



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:17 AM BST

PDB ID : 5GTH  
Title : Native XFEL structure of photosystem II (dark dataset)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2016-08-20  
Resolution : 2.50 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

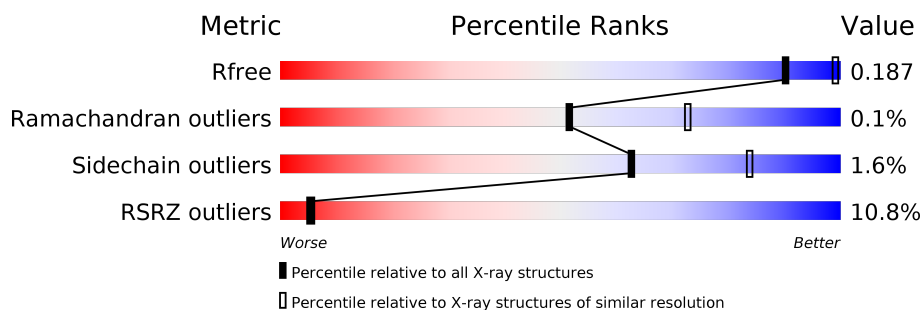
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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>3%</div> <div>97%</div> <div>..</div> </div>
1	a	344	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
2	B	505	<div> <div>10%</div> <div>98%</div> <div>.</div> </div>
2	b	505	<div> <div>11%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>14%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>10%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div>2%</div> <div>100%</div> <div></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	X	40	
17	x	40	
18	Y	30	
18	y	30	
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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
29	PL9	A	414	-	-	-	X
30	UNL	A	415	-	-	-	X
30	UNL	a	415	-	-	-	X
30	UNL	b	626	-	-	-	X
30	UNL	i	101	-	-	-	X
31	LHG	e	101	-	-	-	X
33	LMG	Z	101	-	-	-	X
34	HTG	B	624	-	-	-	X
34	HTG	C	521	-	-	-	X
34	HTG	C	522	-	-	-	X
34	HTG	D	412	-	-	-	X
34	HTG	b	622	-	-	-	X
34	HTG	b	623	-	-	-	X
34	HTG	c	522	-	-	-	X
35	LMT	B	630	-	-	-	X
35	LMT	E	102	-	-	-	X
35	LMT	I	101	-	-	-	X
35	LMT	e	102	-	-	-	X
35	LMT	m	102	-	-	-	X

## 2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 52773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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	5	0
			2639	1732	431	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

- Molecule 3 is a protein called Photosystem II CP43 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	5	0
			3537	2317	589	618	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	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

- 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	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	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
			277	185	43	48	1			

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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	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	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	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	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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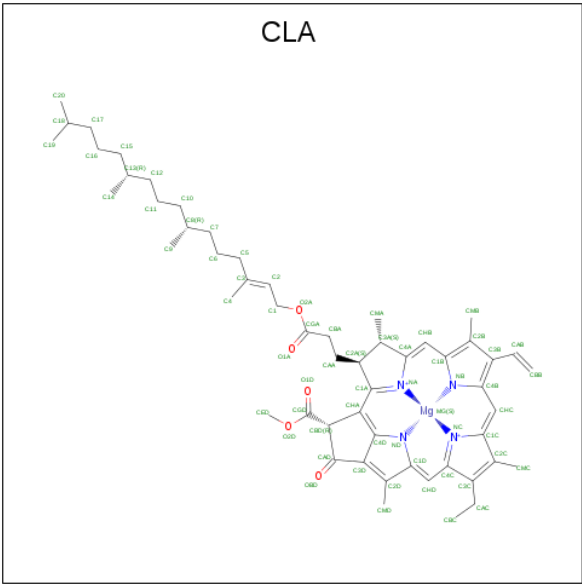
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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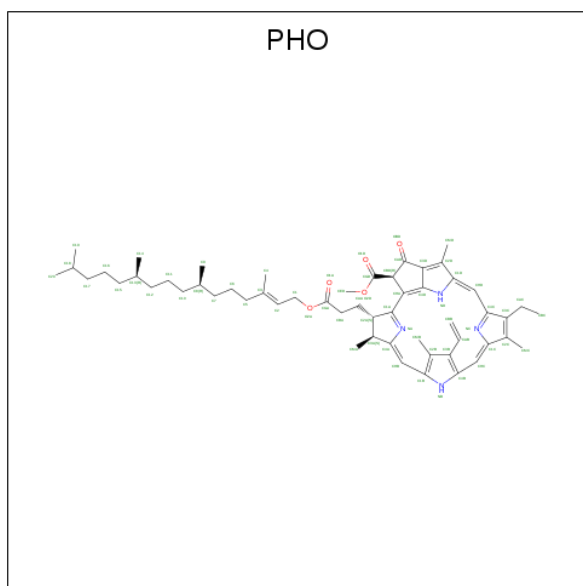
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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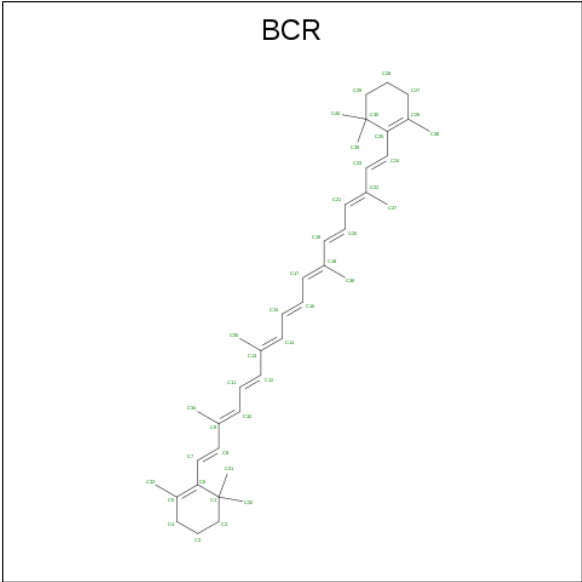
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



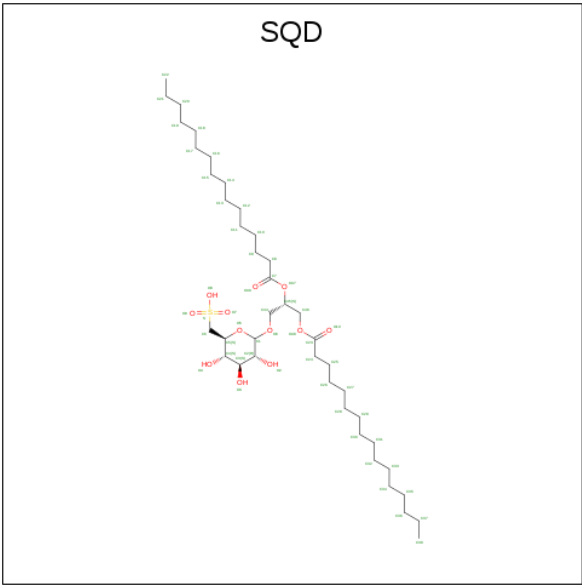
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	h	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



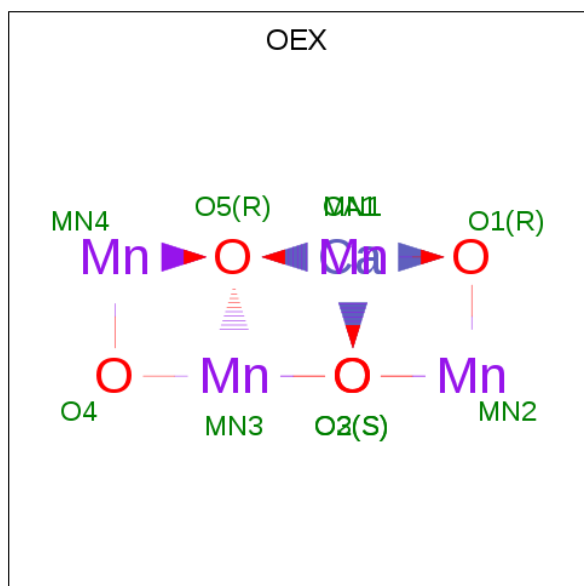
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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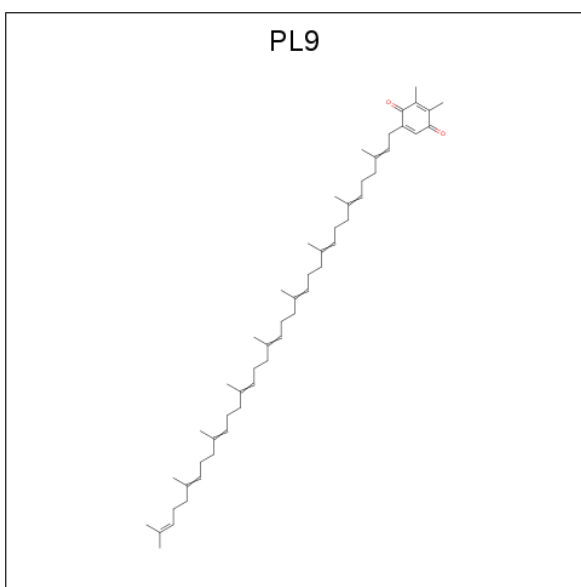
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	d	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 29 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
29	A	1	Total	C	O	0	0
			55	53	2		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	0
			55	53	2		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

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

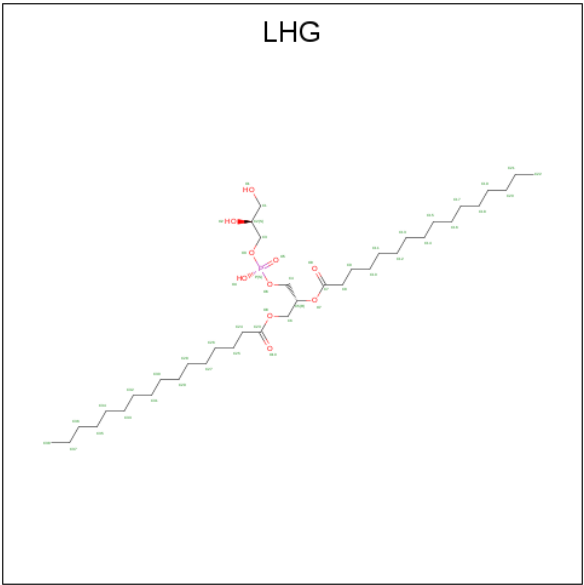
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	x	1	Total	C	O	0	0
			18	16	2		
30	A	1	Total	C	O	0	0
			28	23	5		
30	j	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	d	1	Total	C	O	0	0
			17	16	1		
30	m	1	Total	C		0	0
			10	10			
30	b	2	Total	C	O	0	0
			69	59	10		
30	M	1	Total	C		0	0
			10	10			

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



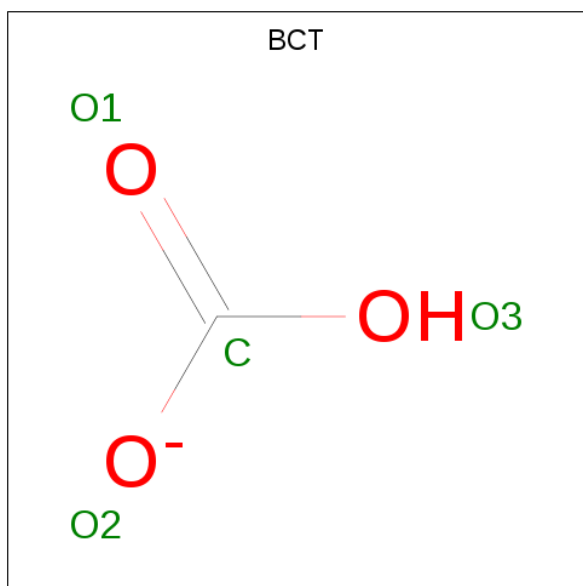
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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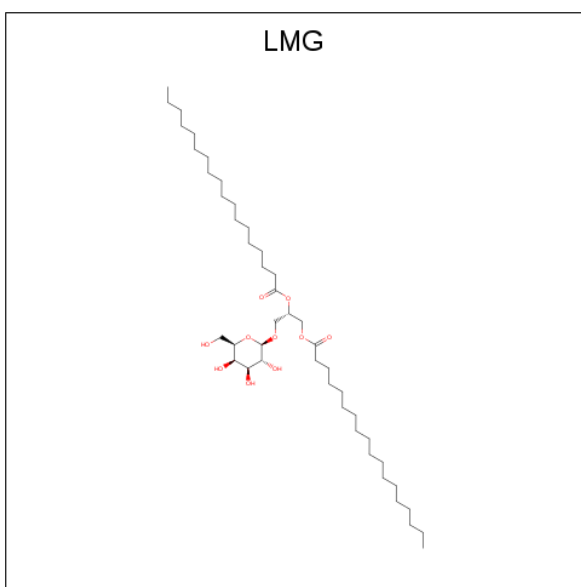
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



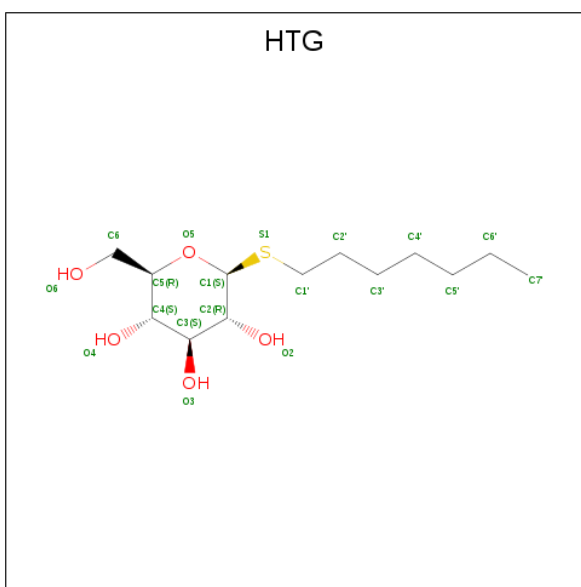
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $\text{C}_{45}\text{H}_{86}\text{O}_{10}$ ).



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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C<sub>13</sub>H<sub>26</sub>O<sub>5</sub>S).



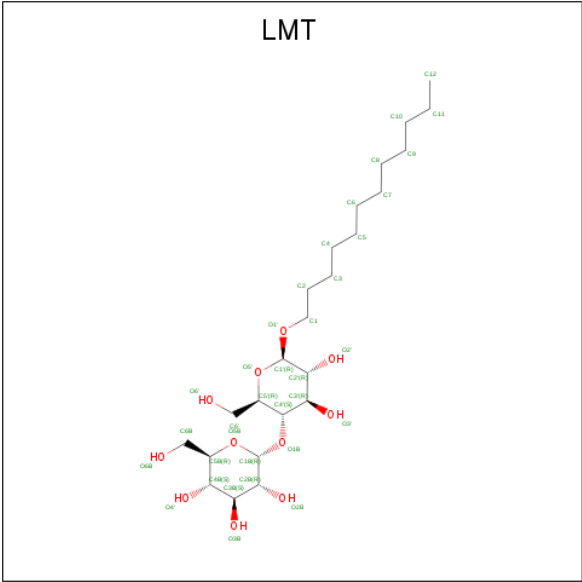
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total 19	C 13	O 5	S 1	0	0
34	B	1	Total 19	C 13	O 5	S 1	0	0
34	B	1	Total 19	C 13	O 5	S 1	0	0
34	B	1	Total 19	C 13	O 5	S 1	0	0
34	C	1	Total 19	C 13	O 5	S 1	0	0
34	C	1	Total 19	C 13	O 5	S 1	0	0
34	D	1	Total 16	C 10	O 5	S 1	0	0
34	V	1	Total 11	C 6	O 5		0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	b	1	Total 19	C 13	O 5	S 1	0	0
34	c	1	Total 19	C 13	O 5	S 1	0	0
34	c	1	Total 19	C 13	O 5	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



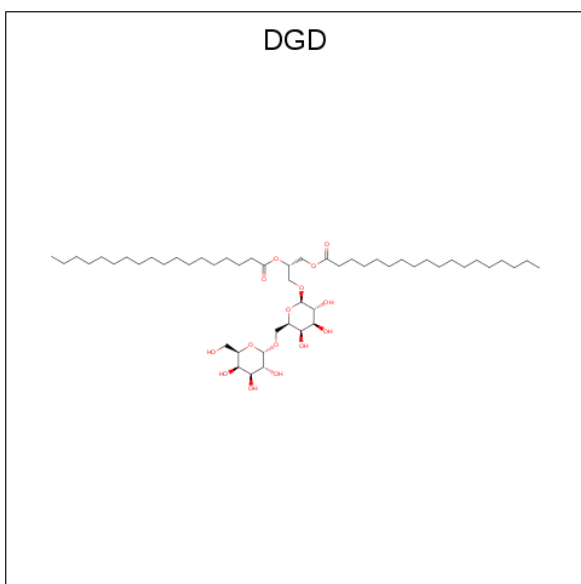
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O		0	0
			25	19	6			
35	B	1	Total	C	O		0	0
			35	24	11			
35	B	1	Total	C	O		0	0
			26	19	7			
35	D	1	Total	C	O		0	0
			35	24	11			
35	D	1	Total	C	O		0	0
			35	24	11			
35	E	1	Total	C	O		0	0
			35	24	11			
35	I	1	Total	C	O		0	0
			35	24	11			
35	M	1	Total	C	O		0	0
			35	24	11			
35	M	1	Total	C	O		0	0
			35	24	11			
35	a	1	Total	C	O		0	0
			35	24	11			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	b	1	Total	C	O	0	0
			25	19	6		
35	b	1	Total	C	O	0	0
			25	19	6		
35	e	1	Total	C	O	0	0
			35	24	11		
35	m	1	Total	C	O	0	0
			35	24	11		

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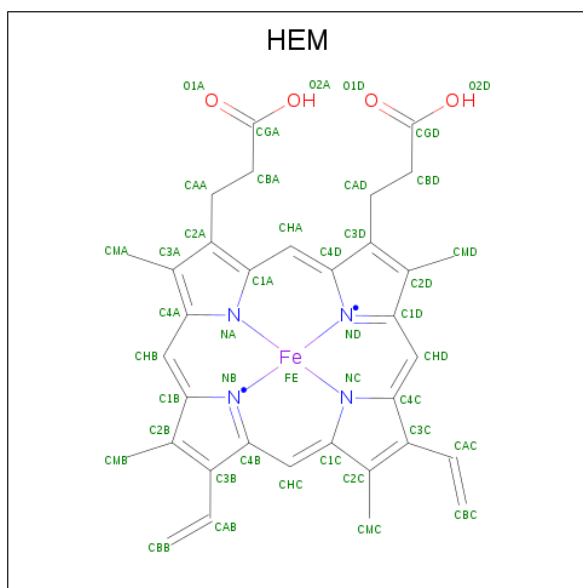
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	o	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	C	1	Total	Ca	0	0
			1	1		
37	V	1	Total	Ca	0	0
			1	1		
37	c	2	Total	Ca	0	0
			2	2		

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

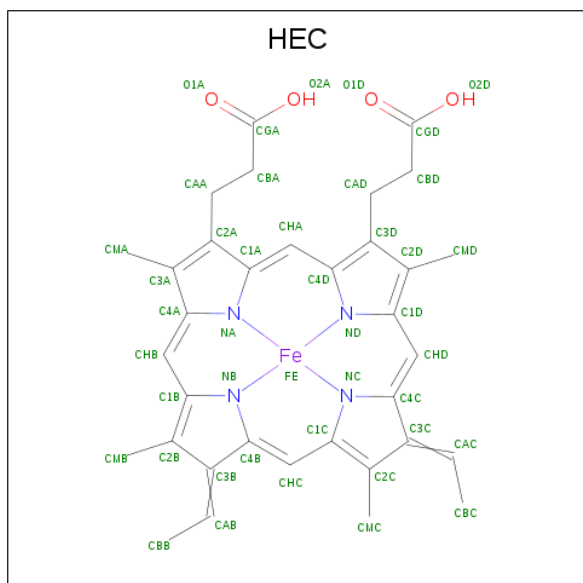


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
38	e	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	J	1	Total Mg 1 1	0	0
39	j	1	Total Mg 1 1	0	0

- Molecule 40 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	127	Total O 127 127	0	0
41	B	175	Total O 175 175	0	0
41	C	148	Total O 148 148	0	0
41	D	111	Total O 111 111	0	0
41	E	18	Total O 18 18	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	F	5	Total O 5 5	0	0
41	H	19	Total O 19 19	0	0
41	I	6	Total O 6 6	0	0
41	J	5	Total O 5 5	0	0
41	K	6	Total O 6 6	0	0
41	L	9	Total O 9 9	0	0
41	M	14	Total O 14 14	0	0
41	O	100	Total O 100 100	0	0
41	T	10	Total O 10 10	0	0
41	U	46	Total O 46 46	0	0
41	V	78	Total O 79 79	0	1
41	X	3	Total O 3 3	0	0
41	Y	1	Total O 1 1	0	0
41	a	130	Total O 130 130	0	0
41	b	192	Total O 192 192	0	0
41	c	136	Total O 136 136	0	0
41	d	108	Total O 108 108	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	28	Total O 28 28	0	0
41	i	4	Total O 4 4	0	0

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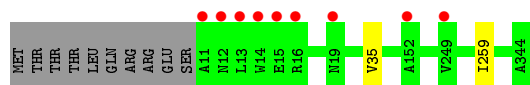
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	j	3	Total 3	O 3	0	0
41	k	4	Total 4	O 4	0	0
41	l	7	Total 7	O 7	0	0
41	m	11	Total 11	O 11	0	0
41	o	109	Total 109	O 109	0	0
41	t	7	Total 7	O 7	0	0
41	u	64	Total 64	O 64	0	0
41	v	71	Total 71	O 71	0	0
41	x	4	Total 4	O 4	0	0
41	y	2	Total 2	O 2	0	0

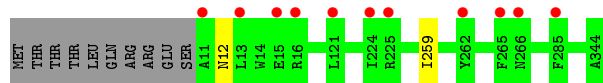
### 3 Residue-property plots [i](#)

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

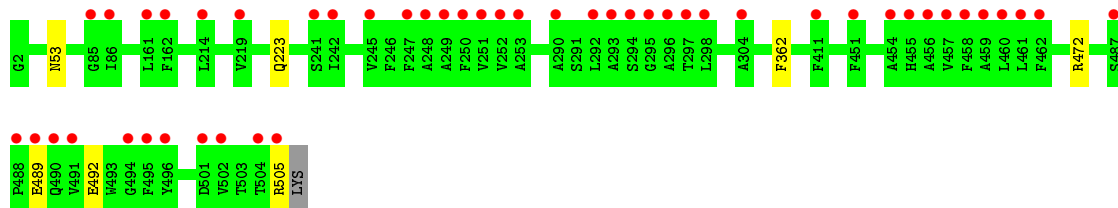
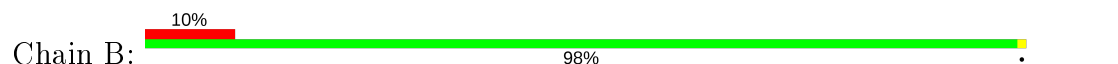
- Molecule 1: Photosystem II protein D1



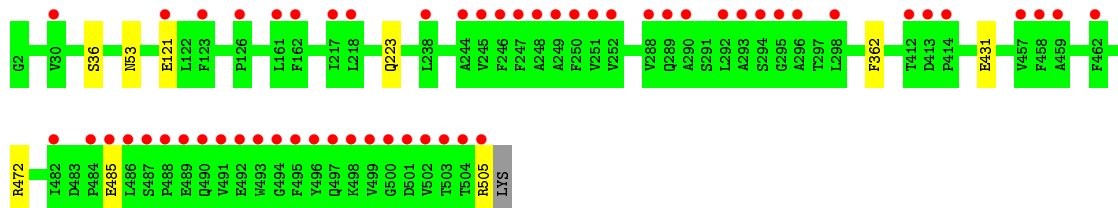
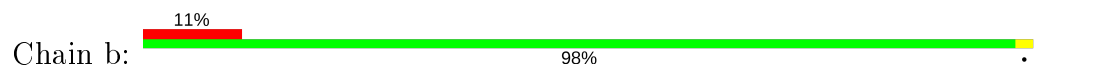
- Molecule 1: Photosystem II protein D1



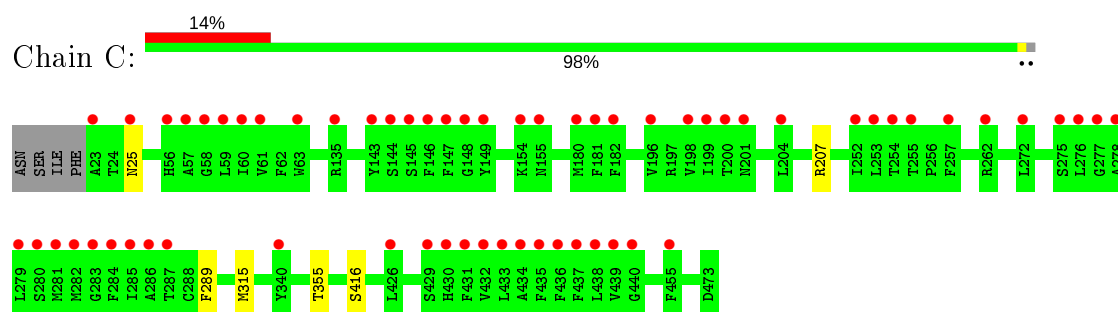
- Molecule 2: Photosystem II CP47 reaction center protein



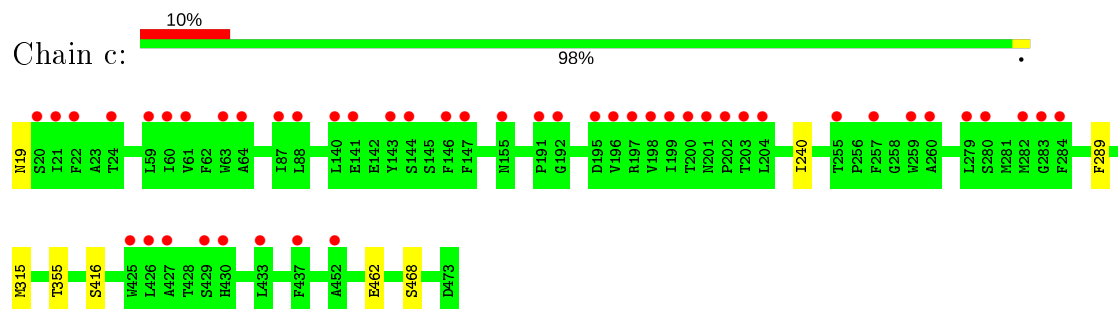
- Molecule 2: Photosystem II CP47 reaction center protein



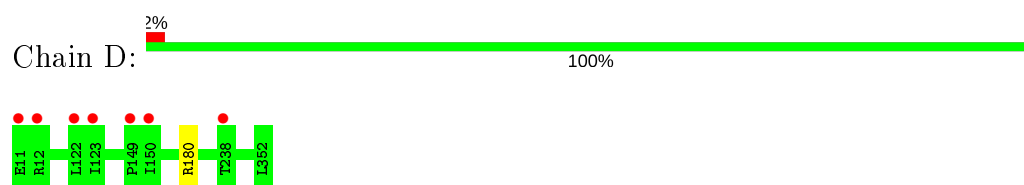
- Molecule 3: Photosystem II CP43 reaction center protein



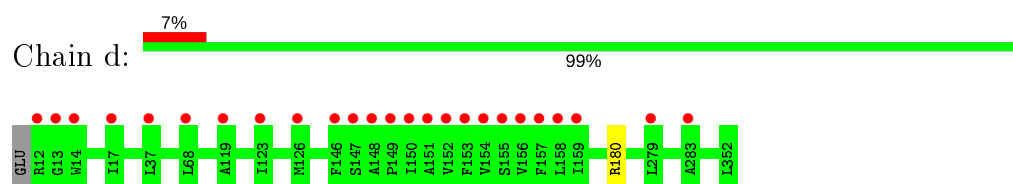
- Molecule 3: Photosystem II CP43 reaction center protein



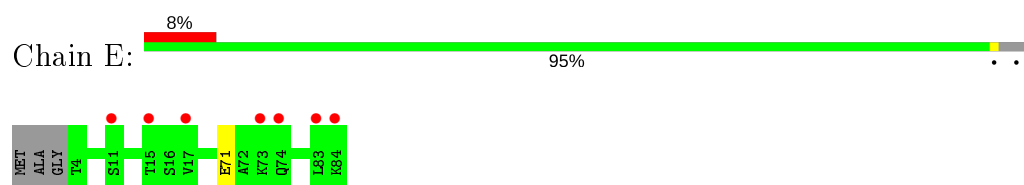
- Molecule 4: Photosystem II D2 protein



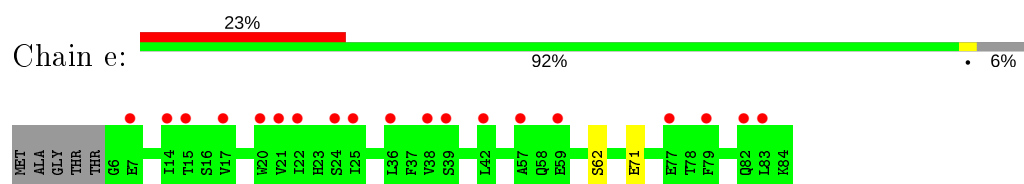
- Molecule 4: Photosystem II D2 protein




- Molecule 5: Cytochrome b559 subunit alpha

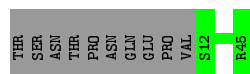


- Molecule 5: Cytochrome b559 subunit alpha



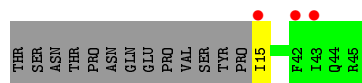
- Molecule 6: Cytochrome b559 subunit beta

Chain F:  77% 23%



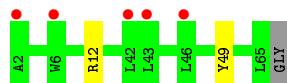
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  7% 68% 30%



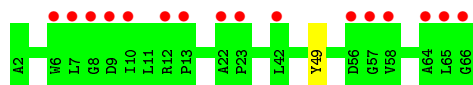
- Molecule 7: Photosystem II reaction center protein H

Chain H:  8% 95%



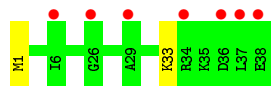
- Molecule 7: Photosystem II reaction center protein H

Chain h:  25% 98%




- Molecule 8: Photosystem II reaction center protein I

Chain I:  18% 95% 5%



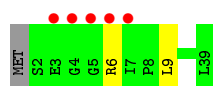
- Molecule 8: Photosystem II reaction center protein I

Chain i:  8% 92% 5%

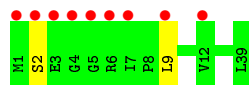


- Molecule 9: Photosystem II reaction center protein J

Chain J:  13% 92% 5%



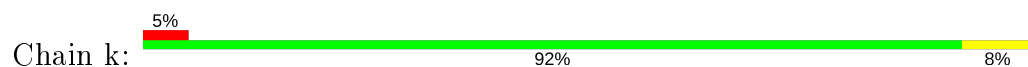
- Molecule 9: Photosystem II reaction center protein J



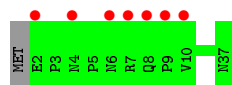
- Molecule 10: Photosystem II reaction center protein K



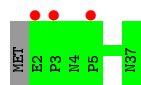
- Molecule 10: Photosystem II reaction center protein K



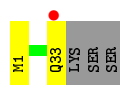
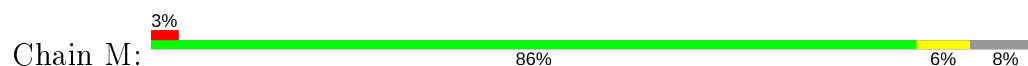
- Molecule 11: Photosystem II reaction center protein L



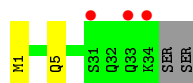
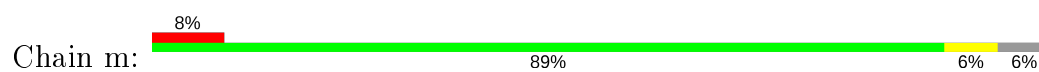
- Molecule 11: Photosystem II reaction center protein L



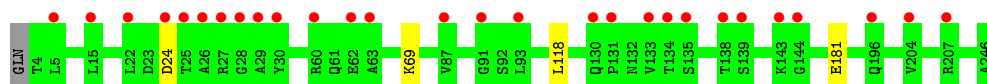
- Molecule 12: Photosystem II reaction center protein M



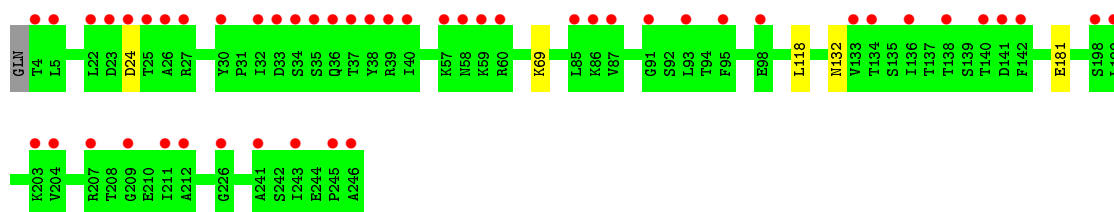
- Molecule 12: Photosystem II reaction center protein M



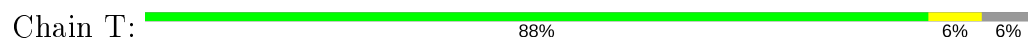
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



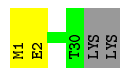
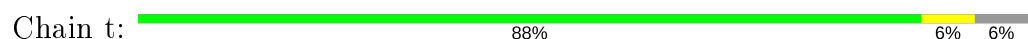
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



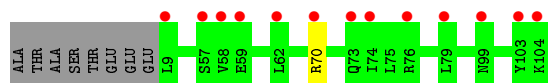
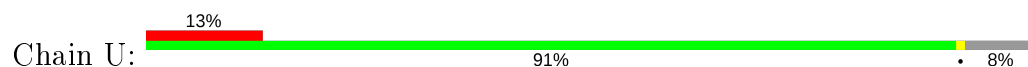
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T

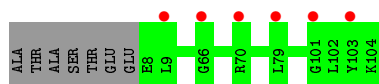


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

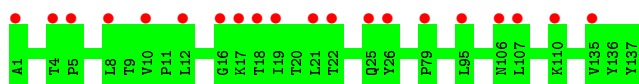




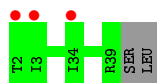
- Molecule 16: Cytochrome c-550



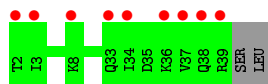
- Molecule 16: Cytochrome c-550



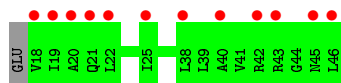
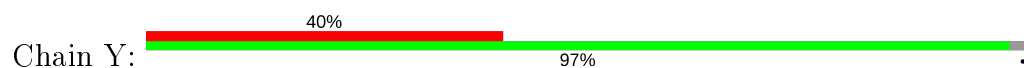
- Molecule 17: Photosystem II reaction center protein X



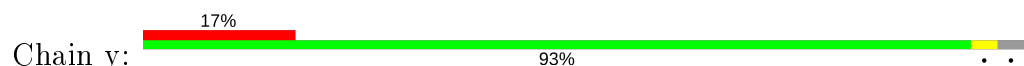
- Molecule 17: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein Ycf12

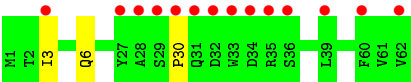


- Molecule 18: Photosystem II reaction center protein Ycf12



- Molecule 19: Photosystem II reaction center protein Z

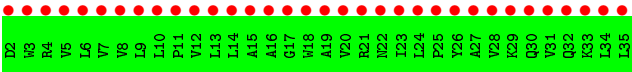




● Molecule 19: Photosystem II reaction center protein Z



● 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, $\alpha$ , $\beta$ , $\gamma$	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 46.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 100.0 (46.51-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.139 , 0.186 0.142 , 0.187	Depositor DCC
$R_{free}$ test set	14614 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 70.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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	0.44	0/2728	0.56	0/3719
1	a	0.45	0/2739	0.56	0/3735
2	B	0.42	0/4171	0.55	0/5683
2	b	0.42	0/4138	0.55	0/5640
3	C	0.40	0/3626	0.53	0/4936
3	c	0.41	0/3670	0.53	0/4996
4	D	0.45	0/2827	0.55	0/3852
4	d	0.45	0/2818	0.53	0/3840
5	E	0.34	0/687	0.53	0/936
5	e	0.34	0/667	0.50	0/908
6	F	0.34	0/284	0.47	0/387
6	f	0.38	0/257	0.48	0/349
7	H	0.35	0/530	0.51	0/723
7	h	0.34	0/524	0.50	0/713
8	I	0.37	0/311	0.49	0/419
8	i	0.37	0/311	0.52	0/419
9	J	0.36	0/278	0.48	0/376
9	j	0.37	0/283	0.50	0/383
10	K	0.36	0/303	0.54	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.43	0/311	0.48	0/423
11	l	0.39	0/311	0.50	0/423
12	M	0.44	0/261	0.55	0/357
12	m	0.44	0/262	0.60	0/357
13	O	0.37	0/1935	0.57	0/2623
13	o	0.37	0/1910	0.56	0/2589
14	T	0.51	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.58	0/1052
15	u	0.40	0/785	0.57	0/1064
16	V	0.38	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1085	0.52	0/1473
17	X	0.35	0/284	0.48	0/384
17	x	0.31	0/284	0.49	0/384
18	Y	0.30	0/216	0.45	0/289
18	y	0.32	0/216	0.52	0/289
19	Z	0.32	0/490	0.45	0/669
19	z	0.34	0/490	0.45	0/669
20	R	0.28	0/279	0.43	0/383
All	All	0.41	0/42949	0.54	0/58445

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%)	328 (98%)	6 (2%)	1 (0%)	41	61
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	41	61
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	34	54
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	34	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	5	7
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	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	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
13	o	243/244 (100%)	234 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	9	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	16
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	51	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	Z	30	PRO
19	z	30	PRO
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%)	271 (100%)	1 (0%)	91	97
1	a	274/279 (98%)	273 (100%)	1 (0%)	91	97
2	B	410/403 (102%)	403 (98%)	7 (2%)	60	82
2	b	406/403 (101%)	397 (98%)	9 (2%)	52	77
3	C	356/356 (100%)	351 (99%)	5 (1%)	67	86
3	c	361/356 (101%)	353 (98%)	8 (2%)	52	77
4	D	278/277 (100%)	277 (100%)	1 (0%)	91	97
4	d	277/277 (100%)	276 (100%)	1 (0%)	91	97
5	E	73/73 (100%)	72 (99%)	1 (1%)	67	86
5	e	70/73 (96%)	68 (97%)	2 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	31	56
7	H	55/54 (102%)	52 (94%)	3 (6%)	21	41
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	80
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	69
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	37
9	J	26/27 (96%)	24 (92%)	2 (8%)	13	25
9	j	26/27 (96%)	24 (92%)	2 (8%)	13	25
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	15
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	15
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	29 (97%)	1 (3%)	38	64
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	64
13	O	211/207 (102%)	207 (98%)	4 (2%)	57	80
13	o	208/207 (100%)	203 (98%)	5 (2%)	49	74
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	58
14	t	26/28 (93%)	25 (96%)	1 (4%)	33	58
15	U	83/89 (93%)	82 (99%)	1 (1%)	71	88
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	21 (96%)	1 (4%)	27	51
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	80
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4360/4403 (99%)	4288 (98%)	72 (2%)	62	82

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
2	B	53	ASN
2	B	223	GLN
2	B	362	PHE
2	B	472	ARG
2	B	489	GLU
2	B	492	GLU
2	B	505	ARG
3	C	25	ASN
3	C	207	ARG
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	180	ARG
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
8	I	33	LYS
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
12	M	33	GLN
13	O	24	ASP
13	O	69	LYS
13	O	118	LEU
13	O	181	GLU
14	T	2	GLU
15	U	70	ARG
19	Z	3	ILE
19	Z	6	GLN
1	a	12	ASN
2	b	36	SER
2	b	53	ASN
2	b	121	GLU
2	b	223	GLN
2	b	362	PHE
2	b	431	GLU
2	b	472	ARG
2	b	485	GLU
2	b	505	ARG

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Mol	Chain	Res	Type
3	c	19	ASN
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	462[A]	GLU
3	c	462[B]	GLU
3	c	468	SER
4	d	180	ARG
5	e	62	SER
5	e	71	GLU
6	f	15	ILE
7	h	49	TYR
8	i	33	LYS
8	i	36	ASP
9	j	2	SER
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	o	24	ASP
13	o	69	LYS
13	o	118	LEU
13	o	132	ASN
13	o	181	GLU
14	t	2	GLU
18	y	45	ASN
19	z	6	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	331	ASN
3	C	201	ASN
4	D	61	HIS
4	D	83	ASN
4	D	142	ASN
5	E	60	GLN
6	F	44	GLN
12	M	5	GLN

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Mol	Chain	Res	Type
13	O	124	ASN
13	O	130	GLN
15	U	73	GLN
15	U	78	ASN
15	U	81	HIS
17	X	33	GLN
19	Z	58	ASN
2	b	14	ASN
2	b	53	ASN
2	b	223	GLN
2	b	331	ASN
3	c	201	ASN
4	d	83	ASN
5	e	60	GLN
5	e	75	GLN
6	f	44	GLN
12	m	5	GLN
13	o	124	ASN
13	o	130	GLN
19	z	58	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	M	1	12	8,9,10	0.58	0	7,9,11	1.50	2 (28%)
14	FME	T	1	14	8,9,10	0.62	0	7,9,11	1.31	1 (14%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.09	1 (14%)

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	0.63	0	7,9,11	1.37	1 (14%)
14	FME	t	1	14	8,9,10	0.64	0	7,9,11	1.85	3 (42%)
12	FME	m	1	12	8,9,10	0.58	0	7,9,11	1.38	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	3/7/9/11	-
14	FME	T	1	14	-	4/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.73	117.62	124.78
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82
12	M	1	FME	CA-N-CN	-2.31	119.27	122.82
8	I	1	FME	O-C-CA	-2.29	118.77	124.78
14	T	1	FME	O-C-CA	-2.25	118.88	124.78
12	M	1	FME	O-C-CA	-2.22	118.95	124.78
12	m	1	FME	CA-N-CN	-2.19	119.45	122.82
8	i	1	FME	O-C-CA	-2.13	119.18	124.78
12	m	1	FME	O1-CN-N	-2.09	119.77	125.27
14	t	1	FME	O1-CN-N	-2.07	119.81	125.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	M	1	FME	O-C-CA-CB
14	T	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 214 ligands modelled in this entry, 18 are unknown and 14 are monoatomic - leaving 182 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
23	CLA	a	408	1	59,73,73	2.02	14 (23%)	67,113,113	2.22	25 (37%)
27	GOL	C	523	-	5,5,5	0.40	0	5,5,5	0.25	0
23	CLA	d	404	4	59,73,73	2.05	12 (20%)	67,113,113	2.16	26 (38%)
36	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.00	6 (7%)
23	CLA	B	608	2	59,73,73	1.96	12 (20%)	67,113,113	2.19	23 (34%)
38	HEM	e	103	5,6	27,50,50	0.81	1 (3%)	17,82,82	1.89	3 (17%)
23	CLA	B	603	2	59,73,73	1.99	13 (22%)	67,113,113	2.26	21 (31%)
23	CLA	b	607	41	59,73,73	1.96	14 (23%)	67,113,113	2.13	20 (29%)
23	CLA	C	502	3	59,73,73	1.96	13 (22%)	67,113,113	2.32	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	j	101	39	51,51,55	0.88	2 (3%)	59,59,63	1.07	5 (8%)
31	LHG	l	101	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
23	CLA	C	514	3	59,73,73	2.02	13 (22%)	67,113,113	2.11	20 (29%)
31	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	5 (9%)
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
23	CLA	c	513	3	59,73,73	2.04	13 (22%)	67,113,113	2.24	21 (31%)
23	CLA	b	613	2	59,73,73	2.04	13 (22%)	67,113,113	2.19	23 (34%)
25	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.73	13 (23%)
24	PHO	D	401	-	67,69,69	2.13	19 (28%)	85,99,99	2.10	24 (28%)
23	CLA	A	406	41	59,73,73	2.02	13 (22%)	67,113,113	2.05	22 (32%)
23	CLA	D	405	4	59,73,73	1.99	12 (20%)	67,113,113	2.25	22 (32%)
31	LHG	D	408	-	48,48,48	0.88	2 (4%)	51,54,54	0.96	3 (5%)
33	LMG	Z	101	-	51,51,55	0.99	2 (3%)	59,59,63	1.27	5 (8%)
23	CLA	b	605	2	59,73,73	2.02	14 (23%)	67,113,113	2.21	20 (29%)
23	CLA	B	616	2	59,73,73	2.05	13 (22%)	67,113,113	2.22	19 (28%)
31	LHG	d	409	-	48,48,48	0.97	2 (4%)	51,54,54	1.00	3 (5%)
31	LHG	d	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.91	3 (5%)
23	CLA	B	613	2	59,73,73	2.06	13 (22%)	67,113,113	2.26	25 (37%)
23	CLA	C	508	41	59,73,73	2.00	12 (20%)	67,113,113	2.22	23 (34%)
27	GOL	a	411	-	5,5,5	0.38	0	5,5,5	0.41	0
23	CLA	c	510	3	59,73,73	1.92	13 (22%)	67,113,113	2.25	26 (38%)
23	CLA	B	605	2	59,73,73	1.99	14 (23%)	67,113,113	2.11	21 (31%)
34	HTG	B	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.74	3 (13%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
23	CLA	c	512	3	59,73,73	2.00	13 (22%)	67,113,113	2.22	20 (29%)
23	CLA	B	604	2	59,73,73	1.96	13 (22%)	67,113,113	2.22	22 (32%)
29	PL9	A	414	-	55,55,55	0.65	2 (3%)	68,69,69	1.95	21 (30%)
25	BCR	d	405	-	41,41,41	1.09	1 (2%)	56,56,56	1.86	14 (25%)
23	CLA	a	404	1	59,73,73	2.00	12 (20%)	67,113,113	2.30	26 (38%)
23	CLA	c	508	3	59,73,73	2.09	13 (22%)	67,113,113	2.27	21 (31%)
23	CLA	C	507	3	59,73,73	2.01	13 (22%)	67,113,113	2.22	25 (37%)
25	BCR	c	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.79	13 (23%)
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.37	0
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.77	1 (2%)
25	BCR	a	409	-	41,41,41	0.95	1 (2%)	56,56,56	1.51	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	615	2	59,73,73	1.98	11 (18%)	67,113,113	2.15	22 (32%)
23	CLA	C	509	3	59,73,73	2.12	14 (23%)	67,113,113	2.26	21 (31%)
35	LMT	b	627	-	25,25,36	0.56	1 (4%)	30,30,47	1.07	3 (10%)
23	CLA	C	513	3	59,73,73	2.02	13 (22%)	67,113,113	2.23	26 (38%)
23	CLA	c	503	3	59,73,73	1.98	13 (22%)	67,113,113	2.18	20 (29%)
33	LMG	a	416	-	51,51,55	0.95	2 (3%)	59,59,63	1.07	3 (5%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.68	11 (19%)
26	SQD	L	101	-	53,54,54	1.02	3 (5%)	62,65,65	1.53	9 (14%)
31	LHG	A	416	-	48,48,48	0.90	3 (6%)	51,54,54	1.10	4 (7%)
23	CLA	B	611	2	59,73,73	2.01	13 (22%)	67,113,113	2.16	22 (32%)
23	CLA	b	616	2	59,73,73	2.01	12 (20%)	67,113,113	2.29	23 (34%)
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	4 (7%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.84	0
25	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.39	10 (17%)
24	PHO	A	407	-	67,69,69	2.15	17 (25%)	85,99,99	2.04	25 (29%)
35	LMT	B	631	-	26,26,36	0.50	0	31,31,47	0.81	1 (3%)
23	CLA	C	511	3	59,73,73	2.00	13 (22%)	67,113,113	2.18	22 (32%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.92	2 (4%)
33	LMG	c	520	-	51,51,55	0.97	3 (5%)	59,59,63	1.24	6 (10%)
29	PL9	d	406	-	55,55,55	0.63	1 (1%)	68,69,69	1.82	20 (29%)
36	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	6 (7%)
33	LMG	c	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	3 (5%)
35	LMT	B	629	-	25,25,36	0.46	0	30,30,47	0.70	0
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
34	HTG	B	622	-	19,19,19	1.01	1 (5%)	23,24,24	1.44	4 (17%)
36	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.02	6 (7%)
23	CLA	B	612	2	59,73,73	2.00	13 (22%)	67,113,113	2.25	23 (34%)
38	HEM	E	103	5,6	27,50,50	0.81	0	17,82,82	2.19	4 (23%)
33	LMG	Z	102	-	37,37,55	1.01	3 (8%)	45,45,63	1.64	9 (20%)
25	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.73	16 (28%)
40	HEC	v	201	16	26,50,50	1.60	4 (15%)	18,82,82	1.60	4 (22%)
34	HTG	c	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.51	1 (4%)
23	CLA	A	408	1	59,73,73	1.98	14 (23%)	67,113,113	2.26	23 (34%)
23	CLA	b	615	2	59,73,73	1.93	12 (20%)	67,113,113	2.13	21 (31%)
23	CLA	D	404	4	59,73,73	2.00	12 (20%)	67,113,113	2.37	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	609	2	59,73,73	2.00	13 (22%)	67,113,113	2.23	21 (31%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.70	17 (30%)
25	BCR	D	406	-	41,41,41	1.04	1 (2%)	56,56,56	1.81	14 (25%)
23	CLA	C	503	3	59,73,73	2.00	12 (20%)	67,113,113	2.10	20 (29%)
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.07	3 (6%)
23	CLA	C	506	3	59,73,73	1.97	13 (22%)	67,113,113	2.26	21 (31%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.48	10 (16%)
35	LMT	b	621	-	25,25,36	0.46	0	30,30,47	0.66	0
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.67	13 (23%)
23	CLA	c	501	3	59,73,73	1.96	13 (22%)	67,113,113	2.15	21 (31%)
23	CLA	b	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.15	21 (31%)
23	CLA	C	505	41	59,73,73	2.08	13 (22%)	67,113,113	2.22	24 (35%)
32	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
27	GOL	d	402	-	5,5,5	0.32	0	5,5,5	0.55	0
23	CLA	B	609	2	59,73,73	1.97	12 (20%)	67,113,113	2.14	19 (28%)
27	GOL	B	626	-	5,5,5	0.52	0	5,5,5	0.40	0
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
25	BCR	b	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.69	13 (23%)
23	CLA	c	507	41	59,73,73	2.00	13 (22%)	67,113,113	2.11	22 (32%)
23	CLA	b	614	2	59,73,73	2.00	13 (22%)	67,113,113	2.21	23 (34%)
33	LMG	C	501	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	4 (6%)
23	CLA	c	505	3	59,73,73	1.97	13 (22%)	67,113,113	2.13	20 (29%)
23	CLA	d	401	41	59,73,73	2.04	12 (20%)	67,113,113	2.25	25 (37%)
36	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	c	509	3	59,73,73	2.08	13 (22%)	67,113,113	2.17	20 (29%)
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.02	2 (4%)
34	HTG	V	203	-	11,11,19	0.25	0	15,15,24	1.12	2 (13%)
23	CLA	b	612	2	59,73,73	2.06	13 (22%)	67,113,113	2.16	20 (29%)
34	HTG	B	623	-	19,19,19	0.84	1 (5%)	23,24,24	1.67	1 (4%)
23	CLA	c	502	3	59,73,73	2.02	12 (20%)	67,113,113	2.22	21 (31%)
23	CLA	C	510	3	59,73,73	2.08	13 (22%)	67,113,113	2.16	22 (32%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.77	1 (2%)
31	LHG	A	417	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	2 (3%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.52	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	610	41	59,73,73	2.06	13 (22%)	67,113,113	2.24	24 (35%)
34	HTG	C	522	-	19,19,19	1.05	2 (10%)	23,24,24	1.89	5 (21%)
27	GOL	b	624	-	5,5,5	0.33	0	5,5,5	0.45	0
36	DGD	c	516	-	63,63,67	0.83	2 (3%)	77,77,81	1.16	6 (7%)
23	CLA	A	405	41	59,73,73	2.06	12 (20%)	67,113,113	2.20	25 (37%)
23	CLA	b	606	2	59,73,73	1.94	12 (20%)	67,113,113	2.23	24 (35%)
34	HTG	D	412	-	16,16,19	1.04	2 (12%)	20,21,24	1.45	1 (5%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.72	3 (13%)
35	LMT	D	402	-	36,36,36	0.64	1 (2%)	47,47,47	1.26	4 (8%)
34	HTG	B	627	-	19,19,19	0.97	2 (10%)	23,24,24	1.40	2 (8%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	b	602	2	59,73,73	2.05	13 (22%)	67,113,113	2.31	27 (40%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.32	7 (14%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.58	12 (21%)
25	BCR	b	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
34	HTG	b	628	-	19,19,19	1.01	1 (5%)	23,24,24	1.83	4 (17%)
32	BCT	A	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	608	2	59,73,73	2.07	14 (23%)	67,113,113	2.20	22 (32%)
35	LMT	B	630	-	36,36,36	0.52	1 (2%)	47,47,47	0.94	2 (4%)
23	CLA	a	405	41	59,73,73	2.04	13 (22%)	67,113,113	2.09	24 (35%)
23	CLA	d	403	4	59,73,73	2.03	14 (23%)	67,113,113	2.19	24 (35%)
31	LHG	e	101	-	41,41,48	1.03	2 (4%)	44,47,54	0.95	2 (4%)
23	CLA	b	611	2	59,73,73	2.04	13 (22%)	67,113,113	2.22	21 (31%)
26	SQD	D	413	-	42,43,54	1.15	3 (7%)	51,54,65	1.78	12 (23%)
29	PL9	a	414	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	20 (29%)
26	SQD	a	412	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	7 (11%)
24	PHO	a	407	-	67,69,69	2.18	15 (22%)	85,99,99	1.98	19 (22%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	1.07	5 (6%)
23	CLA	c	506	3	59,73,73	2.01	14 (23%)	67,113,113	2.16	25 (37%)
34	HTG	d	411	-	16,16,19	1.12	2 (12%)	20,21,24	1.50	1 (5%)
25	BCR	B	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	10 (17%)
23	CLA	b	610	41	59,73,73	2.11	13 (22%)	67,113,113	2.27	23 (34%)
24	PHO	a	406	-	67,69,69	2.10	17 (25%)	85,99,99	1.94	24 (28%)
26	SQD	a	410	-	53,54,54	0.96	3 (5%)	62,65,65	1.73	12 (19%)
23	CLA	B	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.17	21 (31%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LMG	b	620	-	51,51,55	0.86	2 (3%)	59,59,63	1.26	8 (13%)
34	HTG	c	522	-	19,19,19	0.96	2 (10%)	23,24,24	1.49	3 (13%)
29	PL9	D	407	-	55,55,55	0.65	1 (1%)	68,69,69	1.74	21 (30%)
36	DGD	c	518	-	63,63,67	0.86	3 (4%)	77,77,81	1.09	6 (7%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.10	6 (9%)
40	HEC	V	202	16	26,50,50	1.58	4 (15%)	18,82,82	1.60	3 (16%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.11	5 (11%)
23	CLA	B	614	2	59,73,73	1.97	14 (23%)	67,113,113	2.29	24 (35%)
28	OEX	a	413	1,3,41	0,15,15	0.00	-	-	-	-
26	SQD	A	410	-	53,54,54	0.97	3 (5%)	62,65,65	1.86	12 (19%)
23	CLA	C	512	3	59,73,73	2.03	13 (22%)	67,113,113	2.13	22 (32%)
23	CLA	B	607	41	59,73,73	2.01	13 (22%)	67,113,113	2.20	22 (32%)
23	CLA	b	604	2	59,73,73	1.99	12 (20%)	67,113,113	2.23	20 (29%)
23	CLA	A	404	1	59,73,73	2.07	14 (23%)	67,113,113	2.22	26 (38%)
23	CLA	C	504	3	59,73,73	1.95	12 (20%)	67,113,113	2.06	19 (28%)
26	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.38	7 (13%)
28	OEX	A	413	1,3,41	0,15,15	0.00	-	-	-	-
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	11 (19%)
25	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	c	511	3	59,73,73	2.06	13 (22%)	67,113,113	2.15	20 (29%)
27	GOL	A	411	-	5,5,5	0.40	0	5,5,5	0.29	0
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.81	2 (4%)
33	LMG	J	101	39	51,51,55	0.91	2 (3%)	59,59,63	0.98	5 (8%)
34	HTG	b	623	-	19,19,19	1.07	2 (10%)	23,24,24	1.81	3 (13%)
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.57	10 (17%)
34	HTG	b	622	-	19,19,19	0.96	1 (5%)	23,24,24	1.52	3 (13%)
23	CLA	c	504	41	59,73,73	2.06	13 (22%)	67,113,113	2.15	24 (35%)
23	CLA	b	603	2	59,73,73	2.04	14 (23%)	67,113,113	2.18	19 (28%)
23	CLA	B	606	2	59,73,73	1.97	12 (20%)	67,113,113	2.26	21 (31%)
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.75	13 (23%)
36	DGD	c	517	-	63,63,67	0.91	3 (4%)	77,77,81	0.99	6 (7%)
23	CLA	B	602	2	59,73,73	2.05	13 (22%)	67,113,113	2.20	25 (37%)
34	HTG	C	521	-	19,19,19	0.92	1 (5%)	23,24,24	1.44	3 (13%)

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
23	CLA	a	408	1	3/3/20/25	8/37/135/135	-
27	GOL	C	523	-	-	2/4/4/4	-
23	CLA	d	404	4	3/3/20/25	12/37/135/135	-
36	DGD	H	102	-	-	14/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	B	608	2	3/3/20/25	4/37/135/135	-
38	HEM	e	103	5,6	-	0/6/54/54	-
23	CLA	B	603	2	3/3/20/25	4/37/135/135	-
23	CLA	b	607	41	3/3/20/25	4/37/135/135	-
23	CLA	C	502	3	3/3/20/25	8/37/135/135	-
33	LMG	j	101	39	-	12/46/66/70	0/1/1/1
35	LMT	B	631	-	-	7/17/38/61	0/1/1/2
35	LMT	E	102	-	-	11/21/61/61	0/2/2/2
31	LHG	d	407	-	-	14/53/53/53	-
33	LMG	z	101	-	-	6/34/54/70	0/1/1/1
23	CLA	c	513	3	3/3/20/25	1/37/135/135	-
23	CLA	b	613	2	3/3/20/25	10/37/135/135	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
24	PHO	D	401	-	-	6/53/103/103	0/5/6/6
23	CLA	A	406	41	3/3/20/25	11/37/135/135	-
23	CLA	D	405	4	3/3/20/25	11/37/135/135	-
31	LHG	D	408	-	-	15/53/53/53	-
33	LMG	Z	101	-	-	9/46/66/70	0/1/1/1
23	CLA	b	605	2	3/3/20/25	10/37/135/135	-
23	CLA	B	616	2	3/3/20/25	8/37/135/135	-
31	LHG	d	409	-	-	16/53/53/53	-
31	LHG	d	408	-	-	20/53/53/53	-
23	CLA	B	613	2	3/3/20/25	6/37/135/135	-
23	CLA	C	508	41	3/3/20/25	6/37/135/135	-
27	GOL	a	411	-	-	2/4/4/4	-
23	CLA	c	510	3	3/3/20/25	10/37/135/135	-
23	CLA	B	605	2	3/3/20/25	9/37/135/135	-
34	HTG	B	624	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	2	3/3/20/25	12/37/135/135	-
23	CLA	c	512	3	3/3/20/25	12/37/135/135	-
23	CLA	B	604	2	3/3/20/25	11/37/135/135	-
29	PL9	A	414	-	-	11/53/73/73	0/1/1/1
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
23	CLA	a	404	1	3/3/20/25	10/37/135/135	-
23	CLA	c	508	3	3/3/20/25	5/37/135/135	-
23	CLA	C	507	3	3/3/20/25	13/37/135/135	-
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	GOL	B	625	-	-	3/4/4/4	-
35	LMT	M	103	-	-	11/21/61/61	0/2/2/2
25	BCR	a	409	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	2	3/3/20/25	12/37/135/135	-
23	CLA	C	509	3	3/3/20/25	5/37/135/135	-
35	LMT	b	627	-	-	6/17/37/61	0/1/1/2
23	CLA	C	513	3	3/3/20/25	8/37/135/135	-
23	CLA	c	503	3	3/3/20/25	2/37/135/135	-
33	LMG	a	416	-	-	15/46/66/70	0/1/1/1
35	LMT	B	629	-	-	10/17/37/61	0/1/1/2
26	SQD	L	101	-	-	23/49/69/69	0/1/1/1
31	LHG	A	416	-	-	11/53/53/53	-
23	CLA	B	611	2	3/3/20/25	3/37/135/135	-
23	CLA	b	616	2	3/3/20/25	13/37/135/135	-
31	LHG	D	409	-	-	15/53/53/53	-
23	CLA	C	514	3	2/2/20/25	11/37/135/135	-
23	CLA	B	607	41	3/3/20/25	2/37/135/135	-
24	PHO	A	407	-	-	2/53/103/103	0/5/6/6
31	LHG	l	101	-	-	19/53/53/53	-
23	CLA	C	511	3	3/3/20/25	14/37/135/135	-
35	LMT	m	102	-	-	7/21/61/61	0/2/2/2
33	LMG	c	520	-	-	7/46/66/70	0/1/1/1
29	PL9	d	406	-	-	6/53/73/73	0/1/1/1
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
33	LMG	c	519	-	-	13/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
36	DGD	C	518	-	-	13/51/91/95	0/2/2/2
23	CLA	B	612	2	3/3/20/25	9/37/135/135	-
38	HEM	E	103	5,6	-	0/6/54/54	-
33	LMG	C	520	-	-	15/46/66/70	0/1/1/1
33	LMG	Z	102	-	-	14/31/51/70	0/1/1/1
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
40	HEC	v	201	16	-	0/6/54/54	-
34	HTG	c	521	-	-	7/10/30/30	0/1/1/1
23	CLA	A	408	1	3/3/20/25	11/37/135/135	-
23	CLA	b	615	2	3/3/20/25	6/37/135/135	-
23	CLA	D	404	4	1/1/20/25	2/37/135/135	-
23	CLA	b	609	2	3/3/20/25	6/37/135/135	-
36	DGD	c	516	-	-	13/51/91/95	0/2/2/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	BCR	D	406	-	-	7/29/63/63	0/2/2/2
23	CLA	C	503	3	3/3/20/25	7/37/135/135	-
33	LMG	B	621	-	-	13/46/66/70	0/1/1/1
35	LMT	I	101	-	-	10/21/61/61	0/2/2/2
23	CLA	C	506	3	1/1/20/25	8/37/135/135	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
35	LMT	b	621	-	-	7/17/37/61	0/1/1/2
23	CLA	B	606	2	3/3/20/25	7/37/135/135	-
23	CLA	c	501	3	3/3/20/25	6/37/135/135	-
23	CLA	b	601	41	3/3/20/25	15/37/135/135	-
23	CLA	C	505	41	3/3/20/25	7/37/135/135	-
27	GOL	d	402	-	-	2/4/4/4	-
23	CLA	B	609	2	3/3/20/25	6/37/135/135	-
27	GOL	B	626	-	-	3/4/4/4	-
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	c	507	41	3/3/20/25	7/37/135/135	-
23	CLA	b	614	2	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	501	-	-	9/46/66/70	0/1/1/1
23	CLA	c	505	3	1/1/20/25	10/37/135/135	-
23	CLA	d	401	41	3/3/20/25	6/37/135/135	-
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	c	509	3	3/3/20/25	12/37/135/135	-
35	LMT	M	101	-	-	2/21/61/61	0/2/2/2
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
23	CLA	b	612	2	3/3/20/25	8/37/135/135	-
34	HTG	B	623	-	-	6/10/30/30	0/1/1/1
23	CLA	c	502	3	3/3/20/25	6/37/135/135	-
23	CLA	C	510	3	3/3/20/25	6/37/135/135	-
35	LMT	a	417	-	-	4/21/61/61	0/2/2/2
31	LHG	A	417	-	-	21/53/53/53	-
23	CLA	B	610	41	3/3/20/25	8/37/135/135	-
34	HTG	C	522	-	-	2/10/30/30	0/1/1/1
27	GOL	b	624	-	-	1/4/4/4	-
23	CLA	b	604	2	3/3/20/25	13/37/135/135	-
23	CLA	A	405	41	3/3/20/25	7/37/135/135	-
35	LMT	e	102	-	-	9/21/61/61	0/2/2/2
34	HTG	D	412	-	-	0/7/27/30	0/1/1/1
34	HTG	b	625	-	-	6/10/30/30	0/1/1/1
35	LMT	D	402	-	-	6/21/61/61	0/2/2/2
34	HTG	B	627	-	-	2/10/30/30	0/1/1/1
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	b	602	2	3/3/20/25	6/37/135/135	-
35	LMT	D	403	-	-	9/21/61/61	0/2/2/2
25	BCR	A	409	-	-	2/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
34	HTG	b	628	-	-	6/10/30/30	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	608	2	2/2/20/25	4/37/135/135	-
35	LMT	B	630	-	-	7/21/61/61	0/2/2/2
23	CLA	a	405	41	2/2/20/25	5/37/135/135	-
23	CLA	d	403	4	1/1/20/25	3/37/135/135	-
31	LHG	e	101	-	-	14/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	611	2	3/3/20/25	6/37/135/135	-
26	SQD	D	413	-	-	14/38/58/69	0/1/1/1
29	PL9	a	414	-	-	13/53/73/73	0/1/1/1
26	SQD	a	412	-	-	11/49/69/69	0/1/1/1
24	PHO	a	407	-	-	4/53/103/103	0/5/6/6
36	DGD	C	517	-	-	14/51/91/95	0/2/2/2
23	CLA	c	506	3	2/2/20/25	8/37/135/135	-
34	HTG	d	411	-	-	3/7/27/30	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	b	610	41	3/3/20/25	5/37/135/135	-
24	PHO	a	406	-	-	4/53/103/103	0/5/6/6
26	SQD	a	410	-	-	12/49/69/69	0/1/1/1
23	CLA	B	601	41	3/3/20/25	13/37/135/135	-
33	LMG	b	620	-	-	14/46/66/70	0/1/1/1
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
29	PL9	D	407	-	-	11/53/73/73	0/1/1/1
36	DGD	c	518	-	-	5/51/91/95	0/2/2/2
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
40	HEC	V	202	16	-	0/6/54/54	-
31	LHG	E	101	-	-	20/46/46/53	-
23	CLA	B	614	2	3/3/20/25	13/37/135/135	-
26	SQD	A	410	-	-	13/49/69/69	0/1/1/1
23	CLA	C	512	3	3/3/20/25	4/37/135/135	-
23	CLA	A	404	1	3/3/20/25	6/37/135/135	-
23	CLA	C	504	3	2/2/20/25	2/37/135/135	-
26	SQD	f	101	-	-	16/38/58/69	0/1/1/1
25	BCR	y	101	-	-	7/29/63/63	0/2/2/2
25	BCR	k	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	511	3	3/3/20/25	3/37/135/135	-
27	GOL	A	411	-	-	2/4/4/4	-
33	LMG	J	101	39	-	9/46/66/70	0/1/1/1
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
25	BCR	C	516	-	-	2/29/63/63	0/2/2/2
34	HTG	b	622	-	-	2/10/30/30	0/1/1/1
23	CLA	c	504	41	3/3/20/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	603	2	2/2/20/25	10/37/135/135	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
36	DGD	c	517	-	-	14/51/91/95	0/2/2/2
23	CLA	B	602	2	3/3/20/25	6/37/135/135	-
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1

All (1126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3B-C2B	6.82	1.49	1.40
23	C	509	CLA	C3B-C2B	6.72	1.49	1.40
23	C	510	CLA	C3B-C2B	6.65	1.49	1.40
23	C	502	CLA	C3B-C2B	6.54	1.49	1.40
23	b	612	CLA	C3B-C2B	6.53	1.49	1.40
23	D	404	CLA	C3B-C2B	6.43	1.49	1.40
23	b	613	CLA	C3B-C2B	6.39	1.49	1.40
23	a	405	CLA	C3B-C2B	6.39	1.49	1.40
23	b	614	CLA	C3B-C2B	6.39	1.49	1.40
23	B	613	CLA	C3B-C2B	6.38	1.49	1.40
23	c	504	CLA	C3B-C2B	6.38	1.49	1.40
23	b	611	CLA	C3B-C2B	6.36	1.49	1.40
23	b	610	CLA	C3B-C2B	6.32	1.49	1.40
23	c	511	CLA	C3B-C2B	6.30	1.49	1.40
23	c	508	CLA	C3B-C2B	6.30	1.49	1.40
23	A	404	CLA	C3B-C2B	6.28	1.49	1.40
23	c	502	CLA	C3B-C2B	6.28	1.49	1.40
23	b	602	CLA	C3B-C2B	6.27	1.49	1.40
23	B	611	CLA	C3B-C2B	6.26	1.49	1.40
23	b	608	CLA	C3B-C2B	6.24	1.49	1.40
23	d	401	CLA	C3D-C2D	6.20	1.50	1.39
23	a	404	CLA	C3B-C2B	6.19	1.49	1.40
23	b	604	CLA	C3B-C2B	6.17	1.48	1.40
23	C	508	CLA	C3D-C2D	6.13	1.50	1.39
23	B	603	CLA	C3B-C2B	6.12	1.48	1.40
23	d	401	CLA	C3B-C2B	6.10	1.48	1.40
23	B	616	CLA	C3B-C2B	6.09	1.48	1.40
23	c	508	CLA	C3D-C2D	6.09	1.50	1.39
24	D	401	PHO	C3B-C2B	6.09	1.49	1.37
23	C	509	CLA	C3D-C2D	6.07	1.50	1.39
23	B	615	CLA	C3D-C2D	6.06	1.50	1.39
23	C	512	CLA	C3B-C2B	6.05	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C3D-C2D	6.05	1.50	1.39
23	b	608	CLA	C3D-C2D	6.04	1.50	1.39
23	b	601	CLA	C3D-C2D	6.03	1.50	1.39
23	c	509	CLA	C3B-C2B	6.02	1.48	1.40
23	d	404	CLA	C3D-C2D	6.02	1.50	1.39
24	a	406	PHO	C3B-C2B	6.01	1.49	1.37
23	b	613	CLA	C3D-C2D	6.01	1.50	1.39
23	B	602	CLA	C3D-C2D	6.00	1.50	1.39
23	A	405	CLA	C3B-C2B	6.00	1.48	1.40
23	c	502	CLA	C3D-C2D	6.00	1.50	1.39
23	b	605	CLA	C3D-C2D	5.99	1.50	1.39
23	B	601	CLA	C3D-C2D	5.98	1.50	1.39
23	C	503	CLA	C3B-C2B	5.96	1.48	1.40
23	B	601	CLA	C3B-C2B	5.95	1.48	1.40
24	a	407	PHO	C3B-C2B	5.94	1.49	1.37
23	B	612	CLA	C3B-C2B	5.91	1.48	1.40
23	b	601	CLA	C3B-C2B	5.89	1.48	1.40
23	A	405	CLA	C3D-C2D	5.89	1.50	1.39
23	B	616	CLA	C3D-C2D	5.89	1.50	1.39
23	C	513	CLA	C3B-C2B	5.88	1.48	1.40
23	B	607	CLA	C3B-C2B	5.88	1.48	1.40
23	b	616	CLA	C3D-C2D	5.87	1.50	1.39
23	B	602	CLA	C3B-C2B	5.87	1.48	1.40
23	b	607	CLA	C3D-C2D	5.87	1.49	1.39
23	b	611	CLA	C3D-C2D	5.85	1.49	1.39
23	B	610	CLA	C3D-C2D	5.85	1.49	1.39
23	c	509	CLA	C3D-C2D	5.85	1.49	1.39
23	C	506	CLA	C3B-C2B	5.84	1.48	1.40
24	A	407	PHO	C3C-C2C	5.83	1.49	1.36
23	d	404	CLA	C3B-C2B	5.83	1.48	1.40
24	a	407	PHO	C3C-C2C	5.82	1.49	1.36
23	c	503	CLA	C3B-C2B	5.82	1.48	1.40
23	C	507	CLA	C3B-C2B	5.82	1.48	1.40
23	C	513	CLA	C3D-C2D	5.81	1.49	1.39
24	a	406	PHO	C3C-C2C	5.79	1.49	1.36
23	b	602	CLA	C3D-C2D	5.79	1.49	1.39
23	b	605	CLA	C3B-C2B	5.77	1.48	1.40
23	B	609	CLA	C3D-C2D	5.77	1.49	1.39
23	c	512	CLA	C3C-C2C	5.77	1.49	1.36
23	b	610	CLA	C3C-C2C	5.77	1.49	1.36
24	A	407	PHO	C3B-C2B	5.75	1.48	1.37
23	C	505	CLA	C3D-C2D	5.74	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C3D-C2D	5.74	1.49	1.39
23	C	511	CLA	C3B-C2B	5.73	1.48	1.40
23	c	504	CLA	C3D-C2D	5.72	1.49	1.39
23	A	408	CLA	C3B-C2B	5.71	1.48	1.40
23	b	606	CLA	C3B-C2B	5.71	1.48	1.40
23	a	405	CLA	C3D-C2D	5.71	1.49	1.39
23	B	603	CLA	C3D-C2D	5.70	1.49	1.39
23	c	513	CLA	C3B-C2B	5.70	1.48	1.40
23	B	614	CLA	C3D-C2D	5.69	1.49	1.39
23	c	513	CLA	C3D-C2D	5.69	1.49	1.39
23	A	404	CLA	C3D-C2D	5.69	1.49	1.39
23	b	603	CLA	C3C-C2C	5.69	1.48	1.36
23	c	506	CLA	C3D-C2D	5.68	1.49	1.39
23	B	610	CLA	C3B-C2B	5.68	1.48	1.40
23	c	506	CLA	C3B-C2B	5.68	1.48	1.40
23	C	514	CLA	C3D-C2D	5.68	1.49	1.39
23	C	503	CLA	C3D-C2D	5.67	1.49	1.39
23	c	510	CLA	C3B-C2B	5.66	1.48	1.40
23	C	514	CLA	C3B-C2B	5.65	1.48	1.40
23	C	509	CLA	C3C-C2C	5.64	1.48	1.36
23	a	404	CLA	C3D-C2D	5.64	1.49	1.39
23	b	609	CLA	C3D-C2D	5.64	1.49	1.39
23	C	508	CLA	C3C-C2C	5.63	1.48	1.36
23	b	610	CLA	C3D-C2D	5.63	1.49	1.39
24	a	407	PHO	CHC-C1C	5.62	1.49	1.38
23	B	604	CLA	C3B-C2B	5.62	1.48	1.40
23	B	611	CLA	C3D-C2D	5.62	1.49	1.39
23	B	612	CLA	C3D-C2D	5.61	1.49	1.39
23	A	406	CLA	C3D-C2D	5.60	1.49	1.39
23	b	612	CLA	C3D-C2D	5.60	1.49	1.39
23	c	512	CLA	C3D-C2D	5.59	1.49	1.39
23	A	408	CLA	C3C-C2C	5.59	1.48	1.36
23	C	510	CLA	C3D-C2D	5.59	1.49	1.39
23	B	608	CLA	C3B-C2B	5.59	1.48	1.40
23	B	601	CLA	C3C-C2C	5.58	1.48	1.36
23	c	501	CLA	C3D-C2D	5.58	1.49	1.39
23	b	606	CLA	C3D-C2D	5.57	1.49	1.39
23	B	606	CLA	C3D-C2D	5.57	1.49	1.39
23	a	408	CLA	C3D-C2D	5.56	1.49	1.39
23	b	616	CLA	CHC-C1C	5.56	1.49	1.35
23	A	406	CLA	CHC-C1C	5.56	1.49	1.35
23	B	614	CLA	C3B-C2B	5.55	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C3B-C2B	5.54	1.48	1.40
23	B	602	CLA	C3C-C2C	5.54	1.48	1.36
23	b	613	CLA	C3C-C2C	5.53	1.48	1.36
23	d	403	CLA	C3B-C2B	5.53	1.48	1.40
23	B	607	CLA	C3D-C2D	5.53	1.49	1.39
23	B	605	CLA	C3D-C2D	5.52	1.49	1.39
23	B	610	CLA	OBD-CAD	5.52	1.30	1.22
23	C	513	CLA	C3C-C2C	5.51	1.48	1.36
23	B	616	CLA	C3C-C2C	5.51	1.48	1.36
23	c	508	CLA	C3C-C2C	5.51	1.48	1.36
23	B	610	CLA	C3C-C2C	5.51	1.48	1.36
23	B	608	CLA	C3C-C2C	5.50	1.48	1.36
23	D	405	CLA	CHC-C1C	5.50	1.49	1.35
23	B	608	CLA	C3D-C2D	5.49	1.49	1.39
23	b	605	CLA	C3C-C2C	5.49	1.48	1.36
23	B	603	CLA	C3C-C2C	5.47	1.48	1.36
23	C	512	CLA	C3D-C2D	5.46	1.49	1.39
23	A	406	CLA	C3C-C2C	5.46	1.48	1.36
23	D	405	CLA	C3D-C2D	5.46	1.49	1.39
23	b	614	CLA	C3D-C2D	5.46	1.49	1.39
23	C	504	CLA	C3D-C2D	5.45	1.49	1.39
23	D	404	CLA	C3D-C2D	5.45	1.49	1.39
23	C	507	CLA	C3D-C2D	5.45	1.49	1.39
23	C	504	CLA	C3C-C2C	5.44	1.48	1.36
23	b	615	CLA	C3C-C2C	5.44	1.48	1.36
23	c	505	CLA	C3B-C2B	5.43	1.47	1.40
23	C	507	CLA	O2D-CGD	5.43	1.46	1.33
23	b	603	CLA	CHC-C1C	5.41	1.48	1.35
23	b	609	CLA	C3B-C2B	5.41	1.47	1.40
23	B	616	CLA	CHC-C1C	5.41	1.48	1.35
23	a	408	CLA	C3B-C2B	5.40	1.47	1.40
23	b	606	CLA	C3C-C2C	5.39	1.48	1.36
23	B	607	CLA	C3C-C2C	5.39	1.48	1.36
23	a	405	CLA	C3C-C2C	5.39	1.48	1.36
23	c	501	CLA	C3B-C2B	5.39	1.47	1.40
23	d	404	CLA	CHC-C1C	5.39	1.48	1.35
23	d	403	CLA	C3D-C2D	5.38	1.49	1.39
23	B	609	CLA	CHC-C1C	5.37	1.48	1.35
23	b	612	CLA	C3C-C2C	5.37	1.48	1.36
23	C	502	CLA	C3D-C2D	5.37	1.49	1.39
23	c	501	CLA	C3C-C2C	5.36	1.48	1.36
23	D	404	CLA	C3C-C2C	5.35	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C3C-C2C	5.35	1.48	1.36
23	d	404	CLA	C3C-C2C	5.35	1.48	1.36
23	d	401	CLA	C3C-C2C	5.35	1.48	1.36
23	C	506	CLA	CHC-C1C	5.34	1.48	1.35
23	c	509	CLA	C3C-C2C	5.34	1.48	1.36
23	b	616	CLA	C3C-C2C	5.34	1.48	1.36
23	A	405	CLA	C3C-C2C	5.34	1.48	1.36
23	D	405	CLA	C3B-C2B	5.33	1.47	1.40
23	B	606	CLA	C3B-C2B	5.33	1.47	1.40
23	b	602	CLA	C3C-C2C	5.33	1.48	1.36
23	C	514	CLA	CHC-C1C	5.33	1.48	1.35
23	C	504	CLA	C3B-C2B	5.33	1.47	1.40
23	C	503	CLA	C3C-C2C	5.33	1.48	1.36
23	A	408	CLA	C3D-C2D	5.33	1.49	1.39
23	C	511	CLA	C3C-C2C	5.32	1.48	1.36
23	b	603	CLA	C3D-C2D	5.32	1.49	1.39
23	c	503	CLA	C3D-C2D	5.31	1.48	1.39
23	b	603	CLA	C3B-C2B	5.31	1.47	1.40
23	c	512	CLA	C3B-C2B	5.30	1.47	1.40
23	B	606	CLA	C3C-C2C	5.30	1.48	1.36
23	b	615	CLA	C3D-C2D	5.29	1.48	1.39
23	C	505	CLA	C3C-C2C	5.29	1.48	1.36
23	D	405	CLA	C3C-C2C	5.28	1.48	1.36
23	B	610	CLA	CHC-C1C	5.28	1.48	1.35
23	A	405	CLA	CHC-C1C	5.28	1.48	1.35
23	b	601	CLA	O2D-CGD	5.28	1.46	1.33
23	c	505	CLA	CHC-C1C	5.28	1.48	1.35
23	c	505	CLA	C3C-C2C	5.27	1.47	1.36
23	b	601	CLA	C3C-C2C	5.27	1.47	1.36
23	a	408	CLA	C3C-C2C	5.27	1.47	1.36
23	b	610	CLA	CHC-C1C	5.27	1.48	1.35
23	C	512	CLA	O2D-CGD	5.26	1.46	1.33
23	b	604	CLA	C3C-C2C	5.26	1.47	1.36
25	K	102	BCR	C23-C22	-5.26	1.34	1.45
23	c	513	CLA	CHC-C1C	5.25	1.48	1.35
23	b	603	CLA	O2D-CGD	5.25	1.46	1.33
23	B	604	CLA	CHC-C1C	5.25	1.48	1.35
23	C	510	CLA	C3C-C2C	5.25	1.47	1.36
23	C	513	CLA	CHC-C1C	5.25	1.48	1.35
23	C	511	CLA	C3D-C2D	5.24	1.48	1.39
23	c	507	CLA	CHC-C1C	5.24	1.48	1.35
23	A	404	CLA	CHC-C1C	5.24	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	O2D-CGD	5.24	1.46	1.33
25	C	515	BCR	C23-C22	-5.24	1.34	1.45
23	A	404	CLA	C3C-C2C	5.23	1.47	1.36
23	B	612	CLA	C3C-C2C	5.23	1.47	1.36
23	c	511	CLA	C3D-C2D	5.23	1.48	1.39
23	b	612	CLA	CHC-C1C	5.22	1.48	1.35
23	c	506	CLA	O2D-CGD	5.22	1.45	1.33
23	C	514	CLA	C3C-C2C	5.21	1.47	1.36
23	b	608	CLA	C3C-C2C	5.21	1.47	1.36
23	b	602	CLA	O2D-CGD	5.21	1.45	1.33
23	b	611	CLA	C3C-C2C	5.21	1.47	1.36
23	B	606	CLA	CHC-C1C	5.21	1.48	1.35
23	b	609	CLA	CHC-C1C	5.21	1.48	1.35
23	c	513	CLA	C3C-C2C	5.20	1.47	1.36
23	c	511	CLA	C3C-C2C	5.20	1.47	1.36
23	a	408	CLA	CHC-C1C	5.20	1.48	1.35
23	C	502	CLA	C3C-C2C	5.20	1.47	1.36
24	a	407	PHO	O2D-CGD	5.19	1.45	1.33
23	c	503	CLA	C3C-C2C	5.19	1.47	1.36
23	B	605	CLA	C3C-C2C	5.18	1.47	1.36
23	c	507	CLA	C3C-C2C	5.18	1.47	1.36
23	b	615	CLA	C3B-C2B	5.18	1.47	1.40
23	c	507	CLA	C3B-C2B	5.18	1.47	1.40
23	b	604	CLA	CHC-C1C	5.18	1.48	1.35
23	c	502	CLA	C3C-C2C	5.18	1.47	1.36
23	C	503	CLA	CHC-C1C	5.17	1.48	1.35
23	B	605	CLA	CHC-C1C	5.17	1.48	1.35
23	C	511	CLA	CHC-C1C	5.17	1.48	1.35
23	c	511	CLA	CHC-C1C	5.17	1.48	1.35
23	c	508	CLA	CHC-C1C	5.17	1.48	1.35
23	B	615	CLA	C3B-C2B	5.16	1.47	1.40
23	C	508	CLA	C3B-C2B	5.15	1.47	1.40
24	D	401	PHO	C3C-C2C	5.15	1.47	1.36
23	b	611	CLA	O2D-CGD	5.15	1.45	1.33
23	c	509	CLA	O2D-CGD	5.14	1.45	1.33
25	k	101	BCR	C23-C22	-5.14	1.34	1.45
23	B	601	CLA	O2D-CGD	5.14	1.45	1.33
23	c	503	CLA	CHC-C1C	5.14	1.48	1.35
24	D	401	PHO	CHB-C1B	5.14	1.48	1.38
23	c	506	CLA	C3C-C2C	5.14	1.47	1.36
23	B	615	CLA	O2D-CGD	5.14	1.45	1.33
25	b	619	BCR	C23-C22	-5.13	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	O2D-CGD	5.12	1.45	1.33
23	d	403	CLA	C3C-C2C	5.12	1.47	1.36
23	B	602	CLA	O2D-CGD	5.12	1.45	1.33
23	A	408	CLA	CHC-C1C	5.12	1.48	1.35
23	c	513	CLA	O2D-CGD	5.12	1.45	1.33
23	B	609	CLA	O2D-CGD	5.12	1.45	1.33
24	a	406	PHO	CHB-C1B	5.12	1.48	1.38
23	b	602	CLA	CHC-C1C	5.11	1.48	1.35
23	B	615	CLA	OBD-CAD	5.11	1.29	1.22
23	B	611	CLA	O2D-CGD	5.11	1.45	1.33
23	c	504	CLA	O2D-CGD	5.11	1.45	1.33
23	d	403	CLA	CHC-C1C	5.11	1.48	1.35
23	b	601	CLA	CHC-C1C	5.10	1.48	1.35
23	d	401	CLA	CHC-C1C	5.10	1.48	1.35
23	C	504	CLA	CHC-C1C	5.10	1.48	1.35
23	A	406	CLA	C3B-C2B	5.09	1.47	1.40
23	B	615	CLA	C3C-C2C	5.09	1.47	1.36
23	b	613	CLA	O2D-CGD	5.08	1.45	1.33
23	c	505	CLA	C3D-C2D	5.08	1.48	1.39
23	a	405	CLA	CHC-C1C	5.08	1.48	1.35
23	c	512	CLA	CHC-C1C	5.08	1.48	1.35
23	A	406	CLA	O2D-CGD	5.08	1.45	1.33
23	b	609	CLA	O2D-CGD	5.07	1.45	1.33
23	B	607	CLA	CHC-C1C	5.07	1.48	1.35
23	c	510	CLA	O2D-CGD	5.07	1.45	1.33
23	c	511	CLA	OBD-CAD	5.06	1.29	1.22
23	B	614	CLA	O2D-CGD	5.06	1.45	1.33
25	d	405	BCR	C23-C22	-5.06	1.35	1.45
23	c	509	CLA	CHC-C1C	5.05	1.47	1.35
23	c	501	CLA	CHC-C1C	5.05	1.47	1.35
23	b	608	CLA	CHC-C1C	5.04	1.47	1.35
23	B	613	CLA	C3C-C2C	5.04	1.47	1.36
23	C	509	CLA	OBD-CAD	5.04	1.29	1.22
23	C	506	CLA	C3C-C2C	5.04	1.47	1.36
23	b	607	CLA	C3C-C2C	5.04	1.47	1.36
23	b	607	CLA	C3B-C2B	5.04	1.47	1.40
24	D	401	PHO	CHC-C1C	5.03	1.48	1.38
23	b	607	CLA	CHC-C1C	5.03	1.47	1.35
23	a	404	CLA	C3C-C2C	5.03	1.47	1.36
23	B	608	CLA	O2D-CGD	5.03	1.45	1.33
23	C	512	CLA	C3C-C2C	5.02	1.47	1.36
25	D	406	BCR	C23-C22	-5.02	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	O2D-CGD	5.02	1.45	1.33
23	B	613	CLA	O2D-CGD	5.02	1.45	1.33
23	B	604	CLA	C3C-C2C	5.02	1.47	1.36
23	C	510	CLA	O2D-CGD	5.02	1.45	1.33
23	C	507	CLA	CHC-C1C	5.01	1.47	1.35
23	D	405	CLA	OBD-CAD	5.01	1.29	1.22
23	c	502	CLA	O2D-CGD	5.00	1.45	1.33
23	B	601	CLA	CHC-C1C	5.00	1.47	1.35
23	B	602	CLA	CHC-C1C	4.99	1.47	1.35
23	b	609	CLA	OBD-CAD	4.99	1.29	1.22
23	b	608	CLA	O2D-CGD	4.99	1.45	1.33
23	b	614	CLA	O2D-CGD	4.99	1.45	1.33
23	C	510	CLA	CHC-C1C	4.98	1.47	1.35
23	b	615	CLA	CHC-C1C	4.98	1.47	1.35
23	C	512	CLA	CHC-C1C	4.98	1.47	1.35
23	B	613	CLA	CHC-C1C	4.98	1.47	1.35
23	d	403	CLA	O2D-CGD	4.97	1.45	1.33
23	B	608	CLA	CHC-C1C	4.97	1.47	1.35
23	c	510	CLA	C3C-C2C	4.97	1.47	1.36
25	c	514	BCR	C23-C22	-4.96	1.35	1.45
23	b	616	CLA	O2D-CGD	4.96	1.45	1.33
23	b	604	CLA	C3D-C2D	4.96	1.48	1.39
23	C	508	CLA	CHC-C1C	4.96	1.47	1.35
23	C	510	CLA	OBD-CAD	4.96	1.29	1.22
23	c	504	CLA	C3C-C2C	4.96	1.47	1.36
23	c	508	CLA	OBD-CAD	4.96	1.29	1.22
23	C	502	CLA	CHC-C1C	4.95	1.47	1.35
23	b	606	CLA	CHC-C1C	4.94	1.47	1.35
23	c	512	CLA	O2D-CGD	4.94	1.45	1.33
23	b	607	CLA	O2D-CGD	4.94	1.45	1.33
25	t	101	BCR	C23-C22	-4.94	1.35	1.45
23	B	611	CLA	C3C-C2C	4.94	1.47	1.36
23	c	504	CLA	CHC-C1C	4.93	1.47	1.35
23	B	604	CLA	OBD-CAD	4.93	1.29	1.22
23	B	603	CLA	CHC-C1C	4.93	1.47	1.35
23	B	605	CLA	O2D-CGD	4.93	1.45	1.33
23	C	507	CLA	C3C-C2C	4.93	1.47	1.36
23	B	609	CLA	C3C-C2C	4.93	1.47	1.36
23	D	404	CLA	O2D-CGD	4.92	1.45	1.33
23	B	611	CLA	CHC-C1C	4.92	1.47	1.35
24	D	401	PHO	CHD-C1D	4.92	1.48	1.38
23	b	604	CLA	OBD-CAD	4.92	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	OBD-CAD	4.92	1.29	1.22
23	b	612	CLA	O2D-CGD	4.92	1.45	1.33
25	C	516	BCR	C23-C22	-4.92	1.35	1.45
24	D	401	PHO	O2D-CGD	4.91	1.45	1.33
23	a	404	CLA	OBD-CAD	4.91	1.29	1.22
23	b	613	CLA	CHC-C1C	4.91	1.47	1.35
23	C	506	CLA	O2D-CGD	4.90	1.45	1.33
24	A	407	PHO	CHD-C1D	4.90	1.48	1.38
23	b	610	CLA	OBD-CAD	4.89	1.29	1.22
23	b	603	CLA	OBD-CAD	4.89	1.29	1.22
23	b	611	CLA	CHC-C1C	4.89	1.47	1.35
23	c	507	CLA	O2D-CGD	4.88	1.45	1.33
25	b	618	BCR	C23-C22	-4.88	1.35	1.45
23	C	508	CLA	O2D-CGD	4.88	1.45	1.33
23	a	404	CLA	CHC-C1C	4.87	1.47	1.35
23	b	614	CLA	OBD-CAD	4.87	1.29	1.22
24	a	407	PHO	CHD-C1D	4.87	1.48	1.38
23	B	604	CLA	O2D-CGD	4.87	1.45	1.33
25	B	619	BCR	C23-C22	-4.87	1.35	1.45
25	A	409	BCR	C23-C22	-4.86	1.35	1.45
23	D	405	CLA	O2D-CGD	4.86	1.45	1.33
23	c	510	CLA	C3D-C2D	4.86	1.48	1.39
23	b	604	CLA	O2D-CGD	4.86	1.45	1.33
23	a	408	CLA	O2D-CGD	4.86	1.45	1.33
23	B	610	CLA	O2D-CGD	4.86	1.45	1.33
23	b	614	CLA	C3C-C2C	4.86	1.47	1.36
23	B	606	CLA	O2D-CGD	4.85	1.45	1.33
23	b	605	CLA	O2D-CGD	4.85	1.45	1.33
23	C	509	CLA	O2D-CGD	4.84	1.45	1.33
23	c	506	CLA	OBD-CAD	4.84	1.29	1.22
23	B	612	CLA	CHC-C1C	4.84	1.47	1.35
25	H	101	BCR	C23-C22	-4.84	1.35	1.45
23	c	506	CLA	CHC-C1C	4.83	1.47	1.35
23	C	511	CLA	OBD-CAD	4.82	1.29	1.22
23	c	510	CLA	CHC-C1C	4.82	1.47	1.35
23	B	615	CLA	CHC-C1C	4.82	1.47	1.35
23	b	614	CLA	CHC-C1C	4.81	1.47	1.35
23	B	605	CLA	C3B-C2B	4.81	1.47	1.40
23	a	404	CLA	O2D-CGD	4.81	1.44	1.33
25	y	101	BCR	C23-C22	-4.81	1.35	1.45
23	C	505	CLA	CHC-C1C	4.81	1.47	1.35
23	B	604	CLA	C3D-C2D	4.80	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	617	BCR	C23-C22	-4.80	1.35	1.45
23	D	404	CLA	CHC-C1C	4.80	1.47	1.35
23	b	605	CLA	OBD-CAD	4.80	1.29	1.22
23	a	405	CLA	OBD-CAD	4.80	1.29	1.22
23	b	609	CLA	C3C-C2C	4.80	1.46	1.36
25	T	101	BCR	C23-C22	-4.80	1.35	1.45
23	d	401	CLA	O2D-CGD	4.80	1.44	1.33
23	b	615	CLA	O2D-CGD	4.79	1.44	1.33
23	b	601	CLA	OBD-CAD	4.79	1.29	1.22
23	c	503	CLA	O2D-CGD	4.79	1.44	1.33
23	B	601	CLA	OBD-CAD	4.78	1.29	1.22
24	A	407	PHO	CHC-C1C	4.78	1.47	1.38
23	B	609	CLA	C3B-C2B	4.78	1.47	1.40
23	A	404	CLA	O2D-CGD	4.77	1.44	1.33
23	B	613	CLA	OBD-CAD	4.77	1.29	1.22
23	b	608	CLA	OBD-CAD	4.76	1.29	1.22
23	a	405	CLA	O2D-CGD	4.76	1.44	1.33
23	C	506	CLA	C3D-C2D	4.76	1.48	1.39
23	C	511	CLA	O2D-CGD	4.76	1.44	1.33
23	c	512	CLA	OBD-CAD	4.76	1.29	1.22
23	C	514	CLA	O2D-CGD	4.74	1.44	1.33
23	B	609	CLA	O2A-CGA	4.74	1.47	1.33
23	B	616	CLA	O2D-CGD	4.73	1.44	1.33
24	a	407	PHO	CHB-C1B	4.73	1.47	1.38
23	B	612	CLA	O2D-CGD	4.72	1.44	1.33
23	c	505	CLA	O2D-CGD	4.72	1.44	1.33
23	c	502	CLA	CHC-C1C	4.72	1.47	1.35
23	C	509	CLA	CHC-C1C	4.72	1.47	1.35
23	B	616	CLA	OBD-CAD	4.72	1.28	1.22
25	c	515	BCR	C23-C22	-4.72	1.35	1.45
23	A	406	CLA	OBD-CAD	4.72	1.28	1.22
23	d	404	CLA	OBD-CAD	4.71	1.28	1.22
23	C	513	CLA	OBD-CAD	4.71	1.28	1.22
23	B	605	CLA	OBD-CAD	4.71	1.28	1.22
23	c	508	CLA	O2D-CGD	4.71	1.44	1.33
23	c	511	CLA	O2D-CGD	4.69	1.44	1.33
25	h	101	BCR	C23-C22	-4.68	1.35	1.45
23	b	605	CLA	CHC-C1C	4.68	1.47	1.35
24	a	406	PHO	CHD-C1D	4.68	1.47	1.38
23	B	603	CLA	O2D-CGD	4.68	1.44	1.33
23	C	507	CLA	OBD-CAD	4.67	1.28	1.22
23	A	404	CLA	OBD-CAD	4.67	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	O2D-CGD	4.67	1.44	1.33
23	c	509	CLA	OBD-CAD	4.67	1.28	1.22
23	A	405	CLA	O2D-CGD	4.67	1.44	1.33
23	b	606	CLA	O2D-CGD	4.65	1.44	1.33
23	c	505	CLA	OBD-CAD	4.64	1.28	1.22
23	b	610	CLA	O2D-CGD	4.63	1.44	1.33
24	A	407	PHO	CHB-C1B	4.63	1.47	1.38
23	d	404	CLA	O2D-CGD	4.62	1.44	1.33
23	B	607	CLA	O2D-CGD	4.61	1.44	1.33
23	B	611	CLA	OBD-CAD	4.61	1.28	1.22
23	a	408	CLA	OBD-CAD	4.60	1.28	1.22
23	B	614	CLA	CHC-C1C	4.60	1.46	1.35
24	a	406	PHO	O2D-CGD	4.59	1.44	1.33
23	c	504	CLA	OBD-CAD	4.59	1.28	1.22
23	b	607	CLA	OBD-CAD	4.59	1.28	1.22
25	Y	101	BCR	C23-C22	-4.59	1.36	1.45
23	C	512	CLA	OBD-CAD	4.59	1.28	1.22
23	C	514	CLA	OBD-CAD	4.58	1.28	1.22
23	c	502	CLA	OBD-CAD	4.58	1.28	1.22
23	C	505	CLA	OBD-CAD	4.56	1.28	1.22
23	C	502	CLA	O2D-CGD	4.56	1.44	1.33
33	z	101	LMG	O8-C28	4.56	1.46	1.33
23	d	403	CLA	OBD-CAD	4.56	1.28	1.22
23	c	513	CLA	OBD-CAD	4.55	1.28	1.22
23	B	601	CLA	O2A-CGA	4.54	1.46	1.33
23	b	616	CLA	OBD-CAD	4.54	1.28	1.22
23	B	612	CLA	OBD-CAD	4.54	1.28	1.22
25	B	617	BCR	C23-C22	-4.53	1.36	1.45
23	C	503	CLA	O2D-CGD	4.53	1.44	1.33
23	C	506	CLA	OBD-CAD	4.52	1.28	1.22
23	B	602	CLA	OBD-CAD	4.51	1.28	1.22
26	D	413	SQD	O47-C7	4.51	1.47	1.34
23	C	503	CLA	O2A-CGA	4.50	1.46	1.33
26	a	412	SQD	O48-C23	4.49	1.46	1.33
31	E	101	LHG	O8-C23	4.48	1.46	1.33
26	f	101	SQD	O47-C7	4.47	1.46	1.34
24	a	406	PHO	CHC-C1C	4.46	1.47	1.38
23	c	508	CLA	O2A-CGA	4.46	1.46	1.33
23	d	401	CLA	O2A-CGA	4.45	1.46	1.33
26	B	620	SQD	O47-C7	4.44	1.46	1.34
23	b	602	CLA	OBD-CAD	4.44	1.28	1.22
23	C	503	CLA	OBD-CAD	4.44	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	OBD-CAD	4.43	1.28	1.22
23	c	501	CLA	O2D-CGD	4.43	1.44	1.33
23	C	504	CLA	O2D-CGD	4.43	1.44	1.33
23	b	601	CLA	O2A-CGA	4.43	1.46	1.33
23	C	508	CLA	OBD-CAD	4.42	1.28	1.22
23	d	404	CLA	O2A-CGA	4.41	1.46	1.33
23	C	508	CLA	O2A-CGA	4.41	1.46	1.33
23	b	611	CLA	O2A-CGA	4.41	1.46	1.33
36	c	517	DGD	O1G-C1A	4.40	1.46	1.33
23	b	612	CLA	OBD-CAD	4.40	1.28	1.22
23	d	403	CLA	O2A-CGA	4.40	1.46	1.33
25	a	409	BCR	C23-C22	-4.40	1.36	1.45
23	b	612	CLA	O2A-CGA	4.39	1.46	1.33
26	A	412	SQD	O47-C7	4.39	1.46	1.34
33	Z	101	LMG	O7-C10	4.39	1.46	1.34
31	d	409	LHG	O7-C7	4.38	1.46	1.34
23	B	608	CLA	OBD-CAD	4.37	1.28	1.22
23	A	405	CLA	OBD-CAD	4.36	1.28	1.22
23	c	507	CLA	O2A-CGA	4.35	1.46	1.33
23	C	512	CLA	O2A-CGA	4.35	1.46	1.33
23	C	505	CLA	O2A-CGA	4.35	1.46	1.33
23	b	608	CLA	O2A-CGA	4.35	1.46	1.33
23	c	512	CLA	O2A-CGA	4.35	1.46	1.33
23	d	401	CLA	OBD-CAD	4.34	1.28	1.22
26	B	620	SQD	O48-C23	4.34	1.46	1.33
33	C	501	LMG	O8-C28	4.34	1.46	1.33
33	Z	101	LMG	O8-C28	4.34	1.46	1.33
26	A	412	SQD	O48-C23	4.34	1.46	1.33
23	c	501	CLA	OBD-CAD	4.32	1.28	1.22
31	l	101	LHG	O8-C23	4.31	1.45	1.33
23	B	603	CLA	OBD-CAD	4.31	1.28	1.22
23	C	506	CLA	O2A-CGA	4.30	1.45	1.33
23	B	607	CLA	OBD-CAD	4.30	1.28	1.22
31	e	101	LHG	O8-C23	4.30	1.45	1.33
23	C	514	CLA	O2A-CGA	4.30	1.45	1.33
23	A	405	CLA	O2A-CGA	4.30	1.45	1.33
26	L	101	SQD	O48-C23	4.29	1.45	1.33
23	B	607	CLA	O2A-CGA	4.29	1.45	1.33
23	c	509	CLA	O2A-CGA	4.28	1.45	1.33
23	b	615	CLA	OBD-CAD	4.28	1.28	1.22
33	c	520	LMG	O7-C10	4.28	1.46	1.34
23	B	614	CLA	OBD-CAD	4.28	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	O2A-CGA	4.28	1.45	1.33
33	c	520	LMG	O8-C28	4.27	1.45	1.33
26	A	410	SQD	O48-C23	4.27	1.45	1.33
23	c	502	CLA	O2A-CGA	4.27	1.45	1.33
31	A	417	LHG	O8-C23	4.26	1.45	1.33
40	V	202	HEC	CBC-CAC	-4.26	1.33	1.49
23	c	504	CLA	O2A-CGA	4.25	1.45	1.33
23	c	513	CLA	O2A-CGA	4.25	1.45	1.33
33	Z	102	LMG	O7-C10	4.25	1.46	1.34
26	L	101	SQD	O47-C7	4.25	1.46	1.34
33	B	621	LMG	O8-C28	4.25	1.45	1.33
23	b	615	CLA	O2A-CGA	4.24	1.45	1.33
33	c	519	LMG	O8-C28	4.24	1.45	1.33
23	C	511	CLA	O2A-CGA	4.24	1.45	1.33
23	c	503	CLA	OBD-CAD	4.24	1.28	1.22
23	B	606	CLA	O2A-CGA	4.23	1.45	1.33
26	f	101	SQD	O48-C23	4.23	1.45	1.33
33	a	416	LMG	O7-C10	4.23	1.46	1.34
23	c	510	CLA	OBD-CAD	4.22	1.28	1.22
33	C	501	LMG	O7-C10	4.22	1.46	1.34
23	C	502	CLA	O2A-CGA	4.22	1.45	1.33
23	C	513	CLA	O2A-CGA	4.20	1.45	1.33
40	v	201	HEC	CBC-CAC	-4.19	1.33	1.49
31	e	101	LHG	O7-C7	4.19	1.46	1.34
23	A	406	CLA	O2A-CGA	4.18	1.45	1.33
24	a	407	PHO	O2A-CGA	4.17	1.45	1.33
23	a	405	CLA	O2A-CGA	4.16	1.45	1.33
40	v	201	HEC	CBB-CAB	-4.16	1.33	1.49
23	c	506	CLA	O2A-CGA	4.15	1.45	1.33
23	C	507	CLA	O2A-CGA	4.15	1.45	1.33
23	c	511	CLA	O2A-CGA	4.15	1.45	1.33
33	C	520	LMG	O8-C28	4.15	1.45	1.33
40	V	202	HEC	CBB-CAB	-4.15	1.33	1.49
31	d	409	LHG	O8-C23	4.14	1.45	1.33
23	c	505	CLA	O2A-CGA	4.14	1.45	1.33
23	B	616	CLA	O2A-CGA	4.14	1.45	1.33
31	D	409	LHG	O7-C7	4.14	1.46	1.34
33	J	101	LMG	O8-C28	4.14	1.45	1.33
24	D	401	PHO	O2A-CGA	4.13	1.45	1.33
23	B	604	CLA	O2A-CGA	4.13	1.45	1.33
23	C	510	CLA	O2A-CGA	4.12	1.45	1.33
33	c	519	LMG	O7-C10	4.12	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	O2A-CGA	4.11	1.45	1.33
33	a	416	LMG	O8-C28	4.11	1.45	1.33
23	b	611	CLA	OBD-CAD	4.10	1.28	1.22
23	b	613	CLA	OBD-CAD	4.10	1.28	1.22
36	h	102	DGD	O2G-C1B	4.10	1.45	1.34
33	C	520	LMG	O7-C10	4.10	1.45	1.34
26	a	412	SQD	O47-C7	4.10	1.45	1.34
36	H	102	DGD	O2G-C1B	4.09	1.45	1.34
26	a	410	SQD	O48-C23	4.09	1.45	1.33
23	a	408	CLA	O2A-CGA	4.09	1.45	1.33
36	H	102	DGD	O1G-C1A	4.08	1.45	1.33
33	j	101	LMG	O8-C28	4.08	1.45	1.33
23	C	504	CLA	O2A-CGA	4.08	1.45	1.33
31	l	101	LHG	O7-C7	4.07	1.45	1.34
23	D	404	CLA	O2A-CGA	4.06	1.45	1.33
26	D	413	SQD	O48-C23	4.06	1.45	1.33
33	z	101	LMG	O7-C10	4.05	1.45	1.34
33	b	620	LMG	O8-C28	4.05	1.45	1.33
23	B	606	CLA	OBD-CAD	4.05	1.28	1.22
23	b	613	CLA	O2A-CGA	4.04	1.45	1.33
36	c	518	DGD	O1G-C1A	4.04	1.45	1.33
23	B	612	CLA	O2A-CGA	4.03	1.45	1.33
36	h	102	DGD	O1G-C1A	4.03	1.45	1.33
36	c	516	DGD	O1G-C1A	4.03	1.45	1.33
23	C	509	CLA	O2A-CGA	4.03	1.45	1.33
23	B	611	CLA	O2A-CGA	4.02	1.45	1.33
25	B	618	BCR	C23-C22	-4.02	1.37	1.45
23	c	510	CLA	O2A-CGA	4.01	1.45	1.33
23	B	613	CLA	O2A-CGA	4.00	1.45	1.33
31	E	101	LHG	O7-C7	3.99	1.45	1.34
24	a	407	PHO	OBD-CAD	3.99	1.29	1.22
26	a	410	SQD	O47-C7	3.99	1.45	1.34
23	c	501	CLA	O2A-CGA	3.98	1.45	1.33
23	b	602	CLA	O2A-CGA	3.98	1.45	1.33
23	D	404	CLA	OBD-CAD	3.96	1.27	1.22
23	B	609	CLA	OBD-CAD	3.96	1.27	1.22
31	A	417	LHG	O7-C7	3.95	1.45	1.34
36	C	518	DGD	O2G-C1B	3.95	1.45	1.34
23	b	606	CLA	OBD-CAD	3.95	1.27	1.22
23	b	606	CLA	O2A-CGA	3.95	1.44	1.33
31	d	408	LHG	O7-C7	3.94	1.45	1.34
23	b	605	CLA	O2A-CGA	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	408	LHG	O7-C7	3.94	1.45	1.34
23	B	602	CLA	O2A-CGA	3.94	1.44	1.33
36	c	516	DGD	O2G-C1B	3.94	1.45	1.34
23	B	614	CLA	O2A-CGA	3.93	1.44	1.33
23	b	609	CLA	O2A-CGA	3.93	1.44	1.33
23	b	614	CLA	O2A-CGA	3.92	1.44	1.33
36	C	517	DGD	O2G-C1B	3.91	1.45	1.34
23	b	604	CLA	O2A-CGA	3.91	1.44	1.33
23	b	616	CLA	O2A-CGA	3.90	1.44	1.33
33	B	621	LMG	O7-C10	3.90	1.45	1.34
23	B	605	CLA	O2A-CGA	3.89	1.44	1.33
24	A	407	PHO	C4A-NA	-3.88	1.25	1.35
23	b	603	CLA	O2A-CGA	3.88	1.44	1.33
34	B	622	HTG	C1'-S1	-3.88	1.76	1.81
23	A	408	CLA	O2A-CGA	3.86	1.44	1.33
36	C	519	DGD	O1G-C1A	3.86	1.44	1.33
31	D	409	LHG	O8-C23	3.85	1.44	1.33
23	B	610	CLA	O2A-CGA	3.85	1.44	1.33
23	B	608	CLA	O2A-CGA	3.85	1.44	1.33
24	a	406	PHO	O2A-CGA	3.84	1.44	1.33
36	C	518	DGD	O1G-C1A	3.83	1.44	1.33
36	C	519	DGD	O2G-C1B	3.83	1.45	1.34
23	b	610	CLA	O2A-CGA	3.82	1.44	1.33
34	b	628	HTG	C1'-S1	-3.82	1.76	1.81
36	c	518	DGD	O2G-C1B	3.82	1.45	1.34
36	c	517	DGD	O2G-C1B	3.82	1.45	1.34
31	d	407	LHG	O8-C23	3.81	1.44	1.33
34	b	623	HTG	C1'-S1	-3.80	1.76	1.81
31	A	416	LHG	O7-C7	3.78	1.45	1.34
33	J	101	LMG	O7-C10	3.78	1.45	1.34
23	C	502	CLA	OBD-CAD	3.77	1.27	1.22
26	A	410	SQD	O47-C7	3.74	1.44	1.34
31	A	416	LHG	O8-C23	3.73	1.44	1.33
23	A	404	CLA	O2A-CGA	3.73	1.44	1.33
23	B	603	CLA	O2A-CGA	3.72	1.44	1.33
24	a	406	PHO	C3D-C2D	3.71	1.49	1.39
23	A	408	CLA	OBD-CAD	3.70	1.27	1.22
24	D	401	PHO	C3D-C2D	3.70	1.49	1.39
23	D	405	CLA	O2A-CGA	3.69	1.44	1.33
24	D	401	PHO	CHD-C4C	3.69	1.49	1.40
31	d	408	LHG	O8-C23	3.68	1.44	1.33
24	A	407	PHO	OBD-CAD	3.66	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	517	DGD	O1G-C1A	3.66	1.44	1.33
33	b	620	LMG	O7-C10	3.66	1.44	1.34
24	a	407	PHO	C3D-C2D	3.66	1.49	1.39
24	a	407	PHO	CHC-C4B	3.63	1.48	1.40
24	A	407	PHO	C3D-C2D	3.61	1.49	1.39
34	C	522	HTG	C1'-S1	-3.61	1.76	1.81
34	d	411	HTG	C1'-S1	-3.61	1.76	1.81
23	b	607	CLA	O2A-CGA	3.58	1.43	1.33
24	A	407	PHO	O2A-CGA	3.58	1.43	1.33
24	a	407	PHO	CHD-C4C	3.57	1.48	1.40
34	B	624	HTG	C1'-S1	-3.56	1.76	1.81
33	j	101	LMG	O7-C10	3.56	1.44	1.34
24	D	401	PHO	OBD-CAD	3.56	1.28	1.22
31	d	407	LHG	O7-C7	3.55	1.44	1.34
24	a	406	PHO	OBD-CAD	3.53	1.28	1.22
24	A	407	PHO	CHD-C4C	3.47	1.48	1.40
23	d	403	CLA	C1B-NB	-3.39	1.32	1.35
31	D	408	LHG	O8-C23	3.39	1.43	1.33
40	V	202	HEC	C3B-C2B	-3.37	1.37	1.40
24	A	407	PHO	CHC-C4B	3.36	1.48	1.40
34	B	627	HTG	C1'-S1	-3.35	1.77	1.81
34	b	622	HTG	C1'-S1	-3.35	1.77	1.81
23	a	404	CLA	O2A-CGA	3.33	1.43	1.33
24	D	401	PHO	C4A-NA	-3.31	1.27	1.35
34	c	522	HTG	C1'-S1	-3.30	1.77	1.81
23	B	612	CLA	C1B-NB	-3.30	1.32	1.35
24	a	407	PHO	C4A-NA	-3.29	1.27	1.35
24	a	406	PHO	CHC-C4B	3.26	1.48	1.40
40	v	201	HEC	C3B-C2B	-3.24	1.37	1.40
24	a	407	PHO	C3B-C4B	3.23	1.50	1.43
24	A	407	PHO	C3B-C4B	3.21	1.49	1.43
23	A	405	CLA	C4B-CHC	3.20	1.49	1.41
34	C	521	HTG	C1'-S1	-3.18	1.77	1.81
24	a	406	PHO	C4A-NA	-3.17	1.27	1.35
23	c	511	CLA	C1D-C2D	3.17	1.49	1.42
23	d	401	CLA	C1D-C2D	3.17	1.49	1.42
24	D	401	PHO	CHC-C4B	3.16	1.47	1.40
23	a	408	CLA	C1D-C2D	3.14	1.49	1.42
23	C	507	CLA	C1D-C2D	3.14	1.49	1.42
23	A	404	CLA	C1D-C2D	3.13	1.49	1.42
23	A	405	CLA	C1C-C2C	3.12	1.50	1.44
34	D	412	HTG	C1'-S1	-3.11	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C1D-C2D	3.09	1.49	1.42
24	a	406	PHO	CHD-C4C	3.06	1.47	1.40
23	b	610	CLA	C4C-C3C	3.06	1.50	1.45
34	c	521	HTG	C1'-S1	-3.05	1.77	1.81
23	B	602	CLA	C1D-C2D	3.05	1.49	1.42
24	a	406	PHO	CHB-C4A	3.04	1.47	1.40
40	V	202	HEC	C3B-C4B	3.03	1.48	1.43
24	D	401	PHO	CHB-C4A	3.03	1.47	1.40
23	d	404	CLA	C1D-C2D	3.03	1.49	1.42
24	a	407	PHO	CHB-C4A	3.03	1.47	1.40
23	D	404	CLA	C4C-C3C	3.02	1.50	1.45
40	v	201	HEC	C3B-C4B	3.02	1.48	1.43
23	A	405	CLA	C1D-C2D	3.02	1.49	1.42
23	c	501	CLA	C1D-C2D	3.01	1.49	1.42
23	C	514	CLA	C1D-C2D	3.01	1.49	1.42
23	b	603	CLA	C1D-C2D	2.97	1.49	1.42
23	A	404	CLA	C4C-C3C	2.97	1.50	1.45
23	b	609	CLA	C1D-C2D	2.97	1.49	1.42
23	b	605	CLA	C1D-C2D	2.97	1.49	1.42
23	B	605	CLA	C1D-C2D	2.97	1.49	1.42
23	B	609	CLA	C1D-C2D	2.96	1.49	1.42
23	C	510	CLA	C1C-C2C	2.96	1.50	1.44
34	B	623	HTG	C1'-S1	-2.94	1.77	1.81
23	C	506	CLA	C1C-C2C	2.94	1.50	1.44
23	c	505	CLA	C1C-C2C	2.94	1.50	1.44
23	a	405	CLA	C1D-C2D	2.94	1.49	1.42
23	c	504	CLA	C1D-C2D	2.93	1.49	1.42
23	c	513	CLA	C1C-C2C	2.93	1.50	1.44
23	c	509	CLA	C4C-C3C	2.92	1.50	1.45
23	C	511	CLA	C1D-C2D	2.92	1.49	1.42
23	B	606	CLA	C1D-C2D	2.91	1.49	1.42
23	b	610	CLA	C1D-C2D	2.91	1.49	1.42
23	B	601	CLA	C1D-C2D	2.91	1.49	1.42
23	b	603	CLA	C1C-C2C	2.91	1.50	1.44
23	c	507	CLA	C1D-C2D	2.91	1.49	1.42
34	b	625	HTG	C1'-S1	-2.90	1.77	1.81
35	D	402	LMT	O1'-C1'	2.90	1.45	1.40
23	B	607	CLA	C1D-C2D	2.89	1.49	1.42
23	D	404	CLA	C1C-C2C	2.89	1.50	1.44
23	b	601	CLA	C1D-C2D	2.88	1.49	1.42
23	c	510	CLA	C1D-C2D	2.88	1.49	1.42
23	b	610	CLA	C1C-C2C	2.87	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1D-C2D	2.87	1.49	1.42
23	b	604	CLA	C1C-C2C	2.87	1.50	1.44
23	D	405	CLA	C1D-C2D	2.86	1.49	1.42
26	f	101	SQD	C6-S	-2.85	1.66	1.77
23	C	512	CLA	C1C-C2C	2.85	1.50	1.44
23	C	514	CLA	C1C-C2C	2.84	1.50	1.44
23	b	611	CLA	C1B-CHB	2.84	1.48	1.41
23	C	505	CLA	C1C-C2C	2.83	1.50	1.44
23	b	616	CLA	C4B-CHC	2.82	1.48	1.41
26	A	412	SQD	C6-S	-2.82	1.67	1.77
24	A	407	PHO	CHB-C4A	2.81	1.47	1.40
23	D	405	CLA	C1C-C2C	2.81	1.50	1.44
23	c	511	CLA	C1B-CHB	2.80	1.48	1.41
23	c	505	CLA	C1B-CHB	2.80	1.48	1.41
23	c	504	CLA	C1C-C2C	2.80	1.50	1.44
23	C	510	CLA	C1D-C2D	2.79	1.48	1.42
23	B	611	CLA	C1C-C2C	2.78	1.50	1.44
23	b	611	CLA	C4C-C3C	2.78	1.49	1.45
23	B	605	CLA	C4B-CHC	2.78	1.48	1.41
29	a	414	PL9	C6-C5	2.78	1.49	1.35
23	c	503	CLA	C4B-CHC	2.77	1.48	1.41
23	C	512	CLA	C1D-C2D	2.77	1.48	1.42
23	c	508	CLA	C1C-C2C	2.76	1.49	1.44
23	C	509	CLA	C4C-C3C	2.75	1.49	1.45
23	b	610	CLA	C4B-CHC	2.75	1.48	1.41
23	a	404	CLA	C1D-C2D	2.75	1.48	1.42
23	b	604	CLA	C1D-C2D	2.74	1.48	1.42
26	B	620	SQD	C6-S	-2.74	1.67	1.77
26	a	412	SQD	C6-S	-2.74	1.67	1.77
23	B	607	CLA	C1C-C2C	2.73	1.49	1.44
29	A	414	PL9	C6-C5	2.73	1.49	1.35
26	D	413	SQD	C6-S	-2.72	1.67	1.77
23	C	511	CLA	C4C-C3C	2.72	1.49	1.45
23	C	502	CLA	C1D-C2D	2.72	1.48	1.42
23	C	504	CLA	CHD-C4C	2.72	1.48	1.41
23	c	501	CLA	C1B-CHB	2.72	1.48	1.41
23	b	602	CLA	C1C-C2C	2.71	1.49	1.44
23	B	611	CLA	C1B-CHB	2.70	1.48	1.41
23	B	602	CLA	CHD-C4C	2.70	1.48	1.41
23	B	613	CLA	C1C-C2C	2.70	1.49	1.44
23	b	601	CLA	CHD-C4C	2.70	1.48	1.41
23	b	602	CLA	C1D-C2D	2.69	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C1D-C2D	2.69	1.48	1.42
23	c	511	CLA	CHD-C4C	2.69	1.48	1.41
23	B	602	CLA	C4C-C3C	2.69	1.49	1.45
23	b	611	CLA	C1D-C2D	2.68	1.48	1.42
23	c	503	CLA	C1C-C2C	2.68	1.49	1.44
23	b	616	CLA	C1C-C2C	2.68	1.49	1.44
26	A	410	SQD	C6-S	-2.68	1.67	1.77
23	d	403	CLA	C4C-C3C	2.68	1.49	1.45
23	C	503	CLA	C1D-C2D	2.67	1.48	1.42
23	c	509	CLA	C1D-C2D	2.67	1.48	1.42
23	A	406	CLA	C1C-C2C	2.66	1.49	1.44
23	b	615	CLA	C1D-C2D	2.66	1.48	1.42
23	a	408	CLA	C4C-C3C	2.66	1.49	1.45
23	c	501	CLA	C4B-CHC	2.66	1.48	1.41
23	B	603	CLA	C4C-C3C	2.65	1.49	1.45
23	C	509	CLA	C1B-CHB	2.65	1.48	1.41
23	B	611	CLA	C1D-C2D	2.65	1.48	1.42
23	B	615	CLA	C1D-C2D	2.65	1.48	1.42
23	C	504	CLA	C1D-C2D	2.65	1.48	1.42
23	c	507	CLA	C1C-C2C	2.65	1.49	1.44
23	B	612	CLA	C1C-C2C	2.65	1.49	1.44
23	B	610	CLA	C4B-CHC	2.64	1.48	1.41
23	C	511	CLA	CHD-C4C	2.64	1.48	1.41
23	C	507	CLA	CHD-C4C	2.64	1.48	1.41
23	b	608	CLA	C4B-CHC	2.64	1.48	1.41
23	c	512	CLA	C1D-C2D	2.64	1.48	1.42
23	B	614	CLA	C1D-C2D	2.64	1.48	1.42
26	L	101	SQD	C6-S	-2.63	1.67	1.77
23	B	607	CLA	CHD-C4C	2.63	1.48	1.41
23	b	616	CLA	C1D-C2D	2.62	1.48	1.42
23	C	513	CLA	CHD-C4C	2.62	1.48	1.41
23	b	607	CLA	C1C-C2C	2.61	1.49	1.44
23	d	404	CLA	C4B-CHC	2.61	1.48	1.41
23	c	509	CLA	C1C-C2C	2.61	1.49	1.44
23	c	506	CLA	C1D-C2D	2.61	1.48	1.42
23	B	605	CLA	C1B-CHB	2.61	1.48	1.41
33	Z	102	LMG	O8-C28	2.61	1.46	1.33
23	b	602	CLA	CHD-C4C	2.61	1.48	1.41
23	b	605	CLA	C1B-CHB	2.60	1.48	1.41
23	b	612	CLA	C4B-CHC	2.60	1.48	1.41
23	B	604	CLA	C1B-CHB	2.60	1.48	1.41
23	A	408	CLA	C1D-C2D	2.60	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	408	CLA	C1C-C2C	2.59	1.49	1.44
26	a	410	SQD	C6-S	-2.59	1.67	1.77
23	B	616	CLA	C1D-C2D	2.59	1.48	1.42
23	D	405	CLA	C4B-CHC	2.59	1.48	1.41
23	B	613	CLA	C4C-C3C	2.58	1.49	1.45
23	c	513	CLA	CHD-C4C	2.58	1.48	1.41
23	A	404	CLA	CHD-C4C	2.58	1.48	1.41
23	c	504	CLA	C4C-C3C	2.58	1.49	1.45
24	a	406	PHO	C3B-C4B	2.57	1.48	1.43
23	C	510	CLA	CHD-C4C	2.57	1.48	1.41
23	B	609	CLA	C1C-C2C	2.57	1.49	1.44
23	c	505	CLA	C4B-CHC	2.57	1.48	1.41
23	B	605	CLA	C1C-C2C	2.57	1.49	1.44
23	c	509	CLA	CHD-C4C	2.56	1.48	1.41
23	c	510	CLA	CHD-C4C	2.56	1.48	1.41
23	C	513	CLA	C1D-C2D	2.56	1.48	1.42
23	c	501	CLA	CHD-C4C	2.56	1.48	1.41
23	c	508	CLA	C1D-C2D	2.56	1.48	1.42
23	C	513	CLA	C1C-C2C	2.56	1.49	1.44
23	A	404	CLA	C1B-NB	-2.55	1.32	1.35
23	b	614	CLA	CHD-C4C	2.55	1.48	1.41
23	C	514	CLA	CHD-C4C	2.55	1.48	1.41
23	D	404	CLA	CHD-C4C	2.55	1.48	1.41
23	B	613	CLA	C1B-CHB	2.55	1.48	1.41
23	B	616	CLA	C1C-C2C	2.54	1.49	1.44
24	a	406	PHO	C4C-C3C	2.54	1.49	1.45
23	B	609	CLA	C4B-CHC	2.54	1.48	1.41
23	b	603	CLA	C4B-CHC	2.54	1.48	1.41
29	d	406	PL9	C6-C5	2.54	1.48	1.35
23	b	603	CLA	CHD-C4C	2.54	1.48	1.41
23	C	507	CLA	C4C-C3C	2.54	1.49	1.45
23	B	606	CLA	C4B-CHC	2.54	1.48	1.41
23	B	603	CLA	CHD-C4C	2.53	1.48	1.41
23	C	504	CLA	C4C-C3C	2.53	1.49	1.45
23	a	408	CLA	CHD-C4C	2.53	1.48	1.41
23	b	610	CLA	C1B-CHB	2.53	1.48	1.41
23	B	606	CLA	C1C-C2C	2.52	1.49	1.44
23	B	607	CLA	C4C-C3C	2.52	1.49	1.45
23	b	612	CLA	C1D-C2D	2.52	1.48	1.42
23	b	609	CLA	CHD-C4C	2.52	1.48	1.41
23	d	403	CLA	C1D-C2D	2.52	1.48	1.42
23	b	602	CLA	C4B-CHC	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C4C-C3C	2.52	1.49	1.45
23	C	508	CLA	CHD-C4C	2.52	1.48	1.41
23	C	506	CLA	C1B-CHB	2.52	1.48	1.41
23	B	613	CLA	C4B-CHC	2.52	1.48	1.41
23	C	503	CLA	CHD-C4C	2.52	1.48	1.41
23	b	611	CLA	C4B-CHC	2.52	1.48	1.41
23	C	512	CLA	C4C-C3C	2.52	1.49	1.45
23	B	615	CLA	CHD-C4C	2.52	1.48	1.41
23	c	510	CLA	C1B-CHB	2.52	1.48	1.41
23	B	614	CLA	C1B-CHB	2.51	1.48	1.41
23	b	605	CLA	CHD-C4C	2.51	1.48	1.41
23	B	610	CLA	C1B-CHB	2.51	1.48	1.41
23	C	506	CLA	C1D-C2D	2.51	1.48	1.42
23	A	408	CLA	CHD-C4C	2.51	1.48	1.41
23	B	610	CLA	C1D-C2D	2.51	1.48	1.42
23	C	508	CLA	C1D-C2D	2.51	1.48	1.42
23	d	404	CLA	CHD-C4C	2.51	1.48	1.41
23	c	502	CLA	C1D-C2D	2.51	1.48	1.42
23	C	505	CLA	C4B-CHC	2.51	1.48	1.41
23	B	605	CLA	CHD-C4C	2.50	1.48	1.41
23	B	601	CLA	CHD-C4C	2.50	1.48	1.41
23	D	404	CLA	C1D-C2D	2.50	1.48	1.42
23	c	503	CLA	CHD-C4C	2.50	1.48	1.41
23	b	608	CLA	C1D-C2D	2.50	1.48	1.42
24	A	407	PHO	C4C-C3C	2.50	1.49	1.45
23	B	614	CLA	CHD-C4C	2.50	1.48	1.41
23	b	601	CLA	C4B-CHC	2.50	1.47	1.41
23	b	612	CLA	C1C-C2C	2.50	1.49	1.44
23	A	405	CLA	C1B-CHB	2.50	1.47	1.41
23	B	615	CLA	C1C-C2C	2.50	1.49	1.44
23	b	610	CLA	CHD-C4C	2.50	1.48	1.41
23	c	502	CLA	C1B-CHB	2.49	1.47	1.41
23	B	616	CLA	CHD-C4C	2.49	1.48	1.41
23	C	509	CLA	C1C-C2C	2.49	1.49	1.44
23	b	609	CLA	C1B-CHB	2.49	1.47	1.41
23	b	614	CLA	C1D-C2D	2.49	1.48	1.42
23	b	606	CLA	C1C-C2C	2.49	1.49	1.44
23	B	608	CLA	C1D-C2D	2.49	1.48	1.42
24	A	407	PHO	C1A-NA	-2.49	1.32	1.37
23	c	502	CLA	CHD-C4C	2.49	1.48	1.41
23	b	606	CLA	CHD-C4C	2.48	1.48	1.41
23	C	512	CLA	C1B-CHB	2.48	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	CHD-C4C	2.48	1.48	1.41
23	c	507	CLA	CHD-C4C	2.47	1.48	1.41
23	b	613	CLA	C1B-CHB	2.47	1.47	1.41
23	C	510	CLA	C4C-C3C	2.47	1.49	1.45
23	b	613	CLA	C1C-C2C	2.47	1.49	1.44
23	B	605	CLA	C4C-C3C	2.47	1.49	1.45
23	b	611	CLA	CHD-C4C	2.47	1.48	1.41
23	b	608	CLA	C1C-C2C	2.47	1.49	1.44
23	B	609	CLA	C1B-CHB	2.47	1.47	1.41
23	c	511	CLA	C1C-C2C	2.47	1.49	1.44
23	C	505	CLA	C1B-CHB	2.47	1.47	1.41
29	D	407	PL9	C6-C5	2.47	1.48	1.35
23	d	403	CLA	C1B-CHB	2.46	1.47	1.41
23	c	505	CLA	CHD-C4C	2.46	1.48	1.41
23	b	614	CLA	C1B-CHB	2.46	1.47	1.41
23	b	604	CLA	C1B-CHB	2.46	1.47	1.41
23	a	405	CLA	CHD-C4C	2.46	1.48	1.41
23	b	613	CLA	CHD-C4C	2.46	1.48	1.41
23	c	501	CLA	C4C-C3C	2.46	1.49	1.45
23	C	508	CLA	C1C-C2C	2.45	1.49	1.44
23	A	404	CLA	C4B-CHC	2.45	1.47	1.41
23	B	603	CLA	C1D-C2D	2.45	1.48	1.42
23	c	509	CLA	C1B-CHB	2.45	1.47	1.41
23	B	606	CLA	CHD-C4C	2.44	1.48	1.41
23	c	508	CLA	C1B-CHB	2.44	1.47	1.41
23	C	510	CLA	C4B-CHC	2.43	1.47	1.41
23	c	513	CLA	C4B-CHC	2.43	1.47	1.41
23	b	608	CLA	CHD-C4C	2.43	1.48	1.41
23	b	604	CLA	C4B-CHC	2.43	1.47	1.41
23	C	503	CLA	C4B-CHC	2.43	1.47	1.41
23	C	509	CLA	C1D-C2D	2.43	1.48	1.42
23	B	606	CLA	C1B-CHB	2.42	1.47	1.41
23	d	403	CLA	C4B-CHC	2.42	1.47	1.41
23	b	616	CLA	CHD-C4C	2.42	1.48	1.41
23	c	510	CLA	C4C-C3C	2.42	1.49	1.45
23	b	612	CLA	C1B-CHB	2.42	1.47	1.41
23	C	502	CLA	C4C-C3C	2.42	1.49	1.45
23	B	601	CLA	C4C-C3C	2.42	1.49	1.45
38	e	103	HEM	C3B-C2B	-2.42	1.37	1.40
23	D	405	CLA	CHD-C4C	2.42	1.48	1.41
23	B	604	CLA	C1C-C2C	2.42	1.49	1.44
23	b	615	CLA	C1B-CHB	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C4B-CHC	2.41	1.47	1.41
23	A	408	CLA	C1C-C2C	2.41	1.49	1.44
23	c	506	CLA	CHD-C4C	2.41	1.48	1.41
23	c	512	CLA	CHD-C4C	2.41	1.48	1.41
23	b	609	CLA	C1C-C2C	2.41	1.49	1.44
23	b	607	CLA	C4C-C3C	2.41	1.49	1.45
23	C	511	CLA	C1B-CHB	2.41	1.47	1.41
23	C	513	CLA	C4B-CHC	2.41	1.47	1.41
23	B	616	CLA	C1B-CHB	2.40	1.47	1.41
23	B	602	CLA	C1C-C2C	2.40	1.49	1.44
23	B	608	CLA	C1B-CHB	2.40	1.47	1.41
23	B	611	CLA	CHD-C4C	2.40	1.48	1.41
23	B	601	CLA	C4B-CHC	2.40	1.47	1.41
23	C	512	CLA	CHD-C4C	2.40	1.48	1.41
23	c	504	CLA	C1B-CHB	2.40	1.47	1.41
23	C	511	CLA	C1C-C2C	2.40	1.49	1.44
23	d	403	CLA	CHD-C4C	2.40	1.48	1.41
23	b	602	CLA	C1B-CHB	2.40	1.47	1.41
24	D	401	PHO	C4C-C3C	2.40	1.49	1.45
23	c	508	CLA	CHD-C4C	2.40	1.48	1.41
23	d	401	CLA	CHD-C4C	2.39	1.48	1.41
23	c	512	CLA	C4B-CHC	2.39	1.47	1.41
23	D	404	CLA	C1B-CHB	2.39	1.47	1.41
23	a	404	CLA	CHD-C4C	2.39	1.48	1.41
23	c	508	CLA	C4C-C3C	2.39	1.49	1.45
23	B	609	CLA	CHD-C4C	2.39	1.48	1.41
23	b	607	CLA	C1D-C2D	2.39	1.48	1.42
24	a	407	PHO	C1A-NA	-2.39	1.32	1.37
23	C	508	CLA	C4B-CHC	2.39	1.47	1.41
23	c	505	CLA	C1D-C2D	2.39	1.48	1.42
23	c	511	CLA	C4B-CHC	2.39	1.47	1.41
23	B	601	CLA	C1C-C2C	2.39	1.49	1.44
23	c	509	CLA	C4B-CHC	2.39	1.47	1.41
23	C	508	CLA	C4C-C3C	2.39	1.49	1.45
23	a	404	CLA	C1B-CHB	2.38	1.47	1.41
23	d	404	CLA	C1C-C2C	2.38	1.49	1.44
23	b	613	CLA	C1D-C2D	2.38	1.47	1.42
23	b	606	CLA	C1D-C2D	2.37	1.47	1.42
23	B	613	CLA	C1D-C2D	2.37	1.47	1.42
23	C	502	CLA	C1B-CHB	2.37	1.47	1.41
23	B	610	CLA	C4C-C3C	2.36	1.49	1.45
23	C	502	CLA	C1C-C2C	2.36	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4B-CHC	2.36	1.47	1.41
24	a	406	PHO	C4D-CHA	2.36	1.50	1.43
23	c	504	CLA	CHD-C4C	2.36	1.47	1.41
23	C	506	CLA	CHD-C4C	2.36	1.47	1.41
23	b	609	CLA	C4B-CHC	2.35	1.47	1.41
23	b	615	CLA	CHD-C4C	2.35	1.47	1.41
23	B	604	CLA	C1B-NB	-2.35	1.33	1.35
23	c	501	CLA	C1C-C2C	2.35	1.49	1.44
23	C	514	CLA	C1B-CHB	2.35	1.47	1.41
23	b	613	CLA	C4B-CHC	2.35	1.47	1.41
23	c	512	CLA	C4C-C3C	2.34	1.49	1.45
23	c	503	CLA	C4C-C3C	2.34	1.49	1.45
23	B	612	CLA	C1B-CHB	2.33	1.47	1.41
23	A	408	CLA	C4B-CHC	2.33	1.47	1.41
23	b	605	CLA	C4C-C3C	2.33	1.49	1.45
36	c	518	DGD	O2G-C2G	-2.33	1.40	1.46
23	b	601	CLA	C1C-C2C	2.33	1.49	1.44
23	c	507	CLA	C4B-CHC	2.32	1.47	1.41
34	b	625	HTG	C1-S1	-2.32	1.77	1.80
23	b	606	CLA	C1B-CHB	2.32	1.47	1.41
23	C	512	CLA	C4B-CHC	2.32	1.47	1.41
23	a	408	CLA	C1B-NB	-2.32	1.33	1.35
23	a	405	CLA	C4C-C3C	2.32	1.49	1.45
23	C	505	CLA	CHD-C4C	2.32	1.47	1.41
23	A	404	CLA	C1C-C2C	2.32	1.49	1.44
23	b	609	CLA	C4C-C3C	2.32	1.49	1.45
23	D	405	CLA	C1B-CHB	2.32	1.47	1.41
23	b	607	CLA	C1B-NB	-2.31	1.33	1.35
23	C	506	CLA	C4B-CHC	2.31	1.47	1.41
23	C	510	CLA	C1B-CHB	2.31	1.47	1.41
23	b	607	CLA	C1B-CHB	2.31	1.47	1.41
23	c	504	CLA	C4B-CHC	2.31	1.47	1.41
23	c	513	CLA	C1B-CHB	2.31	1.47	1.41
23	c	503	CLA	C1B-CHB	2.31	1.47	1.41
23	B	614	CLA	C4C-C3C	2.30	1.49	1.45
23	B	602	CLA	C1B-CHB	2.30	1.47	1.41
23	b	605	CLA	C1C-C2C	2.29	1.49	1.44
23	B	612	CLA	C4B-CHC	2.29	1.47	1.41
33	Z	102	LMG	O1-C1	2.29	1.44	1.40
34	B	627	HTG	C1-S1	-2.29	1.77	1.80
23	B	610	CLA	CHD-C4C	2.29	1.47	1.41
23	b	608	CLA	C1B-CHB	2.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1C-C2C	2.29	1.49	1.44
23	c	511	CLA	C4C-C3C	2.29	1.49	1.45
23	B	614	CLA	C1C-NC	-2.28	1.34	1.37
23	a	408	CLA	C1B-CHB	2.28	1.47	1.41
23	C	504	CLA	C1B-CHB	2.28	1.47	1.41
23	C	504	CLA	C4B-CHC	2.28	1.47	1.41
23	b	606	CLA	C4B-CHC	2.27	1.47	1.41
23	B	616	CLA	C4C-C3C	2.27	1.49	1.45
23	a	404	CLA	C4B-CHC	2.27	1.47	1.41
23	b	603	CLA	C4C-C3C	2.27	1.48	1.45
23	C	506	CLA	C4C-C3C	2.27	1.48	1.45
23	c	512	CLA	C1B-CHB	2.27	1.47	1.41
34	D	412	HTG	C1-S1	-2.26	1.77	1.80
23	B	608	CLA	CHD-C4C	2.26	1.47	1.41
23	B	607	CLA	C4B-CHC	2.26	1.47	1.41
23	a	408	CLA	C4B-CHC	2.25	1.47	1.41
23	B	604	CLA	C4B-CHC	2.25	1.47	1.41
23	B	604	CLA	CHD-C4C	2.25	1.47	1.41
23	a	405	CLA	C1C-C2C	2.25	1.48	1.44
23	c	508	CLA	C4B-CHC	2.24	1.47	1.41
23	C	502	CLA	CHD-C4C	2.24	1.47	1.41
23	B	608	CLA	C1C-C2C	2.24	1.48	1.44
23	B	610	CLA	C1C-C2C	2.24	1.48	1.44
23	B	611	CLA	C4B-CHC	2.24	1.47	1.41
23	b	616	CLA	C1B-CHB	2.24	1.47	1.41
23	c	507	CLA	C1B-CHB	2.23	1.47	1.41
23	b	614	CLA	C4B-CHC	2.23	1.47	1.41
23	C	503	CLA	C1C-C2C	2.23	1.48	1.44
23	a	405	CLA	C1B-CHB	2.23	1.47	1.41
23	B	604	CLA	C1D-C2D	2.23	1.47	1.42
23	B	613	CLA	CHD-C4C	2.23	1.47	1.41
23	d	403	CLA	C1C-C2C	2.23	1.48	1.44
23	B	603	CLA	C4B-CHC	2.23	1.47	1.41
24	a	406	PHO	C1A-NA	-2.22	1.33	1.37
23	C	505	CLA	C1D-C2D	2.22	1.47	1.42
23	B	605	CLA	C4B-NB	-2.22	1.33	1.35
23	C	514	CLA	C4B-CHC	2.22	1.47	1.41
23	c	513	CLA	C4C-C3C	2.22	1.48	1.45
23	B	601	CLA	C1B-CHB	2.22	1.47	1.41
23	b	615	CLA	C4B-CHC	2.22	1.47	1.41
23	A	405	CLA	CHD-C4C	2.22	1.47	1.41
23	B	608	CLA	C4B-CHC	2.22	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4C-C3C	2.21	1.48	1.45
24	D	401	PHO	C3B-C4B	2.21	1.47	1.43
23	c	506	CLA	C4B-CHC	2.21	1.47	1.41
23	B	607	CLA	C1B-CHB	2.21	1.47	1.41
23	C	503	CLA	C1B-CHB	2.21	1.47	1.41
35	b	627	LMT	O1'-C1'	2.21	1.44	1.40
23	b	601	CLA	C1B-CHB	2.21	1.47	1.41
23	c	512	CLA	C1C-C2C	2.20	1.48	1.44
23	d	401	CLA	C1B-CHB	2.20	1.47	1.41
23	B	612	CLA	C1D-C2D	2.20	1.47	1.42
23	a	405	CLA	C4B-CHC	2.20	1.47	1.41
23	c	502	CLA	C4C-C3C	2.20	1.48	1.45
23	c	506	CLA	C1B-CHB	2.20	1.47	1.41
23	a	404	CLA	C1C-C2C	2.20	1.48	1.44
26	B	620	SQD	O6-C1	2.19	1.43	1.40
23	c	510	CLA	C1C-C2C	2.19	1.48	1.44
23	c	502	CLA	C1C-C2C	2.19	1.48	1.44
23	c	506	CLA	C4C-C3C	2.19	1.48	1.45
23	B	612	CLA	C4C-C3C	2.19	1.48	1.45
23	C	511	CLA	C4B-CHC	2.19	1.47	1.41
23	b	614	CLA	C1C-C2C	2.19	1.48	1.44
23	B	615	CLA	C1B-CHB	2.19	1.47	1.41
23	b	615	CLA	C4C-C3C	2.18	1.48	1.45
35	E	102	LMT	O1'-C1'	2.18	1.43	1.40
35	B	630	LMT	O1'-C1'	2.18	1.43	1.40
23	C	507	CLA	C1B-CHB	2.18	1.47	1.41
23	b	605	CLA	C1C-NC	-2.17	1.34	1.37
23	d	401	CLA	C4B-CHC	2.17	1.47	1.41
23	b	604	CLA	CHD-C4C	2.17	1.47	1.41
24	A	407	PHO	C4D-CHA	2.17	1.49	1.43
23	b	607	CLA	CHD-C4C	2.17	1.47	1.41
23	c	506	CLA	C1B-NB	-2.17	1.33	1.35
36	c	517	DGD	O3G-C1D	2.16	1.43	1.40
23	B	614	CLA	C4B-NB	-2.16	1.33	1.35
23	C	502	CLA	C4B-CHC	2.16	1.47	1.41
23	c	510	CLA	C4B-CHC	2.16	1.47	1.41
23	C	509	CLA	CHD-C4C	2.16	1.47	1.41
23	b	611	CLA	C1C-C2C	2.16	1.48	1.44
24	D	401	PHO	C1A-NA	-2.15	1.33	1.37
23	c	506	CLA	C1C-NC	-2.15	1.34	1.37
23	b	605	CLA	C4B-CHC	2.14	1.46	1.41
23	A	406	CLA	CHD-C4C	2.14	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C4B-CHC	2.14	1.46	1.41
23	A	408	CLA	C1C-NC	-2.14	1.34	1.37
23	B	603	CLA	C1B-NB	-2.13	1.33	1.35
34	d	411	HTG	C1-S1	-2.13	1.77	1.80
23	B	614	CLA	C1C-C2C	2.13	1.48	1.44
36	h	102	DGD	O5D-C1E	2.13	1.43	1.40
23	b	601	CLA	C4C-C3C	2.13	1.48	1.45
24	D	401	PHO	C4D-CHA	2.13	1.49	1.43
23	C	514	CLA	C4C-C3C	2.13	1.48	1.45
23	A	406	CLA	C4B-CHC	2.12	1.46	1.41
34	C	522	HTG	C1-S1	-2.12	1.77	1.80
23	b	613	CLA	C4C-C3C	2.11	1.48	1.45
23	C	509	CLA	C1C-NC	-2.11	1.34	1.37
23	b	608	CLA	C1B-NB	-2.11	1.33	1.35
23	A	406	CLA	C4C-C3C	2.10	1.48	1.45
23	A	408	CLA	C4C-C3C	2.10	1.48	1.45
23	A	408	CLA	C1B-CHB	2.10	1.46	1.41
23	C	509	CLA	C4B-CHC	2.09	1.46	1.41
23	d	401	CLA	C1C-C2C	2.09	1.48	1.44
23	A	406	CLA	C1B-CHB	2.08	1.46	1.41
23	B	603	CLA	C1B-CHB	2.08	1.46	1.41
35	I	101	LMT	O1'-C1'	2.08	1.43	1.40
23	b	614	CLA	C4C-C3C	2.08	1.48	1.45
34	c	522	HTG	C1-S1	-2.08	1.77	1.80
23	C	505	CLA	C4C-C3C	2.08	1.48	1.45
23	B	602	CLA	C4B-CHC	2.08	1.46	1.41
23	C	513	CLA	C1B-CHB	2.06	1.46	1.41
29	A	414	PL9	C2-C3	2.05	1.40	1.34
23	b	608	CLA	C4C-C3C	2.05	1.48	1.45
36	H	102	DGD	O5D-C1E	2.05	1.43	1.40
31	A	416	LHG	O7-C5	-2.04	1.41	1.46
23	A	404	CLA	C1B-CHB	2.04	1.46	1.41
23	C	513	CLA	C4C-C3C	2.04	1.48	1.45
24	D	401	PHO	C1D-C2D	2.03	1.50	1.45
29	a	414	PL9	C2-C3	2.03	1.40	1.34
23	c	505	CLA	C4C-C3C	2.03	1.48	1.45
23	c	507	CLA	C4C-C3C	2.03	1.48	1.45
34	b	623	HTG	C1-S1	-2.02	1.77	1.80
33	c	520	LMG	O1-C1	2.02	1.43	1.40
24	D	401	PHO	C1B-NB	-2.01	1.34	1.38
23	B	611	CLA	C4C-C3C	2.00	1.48	1.45
23	d	404	CLA	C1B-CHB	2.00	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C1B-CHB	2.00	1.46	1.41
23	b	603	CLA	C1B-NB	-2.00	1.33	1.35

All (2293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	401	PHO	CMD-C2D-C1D	8.00	137.38	125.06
24	A	407	PHO	CMD-C2D-C1D	7.45	136.53	125.06
23	B	606	CLA	C4A-NA-C1A	-7.40	103.38	106.71
24	a	407	PHO	CMD-C2D-C1D	7.33	136.36	125.06
23	C	504	CLA	C4A-NA-C1A	-7.18	103.48	106.71
23	A	408	CLA	C4A-NA-C1A	-7.10	103.51	106.71
23	b	616	CLA	C4A-NA-C1A	-7.05	103.54	106.71
23	B	607	CLA	C4A-NA-C1A	-6.99	103.56	106.71
23	D	404	CLA	C4A-NA-C1A	-6.96	103.58	106.71
34	B	624	HTG	C1'-S1-C1	6.85	112.91	100.09
23	A	405	CLA	CHD-C4C-C3C	-6.85	114.77	124.84
23	c	513	CLA	C4A-NA-C1A	-6.77	103.66	106.71
34	b	623	HTG	C1'-S1-C1	6.76	112.73	100.09
23	D	404	CLA	C2C-C1C-NC	6.72	116.26	109.97
34	B	623	HTG	C1'-S1-C1	6.64	112.50	100.09
23	B	609	CLA	CHD-C4C-C3C	-6.58	115.16	124.84
23	C	511	CLA	C4A-NA-C1A	-6.55	103.76	106.71
23	b	616	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
23	c	505	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
38	E	103	HEM	CAD-CBD-CGD	6.48	123.55	112.67
23	D	405	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
23	B	608	CLA	CHD-C4C-C3C	-6.46	115.34	124.84
26	A	410	SQD	O6-C1-C2	6.46	118.38	108.30
23	B	616	CLA	C4A-NA-C1A	-6.44	103.81	106.71
23	C	507	CLA	C4A-NA-C1A	-6.43	103.81	106.71
24	a	406	PHO	CMD-C2D-C1D	6.42	134.95	125.06
23	d	403	CLA	C4A-NA-C1A	-6.41	103.83	106.71
23	C	506	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
23	B	616	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
23	c	508	CLA	O2D-CGD-CBD	6.31	122.48	111.27
23	a	404	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	C	508	CLA	O2D-CGD-CBD	6.29	122.45	111.27
23	B	612	CLA	CHD-C4C-C3C	-6.28	115.60	124.84
23	b	604	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	C	509	CLA	C2C-C1C-NC	6.27	115.85	109.97
23	B	616	CLA	O2D-CGD-CBD	6.27	122.41	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C2C-C1C-NC	6.27	115.84	109.97
23	C	513	CLA	C4A-NA-C1A	-6.24	103.90	106.71
23	B	615	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
23	B	611	CLA	CHD-C4C-C3C	-6.22	115.69	124.84
23	C	506	CLA	O2D-CGD-CBD	6.22	122.33	111.27
23	B	604	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	610	CLA	CHD-C4C-C3C	-6.21	115.70	124.84
23	b	602	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	b	604	CLA	O2D-CGD-CBD	6.17	122.22	111.27
23	b	608	CLA	CHD-C4C-C3C	-6.15	115.81	124.84
23	b	606	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	d	401	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	c	503	CLA	C4A-NA-C1A	-6.12	103.95	106.71
23	d	403	CLA	C2C-C1C-NC	6.12	115.71	109.97
23	b	601	CLA	C4A-NA-C1A	-6.10	103.96	106.71
23	C	505	CLA	C2C-C1C-NC	6.10	115.69	109.97
23	b	603	CLA	C4A-NA-C1A	-6.10	103.97	106.71
23	b	610	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	b	602	CLA	O2D-CGD-CBD	6.09	122.09	111.27
23	b	613	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	c	503	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	D	405	CLA	O2D-CGD-CBD	6.06	122.04	111.27
23	C	506	CLA	C4A-NA-C1A	-6.06	103.98	106.71
23	b	605	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	b	606	CLA	C4A-NA-C1A	-6.06	103.98	106.71
23	C	512	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	B	614	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	B	602	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	c	506	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	c	512	CLA	O2D-CGD-CBD	6.02	121.96	111.27
23	a	405	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	b	601	CLA	O2D-CGD-CBD	5.98	121.89	111.27
23	c	507	CLA	O2D-CGD-CBD	5.97	121.88	111.27
24	D	401	PHO	C3D-C2D-C1D	-5.96	97.19	105.87
23	B	605	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	C	510	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	c	511	CLA	CHD-C4C-C3C	-5.94	116.10	124.84
23	b	614	CLA	O2D-CGD-CBD	5.93	121.81	111.27
34	c	521	HTG	C1'-S1-C1	5.93	111.18	100.09
23	d	404	CLA	C4A-NA-C1A	-5.93	104.04	106.71
23	B	601	CLA	O2D-CGD-CBD	5.91	121.77	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C2C-C1C-NC	5.91	115.51	109.97
23	A	406	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
23	B	614	CLA	O2D-CGD-CBD	5.89	121.73	111.27
26	D	413	SQD	O47-C7-C8	5.87	124.15	111.50
25	D	406	BCR	C7-C8-C9	-5.86	117.38	126.23
23	C	514	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	C	505	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	B	613	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	b	613	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	b	603	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	d	404	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
23	B	612	CLA	O2D-CGD-CBD	5.82	121.61	111.27
23	c	507	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	b	616	CLA	O2D-CGD-CBD	5.81	121.59	111.27
34	D	412	HTG	C1'-S1-C1	5.81	110.95	100.09
23	A	408	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	C	513	CLA	O2D-CGD-CBD	5.80	121.57	111.27
23	B	604	CLA	O2D-CGD-CBD	5.79	121.56	111.27
23	B	603	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	c	512	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
23	c	508	CLA	C4A-NA-C1A	-5.78	104.11	106.71
23	b	611	CLA	C2C-C1C-NC	5.78	115.38	109.97
23	C	513	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	B	614	CLA	CHD-C4C-C3C	-5.77	116.35	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	A	404	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	b	611	CLA	O2D-CGD-CBD	5.75	121.49	111.27
23	b	601	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
34	d	411	HTG	C1'-S1-C1	5.73	110.80	100.09
23	c	501	CLA	C4A-NA-C1A	-5.73	104.13	106.71
23	B	609	CLA	C4A-NA-C1A	-5.72	104.14	106.71
23	B	602	CLA	C2C-C1C-NC	5.72	115.33	109.97
34	b	625	HTG	C1'-S1-C1	5.72	110.78	100.09
23	c	508	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	B	601	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	b	615	CLA	CHD-C4C-C3C	-5.70	116.45	124.84
23	b	614	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	b	609	CLA	C4A-NA-C1A	-5.70	104.14	106.71
23	B	604	CLA	C2C-C1C-NC	5.69	115.31	109.97
23	b	612	CLA	CHD-C4C-C3C	-5.68	116.49	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	b	603	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	C	503	CLA	CHD-C4C-C3C	-5.66	116.51	124.84
38	e	103	HEM	CAD-CBD-CGD	5.65	122.15	112.67
23	C	502	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	c	501	CLA	O2D-CGD-CBD	5.64	121.29	111.27
23	C	502	CLA	O2D-CGD-CBD	5.64	121.29	111.27
23	b	607	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	C	507	CLA	C2C-C1C-NC	5.62	115.24	109.97
23	B	606	CLA	O2D-CGD-CBD	5.62	121.25	111.27
23	b	615	CLA	C2C-C1C-NC	5.62	115.23	109.97
25	Y	101	BCR	C33-C5-C6	-5.61	118.22	124.53
23	c	504	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
23	B	603	CLA	C2C-C1C-NC	5.59	115.21	109.97
23	b	610	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
23	C	502	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	B	610	CLA	O2D-CGD-CBD	5.57	121.17	111.27
23	B	607	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	C	503	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	d	401	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	B	607	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	C	503	CLA	O2D-CGD-CBD	5.53	121.10	111.27
26	D	413	SQD	O6-C1-C2	5.53	116.94	108.30
24	D	401	PHO	O2D-CGD-CBD	5.53	121.10	111.27
23	C	508	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
23	b	607	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	b	604	CLA	C4A-NA-C1A	-5.48	104.24	106.71
23	c	508	CLA	C2C-C1C-NC	5.48	115.10	109.97
23	b	611	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	c	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	C	509	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
23	c	509	CLA	C2C-C1C-NC	5.45	115.07	109.97
23	b	605	CLA	O2D-CGD-CBD	5.44	120.94	111.27
23	B	612	CLA	C3C-C4C-NC	5.42	116.65	110.57
24	D	401	PHO	C2D-C1D-ND	5.41	117.96	109.79
23	c	510	CLA	C2C-C1C-NC	5.41	115.04	109.97
29	a	414	PL9	C7-C3-C4	5.40	121.27	116.88
23	C	511	CLA	O2D-CGD-CBD	5.40	120.86	111.27
23	C	511	CLA	C2C-C1C-NC	5.39	115.03	109.97
23	b	610	CLA	C2C-C1C-NC	5.39	115.03	109.97
24	a	406	PHO	C3D-C2D-C1D	-5.39	98.02	105.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	PHO	C2D-C1D-ND	5.39	117.92	109.79
23	B	613	CLA	C4A-NA-C1A	-5.39	104.28	106.71
23	a	408	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	A	404	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	b	610	CLA	O2D-CGD-CBD	5.38	120.82	111.27
23	B	605	CLA	O2D-CGD-CBD	5.37	120.82	111.27
23	B	615	CLA	C4A-NA-C1A	-5.37	104.29	106.71
23	c	512	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	c	503	CLA	O2D-CGD-CBD	5.36	120.79	111.27
23	C	514	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	C	509	CLA	O2D-CGD-CBD	5.34	120.76	111.27
23	B	611	CLA	C2C-C1C-NC	5.34	114.97	109.97
26	a	410	SQD	O47-C7-C8	5.33	122.99	111.50
23	b	605	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	c	510	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	c	510	CLA	C1-C2-C3	-5.32	116.84	126.04
23	b	609	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
23	b	606	CLA	O2D-CGD-CBD	5.30	120.69	111.27
23	C	508	CLA	C2C-C1C-NC	5.29	114.93	109.97
23	C	505	CLA	O2D-CGD-CBD	5.28	120.66	111.27
23	b	608	CLA	O2D-CGD-CBD	5.28	120.64	111.27
24	a	407	PHO	O2D-CGD-CBD	5.27	120.64	111.27
23	b	604	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	a	406	PHO	O2D-CGD-CBD	5.27	120.63	111.27
23	c	501	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
24	A	407	PHO	C3D-C2D-C1D	-5.26	98.21	105.87
23	c	511	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	c	502	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	a	408	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	C	508	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	a	404	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	c	503	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	C	506	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	c	509	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
23	B	612	CLA	C2C-C1C-NC	5.21	114.86	109.97
23	B	607	CLA	O2D-CGD-CBD	5.21	120.53	111.27
23	B	610	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	b	609	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	C	512	CLA	C2C-C1C-NC	5.19	114.84	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
23	B	601	CLA	C2C-C1C-NC	5.18	114.83	109.97
23	a	404	CLA	CHD-C4C-C3C	-5.18	117.23	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	C4A-NA-C1A	-5.16	104.38	106.71
23	C	504	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	b	608	CLA	C4A-NA-C1A	-5.16	104.39	106.71
23	b	602	CLA	C2C-C1C-NC	5.16	114.80	109.97
23	b	609	CLA	O2D-CGD-CBD	5.16	120.43	111.27
23	c	509	CLA	O2D-CGD-CBD	5.16	120.43	111.27
23	c	509	CLA	C4A-NA-C1A	-5.15	104.39	106.71
34	b	628	HTG	C1'-S1-C1	5.15	109.73	100.09
24	A	407	PHO	C2D-C1D-ND	5.15	117.56	109.79
23	b	614	CLA	C2C-C1C-NC	5.15	114.79	109.97
23	a	408	CLA	C2C-C1C-NC	5.14	114.78	109.97
23	C	503	CLA	C2C-C1C-NC	5.13	114.78	109.97
23	a	408	CLA	O2D-CGD-CBD	5.13	120.38	111.27
23	B	603	CLA	O2D-CGD-CBD	5.13	120.38	111.27
23	c	504	CLA	C2C-C1C-NC	5.12	114.76	109.97
34	C	522	HTG	C1'-S1-C1	5.11	109.65	100.09
23	d	404	CLA	O2D-CGD-CBD	5.11	120.35	111.27
23	D	404	CLA	CHD-C4C-C3C	-5.10	117.34	124.84
26	a	410	SQD	O6-C1-C2	5.07	116.22	108.30
34	b	622	HTG	C1'-S1-C1	5.07	109.57	100.09
23	b	601	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	B	602	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
24	A	407	PHO	C1-C2-C3	-5.06	117.30	126.04
23	C	510	CLA	C4A-NA-C1A	-5.05	104.44	106.71
24	a	407	PHO	C1-C2-C3	-5.05	117.31	126.04
23	B	603	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
23	a	405	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	b	612	CLA	C2C-C1C-NC	5.04	114.69	109.97
25	t	101	BCR	C33-C5-C6	-5.03	118.88	124.53
24	a	407	PHO	C3D-C2D-C1D	-5.01	98.58	105.87
23	B	615	CLA	C2C-C1C-NC	5.01	114.66	109.97
23	C	504	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
26	L	101	SQD	O47-C7-C8	5.00	122.27	111.50
34	B	627	HTG	C1'-S1-C1	5.00	109.43	100.09
23	c	501	CLA	C2C-C1C-NC	4.99	114.65	109.97
26	f	101	SQD	O47-C7-C8	4.99	122.25	111.50
23	C	507	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
23	c	505	CLA	C3C-C4C-NC	4.99	116.16	110.57
23	b	604	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	c	505	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	C	509	CLA	C3C-C4C-NC	4.97	116.15	110.57
23	c	505	CLA	O2D-CGD-CBD	4.96	120.08	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	D	405	CLA	C4A-NA-C1A	-4.94	104.48	106.71
26	B	620	SQD	O6-C1-C2	4.94	116.01	108.30
23	d	403	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
34	C	522	HTG	C1-O5-C5	4.94	121.68	112.58
23	c	512	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	b	612	CLA	O2D-CGD-CBD	4.93	120.03	111.27
25	c	515	BCR	C7-C8-C9	-4.93	118.79	126.23
23	b	615	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	B	601	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	c	505	CLA	C2C-C1C-NC	4.91	114.58	109.97
23	b	612	CLA	C4A-NA-C1A	-4.91	104.50	106.71
23	C	510	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	b	608	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	b	614	CLA	C4A-NA-C1A	-4.91	104.50	106.71
23	d	401	CLA	C1C-C2C-C3C	-4.90	101.80	106.96
23	c	507	CLA	C2C-C1C-NC	4.90	114.56	109.97
34	c	522	HTG	C1'-S1-C1	4.90	109.25	100.09
23	A	408	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	B	609	CLA	C2C-C1C-NC	4.89	114.55	109.97
23	c	513	CLA	O2D-CGD-CBD	4.89	119.95	111.27
34	C	521	HTG	C1'-S1-C1	4.87	109.21	100.09
23	A	404	CLA	CHD-C4C-C3C	-4.87	117.69	124.84
23	D	404	CLA	C1-C2-C3	-4.86	117.63	126.04
23	B	605	CLA	C2C-C1C-NC	4.86	114.53	109.97
33	C	501	LMG	O7-C10-C11	4.86	121.98	111.50
23	A	405	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	C	510	CLA	C2C-C1C-NC	4.85	114.51	109.97
25	T	101	BCR	C15-C16-C17	-4.85	113.55	123.47
23	C	506	CLA	C3C-C4C-NC	4.84	116.00	110.57
23	B	604	CLA	C3C-C4C-NC	4.83	115.98	110.57
23	c	513	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	b	607	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	B	606	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	c	509	CLA	C1-C2-C3	-4.78	117.78	126.04
23	D	404	CLA	O2D-CGD-CBD	4.77	119.75	111.27
23	c	511	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	C	513	CLA	C2C-C1C-NC	4.76	114.43	109.97
23	b	607	CLA	O2D-CGD-CBD	4.76	119.72	111.27
25	y	101	BCR	C33-C5-C6	-4.73	119.21	124.53
23	c	504	CLA	O2D-CGD-CBD	4.72	119.65	111.27
26	A	410	SQD	C1-C2-C3	-4.71	100.18	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	407	PHO	C2D-C1D-ND	4.69	116.87	109.79
23	D	404	CLA	C1C-C2C-C3C	-4.69	102.03	106.96
23	C	505	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
26	A	410	SQD	O47-C7-C8	4.67	121.56	111.50
23	a	404	CLA	C1C-C2C-C3C	-4.66	102.05	106.96
23	B	610	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	b	610	CLA	C1-C2-C3	-4.65	118.01	126.04
23	B	615	CLA	O2D-CGD-CBD	4.64	119.51	111.27
23	B	602	CLA	O2D-CGD-CBD	4.64	119.50	111.27
23	b	607	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	B	611	CLA	C4A-NA-C1A	-4.63	104.63	106.71
23	C	514	CLA	C2C-C1C-NC	4.62	114.30	109.97
23	b	609	CLA	C1-C2-C3	-4.62	118.05	126.04
23	b	606	CLA	C2C-C1C-NC	4.62	114.30	109.97
23	b	613	CLA	C4A-NA-C1A	-4.59	104.64	106.71
31	D	409	LHG	O7-C7-C8	4.59	121.39	111.50
24	A	407	PHO	O2D-CGD-CBD	4.58	119.41	111.27
23	a	405	CLA	O2D-CGD-CBD	4.58	119.41	111.27
23	A	406	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	b	616	CLA	C1D-CHD-C4C	-4.58	116.52	122.56
26	L	101	SQD	O6-C1-C2	4.57	115.43	108.30
29	D	407	PL9	C42-C43-C44	-4.55	116.71	127.66
23	B	609	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	c	508	CLA	O2D-CGD-O1D	-4.53	114.98	123.84
23	B	610	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	c	502	CLA	C1C-C2C-C3C	-4.53	102.20	106.96
23	c	504	CLA	C4A-NA-C1A	-4.52	104.67	106.71
25	H	101	BCR	C11-C10-C9	-4.52	120.86	127.31
23	c	510	CLA	O2D-CGD-CBD	4.52	119.30	111.27
23	B	605	CLA	C4A-NA-C1A	-4.52	104.67	106.71
25	c	514	BCR	C11-C10-C9	-4.52	120.86	127.31
25	T	101	BCR	C33-C5-C6	-4.51	119.46	124.53
25	d	405	BCR	C15-C14-C13	-4.50	120.89	127.31
23	b	603	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	B	608	CLA	O2D-CGD-CBD	4.49	119.24	111.27
23	a	405	CLA	C4A-NA-C1A	-4.45	104.70	106.71
23	B	613	CLA	C1-C2-C3	-4.45	118.35	126.04
23	B	613	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	c	508	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	b	613	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	B	606	CLA	C3C-C4C-NC	4.42	115.52	110.57
25	B	617	BCR	C33-C5-C6	-4.40	119.59	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	Z	102	LMG	O7-C10-C11	4.40	120.97	111.50
23	A	406	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	b	605	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	C	512	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	b	615	CLA	O2D-CGD-CBD	4.38	119.04	111.27
23	A	405	CLA	C2C-C1C-NC	4.38	114.07	109.97
23	c	503	CLA	C3C-C4C-NC	4.37	115.47	110.57
23	B	614	CLA	C1D-CHD-C4C	-4.37	116.79	122.56
26	A	410	SQD	C1-O5-C5	-4.36	105.12	113.69
26	L	101	SQD	O7-S-C6	4.36	112.12	106.94
23	B	616	CLA	C3C-C4C-NC	4.36	115.46	110.57
23	C	507	CLA	O2D-CGD-CBD	4.35	119.00	111.27
26	B	620	SQD	O47-C7-C8	4.34	120.86	111.50
23	b	613	CLA	O2D-CGD-CBD	4.34	118.97	111.27
23	C	514	CLA	O2D-CGD-CBD	4.33	118.97	111.27
23	C	505	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	C	502	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
23	B	616	CLA	C2C-C1C-NC	4.33	114.03	109.97
23	B	609	CLA	O2D-CGD-CBD	4.32	118.95	111.27
34	b	628	HTG	C1-O5-C5	4.32	120.54	112.58
23	d	403	CLA	O2D-CGD-CBD	4.31	118.93	111.27
23	d	403	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	D	404	CLA	C3C-C4C-NC	4.29	115.39	110.57
23	C	505	CLA	C1D-CHD-C4C	-4.29	116.90	122.56
25	b	619	BCR	C3-C4-C5	-4.28	106.43	114.08
23	a	404	CLA	C1D-CHD-C4C	-4.28	116.91	122.56
23	c	507	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	C	509	CLA	C3B-C4B-NB	4.27	114.73	109.21
23	c	501	CLA	O2D-CGD-O1D	-4.27	115.49	123.84
23	B	611	CLA	O2D-CGD-CBD	4.27	118.85	111.27
23	A	408	CLA	C4-C3-C5	4.27	122.45	115.27
23	C	508	CLA	C1D-CHD-C4C	-4.25	116.95	122.56
25	d	405	BCR	C28-C27-C26	-4.24	106.50	114.08
23	B	615	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	c	513	CLA	C3C-C4C-NC	4.24	115.32	110.57
23	b	610	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	b	616	CLA	C3C-C4C-NC	4.23	115.32	110.57
35	D	402	LMT	C1'-O5'-C5'	4.22	121.98	113.69
23	c	506	CLA	O2D-CGD-CBD	4.22	118.77	111.27
25	C	515	BCR	C15-C14-C13	-4.22	121.29	127.31
23	b	606	CLA	C1D-CHD-C4C	-4.21	117.00	122.56
25	B	617	BCR	C7-C8-C9	-4.21	119.88	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	Z	101	LMG	C3-C4-C5	4.19	117.72	110.24
23	c	509	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	C	508	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	B	611	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	D	405	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
23	b	614	CLA	C3C-C4C-NC	4.17	115.25	110.57
23	c	510	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	B	603	CLA	C1D-CHD-C4C	-4.16	117.06	122.56
23	c	503	CLA	C1D-CHD-C4C	-4.16	117.07	122.56
23	C	502	CLA	C1D-CHD-C4C	-4.16	117.07	122.56
29	a	414	PL9	C32-C33-C34	-4.15	117.67	127.66
23	C	510	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	b	606	CLA	C3C-C4C-NC	4.13	115.21	110.57
23	A	405	CLA	O2D-CGD-CBD	4.13	118.61	111.27
26	A	410	SQD	C44-O6-C1	-4.13	105.67	113.74
23	A	408	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	c	511	CLA	O2D-CGD-CBD	4.12	118.59	111.27
23	A	405	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
36	c	516	DGD	O2G-C1B-C2B	4.12	120.37	111.50
23	C	512	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	B	604	CLA	C4A-NA-C1A	-4.11	104.86	106.71
23	c	502	CLA	C4A-NA-C1A	-4.11	104.86	106.71
23	D	405	CLA	C3C-C4C-NC	4.11	115.18	110.57
23	b	612	CLA	C3C-C4C-NC	4.11	115.17	110.57
23	C	505	CLA	C3B-C4B-NB	4.10	114.51	109.21
23	B	614	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
23	C	507	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
25	b	617	BCR	C33-C5-C6	-4.09	119.93	124.53
29	A	414	PL9	C7-C3-C4	4.09	120.20	116.88
23	a	404	CLA	C3B-C4B-NB	4.09	114.49	109.21
23	b	613	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	c	512	CLA	C3C-C4C-NC	4.09	115.15	110.57
35	D	402	LMT	O5'-C5'-C4'	4.08	118.36	109.75
24	a	406	PHO	C4C-C3C-C2C	-4.08	102.27	106.78
23	A	406	CLA	C2C-C1C-NC	4.07	113.79	109.97
23	b	611	CLA	C1-C2-C3	-4.07	119.01	126.04
25	H	101	BCR	C7-C8-C9	-4.06	120.10	126.23
29	a	414	PL9	C15-C14-C16	4.06	122.10	115.27
25	b	619	BCR	C7-C8-C9	-4.06	120.10	126.23
23	A	408	CLA	O2D-CGD-CBD	4.06	118.47	111.27
23	B	612	CLA	O2D-CGD-O1D	-4.05	115.91	123.84
25	k	101	BCR	C11-C10-C9	-4.05	121.53	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	C2C-C1C-NC	4.05	113.76	109.97
23	c	506	CLA	C3B-C4B-NB	4.04	114.44	109.21
23	A	404	CLA	O2A-CGA-CBA	4.04	124.60	111.91
23	B	613	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	c	506	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	B	612	CLA	C1-C2-C3	-4.03	119.07	126.04
33	c	520	LMG	O7-C10-C11	4.03	120.18	111.50
23	c	511	CLA	C4-C3-C5	4.02	122.04	115.27
23	c	502	CLA	C3B-C4B-NB	4.01	114.39	109.21
34	b	625	HTG	C1-O5-C5	4.01	119.97	112.58
31	E	101	LHG	O7-C7-C8	4.01	120.14	111.50
23	D	405	CLA	C2C-C1C-NC	4.01	113.72	109.97
23	A	406	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	B	611	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	608	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	607	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
33	J	101	LMG	O7-C10-C11	4.00	120.11	111.50
25	c	514	BCR	C20-C21-C22	-4.00	121.61	127.31
23	C	514	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	B	608	CLA	C4A-NA-C1A	-3.99	104.91	106.71
23	b	605	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	C	512	CLA	O2D-CGD-CBD	3.98	118.34	111.27
23	A	404	CLA	CAC-C3C-C4C	3.98	129.97	124.81
23	c	507	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	a	408	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	B	604	CLA	C1D-CHD-C4C	-3.97	117.32	122.56
23	C	503	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	a	408	CLA	C1-C2-C3	-3.96	119.19	126.04
23	B	605	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
23	c	512	CLA	C1-C2-C3	-3.96	119.20	126.04
23	b	608	CLA	C3C-C4C-NC	3.96	115.01	110.57
35	I	101	LMT	C1'-O5'-C5'	3.95	121.45	113.69
23	B	604	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
23	A	404	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	B	614	CLA	C3B-C4B-NB	3.94	114.31	109.21
23	C	503	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	C	511	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
25	H	101	BCR	C16-C17-C18	-3.94	121.69	127.31
25	b	618	BCR	C7-C8-C9	-3.94	120.28	126.23
25	d	405	BCR	C29-C30-C25	3.94	116.54	110.48
23	B	607	CLA	C3C-C4C-NC	3.94	114.98	110.57
29	A	414	PL9	C7-C8-C9	-3.93	120.25	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	CMC-C2C-C1C	3.93	131.02	125.04
29	a	414	PL9	C27-C28-C29	-3.92	118.21	127.66
24	D	401	PHO	C1-C2-C3	-3.92	119.26	126.04
23	b	606	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	D	405	CLA	C1-C2-C3	-3.92	119.26	126.04
23	B	608	CLA	C3C-C4C-NC	3.92	114.97	110.57
36	H	102	DGD	O2G-C1B-C2B	3.92	119.94	111.50
23	d	401	CLA	C1D-CHD-C4C	-3.91	117.40	122.56
23	C	507	CLA	C1-C2-C3	-3.91	119.28	126.04
33	Z	101	LMG	O7-C10-C11	3.90	119.92	111.50
23	a	404	CLA	O2D-CGD-CBD	3.90	118.20	111.27
23	b	601	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	c	504	CLA	C3C-C4C-NC	3.89	114.94	110.57
23	C	502	CLA	C1-C2-C3	-3.89	119.31	126.04
23	b	603	CLA	C1D-CHD-C4C	-3.89	117.42	122.56
23	A	404	CLA	CAA-C2A-C3A	-3.89	102.12	112.78
29	a	414	PL9	C7-C3-C2	-3.89	118.19	123.30
23	A	405	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	c	506	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
23	D	405	CLA	C1D-CHD-C4C	-3.88	117.44	122.56
23	B	616	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
23	A	405	CLA	CHD-C4C-NC	3.87	130.30	124.20
23	c	502	CLA	C4D-C3D-CAD	-3.87	106.31	108.47
23	C	502	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	b	615	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	A	405	CLA	CMC-C2C-C1C	3.87	130.93	125.04
26	a	410	SQD	C45-O47-C7	-3.86	108.28	117.79
23	C	513	CLA	C3C-C4C-NC	3.86	114.90	110.57
23	B	606	CLA	C1D-CHD-C4C	-3.86	117.46	122.56
23	b	615	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
23	d	403	CLA	C3C-C4C-NC	3.86	114.90	110.57
23	C	507	CLA	CAC-C3C-C4C	3.85	129.81	124.81
29	a	414	PL9	C22-C23-C24	-3.85	118.39	127.66
26	a	410	SQD	O8-S-C6	3.85	111.87	105.74
23	a	404	CLA	CAA-C2A-C3A	-3.85	102.24	112.78
25	C	515	BCR	C16-C17-C18	-3.84	121.82	127.31
23	C	513	CLA	C1D-CHD-C4C	-3.84	117.49	122.56
23	c	502	CLA	C3C-C4C-NC	3.84	114.88	110.57
23	b	604	CLA	C1C-C2C-C3C	-3.83	102.92	106.96
23	b	602	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	b	612	CLA	C1-C2-C3	-3.83	119.42	126.04
23	b	611	CLA	C3C-C4C-NC	3.83	114.86	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C15-C14-C13	-3.82	121.85	127.31
23	B	602	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	c	501	CLA	C3C-C4C-NC	3.82	114.85	110.57
29	d	406	PL9	C10-C9-C11	3.81	121.68	115.27
33	B	621	LMG	O7-C10-C11	3.81	119.71	111.50
25	d	405	BCR	C7-C8-C9	-3.81	120.48	126.23
29	d	406	PL9	C42-C43-C44	-3.81	118.50	127.66
23	b	603	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	C	512	CLA	C3B-C4B-NB	3.80	114.12	109.21
23	B	605	CLA	C1-C2-C3	-3.80	119.47	126.04
23	C	510	CLA	C1-C2-C3	-3.80	119.47	126.04
33	c	519	LMG	O7-C10-C11	3.80	119.68	111.50
29	d	406	PL9	C7-C8-C9	-3.79	120.48	126.79
38	E	103	HEM	CBD-CAD-C3D	-3.79	105.50	112.48
25	B	618	BCR	C37-C22-C21	-3.78	117.63	122.92
25	c	514	BCR	C15-C14-C13	-3.78	121.92	127.31
23	b	614	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
23	B	605	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	C	508	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
23	b	608	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	B	614	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	c	508	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	b	602	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	c	511	CLA	C1-C2-C3	-3.77	119.52	126.04
23	B	615	CLA	C1D-CHD-C4C	-3.77	117.58	122.56
23	B	612	CLA	C4C-C3C-C2C	-3.77	101.41	106.90
23	a	405	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
31	A	417	LHG	O7-C7-C8	3.75	119.59	111.50
23	c	511	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	A	404	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
23	d	401	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	b	611	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
25	b	619	BCR	C38-C26-C25	-3.74	120.32	124.53
33	j	101	LMG	O7-C10-C11	3.74	119.57	111.50
23	b	605	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
23	B	612	CLA	C4A-NA-C1A	-3.74	105.03	106.71
33	c	520	LMG	O6-C5-C4	3.73	116.47	109.69
23	b	613	CLA	C1D-CHD-C4C	-3.73	117.64	122.56
23	a	404	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	d	401	CLA	C4A-NA-C1A	-3.72	105.03	106.71
23	b	614	CLA	C1D-CHD-C4C	-3.72	117.64	122.56
25	c	514	BCR	C16-C17-C18	-3.71	122.01	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CAA-C2A-C3A	-3.71	102.61	112.78
23	a	405	CLA	C3C-C4C-NC	3.71	114.73	110.57
23	c	506	CLA	C1D-CHD-C4C	-3.71	117.66	122.56
26	B	620	SQD	O7-S-C6	3.71	111.34	106.94
33	a	416	LMG	O7-C10-C11	3.71	119.49	111.50
23	B	610	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
23	d	403	CLA	C3B-C4B-NB	3.70	114.00	109.21
23	c	513	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
23	c	506	CLA	C4A-NA-C1A	-3.70	105.04	106.71
23	C	505	CLA	C4A-NA-C1A	-3.70	105.04	106.71
23	d	401	CLA	O2D-CGD-CBD	3.70	117.84	111.27
23	B	601	CLA	C3C-C4C-NC	3.70	114.72	110.57
23	b	609	CLA	C1C-C2C-C3C	-3.69	103.07	106.96
23	a	408	CLA	C3B-C4B-NB	3.69	113.99	109.21
34	C	522	HTG	O5-C5-C4	3.69	116.40	109.69
23	C	506	CLA	C1D-CHD-C4C	-3.69	117.68	122.56
23	d	404	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	d	404	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	a	405	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
23	C	509	CLA	C4C-C3C-C2C	-3.68	101.53	106.90
23	b	612	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
29	A	414	PL9	C7-C3-C2	-3.68	118.46	123.30
23	B	601	CLA	C1-C2-C3	-3.68	119.68	126.04
23	b	605	CLA	C3B-C4B-NB	3.68	113.97	109.21
23	C	509	CLA	O2D-CGD-O1D	-3.67	116.65	123.84
25	B	618	BCR	C29-C30-C25	3.67	116.13	110.48
25	Y	101	BCR	C15-C14-C13	-3.66	122.08	127.31
33	Z	102	LMG	C3-C4-C5	3.66	116.77	110.24
23	C	502	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	A	407	PHO	C4C-C3C-C2C	-3.66	102.73	106.78
33	Z	101	LMG	O6-C5-C4	3.66	116.33	109.69
23	b	605	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
23	C	504	CLA	O2D-CGD-CBD	3.65	117.76	111.27
23	b	607	CLA	C3B-C4B-NB	3.65	113.93	109.21
29	a	414	PL9	C37-C38-C39	-3.65	118.88	127.66
23	b	609	CLA	C3C-C4C-NC	3.64	114.65	110.57
25	C	516	BCR	C7-C8-C9	-3.64	120.73	126.23
23	B	613	CLA	CAC-C3C-C4C	3.64	129.53	124.81
23	B	612	CLA	C1D-CHD-C4C	-3.63	117.76	122.56
23	c	504	CLA	CAC-C3C-C4C	3.63	129.53	124.81
23	B	603	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	C	509	CLA	C1C-C2C-C3C	-3.63	103.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C1D-CHD-C4C	-3.63	117.77	122.56
23	C	502	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
23	c	504	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
25	k	101	BCR	C24-C23-C22	-3.63	120.75	126.23
23	c	510	CLA	C3B-C4B-NB	3.63	113.90	109.21
23	b	611	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	B	605	CLA	C1D-CHD-C4C	-3.62	117.78	122.56
23	b	602	CLA	C1D-CHD-C4C	-3.62	117.78	122.56
23	B	608	CLA	C1-C2-C3	-3.62	119.78	126.04
25	h	101	BCR	C7-C8-C9	-3.62	120.77	126.23
23	b	615	CLA	C1D-CHD-C4C	-3.61	117.79	122.56
23	b	608	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	A	408	CLA	C1-C2-C3	-3.61	119.80	126.04
23	B	610	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
23	B	616	CLA	C4C-C3C-C2C	-3.61	101.64	106.90
29	A	414	PL9	C27-C28-C29	-3.60	118.98	127.66
23	c	512	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	c	508	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	B	602	CLA	C3C-C4C-NC	3.59	114.60	110.57
23	B	601	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	b	614	CLA	C3B-C4B-NB	3.59	113.86	109.21
23	b	607	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	C	510	CLA	CMC-C2C-C1C	3.59	130.50	125.04
23	C	503	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
23	b	604	CLA	C1-C2-C3	-3.59	119.84	126.04
23	d	403	CLA	O2A-CGA-CBA	3.58	123.16	111.91
23	B	603	CLA	O2A-CGA-O1A	-3.58	114.55	123.59
24	D	401	PHO	CAC-C3C-C4C	3.58	129.13	125.22
23	b	616	CLA	C2C-C1C-NC	3.58	113.33	109.97
26	a	410	SQD	C1-O5-C5	-3.58	106.66	113.69
23	c	513	CLA	CMC-C2C-C1C	3.58	130.49	125.04
25	H	101	BCR	C24-C23-C22	-3.58	120.83	126.23
36	C	518	DGD	O2G-C1B-C2B	3.58	119.21	111.50
23	c	505	CLA	C1D-CHD-C4C	-3.58	117.84	122.56
29	D	407	PL9	C53-C6-C1	3.58	122.30	114.99
23	d	401	CLA	CHD-C4C-NC	3.57	129.83	124.20
33	z	101	LMG	O7-C10-C11	3.57	119.20	111.50
40	V	202	HEC	CBA-CAA-C2A	-3.57	105.90	112.48
23	b	609	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
36	C	517	DGD	O2G-C1B-C2B	3.57	119.19	111.50
25	K	102	BCR	C7-C8-C9	-3.56	120.85	126.23
36	c	517	DGD	O2G-C1B-C2B	3.56	119.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	d	401	CLA	CAA-C2A-C3A	-3.56	103.03	112.78
31	d	407	LHG	O7-C7-C8	3.56	119.17	111.50
23	B	608	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
23	D	404	CLA	C3B-C4B-NB	3.56	113.81	109.21
23	B	602	CLA	C3B-C4B-NB	3.56	113.81	109.21
23	B	604	CLA	C1-C2-C3	-3.56	119.89	126.04
26	D	413	SQD	O7-S-C6	3.55	111.16	106.94
23	B	613	CLA	CMB-C2B-C3B	3.55	131.32	124.68
31	l	101	LHG	O7-C7-C8	3.54	119.13	111.50
23	C	508	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
33	Z	102	LMG	C1-C2-C3	3.54	117.36	110.00
23	B	604	CLA	C3B-C4B-NB	3.53	113.78	109.21
23	b	613	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	b	609	CLA	CAC-C3C-C4C	3.53	129.39	124.81
25	A	409	BCR	C33-C5-C6	-3.53	120.57	124.53
23	b	603	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
25	h	101	BCR	C16-C17-C18	-3.52	122.28	127.31
23	B	614	CLA	CHC-C1C-C2C	-3.52	116.98	126.72
23	B	603	CLA	C3B-C4B-NB	3.52	113.76	109.21
23	a	408	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
23	b	615	CLA	C3B-C4B-NB	3.52	113.75	109.21
23	C	509	CLA	C4D-C3D-CAD	-3.51	106.51	108.47
23	B	611	CLA	C1D-CHD-C4C	-3.51	117.92	122.56
31	d	409	LHG	O7-C7-C8	3.51	119.07	111.50
23	C	513	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
23	c	501	CLA	CAC-C3C-C4C	3.50	129.35	124.81
23	C	503	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
23	B	603	CLA	CAA-C2A-C3A	-3.50	103.19	112.78
23	C	504	CLA	C3C-C4C-NC	3.50	114.50	110.57
23	C	506	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
23	C	512	CLA	CMC-C2C-C1C	3.50	130.36	125.04
23	C	504	CLA	C4-C3-C5	3.49	121.15	115.27
23	B	609	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
23	B	601	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
23	A	408	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
23	B	613	CLA	C3B-C4B-NB	3.49	113.72	109.21
25	C	516	BCR	C11-C10-C9	-3.49	122.33	127.31
23	c	513	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	C	512	CLA	CAC-C3C-C4C	3.48	129.33	124.81
23	c	509	CLA	C3B-C4B-NB	3.48	113.71	109.21
23	B	608	CLA	CHD-C4C-NC	3.48	129.69	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	b	615	CLA	C11-C10-C8	-3.48	104.67	115.92
25	H	101	BCR	C38-C26-C25	-3.48	120.62	124.53
23	c	511	CLA	C3B-C4B-NB	3.48	113.70	109.21
23	b	610	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	C	514	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
23	C	512	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	615	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	C	507	CLA	CBC-CAC-C3C	-3.47	102.86	112.43
23	C	502	CLA	CBC-CAC-C3C	-3.47	102.86	112.43
23	B	608	CLA	O2A-CGA-O1A	-3.47	114.84	123.59
23	B	603	CLA	C3C-C4C-NC	3.46	114.46	110.57
23	B	610	CLA	O2A-CGA-CBA	3.46	122.77	111.91
24	a	407	PHO	C4C-C3C-C2C	-3.46	102.95	106.78
23	b	616	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
25	b	617	BCR	C7-C8-C9	-3.46	121.01	126.23
23	b	601	CLA	C1D-CHD-C4C	-3.46	118.00	122.56
23	A	404	CLA	C3C-C4C-NC	3.46	114.45	110.57
23	C	507	CLA	CMC-C2C-C1C	3.45	130.30	125.04
29	A	414	PL9	C22-C23-C24	-3.45	119.35	127.66
23	c	505	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
23	c	510	CLA	C1D-CHD-C4C	-3.45	118.01	122.56
23	b	601	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	b	613	CLA	O2A-CGA-CBA	3.44	122.72	111.91
23	b	605	CLA	C4-C3-C5	3.44	121.06	115.27
23	b	609	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
23	d	401	CLA	CBC-CAC-C3C	-3.44	102.95	112.43
23	c	512	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
23	A	405	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
25	K	102	BCR	C24-C23-C22	-3.43	121.05	126.23
23	b	614	CLA	CAC-C3C-C4C	3.43	129.26	124.81
23	c	504	CLA	CMC-C2C-C1C	3.43	130.26	125.04
23	c	504	CLA	C3B-C4B-NB	3.43	113.64	109.21
25	t	101	BCR	C37-C22-C23	3.42	123.47	118.08
26	A	410	SQD	O7-S-C6	3.42	111.01	106.94
23	C	506	CLA	CMC-C2C-C1C	3.42	130.25	125.04
25	k	101	BCR	C29-C30-C25	3.41	115.74	110.48
23	c	501	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	A	404	CLA	C1D-CHD-C4C	-3.41	118.06	122.56
23	B	606	CLA	C1C-C2C-C3C	-3.41	103.38	106.96
29	a	414	PL9	C10-C9-C11	3.41	121.00	115.27
23	B	615	CLA	CED-O2D-CGD	3.41	123.64	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	SQD	C1-C2-C3	-3.40	102.91	110.00
23	a	408	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
23	B	607	CLA	CAA-C2A-C3A	-3.40	103.47	112.78
23	B	611	CLA	OBD-CAD-C3D	-3.40	122.34	127.98
23	b	606	CLA	C4-C3-C5	3.40	120.99	115.27
34	b	622	HTG	O5-C1-C2	3.40	114.59	110.31
25	d	405	BCR	C33-C5-C6	-3.40	120.71	124.53
23	B	611	CLA	C3B-C4B-NB	3.40	113.60	109.21
23	C	510	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	B	603	CLA	C4-C3-C5	3.39	120.97	115.27
23	b	605	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	C	504	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
23	C	514	CLA	C1-C2-C3	-3.38	120.19	126.04
26	f	101	SQD	O7-S-C6	3.38	110.95	106.94
25	t	101	BCR	C11-C10-C9	-3.38	122.49	127.31
23	C	511	CLA	C1-C2-C3	-3.37	120.21	126.04
23	c	509	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
23	B	614	CLA	O2A-CGA-O1A	-3.37	115.09	123.59
23	C	514	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
23	D	405	CLA	CHD-C4C-NC	3.36	129.50	124.20
33	c	520	LMG	C3-C4-C5	3.36	116.24	110.24
23	c	502	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
29	d	406	PL9	C20-C19-C21	3.35	120.91	115.27
25	A	409	BCR	C24-C23-C22	-3.35	121.17	126.23
23	d	401	CLA	C3C-C4C-NC	3.35	114.33	110.57
23	a	404	CLA	CMB-C2B-C3B	3.35	130.95	124.68
23	c	502	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	C	512	CLA	C1D-CHD-C4C	-3.35	118.14	122.56
23	B	614	CLA	C4A-NA-C1A	-3.35	105.20	106.71
25	D	406	BCR	C38-C26-C25	-3.35	120.77	124.53
31	A	416	LHG	O8-C23-C24	3.35	122.41	111.91
23	d	403	CLA	C1-C2-C3	-3.35	120.26	126.04
26	A	412	SQD	O48-C23-C24	3.34	122.40	111.91
29	A	414	PL9	C15-C14-C16	3.34	120.89	115.27
23	a	405	CLA	C3B-C4B-NB	3.34	113.53	109.21
23	d	401	CLA	C4D-C3D-CAD	-3.34	106.61	108.47
26	a	410	SQD	O9-S-C6	3.33	110.90	106.94
23	A	408	CLA	C3B-C4B-NB	3.33	113.52	109.21
23	B	608	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	a	408	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
33	Z	102	LMG	C4-C3-C2	3.33	116.63	110.82
25	D	406	BCR	C24-C23-C22	-3.32	121.22	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C1D-CHD-C4C	-3.32	118.17	122.56
29	A	414	PL9	C30-C29-C31	3.32	120.86	115.27
23	C	509	CLA	C1-C2-C3	-3.32	120.30	126.04
24	a	406	PHO	CAC-C3C-C4C	3.32	128.84	125.22
23	D	405	CLA	CMC-C2C-C1C	3.31	130.08	125.04
29	A	414	PL9	C32-C33-C34	-3.31	119.69	127.66
23	c	510	CLA	C4-C3-C5	3.31	120.84	115.27
25	h	101	BCR	C38-C26-C25	-3.31	120.81	124.53
23	C	507	CLA	C3C-C4C-NC	3.31	114.28	110.57
26	a	412	SQD	O47-C7-C8	3.31	118.63	111.50
23	A	408	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
23	B	601	CLA	C3B-C4B-NB	3.31	113.49	109.21
23	b	610	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
25	y	101	BCR	C38-C26-C25	-3.31	120.81	124.53
26	f	101	SQD	C1-O5-C5	3.31	120.18	113.69
23	b	614	CLA	C1-C2-C3	-3.30	120.33	126.04
26	A	412	SQD	O8-S-C6	3.30	111.00	105.74
25	T	101	BCR	C7-C8-C9	-3.30	121.25	126.23
23	B	607	CLA	C1D-CHD-C4C	-3.30	118.21	122.56
23	b	609	CLA	CBC-CAC-C3C	-3.30	103.34	112.43
23	C	511	CLA	C1D-CHD-C4C	-3.29	118.21	122.56
23	b	612	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
34	b	623	HTG	O5-C1-C2	3.29	114.46	110.31
29	a	414	PL9	C30-C29-C31	3.29	120.81	115.27
23	D	404	CLA	CAC-C3C-C4C	3.29	129.08	124.81
23	C	509	CLA	C4A-NA-C1A	-3.29	105.23	106.71
23	B	614	CLA	CAC-C3C-C4C	3.29	129.07	124.81
23	b	616	CLA	CHD-C4C-NC	3.28	129.38	124.20
23	C	511	CLA	C3C-C4C-NC	3.28	114.25	110.57
23	b	610	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
23	b	608	CLA	CMB-C2B-C3B	3.28	130.82	124.68
23	C	512	CLA	C4-C3-C5	3.28	120.79	115.27
23	B	605	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	c	507	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	c	509	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
25	D	406	BCR	C3-C4-C5	-3.27	108.24	114.08
23	c	513	CLA	CAC-C3C-C4C	3.27	129.05	124.81
29	A	414	PL9	C20-C19-C21	3.27	120.77	115.27
25	c	515	BCR	C38-C26-C25	-3.27	120.86	124.53
23	b	609	CLA	O2A-CGA-CBA	3.26	122.14	111.91
23	A	408	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	d	404	CLA	C1D-CHD-C4C	-3.26	118.26	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	416	LHG	O8-C23-O10	-3.25	115.38	123.59
23	c	502	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
25	A	409	BCR	C15-C14-C13	-3.25	122.67	127.31
23	A	406	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
23	c	512	CLA	C3B-C4B-NB	3.25	113.41	109.21
23	B	607	CLA	O2D-CGD-O1D	-3.24	117.49	123.84
23	b	604	CLA	CMC-C2C-C1C	3.24	129.98	125.04
25	d	405	BCR	C16-C17-C18	-3.24	122.68	127.31
23	A	404	CLA	O2A-CGA-O1A	-3.24	115.41	123.59
23	b	615	CLA	CHC-C1C-C2C	-3.24	117.75	126.72
23	b	612	CLA	C4-C3-C5	3.24	120.72	115.27
25	t	101	BCR	C21-C20-C19	-3.24	113.11	123.22
23	c	508	CLA	C1D-CHD-C4C	-3.24	118.29	122.56
23	c	506	CLA	C1-C2-C3	-3.24	120.45	126.04
23	b	605	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	b	608	CLA	CMC-C2C-C1C	3.23	129.96	125.04
25	C	515	BCR	C33-C5-C6	-3.23	120.90	124.53
25	D	406	BCR	C28-C27-C26	-3.23	108.32	114.08
23	c	513	CLA	C1-C2-C3	-3.22	120.47	126.04
25	T	101	BCR	C15-C14-C13	3.22	131.91	127.31
23	B	603	CLA	O2A-CGA-CBA	3.22	122.02	111.91
23	A	405	CLA	C4D-C3D-CAD	-3.22	106.67	108.47
40	V	202	HEC	CAD-CBD-CGD	3.22	118.08	112.67
25	b	617	BCR	C16-C17-C18	-3.22	122.71	127.31
23	b	610	CLA	O2A-CGA-CBA	3.22	122.01	111.91
34	c	522	HTG	C1-O5-C5	3.22	118.52	112.58
23	b	606	CLA	C3B-C4B-NB	3.22	113.37	109.21
29	A	414	PL9	C37-C38-C39	-3.21	119.92	127.66
23	b	602	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
23	C	510	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
23	B	612	CLA	C3B-C4B-NB	3.21	113.36	109.21
25	T	101	BCR	C12-C13-C14	-3.21	114.01	118.94
24	A	407	PHO	C2B-C1B-NB	3.21	114.64	109.79
23	c	510	CLA	CBC-CAC-C3C	-3.21	103.58	112.43
23	B	613	CLA	C4-C3-C5	3.21	120.66	115.27
23	D	404	CLA	O2A-CGA-CBA	3.21	121.97	111.91
23	b	610	CLA	CMB-C2B-C3B	3.20	130.67	124.68
23	C	504	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
24	D	401	PHO	C2A-C1A-NA	3.20	115.54	111.86
29	a	414	PL9	C42-C43-C44	-3.20	119.95	127.66
25	B	618	BCR	C2-C1-C6	3.20	115.41	110.48
23	B	610	CLA	C1-C2-C3	-3.20	120.51	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	CAA-C2A-C3A	-3.20	104.02	112.78
23	a	405	CLA	CHD-C4C-NC	3.19	129.24	124.20
23	C	510	CLA	CAC-C3C-C4C	3.19	128.95	124.81
23	B	615	CLA	C3B-C4B-NB	3.19	113.33	109.21
23	A	404	CLA	O2D-CGD-CBD	3.19	116.93	111.27
23	A	406	CLA	C1-C2-C3	-3.19	120.53	126.04
23	B	610	CLA	C1C-C2C-C3C	-3.19	103.61	106.96
23	b	612	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	D	405	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	C	502	CLA	CHC-C1C-C2C	-3.18	117.92	126.72
23	c	509	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	c	504	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
29	d	406	PL9	C25-C24-C26	3.18	120.62	115.27
23	C	508	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
24	D	401	PHO	C1C-C2C-C3C	-3.17	102.87	106.51
23	A	406	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	C	509	CLA	CAC-C3C-C4C	3.17	128.92	124.81
29	d	406	PL9	C36-C37-C38	-3.17	101.46	111.88
23	c	512	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	b	610	CLA	C4-C3-C5	3.16	120.59	115.27
23	b	607	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
24	a	407	PHO	C4-C3-C5	3.16	120.59	115.27
31	A	416	LHG	O7-C7-C8	3.16	118.32	111.50
23	b	604	CLA	C1D-CHD-C4C	-3.16	118.39	122.56
35	M	101	LMT	O1'-C1'-C2'	3.16	113.23	108.30
23	b	606	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
23	b	608	CLA	CHD-C4C-NC	3.16	129.18	124.20
23	c	502	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
23	B	602	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
23	C	506	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	b	602	CLA	C3B-C4B-NB	3.15	113.29	109.21
23	B	616	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
23	b	609	CLA	C3B-C4B-NB	3.15	113.28	109.21
23	a	404	CLA	O2A-CGA-O1A	-3.15	115.64	123.59
26	a	412	SQD	C3-C4-C5	3.15	115.86	110.24
23	C	504	CLA	C3B-C4B-NB	3.15	113.28	109.21
23	C	507	CLA	C4-C3-C5	3.15	120.57	115.27
23	b	612	CLA	C3B-C4B-NB	3.15	113.28	109.21
23	b	613	CLA	O2A-CGA-O1A	-3.15	115.65	123.59
23	B	609	CLA	CHD-C4C-NC	3.14	129.16	124.20
23	C	509	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
23	d	404	CLA	CAC-C3C-C4C	3.14	128.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C3B-C4B-NB	3.14	113.27	109.21
23	b	611	CLA	C1D-CHD-C4C	-3.14	118.41	122.56
23	c	505	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	c	510	CLA	CHD-C4C-NC	3.14	129.15	124.20
34	B	622	HTG	C1-O5-C5	3.14	118.37	112.58
23	a	404	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	b	614	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	a	404	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
23	C	504	CLA	C1D-CHD-C4C	-3.14	118.41	122.56
23	b	614	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
23	C	509	CLA	O2A-CGA-O1A	-3.14	115.68	123.59
23	B	611	CLA	C1-C2-C3	-3.13	120.62	126.04
33	b	620	LMG	O7-C10-C11	3.13	118.25	111.50
23	D	405	CLA	CAA-C2A-C3A	-3.13	104.20	112.78
23	c	505	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
23	c	506	CLA	CHC-C1C-C2C	-3.13	118.06	126.72
31	e	101	LHG	O7-C7-C8	3.13	118.25	111.50
25	c	515	BCR	C15-C14-C13	-3.13	122.84	127.31
26	a	410	SQD	O47-C7-O49	-3.13	116.14	123.70
23	c	510	CLA	CHC-C1C-C2C	-3.13	118.07	126.72
35	D	403	LMT	O1B-C4'-C3'	3.13	115.60	107.28
23	c	508	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	b	603	CLA	O2A-CGA-CBA	3.13	121.72	111.91
23	b	611	CLA	CHC-C1C-C2C	-3.12	118.08	126.72
23	D	404	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	c	513	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
23	b	606	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	a	404	CLA	C1-C2-C3	-3.12	120.65	126.04
23	c	511	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
23	A	406	CLA	C1D-CHD-C4C	-3.12	118.44	122.56
23	C	510	CLA	C3B-C4B-NB	3.12	113.24	109.21
38	E	103	HEM	CBA-CAA-C2A	-3.12	106.74	112.49
40	v	201	HEC	CBA-CAA-C2A	-3.12	106.74	112.48
23	B	608	CLA	O2A-CGA-CBA	3.11	121.68	111.91
23	b	616	CLA	O2A-CGA-CBA	3.11	121.68	111.91
23	B	616	CLA	C3B-C4B-NB	3.11	113.24	109.21
23	c	511	CLA	CHD-C4C-NC	3.11	129.11	124.20
23	A	408	CLA	CAA-C2A-C3A	-3.11	104.25	112.78
29	d	406	PL9	C40-C39-C41	3.11	120.50	115.27
33	C	520	LMG	O7-C10-C11	3.11	118.20	111.50
23	b	604	CLA	O2A-CGA-CBA	3.11	121.67	111.91
23	b	608	CLA	C1-C2-C3	-3.11	120.67	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
23	b	608	CLA	C1D-CHD-C4C	-3.11	118.46	122.56
23	B	611	CLA	CMC-C2C-C1C	3.11	129.77	125.04
23	B	601	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	a	408	CLA	C1D-CHD-C4C	-3.11	118.46	122.56
23	D	404	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
23	C	507	CLA	C3B-C4B-NB	3.10	113.22	109.21
26	B	620	SQD	O48-C23-C24	3.10	121.65	111.91
23	b	611	CLA	CAC-C3C-C4C	3.10	128.84	124.81
23	b	611	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
23	C	512	CLA	C1-C2-C3	-3.10	120.68	126.04
23	B	603	CLA	CHC-C1C-C2C	-3.10	118.14	126.72
23	B	605	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	a	408	CLA	CAC-C3C-C4C	3.10	128.83	124.81
23	c	513	CLA	CMB-C2B-C3B	3.10	130.48	124.68
26	a	410	SQD	C44-O6-C1	-3.10	107.69	113.74
23	c	513	CLA	C3B-C4B-NB	3.10	113.21	109.21
23	C	505	CLA	CMC-C2C-C1C	3.10	129.75	125.04
25	B	618	BCR	C3-C4-C5	-3.10	108.55	114.08
23	B	606	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
25	k	101	BCR	C15-C14-C13	-3.09	122.90	127.31
23	c	503	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	b	607	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	B	606	CLA	C4-C3-C5	3.09	120.46	115.27
25	T	101	BCR	C11-C10-C9	-3.09	122.91	127.31
25	A	409	BCR	C37-C22-C21	-3.08	118.60	122.92
23	c	510	CLA	C3C-C4C-NC	3.08	114.03	110.57
23	b	612	CLA	O2A-CGA-CBA	3.08	121.58	111.91
23	B	612	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
23	C	506	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
29	D	407	PL9	C12-C13-C14	-3.08	120.24	127.66
24	A	407	PHO	C4D-CHA-C1A	-3.08	118.44	125.37
23	C	511	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
23	c	507	CLA	C1D-CHD-C4C	-3.08	118.49	122.56
23	C	511	CLA	C3B-C4B-NB	3.08	113.19	109.21
23	B	616	CLA	CHD-C4C-NC	3.08	129.05	124.20
33	b	620	LMG	O8-C28-C29	3.08	121.56	111.91
23	B	611	CLA	CHD-C4C-NC	3.07	129.05	124.20
23	d	401	CLA	C1-C2-C3	-3.07	120.73	126.04
25	C	516	BCR	C15-C14-C13	-3.07	122.92	127.31
23	c	505	CLA	C3B-C4B-NB	3.07	113.18	109.21
23	b	608	CLA	C3B-C4B-NB	3.07	113.18	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	624	HTG	O5-C1-C2	3.07	114.17	110.31
24	D	401	PHO	C2C-C1C-NC	3.07	114.42	109.79
23	c	507	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	d	401	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
38	e	103	HEM	CBD-CAD-C3D	-3.06	106.84	112.48
25	C	516	BCR	C33-C5-C6	-3.06	121.09	124.53
23	d	404	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	D	401	PHO	CHC-C1C-C2C	-3.06	118.04	125.73
23	c	511	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	b	605	CLA	CHD-C4C-NC	3.05	129.02	124.20
23	b	616	CLA	C4-C3-C5	3.05	120.41	115.27
23	d	404	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	C	510	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	b	612	CLA	CAC-C3C-C4C	3.05	128.77	124.81
26	a	412	SQD	O7-S-C6	3.05	110.56	106.94
23	D	405	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	B	615	CLA	CHD-C4C-NC	3.04	128.99	124.20
29	D	407	PL9	C22-C23-C24	-3.04	120.35	127.66
23	C	512	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	B	604	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
23	c	501	CLA	C1D-CHD-C4C	-3.03	118.55	122.56
25	b	619	BCR	C15-C14-C13	-3.03	122.98	127.31
26	A	410	SQD	O48-C23-C24	3.03	121.42	111.91
23	B	602	CLA	C1D-CHD-C4C	-3.03	118.56	122.56
23	B	609	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	C	511	CLA	O2A-CGA-CBA	3.03	121.40	111.91
23	a	408	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	c	511	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
25	a	409	BCR	C11-C10-C9	-3.02	122.99	127.31
26	L	101	SQD	C3-C4-C5	3.02	115.63	110.24
23	b	616	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	b	606	CLA	CHD-C4C-NC	3.02	128.97	124.20
23	B	613	CLA	O2A-CGA-CBA	3.02	121.39	111.91
24	a	407	PHO	CHC-C1C-C2C	-3.02	118.13	125.73
25	Y	101	BCR	C16-C17-C18	-3.02	123.00	127.31
23	b	604	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
23	B	614	CLA	CBC-CAC-C3C	-3.02	104.10	112.43
23	c	506	CLA	CAC-C3C-C4C	3.02	128.73	124.81
23	b	607	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
23	a	405	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
23	b	605	CLA	O2A-CGA-O1A	-3.02	115.98	123.59
33	b	620	LMG	C7-O1-C1	-3.01	107.85	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	O2A-CGA-CBA	3.01	121.36	111.91
23	B	610	CLA	C3B-C4B-NB	3.01	113.11	109.21
26	D	413	SQD	C44-O6-C1	-3.01	107.85	113.74
26	a	412	SQD	O9-S-C6	3.01	110.52	106.94
25	D	406	BCR	C16-C17-C18	-3.01	123.02	127.31
23	c	513	CLA	C4-C3-C5	3.01	120.33	115.27
23	b	605	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
23	b	607	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
23	B	605	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
23	b	601	CLA	C4-C3-C5	3.01	120.33	115.27
23	a	408	CLA	O2A-CGA-CBA	3.00	121.34	111.91
23	B	607	CLA	C3B-C4B-NB	3.00	113.09	109.21
25	H	101	BCR	C3-C4-C5	-3.00	108.72	114.08
23	b	602	CLA	CMC-C2C-C1C	3.00	129.61	125.04
23	A	408	CLA	C4D-C3D-CAD	-3.00	106.80	108.47
23	c	505	CLA	CAC-C3C-C4C	3.00	128.70	124.81
24	D	401	PHO	C4C-C3C-C2C	-3.00	103.46	106.78
33	C	520	LMG	O8-C28-C29	3.00	121.32	111.91
23	C	503	CLA	C3B-C4B-NB	3.00	113.08	109.21
23	b	603	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
33	B	621	LMG	O8-C28-C29	2.99	121.29	111.91
23	C	507	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
23	c	501	CLA	C1-C2-C3	-2.99	120.87	126.04
23	B	601	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
23	b	607	CLA	C1-O2A-CGA	2.99	124.28	116.44
23	c	501	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
23	C	514	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	b	603	CLA	CHD-C4C-NC	2.98	128.91	124.20
23	a	408	CLA	O2A-CGA-O1A	-2.98	116.06	123.59
23	c	512	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	D	405	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	A	404	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
26	a	412	SQD	O48-C23-C24	2.98	121.26	111.91
31	E	101	LHG	O8-C23-C24	2.98	121.25	111.91
31	l	101	LHG	O8-C23-C24	2.98	121.25	111.91
23	c	506	CLA	C4-C3-C5	2.98	120.28	115.27
23	c	501	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
23	C	505	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	c	503	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
23	c	506	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
23	A	406	CLA	O2A-CGA-CBA	2.97	121.24	111.91
23	c	509	CLA	C1D-CHD-C4C	-2.97	118.64	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	O2A-CGA-CBA	2.97	121.23	111.91
26	B	620	SQD	C3-C4-C5	2.97	115.54	110.24
23	b	615	CLA	C4-C3-C5	2.97	120.27	115.27
23	c	513	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	C	506	CLA	C3B-C4B-NB	2.97	113.05	109.21
23	C	514	CLA	C2A-C1A-CHA	-2.97	118.67	123.86
26	A	412	SQD	O47-C7-C8	2.97	117.90	111.50
23	b	601	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	c	512	CLA	CHC-C1C-C2C	-2.96	118.53	126.72
23	b	613	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	c	502	CLA	O2A-CGA-CBA	2.96	121.20	111.91
23	b	607	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
29	a	414	PL9	C20-C19-C21	2.96	120.25	115.27
23	C	504	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	b	613	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
25	B	619	BCR	C37-C22-C21	-2.96	118.78	122.92
23	B	609	CLA	C3B-C4B-NB	2.96	113.03	109.21
23	d	403	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
23	b	614	CLA	O2A-CGA-CBA	2.96	121.18	111.91
33	c	520	LMG	O8-C28-C29	2.95	121.17	111.91
23	C	502	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	C	514	CLA	C3B-C4B-NB	2.95	113.03	109.21
26	a	412	SQD	C1-O5-C5	2.95	119.48	113.69
23	C	512	CLA	CHD-C4C-NC	2.95	128.85	124.20
29	A	414	PL9	C10-C9-C11	2.95	120.23	115.27
25	t	101	BCR	C35-C13-C12	2.95	122.72	118.08
23	B	601	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
25	A	409	BCR	C38-C26-C25	-2.94	121.22	124.53
23	B	612	CLA	CAC-C3C-C4C	2.94	128.63	124.81
25	A	409	BCR	C11-C10-C9	-2.94	123.11	127.31
23	B	614	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	b	616	CLA	CAC-C3C-C4C	2.94	128.63	124.81
23	d	404	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
23	B	601	CLA	CHD-C4C-NC	2.94	128.83	124.20
34	B	622	HTG	C1'-S1-C1	2.94	105.58	100.09
25	c	514	BCR	C24-C23-C22	-2.94	121.80	126.23
23	C	513	CLA	O2A-CGA-CBA	2.94	121.12	111.91
25	d	405	BCR	C37-C22-C23	2.94	122.70	118.08
26	L	101	SQD	O48-C23-C24	2.94	121.12	111.91
25	B	618	BCR	C38-C26-C25	-2.94	121.23	124.53
31	d	409	LHG	O8-C23-C24	2.93	121.12	111.91
23	b	611	CLA	O2A-CGA-CBA	2.93	121.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C1D-CHD-C4C	-2.93	118.69	122.56
23	B	615	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	B	606	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	C	510	CLA	CMB-C2B-C3B	2.93	130.15	124.68
23	D	404	CLA	O2A-CGA-O1A	-2.93	116.21	123.59
23	B	613	CLA	C1D-CHD-C4C	-2.92	118.70	122.56
23	B	602	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	C	511	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
23	b	610	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	c	505	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	c	508	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
24	A	407	PHO	C4D-ND-C1D	-2.92	101.52	106.76
23	B	601	CLA	O2A-CGA-CBA	2.92	121.06	111.91
25	t	101	BCR	C19-C18-C17	-2.92	114.47	118.94
31	D	408	LHG	O7-C7-C8	2.91	117.78	111.50
23	C	513	CLA	CBC-CAC-C3C	-2.91	104.40	112.43
23	B	615	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
23	a	404	CLA	C4-C3-C5	2.91	120.17	115.27
23	B	606	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	a	407	PHO	C2B-C1B-NB	2.91	114.18	109.79
26	L	101	SQD	C44-O6-C1	-2.91	108.06	113.74
23	c	503	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	d	406	PL9	C35-C34-C36	2.91	120.16	115.27
29	D	407	PL9	C7-C8-C9	-2.91	121.95	126.79
33	z	101	LMG	O8-C28-C29	2.91	121.03	111.91
23	C	502	CLA	OBD-CAD-C3D	-2.91	123.16	127.98
23	C	514	CLA	CAC-C3C-C4C	2.90	128.58	124.81
23	B	615	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
25	B	619	BCR	C24-C23-C22	-2.90	121.85	126.23
35	I	101	LMT	O1B-C4'-C3'	2.90	115.00	107.28
25	K	102	BCR	C3-C4-C5	-2.90	108.90	114.08
23	C	502	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
23	B	609	CLA	C1-C2-C3	-2.90	121.03	126.04
23	a	405	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	B	604	CLA	CMC-C2C-C1C	2.90	129.45	125.04
36	h	102	DGD	O1G-C1A-C2A	2.90	121.00	111.91
23	B	606	CLA	C3B-C4B-NB	2.90	112.95	109.21
36	C	519	DGD	O1G-C1A-C2A	2.90	121.00	111.91
25	c	514	BCR	C38-C26-C25	-2.90	121.28	124.53
24	a	406	PHO	CHC-C1C-C2C	-2.90	118.45	125.73
29	D	407	PL9	C40-C39-C41	2.90	120.14	115.27
23	b	602	CLA	CHD-C4C-NC	2.89	128.76	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CMC-C2C-C1C	2.89	129.45	125.04
23	c	503	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	b	604	CLA	C3B-C4B-NB	2.89	112.95	109.21
25	c	515	BCR	C2-C1-C6	2.89	114.94	110.48
24	A	407	PHO	C2A-C1A-NA	2.89	115.18	111.86
23	C	513	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	a	406	PHO	C2C-C1C-NC	2.89	114.15	109.79
36	h	102	DGD	O2G-C1B-C2B	2.89	117.73	111.50
23	A	406	CLA	CHD-C4C-NC	2.89	128.75	124.20
23	C	503	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	A	407	PHO	CHC-C1C-C2C	-2.88	118.48	125.73
23	B	608	CLA	C4D-C3D-CAD	-2.88	106.86	108.47
23	C	513	CLA	CHD-C4C-NC	2.88	128.75	124.20
36	c	516	DGD	C2G-O2G-C1B	-2.88	110.69	117.79
23	b	613	CLA	C4-C3-C5	2.88	120.12	115.27
33	J	101	LMG	O8-C28-C29	2.87	120.93	111.91
23	c	504	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	C	514	CLA	CHD-C4C-NC	2.87	128.73	124.20
25	c	514	BCR	C34-C9-C10	-2.87	118.90	122.92
23	C	506	CLA	CAC-C3C-C4C	2.87	128.54	124.81
31	A	417	LHG	O8-C23-C24	2.87	120.92	111.91
23	b	612	CLA	CMB-C2B-C3B	2.87	130.05	124.68
23	b	601	CLA	C3B-C4B-NB	2.87	112.92	109.21
25	t	101	BCR	C7-C6-C5	-2.87	114.52	121.46
23	C	514	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	b	615	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
23	A	406	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
23	d	403	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
31	d	409	LHG	O8-C23-O10	-2.86	116.37	123.59
25	Y	101	BCR	C16-C15-C14	-2.86	117.61	123.47
24	a	406	PHO	O2A-CGA-CBA	2.86	120.88	111.91
23	B	614	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
23	b	603	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
29	D	407	PL9	C10-C9-C11	2.86	120.08	115.27
24	A	407	PHO	C1C-C2C-C3C	-2.86	103.23	106.51
23	b	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
23	c	507	CLA	CAC-C3C-C4C	2.86	128.51	124.81
24	a	407	PHO	C2A-C1A-NA	2.86	115.14	111.86
23	B	610	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
29	d	406	PL9	C22-C23-C24	-2.85	120.79	127.66
23	C	511	CLA	CAC-C3C-C4C	2.85	128.51	124.81
29	A	414	PL9	C42-C43-C44	-2.85	120.79	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	CLA	CMB-C2B-C3B	2.85	130.01	124.68
25	c	515	BCR	C16-C17-C18	-2.85	123.24	127.31
23	b	607	CLA	C1D-CHD-C4C	-2.85	118.80	122.56
25	t	101	BCR	C7-C8-C9	-2.85	121.93	126.23
24	a	407	PHO	C4D-CHA-C1A	-2.85	118.95	125.37
23	c	508	CLA	CMB-C2B-C3B	2.85	130.01	124.68
23	c	507	CLA	C3B-C4B-NB	2.85	112.89	109.21
23	C	513	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
23	A	404	CLA	CAA-CBA-CGA	-2.85	104.93	113.25
23	C	513	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	c	506	CLA	CGD-CBD-CAD	-2.85	101.51	110.73
23	c	501	CLA	C4-C3-C5	2.85	120.06	115.27
23	C	508	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
33	j	101	LMG	C8-O7-C10	-2.84	110.79	117.79
34	b	625	HTG	O5-C5-C4	2.84	114.86	109.69
23	D	405	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
23	A	404	CLA	CMB-C2B-C3B	2.84	129.99	124.68
25	y	101	BCR	C21-C20-C19	-2.84	114.35	123.22
23	C	514	CLA	CMC-C2C-C1C	2.84	129.37	125.04
23	C	510	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	b	609	CLA	CMC-C2C-C1C	2.84	129.36	125.04
23	B	602	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
26	A	410	SQD	O9-S-C6	2.84	110.31	106.94
23	B	603	CLA	CAC-C3C-C4C	2.84	128.49	124.81
25	a	409	BCR	C15-C14-C13	-2.84	123.26	127.31
23	C	507	CLA	C1D-CHD-C4C	-2.84	118.81	122.56
23	B	605	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
23	b	601	CLA	CHD-C4C-NC	2.84	128.67	124.20
34	C	521	HTG	O5-C1-C2	2.84	113.88	110.31
25	Y	101	BCR	C38-C26-C25	-2.83	121.34	124.53
23	A	405	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
23	b	614	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
23	b	611	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
23	b	614	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
23	A	406	CLA	C3B-C4B-NB	2.83	112.87	109.21
23	B	613	CLA	O2D-CGD-CBD	2.83	116.29	111.27
31	d	408	LHG	O7-C7-C8	2.83	117.59	111.50
24	D	401	PHO	C4D-CHA-C1A	-2.83	119.01	125.37
23	b	609	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
23	b	608	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
23	A	404	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
25	y	101	BCR	C15-C14-C13	-2.82	123.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	O2A-CGA-CBA	2.82	120.75	111.91
23	C	508	CLA	C4-C3-C5	2.82	120.01	115.27
26	D	413	SQD	C3-C4-C5	2.81	115.26	110.24
23	b	615	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	b	602	CLA	O2A-CGA-CBA	2.81	120.73	111.91
23	B	604	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	b	610	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
33	C	501	LMG	C7-O1-C1	-2.81	108.26	113.74
25	a	409	BCR	C20-C21-C22	-2.80	123.31	127.31
23	c	503	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	C	505	CLA	C1-O2A-CGA	2.80	123.80	116.44
23	B	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	c	502	CLA	C1-C2-C3	-2.80	121.19	126.04
23	B	602	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	b	605	CLA	C4D-C3D-CAD	-2.80	106.91	108.47
23	c	510	CLA	CMC-C2C-C1C	2.80	129.31	125.04
25	B	617	BCR	C38-C26-C25	-2.80	121.38	124.53
23	B	603	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	b	603	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	B	616	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	B	613	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
25	b	618	BCR	C38-C26-C25	-2.80	121.39	124.53
23	C	505	CLA	OBD-CAD-C3D	-2.80	123.34	127.98
23	a	408	CLA	CMA-C3A-C2A	-2.80	102.55	113.83
29	D	407	PL9	C7-C3-C4	2.79	119.15	116.88
35	D	402	LMT	O1'-C1'-C2'	2.79	112.66	108.30
23	b	613	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
23	C	503	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
23	c	509	CLA	C1-O2A-CGA	2.79	123.77	116.44
23	B	603	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	c	509	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
25	t	101	BCR	C1-C6-C7	2.79	123.67	115.78
23	b	611	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
33	b	620	LMG	O6-C5-C4	2.79	114.76	109.69
24	a	406	PHO	C2B-C1B-NB	2.79	114.00	109.79
23	D	404	CLA	CMC-C2C-C1C	2.79	129.28	125.04
23	c	509	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	B	604	CLA	C4-C3-C5	2.78	119.95	115.27
23	c	503	CLA	C4-C3-C5	2.78	119.95	115.27
23	C	507	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	B	613	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
24	D	401	PHO	C4D-ND-C1D	-2.78	101.76	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
34	B	622	HTG	O5-C1-C2	2.78	113.81	110.31
25	B	619	BCR	C15-C14-C13	-2.78	123.34	127.31
23	B	612	CLA	C4-C3-C5	2.78	119.95	115.27
26	D	413	SQD	O47-C7-O49	-2.78	116.99	123.70
29	d	406	PL9	C51-C49-C50	2.78	120.74	114.60
25	d	405	BCR	C40-C30-C25	-2.78	105.79	110.30
23	B	612	CLA	CMC-C2C-C1C	2.77	129.26	125.04
23	b	606	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
23	b	613	CLA	CHD-C4C-NC	2.77	128.57	124.20
31	D	409	LHG	O8-C23-C24	2.77	120.61	111.91
25	B	619	BCR	C38-C26-C25	-2.77	121.42	124.53
23	C	505	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
23	b	602	CLA	CAC-C3C-C4C	2.77	128.40	124.81
23	B	605	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	A	407	PHO	C2C-C1C-NC	2.77	113.97	109.79
23	B	615	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
23	B	614	CLA	C4-C3-C5	2.77	119.92	115.27
23	c	511	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	C	502	CLA	CHD-C4C-NC	2.76	128.56	124.20
23	b	610	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
25	d	405	BCR	C16-C15-C14	-2.76	117.81	123.47
25	b	619	BCR	C24-C23-C22	-2.76	122.06	126.23
23	c	507	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
23	B	603	CLA	C4D-C3D-CAD	-2.76	106.93	108.47
23	c	511	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
33	c	519	LMG	O8-C28-C29	2.76	120.56	111.91
25	c	515	BCR	C21-C20-C19	-2.76	114.61	123.22
23	A	405	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
23	c	511	CLA	CAA-CBA-CGA	-2.76	105.20	113.25
23	A	405	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
23	B	607	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
26	D	413	SQD	C1-C2-C3	-2.75	104.26	110.00
23	b	602	CLA	C4D-C3D-CAD	-2.75	106.93	108.47
25	k	101	BCR	C3-C4-C5	-2.75	109.16	114.08
23	C	509	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	A	406	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
23	C	513	CLA	C4-C3-C5	2.75	119.90	115.27
23	B	613	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
23	c	512	CLA	C4-C3-C5	2.75	119.90	115.27
23	c	504	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
36	C	518	DGD	O1G-C1A-C2A	2.75	120.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	CMA-C3A-C2A	-2.75	102.74	113.83
23	c	507	CLA	C1-C2-C3	-2.75	121.29	126.04
34	b	628	HTG	O5-C5-C4	2.75	114.69	109.69
23	b	601	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
23	c	512	CLA	CBA-CAA-C2A	-2.75	105.76	113.86
25	C	515	BCR	C23-C24-C25	-2.75	119.49	127.20
23	C	511	CLA	CHD-C4C-NC	2.75	128.53	124.20
23	b	615	CLA	C11-C12-C13	-2.75	107.04	115.92
23	c	505	CLA	CHD-C4C-NC	2.75	128.53	124.20
23	a	408	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
25	B	617	BCR	C11-C10-C9	-2.74	123.39	127.31
23	A	404	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
34	c	522	HTG	O5-C1-C2	2.74	113.77	110.31
24	a	406	PHO	C1-C2-C3	-2.74	121.30	126.04
25	b	617	BCR	C15-C14-C13	-2.74	123.40	127.31
23	c	509	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
23	c	512	CLA	O2A-CGA-CBA	2.74	120.51	111.91
33	Z	102	LMG	O6-C5-C4	2.74	114.67	109.69
23	C	507	CLA	O2A-CGA-CBA	2.74	120.51	111.91
23	C	506	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	c	503	CLA	C1-C2-C3	-2.74	121.31	126.04
23	B	611	CLA	C2A-C1A-CHA	-2.74	119.07	123.86
23	b	602	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	c	512	CLA	CHD-C4C-NC	2.73	128.51	124.20
25	k	101	BCR	C2-C1-C6	2.73	114.69	110.48
25	D	406	BCR	C33-C5-C6	-2.73	121.46	124.53
23	a	404	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
24	A	407	PHO	CAC-C3C-C4C	2.73	128.20	125.22
25	a	409	BCR	C37-C22-C21	-2.73	119.10	122.92
23	B	610	CLA	CHD-C4C-NC	2.73	128.50	124.20
23	b	612	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
36	c	516	DGD	O3G-C3G-C2G	-2.73	104.32	110.90
23	D	404	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
23	B	607	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
23	B	608	CLA	C4-C3-C5	2.72	119.85	115.27
25	A	409	BCR	C20-C21-C22	-2.72	123.42	127.31
23	C	508	CLA	C3B-C4B-NB	2.72	112.73	109.21
23	c	512	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	a	405	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
23	b	604	CLA	CAC-C3C-C4C	2.72	128.34	124.81
23	c	501	CLA	C3B-C4B-NB	2.72	112.73	109.21
23	D	404	CLA	C4-C3-C5	2.72	119.85	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	c	502	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	b	610	CLA	C3B-C4B-NB	2.72	112.73	109.21
29	a	414	PL9	C35-C34-C36	2.72	119.84	115.27
23	A	408	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	D	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
23	B	608	CLA	C4C-C3C-C2C	-2.71	102.94	106.90
23	d	404	CLA	C3B-C4B-NB	2.71	112.72	109.21
23	B	611	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
23	c	508	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
23	C	505	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	d	403	CLA	C4-C3-C5	2.71	119.83	115.27
23	a	405	CLA	CAA-C2A-C3A	-2.71	105.35	112.78
23	C	506	CLA	O2A-CGA-CBA	2.71	120.42	111.91
23	A	408	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
23	b	613	CLA	CMB-C2B-C3B	2.71	129.75	124.68
23	b	601	CLA	CMB-C2B-C3B	2.71	129.75	124.68
23	B	613	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
24	a	406	PHO	C3C-C4C-NC	2.71	114.48	110.28
23	c	504	CLA	CHD-C4C-NC	2.71	128.47	124.20
35	B	630	LMT	O5'-C5'-C4'	2.71	115.46	109.75
23	C	508	CLA	CAC-C3C-C4C	2.71	128.32	124.81
23	b	607	CLA	C4-C3-C5	2.71	119.83	115.27
23	B	616	CLA	CHC-C1C-C2C	-2.71	119.24	126.72
36	C	519	DGD	O2G-C1B-C2B	2.71	117.33	111.50
23	c	504	CLA	CED-O2D-CGD	2.70	122.06	115.94
23	c	507	CLA	C4-C3-C5	2.70	119.82	115.27
23	b	612	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
29	A	414	PL9	C12-C13-C14	-2.70	121.16	127.66
23	c	506	CLA	CHD-C4C-NC	2.70	128.46	124.20
29	D	407	PL9	C27-C28-C29	-2.70	121.16	127.66
23	B	608	CLA	CHC-C1C-C2C	-2.70	119.26	126.72
23	c	513	CLA	O2A-CGA-CBA	2.70	120.38	111.91
23	d	404	CLA	O2A-CGA-CBA	2.70	120.37	111.91
23	C	514	CLA	C4-C3-C5	2.70	119.81	115.27
23	d	404	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	a	406	PHO	O2D-CGD-O1D	-2.70	118.56	123.84
23	C	502	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	b	602	CLA	C11-C10-C8	-2.70	107.21	115.92
23	B	612	CLA	O2A-CGA-CBA	2.70	120.37	111.91
23	c	507	CLA	C6-C7-C8	-2.70	107.21	115.92
23	c	504	CLA	O2A-CGA-CBA	2.69	120.36	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	PHO	C4D-CHA-C1A	-2.69	119.31	125.37
23	b	611	CLA	CMB-C2B-C3B	2.69	129.72	124.68
23	b	602	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
25	c	515	BCR	C33-C5-C6	-2.69	121.50	124.53
25	k	101	BCR	C20-C21-C22	-2.69	123.47	127.31
35	D	403	LMT	C4B-C3B-C2B	2.69	115.52	110.82
24	a	407	PHO	C3A-C4A-CHB	-2.69	117.18	121.83
23	b	605	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	c	506	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
23	B	607	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
23	b	613	CLA	C1-C2-C3	-2.69	121.39	126.04
23	A	406	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	C	512	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
23	B	605	CLA	C3B-C4B-NB	2.68	112.68	109.21
29	a	414	PL9	C25-C24-C26	2.68	119.78	115.27
23	B	604	CLA	O2A-CGA-CBA	2.68	120.31	111.91
23	b	603	CLA	CMC-C2C-C1C	2.68	129.12	125.04
25	C	515	BCR	C7-C8-C9	-2.68	122.19	126.23
29	D	407	PL9	C36-C37-C38	-2.67	103.10	111.88
23	C	511	CLA	C4-C3-C5	2.67	119.77	115.27
23	c	504	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	c	506	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	c	501	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	C	512	CLA	O2A-CGA-CBA	2.67	120.29	111.91
25	A	409	BCR	C8-C7-C6	-2.67	119.70	127.20
23	c	510	CLA	O2A-CGA-CBA	2.67	120.28	111.91
23	C	502	CLA	CMB-C2B-C3B	2.67	129.67	124.68
24	a	407	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
24	a	406	PHO	C4D-ND-C1D	-2.67	101.97	106.76
23	b	602	CLA	CMB-C2B-C3B	2.67	129.66	124.68
31	D	409	LHG	O8-C23-O10	-2.67	116.87	123.59
23	B	603	CLA	CBC-CAC-C3C	-2.66	105.08	112.43
33	b	620	LMG	C1-C2-C3	-2.66	104.45	110.00
23	D	405	CLA	C4-C3-C5	2.66	119.75	115.27
23	C	513	CLA	CBA-CAA-C2A	-2.66	106.00	113.86
23	b	604	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
25	b	617	BCR	C20-C21-C22	-2.66	123.51	127.31
23	c	504	CLA	C1-C2-C3	-2.66	121.44	126.04
23	c	508	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	c	508	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	C	504	CLA	O2A-CGA-CBA	2.66	120.25	111.91
34	C	521	HTG	C1-O5-C5	2.66	117.48	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	b	602	CLA	C11-C12-C13	-2.66	107.33	115.92
23	b	605	CLA	CED-O2D-CGD	2.66	121.94	115.94
29	A	414	PL9	C25-C24-C26	2.66	119.74	115.27
29	D	407	PL9	C20-C19-C21	2.66	119.74	115.27
23	B	602	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
23	b	610	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
25	d	405	BCR	C39-C30-C25	-2.65	106.00	110.30
23	B	610	CLA	CAC-C3C-C4C	2.65	128.25	124.81
24	D	401	PHO	C4-C3-C5	2.65	119.73	115.27
36	h	102	DGD	C3G-O3G-C1D	-2.65	108.56	113.74
25	a	409	BCR	C32-C1-C6	-2.65	106.00	110.30
23	A	404	CLA	CMC-C2C-C1C	2.65	129.07	125.04
23	B	609	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
25	K	102	BCR	C15-C14-C13	-2.65	123.53	127.31
23	C	504	CLA	C1-C2-C3	-2.65	121.47	126.04
23	b	608	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
24	D	401	PHO	C2B-C1B-NB	2.64	113.78	109.79
23	c	511	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
29	A	414	PL9	C35-C34-C36	2.64	119.72	115.27
23	b	614	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
23	d	403	CLA	C1D-CHD-C4C	-2.64	119.07	122.56
23	d	401	CLA	C4-C3-C5	2.64	119.72	115.27
23	B	616	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	e	101	LHG	O8-C23-C24	2.64	120.20	111.91
23	a	405	CLA	C1-C2-C3	-2.64	121.47	126.04
23	D	404	CLA	OBD-CAD-C3D	-2.64	123.60	127.98
35	D	403	LMT	O5'-C5'-C4'	2.64	115.32	109.75
29	d	406	PL9	C31-C32-C33	-2.64	103.21	111.88
31	E	101	LHG	C5-O7-C7	-2.64	111.30	117.79
23	c	503	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
25	A	409	BCR	C16-C17-C18	-2.64	123.55	127.31
25	a	409	BCR	C37-C22-C23	2.64	122.23	118.08
29	A	414	PL9	C17-C18-C19	-2.63	121.32	127.66
31	D	408	LHG	O8-C23-O10	-2.63	116.95	123.59
23	c	511	CLA	CMC-C2C-C1C	2.63	129.05	125.04
25	B	618	BCR	C37-C22-C23	2.63	122.22	118.08
23	b	603	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
25	b	619	BCR	C10-C11-C12	-2.63	115.01	123.22
23	c	508	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	d	404	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	C	505	CLA	CBC-CAC-C3C	-2.63	105.18	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	A	408	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
23	C	505	CLA	CHD-C4C-NC	2.63	128.34	124.20
29	D	407	PL9	C51-C49-C50	2.63	120.40	114.60
26	f	101	SQD	O48-C23-C24	2.63	120.15	111.91
23	C	503	CLA	CAC-C3C-C4C	2.63	128.22	124.81
33	Z	101	LMG	O8-C28-C29	2.62	120.14	111.91
23	B	607	CLA	CHD-C4C-NC	2.62	128.34	124.20
23	d	403	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	C	509	CLA	O2A-CGA-CBA	2.62	120.14	111.91
23	b	604	CLA	CHC-C1C-C2C	-2.62	119.47	126.72
25	c	515	BCR	C3-C4-C5	-2.62	109.40	114.08
23	c	507	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	A	412	SQD	O48-C23-O10	-2.62	116.98	123.59
23	b	609	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	B	609	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	b	612	CLA	CHD-C4C-NC	2.62	128.32	124.20
23	b	611	CLA	CHD-C4C-NC	2.62	128.32	124.20
25	K	102	BCR	C2-C1-C6	2.61	114.50	110.48
25	c	514	BCR	C28-C27-C26	-2.61	109.41	114.08
25	D	406	BCR	C40-C30-C25	-2.61	106.06	110.30
23	a	408	CLA	OBD-CAD-C3D	-2.61	123.64	127.98
23	b	612	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	B	604	CLA	CHD-C4C-NC	2.61	128.32	124.20
23	b	603	CLA	C4-C3-C5	2.61	119.67	115.27
25	d	405	BCR	C21-C20-C19	-2.61	115.08	123.22
23	B	608	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
25	B	619	BCR	C21-C20-C19	-2.61	115.08	123.22
23	B	614	CLA	C1-C2-C3	-2.61	121.53	126.04
23	d	404	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
23	a	404	CLA	CHB-C4A-NA	2.61	128.12	124.51
29	A	414	PL9	C53-C6-C1	2.61	120.32	114.99
23	C	505	CLA	C4D-C3D-CAD	-2.61	107.02	108.47
25	D	406	BCR	C29-C30-C25	2.60	114.49	110.48
23	B	615	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
23	C	506	CLA	C1-C2-C3	-2.60	121.54	126.04
23	b	605	CLA	O2A-CGA-CBA	2.60	120.08	111.91
23	b	609	CLA	CHD-C4C-NC	2.60	128.31	124.20
40	v	201	HEC	CBD-CAD-C3D	-2.60	107.69	112.49
29	a	414	PL9	C53-C6-C1	2.60	120.31	114.99
23	b	606	CLA	CMB-C2B-C3B	2.60	129.54	124.68
25	C	516	BCR	C15-C16-C17	-2.60	118.15	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	201	HEC	CAD-CBD-CGD	2.60	117.03	112.67
23	B	611	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	b	606	CLA	C1-C2-C3	-2.60	121.55	126.04
29	A	414	PL9	C40-C39-C41	2.60	119.64	115.27
23	C	503	CLA	C1-C2-C3	-2.60	121.55	126.04
23	B	615	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	C	506	CLA	C4-C3-C5	2.60	119.64	115.27
23	d	401	CLA	CMA-C3A-C2A	-2.60	103.36	113.83
23	B	614	CLA	C4D-C3D-CAD	-2.59	107.02	108.47
23	B	602	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
35	M	101	LMT	C1-O1'-C1'	-2.59	109.54	113.84
24	a	406	PHO	C1C-C2C-C3C	-2.59	103.53	106.51
23	b	614	CLA	CHD-C4C-NC	2.59	128.29	124.20
31	d	407	LHG	O8-C23-O10	-2.59	117.05	123.59
29	d	406	PL9	C15-C14-C16	2.59	119.63	115.27
23	b	601	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	c	511	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	b	608	CLA	O2A-CGA-CBA	2.59	120.04	111.91
23	D	405	CLA	CAC-C3C-C4C	2.59	128.17	124.81
25	b	618	BCR	C28-C27-C26	-2.59	109.45	114.08
23	b	616	CLA	C3B-C4B-NB	2.59	112.56	109.21
25	Y	101	BCR	C10-C11-C12	-2.59	115.14	123.22
23	d	401	CLA	C11-C12-C13	-2.59	107.56	115.92
23	B	604	CLA	C1-O2A-CGA	2.59	123.23	116.44
23	C	502	CLA	O2A-CGA-CBA	2.59	120.02	111.91
29	A	414	PL9	C45-C44-C46	2.58	119.62	115.27
33	b	620	LMG	C8-O7-C10	-2.58	111.43	117.79
23	b	602	CLA	C1-C2-C3	-2.58	121.57	126.04
25	D	406	BCR	C15-C14-C13	-2.58	123.62	127.31
23	b	615	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
23	A	406	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
23	c	509	CLA	CMB-C2B-C3B	2.58	129.51	124.68
23	B	606	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
25	B	617	BCR	C16-C17-C18	-2.58	123.63	127.31
25	D	406	BCR	C37-C22-C23	2.58	122.14	118.08
34	C	522	HTG	C3-C4-C5	2.58	114.84	110.24
23	C	511	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	C	507	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	d	404	CLA	CHC-C1C-C2C	-2.57	119.60	126.72
25	t	101	BCR	C3-C4-C5	-2.57	109.48	114.08
23	B	607	CLA	C4-C3-C5	2.57	119.60	115.27
23	d	404	CLA	C4D-C3D-CAD	-2.57	107.03	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C4-C3-C5	2.57	119.60	115.27
24	a	406	PHO	CBD-CHA-C1A	2.57	132.36	126.40
23	c	502	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	B	604	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
25	B	618	BCR	C28-C27-C26	-2.57	109.49	114.08
36	C	519	DGD	O1G-C1A-O1A	-2.57	117.11	123.59
36	c	516	DGD	C6D-O5D-C1E	-2.57	108.72	113.74
26	a	412	SQD	O5-C5-C4	2.56	114.35	109.69
25	b	618	BCR	C24-C23-C22	-2.56	122.36	126.23
25	b	619	BCR	C39-C30-C25	-2.56	106.14	110.30
23	c	504	CLA	OBD-CAD-C3D	-2.56	123.73	127.98
25	h	101	BCR	C37-C22-C21	-2.56	119.33	122.92
26	A	410	SQD	C45-O47-C7	-2.56	111.49	117.79
25	k	101	BCR	C7-C8-C9	-2.56	122.37	126.23
23	b	601	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	A	408	CLA	CMB-C2B-C3B	2.56	129.46	124.68
25	h	101	BCR	C10-C11-C12	-2.56	115.24	123.22
25	b	619	BCR	C2-C1-C6	2.56	114.42	110.48
36	c	517	DGD	O1G-C1A-C2A	2.56	119.93	111.91
23	b	604	CLA	CHD-C4C-NC	2.56	128.23	124.20
24	a	407	PHO	C4D-ND-C1D	-2.55	102.17	106.76
23	C	504	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	D	401	PHO	CMC-C2C-C1C	2.55	128.99	125.06
24	A	407	PHO	C6-C5-C3	-2.55	106.76	113.45
23	b	608	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
23	b	607	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
23	b	601	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
23	B	612	CLA	CMB-C2B-C3B	2.54	129.44	124.68
23	B	606	CLA	O2A-CGA-CBA	2.54	119.89	111.91
26	D	413	SQD	O8-S-C6	2.54	109.79	105.74
24	a	407	PHO	CAC-C3C-C4C	2.54	127.99	125.22
23	c	506	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
23	C	507	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	c	509	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
24	A	407	PHO	O2D-CGD-O1D	-2.54	118.87	123.84
36	C	518	DGD	O1G-C1A-O1A	-2.54	117.18	123.59
25	b	618	BCR	C29-C30-C25	2.54	114.39	110.48
23	A	405	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	a	404	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
25	b	619	BCR	C4-C5-C6	-2.54	119.05	122.73
23	d	403	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
23	c	501	CLA	OBD-CAD-C3D	-2.54	123.77	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	416	LMG	O6-C5-C4	2.53	114.29	109.69
24	a	406	PHO	CHD-C1D-C2D	-2.53	119.36	125.73
25	B	617	BCR	C31-C1-C6	-2.53	106.20	110.30
25	B	618	BCR	C36-C18-C19	2.53	122.06	118.08
23	b	606	CLA	CAC-C3C-C4C	2.53	128.09	124.81
23	a	408	CLA	CMC-C2C-C1C	2.53	128.89	125.04
23	B	612	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
23	C	506	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
33	C	501	LMG	C9-C8-C7	-2.52	105.82	111.79
26	D	413	SQD	O48-C23-C24	2.52	119.83	111.91
23	b	614	CLA	CMB-C2B-C3B	2.52	129.40	124.68
23	b	610	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	b	613	CLA	CMC-C2C-C1C	2.52	128.88	125.04
25	C	516	BCR	C38-C26-C25	-2.52	121.70	124.53
23	C	506	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
23	C	508	CLA	O2A-CGA-CBA	2.52	119.81	111.91
23	c	513	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	b	604	CLA	C4-C3-C5	2.52	119.51	115.27
23	C	507	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
23	b	611	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
23	c	505	CLA	C1-C2-C3	-2.51	121.70	126.04
23	a	404	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
25	Y	101	BCR	C37-C22-C23	2.51	122.04	118.08
23	C	510	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	B	601	CLA	CAC-C3C-C4C	2.51	128.07	124.81
23	b	616	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
23	C	508	CLA	C1-C2-C3	-2.51	121.70	126.04
23	B	611	CLA	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407	PHO	O2A-CGA-CBA	2.51	119.78	111.91
31	d	407	LHG	O8-C23-C24	2.51	119.78	111.91
25	y	101	BCR	C24-C23-C22	-2.51	122.44	126.23
23	c	513	CLA	CHD-C4C-NC	2.51	128.15	124.20
25	T	101	BCR	C7-C6-C5	-2.51	115.39	121.46
23	B	607	CLA	CMC-C2C-C1C	2.51	128.85	125.04
25	y	101	BCR	C37-C22-C23	2.50	122.02	118.08
23	b	602	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
23	C	508	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
23	b	615	CLA	CAC-C3C-C4C	2.50	128.05	124.81
25	a	409	BCR	C15-C16-C17	-2.50	118.35	123.47
26	a	410	SQD	O48-C23-C24	2.50	119.75	111.91
25	K	102	BCR	C36-C18-C19	2.50	122.01	118.08
25	c	514	BCR	C33-C5-C6	-2.50	121.72	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	b	603	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
23	A	405	CLA	CAA-CBA-CGA	2.50	120.55	113.25
23	c	510	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
25	K	102	BCR	C33-C5-C6	-2.50	121.72	124.53
35	D	403	LMT	C1-O1'-C1'	-2.50	109.70	113.84
23	B	613	CLA	CHD-C4C-NC	2.50	128.14	124.20
25	d	405	BCR	C38-C26-C25	-2.49	121.73	124.53
24	A	407	PHO	CHD-C1D-C2D	-2.49	119.46	125.73
23	B	610	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	B	602	CLA	CED-O2D-CGD	2.49	121.57	115.94
23	b	611	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	C	510	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	C	511	CLA	CMC-C2C-C1C	2.49	128.83	125.04
23	B	610	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
23	B	613	CLA	CED-O2D-CGD	2.49	121.57	115.94
29	D	407	PL9	C37-C38-C39	-2.49	121.67	127.66
23	c	508	CLA	C4-C3-C5	2.49	119.45	115.27
23	B	615	CLA	CAC-C3C-C4C	2.49	128.04	124.81
23	B	603	CLA	CHD-C4C-NC	2.49	128.12	124.20
23	C	510	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
23	C	513	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
35	b	627	LMT	C1'-C2'-C3'	2.48	115.17	110.00
23	c	505	CLA	CED-O2D-CGD	2.48	121.55	115.94
29	d	406	PL9	C37-C38-C39	-2.48	121.69	127.66
23	C	514	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
23	b	602	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
26	A	410	SQD	O48-C23-O10	-2.48	117.34	123.59
25	A	409	BCR	C36-C18-C19	2.47	121.98	118.08
25	C	515	BCR	C11-C10-C9	-2.47	123.78	127.31
33	J	101	LMG	O8-C28-O10	-2.47	117.35	123.59
25	C	515	BCR	C20-C21-C22	-2.47	123.78	127.31
25	h	101	BCR	C16-C15-C14	-2.47	118.41	123.47
23	c	506	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
23	c	503	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
23	C	511	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
33	Z	102	LMG	C9-C8-C7	-2.47	105.95	111.79
23	B	608	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	c	508	CLA	C1-C2-C3	-2.47	121.77	126.04
23	c	501	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
29	d	406	PL9	C17-C18-C19	-2.47	121.72	127.66
23	D	405	CLA	CHC-C1C-C2C	-2.47	119.89	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	b	616	CLA	C1-C2-C3	-2.47	121.78	126.04
23	a	404	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
25	y	101	BCR	C10-C11-C12	-2.46	115.53	123.22
23	C	505	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
36	C	518	DGD	C2G-O2G-C1B	-2.46	111.73	117.79
29	D	407	PL9	C15-C14-C16	2.46	119.41	115.27
23	C	513	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
23	B	606	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	H	101	BCR	C29-C30-C25	2.46	114.27	110.48
23	C	512	CLA	CMB-C2B-C3B	2.46	129.28	124.68
33	c	520	LMG	O8-C28-O10	-2.46	117.39	123.59
33	Z	102	LMG	C1-O6-C5	2.46	118.51	113.69
23	b	616	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
29	d	406	PL9	C12-C13-C14	-2.46	121.75	127.66
23	b	608	CLA	CBC-CAC-C3C	-2.45	105.66	112.43
23	b	604	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
23	B	606	CLA	CAA-C2A-C3A	-2.45	106.07	112.78
29	d	406	PL9	C53-C6-C1	2.45	120.00	114.99
23	d	401	CLA	C1-O2A-CGA	2.45	122.87	116.44
23	B	601	CLA	C4-C3-C5	2.45	119.39	115.27
23	C	502	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
23	c	503	CLA	CAC-C3C-C4C	2.45	127.99	124.81
23	C	502	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
36	H	102	DGD	O1G-C1A-C2A	2.44	119.58	111.91
23	c	510	CLA	C4-C3-C2	-2.44	117.41	123.68
25	B	618	BCR	C36-C18-C17	-2.44	119.50	122.92
23	b	610	CLA	CHD-C4C-NC	2.44	128.05	124.20
24	A	407	PHO	C3C-C4C-NC	2.44	114.06	110.28
23	A	405	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
23	a	408	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	C	516	BCR	C3-C4-C5	-2.44	109.72	114.08
23	c	505	CLA	C4-C3-C5	2.44	119.37	115.27
23	B	608	CLA	CMC-C2C-C1C	2.43	128.75	125.04
23	A	405	CLA	CMB-C2B-C3B	2.43	129.23	124.68
23	c	501	CLA	CHD-C4C-NC	2.43	128.04	124.20
25	B	619	BCR	C7-C8-C9	-2.43	122.56	126.23
23	A	405	CLA	CMA-C3A-C2A	-2.43	104.01	113.83
23	a	408	CLA	C4-C3-C5	2.43	119.36	115.27
24	D	401	PHO	O2D-CGD-O1D	-2.43	119.08	123.84
31	d	408	LHG	O8-C23-C24	2.43	119.54	111.91
23	B	602	CLA	O2A-CGA-CBA	2.43	119.54	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
23	b	611	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	b	612	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
25	b	618	BCR	C37-C22-C21	-2.43	119.52	122.92
23	C	509	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	c	508	CLA	CHD-C4C-NC	2.43	128.03	124.20
25	b	617	BCR	C37-C22-C21	-2.43	119.52	122.92
23	b	606	CLA	CMC-C2C-C1C	2.43	128.73	125.04
25	b	617	BCR	C32-C1-C6	-2.43	106.36	110.30
23	C	502	CLA	C4-C3-C5	2.42	119.35	115.27
36	c	516	DGD	C3G-C2G-C1G	-2.42	106.06	111.79
23	b	616	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
23	a	405	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
23	A	404	CLA	CED-O2D-CGD	2.42	121.42	115.94
23	B	615	CLA	C4-C3-C5	2.42	119.34	115.27
25	t	101	BCR	C37-C22-C21	-2.42	119.53	122.92
23	A	408	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	B	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
33	Z	102	LMG	O6-C1-C2	2.42	115.47	110.35
26	L	101	SQD	O8-S-C6	2.42	109.59	105.74
29	D	407	PL9	C42-C41-C39	-2.42	105.02	112.98
23	C	504	CLA	CHD-C4C-NC	2.42	128.01	124.20
23	a	404	CLA	CHD-C4C-NC	2.42	128.01	124.20
23	b	606	CLA	O2A-CGA-CBA	2.42	119.49	111.91
23	c	504	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
25	d	405	BCR	C38-C26-C27	2.41	118.25	113.62
23	B	601	CLA	CMB-C2B-C3B	2.41	129.19	124.68
23	c	502	CLA	CAC-C3C-C4C	2.41	127.94	124.81
23	c	509	CLA	CMC-C2C-C1C	2.41	128.72	125.04
23	b	609	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
25	c	515	BCR	C37-C22-C23	2.41	121.88	118.08
23	B	605	CLA	CHC-C1C-C2C	-2.41	120.05	126.72
29	a	414	PL9	C7-C8-C9	-2.41	122.78	126.79
26	f	101	SQD	O5-C5-C4	2.41	114.07	109.69
23	B	602	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
23	b	606	CLA	CAA-C2A-C3A	-2.41	106.18	112.78
23	B	616	CLA	CAC-C3C-C4C	2.41	127.94	124.81
24	D	401	PHO	CBD-CHA-C1A	2.41	131.99	126.40
23	A	405	CLA	C4C-C3C-C2C	-2.41	103.39	106.90
23	C	508	CLA	CHD-C4C-NC	2.41	128.00	124.20
23	b	601	CLA	CAC-C3C-C4C	2.41	127.93	124.81
23	C	503	CLA	CMC-C2C-C1C	2.41	128.70	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	CHD-C4C-NC	2.40	127.99	124.20
29	a	414	PL9	C51-C49-C50	2.40	119.91	114.60
23	B	612	CLA	C11-C12-C13	-2.40	108.15	115.92
33	j	101	LMG	O8-C28-C29	2.40	119.45	111.91
23	c	504	CLA	CMB-C2B-C3B	2.40	129.17	124.68
23	B	616	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	B	610	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
23	b	612	CLA	CMC-C2C-C1C	2.40	128.69	125.04
33	C	520	LMG	O8-C28-O10	-2.40	117.54	123.59
23	C	513	CLA	CMB-C2B-C3B	2.40	129.17	124.68
23	b	616	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
23	D	404	CLA	C1D-CHD-C4C	-2.40	119.39	122.56
33	b	620	LMG	O8-C28-O10	-2.40	117.54	123.59
23	B	610	CLA	C4-C3-C5	2.40	119.30	115.27
23	d	403	CLA	CAC-C3C-C4C	2.39	127.92	124.81
23	c	506	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
24	a	407	PHO	CBD-CHA-C1A	2.39	131.95	126.40
23	B	601	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
35	D	403	LMT	O1B-C4'-C5'	-2.39	102.90	109.45
23	d	403	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
25	C	516	BCR	C16-C17-C18	-2.39	123.90	127.31
26	a	410	SQD	O48-C23-O10	-2.39	117.56	123.59
23	C	514	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
25	y	101	BCR	C28-C27-C26	-2.39	109.81	114.08
25	a	409	BCR	C8-C7-C6	-2.39	120.50	127.20
26	L	101	SQD	C1-C2-C3	-2.38	105.03	110.00
23	A	405	CLA	C3B-C4B-NB	2.38	112.29	109.21
40	V	202	HEC	CBD-CAD-C3D	-2.38	108.09	112.49
23	B	605	CLA	C4-C3-C5	2.38	119.28	115.27
23	c	502	CLA	CMC-C2C-C1C	2.38	128.66	125.04
23	B	616	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
23	c	505	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
23	B	613	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
33	B	621	LMG	C7-O1-C1	-2.38	109.10	113.74
23	B	610	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	c	510	CLA	CAC-C3C-C4C	2.38	127.89	124.81
23	C	507	CLA	CGD-CBD-CAD	-2.37	103.04	110.73
23	B	611	CLA	CMB-C2B-C3B	2.37	129.12	124.68
23	B	611	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	B	616	CLA	C4-C3-C5	2.37	119.26	115.27
34	V	203	HTG	C1-C2-C3	2.37	112.58	109.67
29	A	414	PL9	C51-C49-C50	2.37	119.83	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C38-C26-C25	-2.37	121.87	124.53
23	c	508	CLA	CMC-C2C-C1C	2.37	128.64	125.04
36	c	518	DGD	O3G-C3G-C2G	-2.36	105.20	110.90
23	b	610	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
36	C	517	DGD	C4E-C3E-C2E	-2.36	106.70	110.82
23	b	605	CLA	CAC-C3C-C4C	2.36	127.88	124.81
23	c	507	CLA	CMC-C2C-C1C	2.36	128.64	125.04
23	D	404	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
23	c	513	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
23	B	608	CLA	CMB-C2B-C3B	2.36	129.09	124.68
23	b	601	CLA	CMC-C2C-C1C	2.36	128.63	125.04
25	T	101	BCR	C35-C13-C12	2.36	121.80	118.08
23	c	504	CLA	C4-C3-C5	2.36	119.24	115.27
23	d	403	CLA	CMB-C2B-C3B	2.36	129.09	124.68
26	f	101	SQD	C4-C3-C2	-2.36	106.71	110.82
35	b	627	LMT	O5'-C1'-C2'	2.36	115.34	110.35
23	C	507	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
25	T	101	BCR	C1-C6-C7	2.35	122.44	115.78
23	B	606	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
25	a	409	BCR	C33-C5-C6	-2.35	121.89	124.53
23	d	403	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
23	c	505	CLA	O2A-CGA-CBA	2.35	119.27	111.91
23	B	610	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
25	c	515	BCR	C32-C1-C6	-2.34	106.50	110.30
23	C	508	CLA	C6-C7-C8	-2.34	108.35	115.92
23	a	408	CLA	CMA-C3A-C4A	-2.34	105.48	111.77
24	A	407	PHO	C4-C3-C5	2.34	119.21	115.27
23	B	614	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
23	d	403	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
23	C	505	CLA	C4-C3-C5	2.34	119.21	115.27
25	H	101	BCR	C2-C1-C6	2.34	114.08	110.48
23	c	513	CLA	CHC-C1C-C2C	-2.33	120.26	126.72
23	C	507	CLA	C4C-C3C-C2C	-2.33	103.49	106.90
23	b	601	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	C	514	CLA	O2A-CGA-CBA	2.33	119.23	111.91
23	C	504	CLA	CMB-C2B-C3B	2.33	129.04	124.68
23	C	505	CLA	C1-C2-C3	-2.33	122.01	126.04
23	A	406	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
23	b	614	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
23	C	512	CLA	C11-C10-C8	-2.33	108.39	115.92
23	d	404	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
23	b	602	CLA	O2A-CGA-O1A	-2.33	117.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
23	B	608	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	k	101	BCR	C10-C11-C12	-2.33	115.96	123.22
25	t	101	BCR	C20-C21-C22	-2.32	123.99	127.31
23	a	404	CLA	CMC-C2C-C1C	2.32	128.58	125.04
23	A	404	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	b	613	CLA	C4D-C3D-CAD	-2.32	107.17	108.47
26	f	101	SQD	O47-C7-O49	-2.32	118.09	123.70
23	b	608	CLA	C4D-C3D-CAD	-2.32	107.18	108.47
23	c	506	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
23	B	611	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
23	a	404	CLA	CAC-C3C-C4C	2.32	127.81	124.81
23	d	404	CLA	C4-C3-C5	2.31	119.16	115.27
25	B	618	BCR	C10-C11-C12	-2.31	116.00	123.22
33	j	101	LMG	O7-C10-O9	-2.31	118.11	123.70
23	C	511	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
23	A	404	CLA	OBD-CAD-C3D	-2.31	124.14	127.98
23	C	513	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
23	b	616	CLA	CMC-C2C-C1C	2.31	128.56	125.04
26	D	413	SQD	C46-C45-C44	-2.31	106.33	111.79
23	A	405	CLA	C4-C3-C5	2.31	119.15	115.27
23	D	405	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
29	D	407	PL9	C7-C3-C2	-2.31	120.27	123.30
23	C	505	CLA	CAC-C3C-C4C	2.31	127.80	124.81
36	H	102	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
23	B	609	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	b	602	CLA	C4-C3-C5	2.30	119.15	115.27
23	b	601	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
25	y	101	BCR	C40-C30-C25	-2.30	106.56	110.30
36	c	518	DGD	O2G-C1B-C2B	2.30	116.46	111.50
36	h	102	DGD	O1G-C1A-O1A	-2.30	117.78	123.59
25	c	515	BCR	C11-C10-C9	-2.30	124.03	127.31
25	T	101	BCR	C2-C1-C6	2.30	114.02	110.48
36	c	518	DGD	O5D-C6D-C5D	-2.30	104.80	109.05
25	c	514	BCR	C2-C1-C6	2.30	114.02	110.48
23	A	406	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	b	606	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
23	d	404	CLA	C1-C2-C3	-2.30	122.07	126.04
23	C	503	CLA	C4-C3-C5	2.30	119.13	115.27
23	c	510	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
33	z	101	LMG	C8-O7-C10	-2.30	112.14	117.79
23	a	405	CLA	C4-C3-C5	2.30	119.13	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	522	HTG	O5-C1-C2	2.29	113.20	110.31
23	c	505	CLA	C1-O2A-CGA	2.29	122.46	116.44
23	b	606	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
25	a	409	BCR	C38-C26-C25	-2.29	121.96	124.53
23	C	513	CLA	C1-C2-C3	-2.29	122.08	126.04
33	a	416	LMG	O8-C28-C29	2.29	119.09	111.91
23	a	405	CLA	C1-O2A-CGA	2.29	122.45	116.44
23	b	602	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
25	B	619	BCR	C2-C3-C4	-2.29	106.27	111.38
23	A	408	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
23	C	513	CLA	CHB-C4A-NA	2.29	127.67	124.51
23	C	503	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
26	a	410	SQD	C3-C4-C5	2.29	114.32	110.24
25	b	617	BCR	C24-C23-C22	-2.28	122.78	126.23
33	b	620	LMG	C4-C3-C2	-2.28	106.84	110.82
23	B	607	CLA	CAA-CBA-CGA	2.28	119.92	113.25
23	D	404	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
23	B	614	CLA	CMC-C2C-C1C	2.28	128.51	125.04
25	c	515	BCR	C35-C13-C14	-2.28	119.73	122.92
25	H	101	BCR	C2-C3-C4	-2.28	106.28	111.38
31	A	416	LHG	C5-O7-C7	-2.28	112.17	117.79
23	c	512	CLA	C1-O2A-CGA	2.28	122.43	116.44
31	d	408	LHG	O8-C23-O10	-2.28	117.84	123.59
23	A	404	CLA	C4-C3-C5	2.28	119.11	115.27
24	D	401	PHO	O1D-CGD-CBD	-2.28	119.82	124.48
25	k	101	BCR	C39-C30-C25	-2.28	106.60	110.30
23	d	404	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
33	j	101	LMG	O8-C28-O10	-2.28	117.84	123.59
23	B	605	CLA	CAC-C3C-C4C	2.28	127.76	124.81
25	Y	101	BCR	C40-C30-C25	-2.28	106.61	110.30
23	b	608	CLA	C4-C3-C5	2.28	119.10	115.27
23	c	508	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
23	b	606	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
34	b	628	HTG	O5-C1-C2	2.27	113.17	110.31
23	D	404	CLA	CMB-C2B-C3B	2.27	128.93	124.68
23	c	507	CLA	O2A-CGA-CBA	2.27	119.04	111.91
38	E	103	HEM	C3C-C4C-NC	-2.27	106.66	110.94
29	d	406	PL9	C30-C29-C31	2.27	119.09	115.27
23	c	509	CLA	C4-C3-C5	2.27	119.09	115.27
26	L	101	SQD	O47-C7-O49	-2.27	118.22	123.70
23	c	503	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
36	C	517	DGD	O1G-C1A-O1A	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
25	T	101	BCR	C16-C15-C14	2.27	128.12	123.47
33	Z	101	LMG	C4-C3-C2	2.27	114.78	110.82
36	c	518	DGD	O1G-C1A-C2A	2.27	119.02	111.91
23	C	512	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
23	a	405	CLA	CMB-C2B-C3B	2.27	128.92	124.68
23	b	613	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	A	407	PHO	CBD-CHA-C1A	2.26	131.65	126.40
23	C	513	CLA	CMC-C2C-C1C	2.26	128.48	125.04
23	b	614	CLA	OBD-CAD-C3D	-2.26	124.23	127.98
23	c	510	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
23	C	511	CLA	CMB-C2B-C3B	2.26	128.91	124.68
23	C	509	CLA	OBD-CAD-C3D	-2.26	124.23	127.98
23	B	607	CLA	OBD-CAD-C3D	-2.26	124.23	127.98
23	a	405	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	C	508	CLA	CMC-C2C-C1C	2.25	128.47	125.04
25	t	101	BCR	C16-C15-C14	-2.25	118.86	123.47
25	B	617	BCR	C28-C27-C26	-2.25	110.05	114.08
23	B	613	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
23	C	514	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
23	a	404	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
23	A	404	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
23	D	405	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	B	612	CLA	CHD-C4C-NC	2.25	127.75	124.20
23	B	612	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	b	615	CLA	O2A-CGA-CBA	2.25	118.96	111.91
23	A	405	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	B	609	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	b	610	CLA	C4-C3-C2	-2.25	117.91	123.68
25	c	515	BCR	C20-C21-C22	-2.25	124.10	127.31
25	y	101	BCR	C11-C10-C9	-2.25	124.10	127.31
23	B	612	CLA	OBD-CAD-C3D	-2.25	124.25	127.98
29	D	407	PL9	C25-C24-C26	2.25	119.05	115.27
23	d	404	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
23	c	501	CLA	CMC-C2C-C1C	2.24	128.46	125.04
29	a	414	PL9	C40-C39-C41	2.24	119.04	115.27
23	A	408	CLA	O2A-CGA-CBA	2.24	118.95	111.91
23	C	502	CLA	C3D-CAD-CBD	2.24	110.56	107.61
23	D	405	CLA	O2A-CGA-CBA	2.24	118.94	111.91
25	t	101	BCR	C29-C28-C27	-2.24	106.37	111.38
25	D	406	BCR	C21-C20-C19	-2.24	116.23	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	B	611	CLA	CAC-C3C-C4C	2.24	127.71	124.81
25	C	516	BCR	C21-C20-C19	-2.24	116.24	123.22
23	C	503	CLA	C2A-C1A-CHA	-2.23	119.95	123.86
23	B	616	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
23	b	615	CLA	C4D-C3D-CAD	-2.23	107.22	108.47
36	C	517	DGD	O3G-C3G-C2G	-2.23	105.51	110.90
34	B	622	HTG	O2-C2-C3	-2.23	105.19	110.35
23	C	513	CLA	CAC-C3C-C4C	2.23	127.70	124.81
23	b	616	CLA	C11-C12-C13	-2.23	108.71	115.92
23	C	502	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
35	D	403	LMT	C1B-O5B-C5B	-2.23	109.31	113.69
25	c	515	BCR	C37-C22-C21	-2.23	119.80	122.92
23	b	608	CLA	CAC-C3C-C4C	2.23	127.70	124.81
24	a	406	PHO	CBA-CAA-C2A	-2.23	107.28	113.86
23	C	506	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
25	H	101	BCR	C7-C6-C5	2.23	126.86	121.46
23	B	609	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
23	c	504	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	B	609	CLA	CED-O2D-CGD	2.23	120.97	115.94
25	c	515	BCR	C15-C16-C17	-2.23	118.91	123.47
23	b	614	CLA	C4-C3-C5	2.23	119.01	115.27
23	A	408	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
23	b	609	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
23	C	512	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	D	401	PHO	CBA-CAA-C2A	-2.22	107.30	113.86
26	A	410	SQD	O47-C7-O49	-2.22	118.34	123.70
23	B	615	CLA	O2A-CGA-CBA	2.22	118.87	111.91
29	a	414	PL9	C45-C44-C46	2.22	119.00	115.27
23	B	602	CLA	C1-C2-C3	-2.22	122.21	126.04
23	B	605	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	c	501	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
23	a	405	CLA	O2A-CGA-CBA	2.21	118.86	111.91
25	B	619	BCR	C10-C11-C12	-2.21	116.31	123.22
23	b	607	CLA	CHD-C4C-NC	2.21	127.69	124.20
31	D	408	LHG	O8-C23-C24	2.21	118.85	111.91
25	c	515	BCR	C40-C30-C25	-2.21	106.71	110.30
25	y	101	BCR	C16-C15-C14	-2.21	118.95	123.47
23	d	401	CLA	CAA-CBA-CGA	2.21	119.71	113.25
25	c	514	BCR	C37-C22-C21	-2.21	119.83	122.92
25	b	619	BCR	C37-C22-C23	2.21	121.56	118.08
23	b	601	CLA	CAA-C2A-C3A	-2.21	106.73	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	519	DGD	O6D-C1D-O3G	-2.21	104.75	109.97
23	B	611	CLA	CED-O2D-CGD	2.20	120.92	115.94
23	c	510	CLA	CMB-C2B-C3B	2.20	128.80	124.68
33	C	501	LMG	O8-C28-C29	2.20	118.82	111.91
31	d	407	LHG	O7-C7-O9	-2.20	118.38	123.70
23	b	611	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
23	B	602	CLA	C1-O2A-CGA	2.20	122.22	116.44
23	b	606	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
23	b	616	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
23	c	510	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	C	508	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	a	405	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	b	606	CLA	C1-O2A-CGA	2.20	122.21	116.44
25	b	618	BCR	C20-C21-C22	-2.20	124.17	127.31
35	B	631	LMT	O1'-C1'-C2'	2.20	111.73	108.30
24	a	407	PHO	CBA-CAA-C2A	-2.20	107.38	113.86
40	v	201	HEC	CMB-C2B-C1B	-2.20	125.09	128.46
25	H	101	BCR	C31-C1-C6	-2.19	106.74	110.30
23	b	609	CLA	C7-C6-C5	-2.19	107.40	113.36
23	B	604	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
23	C	504	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	c	513	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	B	610	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
25	H	101	BCR	C36-C18-C17	-2.19	119.86	122.92
23	B	604	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
31	E	101	LHG	O8-C23-O10	-2.19	118.07	123.59
23	c	505	CLA	C2A-C1A-CHA	-2.19	120.04	123.86
23	b	616	CLA	OBD-CAD-C3D	-2.19	124.35	127.98
25	A	409	BCR	C31-C1-C6	-2.18	106.75	110.30
23	B	606	CLA	CMC-C2C-C1C	2.18	128.37	125.04
29	d	406	PL9	C45-C44-C46	2.18	118.94	115.27
23	c	507	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	C	507	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
23	c	506	CLA	CHB-C4A-NA	2.18	127.53	124.51
24	A	407	PHO	CED-O2D-CGD	2.18	120.86	115.94
23	c	510	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
29	D	407	PL9	C45-C44-C46	2.18	118.93	115.27
23	b	607	CLA	CMC-C2C-C1C	2.18	128.35	125.04
23	c	512	CLA	CMA-C3A-C4A	-2.18	105.92	111.77
25	H	101	BCR	C16-C15-C14	-2.18	119.02	123.47
23	B	613	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
23	A	406	CLA	CBC-CAC-C3C	-2.18	106.43	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	O2A-CGA-CBA	2.18	118.73	111.91
23	d	404	CLA	C1-O2A-CGA	2.18	122.15	116.44
36	H	102	DGD	C3G-O3G-C1D	-2.17	109.49	113.74
23	c	512	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
23	C	503	CLA	O2A-CGA-CBA	2.17	118.73	111.91
23	b	605	CLA	C1-C2-C3	-2.17	122.29	126.04
23	B	615	CLA	CMB-C2B-C1B	2.17	131.80	128.46
23	c	510	CLA	OBD-CAD-C3D	-2.17	124.38	127.98
23	c	511	CLA	CMB-C2B-C3B	2.17	128.74	124.68
25	k	101	BCR	C36-C18-C19	2.17	121.49	118.08
25	C	516	BCR	C34-C9-C10	-2.17	119.89	122.92
23	d	401	CLA	CHB-C4A-NA	2.17	127.51	124.51
29	A	414	PL9	C47-C48-C49	-2.17	120.34	127.75
33	z	101	LMG	C7-O1-C1	-2.17	109.51	113.74
23	a	405	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
31	D	409	LHG	O7-C7-O9	-2.17	118.47	123.70
25	b	619	BCR	C21-C20-C19	-2.17	116.46	123.22
23	B	603	CLA	C2A-C1A-CHA	-2.16	120.07	123.86
23	C	509	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
23	a	404	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
23	C	510	CLA	C11-C12-C13	-2.16	108.93	115.92
25	T	101	BCR	C37-C22-C23	2.16	121.48	118.08
29	D	407	PL9	C17-C18-C19	-2.16	122.46	127.66
25	c	514	BCR	C3-C4-C5	-2.16	110.22	114.08
24	A	407	PHO	O2A-CGA-O1A	-2.16	118.14	123.59
23	c	504	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
23	B	607	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	B	602	CLA	CMB-C2B-C3B	2.16	128.71	124.68
25	Y	101	BCR	C36-C18-C19	2.15	121.47	118.08
23	a	405	CLA	CHB-C4A-NA	2.15	127.49	124.51
35	b	627	LMT	C3'-C4'-C5'	-2.15	105.99	110.93
23	A	406	CLA	C4-C3-C5	2.15	118.89	115.27
25	B	618	BCR	C16-C17-C18	-2.15	124.24	127.31
23	B	602	CLA	C11-C12-C13	-2.15	108.98	115.92
24	a	406	PHO	CMB-C2B-C1B	2.15	128.37	125.06
23	B	606	CLA	CMB-C2B-C3B	2.14	128.69	124.68
23	C	513	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
34	B	624	HTG	C1-C2-C3	2.14	114.82	110.59
23	c	509	CLA	CHD-C4C-NC	2.14	127.58	124.20
26	A	412	SQD	O9-S-C6	2.14	109.48	106.94
35	m	102	LMT	C1B-O5B-C5B	2.14	117.89	113.69
23	B	601	CLA	CHB-C4A-NA	2.14	127.47	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	h	101	BCR	C20-C21-C22	-2.14	124.26	127.31
23	C	510	CLA	C4-C3-C5	2.14	118.86	115.27
23	b	610	CLA	C11-C12-C13	-2.14	109.02	115.92
23	C	510	CLA	C1-O2A-CGA	2.13	122.05	116.44
23	B	615	CLA	C1-O2A-CGA	2.13	122.04	116.44
23	d	401	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
35	D	403	LMT	C3B-C4B-C5B	2.13	114.05	110.24
25	C	515	BCR	C11-C12-C13	-2.13	120.42	126.42
29	d	406	PL9	C27-C28-C29	-2.13	122.53	127.66
23	B	605	CLA	CMB-C2B-C1B	2.13	131.74	128.46
23	c	502	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	B	603	CLA	C5-C3-C2	-2.13	116.81	121.12
25	a	409	BCR	C28-C27-C26	-2.13	110.28	114.08
23	a	408	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	A	407	PHO	CMB-C2B-C1B	2.13	128.34	125.06
23	b	615	CLA	OBD-CAD-C3D	-2.13	124.45	127.98
23	B	613	CLA	OBD-CAD-C3D	-2.12	124.45	127.98
23	D	404	CLA	C4-C3-C2	-2.12	118.23	123.68
29	D	407	PL9	C30-C29-C31	2.12	118.84	115.27
23	B	608	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
25	c	515	BCR	C35-C13-C12	2.12	121.42	118.08
23	b	603	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
25	t	101	BCR	C33-C5-C4	2.12	117.69	113.62
35	I	101	LMT	O1'-C1'-C2'	2.12	111.61	108.30
23	c	507	CLA	OBD-CAD-C3D	-2.12	124.47	127.98
23	c	502	CLA	CHB-C4A-NA	2.12	127.44	124.51
26	A	410	SQD	O8-S-C6	2.12	109.11	105.74
23	A	406	CLA	CMA-C3A-C4A	-2.11	106.09	111.77
23	C	507	CLA	CMB-C2B-C3B	2.11	128.63	124.68
35	M	103	LMT	O5'-C5'-C4'	2.11	114.21	109.75
23	A	404	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	c	506	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
24	D	401	PHO	C1-O2A-CGA	2.11	121.98	116.44
23	a	405	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	b	608	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
36	c	517	DGD	O5D-C1E-C2E	2.11	111.60	108.30
25	b	618	BCR	C15-C16-C17	-2.11	119.15	123.47
26	D	413	SQD	O5-C1-C2	-2.11	105.88	110.35
23	A	404	CLA	CMA-C3A-C2A	-2.11	105.32	113.83
24	a	406	PHO	O2A-CGA-O1A	-2.11	118.27	123.59
26	B	620	SQD	O48-C46-C45	2.11	114.57	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
34	b	622	HTG	C1-O5-C5	2.11	116.47	112.58
23	C	512	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
24	D	401	PHO	C3C-C4C-NC	2.11	113.55	110.28
25	h	101	BCR	C37-C22-C23	2.11	121.39	118.08
33	c	520	LMG	C9-C8-C7	-2.11	106.81	111.79
31	l	101	LHG	O8-C23-O10	-2.10	118.28	123.59
26	A	412	SQD	C46-C45-C44	-2.10	106.81	111.79
31	d	407	LHG	C5-O7-C7	-2.10	112.61	117.79
35	D	402	LMT	O5B-C5B-C4B	2.10	113.51	109.69
23	B	614	CLA	CHC-C1C-NC	2.10	127.39	124.20
25	K	102	BCR	C11-C10-C9	-2.10	124.31	127.31
23	d	403	CLA	CHD-C4C-NC	2.10	127.52	124.20
33	J	101	LMG	O7-C10-O9	-2.10	118.63	123.70
25	B	617	BCR	C36-C18-C17	-2.10	119.98	122.92
24	a	406	PHO	C2A-C1A-NA	2.10	114.27	111.86
23	C	508	CLA	CMB-C2B-C1B	2.10	131.69	128.46
23	b	613	CLA	CAC-C3C-C4C	2.10	127.53	124.81
25	B	617	BCR	C33-C5-C4	2.10	117.64	113.62
23	A	405	CLA	C1-C2-C3	-2.10	122.42	126.04
23	b	607	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
25	k	101	BCR	C34-C9-C8	2.10	121.38	118.08
23	C	508	CLA	OBD-CAD-C3D	-2.09	124.50	127.98
25	t	101	BCR	C28-C27-C26	-2.09	110.34	114.08
33	c	519	LMG	O8-C28-O10	-2.09	118.31	123.59
23	B	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	C	510	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
23	A	405	CLA	C11-C10-C8	-2.09	109.17	115.92
34	V	203	HTG	C1-O5-C5	2.09	115.02	112.19
23	b	613	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
35	B	630	LMT	C1'-O5'-C5'	2.09	117.79	113.69
26	D	413	SQD	O48-C23-O10	-2.09	118.32	123.59
23	B	615	CLA	CHA-C1A-NA	-2.09	121.62	126.40
23	c	502	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	C	510	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
36	C	519	DGD	O6E-C1E-O5D	-2.08	105.04	109.97
25	b	617	BCR	C11-C10-C9	-2.08	124.34	127.31
23	C	506	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
36	H	102	DGD	O1G-C1A-O1A	-2.08	118.34	123.59
23	B	614	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
25	B	618	BCR	C35-C13-C14	-2.08	120.01	122.92
25	B	619	BCR	C37-C22-C23	2.08	121.35	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	517	DGD	C1D-O6D-C5D	2.08	117.77	113.69
35	m	102	LMT	O1B-C1B-C2B	2.08	113.48	108.10
23	B	606	CLA	OBD-CAD-C3D	-2.08	124.53	127.98
23	C	513	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
33	Z	102	LMG	C7-O1-C1	-2.08	109.69	113.74
23	b	614	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
23	d	403	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	B	617	BCR	C29-C30-C25	2.07	113.67	110.48
36	h	102	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
23	c	506	CLA	CMC-C2C-C1C	2.07	128.19	125.04
35	a	417	LMT	C1B-O1B-C4'	-2.07	112.84	117.96
25	h	101	BCR	C15-C14-C13	-2.07	124.35	127.31
25	k	101	BCR	C34-C9-C10	-2.07	120.02	122.92
23	B	616	CLA	CMB-C2B-C3B	2.07	128.55	124.68
23	B	601	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
25	Y	101	BCR	C28-C27-C26	-2.07	110.38	114.08
23	B	604	CLA	C6-C7-C8	-2.07	109.23	115.92
34	b	623	HTG	C1-O5-C5	2.07	116.39	112.58
23	C	507	CLA	CED-O2D-CGD	2.07	120.61	115.94
23	c	507	CLA	O1D-CGD-CBD	-2.07	120.26	124.48
23	B	604	CLA	CMB-C2B-C3B	2.07	128.54	124.68
25	Y	101	BCR	C29-C28-C27	-2.06	106.76	111.38
38	e	103	HEM	C3C-C4C-NC	-2.06	107.05	110.94
23	c	504	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
23	c	510	CLA	CHB-C4A-NA	2.06	127.37	124.51
23	B	602	CLA	CHB-C4A-NA	2.06	127.37	124.51
23	B	609	CLA	C7-C6-C5	-2.06	107.76	113.36
35	e	102	LMT	C1B-C2B-C3B	2.06	114.29	110.00
23	A	405	CLA	O2A-CGA-CBA	2.06	118.38	111.91
23	a	404	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
25	b	617	BCR	C38-C26-C25	-2.06	122.21	124.53
36	c	516	DGD	O2G-C1B-O1B	-2.06	118.72	123.70
23	C	504	CLA	CHC-C1C-NC	2.06	127.33	124.20
25	b	619	BCR	C20-C21-C22	-2.06	124.37	127.31
26	B	620	SQD	O9-S-C6	2.06	109.38	106.94
23	b	613	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
23	A	404	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
23	d	401	CLA	CMC-C2C-C1C	2.05	128.17	125.04
23	A	408	CLA	C3D-CAD-CBD	2.05	110.31	107.61
29	a	414	PL9	C17-C18-C19	-2.05	122.72	127.66
24	a	406	PHO	CMC-C2C-C1C	2.05	128.22	125.06
36	C	517	DGD	O1G-C1A-C2A	2.05	118.35	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	B	621	LMG	O8-C28-O10	-2.05	118.42	123.59
23	B	607	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	C	505	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
24	a	406	PHO	C3A-C4A-CHB	-2.05	118.29	121.83
23	B	610	CLA	CMB-C2B-C3B	2.05	128.51	124.68
25	D	406	BCR	C10-C11-C12	-2.05	116.83	123.22
23	b	604	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
26	B	620	SQD	O5-C1-C2	-2.05	106.02	110.35
23	C	513	CLA	C11-C12-C13	-2.05	109.31	115.92
26	B	620	SQD	O48-C23-O10	-2.04	118.43	123.59
23	c	503	CLA	C2A-C1A-CHA	-2.04	120.28	123.86
23	B	614	CLA	CHB-C4A-NA	2.04	127.34	124.51
23	B	610	CLA	OBD-CAD-C3D	-2.04	124.59	127.98
25	A	409	BCR	C7-C8-C9	-2.04	123.15	126.23
24	D	401	PHO	C4A-NA-C1A	-2.04	106.49	108.14
36	c	518	DGD	O6D-C1D-O3G	-2.04	105.14	109.97
31	E	101	LHG	O7-C7-O9	-2.04	118.77	123.70
23	C	512	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
25	b	619	BCR	C28-C27-C26	-2.04	110.43	114.08
36	c	517	DGD	O2G-C1B-O1B	-2.04	118.77	123.70
25	b	617	BCR	C15-C16-C17	-2.04	119.30	123.47
23	D	405	CLA	OBD-CAD-C3D	-2.04	124.60	127.98
23	b	615	CLA	C6-C7-C8	-2.04	109.34	115.92
24	a	407	PHO	C1C-C2C-C3C	-2.04	104.17	106.51
29	D	407	PL9	C45-C44-C43	-2.04	118.46	123.68
25	T	101	BCR	C3-C4-C5	-2.04	110.44	114.08
23	B	602	CLA	C11-C10-C8	-2.04	109.34	115.92
23	a	408	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	b	610	CLA	CMC-C2C-C1C	2.03	128.14	125.04
23	d	404	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	c	510	CLA	C11-C10-C8	-2.03	109.35	115.92
36	H	102	DGD	O6E-C5E-C6E	2.03	111.49	106.44
25	B	619	BCR	C29-C30-C25	2.03	113.61	110.48
25	D	406	BCR	C30-C25-C24	2.03	121.52	115.78
25	K	102	BCR	C38-C26-C25	-2.03	122.25	124.53
24	a	407	PHO	C4A-NA-C1A	-2.03	106.50	108.14
23	C	508	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	A	406	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	C	511	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
23	d	403	CLA	CHB-C4A-NA	2.03	127.31	124.51
23	B	607	CLA	C1-O2A-CGA	2.02	121.76	116.44
24	D	401	PHO	CBC-CAC-C3C	-2.02	106.85	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C6-C7-C8	-2.02	109.38	115.92
23	c	506	CLA	CMB-C2B-C3B	2.02	128.46	124.68
23	B	601	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
23	b	602	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
23	B	606	CLA	C1-O2A-CGA	2.02	121.75	116.44
25	a	409	BCR	C2-C1-C6	2.02	113.59	110.48
33	J	101	LMG	C8-O7-C10	-2.02	112.82	117.79
25	c	514	BCR	C21-C20-C19	-2.02	116.91	123.22
23	d	403	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
23	c	507	CLA	C11-C10-C8	-2.02	109.39	115.92
36	c	518	DGD	C3G-C2G-C1G	-2.02	107.01	111.79
36	C	518	DGD	O6E-C5E-C6E	2.02	111.45	106.44
34	B	627	HTG	C1-O5-C5	2.02	116.30	112.58
23	B	612	CLA	C4D-C3D-CAD	-2.02	107.35	108.47
23	C	503	CLA	OBD-CAD-C3D	-2.02	124.64	127.98
23	B	613	CLA	C7-C6-C5	-2.01	107.89	113.36
26	B	620	SQD	O5-C5-C4	2.01	113.35	109.69
29	d	406	PL9	C36-C34-C33	-2.01	117.05	121.12
36	c	517	DGD	O1G-C1A-O1A	-2.01	118.52	123.59
23	C	505	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	b	615	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
23	C	505	CLA	O2A-CGA-CBA	2.01	118.20	111.91
23	b	602	CLA	C7-C6-C5	-2.01	107.91	113.36
36	C	519	DGD	C3G-C2G-C1G	-2.01	107.04	111.79
36	C	518	DGD	C3G-O3G-C1D	-2.01	109.82	113.74
23	d	401	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
25	d	405	BCR	C35-C13-C14	-2.00	120.12	122.92
23	b	607	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
29	a	414	PL9	C12-C13-C14	-2.00	122.84	127.66
35	e	102	LMT	O1B-C1B-C2B	2.00	113.29	108.10
23	b	609	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (196) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	a	408	CLA	NC
23	a	408	CLA	ND
23	a	408	CLA	NA
23	d	404	CLA	NC
23	d	404	CLA	ND
23	d	404	CLA	NA
23	B	608	CLA	NC

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Mol	Chain	Res	Type	Atom
23	B	608	CLA	ND
23	B	608	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	A	406	CLA	NC
23	A	406	CLA	ND
23	A	406	CLA	NA
23	D	405	CLA	NC
23	D	405	CLA	ND
23	D	405	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	B	616	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	b	606	CLA	NC

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Mol	Chain	Res	Type	Atom
23	b	606	CLA	ND
23	b	606	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	404	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	B	615	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	C	514	CLA	NC
23	C	514	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	511	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	ND
23	A	408	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	D	404	CLA	ND
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	C	506	CLA	ND
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	b	601	CLA	NC
23	b	601	CLA	ND
23	b	601	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	B	609	CLA	NC
23	B	609	CLA	ND
23	B	609	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	c	505	CLA	ND
23	d	401	CLA	NC
23	d	401	CLA	ND
23	d	401	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	509	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	602	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	NA
23	d	403	CLA	ND
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	c	506	CLA	ND
23	c	506	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	C	512	CLA	NC

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Mol	Chain	Res	Type	Atom
23	C	512	CLA	ND
23	C	512	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	b	603	CLA	NC
23	b	603	CLA	ND
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA

All (1331) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	C	523	GOL	O1-C1-C2-O2
27	C	523	GOL	O1-C1-C2-C3
23	B	603	CLA	C2-C3-C5-C6
23	B	603	CLA	C4-C3-C5-C6
31	l	101	LHG	C4-O6-P-O4
31	l	101	LHG	C4-O6-P-O5
35	E	102	LMT	C2'-C1'-O1'-C1
35	E	102	LMT	O5'-C1'-O1'-C1
31	d	407	LHG	O1-C1-C2-C3
33	z	101	LMG	C11-C10-O7-C8
31	E	101	LHG	O1-C1-C2-C3
31	E	101	LHG	C1-C2-C3-O3
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
23	D	405	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	D	405	CLA	C4-C3-C5-C6
31	D	408	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O4
31	d	409	LHG	C4-O6-P-O4
31	d	408	LHG	C3-O3-P-O4
31	d	408	LHG	C3-O3-P-O5
31	d	408	LHG	C3-O3-P-O6
31	d	408	LHG	C4-O6-P-O4
27	a	411	GOL	C1-C2-C3-O3
34	B	624	HTG	O5-C1-S1-C1'
23	b	606	CLA	CHA-CBD-CGD-O1D
29	A	414	PL9	C13-C14-C16-C17
29	A	414	PL9	C15-C14-C16-C17
29	A	414	PL9	C23-C24-C26-C27
29	A	414	PL9	C25-C24-C26-C27
25	d	405	BCR	C7-C8-C9-C10
25	d	405	BCR	C7-C8-C9-C34
25	d	405	BCR	C21-C22-C23-C24
25	d	405	BCR	C37-C22-C23-C24
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
35	M	103	LMT	C2'-C1'-O1'-C1
35	M	103	LMT	O5'-C1'-O1'-C1
35	b	627	LMT	O5'-C1'-O1'-C1
35	b	627	LMT	C2-C1-O1'-C1'
33	a	416	LMG	O9-C10-O7-C8
35	B	629	LMT	C2'-C1'-O1'-C1
35	B	629	LMT	O5'-C1'-O1'-C1
26	L	101	SQD	O49-C7-O47-C45
26	L	101	SQD	C5-C6-S-O7
26	L	101	SQD	C5-C6-S-O8
26	L	101	SQD	C5-C6-S-O9
31	A	416	LHG	C4-O6-P-O5
31	D	409	LHG	C4-O6-P-O4
35	B	631	LMT	C2'-C1'-O1'-C1
35	B	631	LMT	O5'-C1'-O1'-C1
35	B	631	LMT	C2-C1-O1'-C1'
33	c	520	LMG	C11-C10-O7-C8
29	d	406	PL9	C39-C41-C42-C43
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
34	B	622	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
33	Z	102	LMG	C2-C1-O1-C7
33	Z	102	LMG	O9-C10-O7-C8
33	Z	102	LMG	C11-C10-O7-C8
27	B	625	GOL	O1-C1-C2-C3
25	D	406	BCR	C7-C8-C9-C10
25	D	406	BCR	C7-C8-C9-C34
25	D	406	BCR	C21-C22-C23-C24
25	D	406	BCR	C37-C22-C23-C24
25	D	406	BCR	C23-C24-C25-C30
35	I	101	LMT	C2'-C1'-O1'-C1
35	I	101	LMT	O5'-C1'-O1'-C1
26	B	620	SQD	O49-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
35	b	621	LMT	O5'-C1'-O1'-C1
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
27	d	402	GOL	O1-C1-C2-C3
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
27	B	626	GOL	C1-C2-C3-O3
23	c	507	CLA	C2-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
33	C	501	LMG	C11-C10-O7-C8
23	c	509	CLA	C2-C1-O2A-CGA
34	B	623	HTG	C2'-C1'-S1-C1
35	a	417	LMT	C2'-C1'-O1'-C1
35	a	417	LMT	O5'-C1'-O1'-C1
31	A	417	LHG	O1-C1-C2-C3
31	A	417	LHG	C3-O3-P-O4
31	A	417	LHG	C4-O6-P-O4
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
35	e	102	LMT	C2'-C1'-O1'-C1
35	e	102	LMT	O5'-C1'-O1'-C1
35	D	402	LMT	C2'-C1'-O1'-C1
35	D	402	LMT	O5'-C1'-O1'-C1
35	B	630	LMT	C2'-C1'-O1'-C1
35	B	630	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	e	101	LHG	C3-O3-P-O5
31	e	101	LHG	C3-O3-P-O6
31	e	101	LHG	O10-C23-O8-C6
31	e	101	LHG	C24-C23-O8-C6
26	D	413	SQD	O49-C7-O47-C45
26	D	413	SQD	C8-C7-O47-C45
26	D	413	SQD	C5-C6-S-O7
26	D	413	SQD	C5-C6-S-O8
26	D	413	SQD	C5-C6-S-O9
26	a	412	SQD	O6-C44-C45-O47
25	b	617	BCR	C1-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	412	SQD	O6-C44-C45-O47
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	B	614	CLA	C2-C3-C5-C6
23	B	614	CLA	C4-C3-C5-C6
26	f	101	SQD	O49-C7-O47-C45
26	f	101	SQD	C8-C7-O47-C45
26	f	101	SQD	C5-C6-S-O7
26	f	101	SQD	C5-C6-S-O8
26	f	101	SQD	C5-C6-S-O9
27	A	411	GOL	O1-C1-C2-C3
23	b	603	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
35	D	403	LMT	C3'-C4'-O1B-C1B
23	C	514	CLA	CBD-CGD-O2D-CED
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	501	CLA	CBD-CGD-O2D-CED
33	z	101	LMG	O9-C10-O7-C8
33	c	520	LMG	O9-C10-O7-C8
35	I	101	LMT	C3'-C4'-O1B-C1B
23	B	616	CLA	C3-C5-C6-C7
23	A	408	CLA	C3-C5-C6-C7
23	B	614	CLA	C3-C5-C6-C7
33	a	416	LMG	C11-C10-O7-C8
26	L	101	SQD	C8-C7-O47-C45
23	d	401	CLA	CBD-CGD-O2D-CED
33	c	520	LMG	O6-C5-C6-O5
23	c	504	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	504	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	a	405	CLA	CBD-CGD-O2D-CED
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	604	CLA	C3-C5-C6-C7
34	c	521	HTG	S1-C1'-C2'-C3'
33	C	501	LMG	O9-C10-O7-C8
35	D	403	LMT	C4'-C5'-C6'-O6'
34	B	624	HTG	O5-C5-C6-O6
23	C	502	CLA	CBD-CGD-O2D-CED
31	E	101	LHG	O2-C2-C3-O3
31	D	408	LHG	O2-C2-C3-O3
31	d	408	LHG	O2-C2-C3-O3
23	b	616	CLA	C3-C5-C6-C7
23	c	506	CLA	C3-C5-C6-C7
33	Z	101	LMG	O6-C5-C6-O5
35	I	101	LMT	O5B-C5B-C6B-O6B
34	b	625	HTG	O5-C5-C6-O6
34	b	628	HTG	S1-C1'-C2'-C3'
35	M	103	LMT	O5'-C5'-C6'-O6'
35	D	403	LMT	O5'-C5'-C6'-O6'
23	d	404	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	d	404	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
33	j	101	LMG	C10-C11-C12-C13
23	b	610	CLA	C2A-CAA-CBA-CGA
23	B	606	CLA	C2A-CAA-CBA-CGA
35	D	403	LMT	O5B-C5B-C6B-O6B
29	A	414	PL9	C14-C16-C17-C18
29	D	407	PL9	C39-C41-C42-C43
35	E	102	LMT	C4'-C5'-C6'-O6'
34	d	411	HTG	C4-C5-C6-O6
31	D	408	LHG	C1-C2-C3-O3
35	D	403	LMT	C4B-C5B-C6B-O6B
23	c	512	CLA	C3-C5-C6-C7
31	D	409	LHG	C24-C23-O8-C6
23	C	511	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	CBA-CGA-O2A-C1
34	B	623	HTG	C4-C5-C6-O6
26	A	412	SQD	C26-C27-C28-C29
33	c	520	LMG	C4-C5-C6-O5
23	C	508	CLA	C5-C6-C7-C8
23	A	405	CLA	C15-C16-C17-C18
35	b	627	LMT	C2'-C1'-O1'-C1
35	b	621	LMT	C2'-C1'-O1'-C1
31	D	408	LHG	C32-C33-C34-C35
23	B	616	CLA	C6-C7-C8-C9
23	B	605	CLA	C6-C7-C8-C9
23	c	512	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	c	502	CLA	C14-C13-C15-C16
23	b	604	CLA	C11-C10-C8-C9
23	B	601	CLA	C11-C10-C8-C9
23	C	502	CLA	C15-C16-C17-C18
25	H	101	BCR	C7-C8-C9-C34
25	Y	101	BCR	C37-C22-C23-C24
25	K	102	BCR	C7-C8-C9-C34
25	y	101	BCR	C37-C22-C23-C24
25	H	101	BCR	C7-C8-C9-C10
33	J	101	LMG	O6-C5-C6-O5
26	A	410	SQD	C8-C7-O47-C45
23	C	511	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	O1A-CGA-O2A-C1
23	b	606	CLA	C10-C11-C12-C13
34	b	623	HTG	O5-C5-C6-O6
23	B	601	CLA	C5-C6-C7-C8
33	Z	102	LMG	C10-C11-C12-C13
23	C	514	CLA	O1D-CGD-O2D-CED
23	a	408	CLA	C5-C6-C7-C8
23	B	605	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
23	b	616	CLA	C5-C6-C7-C8
23	C	506	CLA	C8-C10-C11-C12
23	c	502	CLA	C15-C16-C17-C18
23	b	611	CLA	C15-C16-C17-C18
23	B	601	CLA	C15-C16-C17-C18
23	B	614	CLA	C5-C6-C7-C8
23	B	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C10-C11-C12-C13
33	c	520	LMG	C10-C11-C12-C13
36	C	518	DGD	C1A-C2A-C3A-C4A
23	a	404	CLA	C15-C16-C17-C18
23	B	606	CLA	C13-C15-C16-C17
35	B	631	LMT	O1'-C1-C2-C3
23	b	614	CLA	C13-C15-C16-C17
35	I	101	LMT	O1'-C1-C2-C3
23	c	510	CLA	C10-C11-C12-C13
34	b	628	HTG	O5-C5-C6-O6
23	A	408	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	A	408	CLA	O1A-CGA-O2A-C1
25	T	101	BCR	C13-C14-C15-C16
23	a	408	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	O1D-CGD-O2D-CED
23	b	605	CLA	C8-C10-C11-C12
23	b	601	CLA	C8-C10-C11-C12
31	D	409	LHG	O10-C23-O8-C6
23	b	604	CLA	CBD-CGD-O2D-CED
35	B	631	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
23	B	616	CLA	C10-C11-C12-C13
26	D	413	SQD	C7-C8-C9-C10
36	c	516	DGD	O6D-C5D-C6D-O5D
35	B	631	LMT	O5'-C5'-C6'-O6'
26	A	410	SQD	O49-C7-O47-C45
34	B	624	HTG	C4-C5-C6-O6
23	B	602	CLA	C15-C16-C17-C18
23	d	404	CLA	CBA-CGA-O2A-C1
31	E	101	LHG	C11-C10-C9-C8
35	I	101	LMT	C4B-C5B-C6B-O6B
23	C	511	CLA	C5-C6-C7-C8
23	c	507	CLA	C8-C10-C11-C12
31	l	101	LHG	C4-O6-P-O3
31	E	101	LHG	C3-O3-P-O6
31	D	408	LHG	C4-O6-P-O3
23	D	405	CLA	C3-C5-C6-C7
35	D	402	LMT	C1-C2-C3-C4
23	c	501	CLA	O1D-CGD-O2D-CED
31	d	408	LHG	C1-C2-C3-O3
23	B	604	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
23	b	614	CLA	C3-C5-C6-C7
23	c	512	CLA	C13-C15-C16-C17
26	A	410	SQD	C11-C10-C9-C8
36	C	517	DGD	O6D-C5D-C6D-O5D
23	b	615	CLA	C13-C15-C16-C17
23	b	614	CLA	C15-C16-C17-C18
33	b	620	LMG	C38-C39-C40-C41
35	b	627	LMT	C2-C3-C4-C5
35	m	102	LMT	C11-C10-C9-C8
36	C	517	DGD	CAA-CBA-CCA-CDA
23	a	404	CLA	CBD-CGD-O2D-CED
33	b	620	LMG	C11-C10-O7-C8
33	Z	101	LMG	C16-C17-C18-C19
31	d	409	LHG	C32-C33-C34-C35
33	a	416	LMG	C31-C32-C33-C34
33	B	621	LMG	C17-C18-C19-C20
35	e	102	LMT	C3-C4-C5-C6
26	a	410	SQD	C9-C10-C11-C12
26	a	410	SQD	C11-C12-C13-C14
26	A	412	SQD	C18-C19-C20-C21
36	C	517	DGD	C4D-C5D-C6D-O5D
36	H	102	DGD	CAB-CBB-CCB-CDB
33	Z	101	LMG	C17-C18-C19-C20
31	d	409	LHG	C34-C35-C36-C37
26	L	101	SQD	C14-C15-C16-C17
26	L	101	SQD	C24-C25-C26-C27
36	C	518	DGD	C7B-C8B-C9B-CAB
26	a	410	SQD	C13-C14-C15-C16
26	A	410	SQD	C9-C10-C11-C12
33	b	620	LMG	O9-C10-O7-C8
31	d	408	LHG	C13-C14-C15-C16
33	c	519	LMG	C33-C34-C35-C36
36	C	518	DGD	C9A-CAA-CBA-CCA
31	D	409	LHG	C29-C30-C31-C32
31	A	417	LHG	C17-C18-C19-C20
26	f	101	SQD	C28-C29-C30-C31
36	c	517	DGD	C7A-C8A-C9A-CAA
33	a	416	LMG	C30-C31-C32-C33
35	B	630	LMT	C2-C3-C4-C5
35	E	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
35	m	102	LMT	C2'-C1'-O1'-C1
36	C	518	DGD	C2E-C1E-O5D-C6D
36	C	517	DGD	C2E-C1E-O5D-C6D
33	Z	101	LMG	C15-C16-C17-C18
33	C	520	LMG	C11-C12-C13-C14
33	B	621	LMG	C36-C37-C38-C39
26	D	413	SQD	C30-C31-C32-C33
23	B	615	CLA	C8-C10-C11-C12
23	b	610	CLA	C15-C16-C17-C18
23	C	507	CLA	C16-C17-C18-C20
23	d	401	CLA	O1D-CGD-O2D-CED
34	B	623	HTG	O5-C5-C6-O6
34	d	411	HTG	O5-C5-C6-O6
24	D	401	PHO	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
29	D	407	PL9	C15-C14-C16-C17
31	E	101	LHG	C24-C25-C26-C27
26	a	412	SQD	C25-C26-C27-C28
33	c	519	LMG	C4-C5-C6-O5
23	B	615	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
23	b	616	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	d	401	CLA	C11-C12-C13-C14
31	A	417	LHG	C23-C24-C25-C26
35	b	627	LMT	C3-C4-C5-C6
36	c	516	DGD	C5A-C6A-C7A-C8A
35	b	621	LMT	C3-C4-C5-C6
26	D	413	SQD	C24-C25-C26-C27
26	A	412	SQD	C16-C17-C18-C19
33	J	101	LMG	C30-C31-C32-C33
23	c	507	CLA	C2A-CAA-CBA-CGA
23	a	408	CLA	O1A-CGA-O2A-C1
36	c	516	DGD	C4D-C5D-C6D-O5D
33	b	620	LMG	C14-C15-C16-C17
34	b	625	HTG	C3'-C4'-C5'-C6'
26	A	412	SQD	C25-C26-C27-C28
26	A	410	SQD	C15-C16-C17-C18
31	A	416	LHG	O1-C1-C2-C3
27	B	625	GOL	C1-C2-C3-O3
27	b	624	GOL	O1-C1-C2-C3
23	d	404	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
34	C	522	HTG	O5-C5-C6-O6
23	B	605	CLA	C8-C10-C11-C12
36	H	102	DGD	C6A-C7A-C8A-C9A
33	j	101	LMG	C29-C30-C31-C32
31	D	408	LHG	C13-C14-C15-C16
31	d	408	LHG	C14-C15-C16-C17
33	C	501	LMG	C37-C38-C39-C40
31	A	417	LHG	C13-C14-C15-C16
26	D	413	SQD	C32-C33-C34-C35
26	a	412	SQD	C27-C28-C29-C30
26	f	101	SQD	C25-C26-C27-C28
23	B	608	CLA	C16-C17-C18-C19
35	m	102	LMT	O5'-C1'-O1'-C1
33	Z	102	LMG	O6-C1-O1-C7
36	C	517	DGD	O6E-C1E-O5D-C6D
31	l	101	LHG	C27-C28-C29-C30
33	a	416	LMG	C35-C36-C37-C38
33	C	520	LMG	C12-C13-C14-C15
26	B	620	SQD	C33-C34-C35-C36
31	A	417	LHG	C25-C26-C27-C28
26	a	412	SQD	C10-C11-C12-C13
26	a	410	SQD	C30-C31-C32-C33
33	B	621	LMG	C28-C29-C30-C31
23	d	404	CLA	O1A-CGA-O2A-C1
33	b	620	LMG	C39-C40-C41-C42
23	a	405	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	CBA-CGA-O2A-C1
33	J	101	LMG	C34-C35-C36-C37
23	c	509	CLA	C5-C6-C7-C8
36	H	102	DGD	CCA-CDA-CEA-CFA
35	B	629	LMT	C5-C6-C7-C8
26	B	620	SQD	C18-C19-C20-C21
23	C	502	CLA	O1D-CGD-O2D-CED
23	B	608	CLA	C16-C17-C18-C20
36	H	102	DGD	CBA-CCA-CDA-CEA
36	H	102	DGD	CBB-CCB-CDB-CEB
26	a	410	SQD	C29-C30-C31-C32
34	B	622	HTG	C1'-C2'-C3'-C4'
35	B	629	LMT	C11-C10-C9-C8
33	C	520	LMG	C28-C29-C30-C31
23	C	506	CLA	C4-C3-C5-C6
24	D	401	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C2-C3-C5-C6
29	D	407	PL9	C13-C14-C16-C17
31	d	407	LHG	C25-C26-C27-C28
26	L	101	SQD	C26-C27-C28-C29
36	C	519	DGD	CAA-CBA-CCA-CDA
31	d	407	LHG	O1-C1-C2-O2
27	B	625	GOL	O1-C1-C2-O2
27	d	402	GOL	O1-C1-C2-O2
27	B	626	GOL	O2-C2-C3-O3
27	A	411	GOL	O1-C1-C2-O2
33	z	101	LMG	C18-C19-C20-C21
33	c	520	LMG	C37-C38-C39-C40
23	c	509	CLA	C3-C5-C6-C7
26	L	101	SQD	C27-C28-C29-C30
36	C	518	DGD	CCB-CDB-CEB-CFB
33	Z	102	LMG	C19-C20-C21-C22
23	b	601	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C1-O2A-CGA
33	j	101	LMG	C38-C39-C40-C41
26	L	101	SQD	C13-C14-C15-C16
31	A	417	LHG	C24-C25-C26-C27
31	e	101	LHG	C26-C27-C28-C29
26	a	412	SQD	C24-C25-C26-C27
31	D	409	LHG	C13-C14-C15-C16
25	D	406	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
31	d	408	LHG	C16-C17-C18-C19
31	d	408	LHG	C30-C31-C32-C33
36	C	517	DGD	C3B-C4B-C5B-C6B
31	d	409	LHG	C24-C23-O8-C6
23	b	606	CLA	C8-C10-C11-C12
23	B	601	CLA	C10-C11-C12-C13
33	B	621	LMG	C11-C10-O7-C8
31	d	407	LHG	C34-C35-C36-C37
31	A	416	LHG	C25-C26-C27-C28
31	A	416	LHG	C32-C33-C34-C35
33	J	101	LMG	C36-C37-C38-C39
23	B	601	CLA	O1A-CGA-O2A-C1
23	A	408	CLA	C4-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	C	511	CLA	C6-C7-C8-C10
23	A	408	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	d	401	CLA	C11-C12-C13-C15
23	b	604	CLA	C6-C7-C8-C10
23	b	603	CLA	C6-C7-C8-C10
34	C	522	HTG	S1-C1'-C2'-C3'
23	b	605	CLA	C3-C5-C6-C7
31	d	409	LHG	O10-C23-O8-C6
34	B	624	HTG	C3'-C4'-C5'-C6'
33	J	101	LMG	C20-C21-C22-C23
23	c	513	CLA	C10-C11-C12-C13
23	B	610	CLA	C16-C17-C18-C19
23	b	601	CLA	CBA-CGA-O2A-C1
31	l	101	LHG	C12-C13-C14-C15
31	l	101	LHG	C14-C15-C16-C17
31	D	409	LHG	C15-C16-C17-C18
23	B	610	CLA	C2A-CAA-CBA-CGA
23	A	404	CLA	C2A-CAA-CBA-CGA
23	b	601	CLA	C10-C11-C12-C13
33	B	621	LMG	C18-C19-C20-C21
35	b	621	LMT	C4-C5-C6-C7
34	b	628	HTG	C1'-C2'-C3'-C4'
26	D	413	SQD	C11-C10-C9-C8
35	e	102	LMT	C5-C6-C7-C8
36	h	102	DGD	CBB-CCB-CDB-CEB
36	c	517	DGD	C9A-CAA-CBA-CCA
23	c	502	CLA	C16-C17-C18-C20
36	C	518	DGD	O6E-C1E-O5D-C6D
36	c	516	DGD	O6E-C1E-O5D-C6D
23	b	611	CLA	C8-C10-C11-C12
33	j	101	LMG	C21-C22-C23-C24
33	C	520	LMG	C17-C18-C19-C20
33	B	621	LMG	C32-C33-C34-C35
33	a	416	LMG	C39-C40-C41-C42
23	c	512	CLA	C10-C11-C12-C13
31	d	408	LHG	C9-C10-C11-C12
26	a	410	SQD	C27-C28-C29-C30
33	B	621	LMG	O9-C10-O7-C8
23	b	608	CLA	C3-C5-C6-C7
31	l	101	LHG	C34-C35-C36-C37
23	C	509	CLA	C10-C11-C12-C13
35	E	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
35	b	627	LMT	C11-C10-C9-C8
36	C	518	DGD	CCA-CDA-CEA-CFA
26	a	410	SQD	C34-C35-C36-C37
33	Z	101	LMG	C4-C5-C6-O5
33	c	519	LMG	C34-C35-C36-C37
23	C	511	CLA	C4-C3-C5-C6
36	c	517	DGD	C1B-C2B-C3B-C4B
29	A	414	PL9	C4-C3-C7-C8
29	a	414	PL9	C4-C3-C7-C8
31	d	407	LHG	C33-C34-C35-C36
36	h	102	DGD	C5B-C6B-C7B-C8B
33	J	101	LMG	C14-C15-C16-C17
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	A	408	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	509	CLA	C14-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C9
23	b	603	CLA	C6-C7-C8-C9
23	B	602	CLA	C11-C12-C13-C14
36	c	516	DGD	O6E-C5E-C6E-O5E
36	C	518	DGD	C8A-C9A-CAA-CBA
33	C	520	LMG	C37-C38-C39-C40
23	b	601	CLA	C3-C5-C6-C7
31	d	407	LHG	C32-C33-C34-C35
33	Z	102	LMG	O6-C5-C6-O5
34	B	627	HTG	O5-C5-C6-O6
36	C	517	DGD	O6E-C5E-C6E-O5E
25	b	619	BCR	C37-C22-C23-C24
23	b	605	CLA	C5-C6-C7-C8
23	a	404	CLA	C13-C15-C16-C17
31	D	409	LHG	C28-C29-C30-C31
25	y	101	BCR	C21-C22-C23-C24
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C16-C17-C18-C20
31	A	416	LHG	C18-C19-C20-C21
33	c	519	LMG	C31-C32-C33-C34
23	b	608	CLA	C13-C15-C16-C17
23	c	506	CLA	C13-C15-C16-C17
31	d	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
31	d	408	LHG	C4-O6-P-O3
31	A	417	LHG	C3-O3-P-O6
31	A	417	LHG	C4-O6-P-O3
34	B	623	HTG	C2'-C3'-C4'-C5'
23	C	503	CLA	C3-C5-C6-C7
31	l	101	LHG	C16-C17-C18-C19
35	B	629	LMT	C7-C8-C9-C10
35	m	102	LMT	C7-C8-C9-C10
35	B	631	LMT	C7-C8-C9-C10
34	b	625	HTG	C4-C5-C6-O6
23	C	507	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
31	d	409	LHG	C33-C34-C35-C36
26	f	101	SQD	C31-C32-C33-C34
23	c	508	CLA	C5-C6-C7-C8
35	D	402	LMT	C3-C4-C5-C6
23	B	605	CLA	C4-C3-C5-C6
36	c	518	DGD	CAB-CBB-CCB-CDB
23	b	613	CLA	CBD-CGD-O2D-CED
31	A	417	LHG	C12-C13-C14-C15
23	b	601	CLA	O1A-CGA-O2A-C1
33	Z	101	LMG	C18-C19-C20-C21
33	j	101	LMG	O6-C5-C6-O5
35	I	101	LMT	O5'-C5'-C6'-O6'
26	L	101	SQD	C44-C45-C46-O48
31	D	409	LHG	C4-C5-C6-O8
26	a	412	SQD	O6-C44-C45-C46
26	A	410	SQD	O6-C44-C45-C46
33	Z	101	LMG	C8-C7-O1-C1
36	C	518	DGD	C2G-C3G-O3G-C1D
36	C	518	DGD	C5D-C6D-O5D-C1E
36	c	517	DGD	C5D-C6D-O5D-C1E
31	D	408	LHG	C17-C18-C19-C20
36	C	519	DGD	CBA-CCA-CDA-CEA
34	c	522	HTG	O5-C5-C6-O6
23	d	404	CLA	C5-C6-C7-C8
23	b	613	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
35	D	402	LMT	C5-C6-C7-C8
23	a	404	CLA	O1D-CGD-O2D-CED
29	a	414	PL9	C14-C16-C17-C18
31	D	408	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C15-C16-C17-C18
26	B	620	SQD	C24-C23-O48-C46
31	E	101	LHG	O1-C1-C2-O2
27	a	411	GOL	O2-C2-C3-O3
31	A	416	LHG	O1-C1-C2-O2
31	l	101	LHG	C26-C27-C28-C29
36	c	517	DGD	CBA-CCA-CDA-CEA
23	B	601	CLA	CAA-CBA-CGA-O2A
35	B	629	LMT	C4'-C5'-C6'-O6'
23	A	406	CLA	C2C-C3C-CAC-CBC
35	a	417	LMT	C11-C10-C9-C8
23	B	615	CLA	C13-C15-C16-C17
23	C	514	CLA	C4-C3-C5-C6
33	c	519	LMG	C21-C22-C23-C24
23	c	502	CLA	C16-C17-C18-C19
35	a	417	LMT	C4-C5-C6-C7
26	a	410	SQD	C10-C11-C12-C13
23	c	506	CLA	C10-C11-C12-C13
31	A	416	LHG	C29-C30-C31-C32
23	a	404	CLA	C2A-CAA-CBA-CGA
23	B	616	CLA	C2-C1-O2A-CGA
35	M	103	LMT	C6-C7-C8-C9
33	C	520	LMG	C36-C37-C38-C39
31	E	101	LHG	C25-C26-C27-C28
35	B	630	LMT	C6-C7-C8-C9
23	b	612	CLA	C10-C11-C12-C13
34	b	628	HTG	C3'-C4'-C5'-C6'
36	c	517	DGD	C2E-C1E-O5D-C6D
33	a	416	LMG	O7-C8-C9-O8
26	f	101	SQD	O6-C44-C45-O47
31	e	101	LHG	C11-C12-C13-C14
23	D	405	CLA	C8-C10-C11-C12
23	B	615	CLA	C16-C17-C18-C19
34	B	623	HTG	C3'-C4'-C5'-C6'
29	d	406	PL9	C15-C14-C16-C17
35	M	103	LMT	C4'-C5'-C6'-O6'
23	a	408	CLA	C11-C10-C8-C7
23	B	616	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C12-C13-C15-C16
23	c	509	CLA	C12-C13-C15-C16
23	B	610	CLA	C12-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C15
36	h	102	DGD	O2G-C1B-C2B-C3B
23	b	607	CLA	C3-C5-C6-C7
23	d	404	CLA	C11-C10-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	d	403	CLA	C11-C12-C13-C14
23	c	506	CLA	C6-C7-C8-C9
36	H	102	DGD	C7B-C8B-C9B-CAB
23	B	611	CLA	C13-C15-C16-C17
26	A	410	SQD	C12-C13-C14-C15
26	B	620	SQD	O10-C23-O48-C46
33	B	621	LMG	C14-C15-C16-C17
25	K	102	BCR	C7-C8-C9-C10
34	B	622	HTG	C2'-C3'-C4'-C5'
36	c	517	DGD	C9B-CAB-CBB-CCB
35	e	102	LMT	C4'-C5'-C6'-O6'
23	c	511	CLA	CBA-CGA-O2A-C1
33	B	621	LMG	C37-C38-C39-C40
34	c	521	HTG	C4-C5-C6-O6
29	a	414	PL9	C9-C11-C12-C13
33	j	101	LMG	C35-C36-C37-C38
33	Z	102	LMG	C17-C18-C19-C20
36	c	518	DGD	CBA-CCA-CDA-CEA
36	c	517	DGD	CAA-CBA-CCA-CDA
29	a	414	PL9	C20-C19-C21-C22
23	C	507	CLA	C2-C3-C5-C6
29	d	406	PL9	C13-C14-C16-C17
23	B	613	CLA	C15-C16-C17-C18
35	E	102	LMT	C9-C10-C11-C12
36	c	517	DGD	C7B-C8B-C9B-CAB
23	b	602	CLA	C16-C17-C18-C19
23	b	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	a	412	SQD	C24-C23-O48-C46
23	C	512	CLA	CBA-CGA-O2A-C1
33	C	520	LMG	C10-C11-C12-C13
23	C	507	CLA	C3A-C2A-CAA-CBA
33	B	621	LMG	C33-C34-C35-C36
26	f	101	SQD	C34-C35-C36-C37
36	c	517	DGD	C2B-C3B-C4B-C5B
36	C	519	DGD	CDA-CEA-CFA-CGA
33	Z	101	LMG	C33-C34-C35-C36
24	A	407	PHO	C2C-C3C-CAC-CBC
35	e	102	LMT	C2B-C1B-O1B-C4'
23	b	602	CLA	C16-C17-C18-C20
36	c	516	DGD	C2A-C1A-O1G-C1G
31	e	101	LHG	C14-C15-C16-C17
33	b	620	LMG	O1-C7-C8-C9
31	E	101	LHG	C4-C5-C6-O8
31	e	101	LHG	C4-C5-C6-O8
36	C	517	DGD	C9A-CAA-CBA-CCA
36	C	517	DGD	C8A-C9A-CAA-CBA
29	a	414	PL9	C45-C44-C46-C47
36	C	519	DGD	C2A-C1A-O1G-C1G
23	B	604	CLA	C2-C3-C5-C6
31	d	409	LHG	C30-C31-C32-C33
36	h	102	DGD	CDA-CEA-CFA-CGA
23	c	511	CLA	O1A-CGA-O2A-C1
35	B	629	LMT	O5'-C5'-C6'-O6'
36	H	102	DGD	C9B-CAB-CBB-CCB
23	B	601	CLA	C2A-CAA-CBA-CGA
31	A	417	LHG	O1-C1-C2-O2
23	b	603	CLA	C13-C15-C16-C17
36	c	516	DGD	CDB-CEB-CFB-CGB
23	D	405	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
33	a	416	LMG	C20-C21-C22-C23
34	b	628	HTG	C2'-C3'-C4'-C5'
33	b	620	LMG	O1-C7-C8-O7
26	L	101	SQD	O47-C45-C46-O48
31	D	409	LHG	O7-C5-C6-O8
26	B	620	SQD	O47-C45-C46-O48
26	A	410	SQD	O6-C44-C45-O47
24	a	407	PHO	C2C-C3C-CAC-CBC
36	c	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C5-C6-C7-C8
23	b	613	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
29	a	414	PL9	C18-C19-C21-C22
29	a	414	PL9	C43-C44-C46-C47
33	C	520	LMG	C16-C17-C18-C19
36	h	102	DGD	C9A-CAA-CBA-CCA
23	B	604	CLA	C13-C15-C16-C17
23	D	405	CLA	C11-C10-C8-C9
23	A	408	CLA	C14-C13-C15-C16
23	b	609	CLA	C6-C7-C8-C9
23	C	503	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
33	C	520	LMG	C13-C14-C15-C16
26	A	412	SQD	C15-C16-C17-C18
23	C	510	CLA	CBD-CGD-O2D-CED
33	Z	102	LMG	C11-C12-C13-C14
23	B	612	CLA	C10-C11-C12-C13
31	D	409	LHG	C2-C3-O3-P
23	C	512	CLA	O1A-CGA-O2A-C1
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
25	Y	101	BCR	C21-C22-C23-C24
23	b	603	CLA	C10-C11-C12-C13
31	d	408	LHG	C28-C29-C30-C31
33	a	416	LMG	C36-C37-C38-C39
23	C	507	CLA	C13-C15-C16-C17
23	A	404	CLA	C13-C15-C16-C17
31	l	101	LHG	O6-C4-C5-C6
36	h	102	DGD	C9B-CAB-CBB-CCB
23	d	404	CLA	C11-C10-C8-C7
23	C	502	CLA	C12-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C10
23	B	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C11-C12-C13-C15
23	C	514	CLA	C11-C10-C8-C7
23	C	506	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	c	502	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C11-C10-C8-C7
23	B	614	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
26	L	101	SQD	C12-C13-C14-C15
23	C	508	CLA	C13-C15-C16-C17
31	e	101	LHG	C9-C10-C11-C12
23	C	507	CLA	C8-C10-C11-C12
24	a	407	PHO	C8-C10-C11-C12
23	B	604	CLA	C2C-C3C-CAC-CBC
31	A	416	LHG	C24-C25-C26-C27
23	b	602	CLA	C10-C11-C12-C13
33	b	620	LMG	C35-C36-C37-C38
34	b	625	HTG	C2'-C1'-S1-C1
34	c	521	HTG	C2'-C1'-S1-C1
23	b	611	CLA	C3-C5-C6-C7
33	a	416	LMG	C29-C28-O8-C9
26	L	101	SQD	C24-C23-O48-C46
31	D	409	LHG	C17-C18-C19-C20
24	D	401	PHO	CAD-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
26	L	101	SQD	C46-C45-O47-C7
24	A	407	PHO	CAD-CBD-CGD-O2D
26	B	620	SQD	C46-C45-O47-C7
23	c	501	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
24	a	406	PHO	C2B-C3B-CAB-CBB
23	C	512	CLA	C3-C5-C6-C7
23	B	611	CLA	C8-C10-C11-C12
23	d	401	CLA	C15-C16-C17-C18
23	c	506	CLA	C15-C16-C17-C18
31	d	407	LHG	C24-C23-O8-C6
31	d	408	LHG	C26-C27-C28-C29
31	A	417	LHG	C14-C15-C16-C17
36	C	519	DGD	O6D-C1D-O3G-C3G
23	c	512	CLA	C15-C16-C17-C18
31	E	101	LHG	C23-C24-C25-C26
26	B	620	SQD	C44-C45-C46-O48
26	A	412	SQD	O6-C44-C45-C46
26	f	101	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	CBD-CGD-O2D-CED
23	b	611	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C3-C5-C6-C7
23	A	405	CLA	C2C-C3C-CAC-CBC
36	C	519	DGD	O6E-C5E-C6E-O5E
23	b	602	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C8-C10-C11-C12
26	A	412	SQD	O49-C7-O47-C45
23	b	605	CLA	CHA-CBD-CGD-O1D
23	b	605	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	D	405	CLA	O1A-CGA-O2A-C1
31	D	408	LHG	O10-C23-O8-C6
36	C	519	DGD	O1A-C1A-O1G-C1G
36	c	516	DGD	O1A-C1A-O1G-C1G
26	a	412	SQD	O10-C23-O48-C46
36	h	102	DGD	CBA-CCA-CDA-CEA
36	c	516	DGD	C2E-C1E-O5D-C6D
23	b	604	CLA	C13-C15-C16-C17
29	A	414	PL9	C2-C3-C7-C8
31	A	416	LHG	C11-C12-C13-C14
26	a	410	SQD	O6-C44-C45-O47
26	f	101	SQD	O47-C45-C46-O48
23	B	608	CLA	C8-C10-C11-C12
23	d	401	CLA	C13-C15-C16-C17
23	C	510	CLA	C10-C11-C12-C13
31	d	409	LHG	C9-C10-C11-C12
23	C	510	CLA	C3-C5-C6-C7
26	A	412	SQD	C8-C7-O47-C45
29	A	414	PL9	C30-C29-C31-C32
23	b	601	CLA	C4-C3-C5-C6
36	H	102	DGD	CCB-CDB-CEB-CFB
31	A	416	LHG	C33-C34-C35-C36
26	A	410	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
31	d	407	LHG	O10-C23-O8-C6
36	c	516	DGD	CDA-CEA-CFA-CGA
23	C	502	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
35	e	102	LMT	C4-C5-C6-C7
23	a	408	CLA	C16-C17-C18-C20
34	b	623	HTG	C4-C5-C6-O6
26	D	413	SQD	C27-C28-C29-C30
23	B	604	CLA	C3-C5-C6-C7
33	B	621	LMG	O6-C5-C6-O5
23	A	408	CLA	C16-C17-C18-C19
31	E	101	LHG	C15-C16-C17-C18
36	h	102	DGD	C4B-C5B-C6B-C7B
25	k	101	BCR	C9-C10-C11-C12
31	d	408	LHG	O10-C23-O8-C6
33	a	416	LMG	O10-C28-O8-C9
23	A	405	CLA	C13-C15-C16-C17
31	d	409	LHG	C29-C30-C31-C32
29	A	414	PL9	C45-C44-C46-C47
33	j	101	LMG	C19-C20-C21-C22
31	E	101	LHG	C10-C11-C12-C13
26	L	101	SQD	O10-C23-O48-C46
31	D	408	LHG	C3-O3-P-O4
31	D	408	LHG	C4-O6-P-O5
31	d	409	LHG	C4-O6-P-O5
31	d	408	LHG	C4-O6-P-O5
31	A	417	LHG	C4-O6-P-O5
23	A	406	CLA	C16-C17-C18-C19
35	E	102	LMT	O1'-C1-C2-C3
35	m	102	LMT	C9-C10-C11-C12
26	L	101	SQD	O5-C1-O6-C44
31	d	408	LHG	C24-C23-O8-C6
23	c	512	CLA	CBA-CGA-O2A-C1
29	d	406	PL9	C9-C11-C12-C13
23	C	513	CLA	C3-C5-C6-C7
33	j	101	LMG	C16-C17-C18-C19
31	D	408	LHG	C33-C34-C35-C36
31	d	409	LHG	C26-C27-C28-C29
35	e	102	LMT	O5B-C1B-O1B-C4'
34	B	622	HTG	C3'-C4'-C5'-C6'
23	b	605	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	503	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	B	601	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
34	c	521	HTG	C3'-C4'-C5'-C6'
34	B	623	HTG	C4'-C5'-C6'-C7'
23	b	613	CLA	O1D-CGD-O2D-CED
33	z	101	LMG	C10-C11-C12-C13
23	A	406	CLA	C12-C13-C15-C16
23	B	605	CLA	C6-C7-C8-C10
23	c	512	CLA	C6-C7-C8-C10
23	B	604	CLA	C11-C12-C13-C15
23	C	514	CLA	C6-C7-C8-C10
34	c	521	HTG	C2-C1-S1-C1'
23	b	601	CLA	C2-C3-C5-C6
23	c	509	CLA	C13-C15-C16-C17
23	B	606	CLA	C10-C11-C12-C13
33	Z	101	LMG	C37-C38-C39-C40
23	b	605	CLA	O1A-CGA-O2A-C1
36	h	102	DGD	CAB-CBB-CCB-CDB
33	a	416	LMG	C7-C8-C9-O8
26	f	101	SQD	O6-C44-C45-C46
31	E	101	LHG	O7-C5-C6-O8
31	e	101	LHG	O7-C5-C6-O8
33	j	101	LMG	C14-C15-C16-C17
35	B	629	LMT	C3-C4-C5-C6
33	Z	102	LMG	C15-C16-C17-C18
23	b	609	CLA	O1A-CGA-O2A-C1
31	l	101	LHG	C9-C10-C11-C12
31	d	407	LHG	C11-C12-C13-C14
35	D	403	LMT	C5-C6-C7-C8
35	M	103	LMT	O5B-C5B-C6B-O6B
36	c	517	DGD	C2G-C3G-O3G-C1D
23	c	508	CLA	C16-C17-C18-C19
35	M	103	LMT	O1'-C1-C2-C3
29	D	407	PL9	C30-C29-C31-C32
29	D	407	PL9	C45-C44-C46-C47
29	A	414	PL9	C28-C29-C31-C32
23	A	408	CLA	C2-C3-C5-C6
29	D	407	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
23	b	604	CLA	O1D-CGD-O2D-CED
23	a	408	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C12-C13-C14
23	b	601	CLA	C11-C10-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	c	512	CLA	O1A-CGA-O2A-C1
33	c	519	LMG	C29-C30-C31-C32
23	B	604	CLA	C4C-C3C-CAC-CBC
29	a	414	PL9	C39-C41-C42-C43
36	c	518	DGD	O1A-C1A-O1G-C1G
36	H	102	DGD	O2G-C1B-C2B-C3B
31	D	409	LHG	C30-C31-C32-C33
33	c	519	LMG	C28-C29-C30-C31
23	A	406	CLA	C4C-C3C-CAC-CBC
23	b	601	CLA	CAA-CBA-CGA-O2A
31	D	409	LHG	C10-C11-C12-C13
35	D	402	LMT	O1'-C1-C2-C3
31	d	407	LHG	C24-C25-C26-C27
35	D	403	LMT	C6-C7-C8-C9
35	b	621	LMT	C11-C10-C9-C8
23	C	514	CLA	C2-C3-C5-C6
26	D	413	SQD	C23-C24-C25-C26
33	C	501	LMG	C12-C13-C14-C15
36	H	102	DGD	C4A-C5A-C6A-C7A
33	b	620	LMG	C22-C23-C24-C25
31	e	101	LHG	C24-C25-C26-C27
23	C	502	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	C2-C1-O2A-CGA
23	a	404	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C2-C1-O2A-CGA
33	a	416	LMG	C10-C11-C12-C13
23	c	510	CLA	O1A-CGA-O2A-C1
35	M	103	LMT	O5B-C1B-O1B-C4'
31	d	409	LHG	C2-C3-O3-P
34	b	623	HTG	S1-C1'-C2'-C3'
23	b	616	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C16-C17-C18-C20
23	A	405	CLA	C16-C17-C18-C20
23	C	507	CLA	C5-C6-C7-C8
31	d	407	LHG	C7-C8-C9-C10
25	C	516	BCR	C1-C6-C7-C8
25	C	516	BCR	C5-C6-C7-C8
23	B	605	CLA	C2-C3-C5-C6
29	A	414	PL9	C43-C44-C46-C47
33	b	620	LMG	C37-C38-C39-C40
35	D	403	LMT	C2-C3-C4-C5
23	b	616	CLA	CBA-CGA-O2A-C1
23	b	609	CLA	CBA-CGA-O2A-C1
33	z	101	LMG	O6-C1-O1-C7
23	C	503	CLA	C10-C11-C12-C13
36	C	519	DGD	C2D-C1D-O3G-C3G
31	E	101	LHG	C4-O6-P-O3
36	c	518	DGD	CCB-CDB-CEB-CFB
23	a	404	CLA	C16-C17-C18-C19
31	A	417	LHG	C30-C31-C32-C33
35	B	629	LMT	C4-C5-C6-C7
23	b	612	CLA	C13-C15-C16-C17
23	D	405	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
26	A	410	SQD	C16-C17-C18-C19
23	b	606	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C9
23	C	506	CLA	C5-C6-C7-C8
33	c	520	LMG	C36-C37-C38-C39
33	c	519	LMG	C35-C36-C37-C38
31	A	417	LHG	C16-C17-C18-C19
26	f	101	SQD	C29-C30-C31-C32
23	b	613	CLA	O1A-CGA-O2A-C1
23	d	404	CLA	C16-C17-C18-C20
23	c	510	CLA	CBA-CGA-O2A-C1
35	E	102	LMT	C2B-C1B-O1B-C4'
35	e	102	LMT	C1-C2-C3-C4
29	a	414	PL9	C25-C24-C26-C27
23	C	514	CLA	O1A-CGA-O2A-C1
23	a	408	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	C	514	CLA	CBA-CGA-O2A-C1
36	c	518	DGD	C2A-C1A-O1G-C1G
29	a	414	PL9	C2-C3-C7-C8
23	a	408	CLA	C15-C16-C17-C18
34	b	625	HTG	C1'-C2'-C3'-C4'
23	C	513	CLA	CBA-CGA-O2A-C1
36	C	518	DGD	CDA-CEA-CFA-CGA
25	t	101	BCR	C15-C16-C17-C18
35	M	103	LMT	C2B-C1B-O1B-C4'
23	b	609	CLA	C13-C15-C16-C17
35	m	102	LMT	C6-C7-C8-C9
23	D	404	CLA	C2C-C3C-CAC-CBC
31	A	417	LHG	C11-C12-C13-C14
24	a	406	PHO	C4B-C3B-CAB-CBB
23	C	507	CLA	C3-C5-C6-C7
26	a	412	SQD	C12-C13-C14-C15
33	c	519	LMG	O6-C5-C6-O5
23	C	513	CLA	O1A-CGA-O2A-C1
23	B	608	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	d	403	CLA	C2-C1-O2A-CGA
35	M	103	LMT	C4B-C5B-C6B-O6B
35	E	102	LMT	C3-C4-C5-C6
26	L	101	SQD	C10-C11-C12-C13
33	C	501	LMG	O8-C28-C29-C30
33	z	101	LMG	C12-C13-C14-C15
33	J	101	LMG	C19-C20-C21-C22
36	H	102	DGD	C6B-C7B-C8B-C9B
23	A	406	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	b	608	CLA	C3A-C2A-CAA-CBA
23	A	406	CLA	C16-C17-C18-C20
23	B	612	CLA	CBA-CGA-O2A-C1
33	j	101	LMG	C28-C29-C30-C31
29	D	407	PL9	C43-C44-C46-C47
23	C	502	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C12-C13-C14
23	C	510	CLA	C6-C7-C8-C9
23	A	404	CLA	C14-C13-C15-C16
23	c	508	CLA	C16-C17-C18-C20
24	a	407	PHO	NC-C1C-CHC-C4B

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Mol	Chain	Res	Type	Atoms
31	l	101	LHG	C24-C25-C26-C27
26	B	620	SQD	C11-C10-C9-C8
36	C	517	DGD	CCA-CDA-CEA-CFA
26	a	410	SQD	O6-C44-C45-C46
33	C	501	LMG	C14-C15-C16-C17
24	D	401	PHO	CBA-CGA-O2A-C1
36	C	519	DGD	C9B-CAB-CBB-CCB
23	b	604	CLA	C10-C11-C12-C13
33	b	620	LMG	C19-C20-C21-C22
36	h	102	DGD	O1B-C1B-C2B-C3B
23	c	501	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C12-C13-C15
23	A	404	CLA	C11-C12-C13-C15
31	d	407	LHG	C17-C18-C19-C20
23	B	601	CLA	CAA-CBA-CGA-O1A
26	D	413	SQD	C29-C30-C31-C32
23	C	510	CLA	O1D-CGD-O2D-CED
35	E	102	LMT	O5B-C1B-O1B-C4'
31	l	101	LHG	C13-C14-C15-C16
23	B	613	CLA	C13-C15-C16-C17
31	A	416	LHG	C28-C29-C30-C31
23	b	616	CLA	C4-C3-C5-C6
33	j	101	LMG	C15-C16-C17-C18
31	D	408	LHG	C9-C10-C11-C12
35	M	101	LMT	C2-C3-C4-C5
23	C	508	CLA	C2A-CAA-CBA-CGA
25	a	409	BCR	C19-C20-C21-C22
23	a	405	CLA	C13-C15-C16-C17
31	A	417	LHG	C32-C33-C34-C35
26	A	412	SQD	O5-C1-O6-C44
34	b	622	HTG	C2'-C3'-C4'-C5'
23	c	509	CLA	O1D-CGD-O2D-CED
29	d	406	PL9	C34-C36-C37-C38
23	b	614	CLA	C2-C1-O2A-CGA
23	B	603	CLA	CBD-CGD-O2D-CED
36	C	518	DGD	C4A-C5A-C6A-C7A
31	d	409	LHG	C31-C32-C33-C34
23	c	504	CLA	C11-C12-C13-C14
33	c	519	LMG	C30-C31-C32-C33
23	b	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	620	SQD	C34-C35-C36-C37
31	l	101	LHG	C32-C33-C34-C35
26	D	413	SQD	C28-C29-C30-C31
35	m	102	LMT	O5'-C5'-C6'-O6'
35	M	101	LMT	O5'-C5'-C6'-O6'
25	d	405	BCR	C23-C24-C25-C30
23	B	615	CLA	C3-C5-C6-C7
25	D	406	BCR	C1-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C30
25	b	619	BCR	C23-C24-C25-C30
25	A	409	BCR	C1-C6-C7-C8
34	b	628	HTG	C4-C5-C6-O6
27	B	626	GOL	O1-C1-C2-C3
23	b	613	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	C4-C3-C5-C6
29	a	414	PL9	C15-C14-C16-C17
29	D	407	PL9	C35-C34-C36-C37
23	b	607	CLA	C13-C15-C16-C17
23	D	405	CLA	C10-C11-C12-C13
35	I	101	LMT	C1-C2-C3-C4
31	D	409	LHG	O6-C4-C5-O7
26	a	410	SQD	C31-C32-C33-C34
23	c	503	CLA	C2A-CAA-CBA-CGA
23	A	405	CLA	C4C-C3C-CAC-CBC
33	b	620	LMG	C33-C34-C35-C36
36	C	519	DGD	C8B-C9B-CAB-CBB
24	D	401	PHO	O1A-CGA-O2A-C1
26	L	101	SQD	C11-C10-C9-C8
23	B	616	CLA	C11-C12-C13-C15
23	c	510	CLA	C2-C3-C5-C6
23	c	510	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	C	503	CLA	C12-C13-C15-C16
23	b	603	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C2-C1-O6-C44
33	C	501	LMG	C29-C30-C31-C32
36	C	517	DGD	C7A-C8A-C9A-CAA
34	b	625	HTG	C4'-C5'-C6'-C7'
23	B	609	CLA	O1A-CGA-O2A-C1
23	b	606	CLA	C16-C17-C18-C19
33	Z	102	LMG	C18-C19-C20-C21
35	M	103	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C13-C15-C16-C17
33	a	416	LMG	C29-C30-C31-C32
34	c	521	HTG	O5-C1-S1-C1'
31	l	101	LHG	O7-C7-C8-C9
29	d	406	PL9	C45-C44-C46-C47
23	d	404	CLA	C10-C11-C12-C13
33	a	416	LMG	C21-C22-C23-C24
33	c	519	LMG	C32-C33-C34-C35
23	B	612	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	C2-C3-C5-C6
36	c	516	DGD	C6B-C7B-C8B-C9B
35	I	101	LMT	C5'-C4'-O1B-C1B
23	b	615	CLA	C16-C17-C18-C19
23	A	406	CLA	C14-C13-C15-C16
23	B	605	CLA	C14-C13-C15-C16
23	B	604	CLA	C11-C12-C13-C14
23	B	611	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
31	d	408	LHG	C35-C36-C37-C38
23	B	612	CLA	C3A-C2A-CAA-CBA
23	b	609	CLA	C3A-C2A-CAA-CBA
33	j	101	LMG	C36-C37-C38-C39
23	B	613	CLA	CAA-CBA-CGA-O2A
31	e	101	LHG	O8-C23-C24-C25
23	b	613	CLA	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	B	609	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
24	a	406	PHO	CAD-CBD-CGD-O2D
23	d	404	CLA	C16-C17-C18-C19
23	b	607	CLA	C16-C17-C18-C20
23	B	609	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	c	517	DGD	O1B-C1B-O2G-C2G
23	b	613	CLA	CAA-CBA-CGA-O2A
23	C	511	CLA	CAA-CBA-CGA-O2A
23	B	612	CLA	CAA-CBA-CGA-O2A
33	C	520	LMG	O8-C28-C29-C30
33	Z	102	LMG	O7-C10-C11-C12
26	a	412	SQD	O48-C23-C24-C25
33	C	501	LMG	C16-C17-C18-C19
36	C	519	DGD	C6B-C7B-C8B-C9B
23	B	607	CLA	C4-C3-C5-C6
29	D	407	PL9	C33-C34-C36-C37
33	C	520	LMG	O7-C10-C11-C12
26	f	101	SQD	O47-C7-C8-C9
25	b	619	BCR	C21-C22-C23-C24
26	B	620	SQD	C16-C17-C18-C19
23	b	603	CLA	O1A-CGA-O2A-C1
31	d	408	LHG	C25-C26-C27-C28
23	b	612	CLA	CAA-CBA-CGA-O2A
33	J	101	LMG	O7-C10-C11-C12
34	b	622	HTG	C4'-C5'-C6'-C7'
31	l	101	LHG	C35-C36-C37-C38
23	b	613	CLA	O2A-C1-C2-C3
24	D	401	PHO	O2A-C1-C2-C3
23	b	602	CLA	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
23	B	602	CLA	O2A-C1-C2-C3
36	H	102	DGD	CDB-CEB-CFB-CGB
36	C	519	DGD	C3A-C4A-C5A-C6A
26	A	412	SQD	C30-C31-C32-C33
23	a	405	CLA	C16-C17-C18-C20
36	C	517	DGD	CDB-CEB-CFB-CGB
23	C	508	CLA	CHA-CBD-CGD-O1D
23	B	605	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	A	405	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CHA-CBD-CGD-O2D
25	y	101	BCR	C9-C10-C11-C12
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O2D
31	A	417	LHG	O7-C7-C8-C9
26	L	101	SQD	C29-C30-C31-C32
34	d	411	HTG	C1'-C2'-C3'-C4'
23	c	507	CLA	C5-C6-C7-C8
33	c	519	LMG	O7-C10-C11-C12
36	C	519	DGD	CCB-CDB-CEB-CFB
33	Z	102	LMG	O1-C7-C8-O7
35	b	621	LMT	C6-C7-C8-C9
35	B	630	LMT	C4-C5-C6-C7
23	c	510	CLA	CAA-CBA-CGA-O2A
26	L	101	SQD	C18-C19-C20-C21
23	D	404	CLA	C16-C17-C18-C20
26	A	410	SQD	C13-C14-C15-C16
23	A	406	CLA	CBA-CGA-O2A-C1
35	I	101	LMT	C4-C5-C6-C7
23	A	406	CLA	O1A-CGA-O2A-C1
23	D	405	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	C	505	CLA	C6-C7-C8-C10
23	c	505	CLA	C6-C7-C8-C10
23	A	404	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C10-C8-C7
36	c	517	DGD	CBB-CCB-CDB-CEB
35	B	630	LMT	C3-C4-C5-C6
23	C	505	CLA	C6-C7-C8-C9
23	A	404	CLA	C11-C12-C13-C14
23	c	504	CLA	C14-C13-C15-C16
33	C	501	LMG	C17-C18-C19-C20
34	c	521	HTG	C2'-C3'-C4'-C5'
31	d	409	LHG	O8-C23-C24-C25
26	L	101	SQD	O48-C23-C24-C25
26	A	412	SQD	C5-C6-S-O8
23	a	404	CLA	C16-C17-C18-C20
23	C	511	CLA	C16-C17-C18-C20
29	a	414	PL9	C31-C32-C33-C34
36	h	102	DGD	CAA-CBA-CCA-CDA
33	C	520	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	O10-C28-C29-C30
31	d	408	LHG	C17-C18-C19-C20
31	l	101	LHG	O9-C7-C8-C9
23	b	612	CLA	CAA-CBA-CGA-O1A
26	a	412	SQD	O10-C23-C24-C25
33	C	520	LMG	C32-C33-C34-C35
23	b	604	CLA	C8-C10-C11-C12
31	l	101	LHG	C28-C29-C30-C31
31	E	101	LHG	C12-C13-C14-C15
23	C	507	CLA	C1A-C2A-CAA-CBA
23	b	612	CLA	C1A-C2A-CAA-CBA
36	C	519	DGD	C1B-C2B-C3B-C4B
31	e	101	LHG	O10-C23-C24-C25
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	CAA-CBA-CGA-O1A
26	f	101	SQD	O49-C7-C8-C9
33	J	101	LMG	O9-C10-C11-C12
33	B	621	LMG	O1-C7-C8-C9
23	B	603	CLA	C2A-CAA-CBA-CGA
23	c	501	CLA	C2A-CAA-CBA-CGA
36	h	102	DGD	CDB-CEB-CFB-CGB
34	B	627	HTG	C2'-C3'-C4'-C5'
35	E	102	LMT	C6-C7-C8-C9
23	B	610	CLA	C13-C15-C16-C17
31	E	101	LHG	C4-O6-P-O5
31	D	409	LHG	C4-O6-P-O5
31	A	417	LHG	C3-O3-P-O5
23	B	616	CLA	C16-C17-C18-C20
36	C	519	DGD	C3B-C4B-C5B-C6B
23	b	613	CLA	CAA-CBA-CGA-O1A
33	Z	102	LMG	O9-C10-C11-C12
31	A	417	LHG	O9-C7-C8-C9
36	h	102	DGD	C6A-C7A-C8A-C9A
25	d	405	BCR	C23-C24-C25-C26
25	A	409	BCR	C5-C6-C7-C8
23	B	612	CLA	CAA-CBA-CGA-O1A
26	a	410	SQD	C26-C27-C28-C29
35	B	629	LMT	C3'-C4'-O1B-C1B
23	C	506	CLA	CAA-CBA-CGA-O2A
29	D	407	PL9	C11-C12-C13-C14
29	D	407	PL9	C36-C37-C38-C39
23	b	607	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	A	406	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	612	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
33	c	519	LMG	O9-C10-C11-C12
36	H	102	DGD	C2B-C3B-C4B-C5B
23	D	405	CLA	C14-C13-C15-C16
23	a	404	CLA	C14-C13-C15-C16
23	b	616	CLA	C14-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C9
23	B	606	CLA	C11-C10-C8-C9
31	e	101	LHG	C23-C24-C25-C26
26	A	412	SQD	C28-C29-C30-C31
35	B	630	LMT	C4'-C5'-C6'-O6'
23	b	614	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
31	d	407	LHG	C1-C2-C3-O3
36	H	102	DGD	C5B-C6B-C7B-C8B
36	c	516	DGD	CCB-CDB-CEB-CFB
31	d	407	LHG	C18-C19-C20-C21
31	l	101	LHG	O6-C4-C5-O7
23	a	404	CLA	C12-C13-C15-C16
23	B	615	CLA	C6-C7-C8-C10
23	b	616	CLA	C12-C13-C15-C16
23	c	501	CLA	C11-C12-C13-C15
29	a	414	PL9	C13-C14-C16-C17
23	B	601	CLA	C11-C10-C8-C7
33	b	620	LMG	O7-C10-C11-C12
23	c	512	CLA	CAA-CBA-CGA-O2A
36	C	517	DGD	O2G-C1B-C2B-C3B
26	A	410	SQD	O47-C7-C8-C9
31	d	409	LHG	O10-C23-C24-C25
23	c	512	CLA	CAA-CBA-CGA-O1A
26	A	410	SQD	O49-C7-C8-C9
35	D	403	LMT	C3-C4-C5-C6
23	c	510	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
23	C	509	CLA	C13-C15-C16-C17
36	C	518	DGD	CBA-CCA-CDA-CEA

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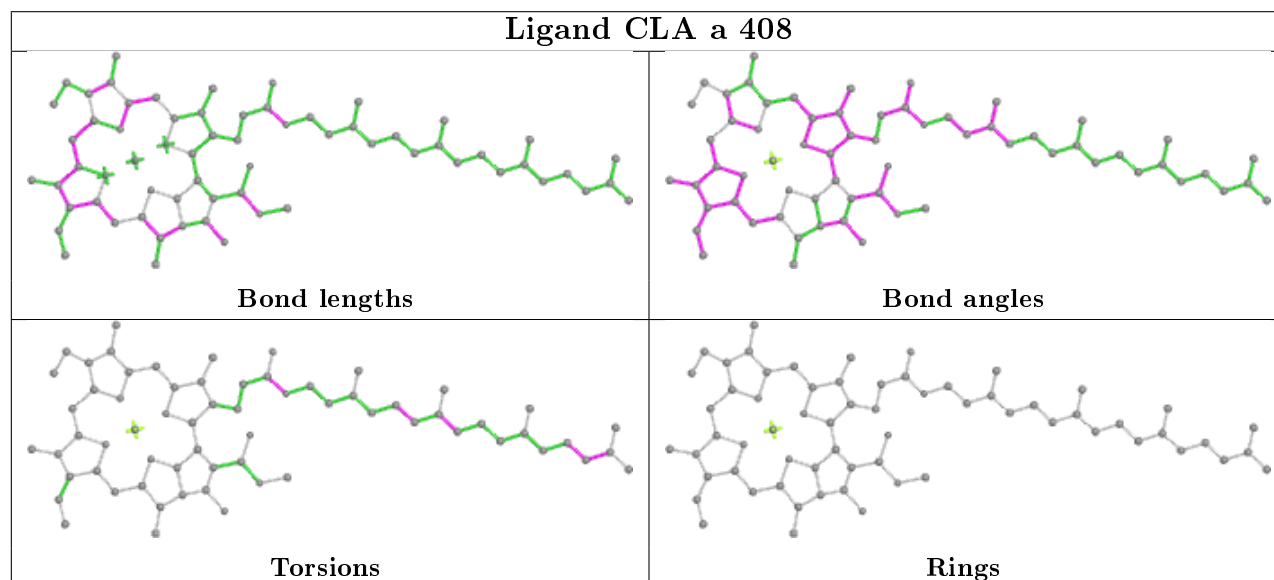
*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
33	b	620	LMG	O9-C10-C11-C12
26	L	101	SQD	O10-C23-C24-C25
33	B	621	LMG	C19-C20-C21-C22
23	b	616	CLA	C10-C11-C12-C13
36	c	516	DGD	O2G-C1B-C2B-C3B
23	B	612	CLA	C13-C15-C16-C17
23	c	510	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	C13-C15-C16-C17
23	c	505	CLA	CAA-CBA-CGA-O2A
23	b	602	CLA	CAA-CBA-CGA-O2A
36	C	517	DGD	O1G-C1A-C2A-C3A
35	b	621	LMT	C3'-C4'-O1B-C1B

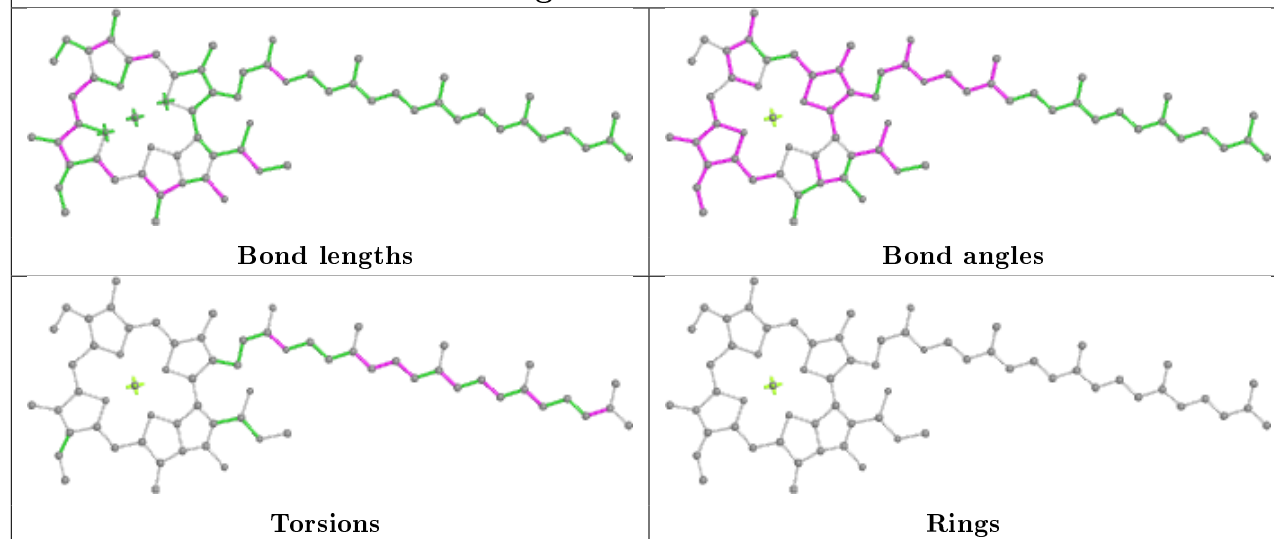
There are no ring outliers.

No monomer is involved in short contacts.

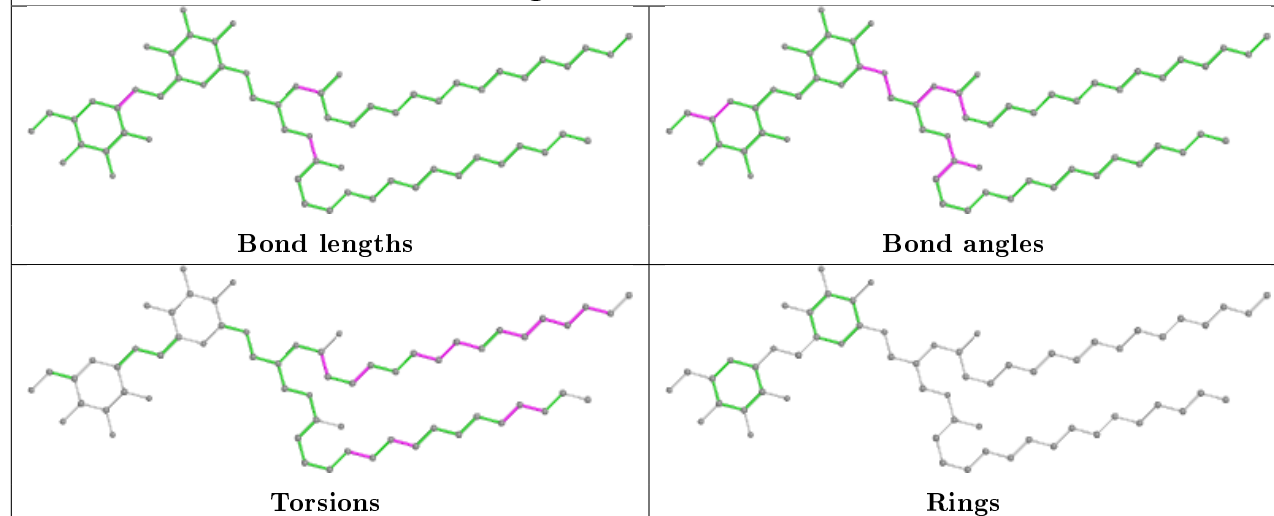
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



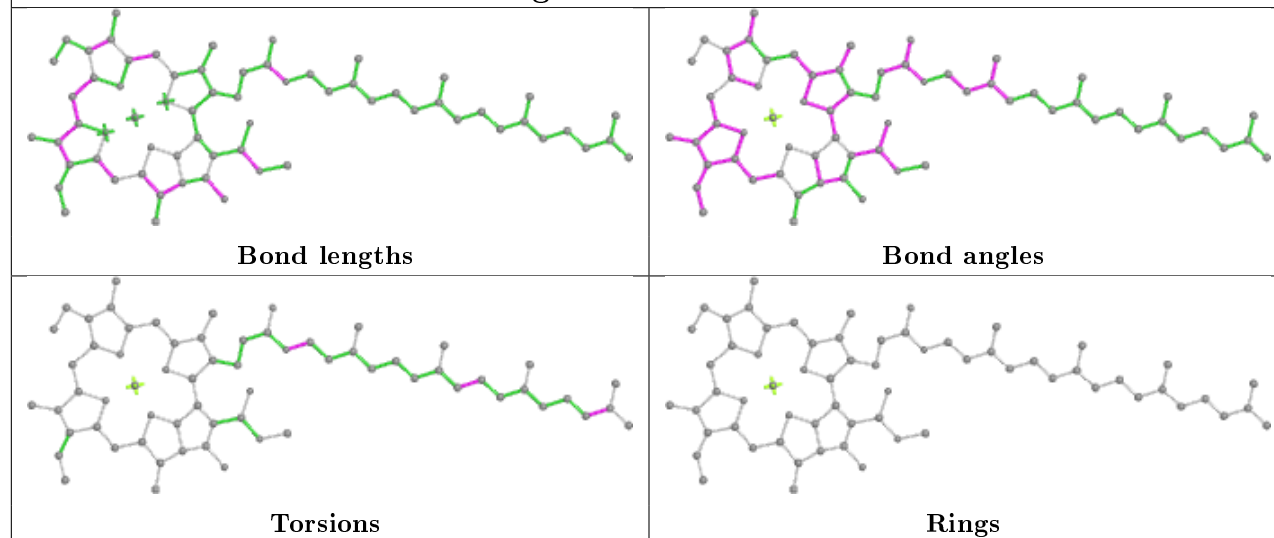
## Ligand CLA d 404



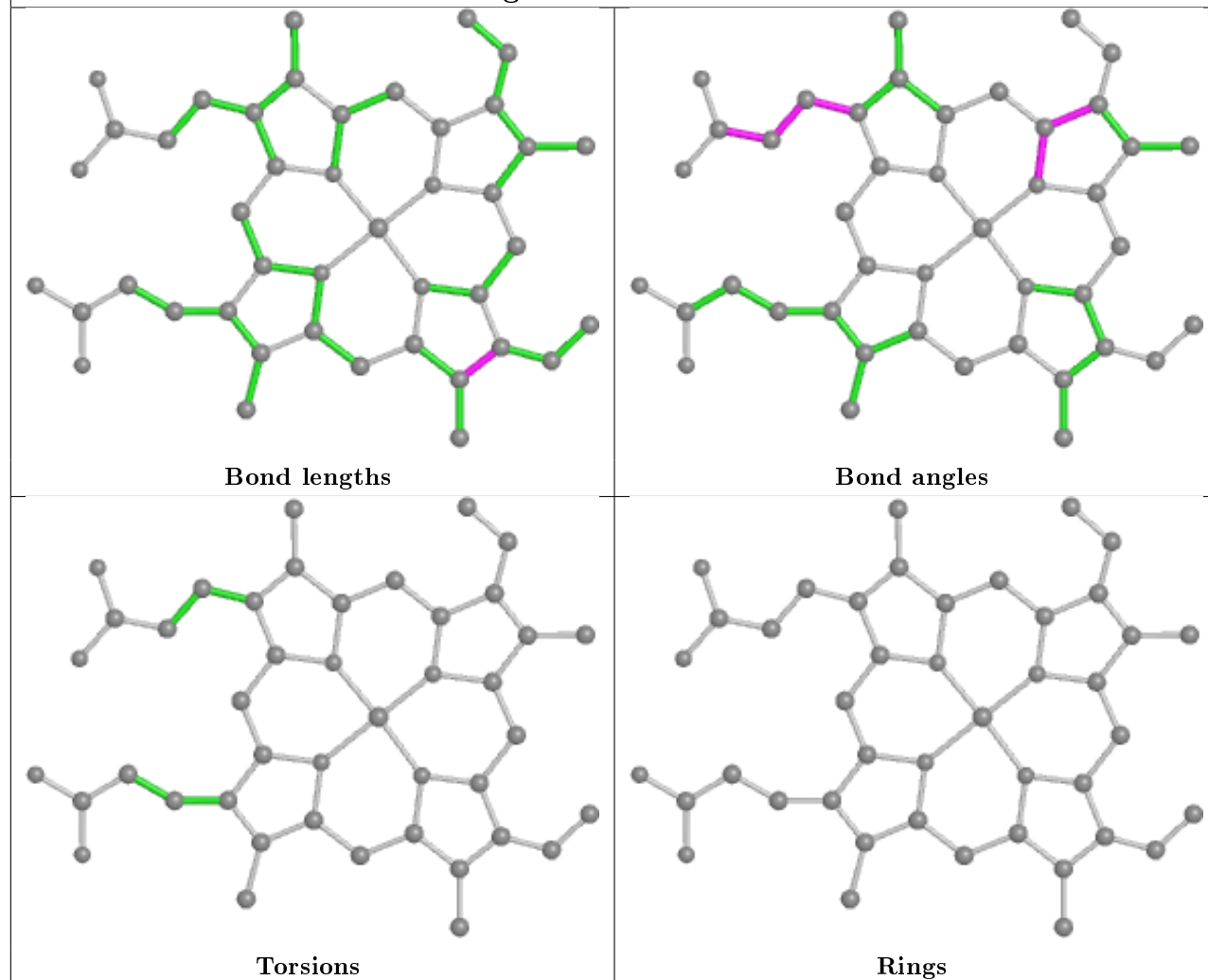
## Ligand DGD H 102



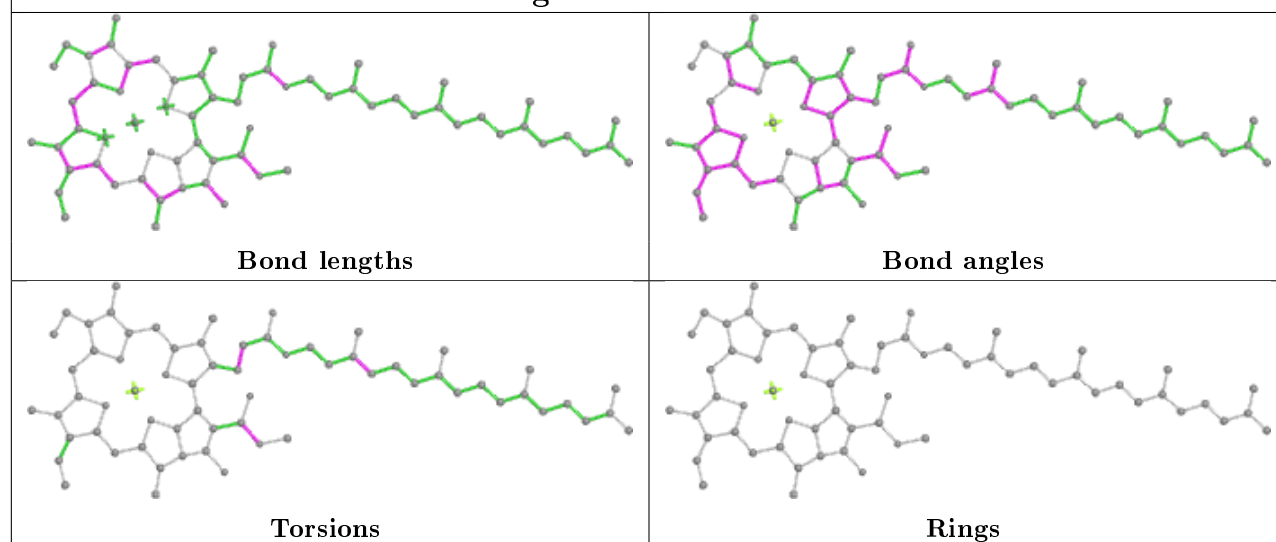
## Ligand CLA B 608



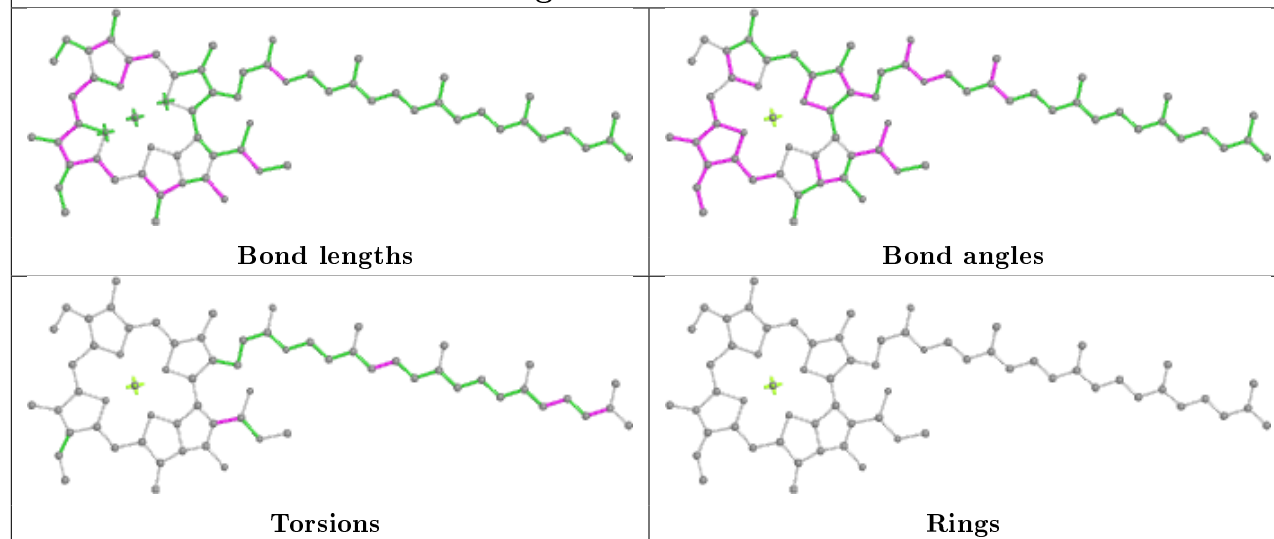
## Ligand HEM e 103



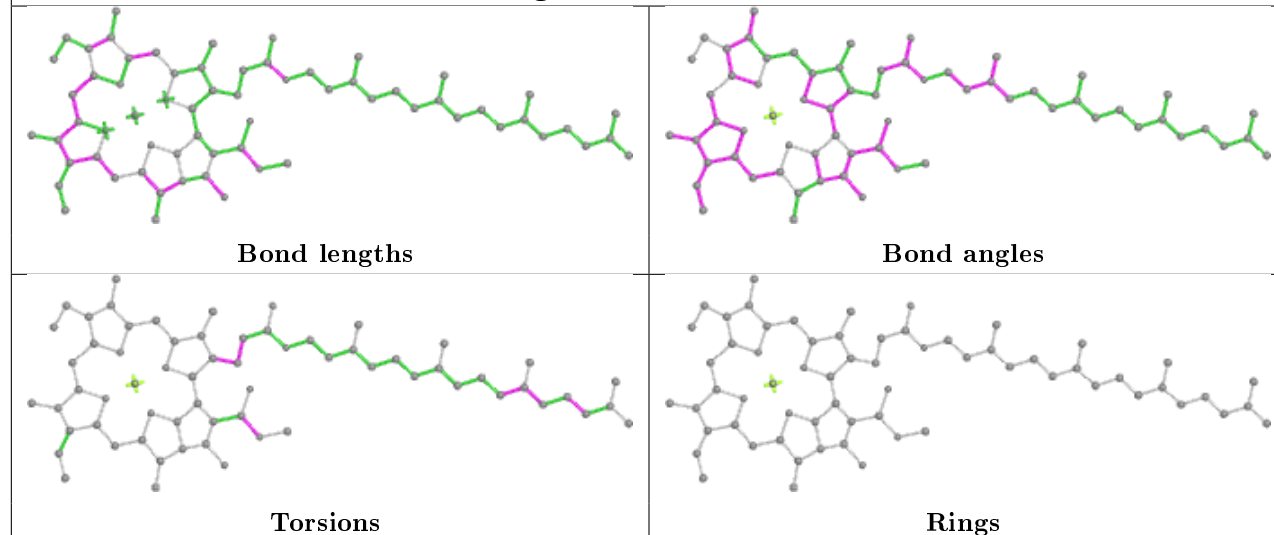
## Ligand CLA B 603



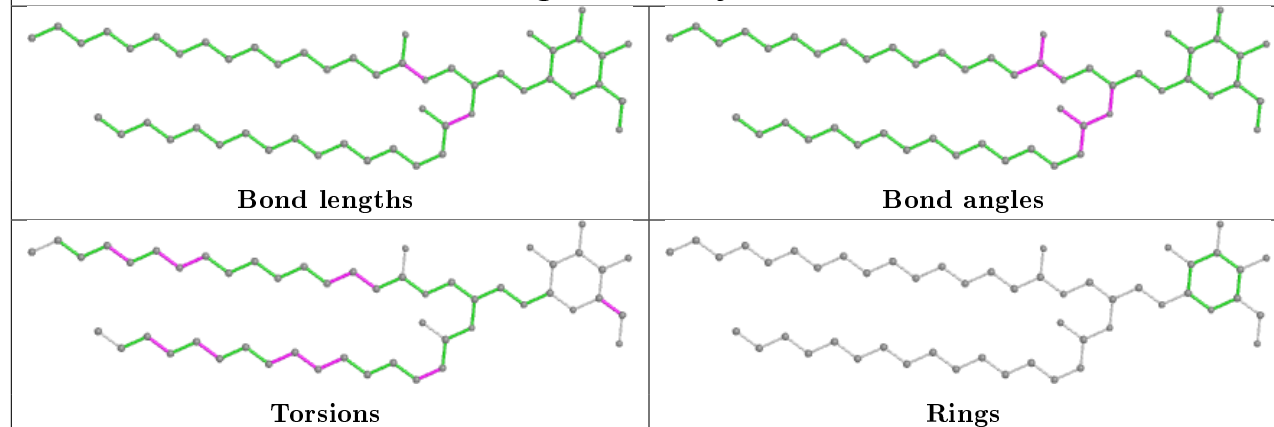
## Ligand CLA b 607



## Ligand CLA C 502

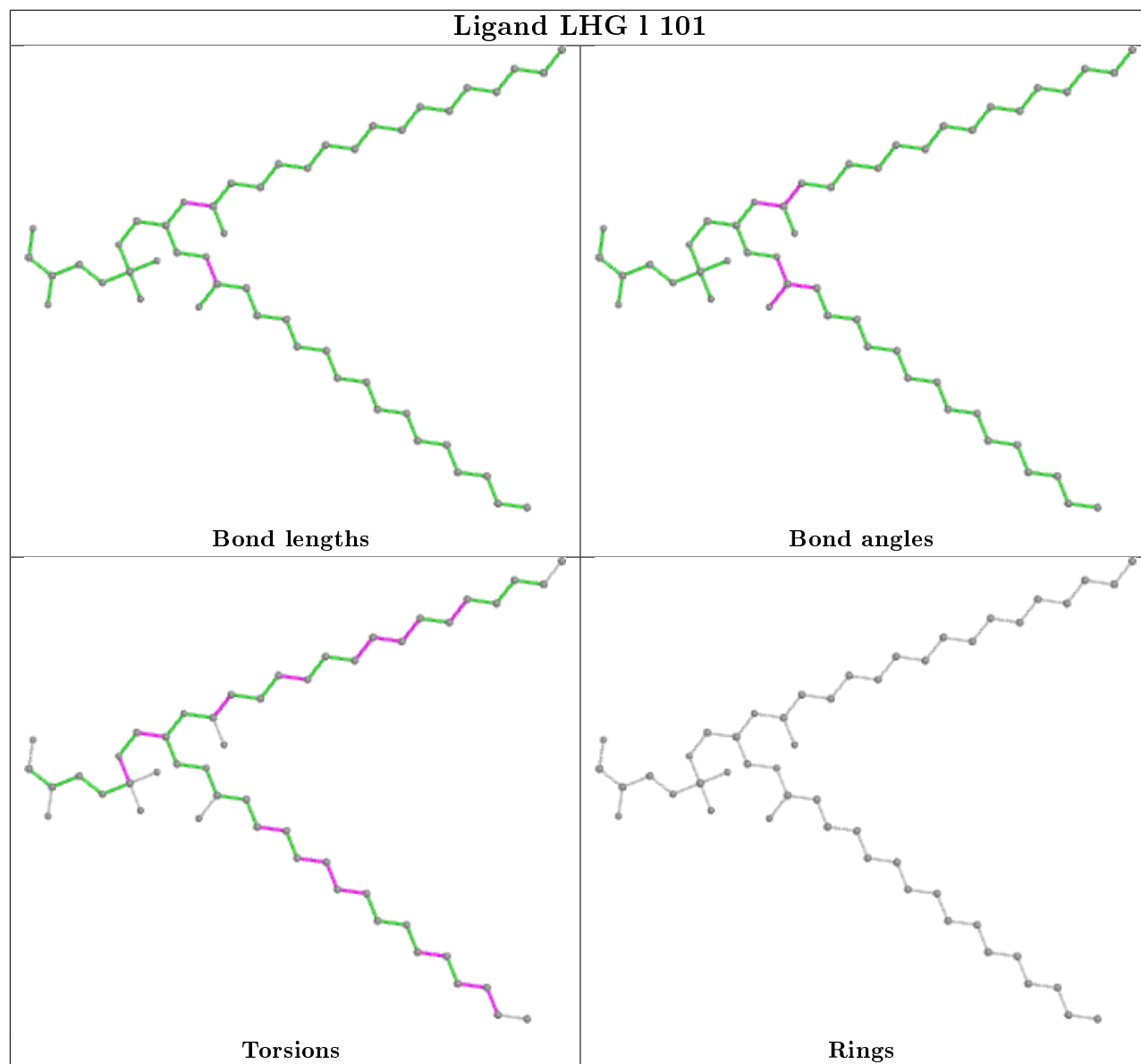


## Ligand LMG j 101

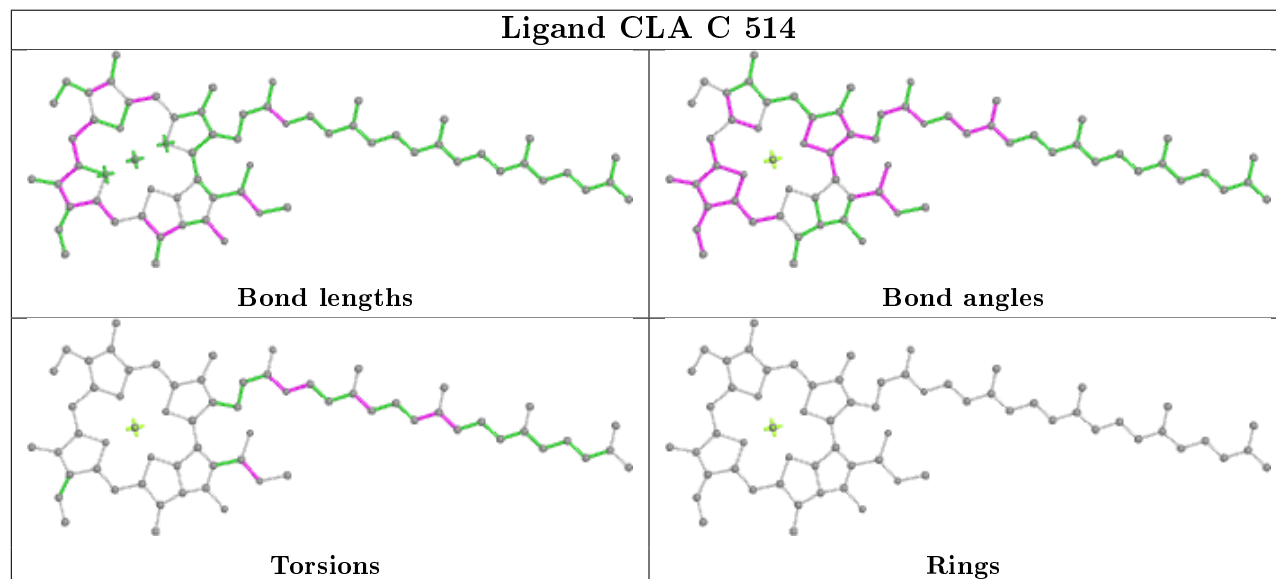


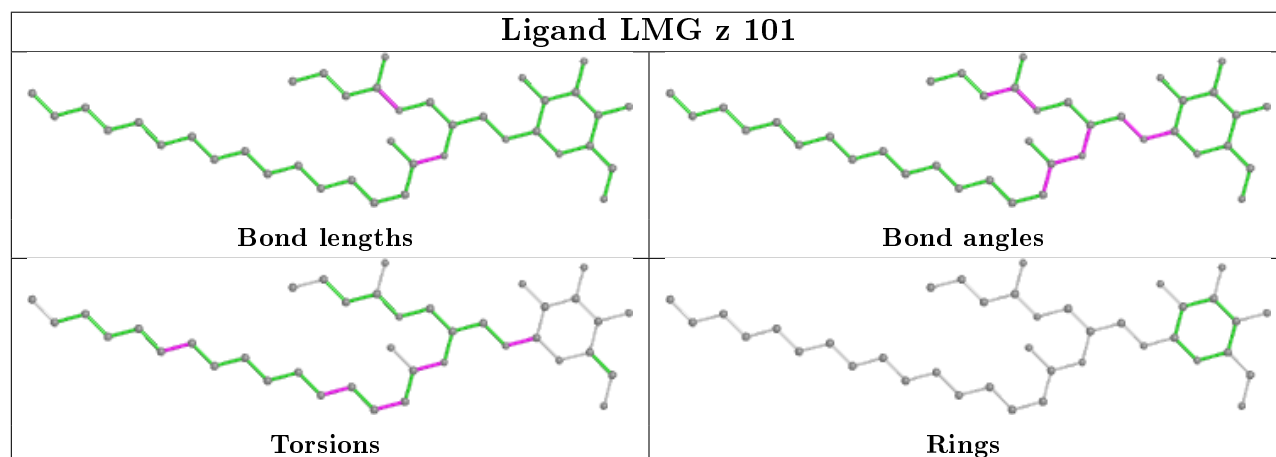
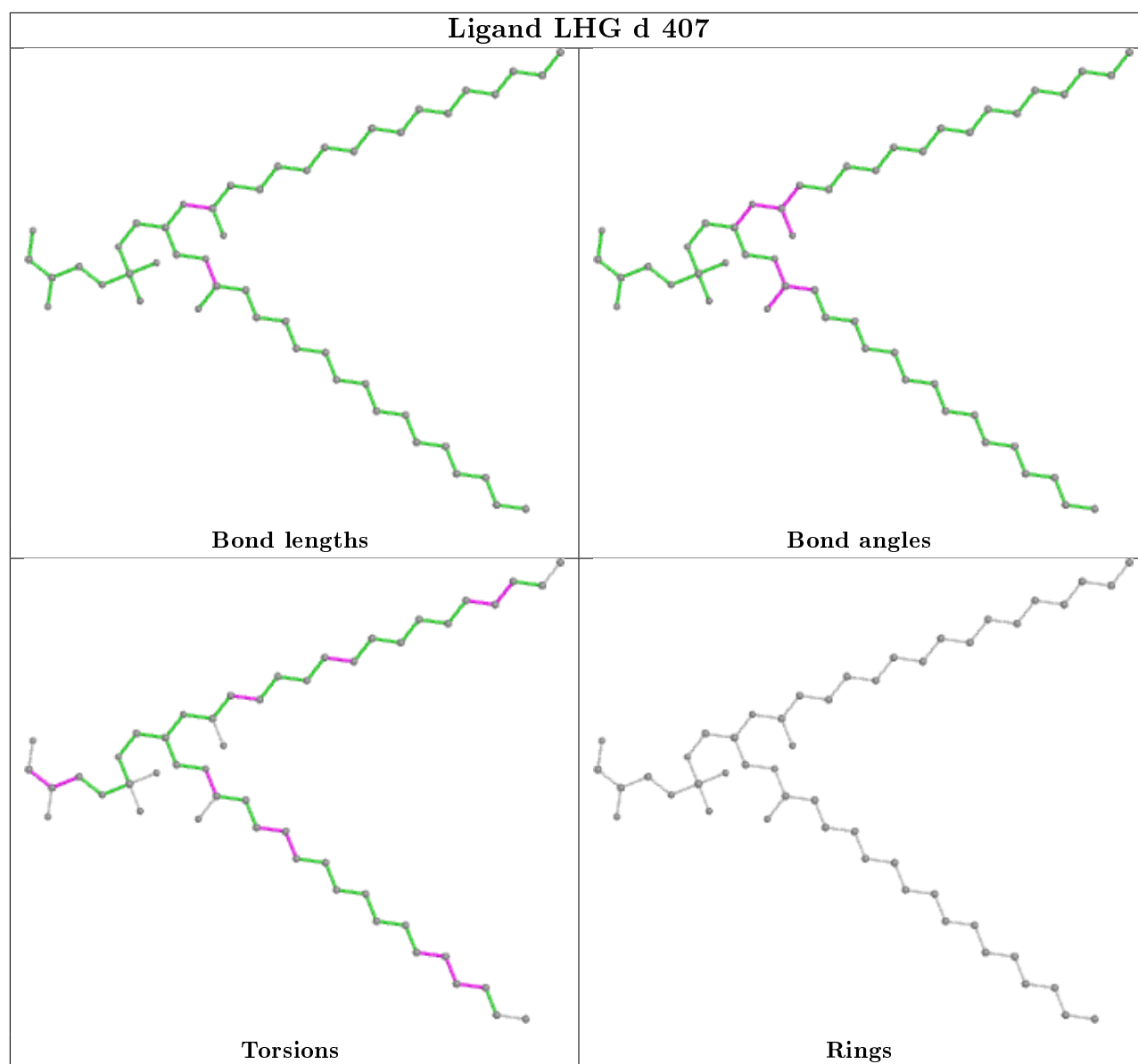


## Ligand LHG 1 101

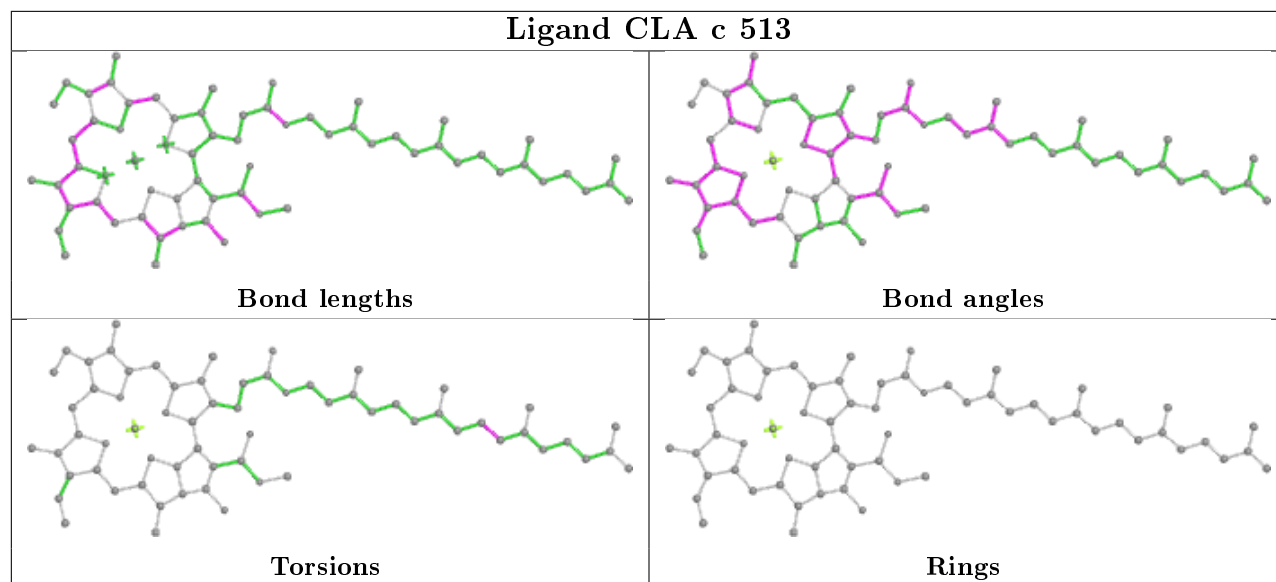


## Ligand CLA C 514

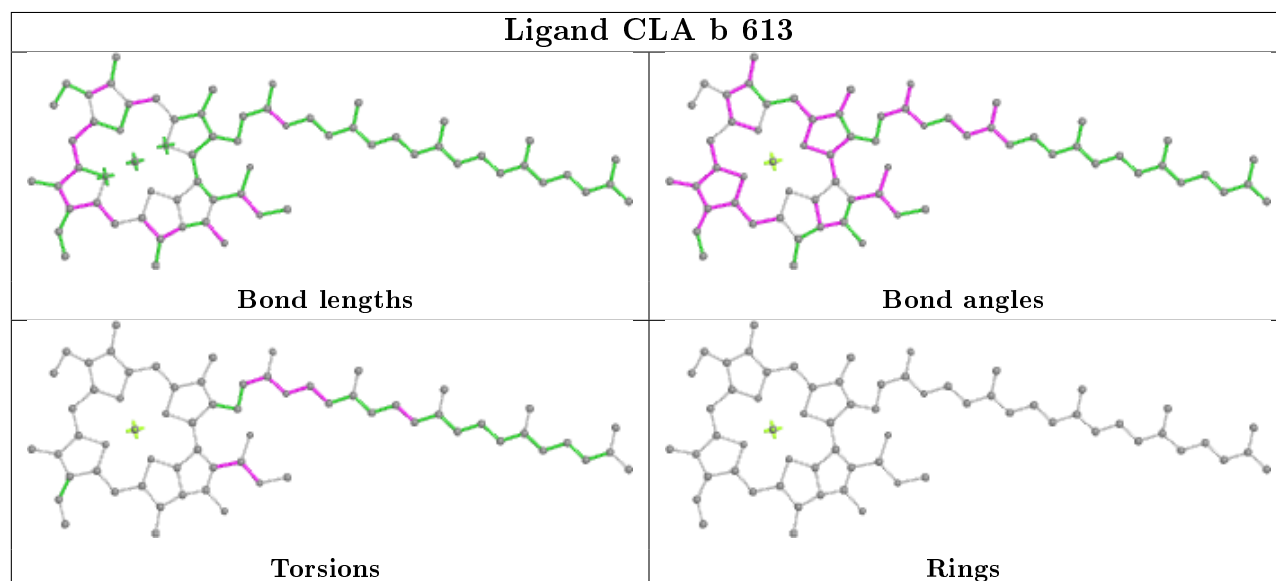




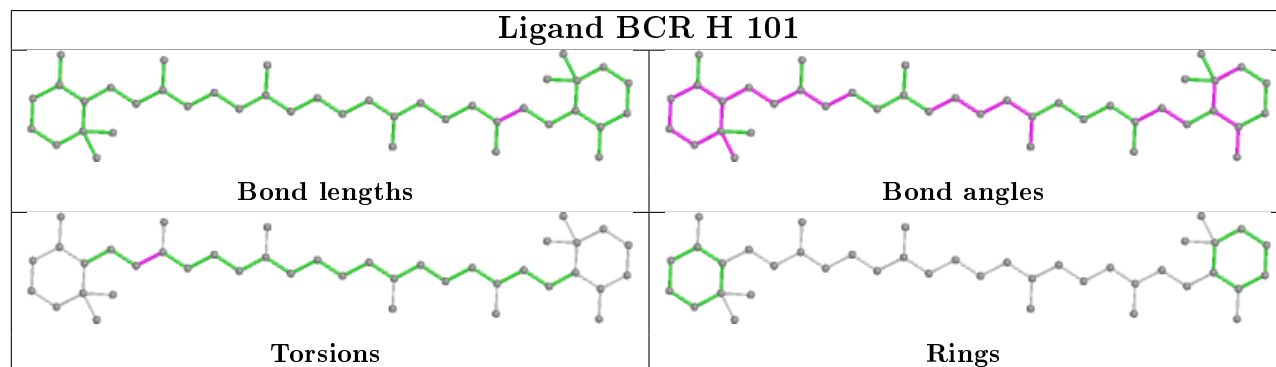
## Ligand CLA c 513

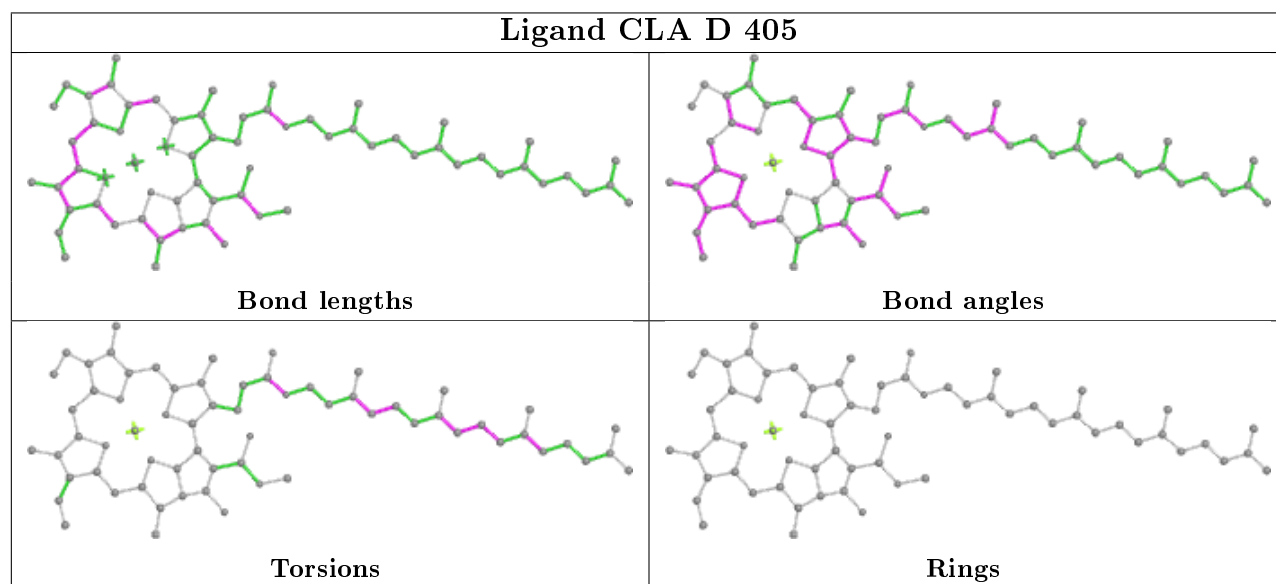
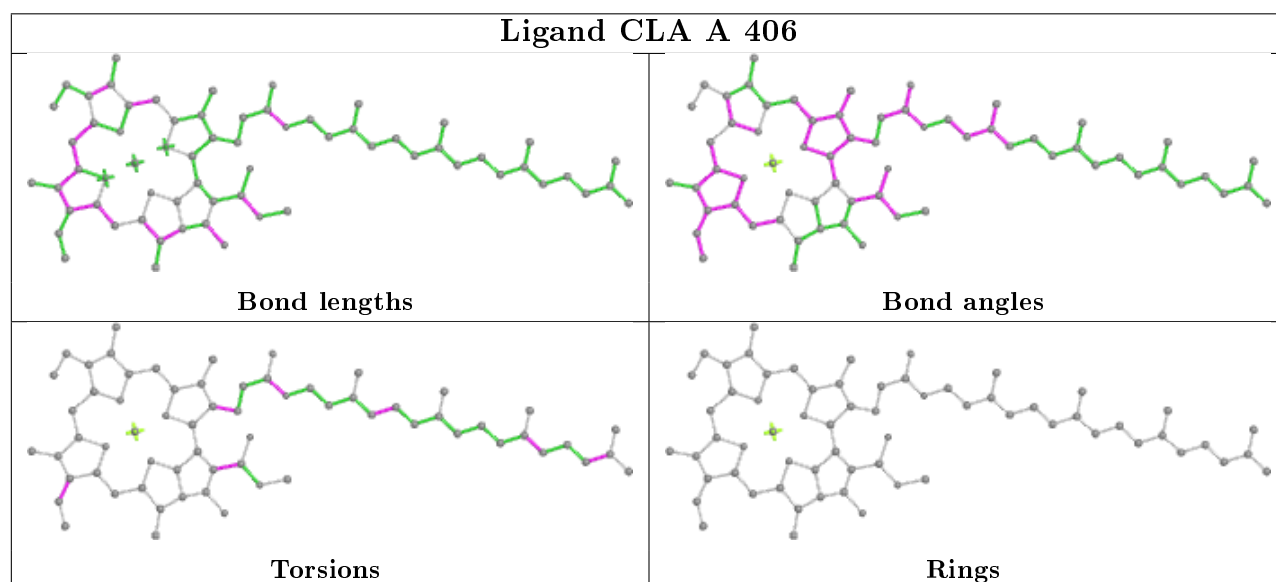
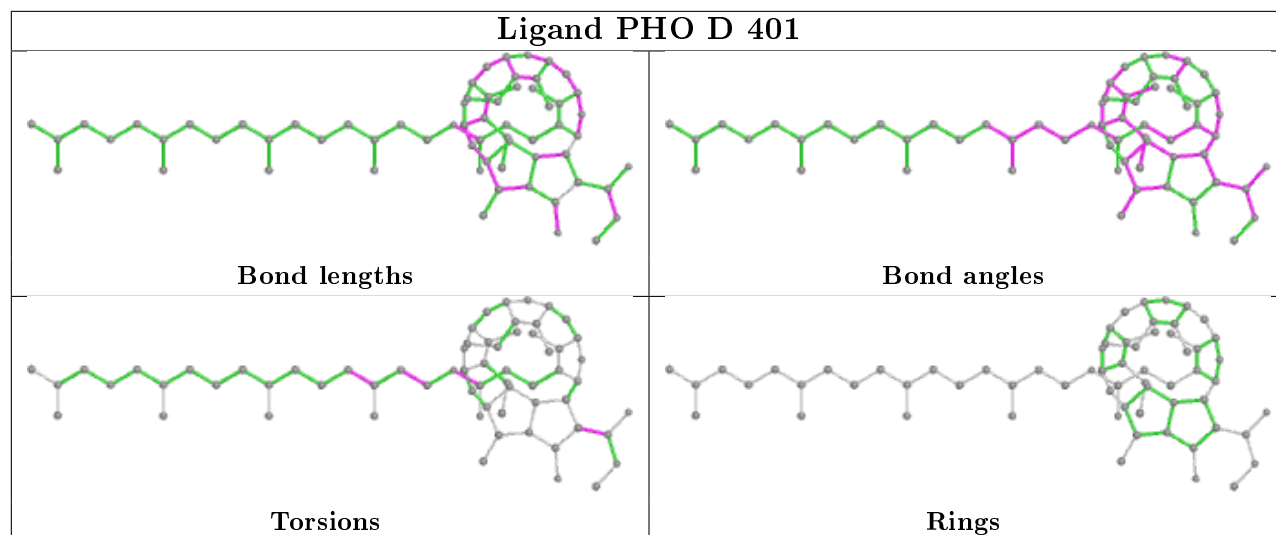


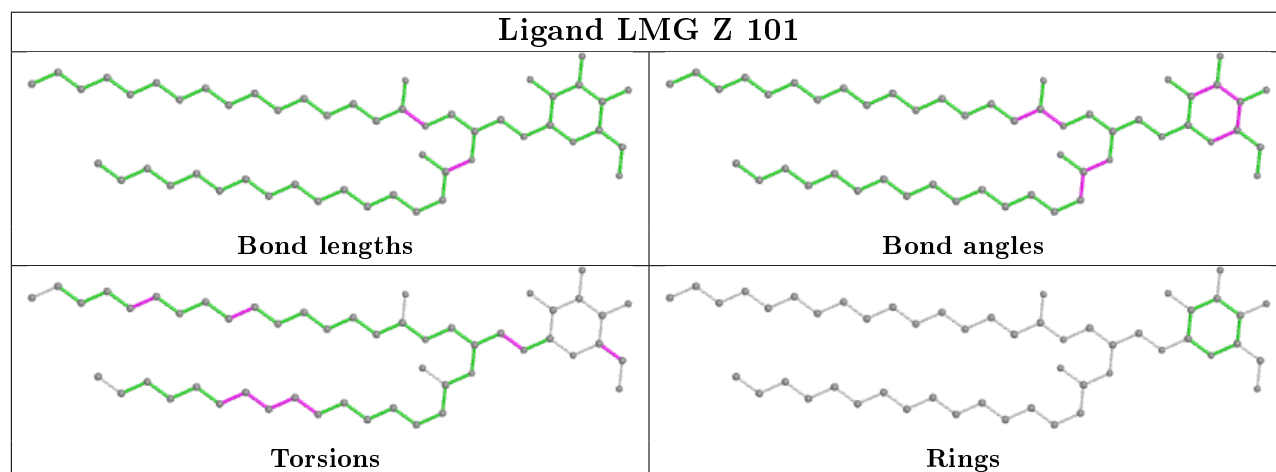
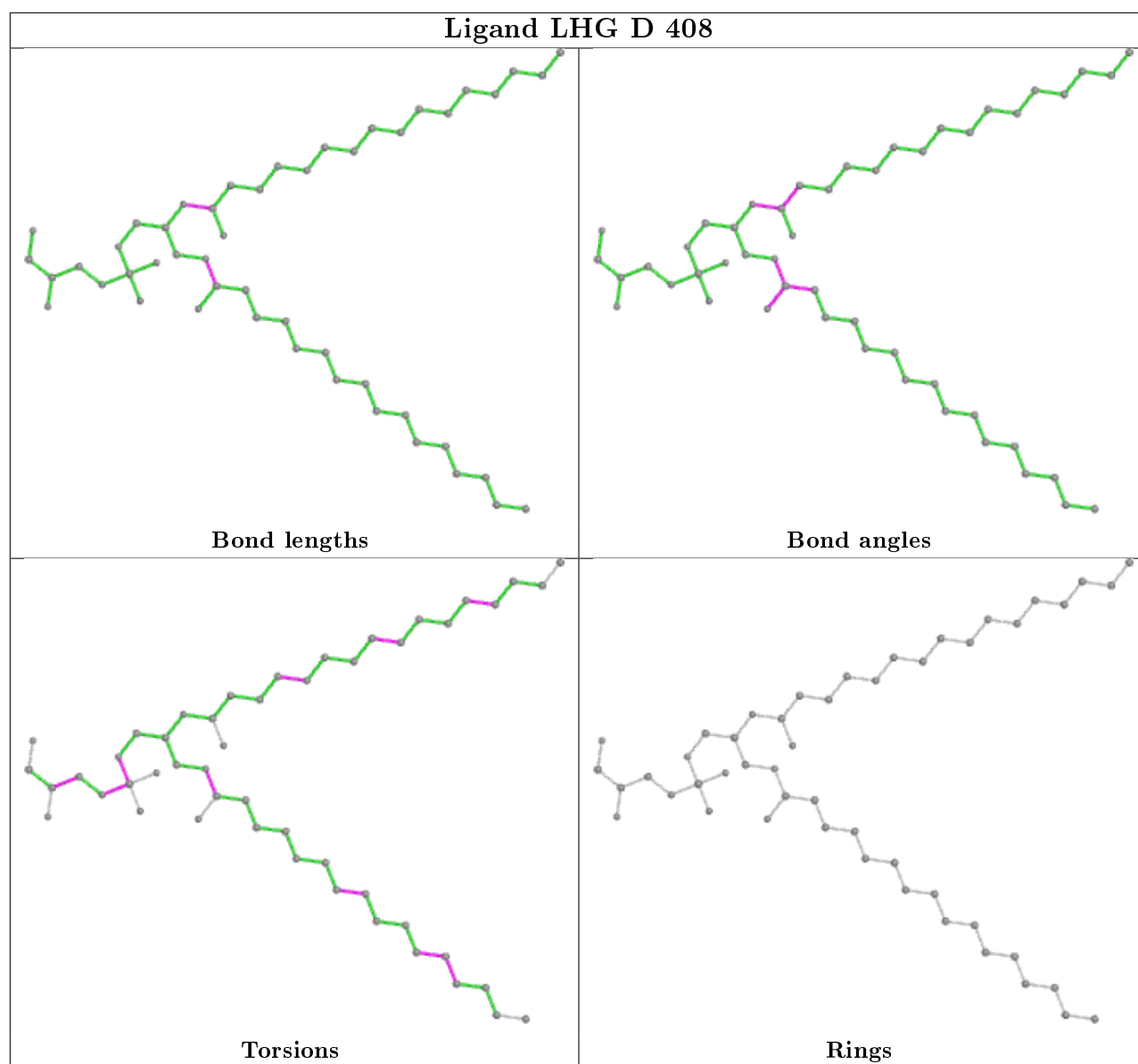
## Ligand CLA b 613



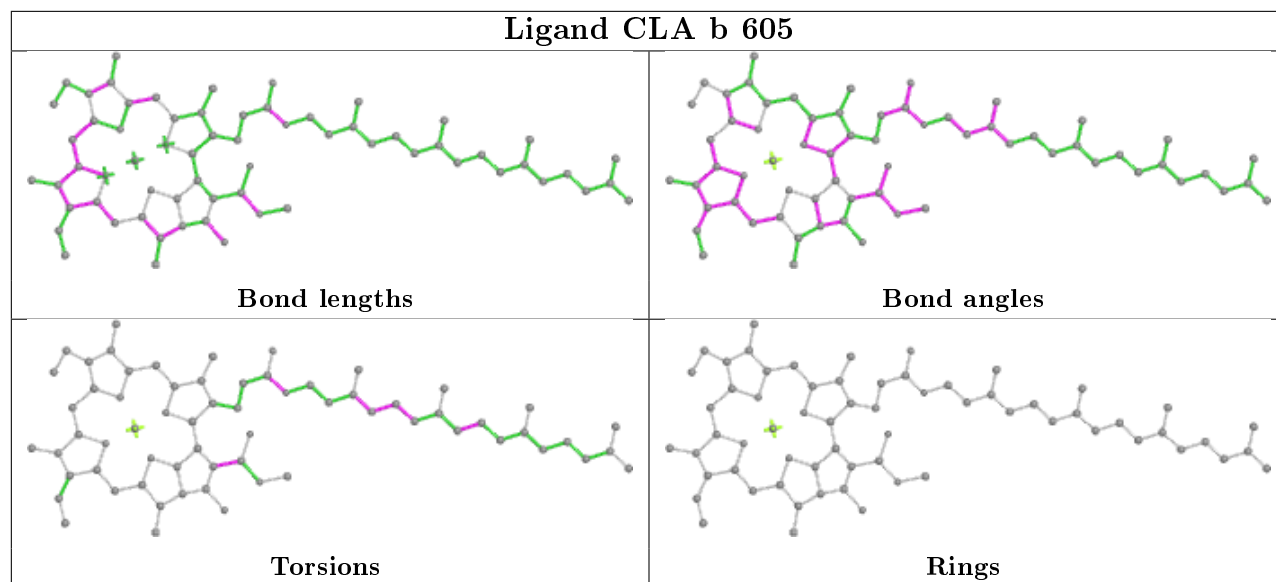
## Ligand BCR H 101



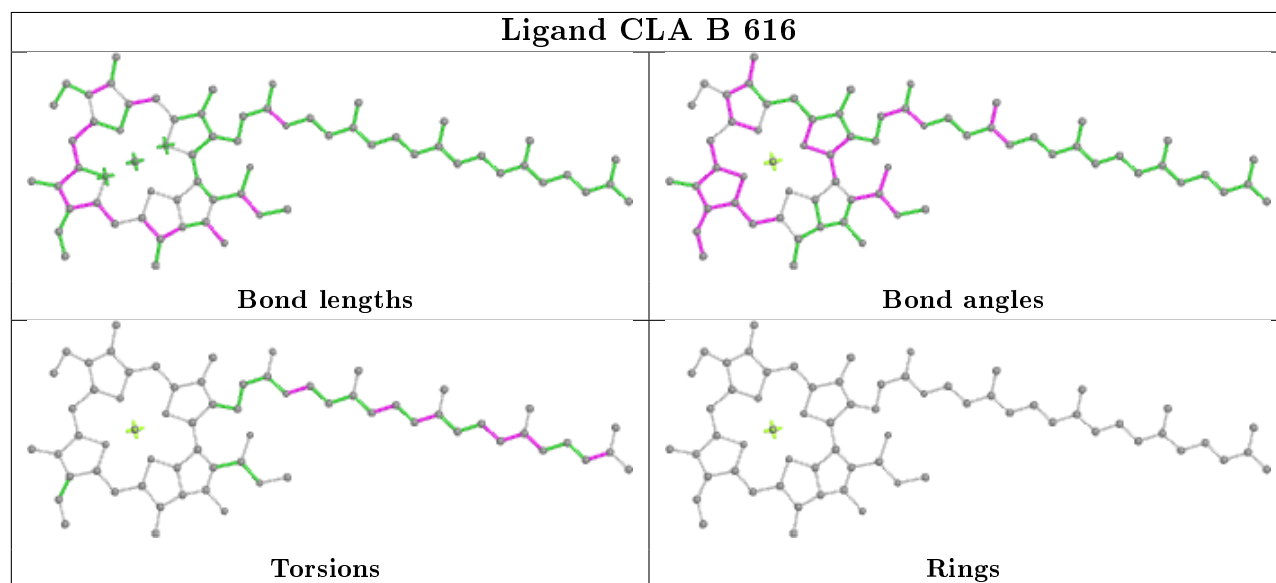


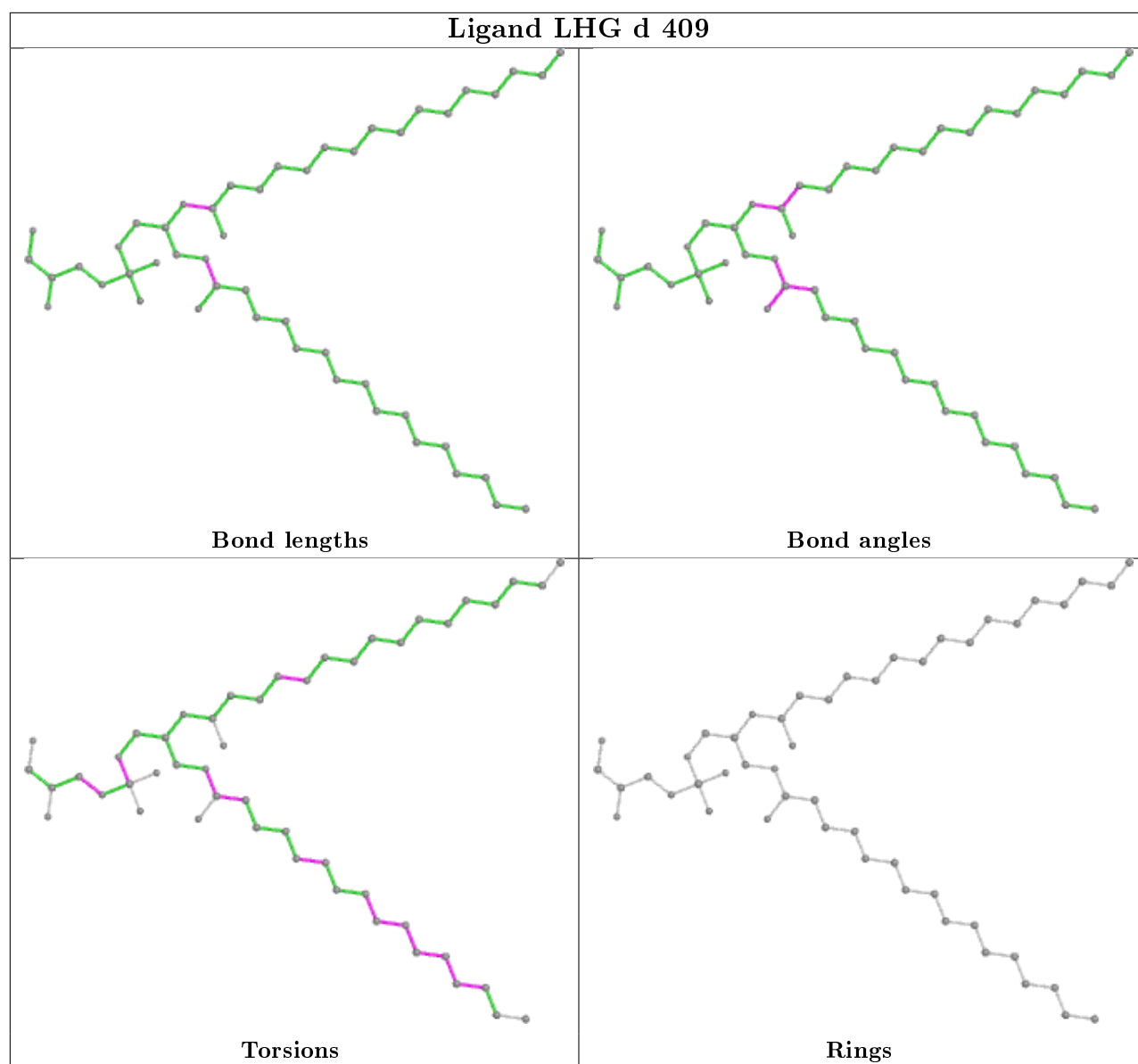


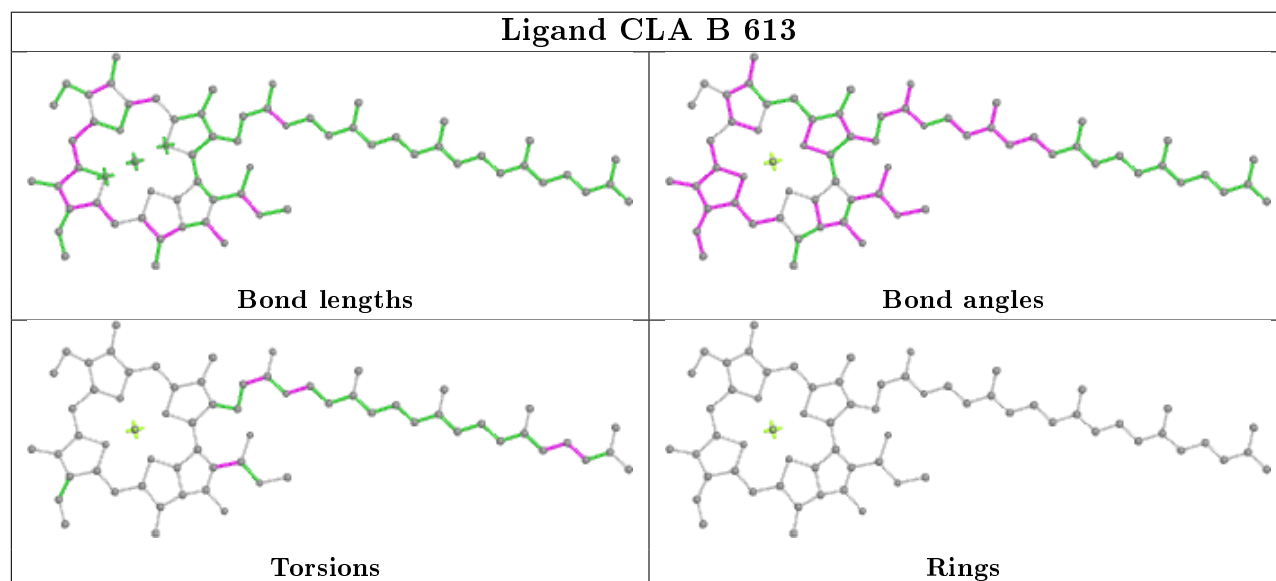
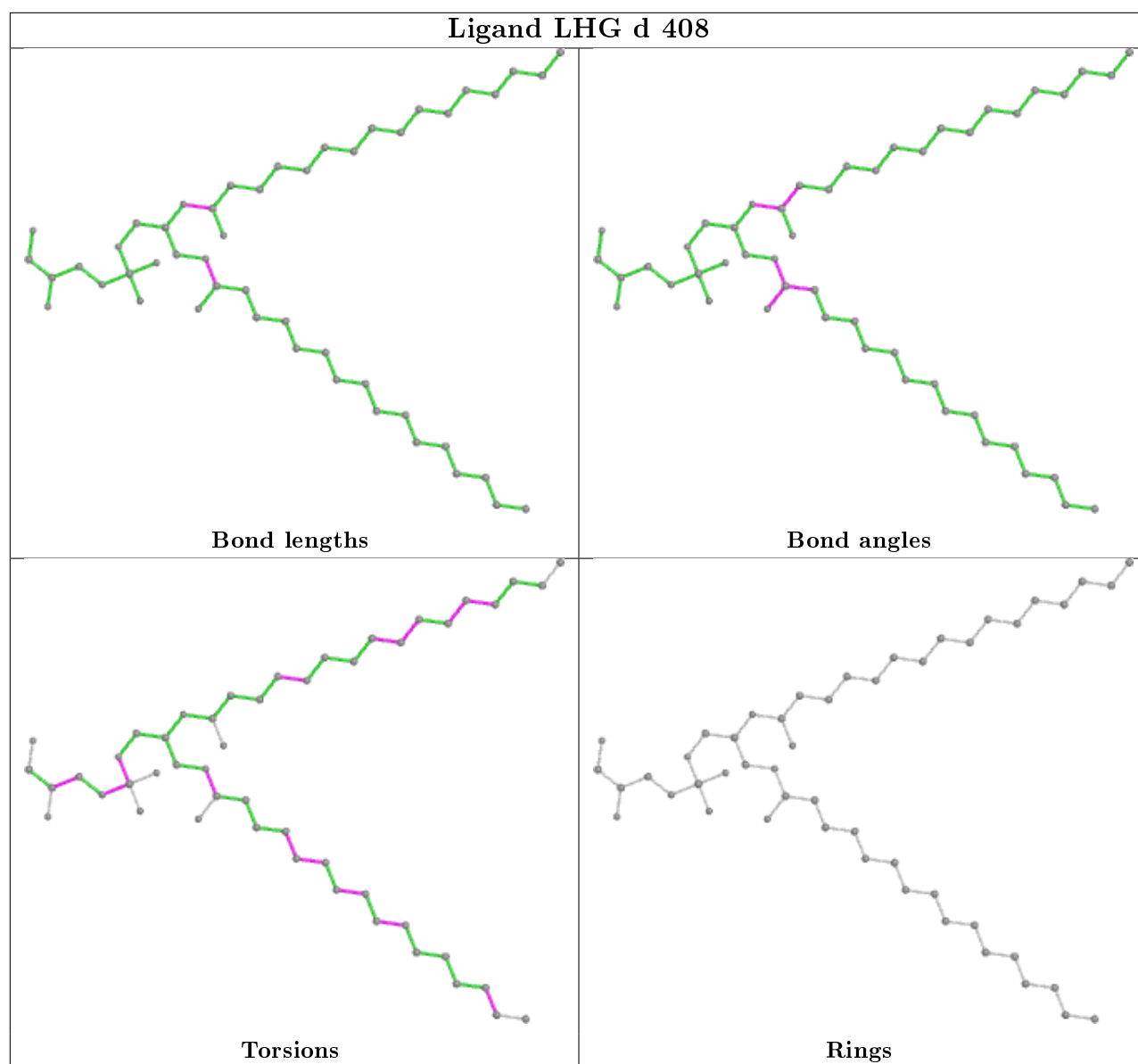
## Ligand CLA b 605



## Ligand CLA B 616

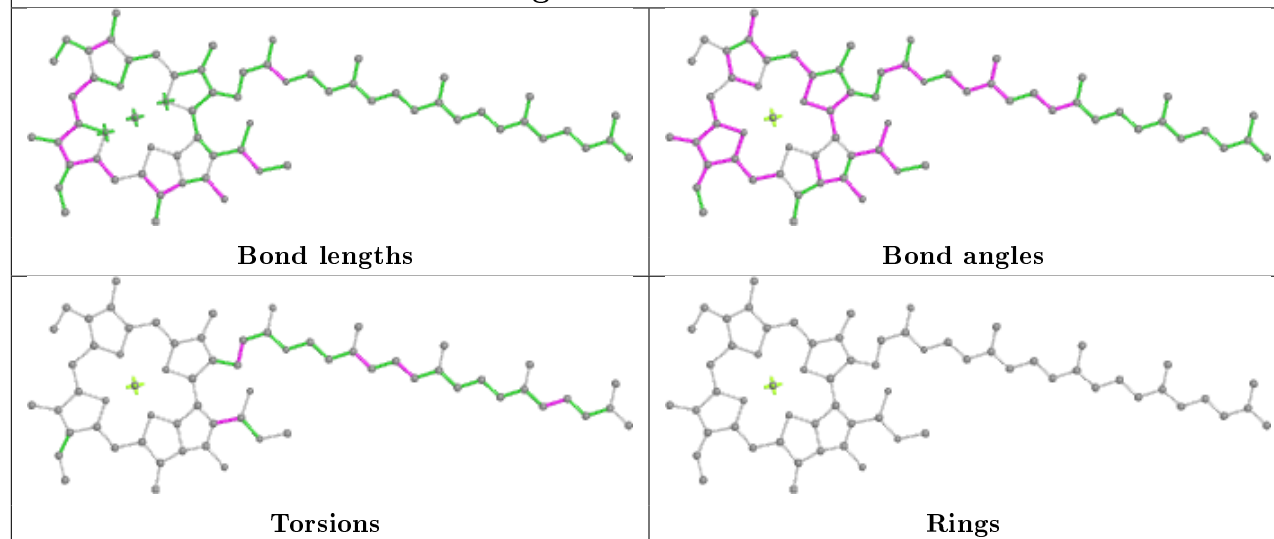




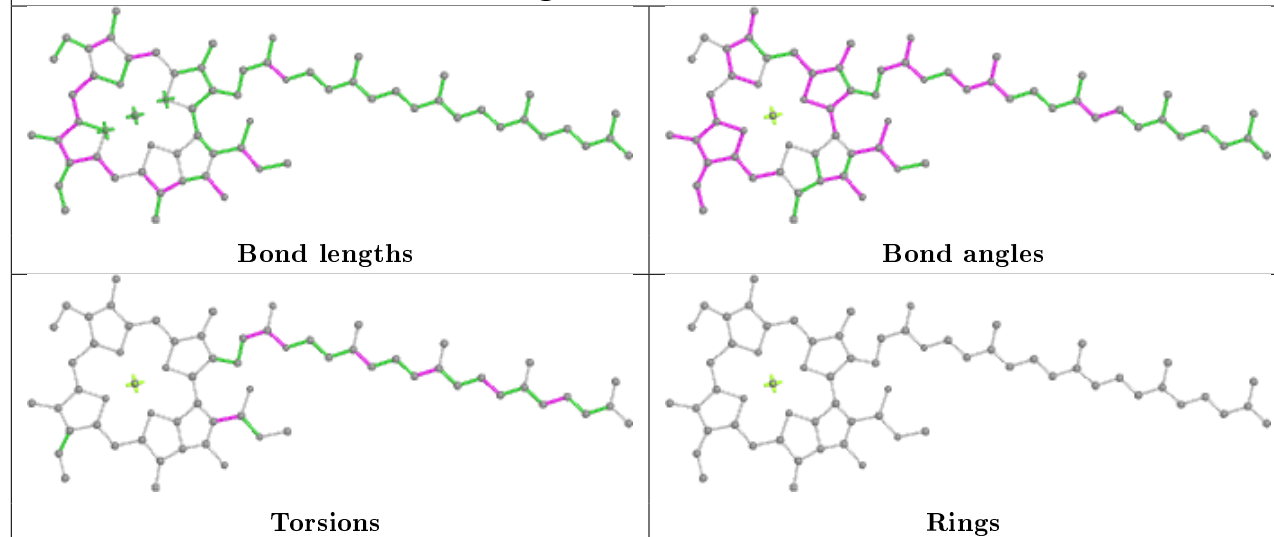




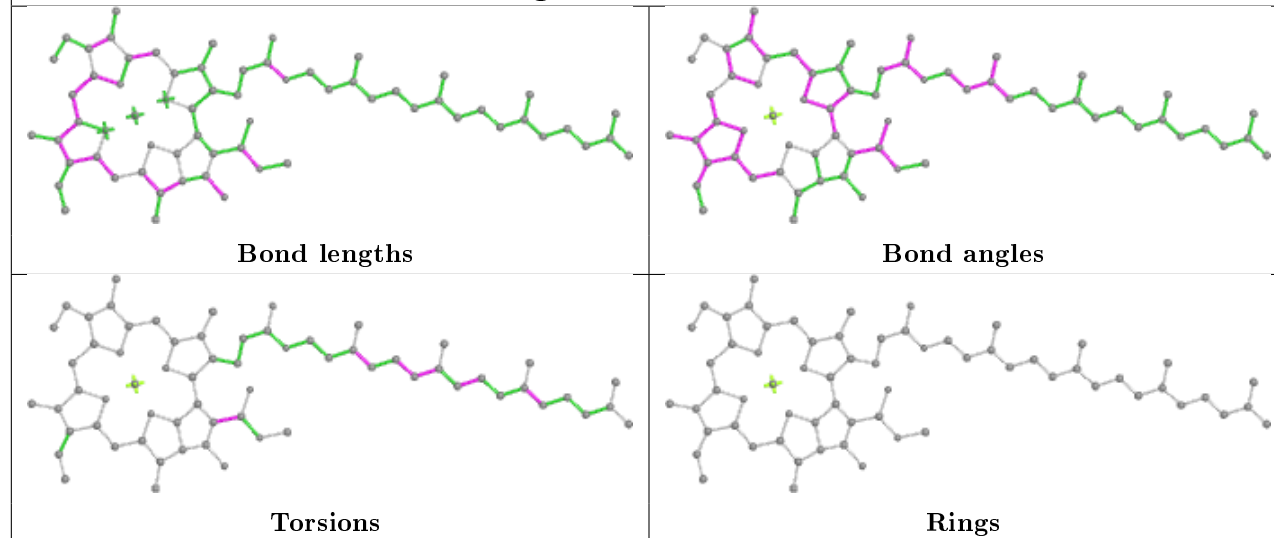
## Ligand CLA C 508

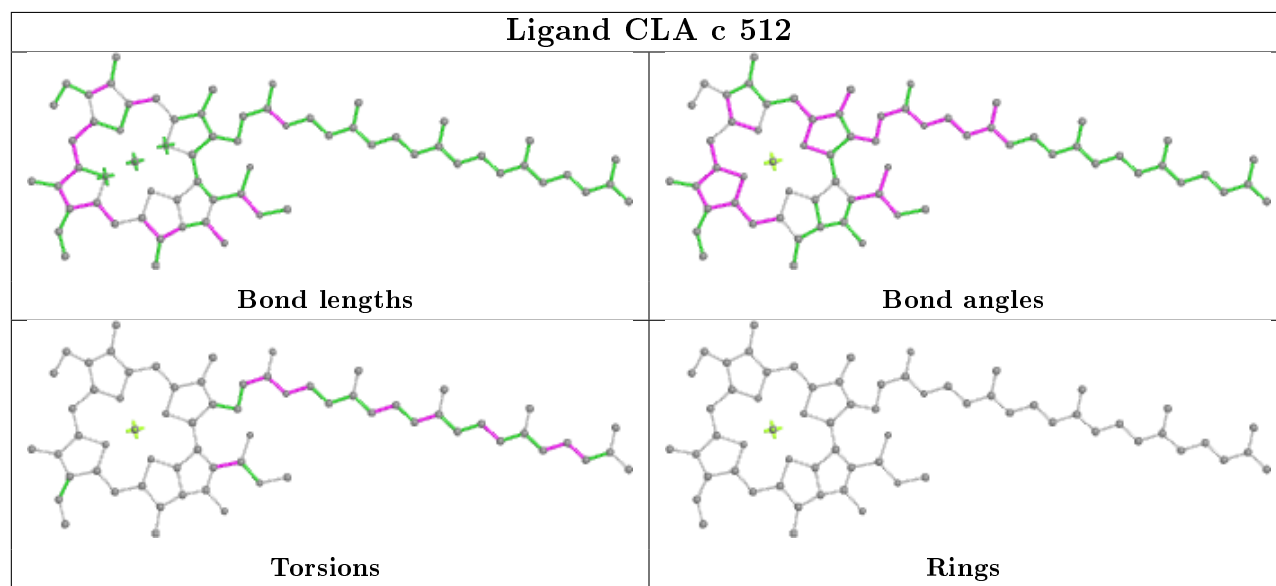
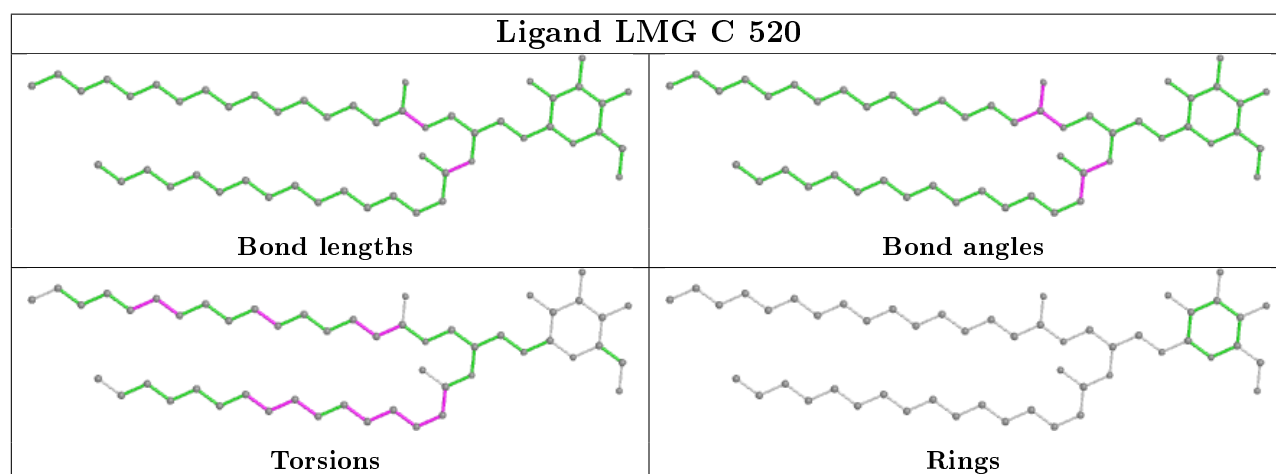
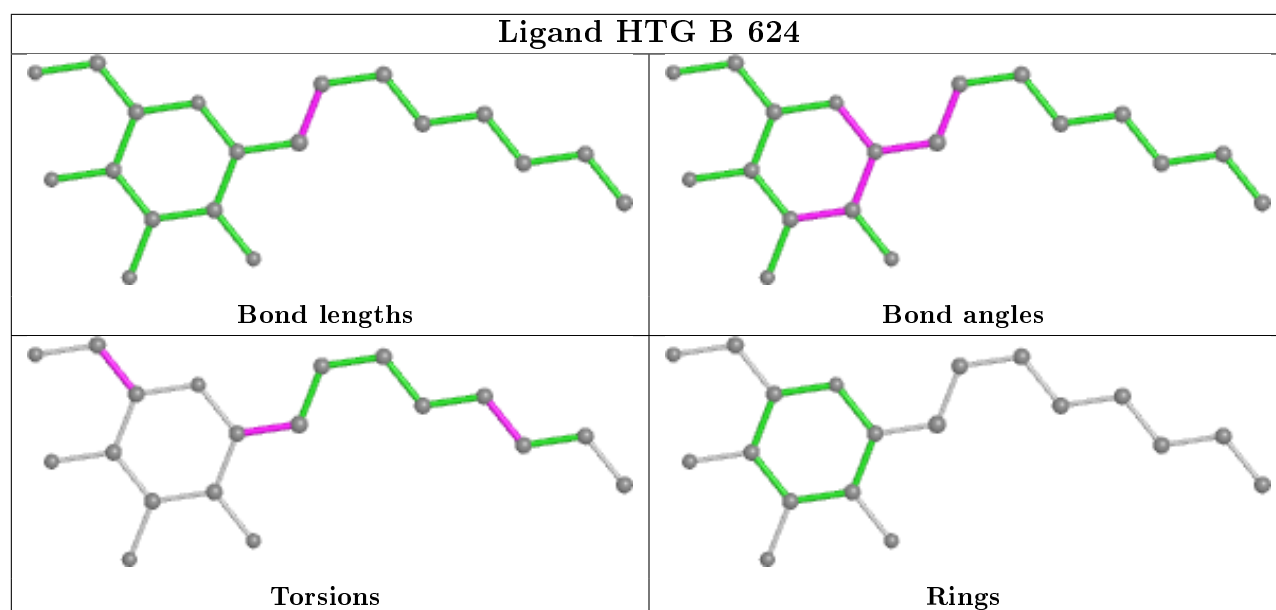


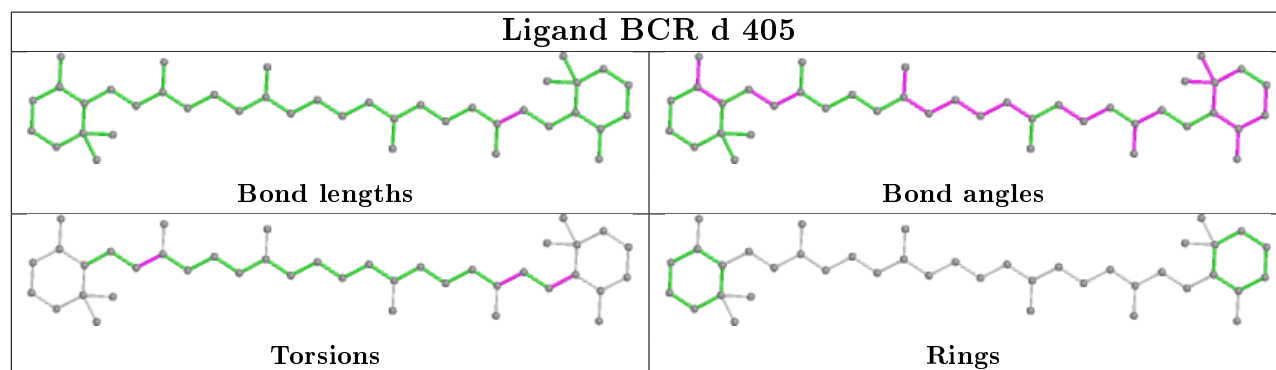
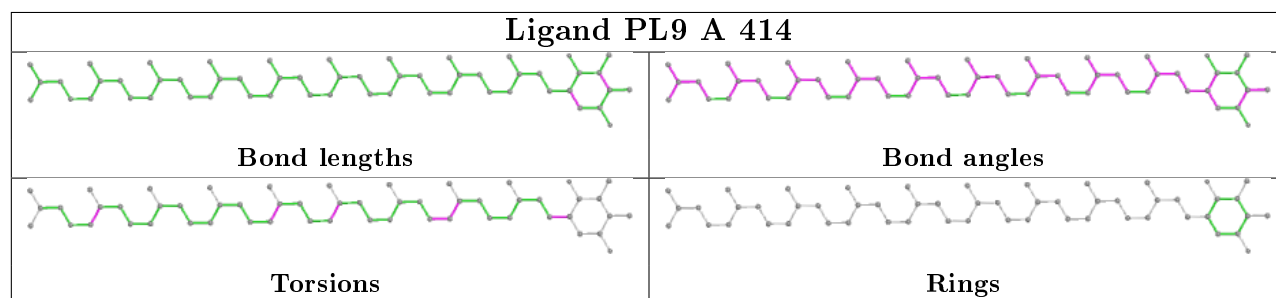
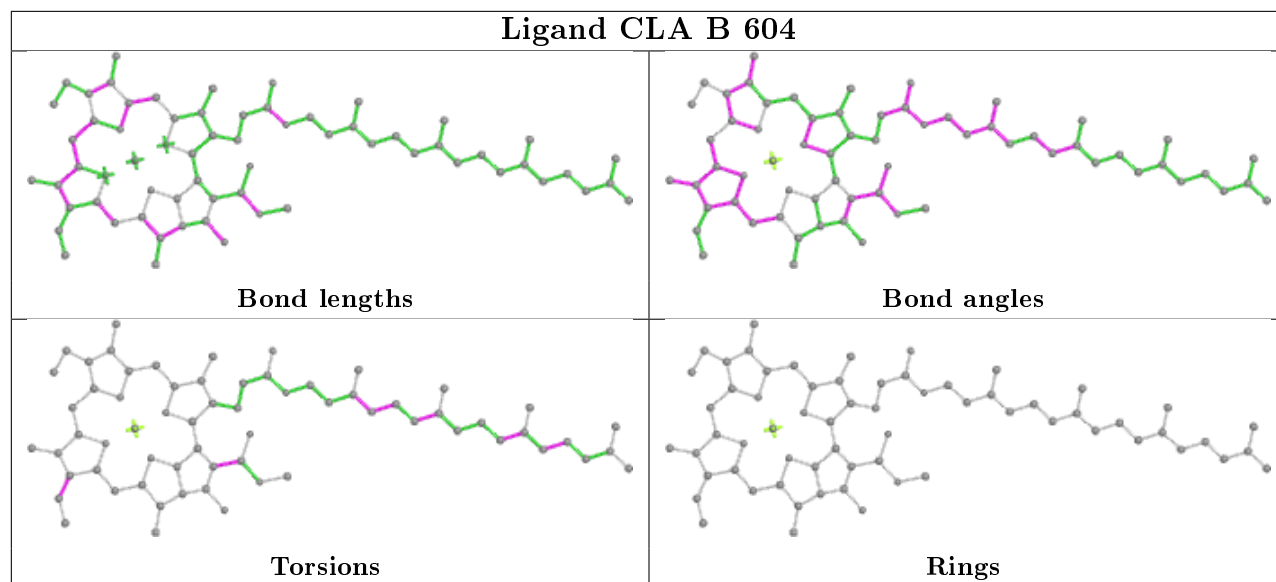
## Ligand CLA c 510



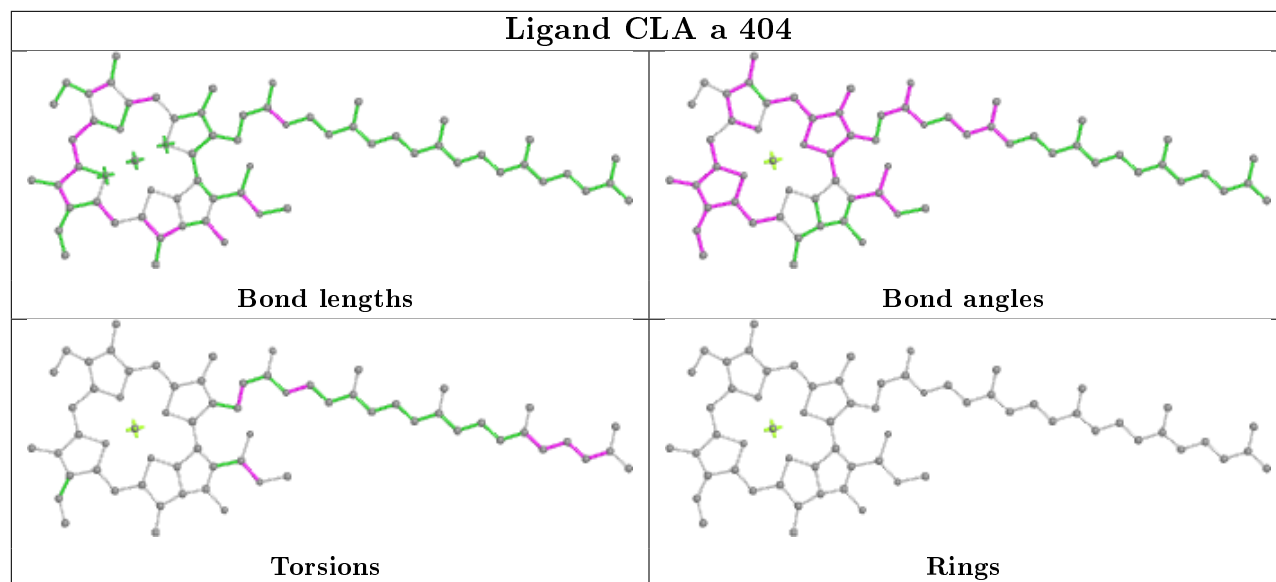
## Ligand CLA B 605



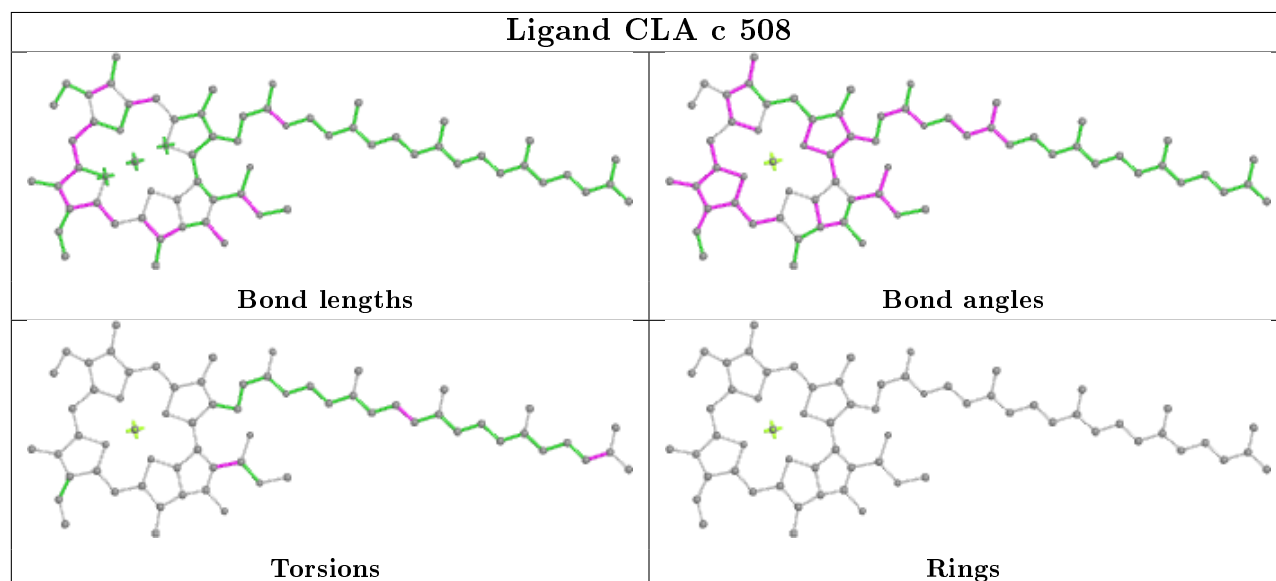




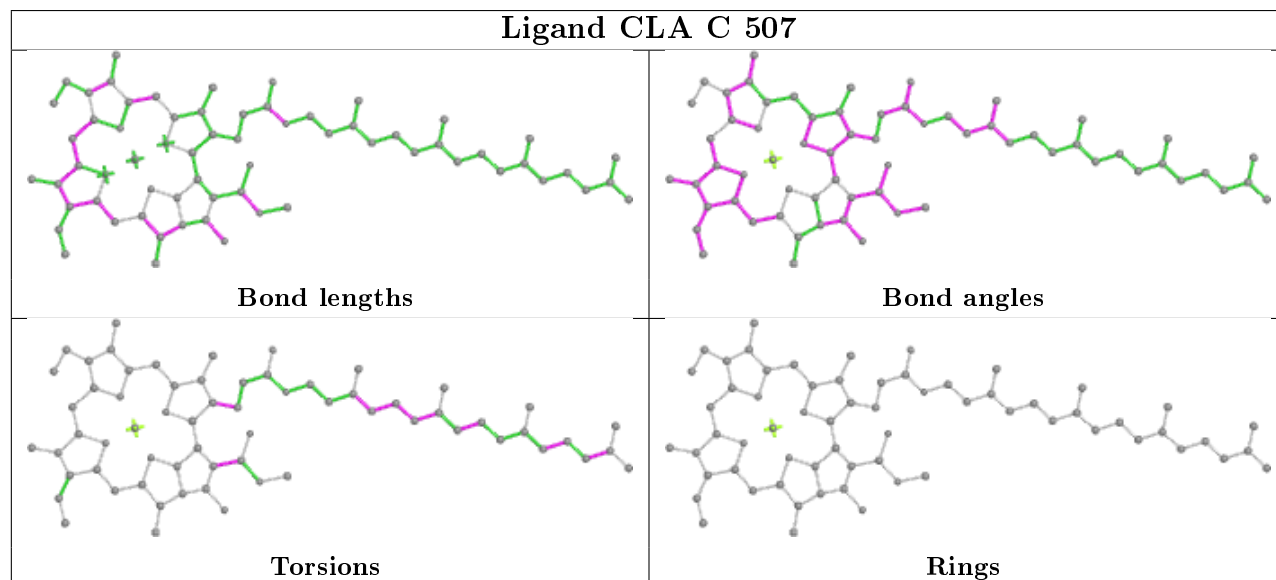
## Ligand CLA a 404

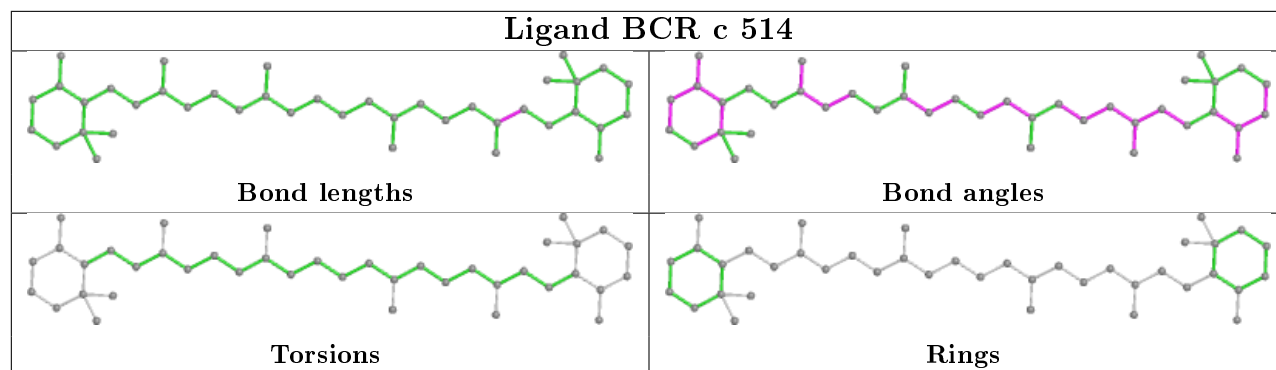
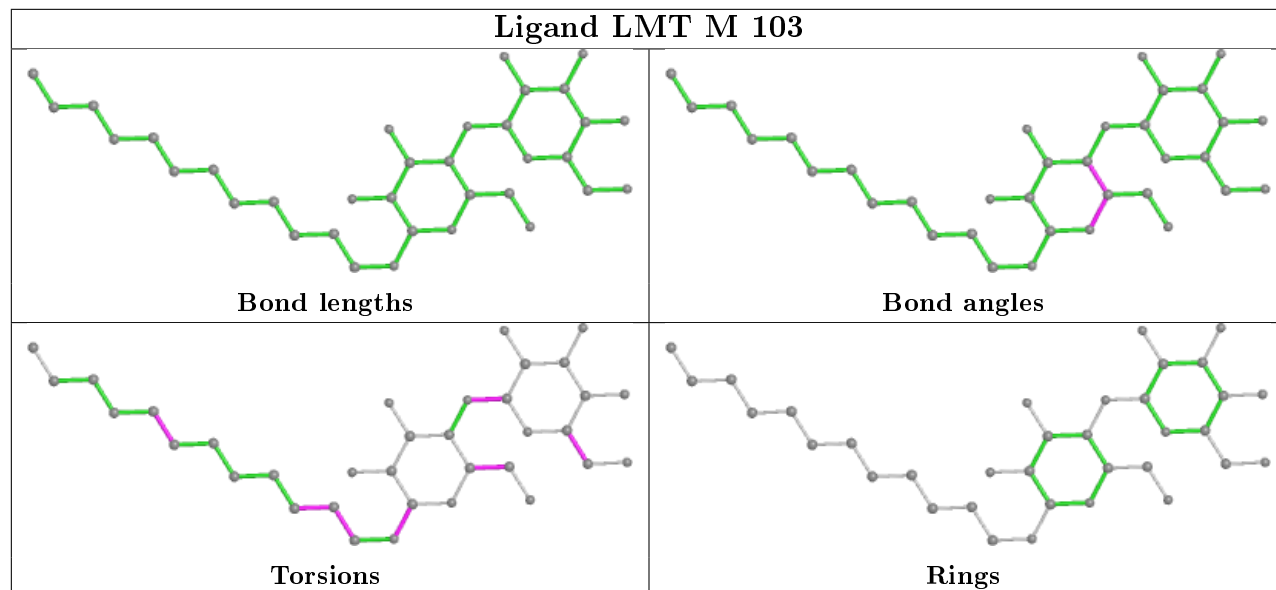
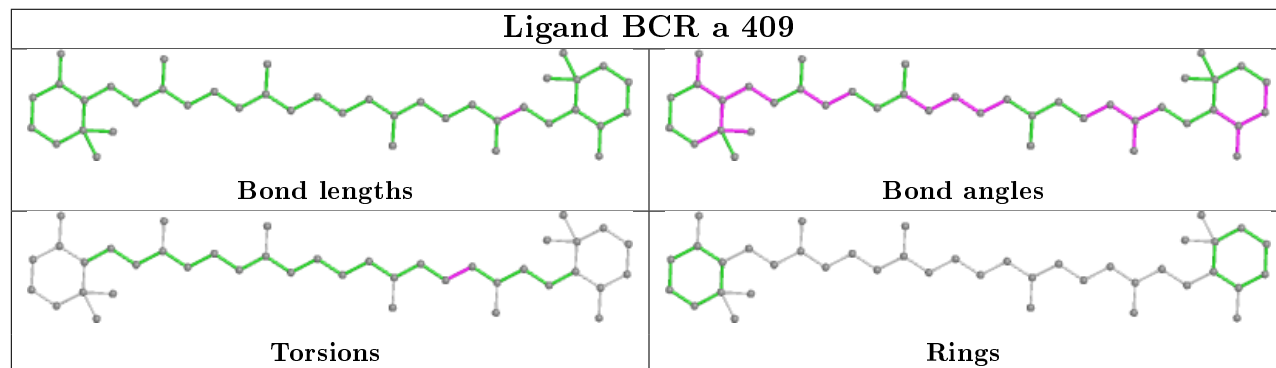


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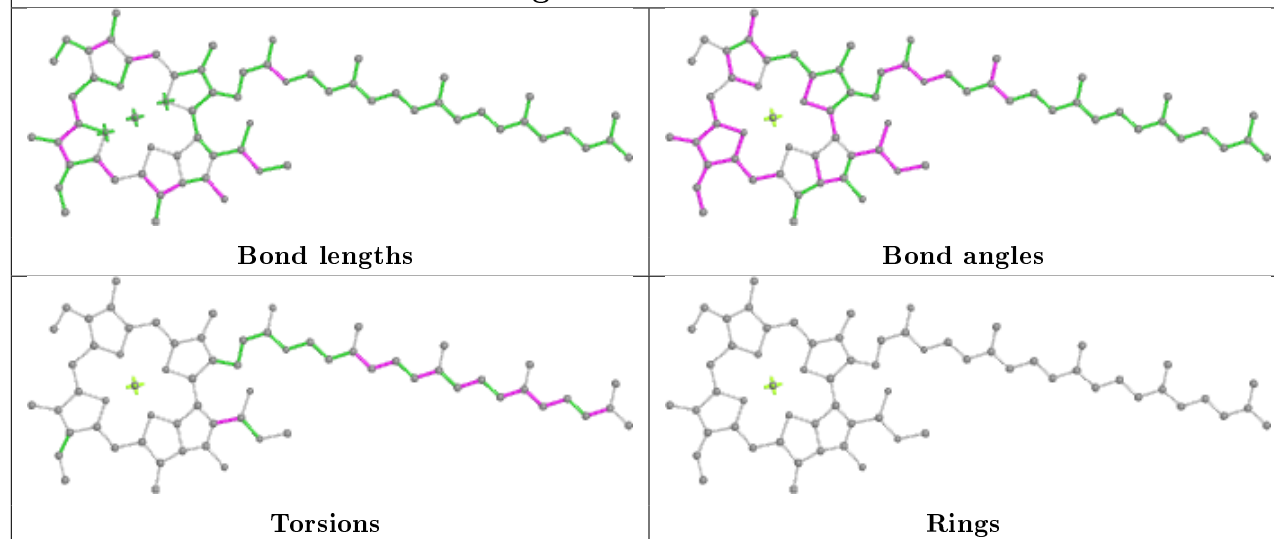


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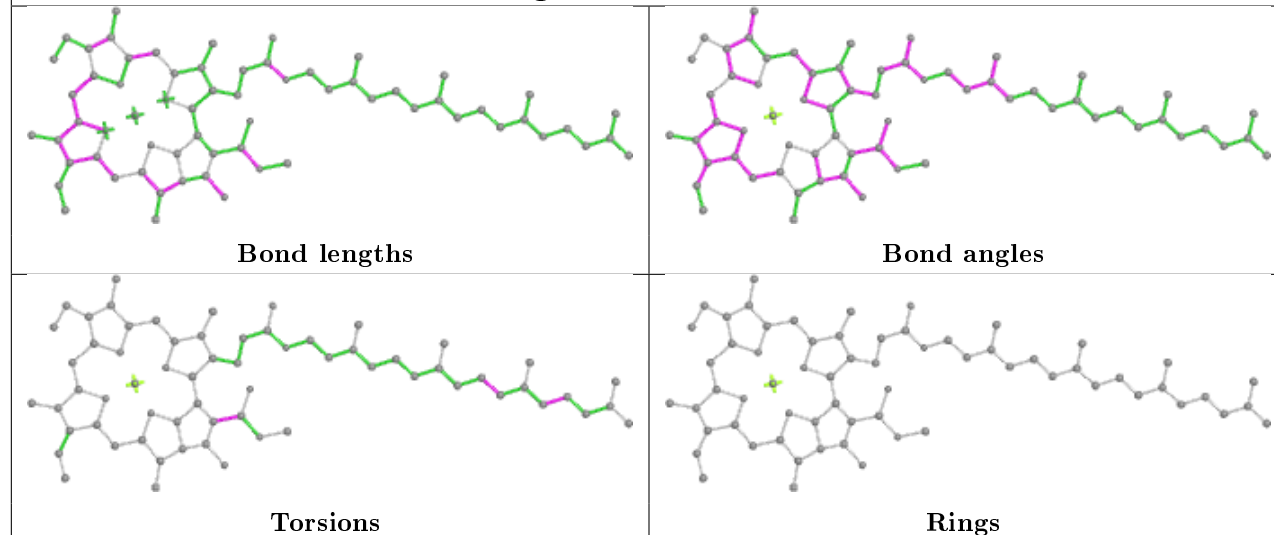


**Ligand BCR c 514****Ligand LMT M 103****Ligand BCR a 409**

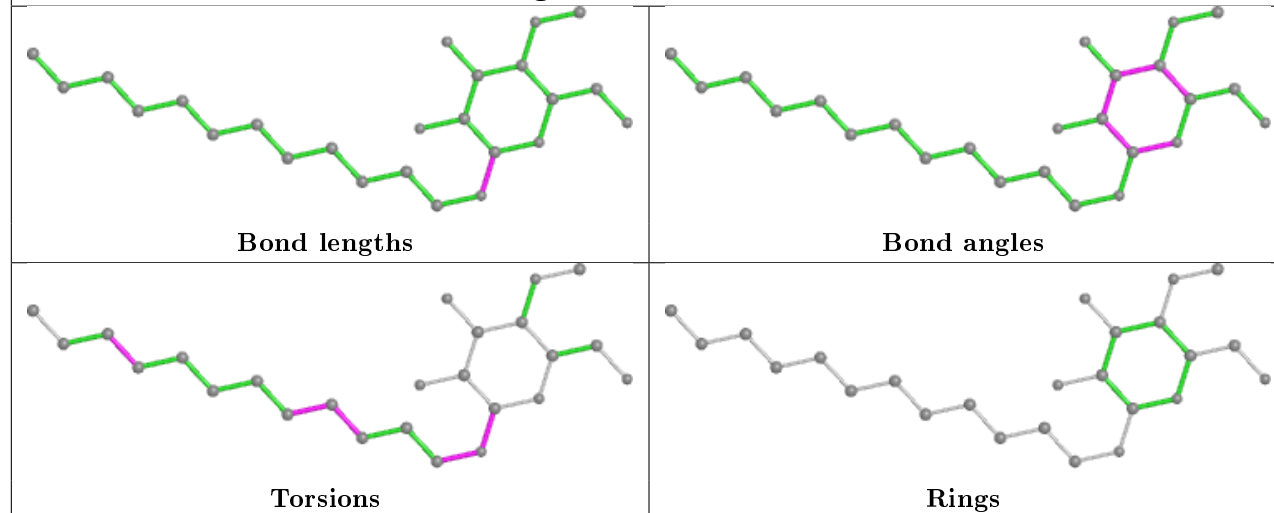
## Ligand CLA B 615

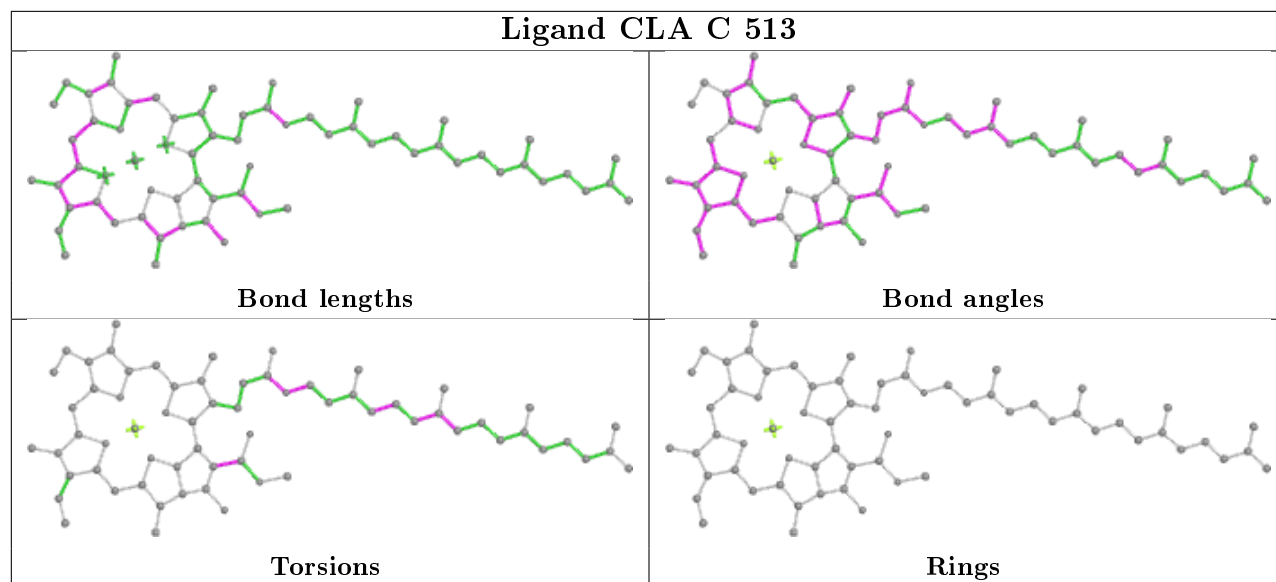
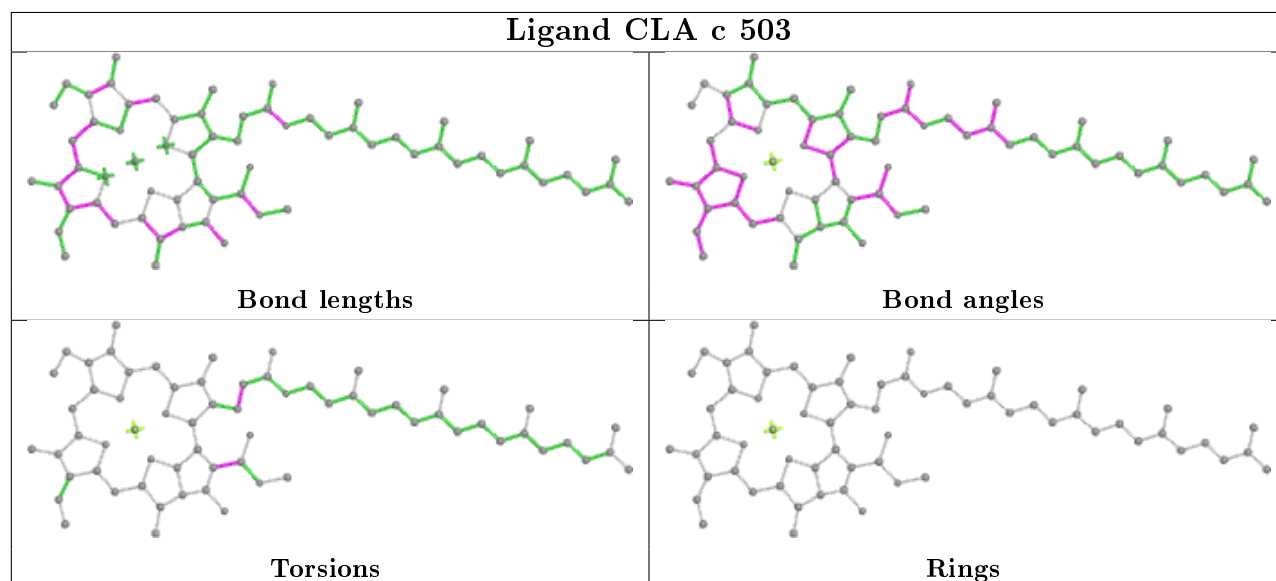
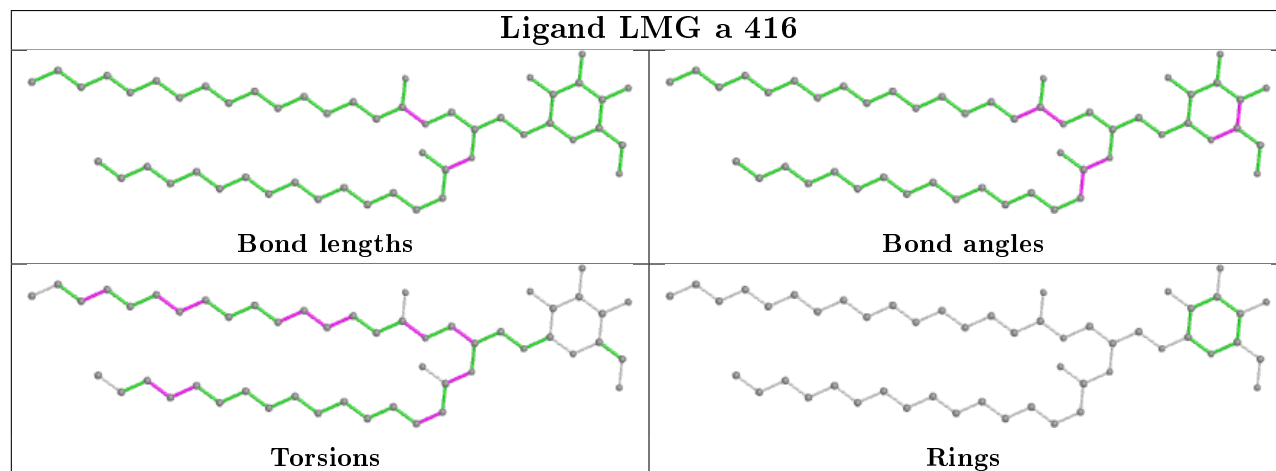


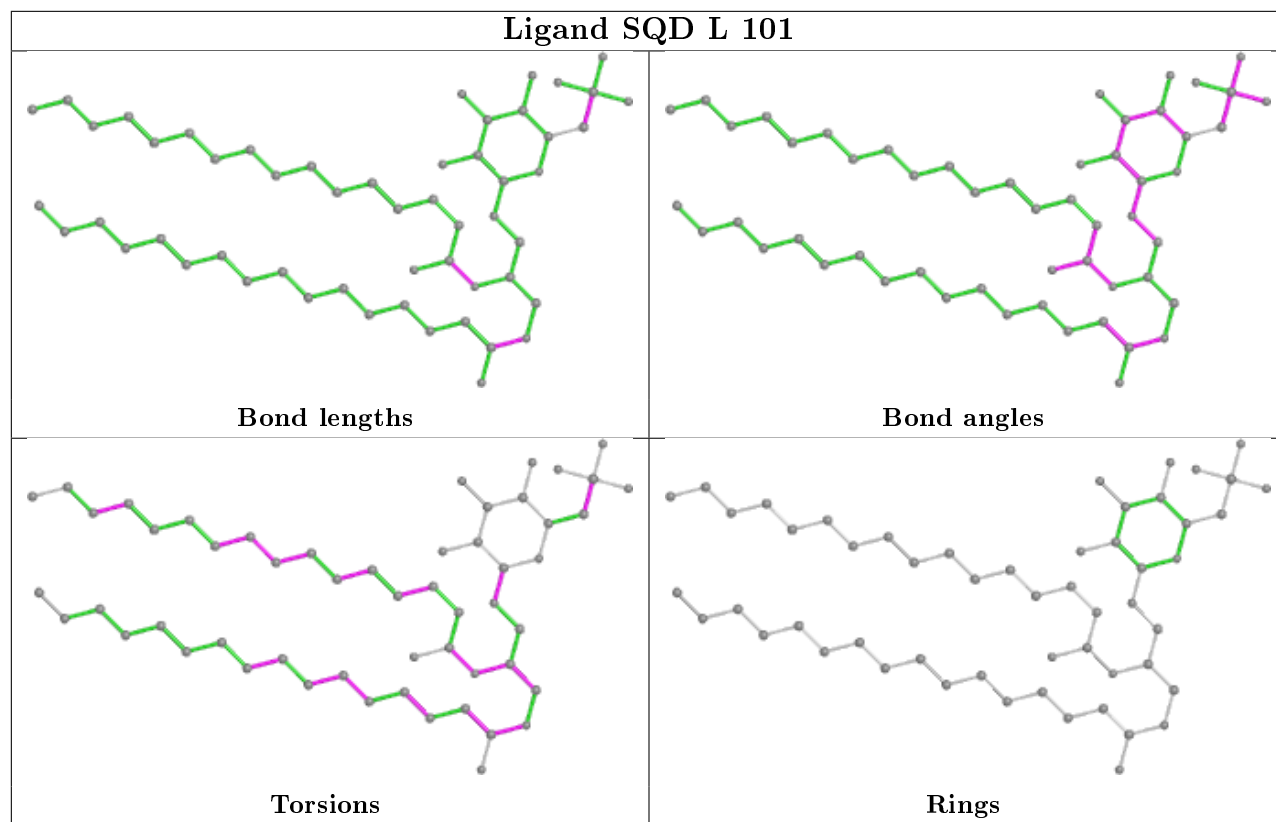
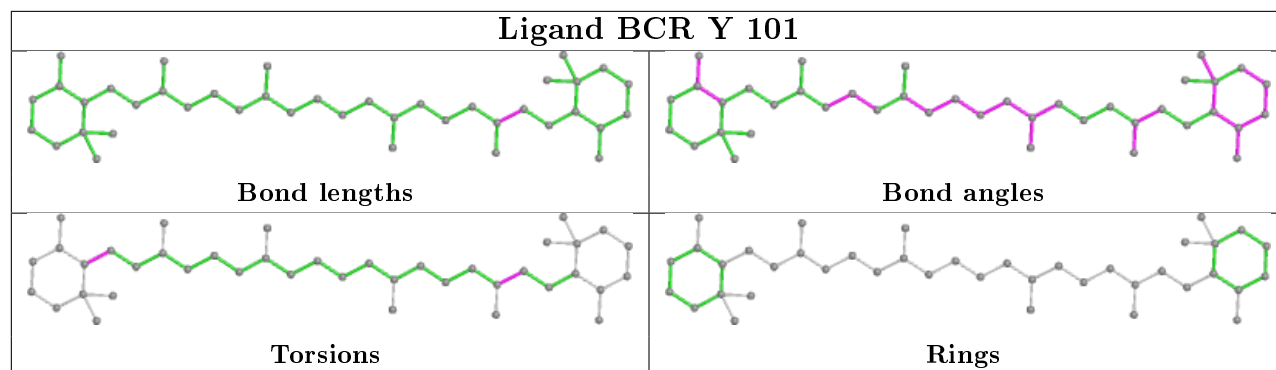
## Ligand CLA C 509



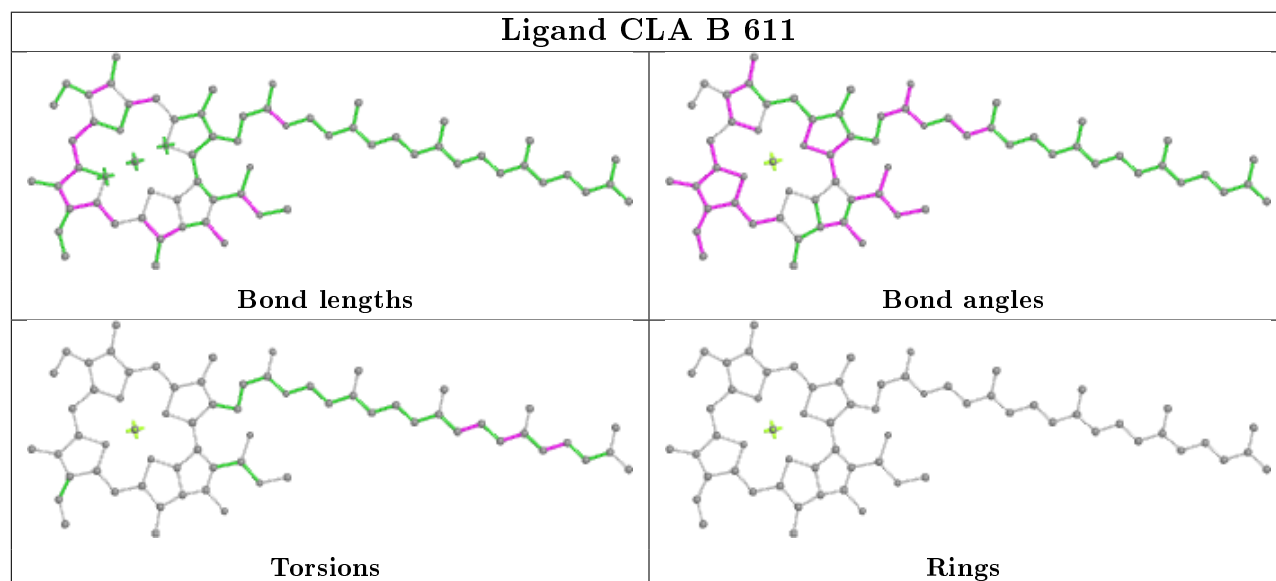
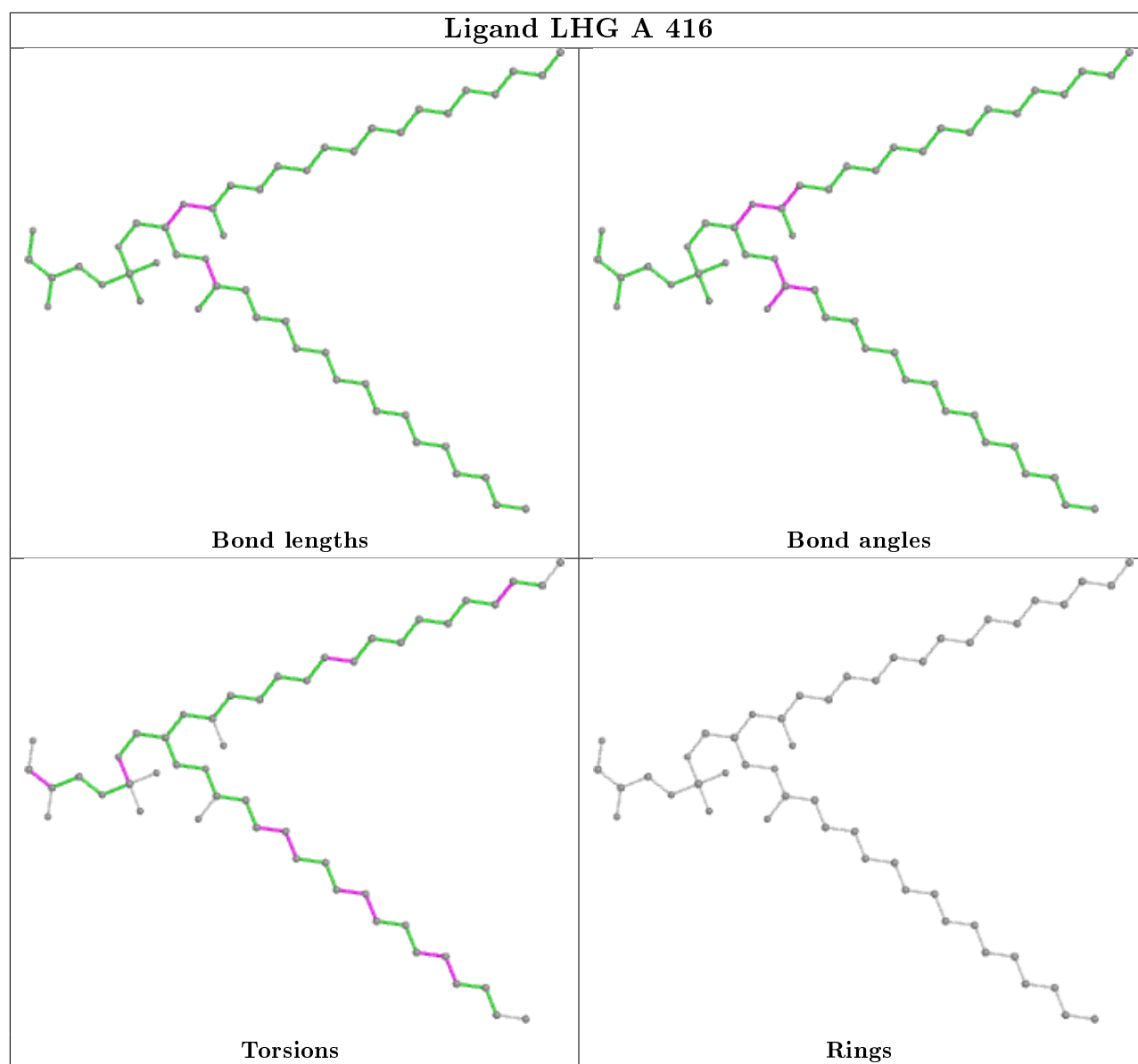
## Ligand LMT b 627



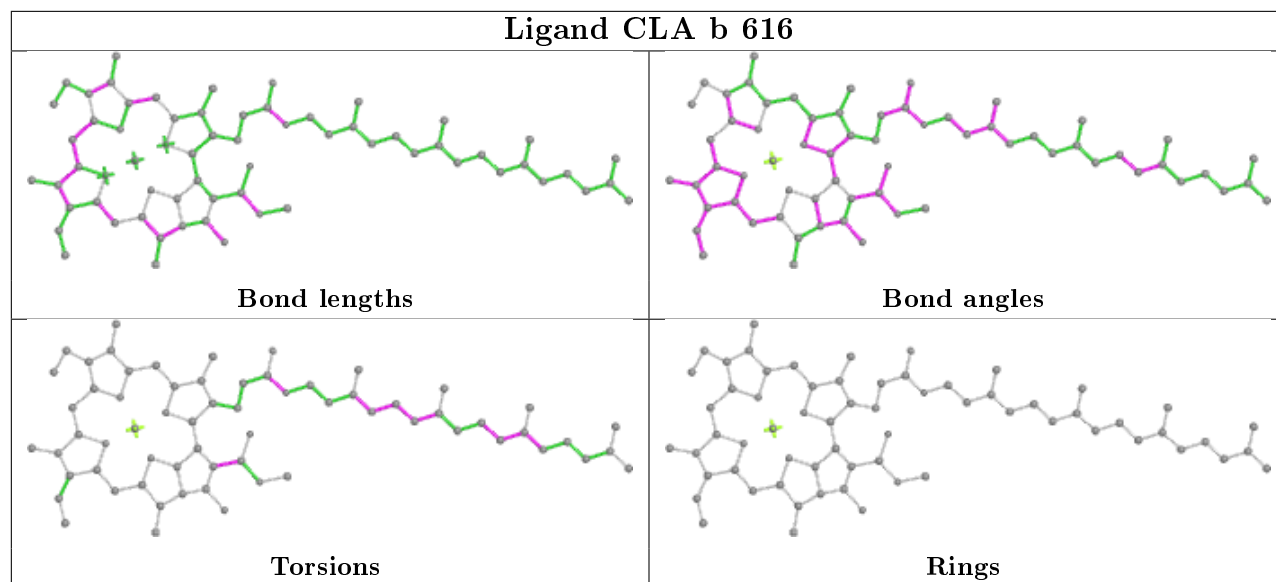
**Ligand CLA C 513****Ligand CLA c 503****Ligand LMG a 416**



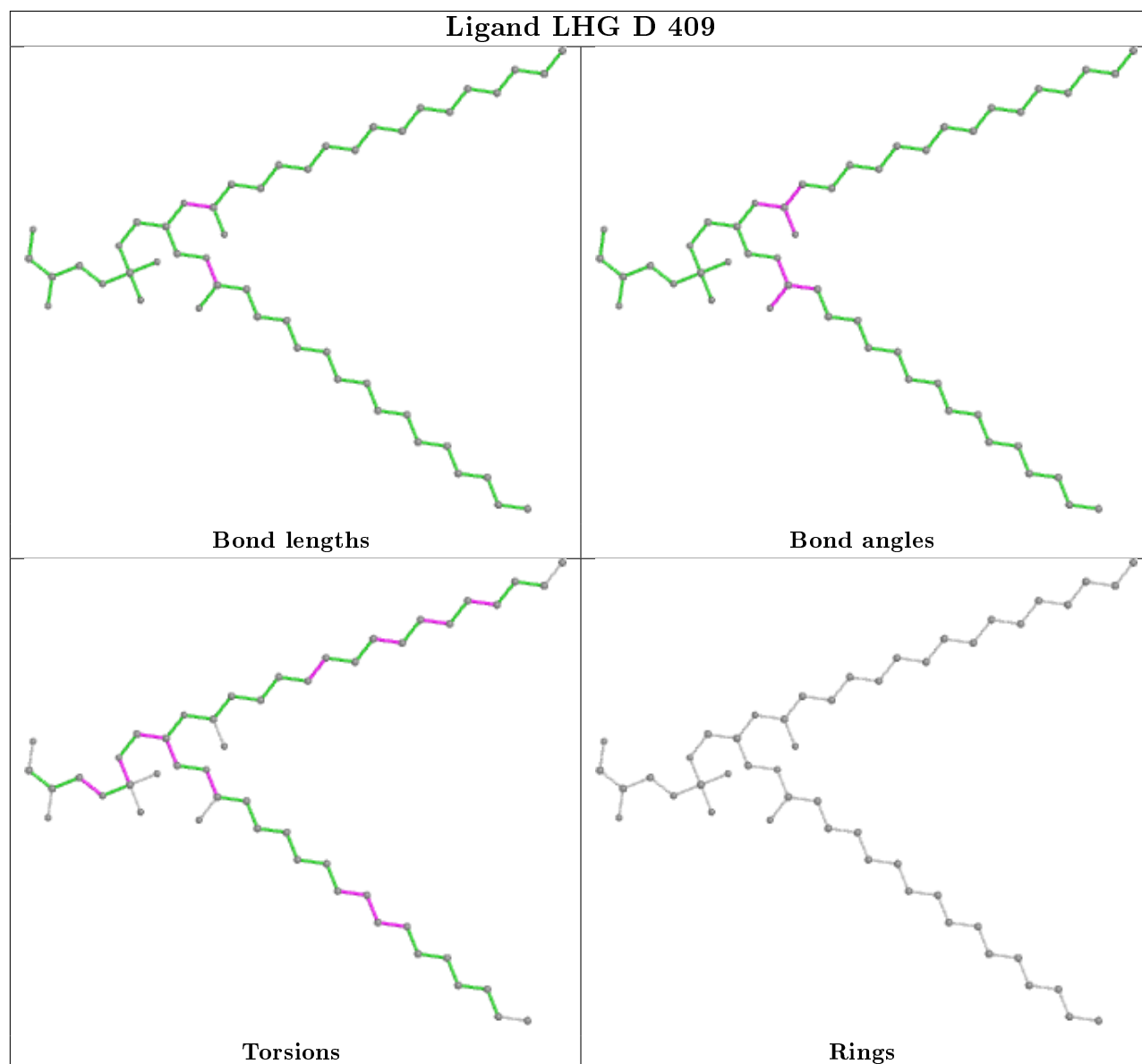


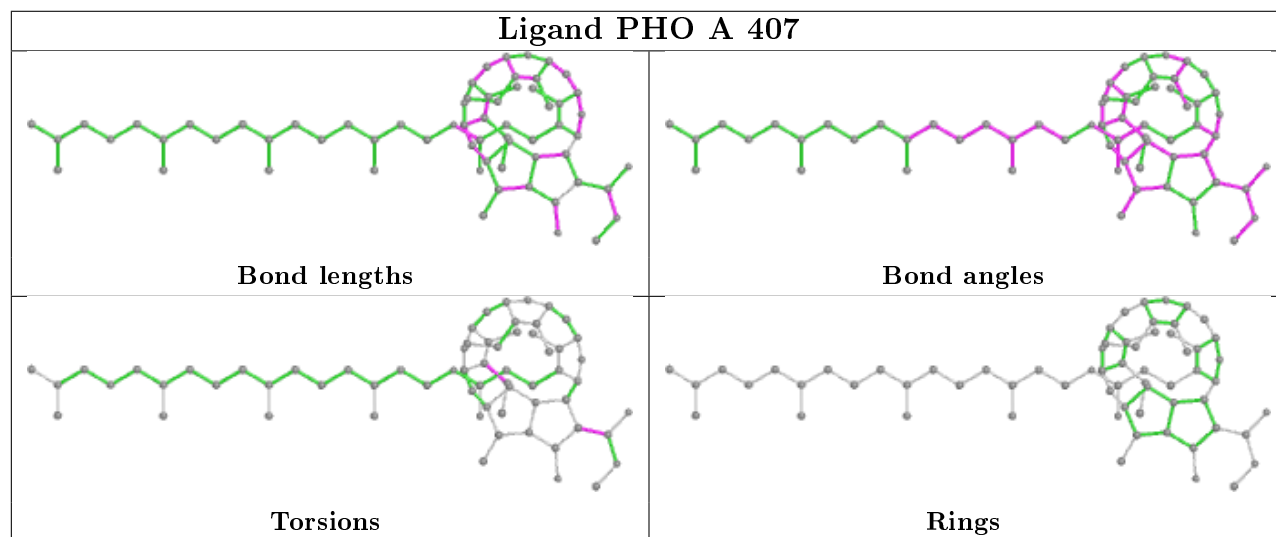
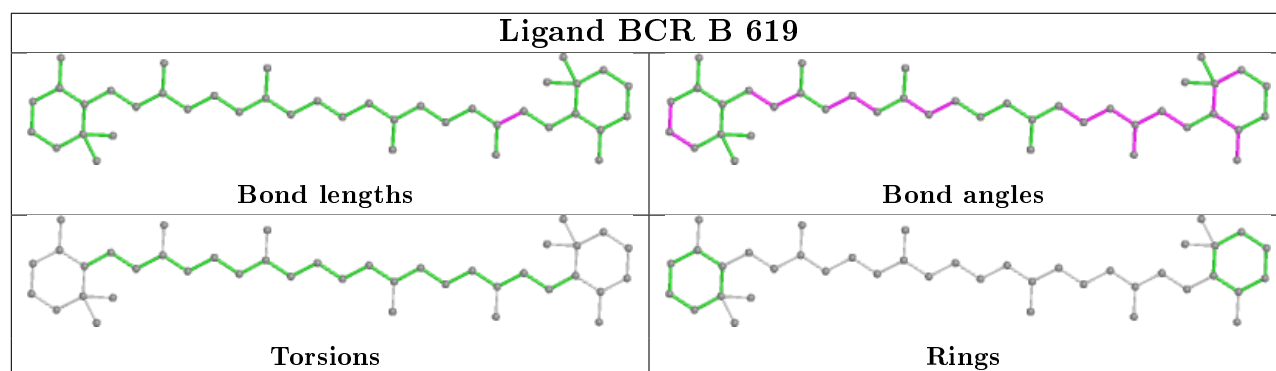
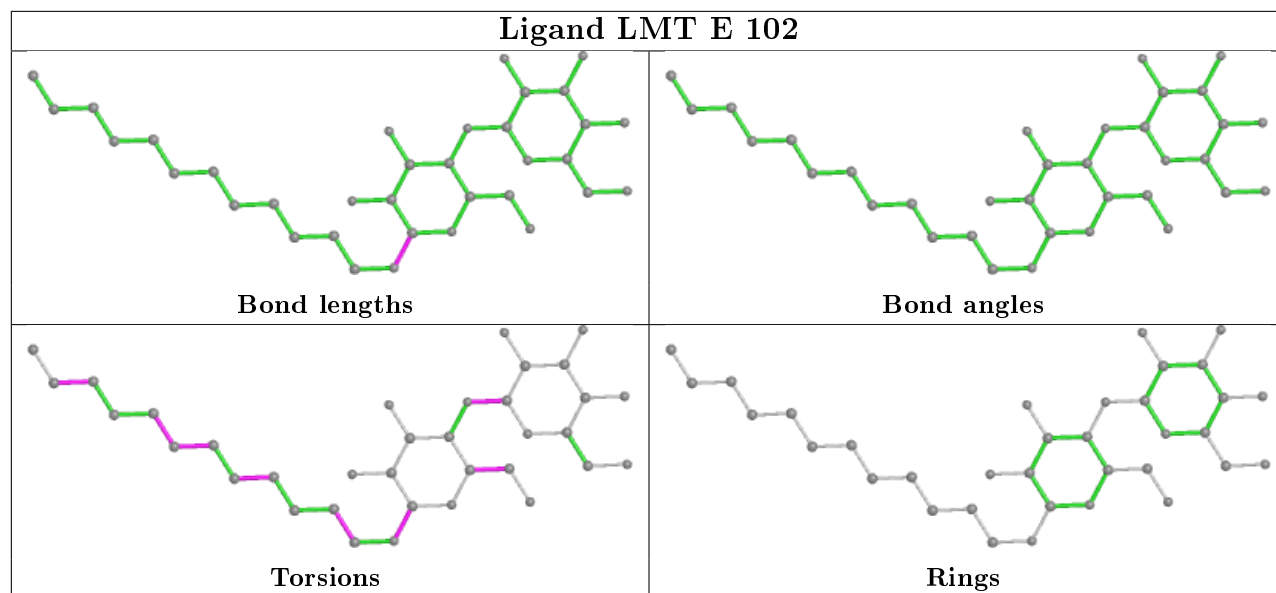


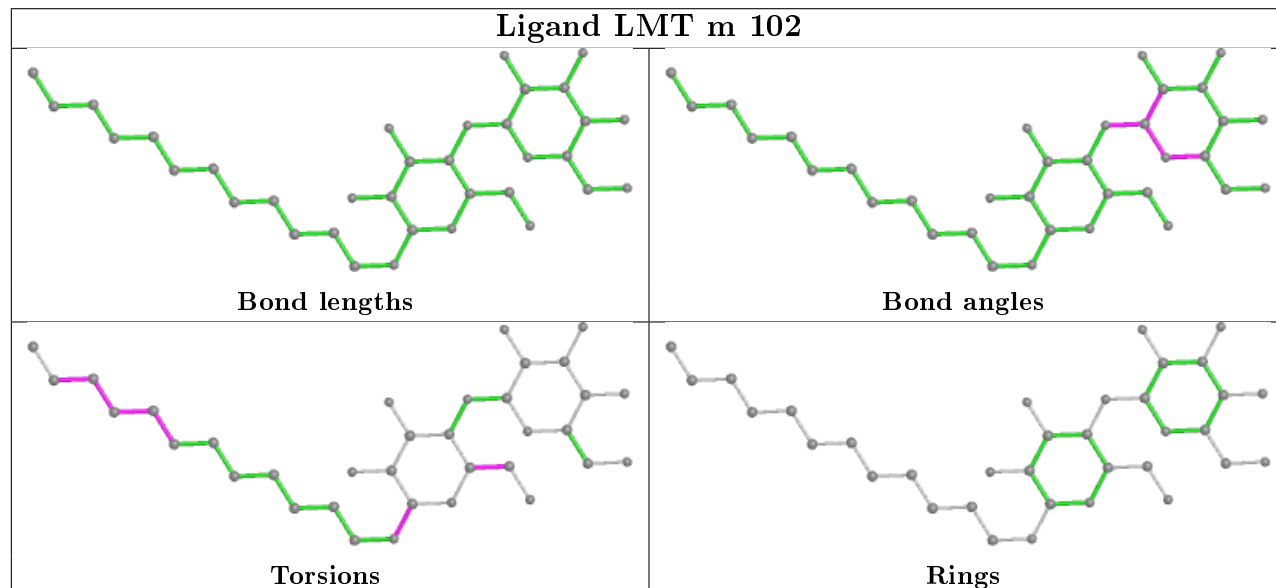
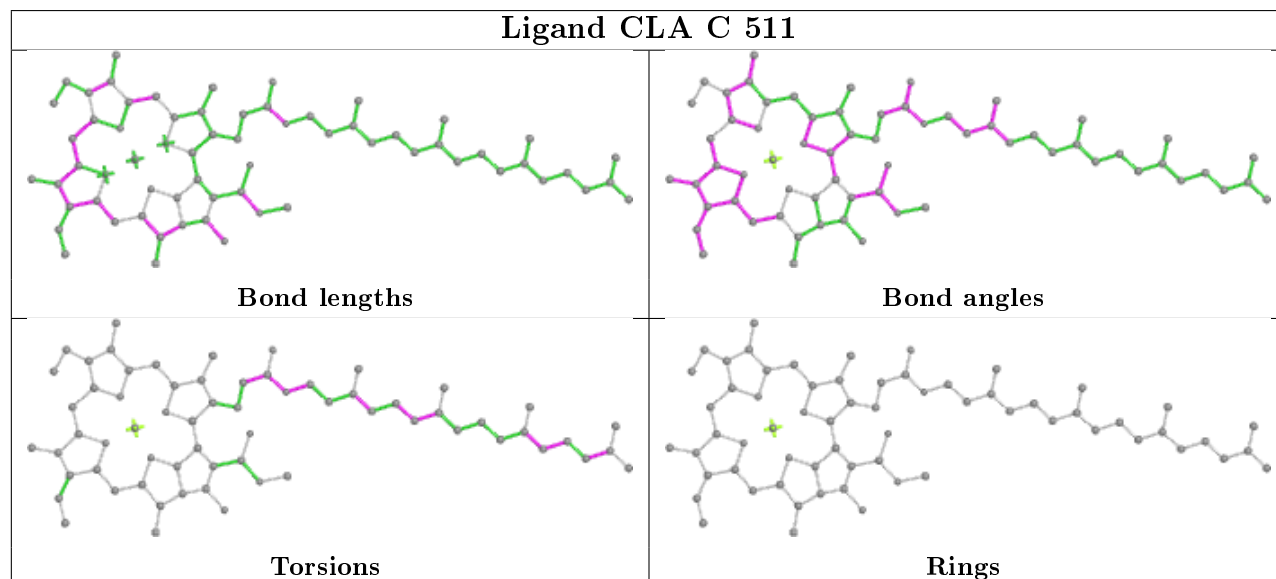
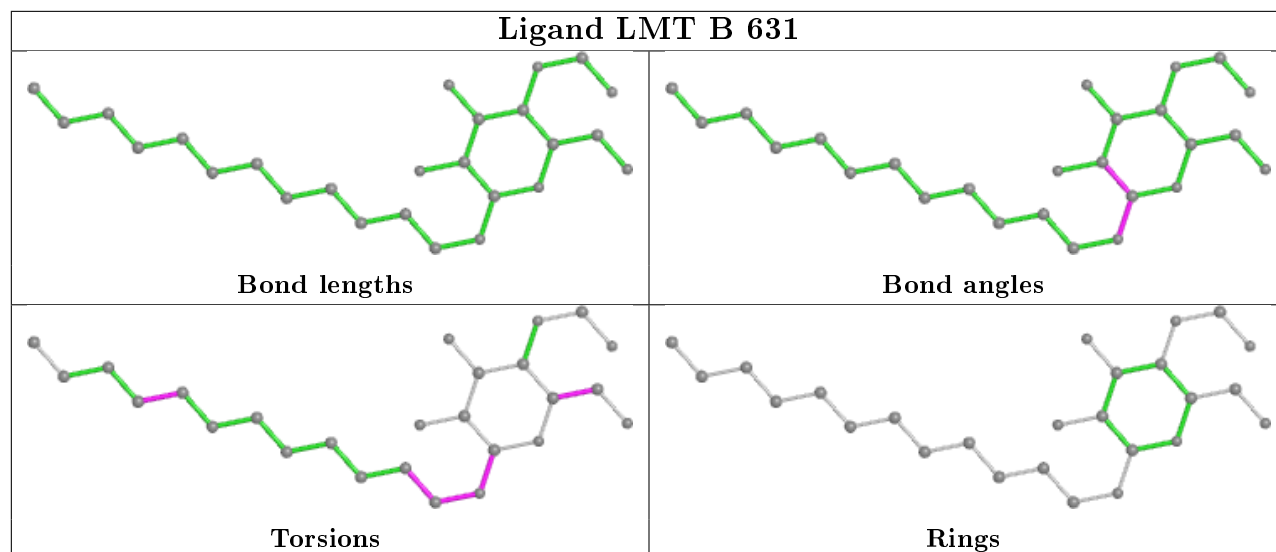
## Ligand CLA b 616

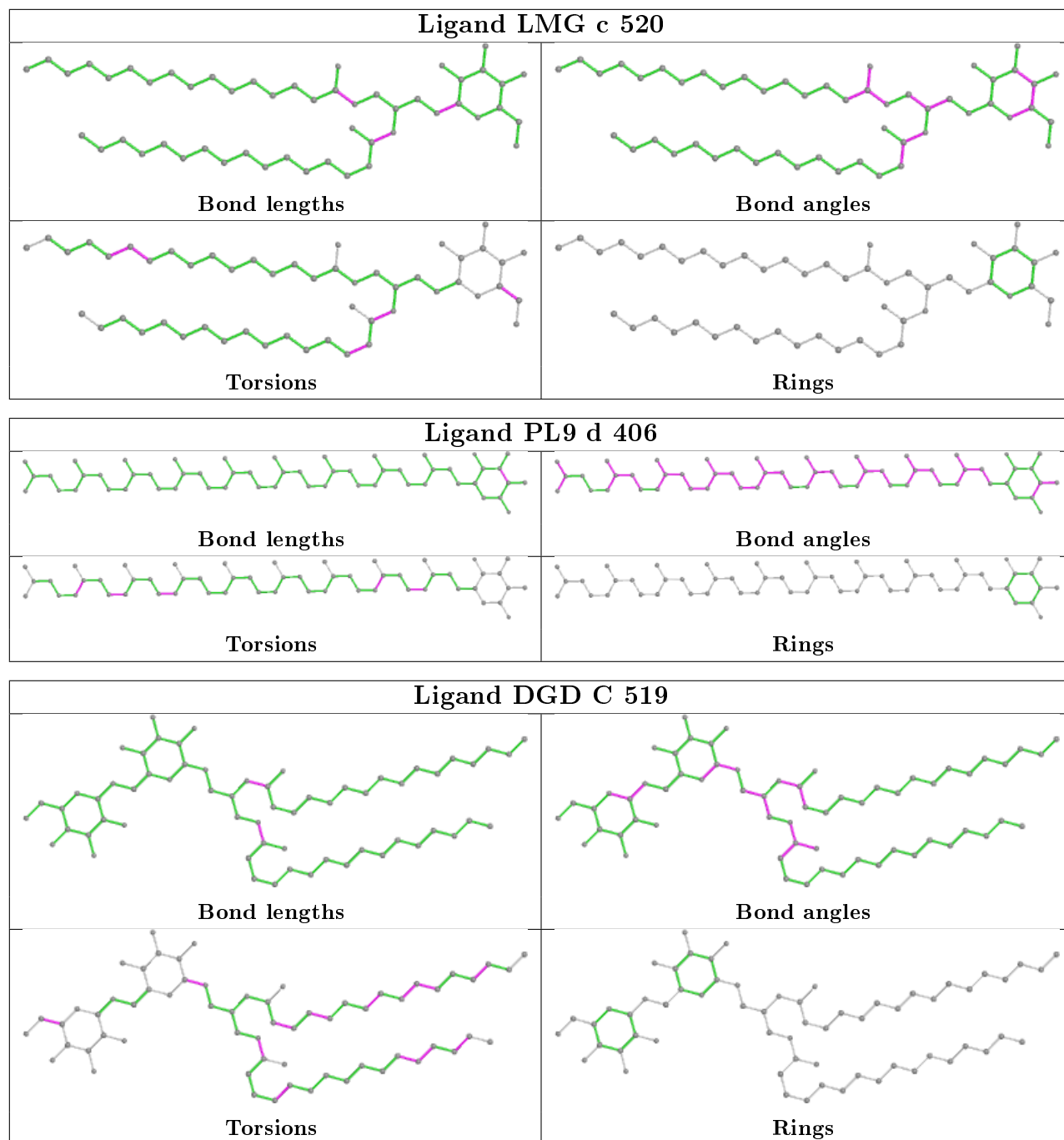


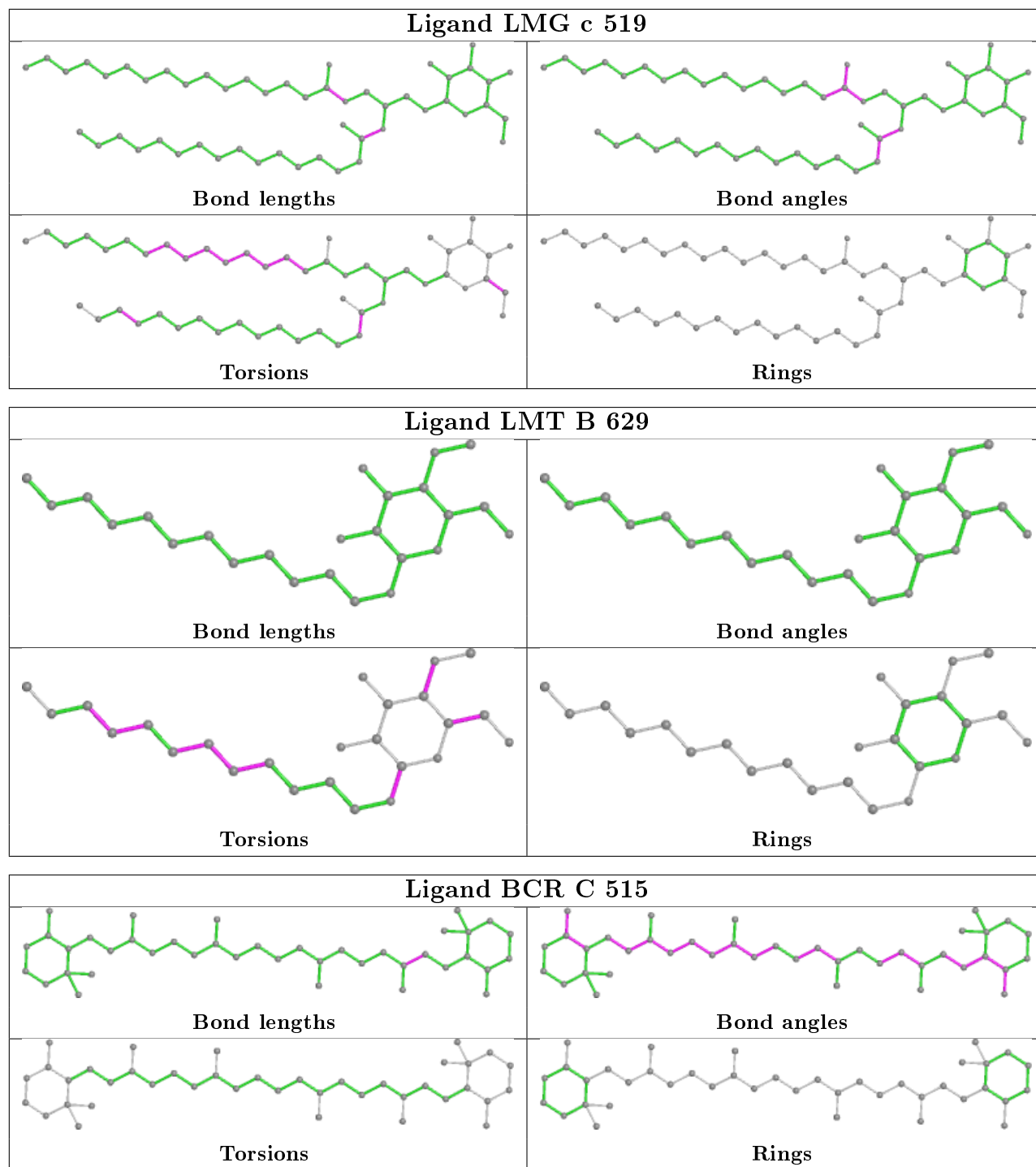
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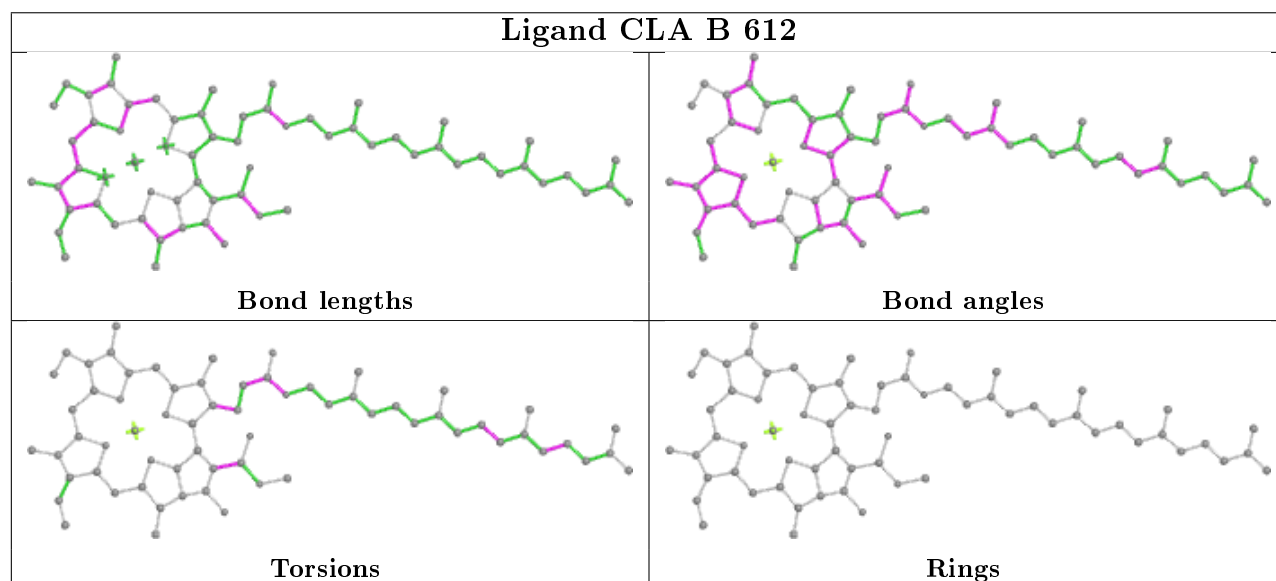
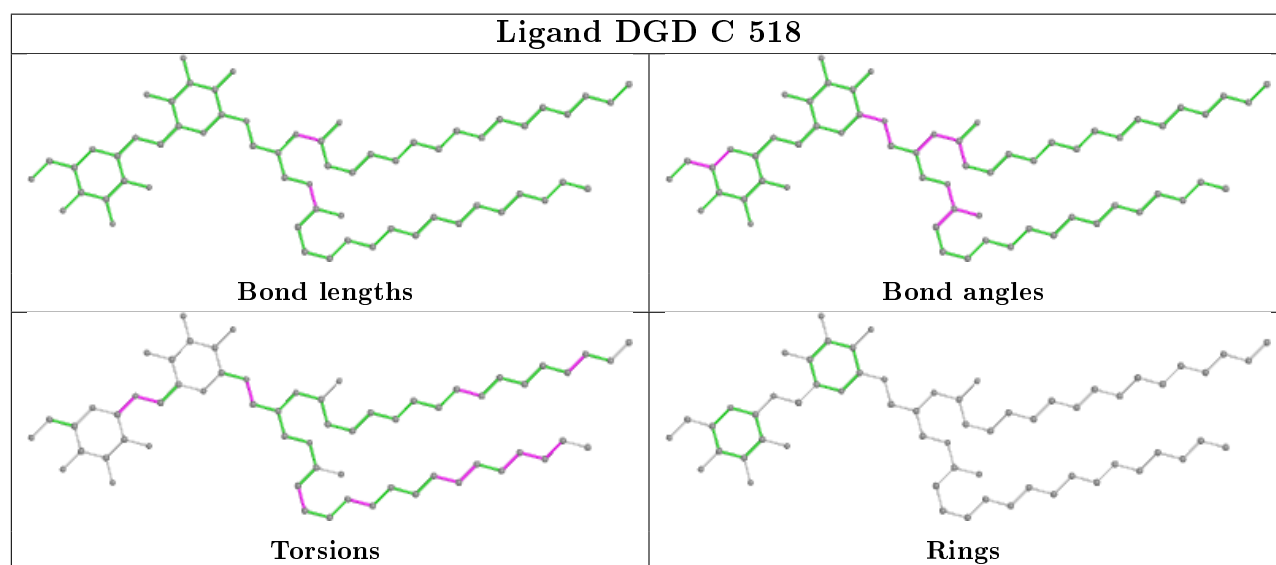
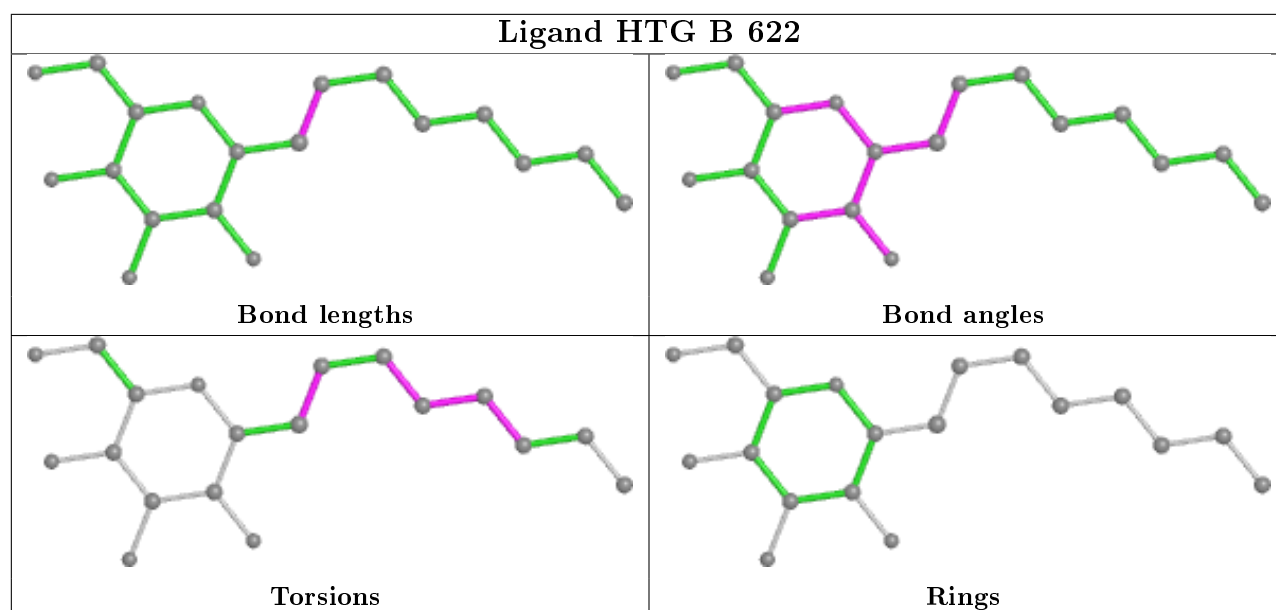


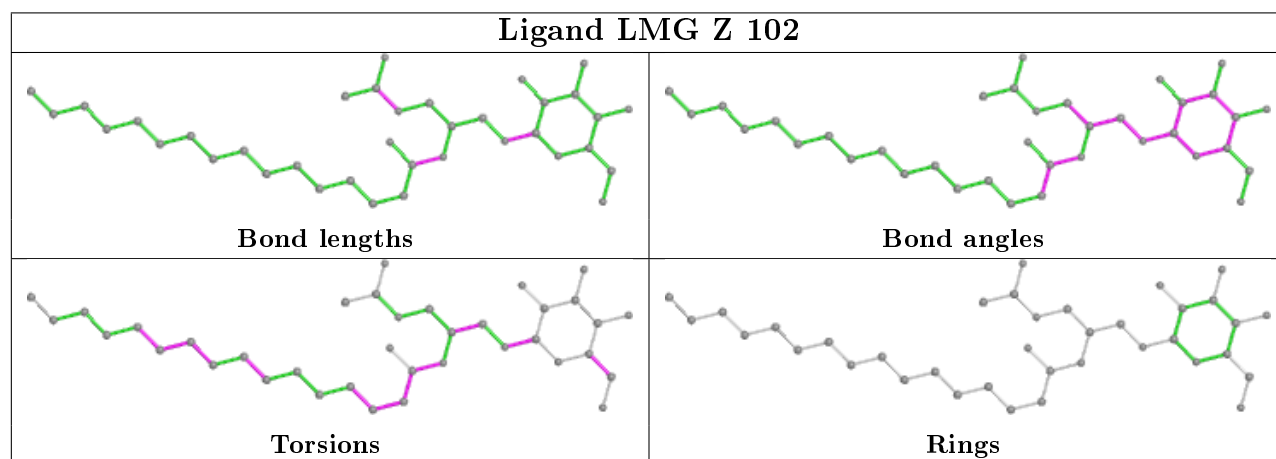
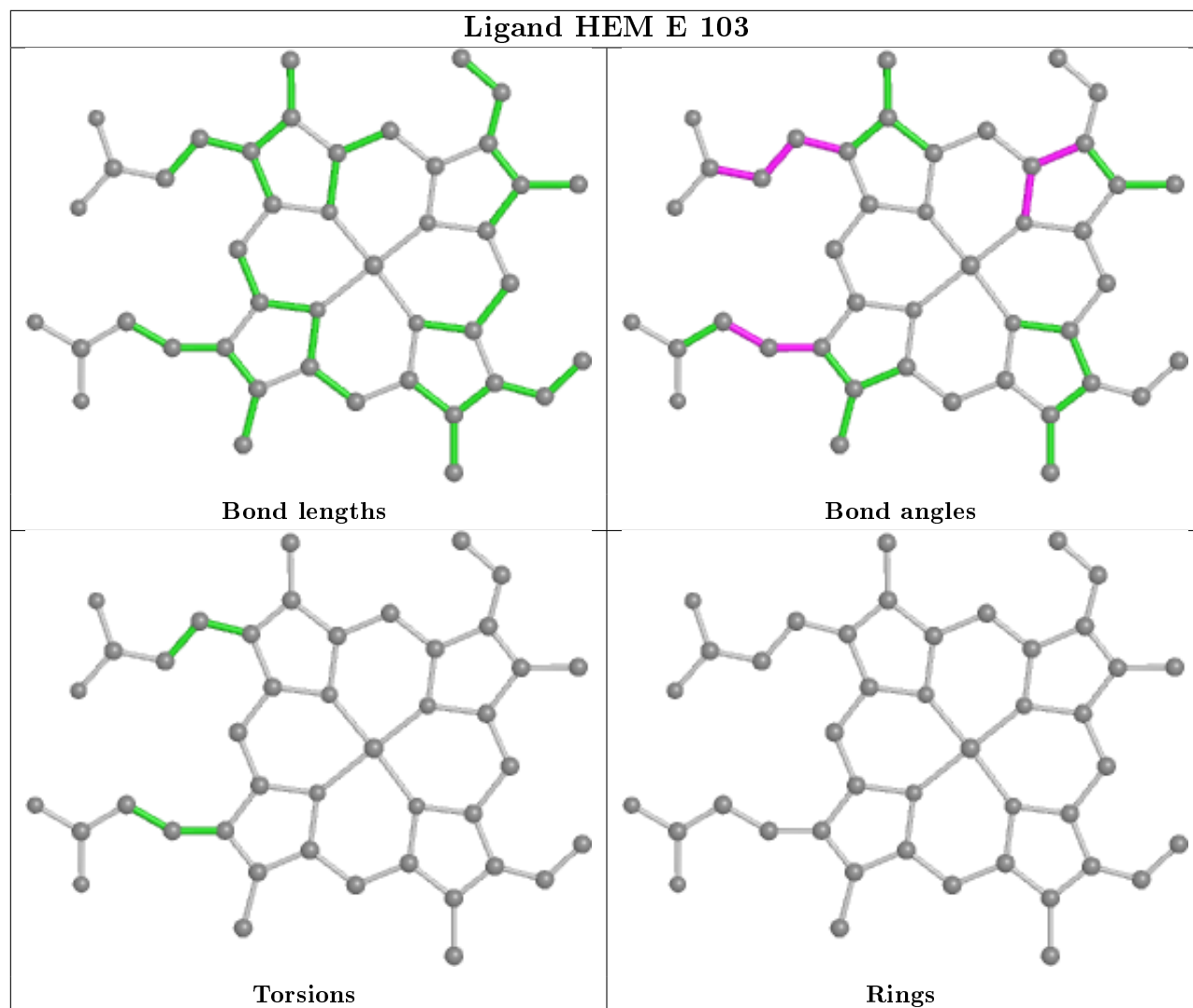




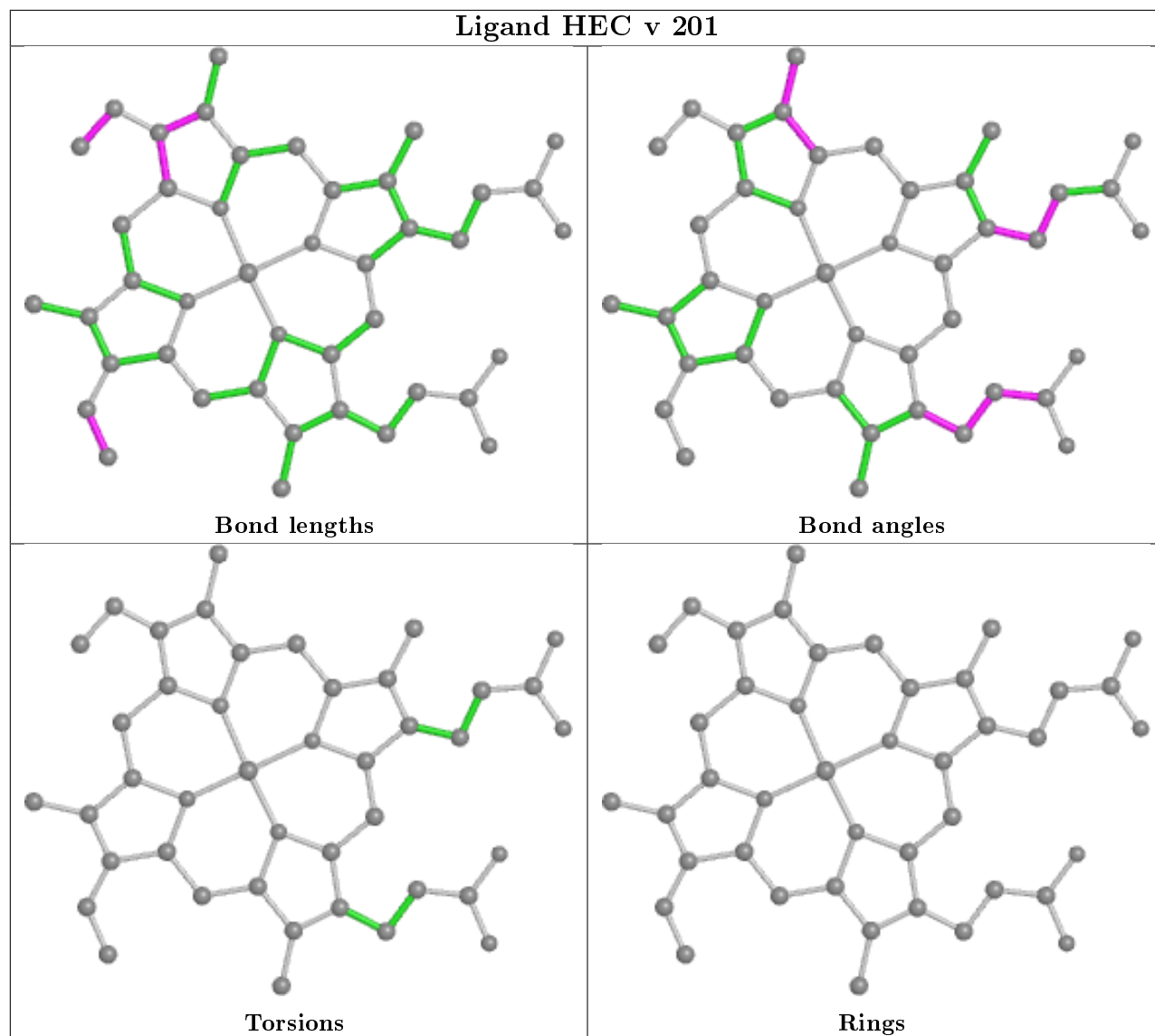
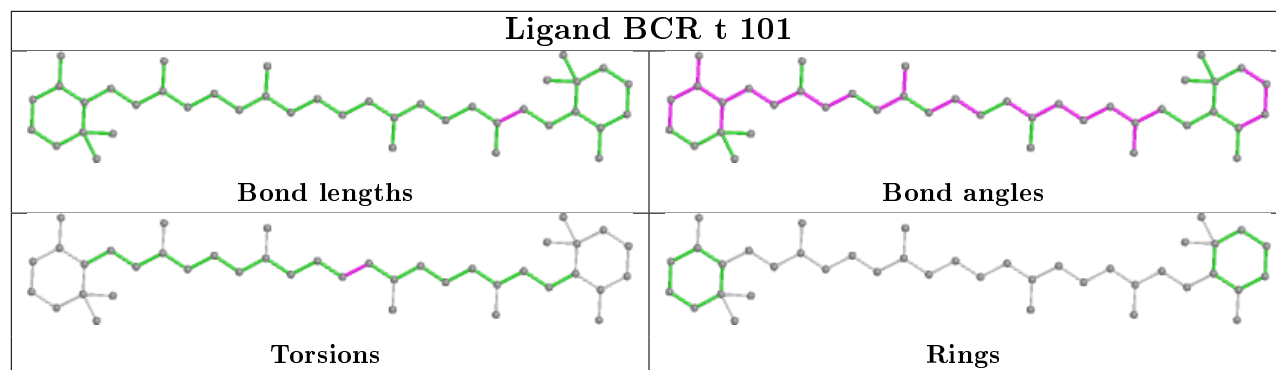


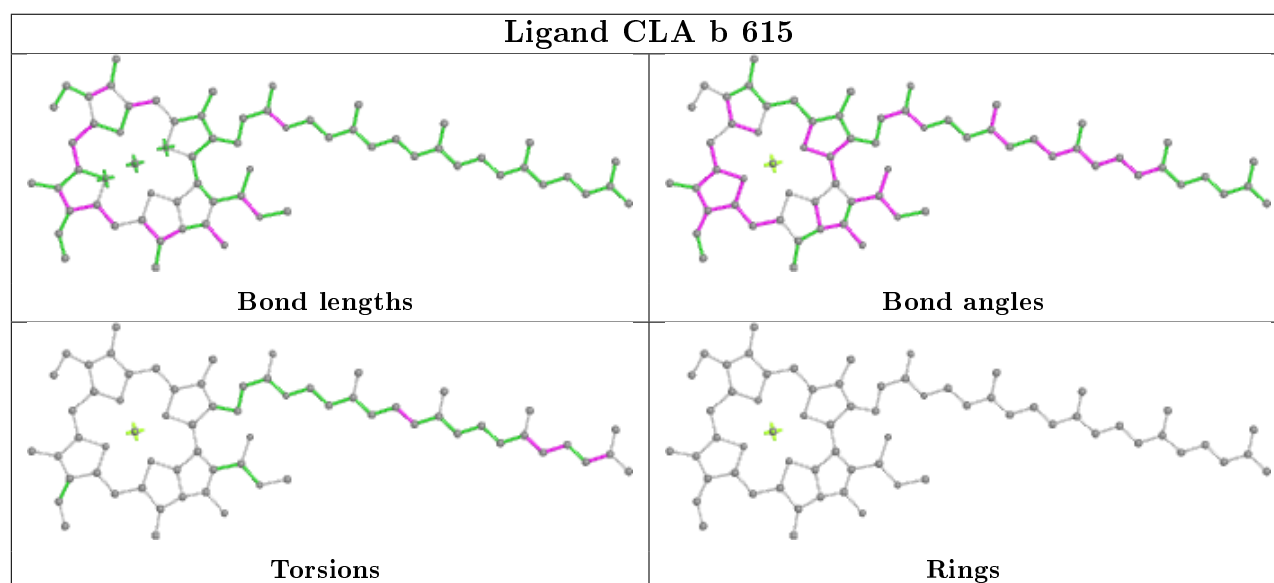
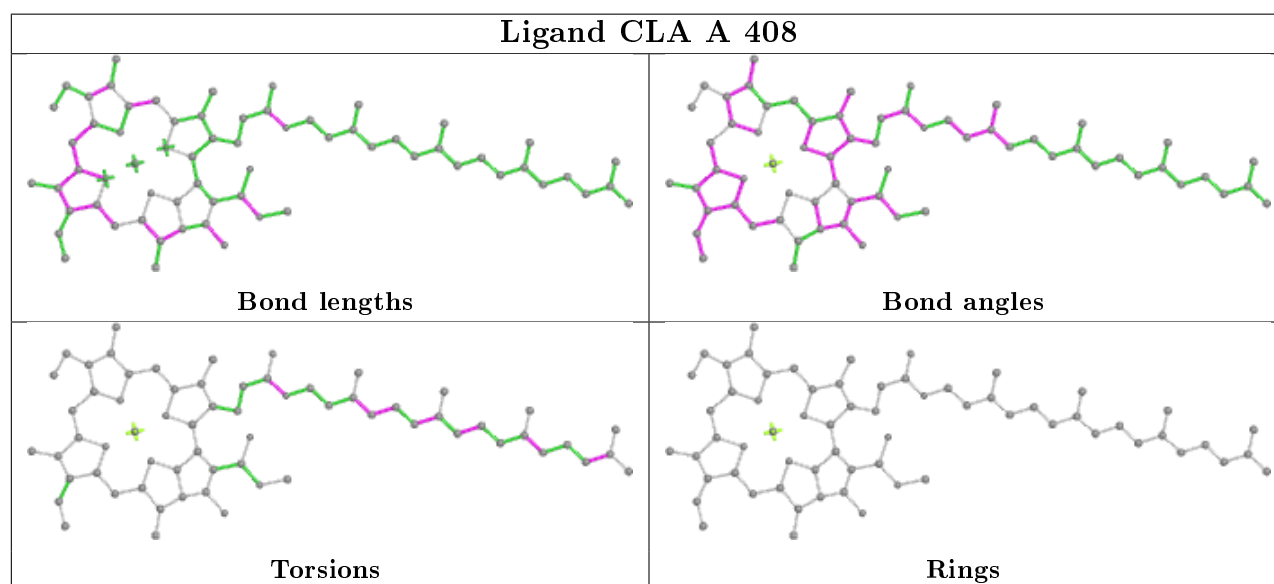
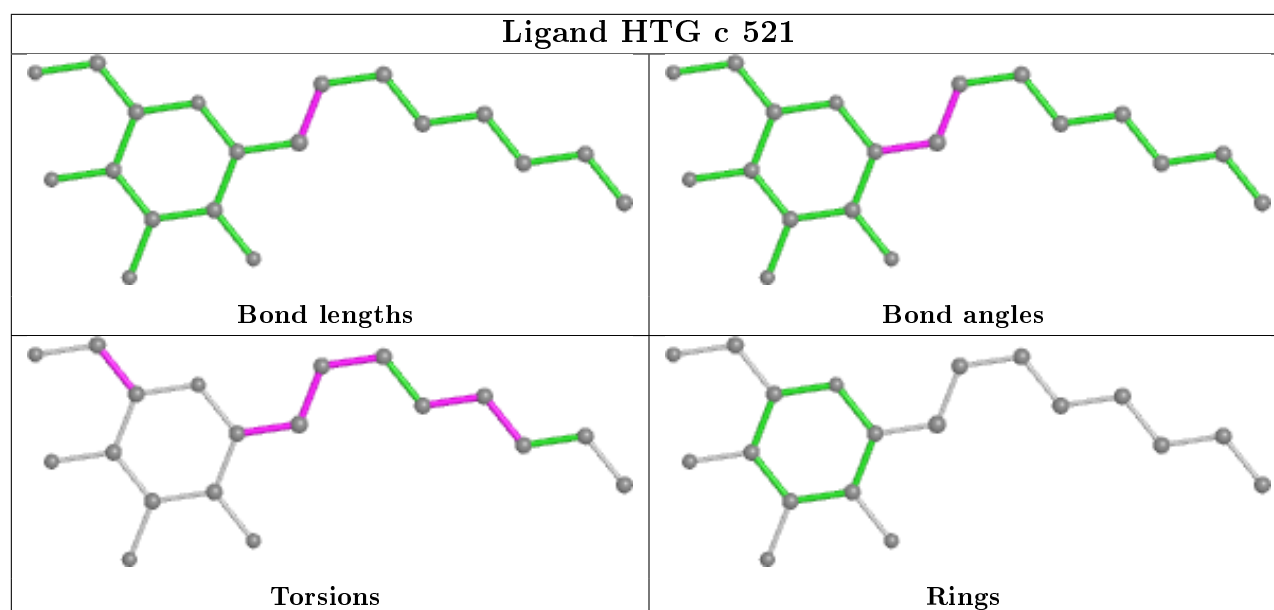




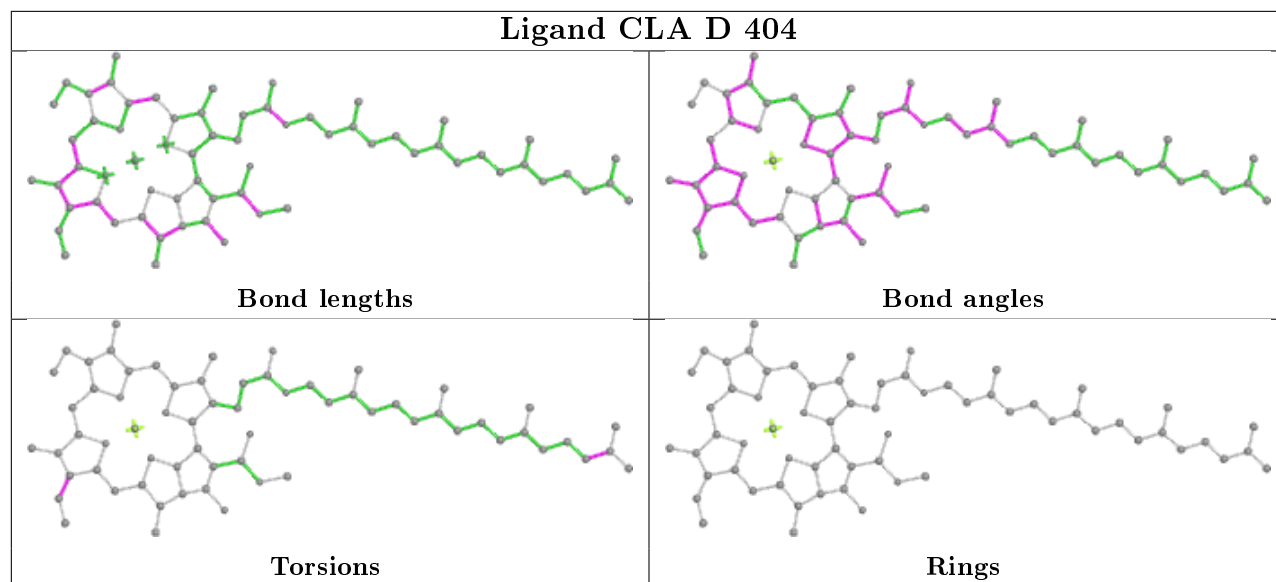




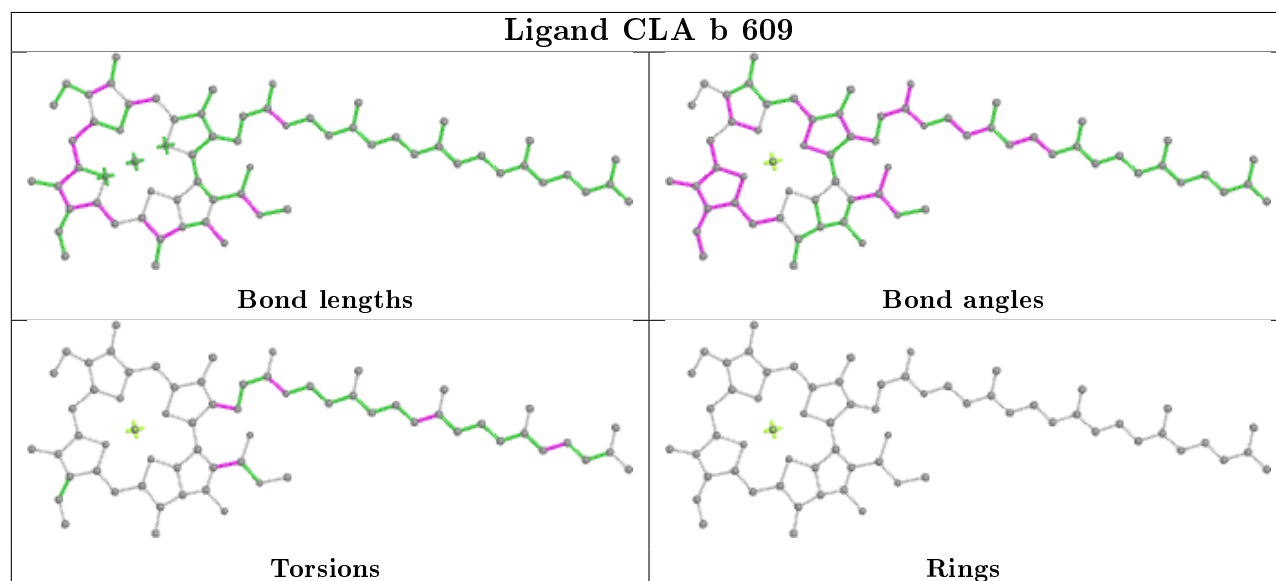




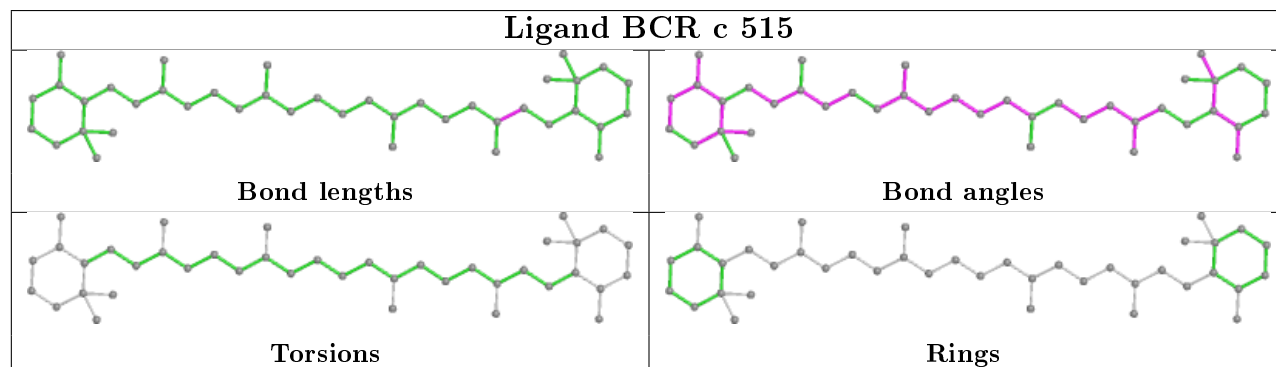
## Ligand CLA D 404

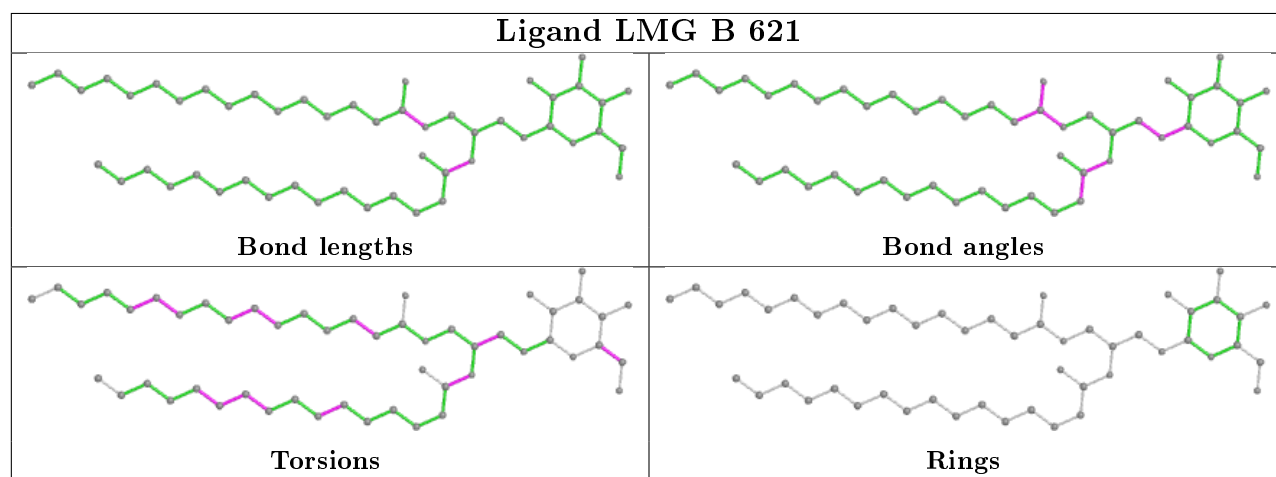
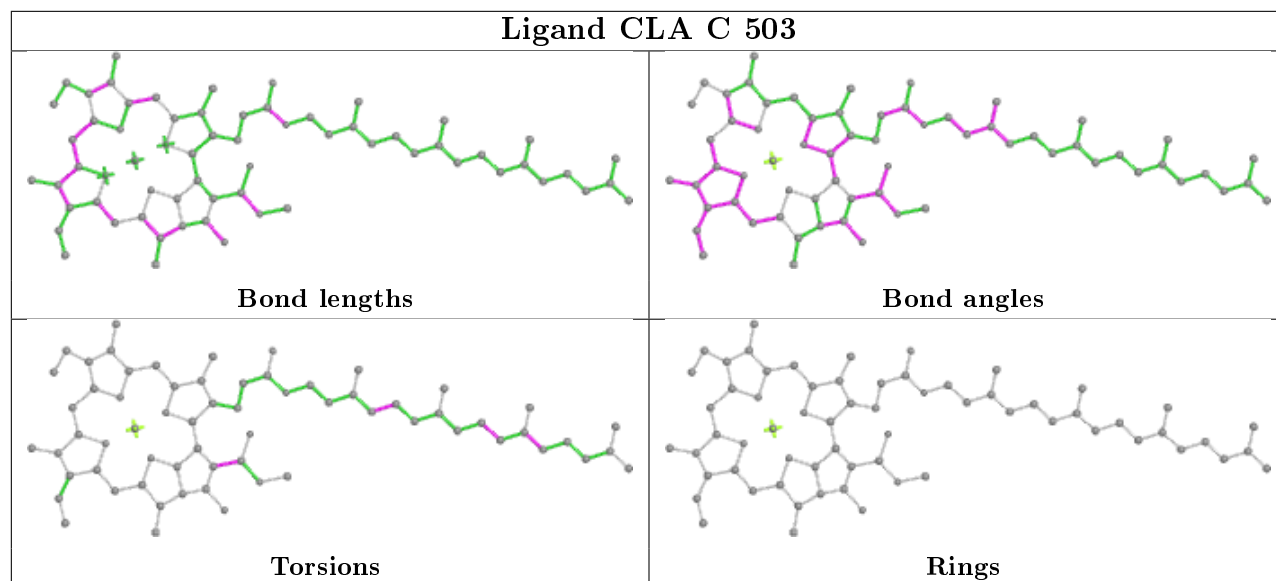
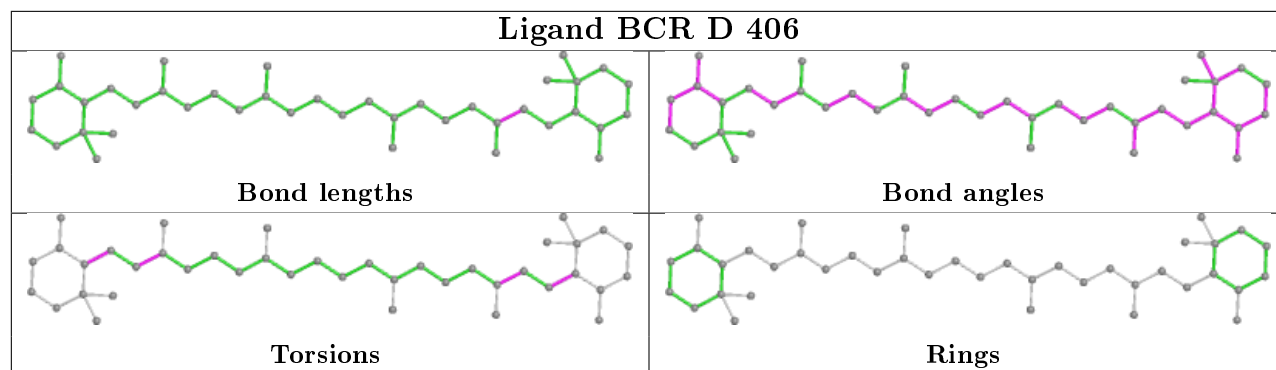


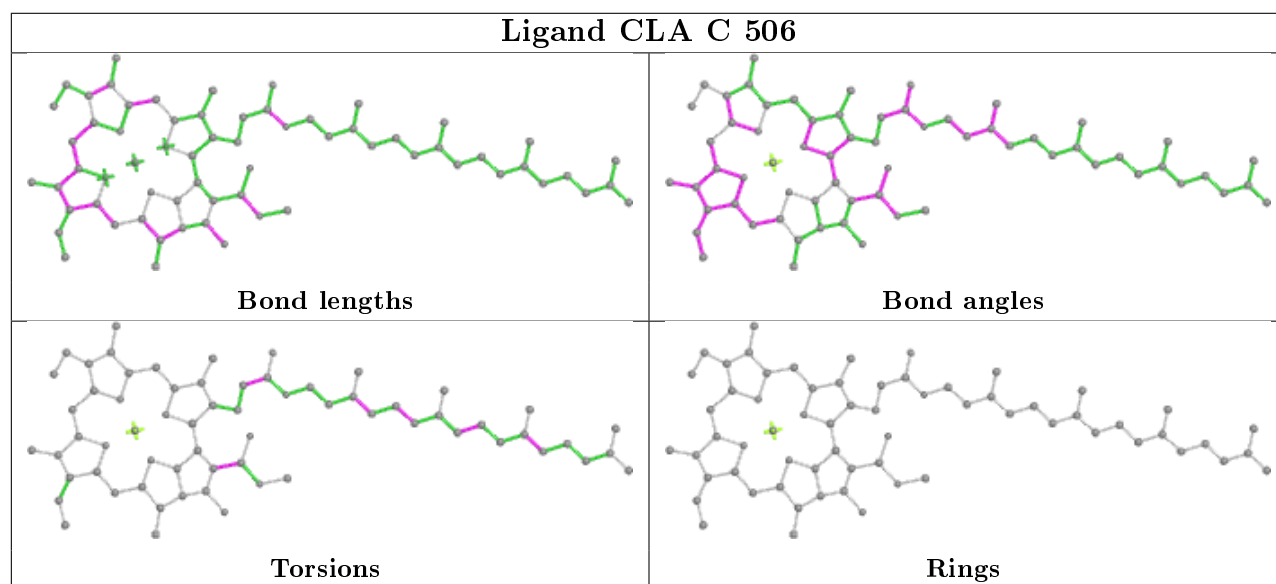
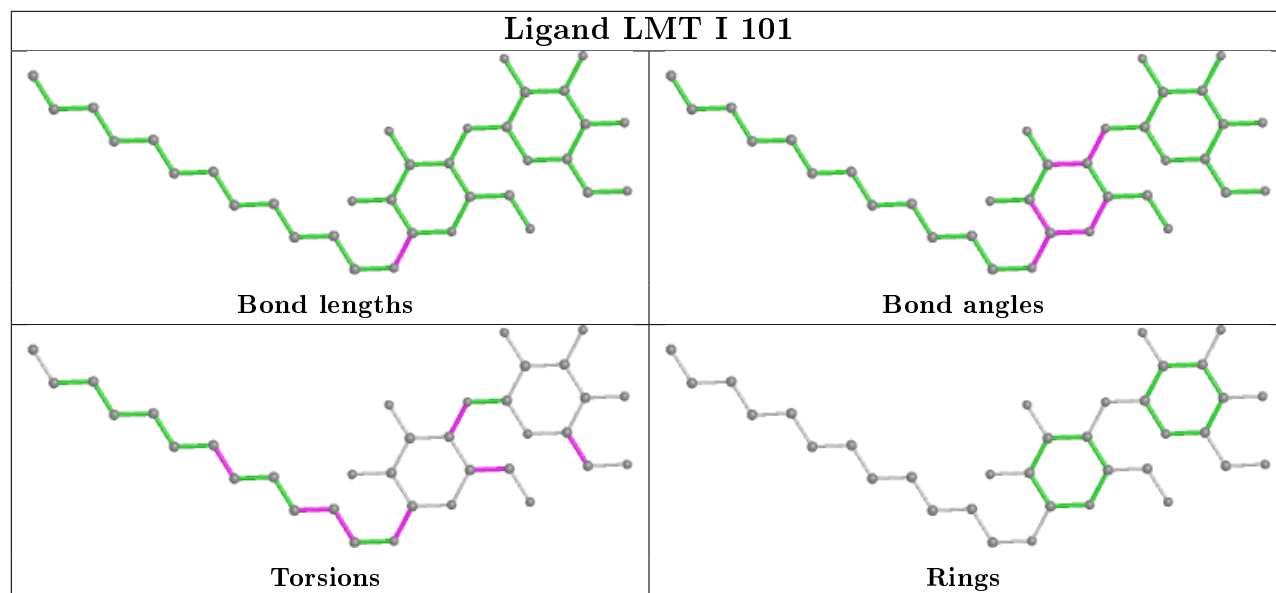
## Ligand CLA b 609

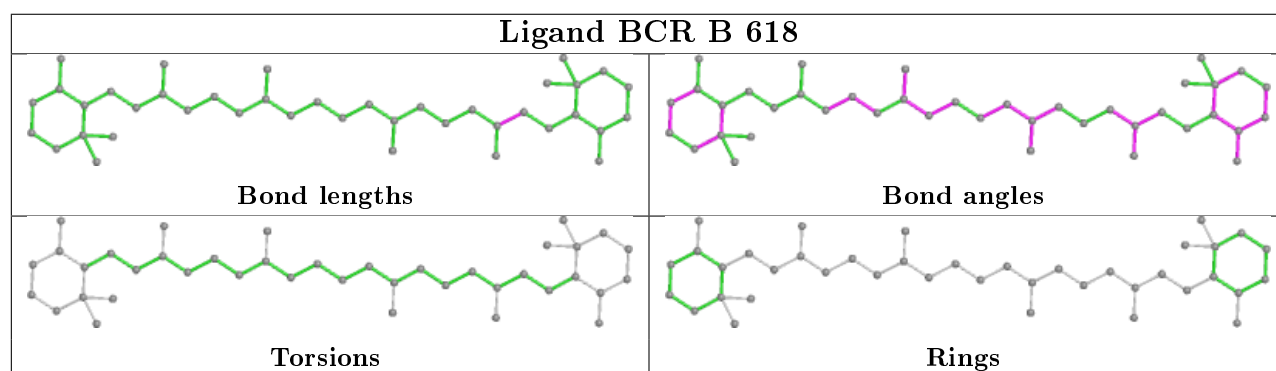
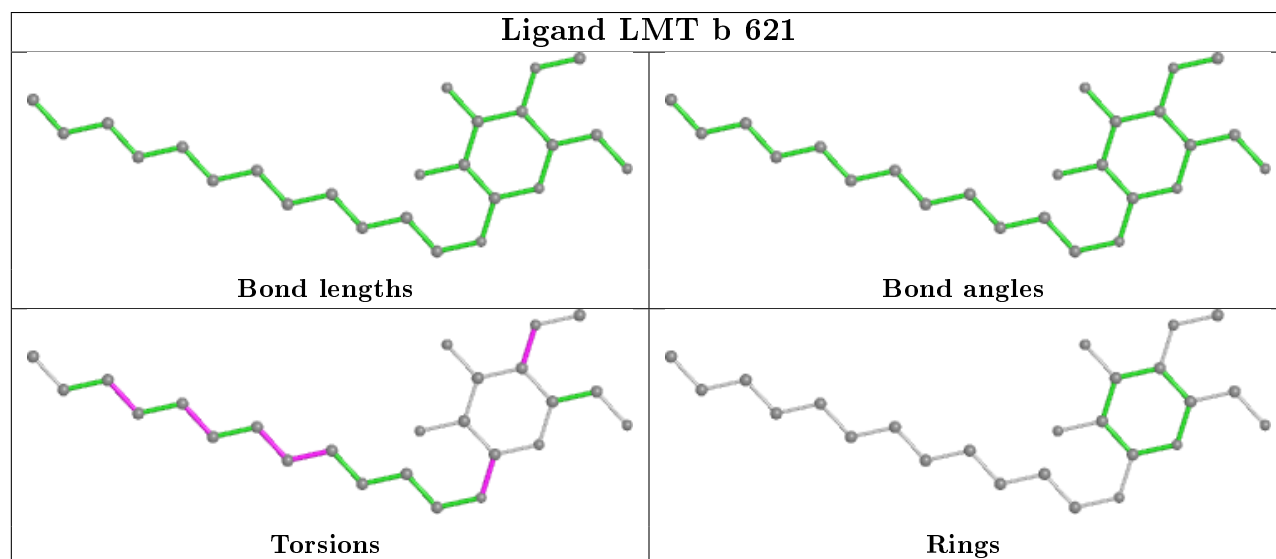
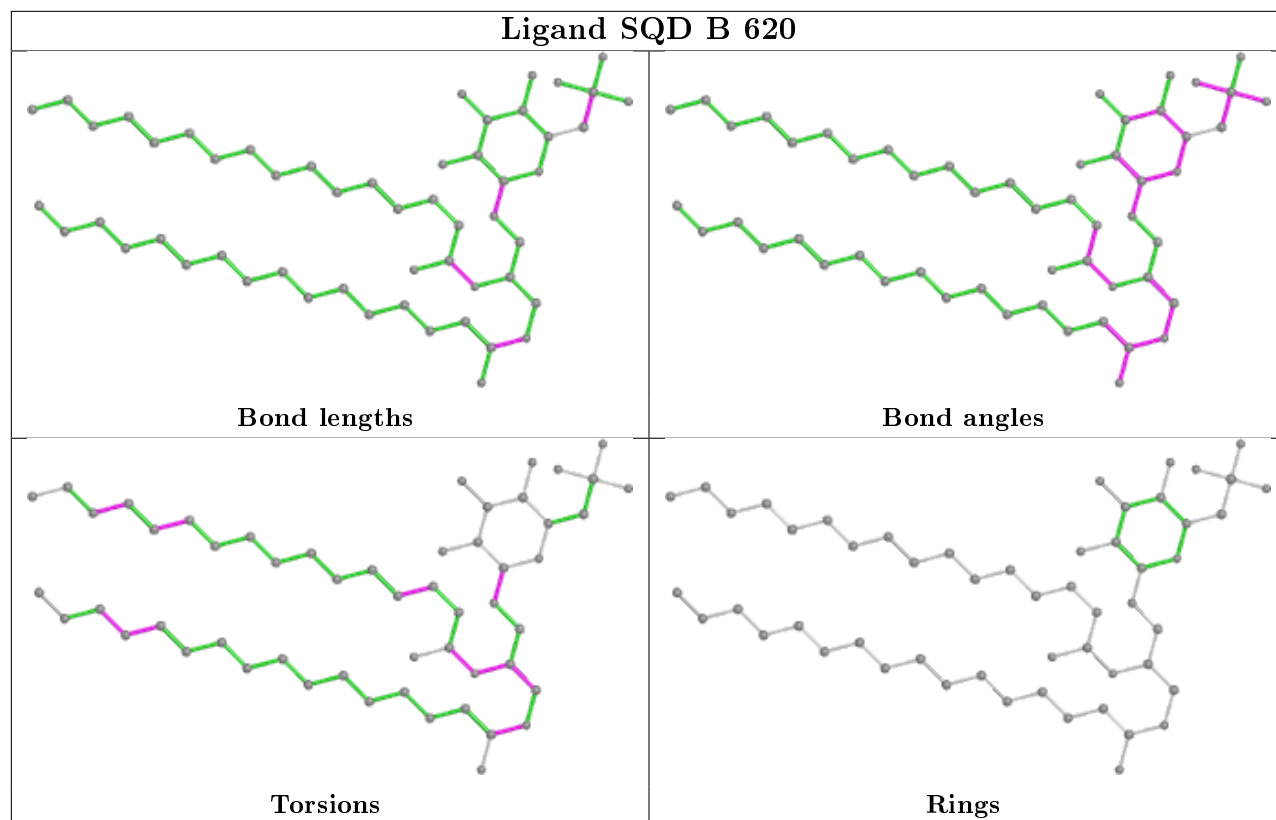


## Ligand BCR c 515

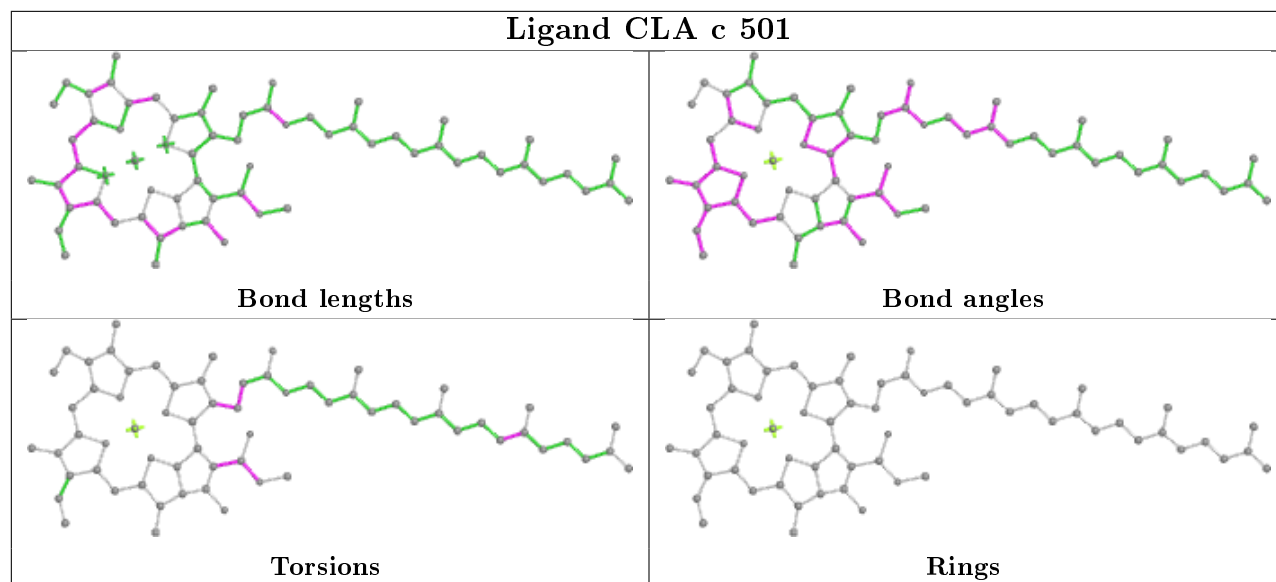




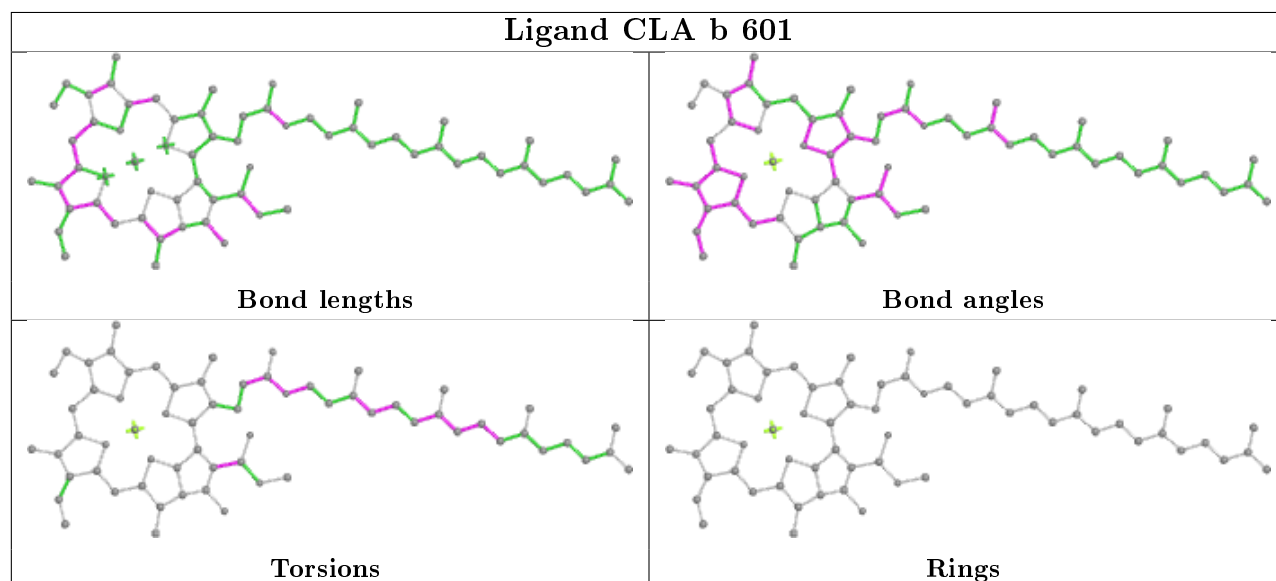




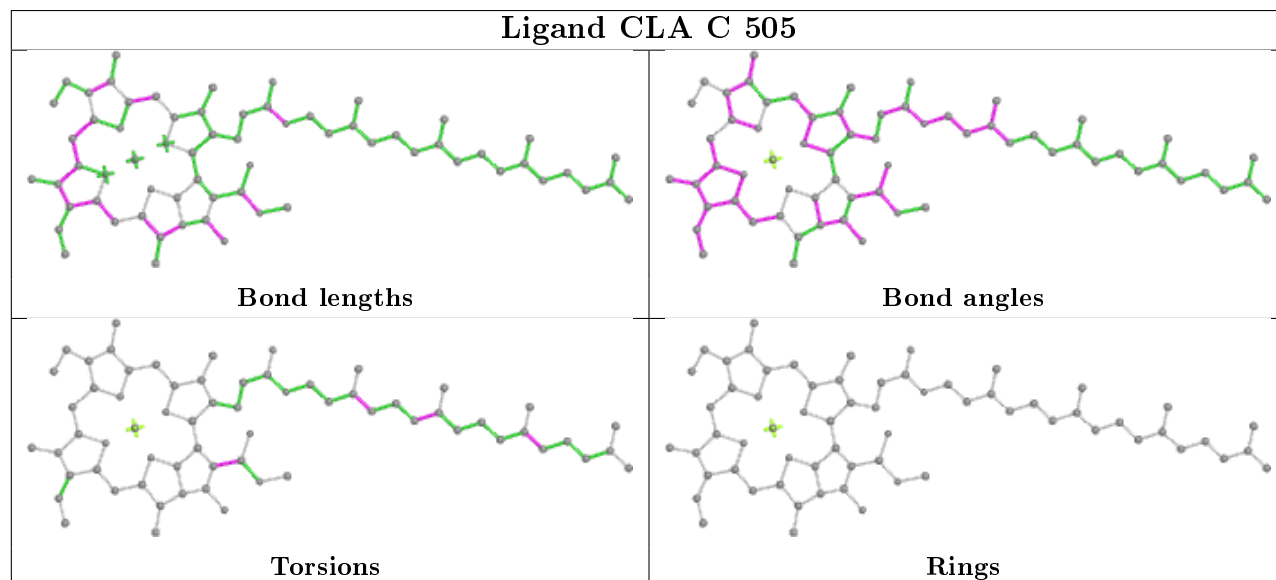
## Ligand CLA c 501

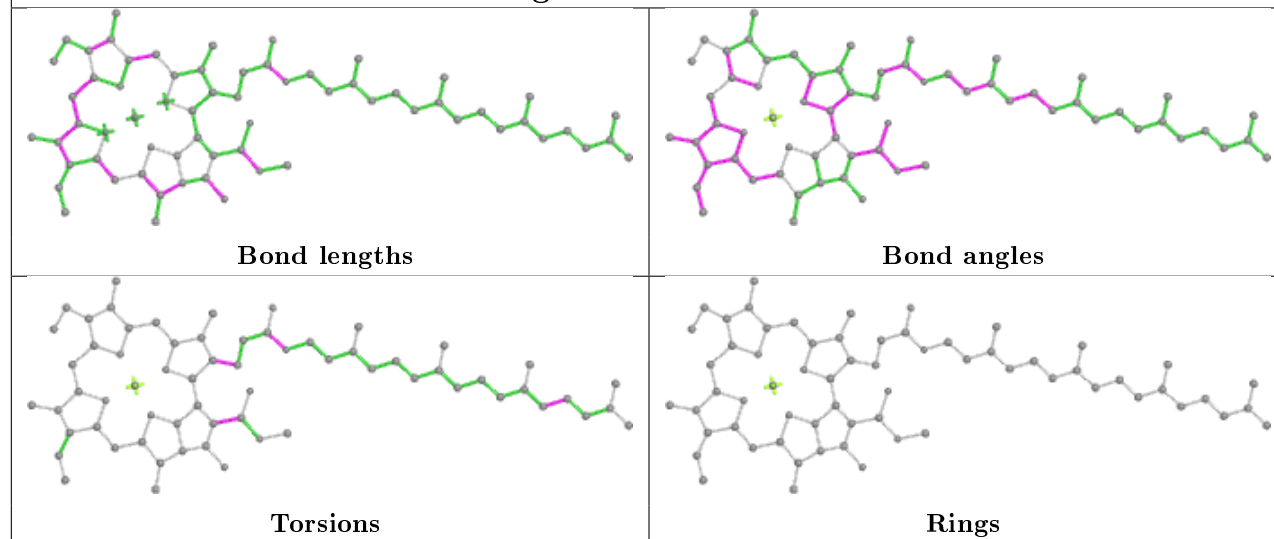
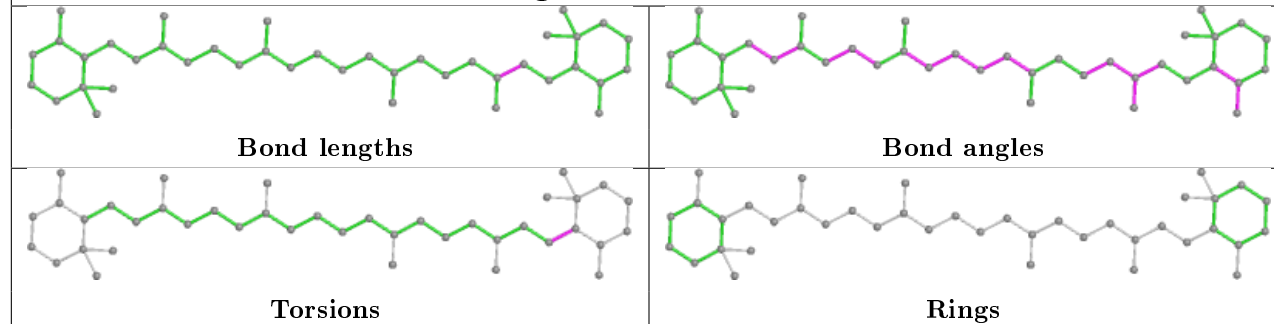
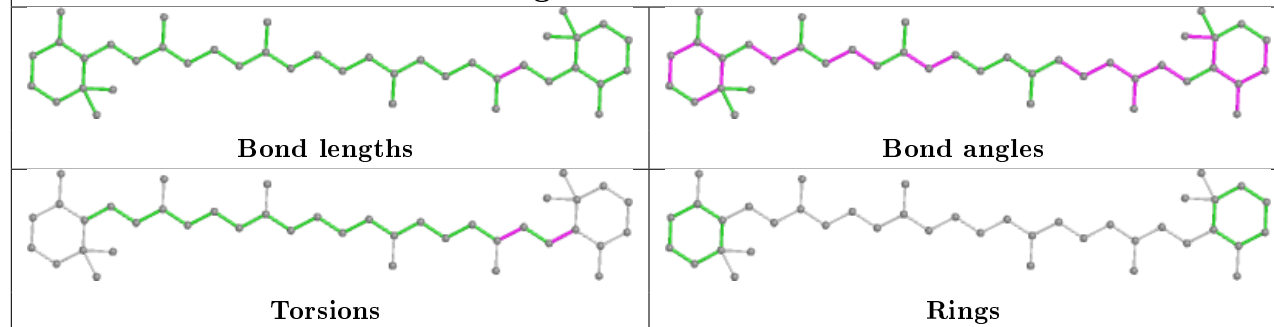


## Ligand CLA b 601



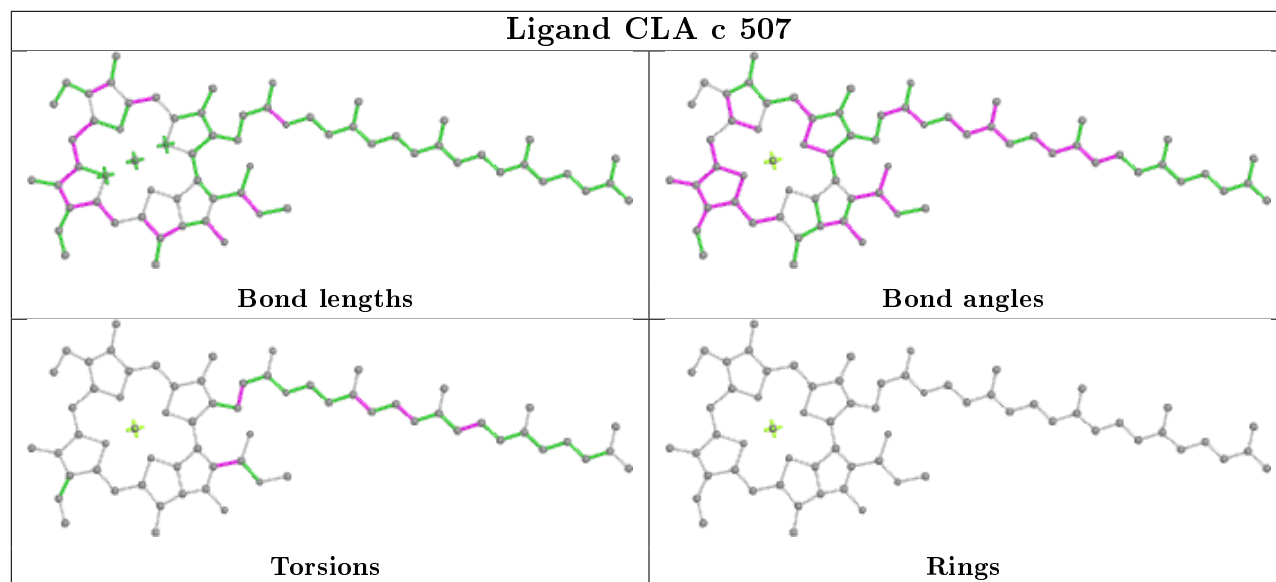
## Ligand CLA C 505



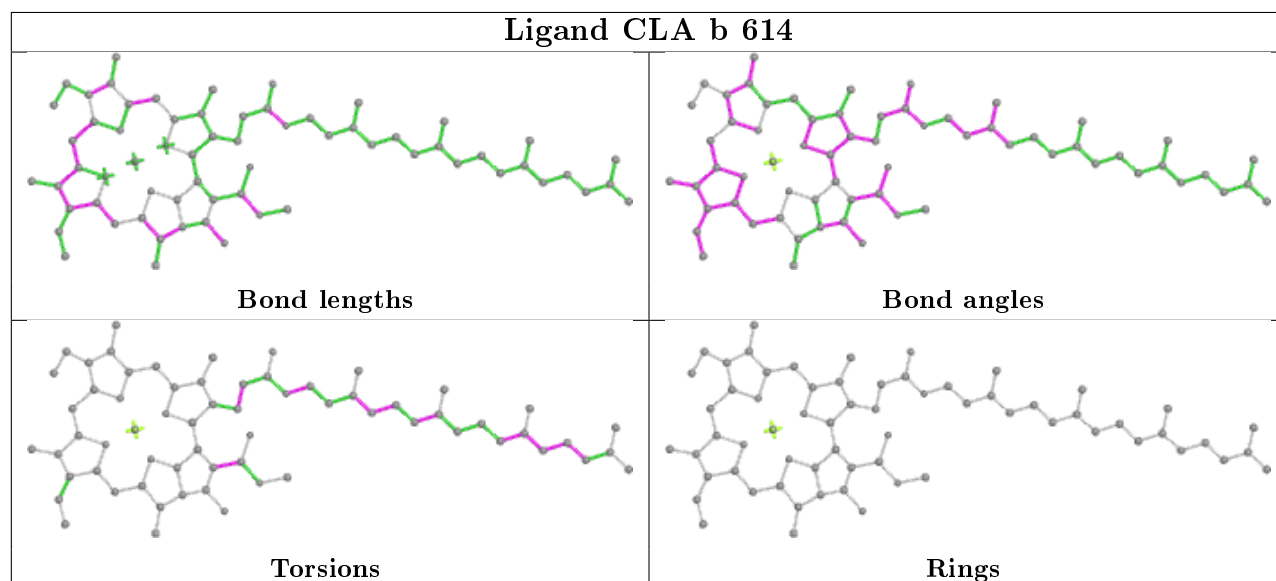
**Ligand CLA B 609****Ligand BCR h 101****Ligand BCR b 619**



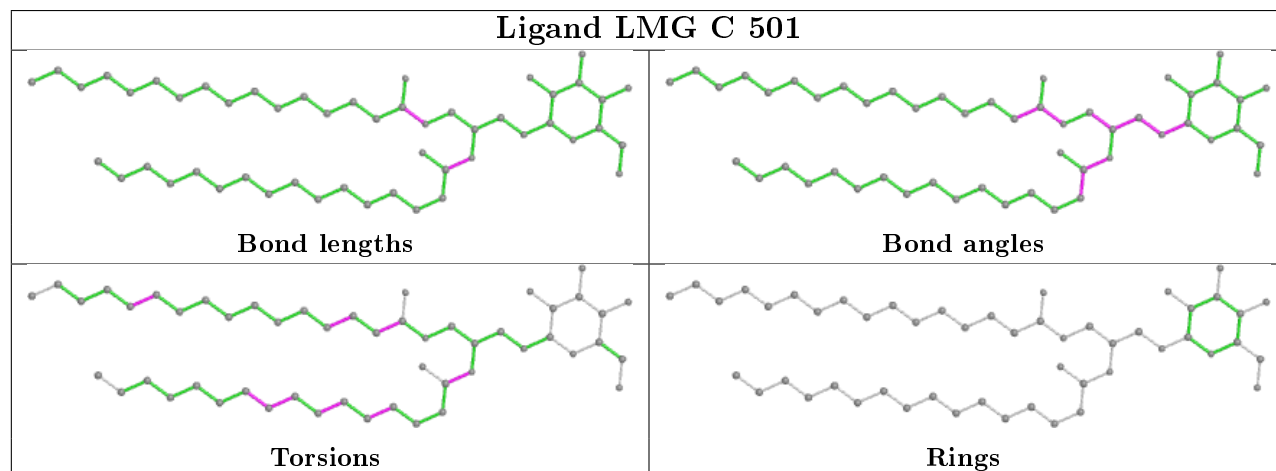
## Ligand CLA c 507



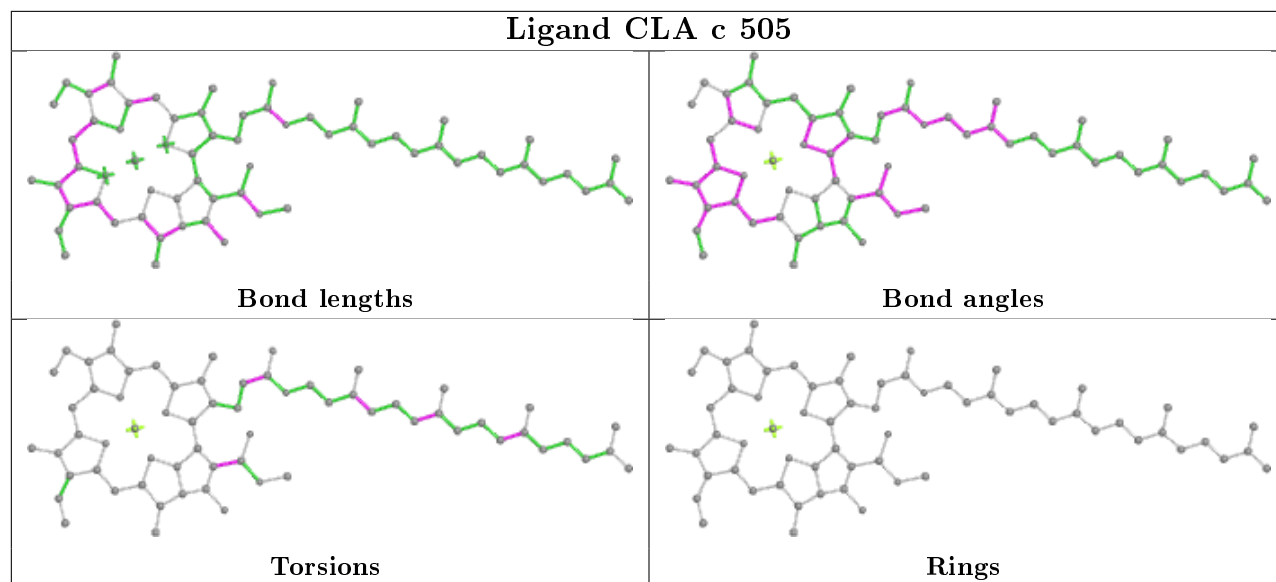
## Ligand CLA b 614



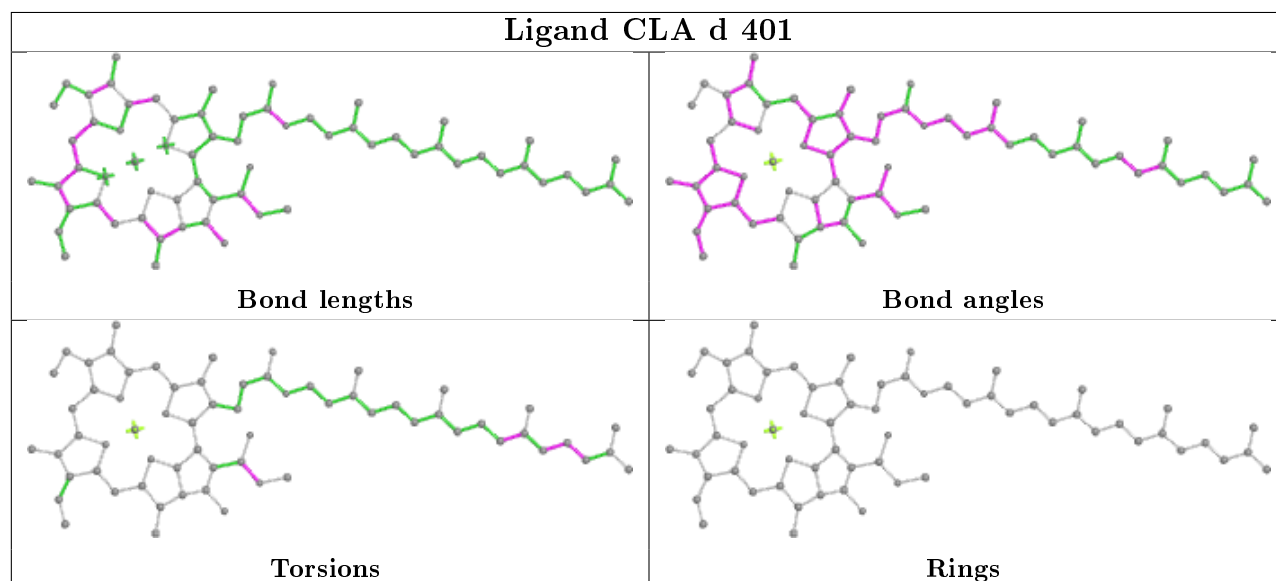
## Ligand LMG C 501



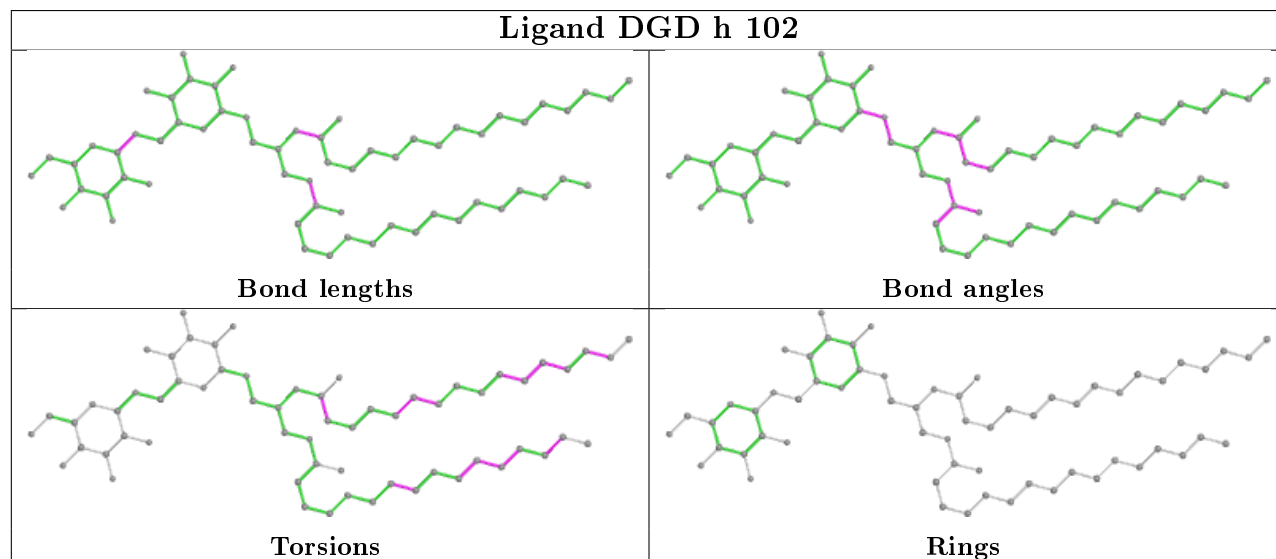
## Ligand CLA c 505



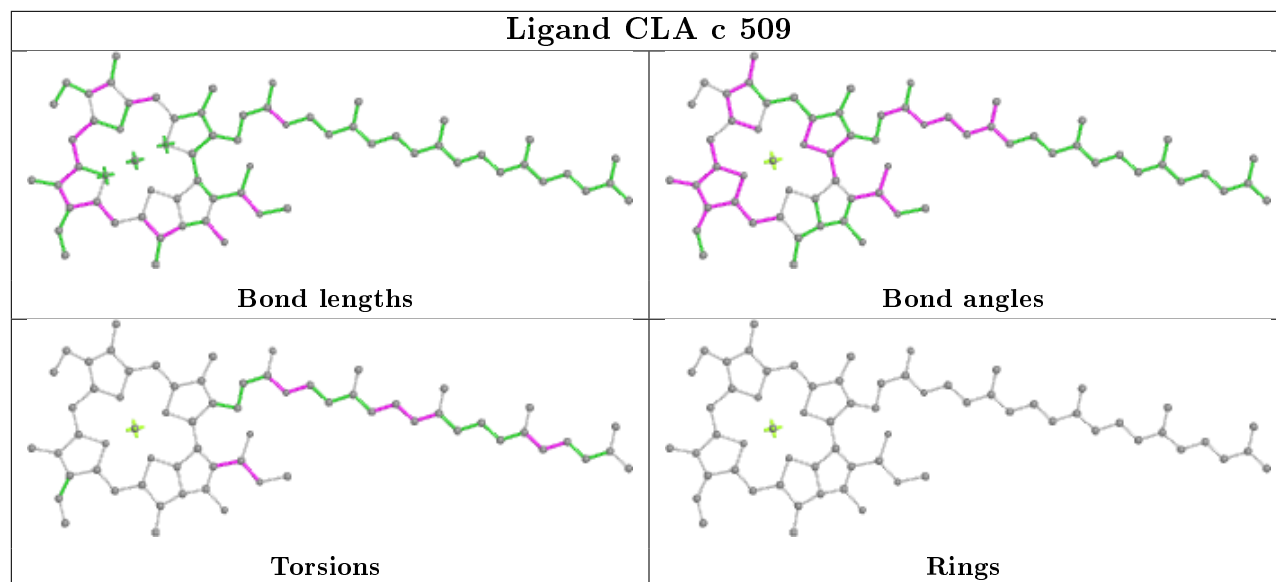
## Ligand CLA d 401



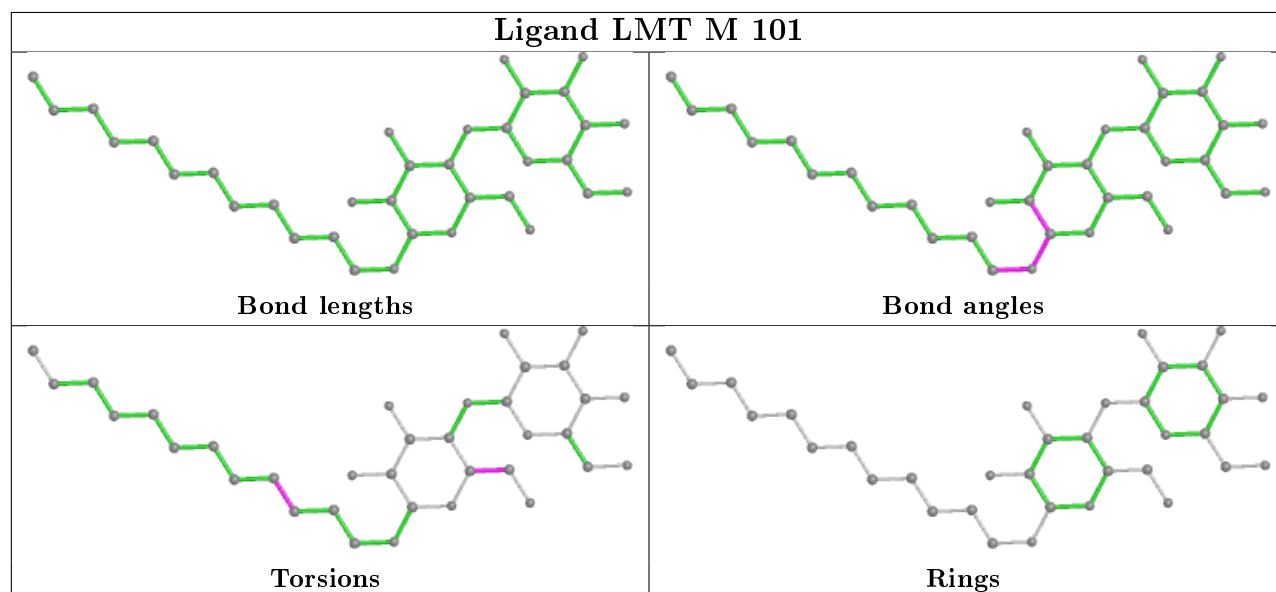
## Ligand DGD h 102

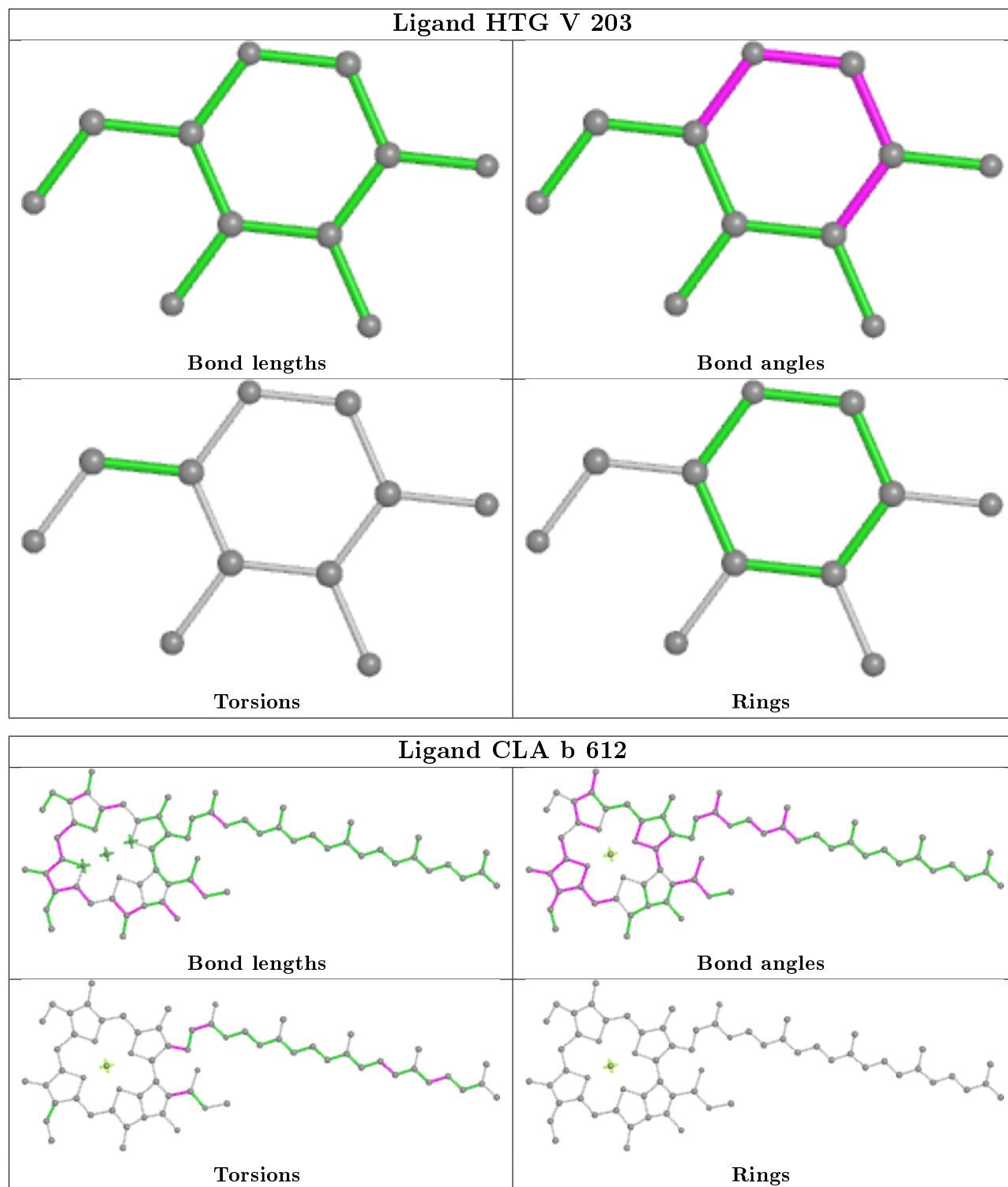


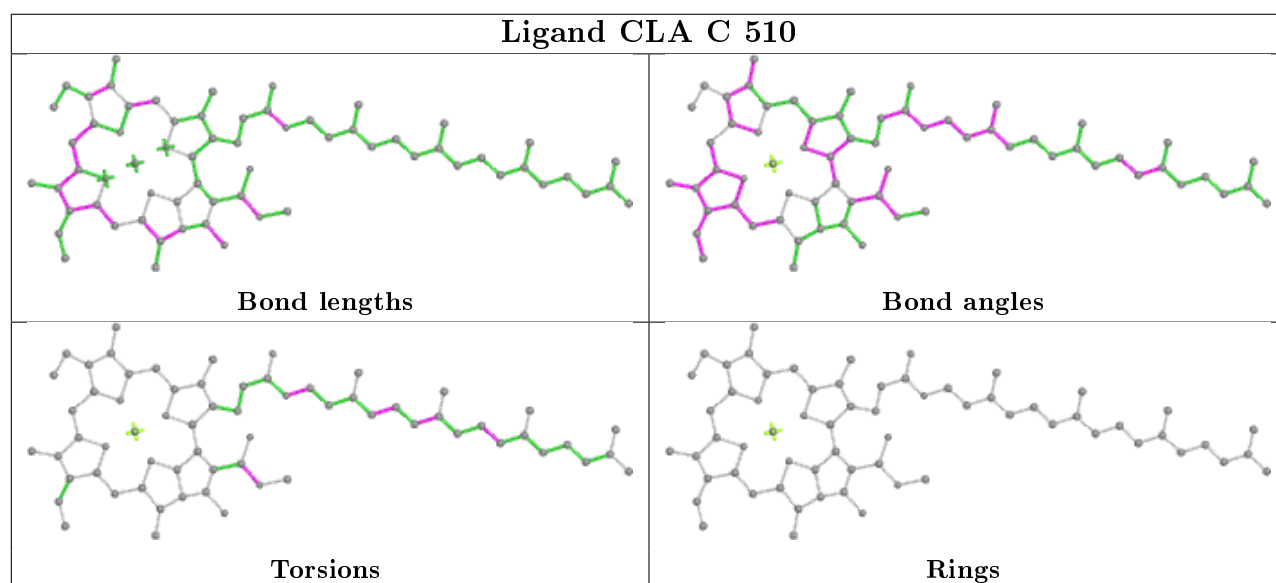
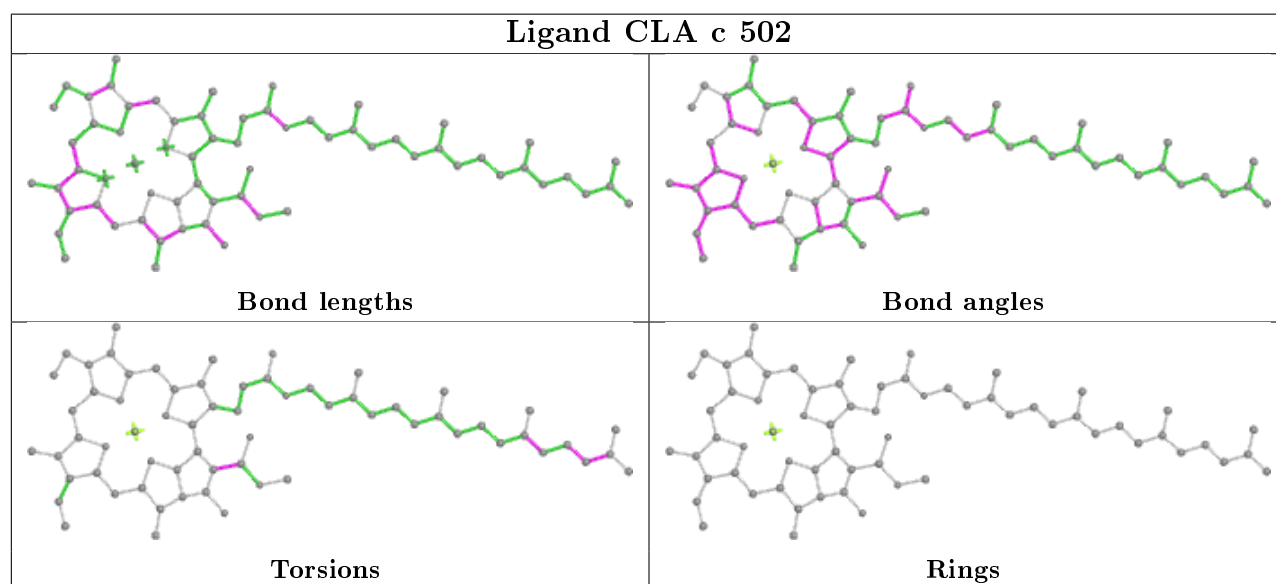
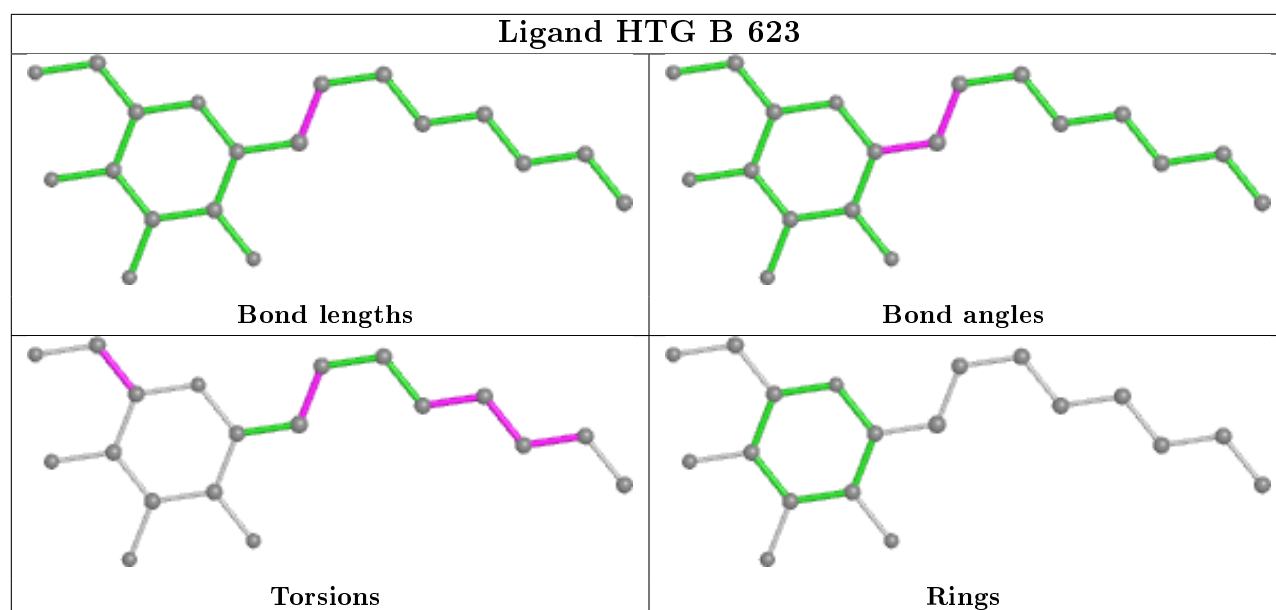
## Ligand CLA c 509

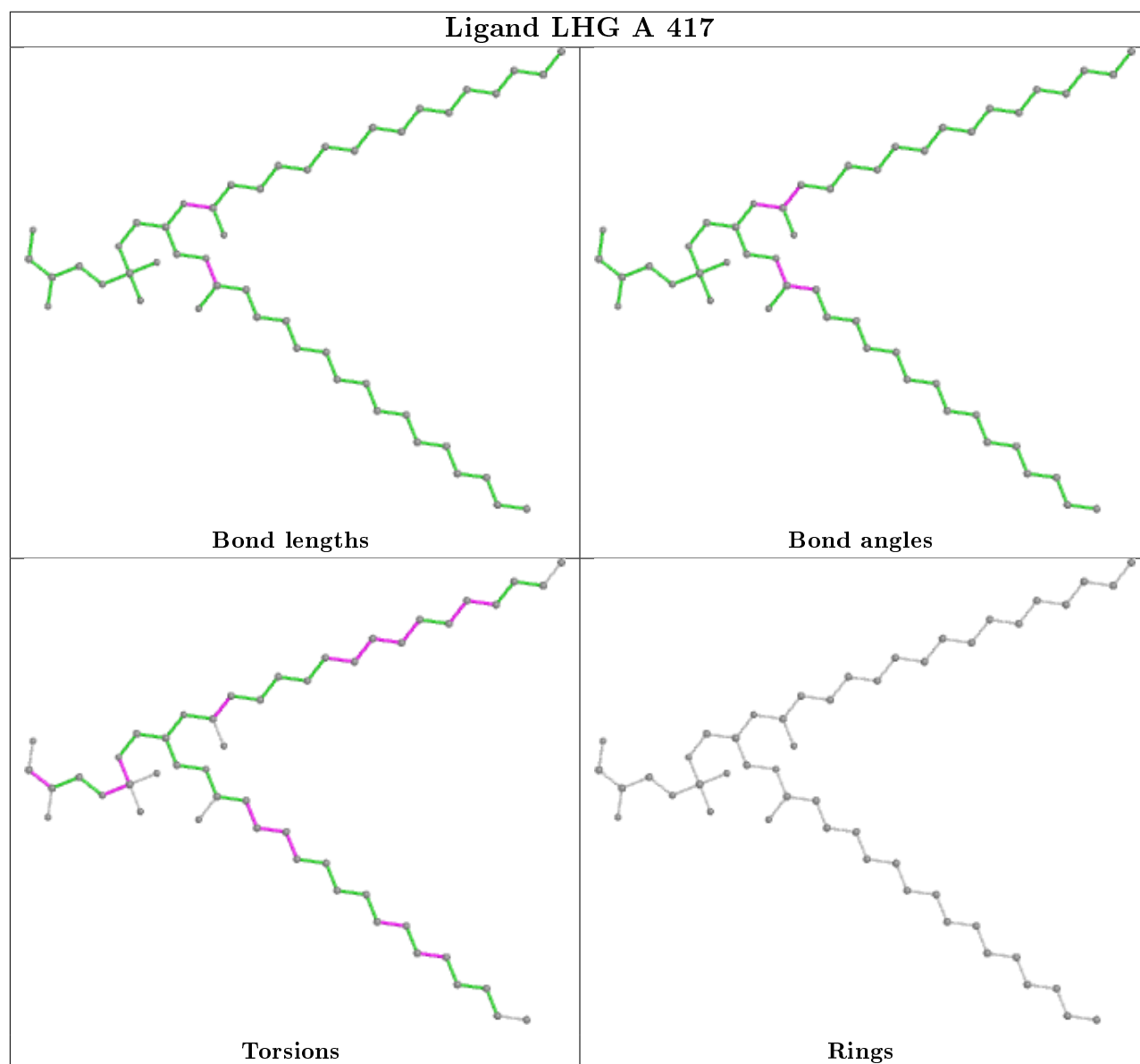
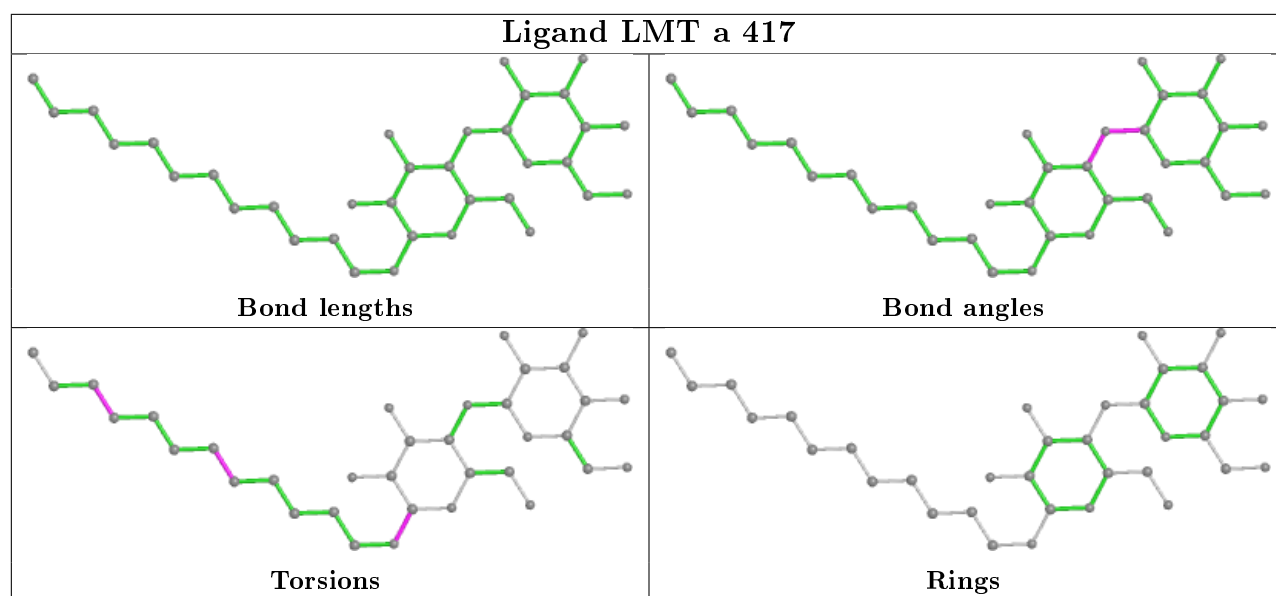


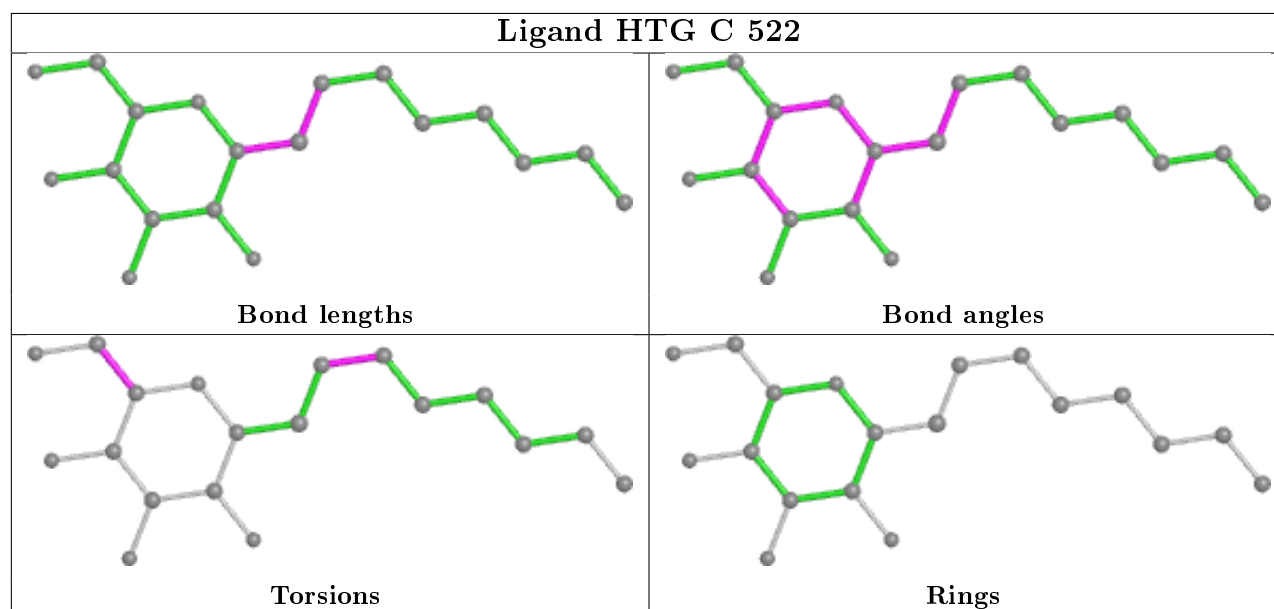
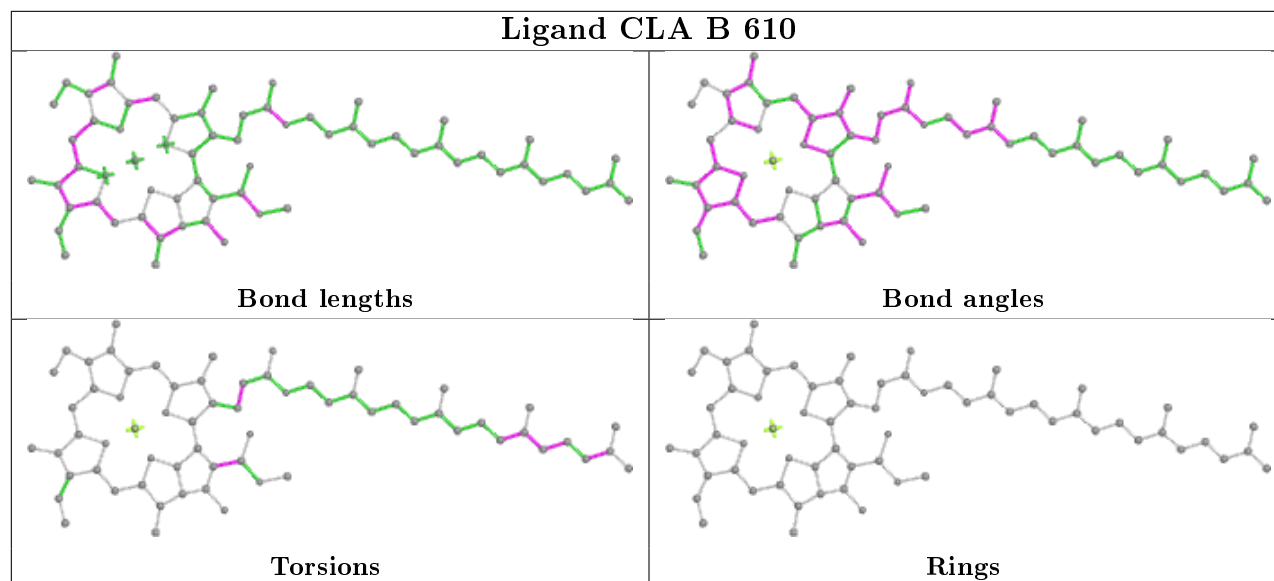
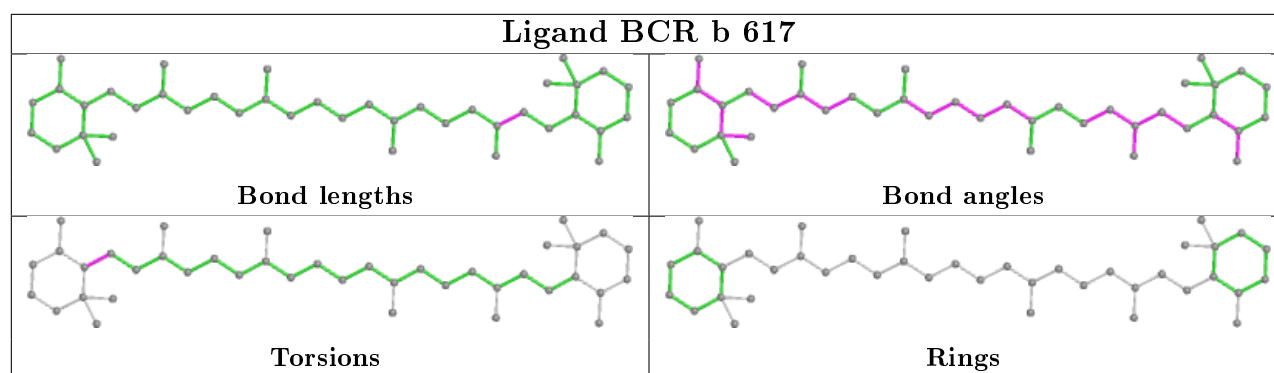
## Ligand LMT M 101



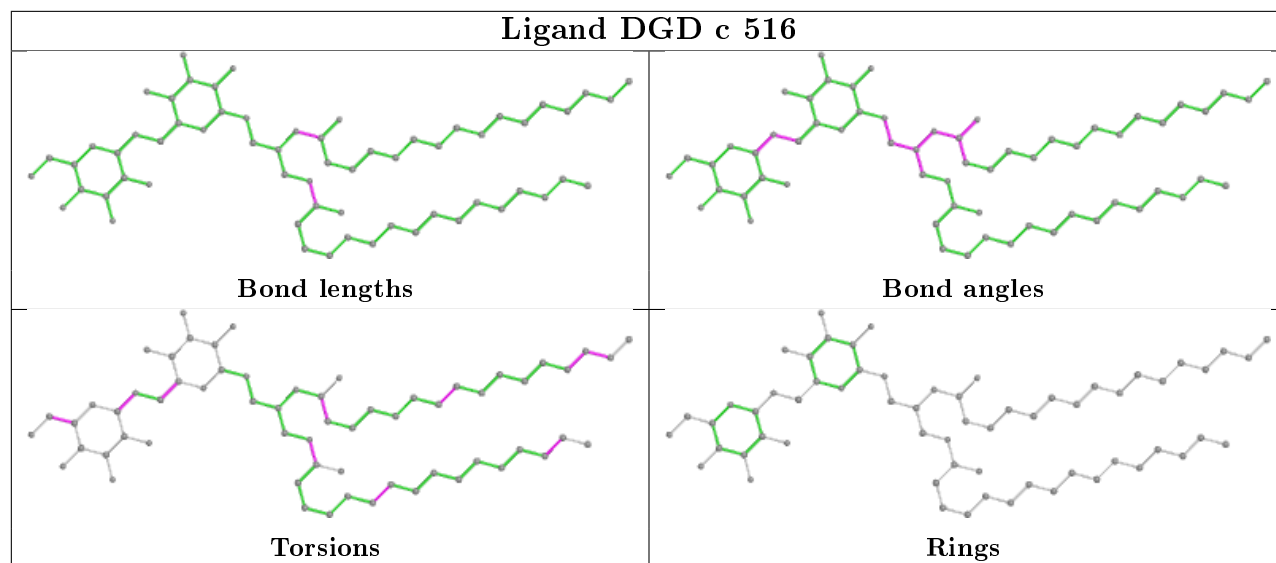




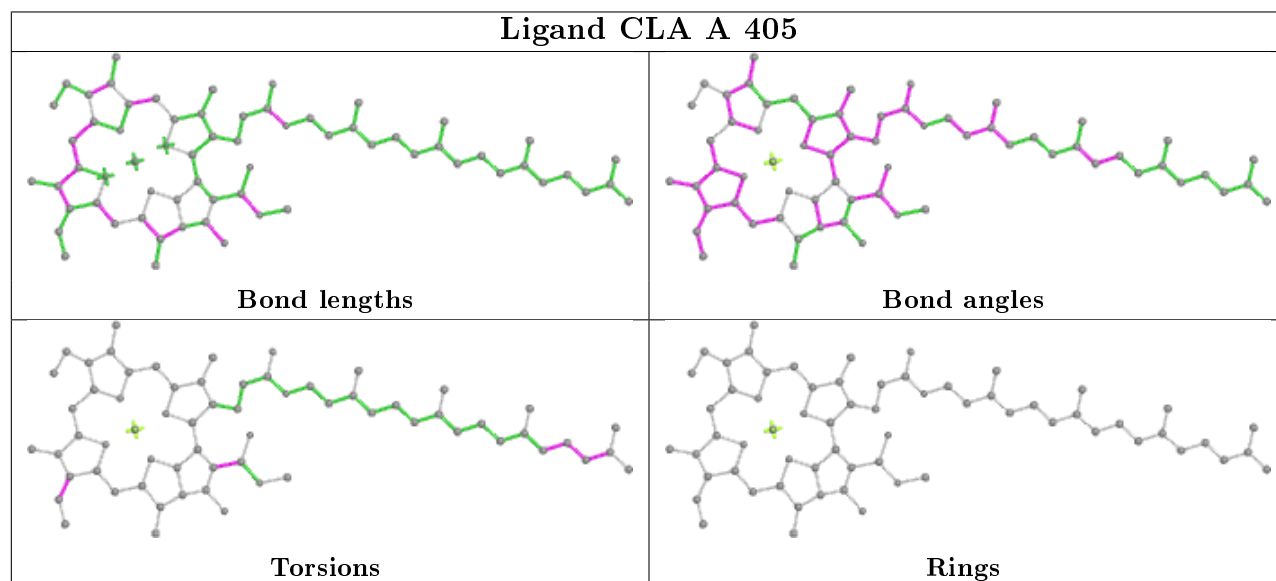




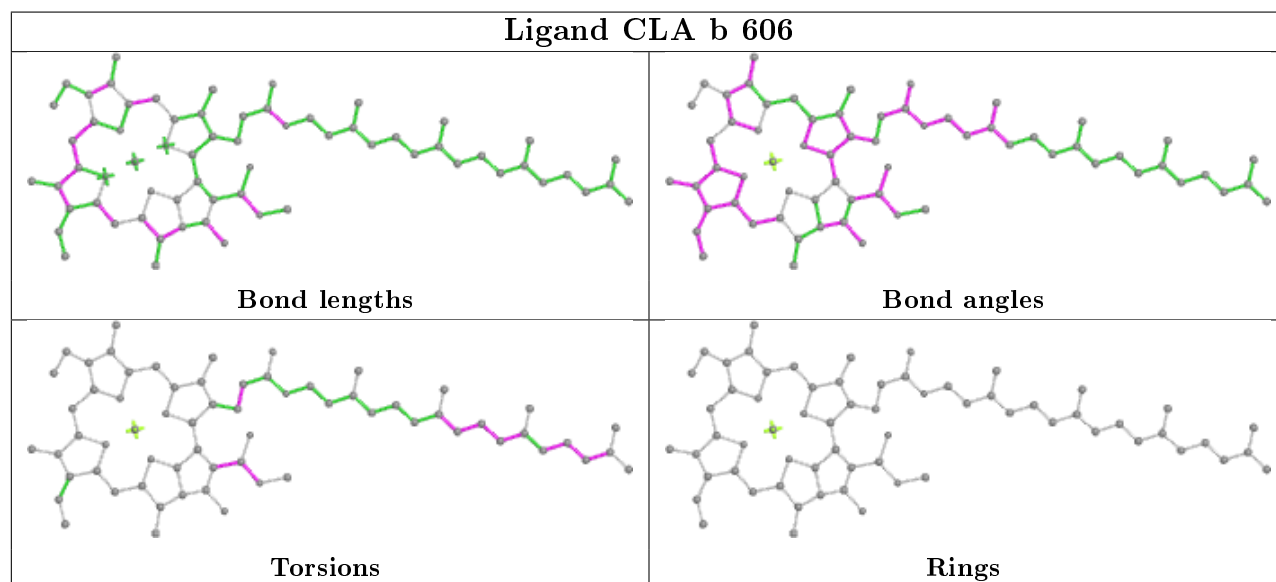
## Ligand DGD c 516



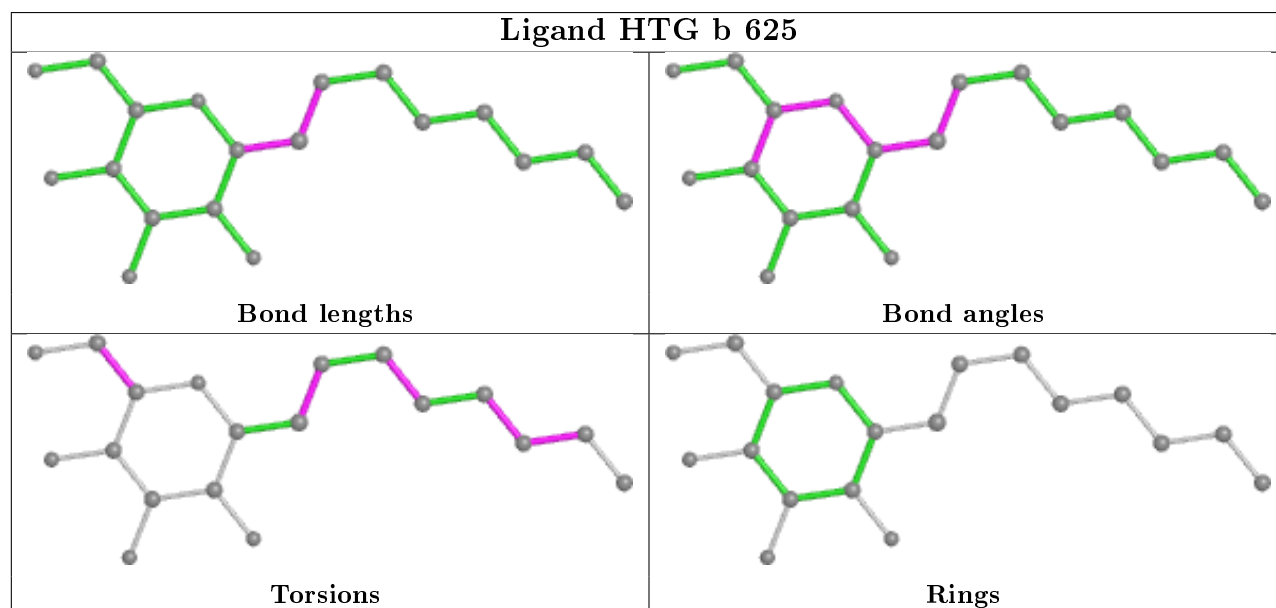
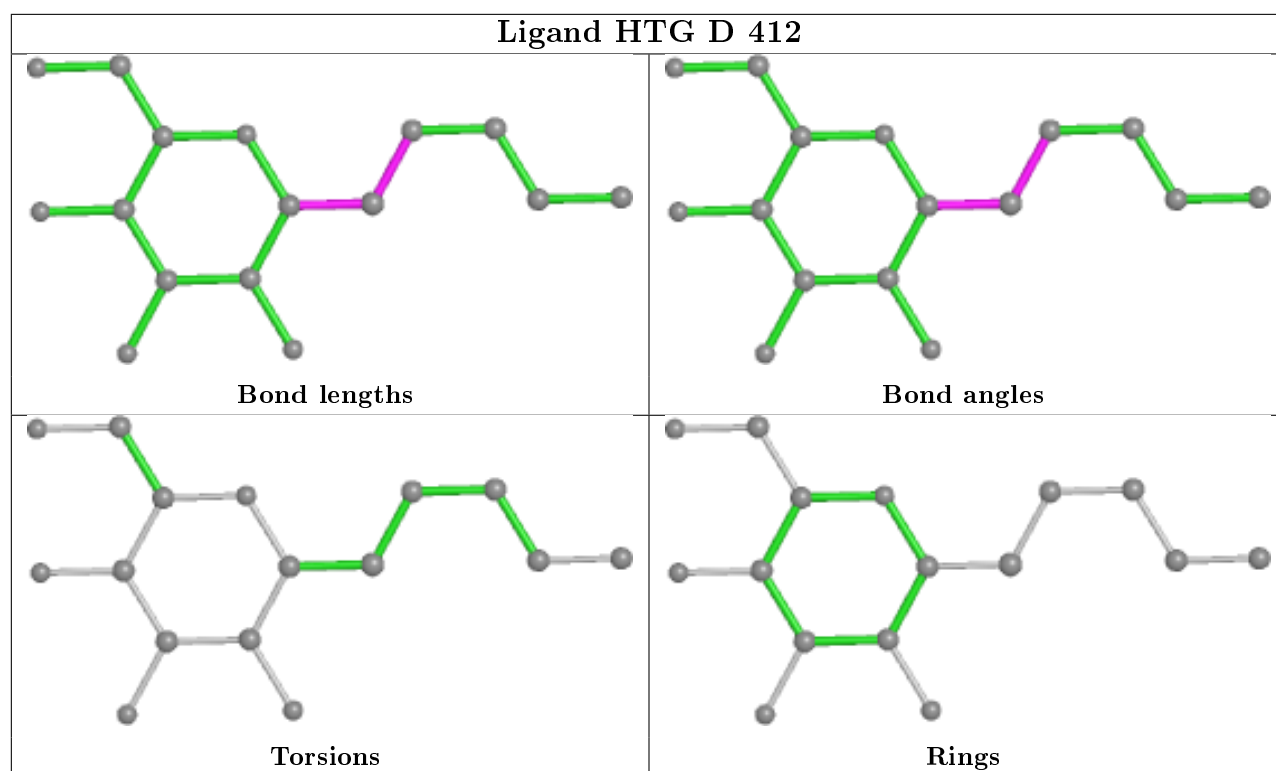
## Ligand CLA A 405

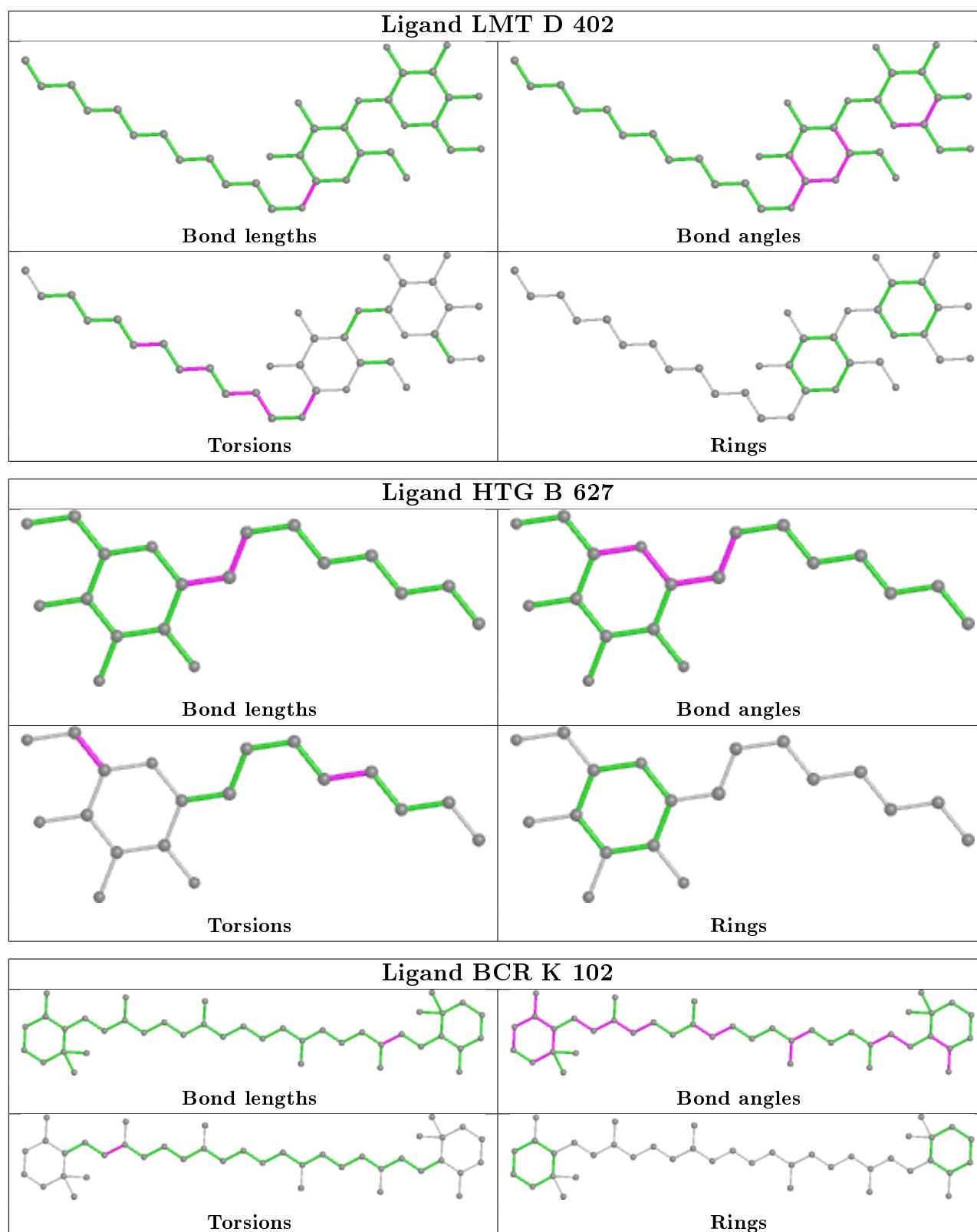


## Ligand CLA b 606

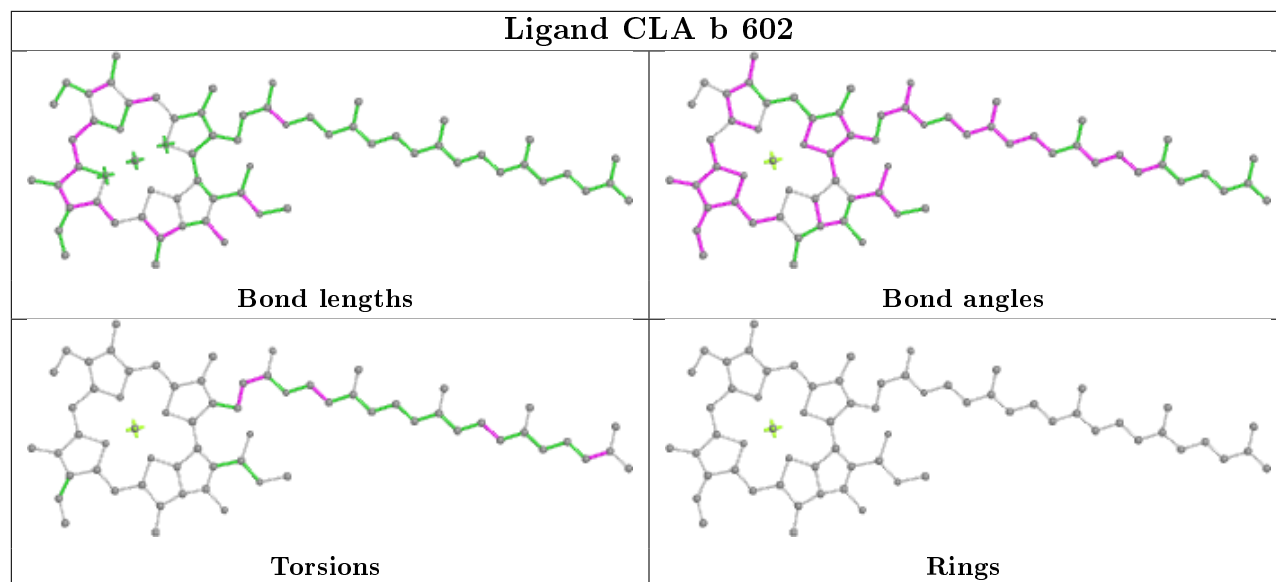




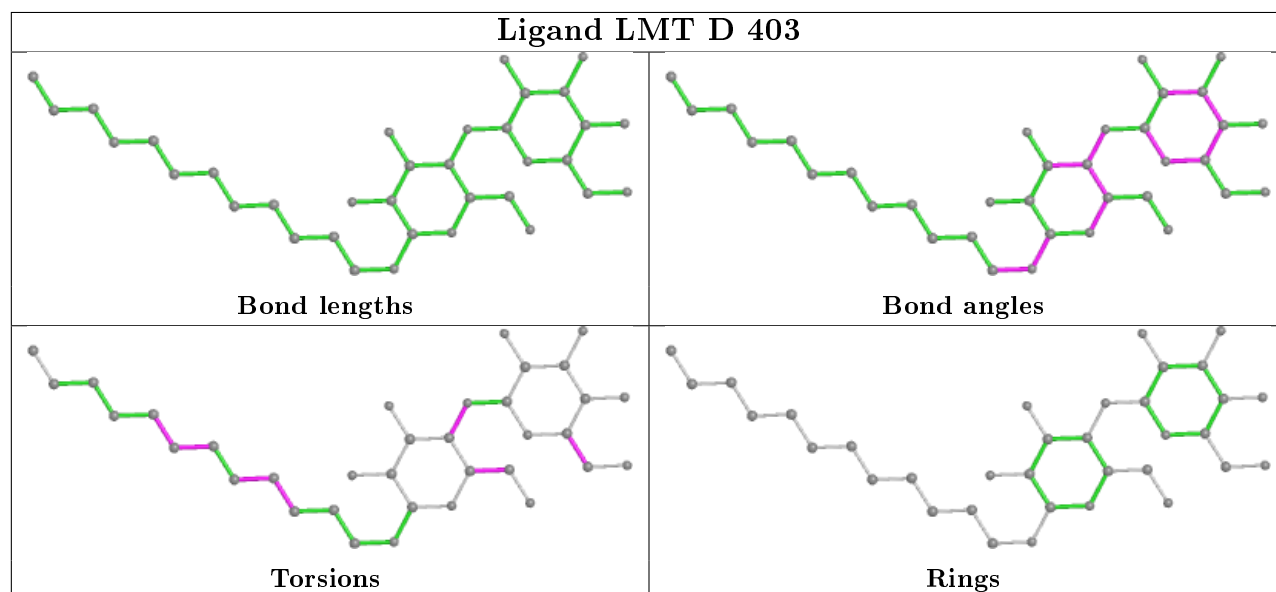




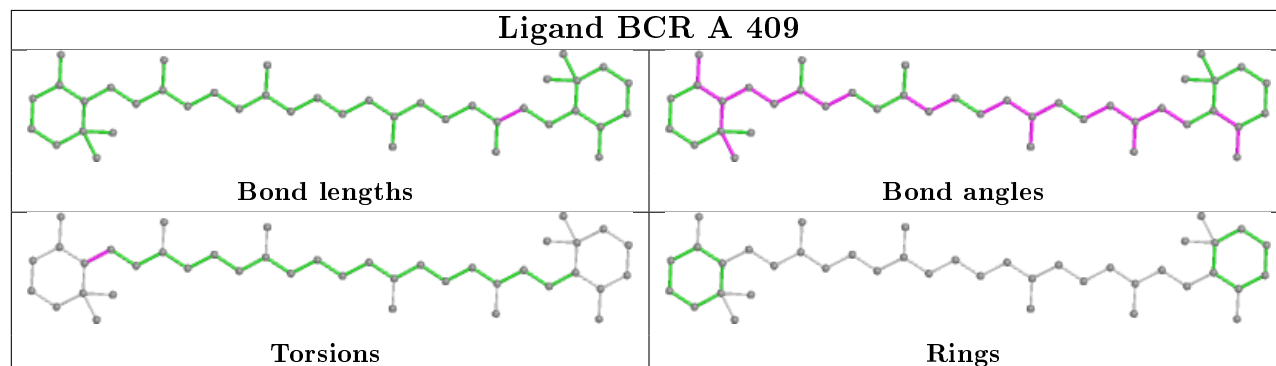
## Ligand CLA b 602



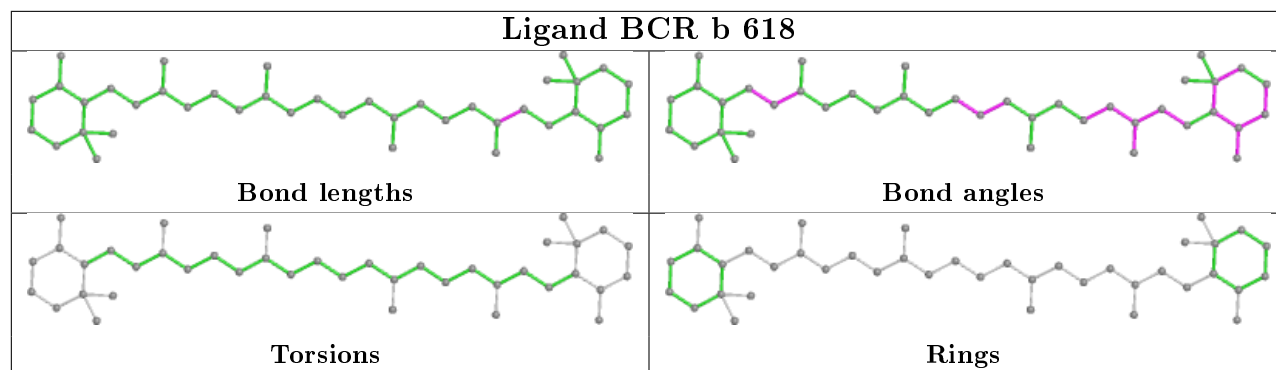
## Ligand LMT D 403



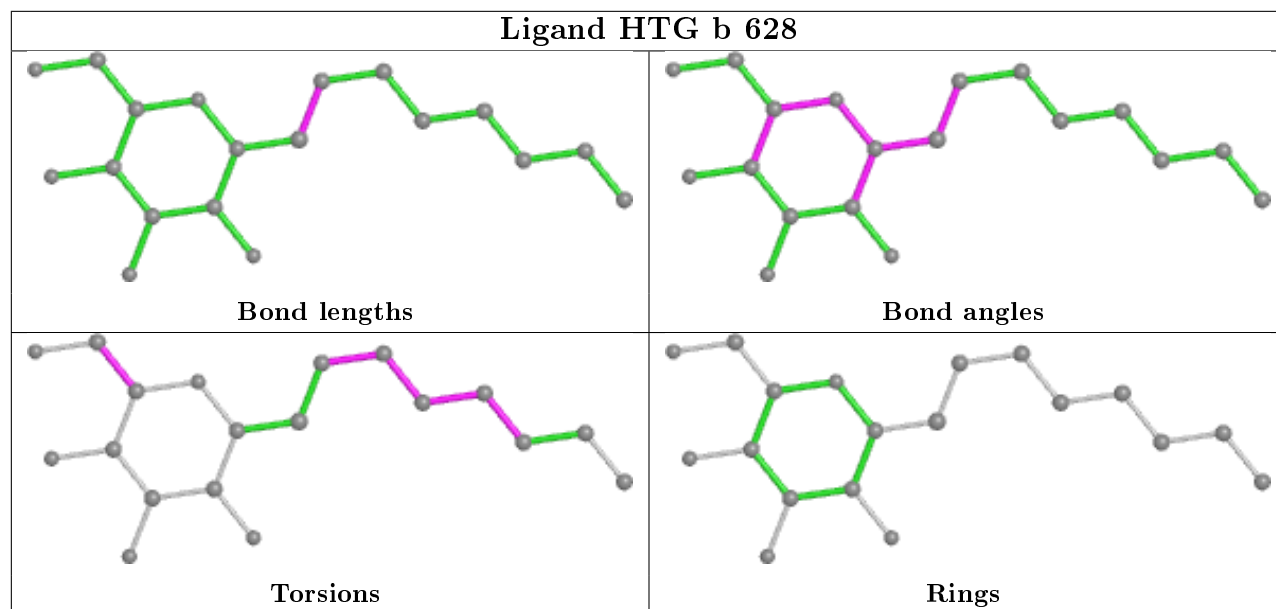
## Ligand BCR A 409



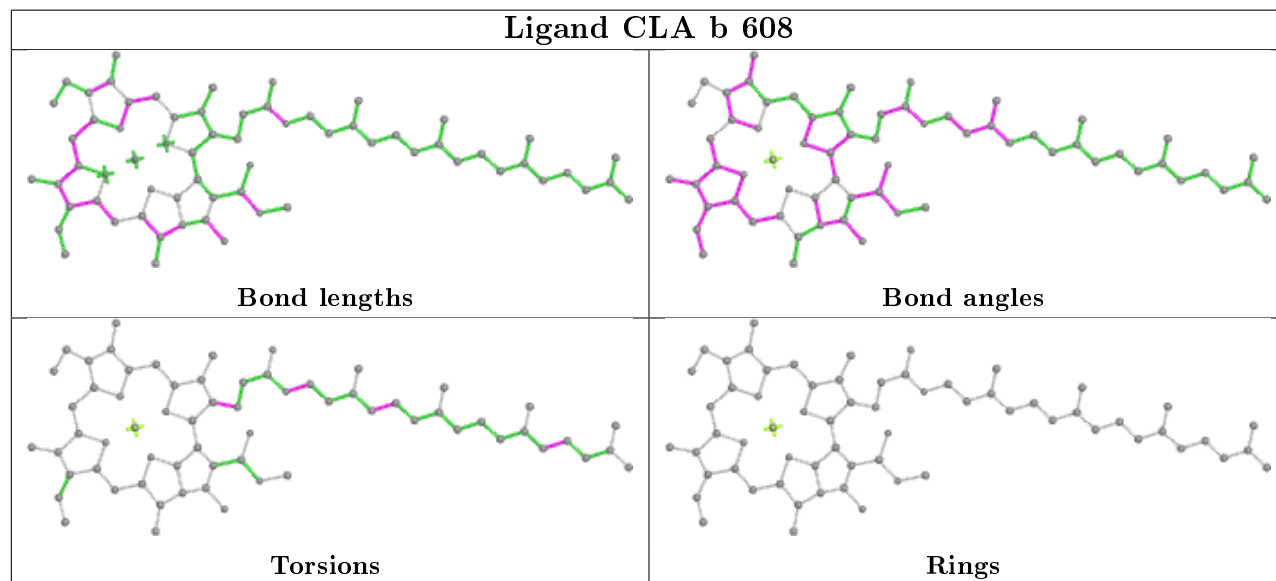
## Ligand BCR b 618

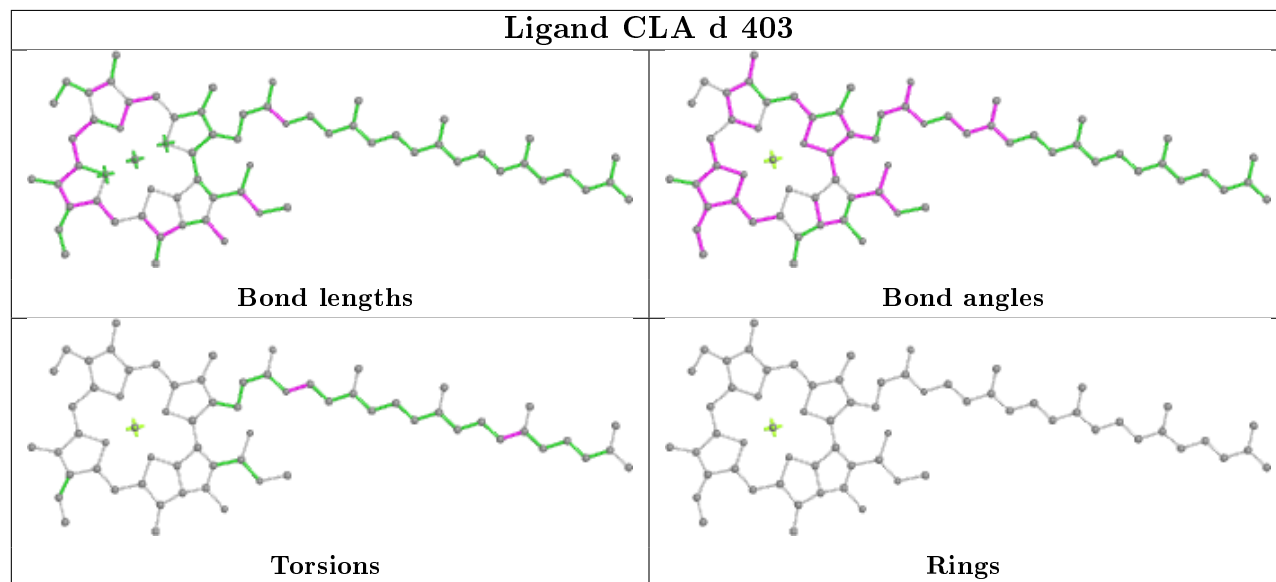
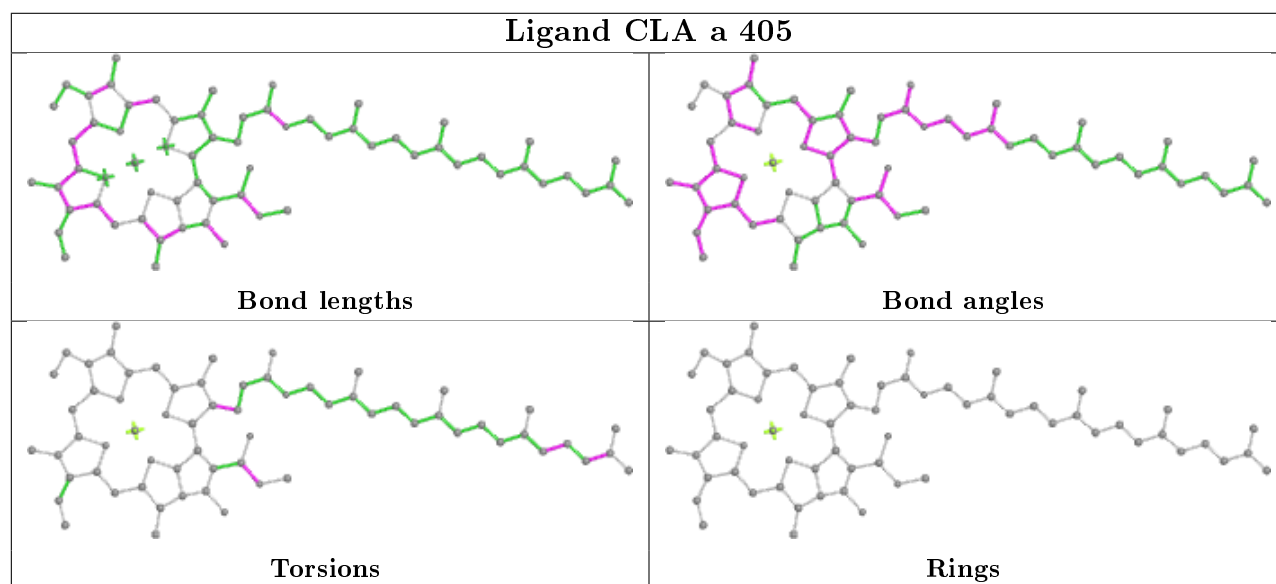
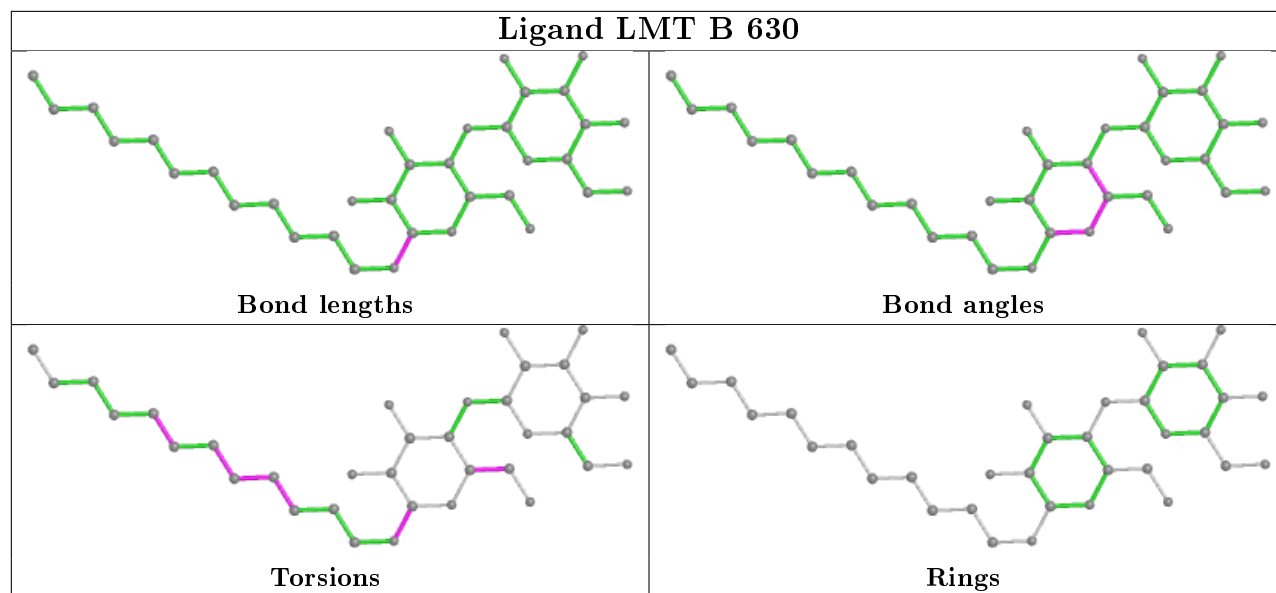


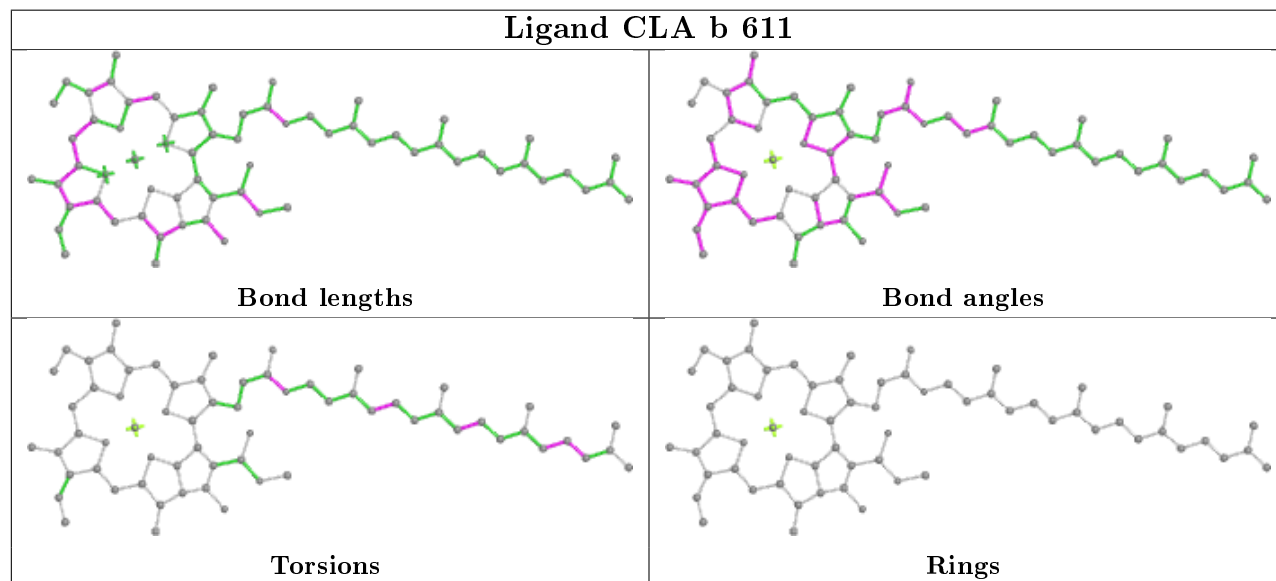
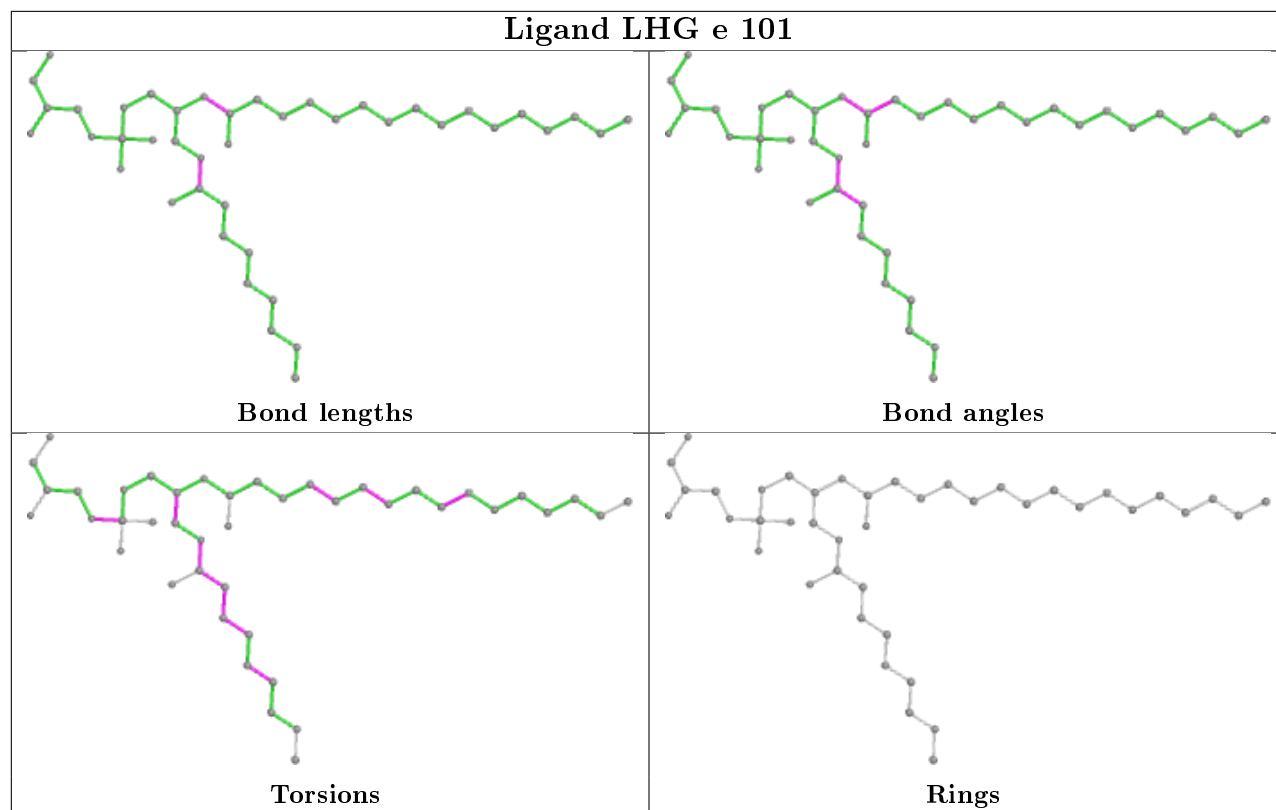
## Ligand HTG b 628

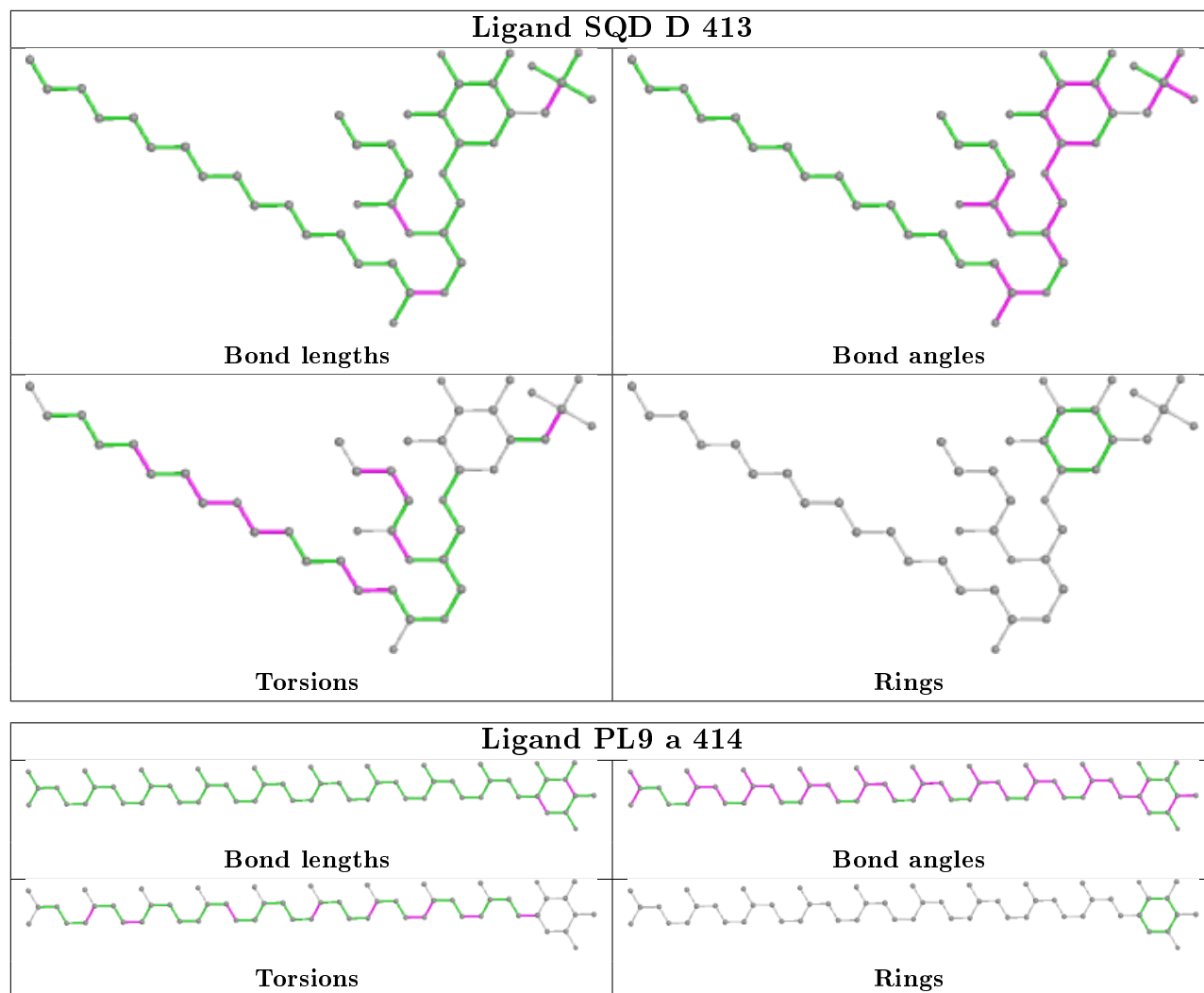


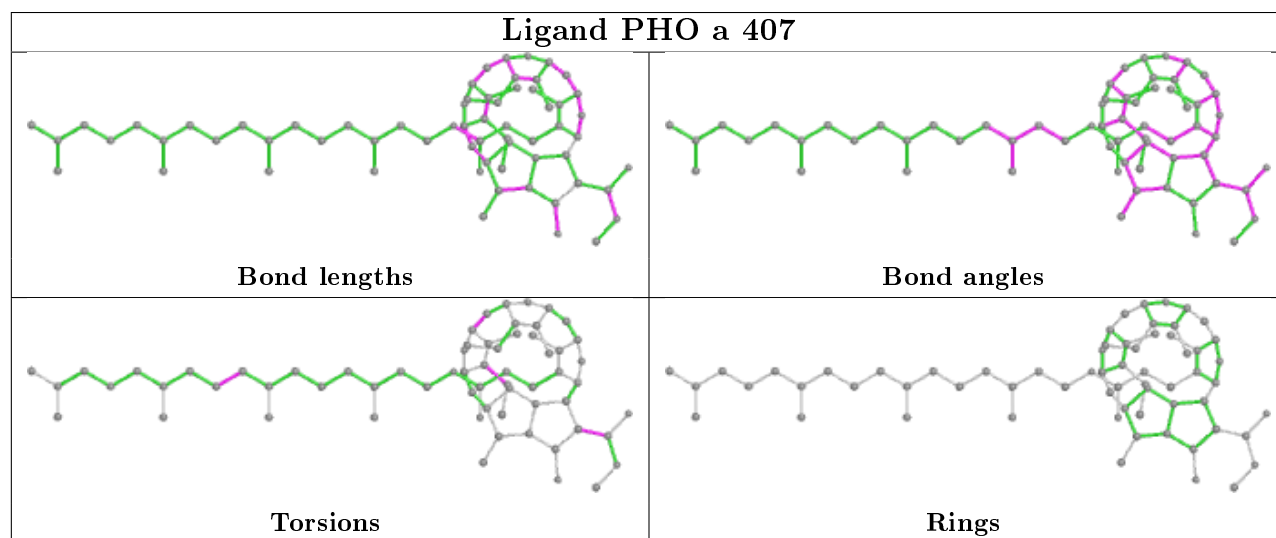
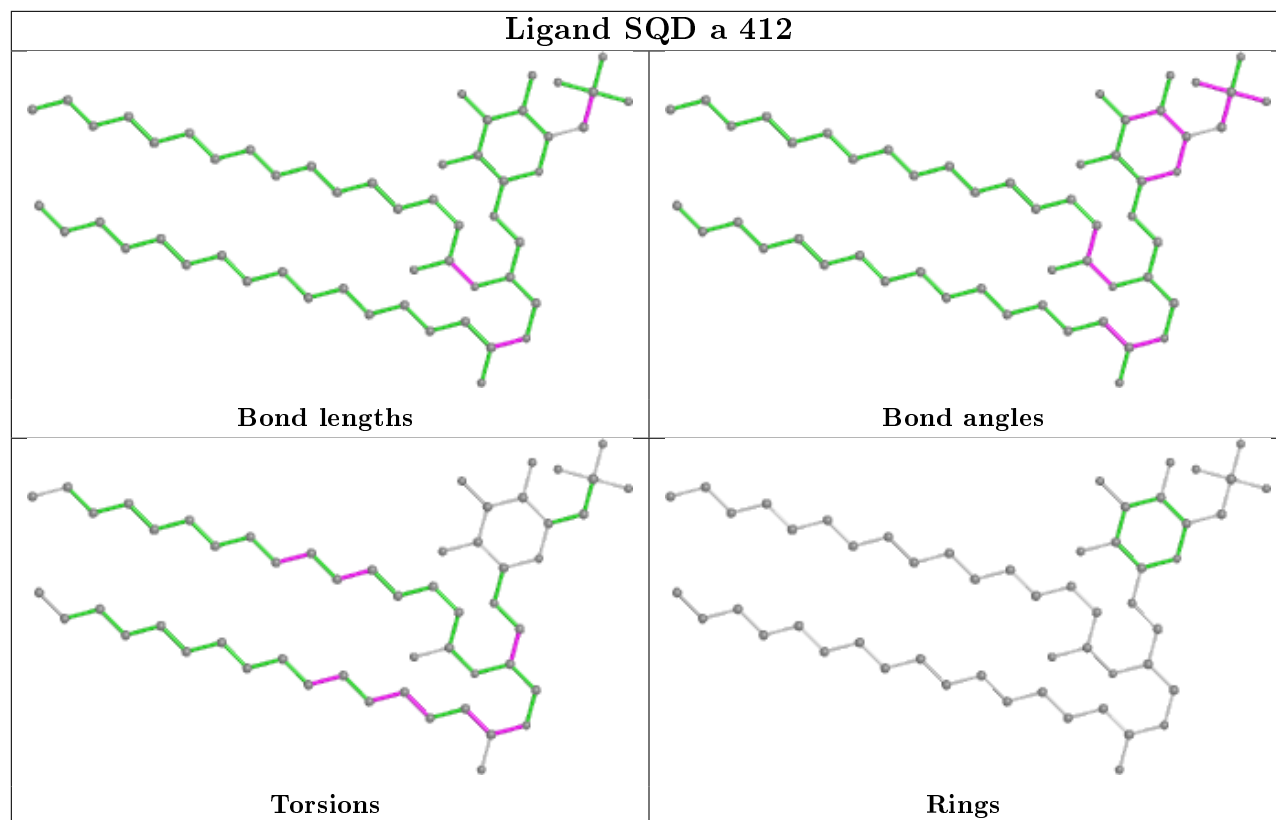
## Ligand CLA b 608



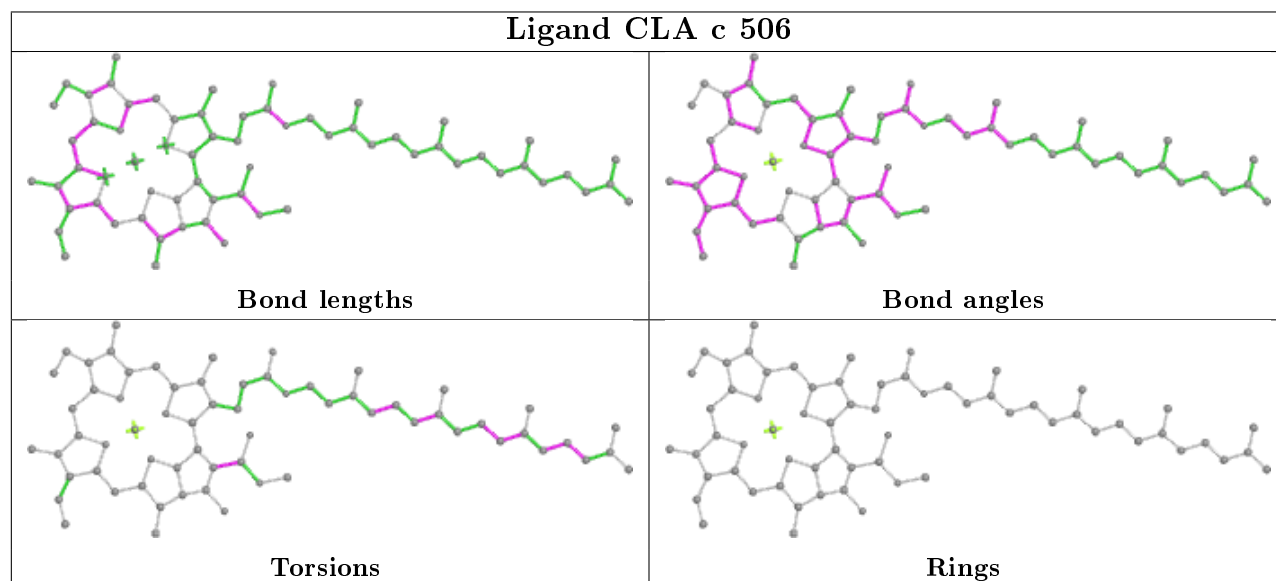
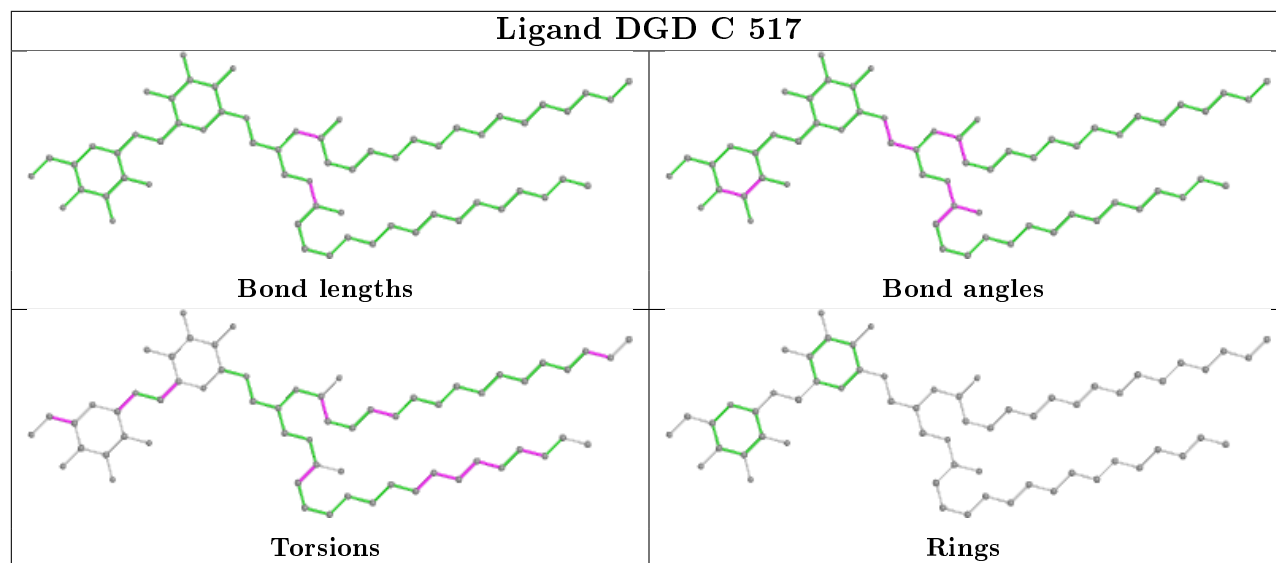


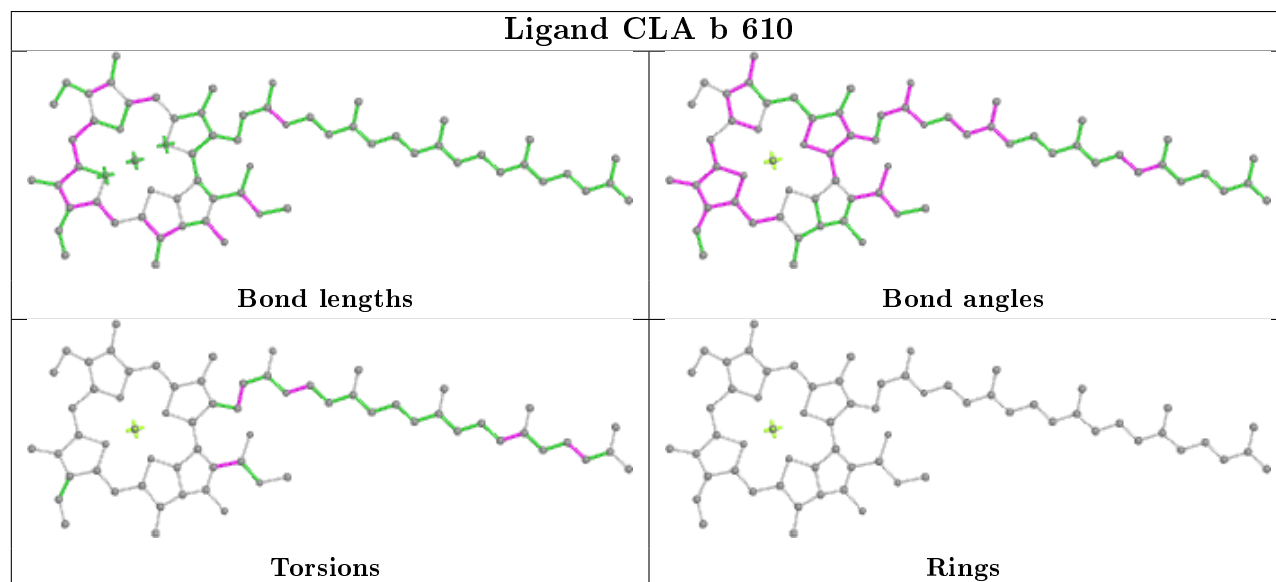
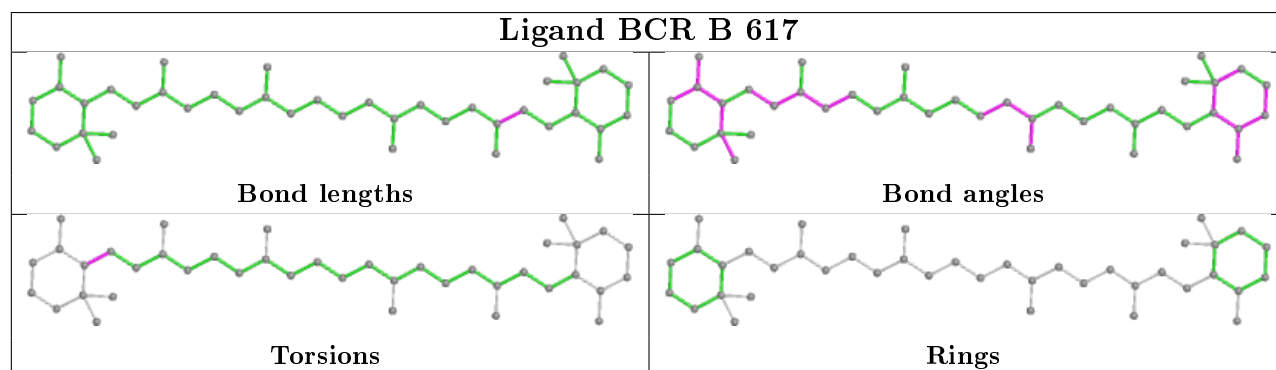
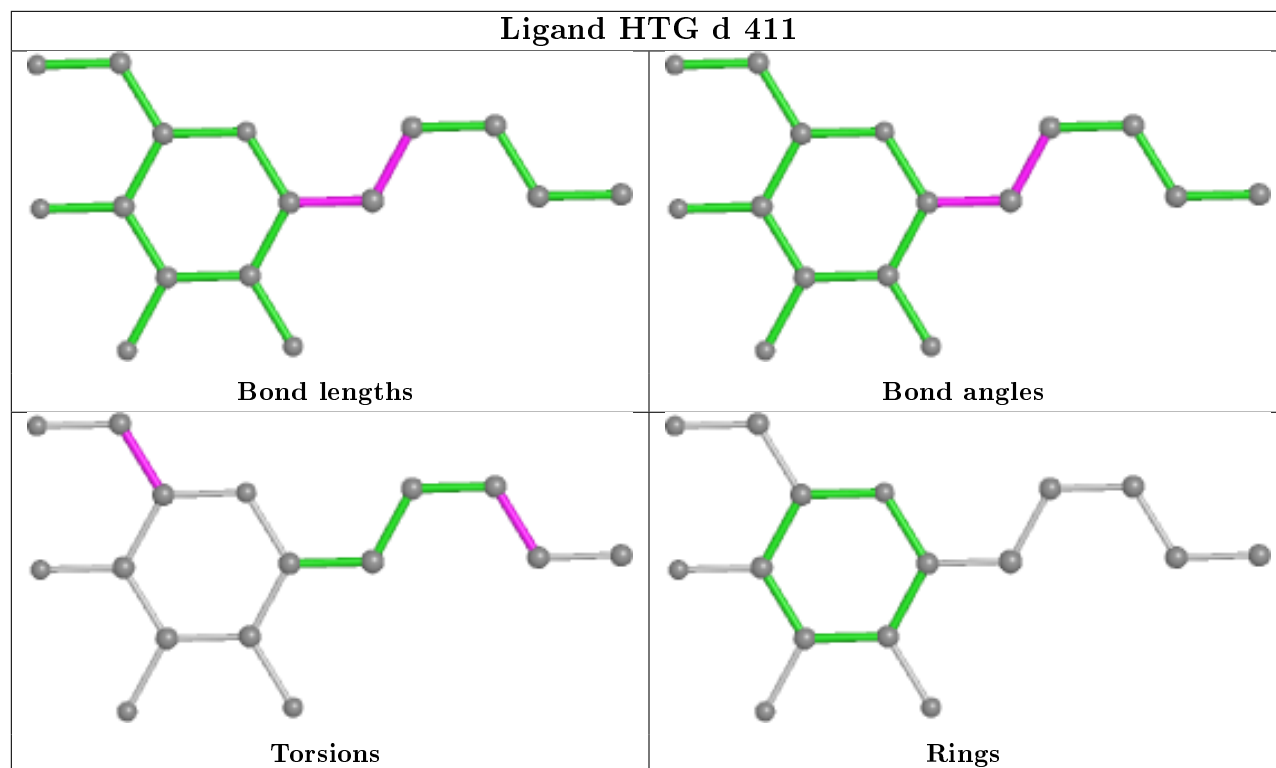


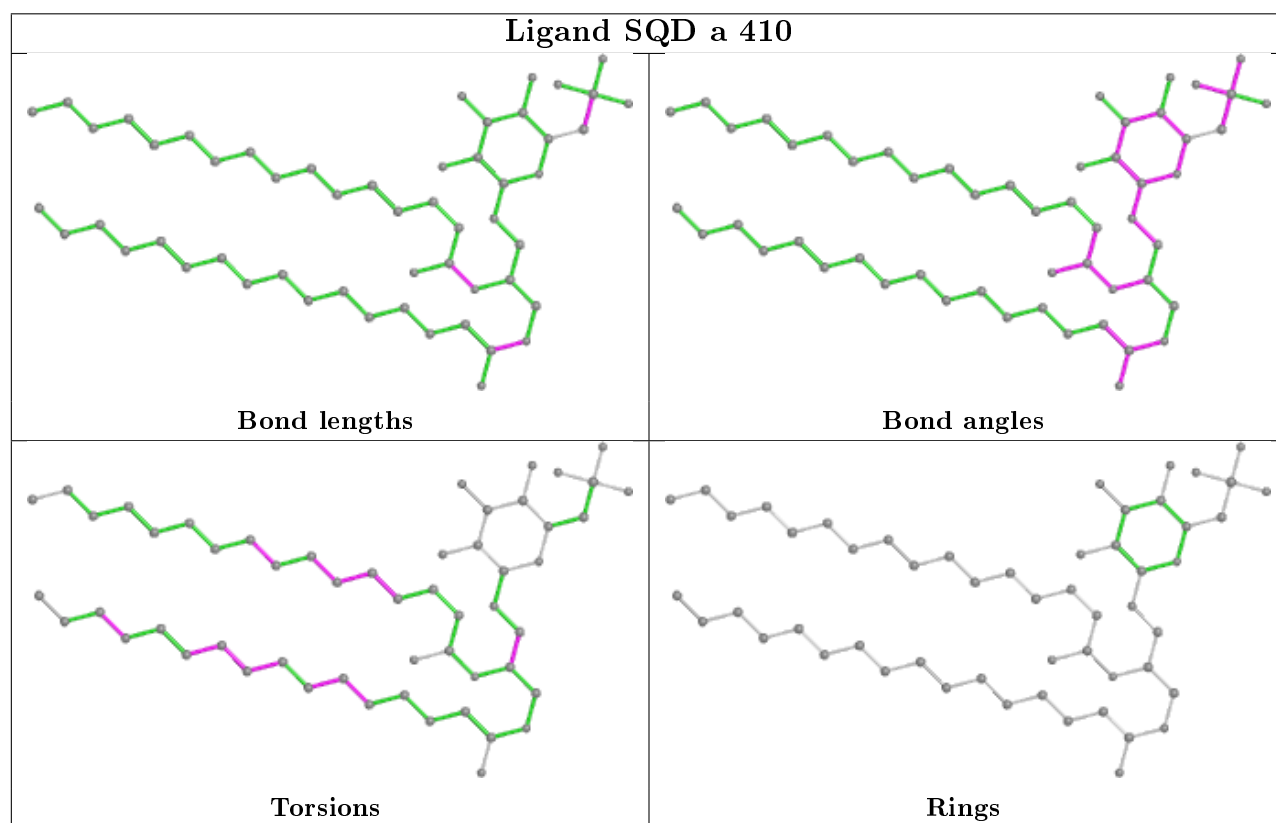
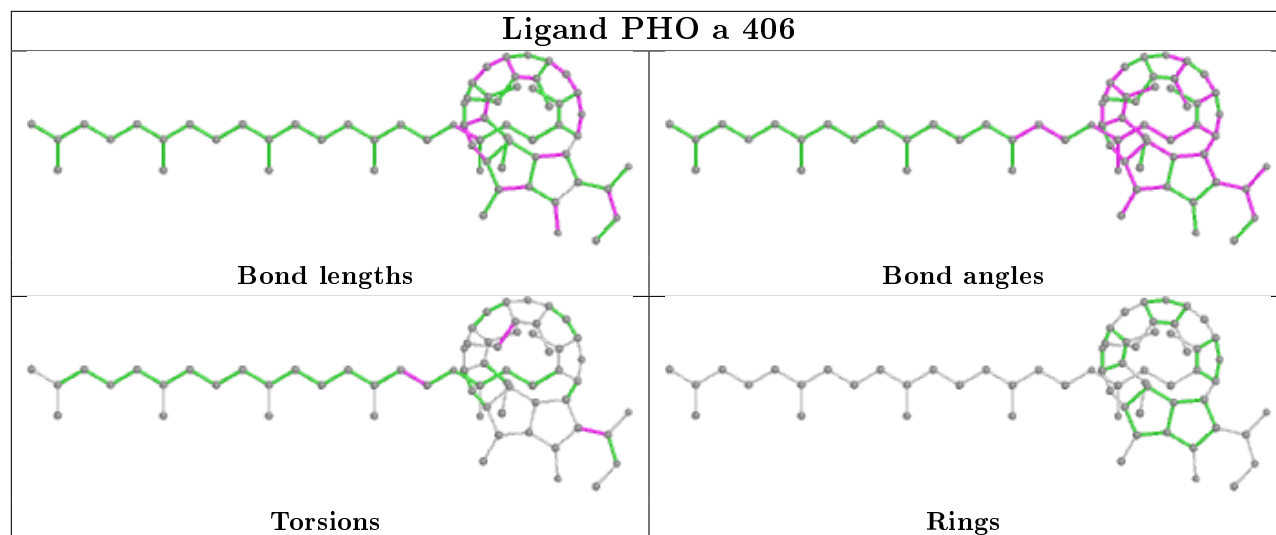




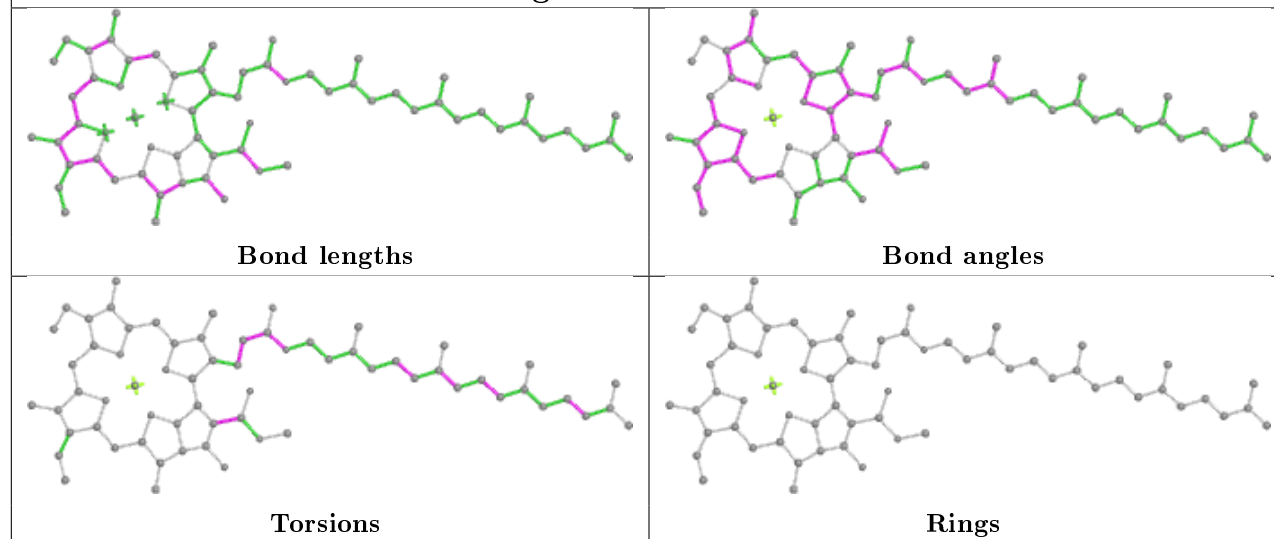




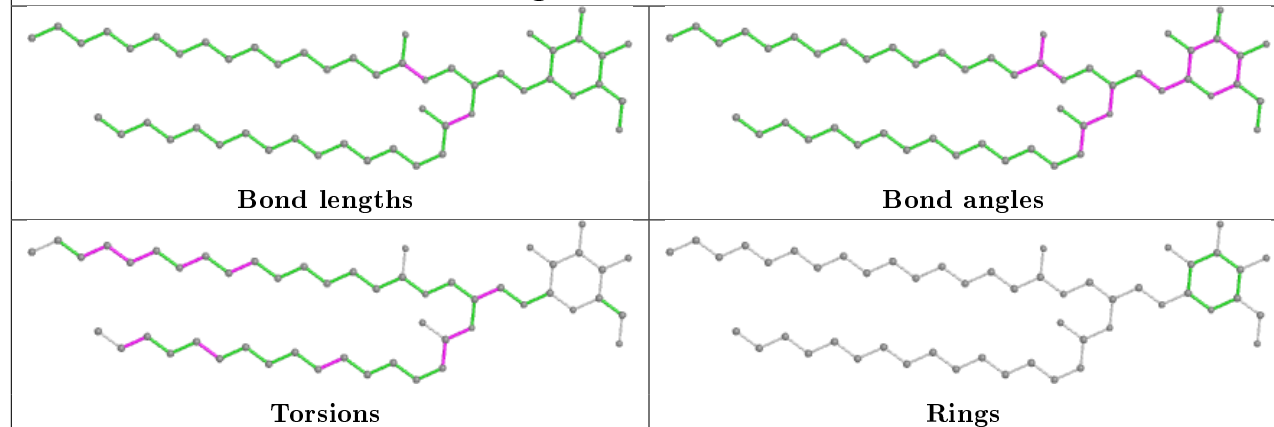




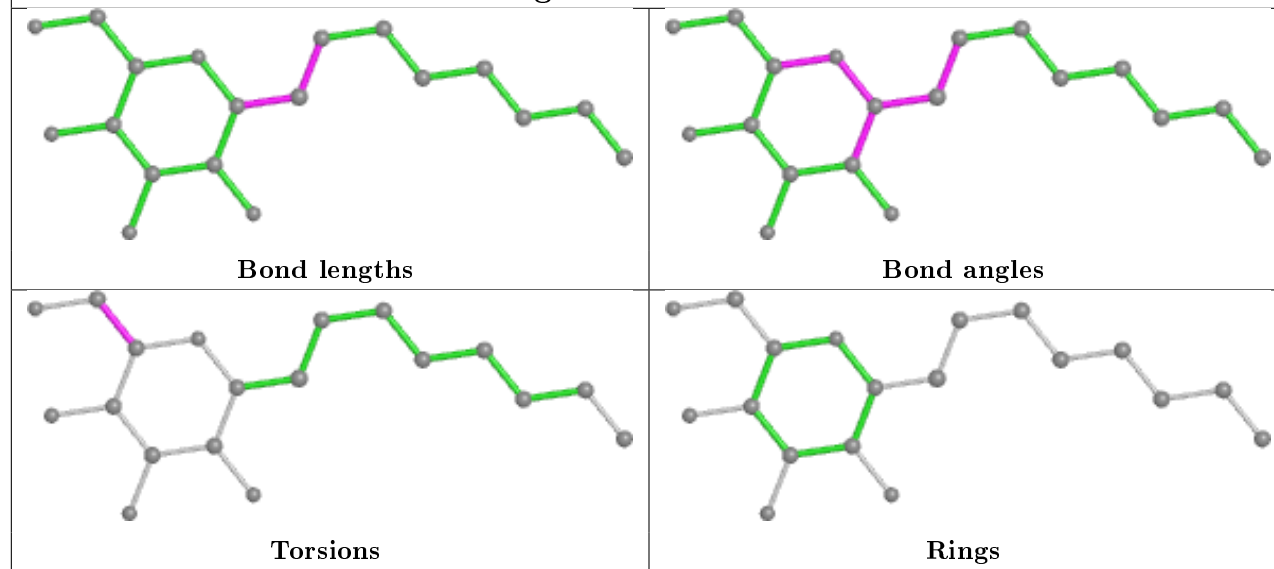
## Ligand CLA B 601

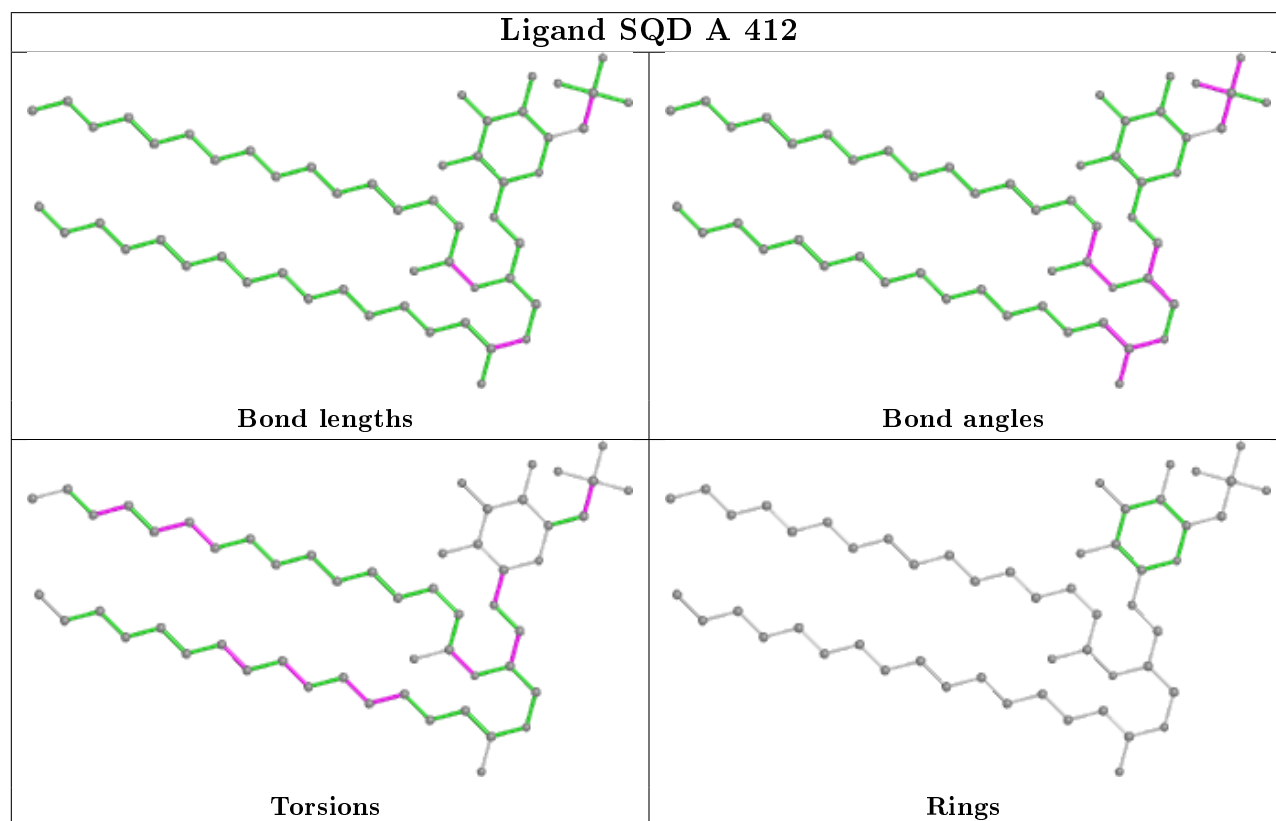
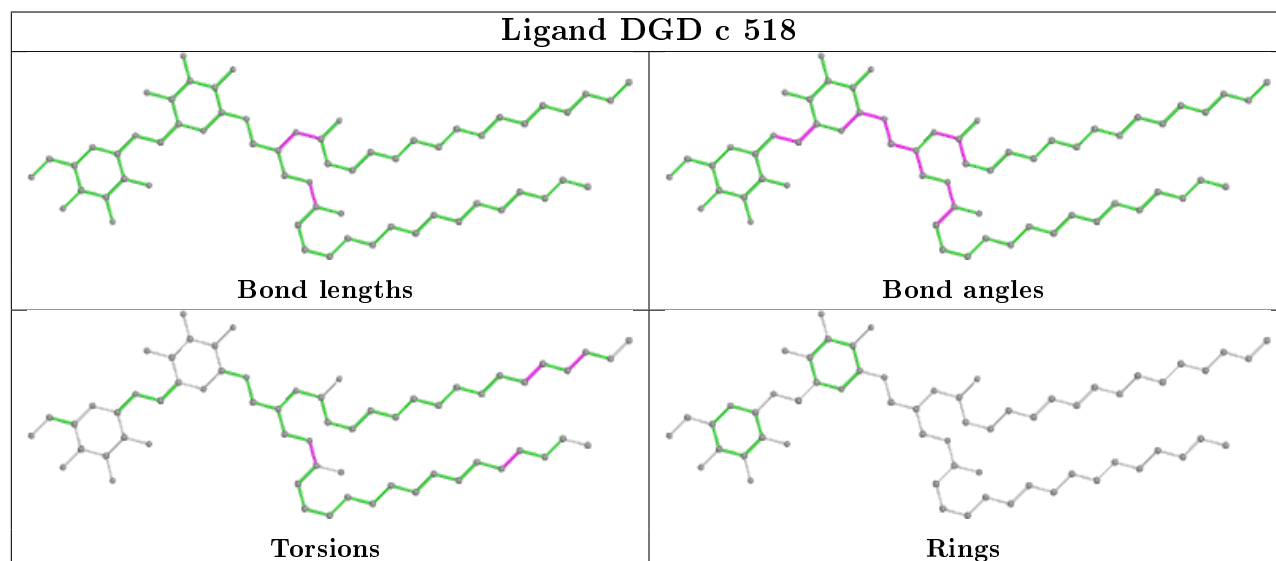
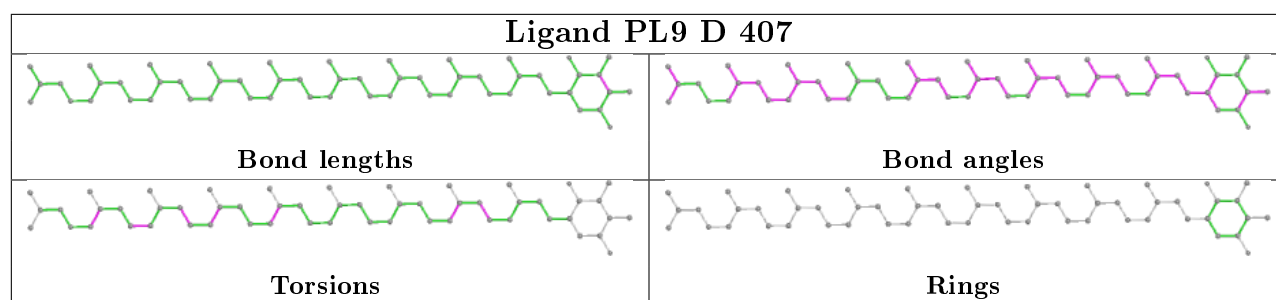


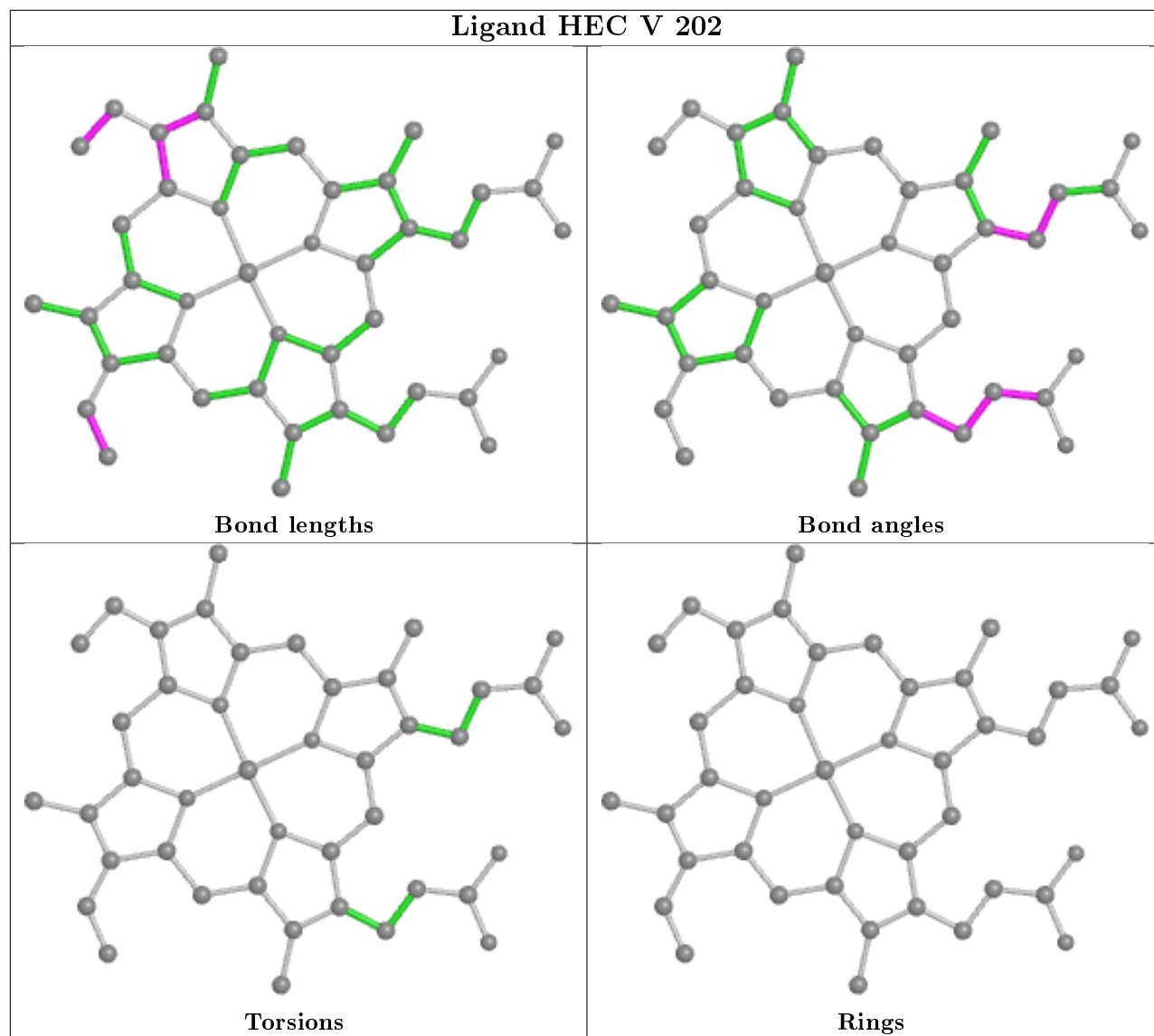
## Ligand LMG b 620

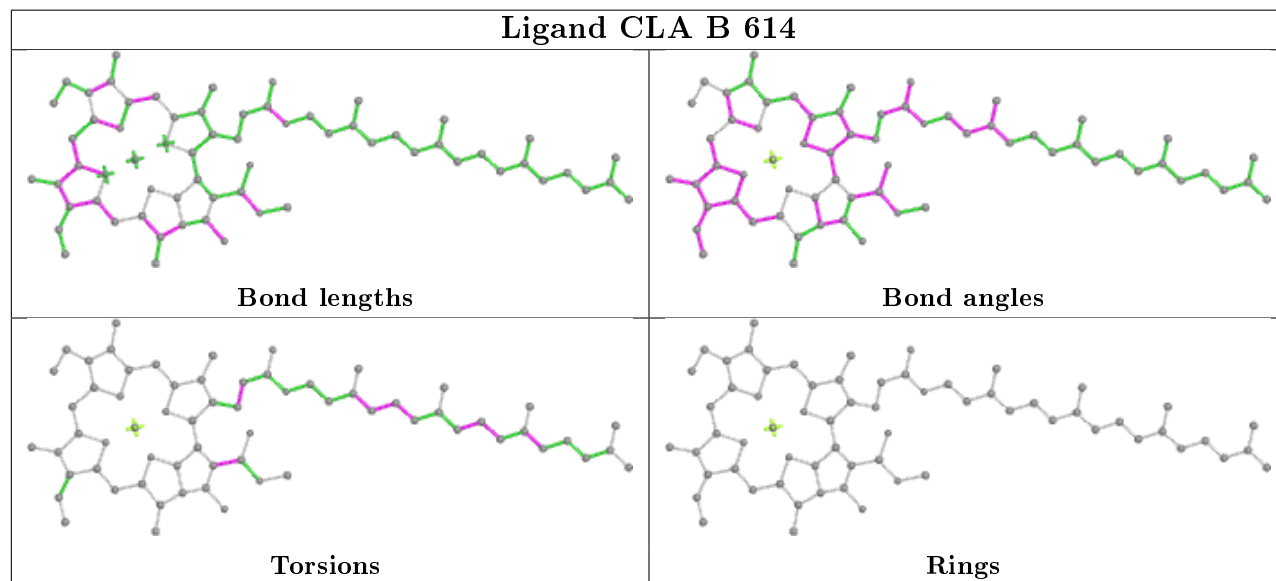
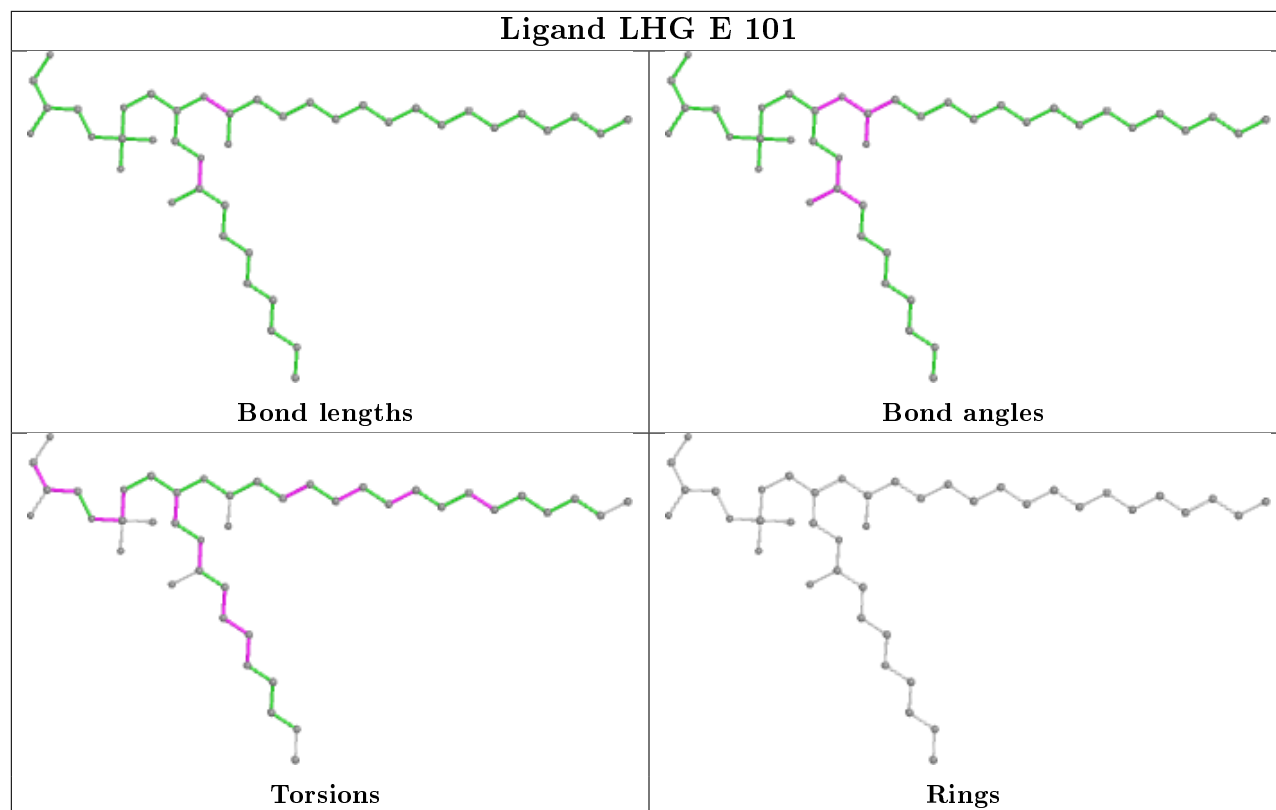


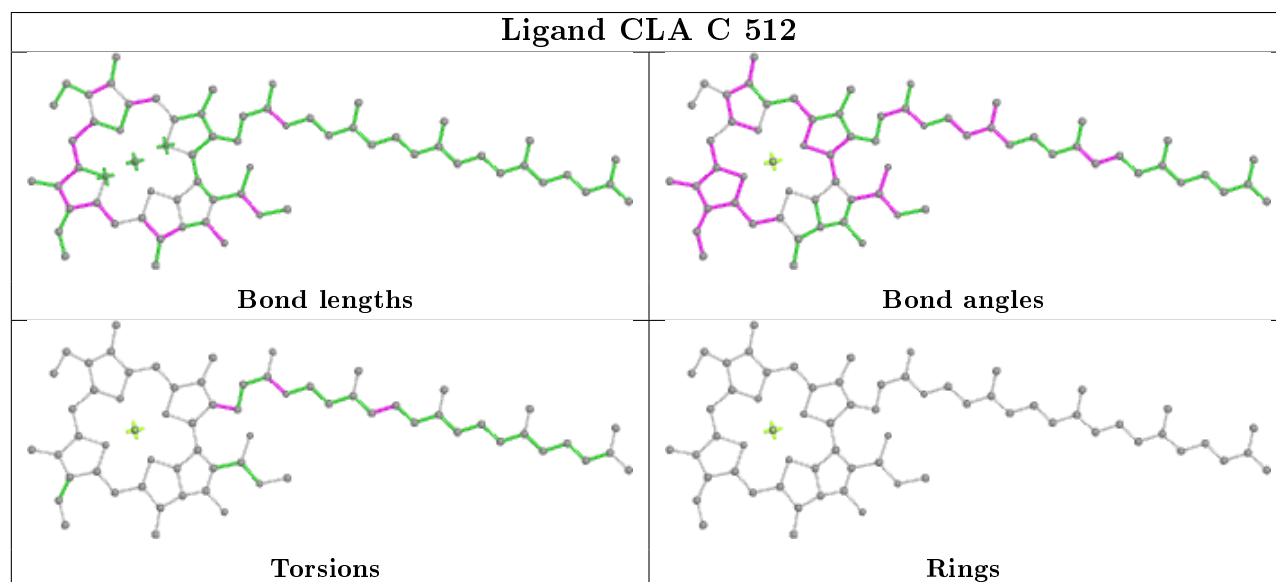
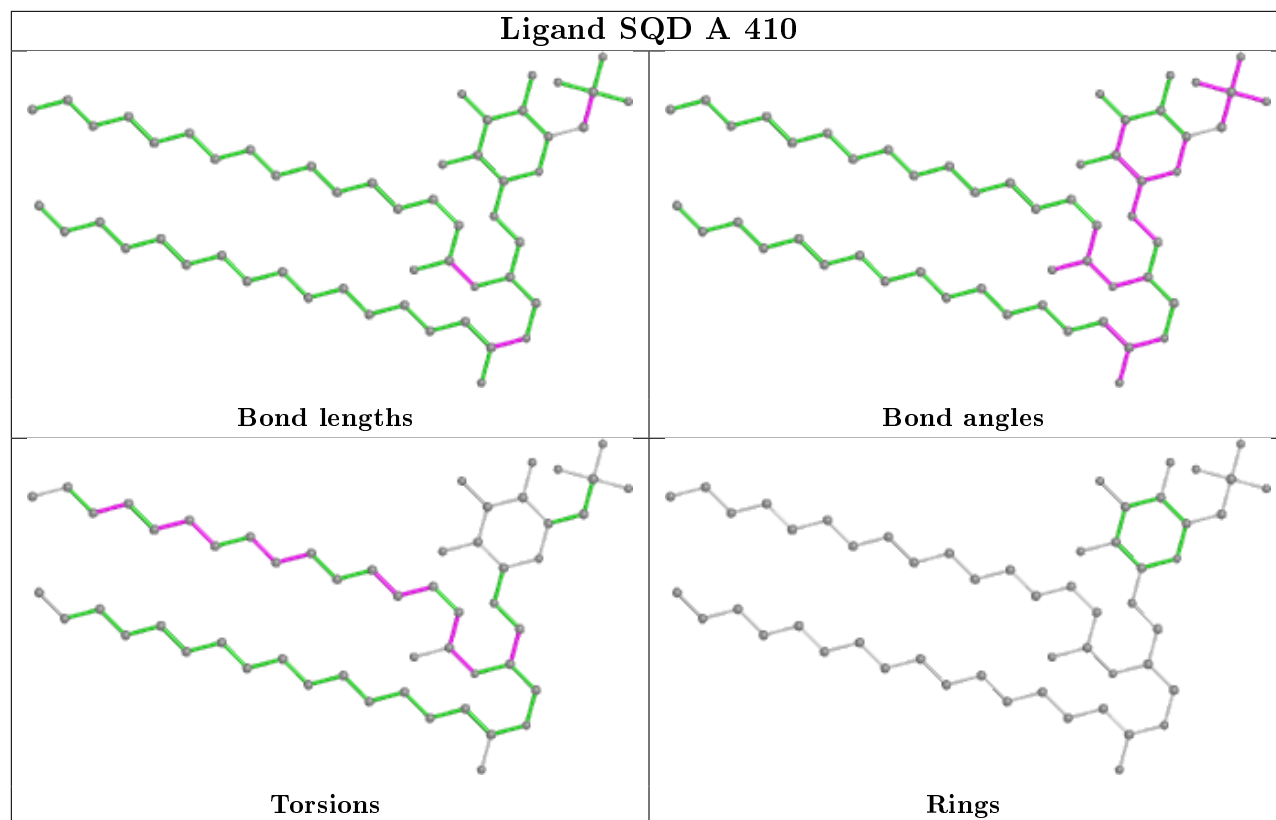
## Ligand HTG c 522





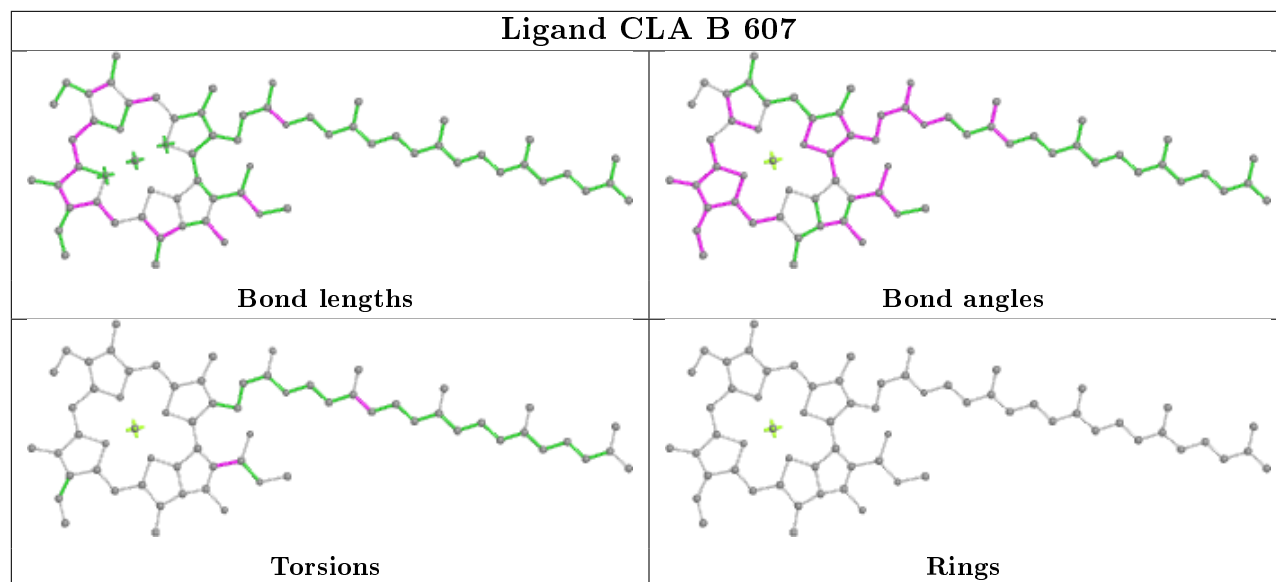




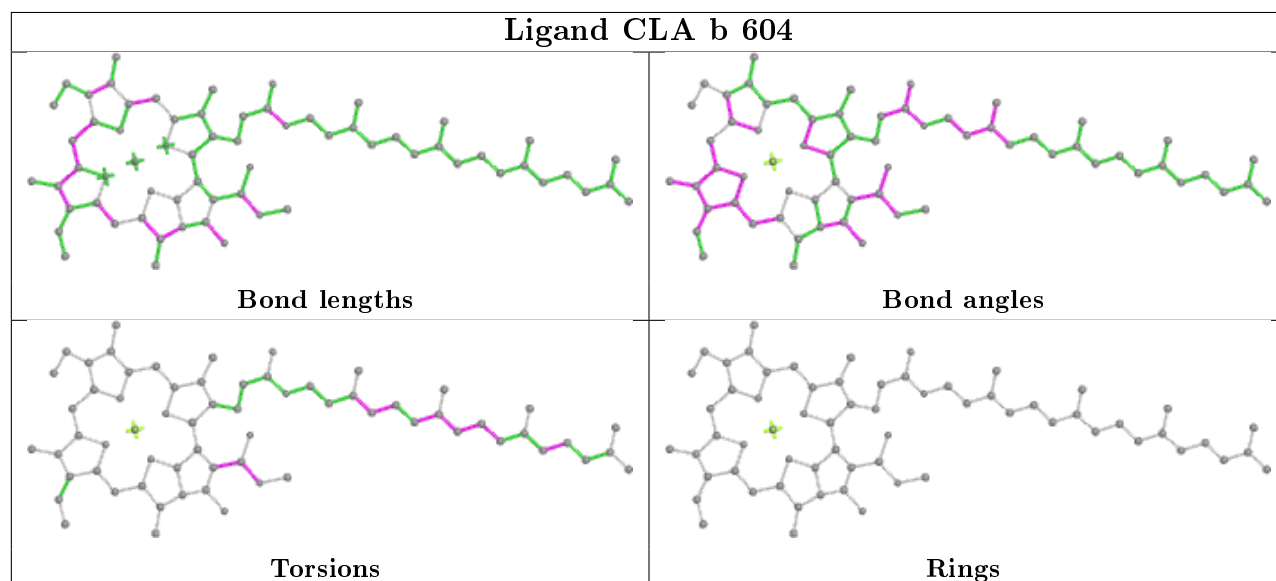




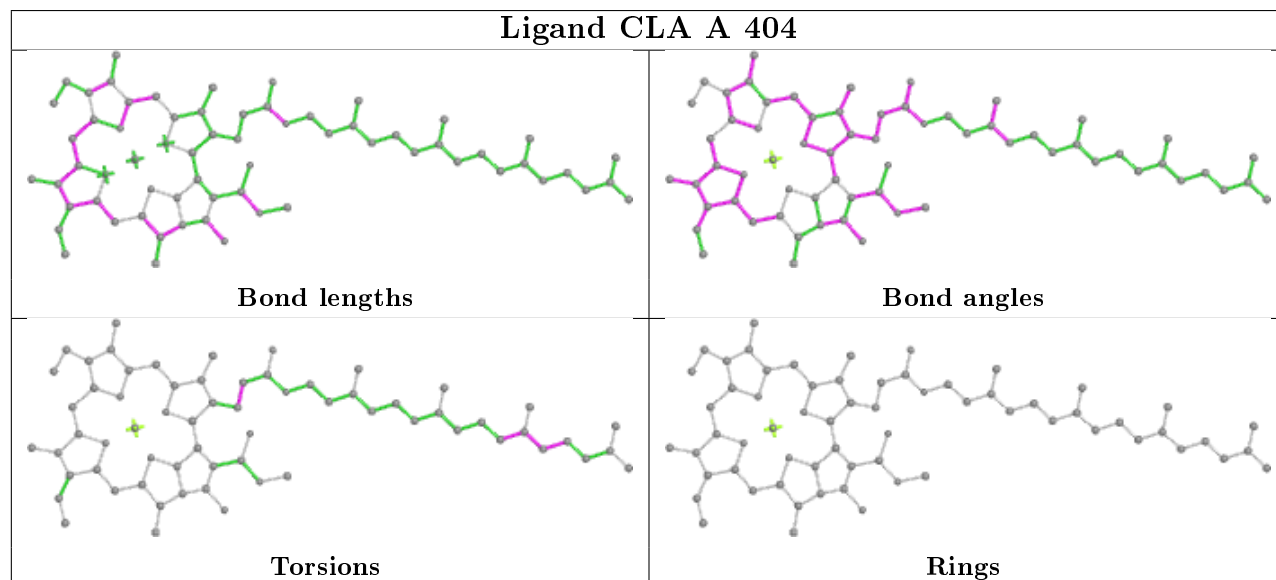
## Ligand CLA B 607



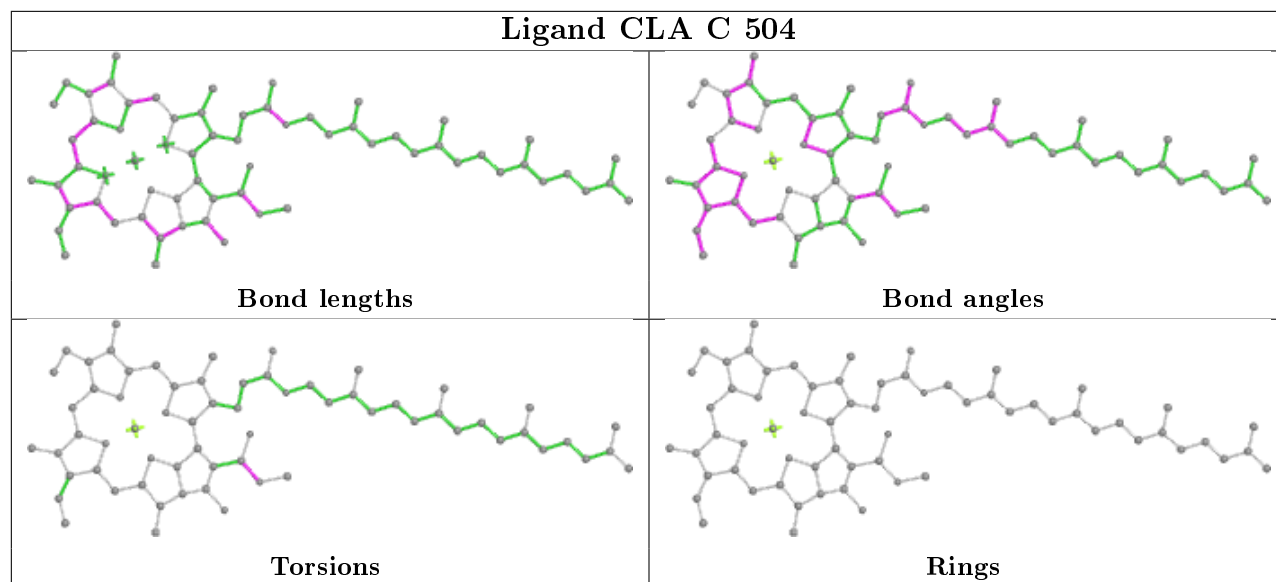
## Ligand CLA b 604



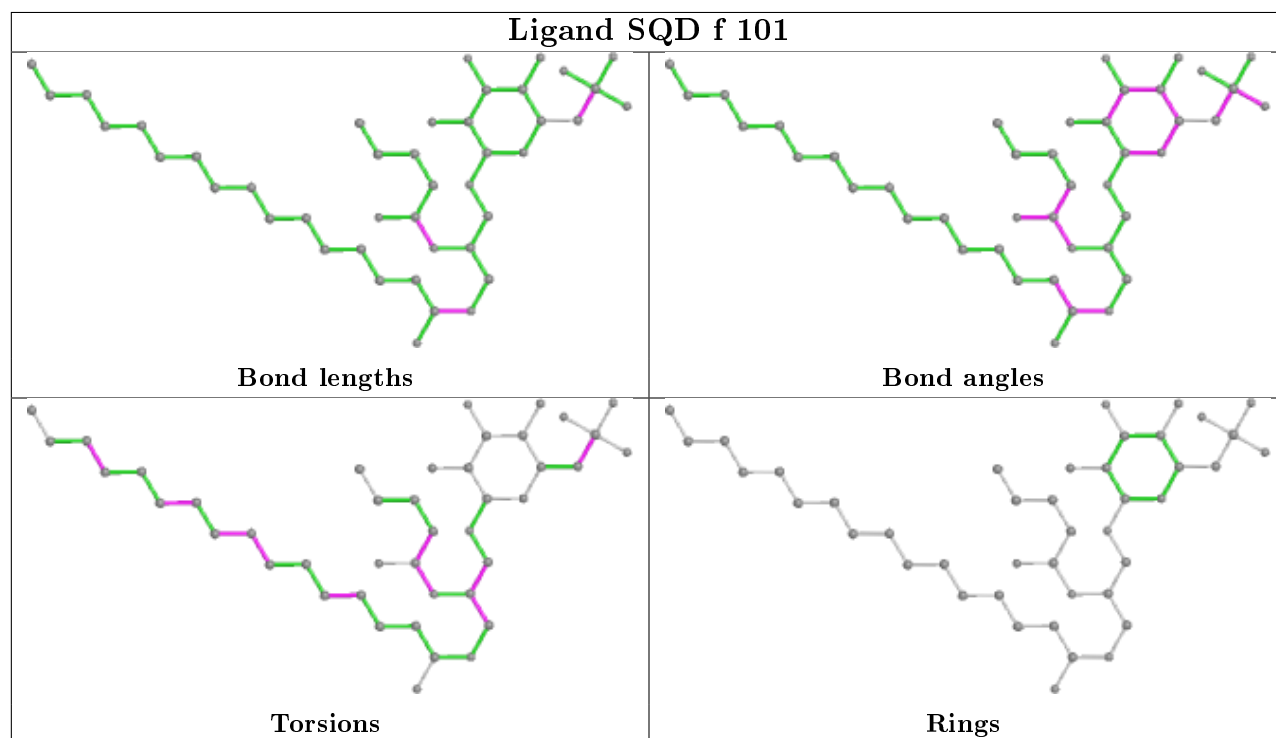
## Ligand CLA A 404



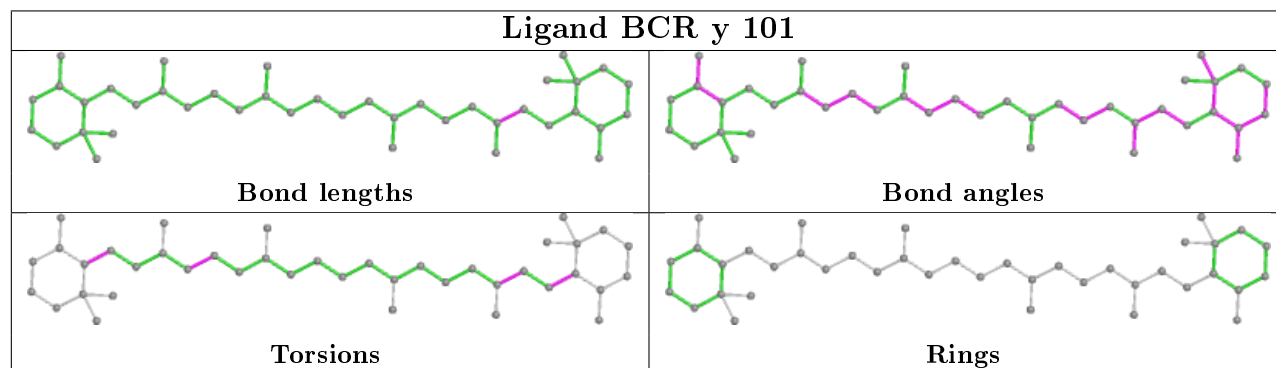
## Ligand CLA C 504

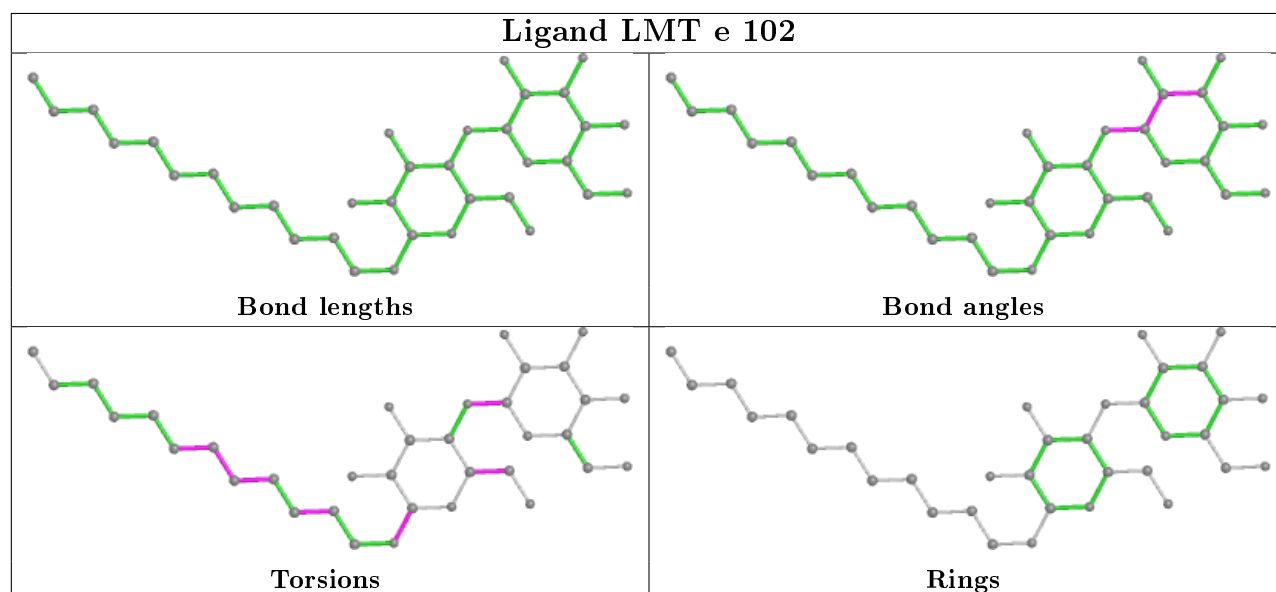
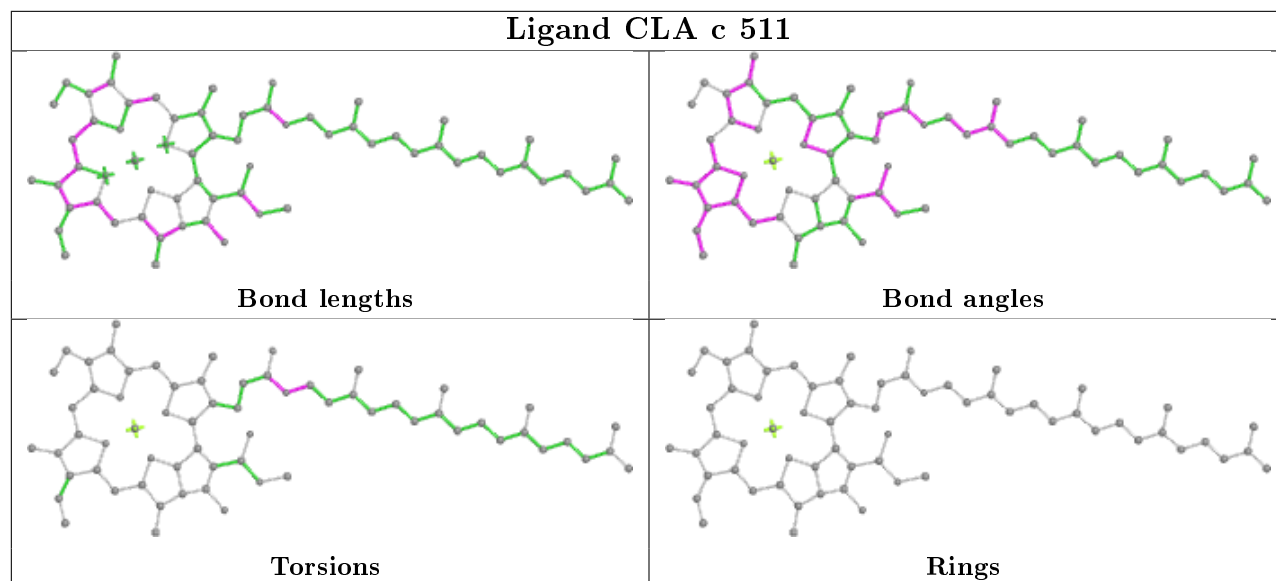
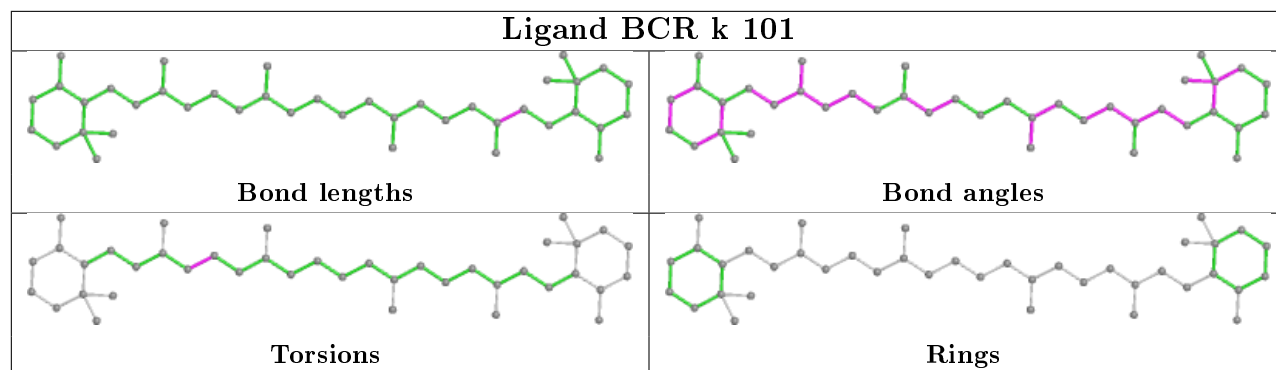


## Ligand SQD f 101

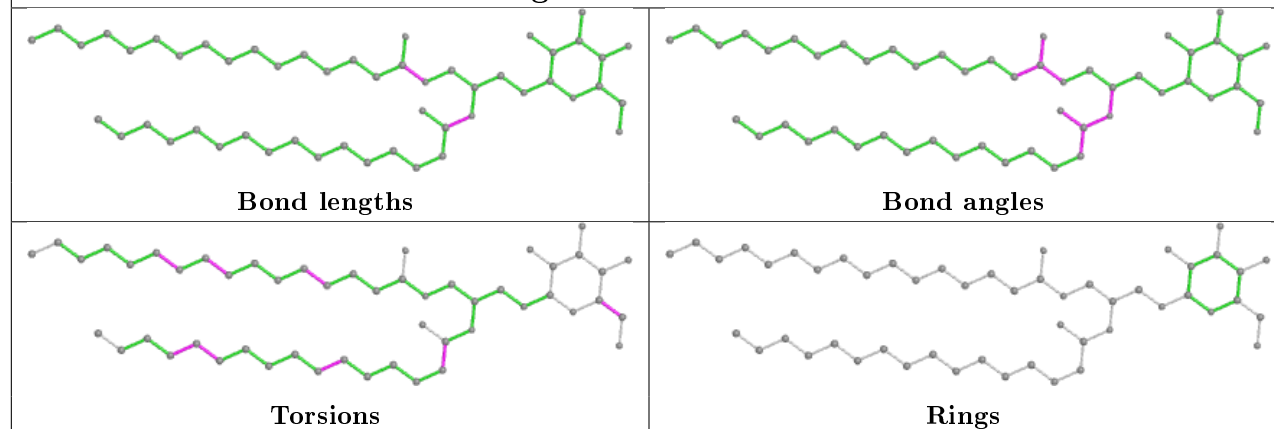


## Ligand BCR y 101

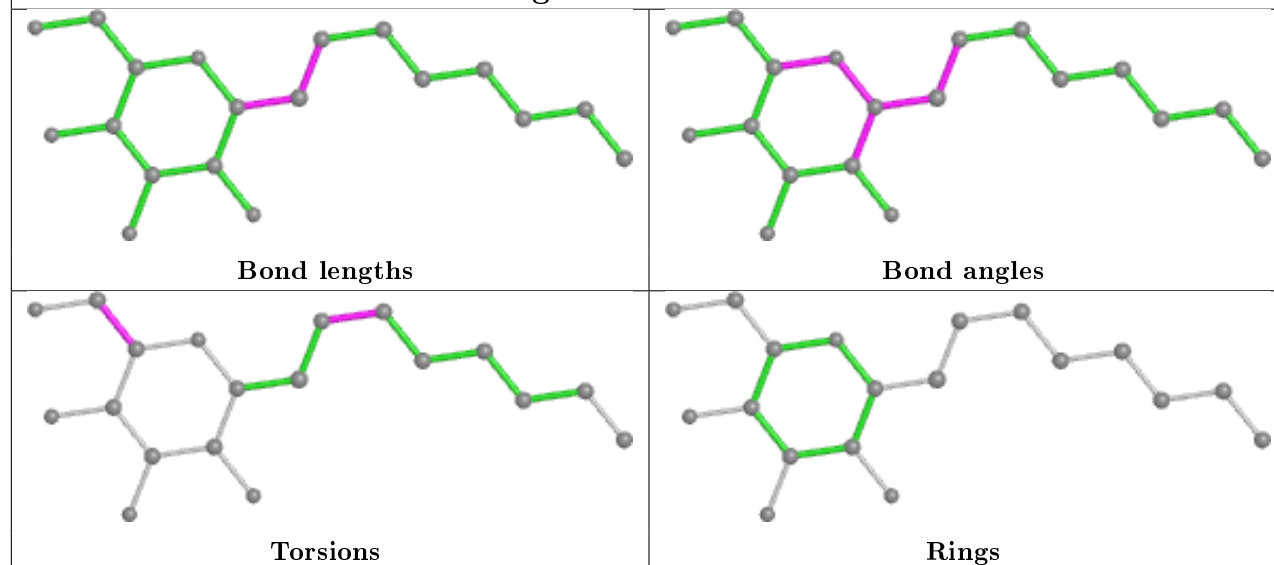




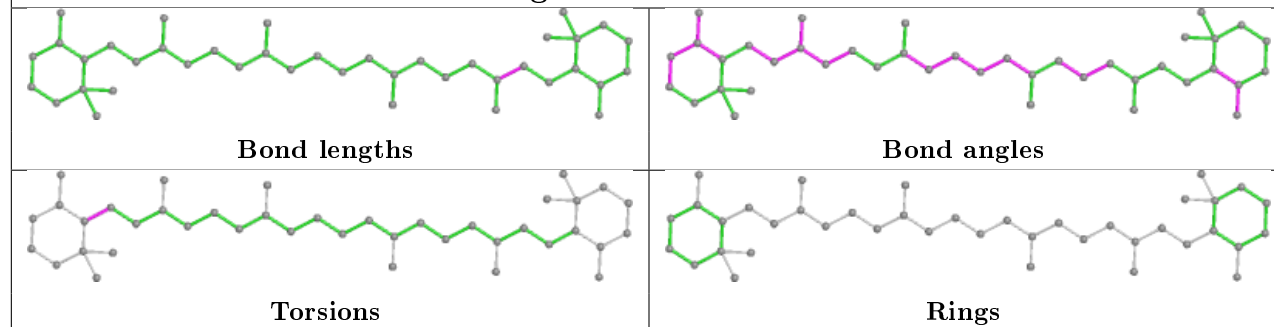
## Ligand LMG J 101

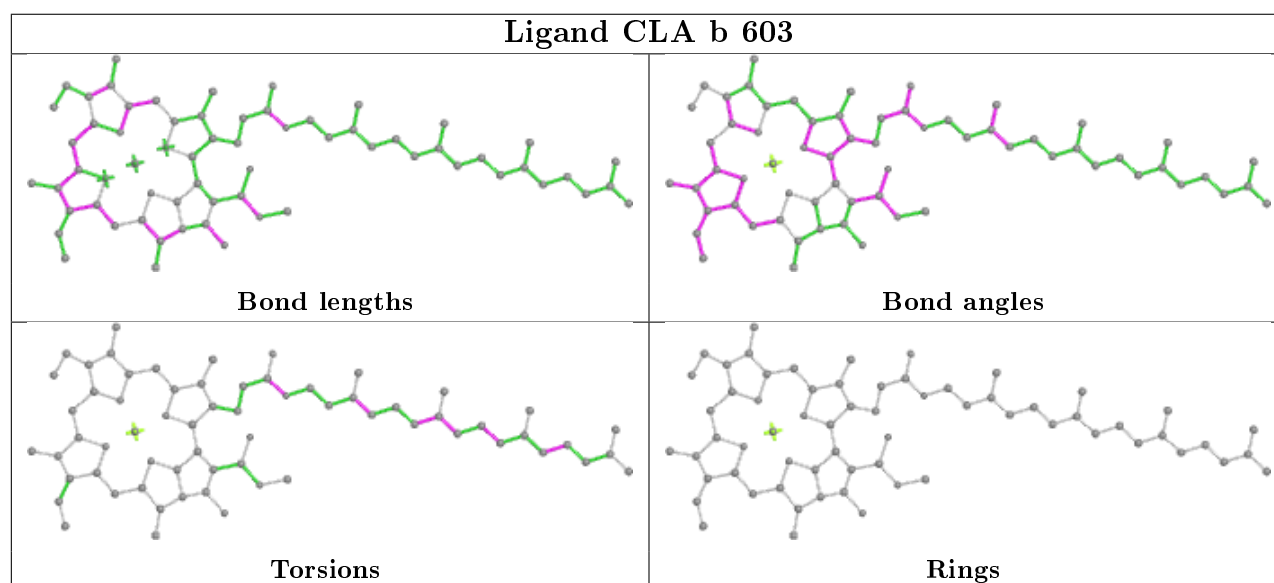
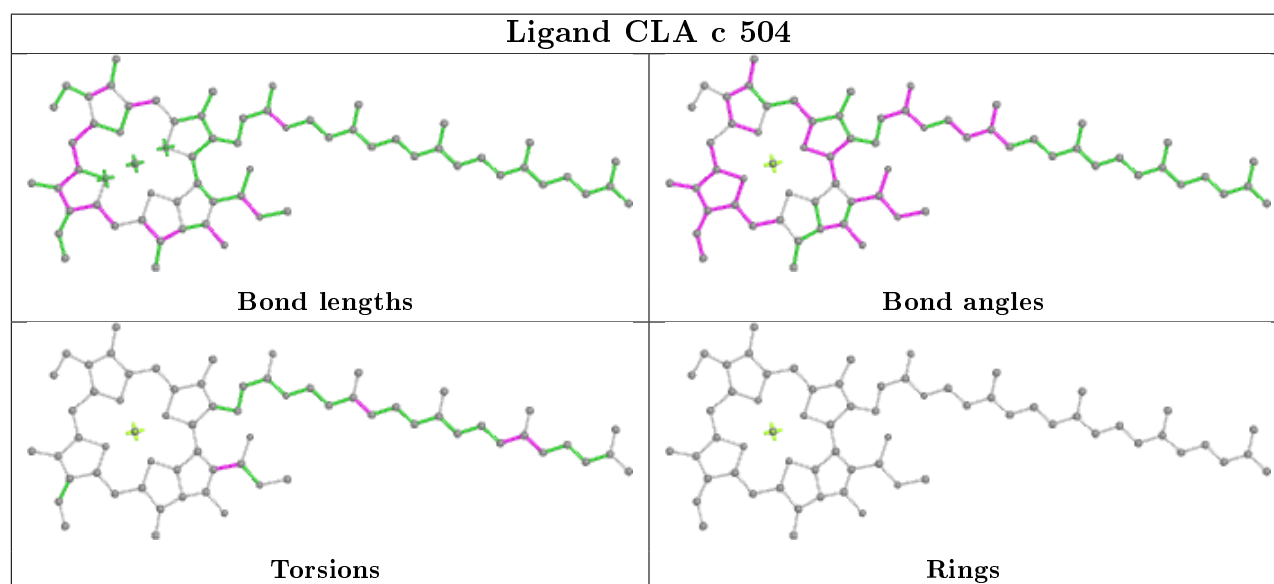
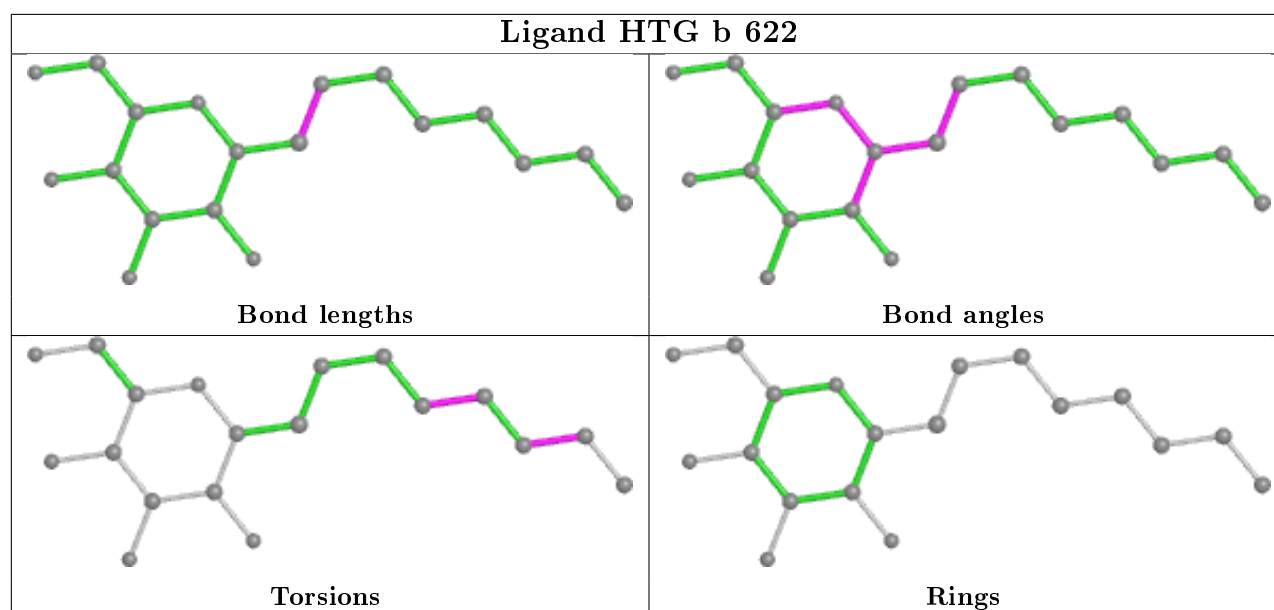


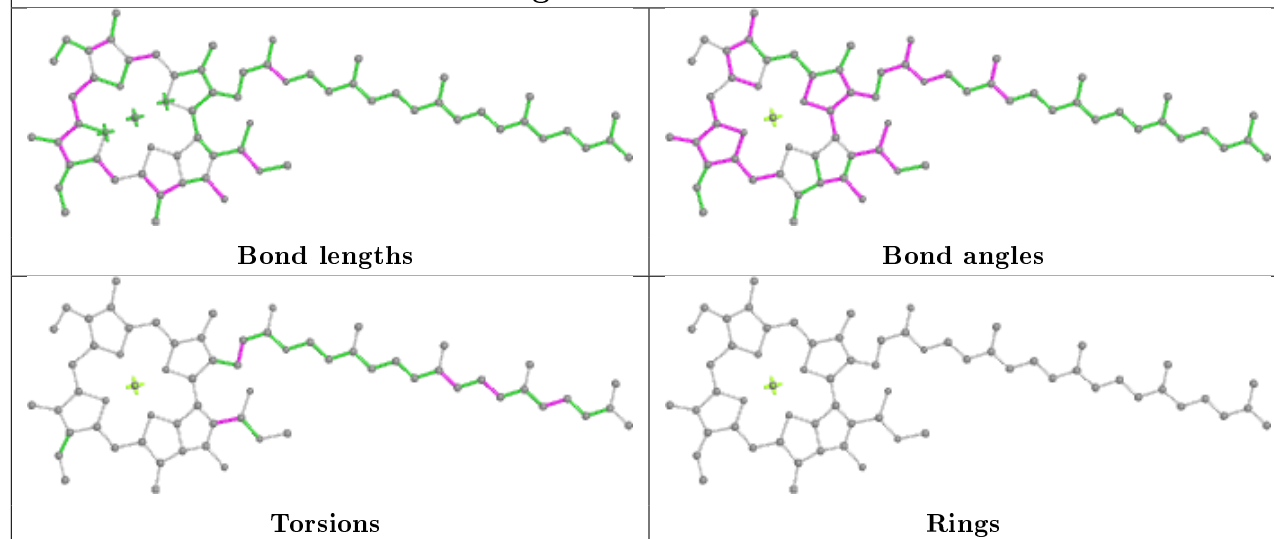
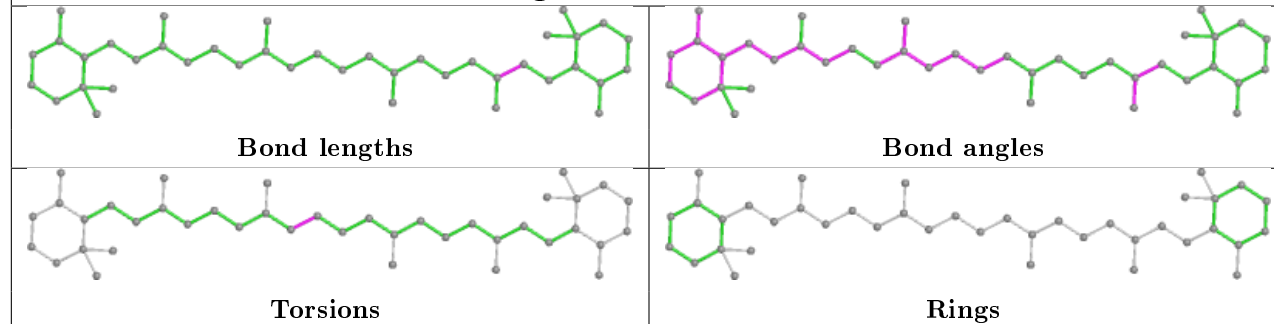
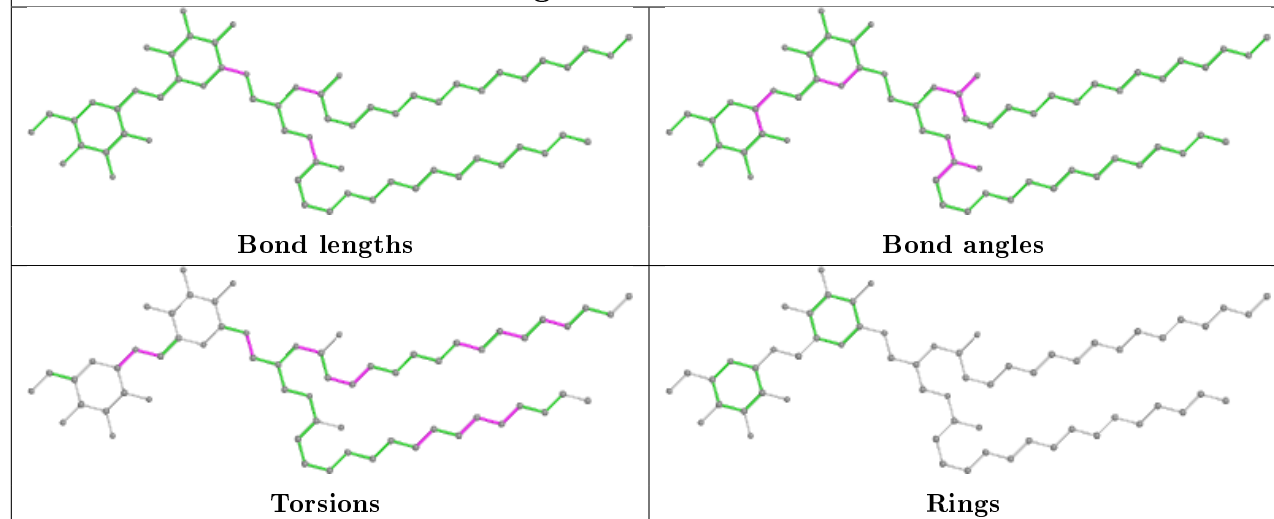
## Ligand HTG b 623



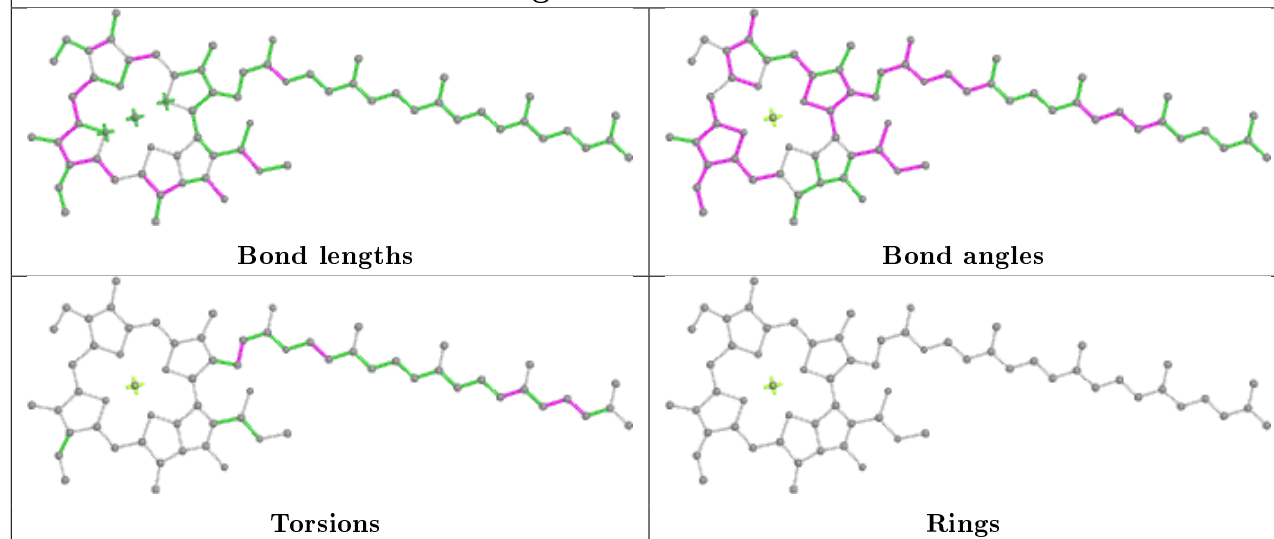
## Ligand BCR C 516



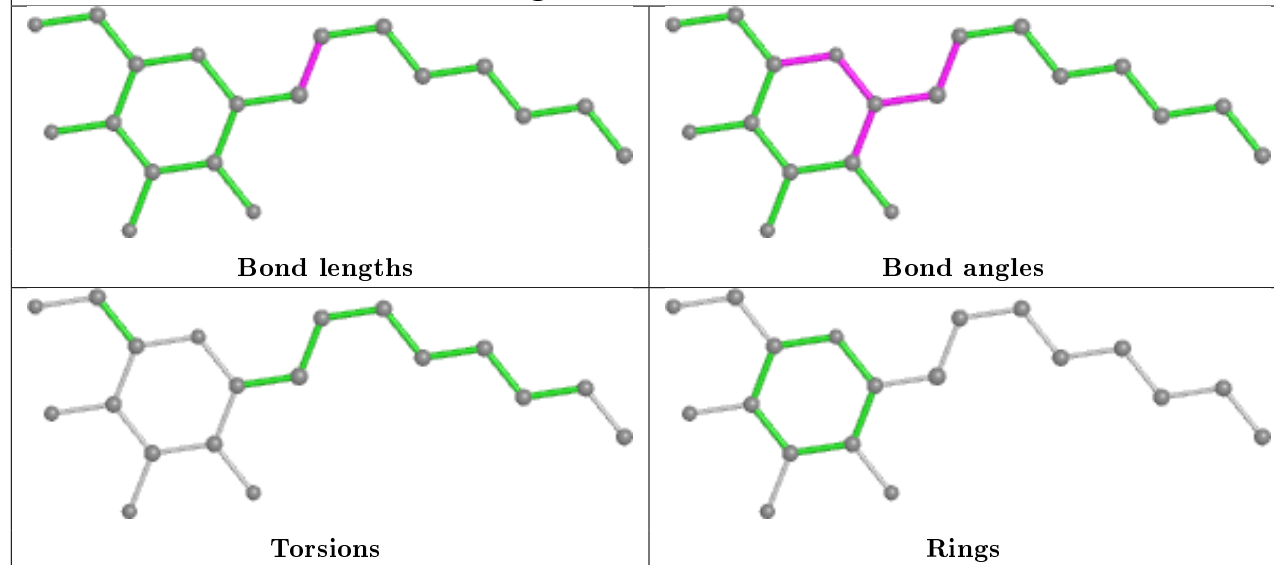


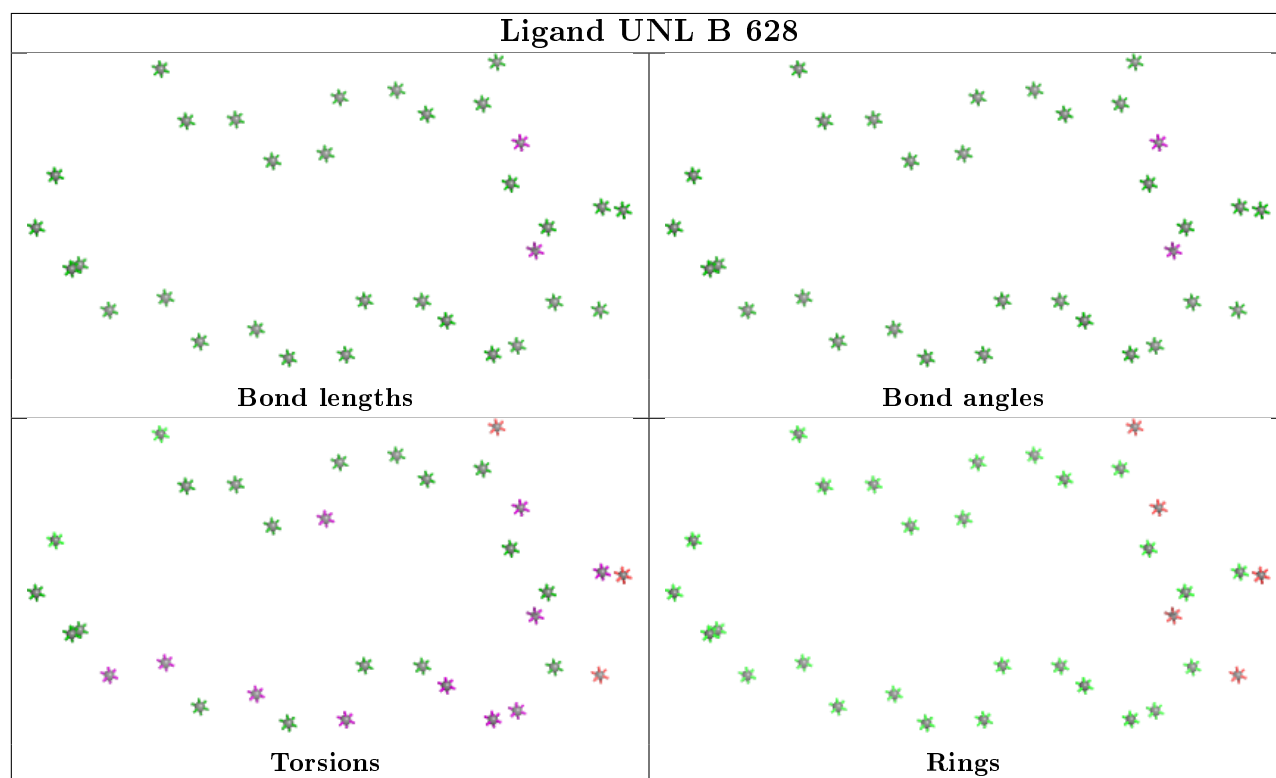
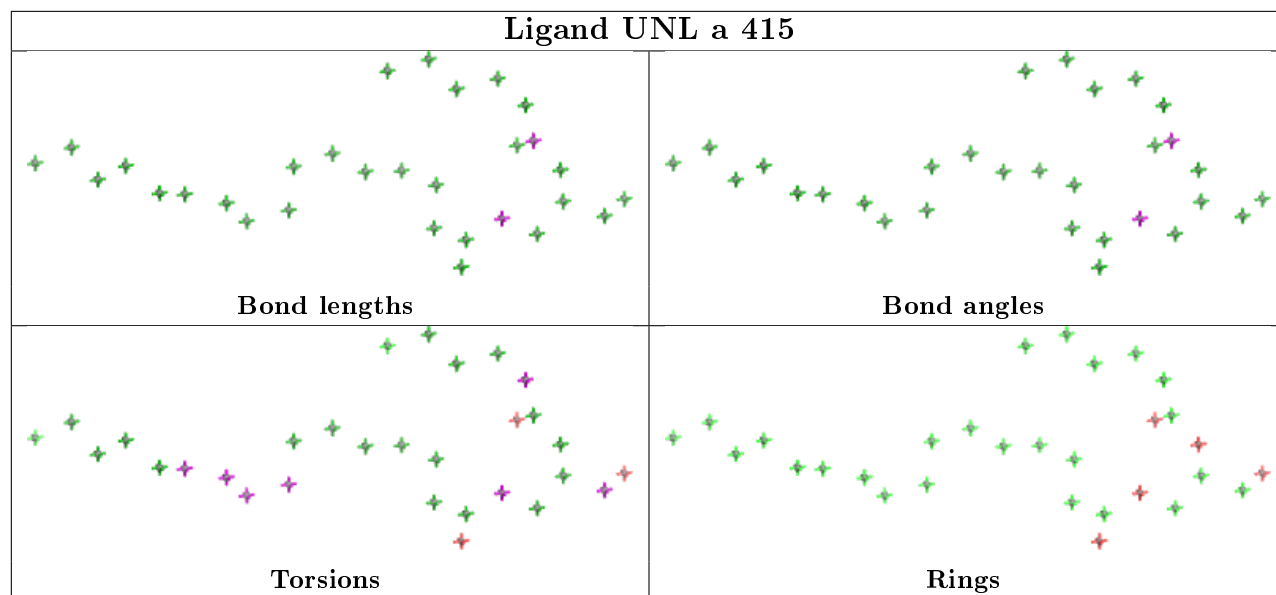
**Ligand CLA B 606****Ligand BCR T 101****Ligand DGD c 517**

## Ligand CLA B 602

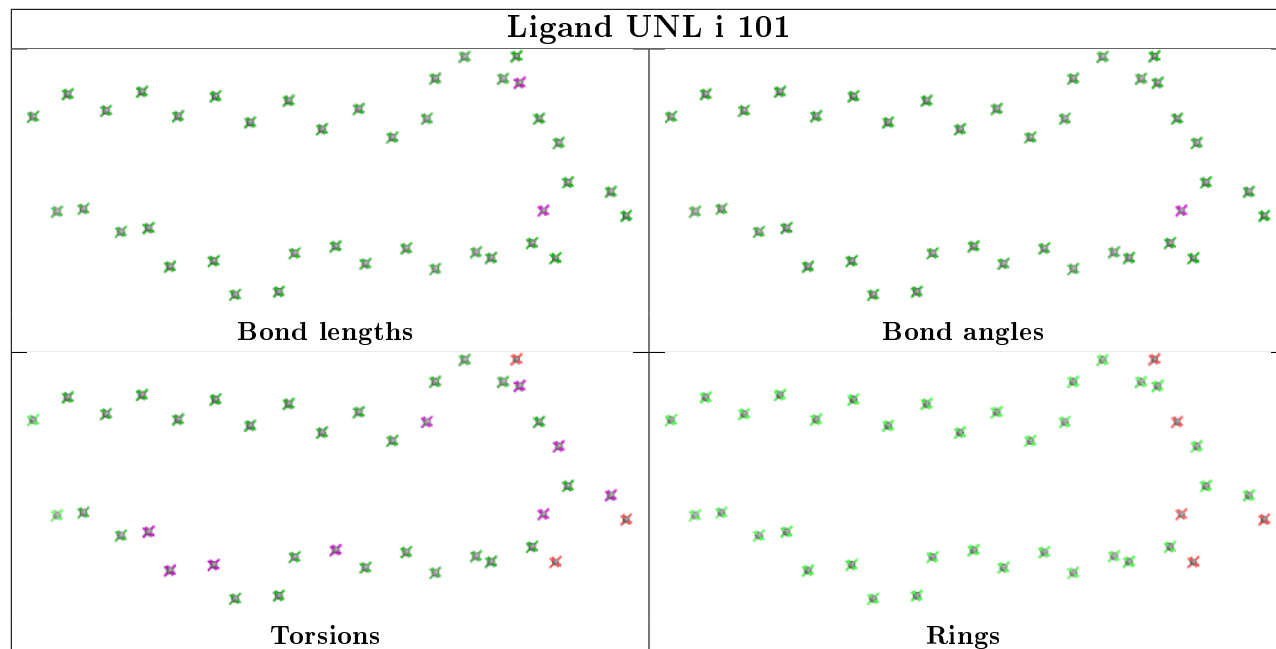
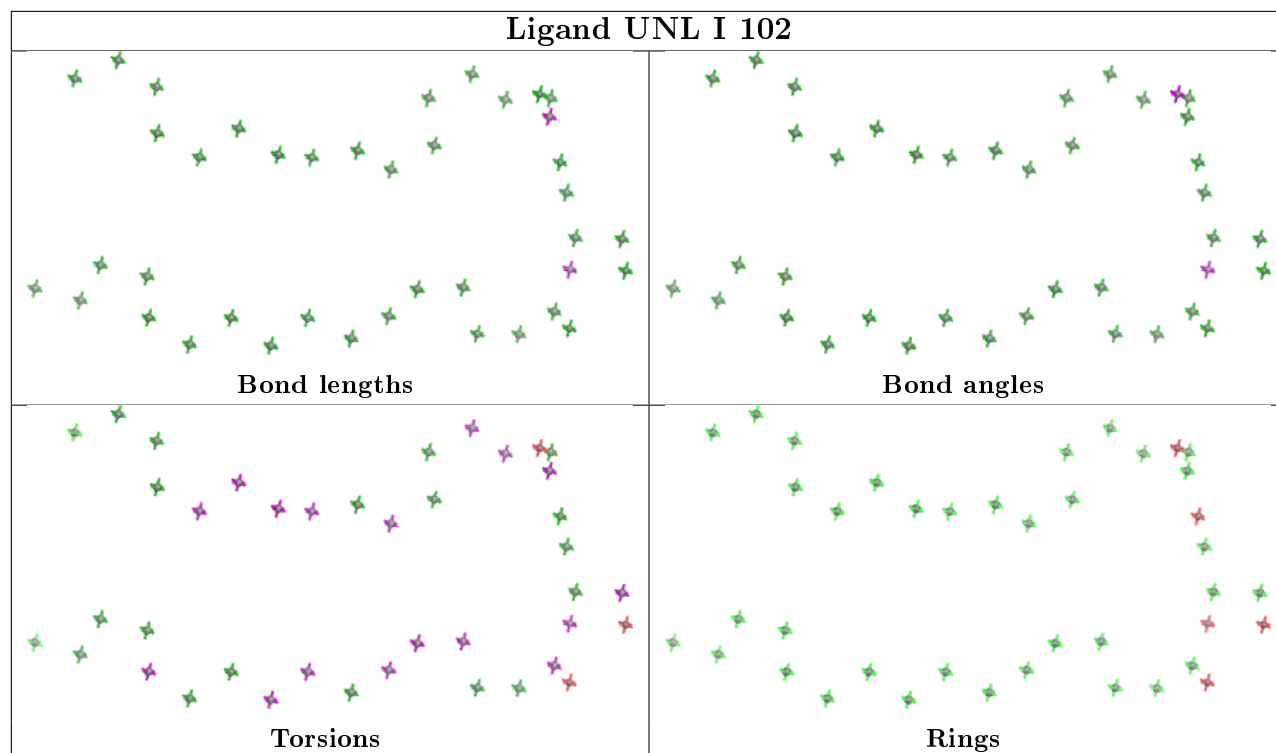


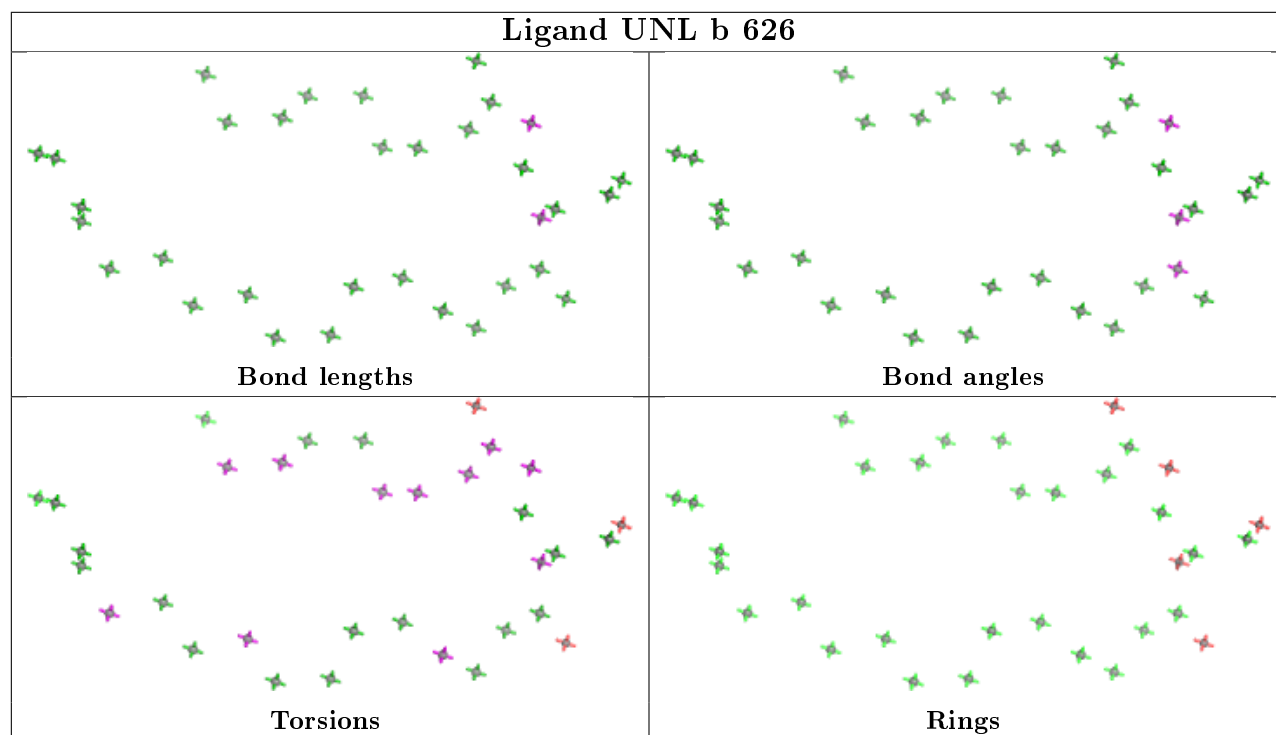
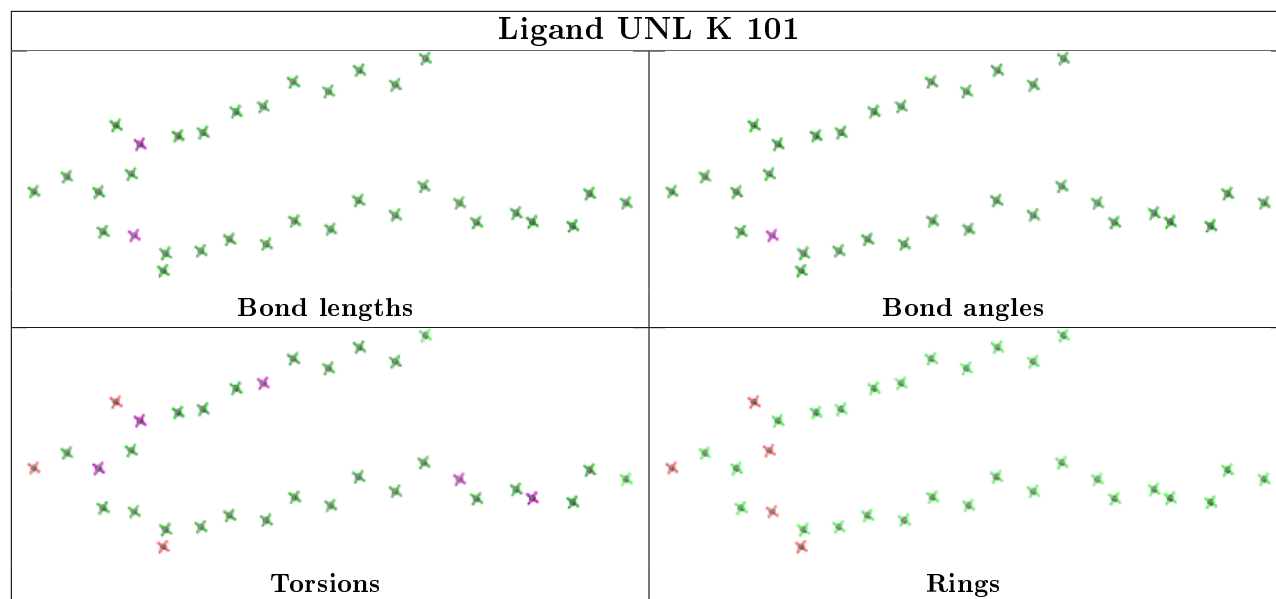
## Ligand HTG C 521

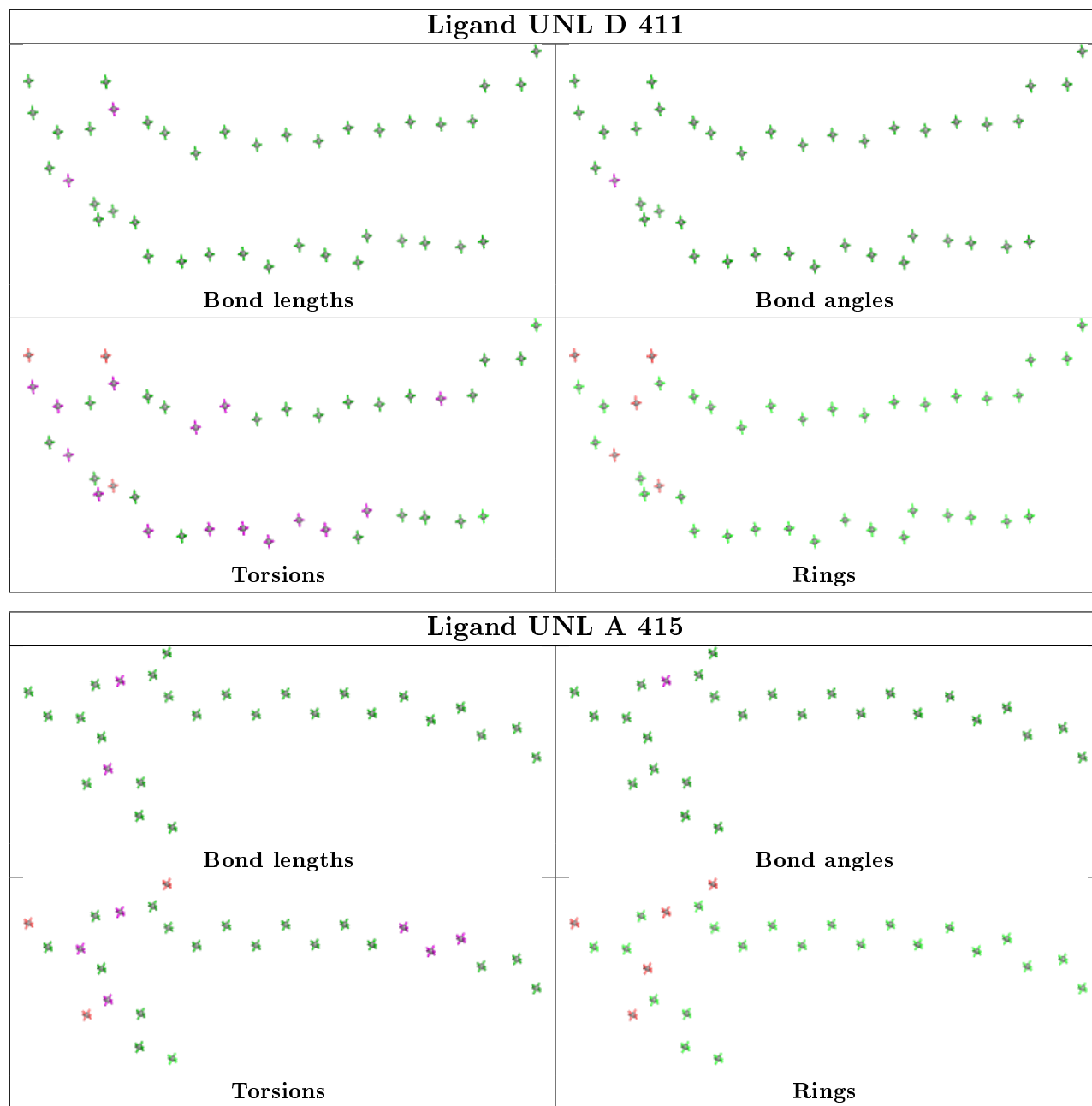


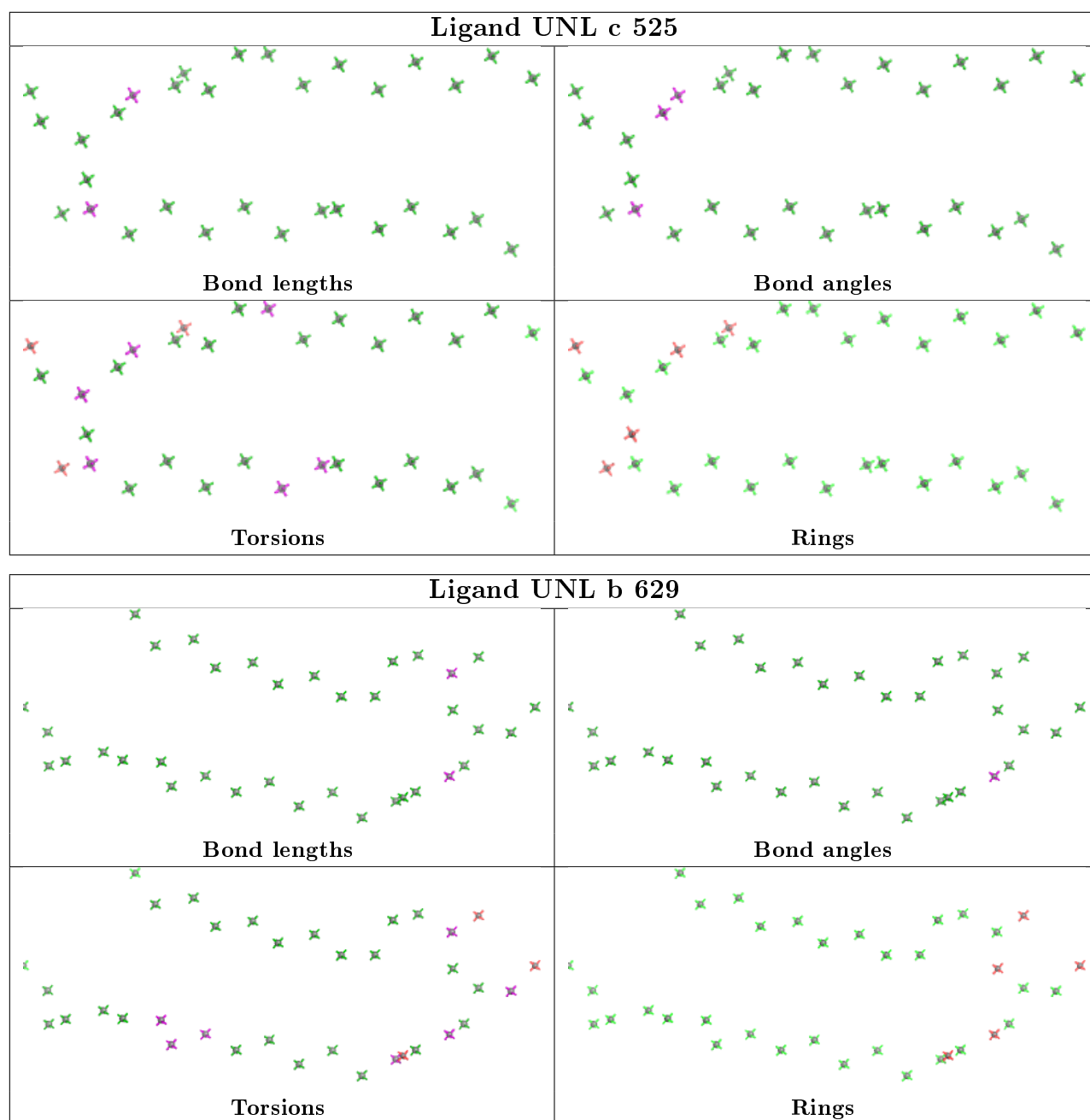












## 5.7 Other polymers [i](#)

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%)	-0.07	9 (2%) 54 58	21, 31, 53, 100	0
1	a	334/344 (97%)	0.08	11 (3%) 46 50	23, 33, 62, 108	0
2	B	504/505 (99%)	0.20	48 (9%) 8 8	21, 36, 65, 109	0
2	b	504/505 (99%)	0.35	57 (11%) 5 4	23, 37, 74, 118	0
3	C	451/455 (99%)	0.51	63 (13%) 2 2	26, 45, 67, 117	0
3	c	455/455 (100%)	0.31	47 (10%) 6 6	30, 48, 69, 109	0
4	D	342/342 (100%)	-0.04	7 (2%) 65 68	21, 32, 53, 108	0
4	d	341/342 (99%)	0.21	25 (7%) 15 15	23, 36, 54, 123	0
5	E	81/84 (96%)	0.20	7 (8%) 10 10	37, 54, 82, 120	0
5	e	79/84 (94%)	1.05	19 (24%) 0 0	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.22	0 100 100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.20	3 (9%) 7 7	44, 50, 86, 122	0
7	H	64/65 (98%)	0.26	5 (7%) 13 13	34, 47, 68, 101	0
7	h	65/65 (100%)	1.07	16 (24%) 0 0	37, 51, 74, 141	0
8	I	37/38 (97%)	0.42	7 (18%) 1 1	37, 46, 88, 130	0
8	i	37/38 (97%)	0.22	3 (8%) 12 12	38, 46, 93, 135	0
9	J	38/39 (97%)	0.20	5 (13%) 3 3	32, 52, 106, 147	0
9	j	39/39 (100%)	0.73	9 (23%) 0 0	40, 51, 107, 129	0
10	K	37/37 (100%)	0.01	3 (8%) 12 12	44, 53, 76, 91	0
10	k	37/37 (100%)	0.29	2 (5%) 25 27	47, 54, 78, 93	0
11	L	36/37 (97%)	0.56	7 (19%) 1 1	20, 26, 89, 129	0
11	l	36/37 (97%)	0.21	3 (8%) 11 11	22, 28, 87, 128	0
12	M	32/36 (88%)	-0.04	1 (3%) 49 52	22, 29, 49, 117	0
12	m	33/36 (91%)	-0.25	3 (9%) 9 9	24, 29, 72, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.25	28 (11%) 4 4	22, 45, 100, 157	0
13	o	243/244 (99%)	0.61	49 (20%) 1 0	24, 46, 99, 144	0
14	T	29/32 (90%)	0.21	0 100 100	23, 28, 60, 96	0
14	t	29/32 (90%)	-0.14	0 100 100	23, 29, 61, 97	0
15	U	96/104 (92%)	0.46	13 (13%) 3 2	31, 40, 66, 84	0
15	u	97/104 (93%)	-0.17	6 (6%) 20 21	32, 43, 68, 101	0
16	V	137/137 (100%)	0.08	2 (1%) 73 75	29, 43, 70, 100	0
16	v	137/137 (100%)	0.45	20 (14%) 2 2	34, 50, 74, 101	0
17	X	38/40 (95%)	0.20	3 (7%) 12 12	44, 56, 82, 110	0
17	x	38/40 (95%)	1.14	9 (23%) 0 0	47, 58, 83, 112	0
18	Y	29/30 (96%)	1.74	12 (41%) 0 0	56, 71, 112, 114	0
18	y	29/30 (96%)	0.94	5 (17%) 1 1	58, 70, 110, 114	0
19	Z	62/62 (100%)	1.06	14 (22%) 0 0	57, 72, 117, 152	0
19	z	62/62 (100%)	1.32	16 (25%) 0 0	60, 74, 117, 153	0
20	R	34/34 (100%)	6.04	34 (100%) 0 0	89, 108, 128, 135	0
All	All	5284/5384 (98%)	0.33	571 (10%) 5 5	20, 41, 82, 157	0

All (571) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	10.4
20	R	35	LEU	9.1
20	R	20	VAL	8.8
20	R	19	ALA	8.7
9	J	5	GLY	8.6
17	x	38	GLN	8.5
20	R	23	ILE	8.4
20	R	6	LEU	8.2
1	A	11	ALA	8.1
20	R	14	LEU	8.0
2	b	495	PHE	7.9
7	h	66	GLY	7.6
20	R	15	ALA	7.4
9	j	3	GLU	7.2
20	R	8	VAL	6.9
9	j	2	SER	6.9
8	I	38	GLU	6.8

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Mol	Chain	Res	Type	RSRZ
20	R	5	VAL	6.7
20	R	13	LEU	6.6
20	R	16	ALA	6.6
20	R	31	VAL	6.6
20	R	3	TRP	6.5
20	R	17	GLY	6.4
2	b	218	LEU	6.3
9	j	5	GLY	6.3
2	b	487	SER	6.3
20	R	24	LEU	6.2
13	o	27	ARG	6.1
18	Y	19	ILE	6.1
17	x	37	VAL	6.0
2	b	494	GLY	5.9
2	b	493	TRP	5.9
20	R	34	LEU	5.9
20	R	4	ARG	5.8
20	R	22	ASN	5.8
3	C	437	PHE	5.8
1	A	13	LEU	5.7
20	R	21	ARG	5.7
13	o	142	PHE	5.7
20	R	7	VAL	5.7
19	z	1	MET	5.6
19	Z	32	ASP	5.6
2	b	491	VAL	5.5
3	C	253	LEU	5.5
3	C	181	PHE	5.4
18	y	19	ILE	5.4
2	b	504	THR	5.4
8	I	37	LEU	5.3
20	R	33	LYS	5.3
2	b	492	GLU	5.3
13	o	4	THR	5.3
2	b	486	LEU	5.2
3	C	60	ILE	5.2
20	R	11	PRO	5.2
7	h	6	TRP	5.2
19	z	7	LEU	5.2
8	i	37	LEU	5.2
20	R	10	LEU	5.2
2	B	496	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
17	x	34	ILE	5.2
2	b	497	GLN	5.1
4	D	238	THR	5.1
17	x	36	LYS	5.0
17	x	33	GLN	5.0
13	o	22	LEU	5.0
19	z	3	ILE	5.0
7	h	65	LEU	4.9
3	c	143	TYR	4.9
19	z	4	LEU	4.9
5	E	84	LYS	4.9
2	B	495	PHE	4.9
3	C	433	LEU	4.8
11	l	3	PRO	4.8
3	C	276	LEU	4.8
19	Z	31	GLN	4.8
2	b	488	PRO	4.8
19	z	57	LEU	4.8
13	o	36	GLN	4.7
20	R	26	TYR	4.7
19	Z	33	TRP	4.7
19	z	61	VAL	4.7
20	R	27	ALA	4.7
2	b	499	VAL	4.7
20	R	12	VAL	4.7
17	x	3	ILE	4.7
20	R	2	ASP	4.7
20	R	32	GLN	4.7
2	b	161	LEU	4.7
3	C	23	ALA	4.6
4	d	12	ARG	4.6
3	C	279	LEU	4.5
4	d	17	ILE	4.5
3	C	143	TYR	4.5
13	o	243	ILE	4.5
13	o	32	ILE	4.4
13	o	211	ILE	4.4
3	c	200	THR	4.4
17	x	2	THR	4.4
1	A	12	ASN	4.4
7	h	22	ALA	4.4
13	o	26	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	4.4
2	B	494	GLY	4.3
3	c	60	ILE	4.3
18	Y	18	VAL	4.3
18	Y	46	LEU	4.3
3	c	20	SER	4.3
3	C	281	MET	4.3
2	b	489	GLU	4.2
19	Z	30	PRO	4.2
19	z	5	PHE	4.2
4	D	12	ARG	4.2
19	Z	34	ASP	4.2
2	b	295	GLY	4.2
3	C	283	GLY	4.2
2	B	489	GLU	4.2
11	L	2	GLU	4.2
13	o	38	TYR	4.1
2	B	461	LEU	4.1
3	C	198	VAL	4.1
9	j	7	ILE	4.1
13	O	27	ARG	4.1
1	A	15	GLU	4.1
3	C	282	MET	4.0
11	L	7	ARG	4.0
3	C	155	ASN	4.0
20	R	28	VAL	4.0
3	c	146	PHE	4.0
19	z	60	PHE	4.0
19	z	2	THR	4.0
2	b	502	VAL	4.0
15	U	62	LEU	3.9
13	o	87	VAL	3.9
15	U	58	VAL	3.9
3	C	280	SER	3.9
13	o	246	ALA	3.9
4	d	154	VAL	3.9
19	z	62	VAL	3.9
3	c	426	LEU	3.9
3	C	285	ILE	3.9
9	j	1	MET	3.9
2	B	505	ARG	3.9
2	b	484	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
7	h	12	ARG	3.9
2	b	293	ALA	3.9
13	o	57	LYS	3.8
3	C	284	PHE	3.8
3	C	438	LEU	3.8
2	B	251	VAL	3.8
3	C	61	VAL	3.8
2	b	503	THR	3.8
8	I	36	ASP	3.8
17	x	39	ARG	3.8
2	b	298	LEU	3.7
3	c	140	LEU	3.7
3	c	199	ILE	3.7
12	m	33	GLN	3.7
13	o	39	ARG	3.7
13	o	133	VAL	3.7
3	C	180	MET	3.7
3	C	434	ALA	3.7
13	o	35	SER	3.7
18	Y	43	ARG	3.6
20	R	9	LEU	3.6
2	B	454	ALA	3.6
16	v	21	LEU	3.6
2	B	296	ALA	3.6
1	a	11	ALA	3.6
3	c	433	LEU	3.6
2	b	249	ALA	3.6
3	C	432	VAL	3.6
13	o	60	ARG	3.6
3	c	279	LEU	3.6
13	o	85	LEU	3.6
18	y	41	VAL	3.6
16	v	17	LYS	3.6
2	B	488	PRO	3.5
5	e	79	PHE	3.5
2	b	248	ALA	3.5
11	L	9	PRO	3.5
2	B	462	PHE	3.5
2	b	246	PHE	3.5
15	U	70	ARG	3.5
3	c	63	TRP	3.5
4	d	148	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	430	HIS	3.5
2	B	253	ALA	3.5
3	c	191	PRO	3.5
15	U	79	LEU	3.5
2	b	296	ALA	3.5
3	c	427	ALA	3.5
5	e	20	TRP	3.5
13	o	134	THR	3.5
4	D	11	GLU	3.4
2	B	298	LEU	3.4
3	C	262	ARG	3.4
3	c	430	HIS	3.4
13	O	25	THR	3.4
18	Y	21	GLN	3.4
3	c	22	PHE	3.4
3	c	155	ASN	3.4
8	i	38	GLU	3.4
2	b	498	LYS	3.4
13	O	62	GLU	3.4
3	C	436	PHE	3.4
13	o	37	THR	3.4
3	C	147	PHE	3.4
3	C	59	LEU	3.4
13	O	93	LEU	3.4
12	m	34	LYS	3.3
5	E	15	THR	3.3
16	v	4	THR	3.3
2	B	458	PHE	3.3
2	b	123	PHE	3.3
10	k	18	PHE	3.3
7	h	64	ALA	3.3
13	o	25	THR	3.3
2	B	252	VAL	3.3
15	U	73	GLN	3.3
1	A	16	ARG	3.3
11	L	10	VAL	3.3
2	b	244	ALA	3.3
2	b	505	ARG	3.3
16	v	5	PRO	3.2
3	C	255	THR	3.2
3	C	145[A]	SER	3.2
19	Z	36	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	b	292	LEU	3.2
2	b	288	VAL	3.2
3	C	439	VAL	3.2
7	H	6	TRP	3.2
10	k	17	ILE	3.2
4	d	155	SER	3.2
13	O	144	GLY	3.2
2	B	250	PHE	3.2
3	C	429	SER	3.2
2	b	245	VAL	3.2
3	C	57	ALA	3.2
17	X	2	THR	3.2
13	o	33	ASP	3.2
2	B	161	LEU	3.2
2	B	457	VAL	3.1
4	d	152	VAL	3.1
18	Y	45	ASN	3.1
3	C	286	ALA	3.1
18	Y	22	LEU	3.1
9	J	6	ARG	3.1
15	U	59	GLU	3.1
13	o	24	ASP	3.1
2	B	504	THR	3.1
5	e	83	LEU	3.1
3	C	201	ASN	3.1
6	f	15	ILE	3.1
5	E	83	LEU	3.1
13	O	5	LEU	3.1
9	j	4	GLY	3.1
3	C	275	SER	3.1
5	E	17	VAL	3.1
3	C	63	TRP	3.1
1	a	265	PHE	3.1
4	d	149	PRO	3.1
11	L	8	GLN	3.1
11	l	2	GLU	3.1
13	O	24	ASP	3.1
20	R	30	GLN	3.1
3	c	280	SER	3.1
7	H	2	ALA	3.1
16	v	107	LEU	3.1
3	C	146	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
3	c	284	PHE	3.0
18	Y	20	ALA	3.0
18	y	37	PHE	3.0
2	b	294	SER	3.0
3	c	198	VAL	3.0
13	O	133	VAL	3.0
19	Z	35	ARG	3.0
17	X	3	ILE	3.0
5	e	59	GLU	3.0
3	C	200	THR	3.0
3	C	278	ALA	3.0
15	U	104	LYS	3.0
19	z	6	GLN	3.0
4	d	150	ILE	3.0
4	d	13	GLY	3.0
4	d	159	ILE	2.9
5	e	25	ILE	2.9
3	C	254	THR	2.9
8	I	34	ARG	2.9
9	j	9	LEU	2.9
4	d	156	VAL	2.9
13	O	139	SER	2.9
3	c	283	GLY	2.9
9	J	4	GLY	2.9
13	o	209	GLY	2.9
18	Y	40	ALA	2.9
2	b	250	PHE	2.9
15	U	74	ILE	2.9
2	B	459	ALA	2.9
13	O	29	ALA	2.9
13	o	212	ALA	2.9
2	b	457	VAL	2.9
2	b	462	PHE	2.9
3	C	435	PHE	2.9
3	c	87	ILE	2.9
16	v	110	LYS	2.9
13	o	199	LEU	2.9
2	B	290	ALA	2.9
9	J	3	GLU	2.9
13	O	22	LEU	2.9
2	B	487	SER	2.9
13	o	58	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	202	PRO	2.9
16	v	95	LEU	2.9
2	B	451	PHE	2.8
4	D	150	ILE	2.8
6	f	42	PHE	2.8
7	h	10	ILE	2.8
2	b	412	THR	2.8
3	C	204	LEU	2.8
1	a	262	TYR	2.8
16	V	135	VAL	2.8
13	o	5	LEU	2.8
13	O	28	GLY	2.8
3	c	196	VAL	2.8
13	o	204	VAL	2.8
4	d	157	PHE	2.8
5	e	36	LEU	2.8
16	v	16	GLY	2.8
2	b	490	GLN	2.8
2	B	460	LEU	2.8
13	O	91	GLY	2.8
4	d	147	SER	2.8
13	o	245	PRO	2.8
15	U	103	TYR	2.8
2	b	247	PHE	2.8
2	b	290	ALA	2.8
3	c	201	ASN	2.8
5	e	15	THR	2.8
2	B	490	GLN	2.8
3	c	64	ALA	2.8
1	a	224	ILE	2.7
2	B	249	ALA	2.7
13	o	140	THR	2.7
5	e	24	SER	2.7
3	c	203	THR	2.7
5	e	14	ILE	2.7
13	O	26	ALA	2.7
2	B	502	VAL	2.7
3	c	61	VAL	2.7
9	J	7	ILE	2.7
2	B	294	SER	2.7
2	b	500	GLY	2.7
2	B	491	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	252	ILE	2.7
13	o	34	SER	2.7
17	X	34	ILE	2.7
2	b	501	ASP	2.7
16	v	1	ALA	2.7
3	C	56	HIS	2.7
16	v	19	ILE	2.7
13	o	30	TYR	2.7
15	U	99	ASN	2.7
13	o	98	GLU	2.6
19	Z	28	ALA	2.6
5	e	42	LEU	2.6
8	I	6	ILE	2.6
13	o	136	ILE	2.6
19	z	59	PHE	2.6
2	b	289	GLN	2.6
3	c	429	SER	2.6
13	O	204	VAL	2.6
2	B	248	ALA	2.6
15	u	103	TYR	2.6
7	h	8	GLY	2.6
13	o	93	LEU	2.6
1	a	225	ARG	2.6
13	O	135	SER	2.6
16	v	10	VAL	2.6
19	Z	29	SER	2.6
3	C	196	VAL	2.6
7	h	9	ASP	2.6
19	z	56	VAL	2.6
3	C	440	GLY	2.6
16	v	26	TYR	2.6
7	h	58	VAL	2.6
16	v	12	LEU	2.6
20	R	25	PRO	2.6
3	C	182	PHE	2.6
4	d	153	PHE	2.6
3	c	257	PHE	2.5
5	e	22	ILE	2.5
16	v	106	ASN	2.5
1	A	14	TRP	2.5
2	B	292	LEU	2.5
19	z	9	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
18	Y	42	ARG	2.5
3	c	144	SER	2.5
2	B	297	THR	2.5
13	O	30	TYR	2.5
1	a	13	LEU	2.5
20	R	29	LYS	2.5
2	b	485	GLU	2.5
3	c	141	GLU	2.5
3	c	255	THR	2.5
4	d	151	ALA	2.5
13	o	86	LYS	2.5
7	h	57	GLY	2.5
3	C	135	ARG	2.5
9	j	6	ARG	2.5
13	o	207	ARG	2.5
7	h	23	PRO	2.5
19	z	46	LEU	2.5
2	B	247	PHE	2.5
5	e	21	VAL	2.5
19	Z	62	VAL	2.5
3	C	431	PHE	2.5
4	d	123	ILE	2.5
3	C	277	GLY	2.5
15	u	9	LEU	2.4
13	o	95	PHE	2.4
13	O	207	ARG	2.4
2	B	241	SER	2.4
19	Z	27	TYR	2.4
2	B	85	GLY	2.4
2	b	126	PRO	2.4
12	M	33	GLN	2.4
13	o	59	LYS	2.4
18	y	43	ARG	2.4
4	d	119	ALA	2.4
15	U	76	ARG	2.4
13	O	138	THR	2.4
13	o	198	SER	2.4
17	x	8	LYS	2.4
13	o	40	ILE	2.4
15	u	66	GLY	2.4
1	a	15	GLU	2.4
5	e	57	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
13	o	241	ALA	2.4
4	D	122	LEU	2.4
2	B	295	GLY	2.4
2	b	413	ASP	2.4
5	E	74	GLN	2.4
18	Y	38	LEU	2.4
19	Z	39	LEU	2.4
2	b	414	PRO	2.4
2	b	482	ILE	2.4
2	b	458	PHE	2.4
7	h	13	PRO	2.4
13	o	141	ASP	2.4
5	e	39	SER	2.4
15	U	57	SER	2.4
3	C	154	LYS	2.3
13	o	203	LYS	2.3
3	C	148	GLY	2.3
13	o	91	GLY	2.3
2	B	245	VAL	2.3
10	K	29	PRO	2.3
3	C	199	ILE	2.3
5	e	7	GLU	2.3
3	c	437	PHE	2.3
2	b	252	VAL	2.3
18	Y	25	ILE	2.3
1	A	19	ASN	2.3
16	V	12	LEU	2.3
16	v	25	GLN	2.3
11	l	5	PRO	2.3
13	O	131	PRO	2.3
2	B	242	ILE	2.3
19	Z	60	PHE	2.3
10	K	14	ALA	2.3
5	e	17	VAL	2.3
4	d	14	TRP	2.3
3	c	192	GLY	2.3
4	d	68	LEU	2.3
2	B	501	ASP	2.3
3	c	195	ASP	2.3
3	c	260	ALA	2.3
3	c	425	TRP	2.3
6	f	43	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
12	m	31	SER	2.3
19	Z	3	ILE	2.3
2	b	251	VAL	2.2
8	I	26	GLY	2.2
13	O	130	GLN	2.2
15	u	101	GLY	2.2
2	b	217	ILE	2.2
3	C	287	THR	2.2
2	b	238	LEU	2.2
7	H	46	LEU	2.2
16	v	8	LEU	2.2
3	c	452	ALA	2.2
4	D	123	ILE	2.2
4	d	37	LEU	2.2
3	C	25	ASN	2.2
2	B	219	VAL	2.2
2	b	459	ALA	2.2
13	o	226	GLY	2.2
3	C	272	LEU	2.2
5	e	38	VAL	2.2
16	v	135	VAL	2.2
4	d	283	ALA	2.2
3	c	21	ILE	2.2
3	c	59	LEU	2.2
3	c	204	LEU	2.2
3	c	282	MET	2.2
1	a	16	ARG	2.2
3	C	58	GLY	2.2
3	c	197	ARG	2.2
7	H	43	LEU	2.2
3	c	259	TRP	2.1
10	K	28	ILE	2.1
18	y	22	LEU	2.1
5	E	11	SER	2.1
3	C	149	TYR	2.1
2	B	293	ALA	2.1
16	v	22	THR	2.1
4	D	149	PRO	2.1
1	a	285	PHE	2.1
2	b	162	PHE	2.1
19	z	38	GLN	2.1
4	d	126	MET	2.1

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Mol	Chain	Res	Type	RSRZ
8	I	29	ALA	2.1
3	c	24	THR	2.1
13	o	138	THR	2.1
1	a	121[A]	LEU	2.1
7	H	42	LEU	2.1
13	O	15	LEU	2.1
7	h	56	ASP	2.1
11	L	4	ASN	2.1
13	O	143	LYS	2.1
2	B	304	ALA	2.1
13	O	60	ARG	2.1
1	a	266	ASN	2.1
13	O	63	ALA	2.1
16	v	18	THR	2.1
3	C	455	PHE	2.1
4	d	146	PHE	2.1
7	h	42	LEU	2.1
11	L	6	ASN	2.1
2	b	121	GLU	2.1
5	e	77	GLU	2.1
1	A	152	ALA	2.1
2	B	456	ALA	2.1
5	E	73	LYS	2.1
15	u	70	ARG	2.1
9	j	12	VAL	2.1
13	O	87	VAL	2.1
3	C	340	TYR	2.1
13	o	23	ASP	2.1
2	B	162	PHE	2.1
3	C	426	LEU	2.1
5	e	82	GLN	2.1
1	A	249	VAL	2.0
13	O	134	THR	2.0
2	B	86	ILE	2.0
2	B	214	LEU	2.0
2	B	411	PHE	2.0
3	C	257	PHE	2.0
8	i	2	GLU	2.0
2	b	30	VAL	2.0
3	C	144	SER	2.0
13	O	196	GLN	2.0
4	d	158	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
4	d	279	LEU	2.0
7	h	7	LEU	2.0
15	u	79	LEU	2.0
3	c	147	PHE	2.0
2	B	455	HIS	2.0
3	c	88	LEU	2.0
15	U	9	LEU	2.0
16	v	79	PRO	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	0.96	0.11	30,42,63,78	0
8	FME	i	1	10/11	0.97	0.09	37,49,57,62	0
12	FME	M	1	10/11	0.97	0.16	18,38,70,79	0
14	FME	T	1	10/11	0.98	0.08	18,32,46,47	0
14	FME	t	1	10/11	0.98	0.10	21,32,41,71	0
8	FME	I	1	10/11	0.98	0.22	31,47,56,62	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
30	UNL	A	415	28/-	0.19	0.56	67,87,108,112	0
35	LMT	B	630	35/35	0.55	0.46	33,105,126,134	0
34	HTG	D	412	16/19	0.55	0.43	48,115,128,130	0
30	UNL	b	626	33/-	0.58	0.44	44,78,131,135	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	LMG	Z	101	51/55	0.59	0.43	46,105,140,150	0
35	LMT	I	101	35/35	0.59	0.65	74,108,131,141	0
30	UNL	a	415	30/-	0.61	0.50	72,90,111,118	0
34	HTG	b	623	19/19	0.62	0.65	71,109,141,169	0
34	HTG	B	624	19/19	0.63	0.68	57,104,140,144	0
35	LMT	D	402	35/35	0.65	0.37	31,97,113,115	0
35	LMT	e	102	35/35	0.66	0.79	76,134,147,156	0
29	PL9	a	414	55/55	0.67	0.40	57,93,112,120	0
34	HTG	C	522	19/19	0.67	0.91	58,139,157,179	0
30	UNL	B	628	33/-	0.67	0.28	29,76,136,139	0
35	LMT	M	103	35/35	0.68	0.34	40,120,148,154	0
35	LMT	M	101	35/35	0.69	0.35	39,80,103,109	0
35	LMT	m	102	35/35	0.70	0.47	34,78,102,109	0
25	BCR	h	101	40/40	0.70	0.27	39,50,64,77	0
33	LMG	c	520	51/55	0.70	0.36	51,102,132,138	0
29	PL9	A	414	55/55	0.71	0.40	41,88,105,119	0
30	UNL	J	102	10/-	0.71	0.39	55,64,89,90	0
30	UNL	i	101	40/-	0.71	0.42	48,88,140,147	0
30	UNL	K	101	34/-	0.72	0.34	55,96,114,125	0
35	LMT	E	102	35/35	0.72	0.55	78,120,147,150	0
30	UNL	I	102	40/-	0.73	0.31	40,85,135,142	0
31	LHG	e	101	42/49	0.73	0.41	81,118,142,148	0
30	UNL	j	102	10/-	0.74	0.30	60,75,88,89	0
34	HTG	c	522	19/19	0.74	0.85	79,124,142,146	0
30	UNL	m	101	10/-	0.74	0.30	40,50,55,56	0
33	LMG	Z	102	37/55	0.74	0.38	47,97,129,137	0
30	UNL	c	525	32/-	0.75	0.30	71,97,113,119	0
34	HTG	B	623	19/19	0.76	0.40	60,84,110,115	0
34	HTG	b	622	19/19	0.76	0.88	74,95,125,130	0
26	SQD	f	101	43/54	0.77	0.36	85,111,157,164	0
26	SQD	L	101	54/54	0.77	0.27	47,71,116,121	0
34	HTG	d	411	16/19	0.77	0.38	81,112,121,122	0
35	LMT	b	621	25/35	0.78	0.24	60,99,144,148	0
34	HTG	c	521	19/19	0.78	0.36	68,112,134,140	0
34	HTG	C	521	19/19	0.79	0.41	66,101,116,120	0
27	GOL	d	402	6/6	0.80	0.59	33,50,65,68	0
31	LHG	E	101	42/49	0.81	0.26	41,93,108,124	0
30	UNL	b	629	36/-	0.81	0.29	49,80,131,138	0
35	LMT	D	403	35/35	0.81	0.32	48,91,116,117	0
30	UNL	x	101	18/-	0.82	0.29	44,63,91,92	0
34	HTG	V	203	11/19	0.82	0.56	71,92,107,108	0
33	LMG	C	520	51/55	0.83	0.28	37,69,104,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	LMT	b	627	25/35	0.83	0.25	29,61,134,139	0
30	UNL	D	411	40/-	0.83	0.24	40,77,117,122	0
35	LMT	B	629	25/35	0.83	0.24	34,68,124,125	0
25	BCR	H	101	40/40	0.84	0.23	33,42,63,67	0
35	LMT	a	417	35/35	0.84	0.55	78,114,130,131	0
33	LMG	C	501	51/55	0.84	0.28	35,74,98,102	0
23	CLA	C	513	65/65	0.84	0.26	43,59,94,101	0
33	LMG	a	416	51/55	0.84	0.25	41,77,102,118	0
34	HTG	b	628	19/19	0.85	0.25	34,65,115,119	0
30	UNL	M	102	10/-	0.85	0.26	33,52,59,69	0
26	SQD	B	620	54/54	0.86	0.21	41,73,108,113	0
27	GOL	B	626	6/6	0.86	0.32	38,51,55,62	0
33	LMG	z	101	39/55	0.88	0.24	63,112,140,147	0
33	LMG	c	519	51/55	0.88	0.27	43,77,114,124	0
26	SQD	a	412	54/54	0.88	0.21	44,73,125,133	0
26	SQD	A	412	54/54	0.89	0.21	39,65,102,118	0
23	CLA	C	514	65/65	0.89	0.23	46,64,87,95	0
36	DGD	h	102	62/66	0.89	0.27	31,46,62,73	0
33	LMG	B	621	51/55	0.89	0.21	32,49,79,105	0
33	LMG	b	620	51/55	0.90	0.19	29,50,88,106	0
36	DGD	C	518	62/66	0.90	0.21	29,46,103,110	0
23	CLA	c	513	65/65	0.90	0.22	52,73,115,119	0
35	LMT	B	631	26/35	0.90	0.17	52,80,105,109	0
23	CLA	C	512	65/65	0.90	0.18	36,52,73,84	0
23	CLA	C	508	65/65	0.91	0.25	36,47,60,70	0
23	CLA	c	502	65/65	0.91	0.41	37,48,68,73	0
23	CLA	c	512	65/65	0.91	0.20	48,64,90,96	0
34	HTG	B	627	19/19	0.91	0.17	45,63,74,75	0
26	SQD	D	413	43/54	0.91	0.27	64,97,112,116	0
27	GOL	a	411	6/6	0.91	0.20	52,60,62,66	0
30	UNL	X	101	18/-	0.91	0.19	40,53,83,90	0
36	DGD	H	102	62/66	0.92	0.25	26,40,58,66	0
25	BCR	y	101	40/40	0.92	0.16	44,54,70,72	0
23	CLA	B	609	65/65	0.92	0.17	29,39,53,63	0
33	LMG	j	101	51/55	0.92	0.18	37,53,102,123	0
23	CLA	b	609	65/65	0.92	0.17	36,44,63,82	0
23	CLA	B	614	65/65	0.92	0.18	21,31,82,100	0
23	CLA	c	507	65/65	0.92	0.18	41,53,65,68	0
34	HTG	B	622	19/19	0.92	0.21	34,61,127,132	0
31	LHG	l	101	49/49	0.92	0.17	25,38,55,60	0
23	CLA	c	511	65/65	0.92	0.21	43,56,74,82	0
33	LMG	J	101	51/55	0.92	0.18	30,51,88,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	c	509	65/65	0.92	0.24	43,52,66,73	0
31	LHG	A	416	49/49	0.92	0.32	26,44,61,77	0
23	CLA	b	602	65/65	0.92	0.23	32,44,60,68	0
36	DGD	c	517	62/66	0.92	0.22	38,53,112,129	0
23	CLA	B	602	65/65	0.92	0.23	29,37,55,67	0
23	CLA	b	616	65/65	0.92	0.18	31,46,98,105	0
25	BCR	d	405	40/40	0.93	0.16	40,50,74,81	0
23	CLA	C	507	65/65	0.93	0.15	39,55,102,106	0
30	UNL	D	410	17/-	0.93	0.29	44,56,91,100	0
23	CLA	b	601	65/65	0.93	0.24	43,69,99,126	0
27	GOL	C	523	6/6	0.93	0.23	44,54,59,60	0
23	CLA	C	510	65/65	0.93	0.29	36,47,67,69	0
34	HTG	b	625	19/19	0.93	0.11	43,56,83,93	0
37	CA	O	301	1/1	0.93	0.11	87,87,87,87	0
23	CLA	b	615	65/65	0.93	0.17	29,40,66,81	0
37	CA	V	201	1/1	0.93	0.15	93,93,93,93	0
36	DGD	C	519	62/66	0.93	0.17	28,44,71,95	0
23	CLA	D	405	65/65	0.93	0.19	31,46,99,111	0
25	BCR	C	516	40/40	0.93	0.21	36,48,66,73	0
23	CLA	C	503	65/65	0.93	0.35	31,42,55,73	0
36	DGD	C	517	62/66	0.93	0.23	27,36,81,92	0
31	LHG	d	408	49/49	0.93	0.22	24,35,53,70	0
23	CLA	c	503	65/65	0.93	0.41	40,51,63,78	0
26	SQD	a	410	54/54	0.93	0.18	41,64,98,105	0
23	CLA	B	601	65/65	0.94	0.22	39,57,88,119	0
25	BCR	Y	101	40/40	0.94	0.15	37,49,59,62	0
25	BCR	K	102	40/40	0.94	0.17	39,47,62,65	0
23	CLA	B	604	65/65	0.94	0.30	21,29,92,104	0
23	CLA	d	404	65/65	0.94	0.17	38,48,98,109	0
23	CLA	B	616	65/65	0.94	0.21	30,45,113,124	0
25	BCR	C	515	40/40	0.94	0.15	46,61,72,73	0
26	SQD	A	410	54/54	0.94	0.15	38,62,99,105	0
23	CLA	b	612	65/65	0.94	0.23	25,35,48,59	0
23	CLA	c	508	65/65	0.94	0.19	35,48,107,118	0
23	CLA	C	504	65/65	0.94	0.27	36,44,65,75	0
23	CLA	C	505	65/65	0.94	0.21	30,41,79,104	0
25	BCR	k	101	40/40	0.94	0.16	47,55,79,81	0
31	LHG	d	409	49/49	0.94	0.20	33,50,98,110	0
37	CA	c	523	1/1	0.94	0.17	68,68,68,68	0
23	CLA	C	502	65/65	0.94	0.22	34,41,60,77	0
29	PL9	d	406	55/55	0.94	0.19	23,30,41,58	0
27	GOL	b	624	6/6	0.94	0.13	58,76,78,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	B	619	40/40	0.94	0.15	28,42,63,67	0
23	CLA	B	606	65/65	0.94	0.15	26,35,76,99	0
25	BCR	b	619	40/40	0.94	0.15	32,45,61,69	0
23	CLA	B	611	65/65	0.94	0.24	23,30,41,45	0
25	BCR	D	406	40/40	0.94	0.17	32,42,87,90	0
23	CLA	c	505	65/65	0.94	0.20	32,45,68,86	0
37	CA	o	301	1/1	0.95	0.10	85,85,85,85	0
23	CLA	c	501	65/65	0.95	0.23	38,49,64,71	0
23	CLA	b	606	65/65	0.95	0.14	27,42,77,106	0
30	UNL	d	410	17/-	0.95	0.29	42,57,85,90	0
23	CLA	B	612	65/65	0.95	0.23	24,29,42,51	0
31	LHG	d	407	49/49	0.95	0.21	25,44,72,87	0
36	DGD	c	516	62/66	0.95	0.23	33,43,73,95	0
25	BCR	c	514	40/40	0.95	0.13	52,65,76,79	0
23	CLA	a	408	65/65	0.95	0.19	28,40,107,115	0
31	LHG	D	409	49/49	0.95	0.19	29,47,107,124	0
23	CLA	B	615	65/65	0.95	0.14	27,34,61,68	0
23	CLA	b	614	65/65	0.95	0.14	23,34,76,89	0
29	PL9	D	407	55/55	0.95	0.23	20,31,45,54	0
23	CLA	c	504	65/65	0.95	0.27	37,50,89,111	0
36	DGD	c	518	62/66	0.95	0.19	36,46,77,96	0
31	LHG	A	417	49/49	0.95	0.23	23,37,55,66	0
27	GOL	B	625	6/6	0.95	0.29	48,76,85,89	0
23	CLA	C	509	65/65	0.95	0.29	30,43,102,115	0
23	CLA	b	604	65/65	0.95	0.31	23,31,85,96	0
23	CLA	A	404	65/65	0.96	0.16	20,23,41,58	0
23	CLA	D	404	65/65	0.96	0.17	20,26,46,52	0
23	CLA	B	605	65/65	0.96	0.20	22,30,44,48	0
31	LHG	D	408	49/49	0.96	0.23	22,34,51,68	0
23	CLA	B	607	65/65	0.96	0.22	18,27,54,66	0
25	BCR	c	515	40/40	0.96	0.14	37,52,65,75	0
23	CLA	b	607	65/65	0.96	0.17	20,31,53,63	0
23	CLA	C	511	65/65	0.96	0.42	33,44,57,61	0
23	CLA	b	605	65/65	0.96	0.23	24,34,52,97	0
25	BCR	b	618	40/40	0.96	0.20	21,34,49,55	0
39	MG	j	103	1/1	0.96	0.14	51,51,51,51	0
23	CLA	b	603	65/65	0.96	0.24	30,40,53,74	0
23	CLA	c	506	65/65	0.96	0.14	44,58,90,111	0
23	CLA	c	510	65/65	0.96	0.31	39,47,62,66	0
25	BCR	T	101	40/40	0.96	0.22	20,36,45,53	0
25	BCR	b	617	40/40	0.96	0.15	20,34,41,44	0
23	CLA	b	610	65/65	0.96	0.20	30,42,51,60	0

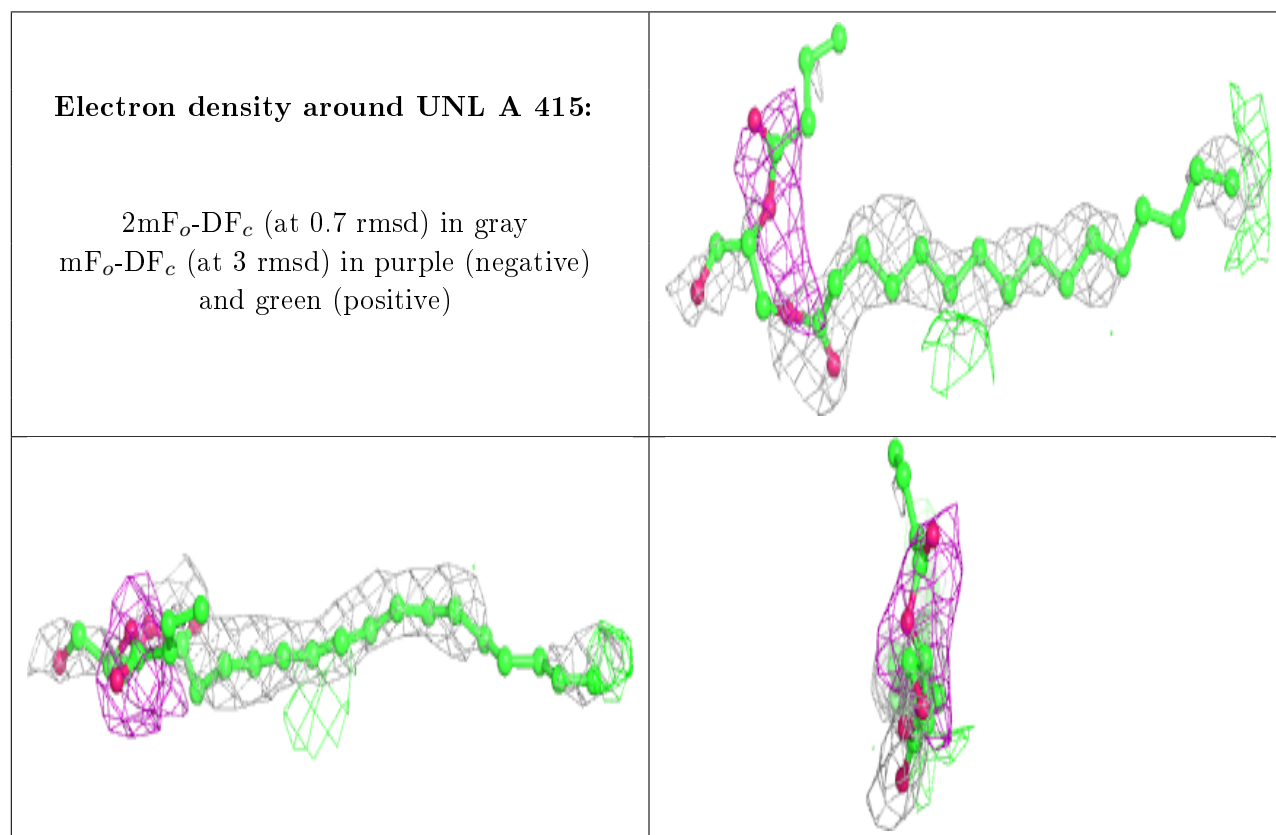
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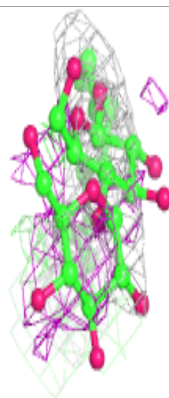
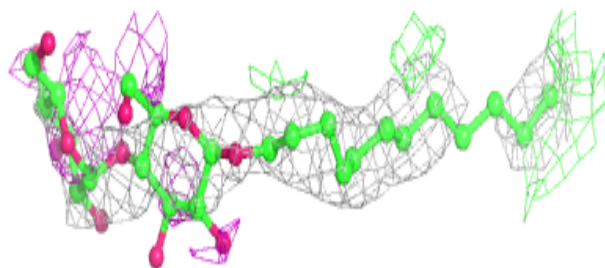
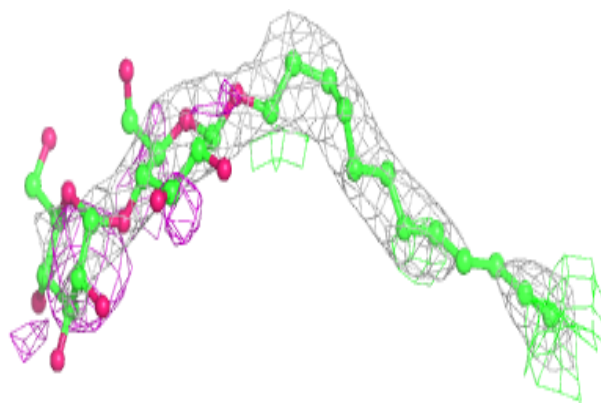
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	506	65/65	0.96	0.26	31,40,71,78	0
24	PHO	a	407	64/64	0.97	0.26	28,35,50,52	0
25	BCR	B	618	40/40	0.97	0.23	21,36,54,69	0
25	BCR	a	409	40/40	0.97	0.14	24,35,45,49	0
23	CLA	B	603	65/65	0.97	0.26	26,39,52,57	0
25	BCR	A	409	40/40	0.97	0.15	22,34,46,49	0
23	CLA	B	610	65/65	0.97	0.23	27,36,52,69	0
23	CLA	d	401	65/65	0.97	0.15	23,26,48,75	0
27	GOL	A	411	6/6	0.97	0.12	50,58,65,79	0
23	CLA	a	404	65/65	0.97	0.17	25,30,50,60	0
23	CLA	b	608	65/65	0.97	0.28	32,41,60,68	0
25	BCR	t	101	40/40	0.97	0.23	19,42,59,62	0
23	CLA	a	405	65/65	0.97	0.22	27,36,105,111	0
23	CLA	d	403	65/65	0.97	0.22	25,29,49,62	0
37	CA	c	524	1/1	0.97	0.09	66,66,66,66	0
24	PHO	A	407	64/64	0.97	0.21	23,31,46,51	0
23	CLA	A	405	65/65	0.97	0.16	19,23,41,47	0
23	CLA	b	611	65/65	0.97	0.19	25,34,49,61	0
23	CLA	B	608	65/65	0.97	0.23	27,37,51,55	0
23	CLA	A	408	65/65	0.97	0.14	26,36,101,109	0
23	CLA	A	406	65/65	0.97	0.14	22,29,80,89	0
23	CLA	b	613	65/65	0.97	0.23	22,33,67,78	0
23	CLA	B	613	65/65	0.97	0.32	21,29,68,78	0
38	HEM	E	103	43/43	0.98	0.09	40,54,66,73	0
40	HEC	V	202	43/43	0.98	0.11	30,33,44,53	0
24	PHO	a	406	64/64	0.98	0.20	22,31,40,51	0
38	HEM	e	103	43/43	0.98	0.19	48,73,98,105	0
37	CA	C	524	1/1	0.98	0.24	62,62,62,62	0
25	BCR	B	617	40/40	0.98	0.16	22,31,46,49	0
24	PHO	D	401	64/64	0.98	0.18	21,27,35,45	0
22	CL	a	403	1/1	0.98	0.19	34,34,34,34	0
39	MG	J	103	1/1	0.98	0.15	39,39,39,39	0
40	HEC	v	201	43/43	0.98	0.13	40,50,59,66	0
32	BCT	a	418	4/4	0.99	0.10	45,52,54,59	0
21	FE2	A	401	1/1	0.99	0.04	42,42,42,42	0
22	CL	a	402	1/1	0.99	0.10	31,31,31,31	0
28	OEX	A	413	10/10	0.99	0.09	22,30,43,45	0
32	BCT	A	418	4/4	0.99	0.08	34,39,47,65	0
21	FE2	a	401	1/1	0.99	0.06	45,45,45,45	0
22	CL	A	402	1/1	0.99	0.07	24,24,24,24	0
22	CL	A	403	1/1	1.00	0.24	27,27,27,27	0
28	OEX	a	413	10/10	1.00	0.09	27,34,45,53	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.

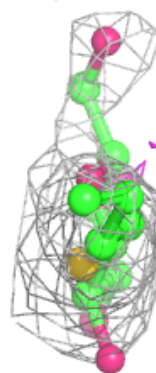
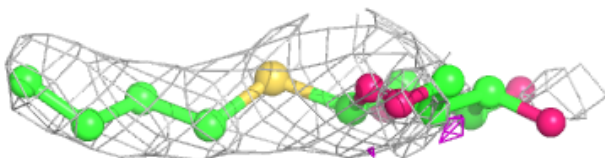
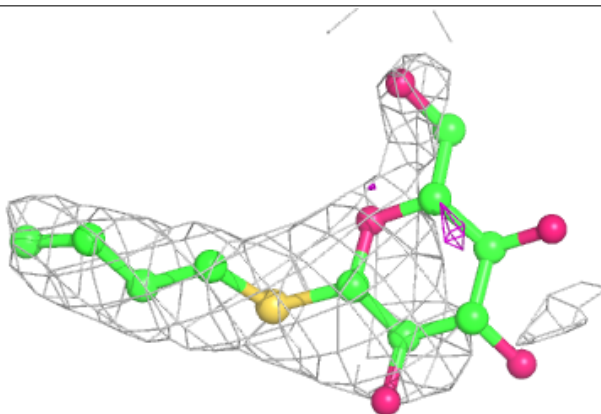


**Electron density around LMT B 630:**

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

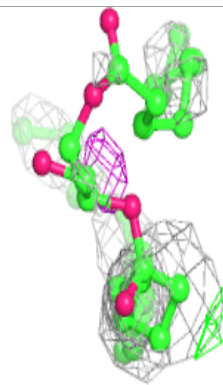
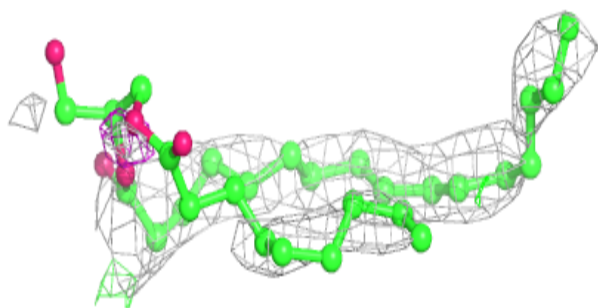
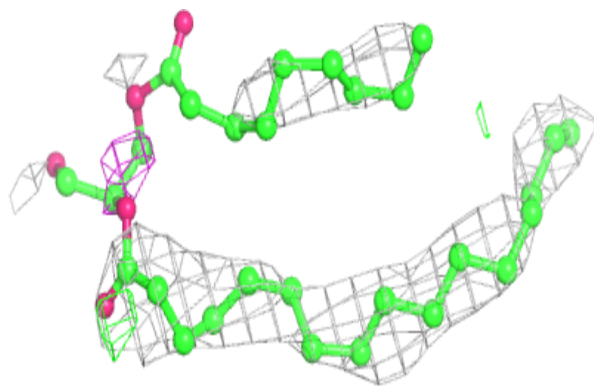
**Electron density around HTG D 412:**

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

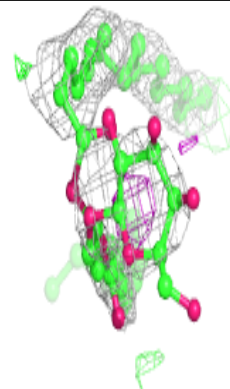
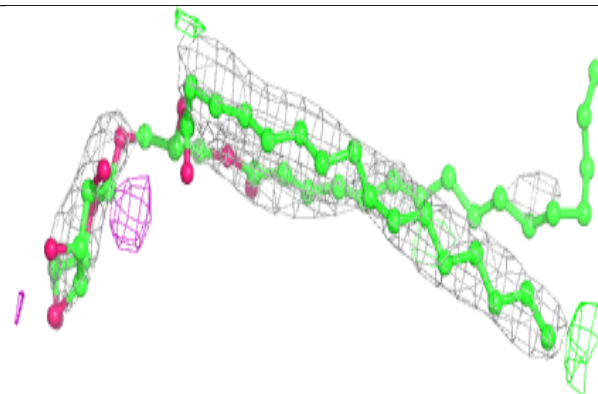
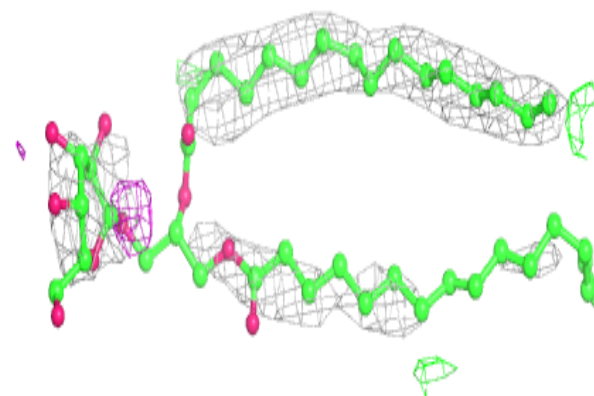


**Electron density around UNL b 626:**

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

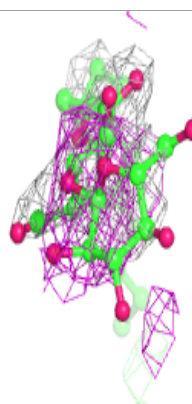
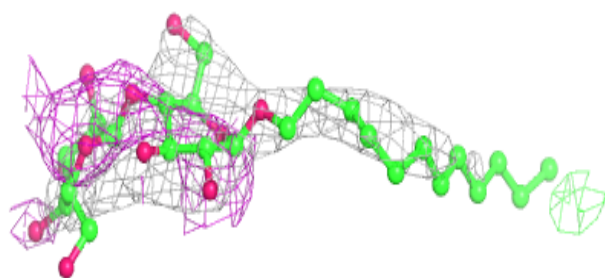
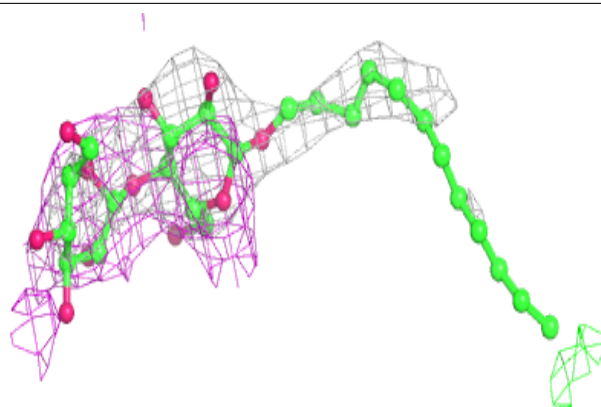
**Electron density around LMG Z 101:**

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

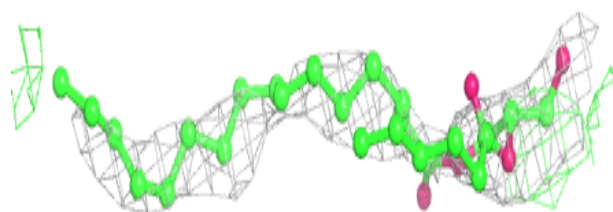
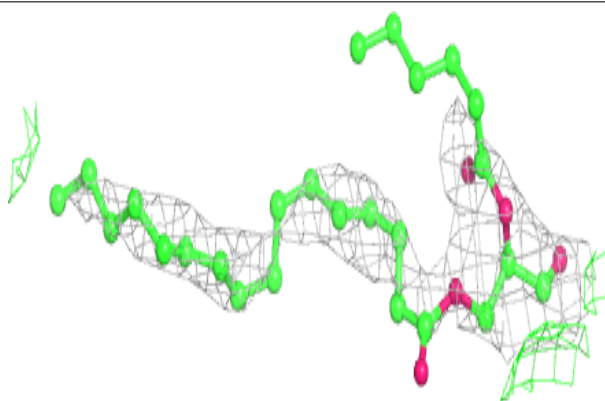


**Electron density around LMT I 101:**

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

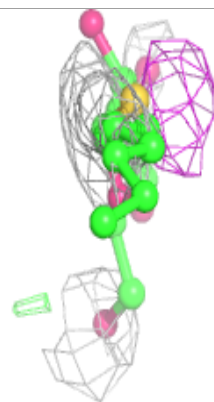
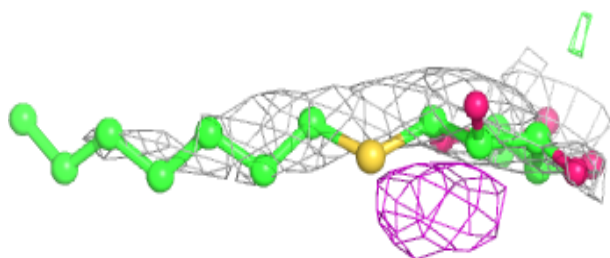
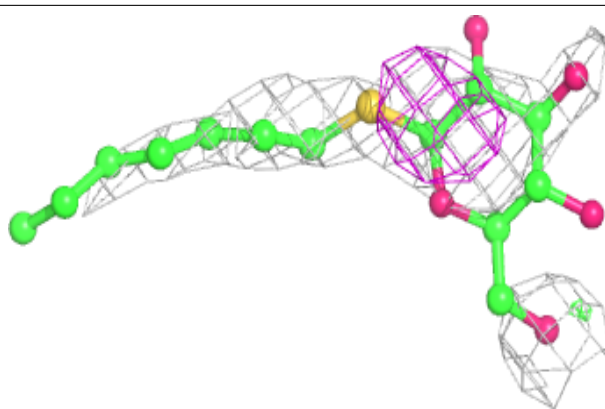
**Electron density around UNL a 415:**

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

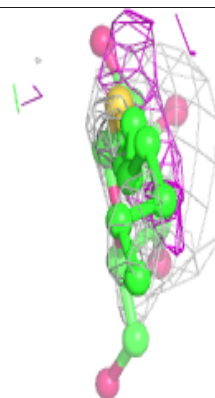
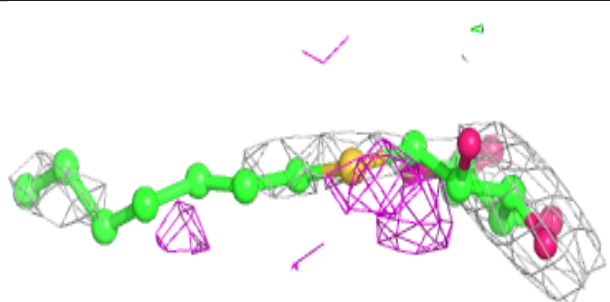
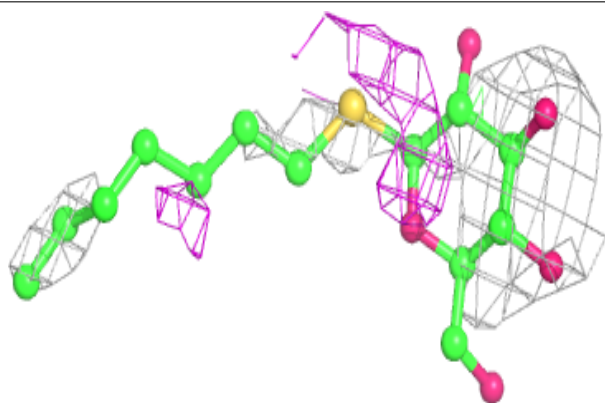


**Electron density around HTG b 623:**

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

**Electron density around HTG B 624:**

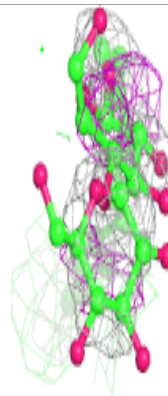
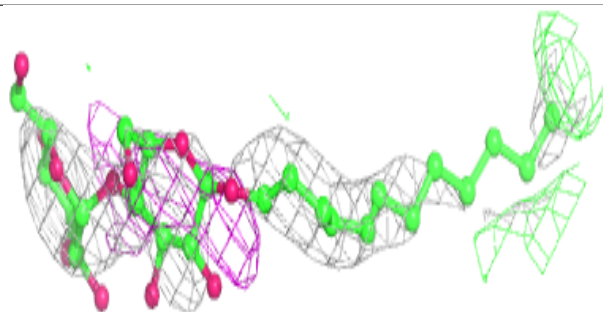
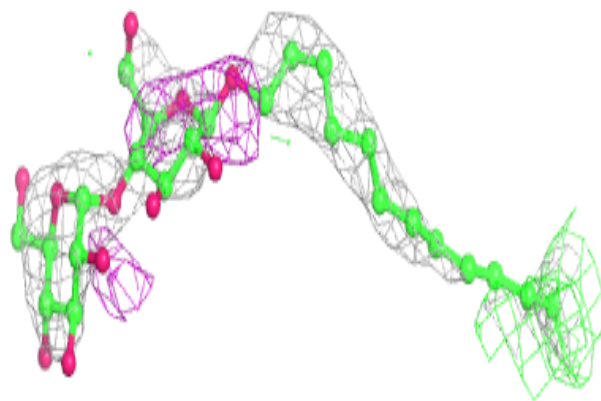
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



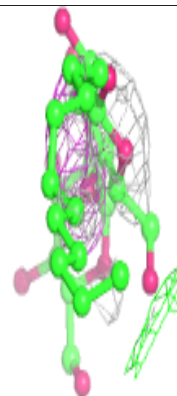
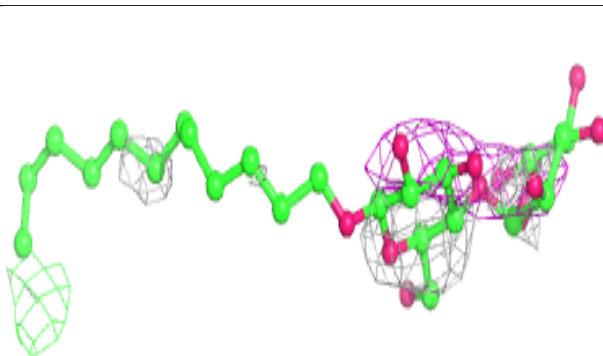
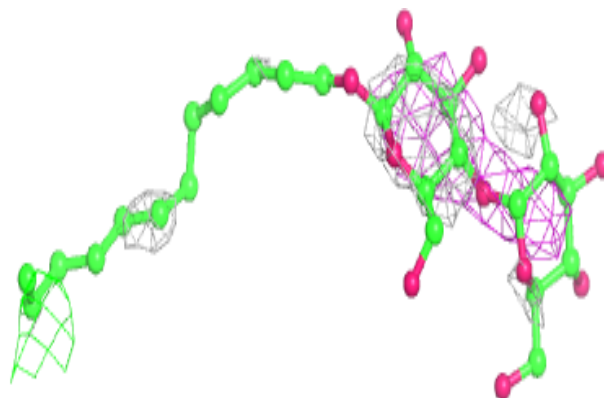


**Electron density around LMT D 402:**

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

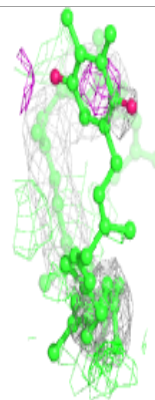
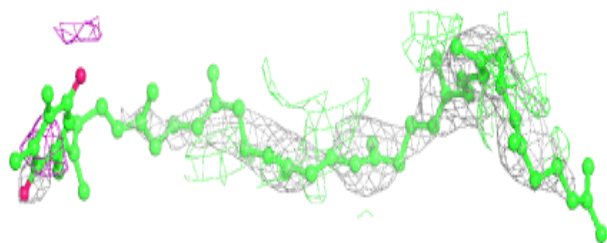
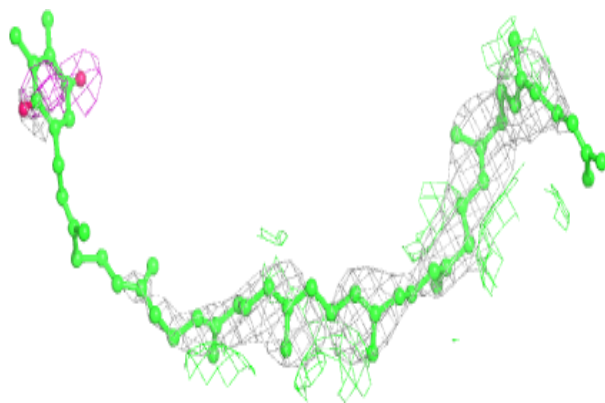
**Electron density around LMT e 102:**

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

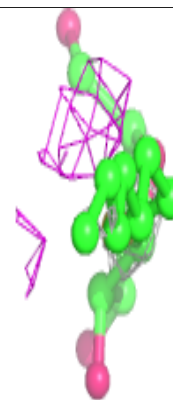
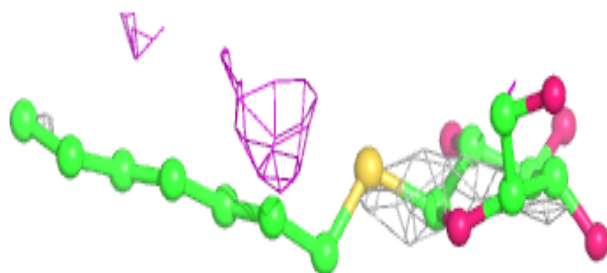
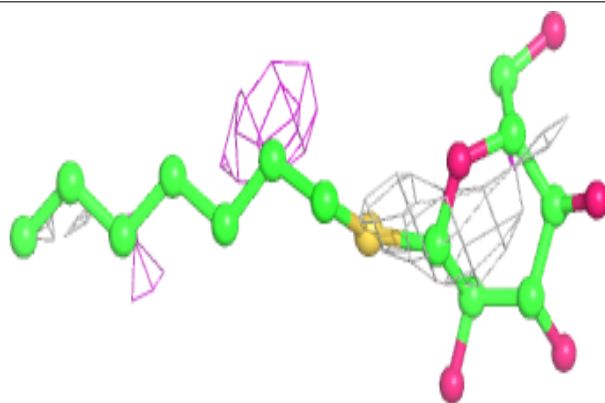


**Electron density around PL9 a 414:**

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

**Electron density around HTG C 522:**

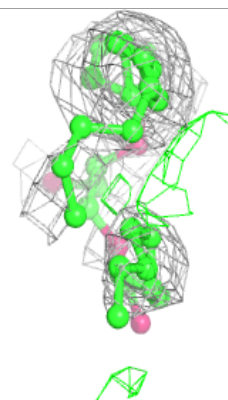
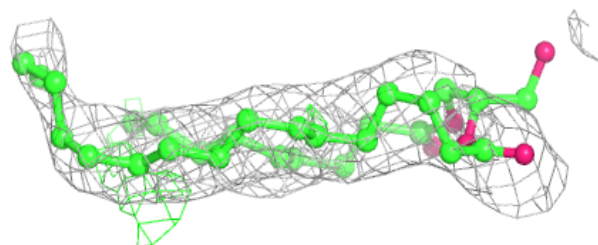
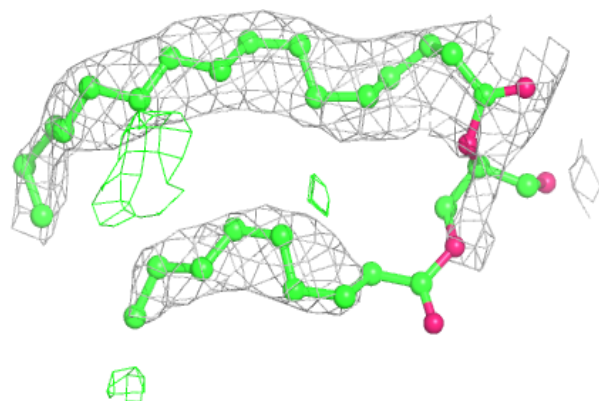
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



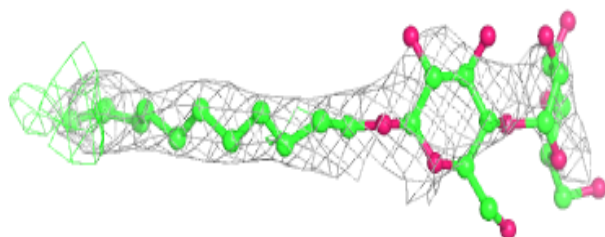
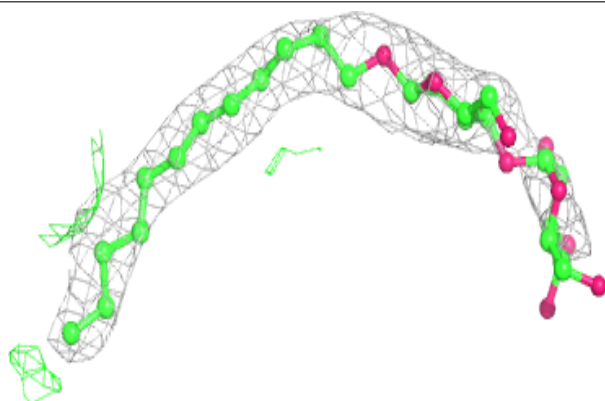


**Electron density around UNL B 628:**

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

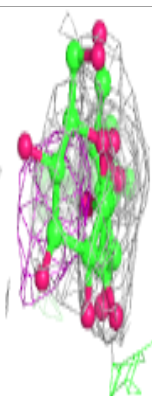
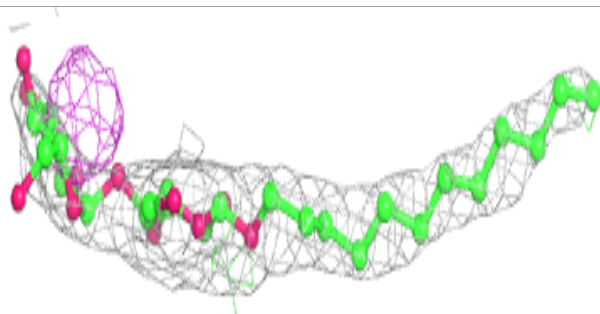
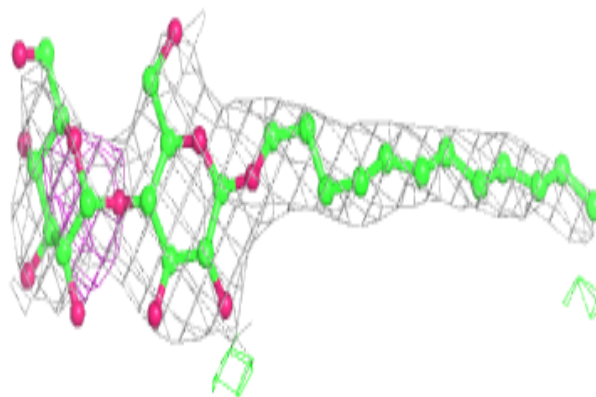
**Electron density around LMT M 103:**

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

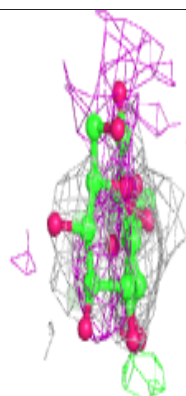
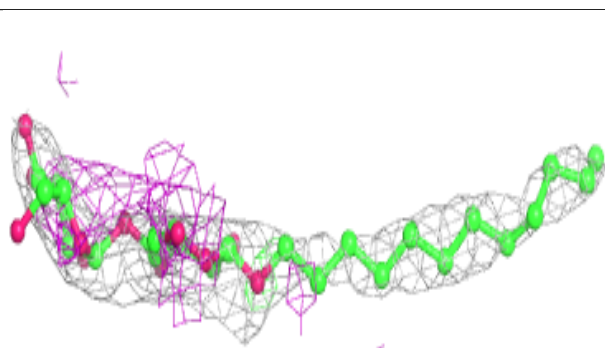
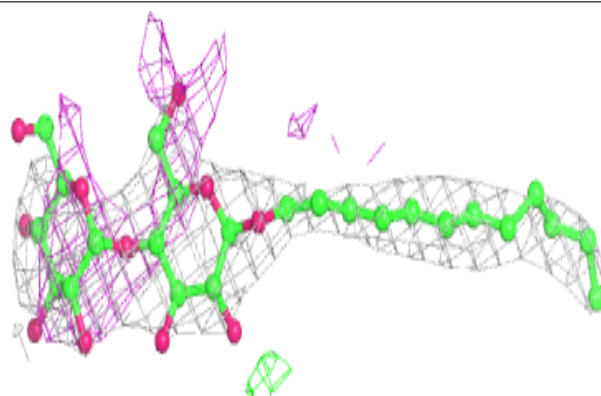


**Electron density around LMT M 101:**

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

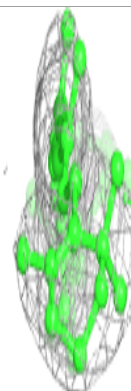
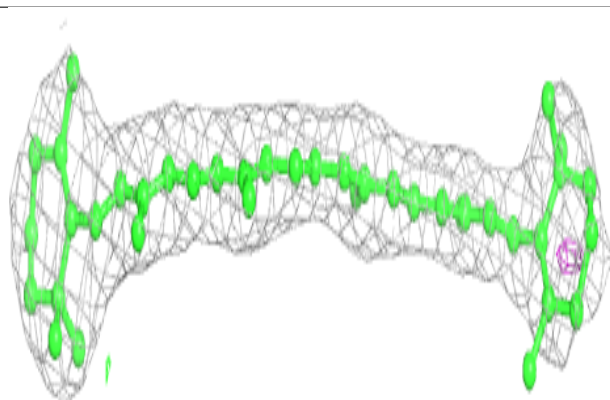
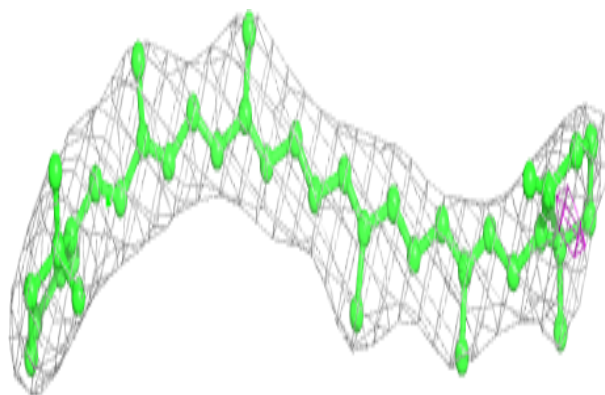
**Electron density around LMT m 102:**

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

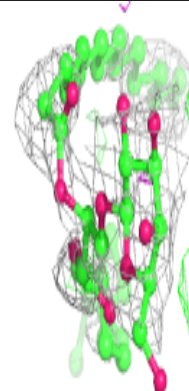
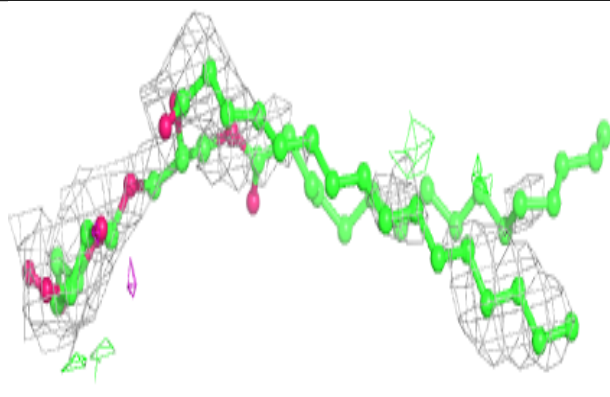
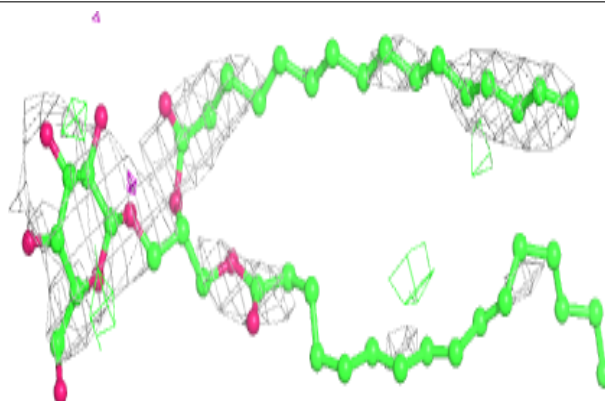


**Electron density around BCR h 101:**

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

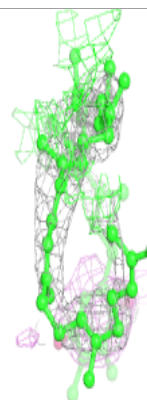
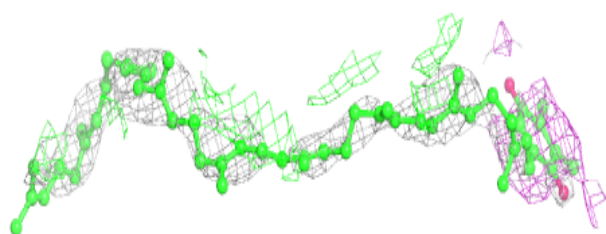
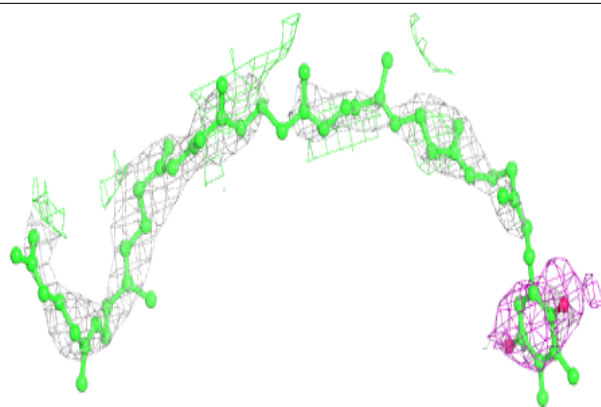
**Electron density around LMG c 520:**

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

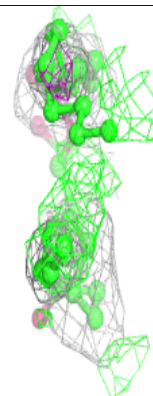
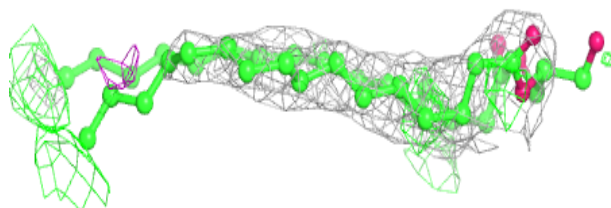
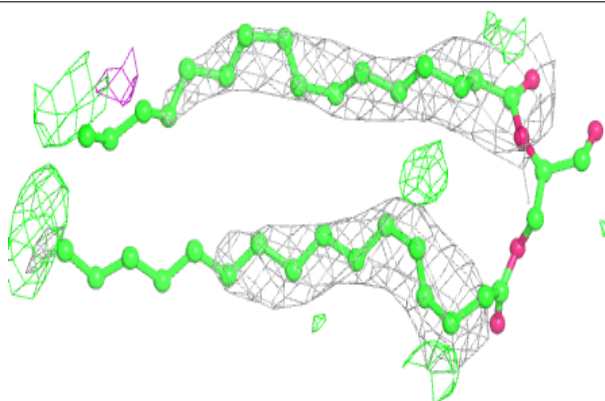


**Electron density around PL9 A 414:**

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

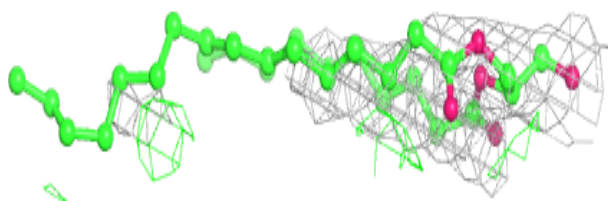
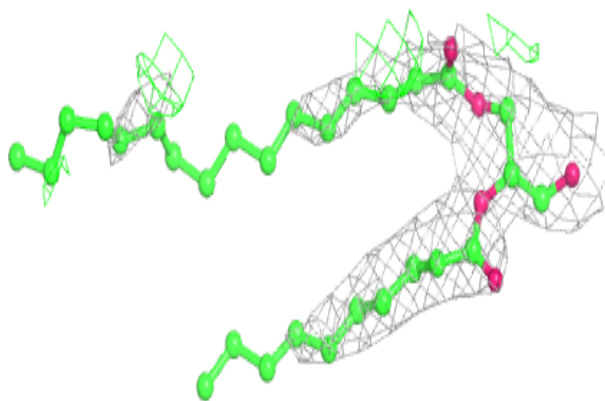
**Electron density around UNL i 101:**

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

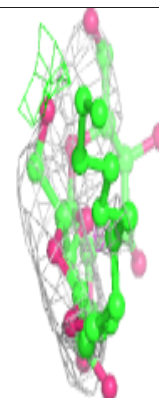
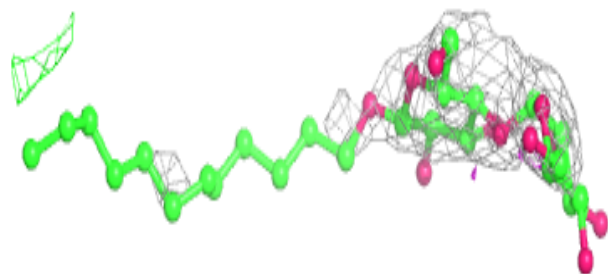
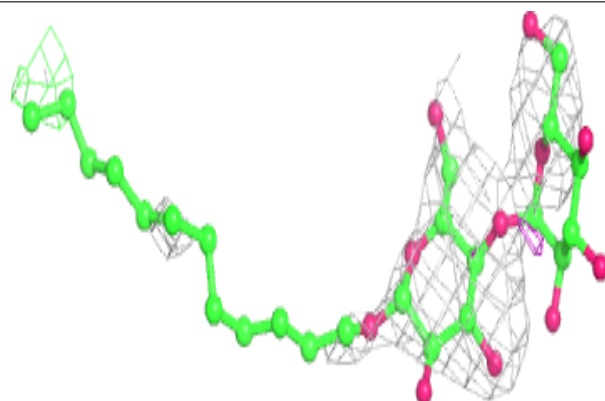


**Electron density around UNL K 101:**

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

**Electron density around LMT E 102:**

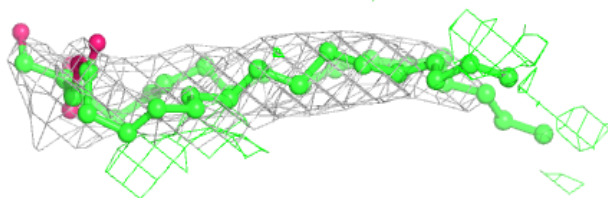
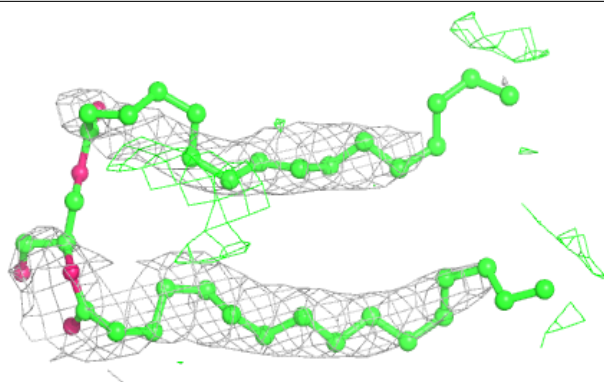
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



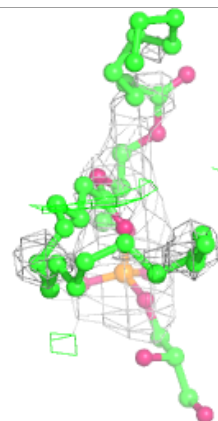
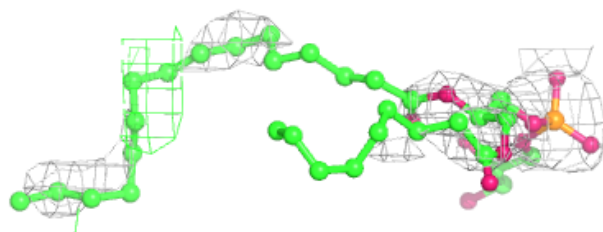
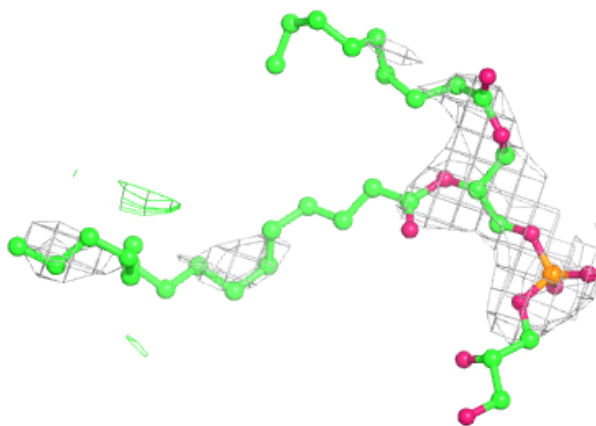


**Electron density around UNL I 102:**

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

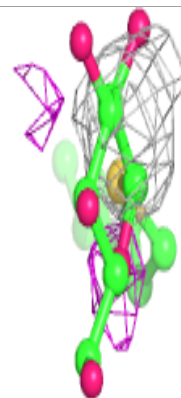
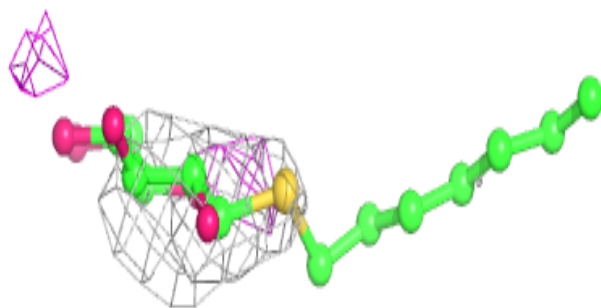
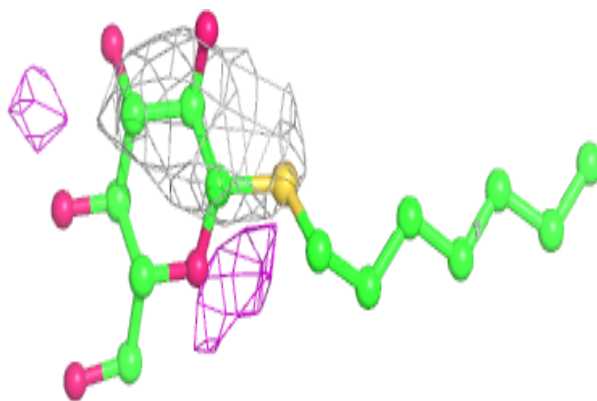
**Electron density around LHG e 101:**

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

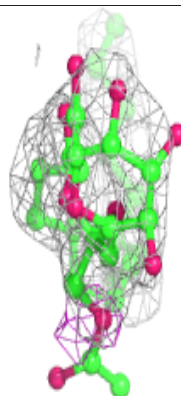
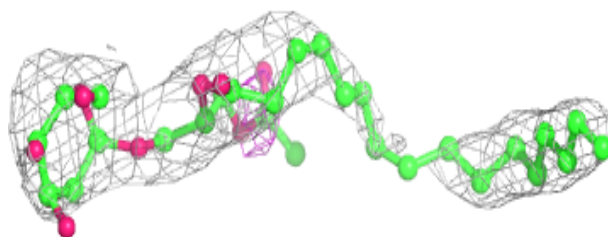
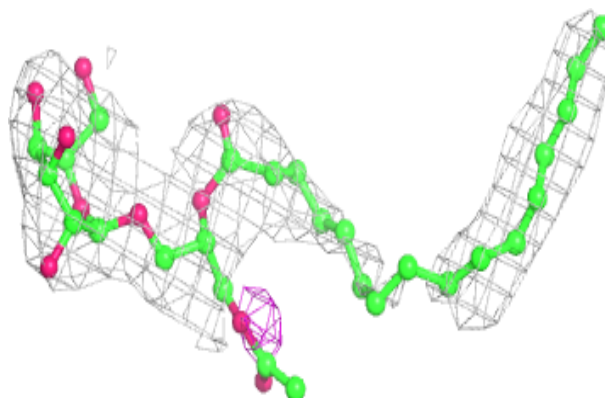


**Electron density around HTG c 522:**

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

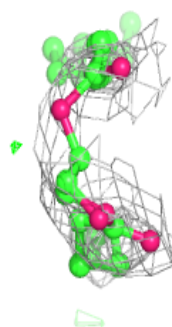
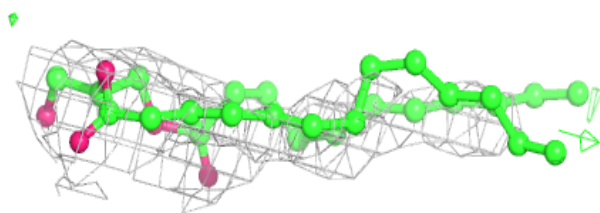
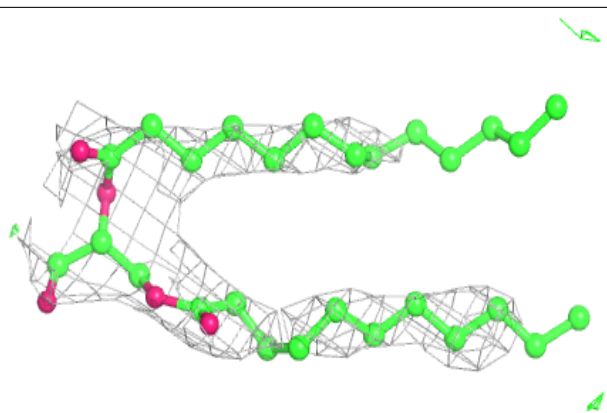
**Electron density around LMG Z 102:**

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

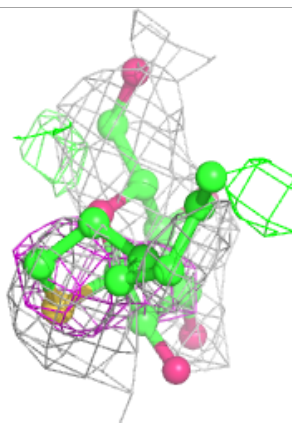
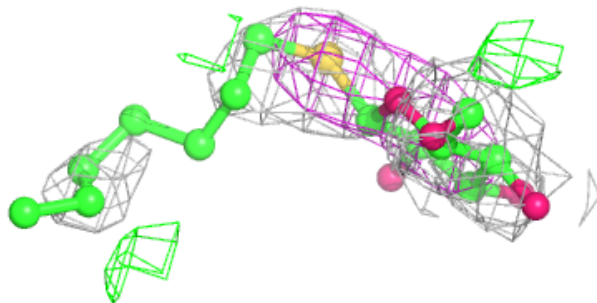
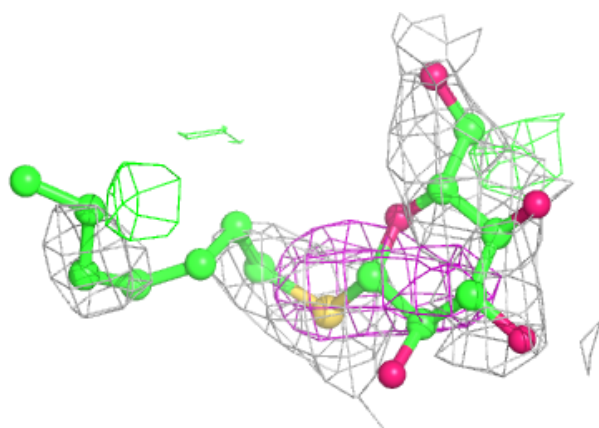


**Electron density around UNL c 525:**

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

**Electron density around HTG B 623:**

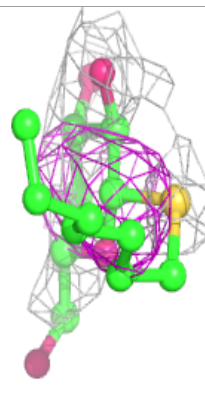
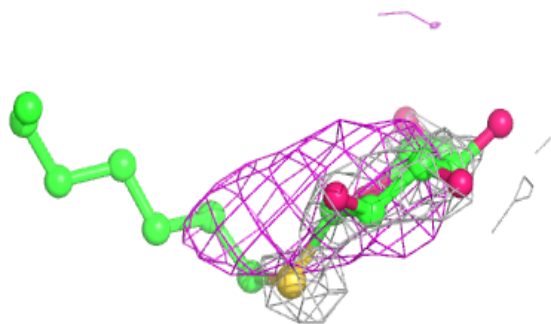
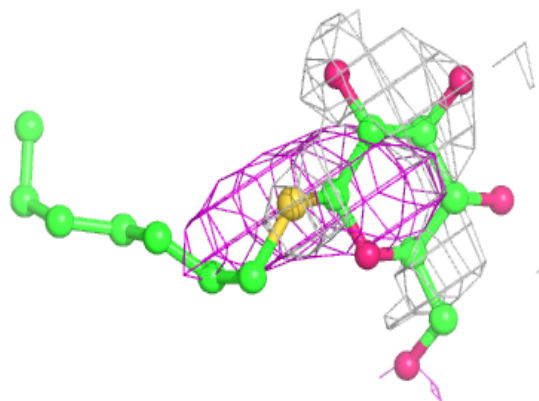
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



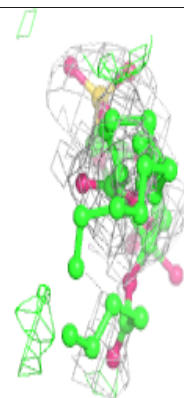
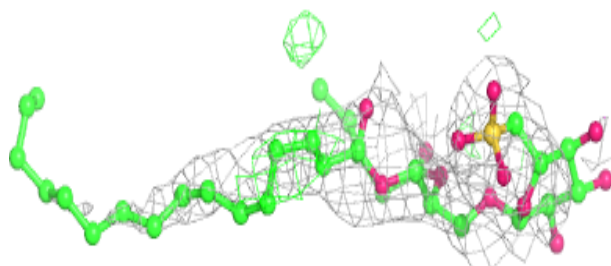
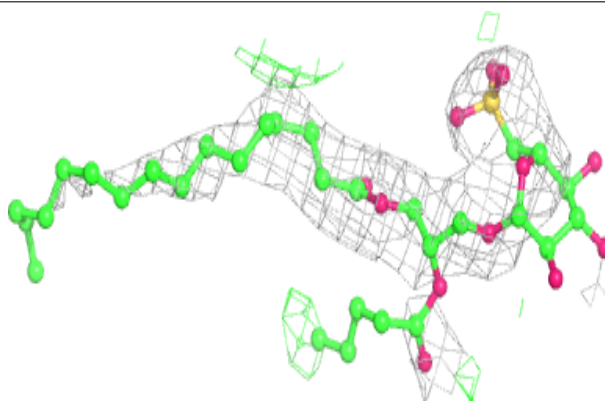


**Electron density around HTG b 622:**

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

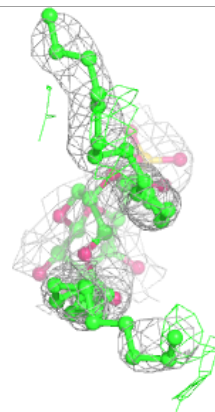
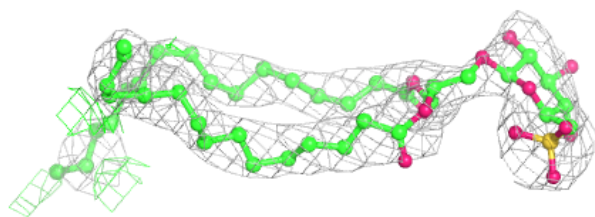
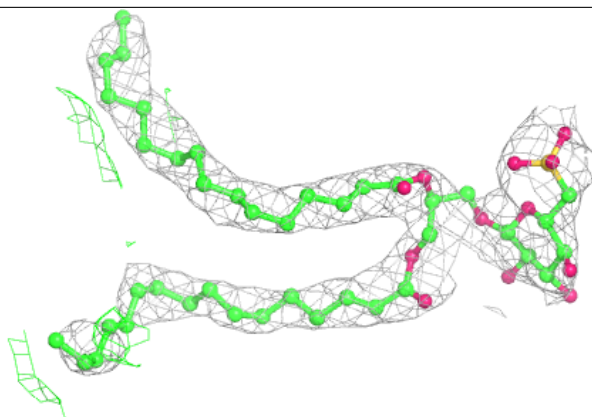
**Electron density around SQD f 101:**

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

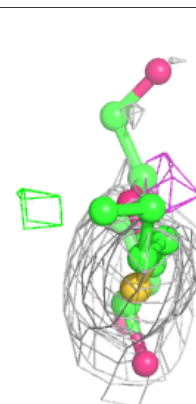
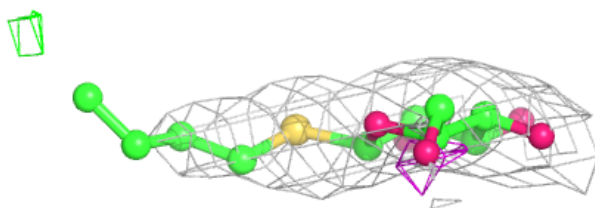
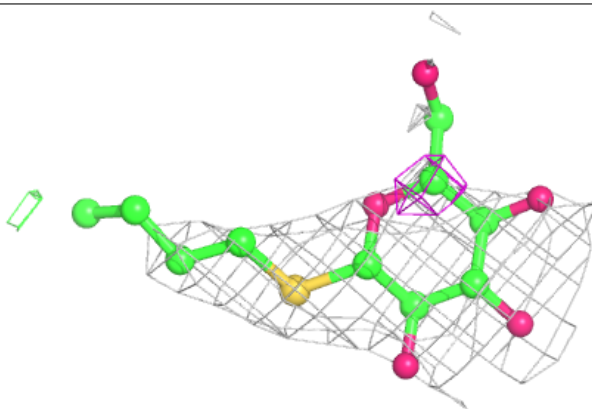


**Electron density around SQD L 101:**

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

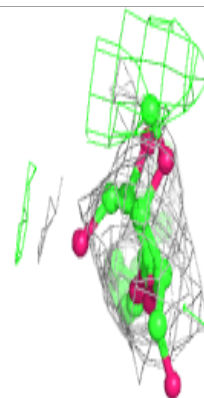
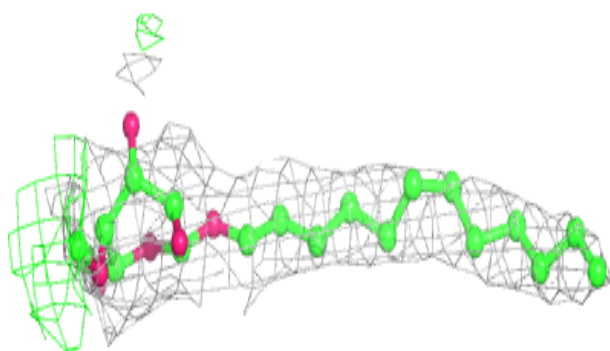
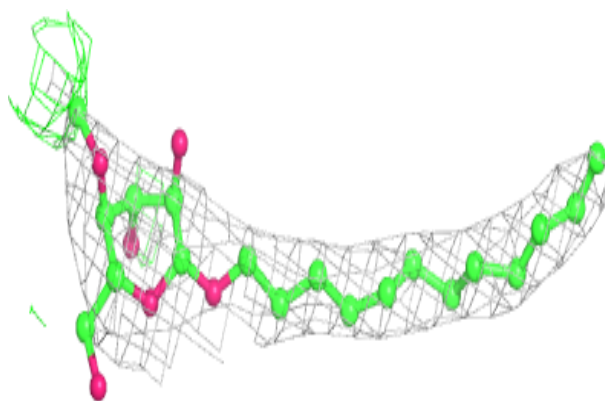
**Electron density around HTG d 411:**

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

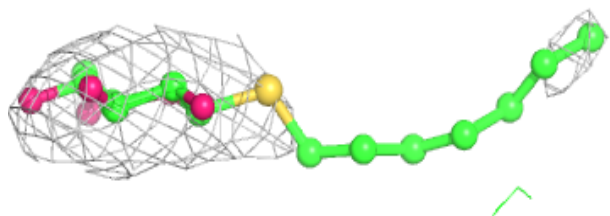
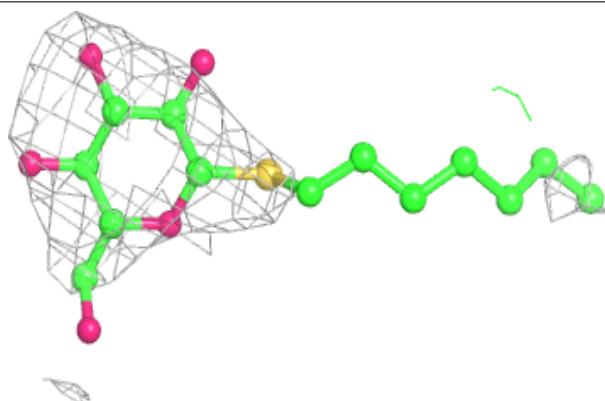


**Electron density around LMT b 621:**

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

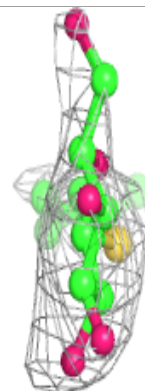
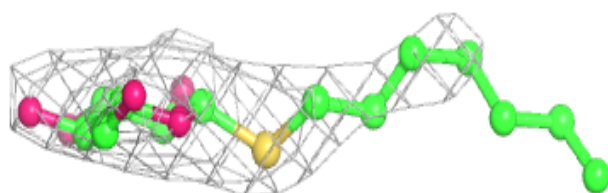
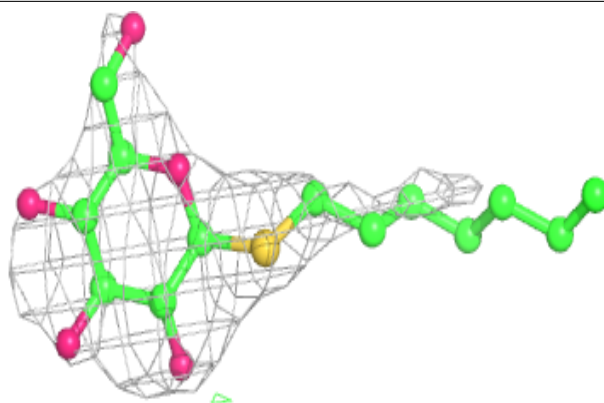
**Electron density around HTG c 521:**

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

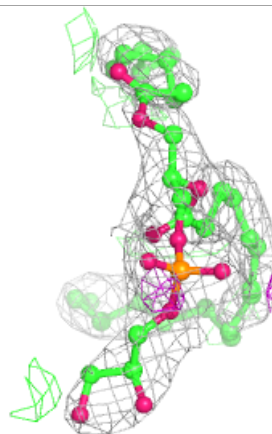
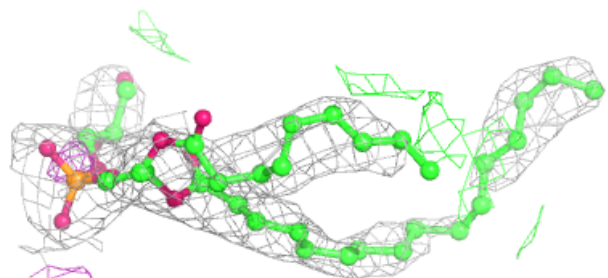
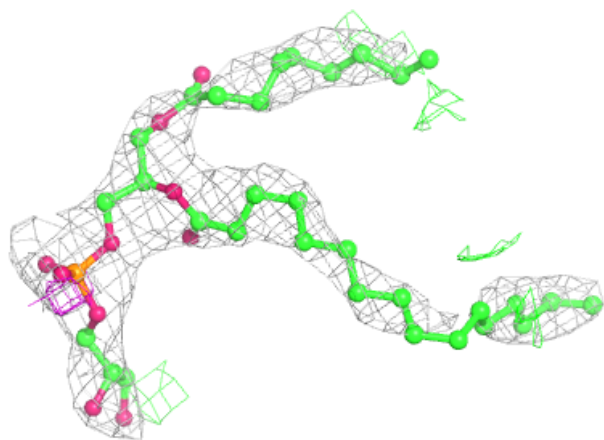


**Electron density around HTG C 521:**

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

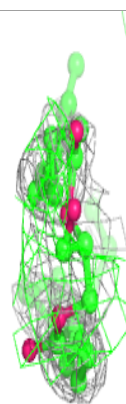
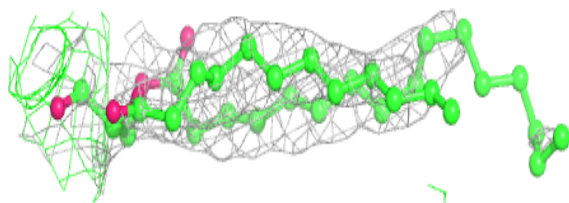
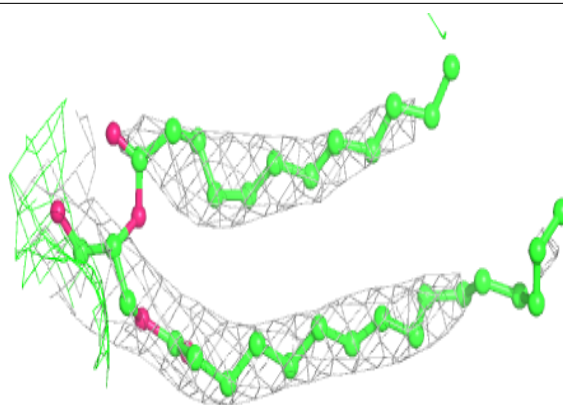
**Electron density around LHG E 101:**

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

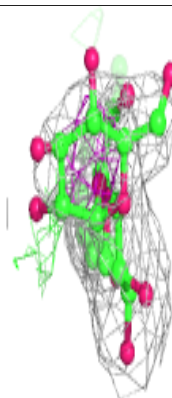
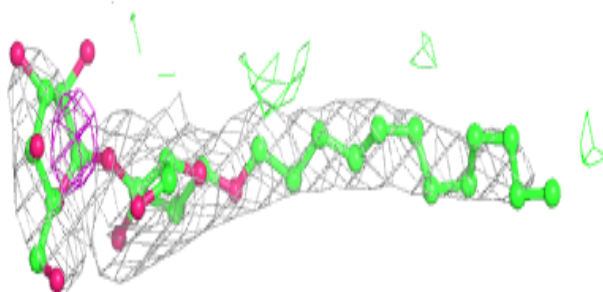
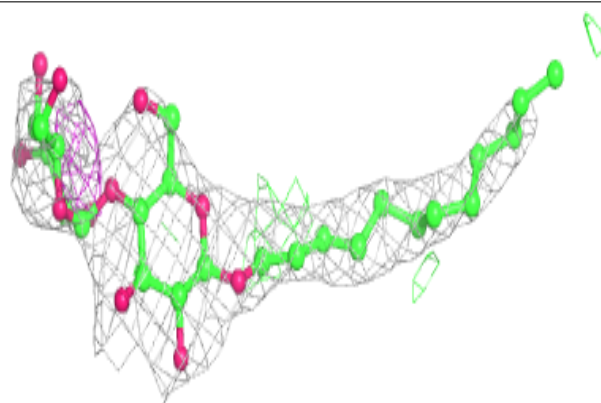


**Electron density around UNL b 629:**

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

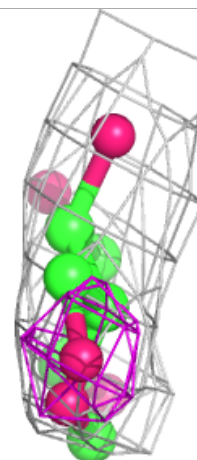
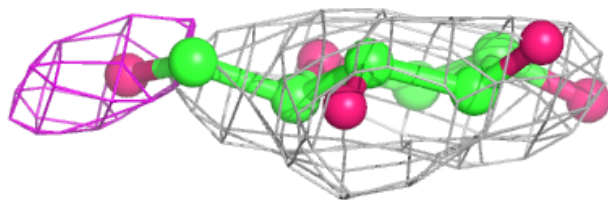
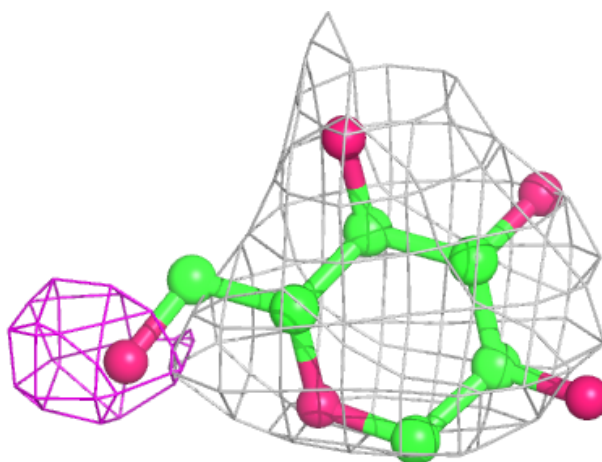
**Electron density around LMT D 403:**

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



**Electron density around HTG V 203:**

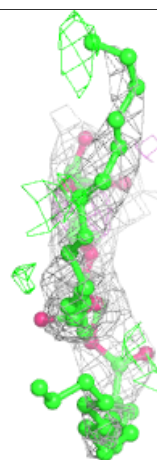
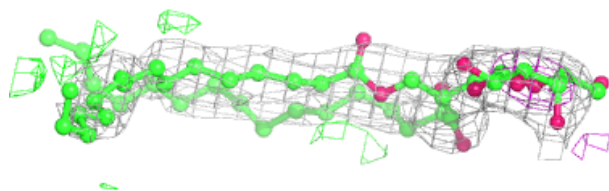
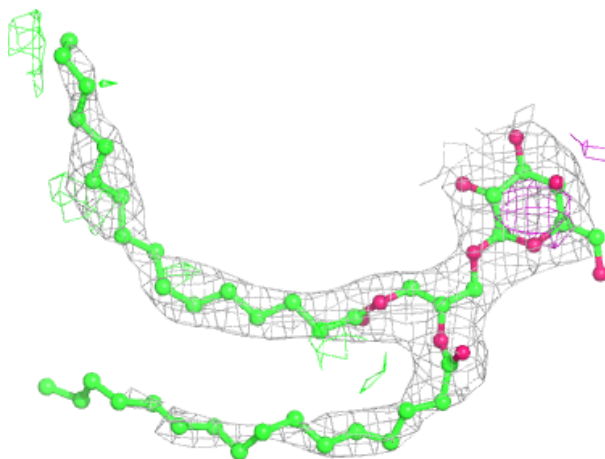
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





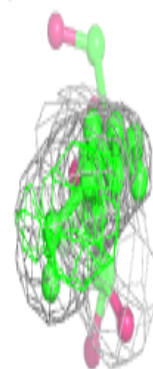
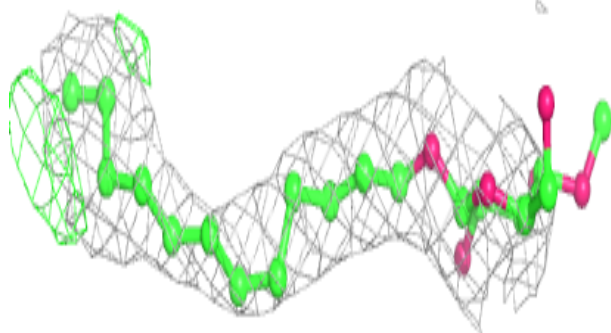
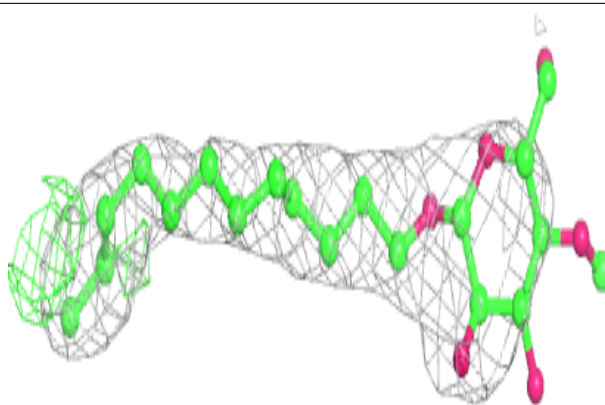
**Electron density around LMG C 520:**

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

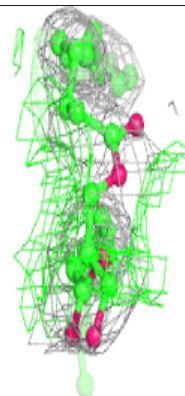
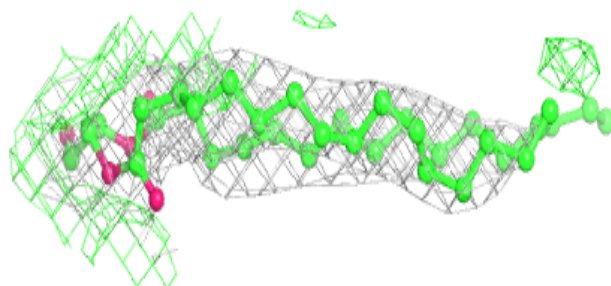
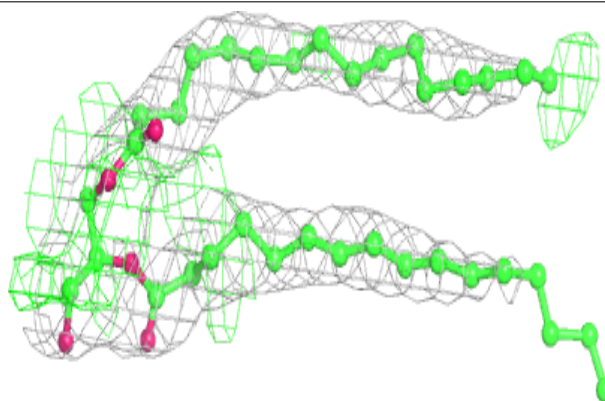


**Electron density around LMT b 627:**

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

**Electron density around UNL D 411:**

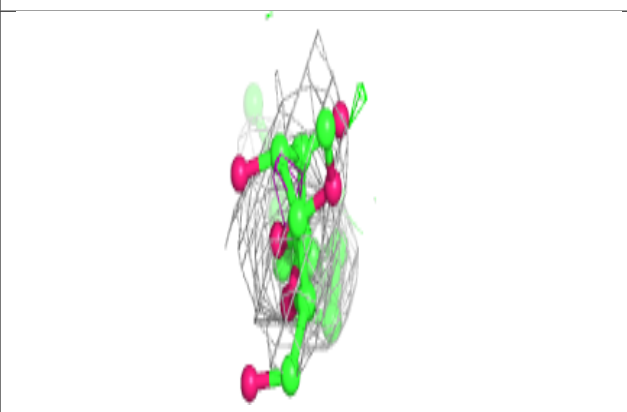
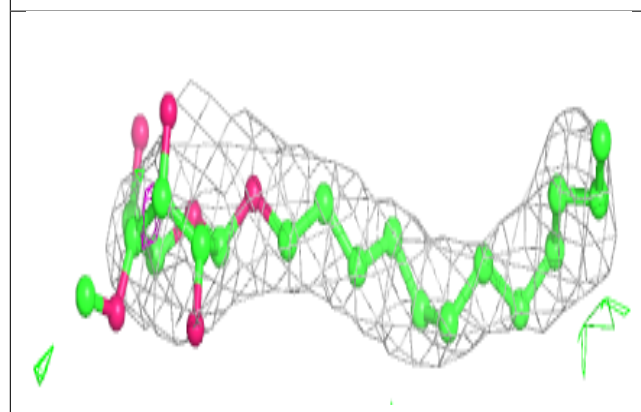
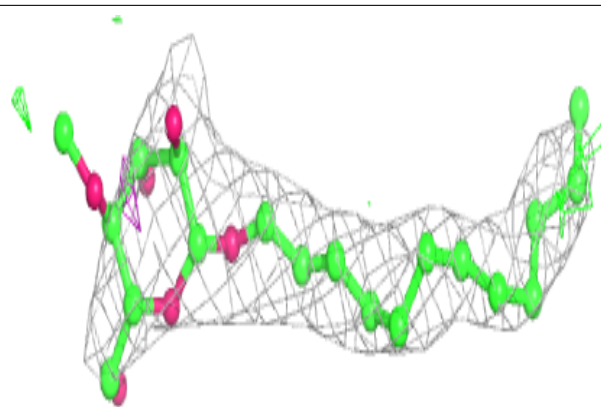
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



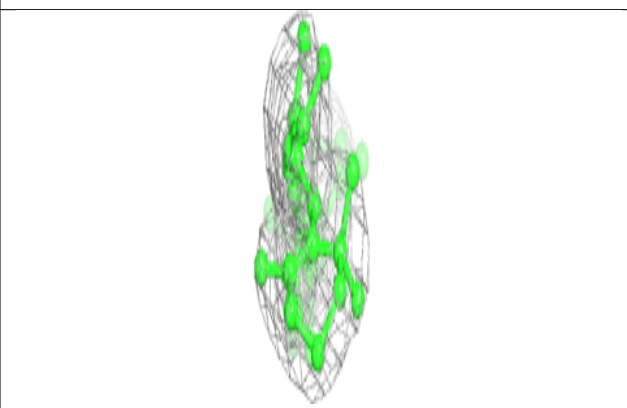
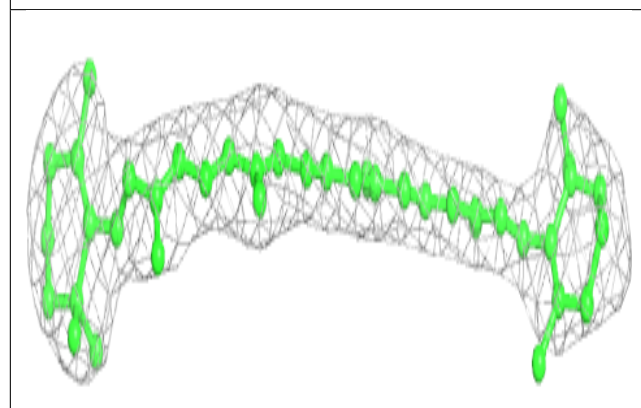
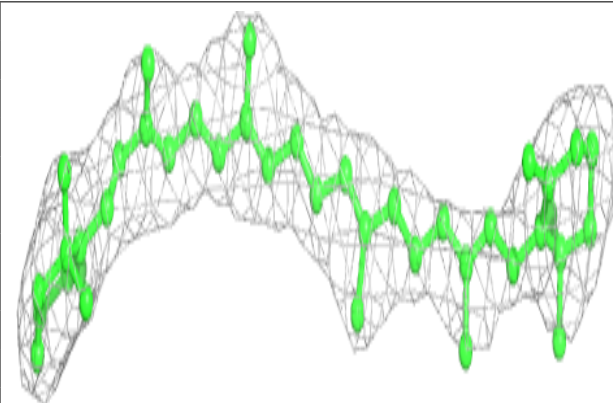


**Electron density around LMT B 629:**

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

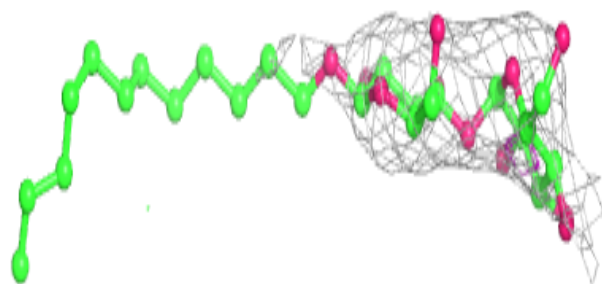
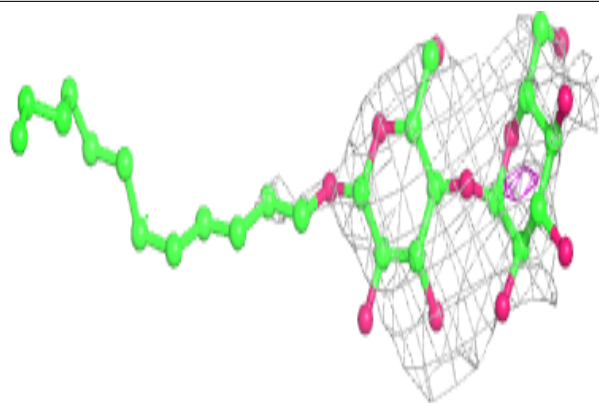
**Electron density around BCR H 101:**

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

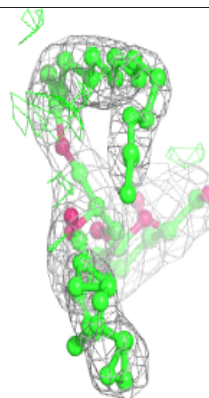
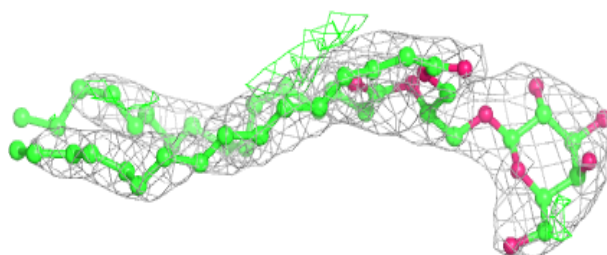
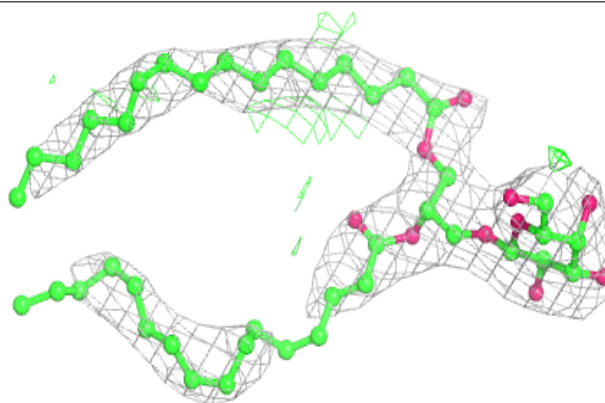


**Electron density around LMT a 417:**

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

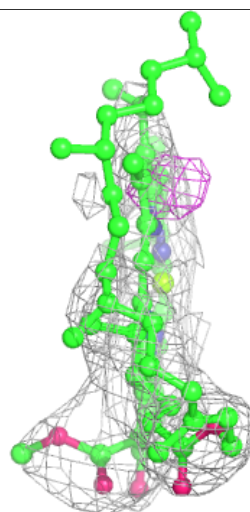
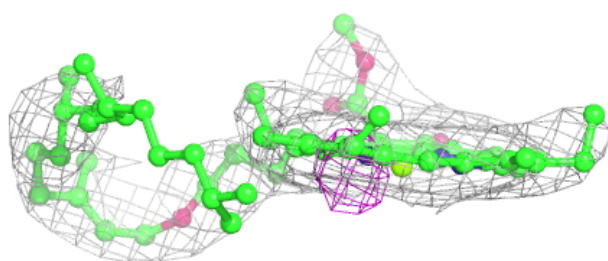
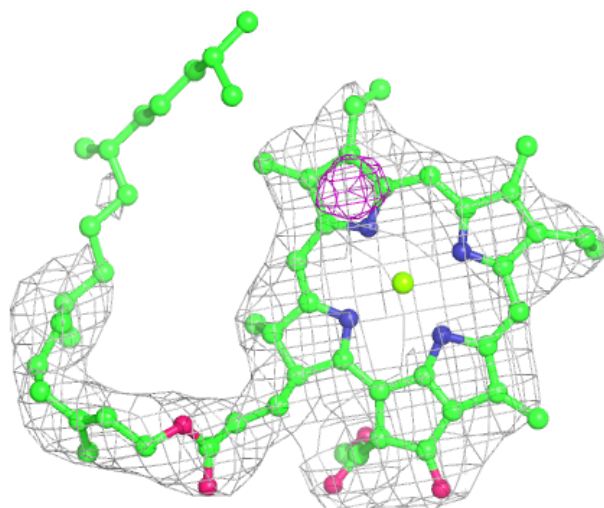
**Electron density around LMG C 501:**

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



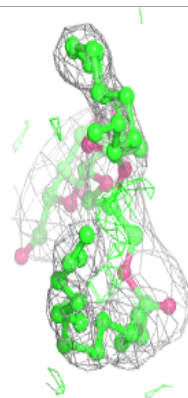
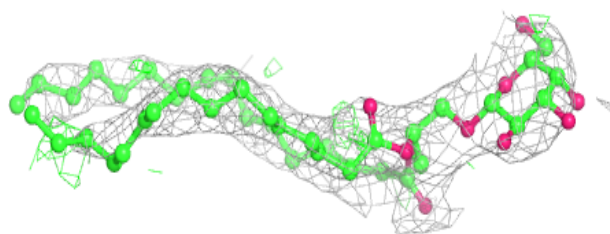
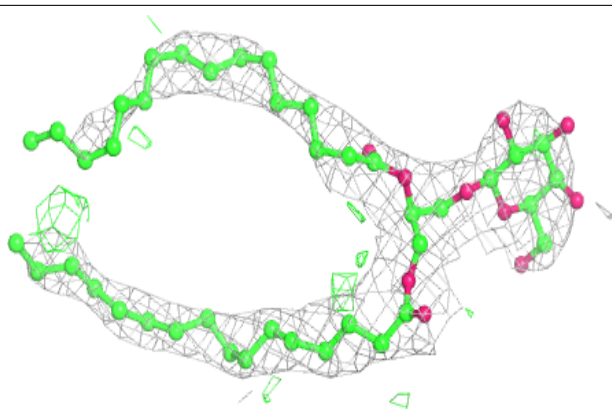
**Electron density around CLA C 513:**

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

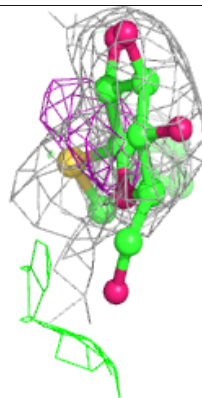
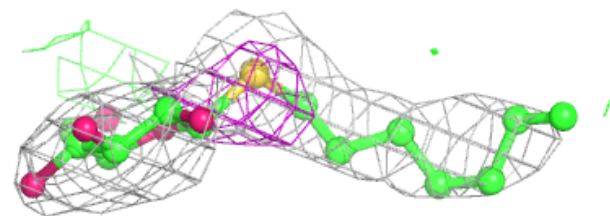
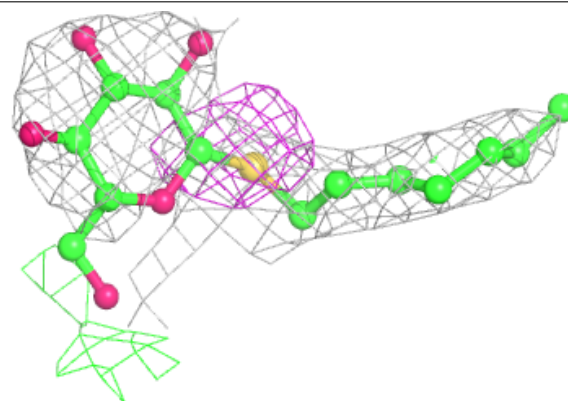


**Electron density around LMG a 416:**

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

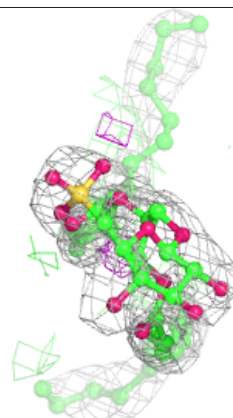
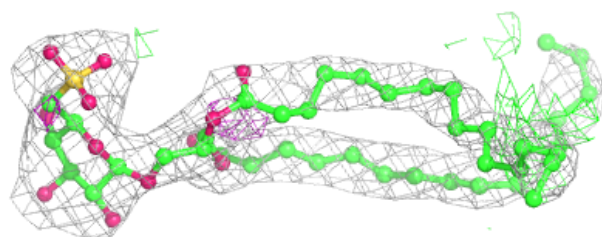
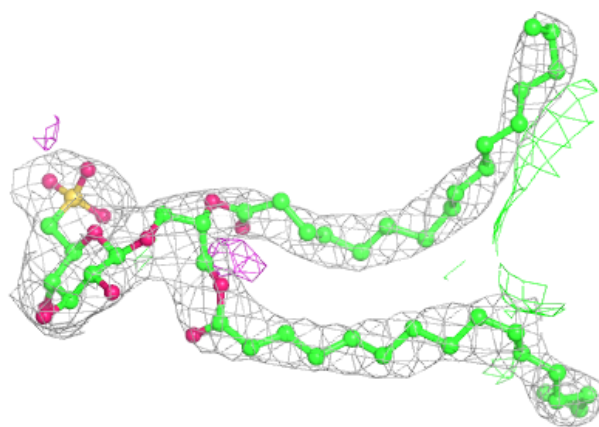
**Electron density around HTG b 628:**

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

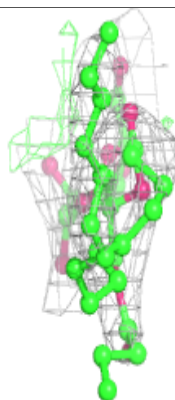
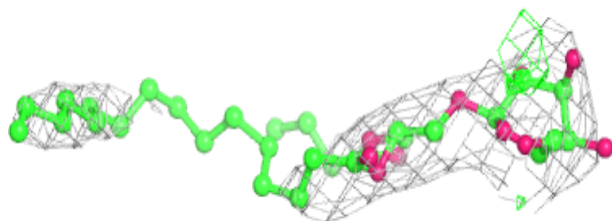
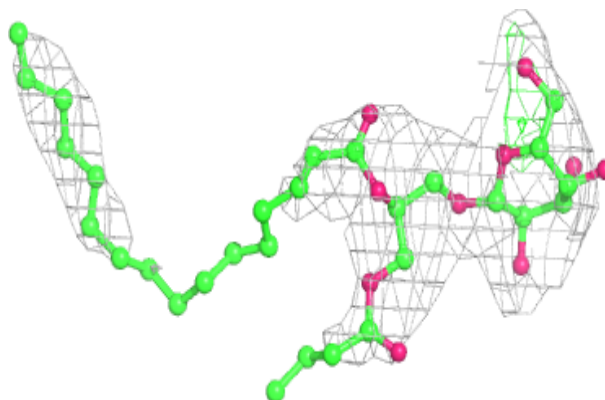


**Electron density around SQD B 620:**

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

**Electron density around LMG z 101:**

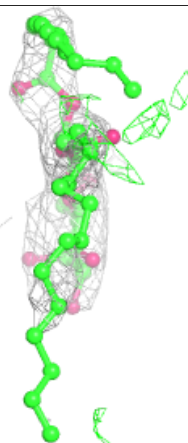
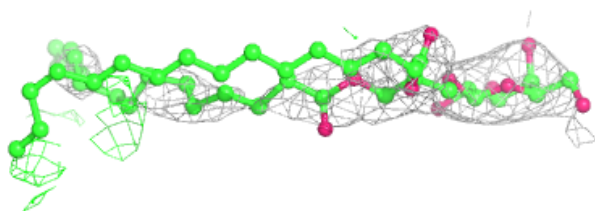
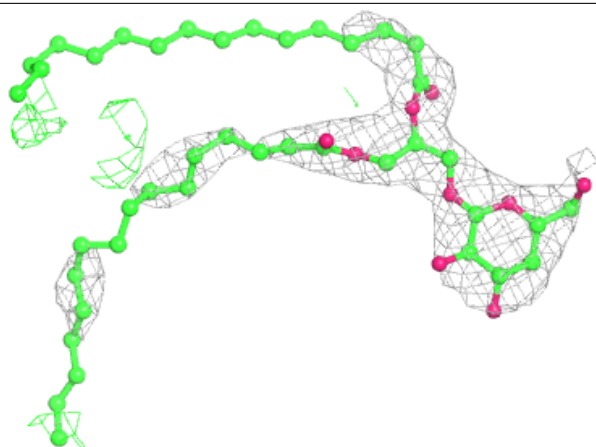
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



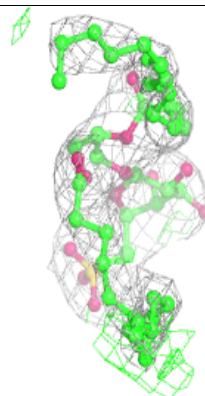
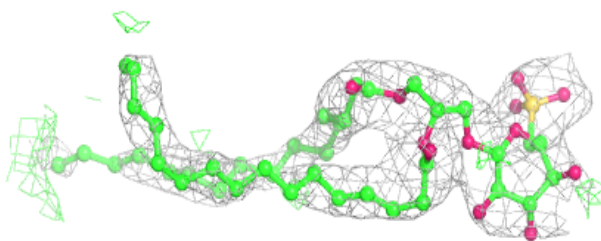
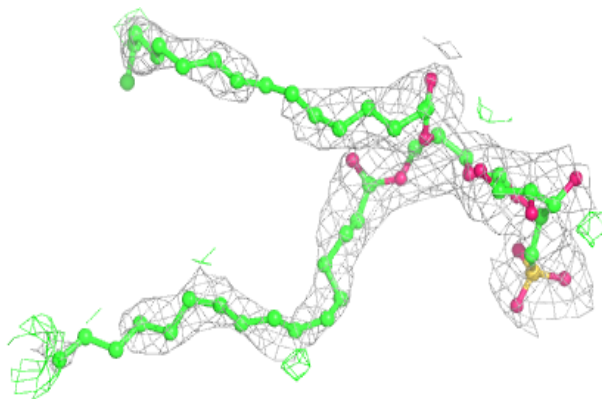


**Electron density around LMG c 519:**

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

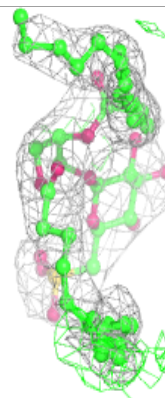
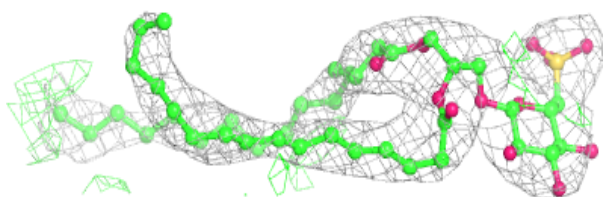
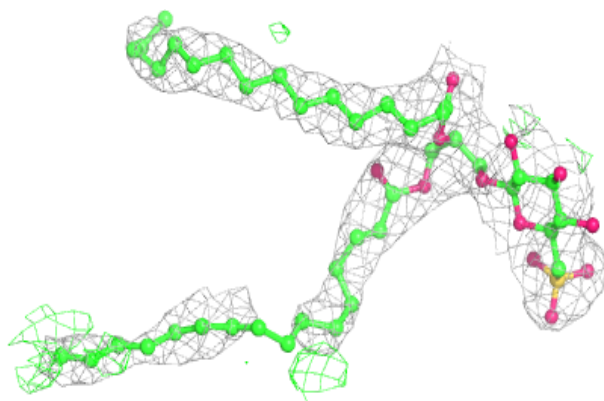
**Electron density around SQD a 412:**

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

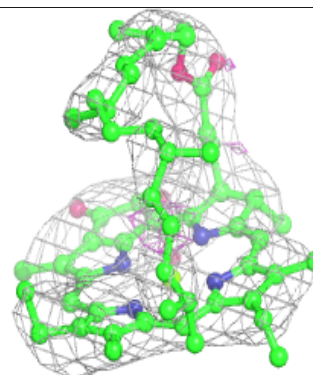
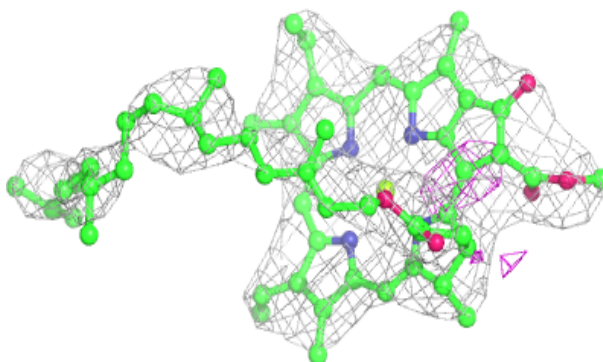
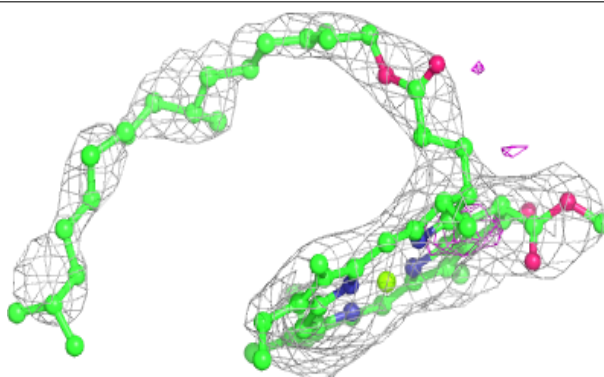


**Electron density around SQD A 412:**

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

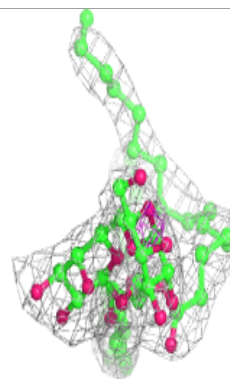
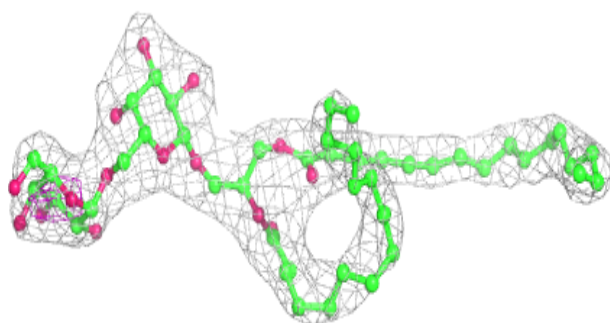
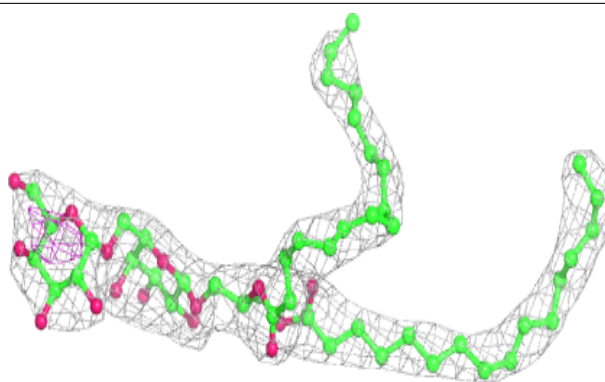
**Electron density around CLA C 514:**

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

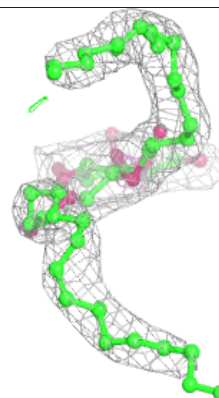
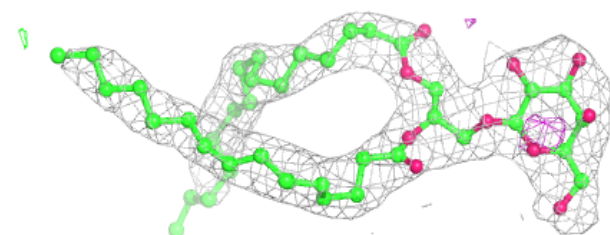
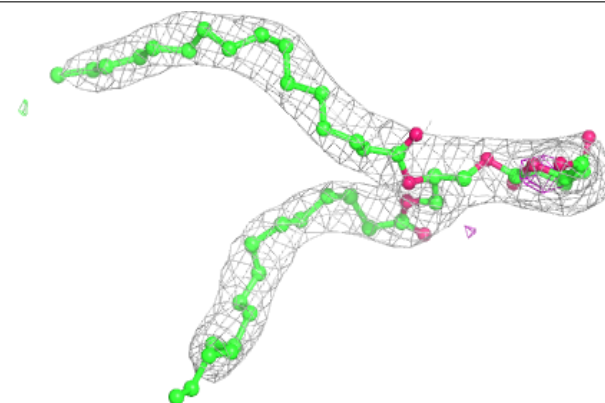


**Electron density around DGD h 102:**

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

**Electron density around LMG B 621:**

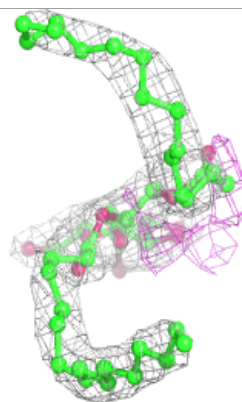
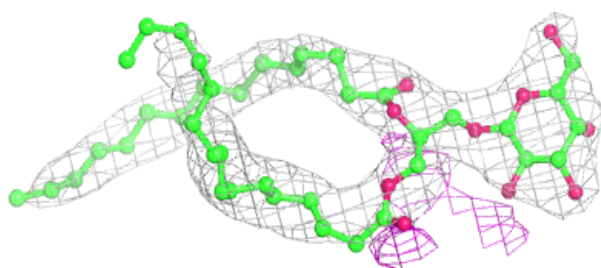
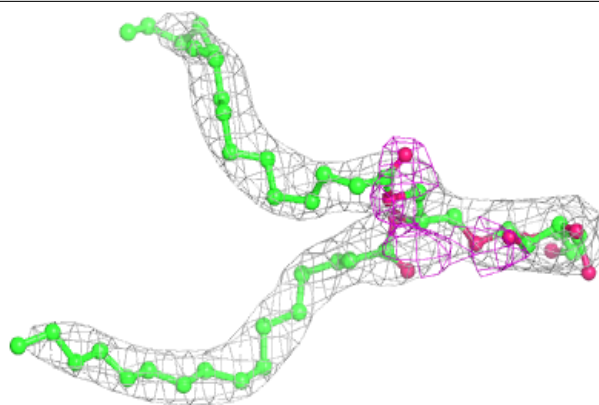
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



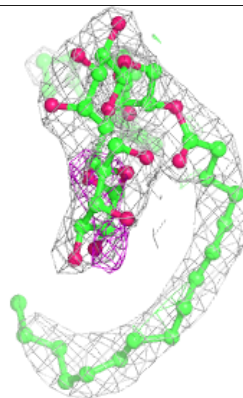
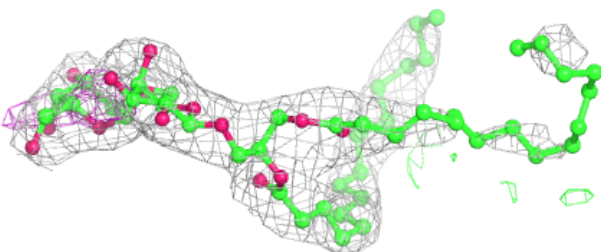
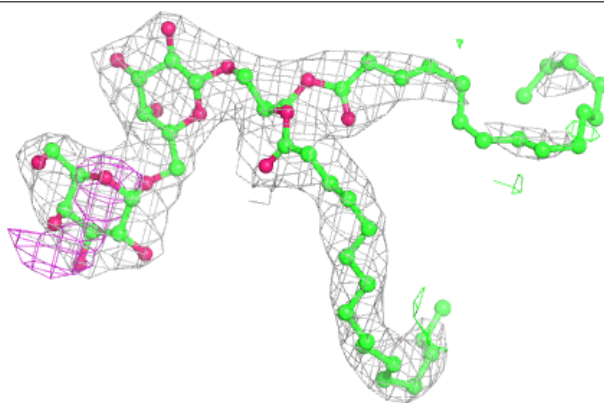


**Electron density around LMG b 620:**

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

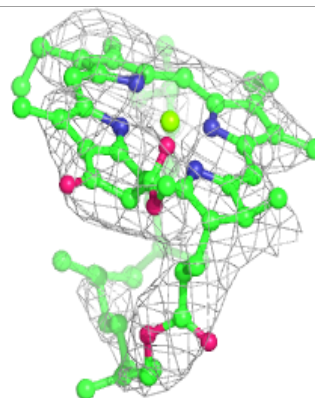
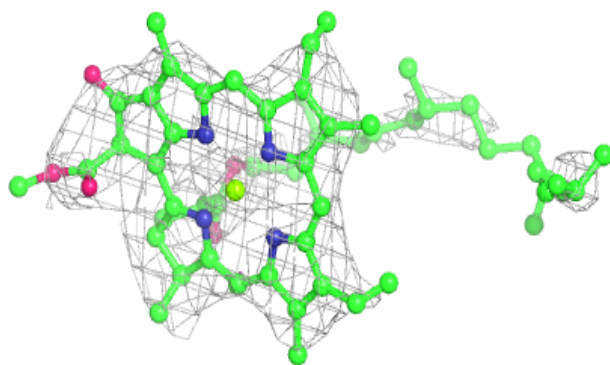
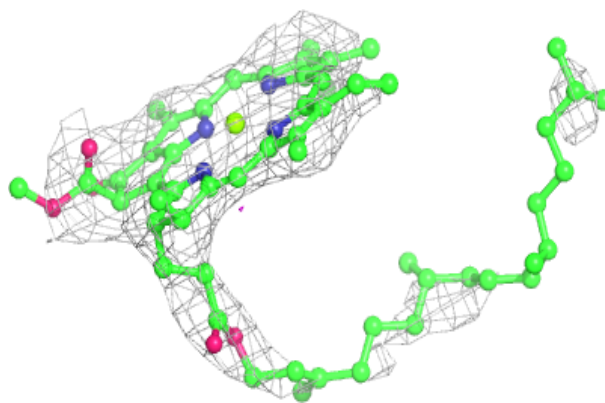
**Electron density around DGD C 518:**

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

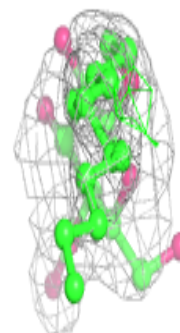
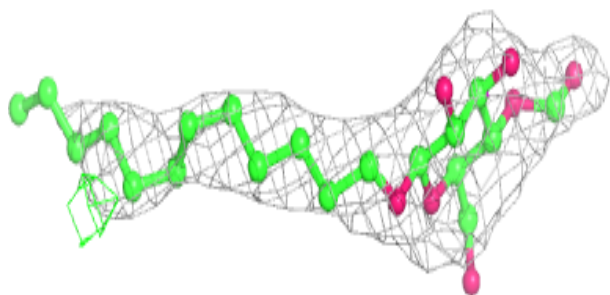
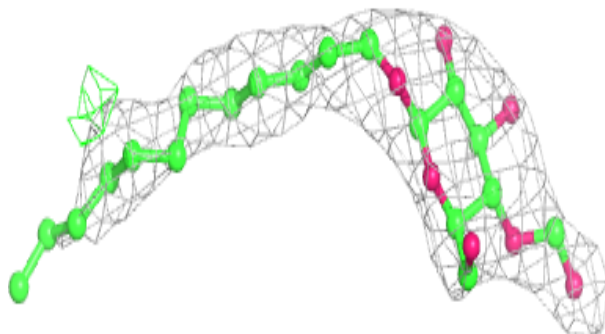


**Electron density around CLA c 513:**

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

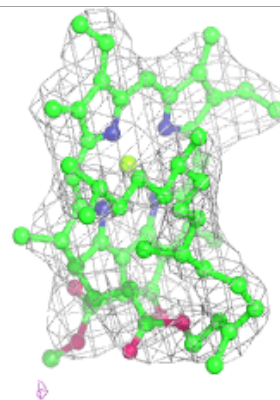
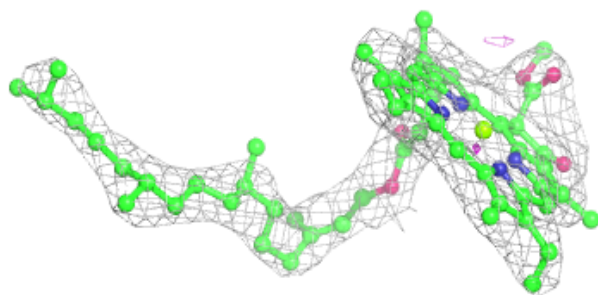
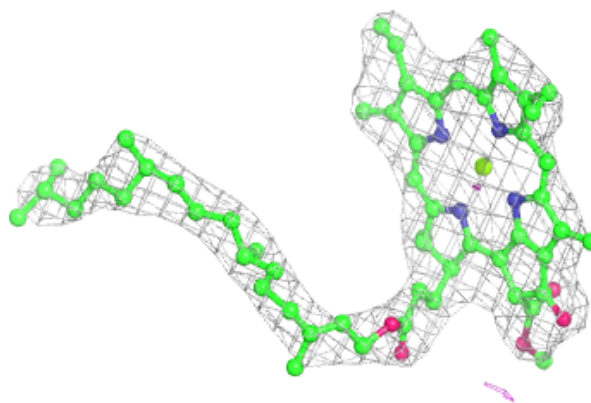
**Electron density around LMT B 631:**

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



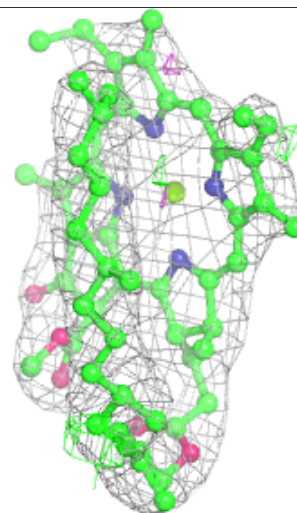
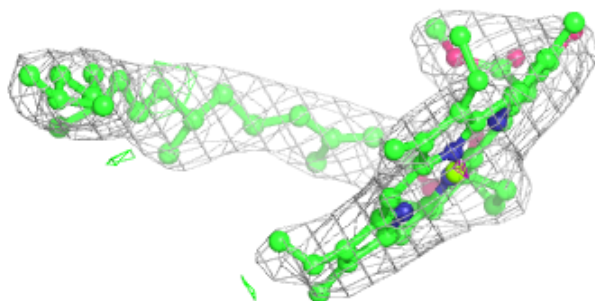
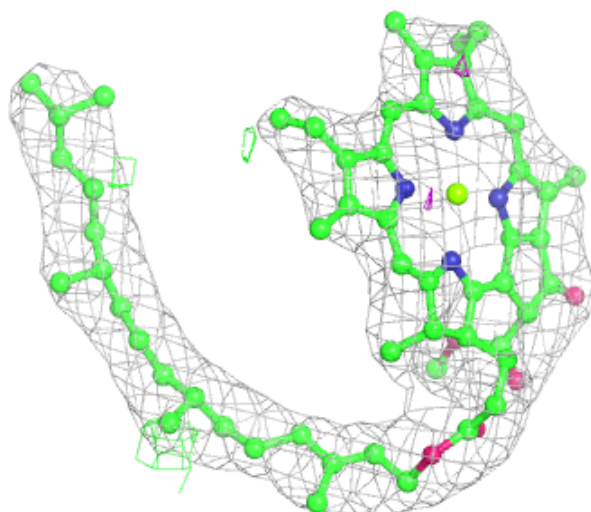
**Electron density around CLA C 512:**

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



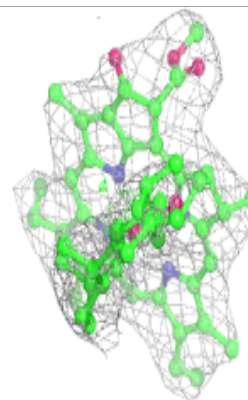
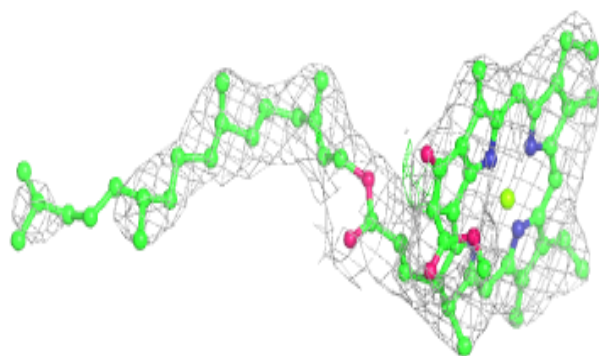
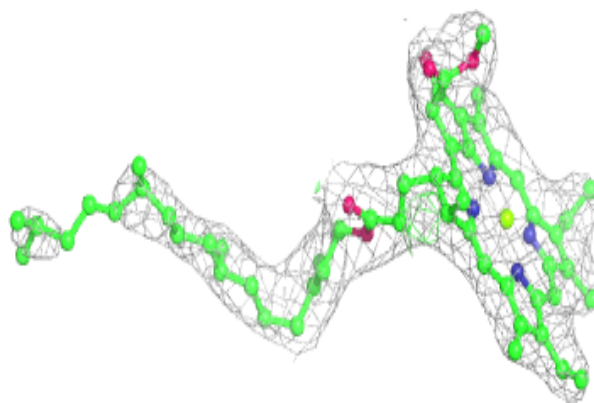
**Electron density around CLA C 508:**

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



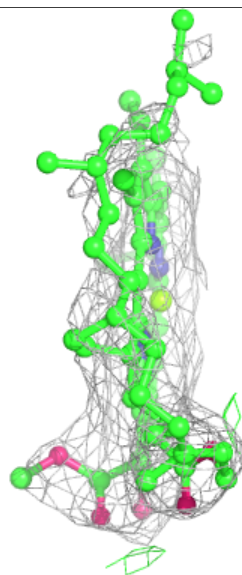
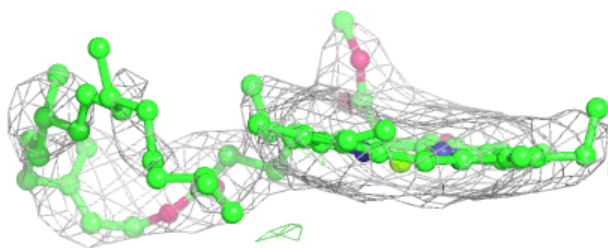
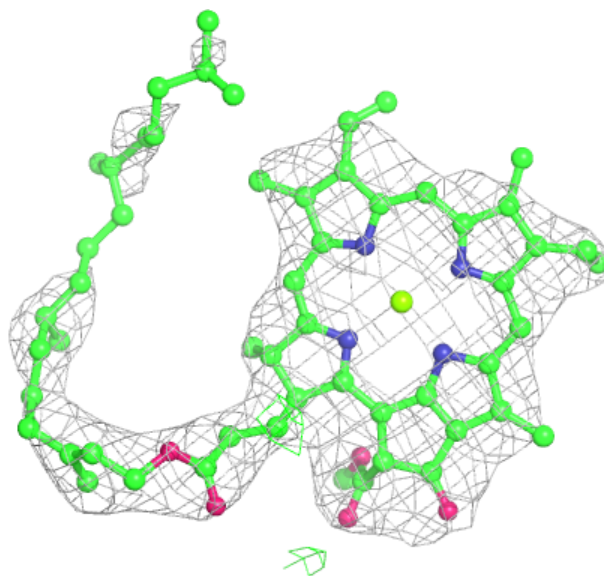
**Electron density around CLA c 502:**

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



**Electron density around CLA c 512:**

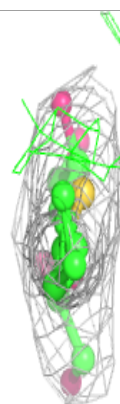
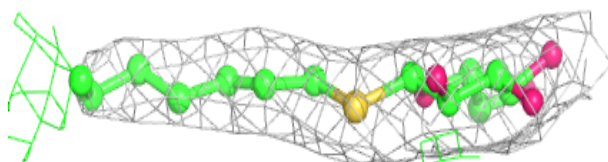
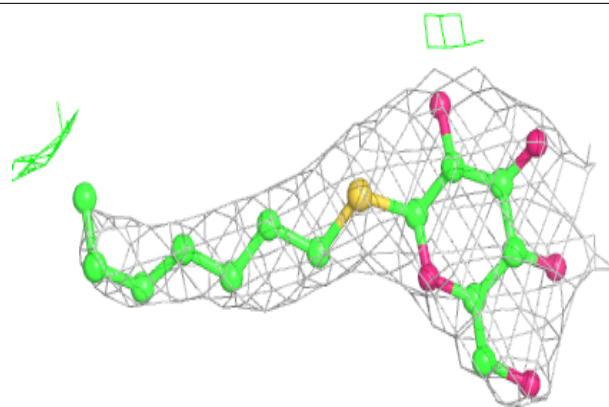
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



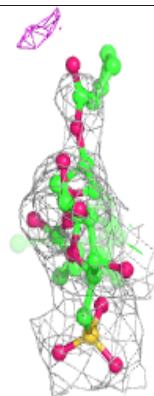
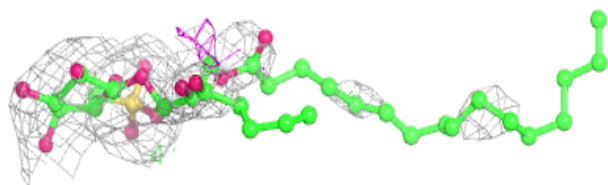
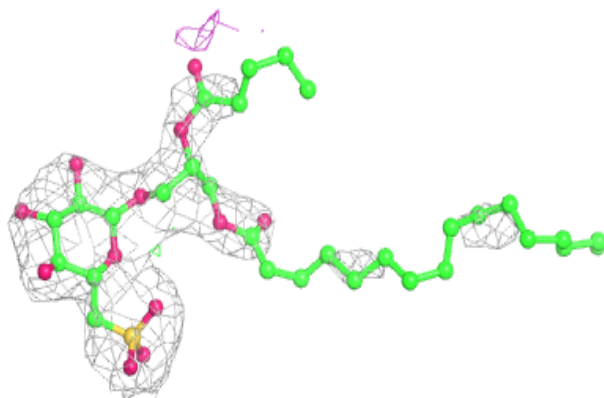


**Electron density around HTG B 627:**

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

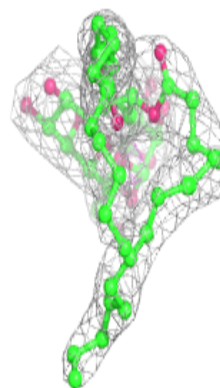
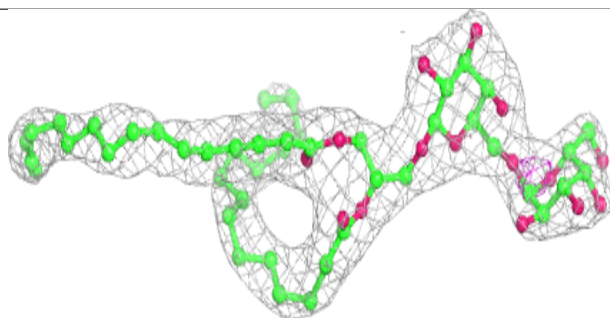
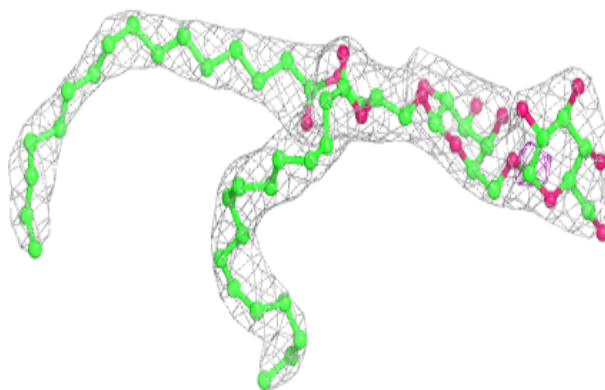
**Electron density around SQD D 413:**

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

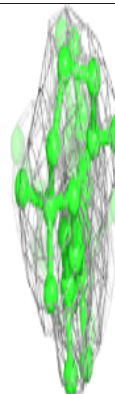
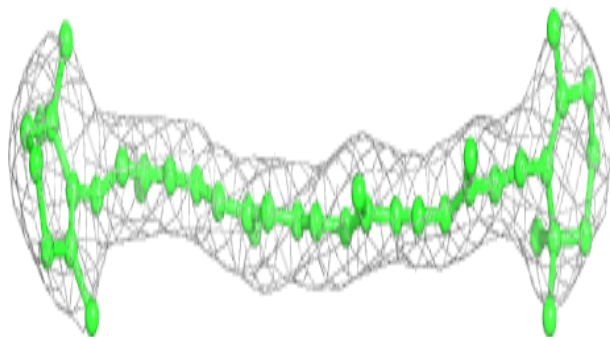
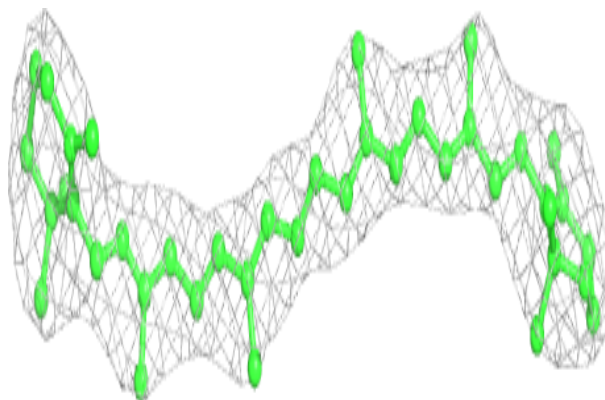


**Electron density around DGD H 102:**

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

**Electron density around BCR y 101:**

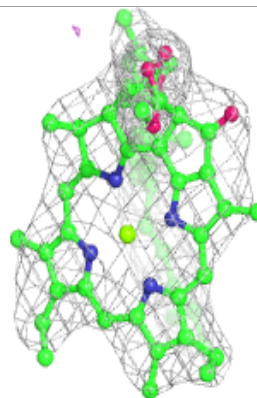
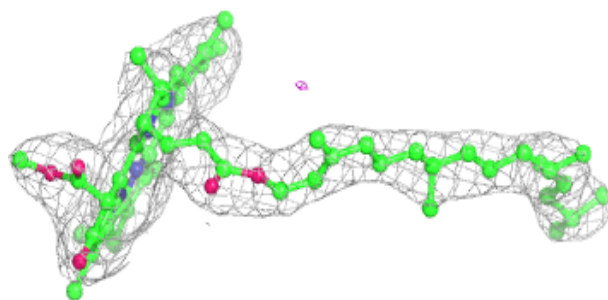
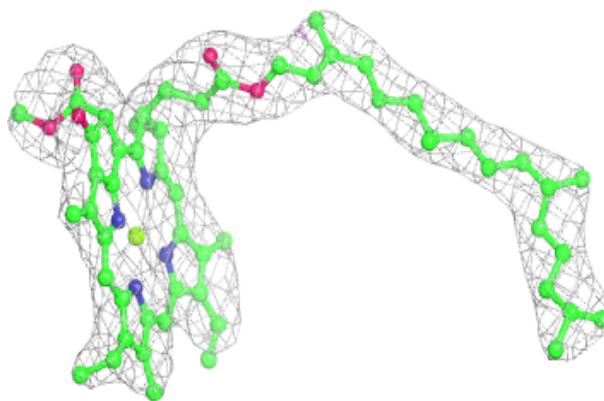
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



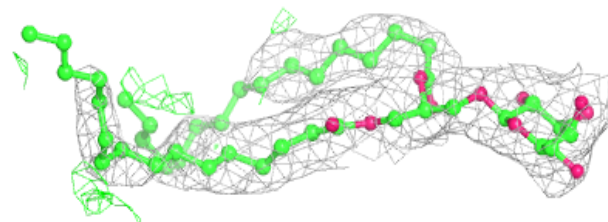
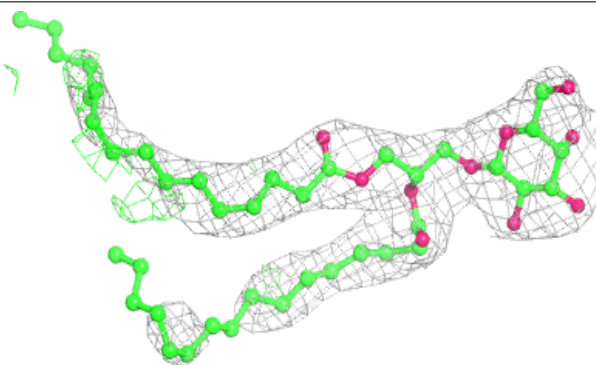


**Electron density around CLA B 609:**

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

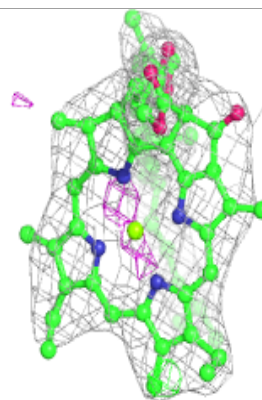
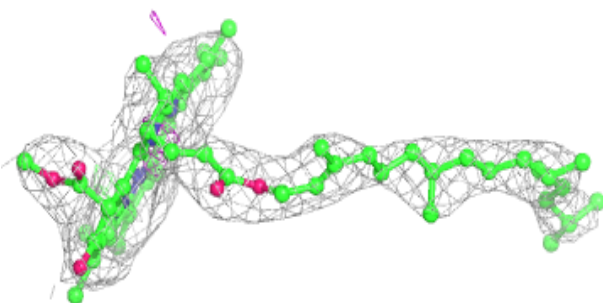
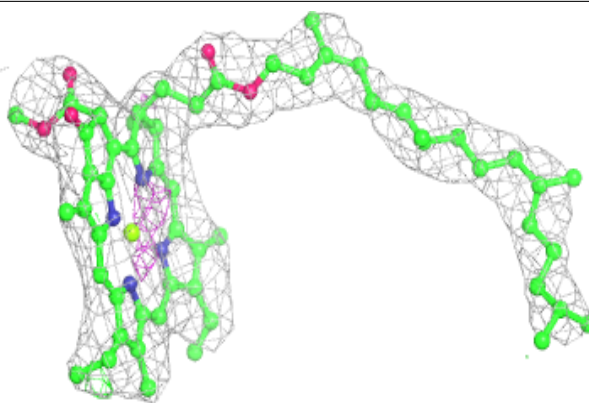
**Electron density around LMG j 101:**

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

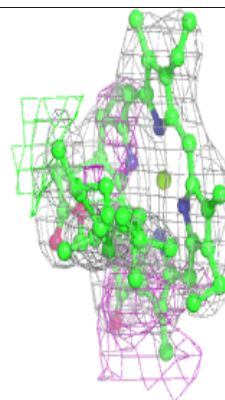
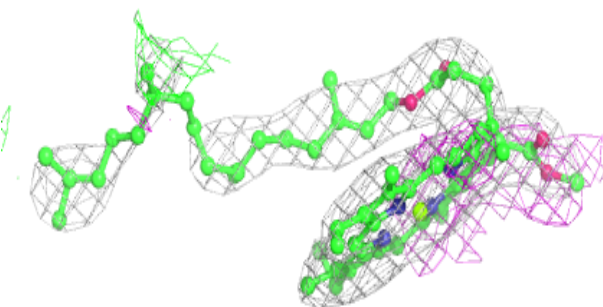
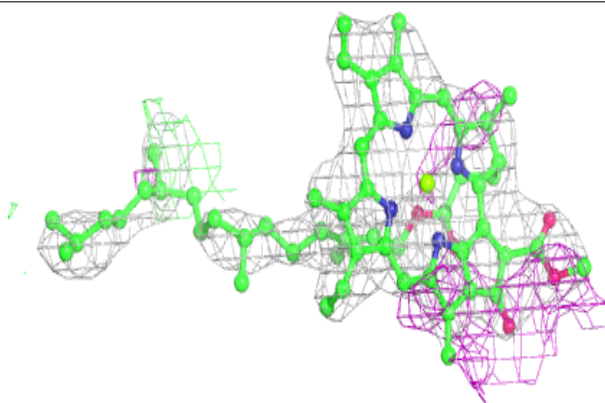


**Electron density around CLA b 609:**

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

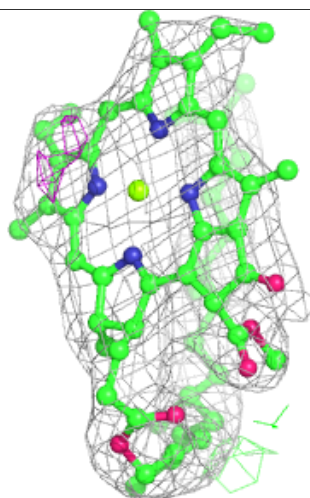
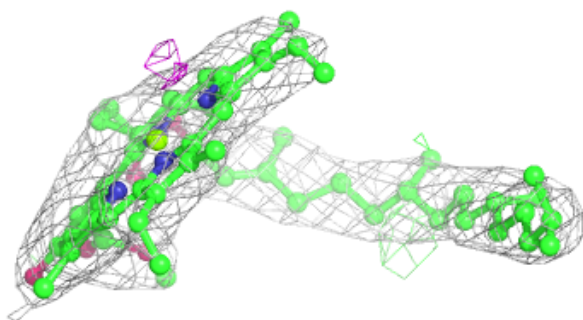
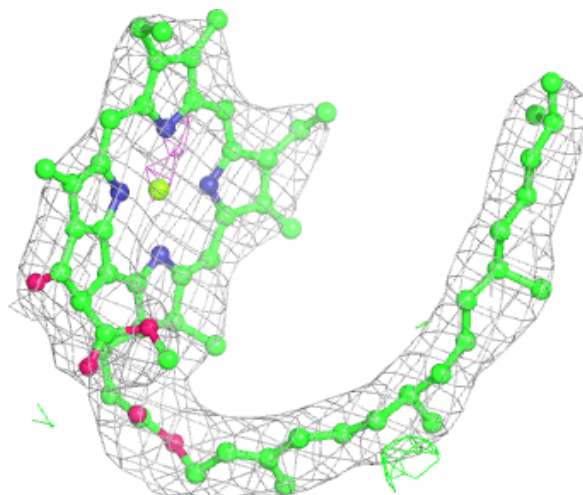
**Electron density around CLA B 614:**

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



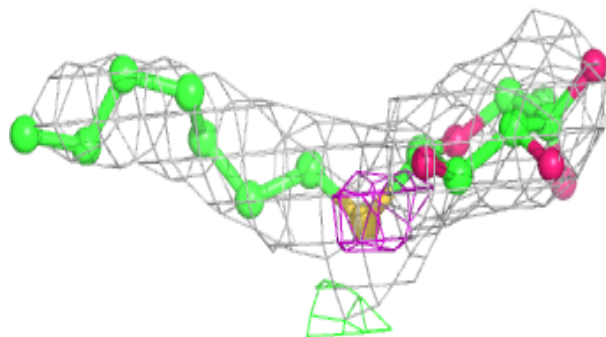
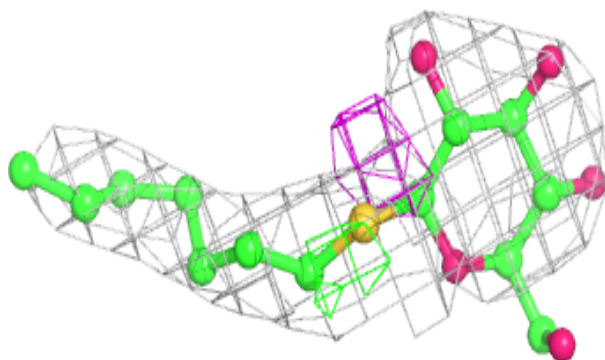
**Electron density around CLA c 507:**

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



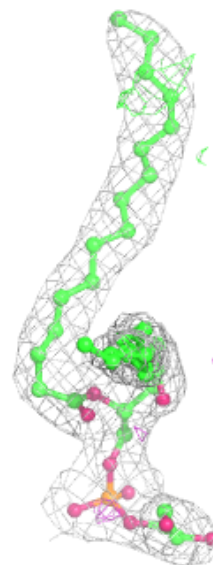
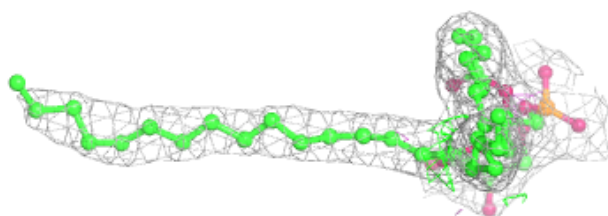
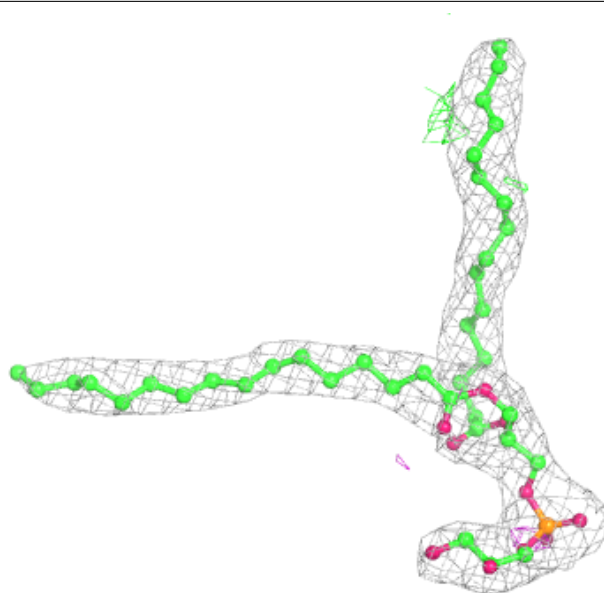
**Electron density around HTG B 622:**

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



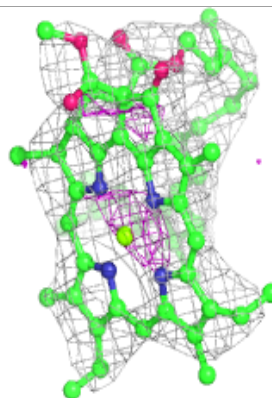
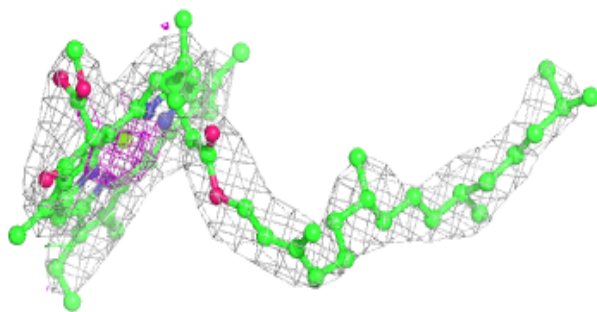
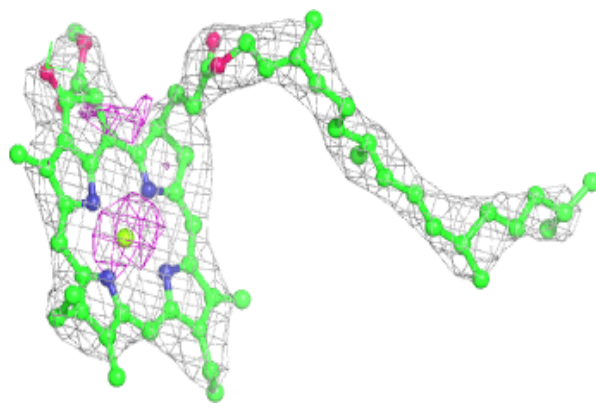
**Electron density around LHG 1 101:**

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

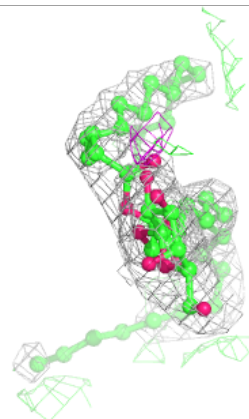
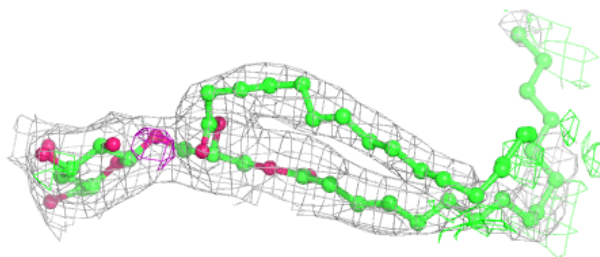
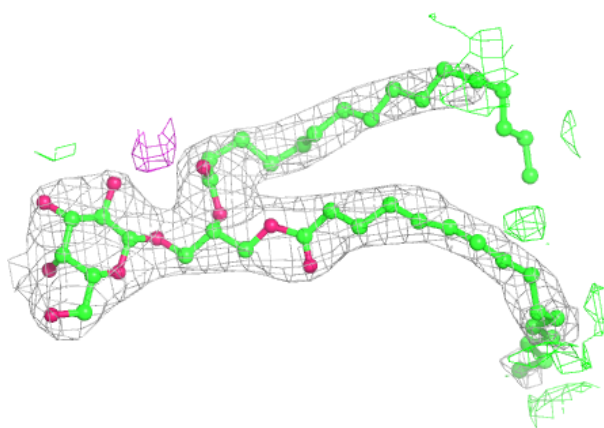


**Electron density around CLA c 511:**

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

**Electron density around LMG J 101:**

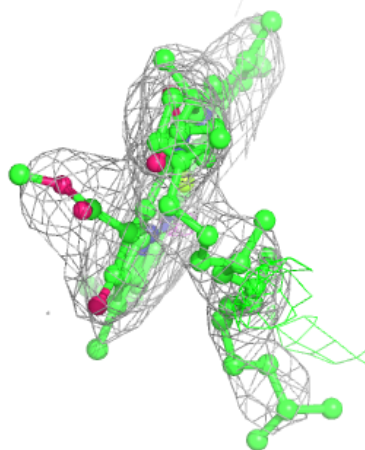
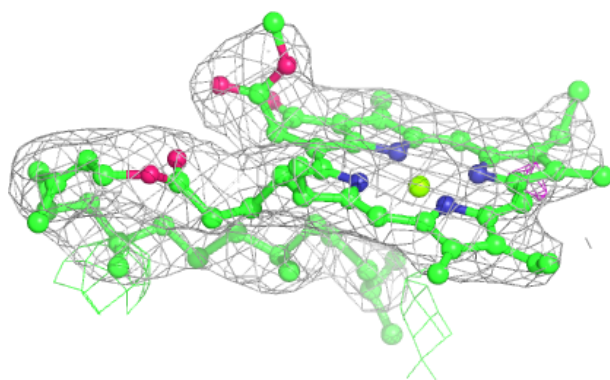
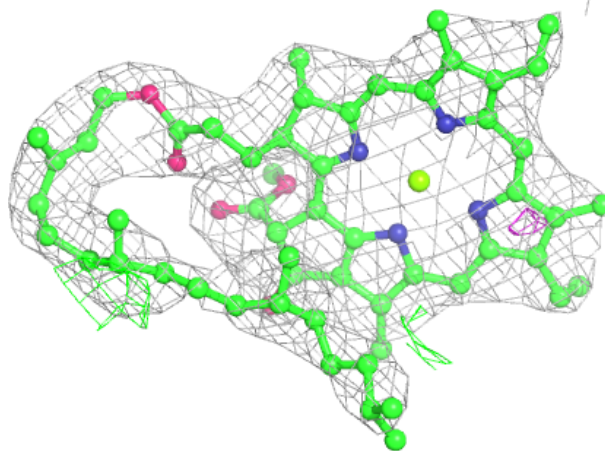
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





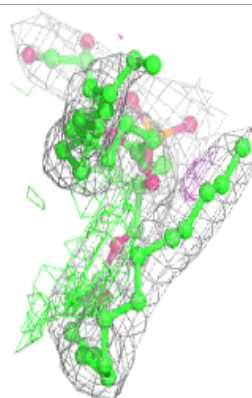
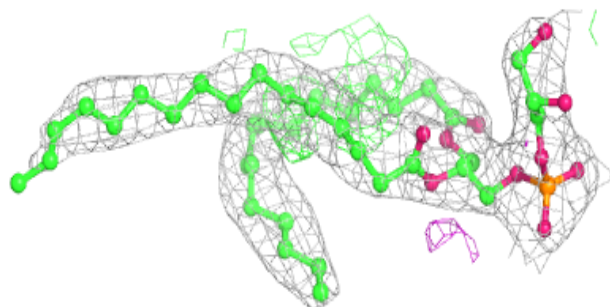
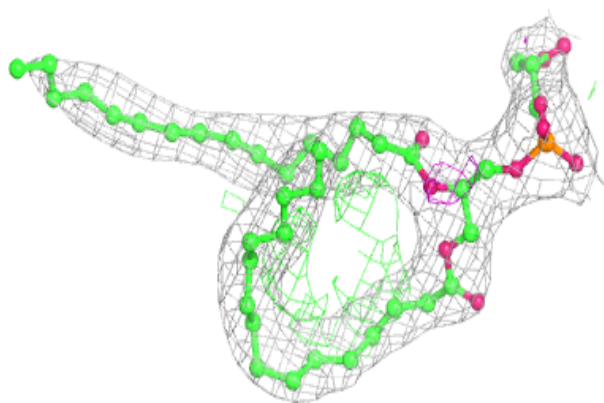
**Electron density around CLA c 509:**

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

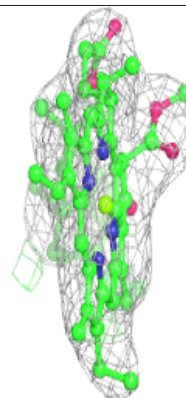
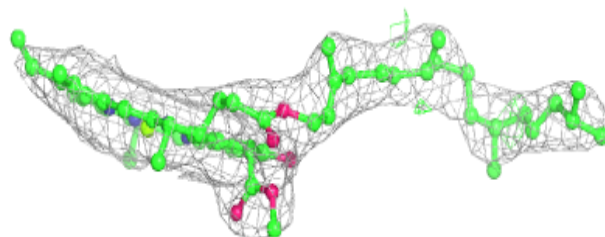
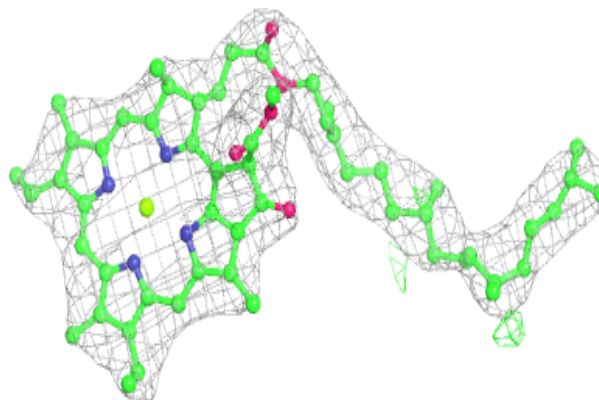


**Electron density around LHG A 416:**

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

**Electron density around CLA b 602:**

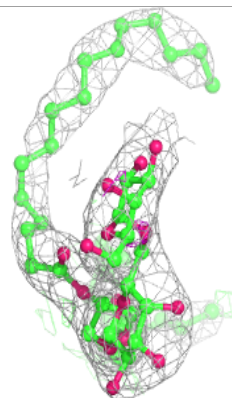
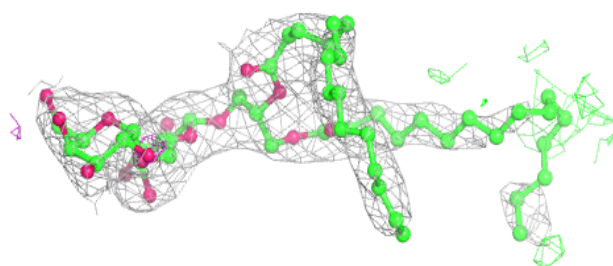
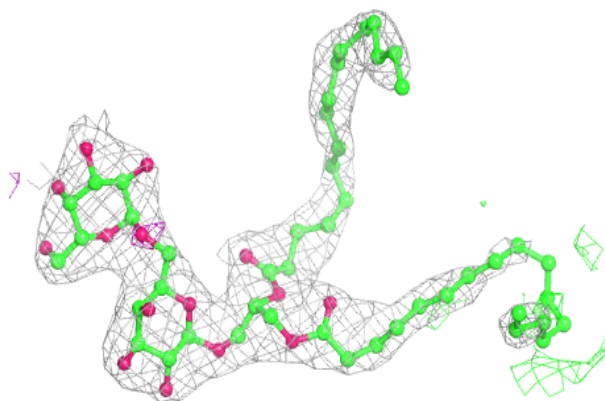
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



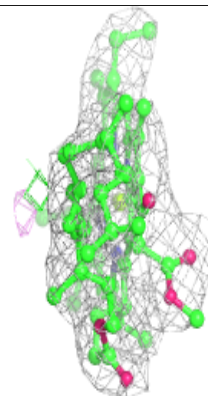
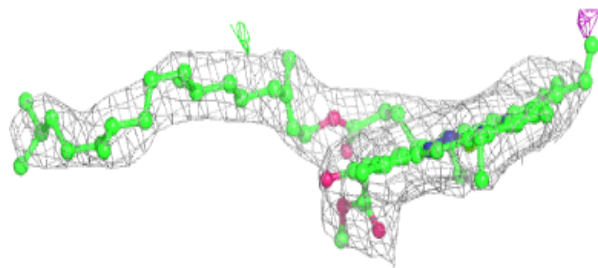
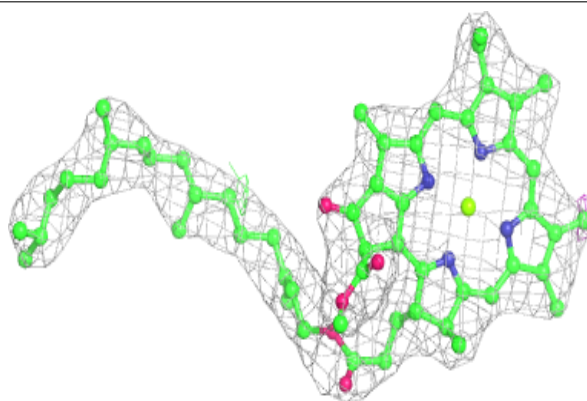


**Electron density around DGD c 517:**

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

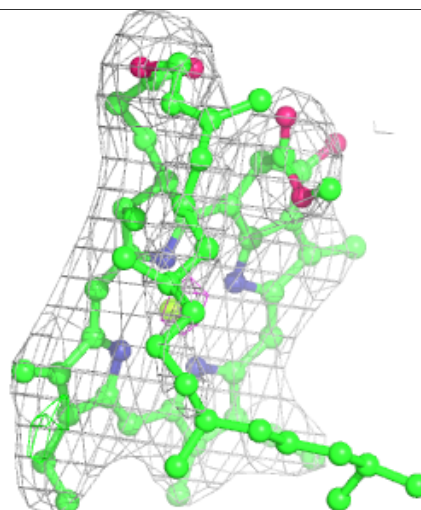
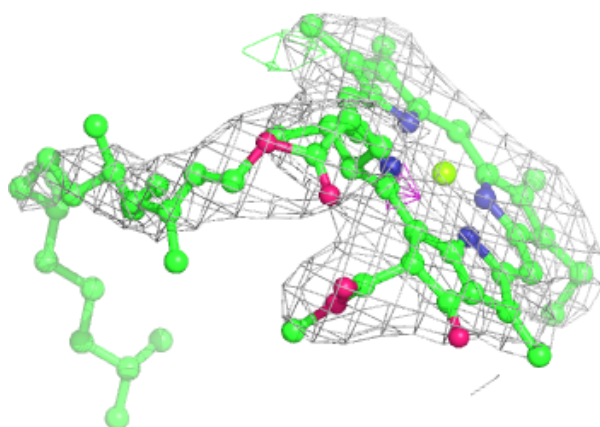
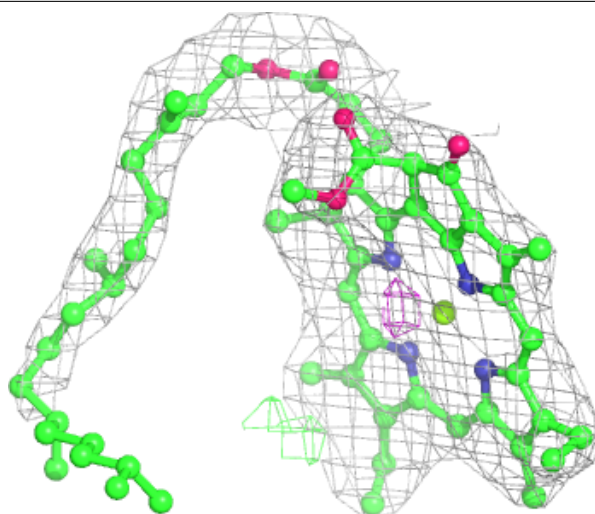
**Electron density around CLA B 602:**

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



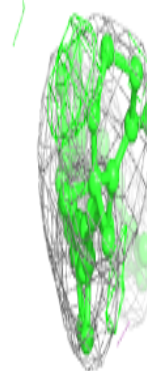
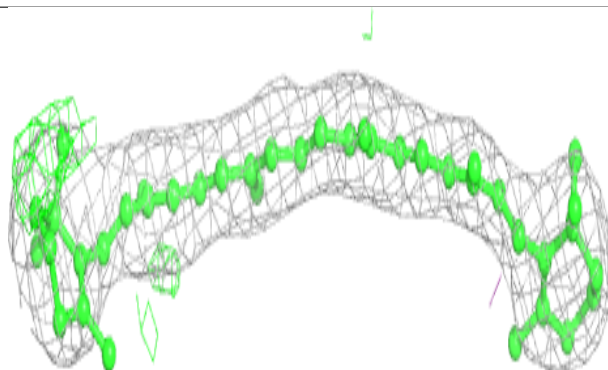
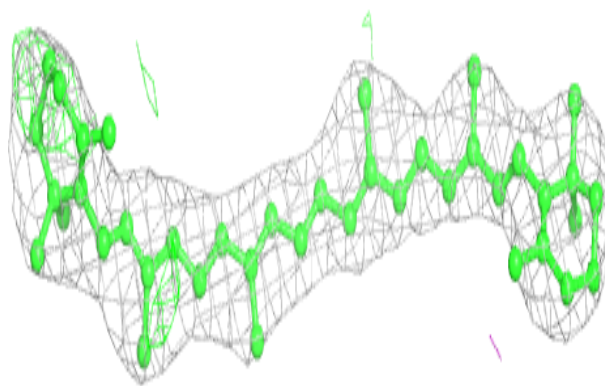
**Electron density around CLA b 616:**

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

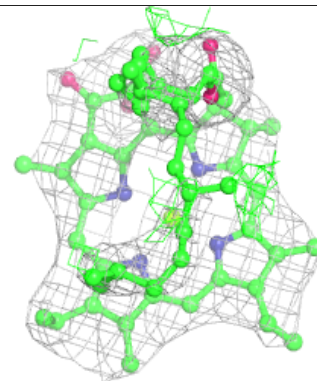
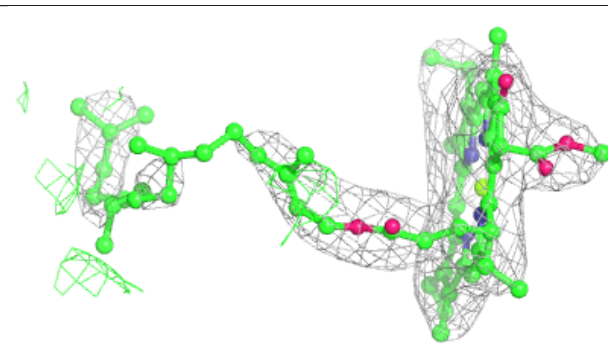
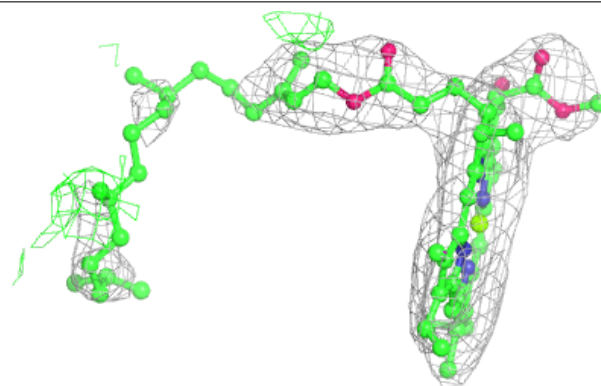


**Electron density around BCR d 405:**

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

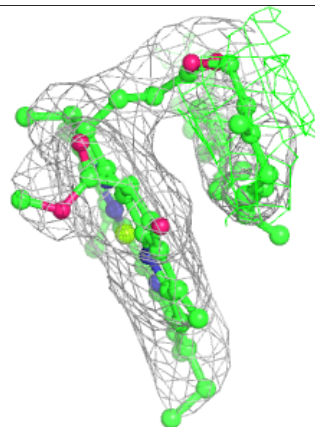
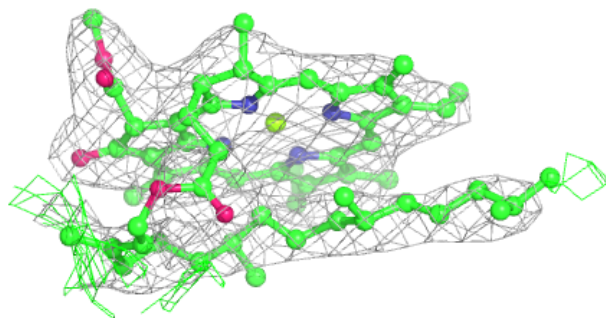
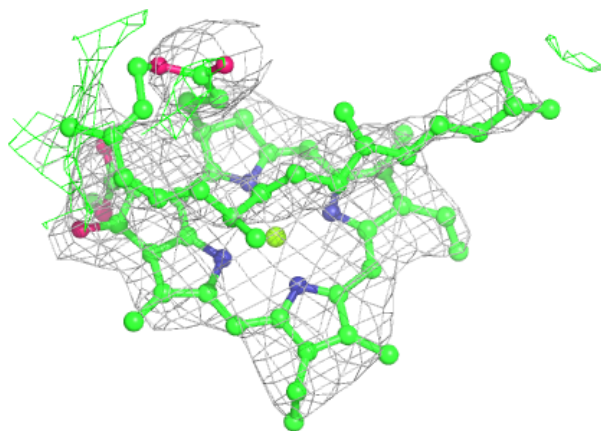
**Electron density around CLA C 507:**

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



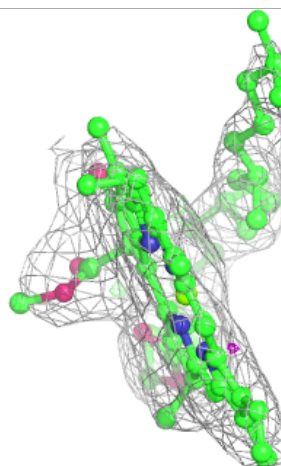
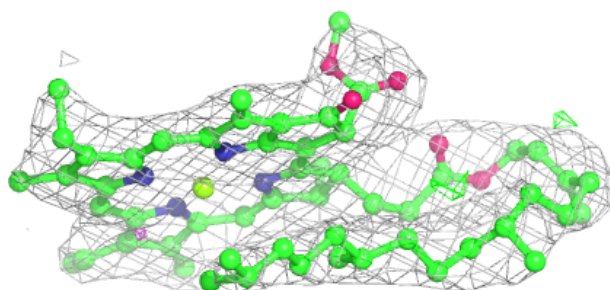
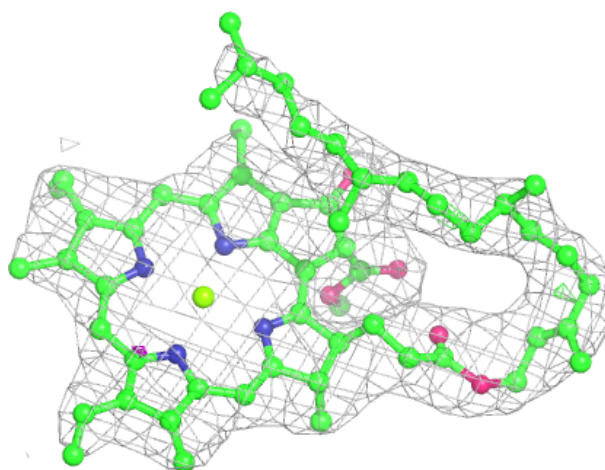
**Electron density around CLA b 601:**

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



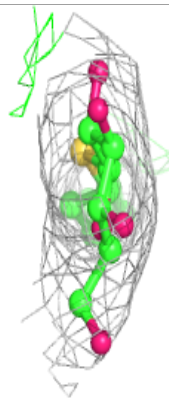
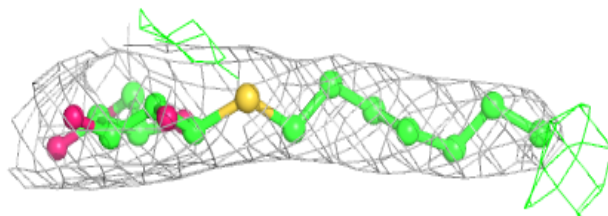
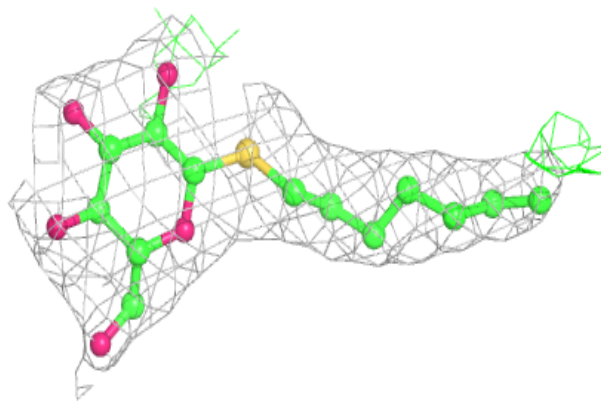
**Electron density around CLA C 510:**

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



**Electron density around HTG b 625:**

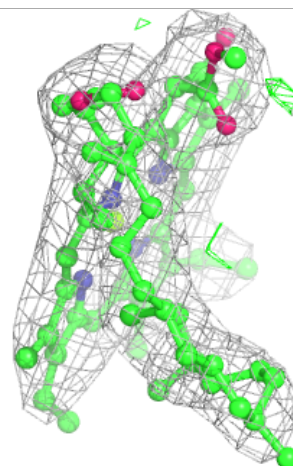
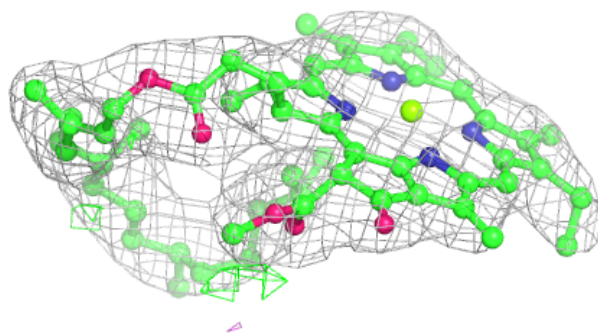
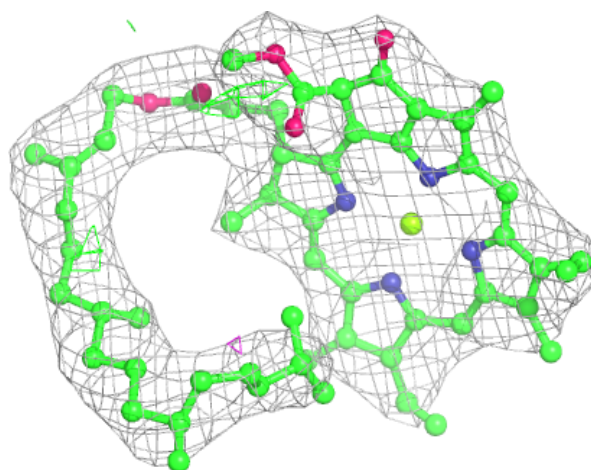
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





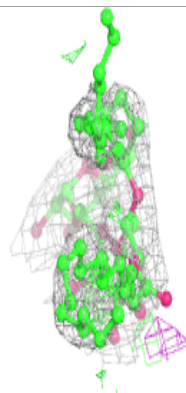
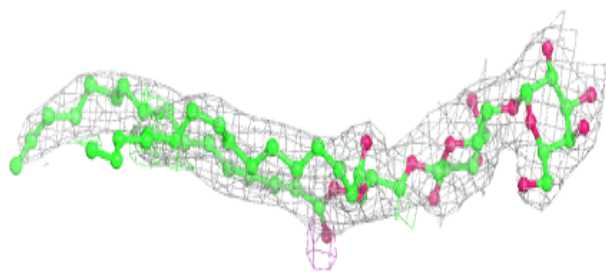
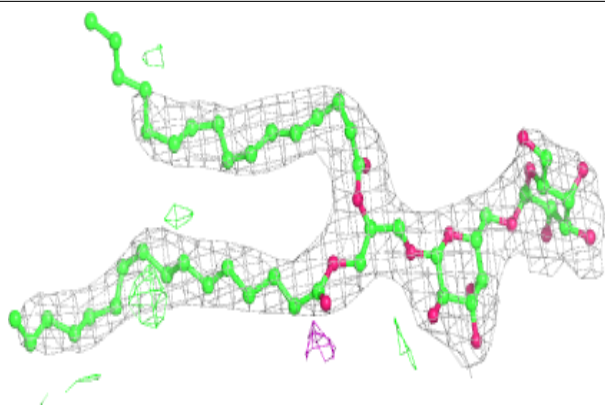
**Electron density around CLA b 615:**

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

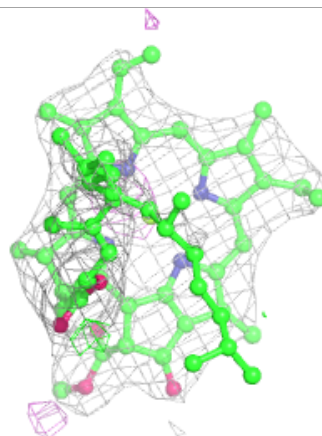
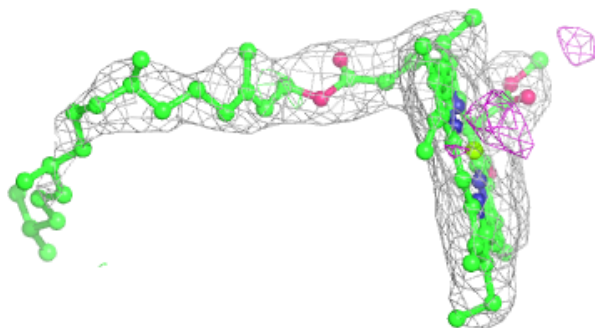
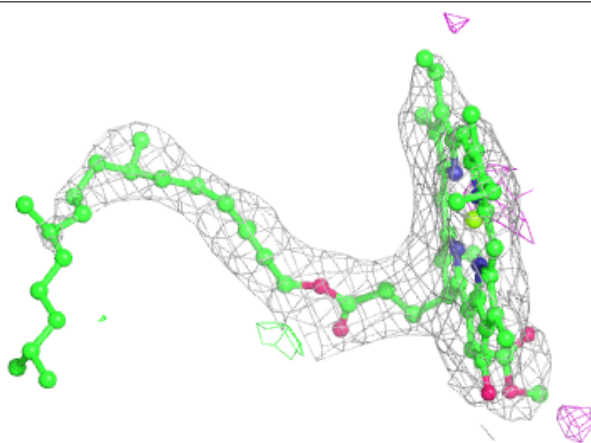


**Electron density around DGD C 519:**

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

**Electron density around CLA D 405:**

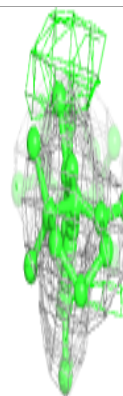
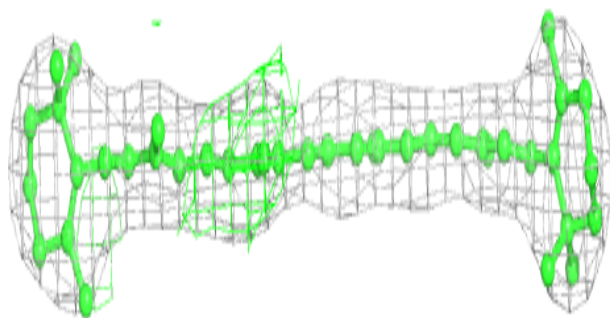
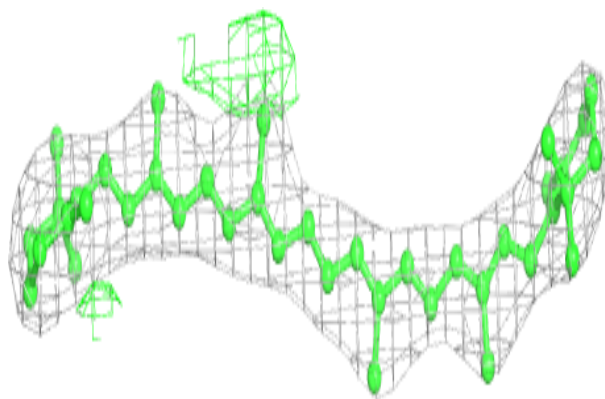
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



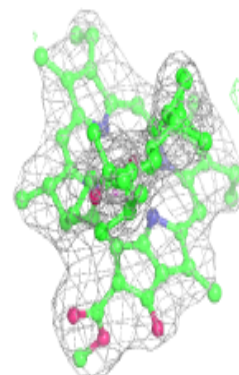
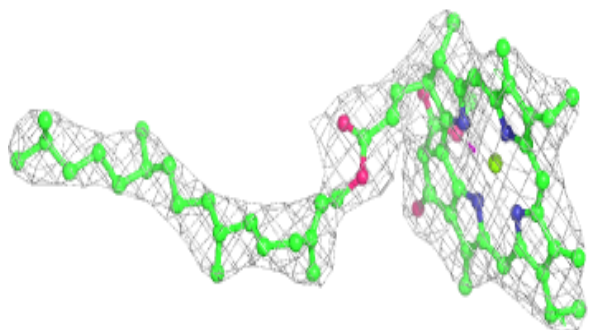
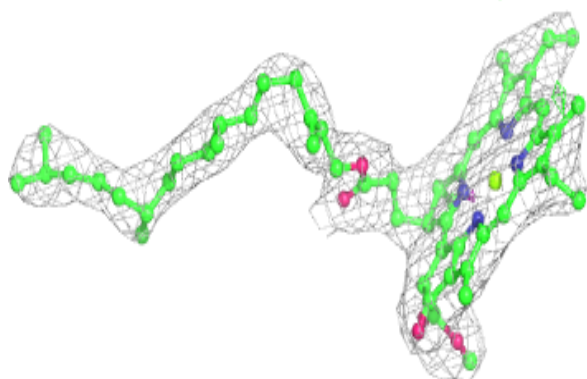


**Electron density around BCR C 516:**

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

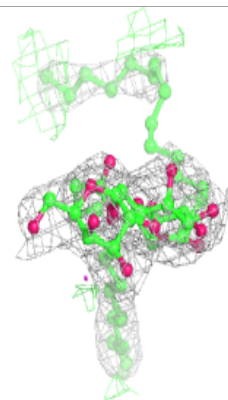
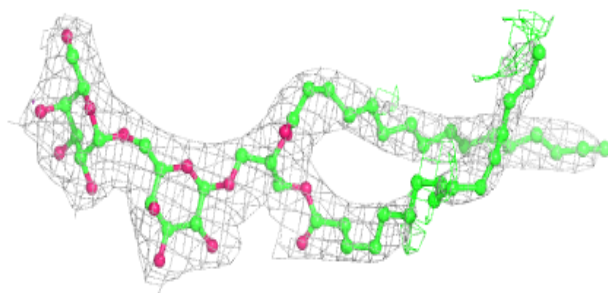
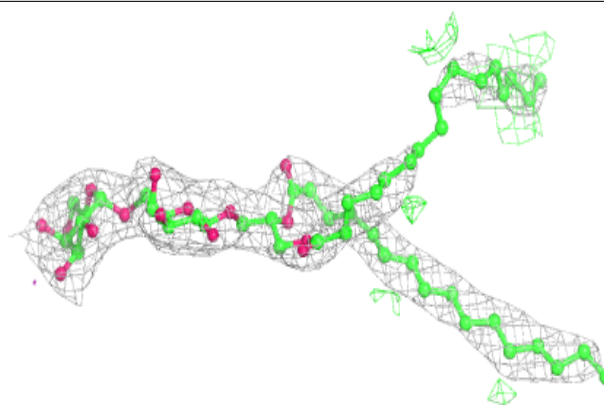
**Electron density around CLA C 503:**

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



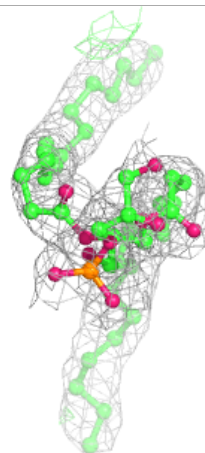
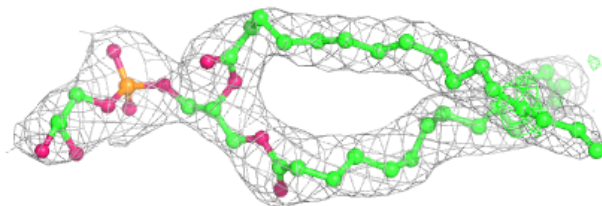
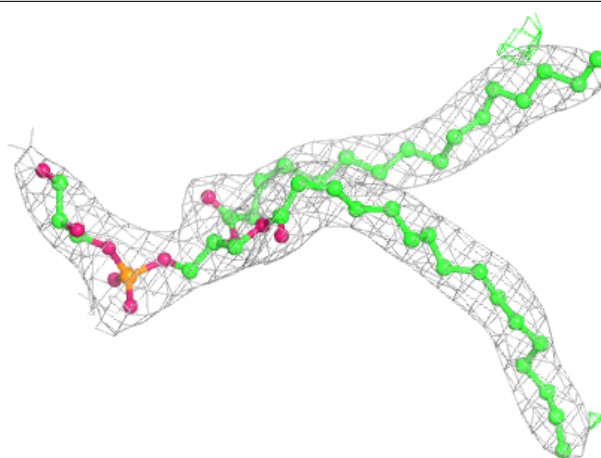
**Electron density around DGD C 517:**

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



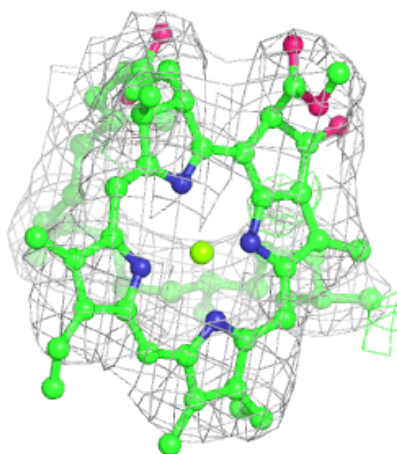
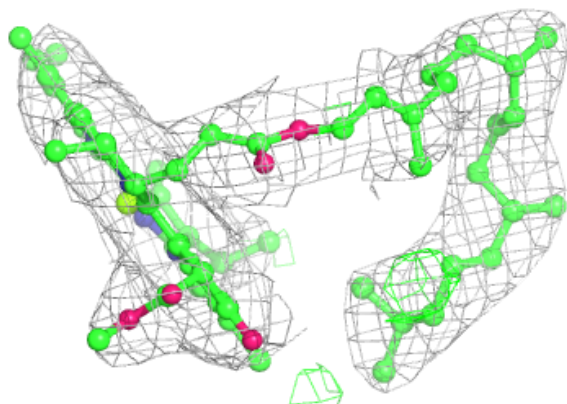
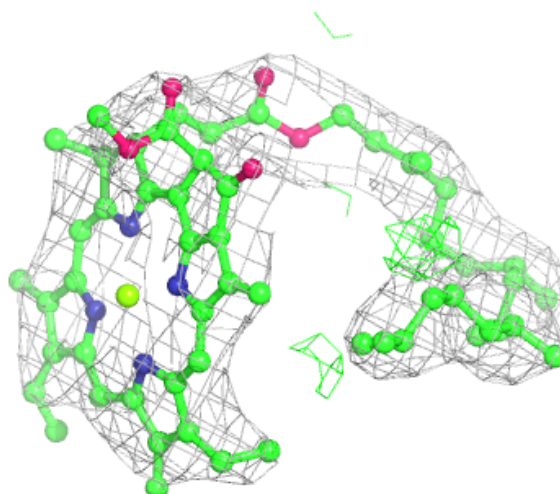
**Electron density around LHG d 408:**

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



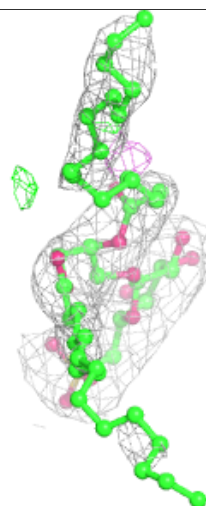
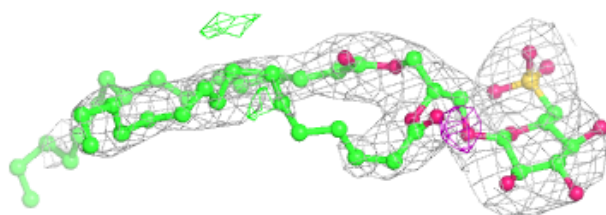
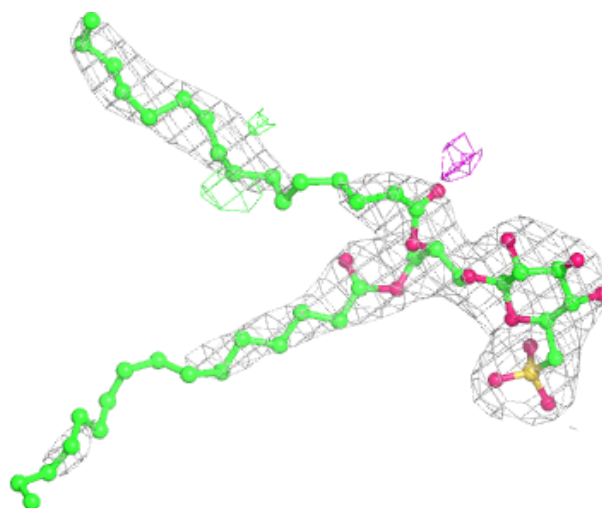
**Electron density around CLA c 503:**

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



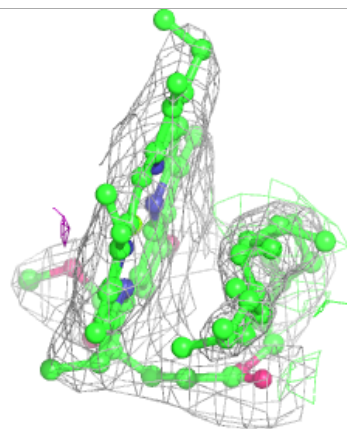
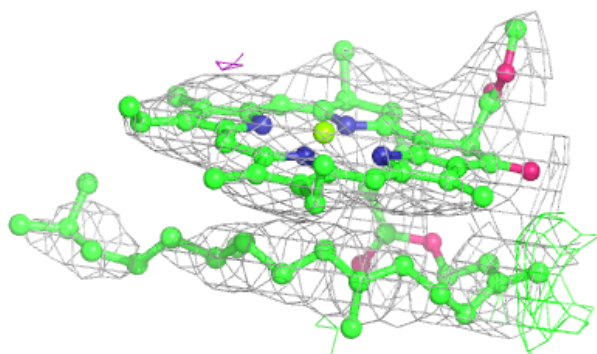
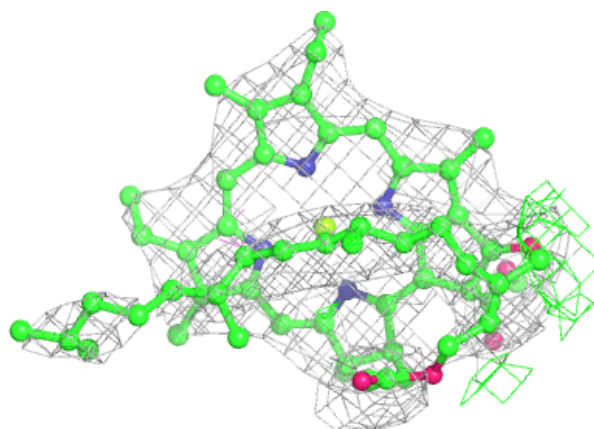
**Electron density around SQD a 410:**

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



**Electron density around CLA B 601:**

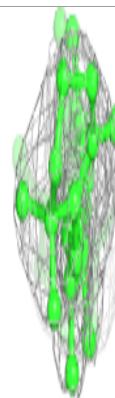
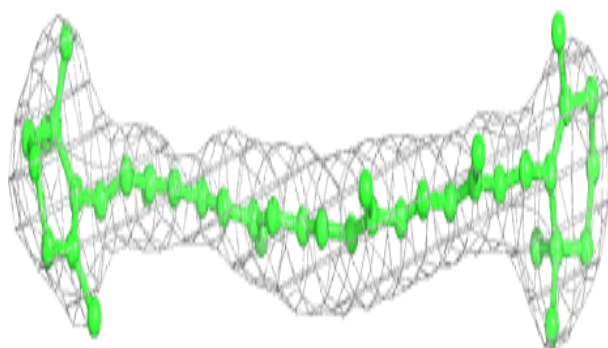
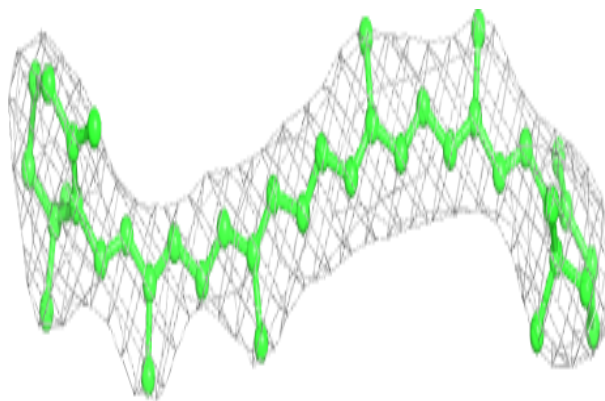
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



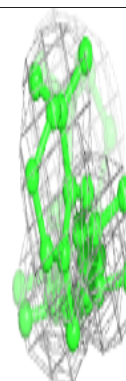
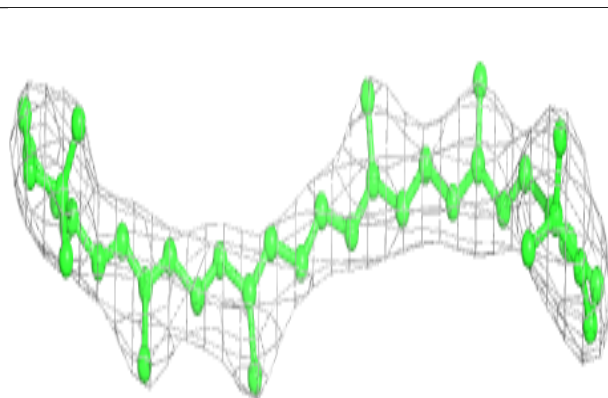
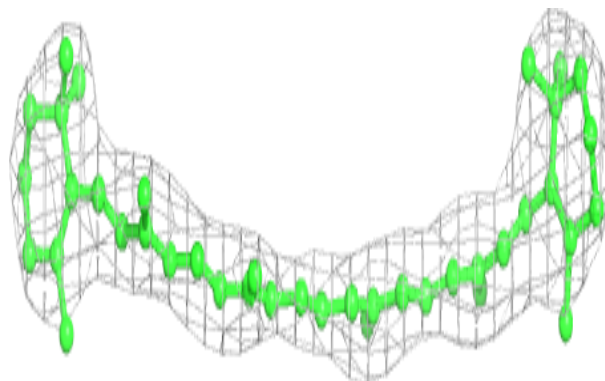


**Electron density around BCR Y 101:**

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

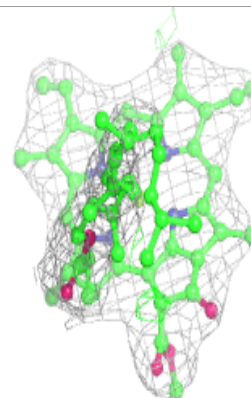
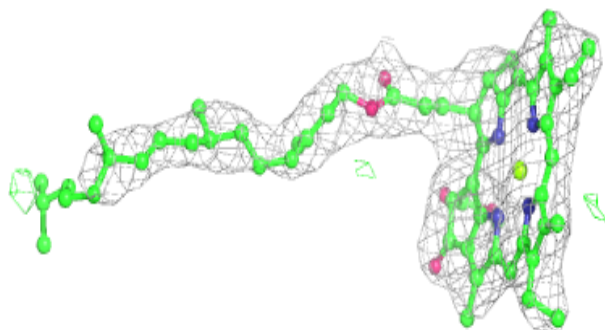
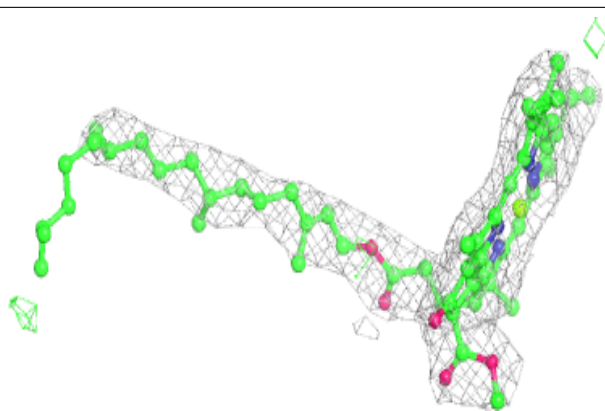
**Electron density around BCR K 102:**

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

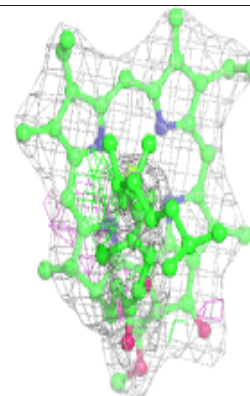
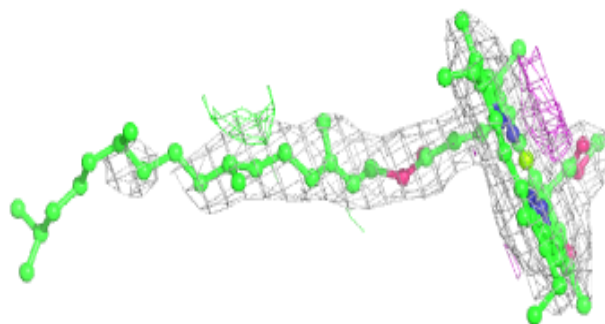
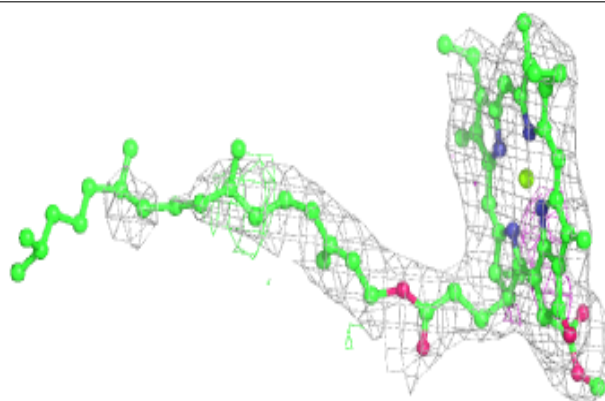


**Electron density around CLA B 604:**

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

**Electron density around CLA d 404:**

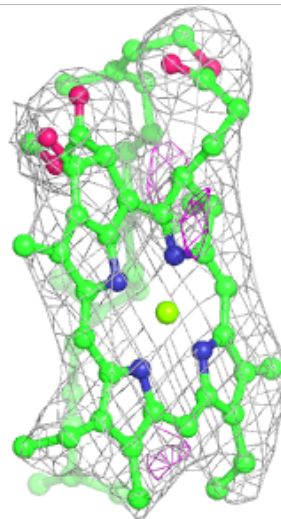
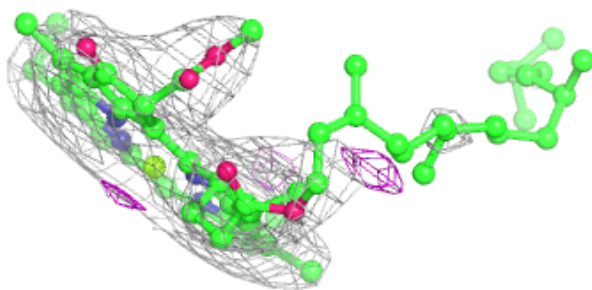
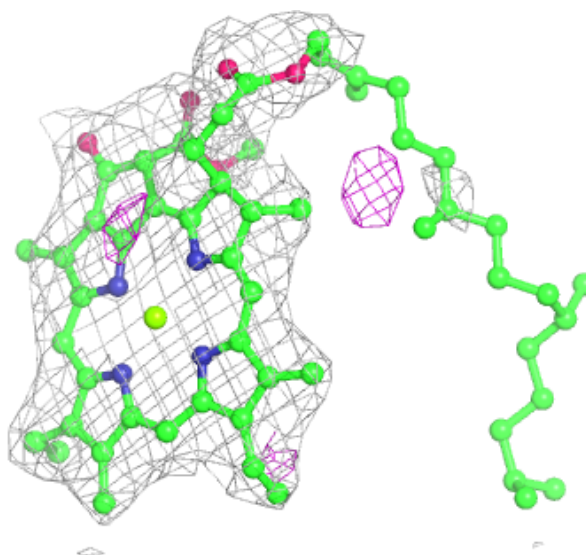
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





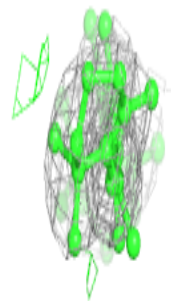
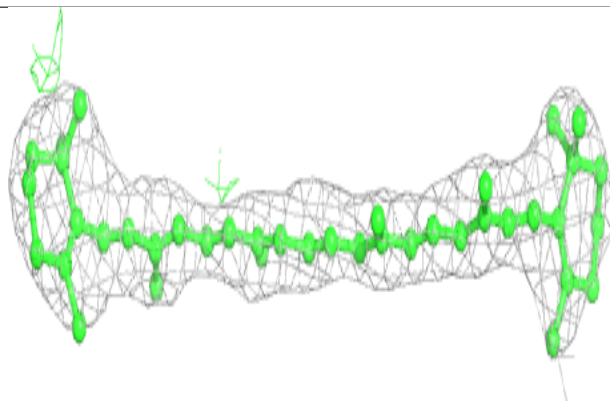
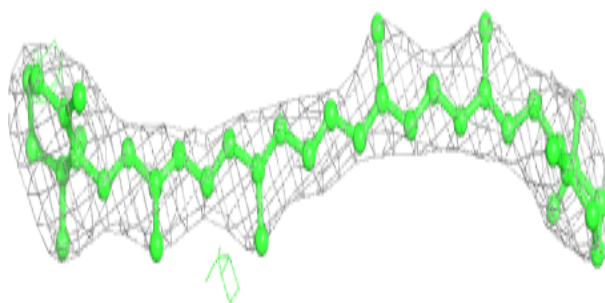
**Electron density around CLA B 616:**

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



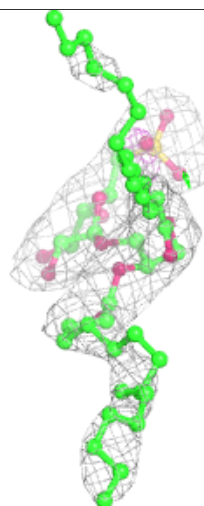
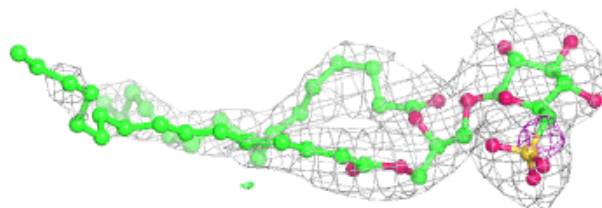
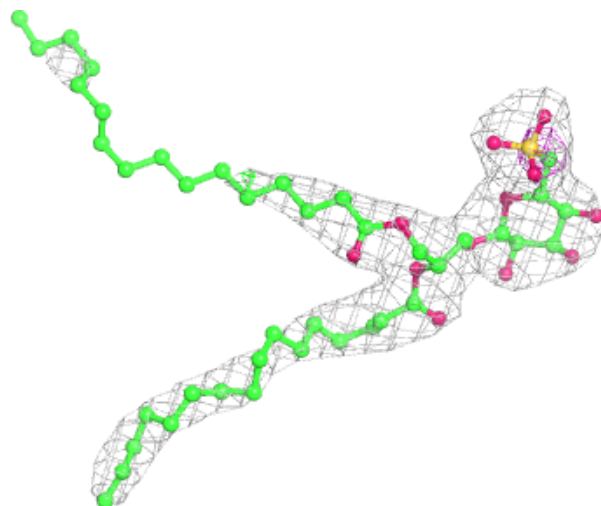
**Electron density around BCR C 515:**

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



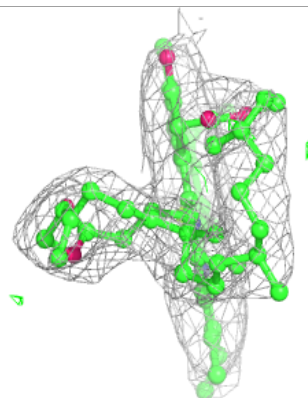
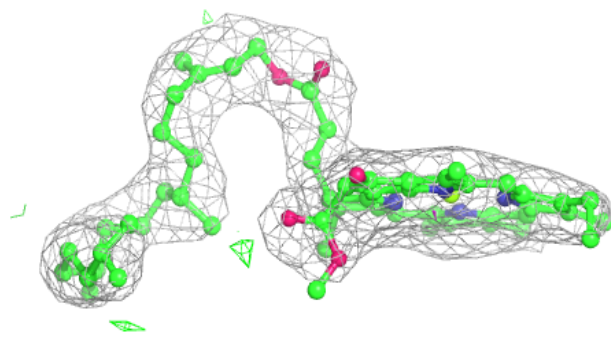
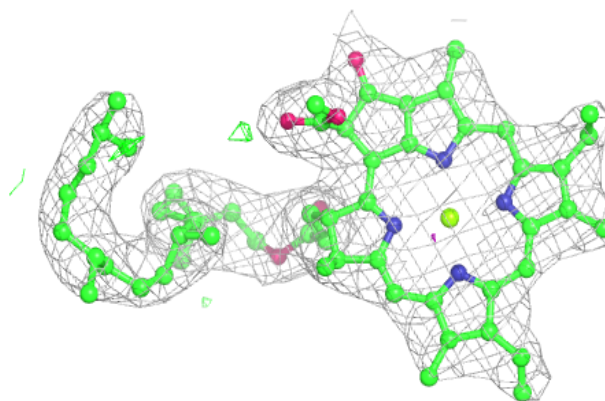
**Electron density around SQD A 410:**

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

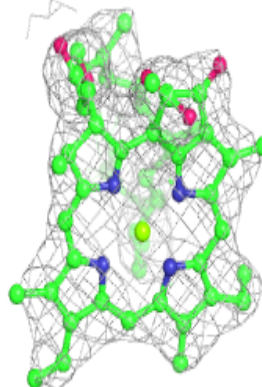
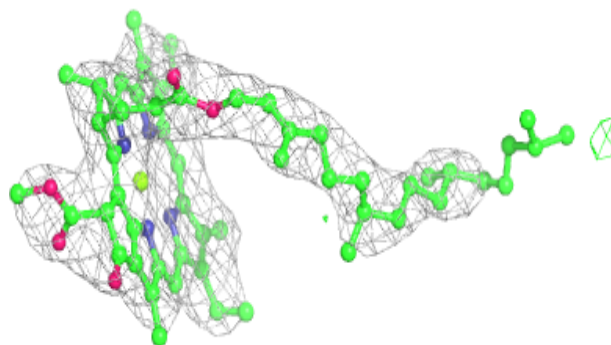
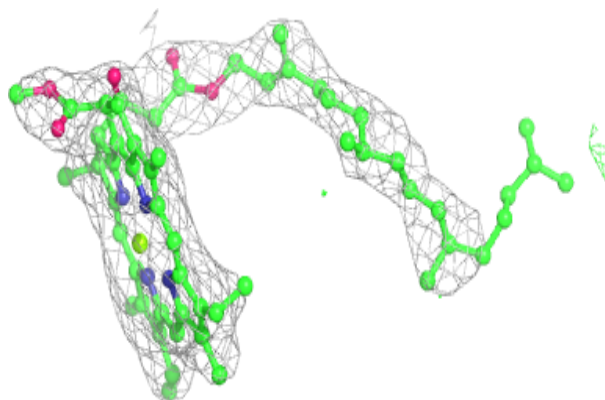


**Electron density around CLA b 612:**

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

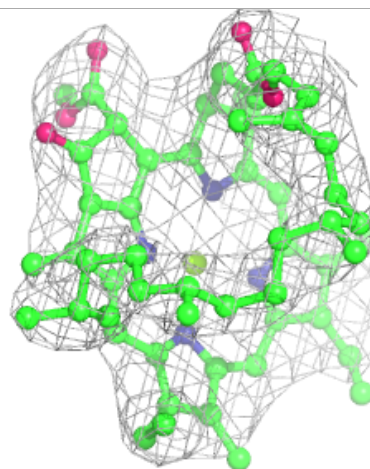
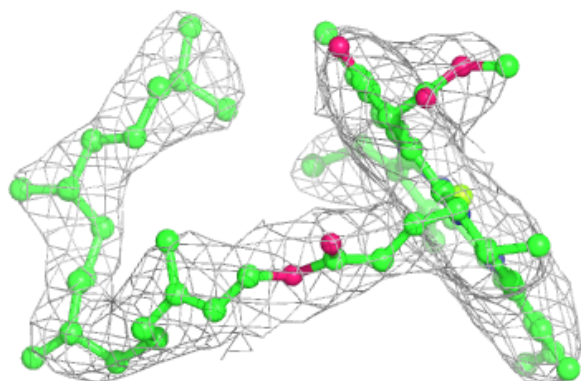
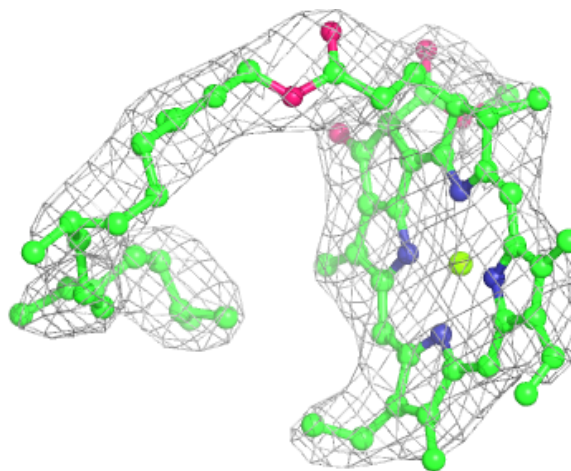
**Electron density around CLA c 508:**

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



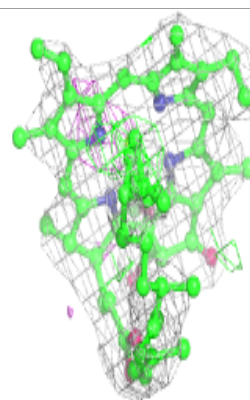
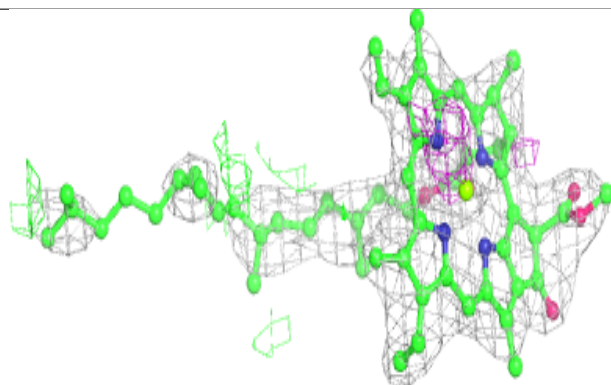
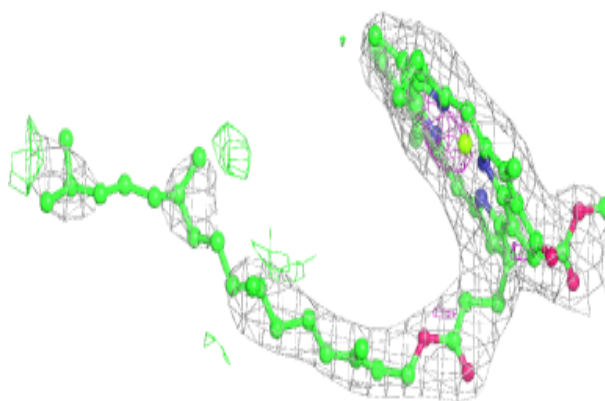
**Electron density around CLA C 504:**

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

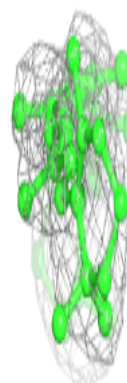
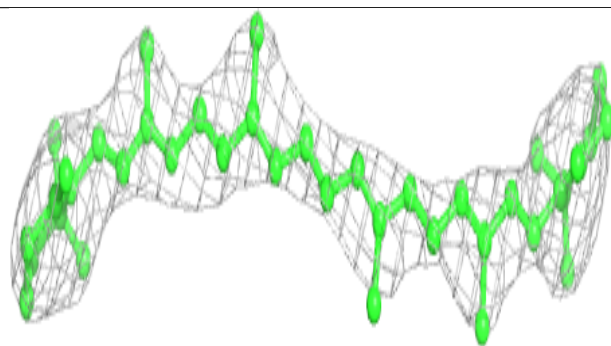
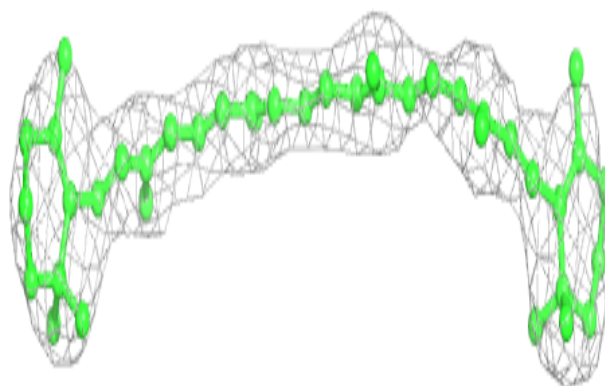


**Electron density around CLA C 505:**

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

**Electron density around BCR k 101:**

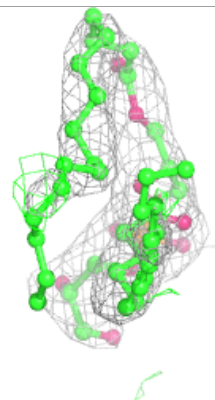
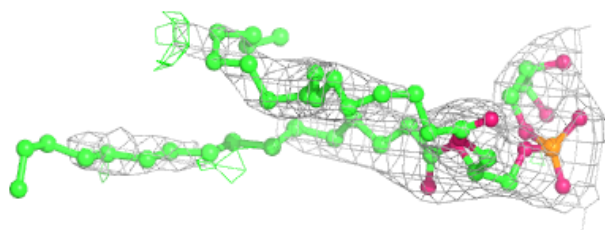
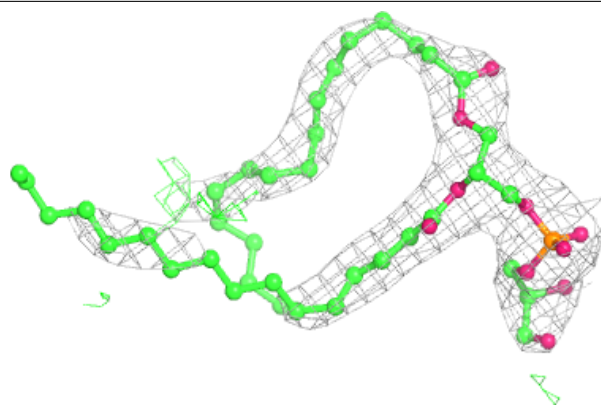
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



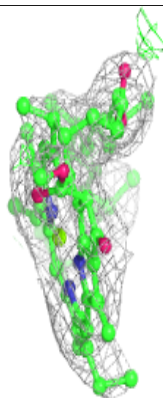
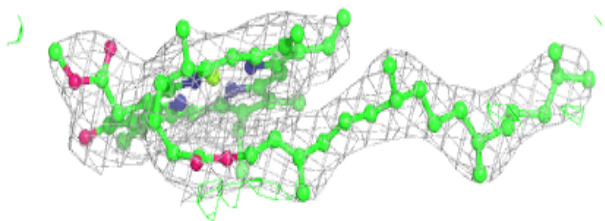
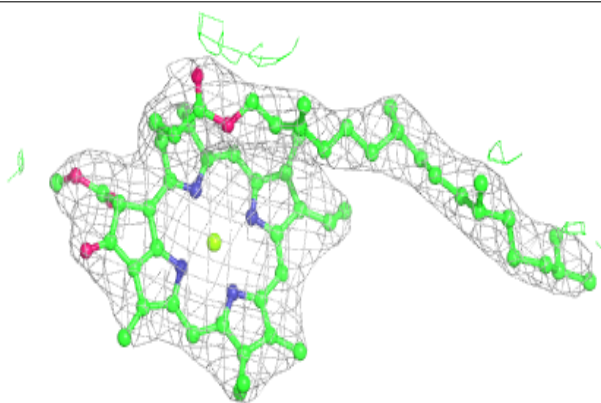


**Electron density around LHG d 409:**

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

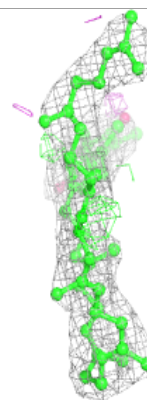
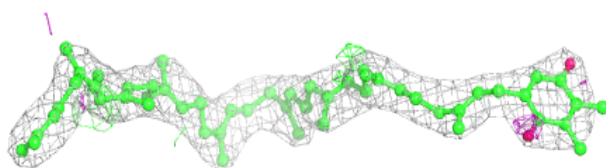
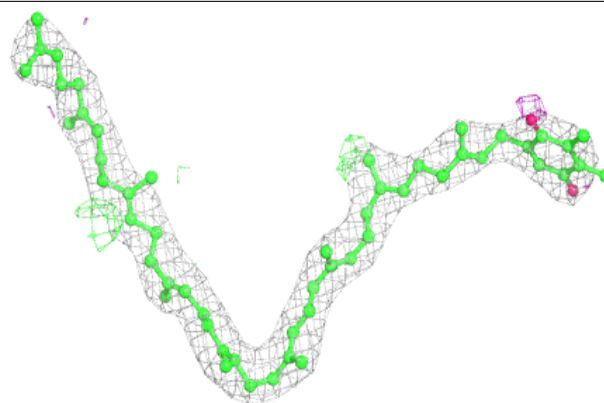
**Electron density around CLA C 502:**

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

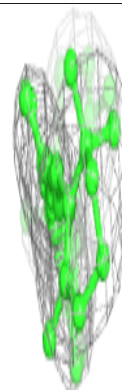
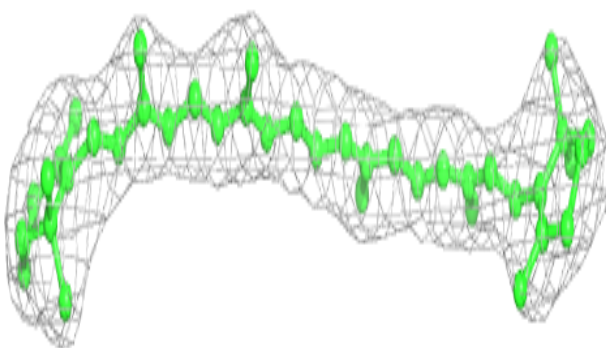
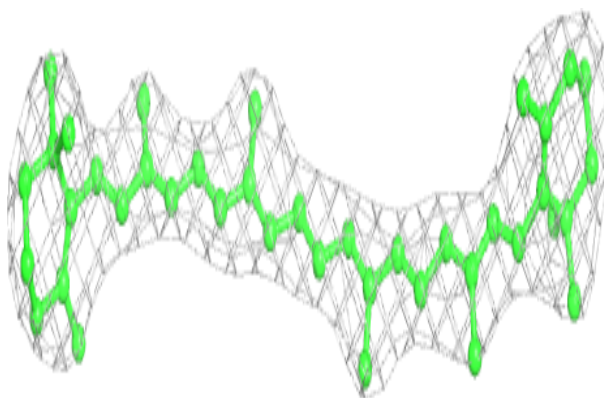


**Electron density around PL9 d 406:**

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

**Electron density around BCR B 619:**

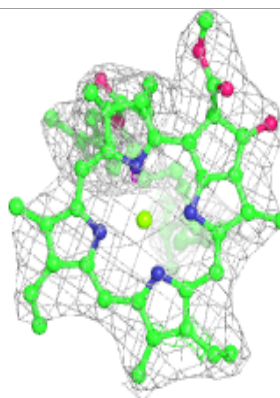
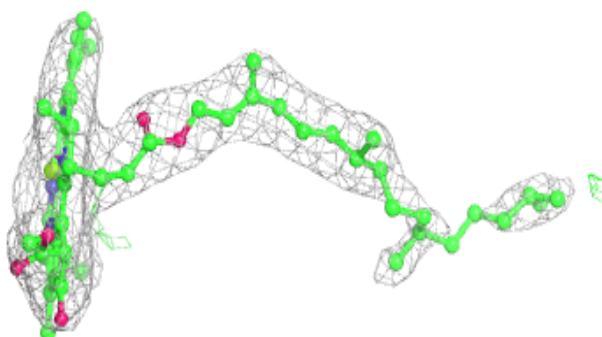
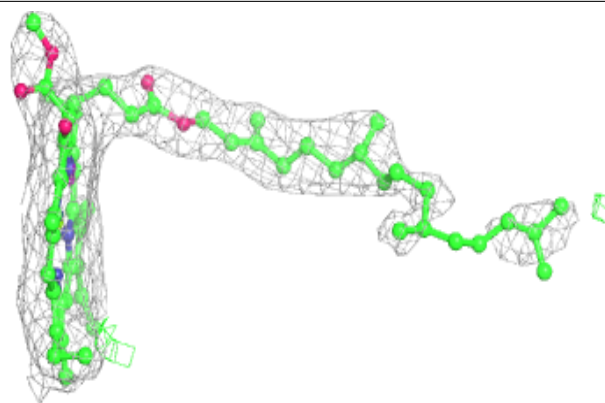
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



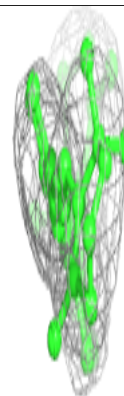
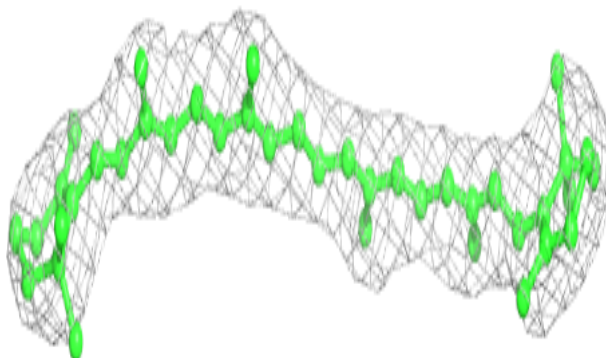
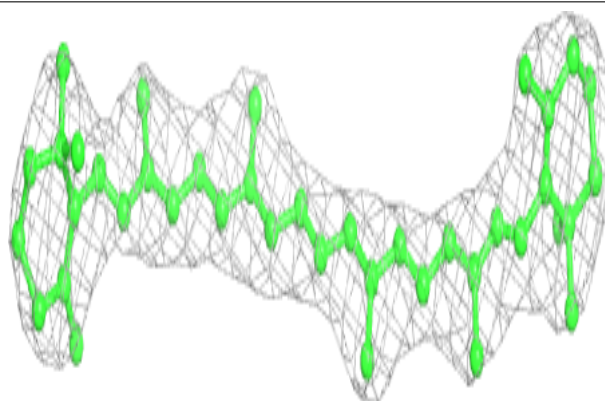


**Electron density around CLA B 606:**

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

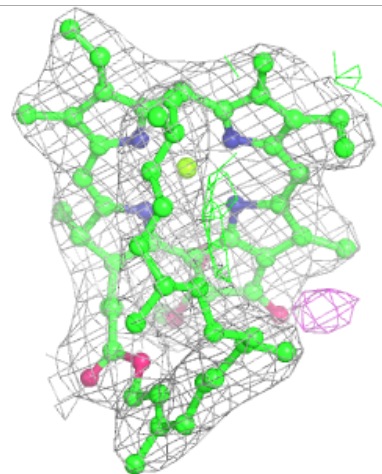
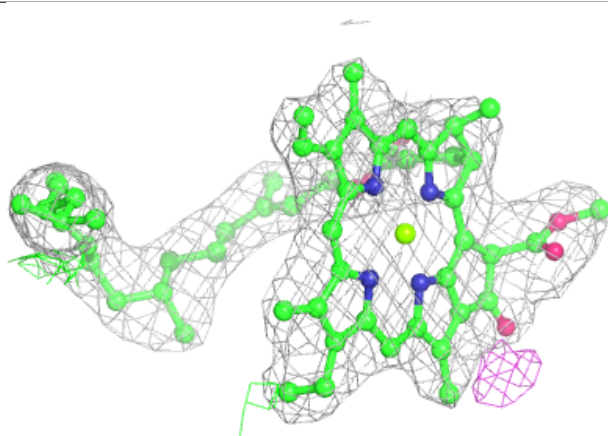
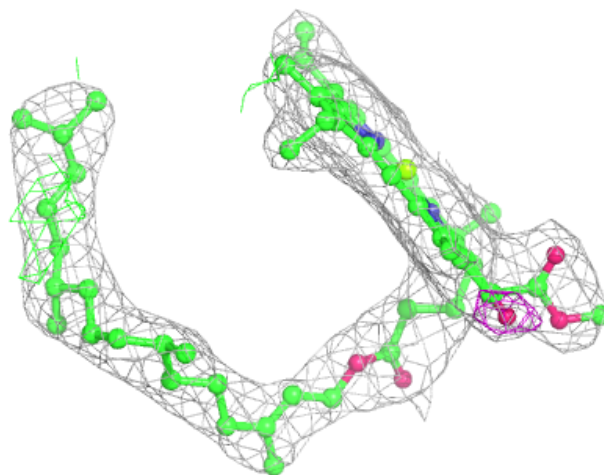
**Electron density around BCR b 619:**

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



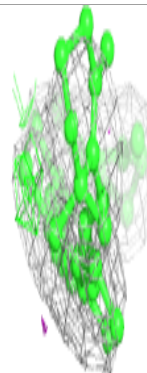
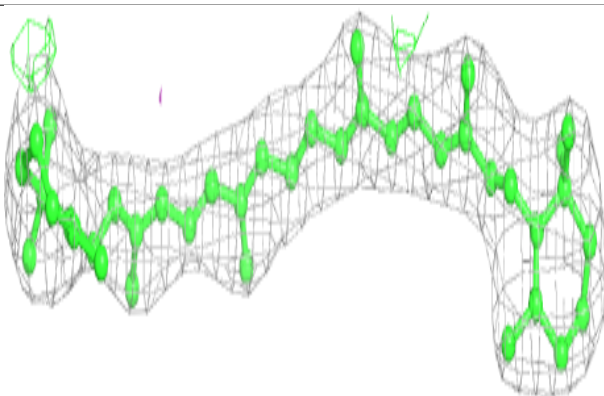
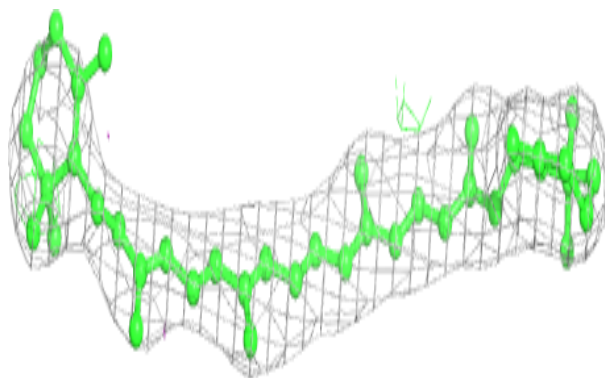
**Electron density around CLA B 611:**

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

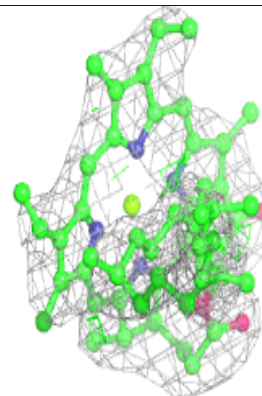
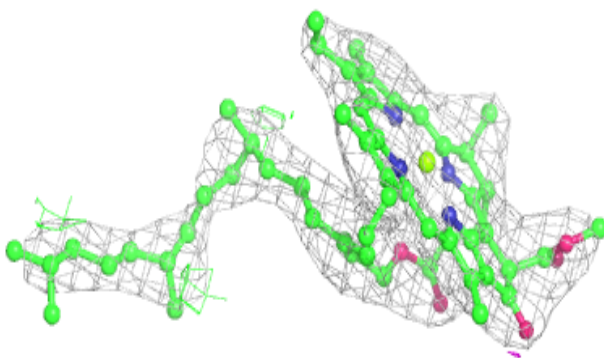
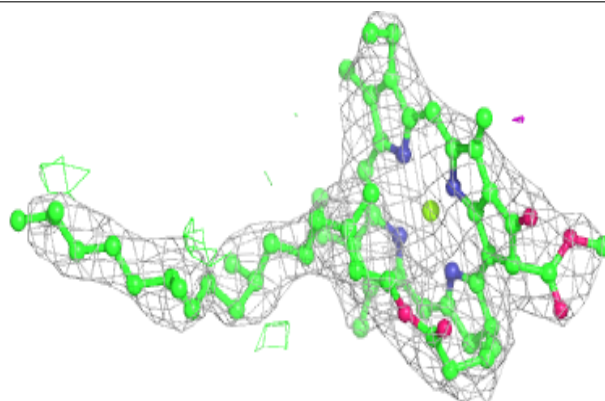


**Electron density around BCR D 406:**

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

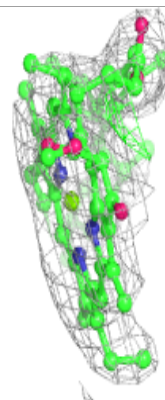
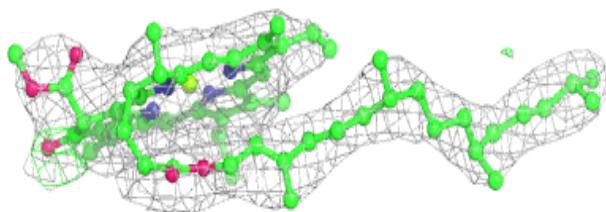
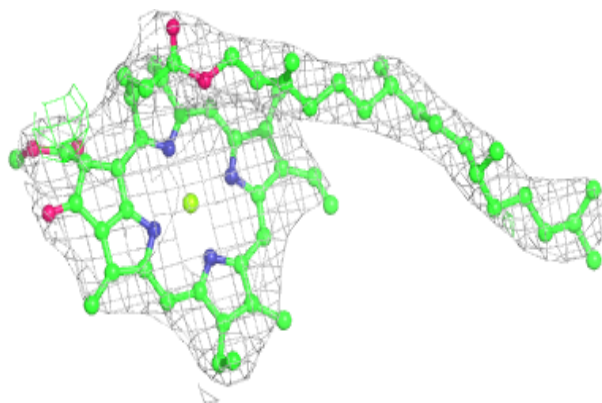
**Electron density around CLA c 505:**

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

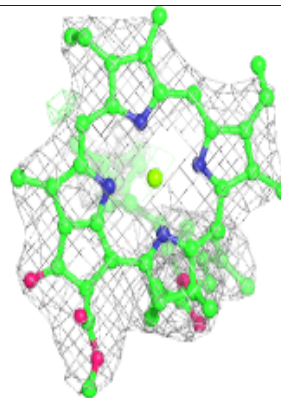
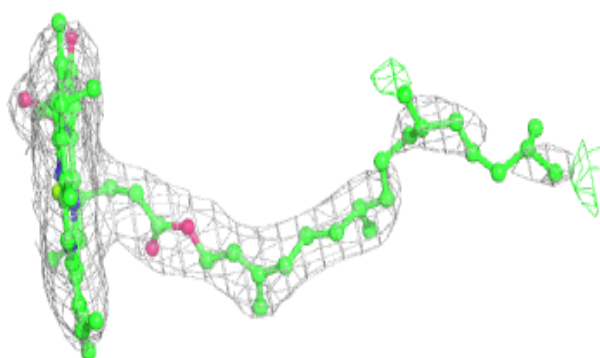
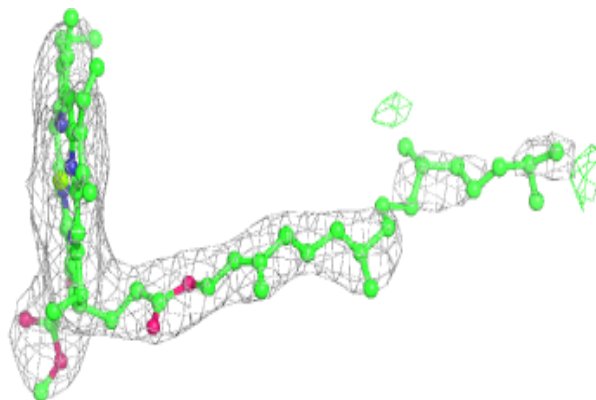


**Electron density around CLA c 501:**

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

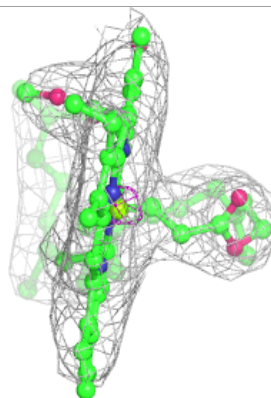
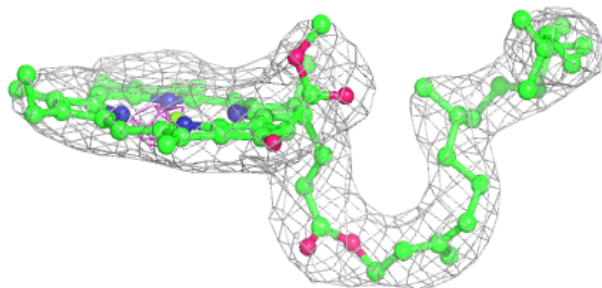
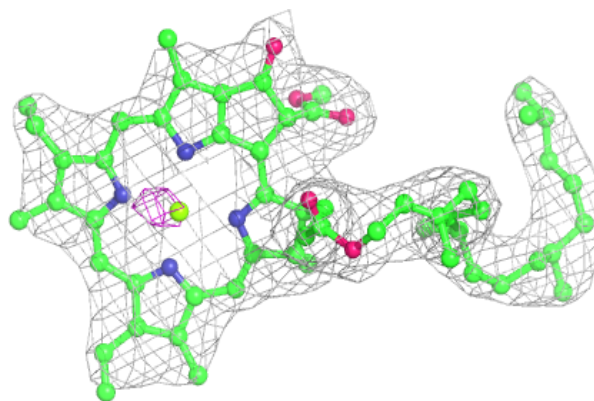
**Electron density around CLA b 606:**

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

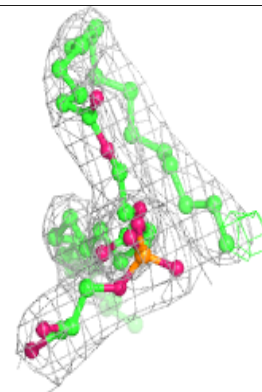
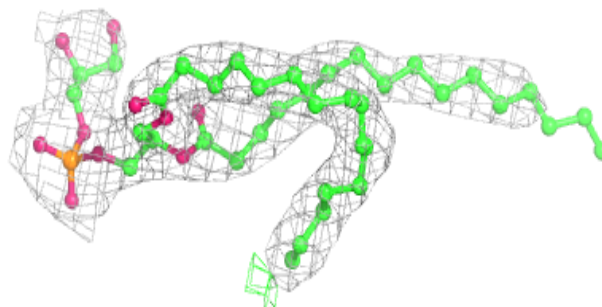
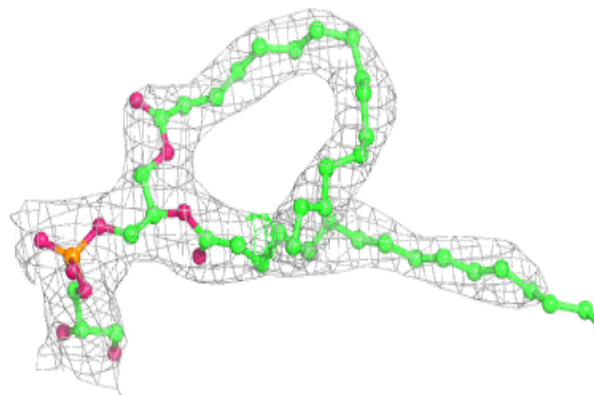


**Electron density around CLA B 612:**

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

**Electron density around LHG d 407:**

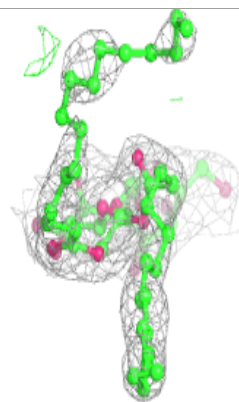
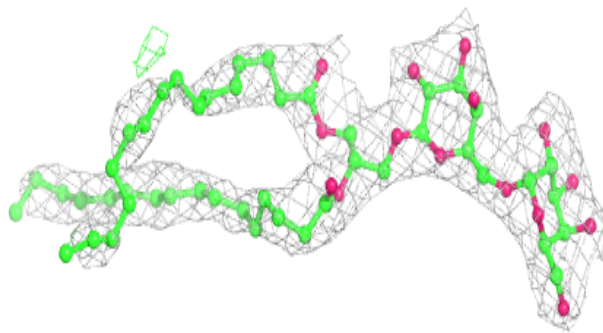
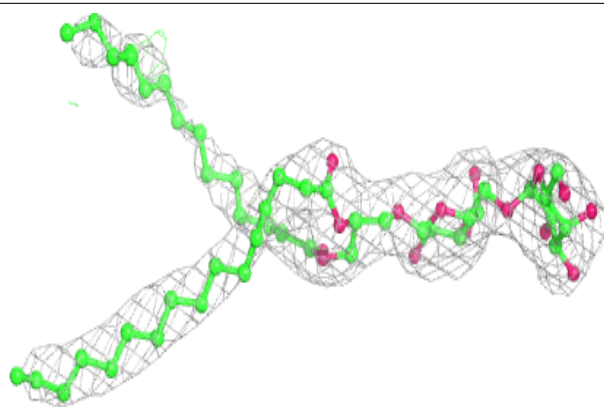
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



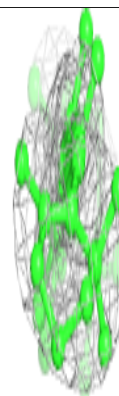
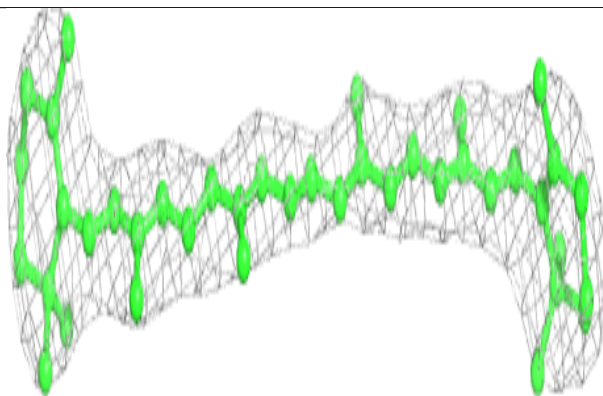
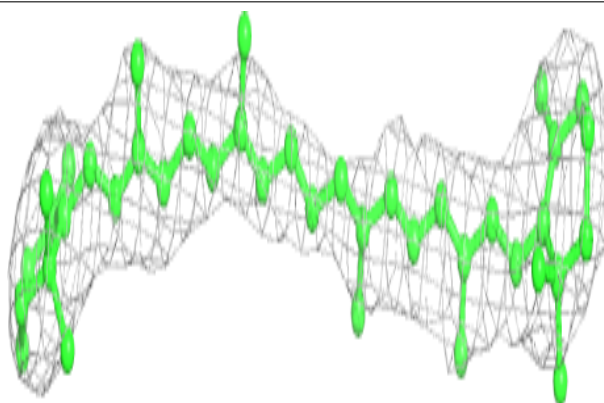


**Electron density around DGD c 516:**

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

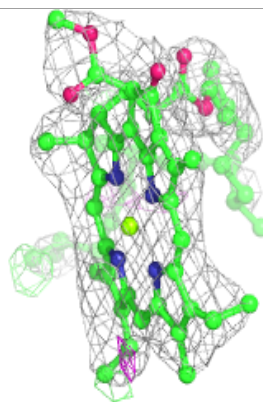
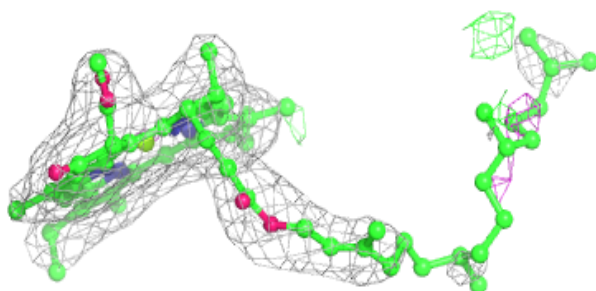
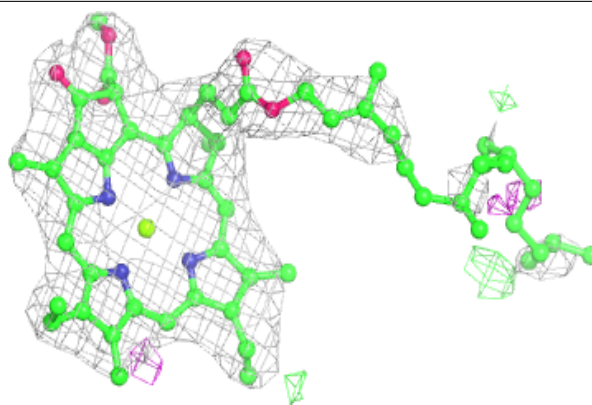
**Electron density around BCR c 514:**

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

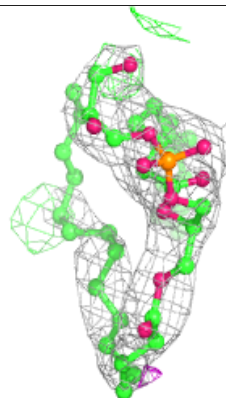
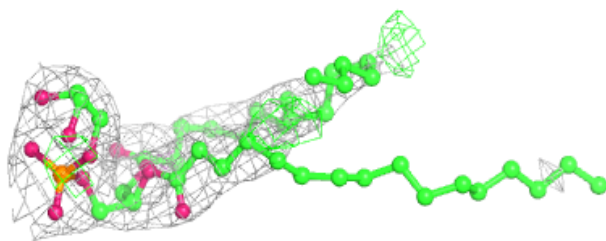
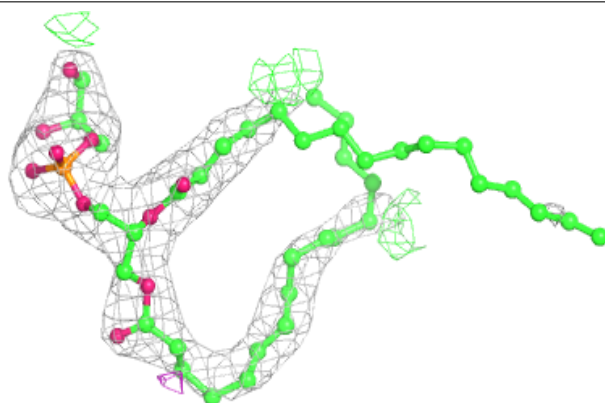


**Electron density around CLA a 408:**

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

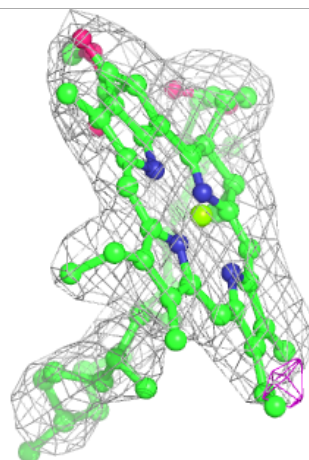
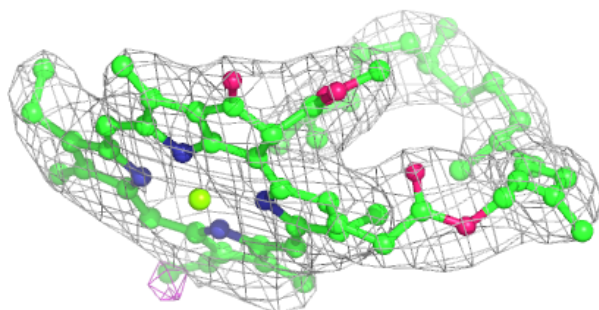
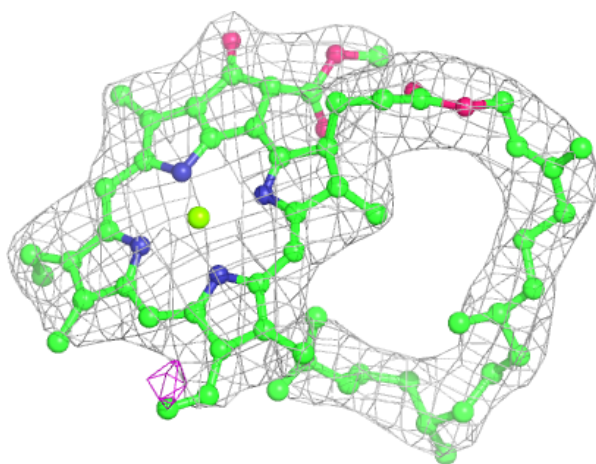
**Electron density around LHG D 409:**

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



**Electron density around CLA B 615:**

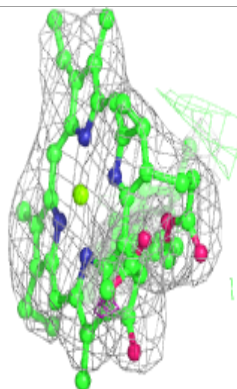
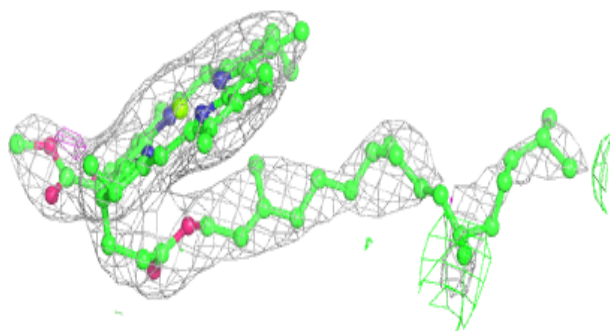
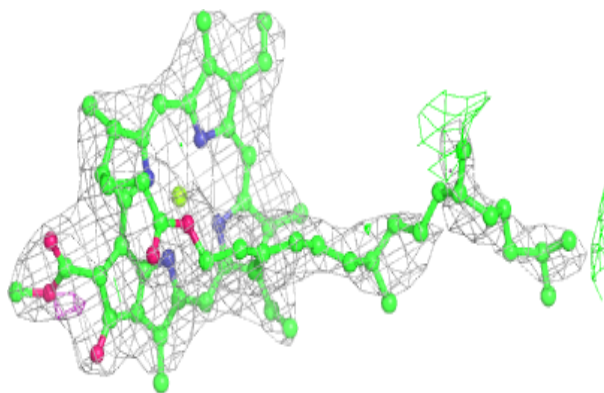
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



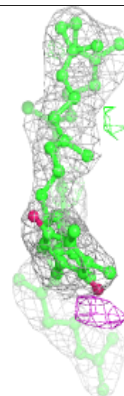
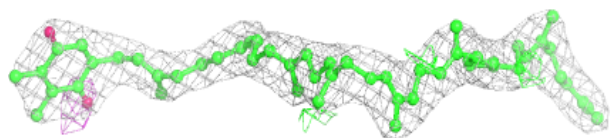
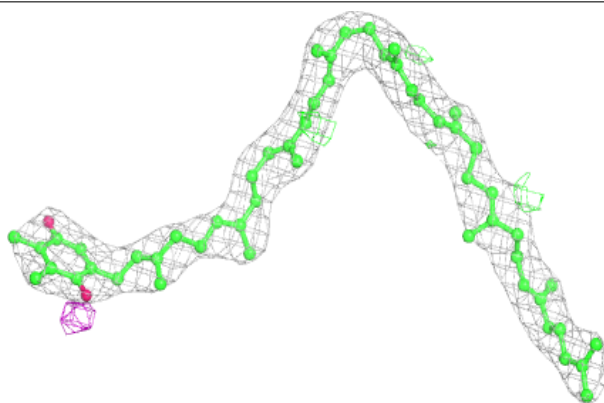


**Electron density around CLA b 614:**

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

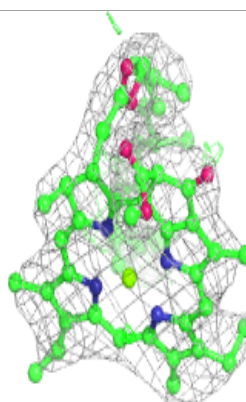
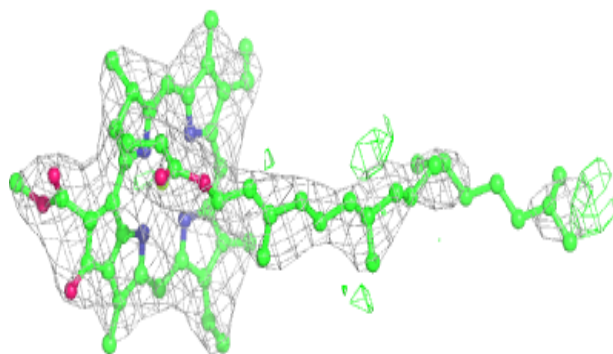
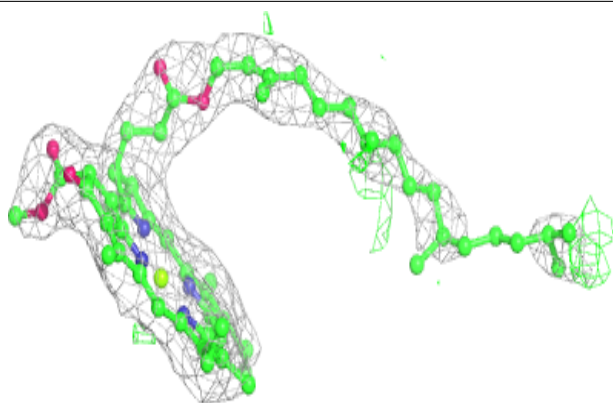
**Electron density around PL9 D 407:**

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

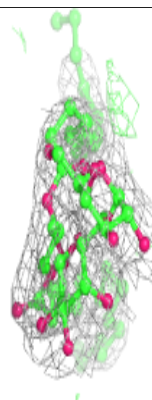
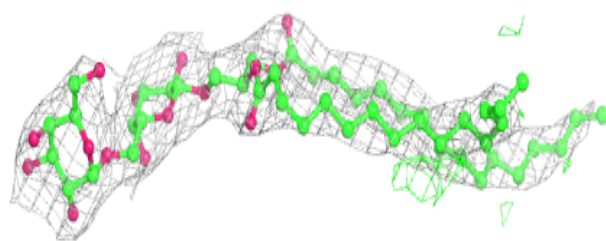
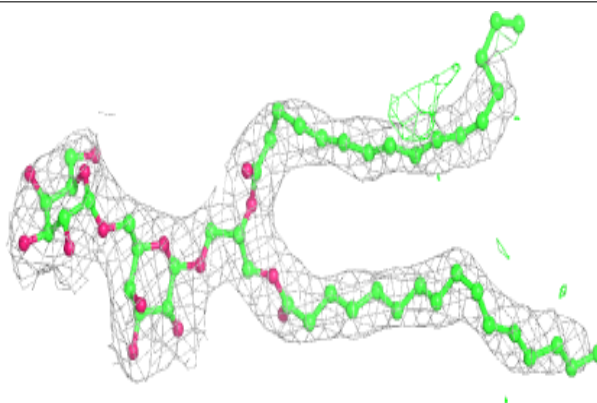


**Electron density around CLA c 504:**

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

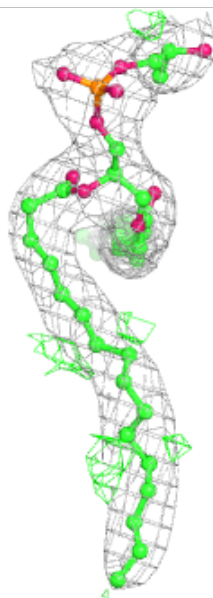
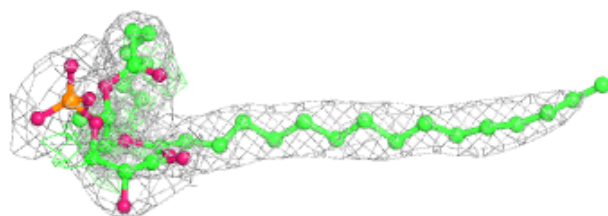
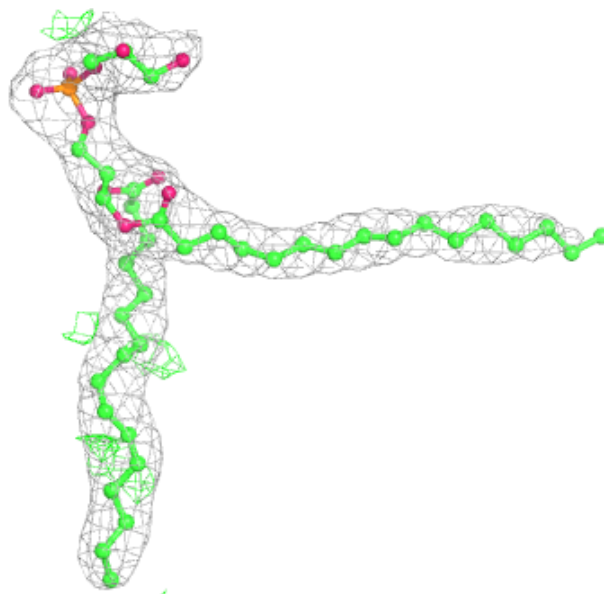
**Electron density around DGD c 518:**

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



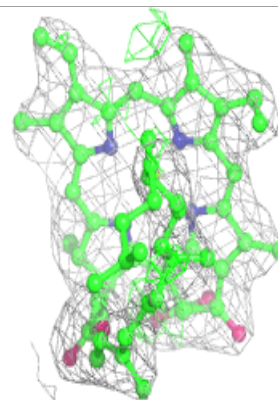
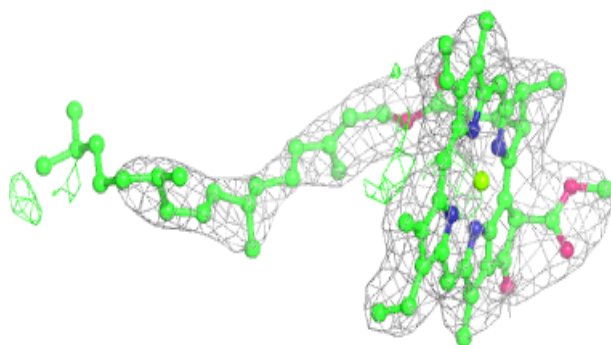
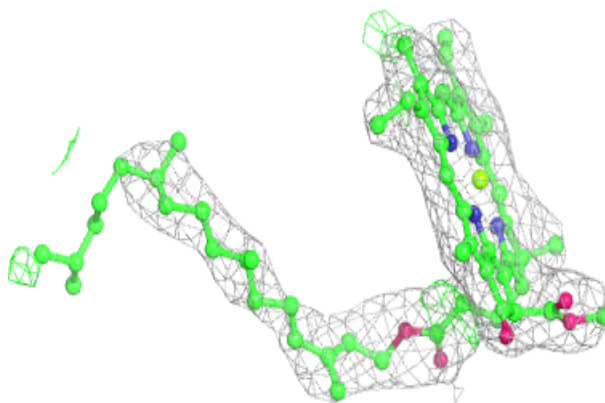
**Electron density around LHG A 417:**

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

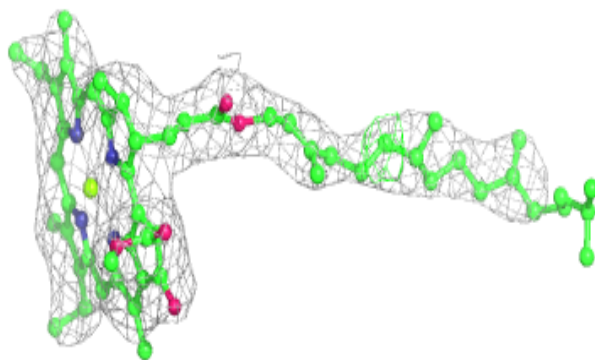
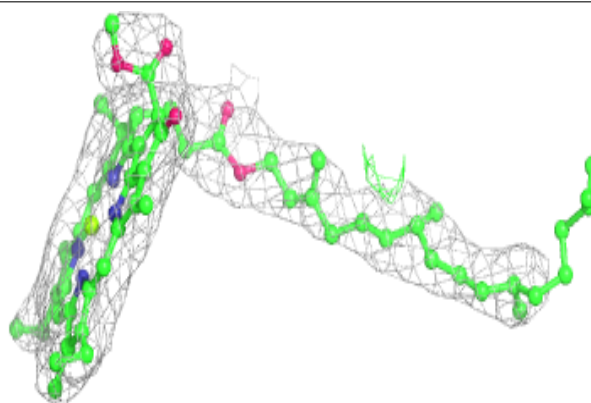


**Electron density around CLA C 509:**

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

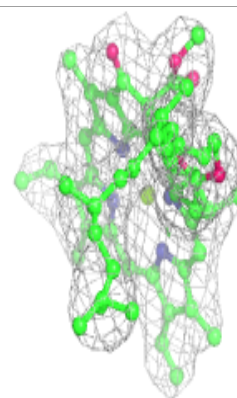
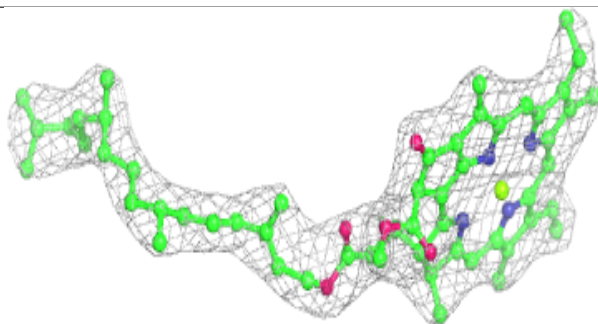
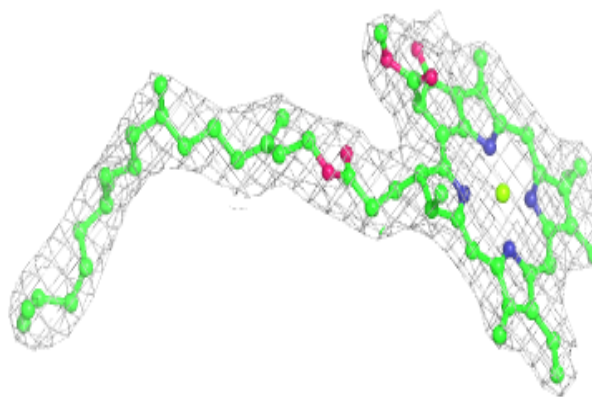
**Electron density around CLA b 604:**

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

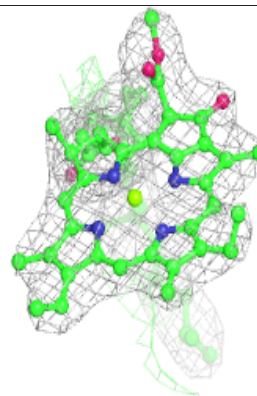
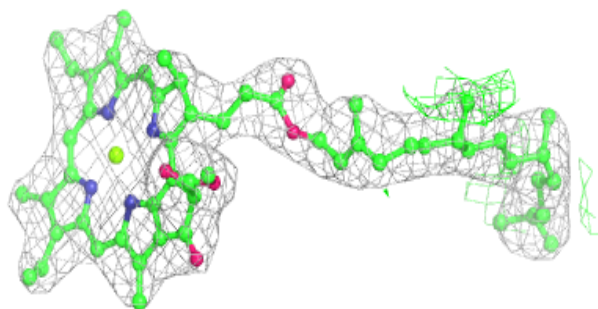
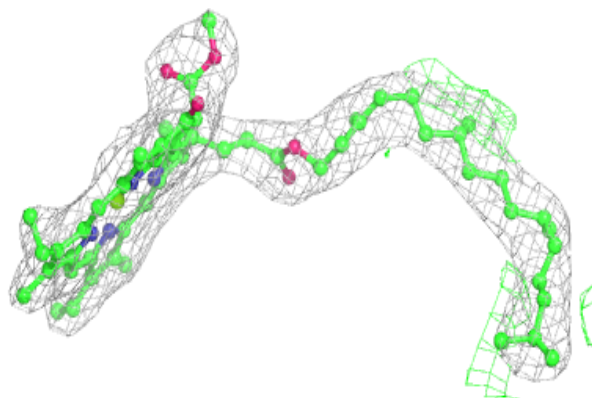


**Electron density around CLA A 404:**

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

**Electron density around CLA D 404:**

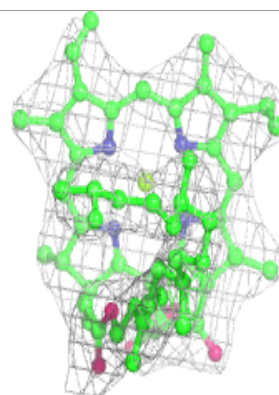
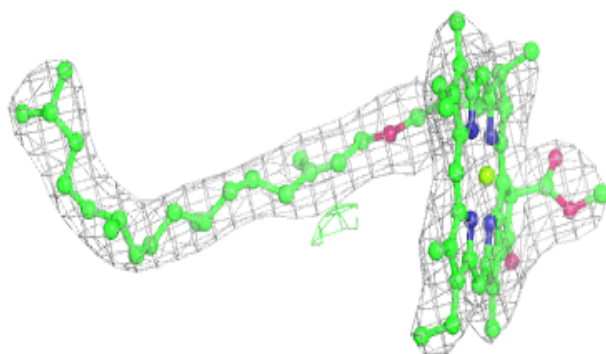
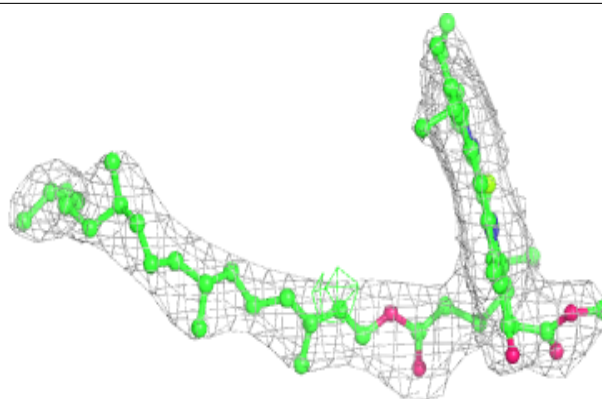
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



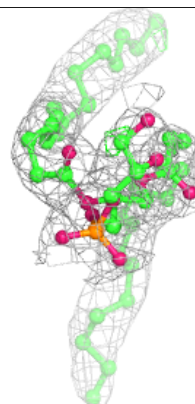
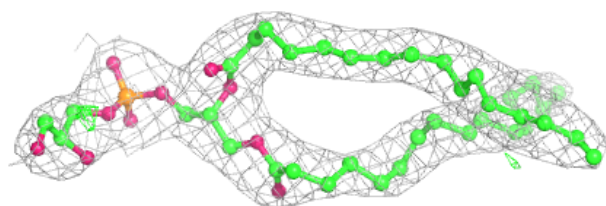
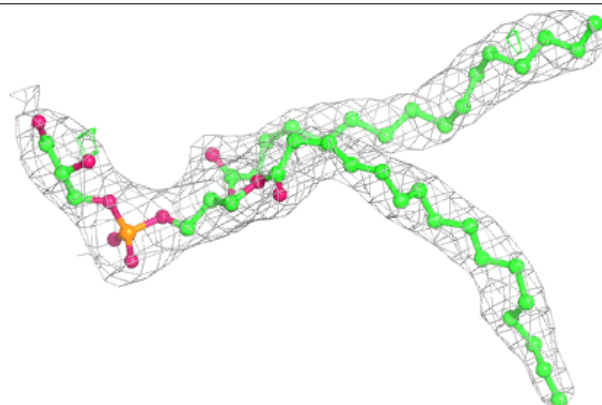


**Electron density around CLA B 605:**

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

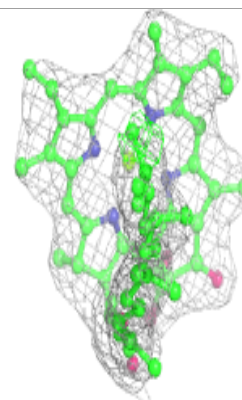
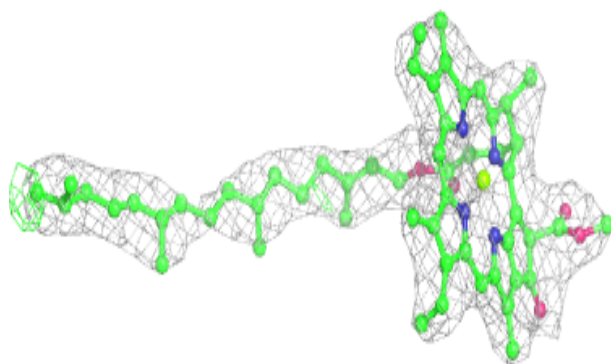
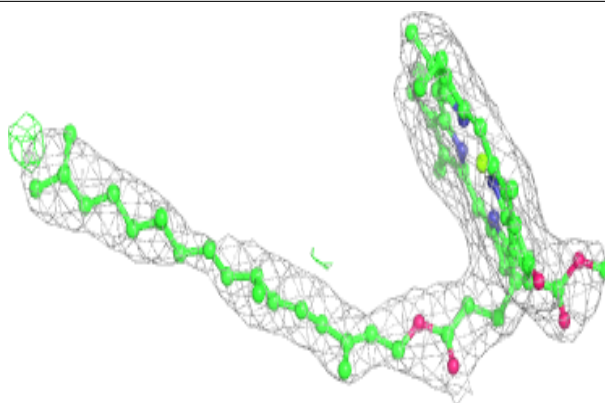
**Electron density around LHG D 408:**

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

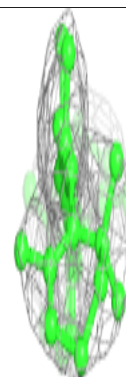
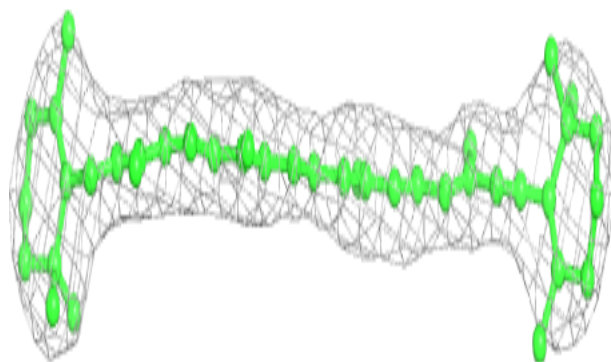
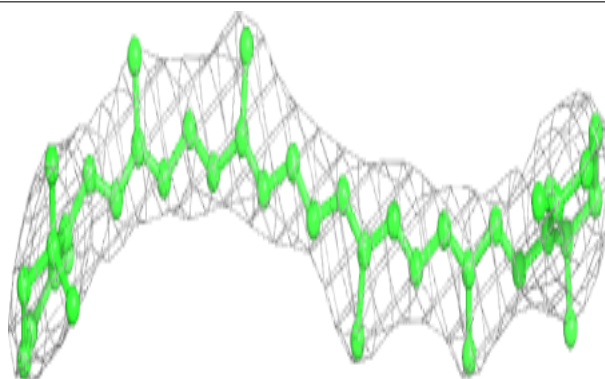


**Electron density around CLA B 607:**

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

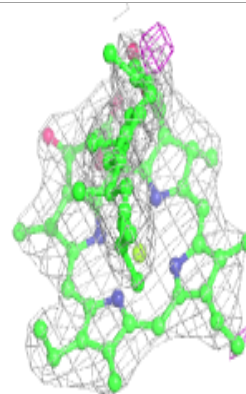
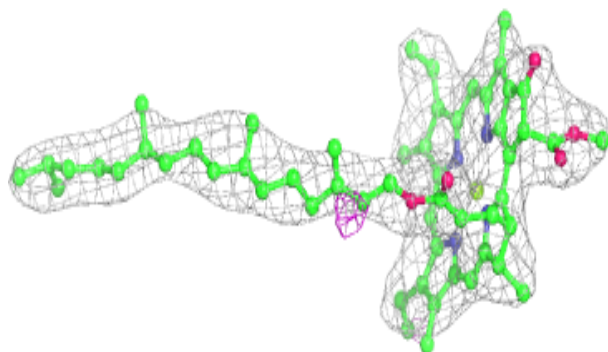
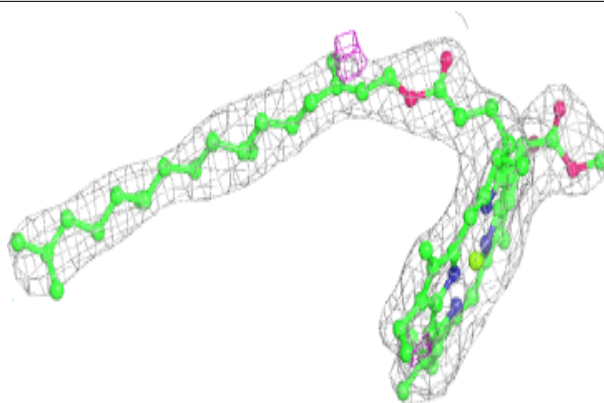
**Electron density around BCR c 515:**

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

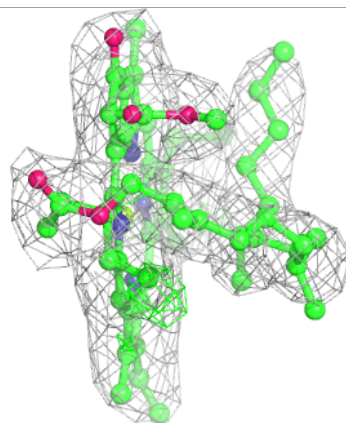
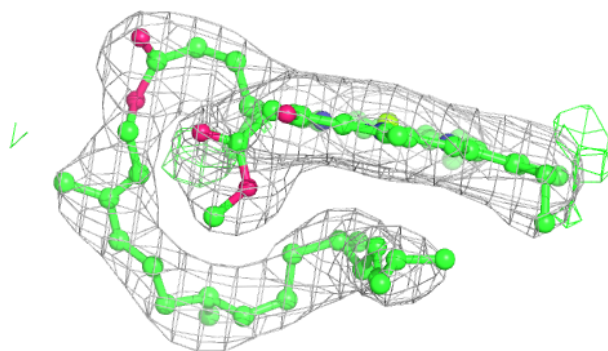
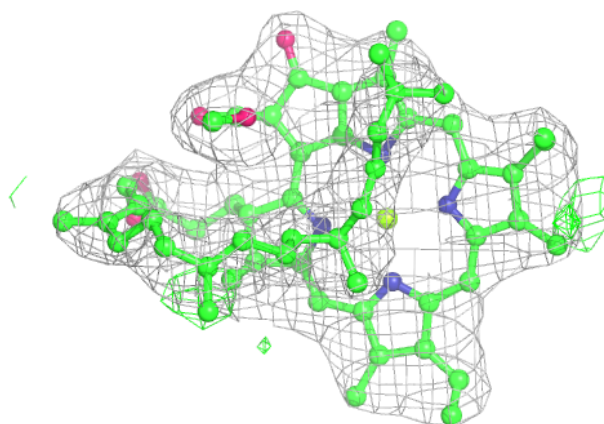


**Electron density around CLA b 607:**

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

**Electron density around CLA C 511:**

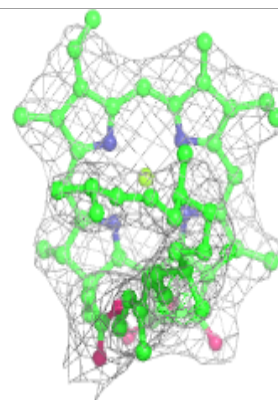
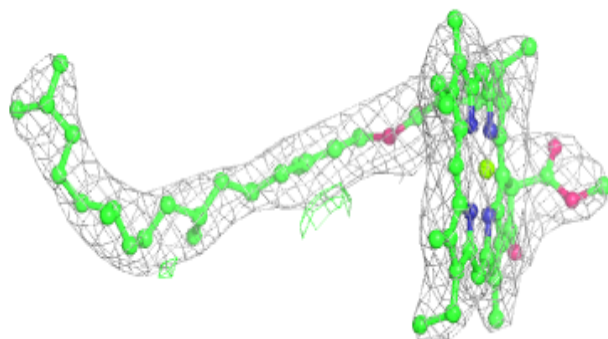
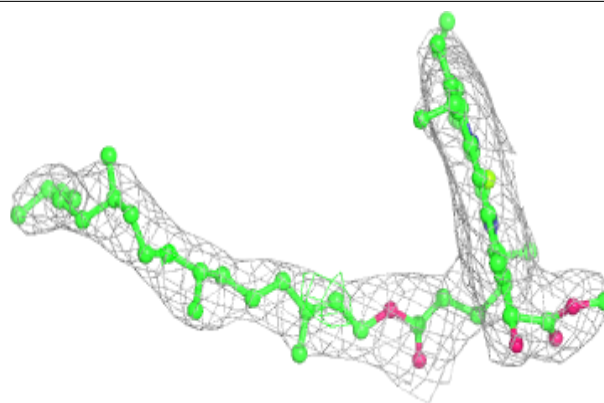
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



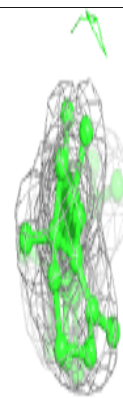
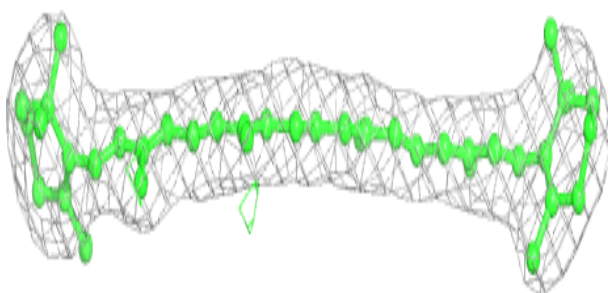
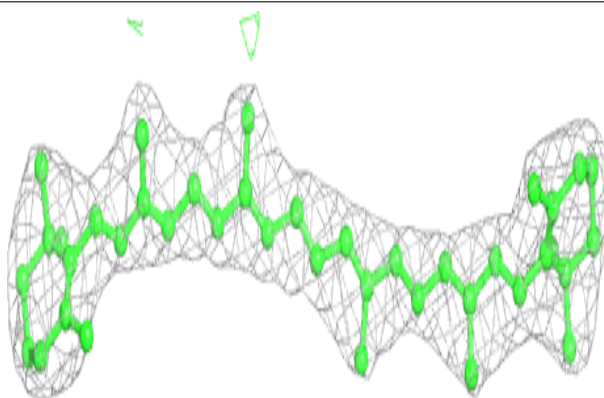


**Electron density around CLA b 605:**

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

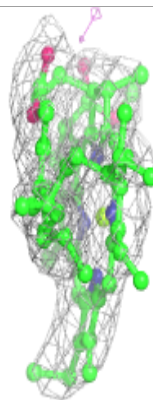
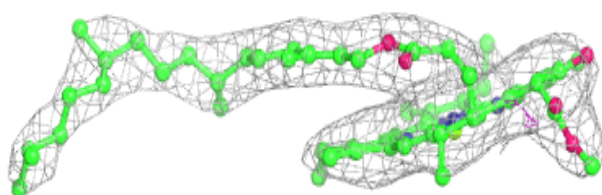
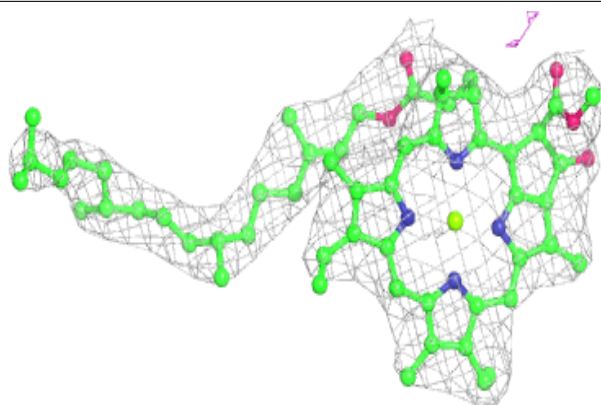
**Electron density around BCR b 618:**

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

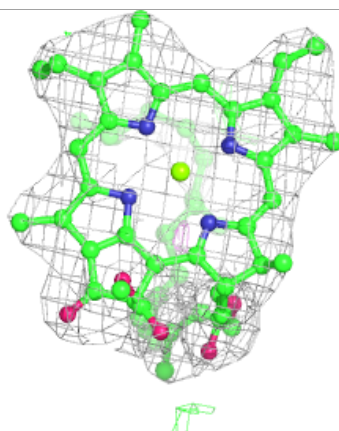
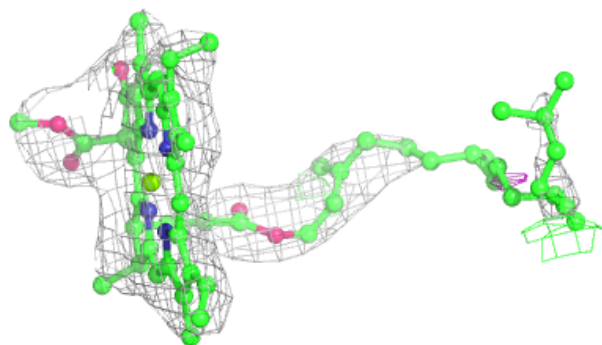
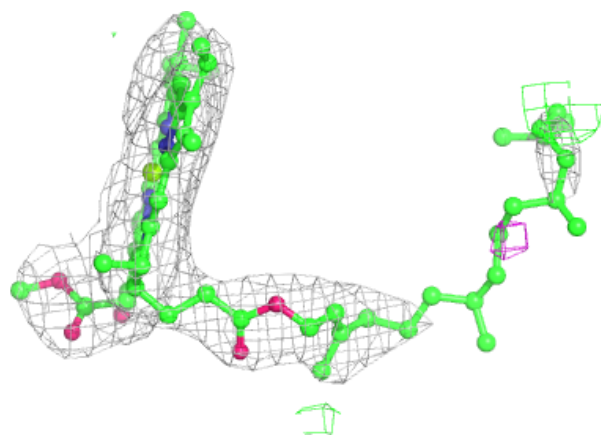


**Electron density around CLA b 603:**

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

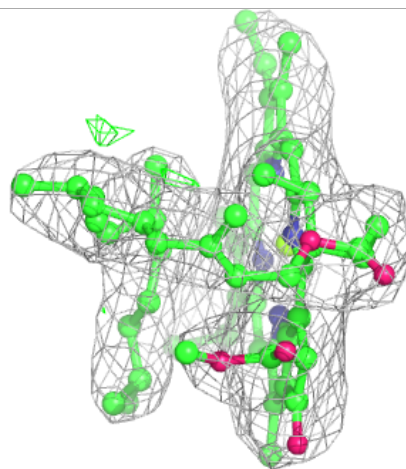
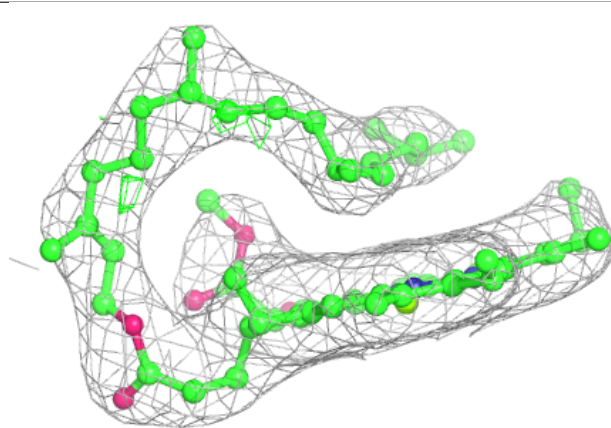
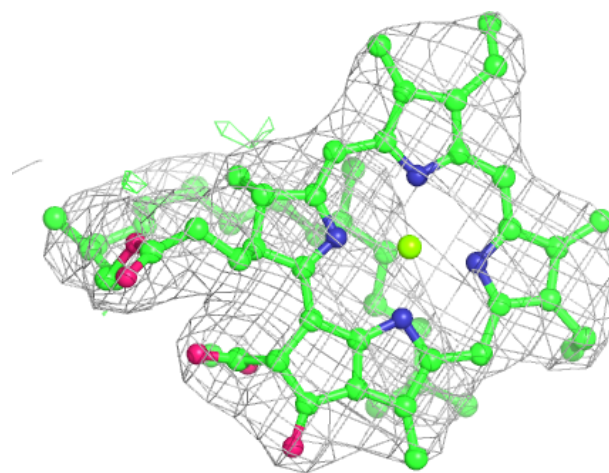
**Electron density around CLA c 506:**

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



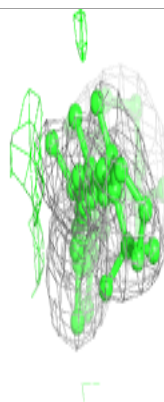
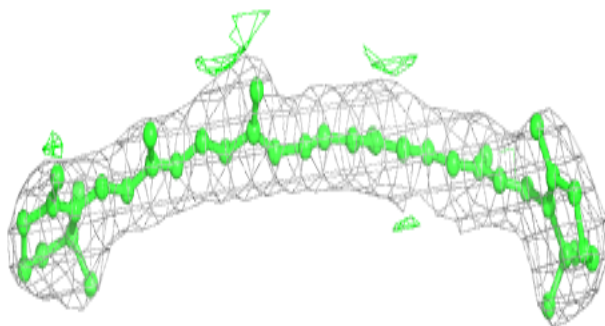
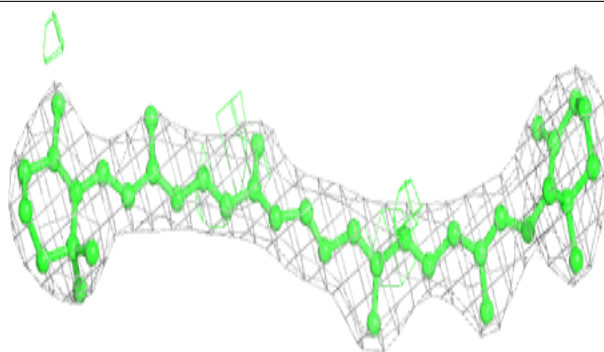
**Electron density around CLA c 510:**

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

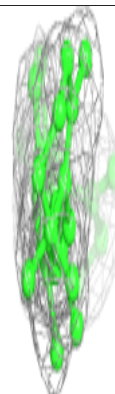
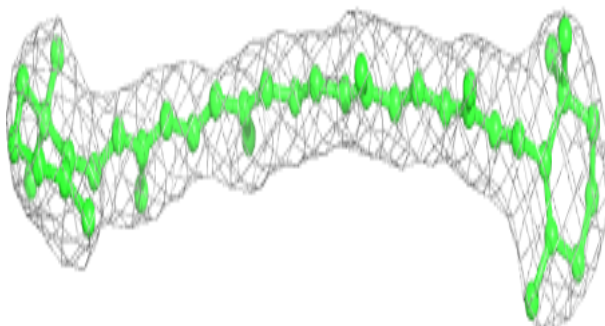
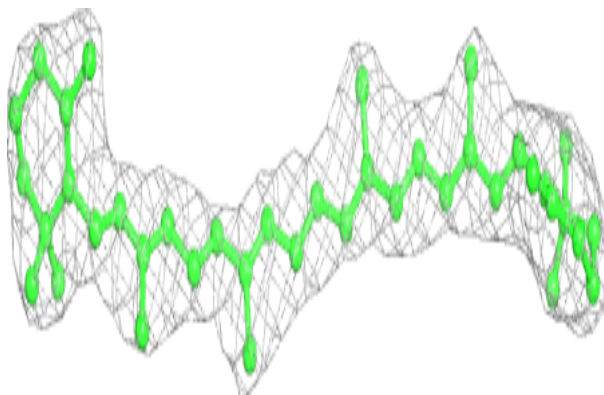


**Electron density around BCR T 101:**

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

**Electron density around BCR b 617:**

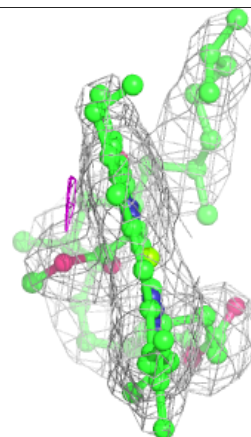
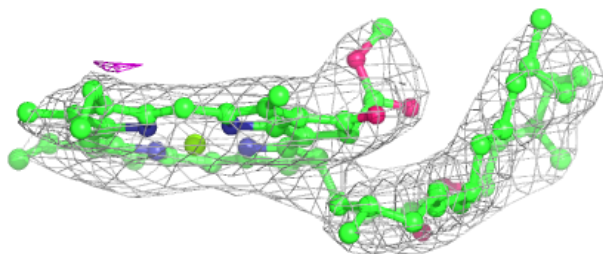
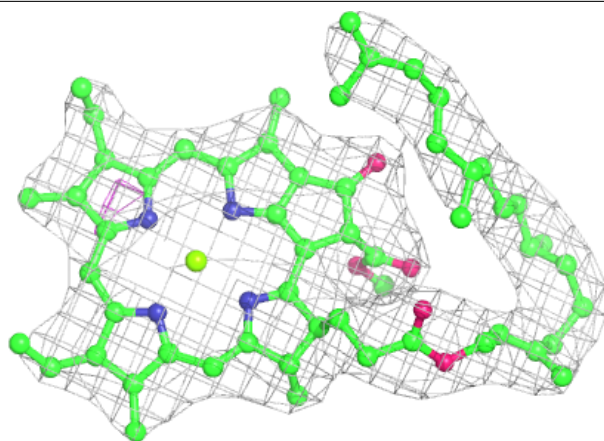
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



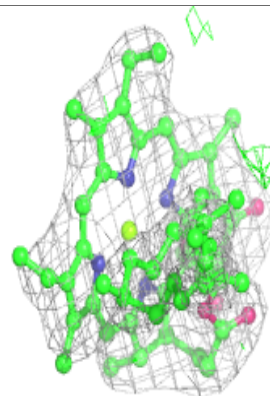
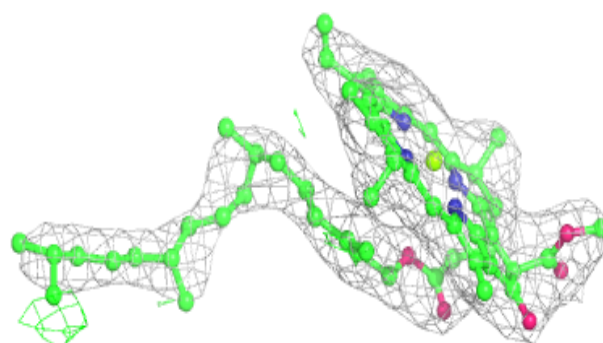
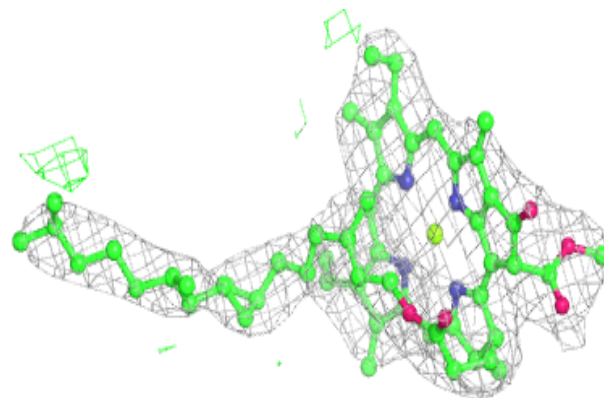


**Electron density around CLA b 610:**

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

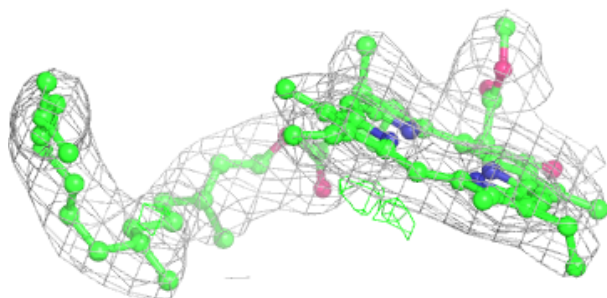
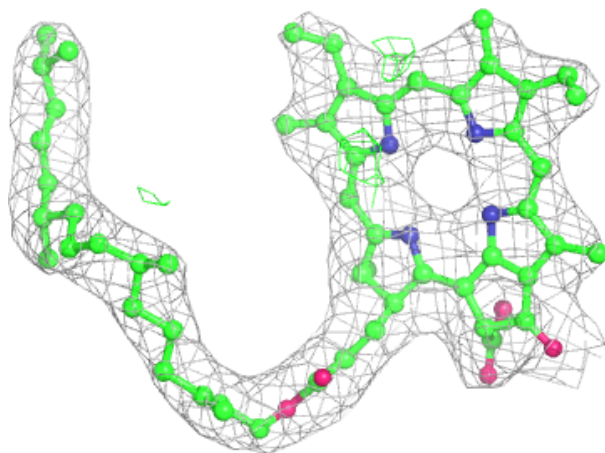
**Electron density around CLA C 506:**

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



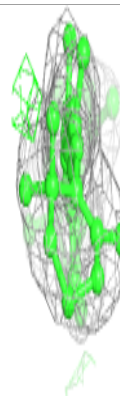
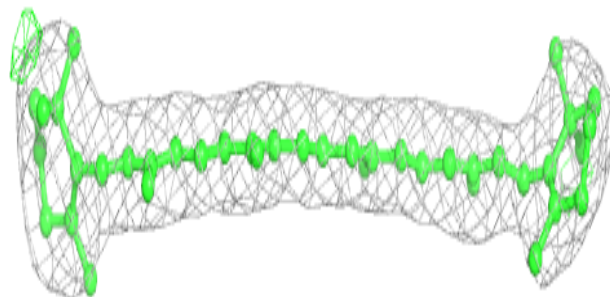
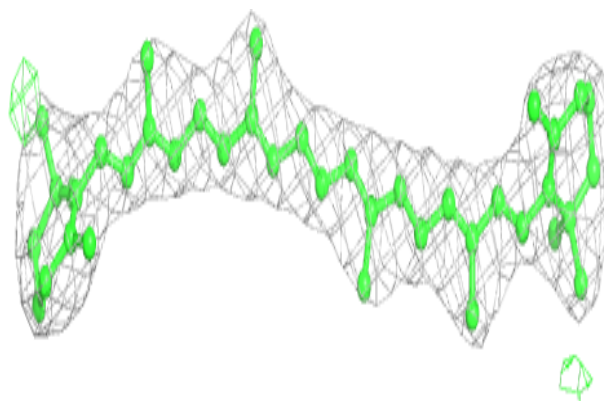
**Electron density around PHO a 407:**

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

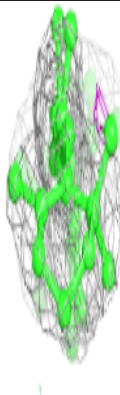
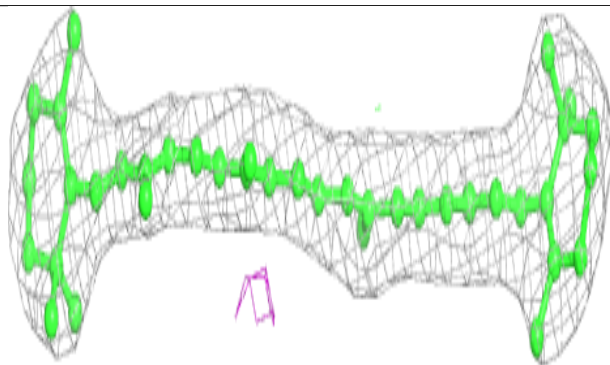
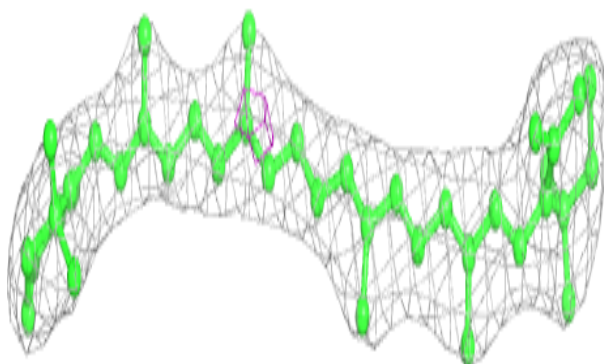


**Electron density around BCR B 618:**

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

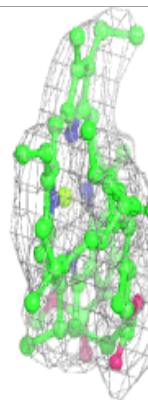
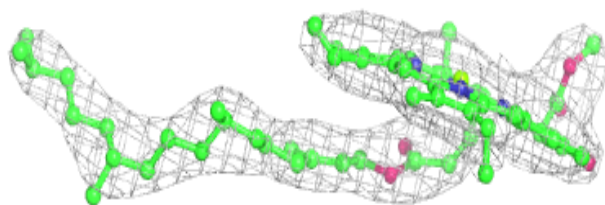
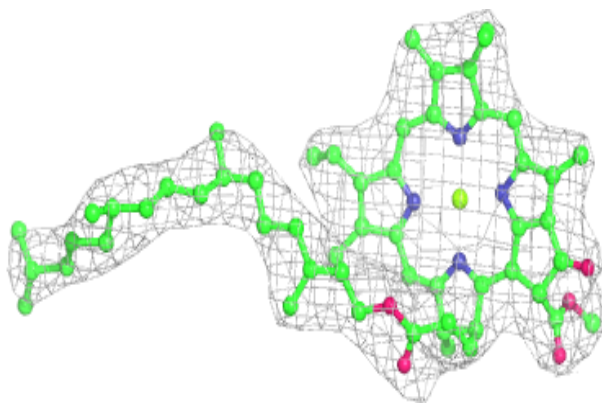
**Electron density around BCR a 409:**

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

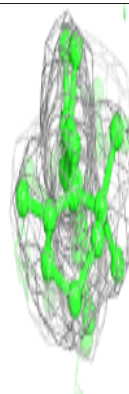
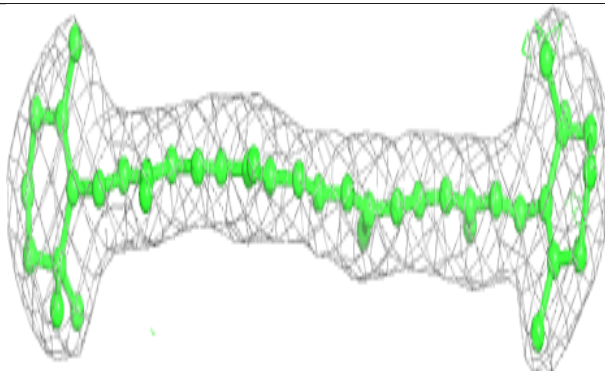
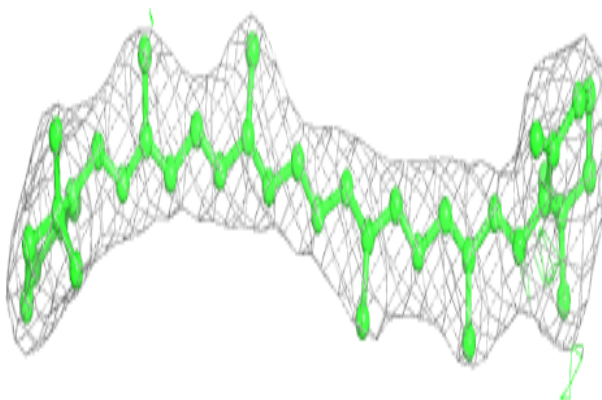


**Electron density around CLA B 603:**

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

**Electron density around BCR A 409:**

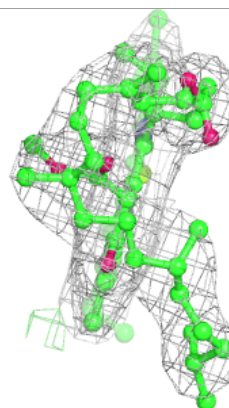
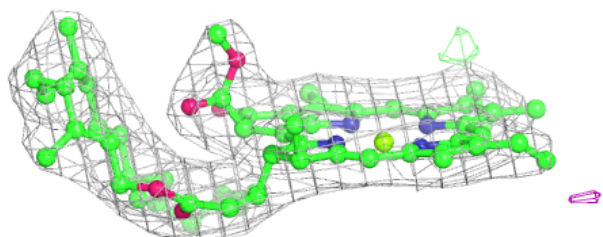
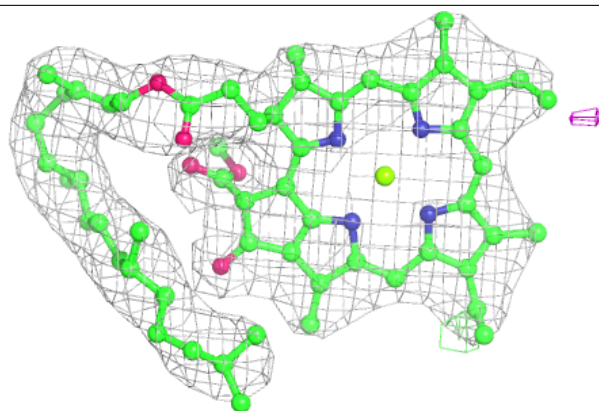
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



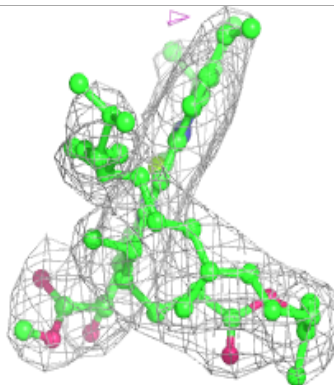
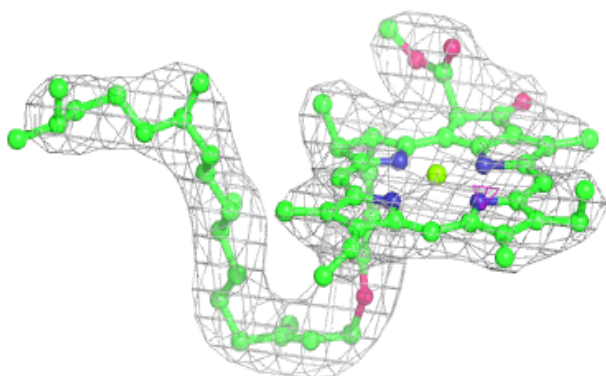
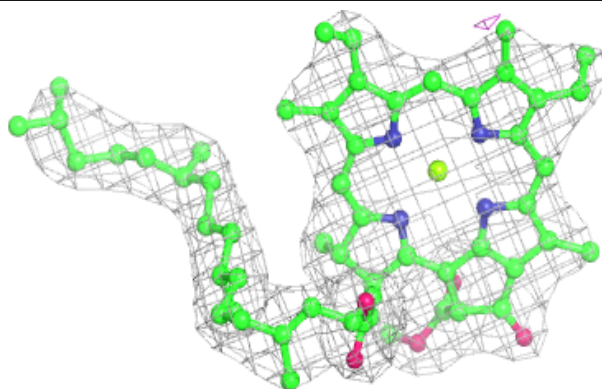


**Electron density around CLA B 610:**

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

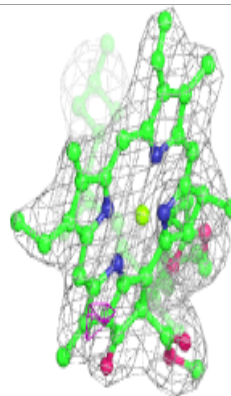
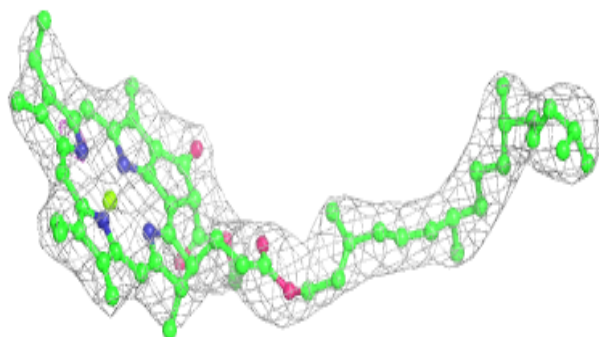
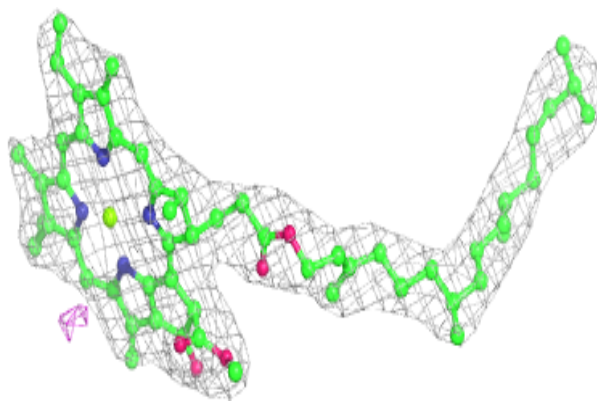
**Electron density around CLA d 401:**

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

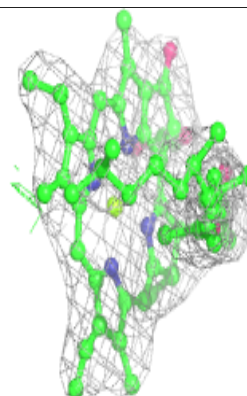
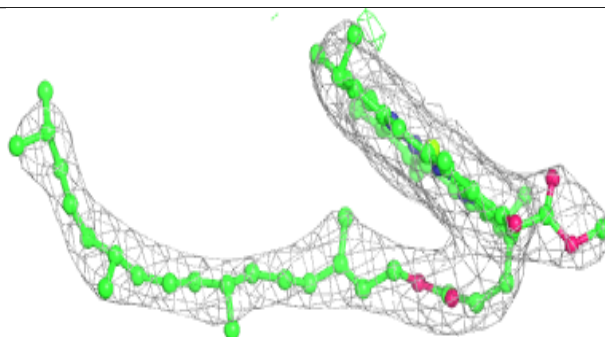
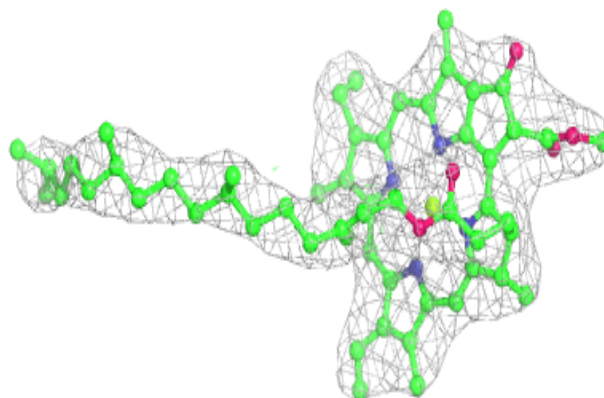


**Electron density around CLA a 404:**

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

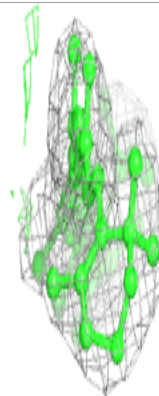
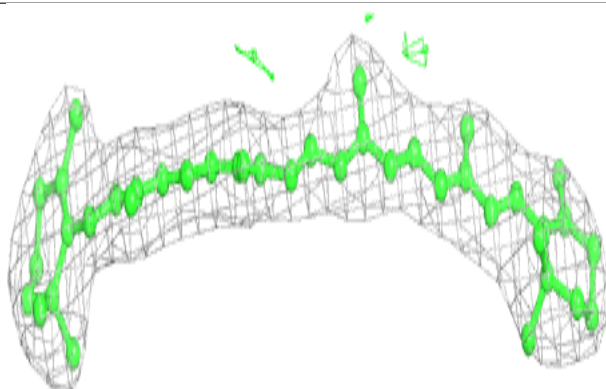
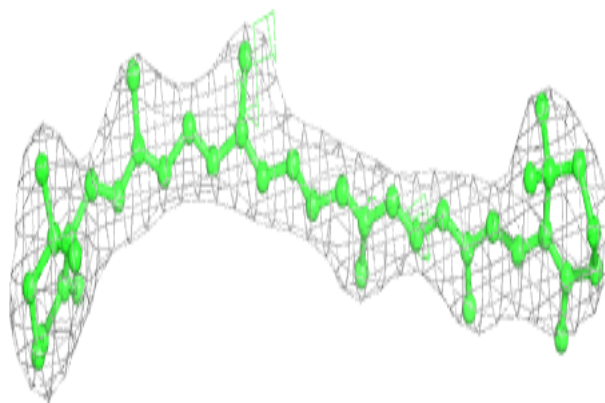
**Electron density around CLA b 608:**

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

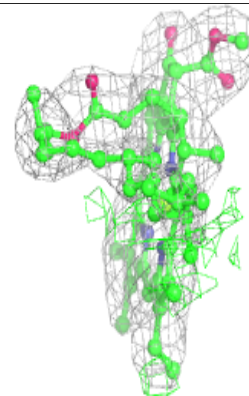
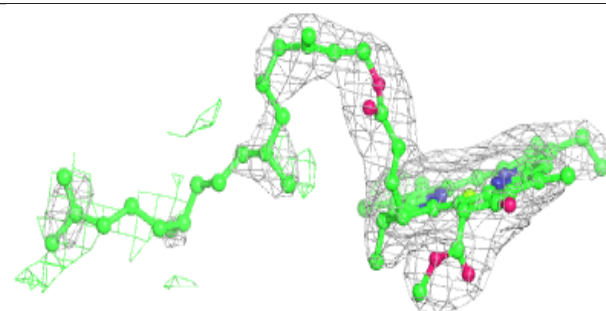
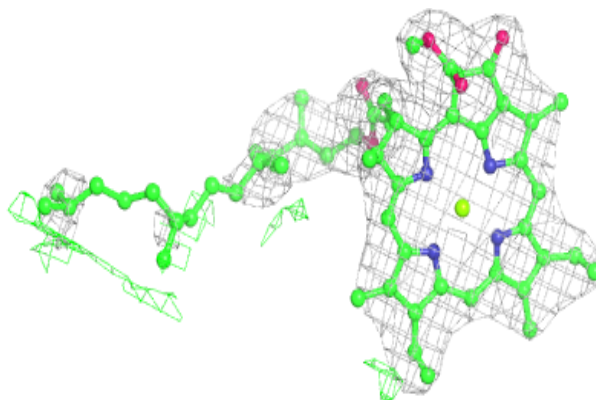


**Electron density around BCR t 101:**

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

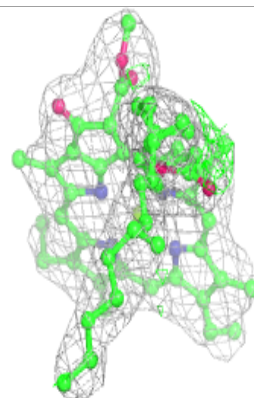
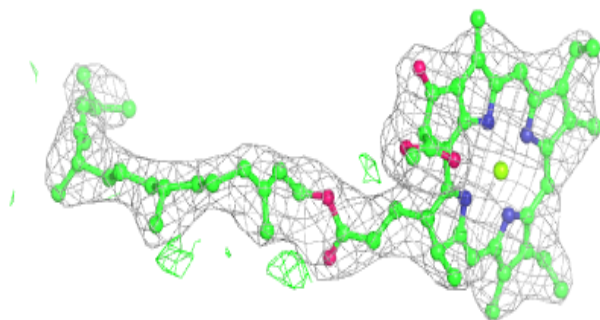
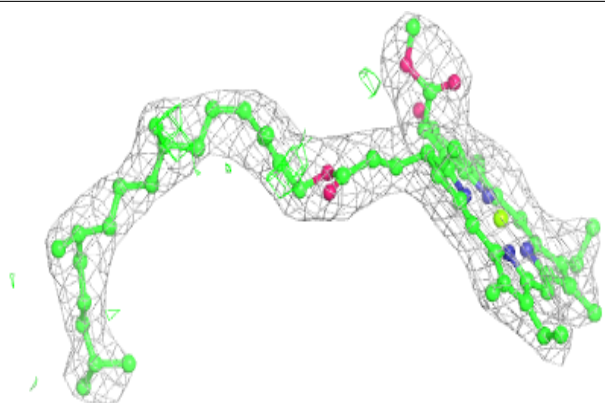
**Electron density around CLA a 405:**

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

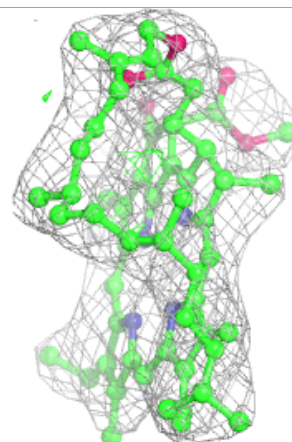
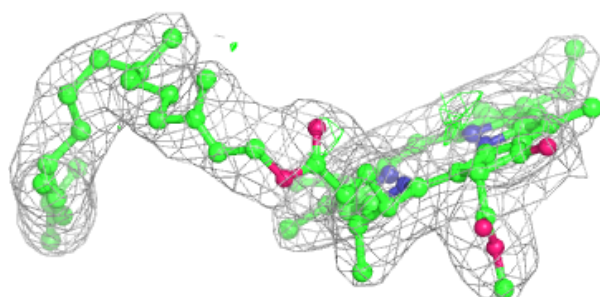
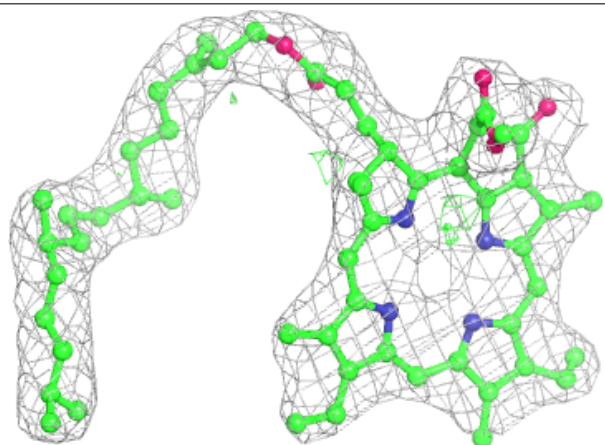


**Electron density around CLA d 403:**

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

**Electron density around PHO A 407:**

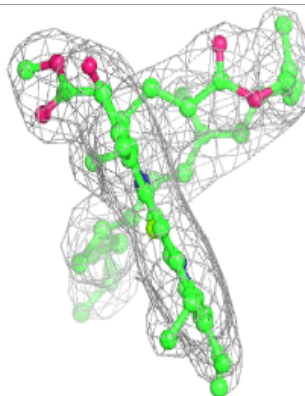
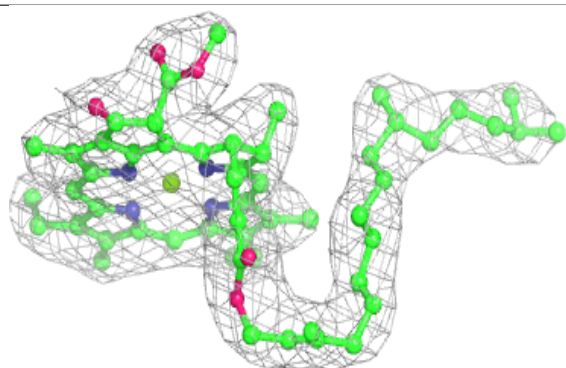
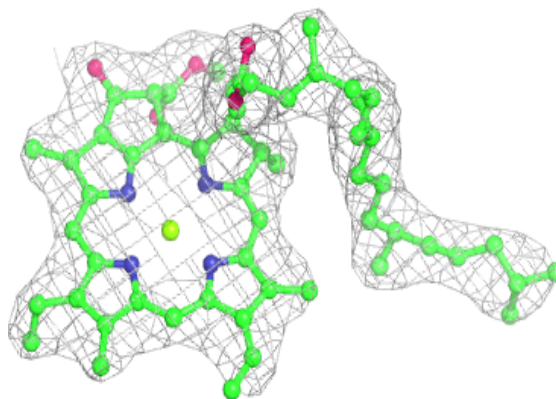
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





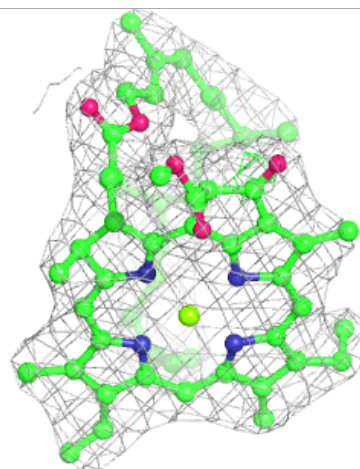
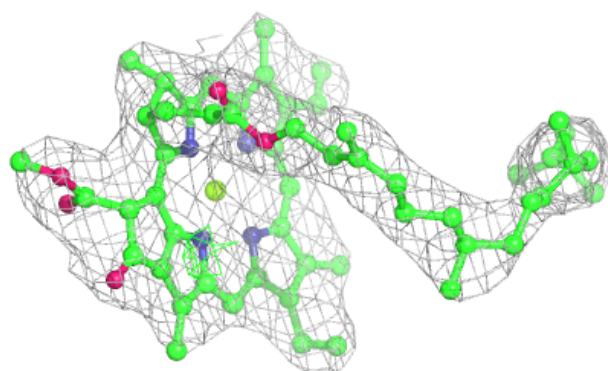
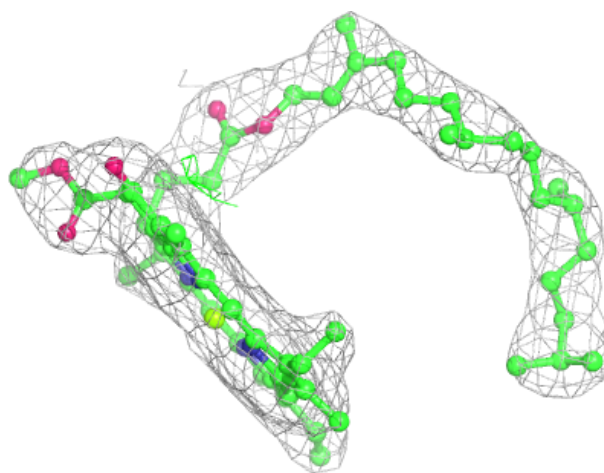
**Electron density around CLA A 405:**

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



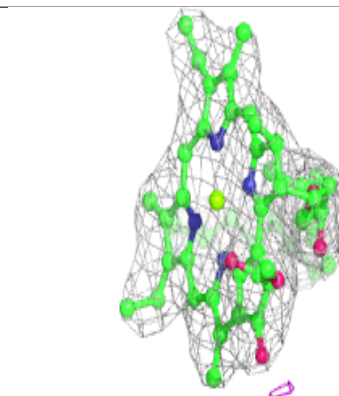
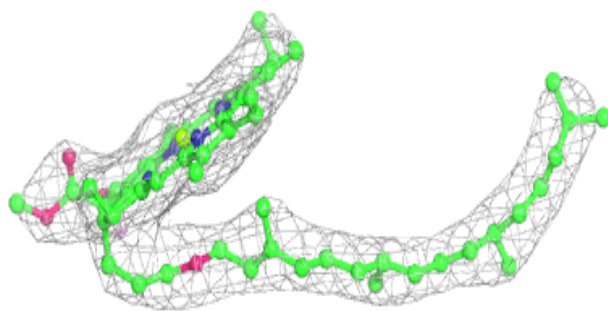
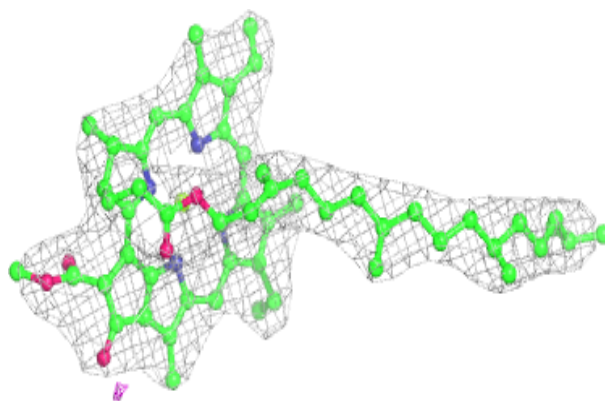
**Electron density around CLA b 611:**

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

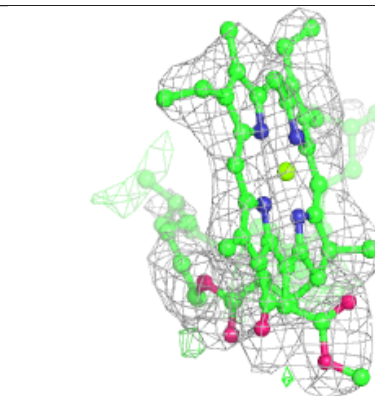
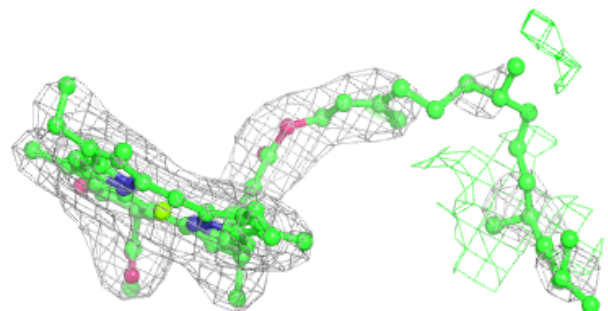
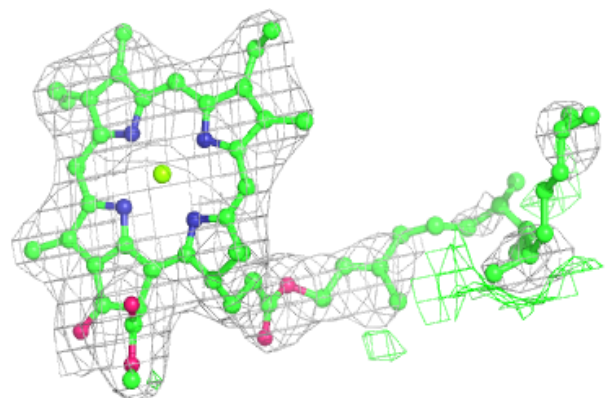


**Electron density around CLA B 608:**

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

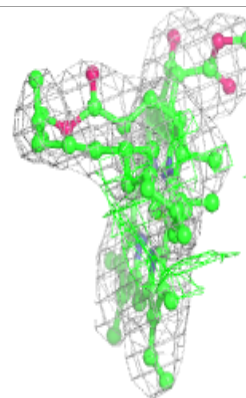
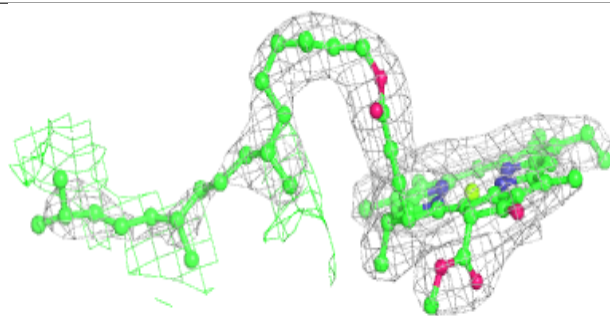
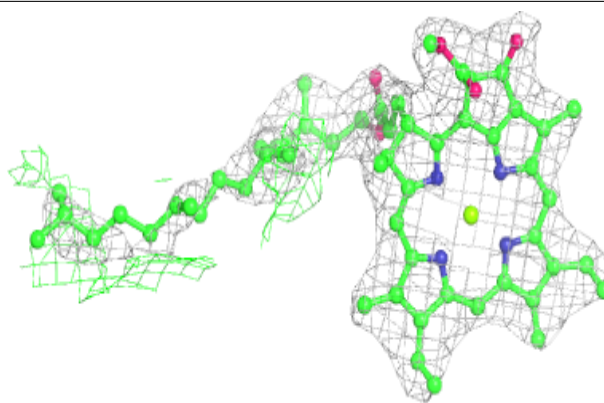
**Electron density around CLA A 408:**

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



**Electron density around CLA A 406:**

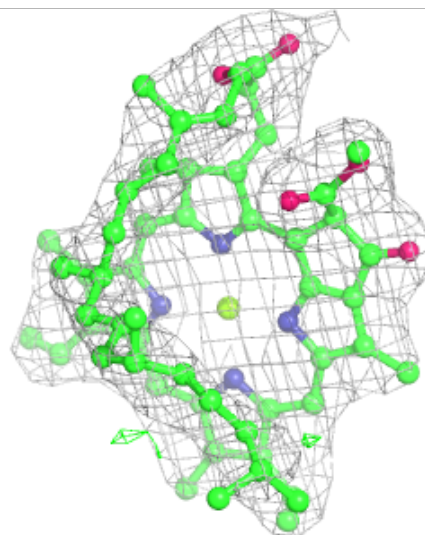
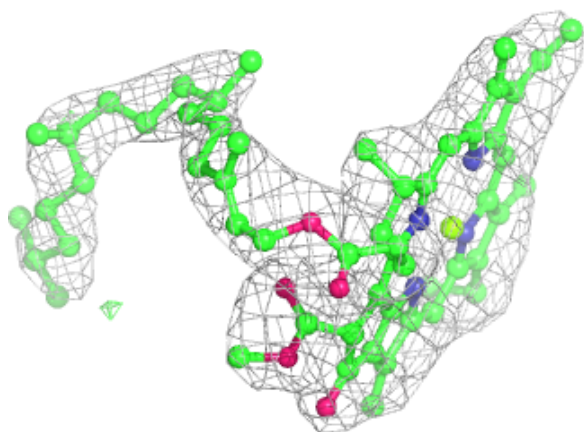
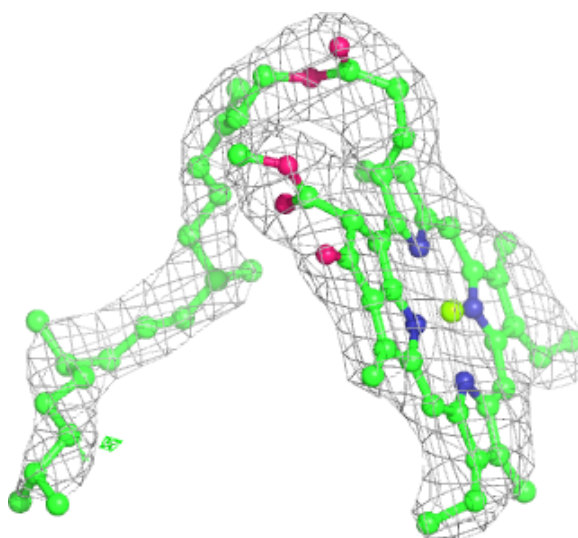
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





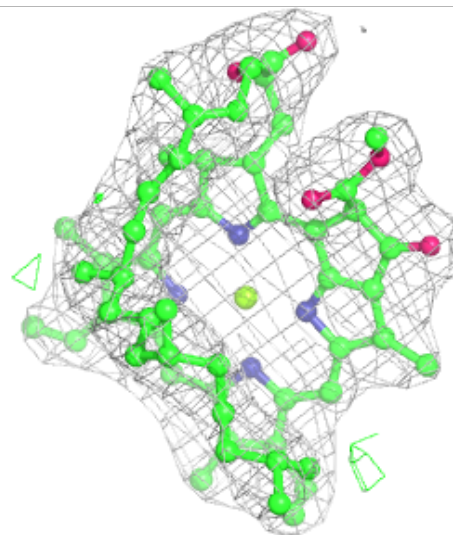
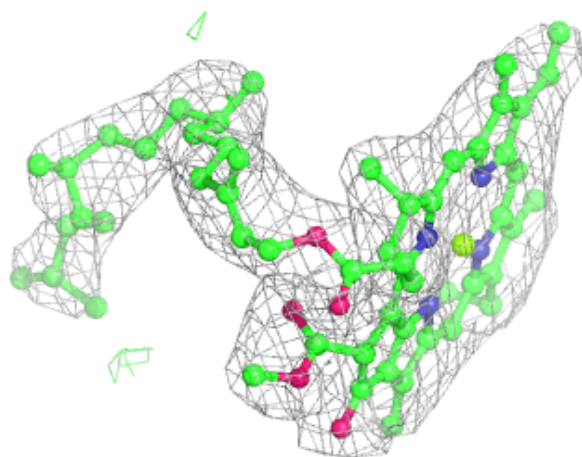
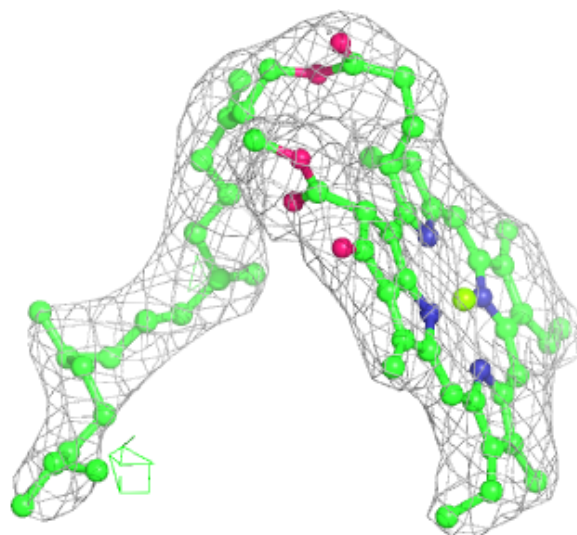
**Electron density around CLA b 613:**

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



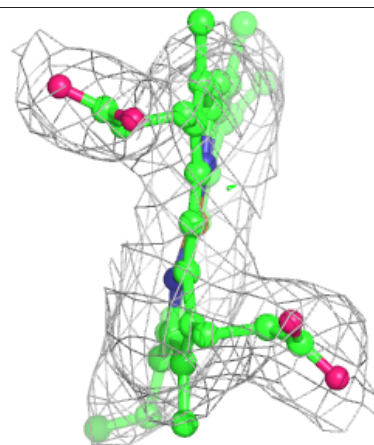
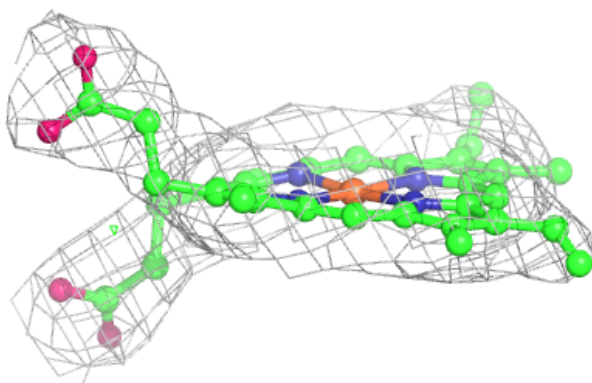
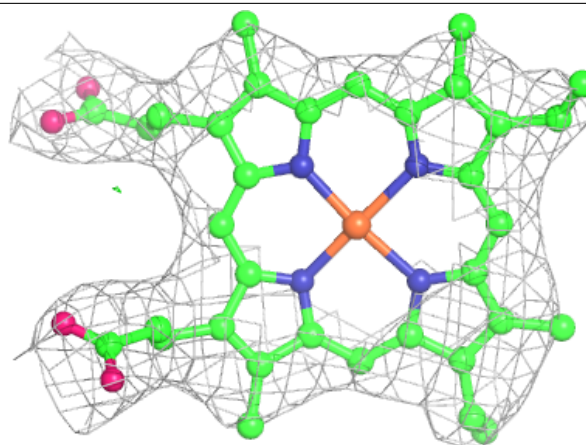
**Electron density around CLA B 613:**

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



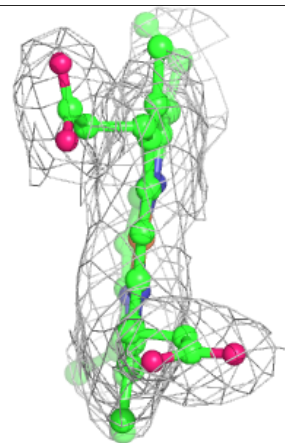
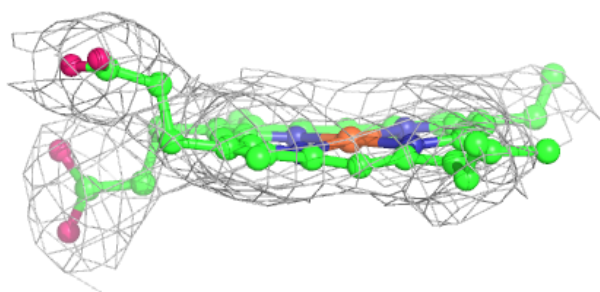
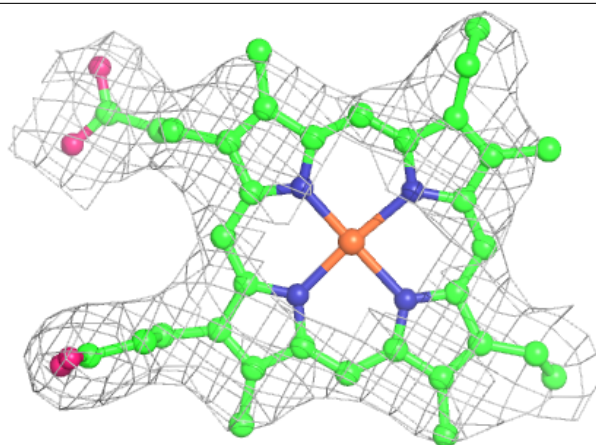
**Electron density around HEM E 103:**

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



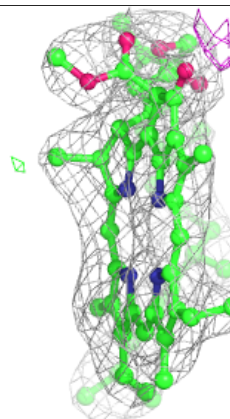
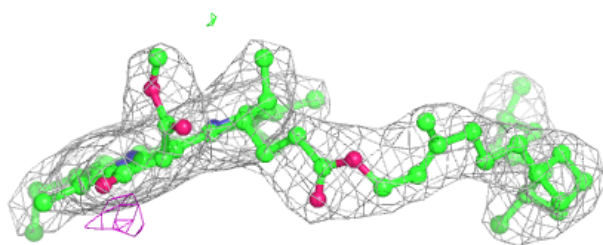
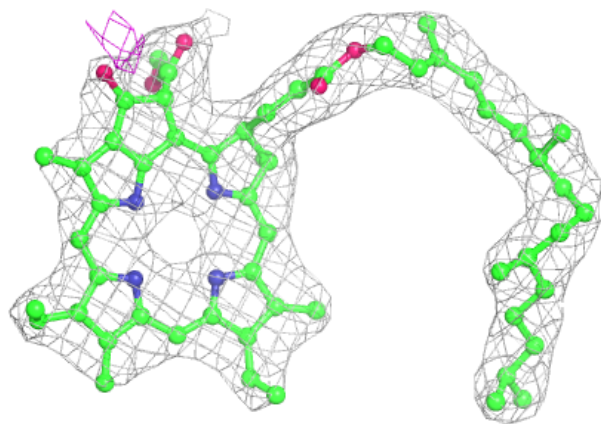
**Electron density around HEC V 202:**

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



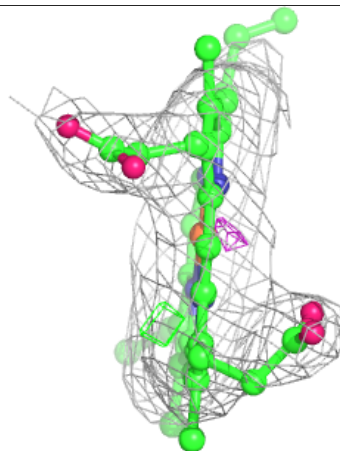
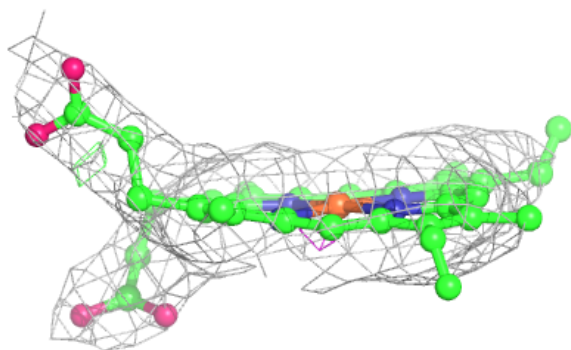
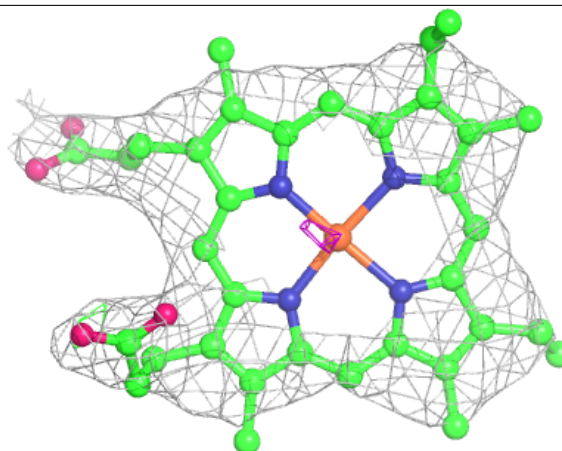
**Electron density around PHO a 406:**

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

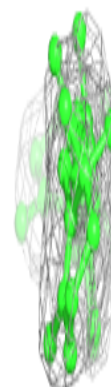
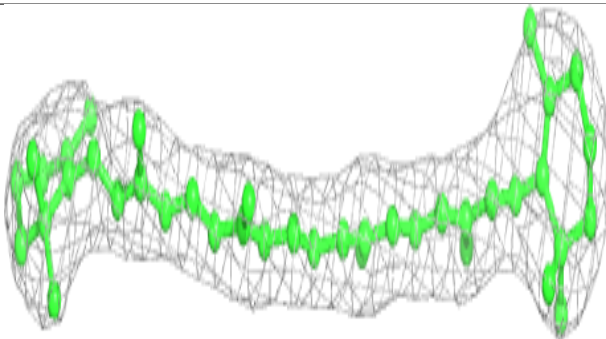
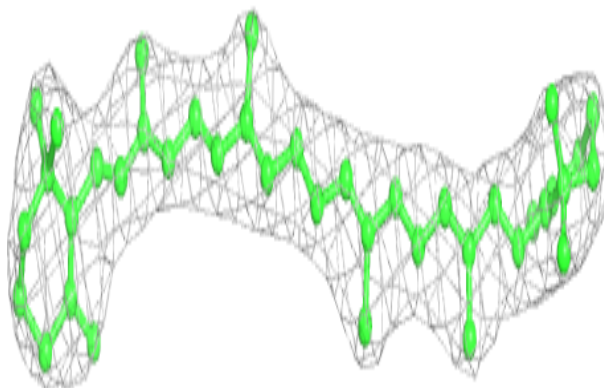


**Electron density around HEM e 103:**

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

**Electron density around BCR B 617:**

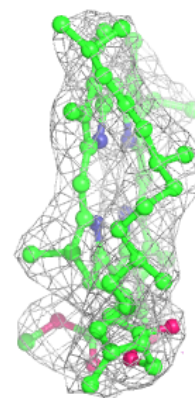
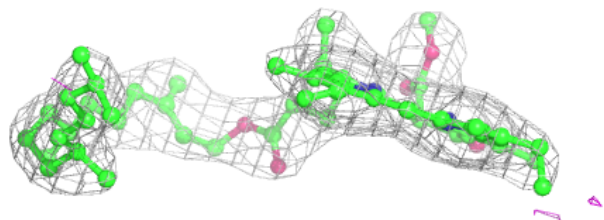
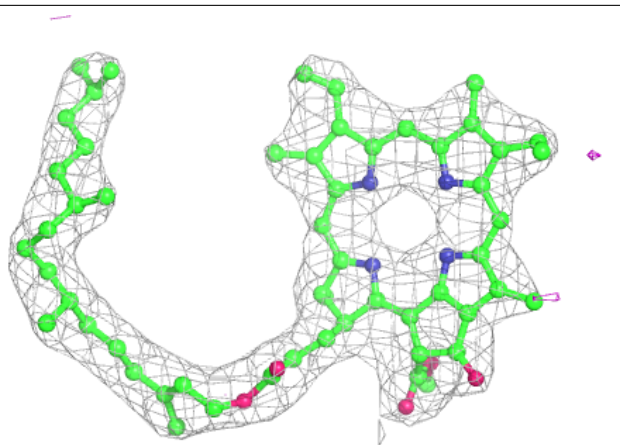
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





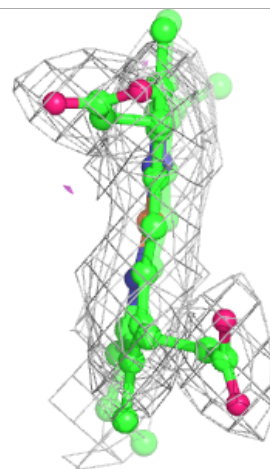
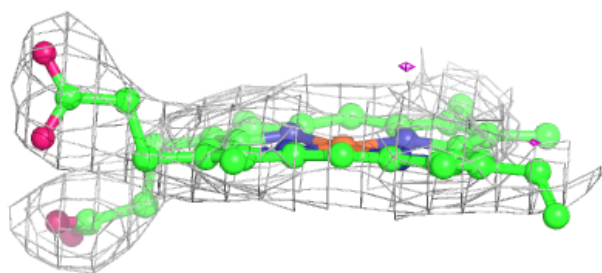
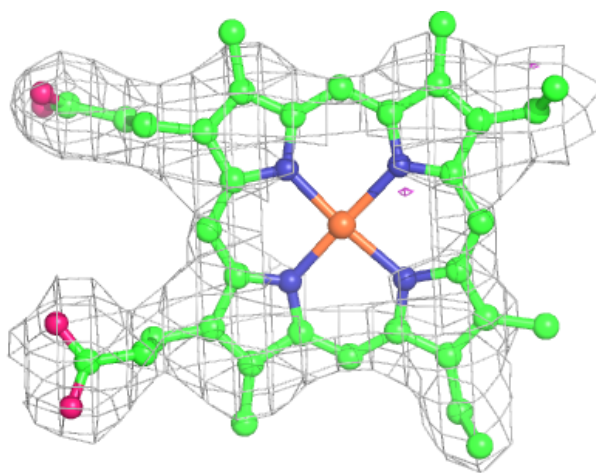
**Electron density around PHO D 401:**

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



**Electron density around HEC v 201:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.