



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2021 – 10:46 AM EDT

PDB ID : 7RF3  
Title : RT XFEL structure of the one-flash state of Photosystem II (1F, S2-rich) at 2.26 Angstrom resolution  
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Deposited on : 2021-07-13  
Resolution : 2.26 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

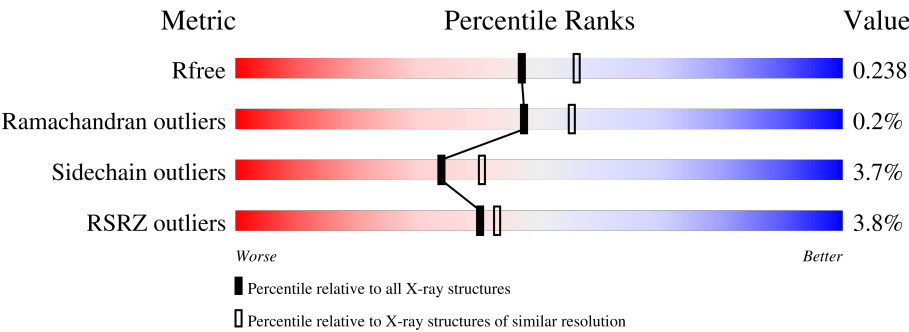


# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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.



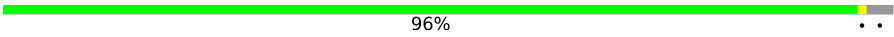
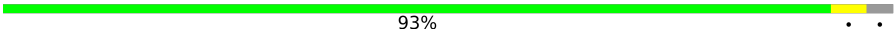
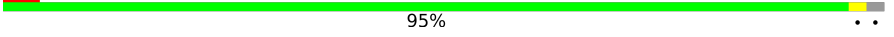
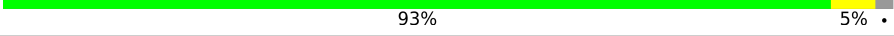


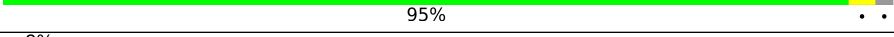

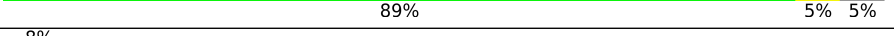
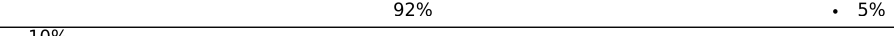
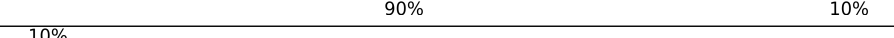
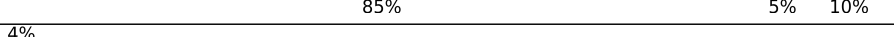

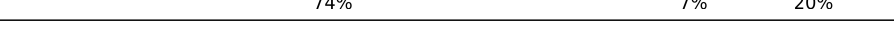
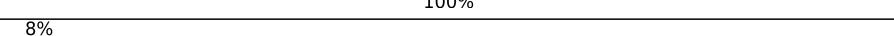

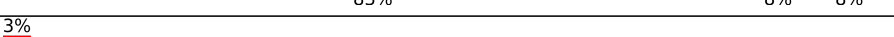

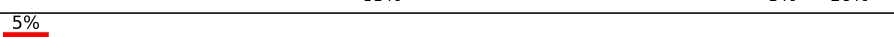






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1377 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>96%</div><div><div></div><div></div></div></div>
1	a	344	<div><div></div><div></div><div></div><div></div><div></div></div> <div>94%</div> <div><div></div><div></div></div>










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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	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	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	B	616	X	-	-	-
22	CLA	C	501	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	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	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	609	X	-	-	-
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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	c	501	X	-	-	-
22	CLA	c	502	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	d	402	X	-	-	-

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103278 atoms, of which 51563 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	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

- 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	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	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
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

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

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

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

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

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

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
			3700	1168	1830	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3720	1170	1846	317	383			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			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
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	129	154			

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

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

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

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

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



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

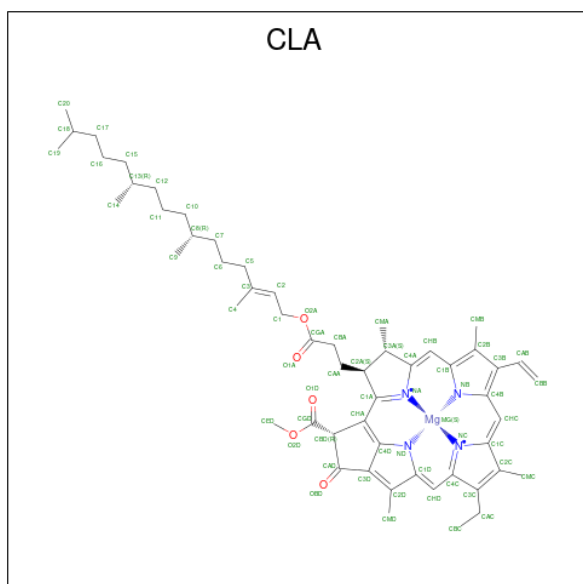
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 21 is 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:  $C_{55}H_{72}MgN_4O_5$ ).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	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
			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
			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	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	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		

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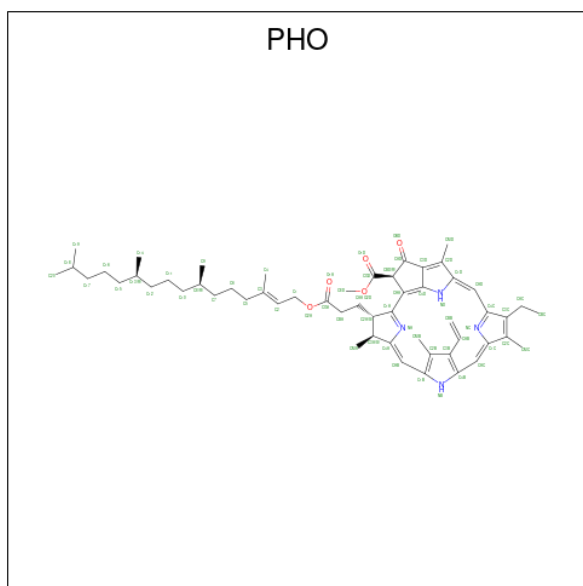
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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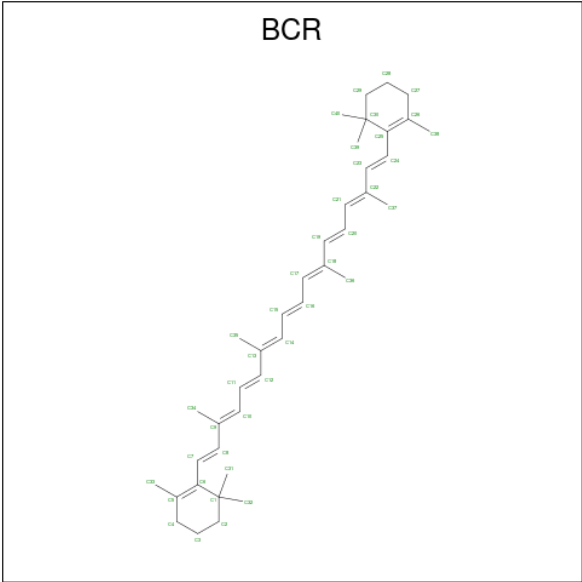
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total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

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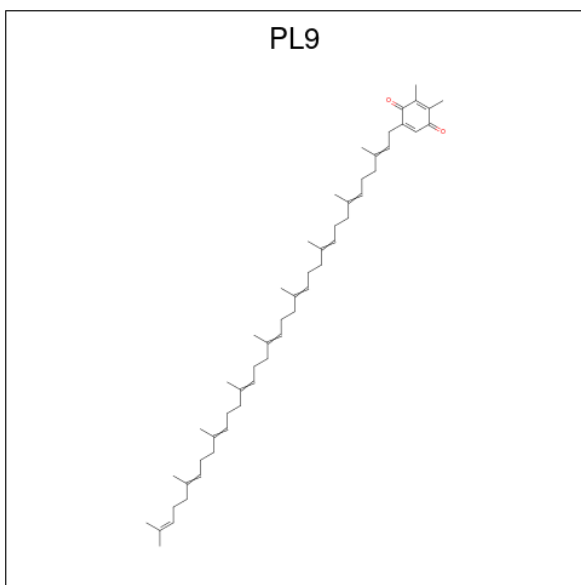
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

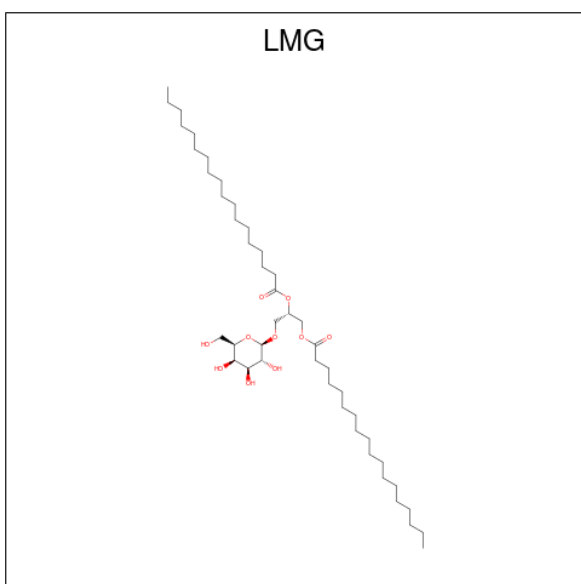
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

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



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

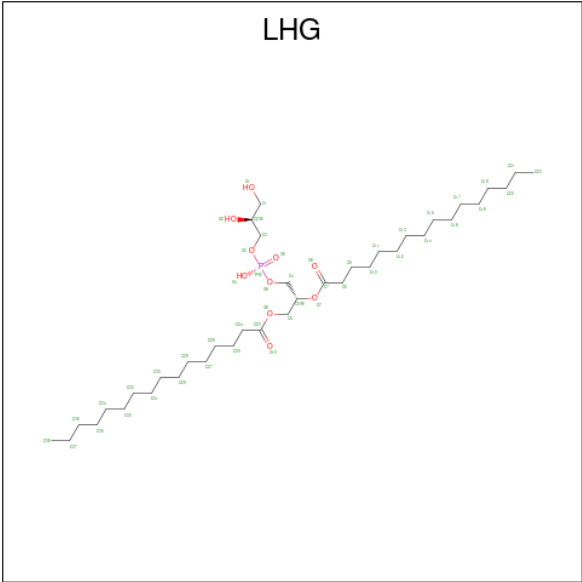
- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





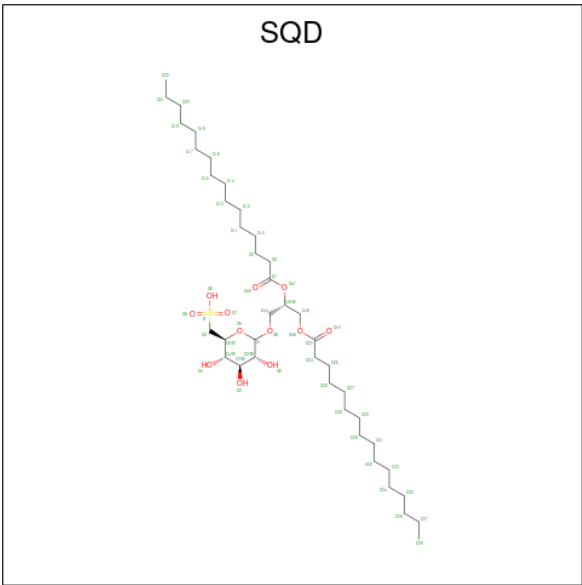
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



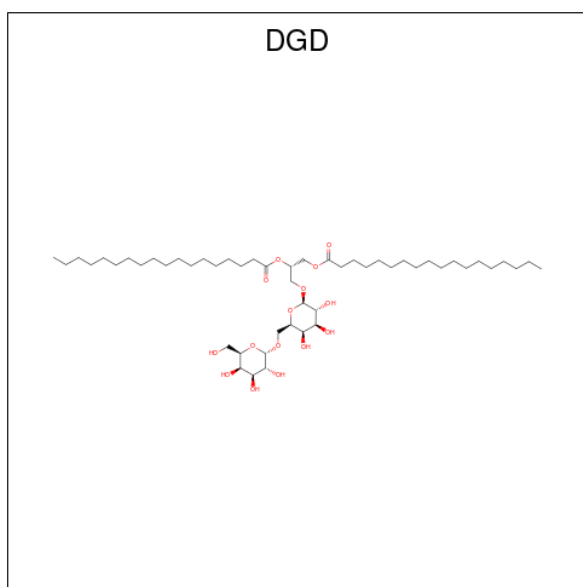
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	b	1	Total	C	H	O	P	0	0
			123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

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



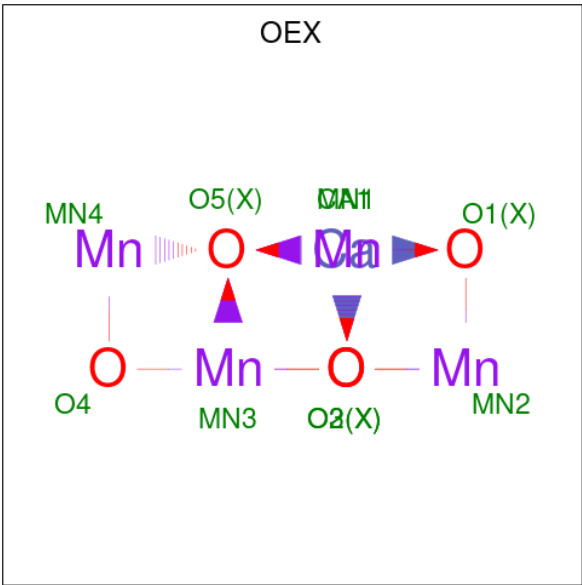
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



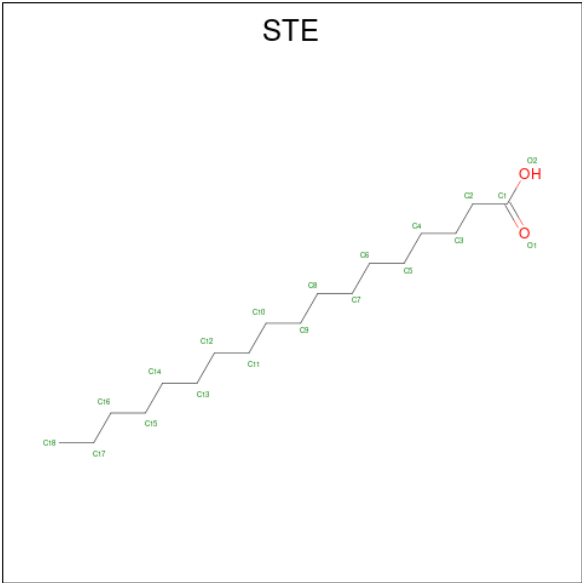
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	B	1	Total	C	H	O	0	0
			119	39	75	5		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		

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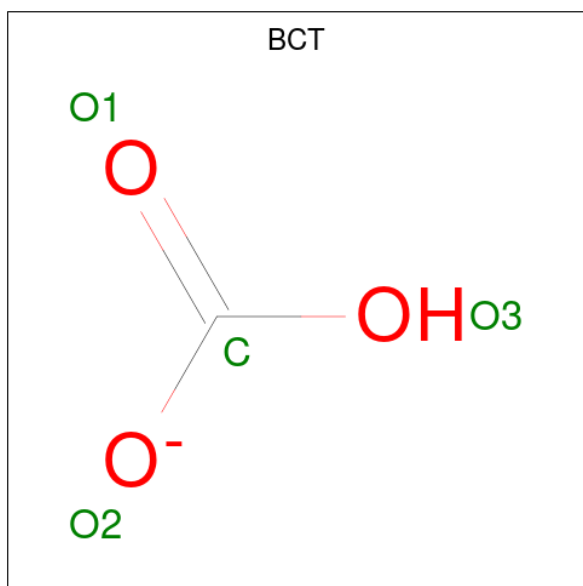
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 46 16 28 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	D	1	Total C H O 55 18 35 2	0	0
32	E	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 44 15 29	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0

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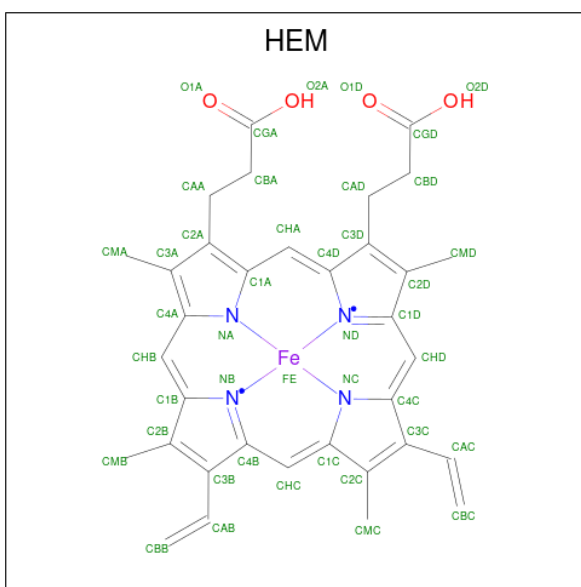
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	k	1	Total	C	H	O	0	0
			28	10	16	2		
32	l	1	Total	C	H		0	0
			53	18	35			
32	m	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		
32	t	1	Total	C	H		0	0
			26	10	16			
32	x	1	Total	C	H	O	0	0
			55	18	35	2		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



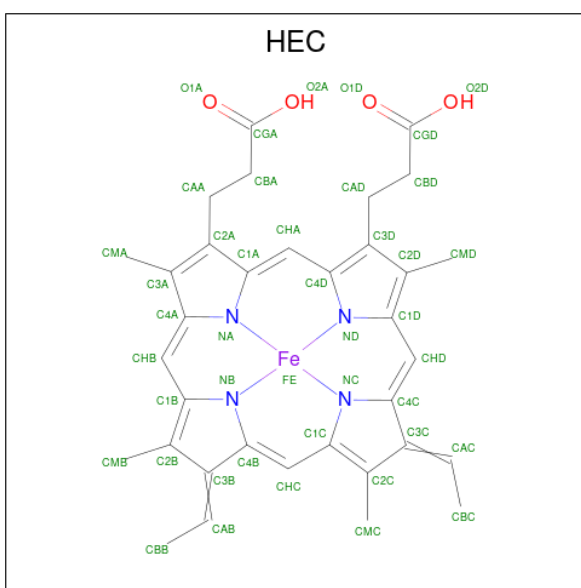
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

- 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	V	1	Total 73	C 34	Fe 1	H 30	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	124	Total O 124 124	0	0
36	B	170	Total O 170 170	0	0
36	C	137	Total O 137 137	0	0
36	D	106	Total O 106 106	0	0
36	E	26	Total O 26 26	0	0
36	F	8	Total O 8 8	0	0
36	H	20	Total O 20 20	0	0
36	I	9	Total O 9 9	0	0
36	J	9	Total O 9 9	0	0
36	K	7	Total O 7 7	0	0
36	L	11	Total O 11 11	0	0
36	M	10	Total O 10 10	0	0
36	O	82	Total O 82 82	0	0
36	R	1	Total O 1 1	0	0
36	T	9	Total O 9 9	0	0
36	U	32	Total O 32 32	0	0
36	V	46	Total O 46 46	0	0
36	X	11	Total O 11 11	0	0
36	Y	3	Total O 3 3	0	0
36	Z	4	Total O 4 4	0	0
36	a	111	Total O 111 111	0	0

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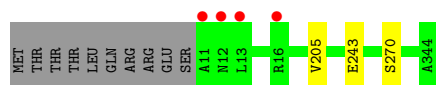
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	b	140	Total 140	O 140	0	0
36	c	115	Total 115	O 115	0	0
36	d	102	Total 102	O 102	0	0
36	e	19	Total 19	O 19	0	0
36	f	10	Total 10	O 10	0	0
36	h	22	Total 22	O 22	0	0
36	i	10	Total 10	O 10	0	0
36	j	10	Total 10	O 10	0	0
36	k	7	Total 7	O 7	0	0
36	l	7	Total 7	O 7	0	0
36	m	7	Total 7	O 7	0	0
36	o	79	Total 79	O 79	0	0
36	r	12	Total 12	O 12	0	0
36	t	10	Total 10	O 10	0	0
36	u	40	Total 40	O 40	0	0
36	v	39	Total 39	O 39	0	0
36	x	5	Total 5	O 5	0	0
36	y	5	Total 5	O 5	0	0
36	z	6	Total 6	O 6	0	0

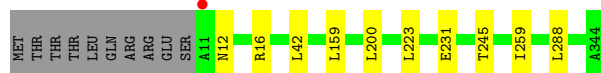
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



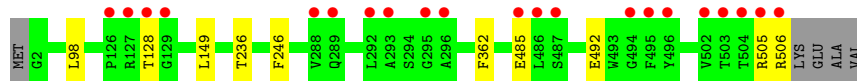
- Molecule 1: Photosystem II protein D1 1



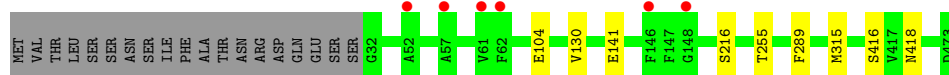
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



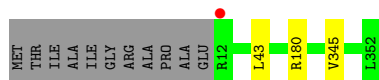
- Molecule 3: Photosystem II CP43 reaction center protein



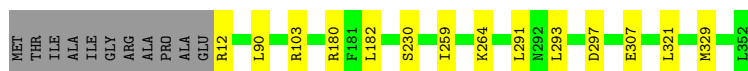
- Molecule 3: Photosystem II CP43 reaction center protein



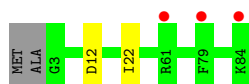
• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein



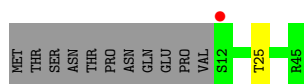
• Molecule 5: Cytochrome b559 subunit alpha



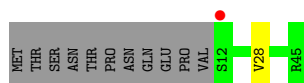
• Molecule 5: Cytochrome b559 subunit alpha



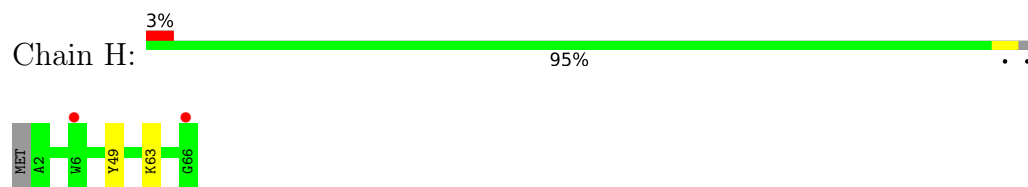
• Molecule 6: Cytochrome b559 subunit beta



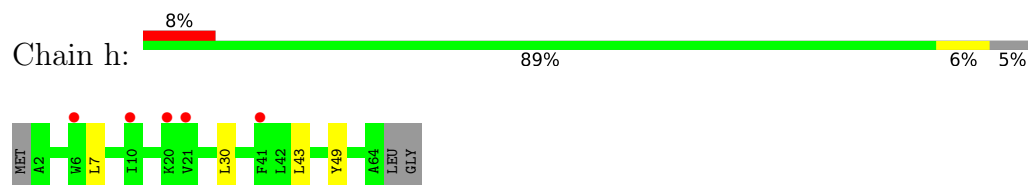
• Molecule 6: Cytochrome b559 subunit beta



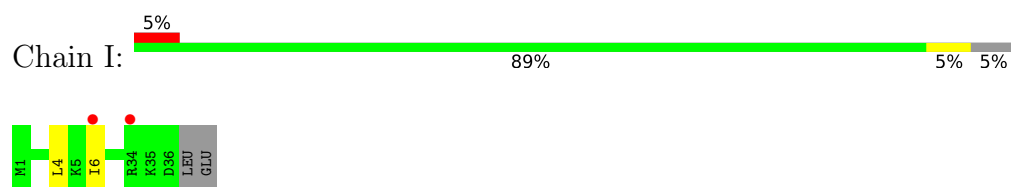
- Molecule 7: Photosystem II reaction center protein H



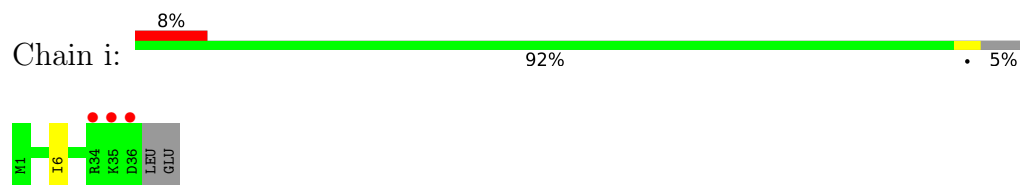
- Molecule 7: Photosystem II reaction center protein H



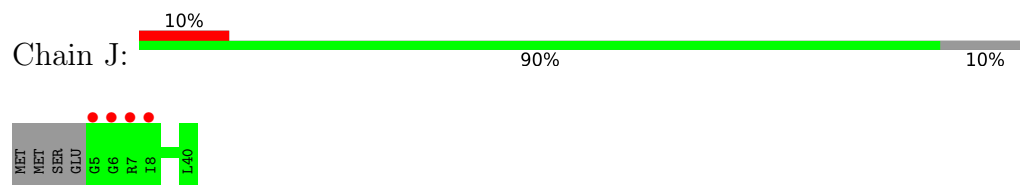
- Molecule 8: Photosystem II reaction center protein I



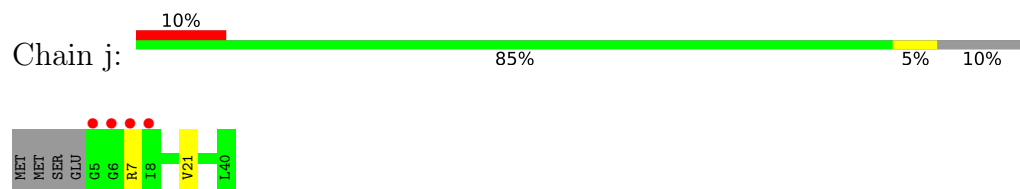
- Molecule 8: Photosystem II reaction center protein I



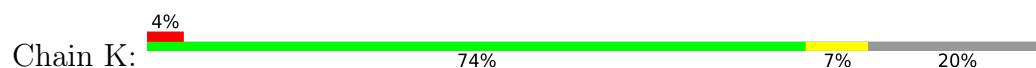
- Molecule 9: Photosystem II reaction center protein J

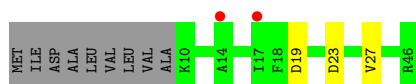


- Molecule 9: Photosystem II reaction center protein J



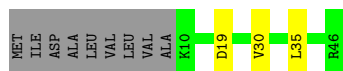
- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

Chain k: 74% 7% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 100%

There are no outlier residues recorded for this chain.

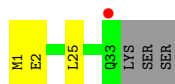
- Molecule 11: Photosystem II reaction center protein L

Chain l: 8% 86% 11%



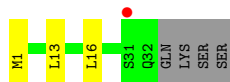
- Molecule 12: Photosystem II reaction center protein M

Chain M: 3% 83% 8% 8%



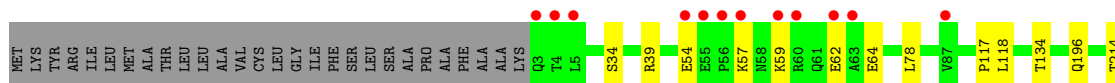
- Molecule 12: Photosystem II reaction center protein M

Chain m: 3% 81% 8% 11%

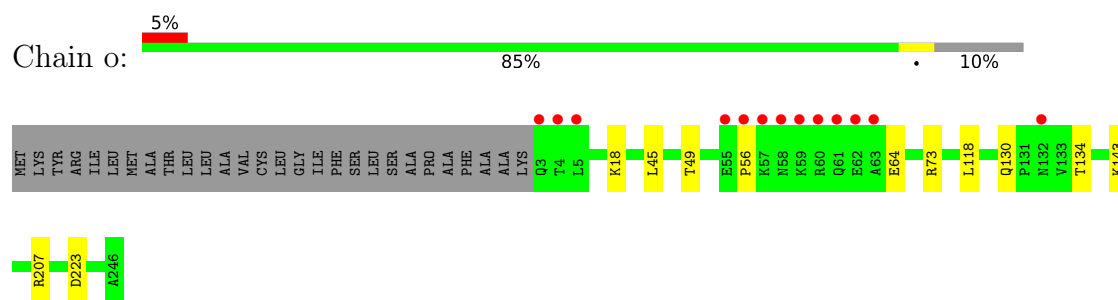


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

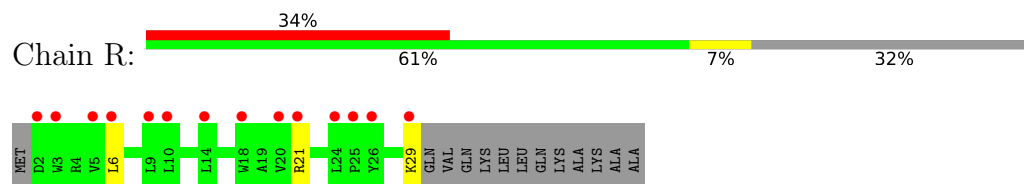
Chain O: 5% 85% 5% 10%



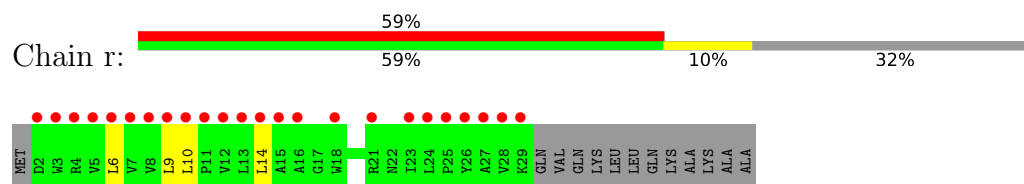
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



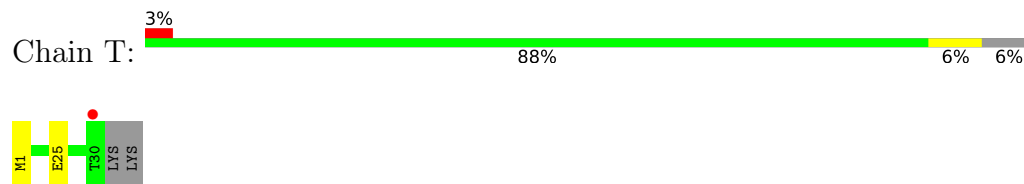
- Molecule 14: Photosystem II protein Y



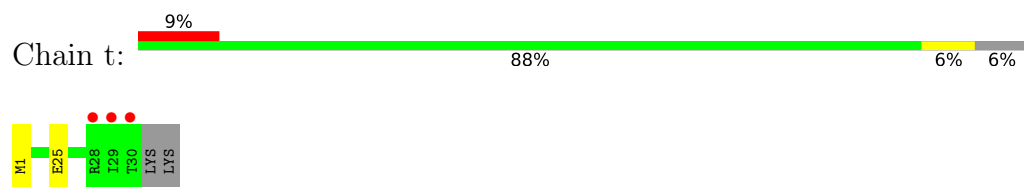
- Molecule 14: Photosystem II protein Y



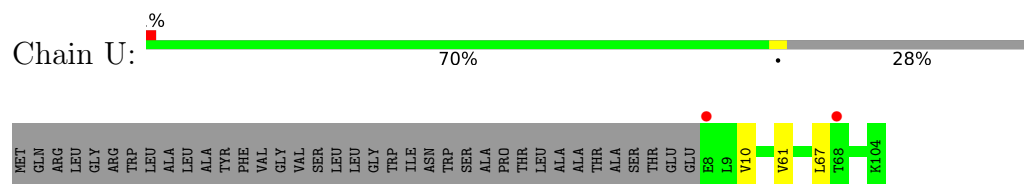
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

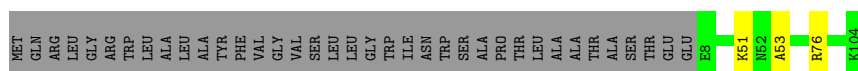


- Molecule 16: Photosystem II 12 kDa extrinsic protein

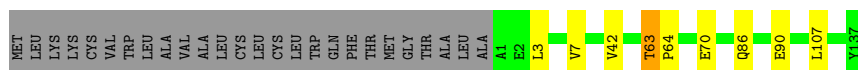
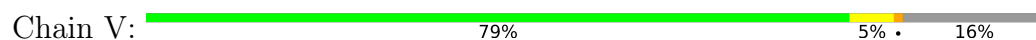


- Molecule 16: Photosystem II 12 kDa extrinsic protein

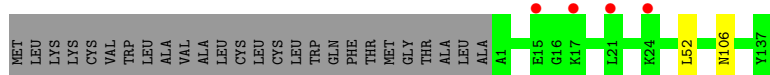
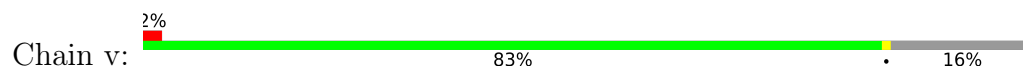




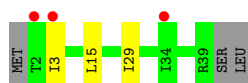
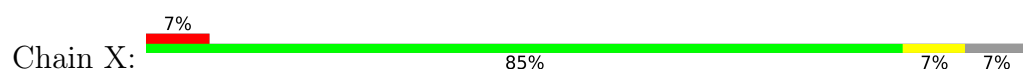
• Molecule 17: Cytochrome c-550



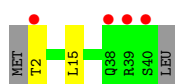
• Molecule 17: Cytochrome c-550



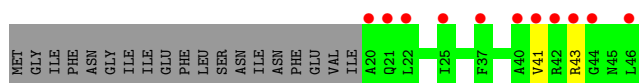
• Molecule 18: Photosystem II reaction center X protein



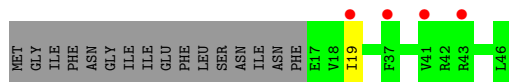
• Molecule 18: Photosystem II reaction center X protein



• Molecule 19: Photosystem II reaction center protein Ycf12

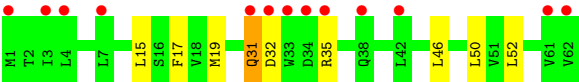
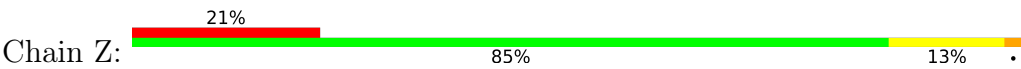


• Molecule 19: Photosystem II reaction center protein Ycf12

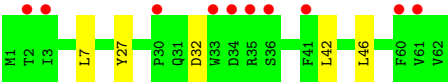
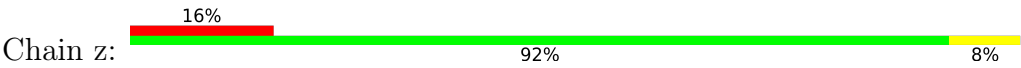


• Molecule 20: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.96Å 221.64Å 307.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.54 – 2.26 33.54 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.54-2.26) 86.8 (33.54-2.26)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.83 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.178 , 0.238 0.178 , 0.238	Depositor DCC
$R_{free}$ test set	3302 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	103278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.64	0/2707	0.67	0/3692
1	a	0.63	0/2704	0.67	0/3688
2	B	0.64	0/4161	0.68	0/5669
2	b	0.61	0/4118	0.67	0/5611
3	C	0.60	0/3547	0.66	0/4830
3	c	0.56	0/3619	0.65	1/4926 (0.0%)
4	D	0.63	0/2812	0.67	0/3832
4	d	0.61	0/2821	0.69	1/3844 (0.0%)
5	E	0.52	0/688	0.62	0/940
5	e	0.53	0/683	0.65	0/932
6	F	0.51	0/284	0.60	0/387
6	f	0.59	0/284	0.62	0/387
7	H	0.64	0/523	0.70	0/713
7	h	0.59	0/511	0.69	0/697
8	I	0.62	0/293	0.66	0/396
8	i	0.62	0/293	0.66	0/396
9	J	0.53	0/263	0.63	0/356
9	j	0.49	0/263	0.62	0/356
10	K	0.50	0/303	0.69	1/416 (0.2%)
10	k	0.48	0/303	0.59	0/416
11	L	0.67	0/311	0.65	0/422
11	l	0.66	0/303	0.70	0/412
12	M	0.65	0/249	0.64	0/341
12	m	0.70	0/244	0.69	0/334
13	O	0.58	0/1904	0.74	1/2585 (0.0%)
13	o	0.61	0/1905	0.73	1/2583 (0.0%)
14	R	0.46	0/227	0.60	0/313
14	r	0.41	0/227	0.58	0/313
15	T	0.68	0/257	0.63	0/349
15	t	0.65	0/255	0.62	0/346
16	U	0.58	0/785	0.68	0/1064
16	u	0.58	0/785	0.71	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	V	0.56	0/1085	0.68	1/1473 (0.1%)
17	v	0.59	0/1085	0.65	0/1473
18	X	0.48	0/284	0.62	0/384
18	x	0.46	0/289	0.58	0/391
19	Y	0.47	0/197	0.61	0/264
19	y	0.38	0/219	0.51	0/294
20	Z	0.47	0/490	0.55	0/669
20	z	0.42	0/488	0.53	0/666
All	All	0.60	0/42769	0.67	6/58224 (0.0%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	V	63	THR	C-N-CD	-6.35	106.63	120.60
4	d	297	ASP	CB-CG-OD1	6.25	123.92	118.30
13	O	223	ASP	CB-CG-OD1	6.22	123.90	118.30
3	c	473	ASP	CB-CG-OD1	5.70	123.43	118.30
10	K	23	ASP	CB-CG-OD1	5.56	123.31	118.30
13	o	223	ASP	CB-CG-OD1	5.23	123.01	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

## 5.2 Too-close contacts ⓘ

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

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	327 (98%)	5 (2%)	0	100	100
1	a	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	41	46
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	493 (98%)	10 (2%)	0	100	100
3	C	442/461 (96%)	431 (98%)	10 (2%)	1 (0%)	47	55
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	47	55
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	328 (96%)	12 (4%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
13	O	243/272 (89%)	232 (96%)	8 (3%)	3 (1%)	13	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	229 (95%)	11 (4%)	2 (1%)	19	17
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	14	10
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	21
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	24 (96%)	0	1 (4%)	3	1
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	9	4
20	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	5231/5700 (92%)	5087 (97%)	132 (2%)	12 (0%)	47	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
16	u	53	ALA
3	C	416	SER
19	Y	43	ARG
20	Z	31	GLN
13	O	57	LYS
1	a	259	ILE
13	o	73	ARG
13	o	56	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	267 (99%)	3 (1%)	73	82
1	a	269/280 (96%)	260 (97%)	9 (3%)	38	46
2	B	408/407 (100%)	400 (98%)	8 (2%)	55	64
2	b	402/407 (99%)	392 (98%)	10 (2%)	47	56
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	59
3	c	354/362 (98%)	339 (96%)	15 (4%)	30	34
4	D	276/283 (98%)	273 (99%)	3 (1%)	73	82
4	d	277/283 (98%)	264 (95%)	13 (5%)	26	29
5	E	72/73 (99%)	69 (96%)	3 (4%)	30	34
5	e	71/73 (97%)	67 (94%)	4 (6%)	21	21
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	42
6	f	28/39 (72%)	27 (96%)	1 (4%)	35	42
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	40
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	12
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	17
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	49
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	9
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	15
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	5
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	26 (93%)	2 (7%)	14	13
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	13
13	O	206/228 (90%)	196 (95%)	10 (5%)	25	27
13	o	207/228 (91%)	198 (96%)	9 (4%)	29	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	22/33 (67%)	19 (86%)	3 (14%)	3	2
14	r	22/33 (67%)	18 (82%)	4 (18%)	1	0
15	T	26/28 (93%)	25 (96%)	1 (4%)	33	39
15	t	25/28 (89%)	24 (96%)	1 (4%)	31	37
16	U	84/112 (75%)	81 (96%)	3 (4%)	35	42
16	u	84/112 (75%)	83 (99%)	1 (1%)	71	80
17	V	117/138 (85%)	111 (95%)	6 (5%)	24	25
17	v	117/138 (85%)	115 (98%)	2 (2%)	60	71
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	6
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	16
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	23
19	y	22/37 (60%)	21 (96%)	1 (4%)	27	31
20	Z	52/52 (100%)	43 (83%)	9 (17%)	2	0
20	z	51/52 (98%)	46 (90%)	5 (10%)	8	6
All	All	4321/4654 (93%)	4158 (96%)	163 (4%)	34	39

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	VAL
1	A	243	GLU
1	A	270	SER
2	B	84	THR
2	B	86	ILE
2	B	127	ARG
2	B	282	GLN
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	505	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	216	SER
3	C	255	THR
3	C	289	PHE
3	C	315	MET

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Mol	Chain	Res	Type
3	C	418	ASN
4	D	43	LEU
4	D	180	ARG
4	D	345	VAL
5	E	12	ASP
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR
7	H	63	LYS
8	I	4	LEU
8	I	6	ILE
10	K	19	ASP
10	K	27	VAL
12	M	2	GLU
12	M	25	LEU
13	O	34	SER
13	O	39	ARG
13	O	54	GLU
13	O	64	GLU
13	O	78	LEU
13	O	117	PRO
13	O	118	LEU
13	O	134	THR
13	O	196	GLN
13	O	214	THR
14	R	6	LEU
14	R	21	ARG
14	R	29	LYS
15	T	25	GLU
16	U	10	VAL
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	42	VAL
17	V	86	GLN
17	V	90	GLU
17	V	107	LEU
18	X	3	ILE
18	X	15	LEU
18	X	29	ILE

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Mol	Chain	Res	Type
19	Y	41	VAL
20	Z	15	LEU
20	Z	17	PHE
20	Z	19	MET
20	Z	31	GLN
20	Z	32	ASP
20	Z	35	ARG
20	Z	46	LEU
20	Z	50	LEU
20	Z	52	LEU
1	a	12	ASN
1	a	16	ARG
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	245	THR
1	a	288	LEU
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	246	PHE
2	b	362	PHE
2	b	485	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	26	ARG
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	165	LEU
3	c	216	SER
3	c	289	PHE
3	c	315	MET
3	c	413[A]	GLU
3	c	413[B]	GLU

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Mol	Chain	Res	Type
3	c	416	SER
3	c	418	ASN
4	d	12	ARG
4	d	90	LEU
4	d	103	ARG
4	d	180	ARG
4	d	182	LEU
4	d	230	SER
4	d	259	ILE
4	d	264	LYS
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	39	SER
5	e	65	LEU
5	e	66	VAL
5	e	83	LEU
6	f	28	VAL
7	h	7	LEU
7	h	30	LEU
7	h	43	LEU
7	h	49	TYR
8	i	6	ILE
9	j	7	ARG
9	j	21	VAL
10	k	19	ASP
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	45	LEU
13	o	49	THR
13	o	64	GLU
13	o	118	LEU
13	o	130	GLN

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Mol	Chain	Res	Type
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	14	LEU
15	t	25	GLU
16	u	51	LYS
17	v	52	LEU
17	v	106	ASN
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
20	z	7	LEU
20	z	27	TYR
20	z	32	ASP
20	z	42	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	338	ASN
3	C	327	ASN
12	M	5	GLN
13	O	36	GLN
13	O	88	ASN
13	O	196	GLN
14	R	22	ASN
16	U	81	HIS
17	V	86	GLN
20	Z	31	GLN
20	Z	38	GLN
1	a	19	ASN
5	e	60	GLN
7	h	59	ASN
12	m	5	GLN
13	o	61	GLN
16	u	78	ASN
20	z	31	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	FME	I	1	8	8,9,10	1.04	0	7,9,11	0.66	0
15	FME	T	1	15	8,9,10	0.82	0	7,9,11	1.33	1 (14%)
12	FME	M	1	12	8,9,10	1.00	0	7,9,11	1.17	1 (14%)
8	FME	i	1	8	8,9,10	0.86	0	7,9,11	0.99	0
15	FME	t	1	15	8,9,10	1.17	1 (12%)	7,9,11	0.87	0
12	FME	m	1	12	8,9,10	1.10	1 (12%)	7,9,11	0.50	0

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	-	0/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.41	1.42	1.46
12	m	1	FME	CA-N	-2.37	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	CA-N-CN	-2.37	119.18	122.82
15	T	1	FME	C-CA-N	2.04	113.42	109.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 186 ligands modelled in this entry, 6 are monoatomic - leaving 180 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	505	-	56,73,73	1.48	7 (12%)	55,113,113	1.41	5 (9%)
32	STE	B	627	-	8,11,19	0.41	0	7,11,19	0.56	0
22	CLA	C	507	36	56,73,73	1.53	7 (12%)	55,113,113	1.58	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	b	605	-	56,73,73	1.41	9 (16%)	55,113,113	1.75	13 (23%)
27	LMG	D	410	-	31,31,55	0.86	1 (3%)	33,33,63	1.18	1 (3%)
32	STE	d	410	-	13,16,19	0.36	0	12,16,19	0.96	0
30	DGD	C	515	-	63,63,67	1.26	8 (12%)	77,77,81	1.42	9 (11%)
22	CLA	b	601	36	56,73,73	1.74	7 (12%)	55,113,113	1.73	10 (18%)
29	SQD	L	101	-	48,49,54	0.97	2 (4%)	57,60,65	2.26	16 (28%)
30	DGD	B	623	-	43,43,67	1.21	6 (13%)	45,45,81	1.26	5 (11%)
22	CLA	c	502	-	56,73,73	1.53	5 (8%)	55,113,113	1.52	9 (16%)
27	LMG	b	622	-	55,55,55	1.13	6 (10%)	63,63,63	1.45	8 (12%)
27	LMG	a	414	-	49,49,55	0.91	1 (2%)	57,57,63	1.34	5 (8%)
22	CLA	C	513	-	56,73,73	1.65	10 (17%)	55,113,113	1.62	11 (20%)
32	STE	x	102	-	16,19,19	0.41	0	15,19,19	0.72	0
35	HEC	v	201	17	26,50,50	2.47	4 (15%)	18,82,82	1.66	5 (27%)
32	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.55	0
22	CLA	d	403	-	56,73,73	1.68	9 (16%)	55,113,113	1.41	9 (16%)
30	DGD	C	517	-	63,63,67	1.14	6 (9%)	77,77,81	1.34	11 (14%)
32	STE	C	521	-	8,11,19	0.42	0	7,11,19	1.07	1 (14%)
26	PL9	A	409	-	55,55,55	1.18	2 (3%)	68,69,69	1.71	15 (22%)
26	PL9	a	410	-	55,55,55	0.83	2 (3%)	68,69,69	1.76	13 (19%)
32	STE	C	519	-	8,11,19	0.47	0	7,11,19	0.56	0
24	BCR	B	617	-	41,41,41	1.24	4 (9%)	56,56,56	1.29	8 (14%)
32	STE	b	624	-	12,15,19	0.45	0	11,15,19	0.73	0
22	CLA	c	504	36	51,68,73	1.68	7 (13%)	49,107,113	1.59	9 (18%)
32	STE	C	520	-	15,15,19	0.53	0	14,14,19	0.60	0
22	CLA	c	510	-	56,73,73	1.68	10 (17%)	55,113,113	1.79	12 (21%)
32	STE	l	102	-	17,17,19	0.41	0	16,16,19	0.79	0
22	CLA	B	614	-	56,73,73	1.62	9 (16%)	55,113,113	1.86	14 (25%)
24	BCR	k	103	-	41,41,41	1.01	2 (4%)	56,56,56	1.18	7 (12%)
22	CLA	c	503	-	56,73,73	1.60	8 (14%)	55,113,113	1.69	10 (18%)
24	BCR	x	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	7 (12%)
32	STE	m	102	-	8,11,19	0.34	0	7,11,19	0.85	0
22	CLA	c	506	-	56,73,73	1.47	8 (14%)	55,113,113	1.46	10 (18%)
22	CLA	b	603	-	56,73,73	1.57	10 (17%)	55,113,113	1.82	10 (18%)
22	CLA	b	613	-	56,73,73	1.44	7 (12%)	55,113,113	1.86	14 (25%)
22	CLA	C	501	-	56,73,73	1.84	11 (19%)	55,113,113	1.41	10 (18%)
22	CLA	D	404	36	56,73,73	1.46	9 (16%)	55,113,113	1.54	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	C	518	-	48,48,55	1.05	6 (12%)	56,56,63	1.37	5 (8%)
27	LMG	d	408	-	18,21,55	0.47	0	16,20,63	1.05	0
22	CLA	C	503	-	56,73,73	1.74	8 (14%)	55,113,113	2.11	11 (20%)
22	CLA	b	610	36	56,73,73	1.52	10 (17%)	55,113,113	1.53	11 (20%)
22	CLA	c	512	-	56,73,73	1.67	9 (16%)	55,113,113	1.77	14 (25%)
22	CLA	C	509	-	56,73,73	1.51	10 (17%)	55,113,113	1.76	9 (16%)
28	LHG	d	406	-	48,48,48	0.70	1 (2%)	51,54,54	1.24	5 (9%)
32	STE	B	626	-	15,15,19	0.45	0	14,14,19	0.72	0
24	BCR	H	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.36	7 (12%)
31	OEX	a	416	3,36,1	0,15,15	-	-	-	-	-
23	PHO	D	401	-	67,69,69	1.35	10 (14%)	85,99,99	1.13	6 (7%)
32	STE	M	103	-	9,9,19	0.38	0	8,8,19	0.74	0
29	SQD	A	413	-	38,38,54	1.05	3 (7%)	40,40,65	1.58	6 (15%)
22	CLA	b	604	-	56,73,73	1.54	8 (14%)	55,113,113	1.99	14 (25%)
30	DGD	c	517	-	63,63,67	1.14	8 (12%)	77,77,81	1.50	14 (18%)
24	BCR	t	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	7 (12%)
24	BCR	T	101	-	41,41,41	1.21	5 (12%)	56,56,56	1.31	6 (10%)
24	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.40	9 (16%)
22	CLA	b	606	-	56,73,73	1.89	9 (16%)	55,113,113	1.81	9 (16%)
22	CLA	c	507	36	56,73,73	1.52	9 (16%)	55,113,113	1.55	10 (18%)
29	SQD	a	412	-	53,54,54	0.99	4 (7%)	62,65,65	1.88	13 (20%)
30	DGD	H	102	-	63,63,67	1.42	14 (22%)	77,77,81	1.38	11 (14%)
34	HEM	F	101	6,5	27,50,50	1.94	5 (18%)	17,82,82	1.93	3 (17%)
22	CLA	b	609	-	56,73,73	1.69	8 (14%)	55,113,113	1.99	13 (23%)
22	CLA	B	603	-	56,73,73	1.54	6 (10%)	55,113,113	1.64	13 (23%)
22	CLA	B	606	-	56,73,73	1.60	8 (14%)	55,113,113	2.01	12 (21%)
22	CLA	c	513	-	56,73,73	1.54	9 (16%)	55,113,113	1.55	10 (18%)
26	PL9	d	405	-	55,55,55	1.42	7 (12%)	68,69,69	1.77	15 (22%)
22	CLA	C	502	-	56,73,73	1.62	9 (16%)	55,113,113	1.56	10 (18%)
22	CLA	C	505	-	56,73,73	1.46	5 (8%)	55,113,113	1.75	9 (16%)
22	CLA	B	609	-	56,73,73	1.41	8 (14%)	55,113,113	1.58	10 (18%)
28	LHG	D	409	-	48,48,48	0.77	3 (6%)	51,54,54	1.31	7 (13%)
30	DGD	c	516	-	63,63,67	1.09	5 (7%)	77,77,81	1.40	11 (14%)
22	CLA	C	506	-	56,73,73	1.42	6 (10%)	55,113,113	1.52	10 (18%)
33	BCT	D	402	21	0,3,3	-	-	0,3,3	-	-
30	DGD	C	516	-	63,63,67	1.25	7 (11%)	77,77,81	1.49	11 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	610	36	56,73,73	1.78	7 (12%)	55,113,113	1.60	11 (20%)
32	STE	c	519	-	16,19,19	0.29	0	15,19,19	1.02	0
32	STE	t	102	-	10,13,19	0.43	0	9,13,19	0.87	0
32	STE	I	101	-	14,14,19	0.51	0	13,13,19	0.58	0
28	LHG	e	102	-	41,41,48	0.93	3 (7%)	44,47,54	1.29	4 (9%)
32	STE	a	415	-	8,11,19	0.52	0	7,11,19	0.70	0
22	CLA	b	612	-	56,73,73	1.31	5 (8%)	55,113,113	1.64	8 (14%)
32	STE	k	104	-	8,11,19	0.46	0	7,11,19	0.74	0
22	CLA	b	616	-	51,68,73	1.59	10 (19%)	49,107,113	1.94	10 (20%)
22	CLA	B	602	-	56,73,73	1.56	8 (14%)	55,113,113	1.63	12 (21%)
22	CLA	a	405	-	56,73,73	1.48	8 (14%)	55,113,113	1.64	12 (21%)
28	LHG	b	623	-	48,48,48	0.99	4 (8%)	51,54,54	1.24	7 (13%)
24	BCR	D	406	-	41,41,41	1.19	2 (4%)	56,56,56	1.13	4 (7%)
27	LMG	D	408	-	51,51,55	1.00	4 (7%)	59,59,63	1.27	6 (10%)
22	CLA	C	504	36	50,67,73	1.67	8 (16%)	47,105,113	1.50	9 (19%)
27	LMG	d	409	-	44,44,55	1.04	4 (9%)	52,52,63	1.35	6 (11%)
27	LMG	m	101	-	51,51,55	1.09	4 (7%)	59,59,63	1.46	8 (13%)
22	CLA	b	608	-	56,73,73	1.66	6 (10%)	55,113,113	1.37	9 (16%)
29	SQD	A	412	-	51,52,54	1.06	5 (9%)	60,63,65	1.99	10 (16%)
22	CLA	c	508	-	55,72,73	1.51	9 (16%)	53,111,113	1.79	10 (18%)
32	STE	B	625	-	14,17,19	0.40	0	13,17,19	0.86	0
29	SQD	F	102	-	35,36,54	0.95	3 (8%)	42,45,65	2.10	13 (30%)
22	CLA	a	403	36	56,73,73	1.61	6 (10%)	55,113,113	1.67	11 (20%)
24	BCR	Z	101	-	41,41,41	1.11	3 (7%)	56,56,56	1.46	11 (19%)
22	CLA	B	601	36	56,73,73	2.00	8 (14%)	55,113,113	1.44	6 (10%)
24	BCR	k	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	5 (8%)
32	STE	b	626	-	9,9,19	0.41	0	8,8,19	0.67	0
23	PHO	a	404	-	67,69,69	1.14	7 (10%)	85,99,99	1.13	6 (7%)
24	BCR	a	406	-	41,41,41	1.09	4 (9%)	56,56,56	1.16	3 (5%)
22	CLA	b	614	-	56,73,73	1.61	8 (14%)	55,113,113	1.53	8 (14%)
22	CLA	c	509	-	56,73,73	1.56	5 (8%)	55,113,113	1.61	7 (12%)
30	DGD	A	414	-	67,67,67	1.23	8 (11%)	81,81,81	1.33	9 (11%)
28	LHG	d	407	-	38,38,48	0.83	2 (5%)	41,44,54	1.19	2 (4%)
27	LMG	D	411	-	20,26,55	0.41	0	18,26,63	1.18	0
32	STE	D	412	-	16,19,19	0.26	0	15,19,19	1.07	0
28	LHG	E	101	-	48,48,48	0.94	4 (8%)	51,54,54	1.24	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	615	-	56,73,73	1.79	7 (12%)	55,113,113	1.59	9 (16%)
22	CLA	D	405	-	56,73,73	1.51	9 (16%)	55,113,113	1.83	12 (21%)
32	STE	j	101	-	8,11,19	0.46	0	7,11,19	0.56	0
32	STE	M	104	-	14,14,19	0.39	0	13,13,19	0.83	0
24	BCR	B	618	-	41,41,41	1.10	3 (7%)	56,56,56	1.12	1 (1%)
24	BCR	C	514	-	41,41,41	1.21	4 (9%)	56,56,56	1.26	4 (7%)
22	CLA	a	402	-	56,73,73	1.65	7 (12%)	55,113,113	1.52	8 (14%)
22	CLA	A	405	-	45,62,73	1.80	8 (17%)	41,99,113	1.97	11 (26%)
22	CLA	B	613	-	56,73,73	1.46	7 (12%)	55,113,113	1.73	12 (21%)
22	CLA	B	607	36	56,73,73	1.47	8 (14%)	55,113,113	1.77	9 (16%)
22	CLA	c	501	-	56,73,73	1.53	9 (16%)	55,113,113	1.76	11 (20%)
24	BCR	b	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.35	8 (14%)
27	LMG	c	520	-	48,48,55	1.10	5 (10%)	56,56,63	1.24	6 (10%)
32	STE	B	624	-	8,11,19	0.45	0	7,11,19	0.69	0
22	CLA	C	508	-	56,73,73	1.78	7 (12%)	55,113,113	1.52	13 (23%)
32	STE	J	101	-	8,11,19	0.29	0	7,11,19	1.10	0
32	STE	M	102	-	11,14,19	0.38	0	10,14,19	0.73	0
32	STE	b	625	-	16,19,19	0.51	0	15,19,19	0.77	0
28	LHG	B	621	-	48,48,48	0.99	2 (4%)	51,54,54	1.33	7 (13%)
23	PHO	A	404	-	67,69,69	1.23	9 (13%)	85,99,99	1.08	6 (7%)
24	BCR	K	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.29	6 (10%)
29	SQD	B	622	-	53,54,54	0.98	3 (5%)	62,65,65	1.91	13 (20%)
28	LHG	A	411	-	46,46,48	0.99	3 (6%)	49,52,54	1.22	3 (6%)
24	BCR	d	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.17	5 (8%)
22	CLA	B	611	-	56,73,73	1.56	7 (12%)	55,113,113	1.63	8 (14%)
32	STE	b	621	-	16,19,19	0.40	0	15,19,19	0.73	0
33	BCT	a	409	21	0,3,3	-	-	0,3,3	-	-
23	PHO	d	401	-	67,69,69	1.28	9 (13%)	85,99,99	1.19	6 (7%)
22	CLA	B	612	-	56,73,73	1.37	5 (8%)	55,113,113	1.75	12 (21%)
24	BCR	B	619	-	41,41,41	1.27	3 (7%)	56,56,56	1.43	9 (16%)
22	CLA	b	602	-	56,73,73	1.73	8 (14%)	55,113,113	1.80	10 (18%)
22	CLA	B	616	-	51,68,73	1.60	10 (19%)	49,107,113	2.06	10 (20%)
32	STE	E	102	-	8,11,19	0.49	0	7,11,19	0.49	0
22	CLA	A	403	36	56,73,73	1.53	7 (12%)	55,113,113	1.44	10 (18%)
22	CLA	B	605	-	56,73,73	1.35	8 (14%)	55,113,113	1.79	12 (21%)
24	BCR	A	406	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	SQD	a	413	-	35,35,54	1.09	2 (5%)	37,37,65	1.33	4 (10%)
22	CLA	b	615	-	56,73,73	1.75	10 (17%)	55,113,113	1.46	7 (12%)
22	CLA	c	511	3	56,73,73	1.82	8 (14%)	55,113,113	1.70	8 (14%)
30	DGD	h	101	-	63,63,67	1.22	9 (14%)	77,77,81	1.47	15 (19%)
22	CLA	d	402	-	56,73,73	1.41	6 (10%)	55,113,113	1.65	8 (14%)
27	LMG	c	518	-	37,37,55	0.98	1 (2%)	45,45,63	1.33	6 (13%)
22	CLA	B	608	-	56,73,73	1.73	11 (19%)	55,113,113	1.48	10 (18%)
35	HEC	V	201	17	26,50,50	2.04	3 (11%)	18,82,82	2.45	6 (33%)
22	CLA	B	604	-	56,73,73	1.29	6 (10%)	55,113,113	2.02	17 (30%)
22	CLA	C	511	3	56,73,73	1.62	5 (8%)	55,113,113	1.70	10 (18%)
26	PL9	D	407	-	55,55,55	1.61	8 (14%)	68,69,69	1.73	16 (23%)
24	BCR	K	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
22	CLA	D	403	-	56,73,73	1.47	8 (14%)	55,113,113	1.74	9 (16%)
34	HEM	e	101	6,5	27,50,50	1.97	4 (14%)	17,82,82	2.14	4 (23%)
22	CLA	b	607	36	56,73,73	1.51	8 (14%)	55,113,113	1.57	6 (10%)
22	CLA	A	402	-	56,73,73	1.50	5 (8%)	55,113,113	1.50	6 (10%)
29	SQD	f	101	-	40,41,54	1.13	5 (12%)	49,52,65	1.88	8 (16%)
24	BCR	b	618	-	41,41,41	1.31	4 (9%)	56,56,56	1.33	8 (14%)
27	LMG	A	410	-	48,48,55	0.94	3 (6%)	56,56,63	1.28	7 (12%)
32	STE	B	620	-	13,16,19	0.43	0	12,16,19	0.62	0
22	CLA	C	512	-	56,73,73	1.56	5 (8%)	55,113,113	1.75	11 (20%)
31	OEX	A	415	3,36,1	0,15,15	-	-	-	-	-
24	BCR	c	514	-	41,41,41	1.13	4 (9%)	56,56,56	1.32	6 (10%)
28	LHG	l	101	-	48,48,48	0.68	0	51,54,54	1.26	6 (11%)
27	LMG	M	101	-	51,51,55	0.96	3 (5%)	59,59,63	1.36	6 (10%)
32	STE	t	103	-	9,9,19	0.39	0	8,8,19	0.63	0
28	LHG	L	102	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	4 (7%)
24	BCR	k	102	-	41,41,41	1.11	3 (7%)	56,56,56	1.23	4 (7%)
32	STE	b	620	-	15,15,19	0.52	0	14,14,19	0.70	0
22	CLA	b	611	-	56,73,73	1.74	6 (10%)	55,113,113	1.62	8 (14%)
22	CLA	C	510	-	56,73,73	1.43	6 (10%)	55,113,113	1.69	11 (20%)
30	DGD	c	515	-	63,63,67	1.12	8 (12%)	77,77,81	1.37	9 (11%)
22	CLA	a	411	36	56,73,73	1.68	8 (14%)	55,113,113	1.54	8 (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
22	CLA	c	505	-	1/1/20/20	7/37/115/115	-
32	STE	B	627	-	-	5/7/9/17	-
22	CLA	C	507	36	1/1/20/20	8/37/115/115	-
22	CLA	b	605	-	1/1/20/20	12/37/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
32	STE	d	410	-	-	8/12/14/17	-
30	DGD	C	515	-	-	21/51/91/95	0/2/2/2
22	CLA	b	601	36	1/1/20/20	17/37/115/115	-
29	SQD	L	101	-	-	25/44/64/69	0/1/1/1
30	DGD	B	623	-	-	24/45/45/95	-
22	CLA	c	502	-	1/1/20/20	15/37/115/115	-
27	LMG	b	622	-	-	24/50/70/70	0/1/1/1
27	LMG	a	414	-	-	21/44/64/70	0/1/1/1
22	CLA	C	513	-	-	16/37/115/115	-
32	STE	x	102	-	-	10/15/17/17	-
35	HEC	v	201	17	-	0/6/54/54	-
32	STE	H	103	-	-	10/15/15/17	-
22	CLA	d	403	-	-	6/37/115/115	-
30	DGD	C	517	-	-	12/51/91/95	0/2/2/2
32	STE	C	521	-	-	1/7/9/17	-
26	PL9	A	409	-	-	24/53/73/73	0/1/1/1
26	PL9	a	410	-	-	26/53/73/73	0/1/1/1
32	STE	C	519	-	-	4/7/9/17	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
32	STE	b	624	-	-	8/11/13/17	-
22	CLA	c	504	36	1/1/19/20	12/31/109/115	-
32	STE	C	520	-	-	4/13/13/17	-
22	CLA	c	510	-	1/1/20/20	10/37/115/115	-
32	STE	l	102	-	-	13/15/15/17	-
22	CLA	B	614	-	1/1/20/20	16/37/115/115	-
24	BCR	k	103	-	-	9/29/63/63	0/2/2/2
22	CLA	c	503	-	1/1/20/20	10/37/115/115	-
24	BCR	x	101	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	m	102	-	-	4/7/9/17	-
22	CLA	c	506	-	1/1/20/20	13/37/115/115	-
22	CLA	b	603	-	1/1/20/20	14/37/115/115	-
22	CLA	b	613	-	1/1/20/20	9/37/115/115	-
22	CLA	C	501	-	1/1/20/20	4/37/115/115	-
22	CLA	D	404	36	1/1/20/20	7/37/115/115	-
27	LMG	C	518	-	-	20/43/63/70	0/1/1/1
27	LMG	d	408	-	-	9/15/17/70	-
22	CLA	C	503	-	1/1/20/20	4/37/115/115	-
22	CLA	b	610	36	1/1/20/20	8/37/115/115	-
22	CLA	c	512	-	1/1/20/20	20/37/115/115	-
22	CLA	C	509	-	1/1/20/20	8/37/115/115	-
28	LHG	d	406	-	-	22/53/53/53	-
32	STE	B	626	-	-	6/13/13/17	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
23	PHO	D	401	-	-	1/53/103/103	0/5/6/6
32	STE	M	103	-	-	3/7/7/17	-
29	SQD	A	413	-	-	12/39/39/69	-
22	CLA	b	604	-	1/1/20/20	8/37/115/115	-
30	DGD	c	517	-	-	19/51/91/95	0/2/2/2
24	BCR	t	101	-	-	8/29/63/63	0/2/2/2
24	BCR	T	101	-	-	10/29/63/63	0/2/2/2
24	BCR	b	619	-	-	14/29/63/63	0/2/2/2
22	CLA	b	606	-	1/1/20/20	11/37/115/115	-
22	CLA	c	507	36	1/1/20/20	10/37/115/115	-
29	SQD	a	412	-	-	21/49/69/69	0/1/1/1
30	DGD	H	102	-	-	19/51/91/95	0/2/2/2
34	HEM	F	101	6,5	-	0/6/54/54	-
22	CLA	b	609	-	1/1/20/20	7/37/115/115	-
22	CLA	B	603	-	1/1/20/20	13/37/115/115	-
22	CLA	B	606	-	1/1/20/20	10/37/115/115	-
22	CLA	c	513	-	1/1/20/20	8/37/115/115	-
26	PL9	d	405	-	-	19/53/73/73	0/1/1/1
22	CLA	C	502	-	1/1/20/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	505	-	1/1/20/20	10/37/115/115	-
22	CLA	B	609	-	-	5/37/115/115	-
28	LHG	D	409	-	-	19/53/53/53	-
30	DGD	c	516	-	-	22/51/91/95	0/2/2/2
22	CLA	C	506	-	1/1/20/20	13/37/115/115	-
30	DGD	C	516	-	-	27/51/91/95	0/2/2/2
22	CLA	B	610	36	1/1/20/20	5/37/115/115	-
32	STE	c	519	-	-	11/15/17/17	-
32	STE	t	102	-	-	3/9/11/17	-
32	STE	I	101	-	-	7/12/12/17	-
28	LHG	e	102	-	-	25/46/46/53	-
32	STE	a	415	-	-	3/7/9/17	-
22	CLA	b	612	-	1/1/20/20	14/37/115/115	-
32	STE	k	104	-	-	0/7/9/17	-
22	CLA	b	616	-	1/1/19/20	6/31/109/115	-
22	CLA	B	602	-	1/1/20/20	12/37/115/115	-
22	CLA	a	405	-	1/1/20/20	11/37/115/115	-
28	LHG	b	623	-	-	24/53/53/53	-
24	BCR	D	406	-	-	6/29/63/63	0/2/2/2
27	LMG	D	408	-	-	17/46/66/70	0/1/1/1
22	CLA	C	504	36	1/1/18/20	9/30/108/115	-
27	LMG	d	409	-	-	12/39/59/70	0/1/1/1
27	LMG	m	101	-	-	23/46/66/70	0/1/1/1
22	CLA	b	608	-	-	8/37/115/115	-
29	SQD	A	412	-	-	17/47/67/69	0/1/1/1
22	CLA	c	508	-	1/1/19/20	17/36/114/115	-
32	STE	B	625	-	-	8/13/15/17	-
29	SQD	F	102	-	-	11/28/48/69	0/1/1/1
22	CLA	a	403	36	1/1/20/20	15/37/115/115	-
24	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
22	CLA	B	601	36	1/1/20/20	17/37/115/115	-
24	BCR	k	101	-	-	13/29/63/63	0/2/2/2
32	STE	b	626	-	-	5/7/7/17	-
23	PHO	a	404	-	-	6/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	a	406	-	-	5/29/63/63	0/2/2/2
22	CLA	b	614	-	1/1/20/20	21/37/115/115	-
22	CLA	c	509	-	1/1/20/20	16/37/115/115	-
30	DGD	A	414	-	-	27/55/95/95	0/2/2/2
28	LHG	d	407	-	-	15/43/43/53	-
27	LMG	D	411	-	-	11/18/22/70	-
32	STE	D	412	-	-	8/15/17/17	-
28	LHG	E	101	-	-	25/53/53/53	-
22	CLA	B	615	-	1/1/20/20	7/37/115/115	-
22	CLA	D	405	-	-	11/37/115/115	-
32	STE	j	101	-	-	2/7/9/17	-
32	STE	M	104	-	-	8/12/12/17	-
24	BCR	B	618	-	-	6/29/63/63	0/2/2/2
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
22	CLA	a	402	-	1/1/20/20	3/37/115/115	-
22	CLA	A	405	-	1/1/17/20	6/24/102/115	-
22	CLA	B	613	-	1/1/20/20	14/37/115/115	-
22	CLA	B	607	36	1/1/20/20	12/37/115/115	-
22	CLA	c	501	-	1/1/20/20	3/37/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
27	LMG	c	520	-	-	26/43/63/70	0/1/1/1
32	STE	B	624	-	-	5/7/9/17	-
22	CLA	C	508	-	-	8/37/115/115	-
32	STE	J	101	-	-	5/7/9/17	-
32	STE	M	102	-	-	3/10/12/17	-
32	STE	b	625	-	-	5/15/17/17	-
28	LHG	B	621	-	-	16/53/53/53	-
23	PHO	A	404	-	-	3/53/103/103	0/5/6/6
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
29	SQD	B	622	-	-	16/49/69/69	0/1/1/1
28	LHG	A	411	-	-	22/51/51/53	-
24	BCR	d	404	-	-	5/29/63/63	0/2/2/2
22	CLA	B	611	-	1/1/20/20	7/37/115/115	-
32	STE	b	621	-	-	7/15/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	d	401	-	-	7/53/103/103	0/5/6/6
22	CLA	B	612	-	1/1/20/20	9/37/115/115	-
24	BCR	B	619	-	-	6/29/63/63	0/2/2/2
22	CLA	b	602	-	1/1/20/20	11/37/115/115	-
22	CLA	B	616	-	1/1/19/20	9/31/109/115	-
32	STE	E	102	-	-	7/7/9/17	-
22	CLA	A	403	36	1/1/20/20	6/37/115/115	-
22	CLA	B	605	-	1/1/20/20	11/37/115/115	-
24	BCR	A	406	-	-	4/29/63/63	0/2/2/2
29	SQD	a	413	-	-	17/37/37/69	-
22	CLA	b	615	-	1/1/20/20	9/37/115/115	-
22	CLA	c	511	3	1/1/20/20	12/37/115/115	-
30	DGD	h	101	-	-	16/51/91/95	0/2/2/2
22	CLA	d	402	-	1/1/20/20	6/37/115/115	-
27	LMG	c	518	-	-	9/31/51/70	0/1/1/1
22	CLA	B	608	-	-	1/37/115/115	-
35	HEC	V	201	17	-	0/6/54/54	-
22	CLA	B	604	-	1/1/20/20	12/37/115/115	-
22	CLA	C	511	3	1/1/20/20	15/37/115/115	-
26	PL9	D	407	-	-	6/53/73/73	0/1/1/1
24	BCR	K	101	-	-	11/29/63/63	0/2/2/2
22	CLA	D	403	-	1/1/20/20	7/37/115/115	-
34	HEM	e	101	6,5	-	0/6/54/54	-
22	CLA	b	607	36	1/1/20/20	13/37/115/115	-
22	CLA	A	402	-	1/1/20/20	3/37/115/115	-
29	SQD	f	101	-	-	13/36/56/69	0/1/1/1
24	BCR	b	618	-	-	1/29/63/63	0/2/2/2
27	LMG	A	410	-	-	24/43/63/70	0/1/1/1
32	STE	B	620	-	-	8/12/14/17	-
22	CLA	C	512	-	1/1/20/20	19/37/115/115	-
24	BCR	c	514	-	-	4/29/63/63	0/2/2/2
28	LHG	l	101	-	-	18/53/53/53	-
27	LMG	M	101	-	-	25/46/66/70	0/1/1/1
32	STE	t	103	-	-	4/7/7/17	-
28	LHG	L	102	-	-	22/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	k	102	-	-	13/29/63/63	0/2/2/2
32	STE	b	620	-	-	7/13/13/17	-
22	CLA	b	611	-	1/1/20/20	11/37/115/115	-
22	CLA	C	510	-	1/1/20/20	9/37/115/115	-
30	DGD	c	515	-	-	24/51/91/95	0/2/2/2
22	CLA	a	411	36	1/1/20/20	13/37/115/115	-

All (844) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	601	CLA	C4B-NB	8.52	1.42	1.35
26	D	407	PL9	C7-C3	-8.51	1.42	1.51
22	b	609	CLA	C4B-NB	8.40	1.42	1.35
22	c	504	CLA	C4B-NB	8.19	1.42	1.35
22	C	508	CLA	C4B-NB	8.18	1.42	1.35
22	b	611	CLA	C4B-NB	7.97	1.42	1.35
22	B	614	CLA	C4B-NB	7.87	1.42	1.35
22	a	403	CLA	C4B-NB	7.86	1.42	1.35
22	c	511	CLA	C4B-NB	7.82	1.42	1.35
22	B	610	CLA	C4B-NB	7.72	1.42	1.35
22	C	505	CLA	C4B-NB	7.66	1.42	1.35
35	v	201	HEC	C3B-C2B	-7.62	1.32	1.40
22	C	507	CLA	C4B-NB	7.44	1.41	1.35
22	b	606	CLA	MG-NA	7.43	2.23	2.06
22	B	615	CLA	C4C-NC	7.40	1.41	1.35
22	C	503	CLA	MG-NA	7.39	2.23	2.06
22	c	512	CLA	C4B-NB	7.36	1.41	1.35
22	C	501	CLA	C4B-NB	7.35	1.41	1.35
22	B	606	CLA	MG-NA	7.31	2.23	2.06
22	d	403	CLA	C4B-NB	7.30	1.41	1.35
22	b	601	CLA	C4B-NB	7.30	1.41	1.35
22	b	602	CLA	C4B-NB	7.25	1.41	1.35
22	C	506	CLA	C4B-NB	7.21	1.41	1.35
22	A	405	CLA	C4B-NB	7.18	1.41	1.35
22	B	615	CLA	C4B-NB	7.12	1.41	1.35
22	c	503	CLA	C4B-NB	7.05	1.41	1.35
22	c	506	CLA	C4B-NB	7.05	1.41	1.35
22	b	604	CLA	C4B-NB	7.00	1.41	1.35
22	B	601	CLA	MG-NA	6.99	2.22	2.06
22	a	402	CLA	C4B-NB	6.96	1.41	1.35
22	c	513	CLA	C4B-NB	6.92	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	C4B-NB	6.89	1.41	1.35
22	A	403	CLA	C4B-NB	6.88	1.41	1.35
22	a	411	CLA	C4B-NB	6.87	1.41	1.35
22	B	602	CLA	C4B-NB	6.86	1.41	1.35
22	C	504	CLA	C4B-NB	6.84	1.41	1.35
22	B	613	CLA	C4B-NB	6.79	1.41	1.35
22	b	608	CLA	C4B-NB	6.77	1.41	1.35
22	b	608	CLA	C4C-NC	6.72	1.41	1.35
22	c	505	CLA	C4B-NB	6.71	1.41	1.35
22	C	511	CLA	C4B-NB	6.71	1.41	1.35
22	C	510	CLA	C4B-NB	6.61	1.41	1.35
22	c	508	CLA	C4B-NB	6.61	1.41	1.35
22	b	607	CLA	C4B-NB	6.56	1.41	1.35
22	B	608	CLA	C4B-NB	6.54	1.41	1.35
22	b	601	CLA	MG-NA	6.53	2.21	2.06
22	b	614	CLA	C4B-NB	6.53	1.41	1.35
35	v	201	HEC	C3C-C2C	-6.51	1.34	1.40
22	B	601	CLA	C4C-NC	6.50	1.41	1.35
35	V	201	HEC	C3B-C2B	-6.44	1.34	1.40
22	B	609	CLA	C4B-NB	6.43	1.40	1.35
22	B	610	CLA	C4C-NC	6.42	1.40	1.35
22	b	603	CLA	C4B-NB	6.41	1.40	1.35
22	b	615	CLA	MG-NA	6.39	2.21	2.06
22	C	513	CLA	C4C-NC	6.35	1.40	1.35
22	b	606	CLA	C4C-NC	6.34	1.40	1.35
22	C	503	CLA	C4B-NB	6.30	1.40	1.35
22	B	608	CLA	MG-NA	6.30	2.21	2.06
22	c	510	CLA	C4C-NC	6.27	1.40	1.35
22	C	502	CLA	C4B-NB	6.24	1.40	1.35
22	B	603	CLA	C4C-NC	6.24	1.40	1.35
22	c	502	CLA	C4B-NB	6.24	1.40	1.35
22	C	501	CLA	C4C-NC	6.21	1.40	1.35
22	a	411	CLA	C4C-NC	6.21	1.40	1.35
22	B	611	CLA	C4B-NB	6.20	1.40	1.35
22	c	512	CLA	C4C-NC	6.19	1.40	1.35
22	D	405	CLA	C4B-NB	6.14	1.40	1.35
22	C	512	CLA	C4B-NB	6.13	1.40	1.35
22	C	508	CLA	MG-NA	6.12	2.20	2.06
22	C	509	CLA	C4C-NC	6.04	1.40	1.35
22	c	501	CLA	C4B-NB	6.03	1.40	1.35
34	e	101	HEM	C3B-C2B	-6.03	1.32	1.40
22	C	513	CLA	C4B-NB	5.96	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	C4C-NC	5.94	1.40	1.35
22	b	612	CLA	C4B-NB	5.94	1.40	1.35
22	c	509	CLA	C4C-NC	5.91	1.40	1.35
22	B	616	CLA	C4B-NB	5.89	1.40	1.35
22	b	616	CLA	C4C-NC	5.89	1.40	1.35
22	A	402	CLA	C4B-NB	5.89	1.40	1.35
22	c	511	CLA	MG-NA	5.88	2.20	2.06
22	d	403	CLA	C4C-NC	5.78	1.40	1.35
22	c	502	CLA	C4C-NC	5.78	1.40	1.35
22	C	502	CLA	C4C-NC	5.77	1.40	1.35
22	b	615	CLA	C4B-NB	5.77	1.40	1.35
22	c	511	CLA	C4C-NC	5.76	1.40	1.35
22	C	511	CLA	C4C-NC	5.71	1.40	1.35
22	b	610	CLA	C4B-NB	5.69	1.40	1.35
22	b	611	CLA	C4C-NC	5.68	1.40	1.35
22	a	402	CLA	C4C-NC	5.63	1.40	1.35
22	B	612	CLA	C4B-NB	5.55	1.40	1.35
22	C	504	CLA	C4C-NC	5.55	1.40	1.35
22	d	402	CLA	C4B-NB	5.53	1.40	1.35
22	D	404	CLA	C4C-NC	5.51	1.40	1.35
22	B	605	CLA	C4B-NB	5.46	1.40	1.35
22	b	606	CLA	C4B-NB	5.45	1.40	1.35
22	b	610	CLA	C4C-NC	5.44	1.40	1.35
22	C	512	CLA	C4C-NC	5.41	1.40	1.35
22	c	510	CLA	MG-NA	5.38	2.19	2.06
22	A	402	CLA	C4C-NC	5.33	1.40	1.35
22	a	405	CLA	C4C-NC	5.31	1.39	1.35
22	B	611	CLA	C4C-NC	5.26	1.39	1.35
22	B	607	CLA	C4B-NB	5.24	1.39	1.35
22	A	405	CLA	C4C-NC	5.24	1.39	1.35
22	a	405	CLA	C4B-NB	5.22	1.39	1.35
22	C	509	CLA	C4B-NB	5.22	1.39	1.35
26	d	405	PL9	C6-C1	-5.21	1.39	1.48
22	b	605	CLA	C4B-NB	5.19	1.39	1.35
22	c	503	CLA	C4C-NC	5.15	1.39	1.35
34	F	101	HEM	C3C-C2C	-5.13	1.33	1.40
22	a	403	CLA	C4C-NC	5.11	1.39	1.35
22	B	607	CLA	C4C-NC	5.10	1.39	1.35
26	A	409	PL9	C7-C3	-5.07	1.46	1.51
22	b	614	CLA	C4C-NC	5.04	1.39	1.35
22	c	507	CLA	C4B-NB	4.96	1.39	1.35
22	D	403	CLA	C4B-NB	4.95	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C4B-NB	4.91	1.39	1.35
22	c	507	CLA	MG-NA	4.86	2.17	2.06
22	b	613	CLA	C4B-NB	4.85	1.39	1.35
22	b	613	CLA	C4C-NC	4.83	1.39	1.35
34	F	101	HEM	C3B-C2B	-4.81	1.33	1.40
22	c	513	CLA	C4C-NC	4.81	1.39	1.35
22	B	616	CLA	C4C-NC	4.81	1.39	1.35
22	c	510	CLA	C4B-NB	4.80	1.39	1.35
22	b	615	CLA	C4C-NC	4.79	1.39	1.35
35	V	201	HEC	C3C-C2C	-4.76	1.35	1.40
22	b	604	CLA	C4C-NC	4.76	1.39	1.35
35	v	201	HEC	C3D-C2D	4.73	1.51	1.37
22	c	504	CLA	C4C-NC	4.60	1.39	1.35
22	c	501	CLA	C4C-NC	4.60	1.39	1.35
22	D	404	CLA	C4B-NB	4.60	1.39	1.35
22	D	405	CLA	C4C-NC	4.56	1.39	1.35
22	b	616	CLA	C4B-NB	4.54	1.39	1.35
34	e	101	HEM	C3C-C2C	-4.49	1.34	1.40
22	C	512	CLA	MG-NA	4.48	2.16	2.06
22	B	603	CLA	MG-NA	4.47	2.16	2.06
22	c	508	CLA	C4C-NC	4.42	1.39	1.35
22	C	507	CLA	C4C-NC	4.41	1.39	1.35
22	A	403	CLA	C4C-NC	4.41	1.39	1.35
22	b	603	CLA	MG-NA	4.39	2.16	2.06
22	B	604	CLA	C4B-NB	4.37	1.39	1.35
24	b	618	BCR	C30-C25	-4.33	1.47	1.53
22	C	501	CLA	MG-NA	4.31	2.16	2.06
24	H	101	BCR	C30-C25	-4.30	1.47	1.53
22	b	602	CLA	MG-NA	4.26	2.16	2.06
22	C	508	CLA	C4C-NC	4.21	1.39	1.35
22	b	601	CLA	C4C-NC	4.21	1.39	1.35
22	B	603	CLA	C4B-NB	4.20	1.39	1.35
22	c	507	CLA	C4C-NC	4.18	1.38	1.35
22	c	505	CLA	C4C-NC	4.17	1.38	1.35
24	B	617	BCR	C30-C25	-4.16	1.48	1.53
24	T	101	BCR	C30-C25	-4.16	1.48	1.53
22	D	403	CLA	C4C-NC	4.15	1.38	1.35
24	B	619	BCR	C30-C25	-4.15	1.48	1.53
24	b	617	BCR	C1-C6	-4.15	1.48	1.53
22	C	511	CLA	MG-NA	4.12	2.16	2.06
27	m	101	LMG	C4-C3	4.11	1.62	1.52
22	B	604	CLA	MG-NA	4.07	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	605	CLA	C4C-NC	4.04	1.38	1.35
35	V	201	HEC	C3D-C2D	4.04	1.49	1.37
22	a	411	CLA	MG-NA	4.01	2.15	2.06
29	a	413	SQD	O47-C7	4.00	1.45	1.34
22	C	510	CLA	C4C-NC	3.98	1.38	1.35
22	C	501	CLA	C3B-C2B	-3.96	1.34	1.40
22	B	602	CLA	C4C-NC	3.96	1.38	1.35
22	D	403	CLA	CMB-C2B	-3.94	1.43	1.51
22	b	606	CLA	C1B-NB	3.93	1.38	1.35
24	b	619	BCR	C30-C25	-3.93	1.48	1.53
24	B	619	BCR	C1-C6	-3.92	1.48	1.53
23	d	401	PHO	CHC-C1C	3.92	1.46	1.38
22	C	503	CLA	C4C-NC	3.92	1.38	1.35
22	B	612	CLA	C4C-NC	3.92	1.38	1.35
24	K	102	BCR	C30-C25	-3.92	1.48	1.53
22	b	603	CLA	C4C-NC	3.89	1.38	1.35
22	B	608	CLA	C4C-NC	3.88	1.38	1.35
22	C	513	CLA	MG-NA	3.86	2.15	2.06
30	C	517	DGD	O2G-C2G	-3.82	1.37	1.46
22	b	609	CLA	CMB-C2B	-3.80	1.43	1.51
22	b	609	CLA	C4C-NC	3.79	1.38	1.35
22	D	403	CLA	MG-NA	3.79	2.15	2.06
22	b	611	CLA	MG-NA	3.76	2.15	2.06
24	D	406	BCR	C30-C25	-3.75	1.48	1.53
28	A	411	LHG	P-O6	3.75	1.74	1.59
24	C	514	BCR	C1-C6	-3.75	1.48	1.53
24	B	617	BCR	C1-C6	-3.75	1.48	1.53
22	b	614	CLA	MG-NA	3.75	2.15	2.06
22	B	610	CLA	CMB-C2B	-3.73	1.43	1.51
29	L	101	SQD	O48-C23	3.70	1.44	1.33
27	b	622	LMG	O6-C1	3.70	1.51	1.41
26	d	405	PL9	C53-C6	-3.69	1.43	1.50
29	A	413	SQD	O47-C7	3.67	1.44	1.34
26	A	409	PL9	C3-C4	-3.66	1.43	1.49
28	b	623	LHG	O7-C5	-3.65	1.37	1.46
29	a	412	SQD	O48-C23	3.64	1.44	1.33
29	B	622	SQD	O47-C7	3.63	1.44	1.34
24	d	404	BCR	C1-C6	-3.62	1.48	1.53
22	c	507	CLA	C3B-C2B	-3.61	1.35	1.40
30	B	623	DGD	O1G-C1A	3.57	1.43	1.33
30	C	516	DGD	C4D-C3D	3.57	1.61	1.52
24	t	101	BCR	C1-C6	-3.56	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	516	DGD	O3D-C3D	-3.55	1.34	1.43
27	M	101	LMG	C9-C8	3.54	1.61	1.50
24	C	514	BCR	C30-C25	-3.54	1.48	1.53
22	d	402	CLA	MG-NA	3.51	2.14	2.06
22	B	615	CLA	MG-NA	3.50	2.14	2.06
24	t	101	BCR	C30-C25	-3.49	1.49	1.53
24	x	101	BCR	C30-C25	-3.49	1.49	1.53
30	C	515	DGD	C4D-C3D	3.46	1.61	1.52
22	a	405	CLA	MG-NA	3.44	2.14	2.06
30	A	414	DGD	C4E-C5E	3.43	1.60	1.53
22	B	616	CLA	MG-NA	3.41	2.14	2.06
22	B	614	CLA	MG-NA	3.40	2.14	2.06
30	c	516	DGD	O2E-C2E	-3.39	1.35	1.43
28	B	621	LHG	O7-C5	-3.39	1.38	1.46
22	C	505	CLA	C4C-NC	3.38	1.38	1.35
23	D	401	PHO	C1A-NA	3.38	1.44	1.37
24	K	101	BCR	C30-C25	-3.37	1.49	1.53
24	k	101	BCR	C30-C25	-3.36	1.49	1.53
30	H	102	DGD	O5D-C1E	3.35	1.45	1.40
29	f	101	SQD	O47-C7	3.35	1.43	1.34
22	c	510	CLA	CMB-C2B	-3.35	1.44	1.51
22	a	402	CLA	MG-NA	3.34	2.14	2.06
22	B	610	CLA	C3B-C2B	-3.34	1.35	1.40
22	b	605	CLA	MG-NA	3.34	2.14	2.06
24	D	406	BCR	C1-C6	-3.31	1.49	1.53
22	b	607	CLA	CMB-C2B	-3.30	1.44	1.51
29	f	101	SQD	O48-C23	3.29	1.43	1.33
34	F	101	HEM	C3C-CAC	3.29	1.54	1.47
22	a	402	CLA	C1D-C2D	3.28	1.50	1.42
22	B	611	CLA	MG-NA	3.28	2.14	2.06
24	B	618	BCR	C30-C25	-3.27	1.49	1.53
22	D	403	CLA	CMD-C2D	-3.27	1.43	1.51
23	D	401	PHO	C3B-C4B	3.27	1.50	1.43
27	b	622	LMG	C3-C2	3.26	1.60	1.52
22	B	605	CLA	C4C-NC	3.24	1.38	1.35
22	b	615	CLA	CMB-C2B	-3.23	1.44	1.51
30	C	515	DGD	C6E-C5E	3.21	1.62	1.51
22	A	403	CLA	CMD-C2D	-3.21	1.43	1.51
30	H	102	DGD	O5D-C6D	-3.20	1.37	1.43
22	C	502	CLA	C3B-C2B	-3.20	1.35	1.40
22	b	608	CLA	C1D-C2D	3.20	1.49	1.42
28	E	101	LHG	P-O6	3.20	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	d	409	LMG	C4-C5	3.19	1.59	1.53
24	b	619	BCR	C1-C6	-3.18	1.49	1.53
22	b	607	CLA	C3B-C2B	-3.17	1.36	1.40
27	D	408	LMG	O2-C2	-3.16	1.35	1.43
24	Z	101	BCR	C1-C6	-3.15	1.49	1.53
22	d	402	CLA	CMB-C2B	-3.15	1.45	1.51
24	k	102	BCR	C1-C6	-3.14	1.49	1.53
29	A	412	SQD	O2-C2	-3.13	1.35	1.43
22	b	616	CLA	MG-NA	3.12	2.13	2.06
22	C	509	CLA	CMB-C2B	-3.12	1.45	1.51
30	A	414	DGD	C3G-C2G	3.11	1.60	1.50
22	c	512	CLA	CMB-C2B	-3.10	1.45	1.51
22	B	603	CLA	C3B-C2B	-3.10	1.36	1.40
27	m	101	LMG	C4-C5	3.09	1.59	1.53
30	c	516	DGD	O3E-C3E	-3.09	1.35	1.43
22	b	607	CLA	C4C-NC	3.09	1.38	1.35
30	H	102	DGD	O4D-C4D	-3.08	1.35	1.43
29	A	413	SQD	O48-C23	3.08	1.42	1.33
30	c	515	DGD	O2G-C2G	-3.08	1.38	1.46
22	B	615	CLA	CMB-C2B	-3.06	1.45	1.51
30	c	515	DGD	O5D-C1E	3.06	1.45	1.40
29	L	101	SQD	O47-C7	3.06	1.42	1.34
22	B	614	CLA	CMB-C2B	-3.05	1.45	1.51
23	d	401	PHO	C3B-C4B	3.05	1.49	1.43
30	B	623	DGD	C1G-C2G	3.05	1.60	1.50
24	K	101	BCR	C1-C6	-3.04	1.49	1.53
22	C	513	CLA	C1D-C2D	3.04	1.49	1.42
22	c	505	CLA	CMB-C2B	-3.03	1.45	1.51
22	C	511	CLA	CMB-C2B	-3.03	1.45	1.51
22	A	405	CLA	MG-NA	-3.03	1.99	2.06
30	C	517	DGD	O1G-C1G	-3.02	1.38	1.45
22	B	613	CLA	C3B-CAB	-3.02	1.41	1.47
29	A	412	SQD	O47-C7	3.02	1.42	1.34
22	D	405	CLA	C3B-C2B	-3.02	1.36	1.40
29	F	102	SQD	O48-C23	3.01	1.42	1.33
22	B	609	CLA	C4C-NC	3.01	1.37	1.35
24	d	404	BCR	C30-C25	-3.00	1.49	1.53
24	Z	101	BCR	C30-C25	-3.00	1.49	1.53
22	b	613	CLA	CMB-C2B	-2.99	1.45	1.51
27	A	410	LMG	C4-C3	2.99	1.59	1.52
27	C	518	LMG	C1-C2	2.99	1.61	1.52
22	d	402	CLA	C4C-NC	2.99	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	C4C-NC	2.98	1.37	1.35
24	c	514	BCR	C1-C6	-2.98	1.49	1.53
22	B	601	CLA	C1D-C2D	2.97	1.49	1.42
22	d	403	CLA	CMB-C2B	-2.97	1.45	1.51
24	b	617	BCR	C30-C25	-2.97	1.49	1.53
22	c	506	CLA	C1D-C2D	2.97	1.49	1.42
27	c	520	LMG	C7-C8	2.97	1.59	1.50
22	B	612	CLA	MG-NA	2.96	2.13	2.06
29	B	622	SQD	O48-C23	2.96	1.42	1.33
22	C	513	CLA	CMB-C2B	-2.95	1.45	1.51
22	b	612	CLA	CMB-C2B	-2.95	1.45	1.51
22	a	402	CLA	CMB-C2B	-2.95	1.45	1.51
22	D	405	CLA	CMB-C2B	-2.95	1.45	1.51
27	C	518	LMG	C4-C5	2.94	1.59	1.53
22	C	508	CLA	C1D-C2D	2.94	1.49	1.42
24	c	514	BCR	C30-C25	-2.94	1.49	1.53
22	B	611	CLA	CMD-C2D	-2.94	1.44	1.51
22	c	510	CLA	C3B-C2B	-2.93	1.36	1.40
29	a	413	SQD	O48-C23	2.93	1.41	1.33
30	c	517	DGD	O2G-C2G	-2.93	1.39	1.46
22	c	501	CLA	MG-NA	2.92	2.13	2.06
22	c	505	CLA	C3B-C2B	-2.92	1.36	1.40
26	d	405	PL9	C31-C29	-2.91	1.45	1.51
30	h	101	DGD	C3G-C2G	2.91	1.59	1.50
22	b	603	CLA	C1D-C2D	2.90	1.49	1.42
22	c	502	CLA	CMD-C2D	-2.90	1.44	1.51
22	C	501	CLA	C1D-C2D	2.90	1.49	1.42
24	k	102	BCR	C30-C25	-2.89	1.49	1.53
26	d	405	PL9	C7-C3	2.89	1.54	1.51
23	a	404	PHO	C3B-C4B	2.89	1.49	1.43
28	L	102	LHG	O8-C23	2.89	1.41	1.33
22	B	614	CLA	C4C-NC	2.89	1.37	1.35
26	D	407	PL9	C11-C9	-2.89	1.45	1.51
22	B	610	CLA	MG-NA	2.89	2.13	2.06
22	B	606	CLA	C4C-NC	2.88	1.37	1.35
24	A	406	BCR	C1-C6	-2.88	1.49	1.53
30	h	101	DGD	O3E-C3E	-2.88	1.36	1.43
22	b	616	CLA	C1D-C2D	2.88	1.49	1.42
22	B	601	CLA	C3B-C2B	-2.87	1.36	1.40
22	b	611	CLA	CMB-C2B	-2.87	1.45	1.51
22	b	602	CLA	CAC-C3C	-2.87	1.45	1.52
22	B	611	CLA	C1D-C2D	2.87	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	501	CLA	CAC-C3C	-2.86	1.45	1.52
30	A	414	DGD	C3E-C2E	2.85	1.59	1.52
22	C	501	CLA	CMD-C2D	-2.84	1.44	1.51
22	B	604	CLA	C1D-C2D	2.84	1.49	1.42
23	A	404	PHO	C1A-NA	2.83	1.43	1.37
22	B	616	CLA	CMD-C2D	-2.82	1.44	1.51
22	b	610	CLA	C3B-C2B	-2.82	1.36	1.40
34	F	101	HEM	C3B-CAB	2.82	1.53	1.47
28	e	102	LHG	P-O6	2.82	1.70	1.59
29	A	413	SQD	O47-C45	-2.81	1.42	1.47
22	B	606	CLA	C3B-CAB	-2.81	1.42	1.47
22	B	602	CLA	OBD-CAD	2.80	1.26	1.22
22	D	405	CLA	C1D-C2D	2.80	1.48	1.42
30	H	102	DGD	O2G-C2G	-2.80	1.39	1.46
27	D	410	LMG	C7-C8	2.79	1.58	1.51
22	C	509	CLA	C1D-C2D	2.79	1.48	1.42
22	B	608	CLA	C1D-C2D	2.79	1.48	1.42
27	d	409	LMG	O6-C5	-2.78	1.37	1.44
23	a	404	PHO	C1C-NC	-2.78	1.32	1.38
34	e	101	HEM	C3C-CAC	2.77	1.53	1.47
22	c	501	CLA	C3B-C2B	-2.77	1.36	1.40
34	e	101	HEM	C3B-CAB	2.77	1.53	1.47
24	B	618	BCR	C1-C6	-2.76	1.50	1.53
30	c	516	DGD	O5D-C1E	2.76	1.44	1.40
22	c	503	CLA	CMB-C2B	-2.76	1.45	1.51
22	C	503	CLA	C1D-C2D	2.75	1.48	1.42
22	B	607	CLA	CMB-C2B	-2.75	1.45	1.51
30	C	516	DGD	C6D-C5D	2.75	1.60	1.51
23	A	404	PHO	CHD-C4C	-2.74	1.34	1.40
23	A	404	PHO	CMD-C2D	-2.74	1.45	1.50
22	b	616	CLA	C3B-C2B	-2.74	1.36	1.40
22	B	609	CLA	CMD-C2D	-2.73	1.45	1.51
23	D	401	PHO	C4C-C3C	2.73	1.50	1.45
22	d	403	CLA	CMD-C2D	-2.73	1.45	1.51
27	M	101	LMG	O7-C8	-2.72	1.39	1.46
27	c	520	LMG	C3-C2	2.72	1.59	1.52
22	B	603	CLA	CMC-C2C	-2.72	1.45	1.51
23	d	401	PHO	C1A-NA	2.71	1.42	1.37
24	a	406	BCR	C1-C6	-2.71	1.50	1.53
23	D	401	PHO	CHC-C1C	2.71	1.44	1.38
22	B	613	CLA	CMB-C2B	-2.71	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.71	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	CMD-C2D	-2.71	1.45	1.51
28	A	411	LHG	O3-C3	-2.70	1.34	1.44
22	B	601	CLA	CMB-C2B	-2.70	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.70	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.69	1.46	1.51
22	c	512	CLA	C3B-C2B	-2.69	1.36	1.40
22	b	613	CLA	MG-NA	2.68	2.12	2.06
30	B	623	DGD	O2G-C1B	2.68	1.41	1.34
27	D	408	LMG	C4-C5	2.68	1.58	1.53
30	H	102	DGD	C4D-C5D	2.68	1.58	1.53
23	A	404	PHO	C1C-NC	-2.67	1.32	1.38
22	b	602	CLA	CMD-C2D	-2.67	1.45	1.51
22	B	616	CLA	CMC-C2C	-2.66	1.45	1.51
30	A	414	DGD	C4D-C3D	2.66	1.59	1.52
22	B	602	CLA	CMB-C2B	-2.66	1.46	1.51
30	B	623	DGD	O2G-C2G	-2.66	1.39	1.46
29	A	412	SQD	O48-C23	2.66	1.41	1.33
30	h	101	DGD	C4E-C5E	2.66	1.58	1.53
22	c	509	CLA	CMB-C2B	-2.66	1.46	1.51
24	a	406	BCR	C38-C26	-2.66	1.46	1.50
22	B	610	CLA	C1D-C2D	2.65	1.48	1.42
22	B	612	CLA	CMC-C2C	-2.65	1.45	1.51
30	C	517	DGD	O6D-C5D	-2.65	1.37	1.44
22	c	511	CLA	C1D-C2D	2.65	1.48	1.42
22	b	604	CLA	C1D-C2D	2.65	1.48	1.42
22	a	405	CLA	CMC-C2C	-2.65	1.45	1.51
22	b	610	CLA	CMD-C2D	-2.65	1.45	1.51
22	c	511	CLA	CMB-C2B	-2.65	1.46	1.51
30	H	102	DGD	C1E-C2E	2.64	1.60	1.52
29	B	622	SQD	O2-C2	-2.64	1.36	1.43
22	a	405	CLA	CMD-C2D	-2.64	1.45	1.51
22	c	503	CLA	CMC-C2C	-2.64	1.45	1.51
22	B	616	CLA	C3B-CAB	-2.63	1.42	1.47
22	b	614	CLA	CMB-C2B	-2.63	1.46	1.51
22	C	502	CLA	CMD-C2D	-2.63	1.45	1.51
30	C	516	DGD	O2D-C2D	-2.63	1.36	1.43
22	A	403	CLA	C3B-C2B	-2.63	1.36	1.40
22	c	513	CLA	CMB-C2B	-2.62	1.46	1.51
22	b	615	CLA	CMC-C2C	-2.62	1.45	1.51
22	b	606	CLA	CMB-C2B	-2.62	1.46	1.51
23	d	401	PHO	C4C-C3C	2.61	1.49	1.45
29	a	412	SQD	O2-C2	-2.61	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	CAC-C3C	-2.61	1.45	1.52
22	b	615	CLA	CMD-C2D	-2.60	1.45	1.51
27	m	101	LMG	O6-C1	2.60	1.48	1.41
22	C	507	CLA	CMB-C2B	-2.60	1.46	1.51
30	A	414	DGD	C6E-C5E	2.60	1.60	1.51
22	b	604	CLA	CMC-C2C	-2.60	1.45	1.51
22	a	402	CLA	CMC-C2C	-2.59	1.45	1.51
22	b	615	CLA	C3B-CAB	-2.59	1.42	1.47
30	c	517	DGD	O5D-C1E	2.59	1.44	1.40
30	C	515	DGD	O2G-C2G	-2.59	1.40	1.46
27	M	101	LMG	C3-C2	2.59	1.58	1.52
22	b	613	CLA	CMD-C2D	-2.59	1.45	1.51
22	c	503	CLA	C3B-CAB	-2.59	1.42	1.47
26	D	407	PL9	C52-C5	-2.59	1.45	1.50
22	b	616	CLA	CMD-C2D	-2.59	1.45	1.51
24	k	103	BCR	C30-C25	-2.58	1.50	1.53
22	c	508	CLA	C1D-C2D	2.58	1.48	1.42
30	H	102	DGD	O2D-C2D	-2.58	1.36	1.43
23	D	401	PHO	CMB-C2B	-2.58	1.45	1.50
22	c	507	CLA	CMB-C2B	-2.57	1.46	1.51
23	D	401	PHO	CHC-C4B	-2.57	1.34	1.40
22	C	503	CLA	CMB-C2B	-2.57	1.46	1.51
22	C	512	CLA	C1D-C2D	2.56	1.48	1.42
27	c	520	LMG	C1-C2	2.56	1.59	1.52
22	b	601	CLA	C1D-C2D	2.56	1.48	1.42
22	b	609	CLA	C1D-C2D	2.56	1.48	1.42
22	D	404	CLA	C1D-C2D	2.56	1.48	1.42
22	B	607	CLA	CMD-C2D	-2.56	1.45	1.51
22	c	508	CLA	MG-NA	2.55	2.12	2.06
22	a	403	CLA	C1D-C2D	2.55	1.48	1.42
22	c	512	CLA	C1D-C2D	2.55	1.48	1.42
22	C	501	CLA	CMC-C2C	-2.55	1.45	1.51
27	b	622	LMG	C1-C2	2.55	1.59	1.52
30	H	102	DGD	C6E-C5E	2.54	1.60	1.51
22	C	502	CLA	CAC-C3C	-2.54	1.45	1.52
22	b	604	CLA	MG-NA	2.54	2.12	2.06
22	b	603	CLA	CMD-C2D	-2.54	1.45	1.51
30	h	101	DGD	O2D-C2D	-2.53	1.37	1.43
22	C	511	CLA	C1D-C2D	2.53	1.48	1.42
22	B	606	CLA	C3B-C2B	-2.53	1.36	1.40
23	a	404	PHO	C4C-NC	2.53	1.42	1.36
30	c	517	DGD	O4D-C4D	-2.52	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	411	CLA	CMB-C2B	-2.52	1.46	1.51
26	a	410	PL9	C53-C6	-2.52	1.45	1.50
26	d	405	PL9	C10-C9	-2.52	1.44	1.50
22	b	602	CLA	CMC-C2C	-2.52	1.45	1.51
22	c	503	CLA	C3B-C2B	-2.52	1.36	1.40
22	B	608	CLA	C3B-CAB	-2.51	1.42	1.47
24	K	102	BCR	C1-C6	-2.51	1.50	1.53
23	A	404	PHO	CHC-C1C	2.51	1.43	1.38
22	B	614	CLA	C3B-CAB	-2.50	1.42	1.47
22	D	404	CLA	C3B-CAB	-2.50	1.42	1.47
22	d	402	CLA	C1D-C2D	2.50	1.48	1.42
28	b	623	LHG	P-O6	2.50	1.69	1.59
30	C	517	DGD	O2E-C2E	-2.50	1.37	1.43
22	C	502	CLA	CMC-C2C	-2.50	1.45	1.51
22	b	609	CLA	CMD-C2D	-2.49	1.45	1.51
22	c	501	CLA	C4B-CHC	-2.49	1.34	1.41
22	C	510	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	603	CLA	C3B-CAB	-2.48	1.42	1.47
22	c	501	CLA	C1D-C2D	2.48	1.48	1.42
22	b	611	CLA	CMD-C2D	-2.48	1.45	1.51
30	C	515	DGD	C3G-C2G	2.47	1.58	1.50
30	H	102	DGD	O1G-C1G	-2.47	1.39	1.45
23	a	404	PHO	C4C-C3C	2.46	1.49	1.45
22	D	404	CLA	CMB-C2B	-2.46	1.46	1.51
28	d	406	LHG	O8-C6	-2.46	1.39	1.45
22	c	505	CLA	CMD-C2D	-2.46	1.45	1.51
28	E	101	LHG	C24-C23	2.46	1.57	1.50
29	a	412	SQD	O47-C7	2.46	1.41	1.34
22	C	503	CLA	C3B-CAB	-2.46	1.42	1.47
26	d	405	PL9	C46-C44	-2.46	1.46	1.51
22	C	506	CLA	C3B-C2B	-2.46	1.37	1.40
22	a	405	CLA	CAC-C3C	-2.46	1.46	1.52
24	C	514	BCR	C33-C5	-2.45	1.46	1.50
22	B	607	CLA	C3B-C2B	-2.45	1.37	1.40
30	h	101	DGD	O5D-C1E	2.45	1.44	1.40
22	C	504	CLA	CMD-C2D	-2.45	1.45	1.51
24	A	406	BCR	C33-C5	-2.45	1.46	1.50
22	a	411	CLA	C3B-C2B	-2.44	1.37	1.40
22	c	507	CLA	CMC-C2C	-2.44	1.45	1.51
30	C	515	DGD	O2D-C2D	-2.44	1.37	1.43
27	c	520	LMG	O1-C1	2.44	1.44	1.40
27	d	409	LMG	O7-C8	-2.44	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	101	BCR	C1-C6	-2.44	1.50	1.53
22	B	601	CLA	C3B-CAB	-2.44	1.43	1.47
22	b	604	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	609	CLA	C4B-CHC	-2.43	1.34	1.41
22	c	503	CLA	C1D-C2D	2.43	1.48	1.42
22	c	501	CLA	CMB-C2B	-2.43	1.46	1.51
29	F	102	SQD	O3-C3	-2.43	1.37	1.43
22	c	512	CLA	CMC-C2C	-2.42	1.45	1.51
22	C	507	CLA	C3B-C2B	-2.42	1.37	1.40
22	d	403	CLA	C1D-C2D	2.42	1.48	1.42
22	c	504	CLA	CAC-C3C	-2.42	1.46	1.52
22	b	613	CLA	C4B-CHC	-2.42	1.34	1.41
22	c	506	CLA	CMD-C2D	-2.42	1.45	1.51
22	c	504	CLA	C1D-C2D	2.41	1.48	1.42
29	F	102	SQD	O2-C2	-2.41	1.37	1.43
23	d	401	PHO	CMC-C2C	-2.41	1.45	1.50
22	c	507	CLA	C3B-CAB	-2.41	1.43	1.47
22	A	403	CLA	CMB-C2B	-2.40	1.46	1.51
28	d	407	LHG	P-O6	2.40	1.69	1.59
24	a	406	BCR	C30-C25	-2.40	1.50	1.53
22	c	508	CLA	CMB-C2B	-2.40	1.46	1.51
23	d	401	PHO	C4C-NC	2.40	1.42	1.36
22	b	604	CLA	C3B-C2B	-2.40	1.37	1.40
30	c	515	DGD	C3G-C2G	2.40	1.58	1.50
22	b	612	CLA	C4C-NC	2.39	1.37	1.35
22	c	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	504	CLA	C4B-CHC	-2.39	1.34	1.41
22	b	614	CLA	CAC-C3C	-2.39	1.46	1.52
22	B	615	CLA	CAC-C3C	-2.38	1.46	1.52
22	B	613	CLA	C1D-C2D	2.38	1.48	1.42
22	B	608	CLA	C3B-C2B	-2.38	1.37	1.40
28	D	409	LHG	O8-C6	-2.38	1.39	1.45
22	b	607	CLA	CMC-C2C	-2.38	1.45	1.51
28	L	102	LHG	O7-C5	-2.38	1.40	1.46
24	x	101	BCR	C1-C6	-2.38	1.50	1.53
30	A	414	DGD	O2G-C1B	2.37	1.41	1.34
22	c	510	CLA	C1D-C2D	2.36	1.47	1.42
22	B	609	CLA	O2D-CGD	2.36	1.39	1.33
22	c	510	CLA	CAA-C2A	-2.36	1.49	1.54
22	a	411	CLA	CMA-C3A	-2.36	1.48	1.53
22	c	513	CLA	CMC-C2C	-2.36	1.45	1.51
22	a	403	CLA	CMD-C2D	-2.36	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	PHO	C4B-NB	2.35	1.42	1.36
24	k	102	BCR	C33-C5	-2.35	1.47	1.50
30	H	102	DGD	O6D-C5D	-2.35	1.38	1.44
22	A	402	CLA	CMB-C2B	-2.35	1.46	1.51
22	c	506	CLA	CAC-C3C	-2.34	1.46	1.52
22	a	403	CLA	CMB-C2B	-2.34	1.46	1.51
30	B	623	DGD	C2A-C1A	2.34	1.57	1.50
27	D	408	LMG	C1-C2	2.34	1.59	1.52
30	h	101	DGD	O5D-C6D	-2.34	1.39	1.43
22	b	609	CLA	MG-NA	2.34	2.11	2.06
27	D	408	LMG	C4-C3	2.34	1.58	1.52
28	B	621	LHG	P-O6	2.34	1.68	1.59
22	b	615	CLA	C4B-CHC	-2.34	1.34	1.41
22	b	614	CLA	C3B-C2B	-2.33	1.37	1.40
24	b	617	BCR	C33-C5	-2.33	1.47	1.50
28	D	409	LHG	O7-C5	-2.33	1.40	1.46
22	a	405	CLA	CMB-C2B	-2.33	1.46	1.51
22	c	510	CLA	CMC-C2C	-2.33	1.46	1.51
30	c	516	DGD	C6E-C5E	2.33	1.59	1.51
22	B	608	CLA	C1B-NB	2.32	1.37	1.35
23	d	401	PHO	CAA-C2A	-2.32	1.49	1.54
22	b	614	CLA	CMC-C2C	-2.32	1.46	1.51
22	c	512	CLA	CMD-C2D	-2.32	1.46	1.51
22	D	404	CLA	CMD-C2D	-2.32	1.46	1.51
23	A	404	PHO	O2D-CGD	2.32	1.38	1.33
22	b	606	CLA	C4B-CHC	-2.32	1.34	1.41
22	b	610	CLA	CMC-C2C	-2.31	1.46	1.51
22	C	507	CLA	C3B-CAB	-2.31	1.43	1.47
28	e	102	LHG	C6-C5	2.31	1.57	1.50
22	b	603	CLA	CMC-C2C	-2.31	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.31	1.46	1.51
27	C	518	LMG	C3-C2	2.31	1.58	1.52
22	d	403	CLA	CMC-C2C	-2.30	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.30	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.30	1.46	1.51
22	c	512	CLA	C3B-CAB	-2.30	1.43	1.47
23	D	401	PHO	CAA-C2A	-2.30	1.49	1.54
24	k	103	BCR	C1-C6	-2.30	1.50	1.53
22	C	504	CLA	CMB-C2B	-2.29	1.46	1.51
30	c	517	DGD	C4E-C3E	-2.29	1.46	1.52
22	a	405	CLA	C4B-CHC	-2.29	1.34	1.41
22	B	614	CLA	C3B-C2B	-2.29	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	CAC-C3C	-2.29	1.46	1.52
22	B	612	CLA	C1D-C2D	2.28	1.47	1.42
30	c	515	DGD	O6E-C1E	-2.28	1.36	1.41
22	b	605	CLA	CAC-C3C	-2.28	1.46	1.52
22	B	605	CLA	CMC-C2C	-2.28	1.46	1.51
30	H	102	DGD	C6D-C5D	2.28	1.58	1.51
22	d	403	CLA	C4B-CHC	-2.28	1.34	1.41
22	A	403	CLA	C3B-CAB	-2.28	1.43	1.47
22	a	403	CLA	CAC-C3C	-2.28	1.46	1.52
30	C	515	DGD	C6D-C5D	2.27	1.58	1.51
22	B	613	CLA	O2D-CED	-2.27	1.40	1.45
22	b	601	CLA	O2A-CGA	2.27	1.40	1.33
22	c	513	CLA	C1D-C2D	2.27	1.47	1.42
22	b	615	CLA	C3B-C2B	-2.27	1.37	1.40
30	H	102	DGD	C3E-C2E	2.27	1.58	1.52
22	D	404	CLA	C3B-C2B	-2.26	1.37	1.40
22	B	601	CLA	CMC-C2C	-2.26	1.46	1.51
29	f	101	SQD	O2-C2	-2.26	1.37	1.43
22	b	616	CLA	CAC-C3C	-2.26	1.46	1.52
26	a	410	PL9	C40-C39	-2.26	1.44	1.50
30	h	101	DGD	C1E-C2E	2.26	1.59	1.52
22	C	507	CLA	CMC-C2C	-2.26	1.46	1.51
30	C	515	DGD	O1G-C1A	2.26	1.39	1.33
30	H	102	DGD	O3G-C1D	2.26	1.44	1.40
22	c	503	CLA	CMD-C2D	-2.26	1.46	1.51
22	B	613	CLA	C4C-NC	2.25	1.37	1.35
30	C	517	DGD	O5D-C6D	2.25	1.47	1.43
22	b	606	CLA	C3B-C2B	-2.25	1.37	1.40
27	m	101	LMG	O7-C8	-2.25	1.41	1.46
22	C	512	CLA	CMB-C2B	-2.25	1.47	1.51
22	b	610	CLA	CAC-C3C	-2.25	1.46	1.52
30	B	623	DGD	C3G-C2G	2.25	1.56	1.51
26	D	407	PL9	C3-C4	-2.25	1.45	1.49
22	c	506	CLA	C4B-CHC	-2.24	1.34	1.41
22	B	615	CLA	C3B-C2B	-2.24	1.37	1.40
22	b	610	CLA	CMB-C2B	-2.24	1.47	1.51
22	C	513	CLA	C4B-CHC	-2.24	1.34	1.41
22	B	605	CLA	OBD-CAD	-2.24	1.19	1.22
30	c	515	DGD	C6D-C5D	2.24	1.58	1.51
24	c	514	BCR	C33-C5	-2.23	1.47	1.50
30	C	516	DGD	O4D-C4D	-2.23	1.37	1.43
22	c	502	CLA	CMC-C2C	-2.23	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C1D-C2D	2.23	1.47	1.42
22	A	402	CLA	CMC-C2C	-2.23	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.22	1.46	1.51
22	b	606	CLA	C1D-C2D	2.22	1.47	1.42
22	c	509	CLA	C1D-C2D	2.22	1.47	1.42
22	C	504	CLA	CAC-C3C	-2.22	1.46	1.52
22	b	609	CLA	CAC-C3C	-2.22	1.46	1.52
22	b	601	CLA	C3B-CAB	-2.22	1.43	1.47
22	D	404	CLA	CAC-C3C	-2.22	1.46	1.52
22	b	610	CLA	C3B-CAB	-2.22	1.43	1.47
22	b	610	CLA	C4B-CHC	-2.22	1.34	1.41
24	T	101	BCR	C27-C26	-2.21	1.46	1.51
30	h	101	DGD	O2E-C2E	-2.21	1.37	1.43
22	c	501	CLA	CMD-C2D	-2.21	1.46	1.51
23	D	401	PHO	CMD-C2D	-2.21	1.46	1.50
22	b	604	CLA	CAC-C3C	-2.21	1.46	1.52
22	b	605	CLA	CMD-C2D	-2.21	1.46	1.51
22	c	504	CLA	CMD-C2D	-2.21	1.46	1.51
22	B	605	CLA	C4B-CHC	-2.21	1.34	1.41
22	C	503	CLA	CMD-C2D	-2.21	1.46	1.51
22	c	513	CLA	MG-NA	-2.21	2.01	2.06
22	b	602	CLA	C3B-CAB	-2.21	1.43	1.47
22	b	611	CLA	C1D-C2D	2.21	1.47	1.42
22	b	616	CLA	CMB-C2B	-2.21	1.47	1.51
23	a	404	PHO	O2D-CGD	2.20	1.38	1.33
24	B	618	BCR	C33-C5	-2.20	1.47	1.50
28	E	101	LHG	O7-C5	-2.20	1.41	1.46
22	c	507	CLA	CMD-C2D	-2.20	1.46	1.51
22	B	616	CLA	C4B-CHC	-2.20	1.34	1.41
22	B	616	CLA	CMB-C2B	-2.20	1.47	1.51
26	D	407	PL9	C26-C24	-2.20	1.46	1.51
22	C	513	CLA	CMD-C2D	-2.20	1.46	1.51
22	A	405	CLA	C3B-CAB	-2.20	1.43	1.47
22	b	608	CLA	C3B-CAB	-2.20	1.43	1.47
22	B	604	CLA	O2D-CGD	2.20	1.38	1.33
22	B	608	CLA	CMD-C2D	-2.20	1.46	1.51
24	b	618	BCR	C33-C5	-2.19	1.47	1.50
22	b	605	CLA	C1D-C2D	2.19	1.47	1.42
22	C	507	CLA	C1D-C2D	2.19	1.47	1.42
23	d	401	PHO	CMD-C2D	-2.19	1.46	1.50
24	t	101	BCR	C27-C26	-2.19	1.46	1.51
22	B	602	CLA	C1D-C2D	2.19	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	CMD-C2D	-2.19	1.46	1.51
22	b	605	CLA	C4B-CHC	-2.19	1.34	1.41
30	C	515	DGD	C2A-C1A	-2.18	1.44	1.50
22	C	504	CLA	C1C-C2C	2.18	1.47	1.42
27	c	520	LMG	O6-C1	2.18	1.47	1.41
29	A	412	SQD	O3-C3	-2.18	1.37	1.43
29	f	101	SQD	O3-C3	-2.18	1.37	1.43
23	A	404	PHO	C3B-C4B	2.18	1.47	1.43
22	b	608	CLA	CMB-C2B	-2.18	1.47	1.51
22	A	405	CLA	CMB-C2B	-2.18	1.47	1.51
22	d	403	CLA	C3B-C2B	-2.18	1.37	1.40
34	F	101	HEM	CAA-C2A	2.18	1.55	1.52
22	a	411	CLA	C1D-C2D	2.18	1.47	1.42
27	d	409	LMG	O8-C28	2.18	1.39	1.33
22	b	608	CLA	CMA-C3A	-2.18	1.48	1.53
30	h	101	DGD	C4D-C3D	2.17	1.57	1.52
27	b	622	LMG	C9-C8	2.17	1.57	1.50
28	e	102	LHG	O8-C23	2.17	1.39	1.33
22	c	513	CLA	C3B-CAB	-2.17	1.43	1.47
28	b	623	LHG	C24-C23	2.17	1.57	1.50
22	b	601	CLA	CAC-C3C	-2.17	1.46	1.52
22	c	502	CLA	C1D-C2D	2.17	1.47	1.42
30	H	102	DGD	C4D-C3D	2.17	1.57	1.52
22	C	510	CLA	CMD-C2D	-2.16	1.46	1.51
27	C	518	LMG	O7-C8	-2.16	1.41	1.46
22	b	609	CLA	CMC-C2C	-2.16	1.46	1.51
22	C	504	CLA	O2D-CGD	2.16	1.38	1.33
24	Z	101	BCR	C33-C5	-2.16	1.47	1.50
22	C	506	CLA	C1D-C2D	2.16	1.47	1.42
24	b	618	BCR	C36-C18	-2.16	1.46	1.50
30	A	414	DGD	O1G-C1G	-2.16	1.40	1.45
22	d	402	CLA	C4B-CHC	-2.15	1.35	1.41
23	A	404	PHO	CMC-C2C	-2.15	1.46	1.50
35	v	201	HEC	C1D-ND	2.15	1.40	1.36
24	C	514	BCR	C36-C18	-2.15	1.46	1.50
22	C	505	CLA	CMC-C2C	-2.15	1.46	1.51
28	d	407	LHG	O6-C4	-2.15	1.36	1.44
22	A	405	CLA	C4B-CHC	-2.15	1.35	1.41
22	B	608	CLA	CMC-C2C	-2.15	1.46	1.51
30	c	515	DGD	C3E-C2E	2.15	1.57	1.52
22	C	508	CLA	CAC-C3C	-2.15	1.46	1.52
22	C	501	CLA	CAC-C3C	-2.15	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	CAC-C3C	-2.15	1.46	1.52
24	b	618	BCR	C1-C6	-2.15	1.50	1.53
24	T	101	BCR	C38-C26	-2.15	1.47	1.50
23	D	401	PHO	O2D-CGD	2.14	1.38	1.33
26	d	405	PL9	C11-C9	-2.14	1.46	1.51
22	B	616	CLA	CAC-C3C	-2.14	1.46	1.52
22	c	512	CLA	CAC-C3C	-2.14	1.46	1.52
22	B	605	CLA	MG-NA	2.14	2.11	2.06
26	D	407	PL9	C35-C34	-2.14	1.45	1.50
22	B	609	CLA	C3B-C2B	-2.14	1.37	1.40
22	D	405	CLA	CMC-C2C	-2.13	1.46	1.51
22	C	509	CLA	O2D-CGD	2.13	1.38	1.33
24	a	406	BCR	C33-C5	-2.13	1.47	1.50
29	A	412	SQD	O4-C4	-2.13	1.38	1.43
27	C	518	LMG	O1-C1	2.13	1.43	1.40
22	B	614	CLA	C1A-CHA	-2.13	1.34	1.43
22	B	609	CLA	C3B-CAB	-2.12	1.43	1.47
22	c	511	CLA	C3B-CAB	-2.12	1.43	1.47
22	B	606	CLA	C1D-C2D	2.12	1.47	1.42
24	B	617	BCR	C33-C5	-2.12	1.47	1.50
22	d	403	CLA	C3B-CAB	-2.12	1.43	1.47
30	A	414	DGD	C1E-C2E	2.12	1.58	1.52
27	a	414	LMG	O7-C8	-2.12	1.41	1.46
22	b	607	CLA	O2D-CED	-2.12	1.40	1.45
22	c	513	CLA	C4B-CHC	-2.12	1.35	1.41
22	B	602	CLA	CAC-C3C	-2.11	1.47	1.52
22	b	603	CLA	C3B-C2B	-2.11	1.37	1.40
22	C	506	CLA	CMB-C2B	-2.11	1.47	1.51
22	c	504	CLA	CMC-C2C	-2.11	1.46	1.51
22	b	612	CLA	C3B-C2B	-2.11	1.37	1.40
22	B	605	CLA	CMB-C2B	-2.11	1.47	1.51
29	a	412	SQD	O3-C3	-2.11	1.38	1.43
22	c	507	CLA	C4B-CHC	-2.11	1.35	1.41
22	C	506	CLA	CMD-C2D	-2.11	1.46	1.51
22	c	505	CLA	C3B-CAB	-2.11	1.43	1.47
30	C	516	DGD	O2E-C2E	-2.10	1.38	1.43
30	c	517	DGD	O2E-C2E	-2.10	1.38	1.43
30	C	516	DGD	O5D-C6D	-2.10	1.39	1.43
30	c	517	DGD	C6D-C5D	2.10	1.58	1.51
22	b	607	CLA	C1D-C2D	2.10	1.47	1.42
26	D	407	PL9	C32-C33	-2.10	1.43	1.50
29	f	101	SQD	O4-C4	-2.10	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	605	CLA	CMB-C2B	-2.10	1.47	1.51
22	b	603	CLA	O2D-CGD	2.10	1.38	1.33
22	A	403	CLA	CAC-C3C	-2.09	1.47	1.52
22	C	510	CLA	O2A-CGA	2.09	1.39	1.33
22	b	612	CLA	C1D-C2D	2.09	1.47	1.42
22	b	616	CLA	CMC-C2C	-2.09	1.46	1.51
22	C	501	CLA	C1B-NB	-2.09	1.33	1.35
24	K	102	BCR	C38-C26	-2.09	1.47	1.50
22	A	402	CLA	C3D-C2D	-2.09	1.35	1.39
22	D	403	CLA	CAC-C3C	-2.09	1.47	1.52
22	D	405	CLA	CMD-C2D	-2.09	1.46	1.51
27	b	622	LMG	C7-C8	2.08	1.57	1.50
30	c	516	DGD	C3G-C2G	2.08	1.57	1.50
22	B	615	CLA	C1D-C2D	2.08	1.47	1.42
24	B	619	BCR	C33-C5	-2.08	1.47	1.50
22	c	505	CLA	CMC-C2C	-2.08	1.46	1.51
30	c	517	DGD	C3E-C2E	2.08	1.57	1.52
30	c	517	DGD	O4E-C4E	-2.08	1.38	1.43
22	a	411	CLA	C3B-CAB	-2.08	1.43	1.47
22	B	607	CLA	CAC-C3C	-2.08	1.47	1.52
22	B	613	CLA	C1B-NB	-2.08	1.33	1.35
22	B	607	CLA	CMC-C2C	-2.07	1.46	1.51
22	a	402	CLA	C3B-C2B	-2.07	1.37	1.40
22	B	607	CLA	C3B-CAB	-2.07	1.43	1.47
22	D	405	CLA	C3B-CAB	-2.07	1.43	1.47
23	a	404	PHO	CMB-C2B	-2.07	1.46	1.50
22	B	604	CLA	C4C-NC	2.07	1.37	1.35
22	B	611	CLA	CAC-C3C	-2.07	1.47	1.52
22	C	513	CLA	C3B-CAB	-2.07	1.43	1.47
22	C	501	CLA	C3B-CAB	-2.06	1.43	1.47
27	b	622	LMG	C4-C5	2.06	1.57	1.53
22	c	506	CLA	CAA-C2A	-2.06	1.50	1.54
24	T	101	BCR	C1-C6	-2.06	1.50	1.53
27	C	518	LMG	O8-C9	-2.06	1.40	1.45
30	c	515	DGD	O3E-C3E	-2.06	1.38	1.43
22	c	508	CLA	CMA-C3A	-2.06	1.48	1.53
26	D	407	PL9	C41-C39	-2.06	1.47	1.51
22	C	513	CLA	CMC-C2C	-2.06	1.46	1.51
30	c	515	DGD	O1G-C1A	2.06	1.39	1.33
22	b	613	CLA	O2D-CED	-2.06	1.40	1.45
22	B	603	CLA	C1D-C2D	2.06	1.47	1.42
23	D	401	PHO	C1C-NC	-2.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C1C-C2C	2.05	1.47	1.42
28	D	409	LHG	P-O3	2.05	1.67	1.59
22	C	502	CLA	C3B-CAB	-2.05	1.43	1.47
22	C	510	CLA	CMC-C2C	-2.05	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.05	1.47	1.51
22	C	502	CLA	C4B-CHC	-2.05	1.35	1.41
22	B	608	CLA	C4B-CHC	-2.05	1.35	1.41
22	D	403	CLA	O2D-CED	-2.04	1.40	1.45
22	B	616	CLA	C1D-C2D	2.04	1.47	1.42
22	c	508	CLA	O2D-CGD	2.04	1.38	1.33
22	b	614	CLA	C1D-C2D	2.04	1.47	1.42
28	A	411	LHG	O8-C23	2.04	1.39	1.33
22	c	513	CLA	CMD-C2D	-2.04	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.04	1.46	1.51
22	b	603	CLA	C1A-CHA	-2.04	1.34	1.43
22	c	511	CLA	CMD-C2D	-2.04	1.46	1.51
22	B	602	CLA	MG-NA	-2.04	2.01	2.06
22	C	505	CLA	C3B-CAB	-2.04	1.43	1.47
22	C	509	CLA	O2A-CGA	2.03	1.39	1.33
22	b	605	CLA	C3B-CAB	-2.03	1.43	1.47
22	C	509	CLA	CMC-C2C	-2.03	1.46	1.51
22	C	509	CLA	C4B-CHC	-2.03	1.35	1.41
22	D	405	CLA	C1C-C2C	2.03	1.47	1.42
24	H	101	BCR	C1-C6	-2.03	1.51	1.53
27	A	410	LMG	C4-C5	2.03	1.57	1.53
22	C	513	CLA	C3B-C2B	-2.03	1.37	1.40
22	b	606	CLA	CAC-C3C	-2.03	1.47	1.52
22	b	602	CLA	CMB-C2B	-2.03	1.47	1.51
22	D	403	CLA	C4B-CHC	-2.03	1.35	1.41
22	c	511	CLA	CMC-C2C	-2.02	1.46	1.51
22	D	404	CLA	C1C-C2C	2.02	1.47	1.42
23	d	401	PHO	CHC-C4B	-2.02	1.35	1.40
22	B	614	CLA	CAC-C3C	-2.02	1.47	1.52
22	b	616	CLA	O2D-CED	-2.02	1.40	1.45
22	B	609	CLA	CAC-C3C	-2.02	1.47	1.52
22	c	508	CLA	CMC-C2C	-2.02	1.46	1.51
22	c	508	CLA	C4B-CHC	-2.02	1.35	1.41
28	b	623	LHG	O8-C23	2.02	1.39	1.33
22	B	606	CLA	CMA-C3A	-2.02	1.48	1.53
23	A	404	PHO	C4C-NC	2.02	1.41	1.36
22	B	610	CLA	C1C-C2C	2.01	1.47	1.42
24	B	617	BCR	C38-C26	-2.01	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	BCR	C38-C26	-2.01	1.47	1.50
22	B	614	CLA	CMC-C2C	-2.01	1.46	1.51
24	T	101	BCR	C4-C5	-2.01	1.47	1.51
22	C	509	CLA	C1C-C2C	2.01	1.47	1.42
22	c	510	CLA	CAC-C3C	-2.01	1.47	1.52
28	E	101	LHG	O8-C6	-2.00	1.40	1.45
27	A	410	LMG	O6-C5	-2.00	1.39	1.44
22	B	605	CLA	C1D-C2D	2.00	1.47	1.42
30	C	517	DGD	C6D-C5D	2.00	1.57	1.51
22	C	506	CLA	C3B-CAB	-2.00	1.43	1.47
27	c	518	LMG	O8-C9	-2.00	1.40	1.45
22	C	508	CLA	CMB-C2B	-2.00	1.47	1.51
22	C	505	CLA	C1D-C2D	2.00	1.47	1.42
22	b	610	CLA	C1D-C2D	2.00	1.47	1.42
22	C	503	CLA	CMC-C2C	-2.00	1.46	1.51

All (1258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	10.28	111.33	106.71
22	B	616	CLA	C4A-NA-C1A	9.55	111.00	106.71
22	B	606	CLA	C4A-NA-C1A	8.85	110.69	106.71
29	a	412	SQD	O6-C1-C2	8.69	121.87	108.30
29	A	412	SQD	O6-C1-C2	8.59	121.72	108.30
29	L	101	SQD	O6-C1-C2	8.41	121.44	108.30
22	B	604	CLA	C4A-NA-C1A	8.24	110.41	106.71
22	b	604	CLA	C4A-NA-C1A	7.95	110.28	106.71
22	D	403	CLA	C4A-NA-C1A	7.79	110.21	106.71
22	b	606	CLA	C4A-NA-C1A	7.76	110.19	106.71
22	b	616	CLA	C4A-NA-C1A	7.71	110.17	106.71
22	d	402	CLA	C4A-NA-C1A	7.68	110.16	106.71
22	c	503	CLA	C4A-NA-C1A	7.51	110.08	106.71
22	C	509	CLA	C4A-NA-C1A	7.21	109.95	106.71
22	b	601	CLA	C4A-NA-C1A	7.18	109.94	106.71
29	B	622	SQD	O6-C1-C2	7.13	119.43	108.30
22	B	607	CLA	C4A-NA-C1A	7.12	109.91	106.71
26	a	410	PL9	C7-C3-C4	7.08	122.63	116.88
22	b	609	CLA	C4A-NA-C1A	6.99	109.85	106.71
29	f	101	SQD	O7-S-C6	6.92	115.16	106.94
22	c	501	CLA	C4A-NA-C1A	6.81	109.77	106.71
26	d	405	PL9	C7-C3-C4	6.77	122.38	116.88
22	C	507	CLA	C4A-NA-C1A	6.63	109.69	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	C4A-NA-C1A	6.55	109.65	106.71
22	c	510	CLA	C4A-NA-C1A	6.53	109.64	106.71
22	b	609	CLA	CMB-C2B-C1B	-6.48	118.51	128.46
22	c	511	CLA	C4A-NA-C1A	6.43	109.60	106.71
29	L	101	SQD	O7-S-C6	6.41	114.56	106.94
22	b	607	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	B	601	CLA	C4A-NA-C1A	6.40	109.58	106.71
26	D	407	PL9	C7-C3-C4	6.32	122.02	116.88
22	C	502	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	c	507	CLA	C4A-NA-C1A	6.21	109.50	106.71
22	C	511	CLA	C4A-NA-C1A	6.15	109.47	106.71
29	F	102	SQD	O6-C1-C2	6.12	117.86	108.30
22	C	510	CLA	C4A-NA-C1A	6.06	109.43	106.71
22	b	614	CLA	C4A-NA-C1A	5.97	109.39	106.71
34	F	101	HEM	CBD-CAD-C3D	-5.97	101.48	112.48
29	A	412	SQD	O7-S-C6	5.93	113.99	106.94
22	B	615	CLA	C4A-NA-C1A	5.88	109.35	106.71
22	B	609	CLA	C4A-NA-C1A	5.88	109.35	106.71
22	a	403	CLA	C4A-NA-C1A	5.86	109.34	106.71
22	C	512	CLA	C4A-NA-C1A	5.78	109.31	106.71
22	b	605	CLA	C4A-NA-C1A	5.72	109.28	106.71
22	c	508	CLA	CMB-C2B-C1B	-5.71	119.69	128.46
34	e	101	HEM	CBA-CAA-C2A	-5.70	101.98	112.49
29	A	413	SQD	C45-O47-C7	5.62	125.10	117.88
29	F	102	SQD	O9-S-C6	5.61	113.60	106.94
22	b	602	CLA	C4A-NA-C1A	5.60	109.22	106.71
22	c	509	CLA	C4A-NA-C1A	5.57	109.21	106.71
22	D	404	CLA	C4A-NA-C1A	5.53	109.19	106.71
22	B	611	CLA	C4A-NA-C1A	5.45	109.16	106.71
22	D	405	CLA	CMB-C2B-C1B	-5.43	120.12	128.46
22	b	612	CLA	CMB-C2B-C1B	-5.41	120.15	128.46
22	B	605	CLA	C4A-NA-C1A	5.38	109.12	106.71
22	b	613	CLA	CMB-C2B-C1B	-5.38	120.20	128.46
35	V	201	HEC	CMC-C2C-C1C	-5.27	120.36	128.46
22	b	615	CLA	C4A-NA-C1A	5.26	109.07	106.71
29	B	622	SQD	O47-C7-C8	5.21	122.73	111.50
26	A	409	PL9	C40-C39-C41	5.20	124.02	115.27
22	B	613	CLA	CMB-C2B-C1B	-5.19	120.48	128.46
22	B	612	CLA	C4A-NA-C1A	5.19	109.04	106.71
29	L	101	SQD	O9-S-C6	5.18	113.09	106.94
22	b	602	CLA	O2D-CGD-O1D	-5.15	113.77	123.84
22	b	606	CLA	O2D-CGD-O1D	-5.15	113.77	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
34	e	101	HEM	CBD-CAD-C3D	-5.13	103.02	112.48
22	c	504	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
29	a	412	SQD	O7-S-C6	5.07	112.97	106.94
22	A	405	CLA	C4A-NA-C1A	5.07	108.98	106.71
22	b	611	CLA	C4A-NA-C1A	5.07	108.98	106.71
29	f	101	SQD	O6-C1-C2	5.05	116.19	108.30
22	B	612	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
22	B	602	CLA	CMB-C2B-C1B	-5.03	120.73	128.46
22	B	603	CLA	C4A-NA-C1A	5.01	108.96	106.71
22	D	405	CLA	C4A-NA-C1A	5.00	108.95	106.71
22	c	505	CLA	C4A-NA-C1A	4.98	108.95	106.71
22	B	614	CLA	O2D-CGD-O1D	-4.94	114.18	123.84
22	b	610	CLA	C4A-NA-C1A	4.91	108.91	106.71
22	C	505	CLA	C4A-NA-C1A	4.90	108.91	106.71
22	d	403	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
22	C	505	CLA	CMB-C2B-C1B	-4.85	121.02	128.46
22	B	604	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
22	C	513	CLA	O2D-CGD-O1D	-4.78	114.50	123.84
22	a	405	CLA	C4A-NA-C1A	4.76	108.85	106.71
22	b	603	CLA	CMB-C2B-C1B	-4.74	121.17	128.46
22	b	603	CLA	CMB-C2B-C3B	4.72	133.51	124.68
22	B	611	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
35	V	201	HEC	CMB-C2B-C1B	-4.69	121.26	128.46
22	C	510	CLA	CMB-C2B-C1B	-4.67	121.28	128.46
22	C	512	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
29	A	412	SQD	O8-S-C6	4.63	113.11	105.74
22	c	508	CLA	CMB-C2B-C3B	4.60	133.29	124.68
29	a	413	SQD	O47-C7-C8	4.60	121.42	111.50
22	A	405	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
22	a	411	CLA	C4A-NA-C1A	4.58	108.76	106.71
22	b	616	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
22	A	402	CLA	CHB-C4A-NA	4.56	130.82	124.51
22	c	510	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
22	c	502	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
26	d	405	PL9	C40-C39-C41	4.52	122.88	115.27
22	A	402	CLA	CMB-C2B-C1B	-4.52	121.52	128.46
22	b	611	CLA	O2D-CGD-O1D	-4.50	115.03	123.84
22	a	402	CLA	CMB-C2B-C1B	-4.49	121.56	128.46
22	C	511	CLA	CMB-C2B-C1B	-4.46	121.61	128.46
22	c	512	CLA	C1-C2-C3	-4.46	118.33	126.04
30	H	102	DGD	O3G-C3G-C2G	-4.44	100.18	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	F	102	SQD	O8-S-C6	4.44	112.81	105.74
22	B	605	CLA	C4D-C3D-CAD	-4.43	106.00	108.47
22	a	403	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
30	C	515	DGD	O3G-C3G-C2G	-4.42	100.23	110.90
22	C	506	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
22	b	601	CLA	O2D-CGD-O1D	-4.41	115.22	123.84
30	c	517	DGD	O5D-C1E-C2E	4.39	115.15	108.30
22	b	603	CLA	O2D-CGD-O1D	-4.38	115.28	123.84
22	c	509	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
22	B	607	CLA	CMB-C2B-C1B	-4.33	121.80	128.46
22	b	609	CLA	CMB-C2B-C3B	4.33	132.78	124.68
22	B	615	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
26	a	410	PL9	C7-C3-C2	-4.32	117.63	123.30
28	D	409	LHG	O4-P-O5	4.32	133.57	112.24
28	L	102	LHG	O4-P-O5	4.29	133.45	112.24
28	l	101	LHG	O4-P-O5	4.28	133.39	112.24
22	B	612	CLA	CMB-C2B-C3B	4.28	132.68	124.68
22	D	405	CLA	O2D-CGD-O1D	-4.28	115.48	123.84
22	B	614	CLA	C4D-C3D-CAD	-4.27	106.09	108.47
22	b	616	CLA	CMB-C2B-C3B	4.26	132.66	124.68
29	F	102	SQD	C1-C2-C3	-4.26	101.12	110.00
22	C	505	CLA	CMB-C2B-C3B	4.24	132.62	124.68
22	B	606	CLA	C4D-C3D-CAD	-4.23	106.11	108.47
22	B	613	CLA	CMB-C2B-C3B	4.23	132.59	124.68
28	d	407	LHG	O4-P-O5	4.23	133.13	112.24
22	C	505	CLA	OBD-CAD-CBD	-4.22	119.86	125.89
22	c	502	CLA	CMB-C2B-C3B	4.21	132.56	124.68
29	A	412	SQD	O47-C7-C8	4.20	120.55	111.50
22	B	603	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
22	C	513	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
29	B	622	SQD	O7-S-C6	4.20	111.92	106.94
22	d	403	CLA	CMB-C2B-C3B	4.19	132.52	124.68
27	b	622	LMG	C1-O6-C5	-4.19	105.47	113.69
22	B	610	CLA	C4A-NA-C1A	4.18	108.59	106.71
22	B	602	CLA	CMB-C2B-C3B	4.18	132.50	124.68
24	b	617	BCR	C2-C1-C6	4.18	116.91	110.48
22	C	509	CLA	CMB-C2B-C3B	4.17	132.49	124.68
22	B	604	CLA	CMB-C2B-C3B	4.17	132.48	124.68
28	B	621	LHG	O4-P-O5	4.17	132.85	112.24
22	b	611	CLA	O2D-CGD-CBD	4.17	118.67	111.27
22	c	513	CLA	C4A-NA-C1A	4.17	108.58	106.71
22	b	604	CLA	C1-C2-C3	-4.15	118.86	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	C4A-NA-C1A	4.14	108.57	106.71
22	b	611	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
22	D	405	CLA	CMB-C2B-C3B	4.13	132.40	124.68
22	c	509	CLA	O2A-CGA-O1A	-4.12	113.19	123.59
22	A	403	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
22	B	613	CLA	C4A-NA-C1A	4.10	108.55	106.71
22	a	402	CLA	C4A-NA-C1A	4.10	108.55	106.71
22	a	405	CLA	CMD-C2D-C3D	4.10	132.35	124.68
28	e	102	LHG	O4-P-O5	4.10	132.50	112.24
22	c	506	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
28	d	406	LHG	O4-P-O5	4.09	132.45	112.24
22	b	615	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
29	A	412	SQD	C1-C2-C3	-4.07	101.52	110.00
22	b	603	CLA	C4A-NA-C1A	4.06	108.53	106.71
22	A	405	CLA	O2D-CGD-CBD	4.06	118.48	111.27
22	c	501	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
22	c	512	CLA	C4A-NA-C1A	4.05	108.53	106.71
22	b	603	CLA	OBD-CAD-CBD	-4.04	120.12	125.89
22	c	506	CLA	C4A-NA-C1A	4.04	108.52	106.71
22	b	612	CLA	CMB-C2B-C3B	4.04	132.24	124.68
22	b	613	CLA	CMB-C2B-C3B	4.04	132.23	124.68
22	b	601	CLA	CHB-C4A-NA	4.01	130.06	124.51
22	B	616	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
35	V	201	HEC	CMB-C2B-C3B	4.00	130.52	125.82
29	L	101	SQD	O47-C7-C8	3.99	120.11	111.50
22	D	404	CLA	CMB-C2B-C3B	3.98	132.13	124.68
22	C	504	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
22	D	403	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
22	b	604	CLA	CMD-C2D-C3D	3.93	132.03	124.68
22	A	403	CLA	CMB-C2B-C3B	3.91	132.00	124.68
22	c	504	CLA	C4A-NA-C1A	3.91	108.46	106.71
22	C	508	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
28	E	101	LHG	O4-P-O5	3.90	131.54	112.24
22	B	603	CLA	CMB-C2B-C3B	3.90	131.97	124.68
22	A	405	CLA	CMB-C2B-C3B	3.89	131.96	124.68
27	m	101	LMG	O3-C3-C2	-3.89	101.36	110.35
28	A	411	LHG	O4-P-O5	3.88	131.42	112.24
22	B	614	CLA	OBD-CAD-CBD	-3.86	120.38	125.89
22	c	509	CLA	CMB-C2B-C3B	3.86	131.90	124.68
22	c	504	CLA	CMB-C2B-C3B	3.85	131.89	124.68
22	B	601	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
22	B	608	CLA	C4A-NA-C1A	3.84	108.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
22	b	613	CLA	C1-C2-C3	-3.83	119.42	126.04
22	b	602	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
22	B	605	CLA	CMD-C2D-C3D	3.83	131.84	124.68
22	c	512	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
22	B	607	CLA	CMB-C2B-C3B	3.82	131.83	124.68
24	H	101	BCR	C36-C18-C17	-3.82	117.57	122.92
22	c	512	CLA	CHB-C4A-NA	3.82	129.79	124.51
22	B	614	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
22	B	611	CLA	CMB-C2B-C3B	3.81	131.80	124.68
22	B	608	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
22	C	512	CLA	CMB-C2B-C3B	3.80	131.78	124.68
30	c	517	DGD	O3G-C3G-C2G	-3.79	101.76	110.90
22	b	604	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
30	C	516	DGD	O3G-C3G-C2G	-3.77	101.81	110.90
22	C	512	CLA	CHB-C4A-NA	3.76	129.71	124.51
22	a	411	CLA	CHB-C4A-NA	3.76	129.71	124.51
22	B	602	CLA	CHB-C4A-NA	3.75	129.70	124.51
22	C	513	CLA	C4D-C3D-CAD	-3.75	106.38	108.47
22	C	510	CLA	CMB-C2B-C3B	3.75	131.69	124.68
24	k	101	BCR	C2-C1-C6	3.74	116.23	110.48
22	b	606	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
22	c	510	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
22	A	402	CLA	CMB-C2B-C3B	3.71	131.62	124.68
22	b	605	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
29	f	101	SQD	O9-S-O7	-3.70	101.15	113.95
22	B	616	CLA	CMB-C2B-C3B	3.69	131.57	124.68
24	Z	101	BCR	C15-C16-C17	-3.67	115.95	123.47
22	b	616	CLA	CHB-C4A-NA	3.67	129.59	124.51
28	b	623	LHG	O4-P-O5	3.67	130.37	112.24
29	B	622	SQD	C1-O5-C5	-3.67	106.49	113.69
22	D	404	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	B	614	CLA	C4A-NA-C1A	3.65	108.34	106.71
22	C	503	CLA	C4D-C3D-CAD	-3.64	106.44	108.47
22	b	613	CLA	CHB-C4A-NA	3.64	129.54	124.51
22	C	503	CLA	O2A-C1-C2	-3.64	99.08	108.64
22	c	512	CLA	C4D-C3D-CAD	-3.63	106.44	108.47
22	c	511	CLA	C4D-C3D-CAD	-3.63	106.45	108.47
22	C	506	CLA	CMB-C2B-C3B	3.63	131.47	124.68
22	c	511	CLA	OBD-CAD-CBD	-3.62	120.72	125.89
24	K	102	BCR	C37-C22-C21	-3.62	117.85	122.92
22	c	505	CLA	O2D-CGD-O1D	-3.62	116.76	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	O1D-CGD-CBD	3.61	131.88	124.48
22	C	511	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
22	a	405	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
22	b	609	CLA	OBD-CAD-CBD	-3.61	120.74	125.89
22	b	613	CLA	C4A-NA-C1A	3.61	108.33	106.71
22	c	511	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
26	D	407	PL9	C7-C3-C2	-3.59	118.58	123.30
26	A	409	PL9	C22-C23-C24	-3.59	119.02	127.66
22	A	405	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
24	B	619	BCR	C2-C1-C6	3.58	116.00	110.48
22	b	601	CLA	O2D-CGD-CBD	3.58	117.63	111.27
22	d	402	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
30	A	414	DGD	O3G-C3G-C2G	-3.57	102.27	110.90
30	C	517	DGD	O3G-C3G-C2G	-3.57	102.27	110.90
35	V	201	HEC	CBD-CAD-C3D	-3.57	105.91	112.49
22	c	511	CLA	CMD-C2D-C3D	3.56	131.34	124.68
27	C	518	LMG	O6-C1-O1	-3.56	101.55	109.97
24	b	617	BCR	C38-C26-C25	-3.55	120.54	124.53
30	h	101	DGD	O6E-C5E-C4E	3.55	116.14	109.69
22	b	602	CLA	CMB-C2B-C3B	3.54	131.31	124.68
22	c	510	CLA	CMB-C2B-C3B	3.54	131.31	124.68
22	a	403	CLA	CMB-C2B-C3B	3.54	131.30	124.68
26	A	409	PL9	C36-C34-C33	-3.54	113.96	121.12
22	a	411	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
22	B	616	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
22	C	513	CLA	CMB-C2B-C3B	3.52	131.27	124.68
22	b	612	CLA	CMD-C2D-C3D	3.51	131.25	124.68
22	B	610	CLA	CMD-C2D-C3D	3.50	131.23	124.68
30	C	516	DGD	O2D-C2D-C1D	-3.49	101.56	110.05
24	b	618	BCR	C36-C18-C17	-3.49	118.03	122.92
24	H	101	BCR	C38-C26-C25	-3.49	120.61	124.53
26	A	409	PL9	C7-C3-C4	3.49	119.71	116.88
29	L	101	SQD	C1-C2-C3	-3.49	102.73	110.00
22	c	513	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
22	B	605	CLA	C4-C3-C5	3.48	121.12	115.27
22	C	504	CLA	C4A-NA-C1A	3.48	108.27	106.71
22	D	405	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
29	A	413	SQD	O48-C23-C24	3.46	122.76	111.91
22	C	508	CLA	C4A-NA-C1A	3.45	108.26	106.71
22	C	505	CLA	CMD-C2D-C3D	3.45	131.13	124.68
22	C	503	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
35	v	201	HEC	CBD-CAD-C3D	-3.43	106.15	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
29	B	622	SQD	O9-S-O7	-3.42	102.10	113.95
22	B	604	CLA	OBD-CAD-CBD	-3.42	121.00	125.89
22	B	603	CLA	OBD-CAD-CBD	-3.42	121.01	125.89
22	A	402	CLA	C7-C6-C5	-3.42	104.07	113.36
30	h	101	DGD	O3G-C3G-C2G	-3.41	102.66	110.90
30	c	517	DGD	O6E-C5E-C4E	3.41	115.89	109.69
22	D	404	CLA	CHB-C4A-NA	3.41	129.23	124.51
28	e	102	LHG	O8-C23-C24	3.41	122.61	111.91
22	b	603	CLA	O2D-CGD-CBD	3.41	117.32	111.27
22	b	605	CLA	C4-C3-C5	3.40	121.00	115.27
22	c	506	CLA	CMB-C2B-C3B	3.40	131.04	124.68
22	C	501	CLA	C4A-NA-C1A	3.40	108.23	106.71
29	F	102	SQD	C1-O5-C5	-3.40	107.02	113.69
22	B	613	CLA	C1-C2-C3	-3.40	120.17	126.04
22	a	405	CLA	OBD-CAD-CBD	-3.38	121.06	125.89
22	B	612	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
29	L	101	SQD	C3-C4-C5	3.38	116.27	110.24
22	a	403	CLA	CHB-C4A-NA	3.38	129.18	124.51
27	m	101	LMG	O1-C1-C2	-3.38	103.03	108.30
22	b	615	CLA	CMD-C2D-C3D	3.38	131.00	124.68
22	B	610	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
22	B	606	CLA	CMD-C2D-C3D	3.37	130.98	124.68
22	c	513	CLA	CHB-C4A-NA	3.36	129.16	124.51
22	B	606	CLA	OBD-CAD-CBD	-3.36	121.10	125.89
22	c	513	CLA	CMB-C2B-C3B	3.35	130.95	124.68
30	C	515	DGD	O1G-C1A-C2A	-3.35	101.39	111.91
22	b	616	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
22	B	606	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	B	605	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	c	513	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
22	d	402	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
22	B	614	CLA	C4-C3-C5	3.33	120.86	115.27
26	D	407	PL9	C20-C19-C21	3.33	120.86	115.27
22	C	513	CLA	CMD-C2D-C3D	3.32	130.90	124.68
22	b	608	CLA	C4D-C3D-CAD	-3.32	106.62	108.47
22	b	608	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
22	B	613	CLA	C4-C3-C5	3.31	120.84	115.27
22	c	513	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
27	b	622	LMG	O1-C1-C2	-3.31	103.14	108.30
24	H	101	BCR	C2-C1-C6	3.31	115.57	110.48
27	d	409	LMG	O6-C1-O1	-3.30	102.16	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	604	CLA	OBD-CAD-CBD	-3.30	121.18	125.89
24	b	619	BCR	C29-C30-C25	3.29	115.55	110.48
22	b	603	CLA	C4-C3-C5	3.29	120.81	115.27
22	A	405	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
22	c	512	CLA	OBD-CAD-CBD	-3.29	121.20	125.89
22	C	509	CLA	CHB-C4A-NA	3.28	129.05	124.51
22	b	609	CLA	CMD-C2D-C3D	3.28	130.82	124.68
22	C	503	CLA	CMD-C2D-C3D	3.28	130.82	124.68
30	C	516	DGD	O5D-C6D-C5D	-3.28	102.98	109.05
22	A	403	CLA	C4A-NA-C1A	3.28	108.18	106.71
22	a	402	CLA	CMB-C2B-C3B	3.27	130.80	124.68
22	C	513	CLA	C4A-NA-C1A	3.27	108.18	106.71
22	b	608	CLA	CMB-C2B-C3B	3.27	130.80	124.68
22	b	604	CLA	CMC-C2C-C3C	3.27	131.11	124.94
29	a	412	SQD	O8-S-C6	3.27	110.95	105.74
24	C	514	BCR	C15-C16-C17	-3.27	116.78	123.47
26	a	410	PL9	C20-C19-C21	3.26	120.75	115.27
26	D	407	PL9	C40-C39-C41	3.26	120.75	115.27
24	C	514	BCR	C2-C1-C6	3.26	115.49	110.48
29	f	101	SQD	O9-S-C6	3.25	110.81	106.94
22	b	608	CLA	CHB-C4A-NA	3.25	129.01	124.51
30	c	516	DGD	O2E-C2E-C1E	-3.25	102.16	110.05
22	C	511	CLA	CMD-C2D-C3D	3.25	130.75	124.68
29	L	101	SQD	O48-C23-C24	3.25	122.09	111.91
29	a	412	SQD	O47-C7-C8	3.24	118.49	111.50
22	c	505	CLA	CHB-C4A-NA	3.24	128.99	124.51
30	C	517	DGD	O3E-C3E-C2E	-3.24	102.87	110.35
22	B	614	CLA	CMD-C2D-C3D	3.24	130.73	124.68
22	B	607	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
22	b	613	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
22	c	503	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
24	T	101	BCR	C31-C1-C6	3.23	115.53	110.30
23	a	404	PHO	CMB-C2B-C1B	-3.22	120.10	125.06
22	C	501	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
22	C	507	CLA	CHB-C4A-NA	3.22	128.97	124.51
22	C	505	CLA	OBD-CAD-C3D	3.21	133.32	127.98
22	B	610	CLA	O2A-CGA-O1A	-3.21	115.49	123.59
26	A	409	PL9	C41-C39-C38	-3.20	114.63	121.12
22	B	607	CLA	CHB-C4A-NA	3.20	128.94	124.51
27	b	622	LMG	O6-C5-C6	3.20	114.39	106.44
24	Z	101	BCR	C11-C10-C9	-3.20	122.75	127.31
24	T	101	BCR	C2-C1-C6	3.19	115.40	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	411	CLA	O2D-CGD-CBD	3.19	116.94	111.27
22	B	610	CLA	CHB-C4A-NA	3.19	128.92	124.51
24	D	406	BCR	C38-C26-C25	-3.18	120.96	124.53
22	b	613	CLA	CMC-C2C-C3C	3.18	130.93	124.94
22	b	605	CLA	CMB-C2B-C3B	3.18	130.62	124.68
22	b	606	CLA	O2D-CGD-CBD	3.17	116.90	111.27
24	c	514	BCR	C36-C18-C17	-3.17	118.48	122.92
22	B	615	CLA	CHB-C4A-NA	3.17	128.90	124.51
30	C	517	DGD	O6D-C1D-O3G	-3.17	102.47	109.97
24	Z	101	BCR	C36-C18-C17	-3.16	118.49	122.92
22	D	405	CLA	O2D-CGD-CBD	3.16	116.89	111.27
24	K	102	BCR	C27-C26-C25	3.16	127.32	122.73
29	B	622	SQD	O8-S-C6	3.16	110.77	105.74
22	b	616	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
22	C	501	CLA	O2A-CGA-O1A	-3.16	115.63	123.59
27	b	622	LMG	O2-C2-C1	-3.15	102.39	110.05
30	C	515	DGD	O2D-C2D-C1D	-3.15	102.39	110.05
22	C	508	CLA	CMB-C2B-C3B	3.15	130.57	124.68
22	c	513	CLA	CMD-C2D-C3D	3.15	130.57	124.68
35	V	201	HEC	C1D-C2D-C3D	-3.15	104.81	107.00
22	c	501	CLA	CED-O2D-CGD	-3.14	108.83	115.94
27	d	409	LMG	O2-C2-C1	-3.14	102.42	110.05
22	c	502	CLA	C4A-NA-C1A	3.14	108.12	106.71
22	C	511	CLA	CMB-C2B-C3B	3.14	130.54	124.68
22	C	512	CLA	O2A-CGA-O1A	-3.13	115.68	123.59
30	C	515	DGD	O5D-C6D-C5D	-3.13	103.26	109.05
29	A	413	SQD	O47-C45-C44	3.13	115.08	107.93
30	C	516	DGD	O3G-C1D-C2D	-3.12	103.43	108.30
22	b	605	CLA	C4D-C3D-CAD	-3.12	106.73	108.47
22	D	403	CLA	CMB-C2B-C3B	3.12	130.51	124.68
22	b	612	CLA	C4A-NA-C1A	3.11	108.10	106.71
24	B	617	BCR	C2-C1-C6	3.10	115.26	110.48
24	c	514	BCR	C2-C1-C6	3.10	115.25	110.48
22	B	608	CLA	O2D-CGD-CBD	3.10	116.77	111.27
22	C	502	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
24	B	619	BCR	C29-C30-C25	3.09	115.24	110.48
26	d	405	PL9	C36-C34-C33	-3.09	114.86	121.12
24	b	619	BCR	C37-C22-C21	-3.09	118.59	122.92
30	h	101	DGD	C4E-C3E-C2E	-3.09	105.43	110.82
22	b	610	CLA	CMD-C2D-C3D	3.09	130.46	124.68
22	D	403	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
24	x	101	BCR	C36-C18-C17	-3.08	118.61	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	LMG	O6-C1-O1	-3.07	102.71	109.97
23	D	401	PHO	C1-C2-C3	-3.07	120.74	126.04
22	b	608	CLA	O2D-CGD-CBD	3.06	116.70	111.27
24	B	617	BCR	C27-C26-C25	3.05	127.16	122.73
22	b	602	CLA	O2D-CGD-CBD	3.05	116.69	111.27
22	B	606	CLA	CMB-C2B-C3B	3.05	130.39	124.68
26	A	409	PL9	C27-C28-C29	-3.05	120.31	127.66
22	c	501	CLA	CMC-C2C-C3C	3.05	130.69	124.94
30	c	515	DGD	O6D-C1D-O3G	-3.05	102.76	109.97
22	B	615	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
22	b	609	CLA	C4D-C3D-CAD	-3.04	106.77	108.47
35	V	201	HEC	CAD-CBD-CGD	-3.04	107.57	112.67
22	B	609	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
29	L	101	SQD	O9-S-O7	-3.03	103.45	113.95
22	b	610	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
24	t	101	BCR	C7-C8-C9	-3.03	121.66	126.23
22	a	402	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
26	d	405	PL9	C35-C34-C36	3.03	120.36	115.27
22	c	501	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
22	a	405	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	D	403	CLA	CMD-C2D-C3D	3.02	130.32	124.68
24	k	103	BCR	C37-C22-C21	-3.01	118.70	122.92
22	c	507	CLA	OBD-CAD-CBD	-3.01	121.59	125.89
22	B	615	CLA	CMB-C2B-C3B	3.01	130.31	124.68
22	b	613	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
29	f	101	SQD	C1-C2-C3	-3.01	103.73	110.00
22	b	610	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	c	510	CLA	CMD-C2D-C3D	3.00	130.30	124.68
35	v	201	HEC	CMC-C2C-C1C	-3.00	123.85	128.46
30	c	516	DGD	O3G-C3G-C2G	-3.00	103.66	110.90
22	B	607	CLA	O2A-CGA-O1A	-3.00	116.02	123.59
22	C	512	CLA	C1-C2-C3	-3.00	120.86	126.04
22	b	602	CLA	C1-C2-C3	-3.00	120.86	126.04
26	a	410	PL9	C26-C24-C23	-2.99	115.06	121.12
22	b	606	CLA	CMC-C2C-C3C	2.99	130.59	124.94
22	B	612	CLA	C11-C12-C13	-2.99	106.24	115.92
29	B	622	SQD	C1-C2-C3	-2.99	103.76	110.00
26	d	405	PL9	C37-C38-C39	-2.99	120.46	127.66
22	B	615	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
27	a	414	LMG	C1-O6-C5	-2.99	107.82	113.69
30	c	517	DGD	O6D-C1D-O3G	-2.99	102.90	109.97
22	B	608	CLA	CMB-C2B-C3B	2.99	130.26	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	405	CLA	CHB-C4A-NA	2.98	128.64	124.51
29	A	412	SQD	O9-S-O7	-2.98	103.63	113.95
22	c	512	CLA	CMD-C2D-C3D	2.98	130.25	124.68
22	c	501	CLA	O2D-CGD-CBD	2.98	116.56	111.27
29	a	413	SQD	O49-C7-C8	-2.97	112.14	123.73
22	C	504	CLA	CMB-C2B-C3B	2.97	130.23	124.68
30	H	102	DGD	O6D-C1D-O3G	-2.97	102.95	109.97
22	A	402	CLA	C4A-NA-C1A	2.96	108.04	106.71
22	B	602	CLA	O2D-CGD-CBD	2.96	116.53	111.27
22	B	603	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	b	606	CLA	CMB-C2B-C3B	2.96	130.21	124.68
29	A	413	SQD	O47-C7-C8	2.95	117.87	111.50
24	T	101	BCR	C7-C8-C9	-2.95	121.77	126.23
24	c	514	BCR	C27-C26-C25	2.95	127.02	122.73
22	c	502	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
28	d	407	LHG	O8-C23-O10	-2.95	116.15	123.59
22	b	614	CLA	CHB-C4A-NA	2.95	128.59	124.51
27	m	101	LMG	C1-O6-C5	-2.95	107.90	113.69
29	f	101	SQD	O47-C7-C8	2.95	119.02	110.80
26	d	405	PL9	C31-C32-C33	-2.95	102.20	111.88
30	C	515	DGD	O3E-C3E-C2E	-2.94	103.55	110.35
26	a	410	PL9	C25-C24-C26	2.94	120.22	115.27
23	D	401	PHO	O1D-CGD-CBD	2.94	130.50	124.48
22	B	609	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
29	a	412	SQD	O47-C7-O49	-2.94	116.60	123.70
26	D	407	PL9	C37-C38-C39	-2.94	120.58	127.66
24	B	618	BCR	C15-C16-C17	-2.93	117.46	123.47
22	b	609	CLA	O1D-CGD-CBD	2.93	130.48	124.48
27	m	101	LMG	O7-C10-O9	-2.93	116.62	123.70
22	B	606	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
22	b	604	CLA	OBD-CAD-C3D	2.93	132.84	127.98
22	b	605	CLA	C1-C2-C3	-2.92	120.99	126.04
23	d	401	PHO	CMB-C2B-C1B	-2.92	120.56	125.06
22	B	608	CLA	CMD-C2D-C3D	2.92	130.15	124.68
24	k	102	BCR	C36-C18-C17	-2.92	118.83	122.92
24	A	406	BCR	C15-C16-C17	-2.92	117.49	123.47
24	Z	101	BCR	C15-C14-C13	-2.92	123.14	127.31
22	a	403	CLA	O2D-CGD-CBD	2.92	116.45	111.27
24	A	406	BCR	C36-C18-C17	-2.92	118.83	122.92
22	b	610	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	B	619	BCR	C37-C22-C21	-2.92	118.84	122.92
24	Z	101	BCR	C7-C8-C9	-2.91	121.83	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	c	506	CLA	OBD-CAD-CBD	-2.91	121.73	125.89
22	C	501	CLA	O2D-CGD-CBD	2.91	116.44	111.27
22	b	602	CLA	CHB-C4A-NA	2.91	128.53	124.51
22	b	604	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	A	406	BCR	C27-C26-C25	2.91	126.95	122.73
22	b	603	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
24	H	101	BCR	C27-C26-C25	2.90	126.94	122.73
26	D	407	PL9	C35-C34-C36	2.90	120.15	115.27
29	a	413	SQD	O48-C23-O10	-2.90	116.28	123.59
29	L	101	SQD	O2-C2-C1	2.90	117.08	110.05
27	M	101	LMG	O6-C1-O1	-2.90	103.12	109.97
24	d	404	BCR	C27-C26-C25	2.89	126.93	122.73
22	B	606	CLA	O2D-CGD-CBD	2.89	116.41	111.27
22	C	504	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
27	c	518	LMG	C9-C8-C7	-2.89	104.95	111.79
22	C	501	CLA	OBD-CAD-C3D	2.89	132.78	127.98
22	a	403	CLA	CMC-C2C-C3C	2.89	130.39	124.94
22	c	501	CLA	OBD-CAD-CBD	-2.89	121.77	125.89
26	d	405	PL9	C22-C23-C24	-2.89	120.71	127.66
22	C	512	CLA	C6-C5-C3	-2.88	105.89	113.45
22	b	613	CLA	CMD-C2D-C3D	2.88	130.06	124.68
28	A	411	LHG	O8-C23-C24	2.88	120.94	111.91
22	D	405	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
22	C	505	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	d	402	CLA	CMB-C2B-C3B	2.87	130.04	124.68
24	t	101	BCR	C1-C6-C5	-2.86	118.58	122.61
22	d	402	CLA	O1D-CGD-CBD	2.86	130.34	124.48
22	b	614	CLA	C4D-C3D-CAD	-2.86	106.88	108.47
22	A	405	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	B	607	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
22	b	607	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
22	C	507	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
22	c	507	CLA	C4D-C3D-CAD	-2.84	106.89	108.47
26	d	405	PL9	C7-C3-C2	-2.84	119.56	123.30
26	A	409	PL9	C40-C39-C38	-2.84	116.39	123.68
22	B	605	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	a	413	SQD	O48-C23-C24	2.84	120.82	111.91
22	C	508	CLA	O2D-CGD-CBD	2.84	116.31	111.27
24	x	101	BCR	C37-C22-C21	-2.83	118.95	122.92
30	c	516	DGD	C6D-O5D-C1E	2.83	119.27	113.74
30	A	414	DGD	CDB-CCB-CBB	-2.83	100.06	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	L	101	SQD	O5-C5-C4	2.83	114.83	109.69
30	A	414	DGD	C3G-C2G-C1G	-2.83	105.10	111.79
22	B	610	CLA	C4D-C3D-CAD	-2.82	106.89	108.47
22	B	612	CLA	O1D-CGD-CBD	2.82	130.26	124.48
23	d	401	PHO	C1-C2-C3	-2.82	121.16	126.04
22	c	510	CLA	OBD-CAD-CBD	-2.82	121.86	125.89
29	A	412	SQD	C1-O5-C5	-2.82	108.15	113.69
24	b	619	BCR	C36-C18-C17	-2.82	118.97	122.92
22	b	616	CLA	O1D-CGD-CBD	2.82	130.25	124.48
29	a	412	SQD	C1-C2-C3	-2.81	104.14	110.00
22	C	503	CLA	C7-C6-C5	-2.81	105.72	113.36
30	c	516	DGD	O3G-C1D-C2D	-2.81	103.91	108.30
28	D	409	LHG	O7-C7-C8	-2.81	105.44	111.50
28	D	409	LHG	O8-C23-C24	2.81	120.72	111.91
22	B	610	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
22	B	609	CLA	CMB-C2B-C3B	2.80	129.92	124.68
30	c	515	DGD	O4D-C4D-C5D	-2.80	102.34	109.30
24	T	101	BCR	C27-C26-C25	2.80	126.80	122.73
23	A	404	PHO	C1B-NB-C4B	2.80	111.79	106.51
27	a	414	LMG	O8-C28-O10	-2.80	116.53	123.59
22	C	506	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
22	b	610	CLA	CAA-CBA-CGA	-2.79	105.10	113.25
30	c	515	DGD	O3G-C3G-C2G	-2.79	104.17	110.90
30	A	414	DGD	O1G-C1A-O1A	-2.78	116.57	123.59
22	B	614	CLA	O1D-CGD-CBD	2.78	130.18	124.48
29	a	412	SQD	O9-S-O7	-2.78	104.32	113.95
22	C	503	CLA	O2A-CGA-O1A	-2.78	116.57	123.59
22	a	403	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
29	a	412	SQD	O48-C23-C24	2.78	120.63	111.91
22	C	511	CLA	C1-C2-C3	-2.78	121.23	126.04
22	C	513	CLA	OBD-CAD-CBD	-2.78	121.93	125.89
22	a	405	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
22	d	403	CLA	C4A-NA-C1A	2.77	107.95	106.71
22	c	507	CLA	CMD-C2D-C3D	2.76	129.85	124.68
30	H	102	DGD	C6D-C5D-C4D	2.76	117.86	112.09
24	C	514	BCR	C38-C26-C25	-2.76	121.43	124.53
22	c	503	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
26	a	410	PL9	C37-C38-C39	-2.75	121.04	127.66
30	c	517	DGD	O5E-C6E-C5E	-2.75	101.85	111.29
26	a	410	PL9	C27-C28-C29	-2.75	121.04	127.66
22	C	512	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
30	h	101	DGD	O6D-C1D-O3G	-2.75	103.47	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	518	LMG	O2-C2-C1	-2.74	103.38	110.05
28	E	101	LHG	O8-C23-C24	2.74	120.51	111.91
22	b	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
22	b	601	CLA	CMD-C2D-C3D	2.74	129.81	124.68
22	C	506	CLA	CMD-C2D-C3D	2.74	129.81	124.68
30	C	516	DGD	C6D-O5D-C1E	2.74	119.09	113.74
29	B	622	SQD	O5-C5-C4	2.74	114.67	109.69
22	B	602	CLA	CMC-C2C-C3C	2.73	130.09	124.94
22	c	501	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
22	B	616	CLA	CAA-CBA-CGA	-2.73	105.28	113.25
28	B	621	LHG	C11-C10-C9	-2.73	100.58	114.42
24	k	102	BCR	C38-C26-C25	-2.73	121.47	124.53
22	B	604	CLA	O2D-CGD-CBD	2.73	116.11	111.27
22	A	403	CLA	O2D-CGD-CBD	2.73	116.11	111.27
35	v	201	HEC	C1D-C2D-C3D	-2.73	105.10	107.00
22	b	608	CLA	CMC-C2C-C3C	2.72	130.08	124.94
22	b	611	CLA	CMB-C2B-C3B	2.72	129.77	124.68
27	d	409	LMG	C40-C39-C38	-2.72	100.61	114.42
29	A	412	SQD	O5-C1-C2	-2.72	104.59	110.35
22	b	613	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
22	B	616	CLA	CHB-C4A-NA	2.72	128.27	124.51
22	B	604	CLA	CHB-C4A-NA	2.71	128.27	124.51
22	b	601	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
26	d	405	PL9	C20-C19-C21	2.71	119.84	115.27
24	k	102	BCR	C27-C26-C25	2.71	126.67	122.73
22	B	602	CLA	C4A-NA-C1A	2.71	107.92	106.71
22	c	510	CLA	O1D-CGD-CBD	2.71	130.03	124.48
24	c	514	BCR	C38-C26-C25	-2.71	121.48	124.53
22	B	614	CLA	CMB-C2B-C3B	2.71	129.75	124.68
22	b	611	CLA	CMC-C2C-C3C	2.71	130.05	124.94
22	B	604	CLA	C1-O2A-CGA	-2.71	109.34	116.44
22	B	612	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
24	Z	101	BCR	C2-C1-C6	2.70	114.64	110.48
24	K	101	BCR	C15-C16-C17	-2.70	117.94	123.47
26	A	409	PL9	O1-C4-C3	-2.70	117.75	120.72
23	D	401	PHO	O2D-CGD-O1D	-2.70	118.56	123.84
22	c	503	CLA	CMB-C2B-C3B	2.70	129.73	124.68
30	c	516	DGD	O3D-C3D-C4D	-2.70	104.11	110.35
27	m	101	LMG	C9-C8-C7	-2.70	105.41	111.79
22	b	605	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	c	511	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
27	b	622	LMG	C3-C4-C5	-2.69	105.43	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	PHO	O1D-CGD-CBD	2.69	129.99	124.48
22	B	616	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
22	C	504	CLA	CED-O2D-CGD	2.69	122.02	115.94
22	b	601	CLA	CMB-C2B-C3B	2.69	129.71	124.68
23	d	401	PHO	C1B-NB-C4B	2.68	111.56	106.51
22	c	504	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	B	605	CLA	CMB-C2B-C3B	2.68	129.69	124.68
30	B	623	DGD	O3G-C3G-C2G	-2.67	104.70	111.78
22	d	403	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
22	C	508	CLA	CMC-C2C-C3C	2.66	129.96	124.94
22	B	608	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
22	B	615	CLA	C2A-C3A-C4A	2.66	106.16	101.87
22	b	610	CLA	CMB-C2B-C3B	2.66	129.65	124.68
27	M	101	LMG	C38-C37-C36	-2.66	100.94	114.42
30	c	516	DGD	C3E-C4E-C5E	-2.66	105.50	110.24
22	C	513	CLA	O2A-CGA-O1A	-2.66	116.89	123.59
22	B	604	CLA	C6-C5-C3	-2.65	106.50	113.45
22	b	603	CLA	OBD-CAD-C3D	2.65	132.38	127.98
24	D	406	BCR	C27-C26-C25	2.65	126.58	122.73
22	B	612	CLA	CMD-C2D-C3D	2.65	129.64	124.68
22	a	402	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
22	B	609	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
29	F	102	SQD	O48-C23-O10	-2.65	116.91	123.59
22	b	613	CLA	C4D-C3D-CAD	-2.65	106.99	108.47
24	b	618	BCR	C15-C16-C17	-2.64	118.06	123.47
29	B	622	SQD	O48-C23-O10	-2.64	116.92	123.59
27	c	518	LMG	O3-C3-C2	-2.64	104.25	110.35
22	B	614	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
22	B	606	CLA	C7-C6-C5	-2.63	106.22	113.36
26	a	410	PL9	C22-C23-C24	-2.63	121.33	127.66
22	D	403	CLA	CHB-C4A-NA	2.63	128.15	124.51
30	c	516	DGD	O6D-C1D-O3G	-2.63	103.75	109.97
22	B	602	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
22	c	503	CLA	C3B-C4B-NB	-2.63	105.81	109.21
24	B	619	BCR	C1-C6-C5	-2.63	118.91	122.61
24	k	101	BCR	C38-C26-C25	-2.63	121.58	124.53
22	c	503	CLA	C4-C3-C5	2.63	119.69	115.27
22	A	403	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
22	B	603	CLA	CMC-C2C-C3C	2.62	129.88	124.94
24	A	406	BCR	C37-C22-C21	-2.62	119.25	122.92
26	a	410	PL9	C21-C19-C18	-2.62	115.82	121.12
22	b	614	CLA	C1-C2-C3	-2.62	121.51	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	O1D-CGD-CBD	2.62	129.84	124.48
22	B	609	CLA	CMD-C2D-C3D	2.61	129.57	124.68
24	C	514	BCR	C27-C26-C25	2.61	126.52	122.73
22	b	610	CLA	CMC-C2C-C3C	2.61	129.86	124.94
22	b	602	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
24	b	619	BCR	C2-C1-C6	2.61	114.50	110.48
24	K	101	BCR	C38-C26-C25	-2.61	121.60	124.53
22	B	613	CLA	O2A-C1-C2	-2.60	101.79	108.64
22	b	614	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
22	b	612	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
22	b	607	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	a	404	PHO	O2D-CGD-O1D	-2.60	118.76	123.84
28	d	406	LHG	C5-O7-C7	-2.59	111.41	117.79
29	a	412	SQD	C1-O5-C5	-2.59	108.60	113.69
22	a	402	CLA	O1D-CGD-CBD	2.59	129.78	124.48
27	d	409	LMG	O1-C1-C2	-2.59	104.26	108.30
22	C	513	CLA	O1D-CGD-CBD	2.59	129.78	124.48
29	L	101	SQD	C45-O47-C7	2.59	124.16	117.79
27	D	408	LMG	O2-C2-C1	-2.59	103.76	110.05
22	B	608	CLA	C6-C7-C8	-2.59	107.56	115.92
22	c	504	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	602	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	k	103	BCR	C36-C18-C17	-2.57	119.32	122.92
27	m	101	LMG	O8-C28-O10	-2.57	117.10	123.59
22	A	403	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	h	101	DGD	C3D-C4D-C5D	-2.57	105.66	110.24
27	d	409	LMG	O6-C5-C4	2.57	114.36	109.69
26	D	407	PL9	C7-C8-C9	-2.57	122.52	126.79
30	C	515	DGD	C3G-C2G-C1G	-2.57	105.72	111.79
28	D	409	LHG	O8-C23-O10	-2.56	117.12	123.59
22	B	605	CLA	C4-C3-C2	-2.56	117.10	123.68
22	C	502	CLA	CMD-C2D-C3D	2.56	129.47	124.68
27	c	520	LMG	O2-C2-C1	-2.56	103.83	110.05
22	C	504	CLA	C4-C3-C5	2.56	119.58	115.27
22	b	604	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	C	513	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	d	403	CLA	CMC-C2C-C3C	2.55	129.76	124.94
24	x	101	BCR	C27-C26-C25	2.55	126.44	122.73
29	L	101	SQD	O47-C7-O49	-2.55	117.53	123.70
22	B	611	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	D	404	CLA	O2D-CGD-CBD	2.55	115.80	111.27
22	c	508	CLA	CHB-C4A-NA	2.55	128.04	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
29	B	622	SQD	C46-C45-C44	-2.55	105.76	111.79
23	d	401	PHO	CBA-CAA-C2A	-2.55	106.34	113.86
22	D	404	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
22	B	606	CLA	CHB-C4A-NA	2.54	128.03	124.51
30	c	515	DGD	C3E-C4E-C5E	-2.54	105.71	110.24
22	B	612	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
22	B	611	CLA	O2D-CGD-CBD	2.53	115.77	111.27
30	C	515	DGD	O6D-C1D-O3G	-2.53	103.97	109.97
27	c	520	LMG	C6-C5-C4	-2.53	107.07	113.00
28	b	623	LHG	O2-C2-C3	-2.53	100.67	109.56
22	B	611	CLA	C5-C3-C2	2.53	126.24	121.12
30	C	516	DGD	C4E-C3E-C2E	-2.52	106.42	110.82
26	D	407	PL9	C42-C43-C44	-2.52	121.58	127.66
22	B	603	CLA	OBD-CAD-C3D	2.52	132.17	127.98
22	B	611	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	a	405	CLA	O2D-CGD-CBD	2.52	115.74	111.27
22	C	507	CLA	CMB-C2B-C3B	2.52	129.39	124.68
24	K	102	BCR	C2-C1-C6	2.52	114.36	110.48
22	A	403	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
29	F	102	SQD	O2-C2-C3	2.51	116.16	110.35
22	b	614	CLA	CMB-C2B-C1B	-2.51	124.60	128.46
28	b	623	LHG	O8-C23-C24	2.51	119.79	111.91
30	c	517	DGD	CDB-CCB-CBB	-2.51	101.68	114.42
22	B	612	CLA	C1-C2-C3	-2.51	121.70	126.04
24	T	101	BCR	C3-C4-C5	-2.51	109.60	114.08
22	c	509	CLA	CMD-C2D-C3D	2.51	129.37	124.68
24	A	406	BCR	C16-C15-C14	-2.50	118.34	123.47
28	e	102	LHG	C11-C10-C9	-2.50	101.72	114.42
22	C	502	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
30	C	516	DGD	C3E-C4E-C5E	-2.50	105.78	110.24
22	C	513	CLA	O2D-CGD-CBD	2.50	115.71	111.27
24	b	617	BCR	C27-C26-C25	2.50	126.36	122.73
27	C	518	LMG	O1-C7-C8	-2.50	104.87	110.90
27	C	518	LMG	C38-C37-C36	-2.49	101.76	114.42
26	A	409	PL9	C35-C34-C36	2.49	119.46	115.27
22	b	605	CLA	O1D-CGD-CBD	2.49	129.58	124.48
22	a	411	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
27	c	518	LMG	O1-C7-C8	-2.49	104.89	110.90
28	D	409	LHG	C20-C19-C18	-2.49	101.79	114.42
30	C	516	DGD	O3E-C3E-C2E	-2.49	104.60	110.35
23	d	401	PHO	O2D-CGD-O1D	-2.49	118.98	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	404	CLA	CMC-C2C-C3C	2.48	129.63	124.94
22	b	609	CLA	CED-O2D-CGD	2.48	121.55	115.94
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	b	608	CLA	CMD-C2D-C3D	2.48	129.32	124.68
26	a	410	PL9	O2-C1-C2	-2.48	116.10	121.78
24	b	618	BCR	C30-C25-C26	-2.48	119.12	122.61
22	B	603	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	C	506	CLA	O1D-CGD-CBD	2.48	129.55	124.48
23	A	404	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
22	C	502	CLA	CMB-C2B-C3B	2.48	129.31	124.68
22	C	503	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
30	C	516	DGD	C5B-C4B-C3B	-2.47	101.88	114.42
27	D	408	LMG	C3-C4-C5	-2.47	105.83	110.24
30	c	517	DGD	O6E-C1E-O5D	-2.47	104.12	109.97
24	k	101	BCR	C15-C16-C17	-2.47	118.41	123.47
29	F	102	SQD	O7-S-C6	-2.47	104.00	106.94
24	b	618	BCR	C37-C22-C21	-2.47	119.46	122.92
22	a	405	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
22	B	603	CLA	C16-C15-C13	-2.47	107.95	115.92
24	B	617	BCR	C30-C25-C26	-2.46	119.15	122.61
22	c	511	CLA	CMC-C2C-C3C	2.46	129.58	124.94
22	C	506	CLA	OBD-CAD-CBD	-2.46	122.38	125.89
22	B	611	CLA	C1-C2-C3	-2.46	121.79	126.04
22	C	509	CLA	CMC-C2C-C3C	2.46	129.57	124.94
28	l	101	LHG	C27-C26-C25	-2.45	101.96	114.42
26	D	407	PL9	C36-C34-C33	-2.45	116.15	121.12
22	c	512	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
22	b	610	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
27	m	101	LMG	O1-C7-C8	-2.45	104.99	110.90
22	B	613	CLA	CMC-C2C-C3C	2.45	129.56	124.94
22	A	405	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
22	D	405	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
22	C	510	CLA	OBD-CAD-CBD	-2.44	122.40	125.89
22	c	504	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
30	c	516	DGD	CDB-CCB-CBB	-2.44	102.03	114.42
29	a	412	SQD	O9-S-C6	2.44	109.84	106.94
22	C	503	CLA	CMB-C2B-C3B	2.44	129.25	124.68
22	C	508	CLA	OBD-CAD-CBD	-2.44	122.41	125.89
26	A	409	PL9	C36-C37-C38	-2.44	103.86	111.88
24	K	101	BCR	C27-C26-C25	2.44	126.27	122.73
22	B	610	CLA	C1-C2-C3	-2.43	121.84	126.04
22	B	614	CLA	O2D-CGD-CBD	2.43	115.59	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C15-C16-C17	-2.43	118.50	123.47
22	b	602	CLA	O1D-CGD-CBD	2.43	129.46	124.48
22	B	603	CLA	O1D-CGD-CBD	2.43	129.45	124.48
24	b	617	BCR	C36-C18-C17	-2.42	119.53	122.92
22	C	503	CLA	O1D-CGD-CBD	2.42	129.44	124.48
22	c	507	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
27	M	101	LMG	O7-C10-O9	-2.42	117.85	123.70
22	A	405	CLA	C4-C3-C5	2.42	119.35	115.27
27	m	101	LMG	C38-C37-C36	-2.42	102.14	114.42
22	c	512	CLA	CMC-C2C-C3C	2.42	129.50	124.94
29	A	412	SQD	O47-C7-O49	-2.42	117.86	123.70
22	C	510	CLA	CMD-C2D-C3D	2.42	129.20	124.68
24	k	103	BCR	C29-C30-C25	2.41	114.20	110.48
28	b	623	LHG	C11-C10-C9	-2.41	102.18	114.42
26	d	405	PL9	C7-C8-C9	-2.41	122.78	126.79
22	c	508	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
28	l	101	LHG	O8-C23-C24	2.41	119.46	111.91
22	c	507	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
30	B	623	DGD	CFB-CEB-CDB	-2.41	102.21	114.42
22	C	507	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
29	L	101	SQD	O5-C1-C2	-2.40	105.26	110.35
26	A	409	PL9	O2-C1-C6	2.40	124.75	120.59
22	B	603	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	C	511	CLA	O2D-CGD-CBD	2.40	115.53	111.27
24	K	102	BCR	C40-C30-C25	2.40	114.19	110.30
27	C	518	LMG	O7-C10-O9	-2.40	117.91	123.70
22	B	609	CLA	CHA-C1A-NA	-2.40	120.91	126.40
26	D	407	PL9	C11-C12-C13	-2.40	104.00	111.88
26	A	409	PL9	O2-C1-C2	-2.40	116.29	121.78
23	D	401	PHO	CMB-C2B-C1B	-2.40	121.37	125.06
24	x	101	BCR	C11-C10-C9	-2.39	123.89	127.31
30	C	516	DGD	CDB-CCB-CBB	-2.39	102.27	114.42
24	x	101	BCR	C2-C1-C6	2.39	114.16	110.48
22	C	509	CLA	C16-C15-C13	-2.39	108.19	115.92
22	c	508	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
30	h	101	DGD	C3G-C2G-C1G	-2.39	106.14	111.79
22	c	508	CLA	CGD-CBD-CAD	-2.39	103.00	110.73
22	B	607	CLA	C2A-C1A-CHA	2.39	128.03	123.86
27	a	414	LMG	O5-C6-C5	-2.39	103.10	111.29
24	d	404	BCR	C30-C25-C26	-2.39	119.25	122.61
22	b	613	CLA	C7-C6-C5	-2.38	106.88	113.36
22	C	501	CLA	C1B-CHB-C4A	-2.38	125.39	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	BCR	C3-C4-C5	-2.38	109.82	114.08
22	b	615	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	c	507	CLA	OBD-CAD-C3D	2.38	131.94	127.98
26	D	407	PL9	C50-C49-C48	-2.38	115.76	122.65
22	b	607	CLA	CMB-C2B-C3B	2.38	129.13	124.68
23	D	401	PHO	CBD-CHA-C1A	2.38	131.92	126.40
27	c	520	LMG	O1-C1-C2	-2.38	104.59	108.30
26	a	410	PL9	O2-C1-C6	2.37	124.70	120.59
34	F	101	HEM	CMA-C3A-C4A	-2.37	124.81	128.46
28	B	621	LHG	O8-C23-O10	-2.37	117.60	123.59
24	a	406	BCR	C33-C5-C6	-2.37	121.86	124.53
22	A	403	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
30	C	517	DGD	C8B-C7B-C6B	-2.37	102.38	114.42
23	a	404	PHO	CHB-C1B-NB	2.37	129.51	124.58
29	F	102	SQD	O5-C5-C4	2.37	113.99	109.69
22	A	405	CLA	CMD-C2D-C3D	2.37	129.11	124.68
30	C	516	DGD	O6D-C1D-O3G	-2.37	104.37	109.97
30	H	102	DGD	C1D-C2D-C3D	-2.37	105.07	110.00
22	c	501	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	a	411	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
23	A	404	PHO	C2B-C1B-NB	-2.37	106.22	109.79
22	c	510	CLA	O2A-C1-C2	-2.37	102.42	108.64
30	A	414	DGD	CBB-CAB-C9B	-2.36	102.42	114.42
22	c	504	CLA	O2D-CGD-CBD	2.36	115.47	111.27
28	B	621	LHG	O8-C23-C24	2.36	119.32	111.91
26	D	407	PL9	O2-C1-C2	-2.36	116.37	121.78
22	B	602	CLA	C11-C12-C13	-2.36	108.29	115.92
30	H	102	DGD	C8B-C7B-C6B	-2.36	102.45	114.42
24	k	103	BCR	C27-C26-C25	2.36	126.16	122.73
24	b	618	BCR	C39-C30-C25	-2.36	106.47	110.30
22	B	604	CLA	C16-C15-C13	-2.36	108.30	115.92
22	b	609	CLA	C5-C3-C2	2.36	125.89	121.12
24	B	617	BCR	C38-C26-C25	-2.36	121.88	124.53
24	B	617	BCR	C23-C22-C21	-2.35	115.33	118.94
26	A	409	PL9	C7-C3-C2	-2.35	120.21	123.30
22	C	507	CLA	CMD-C2D-C3D	2.35	129.08	124.68
22	c	506	CLA	OBD-CAD-C3D	2.35	131.88	127.98
27	b	622	LMG	O7-C10-O9	-2.35	118.02	123.70
29	L	101	SQD	O10-C23-C24	-2.35	114.57	123.73
30	c	516	DGD	O2D-C2D-C1D	-2.35	104.34	110.05
22	b	613	CLA	CED-O2D-CGD	2.35	121.25	115.94
22	B	615	CLA	CMD-C2D-C3D	2.35	129.07	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	414	DGD	C1D-C2D-C3D	-2.34	105.11	110.00
22	c	502	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	613	CLA	CHA-C1A-NA	-2.34	121.03	126.40
22	c	505	CLA	O2D-CGD-CBD	2.34	115.43	111.27
30	c	515	DGD	C4A-C3A-C2A	-2.34	104.77	113.19
24	Z	101	BCR	C38-C26-C25	-2.34	121.90	124.53
22	a	405	CLA	OBD-CAD-C3D	2.34	131.87	127.98
26	d	405	PL9	C50-C49-C48	-2.34	115.89	122.65
22	c	506	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
22	b	604	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
26	a	410	PL9	C30-C29-C31	2.33	119.19	115.27
22	B	602	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
29	L	101	SQD	O47-C45-C46	2.33	116.84	108.40
29	F	102	SQD	C46-C45-C44	-2.33	105.94	113.70
22	B	616	CLA	CMC-C2C-C3C	2.33	129.34	124.94
30	h	101	DGD	C1D-C2D-C3D	-2.33	105.14	110.00
30	C	517	DGD	O3D-C3D-C4D	-2.33	104.96	110.35
24	k	101	BCR	C27-C26-C25	2.33	126.11	122.73
30	h	101	DGD	C7B-C6B-C5B	-2.32	102.64	114.42
23	A	404	PHO	CBD-CHA-C4D	-2.32	105.92	108.54
22	B	614	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	d	405	PL9	C26-C27-C28	-2.32	104.26	111.88
22	D	404	CLA	C7-C6-C5	-2.32	107.06	113.36
22	b	607	CLA	O2A-C1-C2	-2.32	102.55	108.64
24	Z	101	BCR	C36-C18-C19	2.32	121.73	118.08
22	B	608	CLA	CHA-C1A-NA	-2.32	121.10	126.40
28	d	406	LHG	C20-C19-C18	-2.32	102.67	114.42
22	b	605	CLA	CMD-C2D-C3D	2.31	129.01	124.68
22	C	508	CLA	CHB-C4A-NA	2.31	127.71	124.51
30	c	515	DGD	O3G-C1D-C2D	-2.31	104.69	108.30
22	a	402	CLA	CHB-C4A-NA	2.31	127.71	124.51
24	B	619	BCR	C36-C18-C17	-2.31	119.68	122.92
24	d	404	BCR	C24-C23-C22	-2.31	122.74	126.23
24	b	617	BCR	C15-C16-C17	-2.31	118.75	123.47
30	A	414	DGD	O2D-C2D-C1D	-2.30	104.45	110.05
22	C	501	CLA	OBD-CAD-CBD	-2.30	122.61	125.89
22	C	503	CLA	C3A-C2A-C1A	2.30	104.79	101.34
22	C	506	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
29	a	412	SQD	O5-C1-C2	-2.30	105.48	110.35
22	C	512	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	c	511	CLA	CMB-C2B-C3B	2.30	128.98	124.68
24	x	101	BCR	C24-C23-C22	-2.30	122.76	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	SQD	O49-C7-C8	-2.30	114.76	123.73
22	D	403	CLA	CED-O2D-CGD	2.30	121.13	115.94
30	c	515	DGD	O1G-C1A-C2A	-2.30	104.70	111.91
28	L	102	LHG	C18-C17-C16	-2.30	102.76	114.42
22	c	509	CLA	CHB-C4A-NA	2.30	127.69	124.51
22	B	603	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
22	B	604	CLA	C11-C10-C8	-2.29	108.50	115.92
22	b	613	CLA	CAA-CBA-CGA	2.29	119.95	113.25
22	B	613	CLA	O1D-CGD-CBD	2.29	129.17	124.48
28	d	406	LHG	O8-C23-C24	2.29	119.09	111.91
27	D	408	LMG	O4-C4-C5	2.29	114.98	109.30
22	c	502	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
27	c	520	LMG	C9-C8-C7	-2.29	106.37	111.79
29	a	412	SQD	C3-C4-C5	2.29	114.32	110.24
22	B	609	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
24	x	101	BCR	C16-C15-C14	-2.29	118.79	123.47
22	b	616	CLA	OBD-CAD-CBD	-2.29	122.63	125.89
28	E	101	LHG	C11-C10-C9	-2.28	102.84	114.42
22	c	503	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	C	501	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
28	b	623	LHG	O8-C23-O10	-2.28	117.84	123.59
29	f	101	SQD	C3-C4-C5	2.28	114.31	110.24
24	d	404	BCR	C2-C1-C6	2.28	113.99	110.48
22	c	506	CLA	CHB-C4A-NA	2.28	127.66	124.51
29	A	413	SQD	O48-C23-O10	-2.28	117.84	123.59
22	c	507	CLA	CMC-C2C-C3C	2.28	129.23	124.94
26	d	405	PL9	C40-C39-C38	-2.27	117.84	123.68
22	a	405	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
28	E	101	LHG	O8-C23-O10	-2.27	117.85	123.59
30	C	517	DGD	CDB-CCB-CBB	-2.27	102.88	114.42
30	h	101	DGD	O6E-C1E-O5D	-2.27	104.59	109.97
22	C	501	CLA	C3D-CAD-CBD	-2.27	104.62	107.61
22	B	614	CLA	C6-C5-C3	2.27	119.41	113.45
22	d	402	CLA	CMC-C2C-C3C	2.27	129.22	124.94
22	B	609	CLA	C7-C6-C5	-2.27	107.20	113.36
26	a	410	PL9	C12-C13-C14	-2.27	122.20	127.66
22	A	403	CLA	CMD-C2D-C3D	2.27	128.92	124.68
24	d	404	BCR	C38-C26-C25	-2.26	121.98	124.53
22	B	605	CLA	OBD-CAD-CBD	-2.26	122.66	125.89
22	B	601	CLA	CMD-C2D-C3D	2.26	128.91	124.68
27	A	410	LMG	C9-C8-C7	-2.26	106.44	111.79
22	B	606	CLA	O2A-CGA-O1A	-2.26	117.89	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	403	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
28	d	406	LHG	C18-C17-C16	-2.25	102.98	114.42
22	c	508	CLA	C4D-C3D-CAD	-2.25	107.21	108.47
24	A	406	BCR	C38-C26-C27	-2.25	109.29	113.62
22	B	604	CLA	OBD-CAD-C3D	2.25	131.72	127.98
30	c	517	DGD	CAB-C9B-C8B	-2.25	103.00	114.42
22	B	610	CLA	OBD-CAD-CBD	-2.25	122.68	125.89
22	a	403	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
26	D	407	PL9	C30-C29-C31	-2.25	111.49	115.27
30	c	515	DGD	CDB-CCB-CBB	-2.25	103.00	114.42
22	b	614	CLA	CMB-C2B-C3B	2.25	128.88	124.68
24	t	101	BCR	C23-C22-C21	-2.25	115.49	118.94
24	b	618	BCR	C36-C18-C19	2.25	121.62	118.08
22	C	510	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
22	B	612	CLA	CMC-C2C-C3C	2.25	129.18	124.94
22	B	610	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
22	A	402	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
22	b	605	CLA	O1A-CGA-CBA	2.24	132.48	123.73
24	b	619	BCR	C23-C22-C21	2.24	122.38	118.94
29	f	101	SQD	O5-C5-C4	2.24	113.76	109.69
24	A	406	BCR	C2-C1-C6	2.24	113.93	110.48
24	b	619	BCR	C27-C26-C25	2.24	125.98	122.73
22	a	402	CLA	CMD-C2D-C3D	2.24	128.87	124.68
24	B	619	BCR	C34-C9-C10	-2.24	119.79	122.92
27	A	410	LMG	C38-C37-C36	-2.24	103.07	114.42
24	A	406	BCR	C8-C7-C6	-2.24	120.92	127.20
22	b	602	CLA	C4-C3-C5	2.24	119.03	115.27
24	A	406	BCR	C40-C30-C25	2.23	113.92	110.30
27	c	520	LMG	O8-C28-O10	-2.23	117.96	123.59
22	b	609	CLA	OBD-CAD-C3D	2.23	131.68	127.98
22	b	612	CLA	C12-C11-C10	2.23	123.48	113.24
30	B	623	DGD	C7B-C6B-C5B	-2.23	103.12	114.42
22	C	509	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
29	B	622	SQD	O48-C23-C24	2.23	118.89	111.91
22	b	610	CLA	CHA-C1A-NA	-2.23	121.30	126.40
24	B	617	BCR	C15-C16-C17	-2.22	118.92	123.47
30	C	515	DGD	C6D-O5D-C1E	2.22	118.08	113.74
22	c	510	CLA	C16-C15-C13	-2.22	108.74	115.92
22	C	504	CLA	CHA-C1A-NA	-2.22	121.31	126.40
22	c	508	CLA	O2D-CGD-CBD	2.22	115.22	111.27
28	B	621	LHG	C20-C19-C18	-2.22	103.16	114.42
22	b	604	CLA	CAA-CBA-CGA	-2.22	106.77	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	623	DGD	CBB-CAB-C9B	-2.22	103.16	114.42
22	b	601	CLA	CMC-C2C-C3C	2.22	129.12	124.94
22	b	616	CLA	CMC-C2C-C3C	2.22	129.12	124.94
24	b	617	BCR	C11-C10-C9	-2.22	124.15	127.31
24	D	406	BCR	C7-C8-C9	-2.22	122.89	126.23
27	A	410	LMG	O5-C6-C5	-2.21	103.69	111.29
27	A	410	LMG	O6-C1-O1	-2.21	104.73	109.97
24	b	618	BCR	C16-C15-C14	-2.21	118.94	123.47
28	L	102	LHG	C20-C19-C18	-2.21	103.19	114.42
24	B	619	BCR	C15-C16-C17	-2.21	118.94	123.47
30	C	517	DGD	O5E-C6E-C5E	-2.21	103.71	111.29
22	c	506	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
22	B	608	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	a	406	BCR	C27-C26-C25	2.21	125.94	122.73
26	D	407	PL9	C22-C23-C24	-2.21	122.34	127.66
22	C	505	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	H	101	BCR	C29-C30-C25	2.21	113.88	110.48
29	B	622	SQD	C45-O47-C7	2.21	123.22	117.79
30	C	517	DGD	C4D-C3D-C2D	-2.20	106.97	110.82
30	h	101	DGD	C4D-C3D-C2D	-2.20	106.97	110.82
22	C	508	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
22	c	512	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
22	b	606	CLA	O1D-CGD-CBD	2.20	128.99	124.48
24	b	618	BCR	C27-C26-C25	2.20	125.93	122.73
24	t	101	BCR	C24-C23-C22	-2.20	122.91	126.23
22	C	508	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
22	B	604	CLA	CMC-C2C-C3C	2.20	129.09	124.94
22	A	405	CLA	CMC-C2C-C3C	2.20	129.09	124.94
22	C	512	CLA	C2A-C3A-C4A	2.20	105.42	101.87
22	B	604	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	B	605	CLA	CAA-CBA-CGA	-2.20	106.84	113.25
22	D	403	CLA	O2D-CGD-O1D	-2.20	119.55	123.84
22	c	510	CLA	CMA-C3A-C2A	-2.19	104.97	113.83
26	D	407	PL9	C31-C32-C33	-2.19	104.67	111.88
24	t	101	BCR	C40-C30-C25	2.19	113.85	110.30
22	c	512	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
23	a	404	PHO	C2B-C1B-NB	-2.19	106.49	109.79
24	H	101	BCR	C16-C15-C14	-2.19	119.00	123.47
27	a	414	LMG	O6-C1-C2	-2.19	105.72	110.35
28	B	621	LHG	C18-C17-C16	-2.19	103.33	114.42
30	A	414	DGD	O6D-C1D-O3G	-2.18	104.80	109.97
22	B	601	CLA	CMC-C2C-C3C	2.18	129.06	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	103	BCR	C8-C7-C6	-2.18	121.07	127.20
22	C	507	CLA	CAA-CBA-CGA	-2.18	106.88	113.25
22	C	510	CLA	CHA-C1A-NA	-2.18	121.40	126.40
22	b	615	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
27	D	408	LMG	C1-C2-C3	-2.18	105.46	110.00
22	a	403	CLA	C2A-C1A-CHA	2.18	127.67	123.86
22	B	616	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
22	c	513	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
27	M	101	LMG	O1-C7-C8	-2.17	105.66	110.90
22	C	502	CLA	OBD-CAD-CBD	-2.17	122.79	125.89
30	c	517	DGD	C3G-C2G-C1G	-2.17	106.65	111.79
22	D	403	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	a	404	PHO	CBD-CHA-C4D	-2.17	106.09	108.54
24	Z	101	BCR	C35-C13-C14	-2.17	119.88	122.92
22	B	601	CLA	O2D-CGD-CBD	2.17	115.12	111.27
22	C	510	CLA	O2D-CGD-CBD	2.17	115.12	111.27
22	c	510	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
30	B	623	DGD	CAB-C9B-C8B	-2.17	103.42	114.42
24	t	101	BCR	C11-C10-C9	-2.17	124.22	127.31
34	e	101	HEM	C4C-C3C-C2C	2.17	108.41	106.90
22	c	506	CLA	O1D-CGD-CBD	2.16	128.91	124.48
28	E	101	LHG	C18-C17-C16	-2.16	103.44	114.42
22	C	508	CLA	C7-C6-C5	-2.16	107.49	113.36
22	b	605	CLA	CHB-C4A-NA	2.16	127.50	124.51
24	D	406	BCR	C2-C1-C6	2.16	113.81	110.48
24	c	514	BCR	C36-C18-C19	2.16	121.48	118.08
22	D	405	CLA	CMD-C2D-C3D	2.16	128.72	124.68
30	h	101	DGD	C6D-C5D-C4D	2.16	116.60	112.09
24	b	619	BCR	C36-C18-C19	2.16	121.48	118.08
24	B	619	BCR	C36-C18-C19	2.16	121.47	118.08
29	B	622	SQD	C3-C4-C5	2.16	114.08	110.24
28	A	411	LHG	O3-P-O5	-2.16	100.64	109.07
22	b	604	CLA	C4-C3-C5	2.15	118.90	115.27
22	a	411	CLA	C1-C2-C3	-2.15	122.32	126.04
22	c	510	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
29	F	102	SQD	O9-S-O7	-2.15	106.50	113.95
22	B	609	CLA	CMC-C2C-C3C	2.15	129.00	124.94
23	A	404	PHO	OBD-CAD-C3D	2.15	133.70	128.52
22	C	502	CLA	O1D-CGD-CBD	2.15	128.89	124.48
28	B	621	LHG	C27-C26-C25	-2.15	103.50	114.42
22	d	403	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
27	b	622	LMG	C40-C39-C38	-2.15	103.51	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	102	DGD	O3E-C3E-C2E	-2.15	105.38	110.35
22	B	608	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	c	513	CLA	C11-C12-C13	-2.14	108.99	115.92
22	b	609	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	H	102	DGD	O2D-C2D-C1D	-2.14	104.84	110.05
22	B	602	CLA	C3D-CAD-CBD	-2.14	104.78	107.61
29	a	412	SQD	O5-C5-C4	2.14	113.58	109.69
24	B	619	BCR	C32-C1-C6	-2.14	106.83	110.30
27	d	409	LMG	O7-C10-O9	-2.14	118.53	123.70
30	c	516	DGD	C8B-C7B-C6B	-2.14	103.57	114.42
24	k	103	BCR	C2-C1-C6	2.14	113.77	110.48
28	l	101	LHG	C20-C19-C18	-2.14	103.57	114.42
30	c	517	DGD	C3D-C4D-C5D	-2.14	106.43	110.24
35	v	201	HEC	CMB-C2B-C1B	-2.14	125.18	128.46
32	C	521	STE	C4-C3-C2	-2.14	105.46	113.76
22	C	505	CLA	C11-C10-C8	-2.13	109.02	115.92
22	C	504	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
22	c	506	CLA	CMC-C2C-C3C	2.13	128.96	124.94
22	C	508	CLA	CMD-C2D-C3D	2.13	128.66	124.68
22	C	509	CLA	C2A-C3A-C4A	2.13	105.31	101.87
22	C	507	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
22	b	616	CLA	CMD-C2D-C3D	2.12	128.65	124.68
22	b	606	CLA	CMD-C2D-C3D	2.12	128.65	124.68
24	K	101	BCR	C36-C18-C19	2.12	121.42	118.08
22	C	507	CLA	C1-C2-C3	-2.12	122.38	126.04
22	C	508	CLA	CHA-C1A-NA	-2.12	121.54	126.40
27	c	518	LMG	C40-C39-C38	-2.12	103.67	114.42
23	D	401	PHO	C3C-C4C-NC	-2.12	106.99	110.28
22	b	611	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
28	e	102	LHG	C20-C19-C18	-2.12	103.67	114.42
27	c	520	LMG	C3-C4-C5	-2.12	106.46	110.24
22	C	502	CLA	CMA-C3A-C4A	2.12	117.46	111.77
30	H	102	DGD	CEB-CDB-CCB	-2.12	103.69	114.42
28	b	623	LHG	C20-C19-C18	-2.11	103.69	114.42
22	b	606	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
23	a	404	PHO	C1B-NB-C4B	2.11	110.49	106.51
30	c	517	DGD	C1D-C2D-C3D	-2.11	105.59	110.00
22	D	405	CLA	C7-C6-C5	-2.11	107.62	113.36
22	B	612	CLA	CHB-C4A-NA	2.11	127.43	124.51
22	b	611	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	b	608	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
22	c	512	CLA	C4-C3-C5	2.11	118.82	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	CMD-C2D-C3D	2.11	128.63	124.68
26	D	407	PL9	O2-C1-C6	2.11	124.25	120.59
22	c	509	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
22	c	502	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	Z	101	BCR	C29-C30-C25	2.11	113.73	110.48
24	H	101	BCR	C37-C22-C23	2.11	121.40	118.08
22	B	613	CLA	OBD-CAD-C3D	2.11	131.48	127.98
22	B	605	CLA	CMC-C2C-C3C	2.11	128.91	124.94
22	A	403	CLA	C1-C2-C3	-2.11	122.40	126.04
24	K	101	BCR	C12-C13-C14	-2.10	115.71	118.94
22	C	511	CLA	OBD-CAD-CBD	-2.10	122.89	125.89
24	B	617	BCR	C37-C22-C21	-2.10	119.98	122.92
24	K	102	BCR	C38-C26-C27	-2.10	109.58	113.62
24	b	617	BCR	C8-C7-C6	-2.10	121.30	127.20
22	C	509	CLA	C6-C7-C8	-2.10	109.13	115.92
26	A	409	PL9	C12-C13-C14	-2.10	122.60	127.66
30	C	515	DGD	C6B-C5B-C4B	-2.10	103.77	114.42
22	B	604	CLA	C11-C12-C13	-2.10	109.14	115.92
23	A	404	PHO	CMA-C3A-C2A	-2.10	105.37	113.83
27	c	518	LMG	C38-C37-C36	-2.09	103.79	114.42
30	c	517	DGD	C3E-C4E-C5E	-2.09	106.50	110.24
22	c	503	CLA	CHB-C4A-NA	2.09	127.41	124.51
22	c	503	CLA	OBD-CAD-CBD	-2.09	122.91	125.89
30	c	517	DGD	O3E-C3E-C4E	-2.09	105.51	110.35
22	c	507	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
27	c	518	LMG	O6-C1-O1	-2.09	105.02	109.97
22	c	501	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	a	403	CLA	OBD-CAD-CBD	-2.09	122.91	125.89
22	b	603	CLA	O2A-C1-C2	-2.09	103.14	108.64
30	h	101	DGD	CDB-CCB-CBB	-2.09	103.83	114.42
22	c	502	CLA	O1D-CGD-CBD	2.09	128.75	124.48
22	B	602	CLA	C4-C3-C5	2.09	118.78	115.27
22	D	404	CLA	C3D-CAD-CBD	-2.08	104.86	107.61
30	C	517	DGD	CAB-C9B-C8B	-2.08	103.85	114.42
22	b	604	CLA	CMA-C3A-C4A	2.08	117.37	111.77
24	K	102	BCR	C15-C16-C17	-2.08	119.21	123.47
22	b	615	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
30	h	101	DGD	C1E-O6E-C5E	2.08	117.78	113.69
26	A	409	PL9	C31-C29-C28	2.08	125.33	121.12
27	b	622	LMG	O5-C6-C5	-2.08	104.15	111.29
22	c	501	CLA	CMB-C2B-C3B	2.08	128.57	124.68
22	d	402	CLA	O2A-CGA-O1A	-2.08	118.35	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	C4-C3-C5	2.08	118.76	115.27
22	b	607	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	c	503	CLA	CMC-C2C-C3C	2.07	128.85	124.94
22	c	513	CLA	C4D-C3D-CAD	-2.07	107.31	108.47
26	d	405	PL9	C8-C7-C3	2.07	117.84	111.98
22	c	502	CLA	CMC-C2C-C3C	2.07	128.85	124.94
22	B	614	CLA	CMC-C2C-C3C	2.07	128.84	124.94
27	D	408	LMG	C14-C13-C12	-2.07	103.93	114.42
28	E	101	LHG	C5-O7-C7	-2.07	112.70	117.79
22	C	506	CLA	C1-C2-C3	-2.07	122.47	126.04
22	D	404	CLA	CMD-C2D-C3D	2.07	128.54	124.68
27	M	101	LMG	C1-O6-C5	-2.06	109.64	113.69
28	E	101	LHG	C27-C26-C25	-2.06	103.95	114.42
22	C	512	CLA	CMD-C2D-C3D	2.06	128.54	124.68
24	K	101	BCR	C36-C18-C17	-2.06	120.03	122.92
27	D	408	LMG	C38-C37-C36	-2.06	103.95	114.42
22	D	405	CLA	C6-C7-C8	-2.06	109.26	115.92
24	a	406	BCR	C37-C22-C21	-2.06	120.04	122.92
22	B	616	CLA	O1D-CGD-CBD	2.06	128.69	124.48
22	b	609	CLA	CHA-C1A-NA	-2.06	121.69	126.40
27	A	410	LMG	C1-O6-C5	-2.05	109.66	113.69
22	c	507	CLA	CMB-C2B-C3B	2.05	128.52	124.68
22	b	601	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
28	E	101	LHG	C20-C19-C18	-2.05	104.00	114.42
27	M	101	LMG	C1-C2-C3	-2.05	105.72	110.00
22	b	610	CLA	O2D-CGD-CBD	2.05	114.92	111.27
22	d	403	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	F	102	SQD	O8-S-O9	-2.05	106.26	111.27
22	C	511	CLA	CHB-C4A-NA	2.05	127.35	124.51
22	C	504	CLA	CMC-C2C-C3C	2.05	128.81	124.94
24	A	406	BCR	C36-C18-C19	2.05	121.31	118.08
30	c	516	DGD	CBB-CAB-C9B	-2.05	104.02	114.42
22	b	608	CLA	CHA-C1A-NA	-2.05	121.71	126.40
30	h	101	DGD	CBB-CAB-C9B	-2.05	104.03	114.42
30	H	102	DGD	C4D-C3D-C2D	-2.05	107.25	110.82
27	D	410	LMG	C35-C34-C33	-2.05	104.04	114.42
24	B	617	BCR	C33-C5-C6	-2.04	122.23	124.53
35	v	201	HEC	CAD-CBD-CGD	-2.04	109.24	112.67
22	C	511	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	a	411	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
22	B	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	A	412	SQD	O48-C23-O10	-2.04	118.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
22	B	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
28	L	102	LHG	C27-C26-C25	-2.04	104.08	114.42
24	Z	101	BCR	C3-C4-C5	-2.04	110.44	114.08
34	F	101	HEM	CMB-C2B-C3B	2.03	128.48	124.68
30	C	517	DGD	O2E-C2E-C3E	-2.03	105.65	110.35
22	B	613	CLA	CMD-C2D-C3D	2.03	128.48	124.68
30	c	517	DGD	C6B-C5B-C4B	-2.03	104.11	114.42
24	t	101	BCR	C27-C26-C25	2.03	125.68	122.73
22	b	605	CLA	OBD-CAD-CBD	-2.03	123.00	125.89
22	B	603	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	B	615	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
26	d	405	PL9	C41-C39-C38	-2.03	117.01	121.12
28	l	101	LHG	O8-C23-O10	-2.03	118.47	123.59
30	A	414	DGD	O2E-C2E-C1E	-2.03	105.12	110.05
22	a	405	CLA	C16-C15-C13	-2.03	109.37	115.92
22	d	403	CLA	CHB-C4A-NA	2.03	127.31	124.51
22	d	402	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
30	H	102	DGD	C3E-C4E-C5E	-2.02	106.63	110.24
22	c	504	CLA	OBD-CAD-CBD	-2.02	123.00	125.89
22	B	604	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
24	A	406	BCR	C11-C10-C9	-2.02	124.42	127.31
29	F	102	SQD	C3-C4-C5	2.02	113.85	110.24
22	D	405	CLA	CGD-CBD-CAD	-2.02	104.18	110.73
30	c	515	DGD	C8B-C7B-C6B	-2.02	104.16	114.42
22	c	504	CLA	CMC-C2C-C3C	2.02	128.75	124.94
29	L	101	SQD	C1-O5-C5	2.02	117.65	113.69
22	b	605	CLA	C4-C3-C2	-2.02	118.50	123.68
34	e	101	HEM	CMC-C2C-C3C	2.02	128.46	124.68
22	C	510	CLA	C11-C10-C8	-2.02	109.39	115.92
22	d	403	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
28	D	409	LHG	C18-C17-C16	-2.02	104.18	114.42
22	b	604	CLA	C11-C12-C13	-2.01	109.41	115.92
22	C	501	CLA	CMB-C2B-C3B	2.01	128.44	124.68
22	B	604	CLA	CGD-CBD-CAD	-2.01	104.22	110.73
30	H	102	DGD	CAB-C9B-C8B	-2.01	104.22	114.42
24	T	101	BCR	C37-C22-C21	-2.01	120.11	122.92
30	h	101	DGD	O3E-C3E-C2E	-2.01	105.70	110.35
22	b	609	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
24	k	101	BCR	C37-C22-C21	-2.01	120.11	122.92
27	A	410	LMG	O3-C3-C2	-2.01	105.70	110.35
24	k	102	BCR	C8-C7-C6	-2.01	121.56	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	C	502	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
22	C	506	CLA	CHB-C4A-NA	2.01	127.29	124.51
28	b	623	LHG	C27-C26-C25	-2.01	104.24	114.42
22	B	604	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
30	C	517	DGD	C5B-C4B-C3B	-2.00	104.25	114.42
28	D	409	LHG	C27-C26-C25	-2.00	104.25	114.42
22	c	508	CLA	CMD-C2D-C3D	2.00	128.43	124.68
24	b	619	BCR	C15-C16-C17	-2.00	119.37	123.47
22	b	601	CLA	O2A-C1-C2	2.00	113.90	108.64
22	C	502	CLA	C2A-C1A-CHA	2.00	127.36	123.86
22	c	512	CLA	CMB-C2B-C3B	2.00	128.42	124.68
28	l	101	LHG	C11-C10-C9	-2.00	104.26	114.42
24	b	619	BCR	C3-C4-C5	-2.00	110.50	114.08
24	k	103	BCR	C15-C16-C17	-2.00	119.38	123.47
27	A	410	LMG	C40-C39-C38	-2.00	104.27	114.42
22	B	607	CLA	O1A-CGA-CBA	2.00	131.54	123.73

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	402	CLA	ND
22	A	403	CLA	ND
22	A	405	CLA	ND
22	B	601	CLA	ND
22	B	602	CLA	ND
22	B	603	CLA	ND
22	B	604	CLA	ND
22	B	605	CLA	ND
22	B	606	CLA	ND
22	B	607	CLA	ND
22	B	610	CLA	ND
22	B	611	CLA	ND
22	B	612	CLA	ND
22	B	613	CLA	ND
22	B	614	CLA	ND
22	B	615	CLA	ND
22	B	616	CLA	ND
22	C	501	CLA	ND
22	C	502	CLA	ND
22	C	503	CLA	ND
22	C	504	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	505	CLA	ND
22	C	506	CLA	ND
22	C	507	CLA	ND
22	C	509	CLA	ND
22	C	510	CLA	ND
22	C	511	CLA	ND
22	C	512	CLA	ND
22	D	403	CLA	ND
22	D	404	CLA	ND
22	a	402	CLA	ND
22	a	403	CLA	ND
22	a	405	CLA	ND
22	a	411	CLA	ND
22	b	601	CLA	ND
22	b	602	CLA	ND
22	b	603	CLA	ND
22	b	604	CLA	ND
22	b	605	CLA	ND
22	b	606	CLA	ND
22	b	607	CLA	ND
22	b	609	CLA	ND
22	b	610	CLA	ND
22	b	611	CLA	ND
22	b	612	CLA	ND
22	b	613	CLA	ND
22	b	614	CLA	ND
22	b	615	CLA	ND
22	b	616	CLA	ND
22	c	501	CLA	ND
22	c	502	CLA	ND
22	c	503	CLA	ND
22	c	504	CLA	ND
22	c	505	CLA	ND
22	c	506	CLA	ND
22	c	507	CLA	ND
22	c	508	CLA	ND
22	c	509	CLA	ND
22	c	510	CLA	ND
22	c	511	CLA	ND
22	c	512	CLA	ND
22	c	513	CLA	ND
22	d	402	CLA	ND

All (1943) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C4-C3-C5-C6
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	C4-C3-C5-C6
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	C4-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	C	512	CLA	O2A-C1-C2-C3
22	C	512	CLA	C6-C7-C8-C9
22	a	411	CLA	CHA-CBD-CGD-O1D
22	a	411	CLA	CHA-CBD-CGD-O2D
22	b	601	CLA	C11-C10-C8-C9
22	b	603	CLA	C2-C3-C5-C6
22	b	603	CLA	C4-C3-C5-C6
22	b	610	CLA	C2C-C3C-CAC-CBC
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	C6-C7-C8-C9
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	C11-C12-C13-C14
24	A	406	BCR	C20-C21-C22-C37
24	B	617	BCR	C36-C18-C19-C20
24	B	617	BCR	C20-C21-C22-C37
24	B	618	BCR	C7-C8-C9-C34
24	B	618	BCR	C11-C10-C9-C8
24	B	618	BCR	C10-C11-C12-C13
24	B	619	BCR	C7-C8-C9-C34
24	B	619	BCR	C11-C10-C9-C8
24	B	619	BCR	C37-C22-C23-C24
24	C	514	BCR	C11-C12-C13-C14
24	C	514	BCR	C20-C21-C22-C37
24	D	406	BCR	C37-C22-C23-C24
24	D	406	BCR	C22-C23-C24-C25
24	H	101	BCR	C35-C13-C14-C15
24	K	101	BCR	C7-C8-C9-C34
24	K	101	BCR	C21-C22-C23-C24
24	K	101	BCR	C37-C22-C23-C24
24	K	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	T	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C20-C21-C22-C37
24	T	101	BCR	C21-C22-C23-C24
24	Z	101	BCR	C7-C8-C9-C34
24	Z	101	BCR	C14-C15-C16-C17
24	a	406	BCR	C35-C13-C14-C15
24	b	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C20-C21-C22-C37
24	b	617	BCR	C21-C22-C23-C24
24	b	619	BCR	C7-C8-C9-C34
24	b	619	BCR	C11-C12-C13-C14
24	b	619	BCR	C16-C17-C18-C36
24	b	619	BCR	C37-C22-C23-C24
24	c	514	BCR	C35-C13-C14-C15
24	d	404	BCR	C21-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24
24	k	101	BCR	C1-C6-C7-C8
24	k	101	BCR	C11-C12-C13-C14
24	k	101	BCR	C35-C13-C14-C15
24	k	101	BCR	C13-C14-C15-C16
24	k	101	BCR	C17-C18-C19-C20
24	k	102	BCR	C7-C8-C9-C34
24	k	102	BCR	C17-C18-C19-C20
24	k	102	BCR	C36-C18-C19-C20
24	k	103	BCR	C37-C22-C23-C24
24	t	101	BCR	C7-C8-C9-C34
24	t	101	BCR	C20-C21-C22-C37
24	x	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C37-C22-C23-C24
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C23-C24-C26-C27
26	A	409	PL9	C35-C34-C36-C37
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
26	A	409	PL9	C45-C44-C46-C47
26	A	409	PL9	C47-C48-C49-C51
26	a	410	PL9	C12-C13-C14-C15
26	a	410	PL9	C12-C13-C14-C16
26	a	410	PL9	C17-C18-C19-C20
26	a	410	PL9	C17-C18-C19-C21

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C18-C19-C21-C22
26	a	410	PL9	C22-C23-C24-C25
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C25-C24-C26-C27
26	a	410	PL9	C32-C33-C34-C35
26	a	410	PL9	C37-C38-C39-C40
26	a	410	PL9	C42-C43-C44-C45
26	d	405	PL9	C37-C38-C39-C41
26	d	405	PL9	C42-C43-C44-C45
26	d	405	PL9	C42-C43-C44-C46
27	A	410	LMG	O6-C1-O1-C7
27	A	410	LMG	O9-C10-O7-C8
27	C	518	LMG	C2-C1-O1-C7
27	C	518	LMG	O6-C1-O1-C7
27	C	518	LMG	C11-C10-O7-C8
27	D	410	LMG	O1-C7-C8-C9
27	D	410	LMG	O1-C7-C8-O7
27	D	411	LMG	C10-C11-C12-C13
27	D	411	LMG	C28-C29-C30-C31
27	a	414	LMG	O6-C1-O1-C7
27	a	414	LMG	O10-C28-O8-C9
27	a	414	LMG	C29-C28-O8-C9
27	d	408	LMG	C10-C11-C12-C13
28	A	411	LHG	C3-O3-P-O5
28	B	621	LHG	C1-C2-C3-O3
28	B	621	LHG	C3-O3-P-O4
28	B	621	LHG	C3-O3-P-O5
28	B	621	LHG	C3-O3-P-O6
28	D	409	LHG	O1-C1-C2-C3
28	D	409	LHG	O2-C2-C3-O3
28	D	409	LHG	C3-O3-P-O4
28	D	409	LHG	C3-O3-P-O5
28	D	409	LHG	C3-O3-P-O6
28	D	409	LHG	C4-O6-P-O4
28	E	101	LHG	C4-O6-P-O4
28	L	102	LHG	C4-O6-P-O4
28	b	623	LHG	O1-C1-C2-O2
28	b	623	LHG	O1-C1-C2-C3
28	b	623	LHG	C1-C2-C3-O3
28	b	623	LHG	C3-O3-P-O5
28	b	623	LHG	C3-O3-P-O6
28	d	406	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
28	d	406	LHG	C4-O6-P-O4
28	d	407	LHG	C4-O6-P-O4
28	e	102	LHG	O1-C1-C2-C3
28	e	102	LHG	C3-O3-P-O5
28	e	102	LHG	C3-O3-P-O6
28	l	101	LHG	C4-O6-P-O3
28	l	101	LHG	C4-O6-P-O4
28	l	101	LHG	C4-O6-P-O5
29	B	622	SQD	C2-C1-O6-C44
29	B	622	SQD	O5-C1-O6-C44
29	B	622	SQD	O6-C44-C45-O47
29	B	622	SQD	O49-C7-O47-C45
29	B	622	SQD	C8-C7-O47-C45
29	F	102	SQD	C45-C44-O6-C1
29	L	101	SQD	O5-C1-O6-C44
29	L	101	SQD	C8-C7-O47-C45
29	L	101	SQD	O10-C23-O48-C46
29	a	412	SQD	O6-C44-C45-O47
29	a	413	SQD	C8-C7-O47-C45
29	f	101	SQD	O5-C1-O6-C44
30	A	414	DGD	C2B-C1B-O2G-C2G
30	B	623	DGD	C1G-C2G-C3G-O3G
30	B	623	DGD	O2G-C2G-C3G-O3G
32	B	620	STE	C1-C2-C3-C4
32	B	627	STE	C1-C2-C3-C4
32	E	102	STE	C1-C2-C3-C4
32	J	101	STE	C1-C2-C3-C4
32	b	621	STE	C1-C2-C3-C4
32	x	102	STE	C1-C2-C3-C4
22	b	612	CLA	C8-C10-C11-C12
22	b	601	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
30	B	623	DGD	O1A-C1A-O1G-C1G
22	C	513	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	CBA-CGA-O2A-C1
27	c	520	LMG	C29-C28-O8-C9
29	L	101	SQD	C24-C23-O48-C46
29	f	101	SQD	C24-C23-O48-C46
26	a	410	PL9	C47-C48-C49-C51
26	d	405	PL9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	O1A-CGA-O2A-C1
28	e	102	LHG	O10-C23-O8-C6
29	F	102	SQD	O10-C23-O48-C46
29	f	101	SQD	O10-C23-O48-C46
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	O9-C10-O7-C8
27	b	622	LMG	O9-C10-O7-C8
29	L	101	SQD	O49-C7-O47-C45
29	a	413	SQD	O49-C7-O47-C45
29	f	101	SQD	O49-C7-O47-C45
30	A	414	DGD	O1B-C1B-O2G-C2G
22	B	614	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
28	e	102	LHG	C24-C23-O8-C6
29	F	102	SQD	C24-C23-O48-C46
27	A	410	LMG	C11-C10-O7-C8
27	D	410	LMG	C11-C10-O7-C8
26	d	405	PL9	C47-C48-C49-C51
22	C	511	CLA	CBD-CGD-O2D-CED
27	c	520	LMG	O10-C28-O8-C9
22	A	405	CLA	C2-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
26	A	409	PL9	C43-C44-C46-C47
23	d	401	PHO	CBD-CGD-O2D-CED
30	B	623	DGD	C2A-C1A-O1G-C1G
26	A	409	PL9	C47-C48-C49-C50
26	D	407	PL9	C32-C33-C34-C35
26	d	405	PL9	C32-C33-C34-C35
22	D	405	CLA	CBD-CGD-O2D-CED
26	A	409	PL9	C12-C13-C14-C16
26	D	407	PL9	C32-C33-C34-C36
26	a	410	PL9	C37-C38-C39-C41
26	d	405	PL9	C32-C33-C34-C36
22	C	512	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
28	A	411	LHG	O2-C2-C3-O3
28	b	623	LHG	O2-C2-C3-O3
22	B	616	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C47-C48-C49-C50
22	B	613	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
32	b	620	STE	C3-C4-C5-C6
32	b	625	STE	C4-C5-C6-C7
22	b	605	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
26	A	409	PL9	C40-C39-C41-C42
26	a	410	PL9	C30-C29-C31-C32
26	d	405	PL9	C40-C39-C41-C42
22	B	605	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
26	A	409	PL9	C33-C34-C36-C37
26	a	410	PL9	C28-C29-C31-C32
26	d	405	PL9	C38-C39-C41-C42
28	l	101	LHG	C7-C8-C9-C10
22	B	606	CLA	C2A-CAA-CBA-CGA
30	C	517	DGD	C2A-C3A-C4A-C5A
26	A	409	PL9	C19-C21-C22-C23
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
26	a	410	PL9	C9-C11-C12-C13
26	a	410	PL9	C14-C16-C17-C18
26	a	410	PL9	C19-C21-C22-C23
26	d	405	PL9	C34-C36-C37-C38
27	A	410	LMG	O6-C5-C6-O5
28	d	406	LHG	C28-C29-C30-C31
30	H	102	DGD	C2B-C3B-C4B-C5B
28	D	409	LHG	C1-C2-C3-O3
22	c	504	CLA	C3-C5-C6-C7
22	c	506	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9
22	b	602	CLA	CBD-CGD-O2D-CED
24	k	101	BCR	C15-C16-C17-C18
22	b	603	CLA	C5-C6-C7-C8
22	C	502	CLA	C13-C15-C16-C17
22	C	512	CLA	C10-C11-C12-C13
22	D	405	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	B	621	LHG	O2-C2-C3-O3
28	b	623	LHG	C7-C8-C9-C10
27	a	414	LMG	C2-C1-O1-C7
29	f	101	SQD	C2-C1-O6-C44
27	A	410	LMG	O1-C7-C8-O7
26	D	407	PL9	C38-C39-C41-C42
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C6-C7-C8-C9
22	B	601	CLA	C14-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C9
22	B	607	CLA	C14-C13-C15-C16
22	B	614	CLA	C6-C7-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	511	CLA	C14-C13-C15-C16
22	D	403	CLA	C11-C10-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	b	603	CLA	C14-C13-C15-C16
22	b	604	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	607	CLA	C14-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C9
22	c	502	CLA	C6-C7-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
22	c	512	CLA	C6-C7-C8-C9
22	D	405	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	C13-C15-C16-C17
22	C	506	CLA	C13-C15-C16-C17
22	a	403	CLA	C8-C10-C11-C12
22	b	606	CLA	C2A-CAA-CBA-CGA
24	Z	101	BCR	C11-C12-C13-C35
24	b	619	BCR	C11-C12-C13-C35
24	c	514	BCR	C36-C18-C19-C20
24	k	101	BCR	C11-C12-C13-C35
24	k	102	BCR	C37-C22-C23-C24
24	t	101	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C4A-C5A-C6A-C7A
22	c	506	CLA	O1A-CGA-O2A-C1
30	c	517	DGD	O1A-C1A-O1G-C1G
22	B	603	CLA	C8-C10-C11-C12
22	C	512	CLA	C5-C6-C7-C8
22	b	607	CLA	C8-C10-C11-C12
22	b	608	CLA	C8-C10-C11-C12
22	b	612	CLA	C13-C15-C16-C17
22	c	508	CLA	C10-C11-C12-C13
22	c	510	CLA	C8-C10-C11-C12
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	O1D-CGD-O2D-CED
30	h	101	DGD	C4E-C5E-C6E-O5E
22	B	603	CLA	C15-C16-C17-C18
22	B	606	CLA	C15-C16-C17-C18
22	C	512	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
22	c	510	CLA	C10-C11-C12-C13
27	D	410	LMG	C28-C29-C30-C31
29	L	101	SQD	C7-C8-C9-C10
22	B	602	CLA	C13-C15-C16-C17
22	C	509	CLA	C5-C6-C7-C8
22	C	509	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
22	C	511	CLA	C8-C10-C11-C12
22	a	402	CLA	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
22	b	603	CLA	C10-C11-C12-C13
22	b	606	CLA	C15-C16-C17-C18
22	b	614	CLA	C8-C10-C11-C12
22	c	502	CLA	C13-C15-C16-C17
22	c	507	CLA	C13-C15-C16-C17
22	c	511	CLA	C8-C10-C11-C12
27	C	518	LMG	C28-C29-C30-C31
27	d	409	LMG	C28-C29-C30-C31
28	b	623	LHG	C23-C24-C25-C26
28	e	102	LHG	C23-C24-C25-C26
22	c	502	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	C10-C11-C12-C13
22	C	503	CLA	C5-C6-C7-C8
22	C	504	CLA	C8-C10-C11-C12
22	C	505	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C13-C15-C16-C17
22	b	613	CLA	C10-C11-C12-C13
22	b	602	CLA	C15-C16-C17-C18
27	D	408	LMG	C10-C11-C12-C13
27	b	622	LMG	C28-C29-C30-C31
27	m	101	LMG	C10-C11-C12-C13
29	L	101	SQD	C23-C24-C25-C26
30	B	623	DGD	C1B-C2B-C3B-C4B
30	c	516	DGD	C1A-C2A-C3A-C4A
30	c	516	DGD	C1B-C2B-C3B-C4B
22	c	503	CLA	C5-C6-C7-C8
22	B	615	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C12-C13-C15
22	C	508	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	a	403	CLA	C6-C7-C8-C10
22	a	411	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C15
22	c	509	CLA	C6-C7-C8-C10
27	m	101	LMG	C29-C28-O8-C9
22	D	405	CLA	C10-C11-C12-C13
22	c	513	CLA	C5-C6-C7-C8
29	F	102	SQD	C44-C45-C46-O48
30	C	516	DGD	O6E-C1E-O5D-C6D
22	b	612	CLA	C15-C16-C17-C18
26	a	410	PL9	C39-C41-C42-C43
30	C	516	DGD	C1B-C2B-C3B-C4B
24	B	619	BCR	C10-C11-C12-C13
24	C	514	BCR	C18-C19-C20-C21
24	K	102	BCR	C18-C19-C20-C21
24	Z	101	BCR	C10-C11-C12-C13
24	a	406	BCR	C18-C19-C20-C21
24	k	101	BCR	C18-C19-C20-C21
28	e	102	LHG	O2-C2-C3-O3
22	B	601	CLA	C15-C16-C17-C18
22	B	603	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	B	609	CLA	C15-C16-C17-C18
22	B	615	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
22	a	411	CLA	C15-C16-C17-C18
22	b	607	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	C15-C16-C17-C18
22	B	607	CLA	C13-C15-C16-C17
22	B	614	CLA	C8-C10-C11-C12
22	C	508	CLA	C15-C16-C17-C18
22	C	510	CLA	C10-C11-C12-C13
22	C	513	CLA	C15-C16-C17-C18
22	c	511	CLA	C15-C16-C17-C18
22	d	403	CLA	C8-C10-C11-C12
32	B	626	STE	C9-C10-C11-C12
30	A	414	DGD	C4E-C5E-C6E-O5E
27	b	622	LMG	C11-C10-O7-C8
22	B	616	CLA	C5-C6-C7-C8
22	C	507	CLA	C10-C11-C12-C13
22	a	405	CLA	C10-C11-C12-C13
22	b	613	CLA	C15-C16-C17-C18
22	b	614	CLA	C13-C15-C16-C17
28	A	411	LHG	C3-O3-P-O6
28	d	406	LHG	C4-O6-P-O3
22	C	512	CLA	C3-C5-C6-C7
30	A	414	DGD	C2A-C1A-O1G-C1G
22	b	612	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
28	e	102	LHG	C1-C2-C3-O3
27	C	518	LMG	O9-C10-O7-C8
22	b	614	CLA	C5-C6-C7-C8
22	b	614	CLA	C15-C16-C17-C18
29	B	622	SQD	C24-C23-O48-C46
22	b	607	CLA	C10-C11-C12-C13
22	c	509	CLA	C10-C11-C12-C13
24	k	102	BCR	C14-C15-C16-C17
28	d	407	LHG	C23-C24-C25-C26
27	C	518	LMG	C11-C12-C13-C14
29	B	622	SQD	C34-C35-C36-C37
29	f	101	SQD	C29-C30-C31-C32
30	C	516	DGD	CCB-CDB-CEB-CFB
30	c	515	DGD	CAB-CBB-CCB-CDB
32	B	626	STE	C12-C13-C14-C15
32	D	412	STE	C4-C5-C6-C7
24	B	618	BCR	C11-C10-C9-C34
24	C	514	BCR	C35-C13-C14-C15
24	D	406	BCR	C20-C21-C22-C37
24	H	101	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
24	H	101	BCR	C20-C21-C22-C37
24	K	101	BCR	C11-C10-C9-C34
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C20-C21-C22-C37
24	a	406	BCR	C11-C10-C9-C34
24	b	618	BCR	C11-C10-C9-C34
24	b	619	BCR	C11-C10-C9-C34
24	b	619	BCR	C20-C21-C22-C37
24	t	101	BCR	C35-C13-C14-C15
27	A	410	LMG	C33-C34-C35-C36
27	C	518	LMG	C17-C18-C19-C20
27	D	408	LMG	C37-C38-C39-C40
27	D	411	LMG	C36-C37-C38-C39
27	a	414	LMG	C31-C32-C33-C34
27	b	622	LMG	C40-C41-C42-C43
28	A	411	LHG	C30-C31-C32-C33
28	L	102	LHG	C31-C32-C33-C34
29	F	102	SQD	C27-C28-C29-C30
29	F	102	SQD	C33-C34-C35-C36
30	A	414	DGD	C9A-CAA-CBA-CCA
30	C	516	DGD	C9A-CAA-CBA-CCA
30	c	515	DGD	C4A-C5A-C6A-C7A
30	c	515	DGD	C4B-C5B-C6B-C7B
30	c	516	DGD	C2A-C3A-C4A-C5A
32	E	102	STE	C6-C7-C8-C9
32	M	103	STE	C5-C6-C7-C8
32	t	103	STE	C4-C5-C6-C7
22	C	510	CLA	C16-C17-C18-C20
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
28	E	101	LHG	C11-C10-C9-C8
28	b	623	LHG	C33-C34-C35-C36
28	d	406	LHG	C12-C13-C14-C15
28	e	102	LHG	C11-C12-C13-C14
30	A	414	DGD	C4B-C5B-C6B-C7B
30	B	623	DGD	C6A-C7A-C8A-C9A
30	H	102	DGD	C3B-C4B-C5B-C6B
30	c	515	DGD	C8B-C9B-CAB-CBB
30	h	101	DGD	C6B-C7B-C8B-C9B
32	l	102	STE	C12-C13-C14-C15
29	L	101	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C8-C10-C11-C12
27	b	622	LMG	C12-C13-C14-C15
28	A	411	LHG	C12-C13-C14-C15
28	E	101	LHG	C10-C11-C12-C13
28	L	102	LHG	C27-C28-C29-C30
28	b	623	LHG	C15-C16-C17-C18
29	L	101	SQD	C15-C16-C17-C18
29	a	412	SQD	C13-C14-C15-C16
30	C	515	DGD	C6A-C7A-C8A-C9A
30	C	515	DGD	C9A-CAA-CBA-CCA
30	c	516	DGD	CCA-CDA-CEA-CFA
32	B	625	STE	C9-C10-C11-C12
32	C	519	STE	C4-C5-C6-C7
22	c	501	CLA	O1D-CGD-O2D-CED
27	D	411	LMG	C31-C32-C33-C34
27	M	101	LMG	C29-C30-C31-C32
27	a	414	LMG	C12-C13-C14-C15
27	a	414	LMG	C32-C33-C34-C35
27	b	622	LMG	C11-C12-C13-C14
27	c	520	LMG	C11-C12-C13-C14
27	c	520	LMG	C40-C41-C42-C43
27	m	101	LMG	C19-C20-C21-C22
27	m	101	LMG	C31-C32-C33-C34
28	L	102	LHG	C17-C18-C19-C20
29	A	412	SQD	C16-C17-C18-C19
29	F	102	SQD	C28-C29-C30-C31
29	f	101	SQD	C33-C34-C35-C36
30	C	515	DGD	CAB-CBB-CCB-CDB
30	C	517	DGD	C8B-C9B-CAB-CBB
30	c	517	DGD	C5B-C6B-C7B-C8B
32	B	626	STE	C4-C5-C6-C7
32	x	102	STE	C5-C6-C7-C8
27	M	101	LMG	C14-C15-C16-C17
27	b	622	LMG	C30-C31-C32-C33
32	D	412	STE	C11-C10-C9-C8
32	M	102	STE	C11-C10-C9-C8
22	b	615	CLA	C3-C5-C6-C7
30	H	102	DGD	C1A-C2A-C3A-C4A
23	d	401	PHO	O1D-CGD-O2D-CED
24	B	617	BCR	C12-C13-C14-C15
24	C	514	BCR	C20-C21-C22-C23
24	a	406	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	b	619	BCR	C12-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C23
24	k	103	BCR	C20-C21-C22-C23
24	t	101	BCR	C11-C10-C9-C8
24	x	101	BCR	C11-C10-C9-C8
30	C	516	DGD	C2E-C1E-O5D-C6D
22	a	405	CLA	CBA-CGA-O2A-C1
27	A	410	LMG	C29-C30-C31-C32
27	C	518	LMG	C32-C33-C34-C35
27	D	408	LMG	C15-C16-C17-C18
27	c	520	LMG	C16-C17-C18-C19
28	D	409	LHG	C14-C15-C16-C17
28	D	409	LHG	C30-C31-C32-C33
28	d	406	LHG	C11-C12-C13-C14
32	I	101	STE	C11-C10-C9-C8
22	b	602	CLA	C13-C15-C16-C17
22	a	403	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
22	c	509	CLA	C16-C17-C18-C20
22	C	506	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
26	d	405	PL9	C45-C44-C46-C47
27	C	518	LMG	C12-C13-C14-C15
27	D	410	LMG	C12-C13-C14-C15
29	A	412	SQD	C9-C10-C11-C12
29	A	413	SQD	C32-C33-C34-C35
29	L	101	SQD	C16-C17-C18-C19
29	f	101	SQD	C32-C33-C34-C35
30	C	515	DGD	CBB-CCB-CDB-CEB
30	C	516	DGD	C4A-C5A-C6A-C7A
30	C	517	DGD	C7A-C8A-C9A-CAA
32	l	102	STE	C3-C4-C5-C6
26	A	409	PL9	C38-C39-C41-C42
22	B	611	CLA	C11-C12-C13-C14
22	a	405	CLA	C6-C7-C8-C9
22	b	616	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C12-C13-C14
27	C	518	LMG	C37-C38-C39-C40
27	b	622	LMG	C16-C17-C18-C19
27	c	520	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
28	E	101	LHG	C11-C12-C13-C14
28	d	406	LHG	C14-C15-C16-C17
29	A	413	SQD	C17-C18-C19-C20
29	L	101	SQD	C25-C26-C27-C28
29	L	101	SQD	C27-C28-C29-C30
29	a	413	SQD	C15-C16-C17-C18
29	a	413	SQD	C17-C18-C19-C20
30	c	515	DGD	C7B-C8B-C9B-CAB
30	c	516	DGD	C4A-C5A-C6A-C7A
30	c	517	DGD	C6B-C7B-C8B-C9B
32	E	102	STE	C4-C5-C6-C7
32	M	104	STE	C3-C4-C5-C6
27	D	410	LMG	C36-C37-C38-C39
27	d	408	LMG	C31-C32-C33-C34
27	d	408	LMG	C36-C37-C38-C39
28	A	411	LHG	C25-C26-C27-C28
28	b	623	LHG	C11-C10-C9-C8
29	a	412	SQD	C26-C27-C28-C29
30	A	414	DGD	CCA-CDA-CEA-CFA
32	B	626	STE	C3-C4-C5-C6
32	H	103	STE	C7-C8-C9-C10
32	J	101	STE	C6-C7-C8-C9
28	d	407	LHG	O1-C1-C2-C3
27	a	414	LMG	C11-C12-C13-C14
27	c	520	LMG	C30-C31-C32-C33
27	c	520	LMG	C31-C32-C33-C34
27	m	101	LMG	C30-C31-C32-C33
28	B	621	LHG	C28-C29-C30-C31
28	b	623	LHG	C25-C26-C27-C28
30	A	414	DGD	C9B-CAB-CBB-CCB
30	B	623	DGD	CEB-CFB-CGB-CHB
28	E	101	LHG	C23-C24-C25-C26
28	d	406	LHG	C7-C8-C9-C10
30	A	414	DGD	C1A-C2A-C3A-C4A
22	b	609	CLA	O1D-CGD-O2D-CED
27	c	520	LMG	C33-C34-C35-C36
28	d	406	LHG	C29-C30-C31-C32
28	l	101	LHG	C14-C15-C16-C17
29	A	412	SQD	C27-C28-C29-C30
29	A	412	SQD	C29-C30-C31-C32
29	L	101	SQD	C12-C13-C14-C15
30	A	414	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
30	H	102	DGD	C7A-C8A-C9A-CAA
30	h	101	DGD	C3B-C4B-C5B-C6B
32	B	624	STE	C4-C5-C6-C7
32	E	102	STE	C5-C6-C7-C8
32	b	621	STE	C14-C15-C16-C17
32	c	519	STE	C4-C5-C6-C7
32	c	519	STE	C14-C15-C16-C17
32	d	410	STE	C10-C11-C12-C13
32	m	102	STE	C4-C5-C6-C7
32	x	102	STE	C11-C12-C13-C14
22	B	605	CLA	C16-C17-C18-C19
22	B	605	CLA	C16-C17-C18-C20
22	C	512	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
22	b	616	CLA	C11-C12-C13-C14
22	c	510	CLA	C15-C16-C17-C18
22	C	511	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C31-C32-C33-C34
28	L	102	LHG	C14-C15-C16-C17
30	B	623	DGD	CBA-CCA-CDA-CEA
30	H	102	DGD	C8B-C9B-CAB-CBB
32	H	103	STE	C2-C3-C4-C5
32	J	101	STE	C4-C5-C6-C7
22	B	604	CLA	CBD-CGD-O2D-CED
27	a	414	LMG	C33-C34-C35-C36
28	E	101	LHG	C26-C27-C28-C29
28	E	101	LHG	C27-C28-C29-C30
28	E	101	LHG	C33-C34-C35-C36
30	C	515	DGD	C9B-CAB-CBB-CCB
32	B	626	STE	C2-C3-C4-C5
32	H	103	STE	C5-C6-C7-C8
27	C	518	LMG	C39-C40-C41-C42
27	b	622	LMG	C32-C33-C34-C35
28	e	102	LHG	C16-C17-C18-C19
30	c	515	DGD	C9B-CAB-CBB-CCB
30	c	516	DGD	C8B-C9B-CAB-CBB
32	b	625	STE	C11-C12-C13-C14
32	m	102	STE	C5-C6-C7-C8
27	A	410	LMG	C29-C28-O8-C9
27	m	101	LMG	C11-C12-C13-C14
27	m	101	LMG	C39-C40-C41-C42
30	A	414	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
30	B	623	DGD	C5A-C6A-C7A-C8A
30	C	515	DGD	C4B-C5B-C6B-C7B
30	h	101	DGD	CAB-CBB-CCB-CDB
32	c	519	STE	C9-C10-C11-C12
22	B	601	CLA	C3A-C2A-CAA-CBA
28	A	411	LHG	C11-C12-C13-C14
29	B	622	SQD	C13-C14-C15-C16
30	C	516	DGD	C6B-C7B-C8B-C9B
30	C	516	DGD	C8B-C9B-CAB-CBB
30	c	517	DGD	C4B-C5B-C6B-C7B
32	l	102	STE	C7-C8-C9-C10
22	C	512	CLA	O1D-CGD-O2D-CED
22	b	611	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C19
27	M	101	LMG	C38-C39-C40-C41
27	a	414	LMG	C18-C19-C20-C21
29	F	102	SQD	C31-C32-C33-C34
30	A	414	DGD	CBA-CCA-CDA-CEA
30	B	623	DGD	CAB-CBB-CCB-CDB
32	x	102	STE	C10-C11-C12-C13
22	c	511	CLA	O1D-CGD-O2D-CED
30	A	414	DGD	O6E-C5E-C6E-O5E
22	c	508	CLA	CBD-CGD-O2D-CED
30	A	414	DGD	C2A-C3A-C4A-C5A
30	C	515	DGD	CBA-CCA-CDA-CEA
30	C	516	DGD	C3A-C4A-C5A-C6A
30	H	102	DGD	CAB-CBB-CCB-CDB
32	M	104	STE	C10-C11-C12-C13
30	c	515	DGD	O6D-C5D-C6D-O5D
22	B	613	CLA	O1D-CGD-O2D-CED
32	b	621	STE	C2-C3-C4-C5
32	d	410	STE	C9-C10-C11-C12
22	C	513	CLA	CBA-CGA-O2A-C1
28	E	101	LHG	C24-C23-O8-C6
22	b	611	CLA	C2-C3-C5-C6
26	D	407	PL9	C28-C29-C31-C32
26	a	410	PL9	C43-C44-C46-C47
26	d	405	PL9	C28-C29-C31-C32
27	M	101	LMG	C13-C14-C15-C16
30	H	102	DGD	C5A-C6A-C7A-C8A
28	e	102	LHG	O1-C1-C2-O2
27	M	101	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
28	A	411	LHG	C29-C30-C31-C32
28	E	101	LHG	C32-C33-C34-C35
28	b	623	LHG	C18-C19-C20-C21
28	d	407	LHG	C29-C30-C31-C32
30	A	414	DGD	C2B-C3B-C4B-C5B
30	c	515	DGD	CBA-CCA-CDA-CEA
32	J	101	STE	C7-C8-C9-C10
32	b	624	STE	C3-C4-C5-C6
32	b	625	STE	C13-C14-C15-C16
22	a	403	CLA	C16-C17-C18-C20
28	d	407	LHG	C32-C33-C34-C35
32	x	102	STE	C6-C7-C8-C9
28	D	409	LHG	C34-C35-C36-C37
27	M	101	LMG	C20-C21-C22-C23
30	c	517	DGD	CBB-CCB-CDB-CEB
27	D	408	LMG	C30-C31-C32-C33
27	b	622	LMG	C22-C23-C24-C25
32	B	625	STE	C12-C13-C14-C15
32	b	620	STE	C2-C3-C4-C5
27	c	520	LMG	O9-C10-O7-C8
27	M	101	LMG	C12-C13-C14-C15
28	A	411	LHG	C24-C25-C26-C27
28	B	621	LHG	C25-C26-C27-C28
28	B	621	LHG	C29-C30-C31-C32
28	b	623	LHG	C27-C28-C29-C30
29	a	412	SQD	C17-C18-C19-C20
29	a	413	SQD	C24-C25-C26-C27
30	C	516	DGD	CBB-CCB-CDB-CEB
32	E	102	STE	C3-C4-C5-C6
32	M	102	STE	C7-C8-C9-C10
22	B	612	CLA	C10-C11-C12-C13
27	C	518	LMG	O10-C28-O8-C9
27	A	410	LMG	C12-C13-C14-C15
27	d	409	LMG	C11-C12-C13-C14
29	A	412	SQD	C32-C33-C34-C35
30	h	101	DGD	C2B-C3B-C4B-C5B
22	C	510	CLA	C16-C17-C18-C19
27	M	101	LMG	C10-C11-C12-C13
24	D	406	BCR	C23-C24-C25-C26
24	D	406	BCR	C23-C24-C25-C30
24	K	101	BCR	C1-C6-C7-C8
24	K	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	617	BCR	C5-C6-C7-C8
24	d	404	BCR	C23-C24-C25-C26
24	d	404	BCR	C23-C24-C25-C30
24	k	101	BCR	C5-C6-C7-C8
24	k	102	BCR	C1-C6-C7-C8
24	k	102	BCR	C5-C6-C7-C8
24	t	101	BCR	C1-C6-C7-C8
29	A	412	SQD	C11-C12-C13-C14
29	a	412	SQD	C32-C33-C34-C35
30	C	516	DGD	C2B-C3B-C4B-C5B
30	c	515	DGD	C6B-C7B-C8B-C9B
32	b	626	STE	C2-C3-C4-C5
22	C	511	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	C13-C15-C16-C17
29	f	101	SQD	C8-C7-O47-C45
30	B	623	DGD	C2B-C1B-O2G-C2G
27	m	101	LMG	C17-C18-C19-C20
28	b	623	LHG	C16-C17-C18-C19
30	c	517	DGD	C8A-C9A-CAA-CBA
32	b	620	STE	C1-C2-C3-C4
32	l	102	STE	C14-C15-C16-C17
22	c	502	CLA	O1D-CGD-O2D-CED
28	B	621	LHG	C23-C24-C25-C26
27	c	520	LMG	C34-C35-C36-C37
22	b	611	CLA	C15-C16-C17-C18
22	c	504	CLA	C5-C6-C7-C8
27	A	410	LMG	C16-C17-C18-C19
27	b	622	LMG	C34-C35-C36-C37
30	B	623	DGD	CCA-CDA-CEA-CFA
30	c	516	DGD	C5A-C6A-C7A-C8A
32	x	102	STE	C4-C5-C6-C7
22	b	611	CLA	C4-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
26	a	410	PL9	C20-C19-C21-C22
22	B	603	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C12-C13-C15
22	B	611	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C12-C13-C15-C16
22	b	601	CLA	C11-C12-C13-C15
22	b	602	CLA	C12-C13-C15-C16
22	b	603	CLA	C6-C7-C8-C10
22	b	611	CLA	C12-C13-C15-C16
22	b	612	CLA	C11-C10-C8-C7
22	c	502	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
22	c	512	CLA	C11-C12-C13-C15
23	A	404	PHO	C2-C3-C5-C6
22	C	511	CLA	O1A-CGA-O2A-C1
22	C	513	CLA	O1A-CGA-O2A-C1
22	a	405	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	C11-C12-C13-C14
29	a	413	SQD	C11-C12-C13-C14
30	c	517	DGD	C2A-C3A-C4A-C5A
30	h	101	DGD	CCB-CDB-CEB-CFB
22	b	604	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C19
22	c	512	CLA	O1D-CGD-O2D-CED
30	B	623	DGD	C1A-C2A-C3A-C4A
22	B	605	CLA	CBA-CGA-O2A-C1
30	c	517	DGD	C2A-C1A-O1G-C1G
27	c	520	LMG	C36-C37-C38-C39
27	m	101	LMG	C14-C15-C16-C17
30	H	102	DGD	C4B-C5B-C6B-C7B
32	a	415	STE	C6-C7-C8-C9
28	D	409	LHG	C29-C30-C31-C32
32	d	410	STE	C5-C6-C7-C8
27	D	408	LMG	C35-C36-C37-C38
27	D	410	LMG	C31-C32-C33-C34
27	M	101	LMG	C35-C36-C37-C38
28	b	623	LHG	C29-C30-C31-C32
28	d	407	LHG	C33-C34-C35-C36
26	A	409	PL9	C22-C23-C24-C25
30	c	515	DGD	C5B-C6B-C7B-C8B
32	t	103	STE	C6-C7-C8-C9
24	K	101	BCR	C22-C23-C24-C25
22	c	513	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
30	c	515	DGD	O6E-C1E-O5D-C6D
30	c	516	DGD	O6E-C1E-O5D-C6D
22	C	512	CLA	C13-C15-C16-C17
29	L	101	SQD	C14-C15-C16-C17
29	a	412	SQD	C11-C12-C13-C14
30	c	517	DGD	C6A-C7A-C8A-C9A
32	H	103	STE	C11-C12-C13-C14
27	c	520	LMG	C11-C10-O7-C8
28	e	102	LHG	O6-C4-C5-O7
24	k	103	BCR	C10-C11-C12-C13
27	M	101	LMG	C32-C33-C34-C35
28	L	102	LHG	C12-C13-C14-C15
29	A	413	SQD	C12-C13-C14-C15
29	a	412	SQD	C24-C25-C26-C27
22	B	601	CLA	C8-C10-C11-C12
22	c	508	CLA	C13-C15-C16-C17
27	D	408	LMG	C39-C40-C41-C42
27	D	410	LMG	C34-C35-C36-C37
28	d	407	LHG	C34-C35-C36-C37
30	C	517	DGD	C4B-C5B-C6B-C7B
30	c	516	DGD	C2E-C1E-O5D-C6D
29	a	412	SQD	O47-C45-C46-O48
30	A	414	DGD	O2G-C2G-C3G-O3G
30	C	515	DGD	O6E-C5E-C6E-O5E
22	A	405	CLA	C5-C6-C7-C8
32	a	415	STE	C4-C5-C6-C7
32	b	626	STE	C5-C6-C7-C8
22	C	511	CLA	C16-C17-C18-C19
27	m	101	LMG	C20-C21-C22-C23
28	b	623	LHG	C32-C33-C34-C35
32	D	412	STE	C11-C12-C13-C14
30	c	515	DGD	O6E-C5E-C6E-O5E
22	c	502	CLA	C15-C16-C17-C18
26	d	405	PL9	C15-C14-C16-C17
26	d	405	PL9	C43-C44-C46-C47
22	B	606	CLA	C11-C12-C13-C14
22	B	615	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C10-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	a	403	CLA	C6-C7-C8-C9
22	a	411	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C14
22	b	602	CLA	C14-C13-C15-C16
22	b	603	CLA	C11-C10-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	c	502	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
30	B	623	DGD	C5B-C6B-C7B-C8B
32	B	627	STE	C4-C5-C6-C7
30	c	517	DGD	C3A-C4A-C5A-C6A
27	d	409	LMG	O6-C5-C6-O5
22	c	507	CLA	O1D-CGD-O2D-CED
32	C	521	STE	C2-C3-C4-C5
24	B	618	BCR	C11-C12-C13-C14
24	k	102	BCR	C21-C22-C23-C24
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	B	613	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C15
22	d	402	CLA	C16-C17-C18-C20
27	m	101	LMG	O9-C10-O7-C8
27	a	414	LMG	C19-C20-C21-C22
27	b	622	LMG	C39-C40-C41-C42
28	l	101	LHG	C15-C16-C17-C18
32	I	101	STE	C2-C3-C4-C5
22	B	611	CLA	C8-C10-C11-C12
22	b	611	CLA	C13-C15-C16-C17
28	L	102	LHG	C4-O6-P-O3
30	C	515	DGD	C5B-C6B-C7B-C8B
32	H	103	STE	C9-C10-C11-C12
29	a	413	SQD	C29-C30-C31-C32
22	B	606	CLA	C8-C10-C11-C12
22	b	614	CLA	C10-C11-C12-C13
28	e	102	LHG	O6-C4-C5-C6
26	A	409	PL9	C12-C13-C14-C15
28	L	102	LHG	C10-C11-C12-C13
32	b	621	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	h	101	DGD	C6A-C7A-C8A-C9A
32	b	626	STE	C7-C8-C9-C10
27	D	408	LMG	C36-C37-C38-C39
27	M	101	LMG	C39-C40-C41-C42
27	a	414	LMG	C29-C30-C31-C32
32	B	625	STE	C4-C5-C6-C7
27	M	101	LMG	C33-C34-C35-C36
27	b	622	LMG	C31-C32-C33-C34
22	b	605	CLA	C10-C11-C12-C13
30	c	517	DGD	C7A-C8A-C9A-CAA
30	c	515	DGD	C4D-C5D-C6D-O5D
30	c	515	DGD	O1B-C1B-O2G-C2G
26	D	407	PL9	C30-C29-C31-C32
26	a	410	PL9	C45-C44-C46-C47
32	B	627	STE	C5-C6-C7-C8
22	c	510	CLA	CBD-CGD-O2D-CED
27	b	622	LMG	C37-C38-C39-C40
28	D	409	LHG	C8-C7-O7-C5
22	B	605	CLA	O1A-CGA-O2A-C1
28	A	411	LHG	C27-C28-C29-C30
28	E	101	LHG	C12-C13-C14-C15
30	B	623	DGD	C6B-C7B-C8B-C9B
32	H	103	STE	C4-C5-C6-C7
32	l	102	STE	C5-C6-C7-C8
22	C	509	CLA	C3-C5-C6-C7
22	b	612	CLA	C3-C5-C6-C7
27	A	410	LMG	C36-C37-C38-C39
27	C	518	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	c	520	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
28	e	102	LHG	C4-C5-C6-O8
28	l	101	LHG	C9-C10-C11-C12
29	A	412	SQD	O6-C44-C45-C46
29	a	412	SQD	O6-C44-C45-C46
29	f	101	SQD	C27-C28-C29-C30
30	C	516	DGD	C9B-CAB-CBB-CCB
32	x	102	STE	C3-C4-C5-C6
30	C	516	DGD	C5B-C6B-C7B-C8B
32	D	412	STE	C10-C11-C12-C13
22	B	616	CLA	O1A-CGA-O2A-C1
30	C	516	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
30	c	516	DGD	C2G-C3G-O3G-C1D
30	c	516	DGD	C5D-C6D-O5D-C1E
29	a	413	SQD	C14-C15-C16-C17
32	C	519	STE	C2-C3-C4-C5
29	B	622	SQD	C11-C12-C13-C14
28	L	102	LHG	C23-C24-C25-C26
28	D	409	LHG	C9-C10-C11-C12
32	l	102	STE	C13-C14-C15-C16
26	A	409	PL9	C29-C31-C32-C33
27	m	101	LMG	C37-C38-C39-C40
32	b	620	STE	C10-C11-C12-C13
32	b	624	STE	C10-C11-C12-C13
32	d	410	STE	C6-C7-C8-C9
32	l	102	STE	C9-C10-C11-C12
28	D	409	LHG	O1-C1-C2-O2
28	d	407	LHG	O1-C1-C2-O2
29	A	413	SQD	C15-C16-C17-C18
30	C	516	DGD	C4B-C5B-C6B-C7B
28	A	411	LHG	C23-C24-C25-C26
30	h	101	DGD	O6E-C5E-C6E-O5E
27	d	408	LMG	C30-C31-C32-C33
30	C	516	DGD	C3B-C4B-C5B-C6B
30	c	515	DGD	C2B-C3B-C4B-C5B
32	C	520	STE	C4-C5-C6-C7
32	c	519	STE	C15-C16-C17-C18
27	A	410	LMG	C4-C5-C6-O5
28	L	102	LHG	C18-C19-C20-C21
28	d	406	LHG	C15-C16-C17-C18
24	K	102	BCR	C16-C17-C18-C36
24	Z	101	BCR	C35-C13-C14-C15
24	a	406	BCR	C20-C21-C22-C37
27	D	408	LMG	O6-C5-C6-O5
27	b	622	LMG	O6-C5-C6-O5
27	c	520	LMG	O6-C5-C6-O5
22	C	505	CLA	C4-C3-C5-C6
28	E	101	LHG	C15-C16-C17-C18
22	c	509	CLA	C16-C17-C18-C19
27	M	101	LMG	C22-C23-C24-C25
27	d	408	LMG	C11-C12-C13-C14
22	B	616	CLA	CBD-CGD-O2D-CED
22	B	614	CLA	C13-C15-C16-C17
22	C	513	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C10-C11-C12-C13
22	b	604	CLA	C15-C16-C17-C18
22	b	611	CLA	C8-C10-C11-C12
22	c	512	CLA	C13-C15-C16-C17
27	d	408	LMG	C34-C35-C36-C37
30	C	516	DGD	C2A-C3A-C4A-C5A
32	B	620	STE	C12-C13-C14-C15
32	I	101	STE	C1-C2-C3-C4
32	b	620	STE	C13-C14-C15-C16
27	c	518	LMG	O6-C5-C6-O5
28	L	102	LHG	C19-C20-C21-C22
28	d	407	LHG	C27-C28-C29-C30
30	A	414	DGD	CFA-CGA-CHA-CIA
27	A	410	LMG	C32-C33-C34-C35
27	C	518	LMG	C30-C31-C32-C33
27	b	622	LMG	C18-C19-C20-C21
28	d	406	LHG	C17-C18-C19-C20
32	a	415	STE	C7-C8-C9-C10
22	C	512	CLA	C8-C10-C11-C12
22	b	609	CLA	C15-C16-C17-C18
27	D	410	LMG	C35-C36-C37-C38
27	b	622	LMG	C24-C25-C26-C27
28	D	409	LHG	C15-C16-C17-C18
30	c	516	DGD	CDA-CEA-CFA-CGA
32	C	519	STE	C7-C8-C9-C10
32	H	103	STE	C12-C13-C14-C15
32	M	104	STE	C1-C2-C3-C4
27	c	520	LMG	C42-C43-C44-C45
27	d	408	LMG	C35-C36-C37-C38
29	A	412	SQD	C14-C15-C16-C17
22	B	611	CLA	C13-C15-C16-C17
32	c	519	STE	C3-C4-C5-C6
30	c	517	DGD	C1A-C2A-C3A-C4A
22	D	404	CLA	C15-C16-C17-C18
22	b	615	CLA	C10-C11-C12-C13
24	C	514	BCR	C11-C10-C9-C8
24	k	102	BCR	C12-C13-C14-C15
30	B	623	DGD	C4A-C5A-C6A-C7A
29	A	412	SQD	O6-C44-C45-O47
27	m	101	LMG	C40-C41-C42-C43
22	b	604	CLA	C16-C17-C18-C20
27	D	411	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	O6-C5-C6-O5
22	C	510	CLA	C4-C3-C5-C6
28	E	101	LHG	C29-C30-C31-C32
28	d	407	LHG	C24-C25-C26-C27
28	l	101	LHG	C12-C13-C14-C15
32	l	102	STE	C11-C12-C13-C14
22	B	601	CLA	C6-C7-C8-C10
22	B	604	CLA	C12-C13-C15-C16
22	B	607	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C15
22	C	505	CLA	C2-C3-C5-C6
22	C	506	CLA	C2-C3-C5-C6
22	C	506	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C10-C8-C7
22	a	403	CLA	C11-C12-C13-C15
22	b	603	CLA	C11-C10-C8-C7
22	b	605	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C7
22	b	607	CLA	C6-C7-C8-C10
22	b	612	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C12-C13-C15
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C12-C13-C15
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C11-C12-C13-C15
22	c	511	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C10
22	b	606	CLA	C3-C5-C6-C7
29	B	622	SQD	C33-C34-C35-C36
29	a	412	SQD	C10-C11-C12-C13
32	E	102	STE	C7-C8-C9-C10
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	C11-C10-C8-C9
22	b	602	CLA	C6-C7-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
24	c	514	BCR	C14-C15-C16-C17
28	D	409	LHG	C7-C8-C9-C10
30	C	516	DGD	C6A-C7A-C8A-C9A
30	c	515	DGD	C8A-C9A-CAA-CBA
30	c	517	DGD	CCA-CDA-CEA-CFA
28	B	621	LHG	C24-C23-O8-C6
29	a	412	SQD	C24-C23-O48-C46
27	A	410	LMG	C38-C39-C40-C41
27	a	414	LMG	C17-C18-C19-C20
32	c	519	STE	C2-C3-C4-C5
22	b	603	CLA	O1D-CGD-O2D-CED
24	k	101	BCR	C7-C8-C9-C34
22	B	610	CLA	C16-C17-C18-C20
32	x	102	STE	C9-C10-C11-C12
29	L	101	SQD	C30-C31-C32-C33
22	B	607	CLA	C10-C11-C12-C13
27	M	101	LMG	C17-C18-C19-C20
27	c	520	LMG	C14-C15-C16-C17
22	B	616	CLA	CBA-CGA-O2A-C1
28	L	102	LHG	C13-C14-C15-C16
30	c	517	DGD	C5A-C6A-C7A-C8A
30	c	516	DGD	C7A-C8A-C9A-CAA
32	B	620	STE	C7-C8-C9-C10
30	c	516	DGD	C6A-C7A-C8A-C9A
30	h	101	DGD	CBA-CCA-CDA-CEA
32	M	103	STE	C1-C2-C3-C4
28	E	101	LHG	O6-C4-C5-C6
28	l	101	LHG	O6-C4-C5-C6
22	c	507	CLA	C3-C5-C6-C7
26	a	410	PL9	C24-C26-C27-C28
29	L	101	SQD	C10-C11-C12-C13
30	h	101	DGD	C5B-C6B-C7B-C8B
32	b	624	STE	C2-C3-C4-C5
28	B	621	LHG	C33-C34-C35-C36
28	l	101	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	h	101	DGD	C3A-C4A-C5A-C6A
22	D	404	CLA	C13-C15-C16-C17
22	B	616	CLA	O1D-CGD-O2D-CED
30	B	623	DGD	C7B-C8B-C9B-CAB
30	H	102	DGD	CCA-CDA-CEA-CFA
22	C	510	CLA	C2-C3-C5-C6
27	d	409	LMG	C10-C11-C12-C13
30	C	517	DGD	C3B-C4B-C5B-C6B
32	M	104	STE	C11-C10-C9-C8
22	B	615	CLA	C15-C16-C17-C18
22	c	503	CLA	C13-C15-C16-C17
29	a	413	SQD	C11-C10-C9-C8
29	A	412	SQD	C13-C14-C15-C16
32	b	624	STE	C9-C10-C11-C12
27	D	410	LMG	C10-C11-C12-C13
28	L	102	LHG	C32-C33-C34-C35
29	F	102	SQD	C25-C26-C27-C28
32	b	624	STE	C11-C10-C9-C8
27	a	414	LMG	C4-C5-C6-O5
24	T	101	BCR	C13-C14-C15-C16
24	x	101	BCR	C9-C10-C11-C12
27	b	622	LMG	C13-C14-C15-C16
28	d	407	LHG	C35-C36-C37-C38
29	a	412	SQD	C30-C31-C32-C33
29	a	412	SQD	C31-C32-C33-C34
32	B	620	STE	C6-C7-C8-C9
32	M	103	STE	C7-C8-C9-C10
27	D	411	LMG	C12-C13-C14-C15
30	A	414	DGD	CEB-CFB-CGB-CHB
32	D	412	STE	C2-C3-C4-C5
22	c	509	CLA	CAA-CBA-CGA-O2A
22	C	513	CLA	C16-C17-C18-C19
22	D	404	CLA	C16-C17-C18-C20
22	D	405	CLA	CBA-CGA-O2A-C1
27	D	408	LMG	C12-C13-C14-C15
27	A	410	LMG	O1-C7-C8-C9
29	B	622	SQD	O6-C44-C45-C46
29	a	412	SQD	C44-C45-C46-O48
29	a	413	SQD	C44-C45-C46-O48
30	A	414	DGD	O1G-C1G-C2G-C3G
30	A	414	DGD	C1G-C2G-C3G-O3G
28	b	623	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C27-C28-C29-C30
27	A	410	LMG	C19-C20-C21-C22
27	a	414	LMG	C16-C17-C18-C19
28	E	101	LHG	C19-C20-C21-C22
32	D	412	STE	C5-C6-C7-C8
32	t	102	STE	C2-C3-C4-C5
32	x	102	STE	C14-C15-C16-C17
22	C	513	CLA	O2A-C1-C2-C3
22	c	508	CLA	C16-C17-C18-C19
27	A	410	LMG	C14-C15-C16-C17
29	L	101	SQD	C29-C30-C31-C32
22	c	513	CLA	C16-C17-C18-C19
22	c	504	CLA	C2-C3-C5-C6
27	D	411	LMG	C16-C17-C18-C19
28	l	101	LHG	C30-C31-C32-C33
29	L	101	SQD	C17-C18-C19-C20
32	B	620	STE	C4-C5-C6-C7
28	d	406	LHG	O1-C1-C2-O2
22	B	606	CLA	C13-C15-C16-C17
27	a	414	LMG	C14-C15-C16-C17
27	d	409	LMG	C34-C35-C36-C37
28	B	621	LHG	C27-C28-C29-C30
30	H	102	DGD	C9A-CAA-CBA-CCA
27	M	101	LMG	O10-C28-O8-C9
28	e	102	LHG	C7-C8-C9-C10
22	B	610	CLA	C16-C17-C18-C19
28	D	409	LHG	C32-C33-C34-C35
28	l	101	LHG	C35-C36-C37-C38
30	H	102	DGD	CDB-CEB-CFB-CGB
30	B	623	DGD	CBB-CCB-CDB-CEB
27	M	101	LMG	O7-C8-C9-O8
27	c	520	LMG	O1-C7-C8-O7
27	c	520	LMG	O7-C8-C9-O8
28	e	102	LHG	O7-C5-C6-O8
32	B	624	STE	C3-C4-C5-C6
22	B	613	CLA	C16-C17-C18-C19
22	b	610	CLA	C16-C17-C18-C20
27	D	408	LMG	C21-C22-C23-C24
28	E	101	LHG	C16-C17-C18-C19
28	A	411	LHG	C11-C10-C9-C8
22	B	613	CLA	C2-C1-O2A-CGA
22	C	512	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	d	402	CLA	C2-C1-O2A-CGA
32	c	519	STE	C11-C10-C9-C8
22	C	511	CLA	C6-C7-C8-C9
22	a	411	CLA	C11-C12-C13-C14
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C10-C8-C9
22	c	504	CLA	C6-C7-C8-C9
22	c	507	CLA	C14-C13-C15-C16
30	H	102	DGD	C9B-CAB-CBB-CCB
30	c	515	DGD	C2A-C3A-C4A-C5A
32	M	104	STE	C7-C8-C9-C10
30	A	414	DGD	C7B-C8B-C9B-CAB
32	d	410	STE	C11-C10-C9-C8
22	A	403	CLA	C8-C10-C11-C12
28	d	407	LHG	C2-C3-O3-P
28	E	101	LHG	C31-C32-C33-C34
29	A	412	SQD	C30-C31-C32-C33
32	B	625	STE	C11-C12-C13-C14
32	b	624	STE	C6-C7-C8-C9
22	B	611	CLA	C16-C17-C18-C20
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
24	K	101	BCR	C23-C24-C25-C26
24	k	101	BCR	C23-C24-C25-C26
24	k	101	BCR	C23-C24-C25-C30
24	k	103	BCR	C23-C24-C25-C26
24	k	103	BCR	C23-C24-C25-C30
24	t	101	BCR	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
27	m	101	LMG	C13-C14-C15-C16
32	B	626	STE	C6-C7-C8-C9
24	T	101	BCR	C7-C8-C9-C10
24	b	619	BCR	C21-C22-C23-C24
30	c	517	DGD	O6D-C5D-C6D-O5D
24	B	617	BCR	C14-C15-C16-C17
30	C	517	DGD	C9B-CAB-CBB-CCB
32	D	412	STE	C9-C10-C11-C12
32	l	102	STE	C4-C5-C6-C7
22	C	512	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	O1D-CGD-O2D-CED
32	b	621	STE	C12-C13-C14-C15
29	a	412	SQD	C23-C24-C25-C26
28	A	411	LHG	C15-C16-C17-C18
28	l	101	LHG	C34-C35-C36-C37
30	A	414	DGD	CDA-CEA-CFA-CGA
30	A	414	DGD	CEA-CFA-CGA-CHA
32	B	620	STE	C2-C3-C4-C5
32	H	103	STE	C11-C10-C9-C8
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	613	CLA	C6-C7-C8-C10
22	B	614	CLA	C6-C7-C8-C10
22	B	616	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	C	512	CLA	C6-C7-C8-C10
22	C	512	CLA	C12-C13-C15-C16
22	a	411	CLA	C11-C12-C13-C15
22	b	601	CLA	C11-C10-C8-C7
22	b	601	CLA	C12-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C10-C8-C7
22	c	513	CLA	C11-C12-C13-C15
22	B	615	CLA	C3-C5-C6-C7
28	d	406	LHG	C33-C34-C35-C36
32	t	102	STE	C3-C4-C5-C6
22	D	404	CLA	C16-C17-C18-C19
27	c	518	LMG	C29-C28-O8-C9
28	b	623	LHG	C34-C35-C36-C37
22	b	610	CLA	C15-C16-C17-C18
22	b	601	CLA	C2A-CAA-CBA-CGA
27	D	408	LMG	C17-C18-C19-C20
24	A	406	BCR	C11-C10-C9-C34
24	A	406	BCR	C16-C17-C18-C36
24	B	618	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
24	k	102	BCR	C35-C13-C14-C15
27	D	408	LMG	C14-C15-C16-C17
28	A	411	LHG	C10-C11-C12-C13
22	B	602	CLA	C3-C5-C6-C7
27	c	520	LMG	C15-C16-C17-C18
29	B	622	SQD	C17-C18-C19-C20
22	C	513	CLA	C8-C10-C11-C12
27	A	410	LMG	C35-C36-C37-C38
29	f	101	SQD	C28-C29-C30-C31
27	d	408	LMG	C33-C34-C35-C36
22	B	603	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	c	512	CLA	CAD-CBD-CGD-O2D
27	b	622	LMG	C9-C8-O7-C10
29	B	622	SQD	C46-C45-O47-C7
27	c	518	LMG	C35-C36-C37-C38
28	l	101	LHG	C10-C11-C12-C13
29	A	413	SQD	C10-C11-C12-C13
30	C	517	DGD	CAA-CBA-CCA-CDA
30	C	517	DGD	CBA-CCA-CDA-CEA
22	B	613	CLA	C15-C16-C17-C18
22	b	603	CLA	C13-C15-C16-C17
28	A	411	LHG	C9-C10-C11-C12
29	L	101	SQD	C9-C10-C11-C12
24	b	619	BCR	C22-C23-C24-C25
24	k	103	BCR	C22-C23-C24-C25
22	c	504	CLA	C11-C12-C13-C15
30	c	516	DGD	C5B-C6B-C7B-C8B
22	c	503	CLA	C15-C16-C17-C18
22	b	612	CLA	C2C-C3C-CAC-CBC
27	c	520	LMG	C7-C8-C9-O8
30	c	515	DGD	O1G-C1G-C2G-C3G
22	D	405	CLA	O1A-CGA-O2A-C1
30	A	414	DGD	O1A-C1A-O1G-C1G
29	A	412	SQD	C17-C18-C19-C20
28	A	411	LHG	O6-C4-C5-O7
28	l	101	LHG	O6-C4-C5-O7
22	b	605	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	602	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C40-C41-C42-C43
28	L	102	LHG	C29-C30-C31-C32
22	b	608	CLA	C16-C17-C18-C19
28	b	623	LHG	O9-C7-O7-C5
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	C	504	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O1D
22	c	504	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
22	b	606	CLA	C8-C10-C11-C12
32	H	103	STE	C15-C16-C17-C18
24	T	101	BCR	C20-C21-C22-C23
24	Z	101	BCR	C16-C17-C18-C19
30	c	515	DGD	C2E-C1E-O5D-C6D
22	C	505	CLA	C15-C16-C17-C18
28	d	407	LHG	C26-C27-C28-C29
30	A	414	DGD	O1G-C1G-C2G-O2G
30	c	515	DGD	O1G-C1G-C2G-O2G
29	L	101	SQD	C13-C14-C15-C16
30	B	623	DGD	C8B-C9B-CAB-CBB
32	B	625	STE	C10-C11-C12-C13
32	l	102	STE	C11-C10-C9-C8
30	H	102	DGD	CCB-CDB-CEB-CFB
32	b	621	STE	C4-C5-C6-C7
26	A	409	PL9	C12-C11-C9-C10
27	m	101	LMG	C32-C33-C34-C35
30	H	102	DGD	C4A-C5A-C6A-C7A
26	a	410	PL9	C4-C3-C7-C8
28	d	406	LHG	O9-C7-O7-C5
22	B	605	CLA	C10-C11-C12-C13
22	B	616	CLA	C6-C7-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C14-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C9
22	c	513	CLA	C11-C12-C13-C14
28	B	621	LHG	C13-C14-C15-C16
22	B	602	CLA	C8-C10-C11-C12
22	b	602	CLA	C3-C5-C6-C7
32	B	620	STE	C11-C12-C13-C14
24	K	101	BCR	C11-C12-C13-C35
24	b	617	BCR	C7-C8-C9-C34
27	D	410	LMG	C37-C38-C39-C40
30	C	516	DGD	CDB-CEB-CFB-CGB
22	C	508	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C1A-C2A-CAA-CBA
22	b	611	CLA	C1A-C2A-CAA-CBA
29	B	622	SQD	C23-C24-C25-C26
22	b	601	CLA	CBA-CGA-O2A-C1
29	a	413	SQD	C31-C32-C33-C34
24	Z	101	BCR	C15-C16-C17-C18
24	k	102	BCR	C19-C20-C21-C22
22	B	614	CLA	C15-C16-C17-C18
28	E	101	LHG	C4-O6-P-O3
28	d	407	LHG	C4-O6-P-O3
27	d	409	LMG	C14-C15-C16-C17
28	b	623	LHG	C12-C13-C14-C15
27	D	408	LMG	C38-C39-C40-C41
32	C	520	STE	C2-C3-C4-C5
32	b	625	STE	C6-C7-C8-C9
28	A	411	LHG	C2-C3-O3-P
22	B	604	CLA	O1D-CGD-O2D-CED
29	B	622	SQD	C9-C10-C11-C12
22	b	601	CLA	O1A-CGA-O2A-C1
28	d	406	LHG	C3-O3-P-O4
28	e	102	LHG	C3-O3-P-O4
32	B	627	STE	C3-C4-C5-C6
32	M	104	STE	C5-C6-C7-C8
30	C	516	DGD	O6D-C1D-O3G-C3G
22	C	501	CLA	CBA-CGA-O2A-C1
28	A	411	LHG	O6-C4-C5-C6
28	A	411	LHG	C16-C17-C18-C19
22	c	504	CLA	C8-C10-C11-C12
22	C	501	CLA	C2A-CAA-CBA-CGA
27	M	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	c	520	LMG	C38-C39-C40-C41
22	C	513	CLA	C16-C17-C18-C20
27	M	101	LMG	C15-C16-C17-C18
32	b	624	STE	C5-C6-C7-C8
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	513	CLA	CAD-CBD-CGD-O1D
29	a	412	SQD	C5-C6-S-O9
32	B	625	STE	C2-C3-C4-C5
22	A	405	CLA	C6-C7-C8-C9
27	C	518	LMG	C38-C39-C40-C41
30	C	517	DGD	C6B-C7B-C8B-C9B
28	A	411	LHG	C1-C2-C3-O3
32	C	520	STE	C11-C12-C13-C14
22	c	510	CLA	C16-C17-C18-C19
22	B	601	CLA	C4-C3-C5-C6
23	a	404	PHO	C4-C3-C5-C6
22	A	403	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	D	403	CLA	C6-C7-C8-C10
22	a	403	CLA	C12-C13-C15-C16
22	b	604	CLA	C11-C12-C13-C15
22	b	605	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C10-C8-C7
22	c	506	CLA	C6-C7-C8-C10
22	c	507	CLA	C6-C7-C8-C10
23	a	404	PHO	C6-C7-C8-C10
27	A	410	LMG	C28-C29-C30-C31
28	E	101	LHG	O6-C4-C5-O7
32	E	102	STE	C2-C3-C4-C5
32	b	620	STE	C5-C6-C7-C8
28	D	409	LHG	C25-C26-C27-C28
24	b	619	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C34-C35-C36-C37
22	a	403	CLA	C13-C15-C16-C17
30	h	101	DGD	O1A-C1A-O1G-C1G
30	A	414	DGD	CBB-CCB-CDB-CEB
32	c	519	STE	C7-C8-C9-C10
22	B	605	CLA	C8-C10-C11-C12
27	b	622	LMG	C17-C18-C19-C20
29	a	413	SQD	C26-C27-C28-C29
27	C	518	LMG	O1-C7-C8-O7
27	b	622	LMG	O1-C7-C8-O7
27	m	101	LMG	O7-C8-C9-O8
28	E	101	LHG	C18-C19-C20-C21
30	c	517	DGD	CCB-CDB-CEB-CFB
32	I	101	STE	C5-C6-C7-C8
22	C	501	CLA	O1A-CGA-O2A-C1
27	c	520	LMG	C41-C42-C43-C44
30	B	623	DGD	CDA-CEA-CFA-CGA
22	B	601	CLA	C13-C15-C16-C17
22	B	613	CLA	C5-C6-C7-C8
22	a	411	CLA	C8-C10-C11-C12
30	c	517	DGD	CDA-CEA-CFA-CGA
28	E	101	LHG	O10-C23-O8-C6
28	D	409	LHG	C33-C34-C35-C36
29	a	413	SQD	C16-C17-C18-C19
27	A	410	LMG	C39-C40-C41-C42
32	M	104	STE	C2-C3-C4-C5
32	t	103	STE	C7-C8-C9-C10
22	B	603	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	a	402	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	x	101	BCR	C6-C7-C8-C9
30	C	515	DGD	O1A-C1A-O1G-C1G
28	b	623	LHG	C28-C29-C30-C31
32	C	519	STE	C5-C6-C7-C8
27	m	101	LMG	O6-C1-O1-C7
27	a	414	LMG	C36-C37-C38-C39
32	B	624	STE	C7-C8-C9-C10
28	B	621	LHG	C24-C25-C26-C27
28	L	102	LHG	O10-C23-O8-C6
32	m	102	STE	C3-C4-C5-C6
28	d	406	LHG	C31-C32-C33-C34
22	B	603	CLA	C10-C11-C12-C13
27	m	101	LMG	C12-C13-C14-C15
30	H	102	DGD	C8A-C9A-CAA-CBA
30	h	101	DGD	C2A-C3A-C4A-C5A
30	h	101	DGD	O2G-C1B-C2B-C3B
30	C	515	DGD	C3B-C4B-C5B-C6B
22	B	608	CLA	C5-C6-C7-C8
22	c	509	CLA	C13-C15-C16-C17
22	B	611	CLA	C16-C17-C18-C19
30	c	516	DGD	C9A-CAA-CBA-CCA
28	l	101	LHG	C28-C29-C30-C31
30	C	515	DGD	O6D-C5D-C6D-O5D
22	B	605	CLA	C3-C5-C6-C7
30	c	516	DGD	C8A-C9A-CAA-CBA
32	B	627	STE	C6-C7-C8-C9
27	D	410	LMG	C9-C8-O7-C10
30	B	623	DGD	C3G-C2G-O2G-C1B
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	509	CLA	C2A-CAA-CBA-CGA
28	e	102	LHG	C25-C26-C27-C28
22	A	402	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
28	e	102	LHG	C27-C28-C29-C30
29	a	413	SQD	C10-C11-C12-C13
30	c	516	DGD	C7B-C8B-C9B-CAB
22	C	507	CLA	C16-C17-C18-C20
28	A	411	LHG	C31-C32-C33-C34
28	b	623	LHG	C14-C15-C16-C17
29	F	102	SQD	C30-C31-C32-C33
30	H	102	DGD	O2G-C1B-C2B-C3B
32	b	626	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	C13-C15-C16-C17
28	B	621	LHG	C16-C17-C18-C19
27	D	410	LMG	C29-C30-C31-C32
30	H	102	DGD	C5B-C6B-C7B-C8B
22	d	403	CLA	C16-C17-C18-C19
28	L	102	LHG	C30-C31-C32-C33
29	L	101	SQD	C26-C27-C28-C29
32	d	410	STE	C2-C3-C4-C5
24	k	102	BCR	C23-C24-C25-C30
24	k	103	BCR	C1-C6-C7-C8
24	k	103	BCR	C5-C6-C7-C8
22	B	601	CLA	C2-C3-C5-C6
28	L	102	LHG	C24-C25-C26-C27
28	e	102	LHG	C18-C19-C20-C21
22	C	507	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C20
30	C	515	DGD	C4D-C5D-C6D-O5D
27	d	409	LMG	C37-C38-C39-C40
30	c	517	DGD	C7B-C8B-C9B-CAB
24	B	617	BCR	C20-C21-C22-C23
24	B	619	BCR	C20-C21-C22-C23
24	H	101	BCR	C20-C21-C22-C23
24	Z	101	BCR	C11-C10-C9-C8
27	d	409	LMG	C15-C16-C17-C18
27	D	410	LMG	C30-C31-C32-C33
32	l	102	STE	C6-C7-C8-C9
28	d	406	LHG	C3-O3-P-O6
32	l	102	STE	C10-C11-C12-C13
27	D	411	LMG	C32-C33-C34-C35
28	L	102	LHG	C11-C12-C13-C14
27	b	622	LMG	O1-C7-C8-C9
28	d	406	LHG	C32-C33-C34-C35
32	t	102	STE	C6-C7-C8-C9
22	B	606	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C15
22	a	402	CLA	C11-C10-C8-C7
22	a	405	CLA	C6-C7-C8-C10
22	b	604	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
32	c	519	STE	C11-C12-C13-C14
30	C	515	DGD	O1G-C1A-C2A-C3A

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C3-C5-C6-C7
22	B	603	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C12-C13-C14
22	a	403	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C12-C13-C14
22	b	611	CLA	C14-C13-C15-C16
32	I	101	STE	C7-C8-C9-C10
32	b	625	STE	C7-C8-C9-C10
22	d	402	CLA	C13-C15-C16-C17
27	b	622	LMG	C23-C24-C25-C26
27	d	408	LMG	C38-C39-C40-C41
29	L	101	SQD	C24-C25-C26-C27
29	B	622	SQD	C24-C25-C26-C27
22	C	506	CLA	C15-C16-C17-C18
22	B	609	CLA	C4-C3-C5-C6
23	a	404	PHO	C2-C3-C5-C6
28	b	623	LHG	C10-C11-C12-C13
22	b	610	CLA	C16-C17-C18-C19
22	A	405	CLA	CBA-CGA-O2A-C1
32	m	102	STE	C6-C7-C8-C9
24	B	619	BCR	C22-C23-C24-C25
27	c	520	LMG	C28-C29-C30-C31
24	H	101	BCR	C9-C10-C11-C12
24	T	101	BCR	C9-C10-C11-C12
24	Z	101	BCR	C13-C14-C15-C16
24	k	101	BCR	C9-C10-C11-C12
22	A	405	CLA	O1A-CGA-O2A-C1
27	C	518	LMG	C33-C34-C35-C36
27	d	409	LMG	C32-C33-C34-C35
32	I	101	STE	C3-C4-C5-C6
29	A	413	SQD	C27-C28-C29-C30
22	a	411	CLA	C13-C15-C16-C17
27	c	520	LMG	C37-C38-C39-C40
22	a	411	CLA	C16-C17-C18-C19
22	B	614	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
27	c	518	LMG	C38-C39-C40-C41
28	e	102	LHG	C2-C3-O3-P
28	A	411	LHG	C35-C36-C37-C38
30	c	515	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
29	a	412	SQD	C19-C20-C21-C22
30	c	516	DGD	C3A-C4A-C5A-C6A
23	a	404	PHO	C5-C6-C7-C8
22	B	614	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C12-C13-C14
22	c	503	CLA	C11-C10-C8-C9
22	c	510	CLA	C14-C13-C15-C16
27	D	408	LMG	C33-C34-C35-C36
27	c	518	LMG	C31-C32-C33-C34
32	D	412	STE	C14-C15-C16-C17
22	c	512	CLA	C8-C10-C11-C12
30	h	101	DGD	C5A-C6A-C7A-C8A
29	A	413	SQD	C29-C30-C31-C32
32	B	625	STE	C5-C6-C7-C8
24	T	101	BCR	C11-C10-C9-C34
24	Z	101	BCR	C20-C21-C22-C37
24	c	514	BCR	C20-C21-C22-C37
27	D	410	LMG	C7-C8-C9-O8
30	C	515	DGD	O1G-C1G-C2G-C3G
29	A	413	SQD	C25-C26-C27-C28
32	b	620	STE	C7-C8-C9-C10
27	M	101	LMG	C19-C20-C21-C22
22	c	505	CLA	C16-C17-C18-C20
22	D	405	CLA	O2A-C1-C2-C3
22	C	512	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	C15-C16-C17-C18
22	B	607	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C1A-C2A-CAA-CBA
23	d	401	PHO	C1A-C2A-CAA-CBA
27	d	409	LMG	C40-C41-C42-C43
22	B	602	CLA	C6-C7-C8-C10
22	C	513	CLA	C12-C13-C15-C16
22	D	405	CLA	C6-C7-C8-C10
22	b	615	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C12-C13-C15
22	c	512	CLA	C12-C13-C15-C16
29	A	412	SQD	C7-C8-C9-C10
27	D	408	LMG	C11-C12-C13-C14
30	H	102	DGD	CDA-CEA-CFA-CGA
32	j	101	STE	C3-C4-C5-C6
22	C	512	CLA	O1A-CGA-O2A-C1
23	D	401	PHO	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	b	610	CLA	C2A-CAA-CBA-CGA
22	b	615	CLA	C8-C10-C11-C12
28	l	101	LHG	C13-C14-C15-C16
29	F	102	SQD	C34-C35-C36-C37
29	L	101	SQD	C28-C29-C30-C31
30	C	517	DGD	C6A-C7A-C8A-C9A
22	A	402	CLA	C15-C16-C17-C18
27	c	518	LMG	C40-C41-C42-C43
29	A	413	SQD	C11-C10-C9-C8
32	l	102	STE	C15-C16-C17-C18
32	B	625	STE	C6-C7-C8-C9
22	B	603	CLA	C16-C17-C18-C19
30	c	517	DGD	C9B-CAB-CBB-CCB
22	B	604	CLA	C10-C11-C12-C13
27	D	411	LMG	C34-C35-C36-C37
22	b	603	CLA	C15-C16-C17-C18
22	B	604	CLA	O1A-CGA-O2A-C1
29	A	413	SQD	C7-C8-C9-C10
22	c	511	CLA	C16-C17-C18-C19
32	t	103	STE	C5-C6-C7-C8
22	d	402	CLA	C15-C16-C17-C18
27	D	411	LMG	C35-C36-C37-C38
30	C	515	DGD	CDA-CEA-CFA-CGA
22	B	612	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C28-C29-C30-C31
27	b	622	LMG	C10-C11-C12-C13
24	k	103	BCR	C19-C20-C21-C22
22	b	605	CLA	C5-C6-C7-C8
30	h	101	DGD	C7A-C8A-C9A-CAA
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C39-C41-C42-C43
22	c	513	CLA	C3-C5-C6-C7
22	B	601	CLA	C2-C1-O2A-CGA
22	C	509	CLA	C2-C1-O2A-CGA
22	b	610	CLA	C2-C1-O2A-CGA
22	B	607	CLA	C11-C10-C8-C9
28	d	406	LHG	C9-C10-C11-C12
32	M	102	STE	C9-C10-C11-C12
32	M	104	STE	C12-C13-C14-C15
28	e	102	LHG	C14-C15-C16-C17
27	c	518	LMG	C33-C34-C35-C36
22	c	509	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C16-C17-C18-C20
32	B	624	STE	C5-C6-C7-C8
24	A	406	BCR	C23-C24-C25-C30
24	K	102	BCR	C1-C6-C7-C8
24	x	101	BCR	C23-C24-C25-C26
24	x	101	BCR	C23-C24-C25-C30
28	L	102	LHG	C9-C10-C11-C12
30	C	515	DGD	C6B-C7B-C8B-C9B
32	I	101	STE	C10-C11-C12-C13
22	c	508	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
24	d	404	BCR	C7-C8-C9-C10
22	B	609	CLA	C2-C3-C5-C6
22	B	612	CLA	CBD-CGD-O2D-CED
30	C	516	DGD	C5D-C6D-O5D-C1E
22	B	612	CLA	O1D-CGD-O2D-CED
27	c	520	LMG	C29-C30-C31-C32
22	C	508	CLA	C5-C6-C7-C8
22	c	512	CLA	C15-C16-C17-C18
22	B	601	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	CBA-CGA-O2A-C1
32	d	410	STE	C3-C4-C5-C6
28	d	406	LHG	C30-C31-C32-C33
22	a	405	CLA	C15-C16-C17-C18
27	D	408	LMG	C13-C14-C15-C16
27	a	414	LMG	C39-C40-C41-C42
22	C	512	CLA	C4-C3-C5-C6
27	D	410	LMG	C16-C17-C18-C19
22	A	403	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C10-C8-C7
22	C	507	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
32	j	101	STE	C7-C8-C9-C10
22	B	612	CLA	O1A-CGA-O2A-C1
22	c	509	CLA	CAA-CBA-CGA-O1A
24	K	102	BCR	C9-C10-C11-C12
22	b	612	CLA	CAA-CBA-CGA-O2A
30	C	516	DGD	C2D-C1D-O3G-C3G
29	L	101	SQD	O6-C44-C45-O47
29	L	101	SQD	O47-C45-C46-O48
30	c	516	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C3-C5-C6-C7
29	a	412	SQD	O47-C7-C8-C9
30	c	515	DGD	O1G-C1A-C2A-C3A
30	B	623	DGD	C2B-C3B-C4B-C5B
23	A	404	PHO	CBA-CGA-O2A-C1
22	b	610	CLA	C4C-C3C-CAC-CBC
29	f	101	SQD	C26-C27-C28-C29
22	C	513	CLA	C4-C3-C5-C6
26	d	405	PL9	C18-C19-C21-C22
28	E	101	LHG	O8-C23-C24-C25
27	D	408	LMG	C16-C17-C18-C19
22	A	403	CLA	C11-C12-C13-C14
22	C	504	CLA	C11-C10-C8-C9
22	D	403	CLA	C6-C7-C8-C9
22	D	405	CLA	C6-C7-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	c	506	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C12-C13-C14
23	a	404	PHO	C6-C7-C8-C9
29	A	412	SQD	C33-C34-C35-C36
23	d	401	PHO	C3A-C2A-CAA-CBA
27	m	101	LMG	O8-C28-C29-C30
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	616	CLA	CAD-CBD-CGD-O2D
22	C	508	CLA	CAD-CBD-CGD-O2D
22	D	405	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	c	503	CLA	CAD-CBD-CGD-O2D
27	A	410	LMG	C7-C8-O7-C10
30	B	623	DGD	C1G-C2G-O2G-C1B
22	C	502	CLA	CBA-CGA-O2A-C1
26	a	410	PL9	C21-C22-C23-C24
22	D	403	CLA	C3-C5-C6-C7
30	C	516	DGD	O1B-C1B-O2G-C2G
27	d	409	LMG	C35-C36-C37-C38
22	c	505	CLA	C5-C6-C7-C8
30	C	515	DGD	C8B-C9B-CAB-CBB
29	A	412	SQD	O47-C7-C8-C9
29	a	413	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
22	a	405	CLA	C4-C3-C5-C6
22	B	603	CLA	C16-C17-C18-C20
22	c	508	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	B	612	CLA	CAA-CBA-CGA-O2A
28	d	406	LHG	C16-C17-C18-C19
32	x	102	STE	C11-C10-C9-C8
24	H	101	BCR	C17-C18-C19-C20
23	d	401	PHO	C8-C10-C11-C12
22	A	402	CLA	C2C-C3C-CAC-CBC
22	a	411	CLA	C2C-C3C-CAC-CBC
22	b	606	CLA	C2C-C3C-CAC-CBC
22	b	608	CLA	C2C-C3C-CAC-CBC
22	b	616	CLA	C2C-C3C-CAC-CBC
22	c	502	CLA	C2C-C3C-CAC-CBC
22	d	402	CLA	C2C-C3C-CAC-CBC
27	m	101	LMG	C29-C30-C31-C32
32	b	626	STE	C4-C5-C6-C7
32	J	101	STE	C2-C3-C4-C5
27	c	518	LMG	C30-C31-C32-C33
22	b	613	CLA	O2A-C1-C2-C3
22	c	512	CLA	O2A-C1-C2-C3
23	a	404	PHO	O2A-C1-C2-C3
22	C	502	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	C6A-C7A-C8A-C9A
24	b	619	BCR	C14-C15-C16-C17
27	a	414	LMG	C35-C36-C37-C38
30	B	623	DGD	CFA-CGA-CHA-CIA
28	L	102	LHG	C7-C8-C9-C10
22	B	606	CLA	C10-C11-C12-C13
22	b	608	CLA	C16-C17-C18-C20
22	c	502	CLA	C16-C17-C18-C19
22	c	508	CLA	C15-C16-C17-C18
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	D	404	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	CHA-CBD-CGD-O2D
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	c	502	CLA	CHA-CBD-CGD-O2D
22	c	506	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	a	405	CLA	C2-C3-C5-C6
24	b	619	BCR	C16-C17-C18-C19
24	t	101	BCR	C20-C21-C22-C23
27	m	101	LMG	C35-C36-C37-C38
22	c	506	CLA	C10-C11-C12-C13
29	a	412	SQD	C8-C7-O47-C45
27	a	414	LMG	O6-C5-C6-O5
26	d	405	PL9	C30-C29-C31-C32
28	E	101	LHG	C17-C18-C19-C20
29	A	413	SQD	C28-C29-C30-C31
30	C	516	DGD	C5A-C6A-C7A-C8A
22	b	614	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	C11-C10-C8-C7
22	C	513	CLA	C2-C3-C5-C6
22	a	405	CLA	C12-C13-C15-C16
22	b	603	CLA	C12-C13-C15-C16
22	b	613	CLA	C6-C7-C8-C10
22	b	614	CLA	C12-C13-C15-C16
22	b	601	CLA	C16-C17-C18-C19
26	A	409	PL9	C4-C3-C7-C8
28	l	101	LHG	O7-C7-C8-C9
30	C	515	DGD	O2G-C1B-C2B-C3B
22	B	602	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	508	CLA	C11-C10-C8-C9
22	d	403	CLA	C6-C7-C8-C9
22	d	403	CLA	C14-C13-C15-C16
26	d	405	PL9	C44-C46-C47-C48
32	H	103	STE	C1-C2-C3-C4
29	a	412	SQD	C5-C6-S-O8
28	e	102	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C2A-CAA-CBA-CGA
26	A	409	PL9	C21-C22-C23-C24
26	d	405	PL9	C11-C12-C13-C14
32	b	621	STE	C11-C10-C9-C8
22	B	613	CLA	CAA-CBA-CGA-O2A
24	D	406	BCR	C7-C8-C9-C34
22	a	411	CLA	C16-C17-C18-C20
22	c	502	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C20
26	D	407	PL9	C45-C44-C46-C47
22	B	611	CLA	C2-C3-C5-C6
24	x	101	BCR	C7-C8-C9-C10
22	c	507	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	C1A-C2A-CAA-CBA
22	a	411	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
32	c	519	STE	C1-C2-C3-C4
32	d	410	STE	C1-C2-C3-C4
30	c	515	DGD	O1B-C1B-C2B-C3B
30	c	515	DGD	C7A-C8A-C9A-CAA
26	d	405	PL9	C46-C47-C48-C49
29	a	413	SQD	C24-C23-O48-C46
27	M	101	LMG	O10-C28-C29-C30
29	A	412	SQD	O49-C7-C8-C9
27	a	414	LMG	C15-C16-C17-C18
22	B	612	CLA	CAA-CBA-CGA-O1A
30	C	516	DGD	CAA-CBA-CCA-CDA
22	B	613	CLA	CAA-CBA-CGA-O1A
30	C	515	DGD	O1B-C1B-C2B-C3B
28	E	101	LHG	C4-O6-P-O5
28	L	102	LHG	C4-O6-P-O5
28	d	406	LHG	C4-O6-P-O5
28	d	407	LHG	C4-O6-P-O5
22	b	614	CLA	C16-C17-C18-C20
22	b	612	CLA	CAA-CBA-CGA-O1A
24	K	102	BCR	C5-C6-C7-C8
28	E	101	LHG	C34-C35-C36-C37
27	d	409	LMG	C30-C31-C32-C33
28	e	102	LHG	C10-C11-C12-C13
30	A	414	DGD	C6A-C7A-C8A-C9A
30	C	516	DGD	O2G-C1B-C2B-C3B
22	c	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C10-C11-C12-C13
30	C	516	DGD	O1B-C1B-C2B-C3B
29	A	413	SQD	C18-C19-C20-C21
22	B	605	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	B	609	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	a	403	CLA	CAD-CBD-CGD-O1D
27	C	518	LMG	O7-C10-C11-C12
22	C	511	CLA	C15-C16-C17-C18
30	C	517	DGD	O6D-C5D-C6D-O5D
22	B	609	CLA	C11-C10-C8-C9
22	B	610	CLA	C14-C13-C15-C16
22	B	614	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C12-C13-C14
22	c	512	CLA	C14-C13-C15-C16
29	A	412	SQD	C23-C24-C25-C26
22	b	614	CLA	CBA-CGA-O2A-C1
22	B	603	CLA	O1D-CGD-O2D-CED
27	D	411	LMG	C11-C12-C13-C14
22	B	610	CLA	C2A-CAA-CBA-CGA
27	A	410	LMG	C37-C38-C39-C40
28	L	102	LHG	O7-C7-C8-C9
28	e	102	LHG	O8-C23-C24-C25
32	C	520	STE	C5-C6-C7-C8
29	f	101	SQD	C23-C24-C25-C26
24	x	101	BCR	C11-C12-C13-C35
22	B	607	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C12-C13-C15
22	C	509	CLA	C11-C12-C13-C15
22	C	511	CLA	C12-C13-C15-C16
22	D	403	CLA	C11-C10-C8-C7
22	D	403	CLA	C12-C13-C15-C16
22	b	606	CLA	C12-C13-C15-C16
22	c	502	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
29	a	413	SQD	O10-C23-C24-C25
28	B	621	LHG	C32-C33-C34-C35
32	B	620	STE	C9-C10-C11-C12
22	b	613	CLA	CAA-CBA-CGA-O2A

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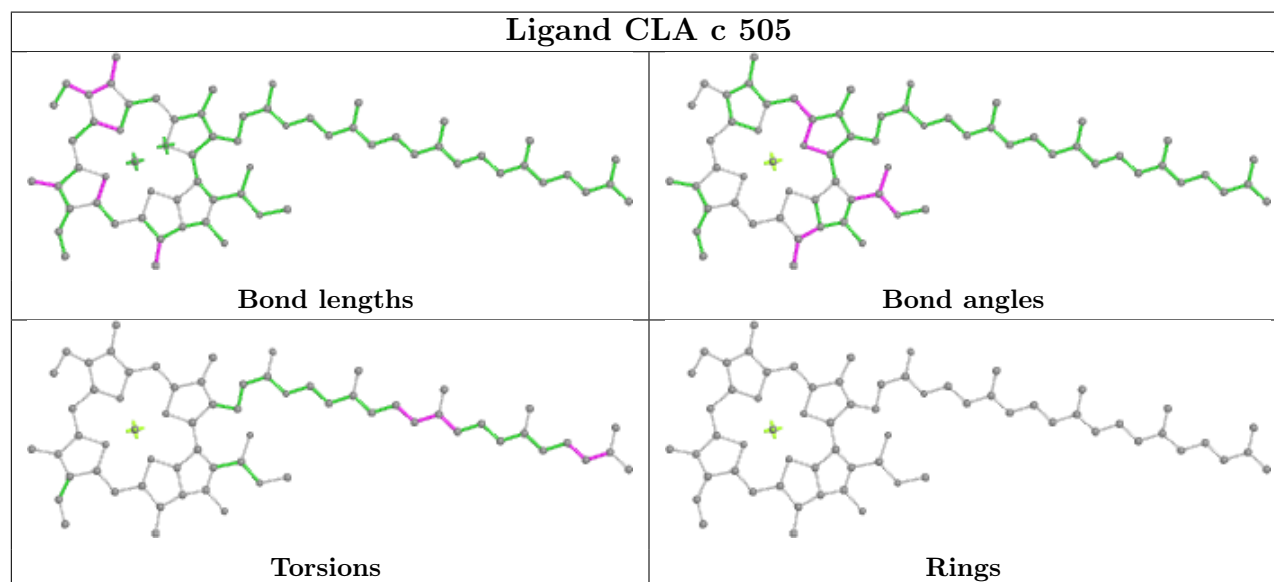
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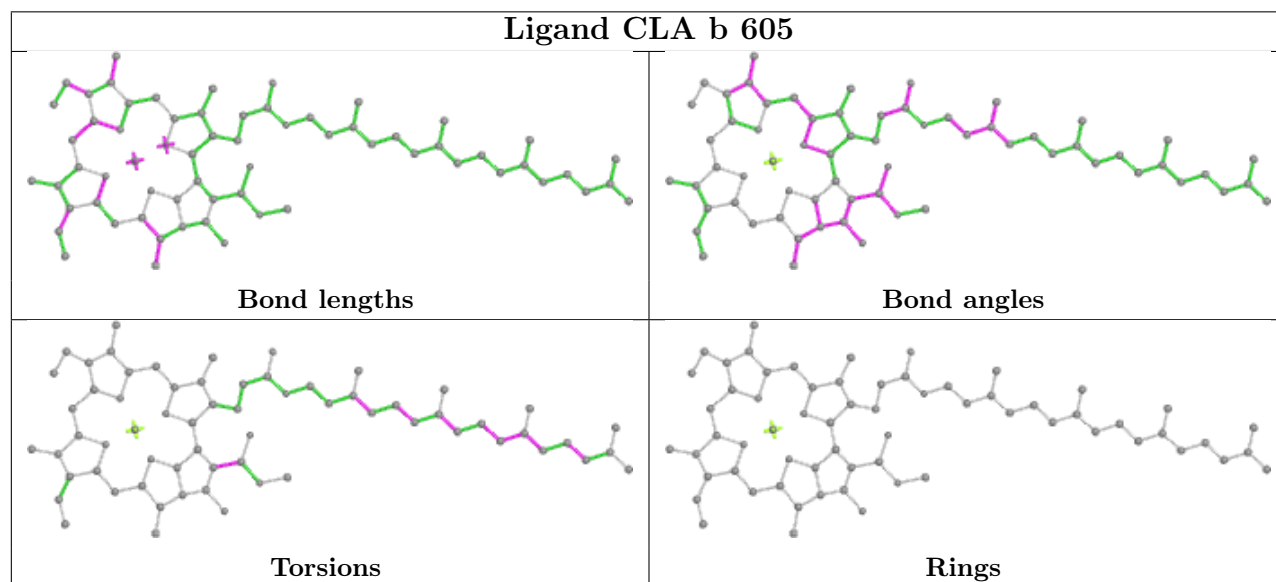
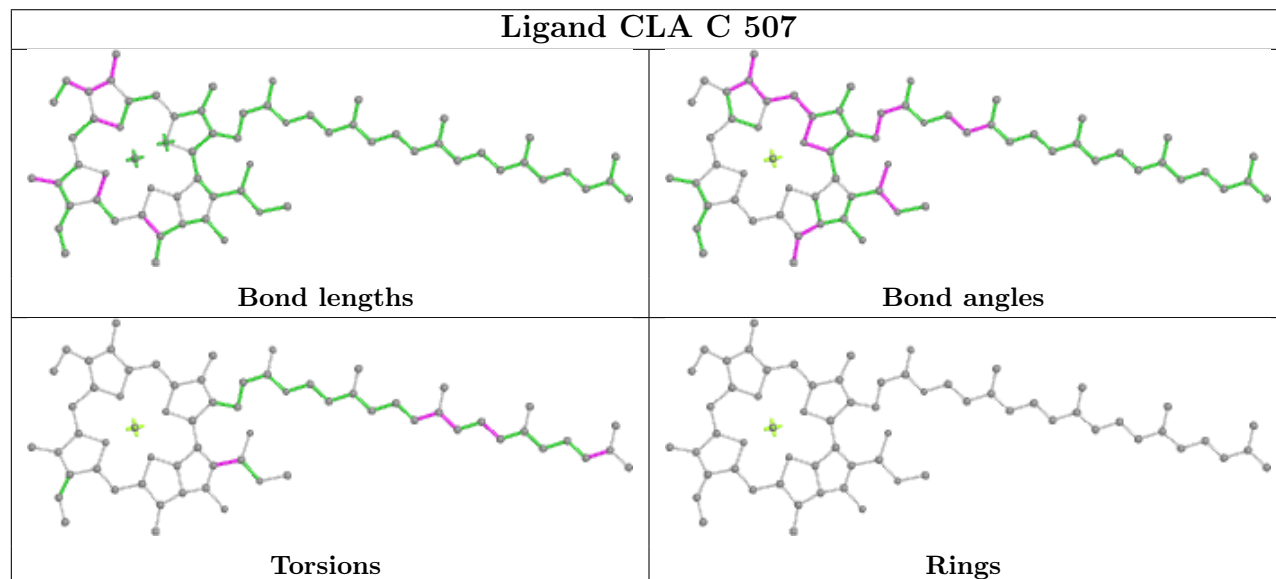
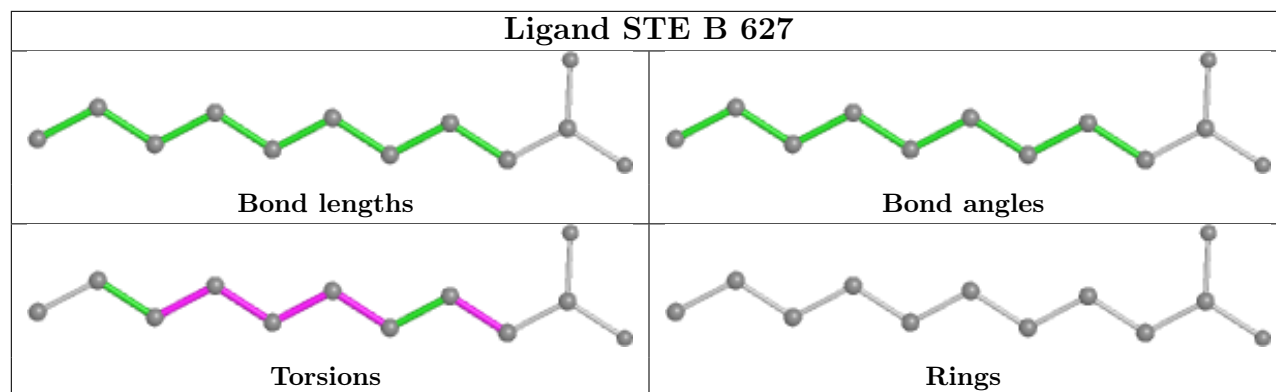
Mol	Chain	Res	Type	Atoms
30	C	515	DGD	C2B-C3B-C4B-C5B
32	c	519	STE	C10-C11-C12-C13
24	k	102	BCR	C7-C8-C9-C10
32	b	624	STE	C11-C12-C13-C14
22	d	403	CLA	C10-C11-C12-C13
30	c	516	DGD	O2G-C1B-C2B-C3B
27	c	518	LMG	C36-C37-C38-C39
22	b	616	CLA	C10-C11-C12-C13
30	c	516	DGD	O1B-C1B-C2B-C3B
27	m	101	LMG	C33-C34-C35-C36
32	B	624	STE	C2-C3-C4-C5

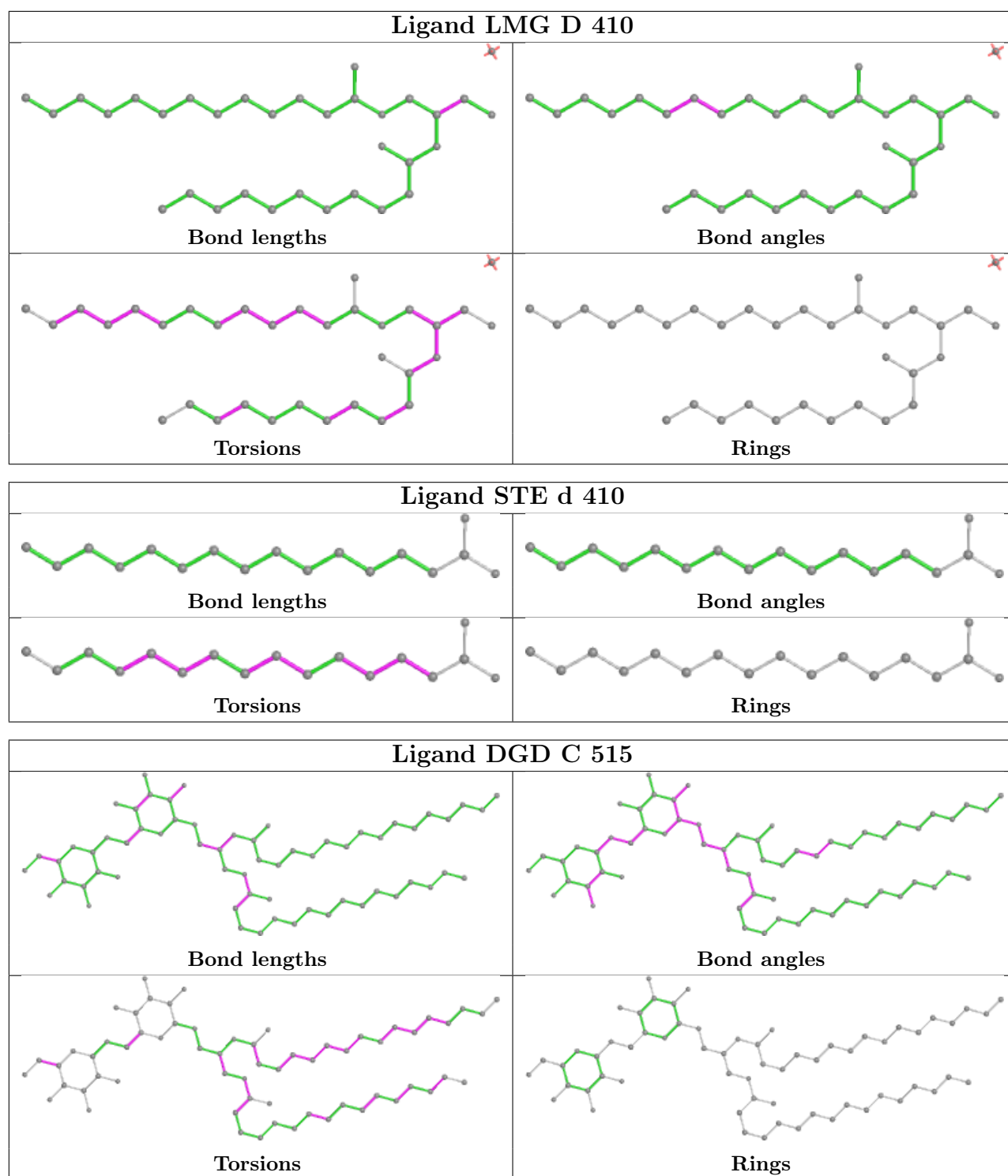
There are no ring outliers.

No monomer is involved in short contacts.

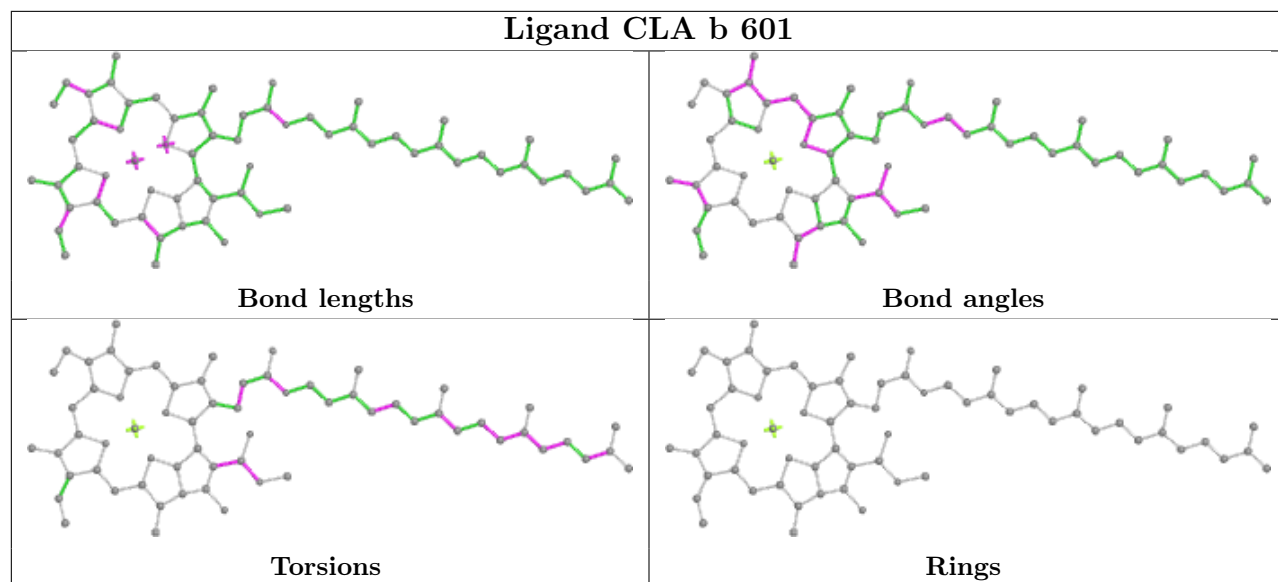
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



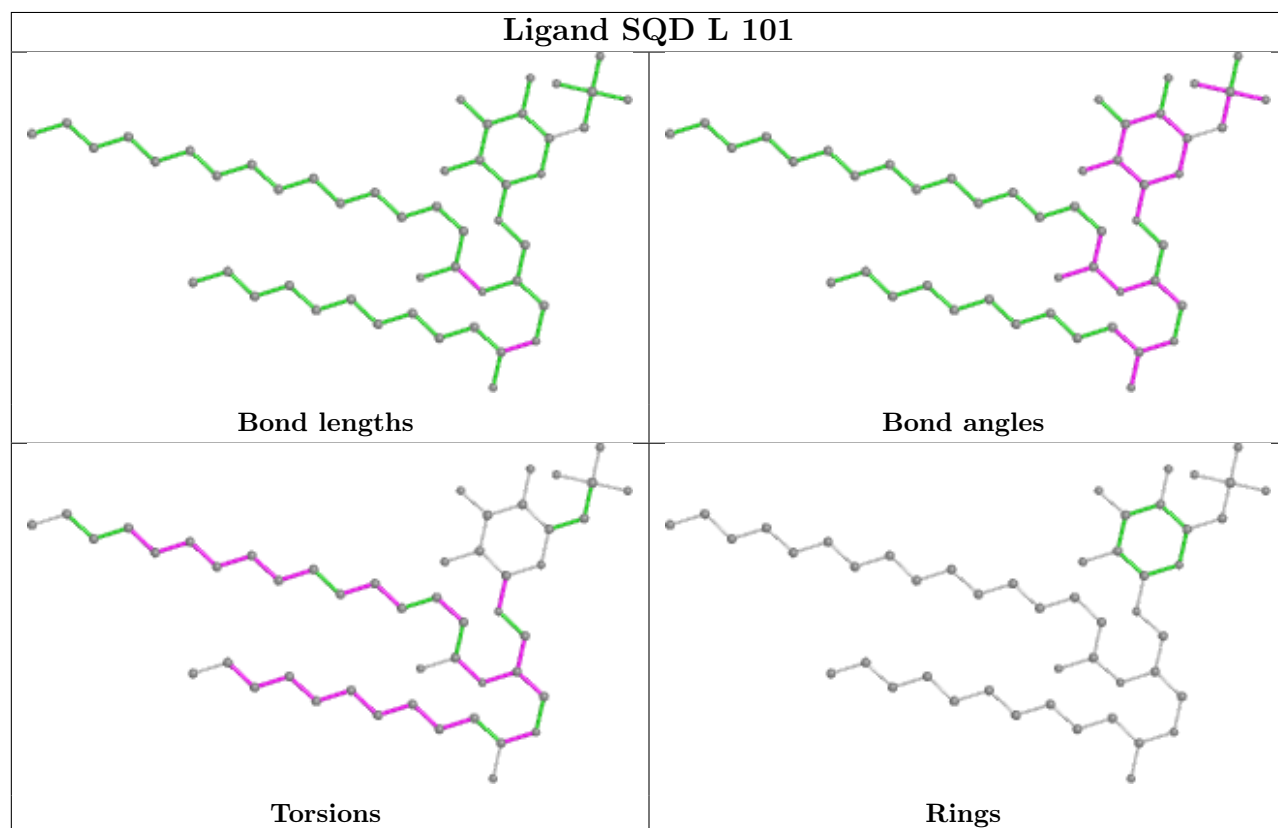


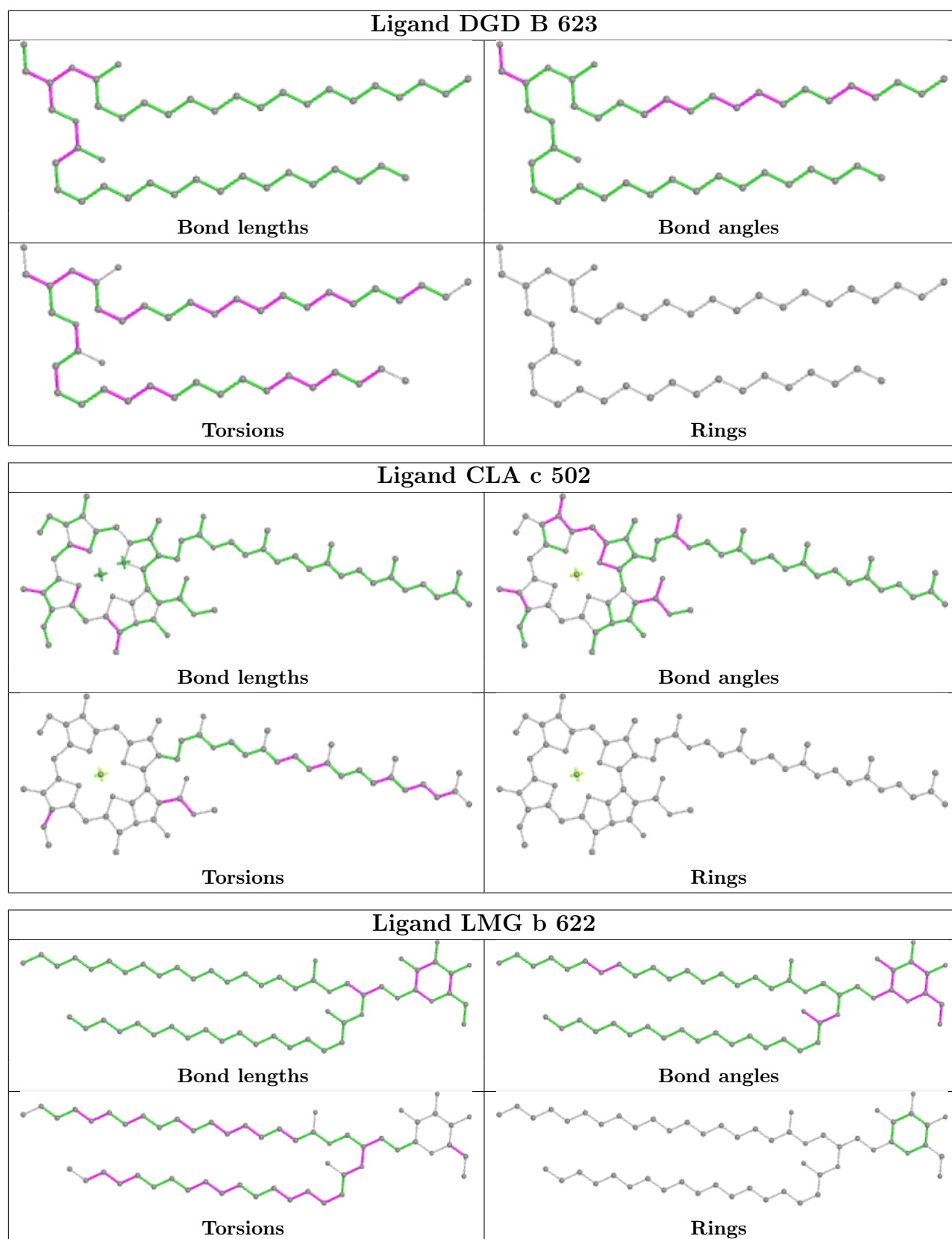


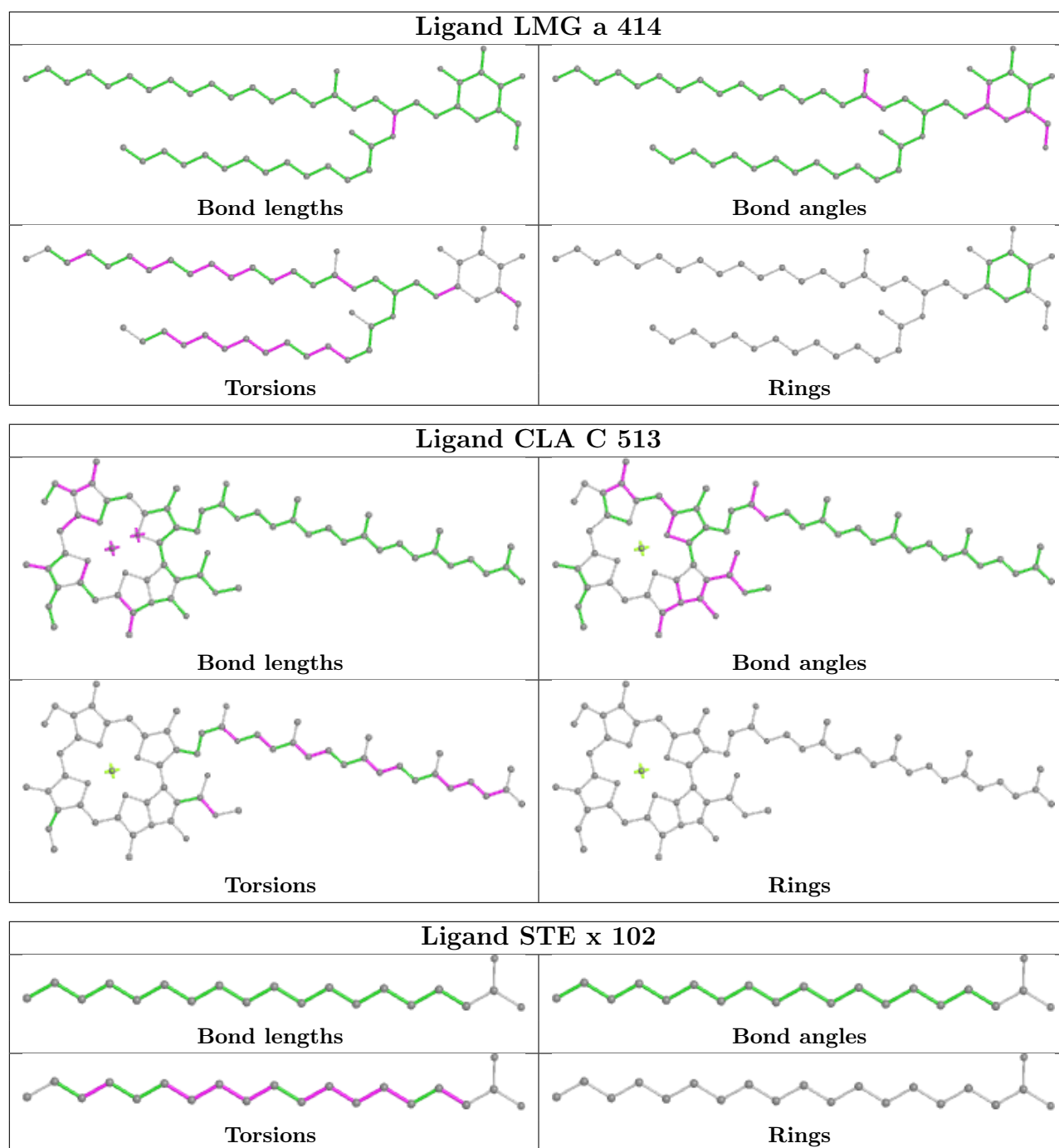
## Ligand CLA b 601



## Ligand SQD L 101

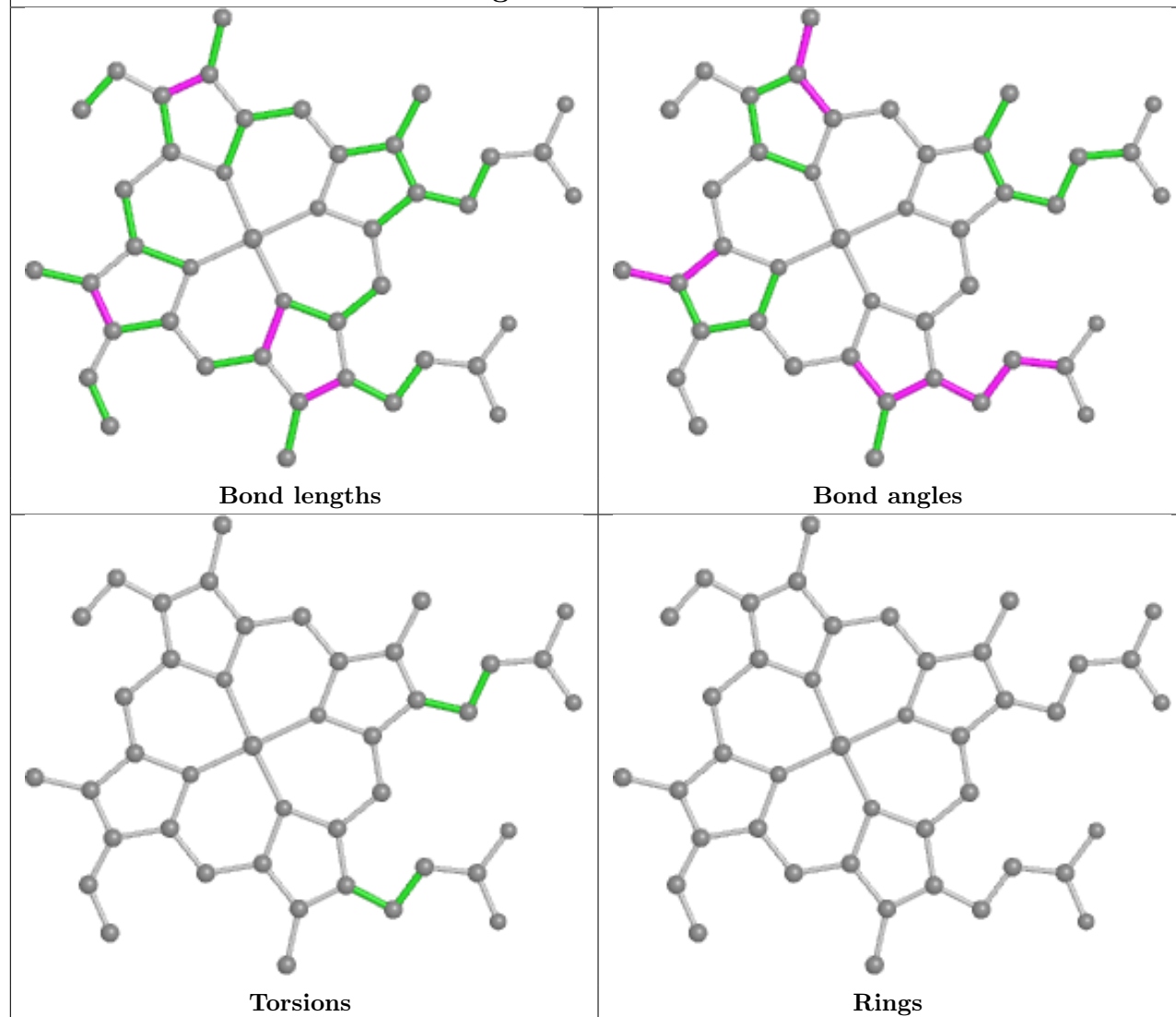




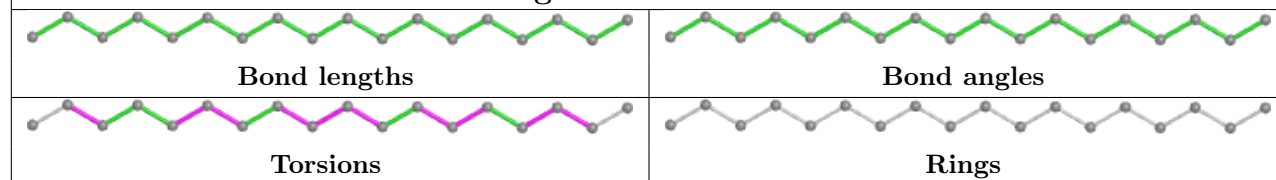




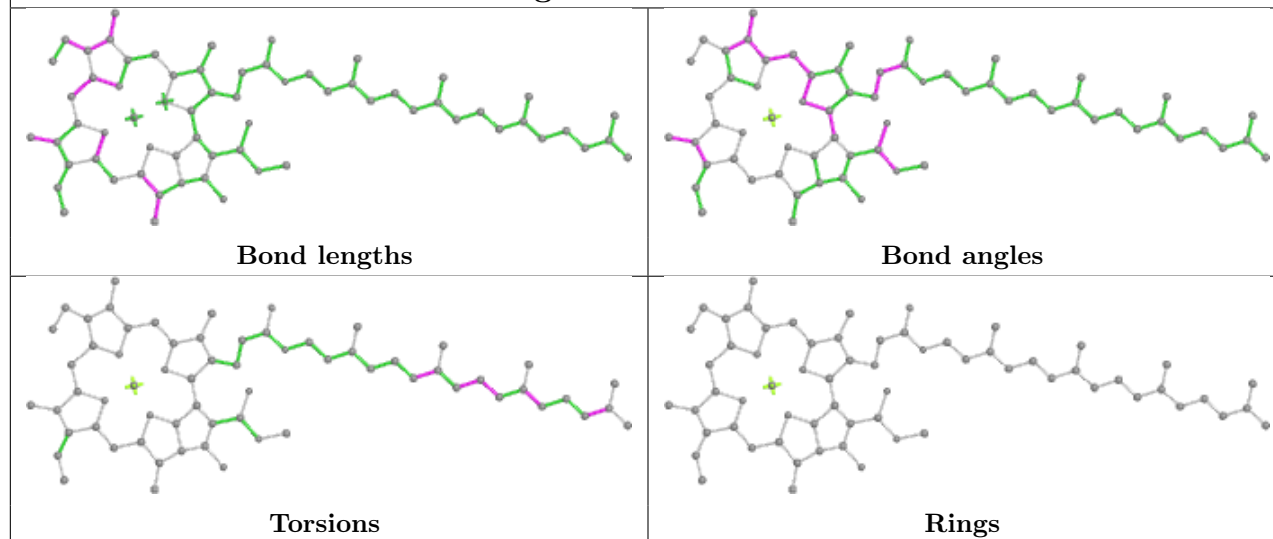
## Ligand HEC v 201



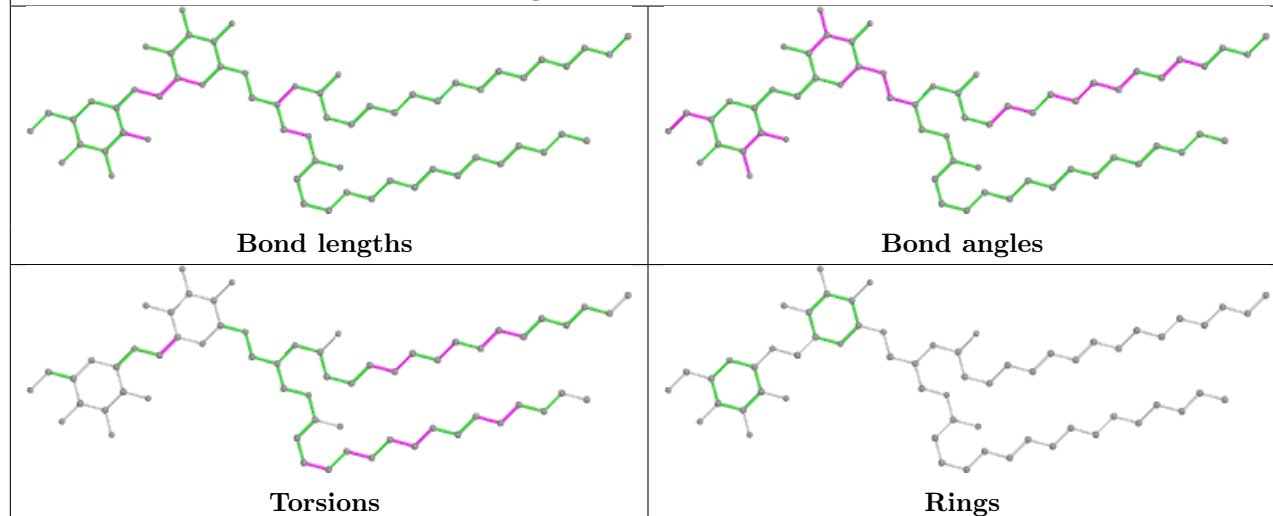
## Ligand STE H 103



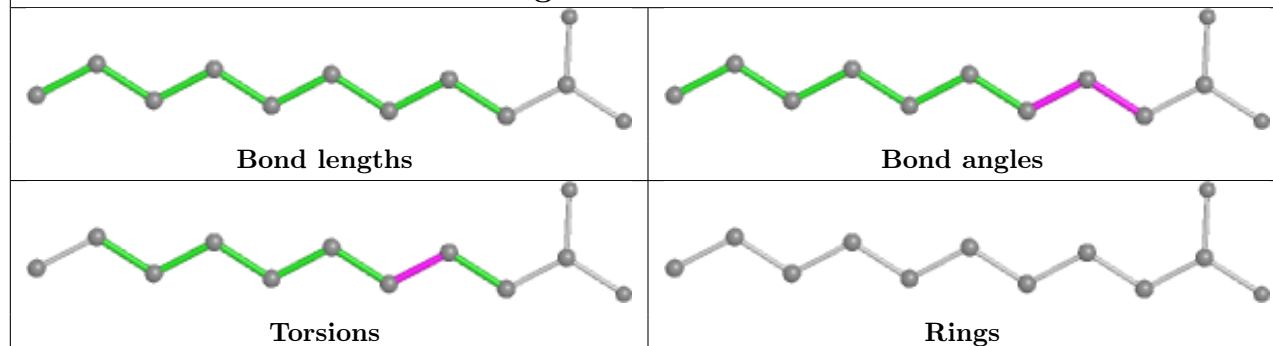
## Ligand CLA d 403

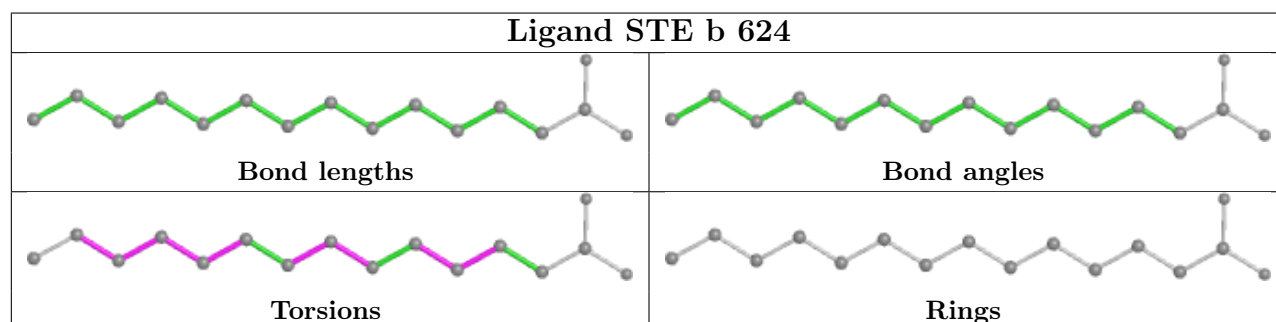
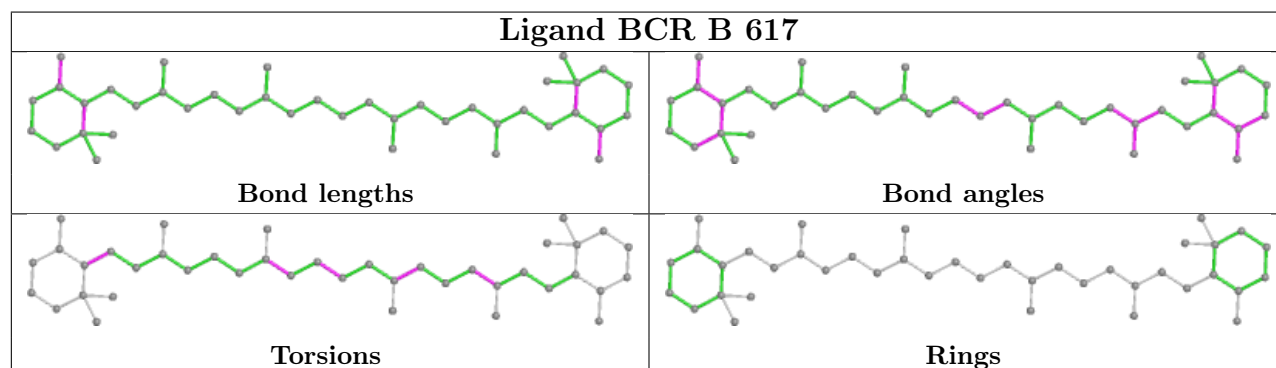
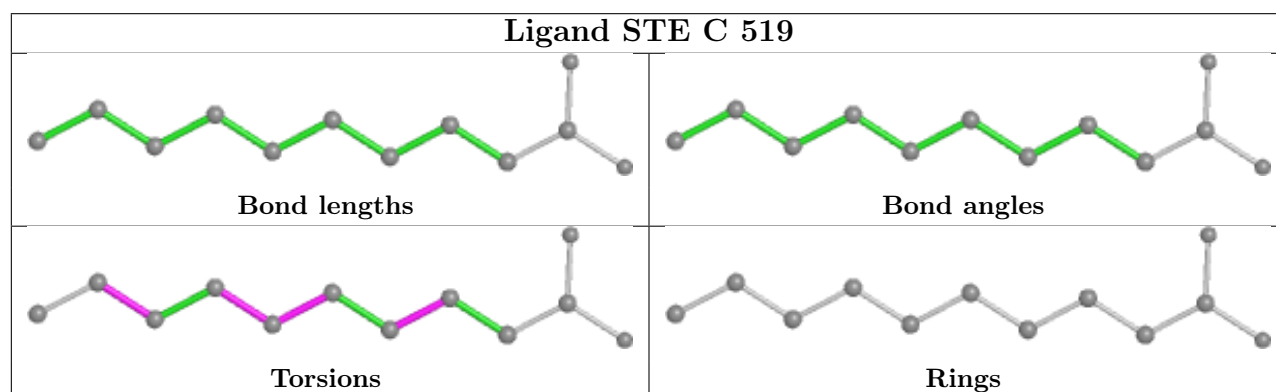
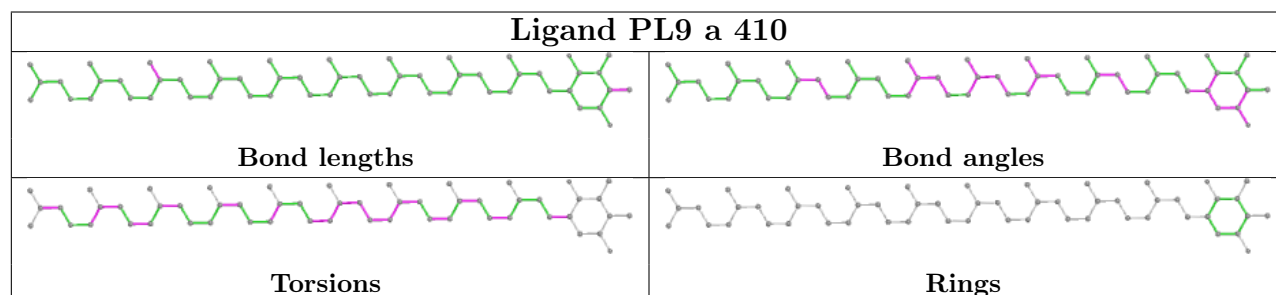
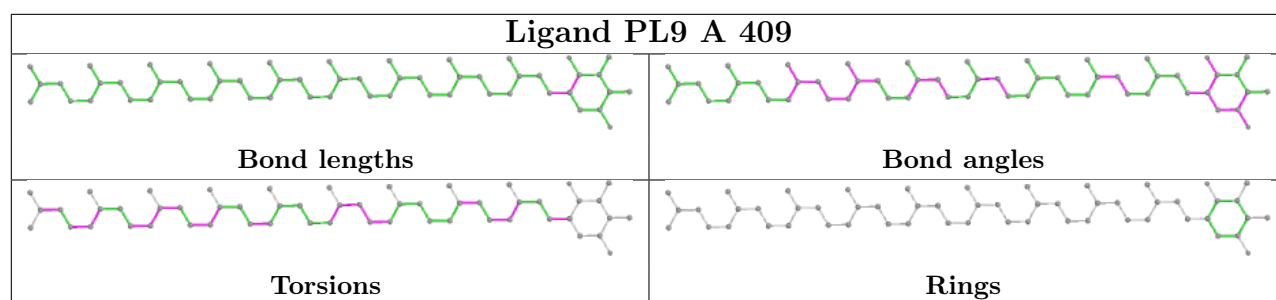


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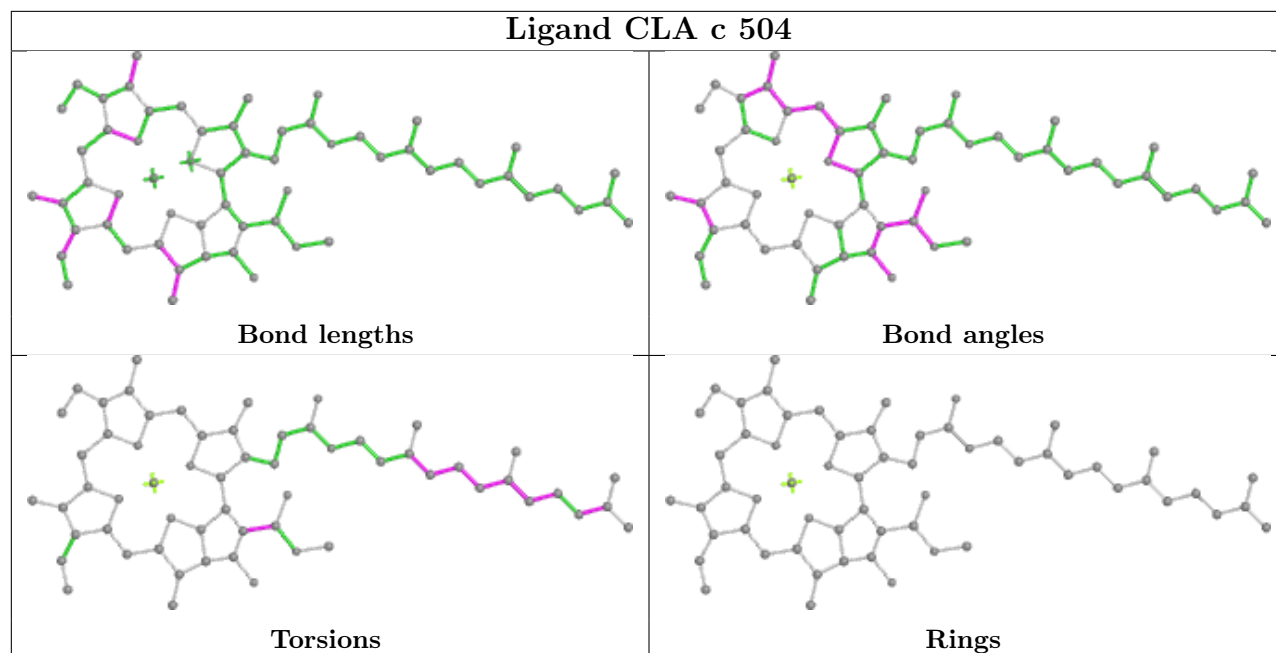


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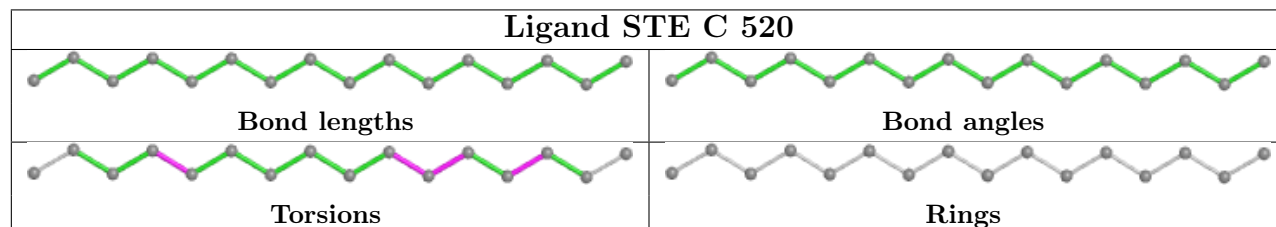




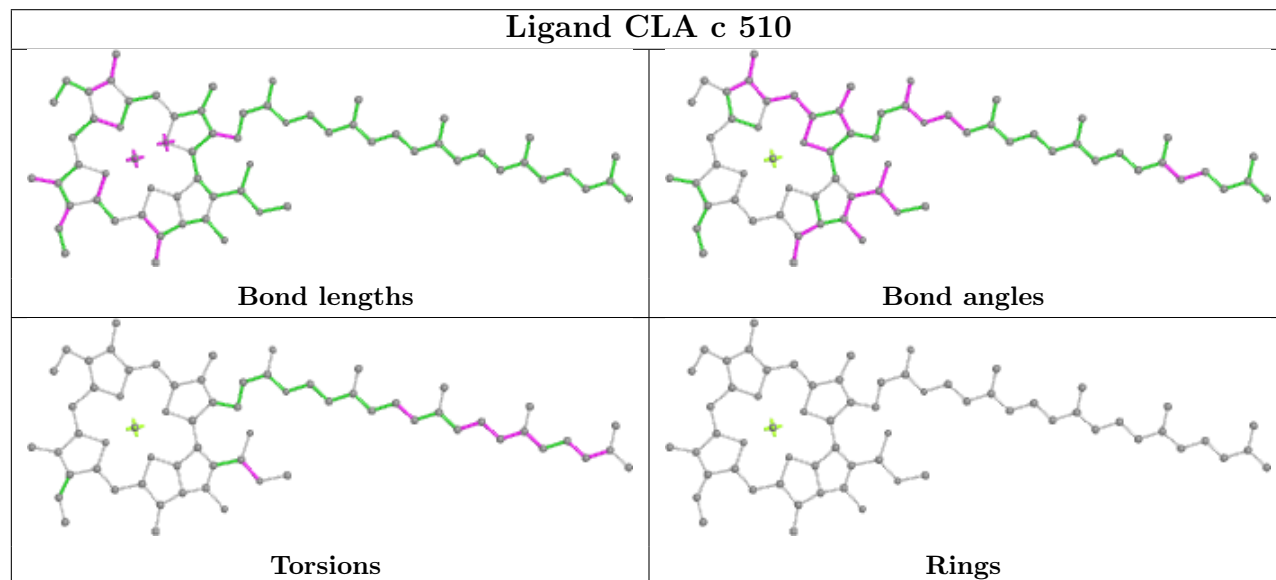
## Ligand CLA c 504



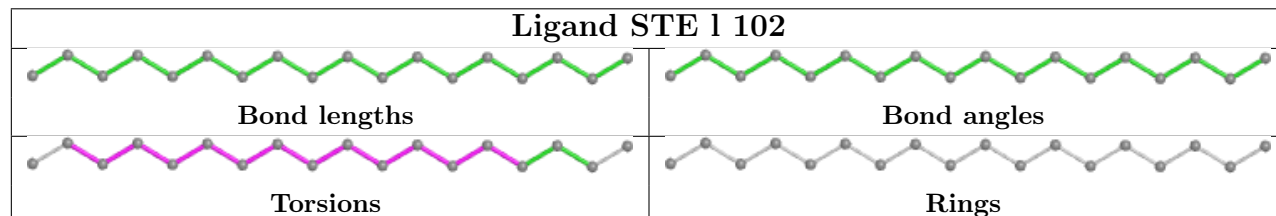
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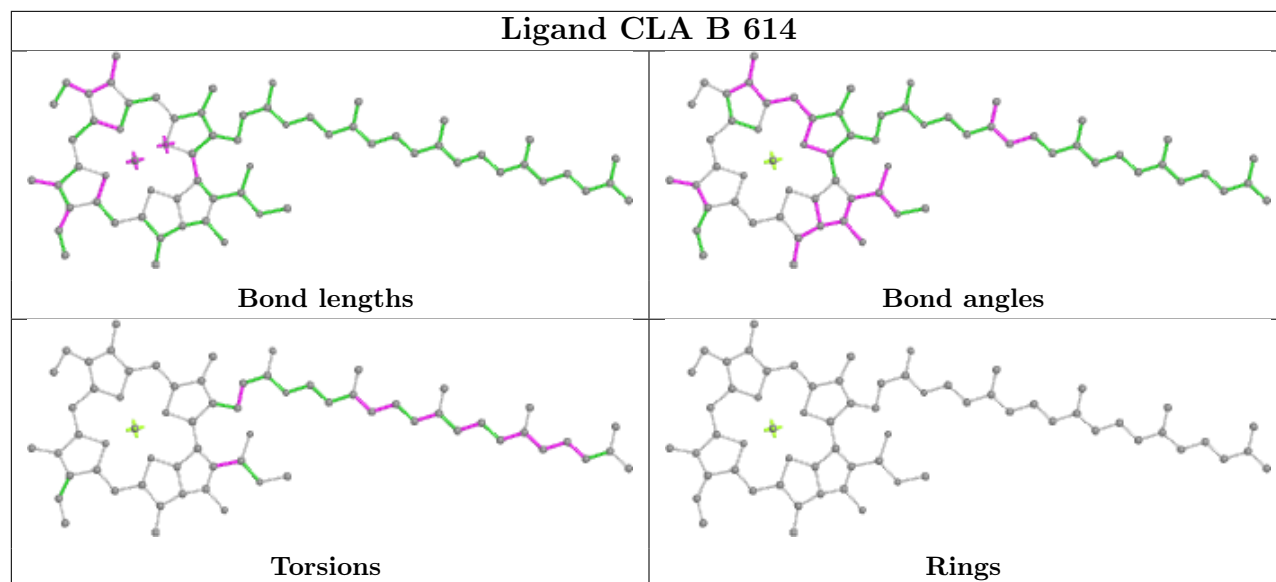
## Ligand CLA c 510



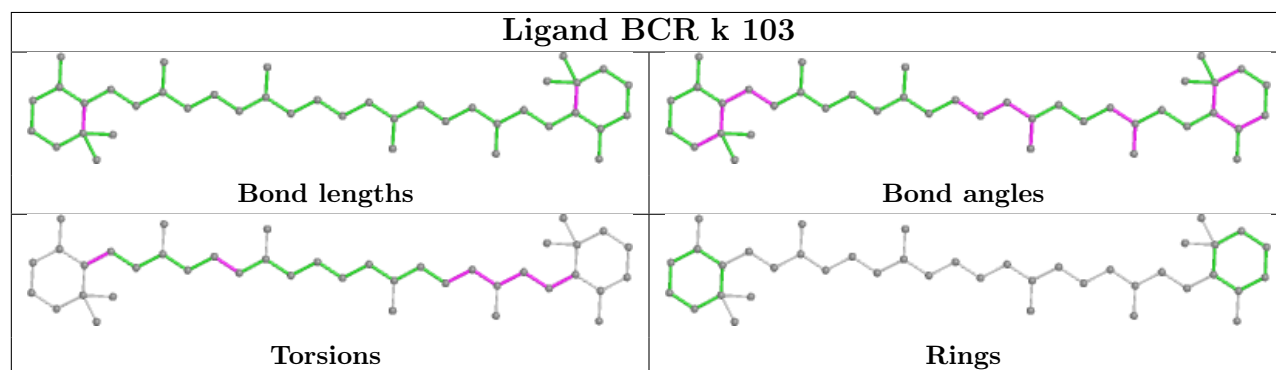
## Ligand STE l 102



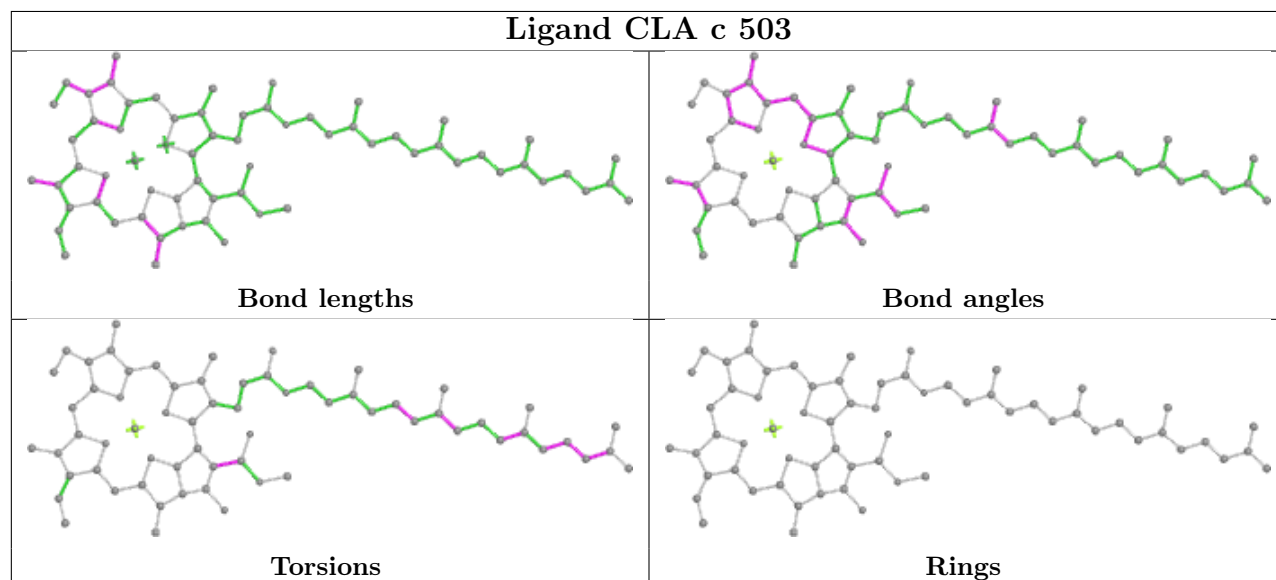
## Ligand CLA B 614

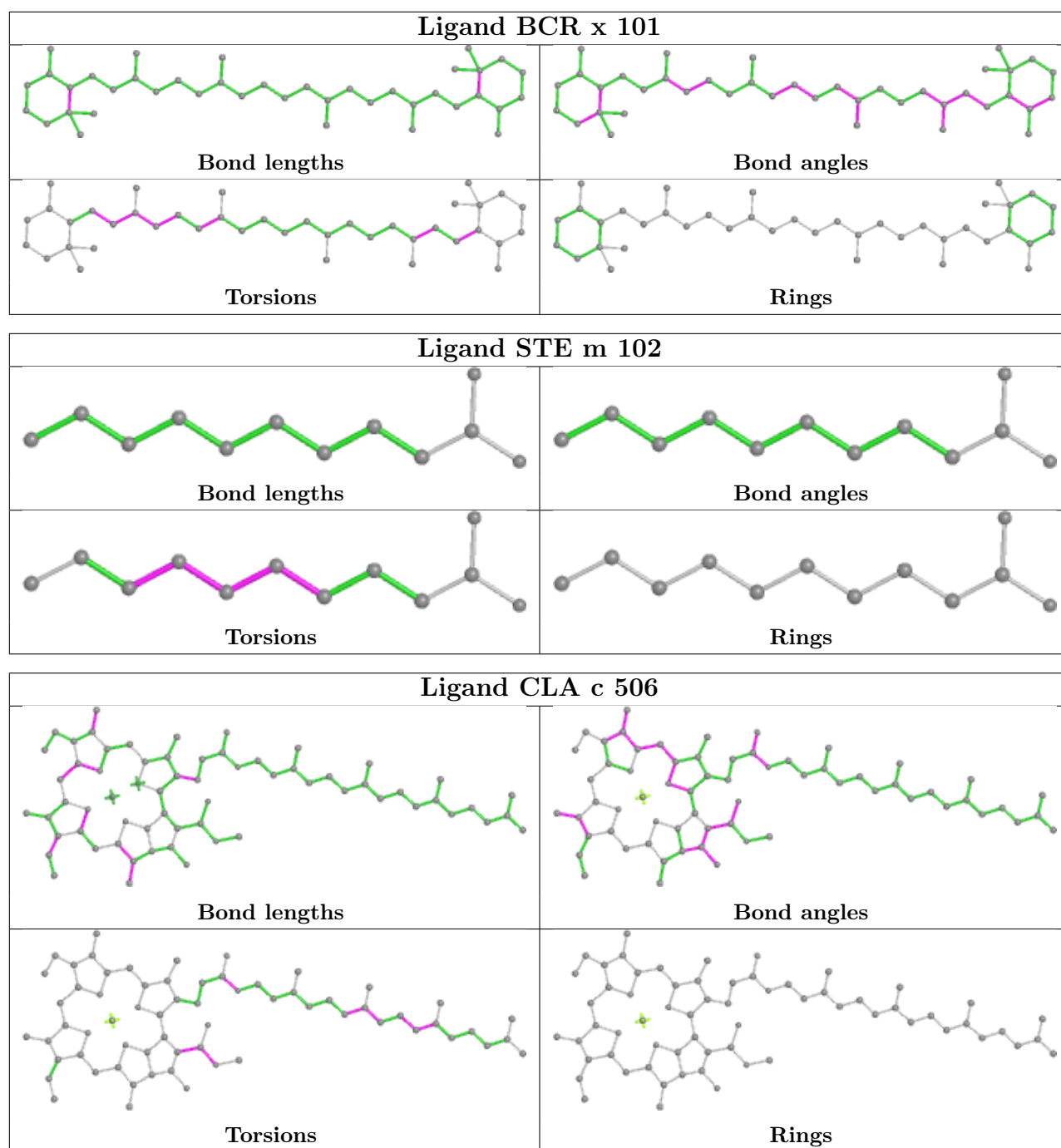


## Ligand BCR k 103

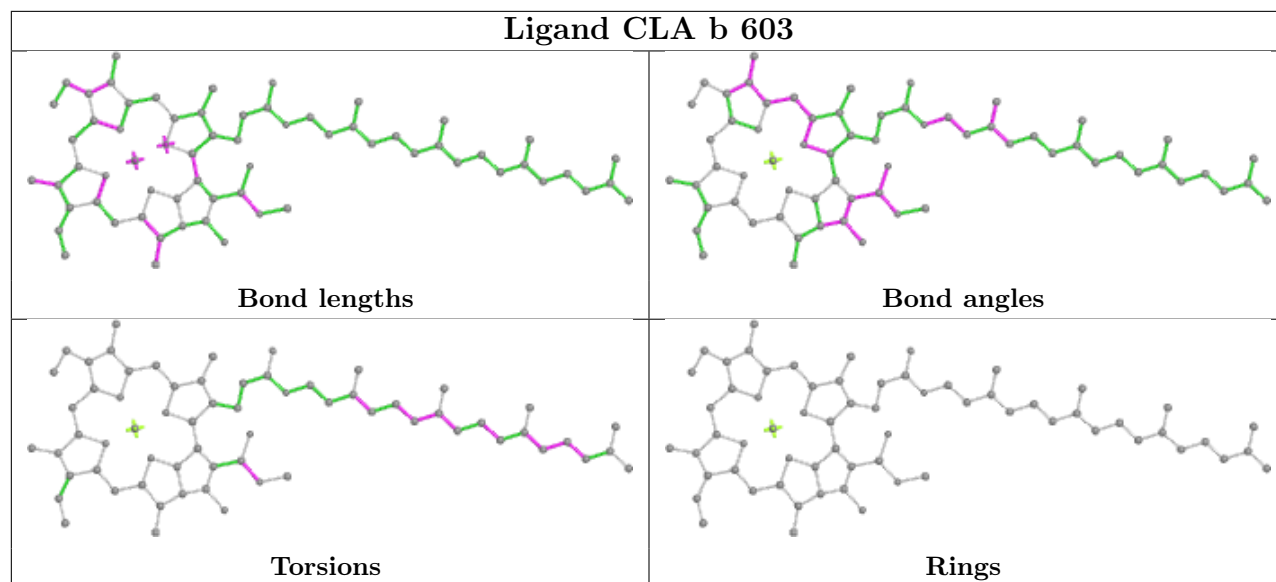


## Ligand CLA c 503

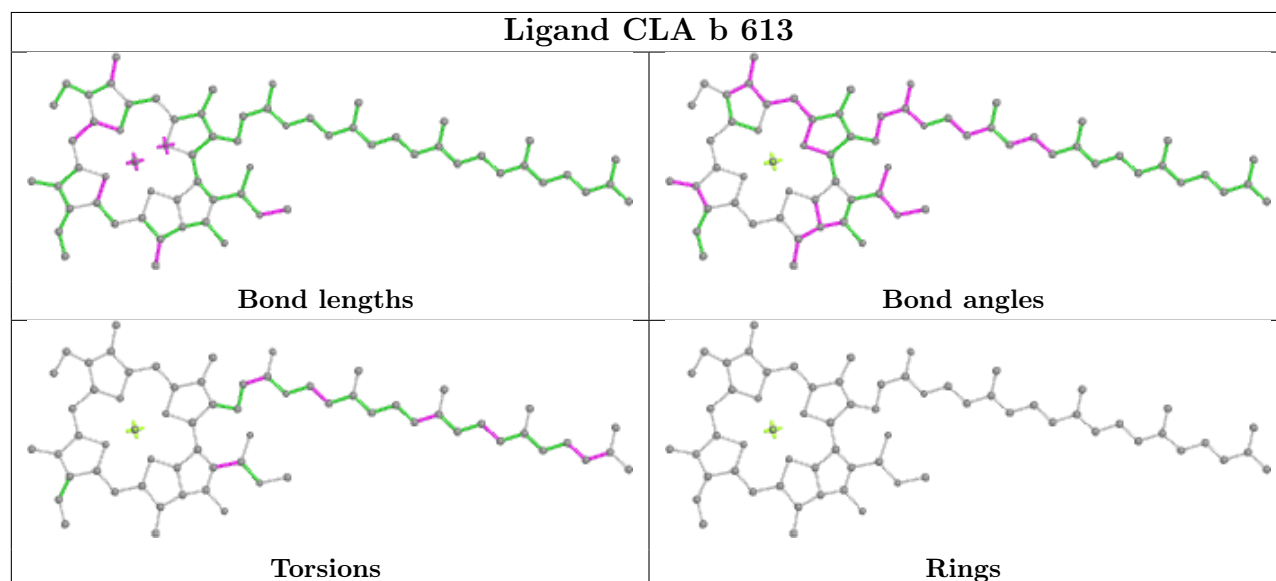




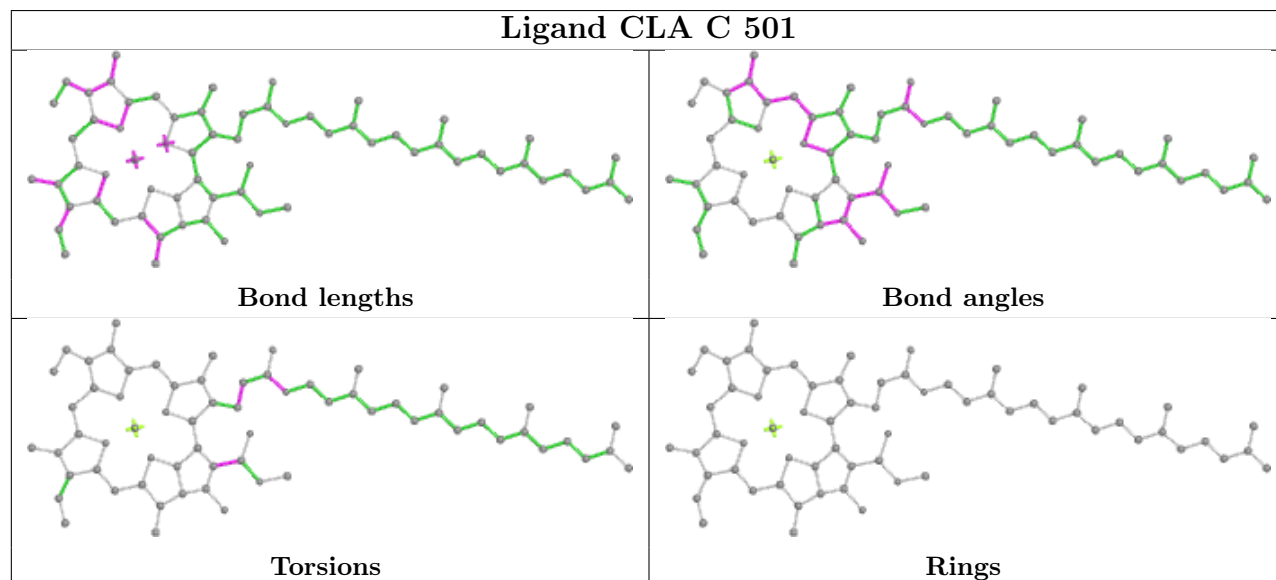
## Ligand CLA b 603



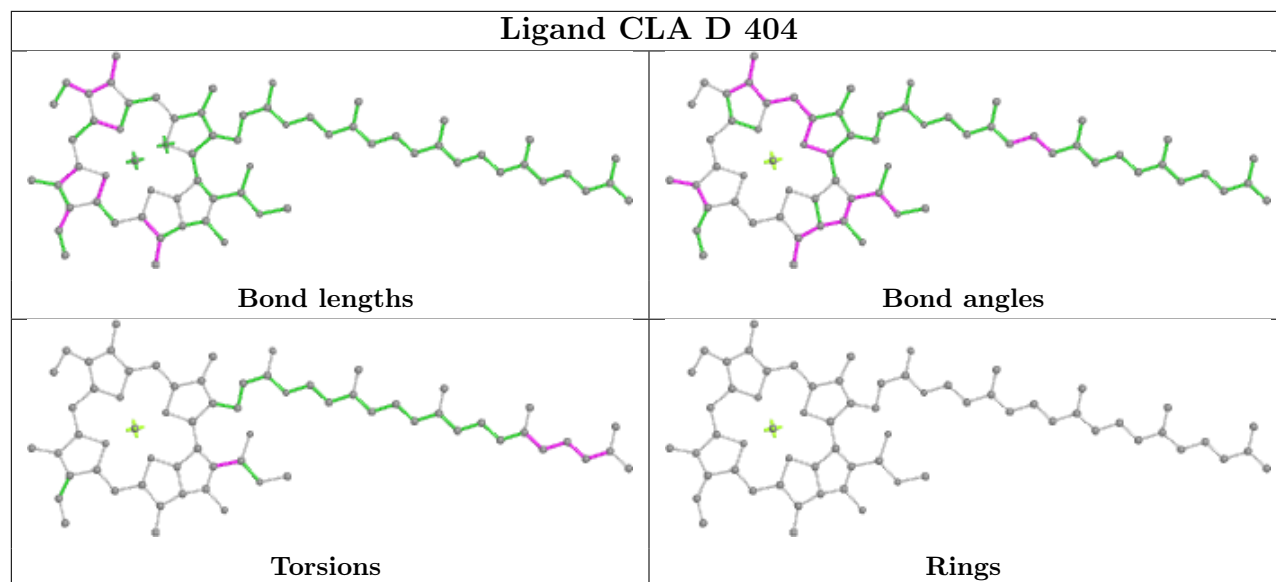
## Ligand CLA b 613



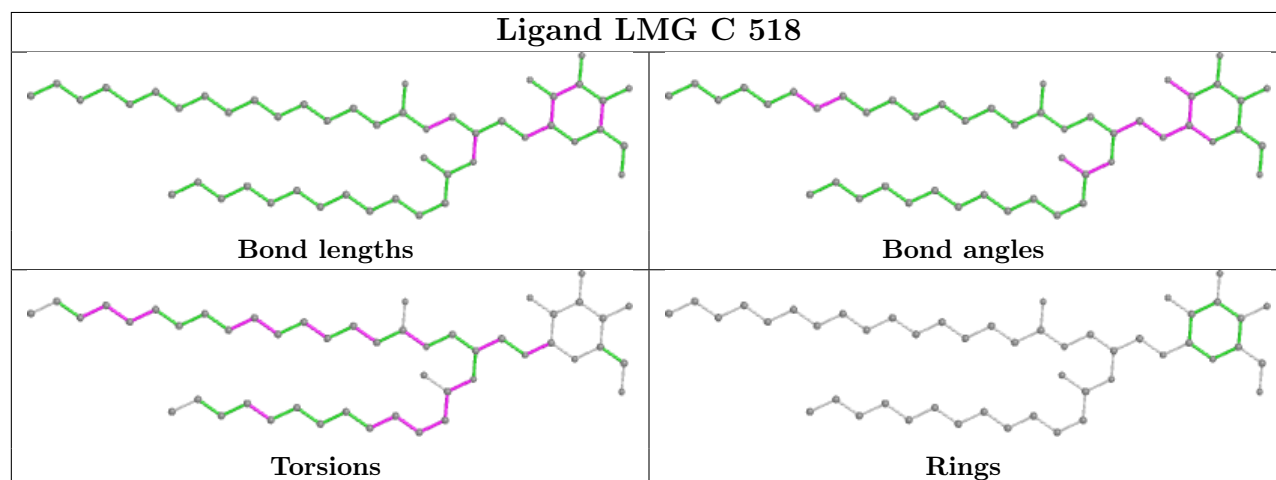
## Ligand CLA C 501



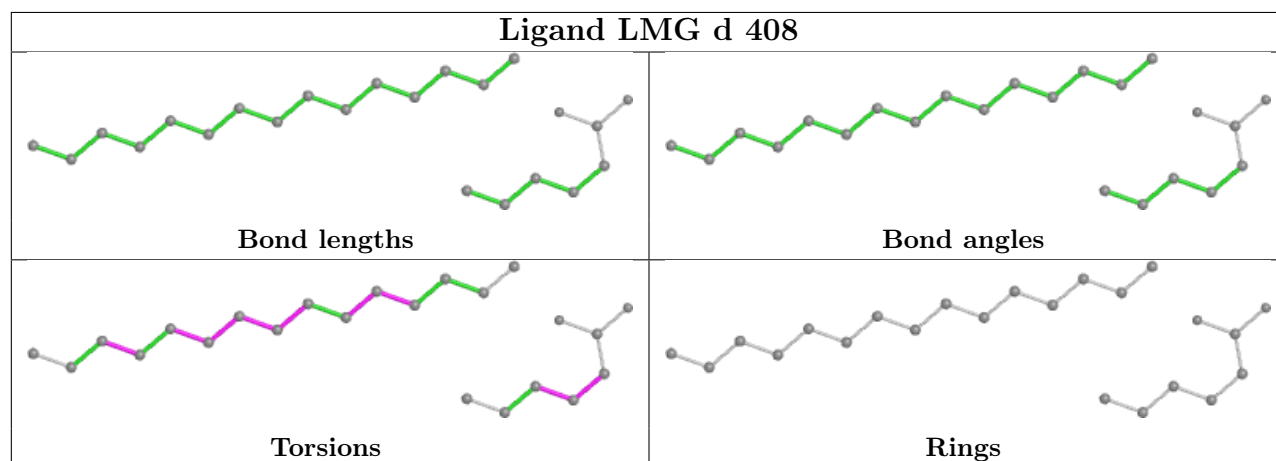
## Ligand CLA D 404



## Ligand LMG C 518

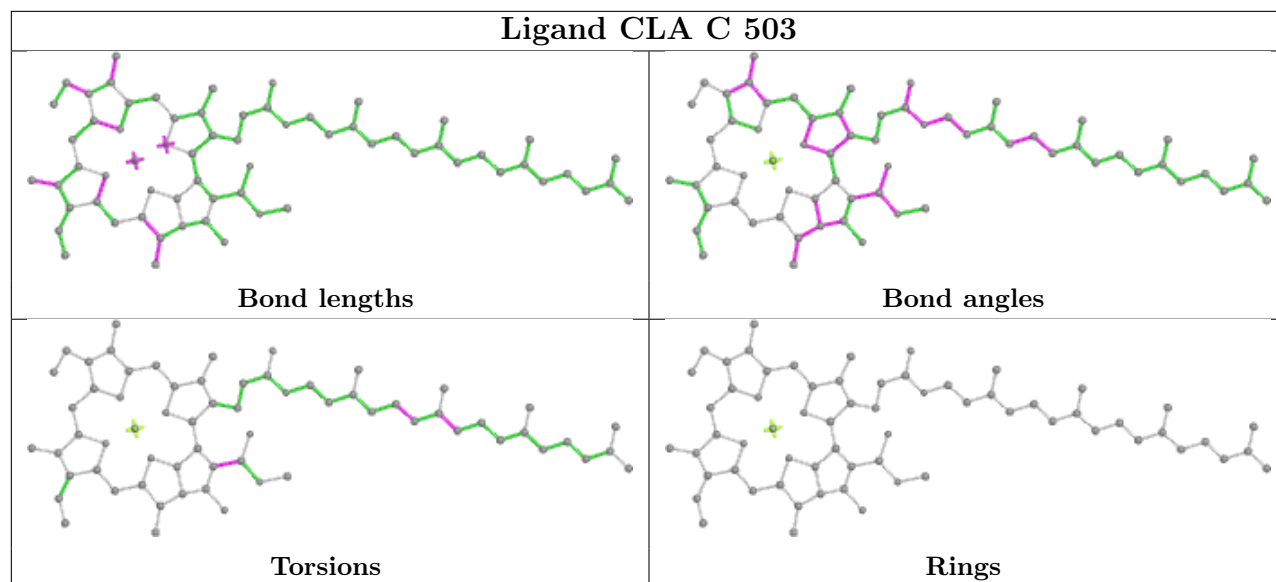


## Ligand LMG d 408

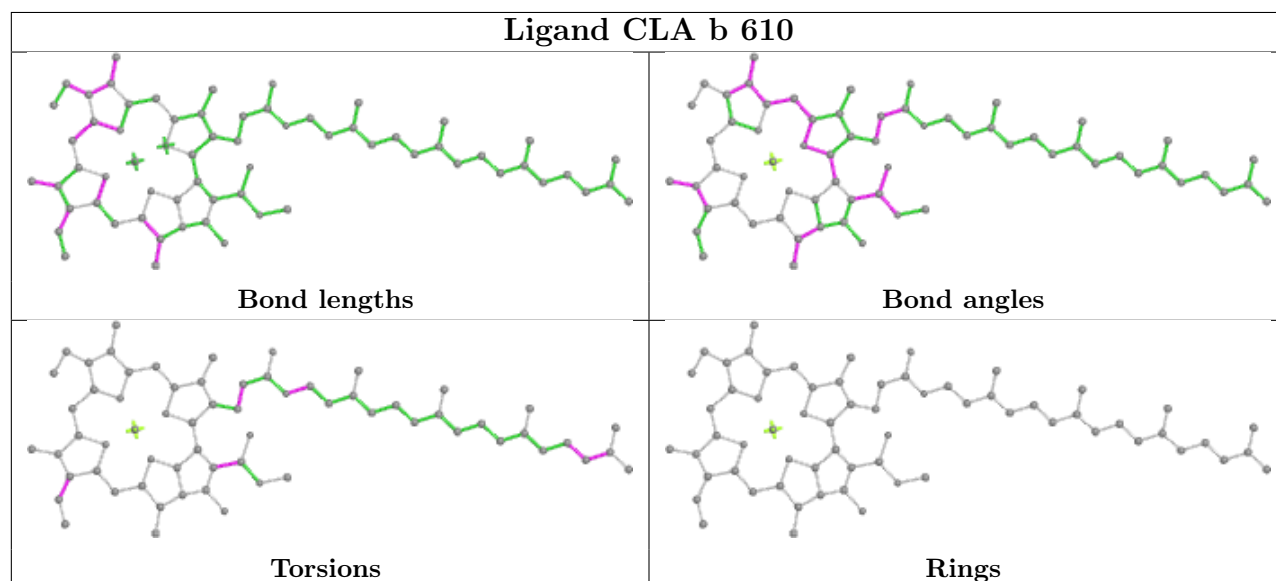




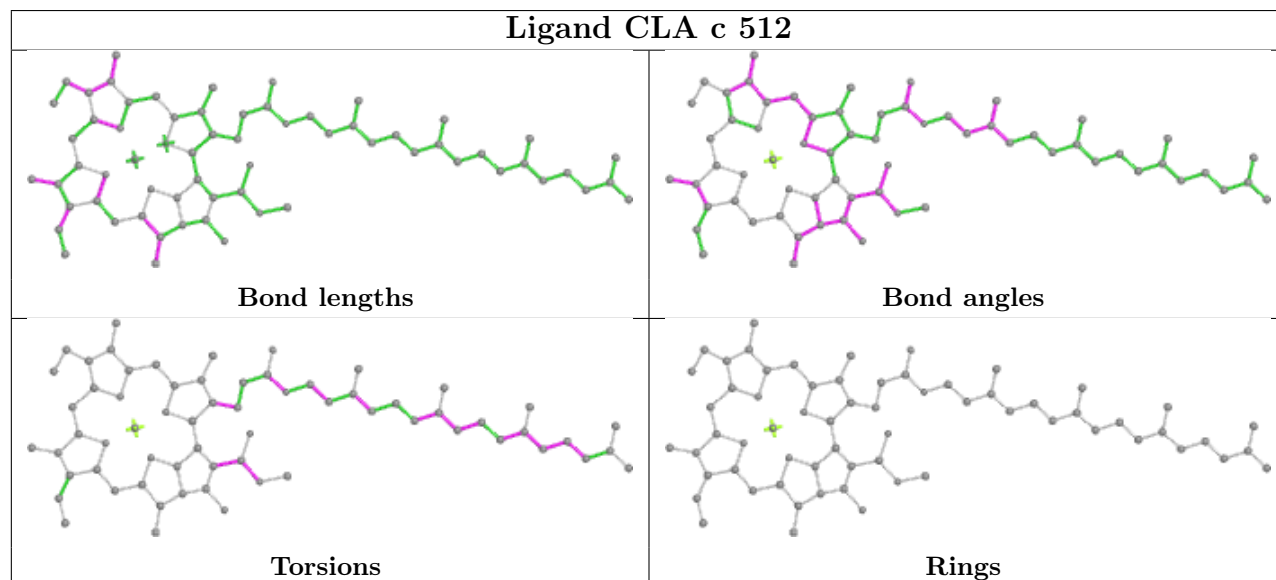
## Ligand CLA C 503



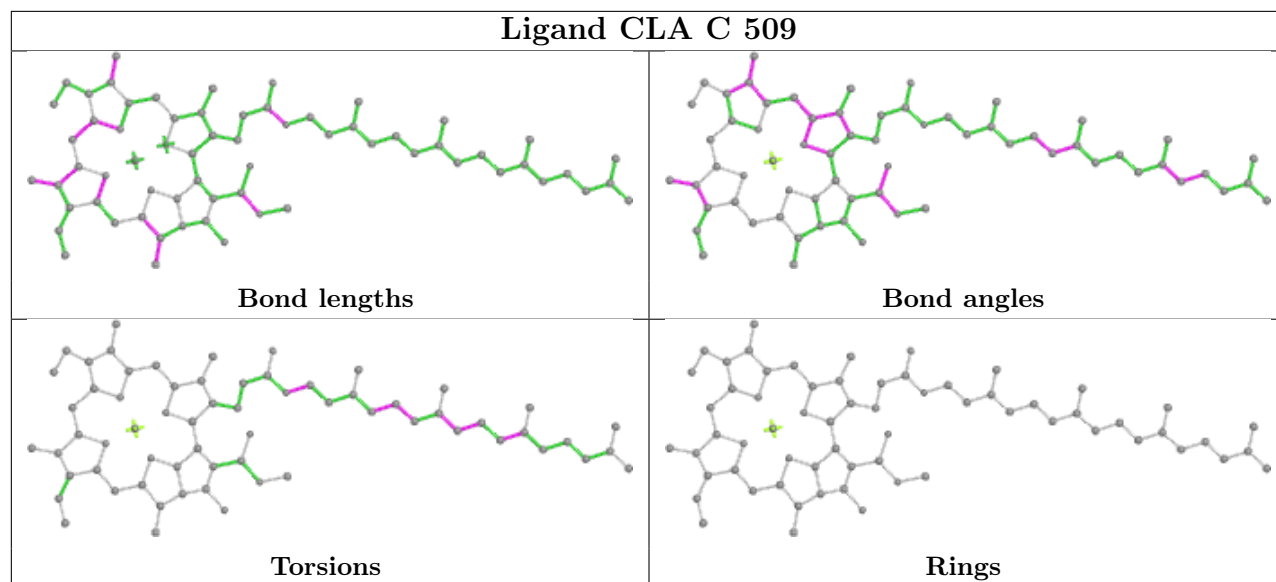
## Ligand CLA b 610



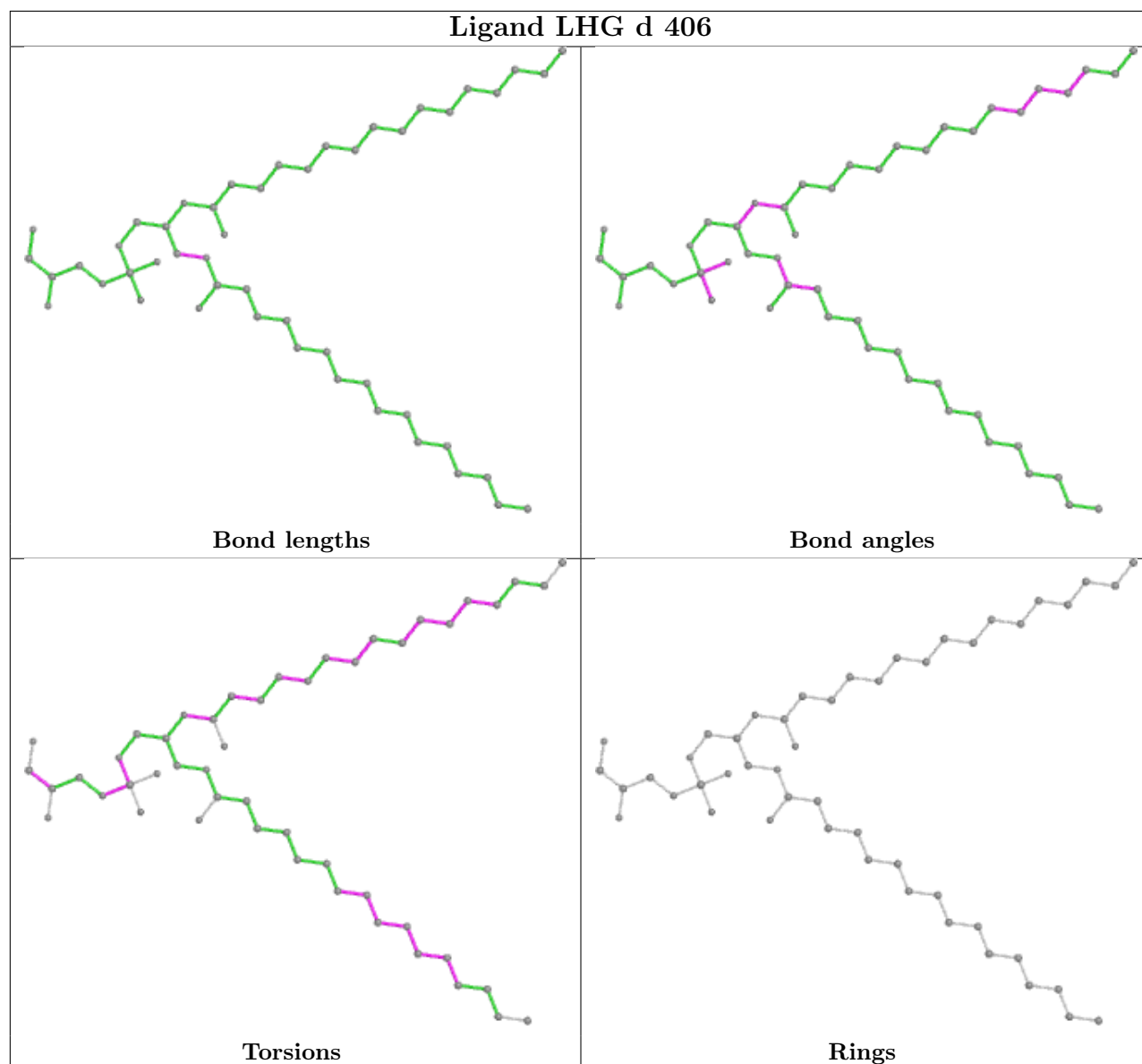
## Ligand CLA c 512

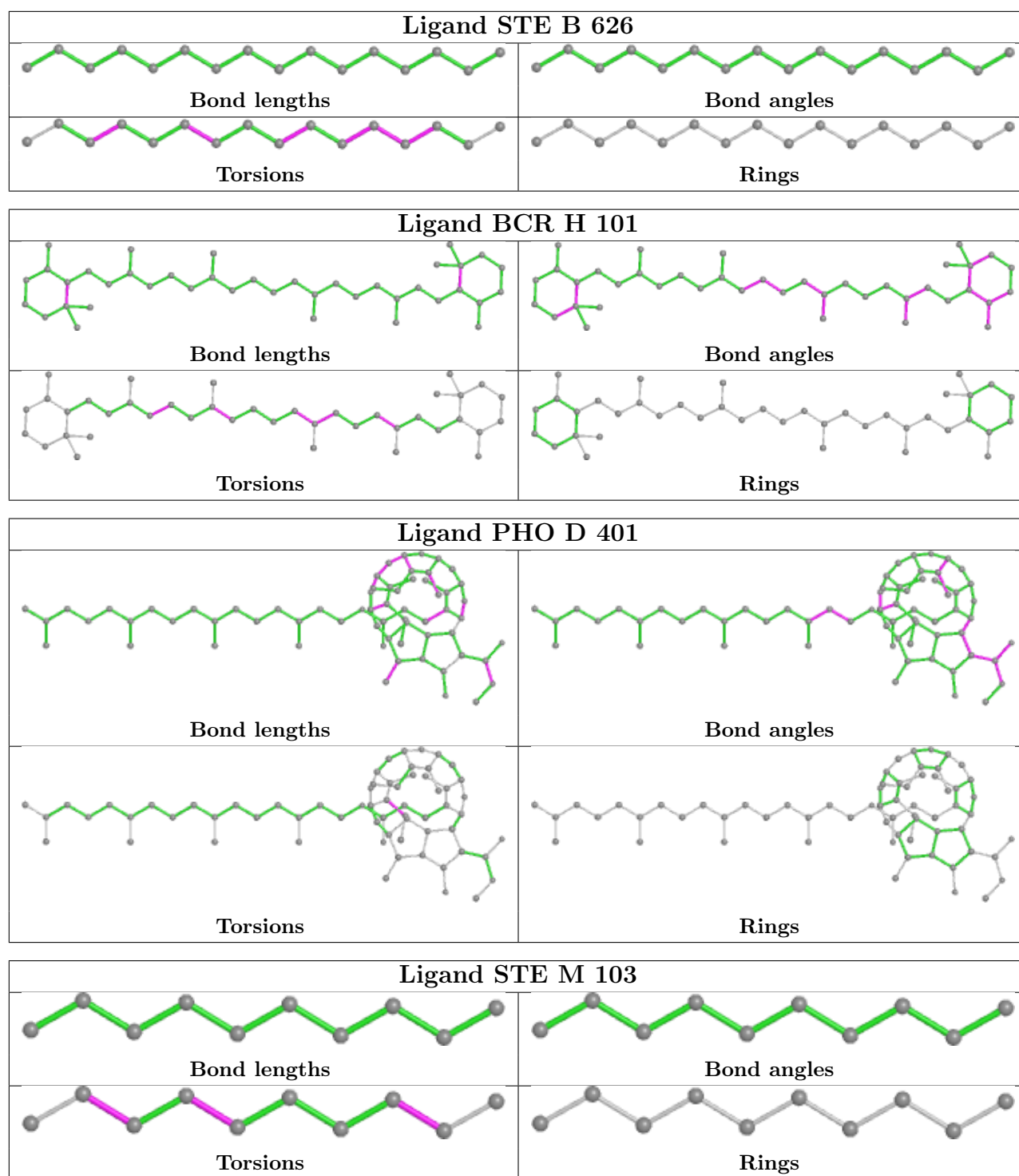


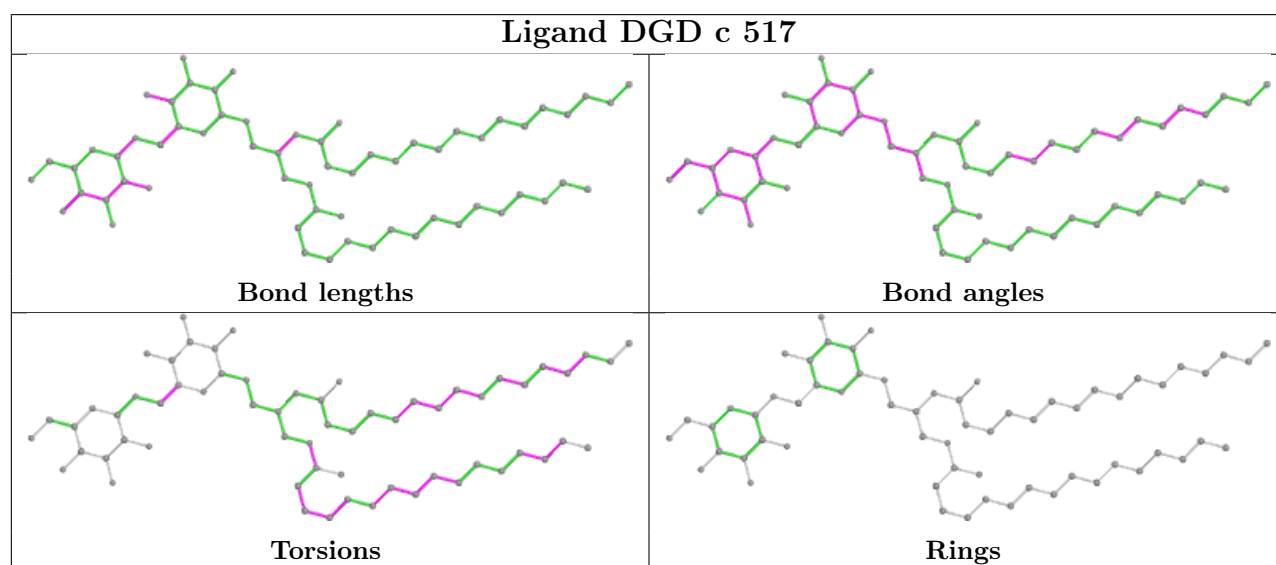
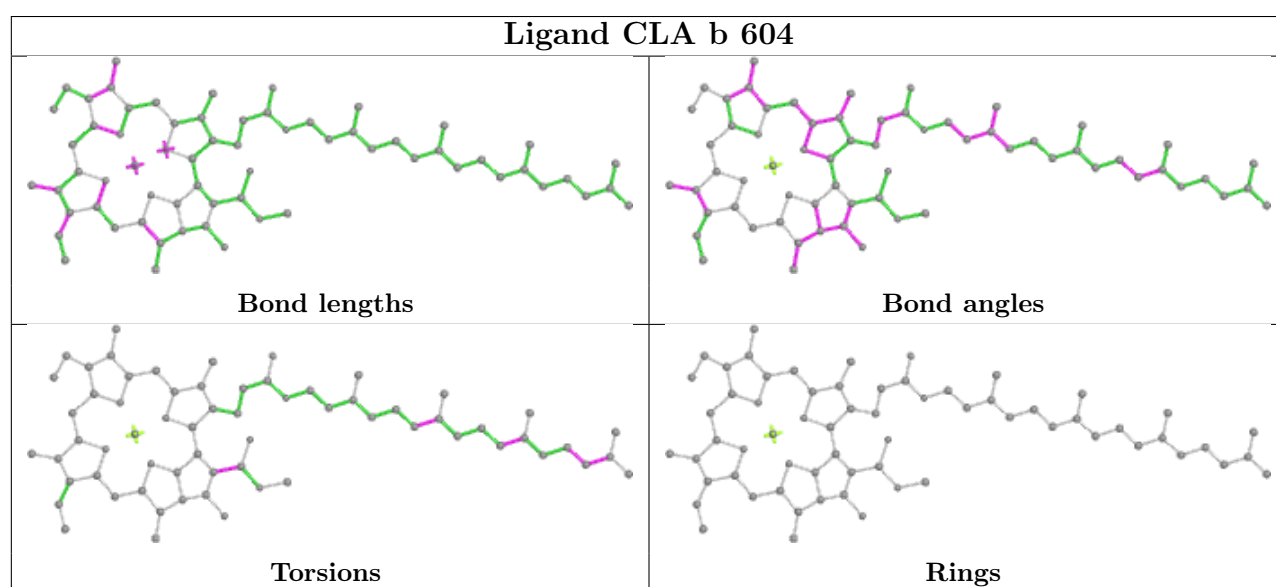
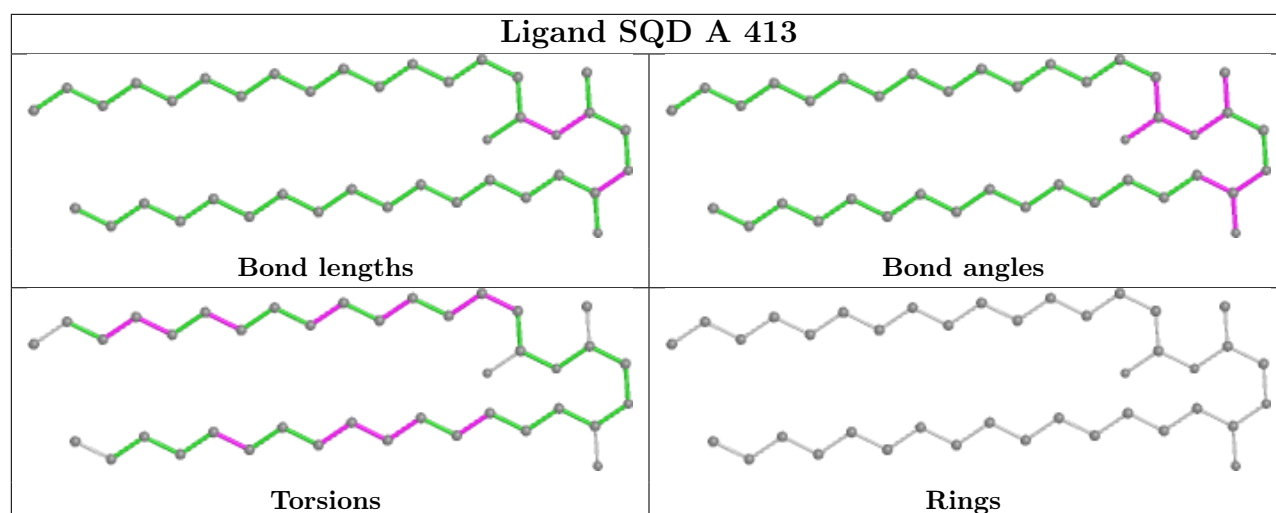
## Ligand CLA C 509

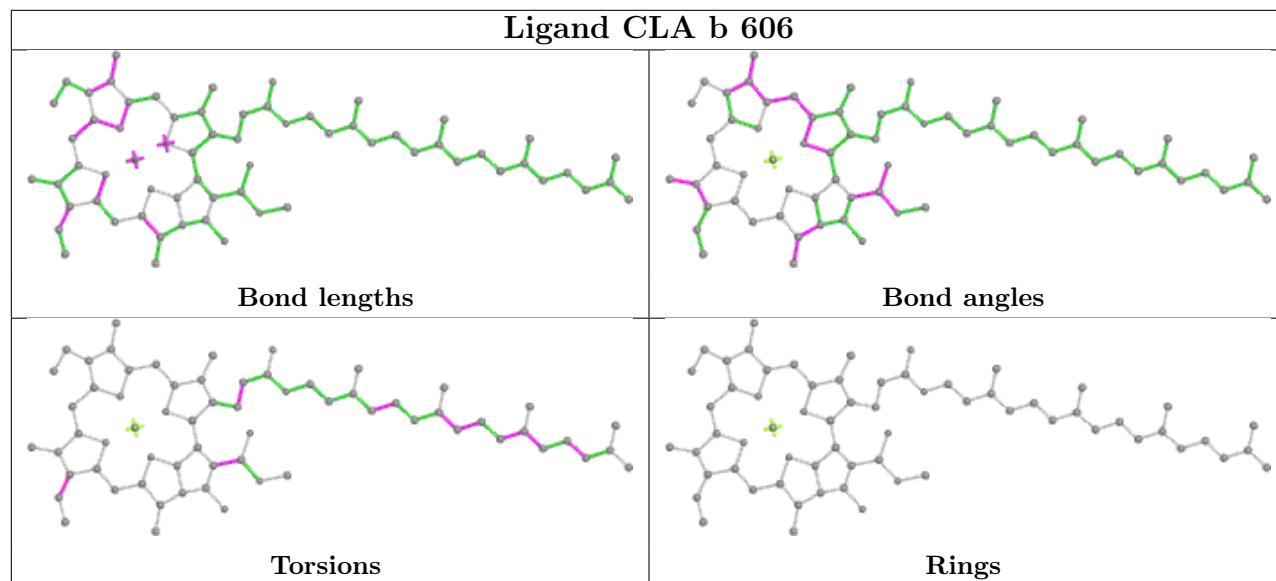
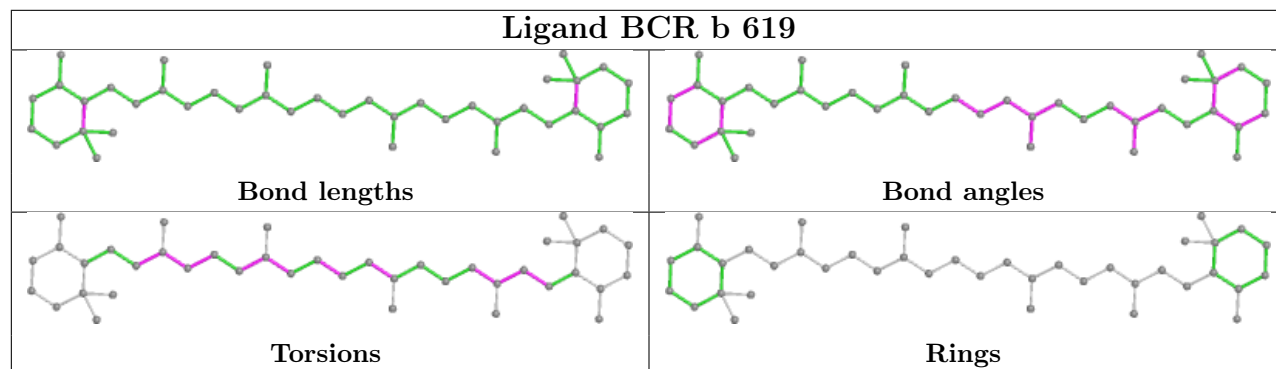
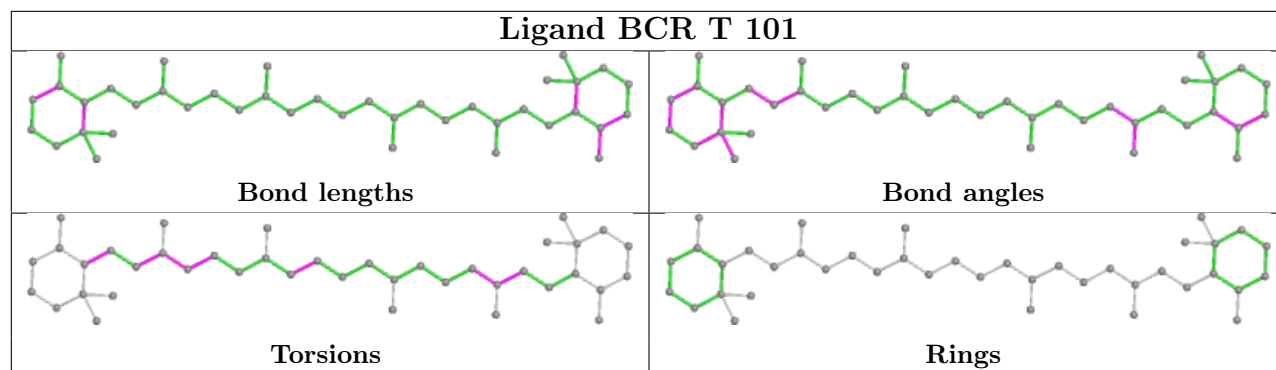
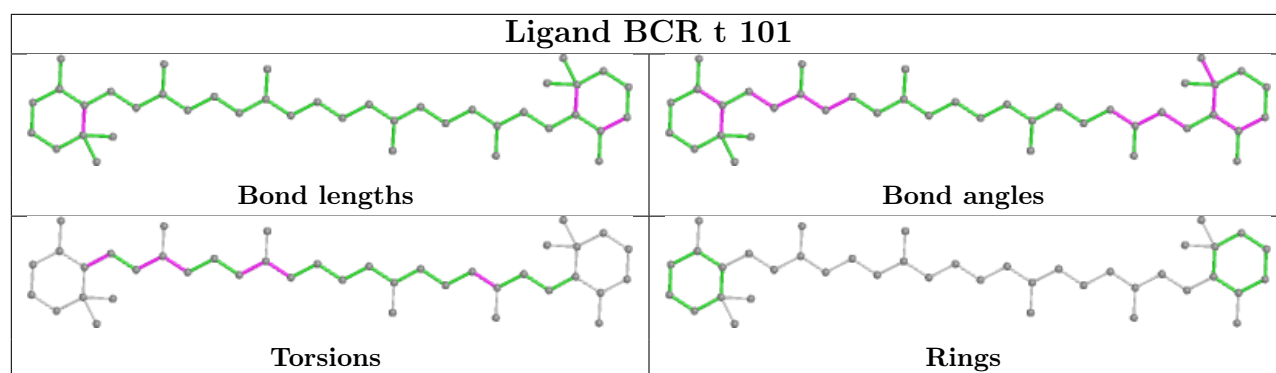


## Ligand LHG d 406

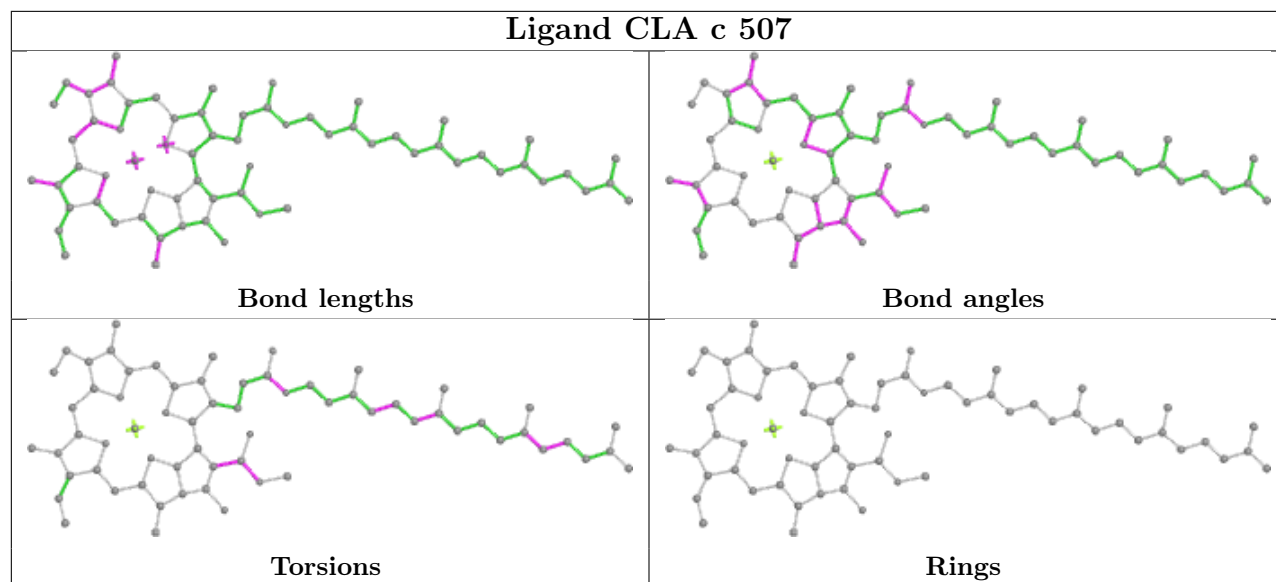




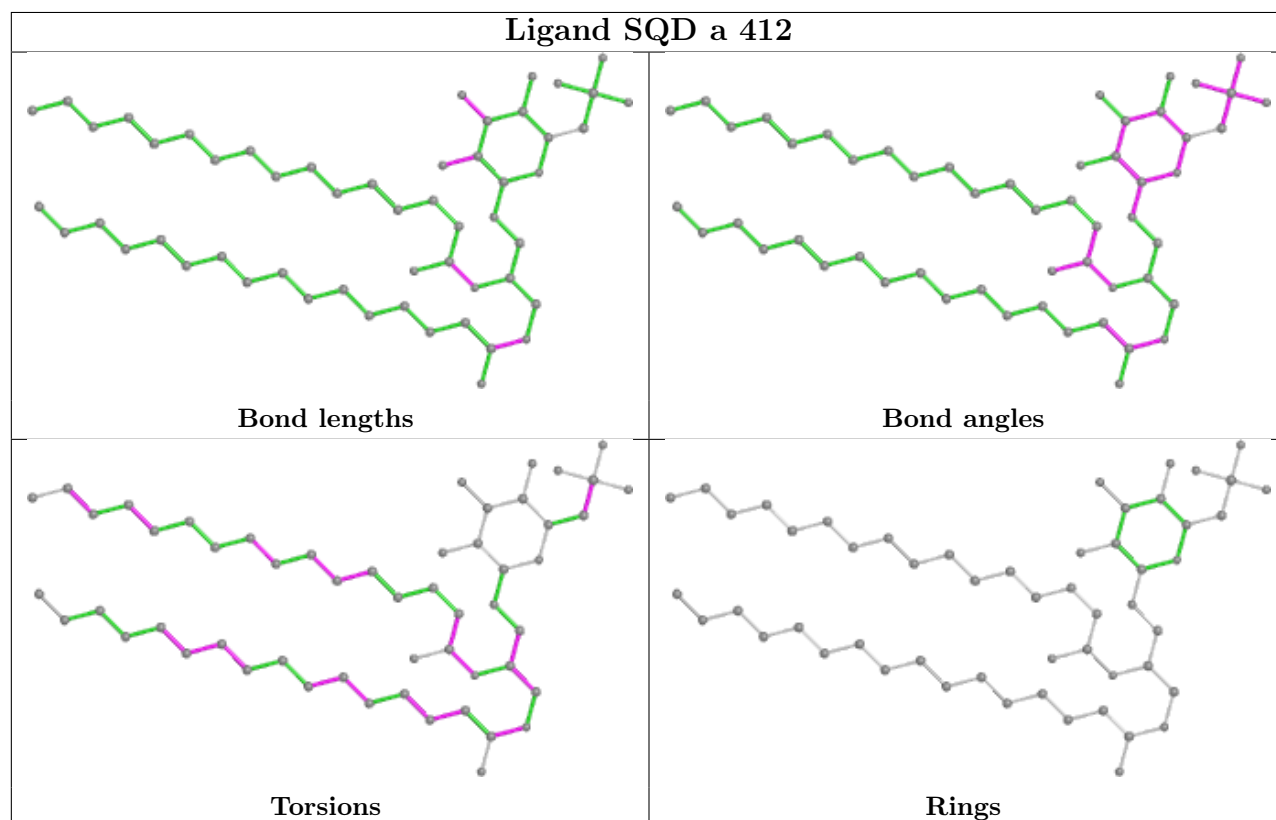


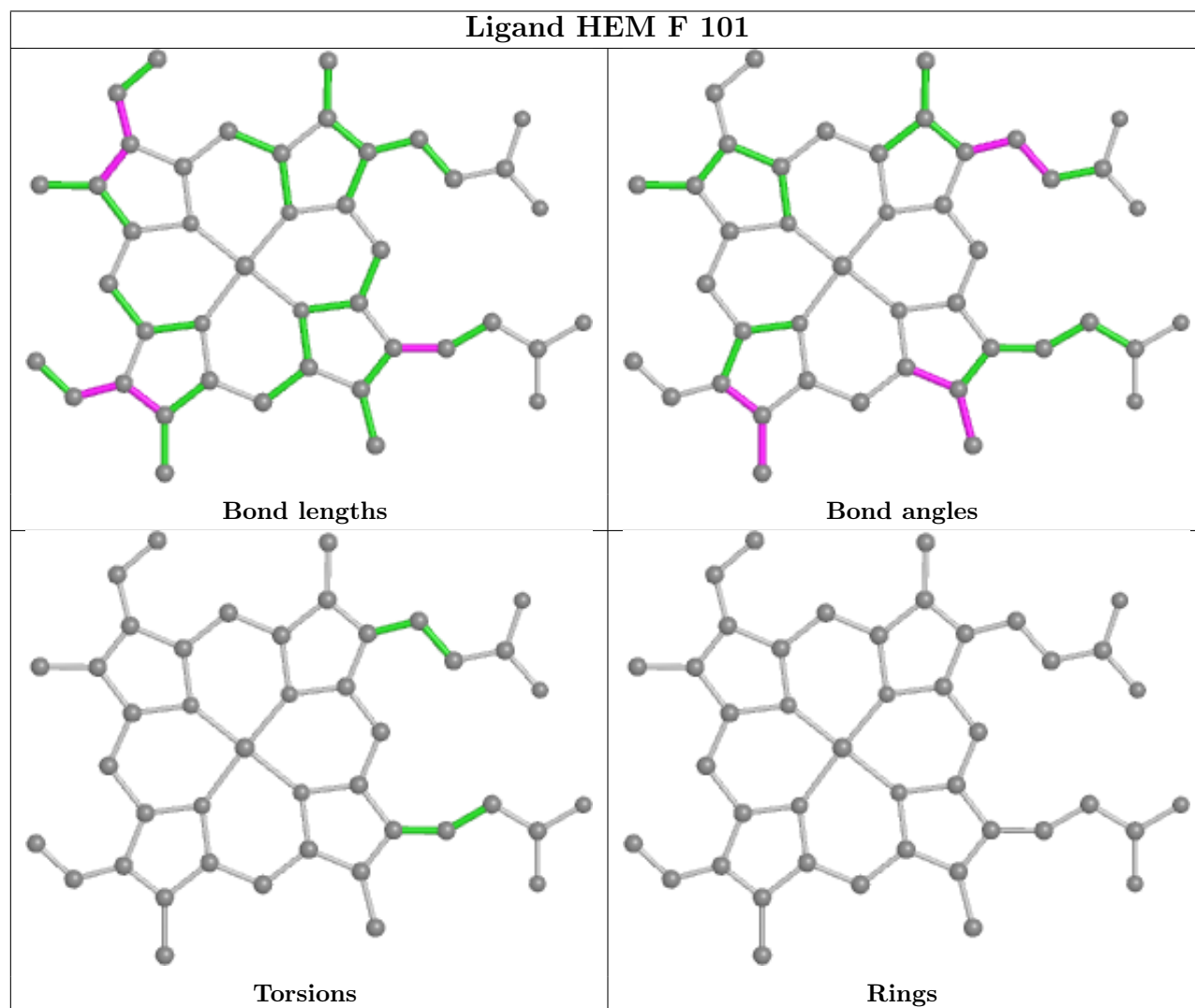
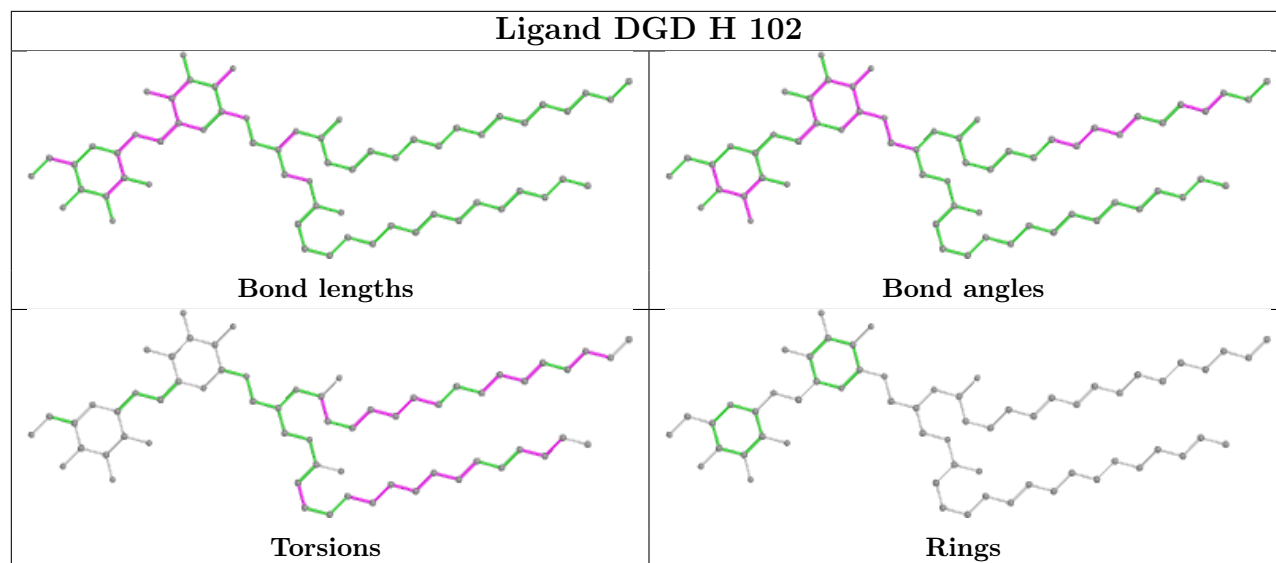


## Ligand CLA c 507

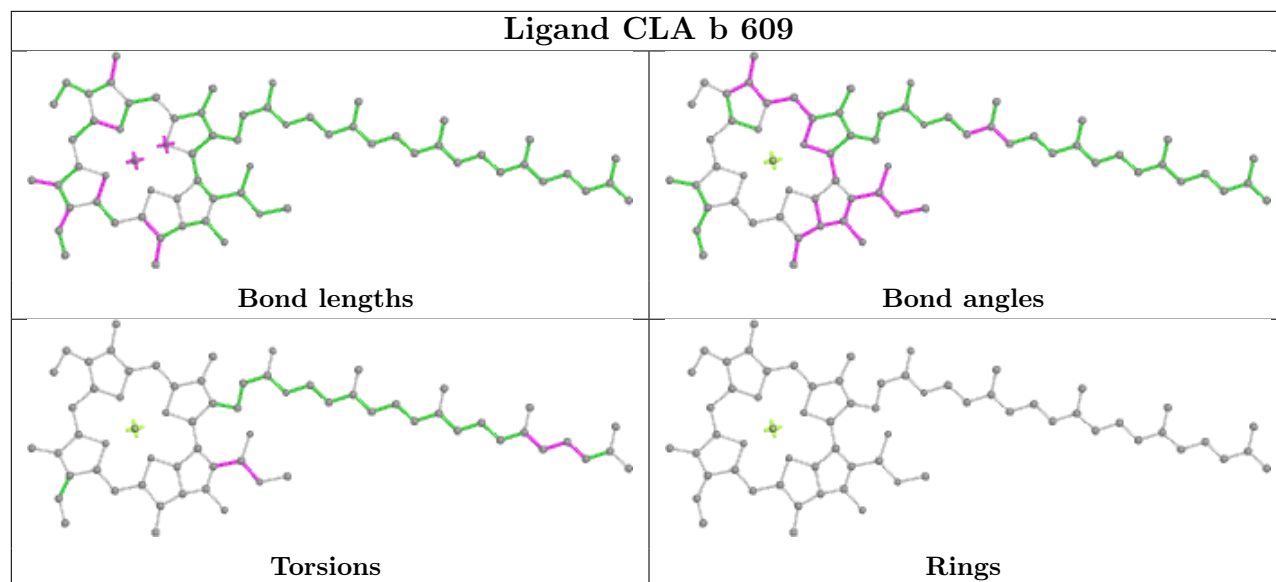


## Ligand SQD a 412

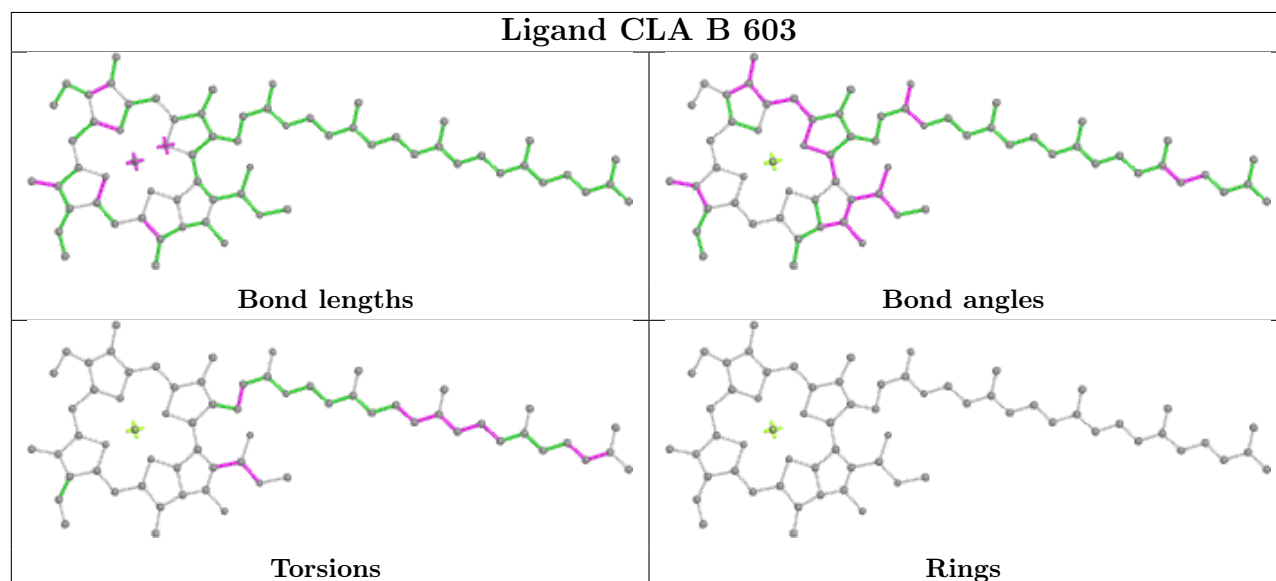




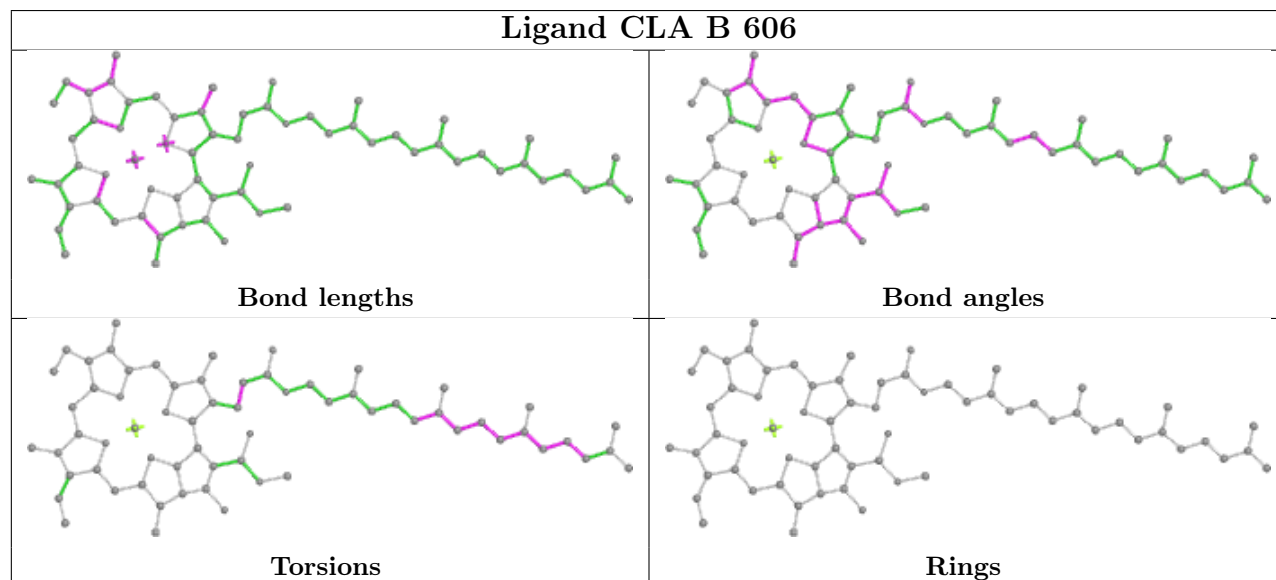
## Ligand CLA b 609



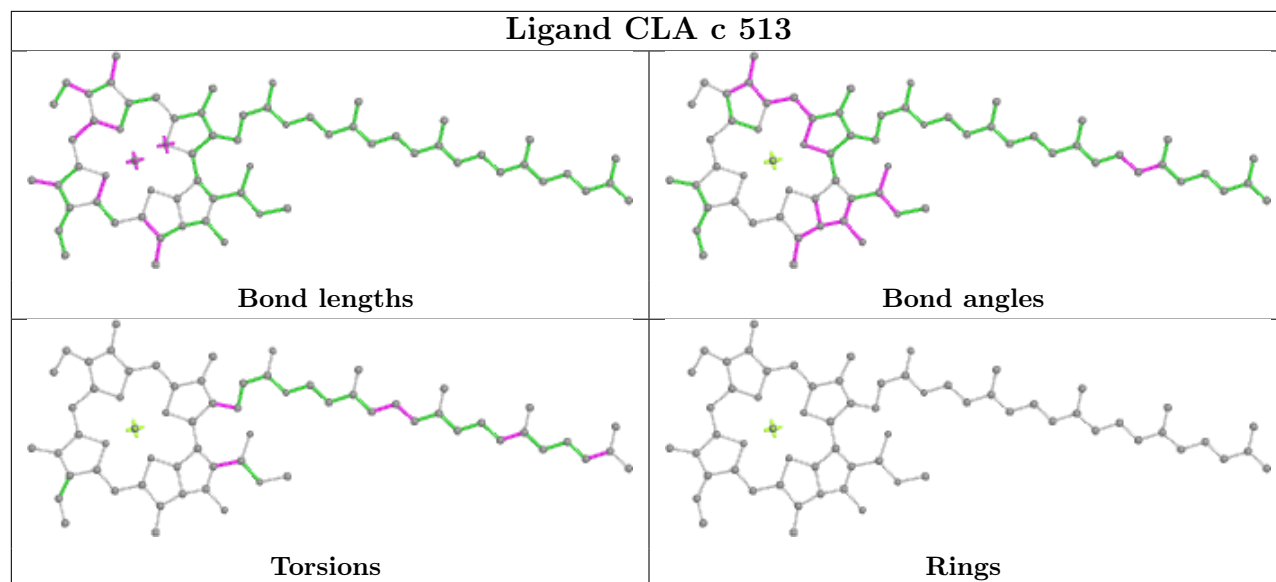
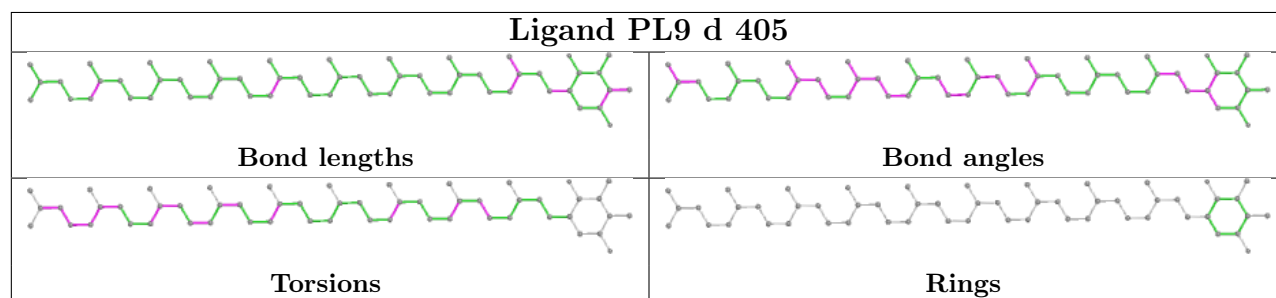
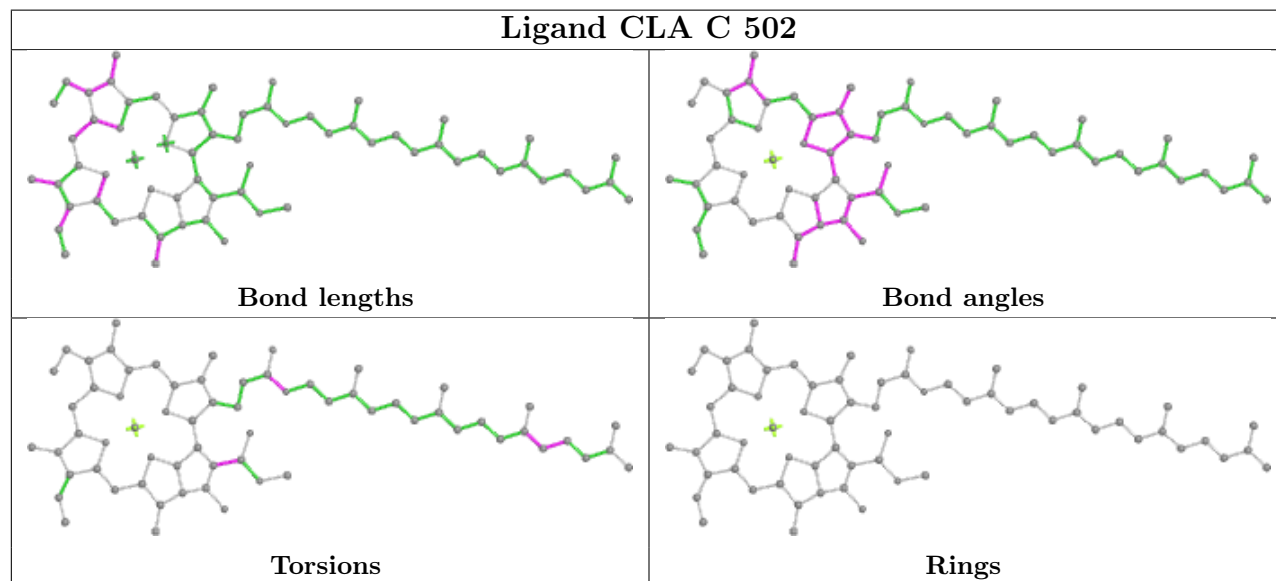
## Ligand CLA B 603

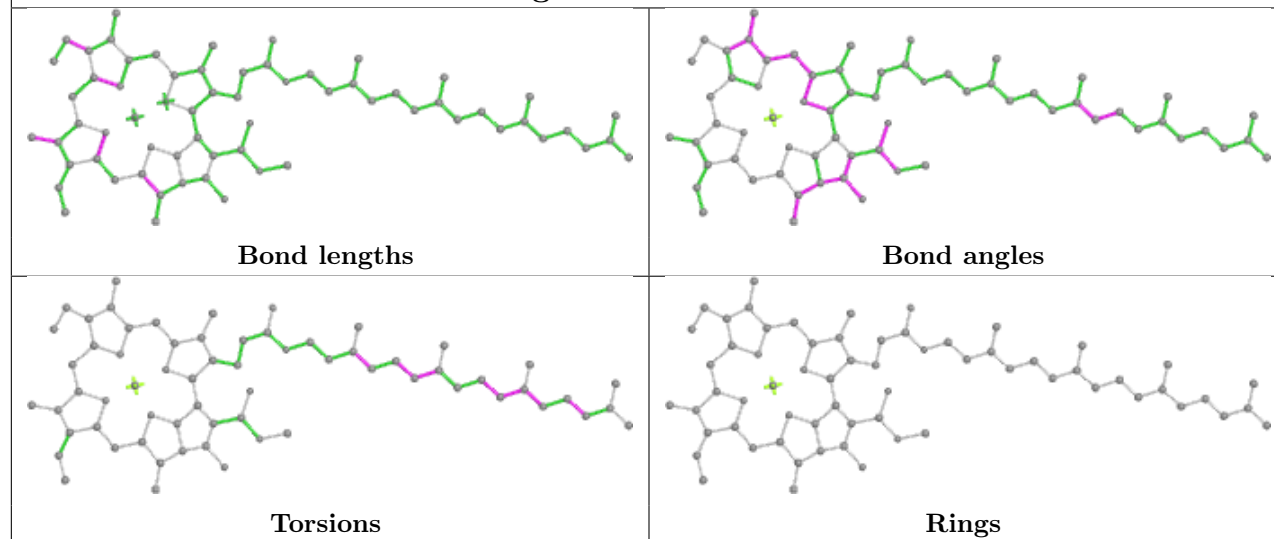
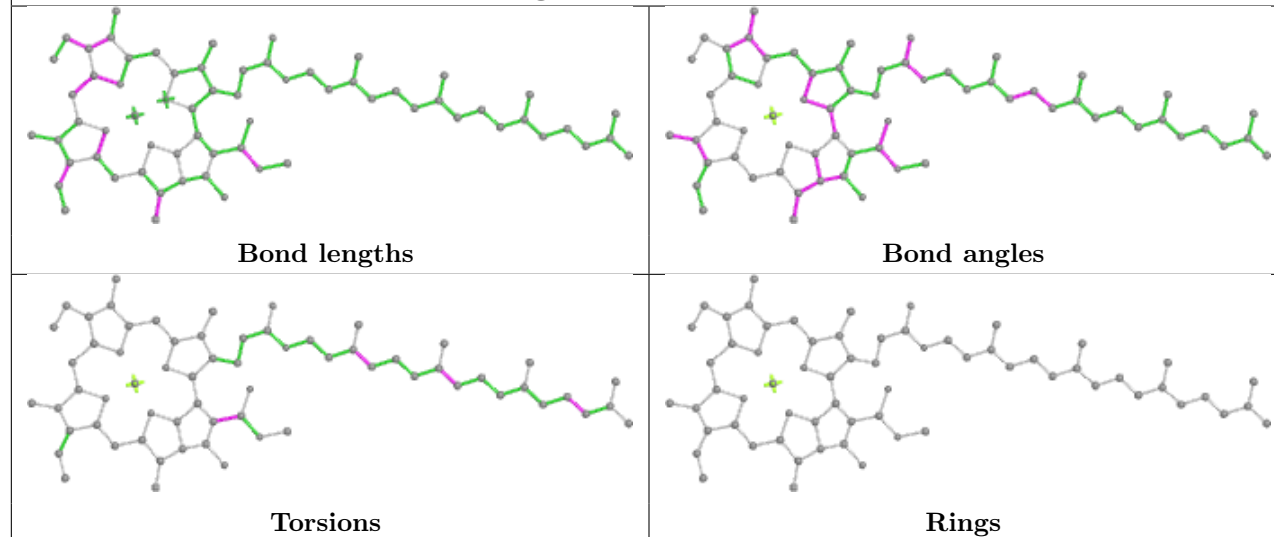


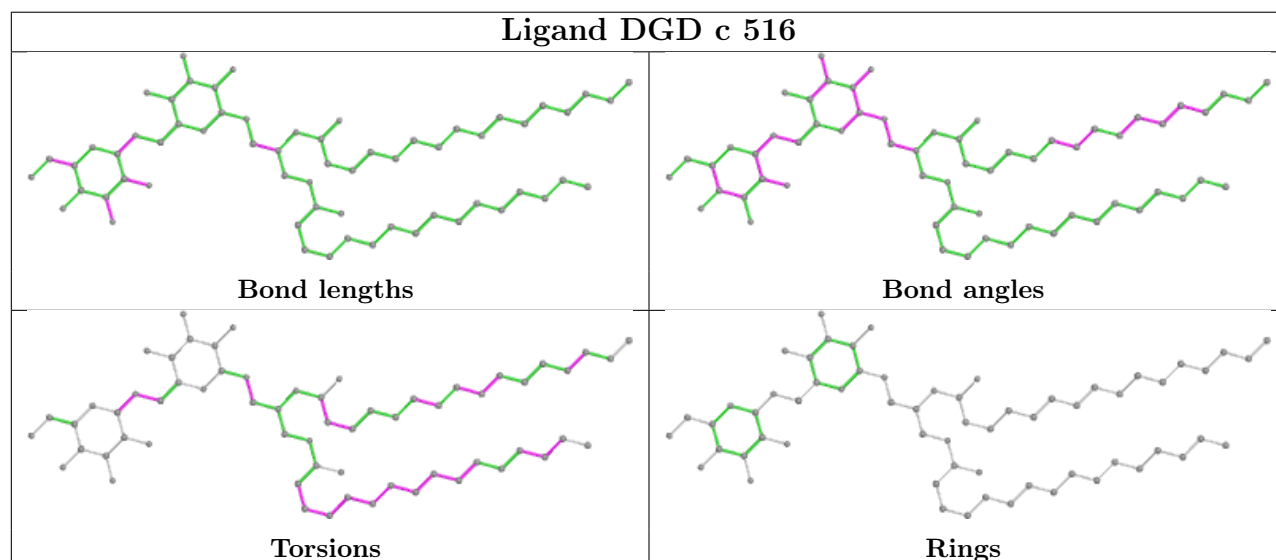
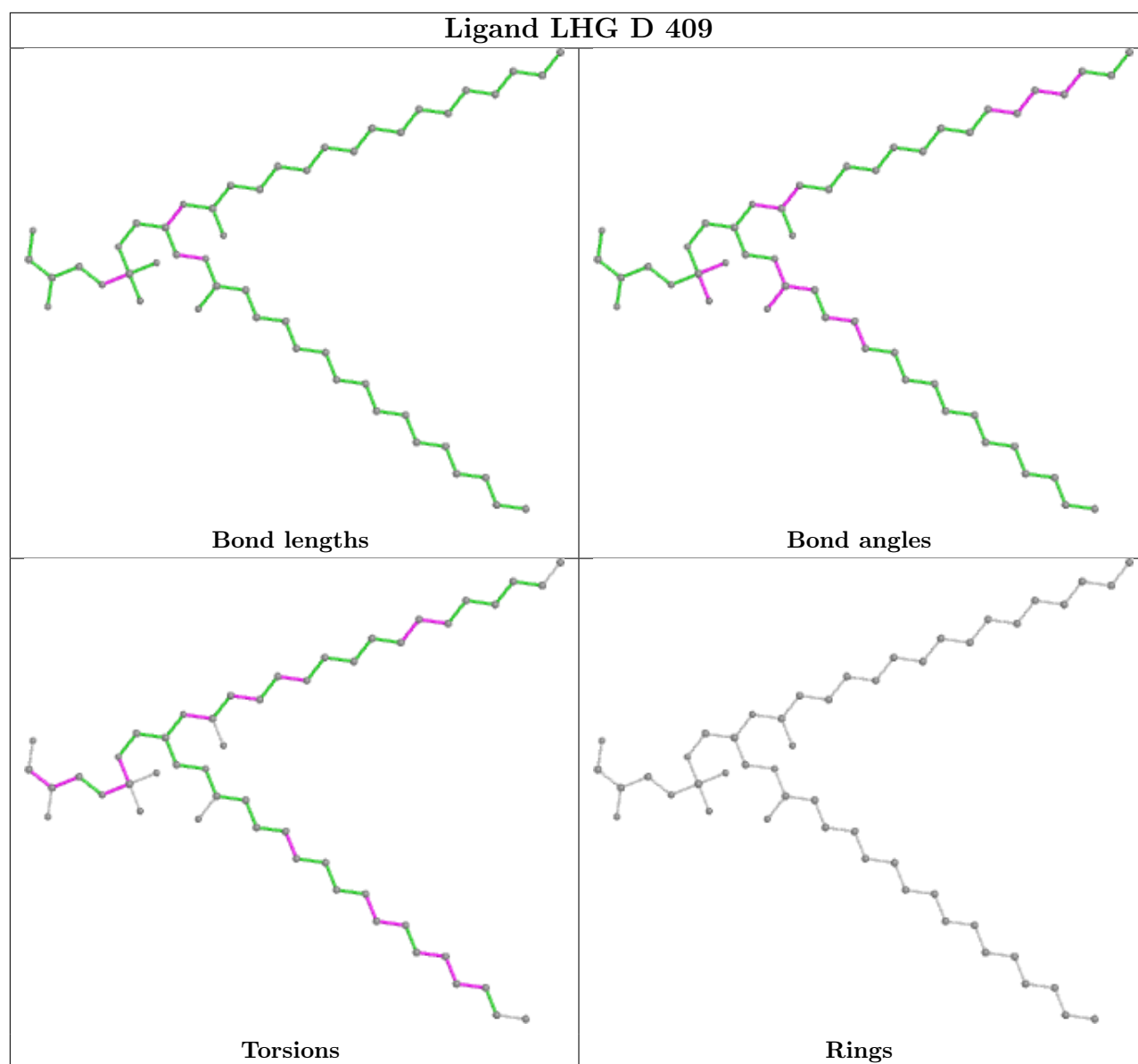
## Ligand CLA B 606



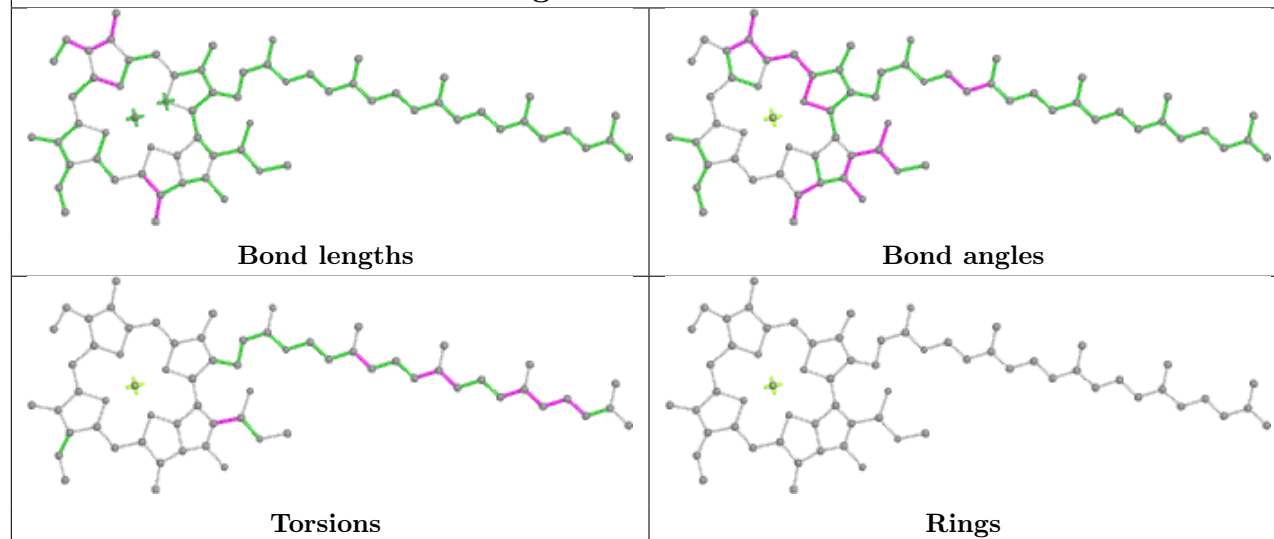


**Ligand CLA c 513****Ligand PL9 d 405****Ligand CLA C 502**

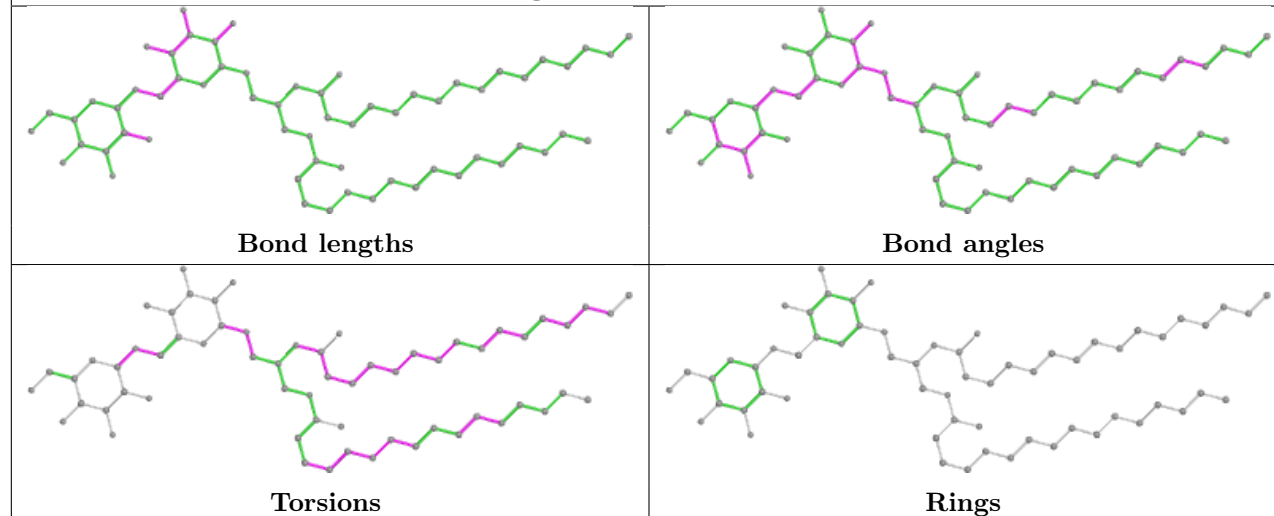
**Ligand CLA C 505****Ligand CLA B 609**



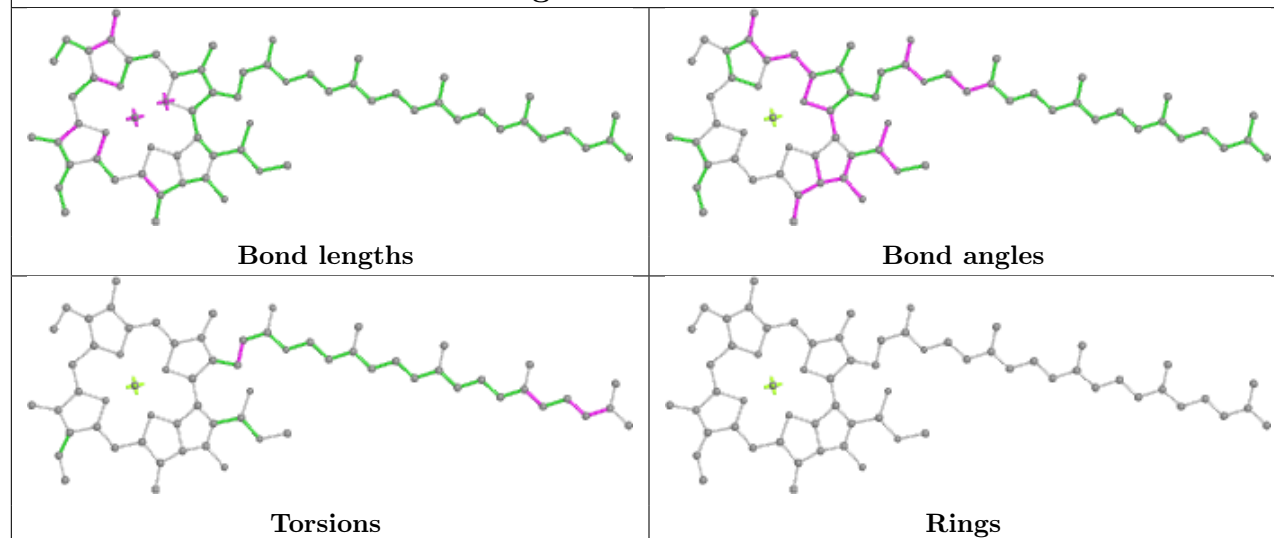
## Ligand CLA C 506

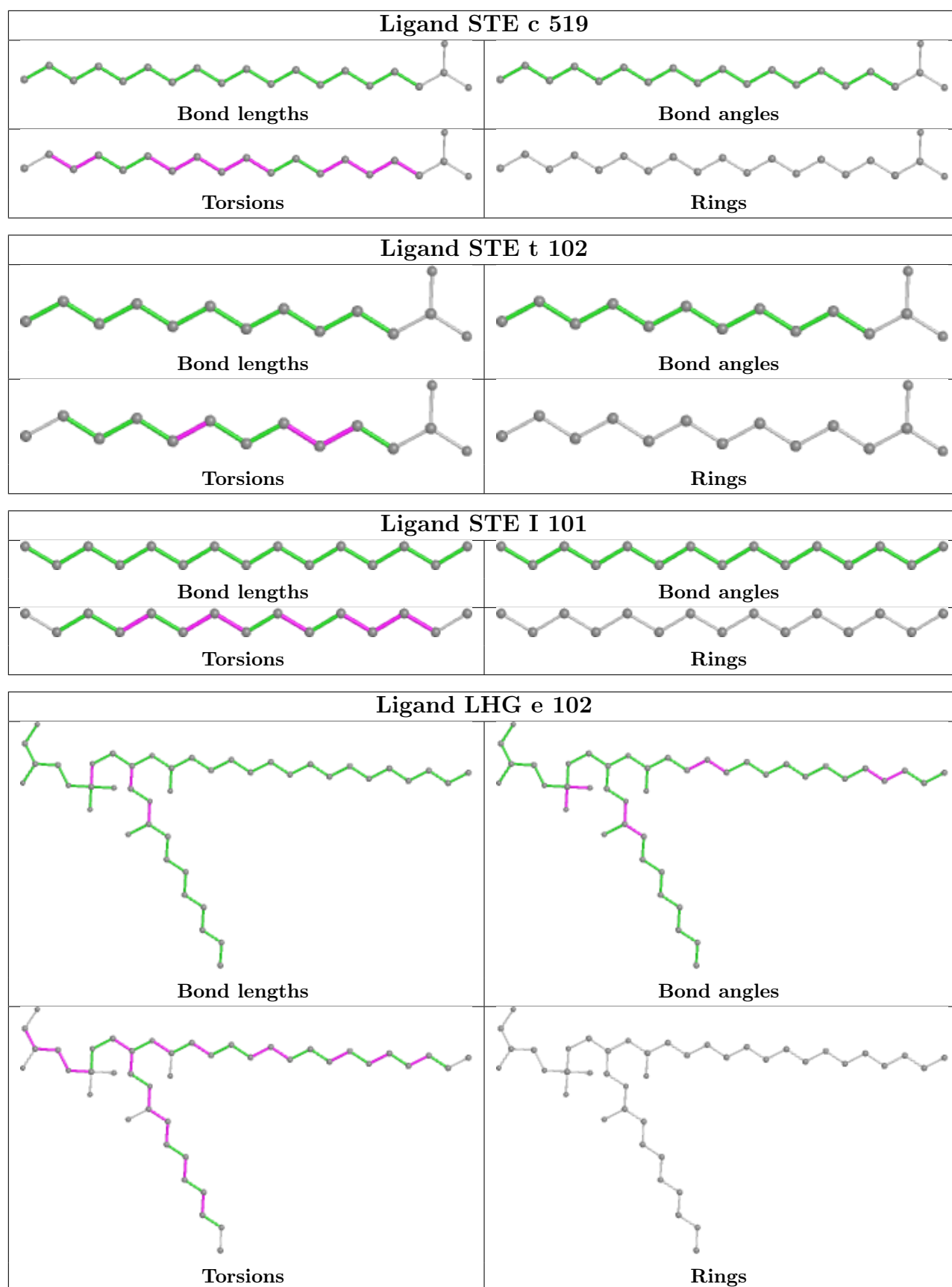


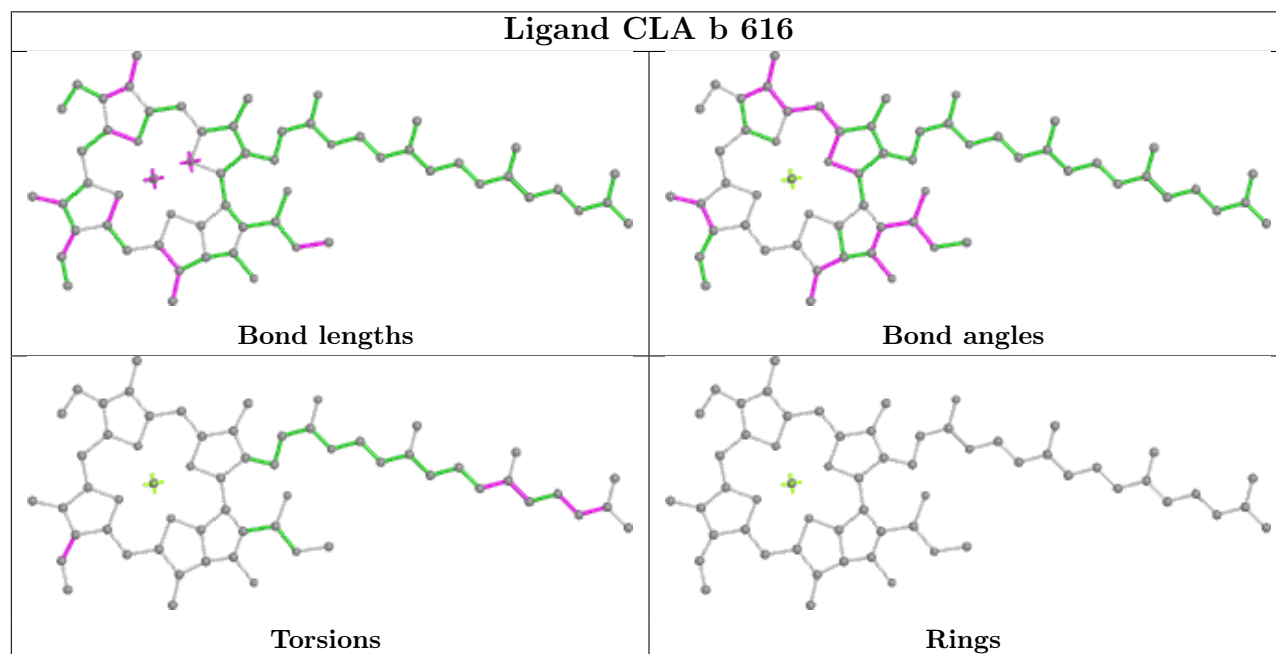
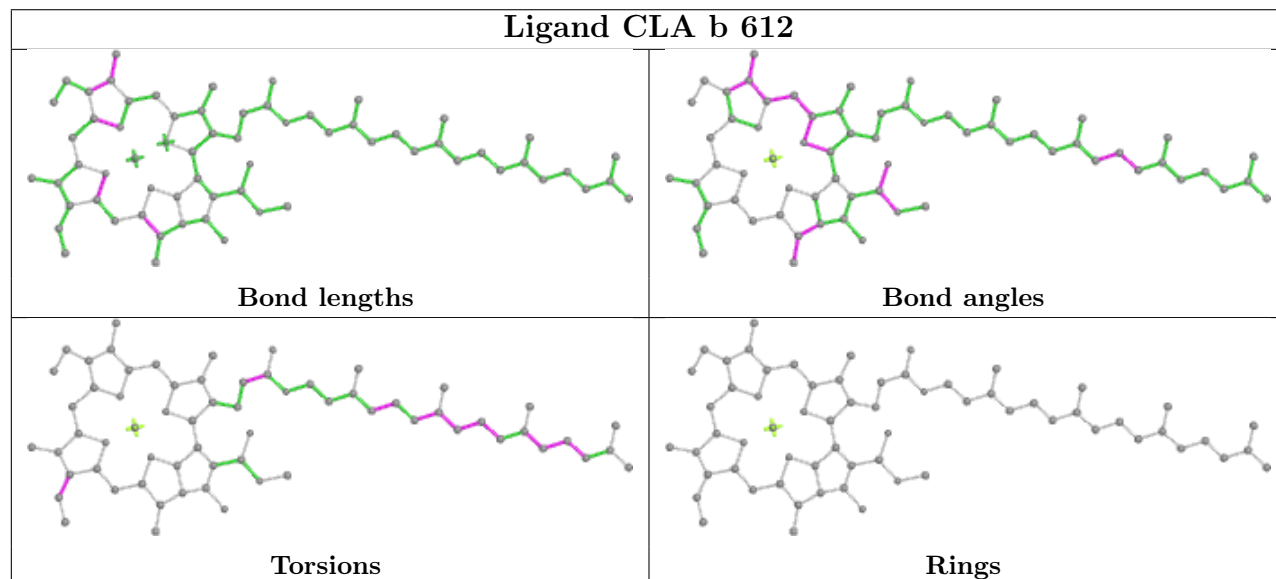
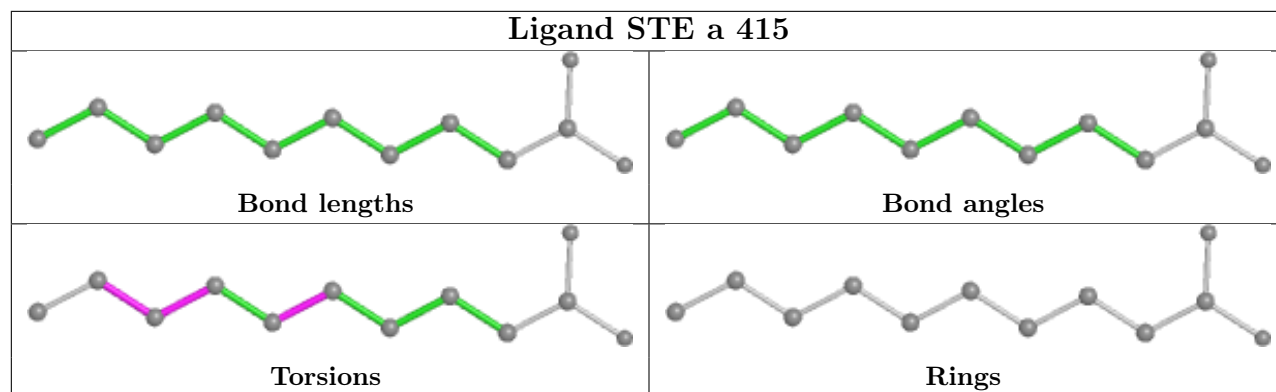
## Ligand DGD C 516

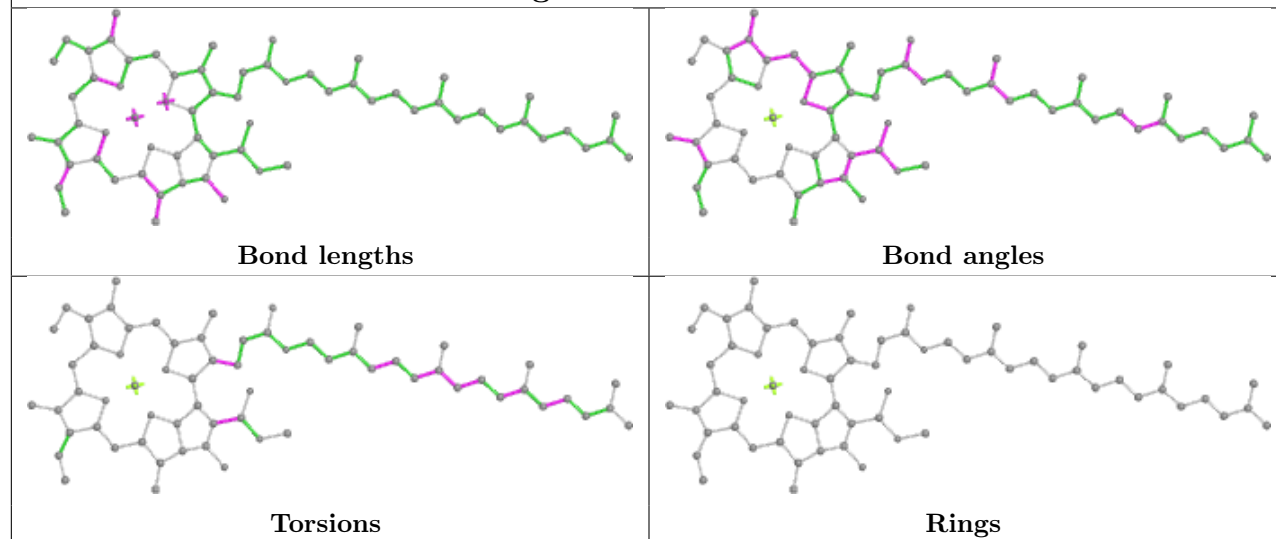
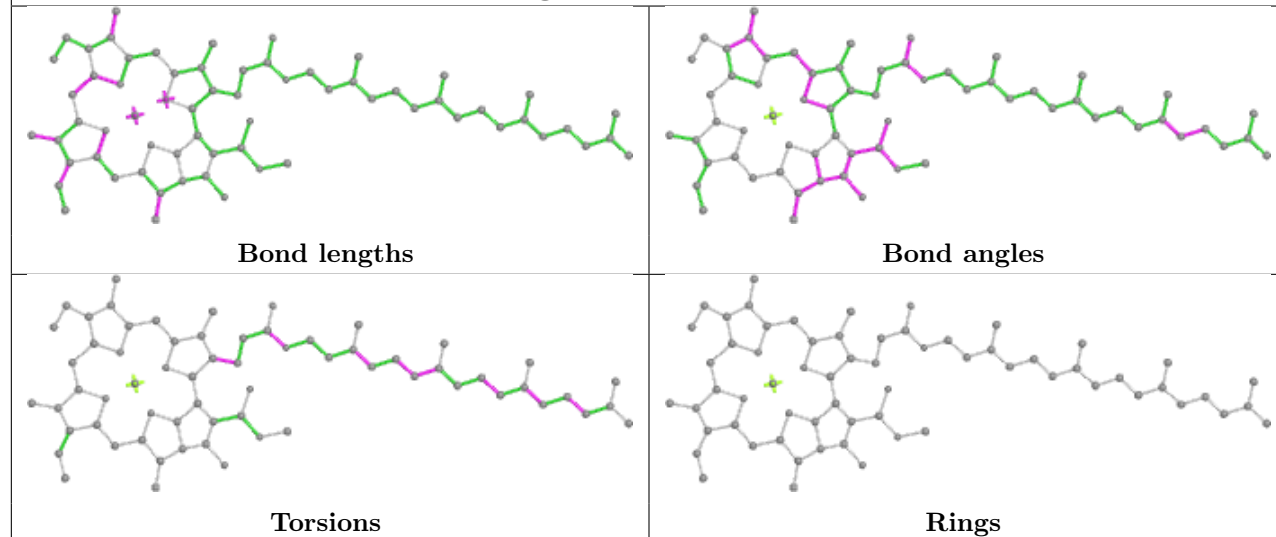


## Ligand CLA B 610

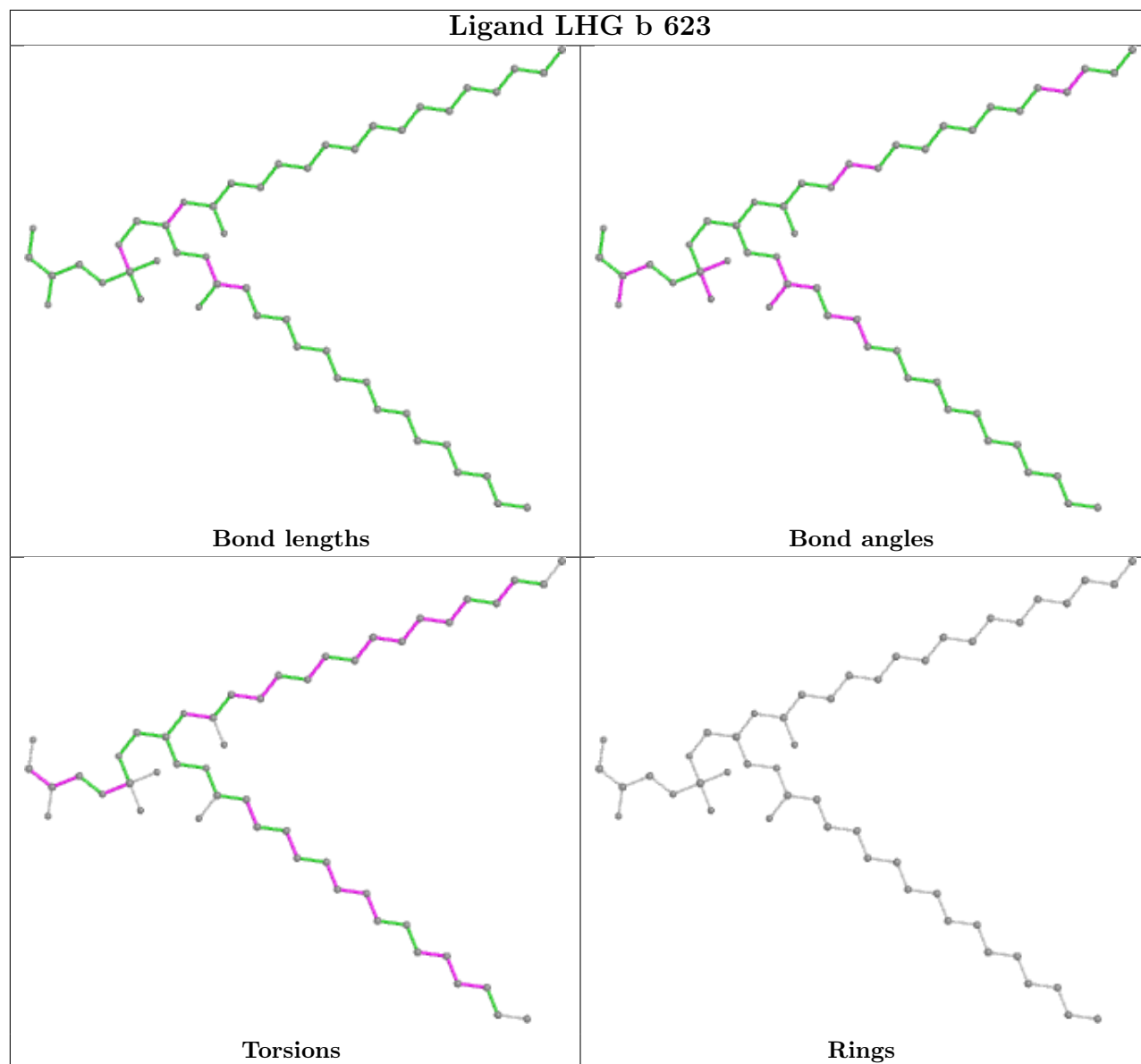




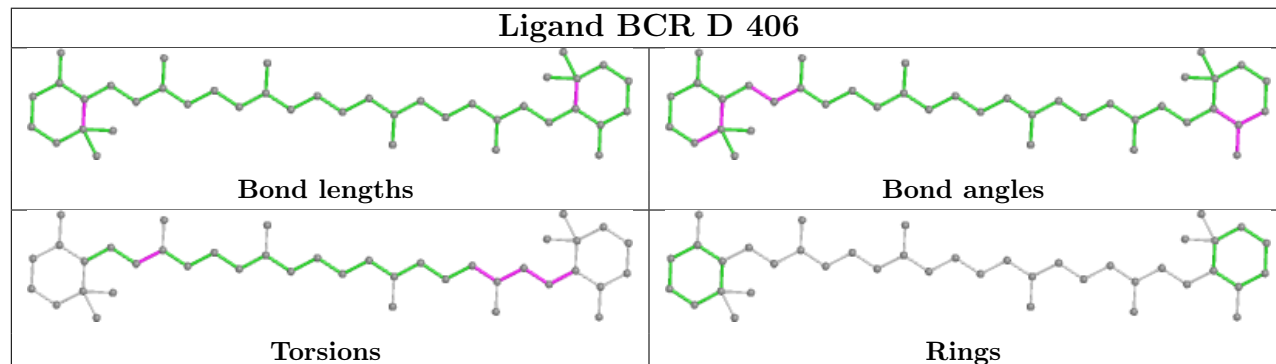


**Ligand CLA B 602****Ligand CLA a 405**

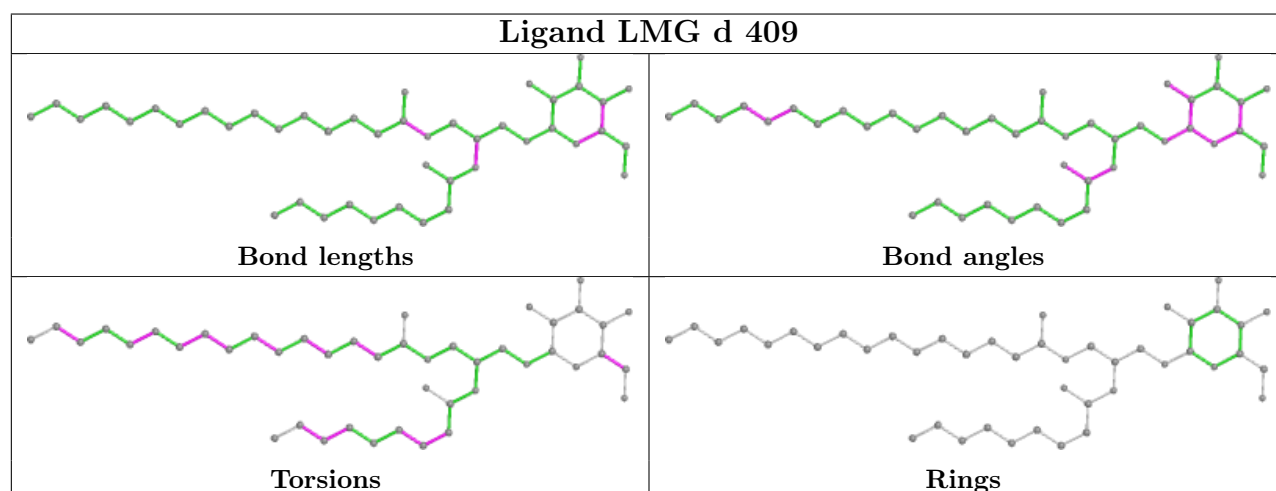
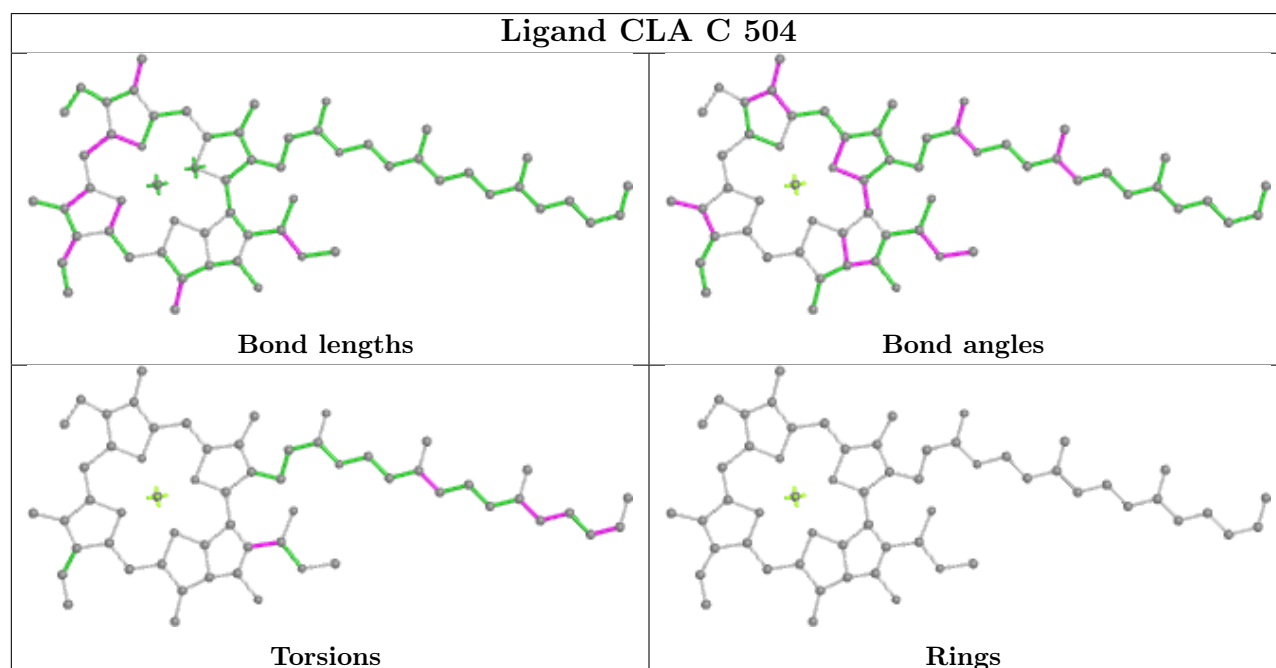
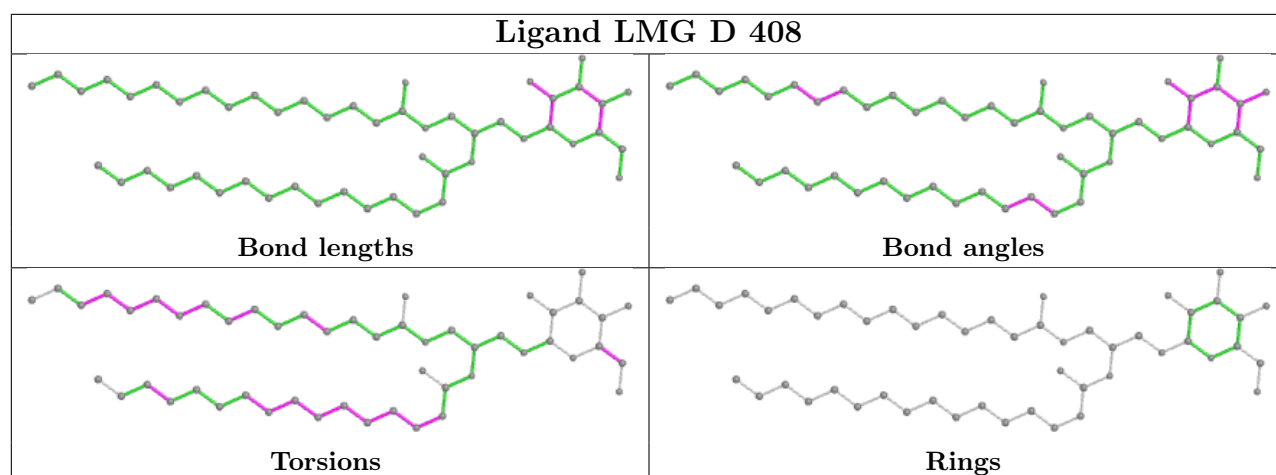
## Ligand LHG b 623

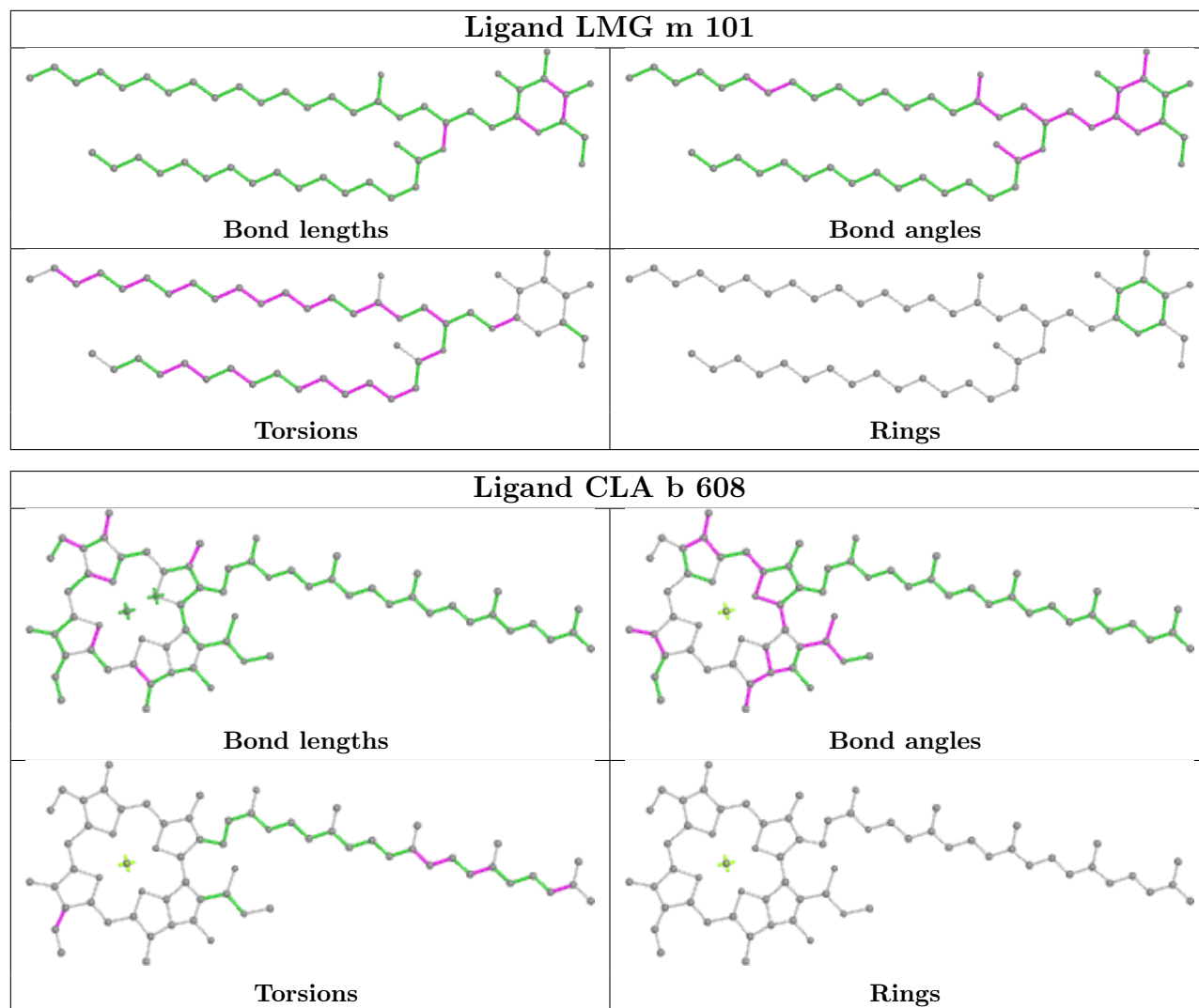


## Ligand BCR D 406

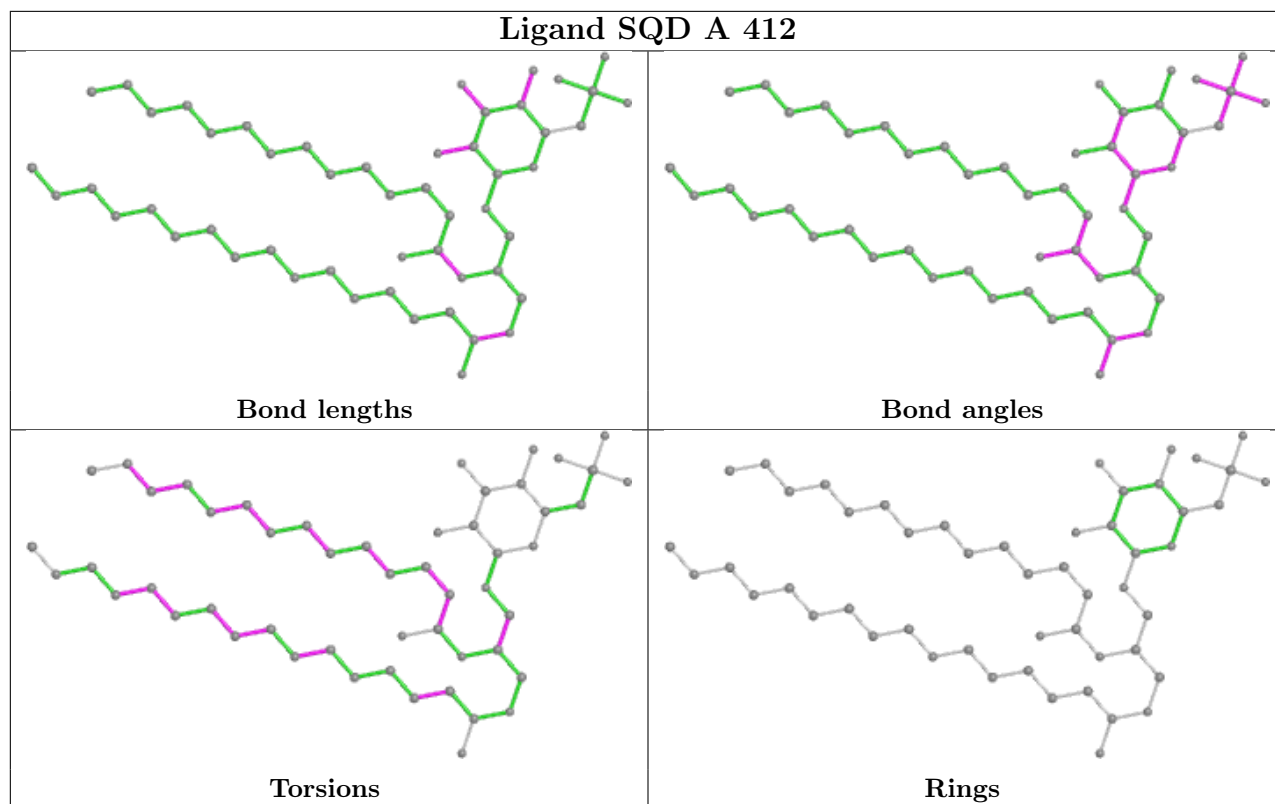




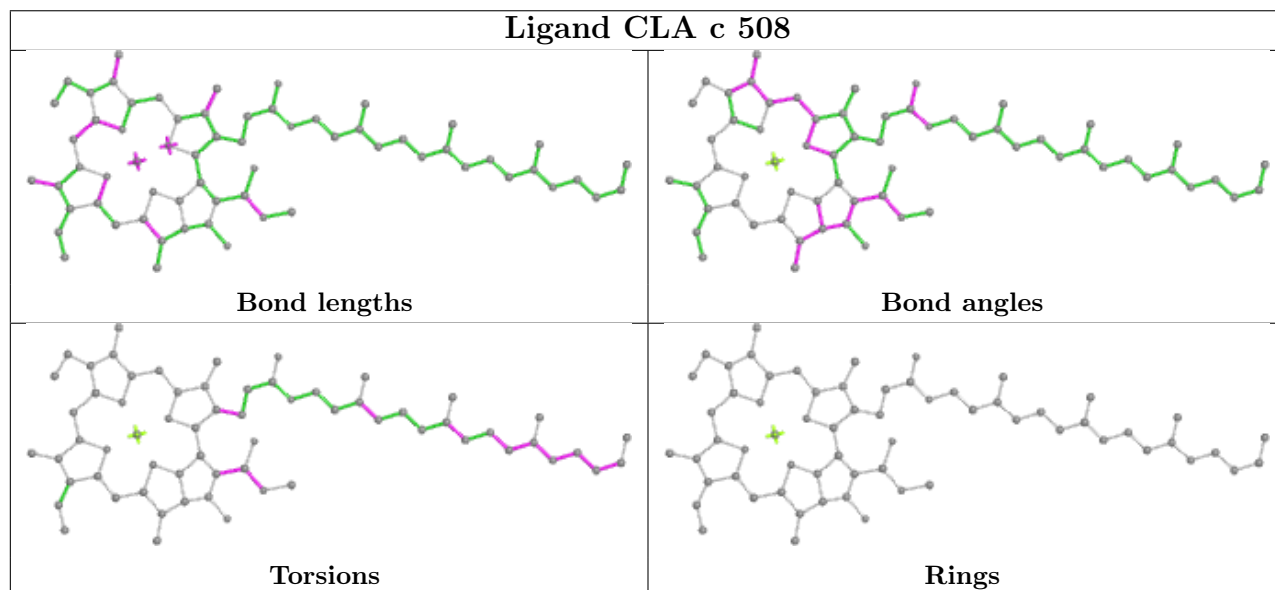




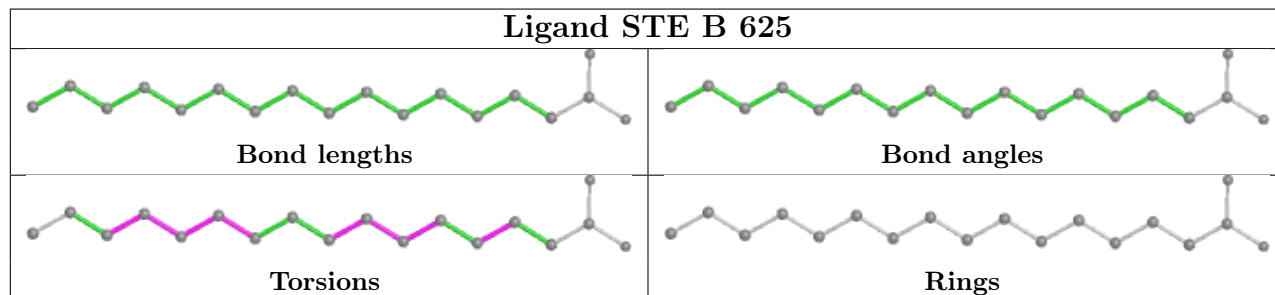
## Ligand SQD A 412

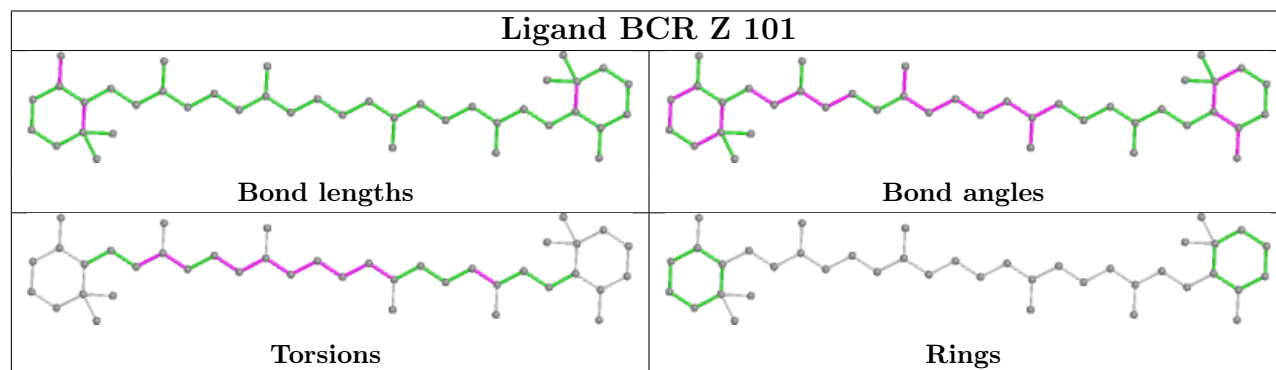
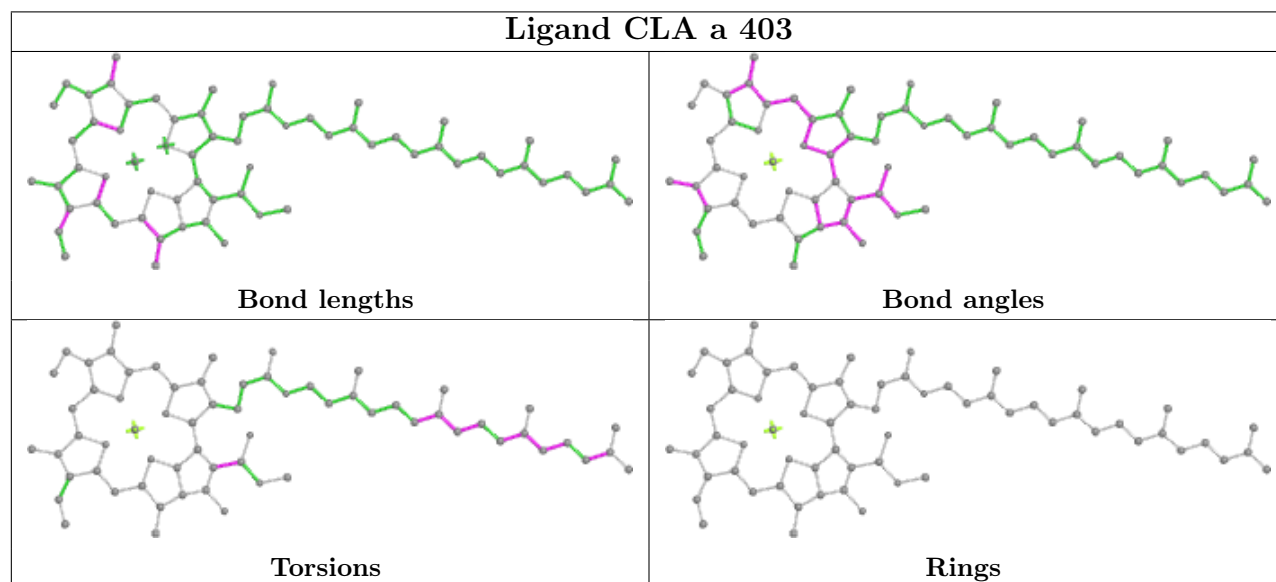
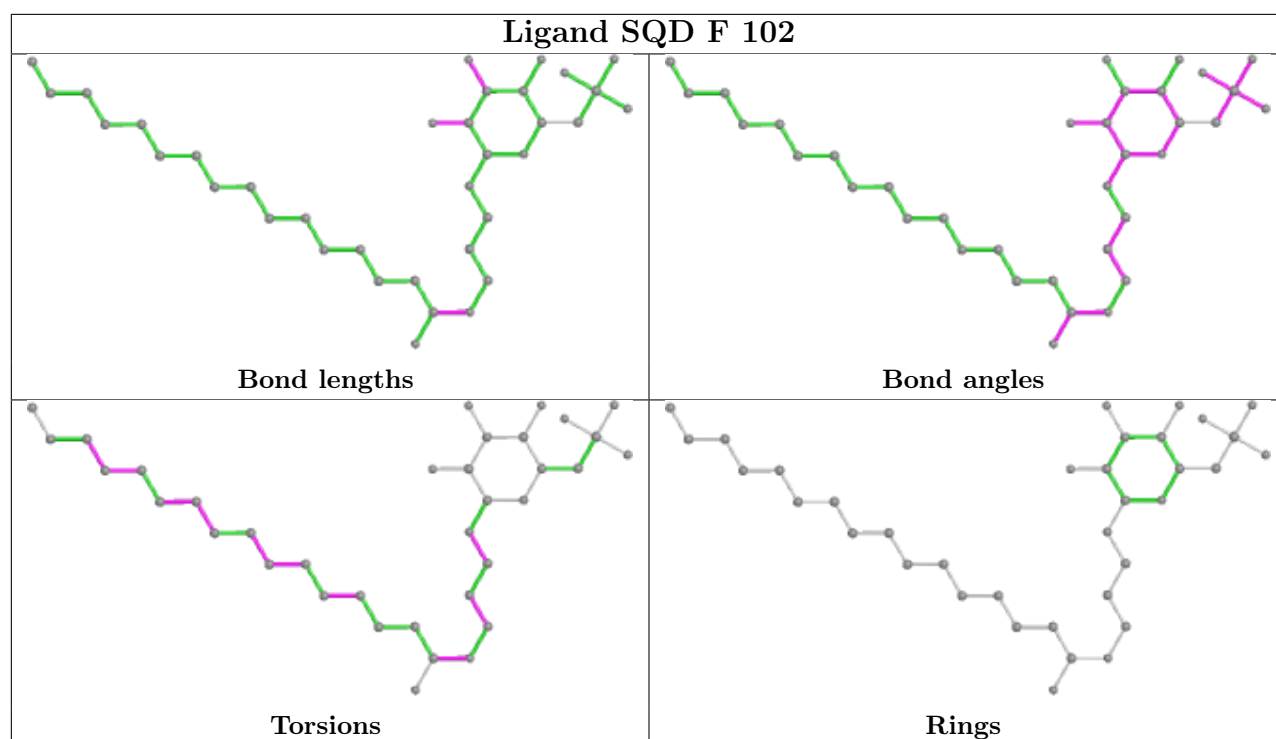


## Ligand CLA c 508

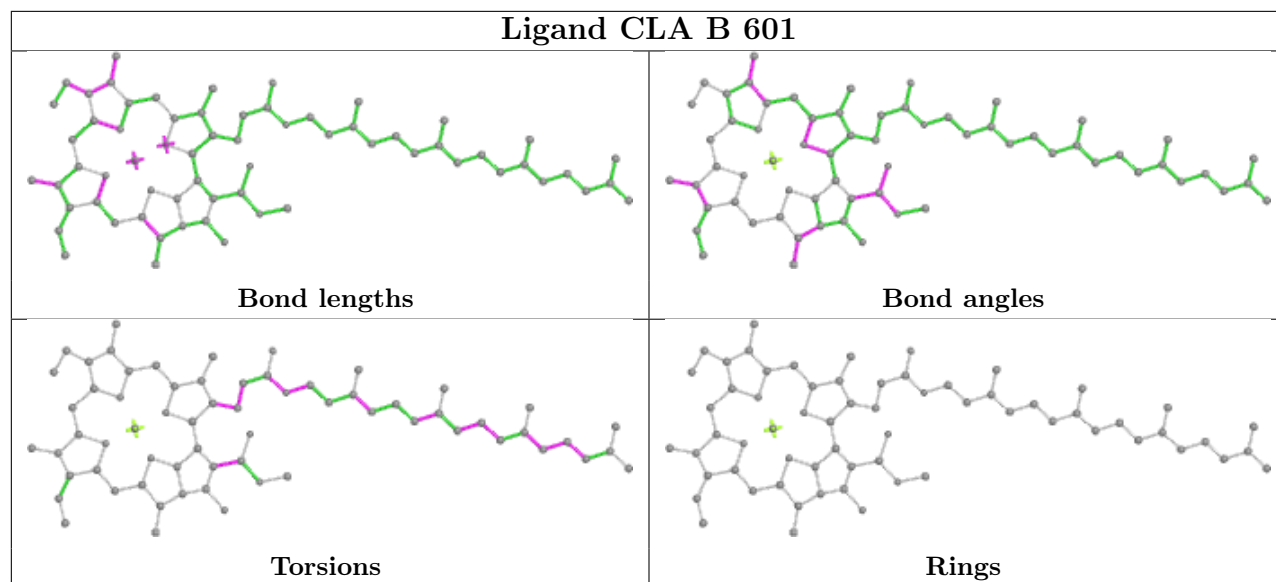


## Ligand STE B 625

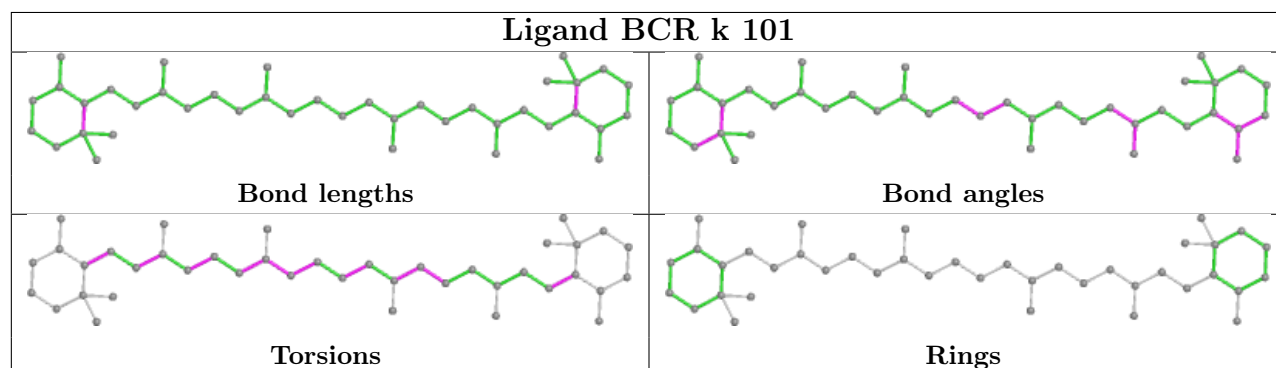




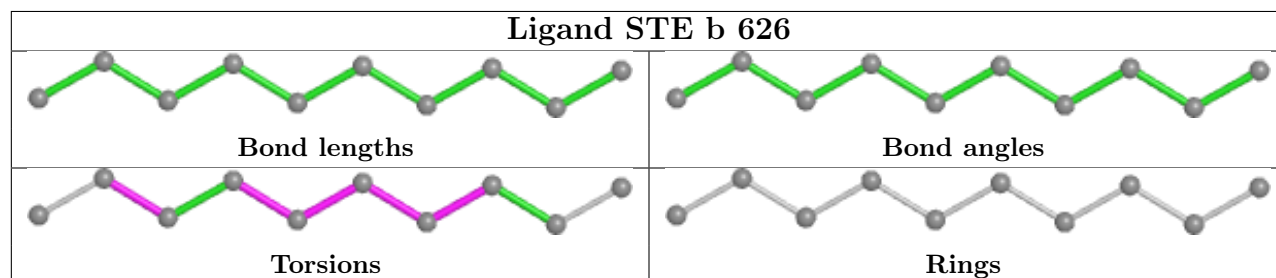
## Ligand CLA B 601



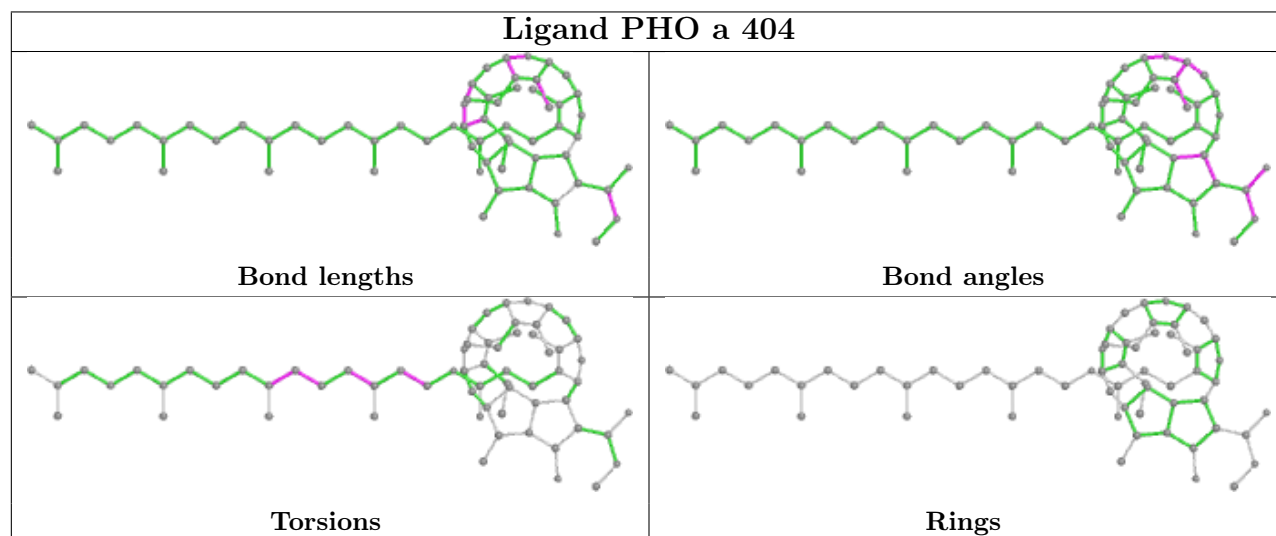
## Ligand BCR k 101



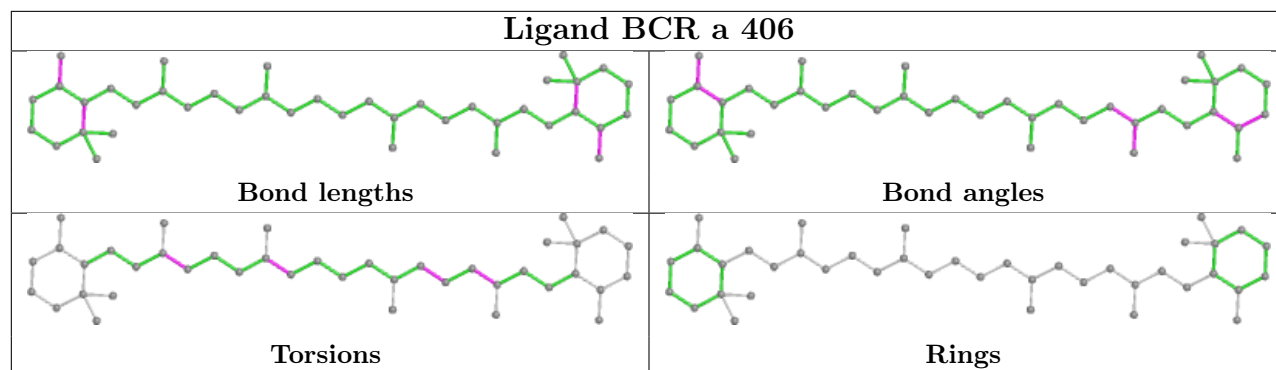
## Ligand STE b 626



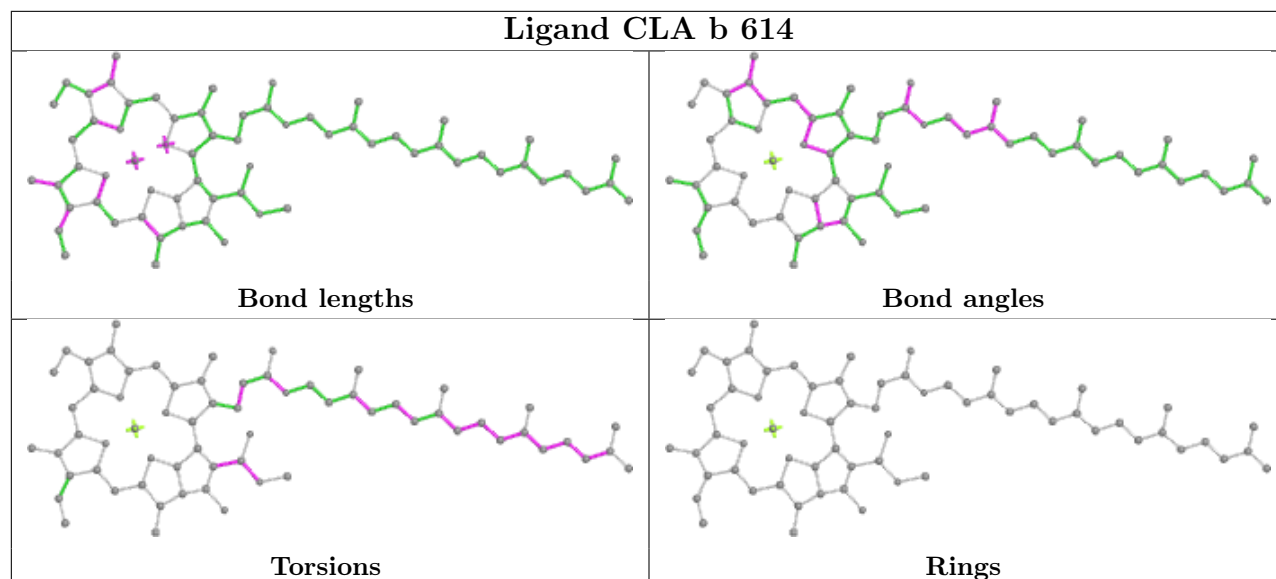
## Ligand PHO a 404



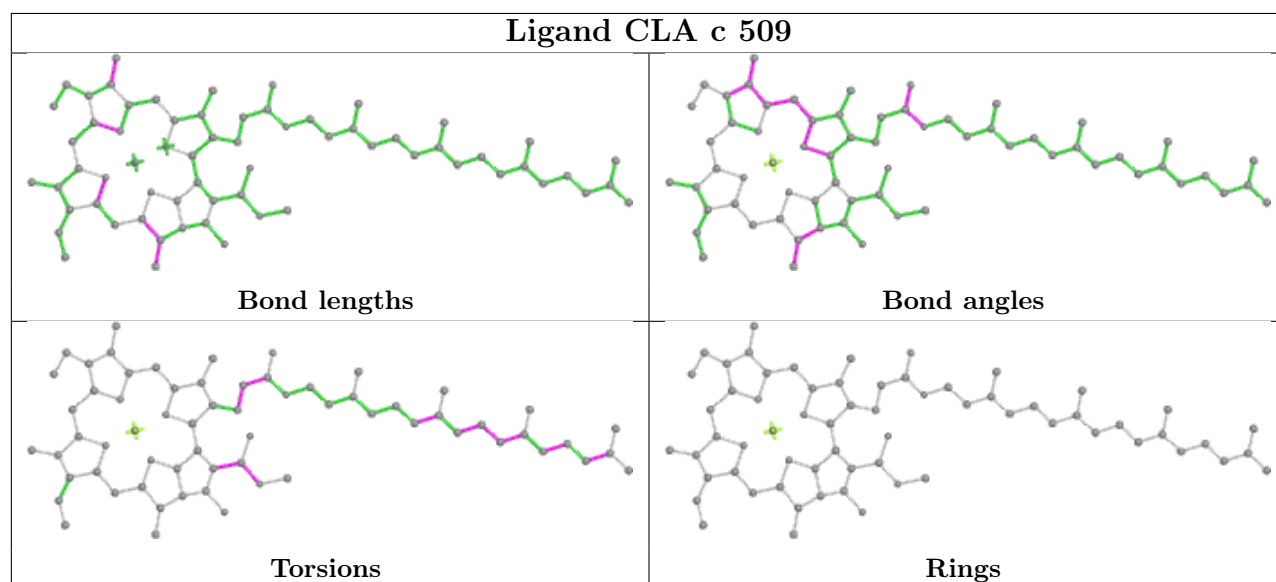
## Ligand BCR a 406

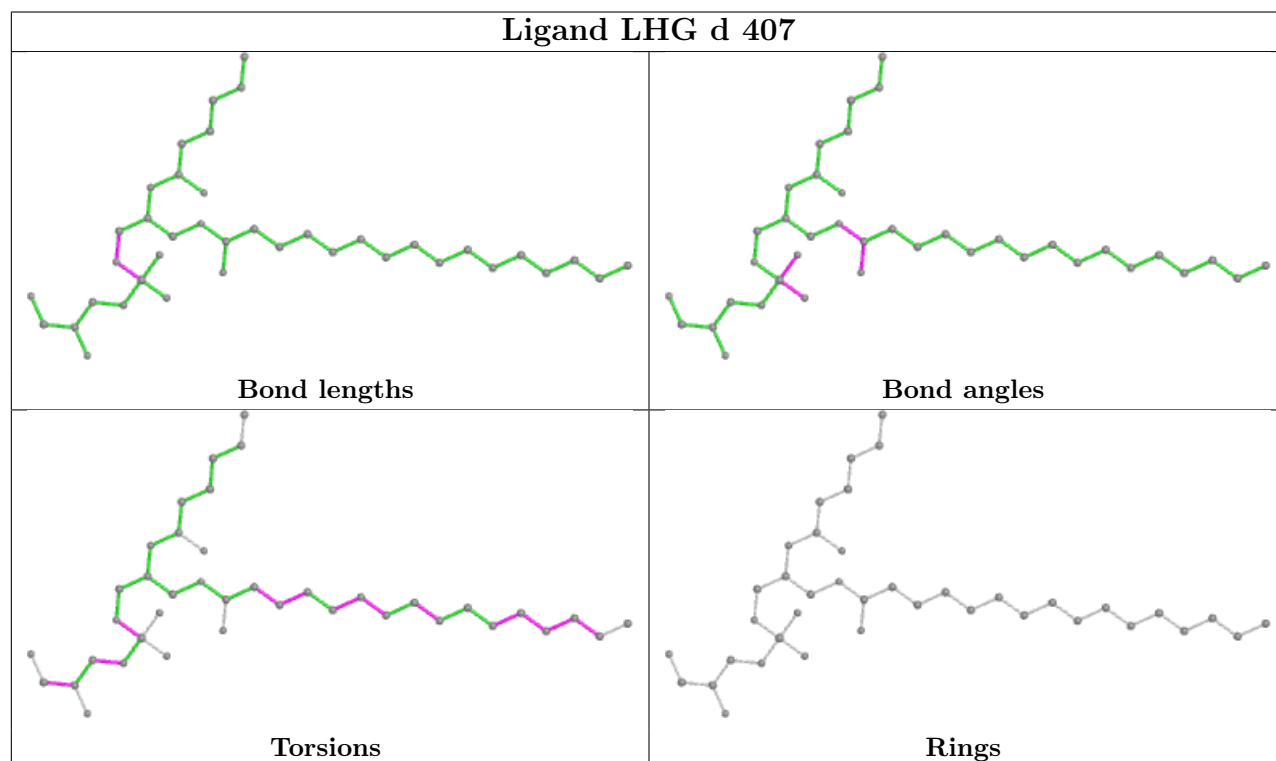
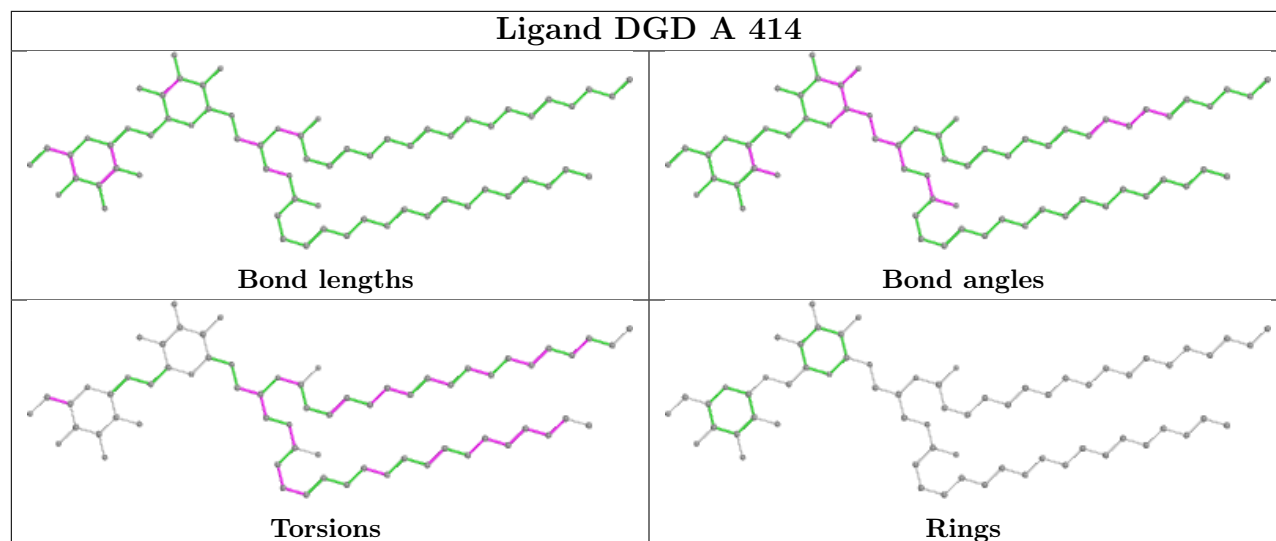


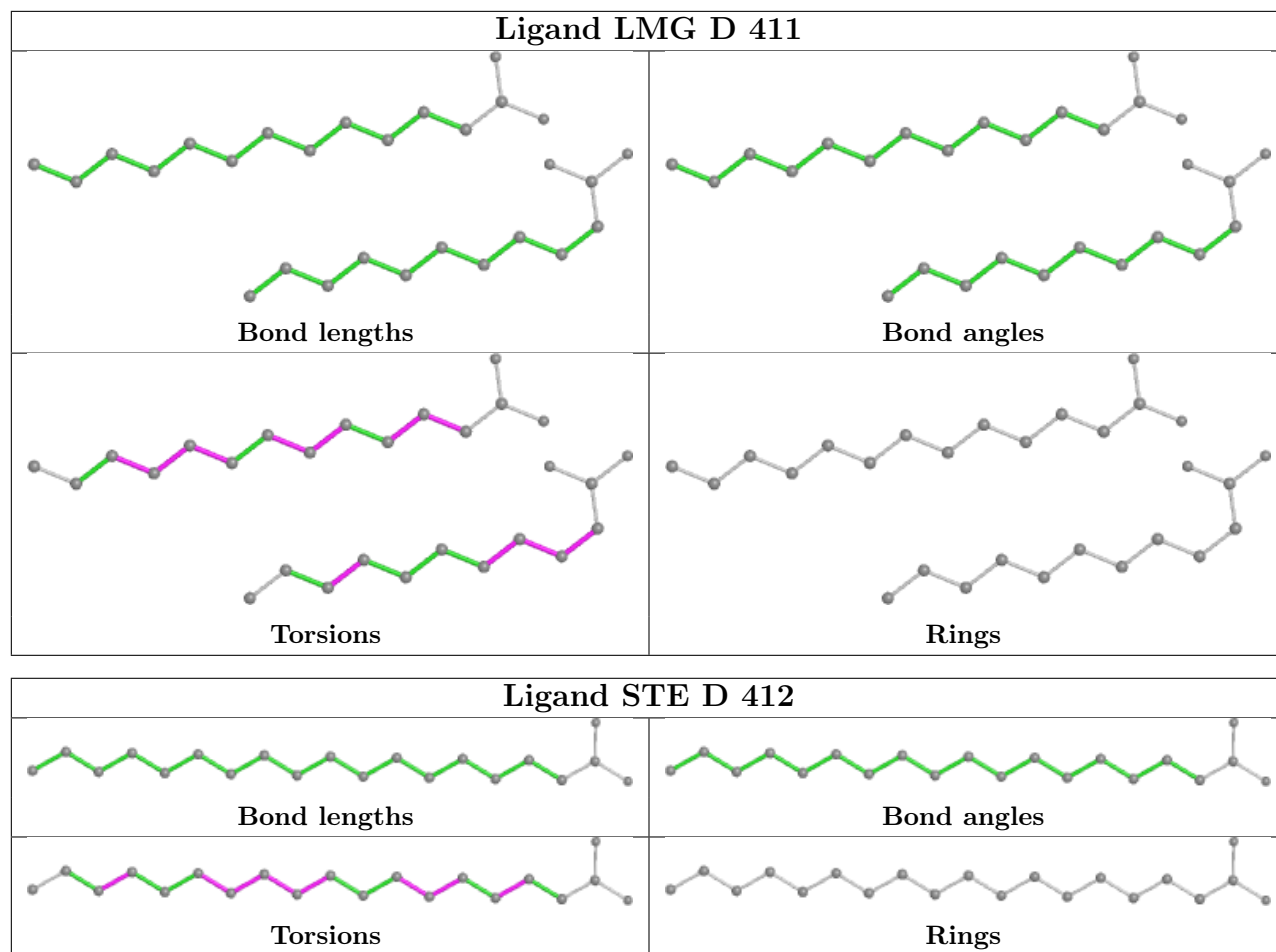
## Ligand CLA b 614



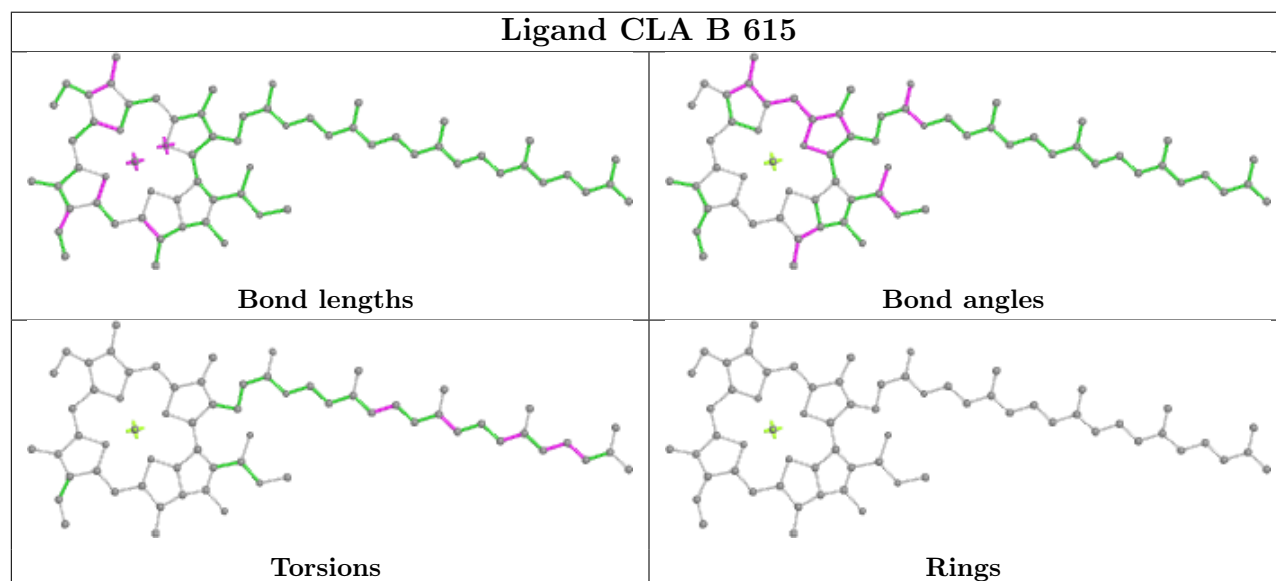
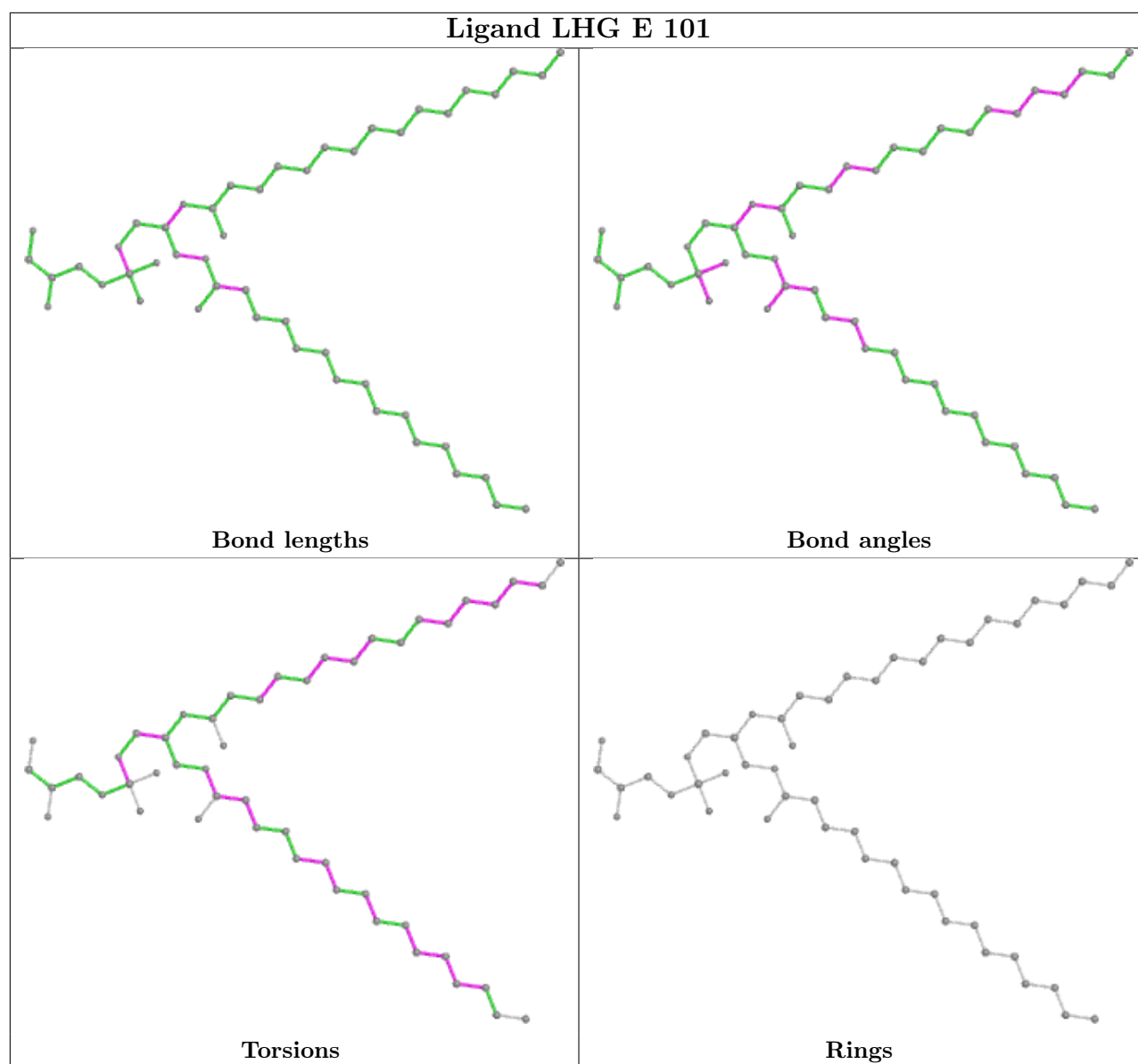
## Ligand CLA c 509

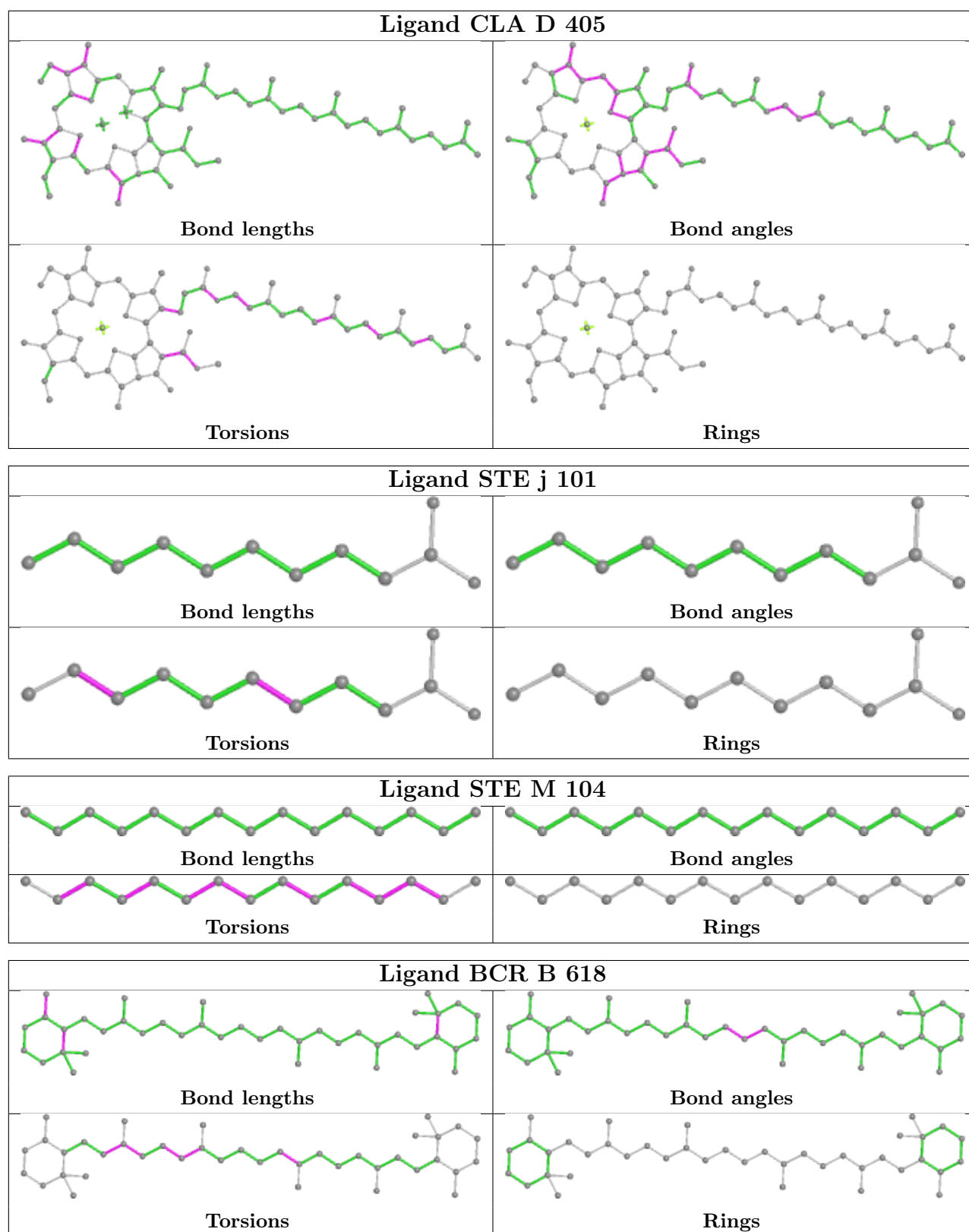


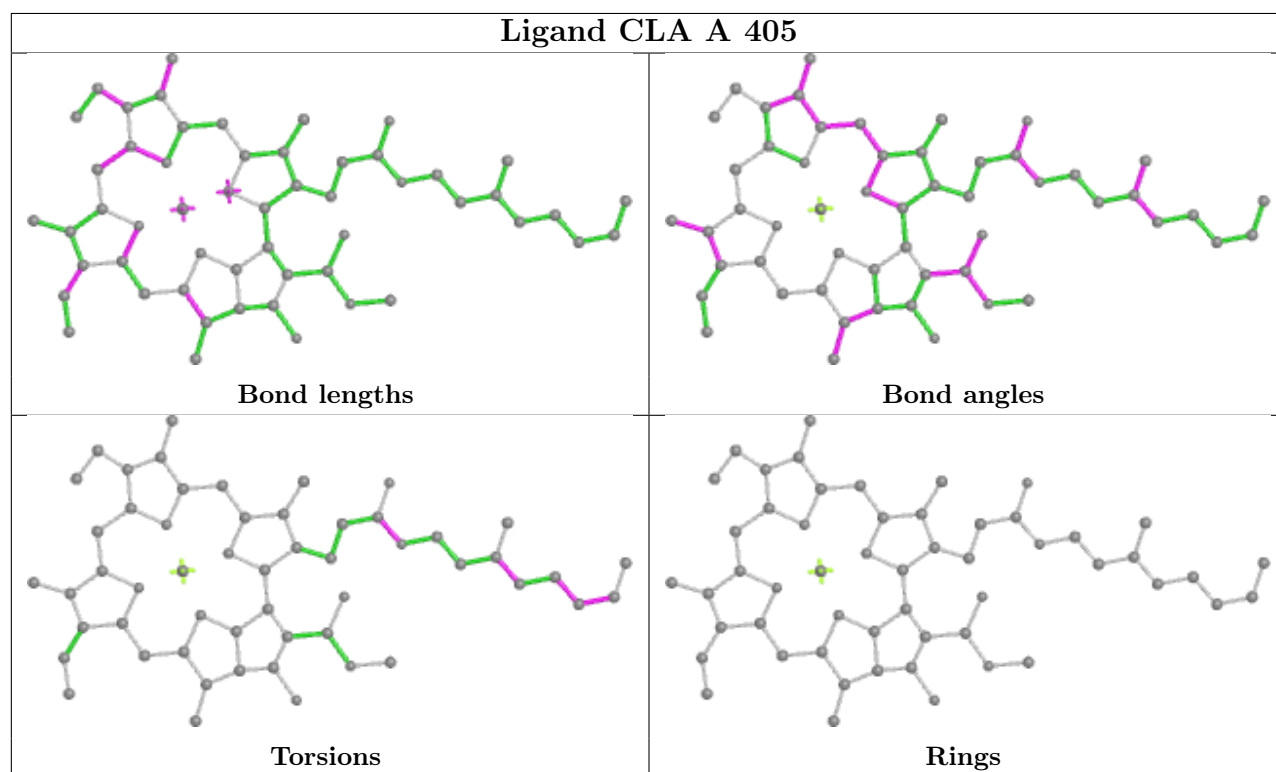
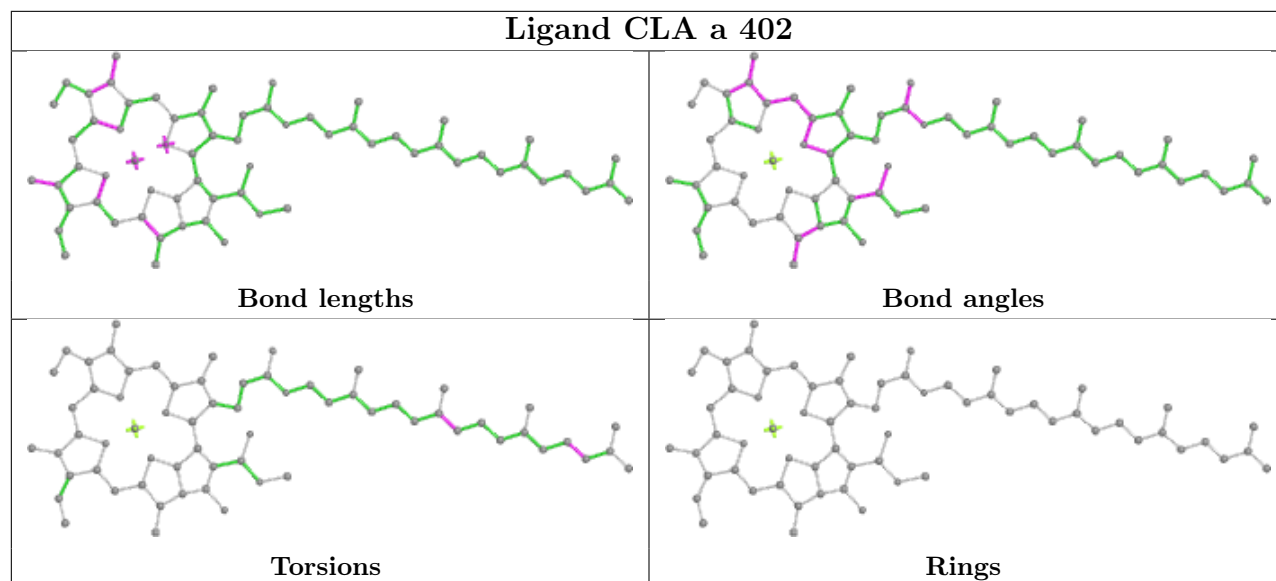
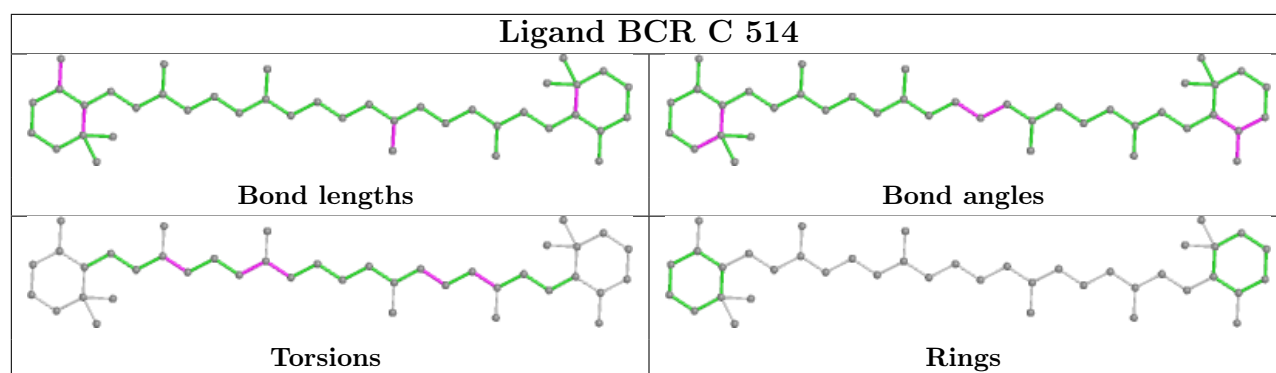


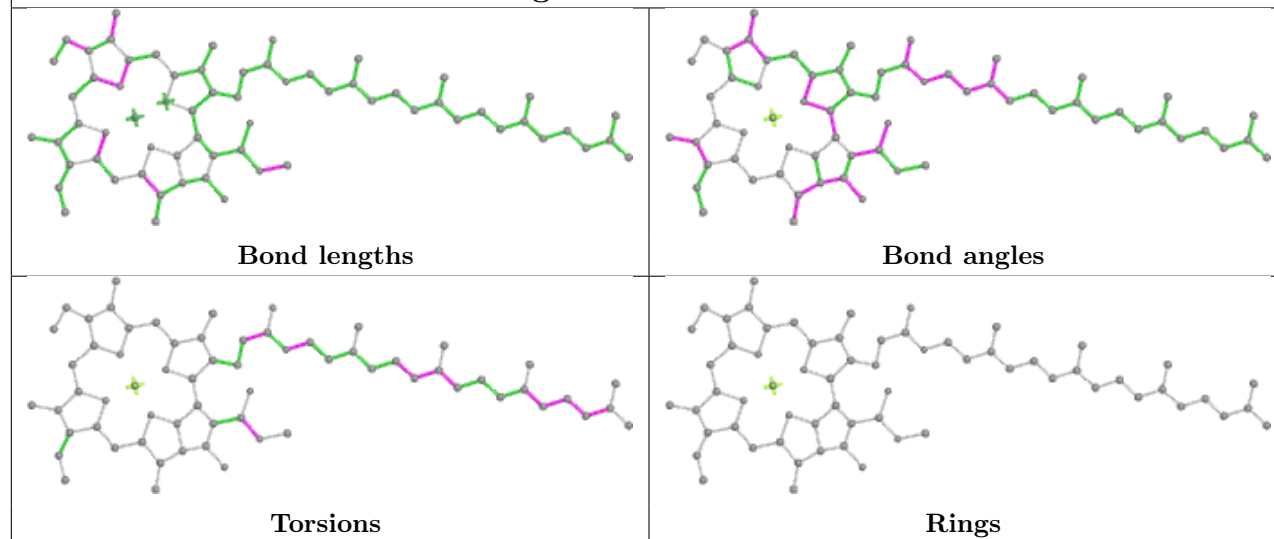
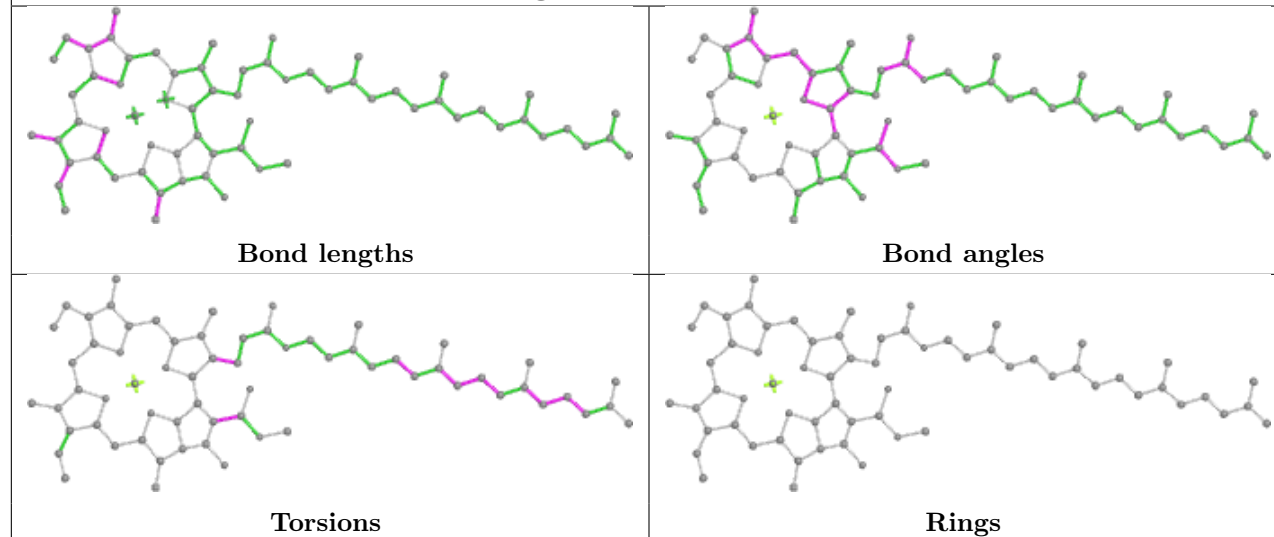
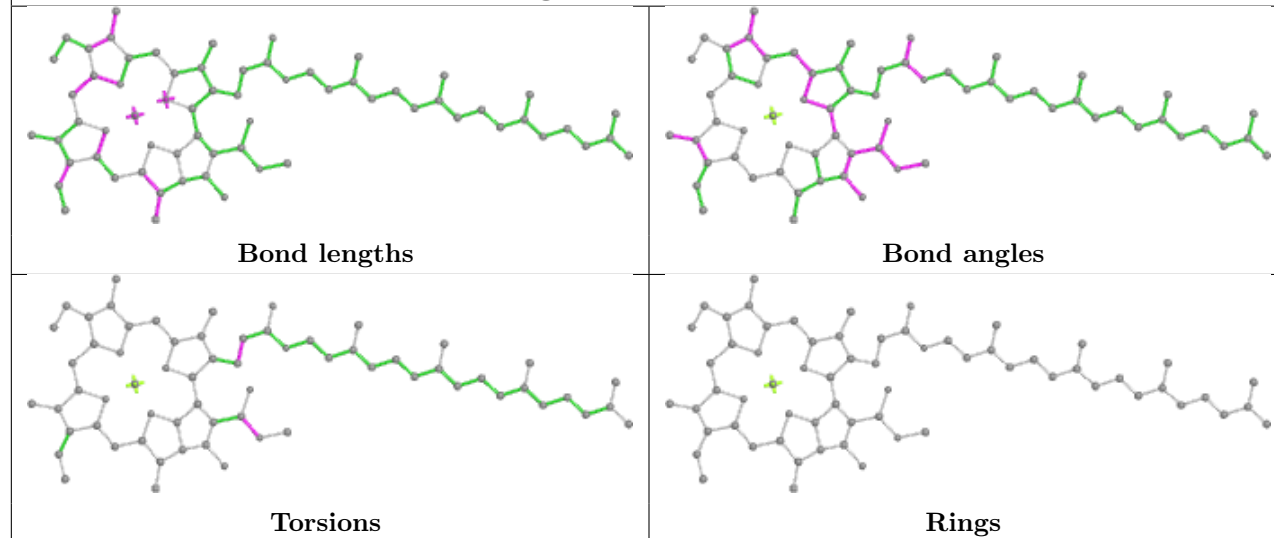




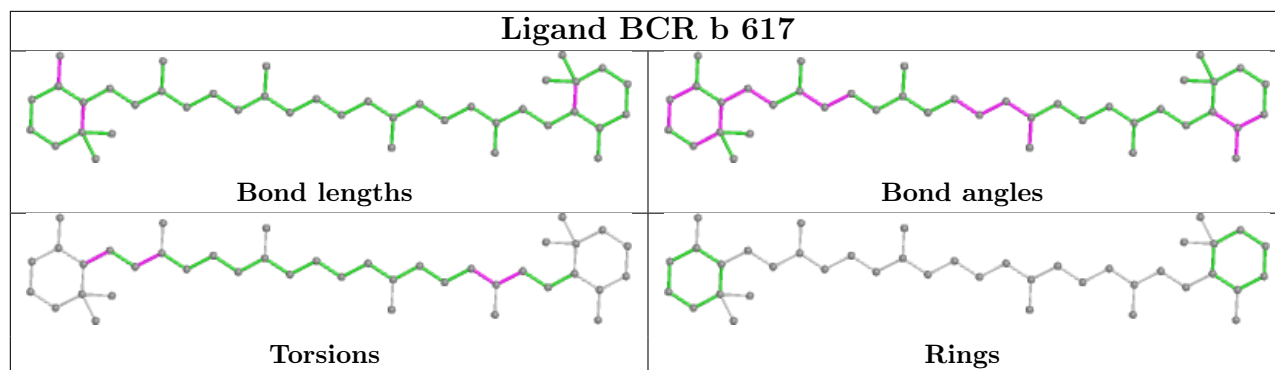




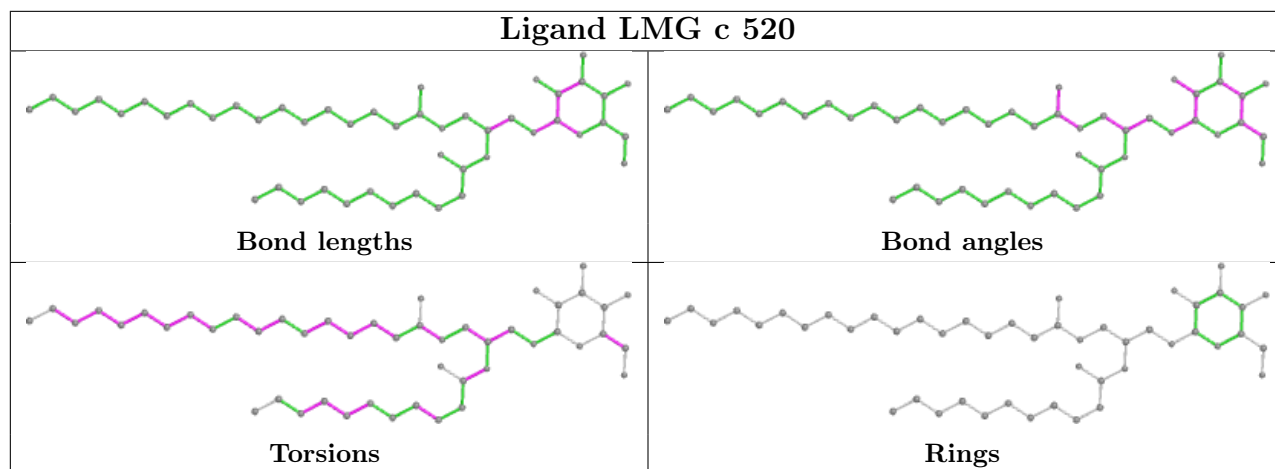


**Ligand CLA B 613****Ligand CLA B 607****Ligand CLA c 501**

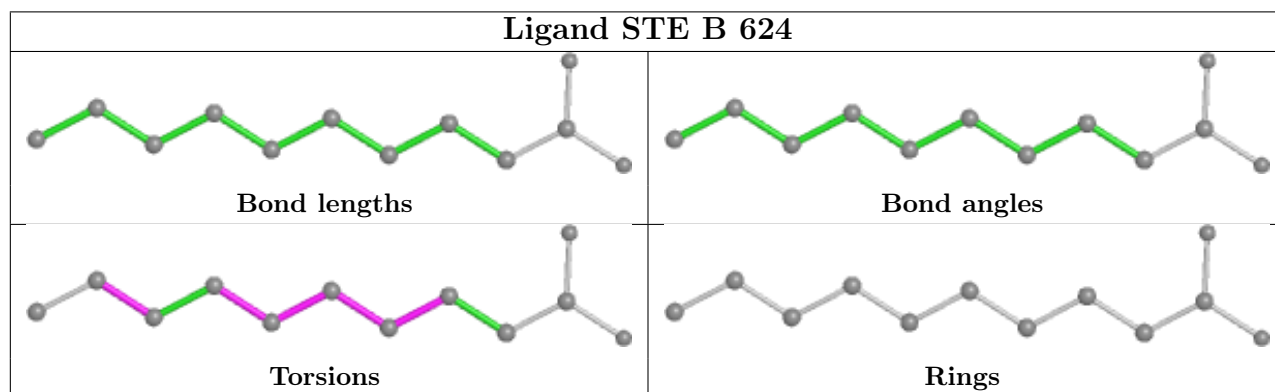
## Ligand BCR b 617

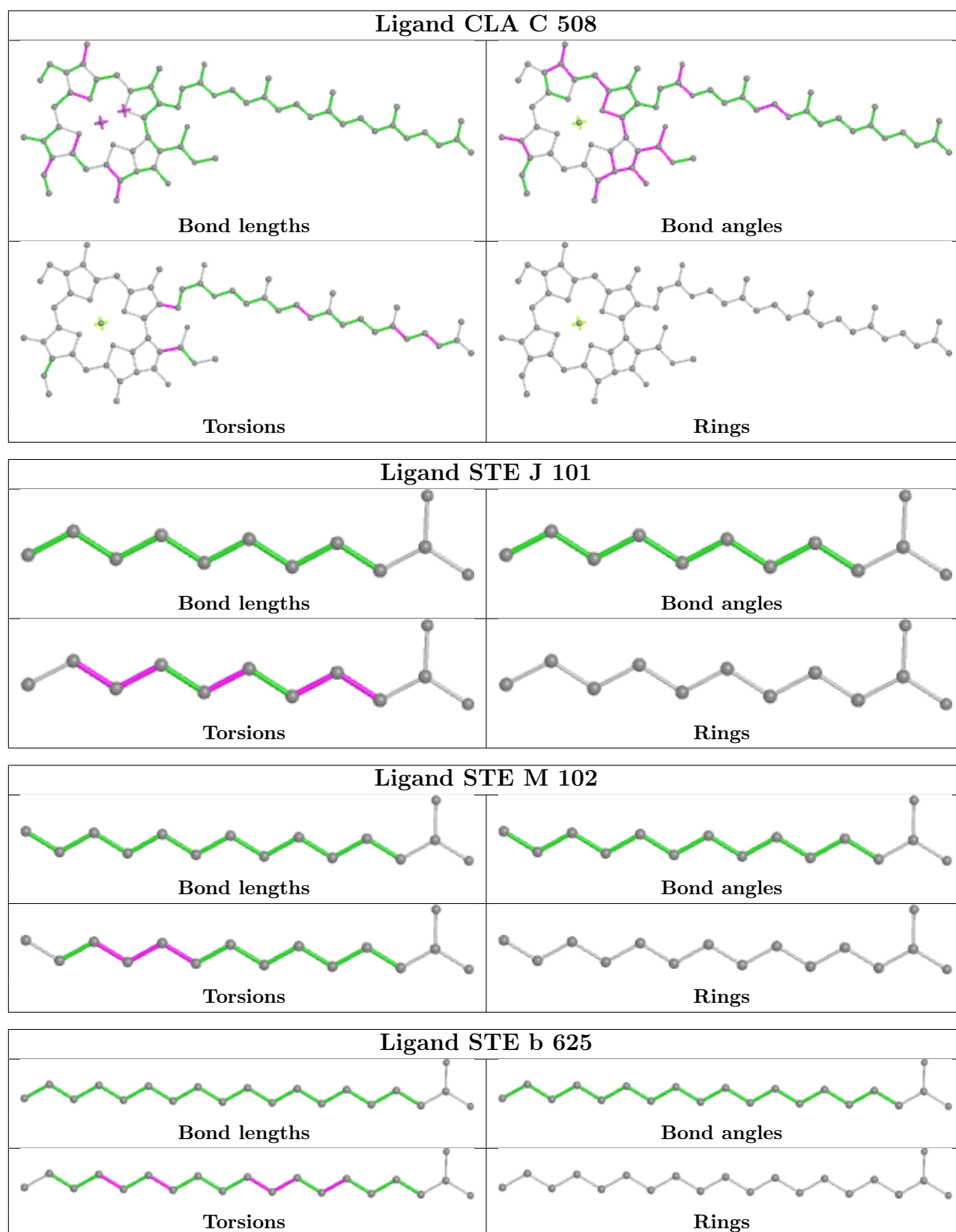


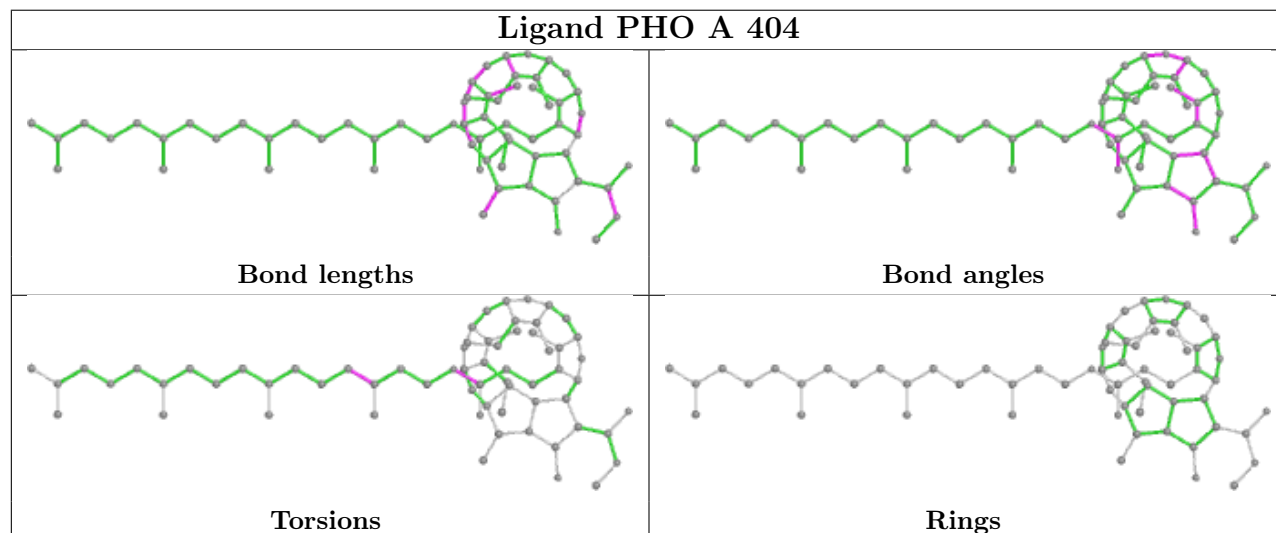
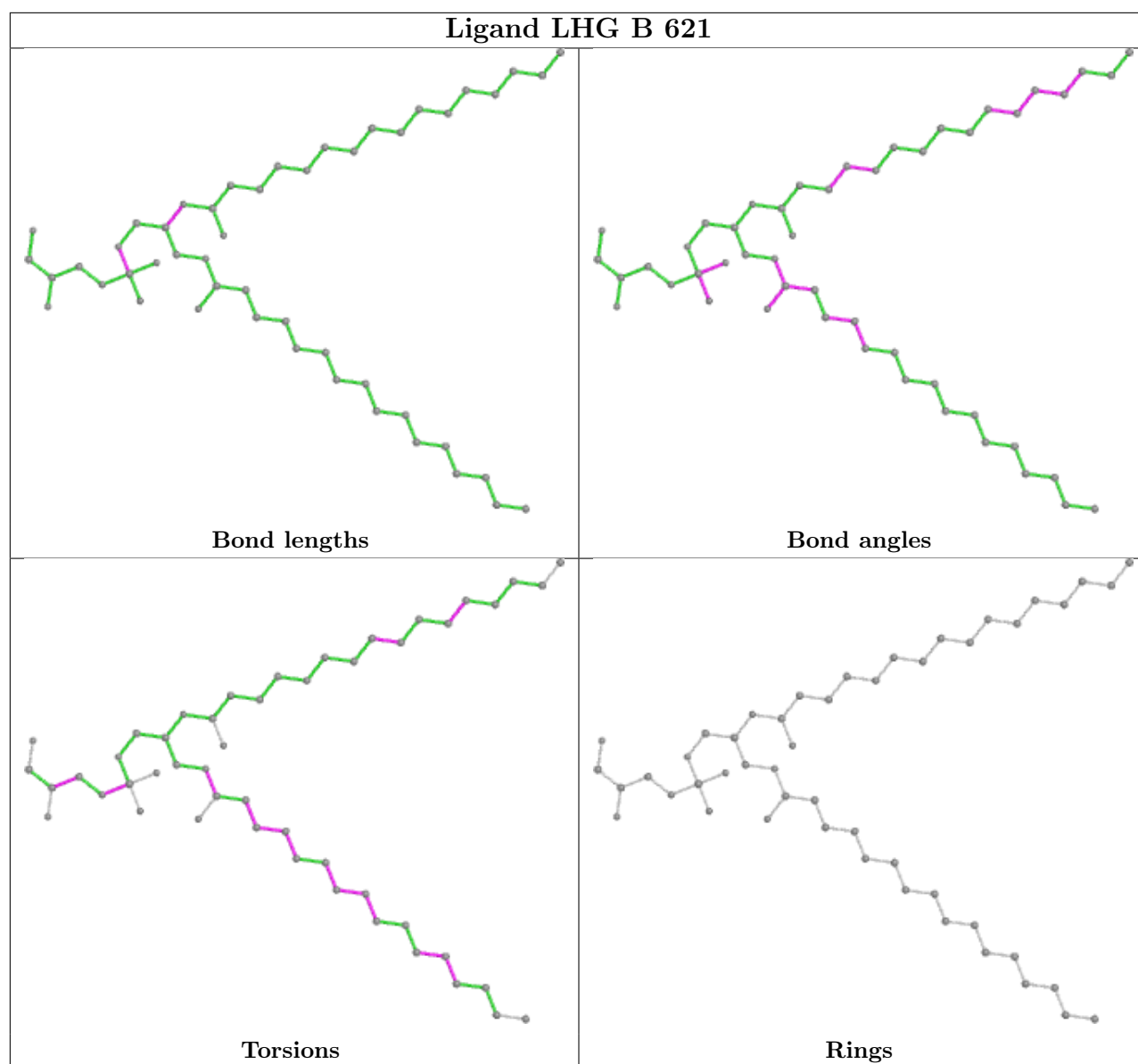
## Ligand LMG c 520

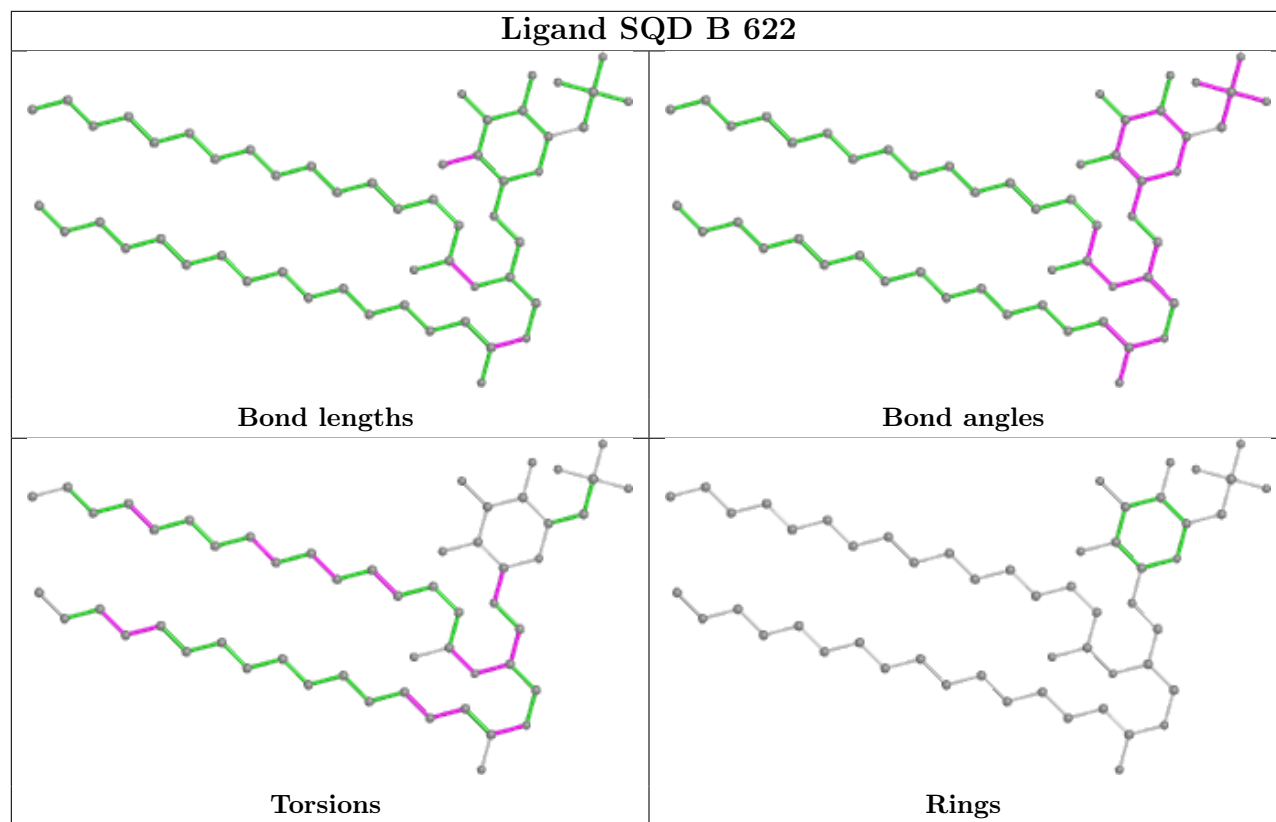
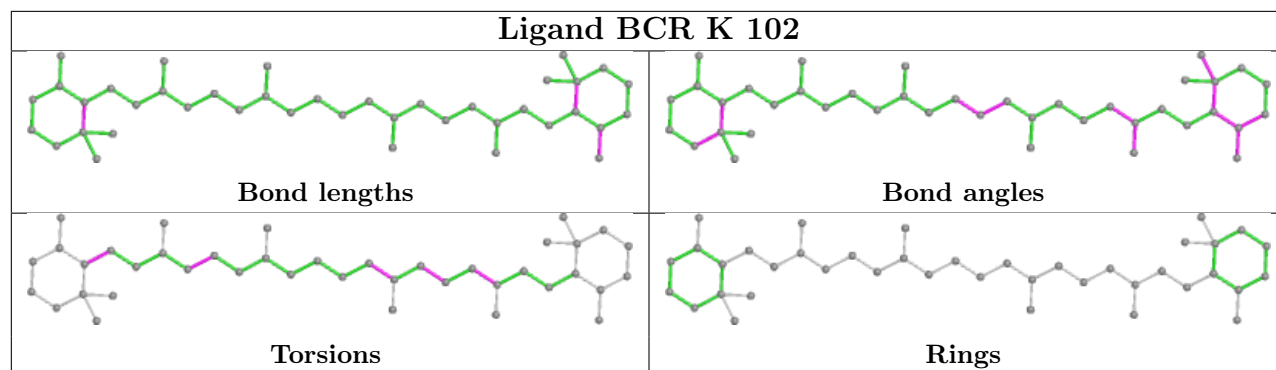


## Ligand STE B 624

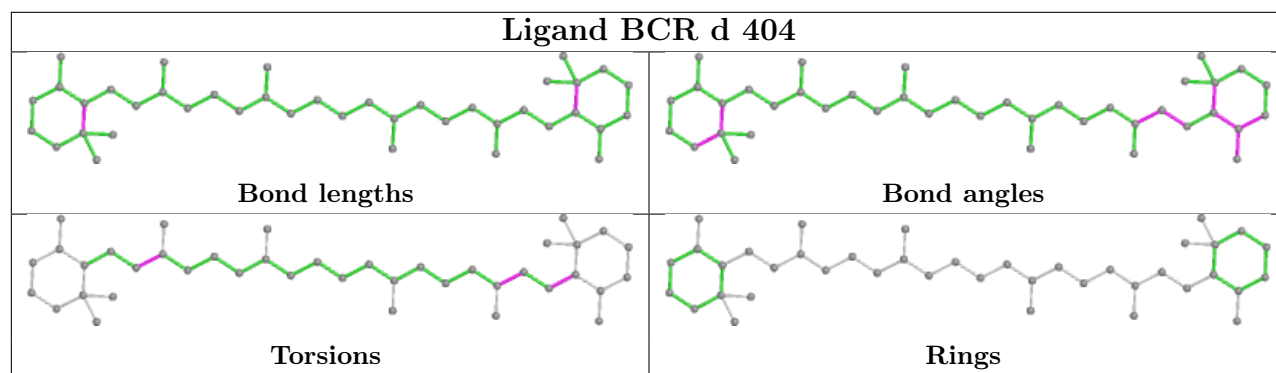
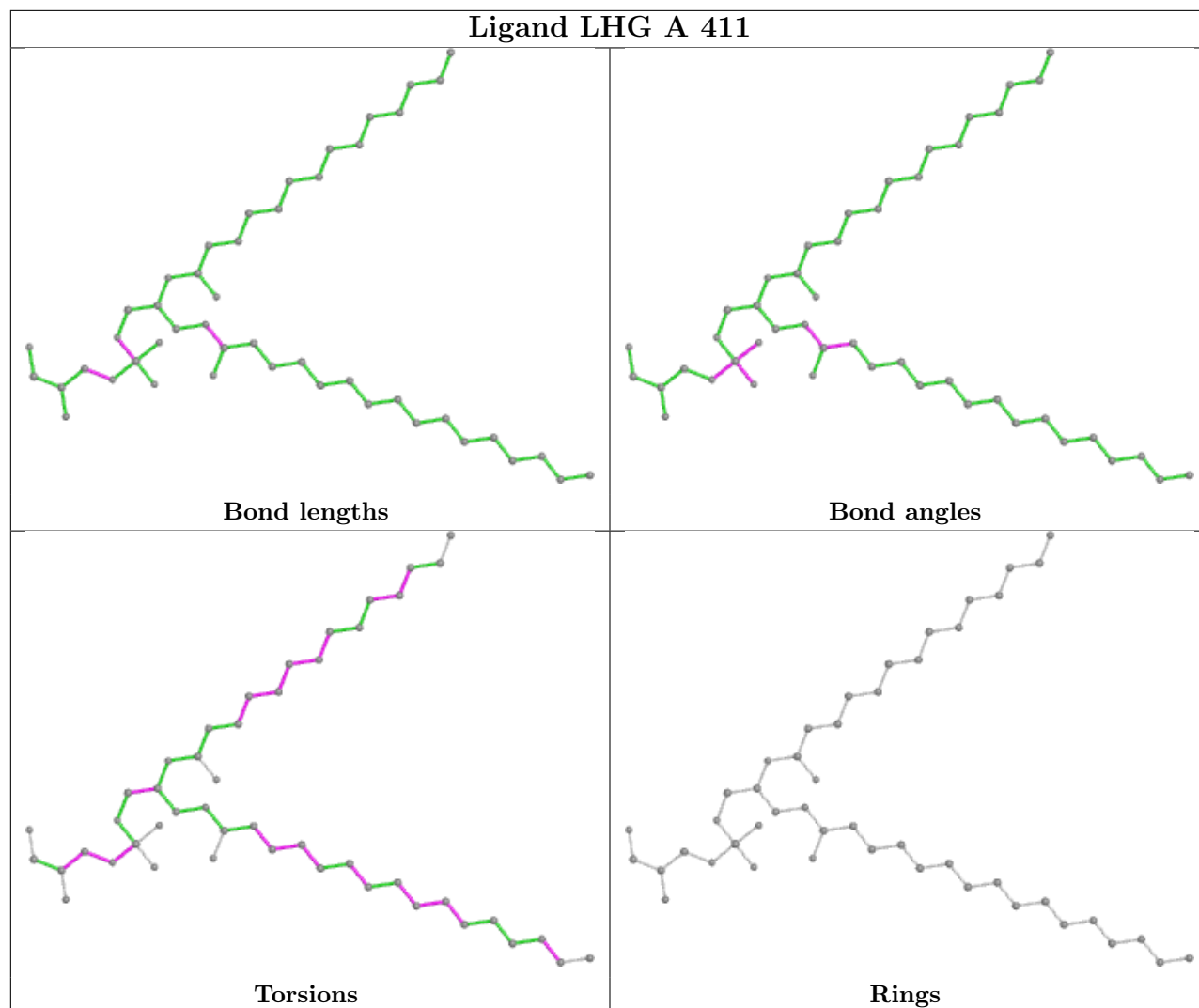




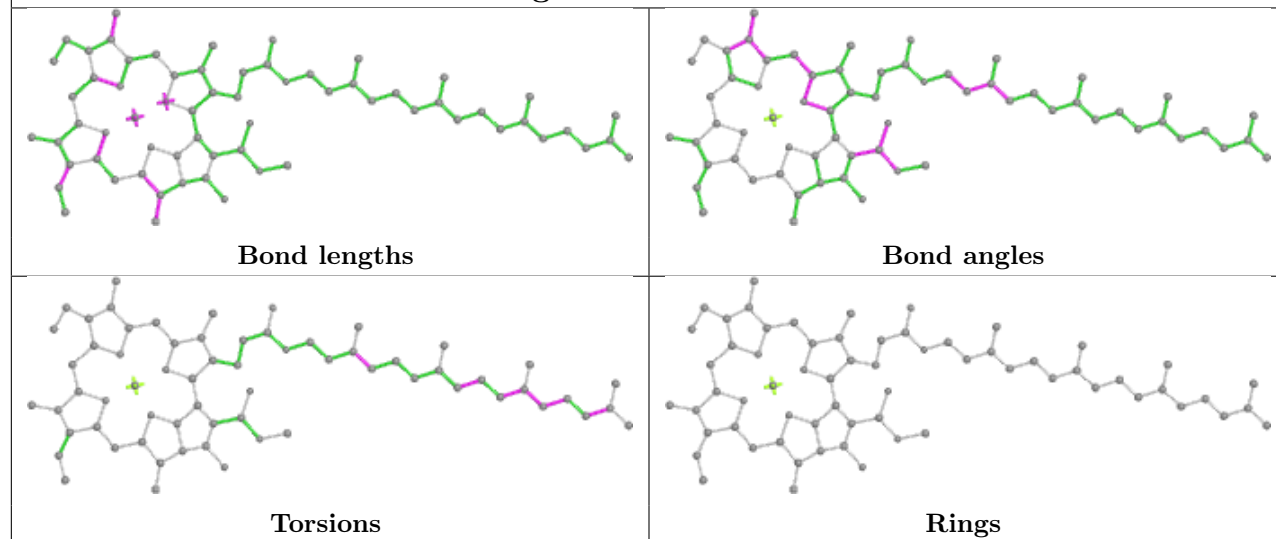




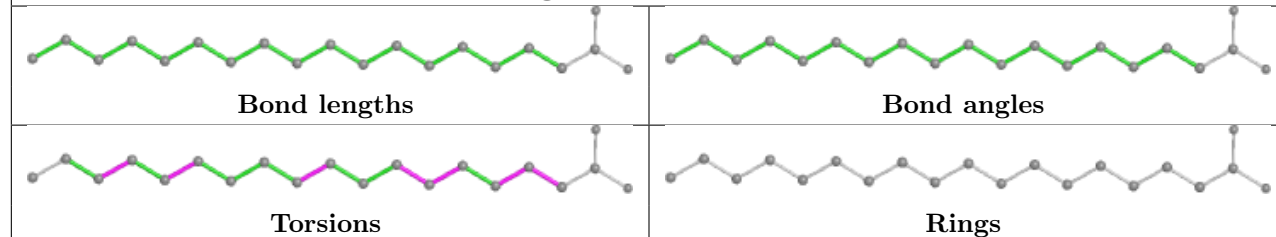




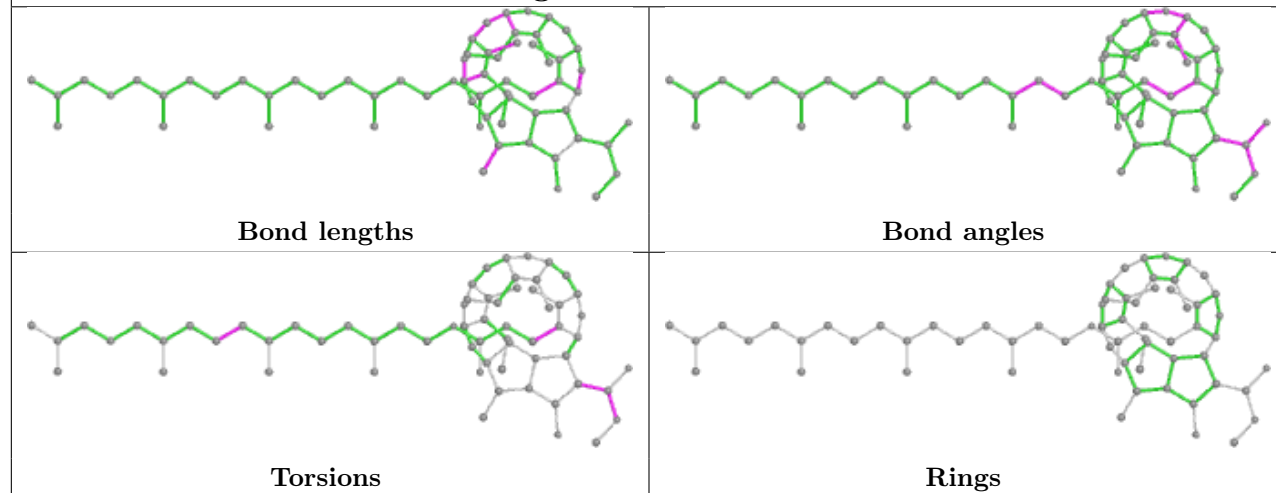
## Ligand CLA B 611

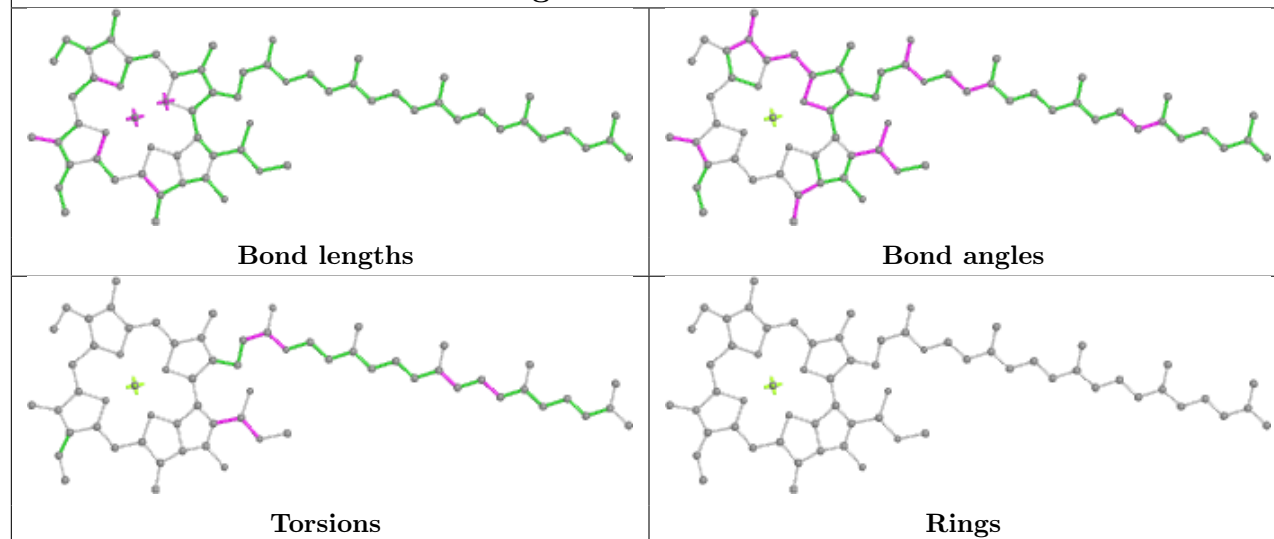
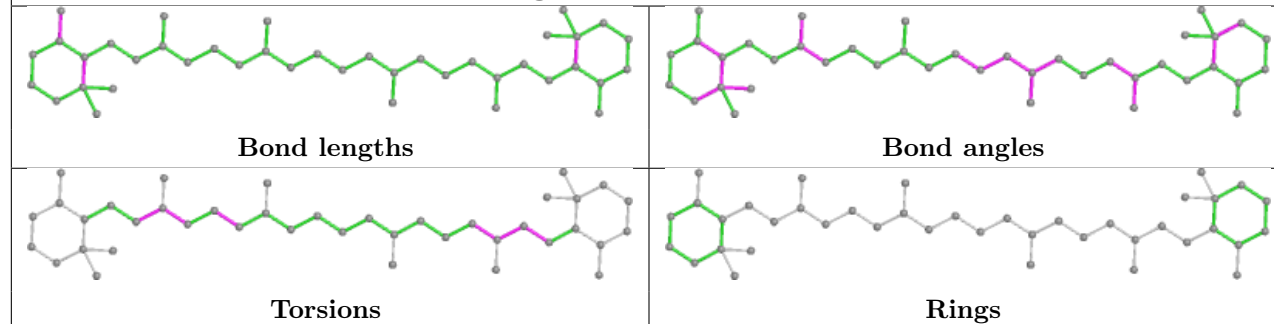
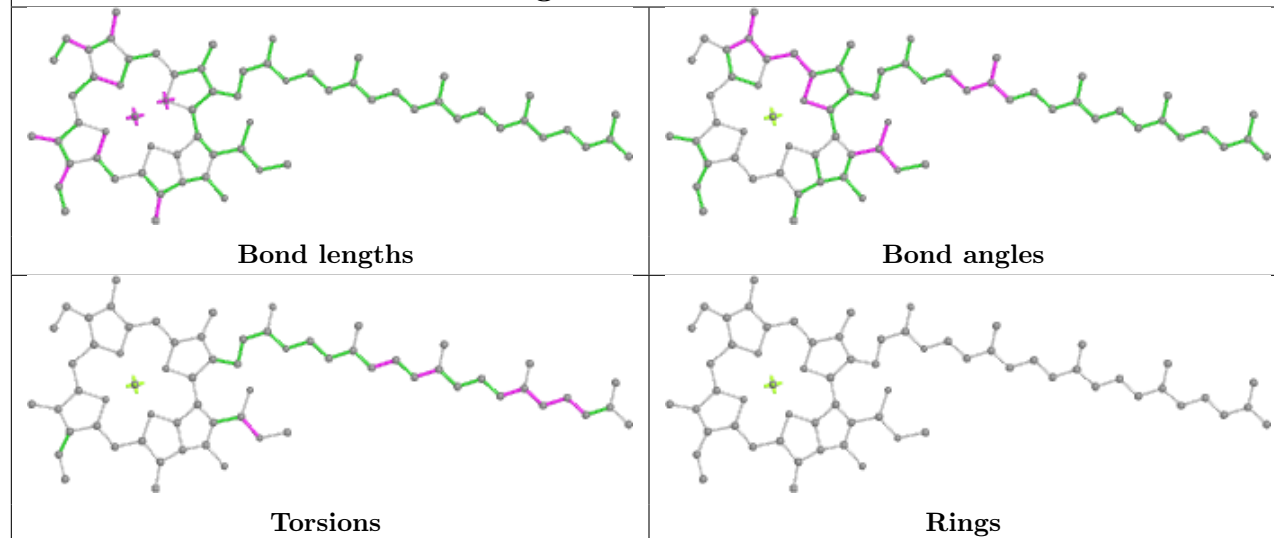


## Ligand STE b 621

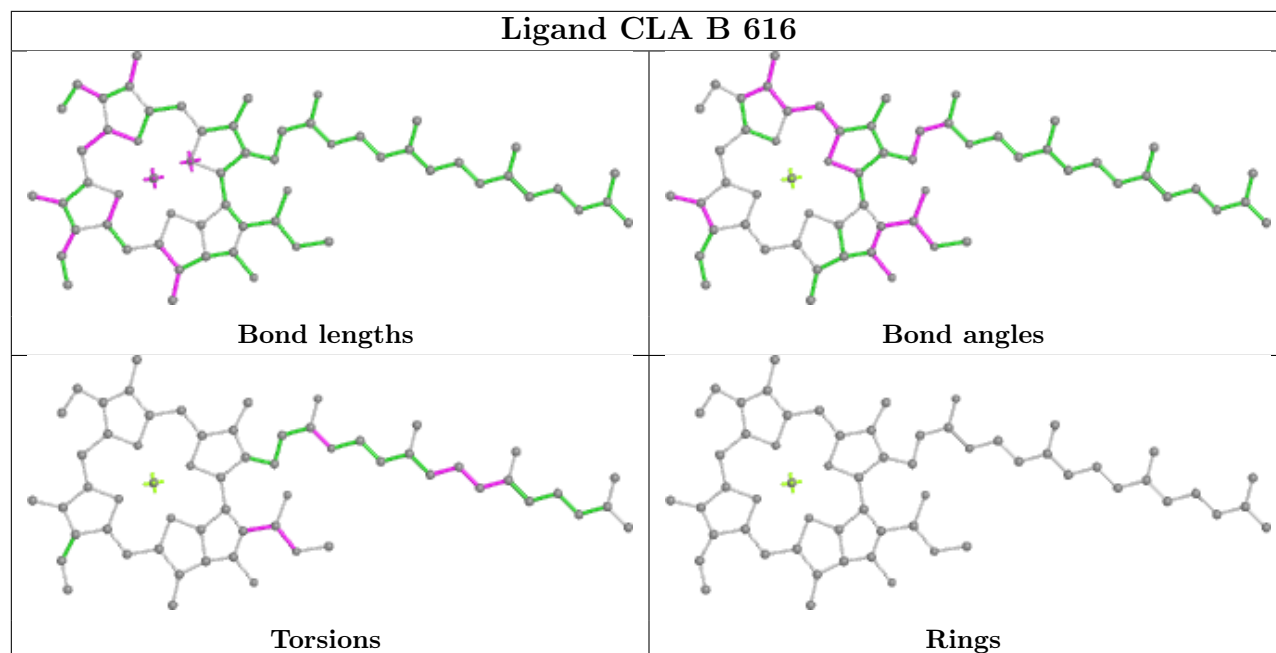


## Ligand PHO d 401

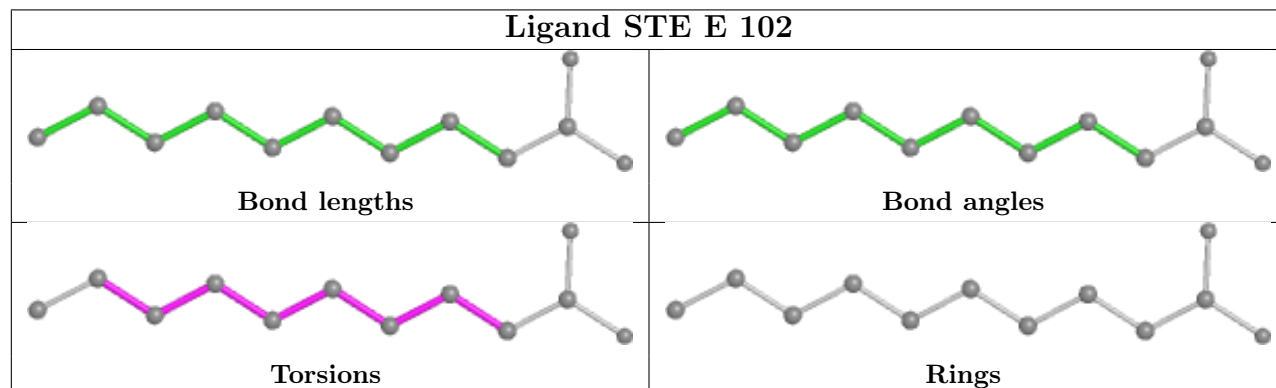


**Ligand CLA B 612****Ligand BCR B 619****Ligand CLA b 602**

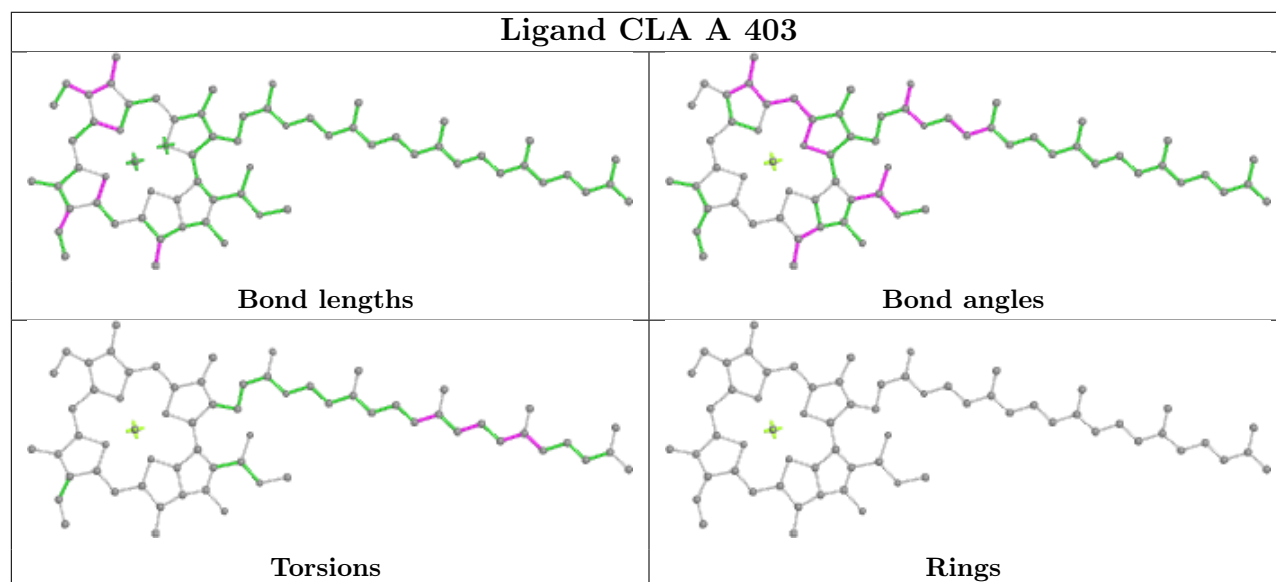
## Ligand CLA B 616



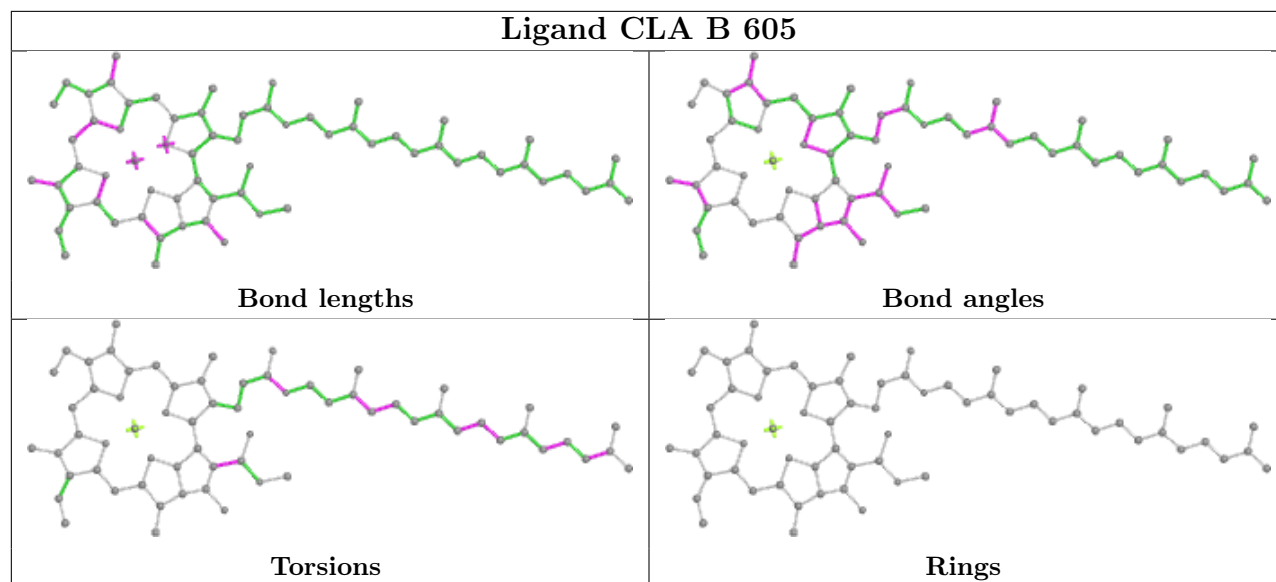
## Ligand STE E 102



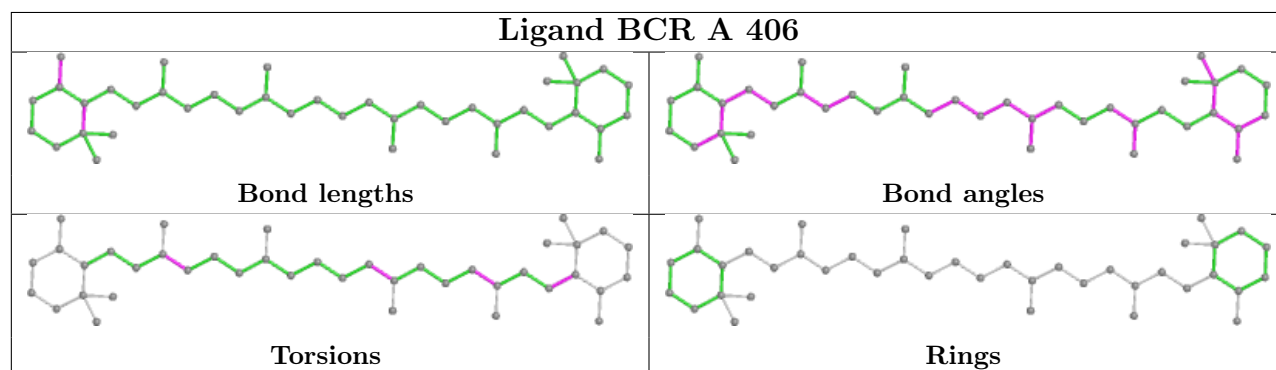
## Ligand CLA A 403



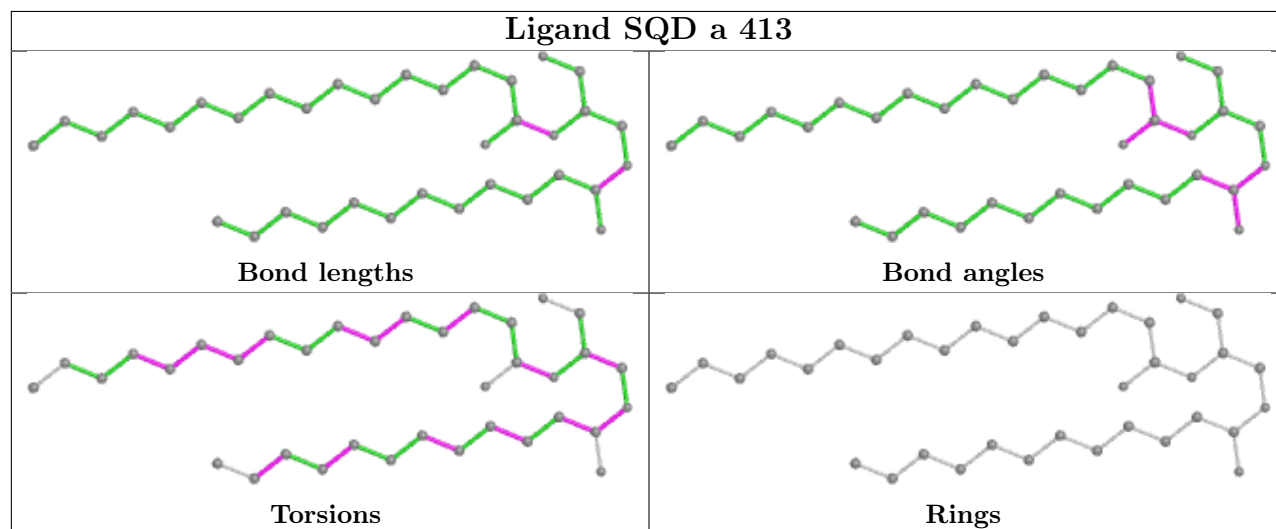
## Ligand CLA B 605



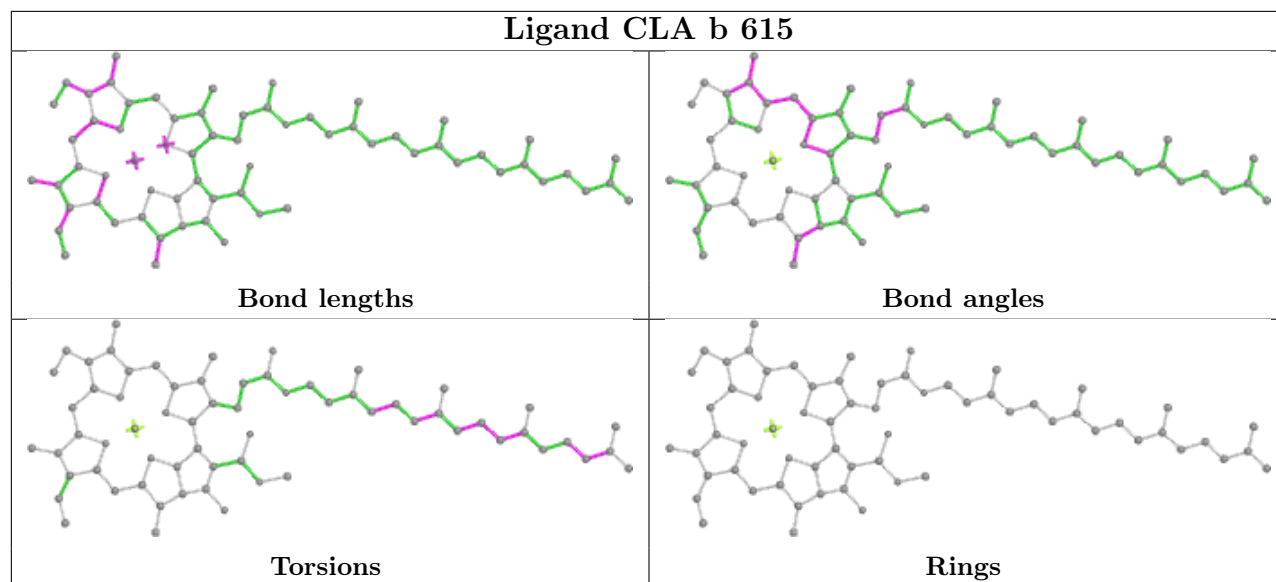
## Ligand BCR A 406



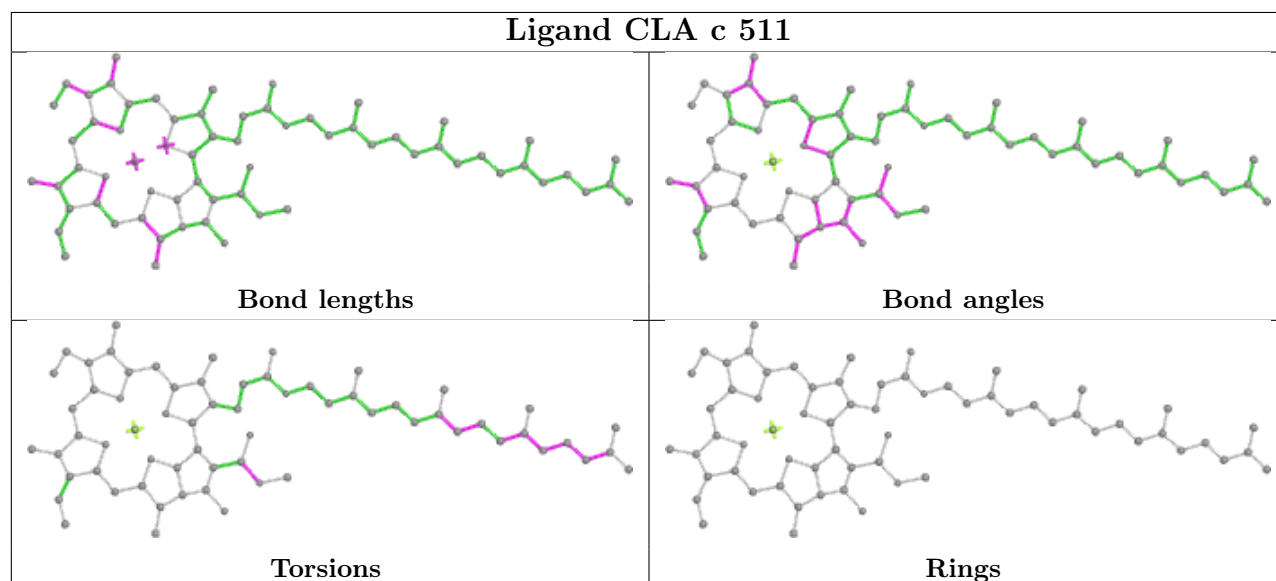
## Ligand SQD a 413



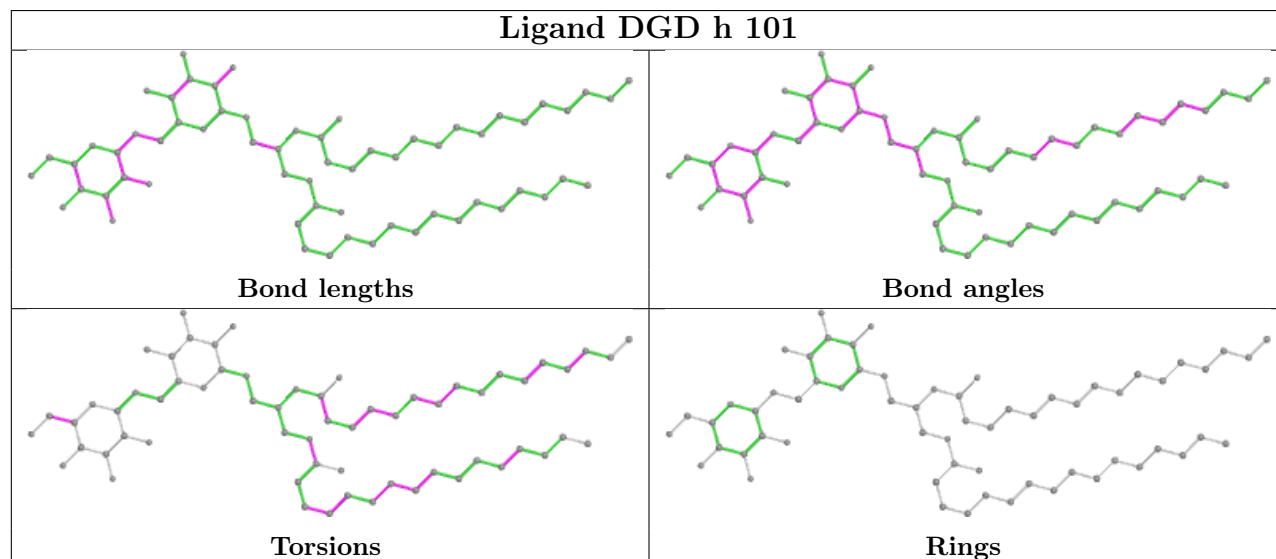
## Ligand CLA b 615



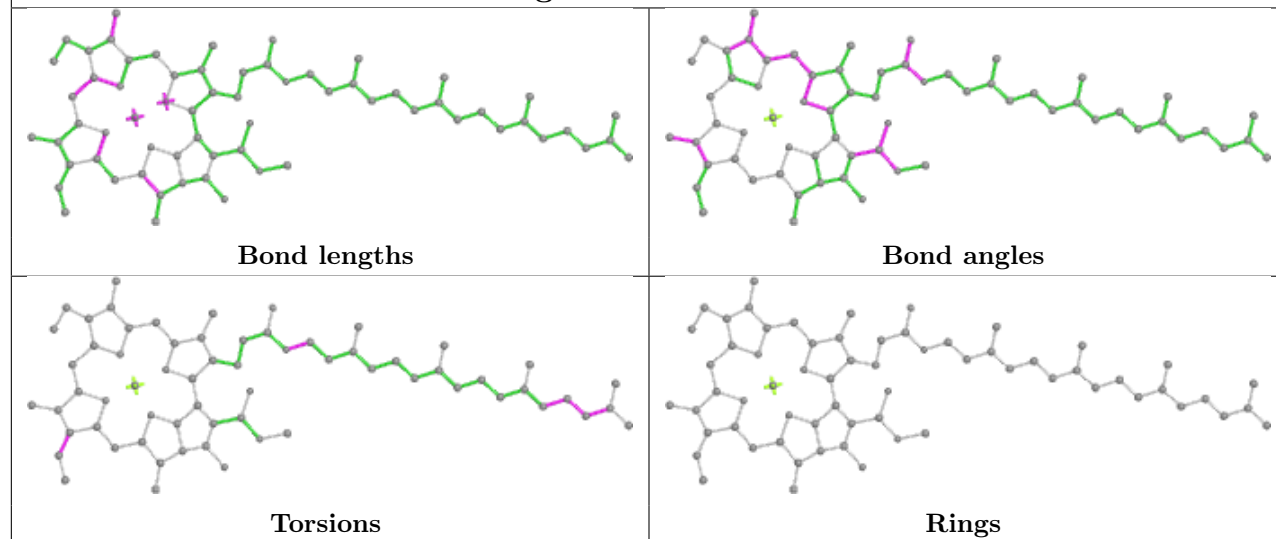
## Ligand CLA c 511



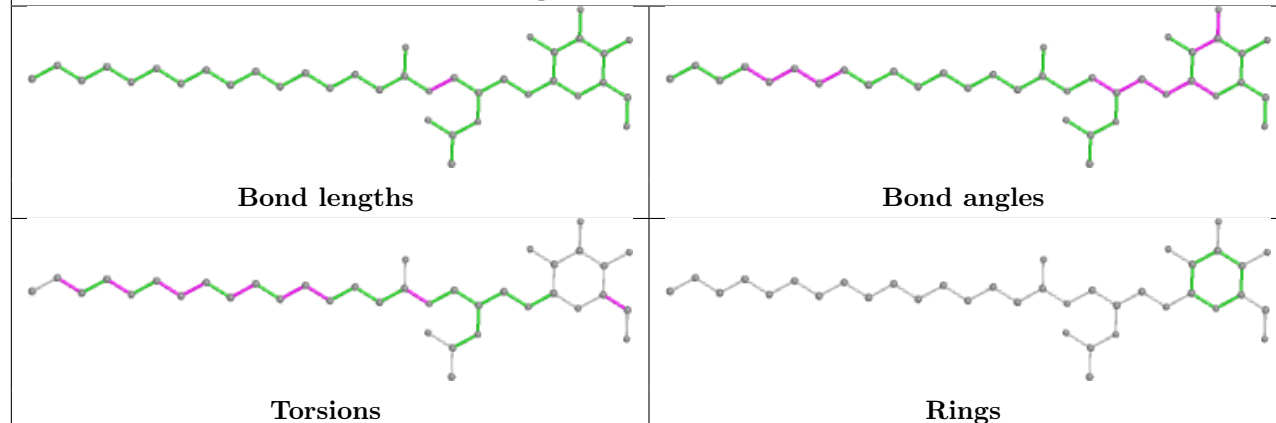
## Ligand DGD h 101



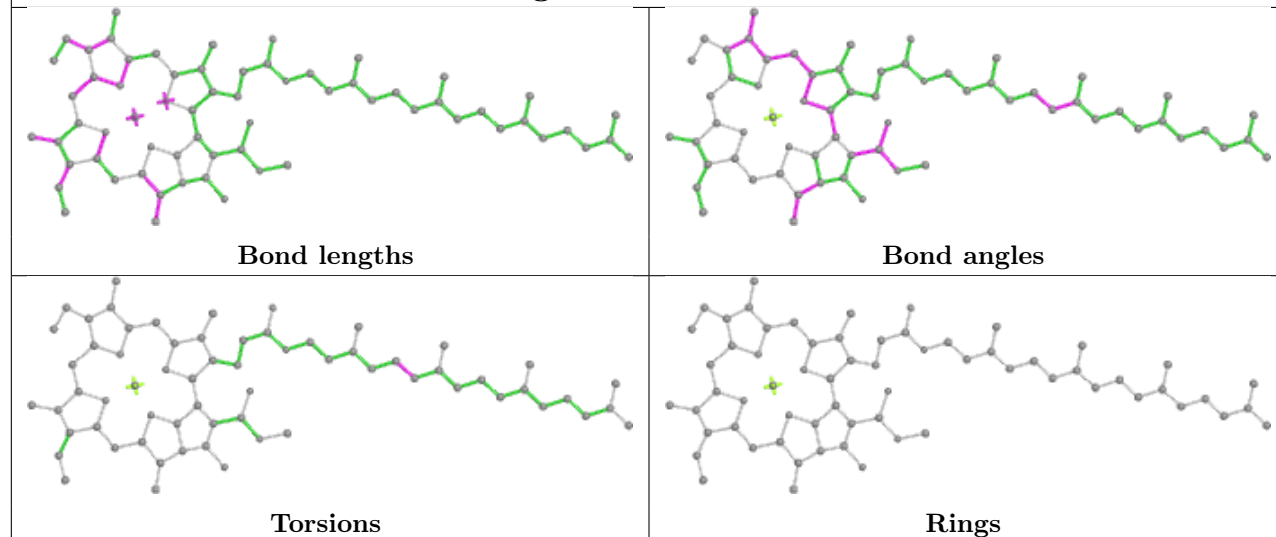
## Ligand CLA d 402



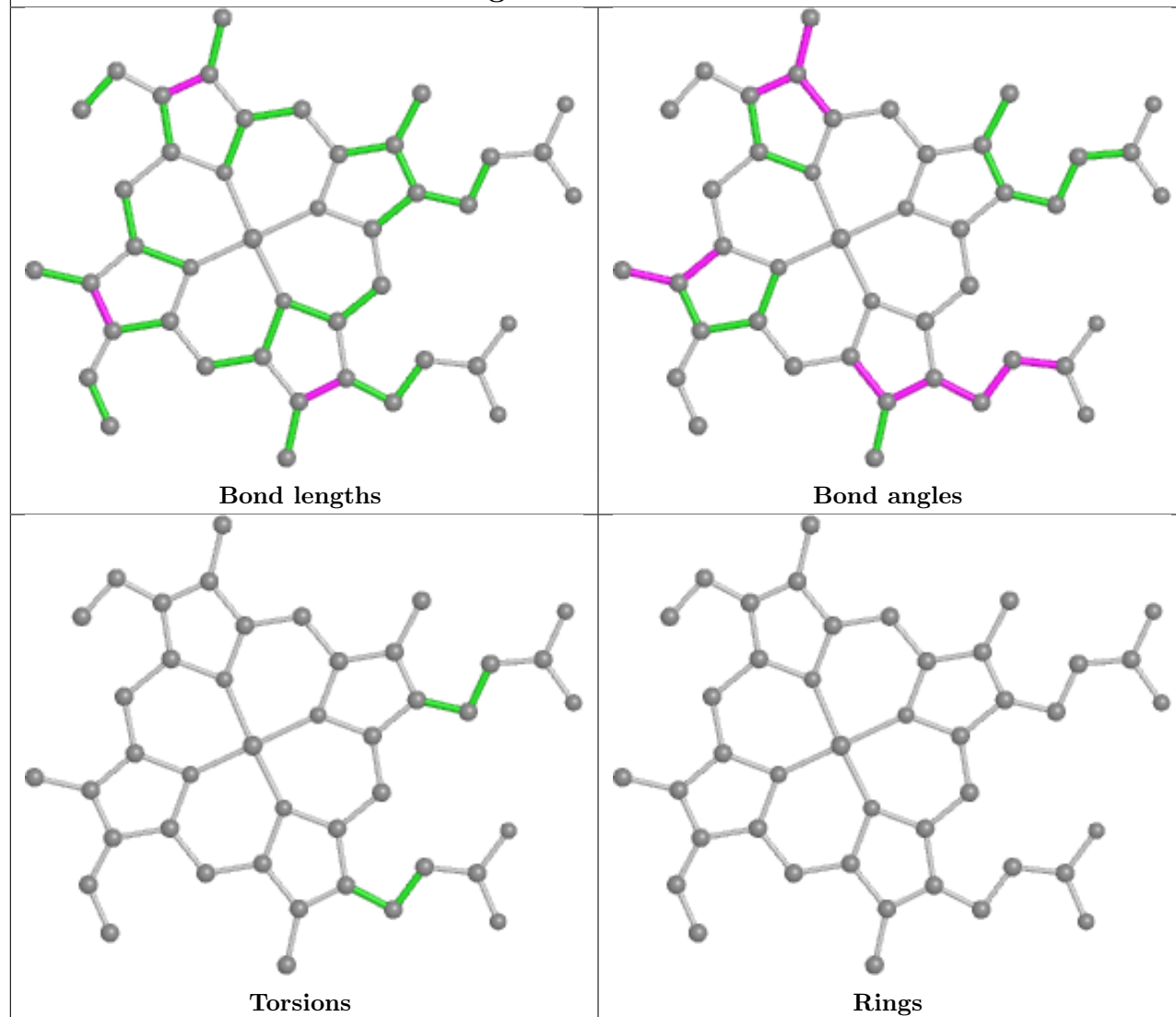
## Ligand LMG c 518



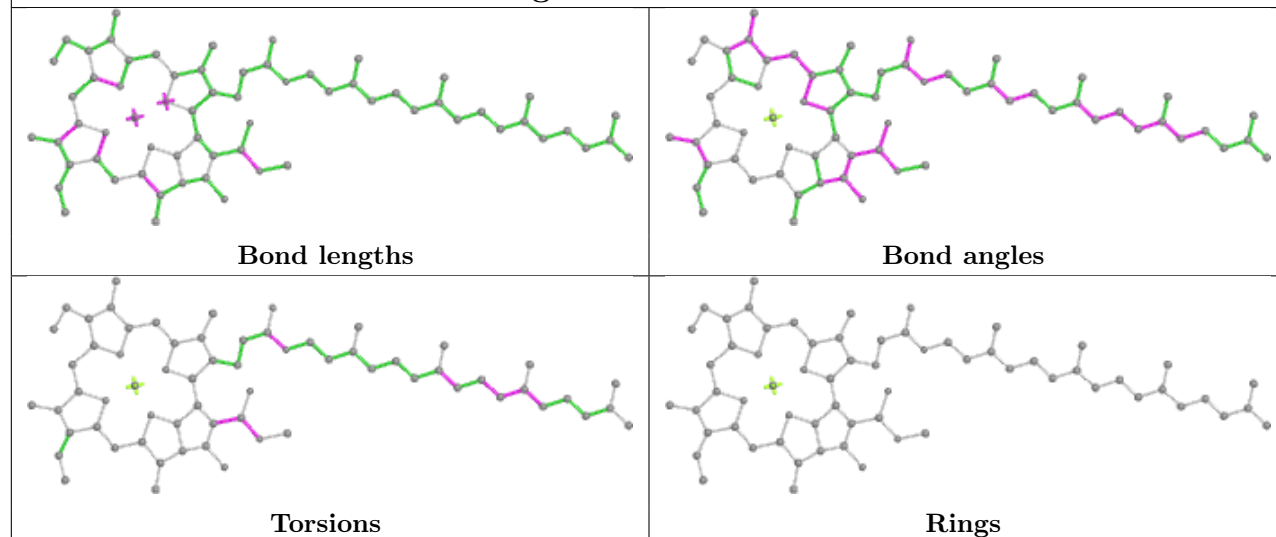
## Ligand CLA B 608



## Ligand HEC V 201

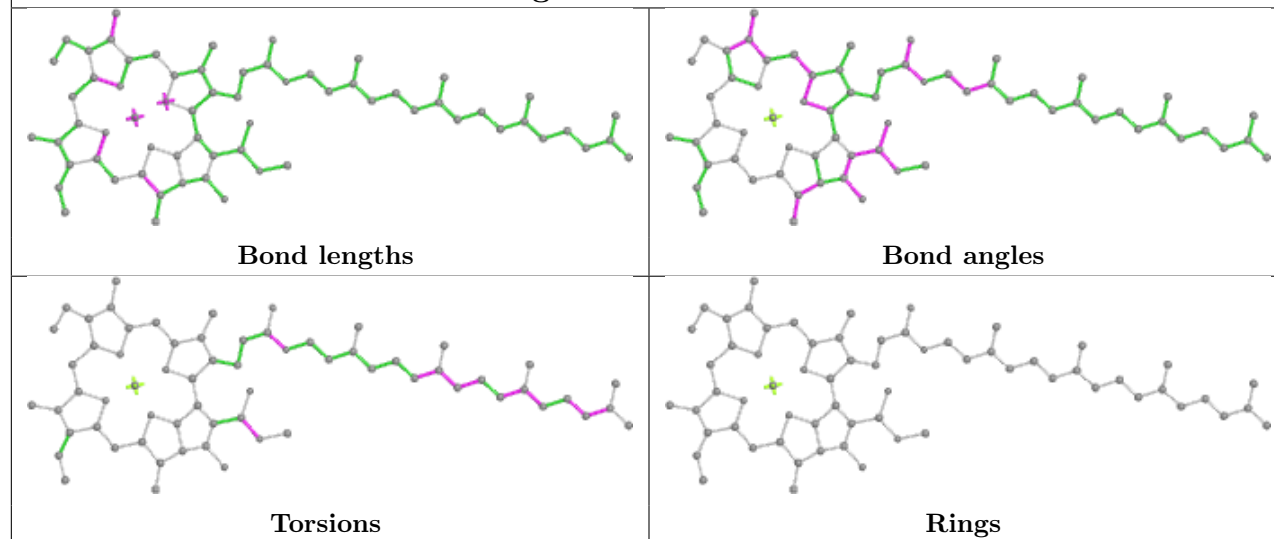


## Ligand CLA B 604

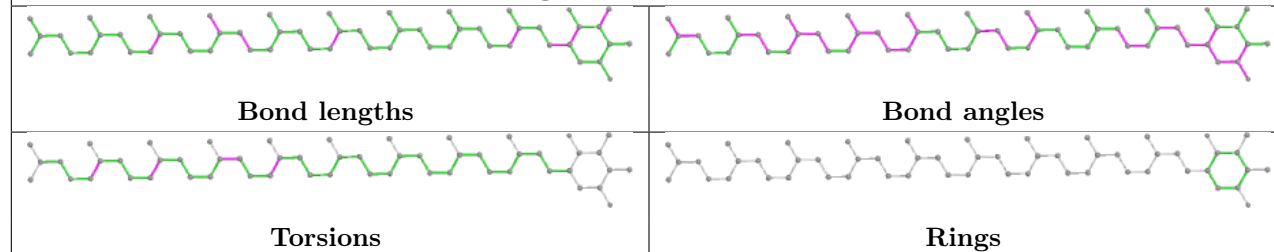




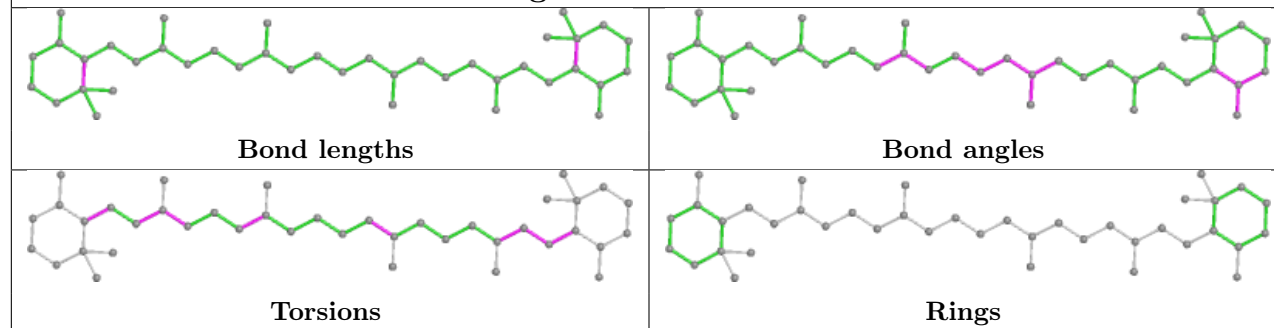
## Ligand CLA C 511



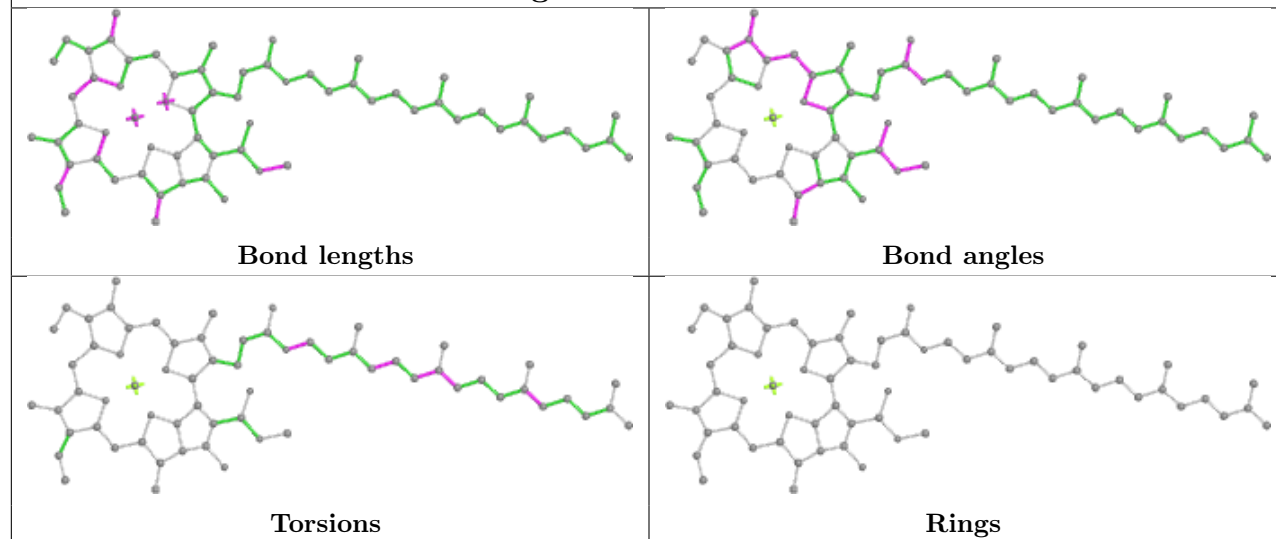
## Ligand PL9 D 407



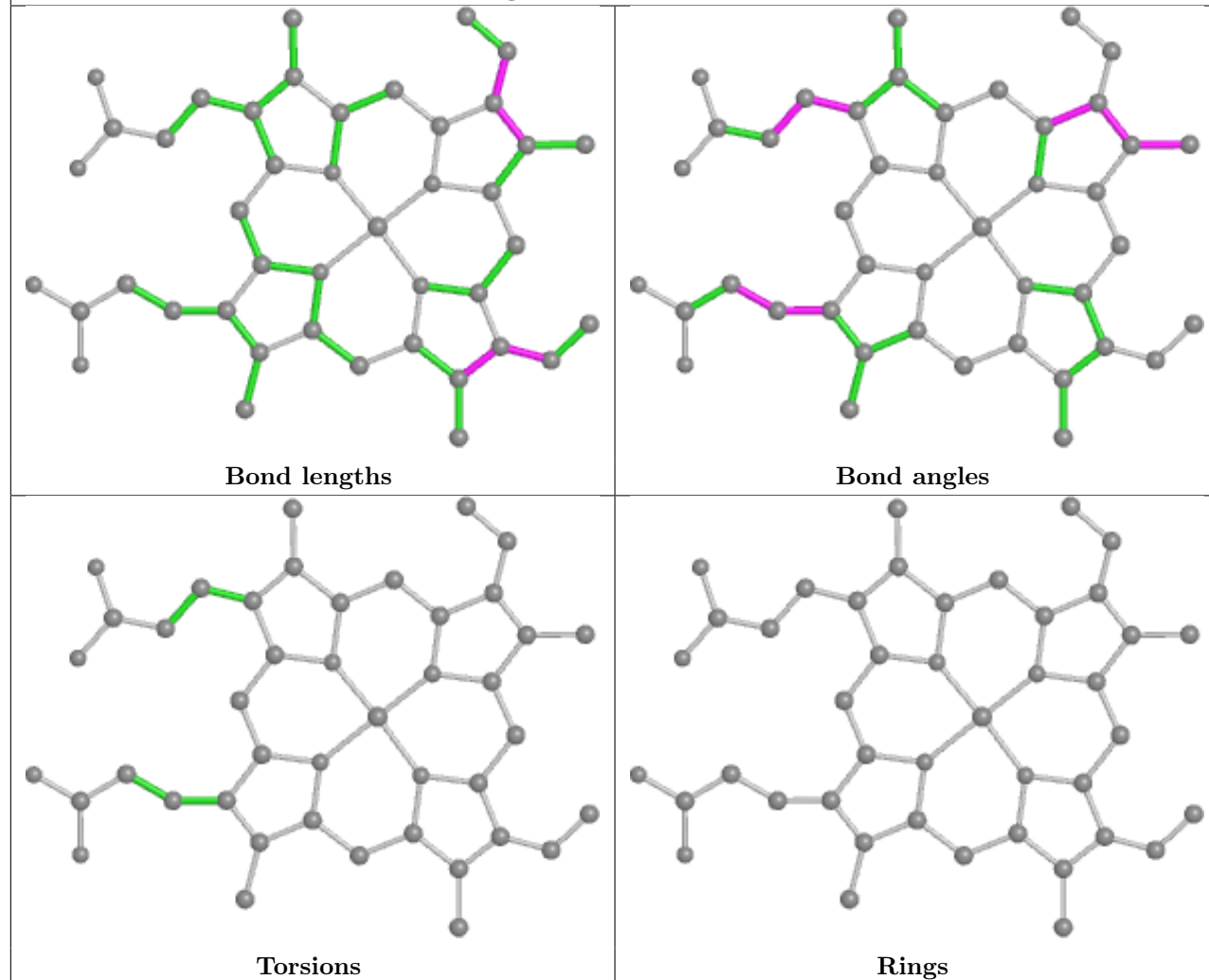
## Ligand BCR K 101



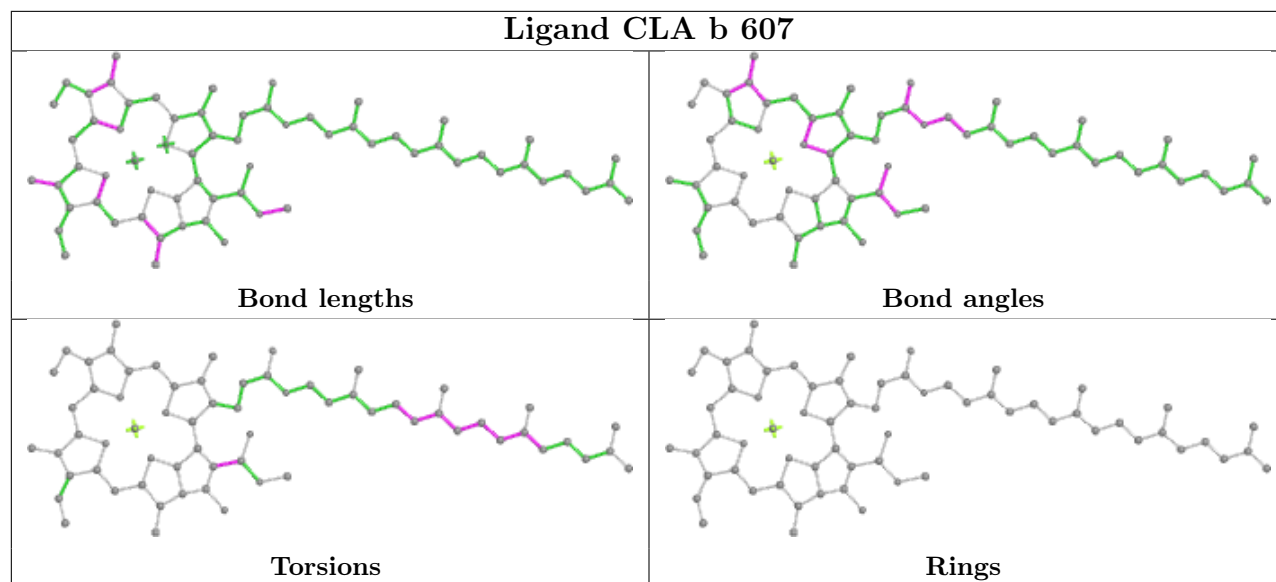
## Ligand CLA D 403



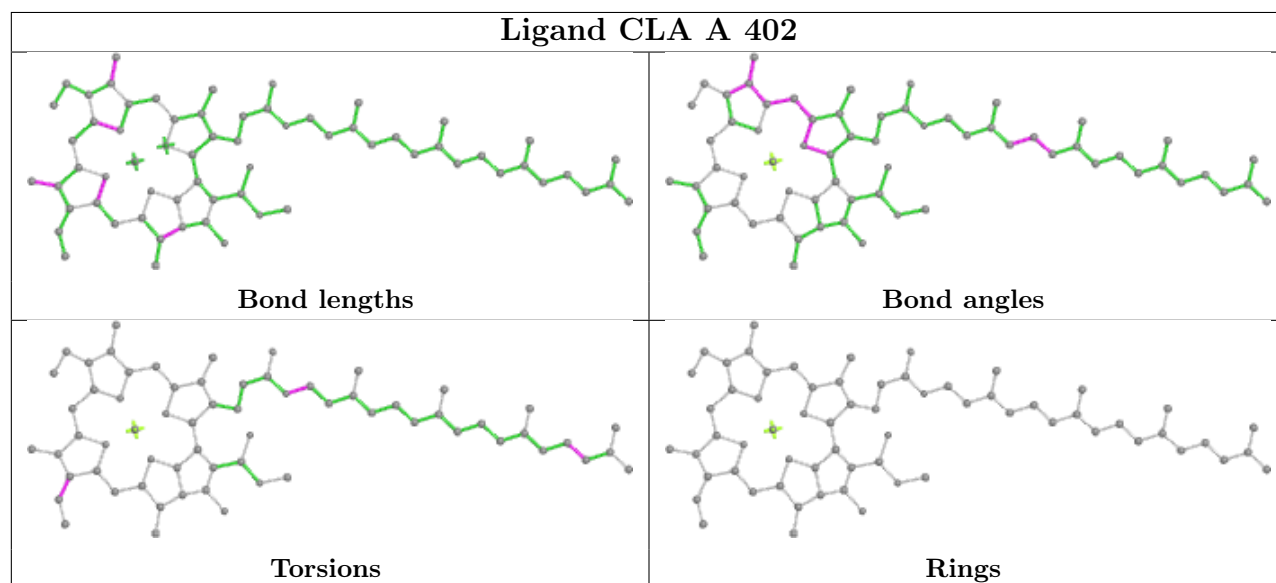
## Ligand HEM e 101

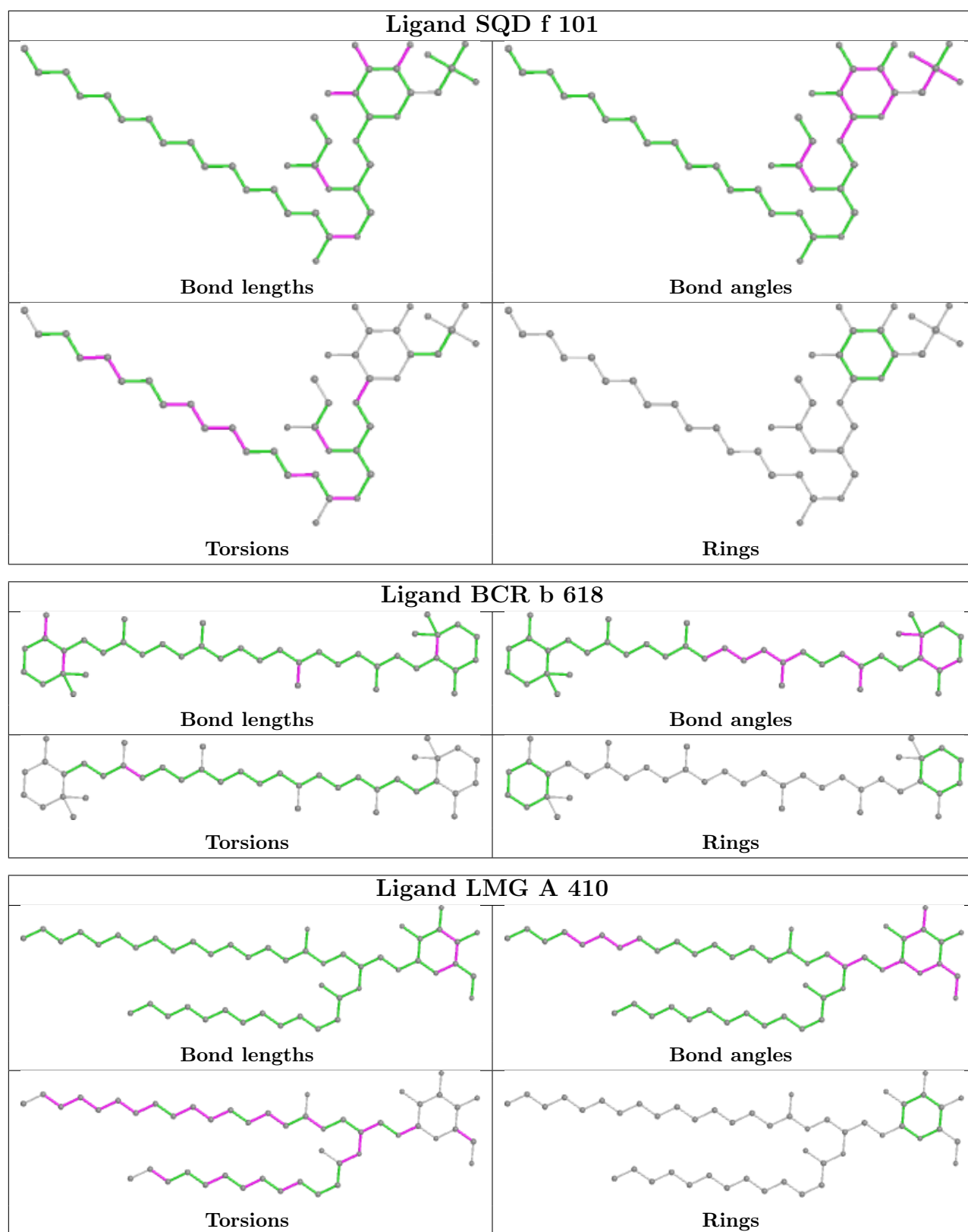


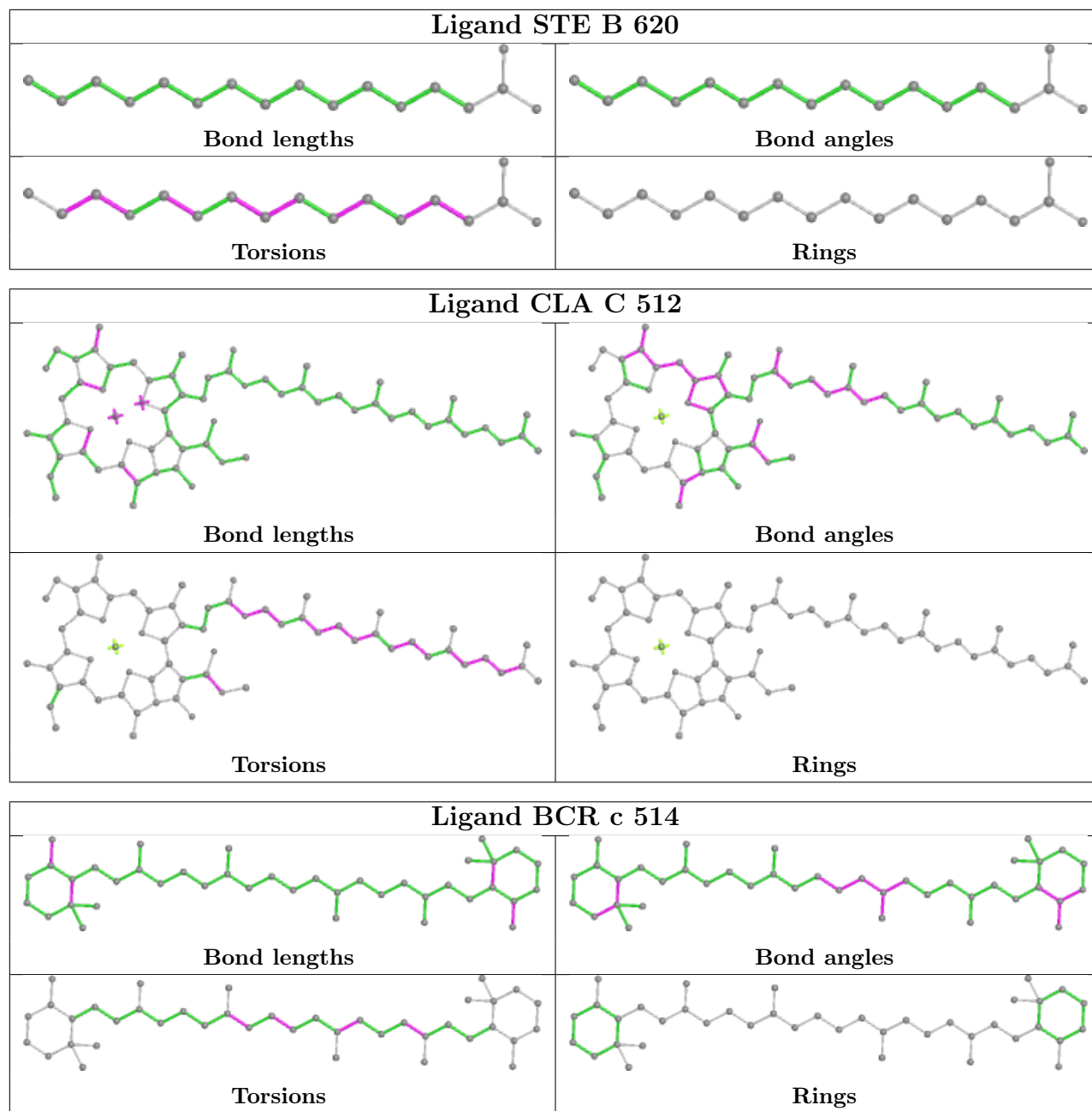
## Ligand CLA b 607

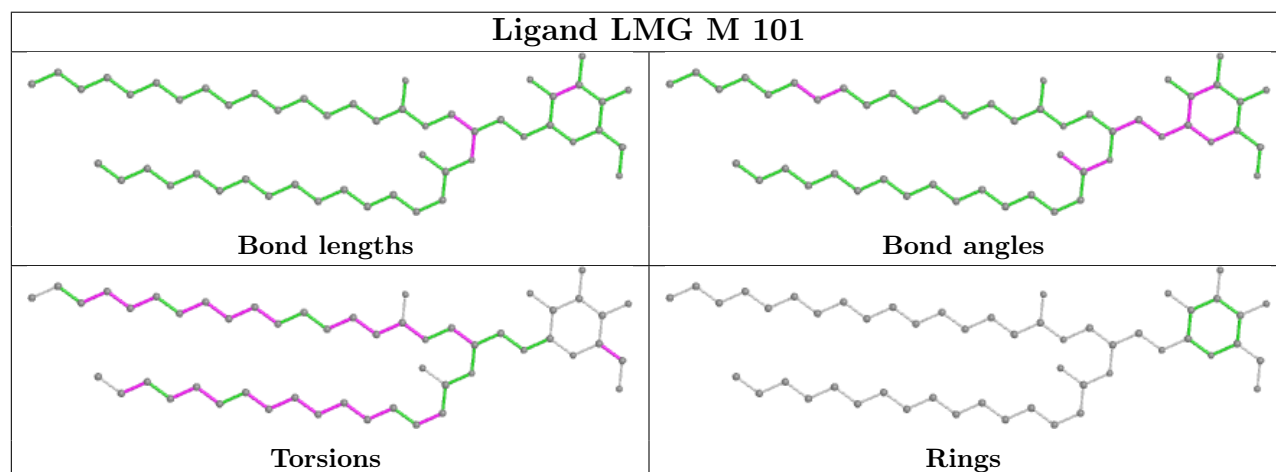
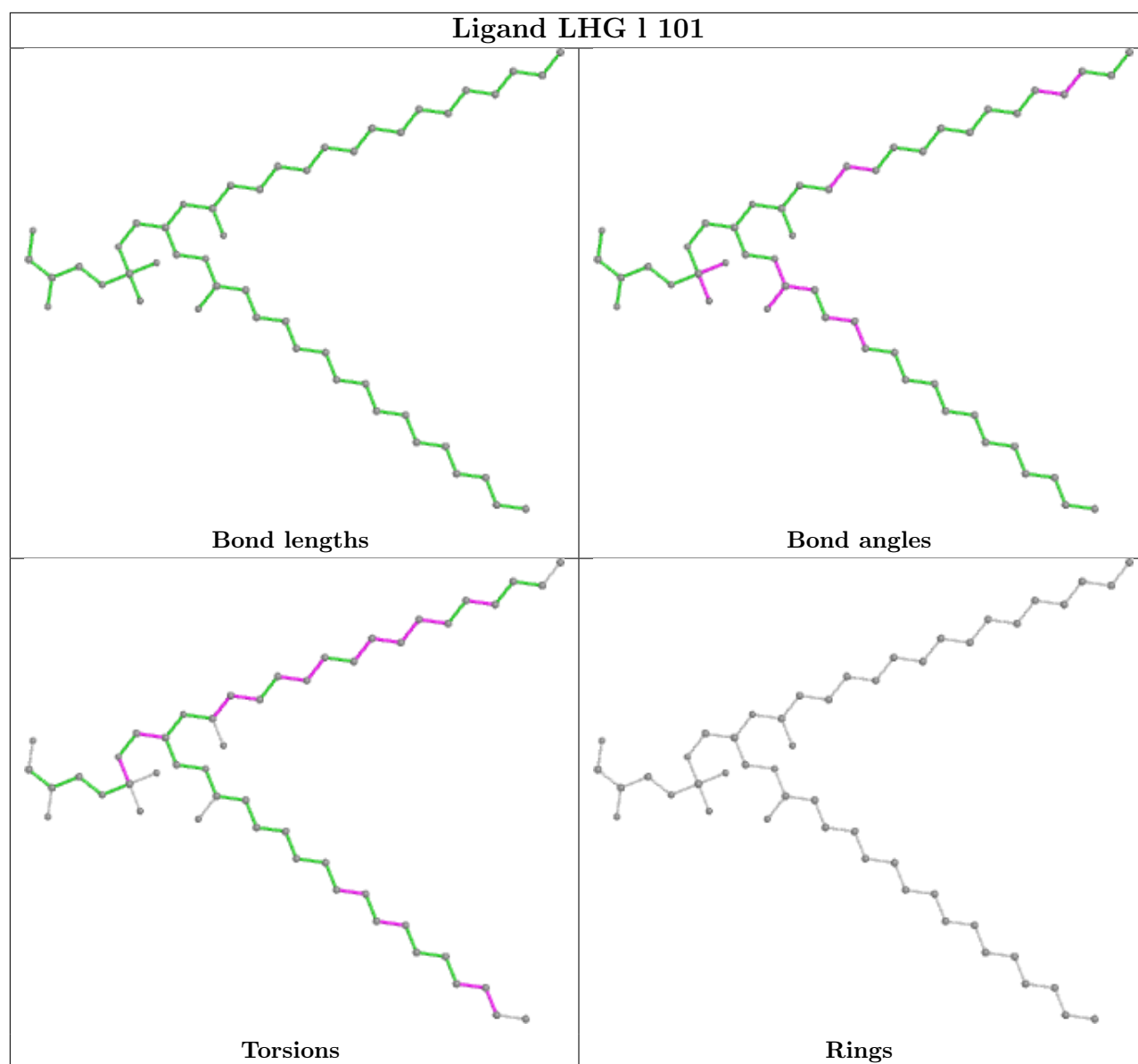


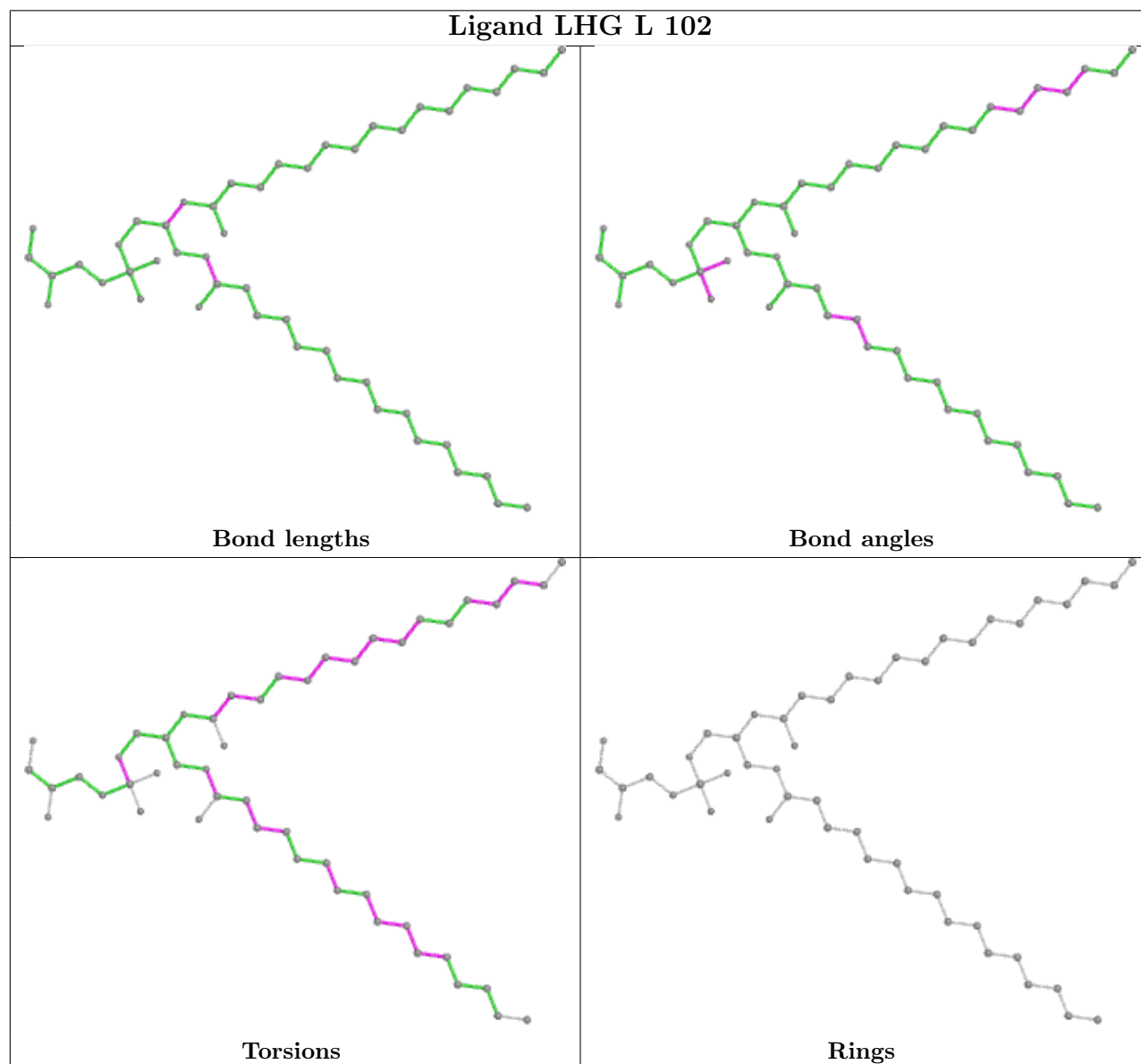
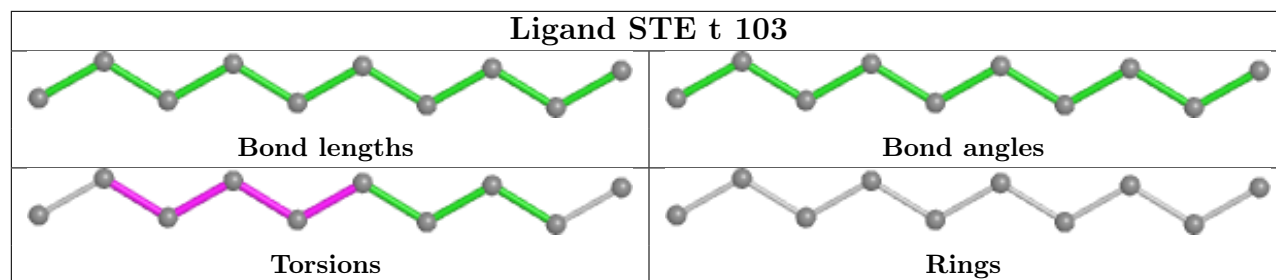
## Ligand CLA A 402

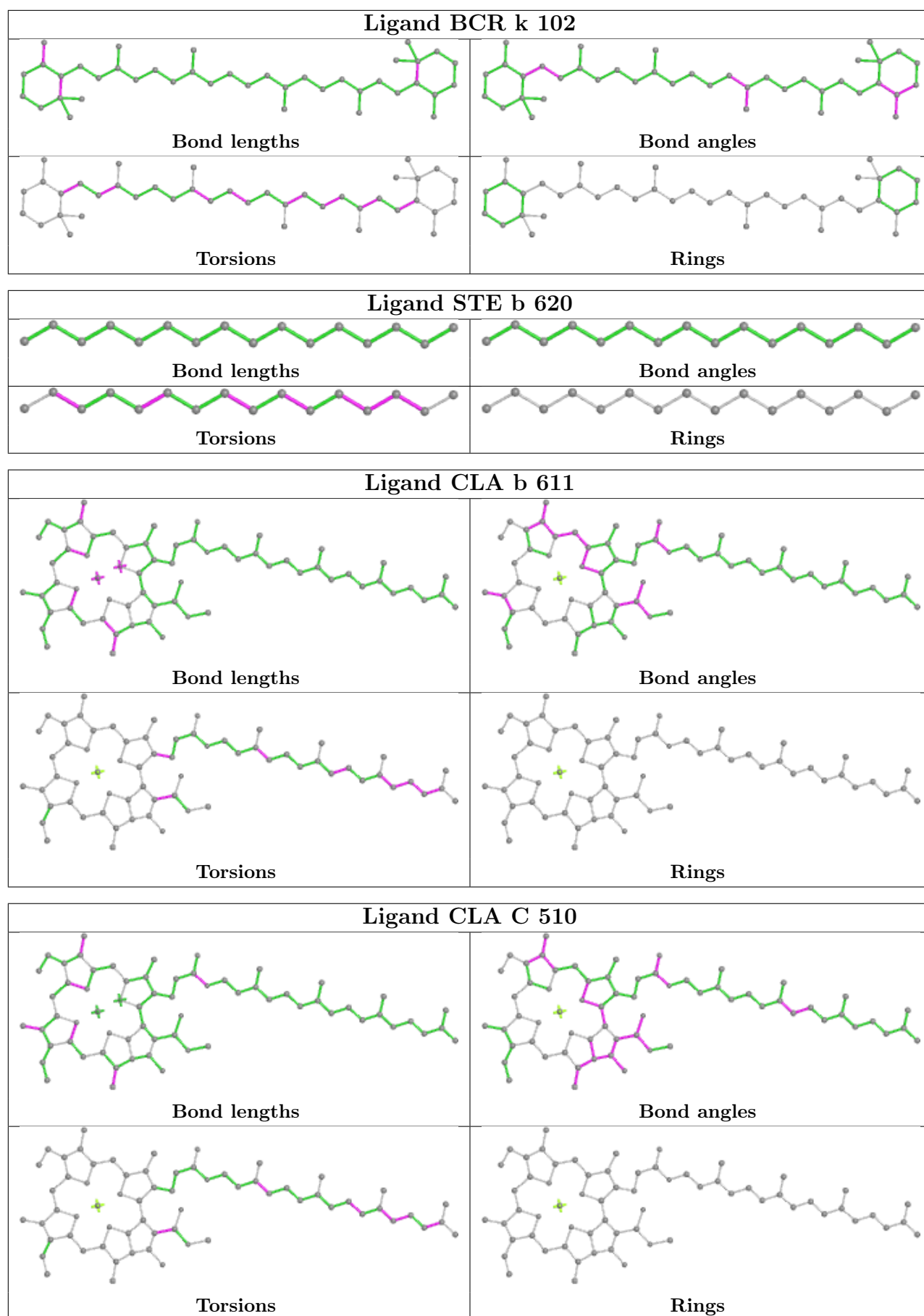




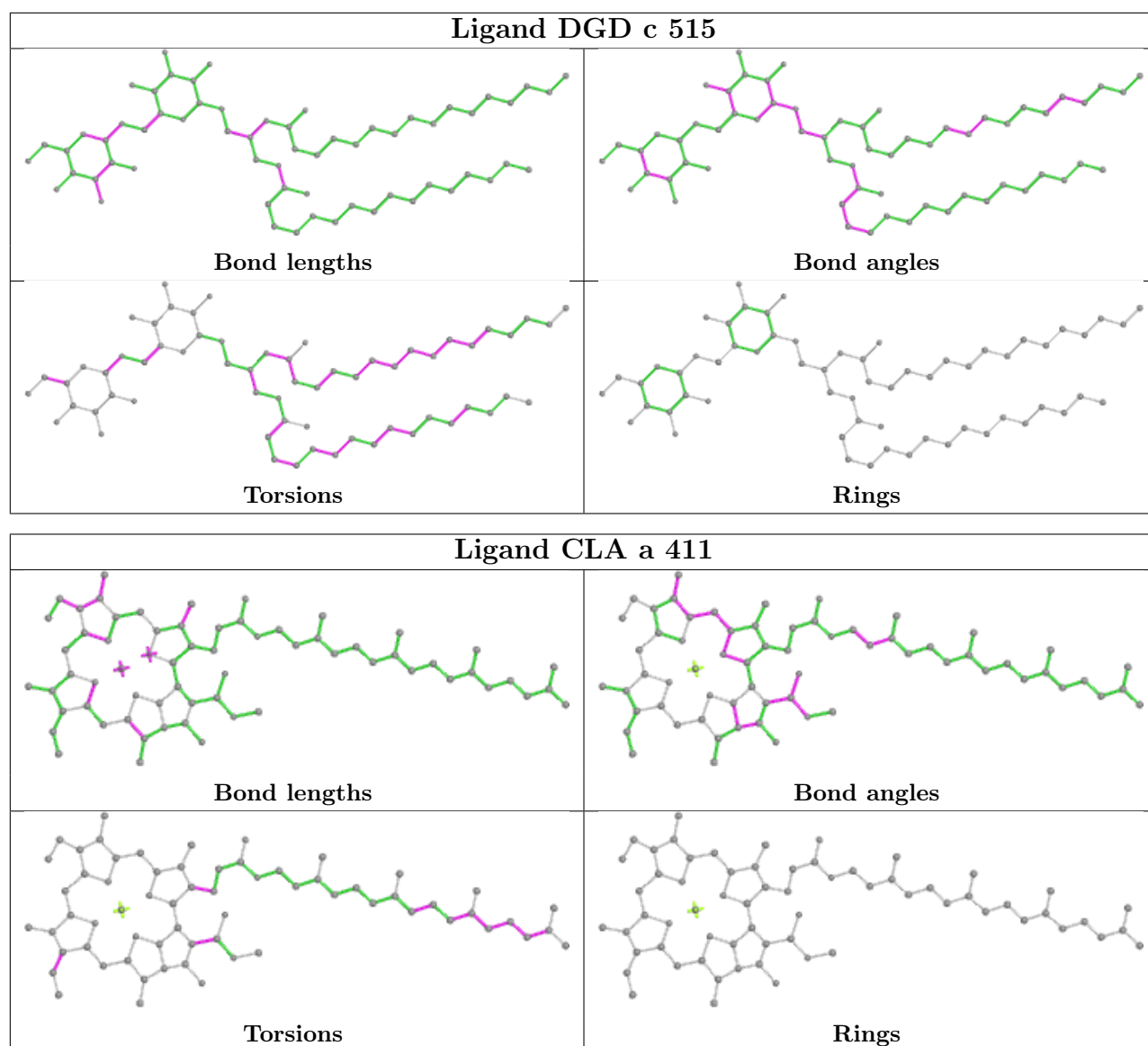












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.44	4 (1%) 79 81	25, 31, 47, 80	0
1	a	334/344 (97%)	-0.47	1 (0%) 94 94	24, 33, 56, 78	0
2	B	505/510 (99%)	-0.41	6 (1%) 79 81	25, 35, 60, 83	0
2	b	505/510 (99%)	-0.23	21 (4%) 36 38	28, 39, 68, 103	0
3	C	442/461 (95%)	-0.33	6 (1%) 75 77	27, 38, 53, 73	0
3	c	451/461 (97%)	-0.26	6 (1%) 77 79	28, 41, 59, 95	0
4	D	341/352 (96%)	-0.40	1 (0%) 94 94	24, 32, 47, 76	0
4	d	341/352 (96%)	-0.31	0 100 100	25, 36, 58, 84	0
5	E	82/84 (97%)	-0.03	3 (3%) 41 44	34, 52, 67, 85	0
5	e	82/84 (97%)	0.18	5 (6%) 21 23	42, 58, 74, 86	0
6	F	34/45 (75%)	-0.51	1 (2%) 51 55	40, 44, 59, 79	0
6	f	34/45 (75%)	-0.25	1 (2%) 51 55	44, 51, 77, 85	0
7	H	65/66 (98%)	-0.06	2 (3%) 49 52	34, 41, 57, 73	0
7	h	63/66 (95%)	0.28	5 (7%) 12 14	41, 51, 61, 65	0
8	I	35/38 (92%)	-0.28	2 (5%) 23 25	35, 41, 64, 77	0
8	i	35/38 (92%)	-0.13	3 (8%) 10 11	33, 41, 75, 84	0
9	J	36/40 (90%)	0.14	4 (11%) 5 5	37, 50, 74, 83	0
9	j	36/40 (90%)	0.11	4 (11%) 5 5	39, 54, 86, 95	0
10	K	37/46 (80%)	0.11	2 (5%) 25 28	45, 52, 69, 78	0
10	k	37/46 (80%)	-0.12	0 100 100	49, 55, 66, 77	0
11	L	37/37 (100%)	-0.48	0 100 100	27, 32, 61, 66	0
11	l	36/37 (97%)	-0.17	3 (8%) 11 12	28, 33, 65, 85	0
12	M	32/36 (88%)	-0.07	1 (3%) 49 52	29, 36, 57, 70	0
12	m	31/36 (86%)	-0.12	1 (3%) 47 50	29, 36, 53, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.08	13 (5%) 26 29	28, 43, 76, 124	0
13	o	244/272 (89%)	-0.16	13 (5%) 26 29	28, 41, 78, 126	0
14	R	28/41 (68%)	1.85	14 (50%) 0 0	57, 67, 81, 88	0
14	r	28/41 (68%)	3.67	24 (85%) 0 0	73, 88, 108, 121	0
15	T	29/32 (90%)	-0.46	1 (3%) 45 47	28, 34, 58, 72	0
15	t	29/32 (90%)	-0.26	3 (10%) 6 6	30, 34, 70, 90	0
16	U	97/134 (72%)	-0.29	2 (2%) 63 66	35, 44, 70, 80	0
16	u	97/134 (72%)	-0.45	0 100 100	32, 42, 57, 84	0
17	V	137/163 (84%)	-0.58	0 100 100	33, 42, 56, 73	0
17	v	137/163 (84%)	-0.21	4 (2%) 51 55	34, 48, 67, 81	0
18	X	38/41 (92%)	0.18	3 (7%) 12 14	40, 50, 63, 74	0
18	x	39/41 (95%)	0.49	4 (10%) 6 6	48, 59, 86, 98	0
19	Y	27/46 (58%)	1.45	11 (40%) 0 0	51, 69, 89, 91	0
19	y	30/46 (65%)	0.48	4 (13%) 3 3	58, 74, 88, 97	0
20	Z	62/62 (100%)	0.75	13 (20%) 1 1	52, 67, 104, 118	0
20	z	62/62 (100%)	0.66	10 (16%) 1 1	55, 70, 106, 115	0
All	All	5293/5700 (92%)	-0.21	201 (3%) 40 43	24, 40, 71, 126	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	10.7
14	r	14	LEU	7.8
13	o	60	ARG	7.3
14	r	9	LEU	7.0
14	r	10	LEU	6.9
1	A	13	LEU	6.7
13	o	57	LYS	6.2
13	O	56	PRO	6.2
14	r	13	LEU	6.0
14	r	28	VAL	5.9
13	O	3	GLN	5.9
14	r	29	LYS	5.9
2	b	495	PHE	5.7
18	X	2	THR	5.4
20	z	33	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
14	r	24	LEU	5.2
15	t	29	ILE	5.2
5	e	79	PHE	5.1
9	j	6	GLY	5.1
14	r	3	TRP	5.1
13	o	56	PRO	5.0
20	Z	1	MET	5.0
20	Z	34	ASP	5.0
14	r	5	VAL	4.9
9	J	7	ARG	4.9
13	o	4	THR	4.9
13	O	62	GLU	4.7
14	r	6	LEU	4.7
20	Z	62	VAL	4.7
13	o	62	GLU	4.7
14	R	3	TRP	4.6
19	Y	25	ILE	4.5
20	Z	35	ARG	4.4
14	R	25	PRO	4.4
5	e	61	ARG	4.4
14	r	25	PRO	4.4
13	O	60	ARG	4.3
20	Z	32	ASP	4.3
7	h	21	VAL	4.3
9	J	6	GLY	4.2
19	Y	20	ALA	4.2
9	j	7	ARG	4.1
13	o	3	GLN	4.1
1	A	11	ALA	4.1
13	O	4	THR	4.0
13	o	59	LYS	4.0
8	i	36	ASP	4.0
20	Z	3	ILE	4.0
7	H	66	GLY	3.8
13	o	5	LEU	3.8
2	b	127	ARG	3.8
9	j	8	ILE	3.7
10	K	17	ILE	3.7
13	o	61	GLN	3.7
9	J	5	GLY	3.7
2	b	502	VAL	3.7
14	r	21	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
2	b	486	LEU	3.7
14	R	6	LEU	3.7
6	f	12	SER	3.7
19	Y	43	ARG	3.7
14	r	26	TYR	3.7
20	z	60	PHE	3.6
9	J	8	ILE	3.6
13	O	63	ALA	3.6
18	x	2	THR	3.6
14	r	2	ASP	3.5
2	b	496	TYR	3.5
13	O	5	LEU	3.5
1	a	11	ALA	3.5
14	R	2	ASP	3.4
20	z	30	PRO	3.4
2	b	506	ARG	3.4
14	R	29	LYS	3.4
2	b	128	THR	3.4
19	Y	40	ALA	3.4
2	b	289	GLN	3.3
3	c	23	ALA	3.3
13	o	63	ALA	3.3
13	o	55	GLU	3.3
14	r	18	TRP	3.3
4	D	12	ARG	3.3
20	Z	42	LEU	3.3
14	R	21	ARG	3.3
5	E	84	LYS	3.2
11	l	7	ARG	3.2
2	B	505	ARG	3.2
3	c	143	TYR	3.2
19	Y	21	GLN	3.1
7	h	6	TRP	3.1
20	Z	33	TRP	3.1
14	R	14	LEU	3.1
20	z	35	ARG	3.1
19	Y	37	PHE	3.0
11	l	3	PRO	3.0
19	y	37	PHE	3.0
20	Z	61	VAL	3.0
15	T	30	THR	3.0
2	b	505	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	293	ALA	3.0
9	j	5	GLY	3.0
14	r	7	VAL	2.9
14	R	18	TRP	2.9
20	Z	31	GLN	2.9
8	i	34	ARG	2.9
5	E	79	PHE	2.9
18	x	39	ARG	2.9
17	v	17	LYS	2.8
18	x	38	GLN	2.8
2	b	487	SER	2.8
17	v	21	LEU	2.8
20	Z	38	GLN	2.7
5	e	74	GLN	2.7
15	t	30	THR	2.7
14	r	23	ILE	2.7
18	x	40	SER	2.7
19	Y	41	VAL	2.7
14	R	10	LEU	2.7
3	C	57	ALA	2.7
13	O	54	GLU	2.6
20	z	3	ILE	2.6
20	z	2	THR	2.6
14	r	15	ALA	2.6
8	I	34	ARG	2.6
14	r	16	ALA	2.6
11	l	2	GLU	2.6
7	h	10	ILE	2.5
5	e	82	GLN	2.5
20	Z	4	LEU	2.5
13	O	55	GLU	2.5
3	C	146	PHE	2.5
3	c	142	GLU	2.5
15	t	28	ARG	2.4
3	c	262	ARG	2.4
20	z	41	PHE	2.4
14	R	26	TYR	2.4
16	U	8	GLU	2.4
14	R	20	VAL	2.4
12	M	33	GLN	2.4
19	y	19	ILE	2.4
2	b	503	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	288	VAL	2.4
1	A	12	ASN	2.4
18	X	3	ILE	2.3
2	B	485	GLU	2.3
3	c	146	PHE	2.3
7	h	41	PHE	2.3
8	I	6	ILE	2.3
7	H	6	TRP	2.3
2	B	127	ARG	2.3
2	b	485	GLU	2.3
19	Y	42	ARG	2.3
2	b	504	THR	2.3
2	b	129	GLY	2.3
19	y	43	ARG	2.3
3	C	61	VAL	2.3
2	b	295	GLY	2.2
14	r	4	ARG	2.2
5	e	84	LYS	2.2
13	O	87	VAL	2.2
14	r	12	VAL	2.2
10	K	14	ALA	2.2
2	B	506	ARG	2.2
19	Y	22	LEU	2.2
17	v	15	GLU	2.2
8	i	35	LYS	2.2
13	o	132	ASN	2.2
19	y	41	VAL	2.2
20	z	36	SER	2.2
2	b	293	ALA	2.2
13	O	246	ALA	2.2
12	m	31	SER	2.2
19	Y	44	GLY	2.2
20	Z	7	LEU	2.1
2	b	126	PRO	2.1
20	z	34	ASP	2.1
18	X	34	ILE	2.1
3	C	148	GLY	2.1
14	r	8	VAL	2.1
14	r	27	ALA	2.1
2	b	494	GLY	2.1
6	F	12	SER	2.1
14	r	11	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
20	z	61	VAL	2.1
1	A	16	ARG	2.1
3	C	62	PHE	2.1
13	O	57	LYS	2.1
5	E	61	ARG	2.1
14	R	5	VAL	2.1
3	c	257	PHE	2.1
19	Y	46	LEU	2.1
2	B	489	GLU	2.0
2	b	296	ALA	2.0
7	h	20	LYS	2.0
17	v	24	LYS	2.0
2	b	292	LEU	2.0
14	R	9	LEU	2.0
14	R	24	LEU	2.0
3	C	52	ALA	2.0
13	O	59	LYS	2.0
16	U	68	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	M	1	10/11	0.92	0.13	41,50,67,78	0
15	FME	t	1	10/11	0.93	0.10	36,48,66,66	0
15	FME	T	1	10/11	0.94	0.12	31,46,69,69	0
8	FME	i	1	10/11	0.96	0.18	45,54,66,70	0
12	FME	m	1	10/11	0.96	0.14	34,46,59,71	0
8	FME	I	1	10/11	0.98	0.13	41,52,63,68	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
32	STE	k	104	12/20	0.71	0.26	50,66,81,84	0
32	STE	H	103	18/20	0.72	0.35	47,75,87,88	0
32	STE	a	415	12/20	0.74	0.31	55,69,75,77	0
32	STE	E	102	12/20	0.77	0.27	53,75,86,89	0
32	STE	B	626	16/20	0.77	0.25	47,64,76,87	0
29	SQD	a	413	36/54	0.80	0.19	31,64,84,89	0
27	LMG	c	520	48/55	0.80	0.25	41,73,104,109	0
32	STE	l	102	18/20	0.80	0.18	36,53,83,90	0
32	STE	C	520	16/20	0.81	0.17	42,56,79,79	0
32	STE	b	624	16/20	0.81	0.18	51,66,80,83	0
27	LMG	D	410	33/55	0.82	0.19	38,56,80,83	0
27	LMG	b	622	55/55	0.82	0.30	49,75,94,103	0
32	STE	B	625	18/20	0.83	0.16	43,59,73,74	0
32	STE	b	625	20/20	0.83	0.18	42,65,80,84	0
28	LHG	e	102	42/49	0.83	0.26	58,82,104,116	0
22	CLA	C	512	65/65	0.83	0.20	37,55,85,90	0
27	LMG	d	408	23/55	0.84	0.23	43,66,82,84	0
32	STE	I	101	15/20	0.84	0.14	45,59,81,82	0
32	STE	c	519	20/20	0.84	0.23	43,61,86,98	0
32	STE	M	104	15/20	0.84	0.18	44,60,84,86	0
30	DGD	B	623	44/66	0.84	0.16	39,56,75,85	0
32	STE	x	102	20/20	0.84	0.22	36,60,76,80	0
28	LHG	E	101	49/49	0.85	0.23	54,79,113,119	0
24	BCR	H	101	40/40	0.85	0.16	31,48,62,70	0
24	BCR	x	101	40/40	0.85	0.16	38,57,78,80	0
22	CLA	b	601	65/65	0.86	0.19	44,68,89,105	0
32	STE	J	101	12/20	0.86	0.17	46,60,71,71	0
30	DGD	A	414	66/66	0.86	0.18	42,65,81,89	0
26	PL9	A	409	55/55	0.86	0.23	37,69,85,88	0
29	SQD	A	413	39/54	0.86	0.18	42,60,87,91	0
22	CLA	c	512	65/65	0.87	0.17	46,59,87,93	0
27	LMG	a	414	49/55	0.87	0.16	37,58,84,101	0
32	STE	d	410	17/20	0.87	0.15	42,58,69,78	0
24	BCR	k	102	40/40	0.87	0.14	45,65,75,78	0
32	STE	b	621	20/20	0.87	0.20	40,56,70,73	0
29	SQD	f	101	41/54	0.87	0.23	62,86,110,115	0
32	STE	B	620	17/20	0.88	0.18	36,50,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	STE	b	620	16/20	0.88	0.18	35,53,66,76	0
22	CLA	B	601	65/65	0.88	0.15	36,63,90,96	0
26	PL9	a	410	55/55	0.88	0.19	40,66,87,94	0
27	LMG	A	410	48/55	0.88	0.14	41,57,75,87	0
32	STE	b	626	10/20	0.88	0.28	43,55,61,65	0
27	LMG	C	518	48/55	0.88	0.19	40,74,93,101	0
24	BCR	K	101	40/40	0.88	0.14	43,57,72,82	0
24	BCR	d	404	40/40	0.88	0.16	36,54,84,98	0
22	CLA	C	513	65/65	0.88	0.20	42,63,92,95	0
22	CLA	c	513	65/65	0.88	0.21	43,67,103,109	0
32	STE	B	624	12/20	0.89	0.10	41,57,67,77	0
32	STE	j	101	12/20	0.89	0.15	42,60,73,77	0
29	SQD	L	101	49/54	0.89	0.14	41,59,89,101	0
24	BCR	k	103	40/40	0.89	0.19	44,58,69,74	0
29	SQD	B	622	54/54	0.89	0.15	36,61,87,102	0
32	STE	C	521	12/20	0.90	0.11	37,48,57,59	0
22	CLA	a	405	65/65	0.90	0.14	21,38,87,98	0
22	CLA	c	508	64/65	0.90	0.17	29,45,85,98	0
22	CLA	d	403	65/65	0.90	0.16	36,53,90,95	0
24	BCR	k	101	40/40	0.90	0.17	42,60,76,77	0
27	LMG	D	411	28/55	0.90	0.15	33,52,63,64	0
32	STE	B	627	12/20	0.90	0.38	51,65,84,84	0
32	STE	C	519	12/20	0.90	0.13	42,57,69,73	0
32	STE	t	103	10/20	0.90	0.18	32,61,69,71	0
27	LMG	M	101	51/55	0.90	0.13	32,52,68,73	0
27	LMG	D	408	51/55	0.91	0.19	29,58,82,92	0
32	STE	D	412	20/20	0.91	0.13	32,53,69,70	0
32	STE	M	102	15/20	0.91	0.14	38,51,67,67	0
32	STE	M	103	10/20	0.91	0.16	38,48,56,65	0
32	STE	m	102	12/20	0.91	0.17	51,64,80,84	0
22	CLA	c	502	65/65	0.91	0.16	31,49,64,70	0
22	CLA	D	405	65/65	0.91	0.14	25,47,98,106	0
27	LMG	m	101	51/55	0.92	0.13	35,54,68,80	0
24	BCR	D	406	40/40	0.92	0.14	31,46,83,87	0
22	CLA	B	615	65/65	0.92	0.14	28,40,71,75	0
22	CLA	B	616	60/65	0.92	0.15	28,44,86,98	0
30	DGD	C	516	62/66	0.92	0.15	35,55,105,118	0
22	CLA	b	616	60/65	0.92	0.14	28,47,91,95	0
22	CLA	C	502	65/65	0.92	0.14	33,45,64,76	0
24	BCR	B	619	40/40	0.93	0.12	28,46,64,68	0
22	CLA	C	507	65/65	0.93	0.15	28,46,61,63	0
22	CLA	c	503	65/65	0.93	0.17	37,48,61,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	c	506	65/65	0.93	0.14	30,54,99,106	0
24	BCR	K	102	40/40	0.93	0.17	40,55,71,75	0
30	DGD	C	517	62/66	0.93	0.14	30,53,74,86	0
30	DGD	c	516	62/66	0.93	0.14	33,56,93,101	0
30	DGD	h	101	62/66	0.93	0.13	30,51,63,69	0
24	BCR	Z	101	40/40	0.93	0.16	40,58,72,79	0
24	BCR	b	617	40/40	0.93	0.13	28,47,58,59	0
27	LMG	c	518	37/55	0.93	0.14	44,65,82,88	0
22	CLA	c	507	65/65	0.93	0.16	30,48,66,67	0
22	CLA	b	602	65/65	0.93	0.16	27,47,66,77	0
22	CLA	c	510	65/65	0.93	0.16	31,50,66,74	0
22	CLA	c	511	65/65	0.93	0.14	40,55,73,77	0
22	CLA	b	606	65/65	0.93	0.12	28,43,75,79	0
22	CLA	b	615	65/65	0.93	0.14	27,42,65,68	0
32	STE	t	102	14/20	0.93	0.12	36,53,59,60	0
22	CLA	C	511	65/65	0.93	0.14	35,52,66,77	0
24	BCR	B	618	40/40	0.93	0.11	26,39,53,56	0
22	CLA	C	505	65/65	0.94	0.15	26,43,71,76	0
22	CLA	C	506	65/65	0.94	0.13	27,49,99,103	0
22	CLA	a	403	65/65	0.94	0.15	26,43,91,102	0
30	DGD	H	102	62/66	0.94	0.11	31,47,60,62	0
22	CLA	B	604	65/65	0.94	0.14	24,36,70,78	0
30	DGD	c	517	62/66	0.94	0.14	32,54,90,96	0
22	CLA	c	505	65/65	0.94	0.17	30,44,71,73	0
27	LMG	d	409	44/55	0.94	0.15	36,56,83,89	0
24	BCR	C	514	40/40	0.94	0.12	28,44,57,62	0
26	PL9	D	407	55/55	0.94	0.12	24,37,51,53	0
22	CLA	C	508	65/65	0.94	0.12	33,47,100,108	0
29	SQD	A	412	52/54	0.94	0.17	33,59,86,89	0
22	CLA	B	606	65/65	0.94	0.12	24,39,76,81	0
22	CLA	B	614	65/65	0.94	0.16	25,40,76,85	0
22	CLA	c	509	65/65	0.94	0.20	36,51,70,74	0
29	SQD	a	412	54/54	0.94	0.17	45,65,85,89	0
22	CLA	b	609	65/65	0.94	0.15	31,48,72,76	0
22	CLA	b	614	65/65	0.94	0.15	27,42,77,88	0
24	BCR	b	619	40/40	0.94	0.10	32,49,67,74	0
22	CLA	C	509	65/65	0.95	0.18	26,49,67,72	0
22	CLA	C	510	65/65	0.95	0.14	30,46,68,74	0
22	CLA	B	603	65/65	0.95	0.16	20,36,62,63	0
22	CLA	A	405	54/65	0.95	0.12	22,37,67,72	0
22	CLA	C	501	65/65	0.95	0.13	23,37,53,58	0
24	BCR	T	101	40/40	0.95	0.09	29,43,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	c	504	60/65	0.95	0.12	34,49,80,87	0
22	CLA	A	403	65/65	0.95	0.14	22,37,83,96	0
28	LHG	A	411	47/49	0.95	0.13	31,51,76,89	0
28	LHG	B	621	49/49	0.95	0.12	31,47,65,80	0
24	BCR	b	618	40/40	0.95	0.10	29,42,53,59	0
28	LHG	b	623	49/49	0.95	0.13	34,52,68,73	0
22	CLA	C	503	65/65	0.95	0.14	33,46,56,58	0
24	BCR	c	514	40/40	0.95	0.12	30,45,60,69	0
22	CLA	C	504	59/65	0.95	0.12	29,47,84,88	0
22	CLA	B	609	65/65	0.95	0.12	28,39,58,68	0
29	SQD	F	102	36/54	0.95	0.17	44,73,93,97	0
22	CLA	B	610	65/65	0.95	0.15	21,36,46,49	0
22	CLA	b	604	65/65	0.95	0.14	25,41,77,86	0
22	CLA	B	613	65/65	0.95	0.15	21,37,68,77	0
22	CLA	b	608	65/65	0.95	0.15	30,46,66,76	0
22	CLA	B	602	65/65	0.95	0.17	26,41,57,65	0
22	CLA	b	610	65/65	0.95	0.18	27,40,51,61	0
30	DGD	C	515	62/66	0.95	0.13	23,43,80,92	0
26	PL9	d	405	55/55	0.95	0.12	24,38,48,52	0
23	PHO	a	404	64/64	0.95	0.13	22,34,42,44	0
24	BCR	A	406	40/40	0.95	0.10	26,38,50,52	0
30	DGD	c	515	62/66	0.95	0.12	26,45,79,86	0
24	BCR	B	617	40/40	0.95	0.12	27,42,58,64	0
22	CLA	b	611	65/65	0.95	0.14	22,35,55,64	0
22	CLA	b	613	65/65	0.95	0.15	25,38,75,78	0
22	CLA	a	411	65/65	0.96	0.12	23,34,52,56	0
24	BCR	t	101	40/40	0.96	0.09	27,42,57,58	0
22	CLA	B	608	65/65	0.96	0.13	25,37,55,61	0
22	CLA	b	612	65/65	0.96	0.17	21,37,49,59	0
22	CLA	D	403	65/65	0.96	0.12	21,33,56,65	0
22	CLA	b	603	65/65	0.96	0.14	24,40,68,75	0
22	CLA	D	404	65/65	0.96	0.11	22,33,50,57	0
28	LHG	l	101	49/49	0.96	0.11	25,47,57,73	0
22	CLA	b	605	65/65	0.96	0.13	23,38,51,57	0
22	CLA	c	501	65/65	0.96	0.14	28,45,56,61	0
22	CLA	d	402	65/65	0.96	0.12	23,36,60,64	0
24	BCR	a	406	40/40	0.96	0.10	22,38,51,55	0
22	CLA	A	402	65/65	0.96	0.11	21,31,44,62	0
23	PHO	A	404	64/64	0.96	0.12	19,31,42,44	0
23	PHO	D	401	64/64	0.96	0.12	23,35,45,49	0
22	CLA	b	607	65/65	0.96	0.13	22,39,66,74	0
23	PHO	d	401	64/64	0.96	0.11	29,42,51,60	0

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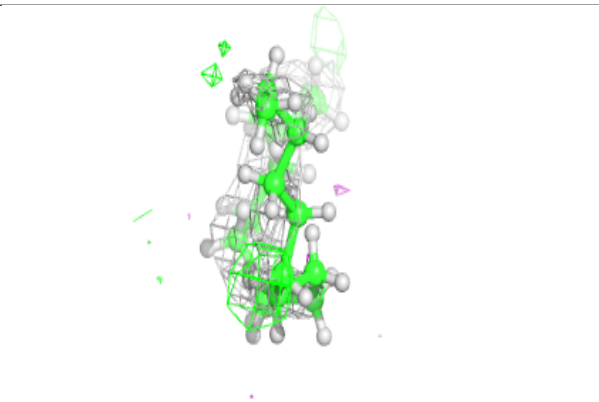
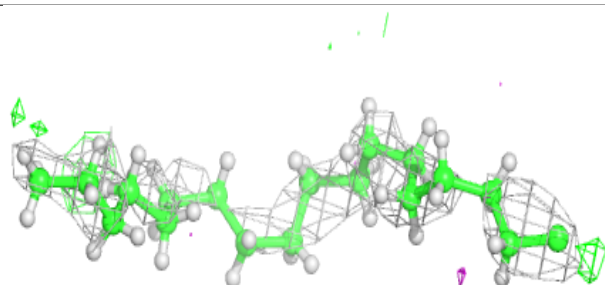
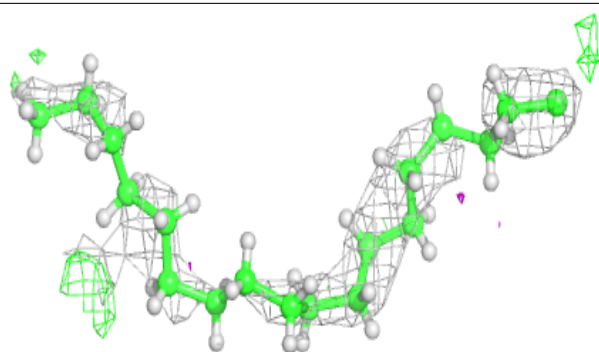
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	B	607	65/65	0.96	0.11	20,36,61,68	0
22	CLA	B	612	65/65	0.96	0.15	22,35,49,58	0
34	HEM	F	101	43/43	0.96	0.13	40,49,68,72	0
34	HEM	e	101	43/43	0.96	0.12	48,59,78,79	0
22	CLA	a	402	65/65	0.97	0.10	22,33,46,56	0
28	LHG	d	406	49/49	0.97	0.10	27,44,56,65	0
28	LHG	d	407	39/49	0.97	0.10	34,50,70,73	0
22	CLA	B	611	65/65	0.97	0.14	21,33,52,55	0
28	LHG	D	409	49/49	0.97	0.10	25,43,55,61	0
22	CLA	B	605	65/65	0.97	0.14	23,35,52,55	0
28	LHG	L	102	49/49	0.97	0.10	29,43,57,69	0
35	HEC	V	201	43/43	0.97	0.14	27,37,46,49	0
33	BCT	D	402	4/4	0.98	0.18	28,32,35,42	0
35	HEC	v	201	43/43	0.98	0.12	33,41,51,58	0
21	FE2	a	401	1/1	0.99	0.09	37,37,37,37	0
25	CL	A	407	1/1	0.99	0.07	34,34,34,34	0
25	CL	a	407	1/1	0.99	0.06	32,32,32,32	0
33	BCT	a	409	4/4	0.99	0.20	33,34,45,51	0
25	CL	a	408	1/1	0.99	0.06	32,32,32,32	0
31	OEX	A	415	10/10	0.99	0.13	26,29,33,36	0
31	OEX	a	416	10/10	0.99	0.12	24,30,33,33	0
21	FE2	A	401	1/1	0.99	0.08	29,29,29,29	0
25	CL	A	408	1/1	1.00	0.04	30,30,30,30	0

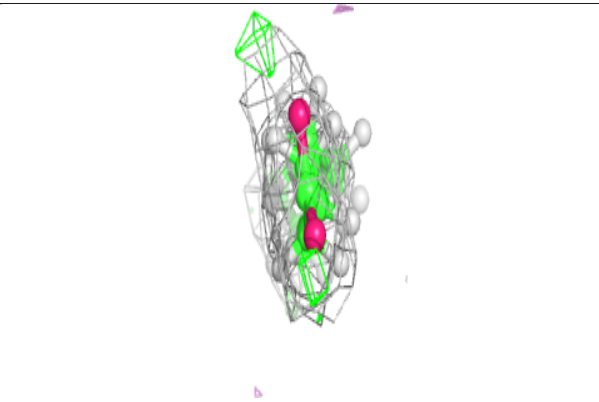
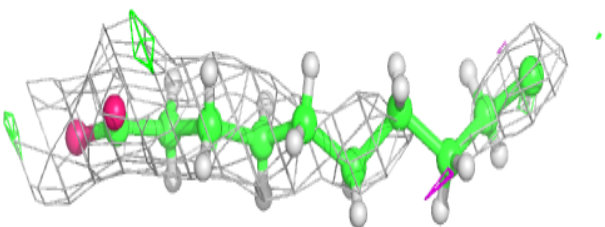
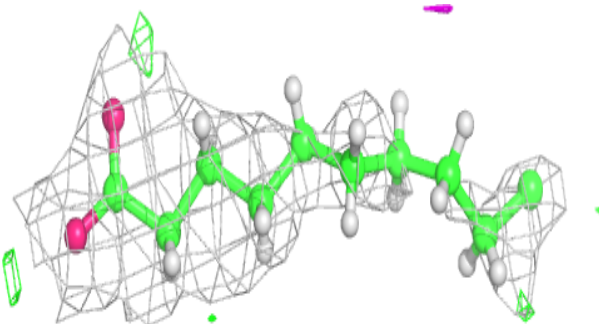
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around STE H 103:**

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

**Electron density around STE a 415:**

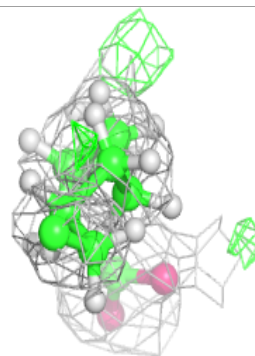
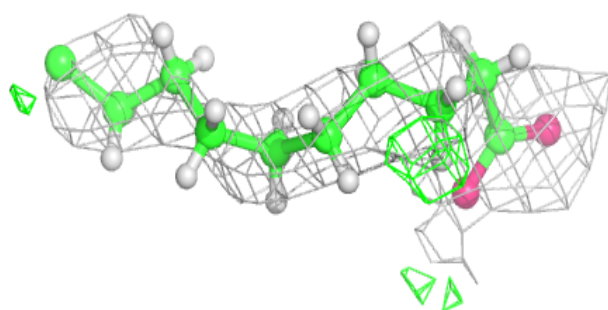
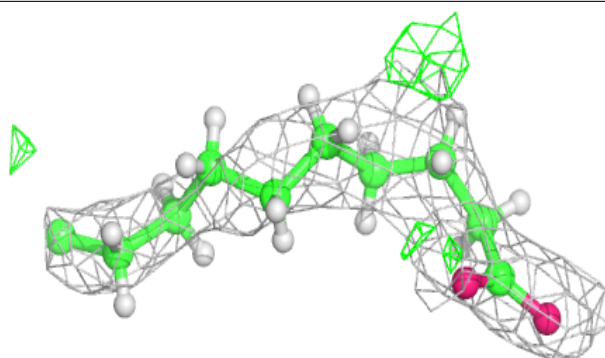
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



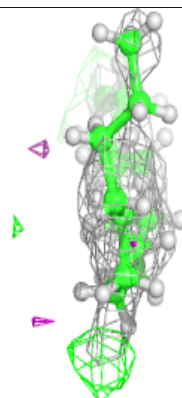
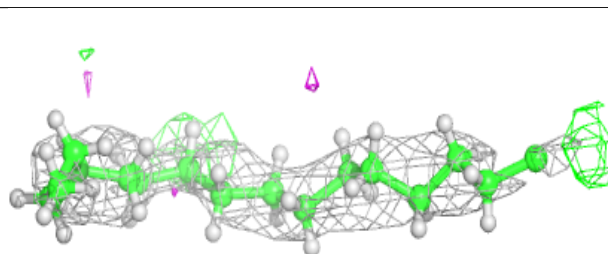
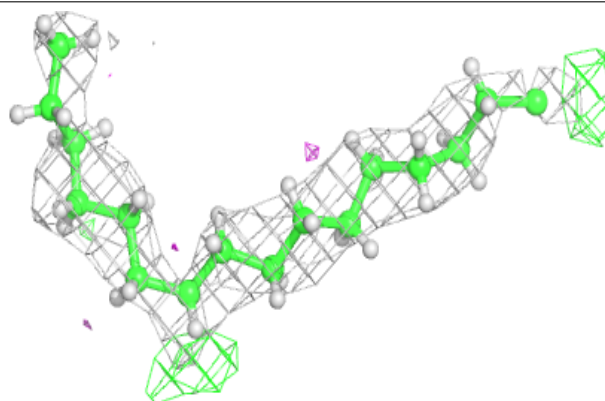


**Electron density around STE E 102:**

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

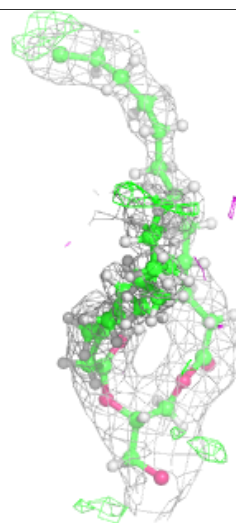
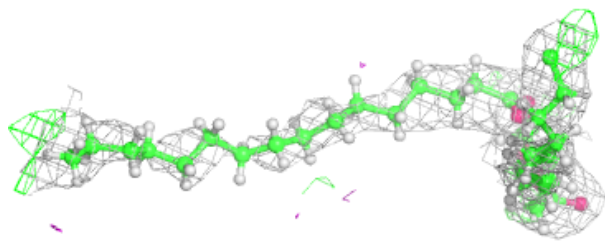
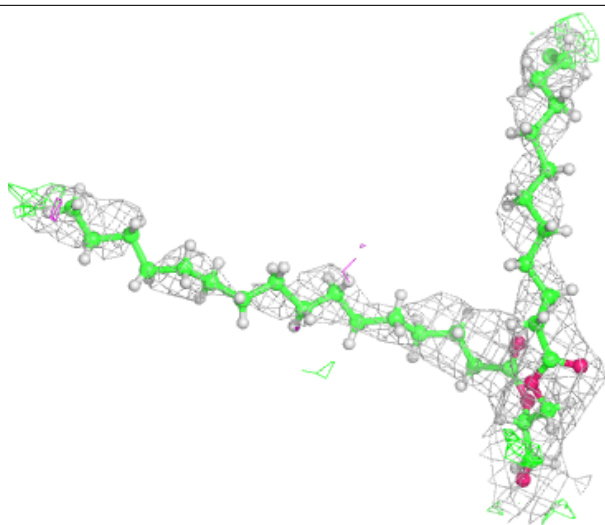
**Electron density around STE B 626:**

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



**Electron density around SQD a 413:**

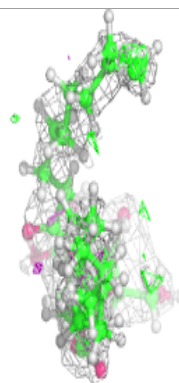
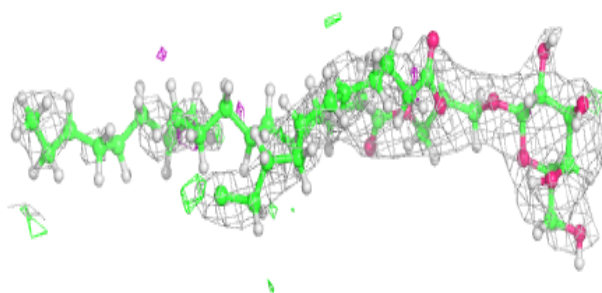
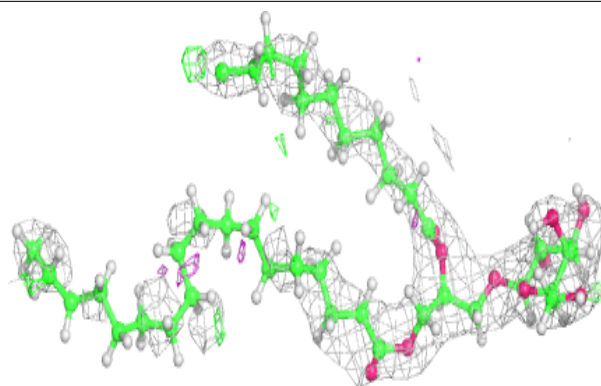
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



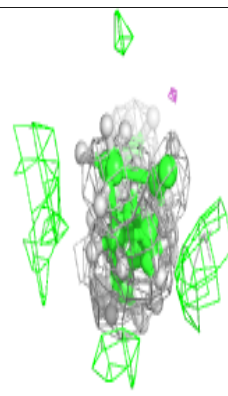
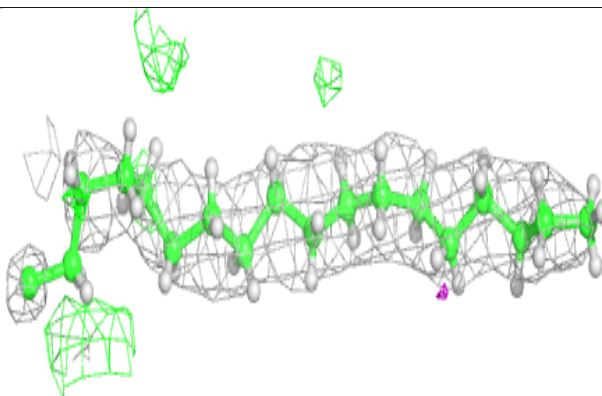
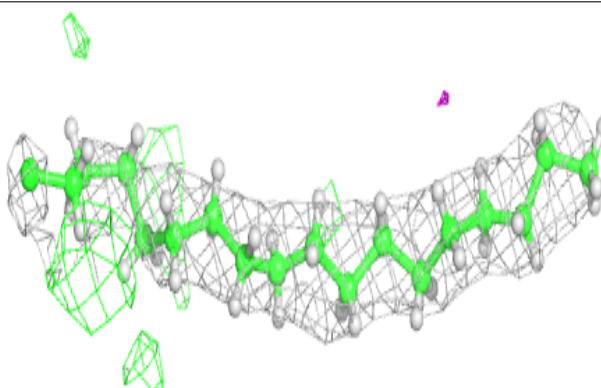


**Electron density around LMG c 520:**

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

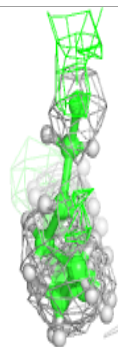
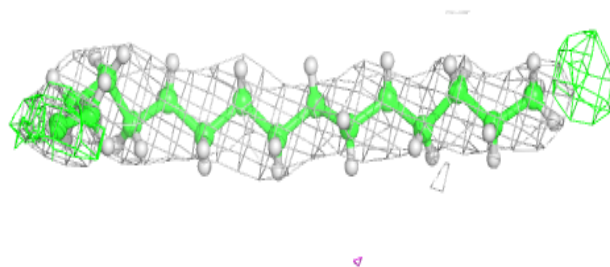
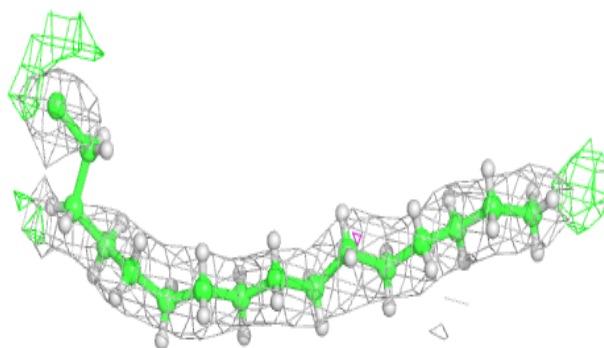
**Electron density around STE l 102:**

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

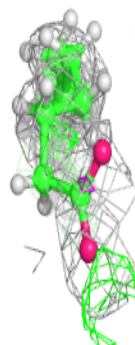
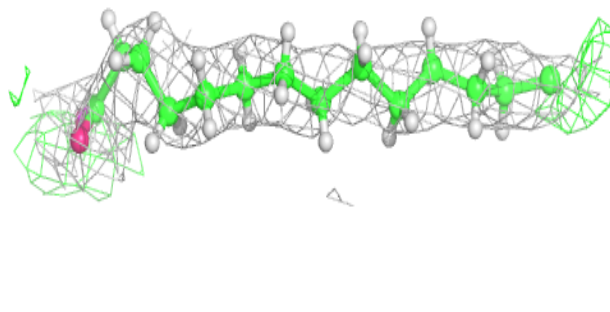
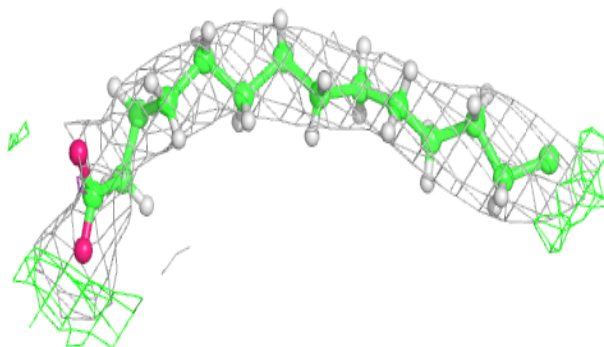


**Electron density around STE C 520:**

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

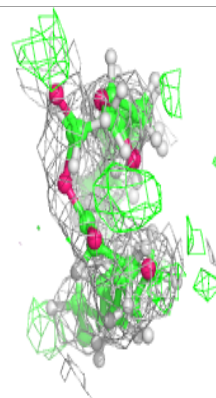
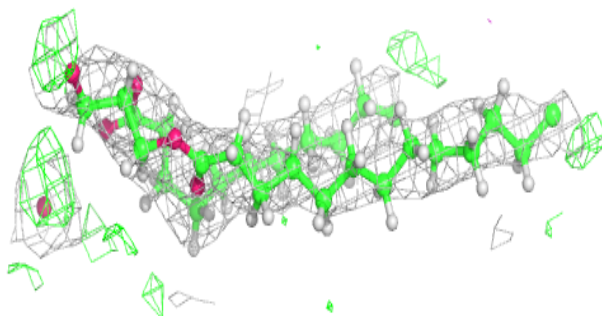
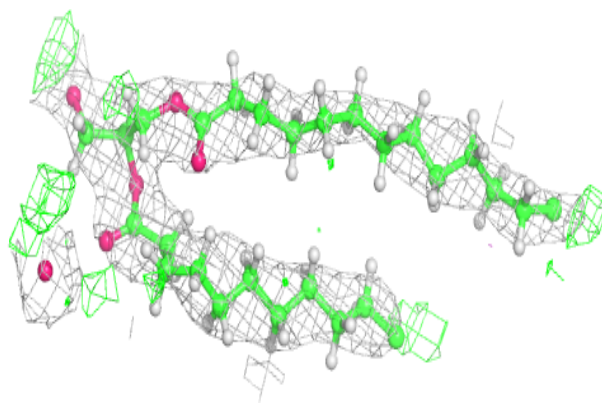
**Electron density around STE b 624:**

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

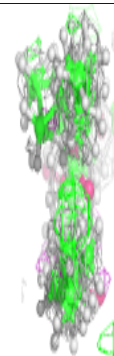
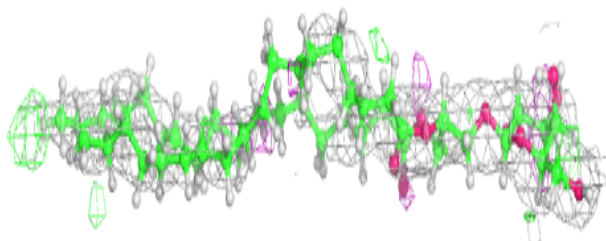
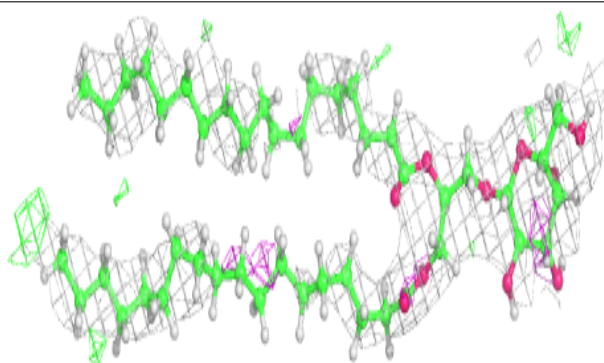


**Electron density around LMG D 410:**

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

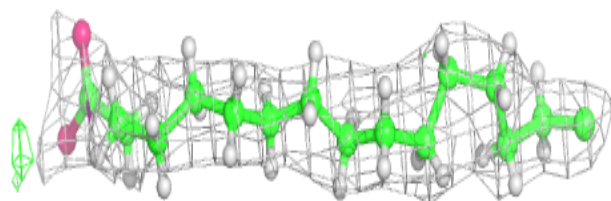
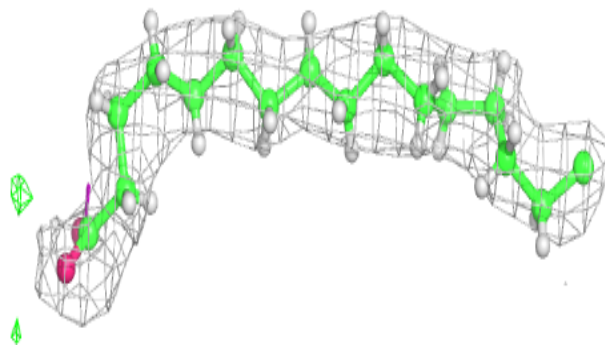
**Electron density around LMG b 622:**

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

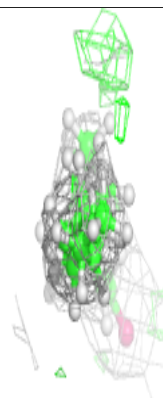
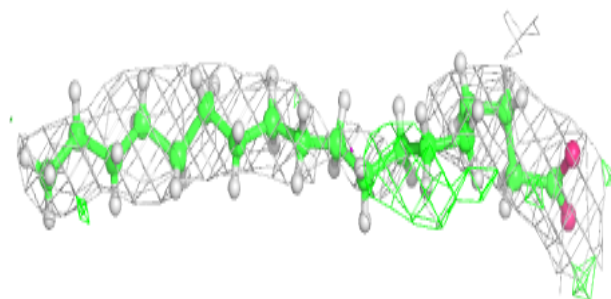
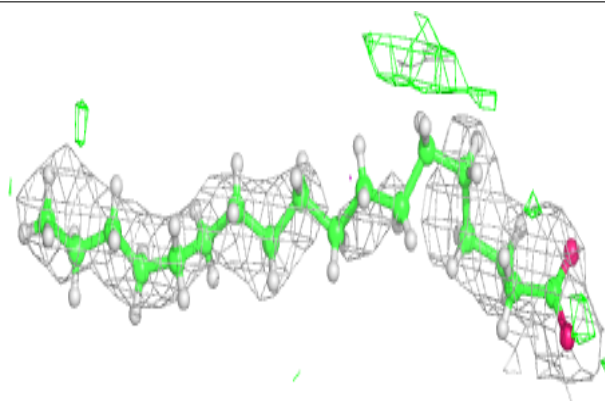


**Electron density around STE B 625:**

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

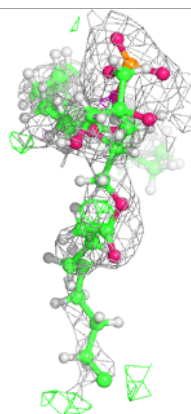
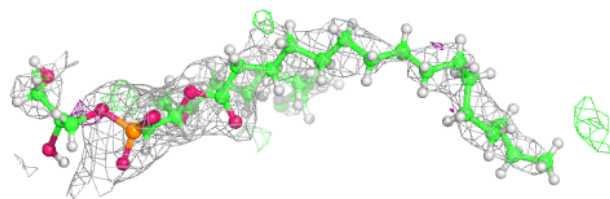
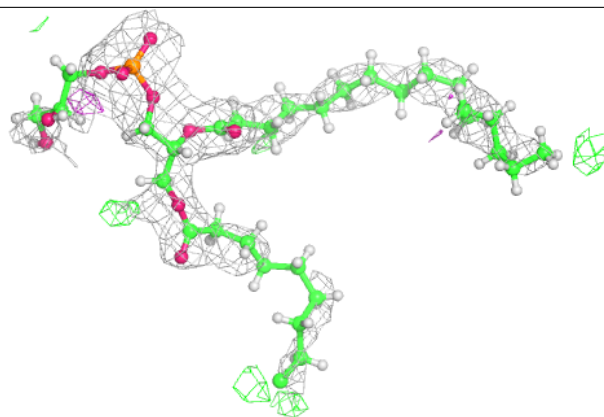
**Electron density around STE b 625:**

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



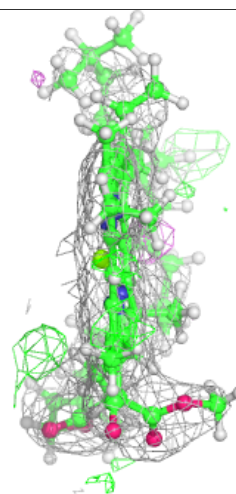
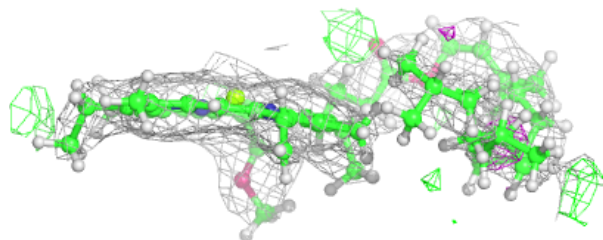
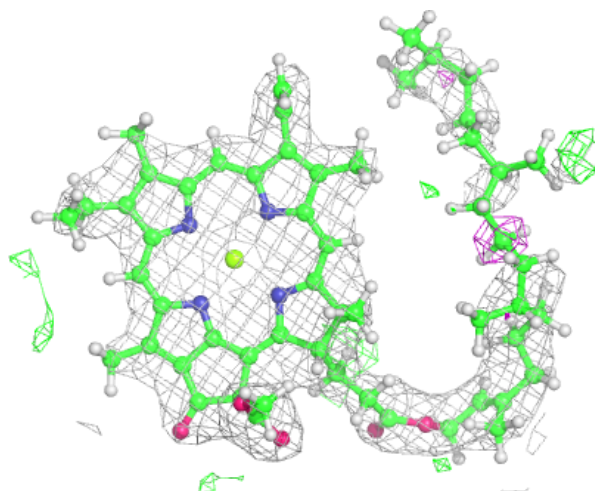
**Electron density around LHG e 102:**

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



**Electron density around CLA C 512:**

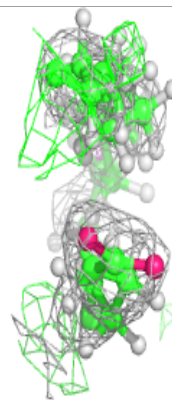
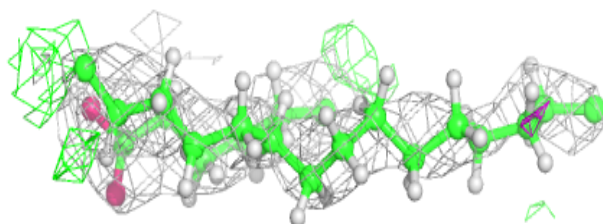
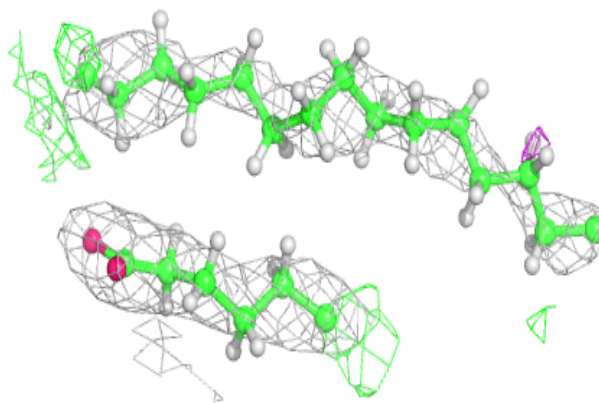
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



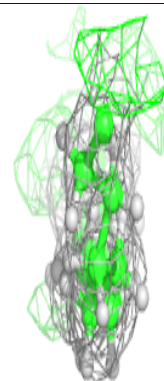
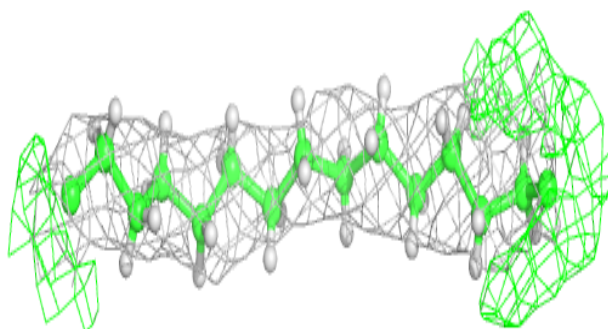
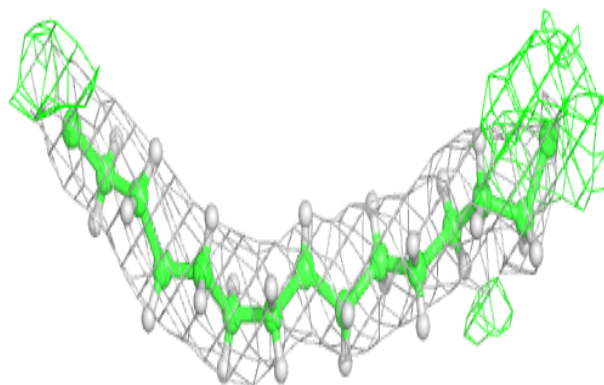


**Electron density around LMG d 408:**

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

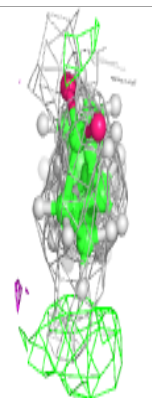
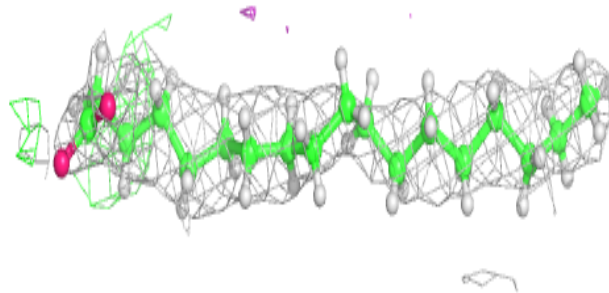
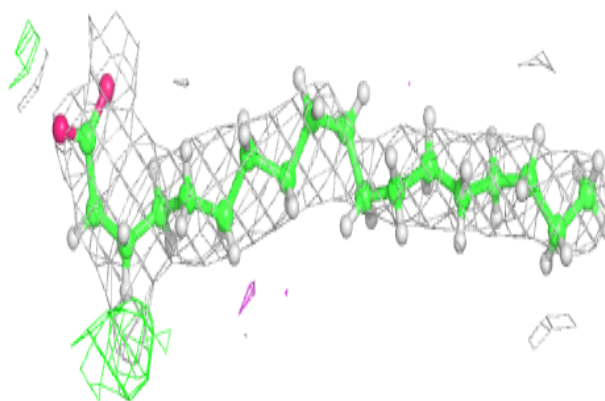
**Electron density around STE I 101:**

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

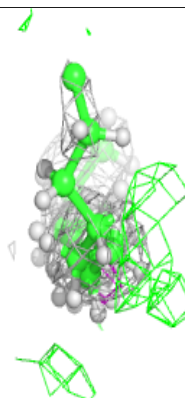
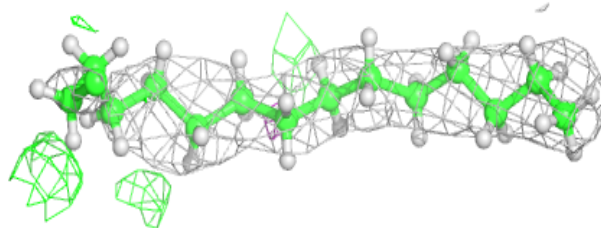
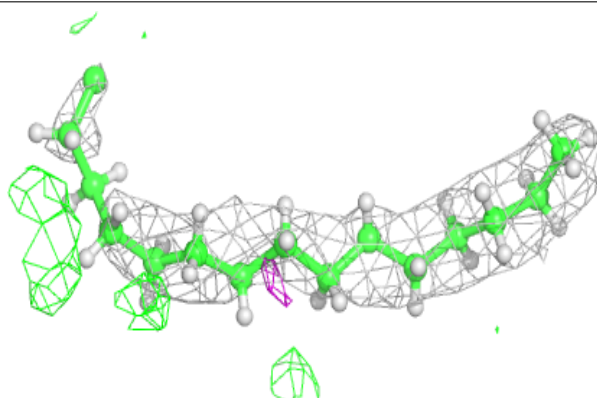


**Electron density around STE c 519:**

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

**Electron density around STE M 104:**

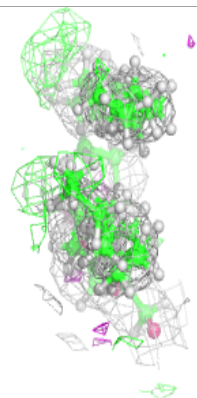
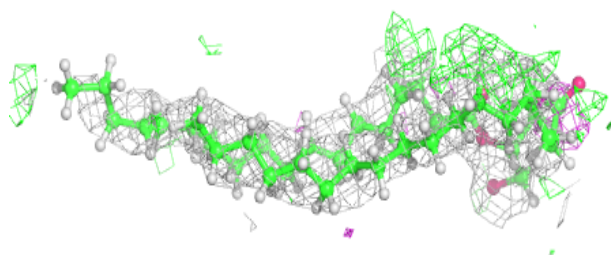
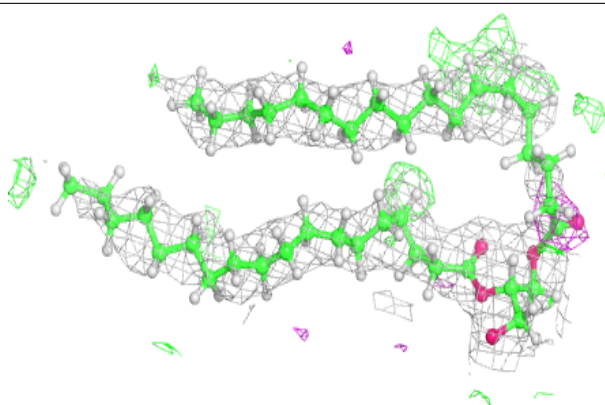
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



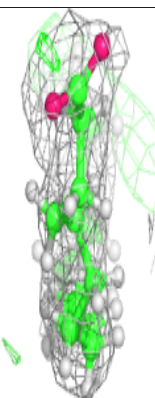
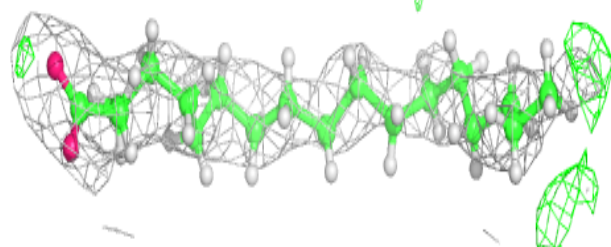
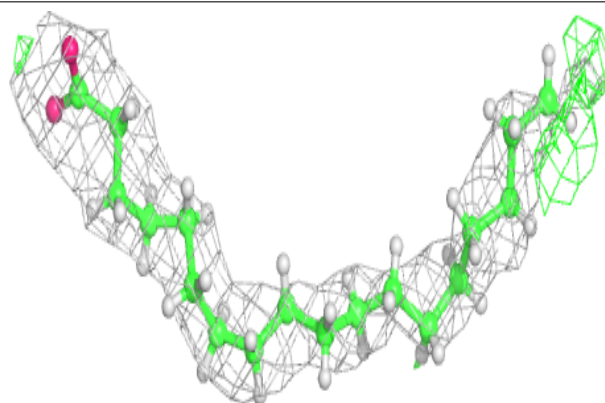


**Electron density around DGD B 623:**

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

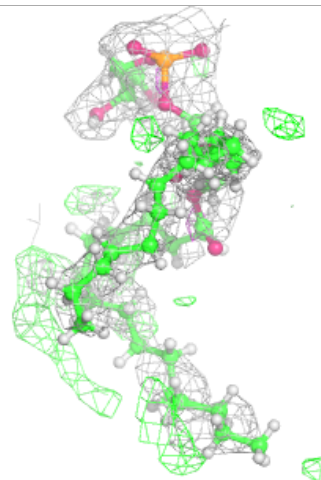
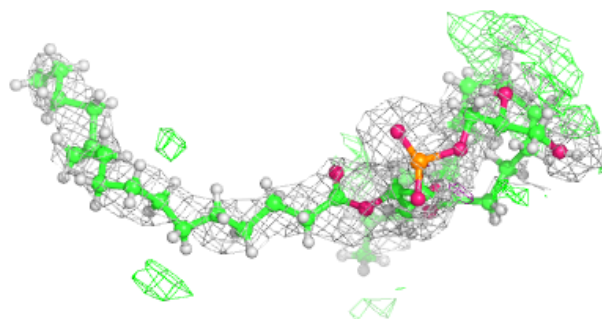
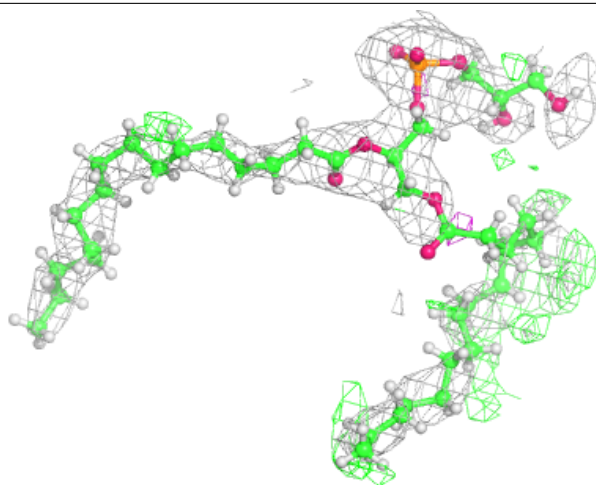
**Electron density around STE x 102:**

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



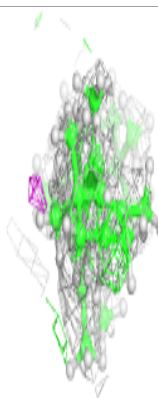
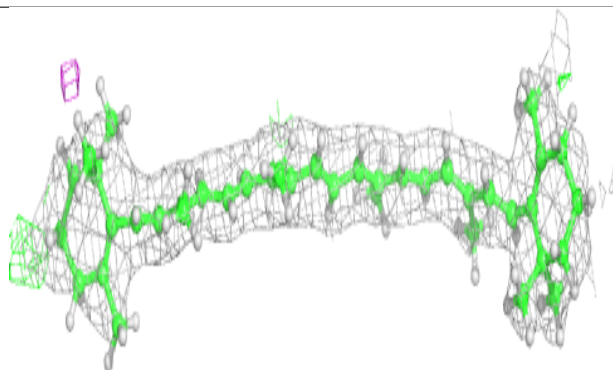
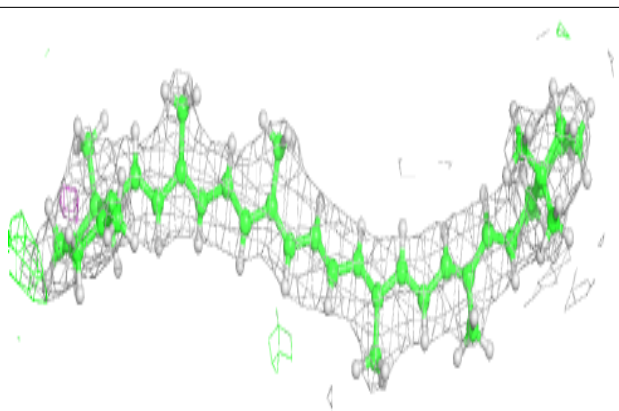
**Electron density around LHG E 101:**

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

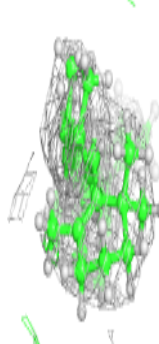
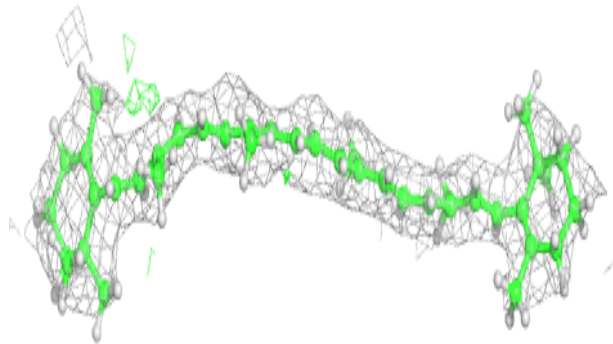
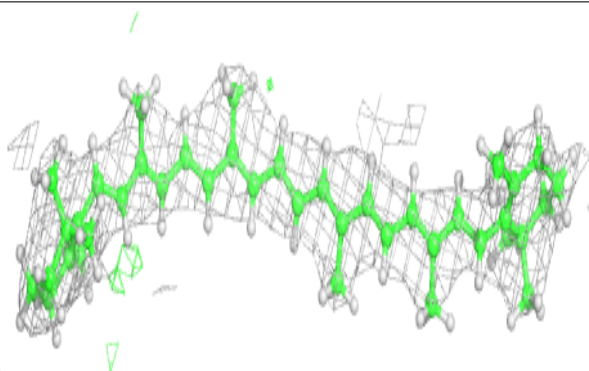


**Electron density around BCR H 101:**

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

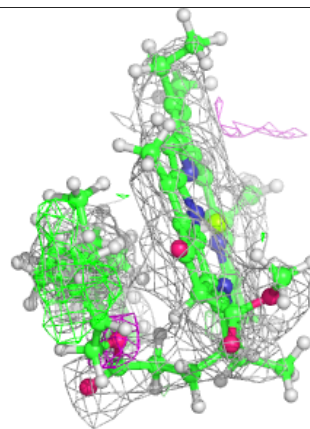
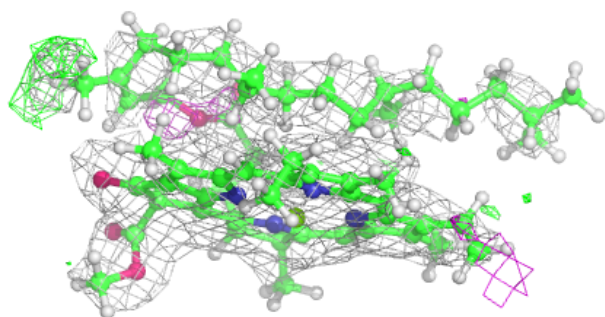
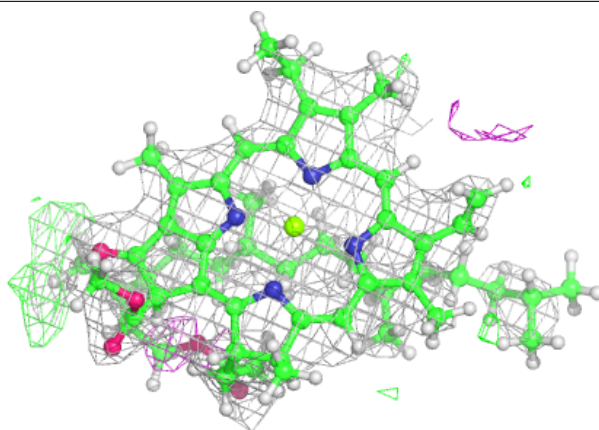
**Electron density around BCR x 101:**

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

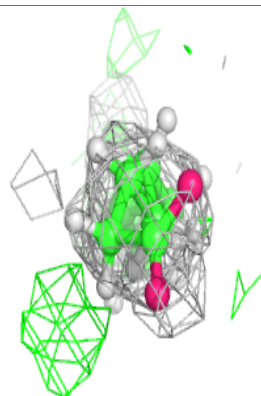
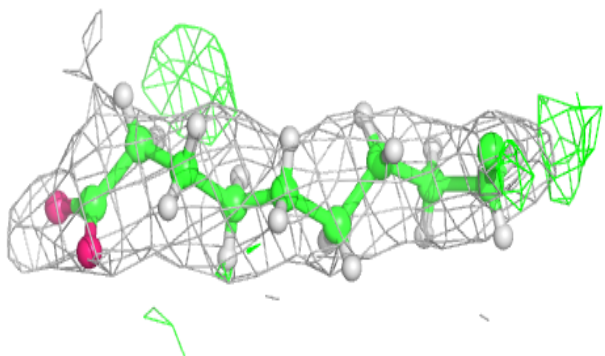
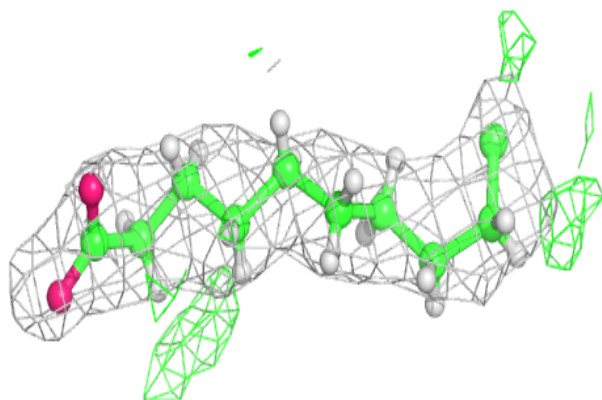


**Electron density around CLA b 601:**

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

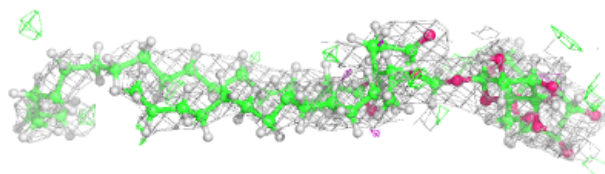
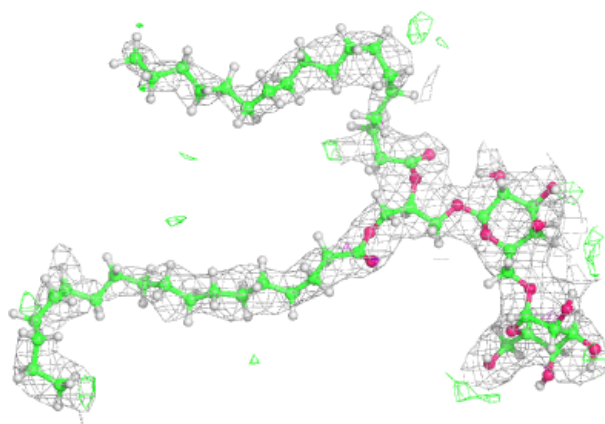
**Electron density around STE J 101:**

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

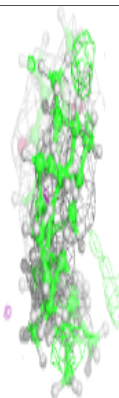
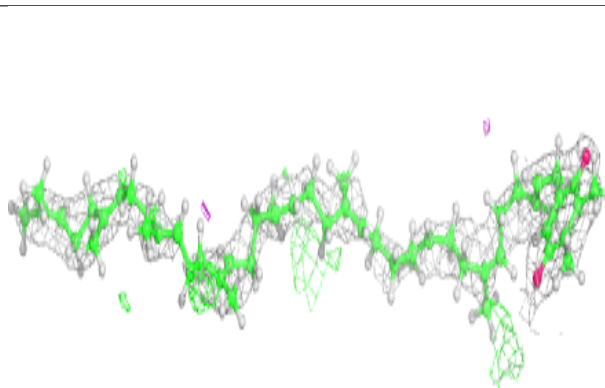
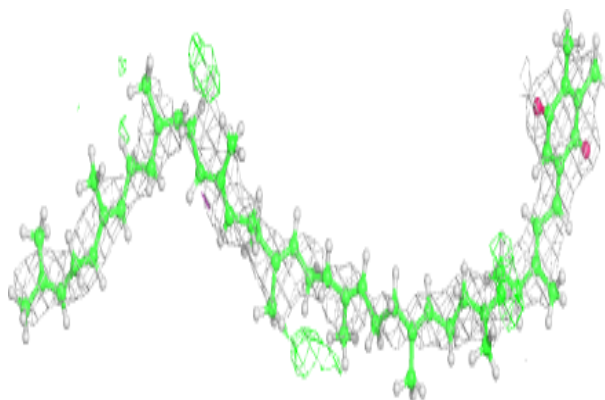


**Electron density around DGD A 414:**

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

**Electron density around PL9 A 409:**

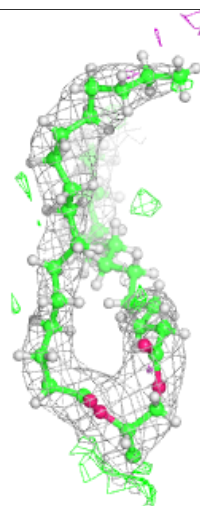
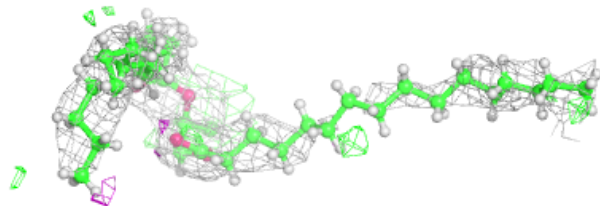
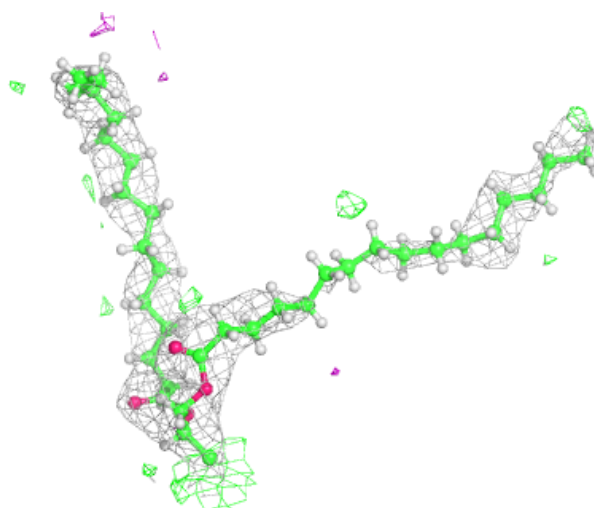
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





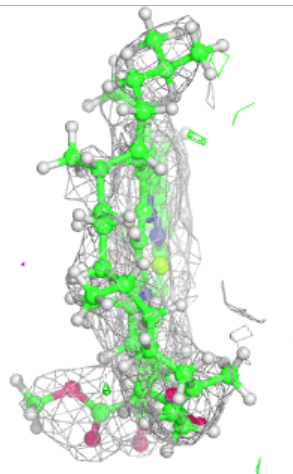
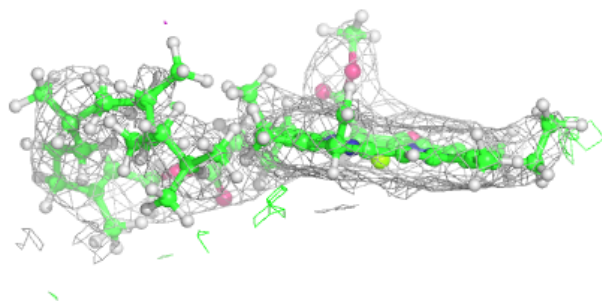
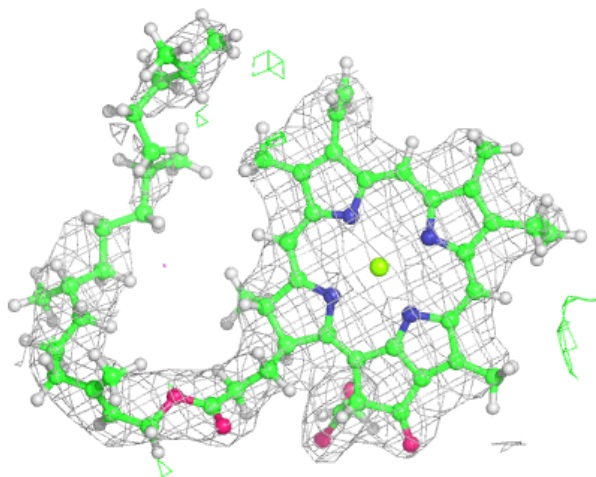
**Electron density around SQD A 413:**

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



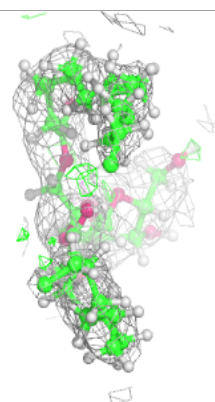
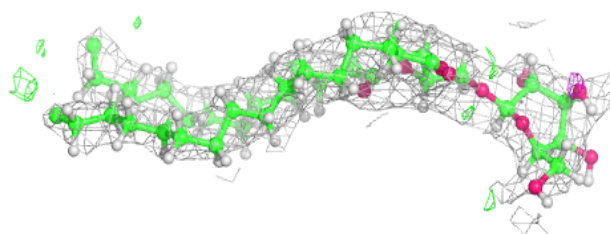
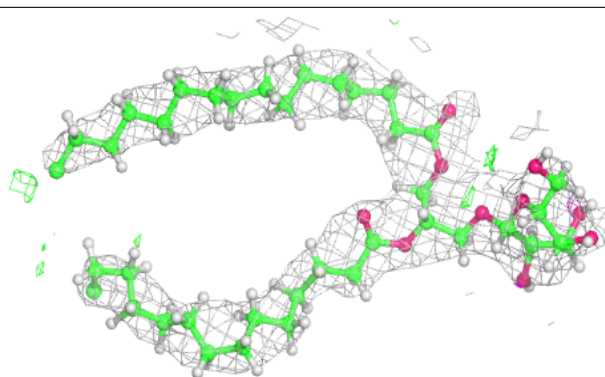
**Electron density around CLA c 512:**

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

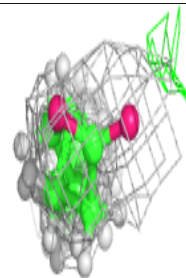
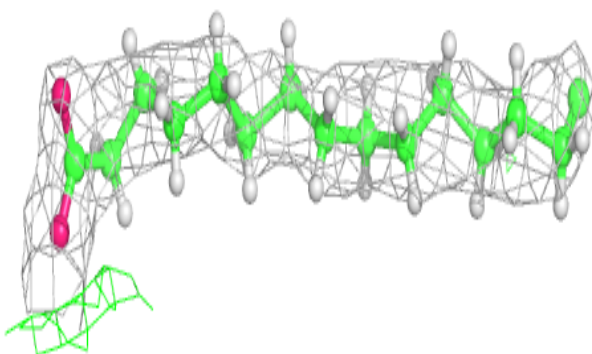
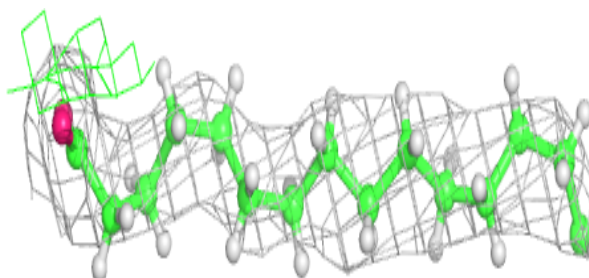


**Electron density around LMG a 414:**

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

**Electron density around STE d 410:**

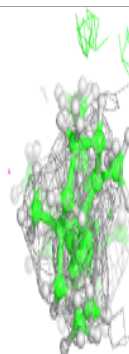
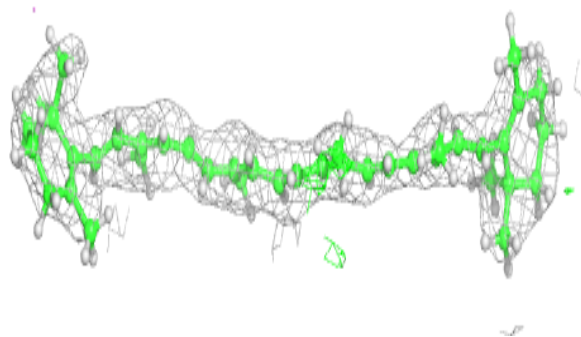
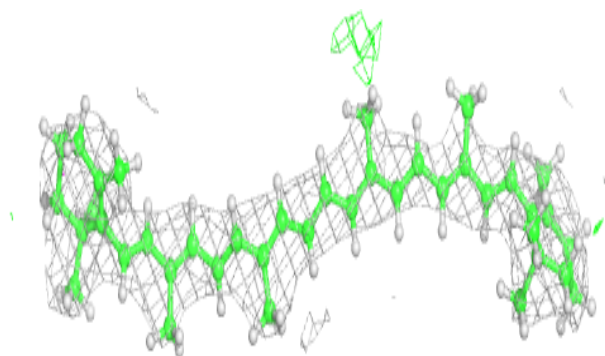
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



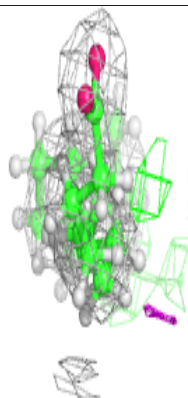
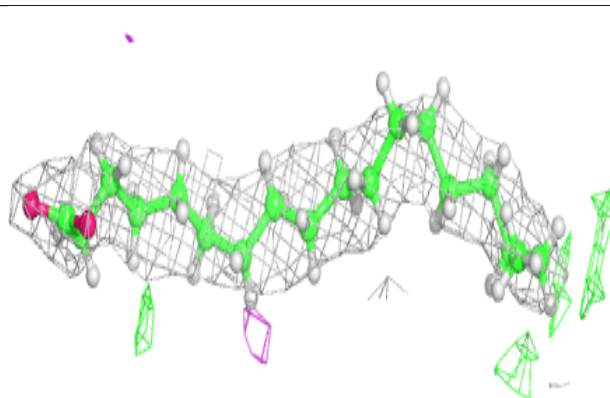
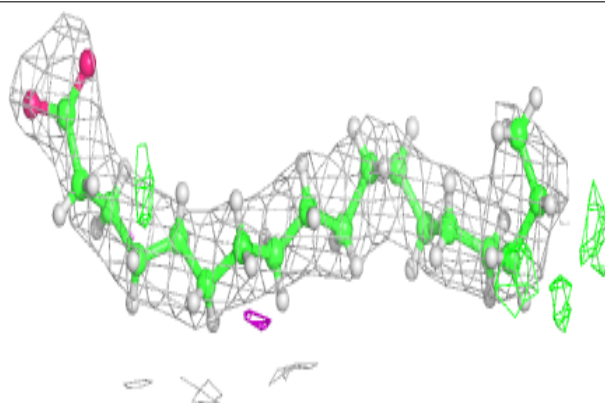


**Electron density around BCR k 102:**

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

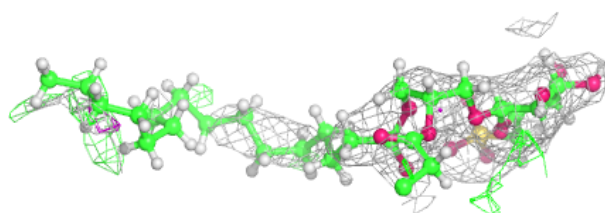
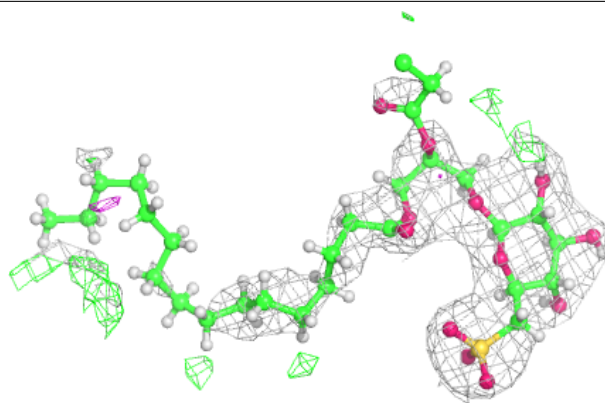
**Electron density around STE b 621:**

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

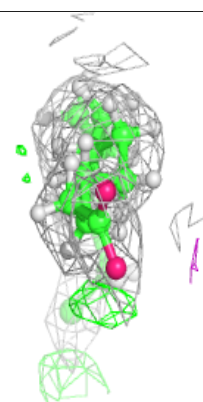
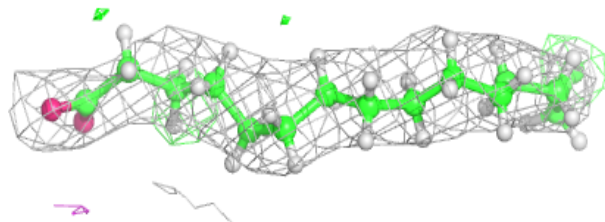
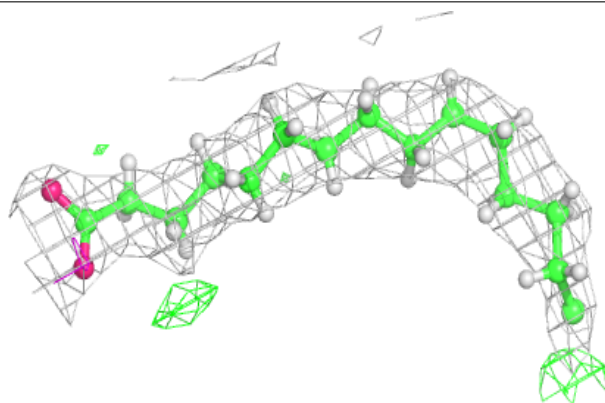


**Electron density around SQD f 101:**

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

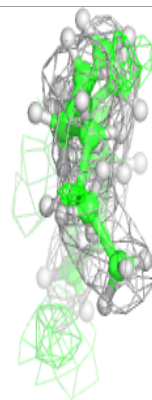
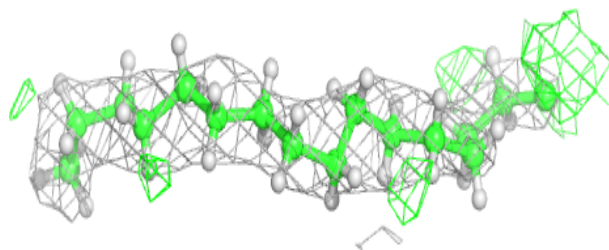
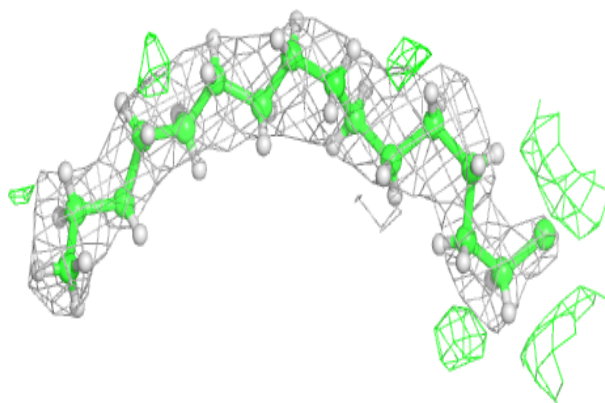
**Electron density around STE B 620:**

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

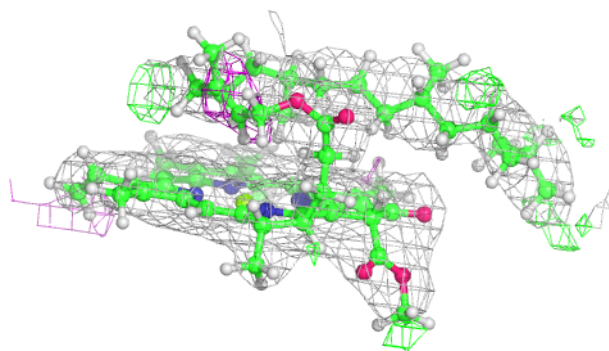
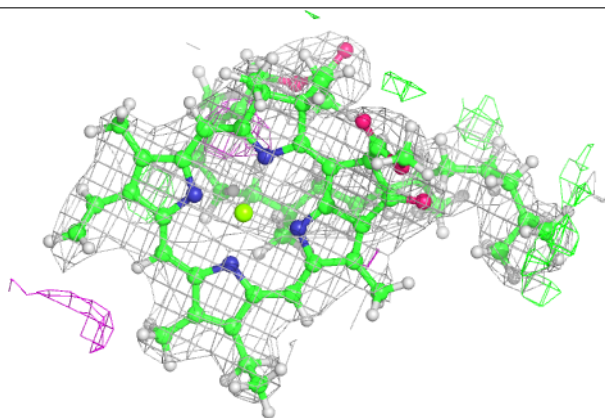


**Electron density around STE b 620:**

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

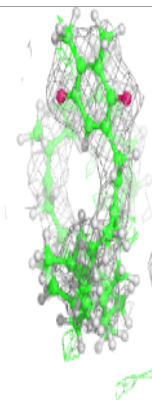
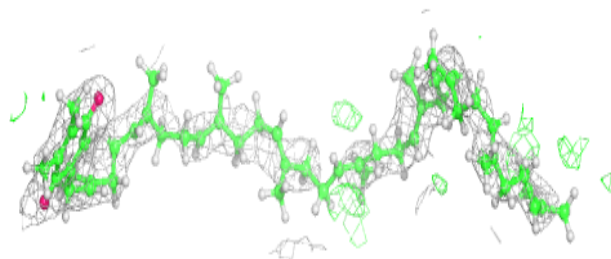
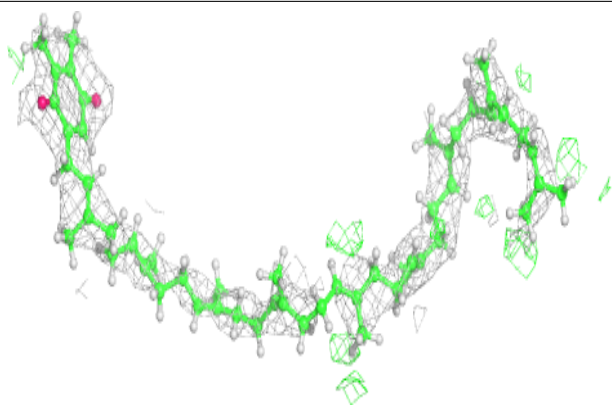
**Electron density around CLA B 601:**

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

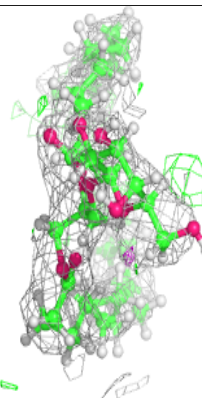
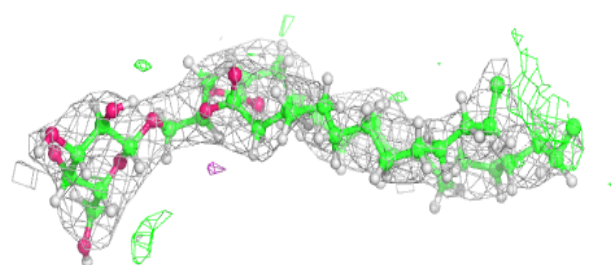
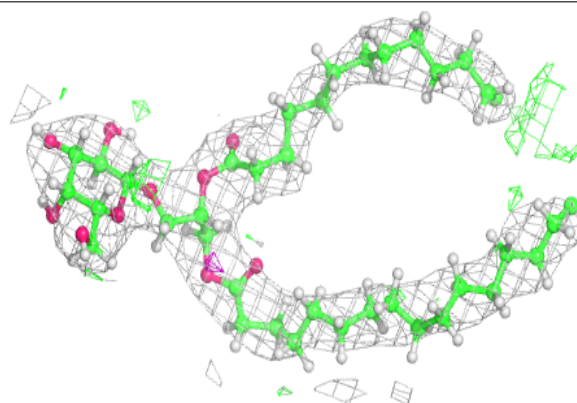


**Electron density around PL9 a 410:**

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

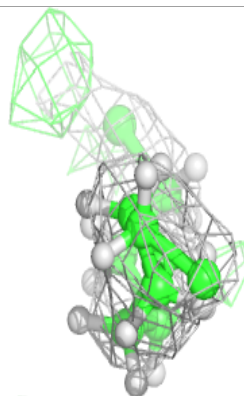
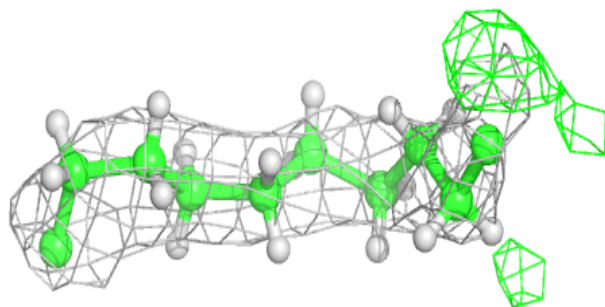
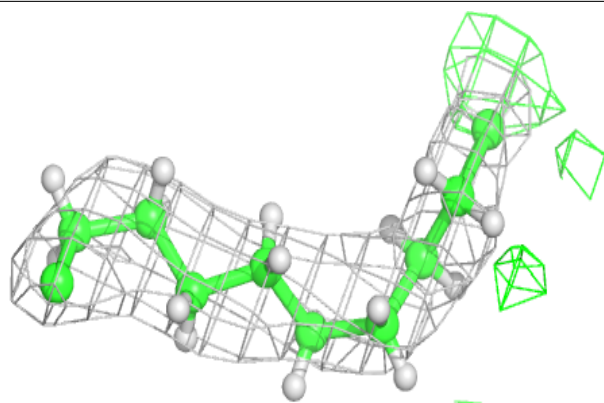
**Electron density around LMG A 410:**

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



**Electron density around STE b 626:**

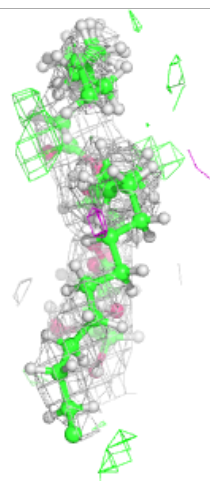
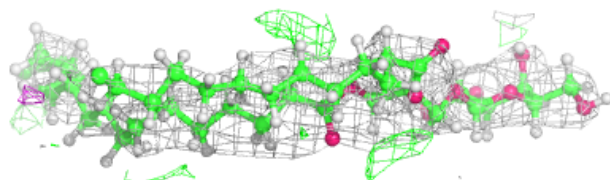
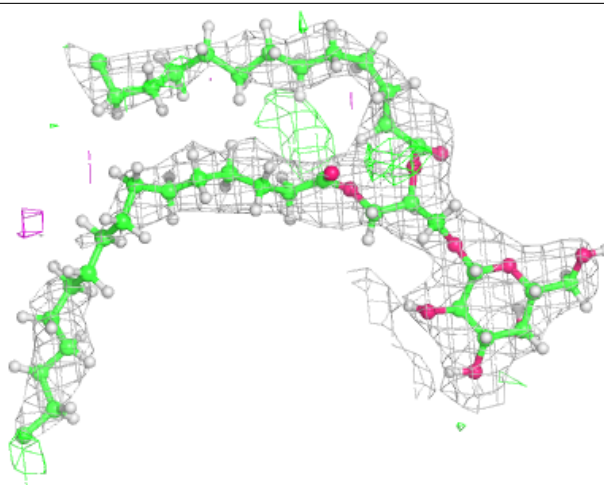
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





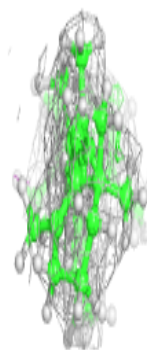
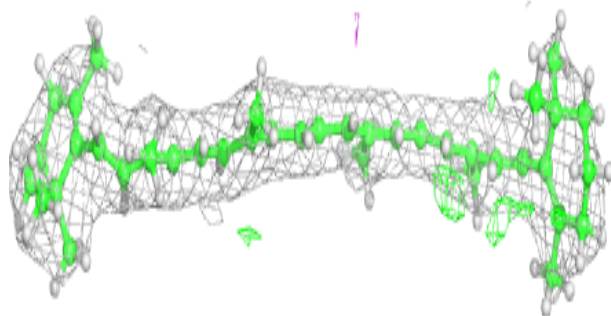
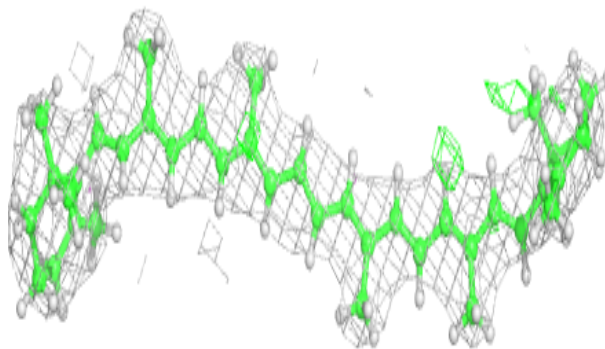
**Electron density around LMG C 518:**

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

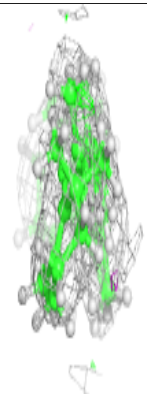
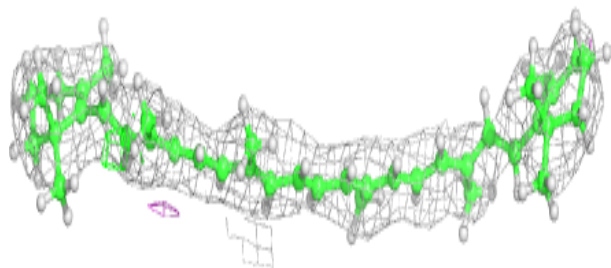
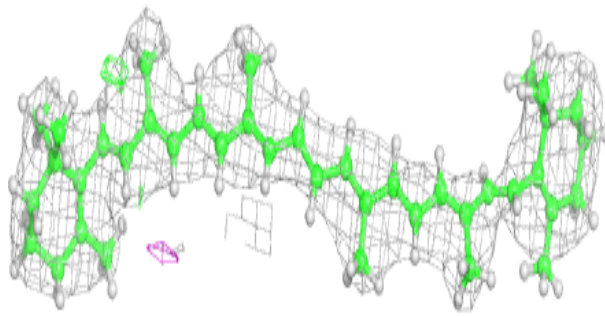


**Electron density around BCR K 101:**

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

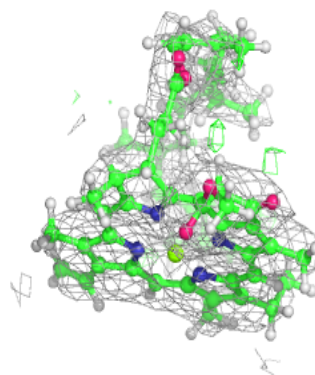
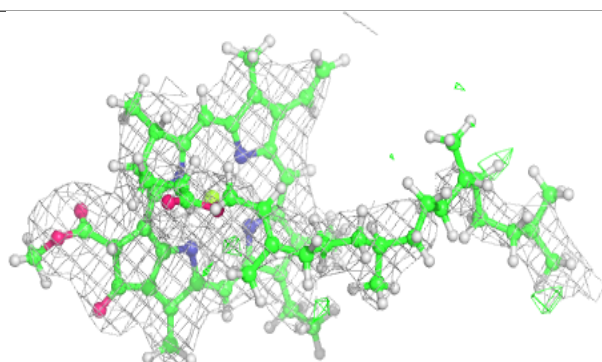
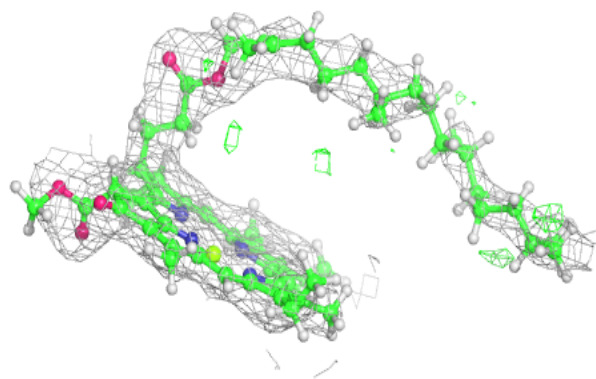
**Electron density around BCR d 404:**

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

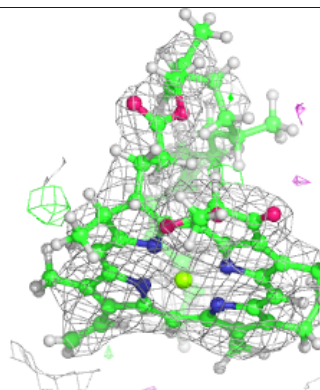
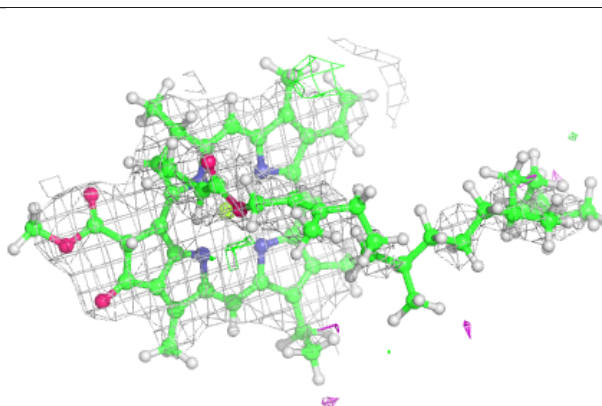
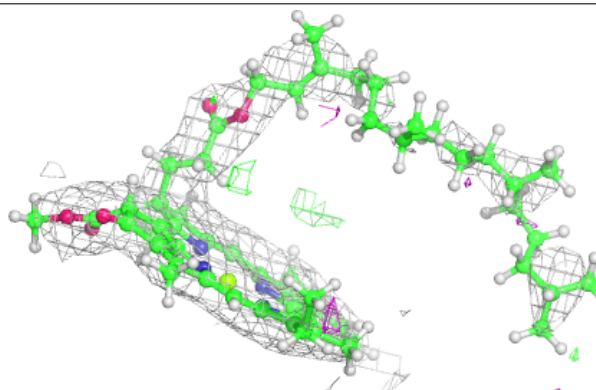


**Electron density around CLA C 513:**

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

**Electron density around CLA c 513:**

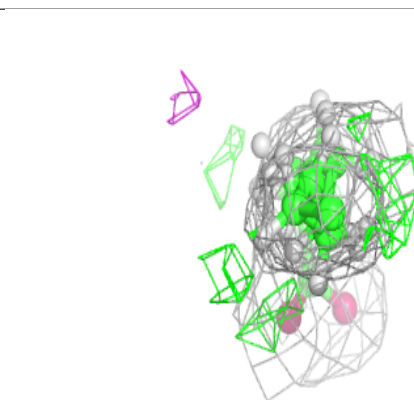
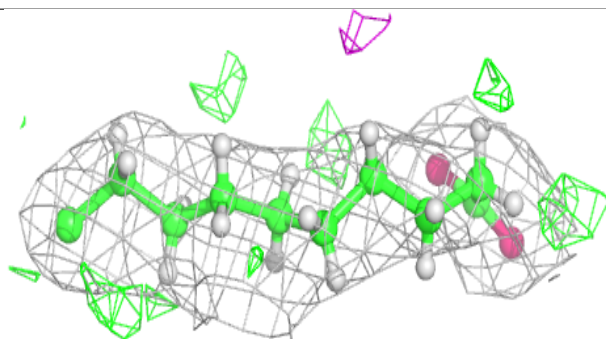
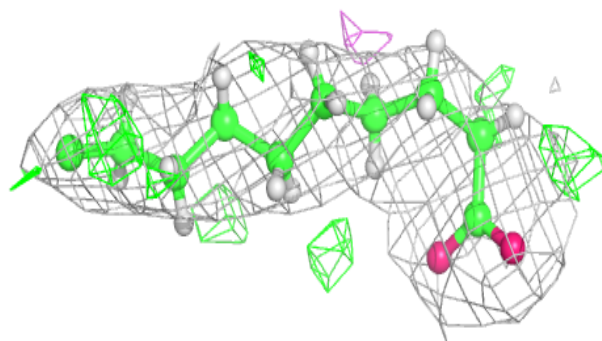
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



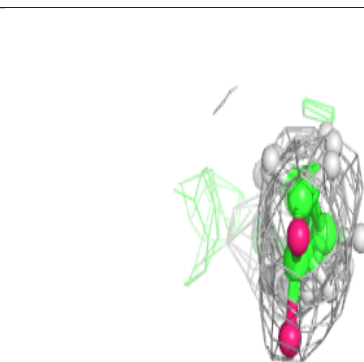
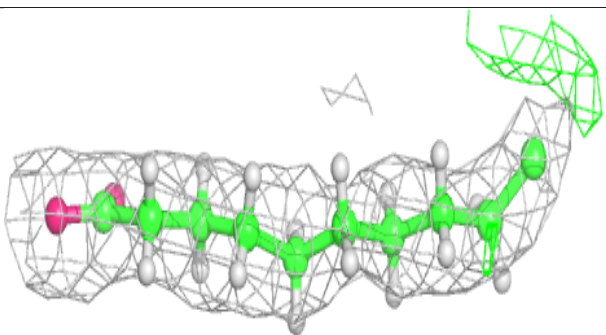
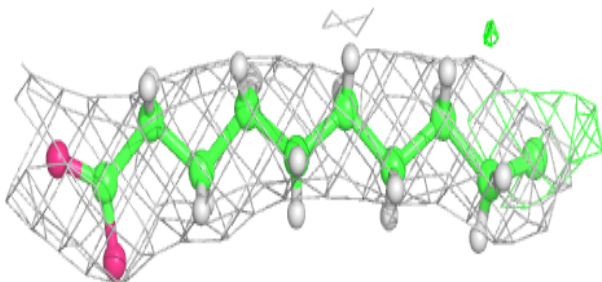


**Electron density around STE B 624:**

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

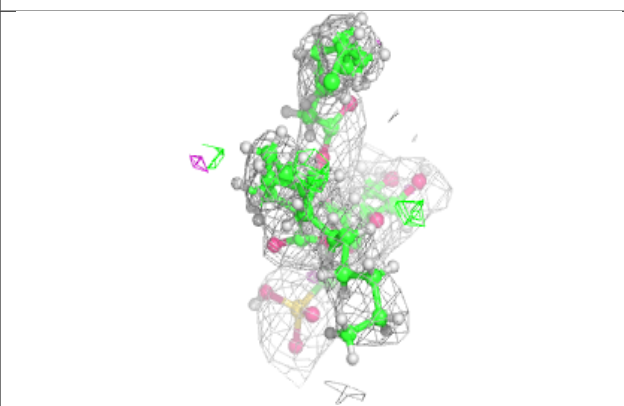
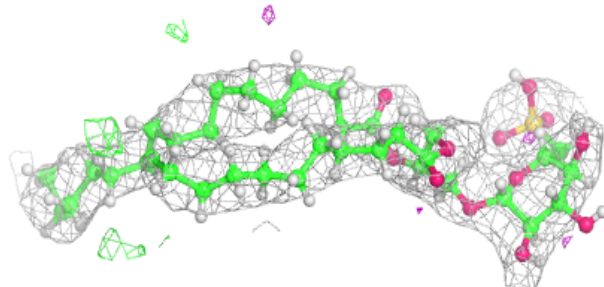
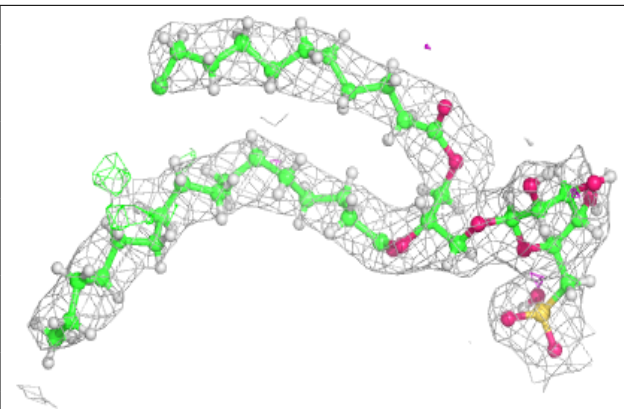
**Electron density around STE j 101:**

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

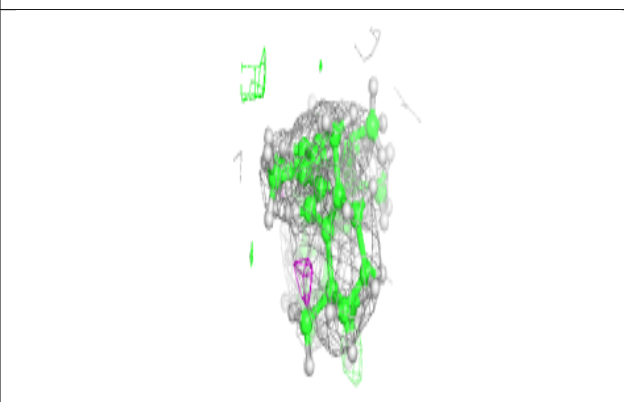
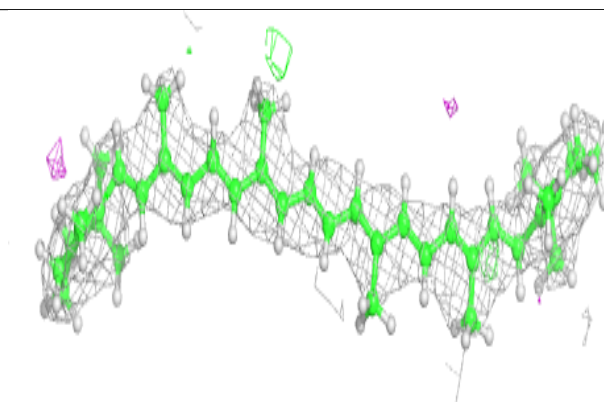
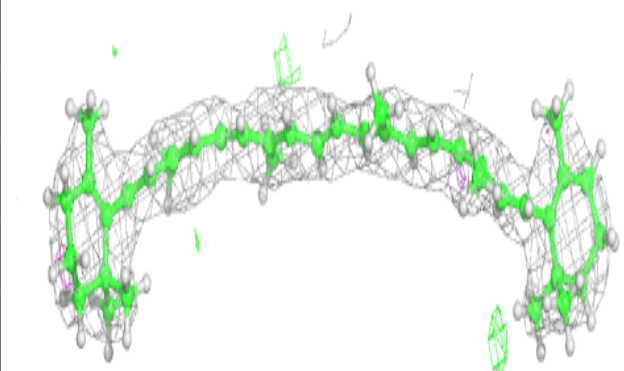


**Electron density around SQD L 101:**

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

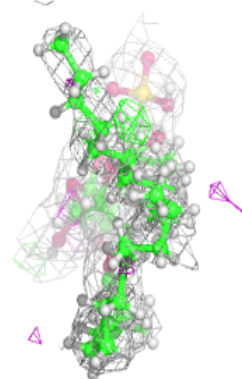
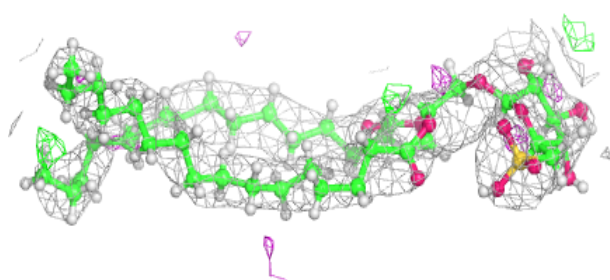
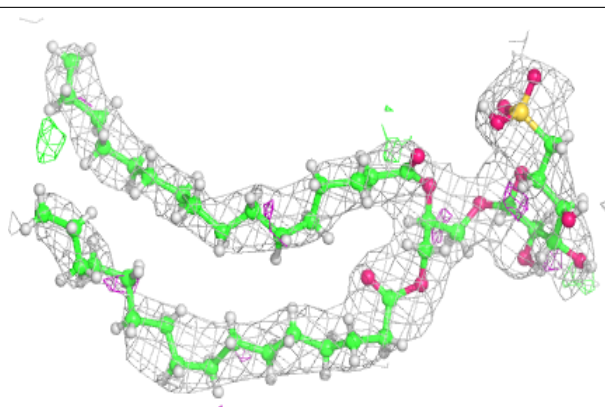
**Electron density around BCR k 103:**

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

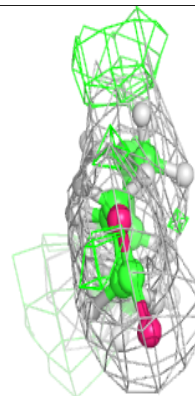
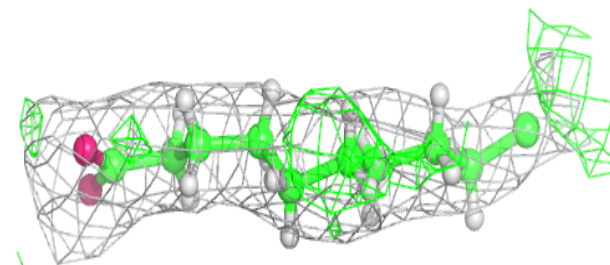
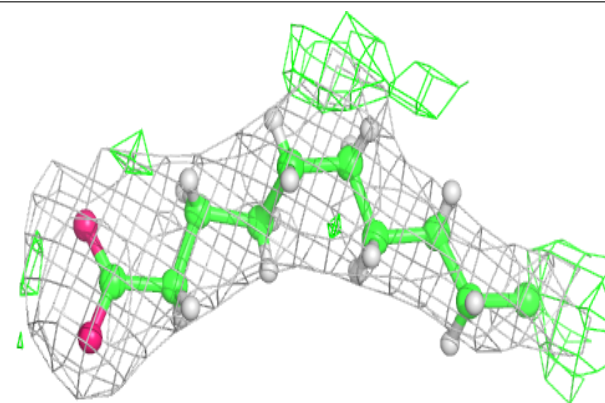


**Electron density around SQD B 622:**

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

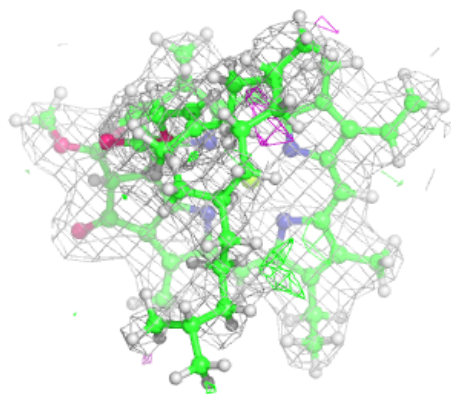
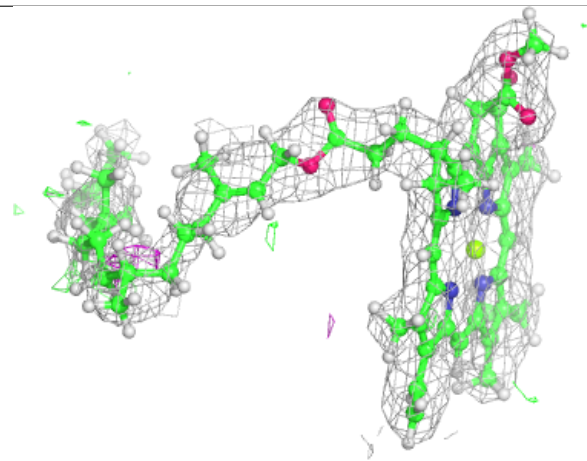
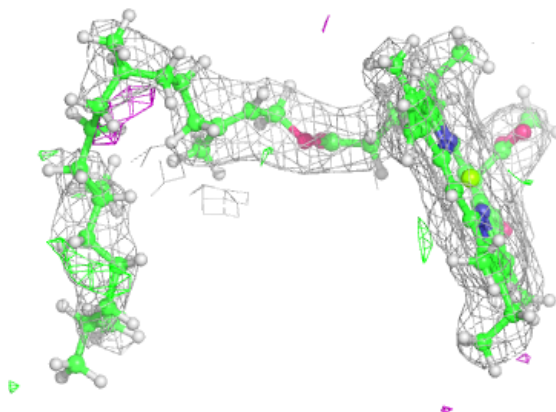
**Electron density around STE C 521:**

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



**Electron density around CLA a 405:**

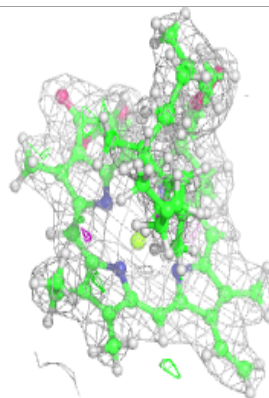
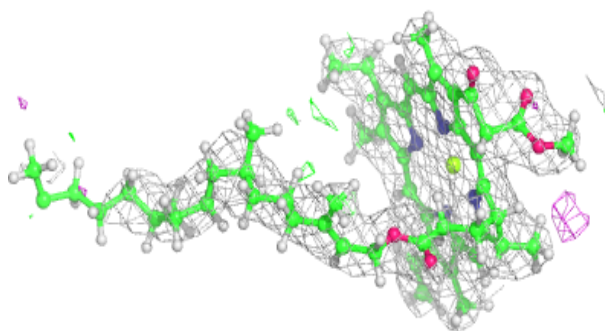
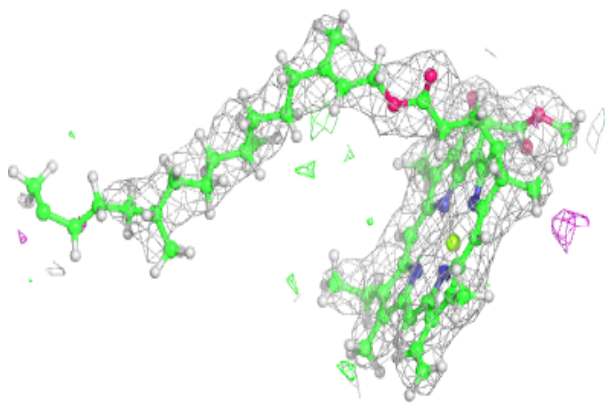
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



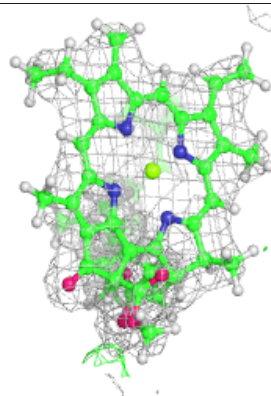
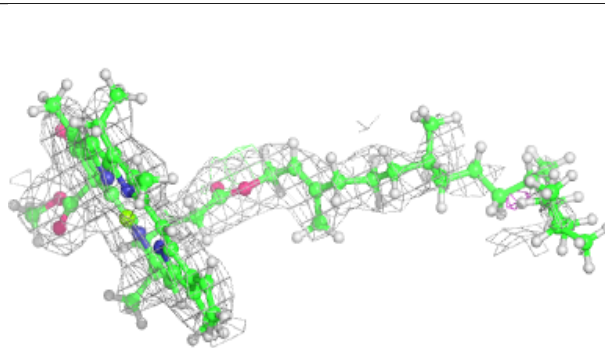
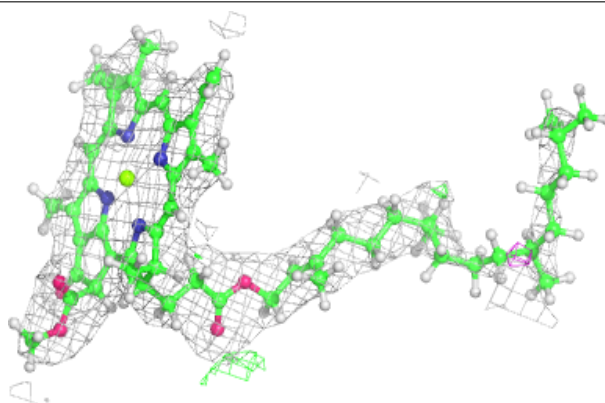


**Electron density around CLA c 508:**

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

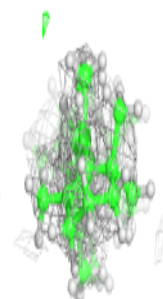
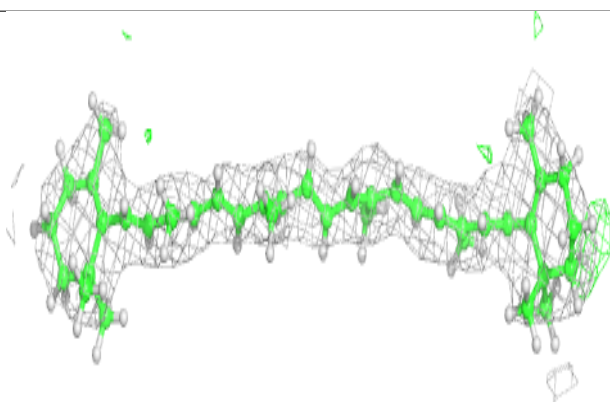
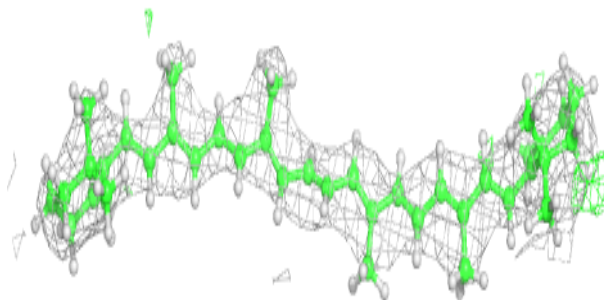
**Electron density around CLA d 403:**

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

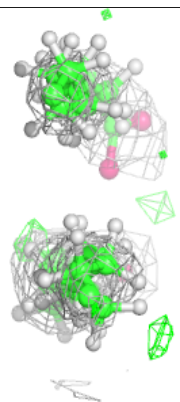
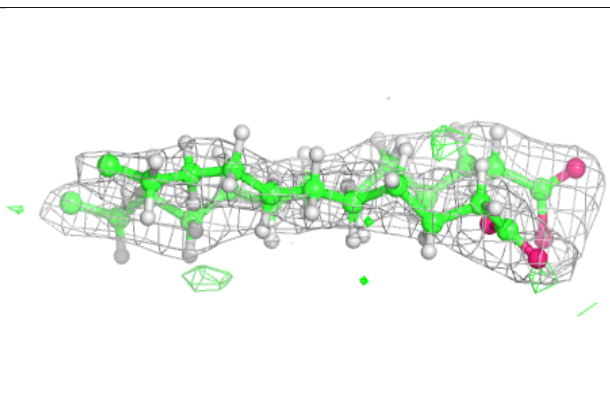
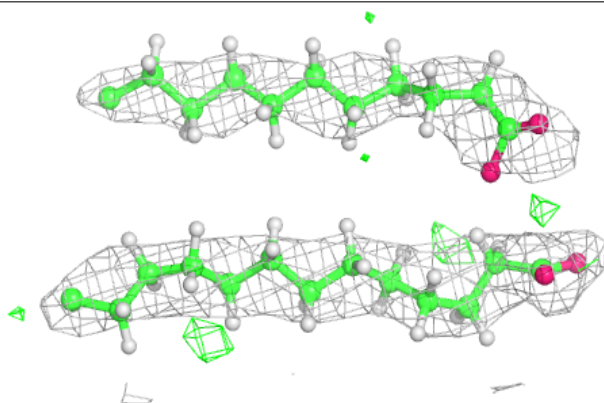


**Electron density around BCR k 101:**

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

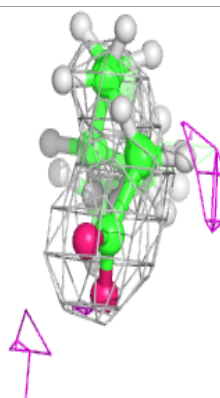
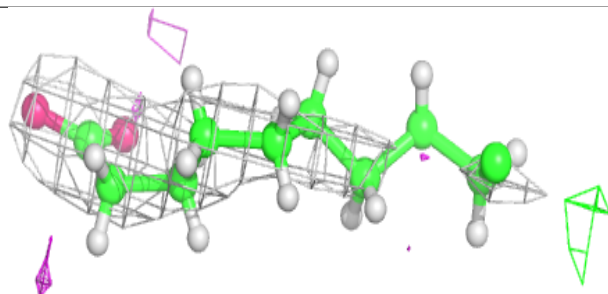
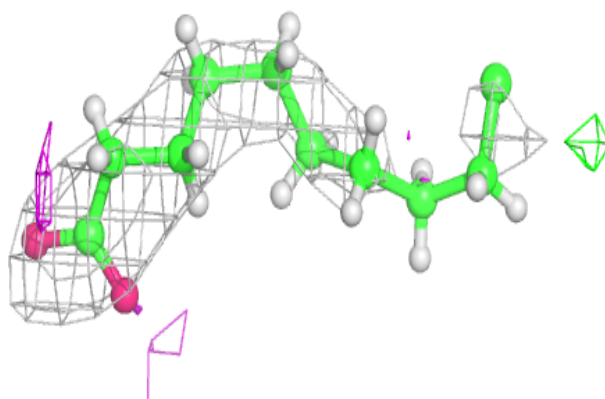
**Electron density around LMG D 411:**

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

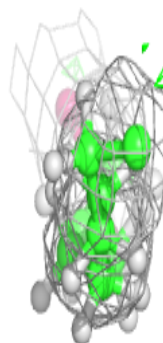
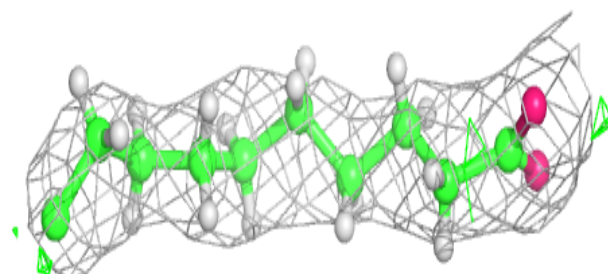
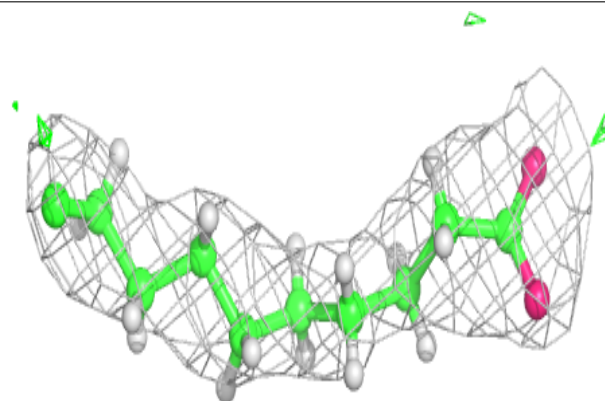


**Electron density around STE B 627:**

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

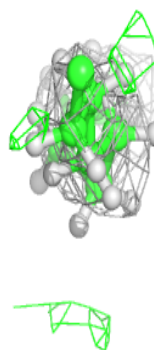
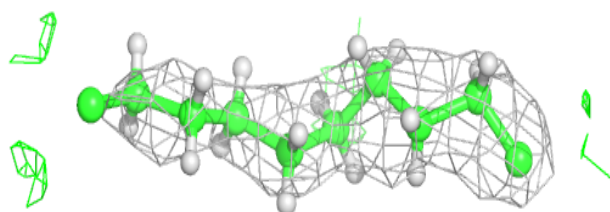
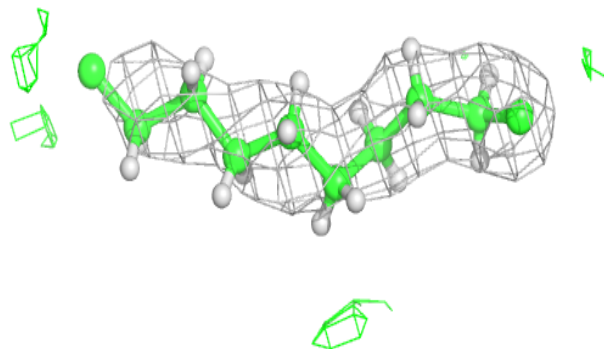
**Electron density around STE C 519:**

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

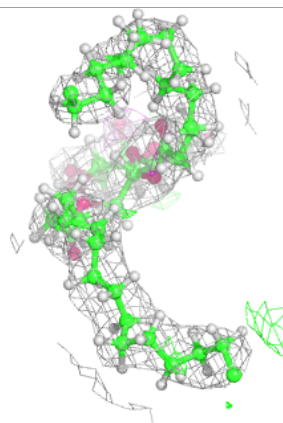
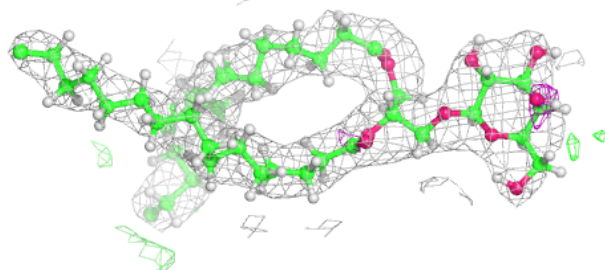
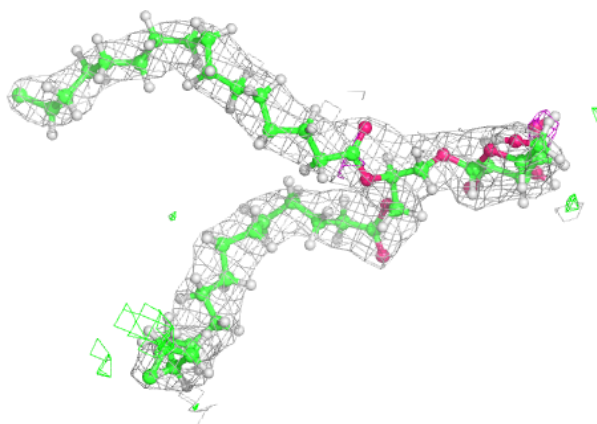


**Electron density around STE t 103:**

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

**Electron density around LMG M 101:**

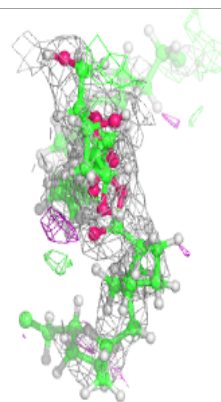
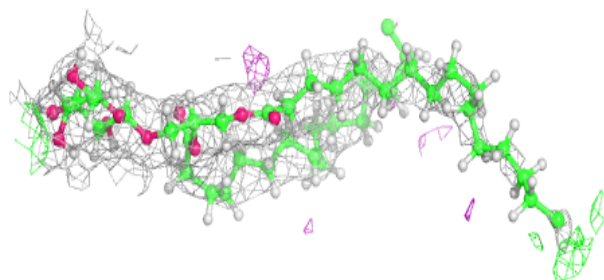
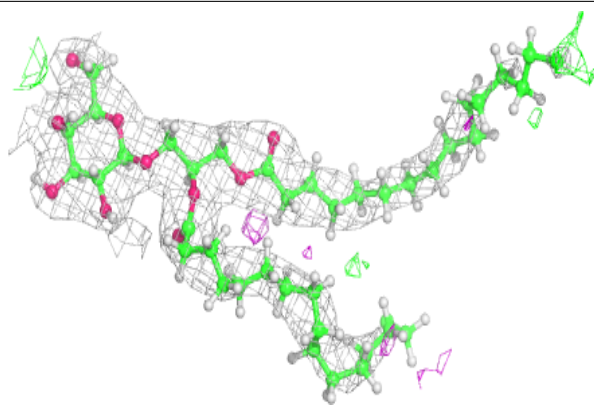
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



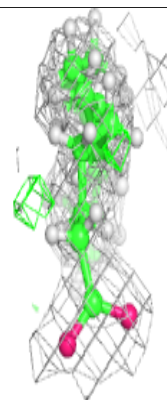
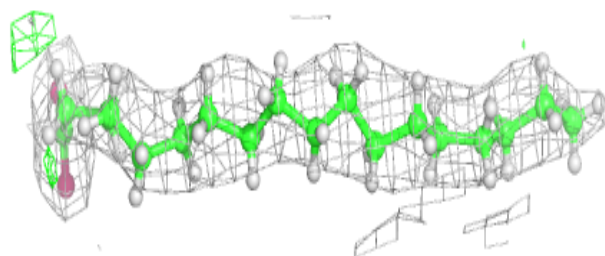
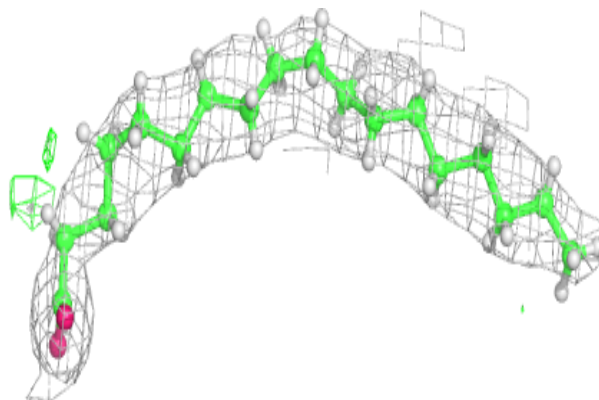


**Electron density around LMG D 408:**

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

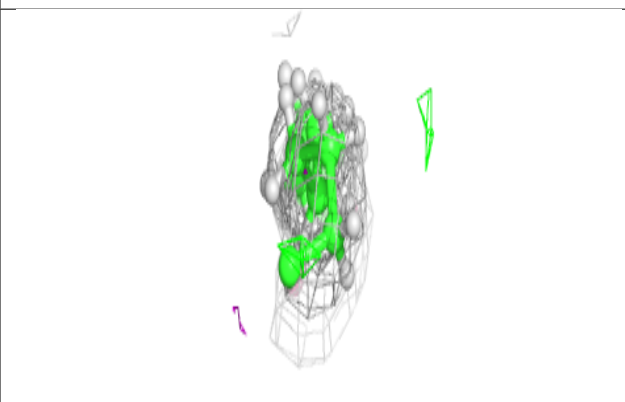
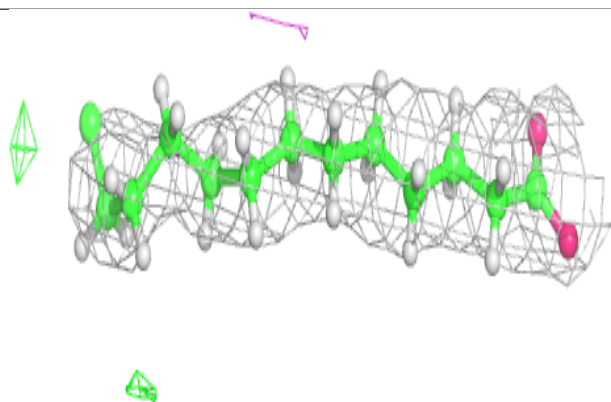
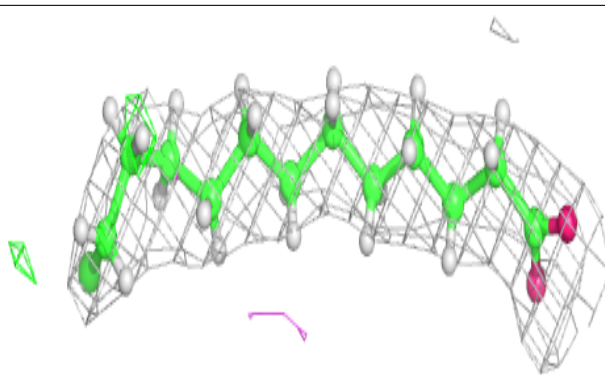
**Electron density around STE D 412:**

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

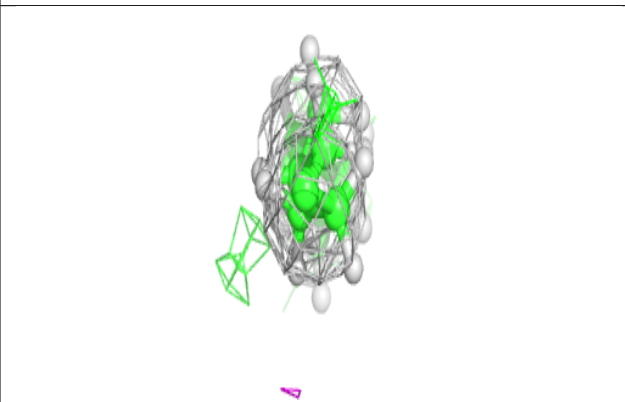
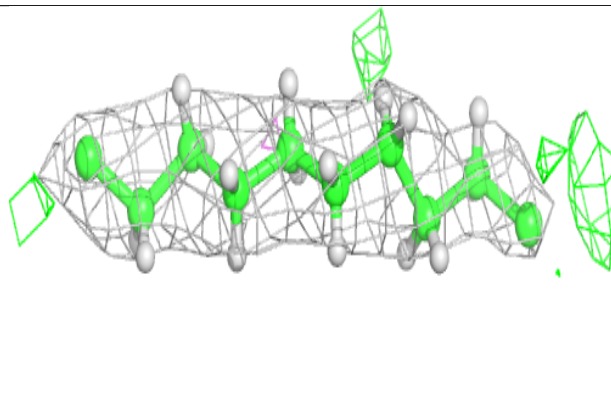
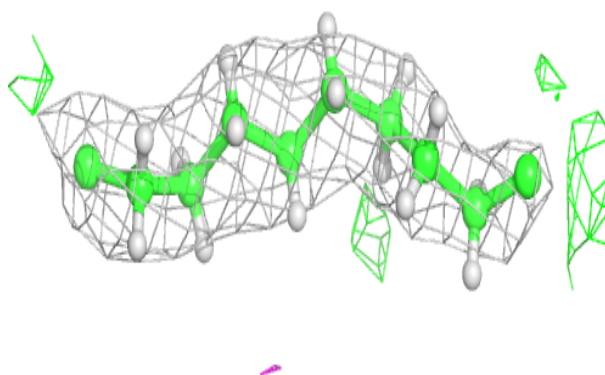


**Electron density around STE M 102:**

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

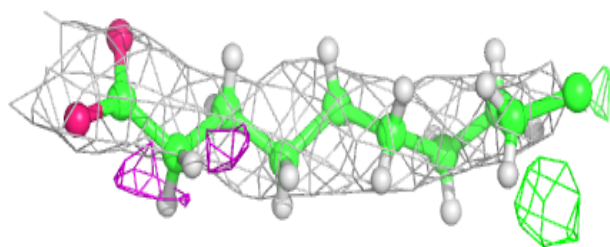
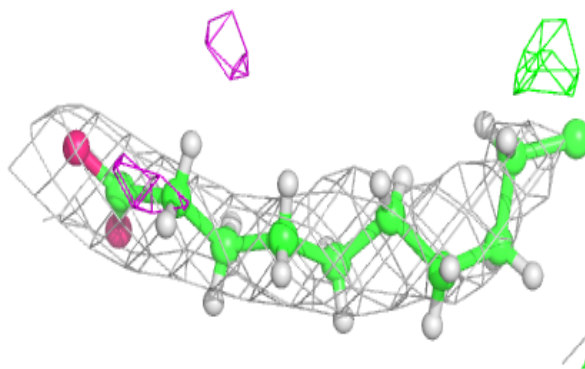
**Electron density around STE M 103:**

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

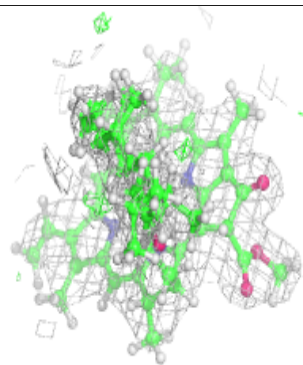
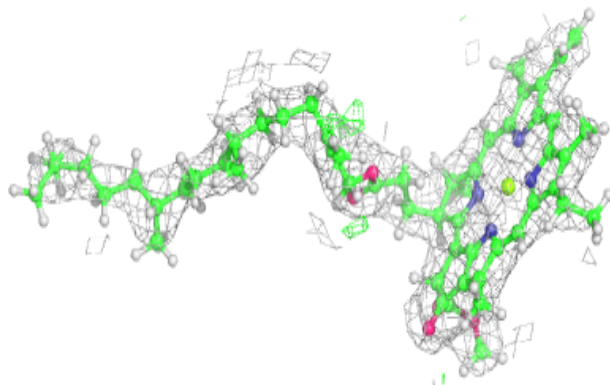
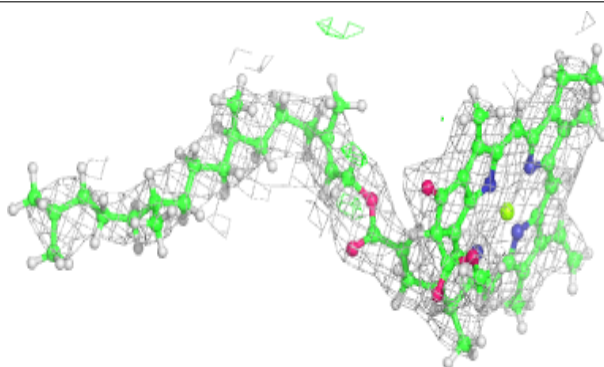


**Electron density around STE m 102:**

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

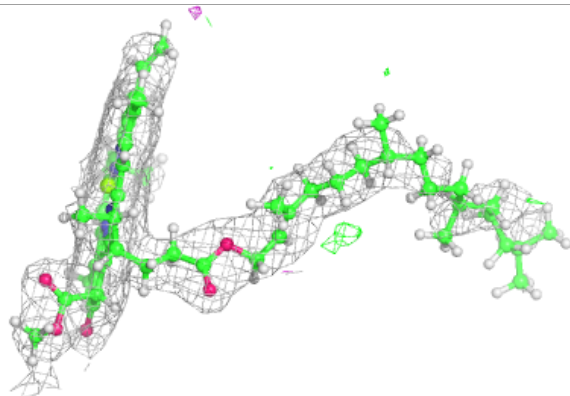
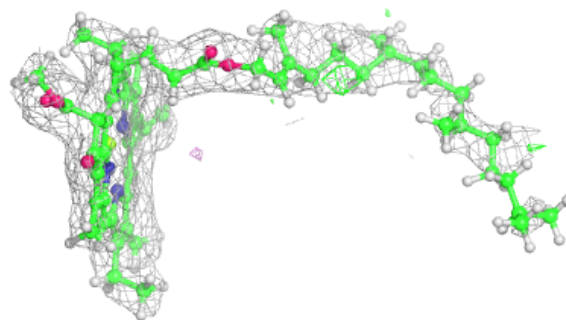
**Electron density around CLA c 502:**

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

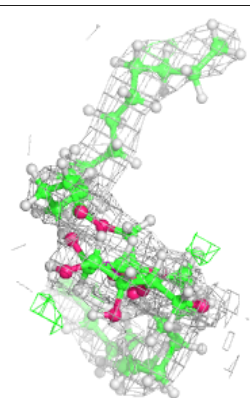
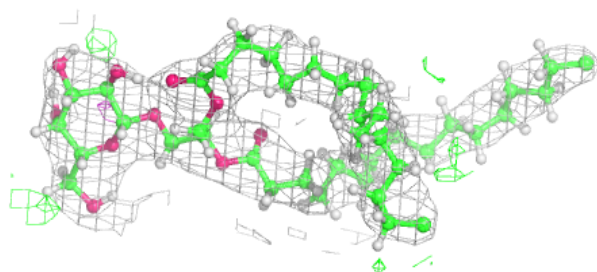
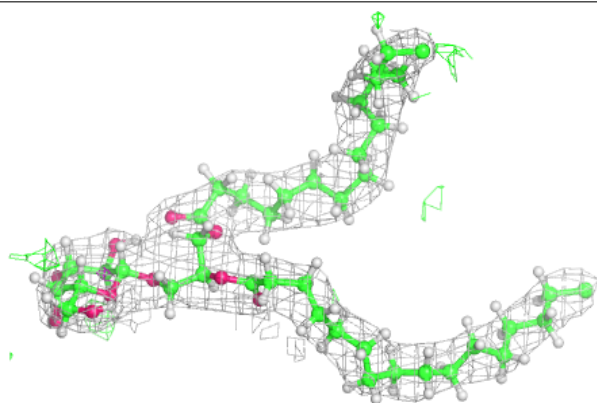


**Electron density around CLA D 405:**

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

**Electron density around LMG m 101:**

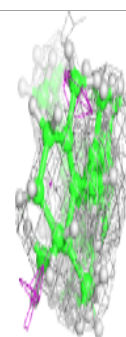
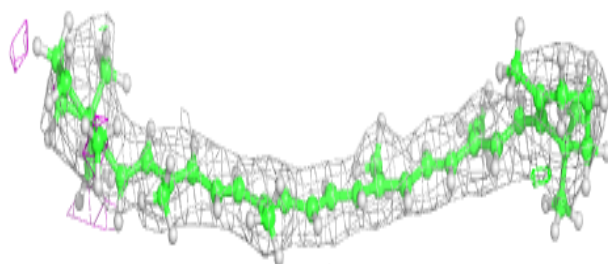
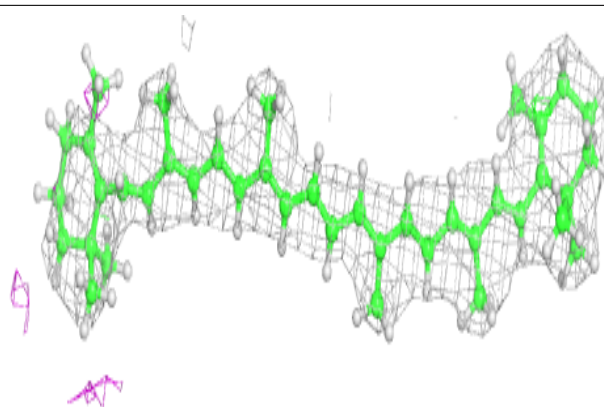
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



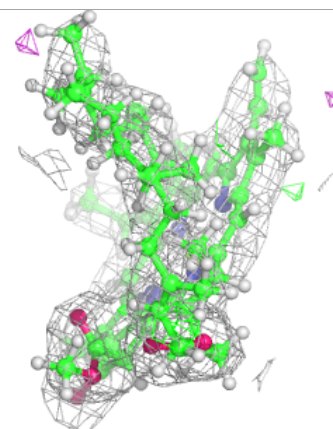
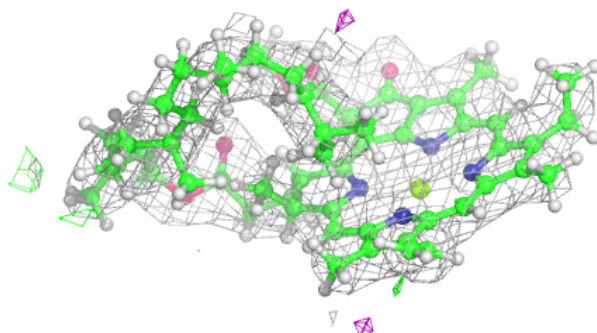
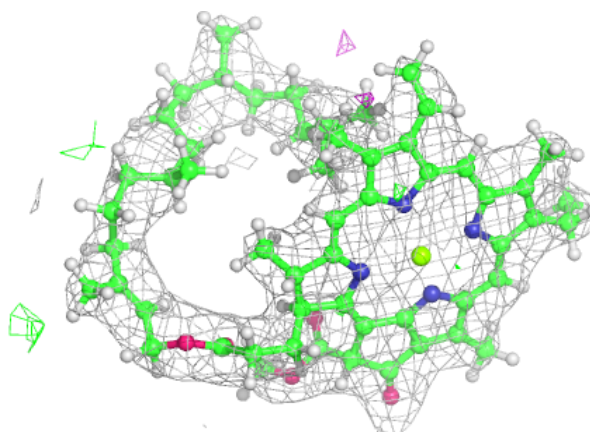


**Electron density around BCR D 406:**

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

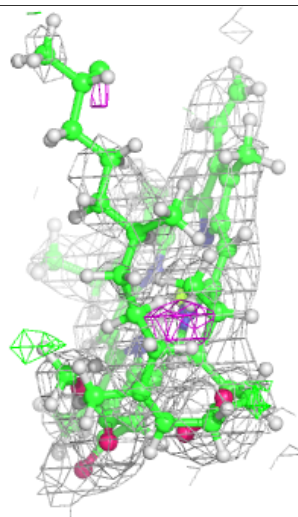
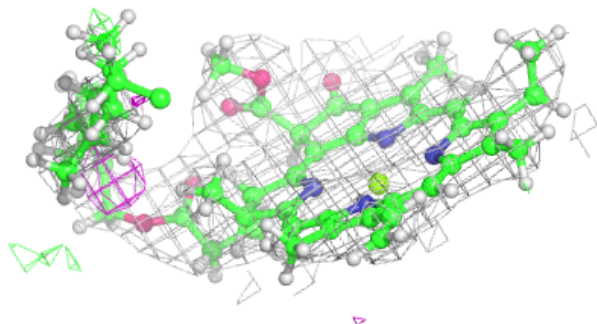
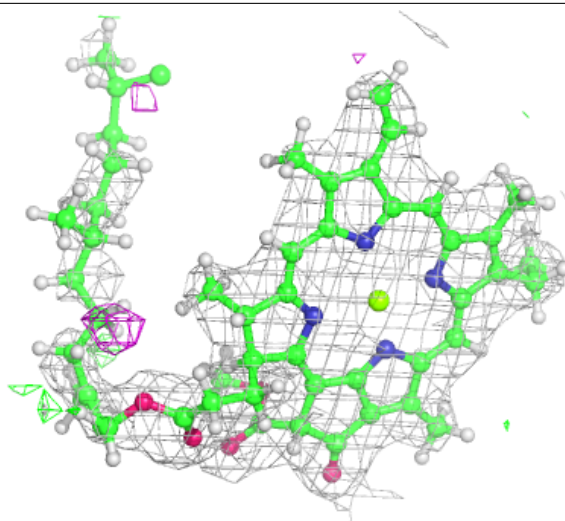
**Electron density around CLA B 615:**

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



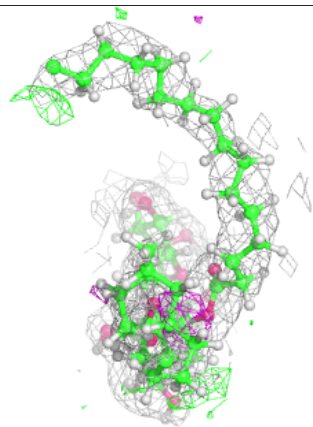
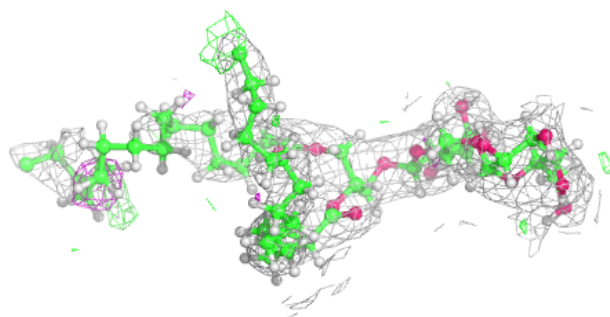
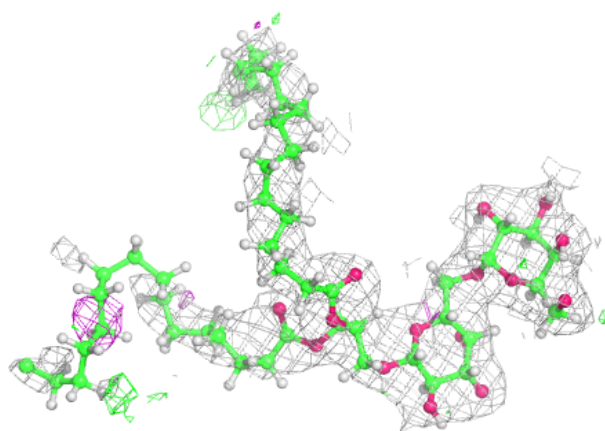
**Electron density around CLA B 616:**

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



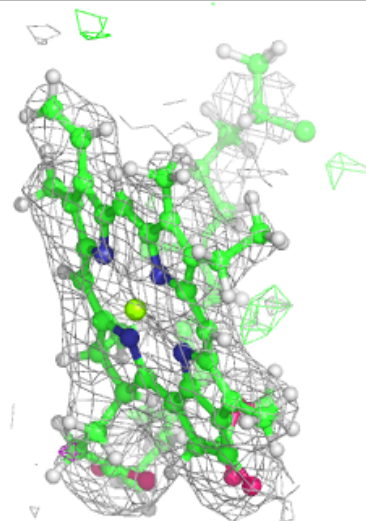
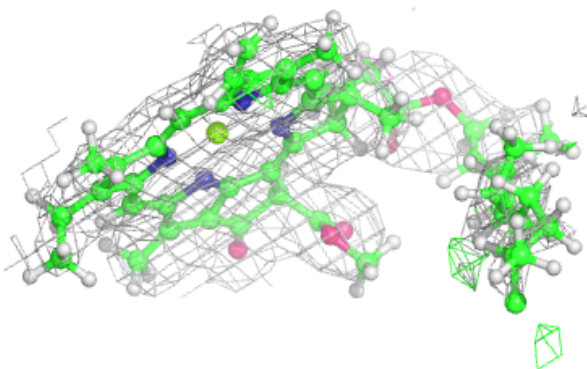
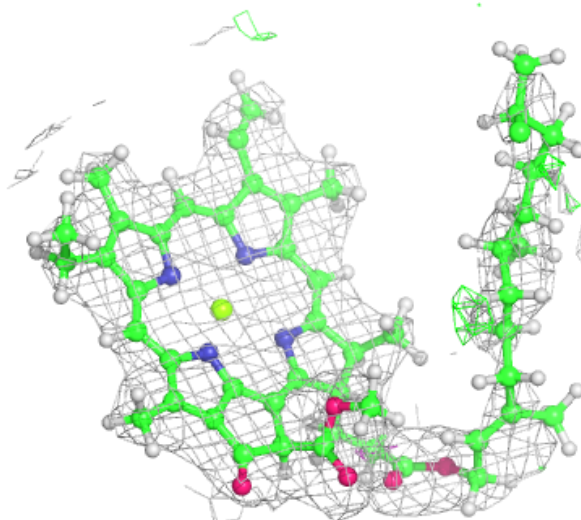
**Electron density around DGD C 516:**

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



**Electron density around CLA b 616:**

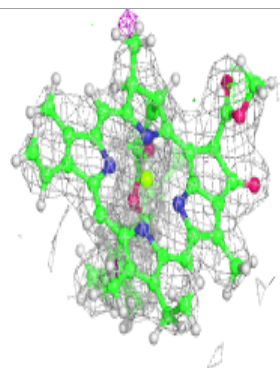
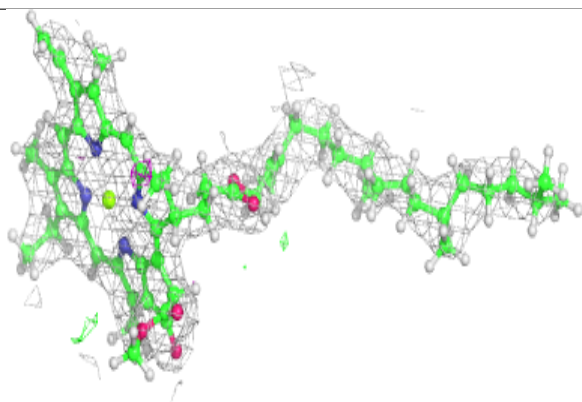
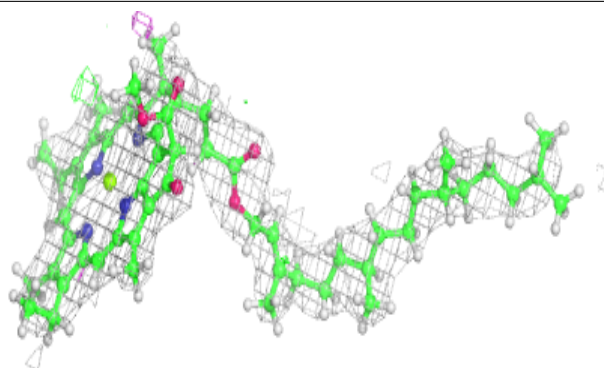
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



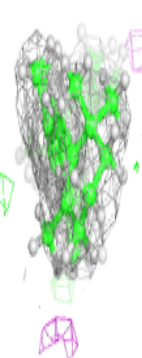
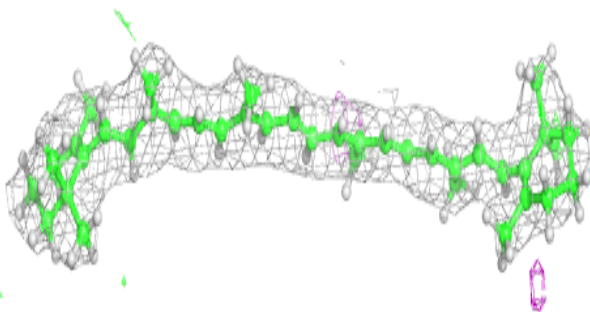
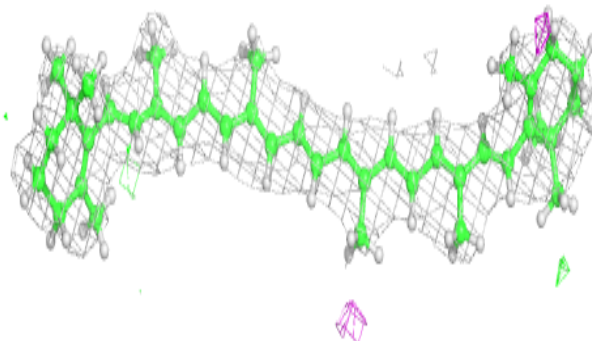


**Electron density around CLA C 502:**

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

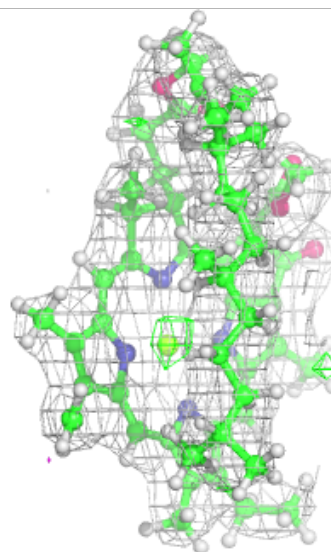
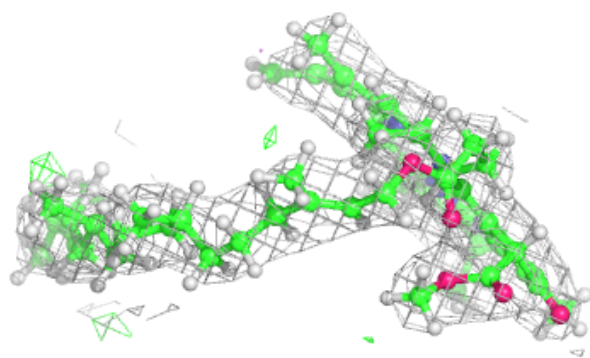
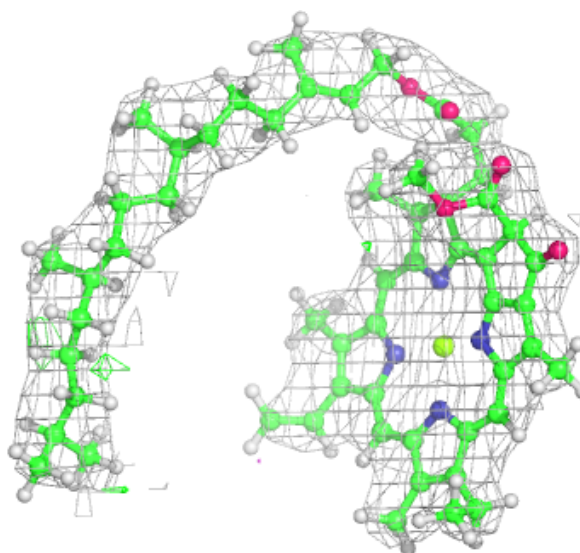
**Electron density around BCR B 619:**

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



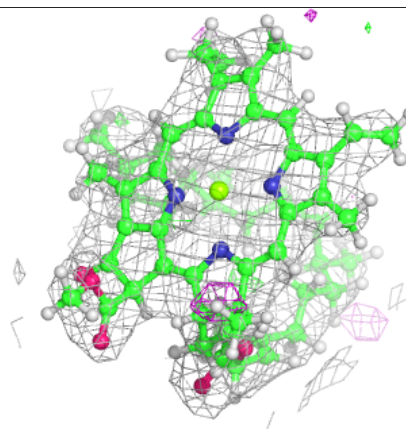
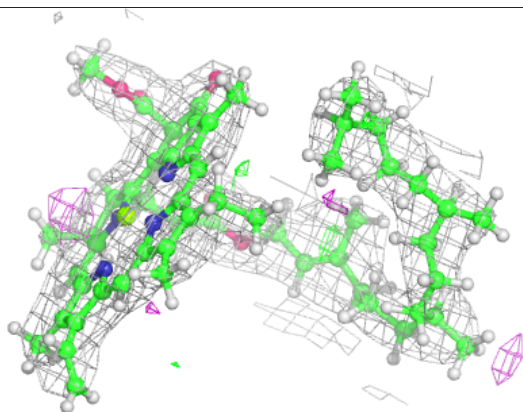
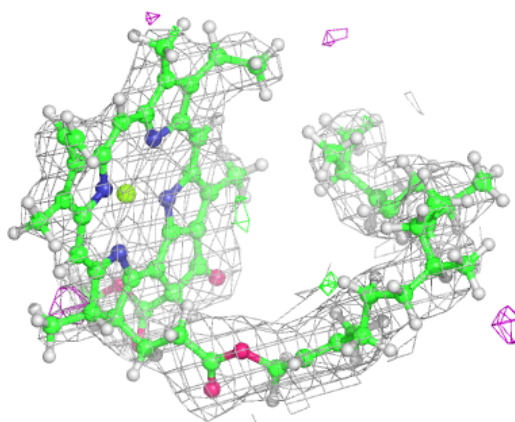
**Electron density around CLA C 507:**

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



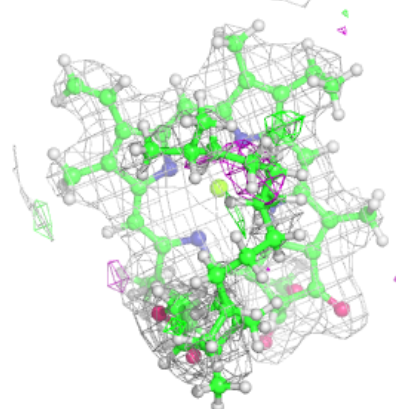
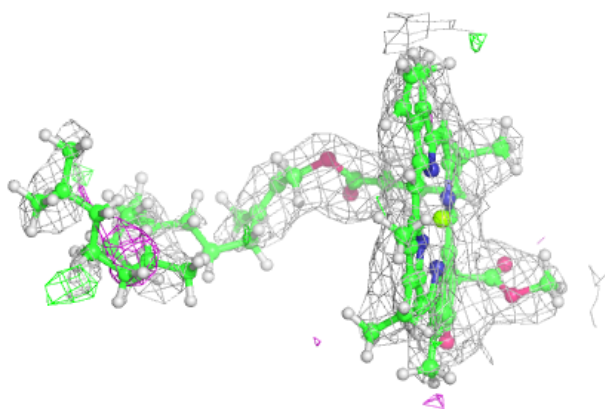
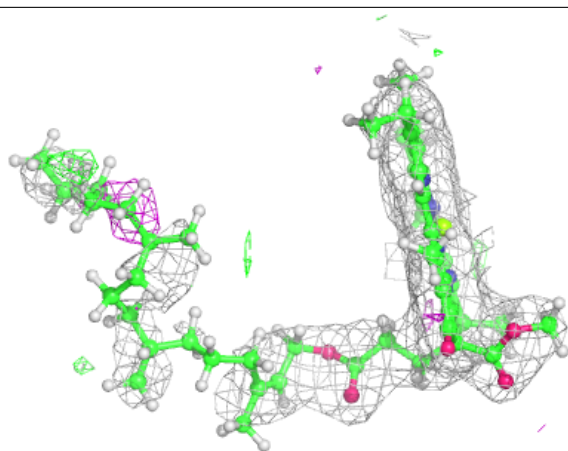
**Electron density around CLA c 503:**

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

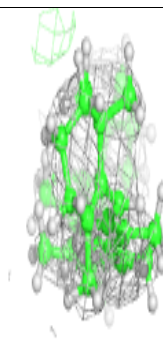
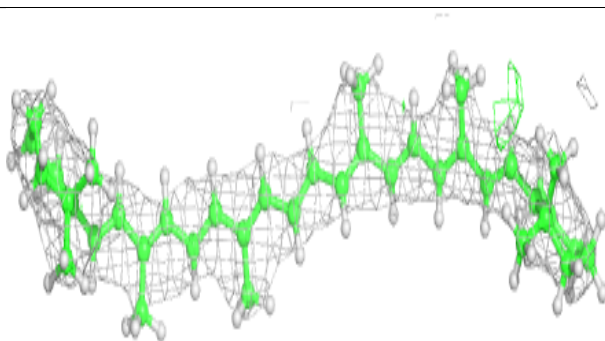
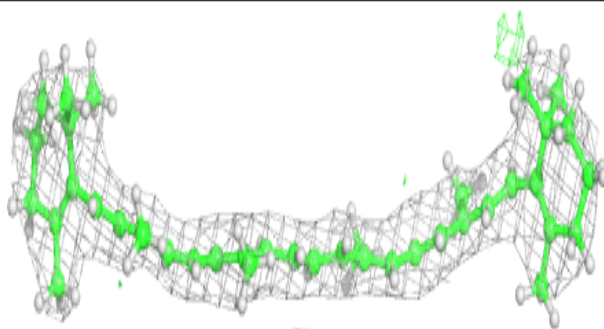


**Electron density around CLA c 506:**

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

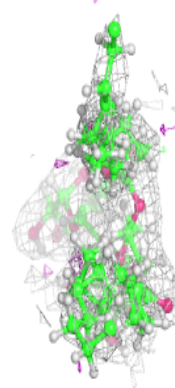
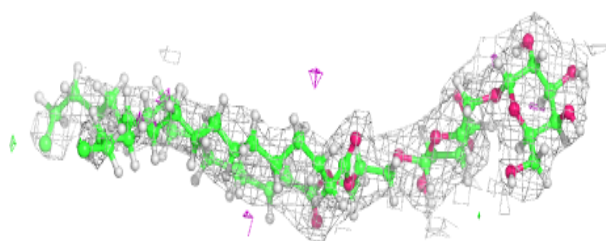
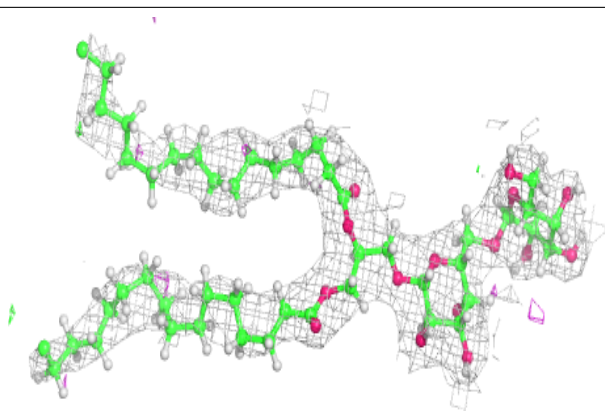
**Electron density around BCR K 102:**

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

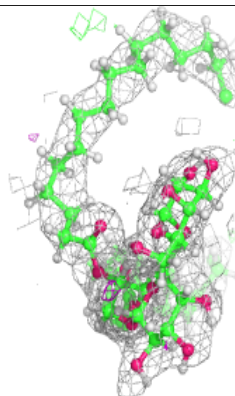
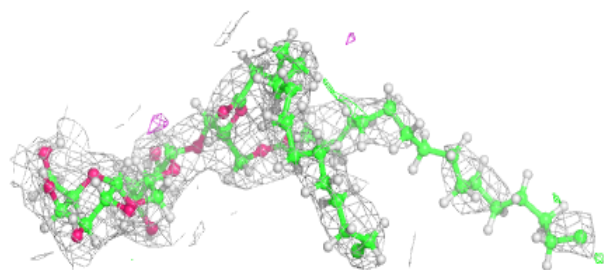
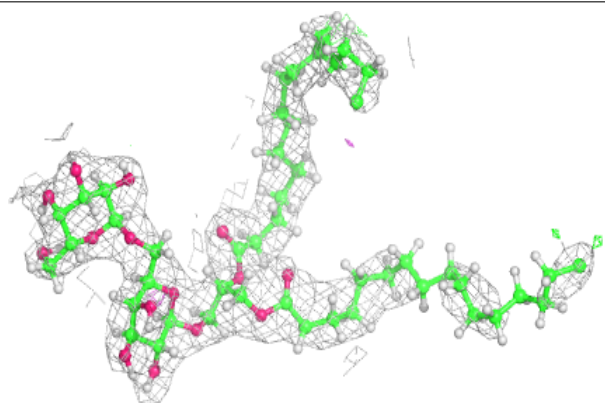


**Electron density around DGD C 517:**

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

**Electron density around DGD c 516:**

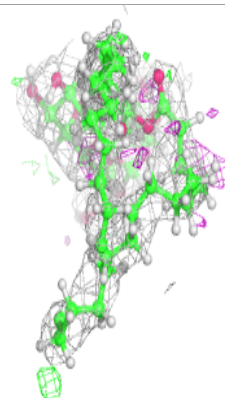
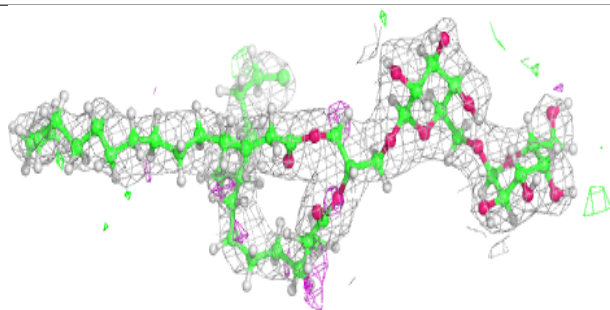
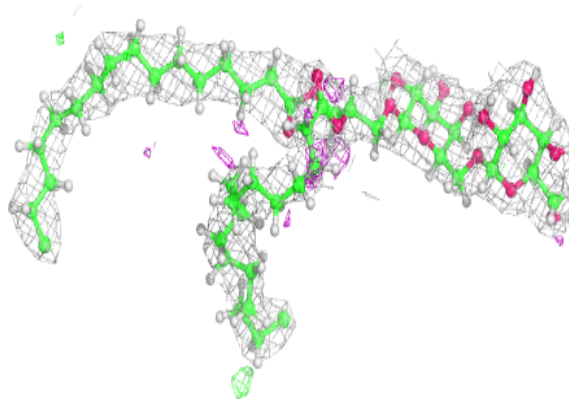
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



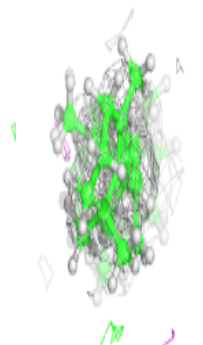
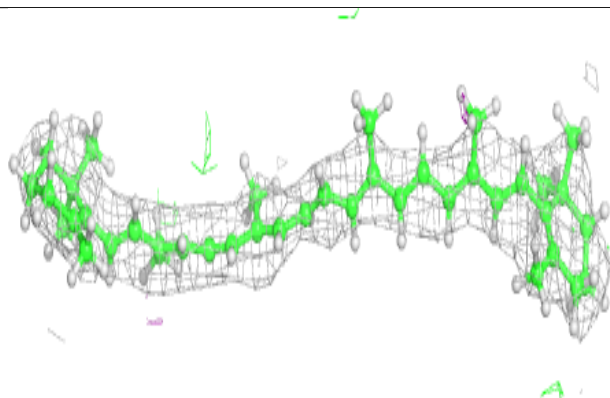
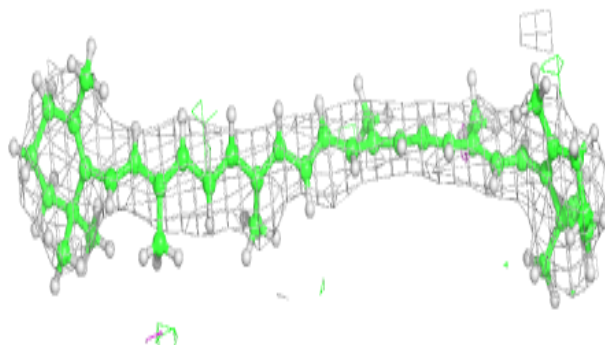


**Electron density around DGD h 101:**

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

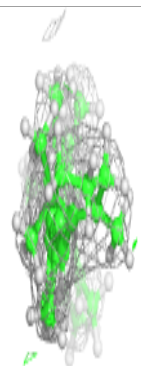
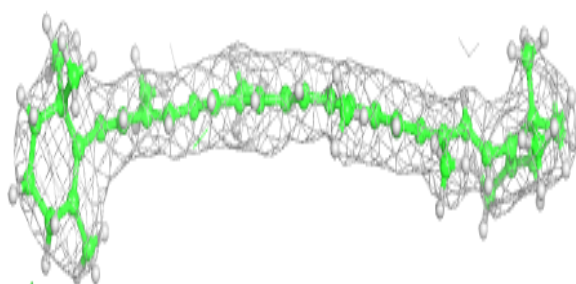
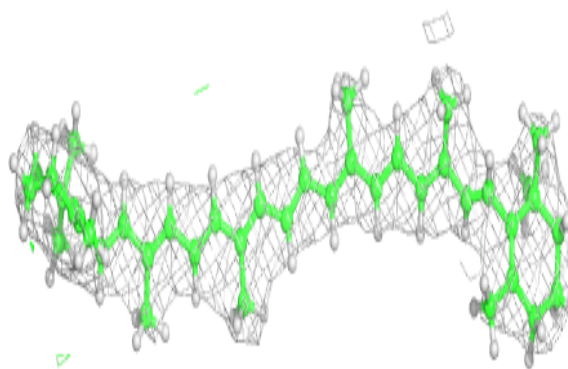
**Electron density around BCR Z 101:**

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

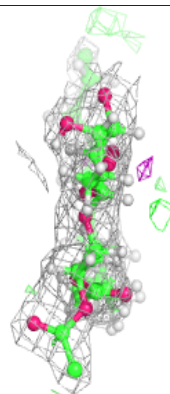
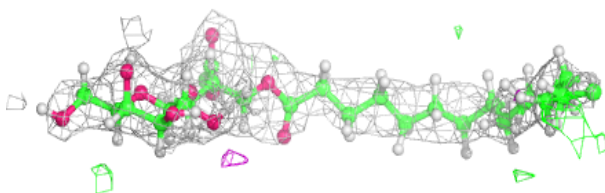
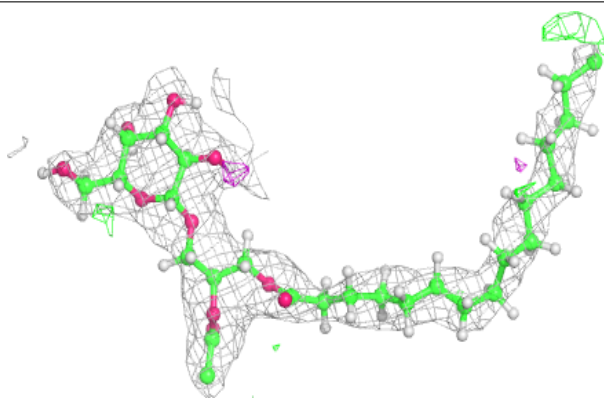


**Electron density around BCR b 617:**

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

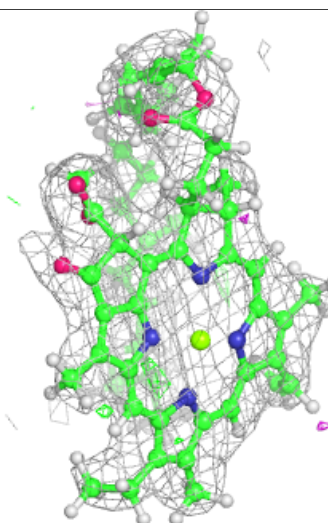
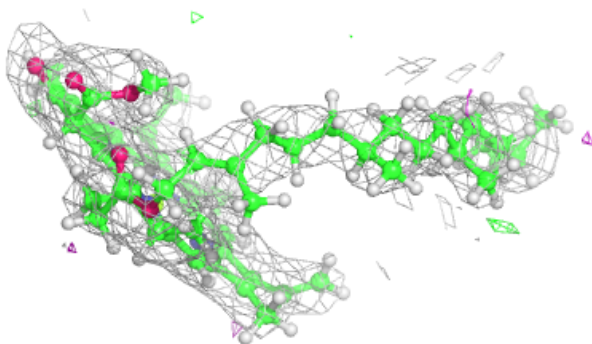
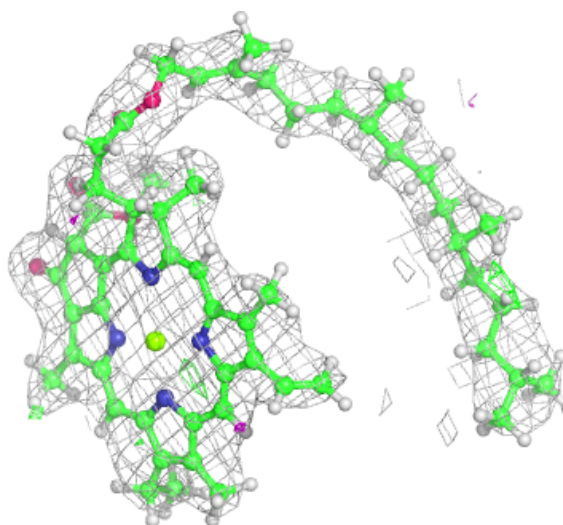
**Electron density around LMG c 518:**

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



**Electron density around CLA c 507:**

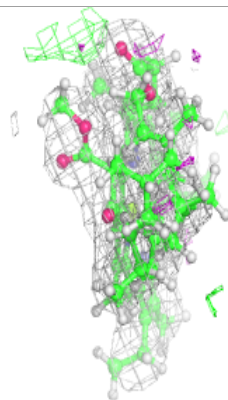
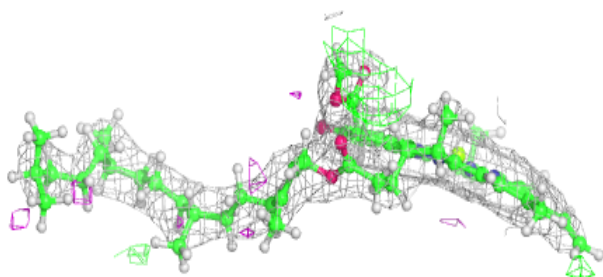
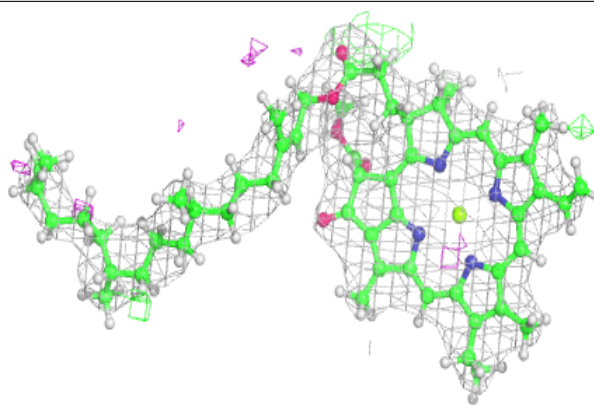
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



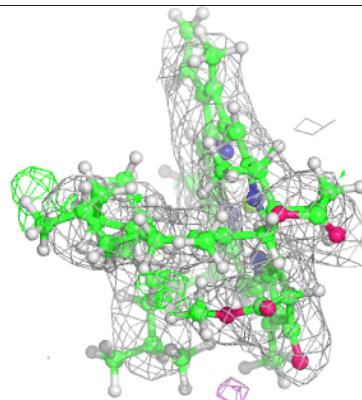
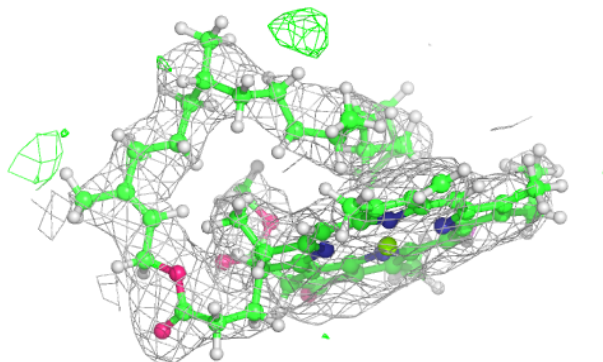
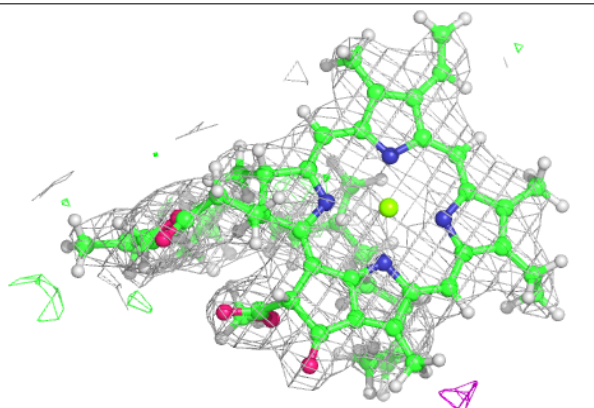


**Electron density around CLA b 602:**

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

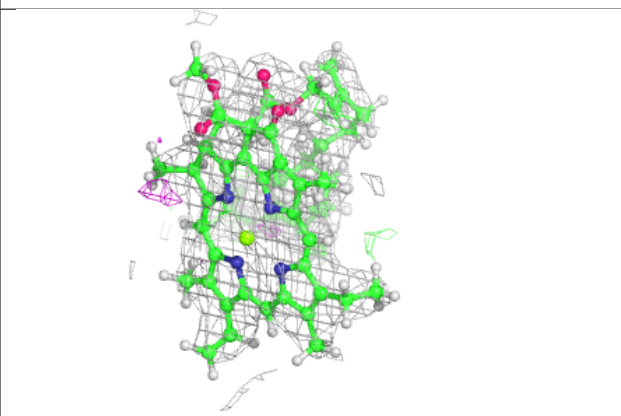
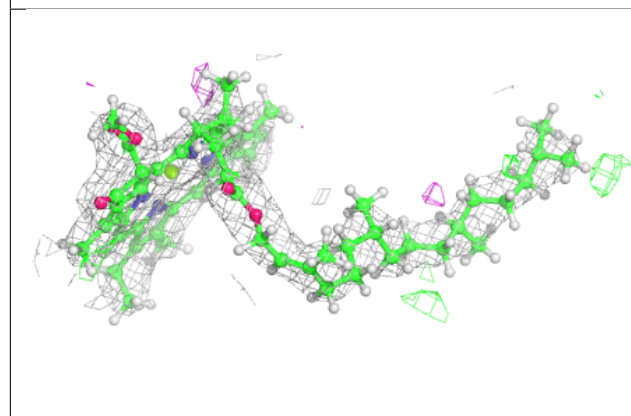
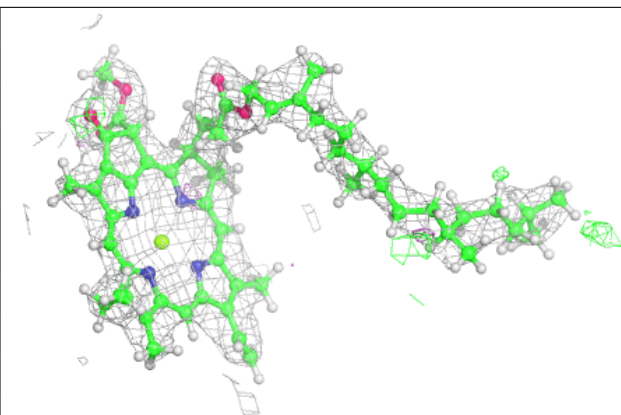
**Electron density around CLA c 510:**

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

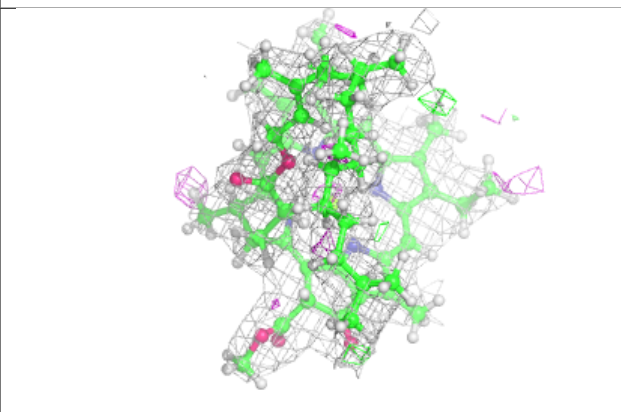
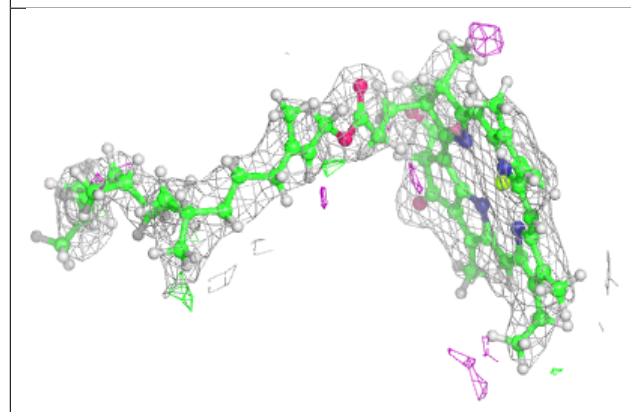
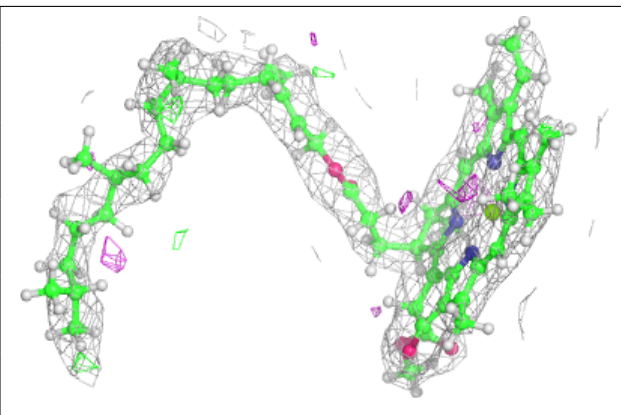


**Electron density around CLA c 511:**

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

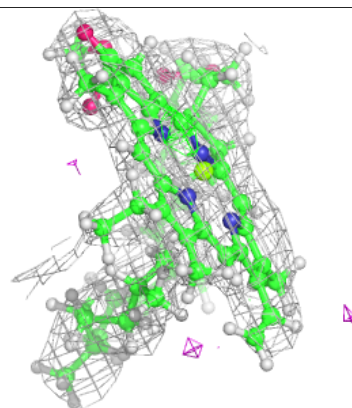
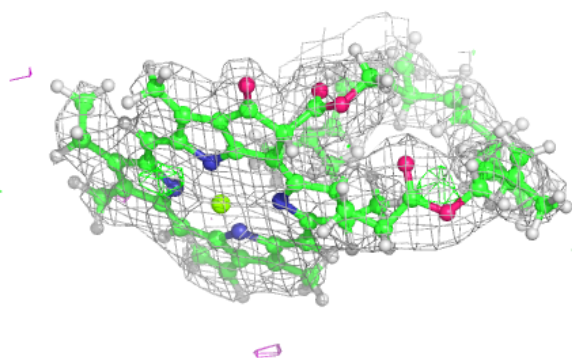
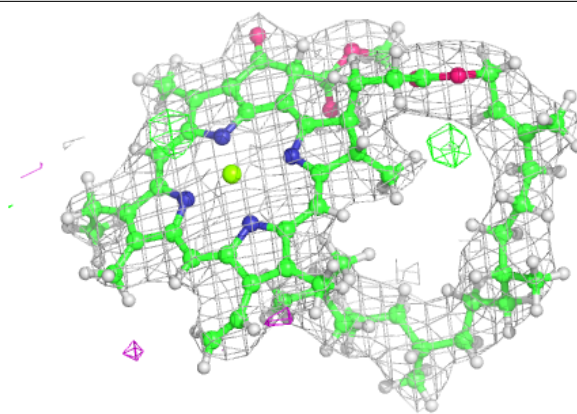
**Electron density around CLA b 606:**

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

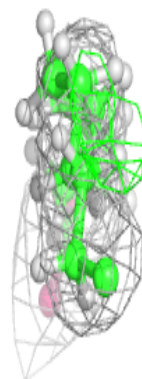
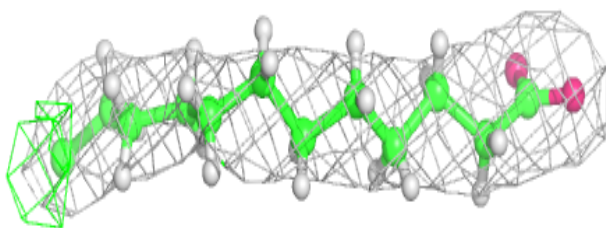
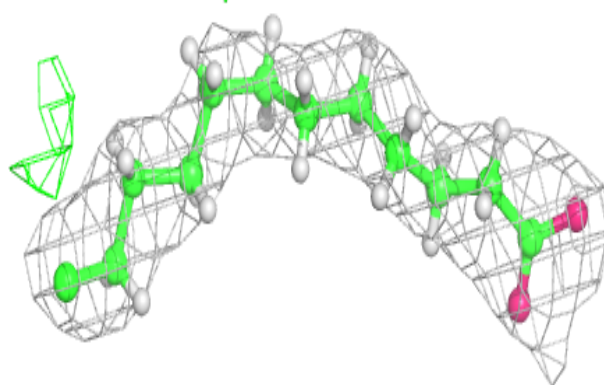


**Electron density around CLA b 615:**

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

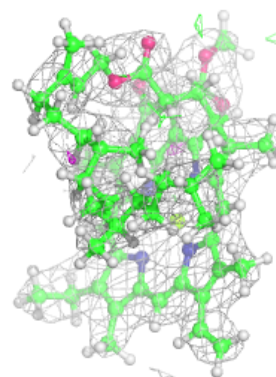
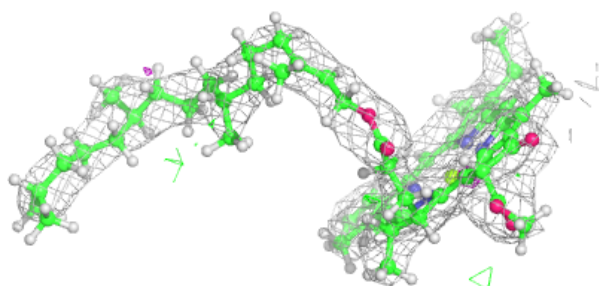
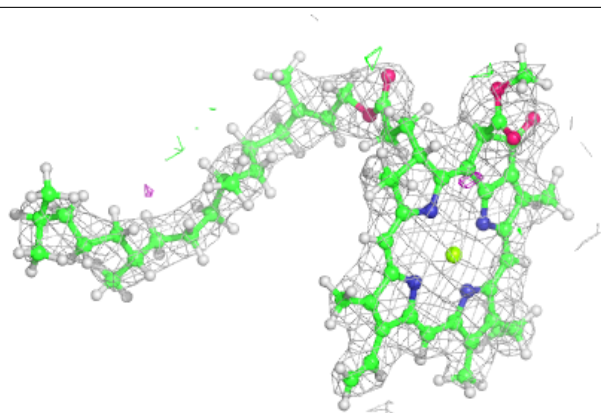
**Electron density around STE t 102:**

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

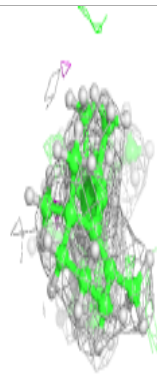
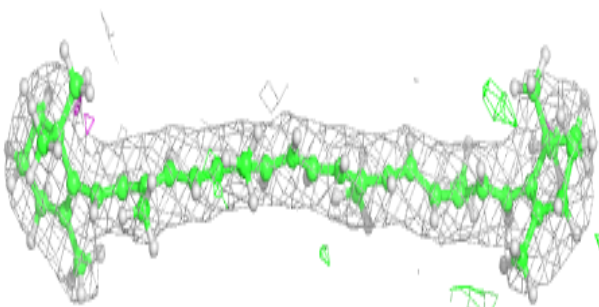
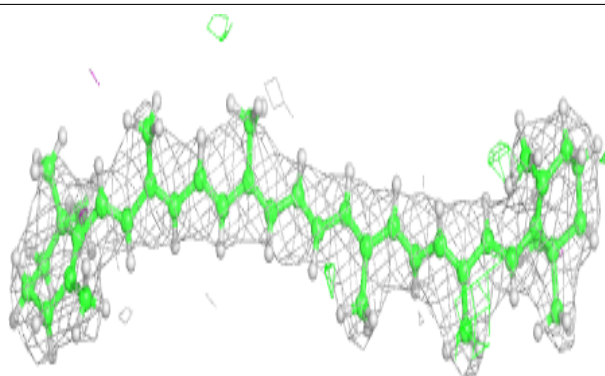


**Electron density around CLA C 511:**

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

**Electron density around BCR B 618:**

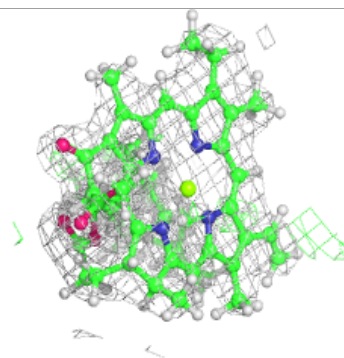
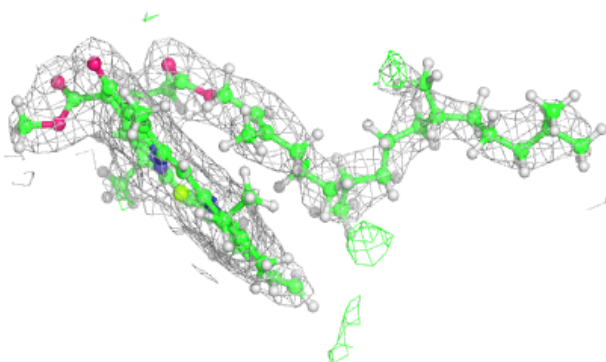
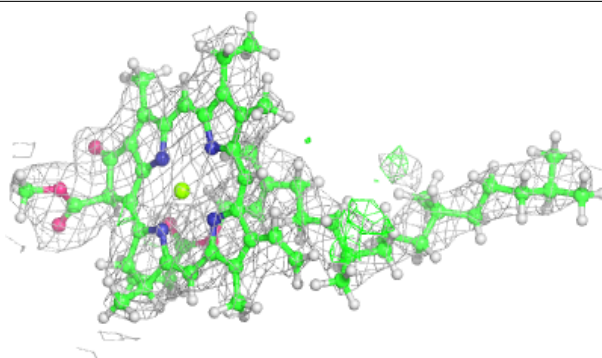
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



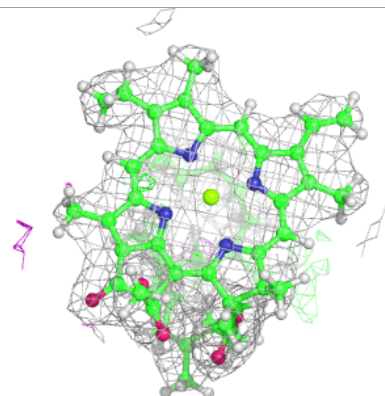
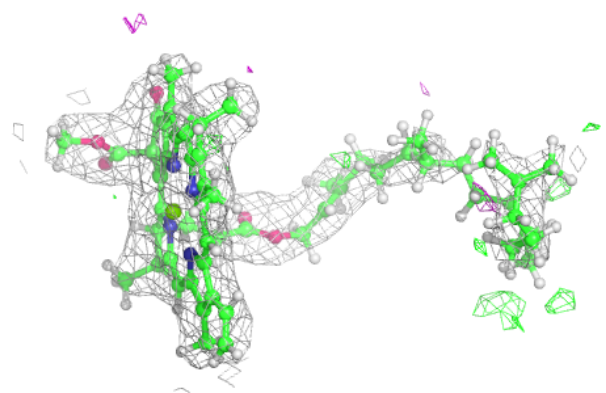
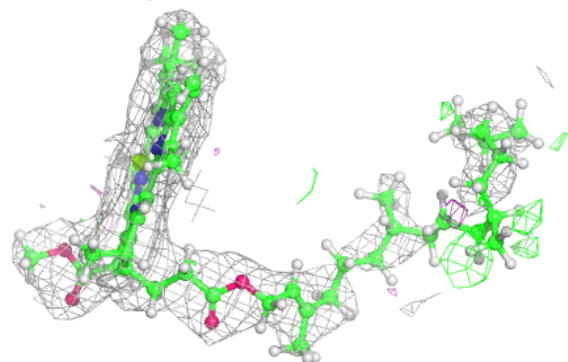


**Electron density around CLA C 505:**

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

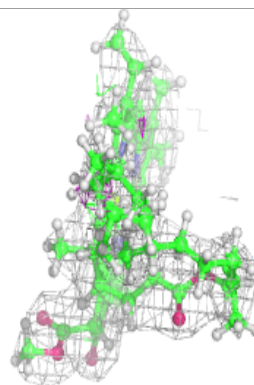
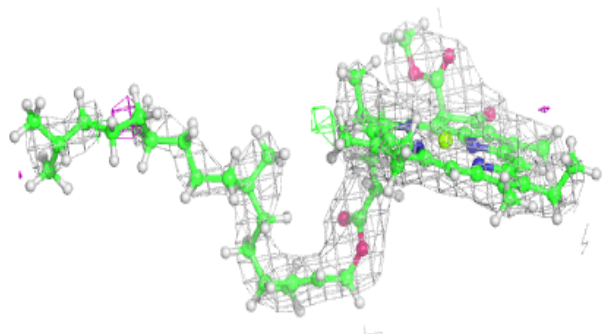
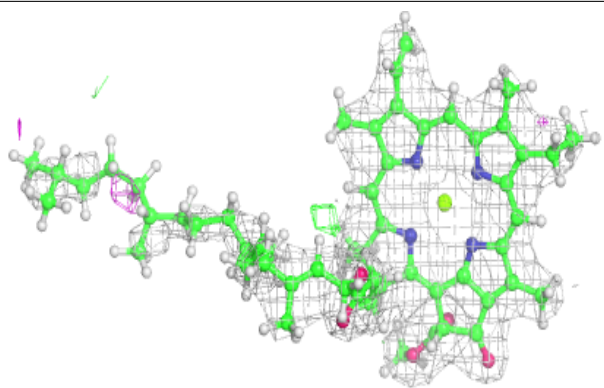
**Electron density around CLA C 506:**

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

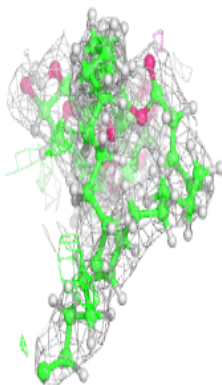
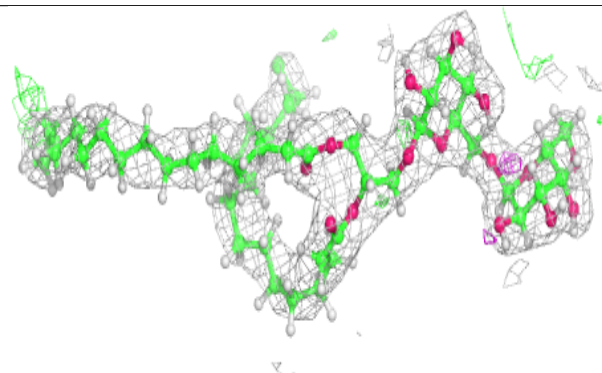
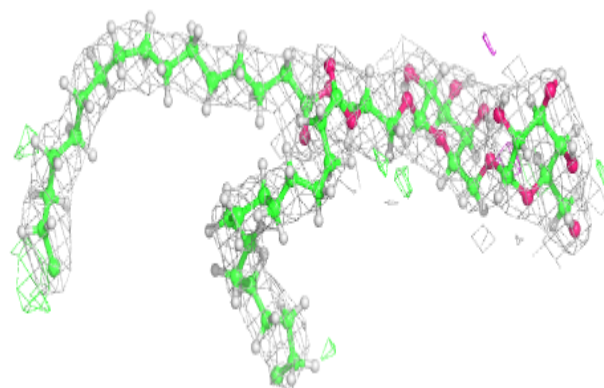


**Electron density around CLA a 403:**

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

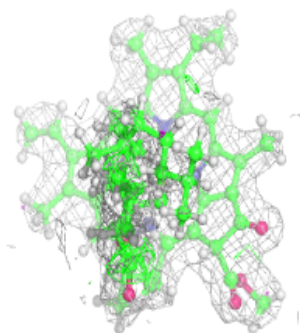
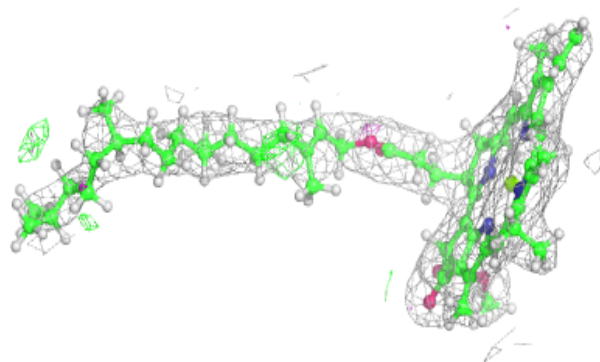
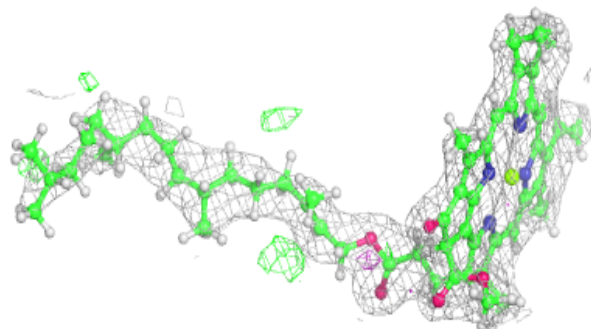
**Electron density around DGD H 102:**

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

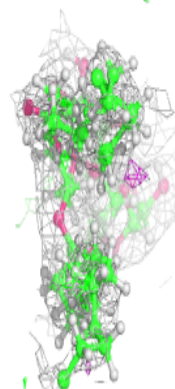
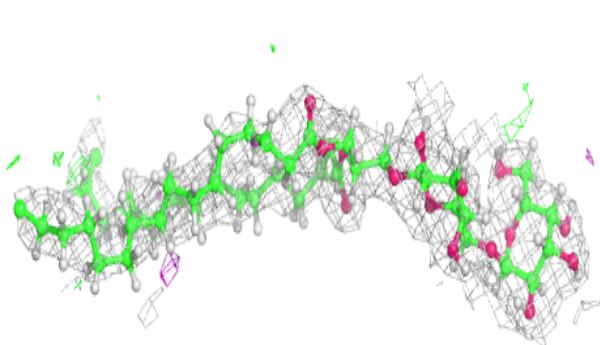
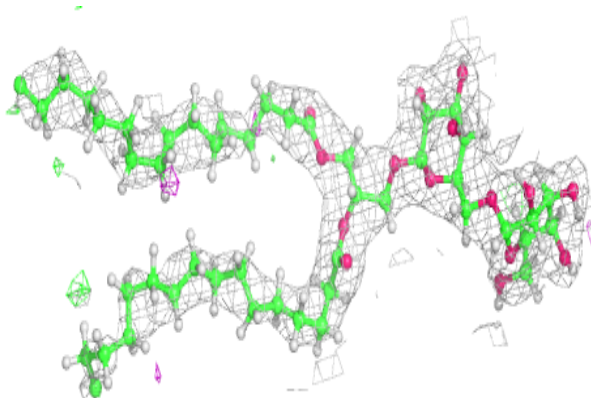


**Electron density around CLA B 604:**

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

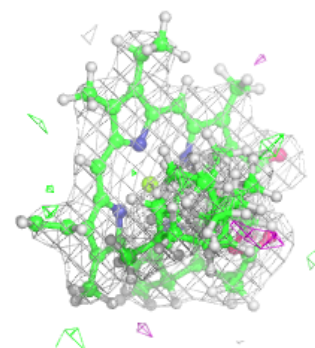
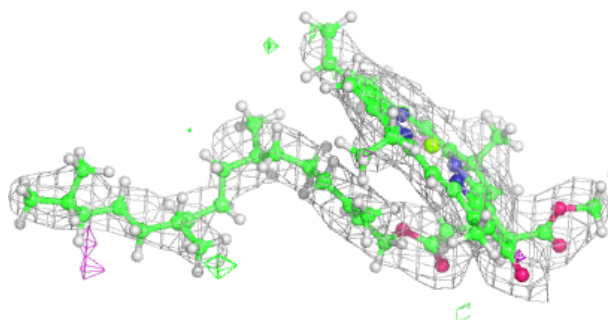
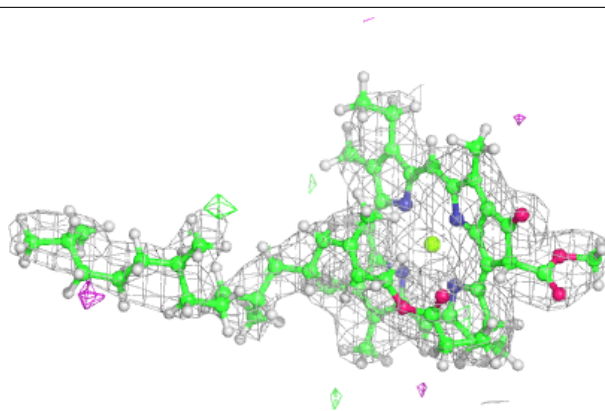
**Electron density around DGD c 517:**

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

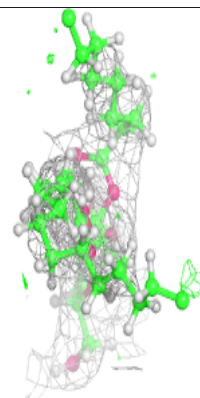
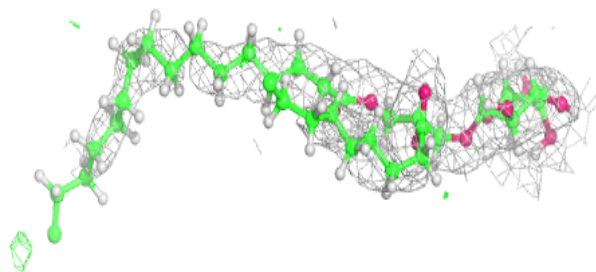
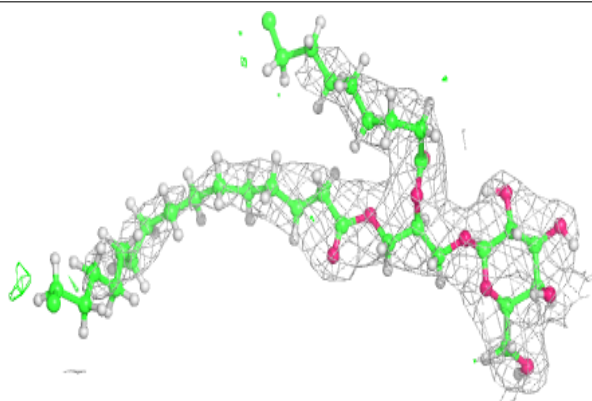


**Electron density around CLA c 505:**

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

**Electron density around LMG d 409:**

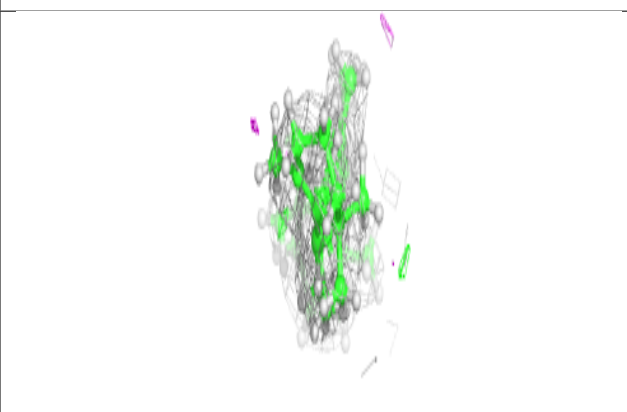
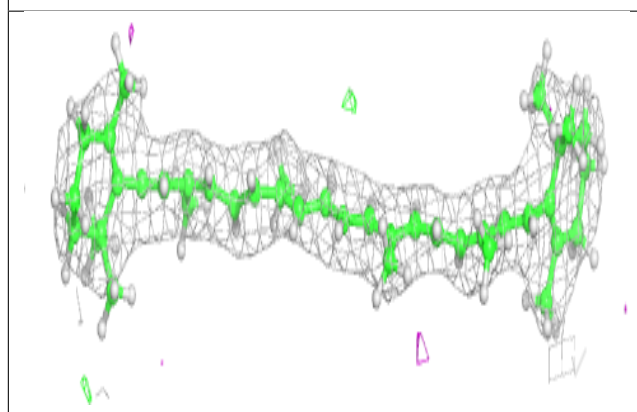
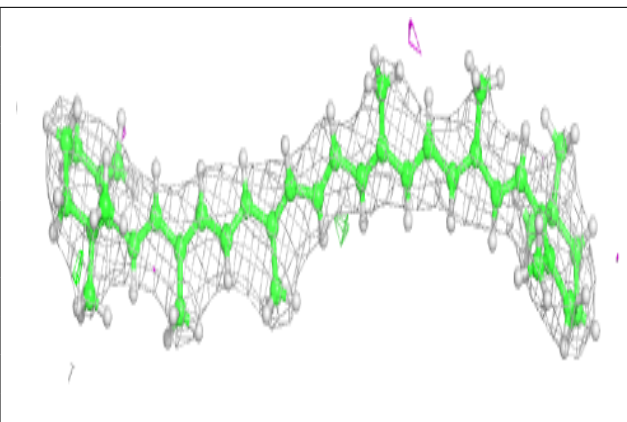
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



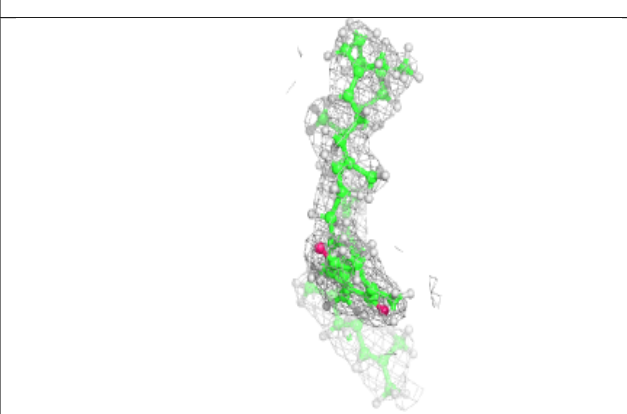
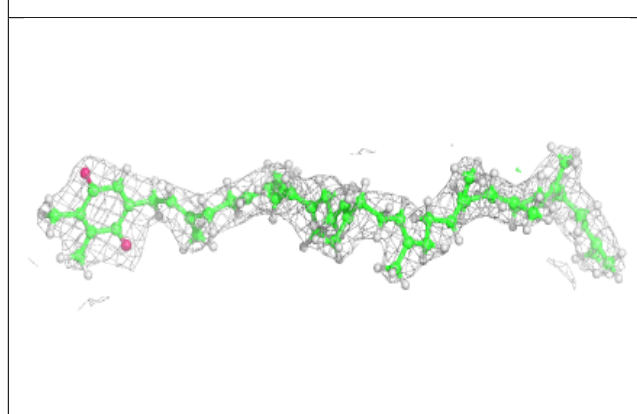
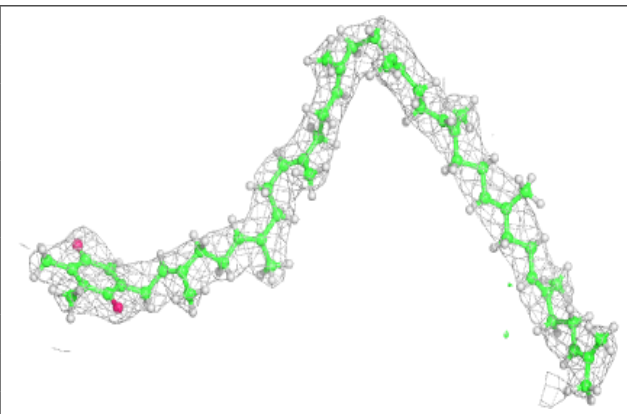


**Electron density around BCR C 514:**

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

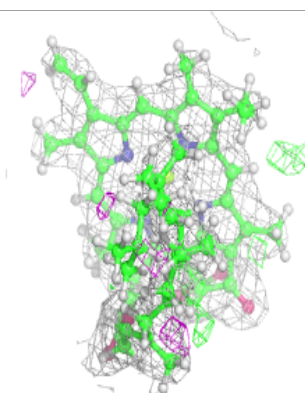
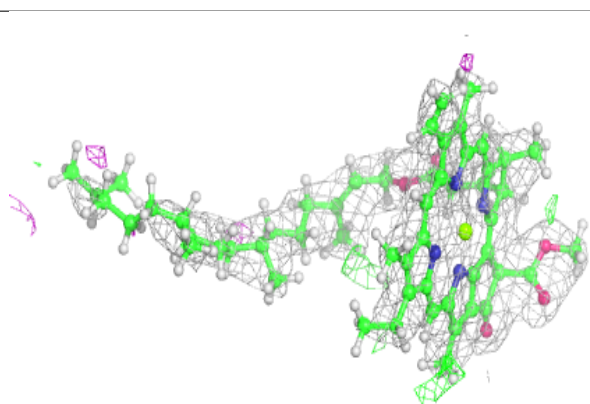
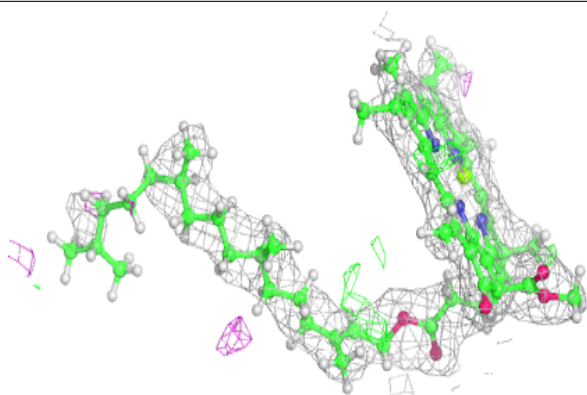
**Electron density around PL9 D 407:**

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



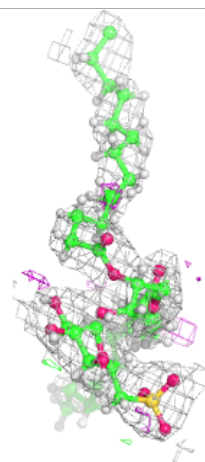
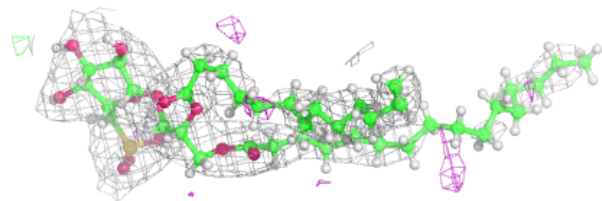
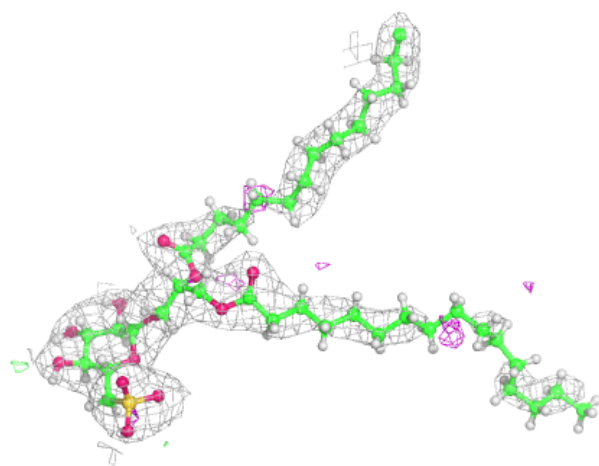
**Electron density around CLA C 508:**

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



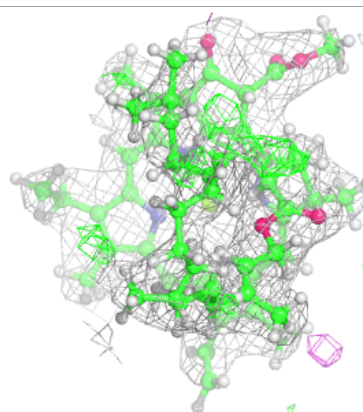
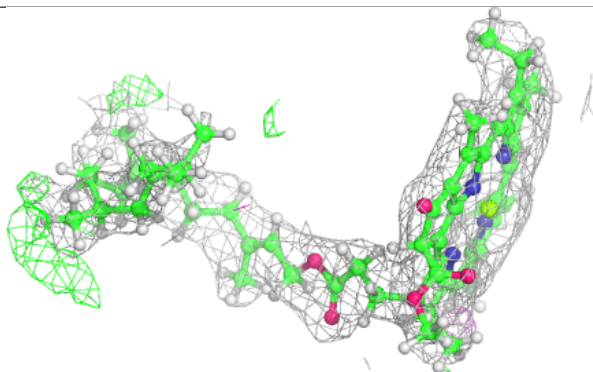
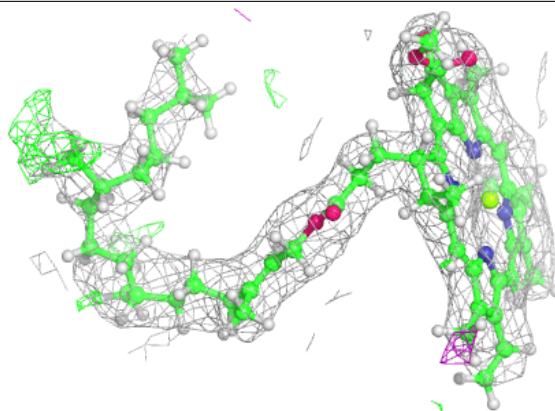
**Electron density around SQD A 412:**

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

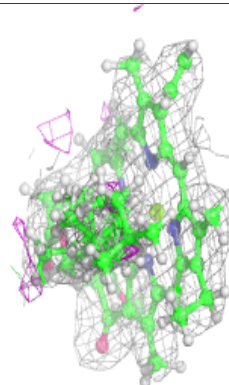
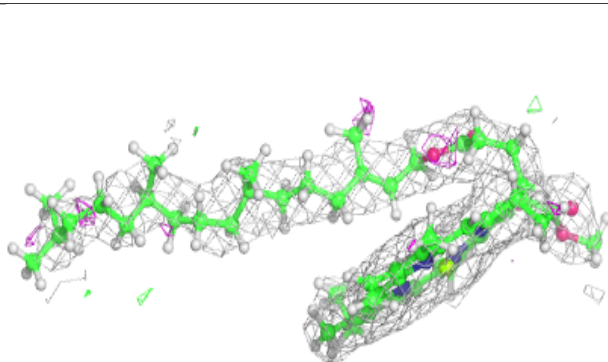
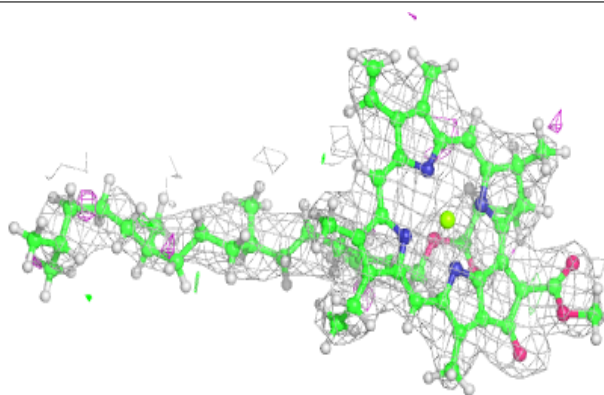


**Electron density around CLA B 606:**

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

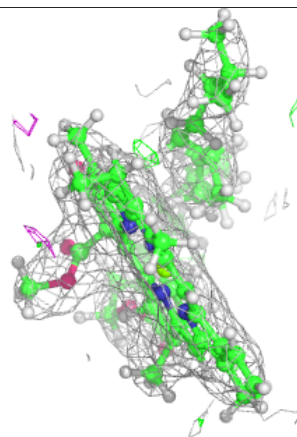
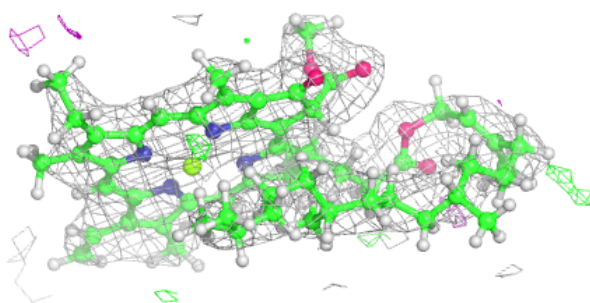
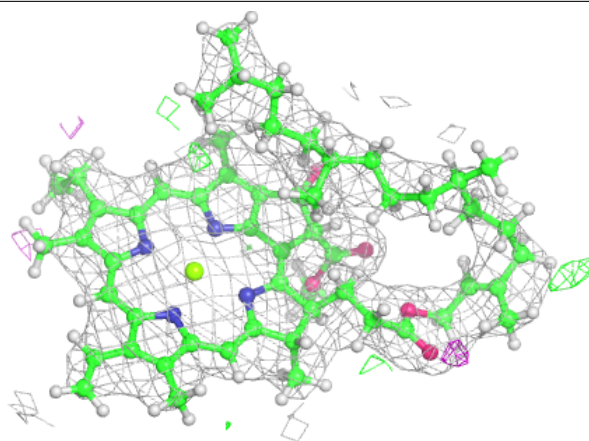
**Electron density around CLA B 614:**

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



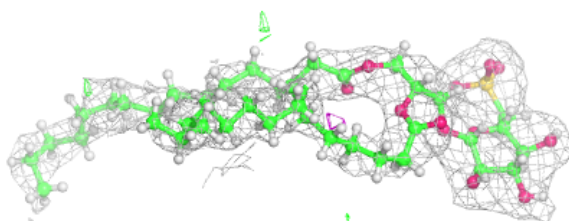
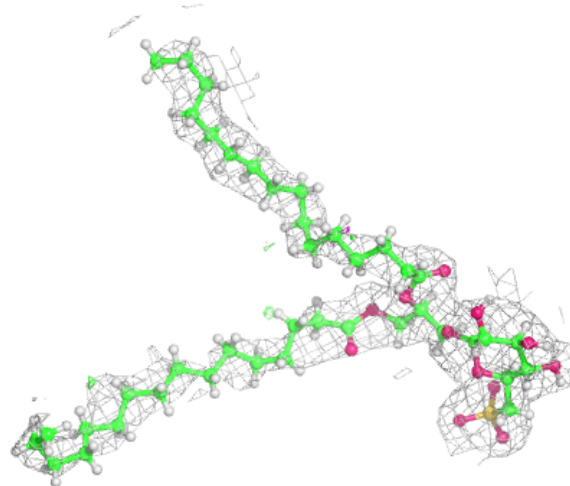
**Electron density around CLA c 509:**

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



**Electron density around SQD a 412:**

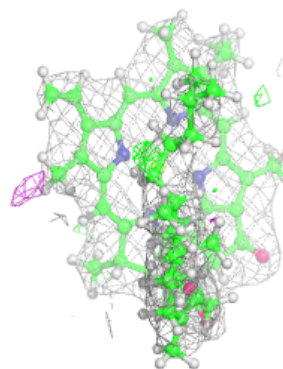
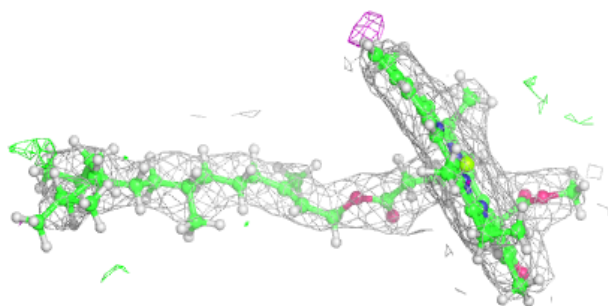
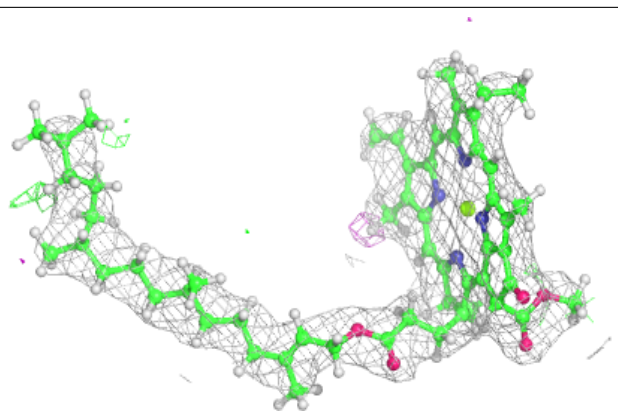
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



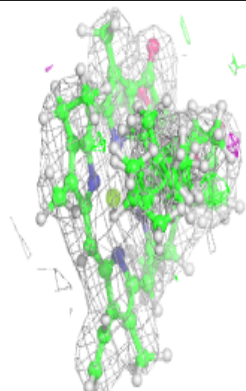
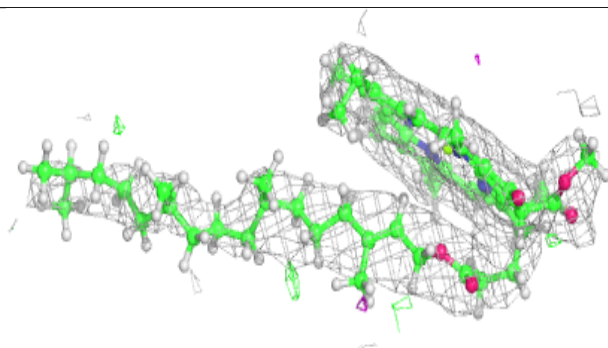
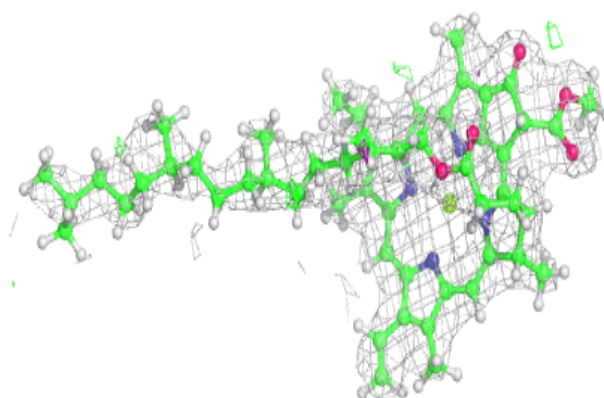


**Electron density around CLA b 609:**

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

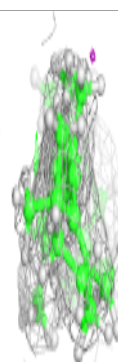
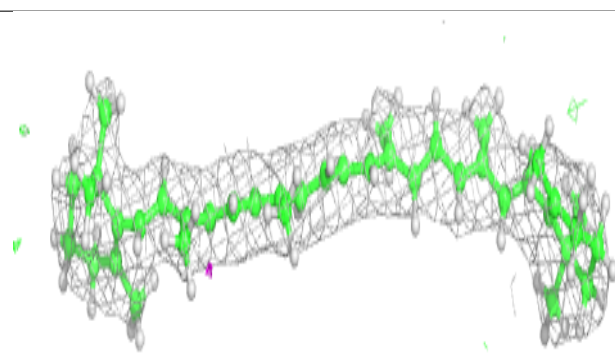
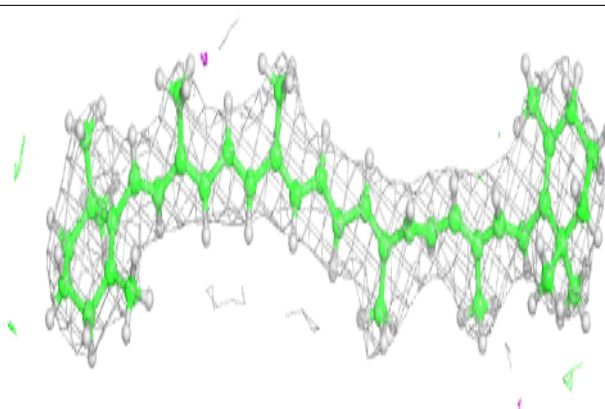
**Electron density around CLA b 614:**

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



**Electron density around BCR b 619:**

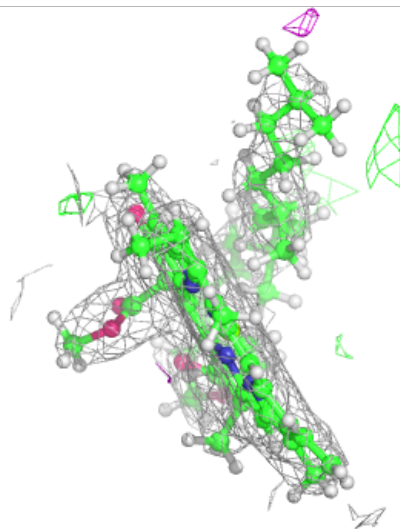
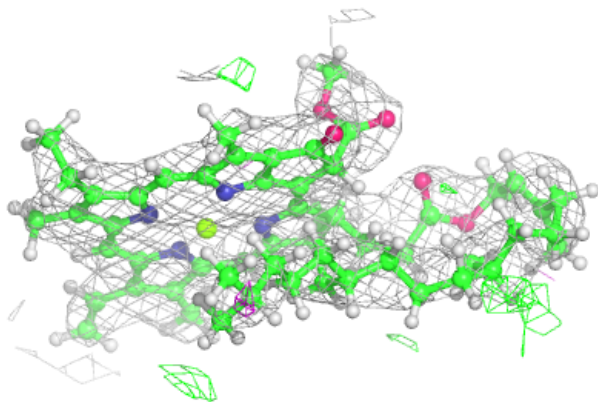
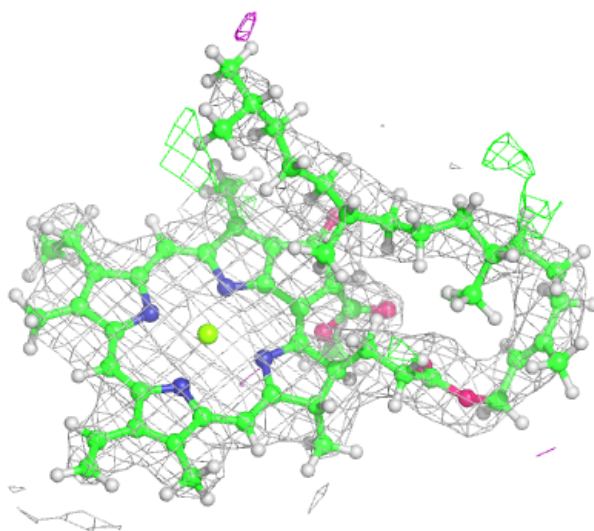
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





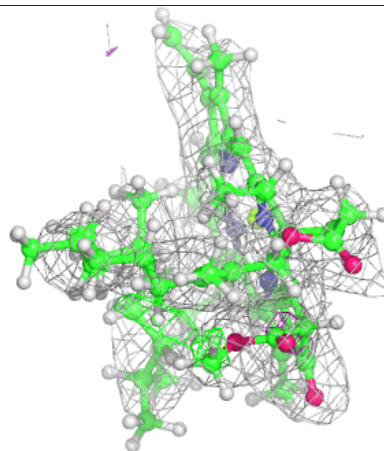
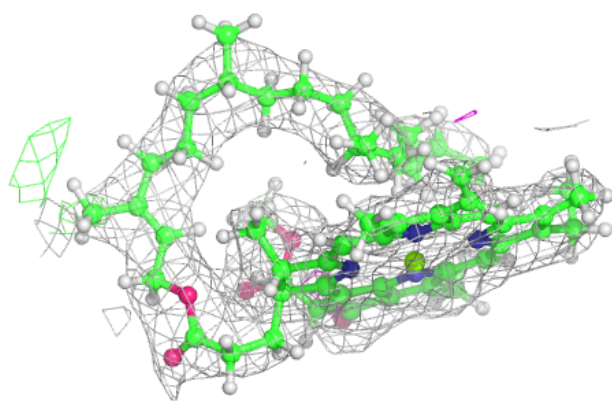
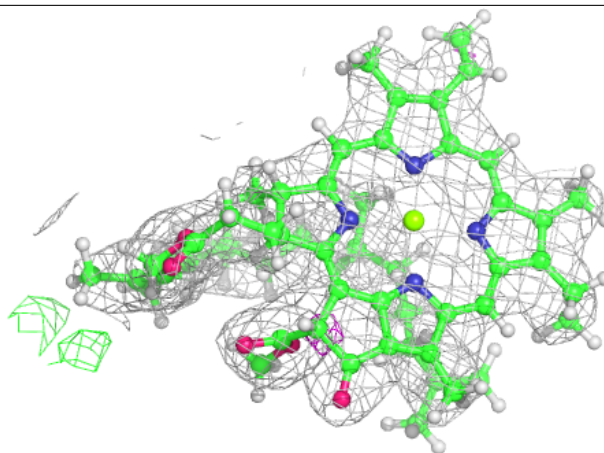
**Electron density around CLA C 509:**

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

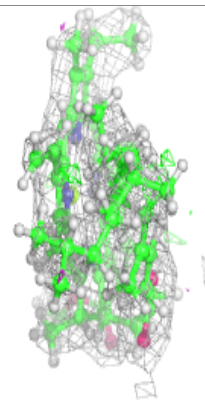
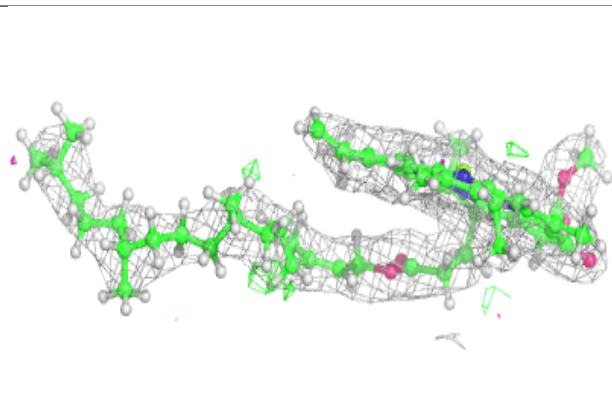
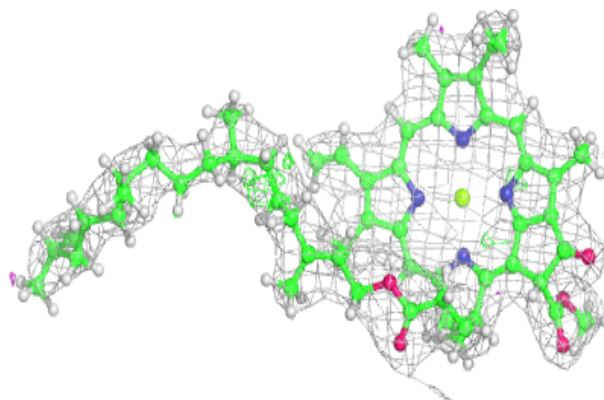


**Electron density around CLA C 510:**

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

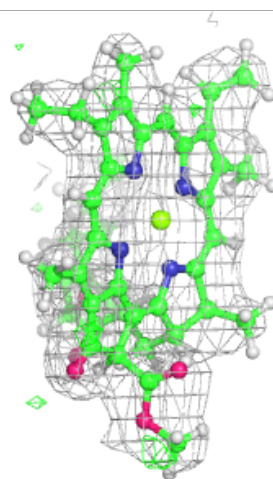
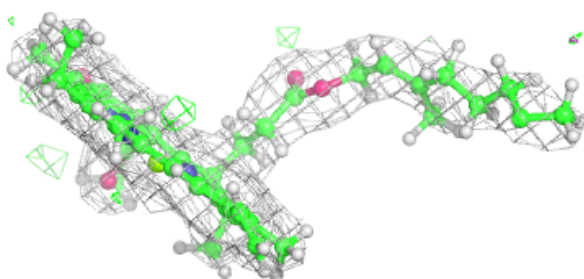
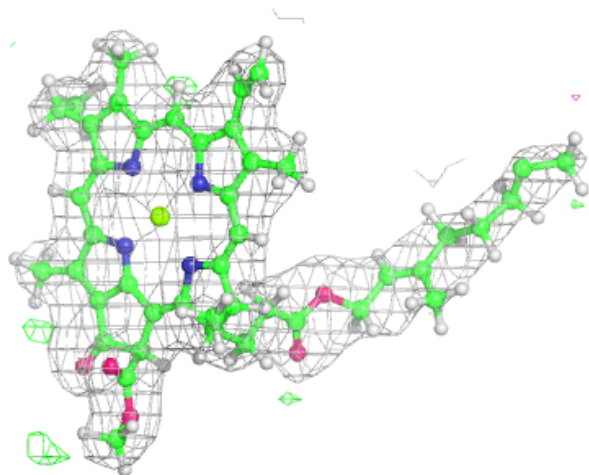
**Electron density around CLA B 603:**

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



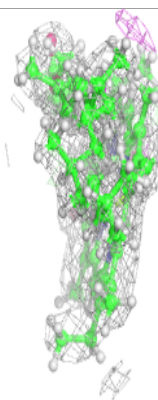
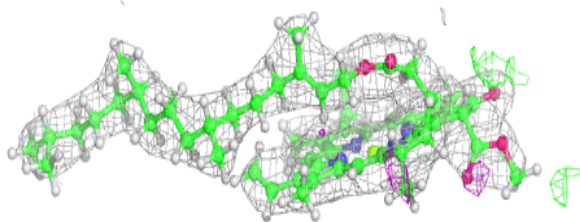
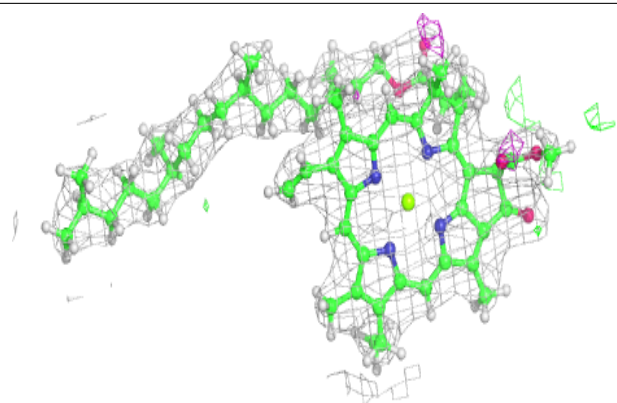
**Electron density around CLA A 405:**

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

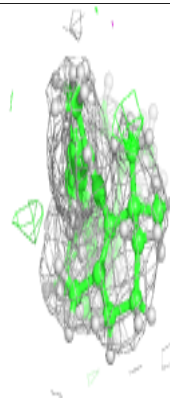
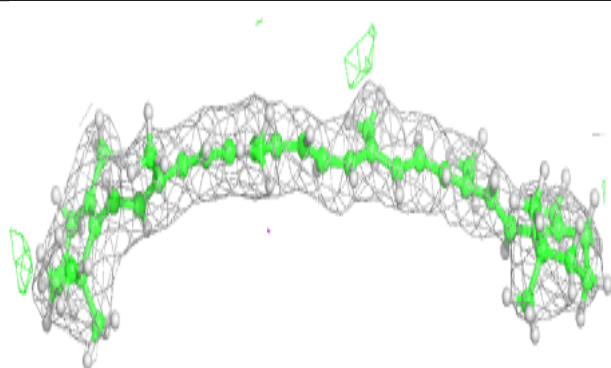
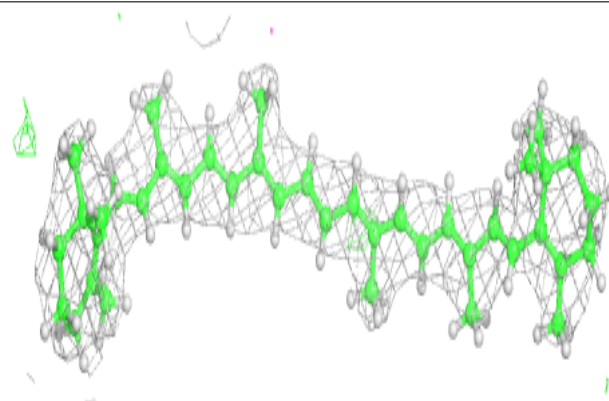


**Electron density around CLA C 501:**

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

**Electron density around BCR T 101:**

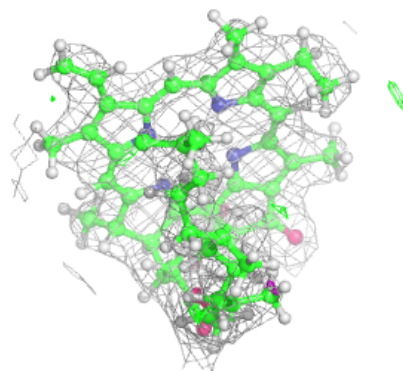
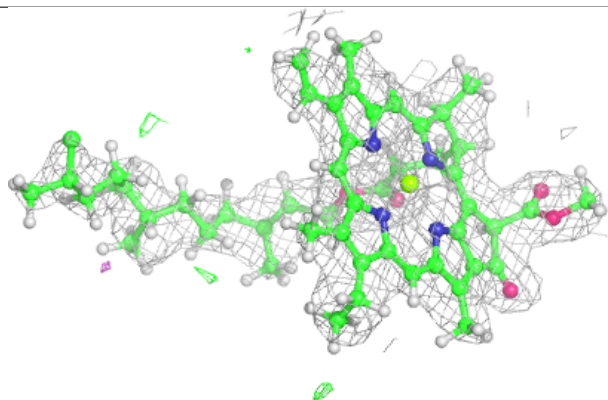
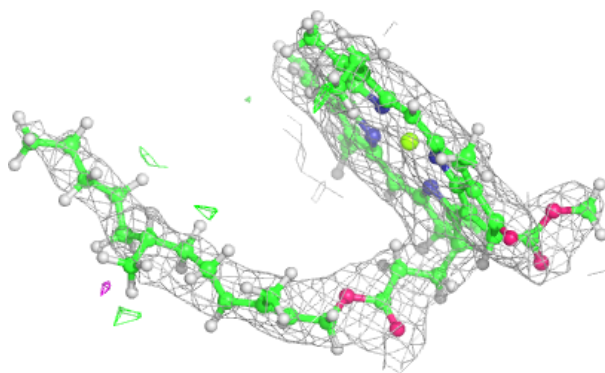
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



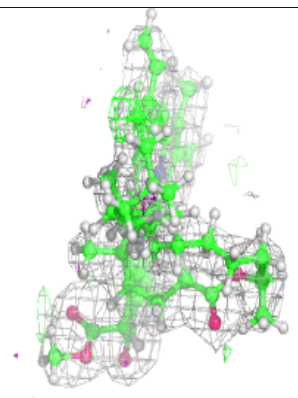
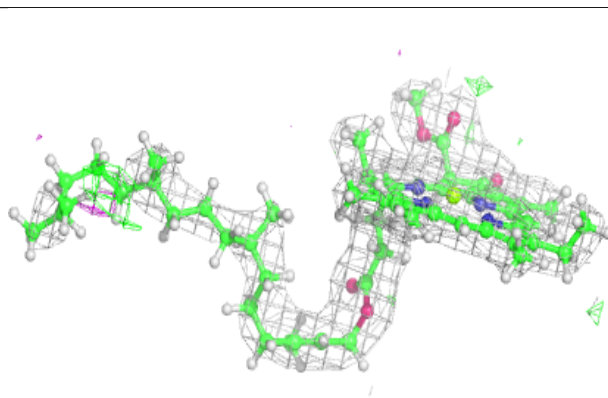
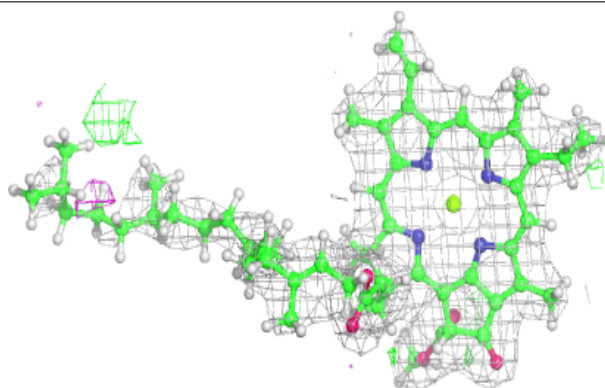


**Electron density around CLA c 504:**

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

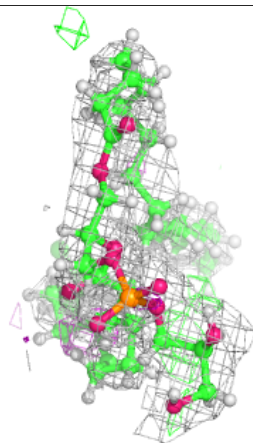
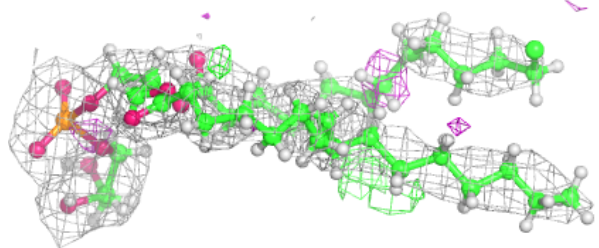
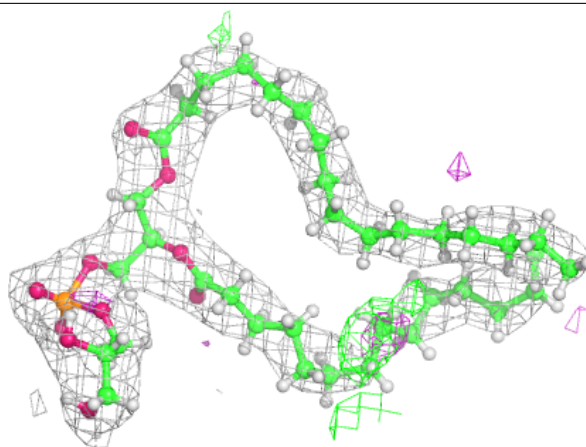
**Electron density around CLA A 403:**

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

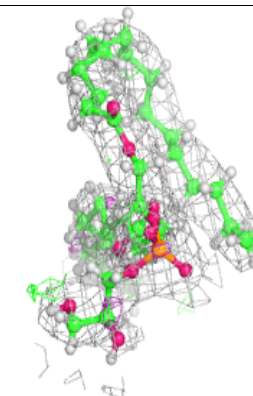
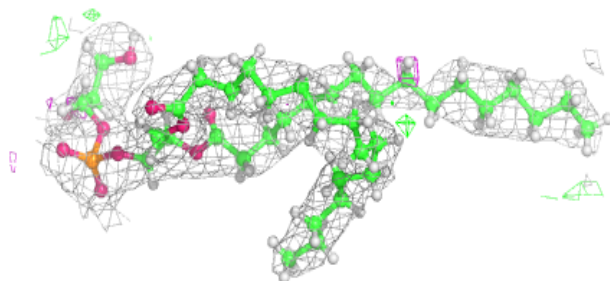
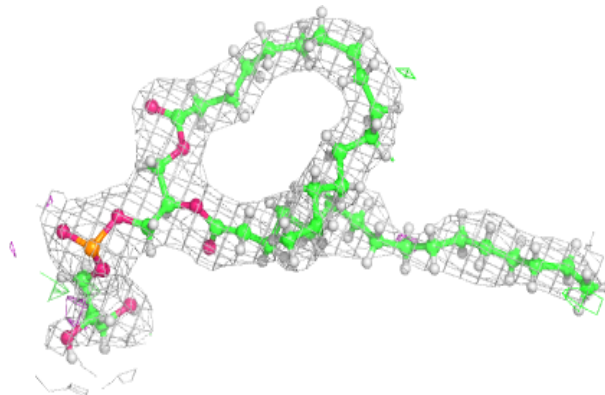


**Electron density around LHG A 411:**

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

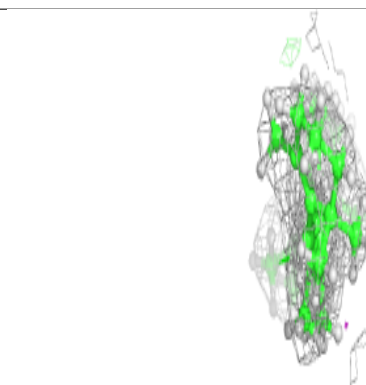
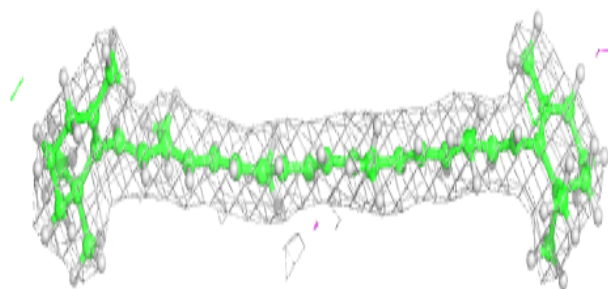
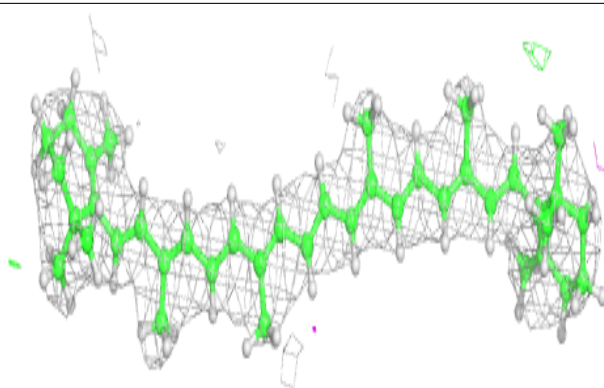
**Electron density around LHG B 621:**

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

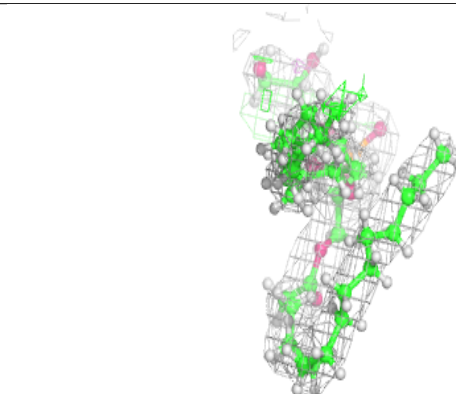
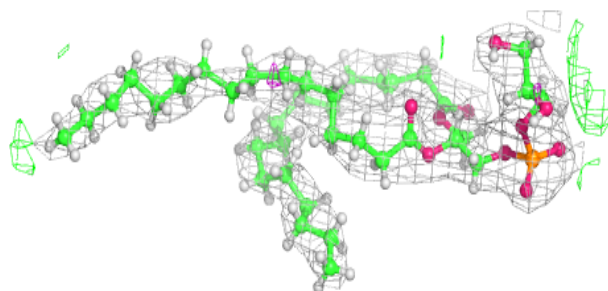
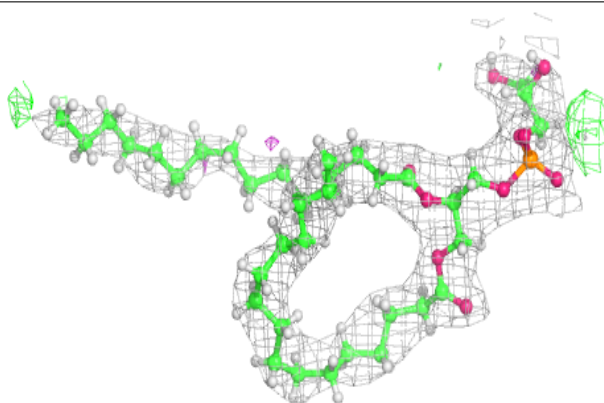


**Electron density around BCR b 618:**

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

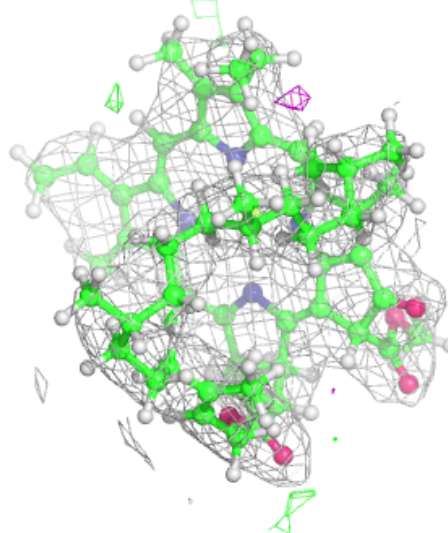
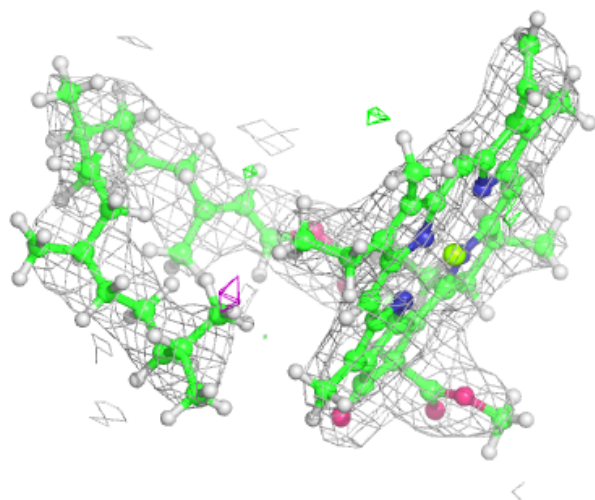
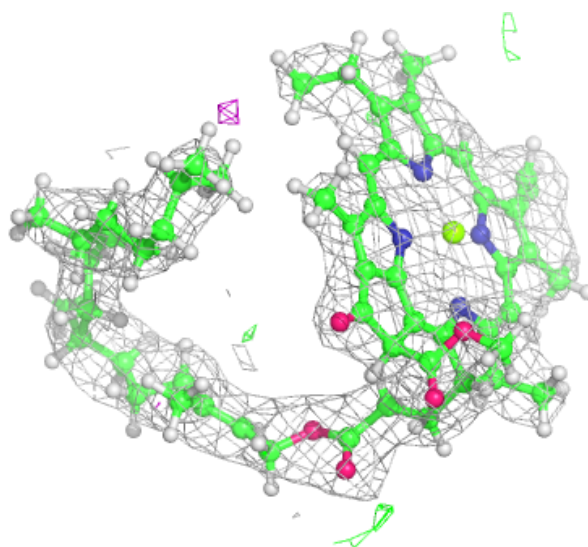
**Electron density around LHG b 623:**

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



**Electron density around CLA C 503:**

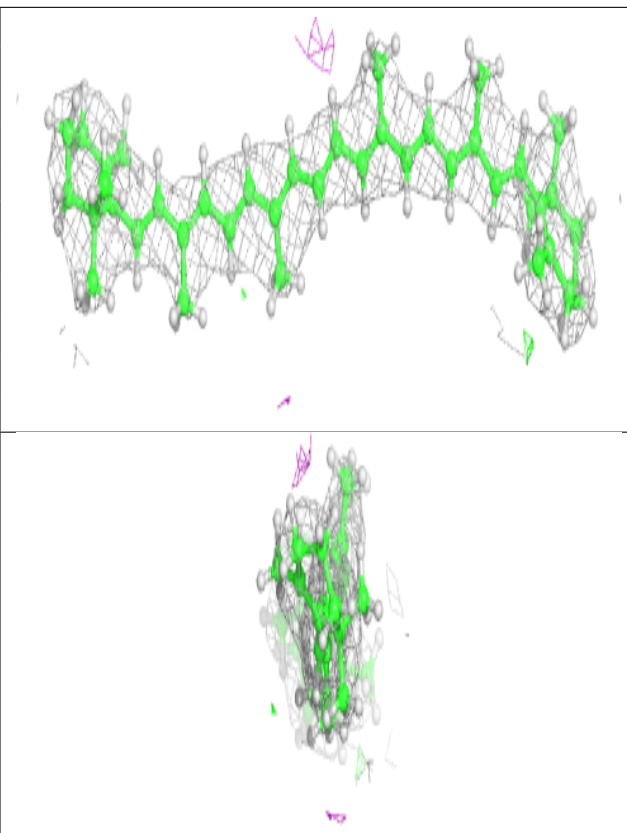
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



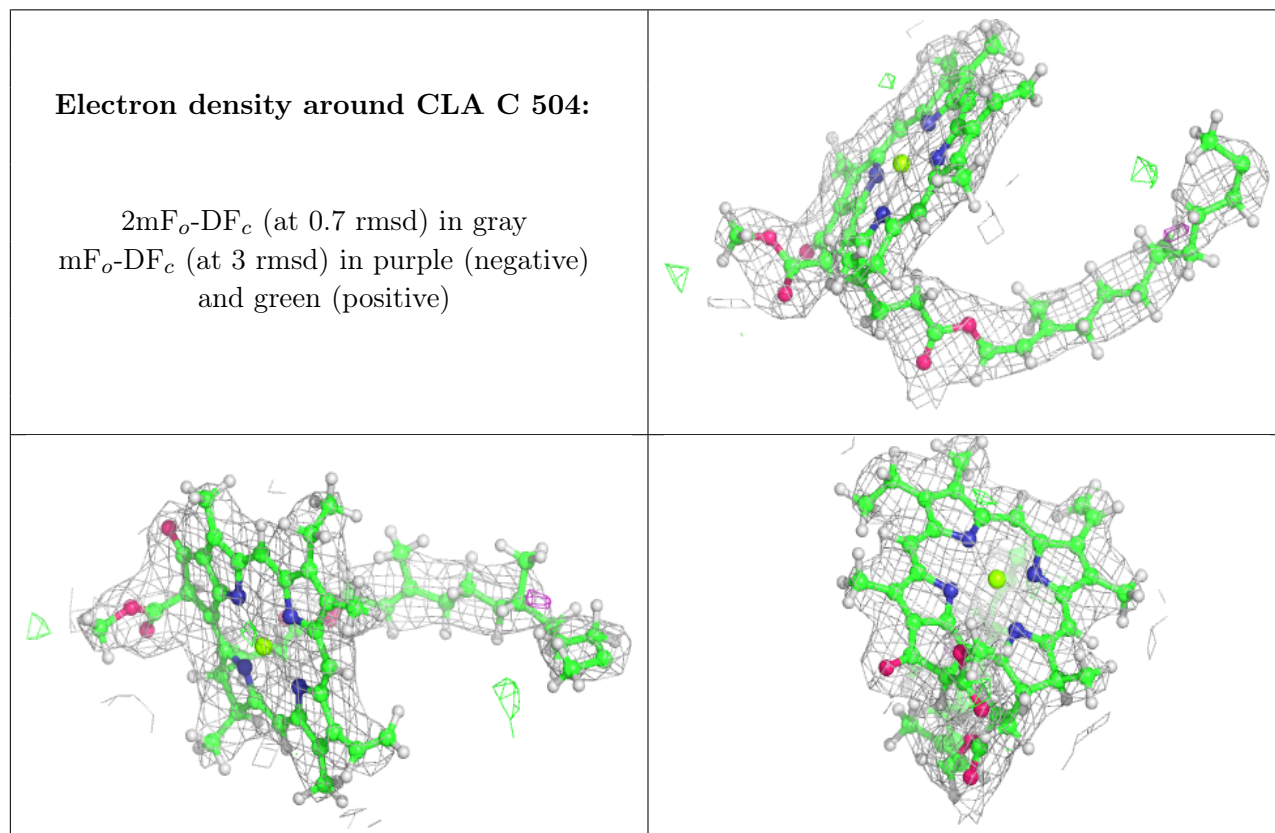


**Electron density around BCR c 514:**

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

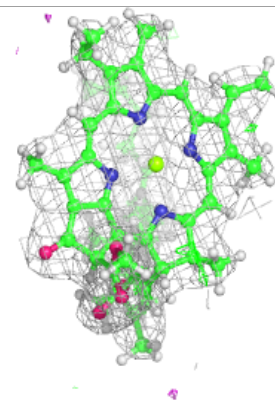
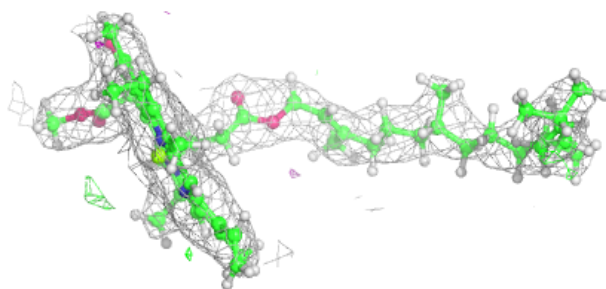
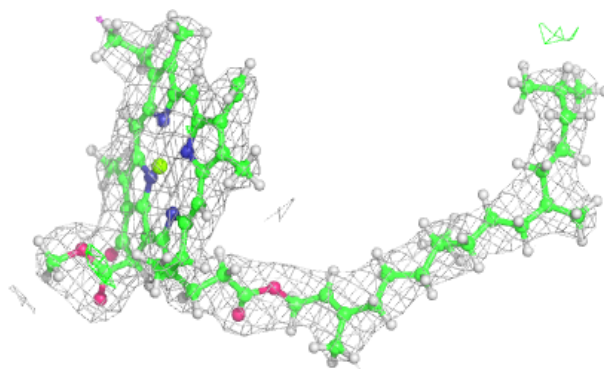
**Electron density around CLA C 504:**

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

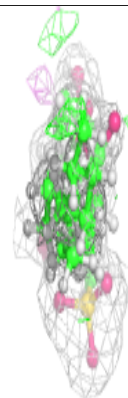
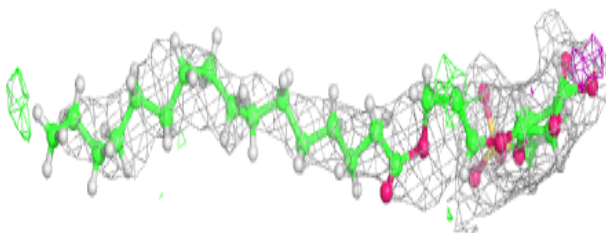
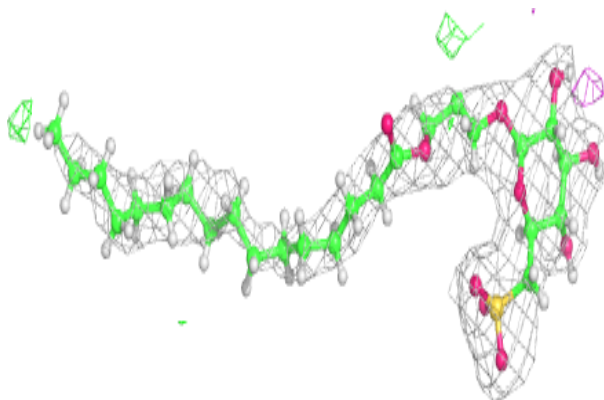


**Electron density around CLA B 609:**

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

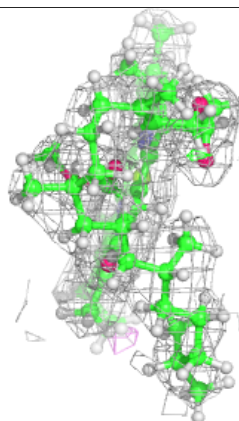
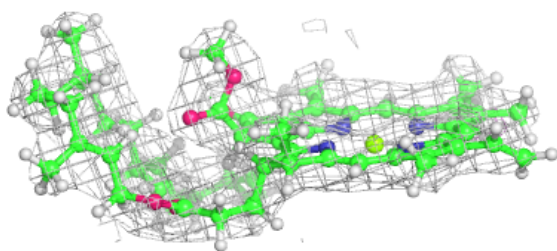
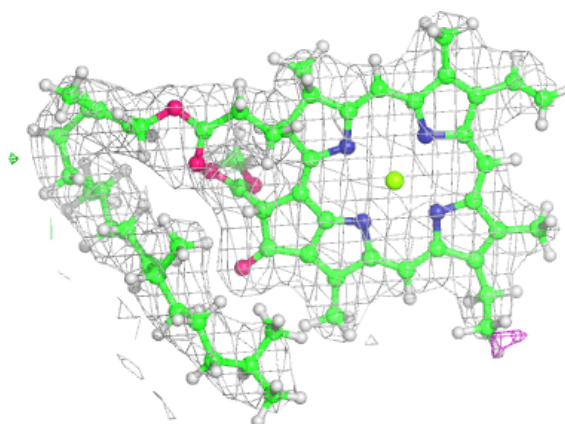
**Electron density around SQD F 102:**

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

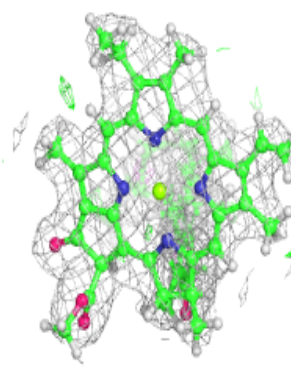
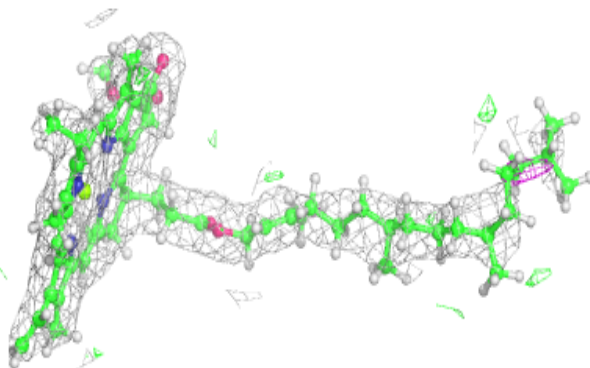
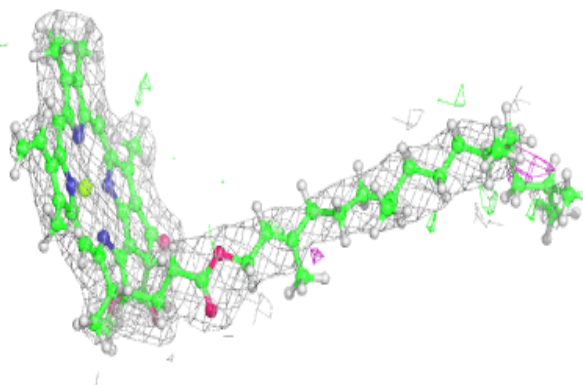


**Electron density around CLA B 610:**

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

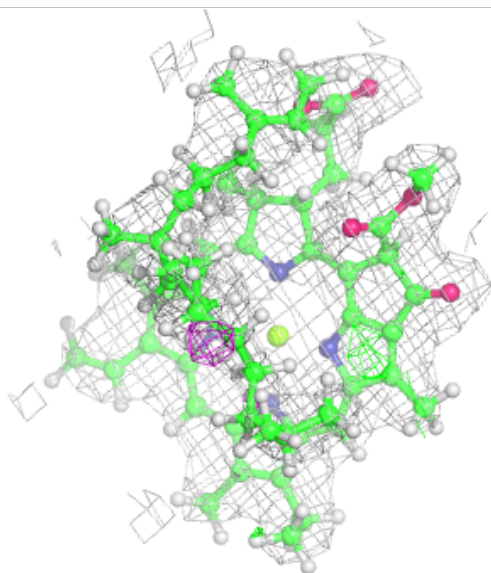
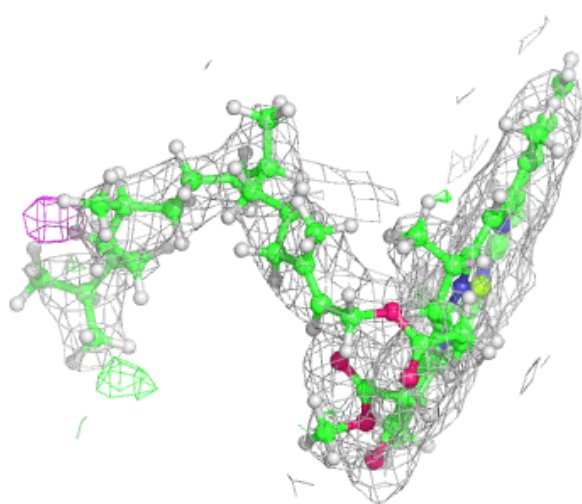
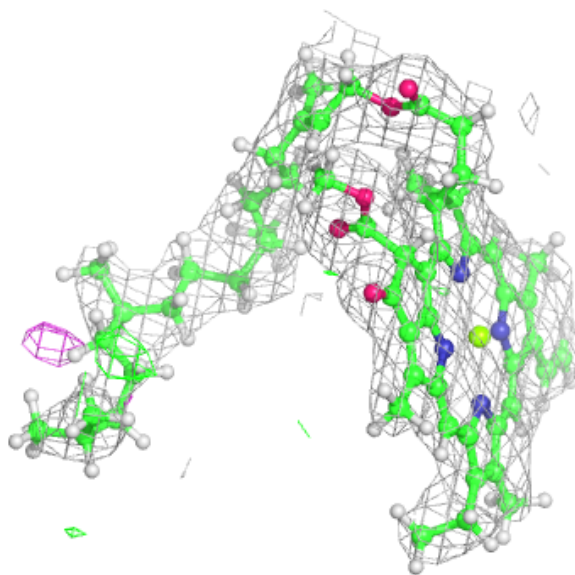
**Electron density around CLA b 604:**

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



**Electron density around CLA B 613:**

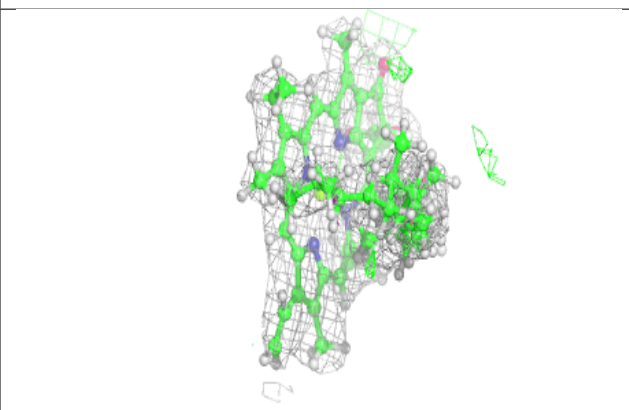
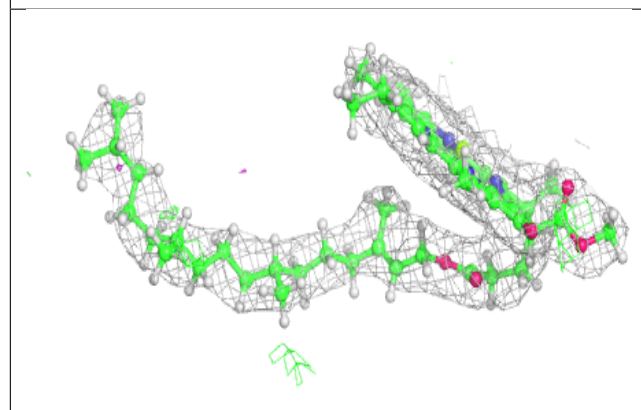
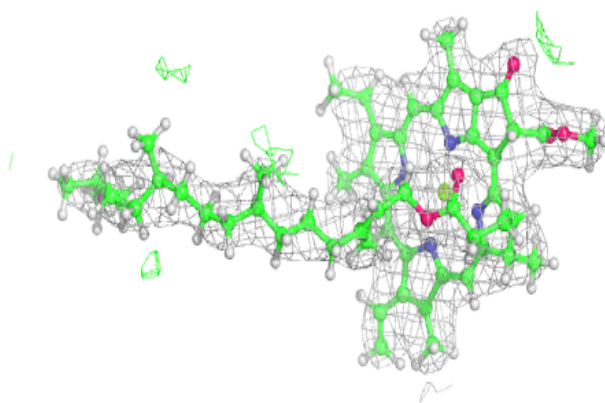
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



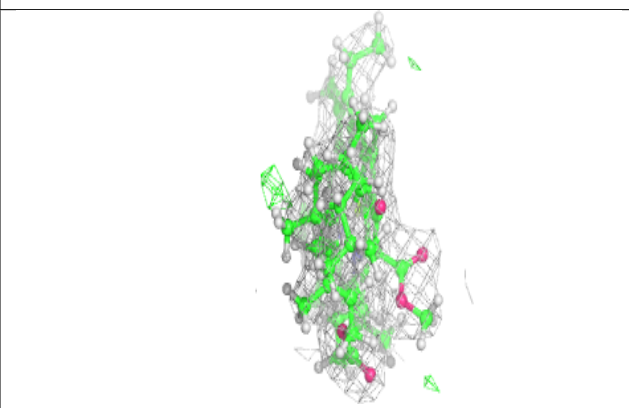
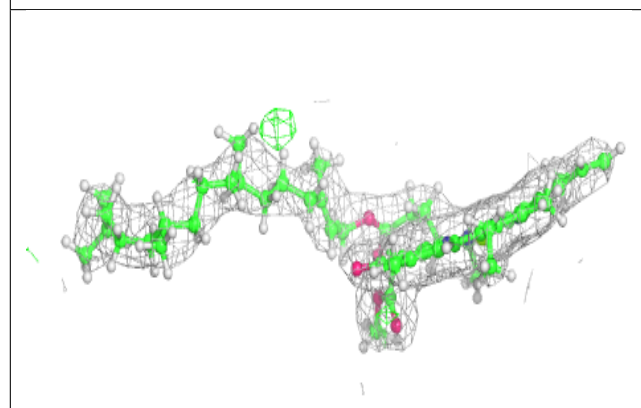
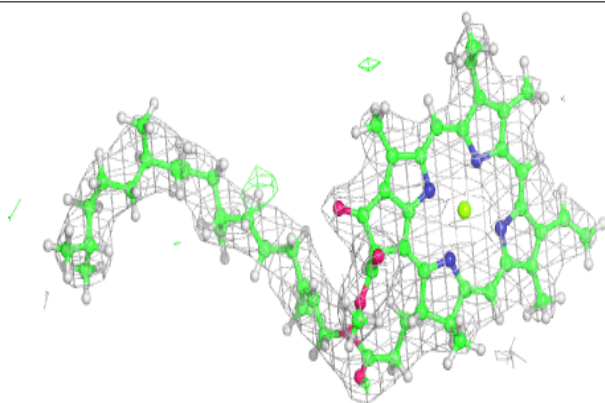


**Electron density around CLA b 608:**

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

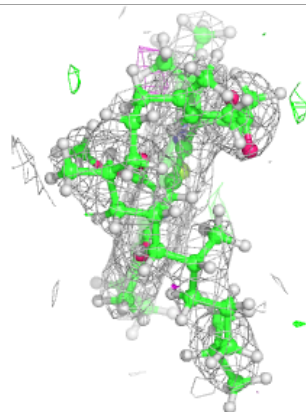
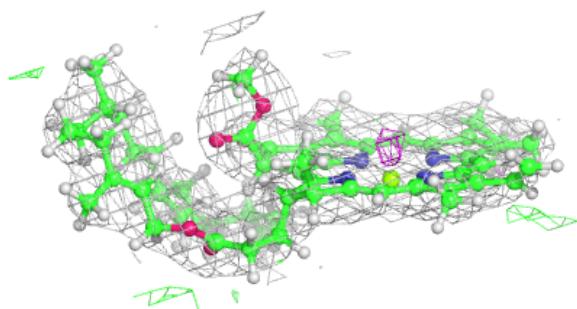
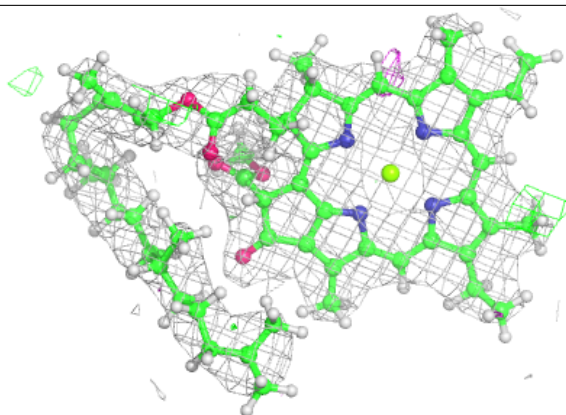
**Electron density around CLA B 602:**

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

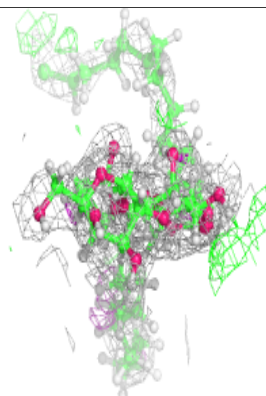
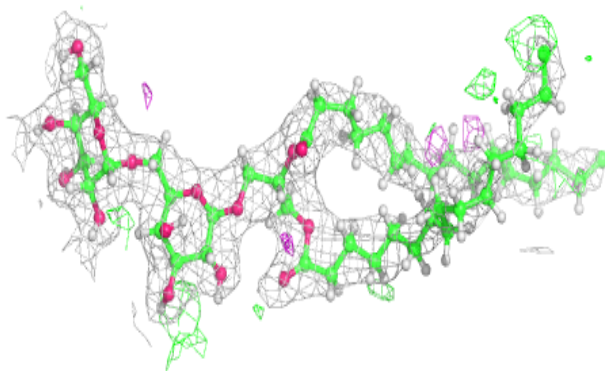
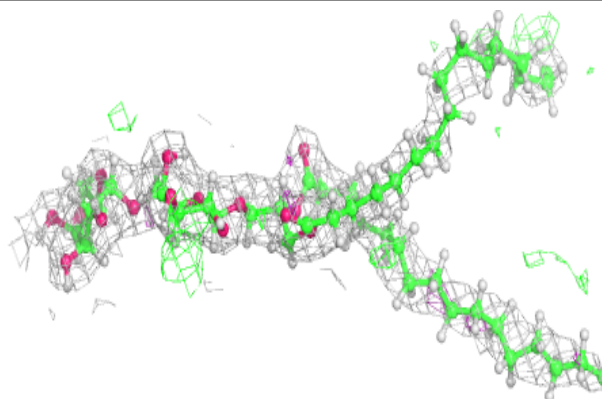


**Electron density around CLA b 610:**

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

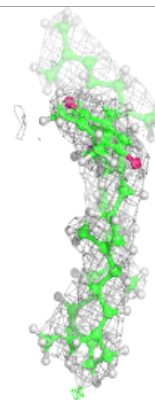
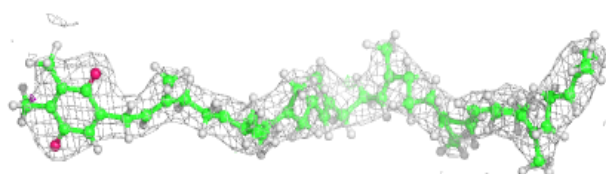
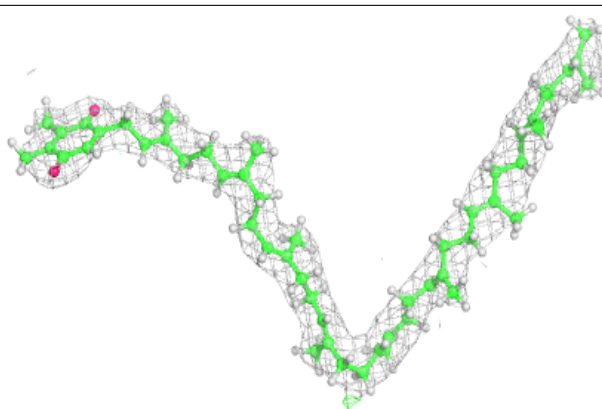
**Electron density around DGD C 515:**

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

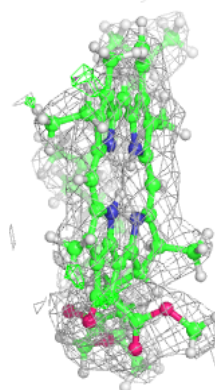
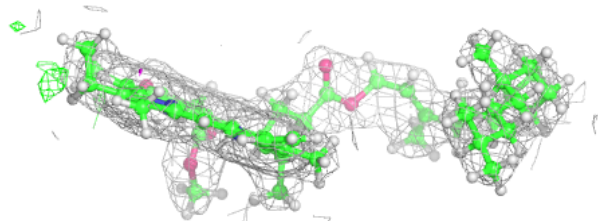
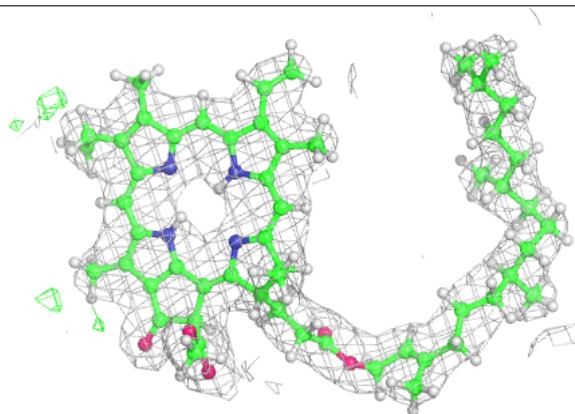


**Electron density around PL9 d 405:**

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

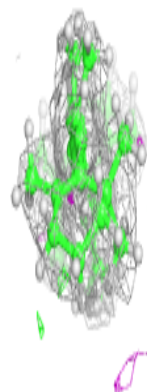
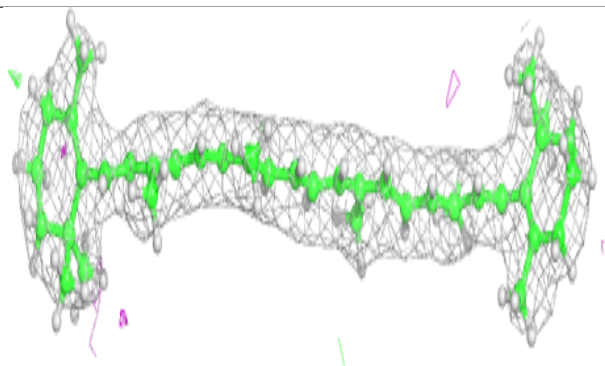
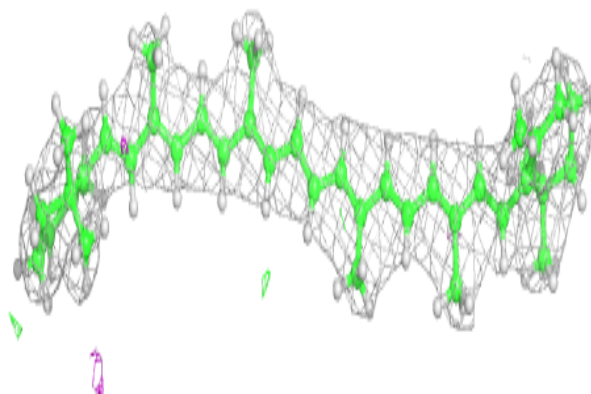
**Electron density around PHO a 404:**

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

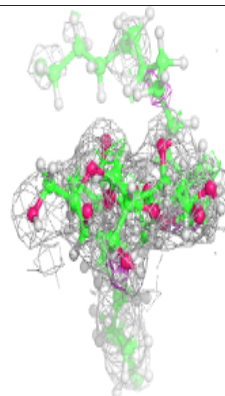
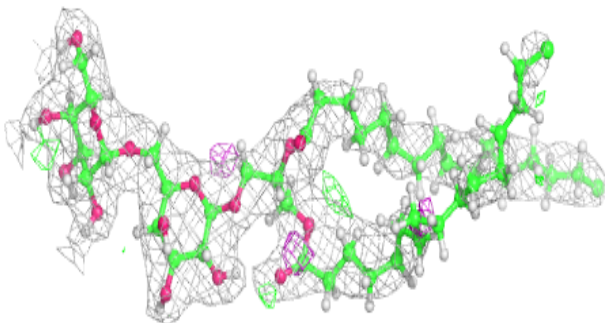
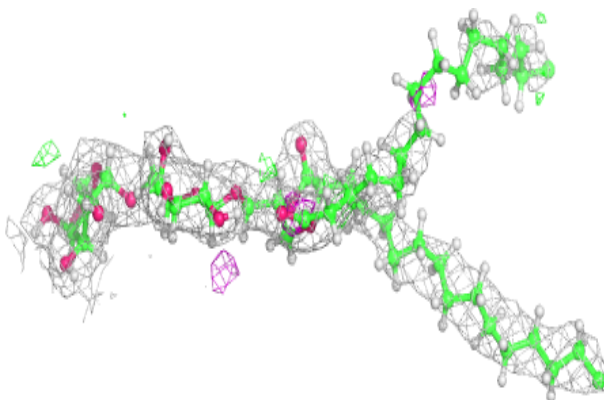


**Electron density around BCR A 406:**

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

**Electron density around DGD c 515:**

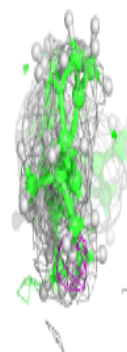
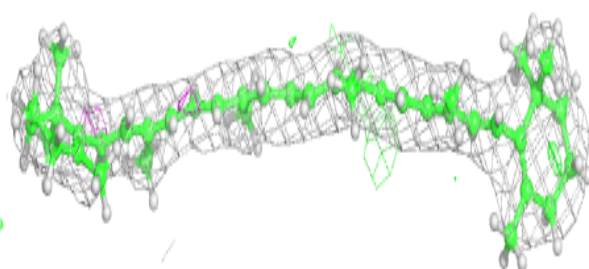
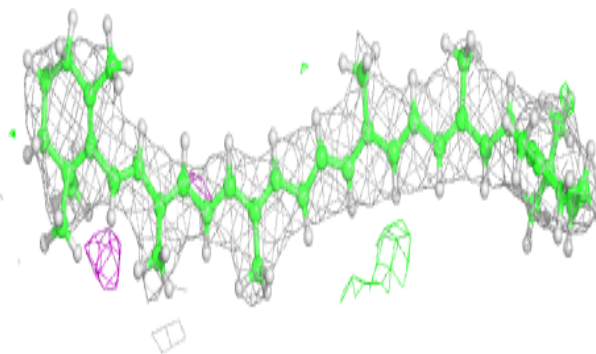
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





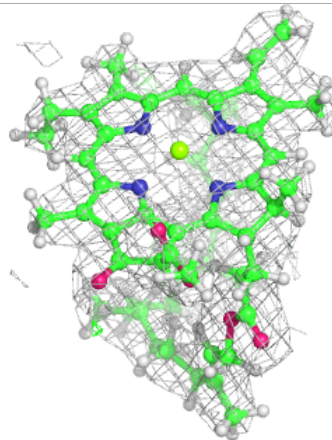
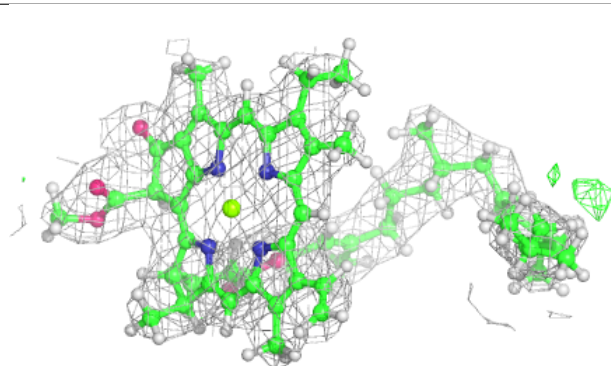
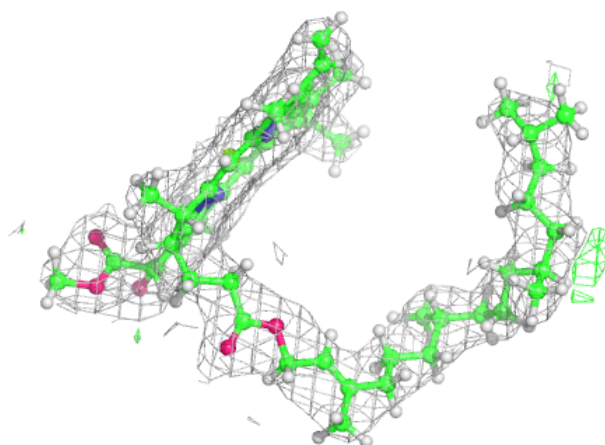
**Electron density around BCR B 617:**

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



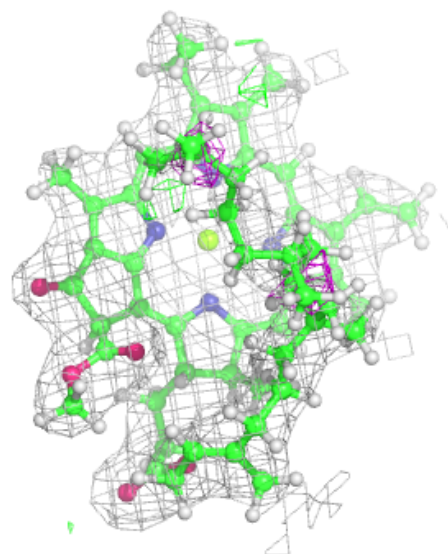
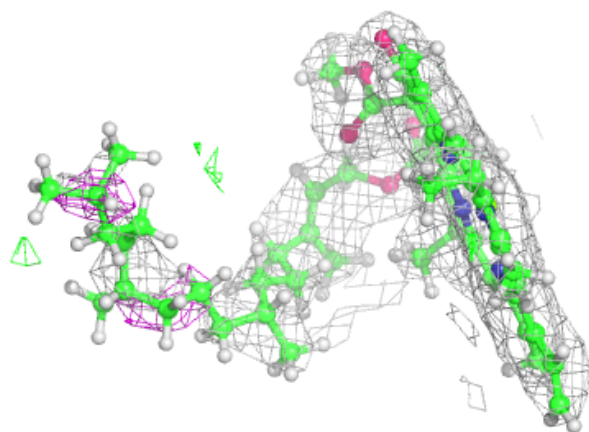
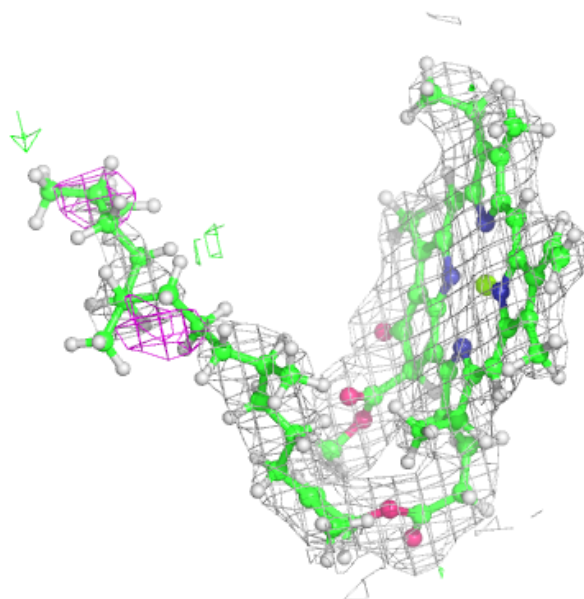
**Electron density around CLA b 611:**

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



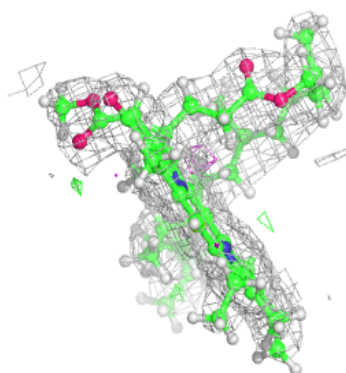
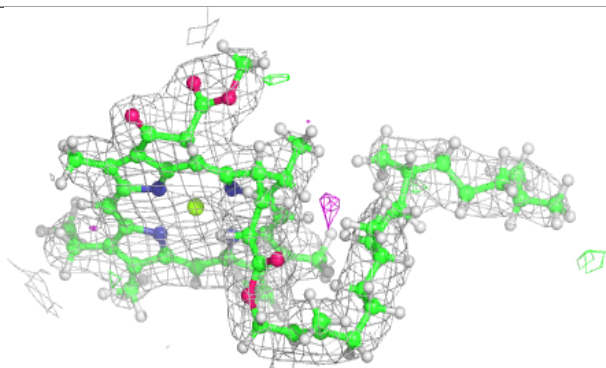
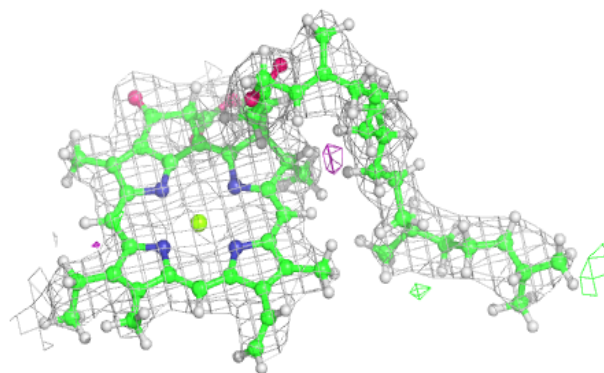
**Electron density around CLA b 613:**

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

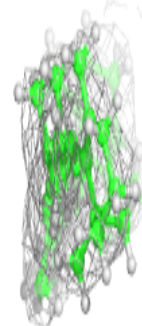
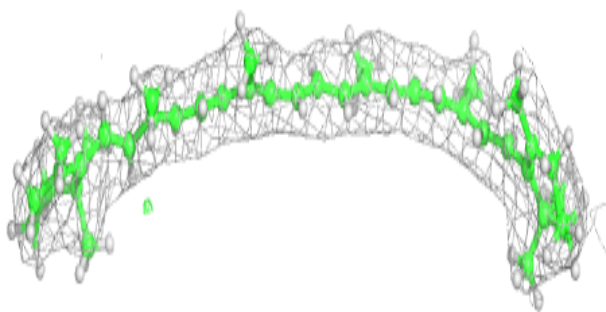
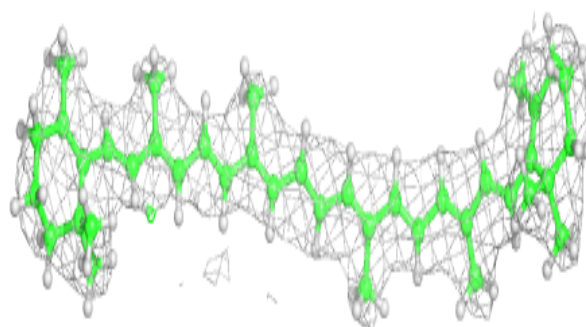


**Electron density around CLA a 411:**

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

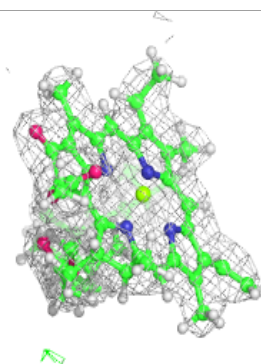
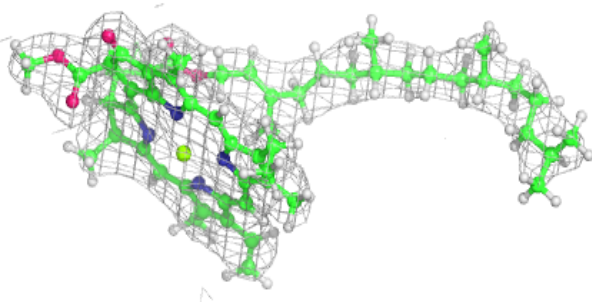
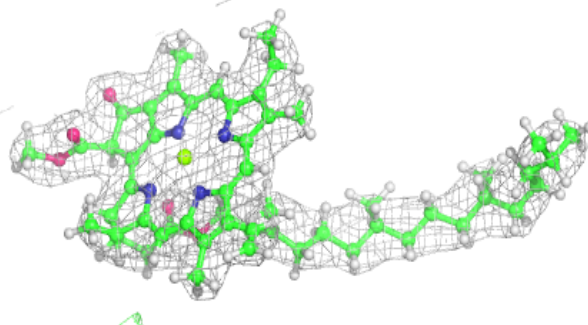
**Electron density around BCR t 101:**

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

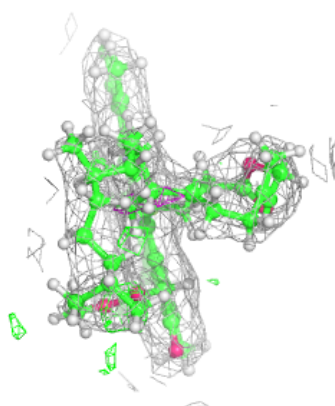
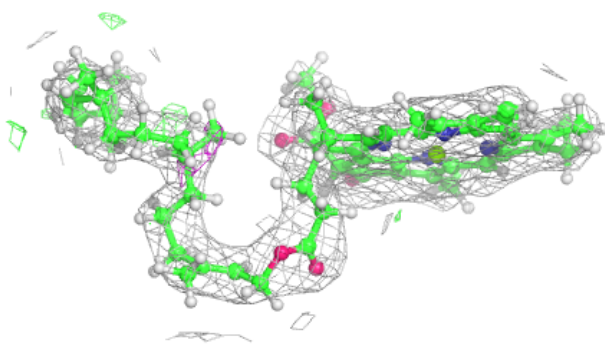
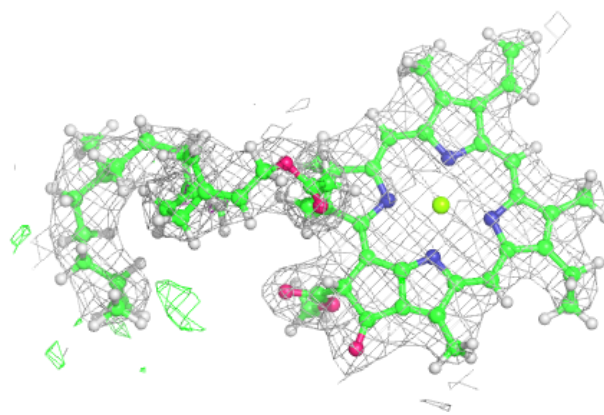


**Electron density around CLA B 608:**

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

**Electron density around CLA b 612:**

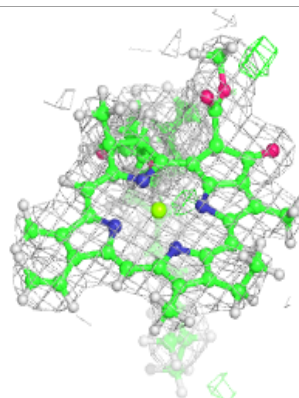
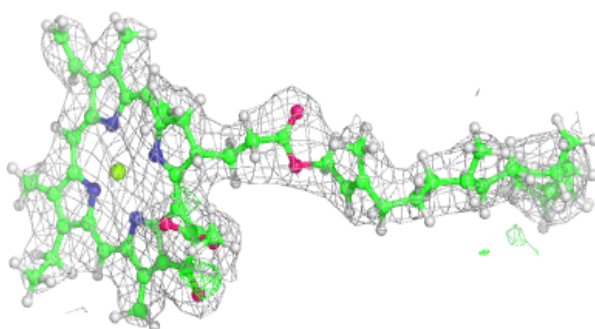
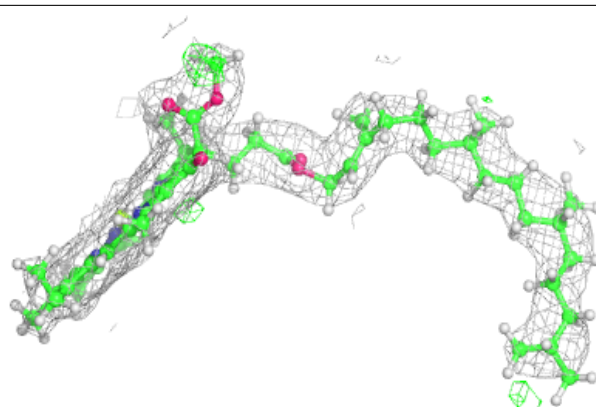
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



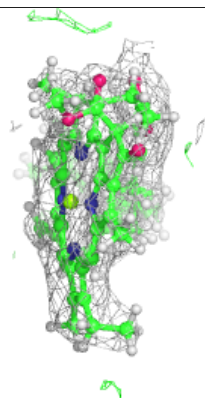
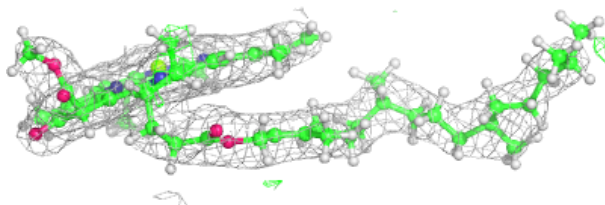
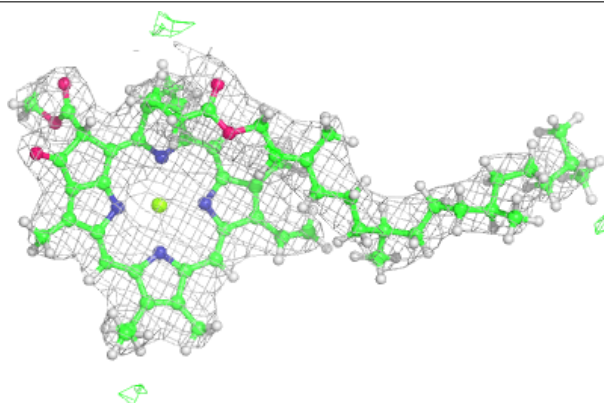


**Electron density around CLA D 403:**

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

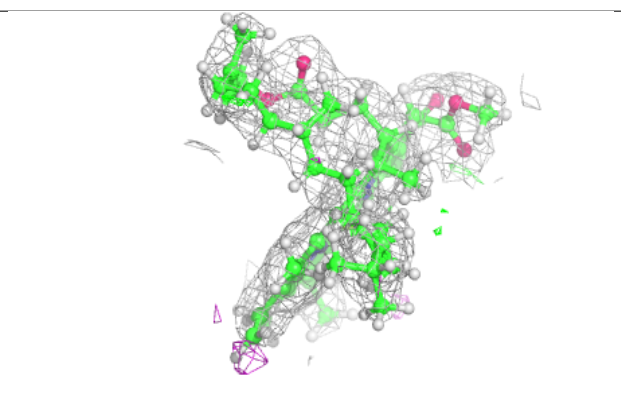
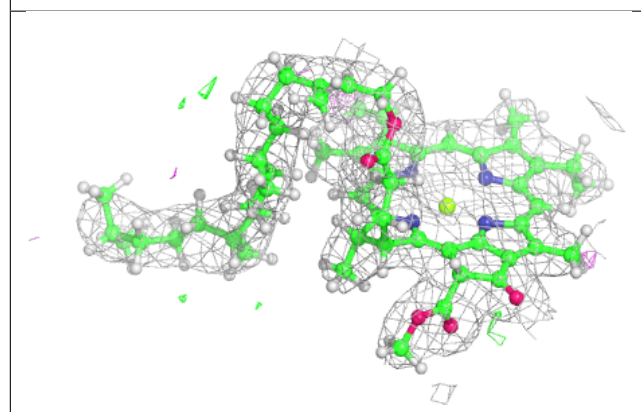
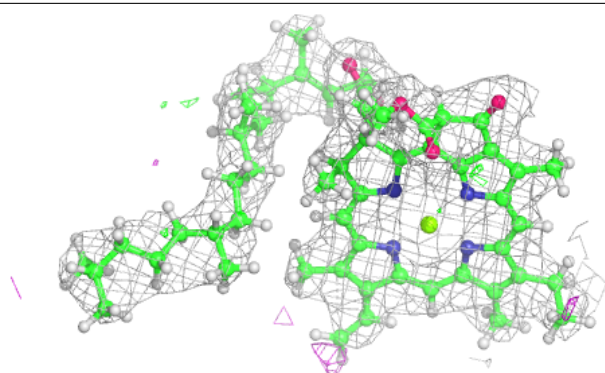
**Electron density around CLA b 603:**

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



**Electron density around CLA D 404:**

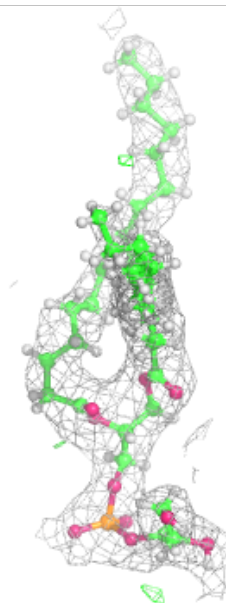
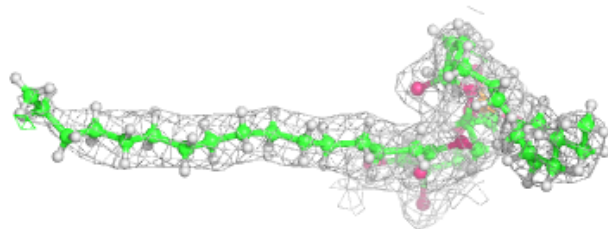
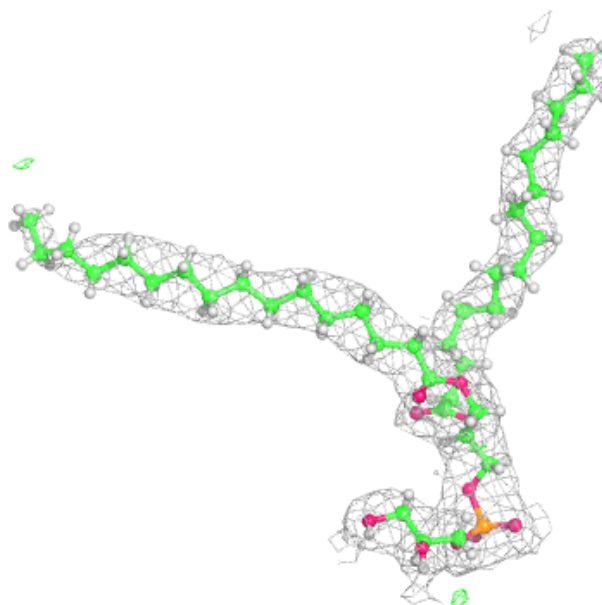
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





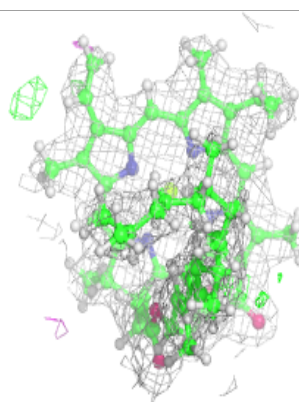
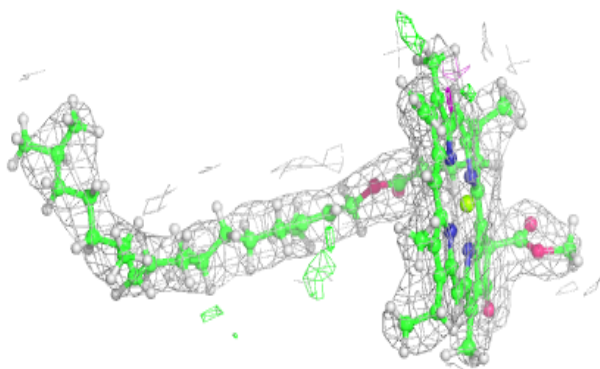
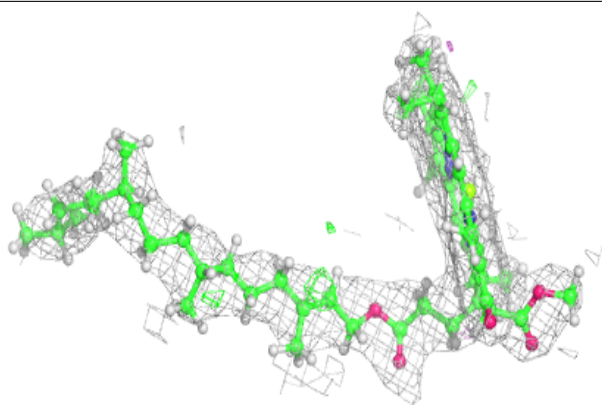
**Electron density around LHG 1 101:**

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

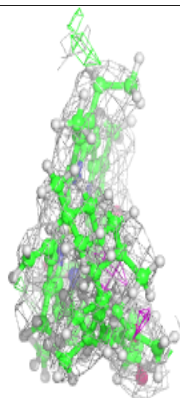
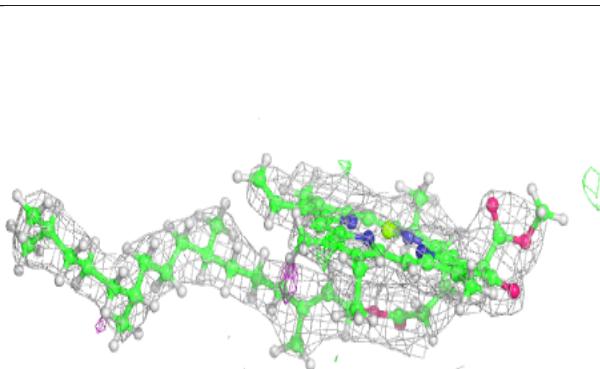
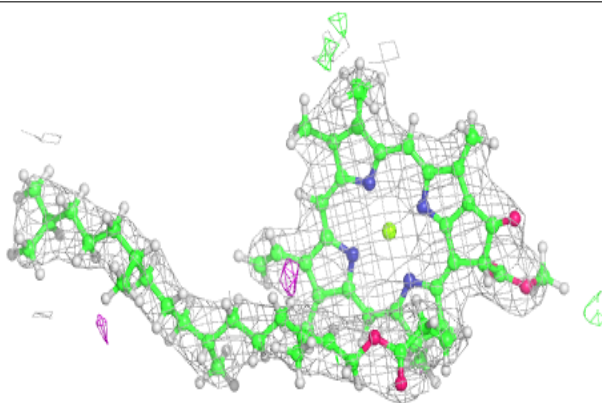


**Electron density around CLA b 605:**

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

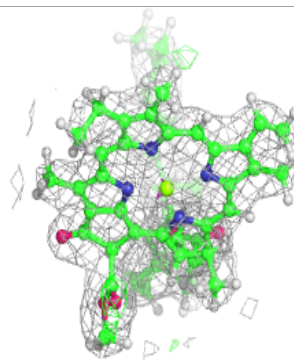
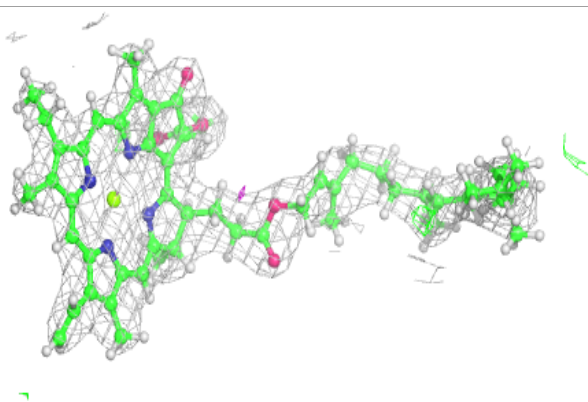
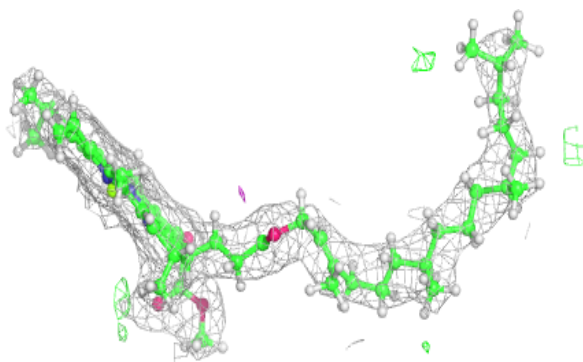
**Electron density around CLA c 501:**

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

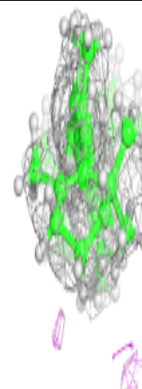
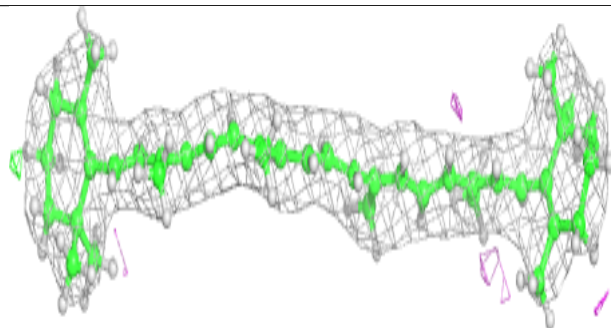
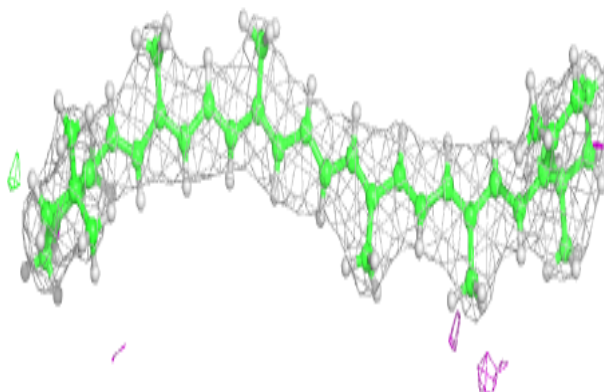


**Electron density around CLA d 402:**

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

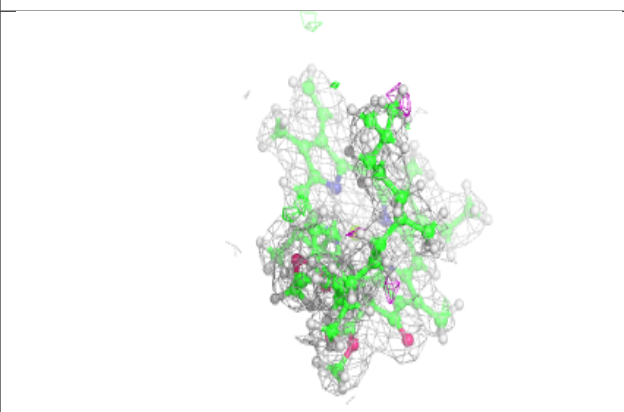
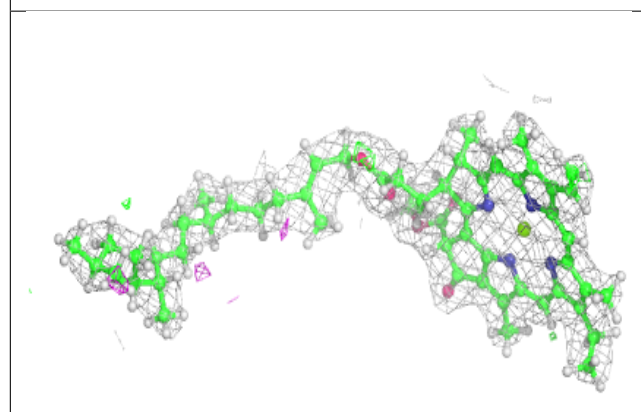
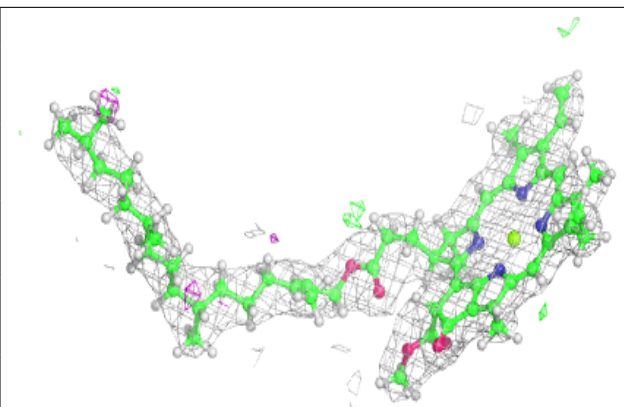
**Electron density around BCR a 406:**

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

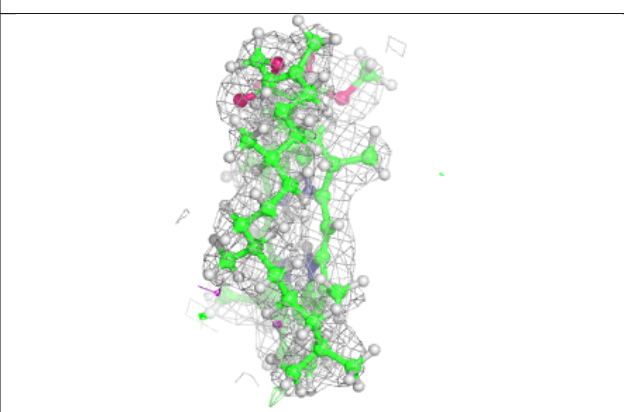
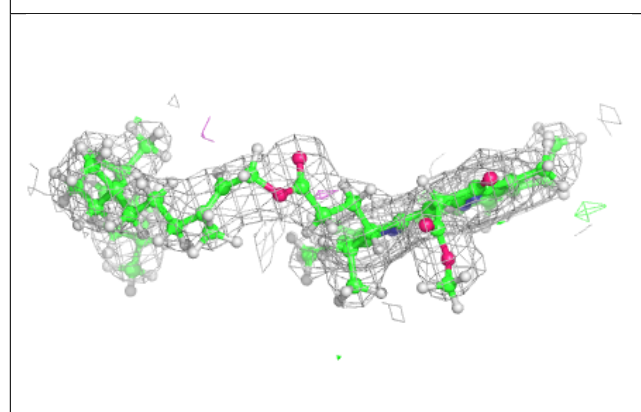
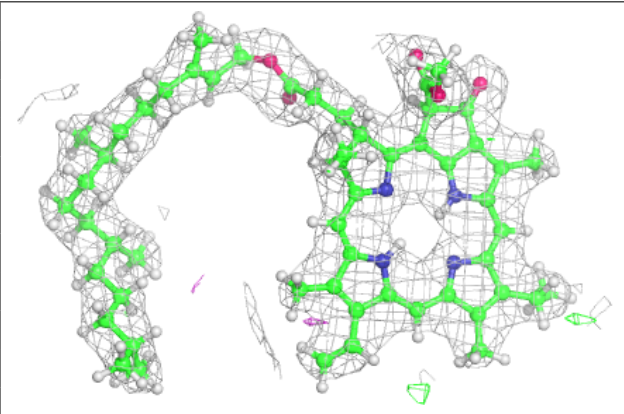


**Electron density around CLA A 402:**

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

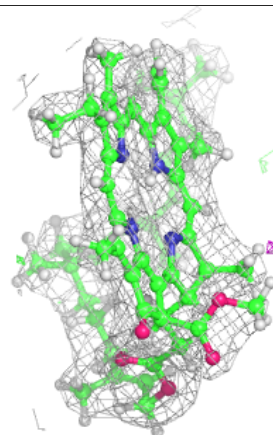
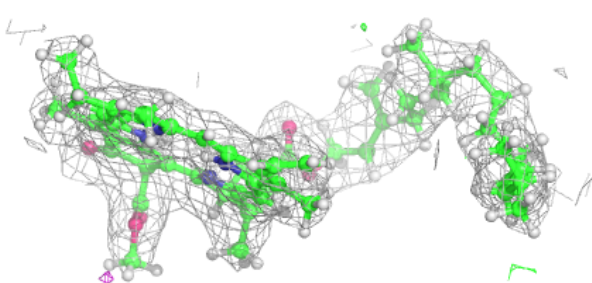
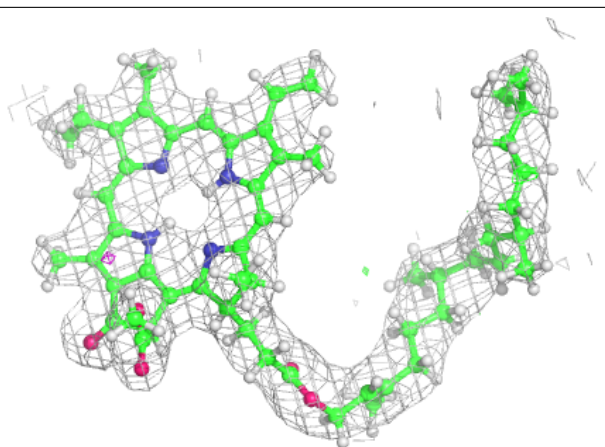
**Electron density around PHO A 404:**

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

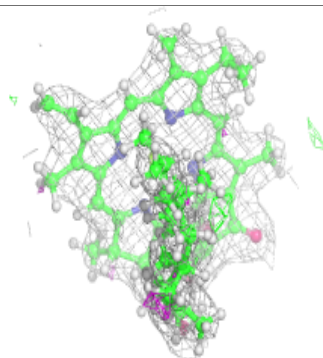
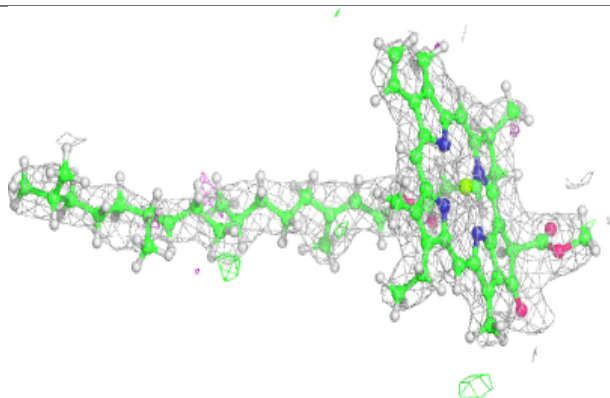
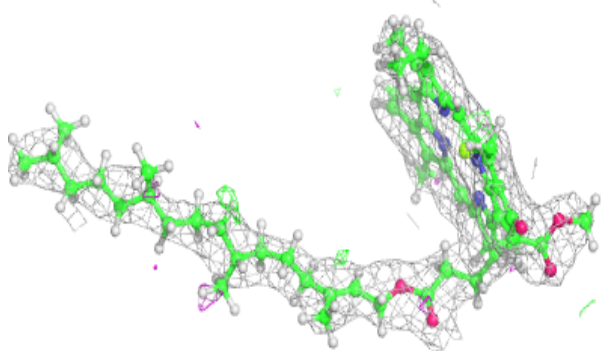


**Electron density around PHO D 401:**

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

**Electron density around CLA b 607:**

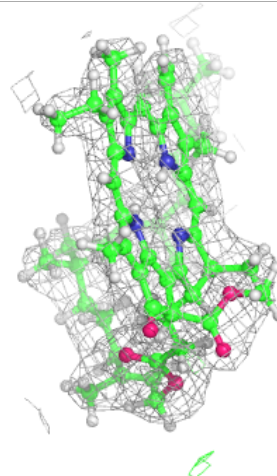
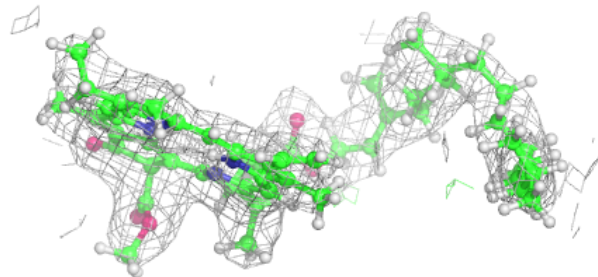
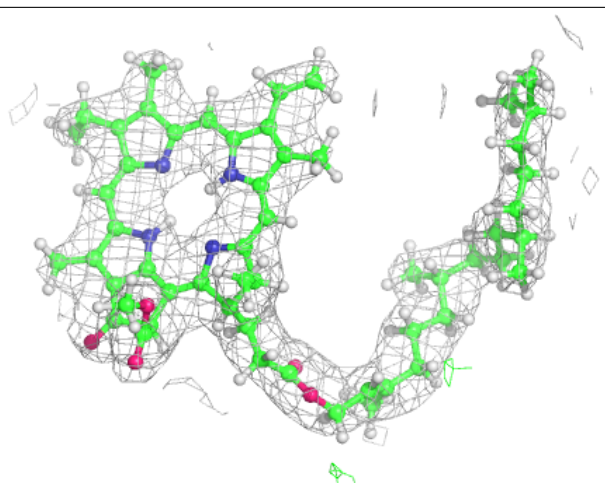
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





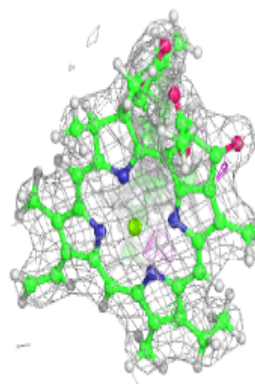
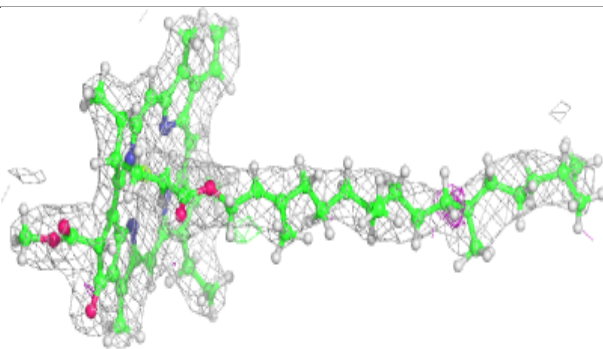
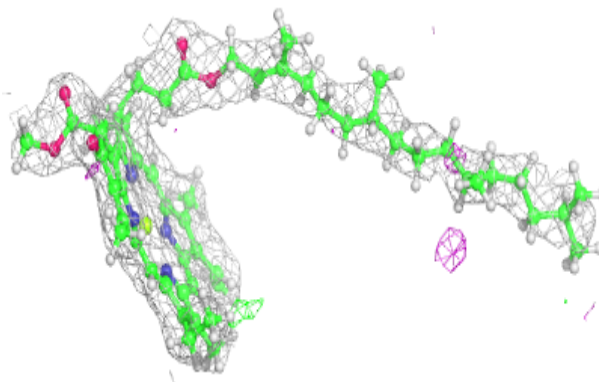
**Electron density around PHO d 401:**

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

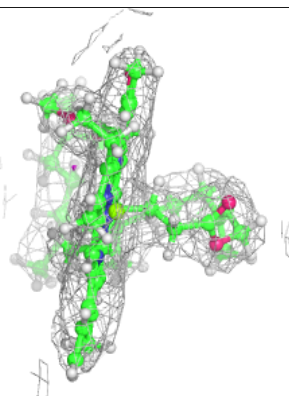
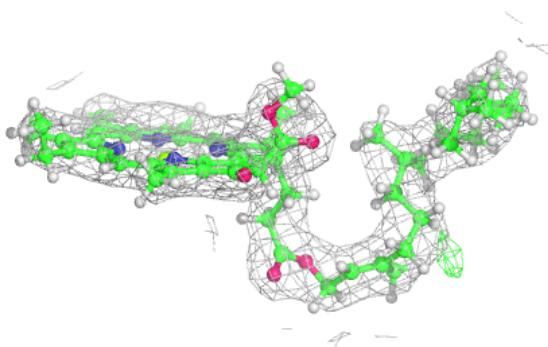
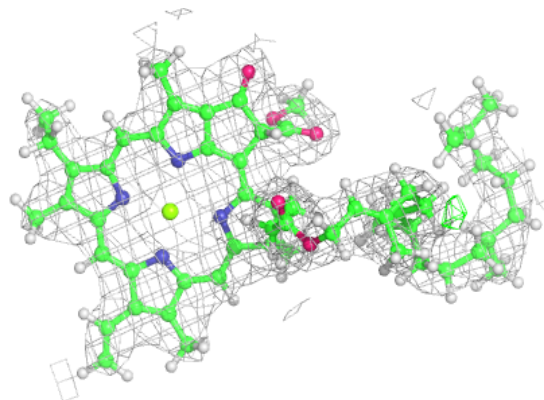


**Electron density around CLA B 607:**

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

**Electron density around CLA B 612:**

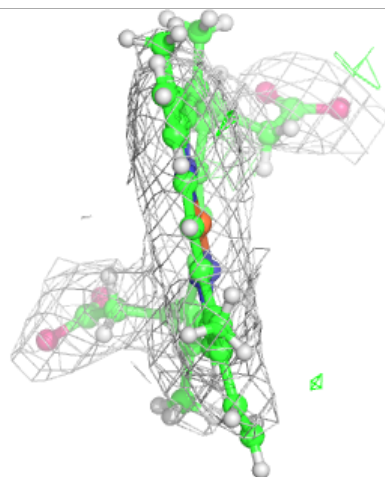
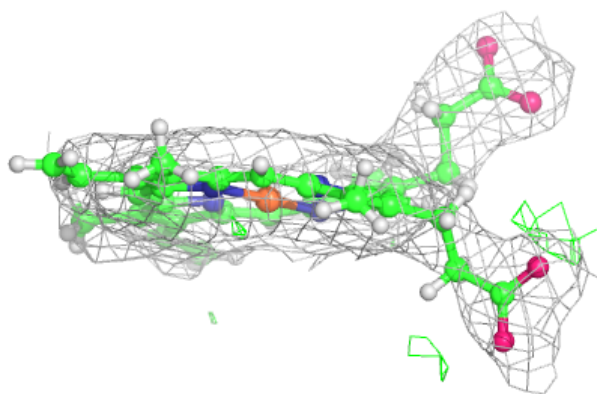
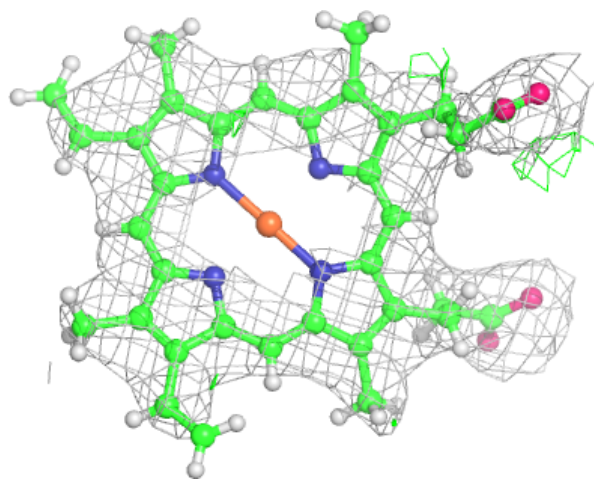
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





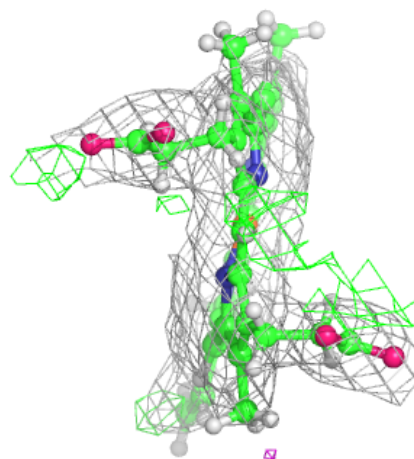
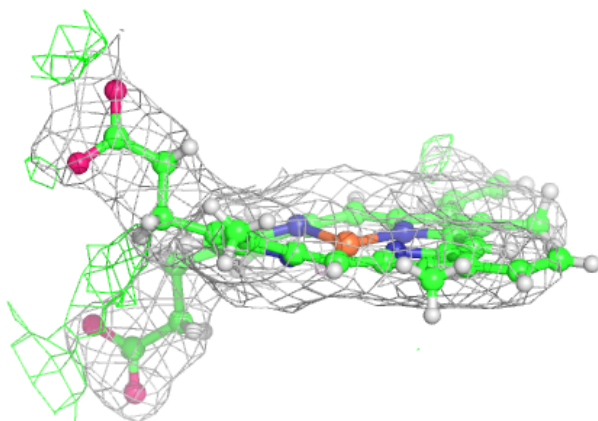
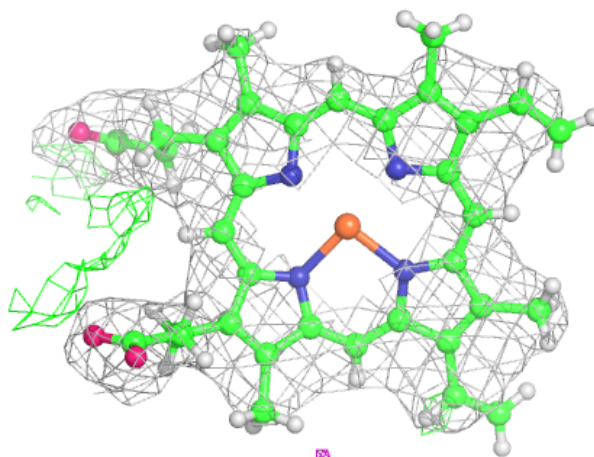
**Electron density around HEM F 101:**

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



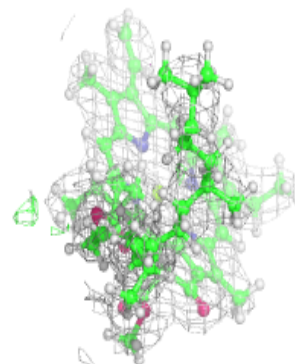
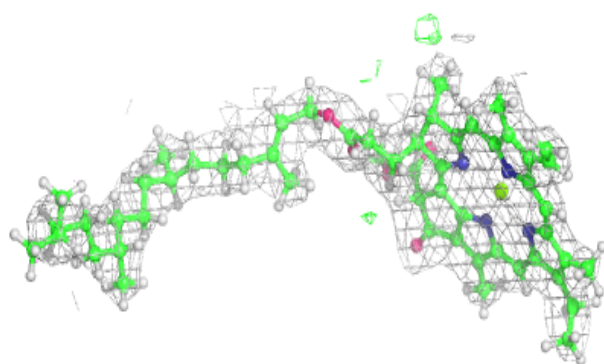
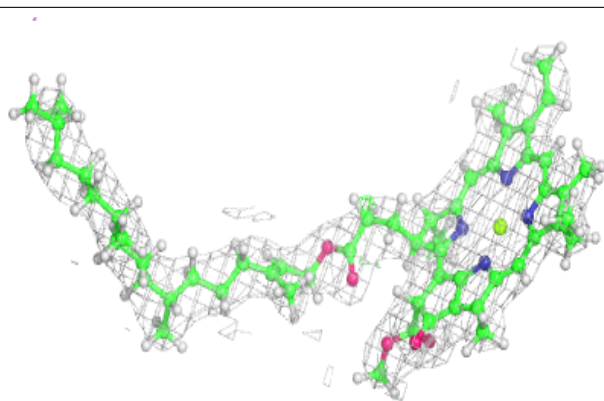
**Electron density around HEM e 101:**

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

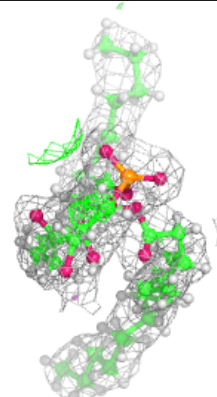
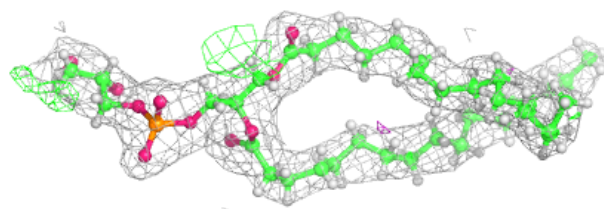
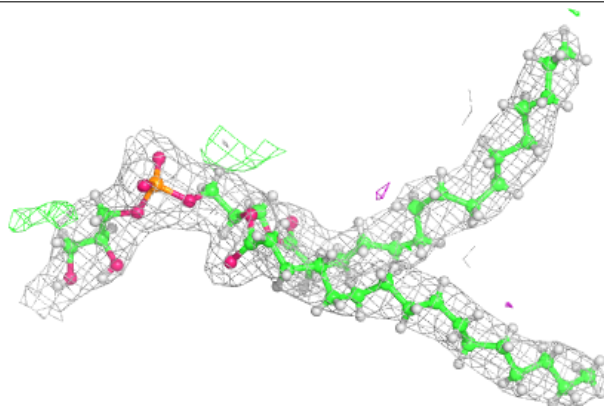


**Electron density around CLA a 402:**

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

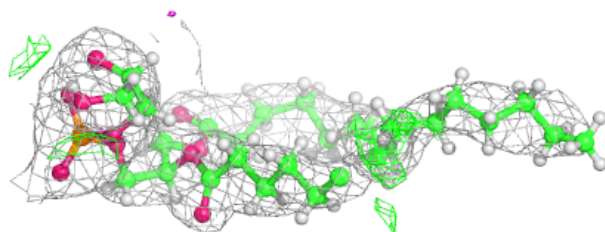
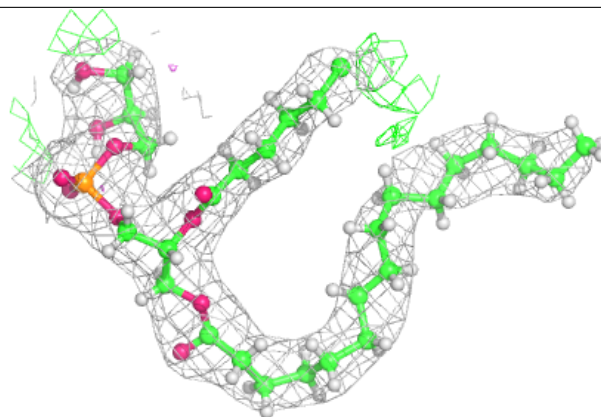
**Electron density around LHG d 406:**

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

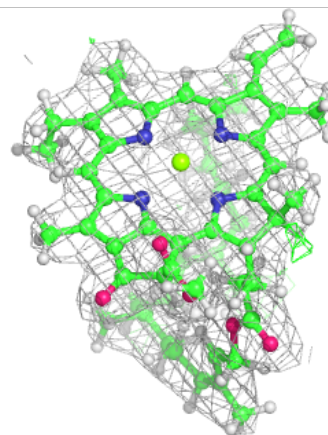
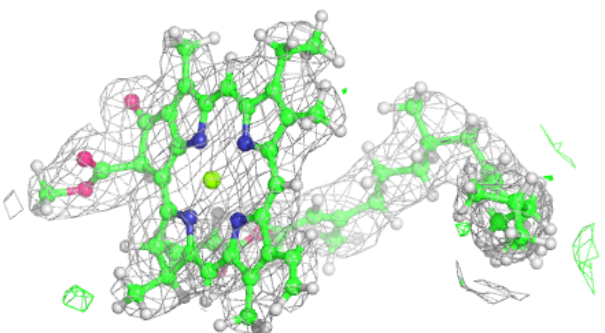
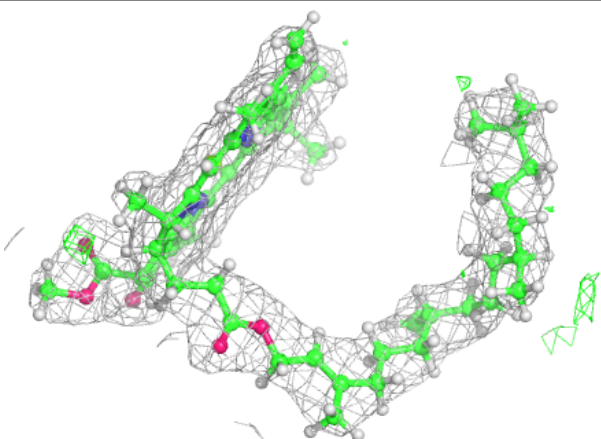


**Electron density around LHG d 407:**

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

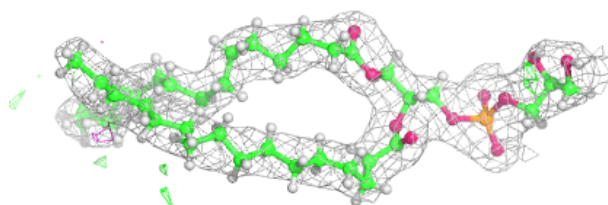
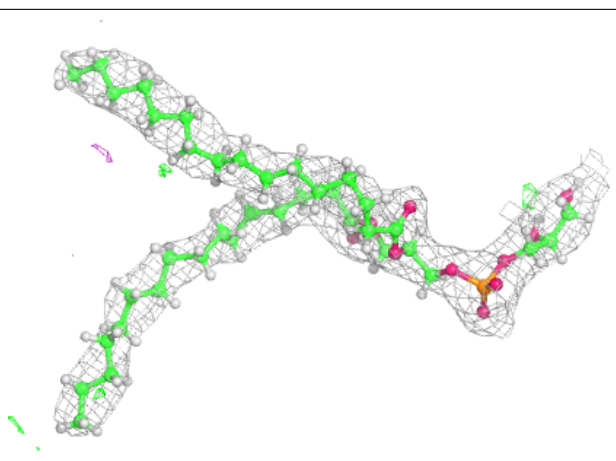
**Electron density around CLA B 611:**

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

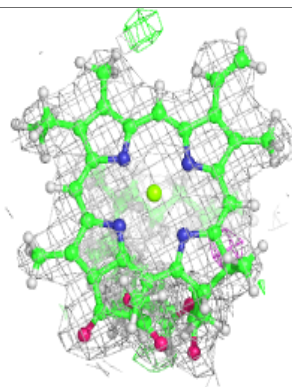
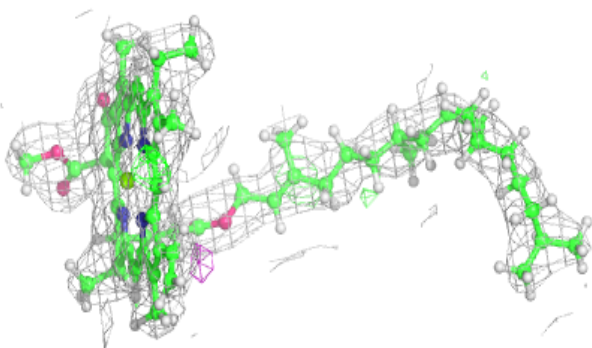
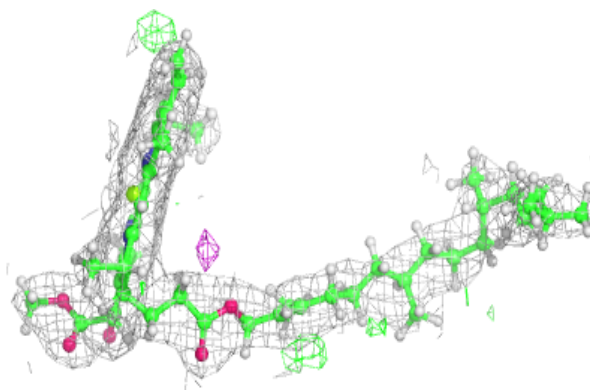


**Electron density around LHG D 409:**

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

**Electron density around CLA B 605:**

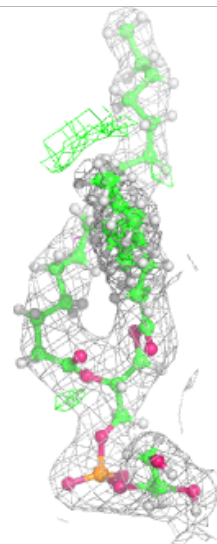
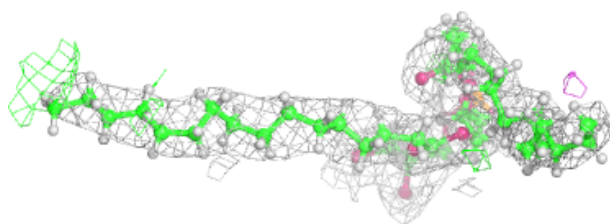
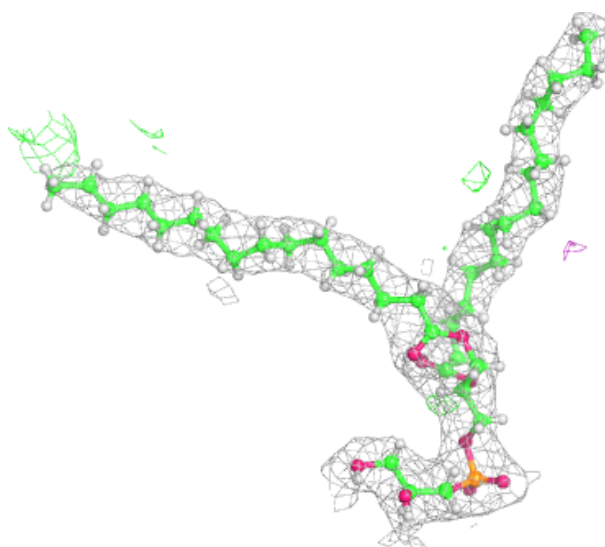
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





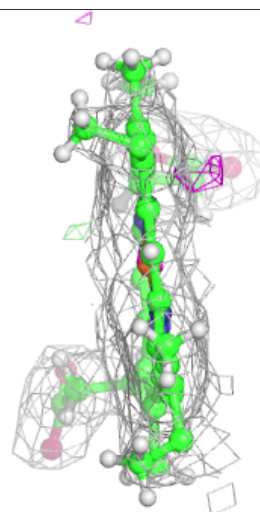
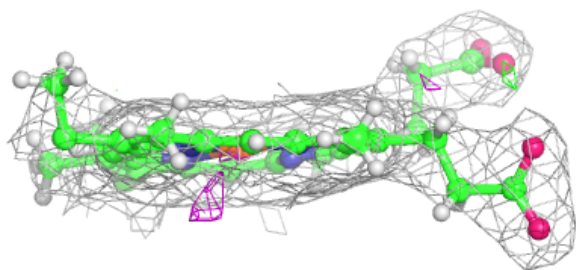
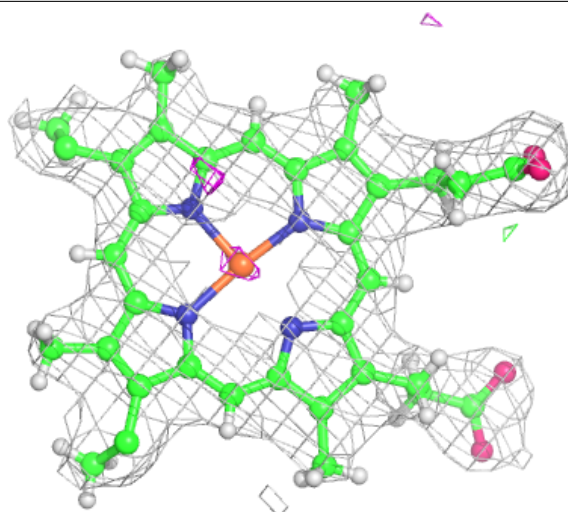
**Electron density around LHG L 102:**

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



**Electron density around HEC V 201:**

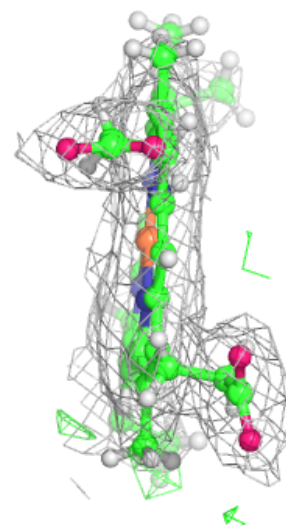
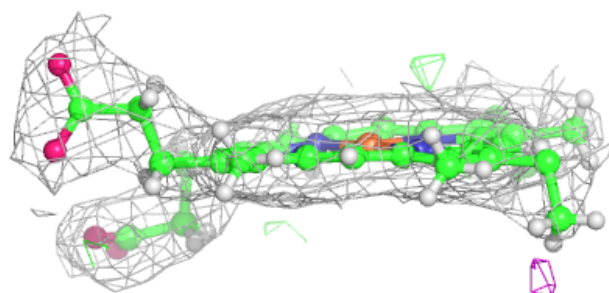
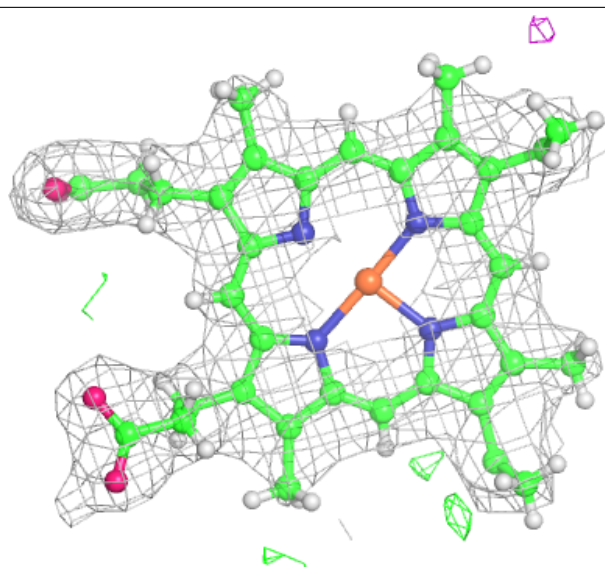
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC v 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.