



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 09:34 PM BST

PDB ID : 4UB6  
Title : Native structure of photosystem II (dataset-1) by a femtosecond X-ray laser  
Authors : Suga, M.; Akita, F.; Hirata, K.; Ueno, G.; Murakami, H.; Nakajima, Y.; Shimizu, T.; Yamashita, K.; Yamamoto, M.; Ago, H.; Shen, J.R.  
Deposited on : 2014-08-12  
Resolution : 1.95 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 ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

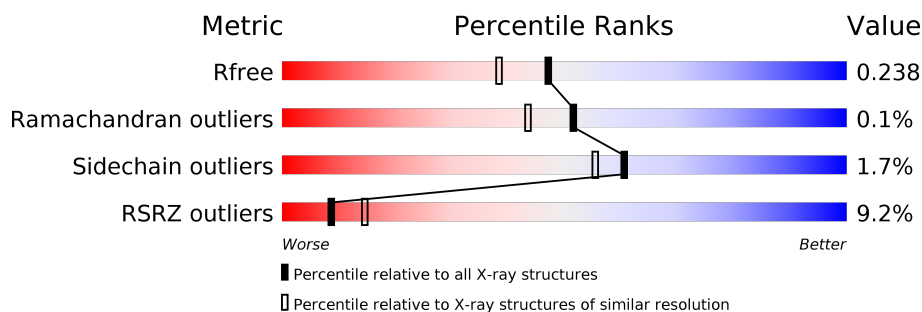
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2580 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>6%</div> <div>97%</div> </div>
1	a	344	<div> <div>10%</div> <div>96%</div> </div>
2	B	505	<div> <div>5%</div> <div>98%</div> </div>
2	b	505	<div> <div>7%</div> <div>98%</div> </div>
3	C	455	<div> <div>4%</div> <div>98%</div> </div>
3	c	455	<div> <div>6%</div> <div>99%</div> </div>
4	D	342	<div> <div>9%</div> <div>99%</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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Mol	Chain	Length	Quality of chain
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	407	X	-	-	-
24	CLA	A	410	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	401	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
28	GOL	V	203	-	-	-	X
36	DGD	d	406	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54195 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	6	0
			2645	1737	432	461	15			

- Molecule 2 is a protein called Photosystem II CP47 chlorophyll apoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	11	0
			4027	2643	668	703	13			
2	b	504	Total	C	N	O	S	0	12	0
			4033	2650	668	702	13			

- Molecule 3 is a protein called Photosystem II 44 kDa reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	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	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	0	0
			287	191	46	50				
18	x	39	Total	C	N	O		0	0	0
			287	191	46	50				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O		0	0	0
			273	186	47	40				

- 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		

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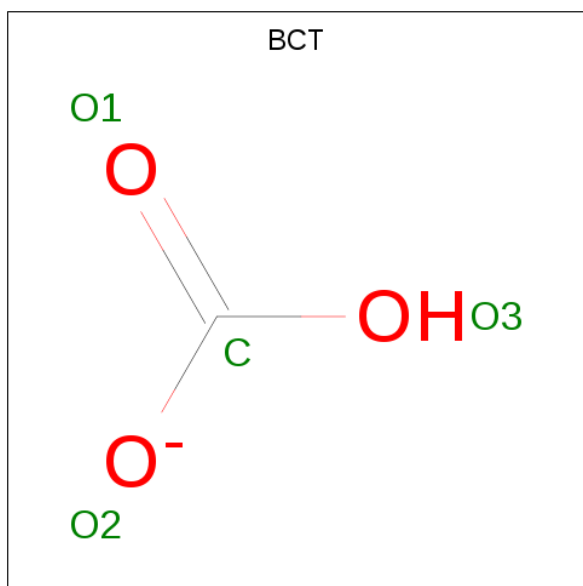
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

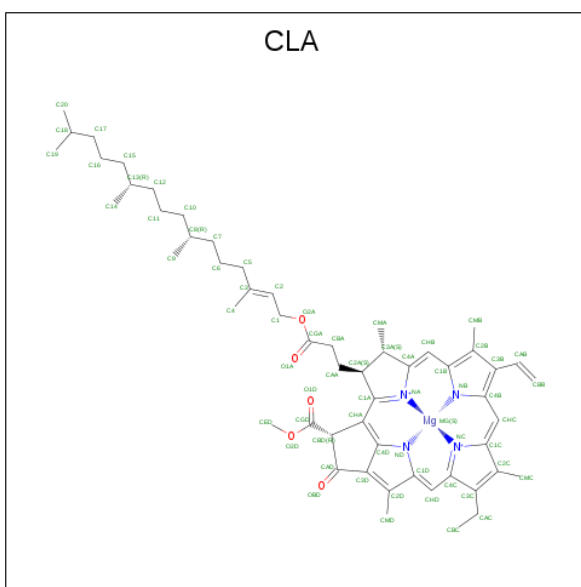
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$ ).

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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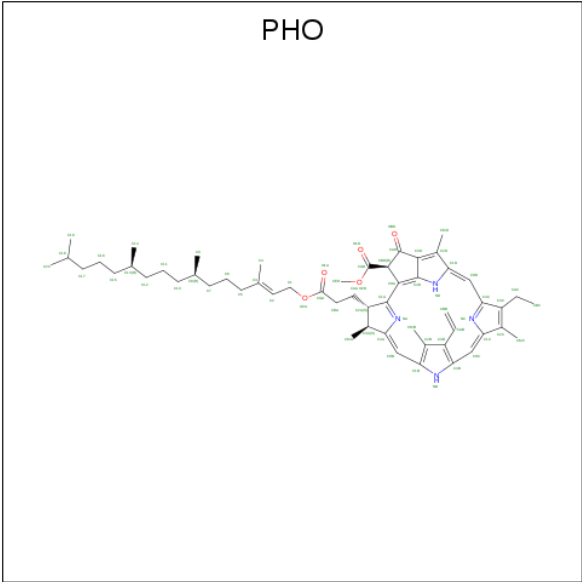
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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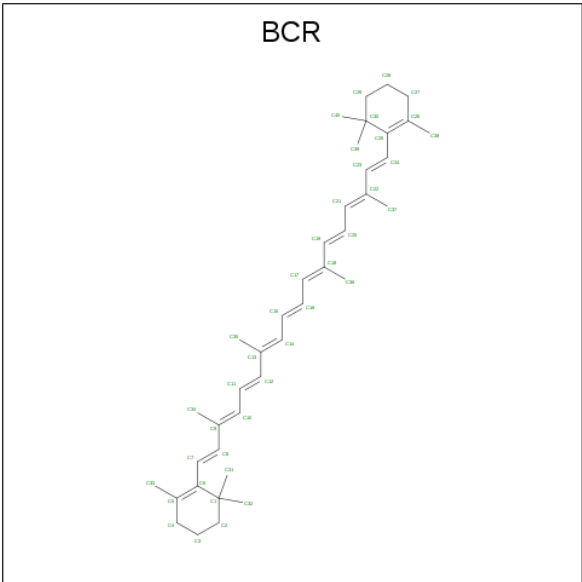
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



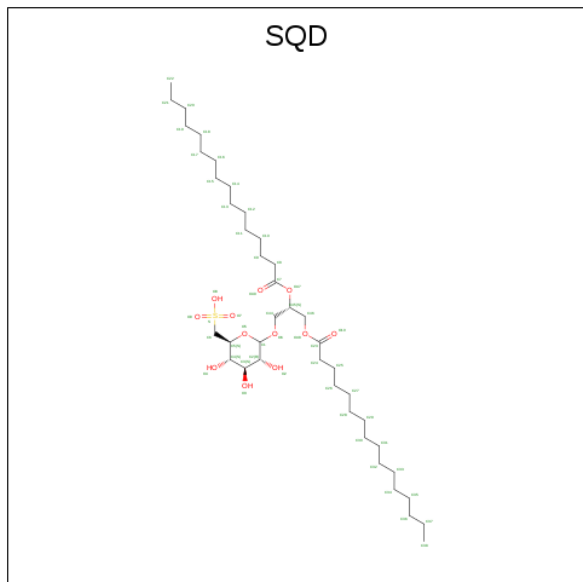
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	F	1	Total	C	O	0	0
			6	3	3		
28	O	1	Total	C	O	0	0
			6	3	3		

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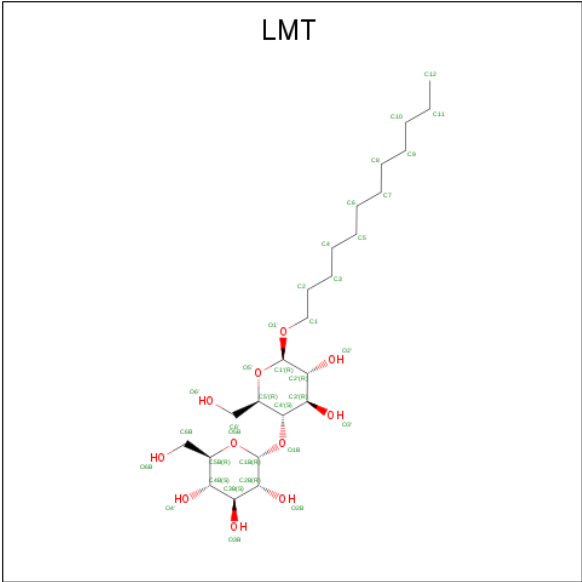
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	f	1	Total 6	C 3	O 3	0	0
28	o	1	Total 6	C 3	O 3	0	0
28	t	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



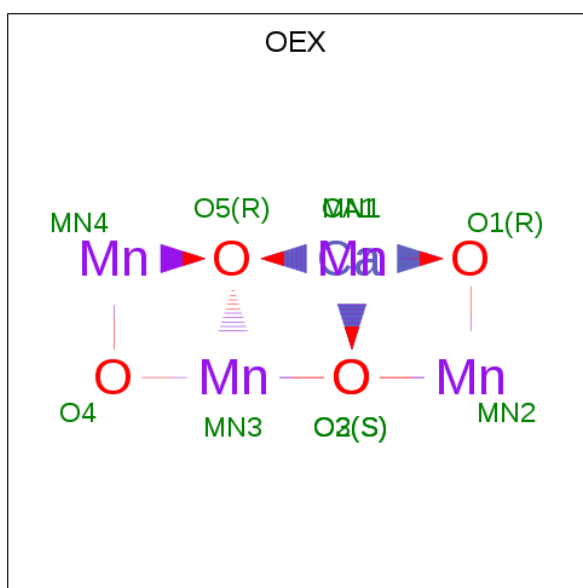
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	b	1	Total	C	O	0	0
			25	19	6		

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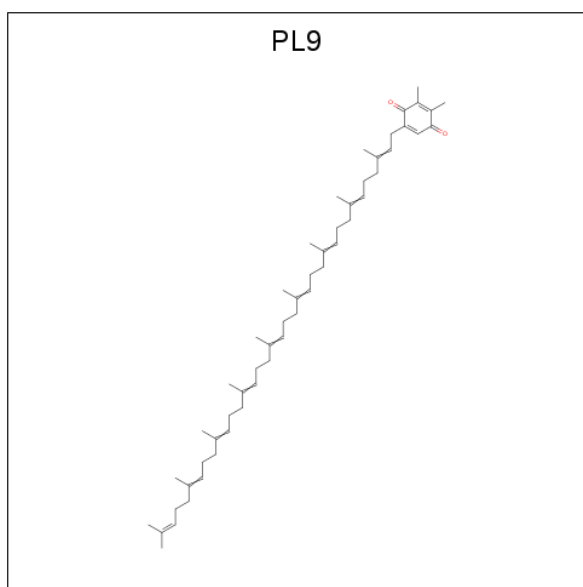
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	c	1	Total	C	O	0	0
			35	24	11		
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 31 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:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



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

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	a	1	Total	C	O	0	0
			30	25	5		

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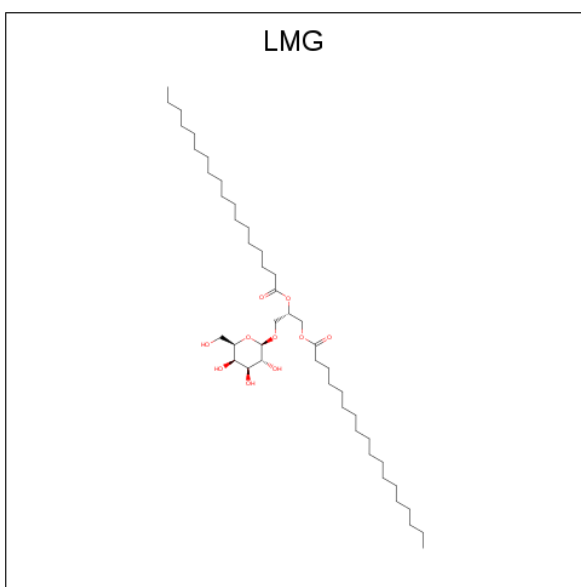
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	j	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	d	3	Total C O 71 63 8	0	0
32	m	1	Total C 10 10	0	0
32	b	1	Total C O 33 28 5	0	0
32	M	1	Total C 10 10	0	0

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

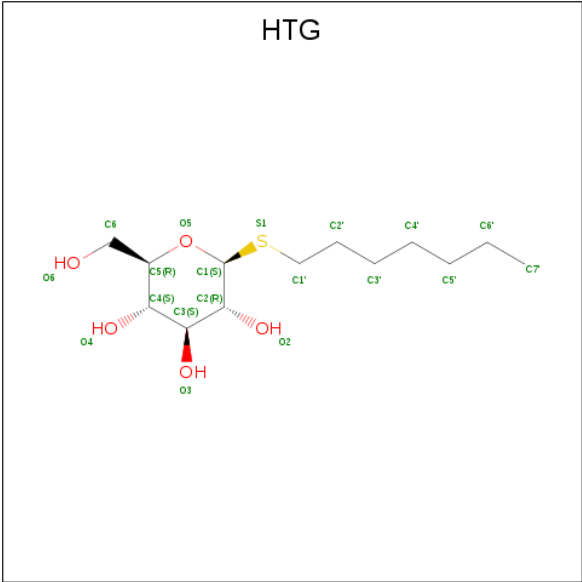
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	c	1	Total Ca 1 1	0	0
33	F	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0
33	O	1	Total Ca 1 1	0	0
33	b	1	Total Ca 1 1	0	0
33	f	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	b	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

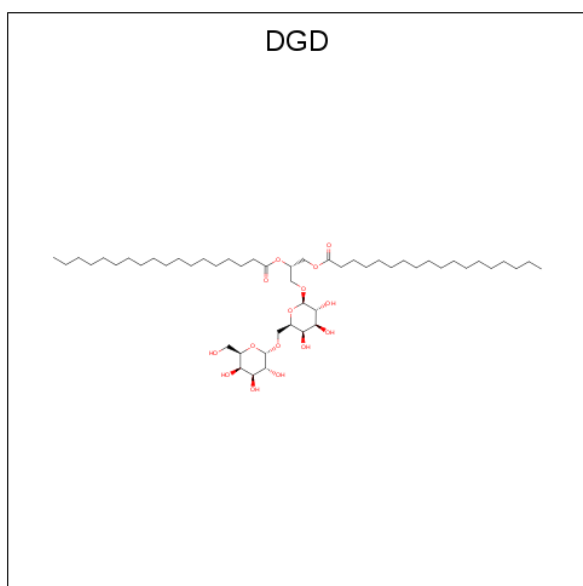
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



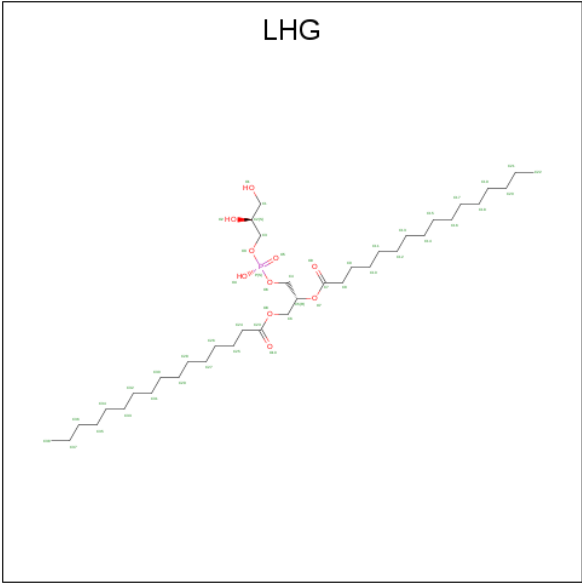
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	d	1	Total	C	O	0	0
			62	47	15		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



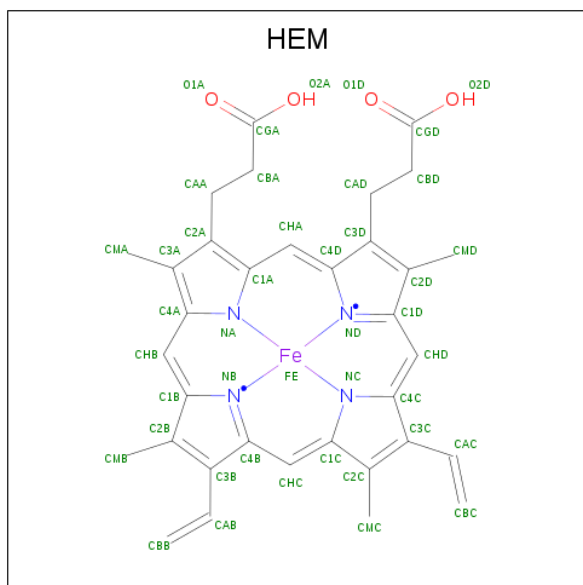
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	e	1	Total	C	O	P	0	0
			42	31	10	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	1	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).





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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	16	Total O 17 17	0	1
41	M	8	Total O 8 8	0	0
41	O	188	Total O 191 191	0	3
41	T	16	Total O 17 17	0	1
41	U	81	Total O 81 81	0	0
41	V	116	Total O 118 118	0	2
41	Y	4	Total O 4 4	0	0
41	X	9	Total O 9 9	0	0
41	Z	1	Total O 1 1	0	0
41	a	153	Total O 154 154	0	1
41	b	261	Total O 264 264	0	3
41	c	197	Total O 199 199	0	2
41	d	132	Total O 137 137	0	5
41	e	17	Total O 17 17	0	0
41	f	5	Total O 5 5	0	0
41	h	41	Total O 41 41	0	0
41	i	6	Total O 6 6	0	0
41	j	7	Total O 7 7	0	0
41	k	6	Total O 6 6	0	0
41	l	10	Total O 10 10	0	0
41	m	18	Total O 18 18	0	0

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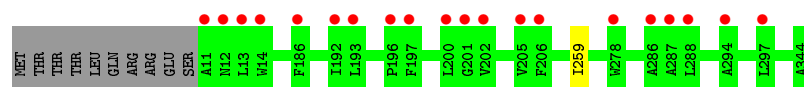
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	154	Total 155	O 155	0	1
41	t	12	Total 12	O 12	0	0
41	u	97	Total 97	O 97	0	0
41	v	89	Total 90	O 90	0	1
41	y	4	Total 4	O 4	0	0
41	x	4	Total 4	O 4	0	0

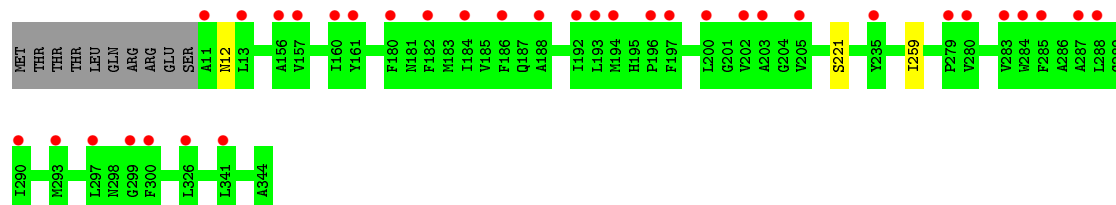
### 3 Residue-property plots

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.

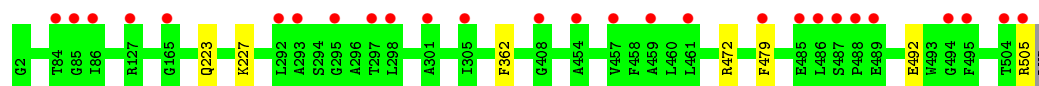
- Molecule 1: Photosystem Q(B) protein



- Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

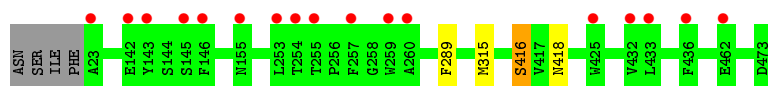


- Molecule 2: Photosystem II CP47 chlorophyll apoprotein

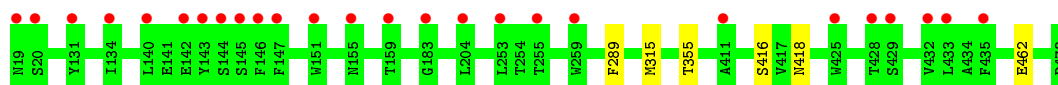


- Molecule 3: Photosystem II 44 kDa reaction center protein

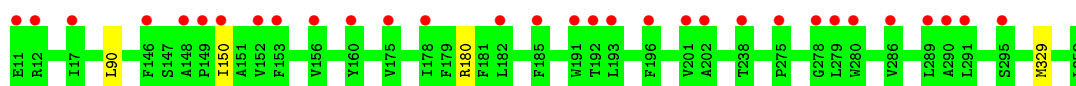




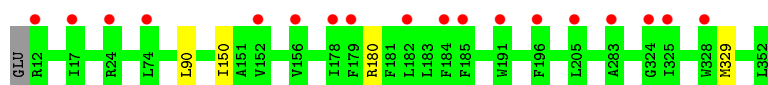
- Molecule 3: Photosystem II 44 kDa reaction center protein



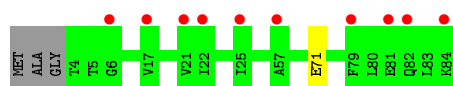
- Molecule 4: Photosystem II D2 protein



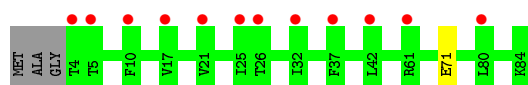
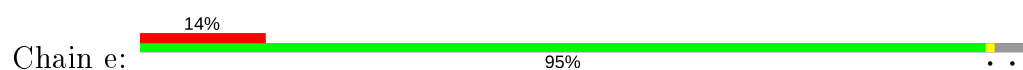
- Molecule 4: Photosystem II D2 protein



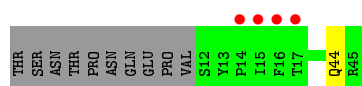
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

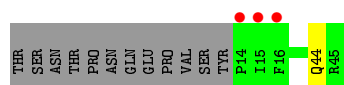


- Molecule 6: Cytochrome b559 subunit beta

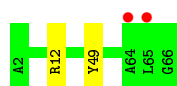


- Molecule 6: Cytochrome b559 subunit beta

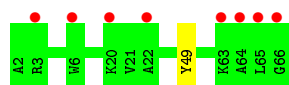




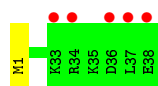
- Molecule 7: Photosystem II reaction center protein H



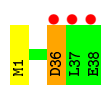
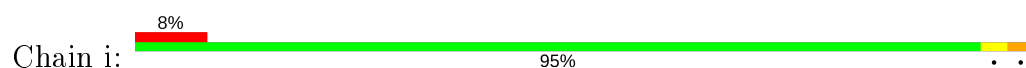
- Molecule 7: Photosystem II reaction center protein H



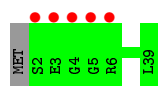
- Molecule 8: Photosystem II reaction center protein I



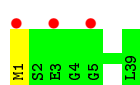
- Molecule 8: Photosystem II reaction center protein I



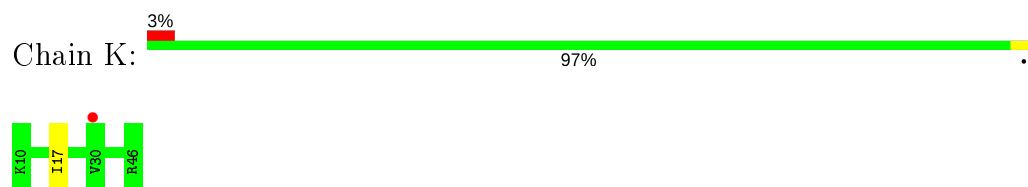
- Molecule 9: Photosystem II reaction center protein J



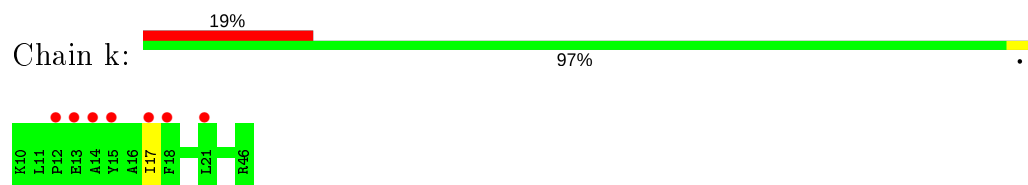
- Molecule 9: Photosystem II reaction center protein J



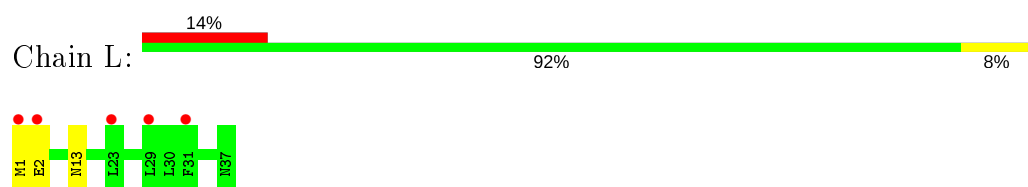
- Molecule 10: Photosystem II reaction center protein K



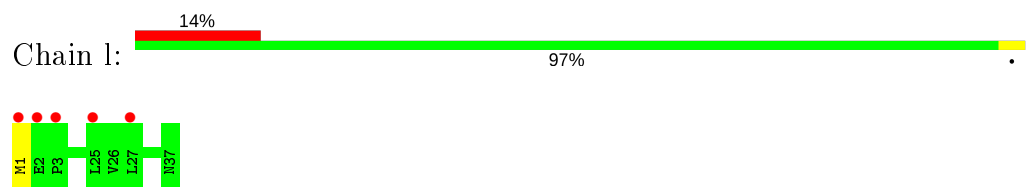
- Molecule 10: Photosystem II reaction center protein K



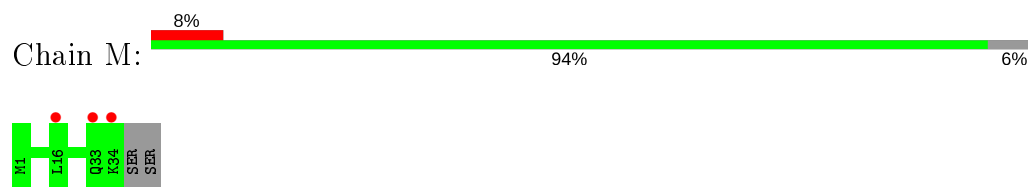
- Molecule 11: Photosystem II reaction center protein L



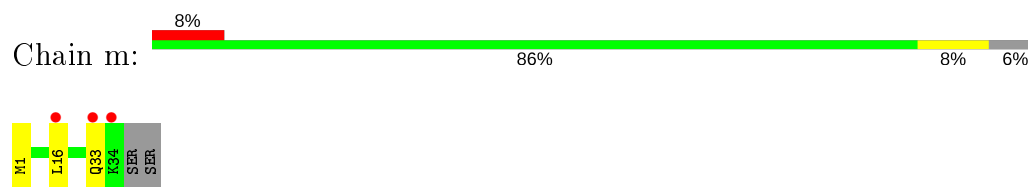
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

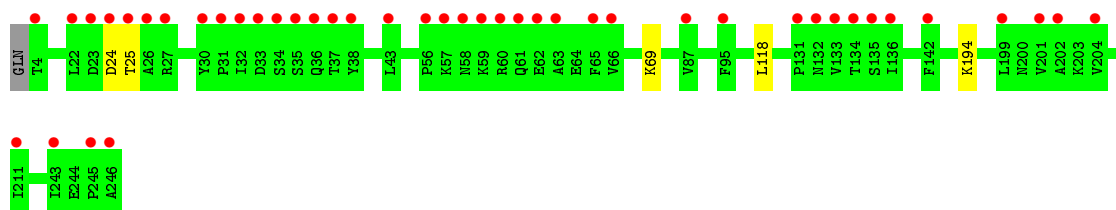


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

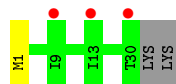
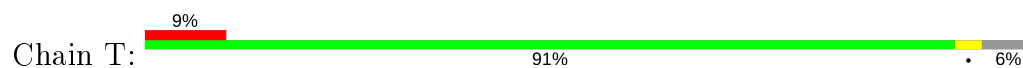




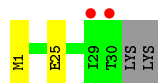
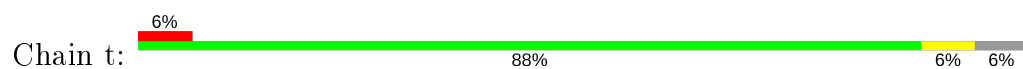
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



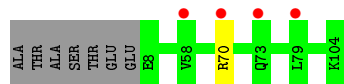
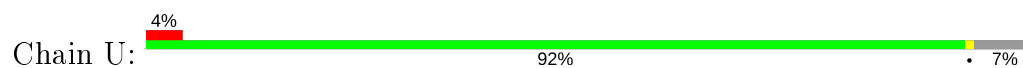
- Molecule 14: Photosystem II reaction center protein T



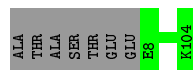
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



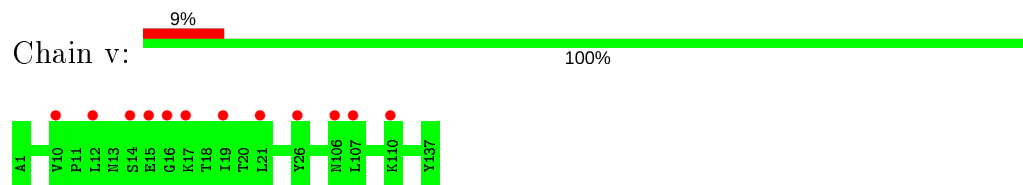
- Molecule 15: Photosystem II 12 kDa extrinsic protein



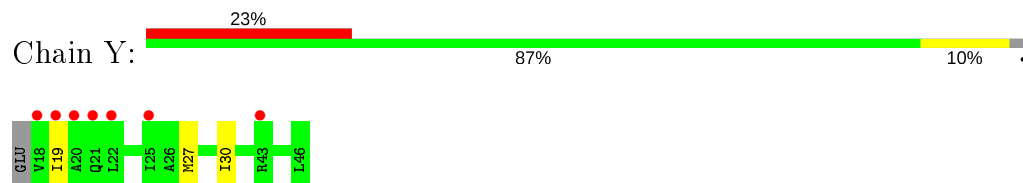
- Molecule 16: Cytochrome c-550



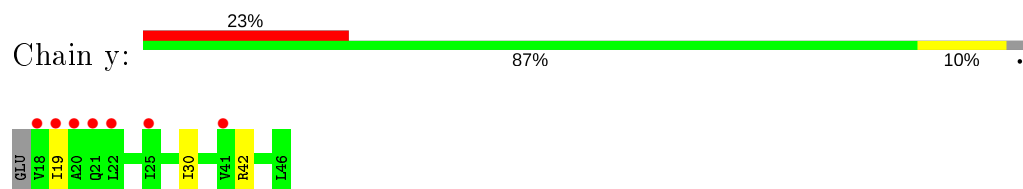
- Molecule 16: Cytochrome c-550



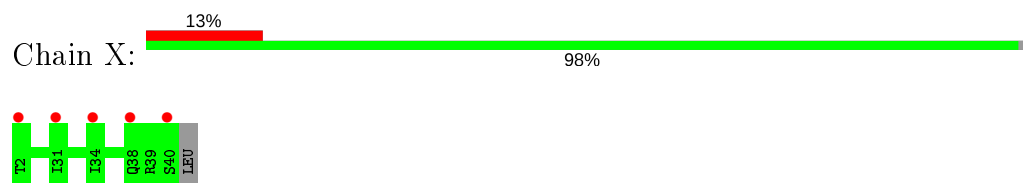
- Molecule 17: Photosystem II reaction center protein Ycf12



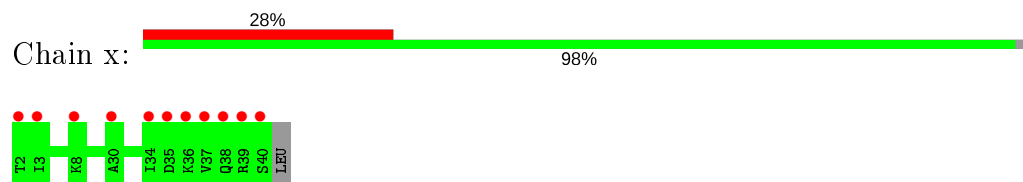
- Molecule 17: Photosystem II reaction center protein Ycf12



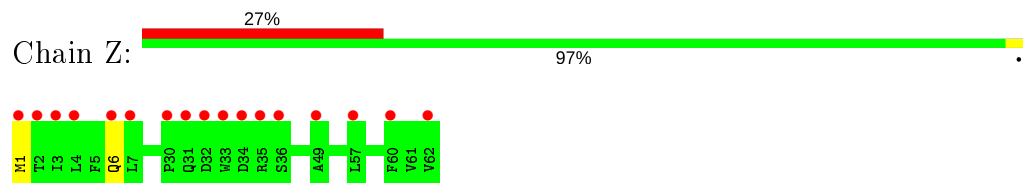
- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X

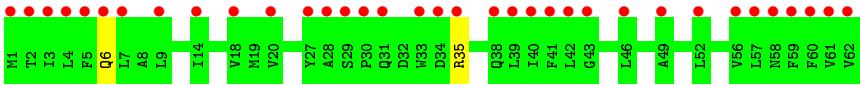


- Molecule 19: Photosystem II reaction center protein Z

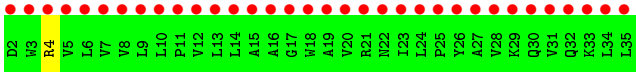


- Molecule 19: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.74Å 229.99Å 288.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.29 – 1.95 62.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (62.29-1.95) 92.0 (62.29-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.67 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.198 , 0.238 0.198 , 0.238	Depositor DCC
$R_{free}$ test set	29338 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	54195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, LMG, FE2, HEC, BCT, HEM, FME, UNL, HTG, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.52	0/2728	0.59	0/3719
1	a	0.52	0/2748	0.57	0/3746
2	B	0.49	0/4200	0.56	0/5721
2	b	0.47	0/4209	0.56	0/5734
3	C	0.45	0/3626	0.54	0/4936
3	c	0.45	0/3676	0.53	0/5004
4	D	0.53	0/2827	0.57	0/3852
4	d	0.51	0/2818	0.56	0/3840
5	E	0.37	0/693	0.54	0/944
5	e	0.35	0/695	0.50	0/948
6	F	0.40	0/284	0.52	0/387
6	f	0.39	0/265	0.52	0/360
7	H	0.37	0/535	0.53	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.38	0/311	0.55	0/419
8	i	0.38	0/311	0.51	0/419
9	J	0.42	0/278	0.47	0/376
9	j	0.41	0/286	0.47	0/386
10	K	0.33	0/303	0.52	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.47	0/319	0.51	0/433
11	l	0.45	0/319	0.50	0/433
12	M	0.45	0/270	0.58	0/368
12	m	0.55	0/262	0.63	0/357
13	O	0.40	0/1958	0.58	0/2654
13	o	0.39	0/1937	0.58	0/2625
14	T	0.55	0/266	0.54	0/362
14	t	0.56	0/266	0.57	0/362
15	U	0.45	0/785	0.58	0/1064
15	u	0.42	0/785	0.56	0/1064
16	V	0.42	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.39	0/1085	0.52	0/1473
17	Y	0.32	0/216	0.46	0/289
17	y	0.33	0/216	0.51	0/289
18	X	0.37	0/290	0.42	0/392
18	x	0.35	0/290	0.46	0/392
19	Z	0.33	0/490	0.43	0/669
19	z	0.33	0/490	0.45	0/669
20	R	0.26	0/279	0.38	0/383
All	All	0.46	0/43239	0.55	0/58829

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	335/344 (97%)	331 (99%)	3 (1%)	1 (0%)	41	30
1	a	338/344 (98%)	333 (98%)	4 (1%)	1 (0%)	41	30
2	B	513/505 (102%)	506 (99%)	7 (1%)	0	100	100
2	b	514/505 (102%)	506 (98%)	8 (2%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	34	22
3	c	459/455 (101%)	445 (97%)	12 (3%)	2 (0%)	34	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	1
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	240 (96%)	8 (3%)	1 (0%)	34	22
13	o	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5290/5384 (98%)	5170 (98%)	112 (2%)	8 (0%)	51	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
13	O	62	GLU
8	i	36	ASP
1	a	259	ILE
1	A	259	ILE

### 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	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	272 (99%)	3 (1%)	73	71
2	B	413/403 (102%)	405 (98%)	8 (2%)	57	50
2	b	414/403 (103%)	406 (98%)	8 (2%)	57	50
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	62
3	c	362/356 (102%)	356 (98%)	6 (2%)	60	55
4	D	278/277 (100%)	274 (99%)	4 (1%)	67	62
4	d	277/277 (100%)	273 (99%)	4 (1%)	67	62
5	E	74/73 (101%)	73 (99%)	1 (1%)	67	62
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	62
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	21
7	H	55/54 (102%)	52 (94%)	3 (6%)	21	9
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	50
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	31
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	22
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	26
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	26
11	L	36/35 (103%)	33 (92%)	3 (8%)	11	3
11	l	36/35 (103%)	35 (97%)	1 (3%)	43	33
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	16	5
13	O	214/207 (103%)	210 (98%)	4 (2%)	57	50
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	40
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	4
15	U	84/89 (94%)	83 (99%)	1 (1%)	71	68
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	80
16	v	117/117 (100%)	117 (100%)	0	100	100
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3	0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	0
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	32/33 (97%)	32 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	21
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	21
20	R	29/29 (100%)	28 (97%)	1 (3%)	37	25
All	All	4395/4403 (100%)	4315 (98%)	80 (2%)	60	53

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	223[A]	GLN
2	B	223[B]	GLN
2	B	227	LYS
2	B	362	PHE
2	B	472	ARG
2	B	479	PHE
2	B	492	GLU
2	B	505	ARG
3	C	289	PHE
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER
3	C	418	ASN
4	D	90	LEU
4	D	150	ILE
4	D	180	ARG
4	D	329	MET
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	17	ILE
11	L	1	MET
11	L	2	GLU
11	L	13	ASN
13	O	49[A]	THR
13	O	49[B]	THR
13	O	118	LEU
13	O	194	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	19	ILE
17	Y	27	MET
17	Y	30	ILE
19	Z	1	MET
19	Z	6	GLN
20	R	4	ARG
1	a	12	ASN
1	a	221[A]	SER
1	a	221[B]	SER
2	b	53	ASN
2	b	84	THR

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Mol	Chain	Res	Type
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	485	GLU
2	b	491	VAL
2	b	505	ARG
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	150	ILE
4	d	180	ARG
4	d	329	MET
5	e	71	GLU
6	f	44	GLN
7	h	49	TYR
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
11	l	1	MET
12	m	16	LEU
12	m	33	GLN
13	o	24	ASP
13	o	25	THR
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
17	y	19	ILE
17	y	30	ILE
17	y	42	ARG
19	z	6	GLN
19	z	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	331	ASN
2	B	490	GLN
4	D	83	ASN
4	D	332	GLN
6	F	44	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN
16	V	86	GLN
19	Z	31	GLN
19	Z	58	ASN
1	a	315	ASN
2	b	53	ASN
2	b	289	GLN
2	b	331	ASN
2	b	490	GLN
3	c	201	ASN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
5	e	75	GLN
6	f	44	GLN
13	o	124	ASN
13	o	147	ASN
16	v	118	HIS
19	z	6	GLN
19	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	0.69	0	7,9,11	1.37	1 (14%)
12	FME	M	1	12	8,9,10	0.65	0	7,9,11	1.11	0
12	FME	m	1	12	8,9,10	0.72	0	7,9,11	1.11	1 (14%)
14	FME	T	1	14	8,9,10	0.64	0	7,9,11	1.56	1 (14%)
8	FME	I	1	8	8,9,10	0.57	0	7,9,11	1.32	2 (28%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	2.10	4 (57%)

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	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.07	115.27	109.73
14	T	1	FME	C-CA-N	2.67	114.55	109.73
14	t	1	FME	O-C-CA	-2.63	117.88	124.78
14	t	1	FME	CA-N-CN	-2.56	118.89	122.82
8	I	1	FME	O-C-CA	-2.36	118.59	124.78
8	i	1	FME	CA-N-CN	-2.29	119.30	122.82
8	I	1	FME	CA-N-CN	-2.19	119.45	122.82
12	m	1	FME	O-C-CA	-2.16	119.12	124.78
14	t	1	FME	CE-SD-CG	-2.00	93.52	100.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	N-CA-CB-CG
14	t	1	FME	O1-CN-N-CA
14	T	1	FME	C-CA-CB-CG
12	M	1	FME	CA-CB-CG-SD
8	I	1	FME	CA-CB-CG-SD
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 251 ligands modelled in this entry, 18 are unknown and 17 are monoatomic - leaving 216 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	$\# Z  > 2$
35	HTG	B	625	-	19,19,19	0.83	1 (5%)	23,24,24	1.18	2 (8%)
36	DGD	D	405	-	63,63,67	0.98	3 (4%)	77,77,81	1.24	7 (9%)
24	CLA	c	904	-	59,73,73	1.96	13 (22%)	67,113,113	2.18	21 (31%)
24	CLA	C	506	-	59,73,73	2.02	14 (23%)	67,113,113	2.20	19 (28%)
27	SQD	f	102	-	42,43,54	1.17	3 (7%)	51,54,65	1.45	8 (15%)
26	BCR	A	411	-	41,41,41	1.02	1 (2%)	56,56,56	1.22	5 (8%)
24	CLA	C	503	-	59,73,73	2.00	13 (22%)	67,113,113	2.22	23 (34%)
27	SQD	A	412	-	53,54,54	0.99	3 (5%)	62,65,65	1.77	12 (19%)
28	GOL	b	629	-	5,5,5	0.34	0	5,5,5	0.15	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	609	-	59,73,73	1.98	12 (20%)	67,113,113	2.30	22 (32%)
24	CLA	D	401	-	59,73,73	1.95	13 (22%)	67,113,113	2.23	21 (31%)
36	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	1.22	6 (7%)
24	CLA	a	407	41	59,73,73	1.98	13 (22%)	67,113,113	2.28	26 (38%)
24	CLA	A	410	-	59,73,73	2.05	12 (20%)	67,113,113	2.10	24 (35%)
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	618	-	59,73,73	1.97	13 (22%)	67,113,113	2.34	23 (34%)
25	PHO	a	408	-	67,69,69	2.02	15 (22%)	85,99,99	1.90	20 (23%)
26	BCR	c	915	-	41,41,41	1.07	1 (2%)	56,56,56	1.43	9 (16%)
26	BCR	T	102	-	41,41,41	0.97	1 (2%)	56,56,56	1.38	11 (19%)
29	LMT	E	102	-	36,36,36	0.48	0	47,47,47	0.86	0
24	CLA	C	513	-	59,73,73	2.00	12 (20%)	67,113,113	2.25	26 (38%)
24	CLA	b	605	41	59,73,73	2.04	12 (20%)	67,113,113	2.14	19 (28%)
28	GOL	b	630	-	5,5,5	0.32	0	5,5,5	0.52	0
25	PHO	a	420	-	67,69,69	2.19	17 (25%)	85,99,99	1.98	20 (23%)
24	CLA	C	505	41	59,73,73	2.04	13 (22%)	67,113,113	2.20	22 (32%)
24	CLA	B	615	-	59,73,73	1.98	13 (22%)	67,113,113	2.33	25 (37%)
28	GOL	b	632	-	5,5,5	0.37	0	5,5,5	0.56	0
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.46	7 (14%)
24	CLA	B	602	41	59,73,73	2.00	14 (23%)	67,113,113	2.18	24 (35%)
26	BCR	b	621	-	41,41,41	1.12	1 (2%)	56,56,56	1.19	2 (3%)
29	LMT	c	921	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
24	CLA	B	607	-	59,73,73	2.04	14 (23%)	67,113,113	2.37	23 (34%)
24	CLA	B	612	-	59,73,73	2.02	13 (22%)	67,113,113	2.15	22 (32%)
28	GOL	b	631	-	5,5,5	0.33	0	5,5,5	0.46	0
38	HEM	e	102	5,6	27,50,50	0.83	1 (3%)	17,82,82	2.15	3 (17%)
28	GOL	b	633	-	5,5,5	0.36	0	5,5,5	0.35	0
24	CLA	b	619	-	59,73,73	2.03	12 (20%)	67,113,113	2.26	23 (34%)
24	CLA	d	402	-	59,73,73	1.92	14 (23%)	67,113,113	2.36	22 (32%)
28	GOL	b	628	-	5,5,5	0.36	0	5,5,5	0.30	0
24	CLA	c	914	-	59,73,73	2.00	13 (22%)	67,113,113	2.06	22 (32%)
24	CLA	c	911	-	59,73,73	2.02	13 (22%)	67,113,113	2.15	22 (32%)
26	BCR	a	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	5 (8%)
36	DGD	H	102	-	63,63,67	0.94	3 (4%)	77,77,81	0.93	4 (5%)
27	SQD	B	621	-	53,54,54	1.05	4 (7%)	62,65,65	1.48	9 (14%)
31	PL9	d	405	-	55,55,55	0.73	2 (3%)	68,69,69	1.55	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	608	41	59,73,73	2.04	13 (22%)	67,113,113	2.13	20 (29%)
28	GOL	B	629	-	5,5,5	0.41	0	5,5,5	0.56	0
28	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.61	0
28	GOL	C	526	-	5,5,5	0.22	0	5,5,5	0.43	0
29	LMT	C	522	-	36,36,36	0.48	0	47,47,47	1.27	5 (10%)
26	BCR	k	101	-	41,41,41	1.10	1 (2%)	56,56,56	1.46	10 (17%)
37	LHG	d	407	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	4 (7%)
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
28	GOL	A	413	-	5,5,5	0.25	0	5,5,5	0.52	0
24	CLA	B	606	-	59,73,73	1.98	12 (20%)	67,113,113	2.27	21 (31%)
36	DGD	c	917	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	2 (2%)
24	CLA	B	604	-	59,73,73	2.04	13 (22%)	67,113,113	2.33	22 (32%)
28	GOL	V	205	-	5,5,5	0.36	0	5,5,5	0.38	0
24	CLA	a	409	-	59,73,73	1.99	13 (22%)	67,113,113	2.26	26 (38%)
25	PHO	A	409	-	67,69,69	2.14	16 (23%)	85,99,99	1.84	21 (24%)
26	BCR	B	618	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	8 (14%)
35	HTG	b	602	-	19,19,19	1.14	2 (10%)	23,24,24	1.22	1 (4%)
29	LMT	B	636	-	25,25,36	0.43	0	30,30,47	0.65	0
30	OEX	A	418	1,3,41	0,15,15	0.00	-	-	-	-
24	CLA	d	403	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	22 (32%)
31	PL9	D	404	-	55,55,55	0.73	2 (3%)	68,69,69	1.58	14 (20%)
27	SQD	F	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.96	10 (19%)
28	GOL	B	637	-	5,5,5	0.40	0	5,5,5	0.30	0
23	BCT	a	419	21	0,3,3	0.00	-	0,3,3	0.00	-
26	BCR	b	623	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	9 (16%)
28	GOL	B	630	-	5,5,5	0.33	0	5,5,5	0.36	0
28	GOL	a	414	-	5,5,5	0.39	0	5,5,5	0.43	0
28	GOL	a	415	-	5,5,5	0.40	0	5,5,5	0.46	0
24	CLA	c	912	3	59,73,73	2.03	13 (22%)	67,113,113	2.08	21 (31%)
37	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	1.09	5 (9%)
28	GOL	F	103	33	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	B	610	-	59,73,73	1.94	13 (22%)	67,113,113	2.22	24 (35%)
35	HTG	D	411	-	16,16,19	1.16	2 (12%)	20,21,24	1.00	1 (5%)
24	CLA	c	905	41	59,73,73	2.04	13 (22%)	67,113,113	2.16	25 (37%)
24	CLA	C	514	-	59,73,73	2.02	13 (22%)	67,113,113	2.16	23 (34%)
24	CLA	b	613	-	59,73,73	1.96	13 (22%)	67,113,113	2.25	24 (35%)
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.57	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	GOL	f	101	33	5,5,5	0.37	0	5,5,5	0.40	0
24	CLA	b	616	-	59,73,73	1.96	11 (18%)	67,113,113	2.20	20 (29%)
28	GOL	V	203	-	5,5,5	0.38	0	5,5,5	0.15	0
24	CLA	c	913	-	59,73,73	1.96	13 (22%)	67,113,113	2.20	24 (35%)
26	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.37	7 (12%)
35	HTG	b	603	-	19,19,19	1.03	2 (10%)	23,24,24	1.47	3 (13%)
24	CLA	C	511	-	59,73,73	2.03	13 (22%)	67,113,113	2.23	22 (32%)
35	HTG	B	624	-	19,19,19	1.13	1 (5%)	23,24,24	1.39	1 (4%)
34	LMG	C	521	-	51,51,55	0.96	2 (3%)	59,59,63	1.07	4 (6%)
29	LMT	A	417	-	36,36,36	0.50	1 (2%)	47,47,47	1.06	2 (4%)
24	CLA	b	607	-	59,73,73	2.01	13 (22%)	67,113,113	2.40	26 (38%)
35	HTG	d	412	-	16,16,19	1.11	2 (12%)	20,21,24	1.38	1 (5%)
24	CLA	B	603	-	59,73,73	2.00	13 (22%)	67,113,113	2.30	28 (41%)
34	LMG	B	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.16	3 (5%)
24	CLA	B	609	-	59,73,73	2.10	13 (22%)	67,113,113	2.24	25 (37%)
24	CLA	d	401	41	59,73,73	2.01	12 (20%)	67,113,113	2.20	24 (35%)
24	CLA	C	512	3	59,73,73	2.01	15 (25%)	67,113,113	2.10	21 (31%)
28	GOL	c	925	-	5,5,5	0.36	0	5,5,5	0.56	0
26	BCR	D	403	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	14 (25%)
24	CLA	D	402	-	59,73,73	1.98	13 (22%)	67,113,113	2.03	21 (31%)
24	CLA	C	507	-	59,73,73	2.02	13 (22%)	67,113,113	2.17	24 (35%)
24	CLA	B	614	-	59,73,73	2.06	13 (22%)	67,113,113	2.15	22 (32%)
28	GOL	v	205	-	5,5,5	0.39	0	5,5,5	0.35	0
28	GOL	V	206	-	5,5,5	0.32	0	5,5,5	0.30	0
24	CLA	c	903	-	59,73,73	1.97	13 (22%)	67,113,113	2.15	20 (29%)
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.27	0
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	B	627	-	5,5,5	0.41	0	5,5,5	0.57	0
37	LHG	d	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	4 (7%)
26	BCR	b	622	-	41,41,41	1.06	1 (2%)	56,56,56	1.27	5 (8%)
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	0.85	2 (3%)
35	HTG	c	922	-	19,19,19	0.90	1 (5%)	23,24,24	1.34	1 (4%)
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.91	3 (5%)
24	CLA	b	620	-	59,73,73	2.03	14 (23%)	67,113,113	2.26	20 (29%)
35	HTG	B	626	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	2 (8%)
30	OEX	a	416	1,3,41	0,15,15	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	SQD	a	402	-	53,54,54	1.06	3 (5%)	62,65,65	1.16	7 (11%)
26	BCR	K	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
24	CLA	b	614	41	59,73,73	2.04	13 (22%)	67,113,113	2.22	26 (38%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
24	CLA	B	613	-	59,73,73	2.03	13 (22%)	67,113,113	2.19	17 (25%)
26	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.23	5 (8%)
34	LMG	a	412	-	51,51,55	0.91	2 (3%)	59,59,63	1.15	6 (10%)
28	GOL	B	631	-	5,5,5	0.42	0	5,5,5	0.47	0
29	LMT	b	601	-	25,25,36	0.46	0	30,30,47	1.35	3 (10%)
24	CLA	B	616	-	59,73,73	1.93	13 (22%)	67,113,113	2.28	26 (38%)
36	DGD	c	918	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	4 (5%)
29	LMT	B	623	-	36,36,36	0.43	0	47,47,47	1.40	5 (10%)
31	PL9	a	417	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	18 (26%)
29	LMT	a	401	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
24	CLA	b	611	41	59,73,73	2.05	14 (23%)	67,113,113	2.23	23 (34%)
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.31	0
28	GOL	V	204	-	5,5,5	0.43	0	5,5,5	0.44	0
28	GOL	T	103	-	5,5,5	0.39	0	5,5,5	0.19	0
28	GOL	T	101	-	5,5,5	0.41	0	5,5,5	0.31	0
24	CLA	a	406	-	59,73,73	2.05	13 (22%)	67,113,113	2.22	27 (40%)
35	HTG	B	633	-	19,19,19	1.12	2 (10%)	23,24,24	1.30	1 (4%)
29	LMT	b	625	-	25,25,36	0.52	1 (4%)	30,30,47	0.60	0
29	LMT	f	103	-	36,36,36	0.54	1 (2%)	47,47,47	0.93	4 (8%)
36	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	6 (7%)
24	CLA	A	405	-	59,73,73	1.98	13 (22%)	67,113,113	2.22	18 (26%)
24	CLA	c	909	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	21 (31%)
35	HTG	B	634	-	19,19,19	1.04	2 (10%)	23,24,24	1.59	3 (13%)
24	CLA	b	617	-	59,73,73	2.02	14 (23%)	67,113,113	2.21	26 (38%)
35	HTG	C	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.64	4 (17%)
34	LMG	j	101	39	51,51,55	0.89	2 (3%)	59,59,63	0.99	4 (6%)
35	HTG	b	626	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	3 (13%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.90	1 (2%)
24	CLA	b	615	-	59,73,73	1.97	13 (22%)	67,113,113	2.24	20 (29%)
26	BCR	d	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.78	16 (28%)
34	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
34	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.31	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	610	-	59,73,73	1.96	12 (20%)	67,113,113	2.33	23 (34%)
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.34	0
34	LMG	b	624	-	51,51,55	0.91	3 (5%)	59,59,63	1.05	3 (5%)
36	DGD	C	517	-	63,63,67	0.86	3 (4%)	77,77,81	1.04	4 (5%)
24	CLA	c	910	-	59,73,73	2.06	13 (22%)	67,113,113	2.21	23 (34%)
37	LHG	e	101	-	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
24	CLA	b	612	-	59,73,73	2.02	13 (22%)	67,113,113	2.19	22 (32%)
24	CLA	c	906	-	59,73,73	1.93	12 (20%)	67,113,113	2.17	18 (26%)
24	CLA	C	504	-	59,73,73	2.01	13 (22%)	67,113,113	2.15	20 (29%)
40	HEC	V	201	16	26,50,50	1.55	4 (15%)	18,82,82	1.53	6 (33%)
40	HEC	v	202	16	26,50,50	1.56	4 (15%)	18,82,82	1.36	4 (22%)
26	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)
24	CLA	c	908	41	59,73,73	1.99	13 (22%)	67,113,113	2.26	24 (35%)
24	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	23 (34%)
28	GOL	B	632	-	5,5,5	0.35	0	5,5,5	0.36	0
25	PHO	A	408	-	67,69,69	2.16	16 (23%)	85,99,99	1.97	20 (23%)
35	HTG	C	523	-	19,19,19	0.98	2 (10%)	23,24,24	1.37	2 (8%)
24	CLA	b	608	-	59,73,73	2.01	13 (22%)	67,113,113	2.20	19 (28%)
28	GOL	O	302	-	5,5,5	0.32	0	5,5,5	0.44	0
31	PL9	A	419	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)
24	CLA	B	605	-	59,73,73	1.90	12 (20%)	67,113,113	2.10	19 (28%)
24	CLA	B	611	41	59,73,73	2.02	13 (22%)	67,113,113	2.28	25 (37%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.29	5 (8%)
28	GOL	t	102	-	5,5,5	0.40	0	5,5,5	0.23	0
34	LMG	c	919	-	51,51,55	0.97	3 (5%)	59,59,63	1.01	2 (3%)
24	CLA	b	606	-	59,73,73	2.00	14 (23%)	67,113,113	2.31	24 (35%)
26	BCR	t	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	7 (12%)
24	CLA	C	508	41	59,73,73	1.97	13 (22%)	67,113,113	2.14	20 (29%)
24	CLA	B	617	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	20 (29%)
28	GOL	o	302	-	5,5,5	0.39	0	5,5,5	0.48	0
26	BCR	K	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	7 (12%)
37	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	A	407	41	59,73,73	2.02	13 (22%)	67,113,113	2.25	25 (37%)
34	LMG	C	501	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
37	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.06	4 (7%)
38	HEM	E	103	5,6	27,50,50	0.80	1 (3%)	17,82,82	2.34	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMT	m	104	-	36,36,36	0.51	0	47,47,47	1.01	2 (4%)
28	GOL	B	628	-	5,5,5	0.27	0	5,5,5	0.42	0
24	CLA	C	510	-	59,73,73	2.08	13 (22%)	67,113,113	2.21	27 (40%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.61	12 (21%)
35	HTG	O	303	-	19,19,19	0.95	1 (5%)	23,24,24	0.71	0
29	LMT	m	103	-	36,36,36	0.48	0	47,47,47	0.99	1 (2%)
28	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.61	0
29	LMT	m	102	-	36,36,36	0.48	0	47,47,47	0.91	1 (2%)
28	GOL	a	413	-	5,5,5	0.31	0	5,5,5	0.65	0
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.37	0
24	CLA	A	406	41	59,73,73	1.98	11 (18%)	67,113,113	2.42	27 (40%)
27	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.60	10 (16%)
37	LHG	E	101	-	41,41,48	1.05	2 (4%)	44,47,54	1.09	3 (6%)
27	SQD	A	416	-	53,54,54	1.03	3 (5%)	62,65,65	1.21	6 (9%)
35	HTG	V	202	-	19,19,19	1.01	2 (10%)	23,24,24	1.54	3 (13%)
24	CLA	c	902	-	59,73,73	1.98	12 (20%)	67,113,113	2.18	22 (32%)
26	BCR	B	620	-	41,41,41	1.09	1 (2%)	56,56,56	1.22	4 (7%)
35	HTG	b	627	-	19,19,19	1.09	2 (10%)	23,24,24	1.97	4 (17%)
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.33	4 (7%)
24	CLA	c	907	-	59,73,73	1.99	14 (23%)	67,113,113	2.26	25 (37%)
34	LMG	J	101	39	51,51,55	0.88	2 (3%)	59,59,63	0.89	3 (5%)
35	HTG	c	923	-	19,19,19	1.14	2 (10%)	23,24,24	1.84	5 (21%)
36	DGD	C	519	-	63,63,67	0.84	3 (4%)	77,77,81	0.95	5 (6%)
24	CLA	C	509	-	59,73,73	2.05	13 (22%)	67,113,113	2.41	25 (37%)
36	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	6 (7%)
26	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.39	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	B	625	-	-	3/10/30/30	0/1/1/1
36	DGD	D	405	-	-	22/51/91/95	0/2/2/2
24	CLA	c	904	-	3/3/20/25	3/37/135/135	-
24	CLA	C	506	-	1/1/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
26	BCR	A	411	-	-	1/29/63/63	0/2/2/2
24	CLA	C	503	-	2/2/20/25	4/37/135/135	-
27	SQD	A	412	-	-	11/49/69/69	0/1/1/1
28	GOL	b	629	-	-	0/4/4/4	-
24	CLA	b	609	-	3/3/20/25	9/37/135/135	-
24	CLA	D	401	-	2/2/20/25	0/37/135/135	-
36	DGD	d	406	-	-	28/51/91/95	0/2/2/2
24	CLA	a	407	41	2/2/20/25	6/37/135/135	-
24	CLA	A	410	-	2/2/20/25	9/37/135/135	-
36	DGD	C	518	-	-	15/51/91/95	0/2/2/2
24	CLA	d	403	-	2/2/20/25	7/37/135/135	-
25	PHO	a	408	-	-	2/53/103/103	0/5/6/6
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
29	LMT	E	102	-	-	7/21/61/61	0/2/2/2
24	CLA	C	513	-	3/3/20/25	10/37/135/135	-
24	CLA	b	605	41	3/3/20/25	12/37/135/135	-
28	GOL	b	630	-	-	0/4/4/4	-
25	PHO	a	420	-	-	4/53/103/103	0/5/6/6
24	CLA	C	505	41	3/3/20/25	5/37/135/135	-
24	CLA	B	615	-	2/2/20/25	18/37/135/135	-
28	GOL	b	632	-	-	2/4/4/4	-
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
24	CLA	B	602	41	3/3/20/25	16/37/135/135	-
26	BCR	b	621	-	-	2/29/63/63	0/2/2/2
28	GOL	b	633	-	-	2/4/4/4	-
24	CLA	B	607	-	2/2/20/25	7/37/135/135	-
24	CLA	B	612	-	3/3/20/25	2/37/135/135	-
28	GOL	b	631	-	-	2/4/4/4	-
38	HEM	e	102	5,6	-	0/6/54/54	-
29	LMT	c	921	-	-	4/21/61/61	0/2/2/2
24	CLA	b	619	-	3/3/20/25	4/37/135/135	-
24	CLA	d	402	-	1/1/20/25	0/37/135/135	-
28	GOL	b	628	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	914	-	3/3/20/25	10/37/135/135	-
24	CLA	c	911	-	3/3/20/25	9/37/135/135	-
26	BCR	a	410	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	9/51/91/95	0/2/2/2
28	GOL	V	205	-	-	1/4/4/4	-
31	PL9	d	405	-	-	5/53/73/73	0/1/1/1
24	CLA	B	608	41	3/3/20/25	2/37/135/135	-
28	GOL	a	415	-	-	2/4/4/4	-
28	GOL	v	203	-	-	4/4/4/4	-
28	GOL	C	526	-	-	0/4/4/4	-
29	LMT	C	522	-	-	9/21/61/61	0/2/2/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
37	LHG	d	407	-	-	9/53/53/53	-
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
28	GOL	A	413	-	-	2/4/4/4	-
24	CLA	B	606	-	3/3/20/25	7/37/135/135	-
36	DGD	c	917	-	-	14/51/91/95	0/2/2/2
26	BCR	y	101	-	-	3/29/63/63	0/2/2/2
24	CLA	B	604	-	2/2/20/25	6/37/135/135	-
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
24	CLA	a	409	-	3/3/20/25	7/37/135/135	-
25	PHO	A	409	-	-	2/53/103/103	0/5/6/6
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
35	HTG	b	602	-	-	1/10/30/30	0/1/1/1
29	LMT	B	636	-	-	8/17/37/61	0/1/1/2
24	CLA	b	618	-	2/2/20/25	17/37/135/135	-
31	PL9	D	404	-	-	3/53/73/73	0/1/1/1
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
28	GOL	B	637	-	-	2/4/4/4	-
26	BCR	b	623	-	-	3/29/63/63	0/2/2/2
28	GOL	B	630	-	-	0/4/4/4	-
28	GOL	a	414	-	-	2/4/4/4	-
28	GOL	B	629	-	-	2/4/4/4	-
24	CLA	c	912	3	3/3/20/25	5/37/135/135	-
37	LHG	D	406	-	-	6/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	511	-	3/3/20/25	9/37/135/135	-
24	CLA	B	610	-	2/2/20/25	3/37/135/135	-
35	HTG	D	411	-	-	1/7/27/30	0/1/1/1
24	CLA	c	905	41	3/3/20/25	5/37/135/135	-
24	CLA	C	514	-	2/2/20/25	2/37/135/135	-
24	CLA	b	613	-	3/3/20/25	2/37/135/135	-
27	SQD	L	102	-	-	25/49/69/69	0/1/1/1
28	GOL	f	101	33	-	4/4/4/4	-
24	CLA	b	616	-	3/3/20/25	1/37/135/135	-
28	GOL	V	203	-	-	4/4/4/4	-
24	CLA	c	913	-	3/3/20/25	7/37/135/135	-
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
35	HTG	b	603	-	-	0/10/30/30	0/1/1/1
34	LMG	c	920	-	-	4/46/66/70	0/1/1/1
35	HTG	B	624	-	-	1/10/30/30	0/1/1/1
34	LMG	C	521	-	-	12/46/66/70	0/1/1/1
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
24	CLA	b	607	-	2/2/20/25	8/37/135/135	-
35	HTG	d	412	-	-	0/7/27/30	0/1/1/1
24	CLA	B	603	-	2/2/20/25	5/37/135/135	-
34	LMG	B	622	-	-	12/46/66/70	0/1/1/1
24	CLA	B	609	-	2/2/20/25	0/37/135/135	-
24	CLA	d	401	41	2/2/20/25	7/37/135/135	-
24	CLA	C	512	3	3/3/20/25	2/37/135/135	-
28	GOL	c	925	-	-	0/4/4/4	-
26	BCR	D	403	-	-	6/29/63/63	0/2/2/2
24	CLA	D	402	-	3/3/20/25	9/37/135/135	-
24	CLA	C	507	-	3/3/20/25	11/37/135/135	-
24	CLA	B	614	-	3/3/20/25	9/37/135/135	-
28	GOL	v	205	-	-	2/4/4/4	-
28	GOL	V	206	-	-	1/4/4/4	-
24	CLA	c	903	-	3/3/20/25	4/37/135/135	-
28	GOL	A	415	-	-	2/4/4/4	-
28	GOL	B	627	-	-	1/4/4/4	-
37	LHG	d	409	-	-	12/53/53/53	-
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	D	407	-	-	5/53/53/53	-
35	HTG	c	922	-	-	4/10/30/30	0/1/1/1
37	LHG	d	408	-	-	11/53/53/53	-
24	CLA	b	620	-	3/3/20/25	8/37/135/135	-
35	HTG	B	626	-	-	4/10/30/30	0/1/1/1
27	SQD	a	402	-	-	17/49/69/69	0/1/1/1
26	BCR	K	103	-	-	2/29/63/63	0/2/2/2
24	CLA	b	614	41	3/3/20/25	3/37/135/135	-
37	LHG	l	101	-	-	15/53/53/53	-
24	CLA	B	613	-	3/3/20/25	4/37/135/135	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
34	LMG	a	412	-	-	10/46/66/70	0/1/1/1
28	GOL	B	631	-	-	4/4/4/4	-
29	LMT	b	601	-	-	8/17/37/61	0/1/1/2
24	CLA	B	616	-	3/3/20/25	10/37/135/135	-
36	DGD	c	918	-	-	17/51/91/95	0/2/2/2
29	LMT	B	623	-	-	7/21/61/61	0/2/2/2
28	GOL	F	103	33	-	2/4/4/4	-
29	LMT	a	401	-	-	11/21/61/61	0/2/2/2
24	CLA	b	611	41	2/2/20/25	2/37/135/135	-
28	GOL	c	924	-	-	0/4/4/4	-
28	GOL	V	204	-	-	2/4/4/4	-
28	GOL	T	103	-	-	4/4/4/4	-
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	a	406	-	3/3/20/25	2/37/135/135	-
35	HTG	B	633	-	-	3/10/30/30	0/1/1/1
29	LMT	b	625	-	-	4/17/37/61	0/1/1/2
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
24	CLA	A	405	-	2/2/20/25	2/37/135/135	-
24	CLA	c	909	-	3/3/20/25	3/37/135/135	-
35	HTG	B	634	-	-	2/10/30/30	0/1/1/1
24	CLA	b	617	-	3/3/20/25	4/37/135/135	-
35	HTG	C	524	-	-	2/10/30/30	0/1/1/1
34	LMG	j	101	39	-	11/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	b	626	-	-	1/10/30/30	0/1/1/1
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
24	CLA	b	615	-	2/2/20/25	5/37/135/135	-
26	BCR	d	404	-	-	4/29/63/63	0/2/2/2
34	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
24	CLA	b	610	-	3/3/20/25	16/37/135/135	-
28	GOL	A	414	-	-	2/4/4/4	-
34	LMG	b	624	-	-	14/46/66/70	0/1/1/1
36	DGD	C	517	-	-	15/51/91/95	0/2/2/2
24	CLA	c	910	-	3/3/20/25	9/37/135/135	-
37	LHG	e	101	-	-	10/46/46/53	-
24	CLA	b	612	-	2/2/20/25	4/37/135/135	-
24	CLA	c	906	-	1/1/20/25	4/37/135/135	-
24	CLA	C	504	-	3/3/20/25	5/37/135/135	-
40	HEC	V	201	16	-	0/6/54/54	-
40	HEC	v	202	16	-	0/6/54/54	-
26	BCR	C	516	-	-	2/29/63/63	0/2/2/2
24	CLA	c	908	41	3/3/20/25	2/37/135/135	-
24	CLA	C	502	-	3/3/20/25	9/37/135/135	-
28	GOL	B	632	-	-	2/4/4/4	-
25	PHO	A	408	-	-	4/53/103/103	0/5/6/6
35	HTG	C	523	-	-	1/10/30/30	0/1/1/1
24	CLA	b	608	-	3/3/20/25	7/37/135/135	-
28	GOL	O	302	-	-	2/4/4/4	-
31	PL9	A	419	-	-	7/53/73/73	0/1/1/1
24	CLA	B	605	-	3/3/20/25	4/37/135/135	-
24	CLA	B	611	41	3/3/20/25	7/37/135/135	-
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
28	GOL	t	102	-	-	0/4/4/4	-
34	LMG	c	919	-	-	16/46/66/70	0/1/1/1
24	CLA	b	606	-	2/2/20/25	3/37/135/135	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	508	41	3/3/20/25	6/37/135/135	-
24	CLA	B	617	-	3/3/20/25	9/37/135/135	-
28	GOL	o	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
37	LHG	L	101	-	-	15/53/53/53	-
24	CLA	A	407	41	2/2/20/25	2/37/135/135	-
34	LMG	C	501	-	-	19/46/66/70	0/1/1/1
37	LHG	D	408	-	-	11/53/53/53	-
38	HEM	E	103	5,6	-	0/6/54/54	-
29	LMT	m	104	-	-	7/21/61/61	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
24	CLA	C	510	-	3/3/20/25	7/37/135/135	-
31	PL9	a	417	-	-	12/53/73/73	0/1/1/1
35	HTG	O	303	-	-	1/10/30/30	0/1/1/1
29	LMT	m	103	-	-	3/21/61/61	0/2/2/2
28	GOL	C	525	-	-	0/4/4/4	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
28	GOL	a	413	-	-	0/4/4/4	-
28	GOL	v	204	-	-	3/4/4/4	-
24	CLA	A	406	41	3/3/20/25	4/37/135/135	-
27	SQD	a	411	-	-	11/49/69/69	0/1/1/1
37	LHG	E	101	-	-	21/46/46/53	-
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
35	HTG	V	202	-	-	5/10/30/30	0/1/1/1
24	CLA	c	902	-	3/3/20/25	4/37/135/135	-
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
35	HTG	b	627	-	-	3/10/30/30	0/1/1/1
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
24	CLA	c	907	-	3/3/20/25	9/37/135/135	-
34	LMG	J	101	39	-	13/46/66/70	0/1/1/1
35	HTG	c	923	-	-	0/10/30/30	0/1/1/1
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
24	CLA	C	509	-	2/2/20/25	7/37/135/135	-
36	DGD	c	916	-	-	10/51/91/95	0/2/2/2
26	BCR	H	101	-	-	3/29/63/63	0/2/2/2

All (1140) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-C2B	6.98	1.50	1.40
24	b	620	CLA	C3B-C2B	6.75	1.49	1.40
24	a	406	CLA	C3B-C2B	6.74	1.49	1.40
24	B	617	CLA	C3B-C2B	6.73	1.49	1.40
24	c	910	CLA	C3B-C2B	6.65	1.49	1.40
24	B	604	CLA	C3B-C2B	6.59	1.49	1.40
24	C	510	CLA	C3B-C2B	6.58	1.49	1.40
24	C	514	CLA	C3B-C2B	6.56	1.49	1.40
24	C	509	CLA	C3D-C2D	6.53	1.51	1.39
24	C	511	CLA	C3B-C2B	6.52	1.49	1.40
24	b	608	CLA	C3B-C2B	6.51	1.49	1.40
24	B	613	CLA	C3B-C2B	6.50	1.49	1.40
24	B	605	CLA	C3B-C2B	6.46	1.49	1.40
24	b	619	CLA	C3D-C2D	6.43	1.51	1.39
24	b	619	CLA	C3B-C2B	6.38	1.49	1.40
24	c	909	CLA	C3B-C2B	6.38	1.49	1.40
24	C	502	CLA	C3B-C2B	6.37	1.49	1.40
24	B	609	CLA	C3B-C2B	6.34	1.49	1.40
24	d	403	CLA	C3B-C2B	6.34	1.49	1.40
24	A	406	CLA	C3D-C2D	6.30	1.50	1.39
24	b	614	CLA	C3B-C2B	6.30	1.49	1.40
24	b	617	CLA	C3B-C2B	6.30	1.49	1.40
24	B	609	CLA	C3D-C2D	6.29	1.50	1.39
24	B	607	CLA	C3B-C2B	6.27	1.49	1.40
24	b	615	CLA	C3B-C2B	6.20	1.49	1.40
24	c	902	CLA	C3B-C2B	6.19	1.49	1.40
24	B	612	CLA	C3B-C2B	6.18	1.48	1.40
24	A	406	CLA	C3B-C2B	6.17	1.48	1.40
24	C	503	CLA	C3D-C2D	6.16	1.50	1.39
24	C	509	CLA	C3B-C2B	6.16	1.48	1.40
24	c	912	CLA	C3B-C2B	6.13	1.48	1.40
25	a	420	PHO	C3B-C2B	6.13	1.49	1.37
24	b	606	CLA	C3B-C2B	6.09	1.48	1.40
25	A	408	PHO	C3C-C2C	6.06	1.49	1.36
25	A	409	PHO	C3B-C2B	6.06	1.49	1.37
24	b	605	CLA	C3D-C2D	6.04	1.50	1.39
24	b	607	CLA	C3B-C2B	6.04	1.48	1.40
24	C	507	CLA	C3B-C2B	6.03	1.48	1.40
24	B	602	CLA	C3D-C2D	6.00	1.50	1.39
24	C	512	CLA	C3B-C2B	5.99	1.48	1.40
24	B	603	CLA	C3B-C2B	5.98	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3D-C2D	5.98	1.50	1.39
24	B	611	CLA	C3B-C2B	5.98	1.48	1.40
24	c	907	CLA	C3B-C2B	5.97	1.48	1.40
24	B	608	CLA	C3B-C2B	5.97	1.48	1.40
24	A	410	CLA	C3B-C2B	5.96	1.48	1.40
24	c	909	CLA	C3D-C2D	5.96	1.50	1.39
24	C	511	CLA	C3D-C2D	5.96	1.50	1.39
24	C	504	CLA	C3B-C2B	5.96	1.48	1.40
24	B	616	CLA	C3D-C2D	5.96	1.50	1.39
24	c	905	CLA	C3D-C2D	5.96	1.50	1.39
24	A	410	CLA	C3D-C2D	5.95	1.50	1.39
24	d	401	CLA	C3D-C2D	5.93	1.50	1.39
24	a	409	CLA	C3D-C2D	5.92	1.50	1.39
24	b	612	CLA	C3B-C2B	5.92	1.48	1.40
25	a	420	PHO	CHB-C1B	5.91	1.50	1.38
24	B	613	CLA	C3D-C2D	5.90	1.50	1.39
24	C	513	CLA	C3B-C2B	5.90	1.48	1.40
24	b	611	CLA	C3B-C2B	5.89	1.48	1.40
24	D	401	CLA	C3B-C2B	5.88	1.48	1.40
24	c	911	CLA	C3B-C2B	5.86	1.48	1.40
24	c	910	CLA	C3D-C2D	5.83	1.49	1.39
24	C	505	CLA	C3B-C2B	5.81	1.48	1.40
24	b	610	CLA	C3B-C2B	5.80	1.48	1.40
24	d	402	CLA	C3B-C2B	5.79	1.48	1.40
25	A	408	PHO	C3B-C2B	5.78	1.49	1.37
24	c	905	CLA	C3B-C2B	5.78	1.48	1.40
24	B	610	CLA	C3D-C2D	5.78	1.49	1.39
24	C	513	CLA	C3D-C2D	5.78	1.49	1.39
24	c	907	CLA	C3D-C2D	5.77	1.49	1.39
24	B	606	CLA	C3D-C2D	5.77	1.49	1.39
24	B	611	CLA	C3D-C2D	5.77	1.49	1.39
24	A	405	CLA	C3B-C2B	5.77	1.48	1.40
24	c	908	CLA	C3B-C2B	5.77	1.48	1.40
24	B	611	CLA	C3C-C2C	5.77	1.49	1.36
24	b	605	CLA	C3B-C2B	5.76	1.48	1.40
24	C	507	CLA	C3D-C2D	5.75	1.49	1.39
24	b	620	CLA	C3D-C2D	5.75	1.49	1.39
24	c	903	CLA	C3D-C2D	5.73	1.49	1.39
24	c	914	CLA	C3B-C2B	5.72	1.48	1.40
25	A	409	PHO	C3C-C2C	5.72	1.48	1.36
24	b	605	CLA	C3C-C2C	5.71	1.48	1.36
24	D	401	CLA	C3D-C2D	5.69	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	C3B-C2B	5.69	1.48	1.40
24	B	612	CLA	C3D-C2D	5.69	1.49	1.39
24	C	508	CLA	C3D-C2D	5.69	1.49	1.39
24	B	614	CLA	C3D-C2D	5.69	1.49	1.39
24	A	407	CLA	C3D-C2D	5.68	1.49	1.39
24	b	609	CLA	C3B-C2B	5.68	1.48	1.40
24	C	514	CLA	C3D-C2D	5.68	1.49	1.39
24	d	403	CLA	C3D-C2D	5.67	1.49	1.39
24	C	506	CLA	C3B-C2B	5.67	1.48	1.40
24	A	405	CLA	C3D-C2D	5.67	1.49	1.39
24	C	503	CLA	C3B-C2B	5.66	1.48	1.40
24	A	407	CLA	C3C-C2C	5.65	1.48	1.36
24	b	610	CLA	C3D-C2D	5.65	1.49	1.39
24	C	508	CLA	C3B-C2B	5.64	1.48	1.40
24	b	617	CLA	C3D-C2D	5.64	1.49	1.39
24	a	407	CLA	C3B-C2B	5.63	1.48	1.40
24	b	615	CLA	C3D-C2D	5.62	1.49	1.39
24	B	608	CLA	OBD-CAD	5.62	1.30	1.22
24	b	618	CLA	C3B-C2B	5.61	1.48	1.40
25	a	408	PHO	C3B-C2B	5.61	1.48	1.37
24	B	617	CLA	C3D-C2D	5.60	1.49	1.39
24	B	616	CLA	C3B-C2B	5.60	1.48	1.40
24	a	406	CLA	C3D-C2D	5.60	1.49	1.39
24	C	504	CLA	C3D-C2D	5.60	1.49	1.39
24	c	912	CLA	C3D-C2D	5.60	1.49	1.39
24	b	606	CLA	C3D-C2D	5.59	1.49	1.39
24	C	505	CLA	C3D-C2D	5.58	1.49	1.39
24	C	502	CLA	C3D-C2D	5.58	1.49	1.39
24	a	407	CLA	C3D-C2D	5.58	1.49	1.39
24	c	908	CLA	C3D-C2D	5.58	1.49	1.39
24	c	913	CLA	C3D-C2D	5.58	1.49	1.39
24	B	603	CLA	C3D-C2D	5.57	1.49	1.39
24	c	902	CLA	C3D-C2D	5.56	1.49	1.39
24	C	504	CLA	C3C-C2C	5.55	1.48	1.36
24	b	612	CLA	C3D-C2D	5.55	1.49	1.39
24	c	904	CLA	C3D-C2D	5.54	1.49	1.39
24	b	614	CLA	C3D-C2D	5.53	1.49	1.39
24	b	618	CLA	C3C-C2C	5.52	1.48	1.36
24	d	401	CLA	C3B-C2B	5.52	1.48	1.40
24	B	604	CLA	C3D-C2D	5.51	1.49	1.39
24	C	507	CLA	C3C-C2C	5.50	1.48	1.36
24	b	612	CLA	C3C-C2C	5.50	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C3C-C2C	5.49	1.48	1.36
25	a	420	PHO	C3C-C2C	5.49	1.48	1.36
24	c	911	CLA	C3D-C2D	5.49	1.49	1.39
24	B	606	CLA	C3B-C2B	5.47	1.48	1.40
24	c	913	CLA	C3B-C2B	5.47	1.48	1.40
24	B	609	CLA	C3C-C2C	5.47	1.48	1.36
24	C	511	CLA	C3C-C2C	5.47	1.48	1.36
24	B	615	CLA	C3B-C2B	5.46	1.48	1.40
24	C	513	CLA	C3C-C2C	5.45	1.48	1.36
24	B	615	CLA	C3D-C2D	5.44	1.49	1.39
24	b	614	CLA	C3C-C2C	5.44	1.48	1.36
24	B	604	CLA	C3C-C2C	5.43	1.48	1.36
24	b	616	CLA	C3B-C2B	5.43	1.47	1.40
24	B	614	CLA	C3C-C2C	5.42	1.48	1.36
24	d	401	CLA	C3C-C2C	5.40	1.48	1.36
24	D	402	CLA	C3D-C2D	5.39	1.49	1.39
24	C	506	CLA	C3C-C2C	5.39	1.48	1.36
24	C	514	CLA	C3C-C2C	5.39	1.48	1.36
24	b	607	CLA	C3C-C2C	5.38	1.48	1.36
24	d	402	CLA	C3D-C2D	5.38	1.49	1.39
24	A	407	CLA	CHC-C1C	5.38	1.48	1.35
24	C	512	CLA	C3D-C2D	5.38	1.49	1.39
25	a	420	PHO	CHC-C1C	5.38	1.49	1.38
24	b	613	CLA	C3D-C2D	5.38	1.49	1.39
24	a	406	CLA	C3C-C2C	5.37	1.48	1.36
24	C	506	CLA	OBD-CAD	5.37	1.29	1.22
24	D	402	CLA	C3B-C2B	5.36	1.47	1.40
24	c	914	CLA	C3D-C2D	5.36	1.49	1.39
24	a	407	CLA	CHC-C1C	5.35	1.48	1.35
24	c	913	CLA	C3C-C2C	5.35	1.48	1.36
24	c	909	CLA	C3C-C2C	5.35	1.48	1.36
24	b	617	CLA	O2D-CGD	5.34	1.46	1.33
24	b	613	CLA	C3B-C2B	5.34	1.47	1.40
24	b	608	CLA	C3D-C2D	5.33	1.49	1.39
24	A	410	CLA	C3C-C2C	5.33	1.48	1.36
24	c	911	CLA	C3C-C2C	5.33	1.48	1.36
25	A	408	PHO	CHB-C1B	5.32	1.49	1.38
24	a	409	CLA	C3B-C2B	5.31	1.47	1.40
24	a	409	CLA	C3C-C2C	5.31	1.48	1.36
25	A	408	PHO	CHC-C1C	5.31	1.49	1.38
24	C	503	CLA	C3C-C2C	5.30	1.48	1.36
24	A	407	CLA	C3B-C2B	5.29	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	914	CLA	CHC-C1C	5.29	1.48	1.35
24	C	505	CLA	C3C-C2C	5.29	1.48	1.36
25	a	408	PHO	C3C-C2C	5.28	1.48	1.36
24	B	603	CLA	C3C-C2C	5.28	1.47	1.36
24	B	607	CLA	C3D-C2D	5.27	1.48	1.39
24	b	611	CLA	CHC-C1C	5.27	1.48	1.35
24	C	513	CLA	CHC-C1C	5.27	1.48	1.35
24	C	505	CLA	OBD-CAD	5.26	1.29	1.22
24	c	903	CLA	C3C-C2C	5.25	1.47	1.36
24	c	907	CLA	O2D-CGD	5.25	1.46	1.33
24	b	618	CLA	CHC-C1C	5.25	1.48	1.35
24	B	602	CLA	C3B-C2B	5.24	1.47	1.40
24	c	911	CLA	CHC-C1C	5.24	1.48	1.35
24	c	904	CLA	C3C-C2C	5.23	1.47	1.36
24	b	616	CLA	C3C-C2C	5.22	1.47	1.36
24	b	609	CLA	C3D-C2D	5.22	1.48	1.39
24	C	510	CLA	O2D-CGD	5.22	1.45	1.33
24	A	407	CLA	O2D-CGD	5.21	1.45	1.33
24	c	903	CLA	CHC-C1C	5.21	1.48	1.35
24	b	611	CLA	C3D-C2D	5.21	1.48	1.39
24	A	405	CLA	CHC-C1C	5.21	1.48	1.35
24	b	611	CLA	C3C-C2C	5.21	1.47	1.36
24	B	608	CLA	C3C-C2C	5.20	1.47	1.36
24	c	913	CLA	CHC-C1C	5.20	1.48	1.35
24	A	405	CLA	C3C-C2C	5.20	1.47	1.36
24	b	616	CLA	CHC-C1C	5.20	1.48	1.35
24	c	912	CLA	C3C-C2C	5.19	1.47	1.36
24	D	402	CLA	CHC-C1C	5.19	1.48	1.35
24	b	605	CLA	O2D-CGD	5.18	1.45	1.33
24	B	603	CLA	O2D-CGD	5.18	1.45	1.33
24	c	914	CLA	C3C-C2C	5.17	1.47	1.36
24	c	904	CLA	CHC-C1C	5.17	1.48	1.35
24	a	409	CLA	O2D-CGD	5.17	1.45	1.33
24	b	613	CLA	CHC-C1C	5.17	1.48	1.35
24	B	614	CLA	CHC-C1C	5.16	1.48	1.35
24	b	620	CLA	C3C-C2C	5.16	1.47	1.36
24	C	505	CLA	CHC-C1C	5.15	1.48	1.35
24	B	608	CLA	C3D-C2D	5.15	1.48	1.39
24	b	618	CLA	C3D-C2D	5.15	1.48	1.39
24	b	612	CLA	CHC-C1C	5.15	1.48	1.35
24	c	906	CLA	C3B-C2B	5.14	1.47	1.40
24	B	617	CLA	C3C-C2C	5.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	CHC-C1C	5.12	1.48	1.35
24	c	903	CLA	C3B-C2B	5.12	1.47	1.40
24	b	613	CLA	O2D-CGD	5.12	1.45	1.33
24	a	407	CLA	C3C-C2C	5.11	1.47	1.36
24	b	616	CLA	C3D-C2D	5.11	1.48	1.39
24	b	607	CLA	C3D-C2D	5.11	1.48	1.39
24	A	410	CLA	O2D-CGD	5.11	1.45	1.33
24	A	406	CLA	C3C-C2C	5.11	1.47	1.36
24	b	607	CLA	CHC-C1C	5.11	1.48	1.35
24	c	908	CLA	C3C-C2C	5.11	1.47	1.36
24	b	617	CLA	C3C-C2C	5.11	1.47	1.36
24	B	602	CLA	O2D-CGD	5.10	1.45	1.33
24	B	610	CLA	C3C-C2C	5.10	1.47	1.36
24	c	905	CLA	O2D-CGD	5.10	1.45	1.33
26	k	101	BCR	C23-C22	-5.10	1.35	1.45
24	b	606	CLA	O2D-CGD	5.10	1.45	1.33
24	c	910	CLA	C3C-C2C	5.10	1.47	1.36
24	d	403	CLA	C3C-C2C	5.09	1.47	1.36
24	B	610	CLA	CHC-C1C	5.09	1.48	1.35
24	C	506	CLA	O2D-CGD	5.09	1.45	1.33
24	B	603	CLA	CHC-C1C	5.09	1.48	1.35
24	c	905	CLA	C3C-C2C	5.09	1.47	1.36
24	B	605	CLA	C3C-C2C	5.09	1.47	1.36
24	C	503	CLA	O2D-CGD	5.08	1.45	1.33
25	A	409	PHO	CHB-C1B	5.08	1.48	1.38
24	b	608	CLA	CHC-C1C	5.08	1.48	1.35
24	c	910	CLA	CHC-C1C	5.08	1.48	1.35
24	b	616	CLA	O2D-CGD	5.07	1.45	1.33
24	B	613	CLA	CHC-C1C	5.07	1.48	1.35
24	B	602	CLA	CHC-C1C	5.06	1.48	1.35
24	B	602	CLA	C3C-C2C	5.06	1.47	1.36
26	t	101	BCR	C23-C22	-5.06	1.35	1.45
24	C	509	CLA	C3C-C2C	5.06	1.47	1.36
24	c	912	CLA	CHC-C1C	5.05	1.47	1.35
25	a	420	PHO	O2D-CGD	5.05	1.45	1.33
24	b	605	CLA	CHC-C1C	5.05	1.47	1.35
24	c	902	CLA	C3C-C2C	5.05	1.47	1.36
24	b	609	CLA	CHC-C1C	5.04	1.47	1.35
24	B	612	CLA	C3C-C2C	5.04	1.47	1.36
24	c	910	CLA	O2D-CGD	5.03	1.45	1.33
24	b	606	CLA	C3C-C2C	5.03	1.47	1.36
24	b	609	CLA	C3C-C2C	5.03	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C3C-C2C	5.03	1.47	1.36
24	b	610	CLA	C3C-C2C	5.03	1.47	1.36
24	B	612	CLA	CHC-C1C	5.03	1.47	1.35
24	c	906	CLA	O2D-CGD	5.02	1.45	1.33
24	C	509	CLA	O2D-CGD	5.02	1.45	1.33
24	c	907	CLA	C3C-C2C	5.01	1.47	1.36
24	C	510	CLA	C3C-C2C	5.01	1.47	1.36
26	B	620	BCR	C23-C22	-5.01	1.35	1.45
24	b	607	CLA	O2D-CGD	5.00	1.45	1.33
26	b	622	BCR	C23-C22	-4.99	1.35	1.45
24	B	608	CLA	O2D-CGD	4.99	1.45	1.33
24	D	402	CLA	O2D-CGD	4.99	1.45	1.33
24	b	614	CLA	CHC-C1C	4.99	1.47	1.35
24	A	410	CLA	OBD-CAD	4.99	1.29	1.22
24	C	506	CLA	C3D-C2D	4.99	1.48	1.39
24	b	617	CLA	CHC-C1C	4.99	1.47	1.35
24	C	508	CLA	CHC-C1C	4.99	1.47	1.35
24	b	615	CLA	O2D-CGD	4.98	1.45	1.33
24	B	609	CLA	OBD-CAD	4.97	1.29	1.22
24	b	611	CLA	OBD-CAD	4.97	1.29	1.22
24	C	506	CLA	CHC-C1C	4.97	1.47	1.35
24	C	508	CLA	C3C-C2C	4.97	1.47	1.36
24	C	512	CLA	O2D-CGD	4.97	1.45	1.33
24	b	610	CLA	CHC-C1C	4.96	1.47	1.35
24	B	613	CLA	C3C-C2C	4.95	1.47	1.36
24	B	607	CLA	C3C-C2C	4.95	1.47	1.36
24	B	606	CLA	C3C-C2C	4.95	1.47	1.36
24	B	616	CLA	CHC-C1C	4.95	1.47	1.35
24	b	620	CLA	O2D-CGD	4.95	1.45	1.33
24	B	617	CLA	OBD-CAD	4.95	1.29	1.22
24	b	620	CLA	CHC-C1C	4.94	1.47	1.35
26	k	102	BCR	C23-C22	-4.94	1.35	1.45
24	B	613	CLA	O2D-CGD	4.94	1.45	1.33
24	B	607	CLA	O2D-CGD	4.94	1.45	1.33
24	c	905	CLA	CHC-C1C	4.94	1.47	1.35
24	b	606	CLA	CHC-C1C	4.93	1.47	1.35
24	c	905	CLA	OBD-CAD	4.93	1.29	1.22
24	d	403	CLA	CHC-C1C	4.92	1.47	1.35
24	b	608	CLA	C3C-C2C	4.92	1.47	1.36
24	B	612	CLA	O2D-CGD	4.92	1.45	1.33
24	B	606	CLA	O2D-CGD	4.91	1.45	1.33
24	C	514	CLA	CHC-C1C	4.91	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409	PHO	CHC-C1C	4.91	1.48	1.38
24	B	615	CLA	CHC-C1C	4.91	1.47	1.35
24	B	616	CLA	O2D-CGD	4.91	1.45	1.33
24	c	906	CLA	C3D-C2D	4.90	1.48	1.39
25	a	408	PHO	CHB-C1B	4.90	1.48	1.38
24	C	512	CLA	C3C-C2C	4.90	1.47	1.36
24	A	410	CLA	CHC-C1C	4.89	1.47	1.35
24	c	906	CLA	C3C-C2C	4.89	1.47	1.36
24	D	401	CLA	C3C-C2C	4.89	1.47	1.36
24	d	402	CLA	C3C-C2C	4.89	1.47	1.36
24	C	513	CLA	O2D-CGD	4.89	1.45	1.33
24	C	512	CLA	CHC-C1C	4.88	1.47	1.35
24	c	908	CLA	CHC-C1C	4.88	1.47	1.35
24	c	909	CLA	O2D-CGD	4.88	1.45	1.33
24	a	409	CLA	CHC-C1C	4.88	1.47	1.35
24	d	403	CLA	O2D-CGD	4.88	1.45	1.33
25	A	408	PHO	O2D-CGD	4.88	1.45	1.33
24	d	401	CLA	OBD-CAD	4.87	1.29	1.22
24	C	511	CLA	CHC-C1C	4.87	1.47	1.35
24	B	616	CLA	C3C-C2C	4.87	1.47	1.36
24	b	608	CLA	O2D-CGD	4.87	1.45	1.33
24	b	609	CLA	OBD-CAD	4.86	1.29	1.22
24	b	619	CLA	O2D-CGD	4.86	1.45	1.33
24	c	914	CLA	O2D-CGD	4.85	1.45	1.33
24	B	610	CLA	C3B-C2B	4.85	1.47	1.40
24	c	902	CLA	CHC-C1C	4.85	1.47	1.35
24	C	502	CLA	C3C-C2C	4.85	1.47	1.36
24	B	605	CLA	CHC-C1C	4.85	1.47	1.35
24	C	503	CLA	CHC-C1C	4.85	1.47	1.35
24	B	613	CLA	OBD-CAD	4.85	1.29	1.22
24	B	608	CLA	CHC-C1C	4.85	1.47	1.35
24	B	617	CLA	CHC-C1C	4.85	1.47	1.35
24	b	619	CLA	OBD-CAD	4.85	1.29	1.22
24	c	913	CLA	O2D-CGD	4.84	1.45	1.33
24	C	507	CLA	CHC-C1C	4.84	1.47	1.35
24	B	607	CLA	OBD-CAD	4.84	1.29	1.22
24	b	609	CLA	O2D-CGD	4.84	1.45	1.33
24	c	903	CLA	OBD-CAD	4.84	1.29	1.22
24	c	906	CLA	CHC-C1C	4.84	1.47	1.35
26	d	404	BCR	C23-C22	-4.83	1.35	1.45
24	C	514	CLA	O2D-CGD	4.83	1.45	1.33
24	b	612	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	403	BCR	C23-C22	-4.83	1.35	1.45
24	C	502	CLA	O2D-CGD	4.83	1.45	1.33
24	C	512	CLA	OBD-CAD	4.83	1.29	1.22
24	C	504	CLA	CHC-C1C	4.82	1.47	1.35
24	c	912	CLA	O2D-CGD	4.82	1.45	1.33
24	c	911	CLA	O2D-CGD	4.82	1.45	1.33
24	B	606	CLA	OBD-CAD	4.80	1.29	1.22
24	B	609	CLA	O2D-CGD	4.80	1.44	1.33
26	C	515	BCR	C23-C22	-4.79	1.35	1.45
24	C	510	CLA	CHC-C1C	4.79	1.47	1.35
24	B	614	CLA	O2D-CGD	4.79	1.44	1.33
24	B	604	CLA	O2D-CGD	4.79	1.44	1.33
24	b	619	CLA	C3C-C2C	4.79	1.46	1.36
24	A	407	CLA	OBD-CAD	4.79	1.29	1.22
26	C	516	BCR	C23-C22	-4.78	1.35	1.45
24	d	401	CLA	CHC-C1C	4.78	1.47	1.35
24	a	409	CLA	OBD-CAD	4.78	1.29	1.22
24	c	908	CLA	O2D-CGD	4.78	1.44	1.33
24	A	406	CLA	O2D-CGD	4.77	1.44	1.33
24	b	614	CLA	O2D-CGD	4.76	1.44	1.33
24	B	611	CLA	CHC-C1C	4.76	1.47	1.35
24	b	615	CLA	CHC-C1C	4.76	1.47	1.35
24	C	502	CLA	CHC-C1C	4.76	1.47	1.35
24	a	406	CLA	CHC-C1C	4.75	1.47	1.35
24	b	615	CLA	C3C-C2C	4.74	1.46	1.36
24	B	605	CLA	C3D-C2D	4.74	1.47	1.39
26	h	101	BCR	C23-C22	-4.74	1.35	1.45
24	C	509	CLA	CHC-C1C	4.74	1.47	1.35
25	a	408	PHO	CHC-C1C	4.74	1.47	1.38
24	c	909	CLA	CHC-C1C	4.74	1.47	1.35
24	D	401	CLA	CHC-C1C	4.73	1.47	1.35
24	B	615	CLA	OBD-CAD	4.73	1.28	1.22
24	C	507	CLA	O2D-CGD	4.72	1.44	1.33
24	b	614	CLA	OBD-CAD	4.72	1.28	1.22
26	b	623	BCR	C23-C22	-4.71	1.35	1.45
24	c	903	CLA	O2D-CGD	4.71	1.44	1.33
24	b	610	CLA	O2D-CGD	4.71	1.44	1.33
24	a	406	CLA	OBD-CAD	4.70	1.28	1.22
26	K	103	BCR	C23-C22	-4.70	1.35	1.45
24	b	619	CLA	CHC-C1C	4.69	1.47	1.35
24	C	502	CLA	OBD-CAD	4.69	1.28	1.22
25	A	409	PHO	O2D-CGD	4.69	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	CHD-C1D	4.69	1.47	1.38
24	c	906	CLA	OBD-CAD	4.69	1.28	1.22
24	c	912	CLA	OBD-CAD	4.68	1.28	1.22
24	B	617	CLA	O2D-CGD	4.68	1.44	1.33
24	B	610	CLA	OBD-CAD	4.67	1.28	1.22
24	b	613	CLA	C3C-C2C	4.66	1.46	1.36
24	d	401	CLA	O2D-CGD	4.65	1.44	1.33
24	B	607	CLA	CHC-C1C	4.65	1.46	1.35
24	B	611	CLA	O2D-CGD	4.64	1.44	1.33
24	c	911	CLA	OBD-CAD	4.64	1.28	1.22
24	C	511	CLA	O2D-CGD	4.64	1.44	1.33
24	b	611	CLA	O2D-CGD	4.63	1.44	1.33
24	C	504	CLA	O2D-CGD	4.63	1.44	1.33
24	c	907	CLA	CHC-C1C	4.63	1.46	1.35
26	y	101	BCR	C23-C22	-4.63	1.36	1.45
24	B	615	CLA	O2D-CGD	4.63	1.44	1.33
24	c	910	CLA	OBD-CAD	4.63	1.28	1.22
24	B	609	CLA	CHC-C1C	4.63	1.46	1.35
26	b	621	BCR	C23-C22	-4.62	1.36	1.45
24	c	909	CLA	OBD-CAD	4.62	1.28	1.22
24	c	902	CLA	O2D-CGD	4.61	1.44	1.33
37	E	101	LHG	O8-C23	4.61	1.46	1.33
24	c	908	CLA	O2A-CGA	4.60	1.46	1.33
36	D	405	DGD	O1G-C1A	4.59	1.46	1.33
24	B	612	CLA	OBD-CAD	4.59	1.28	1.22
24	a	406	CLA	O2D-CGD	4.59	1.44	1.33
24	b	618	CLA	O2D-CGD	4.58	1.44	1.33
24	B	606	CLA	CHC-C1C	4.58	1.46	1.35
24	C	508	CLA	OBD-CAD	4.58	1.28	1.22
26	H	101	BCR	C23-C22	-4.58	1.36	1.45
24	C	505	CLA	O2A-CGA	4.58	1.46	1.33
24	b	613	CLA	OBD-CAD	4.57	1.28	1.22
24	A	406	CLA	CHC-C1C	4.56	1.46	1.35
25	a	420	PHO	CHD-C1D	4.56	1.47	1.38
24	A	405	CLA	O2D-CGD	4.54	1.44	1.33
24	B	610	CLA	O2D-CGD	4.54	1.44	1.33
24	c	914	CLA	OBD-CAD	4.54	1.28	1.22
24	a	407	CLA	O2D-CGD	4.53	1.44	1.33
26	c	915	BCR	C23-C22	-4.53	1.36	1.45
24	B	615	CLA	O2A-CGA	4.53	1.46	1.33
24	b	616	CLA	OBD-CAD	4.53	1.28	1.22
24	b	612	CLA	OBD-CAD	4.53	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	O2D-CGD	4.52	1.44	1.33
27	B	621	SQD	O47-C7	4.52	1.47	1.34
24	b	611	CLA	O2A-CGA	4.52	1.46	1.33
24	d	402	CLA	CHC-C1C	4.52	1.46	1.35
27	a	402	SQD	O48-C23	4.52	1.46	1.33
34	z	101	LMG	O8-C28	4.52	1.46	1.33
24	d	403	CLA	OBD-CAD	4.52	1.28	1.22
24	C	510	CLA	O2A-CGA	4.51	1.46	1.33
26	T	102	BCR	C23-C22	-4.50	1.36	1.45
34	c	919	LMG	O8-C28	4.49	1.46	1.33
26	A	411	BCR	C23-C22	-4.48	1.36	1.45
27	f	102	SQD	O47-C7	4.48	1.46	1.34
24	B	602	CLA	OBD-CAD	4.47	1.28	1.22
25	a	408	PHO	O2D-CGD	4.47	1.44	1.33
24	c	908	CLA	OBD-CAD	4.47	1.28	1.22
27	F	101	SQD	O47-C7	4.47	1.46	1.34
24	a	407	CLA	OBD-CAD	4.47	1.28	1.22
24	B	602	CLA	O2A-CGA	4.46	1.46	1.33
24	B	604	CLA	OBD-CAD	4.45	1.28	1.22
24	b	606	CLA	OBD-CAD	4.45	1.28	1.22
24	C	505	CLA	O2D-CGD	4.45	1.44	1.33
24	C	504	CLA	OBD-CAD	4.45	1.28	1.22
26	B	619	BCR	C23-C22	-4.45	1.36	1.45
24	b	605	CLA	OBD-CAD	4.44	1.28	1.22
34	C	520	LMG	O8-C28	4.44	1.46	1.33
24	b	607	CLA	O2A-CGA	4.44	1.46	1.33
24	b	618	CLA	OBD-CAD	4.44	1.28	1.22
26	a	410	BCR	C23-C22	-4.44	1.36	1.45
24	b	609	CLA	O2A-CGA	4.42	1.46	1.33
24	b	617	CLA	OBD-CAD	4.41	1.28	1.22
24	d	402	CLA	O2A-CGA	4.41	1.46	1.33
24	d	402	CLA	O2D-CGD	4.40	1.43	1.33
24	C	507	CLA	OBD-CAD	4.38	1.28	1.22
24	b	615	CLA	OBD-CAD	4.38	1.28	1.22
24	b	610	CLA	OBD-CAD	4.36	1.28	1.22
24	C	508	CLA	O2D-CGD	4.36	1.43	1.33
24	D	401	CLA	OBD-CAD	4.35	1.28	1.22
24	c	904	CLA	O2D-CGD	4.35	1.43	1.33
25	A	409	PHO	CHD-C1D	4.35	1.47	1.38
26	K	102	BCR	C23-C22	-4.34	1.36	1.45
24	B	607	CLA	O2A-CGA	4.33	1.46	1.33
24	D	402	CLA	OBD-CAD	4.33	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	405	DGD	O2G-C1B	4.32	1.46	1.34
24	C	513	CLA	O2A-CGA	4.32	1.46	1.33
24	D	401	CLA	O2D-CGD	4.32	1.43	1.33
24	B	603	CLA	OBD-CAD	4.32	1.28	1.22
34	C	521	LMG	O7-C10	4.31	1.46	1.34
24	C	513	CLA	OBD-CAD	4.31	1.28	1.22
36	d	406	DGD	O2G-C1B	4.31	1.46	1.34
24	c	907	CLA	OBD-CAD	4.31	1.28	1.22
24	B	610	CLA	O2A-CGA	4.30	1.45	1.33
37	d	409	LHG	O8-C23	4.30	1.45	1.33
34	C	501	LMG	O7-C10	4.30	1.46	1.34
24	b	619	CLA	O2A-CGA	4.29	1.45	1.33
24	c	914	CLA	O2A-CGA	4.29	1.45	1.33
34	b	624	LMG	O8-C28	4.29	1.45	1.33
34	C	501	LMG	O8-C28	4.28	1.45	1.33
24	C	502	CLA	O2A-CGA	4.28	1.45	1.33
34	c	920	LMG	O8-C28	4.27	1.45	1.33
34	Z	101	LMG	O7-C10	4.27	1.46	1.34
27	A	416	SQD	O47-C7	4.26	1.46	1.34
24	c	909	CLA	O2A-CGA	4.26	1.45	1.33
24	b	605	CLA	O2A-CGA	4.26	1.45	1.33
24	D	402	CLA	O2A-CGA	4.26	1.45	1.33
24	c	913	CLA	OBD-CAD	4.25	1.28	1.22
25	a	408	PHO	CHD-C1D	4.25	1.46	1.38
35	b	602	HTG	C1'-S1	-4.25	1.76	1.81
24	C	514	CLA	OBD-CAD	4.25	1.28	1.22
24	C	508	CLA	O2A-CGA	4.25	1.45	1.33
24	B	606	CLA	O2A-CGA	4.25	1.45	1.33
24	b	612	CLA	O2A-CGA	4.25	1.45	1.33
24	c	906	CLA	O2A-CGA	4.24	1.45	1.33
35	B	624	HTG	C1'-S1	-4.24	1.76	1.81
24	B	609	CLA	O2A-CGA	4.24	1.45	1.33
25	a	408	PHO	O2A-CGA	4.24	1.45	1.33
36	d	406	DGD	O1G-C1A	4.24	1.45	1.33
27	L	102	SQD	O47-C7	4.24	1.46	1.34
34	C	521	LMG	O8-C28	4.23	1.45	1.33
24	b	610	CLA	O2A-CGA	4.23	1.45	1.33
37	e	101	LHG	O8-C23	4.23	1.45	1.33
27	A	412	SQD	O48-C23	4.23	1.45	1.33
34	B	622	LMG	O8-C28	4.23	1.45	1.33
24	B	614	CLA	OBD-CAD	4.23	1.28	1.22
24	c	910	CLA	O2A-CGA	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	410	CLA	O2A-CGA	4.22	1.45	1.33
27	A	416	SQD	O48-C23	4.22	1.45	1.33
36	h	102	DGD	O2G-C1B	4.22	1.46	1.34
24	b	618	CLA	O2A-CGA	4.21	1.45	1.33
24	C	512	CLA	O2A-CGA	4.20	1.45	1.33
24	b	620	CLA	O2A-CGA	4.20	1.45	1.33
40	v	202	HEC	CBC-CAC	-4.20	1.33	1.49
25	a	420	PHO	O2A-CGA	4.20	1.45	1.33
27	F	101	SQD	O48-C23	4.20	1.45	1.33
24	B	603	CLA	O2A-CGA	4.20	1.45	1.33
27	a	411	SQD	O48-C23	4.20	1.45	1.33
24	C	507	CLA	O2A-CGA	4.20	1.45	1.33
24	a	407	CLA	O2A-CGA	4.19	1.45	1.33
24	c	913	CLA	O2A-CGA	4.19	1.45	1.33
34	c	920	LMG	O7-C10	4.18	1.46	1.34
24	b	620	CLA	OBD-CAD	4.18	1.28	1.22
27	f	102	SQD	O48-C23	4.18	1.45	1.33
24	c	904	CLA	OBD-CAD	4.17	1.28	1.22
24	C	510	CLA	OBD-CAD	4.17	1.28	1.22
24	C	509	CLA	OBD-CAD	4.16	1.28	1.22
24	c	912	CLA	O2A-CGA	4.16	1.45	1.33
24	C	514	CLA	O2A-CGA	4.16	1.45	1.33
24	b	616	CLA	O2A-CGA	4.15	1.45	1.33
24	B	617	CLA	O2A-CGA	4.14	1.45	1.33
24	c	902	CLA	O2A-CGA	4.14	1.45	1.33
24	D	401	CLA	O2A-CGA	4.14	1.45	1.33
24	b	608	CLA	OBD-CAD	4.13	1.28	1.22
34	a	412	LMG	O8-C28	4.13	1.45	1.33
24	A	405	CLA	O2A-CGA	4.12	1.45	1.33
24	C	503	CLA	OBD-CAD	4.11	1.28	1.22
24	B	608	CLA	O2A-CGA	4.11	1.45	1.33
24	B	612	CLA	O2A-CGA	4.10	1.45	1.33
37	l	101	LHG	O7-C7	4.10	1.45	1.34
37	e	101	LHG	O7-C7	4.10	1.45	1.34
27	L	102	SQD	O48-C23	4.09	1.45	1.33
24	B	616	CLA	O2A-CGA	4.08	1.45	1.33
24	c	903	CLA	O2A-CGA	4.08	1.45	1.33
24	c	902	CLA	OBD-CAD	4.08	1.28	1.22
37	D	408	LHG	O7-C7	4.08	1.45	1.34
40	V	201	HEC	CBC-CAC	-4.08	1.34	1.49
24	c	904	CLA	O2A-CGA	4.07	1.45	1.33
24	c	905	CLA	O2A-CGA	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	d	407	LHG	O8-C23	4.06	1.45	1.33
24	B	604	CLA	O2A-CGA	4.05	1.45	1.33
24	d	401	CLA	O2A-CGA	4.05	1.45	1.33
24	d	403	CLA	O2A-CGA	4.04	1.45	1.33
24	B	611	CLA	O2A-CGA	4.04	1.45	1.33
37	E	101	LHG	O7-C7	4.03	1.45	1.34
24	b	607	CLA	OBD-CAD	4.02	1.27	1.22
34	z	101	LMG	O7-C10	4.02	1.45	1.34
24	A	405	CLA	OBD-CAD	4.01	1.27	1.22
24	b	615	CLA	O2A-CGA	4.01	1.45	1.33
24	c	907	CLA	O2A-CGA	4.01	1.45	1.33
26	B	618	BCR	C23-C22	-4.01	1.37	1.45
27	a	402	SQD	O47-C7	4.01	1.45	1.34
36	c	918	DGD	O1G-C1A	3.99	1.45	1.33
36	c	917	DGD	O1G-C1A	3.99	1.45	1.33
34	B	622	LMG	O7-C10	3.99	1.45	1.34
24	a	409	CLA	O2A-CGA	3.99	1.45	1.33
24	b	614	CLA	O2A-CGA	3.98	1.45	1.33
34	C	520	LMG	O7-C10	3.98	1.45	1.34
35	c	923	HTG	C1'-S1	-3.97	1.76	1.81
40	v	202	HEC	CBB-CAB	-3.97	1.34	1.49
24	C	511	CLA	OBD-CAD	3.96	1.27	1.22
25	A	408	PHO	O2A-CGA	3.96	1.44	1.33
34	a	412	LMG	O7-C10	3.96	1.45	1.34
36	H	102	DGD	O2G-C1B	3.95	1.45	1.34
24	c	911	CLA	O2A-CGA	3.95	1.44	1.33
24	C	504	CLA	O2A-CGA	3.95	1.44	1.33
37	d	409	LHG	O7-C7	3.95	1.45	1.34
34	c	919	LMG	O7-C10	3.94	1.45	1.34
27	B	621	SQD	O48-C23	3.92	1.44	1.33
36	H	102	DGD	O1G-C1A	3.91	1.44	1.33
24	C	506	CLA	O2A-CGA	3.91	1.44	1.33
24	b	608	CLA	O2A-CGA	3.90	1.44	1.33
36	C	519	DGD	O1G-C1A	3.90	1.44	1.33
37	L	101	LHG	O8-C23	3.90	1.44	1.33
35	B	633	HTG	C1'-S1	-3.89	1.76	1.81
40	V	201	HEC	CBB-CAB	-3.89	1.34	1.49
36	c	917	DGD	O2G-C1B	3.89	1.45	1.34
36	C	518	DGD	O1G-C1A	3.88	1.44	1.33
34	j	101	LMG	O8-C28	3.88	1.44	1.33
37	D	406	LHG	O8-C23	3.88	1.44	1.33
37	d	408	LHG	O7-C7	3.88	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	916	DGD	O1G-C1A	3.88	1.44	1.33
25	A	408	PHO	OBD-CAD	3.88	1.29	1.22
24	C	503	CLA	O2A-CGA	3.87	1.44	1.33
37	l	101	LHG	O8-C23	3.87	1.44	1.33
25	A	409	PHO	C3D-C2D	3.87	1.49	1.39
24	b	617	CLA	O2A-CGA	3.86	1.44	1.33
24	B	605	CLA	O2A-CGA	3.86	1.44	1.33
24	C	509	CLA	O2A-CGA	3.85	1.44	1.33
36	h	102	DGD	O1G-C1A	3.85	1.44	1.33
34	j	101	LMG	O7-C10	3.85	1.45	1.34
36	C	519	DGD	O2G-C1B	3.85	1.45	1.34
24	A	407	CLA	O2A-CGA	3.85	1.44	1.33
24	A	406	CLA	OBD-CAD	3.84	1.27	1.22
36	c	918	DGD	O2G-C1B	3.84	1.45	1.34
27	A	412	SQD	O47-C7	3.84	1.45	1.34
34	J	101	LMG	O8-C28	3.84	1.44	1.33
24	B	613	CLA	O2A-CGA	3.84	1.44	1.33
37	D	407	LHG	O7-C7	3.83	1.45	1.34
36	C	517	DGD	O2G-C1B	3.83	1.45	1.34
24	B	614	CLA	O2A-CGA	3.83	1.44	1.33
35	D	411	HTG	C1'-S1	-3.83	1.76	1.81
34	J	101	LMG	O7-C10	3.82	1.45	1.34
25	A	409	PHO	O2A-CGA	3.82	1.44	1.33
24	B	605	CLA	OBD-CAD	3.82	1.27	1.22
37	L	101	LHG	O7-C7	3.81	1.45	1.34
36	C	517	DGD	O1G-C1A	3.80	1.44	1.33
24	C	511	CLA	O2A-CGA	3.80	1.44	1.33
36	c	916	DGD	O2G-C1B	3.77	1.44	1.34
25	A	409	PHO	OBD-CAD	3.76	1.29	1.22
35	B	634	HTG	C1'-S1	-3.76	1.76	1.81
36	C	518	DGD	O2G-C1B	3.76	1.44	1.34
40	v	202	HEC	C3B-C2B	-3.76	1.36	1.40
35	b	627	HTG	C1'-S1	-3.76	1.76	1.81
34	b	624	LMG	O7-C10	3.75	1.44	1.34
27	a	411	SQD	O47-C7	3.74	1.44	1.34
24	b	613	CLA	O2A-CGA	3.73	1.44	1.33
24	b	606	CLA	O2A-CGA	3.72	1.44	1.33
24	A	406	CLA	O2A-CGA	3.72	1.44	1.33
25	A	408	PHO	C4A-NA	-3.71	1.26	1.35
25	a	420	PHO	C3D-C2D	3.69	1.49	1.39
24	B	611	CLA	OBD-CAD	3.69	1.27	1.22
37	d	407	LHG	O7-C7	3.65	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	OBD-CAD	3.60	1.27	1.22
40	V	201	HEC	C3B-C4B	3.60	1.49	1.43
24	a	406	CLA	O2A-CGA	3.59	1.43	1.33
25	a	420	PHO	CHC-C4B	3.59	1.48	1.40
37	d	408	LHG	O8-C23	3.59	1.43	1.33
37	D	408	LHG	O8-C23	3.58	1.43	1.33
25	A	408	PHO	CHC-C4B	3.55	1.48	1.40
35	b	603	HTG	C1'-S1	-3.50	1.76	1.81
37	D	407	LHG	O8-C23	3.50	1.43	1.33
24	d	402	CLA	OBD-CAD	3.49	1.27	1.22
35	C	524	HTG	C1'-S1	-3.49	1.77	1.81
35	d	412	HTG	C1'-S1	-3.49	1.77	1.81
25	a	408	PHO	CHD-C4C	3.48	1.48	1.40
35	B	626	HTG	C1'-S1	-3.47	1.77	1.81
25	A	409	PHO	CHC-C4B	3.44	1.48	1.40
25	a	420	PHO	CHB-C4A	3.43	1.48	1.40
35	V	202	HTG	C1'-S1	-3.42	1.77	1.81
25	A	409	PHO	C4A-NA	-3.42	1.27	1.35
25	a	408	PHO	C3D-C2D	3.37	1.48	1.39
35	C	523	HTG	C1'-S1	-3.34	1.77	1.81
40	v	202	HEC	C3B-C4B	3.32	1.49	1.43
25	A	409	PHO	C3B-C4B	3.31	1.50	1.43
24	c	912	CLA	C1D-C2D	3.28	1.50	1.42
40	V	201	HEC	C3B-C2B	-3.28	1.37	1.40
35	O	303	HTG	C1'-S1	-3.26	1.77	1.81
35	b	626	HTG	C1'-S1	-3.25	1.77	1.81
25	A	408	PHO	C3B-C4B	3.23	1.50	1.43
25	a	408	PHO	CHC-C4B	3.23	1.48	1.40
37	D	406	LHG	O7-C7	3.23	1.43	1.34
25	A	408	PHO	C3D-C2D	3.22	1.47	1.39
24	d	401	CLA	C1D-C2D	3.20	1.49	1.42
24	c	914	CLA	C1D-C2D	3.19	1.49	1.42
25	A	409	PHO	CHD-C4C	3.14	1.47	1.40
35	B	625	HTG	C1'-S1	-3.14	1.77	1.81
25	a	420	PHO	C3B-C4B	3.13	1.49	1.43
24	b	608	CLA	C4C-C3C	3.11	1.50	1.45
25	A	408	PHO	CHB-C4A	3.11	1.47	1.40
25	a	420	PHO	CHD-C4C	3.10	1.47	1.40
25	a	420	PHO	C4A-NA	-3.09	1.27	1.35
27	a	402	SQD	C6-S	-3.08	1.66	1.77
25	a	408	PHO	C4A-NA	-3.06	1.27	1.35
25	A	408	PHO	CHD-C4C	3.06	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C4C-C3C	3.05	1.50	1.45
24	b	608	CLA	C1C-C2C	3.04	1.50	1.44
25	a	420	PHO	OBD-CAD	3.04	1.27	1.22
24	c	906	CLA	C4C-C3C	3.02	1.50	1.45
24	b	610	CLA	C1C-C2C	3.02	1.50	1.44
24	a	406	CLA	C1B-CHB	3.02	1.49	1.41
35	c	922	HTG	C1'-S1	-2.98	1.77	1.81
25	a	408	PHO	OBD-CAD	2.97	1.27	1.22
24	C	512	CLA	C1D-C2D	2.97	1.49	1.42
24	C	510	CLA	C4C-C3C	2.96	1.50	1.45
24	b	605	CLA	C1D-C2D	2.96	1.49	1.42
24	C	507	CLA	C1D-C2D	2.95	1.49	1.42
24	c	911	CLA	C1B-CHB	2.95	1.49	1.41
24	C	502	CLA	C1D-C2D	2.94	1.49	1.42
27	f	102	SQD	C6-S	-2.94	1.66	1.77
24	b	613	CLA	C1C-C2C	2.93	1.50	1.44
27	A	416	SQD	C6-S	-2.92	1.66	1.77
24	C	509	CLA	C4C-C3C	2.92	1.50	1.45
24	B	607	CLA	C1D-C2D	2.91	1.49	1.42
24	b	609	CLA	C1C-C2C	2.91	1.50	1.44
24	C	513	CLA	C1C-C2C	2.89	1.50	1.44
24	b	608	CLA	C1D-C2D	2.89	1.49	1.42
24	D	401	CLA	C4C-C3C	2.88	1.50	1.45
25	a	408	PHO	CHB-C4A	2.88	1.47	1.40
24	d	403	CLA	C1D-C2D	2.88	1.49	1.42
24	B	611	CLA	C1D-C2D	2.87	1.49	1.42
24	C	506	CLA	C4C-C3C	2.87	1.50	1.45
24	b	618	CLA	C1B-CHB	2.86	1.48	1.41
24	c	905	CLA	C1C-C2C	2.86	1.50	1.44
24	b	611	CLA	C1D-C2D	2.86	1.49	1.42
24	B	607	CLA	C4C-C3C	2.85	1.49	1.45
25	A	409	PHO	CHB-C4A	2.85	1.47	1.40
24	C	511	CLA	C4B-CHC	2.83	1.48	1.41
24	c	909	CLA	C4C-C3C	2.82	1.49	1.45
24	b	615	CLA	C1B-CHB	2.82	1.48	1.41
24	B	615	CLA	C1B-CHB	2.82	1.48	1.41
24	C	511	CLA	C1C-C2C	2.82	1.50	1.44
24	B	613	CLA	C1C-C2C	2.81	1.50	1.44
24	C	505	CLA	C1C-C2C	2.80	1.50	1.44
24	C	503	CLA	C1C-C2C	2.80	1.50	1.44
24	C	504	CLA	C1C-C2C	2.80	1.50	1.44
24	c	902	CLA	C1B-CHB	2.79	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1C-C2C	2.79	1.50	1.44
24	c	904	CLA	C4C-C3C	2.79	1.49	1.45
24	B	606	CLA	C4C-C3C	2.78	1.49	1.45
24	a	406	CLA	C4C-C3C	2.78	1.49	1.45
24	a	406	CLA	C1D-C2D	2.78	1.48	1.42
24	B	611	CLA	C1B-CHB	2.78	1.48	1.41
24	b	614	CLA	C1D-C2D	2.77	1.48	1.42
24	C	505	CLA	C1D-C2D	2.76	1.48	1.42
24	B	612	CLA	C4C-C3C	2.76	1.49	1.45
24	C	507	CLA	C1B-CHB	2.76	1.48	1.41
24	D	402	CLA	C4C-C3C	2.76	1.49	1.45
24	c	913	CLA	C1C-C2C	2.75	1.49	1.44
24	B	607	CLA	C1C-C2C	2.75	1.49	1.44
24	B	602	CLA	C1D-C2D	2.75	1.48	1.42
24	c	914	CLA	CHD-C4C	2.74	1.49	1.41
24	d	402	CLA	C4C-C3C	2.74	1.49	1.45
24	D	401	CLA	C1B-CHB	2.74	1.48	1.41
24	C	502	CLA	C1C-C2C	2.74	1.49	1.44
24	C	510	CLA	C1D-C2D	2.74	1.48	1.42
24	C	503	CLA	C4C-C3C	2.73	1.49	1.45
36	H	102	DGD	O5D-C1E	2.73	1.44	1.40
24	b	612	CLA	C4B-CHC	2.73	1.48	1.41
24	A	410	CLA	C1D-C2D	2.73	1.48	1.42
24	c	910	CLA	C1C-C2C	2.73	1.49	1.44
24	b	611	CLA	C1C-C2C	2.73	1.49	1.44
24	B	614	CLA	C1C-C2C	2.72	1.49	1.44
24	C	505	CLA	C1B-CHB	2.72	1.48	1.41
27	a	411	SQD	C6-S	-2.72	1.67	1.77
25	a	420	PHO	C4D-CHA	2.72	1.51	1.43
24	b	612	CLA	C1D-C2D	2.71	1.48	1.42
24	b	607	CLA	C1D-C2D	2.71	1.48	1.42
24	B	615	CLA	C1C-C2C	2.71	1.49	1.44
24	C	514	CLA	C1D-C2D	2.70	1.48	1.42
24	C	508	CLA	C1D-C2D	2.70	1.48	1.42
27	A	412	SQD	C6-S	-2.70	1.67	1.77
24	C	504	CLA	C4C-C3C	2.70	1.49	1.45
24	B	612	CLA	C1D-C2D	2.70	1.48	1.42
24	C	511	CLA	C1B-CHB	2.69	1.48	1.41
24	B	605	CLA	C1B-CHB	2.69	1.48	1.41
24	a	409	CLA	C1D-C2D	2.69	1.48	1.42
24	A	407	CLA	C4B-CHC	2.68	1.48	1.41
34	Z	101	LMG	O8-C28	2.67	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	CHD-C4C	2.67	1.48	1.41
24	D	402	CLA	C1D-C2D	2.67	1.48	1.42
24	C	510	CLA	C1C-C2C	2.67	1.49	1.44
24	B	615	CLA	C1D-C2D	2.67	1.48	1.42
24	b	610	CLA	C1D-C2D	2.67	1.48	1.42
24	B	610	CLA	C1D-C2D	2.66	1.48	1.42
24	C	507	CLA	C4C-C3C	2.66	1.49	1.45
24	A	407	CLA	CHD-C4C	2.66	1.48	1.41
24	b	616	CLA	C1C-C2C	2.66	1.49	1.44
24	b	617	CLA	C1C-C2C	2.65	1.49	1.44
24	B	614	CLA	C4C-C3C	2.65	1.49	1.45
24	C	504	CLA	C1D-C2D	2.65	1.48	1.42
35	c	923	HTG	C1-S1	-2.65	1.76	1.80
24	c	914	CLA	C1C-C2C	2.65	1.49	1.44
25	a	408	PHO	C3B-C4B	2.65	1.48	1.43
31	A	419	PL9	C6-C5	2.65	1.49	1.35
31	a	417	PL9	C6-C5	2.65	1.49	1.35
24	C	512	CLA	C1B-CHB	2.64	1.48	1.41
24	B	609	CLA	C1C-C2C	2.64	1.49	1.44
24	b	606	CLA	C1C-C2C	2.64	1.49	1.44
24	b	605	CLA	CHD-C4C	2.64	1.48	1.41
24	b	616	CLA	C1B-CHB	2.63	1.48	1.41
24	B	605	CLA	C1C-C2C	2.63	1.49	1.44
24	C	503	CLA	C1B-CHB	2.63	1.48	1.41
24	b	606	CLA	C1D-C2D	2.63	1.48	1.42
24	B	602	CLA	CHD-C4C	2.62	1.48	1.41
24	B	612	CLA	C4B-CHC	2.62	1.48	1.41
24	A	407	CLA	C1D-C2D	2.62	1.48	1.42
24	a	407	CLA	C1D-C2D	2.62	1.48	1.42
24	c	911	CLA	C1C-C2C	2.62	1.49	1.44
24	B	611	CLA	C4C-C3C	2.62	1.49	1.45
24	B	604	CLA	C1C-C2C	2.61	1.49	1.44
24	c	905	CLA	C1D-C2D	2.61	1.48	1.42
24	b	619	CLA	C1D-C2D	2.61	1.48	1.42
24	B	609	CLA	C4C-C3C	2.61	1.49	1.45
31	d	405	PL9	C6-C5	2.61	1.48	1.35
31	D	404	PL9	C6-C5	2.61	1.48	1.35
35	B	633	HTG	C1-S1	-2.61	1.76	1.80
24	D	402	CLA	C1C-C2C	2.61	1.49	1.44
24	c	906	CLA	C1C-C2C	2.61	1.49	1.44
24	c	904	CLA	C1D-C2D	2.60	1.48	1.42
27	B	621	SQD	C6-S	-2.60	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	C1B-CHB	2.60	1.48	1.41
24	B	609	CLA	C1D-C2D	2.59	1.48	1.42
24	B	606	CLA	C1B-CHB	2.59	1.48	1.41
24	c	904	CLA	C1C-C2C	2.59	1.49	1.44
24	b	613	CLA	C1B-CHB	2.59	1.48	1.41
24	c	902	CLA	C1C-C2C	2.58	1.49	1.44
24	C	509	CLA	C1C-C2C	2.58	1.49	1.44
25	a	420	PHO	C1A-NA	-2.58	1.32	1.37
24	b	618	CLA	C1C-C2C	2.58	1.49	1.44
24	C	509	CLA	C1D-C2D	2.58	1.48	1.42
24	b	613	CLA	C4B-CHC	2.58	1.48	1.41
24	C	510	CLA	C1B-CHB	2.57	1.48	1.41
24	b	619	CLA	C4C-C3C	2.57	1.49	1.45
24	b	620	CLA	C1B-CHB	2.57	1.48	1.41
24	b	607	CLA	CHD-C4C	2.57	1.48	1.41
24	B	604	CLA	C1D-C2D	2.57	1.48	1.42
27	L	102	SQD	C6-S	-2.57	1.67	1.77
24	B	610	CLA	C1B-CHB	2.57	1.48	1.41
24	B	617	CLA	C1B-CHB	2.56	1.48	1.41
24	c	911	CLA	C4B-CHC	2.56	1.48	1.41
24	b	607	CLA	C4C-C3C	2.56	1.49	1.45
24	C	512	CLA	CHD-C4C	2.56	1.48	1.41
25	A	409	PHO	C1A-NA	-2.56	1.32	1.37
38	e	102	HEM	C3B-C2B	-2.56	1.36	1.40
24	A	410	CLA	C4B-CHC	2.55	1.48	1.41
24	c	903	CLA	C1B-CHB	2.55	1.48	1.41
24	B	614	CLA	C1D-C2D	2.55	1.48	1.42
24	b	614	CLA	CHD-C4C	2.55	1.48	1.41
24	d	403	CLA	C1B-CHB	2.55	1.48	1.41
24	C	506	CLA	C1D-C2D	2.55	1.48	1.42
24	B	603	CLA	C4C-C3C	2.55	1.49	1.45
24	B	608	CLA	C1D-C2D	2.54	1.48	1.42
24	C	508	CLA	CHD-C4C	2.54	1.48	1.41
24	C	507	CLA	CHD-C4C	2.54	1.48	1.41
24	C	506	CLA	C1C-C2C	2.54	1.49	1.44
24	b	614	CLA	C1B-CHB	2.54	1.48	1.41
24	C	503	CLA	CHD-C4C	2.54	1.48	1.41
24	C	504	CLA	CHD-C4C	2.54	1.48	1.41
24	A	410	CLA	C1C-C2C	2.54	1.49	1.44
24	b	606	CLA	C1B-CHB	2.54	1.48	1.41
24	b	607	CLA	C1C-C2C	2.54	1.49	1.44
24	b	609	CLA	C1B-CHB	2.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C4B-CHC	2.53	1.48	1.41
24	c	907	CLA	CHD-C4C	2.53	1.48	1.41
36	h	102	DGD	O5D-C1E	2.53	1.44	1.40
24	c	910	CLA	C4B-CHC	2.53	1.48	1.41
24	a	407	CLA	CHD-C4C	2.53	1.48	1.41
24	C	511	CLA	C4C-C3C	2.53	1.49	1.45
24	b	612	CLA	C4C-C3C	2.53	1.49	1.45
24	a	407	CLA	C4B-CHC	2.53	1.48	1.41
24	C	502	CLA	C4C-C3C	2.52	1.49	1.45
24	b	608	CLA	CHD-C4C	2.52	1.48	1.41
24	c	912	CLA	C1B-CHB	2.52	1.48	1.41
24	B	612	CLA	C1B-CHB	2.52	1.48	1.41
24	c	906	CLA	C1B-CHB	2.52	1.48	1.41
24	C	509	CLA	C1B-CHB	2.52	1.48	1.41
24	b	608	CLA	C4B-CHC	2.52	1.48	1.41
24	c	907	CLA	C1B-CHB	2.52	1.48	1.41
24	c	903	CLA	C4B-CHC	2.52	1.48	1.41
24	c	908	CLA	C1B-CHB	2.51	1.48	1.41
24	c	912	CLA	CHD-C4C	2.51	1.48	1.41
24	b	613	CLA	C1D-C2D	2.51	1.48	1.42
24	b	620	CLA	C1D-C2D	2.51	1.48	1.42
24	B	611	CLA	C4B-CHC	2.51	1.48	1.41
24	A	410	CLA	CHD-C4C	2.51	1.48	1.41
24	d	401	CLA	C1B-CHB	2.51	1.48	1.41
24	B	606	CLA	C1C-C2C	2.50	1.49	1.44
24	b	618	CLA	CHD-C4C	2.50	1.48	1.41
24	A	406	CLA	CHD-C4C	2.50	1.48	1.41
24	b	615	CLA	C4C-C3C	2.50	1.49	1.45
24	B	613	CLA	C1D-C2D	2.50	1.48	1.42
24	c	913	CLA	C4B-CHC	2.50	1.47	1.41
24	c	903	CLA	C1C-C2C	2.50	1.49	1.44
24	c	907	CLA	C1D-C2D	2.50	1.48	1.42
24	B	610	CLA	C1C-C2C	2.50	1.49	1.44
24	C	514	CLA	C1B-CHB	2.49	1.47	1.41
24	b	614	CLA	C4C-C3C	2.49	1.49	1.45
24	c	902	CLA	C4C-C3C	2.49	1.49	1.45
24	c	904	CLA	CHD-C4C	2.49	1.48	1.41
24	b	605	CLA	C4B-CHC	2.49	1.47	1.41
35	d	412	HTG	C1-S1	-2.49	1.76	1.80
24	c	908	CLA	C4C-C3C	2.49	1.49	1.45
24	C	512	CLA	C4C-C3C	2.48	1.49	1.45
24	C	509	CLA	CHD-C4C	2.48	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C1C-C2C	2.48	1.49	1.44
24	B	611	CLA	CHD-C4C	2.48	1.48	1.41
24	B	603	CLA	C1B-CHB	2.48	1.47	1.41
24	c	913	CLA	C4C-C3C	2.48	1.49	1.45
27	F	101	SQD	C6-S	-2.48	1.68	1.77
24	B	616	CLA	C1D-C2D	2.48	1.48	1.42
24	c	908	CLA	CHD-C4C	2.47	1.48	1.41
24	C	511	CLA	CHD-C4C	2.47	1.48	1.41
24	A	405	CLA	C4B-CHC	2.47	1.47	1.41
24	c	910	CLA	CHD-C4C	2.47	1.48	1.41
24	D	402	CLA	C1B-CHB	2.47	1.47	1.41
24	C	505	CLA	CHD-C4C	2.47	1.48	1.41
24	C	505	CLA	C4C-C3C	2.47	1.49	1.45
24	C	502	CLA	C4B-CHC	2.47	1.47	1.41
24	c	904	CLA	C4B-CHC	2.47	1.47	1.41
24	B	609	CLA	CHD-C4C	2.47	1.48	1.41
24	B	615	CLA	CHD-C4C	2.47	1.48	1.41
24	b	617	CLA	C1B-CHB	2.47	1.47	1.41
24	c	908	CLA	C1D-C2D	2.47	1.48	1.42
24	c	908	CLA	C1C-C2C	2.46	1.49	1.44
24	A	407	CLA	C1B-CHB	2.46	1.47	1.41
24	d	403	CLA	C4C-C3C	2.46	1.49	1.45
24	c	905	CLA	C1B-CHB	2.46	1.47	1.41
24	b	614	CLA	C1C-C2C	2.46	1.49	1.44
24	B	612	CLA	CHD-C4C	2.46	1.48	1.41
24	b	617	CLA	C4C-C3C	2.46	1.49	1.45
24	C	508	CLA	C1C-C2C	2.46	1.49	1.44
24	c	910	CLA	C1D-C2D	2.45	1.48	1.42
24	b	615	CLA	C1D-C2D	2.45	1.48	1.42
24	B	608	CLA	CHD-C4C	2.45	1.48	1.41
24	b	609	CLA	CHD-C4C	2.44	1.48	1.41
24	B	613	CLA	C1B-CHB	2.44	1.47	1.41
24	C	506	CLA	CHD-C4C	2.44	1.48	1.41
24	c	905	CLA	C4C-C3C	2.44	1.49	1.45
24	B	602	CLA	C4B-CHC	2.43	1.47	1.41
24	C	511	CLA	C1D-C2D	2.43	1.48	1.42
24	A	406	CLA	C1D-C2D	2.43	1.48	1.42
24	b	612	CLA	C1C-C2C	2.43	1.49	1.44
24	d	402	CLA	C1D-C2D	2.43	1.48	1.42
24	B	604	CLA	C4B-CHC	2.43	1.47	1.41
24	c	911	CLA	CHD-C4C	2.43	1.48	1.41
24	b	610	CLA	CHD-C4C	2.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1B-CHB	2.42	1.47	1.41
24	c	903	CLA	CHD-C4C	2.42	1.48	1.41
24	B	605	CLA	CHD-C4C	2.42	1.48	1.41
24	b	609	CLA	C4B-CHC	2.42	1.47	1.41
24	b	614	CLA	C4B-CHC	2.42	1.47	1.41
24	c	914	CLA	C4C-C3C	2.42	1.49	1.45
29	a	401	LMT	O1'-C1'	2.42	1.44	1.40
24	b	606	CLA	C4C-C3C	2.42	1.49	1.45
24	c	911	CLA	C4C-C3C	2.42	1.49	1.45
24	b	611	CLA	C1B-CHB	2.41	1.47	1.41
24	C	508	CLA	C4B-CHC	2.41	1.47	1.41
24	b	612	CLA	C1B-CHB	2.41	1.47	1.41
24	b	616	CLA	C4B-CHC	2.41	1.47	1.41
24	b	612	CLA	CHD-C4C	2.41	1.48	1.41
25	a	420	PHO	C1C-NC	-2.41	1.33	1.38
24	a	407	CLA	C1C-C2C	2.41	1.49	1.44
24	A	405	CLA	C1D-C2D	2.40	1.48	1.42
24	c	909	CLA	C1D-C2D	2.40	1.48	1.42
24	c	910	CLA	C1B-CHB	2.40	1.47	1.41
24	B	608	CLA	C4B-CHC	2.40	1.47	1.41
24	C	502	CLA	CHD-C4C	2.40	1.48	1.41
24	C	502	CLA	C1B-CHB	2.40	1.47	1.41
24	b	608	CLA	C1B-CHB	2.40	1.47	1.41
24	D	401	CLA	C1C-C2C	2.39	1.49	1.44
24	A	405	CLA	C4C-C3C	2.39	1.49	1.45
36	D	405	DGD	O3G-C1D	2.39	1.44	1.40
24	C	513	CLA	C4B-CHC	2.39	1.47	1.41
24	C	510	CLA	C4B-CHC	2.39	1.47	1.41
24	B	605	CLA	C4B-CHC	2.39	1.47	1.41
24	b	618	CLA	C1D-C2D	2.39	1.48	1.42
24	B	608	CLA	C1B-CHB	2.38	1.47	1.41
24	b	607	CLA	C4B-CHC	2.38	1.47	1.41
24	B	610	CLA	C4B-CHC	2.38	1.47	1.41
24	C	510	CLA	CHD-C4C	2.38	1.47	1.41
24	b	613	CLA	CHD-C4C	2.38	1.47	1.41
25	A	408	PHO	C1A-NA	-2.38	1.32	1.37
24	C	509	CLA	C4B-CHC	2.38	1.47	1.41
24	b	618	CLA	C4C-C3C	2.37	1.49	1.45
24	c	909	CLA	C1C-C2C	2.37	1.49	1.44
24	c	906	CLA	C1D-C2D	2.37	1.47	1.42
24	C	508	CLA	C1B-CHB	2.37	1.47	1.41
24	c	902	CLA	C1D-C2D	2.37	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C4B-CHC	2.36	1.47	1.41
24	C	512	CLA	C1C-C2C	2.36	1.49	1.44
24	B	614	CLA	C4B-CHC	2.36	1.47	1.41
24	C	512	CLA	C1C-NC	-2.36	1.34	1.37
24	b	615	CLA	C1C-C2C	2.36	1.49	1.44
24	c	904	CLA	C1B-CHB	2.36	1.47	1.41
24	c	903	CLA	C1D-C2D	2.36	1.47	1.42
24	b	611	CLA	C4B-CHC	2.36	1.47	1.41
24	a	407	CLA	C1B-CHB	2.35	1.47	1.41
24	A	410	CLA	C1B-CHB	2.35	1.47	1.41
24	a	409	CLA	C1C-C2C	2.35	1.49	1.44
24	C	503	CLA	C4B-CHC	2.35	1.47	1.41
24	D	402	CLA	C4B-CHC	2.35	1.47	1.41
24	b	605	CLA	C1B-CHB	2.35	1.47	1.41
24	B	616	CLA	C4B-CHC	2.35	1.47	1.41
24	c	912	CLA	C4B-CHC	2.34	1.47	1.41
24	b	620	CLA	C4C-C3C	2.34	1.49	1.45
24	B	613	CLA	C4B-CHC	2.34	1.47	1.41
24	C	514	CLA	CHD-C4C	2.34	1.47	1.41
24	d	402	CLA	C1B-NB	-2.34	1.33	1.35
24	A	405	CLA	C1C-C2C	2.33	1.49	1.44
24	d	402	CLA	C4B-CHC	2.33	1.47	1.41
25	A	408	PHO	C4D-CHA	2.33	1.50	1.43
24	A	406	CLA	C4B-CHC	2.33	1.47	1.41
24	B	603	CLA	CHD-C4C	2.33	1.47	1.41
24	d	403	CLA	CHD-C4C	2.33	1.47	1.41
24	c	906	CLA	CHD-C4C	2.33	1.47	1.41
24	C	505	CLA	C4B-CHC	2.33	1.47	1.41
24	b	605	CLA	C1C-C2C	2.32	1.49	1.44
24	b	619	CLA	CHD-C4C	2.32	1.47	1.41
24	d	401	CLA	CHD-C4C	2.32	1.47	1.41
24	c	913	CLA	CHD-C4C	2.32	1.47	1.41
24	b	620	CLA	CHD-C4C	2.32	1.47	1.41
24	C	504	CLA	C4B-CHC	2.32	1.47	1.41
24	A	407	CLA	C1C-C2C	2.32	1.49	1.44
24	B	607	CLA	C1B-CHB	2.32	1.47	1.41
24	B	607	CLA	CHD-C4C	2.32	1.47	1.41
24	C	506	CLA	C1B-CHB	2.32	1.47	1.41
27	B	621	SQD	O6-C1	2.32	1.44	1.40
24	B	604	CLA	C1B-CHB	2.31	1.47	1.41
24	d	402	CLA	C1B-CHB	2.31	1.47	1.41
24	B	616	CLA	C1C-C2C	2.31	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	CLA	C4B-CHC	2.31	1.47	1.41
24	c	914	CLA	C4B-CHC	2.31	1.47	1.41
35	V	202	HTG	C1-S1	-2.30	1.77	1.80
24	a	407	CLA	C4C-C3C	2.30	1.49	1.45
24	b	618	CLA	C4B-CHC	2.30	1.47	1.41
24	c	910	CLA	C4C-C3C	2.30	1.49	1.45
24	C	514	CLA	C4C-C3C	2.29	1.49	1.45
24	c	911	CLA	C1D-C2D	2.29	1.47	1.42
24	C	513	CLA	C1B-CHB	2.29	1.47	1.41
24	b	617	CLA	C4B-CHC	2.29	1.47	1.41
24	C	503	CLA	C1D-C2D	2.28	1.47	1.42
24	a	406	CLA	C1C-C2C	2.28	1.49	1.44
24	b	615	CLA	C4B-CHC	2.28	1.47	1.41
24	c	913	CLA	C1D-C2D	2.28	1.47	1.42
24	c	907	CLA	C4C-C3C	2.28	1.49	1.45
24	C	506	CLA	C1B-NB	-2.27	1.33	1.35
24	C	507	CLA	C1C-C2C	2.27	1.49	1.44
24	b	606	CLA	CHD-C4C	2.27	1.47	1.41
24	c	909	CLA	C4B-CHC	2.27	1.47	1.41
24	B	606	CLA	C4B-CHC	2.27	1.47	1.41
24	B	616	CLA	CHD-C4C	2.27	1.47	1.41
24	c	909	CLA	C1B-CHB	2.26	1.47	1.41
24	B	610	CLA	CHD-C4C	2.26	1.47	1.41
24	b	609	CLA	C1D-C2D	2.26	1.47	1.42
35	b	602	HTG	C1-S1	-2.26	1.77	1.80
24	a	409	CLA	CHD-C4C	2.26	1.47	1.41
24	c	909	CLA	CHD-C4C	2.26	1.47	1.41
35	D	411	HTG	C1-S1	-2.25	1.77	1.80
24	d	403	CLA	C4B-CHC	2.25	1.47	1.41
24	B	614	CLA	CHD-C4C	2.25	1.47	1.41
29	A	417	LMT	O1'-C1'	2.24	1.44	1.40
24	c	913	CLA	C1B-CHB	2.24	1.47	1.41
24	B	617	CLA	C4B-NB	-2.24	1.33	1.35
24	B	609	CLA	C1C-NC	-2.24	1.34	1.37
24	b	620	CLA	C1C-C2C	2.24	1.48	1.44
24	D	401	CLA	C1D-C2D	2.24	1.47	1.42
24	C	508	CLA	C4C-C3C	2.24	1.48	1.45
24	C	513	CLA	CHD-C4C	2.24	1.47	1.41
24	B	617	CLA	C1C-NC	-2.23	1.34	1.37
24	a	409	CLA	C1B-CHB	2.23	1.47	1.41
24	B	604	CLA	CHD-C4C	2.23	1.47	1.41
24	C	514	CLA	C1C-C2C	2.23	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	902	CLA	CHD-C4C	2.22	1.47	1.41
24	B	603	CLA	C1D-C2D	2.22	1.47	1.42
35	b	603	HTG	C1-S1	-2.22	1.77	1.80
24	B	602	CLA	C1C-C2C	2.22	1.48	1.44
24	b	606	CLA	C4B-CHC	2.21	1.47	1.41
24	D	402	CLA	CHD-C4C	2.21	1.47	1.41
24	B	602	CLA	C4C-C3C	2.21	1.48	1.45
24	b	611	CLA	C4C-C3C	2.21	1.48	1.45
24	b	610	CLA	C4B-CHC	2.21	1.47	1.41
24	b	620	CLA	C4B-CHC	2.21	1.47	1.41
24	C	514	CLA	C4B-CHC	2.20	1.47	1.41
24	d	401	CLA	C4B-CHC	2.20	1.47	1.41
24	c	914	CLA	C1B-CHB	2.20	1.47	1.41
24	b	607	CLA	C1B-CHB	2.20	1.47	1.41
24	c	907	CLA	C1C-C2C	2.20	1.48	1.44
24	c	905	CLA	C4B-CHC	2.20	1.47	1.41
35	C	523	HTG	C1-S1	-2.20	1.77	1.80
24	b	616	CLA	C4C-C3C	2.20	1.48	1.45
24	B	611	CLA	C1C-NC	-2.19	1.34	1.37
24	d	402	CLA	CHD-C4C	2.19	1.47	1.41
24	B	605	CLA	C1D-C2D	2.19	1.47	1.42
24	B	617	CLA	C1D-C2D	2.19	1.47	1.42
24	b	619	CLA	C1B-CHB	2.19	1.47	1.41
24	D	401	CLA	CHD-C4C	2.18	1.47	1.41
24	a	409	CLA	C4B-CHC	2.18	1.47	1.41
24	c	907	CLA	C4B-CHC	2.18	1.47	1.41
24	b	617	CLA	C1C-NC	-2.18	1.34	1.37
24	b	613	CLA	C4C-C3C	2.18	1.48	1.45
24	B	602	CLA	C1B-CHB	2.18	1.47	1.41
24	A	407	CLA	C4C-C3C	2.17	1.48	1.45
24	c	907	CLA	C1B-NB	-2.17	1.33	1.35
24	b	615	CLA	CHD-C4C	2.17	1.47	1.41
24	B	613	CLA	CHD-C4C	2.16	1.47	1.41
25	A	409	PHO	C4D-CHA	2.16	1.49	1.43
24	B	616	CLA	C4C-C3C	2.16	1.48	1.45
24	d	403	CLA	C1C-C2C	2.16	1.48	1.44
35	C	524	HTG	C1-S1	-2.16	1.77	1.80
24	C	513	CLA	C1D-C2D	2.15	1.47	1.42
24	c	905	CLA	CHD-C4C	2.15	1.47	1.41
24	A	405	CLA	CHD-C4C	2.15	1.47	1.41
24	B	607	CLA	C1B-NB	-2.15	1.33	1.35
31	a	417	PL9	C2-C3	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	103	HEM	C3B-C2B	-2.14	1.37	1.40
26	a	410	BCR	C12-C13	2.14	1.50	1.45
24	B	609	CLA	C4B-CHC	2.14	1.46	1.41
24	c	912	CLA	C1C-C2C	2.14	1.48	1.44
24	B	608	CLA	C1C-C2C	2.14	1.48	1.44
35	b	627	HTG	C1-S1	-2.14	1.77	1.80
24	c	912	CLA	C4C-C3C	2.12	1.48	1.45
24	B	612	CLA	C1C-C2C	2.12	1.48	1.44
24	C	512	CLA	C4B-NB	-2.12	1.33	1.35
36	C	517	DGD	O5D-C1E	2.12	1.43	1.40
24	B	607	CLA	C4B-CHC	2.12	1.46	1.41
31	D	404	PL9	C2-C3	2.11	1.40	1.34
24	b	617	CLA	CHD-C4C	2.11	1.47	1.41
24	D	401	CLA	C4B-CHC	2.11	1.46	1.41
24	b	619	CLA	C4B-CHC	2.10	1.46	1.41
24	B	615	CLA	C1C-NC	-2.10	1.34	1.37
24	B	617	CLA	C4B-CHC	2.09	1.46	1.41
24	b	617	CLA	C1D-C2D	2.09	1.47	1.42
24	B	616	CLA	C1C-NC	-2.09	1.34	1.37
24	b	611	CLA	CHD-C4C	2.09	1.47	1.41
24	a	409	CLA	C1C-NC	-2.09	1.34	1.37
24	d	401	CLA	C4C-C3C	2.08	1.48	1.45
25	a	408	PHO	C1D-ND	-2.08	1.34	1.38
24	C	507	CLA	C4B-CHC	2.08	1.46	1.41
34	b	624	LMG	O7-C8	-2.08	1.41	1.46
35	B	634	HTG	C1-S1	-2.08	1.77	1.80
24	b	606	CLA	C1C-NC	-2.07	1.34	1.37
24	B	613	CLA	C4C-C3C	2.07	1.48	1.45
36	d	406	DGD	O5D-C1E	2.06	1.43	1.40
31	A	419	PL9	C2-C3	2.06	1.40	1.34
24	b	610	CLA	C1B-CHB	2.06	1.46	1.41
24	b	620	CLA	C1C-NC	-2.06	1.34	1.37
24	B	606	CLA	C1D-C2D	2.05	1.47	1.42
24	b	611	CLA	C1A-CHA	2.05	1.51	1.43
24	B	610	CLA	C4C-C3C	2.04	1.48	1.45
29	f	103	LMT	O1'-C1'	2.04	1.43	1.40
31	d	405	PL9	C2-C3	2.03	1.40	1.34
36	C	519	DGD	O2G-C2G	-2.03	1.41	1.46
29	b	625	LMT	O1'-C1'	2.03	1.43	1.40
24	c	908	CLA	C4B-CHC	2.03	1.46	1.41
24	B	617	CLA	C1C-C2C	2.03	1.48	1.44
24	C	504	CLA	C1B-CHB	2.02	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C4B-CHC	2.02	1.46	1.41
24	B	615	CLA	C4B-CHC	2.02	1.46	1.41
24	B	602	CLA	C1C-NC	-2.01	1.34	1.37
24	A	406	CLA	C1C-C2C	2.01	1.48	1.44
24	B	604	CLA	C4C-C3C	2.01	1.48	1.45
34	c	919	LMG	O1-C1	2.01	1.43	1.40
24	c	903	CLA	C4C-C3C	2.00	1.48	1.45

All (2191) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C4A-NA-C1A	-7.78	103.21	106.71
24	d	402	CLA	C4A-NA-C1A	-7.52	103.33	106.71
25	A	408	PHO	CMD-C2D-C1D	7.42	136.50	125.06
24	b	613	CLA	C4A-NA-C1A	-7.29	103.43	106.71
24	B	616	CLA	C4A-NA-C1A	-7.09	103.52	106.71
24	A	405	CLA	C4A-NA-C1A	-6.94	103.59	106.71
24	c	908	CLA	O2D-CGD-CBD	6.91	123.54	111.27
24	B	606	CLA	C2C-C1C-NC	6.83	116.37	109.97
25	a	420	PHO	CMD-C2D-C1D	6.81	135.55	125.06
25	a	408	PHO	CMD-C2D-C1D	6.78	135.50	125.06
24	C	509	CLA	C4A-NA-C1A	-6.75	103.67	106.71
24	b	607	CLA	C4A-NA-C1A	-6.72	103.68	106.71
24	b	609	CLA	CHD-C4C-C3C	-6.72	114.96	124.84
24	b	611	CLA	CHD-C4C-C3C	-6.67	115.04	124.84
27	F	101	SQD	O6-C1-C2	6.65	118.69	108.30
24	C	513	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
24	B	615	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
35	B	626	HTG	C1'-S1-C1	6.58	112.39	100.09
24	B	607	CLA	C2C-C1C-NC	6.56	116.12	109.97
24	b	610	CLA	C4A-NA-C1A	-6.48	103.79	106.71
24	B	617	CLA	CHD-C4C-C3C	-6.47	115.32	124.84
24	D	401	CLA	C2C-C1C-NC	6.47	116.03	109.97
24	a	406	CLA	C2C-C1C-NC	6.43	116.00	109.97
24	C	506	CLA	C4A-NA-C1A	-6.43	103.82	106.71
24	c	906	CLA	C2C-C1C-NC	6.41	115.98	109.97
24	a	407	CLA	C4A-NA-C1A	-6.40	103.83	106.71
24	b	605	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	b	617	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	B	609	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	b	615	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
24	B	604	CLA	CHD-C4C-C3C	-6.32	115.55	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C2C-C1C-NC	6.31	115.89	109.97
24	d	403	CLA	C2C-C1C-NC	6.31	115.88	109.97
24	c	904	CLA	C4A-NA-C1A	-6.31	103.87	106.71
24	B	617	CLA	O2D-CGD-CBD	6.30	122.46	111.27
24	B	605	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
24	B	603	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
24	b	606	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
24	C	507	CLA	C2C-C1C-NC	6.26	115.83	109.97
24	A	405	CLA	C2C-C1C-NC	6.25	115.83	109.97
24	B	610	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
24	C	509	CLA	C2C-C1C-NC	6.23	115.81	109.97
24	B	608	CLA	C2C-C1C-NC	6.23	115.80	109.97
24	b	619	CLA	C4A-NA-C1A	-6.21	103.91	106.71
24	b	618	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
24	c	908	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	d	402	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	b	619	CLA	C2C-C1C-NC	6.17	115.76	109.97
24	B	616	CLA	CHD-C4C-C3C	-6.17	115.76	124.84
24	a	409	CLA	CHD-C4C-C3C	-6.17	115.76	124.84
24	b	610	CLA	O2D-CGD-CBD	6.16	122.21	111.27
24	c	907	CLA	C2C-C1C-NC	6.11	115.70	109.97
24	A	410	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	C	509	CLA	O2D-CGD-CBD	6.10	122.11	111.27
24	B	609	CLA	C4A-NA-C1A	-6.10	103.97	106.71
24	A	406	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
24	C	504	CLA	C4A-NA-C1A	-6.08	103.97	106.71
24	b	608	CLA	C2C-C1C-NC	6.05	115.64	109.97
24	c	913	CLA	CHD-C4C-C3C	-6.04	115.95	124.84
24	C	508	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
25	A	408	PHO	O2D-CGD-CBD	6.01	121.95	111.27
24	D	401	CLA	C4A-NA-C1A	-6.01	104.00	106.71
24	b	616	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
35	B	634	HTG	C1'-S1-C1	6.01	111.33	100.09
24	b	608	CLA	O2D-CGD-CBD	6.00	121.94	111.27
24	C	512	CLA	C2C-C1C-NC	6.00	115.59	109.97
24	b	614	CLA	C2C-C1C-NC	6.00	115.59	109.97
24	b	611	CLA	C2C-C1C-NC	5.99	115.59	109.97
24	c	903	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	a	407	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
24	A	407	CLA	C4A-NA-C1A	-5.97	104.02	106.71
24	b	613	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
24	b	618	CLA	O2D-CGD-CBD	5.95	121.85	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	b	615	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	B	613	CLA	O2D-CGD-CBD	5.92	121.79	111.27
24	b	617	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
38	E	103	HEM	CAD-CBD-CGD	5.92	122.60	112.67
24	B	608	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	b	612	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	c	902	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
24	C	510	CLA	C2C-C1C-NC	5.91	115.50	109.97
24	c	902	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	d	403	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
24	C	512	CLA	CHD-C4C-C3C	-5.89	116.17	124.84
24	c	904	CLA	C2C-C1C-NC	5.88	115.48	109.97
24	c	911	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
24	b	610	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
24	b	607	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	C	504	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
24	D	402	CLA	CHD-C4C-C3C	-5.85	116.23	124.84
24	C	502	CLA	C2C-C1C-NC	5.85	115.45	109.97
24	c	912	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	C	506	CLA	C2C-C1C-NC	5.83	115.44	109.97
24	C	511	CLA	O2D-CGD-CBD	5.83	121.63	111.27
24	c	910	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	C	505	CLA	O2D-CGD-CBD	5.82	121.62	111.27
24	A	407	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
24	B	611	CLA	C2C-C1C-NC	5.81	115.42	109.97
24	B	606	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	B	614	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	b	620	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	B	613	CLA	C4A-NA-C1A	-5.79	104.10	106.71
24	c	909	CLA	C2C-C1C-NC	5.77	115.38	109.97
24	B	610	CLA	C4A-NA-C1A	-5.77	104.11	106.71
24	b	620	CLA	CHD-C4C-C3C	-5.76	116.36	124.84
24	B	615	CLA	C2C-C1C-NC	5.76	115.37	109.97
24	c	904	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
24	c	905	CLA	O2D-CGD-CBD	5.75	121.48	111.27
24	C	508	CLA	C2C-C1C-NC	5.74	115.35	109.97
35	c	923	HTG	C1'-S1-C1	5.74	110.83	100.09
24	c	906	CLA	O2D-CGD-CBD	5.74	121.46	111.27
24	C	506	CLA	O2D-CGD-CBD	5.73	121.45	111.27
24	B	605	CLA	C2C-C1C-NC	5.71	115.32	109.97
24	B	603	CLA	C4A-NA-C1A	-5.71	104.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	C	503	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
24	c	908	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
25	a	408	PHO	C3D-C2D-C1D	-5.70	97.57	105.87
24	b	612	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
38	e	102	HEM	CAD-CBD-CGD	5.69	122.22	112.67
24	a	409	CLA	C2C-C1C-NC	5.69	115.30	109.97
35	b	603	HTG	C1'-S1-C1	5.68	110.71	100.09
24	B	602	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
24	C	509	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
24	B	614	CLA	C4A-NA-C1A	-5.67	104.16	106.71
25	a	408	PHO	C2D-C1D-ND	5.65	118.32	109.79
24	A	405	CLA	CHD-C4C-C3C	-5.64	116.54	124.84
24	B	611	CLA	C4A-NA-C1A	-5.63	104.18	106.71
24	B	602	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	B	611	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	C	502	CLA	O2D-CGD-CBD	5.61	121.24	111.27
24	b	612	CLA	C2C-C1C-NC	5.60	115.22	109.97
24	c	914	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
24	C	503	CLA	C2C-C1C-NC	5.59	115.21	109.97
24	C	514	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
27	L	102	SQD	O7-S-C6	5.58	113.57	106.94
24	c	905	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
25	a	420	PHO	O2D-CGD-CBD	5.57	121.16	111.27
24	C	511	CLA	C4A-NA-C1A	-5.56	104.21	106.71
24	B	614	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
24	b	618	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	c	905	CLA	C2C-C1C-NC	5.53	115.16	109.97
24	b	614	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
24	c	910	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	C	502	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
24	b	606	CLA	C4A-NA-C1A	-5.51	104.23	106.71
24	b	620	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	C	506	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	C	505	CLA	C2C-C1C-NC	5.50	115.12	109.97
25	A	408	PHO	C3D-C2D-C1D	-5.50	97.86	105.87
24	c	902	CLA	O2D-CGD-CBD	5.50	121.03	111.27
24	C	508	CLA	O2D-CGD-CBD	5.49	121.03	111.27
24	b	616	CLA	O2D-CGD-CBD	5.49	121.03	111.27
24	B	609	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	B	613	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	b	611	CLA	C3C-C4C-NC	5.48	116.72	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C2C-C1C-NC	5.48	115.11	109.97
24	c	906	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
24	A	406	CLA	C2C-C1C-NC	5.46	115.09	109.97
24	c	909	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	c	903	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	b	616	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	c	907	CLA	CHD-C4C-C3C	-5.43	116.86	124.84
24	b	609	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	b	618	CLA	C4A-NA-C1A	-5.42	104.27	106.71
24	c	912	CLA	C4A-NA-C1A	-5.42	104.27	106.71
24	C	510	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
24	b	606	CLA	O2D-CGD-CBD	5.42	120.89	111.27
25	a	420	PHO	C3D-C2D-C1D	-5.39	98.02	105.87
24	B	612	CLA	C2C-C1C-NC	5.39	115.02	109.97
24	d	401	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
24	B	602	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	c	910	CLA	C2C-C1C-NC	5.37	115.00	109.97
25	A	409	PHO	CMD-C2D-C1D	5.37	133.33	125.06
24	C	514	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	C	504	CLA	C2C-C1C-NC	5.36	114.99	109.97
27	a	411	SQD	O47-C7-C8	5.35	123.03	111.50
24	B	607	CLA	O2D-CGD-CBD	5.35	120.77	111.27
24	b	614	CLA	C4A-NA-C1A	-5.34	104.31	106.71
24	b	605	CLA	O2D-CGD-CBD	5.34	120.76	111.27
35	b	626	HTG	C1'-S1-C1	5.33	110.06	100.09
27	a	411	SQD	O6-C1-C2	5.33	116.62	108.30
24	d	402	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
24	c	913	CLA	C4A-NA-C1A	-5.32	104.32	106.71
38	E	103	HEM	CBD-CAD-C3D	-5.31	102.69	112.48
24	B	604	CLA	O2D-CGD-CBD	5.31	120.70	111.27
25	A	408	PHO	C2D-C1D-ND	5.30	117.79	109.79
24	c	903	CLA	O2D-CGD-CBD	5.30	120.68	111.27
24	c	911	CLA	C2C-C1C-NC	5.29	114.93	109.97
24	b	609	CLA	O2D-CGD-CBD	5.29	120.67	111.27
24	B	615	CLA	O2D-CGD-CBD	5.29	120.67	111.27
24	B	606	CLA	C3C-C4C-NC	5.29	116.50	110.57
24	b	620	CLA	O2D-CGD-CBD	5.28	120.66	111.27
24	B	615	CLA	C4A-NA-C1A	-5.28	104.33	106.71
24	B	607	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
24	b	607	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	C	505	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
24	b	606	CLA	C2C-C1C-NC	5.25	114.89	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C2C-C1C-NC	5.24	114.88	109.97
27	A	412	SQD	O6-C1-C2	5.24	116.49	108.30
24	C	505	CLA	C4A-NA-C1A	-5.24	104.35	106.71
24	B	616	CLA	C2C-C1C-NC	5.24	114.88	109.97
24	B	613	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	B	612	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	b	605	CLA	C4A-NA-C1A	-5.22	104.36	106.71
35	c	922	HTG	C1'-S1-C1	5.21	109.84	100.09
24	b	610	CLA	C2C-C1C-NC	5.21	114.85	109.97
24	c	903	CLA	C2C-C1C-NC	5.21	114.85	109.97
24	c	913	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	B	604	CLA	C2C-C1C-NC	5.20	114.84	109.97
24	a	407	CLA	O2D-CGD-CBD	5.19	120.49	111.27
24	b	609	CLA	C4A-NA-C1A	-5.19	104.37	106.71
27	f	102	SQD	O47-C7-C8	5.18	122.67	111.50
24	b	608	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
24	B	603	CLA	O2D-CGD-CBD	5.17	120.46	111.27
24	C	510	CLA	O2D-CGD-CBD	5.17	120.46	111.27
24	C	513	CLA	C4A-NA-C1A	-5.17	104.38	106.71
24	c	914	CLA	C2C-C1C-NC	5.16	114.80	109.97
27	A	412	SQD	O47-C7-C8	5.13	122.56	111.50
24	C	513	CLA	O2D-CGD-CBD	5.12	120.37	111.27
24	b	607	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
24	D	402	CLA	C2C-C1C-NC	5.11	114.76	109.97
24	b	616	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	c	913	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	b	615	CLA	C3C-C4C-NC	5.08	116.27	110.57
24	C	507	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
24	B	606	CLA	C4A-NA-C1A	-5.06	104.43	106.71
25	A	409	PHO	C2D-C1D-ND	5.06	117.42	109.79
24	b	619	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
24	B	610	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	A	410	CLA	C2C-C1C-NC	5.05	114.70	109.97
27	F	101	SQD	O47-C7-C8	5.04	122.37	111.50
36	d	406	DGD	O6E-C5E-C4E	5.04	118.85	109.69
24	C	508	CLA	C4A-NA-C1A	-5.04	104.44	106.71
24	B	617	CLA	C2C-C1C-NC	5.03	114.69	109.97
24	b	606	CLA	C3C-C4C-NC	5.03	116.21	110.57
24	c	912	CLA	C2C-C1C-NC	5.03	114.68	109.97
25	a	420	PHO	C2D-C1D-ND	5.02	117.36	109.79
35	b	627	HTG	O5-C1-C2	5.02	116.62	110.31
24	c	910	CLA	C4A-NA-C1A	-5.01	104.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C3C-C4C-NC	5.00	116.18	110.57
26	K	103	BCR	C7-C8-C9	-4.99	118.70	126.23
24	c	909	CLA	O2D-CGD-CBD	4.98	120.11	111.27
24	b	611	CLA	O2D-CGD-CBD	4.97	120.09	111.27
24	A	405	CLA	C3C-C4C-NC	4.96	116.14	110.57
24	D	401	CLA	O2D-CGD-CBD	4.96	120.08	111.27
35	b	627	HTG	C1'-S1-C1	4.96	109.36	100.09
24	b	605	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	B	606	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	b	615	CLA	O2D-CGD-CBD	4.93	120.03	111.27
24	b	615	CLA	C4A-NA-C1A	-4.92	104.50	106.71
25	A	409	PHO	C3D-C2D-C1D	-4.91	98.71	105.87
24	D	401	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
35	C	523	HTG	C1'-S1-C1	4.90	109.26	100.09
24	B	604	CLA	C4A-NA-C1A	-4.90	104.50	106.71
35	C	524	HTG	C1'-S1-C1	4.88	109.22	100.09
24	d	402	CLA	O2D-CGD-CBD	4.87	119.93	111.27
24	d	403	CLA	C4A-NA-C1A	-4.84	104.53	106.71
35	d	412	HTG	C1'-S1-C1	4.84	109.15	100.09
24	C	513	CLA	C2C-C1C-NC	4.84	114.50	109.97
27	B	621	SQD	O6-C1-C2	4.81	115.82	108.30
24	B	615	CLA	C1D-CHD-C4C	-4.81	116.21	122.56
27	B	621	SQD	O47-C7-C8	4.80	121.85	111.50
24	b	617	CLA	C3C-C4C-NC	4.80	115.95	110.57
24	C	514	CLA	O2D-CGD-CBD	4.79	119.79	111.27
24	b	613	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	b	609	CLA	C3C-C4C-NC	4.79	115.94	110.57
24	B	613	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	d	402	CLA	C3C-C4C-NC	4.76	115.91	110.57
38	e	102	HEM	CBA-CAA-C2A	-4.74	103.75	112.49
26	D	403	BCR	C7-C8-C9	-4.73	119.08	126.23
25	a	420	PHO	C4C-C3C-C2C	-4.73	101.54	106.78
24	b	614	CLA	O2D-CGD-CBD	4.73	119.68	111.27
24	c	906	CLA	C3C-C4C-NC	4.71	115.85	110.57
24	C	503	CLA	C4A-NA-C1A	-4.71	104.59	106.71
24	C	507	CLA	O2D-CGD-CBD	4.70	119.62	111.27
25	A	409	PHO	C1-C2-C3	-4.70	117.92	126.04
24	c	907	CLA	O2D-CGD-CBD	4.69	119.60	111.27
24	C	502	CLA	C4A-NA-C1A	-4.68	104.60	106.71
24	a	406	CLA	C1C-C2C-C3C	-4.68	102.03	106.96
29	b	601	LMT	C1'-O5'-C5'	4.68	122.87	113.69
24	a	407	CLA	C2C-C1C-NC	4.68	114.35	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	408	PHO	O2D-CGD-CBD	4.66	119.55	111.27
24	A	407	CLA	O2D-CGD-CBD	4.65	119.53	111.27
24	d	401	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	a	409	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	c	902	CLA	O2D-CGD-O1D	-4.64	114.77	123.84
24	A	406	CLA	O2D-CGD-CBD	4.63	119.50	111.27
24	B	612	CLA	O2D-CGD-CBD	4.63	119.49	111.27
24	C	504	CLA	O2D-CGD-CBD	4.63	119.49	111.27
27	L	102	SQD	O47-C7-C8	4.62	121.47	111.50
24	c	911	CLA	C4A-NA-C1A	-4.62	104.63	106.71
35	B	633	HTG	C1'-S1-C1	4.62	108.73	100.09
24	D	401	CLA	C3C-C4C-NC	4.62	115.75	110.57
24	A	406	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
36	D	405	DGD	O2G-C1B-C2B	4.61	121.44	111.50
24	b	620	CLA	C3C-C4C-NC	4.61	115.74	110.57
24	B	605	CLA	C3C-C4C-NC	4.61	115.74	110.57
26	K	102	BCR	C33-C5-C6	-4.60	119.36	124.53
24	c	909	CLA	C3C-C4C-NC	4.60	115.73	110.57
24	B	605	CLA	O2D-CGD-CBD	4.59	119.43	111.27
24	c	911	CLA	O2D-CGD-CBD	4.59	119.42	111.27
24	B	617	CLA	C3C-C4C-NC	4.58	115.71	110.57
35	b	627	HTG	C1-O5-C5	4.58	121.02	112.58
27	L	102	SQD	O6-C1-C2	4.57	115.44	108.30
24	b	616	CLA	C2C-C1C-NC	4.57	114.26	109.97
27	A	412	SQD	C45-O47-C7	-4.57	106.55	117.79
24	B	615	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
24	b	613	CLA	O2D-CGD-CBD	4.55	119.36	111.27
24	B	607	CLA	C3C-C4C-NC	4.55	115.68	110.57
24	C	507	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
24	B	603	CLA	C3C-C4C-NC	4.55	115.67	110.57
24	b	618	CLA	C1-C2-C3	-4.55	118.18	126.04
24	C	504	CLA	C3C-C4C-NC	4.54	115.67	110.57
24	B	617	CLA	C1D-CHD-C4C	-4.54	116.56	122.56
24	D	402	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	B	604	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	c	908	CLA	C3C-C4C-NC	4.52	115.64	110.57
24	a	406	CLA	CHD-C4C-C3C	-4.51	118.20	124.84
24	c	904	CLA	C1D-CHD-C4C	-4.51	116.61	122.56
24	B	607	CLA	C1C-C2C-C3C	-4.50	102.22	106.96
24	a	409	CLA	C3C-C4C-NC	4.50	115.61	110.57
26	d	404	BCR	C28-C27-C26	-4.49	106.05	114.08
24	C	503	CLA	C3C-C4C-NC	4.49	115.61	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C3B-C4B-NB	4.49	115.01	109.21
24	c	907	CLA	C4A-NA-C1A	-4.48	104.69	106.71
24	a	407	CLA	C1D-CHD-C4C	-4.48	116.64	122.56
24	C	513	CLA	C3C-C4C-NC	4.48	115.59	110.57
26	C	516	BCR	C7-C8-C9	-4.48	119.47	126.23
34	c	920	LMG	O7-C10-C11	4.48	121.15	111.50
26	y	101	BCR	C33-C5-C6	-4.47	119.50	124.53
24	B	608	CLA	CHD-C4C-C3C	-4.47	118.27	124.84
24	a	406	CLA	C4A-NA-C1A	-4.47	104.70	106.71
24	B	608	CLA	O2D-CGD-CBD	4.46	119.20	111.27
24	B	614	CLA	C3C-C4C-NC	4.46	115.58	110.57
24	c	902	CLA	C3C-C4C-NC	4.46	115.57	110.57
34	z	101	LMG	C3-C4-C5	4.45	118.17	110.24
24	b	608	CLA	C4A-NA-C1A	-4.44	104.71	106.71
24	C	506	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	C	508	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	c	903	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	b	613	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	B	617	CLA	C4A-NA-C1A	-4.43	104.71	106.71
24	b	619	CLA	C3B-C4B-NB	4.43	114.93	109.21
24	d	401	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
24	B	609	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
24	B	605	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
24	A	410	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	B	610	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	b	608	CLA	C3C-C4C-NC	4.38	115.49	110.57
24	B	609	CLA	O2D-CGD-CBD	4.38	119.06	111.27
24	c	914	CLA	C4A-NA-C1A	-4.37	104.74	106.71
24	B	611	CLA	O2D-CGD-CBD	4.36	119.02	111.27
36	d	406	DGD	O2G-C1B-C2B	4.35	120.88	111.50
24	B	602	CLA	C4A-NA-C1A	-4.35	104.75	106.71
24	d	401	CLA	C4A-NA-C1A	-4.35	104.75	106.71
25	a	420	PHO	O2D-CGD-O1D	-4.34	115.35	123.84
31	a	417	PL9	C15-C14-C16	4.34	122.57	115.27
24	b	619	CLA	O2D-CGD-CBD	4.33	118.97	111.27
24	d	403	CLA	C3C-C4C-NC	4.33	115.43	110.57
34	C	521	LMG	O7-C10-C11	4.33	120.83	111.50
26	y	101	BCR	C15-C14-C13	-4.33	121.13	127.31
24	c	904	CLA	C3C-C4C-NC	4.33	115.42	110.57
24	A	407	CLA	C2C-C1C-NC	4.32	114.02	109.97
24	c	905	CLA	C4A-NA-C1A	-4.32	104.76	106.71
24	B	608	CLA	C1C-C2C-C3C	-4.31	102.42	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	917	DGD	O2G-C1B-C2B	4.31	120.79	111.50
34	C	501	LMG	O7-C10-C11	4.29	120.76	111.50
26	t	101	BCR	C33-C5-C6	-4.29	119.71	124.53
24	C	512	CLA	C4A-NA-C1A	-4.29	104.78	106.71
24	C	510	CLA	C4A-NA-C1A	-4.29	104.78	106.71
24	C	514	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	b	610	CLA	C3C-C4C-NC	4.28	115.38	110.57
27	F	101	SQD	C44-O6-C1	-4.28	105.38	113.74
24	C	512	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	b	618	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
31	a	417	PL9	C32-C33-C34	-4.27	117.38	127.66
24	b	610	CLA	CMC-C2C-C1C	4.27	131.54	125.04
24	c	905	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	b	614	CLA	C3C-C4C-NC	4.26	115.35	110.57
24	B	611	CLA	C3C-C4C-NC	4.26	115.35	110.57
24	C	509	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
24	c	911	CLA	C3C-C4C-NC	4.24	115.33	110.57
35	C	524	HTG	C1-O5-C5	4.24	120.40	112.58
24	C	511	CLA	C3C-C4C-NC	4.24	115.32	110.57
26	D	403	BCR	C24-C23-C22	-4.24	119.83	126.23
24	B	610	CLA	O2D-CGD-CBD	4.22	118.77	111.27
24	b	619	CLA	CAC-C3C-C4C	4.22	130.28	124.81
37	l	101	LHG	O7-C7-C8	4.22	120.59	111.50
24	B	609	CLA	C3C-C4C-NC	4.21	115.30	110.57
24	b	612	CLA	O2D-CGD-CBD	4.21	118.74	111.27
24	B	604	CLA	C1D-CHD-C4C	-4.20	117.01	122.56
29	B	623	LMT	O1B-C4'-C3'	4.19	118.44	107.28
24	c	911	CLA	C1-C2-C3	-4.18	118.81	126.04
24	C	507	CLA	C4A-NA-C1A	-4.18	104.83	106.71
24	A	410	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
24	D	402	CLA	O2D-CGD-CBD	4.18	118.69	111.27
24	C	503	CLA	O2D-CGD-CBD	4.18	118.69	111.27
24	C	509	CLA	O2D-CGD-O1D	-4.17	115.68	123.84
34	Z	101	LMG	O7-C10-C11	4.17	120.49	111.50
24	C	503	CLA	C1-C2-C3	-4.16	118.86	126.04
24	B	615	CLA	O2D-CGD-O1D	-4.15	115.72	123.84
24	a	409	CLA	C1-C2-C3	-4.15	118.87	126.04
24	C	502	CLA	C1C-C2C-C3C	-4.15	102.60	106.96
24	A	406	CLA	C4-C3-C5	4.14	122.24	115.27
24	C	512	CLA	C3B-C4B-NB	4.14	114.56	109.21
24	b	608	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
24	c	906	CLA	C3B-C4B-NB	4.14	114.56	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	514	CLA	C3C-C4C-NC	4.13	115.21	110.57
24	B	614	CLA	C3B-C4B-NB	4.13	114.55	109.21
24	b	609	CLA	C1D-CHD-C4C	-4.13	117.10	122.56
24	c	907	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
25	A	408	PHO	C4C-C3C-C2C	-4.12	102.22	106.78
24	b	615	CLA	CAC-C3C-C4C	4.11	130.15	124.81
25	A	409	PHO	O2D-CGD-CBD	4.11	118.58	111.27
34	a	412	LMG	O7-C10-C11	4.11	120.36	111.50
24	c	908	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
24	c	904	CLA	O2D-CGD-CBD	4.11	118.57	111.27
24	b	613	CLA	CMC-C2C-C1C	4.11	131.29	125.04
24	b	619	CLA	C3C-C4C-NC	4.11	115.17	110.57
24	b	610	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
24	c	905	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
35	V	202	HTG	C1'-S1-C1	4.10	107.76	100.09
24	d	403	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
24	B	606	CLA	O2D-CGD-O1D	-4.10	115.83	123.84
24	c	910	CLA	C3C-C4C-NC	4.09	115.16	110.57
34	B	622	LMG	O7-C10-C11	4.09	120.32	111.50
24	b	609	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
24	c	908	CLA	C4A-NA-C1A	-4.09	104.87	106.71
24	C	509	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	C	502	CLA	CBC-CAC-C3C	-4.09	101.16	112.43
27	F	101	SQD	O7-S-C6	4.09	111.80	106.94
24	c	902	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	c	912	CLA	C3C-C4C-NC	4.08	115.15	110.57
24	A	406	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	A	406	CLA	C1D-CHD-C4C	-4.08	117.17	122.56
24	B	616	CLA	C3C-C4C-NC	4.08	115.14	110.57
31	A	419	PL9	C27-C28-C29	-4.07	117.86	127.66
24	A	406	CLA	CMA-C3A-C4A	-4.07	100.84	111.77
35	c	923	HTG	C1-O5-C5	4.06	120.07	112.58
24	C	510	CLA	C3C-C4C-NC	4.05	115.12	110.57
24	c	909	CLA	C3B-C4B-NB	4.05	114.45	109.21
24	B	615	CLA	C3C-C4C-NC	4.05	115.12	110.57
24	C	505	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
31	a	417	PL9	C37-C38-C39	-4.05	117.92	127.66
24	b	617	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	c	902	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	B	605	CLA	C4A-NA-C1A	-4.03	104.89	106.71
24	b	607	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
31	A	419	PL9	C37-C38-C39	-4.03	117.96	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C3B-C4B-NB	4.03	114.42	109.21
37	d	409	LHG	O7-C7-C8	4.02	120.17	111.50
36	C	517	DGD	O2G-C1B-C2B	4.02	120.17	111.50
24	A	407	CLA	CBC-CAC-C3C	-4.02	101.35	112.43
24	C	508	CLA	C1D-CHD-C4C	-4.01	117.27	122.56
24	a	407	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	C	509	CLA	C4D-C3D-CAD	-4.00	106.24	108.47
24	C	512	CLA	C1D-CHD-C4C	-4.00	117.28	122.56
27	B	621	SQD	O7-S-C6	3.99	111.68	106.94
24	c	913	CLA	C3C-C4C-NC	3.99	115.05	110.57
24	d	402	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
24	C	510	CLA	CAC-C3C-C4C	3.99	129.98	124.81
26	c	915	BCR	C7-C8-C9	-3.99	120.21	126.23
24	d	402	CLA	CAC-C3C-C4C	3.98	129.98	124.81
24	c	906	CLA	CAC-C3C-C4C	3.98	129.97	124.81
26	T	102	BCR	C33-C5-C6	-3.98	120.06	124.53
24	C	505	CLA	C3C-C4C-NC	3.97	115.03	110.57
24	C	503	CLA	C4D-C3D-CAD	-3.97	106.25	108.47
24	c	913	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	D	401	CLA	C3B-C4B-NB	3.97	114.34	109.21
24	c	914	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	C	502	CLA	C3C-C4C-NC	3.97	115.02	110.57
24	B	611	CLA	C1D-CHD-C4C	-3.97	117.32	122.56
24	a	409	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
24	b	608	CLA	CAC-C3C-C4C	3.96	129.95	124.81
26	C	515	BCR	C7-C8-C9	-3.95	120.26	126.23
29	C	522	LMT	C1'-O5'-C5'	3.95	121.43	113.69
24	B	606	CLA	C1D-CHD-C4C	-3.95	117.35	122.56
24	b	612	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	b	607	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	B	606	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
24	B	614	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
24	C	508	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
27	A	412	SQD	C1-O5-C5	-3.94	105.96	113.69
24	b	608	CLA	C1-C2-C3	-3.93	119.24	126.04
26	D	403	BCR	C28-C27-C26	-3.93	107.06	114.08
24	A	407	CLA	C1D-CHD-C4C	-3.93	117.37	122.56
24	b	609	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	b	605	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	C	513	CLA	C1D-CHD-C4C	-3.92	117.38	122.56
24	C	510	CLA	C1-C2-C3	-3.91	119.27	126.04
24	c	912	CLA	O2D-CGD-CBD	3.91	118.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	C3B-C4B-NB	3.90	114.26	109.21
27	F	101	SQD	C1-C2-C3	-3.90	101.88	110.00
24	A	405	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
26	h	101	BCR	C38-C26-C25	-3.90	120.15	124.53
26	B	620	BCR	C38-C26-C25	-3.89	120.16	124.53
24	B	608	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	D	401	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	a	406	CLA	C3B-C4B-NB	3.87	114.21	109.21
24	C	504	CLA	C1D-CHD-C4C	-3.85	117.47	122.56
24	B	613	CLA	CMC-C2C-C1C	3.85	130.91	125.04
24	B	602	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	D	402	CLA	C4A-NA-C1A	-3.85	104.98	106.71
36	d	406	DGD	C3E-C4E-C5E	3.85	117.10	110.24
24	b	612	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	c	907	CLA	C3C-C4C-NC	3.84	114.88	110.57
24	B	610	CLA	C1D-CHD-C4C	-3.83	117.50	122.56
24	B	616	CLA	C4D-C3D-CAD	-3.83	106.33	108.47
26	b	621	BCR	C33-C5-C6	-3.83	120.23	124.53
29	B	623	LMT	C3B-C4B-C5B	3.83	117.06	110.24
24	c	910	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	b	616	CLA	C4C-C3C-C2C	-3.82	101.33	106.90
24	B	604	CLA	C4-C3-C5	3.82	121.69	115.27
25	a	420	PHO	C1-C2-C3	-3.81	119.45	126.04
24	c	911	CLA	C1D-CHD-C4C	-3.81	117.53	122.56
24	b	606	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
24	c	907	CLA	C3B-C4B-NB	3.81	114.14	109.21
26	d	404	BCR	C7-C8-C9	-3.81	120.48	126.23
24	b	605	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	C	507	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	b	607	CLA	C1D-CHD-C4C	-3.80	117.54	122.56
24	a	409	CLA	C1D-CHD-C4C	-3.80	117.54	122.56
24	D	401	CLA	C1-C2-C3	-3.80	119.48	126.04
24	b	611	CLA	C4A-NA-C1A	-3.79	105.00	106.71
24	b	611	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	a	406	CLA	CAC-C3C-C4C	3.79	129.73	124.81
29	C	522	LMT	O1B-C4'-C3'	3.79	117.36	107.28
24	c	908	CLA	C1D-CHD-C4C	-3.79	117.56	122.56
25	a	420	PHO	CAC-C3C-C4C	3.79	129.35	125.22
24	b	614	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
24	b	606	CLA	C4C-C3C-C2C	-3.78	101.39	106.90
24	B	613	CLA	CAC-C3C-C4C	3.78	129.72	124.81
24	B	607	CLA	C3B-C4B-NB	3.78	114.09	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	CAC-C3C-C4C	3.78	129.71	124.81
24	C	503	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
37	D	408	LHG	O7-C7-C8	3.77	119.62	111.50
24	C	510	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	b	620	CLA	C3B-C4B-NB	3.76	114.07	109.21
24	B	603	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
24	A	405	CLA	CAA-C2A-C3A	-3.75	102.50	112.78
27	A	412	SQD	C1-C2-C3	-3.75	102.18	110.00
24	C	504	CLA	C1-C2-C3	-3.75	119.56	126.04
24	b	617	CLA	O2D-CGD-CBD	3.75	117.93	111.27
27	A	416	SQD	O47-C7-C8	3.74	119.57	111.50
24	B	617	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
24	c	914	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
24	B	616	CLA	O2D-CGD-CBD	3.74	117.91	111.27
24	C	506	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
35	B	624	HTG	C1'-S1-C1	3.73	107.08	100.09
24	B	602	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
24	c	904	CLA	C1C-C2C-C3C	-3.73	103.03	106.96
25	A	409	PHO	C4C-C3C-C2C	-3.73	102.65	106.78
24	C	502	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	b	615	CLA	C3B-C4B-NB	3.72	114.02	109.21
38	E	103	HEM	CBA-CAA-C2A	-3.72	105.62	112.49
35	b	602	HTG	C1'-S1-C1	3.72	107.05	100.09
34	z	101	LMG	O6-C5-C4	3.72	116.45	109.69
24	B	611	CLA	C3B-C4B-NB	3.72	114.02	109.21
24	b	606	CLA	CAC-C3C-C4C	3.72	129.63	124.81
24	c	909	CLA	CAC-C3C-C4C	3.71	129.63	124.81
24	b	620	CLA	C1D-CHD-C4C	-3.70	117.68	122.56
24	c	902	CLA	C3B-C4B-NB	3.69	113.98	109.21
24	C	514	CLA	C1-C2-C3	-3.69	119.66	126.04
34	z	101	LMG	O7-C10-C11	3.69	119.45	111.50
24	C	511	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	B	612	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	C	502	CLA	CMC-C2C-C1C	3.69	130.65	125.04
36	c	918	DGD	O2G-C1B-C2B	3.68	119.44	111.50
24	a	409	CLA	CAA-C2A-C3A	-3.68	102.69	112.78
24	C	513	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	C	505	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
24	c	910	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
24	b	620	CLA	CAC-C3C-C4C	3.68	129.58	124.81
27	L	102	SQD	C3-C4-C5	3.68	116.80	110.24
25	a	408	PHO	C4C-C3C-C2C	-3.67	102.72	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	411	SQD	C1-O5-C5	-3.67	106.48	113.69
24	B	602	CLA	C1D-CHD-C4C	-3.67	117.72	122.56
24	B	609	CLA	CMB-C2B-C3B	3.67	131.54	124.68
24	b	606	CLA	C1D-CHD-C4C	-3.67	117.72	122.56
24	c	914	CLA	O2D-CGD-CBD	3.66	117.78	111.27
24	b	611	CLA	C3B-C4B-NB	3.66	113.95	109.21
24	b	607	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
24	B	611	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
26	k	102	BCR	C20-C21-C22	-3.66	122.09	127.31
24	A	406	CLA	CHD-C4C-NC	3.66	129.96	124.20
24	A	406	CLA	CBC-CAC-C3C	-3.65	102.36	112.43
24	b	618	CLA	C1D-CHD-C4C	-3.65	117.73	122.56
26	B	618	BCR	C33-C5-C6	-3.65	120.42	124.53
24	b	610	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
24	B	617	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
35	V	202	HTG	C1-C2-C3	-3.65	103.38	110.59
24	d	403	CLA	O2D-CGD-CBD	3.65	117.75	111.27
31	a	417	PL9	C27-C28-C29	-3.65	118.88	127.66
24	b	613	CLA	CAC-C3C-C4C	3.64	129.53	124.81
24	A	410	CLA	CMC-C2C-C1C	3.64	130.58	125.04
25	A	408	PHO	C1-C2-C3	-3.63	119.77	126.04
24	C	505	CLA	C3B-C4B-NB	3.63	113.90	109.21
24	B	617	CLA	C3B-C4B-NB	3.62	113.90	109.21
26	H	101	BCR	C38-C26-C25	-3.62	120.46	124.53
24	C	514	CLA	C1D-CHD-C4C	-3.62	117.78	122.56
24	c	910	CLA	C1D-CHD-C4C	-3.62	117.78	122.56
24	B	615	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	a	407	CLA	CAC-C3C-C4C	3.62	129.50	124.81
24	c	903	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	615	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
34	B	622	LMG	O8-C28-C29	3.61	123.22	111.91
24	b	607	CLA	C4-C3-C5	3.61	121.34	115.27
24	B	604	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	d	401	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	c	906	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	A	410	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	b	618	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	B	604	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
24	B	609	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	A	407	CLA	CAC-C3C-C4C	3.59	129.47	124.81
26	K	103	BCR	C20-C21-C22	-3.59	122.19	127.31
24	b	611	CLA	CAA-C2A-C3A	-3.58	102.97	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	916	DGD	O2G-C1B-C2B	3.58	119.22	111.50
26	D	403	BCR	C38-C26-C25	-3.58	120.51	124.53
27	a	411	SQD	C45-O47-C7	-3.57	108.99	117.79
36	D	405	DGD	C1D-C2D-C3D	3.57	117.44	110.00
24	A	405	CLA	C1D-CHD-C4C	-3.57	117.85	122.56
27	A	416	SQD	O48-C23-C24	3.57	123.10	111.91
24	b	619	CLA	C4-C3-C5	3.57	121.27	115.27
26	k	101	BCR	C15-C14-C13	-3.56	122.23	127.31
24	B	612	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
37	E	101	LHG	O7-C7-C8	3.56	119.17	111.50
26	b	623	BCR	C3-C4-C5	-3.56	107.72	114.08
24	c	908	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
24	B	604	CLA	CAA-C2A-C3A	-3.56	103.04	112.78
29	b	601	LMT	O5'-C5'-C4'	3.56	117.25	109.75
38	e	102	HEM	CBD-CAD-C3D	-3.55	105.93	112.48
24	b	605	CLA	C1D-CHD-C4C	-3.55	117.87	122.56
24	c	911	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	C	510	CLA	C3B-C4B-NB	3.55	113.80	109.21
26	a	410	BCR	C7-C8-C9	-3.55	120.87	126.23
24	c	907	CLA	C1D-CHD-C4C	-3.55	117.87	122.56
24	b	620	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
24	c	911	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
24	c	905	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	b	619	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
24	c	903	CLA	O2D-CGD-O1D	-3.55	116.91	123.84
24	b	607	CLA	O2A-CGA-O1A	-3.55	114.64	123.59
27	F	101	SQD	C1-O5-C5	-3.54	106.73	113.69
24	A	407	CLA	C3C-C4C-NC	3.54	114.54	110.57
34	c	919	LMG	O7-C10-C11	3.54	119.14	111.50
24	C	512	CLA	CAC-C3C-C4C	3.54	129.41	124.81
24	d	402	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	a	407	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
24	c	908	CLA	C3B-C4B-NB	3.54	113.78	109.21
31	A	419	PL9	C7-C8-C9	-3.54	120.90	126.79
24	b	607	CLA	C3B-C4B-NB	3.54	113.78	109.21
24	C	506	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
24	b	620	CLA	C4D-C3D-CAD	-3.53	106.50	108.47
24	B	606	CLA	CAC-C3C-C4C	3.53	129.39	124.81
24	c	907	CLA	C1-C2-C3	-3.53	119.94	126.04
24	b	618	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
24	b	606	CLA	C3B-C4B-NB	3.52	113.77	109.21
24	C	512	CLA	C1C-C2C-C3C	-3.52	103.25	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	C1-C2-C3	-3.52	119.95	126.04
24	b	608	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	b	607	CLA	O2A-CGA-CBA	3.52	122.96	111.91
24	B	607	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	B	616	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
24	c	907	CLA	CBC-CAC-C3C	-3.51	102.75	112.43
37	e	101	LHG	O7-C7-C8	3.51	119.07	111.50
24	b	614	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
24	b	612	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
24	b	619	CLA	C1-C2-C3	-3.51	119.98	126.04
24	b	617	CLA	C3B-C4B-NB	3.50	113.74	109.21
24	C	514	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
24	B	615	CLA	CHD-C4C-NC	3.50	129.72	124.20
24	b	605	CLA	CHD-C4C-NC	3.50	129.72	124.20
31	D	404	PL9	C7-C8-C9	-3.50	120.96	126.79
24	B	611	CLA	CHC-C1C-C2C	-3.50	117.04	126.72
24	a	406	CLA	CHC-C1C-C2C	-3.50	117.04	126.72
24	B	605	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
24	B	612	CLA	CAC-C3C-C4C	3.50	129.35	124.81
24	B	608	CLA	C3B-C4B-NB	3.50	113.73	109.21
24	A	407	CLA	C4-C3-C5	3.49	121.15	115.27
24	a	406	CLA	CAA-C2A-C3A	-3.49	103.21	112.78
24	B	612	CLA	C3B-C4B-NB	3.49	113.72	109.21
24	c	909	CLA	C1-C2-C3	-3.49	120.01	126.04
24	C	505	CLA	C4-C3-C5	3.49	121.14	115.27
24	b	615	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
24	A	406	CLA	CAA-C2A-C3A	-3.49	103.23	112.78
24	a	409	CLA	C3B-C4B-NB	3.48	113.71	109.21
24	c	906	CLA	C4A-NA-C1A	-3.48	105.14	106.71
24	B	610	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
31	a	417	PL9	C22-C23-C24	-3.48	119.29	127.66
24	C	509	CLA	C3B-C4B-NB	3.47	113.70	109.21
24	B	608	CLA	CAA-C2A-C3A	-3.47	103.28	112.78
24	c	909	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
25	a	420	PHO	C4-C3-C5	3.47	121.11	115.27
24	B	616	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
24	c	912	CLA	C1D-CHD-C4C	-3.46	117.99	122.56
24	B	604	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
24	A	405	CLA	C3B-C4B-NB	3.46	113.68	109.21
24	d	402	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
26	C	515	BCR	C38-C26-C25	-3.45	120.65	124.53
24	b	619	CLA	CHC-C1C-C2C	-3.45	117.17	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C4A-NA-C1A	-3.45	105.16	106.71
24	B	604	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	c	910	CLA	C1-C2-C3	-3.45	120.08	126.04
24	C	504	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	b	607	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	C	503	CLA	C1D-CHD-C4C	-3.44	118.01	122.56
24	C	506	CLA	CAC-C3C-C4C	3.44	129.28	124.81
37	D	406	LHG	O8-C23-O10	-3.44	114.91	123.59
35	B	625	HTG	C1'-S1-C1	3.44	106.52	100.09
24	b	610	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
24	C	511	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
24	B	603	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
26	c	915	BCR	C33-C5-C6	-3.43	120.68	124.53
29	B	623	LMT	C4B-C3B-C2B	3.43	116.81	110.82
24	a	406	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
31	d	405	PL9	C53-C6-C1	3.42	121.98	114.99
24	C	511	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
24	C	514	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	B	613	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	A	406	CLA	O2A-CGA-O1A	-3.41	114.98	123.59
26	B	619	BCR	C29-C30-C25	3.41	115.73	110.48
24	b	610	CLA	C3B-C4B-NB	3.41	113.62	109.21
27	f	102	SQD	C1-O5-C5	3.41	120.38	113.69
24	c	909	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
24	C	504	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
24	B	605	CLA	C3B-C4B-NB	3.40	113.61	109.21
34	C	520	LMG	O7-C10-C11	3.40	118.84	111.50
24	c	906	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
24	c	910	CLA	C3B-C4B-NB	3.40	113.61	109.21
24	b	611	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
24	c	907	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	B	612	CLA	C1-C2-C3	-3.40	120.16	126.04
24	D	402	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
24	C	502	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	b	616	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
24	C	502	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
24	b	614	CLA	CMA-C3A-C4A	-3.39	102.66	111.77
34	c	920	LMG	C3-C4-C5	3.39	116.29	110.24
24	b	617	CLA	C4A-NA-C1A	-3.39	105.18	106.71
31	D	404	PL9	C53-C6-C1	3.39	121.92	114.99
24	B	613	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
24	B	606	CLA	C4C-C3C-C2C	-3.39	101.96	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C1-C2-C3	-3.38	120.19	126.04
26	k	102	BCR	C24-C23-C22	-3.38	121.13	126.23
24	b	617	CLA	C1-C2-C3	-3.38	120.20	126.04
24	c	913	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
24	A	410	CLA	CHD-C4C-NC	3.38	129.52	124.20
24	b	617	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
24	d	402	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
24	d	401	CLA	C1D-CHD-C4C	-3.37	118.12	122.56
31	d	405	PL9	C10-C9-C11	3.36	120.93	115.27
34	C	520	LMG	O8-C28-C29	3.36	122.46	111.91
24	b	616	CLA	CAC-C3C-C4C	3.36	129.17	124.81
24	B	611	CLA	CAC-C3C-C4C	3.36	129.17	124.81
24	B	605	CLA	C1-C2-C3	-3.36	120.24	126.04
24	b	613	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
24	d	401	CLA	CHC-C1C-C2C	-3.35	117.44	126.72
24	A	406	CLA	C4D-C3D-CAD	-3.35	106.60	108.47
24	C	507	CLA	CHC-C1C-C2C	-3.35	117.45	126.72
24	B	612	CLA	C1D-CHD-C4C	-3.35	118.13	122.56
24	C	509	CLA	C1-C2-C3	-3.35	120.25	126.04
24	b	615	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
27	a	411	SQD	O47-C7-O49	-3.35	115.61	123.70
24	b	607	CLA	CAC-C3C-C4C	3.34	129.15	124.81
27	A	412	SQD	C44-O6-C1	-3.34	107.21	113.74
24	C	510	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	C	505	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
31	d	405	PL9	C7-C8-C9	-3.34	121.24	126.79
24	c	910	CLA	CMC-C2C-C1C	3.34	130.12	125.04
24	C	511	CLA	C3B-C4B-NB	3.33	113.52	109.21
35	c	923	HTG	O5-C1-C2	3.33	114.50	110.31
24	c	904	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	B	610	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	c	904	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	b	618	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
26	K	102	BCR	C38-C26-C25	-3.33	120.79	124.53
24	B	611	CLA	OBD-CAD-C3D	-3.32	122.46	127.98
26	b	623	BCR	C38-C26-C25	-3.32	120.80	124.53
24	C	507	CLA	C3C-C4C-NC	3.32	114.30	110.57
24	d	402	CLA	O2A-CGA-CBA	3.32	122.33	111.91
24	a	407	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
24	d	403	CLA	C1D-CHD-C4C	-3.32	118.18	122.56
24	B	609	CLA	C1D-CHD-C4C	-3.32	118.18	122.56
24	c	914	CLA	CAC-C3C-C4C	3.31	129.11	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C3B-C4B-NB	3.31	113.49	109.21
26	d	404	BCR	C33-C5-C6	-3.31	120.81	124.53
24	D	402	CLA	C3B-C4B-NB	3.31	113.48	109.21
24	C	509	CLA	C1D-CHD-C4C	-3.31	118.19	122.56
24	C	507	CLA	CBC-CAC-C3C	-3.31	103.32	112.43
24	C	503	CLA	OBD-CAD-C3D	-3.30	122.50	127.98
24	b	616	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
24	b	616	CLA	OBD-CAD-C3D	-3.30	122.50	127.98
24	a	406	CLA	C3C-C4C-NC	3.30	114.27	110.57
31	A	419	PL9	C20-C19-C21	3.30	120.82	115.27
24	c	914	CLA	C1D-CHD-C4C	-3.30	118.21	122.56
24	D	401	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
36	C	518	DGD	O2G-C1B-C2B	3.30	118.60	111.50
24	b	609	CLA	OBD-CAD-C3D	-3.30	122.51	127.98
31	A	419	PL9	C53-C6-C1	3.29	121.72	114.99
24	B	603	CLA	C1D-CHD-C4C	-3.28	118.22	122.56
24	b	609	CLA	CMC-C2C-C1C	3.28	130.04	125.04
27	a	402	SQD	O47-C7-C8	3.28	118.58	111.50
24	B	615	CLA	CMC-C2C-C1C	3.28	130.03	125.04
24	A	410	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
24	b	614	CLA	C3B-C4B-NB	3.28	113.44	109.21
24	D	402	CLA	C4-C3-C5	3.27	120.78	115.27
24	c	912	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
24	C	504	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	b	619	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
24	B	607	CLA	C1D-CHD-C4C	-3.27	118.25	122.56
24	b	610	CLA	C4-C3-C5	3.26	120.76	115.27
24	A	410	CLA	C3B-C4B-NB	3.26	113.43	109.21
24	d	402	CLA	C4D-C3D-CAD	-3.25	106.66	108.47
24	B	604	CLA	CMB-C2B-C3B	3.25	130.77	124.68
24	A	410	CLA	O2D-CGD-CBD	3.25	117.05	111.27
24	B	610	CLA	CMC-C2C-C1C	3.25	129.99	125.04
24	C	513	CLA	CHD-C4C-NC	3.25	129.33	124.20
24	c	906	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
24	c	906	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
34	c	919	LMG	O8-C28-C29	3.25	122.11	111.91
24	b	620	CLA	CMB-C2B-C3B	3.25	130.76	124.68
24	c	905	CLA	CMC-C2C-C1C	3.25	129.98	125.04
24	c	912	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	B	607	CLA	C4-C3-C5	3.24	120.72	115.27
31	A	419	PL9	C22-C23-C24	-3.24	119.86	127.66
24	B	613	CLA	O2D-CGD-O1D	-3.24	117.50	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	407	LHG	O7-C7-C8	3.24	118.47	111.50
31	a	417	PL9	C7-C8-C9	-3.23	121.41	126.79
24	b	613	CLA	C1-C2-C3	-3.23	120.45	126.04
24	A	406	CLA	CMB-C2B-C3B	3.23	130.73	124.68
24	c	907	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
24	C	507	CLA	C1D-CHD-C4C	-3.23	118.29	122.56
37	D	406	LHG	O8-C23-C24	3.22	122.03	111.91
24	B	607	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	C	506	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
24	A	407	CLA	C3B-C4B-NB	3.22	113.37	109.21
24	D	401	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
37	D	407	LHG	O7-C7-C8	3.22	118.44	111.50
24	C	502	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
24	c	909	CLA	C4-C3-C5	3.22	120.68	115.27
24	D	402	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
24	b	609	CLA	C4-C3-C5	3.21	120.68	115.27
24	d	401	CLA	C2A-C1A-CHA	-3.21	118.24	123.86
27	A	412	SQD	O48-C23-C24	3.21	121.99	111.91
24	c	906	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
24	b	617	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	b	608	CLA	C3B-C4B-NB	3.21	113.36	109.21
24	C	512	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
24	d	403	CLA	CAC-C3C-C4C	3.21	128.97	124.81
24	C	503	CLA	C3B-C4B-NB	3.21	113.35	109.21
24	C	512	CLA	O2D-CGD-CBD	3.20	116.96	111.27
24	A	406	CLA	C3C-C4C-NC	3.20	114.16	110.57
26	D	403	BCR	C15-C14-C13	-3.20	122.75	127.31
27	f	102	SQD	O5-C5-C4	3.19	115.50	109.69
24	C	507	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
37	d	408	LHG	O7-C7-C8	3.19	118.38	111.50
24	A	410	CLA	C4-C3-C5	3.19	120.64	115.27
24	C	509	CLA	C2A-C1A-CHA	-3.19	118.28	123.86
24	b	616	CLA	C4-C3-C5	3.19	120.64	115.27
24	B	604	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
24	b	612	CLA	C3B-C4B-NB	3.19	113.33	109.21
37	E	101	LHG	O8-C23-C24	3.19	121.91	111.91
24	c	914	CLA	CMC-C2C-C1C	3.19	129.89	125.04
26	d	404	BCR	C29-C30-C25	3.18	115.38	110.48
24	a	407	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	B	614	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
35	V	202	HTG	O5-C1-C2	-3.18	106.32	110.31
34	b	624	LMG	O8-C28-C29	3.17	121.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	O2A-CGA-CBA	3.17	121.86	111.91
24	C	507	CLA	C1-C2-C3	-3.17	120.56	126.04
24	c	912	CLA	CMB-C2B-C3B	3.17	130.61	124.68
24	A	405	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	c	905	CLA	C1-C2-C3	-3.17	120.56	126.04
24	A	406	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
24	b	616	CLA	C3B-C4B-NB	3.16	113.30	109.21
24	d	403	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
27	a	402	SQD	O48-C23-C24	3.16	121.82	111.91
24	D	401	CLA	CHC-C1C-C2C	-3.16	117.99	126.72
25	A	408	PHO	C2A-C1A-NA	3.16	115.48	111.86
24	b	612	CLA	O2A-CGA-CBA	3.16	121.81	111.91
24	b	617	CLA	CMC-C2C-C1C	3.16	129.84	125.04
27	A	412	SQD	O8-S-C6	3.15	110.77	105.74
24	B	616	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	514	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
24	C	510	CLA	C1D-CHD-C4C	-3.15	118.40	122.56
27	f	102	SQD	O7-S-C6	3.15	110.69	106.94
26	c	915	BCR	C38-C26-C25	-3.15	120.99	124.53
26	d	404	BCR	C3-C4-C5	-3.15	108.45	114.08
24	B	604	CLA	O2A-CGA-CBA	3.15	121.80	111.91
24	A	407	CLA	CHD-C4C-NC	3.15	129.17	124.20
24	A	405	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	b	617	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	503	CLA	CAC-C3C-C4C	3.15	128.90	124.81
24	C	505	CLA	CMC-C2C-C1C	3.15	129.83	125.04
24	c	903	CLA	C1D-CHD-C4C	-3.14	118.41	122.56
24	b	618	CLA	CAC-C3C-C4C	3.14	128.89	124.81
24	B	611	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
31	a	417	PL9	C10-C9-C11	3.14	120.55	115.27
24	b	619	CLA	C1D-CHD-C4C	-3.14	118.42	122.56
24	c	909	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
25	a	408	PHO	CMB-C2B-C1B	3.14	129.90	125.06
24	B	616	CLA	C3B-C4B-NB	3.14	113.26	109.21
26	H	101	BCR	C37-C22-C21	-3.13	118.54	122.92
24	c	913	CLA	C3B-C4B-NB	3.13	113.25	109.21
24	b	618	CLA	OBD-CAD-C3D	-3.12	122.80	127.98
24	a	406	CLA	C2A-C1A-CHA	-3.12	118.40	123.86
24	B	603	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	d	401	CLA	CBC-CAC-C3C	-3.12	103.83	112.43
24	A	407	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
24	B	616	CLA	O2D-CGD-O1D	-3.12	117.74	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
24	C	503	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
24	C	513	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	c	914	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	A	406	CLA	CMC-C2C-C1C	3.11	129.78	125.04
24	a	406	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
24	C	512	CLA	C4-C3-C5	3.11	120.50	115.27
24	b	609	CLA	CHD-C4C-NC	3.11	129.10	124.20
25	a	408	PHO	CAC-C3C-C4C	3.11	128.61	125.22
24	C	504	CLA	C4-C3-C5	3.11	120.50	115.27
24	d	402	CLA	CHC-C1C-C2C	-3.10	118.13	126.72
24	B	611	CLA	C4D-C3D-CAD	-3.10	106.74	108.47
31	a	417	PL9	C30-C29-C31	3.10	120.49	115.27
24	B	616	CLA	CHD-C4C-NC	3.10	129.09	124.20
24	c	910	CLA	CAC-C3C-C4C	3.10	128.83	124.81
24	B	605	CLA	O2A-CGA-O1A	-3.10	115.77	123.59
24	B	613	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
26	b	622	BCR	C28-C27-C26	-3.09	108.55	114.08
27	a	411	SQD	O8-S-C6	3.09	110.67	105.74
31	a	417	PL9	C17-C18-C19	-3.09	120.21	127.66
24	a	406	CLA	CAA-C2A-C1A	-3.09	101.85	111.97
29	m	104	LMT	C1'-O5'-C5'	3.09	119.75	113.69
24	c	910	CLA	CMB-C2B-C3B	3.09	130.46	124.68
31	A	419	PL9	C32-C33-C34	-3.09	120.23	127.66
24	a	406	CLA	O2A-CGA-CBA	3.09	121.59	111.91
24	C	509	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
24	c	902	CLA	C1D-CHD-C4C	-3.08	118.49	122.56
24	b	607	CLA	C5-C3-C2	-3.08	114.88	121.12
24	B	603	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	C	504	CLA	CAC-C3C-C4C	3.08	128.81	124.81
24	b	619	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	c	909	CLA	C4A-NA-C1A	-3.08	105.32	106.71
24	a	407	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
31	D	404	PL9	C10-C9-C11	3.07	120.44	115.27
24	A	405	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
31	a	417	PL9	C42-C43-C44	-3.07	120.27	127.66
26	k	101	BCR	C33-C5-C6	-3.07	121.08	124.53
24	B	610	CLA	CAC-C3C-C4C	3.07	128.79	124.81
24	b	605	CLA	C4-C3-C5	3.07	120.43	115.27
24	B	610	CLA	O2A-CGA-CBA	3.07	121.53	111.91
24	b	614	CLA	CAC-C3C-C4C	3.07	128.79	124.81
24	b	616	CLA	C1-C2-C3	-3.07	120.74	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	c	912	CLA	CAC-C3C-C4C	3.06	128.79	124.81
24	c	912	CLA	C1-C2-C3	-3.06	120.74	126.04
24	b	614	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	C	509	CLA	C4-C3-C5	3.06	120.41	115.27
24	B	612	CLA	C4-C3-C5	3.06	120.41	115.27
24	b	618	CLA	C2A-C1A-CHA	-3.06	118.52	123.86
24	c	903	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
24	B	614	CLA	C4-C3-C5	3.05	120.41	115.27
24	C	514	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
24	b	610	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
24	c	908	CLA	CAC-C3C-C4C	3.05	128.76	124.81
24	B	608	CLA	CAC-C3C-C4C	3.04	128.76	124.81
24	c	913	CLA	CHD-C4C-NC	3.04	129.00	124.20
24	b	615	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	c	903	CLA	CAC-C3C-C4C	3.03	128.75	124.81
26	y	101	BCR	C40-C30-C25	-3.03	105.38	110.30
24	C	513	CLA	C1-C2-C3	-3.03	120.80	126.04
24	c	908	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	B	616	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
29	C	522	LMT	C2'-C3'-C4'	-3.03	102.77	109.68
24	b	620	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
24	b	609	CLA	C3B-C4B-NB	3.03	113.12	109.21
24	B	611	CLA	CAA-C2A-C3A	-3.03	104.49	112.78
24	b	605	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	d	404	BCR	C38-C26-C25	-3.02	121.13	124.53
24	B	617	CLA	CHD-C4C-NC	3.02	128.97	124.20
26	H	101	BCR	C16-C17-C18	-3.02	123.00	127.31
24	C	503	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
24	B	612	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
24	a	409	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	c	902	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
24	B	606	CLA	C3B-C4B-NB	3.02	113.11	109.21
24	b	606	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	C	508	CLA	C3B-C4B-NB	3.01	113.10	109.21
24	a	407	CLA	OBD-CAD-C3D	-3.01	122.98	127.98
24	c	913	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	B	616	CLA	C11-C10-C8	-3.01	106.19	115.92
24	b	612	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
24	c	909	CLA	C4D-C3D-CAD	-3.01	106.79	108.47
24	B	608	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
24	c	904	CLA	CMC-C2C-C1C	3.01	129.62	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	O2A-CGA-O1A	-3.00	116.01	123.59
36	H	102	DGD	O1G-C1A-O1A	-3.00	116.01	123.59
24	c	909	CLA	C1D-CHD-C4C	-3.00	118.59	122.56
24	b	614	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
24	c	912	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
24	b	615	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
31	A	419	PL9	C15-C14-C16	3.00	120.32	115.27
24	b	612	CLA	C1-C2-C3	-3.00	120.86	126.04
24	C	506	CLA	C4-C3-C5	3.00	120.31	115.27
24	B	614	CLA	O2A-CGA-CBA	3.00	121.31	111.91
25	A	409	PHO	C4-C3-C5	2.99	120.31	115.27
24	B	613	CLA	C2A-C1A-CHA	-2.99	118.62	123.86
24	B	615	CLA	CBC-CAC-C3C	-2.99	104.18	112.43
24	B	602	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	B	615	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
24	a	409	CLA	CBC-CAC-C3C	-2.99	104.19	112.43
24	B	606	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	B	617	CLA	OBD-CAD-C3D	-2.99	123.02	127.98
31	d	405	PL9	C27-C28-C29	-2.99	120.46	127.66
24	D	401	CLA	CAC-C3C-C4C	2.99	128.69	124.81
24	b	614	CLA	O2A-CGA-CBA	2.99	121.28	111.91
24	A	407	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
24	d	401	CLA	CAA-C2A-C3A	-2.98	104.60	112.78
24	c	908	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
24	b	613	CLA	O2A-CGA-O1A	-2.98	116.06	123.59
24	c	911	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	C	510	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
24	b	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	c	911	CLA	CAC-C3C-C4C	2.98	128.68	124.81
26	h	101	BCR	C7-C8-C9	-2.98	121.74	126.23
24	B	602	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
24	a	407	CLA	CHD-C4C-NC	2.98	128.89	124.20
24	b	607	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
24	c	902	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
24	C	506	CLA	C3B-C4B-NB	2.97	113.05	109.21
37	D	406	LHG	O7-C7-C8	2.97	117.91	111.50
24	B	611	CLA	O2A-CGA-CBA	2.97	121.24	111.91
24	C	512	CLA	CHC-C1C-C2C	-2.97	118.50	126.72
24	b	611	CLA	C1D-CHD-C4C	-2.97	118.64	122.56
26	b	623	BCR	C37-C22-C23	2.97	122.75	118.08
24	C	505	CLA	CAC-C3C-C4C	2.97	128.66	124.81
24	C	514	CLA	CHC-C1C-C2C	-2.97	118.52	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
24	A	407	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	C	506	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
24	C	502	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
26	b	622	BCR	C29-C30-C25	2.96	115.04	110.48
24	b	605	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
24	C	514	CLA	C4-C3-C5	2.96	120.25	115.27
31	D	404	PL9	C27-C28-C29	-2.96	120.53	127.66
24	B	609	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
37	L	101	LHG	O7-C7-C8	2.95	117.87	111.50
24	c	905	CLA	CAC-C3C-C4C	2.95	128.64	124.81
24	B	616	CLA	CBC-CAC-C3C	-2.95	104.30	112.43
24	b	615	CLA	C1-C2-C3	-2.95	120.94	126.04
24	A	405	CLA	CAA-C2A-C1A	-2.95	102.31	111.97
24	B	605	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
35	D	411	HTG	C1'-S1-C1	2.95	105.61	100.09
24	C	513	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	C	507	CLA	CAC-C3C-C4C	2.95	128.63	124.81
24	b	613	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	C	508	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
24	b	620	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
24	a	406	CLA	O2D-CGD-CBD	2.95	116.50	111.27
24	d	401	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	c	914	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	b	611	CLA	CMC-C2C-C1C	2.94	129.52	125.04
24	B	607	CLA	CMB-C2B-C3B	2.94	130.18	124.68
24	b	608	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
25	A	408	PHO	O1D-CGD-CBD	-2.94	118.47	124.48
24	c	913	CLA	CBC-CAC-C3C	-2.94	104.32	112.43
24	C	514	CLA	CMB-C2B-C3B	2.94	130.18	124.68
24	c	907	CLA	CMC-C2C-C1C	2.94	129.52	125.04
24	B	610	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	b	615	CLA	CMC-C2C-C1C	2.94	129.51	125.04
24	C	510	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	d	402	CLA	C1D-CHD-C4C	-2.93	118.69	122.56
24	a	409	CLA	CHC-C1C-C2C	-2.93	118.60	126.72
24	B	603	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
24	C	503	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
24	c	909	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	B	610	CLA	CHD-C4C-NC	2.93	128.82	124.20
24	C	508	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
24	c	905	CLA	O2D-CGD-O1D	-2.93	118.12	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	b	609	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	C	509	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
31	A	419	PL9	C10-C9-C11	2.92	120.19	115.27
24	B	604	CLA	CHD-C4C-NC	2.92	128.81	124.20
24	a	409	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
24	a	409	CLA	CHB-C4A-NA	2.92	128.55	124.51
31	a	417	PL9	C53-C6-C1	2.92	120.96	114.99
24	C	513	CLA	C1-O2A-CGA	2.92	124.10	116.44
24	b	605	CLA	C3B-C4B-NB	2.92	112.98	109.21
25	a	408	PHO	C4D-ND-C1D	-2.92	101.52	106.76
24	B	612	CLA	CHD-C4C-NC	2.92	128.80	124.20
24	C	514	CLA	CAC-C3C-C4C	2.91	128.59	124.81
26	B	620	BCR	C24-C23-C22	-2.91	121.83	126.23
26	C	516	BCR	C15-C14-C13	-2.91	123.15	127.31
24	b	607	CLA	CMB-C2B-C3B	2.91	130.12	124.68
29	f	103	LMT	C1B-O5B-C5B	2.91	119.40	113.69
24	C	511	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	d	403	CLA	CMC-C2C-C1C	2.91	129.46	125.04
24	D	401	CLA	O2A-CGA-CBA	2.90	121.02	111.91
29	A	417	LMT	O5'-C5'-C4'	2.90	115.87	109.75
24	A	405	CLA	CMC-C2C-C1C	2.90	129.46	125.04
24	B	607	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
36	D	405	DGD	C4D-C3D-C2D	2.90	115.88	110.82
24	c	903	CLA	C3B-C4B-NB	2.89	112.95	109.21
26	b	621	BCR	C7-C8-C9	-2.89	121.86	126.23
24	b	617	CLA	O2A-CGA-CBA	2.89	120.98	111.91
24	c	907	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	c	911	CLA	C4-C3-C5	2.89	120.13	115.27
24	c	904	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
26	t	101	BCR	C15-C16-C17	-2.88	117.56	123.47
36	C	519	DGD	O3G-C3G-C2G	-2.88	103.95	110.90
24	B	602	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
29	C	522	LMT	C1B-O5B-C5B	2.88	119.34	113.69
34	J	101	LMG	O7-C10-C11	2.88	117.70	111.50
24	B	602	CLA	C4D-C3D-CAD	-2.88	106.86	108.47
24	C	505	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
26	d	404	BCR	C16-C17-C18	-2.87	123.21	127.31
35	B	626	HTG	O5-C1-C2	2.87	113.93	110.31
24	B	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	B	609	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	B	603	CLA	CHD-C4C-NC	2.87	128.72	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
36	h	102	DGD	O2G-C1B-C2B	2.87	117.68	111.50
24	b	614	CLA	C1-C2-C3	-2.87	121.08	126.04
26	C	516	BCR	C33-C5-C6	-2.87	121.31	124.53
24	B	616	CLA	CMC-C2C-C1C	2.87	129.40	125.04
24	C	511	CLA	CMC-C2C-C1C	2.87	129.40	125.04
24	B	615	CLA	C2A-C1A-CHA	-2.87	118.85	123.86
24	C	505	CLA	CMB-C2B-C3B	2.86	130.04	124.68
24	c	902	CLA	CAC-C3C-C4C	2.86	128.53	124.81
24	b	620	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
36	h	102	DGD	O1G-C1A-C2A	2.86	120.89	111.91
36	C	517	DGD	O3G-C3G-C2G	-2.86	103.99	110.90
24	B	611	CLA	C4-C3-C5	2.86	120.08	115.27
24	A	410	CLA	CBC-CAC-C3C	-2.86	104.54	112.43
24	c	912	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
24	d	403	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
31	D	404	PL9	C40-C39-C41	2.86	120.08	115.27
24	b	619	CLA	C4D-C3D-CAD	-2.86	106.88	108.47
25	a	420	PHO	C3C-C4C-NC	2.86	114.71	110.28
24	a	407	CLA	O2A-CGA-CBA	2.86	120.87	111.91
24	C	503	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
24	b	612	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
24	B	617	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
24	b	618	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
27	A	416	SQD	O48-C23-O10	-2.85	116.39	123.59
24	a	407	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
31	D	404	PL9	C42-C43-C44	-2.85	120.79	127.66
24	b	611	CLA	CAA-CBA-CGA	2.85	121.58	113.25
25	a	408	PHO	C2A-C1A-NA	2.85	115.13	111.86
24	c	913	CLA	C1-C2-C3	-2.85	121.12	126.04
24	b	611	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
24	B	612	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
24	B	609	CLA	O2A-CGA-CBA	2.84	120.83	111.91
24	d	402	CLA	C1-C2-C3	-2.84	121.13	126.04
25	a	420	PHO	CHD-C1D-C2D	-2.84	118.58	125.73
25	A	409	PHO	CHD-C1D-C2D	-2.84	118.59	125.73
37	D	408	LHG	O8-C23-O10	-2.84	116.43	123.59
34	a	412	LMG	C8-O7-C10	-2.84	110.81	117.79
24	c	910	CLA	OBD-CAD-C3D	-2.84	123.27	127.98
24	b	620	CLA	C1-C2-C3	-2.84	121.14	126.04
24	B	605	CLA	CHD-C4C-NC	2.84	128.67	124.20
24	A	407	CLA	CED-O2D-CGD	2.83	122.35	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	B	621	SQD	O48-C23-C24	2.83	120.79	111.91
37	d	407	LHG	O8-C23-C24	2.83	120.79	111.91
24	B	603	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
31	D	404	PL9	C20-C19-C21	2.83	120.03	115.27
24	c	913	CLA	C4-C3-C5	2.83	120.02	115.27
24	b	607	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
24	C	503	CLA	C4-C3-C5	2.82	120.02	115.27
36	H	102	DGD	O2G-C1B-C2B	2.82	117.58	111.50
24	B	610	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
31	a	417	PL9	C7-C3-C4	2.82	119.17	116.88
24	B	612	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	A	405	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
24	B	615	CLA	C4-C3-C5	2.82	120.01	115.27
24	c	902	CLA	CMC-C2C-C1C	2.82	129.33	125.04
24	B	614	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
24	c	902	CLA	C1-O2A-CGA	2.81	123.82	116.44
24	b	618	CLA	O2A-CGA-CBA	2.81	120.73	111.91
24	A	406	CLA	CED-O2D-CGD	2.81	122.30	115.94
24	C	512	CLA	C1-O2A-CGA	2.81	123.81	116.44
24	c	907	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
24	c	904	CLA	C4-C3-C5	2.81	120.00	115.27
24	a	406	CLA	C4-C3-C5	2.81	119.99	115.27
24	B	610	CLA	CMB-C2B-C1B	2.81	132.78	128.46
40	V	201	HEC	CAD-CBD-CGD	2.80	117.38	112.67
24	B	615	CLA	O2A-CGA-CBA	2.80	120.71	111.91
24	a	409	CLA	CHD-C4C-NC	2.80	128.62	124.20
25	A	409	PHO	C2A-C1A-NA	2.80	115.08	111.86
24	B	606	CLA	O2A-CGA-O1A	-2.80	116.52	123.59
24	B	602	CLA	CHD-C4C-NC	2.80	128.62	124.20
37	L	101	LHG	O8-C23-C24	2.80	120.69	111.91
24	d	402	CLA	C4-C3-C5	2.80	119.98	115.27
26	b	622	BCR	C38-C26-C25	-2.80	121.39	124.53
24	c	911	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
34	a	412	LMG	C7-O1-C1	-2.80	108.28	113.74
24	a	409	CLA	OBD-CAD-C3D	-2.80	123.34	127.98
24	c	912	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	A	407	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
24	B	616	CLA	C1-C2-C3	-2.80	121.21	126.04
24	c	911	CLA	CMC-C2C-C1C	2.80	129.30	125.04
24	D	402	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
24	c	904	CLA	CHC-C1C-C2C	-2.79	118.99	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	C4-C3-C5	2.79	119.97	115.27
24	c	914	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
24	d	402	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
40	v	202	HEC	CAD-CBD-CGD	2.79	117.36	112.67
25	A	408	PHO	C4D-ND-C1D	-2.79	101.75	106.76
24	B	614	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
31	a	417	PL9	C25-C24-C26	2.79	119.96	115.27
24	c	905	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
24	c	912	CLA	O2A-CGA-CBA	2.78	120.64	111.91
24	c	914	CLA	C2A-C1A-CHA	-2.78	118.99	123.86
24	b	616	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
24	B	616	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
25	a	408	PHO	C2C-C1C-NC	2.78	113.98	109.79
26	d	404	BCR	C38-C26-C27	2.78	118.95	113.62
24	c	908	CLA	O2A-CGA-CBA	2.78	120.62	111.91
24	C	511	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	b	620	CLA	OBD-CAD-C3D	-2.77	123.38	127.98
24	c	910	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	C	511	CLA	C4D-C3D-CAD	-2.77	106.92	108.47
24	b	611	CLA	C4-C3-C5	2.77	119.93	115.27
24	B	602	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	c	903	CLA	O2A-CGA-CBA	2.77	120.60	111.91
24	D	401	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
24	c	907	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
25	a	420	PHO	CHC-C1C-C2C	-2.77	118.77	125.73
24	C	509	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	B	606	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	b	607	CLA	OBD-CAD-C3D	-2.77	123.39	127.98
24	b	606	CLA	C4D-C3D-CAD	-2.77	106.93	108.47
24	A	410	CLA	CHC-C1C-C2C	-2.76	119.07	126.72
24	D	402	CLA	C1D-CHD-C4C	-2.76	118.91	122.56
34	c	920	LMG	O6-C5-C4	2.76	114.71	109.69
24	C	504	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	c	914	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
29	m	102	LMT	O5'-C5'-C4'	2.76	115.57	109.75
24	b	612	CLA	CHD-C4C-NC	2.75	128.54	124.20
24	B	614	CLA	CED-O2D-CGD	2.75	122.16	115.94
24	c	904	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
34	b	624	LMG	O7-C10-C11	2.75	117.42	111.50
24	b	613	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
24	A	406	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	C	504	CLA	CMB-C2B-C3B	2.75	129.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	419	PL9	C7-C3-C4	2.75	119.11	116.88
24	C	502	CLA	CMB-C2B-C3B	2.75	129.82	124.68
24	c	905	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
24	C	502	CLA	C1-C2-C3	-2.74	121.30	126.04
24	C	513	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
24	b	606	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
31	a	417	PL9	C20-C19-C21	2.74	119.89	115.27
24	C	508	CLA	CBC-CAC-C3C	-2.74	104.87	112.43
27	a	402	SQD	O5-C5-C4	2.74	114.67	109.69
27	a	411	SQD	C44-O6-C1	-2.74	108.38	113.74
24	b	606	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
36	c	916	DGD	O5D-C6D-C5D	-2.74	103.98	109.05
24	b	610	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
26	b	623	BCR	C2-C1-C6	2.74	114.69	110.48
34	J	101	LMG	O8-C28-O10	-2.73	116.69	123.59
26	B	619	BCR	C2-C1-C6	2.73	114.69	110.48
24	a	407	CLA	C3B-C4B-NB	2.73	112.74	109.21
24	c	907	CLA	C4-C3-C5	2.73	119.87	115.27
24	c	903	CLA	CHC-C1C-C2C	-2.73	119.16	126.72
24	c	910	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	b	610	CLA	O2A-CGA-CBA	2.73	120.48	111.91
26	h	101	BCR	C24-C23-C22	-2.73	122.11	126.23
24	c	904	CLA	OBD-CAD-C3D	-2.73	123.45	127.98
24	b	616	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
27	F	101	SQD	C3-C4-C5	2.73	115.11	110.24
24	b	614	CLA	C4-C3-C5	2.73	119.86	115.27
24	b	620	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	b	616	CLA	O2A-CGA-CBA	2.73	120.47	111.91
24	A	405	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
31	A	419	PL9	C25-C24-C26	2.72	119.86	115.27
24	b	605	CLA	O2A-CGA-CBA	2.72	120.46	111.91
24	C	510	CLA	OBD-CAD-C3D	-2.72	123.46	127.98
24	a	406	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
24	C	513	CLA	CMC-C2C-C1C	2.72	129.18	125.04
25	A	409	PHO	C4D-ND-C1D	-2.72	101.87	106.76
31	A	419	PL9	C42-C43-C44	-2.72	121.11	127.66
24	B	606	CLA	C1-O2A-CGA	2.72	123.58	116.44
24	C	511	CLA	CMB-C2B-C3B	2.72	129.77	124.68
24	c	907	CLA	OBD-CAD-C3D	-2.72	123.47	127.98
24	b	608	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
25	a	408	PHO	C1C-C2C-C3C	-2.72	103.39	106.51
34	z	101	LMG	O8-C28-C29	2.71	120.42	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	908	CLA	CMC-C2C-C1C	2.71	129.17	125.04
24	C	508	CLA	CHD-C4C-NC	2.71	128.47	124.20
34	C	521	LMG	C8-O7-C10	-2.71	111.12	117.79
24	c	910	CLA	CHC-C1C-C2C	-2.71	119.23	126.72
24	c	903	CLA	CMC-C2C-C1C	2.71	129.16	125.04
24	c	911	CLA	CHD-C4C-NC	2.71	128.47	124.20
36	D	405	DGD	O1G-C1A-C2A	2.70	120.40	111.91
24	b	617	CLA	CMA-C3A-C4A	-2.70	104.50	111.77
24	C	504	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
31	d	405	PL9	C15-C14-C16	2.70	119.82	115.27
24	C	512	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	511	CLA	C4-C3-C5	2.70	119.81	115.27
24	d	401	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	B	610	CLA	CBC-CAC-C3C	-2.70	104.99	112.43
24	B	609	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
24	C	507	CLA	C4-C3-C5	2.70	119.81	115.27
25	a	408	PHO	CHC-C1C-C2C	-2.70	118.95	125.73
31	A	419	PL9	C35-C34-C36	2.70	119.81	115.27
24	b	608	CLA	O2A-CGA-CBA	2.69	120.36	111.91
24	c	913	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
24	C	507	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
27	L	102	SQD	O48-C23-C24	2.69	120.35	111.91
25	A	409	PHO	C1C-C2C-C3C	-2.69	103.42	106.51
24	a	407	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	B	611	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	c	914	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
25	A	408	PHO	CHC-C1C-C2C	-2.69	118.97	125.73
27	f	102	SQD	O48-C23-C24	2.69	120.34	111.91
25	A	408	PHO	C3C-C4C-NC	2.69	114.44	110.28
24	b	612	CLA	CAC-C3C-C4C	2.68	128.29	124.81
24	B	607	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
25	A	409	PHO	C2B-C1B-NB	2.68	113.84	109.79
25	A	409	PHO	C3C-C4C-NC	2.68	114.44	110.28
24	C	505	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
24	B	609	CLA	CMA-C3A-C4A	-2.68	104.57	111.77
24	d	401	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
24	c	903	CLA	CHD-C4C-NC	2.68	128.42	124.20
36	d	406	DGD	C1E-O6E-C5E	2.68	118.94	113.69
34	c	920	LMG	O8-C28-C29	2.67	120.30	111.91
24	c	913	CLA	CED-O2D-CGD	2.67	121.98	115.94
25	A	409	PHO	CHC-C1C-C2C	-2.67	119.01	125.73
24	A	410	CLA	C4D-C3D-CAD	-2.67	106.98	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
24	a	409	CLA	CMA-C3A-C4A	-2.67	104.60	111.77
26	D	403	BCR	C29-C30-C25	2.67	114.59	110.48
24	C	513	CLA	C4-C3-C5	2.67	119.76	115.27
24	c	913	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	A	407	CLA	C1-C2-C3	-2.67	121.43	126.04
24	b	612	CLA	CMB-C2B-C3B	2.67	129.66	124.68
24	b	610	CLA	CHD-C4C-NC	2.67	128.40	124.20
24	b	605	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
25	A	408	PHO	CAC-C3C-C4C	2.66	128.13	125.22
26	k	101	BCR	C24-C23-C22	-2.66	122.21	126.23
24	B	608	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
26	B	619	BCR	C37-C22-C21	-2.66	119.20	122.92
25	A	408	PHO	C3A-C2A-C1A	-2.66	98.47	101.64
26	d	404	BCR	C21-C20-C19	-2.66	114.92	123.22
34	Z	101	LMG	O6-C5-C4	2.66	114.52	109.69
24	C	510	CLA	CMC-C2C-C1C	2.66	129.09	125.04
27	A	412	SQD	O47-C7-O49	-2.66	117.28	123.70
24	B	605	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
27	A	412	SQD	O9-S-C6	2.65	110.09	106.94
24	c	913	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
34	B	622	LMG	O8-C28-O10	-2.65	116.89	123.59
24	B	614	CLA	CAC-C3C-C4C	2.65	128.25	124.81
24	b	613	CLA	CHD-C4C-NC	2.65	128.38	124.20
24	C	514	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
24	d	403	CLA	CHD-C4C-NC	2.65	128.38	124.20
24	B	602	CLA	C1-C2-C3	-2.65	121.46	126.04
24	a	406	CLA	CMB-C2B-C3B	2.65	129.63	124.68
24	c	907	CLA	CMB-C2B-C3B	2.65	129.63	124.68
24	B	608	CLA	OBD-CAD-C3D	-2.65	123.59	127.98
24	B	612	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
36	h	102	DGD	O1G-C1A-O1A	-2.64	116.92	123.59
24	B	613	CLA	C1D-CHD-C4C	-2.64	119.07	122.56
24	b	609	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
24	B	607	CLA	C1-C2-C3	-2.64	121.48	126.04
24	B	611	CLA	C1-C2-C3	-2.64	121.48	126.04
24	c	906	CLA	C1-O2A-CGA	2.64	123.37	116.44
24	b	616	CLA	CMC-C2C-C1C	2.64	129.06	125.04
31	d	405	PL9	C45-C44-C46	2.64	119.71	115.27
24	C	511	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
24	C	505	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
24	d	402	CLA	O2A-CGA-O1A	-2.64	116.94	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	417	PL9	C40-C39-C41	2.64	119.71	115.27
24	C	510	CLA	C4-C3-C5	2.64	119.71	115.27
24	b	617	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
24	B	606	CLA	OBD-CAD-C3D	-2.63	123.61	127.98
31	A	419	PL9	C45-C44-C46	2.63	119.70	115.27
24	B	604	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
24	c	914	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	C	513	CLA	CMB-C2B-C3B	2.63	129.60	124.68
24	b	613	CLA	C1D-CHD-C4C	-2.63	119.08	122.56
24	c	906	CLA	CMC-C2C-C1C	2.63	129.04	125.04
24	c	912	CLA	C4-C3-C5	2.63	119.69	115.27
25	a	408	PHO	C3C-C4C-NC	2.63	114.36	110.28
26	A	411	BCR	C33-C5-C6	-2.63	121.58	124.53
31	D	404	PL9	C7-C3-C4	2.63	119.01	116.88
24	C	509	CLA	CHD-C4C-NC	2.63	128.34	124.20
24	b	613	CLA	C3B-C4B-NB	2.63	112.61	109.21
24	b	607	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
24	C	511	CLA	O2A-CGA-CBA	2.62	120.14	111.91
26	T	102	BCR	C21-C20-C19	-2.62	115.03	123.22
24	b	609	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
25	A	409	PHO	C2C-C1C-NC	2.62	113.75	109.79
24	B	617	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
24	C	507	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	K	103	BCR	C15-C14-C13	-2.62	123.57	127.31
24	D	402	CLA	CAC-C3C-C4C	2.62	128.21	124.81
24	d	401	CLA	CMA-C3A-C2A	-2.62	103.27	113.83
24	A	410	CLA	O2A-CGA-CBA	2.62	120.12	111.91
24	b	609	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
24	B	606	CLA	C4-C3-C5	2.62	119.67	115.27
29	A	417	LMT	C1'-O5'-C5'	2.62	118.82	113.69
31	d	405	PL9	C42-C43-C44	-2.62	121.36	127.66
24	B	608	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	B	603	CLA	CMB-C2B-C3B	2.61	129.57	124.68
24	D	402	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
26	c	915	BCR	C3-C4-C5	-2.61	109.41	114.08
24	c	905	CLA	C1D-CHD-C4C	-2.61	119.11	122.56
24	c	906	CLA	C1-C2-C3	-2.61	121.53	126.04
24	A	410	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
24	b	605	CLA	CMB-C2B-C3B	2.61	129.56	124.68
24	B	605	CLA	O2A-CGA-CBA	2.61	120.09	111.91
35	B	634	HTG	C1-O5-C5	2.61	117.39	112.58
24	c	904	CLA	O2A-CGA-CBA	2.61	120.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	907	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
26	T	102	BCR	C7-C6-C5	-2.60	115.15	121.46
24	b	618	CLA	CMC-C2C-C1C	2.60	129.00	125.04
24	B	613	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
26	b	623	BCR	C15-C14-C13	-2.60	123.59	127.31
25	a	408	PHO	CMC-C2C-C1C	2.60	129.07	125.06
24	B	607	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
24	b	617	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
24	c	903	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
34	J	101	LMG	O8-C28-C29	2.60	120.06	111.91
24	B	606	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	a	409	CLA	C4-C3-C5	2.60	119.64	115.27
24	d	403	CLA	CMB-C2B-C3B	2.60	129.54	124.68
31	a	417	PL9	C37-C36-C34	-2.60	104.44	112.98
24	b	608	CLA	C1D-CHD-C4C	-2.59	119.14	122.56
27	F	101	SQD	O48-C23-C24	2.59	120.04	111.91
24	B	614	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	b	606	CLA	C4-C3-C5	2.59	119.62	115.27
24	c	914	CLA	C4-C3-C5	2.59	119.62	115.27
26	t	101	BCR	C1-C6-C7	2.59	123.10	115.78
37	D	408	LHG	O8-C23-C24	2.59	120.02	111.91
25	a	420	PHO	C2A-C1A-NA	2.58	114.83	111.86
24	c	902	CLA	CHD-C4C-NC	2.58	128.27	124.20
37	L	101	LHG	O8-C23-O10	-2.58	117.08	123.59
24	B	615	CLA	OBD-CAD-C3D	-2.58	123.70	127.98
31	d	405	PL9	C40-C39-C41	2.58	119.61	115.27
24	B	604	CLA	CBC-CAC-C3C	-2.58	105.32	112.43
24	B	613	CLA	CMB-C2B-C3B	2.58	129.50	124.68
24	b	606	CLA	CMC-C2C-C1C	2.58	128.96	125.04
24	B	609	CLA	CHB-C4A-NA	2.58	128.07	124.51
26	k	101	BCR	C7-C8-C9	-2.58	122.34	126.23
24	C	511	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
24	C	508	CLA	CAC-C3C-C4C	2.57	128.15	124.81
24	c	907	CLA	CHD-C4C-NC	2.57	128.26	124.20
35	C	524	HTG	O5-C1-C2	2.57	113.55	110.31
34	z	101	LMG	C7-O1-C1	-2.57	108.72	113.74
24	c	902	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
24	C	502	CLA	CHD-C4C-NC	2.57	128.25	124.20
24	a	406	CLA	CMA-C3A-C2A	-2.57	103.47	113.83
24	c	912	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
24	C	513	CLA	OBD-CAD-C3D	-2.57	123.72	127.98
26	K	102	BCR	C16-C17-C18	-2.56	123.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C1-O2A-CGA	2.56	123.17	116.44
24	c	903	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	b	611	CLA	CHD-C4C-NC	2.56	128.23	124.20
24	B	609	CLA	CAC-C3C-C4C	2.56	128.13	124.81
24	b	617	CLA	C4-C3-C5	2.56	119.57	115.27
34	c	920	LMG	C8-O7-C10	-2.56	111.50	117.79
24	B	613	CLA	C4-C3-C5	2.55	119.57	115.27
24	A	407	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
24	c	910	CLA	C4-C3-C5	2.55	119.56	115.27
24	B	605	CLA	CMC-C2C-C1C	2.55	128.93	125.04
26	k	101	BCR	C38-C26-C25	-2.55	121.66	124.53
24	B	608	CLA	C4-C3-C5	2.55	119.56	115.27
26	y	101	BCR	C35-C13-C14	-2.55	119.35	122.92
36	D	405	DGD	C3D-C4D-C5D	2.55	114.78	110.24
24	C	508	CLA	CMC-C2C-C1C	2.55	128.92	125.04
26	a	410	BCR	C2-C1-C6	2.55	114.40	110.48
26	D	403	BCR	C33-C5-C6	-2.55	121.67	124.53
24	b	615	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	b	615	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
24	b	612	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
26	y	101	BCR	C10-C11-C12	-2.54	115.29	123.22
24	C	509	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	B	603	CLA	CMA-C3A-C4A	-2.54	104.95	111.77
24	d	401	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
24	B	614	CLA	CMB-C2B-C3B	2.54	129.43	124.68
26	d	404	BCR	C15-C14-C13	-2.54	123.69	127.31
24	c	907	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
24	B	608	CLA	C2A-C1A-CHA	-2.54	119.43	123.86
24	c	910	CLA	O2A-CGA-CBA	2.53	119.86	111.91
35	b	627	HTG	C1-C2-C3	2.53	115.59	110.59
36	c	918	DGD	O1G-C1A-C2A	2.53	119.85	111.91
24	b	610	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
24	D	402	CLA	C4D-C3D-CAD	-2.53	107.06	108.47
24	B	611	CLA	C3D-CAD-CBD	2.53	110.94	107.61
24	b	609	CLA	O2A-CGA-CBA	2.53	119.84	111.91
24	B	617	CLA	O2A-CGA-CBA	2.53	119.84	111.91
24	B	604	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	b	610	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
24	c	903	CLA	C1-C2-C3	-2.53	121.67	126.04
26	K	102	BCR	C24-C23-C22	-2.53	122.42	126.23
24	c	904	CLA	CHD-C4C-NC	2.52	128.18	124.20
26	B	618	BCR	C37-C22-C21	-2.52	119.39	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	902	CLA	OBD-CAD-C3D	-2.52	123.79	127.98
25	A	409	PHO	CAC-C3C-C4C	2.52	127.97	125.22
26	c	915	BCR	C15-C14-C13	-2.52	123.71	127.31
26	t	101	BCR	C29-C28-C27	-2.52	105.75	111.38
24	d	401	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
24	B	608	CLA	CMB-C2B-C3B	2.52	129.39	124.68
24	c	913	CLA	O2A-CGA-CBA	2.52	119.81	111.91
24	a	407	CLA	C1-C2-C3	-2.52	121.69	126.04
24	D	401	CLA	C4D-C3D-CAD	-2.52	107.07	108.47
27	B	621	SQD	O8-S-C6	2.52	109.75	105.74
27	L	102	SQD	C1-C2-C3	-2.52	104.75	110.00
24	C	514	CLA	CHD-C4C-NC	2.52	128.17	124.20
25	A	408	PHO	C2B-C1B-NB	2.52	113.59	109.79
24	b	607	CLA	CMC-C2C-C1C	2.51	128.87	125.04
26	k	102	BCR	C33-C5-C6	-2.51	121.70	124.53
24	b	612	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
24	a	409	CLA	CAC-C3C-C4C	2.51	128.07	124.81
36	d	406	DGD	O1G-C1A-C2A	2.51	119.79	111.91
36	H	102	DGD	O1G-C1A-C2A	2.51	119.79	111.91
24	C	509	CLA	CMB-C2B-C3B	2.51	129.38	124.68
26	t	101	BCR	C7-C6-C5	-2.51	115.38	121.46
24	B	607	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	b	616	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
26	K	103	BCR	C38-C26-C25	-2.51	121.71	124.53
26	k	101	BCR	C35-C13-C14	-2.51	119.41	122.92
24	C	503	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	B	612	CLA	O2A-CGA-CBA	2.51	119.77	111.91
34	a	412	LMG	O8-C28-C29	2.51	119.77	111.91
24	b	606	CLA	CHD-C4C-NC	2.50	128.15	124.20
37	d	409	LHG	O8-C23-C24	2.50	119.76	111.91
36	C	519	DGD	O2G-C1B-C2B	2.50	116.90	111.50
24	C	507	CLA	C4D-C3D-CAD	-2.50	107.07	108.47
26	D	403	BCR	C29-C28-C27	-2.50	105.79	111.38
24	C	503	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
24	C	513	CLA	O2A-CGA-CBA	2.50	119.75	111.91
24	a	407	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
26	y	101	BCR	C28-C27-C26	-2.50	109.62	114.08
24	B	602	CLA	C4-C3-C5	2.50	119.47	115.27
24	B	604	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
26	H	101	BCR	C7-C8-C9	-2.50	122.46	126.23
26	d	404	BCR	C24-C23-C22	-2.49	122.47	126.23
24	B	603	CLA	CBC-CAC-C3C	-2.49	105.55	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C16-C17-C18	-2.49	123.75	127.31
27	f	102	SQD	O47-C7-O49	-2.49	117.67	123.70
24	C	503	CLA	C3D-CAD-CBD	2.49	110.89	107.61
24	A	406	CLA	CMA-C3A-C2A	-2.49	103.77	113.83
24	C	502	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
24	B	608	CLA	C1-O2A-CGA	2.49	122.98	116.44
24	B	614	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
29	m	103	LMT	C1'-C2'-C3'	2.49	115.18	110.00
24	c	905	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
37	d	408	LHG	O8-C23-O10	-2.49	117.31	123.59
24	B	608	CLA	C1D-CHD-C4C	-2.49	119.28	122.56
24	b	619	CLA	CMB-C2B-C3B	2.49	129.33	124.68
24	C	503	CLA	CMC-C2C-C1C	2.49	128.82	125.04
24	B	615	CLA	C4C-C3C-C2C	-2.49	103.28	106.90
24	c	911	CLA	O2A-CGA-CBA	2.48	119.70	111.91
24	A	405	CLA	O2A-CGA-CBA	2.48	119.70	111.91
26	C	515	BCR	C33-C5-C6	-2.48	121.74	124.53
25	a	408	PHO	C4D-CHA-C1A	-2.48	119.79	125.37
24	a	409	CLA	CMC-C2C-C1C	2.48	128.82	125.04
25	A	409	PHO	C4D-CHA-C1A	-2.48	119.79	125.37
24	B	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
34	j	101	LMG	O8-C28-O10	-2.48	117.34	123.59
24	D	402	CLA	CHD-C4C-NC	2.48	128.11	124.20
29	m	104	LMT	O5'-C5'-C4'	2.48	114.98	109.75
24	C	504	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	B	603	CLA	C4-C3-C5	2.48	119.44	115.27
24	B	609	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
24	C	505	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
26	b	623	BCR	C16-C15-C14	-2.48	118.40	123.47
26	T	102	BCR	C1-C6-C7	2.47	122.78	115.78
24	b	606	CLA	O2A-CGA-CBA	2.47	119.67	111.91
34	Z	101	LMG	C8-O7-C10	-2.47	111.70	117.79
24	C	513	CLA	CBC-CAC-C3C	-2.47	105.61	112.43
24	b	618	CLA	CHD-C4C-NC	2.47	128.10	124.20
31	A	419	PL9	C8-C7-C3	2.47	118.97	111.98
31	d	405	PL9	C35-C34-C36	2.47	119.43	115.27
24	B	607	CLA	C1-O2A-CGA	2.47	122.93	116.44
27	A	412	SQD	O48-C23-O10	-2.47	117.36	123.59
35	c	923	HTG	O5-C5-C4	2.47	114.17	109.69
24	A	405	CLA	CMB-C2B-C3B	2.47	129.29	124.68
24	C	503	CLA	O2A-CGA-CBA	2.46	119.64	111.91
25	A	409	PHO	O2D-CGD-O1D	-2.46	119.02	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	524	HTG	O5-C5-C4	2.46	114.17	109.69
24	b	613	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	b	618	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
26	T	102	BCR	C11-C10-C9	-2.46	123.80	127.31
24	b	617	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	a	420	PHO	C4D-ND-C1D	-2.46	102.34	106.76
24	b	613	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
24	a	409	CLA	O2A-CGA-CBA	2.46	119.62	111.91
24	B	615	CLA	CMB-C2B-C3B	2.46	129.27	124.68
29	a	401	LMT	O5'-C5'-C4'	2.45	114.92	109.75
24	B	611	CLA	CHD-C4C-NC	2.45	128.06	124.20
31	d	405	PL9	C20-C19-C21	2.45	119.39	115.27
24	C	506	CLA	CMC-C2C-C1C	2.45	128.77	125.04
26	B	618	BCR	C34-C9-C10	-2.45	119.49	122.92
24	b	615	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	a	407	CLA	CMB-C2B-C3B	2.44	129.25	124.68
24	B	608	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	B	604	CLA	CAC-C3C-C4C	2.44	127.98	124.81
24	C	507	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	a	407	CLA	CMC-C2C-C1C	2.44	128.76	125.04
24	C	512	CLA	CMB-C2B-C3B	2.44	129.25	124.68
27	L	102	SQD	O47-C7-O49	-2.44	117.81	123.70
24	b	608	CLA	C4-C3-C5	2.44	119.37	115.27
36	d	406	DGD	O5D-C1E-C2E	2.44	112.11	108.30
24	B	605	CLA	CMB-C2B-C3B	2.44	129.24	124.68
24	C	509	CLA	OBD-CAD-CBD	-2.44	122.42	125.89
26	a	410	BCR	C3-C4-C5	-2.43	109.73	114.08
36	c	916	DGD	C2G-O2G-C1B	-2.43	111.80	117.79
25	a	420	PHO	O2A-CGA-CBA	2.43	119.55	111.91
24	b	611	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
24	a	407	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	A	408	PHO	C4-C3-C5	2.43	119.36	115.27
31	a	417	PL9	C51-C49-C50	2.43	119.97	114.60
24	c	905	CLA	CMB-C2B-C3B	2.43	129.22	124.68
24	b	606	CLA	C1-C2-C3	-2.43	121.84	126.04
24	b	612	CLA	CMC-C2C-C1C	2.43	128.74	125.04
24	B	617	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	C	502	CLA	OBD-CAD-C3D	-2.43	123.95	127.98
36	C	519	DGD	O1G-C1A-C2A	2.43	119.53	111.91
24	B	603	CLA	OBD-CAD-C3D	-2.43	123.95	127.98
24	B	604	CLA	C5-C3-C2	-2.43	116.21	121.12
24	C	508	CLA	O2A-CGA-CBA	2.43	119.52	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	410	CLA	CMA-C3A-C4A	-2.43	105.25	111.77
24	B	603	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
24	c	913	CLA	CBA-CAA-C2A	-2.42	106.71	113.86
26	B	619	BCR	C28-C27-C26	-2.42	109.75	114.08
26	D	403	BCR	C10-C11-C12	-2.42	115.67	123.22
24	b	610	CLA	CAC-C3C-C4C	2.42	127.95	124.81
35	B	634	HTG	O5-C5-C4	2.41	114.08	109.69
24	c	909	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
29	f	103	LMT	O5B-C5B-C4B	2.41	114.08	109.69
24	C	510	CLA	CHD-C4C-NC	2.41	128.00	124.20
26	B	618	BCR	C7-C8-C9	-2.41	122.59	126.23
24	c	908	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
24	C	512	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
24	b	618	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
26	t	101	BCR	C21-C20-C19	-2.40	115.71	123.22
24	B	605	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
37	l	101	LHG	O7-C7-O9	-2.40	117.89	123.70
31	d	405	PL9	C32-C33-C34	-2.40	121.88	127.66
27	a	411	SQD	O48-C23-C24	2.40	119.44	111.91
24	c	905	CLA	CHD-C4C-NC	2.40	127.99	124.20
24	c	904	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
24	b	605	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
26	h	101	BCR	C10-C11-C12	-2.40	115.73	123.22
37	d	409	LHG	O7-C7-O9	-2.40	117.90	123.70
24	B	616	CLA	OBD-CAD-C3D	-2.40	124.00	127.98
31	A	419	PL9	C30-C29-C31	2.40	119.30	115.27
37	l	101	LHG	O8-C23-C24	2.40	119.43	111.91
24	c	911	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
26	B	620	BCR	C39-C30-C25	-2.39	106.42	110.30
24	C	502	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
31	d	405	PL9	C31-C32-C33	-2.39	104.02	111.88
27	F	101	SQD	O9-S-C6	2.39	109.78	106.94
24	B	610	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
24	C	513	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
27	L	102	SQD	C44-O6-C1	-2.39	109.07	113.74
24	C	504	CLA	CMC-C2C-C1C	2.39	128.68	125.04
24	C	514	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
24	c	909	CLA	CMB-C2B-C3B	2.39	129.14	124.68
26	y	101	BCR	C21-C20-C19	-2.39	115.77	123.22
24	C	507	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
24	C	514	CLA	O2A-CGA-CBA	2.38	119.39	111.91
24	A	405	CLA	O2D-CGD-CBD	2.38	115.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	O2A-CGA-CBA	2.38	119.39	111.91
24	b	616	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
24	B	603	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
24	B	614	CLA	O2D-CGD-CBD	2.38	115.50	111.27
31	D	404	PL9	C25-C24-C26	2.38	119.27	115.27
24	B	610	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
31	d	405	PL9	C37-C38-C39	-2.38	121.94	127.66
24	b	605	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	b	615	CLA	O2A-CGA-CBA	2.38	119.37	111.91
26	c	915	BCR	C15-C16-C17	-2.38	118.61	123.47
24	c	912	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
24	B	615	CLA	CAA-C2A-C3A	-2.37	106.28	112.78
24	b	611	CLA	OBD-CAD-C3D	-2.37	124.04	127.98
24	c	907	CLA	CGD-CBD-CAD	-2.37	103.05	110.73
24	B	617	CLA	C1-O2A-CGA	2.37	122.66	116.44
24	b	614	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	C	513	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
24	b	614	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	B	609	CLA	CHD-C4C-NC	2.37	127.94	124.20
25	a	408	PHO	CBA-CAA-C2A	-2.37	106.87	113.86
24	B	610	CLA	CMA-C3A-C4A	-2.37	105.41	111.77
27	B	621	SQD	C1-C2-C3	-2.37	105.07	110.00
24	C	503	CLA	CHD-C4C-NC	2.37	127.93	124.20
34	z	101	LMG	O1-C1-C2	2.37	112.00	108.30
24	B	610	CLA	CGD-CBD-CAD	-2.37	103.07	110.73
29	b	601	LMT	O5'-C1'-C2'	2.36	115.35	110.35
24	C	504	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
27	A	416	SQD	C3-C4-C5	2.36	114.45	110.24
27	F	101	SQD	O47-C7-O49	-2.36	117.99	123.70
24	c	909	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
24	d	403	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
24	b	611	CLA	CAC-C3C-C4C	2.36	127.87	124.81
24	d	403	CLA	C4-C3-C5	2.36	119.24	115.27
24	B	609	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
26	D	403	BCR	C16-C17-C18	-2.36	123.94	127.31
24	b	620	CLA	C4-C3-C5	2.36	119.24	115.27
24	b	608	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
24	b	617	CLA	CHD-C4C-NC	2.36	127.92	124.20
24	C	513	CLA	CMA-C3A-C4A	-2.35	105.44	111.77
24	C	509	CLA	O2A-CGA-CBA	2.35	119.29	111.91
24	B	612	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
24	b	606	CLA	CMB-C2B-C3B	2.35	129.08	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	404	PL9	C22-C23-C24	-2.35	121.99	127.66
24	C	502	CLA	C4-C3-C5	2.35	119.23	115.27
24	A	406	CLA	CAA-CBA-CGA	2.35	120.12	113.25
24	B	602	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
24	C	511	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
24	b	614	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
24	b	608	CLA	CMB-C2B-C3B	2.35	129.07	124.68
24	C	502	CLA	O2A-CGA-CBA	2.35	119.28	111.91
24	b	609	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
24	d	402	CLA	C3D-CAD-CBD	2.34	110.69	107.61
24	C	502	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
24	B	607	CLA	O2A-CGA-CBA	2.34	119.26	111.91
24	B	607	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
24	b	620	CLA	CHD-C4C-NC	2.34	127.89	124.20
31	D	404	PL9	C12-C13-C14	-2.34	122.02	127.66
29	B	623	LMT	O1B-C4'-C5'	-2.34	103.04	109.45
29	B	623	LMT	C1-O1'-C1'	-2.34	109.96	113.84
24	C	509	CLA	CMC-C2C-C1C	2.34	128.60	125.04
24	B	617	CLA	CMB-C2B-C3B	2.34	129.05	124.68
24	B	615	CLA	C1-C2-C3	-2.34	122.00	126.04
24	b	613	CLA	OBD-CAD-C3D	-2.34	124.10	127.98
24	b	619	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
24	a	409	CLA	CMB-C2B-C3B	2.33	129.04	124.68
24	b	617	CLA	OBD-CAD-C3D	-2.33	124.11	127.98
24	c	908	CLA	CHD-C4C-NC	2.33	127.88	124.20
24	b	606	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
24	D	401	CLA	CMC-C2C-C1C	2.33	128.59	125.04
36	c	918	DGD	O1G-C1A-O1A	-2.33	117.71	123.59
36	C	518	DGD	O1G-C1A-C2A	2.33	119.22	111.91
24	b	617	CLA	C6-C7-C8	-2.33	108.39	115.92
24	c	910	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
24	b	615	CLA	OBD-CAD-C3D	-2.33	124.11	127.98
24	C	505	CLA	CHD-C4C-NC	2.33	127.87	124.20
26	A	411	BCR	C37-C22-C21	-2.32	119.67	122.92
24	a	409	CLA	CMA-C3A-C2A	-2.32	104.47	113.83
35	b	626	HTG	O5-C1-C2	2.32	113.23	110.31
24	D	402	CLA	OBD-CAD-C3D	-2.32	124.14	127.98
26	k	102	BCR	C36-C18-C19	2.31	121.72	118.08
24	B	603	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
24	D	401	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
35	b	603	HTG	C1-O5-C5	2.31	116.84	112.58
24	A	410	CLA	C4C-C3C-C2C	-2.31	103.53	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CMB-C2B-C3B	2.31	129.00	124.68
24	C	510	CLA	CMB-C2B-C3B	2.31	129.00	124.68
24	d	403	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
24	C	511	CLA	C6-C7-C8	-2.31	108.46	115.92
24	b	613	CLA	CMA-C3A-C2A	-2.31	104.52	113.83
25	a	408	PHO	C2B-C1B-NB	2.31	113.27	109.79
26	B	618	BCR	C29-C30-C25	2.31	114.03	110.48
31	A	419	PL9	C40-C39-C41	2.30	119.15	115.27
24	b	609	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
24	B	607	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
24	B	609	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	d	404	BCR	C40-C30-C25	-2.30	106.56	110.30
24	A	407	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	a	408	PHO	CBD-CHA-C1A	2.30	131.74	126.40
24	C	507	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
26	d	404	BCR	C30-C25-C26	-2.30	119.38	122.61
26	C	516	BCR	C3-C4-C5	-2.30	109.97	114.08
25	a	420	PHO	C2B-C1B-NB	2.30	113.26	109.79
24	A	407	CLA	CMA-C3A-C2A	-2.30	104.56	113.83
40	V	201	HEC	CBD-CAD-C3D	-2.30	108.25	112.49
24	b	606	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
24	A	406	CLA	CAC-C3C-C4C	2.30	127.79	124.81
24	C	506	CLA	O2A-CGA-CBA	2.30	119.11	111.91
27	A	416	SQD	O5-C5-C4	2.30	113.86	109.69
24	C	514	CLA	OBD-CAD-C3D	-2.29	124.17	127.98
31	D	404	PL9	C51-C49-C50	2.29	119.67	114.60
24	C	508	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
26	c	915	BCR	C37-C22-C21	-2.29	119.71	122.92
36	D	405	DGD	O6D-C5D-C6D	2.29	111.29	106.67
37	l	101	LHG	C6-C5-C4	-2.29	106.37	111.79
24	c	906	CLA	OBD-CAD-C3D	-2.29	124.19	127.98
24	A	410	CLA	CAC-C3C-C4C	2.29	127.78	124.81
24	C	513	CLA	CHB-C4A-NA	2.28	127.67	124.51
31	D	404	PL9	C37-C38-C39	-2.28	122.16	127.66
24	B	602	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	b	614	CLA	C11-C12-C13	-2.28	108.54	115.92
24	b	612	CLA	C11-C10-C8	-2.28	108.54	115.92
26	k	102	BCR	C2-C1-C6	2.28	113.99	110.48
34	C	520	LMG	C8-O7-C10	-2.28	112.17	117.79
37	D	406	LHG	O7-C7-O9	-2.28	118.19	123.70
24	A	407	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
24	B	616	CLA	C3D-CAD-CBD	2.28	110.61	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CHB-C4A-NA	2.28	127.66	124.51
24	C	510	CLA	C16-C15-C13	-2.28	108.56	115.92
24	b	608	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
24	C	505	CLA	OBD-CAD-C3D	-2.27	124.21	127.98
24	a	407	CLA	C4-C3-C5	2.27	119.09	115.27
26	y	101	BCR	C37-C22-C21	-2.27	119.74	122.92
26	B	620	BCR	C3-C4-C5	-2.27	110.03	114.08
24	d	402	CLA	C1-O2A-CGA	2.27	122.39	116.44
34	a	412	LMG	O1-C1-C2	2.27	111.84	108.30
24	A	410	CLA	CMA-C3A-C2A	-2.27	104.68	113.83
24	B	615	CLA	CAC-C3C-C4C	2.27	127.75	124.81
25	A	408	PHO	C2C-C1C-NC	2.27	113.21	109.79
24	B	605	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
24	c	902	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
24	B	608	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	B	602	CLA	CMC-C2C-C1C	2.26	128.49	125.04
24	c	911	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
24	B	612	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
24	b	617	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
24	B	615	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
34	z	101	LMG	C8-O7-C10	-2.26	112.23	117.79
24	a	406	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
24	c	912	CLA	C1-O2A-CGA	2.26	122.37	116.44
24	C	512	CLA	CMC-C2C-C1C	2.26	128.47	125.04
24	B	611	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
26	d	404	BCR	C37-C22-C23	2.26	121.63	118.08
24	c	911	CLA	CMB-C2B-C3B	2.25	128.90	124.68
26	C	515	BCR	C2-C1-C6	2.25	113.95	110.48
24	b	610	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
27	f	102	SQD	C3-C4-C5	2.25	114.26	110.24
24	B	617	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
24	B	614	CLA	CHD-C4C-NC	2.25	127.75	124.20
26	b	623	BCR	C10-C11-C12	-2.25	116.19	123.22
24	B	616	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	C	510	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
26	B	618	BCR	C37-C22-C23	2.25	121.62	118.08
24	b	618	CLA	C4-C3-C5	2.25	119.06	115.27
24	A	410	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
24	C	505	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
24	b	618	CLA	CMB-C2B-C3B	2.25	128.89	124.68
25	A	408	PHO	CHD-C1D-C2D	-2.25	120.07	125.73
24	D	402	CLA	C1-C2-C3	-2.25	122.16	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C15-C16-C17	-2.25	118.87	123.47
26	y	101	BCR	C38-C26-C25	-2.25	122.00	124.53
25	a	408	PHO	CHD-C1D-C2D	-2.25	120.08	125.73
36	C	518	DGD	O6E-C5E-C6E	2.25	112.02	106.44
27	a	411	SQD	O9-S-C6	2.24	109.61	106.94
26	k	101	BCR	C21-C20-C19	-2.24	116.22	123.22
37	D	406	LHG	O4-P-O5	2.24	123.32	112.24
24	c	912	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
24	B	616	CLA	CHA-C1A-NA	-2.24	121.27	126.40
24	b	611	CLA	CMB-C2B-C3B	2.24	128.87	124.68
37	e	101	LHG	O8-C23-C24	2.24	118.93	111.91
24	C	511	CLA	CAC-C3C-C4C	2.24	127.71	124.81
29	a	401	LMT	C1'-O5'-C5'	2.24	118.08	113.69
35	b	626	HTG	C1-C2-C3	2.23	115.00	110.59
24	b	619	CLA	O2A-CGA-CBA	2.23	118.92	111.91
24	C	514	CLA	C1-O2A-CGA	2.23	122.30	116.44
24	d	401	CLA	CAA-CBA-CGA	2.23	119.78	113.25
36	C	518	DGD	C6D-C5D-C4D	2.23	116.75	112.09
24	C	504	CLA	O2A-CGA-CBA	2.23	118.91	111.91
24	B	616	CLA	CED-O2D-CGD	2.23	120.98	115.94
24	D	401	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	B	612	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	B	615	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
35	B	625	HTG	C1-C2-C3	2.23	114.99	110.59
25	a	408	PHO	O2D-CGD-O1D	-2.23	119.48	123.84
24	b	605	CLA	C4D-C3D-CAD	-2.23	107.23	108.47
25	A	409	PHO	CMC-C2C-C1C	2.23	128.49	125.06
24	D	401	CLA	OBD-CAD-C3D	-2.23	124.28	127.98
24	B	607	CLA	O2D-CGD-O1D	-2.23	119.49	123.84
24	b	619	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	C	510	CLA	CBC-CAC-C3C	-2.22	106.30	112.43
37	d	407	LHG	O8-C23-O10	-2.22	117.98	123.59
26	d	404	BCR	C35-C13-C12	2.22	121.58	118.08
24	C	512	CLA	CED-O2D-CGD	2.22	120.97	115.94
24	b	616	CLA	CHD-C4C-NC	2.22	127.71	124.20
24	A	410	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	B	610	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
34	b	624	LMG	O8-C28-O10	-2.22	117.99	123.59
24	C	513	CLA	CAA-C2A-C1A	2.22	119.25	111.97
24	b	609	CLA	C1-C2-C3	-2.22	122.20	126.04
27	B	621	SQD	C3-C4-C5	2.22	114.20	110.24
24	B	613	CLA	C1-C2-C3	-2.22	122.21	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
24	B	611	CLA	CMA-C3A-C4A	-2.22	105.82	111.77
24	C	506	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	B	603	CLA	CMC-C2C-C1C	2.21	128.41	125.04
24	C	512	CLA	C11-C10-C8	-2.21	108.77	115.92
40	V	201	HEC	CMB-C2B-C1B	-2.21	125.06	128.46
29	M	101	LMT	O5B-C5B-C6B	2.21	111.93	106.44
24	C	510	CLA	C11-C12-C13	-2.21	108.77	115.92
34	Z	101	LMG	C1-O6-C5	2.21	118.02	113.69
24	b	607	CLA	CHD-C4C-NC	2.21	127.68	124.20
24	d	401	CLA	O2A-CGA-CBA	2.21	118.84	111.91
24	a	407	CLA	C1-O2A-CGA	2.21	122.24	116.44
24	A	410	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	d	402	CLA	CMB-C2B-C3B	2.21	128.81	124.68
40	v	202	HEC	CBA-CAA-C2A	-2.21	108.41	112.48
26	b	623	BCR	C7-C8-C9	-2.21	122.90	126.23
26	K	102	BCR	C15-C14-C13	-2.20	124.16	127.31
27	a	411	SQD	C1-C2-C3	-2.20	105.41	110.00
24	c	914	CLA	CED-O2D-CGD	2.20	120.92	115.94
24	a	407	CLA	CMA-C3A-C2A	-2.20	104.94	113.83
26	K	102	BCR	C10-C11-C12	-2.20	116.34	123.22
24	b	617	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	B	603	CLA	C1-C2-C3	-2.20	122.24	126.04
24	c	905	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
24	c	905	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
37	D	407	LHG	O8-C23-O10	-2.20	118.04	123.59
24	A	410	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
25	A	408	PHO	O2D-CGD-O1D	-2.20	119.54	123.84
24	C	504	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	c	908	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	B	606	CLA	CMC-C2C-C1C	2.20	128.38	125.04
24	c	908	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
24	B	611	CLA	CHC-C1C-NC	2.19	127.53	124.20
26	T	102	BCR	C37-C22-C23	2.19	121.53	118.08
24	B	612	CLA	CMB-C2B-C3B	2.19	128.78	124.68
26	A	411	BCR	C8-C7-C6	-2.19	121.05	127.20
24	C	508	CLA	CMB-C2B-C3B	2.19	128.78	124.68
24	D	401	CLA	CED-O2D-CGD	2.19	120.89	115.94
24	c	914	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	B	609	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
26	k	101	BCR	C16-C17-C18	-2.19	124.18	127.31
34	c	920	LMG	O7-C10-O9	-2.19	118.41	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	b	619	CLA	CMC-C2C-C1C	2.19	128.37	125.04
26	D	403	BCR	C30-C25-C24	2.19	121.97	115.78
24	c	903	CLA	OBD-CAD-C3D	-2.19	124.35	127.98
24	c	911	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
24	c	908	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
24	B	610	CLA	C1-O2A-CGA	2.18	122.17	116.44
26	H	101	BCR	C20-C21-C22	-2.18	124.19	127.31
24	c	905	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
24	b	605	CLA	CAC-C3C-C2C	2.18	131.26	127.53
24	A	407	CLA	C1-O2A-CGA	2.18	122.17	116.44
26	b	623	BCR	C21-C20-C19	-2.18	116.41	123.22
24	c	913	CLA	C1-O2A-CGA	2.18	122.16	116.44
26	T	102	BCR	C37-C22-C21	-2.18	119.87	122.92
27	A	416	SQD	O8-S-C6	2.18	109.21	105.74
24	C	514	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
24	B	617	CLA	C4-C3-C5	2.18	118.93	115.27
24	C	507	CLA	O2A-CGA-CBA	2.18	118.74	111.91
26	A	411	BCR	C16-C17-C18	-2.18	124.20	127.31
26	D	403	BCR	C38-C26-C27	2.18	117.80	113.62
25	a	420	PHO	CMB-C2B-C1B	2.18	128.41	125.06
24	C	506	CLA	C1-O2A-CGA	2.17	122.15	116.44
34	a	412	LMG	O7-C10-O9	-2.17	118.45	123.70
24	C	506	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	b	619	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	b	606	CLA	CMA-C3A-C2A	-2.17	105.07	113.83
24	A	407	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
24	B	603	CLA	CAC-C3C-C4C	2.17	127.63	124.81
24	B	607	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	b	607	CLA	CHB-C4A-NA	2.17	127.51	124.51
35	b	603	HTG	O5-C1-C2	2.17	113.04	110.31
24	B	612	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
31	D	404	PL9	C36-C37-C38	-2.17	104.76	111.88
24	C	509	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
36	C	517	DGD	C2G-O2G-C1B	-2.17	112.46	117.79
24	c	905	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
24	B	606	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
26	y	101	BCR	C37-C22-C23	2.16	121.49	118.08
24	D	402	CLA	O2A-CGA-CBA	2.16	118.70	111.91
24	B	614	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
34	Z	101	LMG	C7-O1-C1	-2.16	109.51	113.74
26	T	102	BCR	C29-C28-C27	-2.16	106.55	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C1-O2A-CGA	2.16	122.12	116.44
26	K	102	BCR	C37-C22-C23	2.16	121.48	118.08
27	a	402	SQD	O9-S-C6	2.16	109.51	106.94
24	B	615	CLA	C1-O2A-CGA	2.16	122.11	116.44
25	a	420	PHO	C4D-CHA-C1A	-2.16	120.51	125.37
24	B	603	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	D	402	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
29	C	522	LMT	O5'-C5'-C4'	2.16	114.31	109.75
27	a	402	SQD	O6-C1-C2	2.16	111.67	108.30
24	d	401	CLA	CMB-C2B-C1B	2.16	131.78	128.46
24	b	611	CLA	C1-O2A-CGA	2.16	122.10	116.44
36	C	519	DGD	O1G-C1A-O1A	-2.16	118.15	123.59
24	b	617	CLA	CMB-C2B-C3B	2.16	128.71	124.68
24	C	507	CLA	CGD-CBD-CAD	-2.16	103.75	110.73
24	c	904	CLA	C1-C2-C3	-2.15	122.32	126.04
36	h	102	DGD	C3B-C2B-C1B	-2.15	105.79	113.62
27	a	402	SQD	O48-C23-O10	-2.15	118.16	123.59
25	A	408	PHO	C4D-CHA-C1A	-2.15	120.52	125.37
26	D	403	BCR	C37-C22-C23	2.15	121.47	118.08
24	c	908	CLA	OBD-CAD-C3D	-2.15	124.41	127.98
27	a	402	SQD	C3-C4-C5	2.15	114.08	110.24
24	C	508	CLA	C4-C3-C5	2.15	118.89	115.27
24	d	403	CLA	C4D-C3D-CAD	-2.15	107.27	108.47
34	Z	101	LMG	C9-O8-C28	2.15	122.50	117.10
24	C	512	CLA	OBD-CAD-C3D	-2.15	124.42	127.98
24	c	902	CLA	C4D-C3D-CAD	-2.15	107.27	108.47
26	h	101	BCR	C7-C6-C5	2.15	126.66	121.46
25	A	409	PHO	O2A-CGA-CBA	2.14	118.62	111.91
25	A	408	PHO	C1C-C2C-C3C	-2.14	104.05	106.51
24	B	616	CLA	C1-O2A-CGA	2.14	122.05	116.44
37	d	407	LHG	O7-C7-O9	-2.14	118.54	123.70
24	d	401	CLA	CED-O2D-CGD	2.14	120.77	115.94
27	B	621	SQD	O47-C7-O49	-2.14	118.54	123.70
36	C	519	DGD	C4D-C3D-C2D	-2.13	107.10	110.82
24	c	913	CLA	OBD-CAD-C3D	-2.13	124.44	127.98
26	k	102	BCR	C37-C22-C21	-2.13	119.94	122.92
27	L	102	SQD	C45-O47-C7	-2.13	112.54	117.79
24	C	510	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
24	c	908	CLA	C4-C3-C5	2.13	118.86	115.27
24	C	512	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	b	611	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
26	T	102	BCR	C15-C16-C17	-2.13	119.11	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	102	BCR	C29-C30-C25	2.13	113.76	110.48
34	C	521	LMG	O7-C10-O9	-2.13	118.56	123.70
24	B	614	CLA	C1D-CHD-C4C	-2.13	119.75	122.56
26	t	101	BCR	C31-C1-C6	2.13	113.75	110.30
24	b	613	CLA	C7-C6-C5	-2.12	107.59	113.36
24	a	406	CLA	C11-C10-C8	-2.12	109.05	115.92
35	c	923	HTG	C4-C3-C2	-2.12	107.12	110.82
24	b	609	CLA	CAC-C3C-C4C	2.12	127.56	124.81
24	c	904	CLA	CMB-C2B-C3B	2.12	128.65	124.68
36	c	916	DGD	O6E-C5E-C4E	2.12	113.55	109.69
24	B	606	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
24	A	406	CLA	C4C-C3C-C2C	-2.12	103.81	106.90
24	a	406	CLA	C11-C12-C13	-2.12	109.07	115.92
24	c	910	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
31	A	419	PL9	C17-C18-C19	-2.12	122.56	127.66
37	D	408	LHG	O4-P-O5	2.12	122.71	112.24
31	A	419	PL9	C16-C17-C18	-2.12	104.92	111.88
26	b	622	BCR	C11-C10-C9	-2.12	124.29	127.31
24	b	618	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	B	610	CLA	C7-C6-C5	-2.12	107.61	113.36
37	E	101	LHG	C5-O7-C7	-2.11	112.58	117.79
24	b	614	CLA	CED-O2D-CGD	2.11	120.72	115.94
24	C	514	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
24	a	409	CLA	CED-O2D-CGD	2.11	120.72	115.94
26	c	915	BCR	C39-C30-C25	-2.11	106.87	110.30
36	c	918	DGD	O2G-C1B-O1B	-2.11	118.59	123.70
24	B	614	CLA	CMC-C2C-C1C	2.11	128.26	125.04
24	a	406	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
24	c	913	CLA	CAC-C3C-C4C	2.11	127.55	124.81
25	a	420	PHO	C4-C3-C2	-2.11	118.27	123.68
24	C	505	CLA	C1-O2A-CGA	2.11	121.97	116.44
24	b	617	CLA	CED-O2D-CGD	2.11	120.70	115.94
34	c	920	LMG	O8-C28-O10	-2.11	118.27	123.59
24	c	908	CLA	CAA-C2A-C1A	2.11	118.88	111.97
24	d	403	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
26	B	618	BCR	C21-C20-C19	-2.11	116.65	123.22
35	C	523	HTG	C1-O5-C5	2.10	116.46	112.58
37	d	408	LHG	O8-C23-C24	2.10	118.51	111.91
24	b	620	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
36	C	517	DGD	O1G-C1A-O1A	-2.10	118.28	123.59
24	B	603	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
24	D	401	CLA	C4-C3-C5	2.10	118.81	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	908	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
34	C	501	LMG	O8-C28-C29	2.10	118.50	111.91
24	B	611	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	B	609	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
27	A	412	SQD	C3-C4-C5	2.10	113.99	110.24
27	B	621	SQD	C25-C24-C23	-2.10	105.98	113.62
34	C	501	LMG	O6-C5-C4	2.10	113.51	109.69
24	c	911	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
26	k	101	BCR	C11-C10-C9	-2.10	124.31	127.31
24	b	617	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
26	T	102	BCR	C3-C4-C5	-2.10	110.33	114.08
24	c	914	CLA	CMB-C2B-C3B	2.10	128.60	124.68
24	c	910	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
26	d	404	BCR	C35-C13-C14	-2.10	119.99	122.92
24	B	605	CLA	C4-C3-C5	2.09	118.80	115.27
24	B	609	CLA	C1-C2-C3	-2.09	122.42	126.04
24	c	904	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
24	B	603	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	A	406	CLA	O2A-CGA-CBA	2.09	118.47	111.91
24	C	509	CLA	C7-C6-C5	-2.09	107.68	113.36
24	c	909	CLA	O2A-CGA-CBA	2.09	118.47	111.91
24	c	912	CLA	CED-O2D-CGD	2.09	120.66	115.94
24	c	913	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
24	a	409	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	a	410	BCR	C38-C26-C25	-2.09	122.18	124.53
24	C	510	CLA	C3D-CAD-CBD	2.09	110.35	107.61
24	b	614	CLA	CMC-C2C-C1C	2.08	128.21	125.04
26	a	410	BCR	C16-C17-C18	-2.08	124.34	127.31
26	b	622	BCR	C20-C21-C22	-2.08	124.34	127.31
29	c	921	LMT	C1B-O1B-C4'	-2.08	112.81	117.96
24	c	914	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
26	H	101	BCR	C24-C23-C22	-2.08	123.09	126.23
24	b	606	CLA	OBD-CAD-C3D	-2.08	124.53	127.98
24	c	907	CLA	CAA-CBA-CGA	2.08	119.33	113.25
24	A	406	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
36	c	916	DGD	O2G-C1B-O1B	-2.08	118.68	123.70
34	C	501	LMG	C8-O7-C10	-2.08	112.67	117.79
24	C	510	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	y	101	BCR	C8-C7-C6	-2.08	121.37	127.20
24	c	907	CLA	CED-O2D-CGD	2.08	120.64	115.94
24	b	610	CLA	C11-C10-C8	-2.08	109.21	115.92
31	A	419	PL9	C37-C36-C34	-2.08	106.15	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	411	BCR	C11-C10-C9	-2.07	124.35	127.31
26	K	103	BCR	C33-C5-C6	-2.07	122.20	124.53
25	a	420	PHO	C2C-C1C-NC	2.07	112.92	109.79
24	d	403	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
36	D	405	DGD	C1E-O6E-C5E	2.07	117.75	113.69
24	C	508	CLA	C1-C2-C3	-2.07	122.46	126.04
24	b	607	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
26	T	102	BCR	C7-C8-C9	-2.07	123.11	126.23
24	c	909	CLA	CHD-C4C-NC	2.07	127.46	124.20
34	j	101	LMG	O7-C10-C11	2.07	115.96	111.50
24	B	611	CLA	CHA-C1A-NA	-2.07	121.66	126.40
36	c	916	DGD	C3G-C2G-C1G	-2.07	106.90	111.79
24	C	506	CLA	CHA-C1A-NA	-2.07	121.67	126.40
24	b	615	CLA	C7-C6-C5	-2.07	107.75	113.36
24	d	401	CLA	OBD-CAD-C3D	-2.06	124.55	127.98
24	B	602	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
24	C	513	CLA	CHA-C1A-NA	-2.06	121.68	126.40
24	c	908	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
36	C	518	DGD	C2G-O2G-C1B	-2.06	112.72	117.79
24	d	403	CLA	O2A-CGA-CBA	2.06	118.37	111.91
37	d	409	LHG	O8-C23-O10	-2.06	118.39	123.59
24	c	914	CLA	CHB-C4A-NA	2.06	127.36	124.51
24	b	611	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	c	909	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
24	c	902	CLA	CMB-C2B-C3B	2.06	128.53	124.68
24	A	407	CLA	OBD-CAD-C3D	-2.06	124.57	127.98
26	B	618	BCR	C16-C17-C18	-2.06	124.38	127.31
24	B	602	CLA	CMB-C2B-C3B	2.06	128.52	124.68
24	b	607	CLA	CMA-C3A-C2A	-2.05	105.54	113.83
36	h	102	DGD	C3E-C4E-C5E	-2.05	106.58	110.24
24	C	513	CLA	CBA-CAA-C2A	-2.05	107.80	113.86
24	c	905	CLA	O2A-CGA-CBA	2.05	118.35	111.91
24	b	607	CLA	C3D-CAD-CBD	2.05	110.31	107.61
24	b	610	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
24	a	407	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
24	c	911	CLA	C4-C3-C2	-2.05	118.42	123.68
24	a	406	CLA	CMC-C2C-C1C	2.05	128.16	125.04
24	a	406	CLA	CHD-C4C-NC	2.05	127.43	124.20
34	C	520	LMG	O6-C5-C6	2.05	111.52	106.44
36	H	102	DGD	O6E-C5E-C6E	2.05	111.52	106.44
24	b	614	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
25	A	409	PHO	C4A-NA-C1A	-2.05	106.49	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
31	a	417	PL9	C45-C44-C46	2.04	118.71	115.27
24	b	614	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
26	c	915	BCR	C20-C21-C22	-2.04	124.40	127.31
24	D	402	CLA	CMB-C2B-C1B	2.04	131.60	128.46
24	b	612	CLA	C4-C3-C5	2.04	118.70	115.27
40	V	201	HEC	CBA-CAA-C2A	-2.04	108.72	112.48
24	c	902	CLA	O2A-CGA-CBA	2.04	118.30	111.91
24	b	619	CLA	CHD-C4C-NC	2.04	127.42	124.20
24	B	616	CLA	C6-C7-C8	-2.04	109.33	115.92
26	H	101	BCR	C29-C30-C25	2.04	113.62	110.48
29	f	103	LMT	O1B-C1B-C2B	2.04	113.38	108.10
24	b	611	CLA	CED-O2D-CGD	2.04	120.54	115.94
31	d	405	PL9	C30-C29-C31	2.03	118.69	115.27
24	C	507	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
29	f	103	LMT	O5'-C5'-C4'	2.03	114.03	109.75
26	k	101	BCR	C20-C21-C22	-2.03	124.41	127.31
27	f	102	SQD	O48-C23-O10	-2.03	118.47	123.59
24	a	406	CLA	C5-C3-C2	-2.03	117.01	121.12
24	c	905	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
24	a	406	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
24	A	406	CLA	C3D-CAD-CBD	2.03	110.27	107.61
24	B	602	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
34	j	101	LMG	O8-C28-C29	2.03	118.26	111.91
36	h	102	DGD	O4E-C4E-C5E	2.02	114.33	109.30
24	b	619	CLA	C11-C10-C8	-2.02	109.37	115.92
24	d	401	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
24	B	616	CLA	O2A-CGA-CBA	2.02	118.26	111.91
26	K	103	BCR	C2-C1-C6	2.02	113.60	110.48
37	L	101	LHG	C6-C5-C4	-2.02	107.00	111.79
26	C	516	BCR	C11-C10-C9	-2.02	124.42	127.31
27	L	102	SQD	O48-C23-O10	-2.02	118.49	123.59
24	c	910	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	C	509	CLA	C3D-CAD-CBD	2.02	110.27	107.61
40	v	202	HEC	CMC-C2C-C1C	-2.02	125.36	128.46
40	V	201	HEC	CMC-C2C-C1C	-2.02	125.36	128.46
24	b	613	CLA	CED-O2D-CGD	2.02	120.50	115.94
27	L	102	SQD	O8-S-C6	2.02	108.96	105.74
40	v	202	HEC	C3C-C4C-NC	-2.02	107.13	110.94
24	c	906	CLA	CHB-C4A-NA	2.02	127.30	124.51
36	C	518	DGD	O6D-C1D-O3G	-2.02	105.20	109.97
24	C	510	CLA	O2A-CGA-CBA	2.02	118.23	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C4-C3-C5	2.02	118.66	115.27
24	c	913	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	D	402	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
24	c	902	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
34	j	101	LMG	O6-C5-C4	2.01	113.35	109.69
36	c	917	DGD	O2G-C1B-O1B	-2.01	118.84	123.70
31	A	419	PL9	C12-C13-C14	-2.01	122.82	127.66
24	c	905	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
26	D	403	BCR	C11-C10-C9	-2.01	124.44	127.31
24	b	613	CLA	CMB-C2B-C3B	2.01	128.44	124.68
34	C	521	LMG	O8-C28-C29	2.01	118.21	111.91
24	c	903	CLA	O2A-C1-C2	2.01	113.91	108.64
40	V	201	HEC	C3B-C4B-NB	-2.01	107.15	110.94
24	b	613	CLA	C4-C3-C5	2.00	118.64	115.27
24	C	507	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	A	407	CLA	CMC-C2C-C1C	2.00	128.09	125.04
24	c	906	CLA	CHD-C4C-NC	2.00	127.36	124.20
24	C	505	CLA	CAA-CBA-CGA	2.00	119.11	113.25

All (182) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	c	904	CLA	NC
24	c	904	CLA	ND
24	c	904	CLA	NA
24	C	506	CLA	ND
24	C	503	CLA	NC
24	C	503	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	D	401	CLA	ND
24	D	401	CLA	NA
24	a	407	CLA	NC
24	a	407	CLA	NA
24	A	410	CLA	NC
24	A	410	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA

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Mol	Chain	Res	Type	Atom
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND
24	C	505	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	b	619	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	d	402	CLA	ND
24	c	914	CLA	NC
24	c	914	CLA	ND
24	c	914	CLA	NA
24	c	911	CLA	NC
24	c	911	CLA	ND
24	c	911	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	a	409	CLA	NC
24	a	409	CLA	ND
24	a	409	CLA	NA
24	d	403	CLA	NC
24	d	403	CLA	NA
24	c	912	CLA	NC
24	c	912	CLA	ND
24	c	912	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	c	905	CLA	NC
24	c	905	CLA	ND
24	c	905	CLA	NA
24	C	514	CLA	NC
24	C	514	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	c	913	CLA	NC
24	c	913	CLA	ND
24	c	913	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	609	CLA	NC
24	B	609	CLA	NA
24	d	401	CLA	ND
24	d	401	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	D	402	CLA	NC
24	D	402	CLA	ND
24	D	402	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	c	903	CLA	NC
24	c	903	CLA	ND
24	c	903	CLA	NA

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Mol	Chain	Res	Type	Atom
24	c	908	CLA	NC
24	c	908	CLA	ND
24	c	908	CLA	NA
24	b	620	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	ND
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	b	611	CLA	NC
24	b	611	CLA	ND
24	a	406	CLA	NC
24	a	406	CLA	ND
24	a	406	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	c	909	CLA	NC
24	c	909	CLA	ND
24	c	909	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	c	910	CLA	NC
24	c	910	CLA	ND
24	c	910	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	NA
24	c	906	CLA	ND
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	608	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	A	407	CLA	NC
24	A	407	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	c	902	CLA	NC
24	c	902	CLA	ND
24	c	902	CLA	NA
24	c	907	CLA	NC
24	c	907	CLA	ND
24	c	907	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	NA

All (1245) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	625	HTG	C2'-C1'-S1-C1
36	D	405	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
36	D	405	DGD	C2D-C1D-O3G-C3G
36	D	405	DGD	O6D-C1D-O3G-C3G
36	D	405	DGD	O6E-C1E-O5D-C6D
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
24	b	609	CLA	C2-C3-C5-C6
24	b	609	CLA	C4-C3-C5-C6
36	d	406	DGD	C2B-C1B-O2G-C2G
36	d	406	DGD	O1B-C1B-O2G-C2G
36	d	406	DGD	C2E-C1E-O5D-C6D
36	d	406	DGD	O6E-C1E-O5D-C6D
24	A	410	CLA	C2-C3-C5-C6
24	A	410	CLA	C4-C3-C5-C6
24	b	618	CLA	CHA-CBD-CGD-O1D
24	b	618	CLA	CHA-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	C2-C3-C5-C6
24	b	618	CLA	C4-C3-C5-C6
29	E	102	LMT	C2'-C1'-O1'-C1
29	E	102	LMT	O5'-C1'-O1'-C1
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
34	z	101	LMG	O9-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
28	b	631	GOL	O1-C1-C2-C3
28	v	205	GOL	O1-C1-C2-C3
28	b	633	GOL	O1-C1-C2-O2
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
28	B	629	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
29	C	522	LMT	C2'-C1'-O1'-C1
29	C	522	LMT	O5'-C1'-O1'-C1
29	B	636	LMT	C2'-C1'-O1'-C1
29	B	636	LMT	O5'-C1'-O1'-C1
27	F	101	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
27	F	101	SQD	C8-C7-O47-C45
28	a	415	GOL	O1-C1-C2-C3
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	L	102	SQD	C5-C6-S-O7
27	L	102	SQD	C5-C6-S-O8
27	L	102	SQD	C5-C6-S-O9
28	f	101	GOL	O1-C1-C2-C3
28	V	203	GOL	O1-C1-C2-C3
28	V	203	GOL	C1-C2-C3-O3
37	d	408	LHG	C3-O3-P-O6
37	d	408	LHG	C4-O6-P-O4
28	A	415	GOL	O1-C1-C2-C3
28	B	637	GOL	O1-C1-C2-C3
37	D	407	LHG	C3-O3-P-O6
35	c	922	HTG	C2'-C1'-S1-C1
31	a	417	PL9	C9-C11-C12-C13
31	a	417	PL9	C13-C14-C16-C17
31	a	417	PL9	C15-C14-C16-C17
27	a	402	SQD	O6-C44-C45-O47
37	l	101	LHG	C4-O6-P-O3
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
28	B	631	GOL	O1-C1-C2-C3
29	b	601	LMT	C2'-C1'-O1'-C1
29	b	601	LMT	O5'-C1'-O1'-C1
28	F	103	GOL	O1-C1-C2-C3
28	T	103	GOL	O1-C1-C2-C3
29	b	625	LMT	C2'-C1'-O1'-C1
29	b	625	LMT	O5'-C1'-O1'-C1
24	c	909	CLA	CHA-CBD-CGD-O1D
24	c	909	CLA	CHA-CBD-CGD-O2D
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	D	403	BCR	C21-C22-C23-C24
26	D	403	BCR	C37-C22-C23-C24
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D
28	A	414	GOL	C1-C2-C3-O3
28	A	414	GOL	O2-C2-C3-O3
28	O	302	GOL	O1-C1-C2-C3
24	C	508	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	C	508	CLA	C2-C3-C5-C6
24	C	508	CLA	C4-C3-C5-C6
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C21-C22-C23-C24
26	K	102	BCR	C37-C22-C23-C24
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
29	m	102	LMT	O5'-C1'-O1'-C1
29	m	102	LMT	C2-C1-O1'-C1'
37	E	101	LHG	C24-C23-O8-C6
27	A	416	SQD	O6-C44-C45-O47
35	V	202	HTG	C2-C1-S1-C1'
35	V	202	HTG	O5-C1-S1-C1'
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
26	H	101	BCR	C7-C8-C9-C10
29	C	522	LMT	C3'-C4'-O1B-C1B
29	B	623	LMT	C3'-C4'-O1B-C1B
37	e	101	LHG	O10-C23-O8-C6
37	E	101	LHG	O10-C23-O8-C6
37	e	101	LHG	C24-C23-O8-C6
36	D	405	DGD	O1B-C1B-O2G-C2G
24	B	605	CLA	C3-C5-C6-C7
27	L	102	SQD	C8-C7-O47-C45
24	c	902	CLA	CBD-CGD-O2D-CED
24	B	615	CLA	C4-C3-C5-C6
24	B	604	CLA	C4-C3-C5-C6
24	b	607	CLA	C4-C3-C5-C6
24	b	607	CLA	C2-C3-C5-C6
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C3-C5-C6-C7
29	B	623	LMT	O5B-C5B-C6B-O6B
24	d	401	CLA	CBD-CGD-O2D-CED
24	b	618	CLA	C3-C5-C6-C7
37	E	101	LHG	C8-C7-O7-C5
24	B	617	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
35	B	633	HTG	O5-C5-C6-O6
29	f	103	LMT	O5'-C5'-C6'-O6'
31	A	419	PL9	C25-C24-C26-C27
35	V	202	HTG	C4-C5-C6-O6
24	B	615	CLA	C2-C3-C5-C6
31	A	419	PL9	C23-C24-C26-C27
29	m	102	LMT	C4'-C5'-C6'-O6'
34	C	521	LMG	O6-C5-C6-O5
24	d	403	CLA	C3-C5-C6-C7
24	C	510	CLA	C3-C5-C6-C7
29	B	623	LMT	C4B-C5B-C6B-O6B
37	E	101	LHG	O6-C4-C5-O7
24	a	409	CLA	C5-C6-C7-C8
27	B	621	SQD	C7-C8-C9-C10
27	F	101	SQD	C7-C8-C9-C10
36	D	405	DGD	C2E-C1E-O5D-C6D
34	Z	101	LMG	C2-C1-O1-C7
24	D	402	CLA	C4-C3-C5-C6
24	B	604	CLA	C2-C3-C5-C6
24	a	407	CLA	C14-C13-C15-C16
24	C	513	CLA	C6-C7-C8-C9
24	c	911	CLA	C11-C12-C13-C14
24	C	502	CLA	C11-C12-C13-C14
24	B	617	CLA	C6-C7-C8-C9
24	c	907	CLA	C6-C7-C8-C9
24	C	510	CLA	C8-C10-C11-C12
26	b	623	BCR	C37-C22-C23-C24
26	K	103	BCR	C7-C8-C9-C34
26	D	403	BCR	C7-C8-C9-C34
26	H	101	BCR	C7-C8-C9-C34
35	B	633	HTG	C4-C5-C6-O6
24	B	615	CLA	C5-C6-C7-C8
24	B	604	CLA	C5-C6-C7-C8
24	c	907	CLA	C10-C11-C12-C13
24	c	911	CLA	C8-C10-C11-C12
24	a	409	CLA	C8-C10-C11-C12
24	b	620	CLA	C15-C16-C17-C18
24	b	610	CLA	C10-C11-C12-C13
24	C	509	CLA	C10-C11-C12-C13
35	B	626	HTG	O5-C5-C6-O6
24	b	618	CLA	C15-C16-C17-C18
24	B	602	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	b	607	CLA	C5-C6-C7-C8
29	a	401	LMT	C3-C4-C5-C6
28	B	629	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
28	b	632	GOL	O2-C2-C3-O3
28	B	631	GOL	O1-C1-C2-O2
28	T	103	GOL	O1-C1-C2-O2
27	A	416	SQD	C23-C24-C25-C26
29	m	104	LMT	O5'-C5'-C6'-O6'
35	V	202	HTG	O5-C5-C6-O6
24	a	409	CLA	C15-C16-C17-C18
37	d	409	LHG	C30-C31-C32-C33
29	m	103	LMT	O5'-C5'-C6'-O6'
37	E	101	LHG	O9-C7-O7-C5
34	C	521	LMG	C11-C10-O7-C8
24	B	617	CLA	C10-C11-C12-C13
24	A	410	CLA	C6-C7-C8-C10
24	A	410	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C7
24	b	610	CLA	C12-C13-C15-C16
24	b	618	CLA	C10-C11-C12-C13
24	C	507	CLA	C13-C15-C16-C17
34	b	624	LMG	C30-C31-C32-C33
24	b	610	CLA	CBD-CGD-O2D-CED
29	f	103	LMT	C4'-C5'-C6'-O6'
29	f	103	LMT	O5'-C1'-O1'-C1
24	D	402	CLA	C5-C6-C7-C8
34	C	520	LMG	C28-C29-C30-C31
29	C	522	LMT	O5B-C5B-C6B-O6B
24	c	907	CLA	C15-C16-C17-C18
29	m	102	LMT	O5'-C5'-C6'-O6'
24	b	605	CLA	C8-C10-C11-C12
37	e	101	LHG	C3-O3-P-O6
37	L	101	LHG	C4-O6-P-O3
37	E	101	LHG	C4-O6-P-O3
35	C	524	HTG	O5-C5-C6-O6
24	c	907	CLA	C3-C5-C6-C7
27	F	101	SQD	C23-C24-C25-C26
34	C	521	LMG	O9-C10-O7-C8
24	B	615	CLA	C10-C11-C12-C13
36	c	917	DGD	C3B-C4B-C5B-C6B
24	C	508	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
36	d	406	DGD	C4E-C5E-C6E-O5E
37	D	407	LHG	C32-C33-C34-C35
37	d	407	LHG	C27-C28-C29-C30
27	L	102	SQD	C30-C31-C32-C33
29	b	601	LMT	C3-C4-C5-C6
34	C	501	LMG	C11-C10-O7-C8
29	M	101	LMT	O5'-C5'-C6'-O6'
24	B	602	CLA	C3-C5-C6-C7
36	H	102	DGD	C7A-C8A-C9A-CAA
27	L	102	SQD	C14-C15-C16-C17
34	B	622	LMG	C31-C32-C33-C34
27	a	411	SQD	C25-C26-C27-C28
24	a	409	CLA	C16-C17-C18-C19
24	b	605	CLA	CBA-CGA-O2A-C1
27	f	102	SQD	C29-C30-C31-C32
27	a	402	SQD	C10-C11-C12-C13
37	L	101	LHG	C12-C13-C14-C15
34	Z	101	LMG	C19-C20-C21-C22
36	C	519	DGD	C2A-C3A-C4A-C5A
34	c	919	LMG	O9-C10-O7-C8
34	C	501	LMG	O9-C10-O7-C8
36	D	405	DGD	C1A-C2A-C3A-C4A
35	B	625	HTG	C2'-C3'-C4'-C5'
29	C	522	LMT	C4-C5-C6-C7
36	c	918	DGD	C5A-C6A-C7A-C8A
34	C	501	LMG	C37-C38-C39-C40
37	D	408	LHG	C29-C30-C31-C32
27	a	411	SQD	C9-C10-C11-C12
34	j	101	LMG	C17-C18-C19-C20
37	d	407	LHG	C32-C33-C34-C35
36	H	102	DGD	CCB-CDB-CEB-CFB
27	L	102	SQD	C26-C27-C28-C29
36	c	918	DGD	C2B-C3B-C4B-C5B
36	C	517	DGD	C3B-C4B-C5B-C6B
27	a	411	SQD	C34-C35-C36-C37
34	J	101	LMG	C20-C21-C22-C23
27	A	412	SQD	C9-C10-C11-C12
27	B	621	SQD	C31-C32-C33-C34
34	C	520	LMG	C17-C18-C19-C20
34	b	624	LMG	C38-C39-C40-C41
36	d	406	DGD	C2D-C1D-O3G-C3G
29	c	921	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	a	401	LMT	C2'-C1'-O1'-C1
29	f	103	LMT	C2'-C1'-O1'-C1
29	m	102	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C4B-C5B-C6B-C7B
27	a	411	SQD	C30-C31-C32-C33
24	C	507	CLA	C16-C17-C18-C20
24	c	903	CLA	C16-C17-C18-C20
24	c	902	CLA	O1D-CGD-O2D-CED
25	A	408	PHO	C4-C3-C5-C6
27	f	102	SQD	C25-C26-C27-C28
27	A	412	SQD	C32-C33-C34-C35
36	c	917	DGD	C9B-CAB-CBB-CCB
37	L	101	LHG	C13-C14-C15-C16
34	J	101	LMG	C14-C15-C16-C17
24	A	410	CLA	C14-C13-C15-C16
24	d	403	CLA	C14-C13-C15-C16
24	c	912	CLA	C6-C7-C8-C9
24	b	610	CLA	C11-C10-C8-C9
24	B	605	CLA	C6-C7-C8-C9
36	c	916	DGD	O6D-C5D-C6D-O5D
36	c	918	DGD	C1A-C2A-C3A-C4A
27	L	102	SQD	C34-C35-C36-C37
37	l	101	LHG	C25-C26-C27-C28
34	c	919	LMG	C13-C14-C15-C16
34	C	501	LMG	C12-C13-C14-C15
29	a	401	LMT	C4B-C5B-C6B-O6B
26	c	915	BCR	C7-C8-C9-C34
36	d	406	DGD	C8B-C9B-CAB-CBB
34	z	101	LMG	C15-C16-C17-C18
37	d	409	LHG	C29-C30-C31-C32
28	b	633	GOL	O1-C1-C2-C3
28	b	628	GOL	C1-C2-C3-O3
28	A	413	GOL	O1-C1-C2-C3
28	V	205	GOL	O1-C1-C2-C3
28	f	101	GOL	C1-C2-C3-O3
28	b	632	GOL	C1-C2-C3-O3
28	B	627	GOL	O1-C1-C2-C3
28	V	204	GOL	O1-C1-C2-C3
28	T	103	GOL	C1-C2-C3-O3
28	B	632	GOL	O1-C1-C2-C3
28	o	302	GOL	O1-C1-C2-C3
26	b	623	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	C	513	CLA	C3-C5-C6-C7
24	b	605	CLA	C3-C5-C6-C7
24	C	502	CLA	C15-C16-C17-C18
34	c	919	LMG	C11-C10-O7-C8
34	C	520	LMG	C12-C13-C14-C15
29	B	636	LMT	C3-C4-C5-C6
36	c	918	DGD	C3B-C4B-C5B-C6B
36	D	405	DGD	C1B-C2B-C3B-C4B
36	D	405	DGD	C2A-C3A-C4A-C5A
34	z	101	LMG	C12-C13-C14-C15
27	B	621	SQD	C11-C10-C9-C8
36	H	102	DGD	CBA-CCA-CDA-CEA
36	H	102	DGD	CAB-CBB-CCB-CDB
27	L	102	SQD	C28-C29-C30-C31
37	l	101	LHG	C13-C14-C15-C16
36	c	918	DGD	C2A-C3A-C4A-C5A
36	h	102	DGD	CBB-CCB-CDB-CEB
37	L	101	LHG	C14-C15-C16-C17
37	E	101	LHG	C10-C11-C12-C13
37	E	101	LHG	C25-C26-C27-C28
34	j	101	LMG	O6-C5-C6-O5
35	b	627	HTG	O5-C5-C6-O6
34	J	101	LMG	O6-C5-C6-O5
36	d	406	DGD	O6D-C1D-O3G-C3G
29	c	921	LMT	O5'-C1'-O1'-C1
29	a	401	LMT	O5'-C1'-O1'-C1
36	d	406	DGD	C2A-C3A-C4A-C5A
36	C	518	DGD	CAB-CBB-CCB-CDB
36	h	102	DGD	C5B-C6B-C7B-C8B
34	C	501	LMG	C14-C15-C16-C17
27	a	411	SQD	C16-C17-C18-C19
37	E	101	LHG	C24-C25-C26-C27
27	f	102	SQD	C26-C27-C28-C29
36	c	917	DGD	C2B-C3B-C4B-C5B
29	B	636	LMT	C6-C7-C8-C9
37	e	101	LHG	C9-C10-C11-C12
24	B	614	CLA	C13-C15-C16-C17
36	C	518	DGD	CAA-CBA-CCA-CDA
34	C	520	LMG	C11-C12-C13-C14
27	F	101	SQD	C32-C33-C34-C35
37	l	101	LHG	C33-C34-C35-C36
37	d	409	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CBA-CGA-O2A-C1
24	d	401	CLA	O1D-CGD-O2D-CED
24	c	910	CLA	C13-C15-C16-C17
24	b	612	CLA	C13-C15-C16-C17
34	B	622	LMG	C30-C31-C32-C33
34	J	101	LMG	C16-C17-C18-C19
27	a	402	SQD	C16-C17-C18-C19
36	c	918	DGD	CBA-CCA-CDA-CEA
34	C	501	LMG	C11-C12-C13-C14
34	J	101	LMG	C11-C12-C13-C14
36	C	517	DGD	O6D-C5D-C6D-O5D
24	b	608	CLA	C3-C5-C6-C7
37	D	408	LHG	C13-C14-C15-C16
29	m	102	LMT	O1'-C1-C2-C3
31	A	419	PL9	C30-C29-C31-C32
25	A	408	PHO	C2-C3-C5-C6
31	A	419	PL9	C28-C29-C31-C32
34	j	101	LMG	C16-C17-C18-C19
28	v	205	GOL	O1-C1-C2-O2
28	a	415	GOL	O1-C1-C2-O2
28	f	101	GOL	O2-C2-C3-O3
28	A	415	GOL	O1-C1-C2-O2
28	B	637	GOL	O1-C1-C2-O2
28	F	103	GOL	O1-C1-C2-O2
28	T	103	GOL	O2-C2-C3-O3
28	O	302	GOL	O1-C1-C2-O2
37	D	406	LHG	C28-C29-C30-C31
34	C	521	LMG	C11-C12-C13-C14
37	E	101	LHG	C23-C24-C25-C26
36	d	406	DGD	C9B-CAB-CBB-CCB
27	L	102	SQD	C12-C13-C14-C15
24	c	913	CLA	CBD-CGD-O2D-CED
27	a	411	SQD	C10-C11-C12-C13
35	V	202	HTG	C2'-C3'-C4'-C5'
34	J	101	LMG	C35-C36-C37-C38
24	b	605	CLA	C2-C1-O2A-CGA
24	B	617	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
34	j	101	LMG	C32-C33-C34-C35
35	B	626	HTG	C3'-C4'-C5'-C6'
24	b	610	CLA	C13-C15-C16-C17
24	C	502	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	O1A-CGA-O2A-C1
36	D	405	DGD	C4A-C5A-C6A-C7A
36	d	406	DGD	CAA-CBA-CCA-CDA
36	h	102	DGD	CAA-CBA-CCA-CDA
26	b	621	BCR	C1-C6-C7-C8
26	b	621	BCR	C5-C6-C7-C8
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	h	101	BCR	C23-C24-C25-C26
26	h	101	BCR	C23-C24-C25-C30
26	K	102	BCR	C1-C6-C7-C8
26	H	101	BCR	C5-C6-C7-C8
27	B	621	SQD	C24-C23-O48-C46
36	c	918	DGD	C6A-C7A-C8A-C9A
36	C	517	DGD	C7A-C8A-C9A-CAA
34	c	919	LMG	C20-C21-C22-C23
24	B	602	CLA	O1A-CGA-O2A-C1
29	M	101	LMT	C4B-C5B-C6B-O6B
24	B	607	CLA	C10-C11-C12-C13
37	l	101	LHG	C14-C15-C16-C17
24	c	911	CLA	C4-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	a	407	CLA	C12-C13-C15-C16
24	c	911	CLA	C11-C12-C13-C15
24	B	606	CLA	C2-C3-C5-C6
24	d	403	CLA	C12-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C10
24	D	402	CLA	C2-C3-C5-C6
24	B	616	CLA	C11-C12-C13-C15
24	b	610	CLA	C11-C10-C8-C7
24	b	608	CLA	C11-C12-C13-C15
24	c	907	CLA	C11-C10-C8-C7
35	C	524	HTG	S1-C1'-C2'-C3'
24	b	620	CLA	C3-C5-C6-C7
36	d	406	DGD	C7A-C8A-C9A-CAA
37	d	407	LHG	C28-C29-C30-C31
24	A	405	CLA	C2C-C3C-CAC-CBC
36	H	102	DGD	C9B-CAB-CBB-CCB
35	B	625	HTG	C1'-C2'-C3'-C4'
34	Z	101	LMG	C10-C11-C12-C13
29	E	102	LMT	C4'-C5'-C6'-O6'
34	j	101	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	l	101	LHG	C12-C13-C14-C15
36	h	102	DGD	CCA-CDA-CEA-CFA
24	b	619	CLA	C10-C11-C12-C13
36	d	406	DGD	C3A-C4A-C5A-C6A
27	a	402	SQD	C31-C32-C33-C34
24	a	406	CLA	C2C-C3C-CAC-CBC
35	c	922	HTG	S1-C1'-C2'-C3'
37	d	407	LHG	C30-C31-C32-C33
34	C	521	LMG	C16-C17-C18-C19
36	H	102	DGD	C5B-C6B-C7B-C8B
36	h	102	DGD	C8A-C9A-CAA-CBA
24	B	607	CLA	C13-C15-C16-C17
29	M	101	LMT	O5B-C5B-C6B-O6B
34	Z	101	LMG	O6-C5-C6-O5
34	a	412	LMG	C29-C30-C31-C32
27	L	102	SQD	C15-C16-C17-C18
24	a	409	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C19
24	c	911	CLA	C2-C3-C5-C6
24	C	511	CLA	C2-C3-C5-C6
24	B	616	CLA	C2-C3-C5-C6
31	a	417	PL9	C4-C3-C7-C8
31	A	419	PL9	C4-C3-C7-C8
24	A	410	CLA	C6-C7-C8-C9
24	b	618	CLA	C6-C7-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	b	608	CLA	C11-C12-C13-C14
24	c	907	CLA	C11-C10-C8-C9
27	a	402	SQD	C25-C26-C27-C28
37	d	409	LHG	C32-C33-C34-C35
27	F	101	SQD	C31-C32-C33-C34
29	f	103	LMT	C5-C6-C7-C8
36	c	917	DGD	C1A-C2A-C3A-C4A
37	l	101	LHG	C31-C32-C33-C34
29	m	104	LMT	C2-C3-C4-C5
36	C	517	DGD	O6E-C5E-C6E-O5E
24	c	903	CLA	C16-C17-C18-C19
29	B	623	LMT	C5-C6-C7-C8
34	b	624	LMG	C17-C18-C19-C20
37	L	101	LHG	C32-C33-C34-C35
24	c	904	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	b	620	CLA	C10-C11-C12-C13
36	c	917	DGD	CAA-CBA-CCA-CDA
29	A	417	LMT	O1'-C1-C2-C3
29	b	601	LMT	C2-C3-C4-C5
34	C	521	LMG	C17-C18-C19-C20
36	C	517	DGD	C5B-C6B-C7B-C8B
34	C	520	LMG	C16-C17-C18-C19
29	a	401	LMT	C7-C8-C9-C10
27	F	101	SQD	C30-C31-C32-C33
36	c	916	DGD	CAA-CBA-CCA-CDA
29	a	401	LMT	C1-C2-C3-C4
24	b	619	CLA	C5-C6-C7-C8
34	a	412	LMG	C35-C36-C37-C38
36	d	406	DGD	O6D-C5D-C6D-O5D
36	C	517	DGD	C4D-C5D-C6D-O5D
24	d	403	CLA	C4-C3-C5-C6
24	C	511	CLA	C4-C3-C5-C6
24	B	616	CLA	C4-C3-C5-C6
27	B	621	SQD	C34-C35-C36-C37
24	c	905	CLA	C8-C10-C11-C12
29	B	636	LMT	C5-C6-C7-C8
27	B	621	SQD	O10-C23-O48-C46
27	B	621	SQD	C35-C36-C37-C38
29	b	601	LMT	C4-C5-C6-C7
24	b	618	CLA	C16-C17-C18-C20
36	D	405	DGD	O1G-C1G-C2G-C3G
34	c	919	LMG	C7-C8-C9-O8
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	917	DGD	C2G-C3G-O3G-C1D
36	c	917	DGD	C5D-C6D-O5D-C1E
34	C	521	LMG	C8-C7-O1-C1
34	C	520	LMG	C21-C22-C23-C24
29	f	103	LMT	C2B-C1B-O1B-C4'
36	H	102	DGD	CDB-CEB-CFB-CGB
36	c	918	DGD	C7A-C8A-C9A-CAA
29	c	921	LMT	C6-C7-C8-C9
24	A	410	CLA	C3-C5-C6-C7
24	B	616	CLA	C16-C17-C18-C20
27	f	102	SQD	C32-C33-C34-C35
28	b	631	GOL	O1-C1-C2-O2
28	b	628	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	f	101	GOL	O1-C1-C2-O2
28	V	203	GOL	O1-C1-C2-O2
28	V	203	GOL	O2-C2-C3-O3
28	o	302	GOL	O1-C1-C2-O2
35	B	633	HTG	C4'-C5'-C6'-C7'
34	a	412	LMG	C28-C29-C30-C31
34	C	520	LMG	C22-C23-C24-C25
35	O	303	HTG	C3'-C4'-C5'-C6'
27	A	416	SQD	C26-C27-C28-C29
36	c	916	DGD	O6E-C5E-C6E-O5E
24	b	605	CLA	C2-C3-C5-C6
36	C	519	DGD	C2A-C1A-O1G-C1G
29	C	522	LMT	O5'-C5'-C6'-O6'
36	C	519	DGD	CBA-CCA-CDA-CEA
24	B	603	CLA	C15-C16-C17-C18
24	b	614	CLA	C15-C16-C17-C18
34	a	412	LMG	C21-C22-C23-C24
34	b	624	LMG	C15-C16-C17-C18
34	Z	101	LMG	C29-C28-O8-C9
34	C	521	LMG	C15-C16-C17-C18
24	b	605	CLA	C5-C6-C7-C8
24	C	510	CLA	C10-C11-C12-C13
36	H	102	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	C7-C8-C9-C10
27	a	411	SQD	C31-C32-C33-C34
29	m	103	LMT	C4'-C5'-C6'-O6'
24	b	618	CLA	C13-C15-C16-C17
24	C	508	CLA	C5-C6-C7-C8
24	C	510	CLA	C15-C16-C17-C18
24	B	602	CLA	CAA-CBA-CGA-O2A
29	b	601	LMT	C7-C8-C9-C10
37	L	101	LHG	C24-C25-C26-C27
36	c	916	DGD	C5A-C6A-C7A-C8A
24	b	605	CLA	C4-C3-C5-C6
34	B	622	LMG	C34-C35-C36-C37
24	C	506	CLA	C11-C12-C13-C15
24	b	618	CLA	C6-C7-C8-C10
24	C	513	CLA	C11-C10-C8-C7
24	B	615	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	D	402	CLA	C11-C10-C8-C7
24	C	507	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	b	620	CLA	C11-C12-C13-C15
24	c	910	CLA	C12-C13-C15-C16
24	C	502	CLA	C12-C13-C15-C16
29	c	921	LMT	C7-C8-C9-C10
24	b	609	CLA	C11-C10-C8-C9
24	C	513	CLA	C11-C10-C8-C9
24	B	615	CLA	C11-C10-C8-C9
24	B	602	CLA	C11-C10-C8-C9
24	C	507	CLA	C6-C7-C8-C9
24	b	620	CLA	C11-C12-C13-C14
24	b	610	CLA	C14-C13-C15-C16
24	c	910	CLA	C14-C13-C15-C16
24	C	502	CLA	C14-C13-C15-C16
24	B	611	CLA	C14-C13-C15-C16
37	D	406	LHG	C25-C26-C27-C28
34	C	501	LMG	C13-C14-C15-C16
24	B	616	CLA	C10-C11-C12-C13
36	c	916	DGD	C4D-C5D-C6D-O5D
24	B	616	CLA	C16-C17-C18-C19
34	a	412	LMG	C33-C34-C35-C36
26	K	103	BCR	C7-C8-C9-C10
24	B	614	CLA	C10-C11-C12-C13
37	D	406	LHG	C34-C35-C36-C37
36	d	406	DGD	C2A-C1A-O1G-C1G
37	L	101	LHG	C26-C27-C28-C29
37	l	101	LHG	O6-C4-C5-C6
37	E	101	LHG	O6-C4-C5-C6
31	a	417	PL9	C14-C16-C17-C18
29	b	625	LMT	C3'-C4'-O1B-C1B
27	A	412	SQD	C15-C16-C17-C18
24	c	911	CLA	CBA-CGA-O2A-C1
24	B	616	CLA	C13-C15-C16-C17
24	b	610	CLA	C15-C16-C17-C18
36	C	517	DGD	C6A-C7A-C8A-C9A
36	C	519	DGD	O1A-C1A-O1G-C1G
27	F	101	SQD	C34-C35-C36-C37
29	a	401	LMT	C2-C3-C4-C5
24	b	618	CLA	C16-C17-C18-C19
27	F	101	SQD	C29-C30-C31-C32
37	d	408	LHG	C26-C27-C28-C29
24	A	410	CLA	CBA-CGA-O2A-C1
27	f	102	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
34	c	919	LMG	C10-C11-C12-C13
24	C	514	CLA	C3A-C2A-CAA-CBA
27	A	412	SQD	C13-C14-C15-C16
27	f	102	SQD	C44-C45-C46-O48
36	d	406	DGD	O1G-C1G-C2G-C3G
27	a	402	SQD	O6-C44-C45-C46
37	e	101	LHG	C4-C5-C6-O8
37	E	101	LHG	C4-C5-C6-O8
27	A	416	SQD	O6-C44-C45-C46
29	b	601	LMT	O1'-C1-C2-C3
27	F	101	SQD	C24-C25-C26-C27
36	C	519	DGD	C9B-CAB-CBB-CCB
34	a	412	LMG	C22-C23-C24-C25
37	D	408	LHG	C28-C29-C30-C31
37	d	408	LHG	C4-O6-P-O3
27	a	402	SQD	C23-C24-C25-C26
29	a	401	LMT	O5B-C5B-C6B-O6B
24	d	401	CLA	C15-C16-C17-C18
29	E	102	LMT	C2-C3-C4-C5
36	h	102	DGD	C6A-C7A-C8A-C9A
24	c	912	CLA	CBA-CGA-O2A-C1
27	a	402	SQD	C24-C23-O48-C46
34	C	501	LMG	C38-C39-C40-C41
24	C	506	CLA	C10-C11-C12-C13
35	c	922	HTG	C3'-C4'-C5'-C6'
27	a	402	SQD	C27-C28-C29-C30
37	d	408	LHG	O2-C2-C3-O3
34	J	101	LMG	C13-C14-C15-C16
24	c	911	CLA	O1A-CGA-O2A-C1
36	h	102	DGD	CDA-CEA-CFA-CGA
36	D	405	DGD	O2G-C2G-C3G-O3G
27	A	412	SQD	O6-C44-C45-O47
34	z	101	LMG	O1-C7-C8-O7
27	B	621	SQD	O47-C45-C46-O48
27	F	101	SQD	O47-C45-C46-O48
27	L	102	SQD	O47-C45-C46-O48
34	c	919	LMG	O1-C7-C8-O7
34	c	919	LMG	O7-C8-C9-O8
34	C	501	LMG	O1-C7-C8-O7
34	C	501	LMG	C16-C17-C18-C19
36	C	517	DGD	O6E-C1E-O5D-C6D
24	c	914	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	c	912	CLA	C2-C1-O2A-CGA
24	B	614	CLA	C2-C1-O2A-CGA
24	a	407	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	c	914	CLA	C6-C7-C8-C9
34	B	622	LMG	C36-C37-C38-C39
34	c	919	LMG	C39-C40-C41-C42
29	A	417	LMT	C4B-C5B-C6B-O6B
24	b	617	CLA	C5-C6-C7-C8
24	b	610	CLA	C8-C10-C11-C12
37	D	408	LHG	C2-C3-O3-P
37	d	408	LHG	C34-C35-C36-C37
34	b	624	LMG	C32-C33-C34-C35
26	c	915	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
26	d	404	BCR	C23-C24-C25-C30
26	D	403	BCR	C23-C24-C25-C26
26	D	403	BCR	C23-C24-C25-C30
24	B	612	CLA	C8-C10-C11-C12
29	m	104	LMT	C9-C10-C11-C12
36	c	916	DGD	C8A-C9A-CAA-CBA
37	l	101	LHG	C30-C31-C32-C33
26	c	915	BCR	C7-C8-C9-C10
26	D	403	BCR	C7-C8-C9-C10
36	d	406	DGD	C4D-C5D-C6D-O5D
27	L	102	SQD	C9-C10-C11-C12
37	L	101	LHG	C7-C8-C9-C10
24	c	913	CLA	O1D-CGD-O2D-CED
36	D	405	DGD	C8B-C9B-CAB-CBB
37	d	407	LHG	C25-C26-C27-C28
36	c	917	DGD	C7A-C8A-C9A-CAA
24	b	609	CLA	C10-C11-C12-C13
37	L	101	LHG	C11-C12-C13-C14
24	C	507	CLA	C8-C10-C11-C12
34	J	101	LMG	C10-C11-C12-C13
24	A	405	CLA	C4C-C3C-CAC-CBC
34	J	101	LMG	C15-C16-C17-C18
24	C	505	CLA	C12-C13-C15-C16
24	B	607	CLA	C11-C10-C8-C7
24	c	912	CLA	C6-C7-C8-C10
24	c	905	CLA	C12-C13-C15-C16
24	B	605	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	B	614	CLA	C15-C16-C17-C18
26	h	101	BCR	C9-C10-C11-C12
36	D	405	DGD	CDA-CEA-CFA-CGA
37	d	407	LHG	C23-C24-C25-C26
36	d	406	DGD	O1A-C1A-O1G-C1G
34	z	101	LMG	C16-C17-C18-C19
35	b	626	HTG	C2'-C1'-S1-C1
34	b	624	LMG	C36-C37-C38-C39
29	f	103	LMT	O5B-C1B-O1B-C4'
36	c	918	DGD	CAB-CBB-CCB-CDB
34	C	501	LMG	C17-C18-C19-C20
36	C	518	DGD	C8A-C9A-CAA-CBA
34	j	101	LMG	C18-C19-C20-C21
36	C	517	DGD	C5A-C6A-C7A-C8A
24	c	904	CLA	CAD-CBD-CGD-O2D
24	c	914	CLA	CAD-CBD-CGD-O2D
24	c	911	CLA	CAD-CBD-CGD-O2D
27	B	621	SQD	C46-C45-O47-C7
27	L	102	SQD	C46-C45-O47-C7
24	c	913	CLA	CAD-CBD-CGD-O2D
24	b	620	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
25	a	420	PHO	C2C-C3C-CAC-CBC
24	d	401	CLA	C2C-C3C-CAC-CBC
27	L	102	SQD	C31-C32-C33-C34
27	a	411	SQD	C26-C27-C28-C29
24	C	512	CLA	CBA-CGA-O2A-C1
36	d	406	DGD	C5A-C6A-C7A-C8A
36	C	518	DGD	O6E-C1E-O5D-C6D
36	c	917	DGD	O6E-C1E-O5D-C6D
34	B	622	LMG	C10-C11-C12-C13
34	z	101	LMG	O1-C7-C8-C9
27	B	621	SQD	C44-C45-C46-O48
27	L	102	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
36	h	102	DGD	O1G-C1G-C2G-C3G
34	c	919	LMG	O1-C7-C8-C9
24	c	912	CLA	O1A-CGA-O2A-C1
37	l	101	LHG	O6-C4-C5-O7
27	L	102	SQD	C27-C28-C29-C30
37	l	101	LHG	C35-C36-C37-C38
35	B	624	HTG	S1-C1'-C2'-C3'
29	A	417	LMT	C7-C8-C9-C10
24	C	512	CLA	O1A-CGA-O2A-C1
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	b	609	CLA	CHA-CBD-CGD-O1D
24	b	605	CLA	CHA-CBD-CGD-O1D
24	b	605	CLA	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	CBD-CGD-O2D-CED
24	A	410	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	C13-C14-C15-C16
27	A	416	SQD	C19-C20-C21-C22
27	F	101	SQD	C2-C1-O6-C44
34	C	501	LMG	C2-C1-O1-C7
31	A	419	PL9	C2-C3-C7-C8
36	d	406	DGD	C2B-C3B-C4B-C5B
29	E	102	LMT	C5-C6-C7-C8
36	h	102	DGD	CDB-CEB-CFB-CGB
37	d	409	LHG	C9-C10-C11-C12
27	f	102	SQD	O47-C45-C46-O48
36	d	406	DGD	O1G-C1G-C2G-O2G
37	E	101	LHG	O7-C5-C6-O8
28	B	632	GOL	O1-C1-C2-O2
28	B	628	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
36	c	918	DGD	C4B-C5B-C6B-C7B
24	c	913	CLA	C15-C16-C17-C18
27	a	402	SQD	O10-C23-O48-C46
29	b	625	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	O9-C10-O7-C8
24	B	607	CLA	C11-C10-C8-C9
24	c	905	CLA	C14-C13-C15-C16
24	b	608	CLA	C6-C7-C8-C9
24	C	509	CLA	C11-C10-C8-C9
34	C	521	LMG	C4-C5-C6-O5
29	b	601	LMT	C11-C10-C9-C8
37	d	409	LHG	C17-C18-C19-C20
29	m	104	LMT	C11-C10-C9-C8
27	A	416	SQD	C17-C18-C19-C20
29	m	104	LMT	C6-C7-C8-C9
29	B	636	LMT	C4'-C5'-C6'-O6'
35	B	634	HTG	C4-C5-C6-O6
36	h	102	DGD	O2G-C1B-C2B-C3B
26	y	101	BCR	C36-C18-C19-C20
28	B	628	GOL	O1-C1-C2-C3
34	j	101	LMG	C19-C20-C21-C22
36	d	406	DGD	C1A-C2A-C3A-C4A
34	B	622	LMG	C32-C33-C34-C35
27	B	621	SQD	C9-C10-C11-C12
36	C	518	DGD	C9A-CAA-CBA-CCA
34	C	520	LMG	C37-C38-C39-C40
37	e	101	LHG	C11-C12-C13-C14
37	D	406	LHG	C27-C28-C29-C30
37	d	409	LHG	C2-C3-O3-P
24	d	403	CLA	C2-C3-C5-C6
35	B	634	HTG	C4'-C5'-C6'-C7'
37	d	408	LHG	C3-O3-P-O4
37	d	408	LHG	C4-O6-P-O5
37	D	407	LHG	C3-O3-P-O4
37	e	101	LHG	C3-O3-P-O5
37	E	101	LHG	C4-O6-P-O5
24	b	615	CLA	C16-C17-C18-C20
34	c	919	LMG	O6-C1-O1-C7
34	B	622	LMG	C37-C38-C39-C40
37	D	407	LHG	C33-C34-C35-C36
37	D	408	LHG	C12-C13-C14-C15
25	a	408	PHO	C8-C10-C11-C12
29	a	401	LMT	C6-C7-C8-C9
36	C	519	DGD	C6B-C7B-C8B-C9B
24	C	503	CLA	CAD-CBD-CGD-O1D
24	b	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	CAD-CBD-CGD-O1D
24	C	505	CLA	CAD-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O1D
27	B	621	SQD	C5-C6-S-O7
24	B	606	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
34	a	412	LMG	C10-C11-C12-C13
36	c	918	DGD	C1B-C2B-C3B-C4B
24	B	606	CLA	C8-C10-C11-C12
27	B	621	SQD	C32-C33-C34-C35
34	J	101	LMG	C36-C37-C38-C39
37	d	407	LHG	C33-C34-C35-C36
24	B	615	CLA	C16-C17-C18-C20
24	C	506	CLA	C12-C13-C15-C16
24	a	407	CLA	C11-C12-C13-C15
24	B	602	CLA	C12-C13-C15-C16
24	D	402	CLA	C12-C13-C15-C16
24	B	616	CLA	C12-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C15
24	B	617	CLA	C6-C7-C8-C10
24	B	617	CLA	C12-C13-C15-C16
35	b	627	HTG	C2-C1-S1-C1'
24	c	907	CLA	C6-C7-C8-C10
29	a	401	LMT	O1'-C1-C2-C3
34	B	622	LMG	C11-C10-O7-C8
34	C	521	LMG	C18-C19-C20-C21
27	a	411	SQD	C15-C16-C17-C18
24	b	609	CLA	CBD-CGD-O2D-CED
24	b	607	CLA	CBD-CGD-O2D-CED
24	B	611	CLA	C16-C17-C18-C20
27	a	402	SQD	C34-C35-C36-C37
34	C	501	LMG	C10-C11-C12-C13
34	C	501	LMG	O1-C7-C8-C9
37	e	101	LHG	O7-C5-C6-O8
34	Z	101	LMG	O1-C7-C8-O7
36	C	518	DGD	C3A-C4A-C5A-C6A
27	a	402	SQD	C19-C20-C21-C22
36	C	519	DGD	C2B-C3B-C4B-C5B
27	A	416	SQD	C18-C19-C20-C21
34	B	622	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C27-C28-C29-C30
24	C	506	CLA	C11-C12-C13-C14
24	C	505	CLA	C14-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C9
24	B	616	CLA	C14-C13-C15-C16
24	B	617	CLA	C14-C13-C15-C16
24	b	615	CLA	C16-C17-C18-C19
36	c	918	DGD	C4A-C5A-C6A-C7A
34	C	501	LMG	O6-C1-O1-C7
24	C	511	CLA	O1A-CGA-O2A-C1
28	A	413	GOL	O1-C1-C2-O2
24	A	406	CLA	C15-C16-C17-C18
35	D	411	HTG	O5-C5-C6-O6
27	A	416	SQD	C15-C16-C17-C18
27	A	416	SQD	C24-C23-O48-C46
36	d	406	DGD	CAB-CBB-CCB-CDB
27	F	101	SQD	C11-C10-C9-C8
36	c	918	DGD	CCB-CDB-CEB-CFB
37	d	409	LHG	O10-C23-O8-C6
27	B	621	SQD	C12-C13-C14-C15
37	D	408	LHG	O10-C23-O8-C6
27	A	416	SQD	O10-C23-O48-C46
24	b	610	CLA	O1D-CGD-O2D-CED
24	b	619	CLA	C16-C17-C18-C19
27	L	102	SQD	C18-C19-C20-C21
34	a	412	LMG	C13-C14-C15-C16
29	B	636	LMT	C11-C10-C9-C8
36	C	517	DGD	CDB-CEB-CFB-CGB
34	J	101	LMG	C34-C35-C36-C37
24	a	406	CLA	C4C-C3C-CAC-CBC
24	B	611	CLA	C16-C17-C18-C19
31	a	417	PL9	C2-C3-C7-C8
37	d	407	LHG	C26-C27-C28-C29
27	a	402	SQD	C18-C19-C20-C21
24	C	511	CLA	CBA-CGA-O2A-C1
24	D	402	CLA	C8-C10-C11-C12
34	c	920	LMG	C28-C29-C30-C31
26	c	915	BCR	C1-C6-C7-C8
27	A	412	SQD	O49-C7-O47-C45
24	b	609	CLA	O1D-CGD-O2D-CED
36	C	517	DGD	C1B-C2B-C3B-C4B
37	D	408	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
27	A	412	SQD	C8-C7-O47-C45
24	C	507	CLA	C5-C6-C7-C8
24	B	602	CLA	C2A-CAA-CBA-CGA
36	C	518	DGD	C2E-C1E-O5D-C6D
36	c	917	DGD	C2E-C1E-O5D-C6D
31	D	404	PL9	C39-C41-C42-C43
36	C	517	DGD	C2E-C1E-O5D-C6D
34	c	919	LMG	C2-C1-O1-C7
27	A	416	SQD	C24-C25-C26-C27
36	D	405	DGD	O1G-C1G-C2G-O2G
34	c	920	LMG	O7-C8-C9-O8
27	L	102	SQD	C35-C36-C37-C38
24	b	616	CLA	C3-C5-C6-C7
35	B	626	HTG	C2'-C3'-C4'-C5'
35	b	627	HTG	C1'-C2'-C3'-C4'
35	B	626	HTG	C4-C5-C6-O6
24	B	602	CLA	C11-C10-C8-C7
24	b	608	CLA	C6-C7-C8-C10
24	A	407	CLA	C12-C13-C15-C16
24	b	618	CLA	C11-C12-C13-C14
24	B	615	CLA	C11-C12-C13-C14
24	D	402	CLA	C11-C10-C8-C9
34	j	101	LMG	C13-C14-C15-C16
34	Z	101	LMG	O10-C28-O8-C9
27	B	621	SQD	C19-C20-C21-C22
36	c	917	DGD	C4B-C5B-C6B-C7B
28	B	631	GOL	C1-C2-C3-O3
28	v	204	GOL	C1-C2-C3-O3
24	A	406	CLA	C2C-C3C-CAC-CBC
36	c	916	DGD	C4B-C5B-C6B-C7B
28	V	204	GOL	O1-C1-C2-O2
24	C	513	CLA	CBA-CGA-O2A-C1
34	C	520	LMG	C29-C28-O8-C9
34	b	624	LMG	C29-C28-O8-C9
37	d	409	LHG	C24-C23-O8-C6
24	C	507	CLA	C10-C11-C12-C13
27	A	412	SQD	C34-C35-C36-C37
24	B	614	CLA	CBD-CGD-O2D-CED
24	C	502	CLA	CBD-CGD-O2D-CED
29	B	623	LMT	C3-C4-C5-C6
24	C	511	CLA	C8-C10-C11-C12
24	c	907	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	C	520	LMG	O10-C28-O8-C9
36	c	916	DGD	C5B-C6B-C7B-C8B
29	M	101	LMT	C4'-C5'-C6'-O6'
36	D	405	DGD	C7B-C8B-C9B-CAB
29	B	623	LMT	C4-C5-C6-C7
24	C	513	CLA	O1A-CGA-O2A-C1
34	B	622	LMG	C20-C21-C22-C23
37	L	101	LHG	C31-C32-C33-C34
24	c	910	CLA	C16-C17-C18-C19
36	h	102	DGD	C7A-C8A-C9A-CAA
31	d	405	PL9	C13-C14-C16-C17
24	b	615	CLA	C2-C3-C5-C6
24	b	617	CLA	C2-C1-O2A-CGA
24	B	604	CLA	C16-C17-C18-C20
36	C	517	DGD	CBA-CCA-CDA-CEA
24	B	617	CLA	C8-C10-C11-C12
24	B	603	CLA	C2A-CAA-CBA-CGA
24	b	614	CLA	C2A-CAA-CBA-CGA
24	B	611	CLA	C2A-CAA-CBA-CGA
24	c	902	CLA	C2A-CAA-CBA-CGA
36	d	406	DGD	C6A-C7A-C8A-C9A
24	B	602	CLA	C3A-C2A-CAA-CBA
27	a	411	SQD	C13-C14-C15-C16
29	B	636	LMT	O5'-C5'-C6'-O6'
29	C	522	LMT	C1-C2-C3-C4
37	D	406	LHG	C33-C34-C35-C36
24	B	614	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C14-C13-C15-C16
24	b	619	CLA	C16-C17-C18-C20
36	c	918	DGD	C8B-C9B-CAB-CBB
36	c	917	DGD	C1B-C2B-C3B-C4B
34	a	412	LMG	C15-C16-C17-C18
34	J	101	LMG	C30-C31-C32-C33
34	C	521	LMG	O1-C7-C8-C9
29	m	104	LMT	C1-C2-C3-C4
24	B	602	CLA	CAA-CBA-CGA-O1A
36	c	918	DGD	C2A-C1A-O1G-C1G
29	M	101	LMT	O5'-C1'-O1'-C1
37	d	407	LHG	C11-C10-C9-C8
27	B	621	SQD	C17-C18-C19-C20
34	c	920	LMG	C29-C30-C31-C32
36	d	406	DGD	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
34	b	624	LMG	C10-C11-C12-C13
24	B	612	CLA	C15-C16-C17-C18
24	a	409	CLA	C4-C3-C5-C6
31	a	417	PL9	C45-C44-C46-C47
24	b	615	CLA	C4-C3-C5-C6
24	C	514	CLA	C1A-C2A-CAA-CBA
24	b	607	CLA	C6-C7-C8-C10
24	b	610	CLA	C11-C12-C13-C15
24	B	617	CLA	C11-C12-C13-C15
37	d	409	LHG	C33-C34-C35-C36
29	A	417	LMT	C1-C2-C3-C4
37	L	101	LHG	C25-C26-C27-C28
34	C	501	LMG	C21-C22-C23-C24
37	D	408	LHG	C10-C11-C12-C13
24	b	605	CLA	CAA-CBA-CGA-O2A
36	d	406	DGD	C4A-C5A-C6A-C7A
29	B	623	LMT	C6-C7-C8-C9
25	a	420	PHO	C8-C10-C11-C12
36	C	518	DGD	C4E-C5E-C6E-O5E
34	j	101	LMG	C29-C30-C31-C32
36	c	917	DGD	CBB-CCB-CDB-CEB
27	L	102	SQD	C11-C10-C9-C8
24	B	603	CLA	C13-C15-C16-C17
29	A	417	LMT	O5B-C5B-C6B-O6B
34	b	624	LMG	C18-C19-C20-C21
37	D	408	LHG	C30-C31-C32-C33
29	E	102	LMT	C2B-C1B-O1B-C4'
27	a	411	SQD	O6-C44-C45-O47
29	C	522	LMT	C5-C6-C7-C8
29	a	401	LMT	C9-C10-C11-C12
34	b	624	LMG	C40-C41-C42-C43
34	c	919	LMG	C36-C37-C38-C39
26	t	101	BCR	C13-C14-C15-C16
36	D	405	DGD	CAA-CBA-CCA-CDA
34	C	501	LMG	C15-C16-C17-C18
31	d	405	PL9	C39-C41-C42-C43
31	a	417	PL9	C20-C19-C21-C22
34	Z	101	LMG	C11-C12-C13-C14
24	c	910	CLA	C2-C1-O2A-CGA
35	C	523	HTG	O5-C5-C6-O6
24	d	401	CLA	C4C-C3C-CAC-CBC
24	b	608	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C8-C10-C11-C12
36	c	918	DGD	O1A-C1A-O1G-C1G
34	b	624	LMG	O10-C28-O8-C9
35	b	602	HTG	C4'-C5'-C6'-C7'
24	C	504	CLA	C5-C6-C7-C8
37	E	101	LHG	C17-C18-C19-C20
26	k	101	BCR	C1-C6-C7-C8
26	b	623	BCR	C23-C24-C25-C30
26	k	102	BCR	C1-C6-C7-C8
26	b	622	BCR	C23-C24-C25-C30
26	C	516	BCR	C1-C6-C7-C8
26	K	102	BCR	C23-C24-C25-C30
26	B	620	BCR	C23-C24-C25-C30
27	A	412	SQD	C12-C13-C14-C15
34	c	919	LMG	C21-C22-C23-C24
28	v	203	GOL	C1-C2-C3-O3
28	v	204	GOL	O1-C1-C2-C3
29	f	103	LMT	C4-C5-C6-C7
34	c	919	LMG	C32-C33-C34-C35
24	c	914	CLA	C4-C3-C5-C6
31	a	417	PL9	C12-C11-C9-C10
34	C	501	LMG	C18-C19-C20-C21
36	H	102	DGD	O1B-C1B-C2B-C3B
24	B	615	CLA	C16-C17-C18-C19
34	j	101	LMG	C21-C22-C23-C24
34	j	101	LMG	C36-C37-C38-C39
34	C	520	LMG	C29-C30-C31-C32
31	D	404	PL9	C40-C39-C41-C42
24	b	620	CLA	C4-C3-C5-C6
24	b	618	CLA	C11-C12-C13-C15
24	c	914	CLA	C2-C3-C5-C6
24	a	409	CLA	C2-C3-C5-C6
24	B	610	CLA	C2-C3-C5-C6
25	A	408	PHO	C8-C10-C11-C12
36	D	405	DGD	CBA-CCA-CDA-CEA
27	A	416	SQD	C16-C17-C18-C19
36	c	916	DGD	C7A-C8A-C9A-CAA
37	d	408	LHG	O10-C23-O8-C6
36	C	518	DGD	CCB-CDB-CEB-CFB
27	B	621	SQD	C30-C31-C32-C33
29	f	103	LMT	C9-C10-C11-C12
29	m	104	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	612	CLA	C4-C3-C5-C6
24	B	602	CLA	C15-C16-C17-C18
31	d	405	PL9	C28-C29-C31-C32
34	z	101	LMG	O7-C10-C11-C12
36	D	405	DGD	CAB-CBB-CCB-CDB
24	a	407	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C12-C13-C14
24	B	602	CLA	C14-C13-C15-C16
24	D	402	CLA	C14-C13-C15-C16
24	c	910	CLA	C11-C10-C8-C9
24	A	407	CLA	C14-C13-C15-C16
37	d	409	LHG	C28-C29-C30-C31
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	610	CLA	C3A-C2A-CAA-CBA
24	C	513	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	d	403	CLA	CAD-CBD-CGD-O2D
24	c	906	CLA	CAD-CBD-CGD-O2D
24	b	608	CLA	CAD-CBD-CGD-O2D
24	c	902	CLA	CAD-CBD-CGD-O2D
27	B	621	SQD	C18-C19-C20-C21
24	C	502	CLA	C2A-CAA-CBA-CGA
24	b	612	CLA	C2-C1-O2A-CGA
37	d	409	LHG	C25-C26-C27-C28
37	L	101	LHG	C23-C24-C25-C26
34	c	919	LMG	C37-C38-C39-C40
31	d	405	PL9	C30-C29-C31-C32
31	a	417	PL9	C18-C19-C21-C22
31	a	417	PL9	C43-C44-C46-C47
36	d	406	DGD	O2G-C1B-C2B-C3B
24	C	513	CLA	CAA-CBA-CGA-O2A
37	E	101	LHG	C18-C19-C20-C21
24	c	914	CLA	O1A-CGA-O2A-C1
31	a	417	PL9	C39-C41-C42-C43
36	D	405	DGD	C1G-C2G-C3G-O3G
27	F	101	SQD	C44-C45-C46-O48
34	Z	101	LMG	O1-C7-C8-C9
27	A	412	SQD	C14-C15-C16-C17
37	D	408	LHG	C24-C25-C26-C27
25	a	408	PHO	O2A-C1-C2-C3
24	D	402	CLA	O2A-C1-C2-C3
24	B	614	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
24	c	910	CLA	O2A-C1-C2-C3
37	D	407	LHG	C17-C18-C19-C20
24	b	618	CLA	C8-C10-C11-C12
27	f	102	SQD	O47-C7-C8-C9
24	c	913	CLA	CAA-CBA-CGA-O2A
37	d	408	LHG	C13-C14-C15-C16
34	c	920	LMG	C30-C31-C32-C33
24	B	611	CLA	C15-C16-C17-C18
24	b	609	CLA	CHA-CBD-CGD-O2D
25	a	420	PHO	CHA-CBD-CGD-O1D
25	a	420	PHO	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
25	A	409	PHO	CHA-CBD-CGD-O1D
25	A	409	PHO	CHA-CBD-CGD-O2D
24	c	905	CLA	CHA-CBD-CGD-O1D
24	c	913	CLA	CHA-CBD-CGD-O2D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	c	903	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O1D
24	c	910	CLA	CHA-CBD-CGD-O1D
24	c	910	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	C	510	CLA	CHA-CBD-CGD-O2D
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
36	c	918	DGD	CBB-CCB-CDB-CEB
27	A	416	SQD	C25-C26-C27-C28
24	B	614	CLA	CAA-CBA-CGA-O2A
37	l	101	LHG	C11-C12-C13-C14
37	E	101	LHG	O8-C23-C24-C25
28	v	203	GOL	O2-C2-C3-O3
28	a	414	GOL	O2-C2-C3-O3
28	B	631	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
37	d	408	LHG	C24-C23-O8-C6
24	B	613	CLA	CBA-CGA-O2A-C1
29	E	102	LMT	O5'-C5'-C6'-O6'
24	B	606	CLA	O1D-CGD-O2D-CED
24	c	914	CLA	C12-C13-C15-C16
34	B	622	LMG	O8-C28-C29-C30
24	b	610	CLA	C11-C12-C13-C14
35	c	922	HTG	C2'-C3'-C4'-C5'
24	B	613	CLA	CAA-CBA-CGA-O2A
37	e	101	LHG	O8-C23-C24-C25
27	B	621	SQD	C5-C6-S-O8
27	a	402	SQD	C5-C6-S-O8
27	A	416	SQD	C5-C6-S-O8
27	L	102	SQD	C29-C30-C31-C32
24	B	613	CLA	O1A-CGA-O2A-C1
24	c	904	CLA	C2A-CAA-CBA-CGA
29	C	522	LMT	O1'-C1-C2-C3
36	D	405	DGD	O1G-C1A-C2A-C3A
24	c	911	CLA	CAA-CBA-CGA-O2A
24	c	909	CLA	C13-C15-C16-C17
37	D	408	LHG	C9-C10-C11-C12
34	z	101	LMG	O9-C10-C11-C12
24	B	606	CLA	C16-C17-C18-C19
24	b	610	CLA	C16-C17-C18-C19
37	L	101	LHG	C16-C17-C18-C19
28	a	414	GOL	C1-C2-C3-O3
28	V	206	GOL	C1-C2-C3-O3
24	b	620	CLA	C2-C3-C5-C6
24	C	509	CLA	C1A-C2A-CAA-CBA
36	C	518	DGD	CDA-CEA-CFA-CGA
29	M	101	LMT	C7-C8-C9-C10
34	C	501	LMG	C36-C37-C38-C39
27	B	621	SQD	C28-C29-C30-C31
36	h	102	DGD	C5A-C6A-C7A-C8A
27	A	412	SQD	O6-C44-C45-C46
24	B	604	CLA	C16-C17-C18-C19
27	f	102	SQD	O49-C7-C8-C9
31	d	405	PL9	C15-C14-C16-C17
24	C	506	CLA	CAA-CBA-CGA-O2A
24	b	617	CLA	CAA-CBA-CGA-O2A
36	d	406	DGD	O1B-C1B-C2B-C3B
24	c	913	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
36	c	917	DGD	C9A-CAA-CBA-CCA
24	c	914	CLA	C10-C11-C12-C13
27	f	102	SQD	C34-C35-C36-C37
24	C	511	CLA	C16-C17-C18-C19
36	h	102	DGD	O1G-C1G-C2G-O2G
24	B	613	CLA	CAA-CBA-CGA-O1A
37	l	101	LHG	O7-C7-C8-C9
24	c	914	CLA	CBA-CGA-O2A-C1
26	C	516	BCR	C5-C6-C7-C8
26	K	102	BCR	C23-C24-C25-C26
26	B	620	BCR	C23-C24-C25-C26
31	A	419	PL9	C19-C21-C22-C23
24	C	503	CLA	C13-C15-C16-C17
24	d	403	CLA	C10-C11-C12-C13
34	J	101	LMG	C32-C33-C34-C35
24	C	511	CLA	CAA-CBA-CGA-O2A
24	b	606	CLA	C2A-CAA-CBA-CGA
24	C	513	CLA	CAA-CBA-CGA-O1A
24	C	504	CLA	C4-C3-C5-C6
27	B	621	SQD	O5-C5-C6-S
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	b	613	CLA	CAD-CBD-CGD-O1D
27	a	402	SQD	C5-C6-S-O7
27	a	402	SQD	C5-C6-S-O9
27	A	416	SQD	C5-C6-S-O7
27	A	416	SQD	C5-C6-S-O9
24	c	907	CLA	CAD-CBD-CGD-O1D
37	e	101	LHG	O10-C23-C24-C25
34	b	624	LMG	O8-C28-C29-C30
24	c	914	CLA	C14-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C14
24	c	906	CLA	C11-C12-C13-C14
36	C	518	DGD	CBB-CCB-CDB-CEB
37	E	101	LHG	O7-C7-C8-C9
34	C	521	LMG	C39-C40-C41-C42
37	E	101	LHG	O10-C23-C24-C25
36	C	518	DGD	C5A-C6A-C7A-C8A
36	C	518	DGD	O2G-C1B-C2B-C3B
24	c	906	CLA	CAA-CBA-CGA-O2A
36	C	519	DGD	O1G-C1A-C2A-C3A

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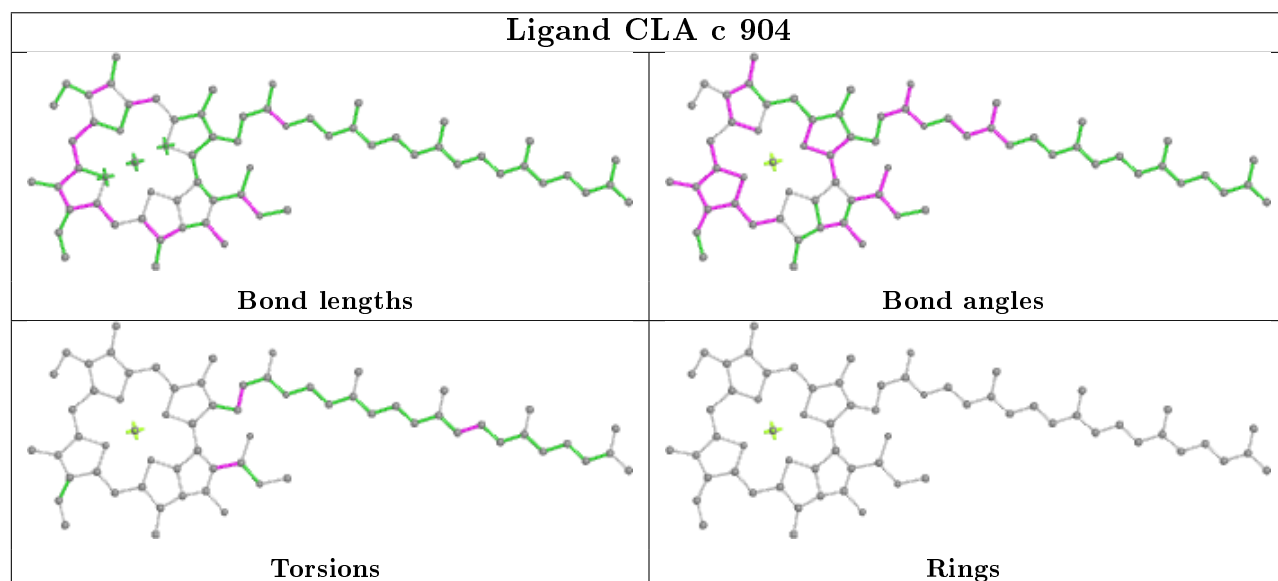
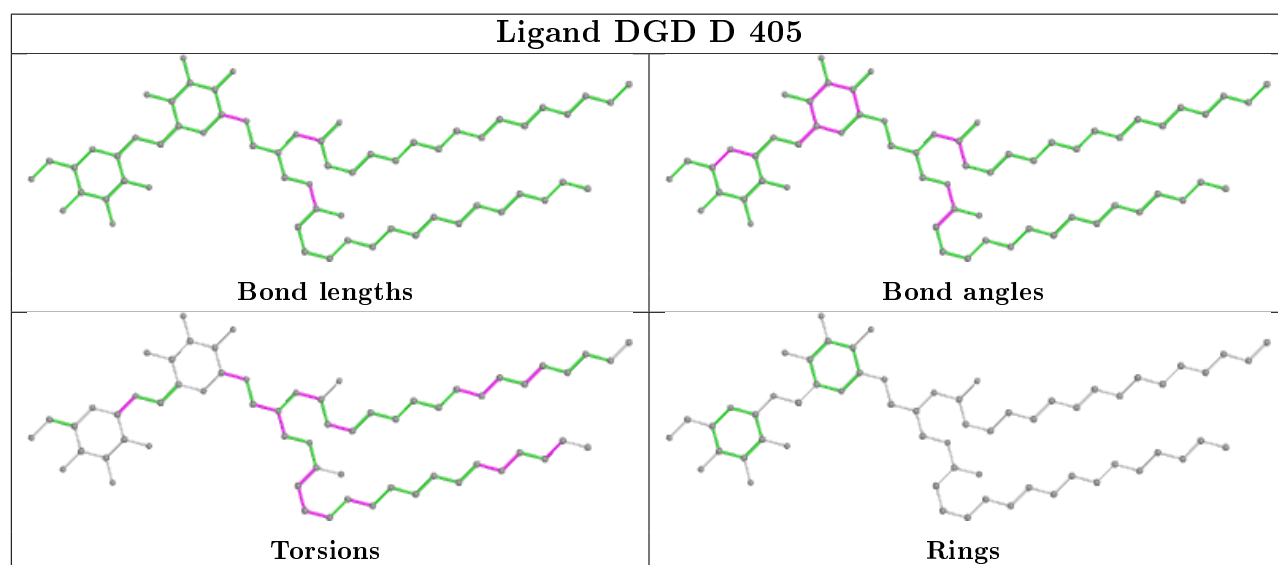
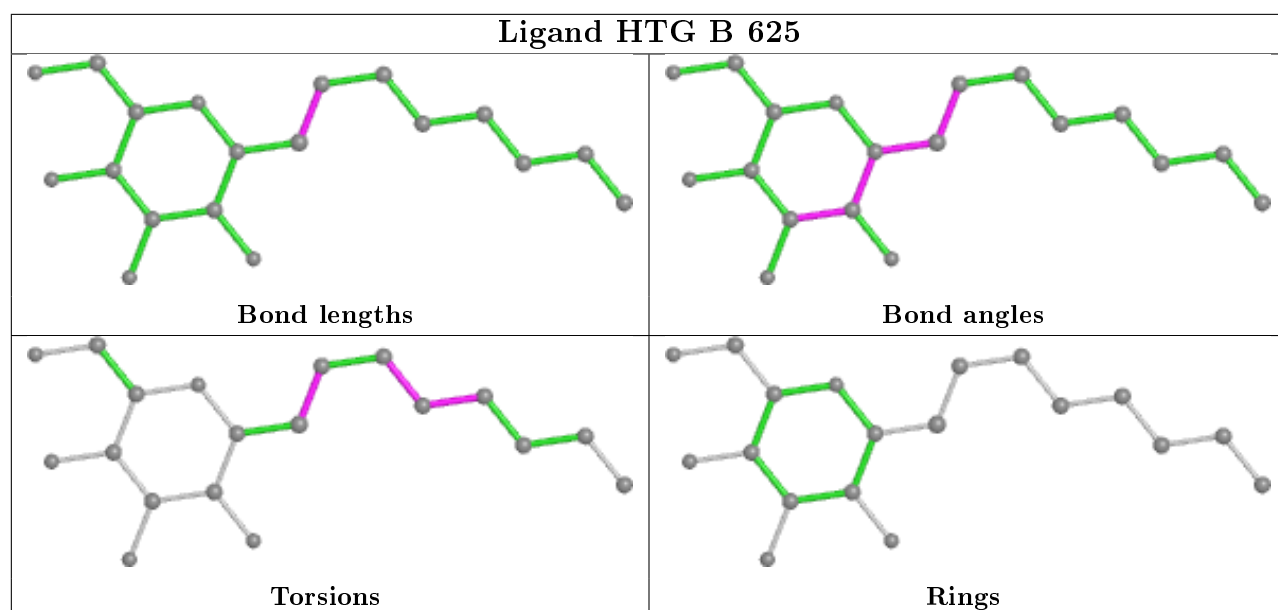
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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C15-C16-C17-C18
31	D	404	PL9	C35-C34-C36-C37
24	C	509	CLA	C5-C6-C7-C8
24	a	407	CLA	C6-C7-C8-C10
24	C	513	CLA	C6-C7-C8-C10
24	b	613	CLA	C2-C3-C5-C6
24	b	612	CLA	C11-C10-C8-C7
34	b	624	LMG	C39-C40-C41-C42
36	C	517	DGD	C2A-C3A-C4A-C5A
37	D	406	LHG	C11-C12-C13-C14
34	b	624	LMG	C31-C32-C33-C34
26	A	411	BCR	C17-C18-C19-C20
26	T	102	BCR	C13-C14-C15-C16
36	c	916	DGD	C2A-C3A-C4A-C5A
34	C	520	LMG	O7-C10-C11-C12
29	m	103	LMT	O5'-C1'-O1'-C1
27	a	402	SQD	C13-C14-C15-C16
24	B	614	CLA	CAA-CBA-CGA-O1A
24	c	906	CLA	CAA-CBA-CGA-O1A
37	E	101	LHG	O9-C7-C8-C9
34	a	412	LMG	C31-C32-C33-C34
27	L	102	SQD	O48-C23-C24-C25
34	Z	101	LMG	O7-C10-C11-C12
24	b	615	CLA	C8-C10-C11-C12
36	D	405	DGD	O1A-C1A-C2A-C3A

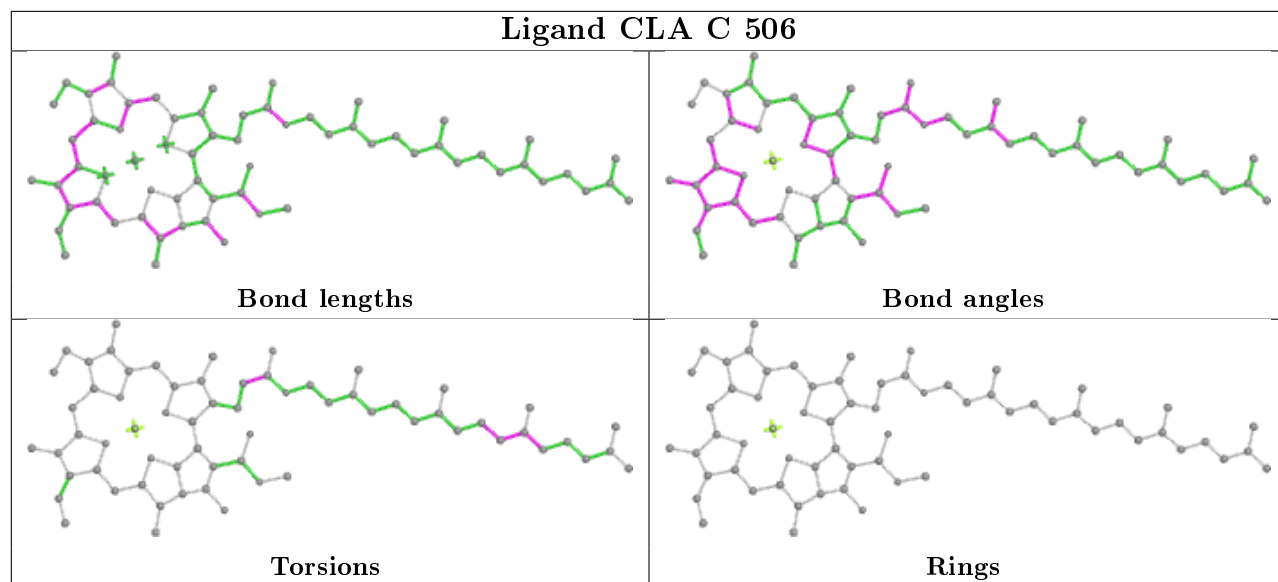
There are no ring outliers.

No monomer is involved in short contacts.

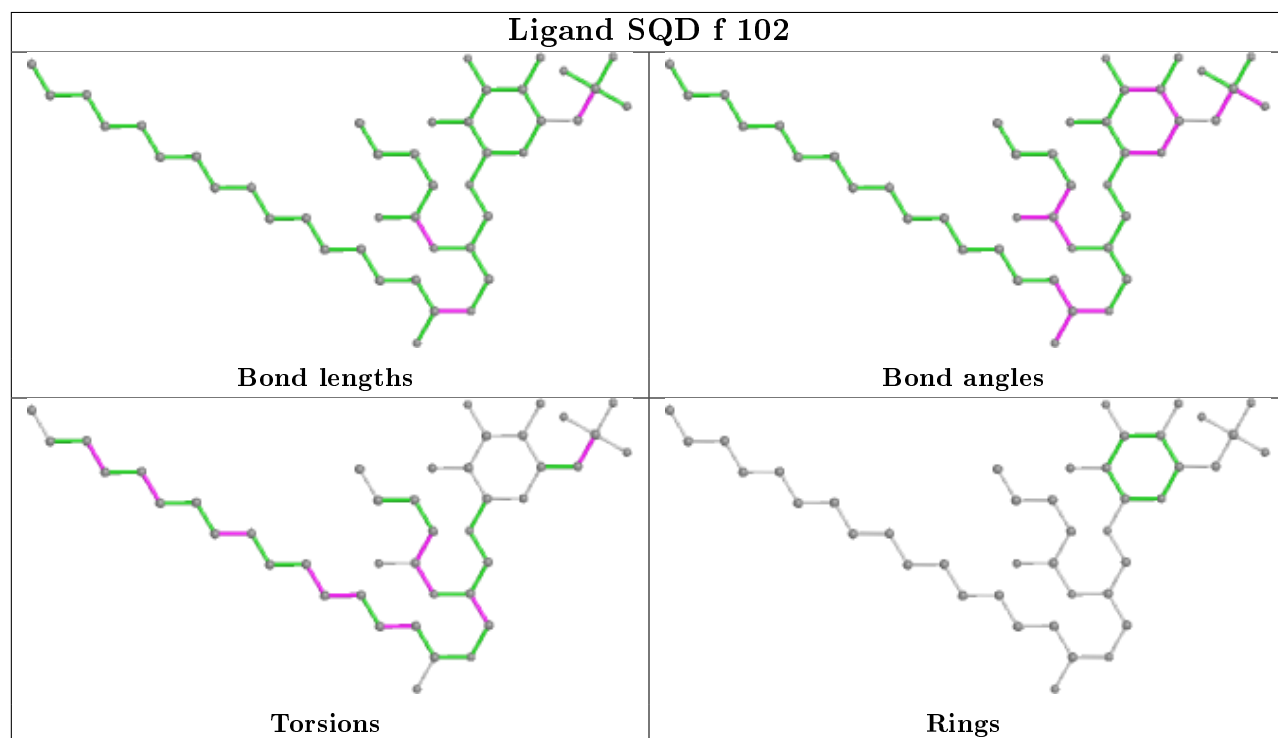
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



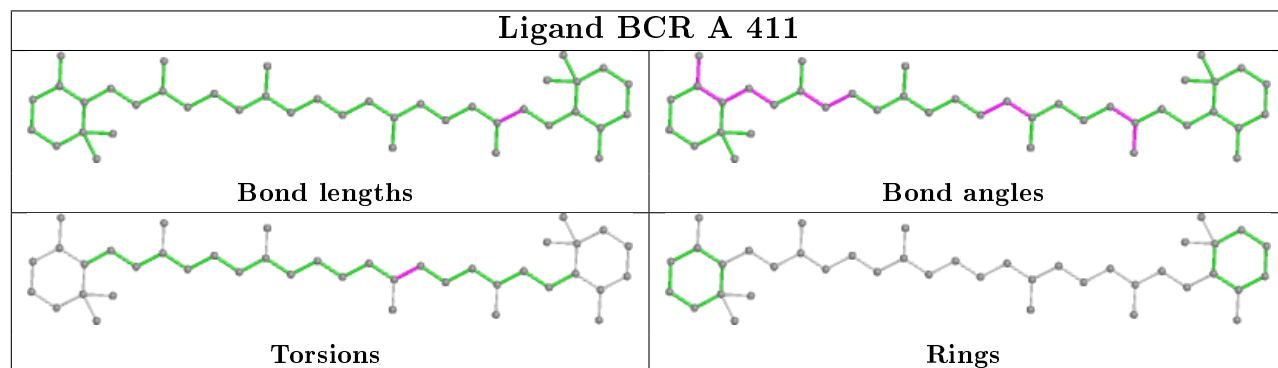
## Ligand CLA C 506



## Ligand SQD f 102

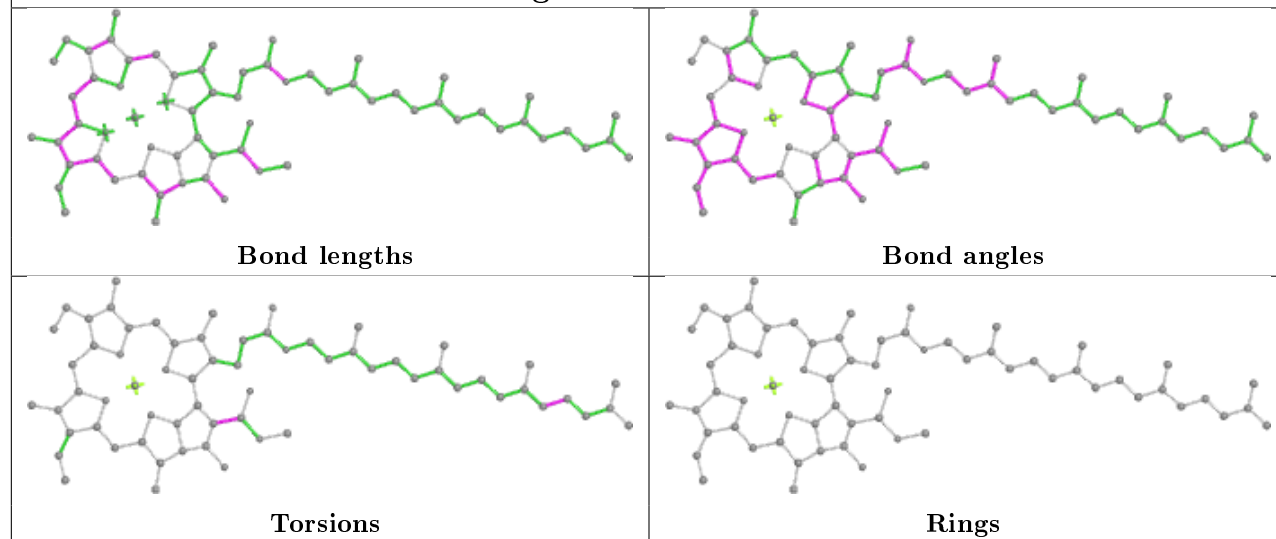


## Ligand BCR A 411

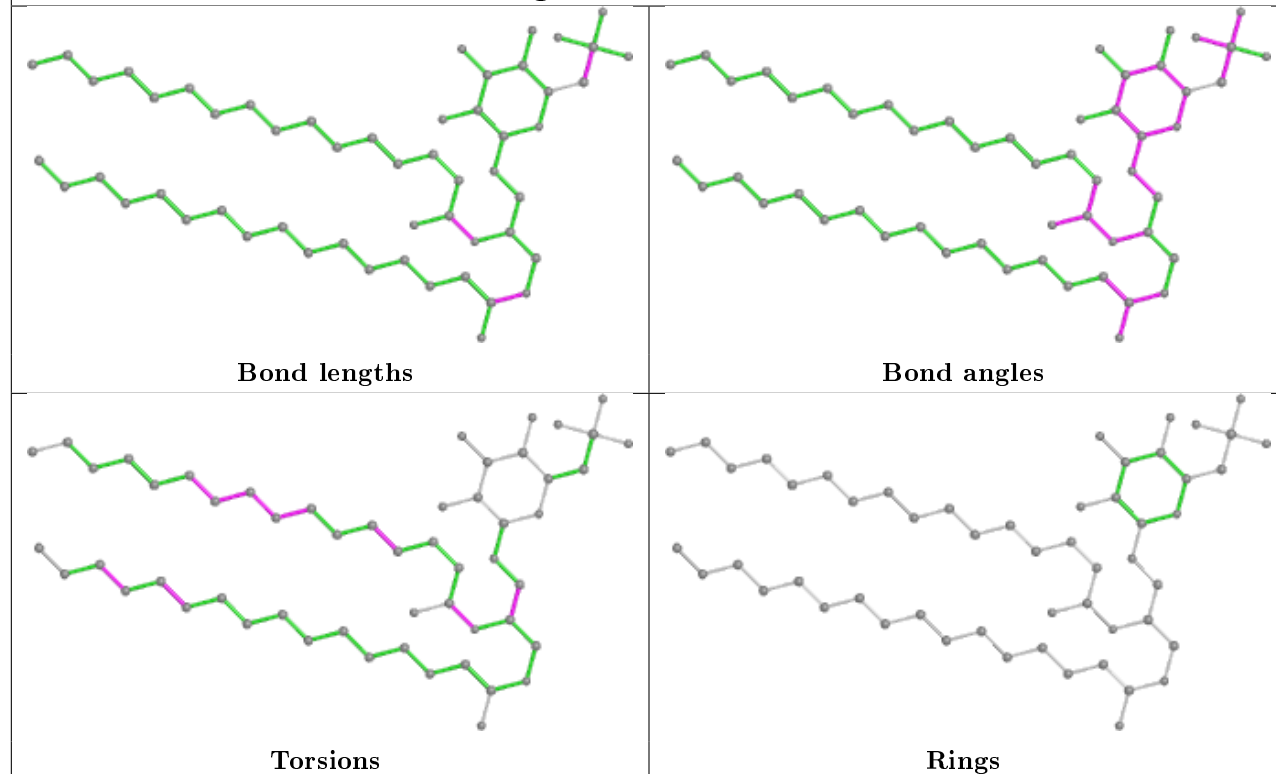




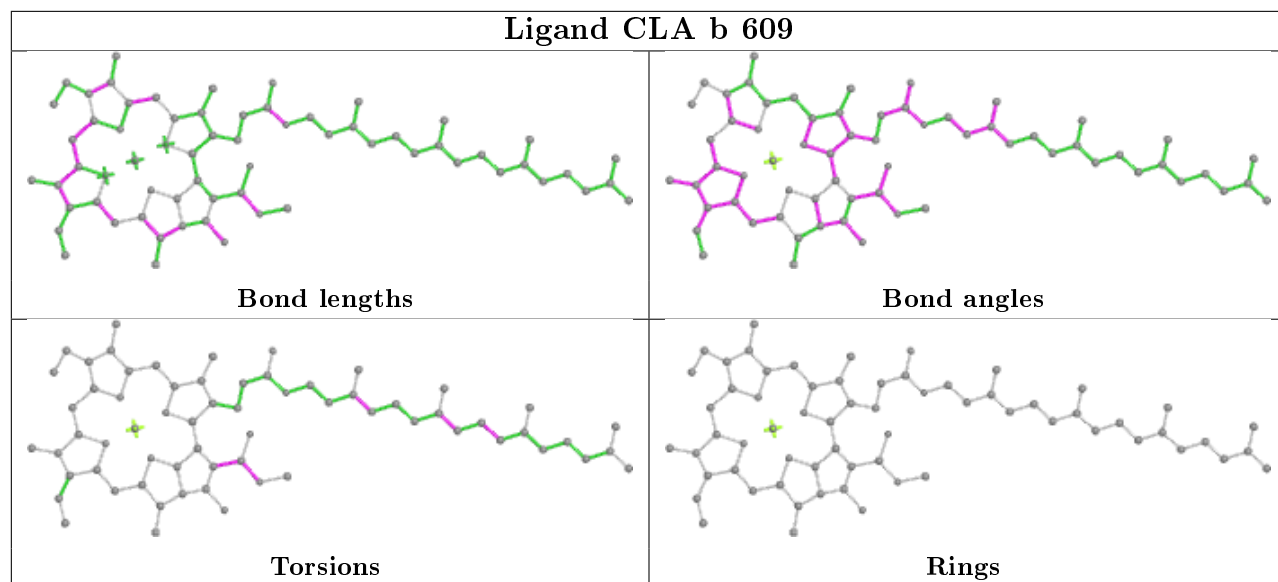
## Ligand CLA C 503



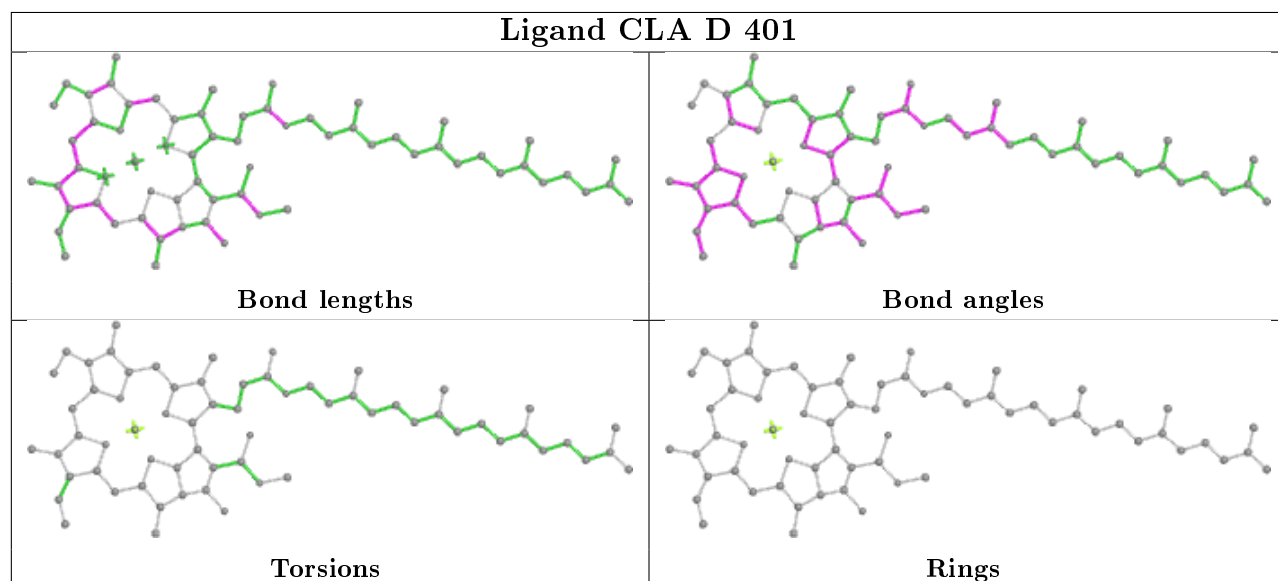
## Ligand SQD A 412



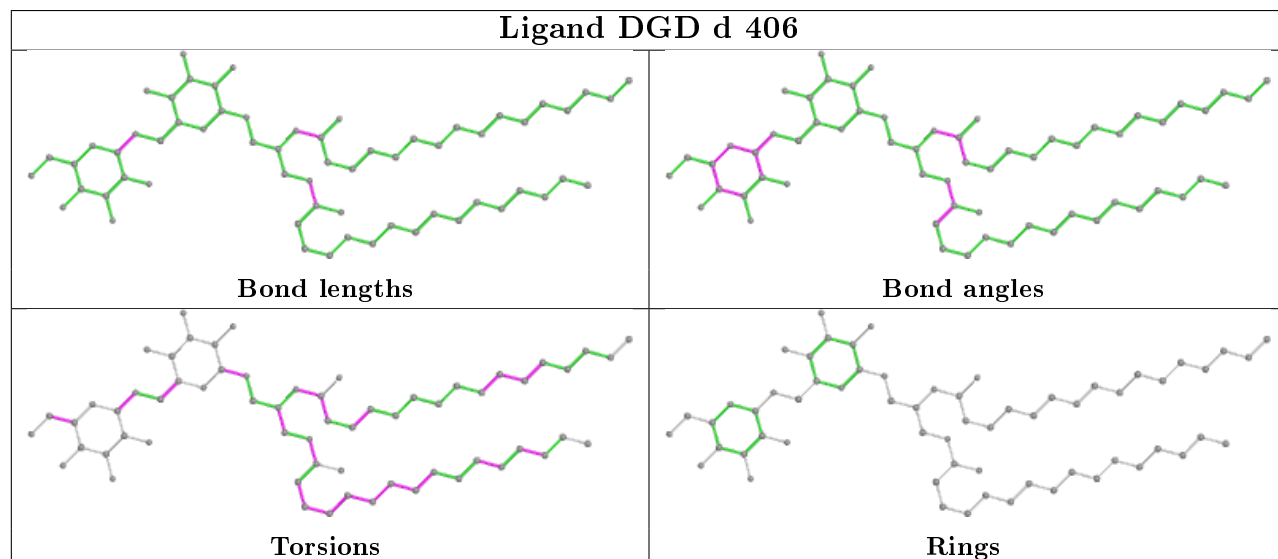
## Ligand CLA b 609



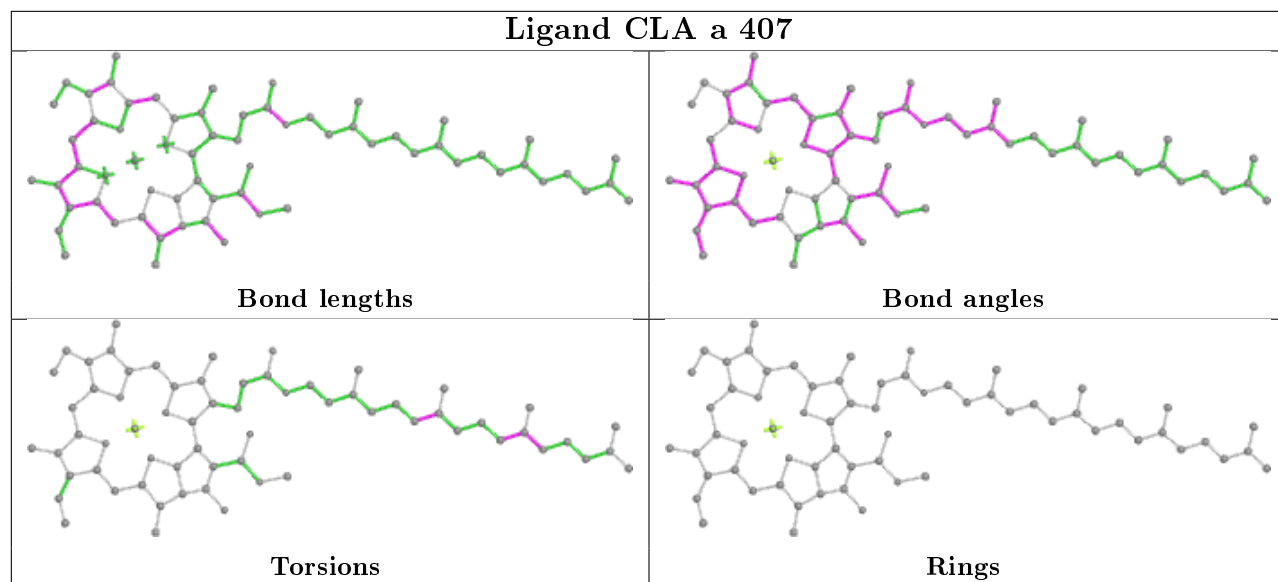
## Ligand CLA D 401



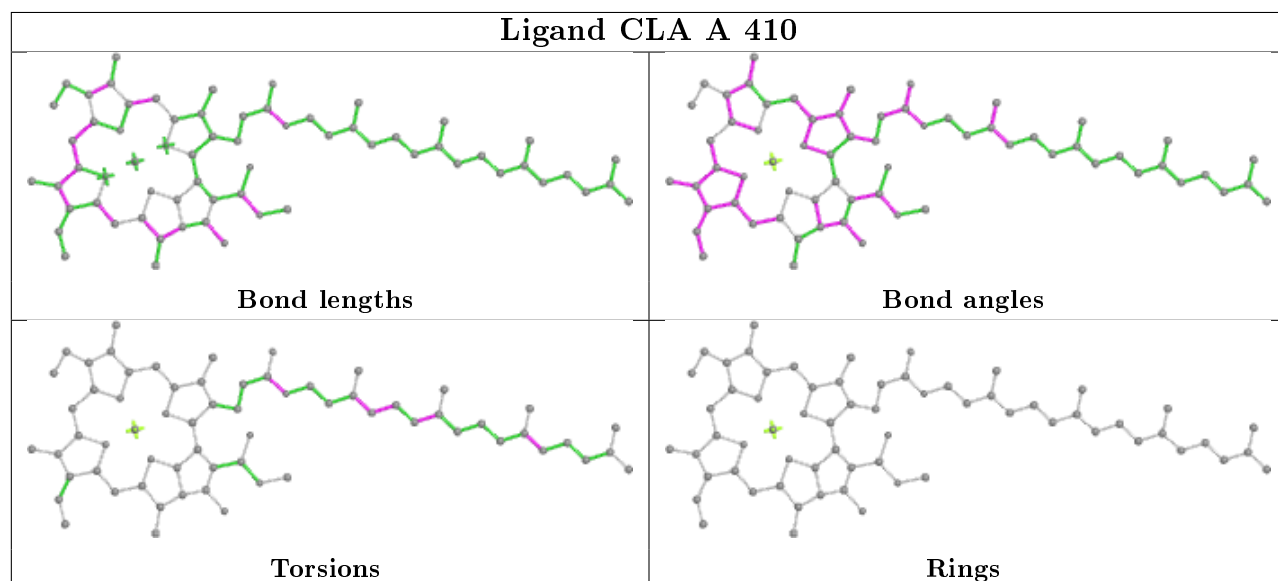
## Ligand DGD d 406



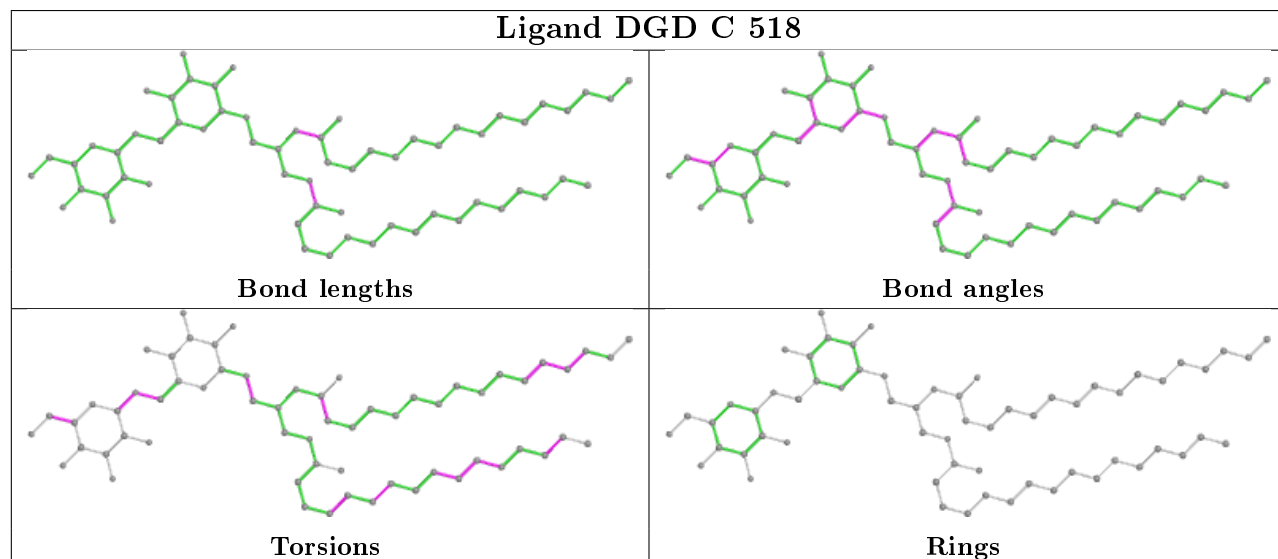
## Ligand CLA a 407



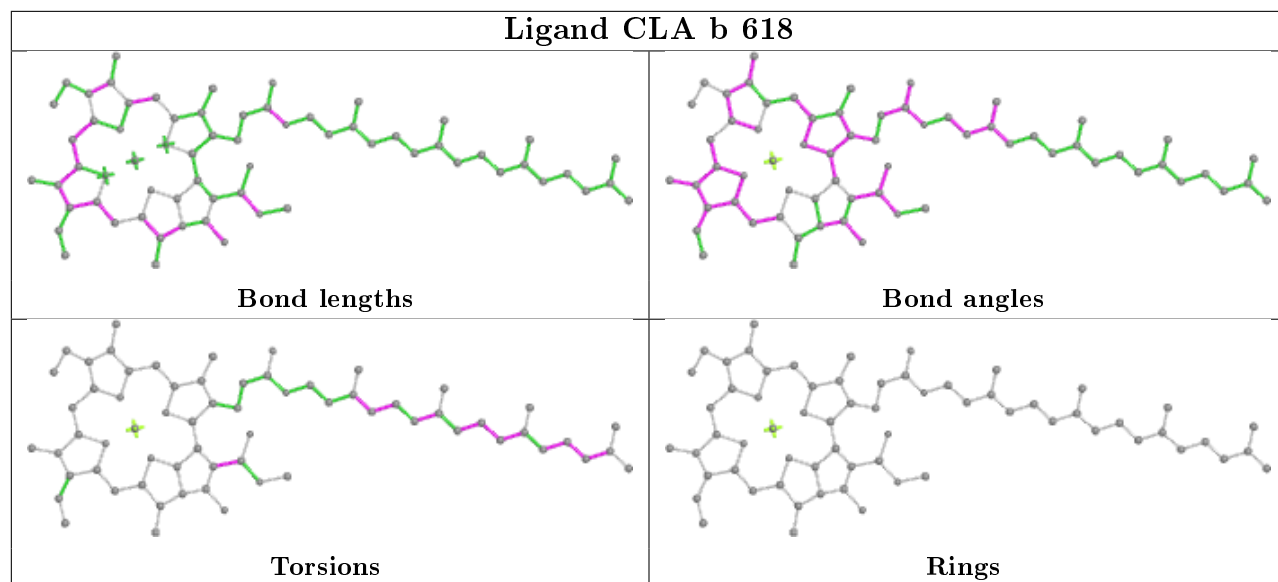
## Ligand CLA A 410



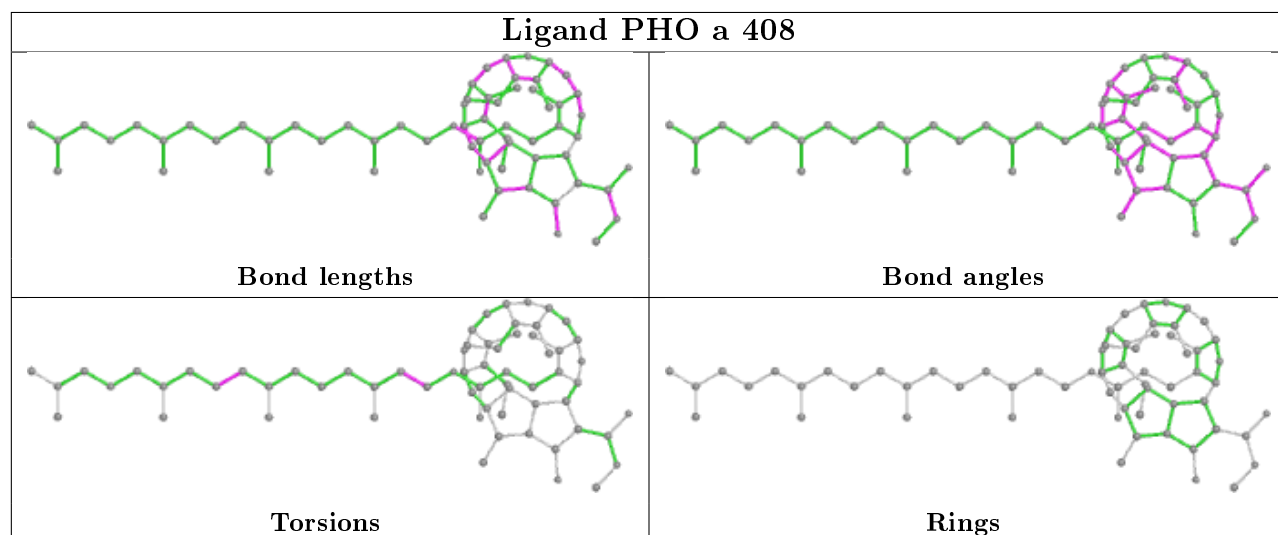
## Ligand DGD C 518



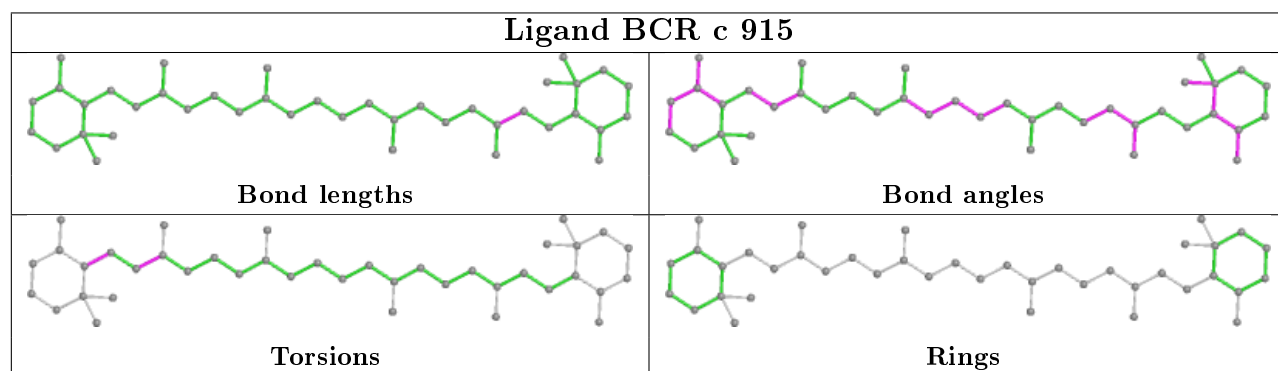
## Ligand CLA b 618

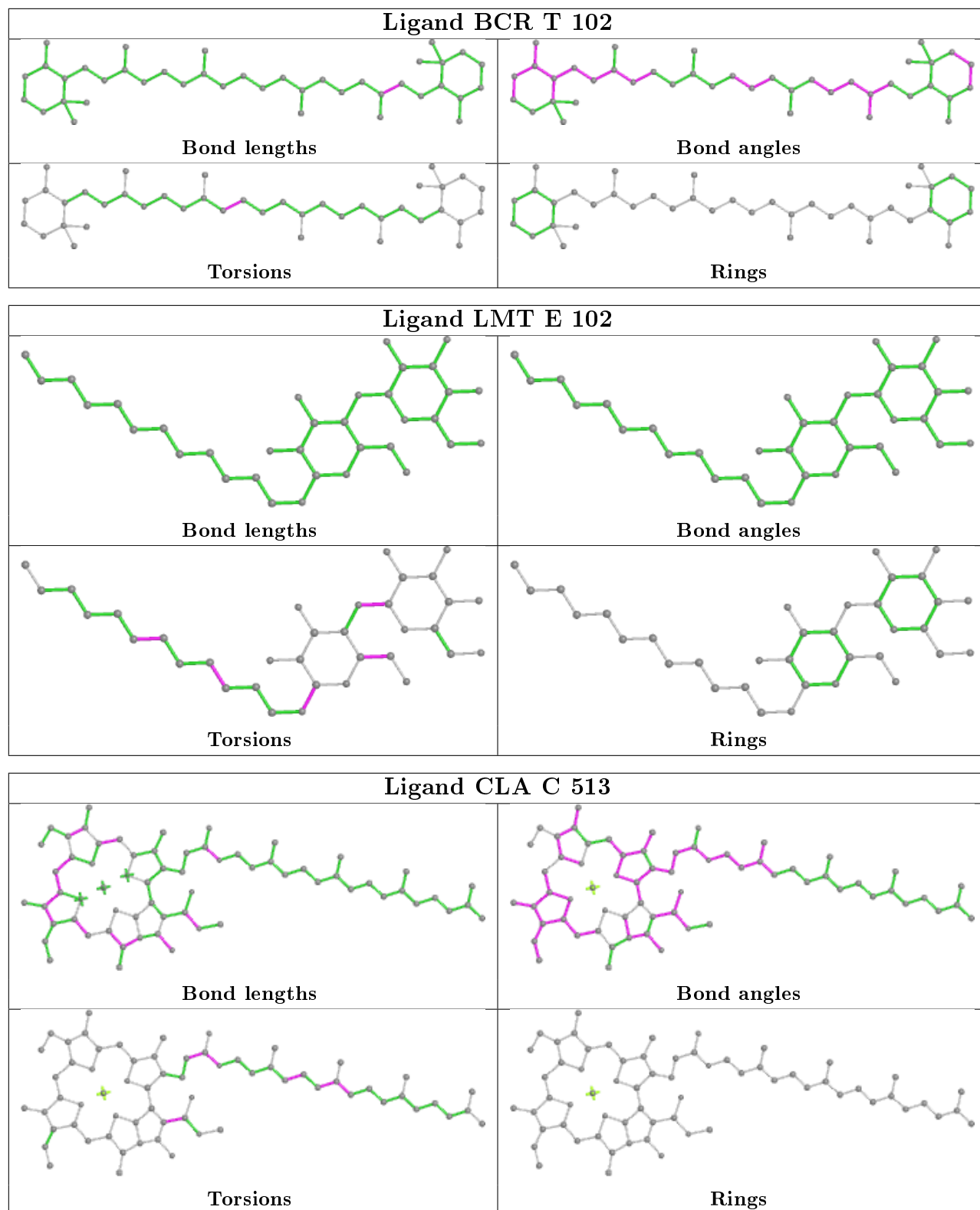


## Ligand PHO a 408

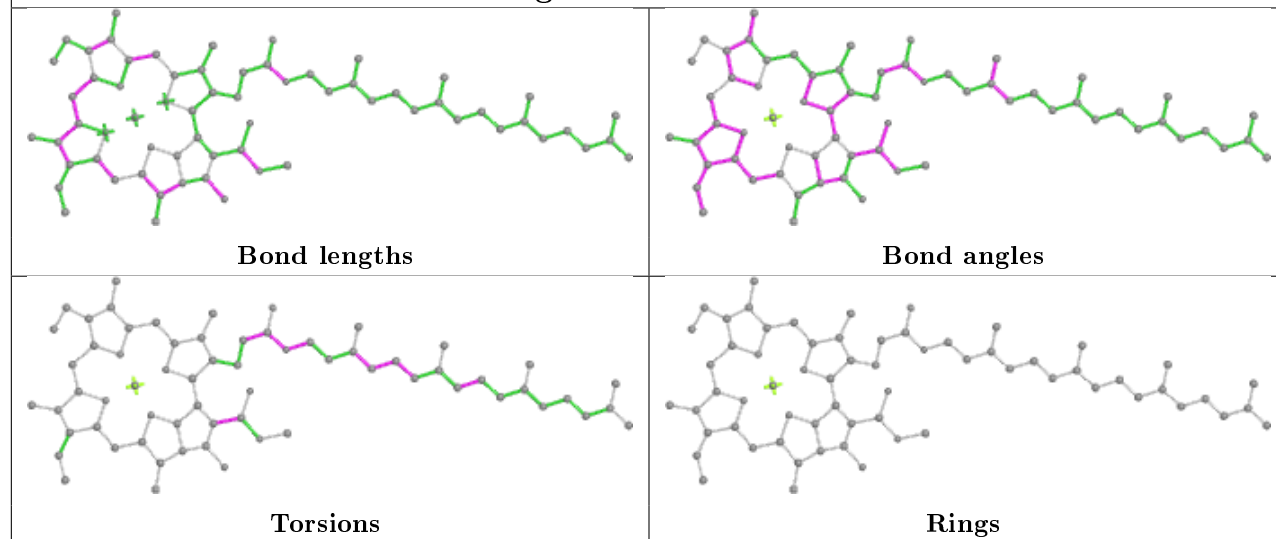


## Ligand BCR c 915

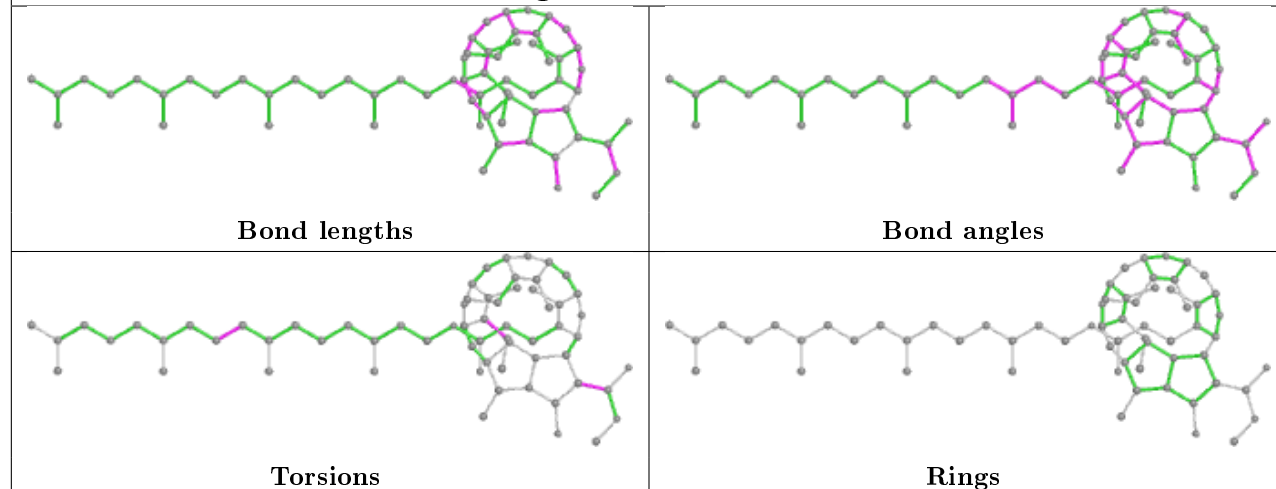




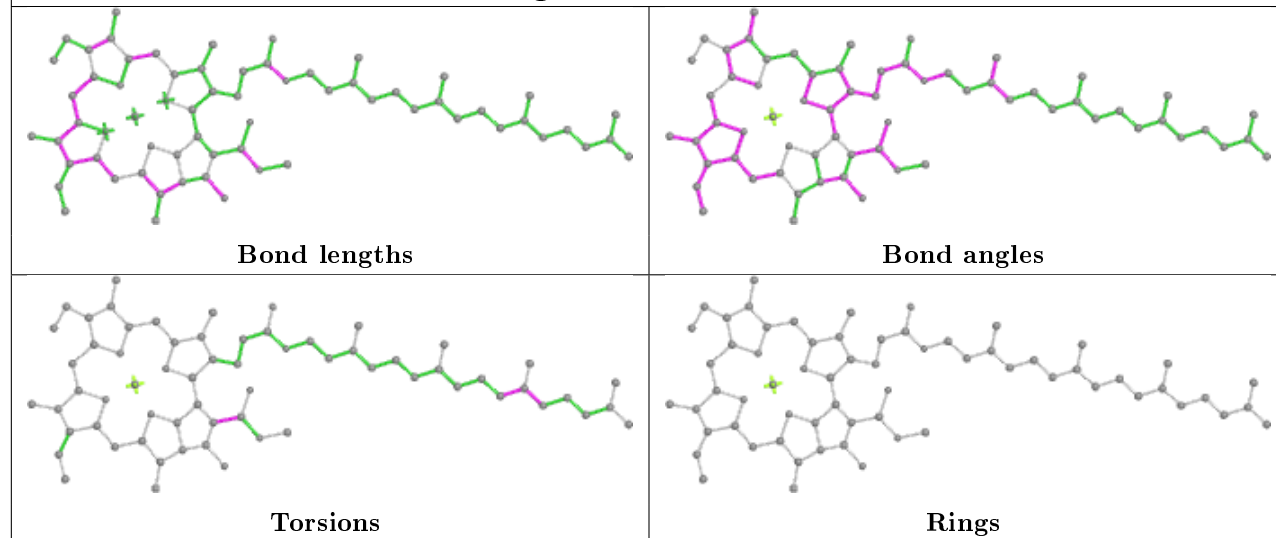
## Ligand CLA b 605



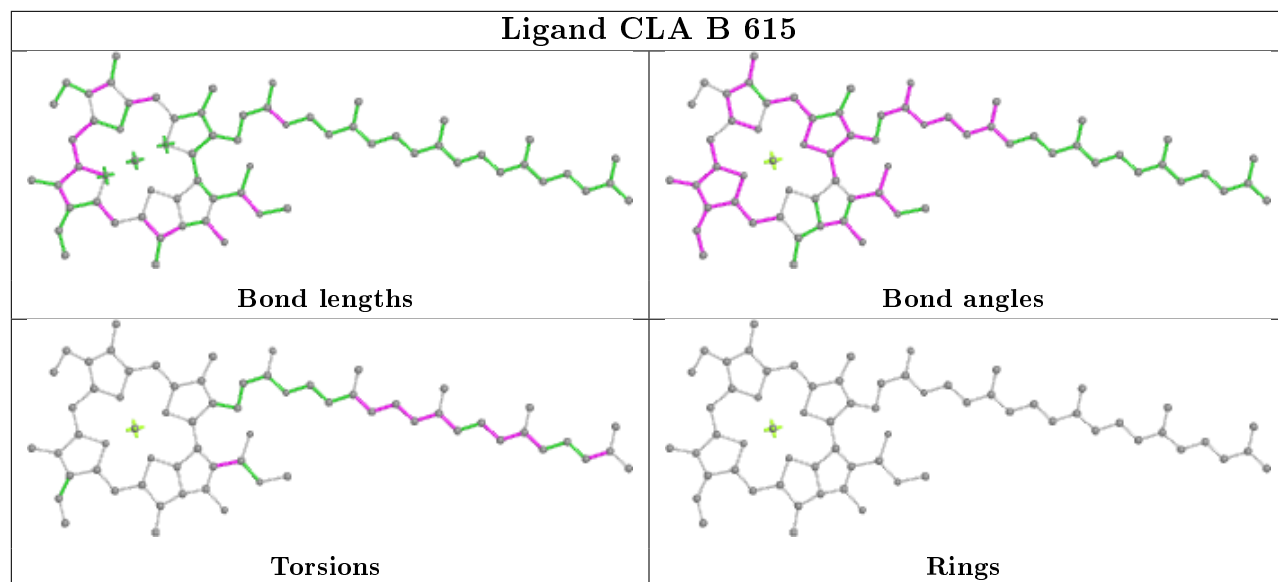
## Ligand PHO a 420



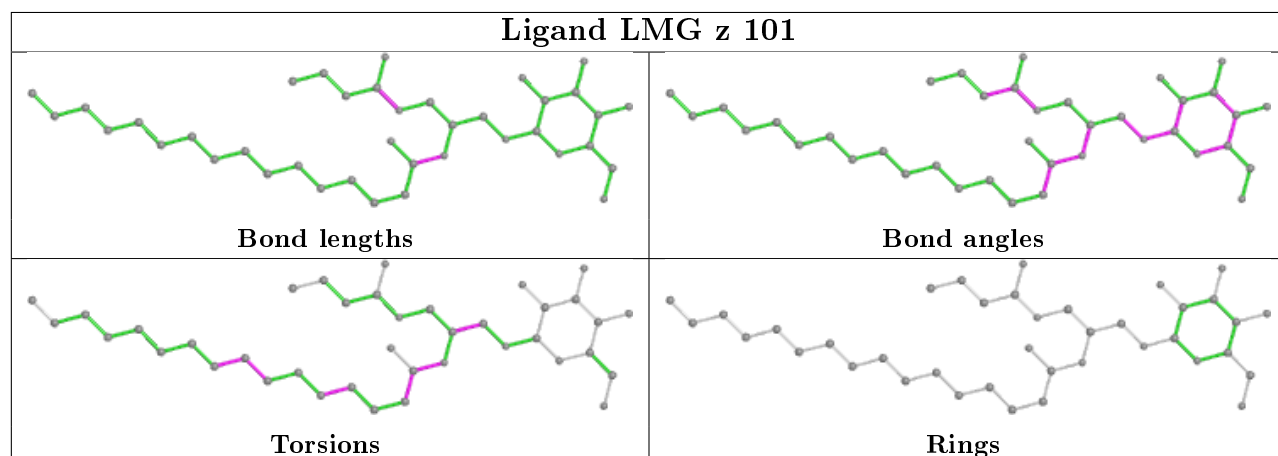
## Ligand CLA C 505



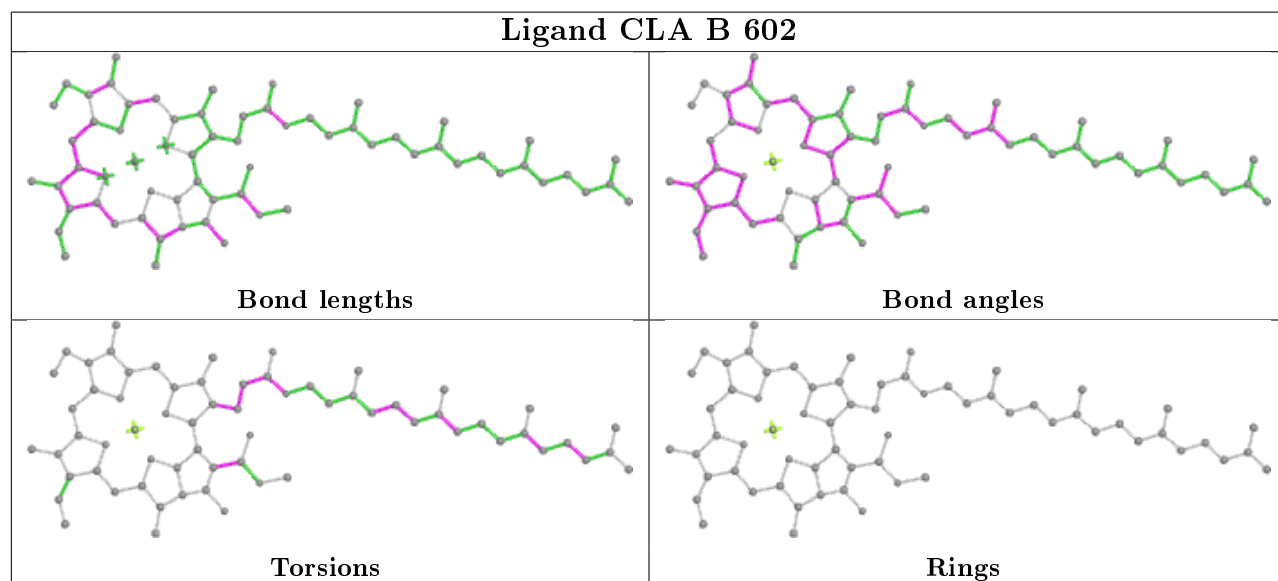
## Ligand CLA B 615



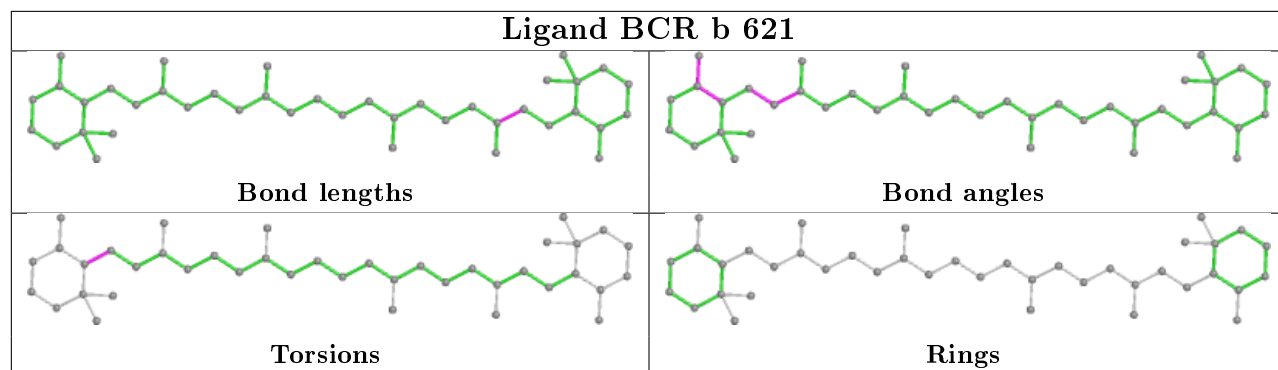
## Ligand LMG z 101



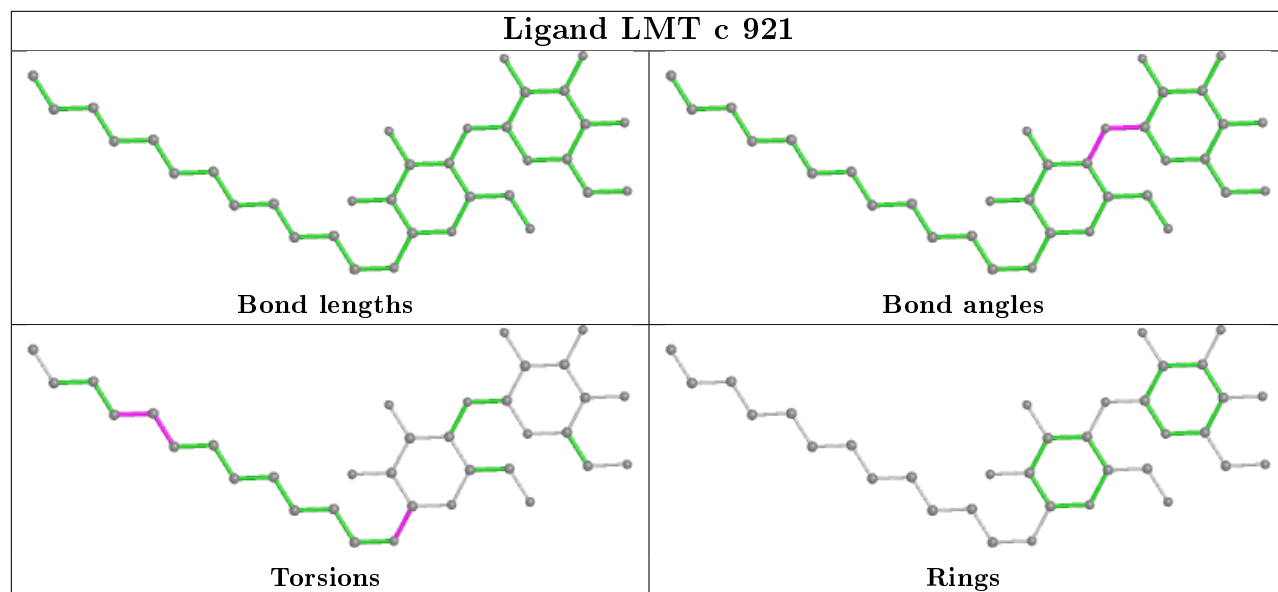
## Ligand CLA B 602



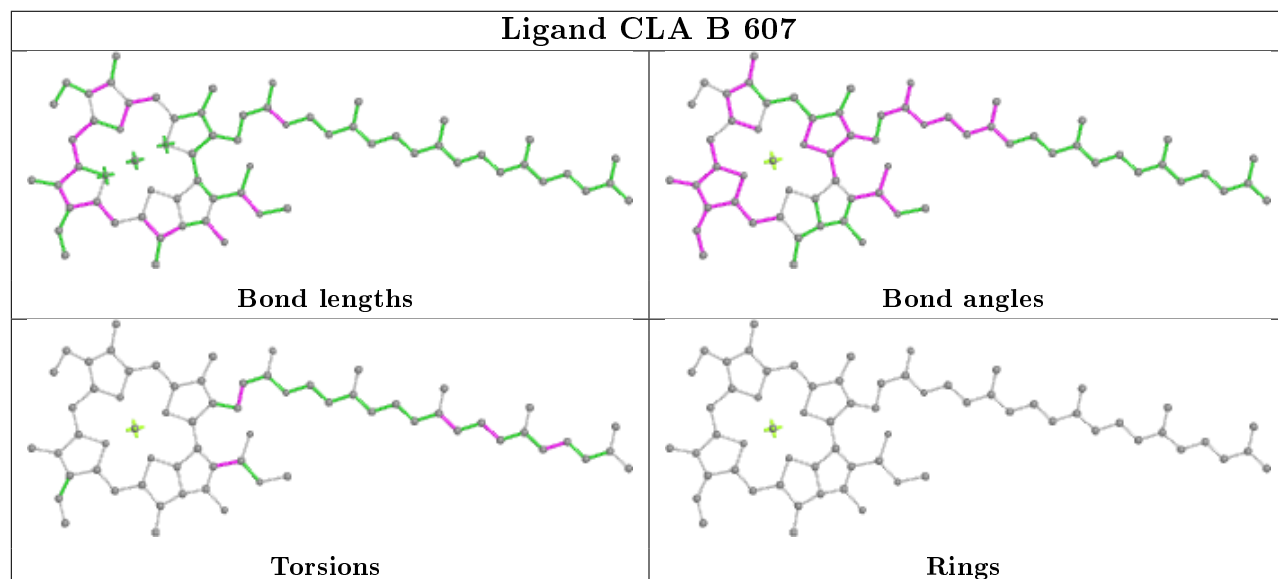
## Ligand BCR b 621



## Ligand LMT c 921

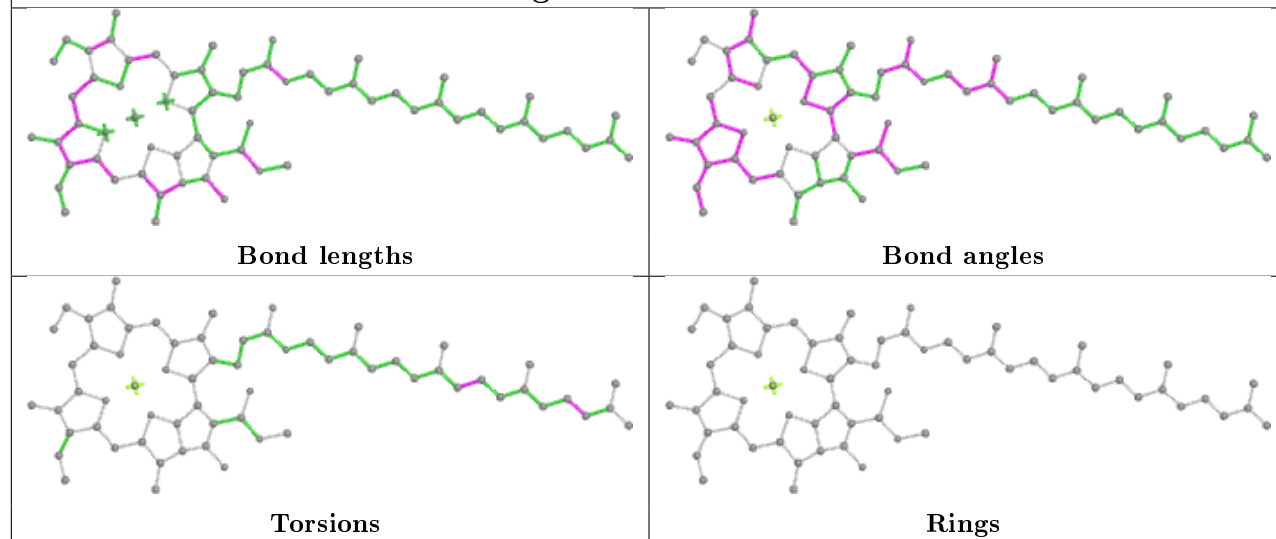


## Ligand CLA B 607

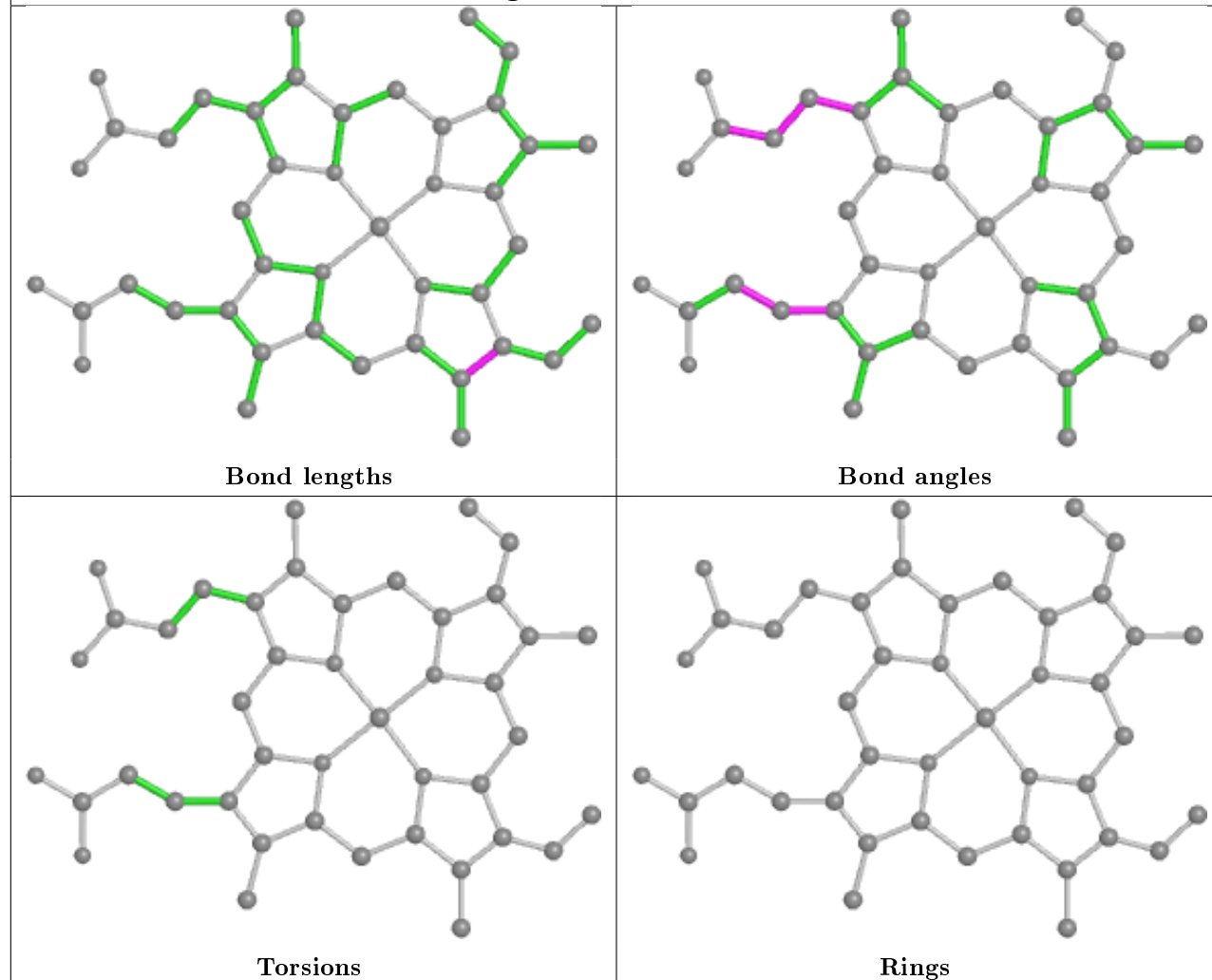




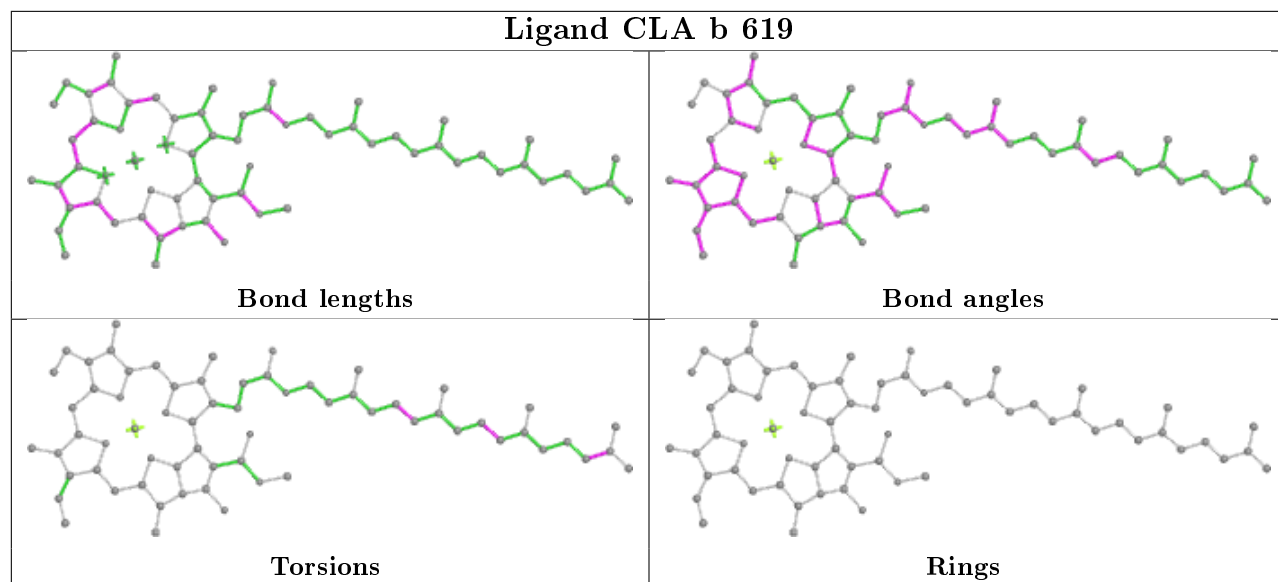
## Ligand CLA B 612



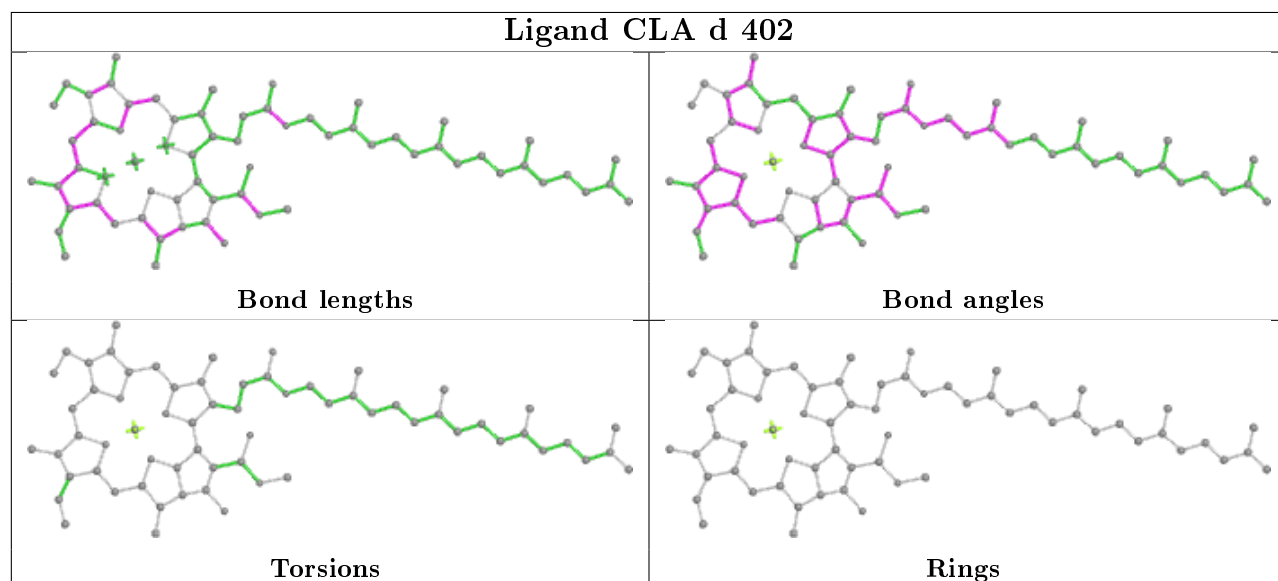
## Ligand HEM e 102



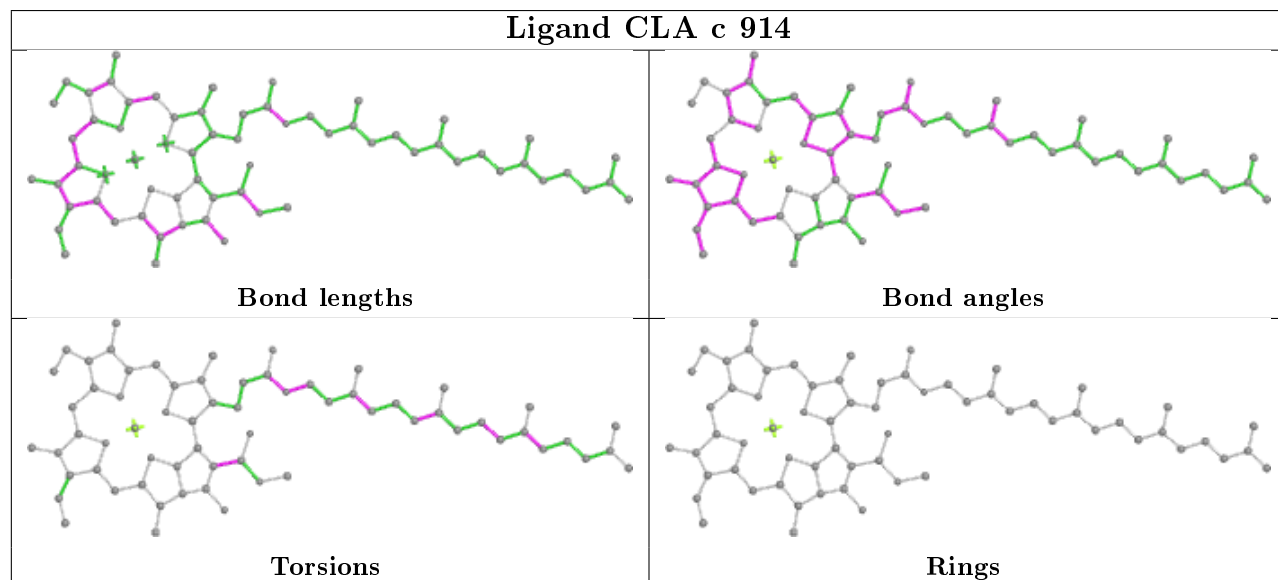
## Ligand CLA b 619

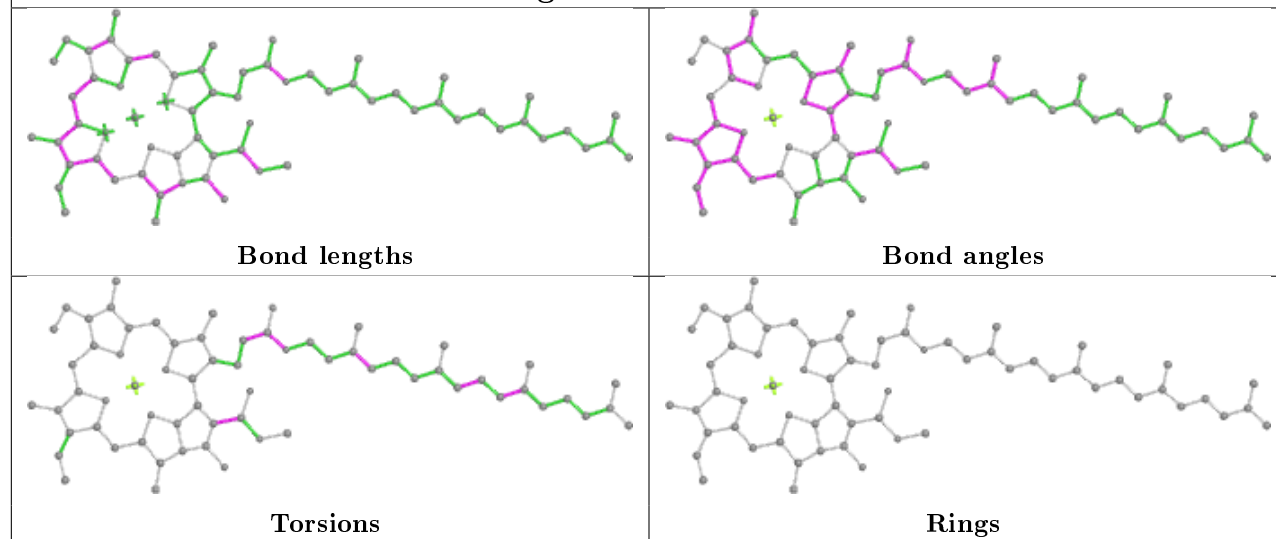
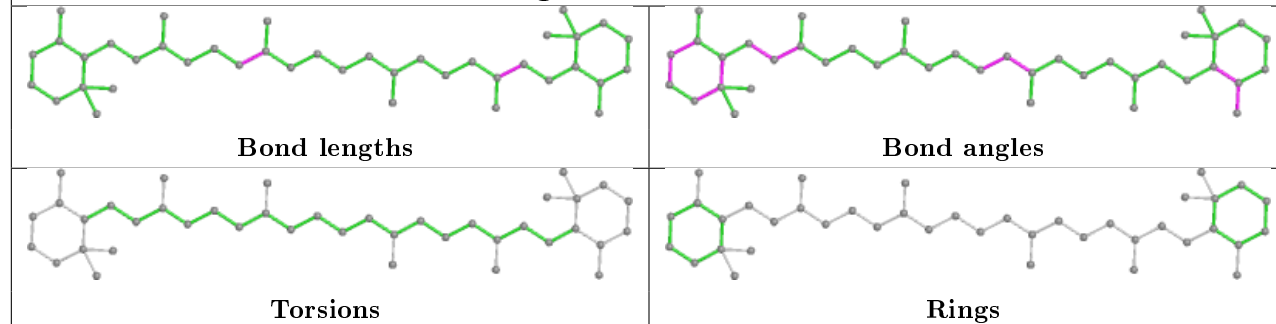
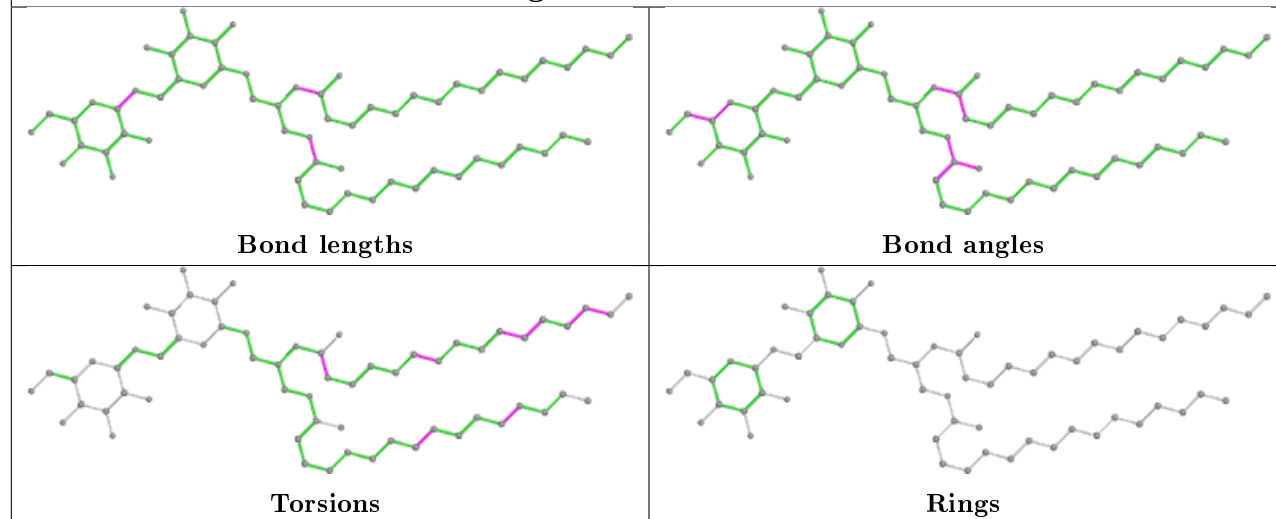


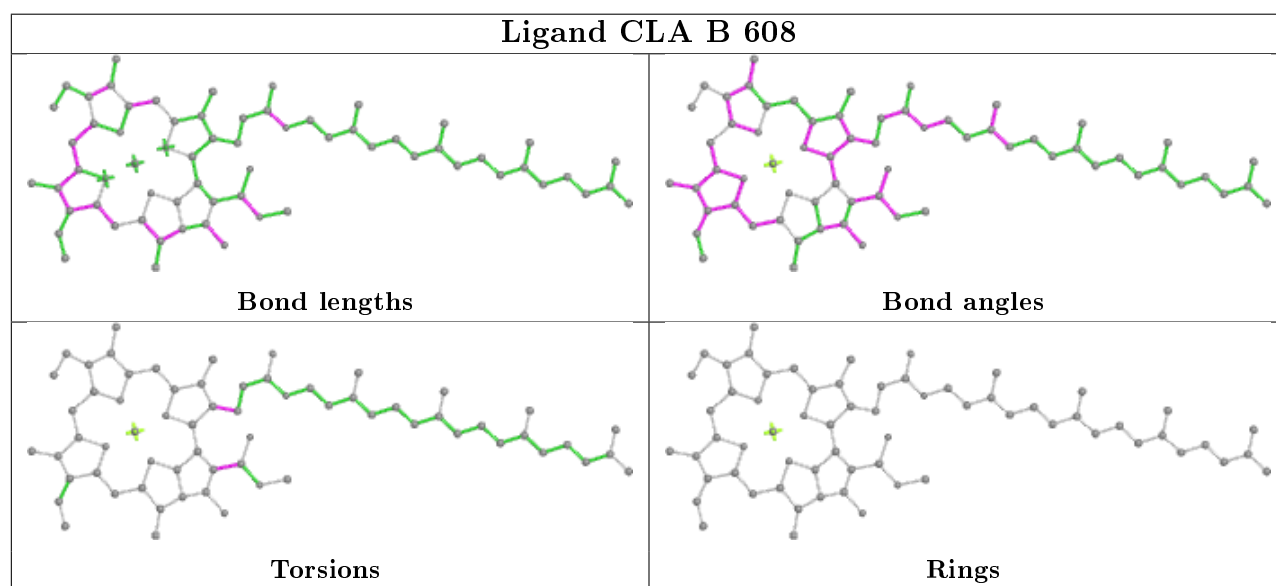
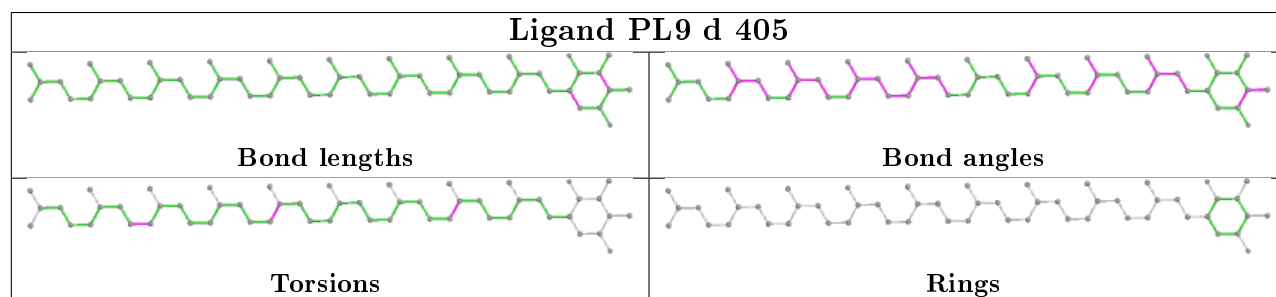
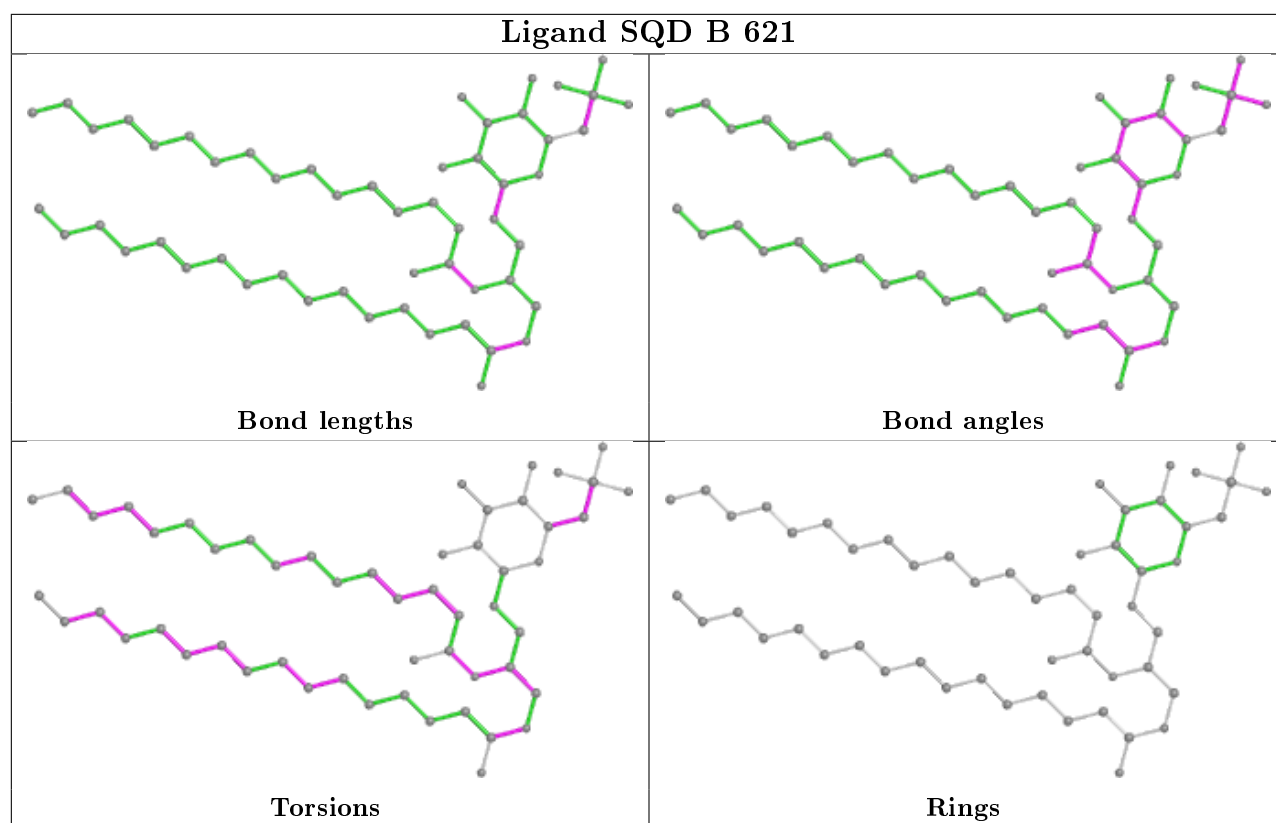
## Ligand CLA d 402

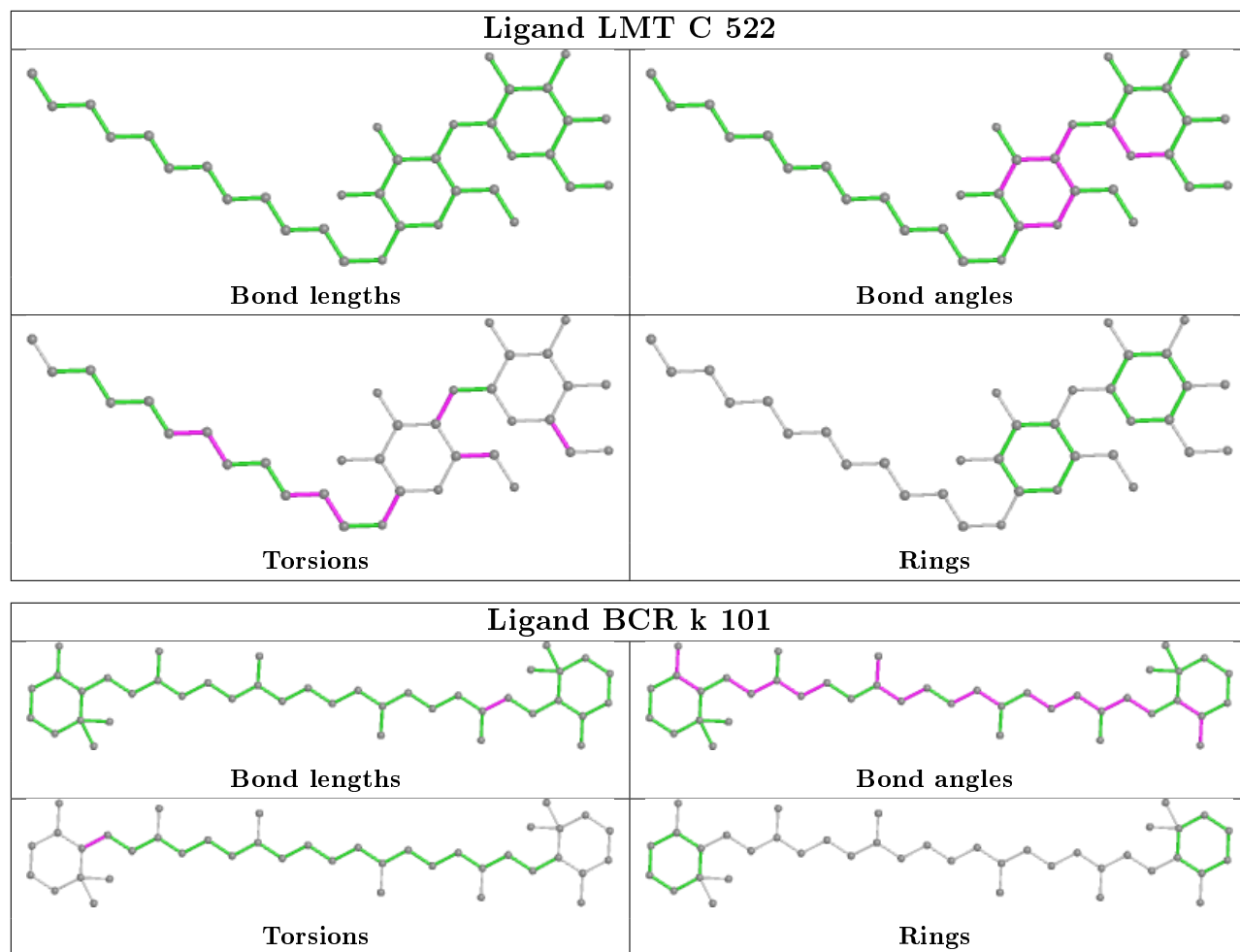


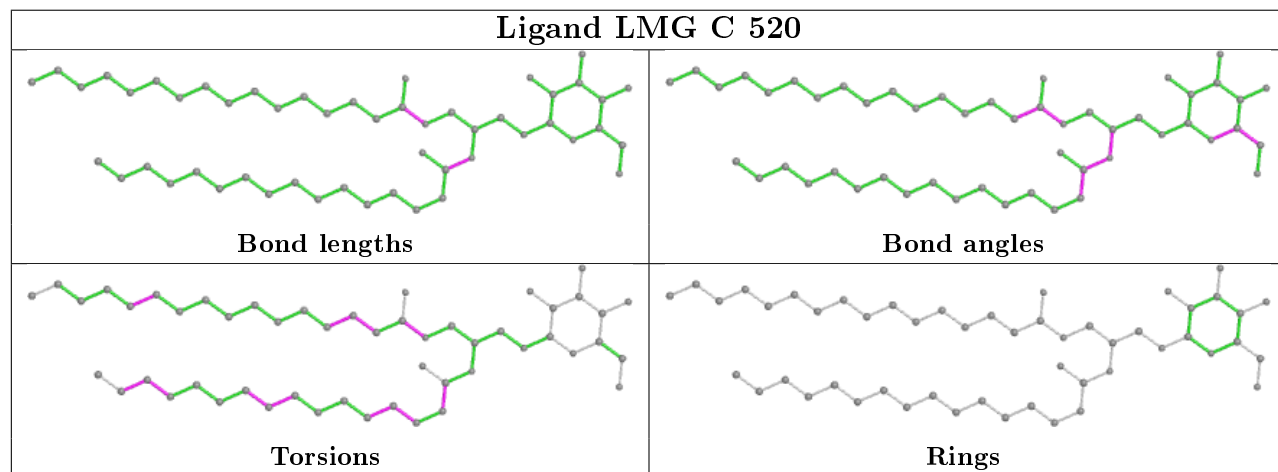
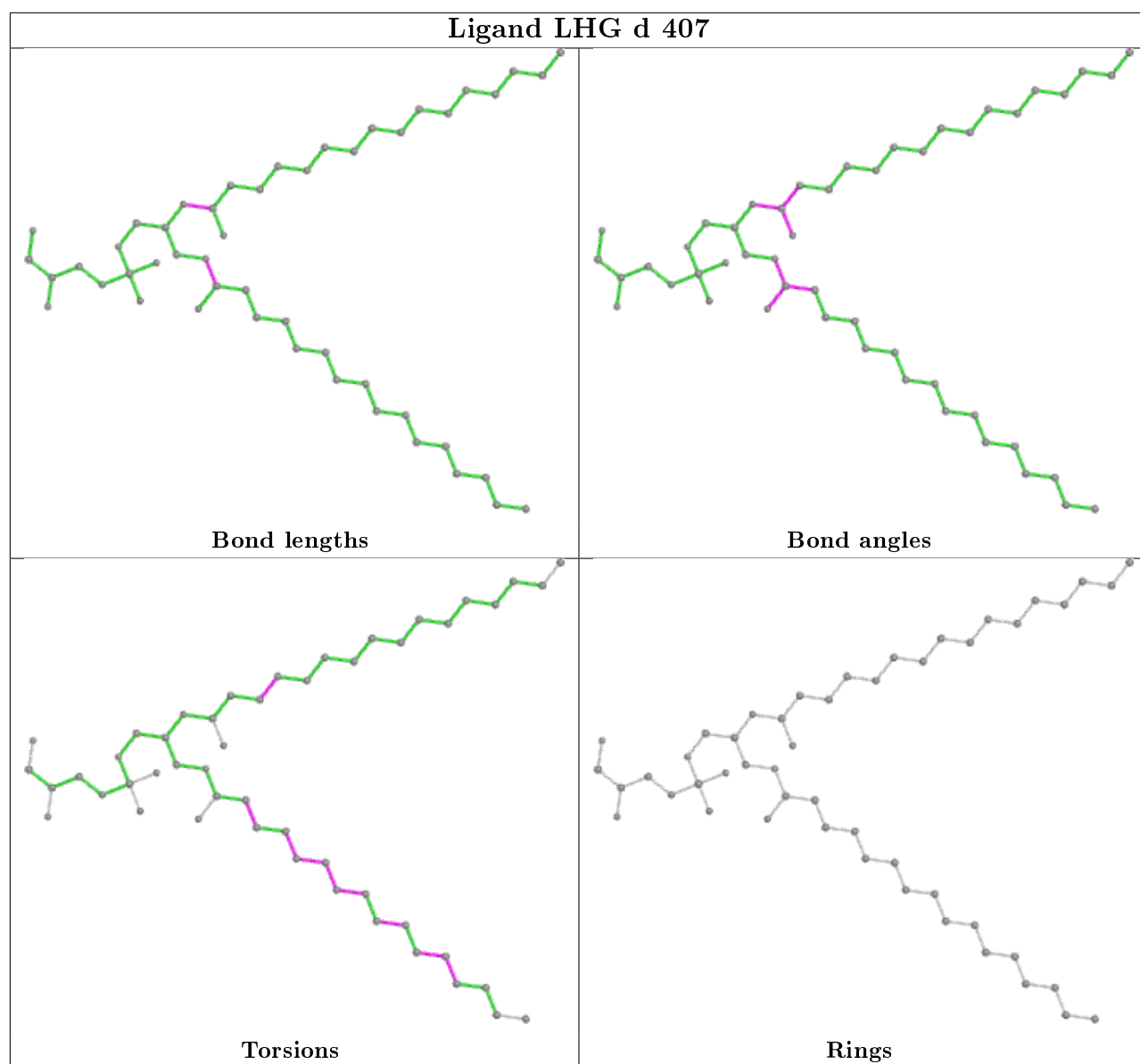
## Ligand CLA c 914



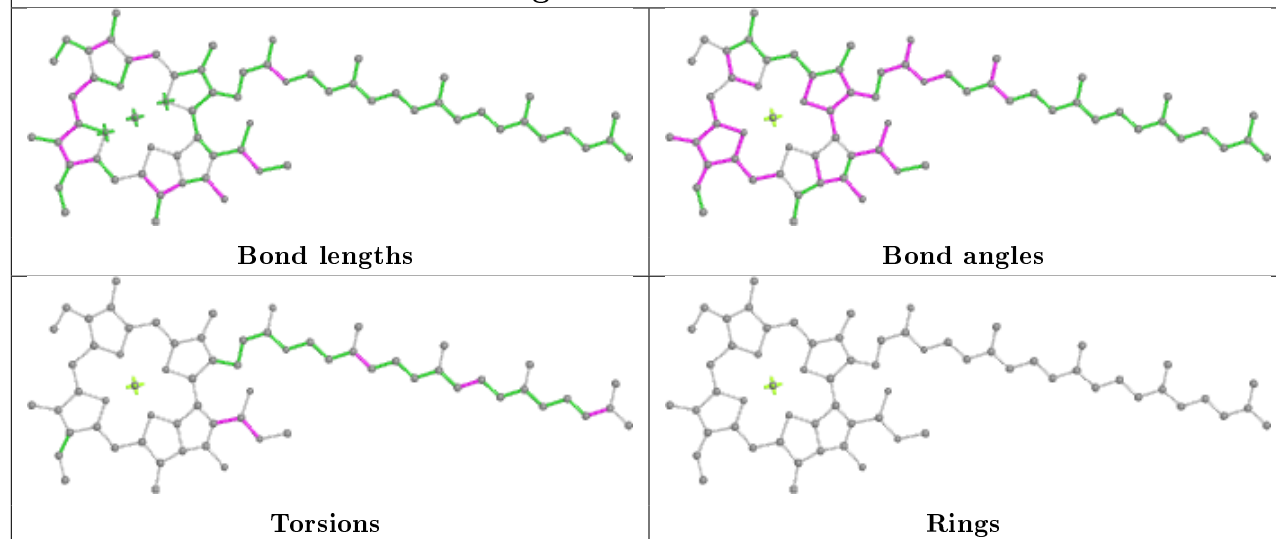
**Ligand CLA c 911****Ligand BCR a 410****Ligand DGD H 102**



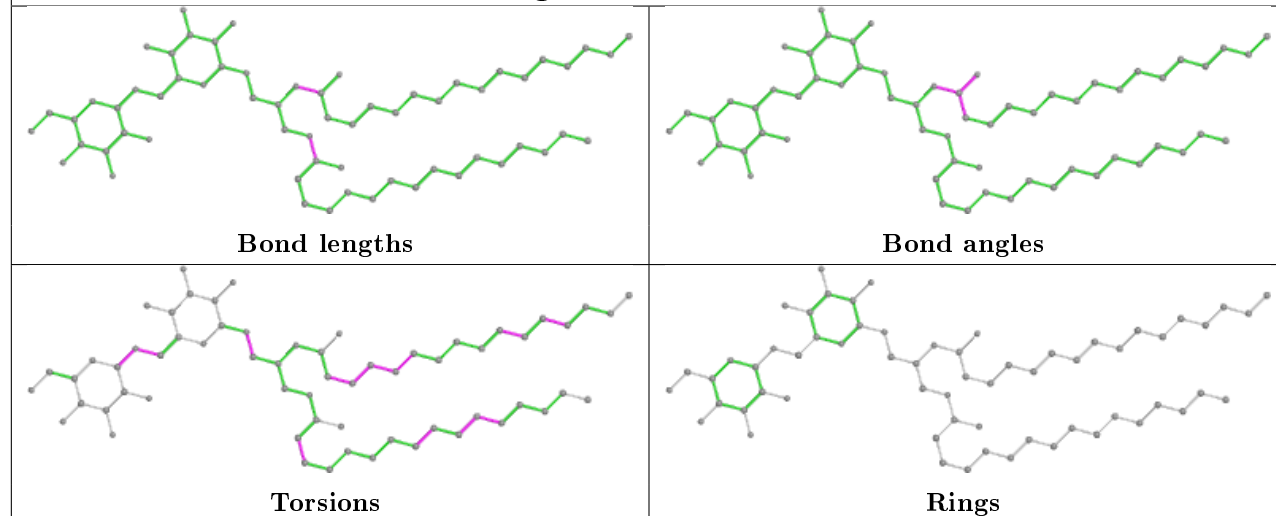




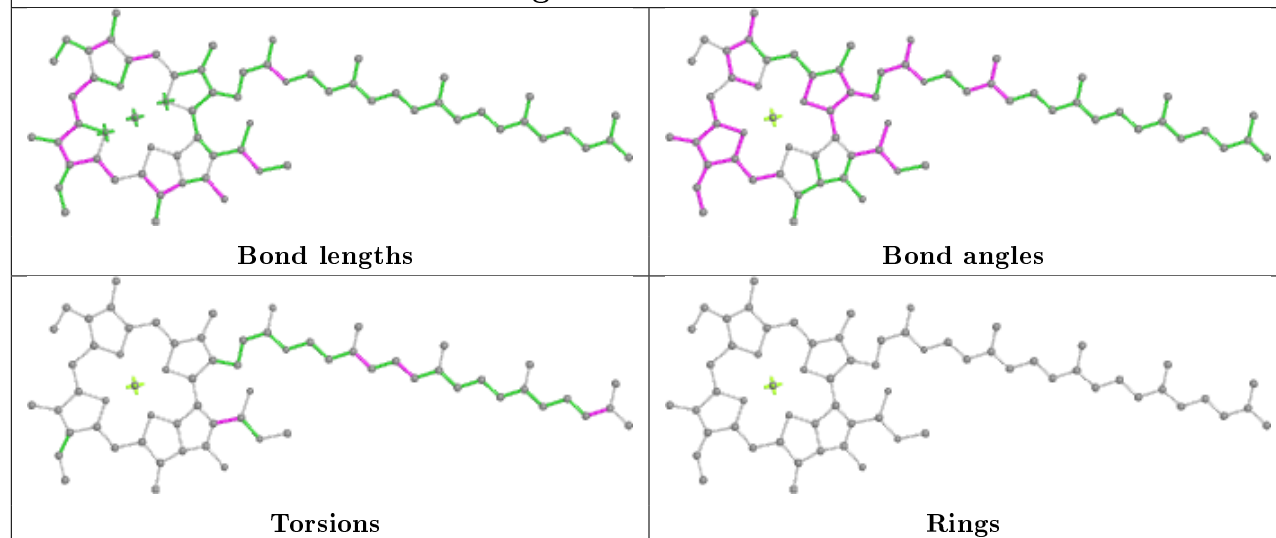
## Ligand CLA B 606



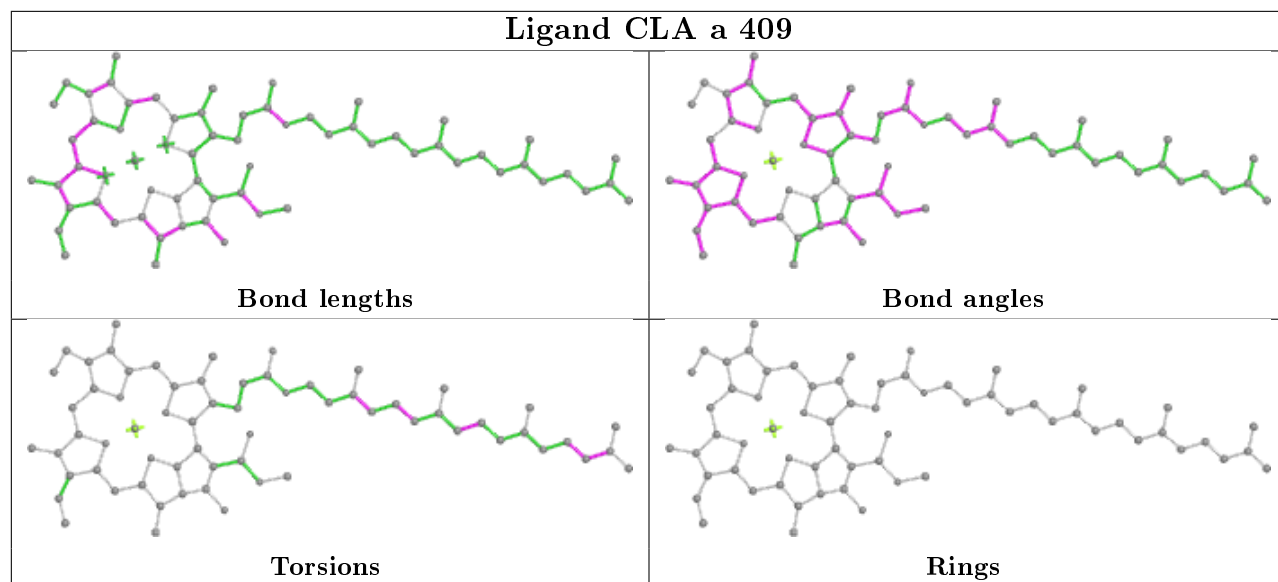
## Ligand DGD c 917



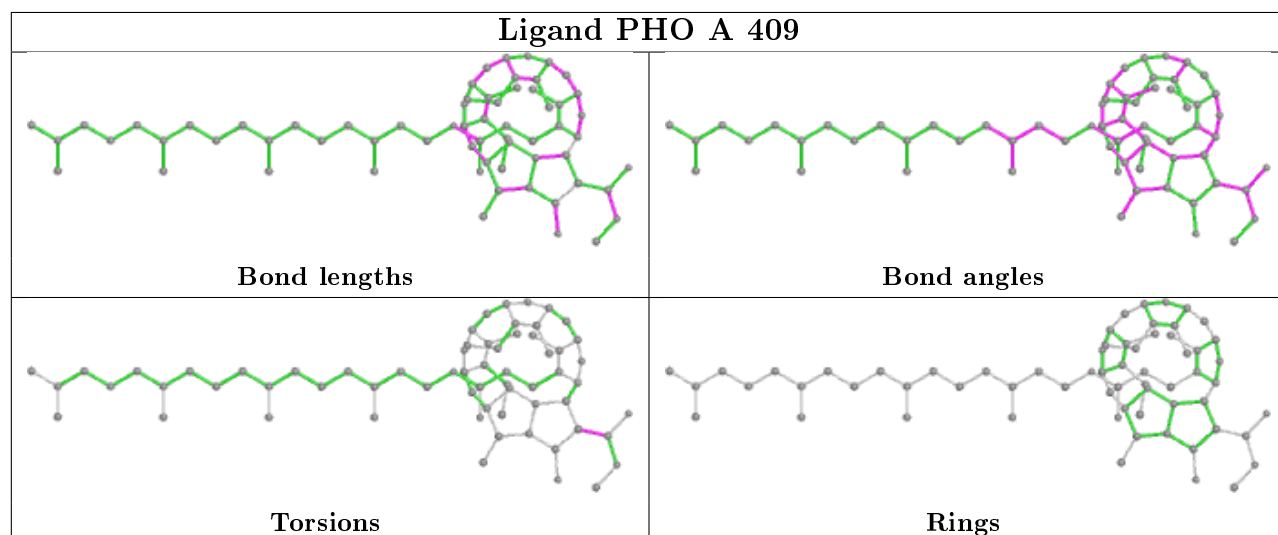
## Ligand CLA B 604



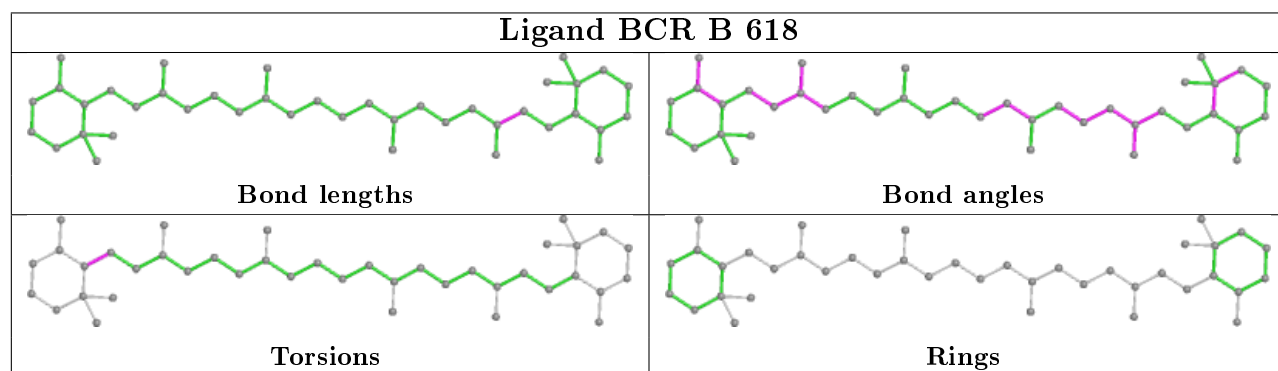
## Ligand CLA a 409



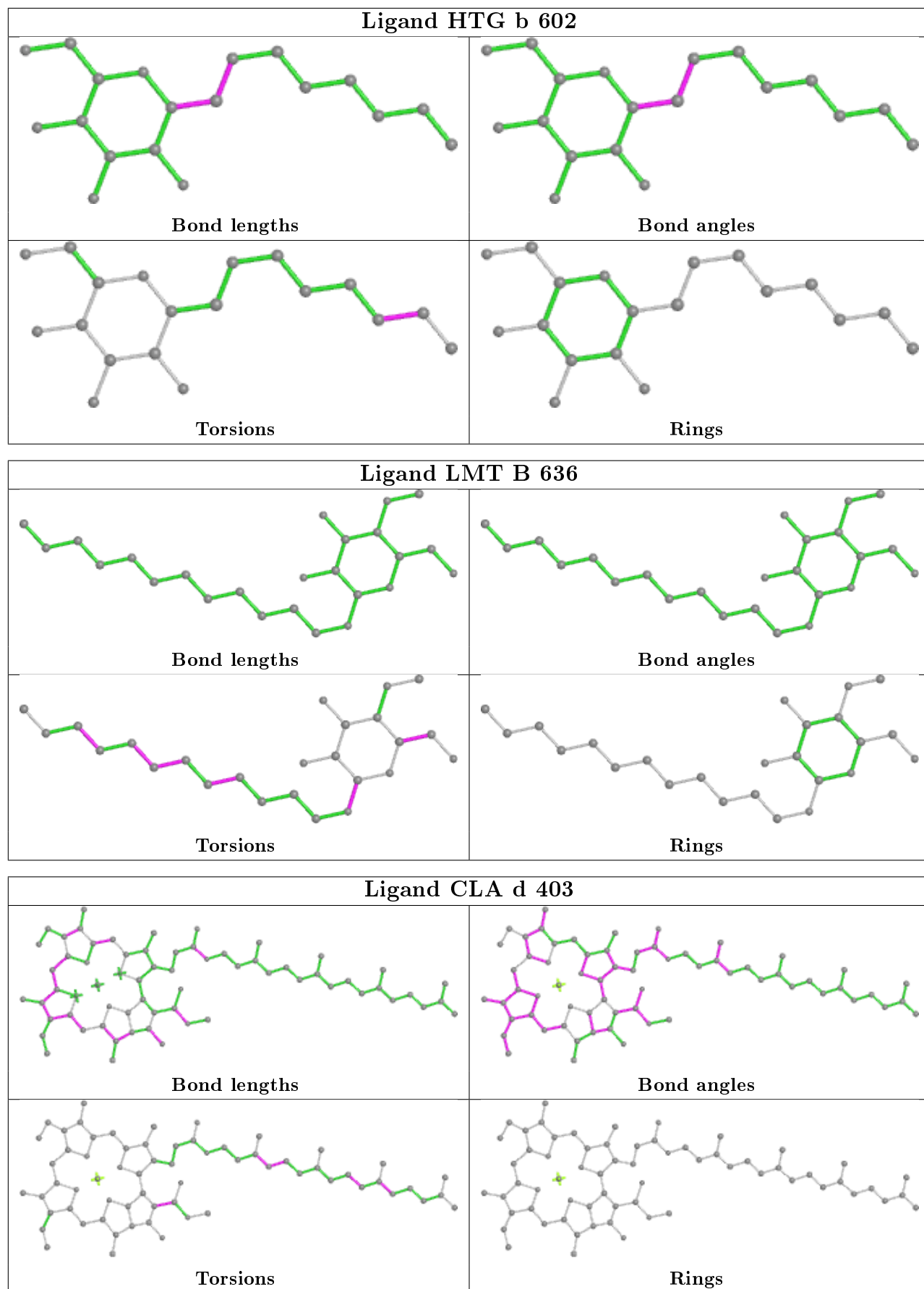
## Ligand PHO A 409

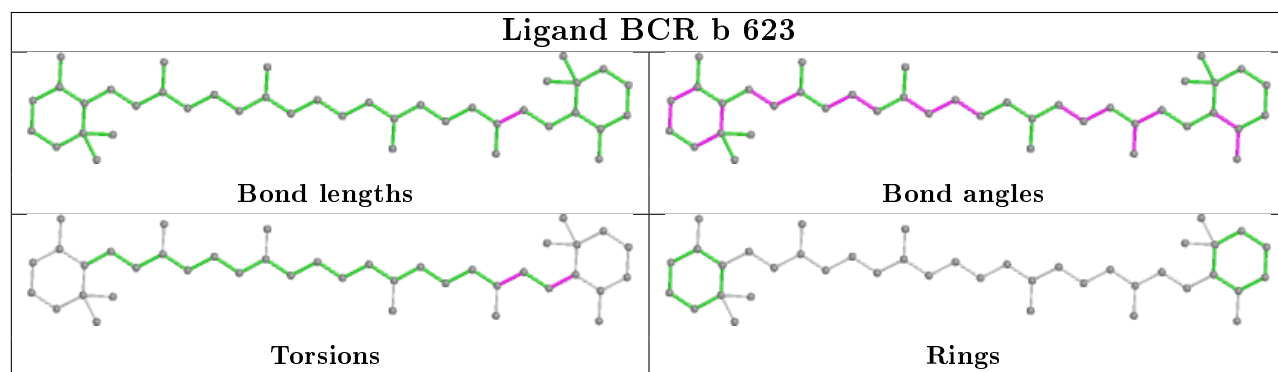
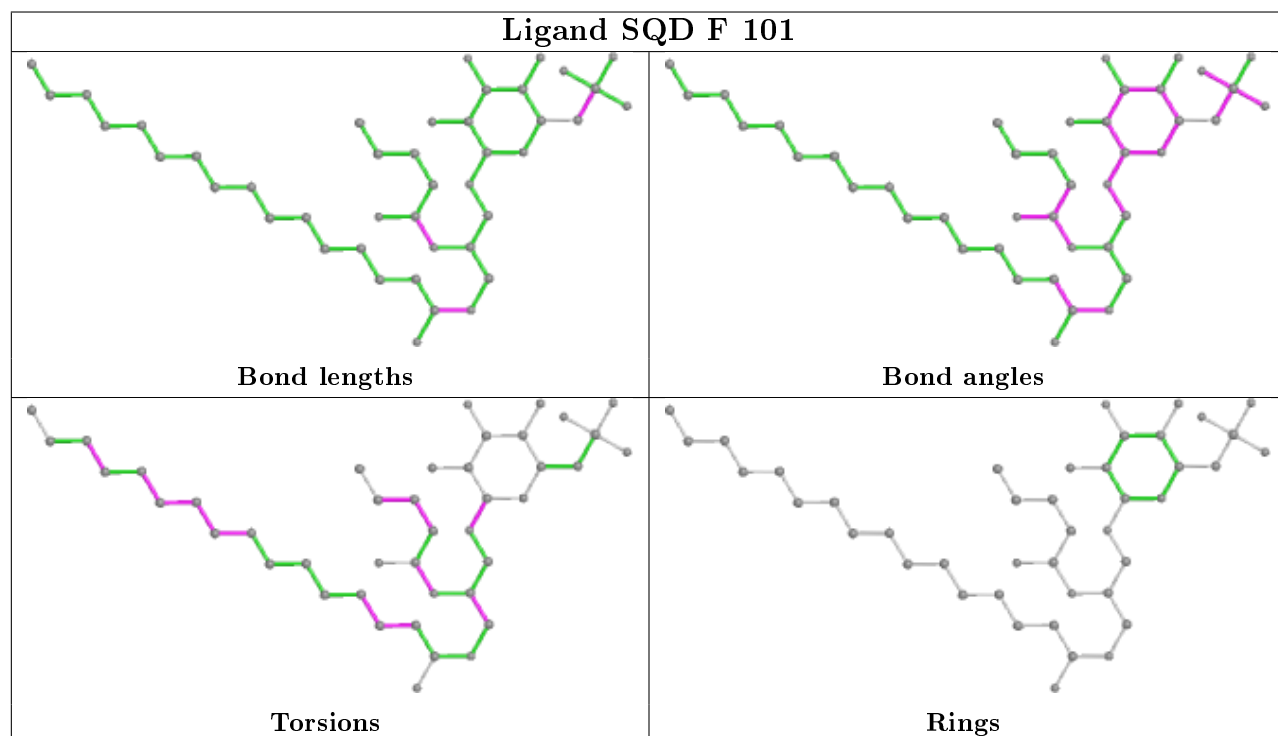
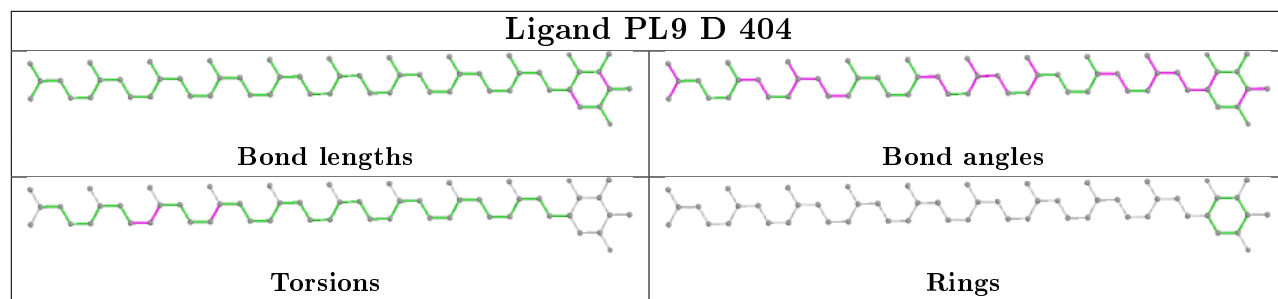


## Ligand BCR B 618

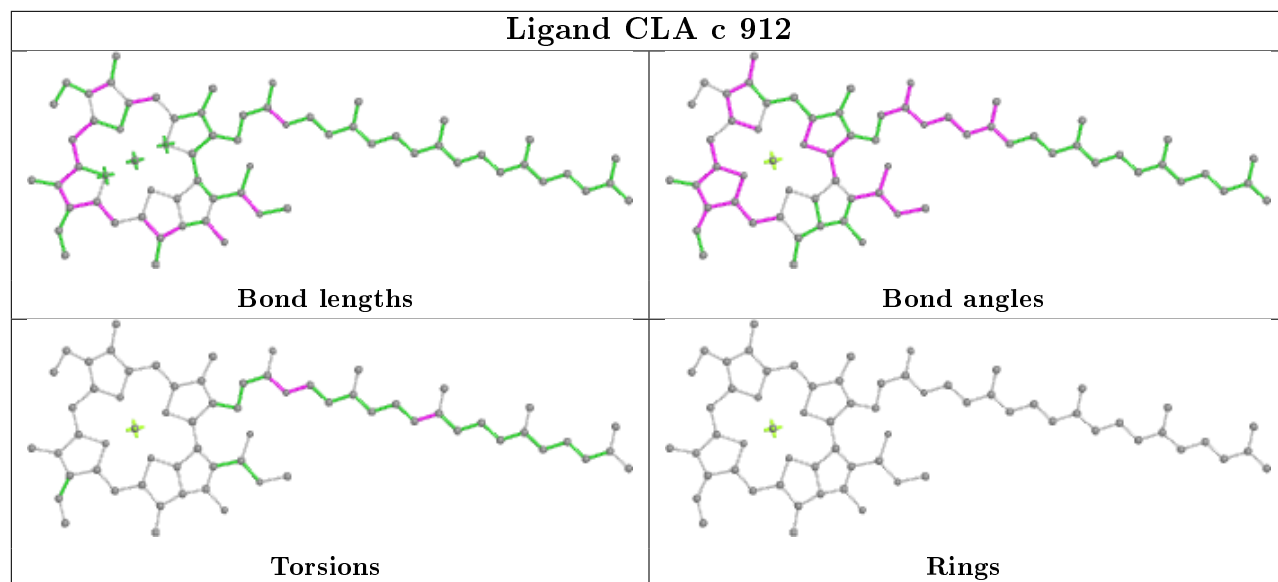




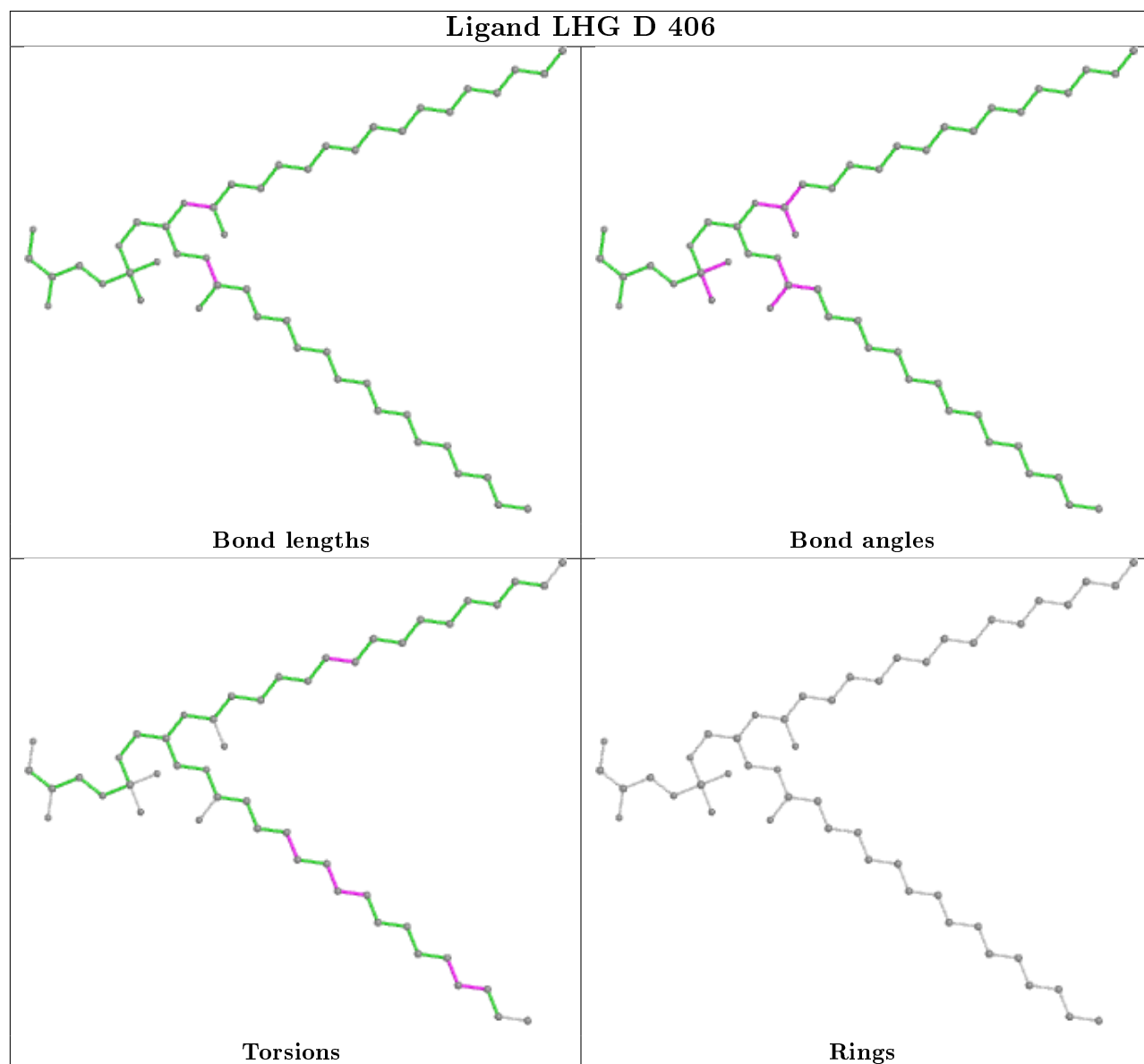




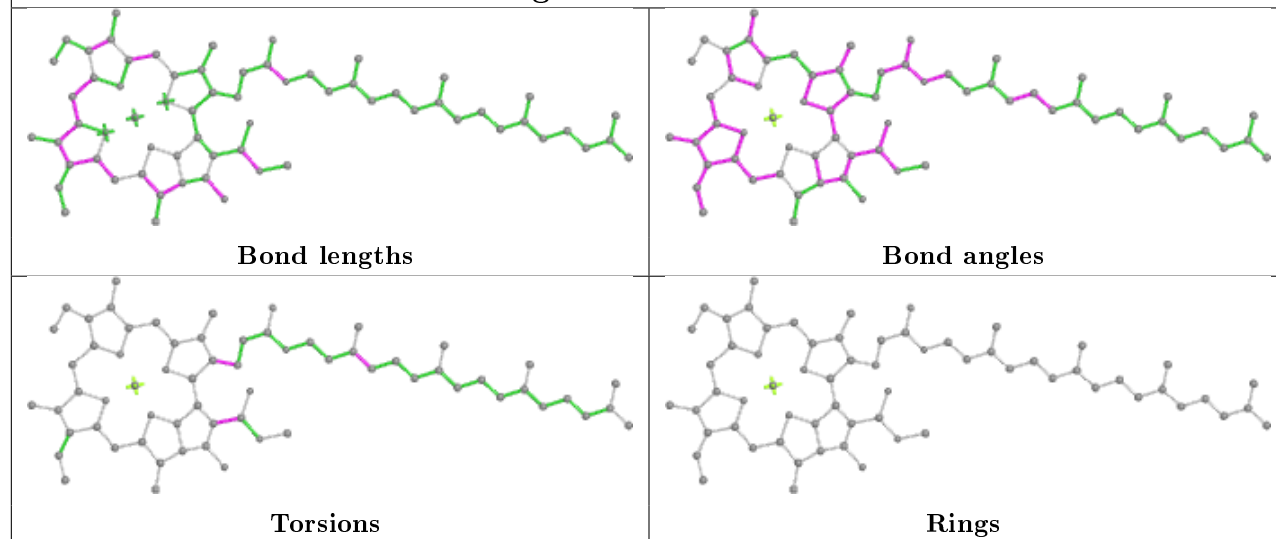
## Ligand CLA c 912



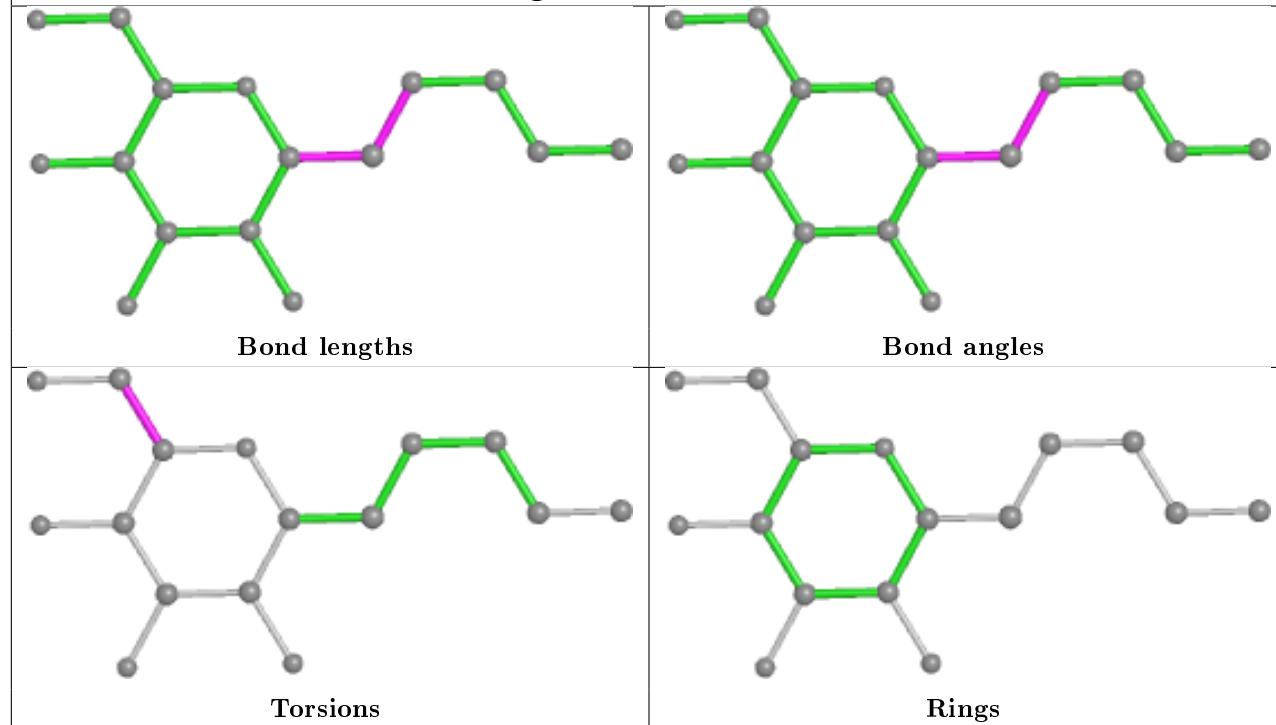
## Ligand LHG D 406



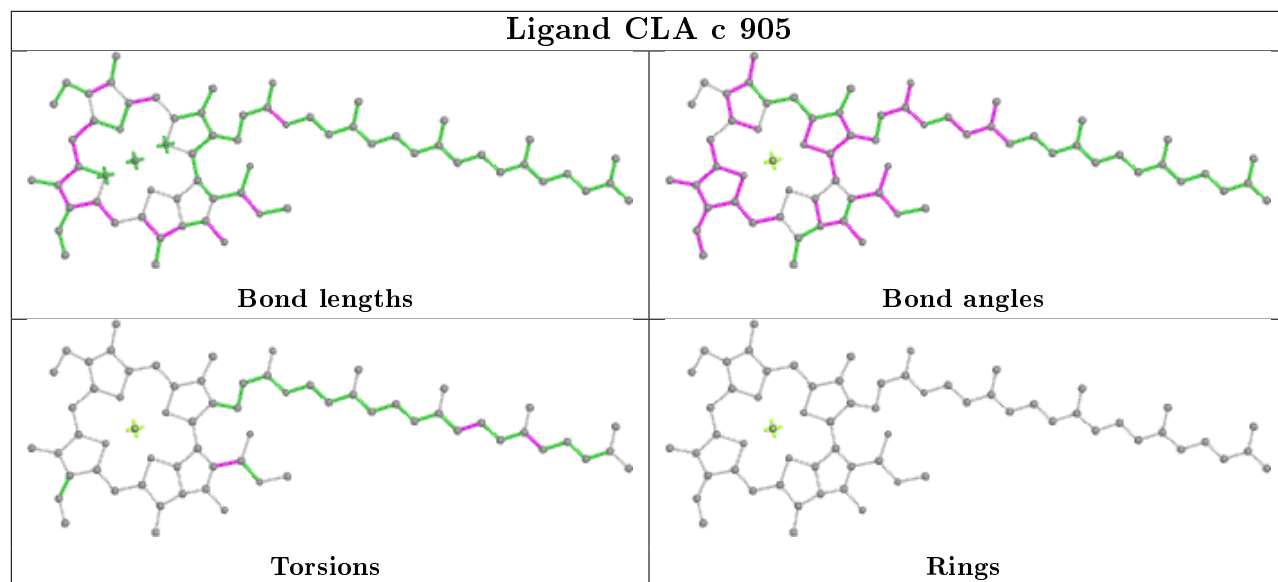
## Ligand CLA B 610



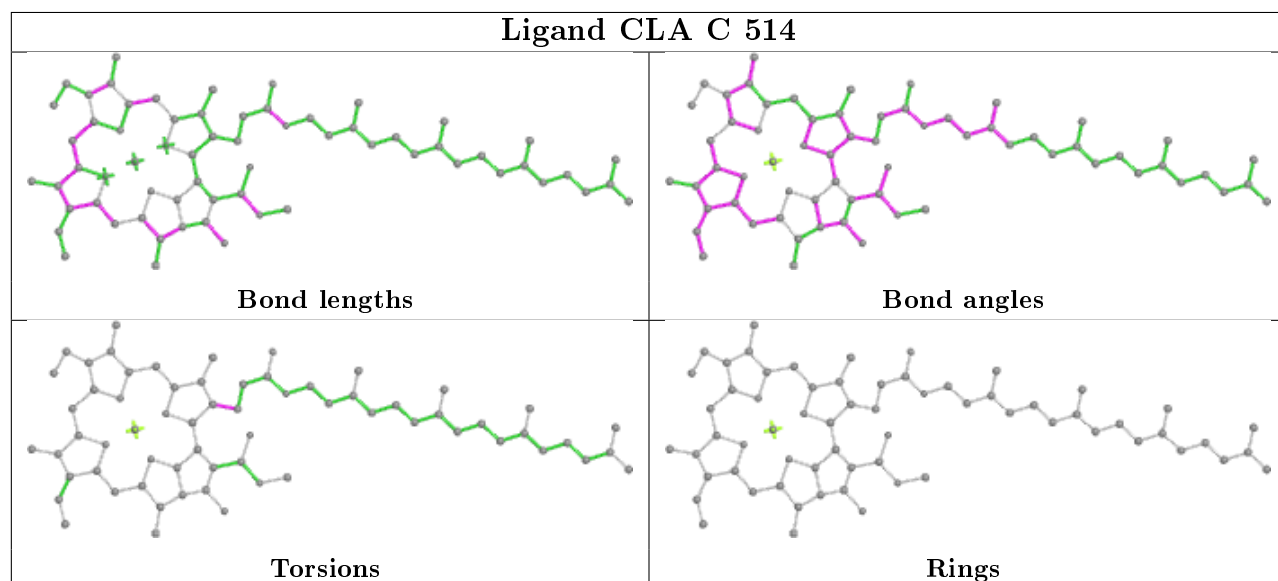
## Ligand HTG D 411



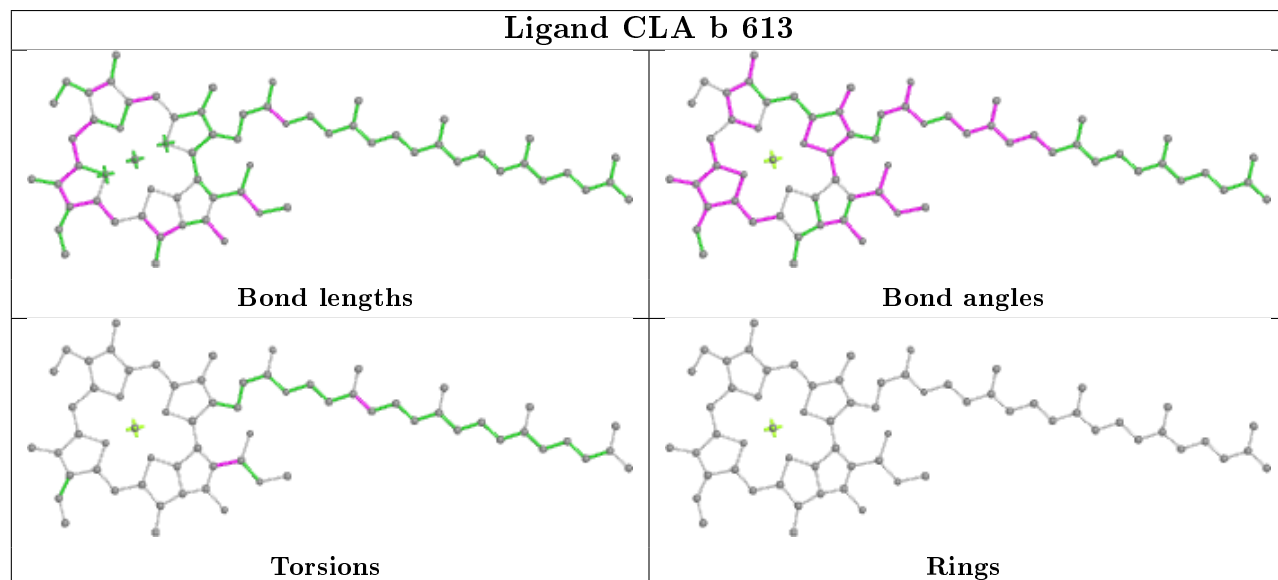
## Ligand CLA c 905

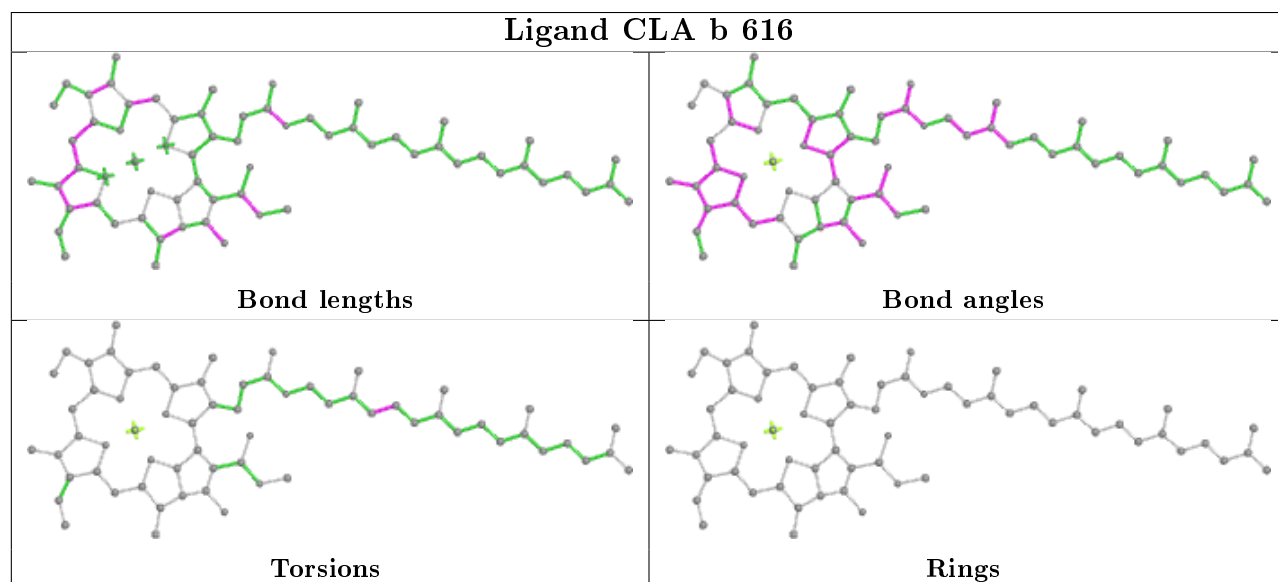
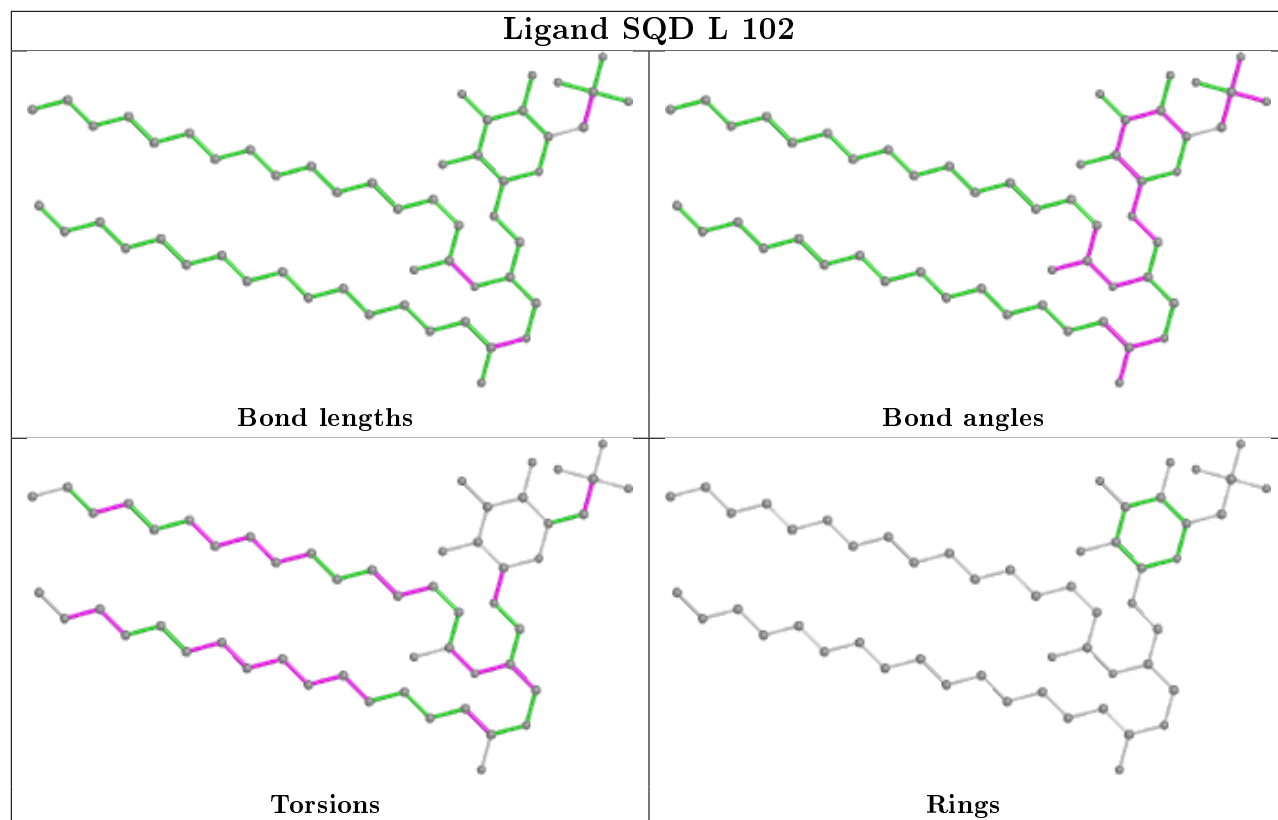


## Ligand CLA C 514

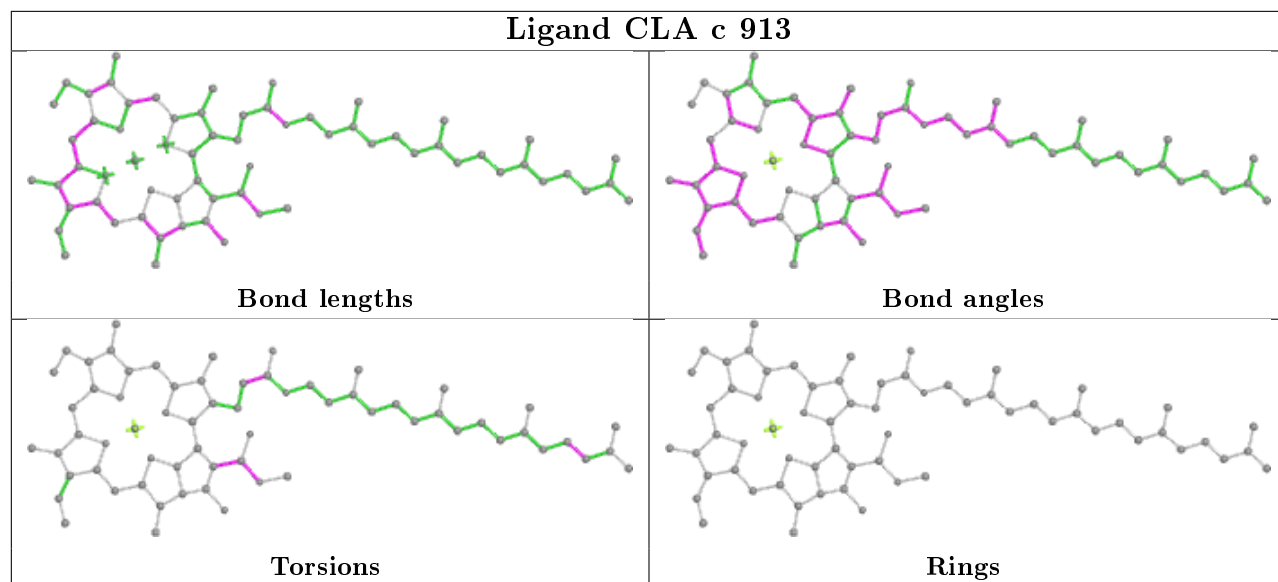


## Ligand CLA b 613

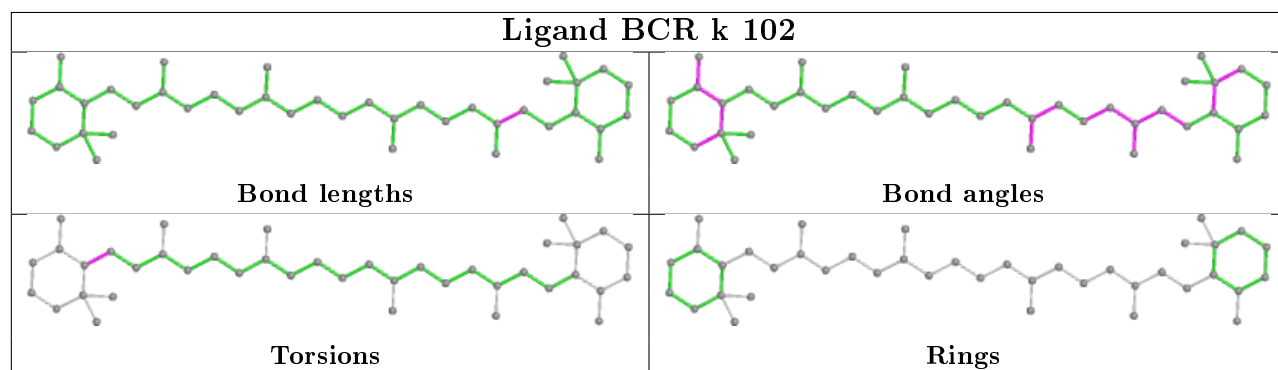




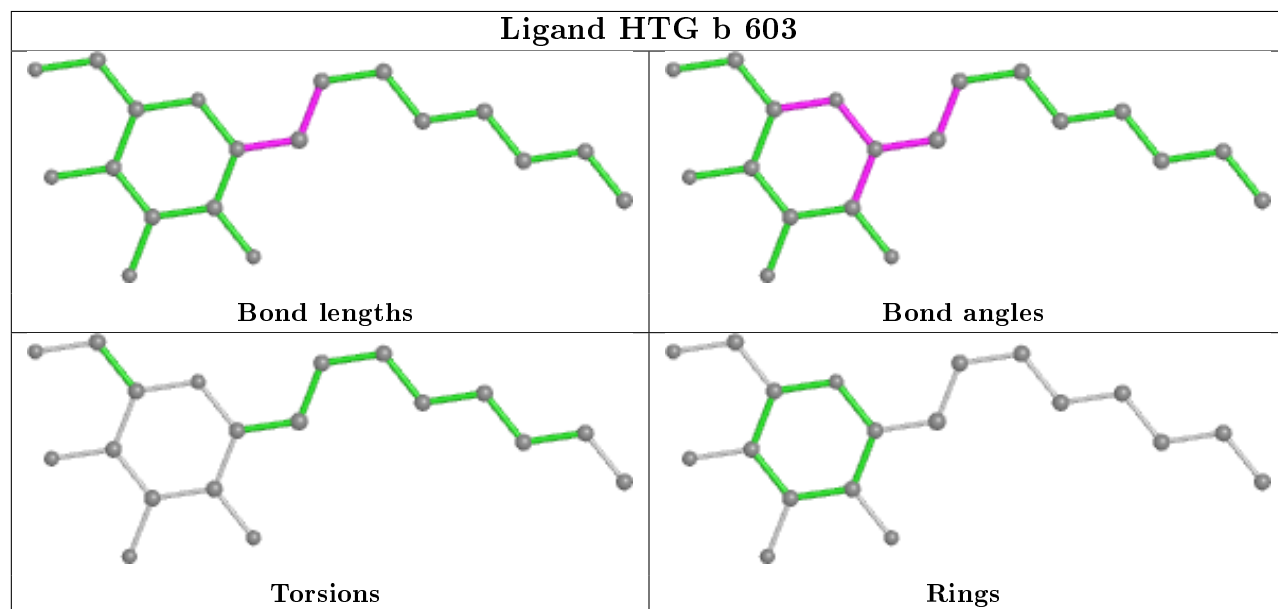
## Ligand CLA c 913



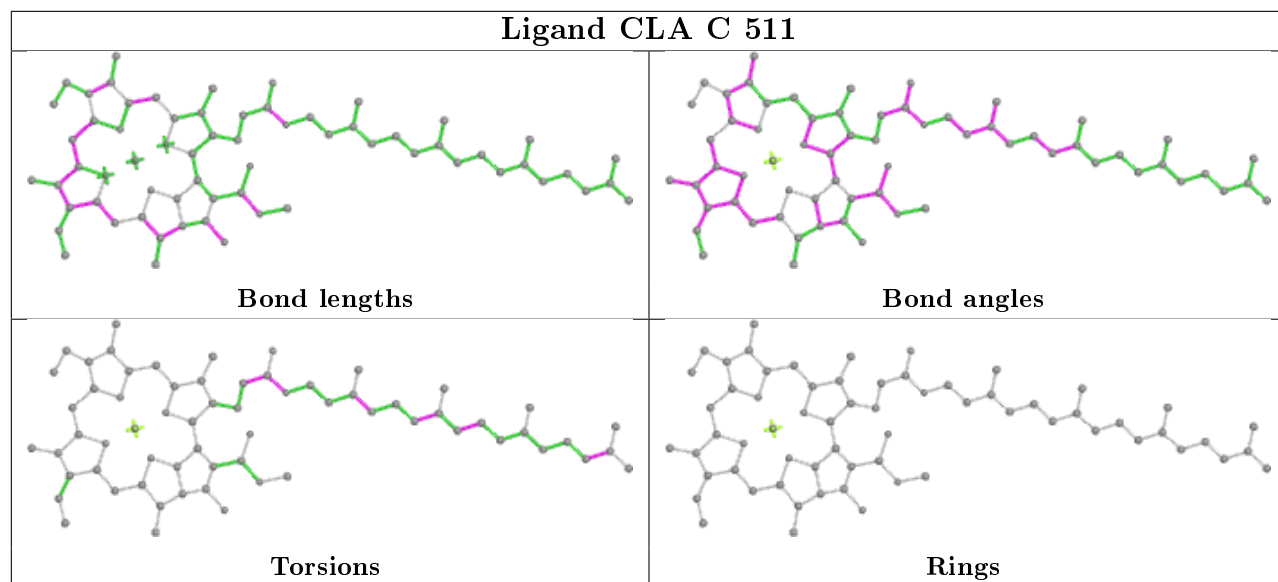
## Ligand BCR k 102



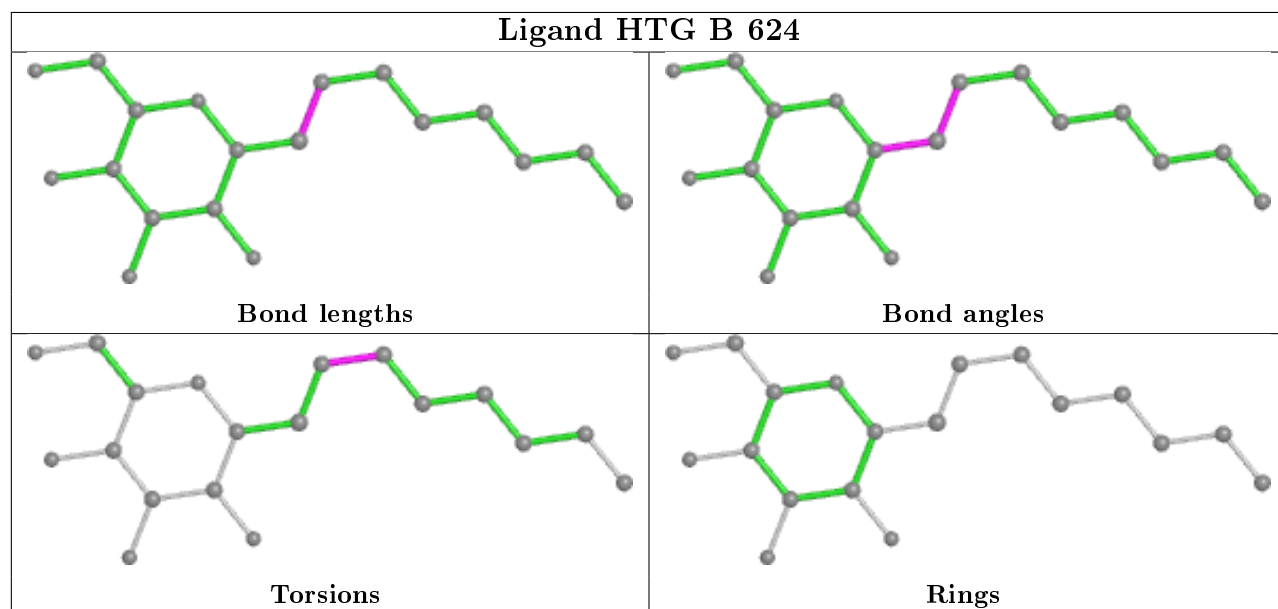
## Ligand HTG b 603



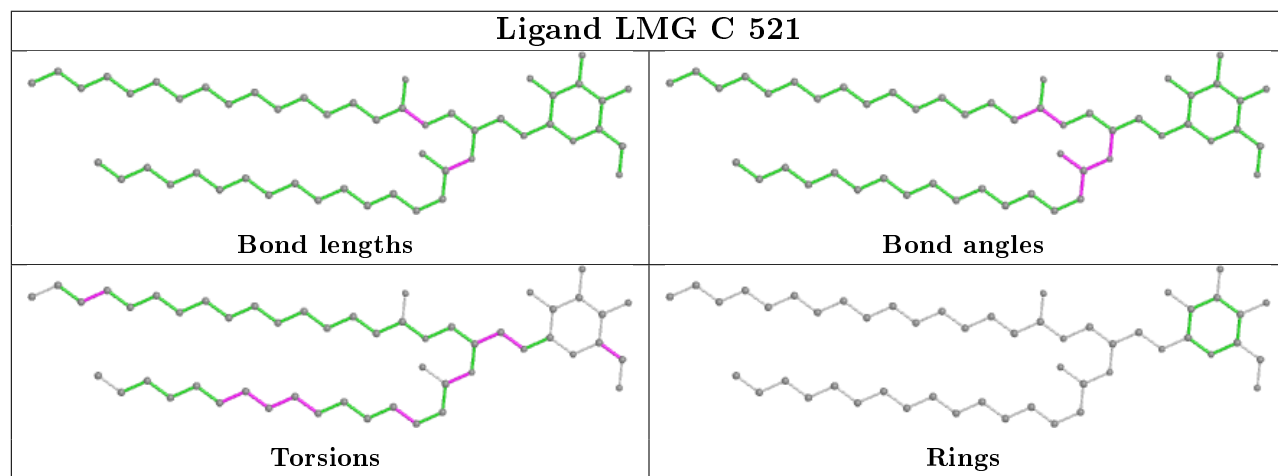
## Ligand CLA C 511



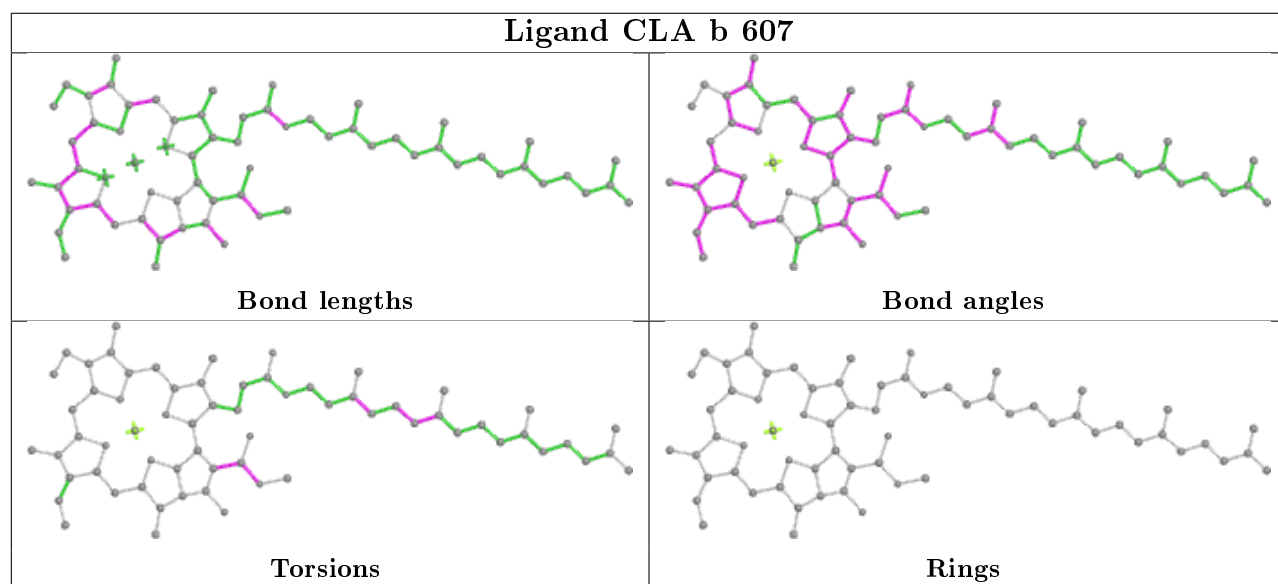
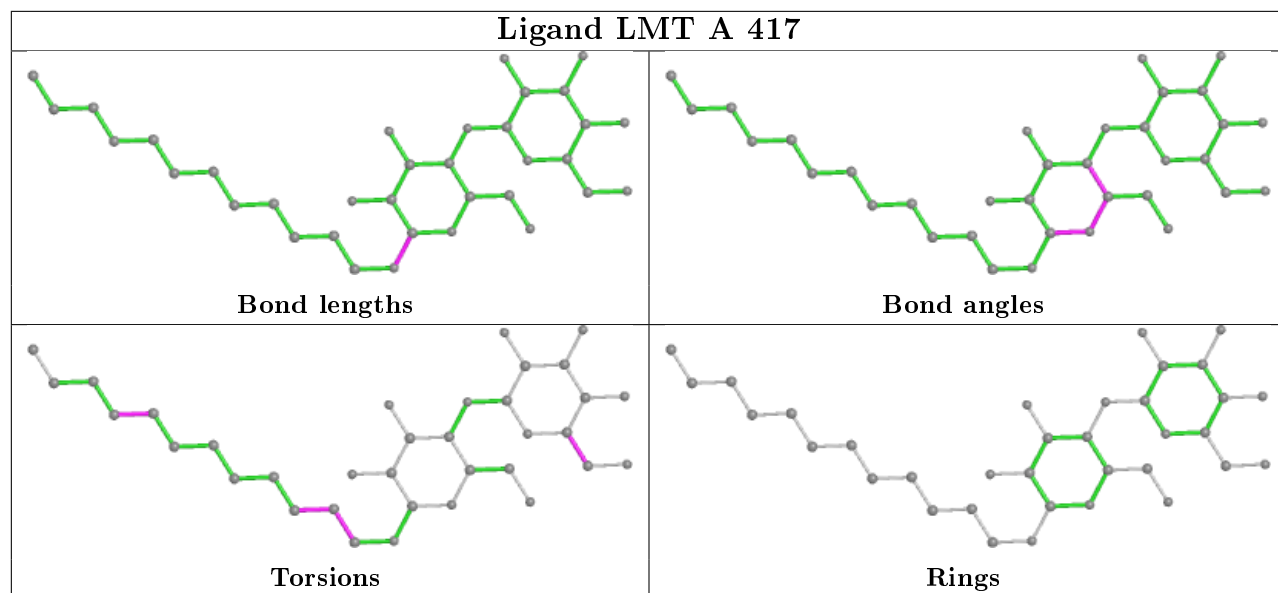
## Ligand HTG B 624

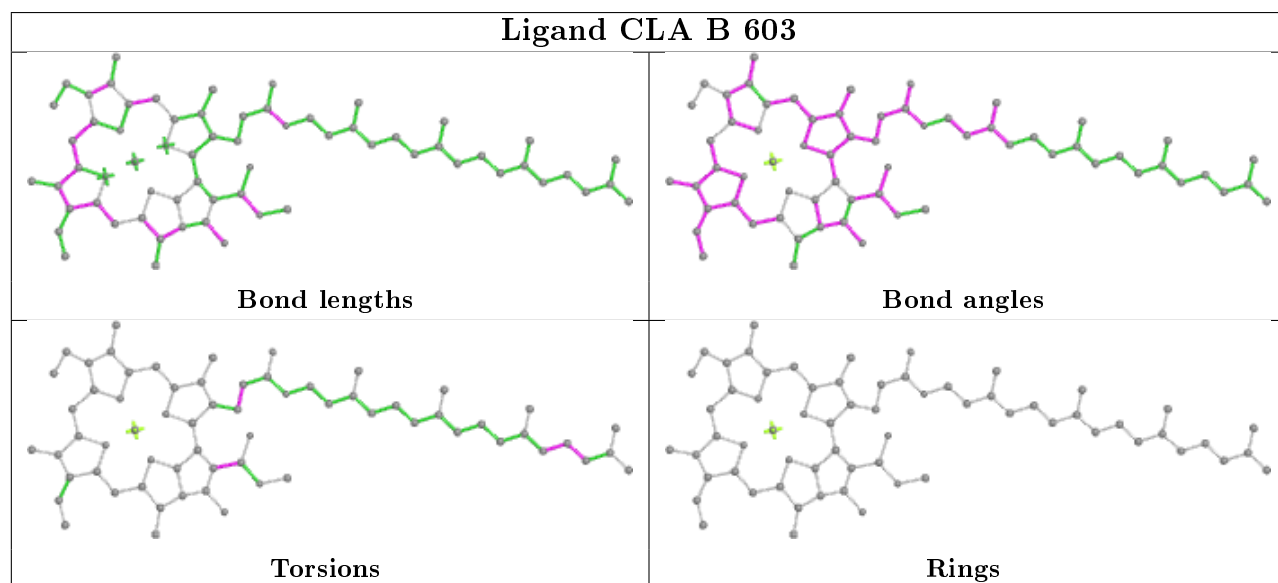
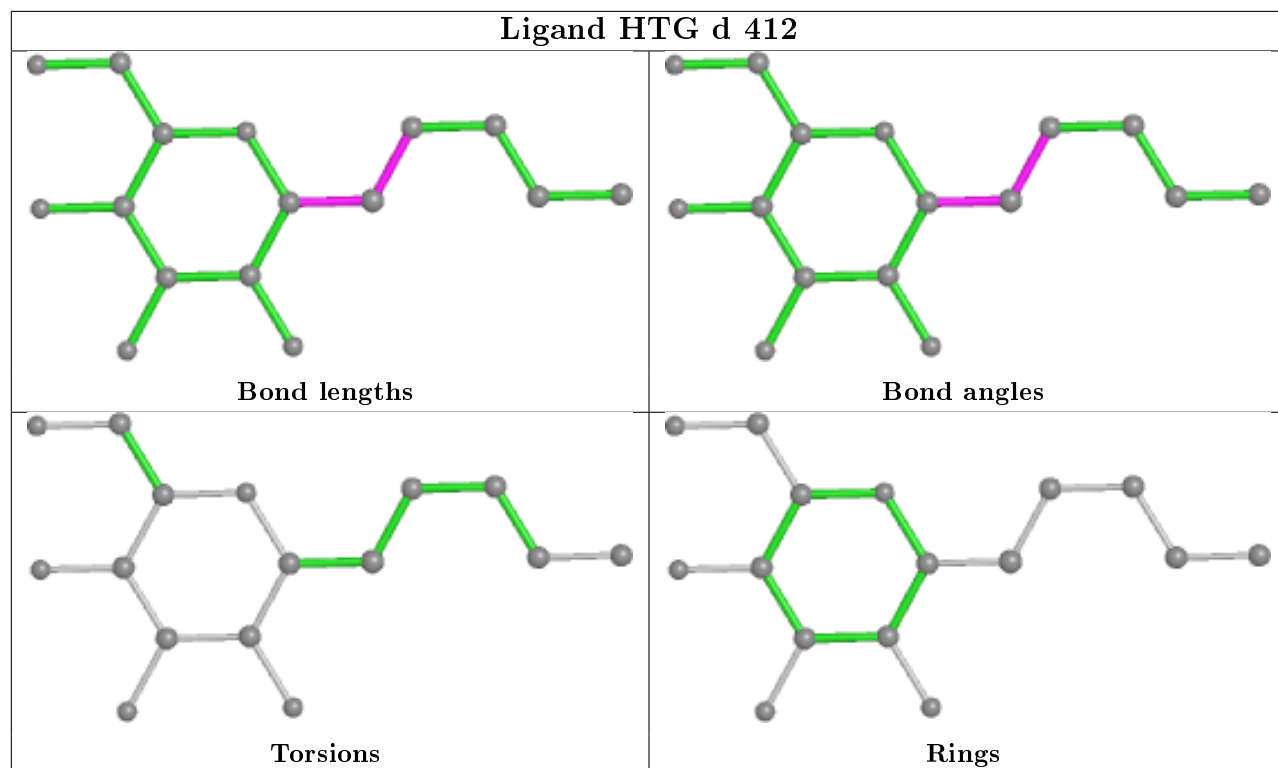


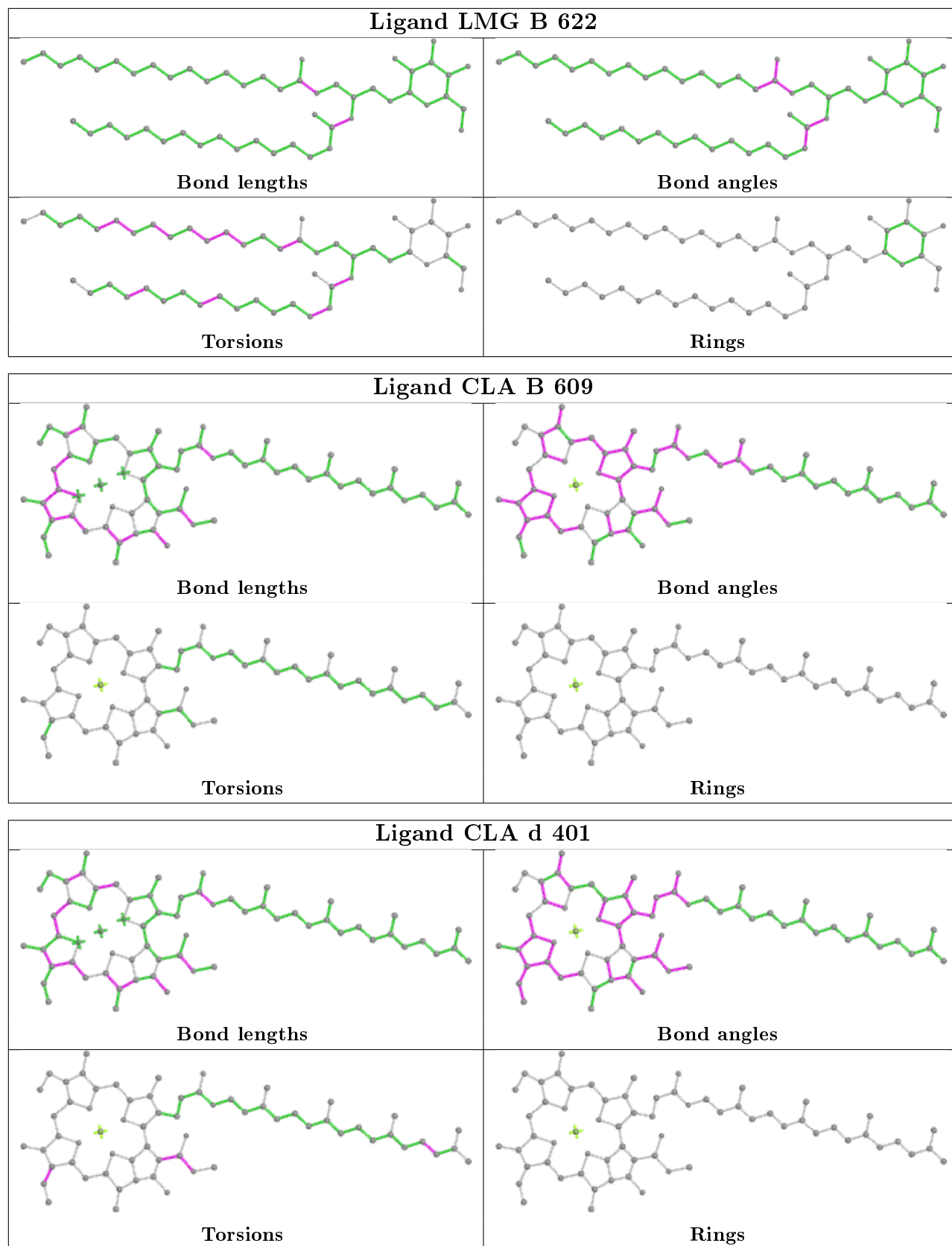
## Ligand LMG C 521



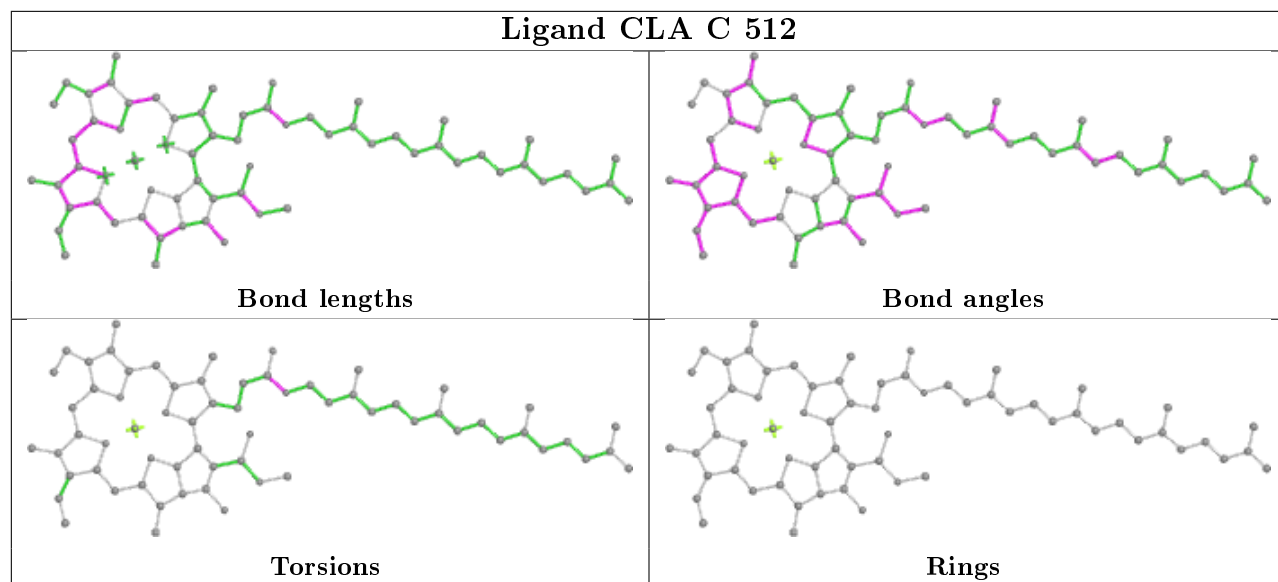




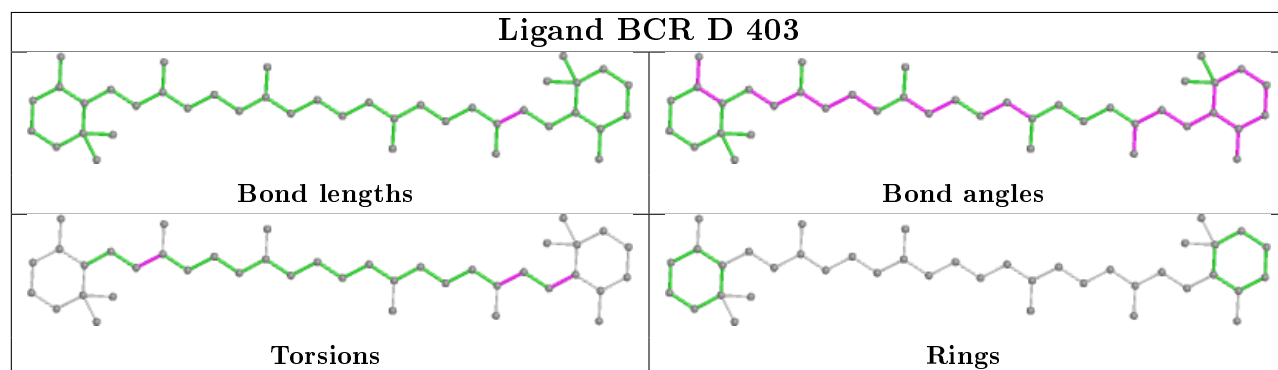




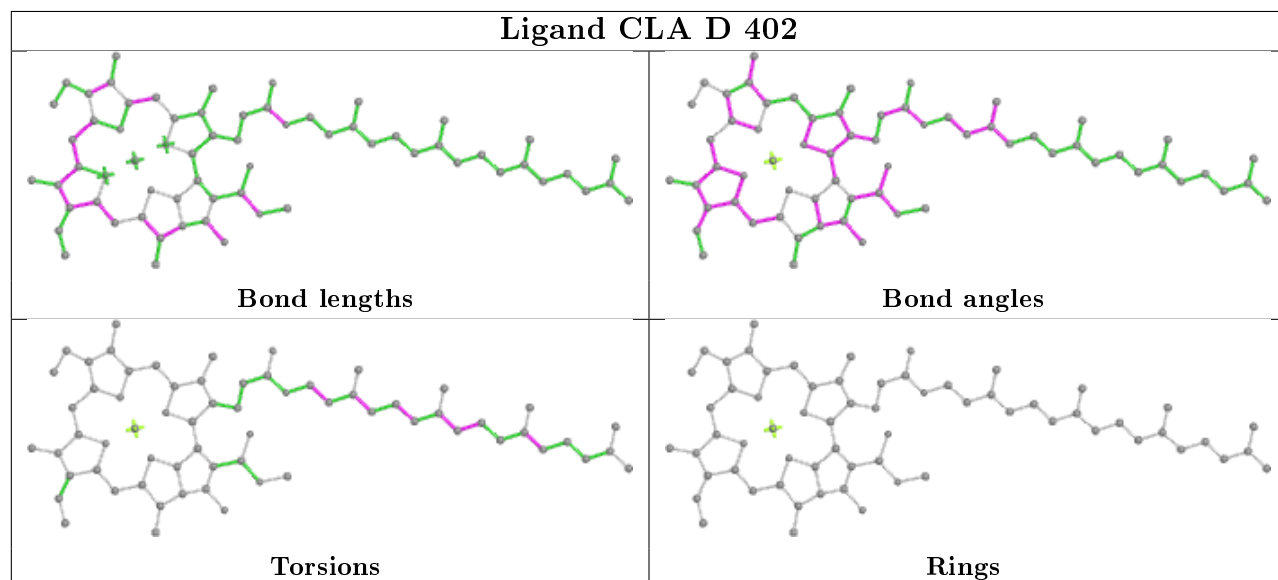
## Ligand CLA C 512



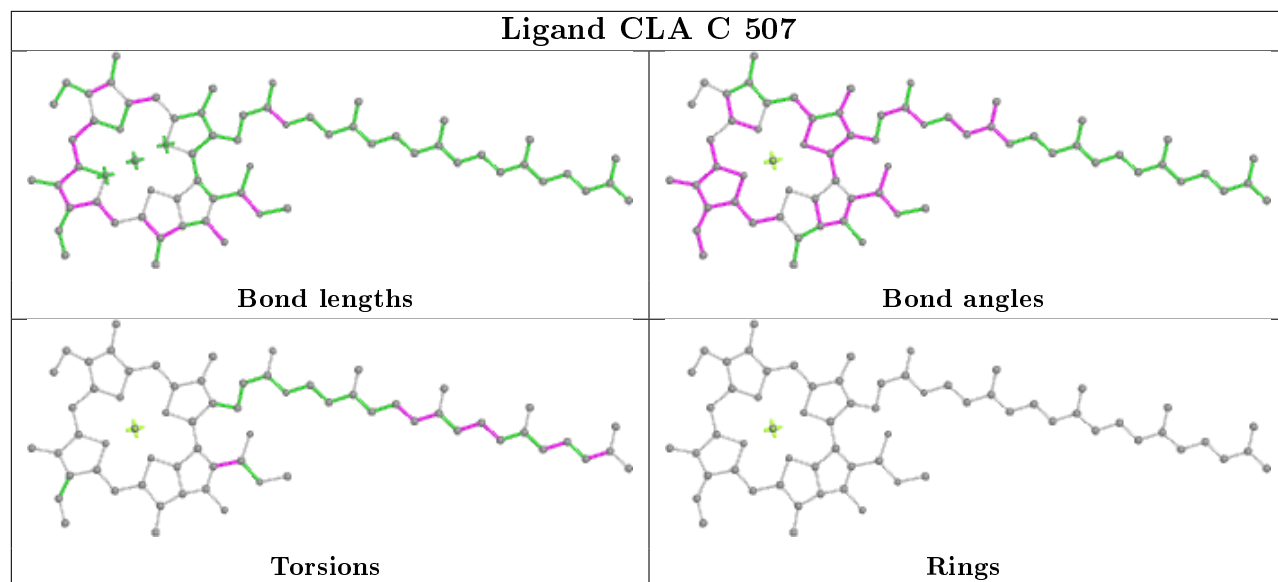
## Ligand BCR D 403



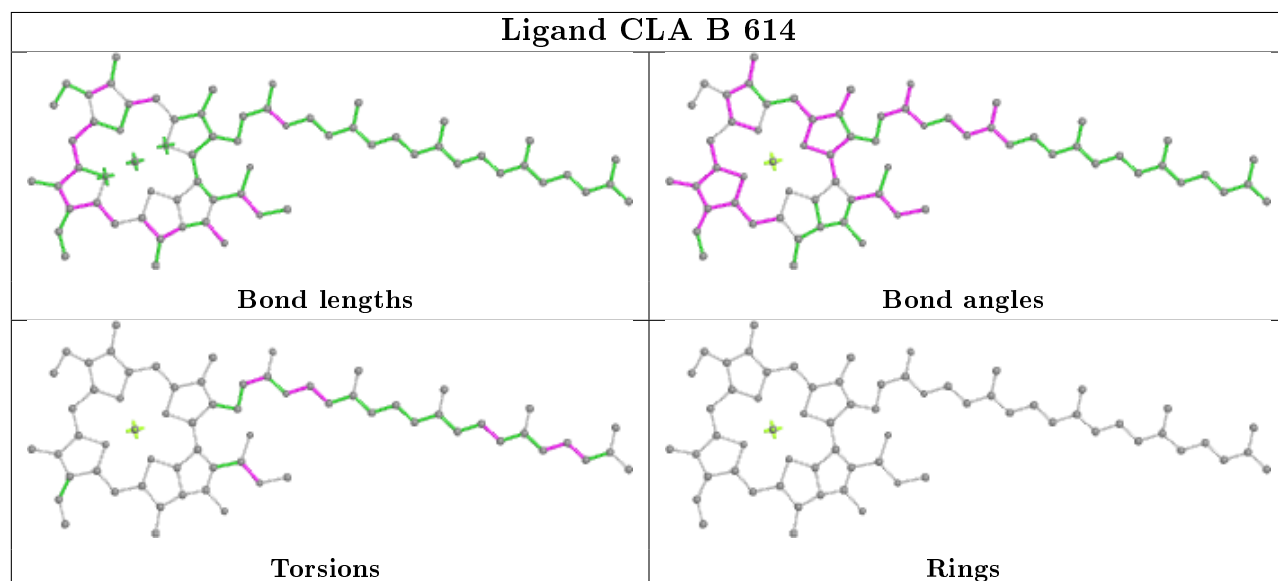
## Ligand CLA D 402



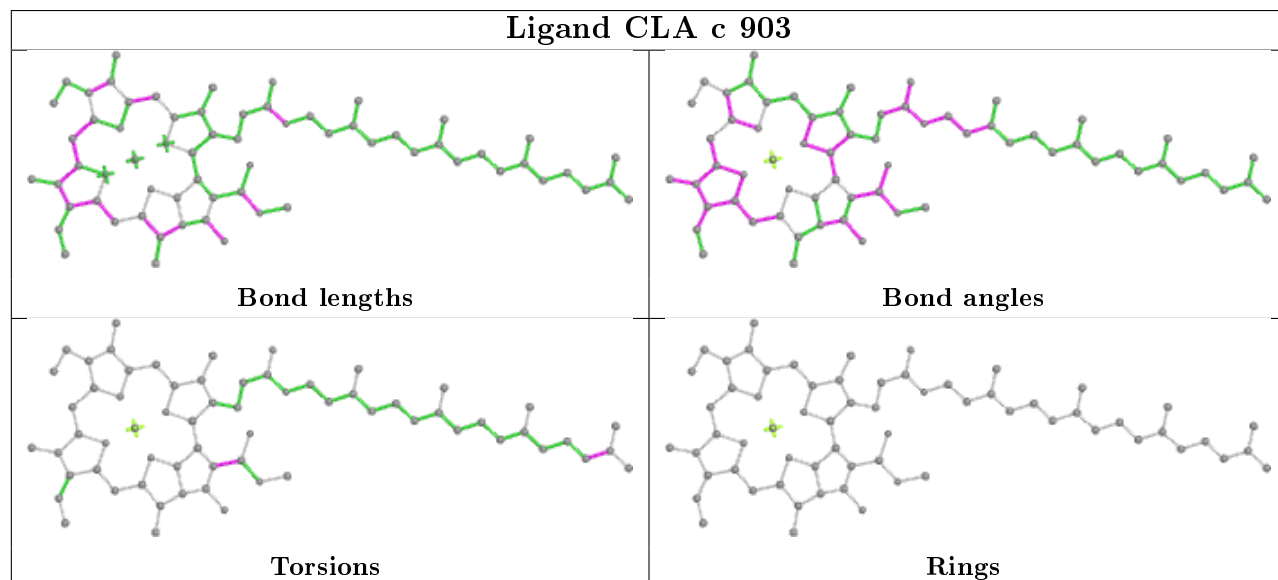
## Ligand CLA C 507



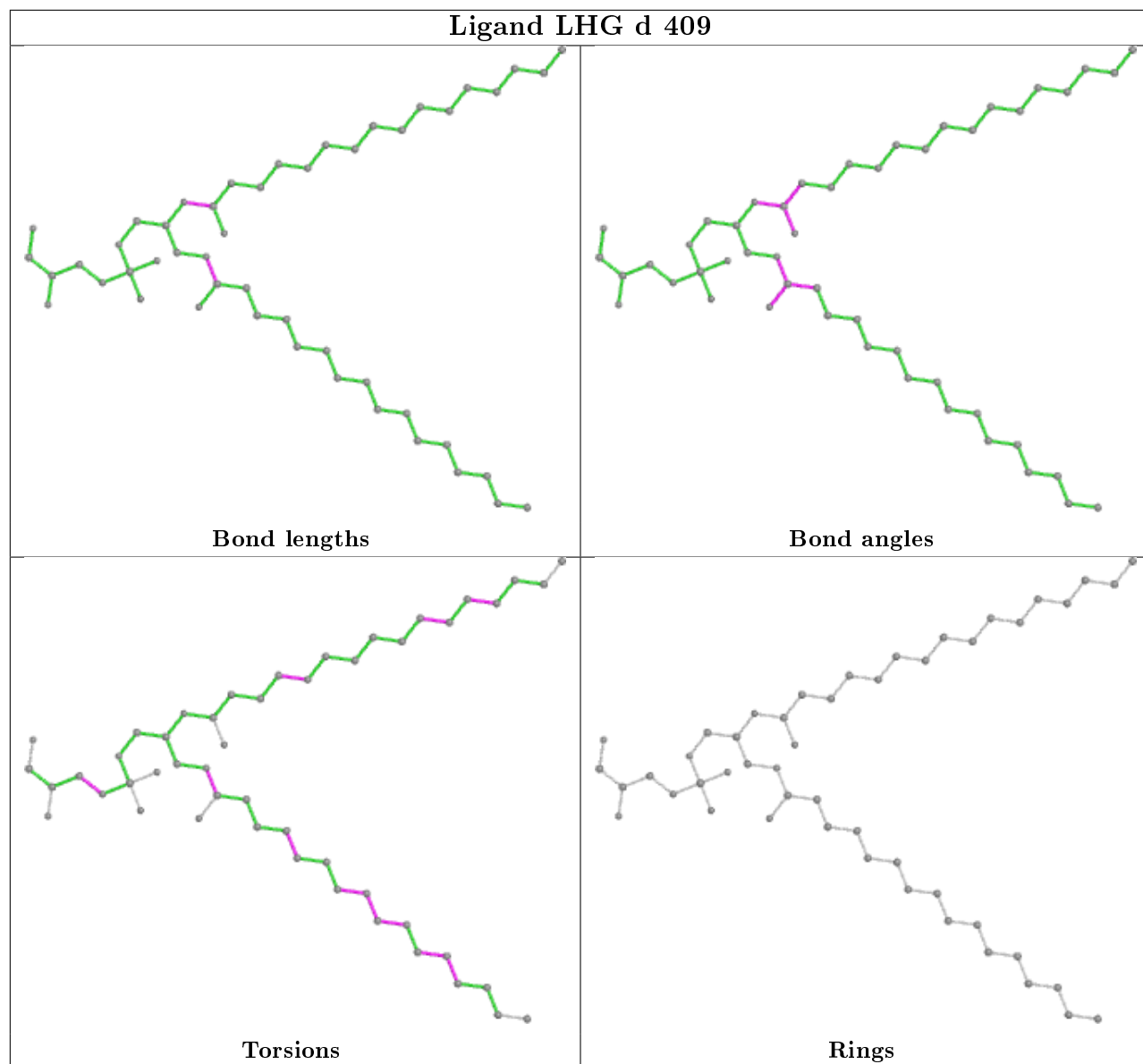
## Ligand CLA B 614



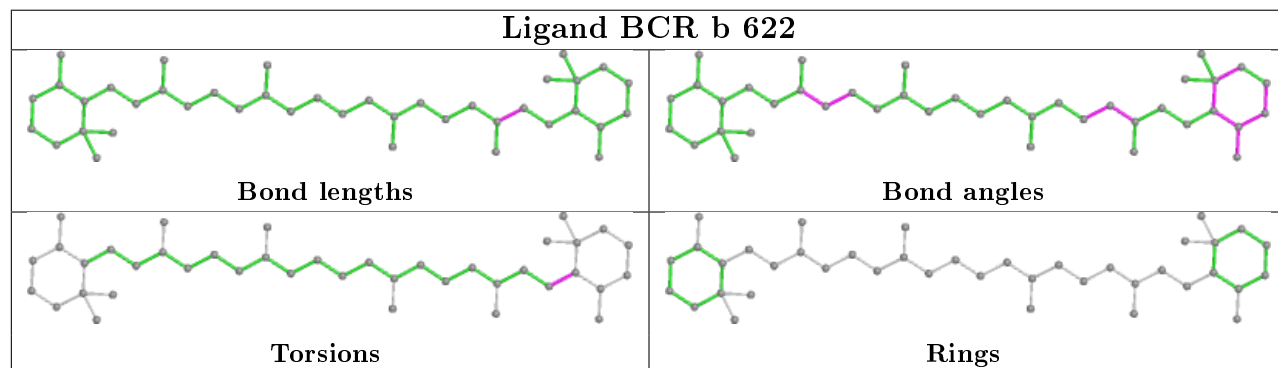
## Ligand CLA c 903

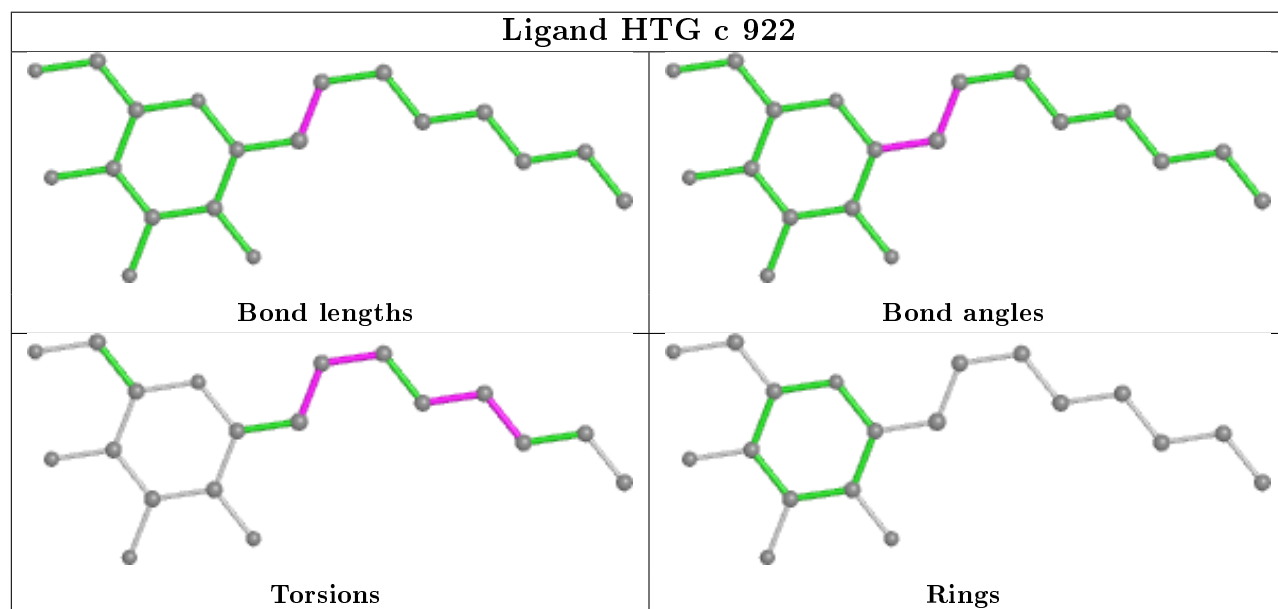
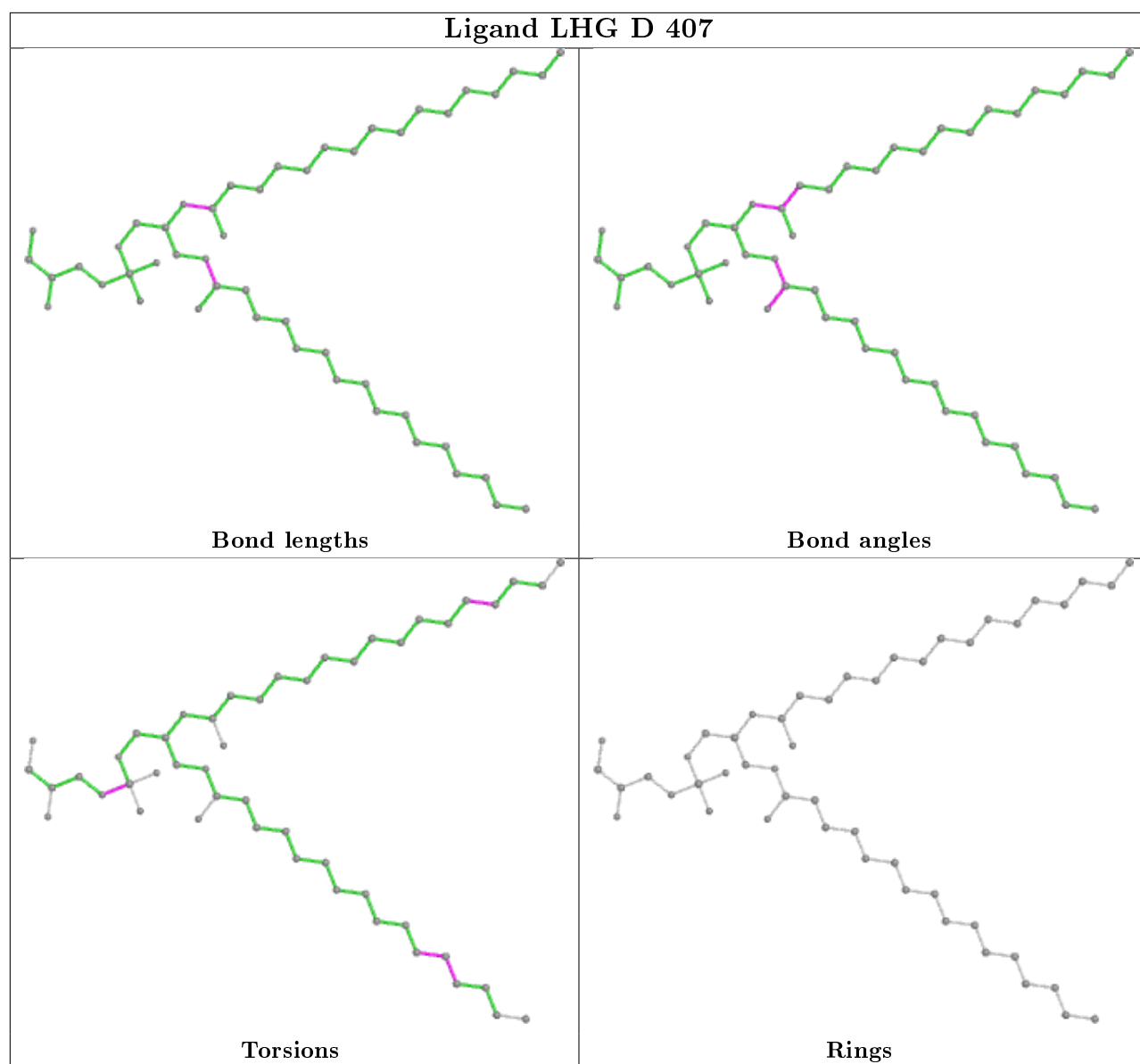


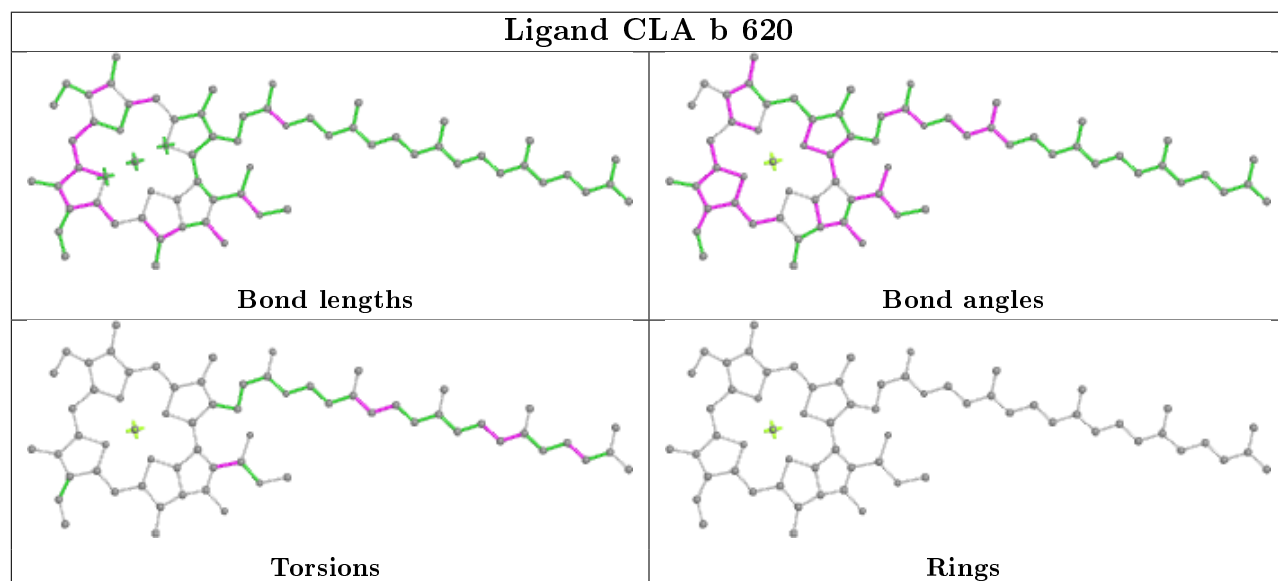
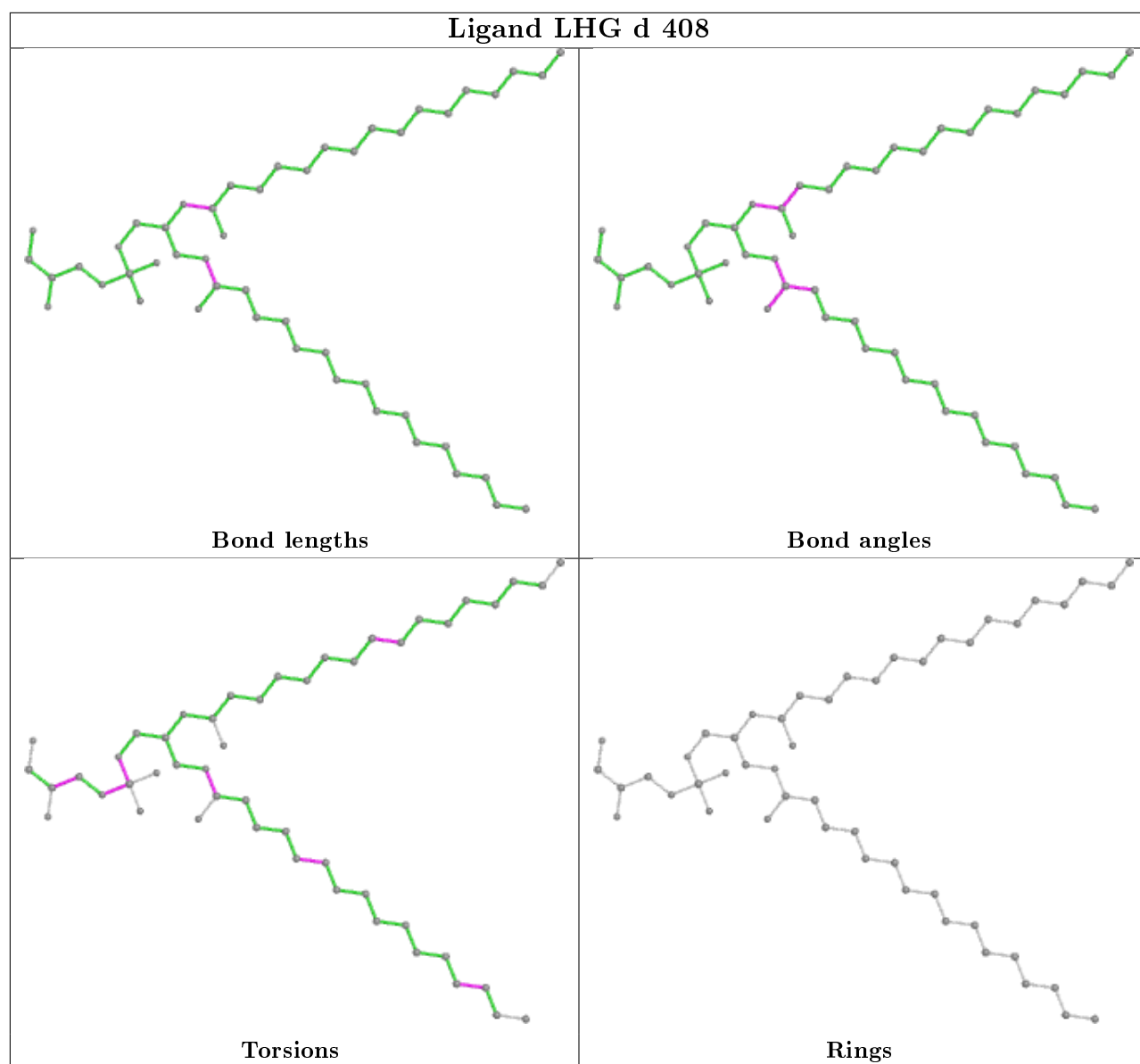
## Ligand LHG d 409



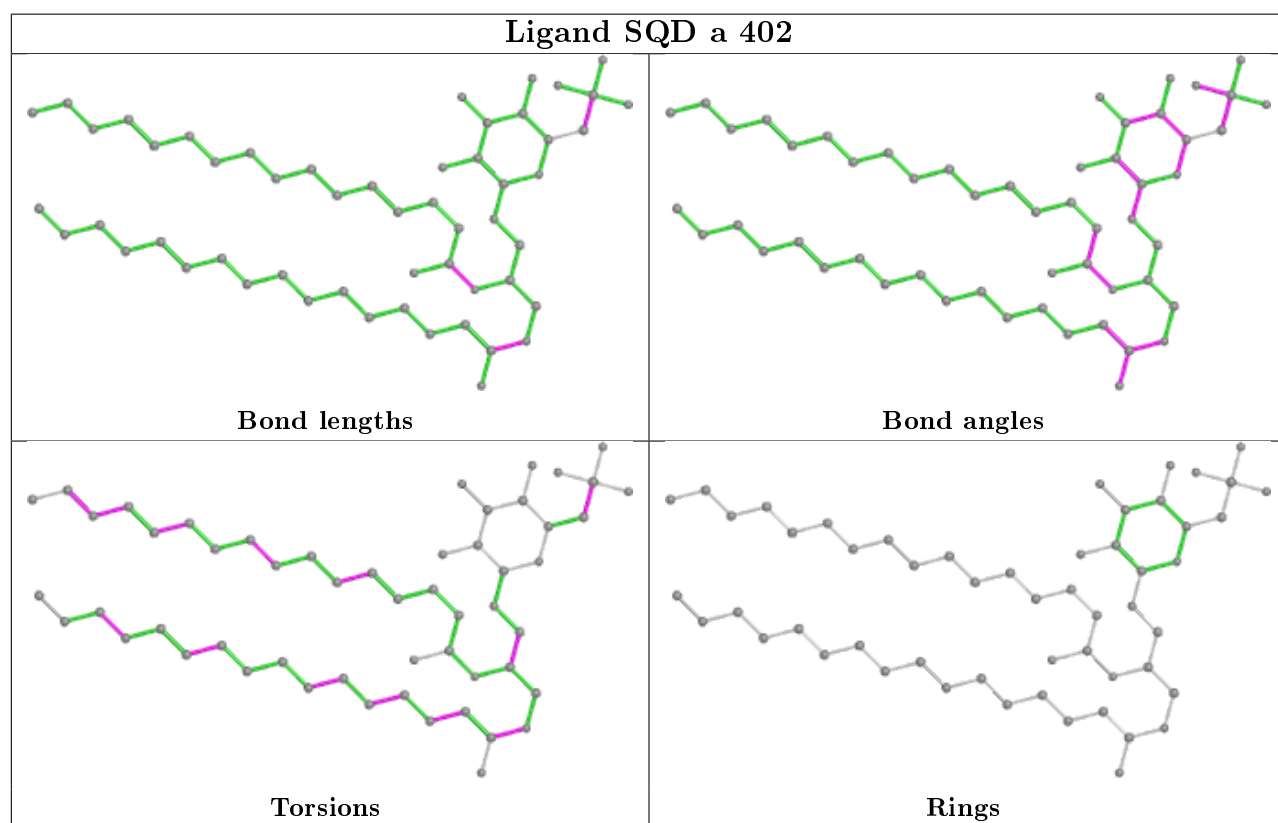
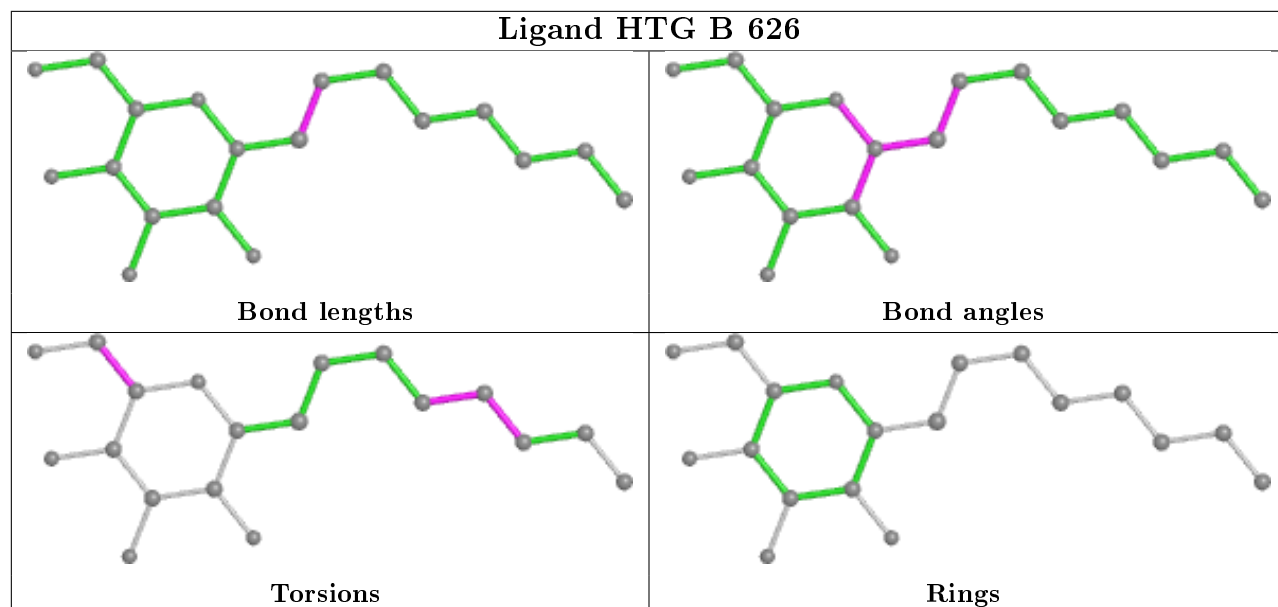
## Ligand BCR b 622

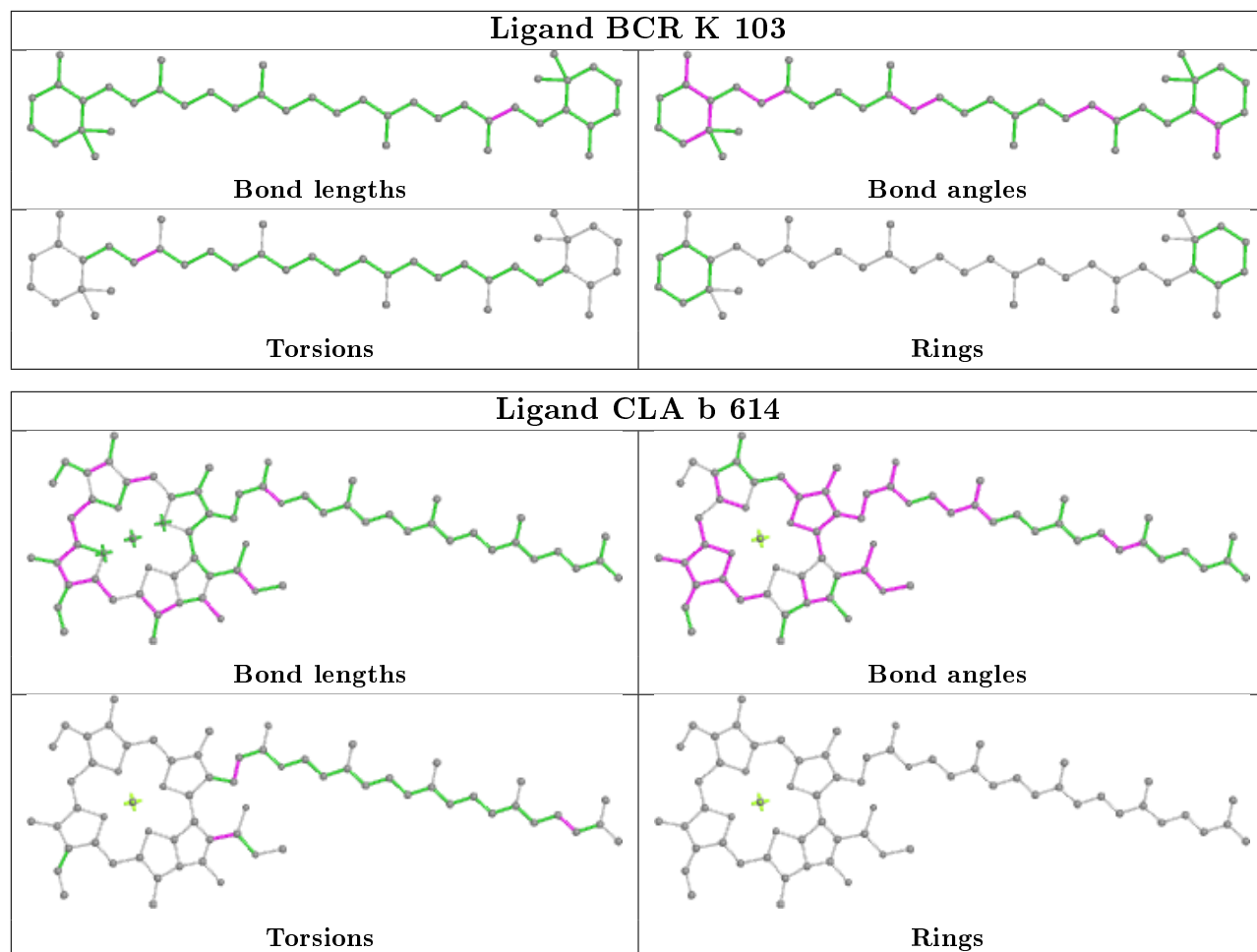


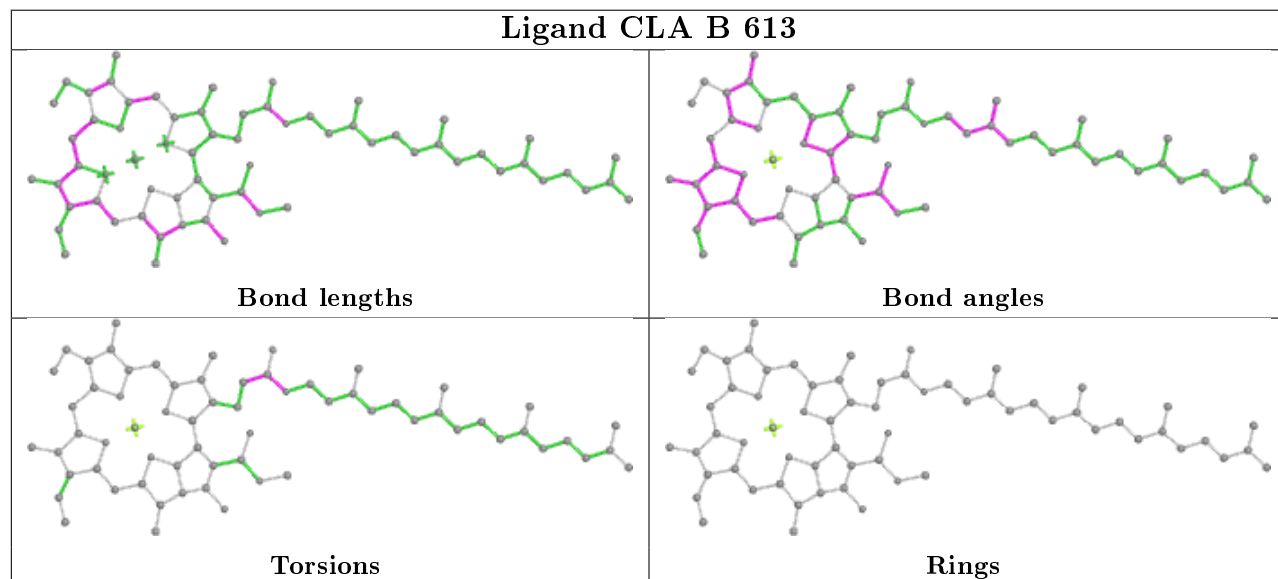
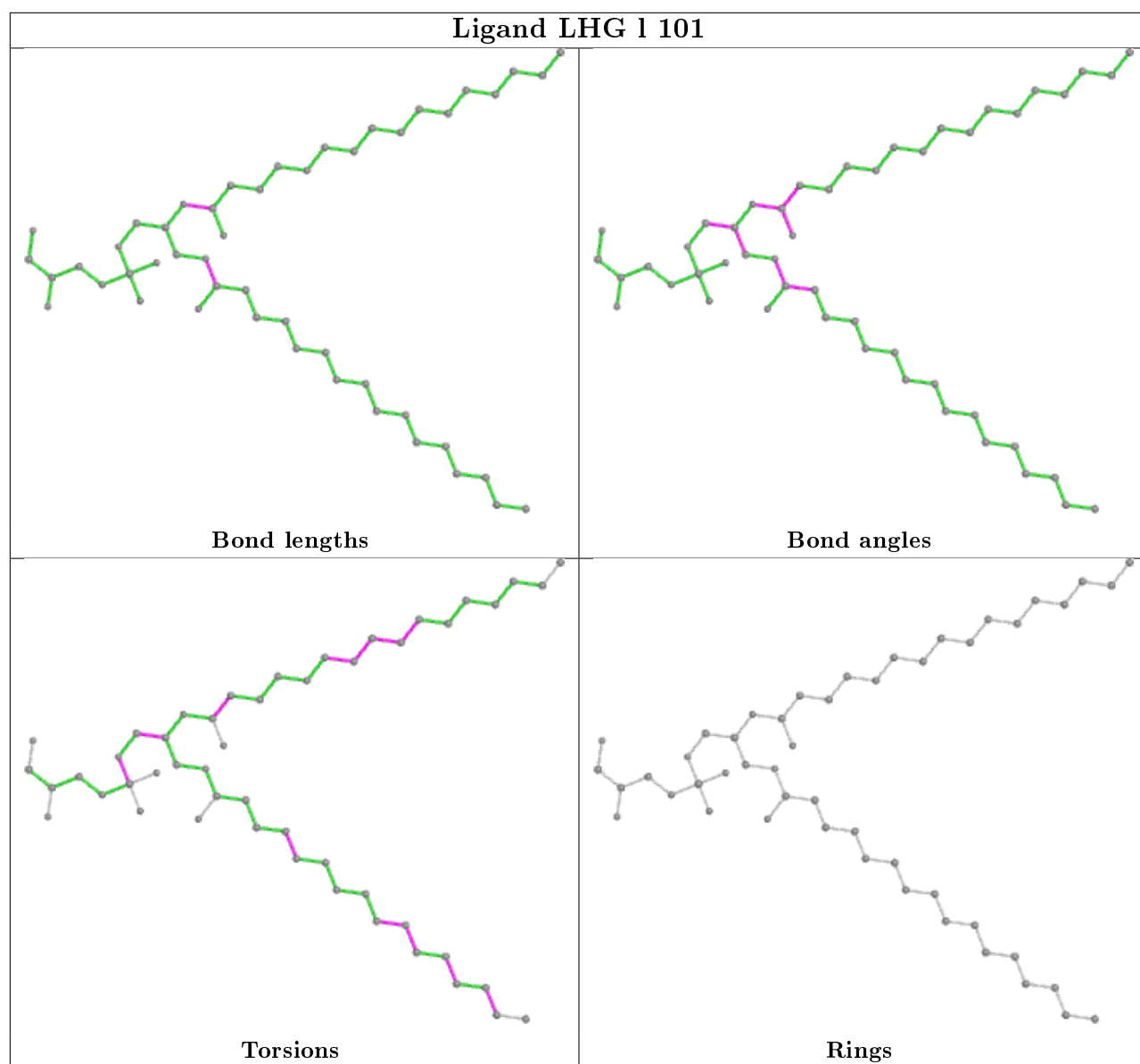


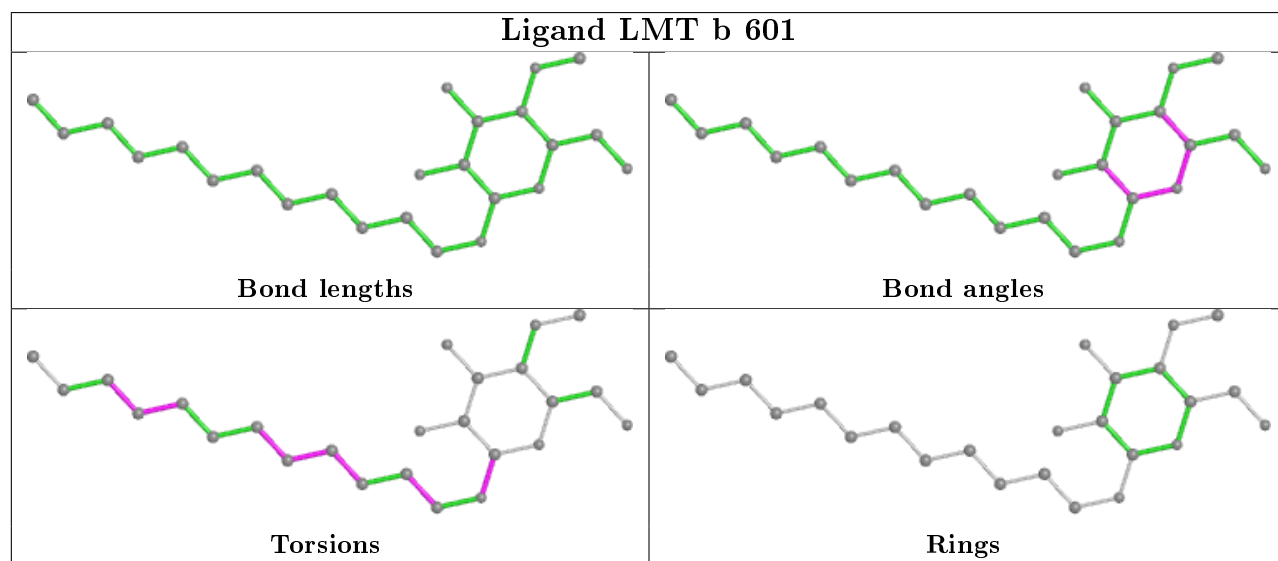
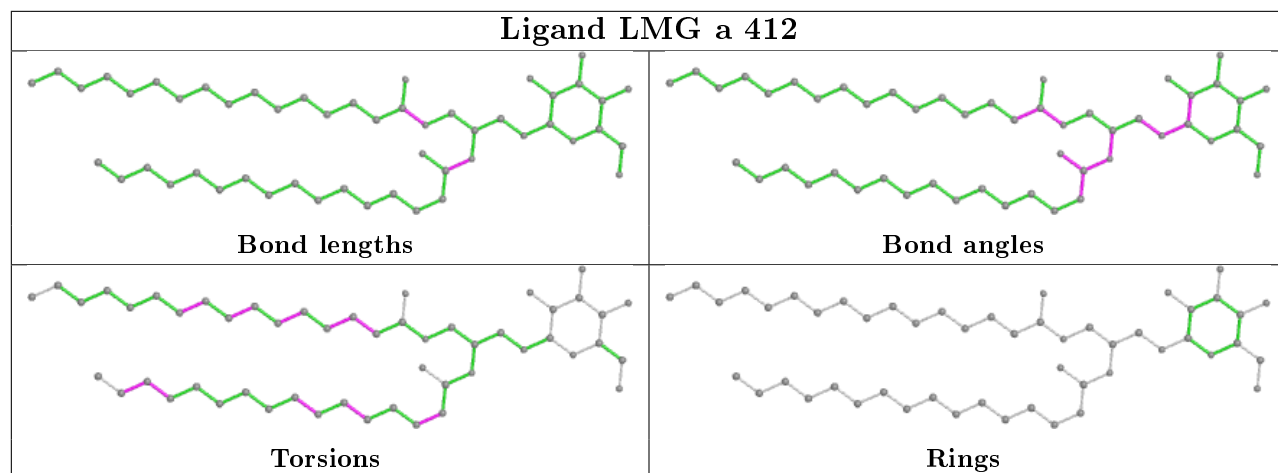
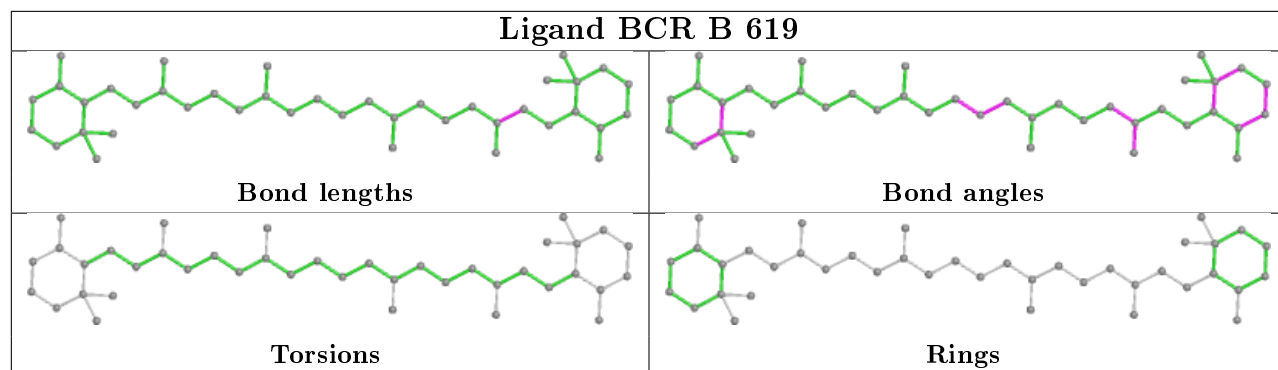


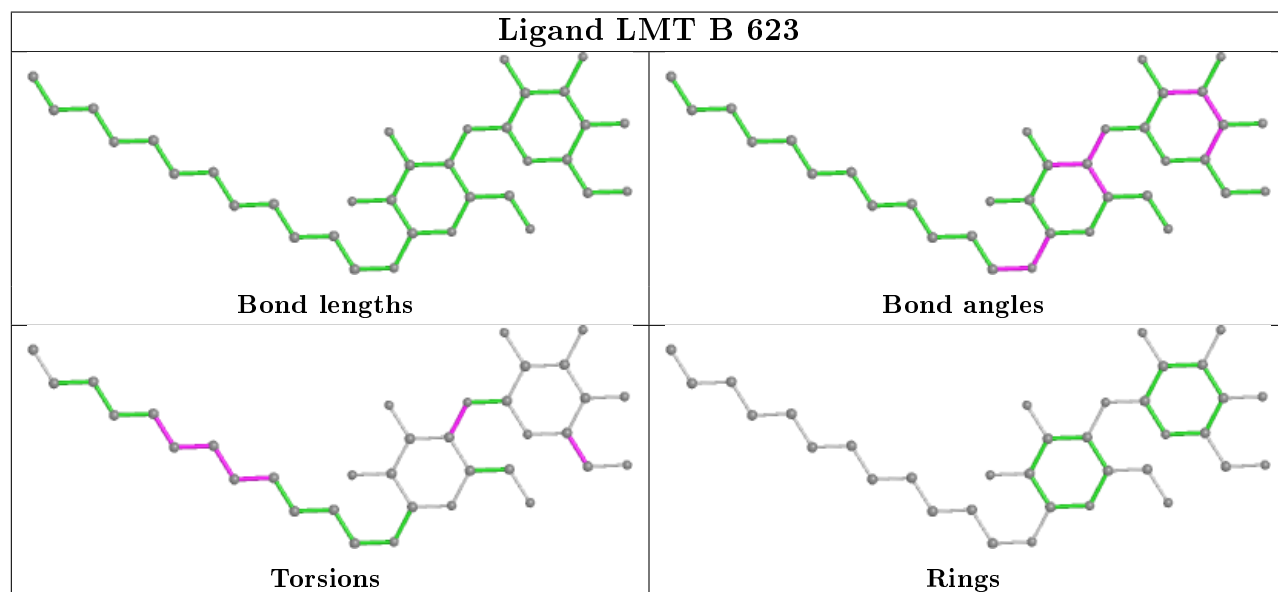
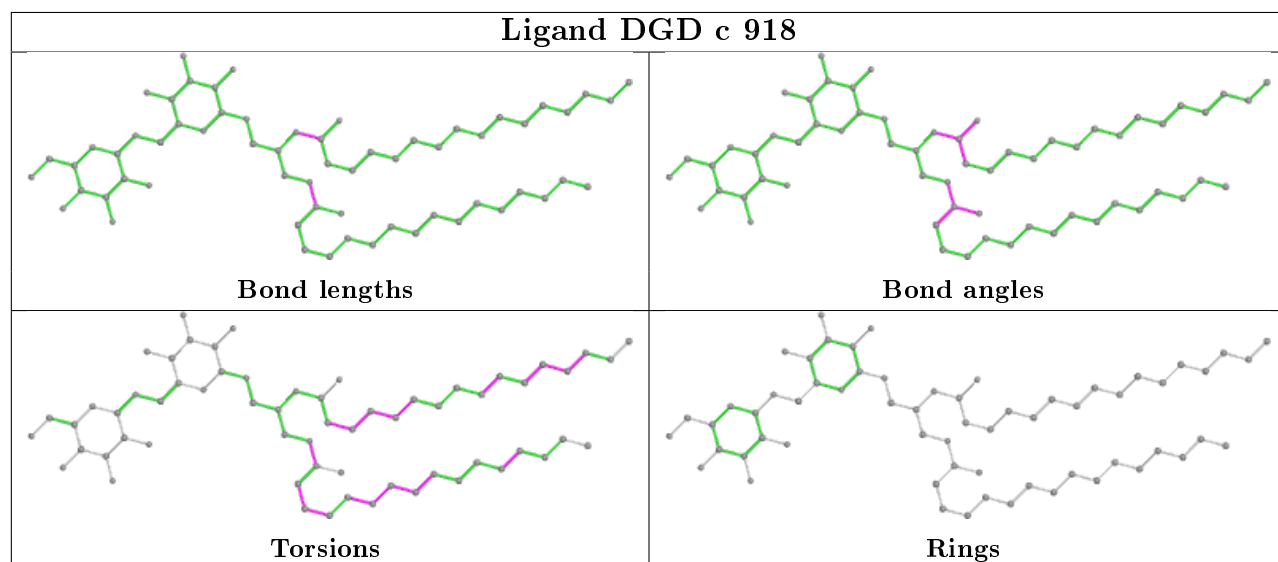
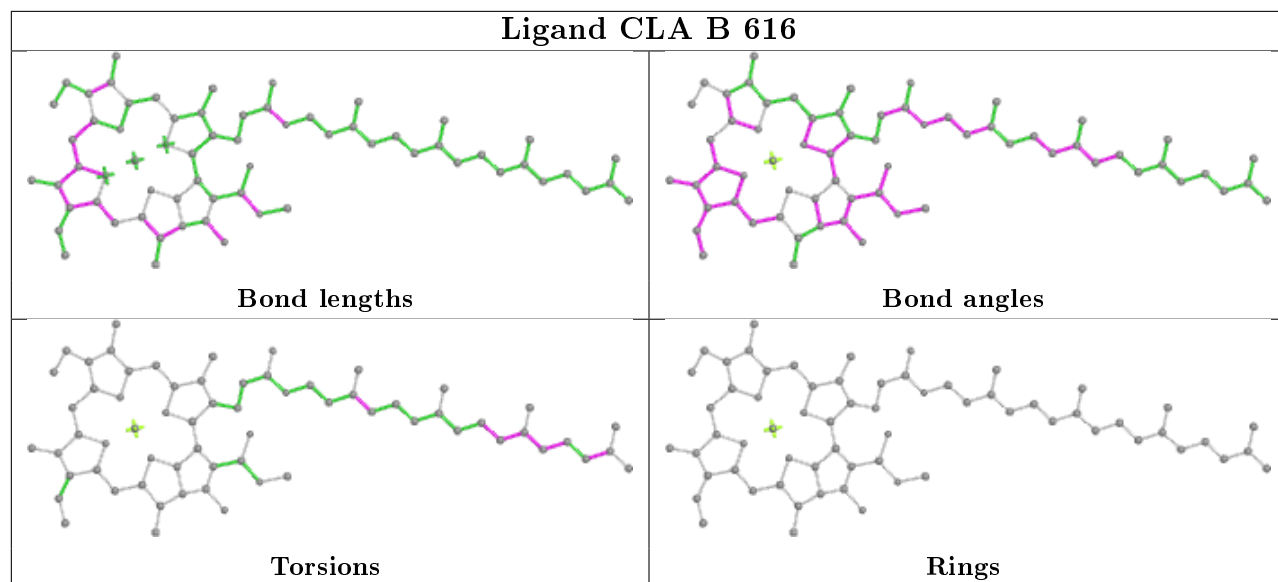


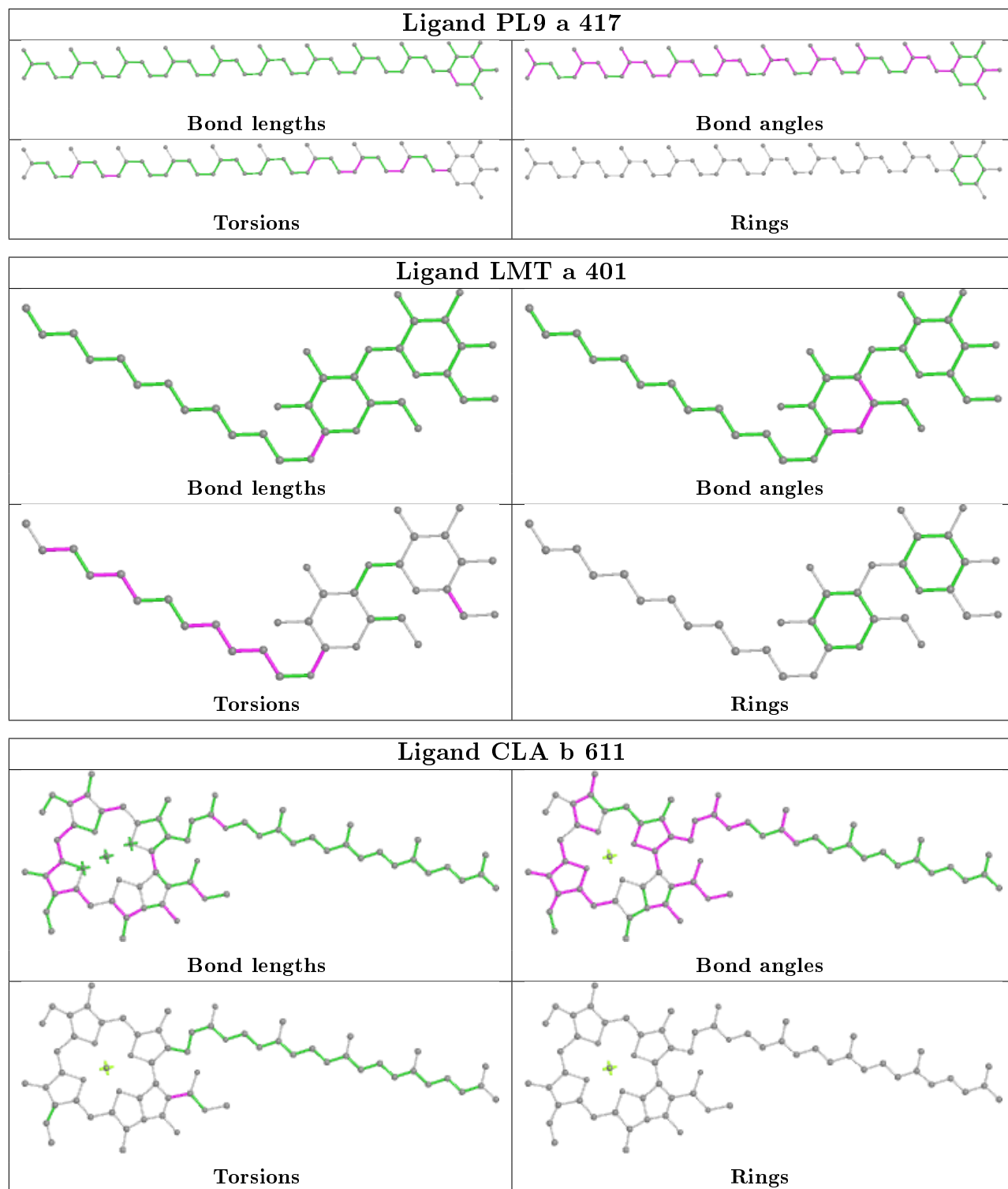




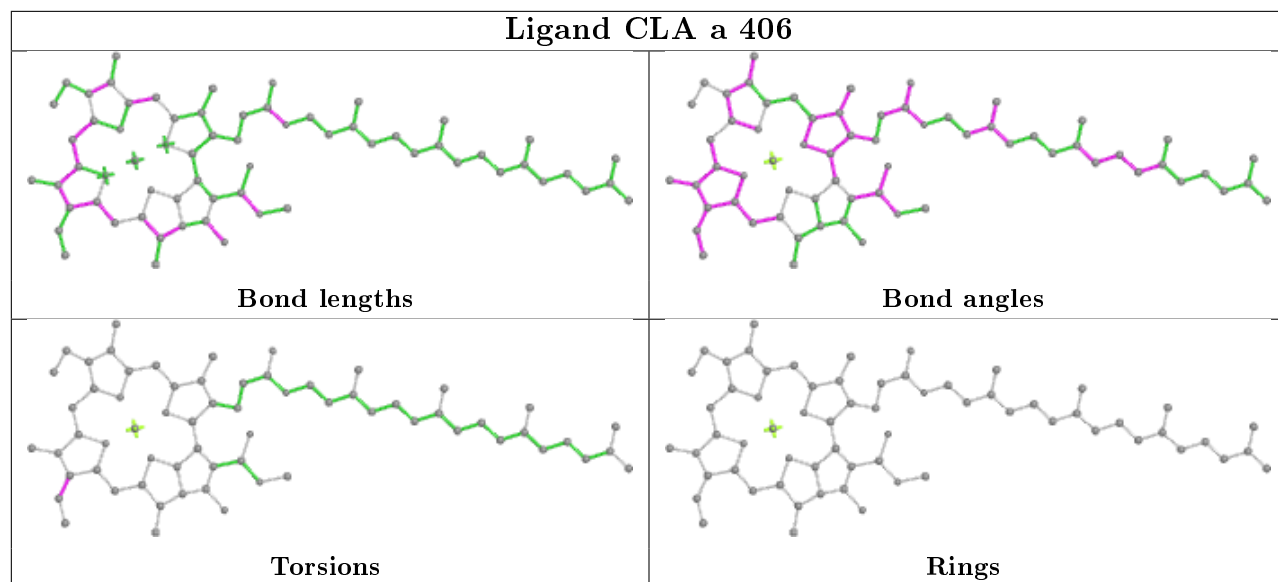




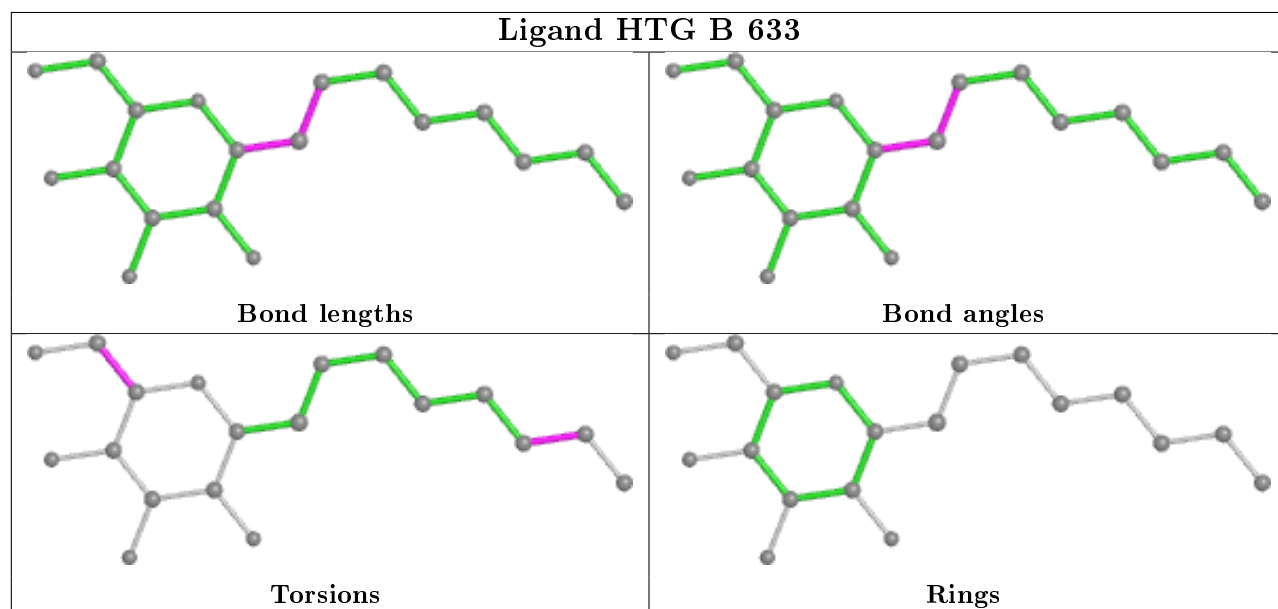




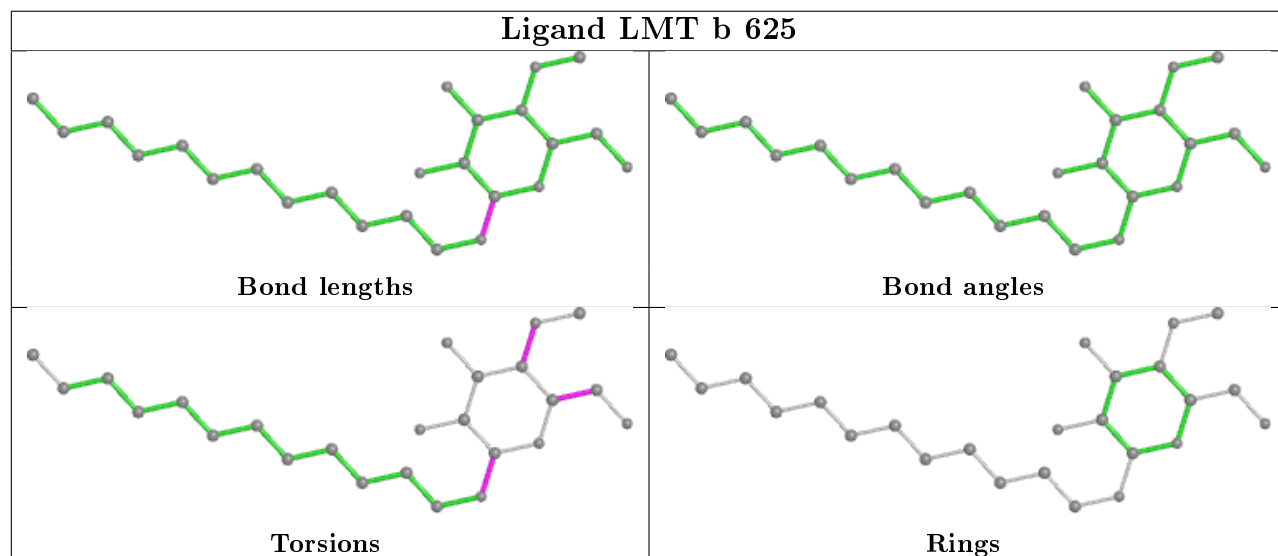
## Ligand CLA a 406

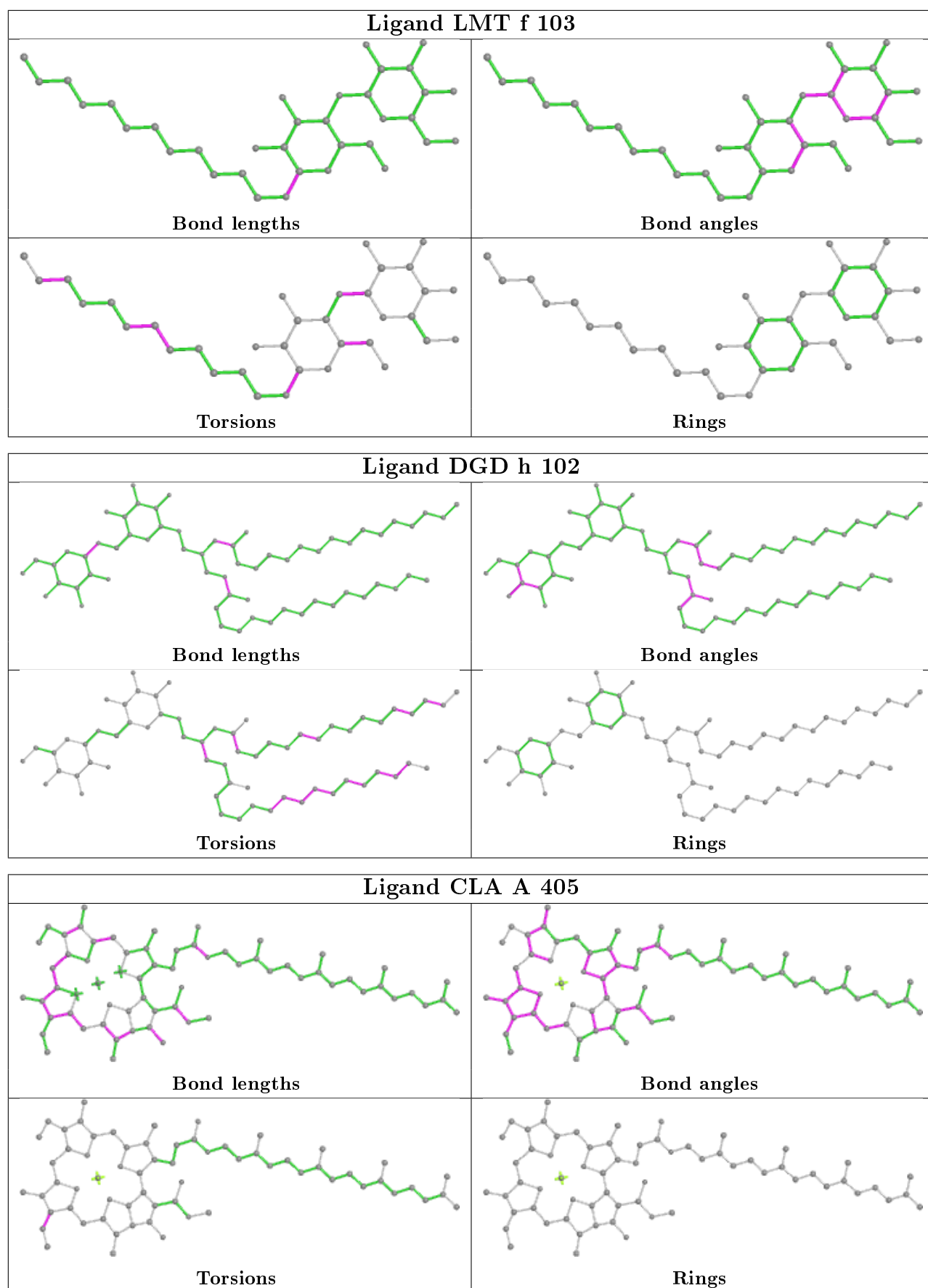


## Ligand HTG B 633



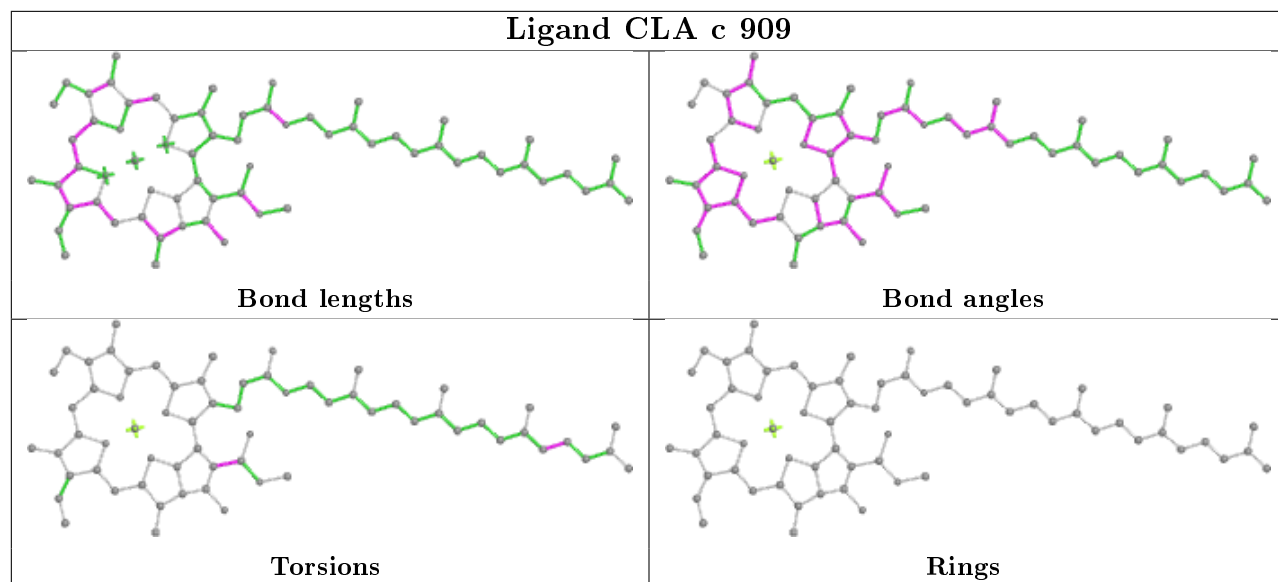
## Ligand LMT b 625



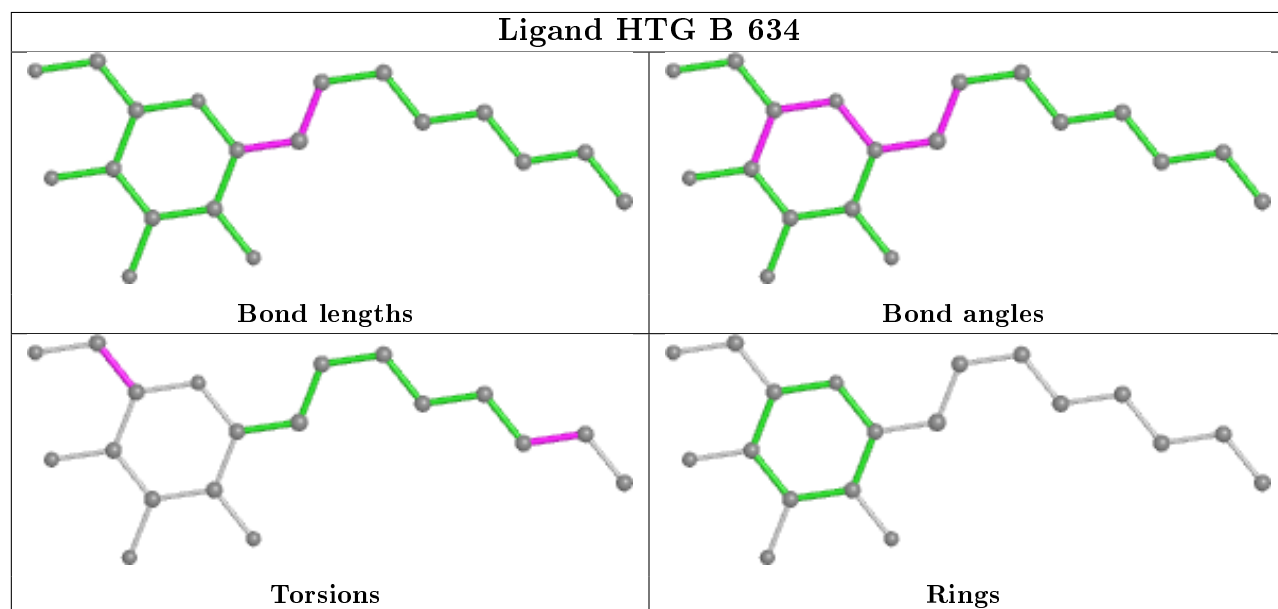




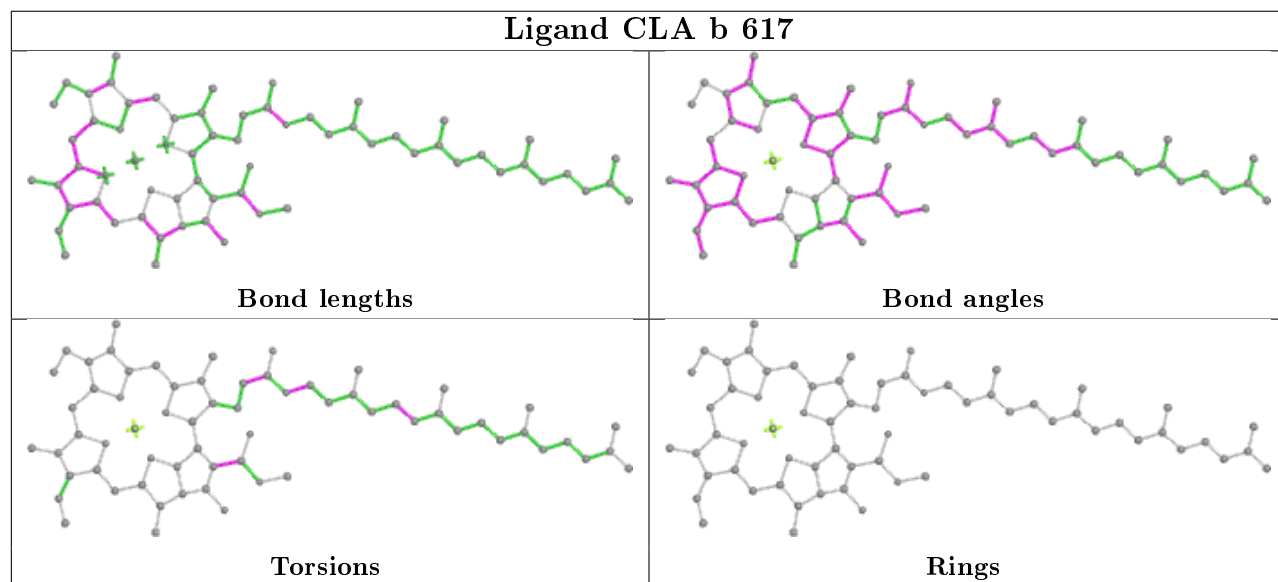
## Ligand CLA c 909

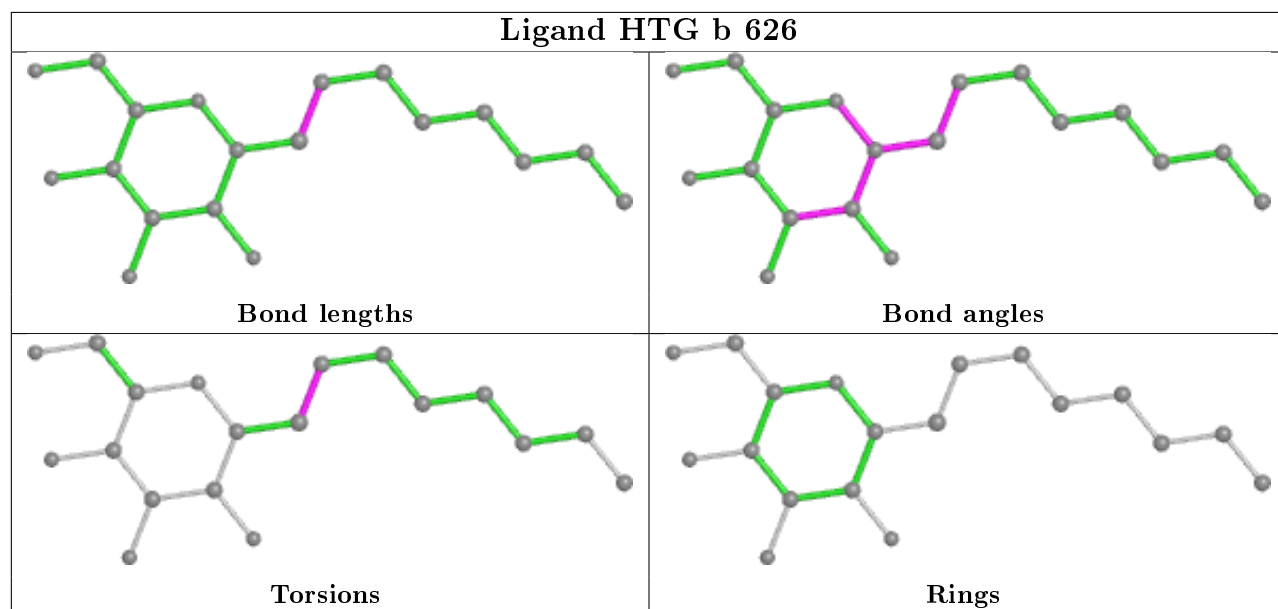
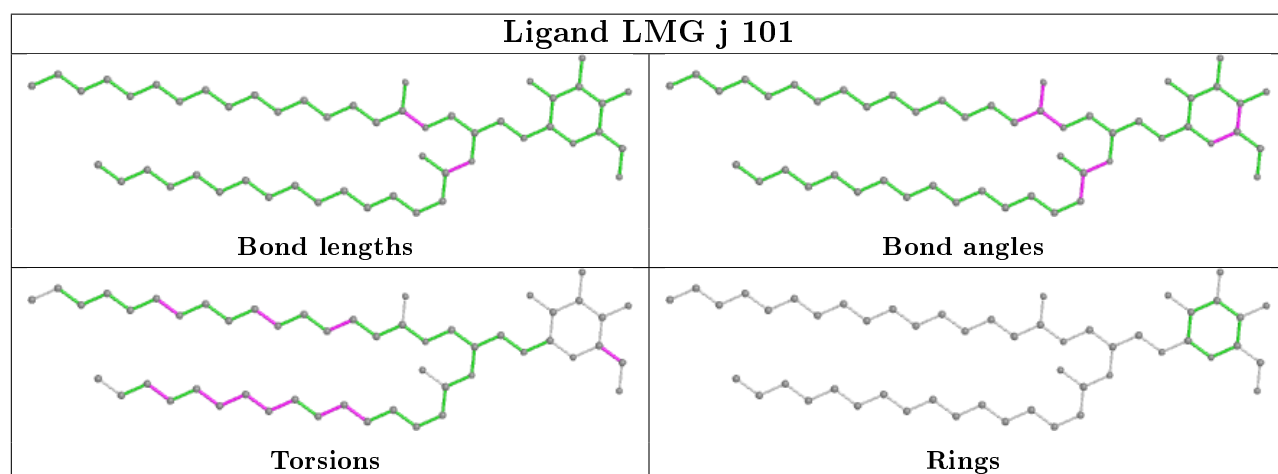
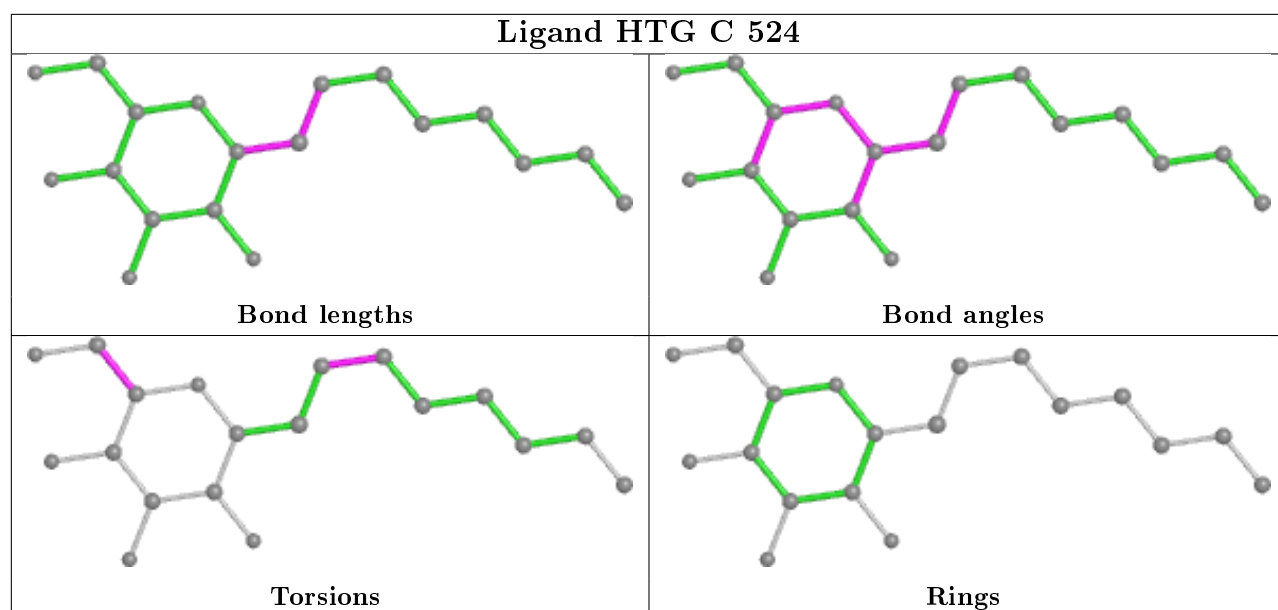


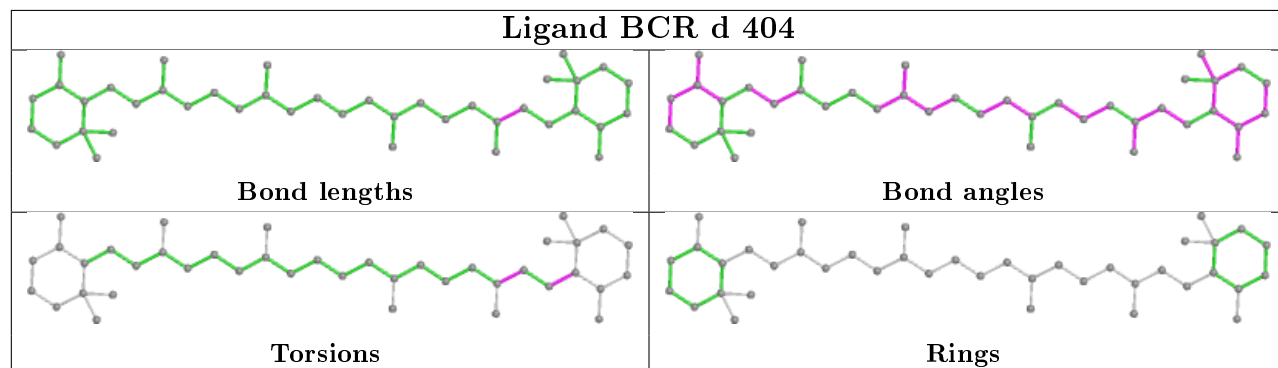
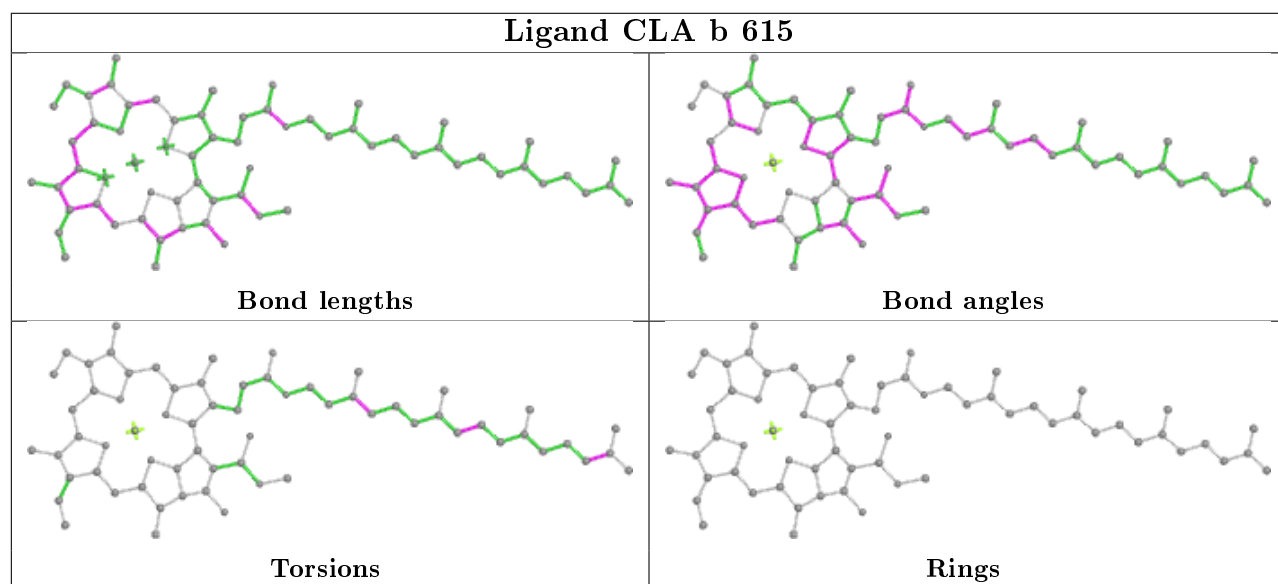
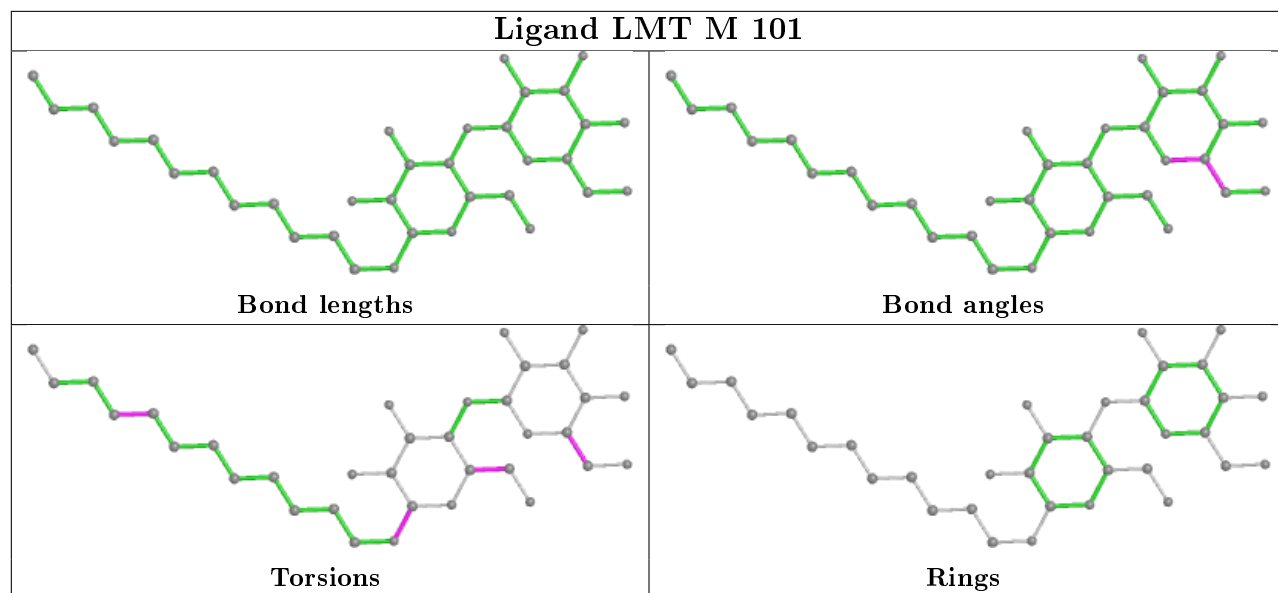
## Ligand HTG B 634

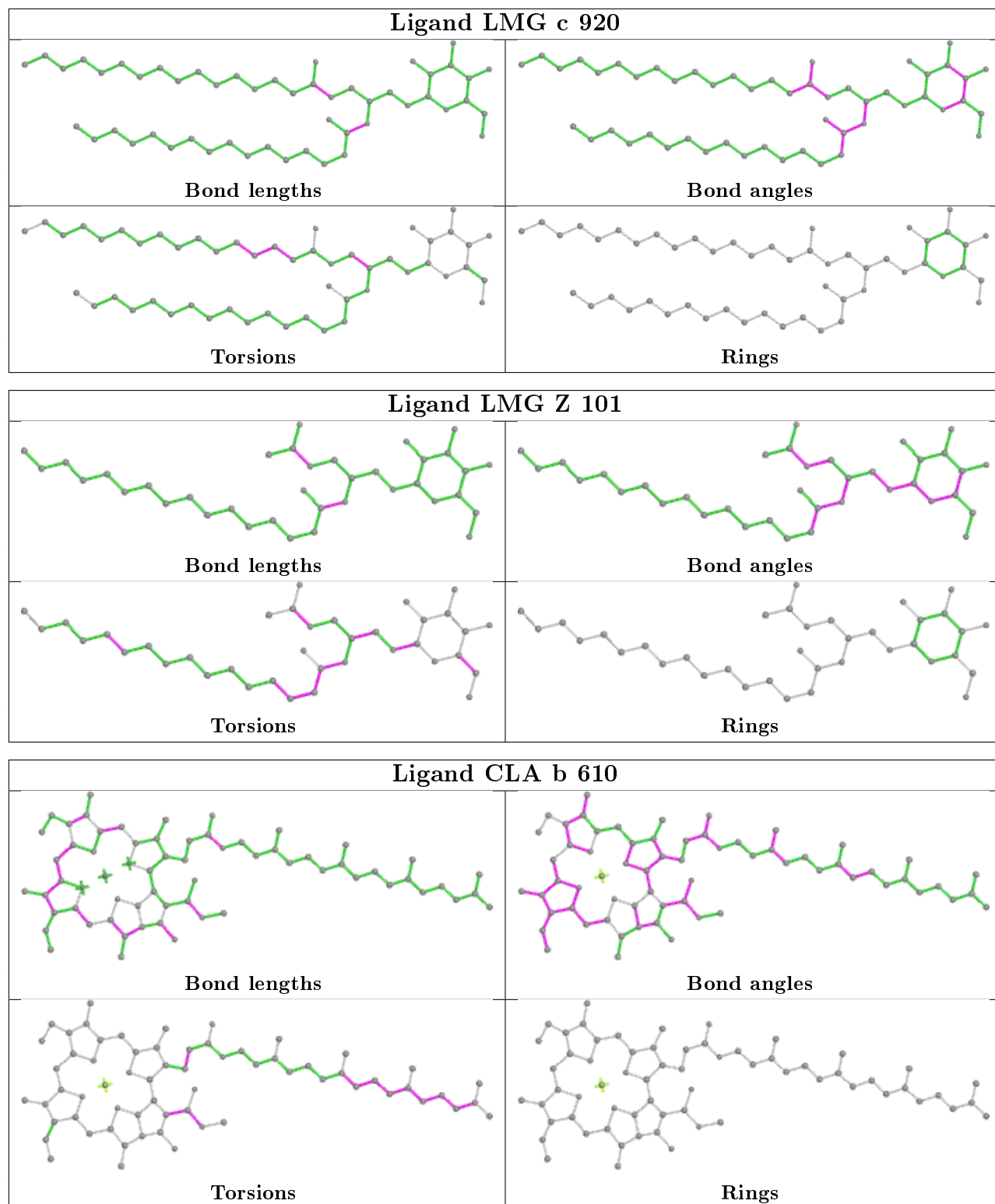


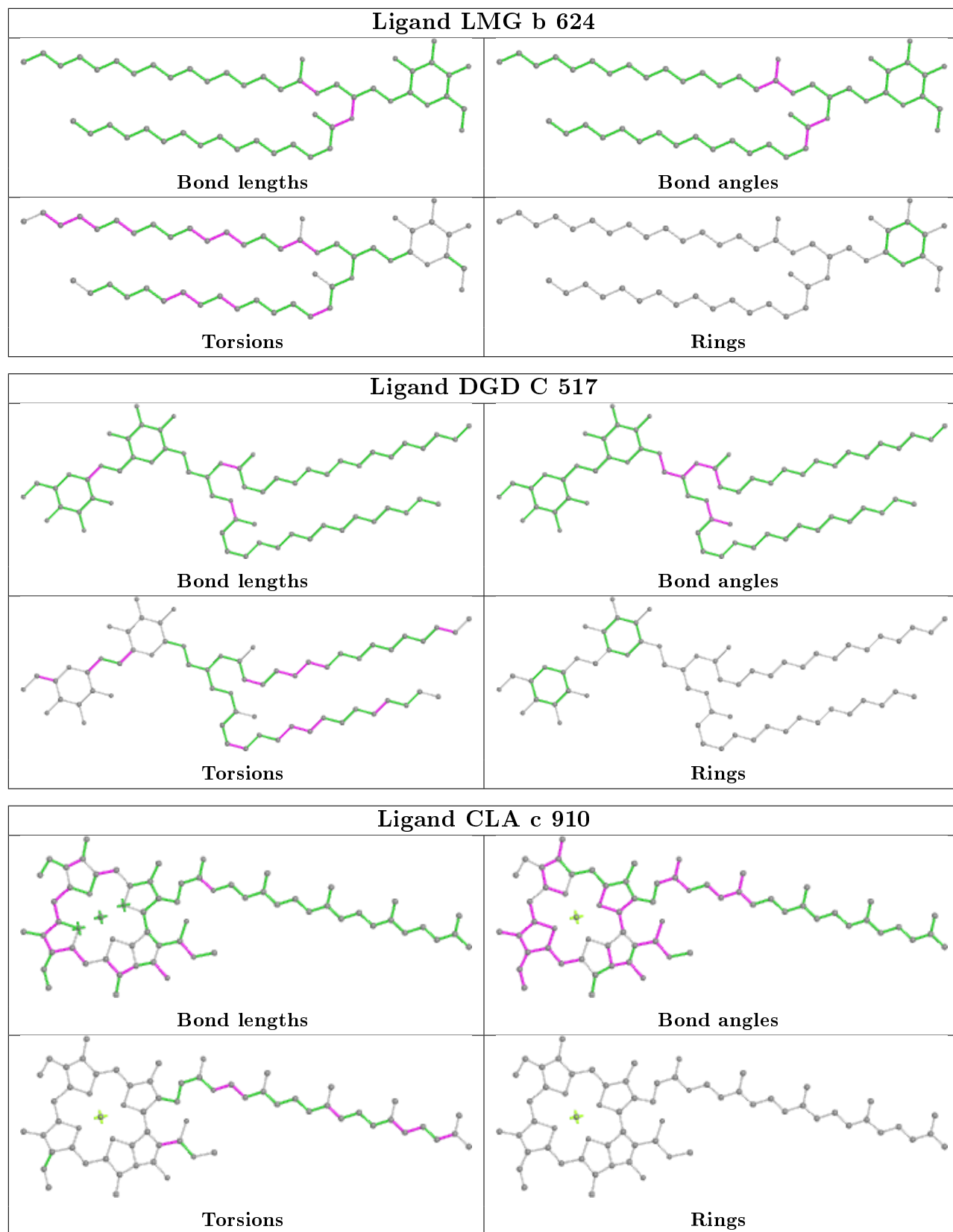
## Ligand CLA b 617

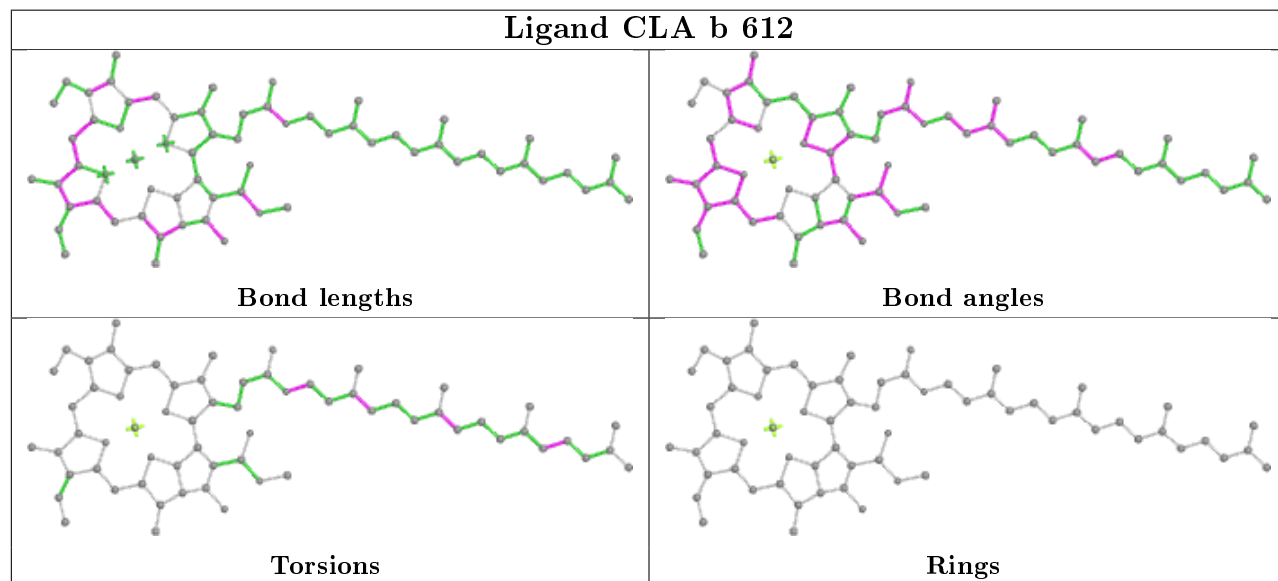
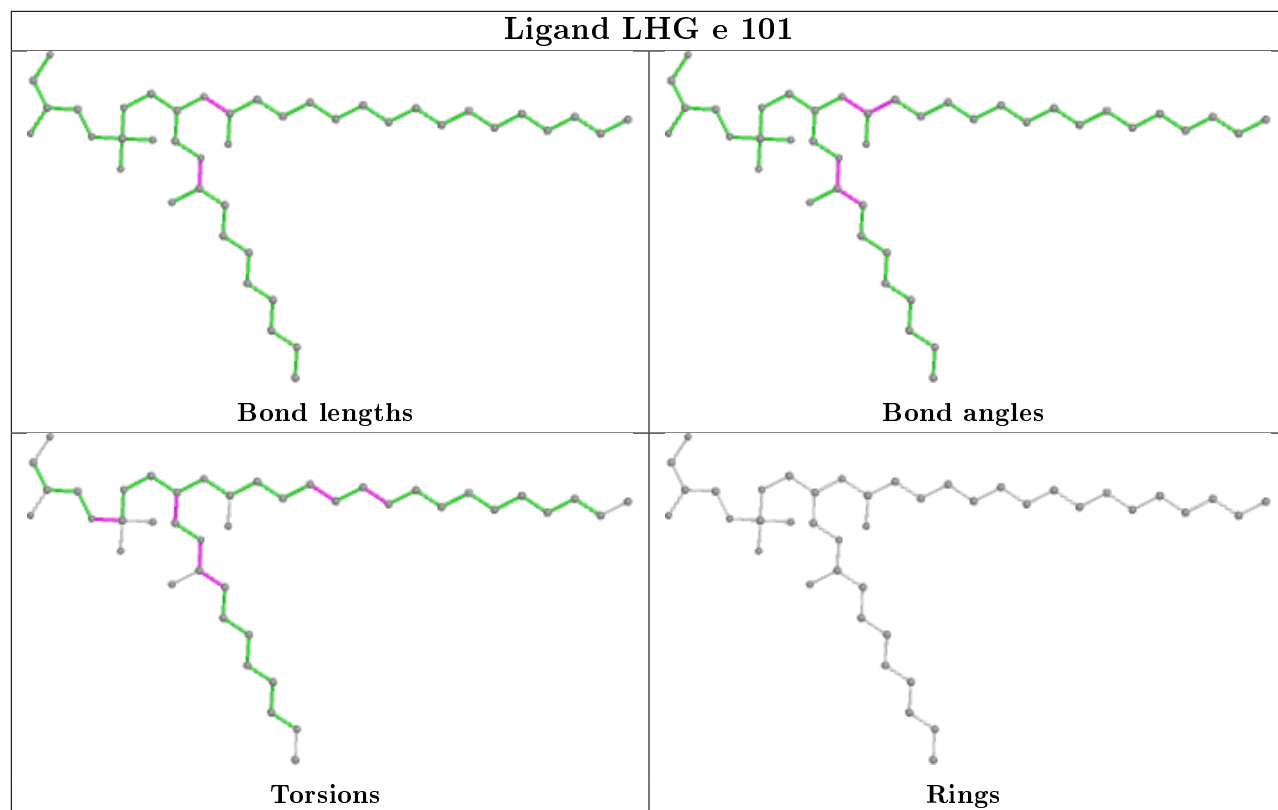


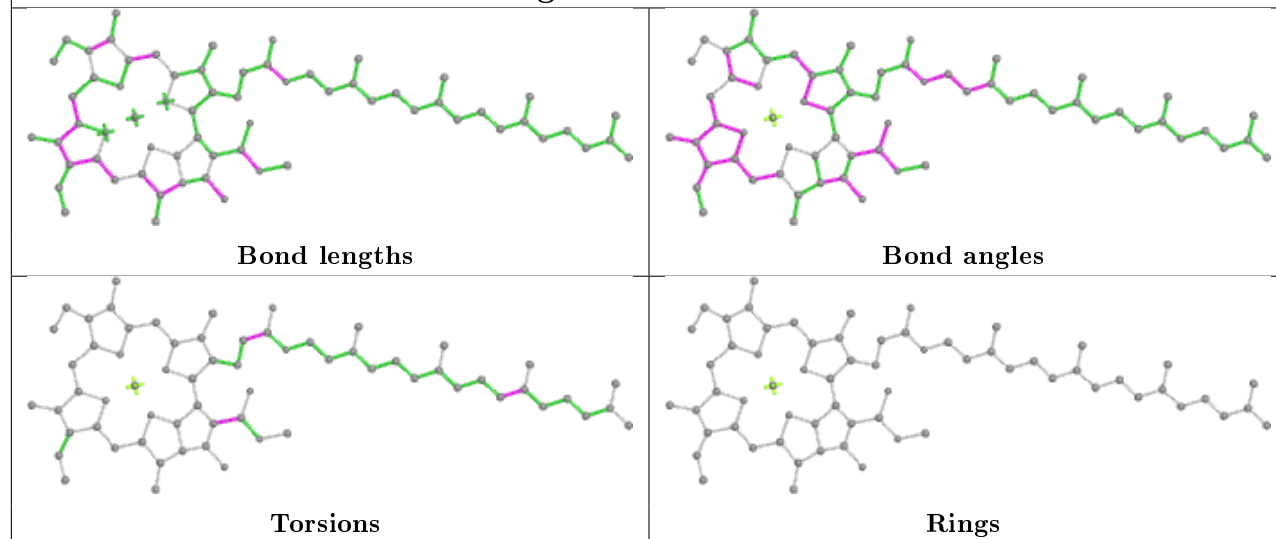
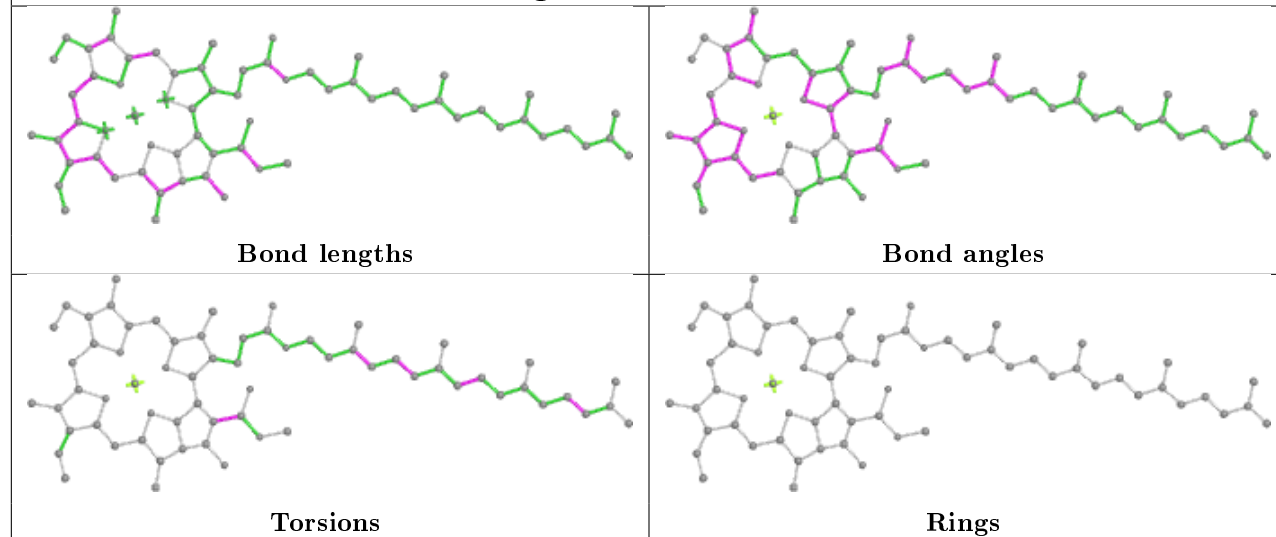


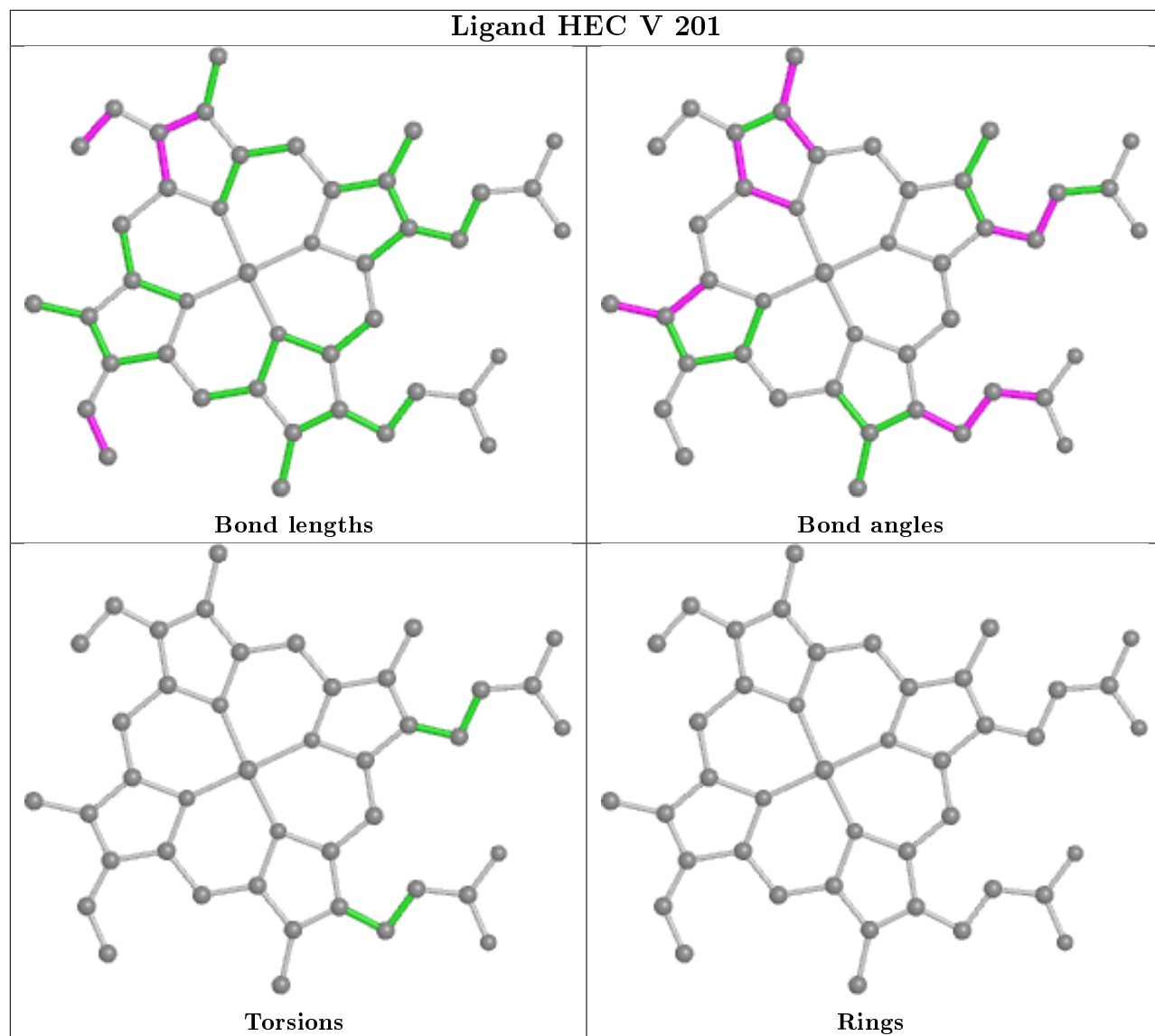






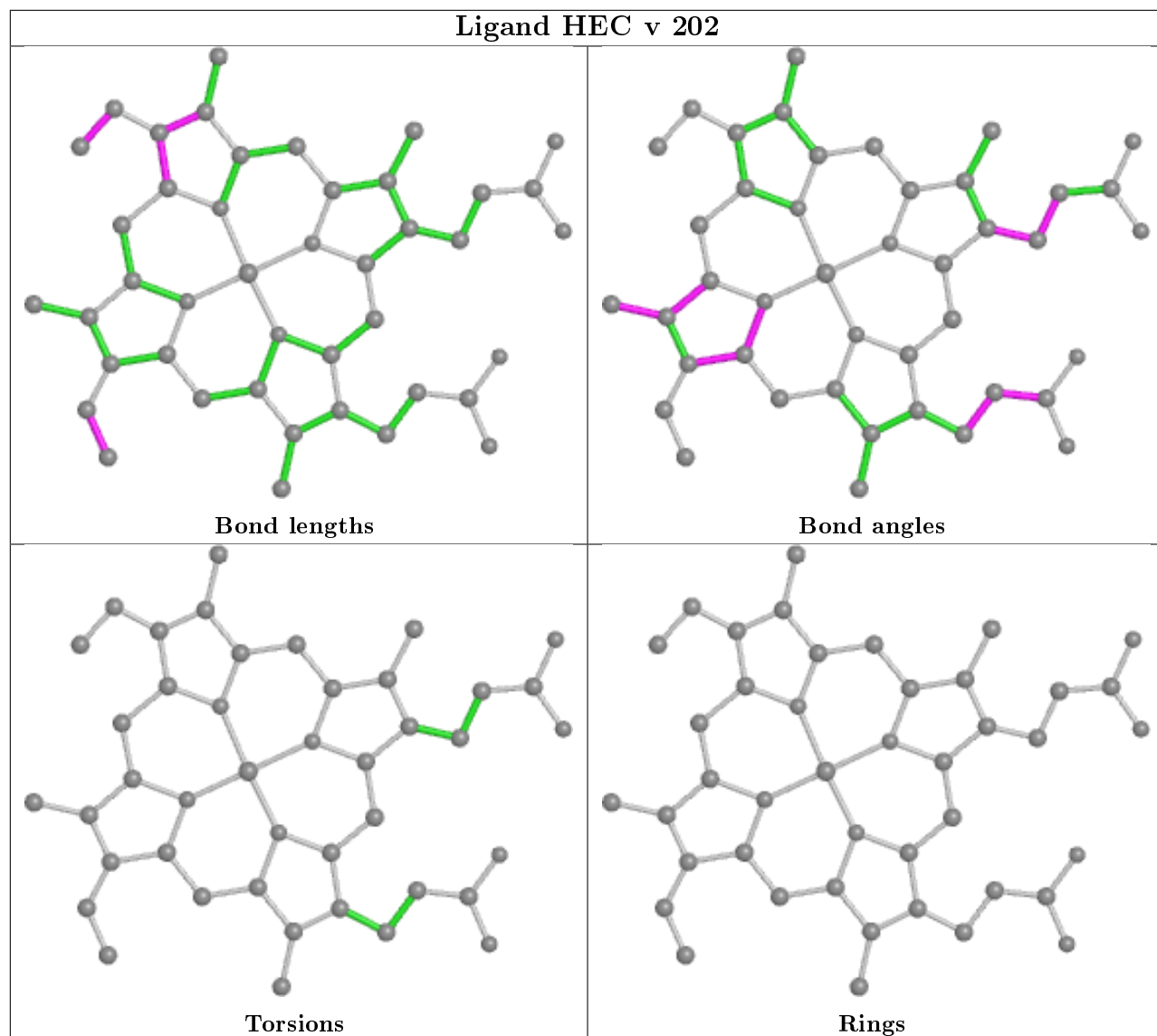


**Ligand CLA c 906****Ligand CLA C 504**

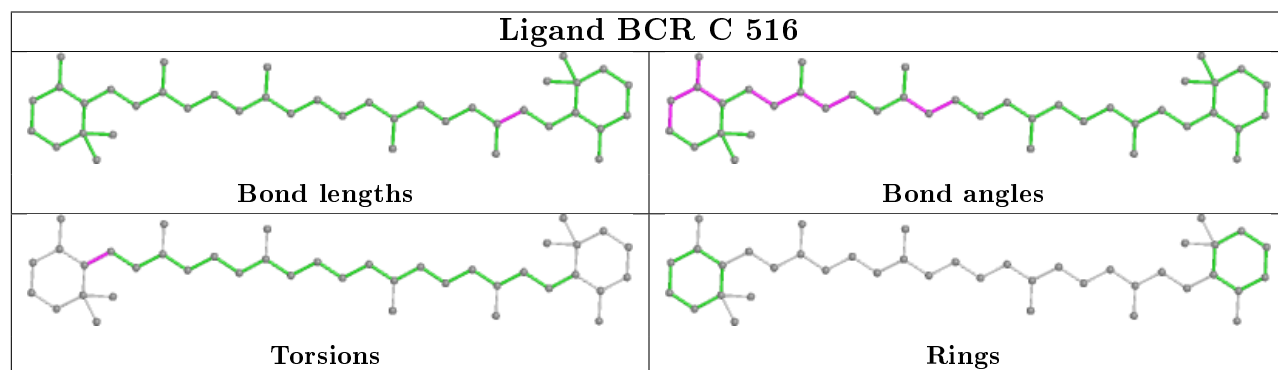




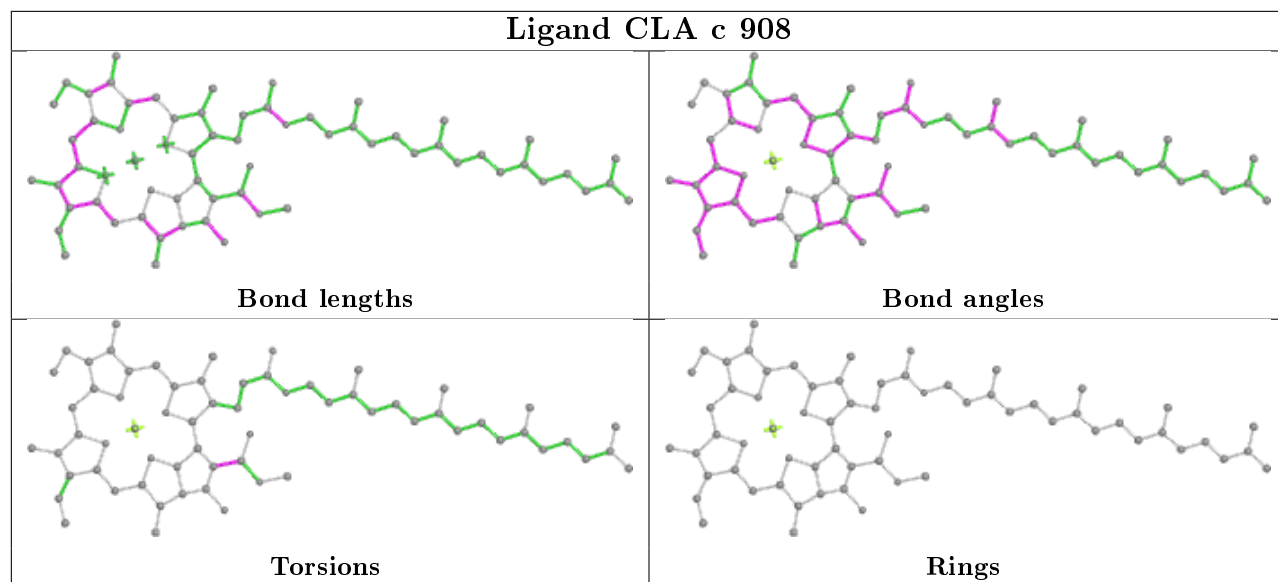
## Ligand HEC v 202



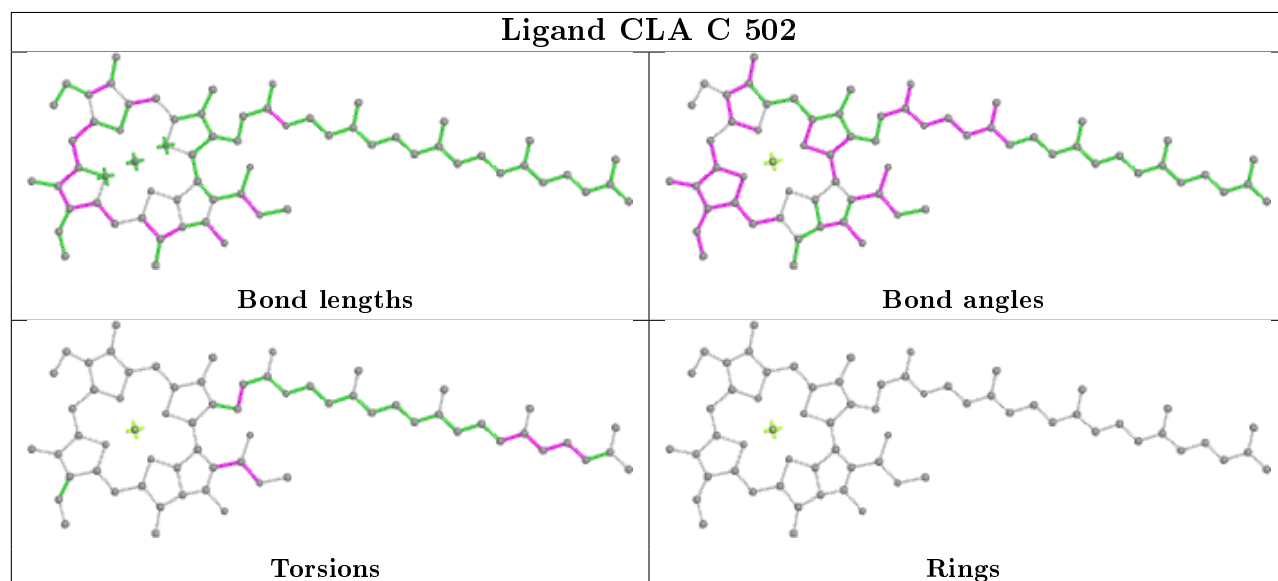
## Ligand BCR C 516



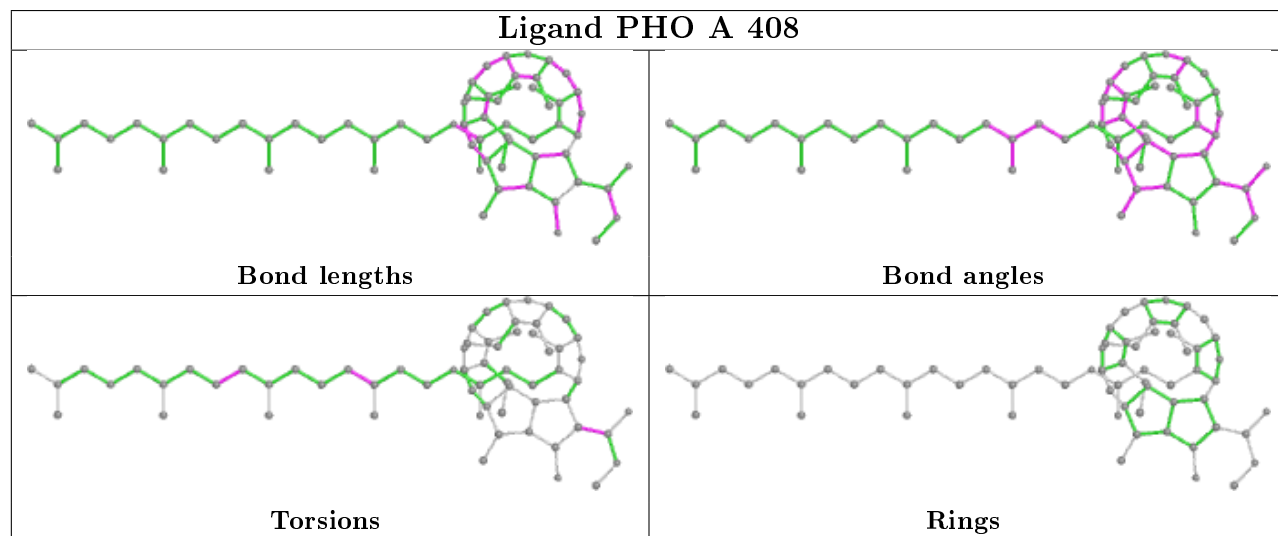
## Ligand CLA c 908

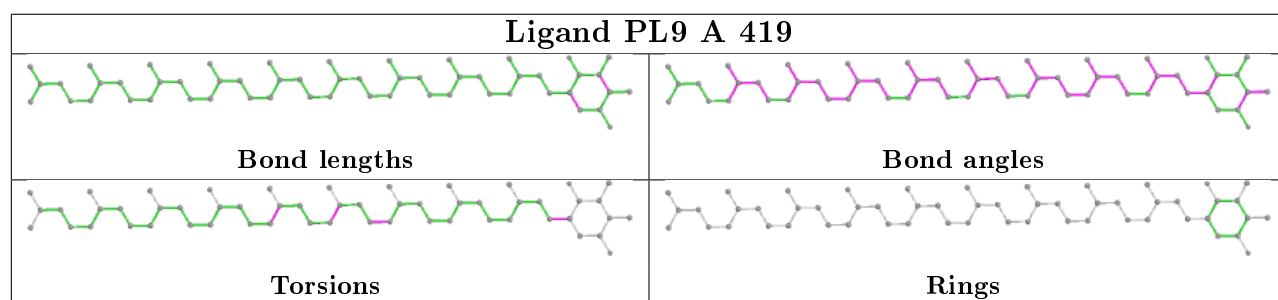
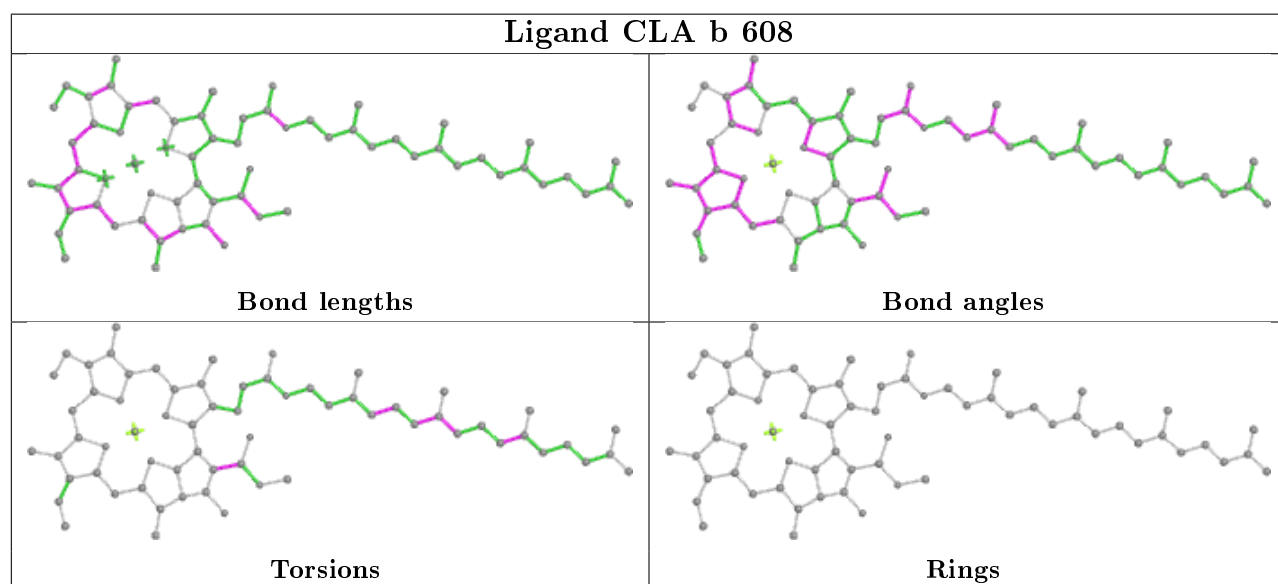
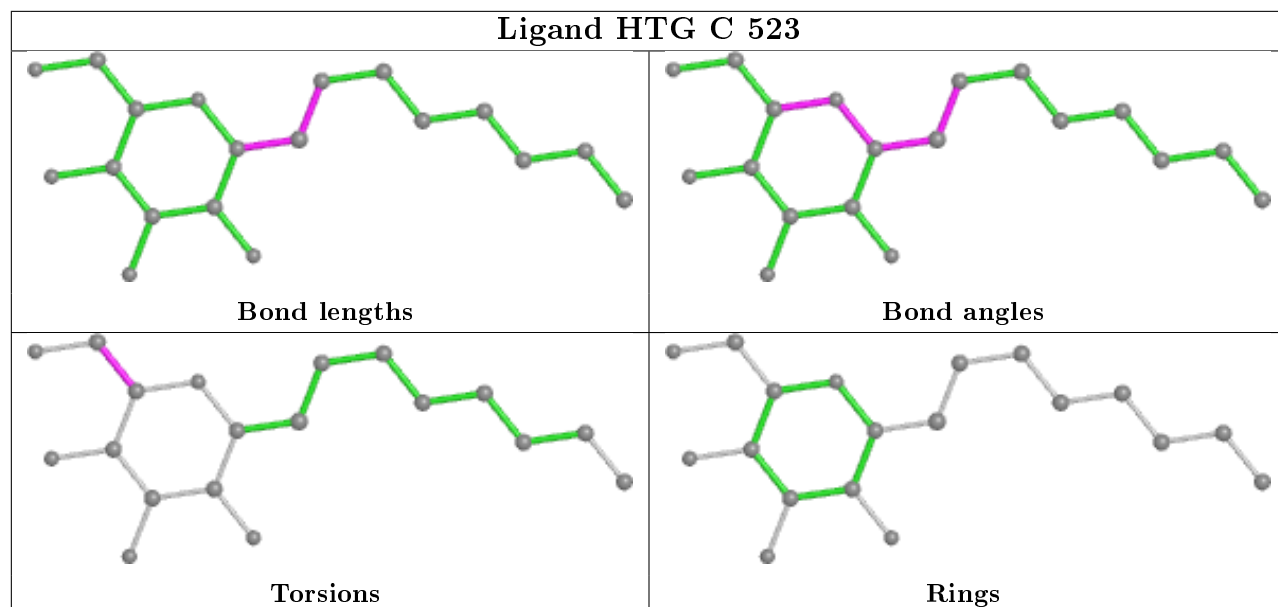


## Ligand CLA C 502

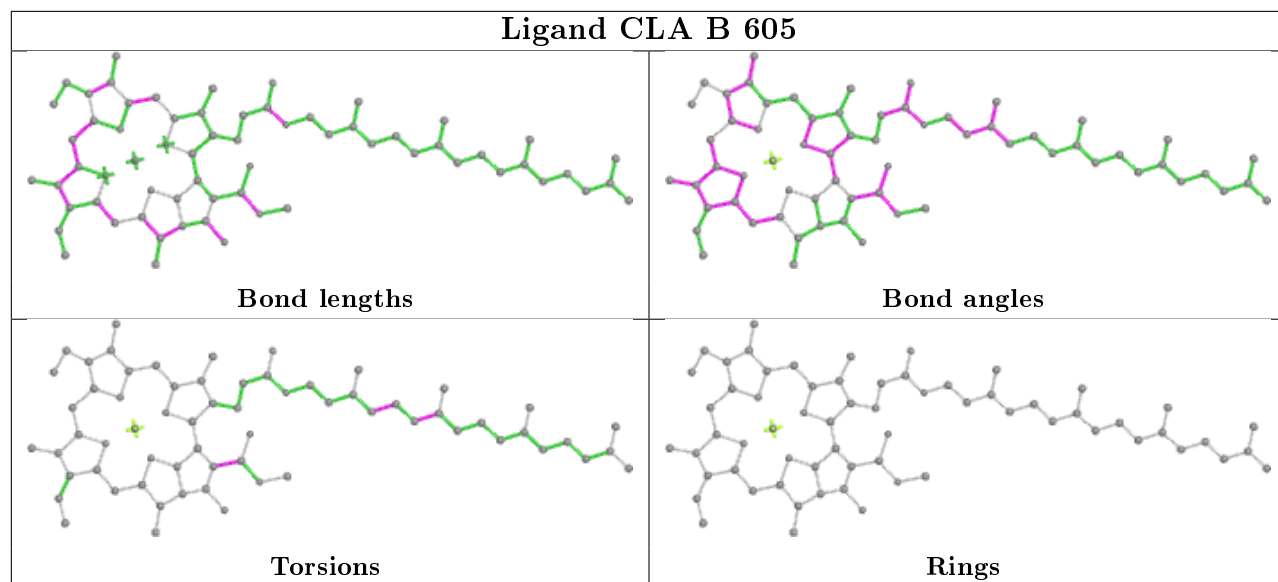


## Ligand PHO A 408

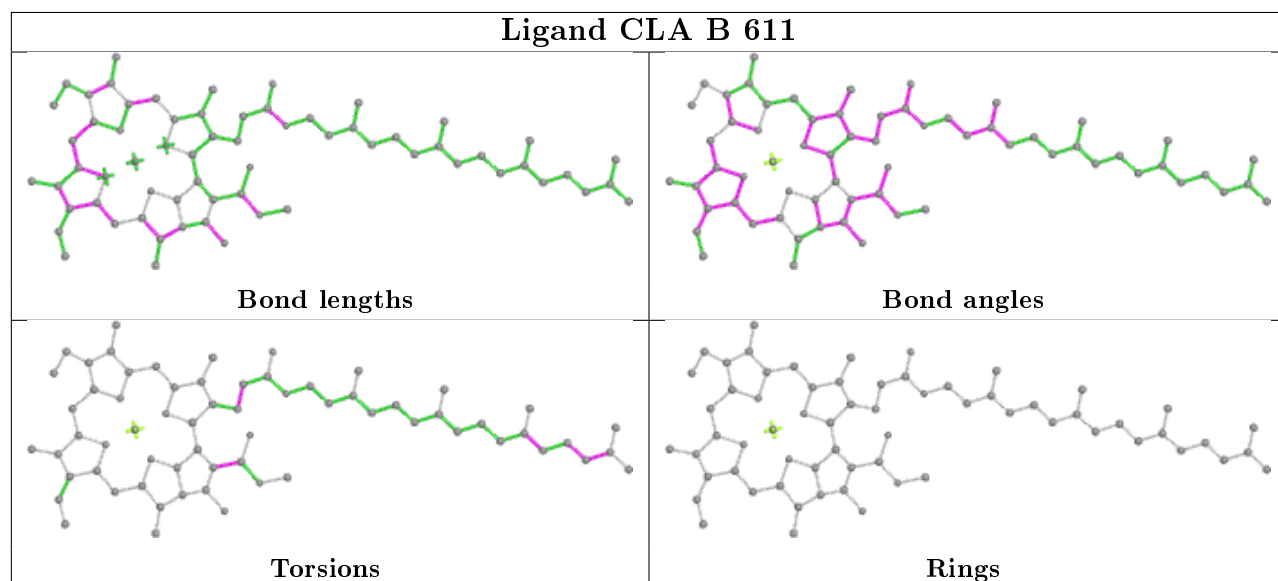




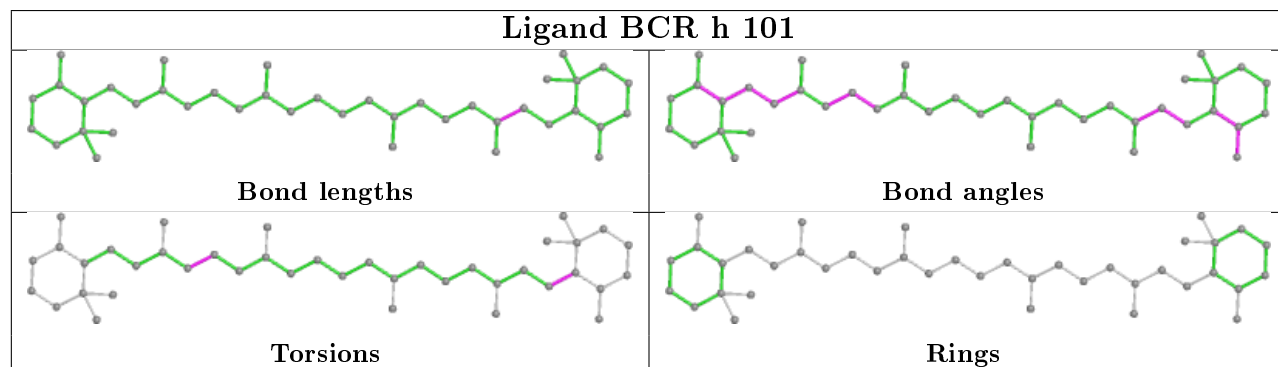
## Ligand CLA B 605

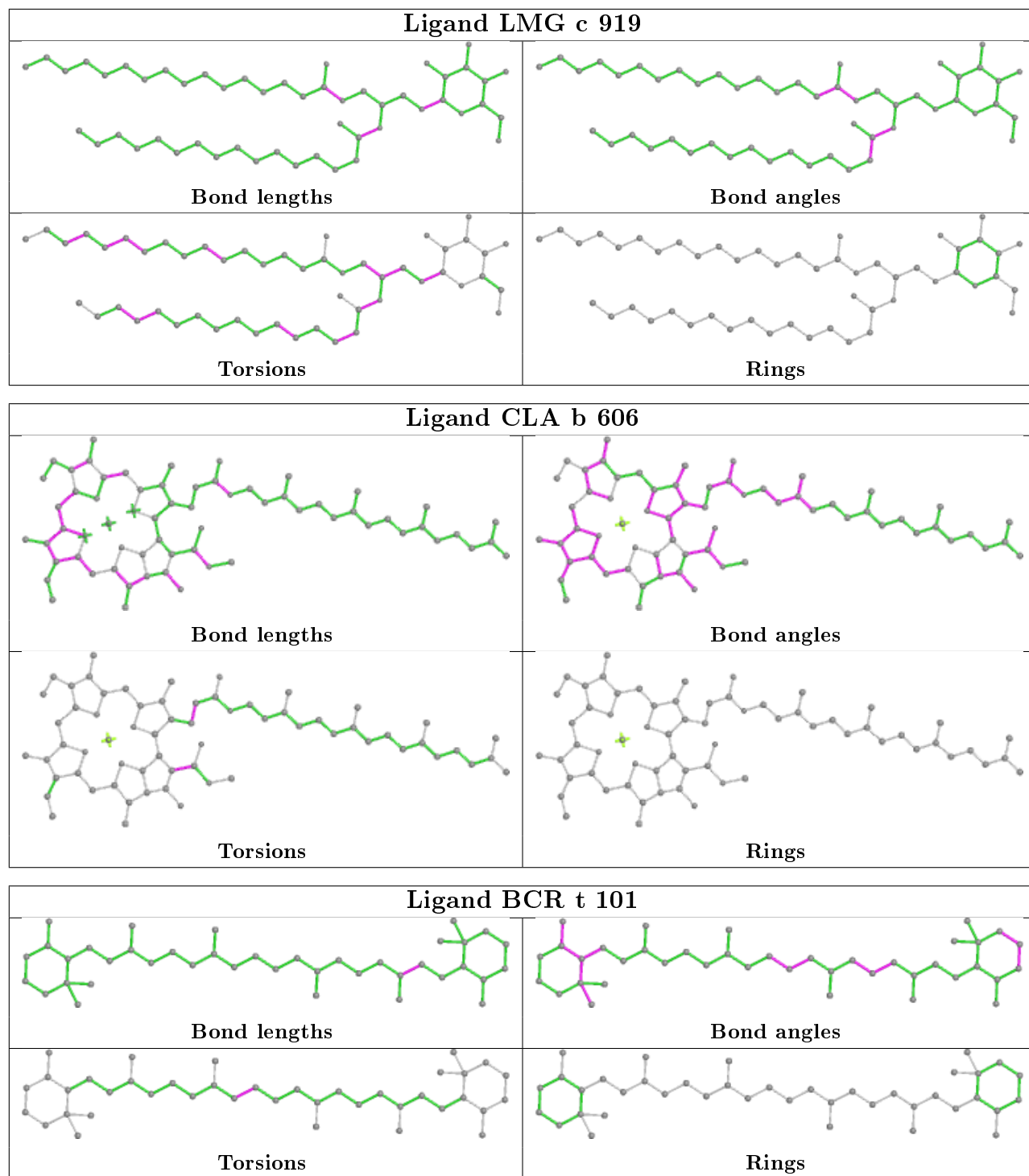


## Ligand CLA B 611

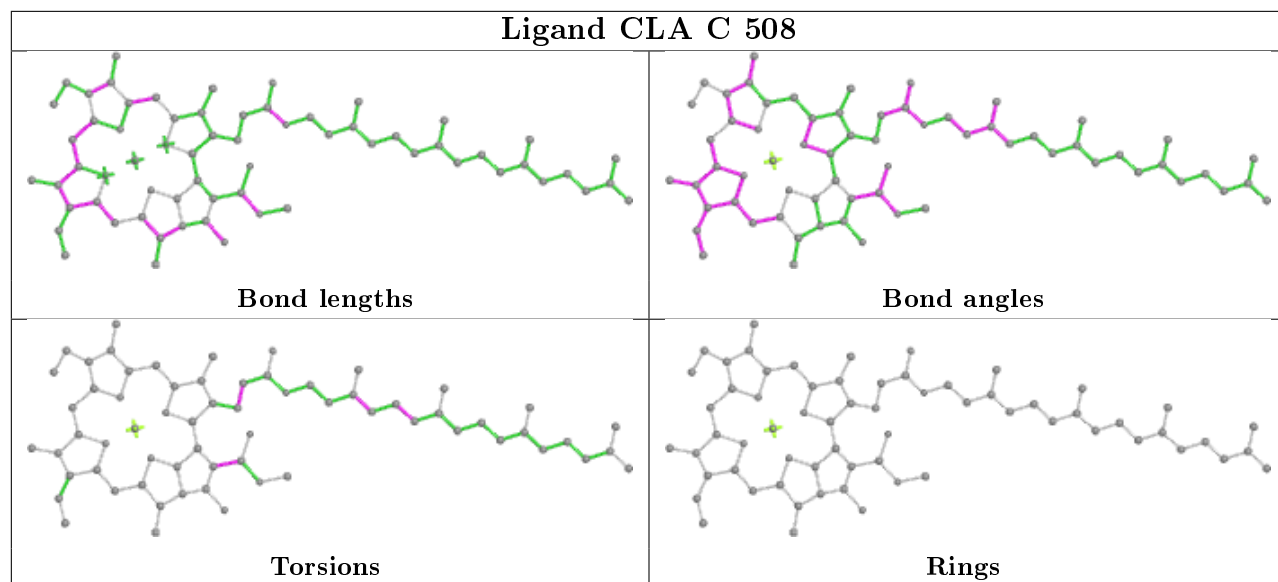


## Ligand BCR h 101

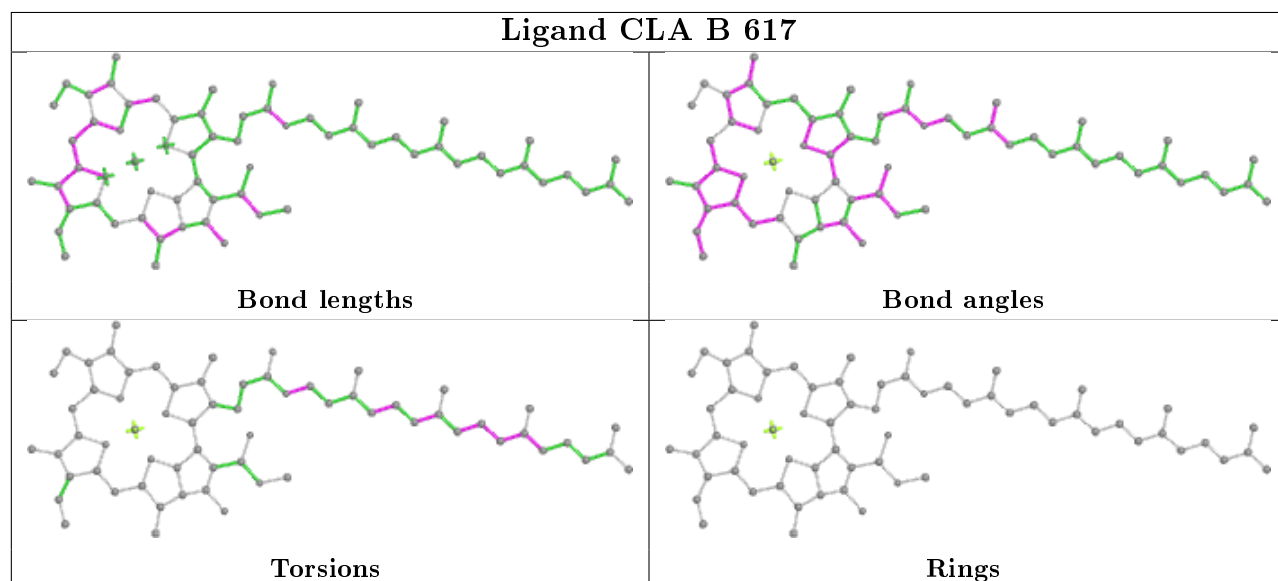




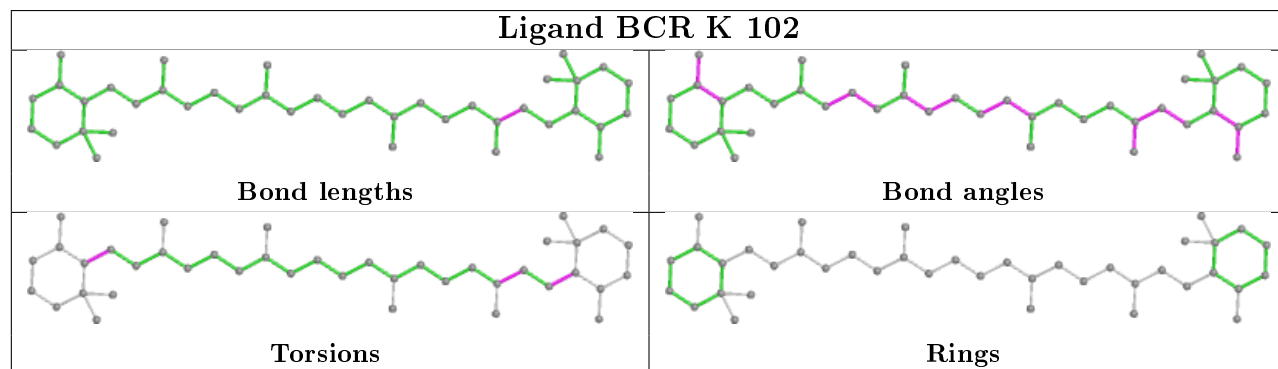
## Ligand CLA C 508

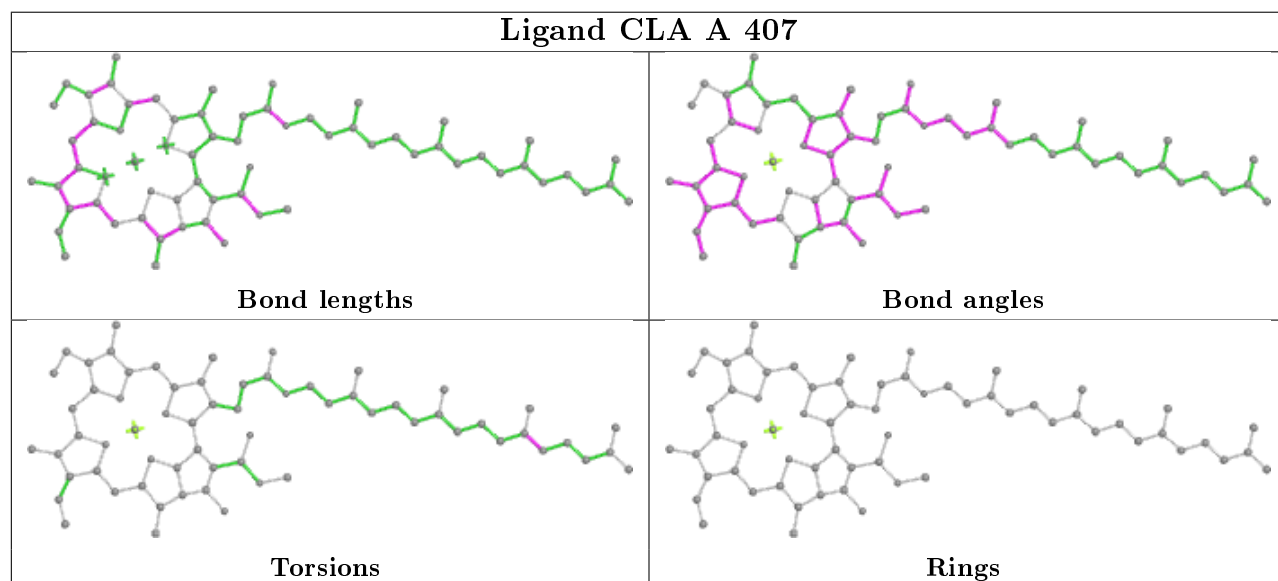
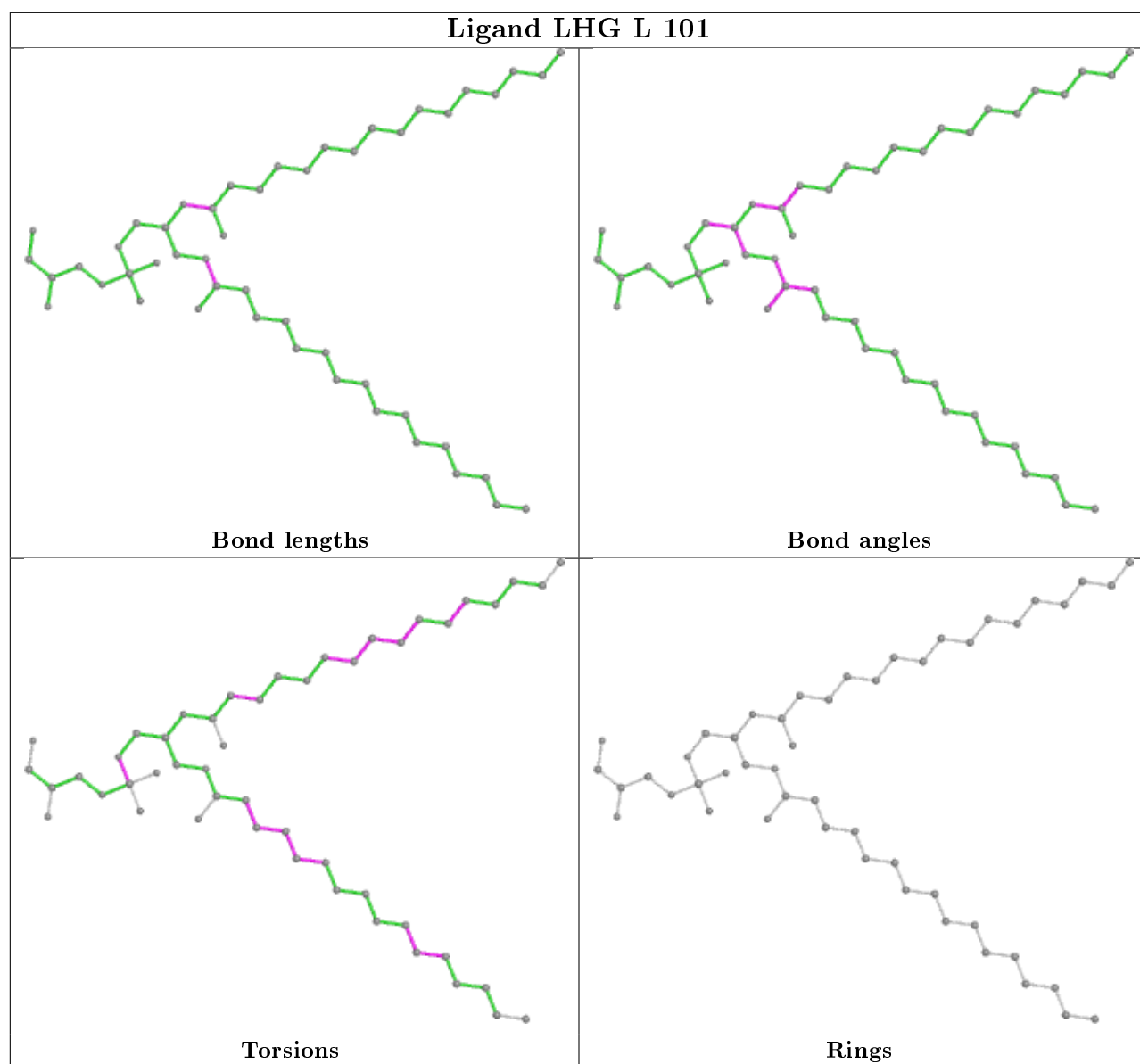


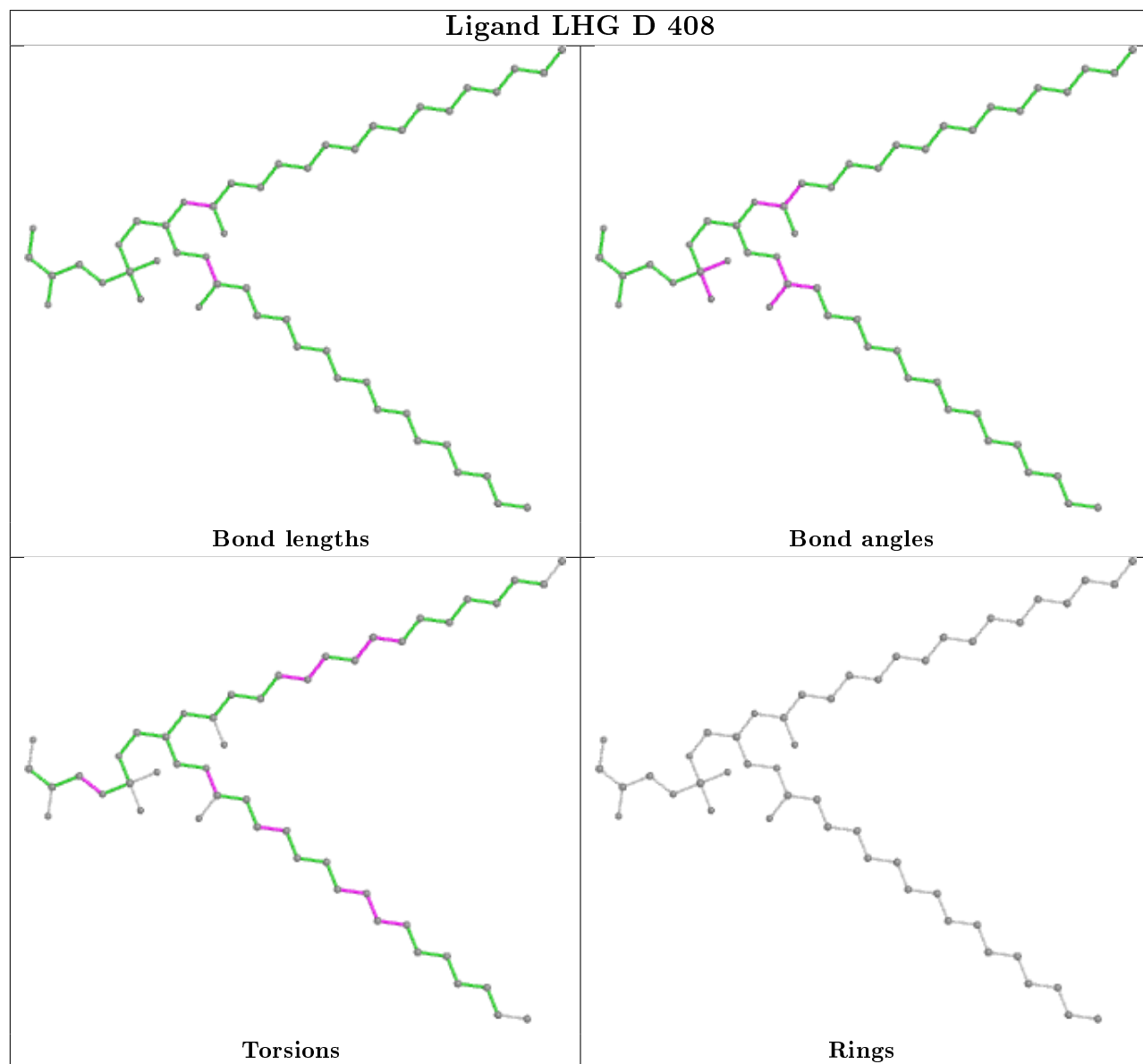
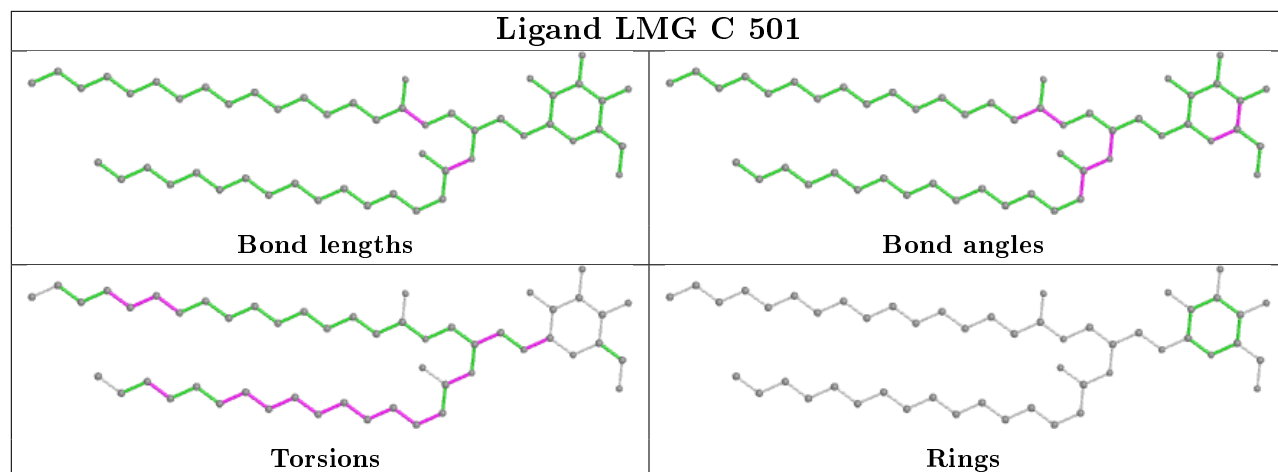
## Ligand CLA B 617



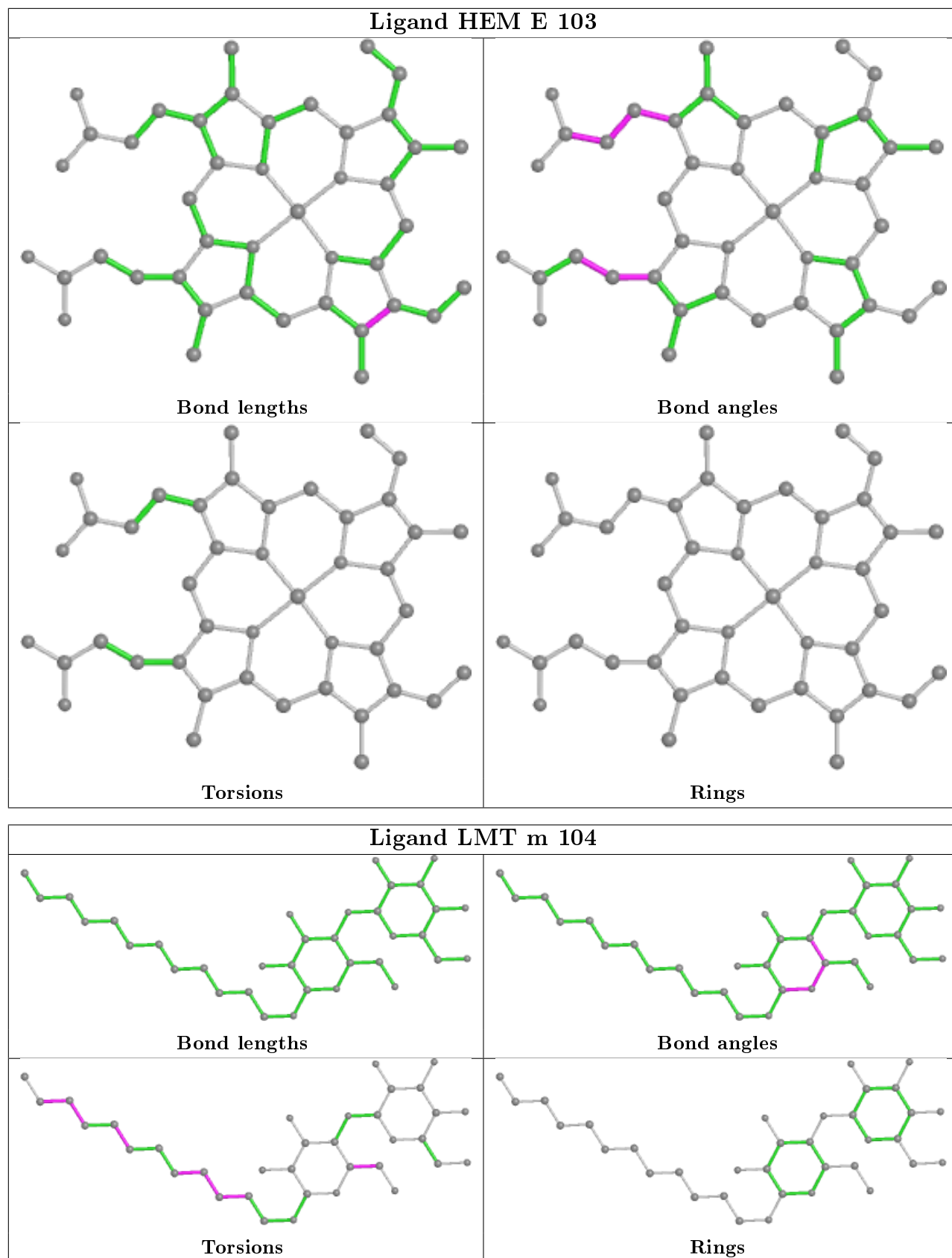
## Ligand BCR K 102



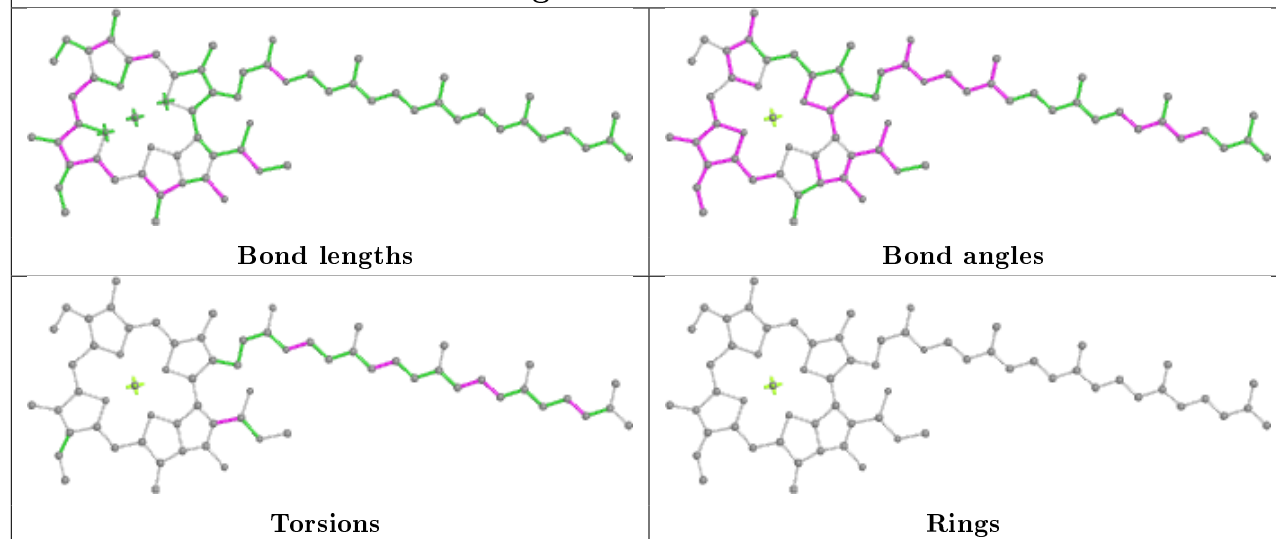




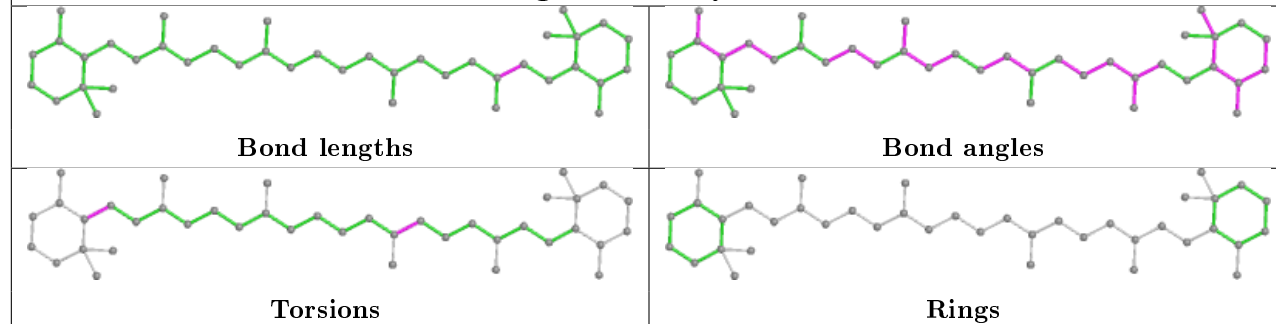




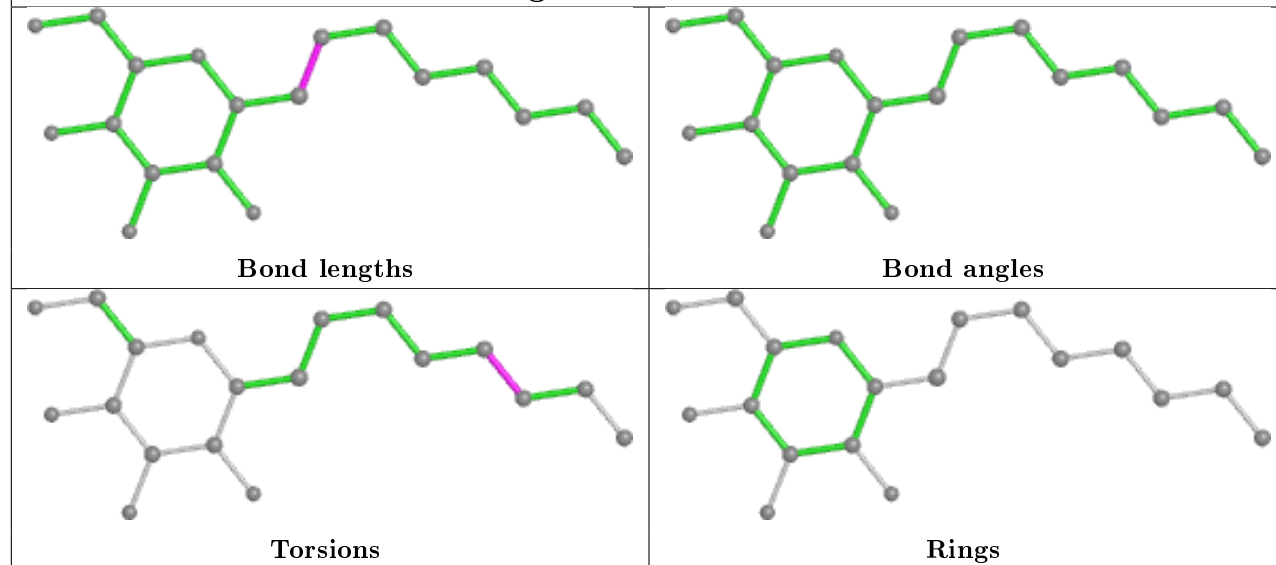
## Ligand CLA C 510

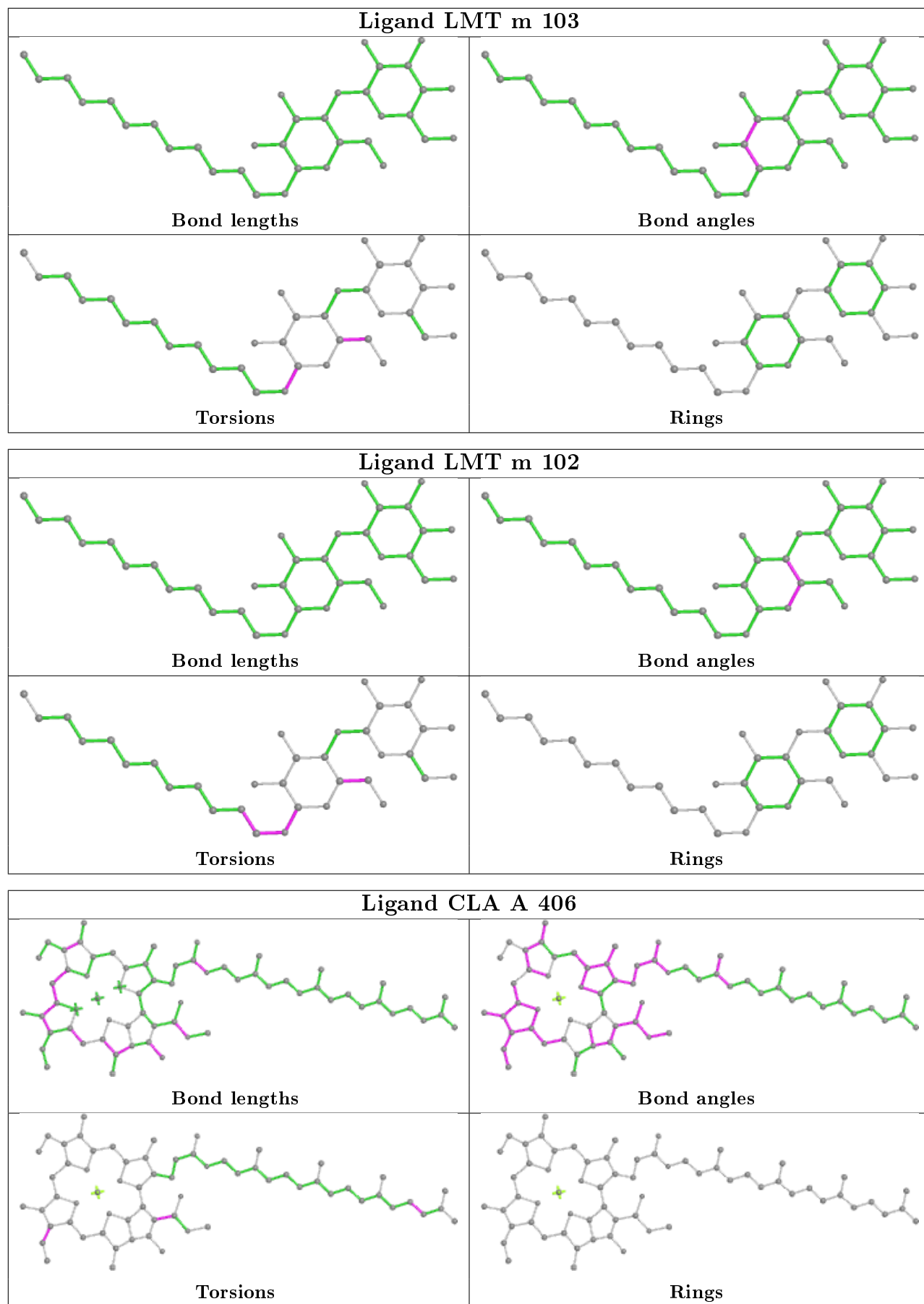


## Ligand BCR y 101

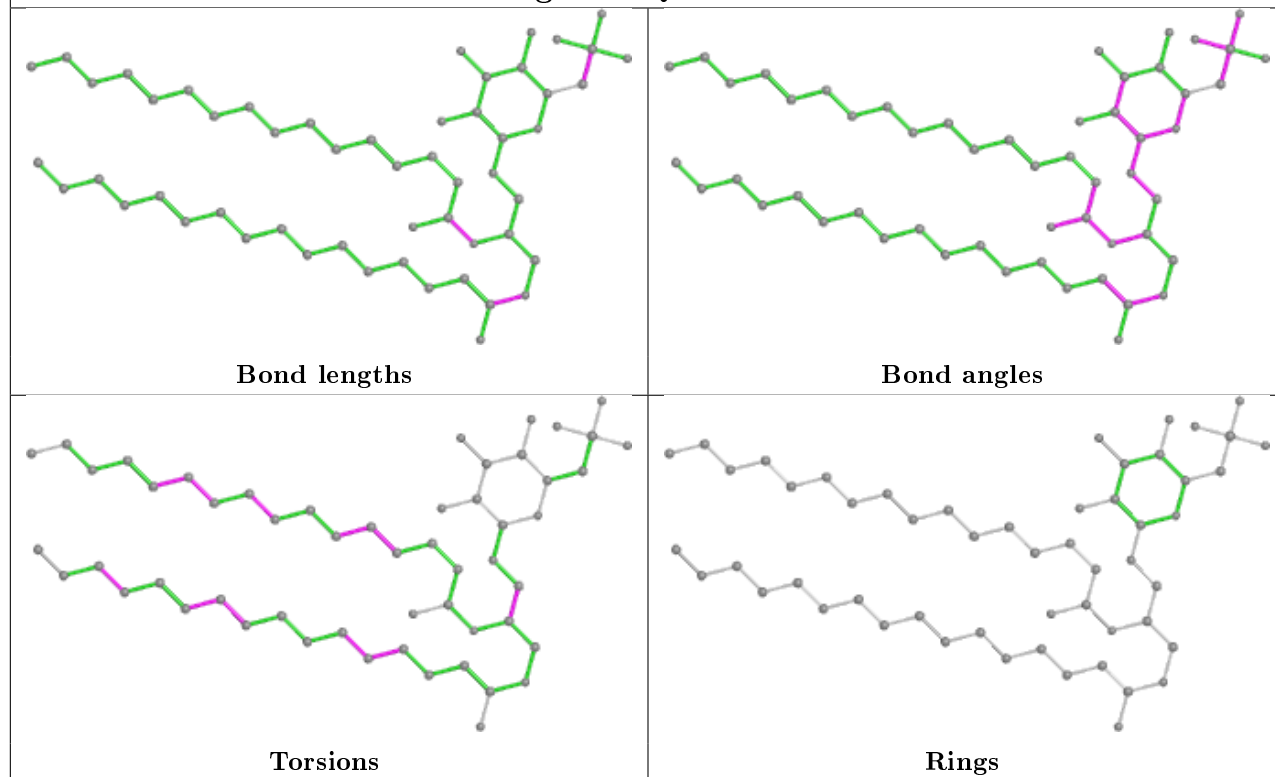


## Ligand HTG O 303

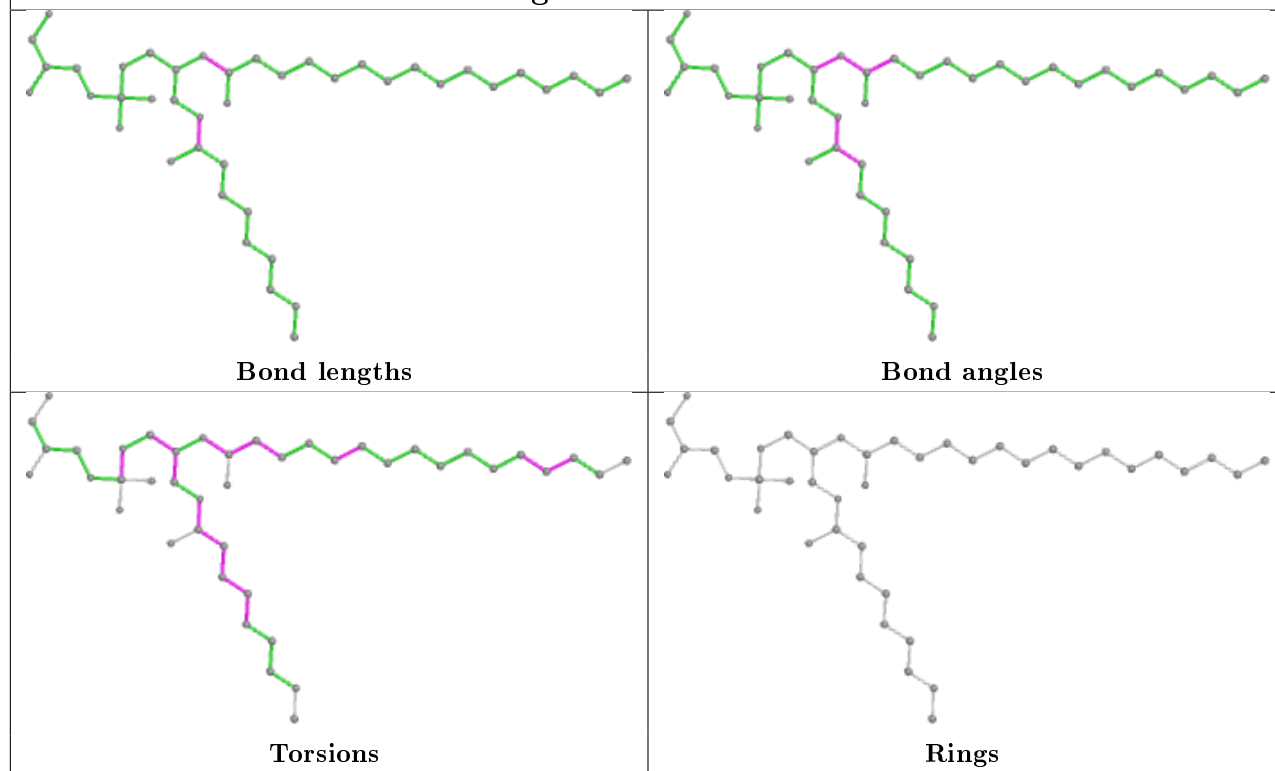


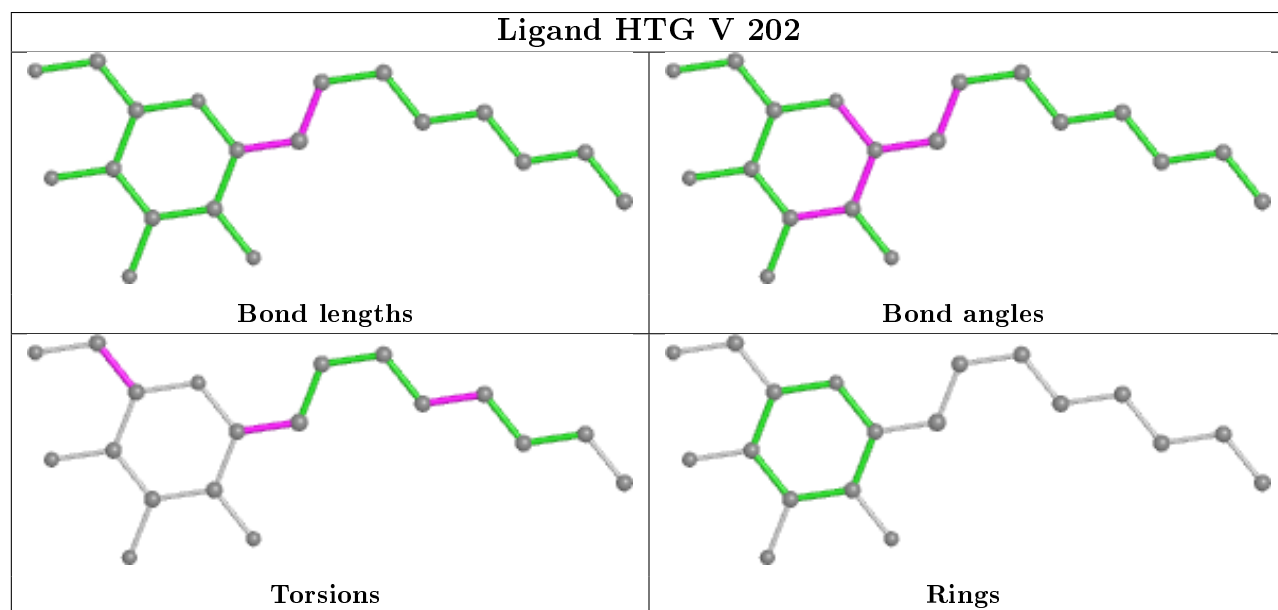
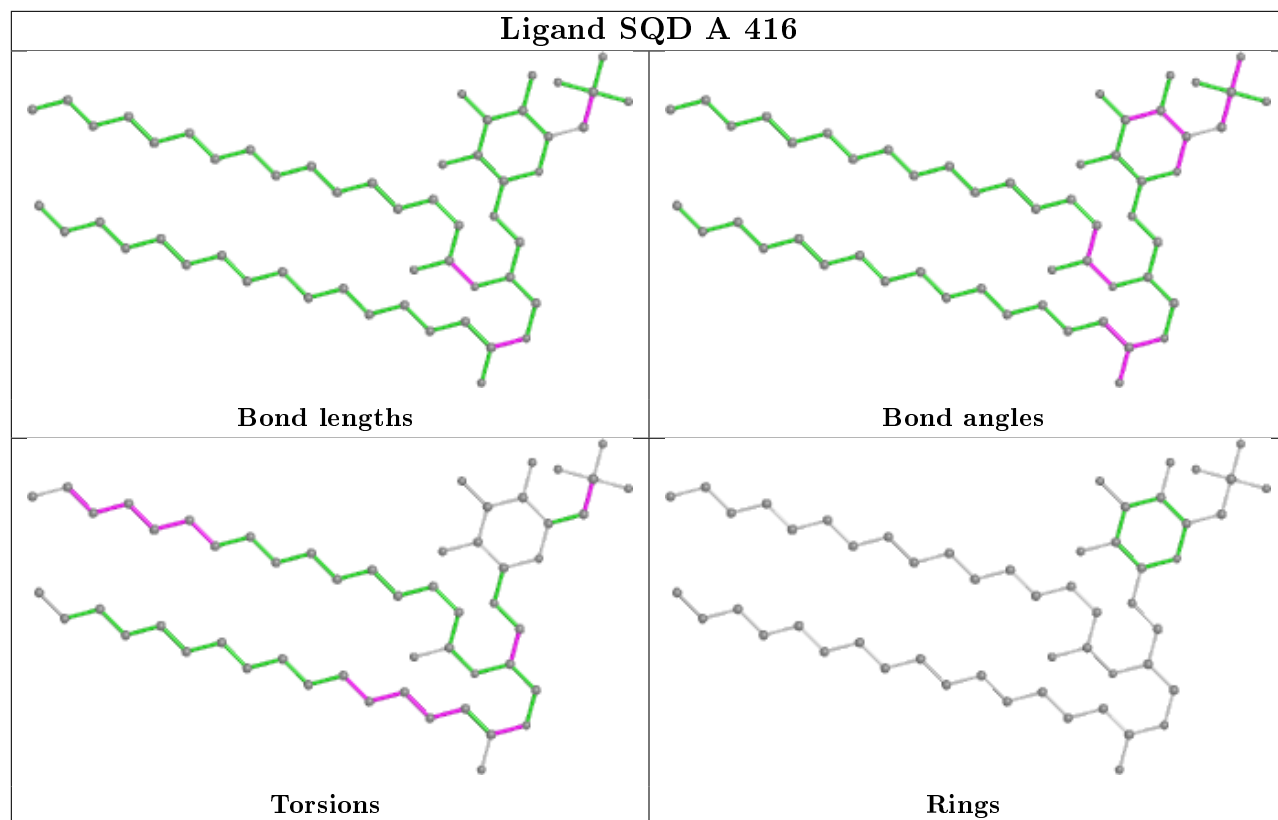


## Ligand SQD a 411

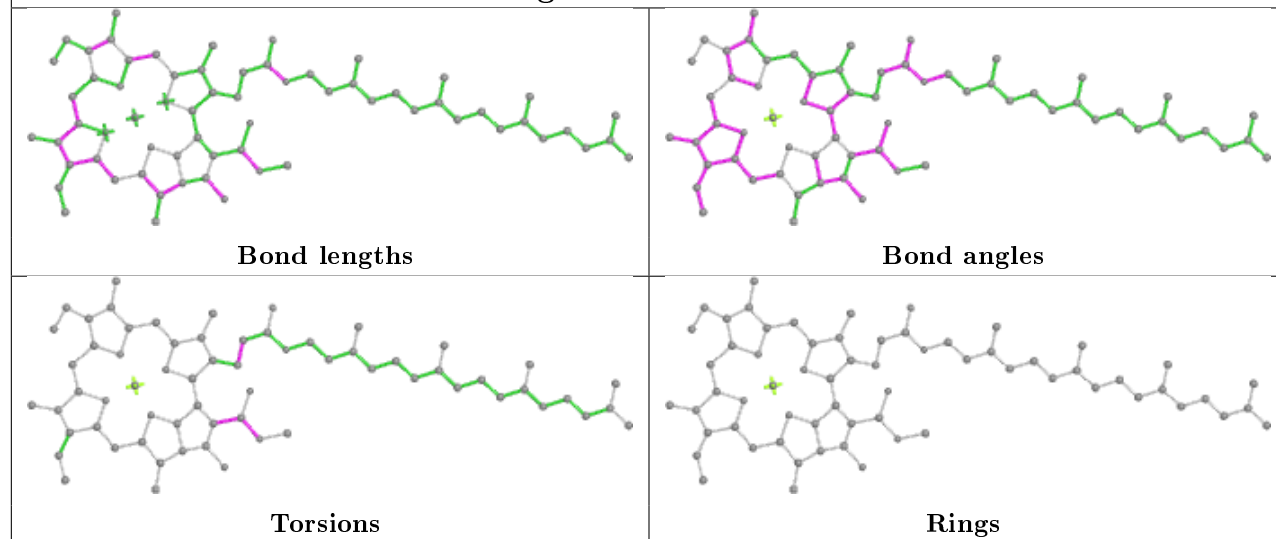


## Ligand LHG E 101

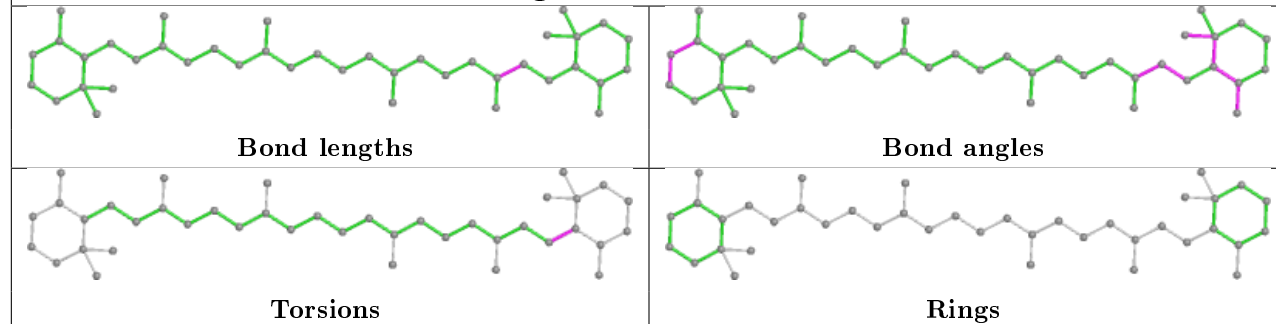




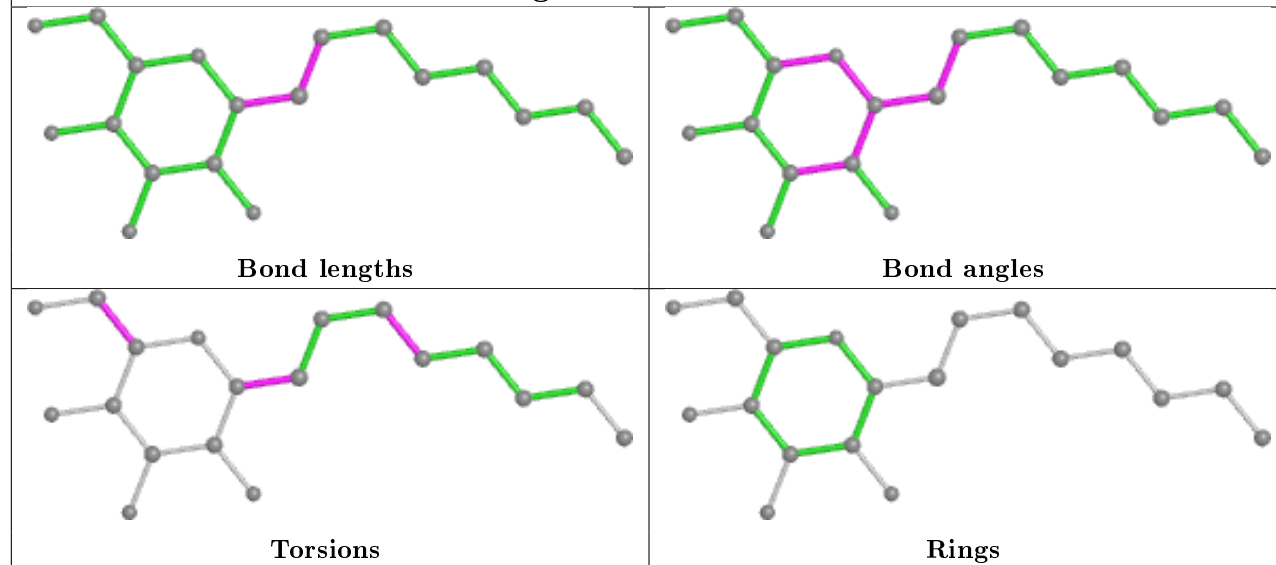
## Ligand CLA c 902

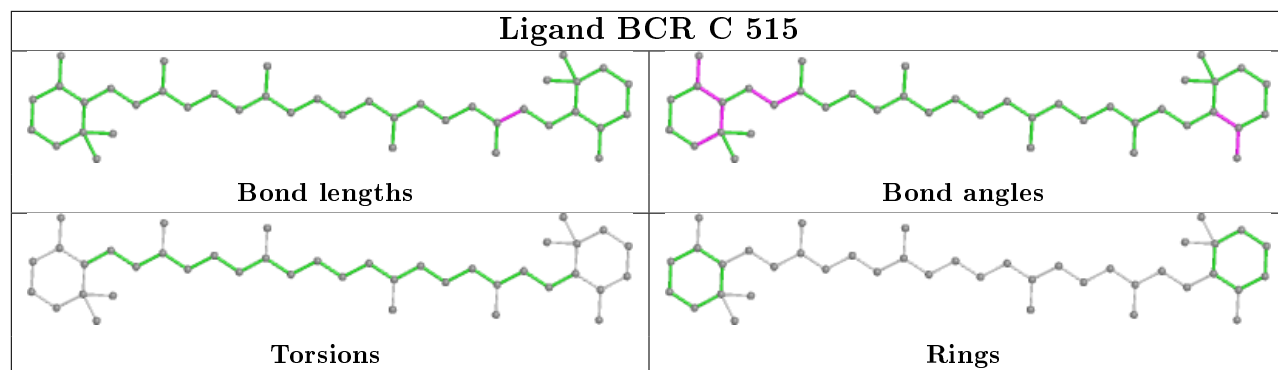
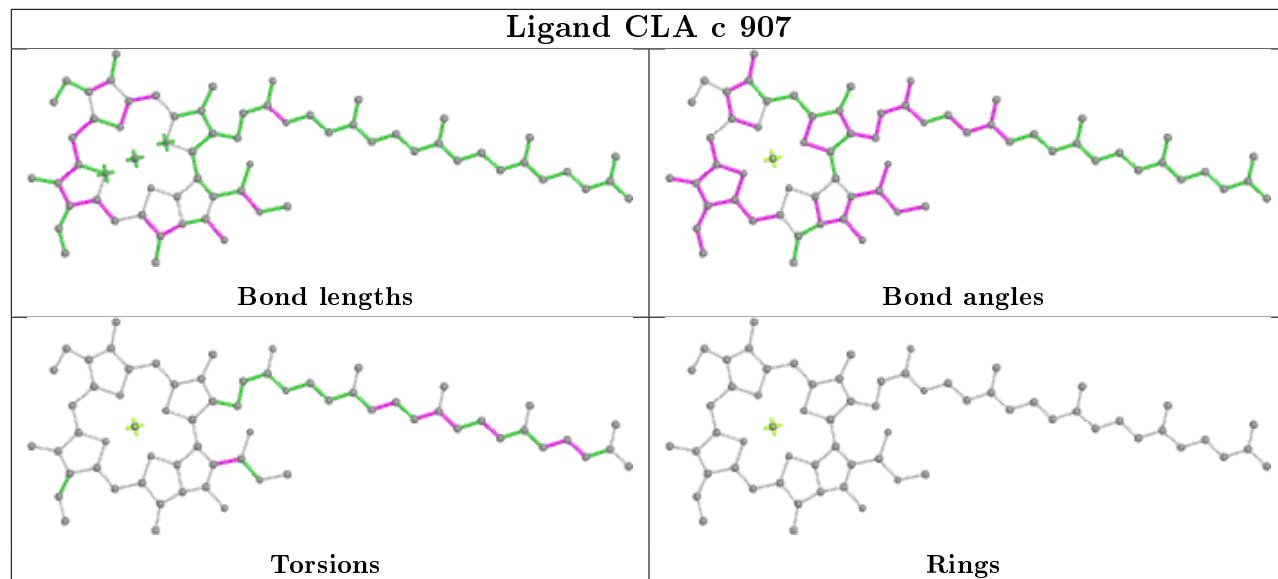
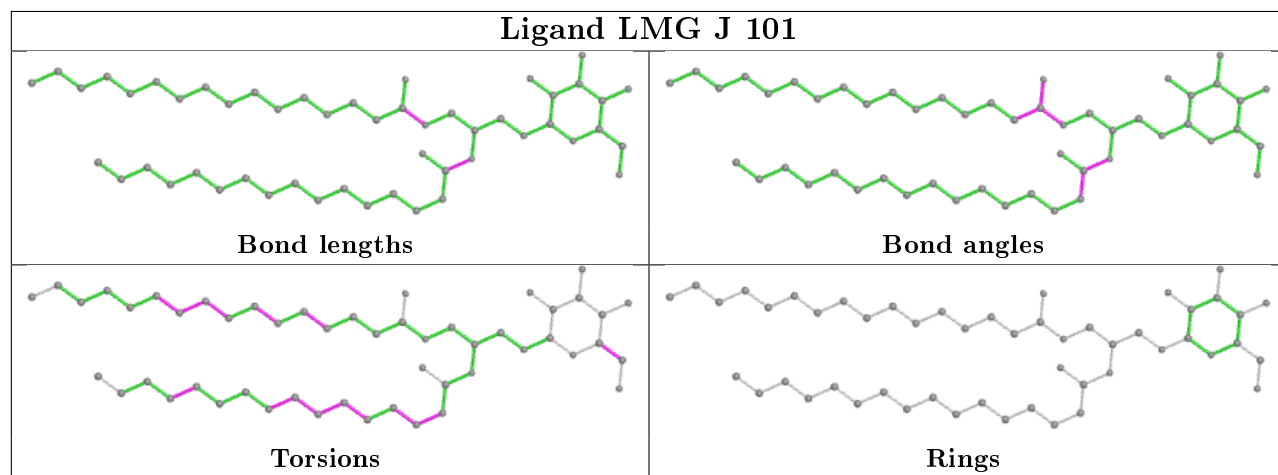


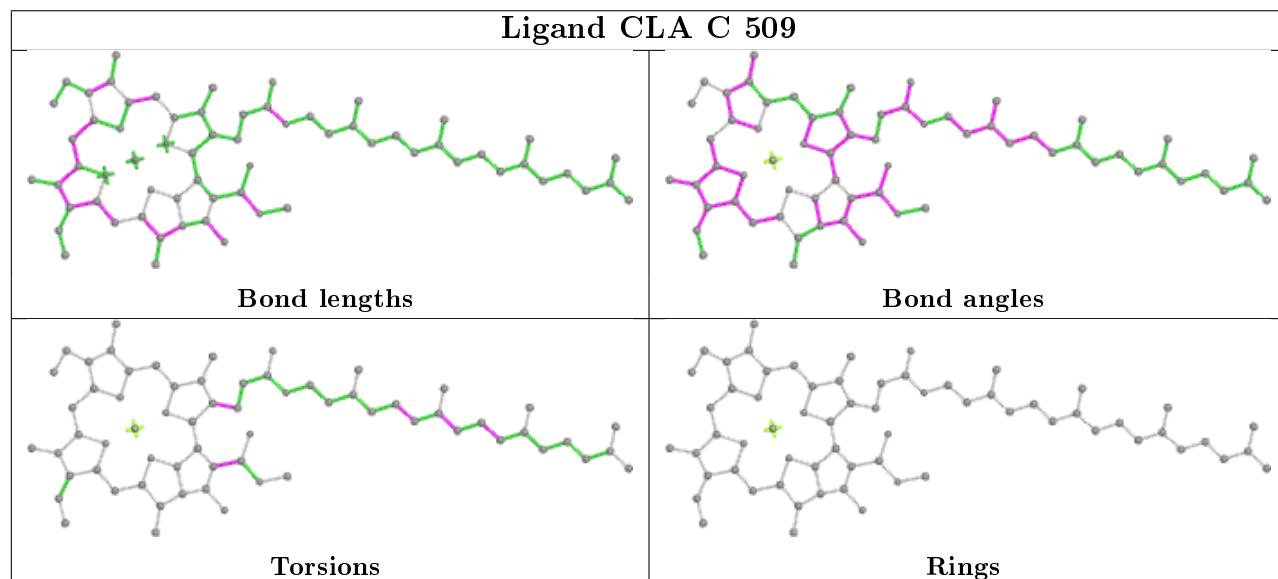
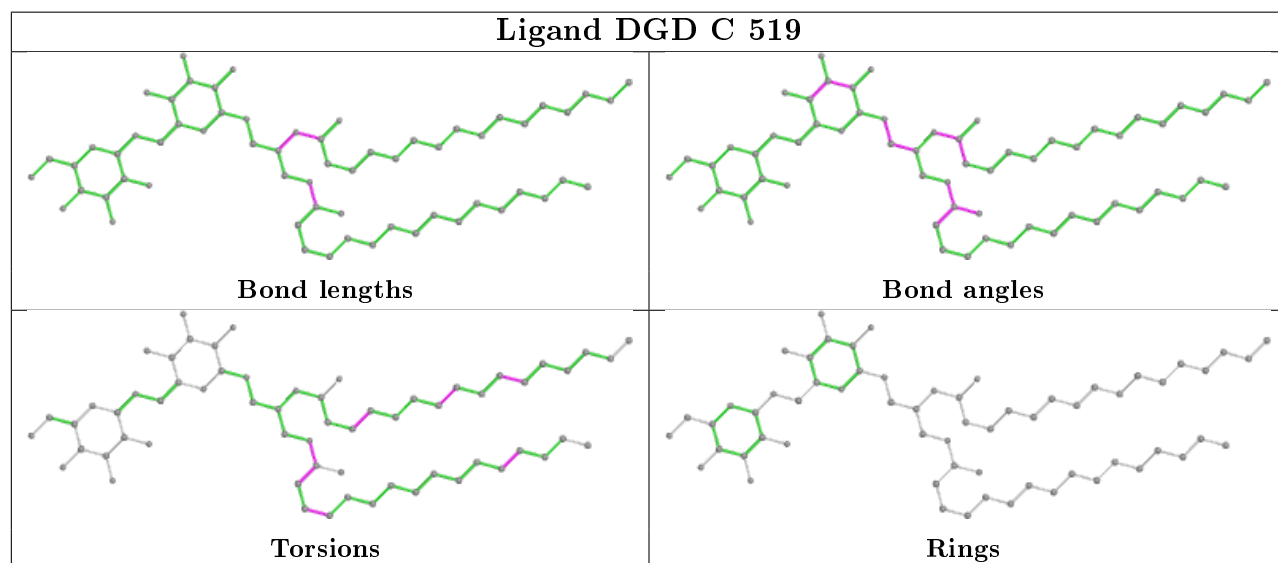
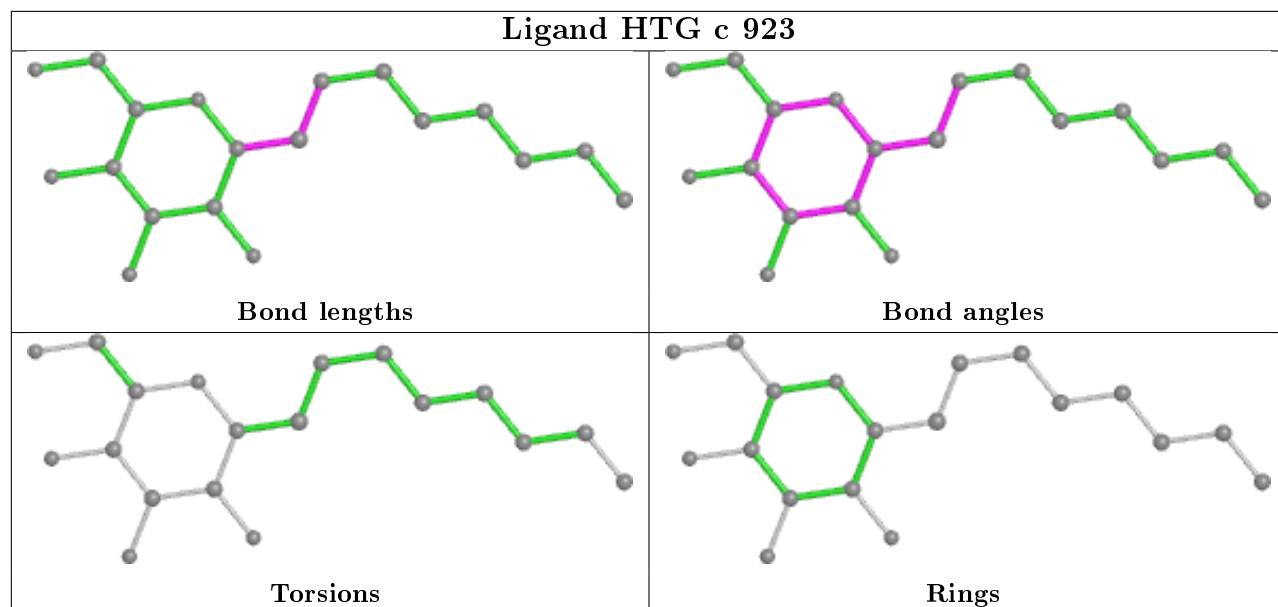
## Ligand BCR B 620



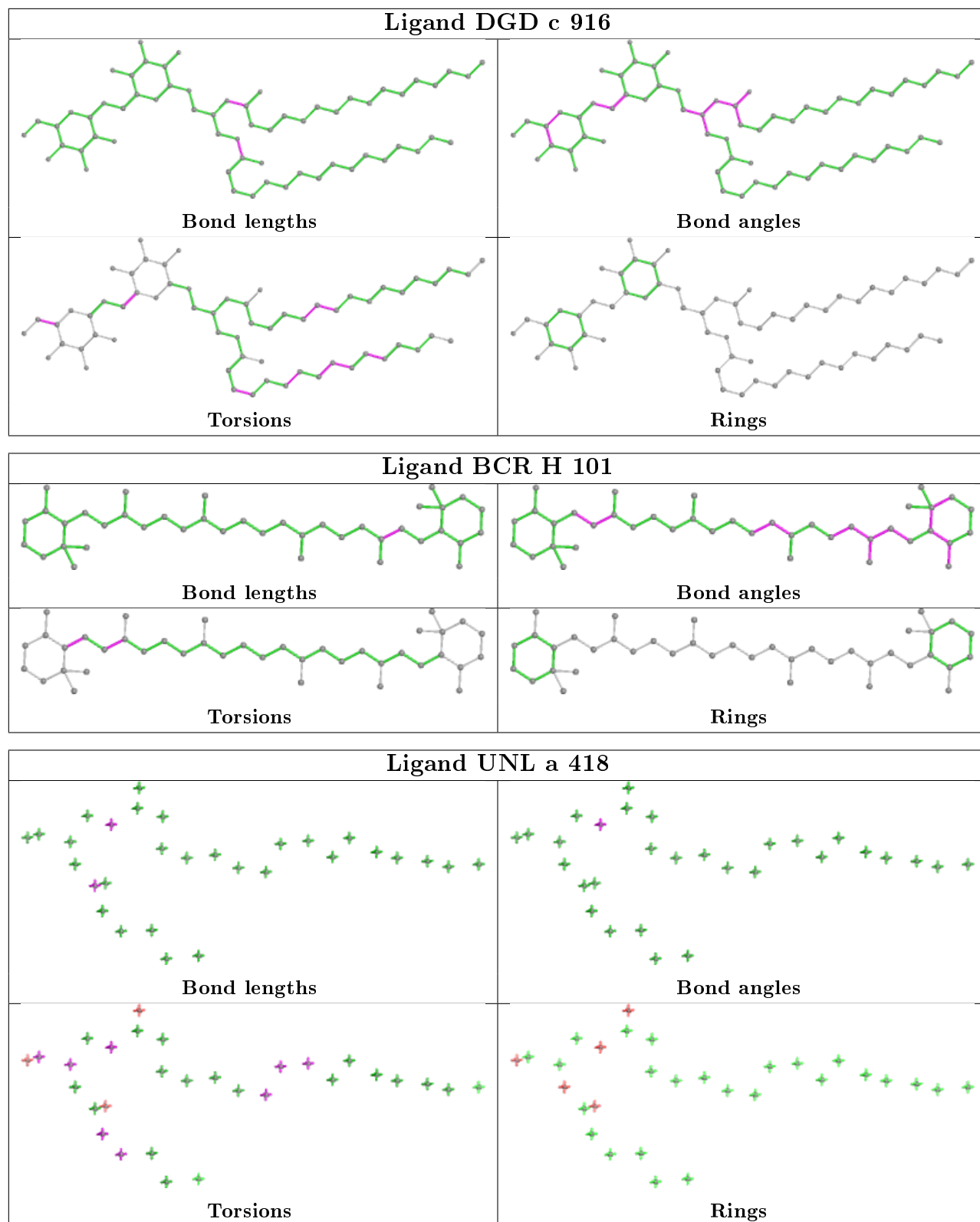
## Ligand HTG b 627

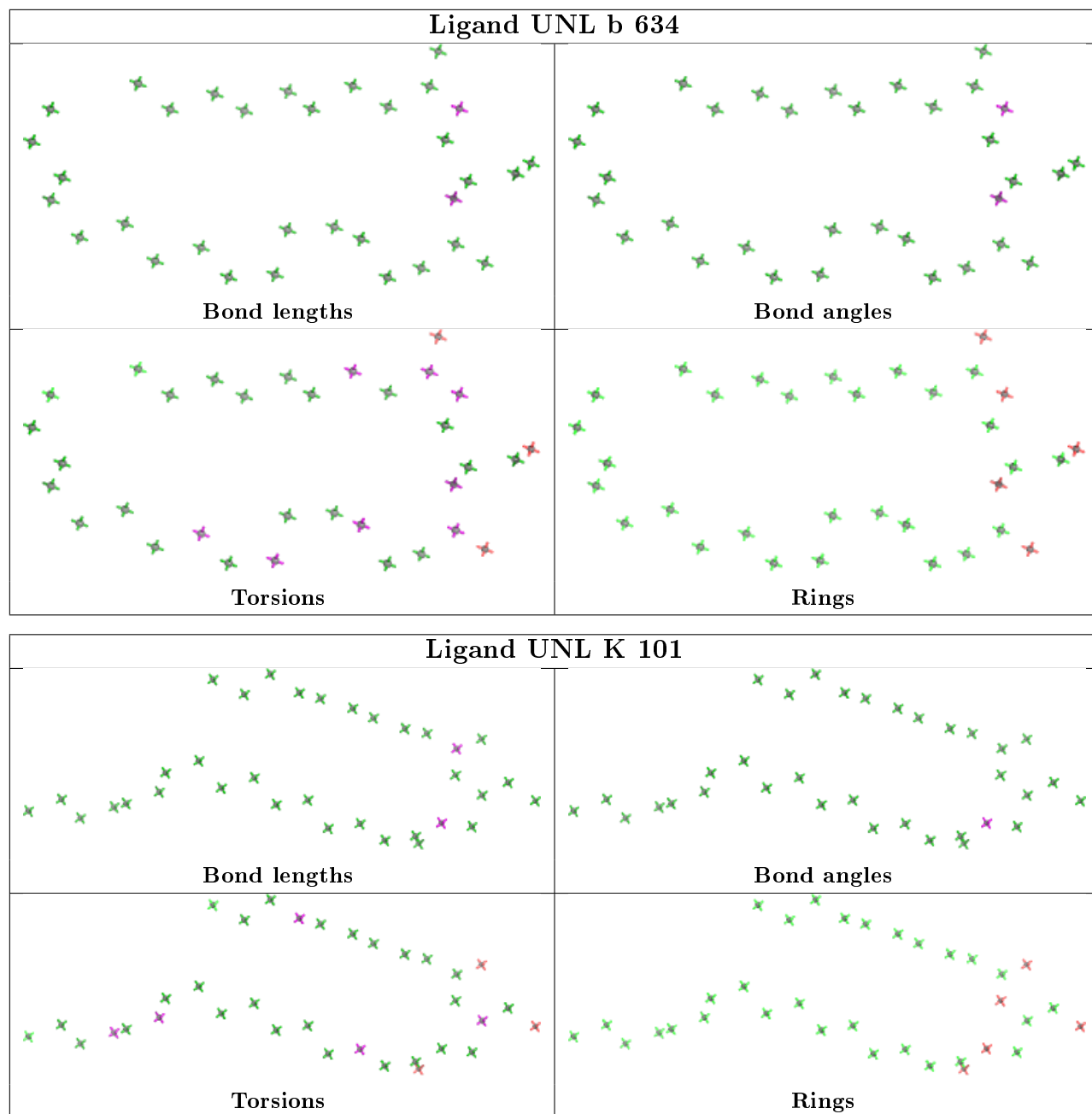


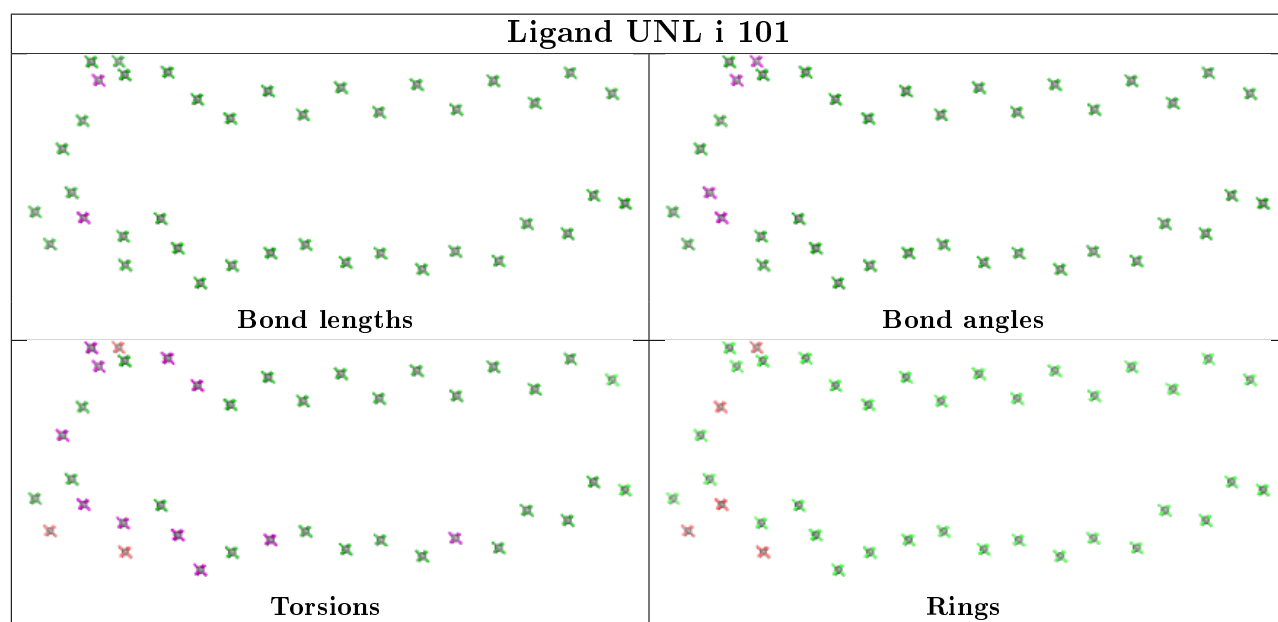
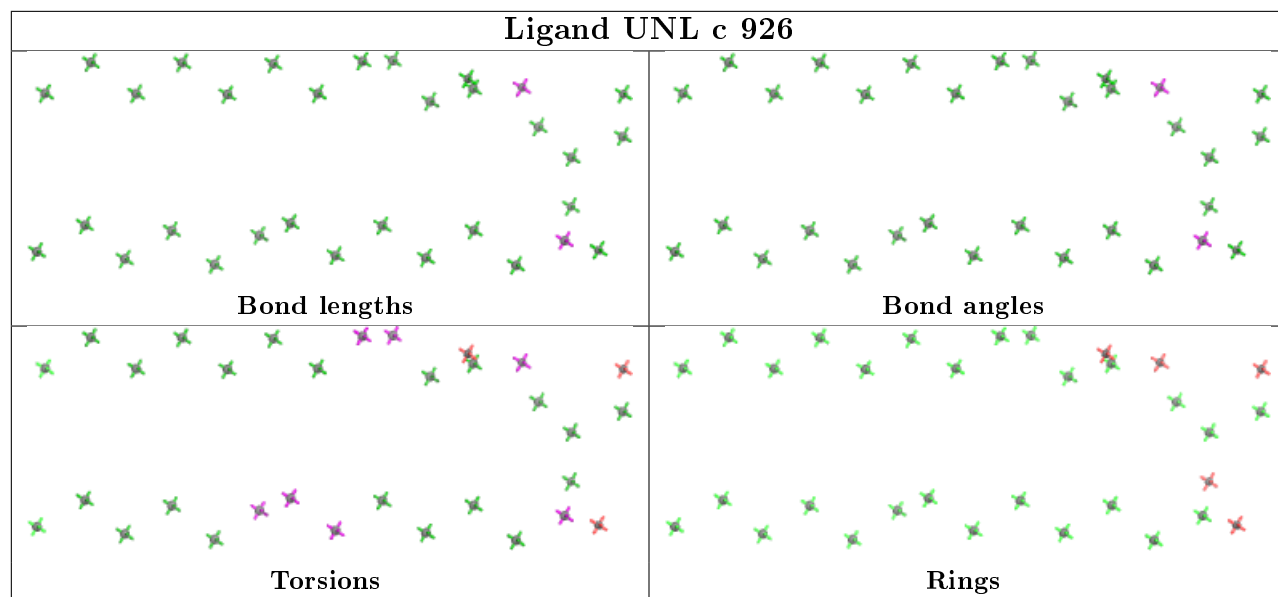
**Ligand BCR C 515****Ligand CLA c 907****Ligand LMG J 101**

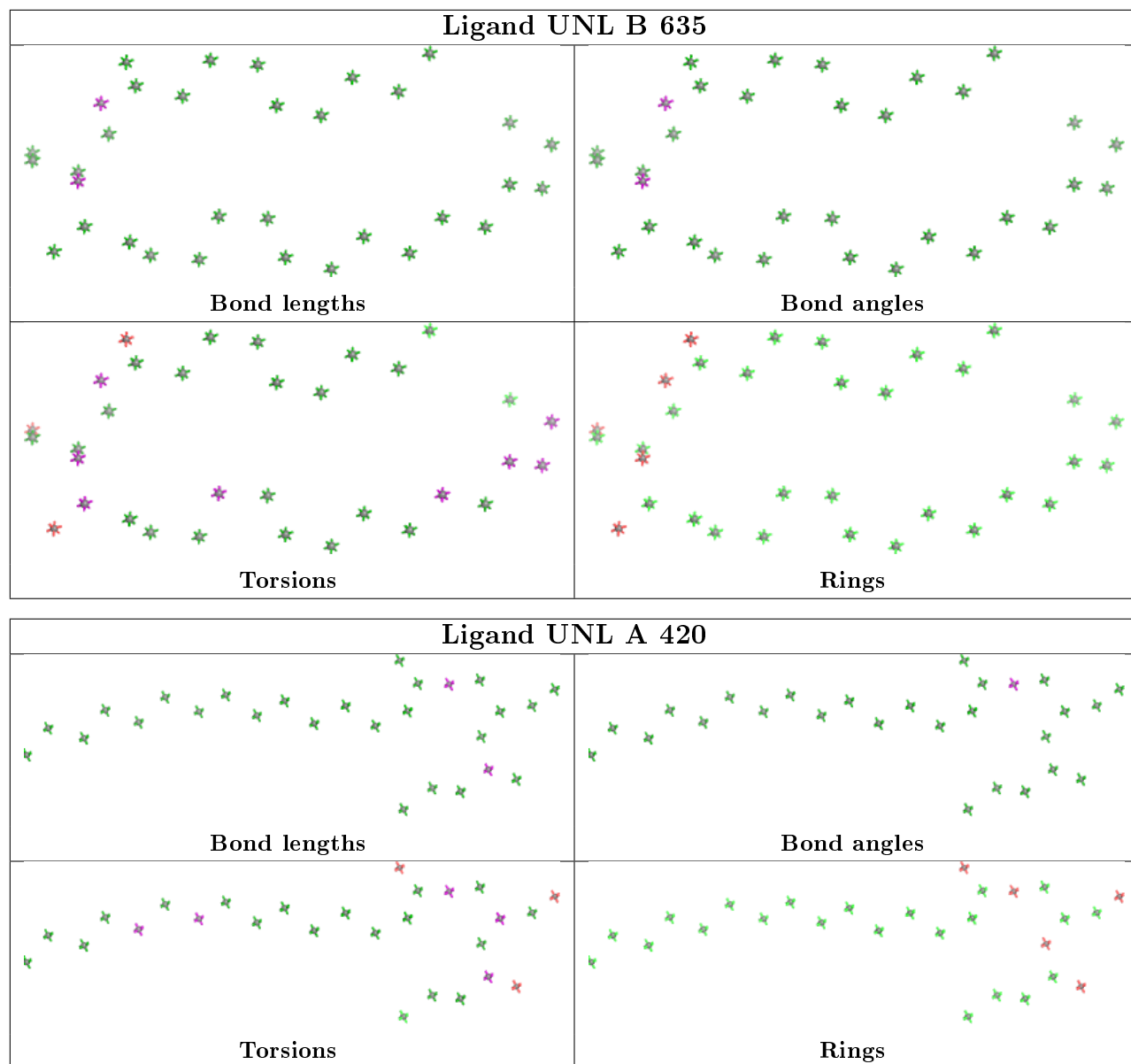


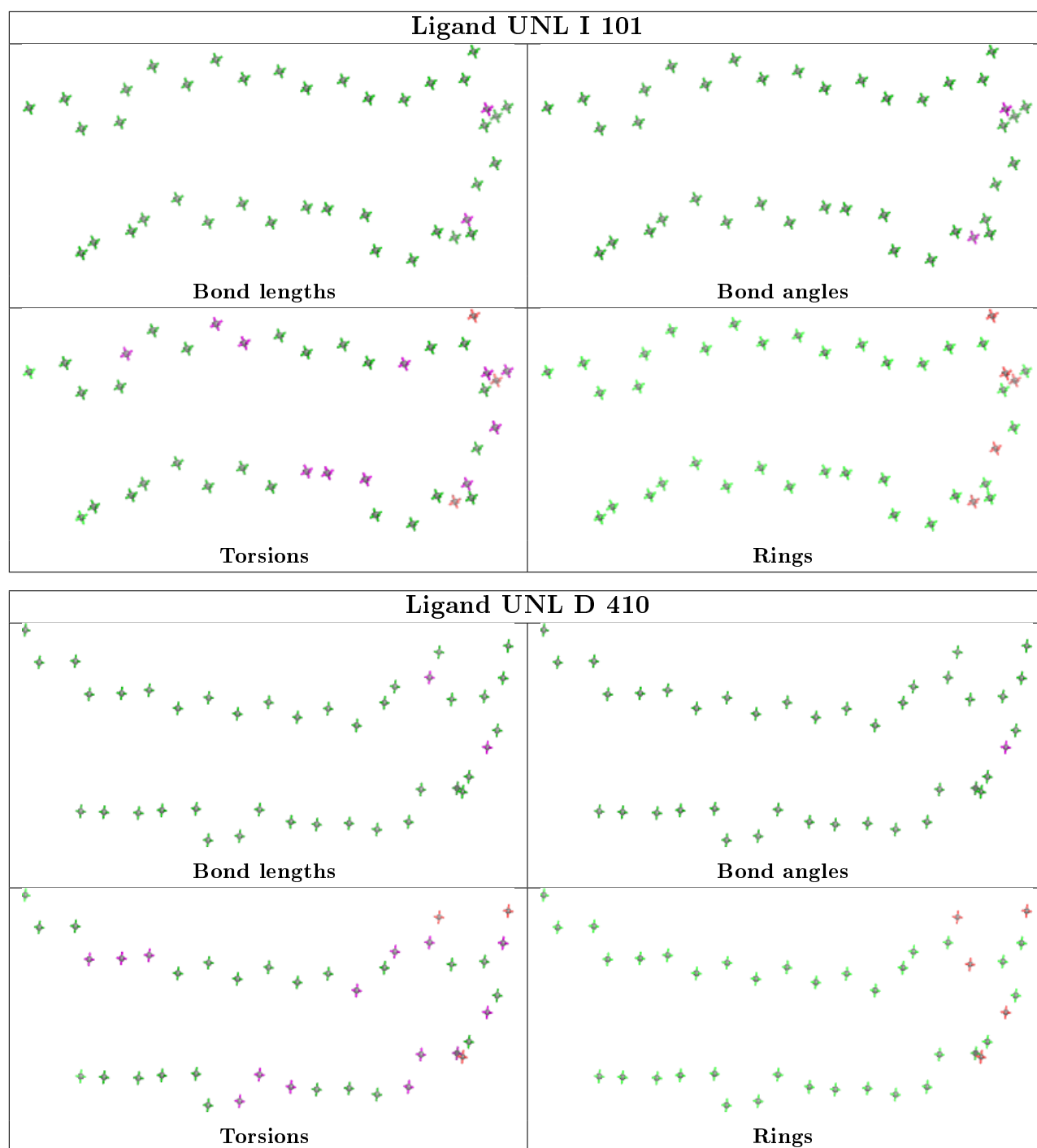


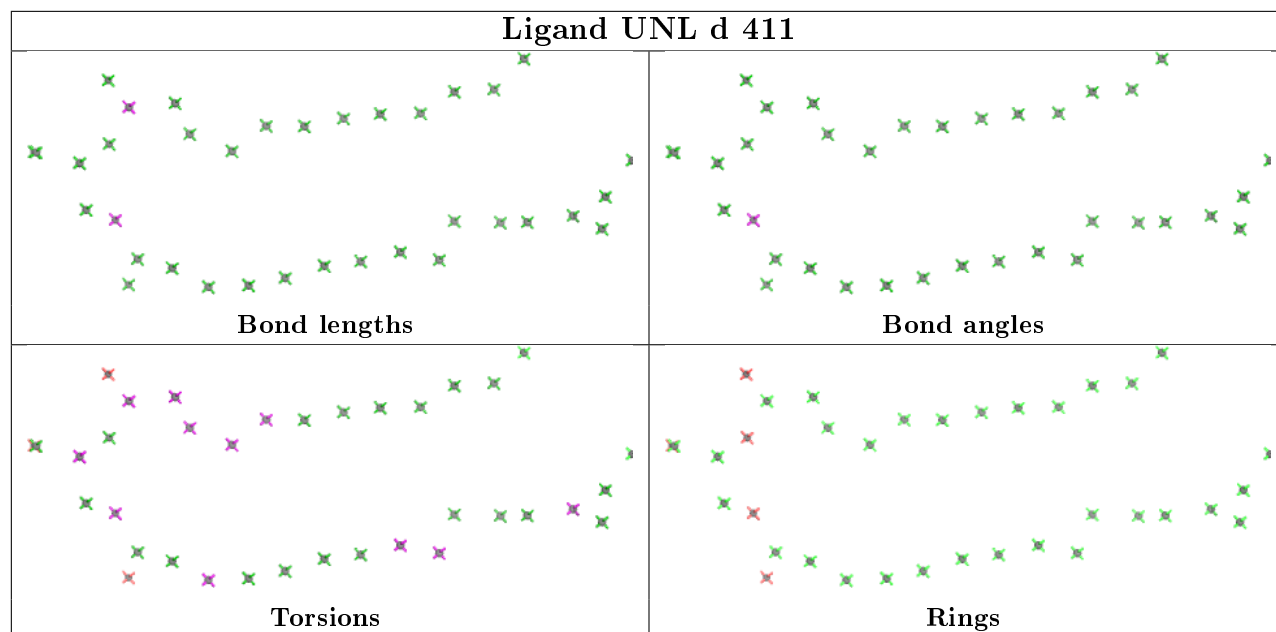












## 5.7 Other polymers [i](#)

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%)	0.43	20 (5%) 21 30	13, 21, 38, 73	0
1	a	334/344 (97%)	0.58	35 (10%) 6 10	15, 23, 47, 90	0
2	B	504/505 (99%)	0.17	27 (5%) 25 34	15, 25, 48, 78	0
2	b	504/505 (99%)	0.26	36 (7%) 16 24	16, 27, 59, 92	0
3	C	451/455 (99%)	0.14	17 (3%) 40 50	18, 30, 46, 73	0
3	c	455/455 (100%)	0.29	26 (5%) 23 32	21, 33, 49, 92	0
4	D	342/342 (100%)	0.56	31 (9%) 9 15	14, 22, 37, 97	0
4	d	341/342 (99%)	0.36	18 (5%) 26 35	16, 25, 39, 90	0
5	E	81/84 (96%)	0.85	10 (12%) 4 6	26, 37, 66, 92	0
5	e	81/84 (96%)	1.10	12 (14%) 2 3	30, 42, 71, 92	0
6	F	34/44 (77%)	0.34	4 (11%) 4 7	23, 30, 50, 61	0
6	f	32/44 (72%)	0.27	3 (9%) 8 13	30, 34, 79, 84	0
7	H	65/65 (100%)	0.22	2 (3%) 49 58	23, 31, 46, 110	0
7	h	65/65 (100%)	0.72	8 (12%) 4 6	27, 35, 52, 105	0
8	I	37/38 (97%)	0.58	5 (13%) 3 5	26, 33, 88, 108	0
8	i	37/38 (97%)	0.52	3 (8%) 12 18	27, 33, 73, 102	0
9	J	38/39 (97%)	0.59	5 (13%) 3 5	24, 35, 84, 98	0
9	j	39/39 (100%)	0.37	3 (7%) 13 21	29, 38, 84, 96	0
10	K	37/37 (100%)	0.22	1 (2%) 54 63	27, 35, 54, 65	0
10	k	37/37 (100%)	0.85	7 (18%) 1 1	30, 38, 55, 68	0
11	L	37/37 (100%)	0.67	5 (13%) 3 5	15, 19, 56, 82	0
11	l	37/37 (100%)	0.79	5 (13%) 3 5	16, 20, 58, 83	0
12	M	33/36 (91%)	0.75	3 (9%) 9 15	15, 21, 45, 89	0
12	m	33/36 (91%)	0.67	3 (9%) 9 15	16, 21, 41, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.27	16 (6%) 18 26	16, 32, 66, 110	0
13	o	243/244 (99%)	0.71	44 (18%) 1 1	19, 33, 71, 125	0
14	T	29/32 (90%)	0.83	3 (10%) 6 10	16, 20, 43, 89	0
14	t	29/32 (90%)	0.45	2 (6%) 16 25	16, 20, 46, 89	0
15	U	97/104 (93%)	0.34	4 (4%) 37 46	21, 31, 54, 84	0
15	u	97/104 (93%)	-0.08	0 100 100	23, 33, 51, 84	0
16	V	137/137 (100%)	-0.09	0 100 100	20, 31, 51, 69	0
16	v	137/137 (100%)	0.47	12 (8%) 10 16	24, 36, 57, 70	0
17	Y	29/30 (96%)	1.56	7 (24%) 0 0	35, 47, 82, 101	0
17	y	29/30 (96%)	1.42	7 (24%) 0 0	38, 50, 83, 100	0
18	X	39/40 (97%)	0.60	5 (12%) 3 6	31, 38, 75, 102	0
18	x	39/40 (97%)	1.50	11 (28%) 0 0	33, 41, 83, 102	0
19	Z	62/62 (100%)	1.29	17 (27%) 0 0	36, 47, 83, 96	0
19	z	62/62 (100%)	2.79	35 (56%) 0 0	42, 49, 82, 96	0
20	R	34/34 (100%)	7.13	34 (100%) 0 0	55, 75, 98, 106	0
All	All	5294/5384 (98%)	0.48	486 (9%) 9 14	13, 29, 61, 125	0

All (486) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	15.8
20	R	18	TRP	11.3
7	H	65	LEU	11.1
17	Y	18	VAL	10.5
20	R	23	ILE	10.4
5	e	5	THR	10.0
20	R	24	LEU	9.9
20	R	3	TRP	9.7
19	z	3	ILE	9.6
20	R	14	LEU	9.2
20	R	20	VAL	9.2
20	R	19	ALA	9.1
20	R	32	GLN	9.0
20	R	31	VAL	8.9
20	R	6	LEU	8.7
17	Y	19	ILE	8.5
20	R	25	PRO	8.1

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Mol	Chain	Res	Type	RSRZ
20	R	7	VAL	7.9
20	R	10	LEU	7.9
13	o	59	LYS	7.8
7	h	65	LEU	7.6
19	Z	3	ILE	7.6
20	R	26	TYR	7.4
19	z	5	PHE	7.4
1	a	11	ALA	7.2
19	z	42	LEU	7.2
18	X	40	SER	7.1
20	R	28	VAL	6.8
20	R	34	LEU	6.8
19	z	4	LEU	6.8
8	I	37	LEU	6.8
17	y	18	VAL	6.8
20	R	9	LEU	6.7
18	x	2	THR	6.7
20	R	5	VAL	6.7
13	O	56	PRO	6.7
9	j	1	MET	6.7
20	R	15	ALA	6.6
20	R	13	LEU	6.5
20	R	21	ARG	6.5
20	R	33	LYS	6.5
19	z	61	VAL	6.4
20	R	29	LYS	6.4
18	x	40	SER	6.3
20	R	27	ALA	6.3
20	R	30	GLN	6.2
17	y	19	ILE	6.2
19	Z	7	LEU	6.2
2	b	486	LEU	6.1
17	Y	22	LEU	6.1
2	b	495	PHE	6.0
5	E	84	LYS	6.0
20	R	35	LEU	6.0
19	Z	1	MET	6.0
1	A	11	ALA	5.9
3	C	23	ALA	5.8
19	Z	62	VAL	5.8
20	R	16	ALA	5.8
2	b	85	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
8	i	37	LEU	5.7
9	J	2	SER	5.6
11	l	1	MET	5.6
19	z	2	THR	5.6
19	Z	4	LEU	5.5
9	J	3	GLU	5.5
20	R	8	VAL	5.4
19	z	60	PHE	5.4
20	R	22	ASN	5.3
20	R	2	ASP	5.3
18	x	37	VAL	5.3
7	h	66	GLY	5.3
13	o	246	ALA	5.2
13	o	61	GLN	5.2
18	x	38	GLN	5.2
14	T	30	THR	5.2
2	b	505	ARG	5.2
20	R	17	GLY	5.1
13	O	62	GLU	5.0
13	o	36	GLN	5.0
13	o	35	SER	4.9
2	B	486	LEU	4.9
10	k	18	PHE	4.8
2	b	487	SER	4.7
7	h	64	ALA	4.7
2	B	86	ILE	4.7
5	e	25	ILE	4.7
19	z	7	LEU	4.7
2	b	293	ALA	4.7
19	z	18	VAL	4.7
4	D	12	ARG	4.6
18	X	2	THR	4.6
13	o	63	ALA	4.6
1	A	13	LEU	4.4
13	o	56	PRO	4.4
3	c	143	TYR	4.4
13	o	26	ALA	4.4
6	f	14	PRO	4.3
8	I	38	GLU	4.3
7	H	64	ALA	4.3
16	v	17	LYS	4.2
19	Z	31	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
8	i	36	ASP	4.2
5	e	4	THR	4.2
2	B	494	GLY	4.2
19	z	1	MET	4.2
13	o	135	SER	4.2
10	k	13	GLU	4.2
2	b	489	GLU	4.1
13	o	24	ASP	4.1
20	R	4	ARG	4.1
19	z	57	LEU	4.1
13	O	61	GLN	4.1
2	b	504	THR	4.0
19	z	9	LEU	4.0
13	o	34	SER	4.0
13	O	4	THR	4.0
2	b	84	THR	4.0
16	v	16	GLY	4.0
10	k	14	ALA	4.0
2	B	298	LEU	3.9
2	b	493	TRP	3.9
3	C	143	TYR	3.8
6	F	16	PHE	3.8
4	D	11	GLU	3.8
6	F	15	ILE	3.8
2	b	484	PRO	3.8
20	R	12	VAL	3.8
6	f	16	PHE	3.7
1	A	12	ASN	3.7
12	M	33	GLN	3.7
8	I	36	ASP	3.7
2	b	496	TYR	3.7
13	o	32	ILE	3.7
3	c	134	ILE	3.6
18	x	30	ALA	3.6
17	Y	20	ALA	3.6
14	t	30	THR	3.6
13	o	25	THR	3.6
1	a	192	ILE	3.5
2	b	294	SER	3.5
18	x	39	ARG	3.5
2	b	497	GLN	3.5
14	t	29	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
13	o	199	LEU	3.4
13	o	4	THR	3.4
2	b	290	ALA	3.4
1	A	202	VAL	3.4
19	Z	33	TRP	3.4
19	z	41	PHE	3.4
19	z	43	GLY	3.4
13	O	27	ARG	3.4
5	e	32	ILE	3.4
5	E	17	VAL	3.4
7	h	6	TRP	3.4
19	Z	35	ARG	3.4
2	b	494	GLY	3.4
13	o	134	THR	3.4
13	O	25	THR	3.3
19	z	46	LEU	3.3
19	z	33	TRP	3.3
18	x	34	ILE	3.3
2	b	490	GLN	3.3
4	D	279	LEU	3.3
13	O	26	ALA	3.3
2	b	488	PRO	3.3
2	b	295	GLY	3.3
17	y	22	LEU	3.3
19	Z	60	PHE	3.2
2	b	86[A]	ILE	3.2
1	a	200	LEU	3.2
19	Z	34	ASP	3.2
12	m	34	LYS	3.2
1	a	197	PHE	3.2
2	B	127	ARG	3.2
1	A	197	PHE	3.2
3	C	254	THR	3.2
13	O	138	THR	3.2
17	y	20	ALA	3.2
5	e	21	VAL	3.2
4	D	153	PHE	3.2
1	A	200	LEU	3.2
2	B	85	GLY	3.2
1	A	206	PHE	3.2
19	z	59	PHE	3.2
2	B	505	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
13	o	37	THR	3.1
16	v	14	SER	3.1
2	b	502	VAL	3.1
3	c	432	VAL	3.1
1	a	290	ILE	3.1
4	d	325	ILE	3.1
13	o	243	ILE	3.1
15	U	79	LEU	3.1
2	B	485	GLU	3.1
2	b	491	VAL	3.1
16	v	106	ASN	3.1
1	a	13	LEU	3.1
2	b	298	LEU	3.1
19	z	39	LEU	3.1
17	Y	21	GLN	3.1
13	o	23	ASP	3.0
2	B	495	PHE	3.0
3	c	140	LEU	3.0
13	o	58	ASN	3.0
13	o	62	GLU	3.0
11	l	3	PRO	3.0
4	D	201	VAL	3.0
3	C	257	PHE	3.0
13	o	95	PHE	3.0
19	z	40	ILE	3.0
4	D	278	GLY	3.0
4	d	152	VAL	3.0
15	U	73	GLN	3.0
16	v	26	TYR	3.0
5	E	21	VAL	3.0
16	v	10	VAL	3.0
12	M	34	LYS	3.0
5	e	26	THR	2.9
11	L	1	MET	2.9
3	c	155	ASN	2.9
2	b	485	GLU	2.9
20	R	11	PRO	2.9
1	A	14	TRP	2.9
4	D	149	PRO	2.9
6	F	14	PRO	2.9
9	J	4	GLY	2.9
3	C	432	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	193	LEU	2.9
18	X	31	ILE	2.9
3	c	146	PHE	2.9
10	k	12	PRO	2.9
19	z	6	GLN	2.9
19	Z	32	ASP	2.9
1	A	205	VAL	2.9
4	D	156	VAL	2.9
15	U	58	VAL	2.9
13	O	137	THR	2.9
4	D	152	VAL	2.9
4	D	289	LEU	2.9
13	o	65	PHE	2.9
10	k	17	ILE	2.8
19	z	27	TYR	2.8
19	z	35	ARG	2.8
2	b	291	SER	2.8
1	A	288	LEU	2.8
2	b	297	THR	2.8
4	D	280	TRP	2.8
13	o	132	ASN	2.8
13	O	60	ARG	2.8
1	a	288	LEU	2.8
11	l	27	LEU	2.8
19	Z	30	PRO	2.8
17	Y	25	ILE	2.8
3	c	145	SER	2.7
4	D	17	ILE	2.7
4	D	191	TRP	2.7
3	c	147	PHE	2.7
5	e	37	PHE	2.7
4	D	148	ALA	2.7
4	d	74	LEU	2.7
19	Z	57	LEU	2.7
1	A	192	ILE	2.7
11	L	31	PHE	2.7
13	o	133	VAL	2.7
2	B	461	LEU	2.7
3	c	159	THR	2.7
1	a	300	PHE	2.7
2	b	302	TRP	2.7
3	c	259	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
17	y	41	VAL	2.7
2	b	296	ALA	2.6
2	B	295	GLY	2.6
4	d	328	TRP	2.6
4	d	12	ARG	2.6
5	e	61	ARG	2.6
13	o	60	ARG	2.6
12	m	16	LEU	2.6
3	C	145[A]	SER	2.6
13	o	33	ASP	2.6
1	A	287	ALA	2.6
5	E	6	GLY	2.6
8	I	34	ARG	2.6
5	e	42	LEU	2.6
12	M	16[A]	LEU	2.6
4	D	202	ALA	2.6
13	o	57	LYS	2.6
4	D	150	ILE	2.6
6	f	15	ILE	2.6
4	d	196	PHE	2.6
1	a	193	LEU	2.6
4	D	182	LEU	2.6
9	J	6	ARG	2.6
7	h	22	ALA	2.6
2	b	126	PRO	2.6
1	a	157	VAL	2.6
1	a	202	VAL	2.6
4	d	182	LEU	2.6
4	D	178	ILE	2.6
18	x	3	ILE	2.6
13	O	130	GLN	2.6
1	a	280	VAL	2.6
13	o	66	VAL	2.6
4	D	196	PHE	2.5
2	B	293	ALA	2.5
3	c	411	ALA	2.5
13	O	24	ASP	2.5
14	T	9	ILE	2.5
17	y	25	ILE	2.5
1	a	205	VAL	2.5
1	a	285	PHE	2.5
3	C	436	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
8	i	38	GLU	2.5
1	a	299	GLY	2.5
18	x	36	LYS	2.5
17	Y	43	ARG	2.5
3	c	19	ASN	2.5
3	C	433	LEU	2.5
7	h	3	ARG	2.5
1	A	278	TRP	2.5
18	x	35	ASP	2.5
2	b	127	ARG	2.5
15	U	70	ARG	2.5
1	a	293	MET	2.5
3	c	131	TYR	2.5
12	m	33	GLN	2.5
19	z	38	GLN	2.5
13	o	136	ILE	2.5
3	C	260	ALA	2.5
3	c	151	TRP	2.5
1	A	186	PHE	2.5
19	Z	2	THR	2.5
13	o	131	PRO	2.4
7	h	63	LYS	2.4
5	E	81	GLU	2.4
16	v	15	GLU	2.4
1	a	156	ALA	2.4
3	c	142	GLU	2.4
3	c	204	LEU	2.4
4	d	205	LEU	2.4
5	E	79	PHE	2.4
10	k	21	LEU	2.4
11	L	29	LEU	2.4
13	o	38	TYR	2.4
2	B	165	GLY	2.4
3	C	155	ASN	2.4
2	B	84	THR	2.4
18	X	34	ILE	2.4
19	z	20	VAL	2.4
1	A	196	PRO	2.4
1	a	196	PRO	2.4
4	D	291	LEU	2.4
19	Z	49	ALA	2.4
19	z	28	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	a	160	ILE	2.4
2	B	457	VAL	2.4
2	b	499	VAL	2.4
4	D	286	VAL	2.4
5	E	25	ILE	2.4
18	X	38	GLN	2.4
10	K	30	VAL	2.4
1	A	297	LEU	2.3
11	L	23	LEU	2.3
1	a	188	ALA	2.3
4	d	184	PHE	2.3
3	c	255	THR	2.3
16	v	19	ILE	2.3
3	C	142	GLU	2.3
4	D	238	THR	2.3
3	c	435	PHE	2.3
4	d	185	PHE	2.3
4	D	275	PRO	2.3
19	Z	6	GLN	2.3
19	z	56	VAL	2.3
2	B	292	LEU	2.3
6	F	17	THR	2.3
2	B	489	GLU	2.3
14	T	13	ILE	2.3
19	z	14	ILE	2.3
13	O	5	LEU	2.3
4	D	146	PHE	2.3
19	z	34	ASP	2.3
3	c	253	LEU	2.3
13	o	22	LEU	2.3
4	d	24	ARG	2.3
2	b	129	GLY	2.2
4	D	185	PHE	2.2
2	B	488	PRO	2.2
4	D	192	THR	2.2
13	o	204	VAL	2.2
1	a	284	TRP	2.2
3	C	259	TRP	2.2
4	D	193	LEU	2.2
13	o	43	LEU	2.2
1	a	235	TYR	2.2
13	o	245	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
19	z	30	PRO	2.2
3	C	255	THR	2.2
3	C	425	TRP	2.2
16	v	21	LEU	2.2
10	k	15	TYR	2.2
3	c	20	SER	2.2
5	e	10	PHE	2.2
4	D	290	ALA	2.2
1	A	201	GLY	2.2
4	D	175	VAL	2.2
5	E	22	ILE	2.2
19	z	58	ASN	2.2
19	z	52	LEU	2.2
1	a	283	VAL	2.2
13	o	27	ARG	2.2
13	o	31	PRO	2.2
19	z	31	GLN	2.2
1	a	161	TYR	2.2
4	d	179	PHE	2.2
17	y	21	GLN	2.2
13	O	131	PRO	2.1
2	B	305	ILE	2.1
1	a	194	MET	2.1
2	B	301	ALA	2.1
2	B	454	ALA	2.1
2	B	459	ALA	2.1
13	o	30	TYR	2.1
1	a	180	PHE	2.1
3	c	144	SER	2.1
3	c	429	SER	2.1
19	Z	36	SER	2.1
2	B	408	GLY	2.1
3	c	183	GLY	2.1
7	h	20	LYS	2.1
9	J	5	GLY	2.1
16	v	110	LYS	2.1
1	a	297	LEU	2.1
5	e	80	LEU	2.1
1	a	203	ALA	2.1
9	j	3	GLU	2.1
2	B	297	THR	2.1
13	o	211	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	a	287	ALA	2.1
2	b	301	ALA	2.1
3	C	253	LEU	2.1
11	l	25	LEU	2.1
16	v	12	LEU	2.1
16	v	107	LEU	2.1
19	z	49	ALA	2.1
19	z	29	SER	2.1
4	D	160	TYR	2.1
3	c	425	TRP	2.1
4	d	324	GLY	2.1
11	L	2	GLU	2.1
4	d	156	VAL	2.1
5	e	17	VAL	2.1
13	O	87	VAL	2.1
13	o	87	VAL	2.1
1	A	294	ALA	2.1
2	B	487	SER	2.1
4	d	283	ALA	2.1
1	a	279	PRO	2.1
2	b	223	GLN	2.1
11	l	2	GLU	2.1
13	O	59	LYS	2.1
18	x	8	LYS	2.1
1	a	182	PHE	2.1
1	a	186	PHE	2.1
4	d	191	TRP	2.1
13	o	142	PHE	2.1
4	D	295[A]	SER	2.1
1	A	286	ALA	2.1
3	C	462[A]	GLU	2.1
13	o	202	ALA	2.1
1	a	184	ILE	2.1
4	d	17	ILE	2.1
1	a	326	LEU	2.1
2	B	504	THR	2.0
5	E	82	GLN	2.0
3	C	146	PHE	2.0
5	E	57	ALA	2.0
9	j	5	GLY	2.0
2	b	120	LEU	2.0
3	c	433	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
4	d	178	ILE	2.0
2	b	501	ASP	2.0
8	I	33	LYS	2.0
13	o	201	VAL	2.0
2	B	479	PHE	2.0
1	a	341	LEU	2.0
3	c	428	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
12	FME	m	1	10/11	0.93	0.16	13,32,67,68	0
8	FME	I	1	10/11	0.95	0.12	22,34,38,38	0
14	FME	T	1	10/11	0.96	0.17	18,26,40,49	0
14	FME	t	1	10/11	0.96	0.12	12,22,31,68	0
12	FME	M	1	10/11	0.97	0.12	23,36,70,74	0
8	FME	i	1	10/11	0.98	0.13	21,31,39,42	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	CA	b	604	1/1	0.47	0.25	117,117,117,117	0
36	DGD	D	405	62/66	0.55	0.40	48,79,113,122	0
29	LMT	E	102	35/35	0.57	0.34	43,80,109,115	0
29	LMT	f	103	35/35	0.59	0.37	43,86,107,111	0
36	DGD	d	406	62/66	0.61	0.45	38,89,122,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	HTG	B	626	19/19	0.61	0.36	48,81,94,95	0
28	GOL	B	637	6/6	0.61	0.26	51,72,83,86	0
35	HTG	B	634	19/19	0.65	0.29	32,76,109,127	0
32	UNL	A	420	28/-	0.66	0.28	50,71,78,86	0
35	HTG	b	603	19/19	0.67	0.24	46,84,110,111	0
32	UNL	b	634	33/-	0.68	0.29	29,62,111,117	0
29	LMT	m	102	35/35	0.68	0.25	33,61,79,95	0
37	LHG	e	101	42/49	0.69	0.28	52,89,118,129	0
32	UNL	K	101	34/-	0.70	0.30	37,61,83,88	0
35	HTG	d	412	16/19	0.70	0.31	38,78,97,98	0
29	LMT	b	625	25/35	0.71	0.29	44,67,109,119	0
32	UNL	c	926	32/-	0.71	0.36	39,79,98,105	0
32	UNL	B	635	33/-	0.72	0.25	33,58,102,102	0
29	LMT	M	101	35/35	0.72	0.21	23,52,69,77	0
35	HTG	b	627	19/19	0.72	0.27	49,86,110,116	0
31	PL9	a	417	55/55	0.73	0.26	41,73,92,99	0
32	UNL	a	418	30/-	0.73	0.31	42,66,98,106	0
34	LMG	z	101	39/55	0.73	0.33	45,82,99,107	0
29	LMT	C	522	35/35	0.74	0.40	52,81,102,104	0
28	GOL	v	203	6/6	0.75	0.31	39,74,86,87	0
32	UNL	j	102	10/-	0.76	0.29	47,57,63,63	0
32	UNL	J	102	10/-	0.76	0.35	39,51,64,67	0
29	LMT	m	104	35/35	0.76	0.24	29,59,85,86	0
34	LMG	Z	101	37/55	0.76	0.28	30,75,96,112	0
28	GOL	a	415	6/6	0.76	0.22	48,62,65,66	0
35	HTG	C	524	19/19	0.76	0.30	41,69,99,100	0
33	CA	B	601	1/1	0.77	0.10	83,83,83,83	0
32	UNL	i	101	40/-	0.77	0.24	28,62,105,117	0
32	UNL	d	413	18/-	0.78	0.19	30,52,81,84	0
34	LMG	C	521	51/55	0.78	0.25	32,69,88,108	0
34	LMG	a	412	51/55	0.78	0.21	33,62,84,90	0
28	GOL	O	302	6/6	0.78	0.23	49,55,57,61	0
32	UNL	I	101	40/-	0.78	0.24	27,62,110,120	0
27	SQD	B	621	54/54	0.78	0.20	26,55,94,104	0
27	SQD	L	102	54/54	0.78	0.22	24,52,86,91	0
28	GOL	V	203	6/6	0.78	0.43	50,64,71,72	0
35	HTG	D	411	16/19	0.78	0.26	38,102,111,112	0
35	HTG	c	923	19/19	0.78	0.30	45,80,94,97	0
34	LMG	C	501	51/55	0.80	0.21	34,56,76,85	0
32	UNL	d	411	36/-	0.80	0.23	32,56,104,111	0
35	HTG	c	922	19/19	0.81	0.21	43,67,84,95	0
31	PL9	A	419	55/55	0.81	0.23	28,56,91,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	LMT	B	623	35/35	0.81	0.22	26,74,96,101	0
28	GOL	A	415	6/6	0.81	0.19	36,49,64,64	0
27	SQD	a	402	54/54	0.81	0.20	29,55,76,90	0
28	GOL	f	101	6/6	0.82	0.25	44,50,62,64	0
28	GOL	T	103	6/6	0.82	0.23	52,68,70,79	0
32	UNL	m	101	10/-	0.82	0.21	35,50,55,61	0
32	UNL	M	102	10/-	0.82	0.21	28,38,57,58	0
34	LMG	c	919	51/55	0.82	0.21	29,57,78,81	0
37	LHG	E	101	42/49	0.82	0.22	22,63,78,93	0
27	SQD	A	416	54/54	0.82	0.20	26,51,78,85	0
34	LMG	c	920	51/55	0.82	0.25	33,74,88,93	0
32	UNL	D	410	40/-	0.82	0.20	24,54,93,101	0
29	LMT	c	921	35/35	0.83	0.40	46,76,97,104	0
29	LMT	a	401	35/35	0.83	0.20	21,53,74,80	0
29	LMT	b	601	25/35	0.83	0.27	18,55,104,111	0
29	LMT	m	103	35/35	0.84	0.17	19,48,62,74	0
28	GOL	V	206	6/6	0.84	0.27	47,63,66,66	0
34	LMG	C	520	51/55	0.84	0.22	22,52,72,90	0
29	LMT	B	636	25/35	0.85	0.23	24,61,106,122	0
29	LMT	A	417	35/35	0.85	0.19	22,57,79,97	0
28	GOL	B	629	6/6	0.85	0.21	28,42,50,56	0
28	GOL	b	632	6/6	0.85	0.20	38,52,59,59	0
28	GOL	B	628	6/6	0.86	0.31	33,42,54,72	0
27	SQD	f	102	43/54	0.86	0.24	41,75,103,108	0
34	LMG	B	622	51/55	0.87	0.23	19,32,49,71	0
28	GOL	B	631	6/6	0.87	0.24	30,48,62,65	0
28	GOL	v	204	6/6	0.87	0.17	54,66,71,80	0
32	UNL	X	101	18/-	0.87	0.15	29,44,62,79	0
32	UNL	D	409	17/-	0.87	0.16	30,40,63,66	0
32	UNL	d	410	17/-	0.87	0.18	34,48,82,82	0
28	GOL	A	414	6/6	0.87	0.18	30,40,43,49	0
35	HTG	B	633	19/19	0.88	0.16	28,54,70,76	0
24	CLA	c	914	65/65	0.88	0.26	35,48,81,87	0
35	HTG	b	602	19/19	0.88	0.15	29,45,65,68	0
28	GOL	t	102	6/6	0.88	0.25	22,59,67,67	0
28	GOL	T	101	6/6	0.88	0.27	54,60,61,69	0
28	GOL	c	925	6/6	0.89	0.23	34,52,63,66	0
26	BCR	d	404	40/40	0.89	0.15	27,36,54,60	0
35	HTG	V	202	19/19	0.89	0.19	40,59,77,163	0
26	BCR	k	102	40/40	0.89	0.15	30,37,50,61	0
34	LMG	b	624	51/55	0.89	0.23	21,36,57,81	0
28	GOL	o	302	6/6	0.90	0.13	44,50,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	DGD	H	102	62/66	0.90	0.16	16,28,46,59	0
28	GOL	F	103	6/6	0.90	0.19	60,65,71,71	0
27	SQD	F	101	43/54	0.90	0.24	34,59,81,90	0
26	BCR	h	101	40/40	0.90	0.12	25,35,48,52	0
35	HTG	b	626	19/19	0.90	0.19	30,50,86,86	0
37	LHG	l	101	49/49	0.90	0.18	15,27,39,56	0
33	CA	f	104	1/1	0.90	0.07	77,77,77,77	0
36	DGD	h	102	62/66	0.90	0.14	19,31,48,60	0
26	BCR	H	101	40/40	0.90	0.13	19,32,45,59	0
24	CLA	c	913	65/65	0.91	0.16	31,40,59,65	0
36	DGD	c	918	62/66	0.91	0.20	25,31,52,70	0
26	BCR	y	101	40/40	0.91	0.14	29,37,57,63	0
24	CLA	c	904	65/65	0.91	0.12	26,33,44,47	0
24	CLA	C	513	65/65	0.91	0.13	27,40,59,71	0
36	DGD	c	917	62/66	0.91	0.18	26,35,61,87	0
28	GOL	a	413	6/6	0.91	0.11	30,32,37,42	0
27	SQD	A	412	54/54	0.91	0.20	15,45,72,85	0
27	SQD	a	411	54/54	0.91	0.21	32,52,73,81	0
35	HTG	B	625	19/19	0.91	0.20	28,43,74,86	0
24	CLA	c	905	65/65	0.91	0.16	25,32,49,68	0
31	PL9	d	405	55/55	0.91	0.18	13,19,33,44	0
28	GOL	b	631	6/6	0.91	0.15	28,41,48,51	0
24	CLA	c	906	65/65	0.91	0.12	21,28,44,56	0
34	LMG	J	101	51/55	0.91	0.18	18,32,75,81	0
28	GOL	b	628	6/6	0.91	0.13	30,35,42,53	0
28	GOL	B	632	6/6	0.91	0.17	24,40,53,57	0
36	DGD	C	518	62/66	0.92	0.20	19,29,78,90	0
24	CLA	b	613	65/65	0.92	0.11	23,29,42,48	0
26	BCR	c	915	40/40	0.92	0.11	25,34,42,45	0
35	HTG	C	523	19/19	0.92	0.20	54,62,86,88	0
34	LMG	j	101	51/55	0.92	0.17	25,35,71,81	0
28	GOL	B	627	6/6	0.92	0.16	23,36,45,72	0
26	BCR	k	101	40/40	0.92	0.18	34,45,63,75	0
31	PL9	D	404	55/55	0.92	0.20	11,18,31,41	0
24	CLA	c	908	65/65	0.92	0.12	26,33,49,60	0
37	LHG	d	407	49/49	0.92	0.20	15,31,44,53	0
24	CLA	B	602	65/65	0.92	0.16	22,40,80,101	0
26	BCR	K	103	40/40	0.92	0.11	24,30,40,43	0
24	CLA	b	605	65/65	0.92	0.18	29,48,89,102	0
24	CLA	c	902	65/65	0.92	0.12	26,32,45,52	0
26	BCR	t	101	40/40	0.92	0.12	12,26,45,48	0
37	LHG	D	406	49/49	0.92	0.22	14,26,38,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	603	65/65	0.92	0.12	17,24,36,47	0
24	CLA	B	610	65/65	0.92	0.12	17,24,36,45	0
36	DGD	c	916	62/66	0.92	0.17	22,31,64,82	0
26	BCR	b	621	40/40	0.92	0.16	14,24,33,38	0
26	BCR	a	410	40/40	0.93	0.10	15,23,28,32	0
24	CLA	b	618	65/65	0.93	0.14	14,24,78,80	0
24	CLA	c	909	65/65	0.93	0.15	23,28,67,91	0
28	GOL	b	629	6/6	0.93	0.15	27,36,50,54	0
26	BCR	b	622	40/40	0.93	0.18	14,24,43,51	0
24	CLA	d	403	65/65	0.93	0.12	26,31,79,93	0
26	BCR	T	102	40/40	0.93	0.14	13,26,37,42	0
28	GOL	b	630	6/6	0.93	0.14	35,39,50,53	0
28	GOL	A	413	6/6	0.93	0.11	23,30,33,36	0
26	BCR	D	403	40/40	0.93	0.14	19,30,58,70	0
24	CLA	b	610	65/65	0.93	0.11	18,31,78,87	0
23	BCT	a	419	4/4	0.93	0.15	21,32,41,50	0
28	GOL	C	525	6/6	0.93	0.20	32,41,61,69	0
28	GOL	B	630	6/6	0.93	0.10	26,32,40,42	0
26	BCR	B	619	40/40	0.93	0.14	15,23,46,49	0
24	CLA	b	619	65/65	0.93	0.11	20,30,49,51	0
24	CLA	c	912	65/65	0.93	0.12	27,36,50,54	0
24	CLA	B	608	65/65	0.93	0.16	11,19,28,40	0
24	CLA	C	511	65/65	0.93	0.15	21,29,38,45	0
24	CLA	C	512	65/65	0.93	0.11	22,30,39,45	0
25	PHO	a	420	64/64	0.93	0.20	17,24,30,33	0
24	CLA	C	505	65/65	0.93	0.18	18,27,47,61	0
26	BCR	C	515	40/40	0.93	0.11	29,38,49,53	0
24	CLA	C	507	65/65	0.93	0.14	25,40,75,77	0
26	BCR	B	618	40/40	0.93	0.14	11,23,32,35	0
24	CLA	C	514	65/65	0.93	0.14	30,42,67,73	0
36	DGD	C	519	62/66	0.93	0.20	18,29,48,55	0
24	CLA	c	903	65/65	0.93	0.15	24,30,41,51	0
24	CLA	b	606	65/65	0.93	0.12	22,28,38,48	0
24	CLA	C	508	65/65	0.94	0.12	23,35,47,54	0
28	GOL	b	633	6/6	0.94	0.36	34,60,65,65	0
26	BCR	K	102	40/40	0.94	0.11	22,30,39,47	0
24	CLA	b	614	65/65	0.94	0.10	20,29,39,42	0
37	LHG	L	101	49/49	0.94	0.21	12,26,38,46	0
24	CLA	b	615	65/65	0.94	0.14	17,22,38,46	0
24	CLA	B	606	65/65	0.94	0.10	13,20,31,41	0
37	LHG	D	408	49/49	0.94	0.18	17,29,88,100	0
24	CLA	C	503	65/65	0.94	0.12	20,25,39,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	D	402	65/65	0.94	0.12	18,27,68,84	0
25	PHO	a	408	64/64	0.94	0.15	15,18,27,30	0
24	CLA	C	510	65/65	0.94	0.10	23,30,45,62	0
22	CL	v	201	1/1	0.94	0.08	62,62,62,62	0
24	CLA	B	614	65/65	0.94	0.16	12,20,43,55	0
24	CLA	c	910	65/65	0.94	0.11	27,34,47,53	0
24	CLA	b	616	65/65	0.94	0.10	16,23,32,44	0
26	BCR	b	623	40/40	0.94	0.09	18,31,42,48	0
24	CLA	C	504	65/65	0.94	0.11	22,28,40,45	0
24	CLA	B	604	65/65	0.94	0.11	16,25,32,38	0
24	CLA	C	502	65/65	0.94	0.11	22,30,42,54	0
28	GOL	V	204	6/6	0.94	0.14	19,26,30,37	0
28	GOL	a	414	6/6	0.94	0.14	25,34,43,53	0
23	BCT	A	404	4/4	0.94	0.17	21,24,36,47	0
37	LHG	d	408	49/49	0.94	0.13	15,23,41,54	0
26	BCR	B	620	40/40	0.94	0.09	16,26,39,49	0
28	GOL	V	205	6/6	0.94	0.16	34,41,45,52	0
24	CLA	B	605	65/65	0.94	0.13	13,19,44,57	0
24	CLA	c	911	65/65	0.94	0.16	24,31,43,53	0
24	CLA	c	907	65/65	0.94	0.12	28,37,64,72	0
24	CLA	B	615	65/65	0.94	0.12	12,21,66,79	0
24	CLA	a	407	65/65	0.94	0.23	18,23,72,84	0
24	CLA	b	620	65/65	0.94	0.14	19,33,77,78	0
24	CLA	C	509	65/65	0.94	0.14	18,25,67,82	0
24	CLA	B	607	65/65	0.94	0.12	16,25,70,76	0
26	BCR	A	411	40/40	0.94	0.11	15,22,29,31	0
24	CLA	A	407	65/65	0.95	0.25	13,20,71,73	0
24	CLA	b	612	65/65	0.95	0.10	21,28,40,43	0
38	HEM	e	102	43/43	0.95	0.18	37,46,76,95	0
28	GOL	v	205	6/6	0.95	0.16	23,35,46,50	0
26	BCR	C	516	40/40	0.95	0.09	23,32,42,43	0
28	GOL	C	526	6/6	0.95	0.18	17,21,26,26	0
37	LHG	d	409	49/49	0.95	0.17	21,32,85,88	0
24	CLA	B	613	65/65	0.95	0.11	13,20,27,33	0
24	CLA	A	405	65/65	0.95	0.23	13,17,27,52	0
25	PHO	A	408	64/64	0.95	0.16	12,16,23,24	0
24	CLA	C	506	65/65	0.95	0.10	18,27,47,54	0
24	CLA	B	609	65/65	0.95	0.14	15,24,30,36	0
24	CLA	b	608	65/65	0.95	0.13	15,23,51,62	0
24	CLA	b	617	65/65	0.95	0.15	14,22,44,52	0
24	CLA	D	401	65/65	0.95	0.24	12,16,32,36	0
35	HTG	O	303	19/19	0.95	0.10	23,32,46,55	0

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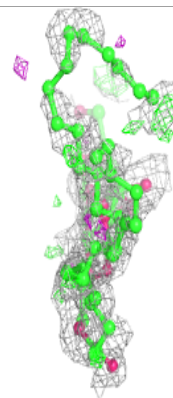
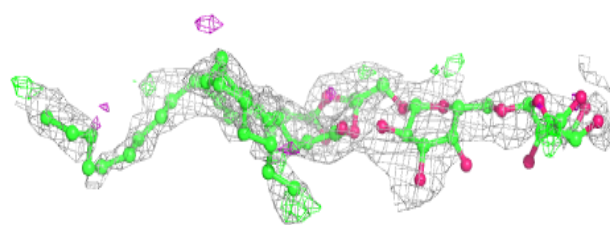
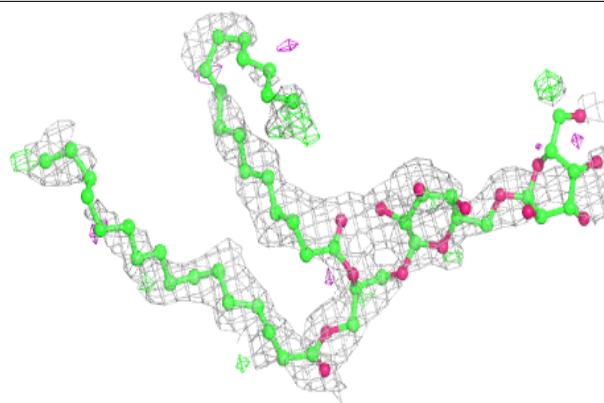
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	611	65/65	0.95	0.10	17,25,33,50	0
24	CLA	d	401	65/65	0.95	0.19	14,18,27,47	0
24	CLA	B	616	65/65	0.95	0.11	16,23,42,45	0
24	CLA	d	402	65/65	0.95	0.23	16,20,36,46	0
37	LHG	D	407	49/49	0.95	0.15	13,22,44,57	0
24	CLA	B	612	65/65	0.95	0.15	12,18,30,37	0
24	CLA	a	409	65/65	0.95	0.12	18,26,79,83	0
24	CLA	b	611	65/65	0.95	0.16	13,20,31,34	0
24	CLA	B	617	65/65	0.95	0.15	16,28,79,88	0
25	PHO	A	409	64/64	0.95	0.21	13,20,29,35	0
36	DGD	C	517	62/66	0.95	0.12	19,28,60,72	0
24	CLA	b	609	65/65	0.95	0.10	16,24,37,44	0
35	HTG	B	624	19/19	0.95	0.10	20,32,43,46	0
24	CLA	a	406	65/65	0.95	0.22	15,17,32,38	0
38	HEM	E	103	43/43	0.96	0.13	23,35,45,56	0
22	CL	U	201	1/1	0.96	0.07	50,50,50,50	0
24	CLA	b	607	65/65	0.96	0.10	21,28,38,50	0
33	CA	c	901	1/1	0.96	0.04	44,44,44,44	0
24	CLA	A	406	65/65	0.96	0.20	12,16,30,35	0
24	CLA	A	410	65/65	0.96	0.11	17,26,80,89	0
33	CA	F	102	1/1	0.96	0.09	69,69,69,69	0
40	HEC	V	201	43/43	0.97	0.09	22,25,32,39	0
39	MG	j	103	1/1	0.97	0.14	33,33,33,33	0
40	HEC	v	202	43/43	0.97	0.11	28,31,40,46	0
28	GOL	c	924	6/6	0.97	0.20	24,24,25,29	0
33	CA	O	301	1/1	0.97	0.14	53,53,53,53	0
30	OEX	a	416	10/10	0.98	0.10	18,21,24,34	0
33	CA	o	301	1/1	0.98	0.04	54,54,54,54	0
22	CL	a	404	1/1	0.98	0.07	20,20,20,20	0
39	MG	J	103	1/1	0.99	0.05	27,27,27,27	0
30	OEX	A	418	10/10	0.99	0.09	15,20,24,28	0
21	FE2	a	403	1/1	0.99	0.08	28,28,28,28	0
22	CL	A	403	1/1	0.99	0.05	19,19,19,19	0
22	CL	a	405	1/1	0.99	0.09	26,26,26,26	0
22	CL	A	402	1/1	1.00	0.07	18,18,18,18	0
21	FE2	A	401	1/1	1.00	0.07	24,24,24,24	0

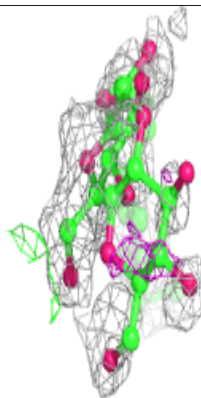
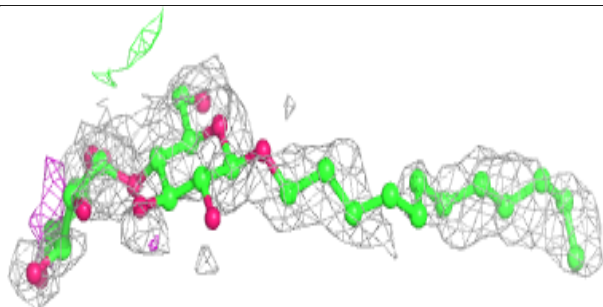
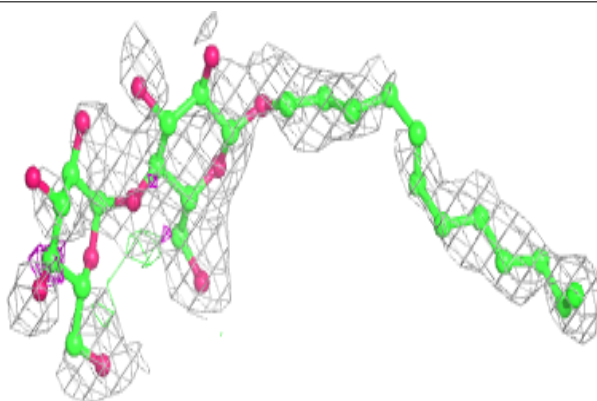
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DGD 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)

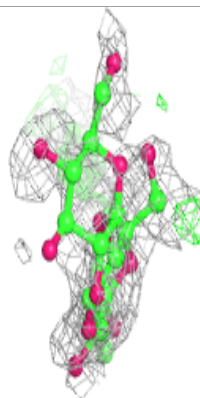
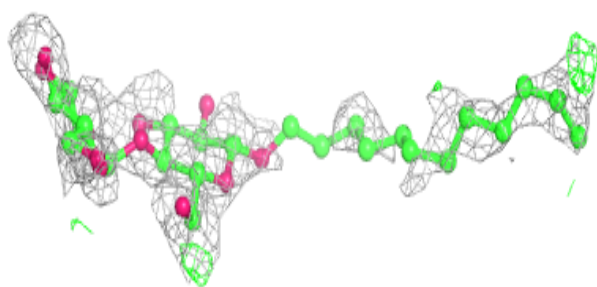
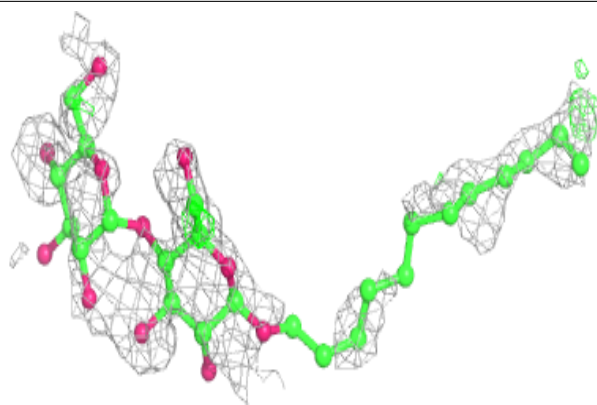
**Electron density around LMT E 102:**

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

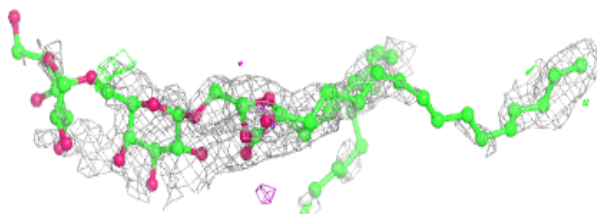
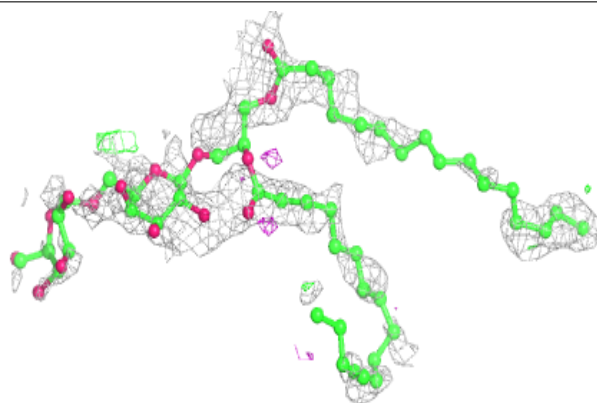


**Electron density around LMT f 103:**

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

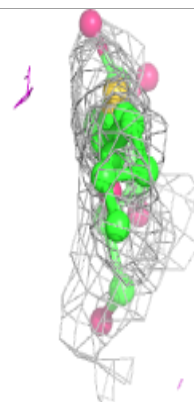
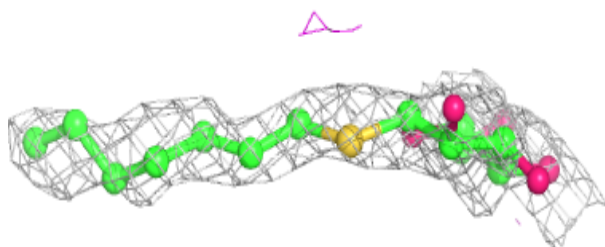
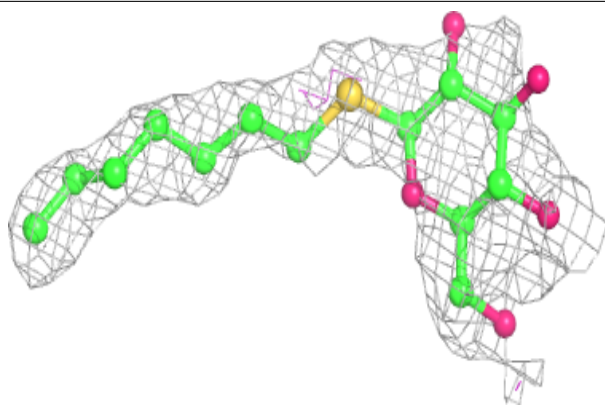
**Electron density around DGD d 406:**

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

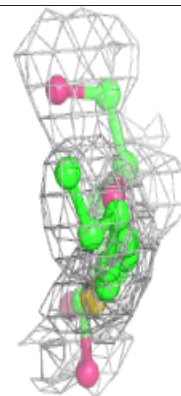
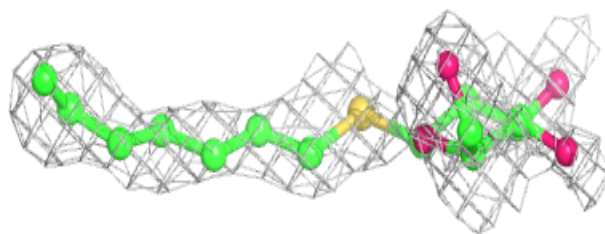
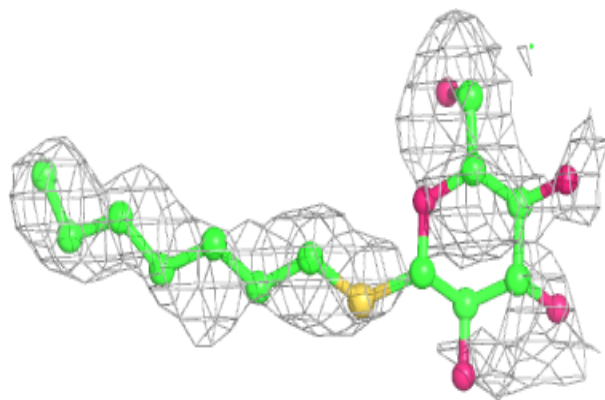


**Electron density around HTG B 626:**

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

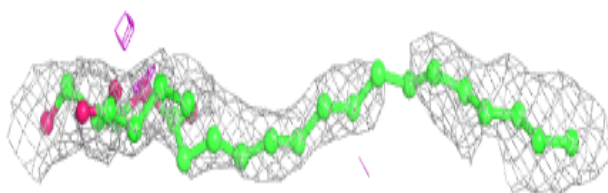
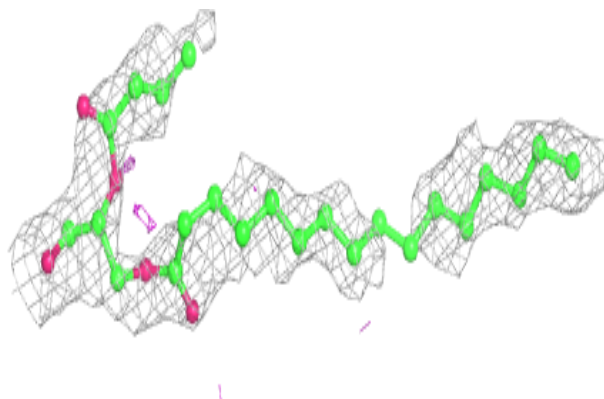
**Electron density around HTG B 634:**

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

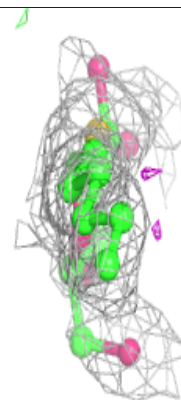
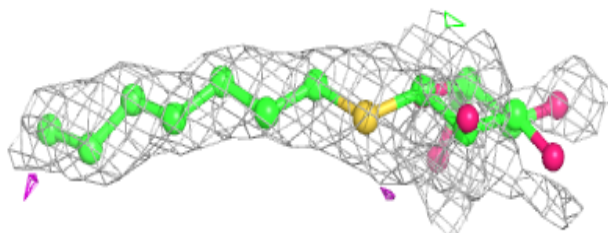
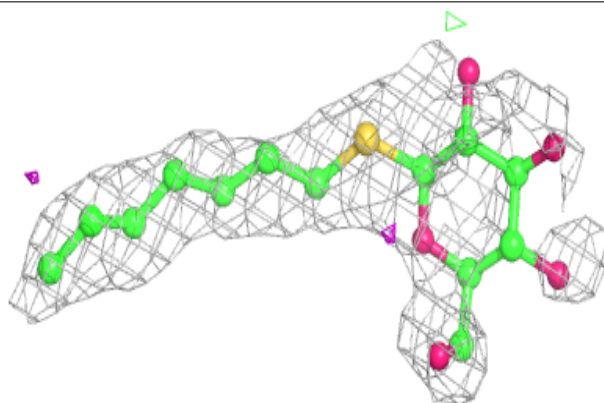


**Electron density around UNL A 420:**

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

**Electron density around HTG b 603:**

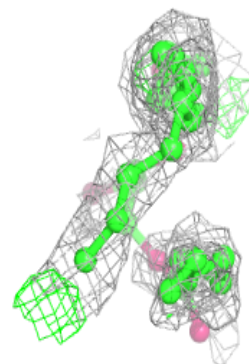
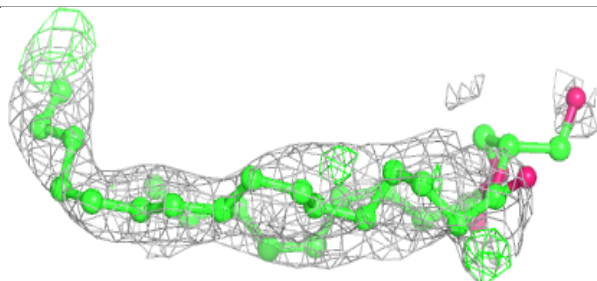
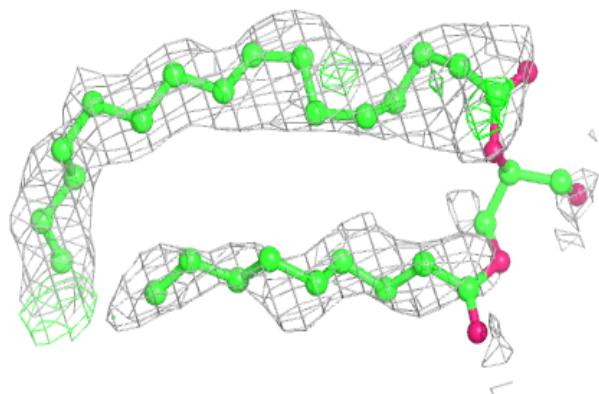
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



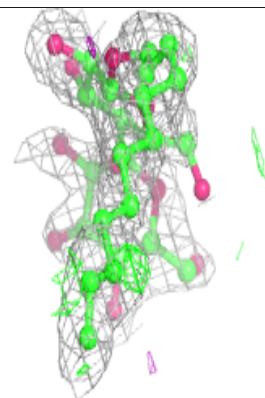
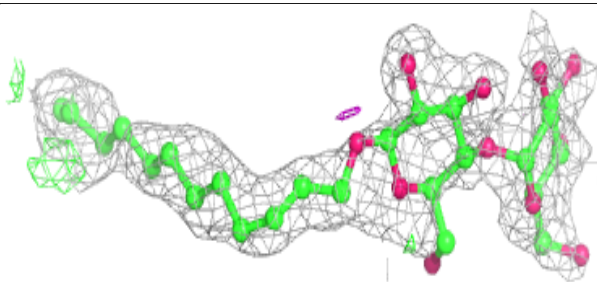
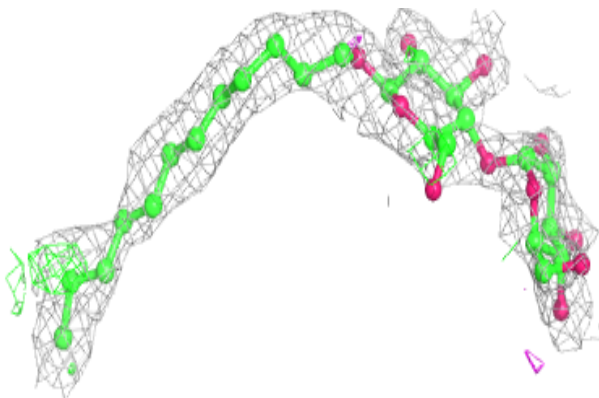


**Electron density around UNL b 634:**

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

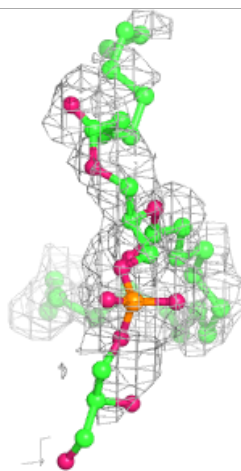
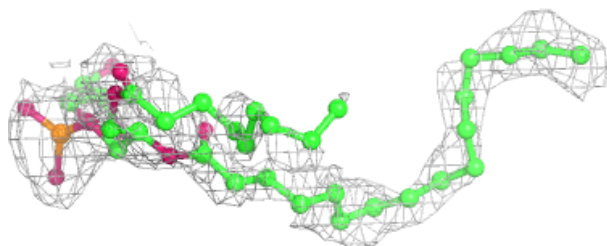
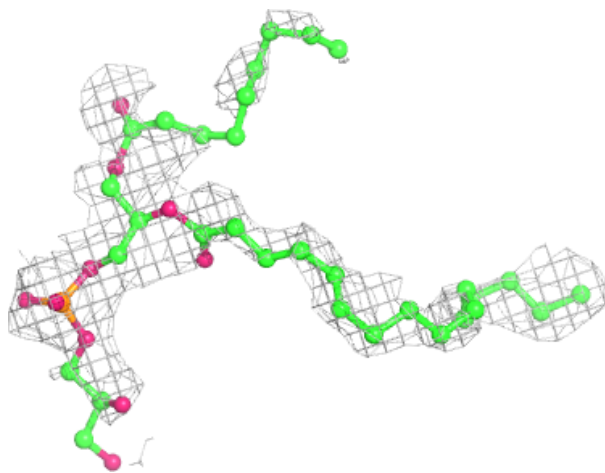
**Electron density around LMT m 102:**

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



**Electron density around LHG e 101:**

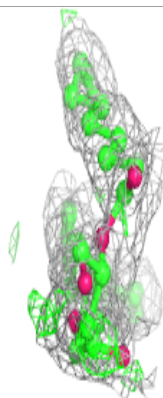
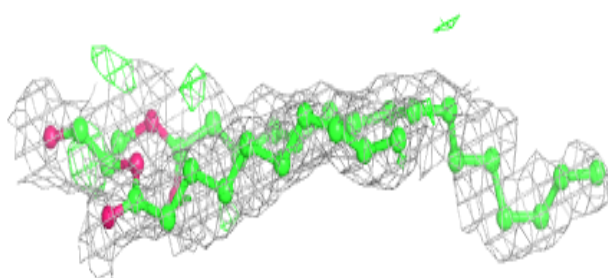
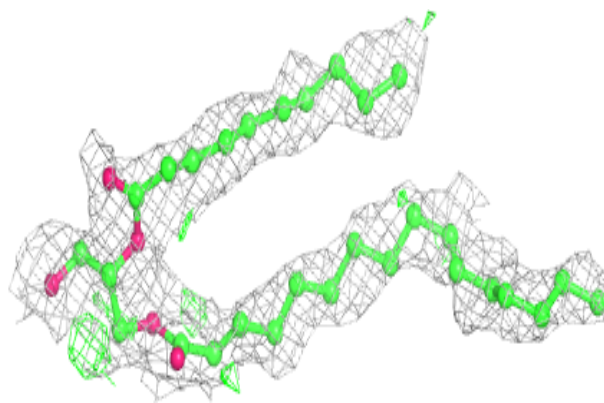
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



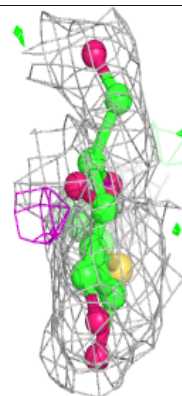
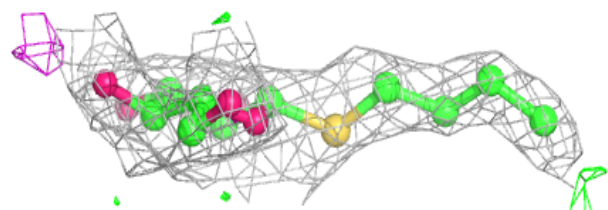
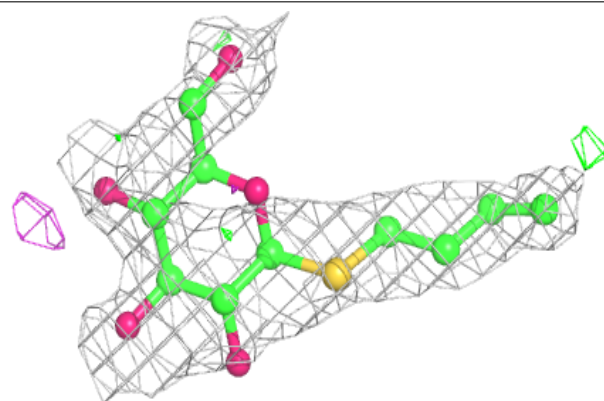


**Electron density around UNL K 101:**

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

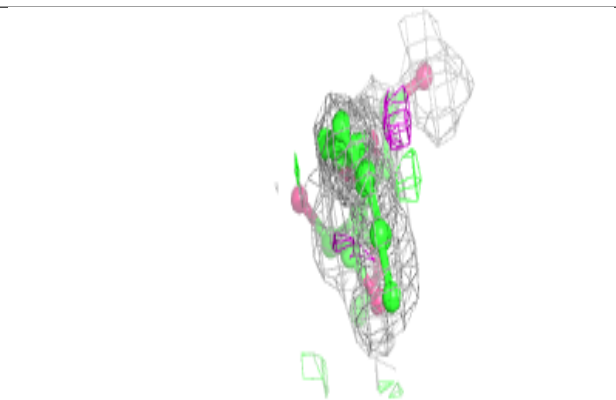
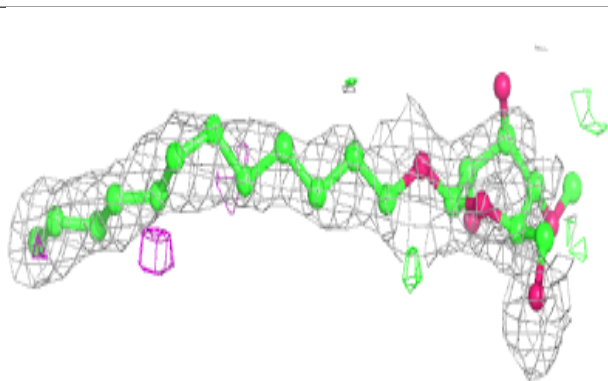
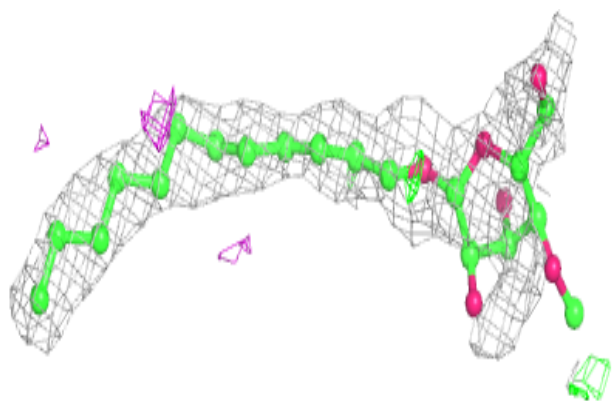
**Electron density around HTG d 412:**

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

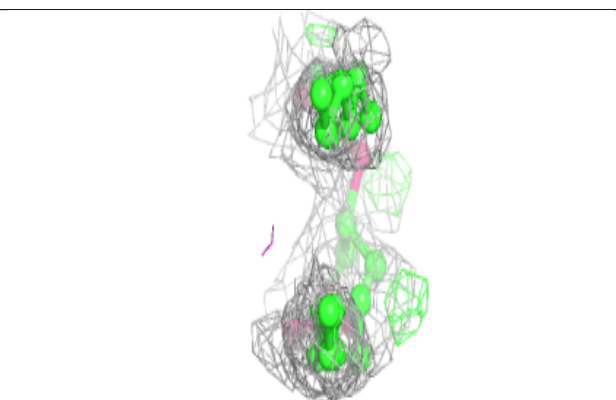
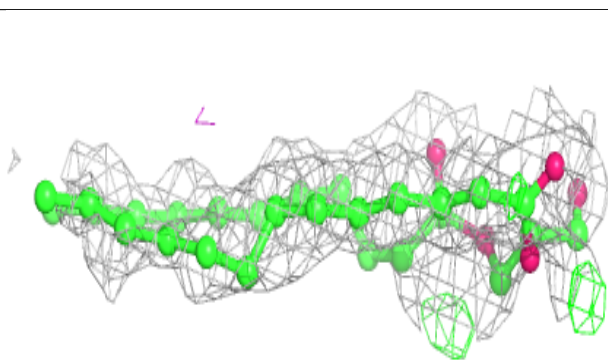
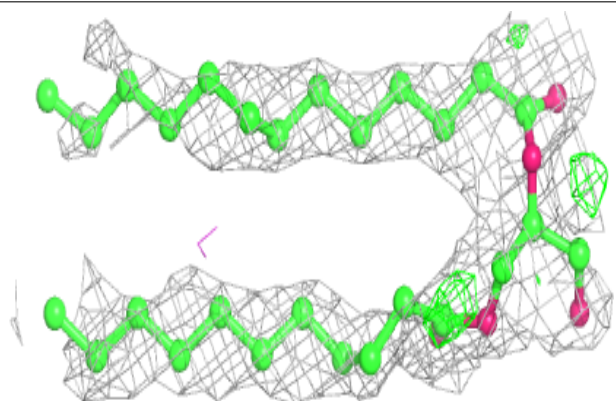


**Electron density around LMT b 625:**

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

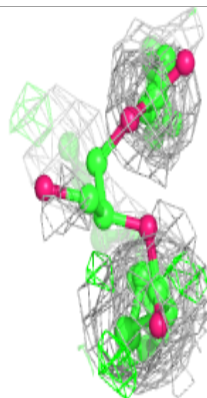
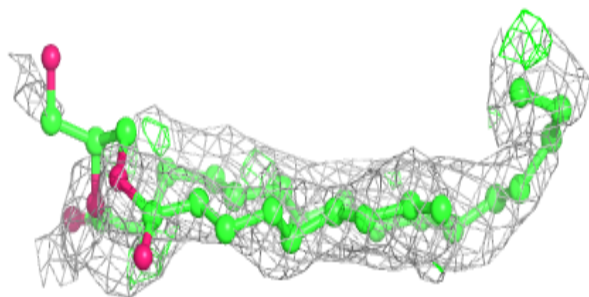
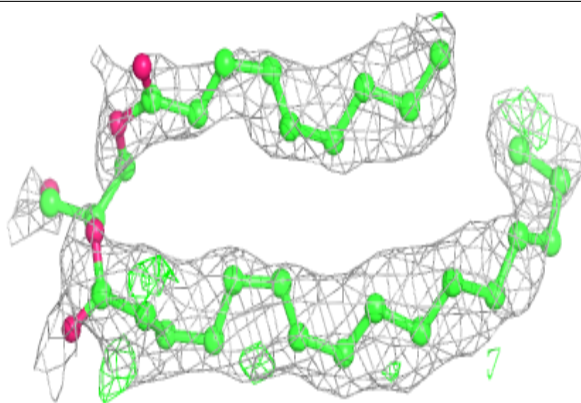
**Electron density around UNL c 926:**

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

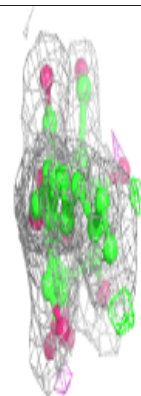
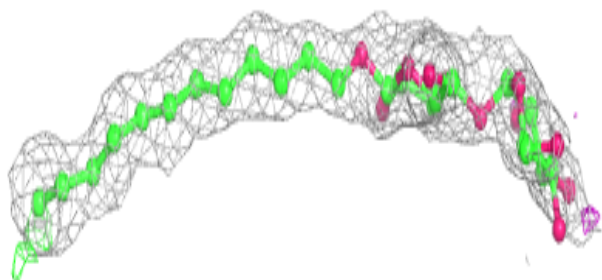
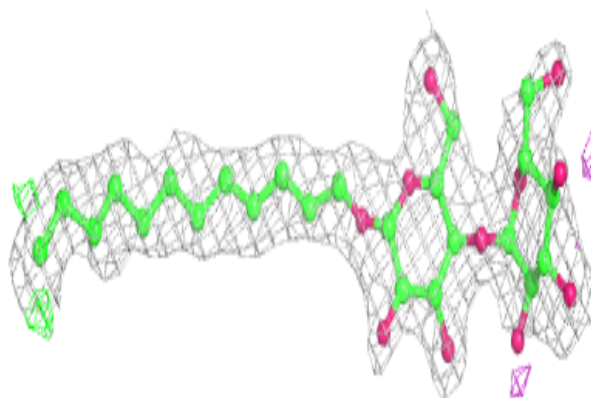


**Electron density around UNL B 635:**

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

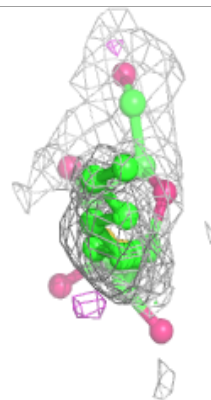
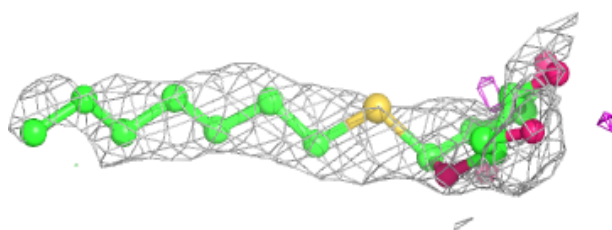
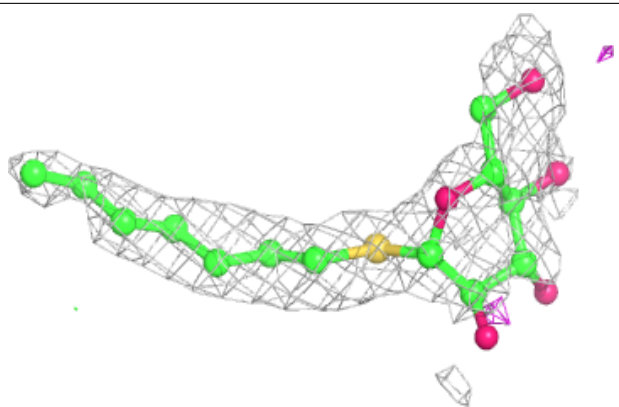
**Electron density around LMT M 101:**

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

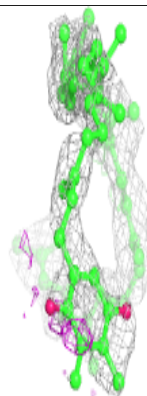
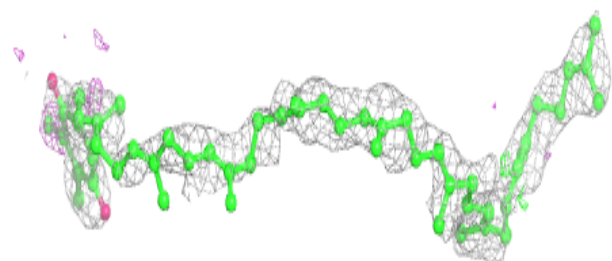
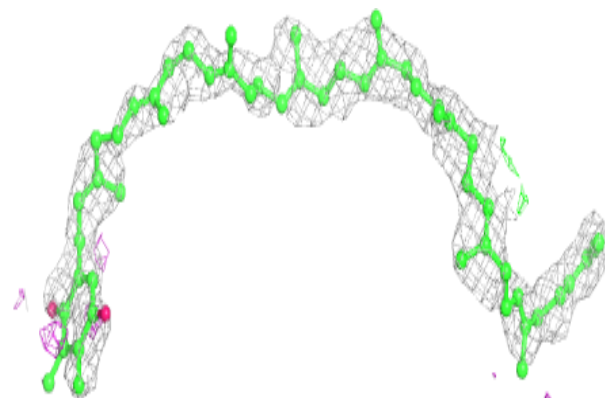


**Electron density around HTG b 627:**

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

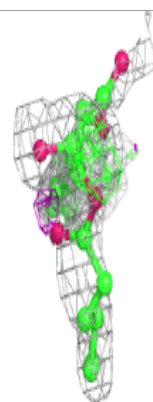
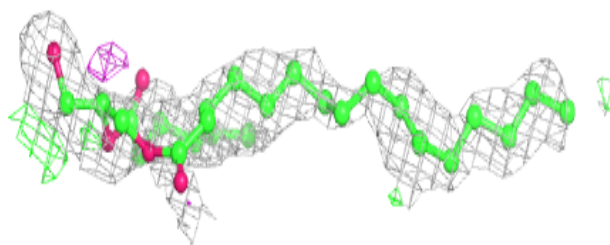
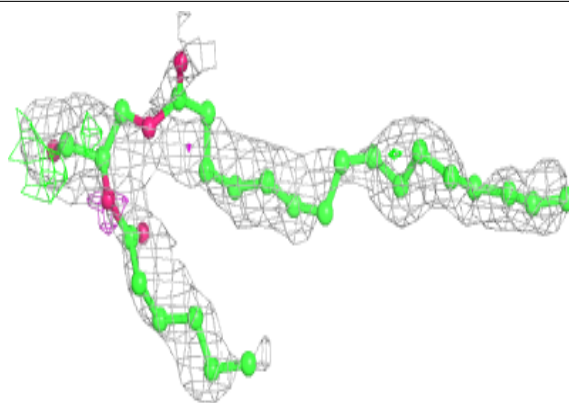
**Electron density around PL9 a 417:**

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

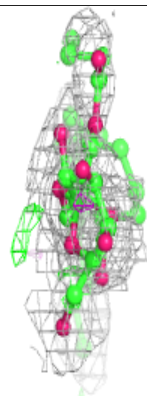
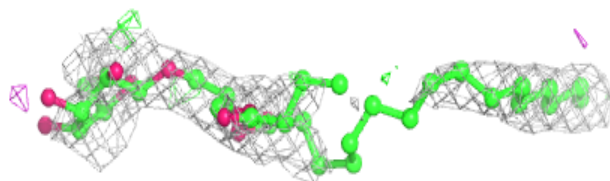
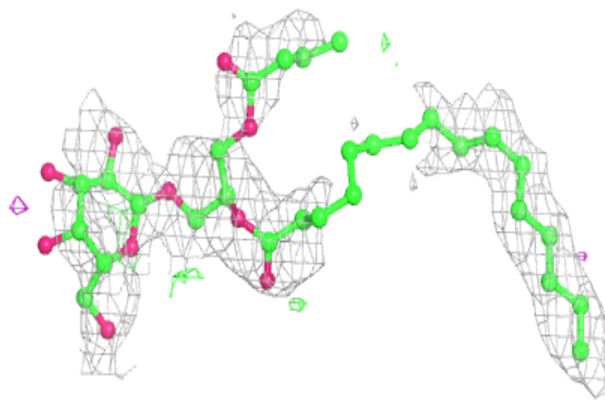


**Electron density around UNL a 418:**

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

**Electron density around LMG z 101:**

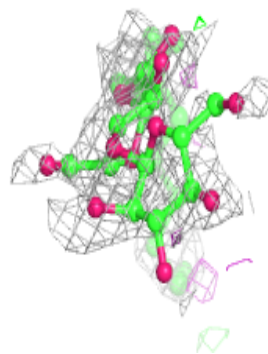
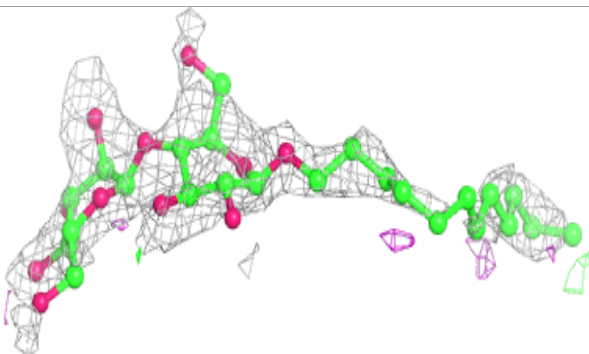
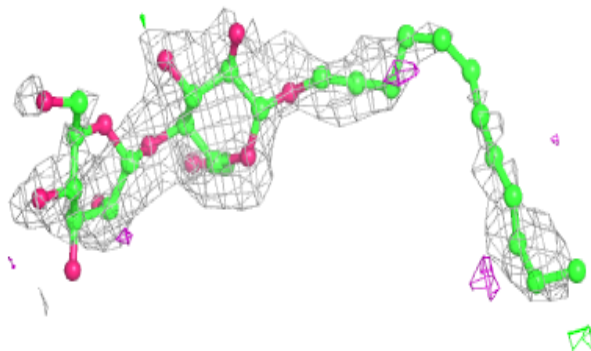
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



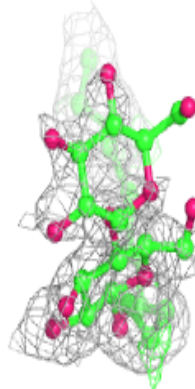
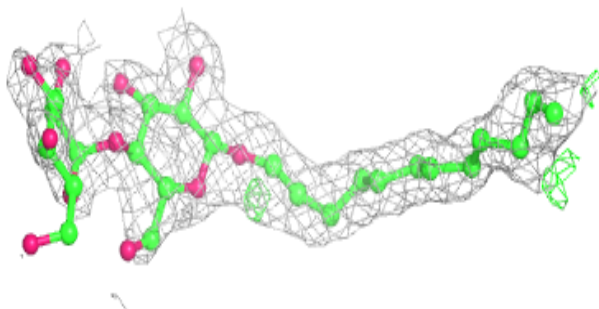
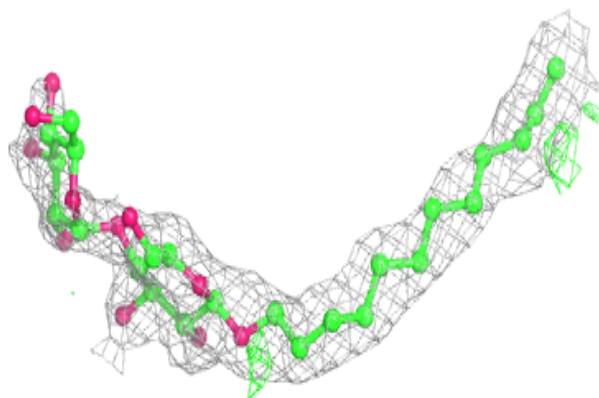


**Electron density around LMT C 522:**

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

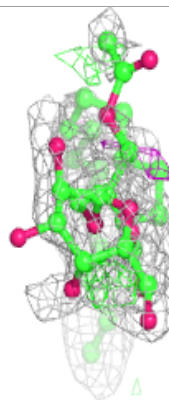
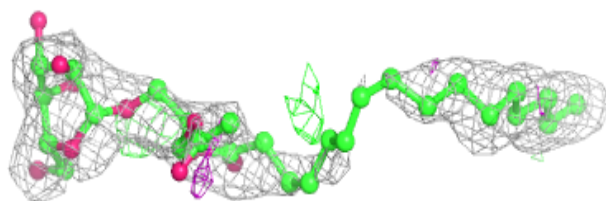
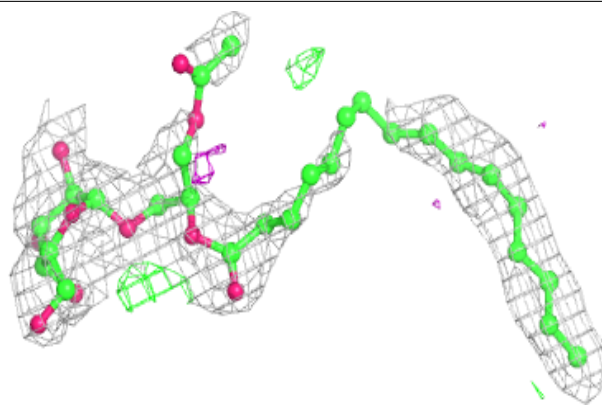
**Electron density around LMT m 104:**

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

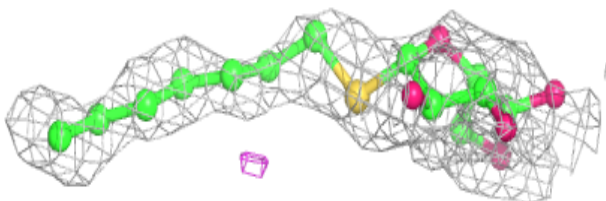
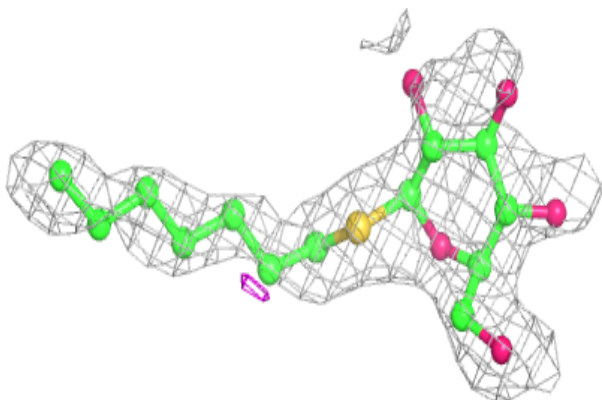


**Electron density around LMG Z 101:**

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

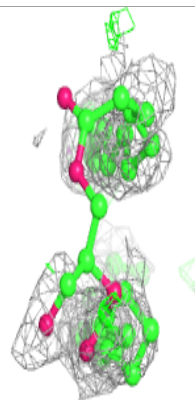
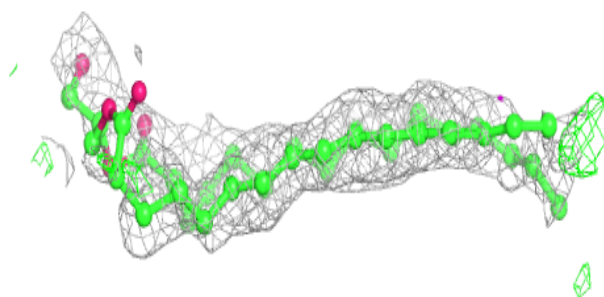
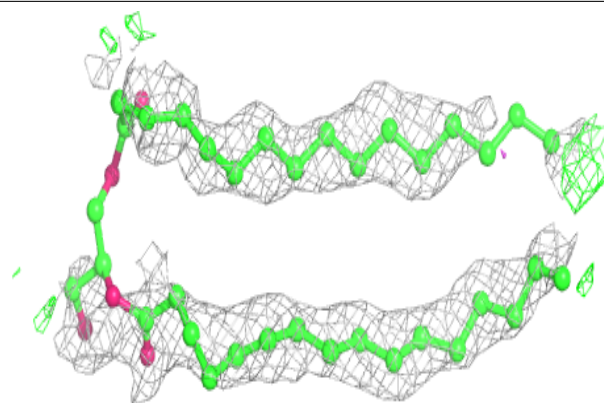
**Electron density around HTG C 524:**

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

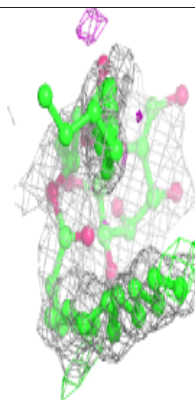
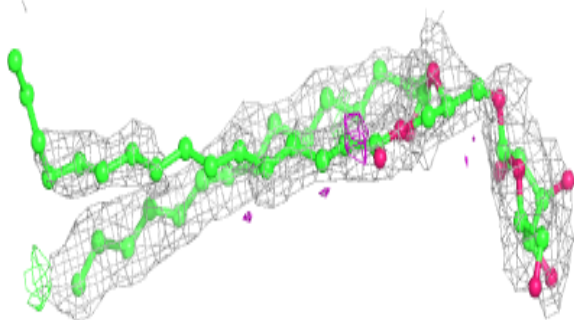
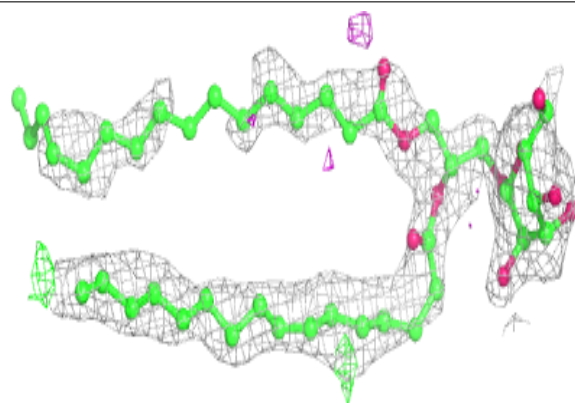


**Electron density around UNL i 101:**

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

**Electron density around LMG C 521:**

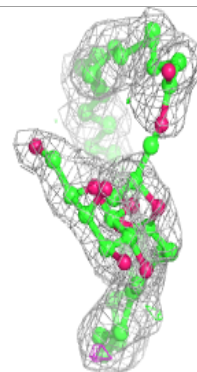
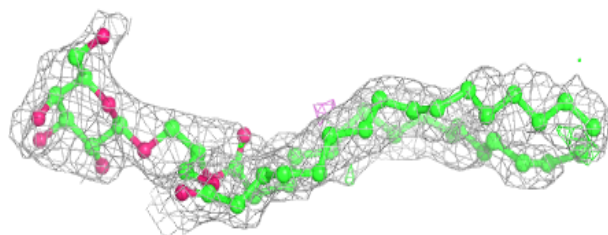
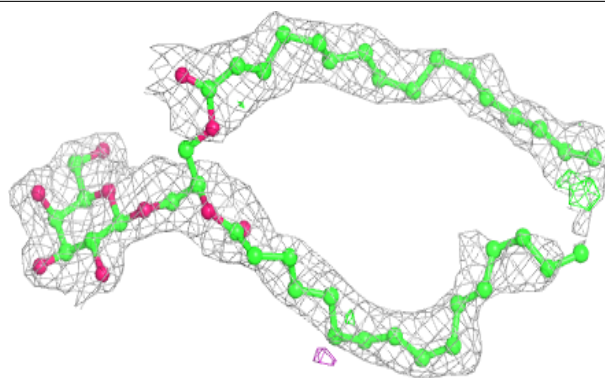
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



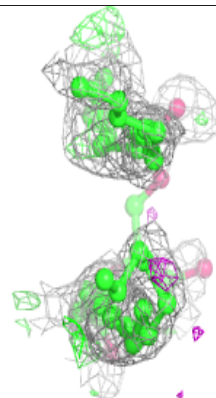
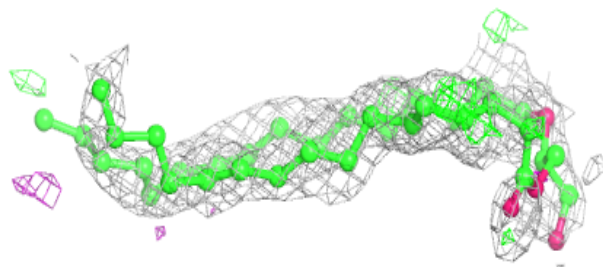
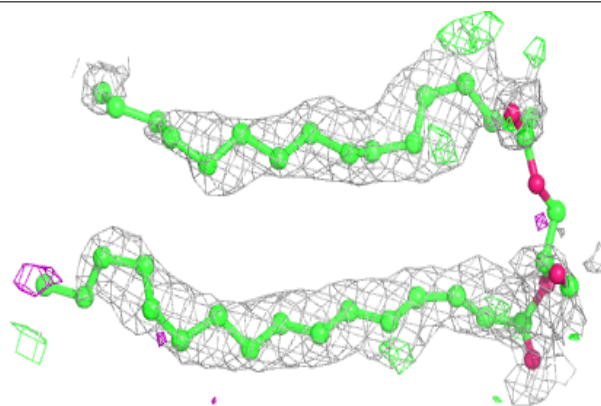


**Electron density around LMG a 412:**

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

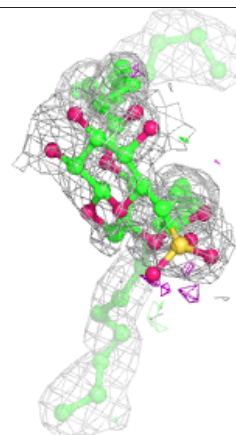
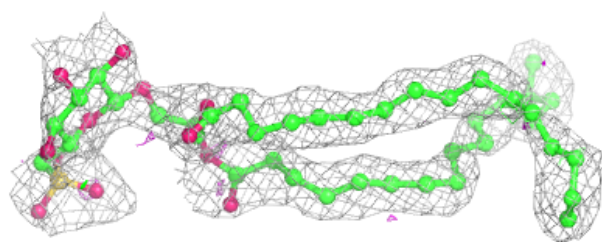
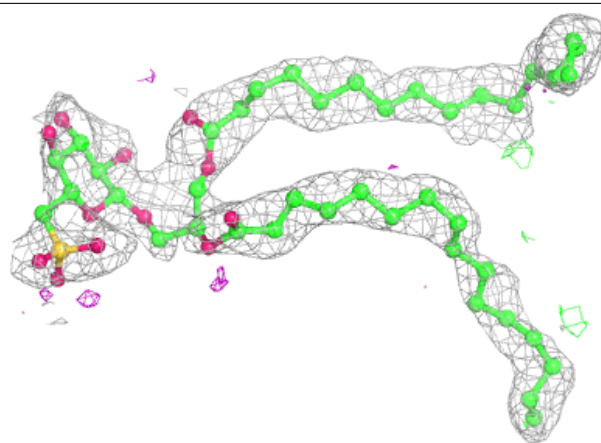
**Electron density around UNL I 101:**

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



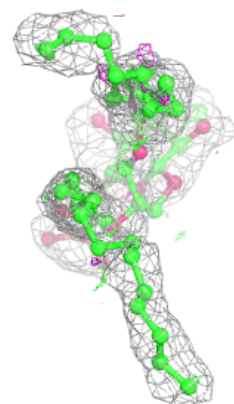
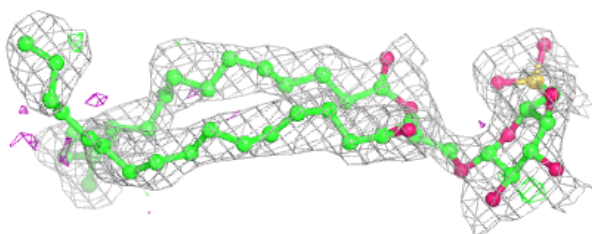
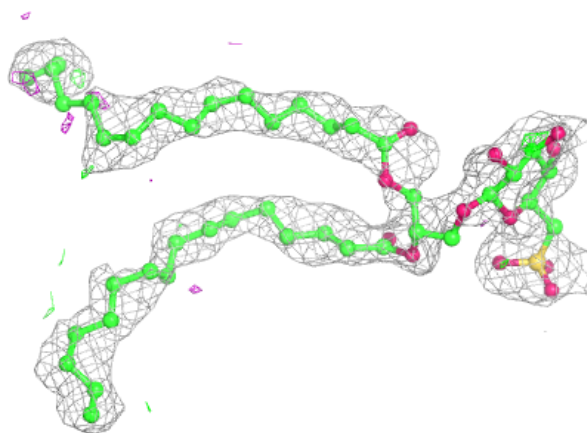
**Electron density around SQD B 621:**

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



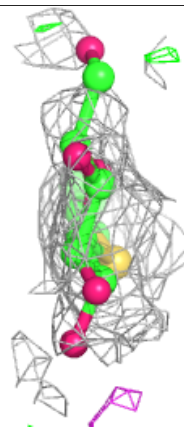
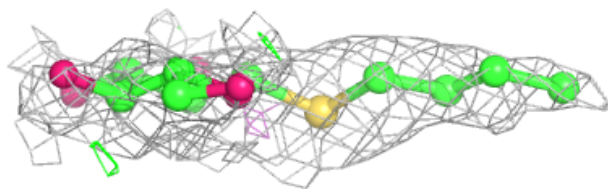
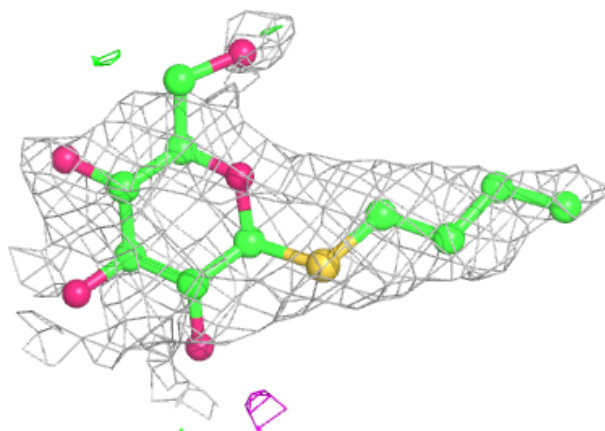
**Electron density around SQD L 102:**

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

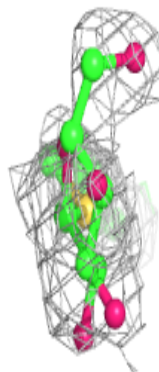
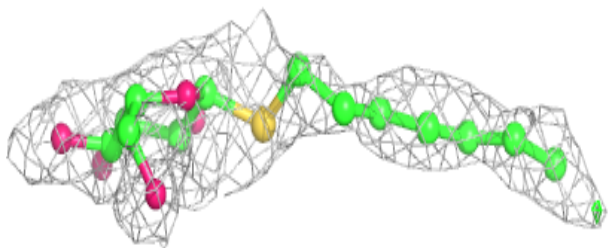
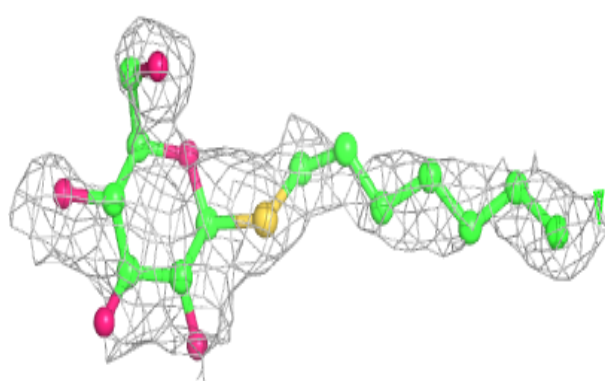


**Electron density around HTG D 411:**

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

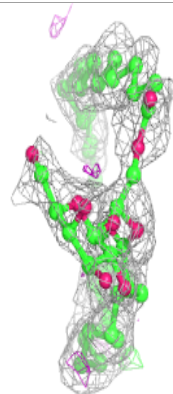
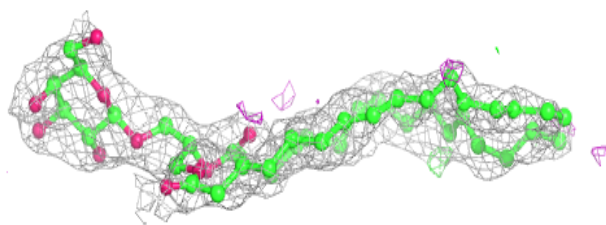
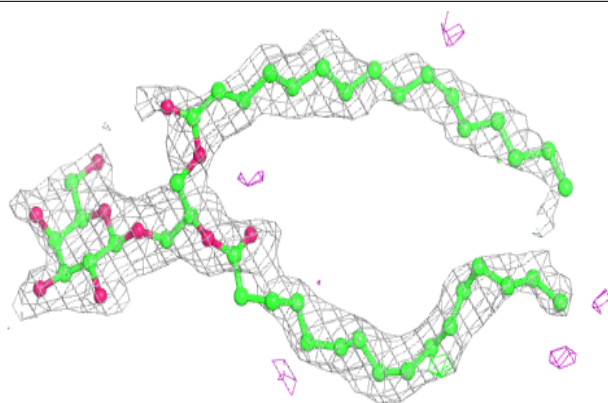
**Electron density around HTG c 923:**

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

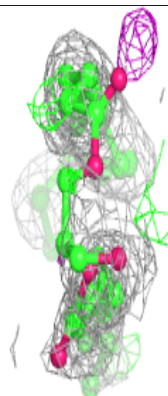
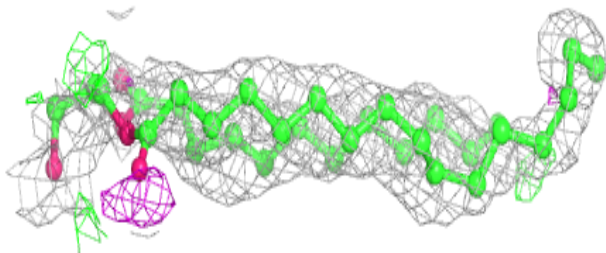
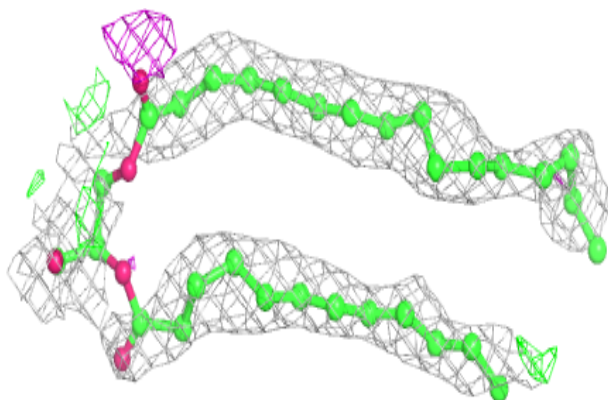


**Electron density around LMG C 501:**

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

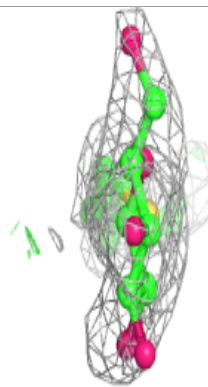
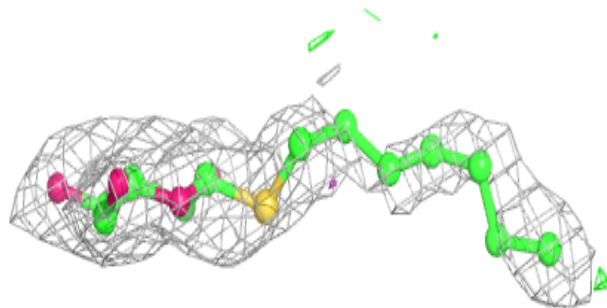
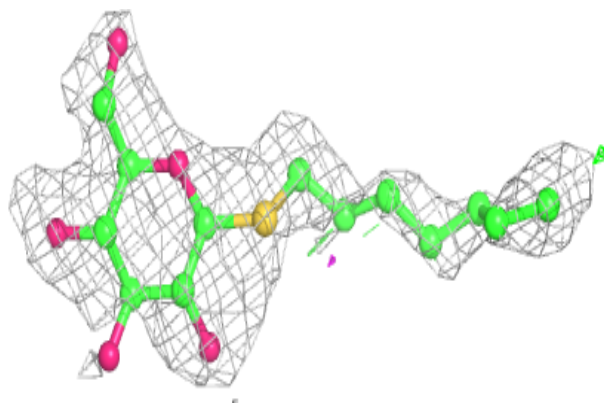
**Electron density around UNL d 411:**

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

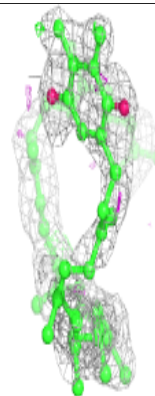
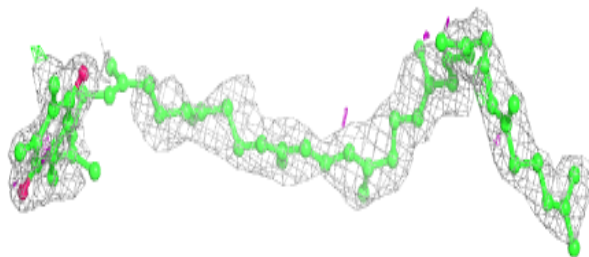
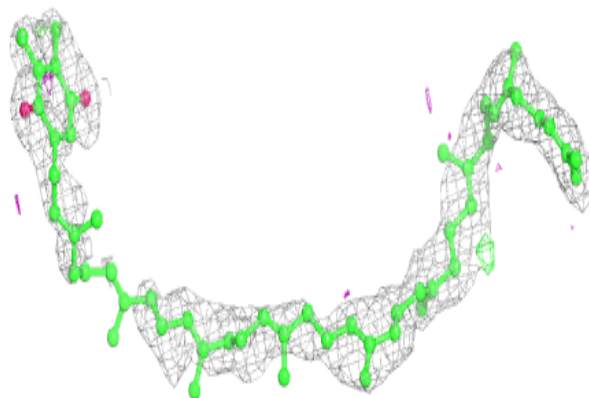


**Electron density around HTG c 922:**

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

**Electron density around PL9 A 419:**

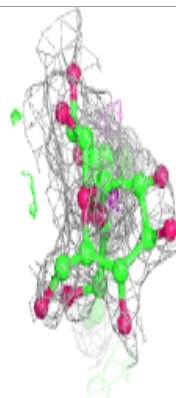
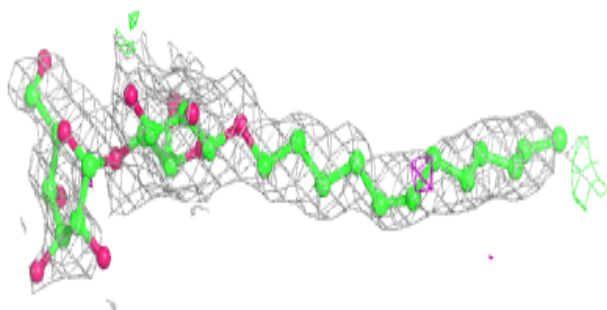
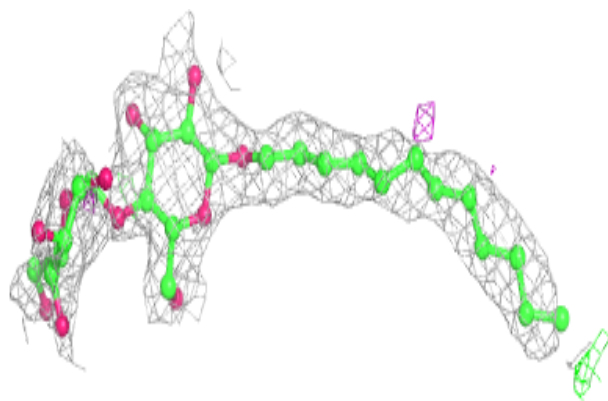
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



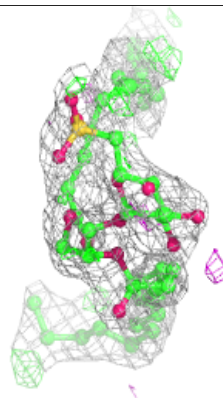
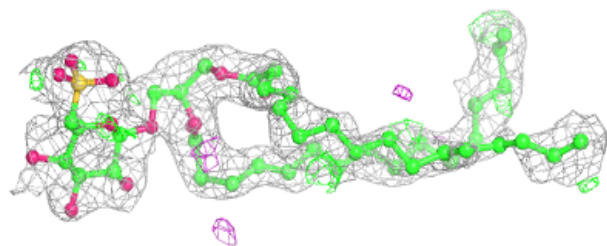
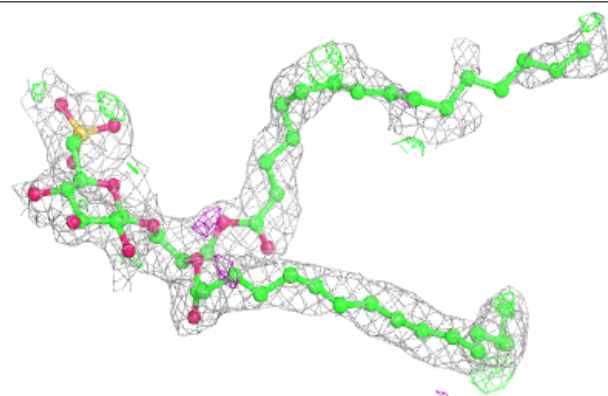


**Electron density around LMT B 623:**

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

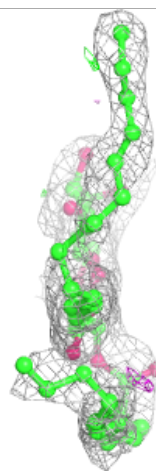
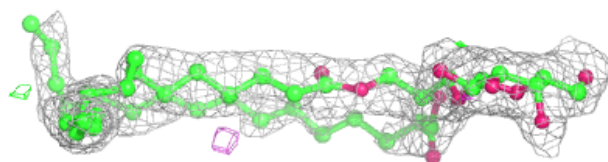
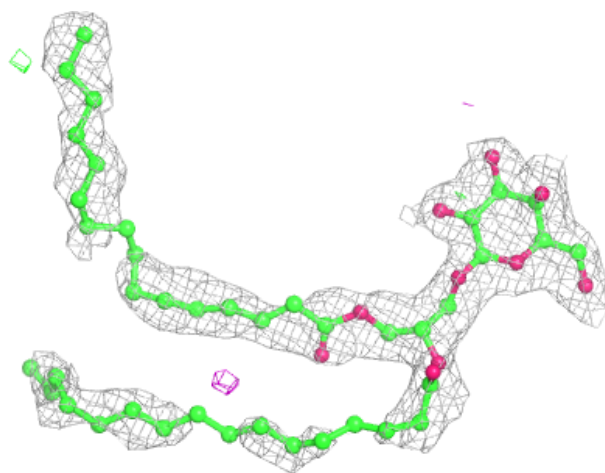
**Electron density around SQD a 402:**

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



**Electron density around LMG c 919:**

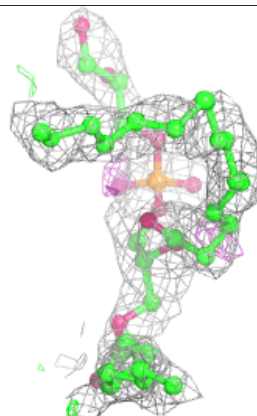
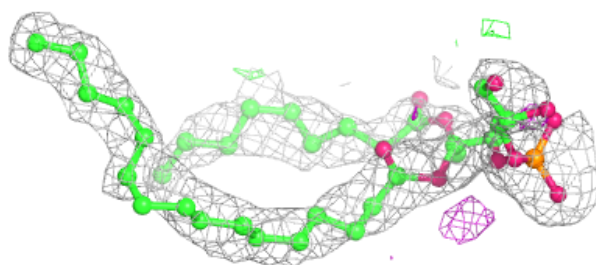
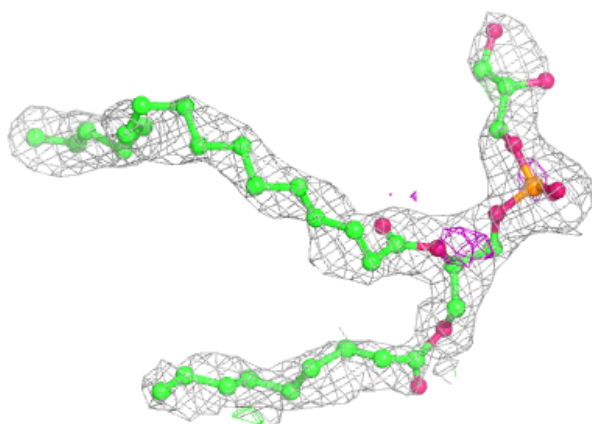
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



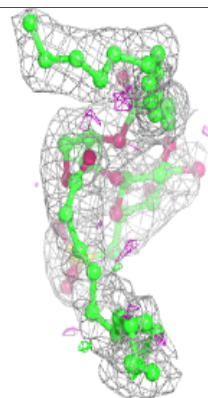
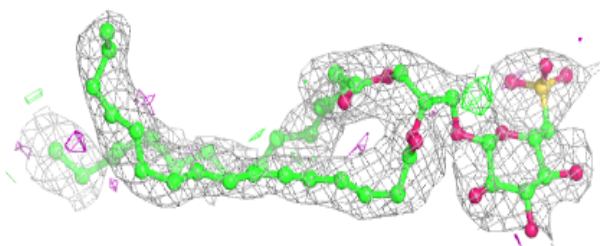
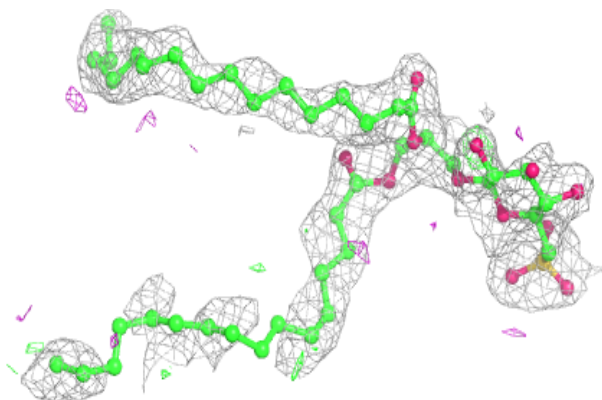


**Electron density around LHG E 101:**

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

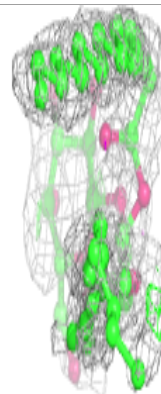
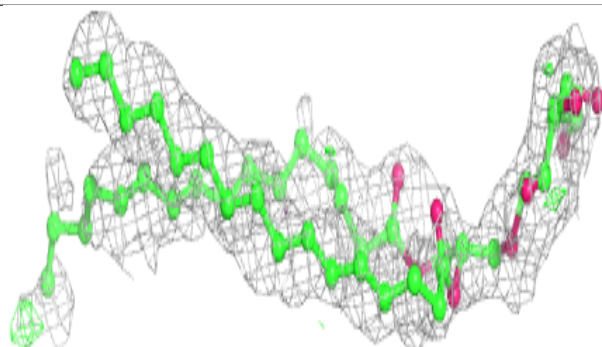
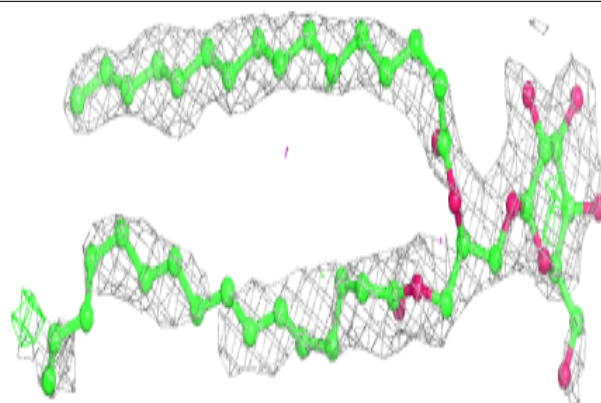
**Electron density around SQD A 416:**

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

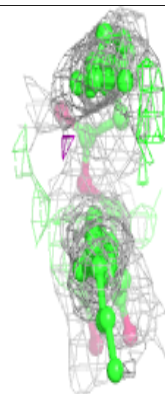
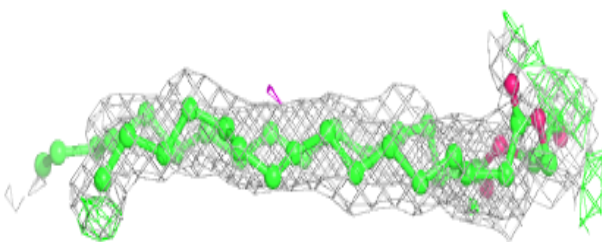
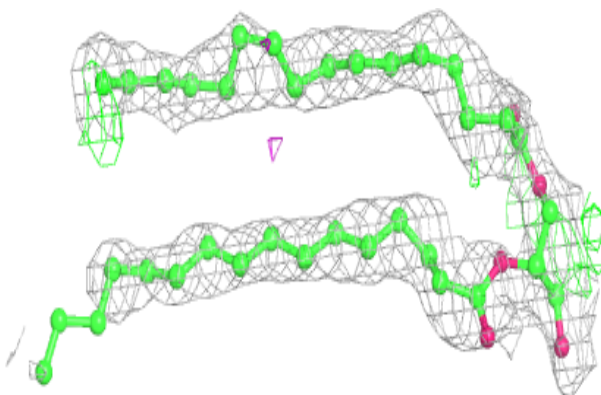


**Electron density around LMG c 920:**

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

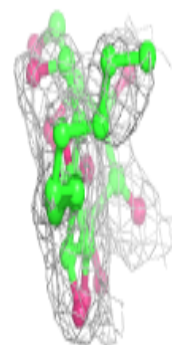
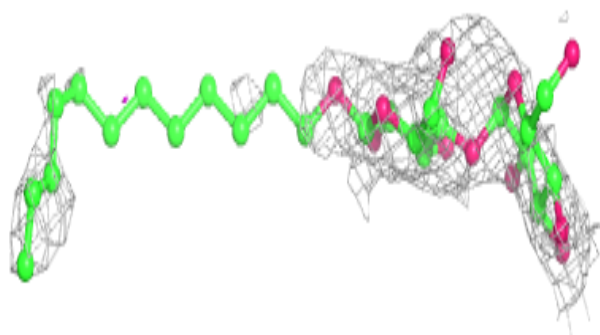
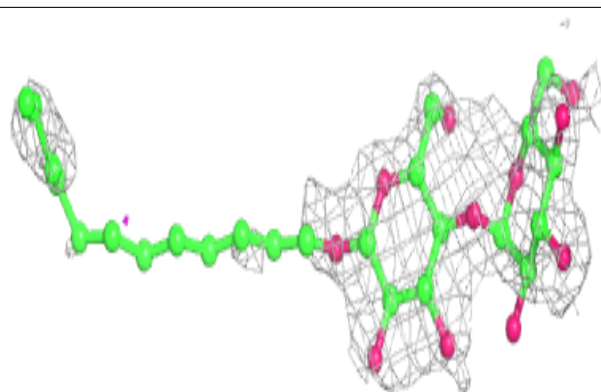
**Electron density around UNL D 410:**

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

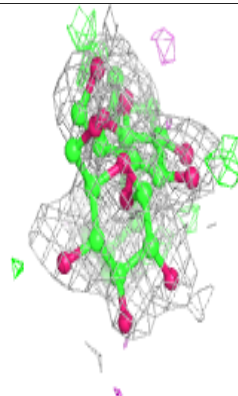
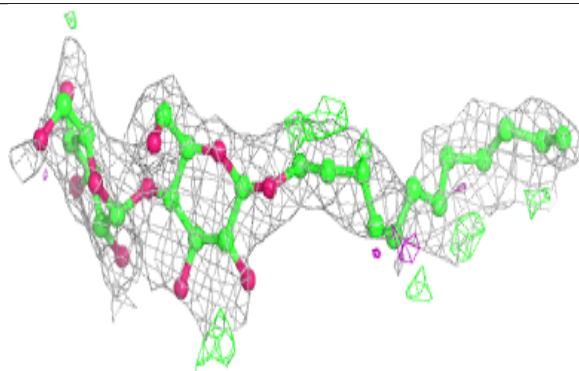
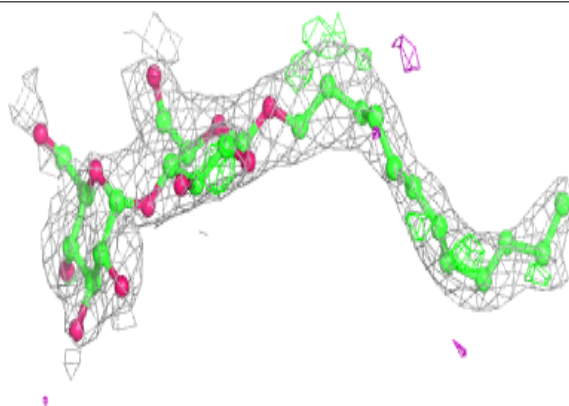


**Electron density around LMT c 921:**

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

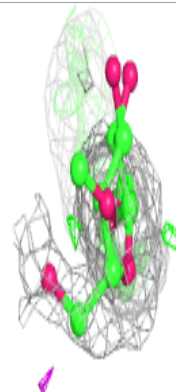
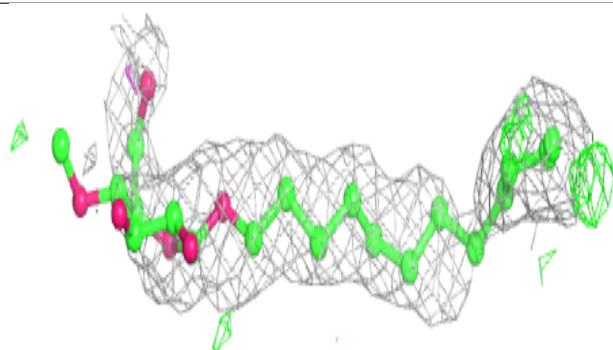
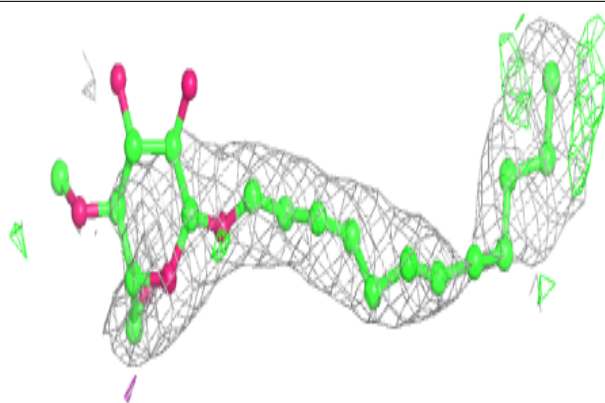
**Electron density around LMT a 401:**

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

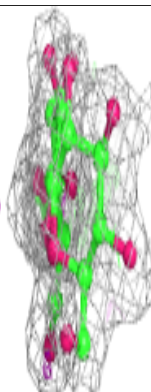
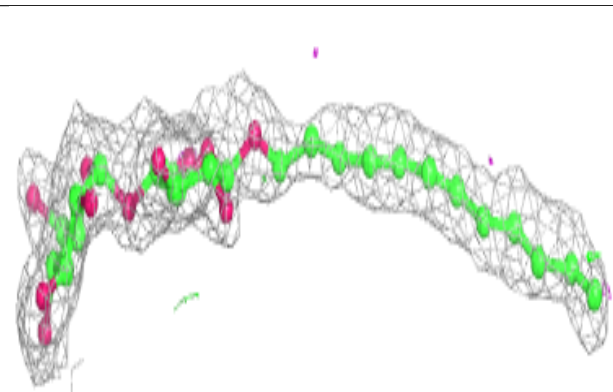
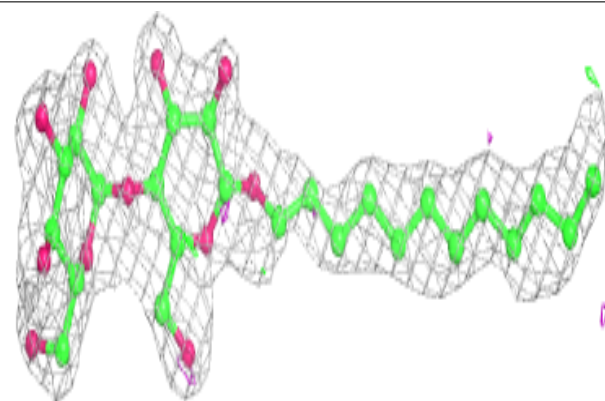


**Electron density around LMT b 601:**

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

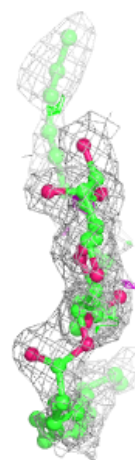
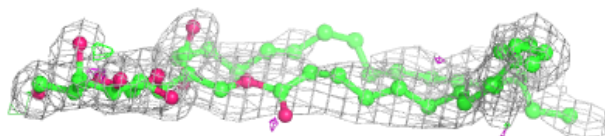
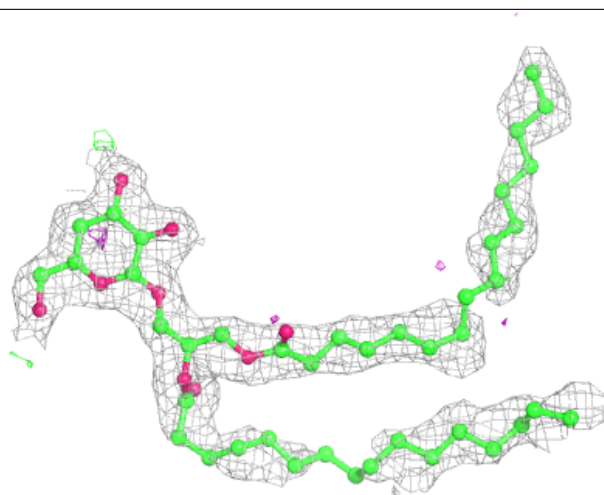
**Electron density around LMT m 103:**

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



**Electron density around LMG C 520:**

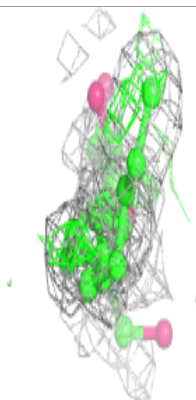
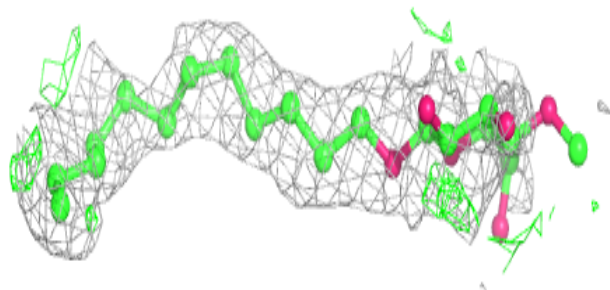
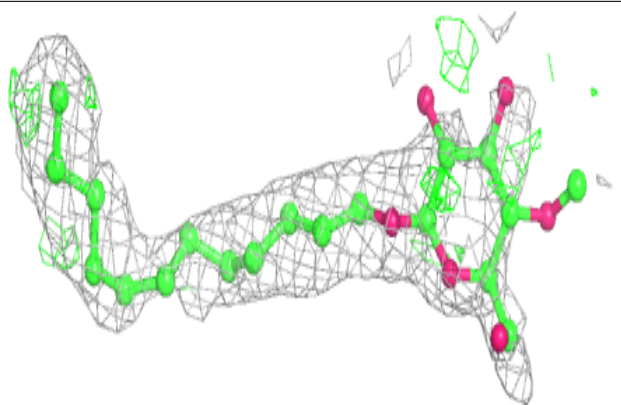
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



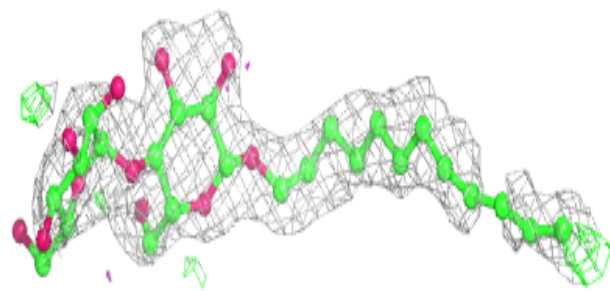
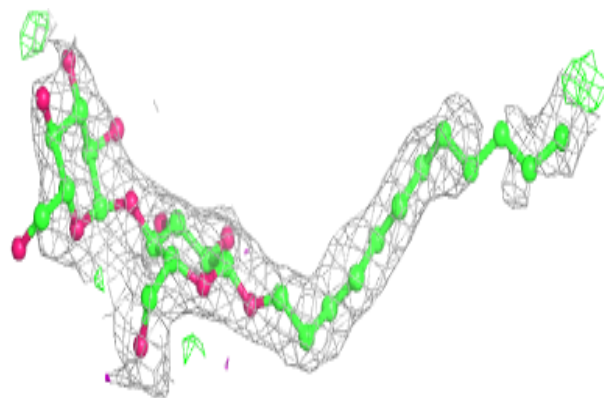


**Electron density around LMT B 636:**

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

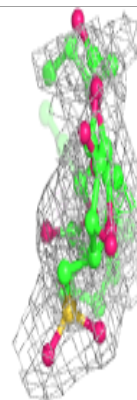
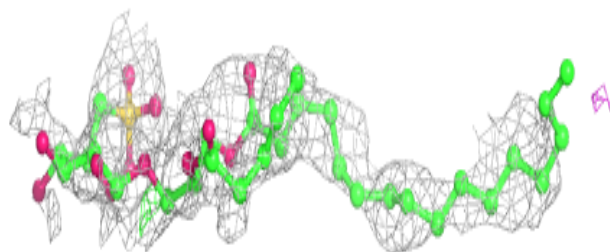
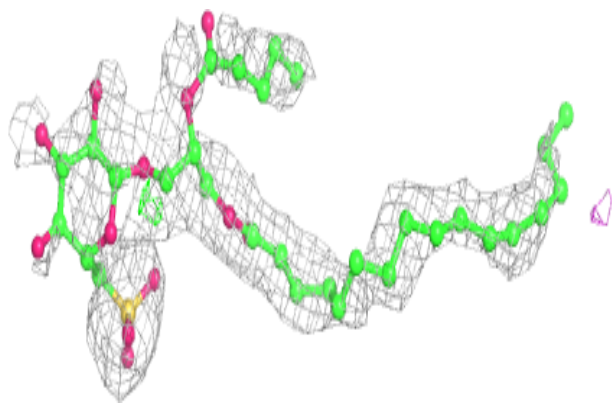
**Electron density around LMT A 417:**

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



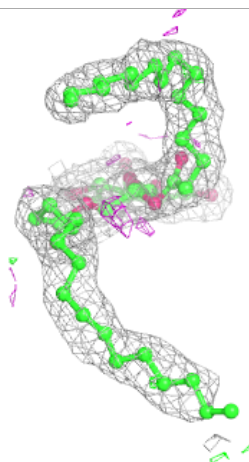
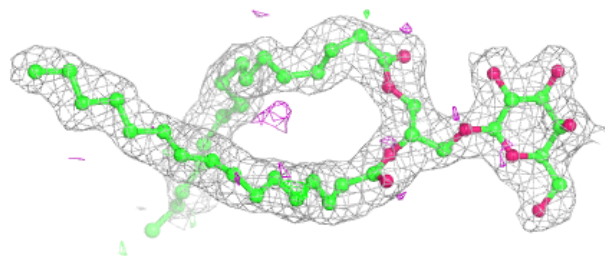
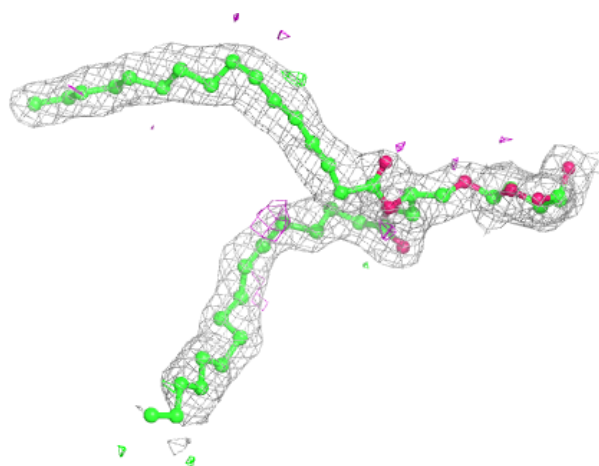
**Electron density around SQD f 102:**

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



**Electron density around LMG B 622:**

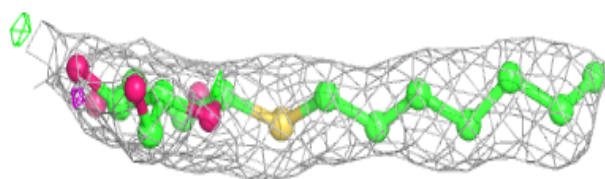
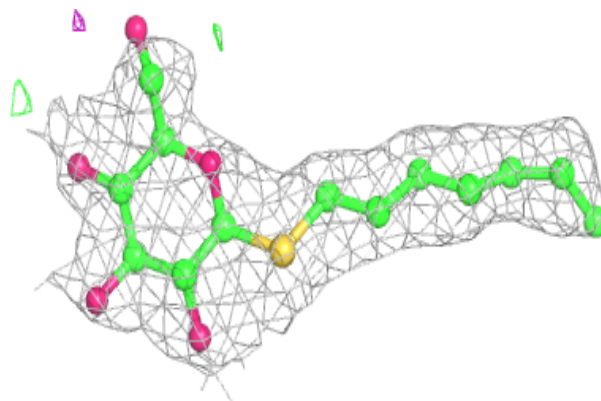
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



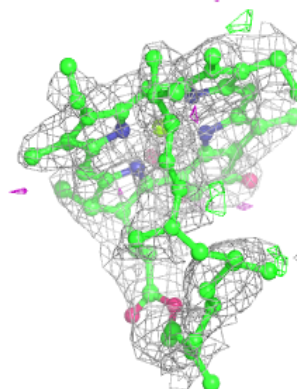
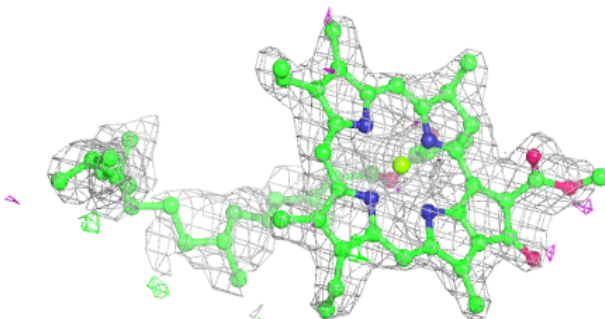
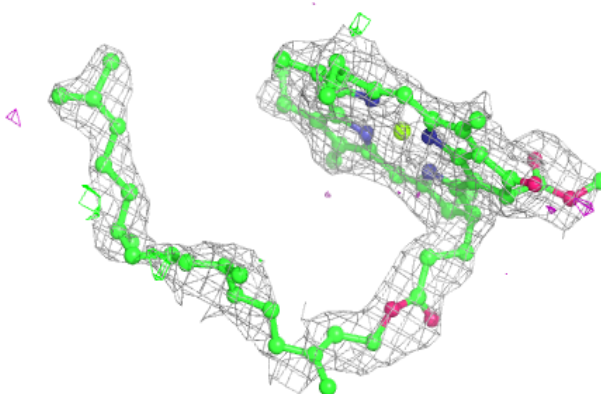


**Electron density around HTG B 633:**

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

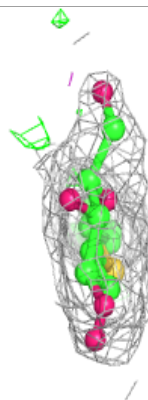
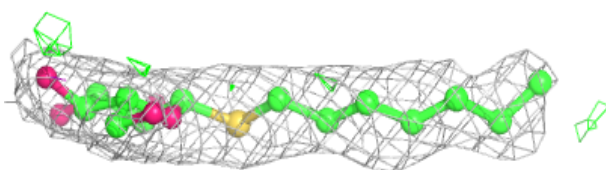
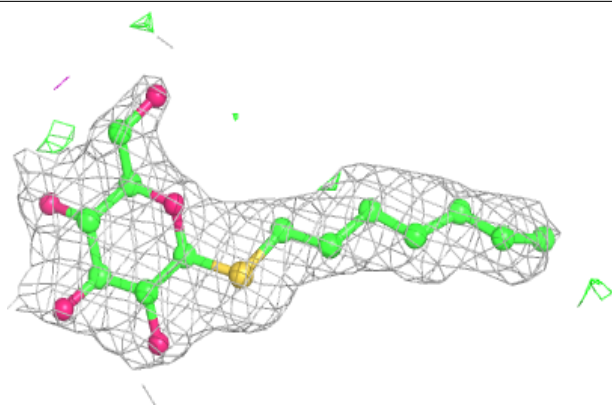
**Electron density around CLA c 914:**

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

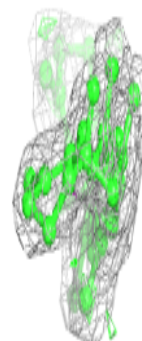
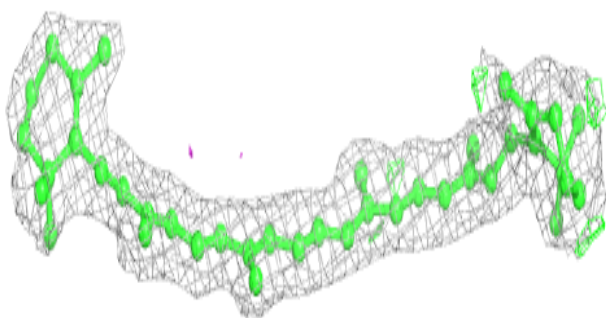
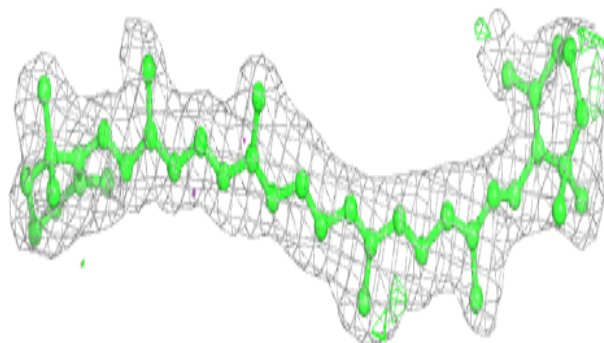


**Electron density around HTG b 602:**

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

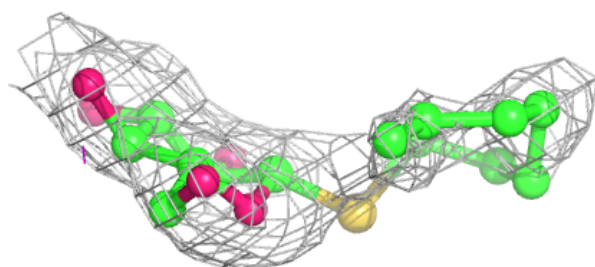
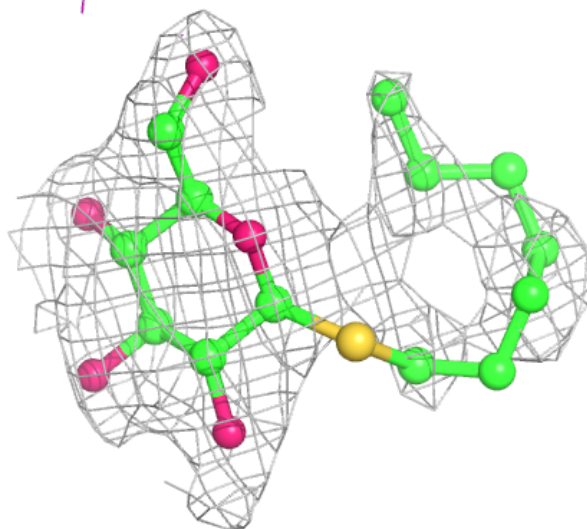
**Electron density around BCR d 404:**

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



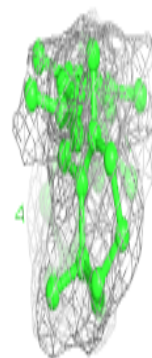
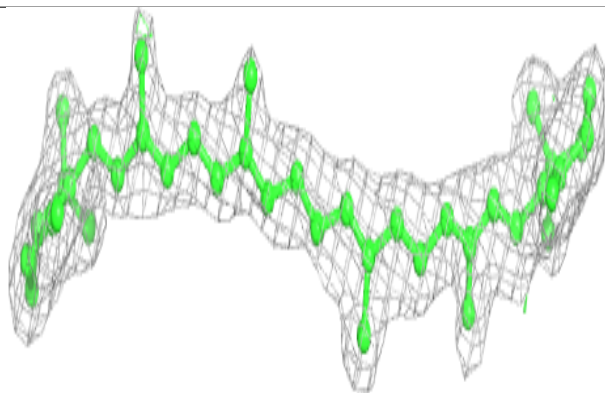
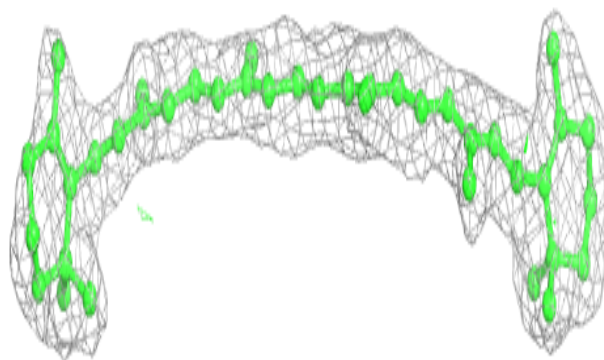
**Electron density around HTG V 202:**

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

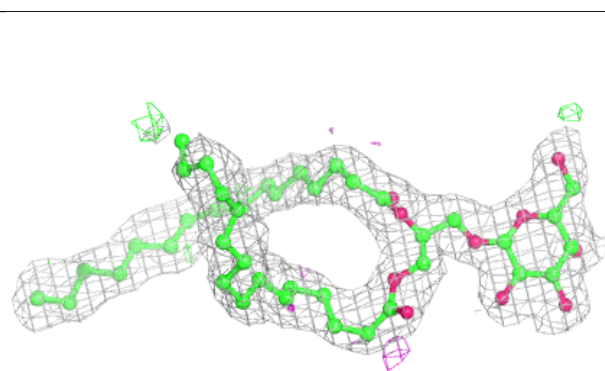
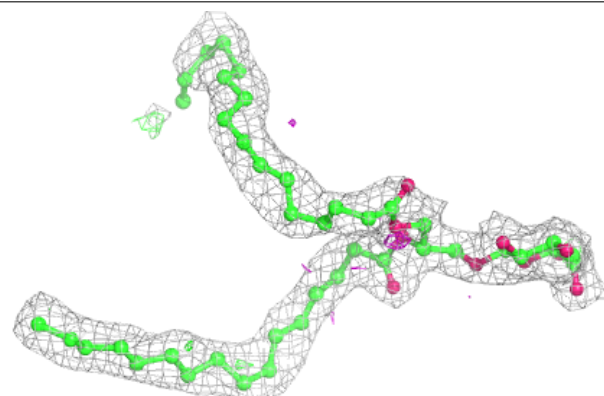


**Electron density around BCR k 102:**

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

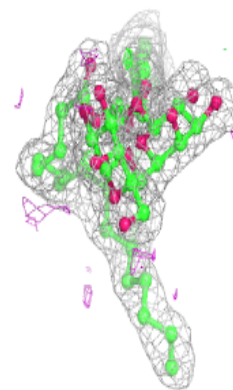
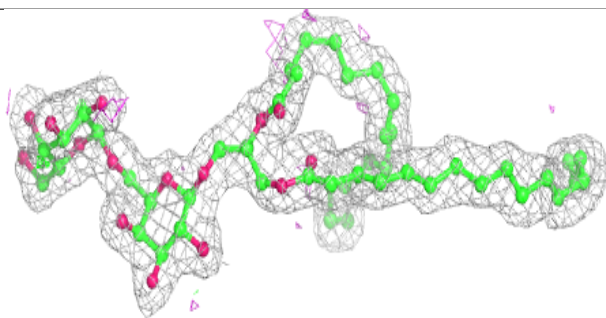
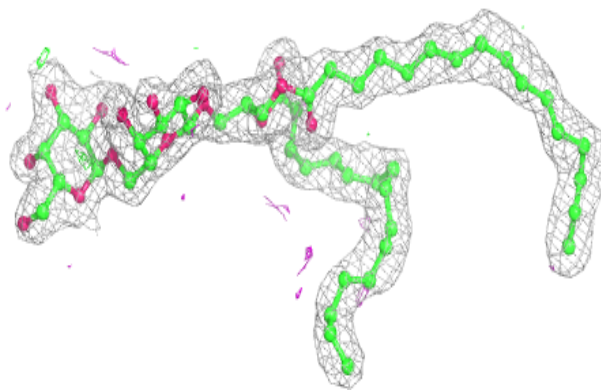
**Electron density around LMG b 624:**

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

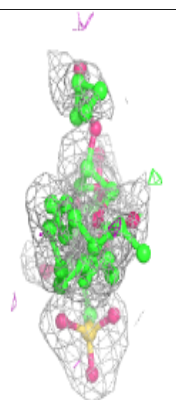
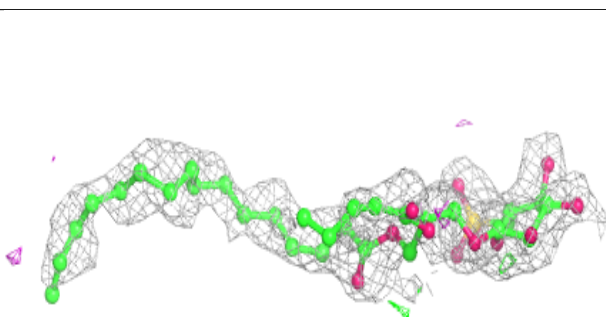
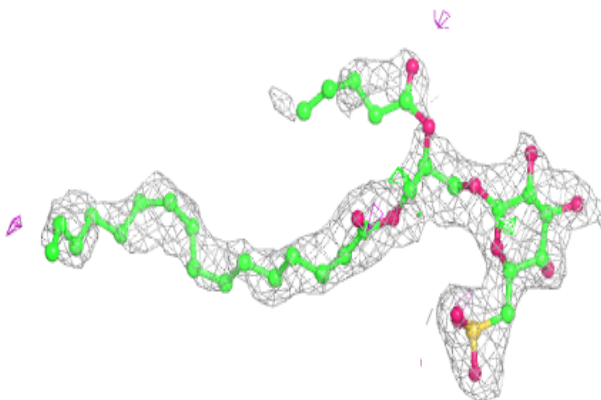


**Electron density around DGD H 102:**

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

**Electron density around SQD F 101:**

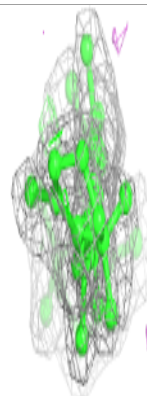
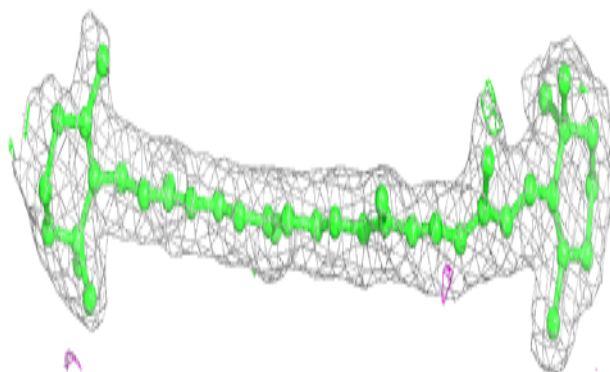
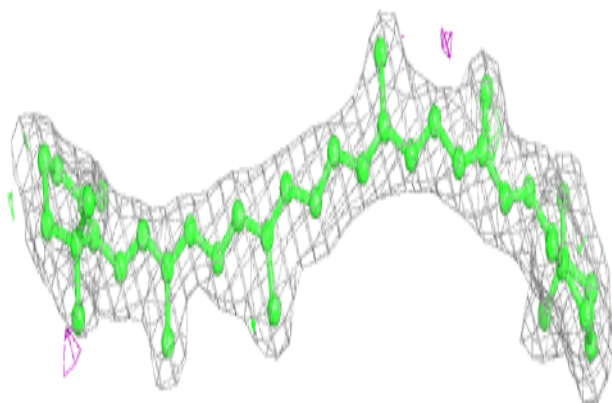
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



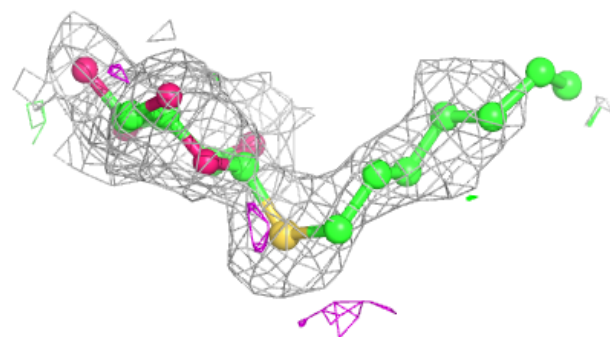
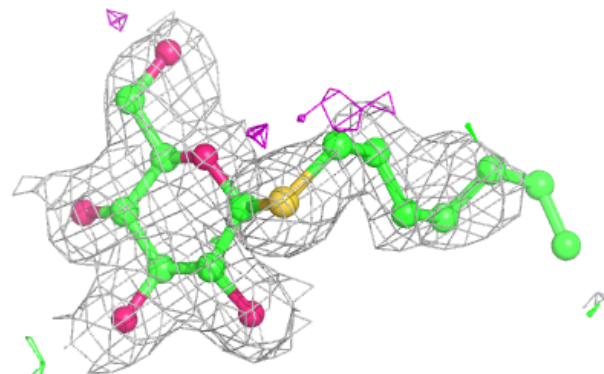


**Electron density around BCR h 101:**

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

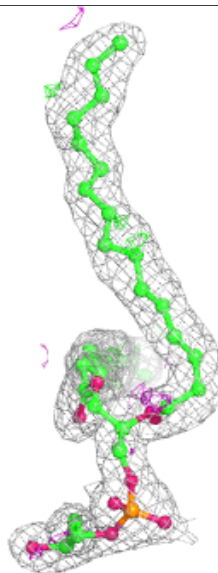
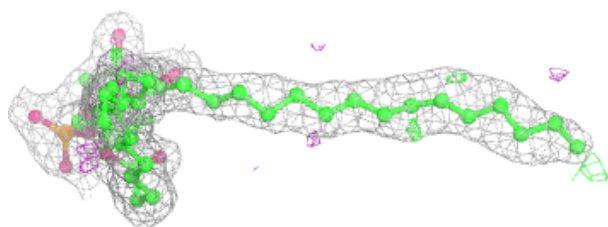
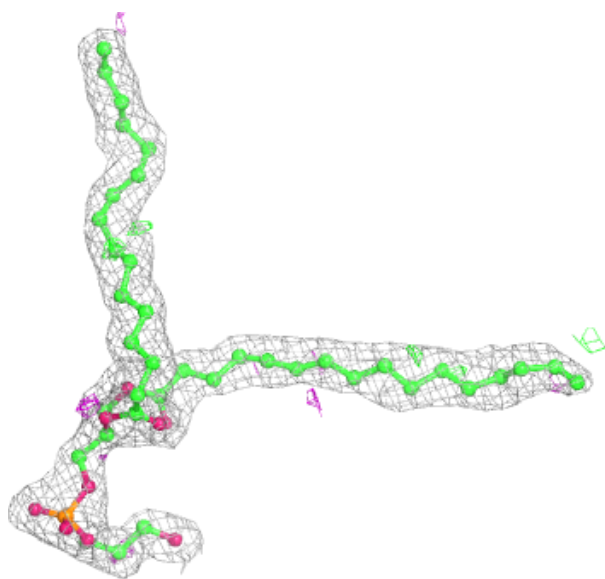
**Electron density around HTG b 626:**

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



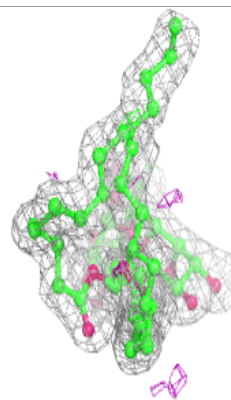
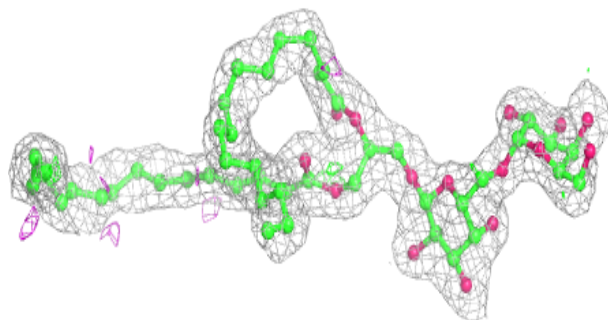
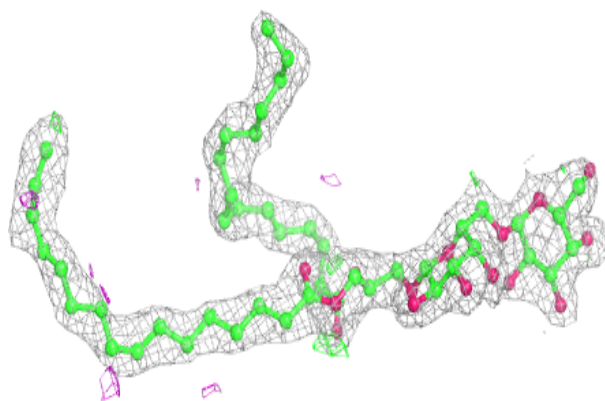
**Electron density around LHG 1 101:**

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

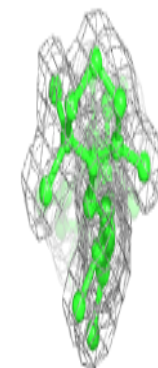
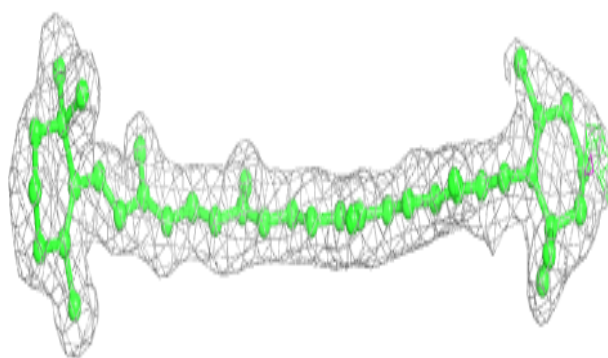
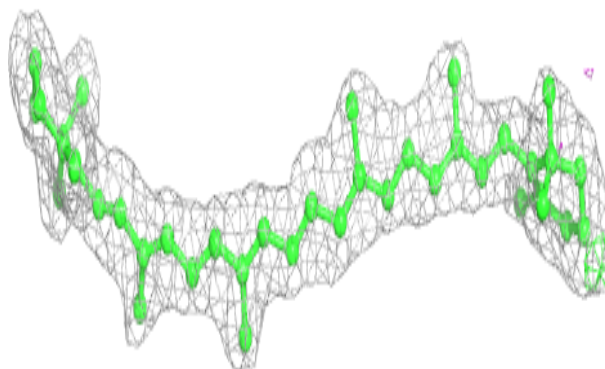


**Electron density around DGD h 102:**

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

**Electron density around BCR H 101:**

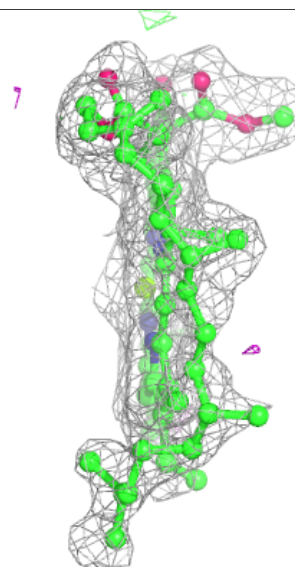
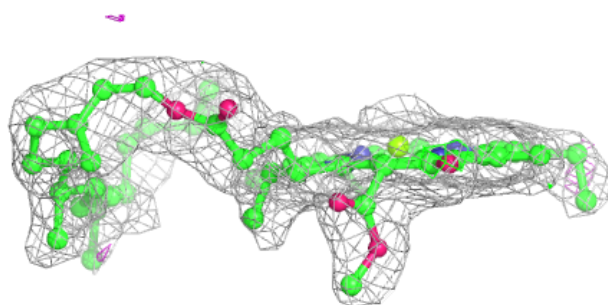
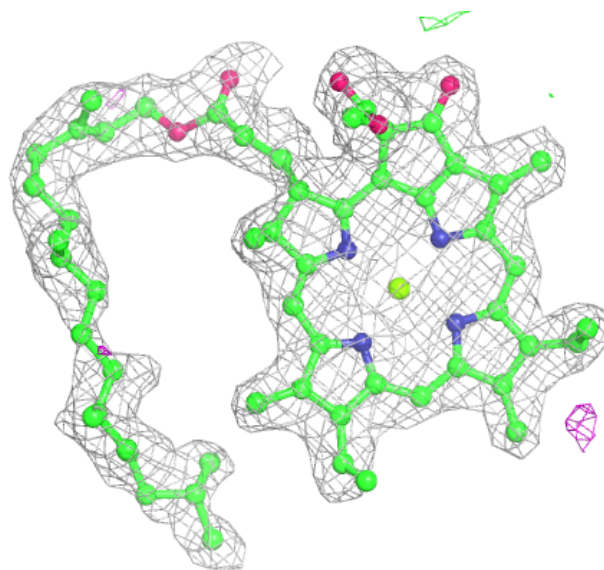
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





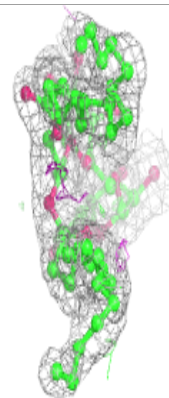
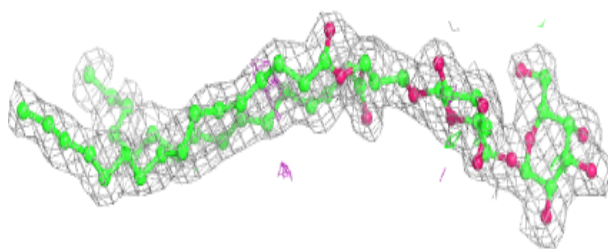
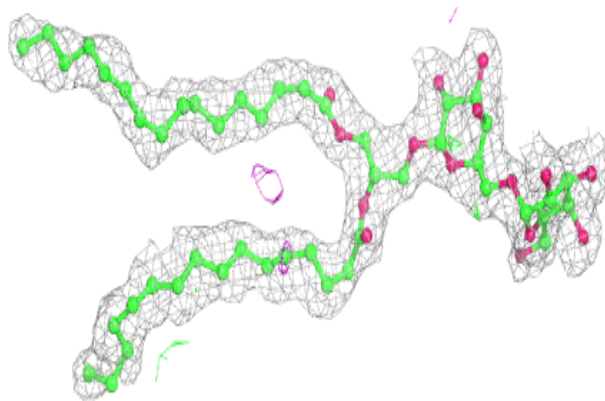
**Electron density around CLA c 913:**

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

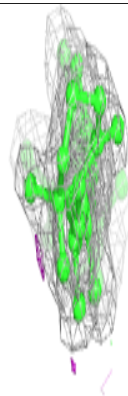
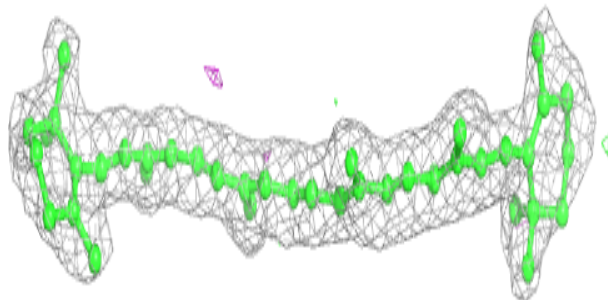
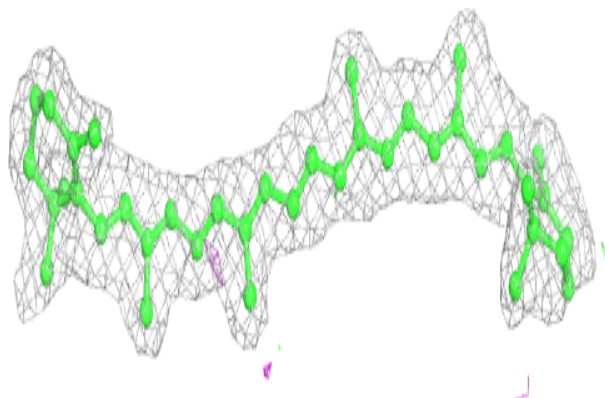


**Electron density around DGD c 918:**

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

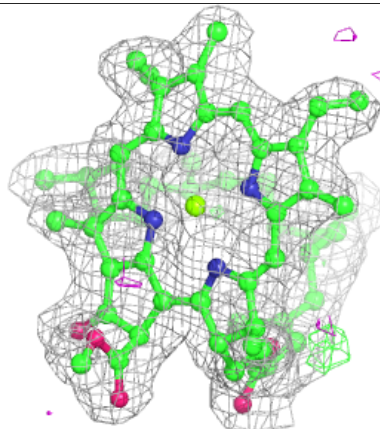
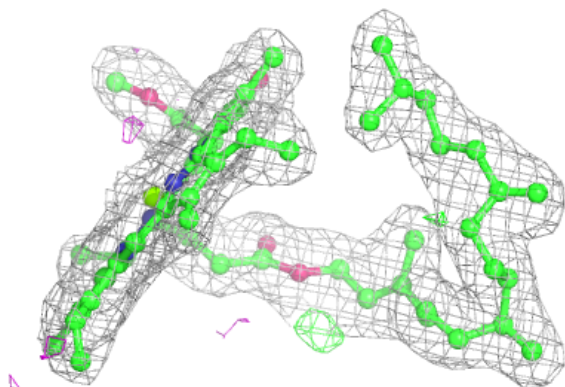
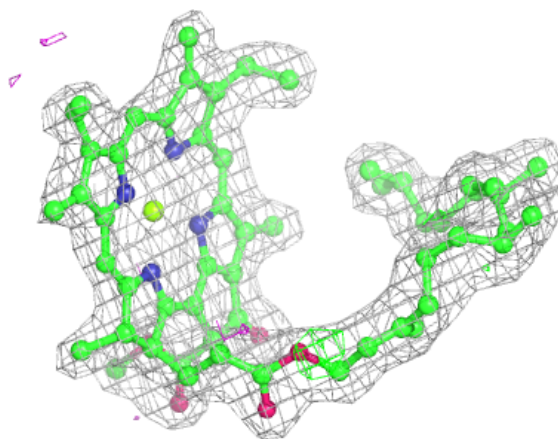
**Electron density around BCR y 101:**

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



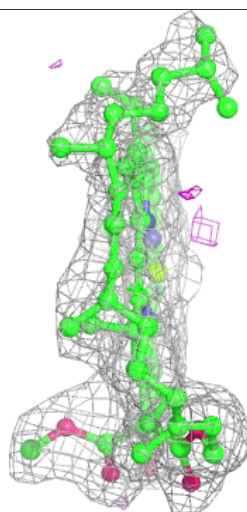
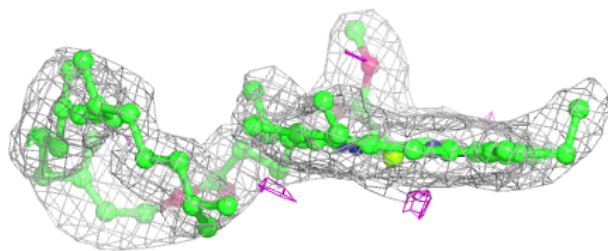
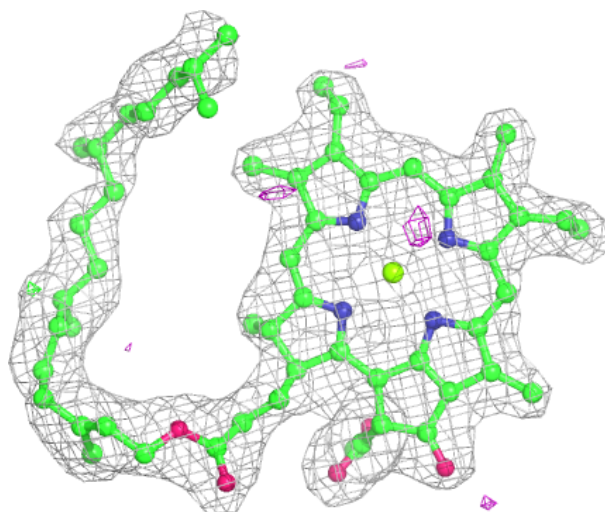
**Electron density around CLA c 904:**

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



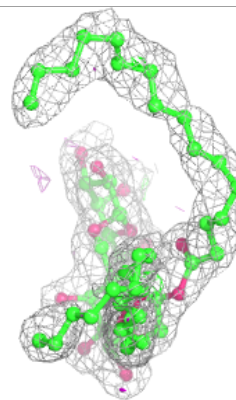
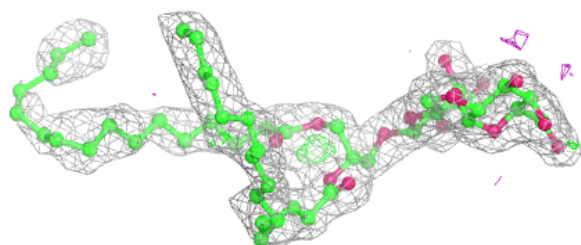
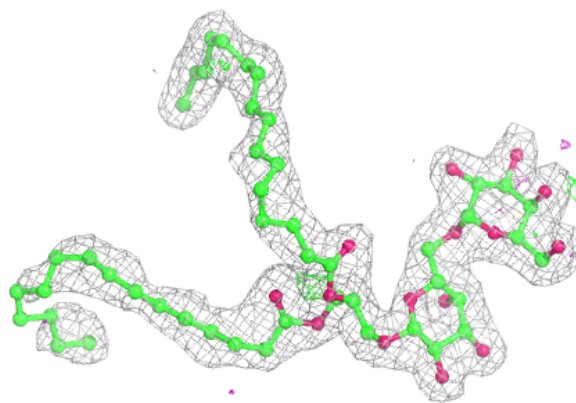
**Electron density around CLA C 513:**

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



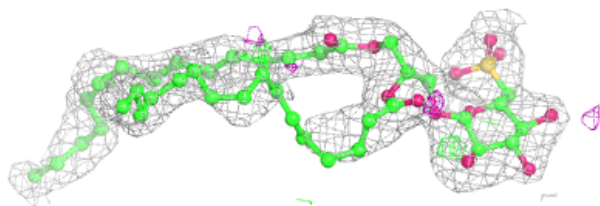
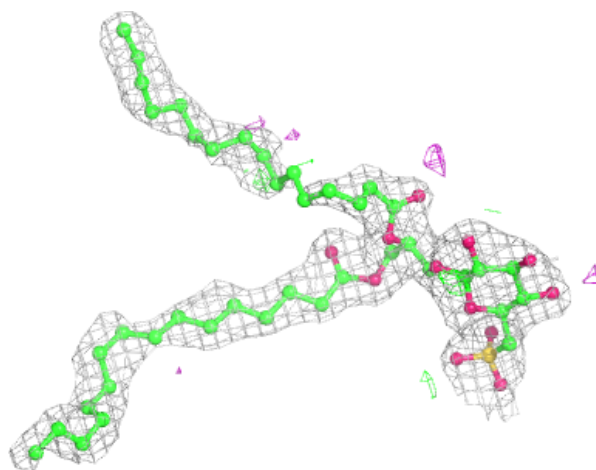
**Electron density around DGD c 917:**

$2mF_o-DF_c$  (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:**

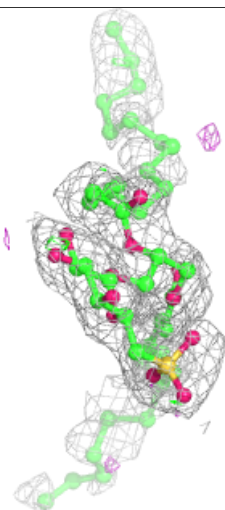
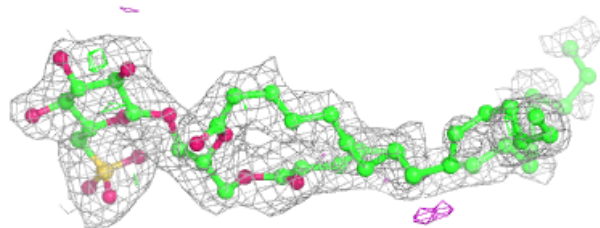
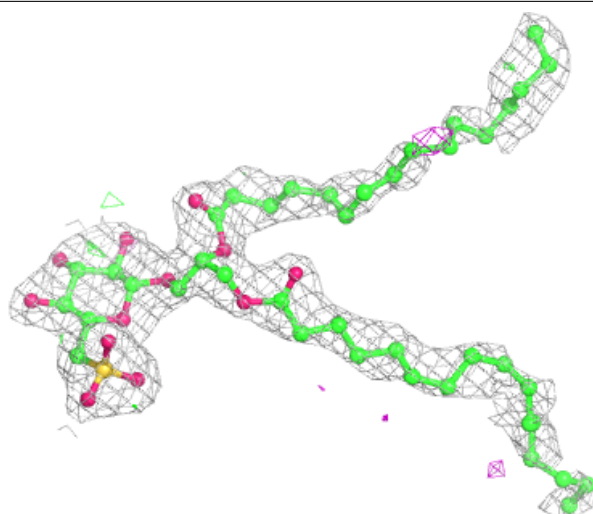
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





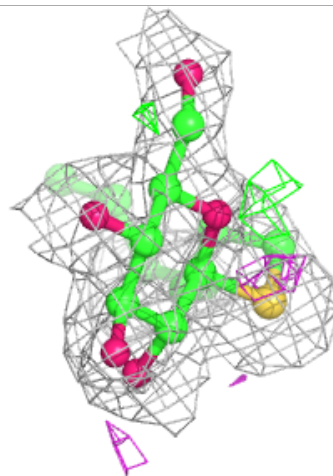
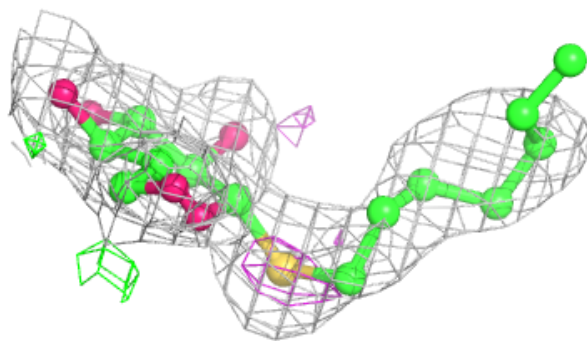
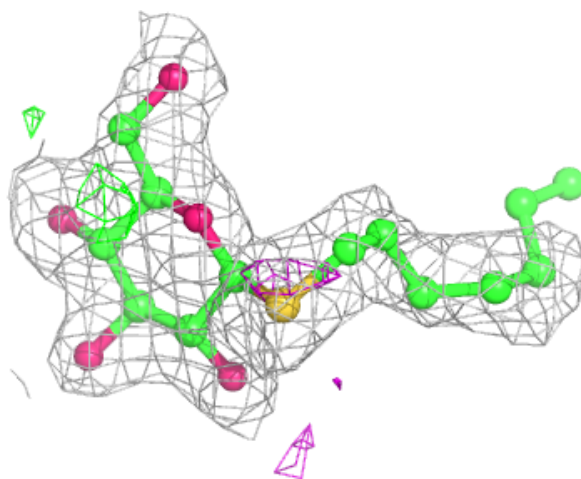
**Electron density around SQD a 411:**

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



**Electron density around HTG B 625:**

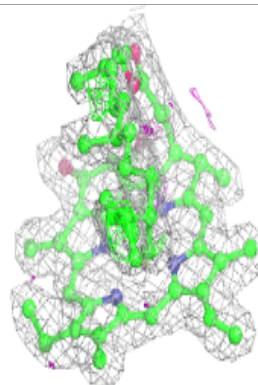
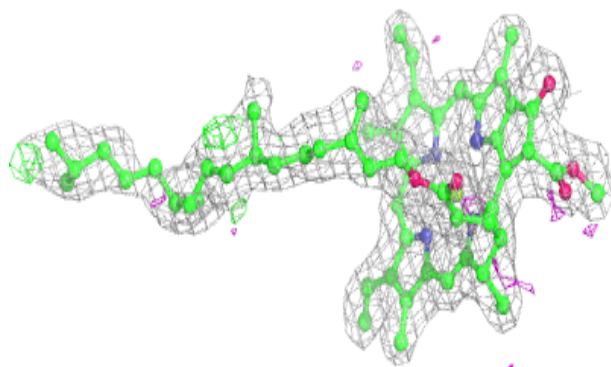
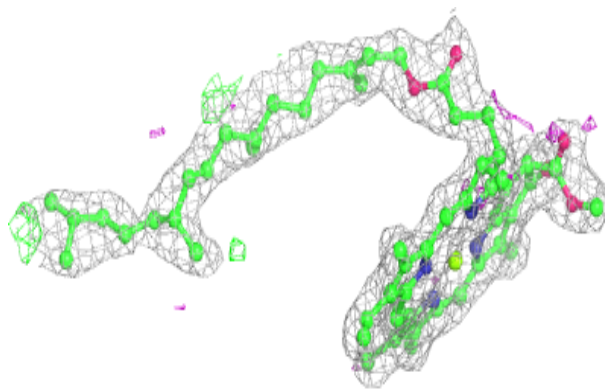
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



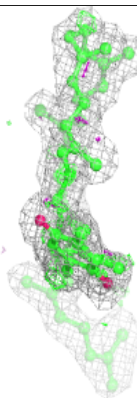
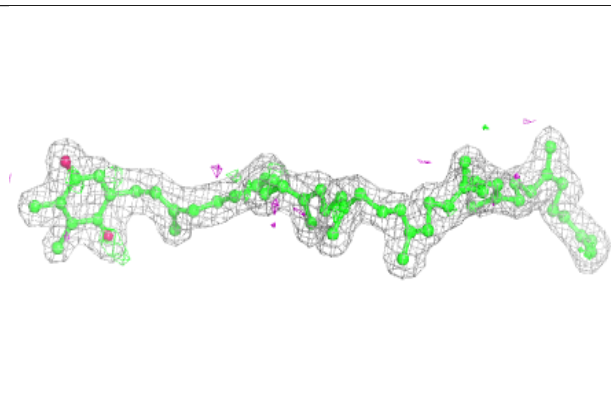
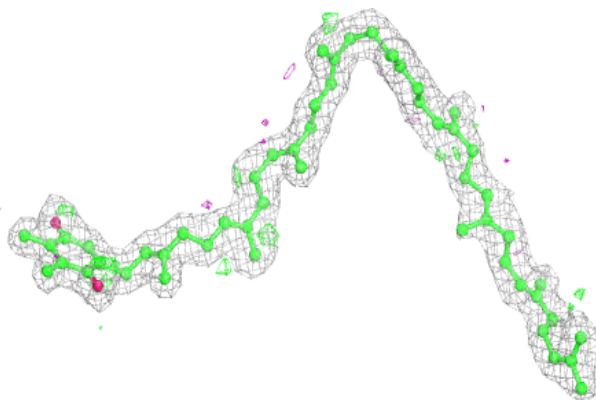


**Electron density around CLA c 905:**

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

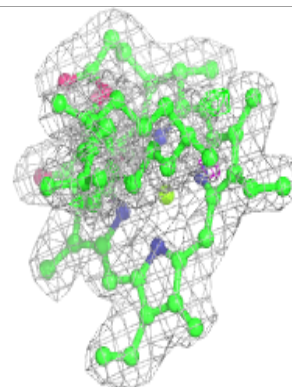
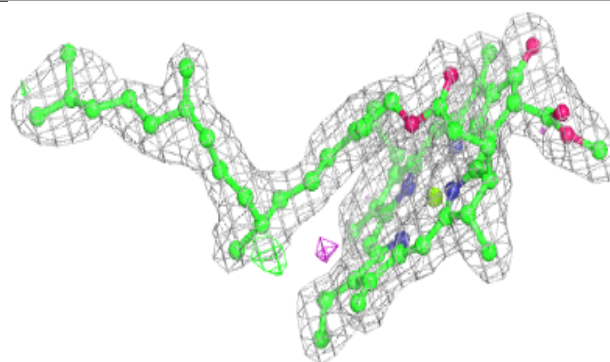
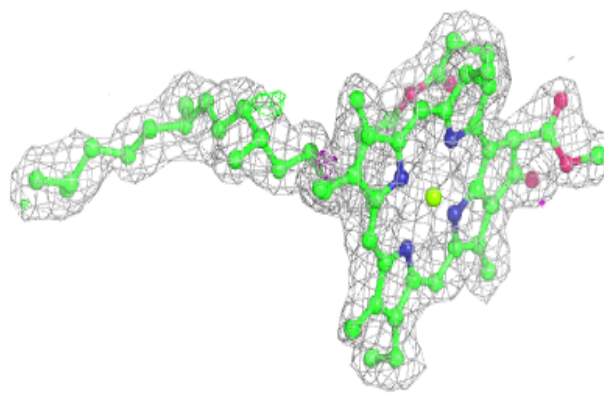
**Electron density around PL9 d 405:**

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

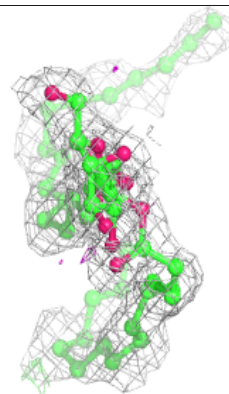
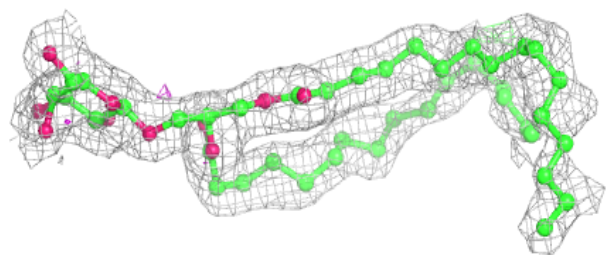
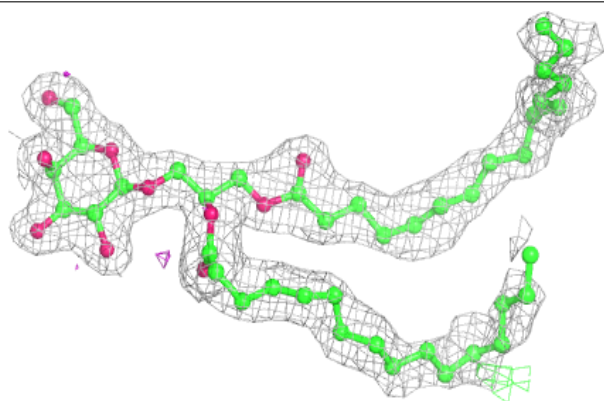


**Electron density around CLA c 906:**

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

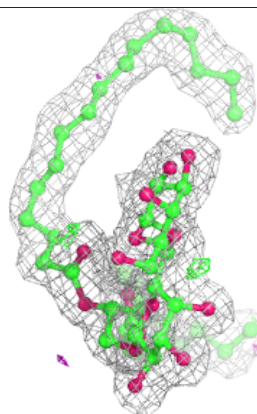
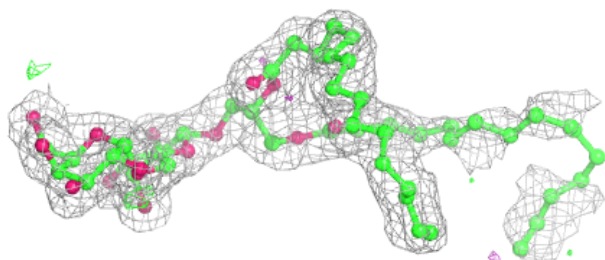
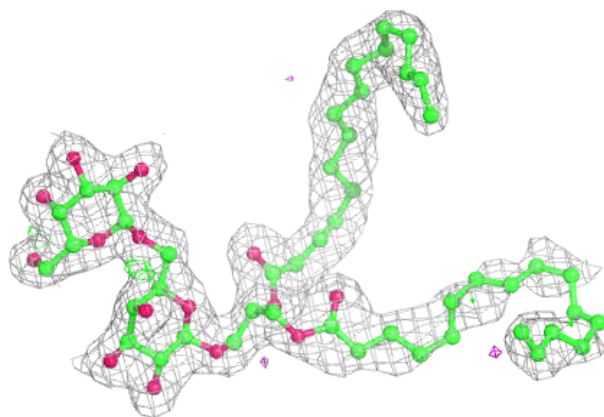
**Electron density around LMG J 101:**

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

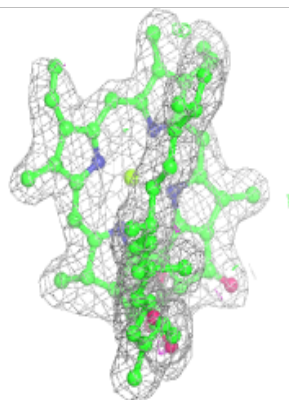
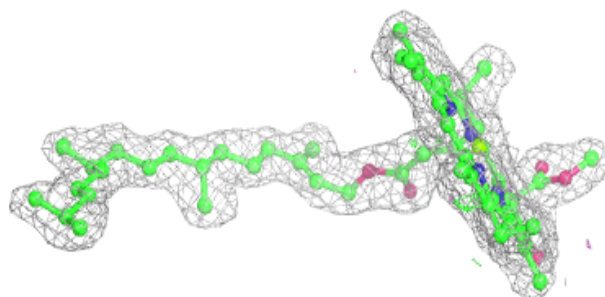
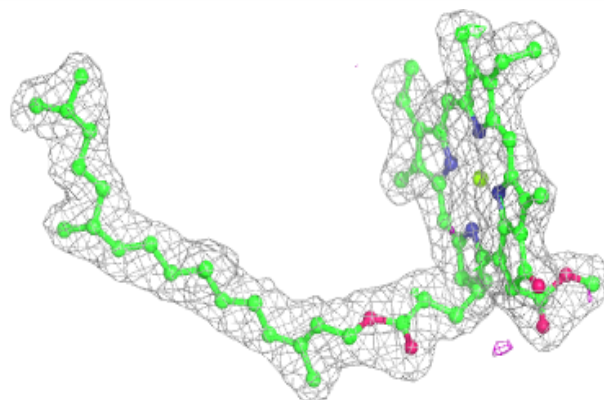


**Electron density around DGD C 518:**

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

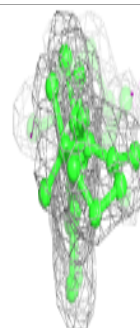
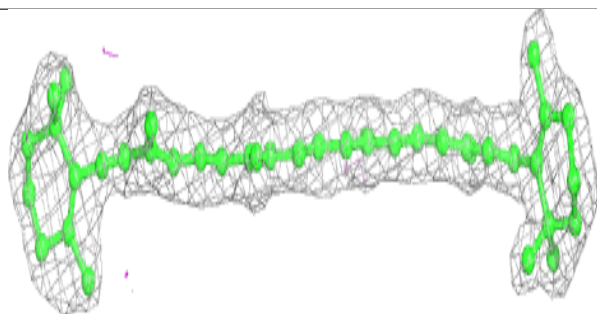
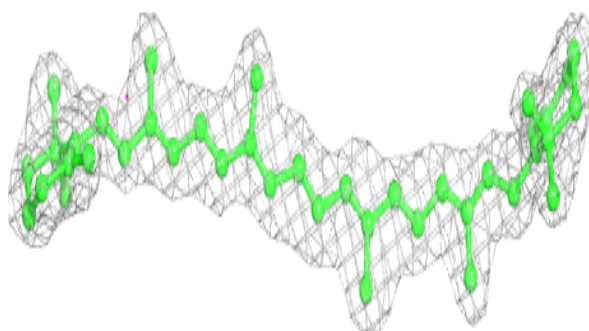
**Electron density around CLA b 613:**

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

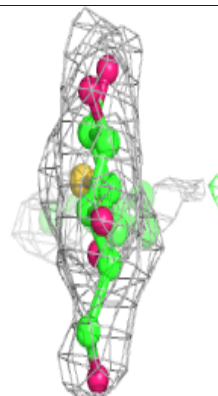
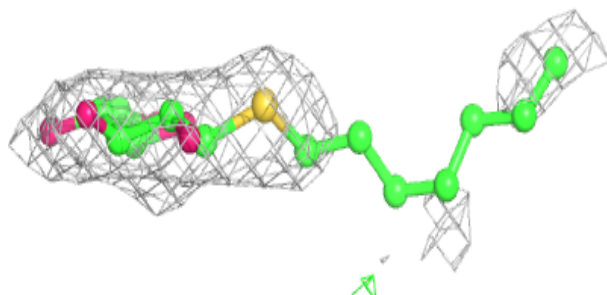
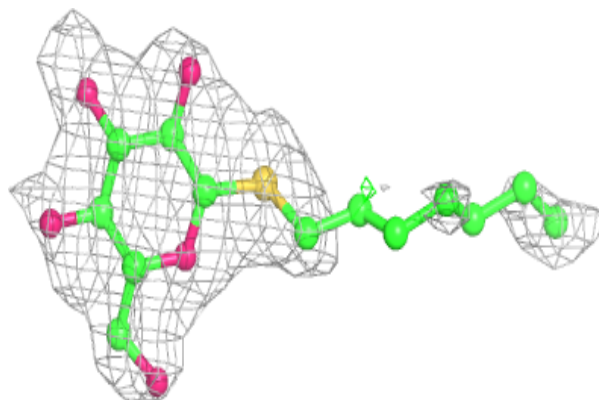


**Electron density around BCR c 915:**

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

**Electron density around HTG C 523:**

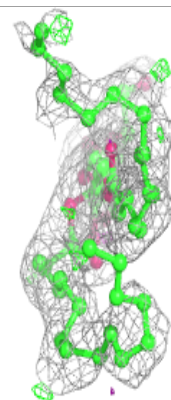
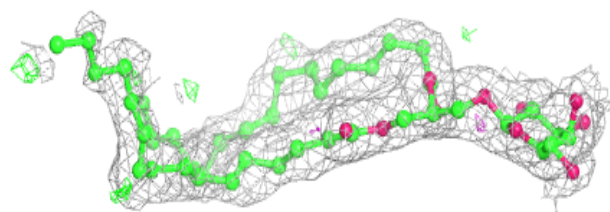
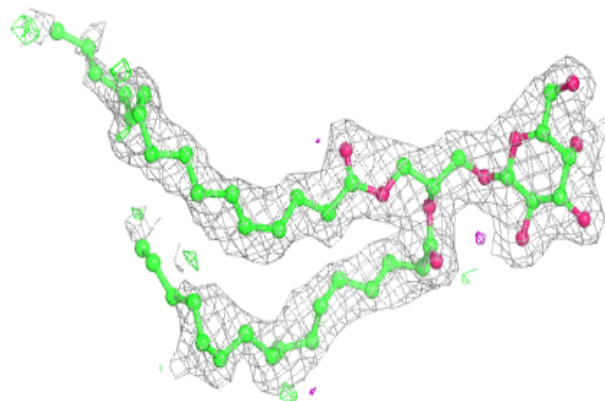
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



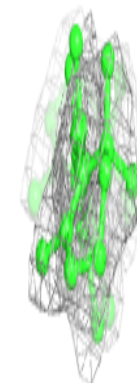
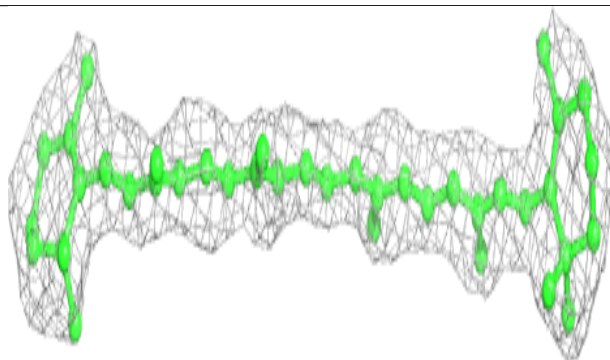
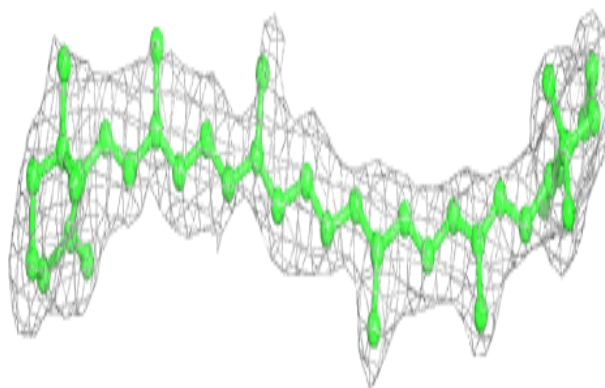


**Electron density around LMG j 101:**

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

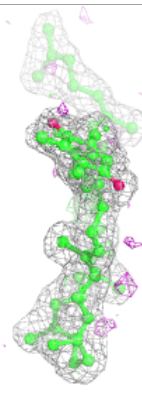
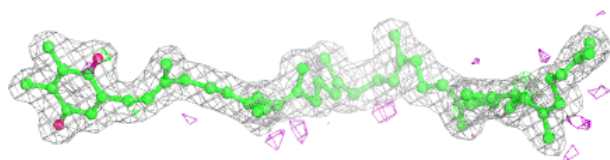
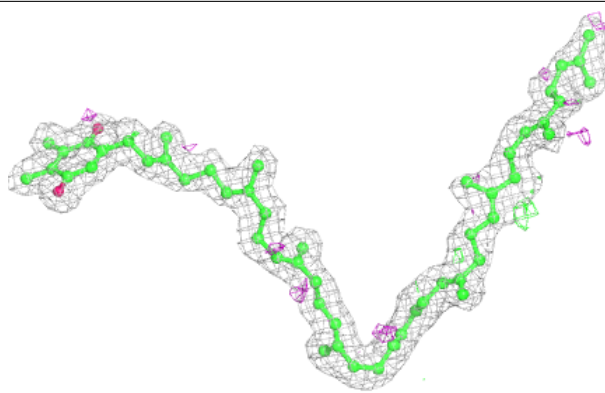
**Electron density around BCR k 101:**

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



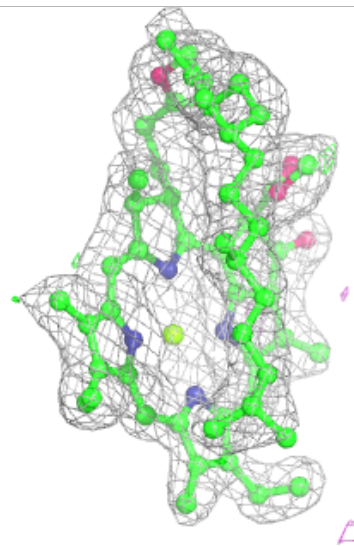
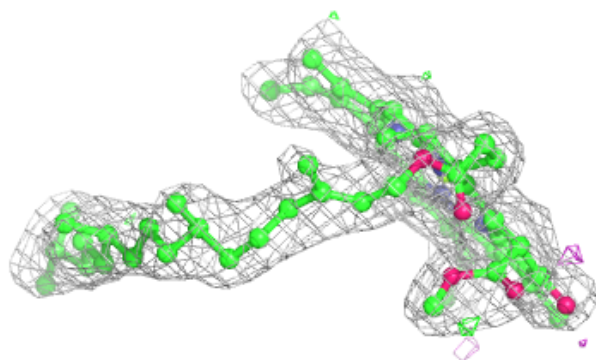
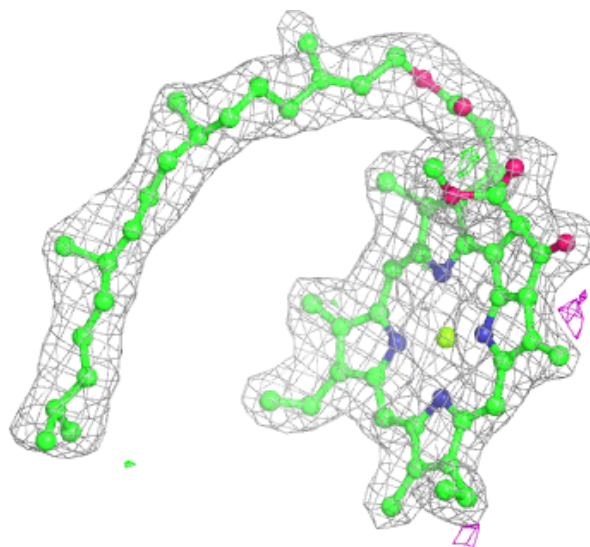
**Electron density around PL9 D 404:**

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



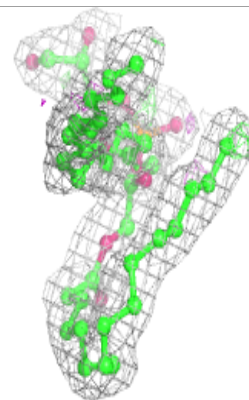
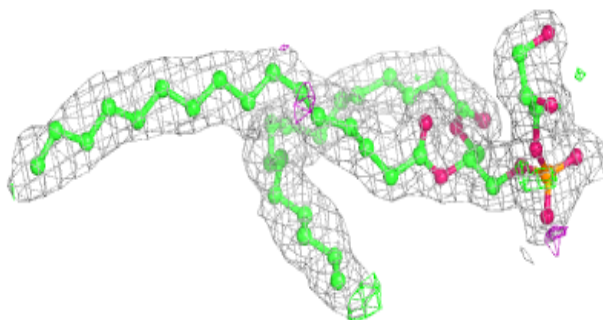
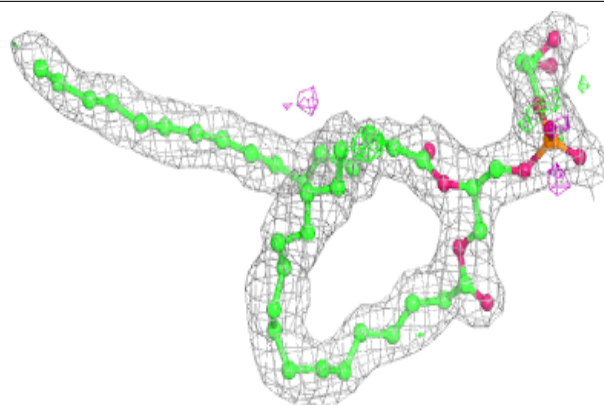
**Electron density around CLA c 908:**

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

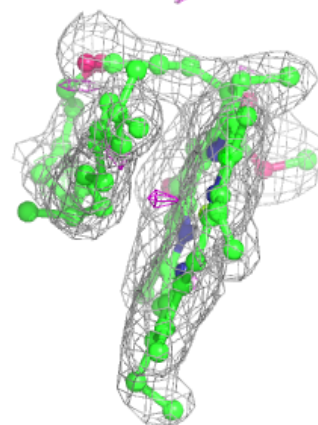
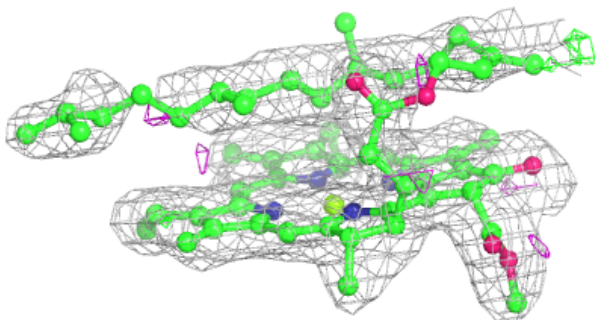
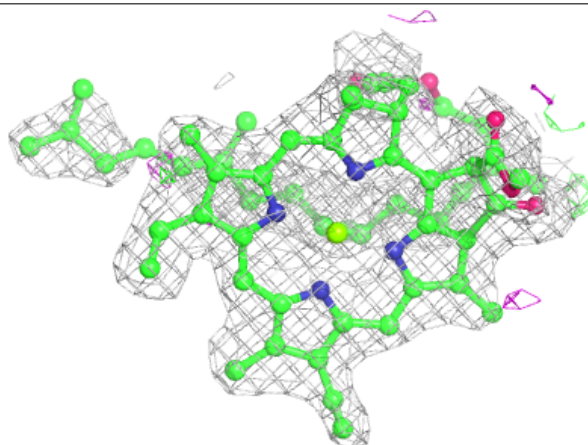


**Electron density around LHG d 407:**

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

**Electron density around CLA B 602:**

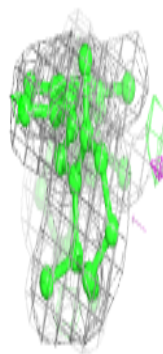
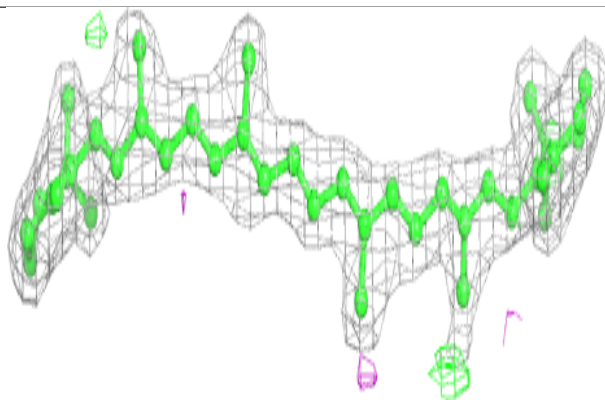
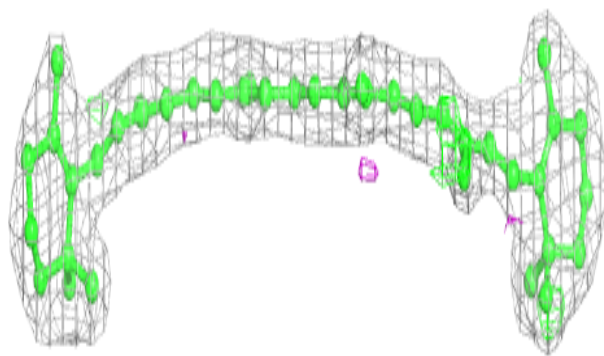
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





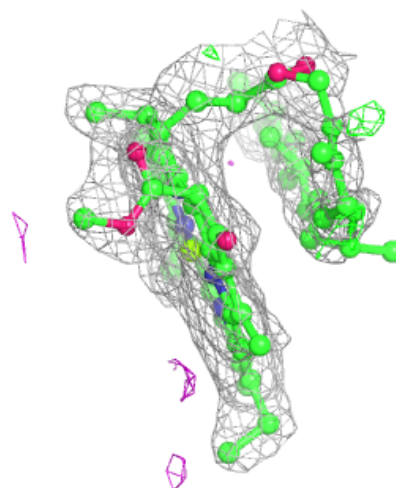
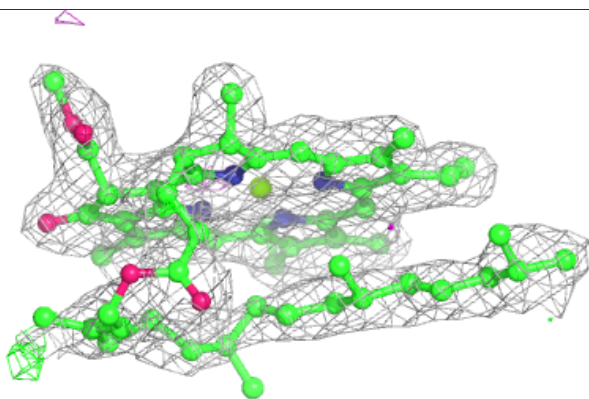
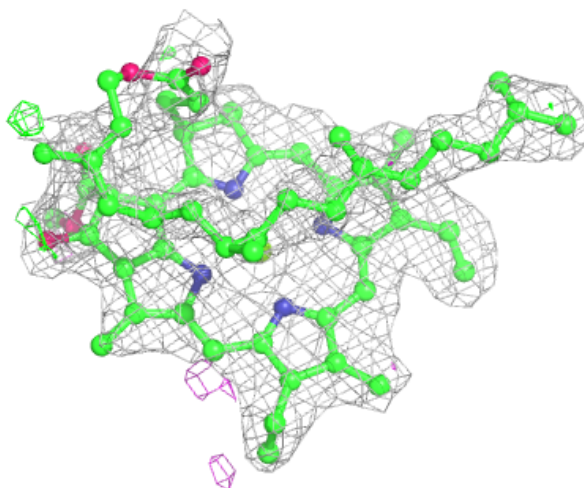
**Electron density around BCR K 103:**

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



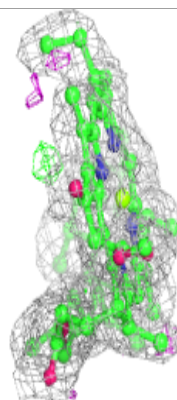
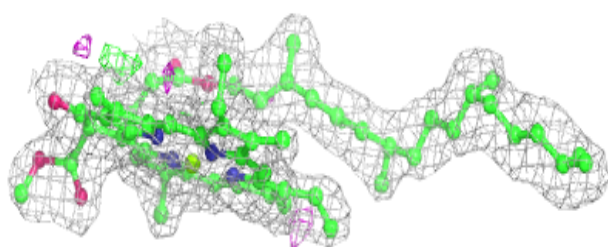
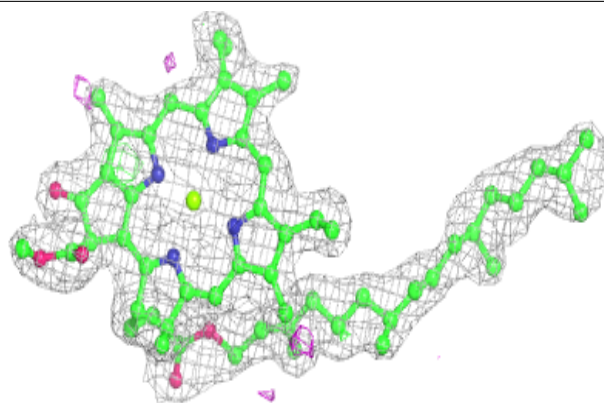
**Electron density around CLA b 605:**

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

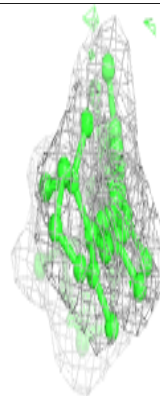
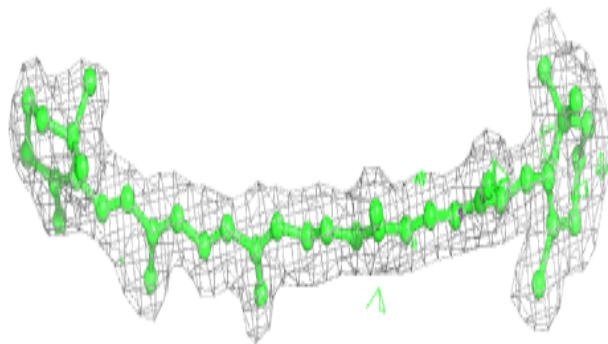
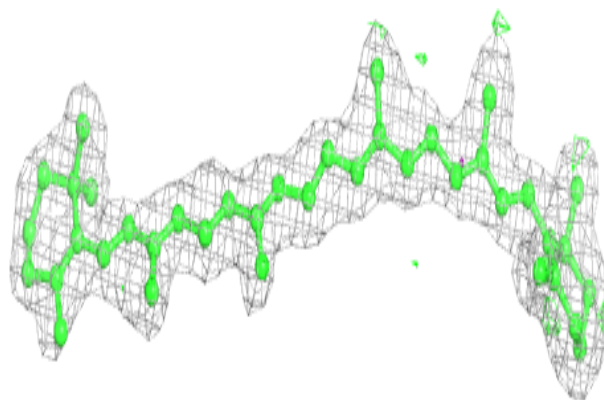


**Electron density around CLA c 902:**

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

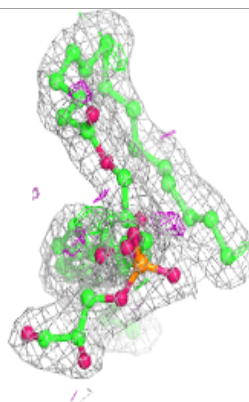
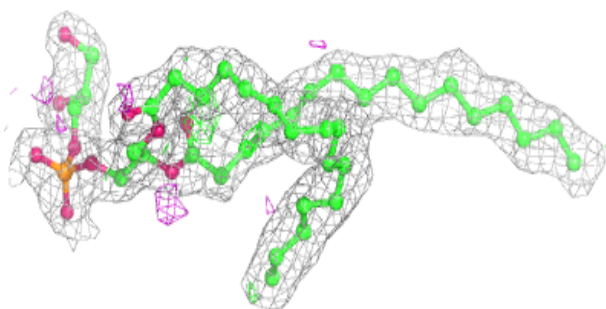
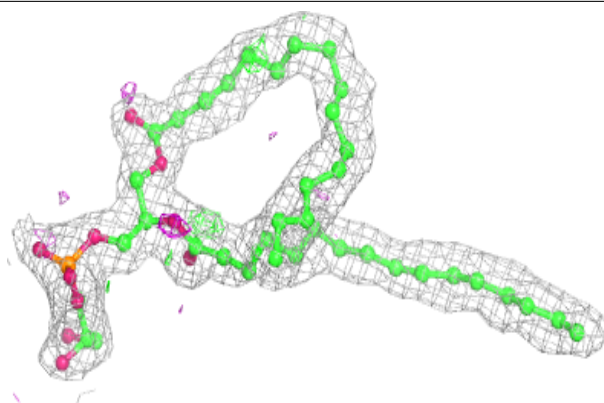
**Electron density around BCR t 101:**

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

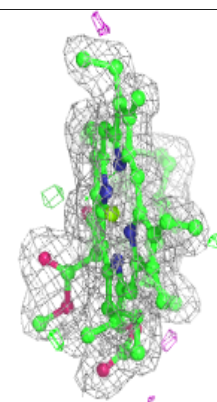
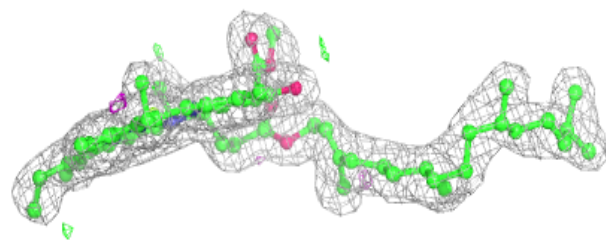
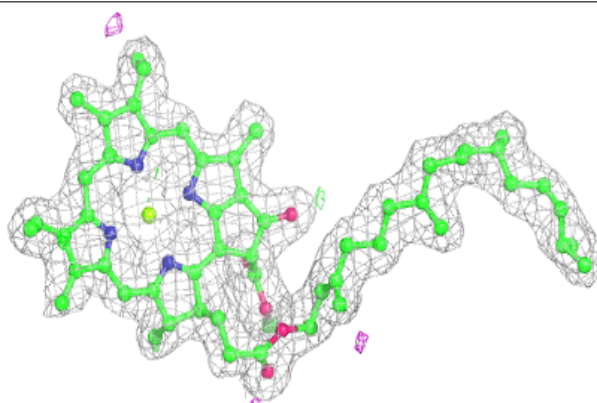


**Electron density around LHG D 406:**

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

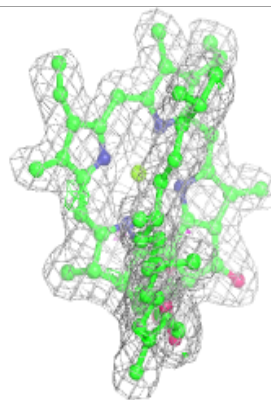
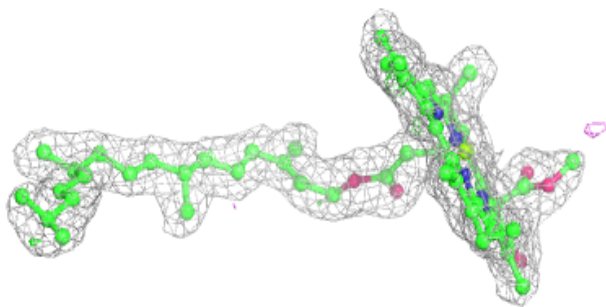
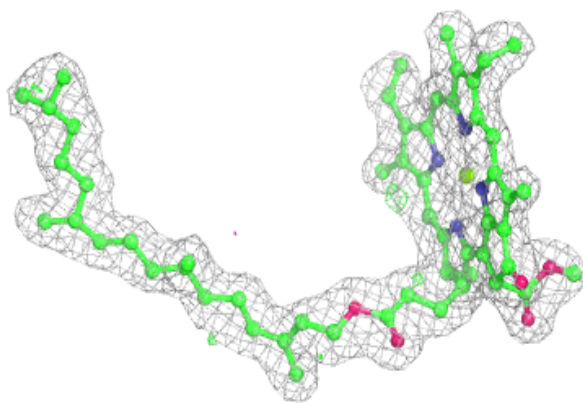
**Electron density around CLA B 603:**

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

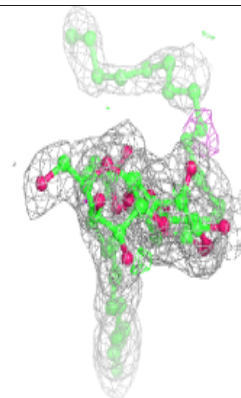
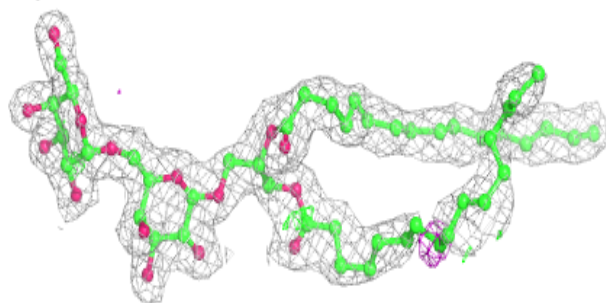
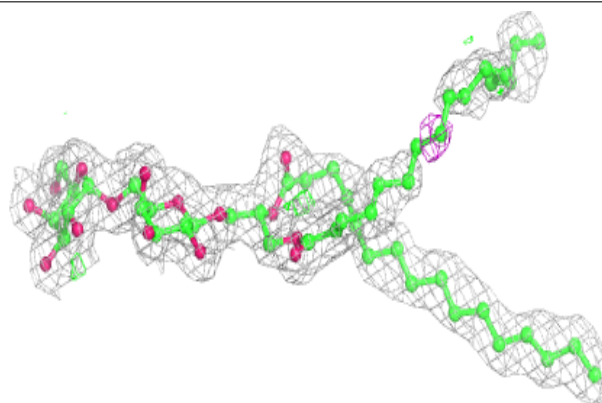


**Electron density around CLA B 610:**

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

**Electron density around DGD c 916:**

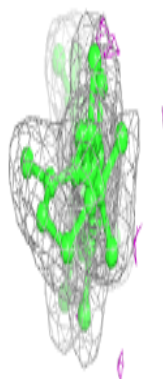
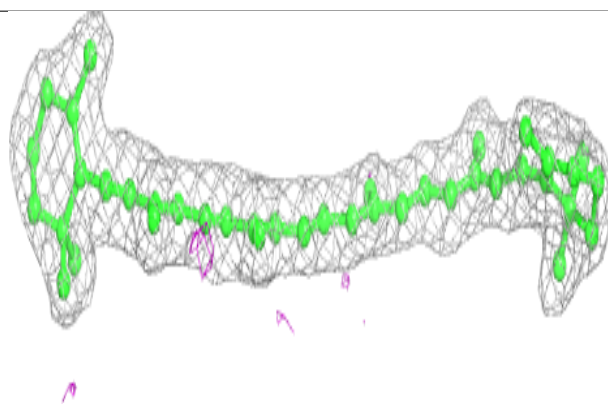
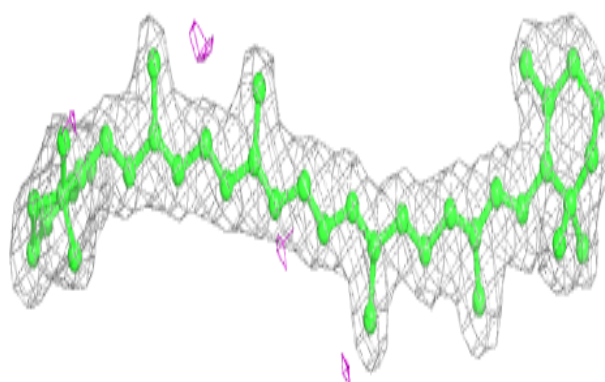
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



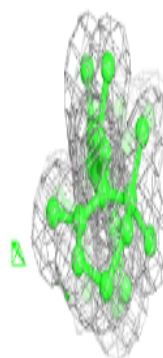
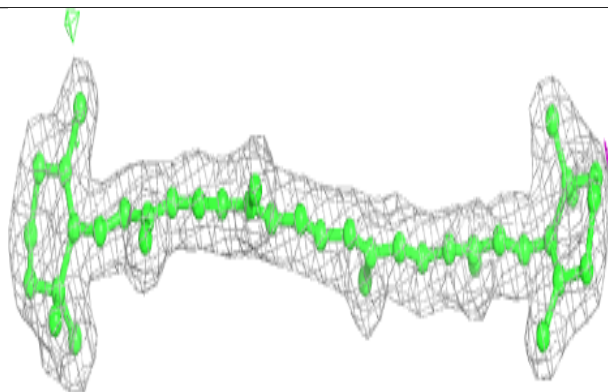
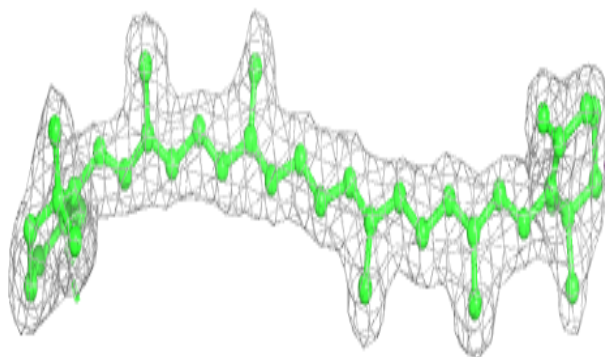


**Electron density around BCR b 621:**

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

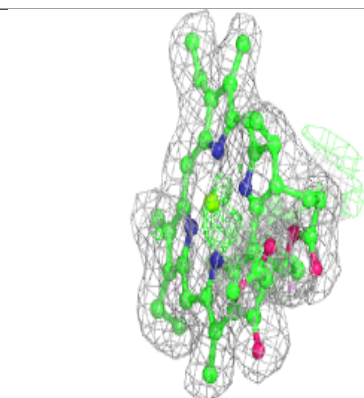
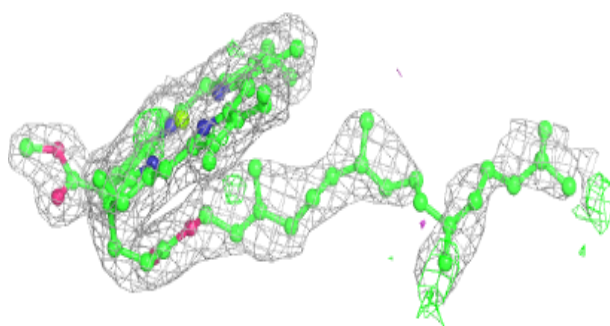
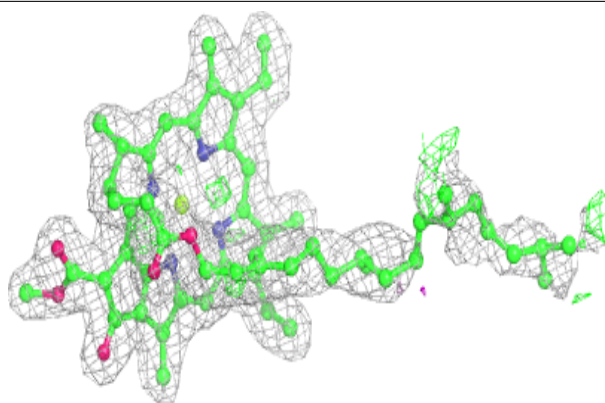
**Electron density around BCR a 410:**

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

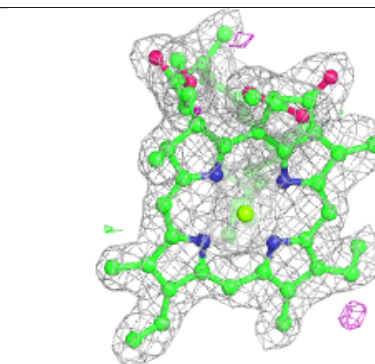
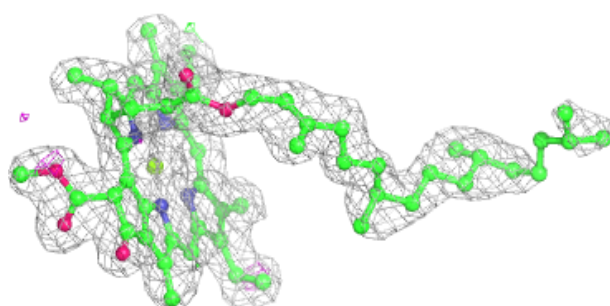
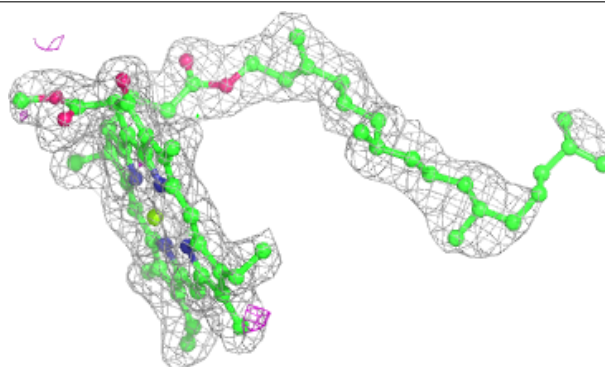


**Electron density around CLA b 618:**

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

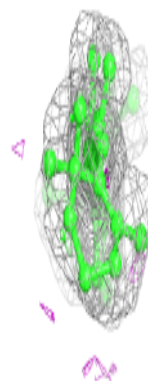
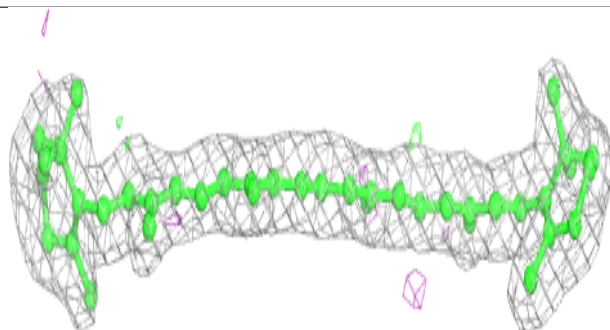
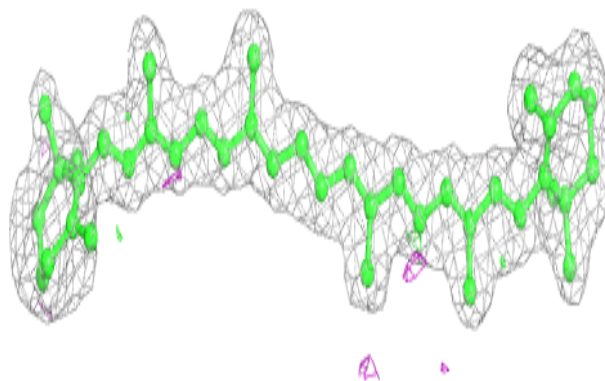
**Electron density around CLA c 909:**

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

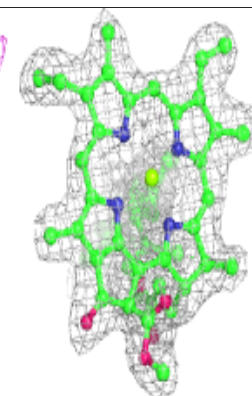
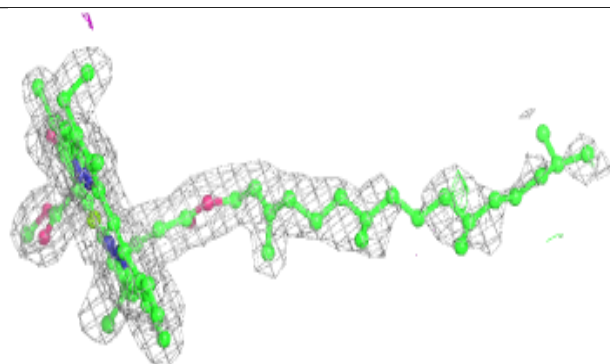
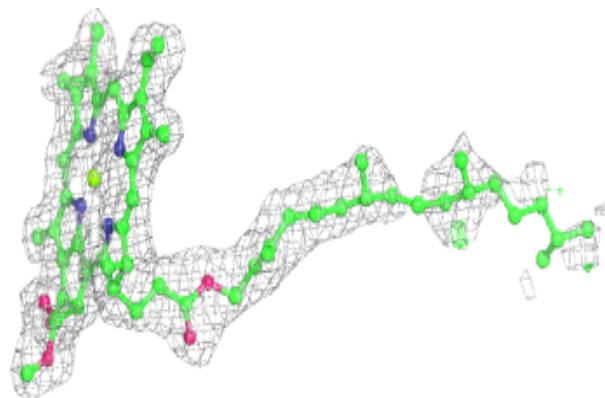


**Electron density around BCR b 622:**

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

**Electron density around CLA d 403:**

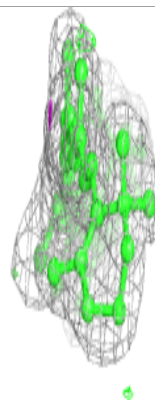
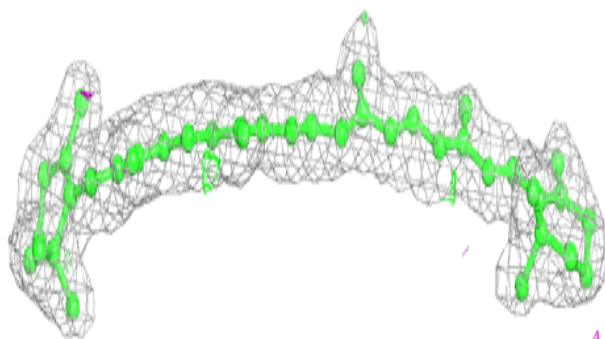
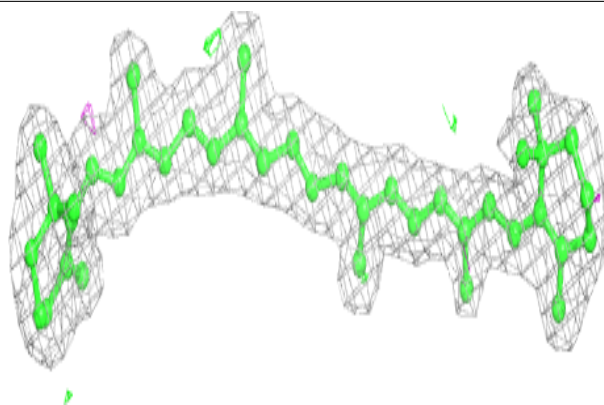
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



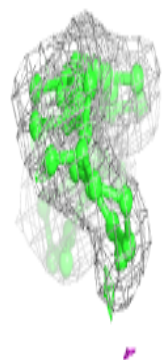
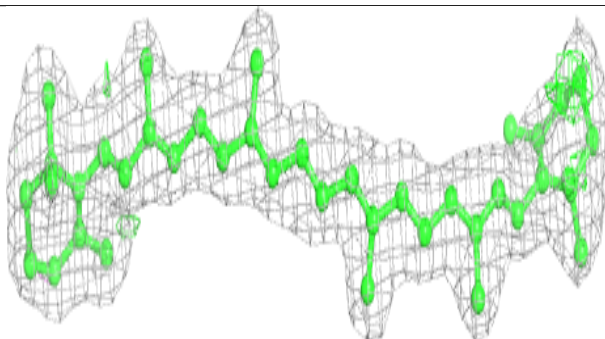
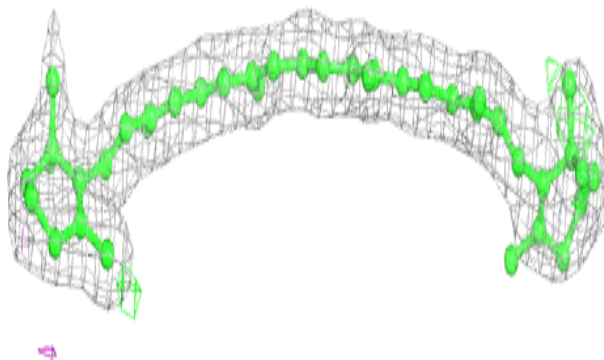


**Electron density around BCR T 102:**

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

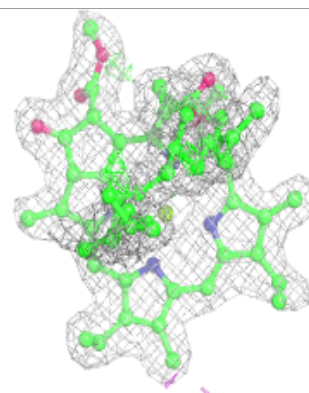
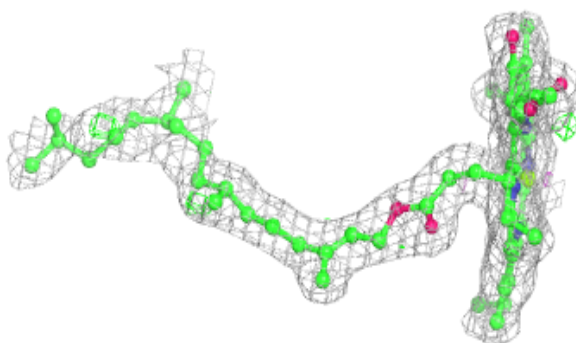
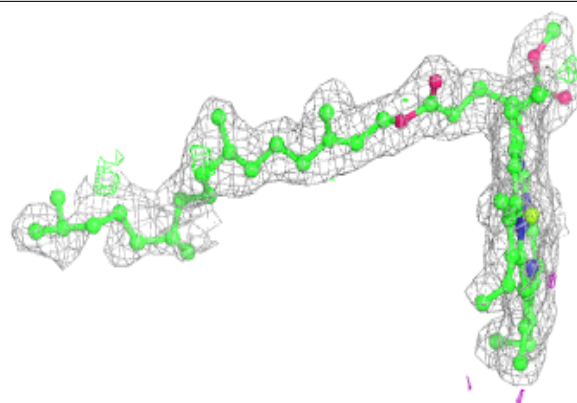
**Electron density around BCR D 403:**

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

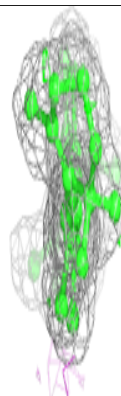
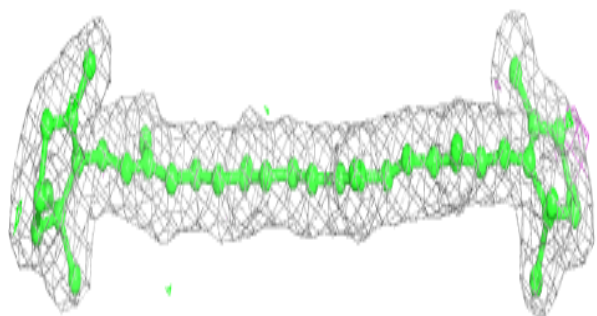
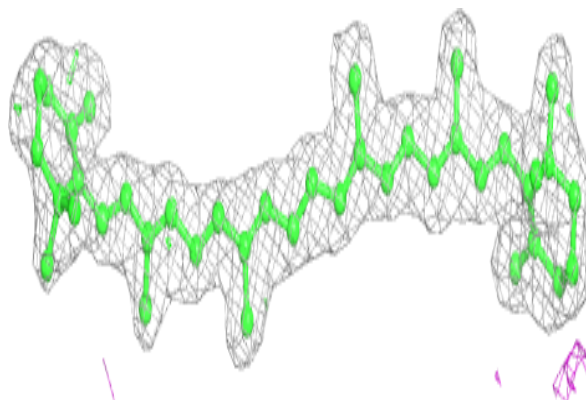


**Electron density around CLA b 610:**

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

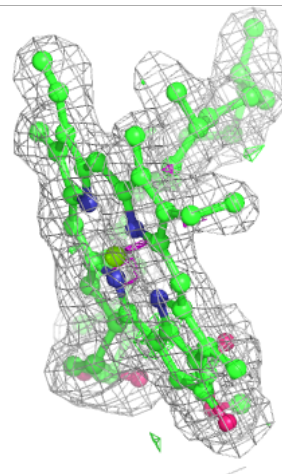
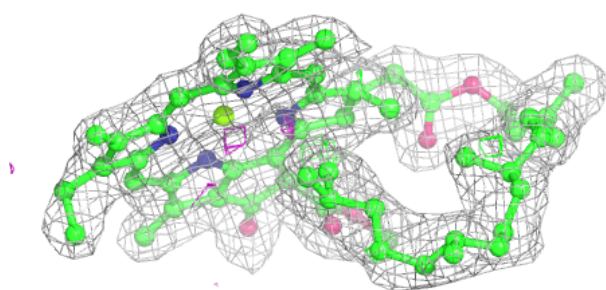
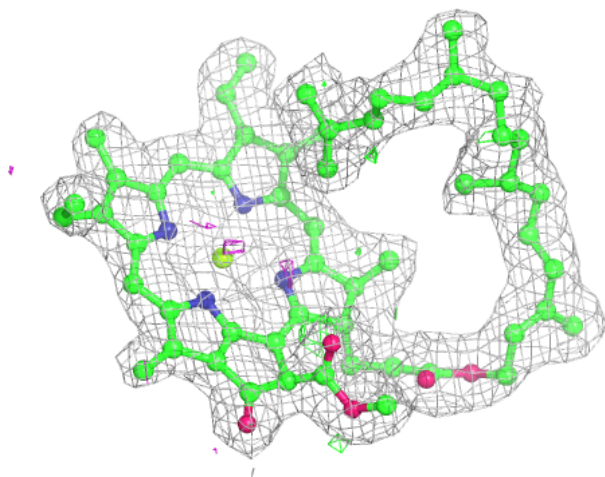
**Electron density around BCR B 619:**

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



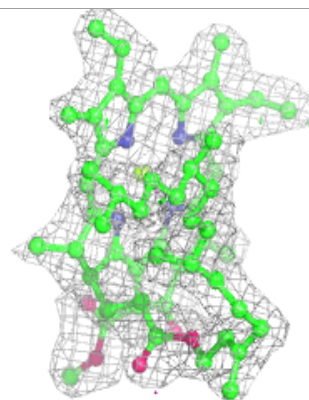
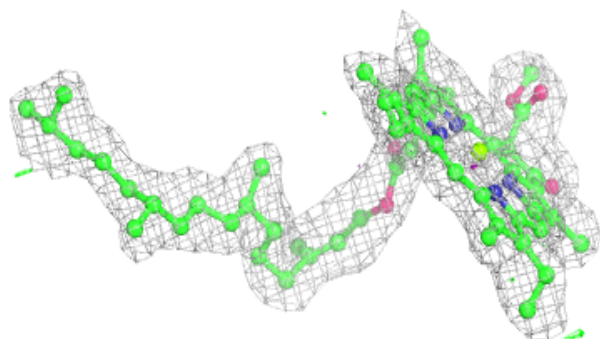
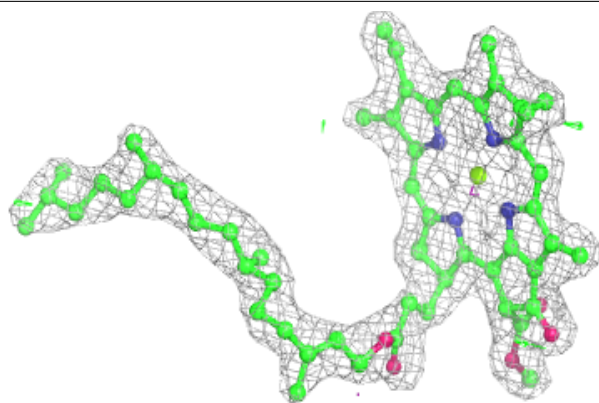
**Electron density around CLA b 619:**

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

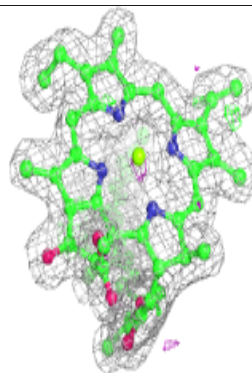
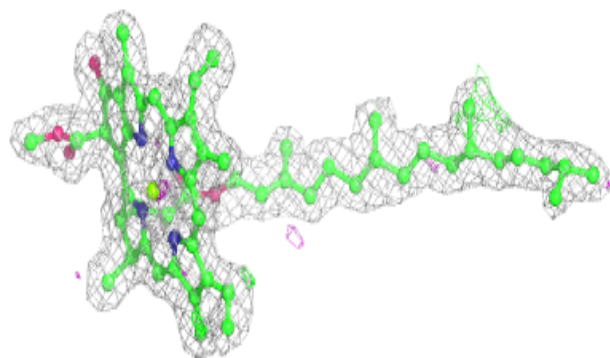
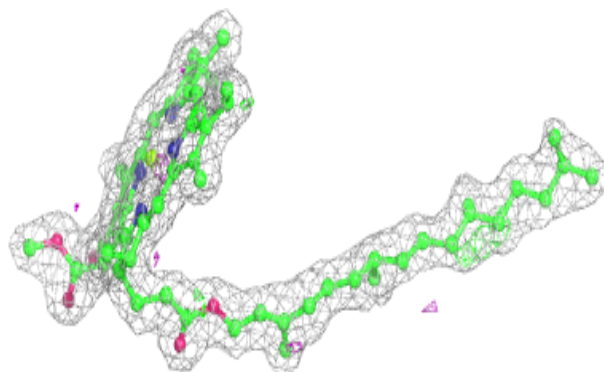


**Electron density around CLA c 912:**

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

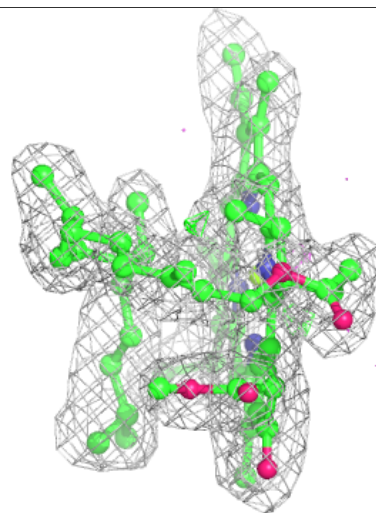
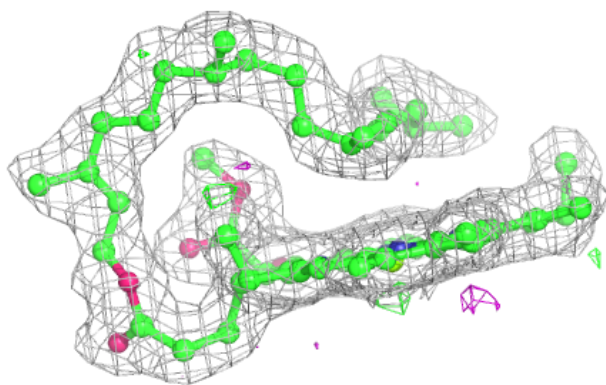
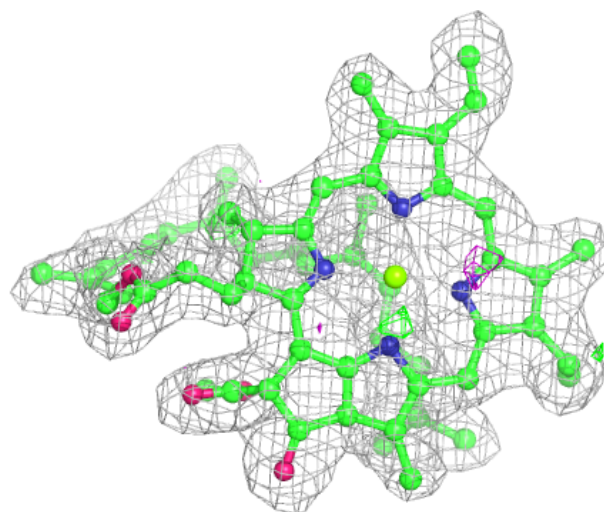
**Electron density around CLA B 608:**

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



**Electron density around CLA C 511:**

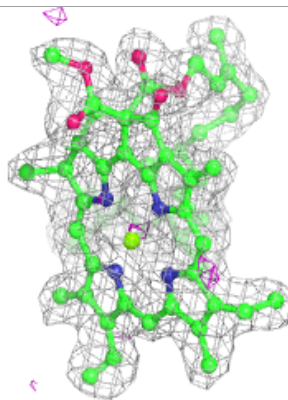
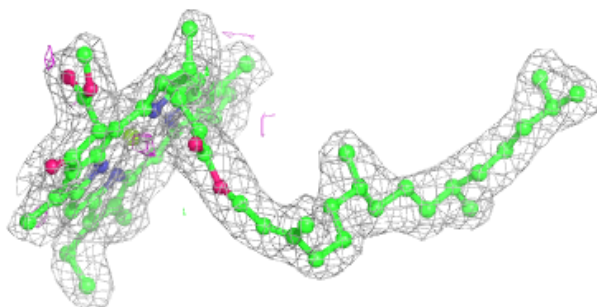
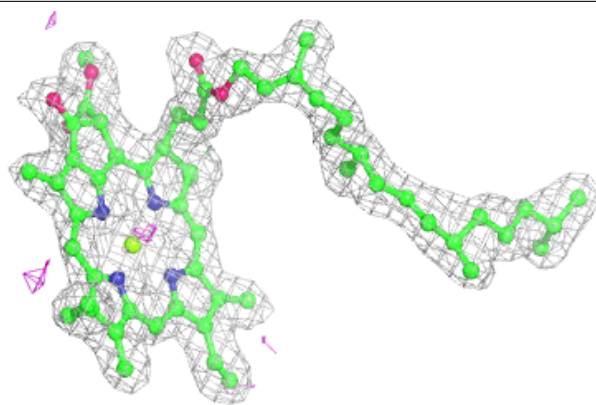
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





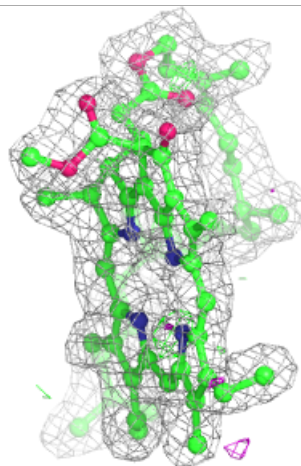
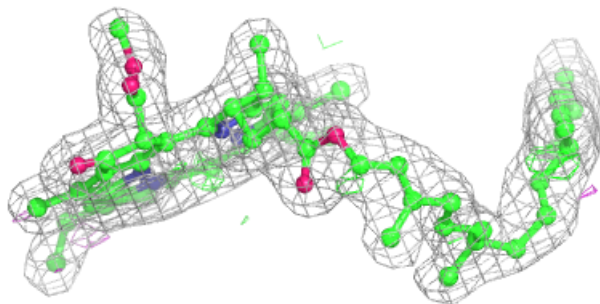
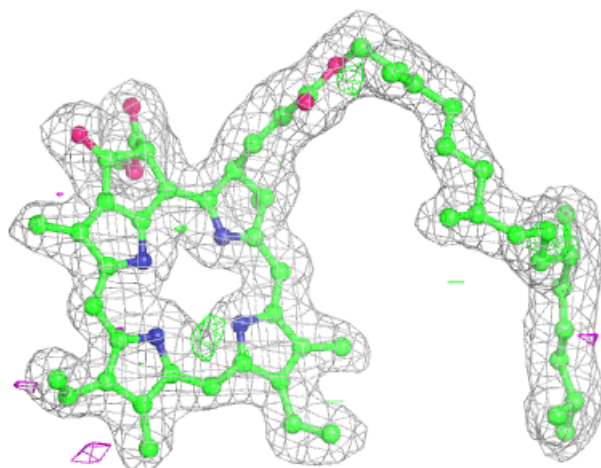
**Electron density around CLA C 512:**

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



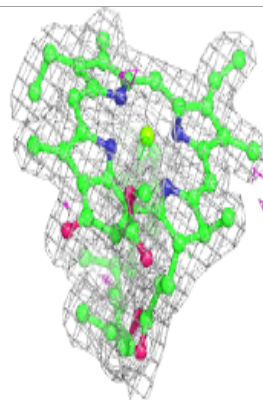
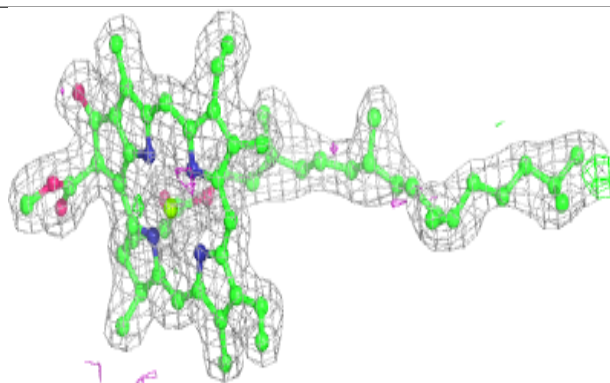
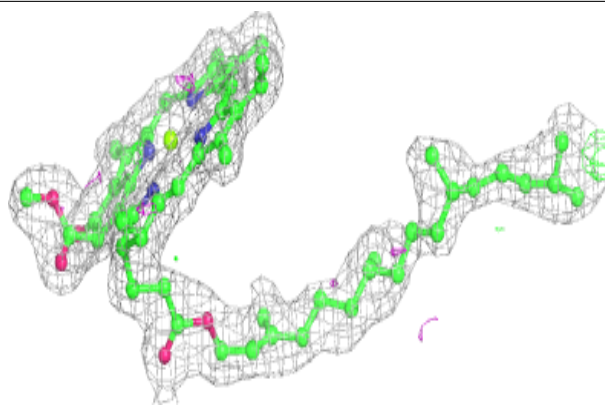
**Electron density around PHO a 420:**

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

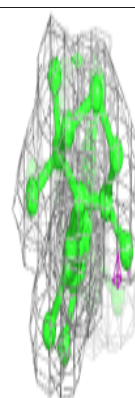
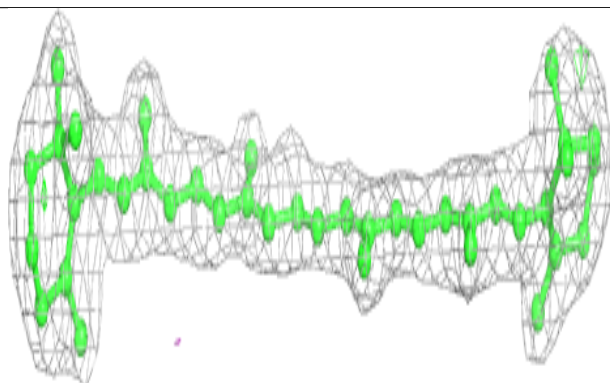
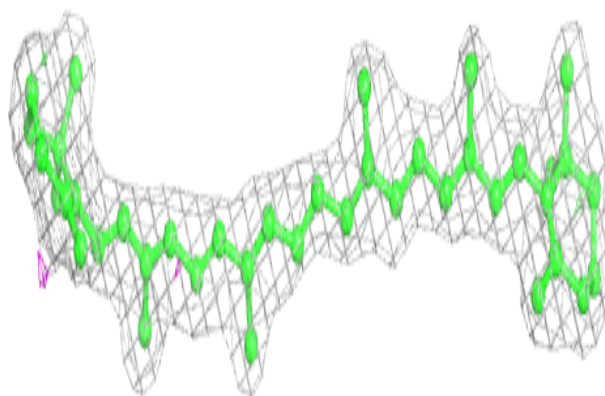


**Electron density around CLA C 505:**

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

**Electron density around BCR C 515:**

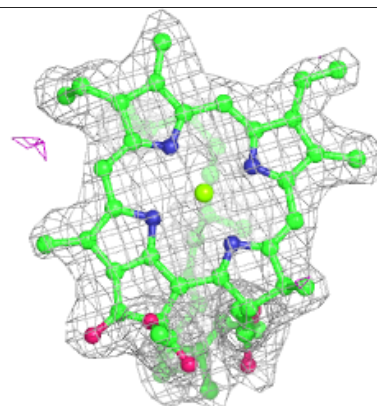
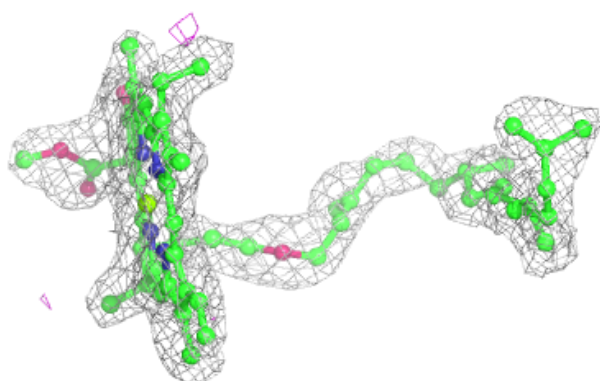
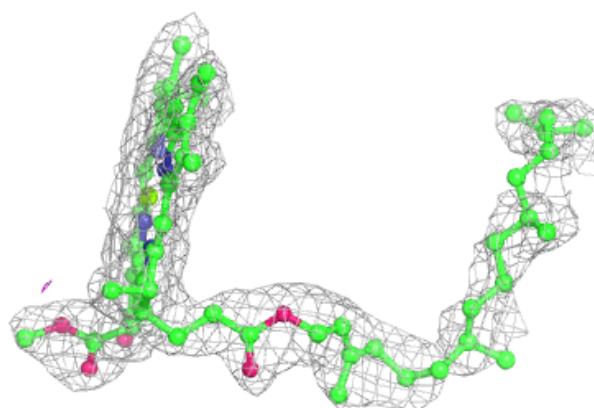
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



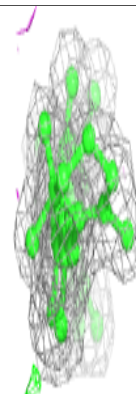
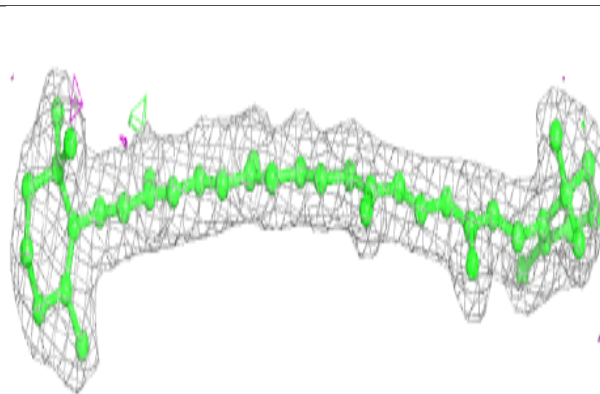
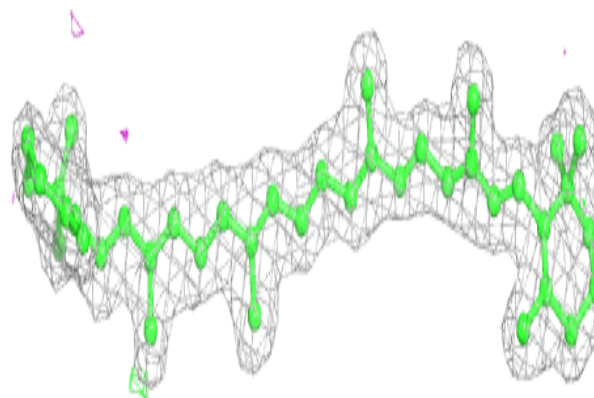


**Electron density around CLA C 507:**

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

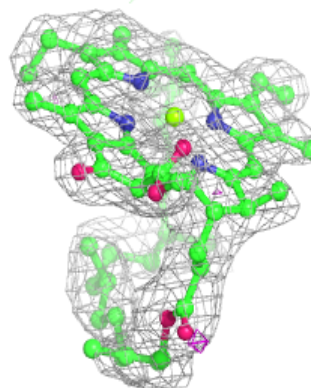
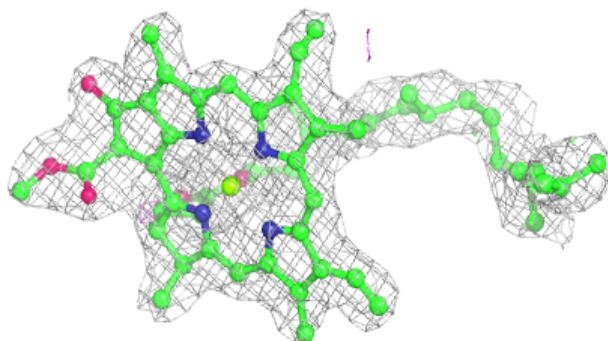
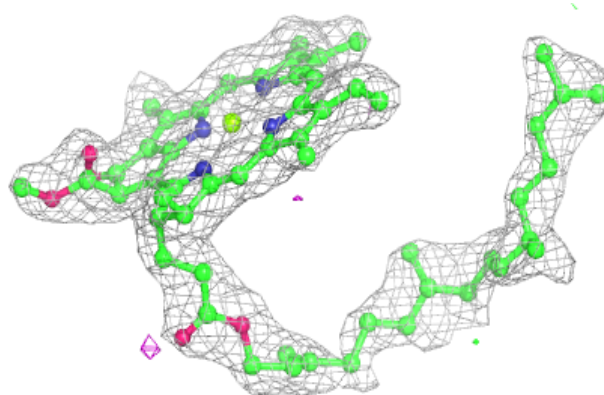
**Electron density around BCR B 618:**

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

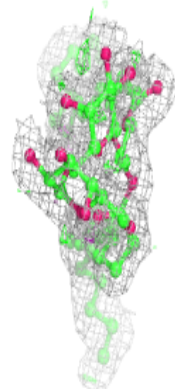
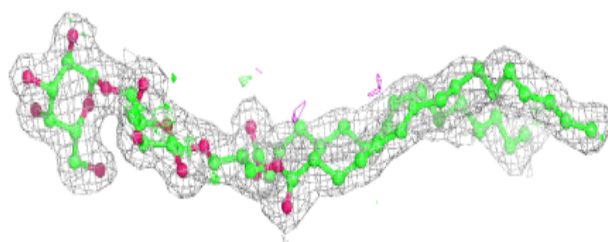
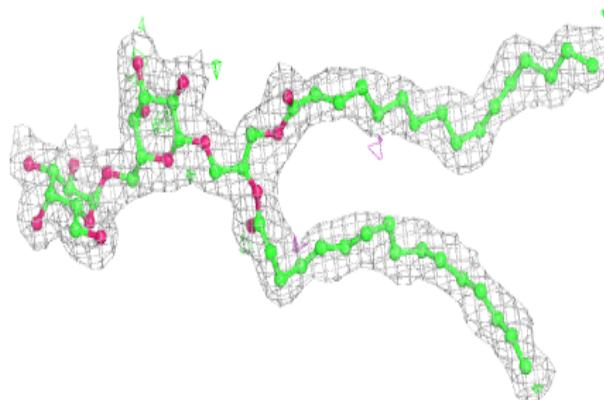


**Electron density around CLA C 514:**

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

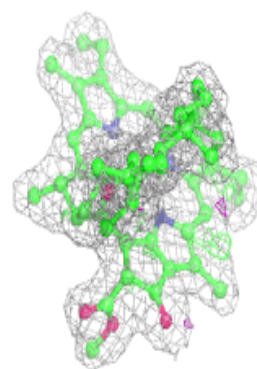
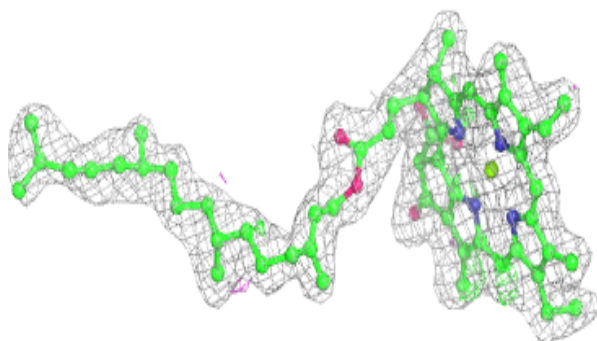
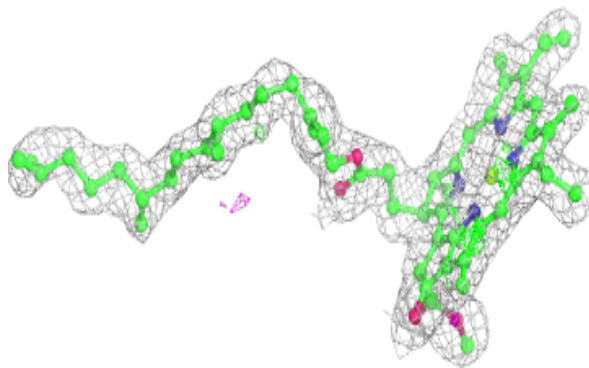
**Electron density around DGD C 519:**

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

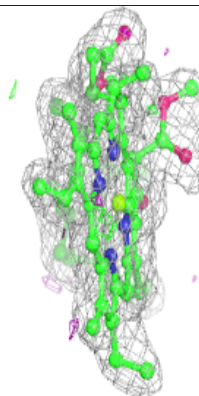
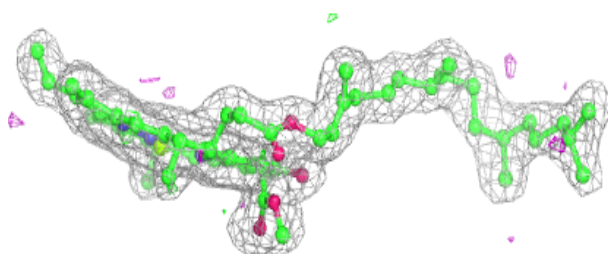
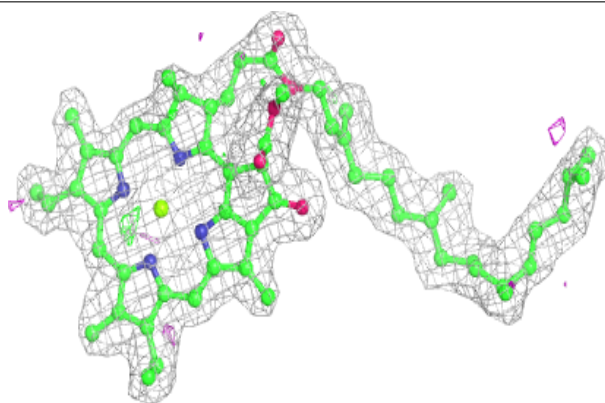


**Electron density around CLA c 903:**

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

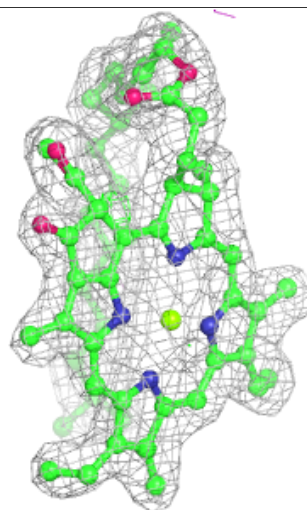
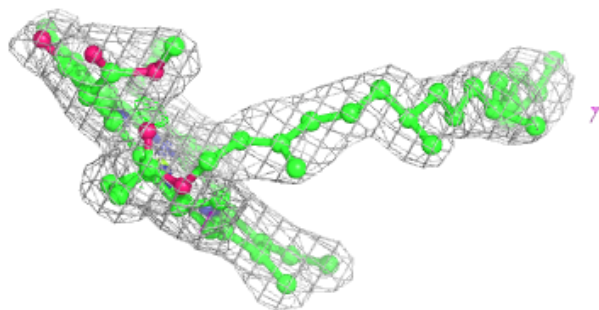
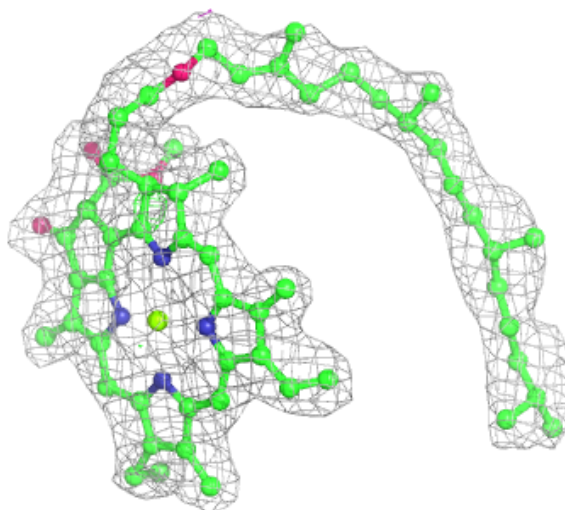
**Electron density around CLA b 606:**

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



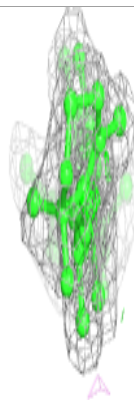
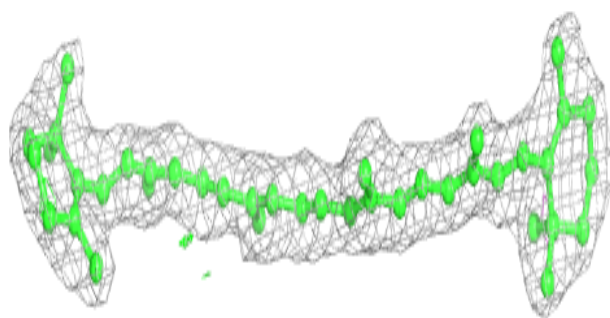
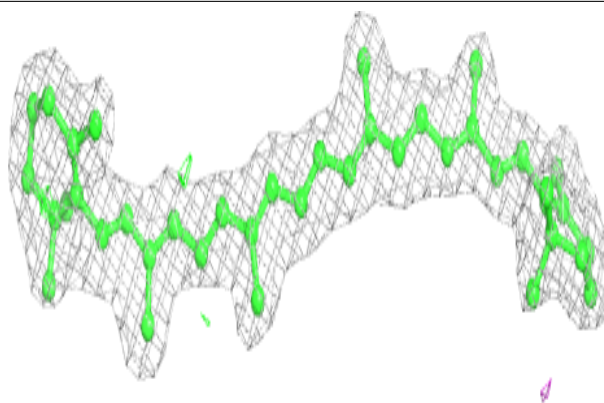
**Electron density around CLA C 508:**

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



**Electron density around BCR K 102:**

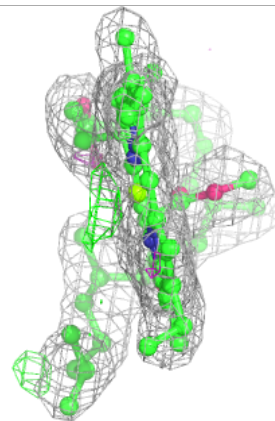
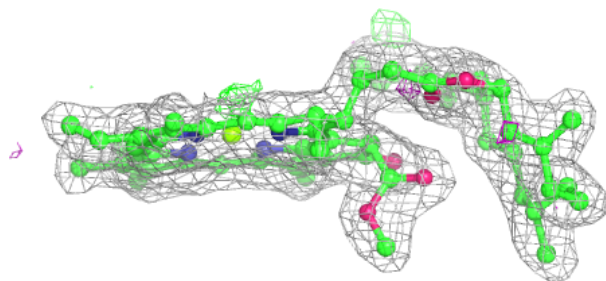
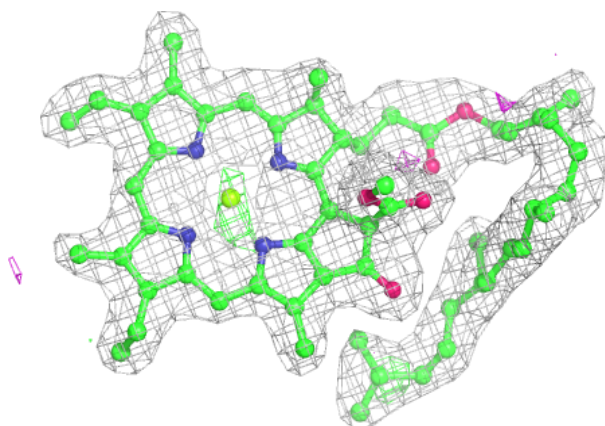
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





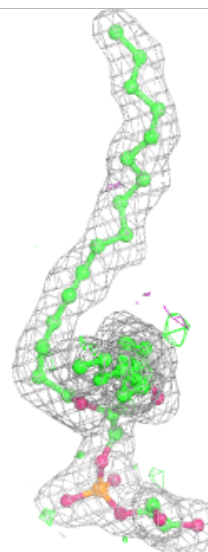
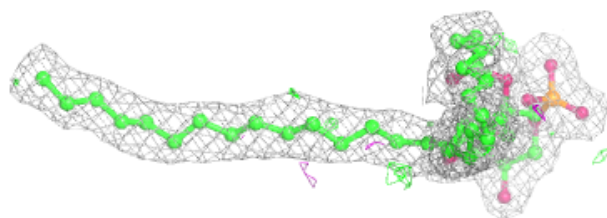
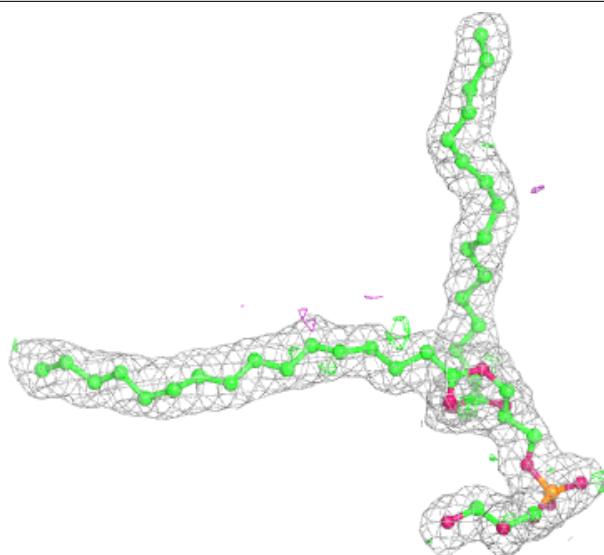
**Electron density around CLA b 614:**

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



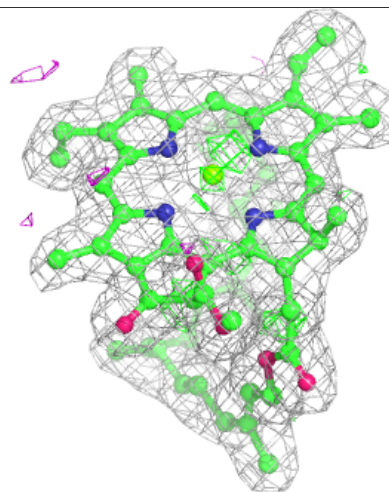
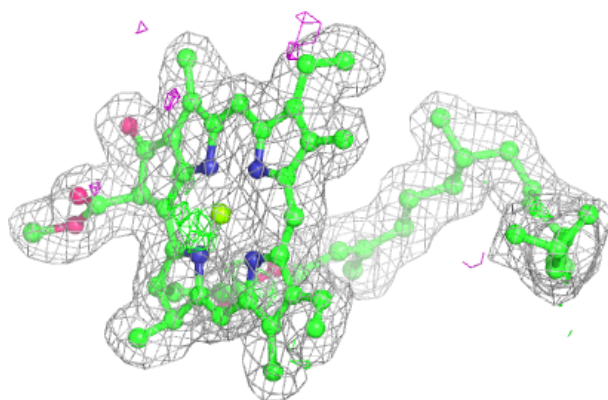
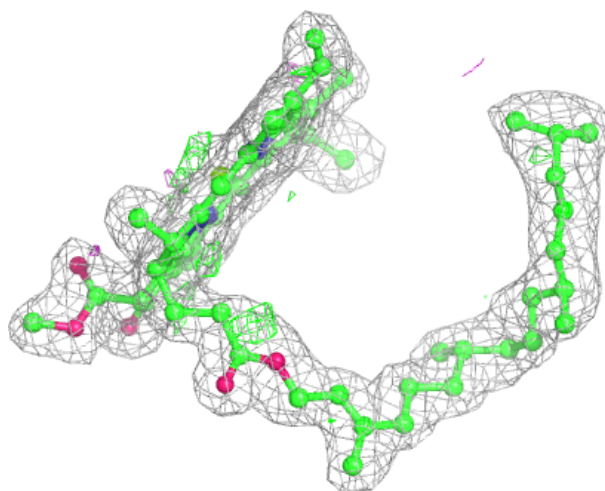
**Electron density around LHG L 101:**

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



**Electron density around CLA b 615:**

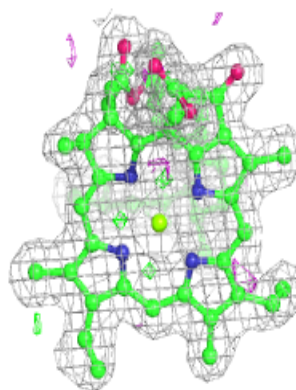
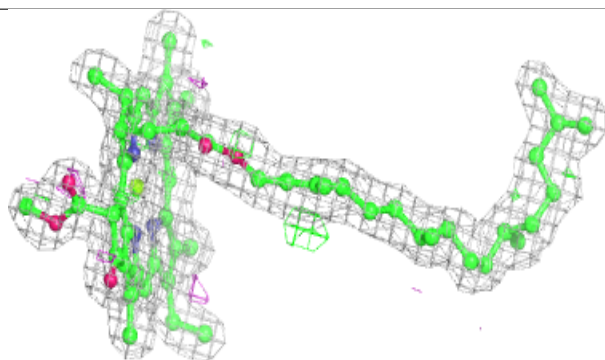
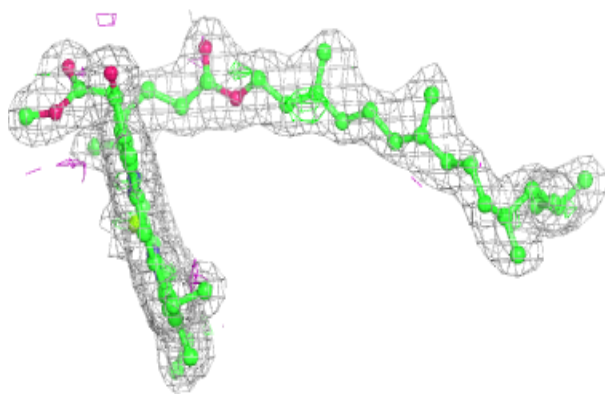
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



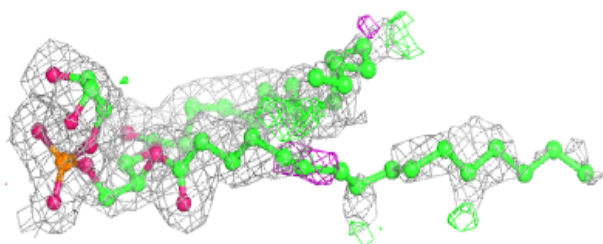
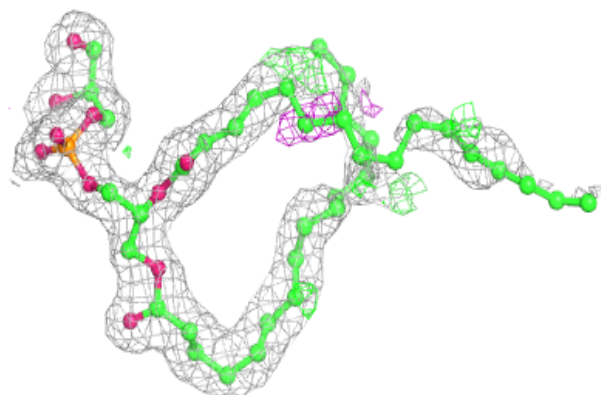


**Electron density around CLA B 606:**

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

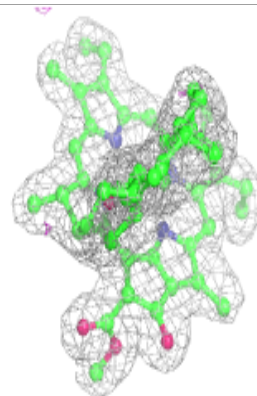
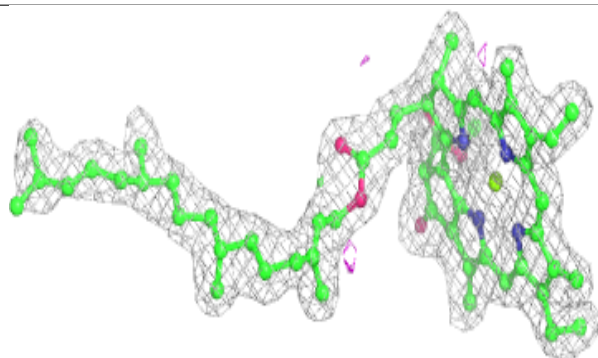
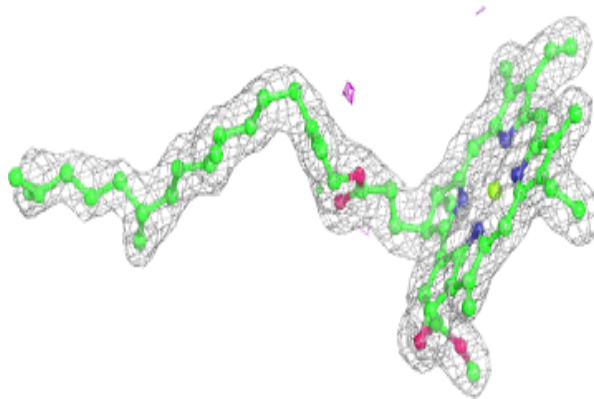
**Electron density around LHG D 408:**

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

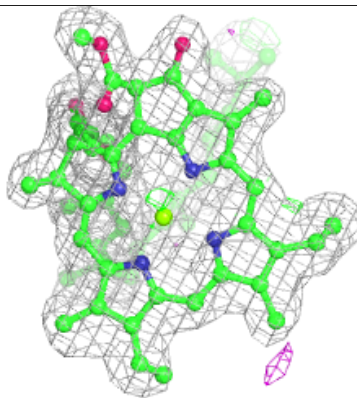
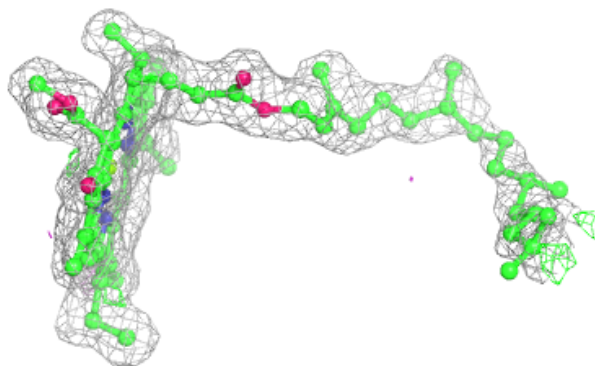
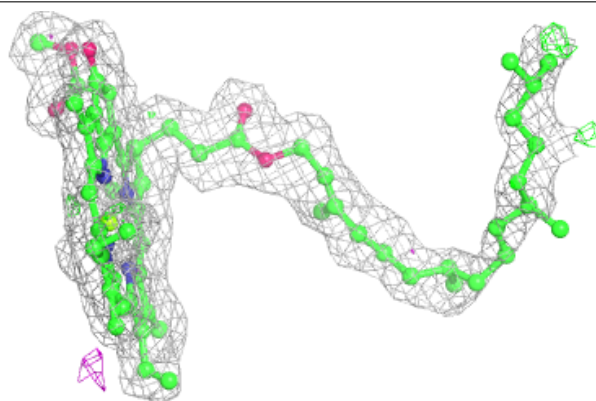


**Electron density around CLA C 503:**

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

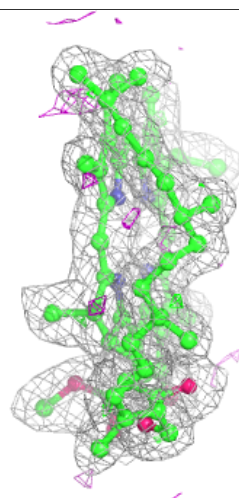
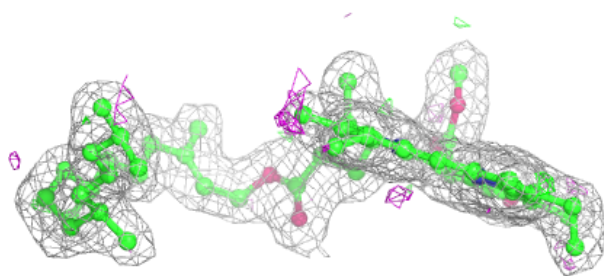
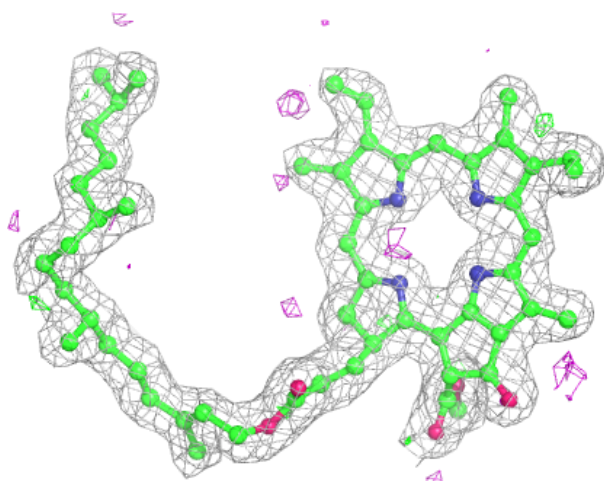
**Electron density around CLA D 402:**

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



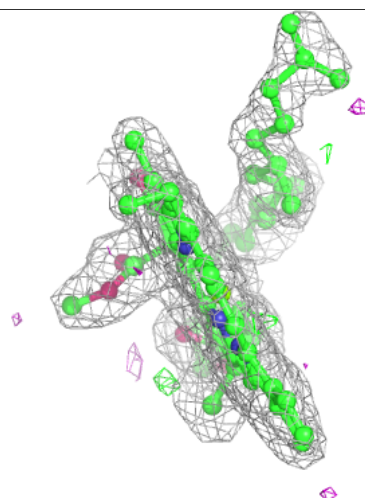
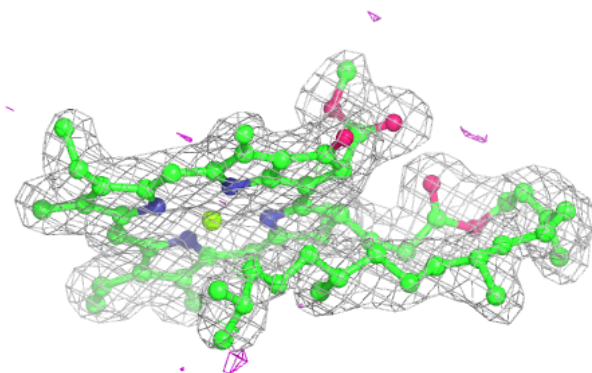
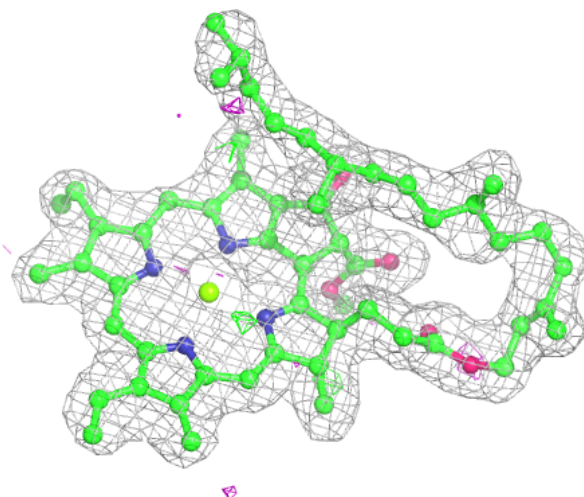
**Electron density around PHO a 408:**

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



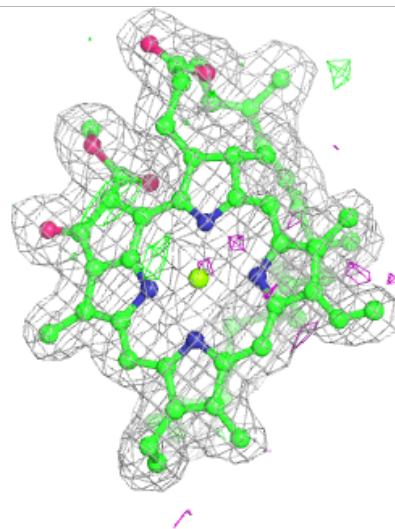
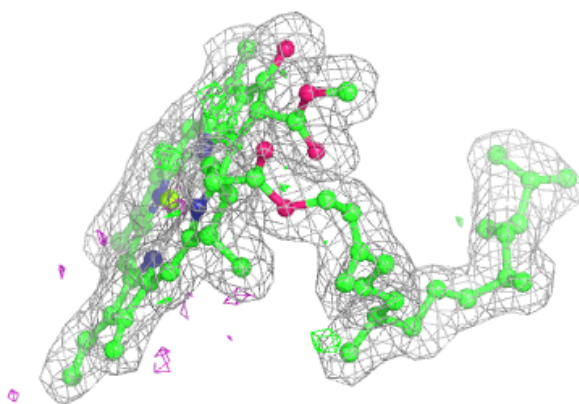
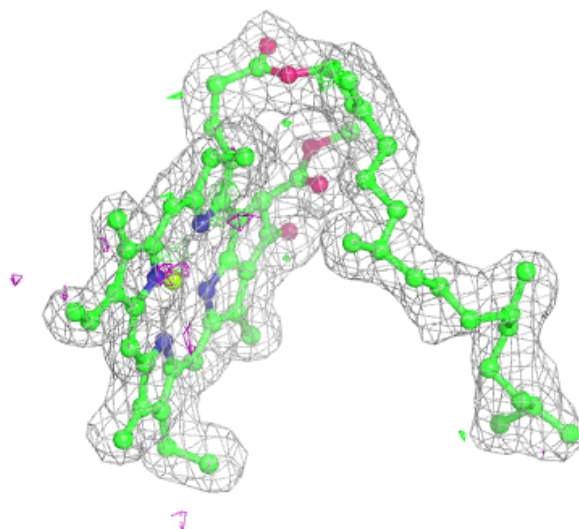
**Electron density around CLA C 510:**

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



**Electron density around CLA B 614:**

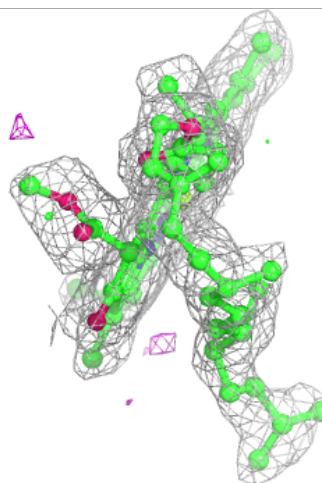
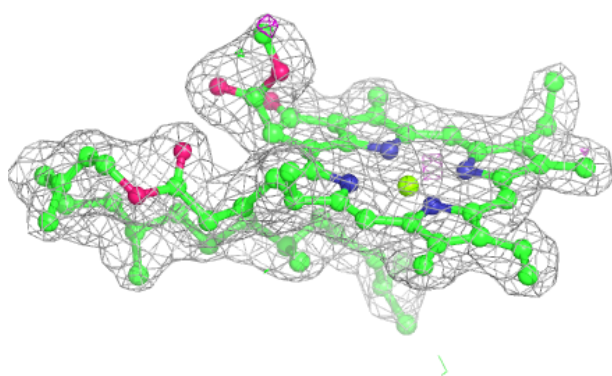
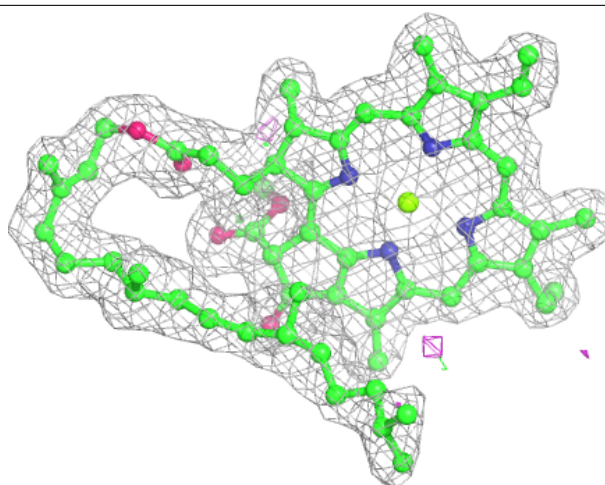
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





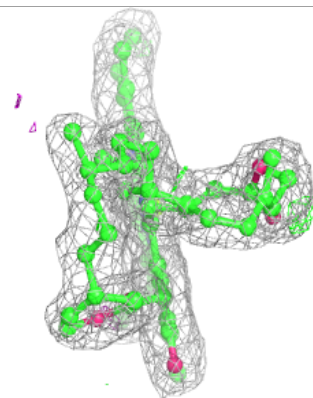
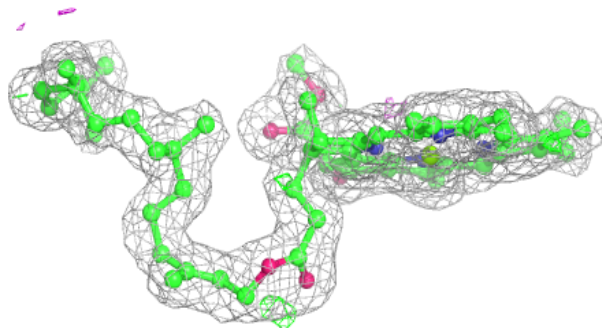
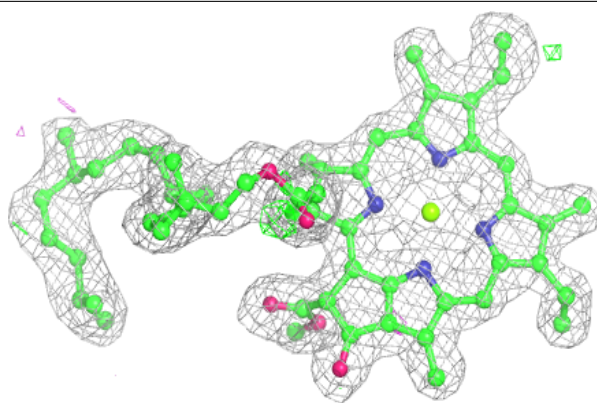
**Electron density around CLA c 910:**

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

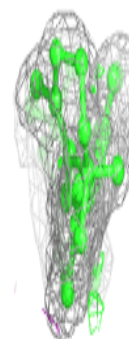
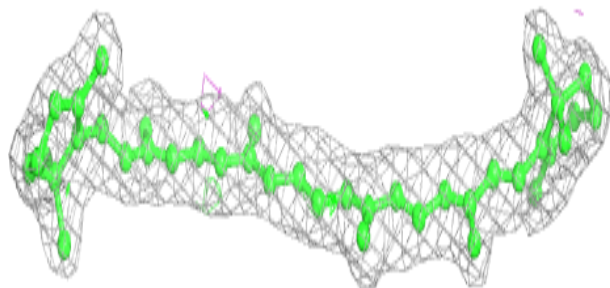
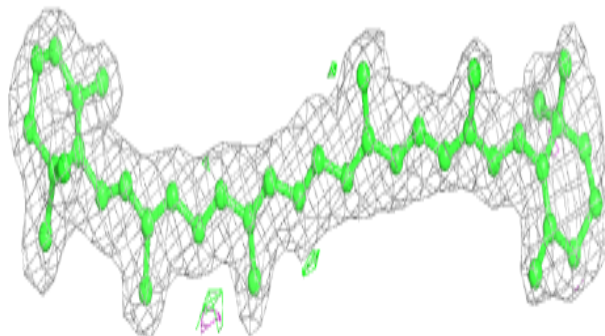


**Electron density around CLA b 616:**

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

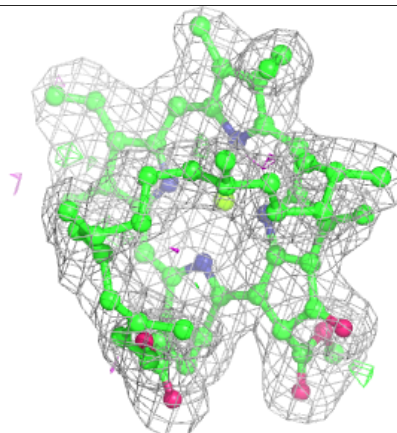
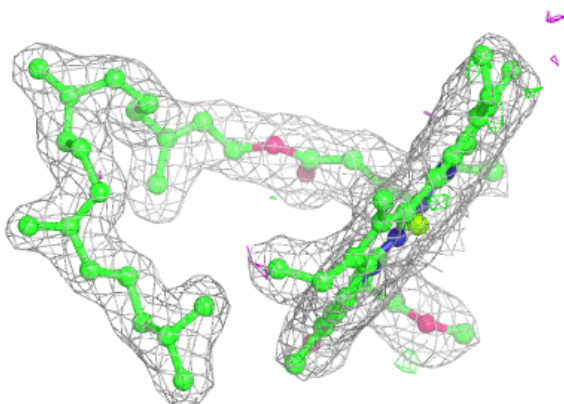
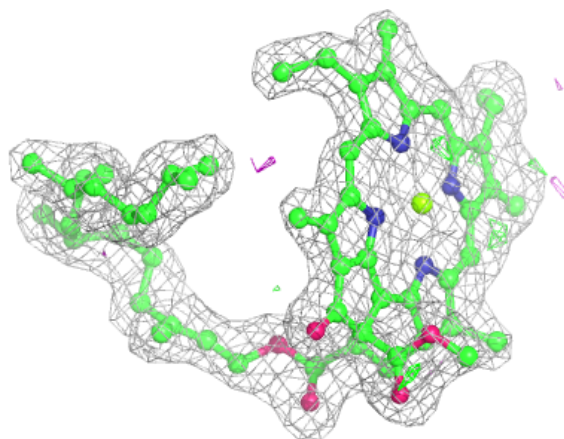
**Electron density around BCR b 623:**

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

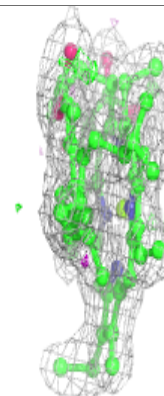
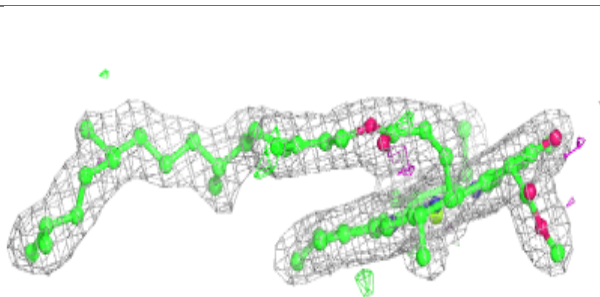
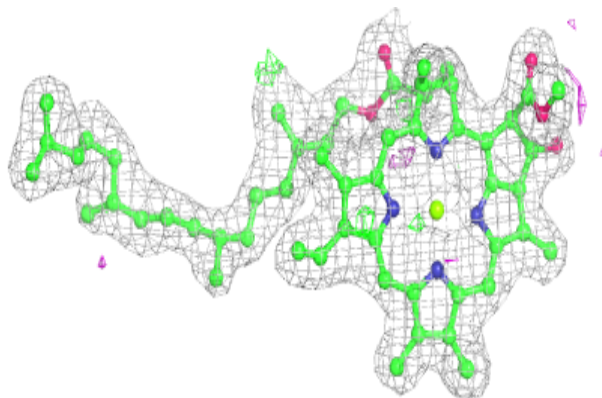


**Electron density around CLA C 504:**

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

**Electron density around CLA B 604:**

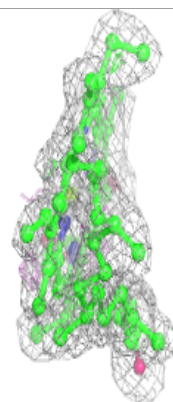
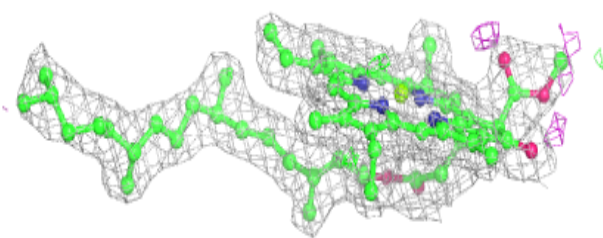
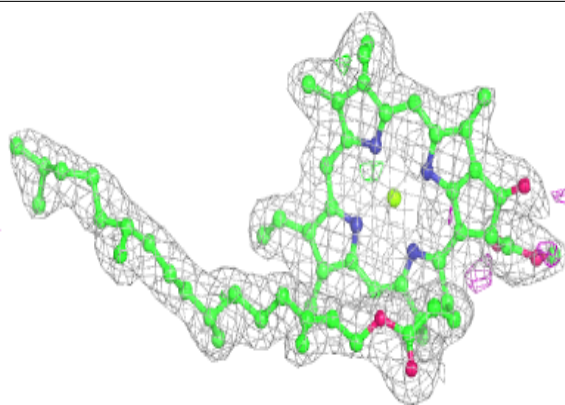
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



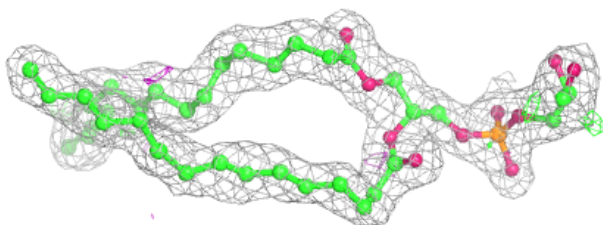
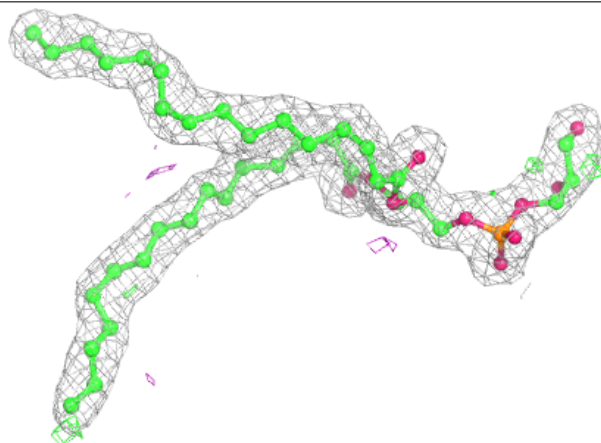


**Electron density around CLA C 502:**

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

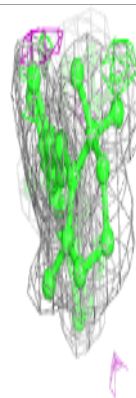
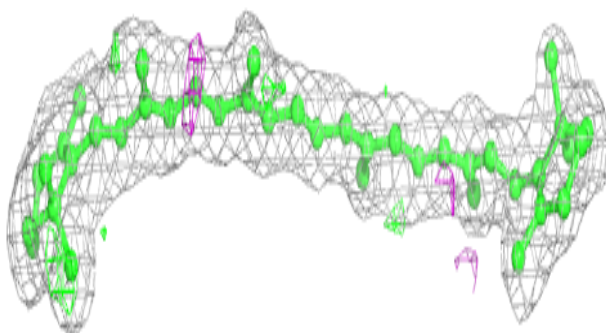
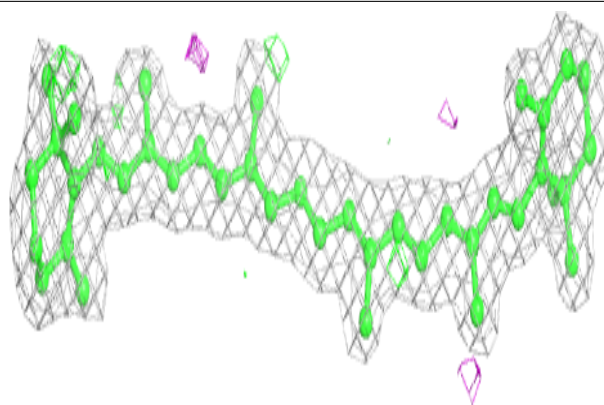
**Electron density around LHG d 408:**

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

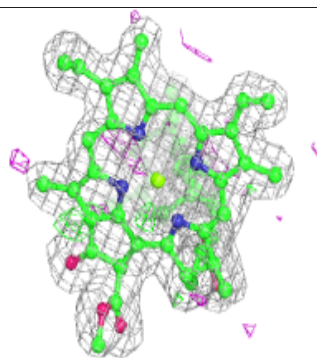
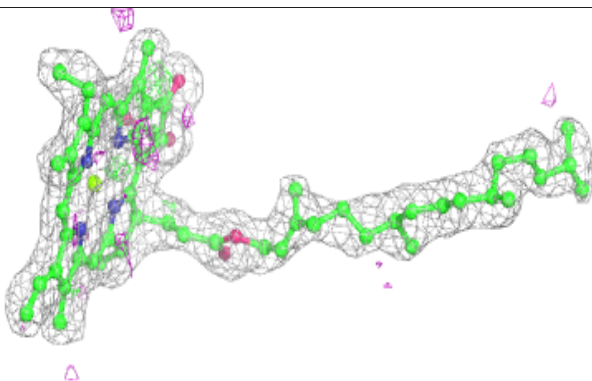
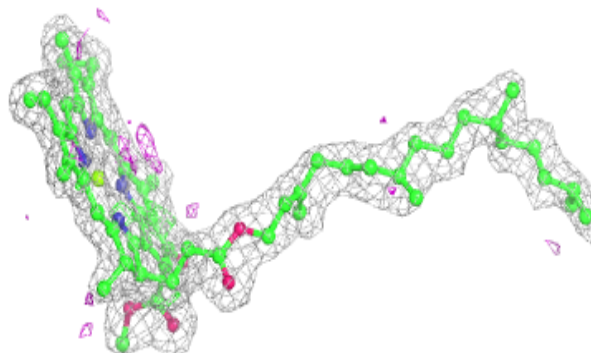


**Electron density around BCR B 620:**

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

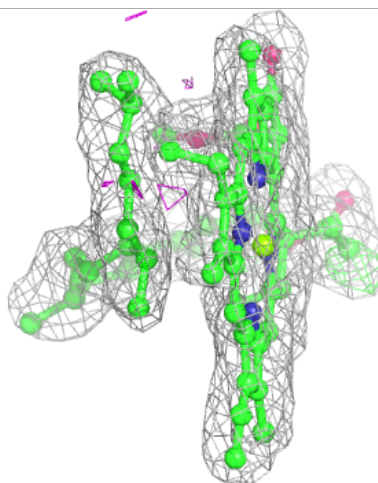
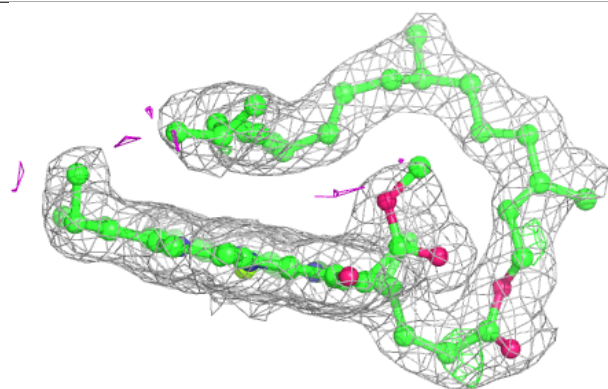
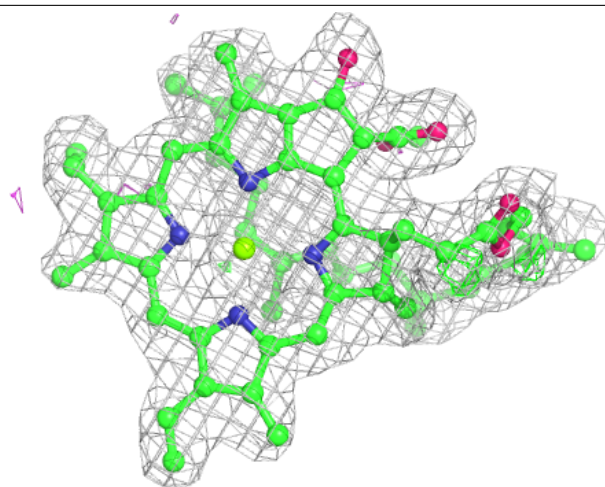
**Electron density around CLA B 605:**

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



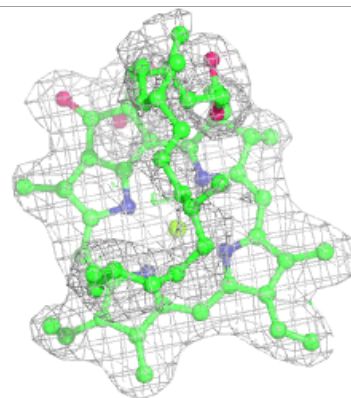
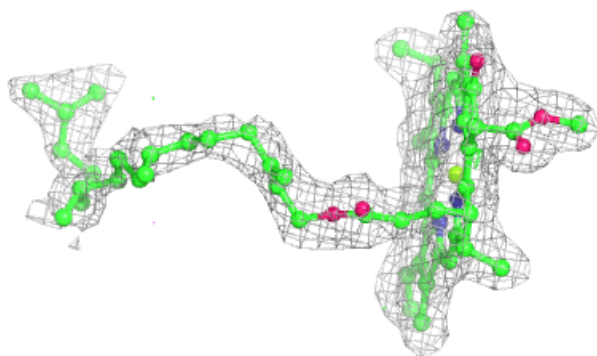
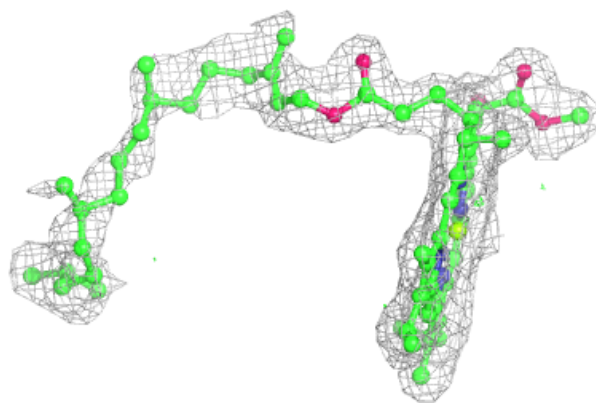
**Electron density around CLA c 911:**

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

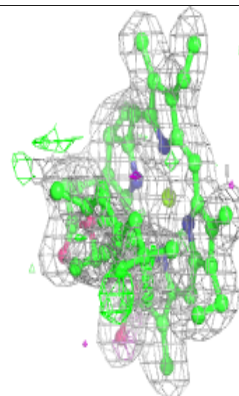
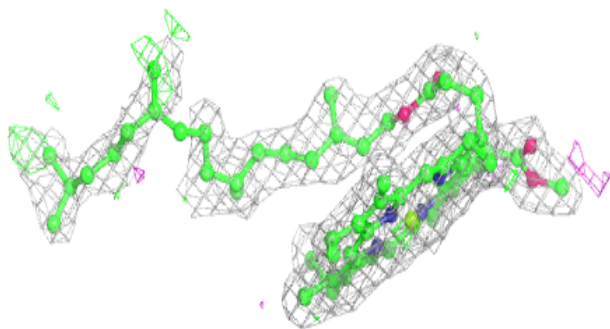
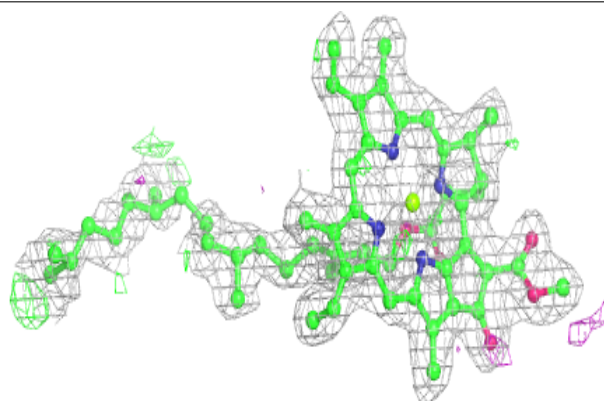


**Electron density around CLA c 907:**

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

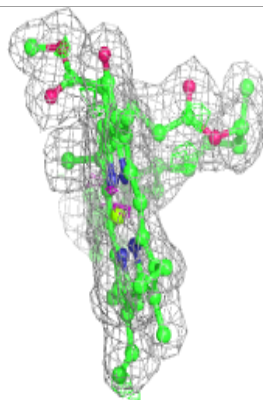
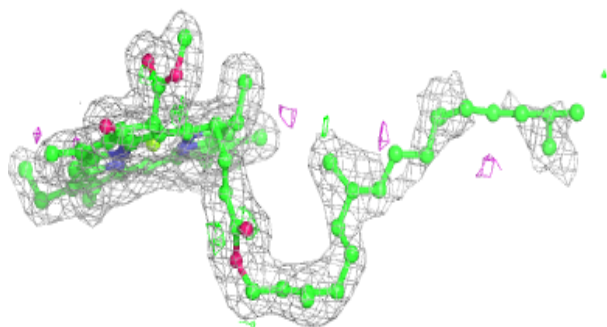
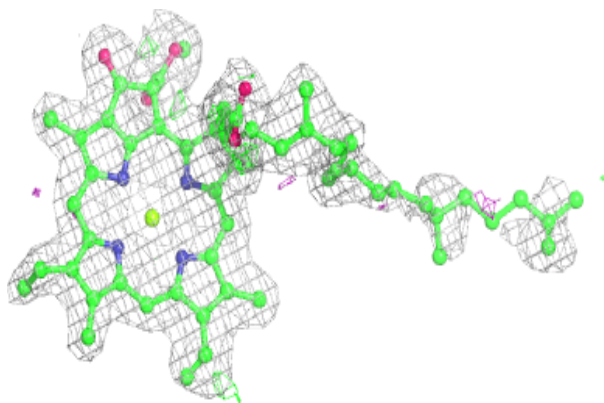
**Electron density around CLA B 615:**

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



**Electron density around CLA a 407:**

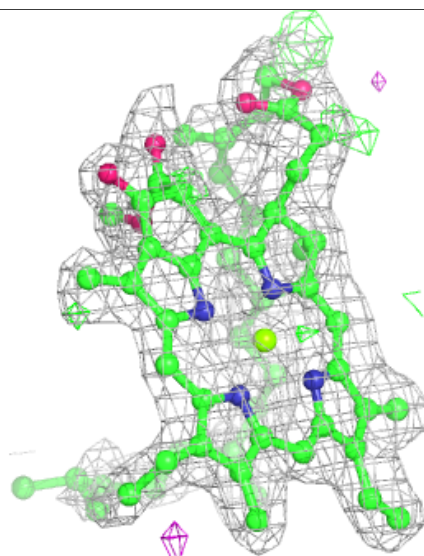
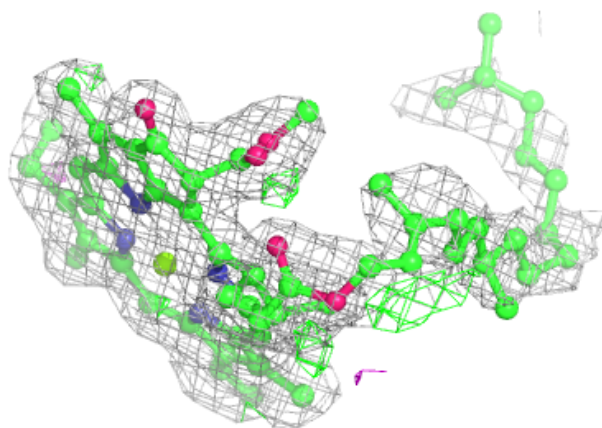
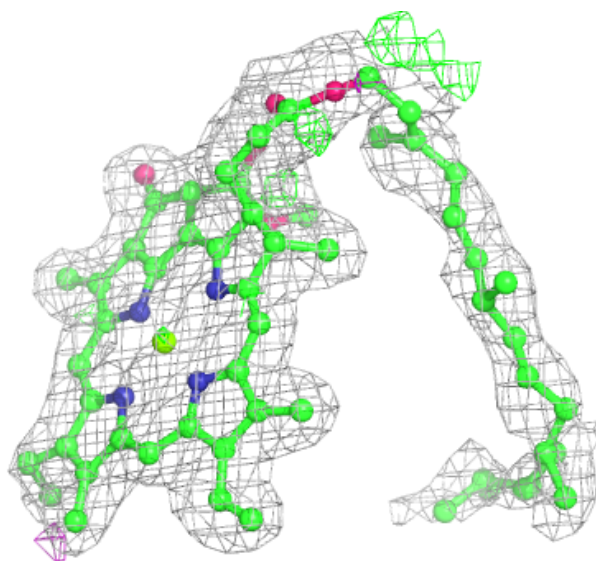
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





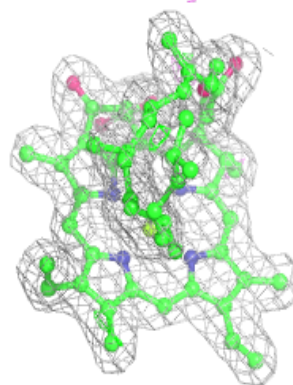
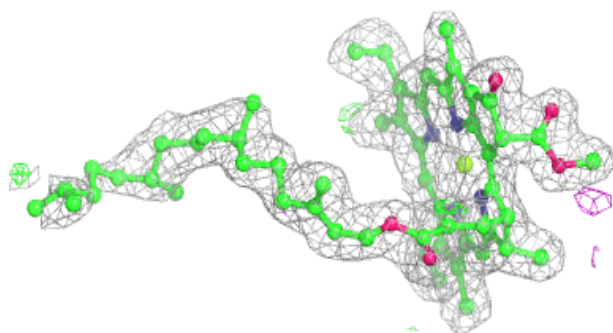
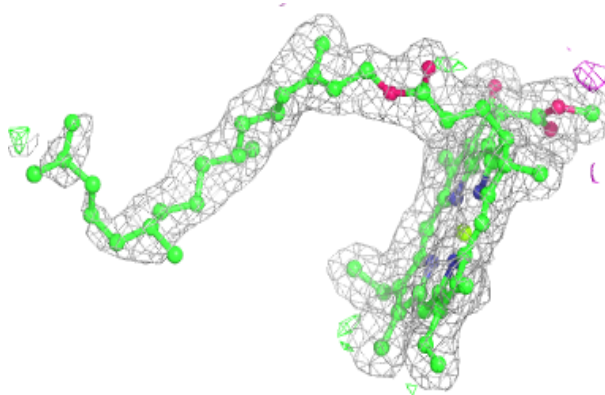
**Electron density around CLA b 620:**

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

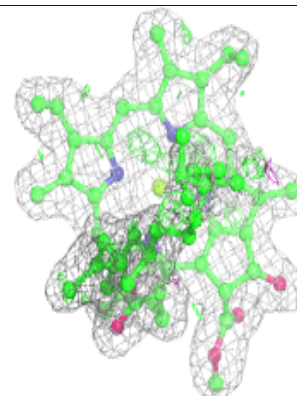
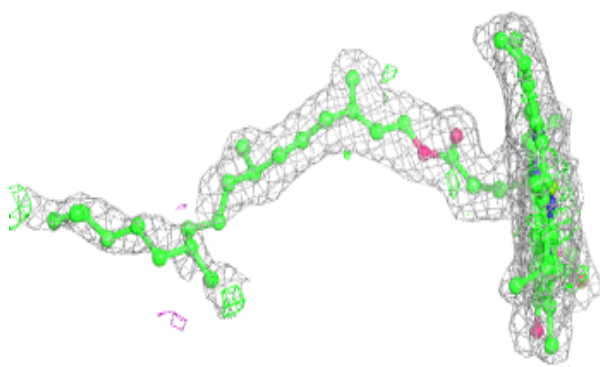
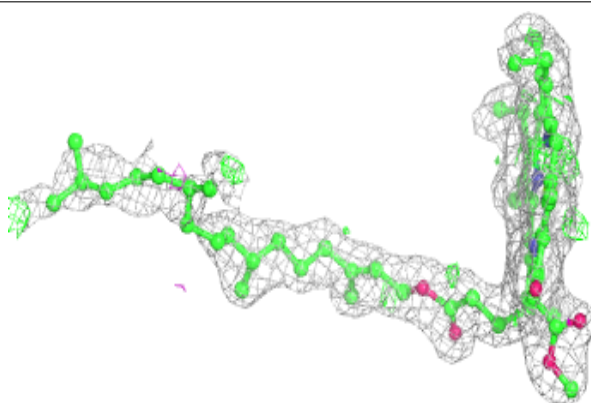


**Electron density around CLA C 509:**

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

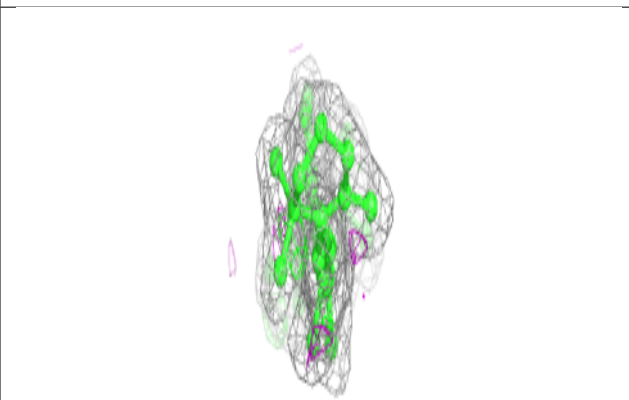
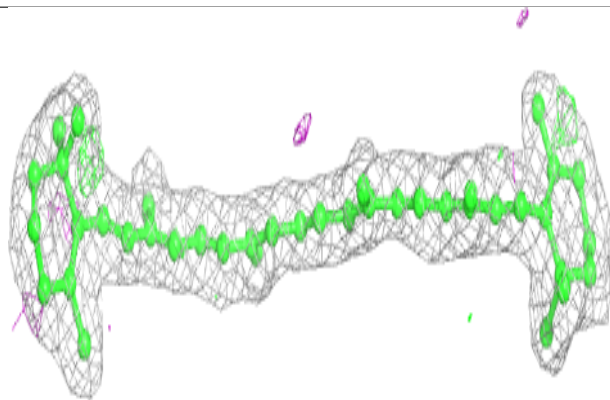
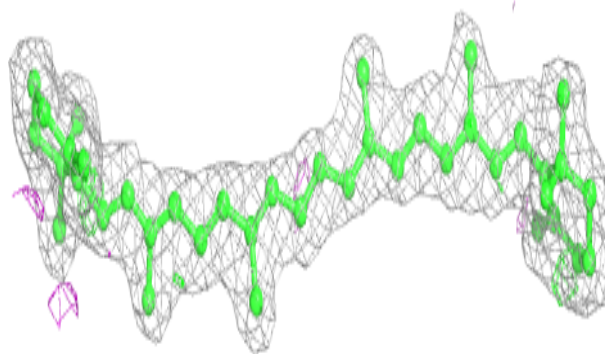
**Electron density around CLA B 607:**

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

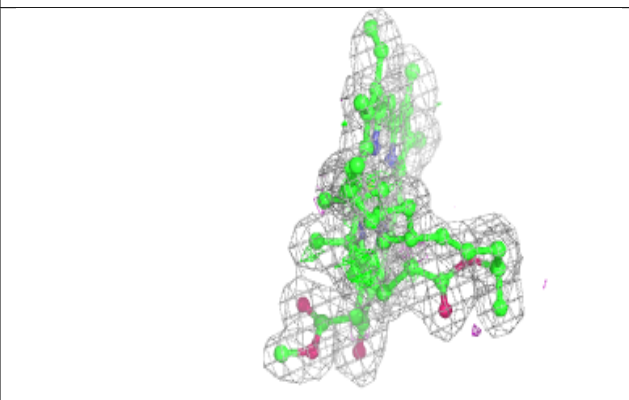
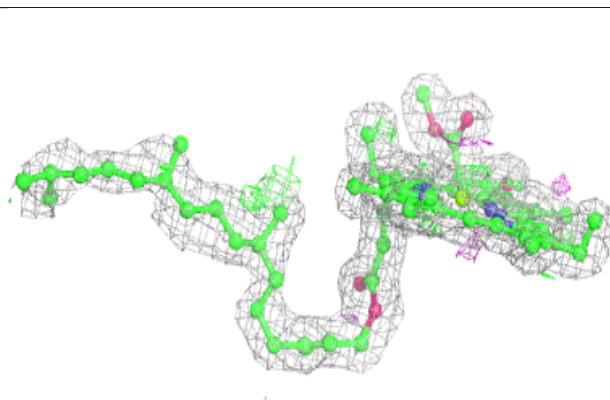
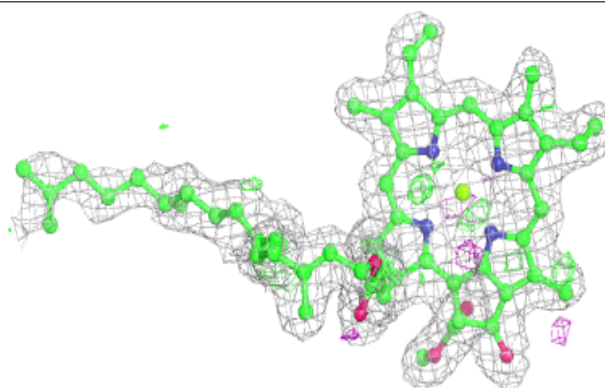


**Electron density around BCR A 411:**

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

**Electron density around CLA A 407:**

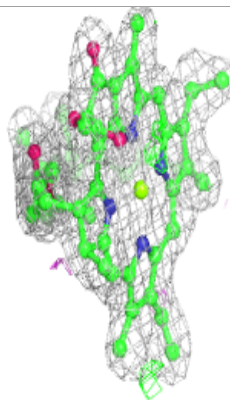
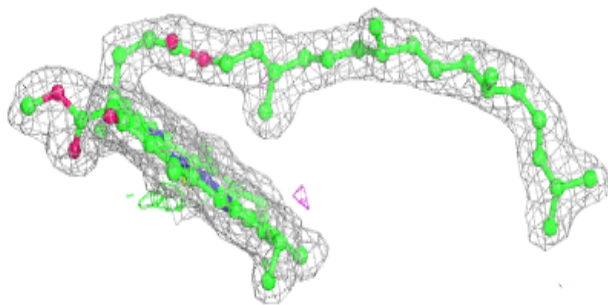
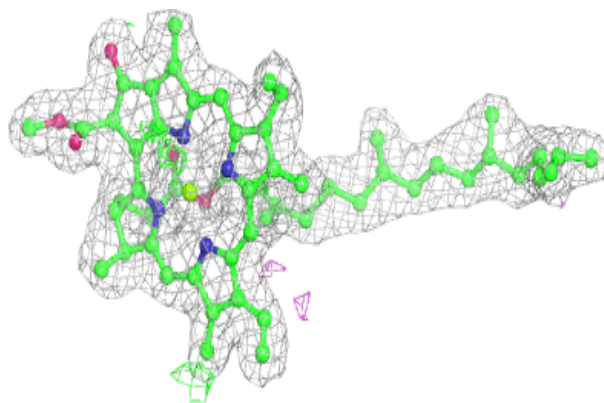
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





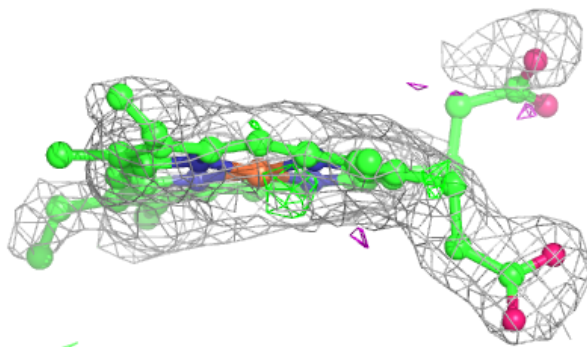
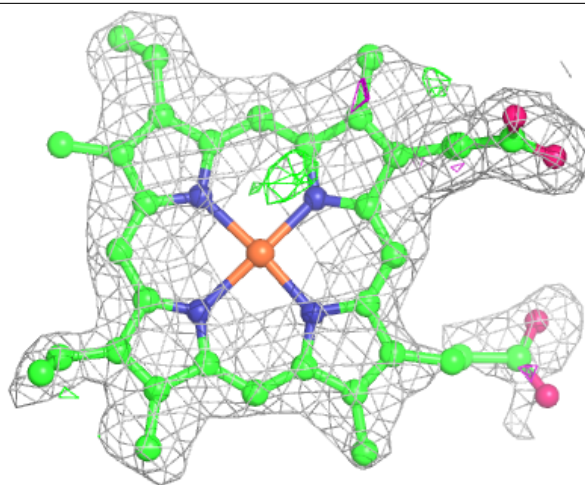
**Electron density around CLA b 612:**

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



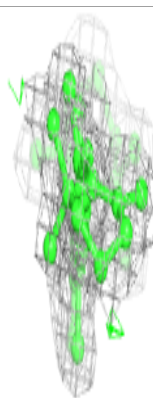
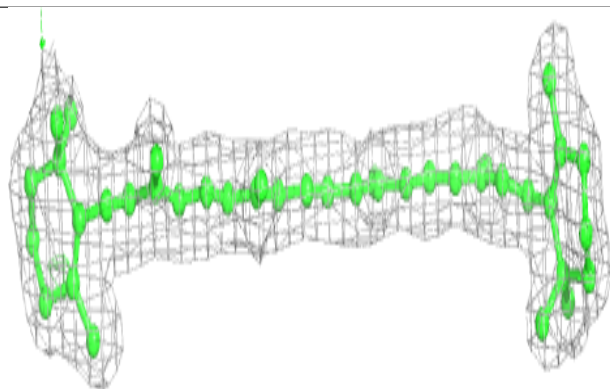
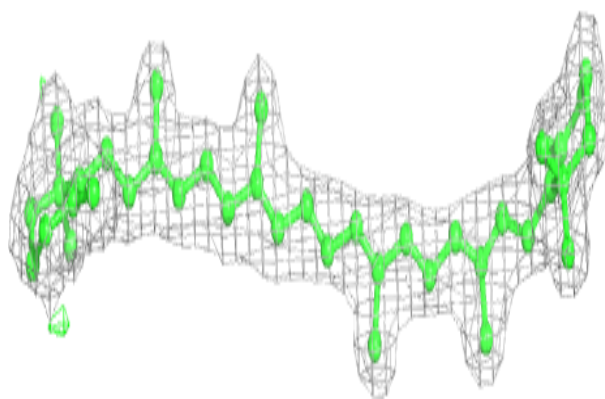
**Electron density around HEM e 102:**

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

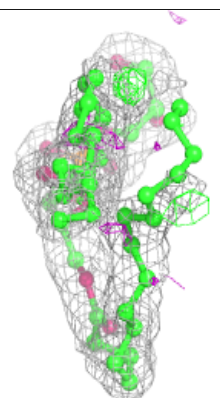
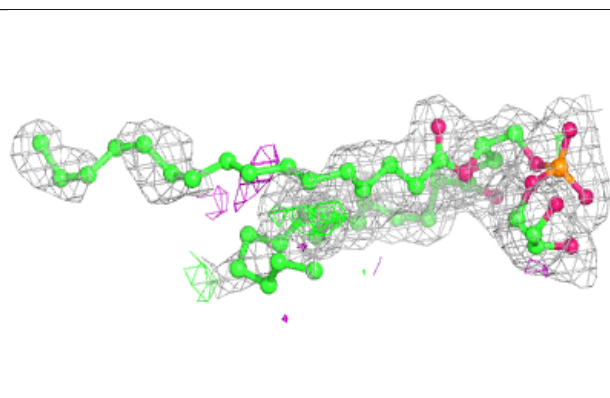
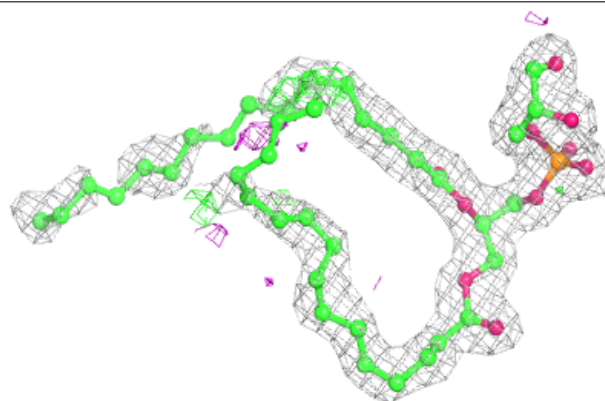


**Electron density around BCR C 516:**

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

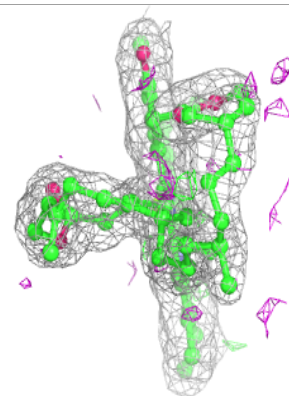
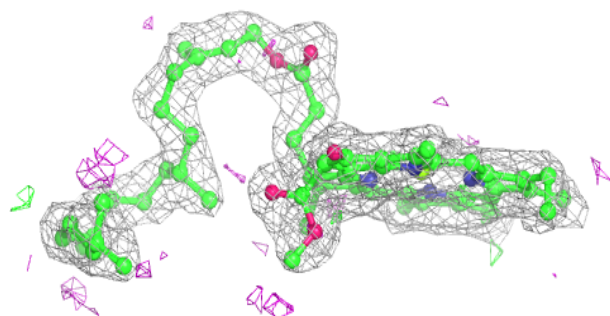
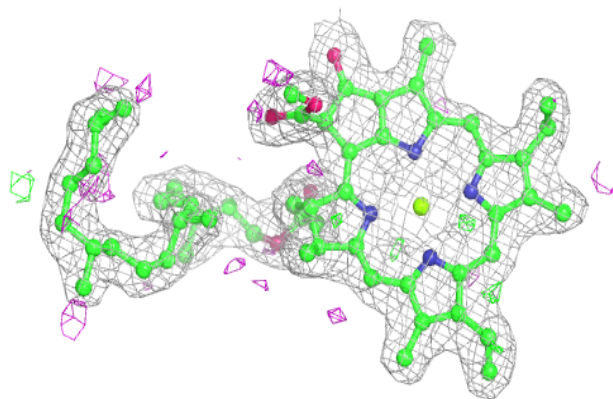
**Electron density around LHG d 409:**

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

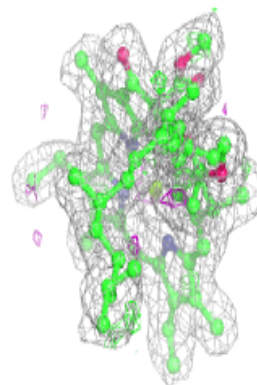
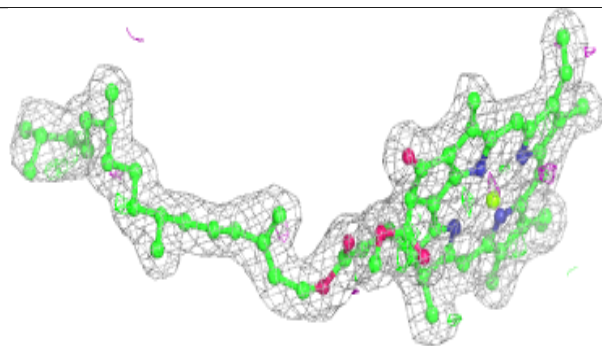
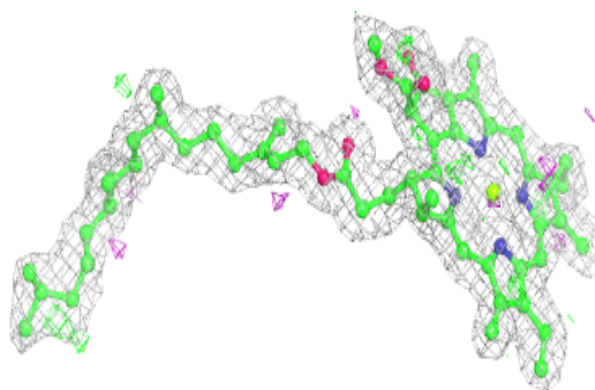


**Electron density around CLA B 613:**

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

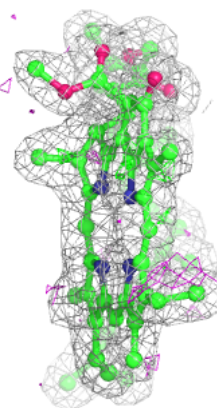
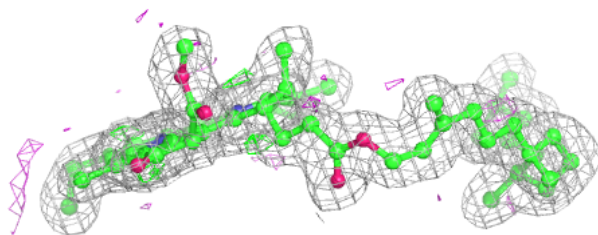
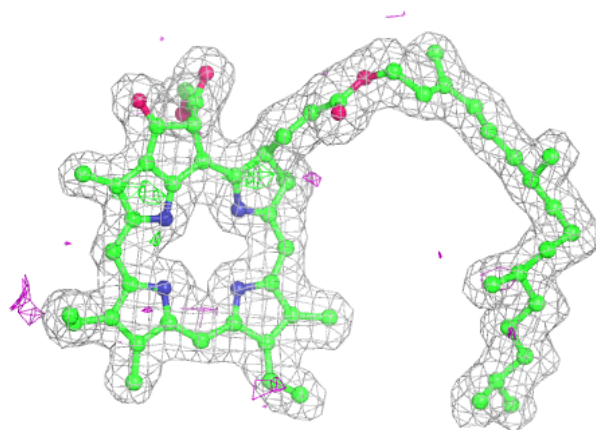
**Electron density around CLA A 405:**

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

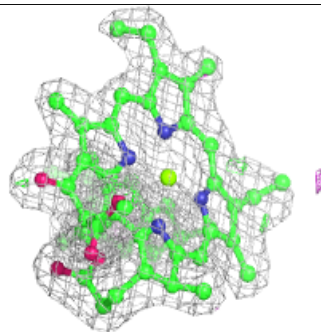
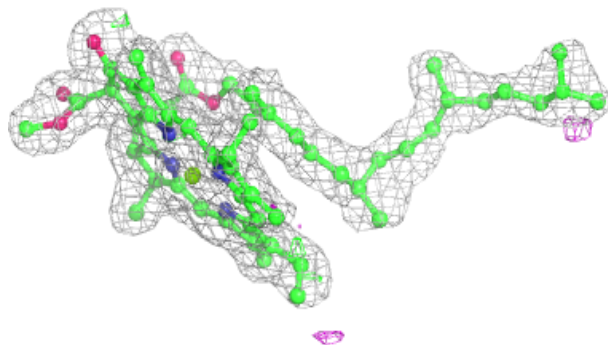
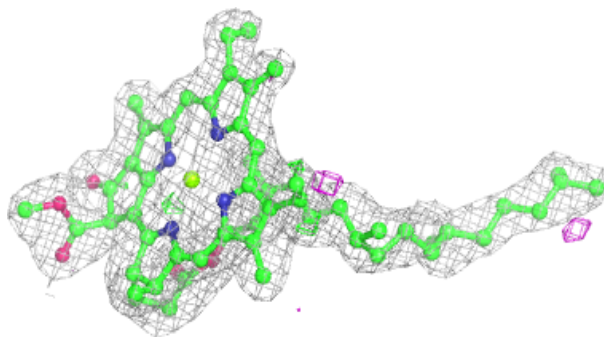


**Electron density around PHO A 408:**

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

**Electron density around CLA C 506:**

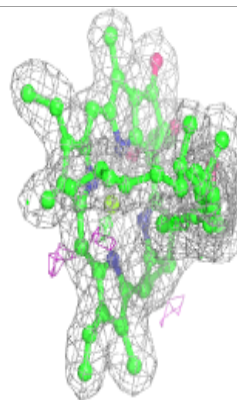
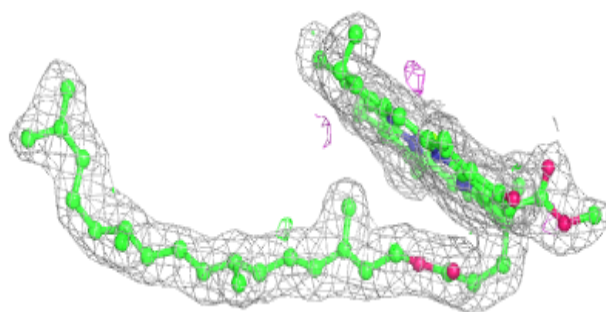
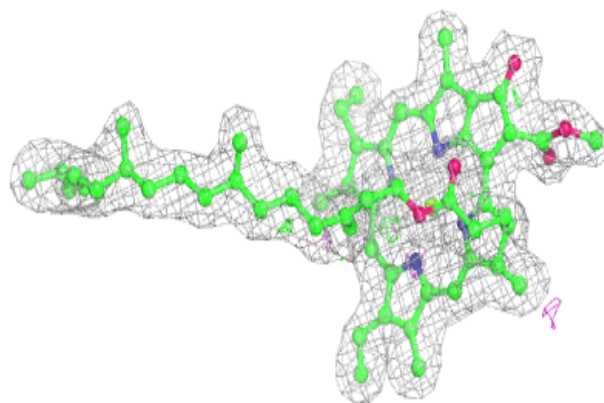
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



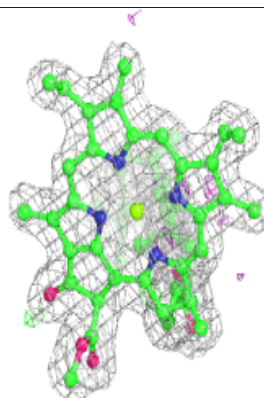
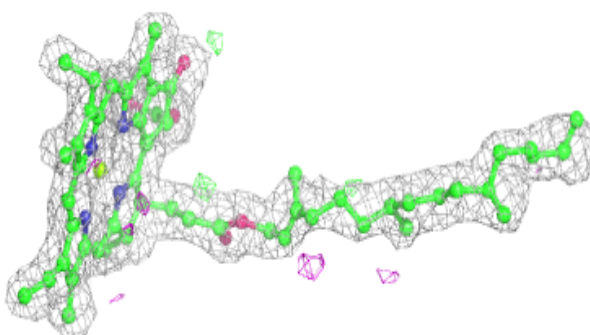
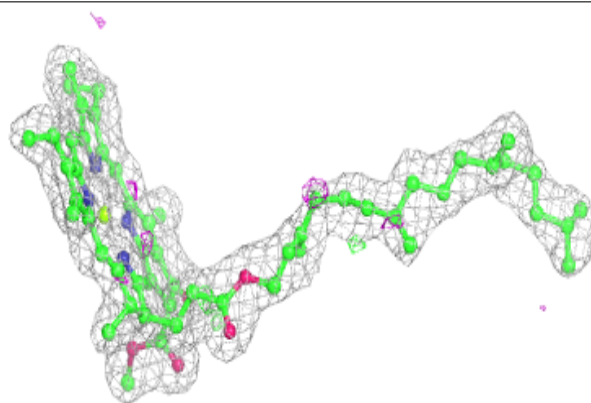


**Electron density around CLA B 609:**

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

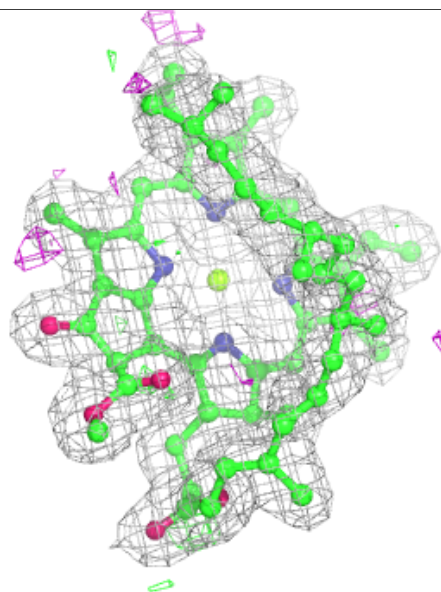
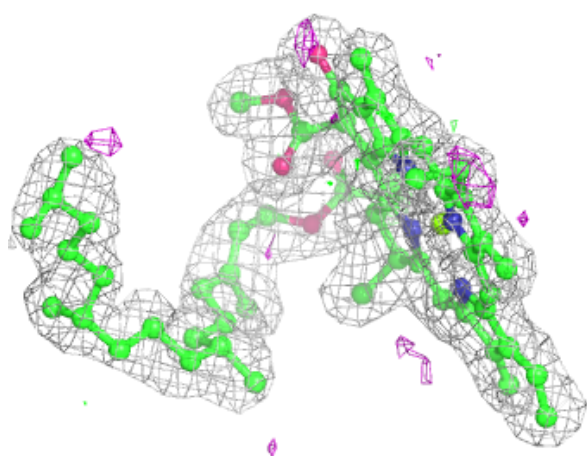
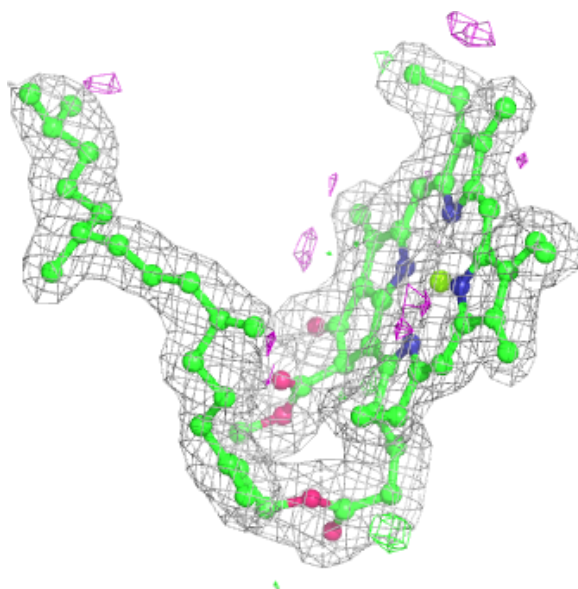
**Electron density around CLA b 608:**

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



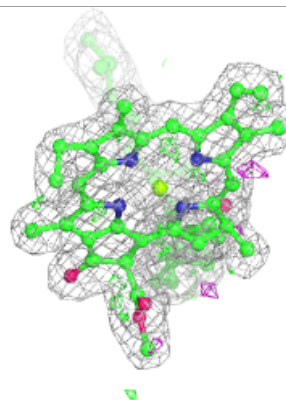
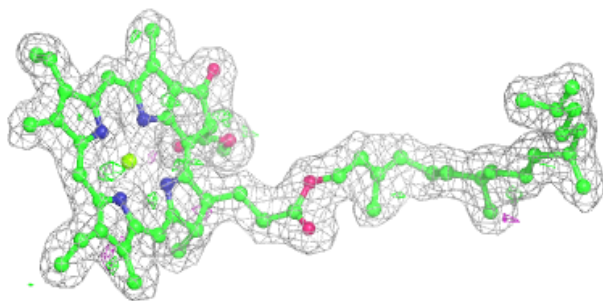
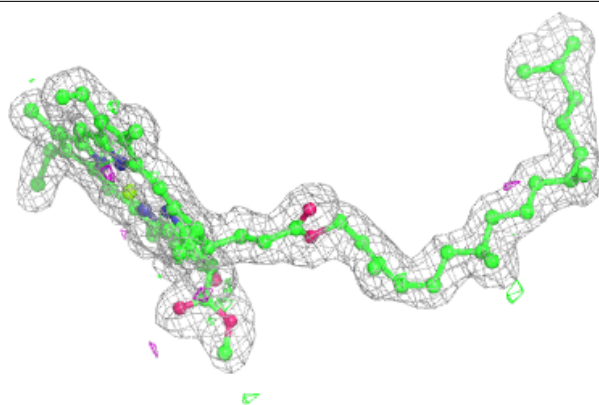
**Electron density around CLA b 617:**

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

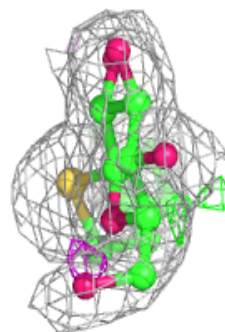
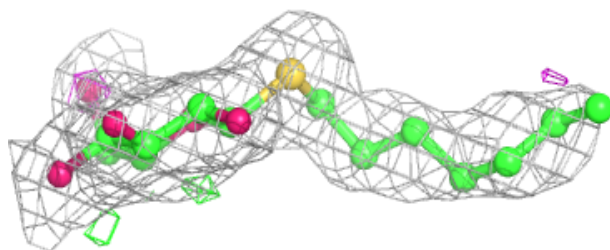
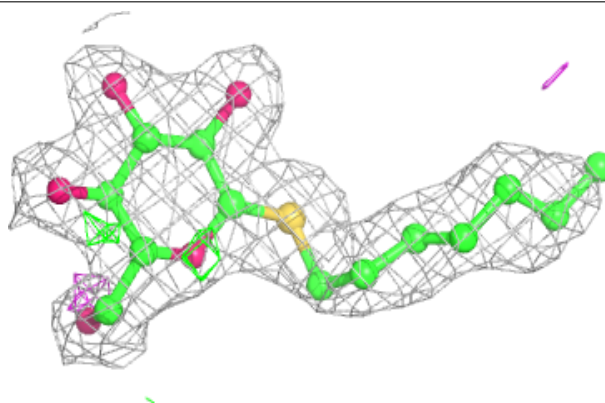


**Electron density around CLA D 401:**

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

**Electron density around HTG O 303:**

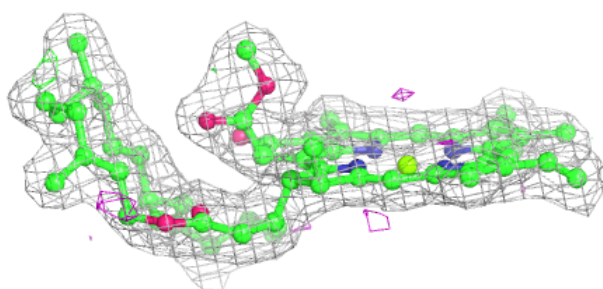
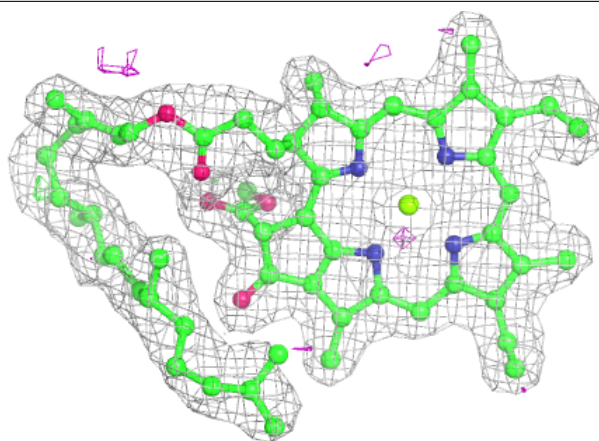
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



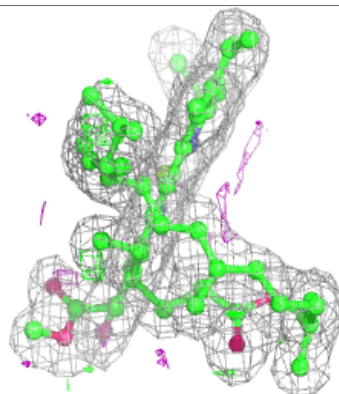
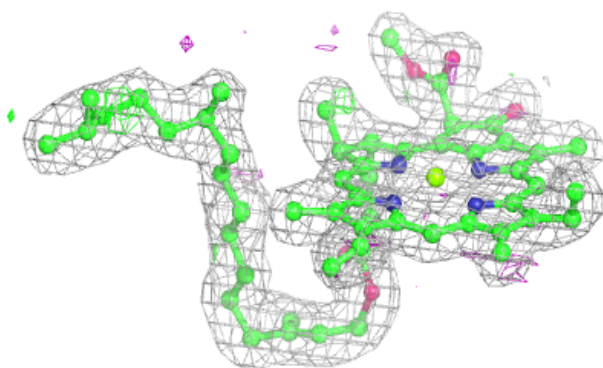
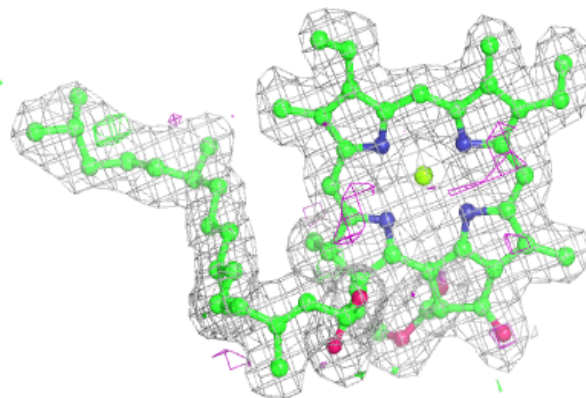


**Electron density around CLA B 611:**

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

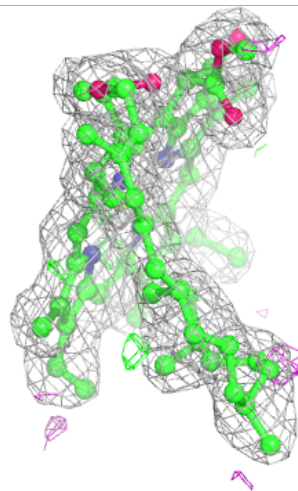
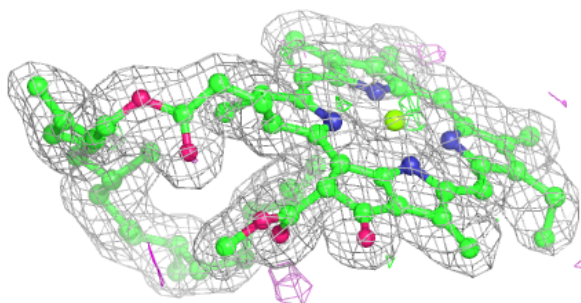
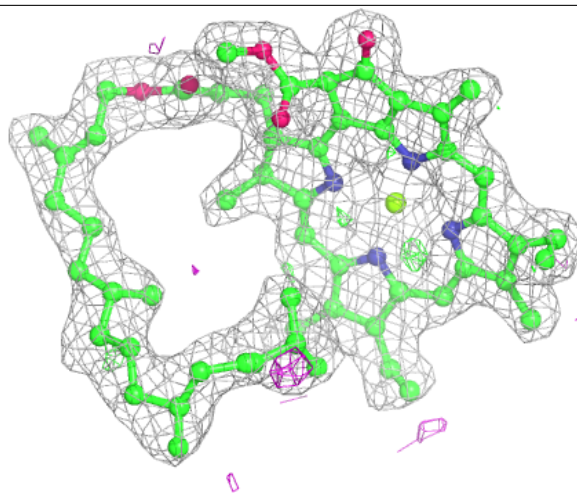
**Electron density around CLA d 401:**

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



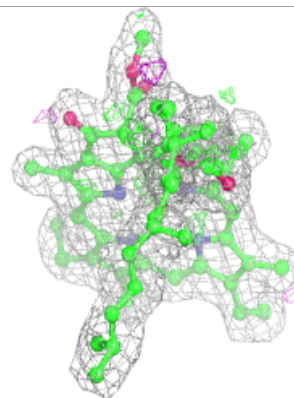
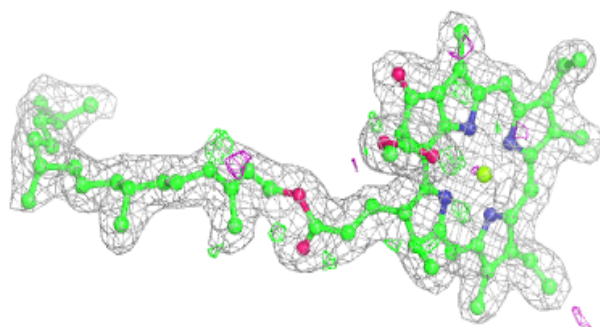
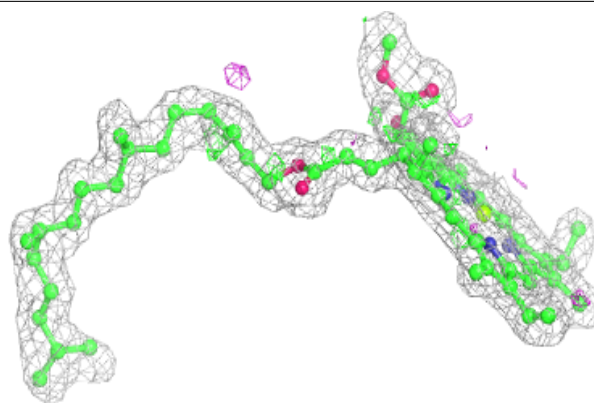
**Electron density around CLA B 616:**

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

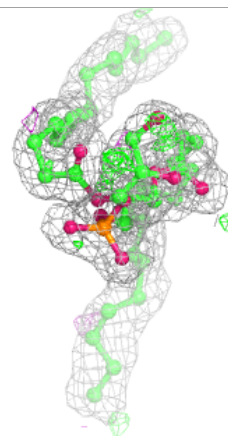
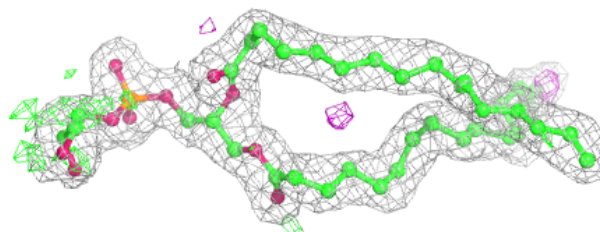
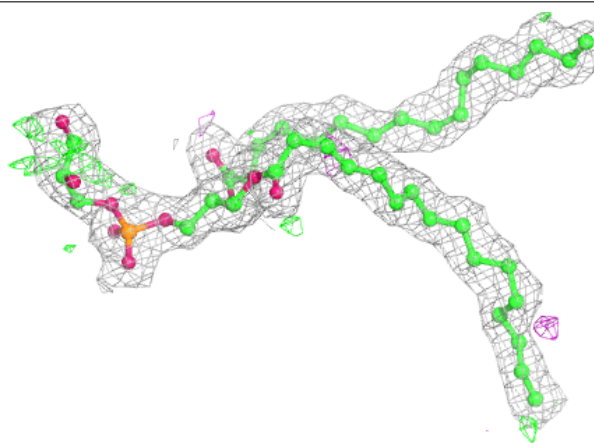


**Electron density around CLA d 402:**

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

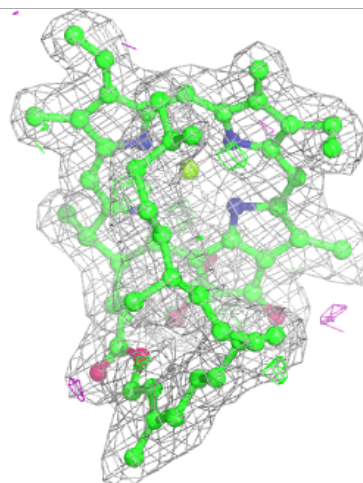
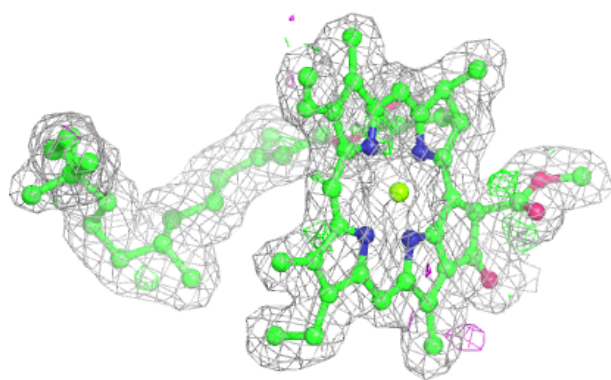
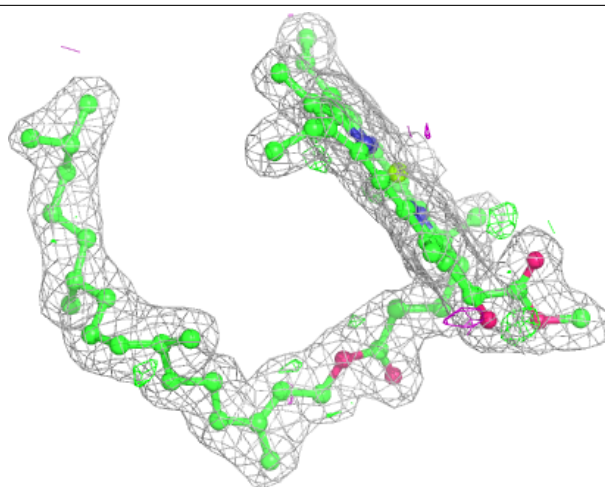
**Electron density around LHG D 407:**

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



**Electron density around CLA B 612:**

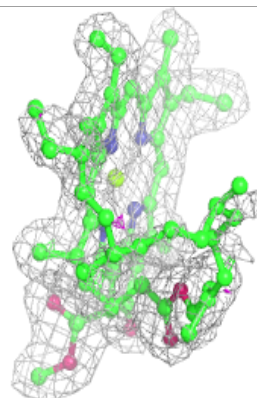
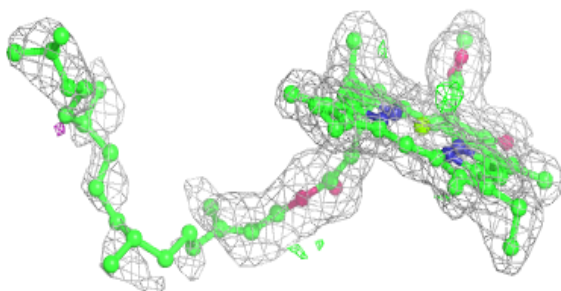
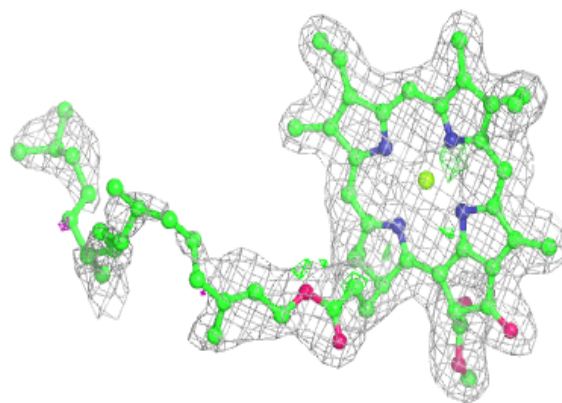
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



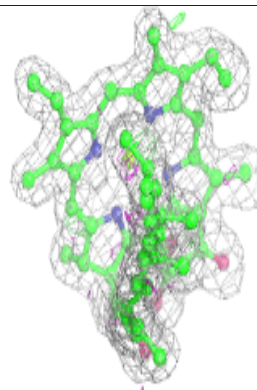
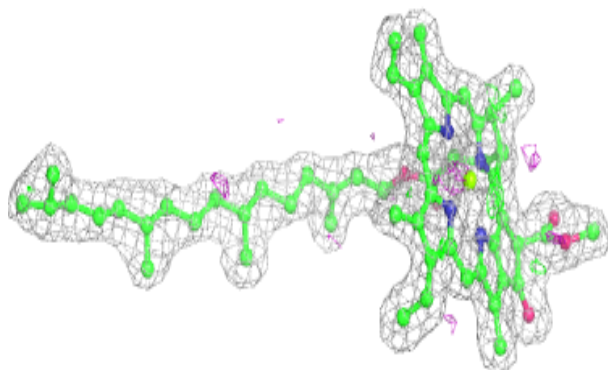
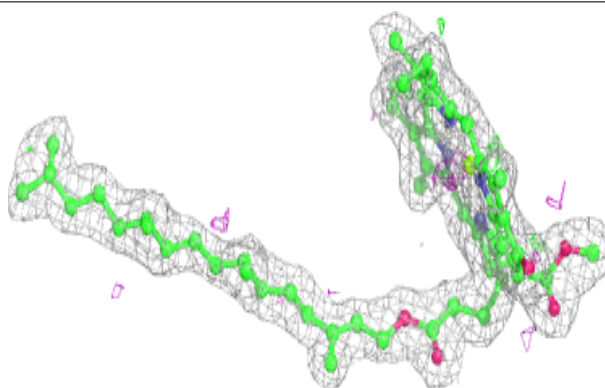


**Electron density around CLA a 409:**

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

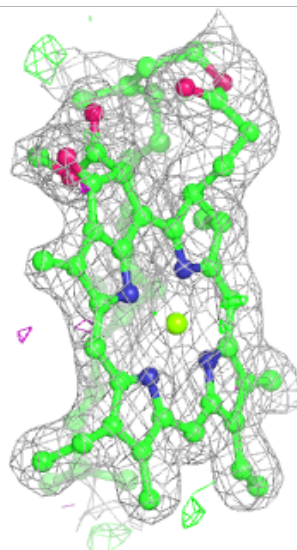
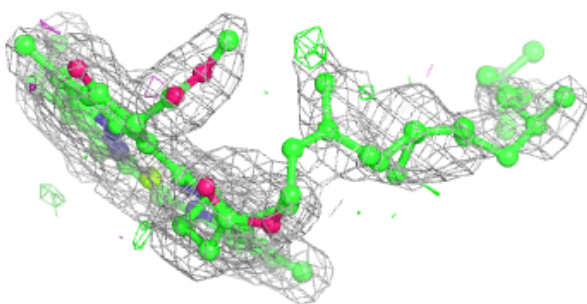
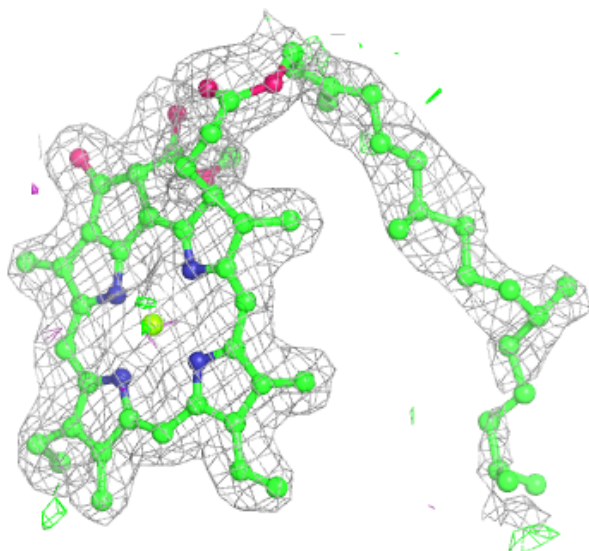
**Electron density around CLA b 611:**

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



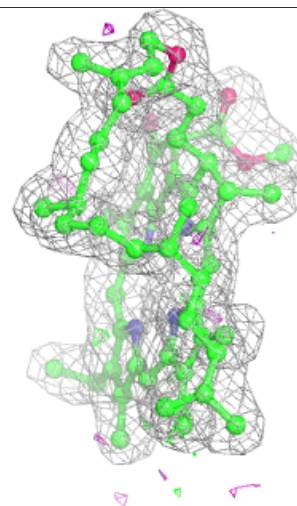
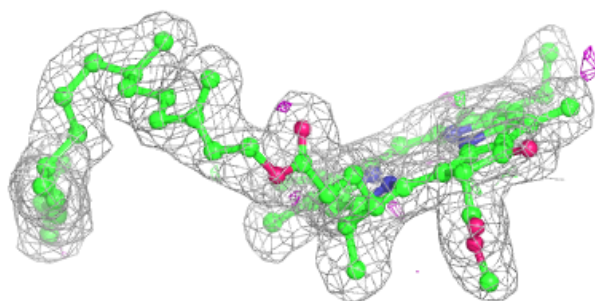
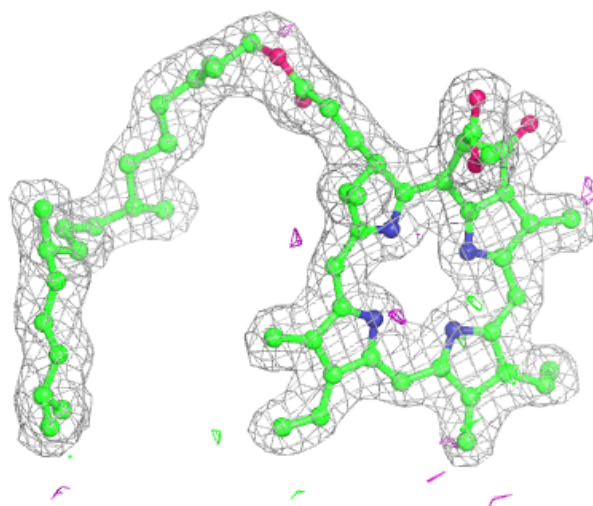
**Electron density around CLA B 617:**

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



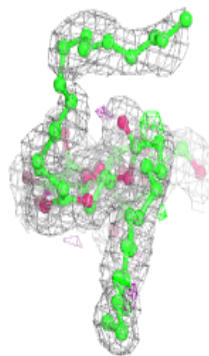
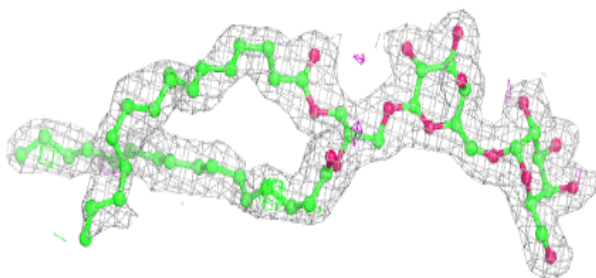
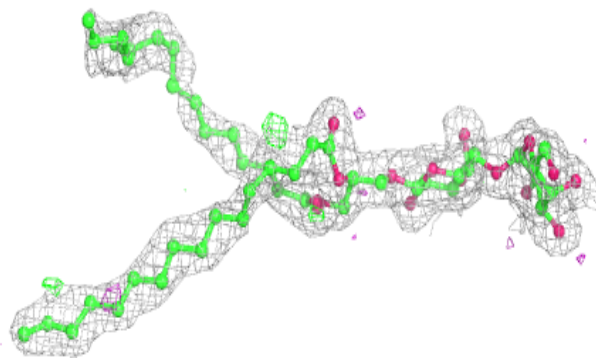
**Electron density around PHO A 409:**

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

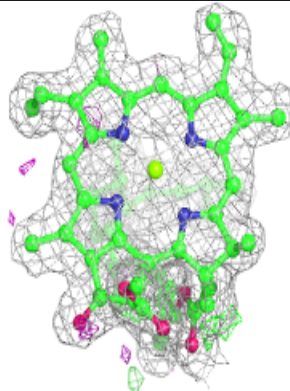
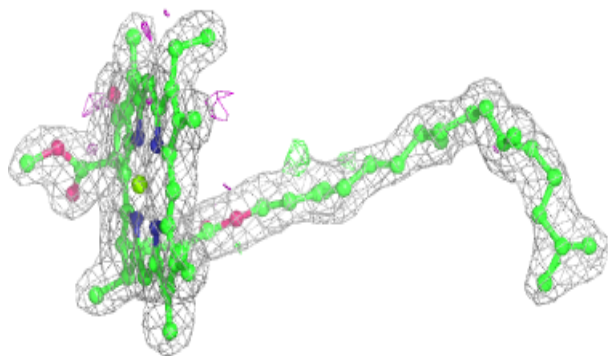
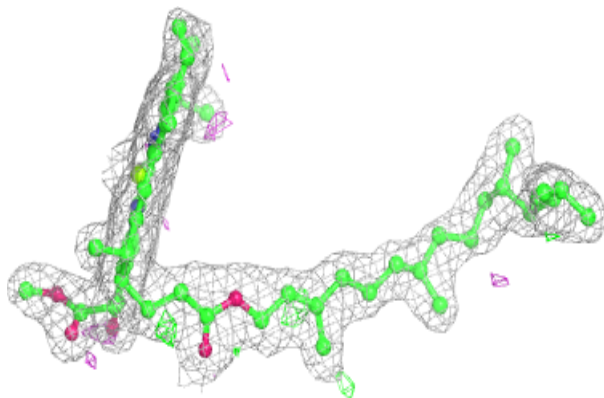


**Electron density around DGD C 517:**

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

**Electron density around CLA b 609:**

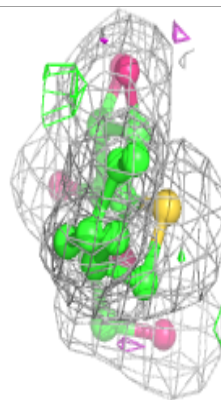
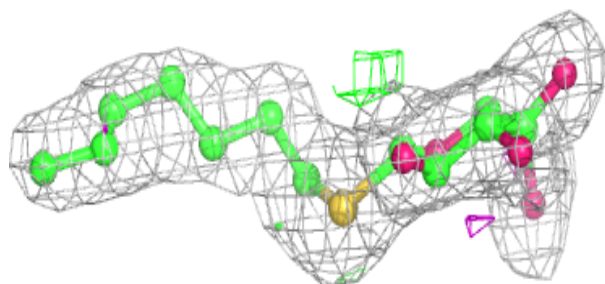
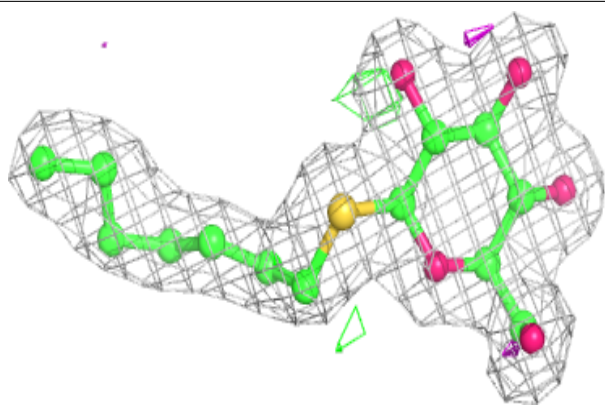
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



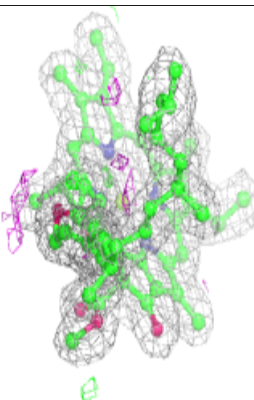
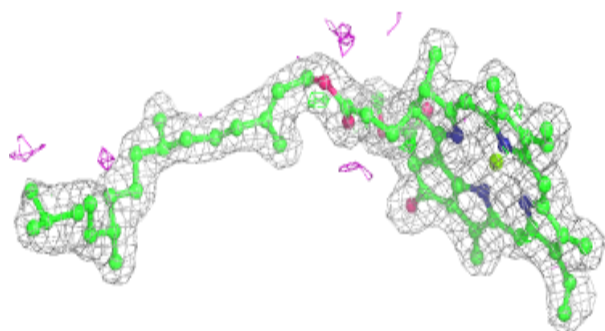
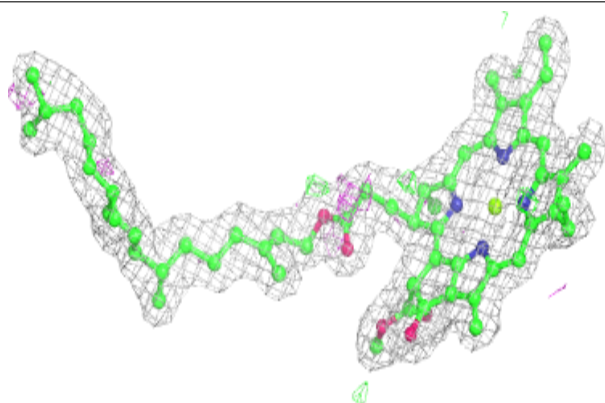


**Electron density around HTG B 624:**

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

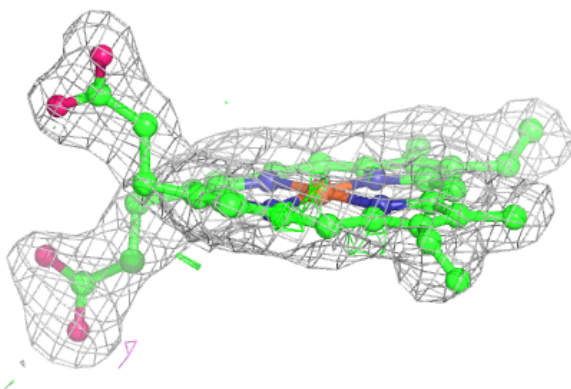
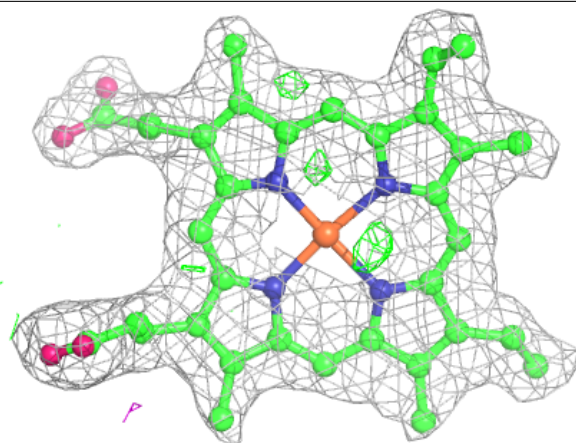
**Electron density around CLA a 406:**

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

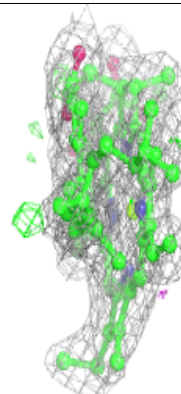
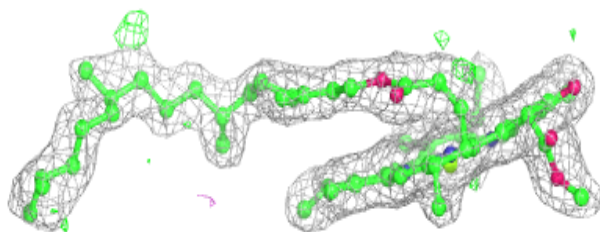
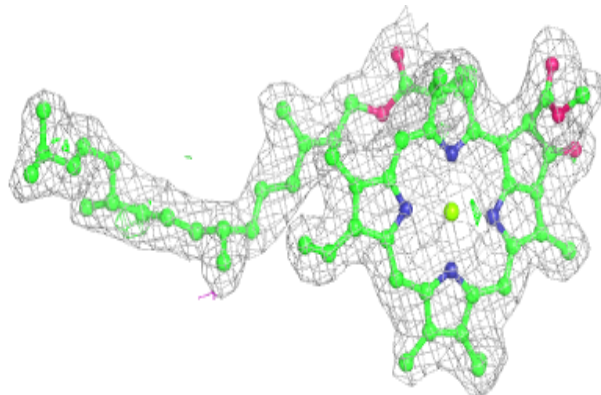


**Electron density around HEM E 103:**

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

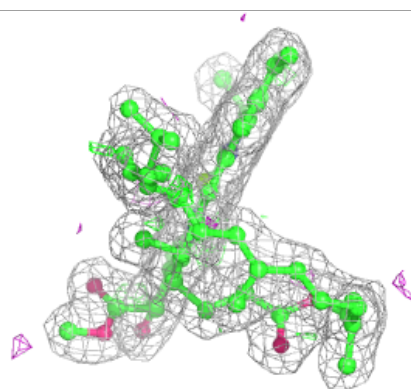
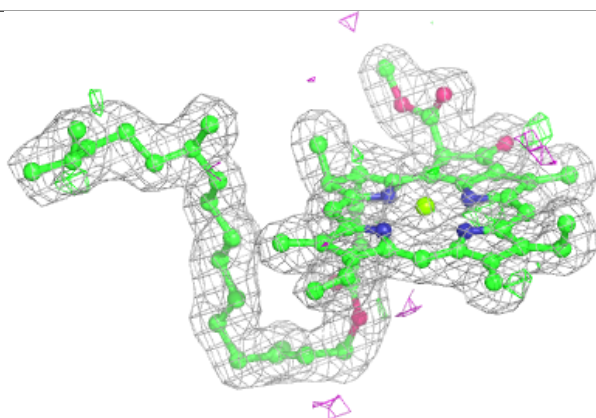
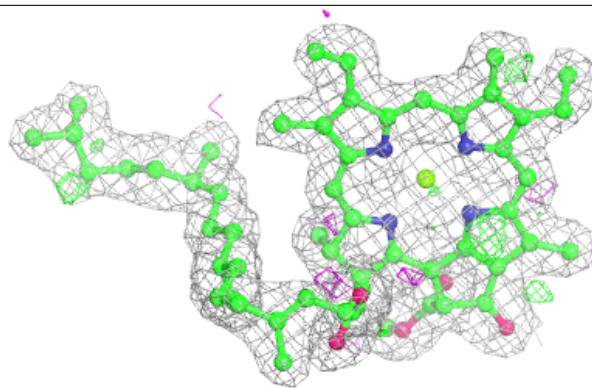
**Electron density around CLA b 607:**

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

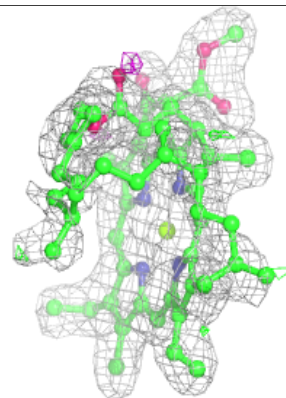
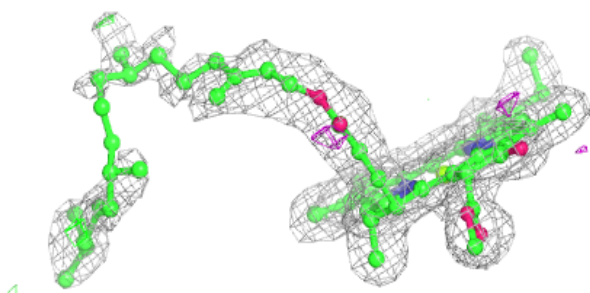
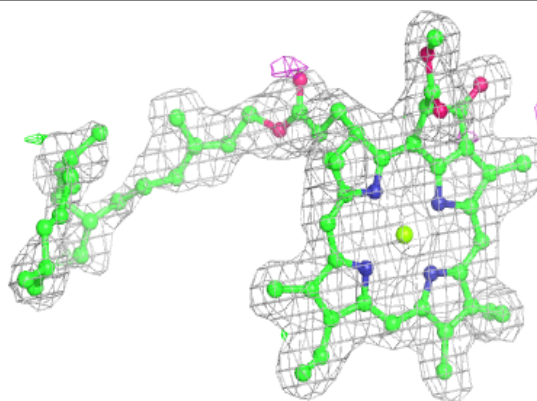


**Electron density around CLA A 406:**

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

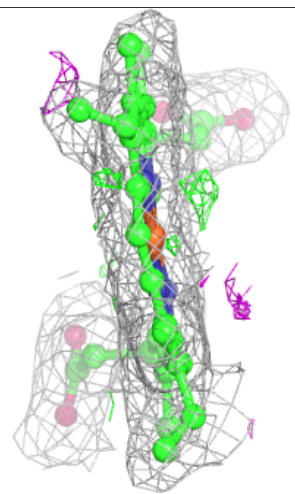
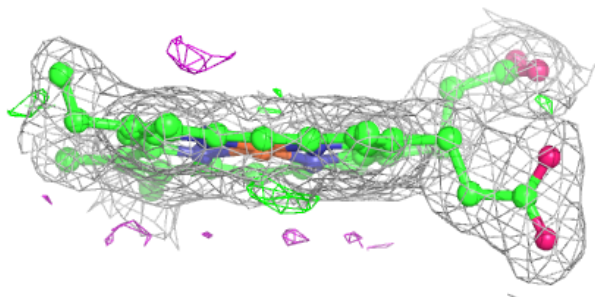
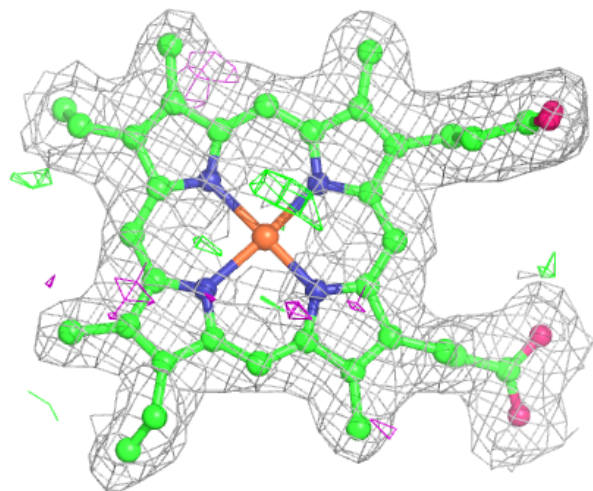
**Electron density around CLA A 410:**

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



**Electron density around HEC V 201:**

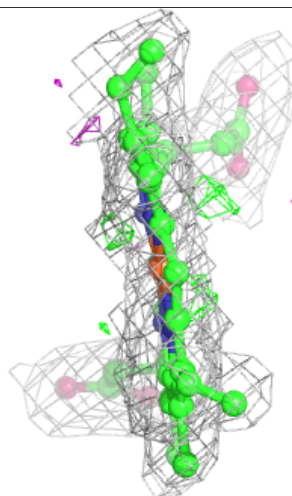
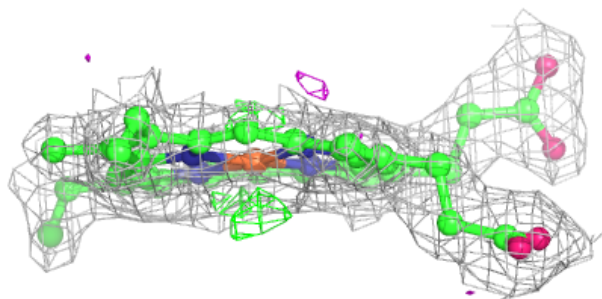
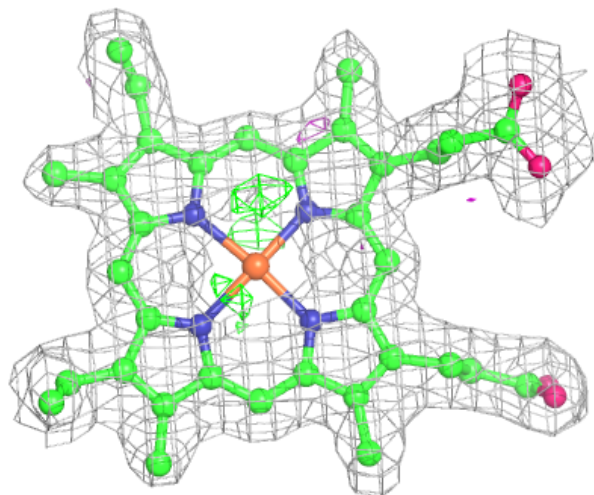
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEC v 202:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.