



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 04:58 AM BST

PDB ID : 6JLO  
Title : XFEL structure of cyanobacterial photosystem II (2F state, dataset2)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
Resolution : 2.40 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

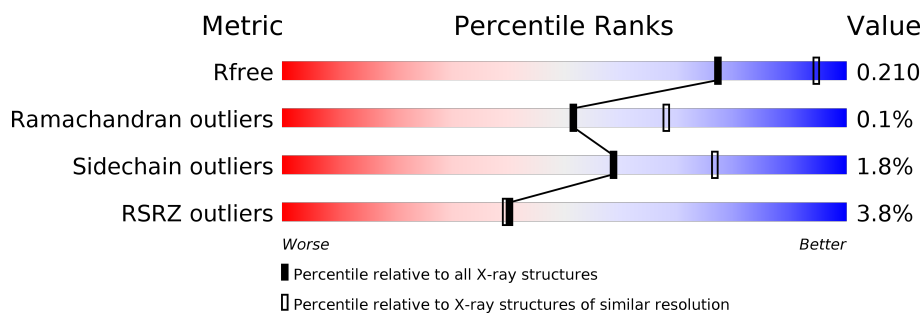
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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></div> <div>97%</div> <div>.</div> </div>
1	a	344	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>3%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div></div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	23% 96%
5	e	84	10% 95%
6	F	44	9% 77% 23%
6	f	44	2% 70% 27%
7	H	65	3% 97%
7	h	65	3% 98%
8	I	38	11% 95% 5%
8	i	38	8% 95% 5%
9	J	39	13% 97%
9	j	39	18% 100%
10	K	37	11% 100%
10	k	37	95% 5%
11	L	37	97%
11	l	37	100%
12	M	36	92% 6%
12	m	36	89% 6% 6%
13	O	244	2% 98%
13	o	244	2% 96%
14	T	32	3% 88% 6% 6%
14	t	32	3% 88% 6% 6%
15	U	104	% 89% 7%
15	u	104	% 91% 7%
16	V	137	% 100%
16	v	137	% 99%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	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	B	617	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	405	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	411	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	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	b	622	X	-	-	-
23	CLA	b	623	X	-	-	-
23	CLA	b	624	X	-	-	-
23	CLA	b	625	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	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	c	517	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-
27	GOL	V	201	-	-	-	X
28	LMT	F	101	-	-	-	X
28	LMT	a	418	-	-	-	X
28	LMT	b	630	-	-	-	X
37	DGD	d	408	-	-	-	X

## 2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 55695 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	54	0
			3024	1969	499	538	18			
1	a	334	Total	C	N	O	S	0	56	0
			3020	1970	497	535	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	UNP P51765

- 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	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	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	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	See sequence details	UNP D0VWR7
C	20	SER	-	See sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	UNP P19054

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	UNP P12312

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

- 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			

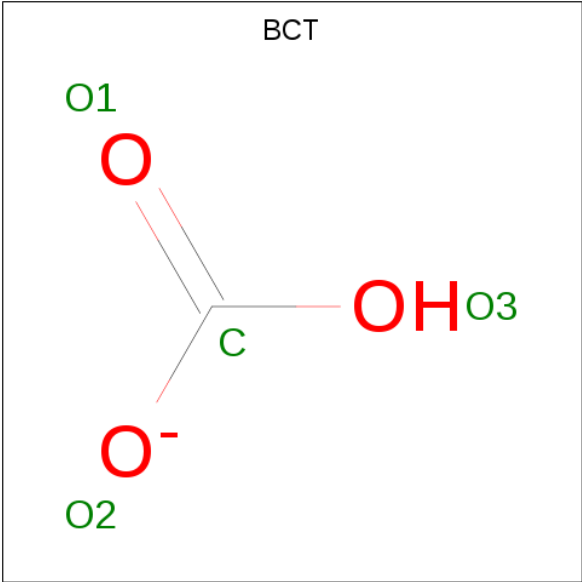
- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	S	98	0	0
			239	163	41	35				

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

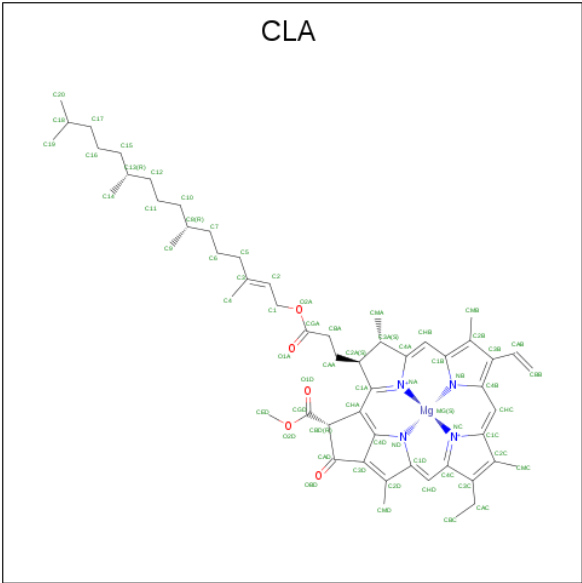
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	2
			4	4		
21	v	1	Total	Cl	0	0
			1	1		
21	a	2	Total	Cl	0	2
			4	4		
21	U	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	1
			8	2	6		
22	d	1	Total	C	O	0	1
			8	2	6		

- 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>).



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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	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	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

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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	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

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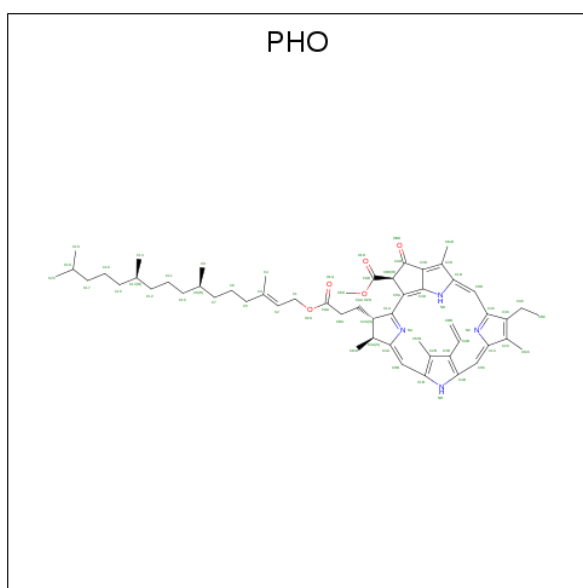
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

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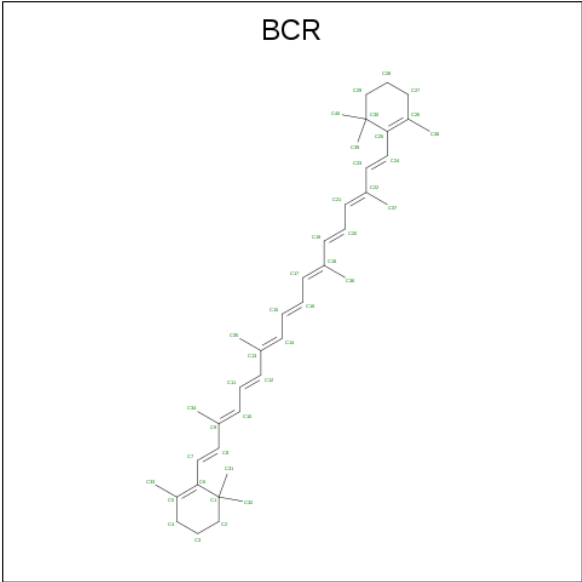
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	d	1	Total	C	N	O	0	1
			128	110	8	10		

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



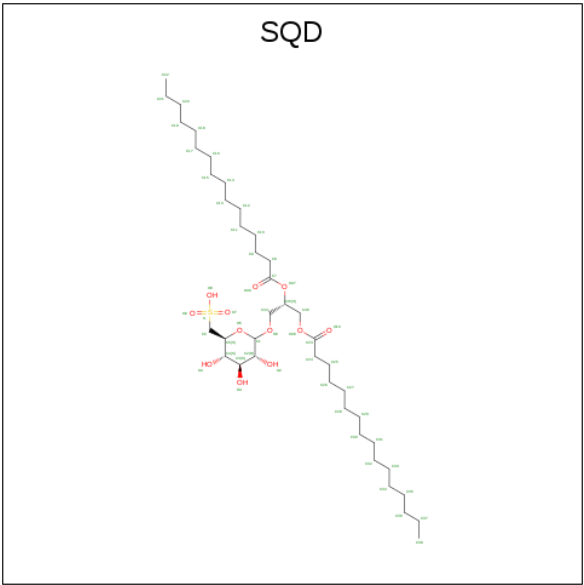
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

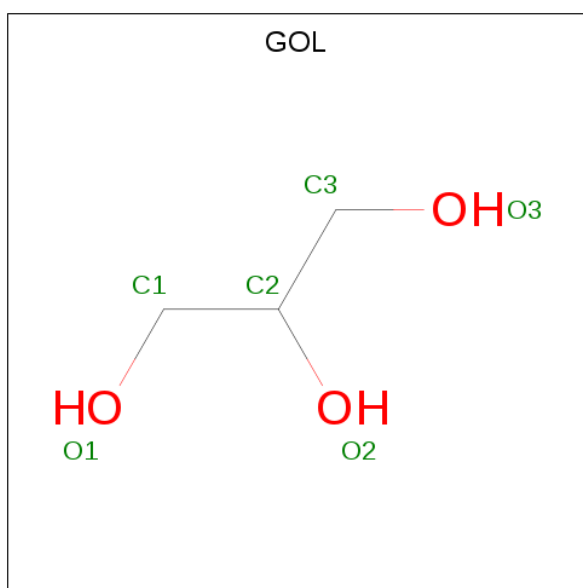
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- 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	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	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		

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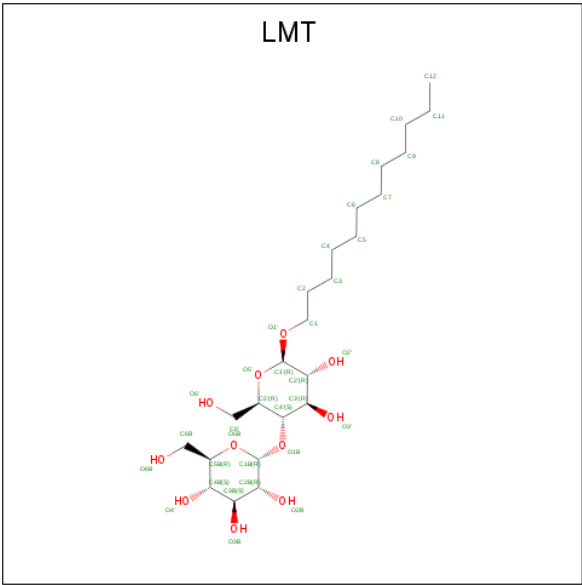
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	B	1	Total 6	C 3	O 3	0	0
27	B	1	Total 6	C 3	O 3	0	0
27	B	1	Total 6	C 3	O 3	0	0
27	C	1	Total 6	C 3	O 3	0	0
27	C	1	Total 6	C 3	O 3	0	0
27	D	1	Total 6	C 3	O 3	0	0
27	F	1	Total 6	C 3	O 3	0	0
27	O	1	Total 6	C 3	O 3	0	0
27	T	1	Total 6	C 3	O 3	0	0
27	T	1	Total 6	C 3	O 3	0	0
27	V	1	Total 6	C 3	O 3	0	0
27	V	1	Total 6	C 3	O 3	0	0
27	V	1	Total 6	C 3	O 3	0	0
27	V	1	Total 6	C 3	O 3	0	0
27	a	1	Total 6	C 3	O 3	0	0
27	a	1	Total 6	C 3	O 3	0	0
27	b	1	Total 6	C 3	O 3	0	0
27	b	1	Total 6	C 3	O 3	0	0
27	b	1	Total 6	C 3	O 3	0	0
27	b	1	Total 6	C 3	O 3	0	0
27	c	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	0
			6	3	3		
27	f	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	t	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



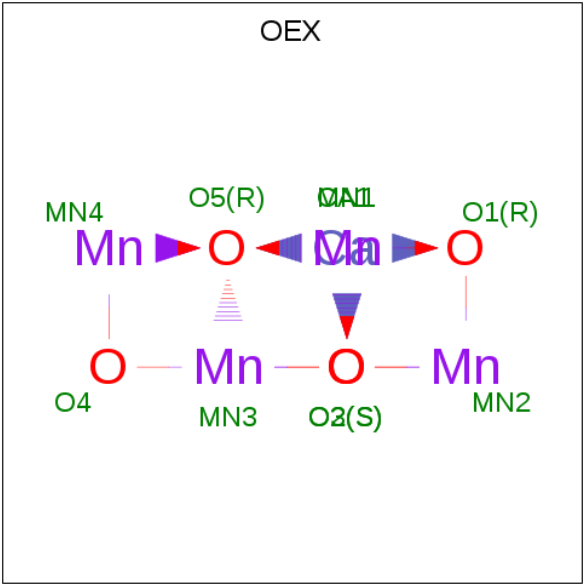
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			35	24	11		
28	B	1	Total	C	O	0	0
			25	19	6		
28	C	1	Total	C	O	0	0
			35	24	11		

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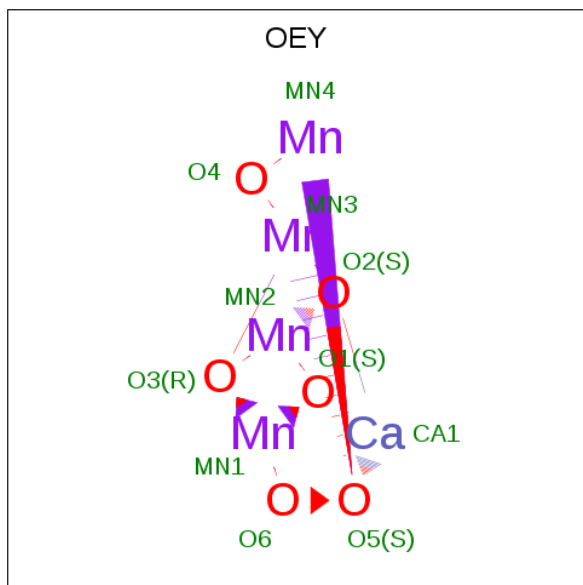
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	D	1	Total	C	O	0	0
			35	24	11		
28	F	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		
28	M	1	Total	C	O	0	0
			35	24	11		
28	T	1	Total	C	O	0	0
			25	19	6		
28	a	1	Total	C	O	0	0
			35	24	11		
28	a	1	Total	C	O	0	0
			35	24	11		
28	b	1	Total	C	O	0	0
			25	19	6		
28	e	1	Total	C	O	0	0
			35	24	11		
28	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



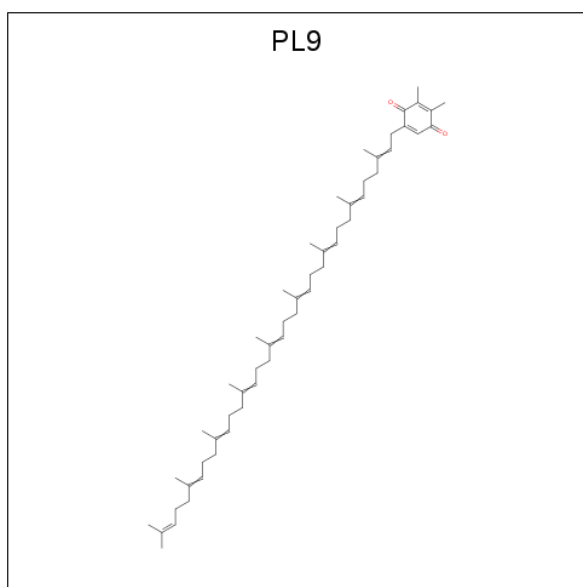
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ).



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

- Molecule 31 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	1
			110	106	4		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	1
			110	106	4		

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

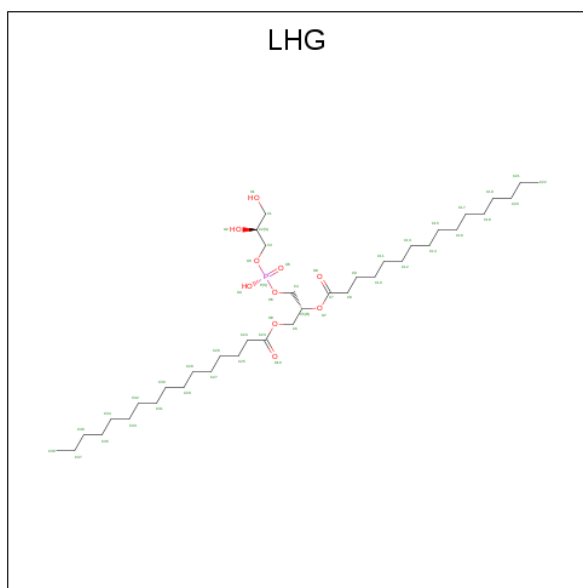
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	a	1	Total	C	O	0	0
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

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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O P 42 31 10 1	0	0
33	D	1	Total C O P 49 38 10 1	0	0
33	D	1	Total C O P 49 38 10 1	0	0
33	D	1	Total C O P 49 38 10 1	0	0

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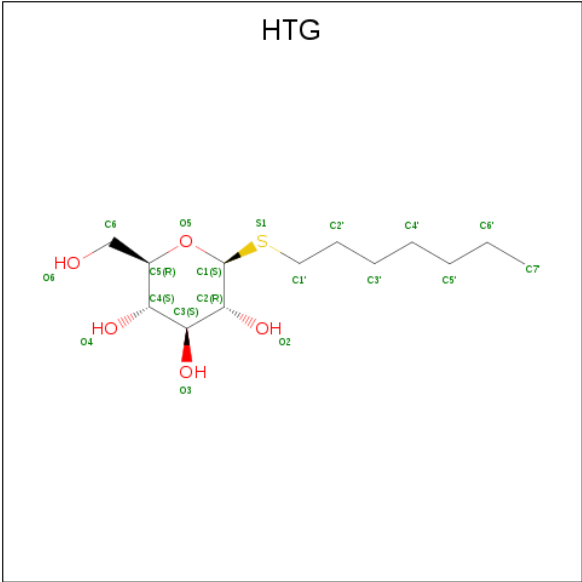
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	L	1	Total	C	O	P	0	0
			49	38	10	1		
33	a	1	Total	C	O	P	0	0
			42	31	10	1		
33	b	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		
33	d	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	1	Total	Ca	0	0
			1	1		
34	C	1	Total	Ca	0	0
			1	1		
34	c	2	Total	Ca	0	0
			2	2		
34	f	1	Total	Ca	0	0
			1	1		
34	o	1	Total	Ca	0	0
			1	1		
34	O	1	Total	Ca	0	0
			1	1		
34	b	1	Total	Ca	0	0
			1	1		
34	F	1	Total	Ca	0	0
			1	1		

- Molecule 35 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).





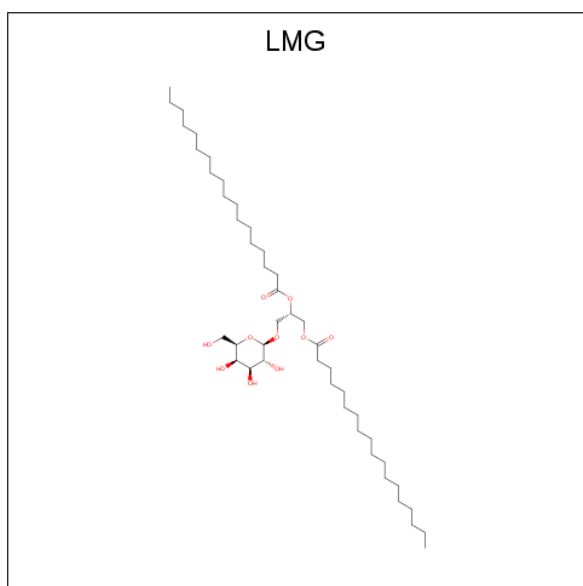
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



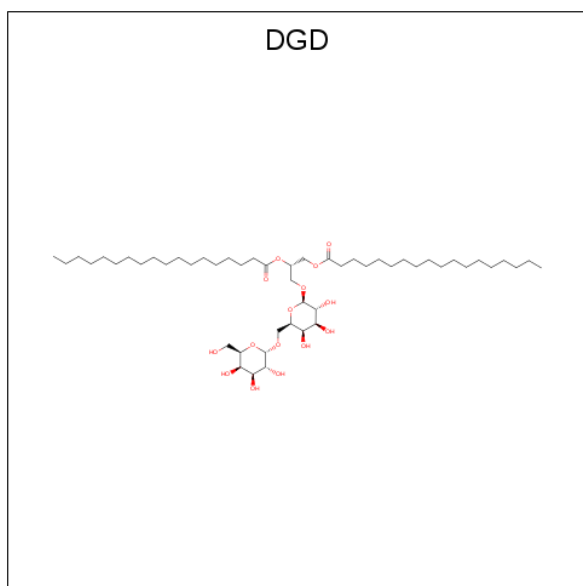
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			51	41	10			
36	C	1	Total	C	O		0	0
			51	41	10			
36	C	1	Total	C	O		0	0
			51	41	10			
36	D	1	Total	C	O		0	0
			51	41	10			
36	M	1	Total	C	O		0	0
			51	41	10			
36	Z	1	Total	C	O		0	0
			37	27	10			
36	a	1	Total	C	O		0	0
			51	41	10			
36	b	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total	C	O	0	0
			51	41	10		
36	d	1	Total	C	O	0	0
			51	41	10		
36	k	1	Total	C	O	0	0
			51	41	10		
36	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		

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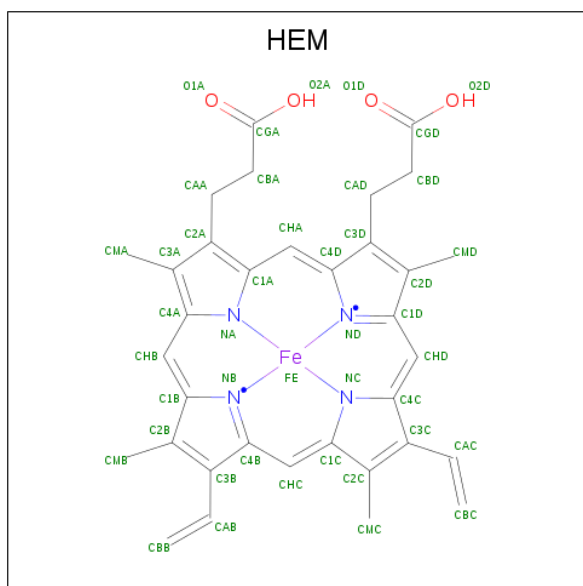
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	c	1	Total 62	C 47	O 15	0	0
37	d	1	Total 62	C 47	O 15	0	0
37	h	1	Total 62	C 47	O 15	0	0

- Molecule 38 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	a	1	Total Fe 1 1	0	1
38	D	1	Total Fe 2 2	0	1

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	157	Total	O	0	14
			169	169		
41	B	287	Total	O	0	4
			291	291		
41	C	231	Total	O	0	4
			235	235		
41	D	143	Total	O	0	5
			147	147		
41	E	32	Total	O	0	1
			33	33		
41	F	11	Total	O	0	0
			11	11		
41	H	44	Total	O	0	0
			44	44		
41	I	5	Total	O	0	0
			5	5		
41	J	10	Total	O	0	0
			10	10		
41	K	10	Total	O	0	0
			10	10		
41	L	11	Total	O	0	1
			12	12		
41	M	25	Total	O	0	0
			25	25		
41	O	178	Total	O	0	2
			180	180		
41	T	16	Total	O	0	1
			17	17		
41	U	80	Total	O	0	0
			80	80		
41	V	114	Total	O	0	2
			116	116		
41	Y	4	Total	O	0	0
			4	4		

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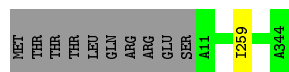
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	X	8	Total 8	O 8	0	0
41	Z	1	Total 1	O 1	0	0
41	a	151	Total 160	O 160	0	11
41	b	260	Total 263	O 263	0	3
41	c	194	Total 199	O 199	0	5
41	d	138	Total 141	O 141	0	4
41	e	20	Total 20	O 20	0	0
41	f	7	Total 7	O 7	0	0
41	h	43	Total 43	O 43	0	0
41	i	3	Total 3	O 3	0	0
41	j	6	Total 6	O 6	0	0
41	k	8	Total 8	O 8	0	0
41	l	8	Total 8	O 8	0	0
41	m	15	Total 15	O 15	0	0
41	o	155	Total 155	O 155	0	0
41	t	14	Total 14	O 14	0	0
41	u	94	Total 94	O 94	0	0
41	v	86	Total 87	O 87	0	1
41	y	1	Total 1	O 1	0	0
41	x	7	Total 7	O 7	0	0

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

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

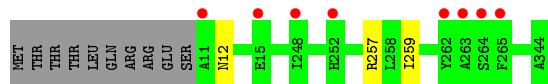
- Molecule 1: Photosystem II protein D1

Chain A:  97%



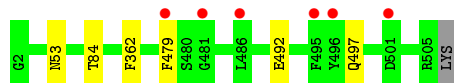
- Molecule 1: Photosystem II protein D1

Chain a:  96%



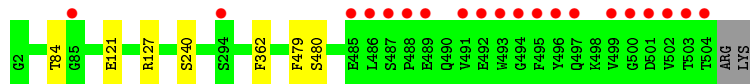
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



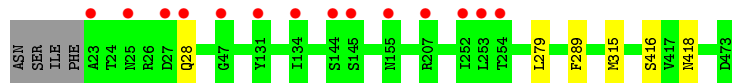
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%

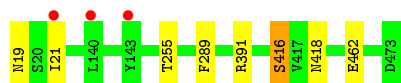


- Molecule 3: Photosystem II CP43 reaction center protein

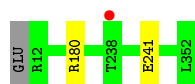
Chain C:  98%



- Molecule 3: Photosystem II CP43 reaction center protein



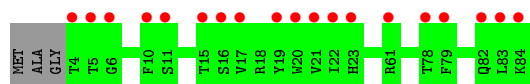
- Molecule 4: Photosystem II D2 protein



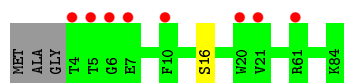
- Molecule 4: Photosystem II D2 protein



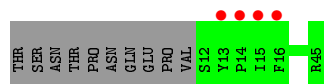
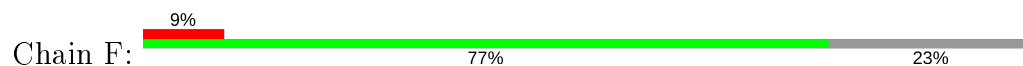
- Molecule 5: Cytochrome b559 subunit alpha



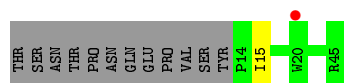
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

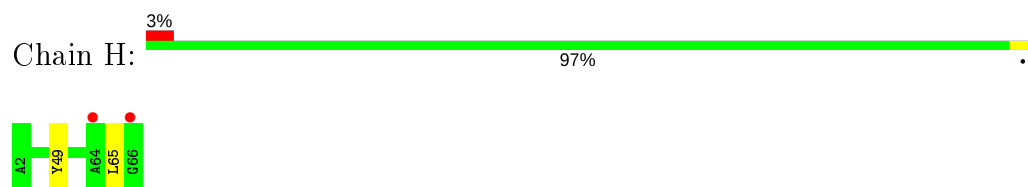


- Molecule 6: Cytochrome b559 subunit beta

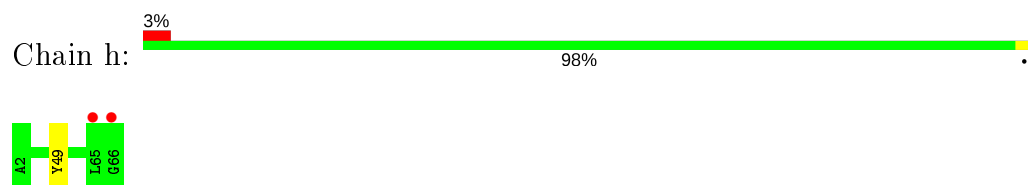




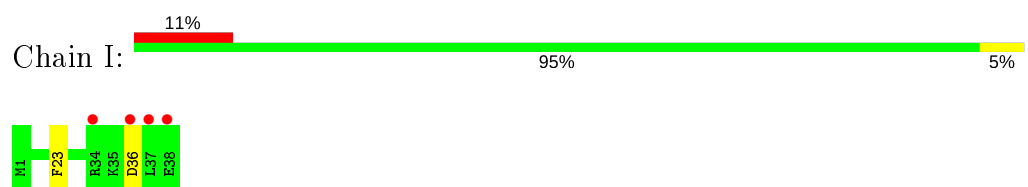
- Molecule 7: Photosystem II reaction center protein H



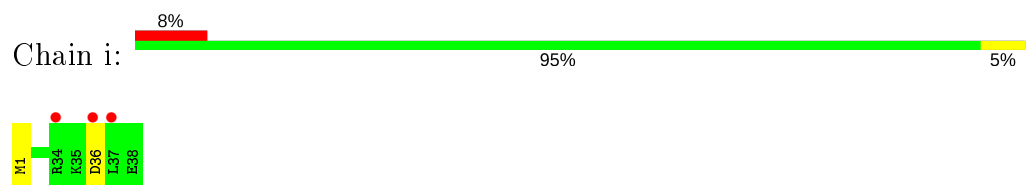
- Molecule 7: Photosystem II reaction center protein H



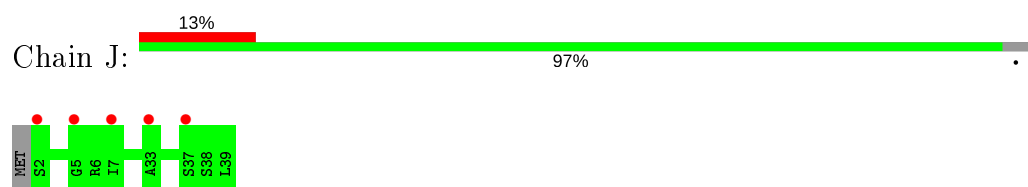
- Molecule 8: Photosystem II reaction center protein I



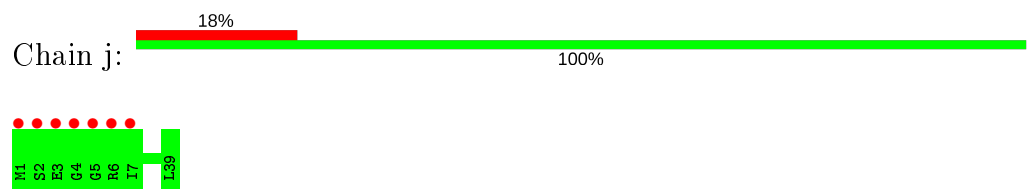
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

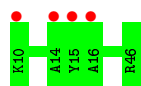


- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

Chain k: 95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 97% .



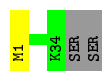
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein M

Chain M: 92% . 6%



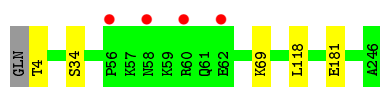
- Molecule 12: Photosystem II reaction center protein M

Chain m: 89% 6% 6%



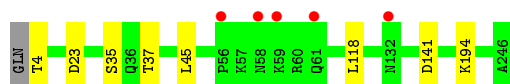
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 2% 98% .

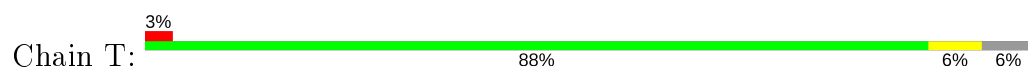


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

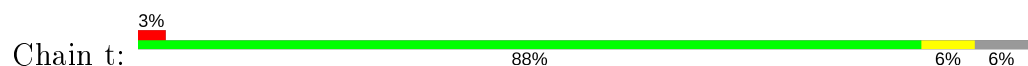
Chain o: 2% 96% .



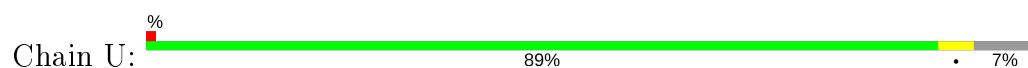
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



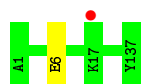
- Molecule 15: Photosystem II 12 kDa extrinsic protein



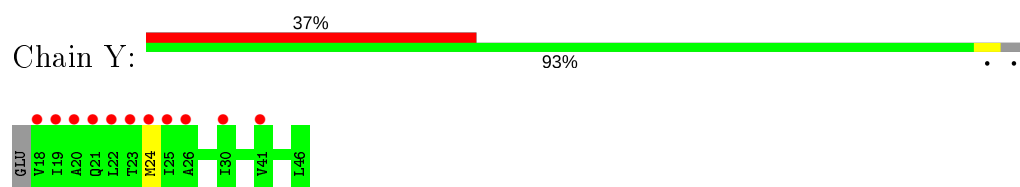
- Molecule 16: Cytochrome c-550



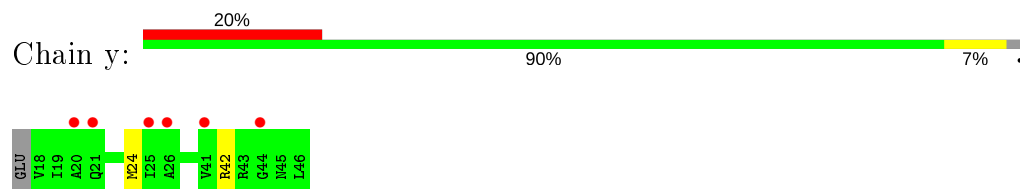
- Molecule 16: Cytochrome c-550



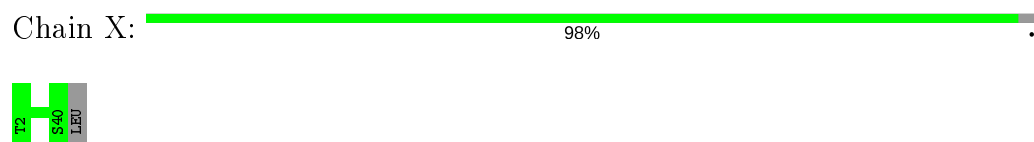
- Molecule 17: Photosystem II reaction center protein Ycf12



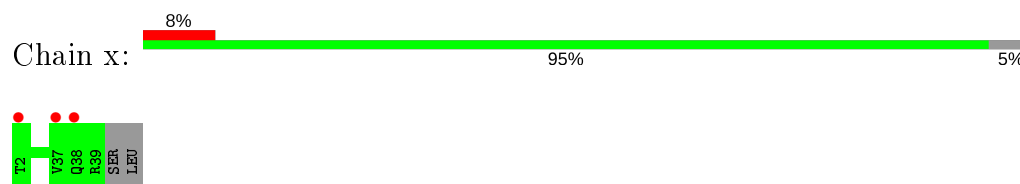
- Molecule 17: Photosystem II reaction center protein Ycf12



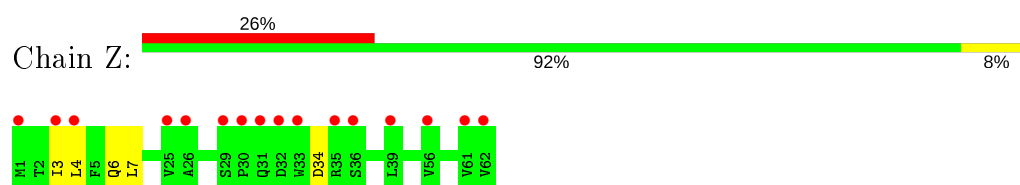
- Molecule 18: Photosystem II reaction center protein X



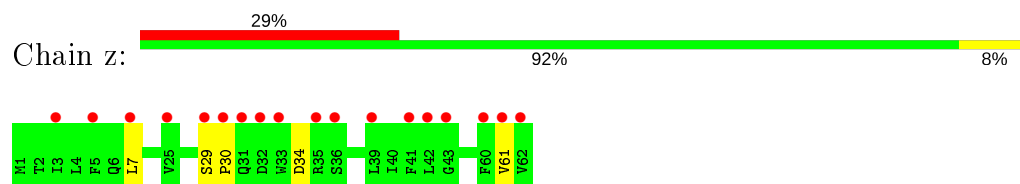
- Molecule 18: Photosystem II reaction center protein X



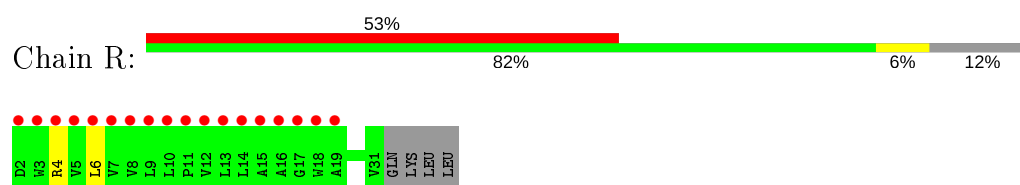
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 121.57 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.40) 99.2 (121.57-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.151 , 0.207 0.156 , 0.210	Depositor DCC
$R_{free}$ test set	17886 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 78.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	55695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, OEY, LMG, FE2, 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	0.42	0/3126	0.54	0/4257
1	a	0.43	0/3128	0.56	0/4260
2	B	0.43	0/4191	0.54	0/5709
2	b	0.43	0/4198	0.54	0/5720
3	C	0.38	0/3678	0.51	0/5007
3	c	0.39	0/3774	0.51	0/5135
4	D	0.46	0/2952	0.55	0/4021
4	d	0.45	0/2952	0.54	0/4021
5	E	0.33	0/693	0.48	0/944
5	e	0.33	0/695	0.50	0/948
6	F	0.39	0/284	0.51	0/387
6	f	0.40	0/265	0.53	0/360
7	H	0.36	0/535	0.54	0/728
7	h	0.35	0/524	0.52	0/713
8	I	0.34	0/311	0.50	0/419
8	i	0.36	0/311	0.52	0/419
9	J	0.36	0/278	0.41	0/376
9	j	0.32	0/286	0.46	0/386
10	K	0.35	0/303	0.50	0/416
10	k	0.35	0/303	0.49	0/416
11	L	0.42	0/319	0.49	0/433
11	l	0.45	0/319	0.50	0/433
12	M	0.46	0/270	0.59	0/368
12	m	0.44	0/262	0.60	0/357
13	O	0.38	0/1958	0.57	0/2654
13	o	0.38	0/1937	0.56	0/2625
14	T	0.44	0/266	0.52	0/362
14	t	0.50	0/266	0.52	0/362
15	U	0.38	0/785	0.54	0/1064
15	u	0.38	0/785	0.55	0/1064
16	V	0.36	0/1109	0.50	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.35	0/1098	0.51	0/1488
17	Y	0.33	0/216	0.46	0/289
17	y	0.31	0/216	0.46	0/289
18	X	0.34	0/290	0.46	0/392
18	x	0.32	0/284	0.47	0/384
19	Z	0.29	0/490	0.42	0/669
19	z	0.29	0/490	0.46	0/669
20	R	0.24	0/245	0.38	0/338
All	All	0.40	0/44392	0.53	0/60384

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	385/344 (112%)	378 (98%)	6 (2%)	1 (0%)	41	55
1	a	385/344 (112%)	381 (99%)	3 (1%)	1 (0%)	41	55
2	B	512/505 (101%)	503 (98%)	9 (2%)	0	100	100
2	b	513/505 (102%)	503 (98%)	9 (2%)	1 (0%)	47	62
3	C	461/455 (101%)	448 (97%)	11 (2%)	2 (0%)	34	48
3	c	473/455 (104%)	455 (96%)	16 (3%)	2 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	344 (97%)	11 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	240 (96%)	9 (4%)	0	100	100
13	o	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	4	3
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5431/5384 (101%)	5280 (97%)	142 (3%)	9 (0%)	51	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	z	30	PRO
2	b	127	ARG
19	z	61	VAL
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	312/279 (112%)	312 (100%)	0	100	100
1	a	312/279 (112%)	310 (99%)	2 (1%)	86	94
2	B	412/403 (102%)	406 (98%)	6 (2%)	65	80
2	b	413/403 (102%)	407 (98%)	6 (2%)	65	80
3	C	361/356 (101%)	356 (99%)	5 (1%)	67	82
3	c	371/356 (104%)	361 (97%)	10 (3%)	44	65
4	D	290/277 (105%)	288 (99%)	2 (1%)	84	92
4	d	290/277 (105%)	288 (99%)	2 (1%)	84	92
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	51
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	54
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	75
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	32
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	62
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	27 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	26
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	63
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	57
13	O	214/207 (103%)	208 (97%)	6 (3%)	43	63
13	o	211/207 (102%)	203 (96%)	8 (4%)	33	51
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	22
15	U	84/89 (94%)	81 (96%)	3 (4%)	35	54
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	68
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	91
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	44
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	14
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	47 (90%)	5 (10%)	8	12
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	32
20	R	25/29 (86%)	23 (92%)	2 (8%)	12	18
All	All	4506/4403 (102%)	4424 (98%)	82 (2%)	59	76

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	84	THR
2	B	362	PHE
2	B	479	PHE
2	B	492	GLU
2	B	497	GLN
3	C	28	GLN
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	180	ARG
4	D	241	GLU
7	H	49	TYR
7	H	65	LEU
8	I	23	PHE
8	I	36	ASP
11	L	13	ASN
13	O	4	THR
13	O	34	SER
13	O	69	LYS
13	O	118	LEU
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	8	GLU
15	U	59	GLU
15	U	70	ARG
17	Y	24	MET
19	Z	3	ILE
19	Z	4	LEU
19	Z	6	GLN
19	Z	7	LEU
19	Z	34	ASP
20	R	4	ARG
20	R	6	LEU
1	a	12	ASN
1	a	257	ARG
2	b	84	THR
2	b	121	GLU
2	b	240	SER
2	b	362	PHE

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Mol	Chain	Res	Type
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	21	ILE
3	c	255	THR
3	c	289	PHE
3	c	391	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	180	ARG
5	e	16	SER
6	f	15	ILE
7	h	49	TYR
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	35	SER
13	o	37	THR
13	o	45	LEU
13	o	118	LEU
13	o	141	ASP
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	61	VAL
15	u	86	GLU
16	v	6	GLU
17	y	24	MET
17	y	42	ARG
19	z	7	LEU
19	z	29	SER
19	z	34	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	53	ASN
2	B	331	ASN
2	B	490	GLN
2	B	497	GLN
3	C	201	ASN
4	D	61	HIS
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN
15	U	81	HIS
16	V	118	HIS
19	Z	31	GLN
19	Z	58	ASN
1	a	12	ASN
1	a	315	ASN
2	b	14	ASN
2	b	53	ASN
2	b	331	ASN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
13	o	124	ASN
13	o	130	GLN
13	o	147	ASN
16	v	86	GLN
19	z	31	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	0.66	0	7,9,11	1.25	1 (14%)
14	FME	T	1	14	8,9,10	0.67	0	7,9,11	1.64	3 (42%)
12	FME	M	1	12	8,9,10	0.67	0	7,9,11	1.37	2 (28%)
14	FME	t	1	14	8,9,10	0.87	0	7,9,11	2.06	3 (42%)
8	FME	I	1	8	8,9,10	0.71	0	7,9,11	1.16	0
8	FME	i	1	8	8,9,10	0.68	0	7,9,11	1.15	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-

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	CA-N-CN	-2.89	118.38	122.82
14	t	1	FME	O-C-CA	-2.72	117.64	124.78
14	T	1	FME	O-C-CA	-2.65	117.83	124.78
12	M	1	FME	CA-N-CN	-2.32	119.26	122.82
14	T	1	FME	C-CA-N	2.30	113.87	109.73
8	i	1	FME	O-C-CA	-2.12	119.21	124.78
14	T	1	FME	CA-N-CN	-2.11	119.58	122.82
12	M	1	FME	O-C-CA	-2.11	119.25	124.78
14	t	1	FME	CG-CB-CA	-2.04	107.29	112.95
12	m	1	FME	O-C-CA	-2.03	119.45	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	m	1	FME	O1-CN-N-CA
8	i	1	FME	O1-CN-N-CA
12	M	1	FME	CA-CB-CG-SD
12	m	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CA-N-CN
8	I	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 266 ligands modelled in this entry, 18 are unknown and 24 are monoatomic - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	HTG	V	206	-	19,19,19	1.04	2 (10%)	23,24,24	1.35	4 (17%)
33	LHG	L	101	-	48,48,48	0.86	2 (4%)	51,54,54	1.11	6 (11%)
23	CLA	C	504	-	59,73,73	2.04	13 (22%)	67,113,113	2.15	18 (26%)
26	SQD	A	410	-	53,54,54	0.99	3 (5%)	62,65,65	1.44	10 (16%)
23	CLA	c	508	41	59,73,73	2.00	13 (22%)	67,113,113	2.20	26 (38%)
33	LHG	d	410	-	48,48,48	0.86	2 (4%)	51,54,54	1.05	3 (5%)
28	LMT	T	104	-	25,25,36	0.57	1 (4%)	30,30,47	0.98	1 (3%)
35	HTG	C	522	-	19,19,19	1.01	2 (10%)	23,24,24	1.58	3 (13%)
26	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.46	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	LMG	b	629	-	51,51,55	0.91	2 (3%)	59,59,63	1.11	3 (5%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	7 (12%)
36	LMG	D	416	40	51,51,55	0.90	2 (3%)	59,59,63	0.96	3 (5%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.06	6 (7%)
23	CLA	C	503	-	59,73,73	2.00	13 (22%)	67,113,113	2.17	22 (32%)
23	CLA	C	507	-	59,73,73	1.97	13 (22%)	67,113,113	2.18	23 (34%)
27	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.36	0
27	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.26	0
23	CLA	b	616	41	59,73,73	1.98	13 (22%)	67,113,113	2.08	22 (32%)
28	LMT	M	104	-	36,36,36	0.55	1 (2%)	47,47,47	1.00	3 (6%)
23	CLA	c	513	-	59,73,73	2.07	13 (22%)	67,113,113	2.25	22 (32%)
36	LMG	c	522	-	51,51,55	0.94	2 (3%)	59,59,63	1.17	7 (11%)
27	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.26	0
25	BCR	Y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.80	14 (25%)
30	OXY	A	416[B]	1,3,41	0,16,16	0.00	-	-	-	-
31	PL9	d	407[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.55	14 (20%)
31	PL9	D	408[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.65	20 (29%)
36	LMG	d	416	40	51,51,55	0.91	2 (3%)	59,59,63	1.10	4 (6%)
35	HTG	b	631	-	19,19,19	0.87	1 (5%)	23,24,24	1.42	1 (4%)
27	GOL	o	301	-	5,5,5	0.41	0	5,5,5	0.32	0
31	PL9	d	407[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.66	17 (25%)
27	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.40	0
25	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.43	7 (12%)
23	CLA	b	619	41	59,73,73	2.00	14 (23%)	67,113,113	2.10	22 (32%)
23	CLA	B	615	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	22 (32%)
23	CLA	a	408	-	59,73,73	2.02	13 (22%)	67,113,113	2.18	25 (37%)
23	CLA	B	610	-	59,73,73	1.96	13 (22%)	67,113,113	2.15	24 (35%)
24	PHO	D	402[A]	-	67,69,69	2.15	16 (23%)	85,99,99	1.94	20 (23%)
23	CLA	A	404	-	59,73,73	2.02	12 (20%)	67,113,113	2.24	27 (40%)
31	PL9	A	417[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
37	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	4 (5%)
27	GOL	t	102	-	5,5,5	0.48	0	5,5,5	0.11	0
23	CLA	c	517	-	59,73,73	2.03	13 (22%)	67,113,113	2.13	24 (35%)
27	GOL	B	627	-	5,5,5	0.37	0	5,5,5	0.42	0
23	CLA	B	607	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	22 (32%)
27	GOL	v	202	-	5,5,5	0.41	0	5,5,5	0.24	0



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	2.08	13 (22%)	67,113,113	2.13	19 (28%)
33	LHG	D	411	-	48,48,48	0.91	3 (6%)	51,54,54	0.90	3 (5%)
33	LHG	d	411	-	48,48,48	0.96	2 (4%)	51,54,54	1.05	2 (3%)
23	CLA	c	511	41	59,73,73	2.04	13 (22%)	67,113,113	2.17	20 (29%)
33	LHG	D	410	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	4 (7%)
23	CLA	B	608	41	59,73,73	1.98	14 (23%)	67,113,113	2.17	24 (35%)
28	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.06	3 (6%)
23	CLA	D	405	-	59,73,73	1.95	13 (22%)	67,113,113	2.26	23 (34%)
27	GOL	B	626	-	5,5,5	0.35	0	5,5,5	0.51	0
29	OEX	A	415[A]	1,3,41	0,15,15	0.00	-	-		
27	GOL	A	411	-	5,5,5	0.39	0	5,5,5	0.39	0
23	CLA	B	616	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	23 (34%)
37	DGD	D	409	-	52,52,67	1.03	3 (5%)	60,60,81	1.12	5 (8%)
25	BCR	d	406	-	41,41,41	1.07	1 (2%)	56,56,56	1.72	15 (26%)
27	GOL	B	629	-	5,5,5	0.42	0	5,5,5	0.45	0
23	CLA	C	511	-	59,73,73	2.06	13 (22%)	67,113,113	2.14	24 (35%)
25	BCR	c	526	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	10 (17%)
28	LMT	D	404	-	36,36,36	0.44	0	47,47,47	0.98	1 (2%)
25	BCR	C	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	8 (14%)
35	HTG	B	623	-	19,19,19	0.83	1 (5%)	23,24,24	1.47	3 (13%)
27	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.53	0
27	GOL	A	412	-	5,5,5	0.43	0	5,5,5	0.28	0
23	CLA	B	612	-	59,73,73	1.99	13 (22%)	67,113,113	2.25	23 (34%)
25	BCR	t	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.68	14 (25%)
30	OXY	a	417[B]	1,3,41	0,16,16	0.00	-	-		
27	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.76	0
24	PHO	d	402[B]	-	67,69,69	2.15	16 (23%)	85,99,99	1.99	21 (24%)
23	CLA	B	604	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	21 (31%)
25	BCR	b	628	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	10 (17%)
24	PHO	d	402[A]	-	67,69,69	2.13	16 (23%)	85,99,99	2.01	22 (25%)
23	CLA	b	623	-	59,73,73	1.98	13 (22%)	67,113,113	2.27	22 (32%)
23	CLA	c	514	-	59,73,73	2.05	13 (22%)	67,113,113	2.18	20 (29%)
23	CLA	D	406	-	59,73,73	1.97	13 (22%)	67,113,113	2.08	23 (34%)
23	CLA	C	513	-	59,73,73	2.06	13 (22%)	67,113,113	2.17	22 (32%)
28	LMT	A	414	-	36,36,36	0.59	1 (2%)	47,47,47	1.37	5 (10%)
27	GOL	V	204	-	5,5,5	0.37	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	LMG	k	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.05	4 (6%)
25	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.31	7 (12%)
23	CLA	B	611	41	59,73,73	2.02	14 (23%)	67,113,113	2.20	22 (32%)
23	CLA	c	515	3	59,73,73	1.97	13 (22%)	67,113,113	2.04	21 (31%)
37	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	3 (3%)
27	GOL	D	403	-	5,5,5	0.44	0	5,5,5	0.29	0
27	GOL	v	201	-	5,5,5	0.34	0	5,5,5	0.20	0
29	OEX	a	416[A]	1,3,41	0,15,15	0.00	-	-		
23	CLA	C	510	-	59,73,73	2.09	13 (22%)	67,113,113	2.09	23 (34%)
33	LHG	A	419	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
26	SQD	F	104	-	42,43,54	1.19	4 (9%)	51,54,65	1.54	9 (17%)
36	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.12	4 (8%)
39	HEM	F	102	5,6	27,50,50	0.85	2 (7%)	17,82,82	2.18	3 (17%)
35	HTG	c	524	-	19,19,19	1.03	2 (10%)	23,24,24	1.50	3 (13%)
23	CLA	b	615	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	23 (34%)
23	CLA	A	408	-	59,73,73	1.99	13 (22%)	67,113,113	2.16	23 (34%)
25	BCR	a	412	-	41,41,41	1.05	1 (2%)	56,56,56	1.30	6 (10%)
22	BCT	A	403[A]	38	0,3,3	0.00	-	0,3,3	0.00	-
36	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	4 (6%)
28	LMT	e	102	-	36,36,36	0.49	0	47,47,47	0.82	0
36	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.04	5 (8%)
35	HTG	b	607	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	4 (17%)
23	CLA	c	516	-	59,73,73	2.03	13 (22%)	67,113,113	2.33	23 (34%)
31	PL9	A	417[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.77	22 (32%)
23	CLA	C	505	41	59,73,73	2.07	14 (23%)	67,113,113	2.29	22 (32%)
25	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	12 (21%)
23	CLA	c	509	-	59,73,73	1.95	13 (22%)	67,113,113	2.09	20 (29%)
23	CLA	d	405	-	59,73,73	2.01	12 (20%)	67,113,113	2.21	25 (37%)
25	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	9 (16%)
23	CLA	a	411	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	23 (34%)
25	BCR	D	407	-	41,41,41	1.05	1 (2%)	56,56,56	1.73	12 (21%)
23	CLA	a	409	41	59,73,73	1.98	12 (20%)	67,113,113	2.18	24 (35%)
36	LMG	M	101	-	51,51,55	0.91	2 (3%)	59,59,63	1.02	3 (5%)
39	HEM	v	206	16	27,50,50	0.87	1 (3%)	17,82,82	1.26	2 (11%)
37	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	4 (5%)
36	LMG	a	414	-	51,51,55	0.90	2 (3%)	59,59,63	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	512	-	59,73,73	2.05	12 (20%)	67,113,113	2.28	23 (34%)
22	BCT	d	401[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	405	41	59,73,73	2.05	13 (22%)	67,113,113	2.34	23 (34%)
23	CLA	C	509	-	59,73,73	2.04	13 (22%)	67,113,113	2.17	23 (34%)
22	BCT	d	401[B]	38	0,3,3	0.00	-	0,3,3	0.00	-
31	PL9	D	408[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.74	20 (29%)
35	HTG	b	602	-	19,19,19	1.02	1 (5%)	23,24,24	1.11	2 (8%)
26	SQD	b	601	-	53,54,54	1.04	3 (5%)	62,65,65	1.58	12 (19%)
28	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.94	1 (2%)
23	CLA	B	613	-	59,73,73	2.04	13 (22%)	67,113,113	2.24	20 (29%)
39	HEM	e	101	5,6	27,50,50	0.81	1 (3%)	17,82,82	2.06	3 (17%)
33	LHG	a	419	-	41,41,48	1.03	2 (4%)	44,47,54	0.97	2 (4%)
35	HTG	B	622	-	19,19,19	1.20	1 (5%)	23,24,24	1.42	2 (8%)
23	CLA	b	624	-	59,73,73	2.01	14 (23%)	67,113,113	2.05	21 (31%)
23	CLA	B	609	-	59,73,73	2.01	12 (20%)	67,113,113	2.14	22 (32%)
23	CLA	B	603	-	59,73,73	2.04	13 (22%)	67,113,113	2.36	28 (41%)
36	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.13	5 (8%)
23	CLA	b	618	-	59,73,73	1.98	13 (22%)	67,113,113	2.24	22 (32%)
25	BCR	y	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	11 (19%)
23	CLA	B	614	-	59,73,73	2.06	14 (23%)	67,113,113	2.18	22 (32%)
23	CLA	b	621	-	59,73,73	2.04	12 (20%)	67,113,113	2.31	24 (35%)
37	DGD	d	408	-	63,63,67	0.93	2 (3%)	77,77,81	1.29	7 (9%)
28	LMT	a	418	-	36,36,36	0.43	0	47,47,47	0.76	0
24	PHO	D	402[B]	-	67,69,69	2.20	17 (25%)	85,99,99	1.85	21 (24%)
23	CLA	b	622	-	59,73,73	1.98	12 (20%)	67,113,113	2.23	25 (37%)
35	HTG	B	624	-	19,19,19	1.03	2 (10%)	23,24,24	2.12	4 (17%)
23	CLA	b	617	-	59,73,73	2.01	13 (22%)	67,113,113	2.15	22 (32%)
27	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.44	0
25	BCR	b	626	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	12 (21%)
35	HTG	b	608	-	19,19,19	1.06	2 (10%)	23,24,24	1.08	2 (8%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.41	9 (16%)
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.14	7 (9%)
25	BCR	T	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.72	15 (26%)
27	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.13	0
23	CLA	B	606	-	59,73,73	2.02	13 (22%)	67,113,113	2.15	21 (31%)
27	GOL	v	204	-	5,5,5	0.34	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	505	-	59,73,73	1.96	13 (22%)	67,113,113	2.16	23 (34%)
37	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	3 (3%)
23	CLA	b	614	-	59,73,73	1.97	13 (22%)	67,113,113	2.28	20 (29%)
23	CLA	b	611	-	59,73,73	2.04	13 (22%)	67,113,113	2.26	24 (35%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	7 (9%)
26	SQD	a	413	-	53,54,54	0.96	3 (5%)	62,65,65	1.56	12 (19%)
33	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.03	4 (7%)
25	BCR	B	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.41	6 (10%)
25	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	10 (17%)
27	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
35	HTG	B	631	-	19,19,19	1.04	1 (5%)	23,24,24	1.43	2 (8%)
27	GOL	B	630	-	5,5,5	0.34	0	5,5,5	0.41	0
36	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.34	6 (13%)
23	CLA	b	620	-	59,73,73	1.94	12 (20%)	67,113,113	2.23	23 (34%)
35	HTG	c	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.55	1 (4%)
27	GOL	v	203	-	5,5,5	0.38	0	5,5,5	0.40	0
25	BCR	A	409	-	41,41,41	1.07	1 (2%)	56,56,56	1.24	7 (12%)
28	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.91	2 (4%)
28	LMT	b	630	-	25,25,36	0.49	0	30,30,47	0.56	0
35	HTG	D	415	-	16,16,19	1.06	2 (12%)	20,21,24	1.47	1 (5%)
27	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.14	0
39	HEM	V	205	16	27,50,50	0.88	2 (7%)	17,82,82	1.61	3 (17%)
35	HTG	B	632	-	19,19,19	1.00	2 (10%)	23,24,24	1.31	1 (4%)
27	GOL	V	202	-	5,5,5	0.36	0	5,5,5	0.41	0
24	PHO	A	407	-	67,69,69	2.16	16 (23%)	85,99,99	1.93	24 (28%)
23	CLA	B	602	41	59,73,73	2.05	14 (23%)	67,113,113	2.12	19 (28%)
28	LMT	m	102	-	36,36,36	0.52	0	47,47,47	1.11	4 (8%)
23	CLA	C	508	41	59,73,73	1.98	13 (22%)	67,113,113	2.10	18 (26%)
35	HTG	d	414	-	16,16,19	1.19	2 (12%)	20,21,24	1.82	3 (15%)
23	CLA	d	403	41	59,73,73	2.03	13 (22%)	67,113,113	2.24	23 (34%)
28	LMT	a	404	-	36,36,36	0.57	1 (2%)	47,47,47	1.15	3 (6%)
23	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.14	20 (29%)
27	GOL	O	301	-	5,5,5	0.38	0	5,5,5	0.36	0
28	LMT	B	634	-	25,25,36	0.52	0	30,30,47	0.79	1 (3%)
23	CLA	c	506	-	59,73,73	2.02	12 (20%)	67,113,113	2.15	22 (32%)
27	GOL	V	201	-	5,5,5	0.34	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	617	-	59,73,73	1.99	12 (20%)	67,113,113	2.28	21 (31%)
27	GOL	B	635	-	5,5,5	0.38	0	5,5,5	0.44	0
28	LMT	M	105	-	36,36,36	0.48	0	47,47,47	0.85	0
23	CLA	c	510	-	59,73,73	1.98	14 (23%)	67,113,113	2.12	23 (34%)
23	CLA	A	406	41	59,73,73	1.98	11 (18%)	67,113,113	2.19	22 (32%)
27	GOL	F	103	34	5,5,5	0.38	0	5,5,5	0.18	0
31	PL9	a	415[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.82	21 (30%)
23	CLA	b	612	-	59,73,73	2.00	14 (23%)	67,113,113	2.30	22 (32%)
23	CLA	C	512	3	59,73,73	2.05	13 (22%)	67,113,113	2.12	24 (35%)
31	PL9	a	415[A]	-	55,55,55	0.61	2 (3%)	68,69,69	1.91	20 (29%)
25	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.69	14 (25%)
26	SQD	A	413	-	53,54,54	1.04	3 (5%)	62,65,65	1.14	6 (9%)
23	CLA	C	506	-	59,73,73	1.95	13 (22%)	67,113,113	2.15	17 (25%)
27	GOL	f	101	34	5,5,5	0.30	0	5,5,5	0.40	0
27	GOL	B	625	-	5,5,5	0.37	0	5,5,5	0.18	0
25	BCR	K	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.50	9 (16%)
23	CLA	C	514	-	59,73,73	2.03	13 (22%)	67,113,113	2.07	21 (31%)
23	CLA	b	613	-	59,73,73	2.01	13 (22%)	67,113,113	2.27	23 (34%)
33	LHG	b	634	-	48,48,48	0.97	2 (4%)	51,54,54	1.08	2 (3%)
26	SQD	B	636	-	53,54,54	1.06	3 (5%)	62,65,65	1.21	4 (6%)
27	GOL	b	605	-	5,5,5	0.36	0	5,5,5	0.24	0
23	CLA	b	625	-	59,73,73	1.96	12 (20%)	67,113,113	2.28	23 (34%)
35	HTG	C	523	-	19,19,19	1.04	2 (10%)	23,24,24	1.81	4 (17%)
27	GOL	V	203	-	5,5,5	0.42	0	5,5,5	0.30	0
26	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.34	7 (11%)
35	HTG	b	632	-	19,19,19	1.16	2 (10%)	23,24,24	1.70	3 (13%)
23	CLA	d	404	-	59,73,73	2.00	14 (23%)	67,113,113	2.27	25 (37%)
23	CLA	B	605	-	59,73,73	1.91	12 (20%)	67,113,113	2.17	22 (32%)
22	BCT	A	403[B]	38	0,3,3	0.00	-	0,3,3	0.00	-
37	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.03	7 (9%)
27	GOL	b	603	-	5,5,5	0.37	0	5,5,5	0.50	0
33	LHG	D	412	-	48,48,48	0.97	2 (4%)	51,54,54	1.11	3 (5%)
24	PHO	a	410	-	67,69,69	2.10	17 (25%)	85,99,99	1.90	23 (27%)
27	GOL	c	502	-	5,5,5	0.39	0	5,5,5	0.42	0
23	CLA	c	507	-	59,73,73	1.97	12 (20%)	67,113,113	2.18	22 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	V	206	-	-	4/10/30/30	0/1/1/1
33	LHG	L	101	-	-	12/53/53/53	-
23	CLA	C	504	-	3/3/20/25	3/37/135/135	-
26	SQD	A	410	-	-	9/49/69/69	0/1/1/1
23	CLA	c	508	41	3/3/20/25	9/37/135/135	-
33	LHG	d	410	-	-	5/53/53/53	-
28	LMT	T	104	-	-	7/17/37/61	0/1/1/2
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
26	SQD	f	102	-	-	14/38/58/69	0/1/1/1
36	LMG	b	629	-	-	8/46/66/70	0/1/1/1
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
36	LMG	D	416	40	-	9/46/66/70	0/1/1/1
37	DGD	H	102	-	-	11/51/91/95	0/2/2/2
23	CLA	C	503	-	2/2/20/25	5/37/135/135	-
23	CLA	C	507	-	3/3/20/25	9/37/135/135	-
27	GOL	a	402	-	-	2/4/4/4	-
23	CLA	D	406	-	3/3/20/25	2/37/135/135	-
23	CLA	b	616	41	3/3/20/25	4/37/135/135	-
28	LMT	M	104	-	-	11/21/61/61	0/2/2/2
23	CLA	c	513	-	3/3/20/25	14/37/135/135	-
36	LMG	c	522	-	-	4/46/66/70	0/1/1/1
27	GOL	b	606	-	-	4/4/4/4	-
35	HTG	b	607	-	-	2/10/30/30	0/1/1/1
31	PL9	d	407[A]	-	-	8/53/73/73	0/1/1/1
31	PL9	D	408[A]	-	-	8/53/73/73	0/1/1/1
36	LMG	d	416	40	-	10/46/66/70	0/1/1/1
27	GOL	t	102	-	-	0/4/4/4	-
27	GOL	o	301	-	-	0/4/4/4	-
27	GOL	V	201	-	-	4/4/4/4	-
31	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
27	GOL	a	401	-	-	2/4/4/4	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	b	619	41	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	615	-	3/3/20/25	18/37/135/135	-
23	CLA	a	408	-	3/3/20/25	6/37/135/135	-
23	CLA	B	610	-	3/3/20/25	4/37/135/135	-
24	PHO	D	402[A]	-	-	2/53/103/103	0/5/6/6
23	CLA	A	404	-	3/3/20/25	4/37/135/135	-
31	PL9	A	417[A]	-	-	10/53/73/73	0/1/1/1
25	BCR	d	406	-	-	5/29/63/63	0/2/2/2
37	DGD	c	521	-	-	12/51/91/95	0/2/2/2
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
23	CLA	c	517	-	2/2/20/25	4/37/135/135	-
27	GOL	B	627	-	-	2/4/4/4	-
23	CLA	B	607	-	3/3/20/25	7/37/135/135	-
27	GOL	v	202	-	-	2/4/4/4	-
23	CLA	b	610	41	3/3/20/25	13/37/135/135	-
33	LHG	D	411	-	-	9/53/53/53	-
25	BCR	t	101	-	-	3/29/63/63	0/2/2/2
23	CLA	c	511	41	3/3/20/25	4/37/135/135	-
33	LHG	D	410	-	-	14/53/53/53	-
23	CLA	B	608	41	3/3/20/25	6/37/135/135	-
37	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	D	405	-	1/1/20/25	2/37/135/135	-
27	GOL	B	626	-	-	0/4/4/4	-
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	616	-	3/3/20/25	9/37/135/135	-
37	DGD	D	409	-	-	19/47/67/95	0/1/1/2
23	CLA	b	621	-	3/3/20/25	2/37/135/135	-
27	GOL	B	629	-	-	2/4/4/4	-
23	CLA	C	511	-	3/3/20/25	11/37/135/135	-
25	BCR	c	526	-	-	3/29/63/63	0/2/2/2
28	LMT	D	404	-	-	8/21/61/61	0/2/2/2
25	BCR	C	515	-	-	6/29/63/63	0/2/2/2
35	HTG	B	623	-	-	6/10/30/30	0/1/1/1
27	GOL	C	525	-	-	0/4/4/4	-
27	GOL	A	412	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	-	3/3/20/25	5/37/135/135	-
33	LHG	d	411	-	-	13/53/53/53	-
27	GOL	C	524	-	-	0/4/4/4	-
24	PHO	d	402[B]	-	-	3/53/103/103	0/5/6/6
23	CLA	B	604	-	3/3/20/25	7/37/135/135	-
25	BCR	b	628	-	-	1/29/63/63	0/2/2/2
24	PHO	d	402[A]	-	-	3/53/103/103	0/5/6/6
23	CLA	c	514	-	3/3/20/25	10/37/135/135	-
27	GOL	B	628	-	-	2/4/4/4	-
23	CLA	C	513	-	3/3/20/25	7/37/135/135	-
28	LMT	A	414	-	-	6/21/61/61	0/2/2/2
27	GOL	V	204	-	-	2/4/4/4	-
36	LMG	k	101	-	-	17/46/66/70	0/1/1/1
25	BCR	b	627	-	-	2/29/63/63	0/2/2/2
23	CLA	B	611	41	3/3/20/25	8/37/135/135	-
23	CLA	c	515	3	3/3/20/25	4/37/135/135	-
28	LMT	C	521	-	-	10/21/61/61	0/2/2/2
27	GOL	D	403	-	-	2/4/4/4	-
27	GOL	v	201	-	-	3/4/4/4	-
39	HEM	V	205	16	-	0/6/54/54	-
23	CLA	C	510	-	3/3/20/25	12/37/135/135	-
33	LHG	A	419	-	-	21/46/46/53	-
26	SQD	F	104	-	-	17/38/58/69	0/1/1/1
36	LMG	z	101	-	-	15/34/54/70	0/1/1/1
39	HEM	F	102	5,6	-	0/6/54/54	-
35	HTG	c	524	-	-	0/10/30/30	0/1/1/1
23	CLA	b	615	-	3/3/20/25	10/37/135/135	-
23	CLA	A	408	-	2/2/20/25	10/37/135/135	-
25	BCR	a	412	-	-	0/29/63/63	0/2/2/2
36	LMG	C	520	-	-	13/46/66/70	0/1/1/1
28	LMT	e	102	-	-	7/21/61/61	0/2/2/2
36	LMG	C	519	-	-	11/46/66/70	0/1/1/1
23	CLA	B	605	-	3/3/20/25	2/37/135/135	-
23	CLA	c	516	-	3/3/20/25	8/37/135/135	-
31	PL9	A	417[B]	-	-	11/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	505	41	3/3/20/25	3/37/135/135	-
25	BCR	K	103	-	-	1/29/63/63	0/2/2/2
23	CLA	c	509	-	2/2/20/25	5/37/135/135	-
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
23	CLA	a	411	-	3/3/20/25	10/37/135/135	-
25	BCR	D	407	-	-	6/29/63/63	0/2/2/2
23	CLA	a	409	41	2/2/20/25	8/37/135/135	-
36	LMG	M	101	-	-	10/46/66/70	0/1/1/1
39	HEM	v	206	16	-	0/6/54/54	-
37	DGD	C	518	-	-	12/51/91/95	0/2/2/2
36	LMG	a	414	-	-	14/46/66/70	0/1/1/1
23	CLA	c	512	-	3/3/20/25	4/37/135/135	-
23	CLA	A	405	41	3/3/20/25	4/37/135/135	-
23	CLA	C	509	-	3/3/20/25	9/37/135/135	-
25	BCR	b	626	-	-	4/29/63/63	0/2/2/2
31	PL9	D	408[B]	-	-	7/53/73/73	0/1/1/1
35	HTG	b	602	-	-	3/10/30/30	0/1/1/1
26	SQD	b	601	-	-	25/49/69/69	0/1/1/1
28	LMT	F	101	-	-	5/21/61/61	0/2/2/2
23	CLA	B	613	-	3/3/20/25	3/37/135/135	-
39	HEM	e	101	5,6	-	0/6/54/54	-
33	LHG	a	419	-	-	17/46/46/53	-
35	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	624	-	3/3/20/25	3/37/135/135	-
23	CLA	B	609	-	2/2/20/25	1/37/135/135	-
23	CLA	B	603	-	2/2/20/25	5/37/135/135	-
36	LMG	C	501	-	-	17/46/66/70	0/1/1/1
23	CLA	d	403	41	3/3/20/25	7/37/135/135	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	614	-	3/3/20/25	9/37/135/135	-
37	DGD	d	408	-	-	28/51/91/95	0/2/2/2
28	LMT	a	418	-	-	4/21/61/61	0/2/2/2
24	PHO	D	402[B]	-	-	2/53/103/103	0/5/6/6
23	CLA	b	622	-	3/3/20/25	5/37/135/135	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	617	-	2/2/20/25	2/37/135/135	-
27	GOL	c	501	-	-	0/4/4/4	-
23	CLA	d	405	-	3/3/20/25	6/37/135/135	-
35	HTG	b	608	-	-	1/10/30/30	0/1/1/1
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
25	BCR	T	103	-	-	3/29/63/63	0/2/2/2
27	GOL	T	101	-	-	0/4/4/4	-
23	CLA	B	606	-	3/3/20/25	3/37/135/135	-
27	GOL	v	204	-	-	2/4/4/4	-
23	CLA	c	505	-	3/3/20/25	5/37/135/135	-
37	DGD	c	520	-	-	19/51/91/95	0/2/2/2
23	CLA	b	614	-	3/3/20/25	8/37/135/135	-
23	CLA	b	611	-	2/2/20/25	4/37/135/135	-
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
33	LHG	d	409	-	-	5/53/53/53	-
25	BCR	B	618	-	-	2/29/63/63	0/2/2/2
25	BCR	c	518	-	-	1/29/63/63	0/2/2/2
27	GOL	T	102	-	-	2/4/4/4	-
35	HTG	B	631	-	-	2/10/30/30	0/1/1/1
27	GOL	B	630	-	-	4/4/4/4	-
36	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
23	CLA	b	620	-	3/3/20/25	5/37/135/135	-
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
27	GOL	v	203	-	-	2/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
28	LMT	M	102	-	-	5/21/61/61	0/2/2/2
28	LMT	b	630	-	-	4/17/37/61	0/1/1/2
35	HTG	D	415	-	-	0/7/27/30	0/1/1/1
27	GOL	b	604	-	-	0/4/4/4	-
35	HTG	B	632	-	-	1/10/30/30	0/1/1/1
27	GOL	V	202	-	-	0/4/4/4	-
23	CLA	b	623	-	3/3/20/25	19/37/135/135	-
23	CLA	B	602	41	3/3/20/25	12/37/135/135	-
23	CLA	C	508	41	3/3/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
23	CLA	b	618	-	2/2/20/25	3/37/135/135	-
28	LMT	a	404	-	-	5/21/61/61	0/2/2/2
23	CLA	C	502	-	3/3/20/25	11/37/135/135	-
24	PHO	A	407	-	-	3/53/103/103	0/5/6/6
28	LMT	B	634	-	-	6/17/37/61	0/1/1/2
23	CLA	c	506	-	3/3/20/25	3/37/135/135	-
27	GOL	O	301	-	-	2/4/4/4	-
23	CLA	B	617	-	3/3/20/25	6/37/135/135	-
27	GOL	B	635	-	-	0/4/4/4	-
28	LMT	M	105	-	-	7/21/61/61	0/2/2/2
23	CLA	c	510	-	3/3/20/25	14/37/135/135	-
23	CLA	A	406	41	2/2/20/25	6/37/135/135	-
27	GOL	F	103	34	-	2/4/4/4	-
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
31	PL9	a	415[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	b	612	-	2/2/20/25	8/37/135/135	-
23	CLA	C	512	3	2/2/20/25	5/37/135/135	-
31	PL9	a	415[A]	-	-	14/53/73/73	0/1/1/1
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	A	413	-	-	14/49/69/69	0/1/1/1
23	CLA	C	506	-	1/1/20/25	6/37/135/135	-
27	GOL	f	101	34	-	2/4/4/4	-
27	GOL	B	625	-	-	0/4/4/4	-
25	BCR	K	101	-	-	2/29/63/63	0/2/2/2
23	CLA	C	514	-	2/2/20/25	7/37/135/135	-
23	CLA	b	613	-	3/3/20/25	4/37/135/135	-
33	LHG	b	634	-	-	17/53/53/53	-
26	SQD	B	636	-	-	15/49/69/69	0/1/1/1
27	GOL	b	605	-	-	2/4/4/4	-
23	CLA	b	625	-	3/3/20/25	10/37/135/135	-
35	HTG	C	523	-	-	3/10/30/30	0/1/1/1
27	GOL	V	203	-	-	2/4/4/4	-
26	SQD	B	621	-	-	20/49/69/69	0/1/1/1
35	HTG	b	632	-	-	4/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	404	-	1/1/20/25	5/37/135/135	-
28	LMT	m	102	-	-	5/21/61/61	0/2/2/2
37	DGD	C	517	-	-	15/51/91/95	0/2/2/2
27	GOL	b	603	-	-	0/4/4/4	-
33	LHG	D	412	-	-	16/53/53/53	-
24	PHO	a	410	-	-	7/53/103/103	0/5/6/6
27	GOL	c	502	-	-	2/4/4/4	-
23	CLA	c	507	-	3/3/20/25	3/37/135/135	-

All (1169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3B-C2B	6.99	1.50	1.40
23	c	513	CLA	C3B-C2B	6.67	1.49	1.40
23	b	613	CLA	C3B-C2B	6.51	1.49	1.40
23	A	405	CLA	C3B-C2B	6.48	1.49	1.40
23	B	613	CLA	C3B-C2B	6.48	1.49	1.40
23	B	617	CLA	C3B-C2B	6.39	1.49	1.40
23	C	505	CLA	C3B-C2B	6.37	1.49	1.40
23	D	405	CLA	C3B-C2B	6.37	1.49	1.40
23	b	622	CLA	C3B-C2B	6.37	1.49	1.40
23	C	505	CLA	C3D-C2D	6.37	1.50	1.39
23	c	514	CLA	C3B-C2B	6.36	1.49	1.40
23	A	404	CLA	C3B-C2B	6.35	1.49	1.40
23	b	620	CLA	C3B-C2B	6.34	1.49	1.40
23	c	512	CLA	C3B-C2B	6.32	1.49	1.40
23	C	510	CLA	C3B-C2B	6.30	1.49	1.40
23	B	614	CLA	C3B-C2B	6.26	1.49	1.40
23	c	508	CLA	C3B-C2B	6.25	1.49	1.40
23	b	611	CLA	C3B-C2B	6.22	1.49	1.40
23	c	515	CLA	C3B-C2B	6.20	1.49	1.40
23	C	509	CLA	C3B-C2B	6.19	1.49	1.40
23	c	506	CLA	C3D-C2D	6.19	1.50	1.39
23	B	606	CLA	C3B-C2B	6.19	1.49	1.40
23	C	512	CLA	C3B-C2B	6.16	1.48	1.40
23	b	621	CLA	C3B-C2B	6.13	1.48	1.40
23	B	615	CLA	C3B-C2B	6.09	1.48	1.40
23	b	610	CLA	C3D-C2D	6.09	1.50	1.39
23	c	512	CLA	C3D-C2D	6.08	1.50	1.39
23	A	406	CLA	C3D-C2D	6.07	1.50	1.39
23	B	616	CLA	C3D-C2D	6.06	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	C3D-C2D	6.06	1.50	1.39
23	d	404	CLA	C3B-C2B	6.06	1.48	1.40
23	d	405	CLA	C3D-C2D	6.05	1.50	1.39
24	D	402[B]	PHO	C3B-C2B	6.05	1.49	1.37
23	B	614	CLA	C3D-C2D	6.04	1.50	1.39
23	b	619	CLA	C3B-C2B	6.02	1.48	1.40
23	a	408	CLA	C3B-C2B	6.02	1.48	1.40
23	b	623	CLA	C3B-C2B	6.02	1.48	1.40
23	c	510	CLA	C3B-C2B	6.02	1.48	1.40
23	C	510	CLA	C3D-C2D	6.01	1.50	1.39
23	B	603	CLA	C3B-C2B	6.01	1.48	1.40
23	B	611	CLA	C3B-C2B	6.00	1.48	1.40
23	B	609	CLA	C3B-C2B	6.00	1.48	1.40
23	b	624	CLA	C3D-C2D	5.99	1.50	1.39
23	C	513	CLA	C3D-C2D	5.99	1.50	1.39
23	b	610	CLA	C3B-C2B	5.98	1.48	1.40
23	d	403	CLA	C3B-C2B	5.98	1.48	1.40
23	A	405	CLA	C3D-C2D	5.98	1.50	1.39
23	d	403	CLA	C3D-C2D	5.98	1.50	1.39
24	d	402[B]	PHO	C3B-C2B	5.97	1.49	1.37
23	C	512	CLA	C3D-C2D	5.95	1.50	1.39
24	D	402[A]	PHO	C3B-C2B	5.94	1.49	1.37
24	A	407	PHO	C3B-C2B	5.93	1.49	1.37
23	B	615	CLA	C3D-C2D	5.92	1.50	1.39
23	B	612	CLA	C3D-C2D	5.92	1.50	1.39
23	A	404	CLA	C3D-C2D	5.92	1.50	1.39
23	C	503	CLA	C3B-C2B	5.91	1.48	1.40
23	c	511	CLA	C3B-C2B	5.91	1.48	1.40
23	c	505	CLA	C3B-C2B	5.90	1.48	1.40
24	d	402[A]	PHO	C3C-C2C	5.87	1.49	1.36
23	C	514	CLA	C3B-C2B	5.82	1.48	1.40
24	A	407	PHO	C3C-C2C	5.82	1.49	1.36
23	b	623	CLA	C3D-C2D	5.82	1.49	1.39
23	C	503	CLA	C3D-C2D	5.81	1.49	1.39
23	c	511	CLA	C3D-C2D	5.81	1.49	1.39
23	c	516	CLA	C3D-C2D	5.81	1.49	1.39
23	B	608	CLA	C3B-C2B	5.81	1.48	1.40
24	D	402[A]	PHO	C3C-C2C	5.81	1.49	1.36
24	D	402[B]	PHO	C3C-C2C	5.81	1.49	1.36
23	B	603	CLA	C3D-C2D	5.80	1.49	1.39
23	C	504	CLA	C3B-C2B	5.78	1.48	1.40
23	B	607	CLA	C3B-C2B	5.78	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	517	CLA	C3D-C2D	5.77	1.49	1.39
23	b	612	CLA	C3B-C2B	5.77	1.48	1.40
23	C	507	CLA	C3D-C2D	5.75	1.49	1.39
23	b	621	CLA	C3D-C2D	5.75	1.49	1.39
23	C	513	CLA	C3B-C2B	5.75	1.48	1.40
23	C	502	CLA	C3B-C2B	5.74	1.48	1.40
23	c	507	CLA	C3B-C2B	5.74	1.48	1.40
23	C	511	CLA	C3B-C2B	5.74	1.48	1.40
24	d	402[B]	PHO	C3C-C2C	5.72	1.48	1.36
23	c	517	CLA	C3B-C2B	5.72	1.48	1.40
24	d	402[A]	PHO	C3B-C2B	5.72	1.48	1.37
23	C	504	CLA	C3D-C2D	5.71	1.49	1.39
23	C	511	CLA	C3D-C2D	5.71	1.49	1.39
23	B	602	CLA	C3B-C2B	5.71	1.48	1.40
23	B	602	CLA	C3D-C2D	5.71	1.49	1.39
23	B	612	CLA	C3B-C2B	5.70	1.48	1.40
23	C	509	CLA	C3C-C2C	5.69	1.48	1.36
23	b	618	CLA	C3D-C2D	5.69	1.49	1.39
23	C	508	CLA	C3D-C2D	5.69	1.49	1.39
23	C	514	CLA	C3D-C2D	5.68	1.49	1.39
23	C	509	CLA	C3D-C2D	5.68	1.49	1.39
23	c	505	CLA	C3D-C2D	5.66	1.49	1.39
23	b	620	CLA	C3D-C2D	5.66	1.49	1.39
24	a	410	PHO	C3B-C2B	5.65	1.48	1.37
23	A	408	CLA	C3D-C2D	5.64	1.49	1.39
23	b	625	CLA	C3D-C2D	5.63	1.49	1.39
23	B	603	CLA	C3C-C2C	5.63	1.48	1.36
23	b	615	CLA	C3B-C2B	5.62	1.48	1.40
23	C	506	CLA	C3B-C2B	5.62	1.48	1.40
23	B	610	CLA	C3D-C2D	5.61	1.49	1.39
23	B	602	CLA	C3C-C2C	5.61	1.48	1.36
23	B	604	CLA	C3C-C2C	5.61	1.48	1.36
23	C	513	CLA	C3C-C2C	5.58	1.48	1.36
23	B	611	CLA	C3C-C2C	5.58	1.48	1.36
23	b	624	CLA	C3B-C2B	5.58	1.48	1.40
23	c	514	CLA	C3D-C2D	5.57	1.49	1.39
23	a	411	CLA	C3C-C2C	5.57	1.48	1.36
23	C	514	CLA	C3C-C2C	5.57	1.48	1.36
23	b	610	CLA	C3C-C2C	5.56	1.48	1.36
23	B	607	CLA	C3C-C2C	5.55	1.48	1.36
23	B	617	CLA	C3D-C2D	5.54	1.49	1.39
23	c	506	CLA	C3B-C2B	5.54	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	C3B-C2B	5.53	1.48	1.40
23	c	516	CLA	C3B-C2B	5.52	1.48	1.40
23	A	408	CLA	C3B-C2B	5.52	1.48	1.40
23	b	617	CLA	C3C-C2C	5.51	1.48	1.36
23	b	612	CLA	C3D-C2D	5.51	1.49	1.39
23	C	508	CLA	C3B-C2B	5.49	1.48	1.40
23	a	411	CLA	C3D-C2D	5.49	1.49	1.39
23	A	404	CLA	CHC-C1C	5.47	1.49	1.35
23	d	404	CLA	C3D-C2D	5.47	1.49	1.39
23	C	502	CLA	C3D-C2D	5.47	1.49	1.39
23	B	611	CLA	C3D-C2D	5.46	1.49	1.39
23	b	614	CLA	C3B-C2B	5.46	1.48	1.40
23	B	613	CLA	CHC-C1C	5.46	1.49	1.35
23	d	405	CLA	CHC-C1C	5.46	1.49	1.35
23	b	625	CLA	C3B-C2B	5.45	1.47	1.40
23	B	606	CLA	C3D-C2D	5.44	1.49	1.39
23	b	622	CLA	C3D-C2D	5.44	1.49	1.39
23	B	616	CLA	O2D-CGD	5.44	1.46	1.33
23	b	611	CLA	C3D-C2D	5.44	1.49	1.39
23	A	406	CLA	C3C-C2C	5.43	1.48	1.36
23	B	604	CLA	C3B-C2B	5.43	1.47	1.40
23	b	614	CLA	C3D-C2D	5.43	1.49	1.39
23	c	517	CLA	C3C-C2C	5.43	1.48	1.36
23	b	615	CLA	C3D-C2D	5.43	1.49	1.39
23	a	408	CLA	C3D-C2D	5.42	1.49	1.39
23	B	613	CLA	C3D-C2D	5.41	1.49	1.39
23	B	604	CLA	C3D-C2D	5.40	1.49	1.39
23	B	609	CLA	C3D-C2D	5.40	1.49	1.39
24	a	410	PHO	C3C-C2C	5.40	1.48	1.36
23	A	406	CLA	CHC-C1C	5.39	1.48	1.35
23	c	509	CLA	C3C-C2C	5.39	1.48	1.36
23	c	513	CLA	C3D-C2D	5.39	1.49	1.39
23	c	516	CLA	CHC-C1C	5.38	1.48	1.35
23	C	511	CLA	C3C-C2C	5.38	1.48	1.36
23	d	403	CLA	C3C-C2C	5.38	1.48	1.36
23	C	510	CLA	C3C-C2C	5.38	1.48	1.36
23	b	615	CLA	C3C-C2C	5.38	1.48	1.36
23	b	619	CLA	C3C-C2C	5.37	1.48	1.36
23	b	613	CLA	C3D-C2D	5.37	1.49	1.39
24	d	402[B]	PHO	CHC-C1C	5.37	1.49	1.38
23	c	514	CLA	C3C-C2C	5.36	1.48	1.36
23	B	616	CLA	C3B-C2B	5.36	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C3B-C2B	5.36	1.47	1.40
23	B	607	CLA	C3D-C2D	5.36	1.49	1.39
23	c	507	CLA	CHC-C1C	5.36	1.48	1.35
23	C	504	CLA	C3C-C2C	5.35	1.48	1.36
23	D	405	CLA	C3C-C2C	5.35	1.48	1.36
23	A	405	CLA	C3C-C2C	5.35	1.48	1.36
23	c	508	CLA	O2D-CGD	5.34	1.46	1.33
23	D	406	CLA	C3D-C2D	5.34	1.49	1.39
23	c	508	CLA	C3D-C2D	5.34	1.49	1.39
23	B	606	CLA	CHC-C1C	5.33	1.48	1.35
24	D	402[B]	PHO	CHB-C1B	5.32	1.49	1.38
24	D	402[B]	PHO	CHC-C1C	5.32	1.49	1.38
23	a	409	CLA	C3D-C2D	5.32	1.49	1.39
23	c	516	CLA	C3C-C2C	5.32	1.48	1.36
23	C	504	CLA	CHC-C1C	5.31	1.48	1.35
23	B	604	CLA	CHC-C1C	5.31	1.48	1.35
23	C	508	CLA	C3C-C2C	5.31	1.48	1.36
24	d	402[A]	PHO	CHC-C1C	5.31	1.49	1.38
23	C	507	CLA	C3B-C2B	5.31	1.47	1.40
23	c	506	CLA	C3C-C2C	5.30	1.48	1.36
23	b	612	CLA	CHC-C1C	5.30	1.48	1.35
23	b	625	CLA	CHC-C1C	5.30	1.48	1.35
23	b	622	CLA	O2D-CGD	5.29	1.46	1.33
23	D	406	CLA	C3B-C2B	5.29	1.47	1.40
23	C	513	CLA	CHC-C1C	5.29	1.48	1.35
23	c	507	CLA	C3C-C2C	5.28	1.48	1.36
23	b	624	CLA	OBD-CAD	5.28	1.29	1.22
25	K	101	BCR	C23-C22	-5.27	1.34	1.45
23	D	406	CLA	C3C-C2C	5.27	1.47	1.36
23	B	611	CLA	CHC-C1C	5.27	1.48	1.35
23	C	508	CLA	CHC-C1C	5.27	1.48	1.35
23	b	618	CLA	O2D-CGD	5.27	1.46	1.33
24	A	407	PHO	CHB-C1B	5.27	1.48	1.38
23	c	515	CLA	C3D-C2D	5.26	1.48	1.39
23	b	617	CLA	CHC-C1C	5.26	1.48	1.35
23	B	617	CLA	C3C-C2C	5.26	1.47	1.36
23	b	616	CLA	C3D-C2D	5.25	1.48	1.39
23	d	405	CLA	C3B-C2B	5.25	1.47	1.40
23	c	512	CLA	C3C-C2C	5.25	1.47	1.36
23	B	609	CLA	C3C-C2C	5.25	1.47	1.36
23	D	405	CLA	C3D-C2D	5.25	1.48	1.39
25	K	103	BCR	C23-C22	-5.24	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3C-C2C	5.24	1.47	1.36
23	A	408	CLA	CHC-C1C	5.24	1.48	1.35
24	D	402[A]	PHO	CHC-C1C	5.24	1.48	1.38
23	a	409	CLA	C3C-C2C	5.24	1.47	1.36
23	B	607	CLA	O2D-CGD	5.23	1.46	1.33
23	C	512	CLA	O2D-CGD	5.23	1.46	1.33
23	b	610	CLA	CHC-C1C	5.23	1.48	1.35
23	a	409	CLA	CHC-C1C	5.23	1.48	1.35
23	b	622	CLA	C3C-C2C	5.23	1.47	1.36
23	b	614	CLA	C3C-C2C	5.23	1.47	1.36
25	k	102	BCR	C23-C22	-5.22	1.34	1.45
23	b	623	CLA	C3C-C2C	5.22	1.47	1.36
23	b	610	CLA	O2D-CGD	5.21	1.45	1.33
23	d	405	CLA	O2D-CGD	5.20	1.45	1.33
23	d	405	CLA	C3C-C2C	5.20	1.47	1.36
23	B	615	CLA	C3C-C2C	5.20	1.47	1.36
23	C	503	CLA	C3C-C2C	5.20	1.47	1.36
23	C	513	CLA	O2D-CGD	5.20	1.45	1.33
23	B	616	CLA	CHC-C1C	5.19	1.48	1.35
23	A	408	CLA	C3C-C2C	5.19	1.47	1.36
23	b	619	CLA	C3D-C2D	5.19	1.48	1.39
23	C	502	CLA	CHC-C1C	5.19	1.48	1.35
23	b	618	CLA	CHC-C1C	5.18	1.48	1.35
23	B	603	CLA	CHC-C1C	5.18	1.48	1.35
23	B	606	CLA	O2D-CGD	5.18	1.45	1.33
23	C	506	CLA	O2D-CGD	5.18	1.45	1.33
23	B	610	CLA	C3C-C2C	5.18	1.47	1.36
23	A	406	CLA	C3B-C2B	5.18	1.47	1.40
23	B	613	CLA	C3C-C2C	5.17	1.47	1.36
23	b	611	CLA	CHC-C1C	5.17	1.48	1.35
23	c	507	CLA	C3D-C2D	5.17	1.48	1.39
23	B	602	CLA	O2D-CGD	5.16	1.45	1.33
23	b	616	CLA	C3B-C2B	5.16	1.47	1.40
23	c	509	CLA	C3D-C2D	5.16	1.48	1.39
23	b	621	CLA	C3C-C2C	5.16	1.47	1.36
23	A	408	CLA	O2D-CGD	5.16	1.45	1.33
23	C	514	CLA	CHC-C1C	5.16	1.48	1.35
23	C	511	CLA	O2D-CGD	5.16	1.45	1.33
23	C	511	CLA	CHC-C1C	5.16	1.48	1.35
23	b	623	CLA	O2D-CGD	5.16	1.45	1.33
23	c	510	CLA	C3C-C2C	5.15	1.47	1.36
23	C	512	CLA	C3C-C2C	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	CHC-C1C	5.15	1.48	1.35
23	c	510	CLA	C3D-C2D	5.14	1.48	1.39
23	c	509	CLA	C3B-C2B	5.14	1.47	1.40
23	b	616	CLA	CHC-C1C	5.14	1.48	1.35
23	B	610	CLA	O2D-CGD	5.13	1.45	1.33
24	D	402[A]	PHO	O2D-CGD	5.13	1.45	1.33
25	A	409	BCR	C23-C22	-5.13	1.34	1.45
23	b	614	CLA	O2D-CGD	5.13	1.45	1.33
23	c	510	CLA	O2D-CGD	5.12	1.45	1.33
23	C	509	CLA	O2D-CGD	5.12	1.45	1.33
23	c	511	CLA	CHC-C1C	5.12	1.48	1.35
23	C	510	CLA	CHC-C1C	5.12	1.48	1.35
23	c	515	CLA	CHC-C1C	5.12	1.48	1.35
24	d	402[B]	PHO	O2D-CGD	5.11	1.45	1.33
23	d	404	CLA	C3C-C2C	5.11	1.47	1.36
23	a	411	CLA	C3B-C2B	5.11	1.47	1.40
24	A	407	PHO	CHC-C1C	5.11	1.48	1.38
23	b	619	CLA	CHC-C1C	5.10	1.48	1.35
23	b	620	CLA	O2D-CGD	5.10	1.45	1.33
23	b	621	CLA	CHC-C1C	5.10	1.48	1.35
23	b	612	CLA	C3C-C2C	5.10	1.47	1.36
23	C	505	CLA	CHC-C1C	5.10	1.48	1.35
23	b	611	CLA	C3C-C2C	5.09	1.47	1.36
23	C	506	CLA	C3C-C2C	5.09	1.47	1.36
24	a	410	PHO	CHC-C1C	5.08	1.48	1.38
23	b	614	CLA	CHC-C1C	5.08	1.48	1.35
23	C	507	CLA	O2D-CGD	5.08	1.45	1.33
25	H	101	BCR	C23-C22	-5.08	1.35	1.45
23	c	506	CLA	O2D-CGD	5.08	1.45	1.33
23	C	503	CLA	CHC-C1C	5.07	1.48	1.35
23	b	616	CLA	O2D-CGD	5.06	1.45	1.33
23	B	617	CLA	O2D-CGD	5.06	1.45	1.33
23	b	621	CLA	O2D-CGD	5.06	1.45	1.33
23	C	510	CLA	O2D-CGD	5.06	1.45	1.33
25	Y	101	BCR	C23-C22	-5.06	1.35	1.45
23	B	607	CLA	CHC-C1C	5.06	1.47	1.35
23	a	411	CLA	O2D-CGD	5.05	1.45	1.33
23	c	508	CLA	CHC-C1C	5.05	1.47	1.35
23	c	513	CLA	C3C-C2C	5.05	1.47	1.36
23	b	613	CLA	C3C-C2C	5.05	1.47	1.36
23	c	513	CLA	CHC-C1C	5.05	1.47	1.35
23	b	621	CLA	OBD-CAD	5.04	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	t	101	BCR	C23-C22	-5.04	1.35	1.45
23	a	408	CLA	C3C-C2C	5.04	1.47	1.36
23	C	505	CLA	C3C-C2C	5.04	1.47	1.36
23	B	614	CLA	C3C-C2C	5.03	1.47	1.36
23	C	514	CLA	O2D-CGD	5.03	1.45	1.33
23	B	613	CLA	OBD-CAD	5.03	1.29	1.22
23	c	512	CLA	O2D-CGD	5.03	1.45	1.33
23	c	505	CLA	C3C-C2C	5.02	1.47	1.36
23	C	509	CLA	CHC-C1C	5.02	1.47	1.35
24	D	402[B]	PHO	O2D-CGD	5.02	1.45	1.33
23	C	503	CLA	O2D-CGD	5.02	1.45	1.33
23	B	617	CLA	CHC-C1C	5.02	1.47	1.35
23	c	511	CLA	C3C-C2C	5.02	1.47	1.36
23	b	611	CLA	OBD-CAD	5.01	1.29	1.22
23	c	516	CLA	OBD-CAD	5.01	1.29	1.22
23	c	517	CLA	CHC-C1C	5.01	1.47	1.35
25	y	101	BCR	C23-C22	-5.00	1.35	1.45
23	c	517	CLA	O2D-CGD	5.00	1.45	1.33
23	b	624	CLA	CHC-C1C	5.00	1.47	1.35
23	b	624	CLA	C3C-C2C	5.00	1.47	1.36
23	D	406	CLA	CHC-C1C	5.00	1.47	1.35
25	c	526	BCR	C23-C22	-4.99	1.35	1.45
23	B	614	CLA	O2D-CGD	4.99	1.45	1.33
23	b	615	CLA	CHC-C1C	4.98	1.47	1.35
24	d	402[A]	PHO	O2D-CGD	4.98	1.45	1.33
23	A	406	CLA	O2D-CGD	4.98	1.45	1.33
23	d	404	CLA	CHC-C1C	4.98	1.47	1.35
23	c	514	CLA	CHC-C1C	4.97	1.47	1.35
23	B	603	CLA	O2D-CGD	4.97	1.45	1.33
23	b	625	CLA	O2D-CGD	4.97	1.45	1.33
23	c	513	CLA	OBD-CAD	4.97	1.29	1.22
23	C	512	CLA	CHC-C1C	4.97	1.47	1.35
23	c	509	CLA	CHC-C1C	4.96	1.47	1.35
23	a	408	CLA	OBD-CAD	4.96	1.29	1.22
23	C	505	CLA	O2D-CGD	4.96	1.45	1.33
23	C	502	CLA	C3C-C2C	4.96	1.47	1.36
23	B	608	CLA	C3D-C2D	4.96	1.48	1.39
23	b	618	CLA	C3C-C2C	4.96	1.47	1.36
23	B	609	CLA	CHC-C1C	4.95	1.47	1.35
25	T	103	BCR	C23-C22	-4.95	1.35	1.45
23	A	404	CLA	C3C-C2C	4.95	1.47	1.36
23	c	513	CLA	O2D-CGD	4.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	CHD-C1D	4.94	1.48	1.38
25	C	515	BCR	C23-C22	-4.94	1.35	1.45
23	b	613	CLA	CHC-C1C	4.94	1.47	1.35
24	D	402[B]	PHO	CHD-C1D	4.93	1.48	1.38
25	h	101	BCR	C23-C22	-4.93	1.35	1.45
23	c	516	CLA	O2D-CGD	4.93	1.45	1.33
23	b	617	CLA	O2D-CGD	4.93	1.45	1.33
23	c	512	CLA	OBD-CAD	4.92	1.29	1.22
23	C	506	CLA	CHC-C1C	4.92	1.47	1.35
23	b	617	CLA	C3B-C2B	4.92	1.47	1.40
23	c	506	CLA	CHC-C1C	4.92	1.47	1.35
23	C	507	CLA	C3C-C2C	4.92	1.47	1.36
23	D	406	CLA	O2D-CGD	4.92	1.45	1.33
23	b	616	CLA	C3C-C2C	4.91	1.47	1.36
23	c	514	CLA	O2D-CGD	4.91	1.45	1.33
23	a	409	CLA	OBD-CAD	4.91	1.29	1.22
23	c	512	CLA	CHC-C1C	4.91	1.47	1.35
23	c	511	CLA	O2D-CGD	4.91	1.45	1.33
23	B	616	CLA	OBD-CAD	4.91	1.29	1.22
24	D	402[A]	PHO	CHB-C1B	4.90	1.48	1.38
23	B	605	CLA	C3C-C2C	4.90	1.47	1.36
23	B	608	CLA	C3C-C2C	4.90	1.47	1.36
23	C	507	CLA	CHC-C1C	4.89	1.47	1.35
23	b	611	CLA	O2D-CGD	4.89	1.45	1.33
23	c	515	CLA	C3C-C2C	4.89	1.47	1.36
23	B	605	CLA	CHC-C1C	4.89	1.47	1.35
23	A	405	CLA	O2D-CGD	4.89	1.45	1.33
23	B	616	CLA	C3C-C2C	4.89	1.47	1.36
23	c	505	CLA	O2D-CGD	4.88	1.45	1.33
23	C	506	CLA	C3D-C2D	4.88	1.48	1.39
23	B	604	CLA	O2D-CGD	4.88	1.45	1.33
23	B	610	CLA	CHC-C1C	4.88	1.47	1.35
23	c	507	CLA	O2D-CGD	4.87	1.45	1.33
23	a	411	CLA	CHC-C1C	4.86	1.47	1.35
23	b	625	CLA	C3C-C2C	4.86	1.47	1.36
23	d	403	CLA	CHC-C1C	4.86	1.47	1.35
23	B	609	CLA	O2D-CGD	4.86	1.45	1.33
25	b	628	BCR	C23-C22	-4.85	1.35	1.45
24	A	407	PHO	O2D-CGD	4.85	1.45	1.33
23	B	602	CLA	CHC-C1C	4.85	1.47	1.35
23	c	514	CLA	OBD-CAD	4.84	1.29	1.22
23	C	504	CLA	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402[A]	PHO	CHB-C1B	4.84	1.48	1.38
23	B	605	CLA	C3D-C2D	4.84	1.48	1.39
23	B	606	CLA	C3C-C2C	4.84	1.47	1.36
23	c	510	CLA	CHC-C1C	4.84	1.47	1.35
24	d	402[B]	PHO	CHD-C1D	4.84	1.48	1.38
23	C	502	CLA	OBD-CAD	4.84	1.29	1.22
23	C	502	CLA	O2D-CGD	4.83	1.45	1.33
23	B	612	CLA	O2D-CGD	4.83	1.45	1.33
23	b	612	CLA	O2D-CGD	4.83	1.45	1.33
24	d	402[B]	PHO	CHB-C1B	4.82	1.48	1.38
23	c	511	CLA	OBD-CAD	4.82	1.29	1.22
23	C	511	CLA	OBD-CAD	4.82	1.29	1.22
24	a	410	PHO	CHD-C1D	4.81	1.48	1.38
23	c	509	CLA	O2D-CGD	4.80	1.44	1.33
24	a	410	PHO	O2D-CGD	4.79	1.44	1.33
23	C	504	CLA	OBD-CAD	4.79	1.29	1.22
23	b	620	CLA	C3C-C2C	4.78	1.46	1.36
23	c	505	CLA	CHC-C1C	4.78	1.47	1.35
24	d	402[A]	PHO	CHD-C1D	4.78	1.47	1.38
23	b	620	CLA	CHC-C1C	4.78	1.47	1.35
23	b	613	CLA	OBD-CAD	4.78	1.29	1.22
35	B	622	HTG	C1'-S1	-4.78	1.75	1.81
23	B	614	CLA	CHC-C1C	4.77	1.47	1.35
23	b	624	CLA	O2D-CGD	4.77	1.44	1.33
23	d	403	CLA	O2D-CGD	4.77	1.44	1.33
23	B	612	CLA	CHC-C1C	4.77	1.47	1.35
23	d	404	CLA	O2D-CGD	4.76	1.44	1.33
23	c	508	CLA	C3C-C2C	4.76	1.46	1.36
23	B	610	CLA	OBD-CAD	4.76	1.29	1.22
23	b	615	CLA	O2D-CGD	4.76	1.44	1.33
23	b	613	CLA	O2D-CGD	4.75	1.44	1.33
23	b	623	CLA	CHC-C1C	4.75	1.47	1.35
23	a	408	CLA	O2D-CGD	4.75	1.44	1.33
25	B	620	BCR	C23-C22	-4.74	1.35	1.45
23	B	612	CLA	OBD-CAD	4.74	1.28	1.22
23	B	603	CLA	OBD-CAD	4.74	1.28	1.22
25	a	412	BCR	C23-C22	-4.74	1.35	1.45
24	a	410	PHO	CHB-C1B	4.73	1.47	1.38
23	B	602	CLA	O2A-CGA	4.73	1.47	1.33
23	D	405	CLA	CHC-C1C	4.72	1.47	1.35
23	B	611	CLA	OBD-CAD	4.71	1.28	1.22
23	B	613	CLA	O2D-CGD	4.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	OBD-CAD	4.71	1.28	1.22
23	a	408	CLA	CHC-C1C	4.69	1.47	1.35
25	B	618	BCR	C23-C22	-4.69	1.35	1.45
23	C	513	CLA	OBD-CAD	4.69	1.28	1.22
23	B	615	CLA	O2D-CGD	4.69	1.44	1.33
23	A	404	CLA	O2D-CGD	4.69	1.44	1.33
23	a	411	CLA	OBD-CAD	4.68	1.28	1.22
23	D	406	CLA	OBD-CAD	4.68	1.28	1.22
23	B	615	CLA	CHC-C1C	4.68	1.47	1.35
23	b	619	CLA	OBD-CAD	4.67	1.28	1.22
25	b	626	BCR	C23-C22	-4.66	1.35	1.45
23	B	610	CLA	C3B-C2B	4.66	1.46	1.40
25	D	407	BCR	C23-C22	-4.66	1.35	1.45
23	a	409	CLA	O2D-CGD	4.65	1.44	1.33
23	c	506	CLA	OBD-CAD	4.64	1.28	1.22
23	B	615	CLA	O2A-CGA	4.64	1.46	1.33
23	b	615	CLA	OBD-CAD	4.64	1.28	1.22
25	d	406	BCR	C23-C22	-4.63	1.36	1.45
23	c	515	CLA	O2D-CGD	4.63	1.44	1.33
23	C	510	CLA	OBD-CAD	4.63	1.28	1.22
23	A	405	CLA	CHC-C1C	4.63	1.46	1.35
23	A	405	CLA	OBD-CAD	4.62	1.28	1.22
23	B	608	CLA	O2D-CGD	4.61	1.44	1.33
23	B	602	CLA	OBD-CAD	4.61	1.28	1.22
24	D	402[A]	PHO	CHD-C1D	4.61	1.47	1.38
23	C	506	CLA	OBD-CAD	4.61	1.28	1.22
26	A	413	SQD	O48-C23	4.61	1.46	1.33
26	f	102	SQD	O47-C7	4.61	1.47	1.34
23	C	508	CLA	O2D-CGD	4.61	1.44	1.33
23	C	514	CLA	OBD-CAD	4.60	1.28	1.22
23	B	609	CLA	OBD-CAD	4.60	1.28	1.22
23	d	403	CLA	OBD-CAD	4.59	1.28	1.22
23	b	610	CLA	OBD-CAD	4.58	1.28	1.22
25	c	518	BCR	C23-C22	-4.57	1.36	1.45
23	b	619	CLA	O2D-CGD	4.56	1.44	1.33
23	c	507	CLA	OBD-CAD	4.56	1.28	1.22
25	B	619	BCR	C23-C22	-4.56	1.36	1.45
23	c	517	CLA	OBD-CAD	4.55	1.28	1.22
23	C	505	CLA	OBD-CAD	4.55	1.28	1.22
23	C	512	CLA	OBD-CAD	4.54	1.28	1.22
23	c	513	CLA	O2A-CGA	4.54	1.46	1.33
36	z	101	LMG	O8-C28	4.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	409	DGD	O1G-C1A	4.52	1.46	1.33
23	c	508	CLA	OBD-CAD	4.52	1.28	1.22
23	C	503	CLA	OBD-CAD	4.52	1.28	1.22
23	C	509	CLA	OBD-CAD	4.50	1.28	1.22
23	B	614	CLA	OBD-CAD	4.49	1.28	1.22
26	B	636	SQD	O48-C23	4.49	1.46	1.33
23	C	510	CLA	O2A-CGA	4.49	1.46	1.33
26	F	104	SQD	O47-C7	4.49	1.47	1.34
23	A	406	CLA	OBD-CAD	4.48	1.28	1.22
23	B	615	CLA	OBD-CAD	4.48	1.28	1.22
23	b	616	CLA	OBD-CAD	4.47	1.28	1.22
23	c	515	CLA	OBD-CAD	4.47	1.28	1.22
23	B	605	CLA	O2D-CGD	4.46	1.44	1.33
23	c	509	CLA	OBD-CAD	4.46	1.28	1.22
23	b	614	CLA	OBD-CAD	4.46	1.28	1.22
33	D	412	LHG	O7-C7	4.45	1.46	1.34
36	C	520	LMG	O7-C10	4.45	1.46	1.34
23	D	405	CLA	O2D-CGD	4.45	1.44	1.33
25	b	627	BCR	C23-C22	-4.44	1.36	1.45
23	b	616	CLA	O2A-CGA	4.44	1.46	1.33
23	b	618	CLA	OBD-CAD	4.44	1.28	1.22
23	b	610	CLA	O2A-CGA	4.44	1.46	1.33
37	D	409	DGD	O2G-C1B	4.43	1.46	1.34
23	a	409	CLA	O2A-CGA	4.42	1.46	1.33
23	B	606	CLA	OBD-CAD	4.42	1.28	1.22
23	C	508	CLA	OBD-CAD	4.40	1.28	1.22
23	B	609	CLA	O2A-CGA	4.40	1.46	1.33
37	d	408	DGD	O2G-C1B	4.39	1.46	1.34
23	c	510	CLA	OBD-CAD	4.39	1.28	1.22
23	A	405	CLA	O2A-CGA	4.38	1.46	1.33
23	b	622	CLA	CHC-C1C	4.37	1.46	1.35
23	c	511	CLA	O2A-CGA	4.37	1.46	1.33
23	B	607	CLA	OBD-CAD	4.36	1.28	1.22
23	b	612	CLA	OBD-CAD	4.35	1.28	1.22
23	C	507	CLA	OBD-CAD	4.35	1.28	1.22
23	C	508	CLA	O2A-CGA	4.34	1.46	1.33
23	d	405	CLA	OBD-CAD	4.33	1.28	1.22
23	B	604	CLA	O2A-CGA	4.33	1.46	1.33
23	B	610	CLA	O2A-CGA	4.33	1.46	1.33
23	A	408	CLA	OBD-CAD	4.32	1.28	1.22
33	a	419	LHG	O8-C23	4.32	1.46	1.33
23	C	513	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C	518	DGD	O1G-C1A	4.31	1.45	1.33
36	C	519	LMG	O8-C28	4.31	1.45	1.33
33	A	419	LHG	O8-C23	4.30	1.45	1.33
26	f	102	SQD	O48-C23	4.30	1.45	1.33
23	c	515	CLA	O2A-CGA	4.30	1.45	1.33
26	B	636	SQD	O47-C7	4.29	1.46	1.34
23	c	517	CLA	O2A-CGA	4.29	1.45	1.33
23	C	511	CLA	O2A-CGA	4.29	1.45	1.33
26	b	601	SQD	O47-C7	4.28	1.46	1.34
36	C	501	LMG	O8-C28	4.28	1.45	1.33
33	d	411	LHG	O8-C23	4.28	1.45	1.33
23	C	509	CLA	O2A-CGA	4.28	1.45	1.33
23	B	607	CLA	O2A-CGA	4.28	1.45	1.33
23	B	611	CLA	O2D-CGD	4.27	1.43	1.33
24	d	402[A]	PHO	O2A-CGA	4.27	1.45	1.33
23	B	608	CLA	OBD-CAD	4.27	1.28	1.22
23	C	502	CLA	O2A-CGA	4.27	1.45	1.33
23	B	617	CLA	O2A-CGA	4.27	1.45	1.33
36	M	101	LMG	O8-C28	4.27	1.45	1.33
23	d	403	CLA	O2A-CGA	4.26	1.45	1.33
37	C	518	DGD	O2G-C1B	4.26	1.46	1.34
23	D	406	CLA	O2A-CGA	4.26	1.45	1.33
23	C	505	CLA	O2A-CGA	4.26	1.45	1.33
37	d	408	DGD	O1G-C1A	4.26	1.45	1.33
23	C	504	CLA	O2A-CGA	4.25	1.45	1.33
33	b	634	LHG	O8-C23	4.25	1.45	1.33
23	c	516	CLA	O2A-CGA	4.25	1.45	1.33
24	d	402[B]	PHO	O2A-CGA	4.24	1.45	1.33
33	b	634	LHG	O7-C7	4.24	1.46	1.34
37	c	521	DGD	O1G-C1A	4.24	1.45	1.33
23	d	404	CLA	O2A-CGA	4.24	1.45	1.33
33	d	411	LHG	O7-C7	4.24	1.46	1.34
23	C	507	CLA	O2A-CGA	4.23	1.45	1.33
26	B	621	SQD	O47-C7	4.23	1.46	1.34
23	C	514	CLA	O2A-CGA	4.22	1.45	1.33
23	c	512	CLA	O2A-CGA	4.22	1.45	1.33
23	b	625	CLA	O2A-CGA	4.22	1.45	1.33
36	C	501	LMG	O7-C10	4.21	1.46	1.34
23	B	613	CLA	O2A-CGA	4.21	1.45	1.33
23	B	617	CLA	OBD-CAD	4.20	1.28	1.22
23	B	616	CLA	O2A-CGA	4.20	1.45	1.33
37	c	520	DGD	O1G-C1A	4.20	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	520	LMG	O8-C28	4.19	1.45	1.33
23	d	405	CLA	O2A-CGA	4.18	1.45	1.33
23	b	617	CLA	O2A-CGA	4.18	1.45	1.33
23	B	614	CLA	O2A-CGA	4.18	1.45	1.33
23	b	615	CLA	O2A-CGA	4.18	1.45	1.33
33	a	419	LHG	O7-C7	4.17	1.46	1.34
23	D	405	CLA	OBD-CAD	4.17	1.28	1.22
36	c	522	LMG	O7-C10	4.16	1.46	1.34
23	a	411	CLA	O2A-CGA	4.16	1.45	1.33
23	A	404	CLA	OBD-CAD	4.15	1.28	1.22
36	c	522	LMG	O8-C28	4.15	1.45	1.33
23	A	404	CLA	O2A-CGA	4.14	1.45	1.33
23	C	512	CLA	O2A-CGA	4.13	1.45	1.33
36	a	414	LMG	O8-C28	4.12	1.45	1.33
24	D	402[A]	PHO	O2A-CGA	4.12	1.45	1.33
37	h	102	DGD	O1G-C1A	4.12	1.45	1.33
23	c	506	CLA	O2A-CGA	4.12	1.45	1.33
23	b	624	CLA	O2A-CGA	4.11	1.45	1.33
26	F	104	SQD	O48-C23	4.11	1.45	1.33
26	b	601	SQD	O48-C23	4.11	1.45	1.33
33	A	419	LHG	O7-C7	4.11	1.45	1.34
36	Z	101	LMG	O7-C10	4.10	1.45	1.34
23	A	408	CLA	O2A-CGA	4.10	1.45	1.33
26	a	413	SQD	O48-C23	4.10	1.45	1.33
24	D	402[B]	PHO	O2A-CGA	4.09	1.45	1.33
23	b	618	CLA	O2A-CGA	4.09	1.45	1.33
23	c	510	CLA	O2A-CGA	4.09	1.45	1.33
36	z	101	LMG	O7-C10	4.08	1.45	1.34
23	b	621	CLA	O2A-CGA	4.08	1.45	1.33
36	d	416	LMG	O7-C10	4.07	1.45	1.34
33	D	412	LHG	O8-C23	4.07	1.45	1.33
23	b	620	CLA	O2A-CGA	4.07	1.45	1.33
36	k	101	LMG	O8-C28	4.07	1.45	1.33
35	b	632	HTG	C1'-S1	-4.06	1.76	1.81
26	B	621	SQD	O48-C23	4.06	1.45	1.33
37	H	102	DGD	O1G-C1A	4.06	1.45	1.33
23	c	505	CLA	O2A-CGA	4.06	1.45	1.33
23	b	623	CLA	O2A-CGA	4.06	1.45	1.33
24	A	407	PHO	O2A-CGA	4.04	1.45	1.33
37	C	516	DGD	O2G-C1B	4.04	1.45	1.34
23	b	625	CLA	OBD-CAD	4.04	1.28	1.22
23	c	509	CLA	O2A-CGA	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	416	LMG	O8-C28	4.02	1.45	1.33
37	C	517	DGD	O1G-C1A	4.02	1.45	1.33
33	D	411	LHG	O8-C23	4.01	1.45	1.33
37	c	520	DGD	O2G-C1B	4.00	1.45	1.34
23	B	606	CLA	O2A-CGA	4.00	1.45	1.33
23	b	613	CLA	O2A-CGA	4.00	1.45	1.33
33	D	410	LHG	O8-C23	4.00	1.45	1.33
23	b	612	CLA	O2A-CGA	4.00	1.45	1.33
23	c	505	CLA	OBD-CAD	3.99	1.27	1.22
37	C	517	DGD	O2G-C1B	3.99	1.45	1.34
23	c	508	CLA	O2A-CGA	3.99	1.45	1.33
23	b	622	CLA	O2A-CGA	3.99	1.45	1.33
36	k	101	LMG	O7-C10	3.99	1.45	1.34
37	C	516	DGD	O1G-C1A	3.98	1.45	1.33
23	B	608	CLA	O2A-CGA	3.98	1.45	1.33
24	a	410	PHO	O2A-CGA	3.98	1.45	1.33
26	A	410	SQD	O47-C7	3.98	1.45	1.34
23	B	605	CLA	OBD-CAD	3.97	1.27	1.22
36	C	519	LMG	O7-C10	3.97	1.45	1.34
37	h	102	DGD	O2G-C1B	3.97	1.45	1.34
26	A	413	SQD	O47-C7	3.96	1.45	1.34
36	D	416	LMG	O8-C28	3.96	1.44	1.33
36	D	416	LMG	O7-C10	3.96	1.45	1.34
23	d	404	CLA	OBD-CAD	3.95	1.27	1.22
23	D	405	CLA	O2A-CGA	3.95	1.44	1.33
26	A	410	SQD	O48-C23	3.93	1.44	1.33
36	M	101	LMG	O7-C10	3.93	1.45	1.34
23	C	503	CLA	O2A-CGA	3.93	1.44	1.33
23	c	507	CLA	O2A-CGA	3.93	1.44	1.33
23	b	623	CLA	OBD-CAD	3.93	1.27	1.22
23	B	612	CLA	O2A-CGA	3.92	1.44	1.33
33	d	410	LHG	O7-C7	3.92	1.45	1.34
37	H	102	DGD	O2G-C1B	3.91	1.45	1.34
37	c	521	DGD	O2G-C1B	3.90	1.45	1.34
36	b	629	LMG	O8-C28	3.90	1.44	1.33
23	b	614	CLA	O2A-CGA	3.90	1.44	1.33
37	c	519	DGD	O1G-C1A	3.90	1.44	1.33
36	b	629	LMG	O7-C10	3.88	1.45	1.34
24	a	410	PHO	OBD-CAD	3.88	1.29	1.22
23	a	408	CLA	O2A-CGA	3.88	1.44	1.33
35	d	414	HTG	C1'-S1	-3.88	1.76	1.81
36	a	414	LMG	O7-C10	3.87	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	O2A-CGA	3.87	1.44	1.33
26	a	413	SQD	O47-C7	3.85	1.45	1.34
37	c	519	DGD	O2G-C1B	3.84	1.45	1.34
33	L	101	LHG	O8-C23	3.83	1.44	1.33
23	c	514	CLA	O2A-CGA	3.83	1.44	1.33
23	B	603	CLA	O2A-CGA	3.80	1.44	1.33
35	B	631	HTG	C1'-S1	-3.80	1.76	1.81
23	C	506	CLA	O2A-CGA	3.79	1.44	1.33
23	A	406	CLA	O2A-CGA	3.79	1.44	1.33
35	b	602	HTG	C1'-S1	-3.79	1.76	1.81
23	B	611	CLA	O2A-CGA	3.78	1.44	1.33
23	b	619	CLA	O2A-CGA	3.77	1.44	1.33
24	d	402[A]	PHO	C3D-C2D	3.77	1.49	1.39
23	b	622	CLA	OBD-CAD	3.76	1.27	1.22
24	D	402[B]	PHO	C3D-C2D	3.74	1.49	1.39
24	D	402[B]	PHO	CHC-C4B	3.74	1.49	1.40
24	a	410	PHO	CHC-C4B	3.72	1.49	1.40
33	d	409	LHG	O8-C23	3.72	1.44	1.33
24	d	402[B]	PHO	CHC-C4B	3.68	1.49	1.40
35	V	206	HTG	C1'-S1	-3.66	1.76	1.81
24	D	402[A]	PHO	C3D-C2D	3.65	1.49	1.39
24	D	402[A]	PHO	C4A-NA	-3.64	1.26	1.35
35	b	607	HTG	C1'-S1	-3.64	1.76	1.81
24	D	402[B]	PHO	C4A-NA	-3.63	1.26	1.35
33	d	409	LHG	O7-C7	3.63	1.44	1.34
24	a	410	PHO	C3D-C2D	3.60	1.48	1.39
23	B	604	CLA	OBD-CAD	3.59	1.27	1.22
24	d	402[B]	PHO	OBD-CAD	3.58	1.28	1.22
35	c	524	HTG	C1'-S1	-3.57	1.76	1.81
24	D	402[B]	PHO	OBD-CAD	3.56	1.28	1.22
35	C	523	HTG	C1'-S1	-3.56	1.76	1.81
24	d	402[A]	PHO	CHC-C4B	3.55	1.48	1.40
24	A	407	PHO	C3D-C2D	3.55	1.48	1.39
35	c	523	HTG	C1'-S1	-3.54	1.76	1.81
23	B	605	CLA	O2A-CGA	3.52	1.43	1.33
35	b	608	HTG	C1'-S1	-3.51	1.76	1.81
24	D	402[A]	PHO	CHC-C4B	3.51	1.48	1.40
35	B	632	HTG	C1'-S1	-3.49	1.77	1.81
33	D	411	LHG	O7-C7	3.49	1.44	1.34
33	d	410	LHG	O8-C23	3.47	1.43	1.33
24	d	402[B]	PHO	C3D-C2D	3.44	1.48	1.39
24	d	402[B]	PHO	C4A-NA	-3.43	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	L	101	LHG	O7-C7	3.43	1.44	1.34
35	C	522	HTG	C1'-S1	-3.43	1.77	1.81
35	B	624	HTG	C1'-S1	-3.41	1.77	1.81
24	A	407	PHO	C4A-NA	-3.41	1.27	1.35
24	A	407	PHO	CHB-C4A	3.40	1.48	1.40
24	a	410	PHO	C4A-NA	-3.40	1.27	1.35
24	A	407	PHO	OBD-CAD	3.38	1.28	1.22
24	A	407	PHO	CHD-C4C	3.38	1.48	1.40
24	D	402[B]	PHO	CHD-C4C	3.34	1.48	1.40
24	D	402[A]	PHO	OBD-CAD	3.33	1.28	1.22
23	b	620	CLA	OBD-CAD	3.31	1.26	1.22
24	A	407	PHO	CHC-C4B	3.31	1.48	1.40
24	d	402[A]	PHO	C4A-NA	-3.30	1.27	1.35
33	D	410	LHG	O7-C7	3.29	1.43	1.34
24	d	402[A]	PHO	OBD-CAD	3.25	1.28	1.22
23	b	624	CLA	C1D-C2D	3.24	1.49	1.42
23	c	509	CLA	C4C-C3C	3.23	1.50	1.45
24	A	407	PHO	C3B-C4B	3.23	1.50	1.43
24	D	402[A]	PHO	CHD-C4C	3.22	1.48	1.40
35	D	415	HTG	C1'-S1	-3.17	1.77	1.81
24	d	402[B]	PHO	CHD-C4C	3.16	1.47	1.40
23	B	606	CLA	C1C-C2C	3.15	1.50	1.44
24	D	402[B]	PHO	C3B-C4B	3.14	1.49	1.43
24	d	402[A]	PHO	CHD-C4C	3.14	1.47	1.40
24	D	402[A]	PHO	C3B-C4B	3.13	1.49	1.43
24	D	402[B]	PHO	CHB-C4A	3.10	1.47	1.40
24	d	402[B]	PHO	C3B-C4B	3.09	1.49	1.43
35	b	631	HTG	C1'-S1	-3.07	1.77	1.81
24	d	402[A]	PHO	C3B-C4B	3.06	1.49	1.43
23	b	622	CLA	C4C-C3C	3.04	1.50	1.45
23	B	602	CLA	C1D-C2D	3.03	1.49	1.42
23	a	408	CLA	C4C-C3C	3.02	1.50	1.45
23	b	612	CLA	C1C-C2C	3.02	1.50	1.44
24	d	402[B]	PHO	CHB-C4A	3.01	1.47	1.40
24	a	410	PHO	C3B-C4B	3.00	1.49	1.43
35	B	623	HTG	C1'-S1	-3.00	1.77	1.81
23	B	614	CLA	C4C-C3C	2.99	1.50	1.45
23	B	603	CLA	C1D-C2D	2.98	1.49	1.42
23	d	405	CLA	C1D-C2D	2.97	1.49	1.42
23	C	502	CLA	C1C-C2C	2.97	1.50	1.44
26	A	413	SQD	C6-S	-2.96	1.66	1.77
23	b	610	CLA	C1D-C2D	2.95	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1D-C2D	2.95	1.49	1.42
23	b	621	CLA	C1C-C2C	2.95	1.50	1.44
23	a	408	CLA	C1D-C2D	2.93	1.49	1.42
23	C	511	CLA	C1D-C2D	2.93	1.49	1.42
26	F	104	SQD	C6-S	-2.93	1.66	1.77
23	C	507	CLA	C1D-C2D	2.92	1.49	1.42
23	a	409	CLA	C1D-C2D	2.92	1.49	1.42
24	a	410	PHO	CHD-C4C	2.92	1.47	1.40
26	f	102	SQD	C6-S	-2.92	1.66	1.77
23	c	511	CLA	C1C-C2C	2.91	1.50	1.44
24	d	402[A]	PHO	CHB-C4A	2.88	1.47	1.40
23	C	514	CLA	C1D-C2D	2.88	1.49	1.42
23	b	619	CLA	C1D-C2D	2.87	1.49	1.42
23	B	614	CLA	C1C-C2C	2.87	1.50	1.44
26	A	410	SQD	C6-S	-2.86	1.66	1.77
23	c	513	CLA	C1C-C2C	2.86	1.50	1.44
23	c	514	CLA	CHD-C4C	2.85	1.49	1.41
23	b	616	CLA	C1D-C2D	2.85	1.49	1.42
23	B	611	CLA	C1D-C2D	2.85	1.49	1.42
23	c	510	CLA	C1D-C2D	2.84	1.49	1.42
23	c	508	CLA	C1D-C2D	2.84	1.49	1.42
23	b	618	CLA	C1D-C2D	2.84	1.49	1.42
23	c	517	CLA	C1D-C2D	2.84	1.49	1.42
23	B	606	CLA	C4B-CHC	2.84	1.48	1.41
23	C	504	CLA	C1D-C2D	2.83	1.49	1.42
23	b	611	CLA	C1D-C2D	2.83	1.49	1.42
23	D	406	CLA	C1D-C2D	2.82	1.49	1.42
39	v	206	HEM	C3B-C2B	-2.82	1.36	1.40
23	C	502	CLA	C1D-C2D	2.82	1.48	1.42
23	C	506	CLA	C4C-C3C	2.81	1.49	1.45
23	C	511	CLA	CHD-C4C	2.81	1.49	1.41
23	c	505	CLA	C1D-C2D	2.80	1.48	1.42
23	B	610	CLA	C1D-C2D	2.80	1.48	1.42
24	a	410	PHO	CHB-C4A	2.80	1.47	1.40
23	C	512	CLA	C4C-C3C	2.79	1.49	1.45
23	d	404	CLA	C1C-C2C	2.79	1.50	1.44
23	c	515	CLA	C1D-C2D	2.78	1.48	1.42
23	c	511	CLA	C1D-C2D	2.78	1.48	1.42
23	d	405	CLA	C1C-C2C	2.78	1.49	1.44
23	B	613	CLA	C1C-C2C	2.78	1.49	1.44
24	D	402[A]	PHO	CHB-C4A	2.77	1.46	1.40
23	b	617	CLA	C1B-CHB	2.77	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	617	CLA	C4B-CHC	2.76	1.48	1.41
23	b	616	CLA	C1B-CHB	2.75	1.48	1.41
23	C	510	CLA	C1D-C2D	2.75	1.48	1.42
23	b	617	CLA	C1D-C2D	2.75	1.48	1.42
23	d	404	CLA	C1B-NB	-2.74	1.32	1.35
23	C	504	CLA	C1C-C2C	2.74	1.49	1.44
23	b	614	CLA	C1C-C2C	2.73	1.49	1.44
23	c	514	CLA	C1D-C2D	2.73	1.48	1.42
23	B	607	CLA	C1D-C2D	2.73	1.48	1.42
23	C	511	CLA	C4C-C3C	2.72	1.49	1.45
23	B	611	CLA	C4B-CHC	2.72	1.48	1.41
23	A	406	CLA	C1D-C2D	2.72	1.48	1.42
23	b	615	CLA	C1D-C2D	2.72	1.48	1.42
23	b	621	CLA	C1B-CHB	2.72	1.48	1.41
23	C	504	CLA	C4B-CHC	2.72	1.48	1.41
23	b	623	CLA	C1D-C2D	2.72	1.48	1.42
23	B	604	CLA	C1B-NB	-2.72	1.32	1.35
23	A	404	CLA	C1C-C2C	2.71	1.49	1.44
23	C	505	CLA	CHD-C4C	2.71	1.48	1.41
23	b	613	CLA	C1C-C2C	2.70	1.49	1.44
23	c	507	CLA	C1C-C2C	2.70	1.49	1.44
23	c	516	CLA	CHD-C4C	2.70	1.48	1.41
23	d	403	CLA	C1D-C2D	2.70	1.48	1.42
23	C	508	CLA	C1C-C2C	2.69	1.49	1.44
23	b	615	CLA	C1B-NB	-2.69	1.32	1.35
23	c	516	CLA	C1C-C2C	2.69	1.49	1.44
26	B	636	SQD	C6-S	-2.68	1.67	1.77
23	A	408	CLA	C4B-CHC	2.68	1.48	1.41
23	b	614	CLA	C1D-C2D	2.68	1.48	1.42
23	B	606	CLA	C1B-CHB	2.67	1.48	1.41
23	C	514	CLA	CHD-C4C	2.67	1.48	1.41
23	C	505	CLA	C1D-C2D	2.67	1.48	1.42
23	c	507	CLA	C4B-CHC	2.67	1.48	1.41
23	d	405	CLA	C4B-CHC	2.67	1.48	1.41
36	Z	101	LMG	O8-C28	2.66	1.46	1.33
23	C	510	CLA	CHD-C4C	2.66	1.48	1.41
23	C	508	CLA	C1D-C2D	2.66	1.48	1.42
23	A	408	CLA	C1D-C2D	2.65	1.48	1.42
23	c	509	CLA	C1B-CHB	2.65	1.48	1.41
23	c	514	CLA	C1B-CHB	2.65	1.48	1.41
23	B	608	CLA	C1B-NB	-2.65	1.32	1.35
23	b	619	CLA	CHD-C4C	2.65	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	625	CLA	C1D-C2D	2.65	1.48	1.42
23	d	404	CLA	C4C-C3C	2.64	1.49	1.45
23	C	513	CLA	C1C-C2C	2.64	1.49	1.44
31	d	407[B]	PL9	C6-C5	2.64	1.49	1.35
23	b	610	CLA	CHD-C4C	2.64	1.48	1.41
23	A	408	CLA	C1C-C2C	2.64	1.49	1.44
23	b	615	CLA	C1C-C2C	2.64	1.49	1.44
23	B	611	CLA	CHD-C4C	2.64	1.48	1.41
23	b	619	CLA	C1B-CHB	2.64	1.48	1.41
23	B	608	CLA	C4B-CHC	2.63	1.48	1.41
23	B	615	CLA	C1D-C2D	2.63	1.48	1.42
23	C	503	CLA	C1B-CHB	2.63	1.48	1.41
23	a	411	CLA	C1D-C2D	2.63	1.48	1.42
23	b	622	CLA	CHD-C4C	2.62	1.48	1.41
23	C	512	CLA	CHD-C4C	2.62	1.48	1.41
23	C	504	CLA	CHD-C4C	2.62	1.48	1.41
23	c	517	CLA	CHD-C4C	2.62	1.48	1.41
23	B	614	CLA	C1D-C2D	2.61	1.48	1.42
23	c	514	CLA	C4C-C3C	2.61	1.49	1.45
23	b	625	CLA	C1B-CHB	2.61	1.48	1.41
23	b	613	CLA	C1B-CHB	2.61	1.48	1.41
26	a	413	SQD	C6-S	-2.61	1.67	1.77
23	b	625	CLA	C4B-CHC	2.61	1.48	1.41
23	B	616	CLA	C4B-CHC	2.61	1.48	1.41
23	C	509	CLA	C1D-C2D	2.60	1.48	1.42
23	c	513	CLA	C1B-CHB	2.60	1.48	1.41
23	d	403	CLA	CHD-C4C	2.60	1.48	1.41
23	b	611	CLA	C1C-C2C	2.60	1.49	1.44
23	b	622	CLA	C1B-CHB	2.60	1.48	1.41
23	c	506	CLA	C1B-CHB	2.60	1.48	1.41
23	C	513	CLA	CHD-C4C	2.60	1.48	1.41
23	C	506	CLA	C1B-CHB	2.60	1.48	1.41
23	B	606	CLA	C1D-C2D	2.60	1.48	1.42
26	B	621	SQD	C6-S	-2.60	1.67	1.77
23	b	611	CLA	C4C-C3C	2.60	1.49	1.45
23	B	607	CLA	C1C-C2C	2.59	1.49	1.44
23	c	513	CLA	C1D-C2D	2.59	1.48	1.42
23	B	608	CLA	C1B-CHB	2.59	1.48	1.41
31	a	415[B]	PL9	C6-C5	2.58	1.48	1.35
23	C	510	CLA	C4C-C3C	2.58	1.49	1.45
23	B	610	CLA	C1B-CHB	2.58	1.48	1.41
23	c	509	CLA	CHD-C4C	2.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C1D-C2D	2.58	1.48	1.42
31	a	415[A]	PL9	C6-C5	2.58	1.48	1.35
26	b	601	SQD	C6-S	-2.58	1.67	1.77
23	B	609	CLA	C1C-C2C	2.57	1.49	1.44
23	c	507	CLA	C1D-C2D	2.57	1.48	1.42
31	D	408[A]	PL9	C6-C5	2.57	1.48	1.35
31	D	408[B]	PL9	C6-C5	2.57	1.48	1.35
23	C	513	CLA	C1D-C2D	2.57	1.48	1.42
23	b	620	CLA	C1B-CHB	2.57	1.48	1.41
23	B	607	CLA	C1B-CHB	2.57	1.48	1.41
23	c	505	CLA	C4C-C3C	2.57	1.49	1.45
23	b	617	CLA	CHD-C4C	2.56	1.48	1.41
23	c	510	CLA	C1B-CHB	2.56	1.48	1.41
23	c	505	CLA	C1B-CHB	2.56	1.48	1.41
23	C	512	CLA	C1D-C2D	2.56	1.48	1.42
28	a	404	LMT	O1'-C1'	2.56	1.44	1.40
23	C	502	CLA	C4C-C3C	2.56	1.49	1.45
23	B	602	CLA	C1B-CHB	2.55	1.48	1.41
23	D	405	CLA	C1C-C2C	2.55	1.49	1.44
31	A	417[B]	PL9	C6-C5	2.55	1.48	1.35
23	B	604	CLA	C1D-C2D	2.55	1.48	1.42
31	d	407[A]	PL9	C6-C5	2.55	1.48	1.35
23	b	611	CLA	C1B-CHB	2.54	1.48	1.41
23	c	508	CLA	C1C-C2C	2.54	1.49	1.44
31	A	417[A]	PL9	C6-C5	2.54	1.48	1.35
23	C	514	CLA	C4B-CHC	2.54	1.48	1.41
23	C	507	CLA	CHD-C4C	2.54	1.48	1.41
23	B	612	CLA	C1D-C2D	2.54	1.48	1.42
23	C	502	CLA	C4B-CHC	2.54	1.48	1.41
23	B	604	CLA	CHD-C4C	2.54	1.48	1.41
23	C	510	CLA	C1C-C2C	2.54	1.49	1.44
23	C	508	CLA	C4B-CHC	2.54	1.48	1.41
23	a	408	CLA	CHD-C4C	2.53	1.48	1.41
23	C	503	CLA	C1C-C2C	2.53	1.49	1.44
35	c	523	HTG	C1-S1	-2.53	1.76	1.80
23	B	613	CLA	C1B-CHB	2.53	1.48	1.41
23	b	611	CLA	CHD-C4C	2.53	1.48	1.41
23	C	511	CLA	C1B-CHB	2.52	1.48	1.41
23	C	511	CLA	C4B-CHC	2.52	1.48	1.41
23	D	405	CLA	C1D-C2D	2.52	1.48	1.42
23	C	506	CLA	C1D-C2D	2.52	1.48	1.42
23	C	513	CLA	C4B-CHC	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	414	LMT	O1'-C1'	2.52	1.44	1.40
23	b	621	CLA	C4B-CHC	2.52	1.48	1.41
23	c	516	CLA	C1D-C2D	2.52	1.48	1.42
23	a	409	CLA	CHD-C4C	2.51	1.48	1.41
23	B	614	CLA	CHD-C4C	2.51	1.48	1.41
23	c	517	CLA	C1C-C2C	2.51	1.49	1.44
23	b	618	CLA	CHD-C4C	2.51	1.48	1.41
23	c	517	CLA	C4B-CHC	2.51	1.48	1.41
23	d	404	CLA	C1D-C2D	2.51	1.48	1.42
23	a	408	CLA	C1B-CHB	2.51	1.48	1.41
23	C	514	CLA	C1B-CHB	2.51	1.48	1.41
23	a	411	CLA	CHD-C4C	2.50	1.48	1.41
23	c	510	CLA	CHD-C4C	2.50	1.48	1.41
23	c	516	CLA	C4B-CHC	2.50	1.48	1.41
23	b	613	CLA	C1D-C2D	2.50	1.48	1.42
39	V	205	HEM	C3B-C2B	-2.50	1.36	1.40
23	B	616	CLA	C1C-C2C	2.50	1.49	1.44
35	b	632	HTG	C1-S1	-2.50	1.76	1.80
23	c	512	CLA	C1D-C2D	2.50	1.48	1.42
23	b	624	CLA	CHD-C4C	2.49	1.48	1.41
35	D	415	HTG	C1-S1	-2.49	1.76	1.80
23	B	608	CLA	C1C-C2C	2.49	1.49	1.44
23	B	610	CLA	C4C-C3C	2.49	1.49	1.45
23	c	506	CLA	CHD-C4C	2.48	1.48	1.41
23	C	512	CLA	C1B-CHB	2.48	1.47	1.41
23	C	509	CLA	C1B-CHB	2.48	1.47	1.41
23	D	406	CLA	C4C-C3C	2.48	1.49	1.45
23	C	512	CLA	C1C-C2C	2.47	1.49	1.44
23	c	511	CLA	CHD-C4C	2.47	1.48	1.41
23	b	623	CLA	CHD-C4C	2.47	1.48	1.41
23	C	511	CLA	C1C-C2C	2.47	1.49	1.44
39	F	102	HEM	C3B-C2B	-2.47	1.36	1.40
23	C	502	CLA	CHD-C4C	2.47	1.48	1.41
23	B	612	CLA	C4C-C3C	2.47	1.49	1.45
23	c	511	CLA	C1B-CHB	2.47	1.47	1.41
23	B	614	CLA	C1B-CHB	2.47	1.47	1.41
23	a	408	CLA	C1C-C2C	2.47	1.49	1.44
23	c	508	CLA	CHD-C4C	2.47	1.48	1.41
23	D	406	CLA	CHD-C4C	2.47	1.48	1.41
23	c	513	CLA	CHD-C4C	2.47	1.48	1.41
23	c	512	CLA	C1B-CHB	2.46	1.47	1.41
23	c	508	CLA	C1B-CHB	2.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	CHD-C4C	2.46	1.48	1.41
23	C	506	CLA	CHD-C4C	2.46	1.48	1.41
23	d	404	CLA	C4B-CHC	2.46	1.47	1.41
23	c	509	CLA	C1D-C2D	2.46	1.48	1.42
23	D	405	CLA	C4C-C3C	2.46	1.49	1.45
35	b	608	HTG	C1-S1	-2.46	1.77	1.80
23	b	616	CLA	C4B-CHC	2.45	1.47	1.41
23	A	404	CLA	C4C-C3C	2.45	1.49	1.45
23	B	607	CLA	C4C-C3C	2.45	1.49	1.45
23	C	510	CLA	C1B-CHB	2.45	1.47	1.41
23	b	618	CLA	C1B-CHB	2.44	1.47	1.41
23	C	505	CLA	C1C-C2C	2.44	1.49	1.44
23	c	511	CLA	C4B-CHC	2.44	1.47	1.41
24	D	402[A]	PHO	C1A-NA	-2.44	1.32	1.37
23	C	510	CLA	C4B-CHC	2.43	1.47	1.41
23	B	605	CLA	C1C-C2C	2.43	1.49	1.44
23	b	612	CLA	C1D-C2D	2.43	1.48	1.42
23	c	512	CLA	CHD-C4C	2.43	1.48	1.41
23	c	505	CLA	CHD-C4C	2.43	1.48	1.41
23	B	607	CLA	C4B-CHC	2.43	1.47	1.41
23	B	612	CLA	CHD-C4C	2.43	1.48	1.41
23	A	406	CLA	CHD-C4C	2.43	1.48	1.41
23	c	513	CLA	C4B-CHC	2.43	1.47	1.41
23	B	608	CLA	CHD-C4C	2.42	1.48	1.41
23	B	615	CLA	CHD-C4C	2.42	1.48	1.41
23	B	603	CLA	C4C-C3C	2.42	1.49	1.45
23	B	615	CLA	C1B-CHB	2.42	1.47	1.41
23	b	620	CLA	C1D-C2D	2.42	1.48	1.42
23	b	616	CLA	C1B-NB	-2.42	1.33	1.35
23	B	613	CLA	C1D-C2D	2.41	1.48	1.42
23	b	610	CLA	C4B-CHC	2.41	1.47	1.41
23	b	624	CLA	C1B-CHB	2.41	1.47	1.41
23	B	602	CLA	CHD-C4C	2.41	1.48	1.41
23	B	608	CLA	C4C-C3C	2.41	1.49	1.45
23	c	509	CLA	C4B-CHC	2.41	1.47	1.41
23	c	514	CLA	C4B-CHC	2.40	1.47	1.41
23	B	617	CLA	C1B-CHB	2.40	1.47	1.41
23	b	619	CLA	C4B-CHC	2.40	1.47	1.41
23	C	503	CLA	C1D-C2D	2.40	1.48	1.42
23	b	625	CLA	C1C-C2C	2.40	1.49	1.44
23	C	505	CLA	C4B-CHC	2.40	1.47	1.41
23	a	411	CLA	C1B-CHB	2.40	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	CHD-C4C	2.40	1.48	1.41
23	b	623	CLA	C1B-CHB	2.39	1.47	1.41
23	B	604	CLA	C1C-C2C	2.39	1.49	1.44
37	D	409	DGD	O3G-C1D	2.39	1.44	1.40
23	A	405	CLA	C1D-C2D	2.39	1.48	1.42
23	a	409	CLA	C1B-NB	-2.38	1.33	1.35
23	C	505	CLA	C4C-C3C	2.38	1.49	1.45
23	B	606	CLA	CHD-C4C	2.38	1.47	1.41
23	C	509	CLA	C1C-C2C	2.38	1.49	1.44
23	A	408	CLA	C1B-CHB	2.38	1.47	1.41
23	c	515	CLA	CHD-C4C	2.38	1.47	1.41
23	B	603	CLA	C1C-C2C	2.38	1.49	1.44
23	b	615	CLA	C1B-CHB	2.38	1.47	1.41
23	d	404	CLA	C1B-CHB	2.37	1.47	1.41
23	D	405	CLA	CHD-C4C	2.37	1.47	1.41
23	B	610	CLA	C1C-C2C	2.37	1.49	1.44
23	A	404	CLA	CHD-C4C	2.37	1.47	1.41
23	B	615	CLA	C1C-C2C	2.37	1.49	1.44
23	b	610	CLA	C1C-C2C	2.36	1.49	1.44
23	C	505	CLA	C1B-CHB	2.36	1.47	1.41
23	c	515	CLA	C1C-C2C	2.36	1.49	1.44
23	c	507	CLA	CHD-C4C	2.36	1.47	1.41
23	b	612	CLA	C4B-CHC	2.36	1.47	1.41
23	B	607	CLA	CHD-C4C	2.36	1.47	1.41
23	B	610	CLA	CHD-C4C	2.35	1.47	1.41
23	A	404	CLA	C1D-C2D	2.35	1.47	1.42
23	B	604	CLA	C4B-CHC	2.35	1.47	1.41
23	d	405	CLA	CHD-C4C	2.35	1.47	1.41
23	b	612	CLA	C4C-C3C	2.35	1.49	1.45
23	c	505	CLA	C1C-C2C	2.35	1.49	1.44
23	b	622	CLA	C1D-C2D	2.35	1.47	1.42
35	C	522	HTG	C1-S1	-2.35	1.77	1.80
23	b	620	CLA	C4C-C3C	2.35	1.49	1.45
23	c	509	CLA	C1C-C2C	2.35	1.49	1.44
23	b	617	CLA	C1C-C2C	2.35	1.49	1.44
23	b	614	CLA	C1B-CHB	2.34	1.47	1.41
23	c	517	CLA	C4C-C3C	2.34	1.49	1.45
23	b	620	CLA	CHD-C4C	2.34	1.47	1.41
23	C	502	CLA	C1B-CHB	2.34	1.47	1.41
23	b	612	CLA	C1B-CHB	2.34	1.47	1.41
24	a	410	PHO	C1A-NA	-2.34	1.32	1.37
23	b	613	CLA	CHD-C4C	2.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C1C-C2C	2.34	1.49	1.44
23	B	609	CLA	C1D-C2D	2.34	1.47	1.42
23	B	612	CLA	C1C-C2C	2.33	1.49	1.44
23	C	504	CLA	C1B-CHB	2.33	1.47	1.41
23	C	503	CLA	CHD-C4C	2.33	1.47	1.41
23	B	602	CLA	C4B-CHC	2.33	1.47	1.41
23	A	408	CLA	CHD-C4C	2.33	1.47	1.41
23	C	503	CLA	C4B-CHC	2.33	1.47	1.41
23	b	615	CLA	CHD-C4C	2.33	1.47	1.41
24	d	402[B]	PHO	C1A-NA	-2.33	1.33	1.37
23	B	617	CLA	CHD-C4C	2.33	1.47	1.41
23	C	507	CLA	C4C-C3C	2.33	1.49	1.45
23	A	406	CLA	C4B-CHC	2.32	1.47	1.41
35	c	524	HTG	C1-S1	-2.32	1.77	1.80
35	V	206	HTG	C1-S1	-2.32	1.77	1.80
23	c	515	CLA	C1B-CHB	2.31	1.47	1.41
23	B	602	CLA	C4C-C3C	2.31	1.49	1.45
23	B	603	CLA	C4B-CHC	2.30	1.47	1.41
23	b	624	CLA	C4C-C3C	2.30	1.49	1.45
23	C	504	CLA	C4C-C3C	2.30	1.49	1.45
23	b	621	CLA	C1D-C2D	2.30	1.47	1.42
23	D	406	CLA	C4B-CHC	2.30	1.47	1.41
23	D	406	CLA	C1B-CHB	2.29	1.47	1.41
23	b	614	CLA	C4B-CHC	2.29	1.47	1.41
23	a	411	CLA	C4C-C3C	2.29	1.49	1.45
23	c	510	CLA	C1B-NB	-2.29	1.33	1.35
23	B	605	CLA	C4B-CHC	2.29	1.47	1.41
23	B	602	CLA	C1C-C2C	2.29	1.49	1.44
23	A	405	CLA	C4C-C3C	2.28	1.49	1.45
23	c	506	CLA	C4B-CHC	2.28	1.47	1.41
23	b	611	CLA	C4B-CHC	2.28	1.47	1.41
23	b	620	CLA	C4B-CHC	2.28	1.47	1.41
23	A	405	CLA	CHD-C4C	2.28	1.47	1.41
23	c	507	CLA	C1B-CHB	2.27	1.47	1.41
23	b	610	CLA	C1B-CHB	2.27	1.47	1.41
24	D	402[A]	PHO	C4D-CHA	2.27	1.49	1.43
23	d	404	CLA	CHD-C4C	2.27	1.47	1.41
23	b	625	CLA	CHD-C4C	2.27	1.47	1.41
23	B	609	CLA	C1B-CHB	2.27	1.47	1.41
23	c	511	CLA	C4C-C3C	2.27	1.48	1.45
24	D	402[B]	PHO	C1A-NA	-2.27	1.33	1.37
23	b	615	CLA	C4B-CHC	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	e	101	HEM	C3B-C2B	-2.27	1.37	1.40
23	B	609	CLA	C4C-C3C	2.26	1.48	1.45
23	B	616	CLA	C1D-C2D	2.26	1.47	1.42
23	C	508	CLA	C1B-CHB	2.26	1.47	1.41
23	B	605	CLA	CHD-C4C	2.26	1.47	1.41
23	B	611	CLA	C1B-CHB	2.26	1.47	1.41
23	A	404	CLA	C4B-CHC	2.26	1.47	1.41
23	C	508	CLA	C4C-C3C	2.26	1.48	1.45
23	C	506	CLA	C4B-CHC	2.25	1.47	1.41
23	B	613	CLA	C4B-CHC	2.25	1.47	1.41
23	B	609	CLA	CHD-C4C	2.25	1.47	1.41
23	C	506	CLA	C1C-C2C	2.25	1.48	1.44
23	b	618	CLA	C4B-CHC	2.24	1.47	1.41
23	b	613	CLA	C4C-C3C	2.24	1.48	1.45
23	B	605	CLA	C1D-C2D	2.24	1.47	1.42
23	c	514	CLA	C1C-C2C	2.24	1.48	1.44
23	D	405	CLA	C1B-CHB	2.24	1.47	1.41
35	d	414	HTG	C1-S1	-2.24	1.77	1.80
23	D	405	CLA	C4B-CHC	2.24	1.47	1.41
23	C	509	CLA	C4B-CHC	2.23	1.47	1.41
23	C	514	CLA	C1C-C2C	2.23	1.48	1.44
23	b	616	CLA	CHD-C4C	2.23	1.47	1.41
23	a	408	CLA	C4B-CHC	2.23	1.47	1.41
23	c	517	CLA	C1B-CHB	2.22	1.47	1.41
23	c	510	CLA	C4B-CHC	2.22	1.47	1.41
23	c	508	CLA	C4B-CHC	2.22	1.47	1.41
23	D	406	CLA	C1C-C2C	2.22	1.48	1.44
23	B	611	CLA	C1C-C2C	2.22	1.48	1.44
23	C	509	CLA	C4C-C3C	2.22	1.48	1.45
23	c	515	CLA	C1C-NC	-2.21	1.34	1.37
23	B	606	CLA	C4C-C3C	2.21	1.48	1.45
23	c	506	CLA	C1C-NC	-2.20	1.34	1.37
23	C	509	CLA	CHD-C4C	2.20	1.47	1.41
23	A	405	CLA	C1B-CHB	2.20	1.47	1.41
23	B	605	CLA	C1B-CHB	2.20	1.47	1.41
23	C	503	CLA	C4C-C3C	2.20	1.48	1.45
23	B	611	CLA	C4C-C3C	2.20	1.48	1.45
24	d	402[A]	PHO	C4D-CHA	2.20	1.49	1.43
23	b	619	CLA	C1B-NB	-2.20	1.33	1.35
23	B	617	CLA	C4B-CHC	2.20	1.47	1.41
23	B	616	CLA	CHD-C4C	2.19	1.47	1.41
23	B	612	CLA	C1B-CHB	2.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CHD-C4C	2.19	1.47	1.41
37	h	102	DGD	O5D-C1E	2.19	1.43	1.40
23	b	612	CLA	CHD-C4C	2.19	1.47	1.41
23	a	409	CLA	C1B-CHB	2.19	1.47	1.41
23	B	617	CLA	C1D-C2D	2.19	1.47	1.42
23	b	619	CLA	C1C-C2C	2.18	1.48	1.44
23	d	403	CLA	C1B-NB	-2.18	1.33	1.35
24	A	407	PHO	C1A-NA	-2.18	1.33	1.37
23	d	403	CLA	C1C-NC	-2.18	1.34	1.37
23	C	513	CLA	C1B-CHB	2.18	1.47	1.41
23	b	624	CLA	C4B-CHC	2.18	1.47	1.41
23	c	515	CLA	C4B-CHC	2.18	1.47	1.41
24	D	402[B]	PHO	C4D-CHA	2.18	1.49	1.43
23	B	615	CLA	C4C-C3C	2.17	1.48	1.45
23	C	512	CLA	C4B-CHC	2.17	1.47	1.41
23	b	610	CLA	C4C-C3C	2.17	1.48	1.45
23	B	613	CLA	CHD-C4C	2.17	1.47	1.41
23	C	507	CLA	C1B-CHB	2.17	1.47	1.41
23	b	624	CLA	C1C-C2C	2.17	1.48	1.44
23	B	614	CLA	C4B-CHC	2.17	1.47	1.41
23	c	510	CLA	C4C-C3C	2.16	1.48	1.45
23	b	613	CLA	C4B-CHC	2.16	1.47	1.41
23	C	513	CLA	C4C-C3C	2.16	1.48	1.45
35	B	632	HTG	C1-S1	-2.16	1.77	1.80
23	B	604	CLA	C1B-CHB	2.15	1.47	1.41
35	B	624	HTG	C1-S1	-2.15	1.77	1.80
23	b	616	CLA	C1C-C2C	2.15	1.48	1.44
23	B	603	CLA	C1B-CHB	2.15	1.47	1.41
23	c	513	CLA	C4C-C3C	2.14	1.48	1.45
23	b	621	CLA	CHD-C4C	2.14	1.47	1.41
39	F	102	HEM	C4D-C3D	2.14	1.47	1.42
23	B	611	CLA	C1B-NB	-2.13	1.33	1.35
24	A	407	PHO	C4D-CHA	2.13	1.49	1.43
23	C	507	CLA	C4B-CHC	2.13	1.46	1.41
23	B	602	CLA	C1C-NC	-2.13	1.34	1.37
28	T	104	LMT	O1'-C1'	2.12	1.43	1.40
24	d	402[B]	PHO	C4D-CHA	2.12	1.49	1.43
23	b	619	CLA	C4C-C3C	2.12	1.48	1.45
23	B	617	CLA	C1C-NC	-2.12	1.34	1.37
23	B	616	CLA	C1B-CHB	2.11	1.46	1.41
23	b	617	CLA	C4C-C3C	2.11	1.48	1.45
23	C	505	CLA	C1B-NB	-2.11	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402[A]	PHO	C1A-NA	-2.11	1.33	1.37
23	A	405	CLA	C4B-CHC	2.11	1.46	1.41
23	b	618	CLA	C4C-C3C	2.11	1.48	1.45
23	B	610	CLA	C4B-CHC	2.10	1.46	1.41
23	a	411	CLA	C1C-C2C	2.10	1.48	1.44
23	d	403	CLA	C4B-CHC	2.10	1.46	1.41
33	D	411	LHG	O7-C5	-2.10	1.41	1.46
23	C	507	CLA	C1B-NB	-2.09	1.33	1.35
23	c	508	CLA	C4C-C3C	2.09	1.48	1.45
23	b	614	CLA	C4C-C3C	2.09	1.48	1.45
23	A	405	CLA	C1C-C2C	2.09	1.48	1.44
23	d	403	CLA	C1B-CHB	2.09	1.46	1.41
23	c	516	CLA	C1B-CHB	2.09	1.46	1.41
39	V	205	HEM	C4D-C3D	2.08	1.47	1.42
23	A	406	CLA	C1C-NC	-2.08	1.34	1.37
23	A	408	CLA	C4C-C3C	2.07	1.48	1.45
23	b	612	CLA	C1B-NB	-2.07	1.33	1.35
23	c	516	CLA	C4C-C3C	2.07	1.48	1.45
24	a	410	PHO	C4D-CHA	2.07	1.49	1.43
35	C	523	HTG	C1-S1	-2.06	1.77	1.80
23	b	623	CLA	C1C-C2C	2.06	1.48	1.44
31	D	408[A]	PL9	C2-C3	2.06	1.40	1.34
23	C	514	CLA	C4C-C3C	2.05	1.48	1.45
23	B	614	CLA	C1B-NB	-2.05	1.33	1.35
23	b	622	CLA	C1C-C2C	2.05	1.48	1.44
23	c	505	CLA	C4B-CHC	2.04	1.46	1.41
23	b	624	CLA	C1C-NC	-2.04	1.34	1.37
28	M	104	LMT	O1'-C1'	2.04	1.43	1.40
23	b	623	CLA	C4B-CHC	2.04	1.46	1.41
23	B	612	CLA	C4B-CHC	2.04	1.46	1.41
31	a	415[B]	PL9	C2-C3	2.03	1.40	1.34
24	a	410	PHO	C1C-C2C	2.03	1.50	1.45
24	D	402[B]	PHO	C4C-C3C	2.03	1.48	1.45
26	F	104	SQD	O6-C1	2.03	1.43	1.40
35	b	607	HTG	C1-S1	-2.03	1.77	1.80
31	a	415[A]	PL9	C2-C3	2.03	1.40	1.34
31	d	407[A]	PL9	C2-C3	2.03	1.40	1.34
31	d	407[B]	PL9	C2-C3	2.03	1.40	1.34
23	c	510	CLA	C1C-C2C	2.02	1.48	1.44
23	a	409	CLA	C1C-C2C	2.02	1.48	1.44
23	b	623	CLA	C4C-C3C	2.02	1.48	1.45
23	a	411	CLA	C4B-CHC	2.02	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C4C-C3C	2.01	1.48	1.45
23	B	613	CLA	C1B-NB	-2.01	1.33	1.35
31	A	417[B]	PL9	C2-C3	2.01	1.39	1.34
23	c	512	CLA	C4B-CHC	2.01	1.46	1.41
23	d	405	CLA	C1B-CHB	2.00	1.46	1.41
31	D	408[B]	PL9	C2-C3	2.00	1.39	1.34

All (2361) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402[B]	PHO	CMD-C2D-C1D	7.50	136.62	125.06
23	B	603	CLA	C4A-NA-C1A	-7.35	103.40	106.71
23	d	404	CLA	C4A-NA-C1A	-7.22	103.46	106.71
23	b	622	CLA	C2C-C1C-NC	7.00	116.53	109.97
23	c	516	CLA	C4A-NA-C1A	-6.92	103.59	106.71
23	B	616	CLA	C4A-NA-C1A	-6.90	103.61	106.71
23	c	516	CLA	O2D-CGD-CBD	6.83	123.41	111.27
23	b	621	CLA	CHD-C4C-C3C	-6.82	114.81	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.79	114.86	124.84
24	D	402[A]	PHO	CMD-C2D-C1D	6.76	135.48	125.06
23	b	611	CLA	C4A-NA-C1A	-6.68	103.70	106.71
24	A	407	PHO	CMD-C2D-C1D	6.64	135.29	125.06
23	b	612	CLA	C4A-NA-C1A	-6.56	103.76	106.71
24	d	402[A]	PHO	CMD-C2D-C1D	6.55	135.15	125.06
23	b	614	CLA	CHD-C4C-C3C	-6.55	115.22	124.84
24	D	402[B]	PHO	CMD-C2D-C1D	6.54	135.13	125.06
23	b	618	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	b	625	CLA	CHD-C4C-C3C	-6.53	115.25	124.84
23	c	507	CLA	CHD-C4C-C3C	-6.51	115.28	124.84
23	B	613	CLA	O2D-CGD-CBD	6.48	122.78	111.27
39	F	102	HEM	CAD-CBD-CGD	6.43	123.46	112.67
23	c	515	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
35	B	624	HTG	C1'-S1-C1	6.42	112.10	100.09
24	a	410	PHO	CMD-C2D-C1D	6.41	134.94	125.06
23	C	503	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	C	508	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
23	c	512	CLA	C2C-C1C-NC	6.34	115.91	109.97
23	B	616	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	B	614	CLA	C2C-C1C-NC	6.28	115.85	109.97
23	a	408	CLA	C2C-C1C-NC	6.27	115.85	109.97
23	B	617	CLA	CHD-C4C-C3C	-6.27	115.63	124.84
23	b	625	CLA	C4A-NA-C1A	-6.25	103.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C4A-NA-C1A	-6.25	103.90	106.71
23	b	615	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
23	d	405	CLA	C4A-NA-C1A	-6.24	103.90	106.71
23	C	504	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	A	408	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.22	115.69	124.84
23	C	513	CLA	CHD-C4C-C3C	-6.22	115.69	124.84
23	C	509	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
23	C	504	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	b	618	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	C	505	CLA	C4A-NA-C1A	-6.13	103.95	106.71
35	C	522	HTG	C1'-S1-C1	6.12	111.54	100.09
23	d	405	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
35	d	414	HTG	C1'-S1-C1	6.12	111.53	100.09
23	b	620	CLA	C2C-C1C-NC	6.11	115.70	109.97
23	B	613	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
23	B	608	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	b	612	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	B	612	CLA	C4A-NA-C1A	-6.08	103.97	106.71
35	c	523	HTG	C1'-S1-C1	6.06	111.42	100.09
23	a	408	CLA	C4A-NA-C1A	-6.05	103.99	106.71
23	B	611	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	C	506	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	B	609	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
23	b	613	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
23	B	617	CLA	O2D-CGD-CBD	6.00	121.94	111.27
23	c	513	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	a	409	CLA	C4A-NA-C1A	-5.99	104.02	106.71
23	b	625	CLA	O2D-CGD-CBD	5.97	121.88	111.27
23	B	602	CLA	O2D-CGD-CBD	5.97	121.88	111.27
23	B	604	CLA	O2D-CGD-CBD	5.97	121.87	111.27
23	c	510	CLA	C2C-C1C-NC	5.95	115.55	109.97
23	B	602	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
23	b	623	CLA	O2D-CGD-CBD	5.94	121.82	111.27
23	b	615	CLA	C4A-NA-C1A	-5.94	104.04	106.71
23	C	506	CLA	C4A-NA-C1A	-5.94	104.04	106.71
23	d	403	CLA	C2C-C1C-NC	5.93	115.53	109.97
26	b	601	SQD	O6-C1-C2	5.92	117.55	108.30
23	b	623	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
39	e	101	HEM	CAD-CBD-CGD	5.91	122.58	112.67
23	b	613	CLA	O2D-CGD-CBD	5.91	121.76	111.27
23	B	607	CLA	C4A-NA-C1A	-5.90	104.05	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C4A-NA-C1A	-5.90	104.05	106.71
23	B	605	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	B	612	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	c	508	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	D	405	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	c	507	CLA	C4A-NA-C1A	-5.88	104.06	106.71
23	B	604	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
23	B	610	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	b	618	CLA	O2D-CGD-CBD	5.86	121.68	111.27
23	c	514	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	B	611	CLA	C4A-NA-C1A	-5.85	104.08	106.71
23	A	404	CLA	C4A-NA-C1A	-5.84	104.08	106.71
23	A	405	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	b	616	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	D	405	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	C	507	CLA	C2C-C1C-NC	5.83	115.44	109.97
35	D	415	HTG	C1'-S1-C1	5.83	110.99	100.09
23	c	516	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
23	c	509	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	a	411	CLA	C2C-C1C-NC	5.79	115.40	109.97
23	B	605	CLA	C2C-C1C-NC	5.79	115.40	109.97
23	c	512	CLA	O2D-CGD-CBD	5.79	121.56	111.27
23	b	610	CLA	O2D-CGD-CBD	5.78	121.55	111.27
23	A	405	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	C	502	CLA	O2D-CGD-CBD	5.76	121.51	111.27
23	b	613	CLA	C2C-C1C-NC	5.76	115.37	109.97
23	B	615	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	d	404	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	b	614	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	B	615	CLA	C2C-C1C-NC	5.71	115.32	109.97
26	f	102	SQD	O47-C7-C8	5.71	123.80	111.50
23	b	617	CLA	C4A-NA-C1A	-5.70	104.14	106.71
23	B	603	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	b	619	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
23	C	513	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	b	624	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	B	607	CLA	C2C-C1C-NC	5.69	115.30	109.97
23	c	505	CLA	C2C-C1C-NC	5.68	115.29	109.97
23	A	406	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
23	C	505	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	a	409	CLA	CHD-C4C-C3C	-5.66	116.51	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	624	HTG	O5-C1-C2	5.66	117.43	110.31
23	c	511	CLA	O2D-CGD-CBD	5.66	121.32	111.27
23	b	610	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	b	617	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
23	b	611	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	c	511	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	c	506	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
25	Y	101	BCR	C33-C5-C6	-5.58	118.27	124.53
23	c	510	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
23	B	609	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	c	517	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	B	614	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	c	514	CLA	C4A-NA-C1A	-5.54	104.22	106.71
23	C	514	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	C	509	CLA	O2D-CGD-CBD	5.52	121.08	111.27
23	B	612	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
23	b	613	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	C	502	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	c	509	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	c	512	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
23	c	505	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
23	C	510	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	c	517	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	a	411	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
23	C	505	CLA	C2C-C1C-NC	5.48	115.11	109.97
23	D	406	CLA	CHD-C4C-C3C	-5.48	116.78	124.84
23	B	617	CLA	C4A-NA-C1A	-5.48	104.24	106.71
24	d	402[B]	PHO	C3D-C2D-C1D	-5.47	97.90	105.87
23	C	512	CLA	C2C-C1C-NC	5.46	115.09	109.97
23	b	623	CLA	C2C-C1C-NC	5.45	115.08	109.97
23	B	604	CLA	C4A-NA-C1A	-5.43	104.26	106.71
23	B	605	CLA	O2D-CGD-CBD	5.43	120.92	111.27
23	A	405	CLA	O2D-CGD-CBD	5.43	120.92	111.27
23	B	613	CLA	C4A-NA-C1A	-5.43	104.27	106.71
23	C	511	CLA	C4A-NA-C1A	-5.42	104.27	106.71
23	d	403	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
23	B	615	CLA	O2D-CGD-CBD	5.41	120.88	111.27
24	A	407	PHO	O2D-CGD-CBD	5.41	120.88	111.27
23	B	610	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	A	404	CLA	CHD-C4C-C3C	-5.40	116.91	124.84
23	b	624	CLA	C2C-C1C-NC	5.39	115.03	109.97
23	C	508	CLA	O2D-CGD-CBD	5.37	120.81	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	PHO	C3D-C2D-C1D	-5.37	98.05	105.87
23	C	514	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	A	406	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	c	508	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	b	620	CLA	C4A-NA-C1A	-5.35	104.30	106.71
24	D	402[B]	PHO	C3D-C2D-C1D	-5.35	98.08	105.87
23	B	608	CLA	C2C-C1C-NC	5.34	114.98	109.97
23	d	404	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
23	c	513	CLA	C2C-C1C-NC	5.34	114.97	109.97
23	B	603	CLA	C2C-C1C-NC	5.34	114.97	109.97
24	d	402[A]	PHO	O2D-CGD-CBD	5.34	120.75	111.27
23	b	620	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
23	C	512	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
23	b	612	CLA	O2D-CGD-CBD	5.33	120.74	111.27
24	D	402[A]	PHO	C3D-C2D-C1D	-5.33	98.11	105.87
23	c	506	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	b	619	CLA	C4A-NA-C1A	-5.31	104.32	106.71
23	B	607	CLA	O2D-CGD-CBD	5.31	120.71	111.27
23	a	409	CLA	O2D-CGD-CBD	5.31	120.71	111.27
23	C	511	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	A	406	CLA	O2D-CGD-CBD	5.30	120.69	111.27
23	C	507	CLA	C4A-NA-C1A	-5.30	104.32	106.71
23	C	506	CLA	O2D-CGD-CBD	5.30	120.69	111.27
23	B	602	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	B	617	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	b	616	CLA	C2C-C1C-NC	5.30	114.93	109.97
23	c	508	CLA	C2C-C1C-NC	5.29	114.93	109.97
23	C	502	CLA	C4A-NA-C1A	-5.27	104.33	106.71
23	C	513	CLA	C4A-NA-C1A	-5.27	104.34	106.71
23	C	504	CLA	O2D-CGD-CBD	5.26	120.62	111.27
35	b	632	HTG	C1'-S1-C1	5.26	109.93	100.09
23	b	618	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	c	514	CLA	CHD-C4C-C3C	-5.25	117.12	124.84
26	F	104	SQD	O47-C7-C8	5.24	122.80	111.50
35	B	623	HTG	C1'-S1-C1	5.24	109.90	100.09
23	b	615	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	C	505	CLA	CHD-C4C-C3C	-5.24	117.14	124.84
35	B	631	HTG	C1'-S1-C1	5.23	109.88	100.09
35	b	631	HTG	C1'-S1-C1	5.23	109.88	100.09
23	b	614	CLA	O2D-CGD-CBD	5.23	120.56	111.27
23	C	510	CLA	C2C-C1C-NC	5.22	114.86	109.97
23	C	503	CLA	C2C-C1C-NC	5.19	114.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	PHO	C2D-C1D-ND	5.19	117.62	109.79
23	b	610	CLA	C4A-NA-C1A	-5.18	104.38	106.71
23	D	406	CLA	C2C-C1C-NC	5.18	114.82	109.97
35	C	523	HTG	C1'-S1-C1	5.18	109.77	100.09
24	d	402[B]	PHO	C2D-C1D-ND	5.16	117.58	109.79
23	b	612	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	b	621	CLA	O2D-CGD-CBD	5.16	120.44	111.27
24	D	402[A]	PHO	C2D-C1D-ND	5.14	117.55	109.79
35	B	622	HTG	C1'-S1-C1	5.13	109.69	100.09
23	c	509	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	b	622	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	b	615	CLA	O2D-CGD-CBD	5.12	120.37	111.27
23	C	502	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
35	B	632	HTG	C1'-S1-C1	5.11	109.65	100.09
23	A	405	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	b	621	CLA	C3C-C4C-NC	5.10	116.29	110.57
23	c	517	CLA	C2C-C1C-NC	5.09	114.75	109.97
23	C	508	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	B	616	CLA	C2C-C1C-NC	5.08	114.73	109.97
24	D	402[B]	PHO	C2D-C1D-ND	5.08	117.46	109.79
24	d	402[A]	PHO	C3D-C2D-C1D	-5.08	98.47	105.87
23	b	614	CLA	C2C-C1C-NC	5.07	114.72	109.97
23	d	405	CLA	O2D-CGD-CBD	5.07	120.27	111.27
23	C	506	CLA	CHD-C4C-C3C	-5.07	117.39	124.84
23	c	513	CLA	O2D-CGD-CBD	5.07	120.27	111.27
23	c	506	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	C	504	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	C	509	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	C	511	CLA	O2D-CGD-CBD	5.04	120.23	111.27
23	B	603	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	c	505	CLA	O2D-CGD-CBD	5.04	120.22	111.27
24	A	407	PHO	C3D-C2D-C1D	-5.02	98.56	105.87
23	a	408	CLA	CHD-C4C-C3C	-5.01	117.48	124.84
23	a	411	CLA	O2D-CGD-CBD	5.01	120.16	111.27
23	b	611	CLA	C2C-C1C-NC	5.00	114.66	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
23	A	404	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	b	617	CLA	O2D-CGD-CBD	4.99	120.13	111.27
23	A	408	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	A	408	CLA	C2C-C1C-NC	4.97	114.63	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	407	BCR	C7-C8-C9	-4.95	118.75	126.23
23	b	621	CLA	C4A-NA-C1A	-4.95	104.48	106.71
24	D	402[A]	PHO	C1-C2-C3	-4.95	117.48	126.04
23	b	611	CLA	O2D-CGD-CBD	4.94	120.04	111.27
23	B	612	CLA	O2D-CGD-CBD	4.94	120.04	111.27
24	d	402[A]	PHO	C2D-C1D-ND	4.90	117.19	109.79
24	A	407	PHO	C2D-C1D-ND	4.90	117.18	109.79
35	c	524	HTG	C1'-S1-C1	4.89	109.24	100.09
23	b	617	CLA	C2C-C1C-NC	4.88	114.55	109.97
23	B	606	CLA	C4A-NA-C1A	-4.88	104.51	106.71
24	d	402[B]	PHO	O2D-CGD-CBD	4.88	119.94	111.27
25	t	101	BCR	C33-C5-C6	-4.88	119.05	124.53
23	B	611	CLA	O2D-CGD-CBD	4.86	119.90	111.27
23	A	406	CLA	C2C-C1C-NC	4.86	114.52	109.97
23	C	513	CLA	C2C-C1C-NC	4.85	114.51	109.97
23	b	623	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	b	614	CLA	C3C-C4C-NC	4.84	116.00	110.57
35	C	523	HTG	C1-O5-C5	4.84	121.50	112.58
23	c	509	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	C	508	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	b	620	CLA	O2D-CGD-CBD	4.82	119.83	111.27
23	C	514	CLA	C2C-C1C-NC	4.81	114.48	109.97
36	c	522	LMG	O7-C10-C11	4.81	121.86	111.50
37	d	408	DGD	O6E-C5E-C4E	4.80	118.40	109.69
23	c	513	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	B	610	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	c	514	CLA	O2D-CGD-CBD	4.78	119.76	111.27
23	B	606	CLA	O2D-CGD-CBD	4.77	119.75	111.27
26	B	636	SQD	O8-S-C6	4.77	113.34	105.74
23	b	610	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	C	503	CLA	O2D-CGD-CBD	4.77	119.74	111.27
23	d	403	CLA	O2D-CGD-CBD	4.76	119.73	111.27
23	c	512	CLA	C4A-NA-C1A	-4.76	104.57	106.71
24	d	402[A]	PHO	C1-C2-C3	-4.76	117.82	126.04
23	b	619	CLA	C2C-C1C-NC	4.75	114.42	109.97
26	a	413	SQD	O47-C7-C8	4.75	121.74	111.50
25	y	101	BCR	C33-C5-C6	-4.75	119.20	124.53
23	b	621	CLA	C2C-C1C-NC	4.74	114.41	109.97
23	c	507	CLA	C2C-C1C-NC	4.74	114.41	109.97
23	b	613	CLA	C3C-C4C-NC	4.74	115.89	110.57
25	b	626	BCR	C7-C8-C9	-4.73	119.09	126.23
23	B	613	CLA	C3C-C4C-NC	4.72	115.86	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C2C-C1C-NC	4.71	114.39	109.97
33	D	412	LHG	O7-C7-C8	4.70	121.64	111.50
26	B	621	SQD	O47-C7-C8	4.69	121.61	111.50
36	a	414	LMG	O7-C10-C11	4.69	121.61	111.50
23	d	403	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
26	A	410	SQD	O47-C7-C8	4.66	121.54	111.50
23	B	613	CLA	C2C-C1C-NC	4.64	114.32	109.97
23	c	507	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	C	511	CLA	C1-C2-C3	-4.63	118.04	126.04
23	B	609	CLA	O2D-CGD-CBD	4.62	119.47	111.27
23	B	608	CLA	O2D-CGD-CBD	4.61	119.46	111.27
23	C	510	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	c	507	CLA	O2D-CGD-CBD	4.59	119.43	111.27
23	C	507	CLA	O2D-CGD-CBD	4.59	119.42	111.27
24	a	410	PHO	O2D-CGD-CBD	4.58	119.41	111.27
33	D	410	LHG	O8-C23-C24	4.57	126.26	111.91
24	d	402[B]	PHO	C1-C2-C3	-4.57	118.14	126.04
25	B	620	BCR	C15-C14-C13	-4.56	120.80	127.31
36	C	501	LMG	O7-C10-C11	4.56	121.33	111.50
23	c	516	CLA	C2C-C1C-NC	4.56	114.24	109.97
23	a	409	CLA	C2C-C1C-NC	4.54	114.23	109.97
23	c	506	CLA	O2D-CGD-CBD	4.54	119.33	111.27
23	B	610	CLA	O2D-CGD-CBD	4.54	119.33	111.27
23	b	625	CLA	C2C-C1C-NC	4.53	114.22	109.97
23	B	606	CLA	C2C-C1C-NC	4.53	114.22	109.97
23	B	615	CLA	C4A-NA-C1A	-4.52	104.67	106.71
23	c	511	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	C	510	CLA	O2D-CGD-CBD	4.51	119.28	111.27
28	A	414	LMT	C1'-O5'-C5'	4.51	122.54	113.69
23	c	505	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	b	625	CLA	C3C-C4C-NC	4.50	115.62	110.57
25	B	618	BCR	C33-C5-C6	-4.50	119.48	124.53
23	C	503	CLA	C4A-NA-C1A	-4.50	104.69	106.71
36	C	520	LMG	O7-C10-C11	4.49	121.17	111.50
23	c	510	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
24	D	402[A]	PHO	O2D-CGD-CBD	4.49	119.24	111.27
23	B	617	CLA	C1D-CHD-C4C	-4.48	116.65	122.56
26	A	410	SQD	O6-C1-C2	4.48	115.29	108.30
37	d	408	DGD	O2G-C1B-C2B	4.47	121.14	111.50
23	c	512	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	b	612	CLA	C3C-C4C-NC	4.46	115.58	110.57
23	C	509	CLA	C3C-C4C-NC	4.46	115.57	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
23	D	405	CLA	O2D-CGD-CBD	4.45	119.17	111.27
25	b	626	BCR	C33-C5-C6	-4.44	119.54	124.53
23	C	504	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	b	622	CLA	C3B-C4B-NB	4.43	114.94	109.21
23	B	606	CLA	C3C-C4C-NC	4.42	115.53	110.57
35	b	607	HTG	C1'-S1-C1	4.42	108.35	100.09
23	c	508	CLA	C4A-NA-C1A	-4.42	104.72	106.71
23	B	605	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	C	503	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	C	509	CLA	C4A-NA-C1A	-4.41	104.72	106.71
23	B	607	CLA	C3C-C4C-NC	4.41	115.51	110.57
26	a	413	SQD	O6-C1-C2	4.38	115.15	108.30
23	B	611	CLA	C2C-C1C-NC	4.37	114.07	109.97
23	c	511	CLA	C4A-NA-C1A	-4.37	104.74	106.71
24	d	402[A]	PHO	C4C-C3C-C2C	-4.36	101.96	106.78
23	C	506	CLA	C3C-C4C-NC	4.36	115.46	110.57
23	c	515	CLA	C2C-C1C-NC	4.35	114.05	109.97
23	C	514	CLA	O2D-CGD-CBD	4.35	118.99	111.27
23	C	512	CLA	C4A-NA-C1A	-4.34	104.75	106.71
23	B	605	CLA	C1C-C2C-C3C	-4.34	102.40	106.96
23	b	622	CLA	C4A-NA-C1A	-4.33	104.76	106.71
26	B	621	SQD	O7-S-C6	4.33	112.08	106.94
23	C	508	CLA	C3C-C4C-NC	4.33	115.42	110.57
23	B	614	CLA	C3C-C4C-NC	4.32	115.42	110.57
23	A	405	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	D	405	CLA	C1-C2-C3	-4.32	118.57	126.04
23	d	403	CLA	C3B-C4B-NB	4.31	114.78	109.21
23	B	616	CLA	O2D-CGD-CBD	4.30	118.91	111.27
23	B	616	CLA	C3C-C4C-NC	4.30	115.39	110.57
25	c	526	BCR	C15-C14-C13	-4.29	121.19	127.31
23	D	405	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	b	622	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	b	618	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	c	513	CLA	C1-C2-C3	-4.28	118.64	126.04
23	b	615	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	c	507	CLA	C1-C2-C3	-4.28	118.65	126.04
23	a	411	CLA	C1C-C2C-C3C	-4.27	102.46	106.96
23	d	404	CLA	C3C-C4C-NC	4.26	115.35	110.57
37	C	516	DGD	O2G-C1B-C2B	4.26	120.67	111.50
23	b	616	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	c	513	CLA	C3C-C4C-NC	4.25	115.34	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C1-C2-C3	-4.25	118.70	126.04
23	d	405	CLA	C2C-C1C-NC	4.24	113.95	109.97
23	A	404	CLA	C3C-C4C-NC	4.24	115.32	110.57
39	e	101	HEM	CBD-CAD-C3D	-4.23	104.69	112.48
23	B	609	CLA	C4A-NA-C1A	-4.23	104.81	106.71
23	b	612	CLA	C1D-CHD-C4C	-4.22	116.99	122.56
25	K	103	BCR	C7-C8-C9	-4.21	119.87	126.23
23	C	503	CLA	C1D-CHD-C4C	-4.20	117.01	122.56
37	D	409	DGD	O2G-C1B-C2B	4.20	120.56	111.50
24	D	402[B]	PHO	C1-C2-C3	-4.18	118.82	126.04
23	c	517	CLA	O2D-CGD-CBD	4.17	118.69	111.27
26	b	601	SQD	O47-C7-C8	4.17	120.50	111.50
28	A	414	LMT	O5'-C5'-C4'	4.17	118.55	109.75
23	c	507	CLA	C1D-CHD-C4C	-4.17	117.06	122.56
23	a	411	CLA	C3B-C4B-NB	4.17	114.60	109.21
23	C	512	CLA	O2D-CGD-CBD	4.15	118.65	111.27
25	T	103	BCR	C33-C5-C6	-4.14	119.88	124.53
23	C	504	CLA	C1D-CHD-C4C	-4.14	117.10	122.56
23	A	408	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	c	509	CLA	C3C-C4C-NC	4.13	115.20	110.57
25	K	101	BCR	C7-C8-C9	-4.13	120.00	126.23
23	B	609	CLA	C3C-C4C-NC	4.12	115.20	110.57
23	b	619	CLA	O2D-CGD-CBD	4.12	118.59	111.27
23	c	515	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	B	608	CLA	C3C-C4C-NC	4.12	115.19	110.57
25	C	515	BCR	C7-C8-C9	-4.11	120.02	126.23
37	c	519	DGD	O2G-C1B-C2B	4.11	120.35	111.50
31	A	417[B]	PL9	C7-C3-C4	4.11	120.21	116.88
23	B	615	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
23	b	622	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	b	623	CLA	C3C-C4C-NC	4.10	115.16	110.57
33	A	419	LHG	O7-C7-C8	4.09	120.31	111.50
23	B	606	CLA	CMC-C2C-C1C	4.08	131.26	125.04
23	C	513	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	510	CLA	C4A-NA-C1A	-4.08	104.87	106.71
23	B	612	CLA	C3C-C4C-NC	4.07	115.14	110.57
23	b	623	CLA	C1-C2-C3	-4.07	119.00	126.04
23	B	613	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	b	611	CLA	C3C-C4C-NC	4.07	115.14	110.57
23	B	609	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
23	C	507	CLA	CBC-CAC-C3C	-4.06	101.24	112.43
23	b	616	CLA	C4A-NA-C1A	-4.06	104.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	623	CLA	C1D-CHD-C4C	-4.06	117.20	122.56
23	c	512	CLA	C3C-C4C-NC	4.05	115.12	110.57
23	D	405	CLA	C3C-C4C-NC	4.05	115.12	110.57
23	C	506	CLA	CAC-C3C-C4C	4.05	130.07	124.81
23	B	615	CLA	C3B-C4B-NB	4.05	114.45	109.21
23	c	511	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	b	621	CLA	C1D-CHD-C4C	-4.05	117.22	122.56
23	B	604	CLA	C3C-C4C-NC	4.05	115.11	110.57
23	B	607	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
31	d	407[B]	PL9	C42-C43-C44	-4.04	117.93	127.66
23	d	404	CLA	O2D-CGD-CBD	4.04	118.45	111.27
35	b	632	HTG	O5-C1-C2	4.03	115.39	110.31
23	c	510	CLA	C3B-C4B-NB	4.03	114.42	109.21
23	c	508	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	b	616	CLA	O2D-CGD-CBD	4.03	118.43	111.27
23	b	615	CLA	C1D-CHD-C4C	-4.03	117.24	122.56
23	C	507	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
37	c	520	DGD	O2G-C1B-C2B	4.02	120.17	111.50
23	C	510	CLA	C3C-C4C-NC	4.02	115.08	110.57
33	d	411	LHG	O7-C7-C8	4.01	120.15	111.50
23	c	509	CLA	CAC-C3C-C4C	4.01	130.02	124.81
23	C	512	CLA	CAC-C3C-C4C	4.01	130.02	124.81
23	c	512	CLA	C3B-C4B-NB	4.01	114.39	109.21
33	b	634	LHG	O7-C7-C8	4.01	120.13	111.50
36	C	519	LMG	O7-C10-C11	4.00	120.12	111.50
37	c	521	DGD	O2G-C1B-C2B	4.00	120.11	111.50
23	B	608	CLA	CAC-C3C-C4C	3.99	129.99	124.81
23	D	406	CLA	O2D-CGD-CBD	3.99	118.36	111.27
28	D	404	LMT	O1B-C4'-C3'	3.99	117.89	107.28
23	a	408	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	C	502	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	b	625	CLA	C1D-CHD-C4C	-3.98	117.30	122.56
23	B	617	CLA	C3C-C4C-NC	3.98	115.04	110.57
23	c	505	CLA	C1C-C2C-C3C	-3.98	102.78	106.96
23	b	610	CLA	C1D-CHD-C4C	-3.97	117.31	122.56
25	y	101	BCR	C15-C14-C13	-3.97	121.64	127.31
23	b	620	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	c	508	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
23	B	602	CLA	C3C-C4C-NC	3.96	115.01	110.57
31	a	415[B]	PL9	C7-C8-C9	-3.96	120.20	126.79
25	Y	101	BCR	C15-C14-C13	-3.96	121.66	127.31
23	b	624	CLA	C4A-NA-C1A	-3.96	104.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
23	c	510	CLA	O2D-CGD-CBD	3.96	118.30	111.27
23	D	406	CLA	C4A-NA-C1A	-3.95	104.93	106.71
23	B	603	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	a	410	PHO	C4C-C3C-C2C	-3.94	102.42	106.78
23	d	404	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
37	d	408	DGD	C3E-C4E-C5E	3.93	117.25	110.24
31	D	408[B]	PL9	C42-C43-C44	-3.93	118.19	127.66
23	A	408	CLA	O2D-CGD-CBD	3.93	118.24	111.27
25	H	101	BCR	C38-C26-C25	-3.92	120.13	124.53
25	C	515	BCR	C33-C5-C6	-3.92	120.13	124.53
23	C	505	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
23	d	403	CLA	C4A-NA-C1A	-3.91	104.95	106.71
23	c	514	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
23	b	613	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
23	B	616	CLA	C1D-CHD-C4C	-3.90	117.41	122.56
23	c	505	CLA	O2D-CGD-O1D	-3.90	116.22	123.84
23	B	612	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
24	D	402[B]	PHO	O2D-CGD-CBD	3.89	118.18	111.27
23	c	506	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	B	605	CLA	C4A-NA-C1A	-3.88	104.96	106.71
23	a	411	CLA	C1D-CHD-C4C	-3.88	117.43	122.56
23	b	620	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	b	624	CLA	C3C-C4C-NC	3.87	114.92	110.57
23	B	610	CLA	C3C-C4C-NC	3.87	114.91	110.57
25	d	406	BCR	C38-C26-C25	-3.87	120.19	124.53
23	C	512	CLA	C3B-C4B-NB	3.86	114.21	109.21
23	B	612	CLA	C3B-C4B-NB	3.86	114.20	109.21
23	b	615	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
23	B	614	CLA	C3B-C4B-NB	3.86	114.19	109.21
25	C	515	BCR	C15-C14-C13	-3.86	121.81	127.31
25	D	407	BCR	C24-C23-C22	-3.85	120.41	126.23
23	c	516	CLA	C1D-CHD-C4C	-3.85	117.47	122.56
31	a	415[A]	PL9	C22-C23-C24	-3.85	118.39	127.66
25	H	101	BCR	C24-C23-C22	-3.85	120.42	126.23
23	c	513	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	D	402[A]	PHO	C4C-C3C-C2C	-3.84	102.53	106.78
25	Y	101	BCR	C16-C17-C18	-3.83	121.84	127.31
31	a	415[A]	PL9	C32-C33-C34	-3.83	118.44	127.66
23	A	405	CLA	C1D-CHD-C4C	-3.83	117.51	122.56
23	b	616	CLA	C1C-C2C-C3C	-3.83	102.94	106.96
23	B	606	CLA	C1D-CHD-C4C	-3.82	117.51	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	CLA	C4A-NA-C1A	-3.82	104.99	106.71
31	D	408[B]	PL9	C40-C39-C41	3.82	121.70	115.27
23	B	607	CLA	C1D-CHD-C4C	-3.82	117.52	122.56
26	B	636	SQD	O47-C7-C8	3.81	119.71	111.50
23	c	515	CLA	C1D-CHD-C4C	-3.80	117.54	122.56
23	d	405	CLA	C3C-C4C-NC	3.80	114.84	110.57
23	B	602	CLA	C4A-NA-C1A	-3.80	105.00	106.71
23	C	502	CLA	CMC-C2C-C1C	3.80	130.82	125.04
23	B	615	CLA	C3C-C4C-NC	3.79	114.83	110.57
23	b	624	CLA	C3B-C4B-NB	3.79	114.11	109.21
25	D	407	BCR	C38-C26-C25	-3.79	120.28	124.53
23	d	403	CLA	CBC-CAC-C3C	-3.78	102.00	112.43
26	b	601	SQD	O8-S-C6	3.78	111.77	105.74
25	H	101	BCR	C7-C8-C9	-3.78	120.52	126.23
23	D	406	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	b	617	CLA	O2D-CGD-O1D	-3.78	116.46	123.84
26	F	104	SQD	O5-C5-C4	3.77	116.55	109.69
23	b	619	CLA	C3C-C4C-NC	3.77	114.80	110.57
31	a	415[A]	PL9	C7-C3-C4	3.77	119.94	116.88
23	c	505	CLA	C3C-C4C-NC	3.76	114.79	110.57
23	b	618	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
23	b	617	CLA	C3C-C4C-NC	3.76	114.78	110.57
23	C	505	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	d	402[B]	PHO	C4C-C3C-C2C	-3.75	102.63	106.78
23	B	603	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	c	517	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	A	404	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
23	b	617	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	508	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
23	c	513	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
23	c	508	CLA	CMC-C2C-C1C	3.73	130.72	125.04
36	Z	101	LMG	O7-C10-C11	3.73	119.54	111.50
23	d	403	CLA	C1D-CHD-C4C	-3.73	117.64	122.56
23	A	404	CLA	CAA-C2A-C3A	-3.73	102.57	112.78
23	B	603	CLA	CAA-C2A-C3A	-3.73	102.58	112.78
23	C	505	CLA	C1D-CHD-C4C	-3.72	117.64	122.56
23	C	510	CLA	C1-C2-C3	-3.72	119.61	126.04
23	c	514	CLA	C4-C3-C5	3.72	121.53	115.27
31	D	408[B]	PL9	C7-C8-C9	-3.72	120.60	126.79
23	b	621	CLA	C1-C2-C3	-3.72	119.61	126.04
33	D	410	LHG	O8-C23-O10	-3.72	114.21	123.59
23	c	515	CLA	O2D-CGD-CBD	3.71	117.87	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
25	d	406	BCR	C28-C27-C26	-3.71	107.45	114.08
25	T	103	BCR	C11-C10-C9	-3.71	122.01	127.31
23	A	406	CLA	C4-C3-C5	3.71	121.51	115.27
23	b	614	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
23	b	619	CLA	C1-C2-C3	-3.70	119.64	126.04
23	c	516	CLA	C3C-C4C-NC	3.70	114.72	110.57
23	B	615	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
36	b	629	LMG	O8-C28-C29	3.70	123.50	111.91
23	c	514	CLA	C3B-C4B-NB	3.69	113.99	109.21
35	V	206	HTG	C1'-S1-C1	3.69	107.00	100.09
23	C	502	CLA	CAC-C3C-C4C	3.69	129.60	124.81
23	B	611	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
23	C	506	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	B	609	CLA	C1D-CHD-C4C	-3.69	117.69	122.56
23	c	508	CLA	C1D-CHD-C4C	-3.69	117.69	122.56
28	a	404	LMT	O5'-C5'-C4'	3.69	117.53	109.75
23	C	502	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
23	b	613	CLA	C1-C2-C3	-3.68	119.67	126.04
23	C	513	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
23	A	406	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
31	a	415[B]	PL9	C7-C3-C4	3.68	119.87	116.88
23	B	607	CLA	C1-C2-C3	-3.68	119.68	126.04
23	B	611	CLA	C3C-C4C-NC	3.68	114.70	110.57
23	C	512	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
23	a	409	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
25	B	619	BCR	C33-C5-C6	-3.67	120.40	124.53
23	c	511	CLA	CMC-C2C-C1C	3.67	130.63	125.04
23	b	618	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
23	C	514	CLA	C1-C2-C3	-3.67	119.69	126.04
23	c	516	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
23	B	617	CLA	C3B-C4B-NB	3.66	113.94	109.21
23	C	502	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
31	A	417[A]	PL9	C7-C3-C4	3.65	119.85	116.88
28	a	404	LMT	C1'-O5'-C5'	3.65	120.85	113.69
23	b	612	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	C	509	CLA	C3B-C4B-NB	3.64	113.92	109.21
23	B	616	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	A	408	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
23	c	509	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
23	C	507	CLA	CAC-C3C-C4C	3.63	129.53	124.81
23	B	610	CLA	C1C-C2C-C3C	-3.63	103.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	517	DGD	O2G-C1B-C2B	3.63	119.33	111.50
37	H	102	DGD	C3G-O3G-C1D	-3.63	106.64	113.74
24	D	402[B]	PHO	C4C-C3C-C2C	-3.63	102.76	106.78
23	b	613	CLA	C3B-C4B-NB	3.63	113.90	109.21
23	b	616	CLA	CBC-CAC-C3C	-3.63	102.44	112.43
23	b	614	CLA	O2D-CGD-O1D	-3.62	116.75	123.84
23	C	512	CLA	C3C-C4C-NC	3.62	114.64	110.57
23	B	609	CLA	C3B-C4B-NB	3.62	113.89	109.21
26	B	636	SQD	O48-C23-C24	3.62	123.28	111.91
23	a	408	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	c	506	CLA	C4D-C3D-CAD	-3.62	106.45	108.47
23	A	405	CLA	CBC-CAC-C3C	-3.62	102.46	112.43
23	B	604	CLA	C1D-CHD-C4C	-3.62	117.79	122.56
23	A	404	CLA	CMB-C2B-C3B	3.61	131.44	124.68
23	C	514	CLA	C3C-C4C-NC	3.61	114.62	110.57
31	a	415[A]	PL9	C15-C14-C16	3.61	121.35	115.27
23	A	405	CLA	C3C-C4C-NC	3.61	114.62	110.57
23	b	622	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
23	b	620	CLA	C1-C2-C3	-3.61	119.80	126.04
23	B	602	CLA	C3B-C4B-NB	3.61	113.87	109.21
26	A	413	SQD	O48-C23-C24	3.60	123.22	111.91
23	c	517	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	c	505	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	B	603	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
23	c	517	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
31	a	415[A]	PL9	C7-C8-C9	-3.59	120.81	126.79
23	B	612	CLA	C1-C2-C3	-3.59	119.83	126.04
23	d	405	CLA	CMC-C2C-C1C	3.59	130.50	125.04
23	C	505	CLA	C3B-C4B-NB	3.59	113.85	109.21
23	B	611	CLA	C1D-CHD-C4C	-3.58	117.83	122.56
23	c	512	CLA	C1D-CHD-C4C	-3.58	117.83	122.56
23	b	623	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
23	b	620	CLA	C3B-C4B-NB	3.58	113.83	109.21
23	B	614	CLA	O2D-CGD-CBD	3.58	117.62	111.27
23	b	619	CLA	C1D-CHD-C4C	-3.57	117.85	122.56
23	A	405	CLA	C3B-C4B-NB	3.57	113.82	109.21
23	c	514	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
36	k	101	LMG	O7-C10-C11	3.56	119.18	111.50
23	b	610	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	A	408	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
25	k	102	BCR	C11-C10-C9	-3.56	122.23	127.31
23	c	514	CLA	C1-C2-C3	-3.56	119.89	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	414	LMG	C8-O7-C10	-3.55	109.04	117.79
36	M	101	LMG	O8-C28-C29	3.55	123.06	111.91
23	b	622	CLA	CAC-C3C-C4C	3.55	129.42	124.81
23	b	623	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	B	612	CLA	C1D-CHD-C4C	-3.55	117.87	122.56
23	b	613	CLA	C1D-CHD-C4C	-3.55	117.87	122.56
23	B	604	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
28	C	521	LMT	C1'-O5'-C5'	3.55	120.65	113.69
37	D	409	DGD	C1D-C2D-C3D	3.55	117.38	110.00
23	C	514	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
37	h	102	DGD	O2G-C1B-C2B	3.55	119.14	111.50
36	d	416	LMG	O7-C10-C11	3.54	119.13	111.50
23	b	622	CLA	CHC-C1C-C2C	-3.54	116.93	126.72
25	K	103	BCR	C24-C23-C22	-3.54	120.89	126.23
23	d	404	CLA	C1-C2-C3	-3.54	119.92	126.04
23	A	404	CLA	O2D-CGD-CBD	3.54	117.55	111.27
36	z	101	LMG	O7-C10-C11	3.53	119.12	111.50
23	C	505	CLA	CBC-CAC-C3C	-3.53	102.69	112.43
23	a	409	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	b	614	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	B	610	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	b	621	CLA	CMC-C2C-C1C	3.53	130.41	125.04
23	a	411	CLA	C1-C2-C3	-3.53	119.94	126.04
25	D	407	BCR	C28-C27-C26	-3.52	107.78	114.08
23	C	513	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	C	514	CLA	C1D-CHD-C4C	-3.52	117.92	122.56
23	C	512	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	A	404	CLA	O2A-CGA-CBA	3.51	122.92	111.91
25	c	526	BCR	C33-C5-C6	-3.51	120.59	124.53
23	B	602	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
26	A	413	SQD	O47-C7-C8	3.51	119.06	111.50
23	b	620	CLA	CAC-C3C-C4C	3.50	129.35	124.81
24	a	410	PHO	CMB-C2B-C1B	3.50	130.46	125.06
23	c	511	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
23	b	623	CLA	C3B-C4B-NB	3.50	113.74	109.21
25	B	620	BCR	C38-C26-C25	-3.50	120.60	124.53
23	B	602	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
23	b	617	CLA	C1-C2-C3	-3.50	120.00	126.04
39	F	102	HEM	CBA-CAA-C2A	-3.49	106.04	112.49
23	b	621	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
23	A	404	CLA	C3B-C4B-NB	3.49	113.72	109.21
23	c	514	CLA	C3C-C4C-NC	3.49	114.49	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	B	605	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
23	B	604	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
26	a	413	SQD	O8-S-C6	3.48	111.29	105.74
24	A	407	PHO	C1C-C2C-C3C	-3.48	102.51	106.51
23	C	511	CLA	C3C-C4C-NC	3.48	114.47	110.57
23	A	406	CLA	C3C-C4C-NC	3.48	114.47	110.57
23	C	509	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
36	D	416	LMG	O7-C10-C11	3.47	118.99	111.50
23	D	406	CLA	C3B-C4B-NB	3.47	113.70	109.21
23	B	605	CLA	C3B-C4B-NB	3.47	113.70	109.21
23	c	513	CLA	C3B-C4B-NB	3.47	113.69	109.21
23	b	610	CLA	C3C-C4C-NC	3.47	114.46	110.57
23	a	409	CLA	C3C-C4C-NC	3.47	114.46	110.57
23	b	611	CLA	CAC-C3C-C4C	3.46	129.30	124.81
23	b	614	CLA	C1-C2-C3	-3.46	120.05	126.04
23	b	624	CLA	C1D-CHD-C4C	-3.46	117.99	122.56
23	c	516	CLA	CBC-CAC-C3C	-3.46	102.89	112.43
23	b	621	CLA	C4-C3-C5	3.46	121.09	115.27
31	A	417[B]	PL9	C37-C38-C39	-3.46	119.34	127.66
25	B	618	BCR	C7-C8-C9	-3.46	121.01	126.23
23	D	406	CLA	C4-C3-C5	3.46	121.08	115.27
24	A	407	PHO	CHC-C1C-C2C	-3.45	117.05	125.73
23	A	404	CLA	C1C-C2C-C3C	-3.44	103.33	106.96
23	B	605	CLA	CMC-C2C-C1C	3.44	130.28	125.04
23	A	406	CLA	CBC-CAC-C3C	-3.44	102.94	112.43
23	D	406	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	d	404	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	b	614	CLA	C4-C3-C5	3.44	121.06	115.27
23	c	510	CLA	C3C-C4C-NC	3.44	114.43	110.57
23	c	505	CLA	CBC-CAC-C3C	-3.44	102.95	112.43
26	a	413	SQD	C1-C2-C3	-3.44	102.83	110.00
33	D	410	LHG	O7-C7-C8	3.44	118.91	111.50
33	a	419	LHG	O7-C7-C8	3.44	118.91	111.50
31	a	415[B]	PL9	C32-C33-C34	-3.44	119.38	127.66
23	B	608	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
23	C	509	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
23	d	405	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
23	b	615	CLA	C3B-C4B-NB	3.43	113.65	109.21
23	B	613	CLA	CMC-C2C-C1C	3.43	130.26	125.04
23	B	606	CLA	CHD-C4C-NC	3.43	129.60	124.20
23	b	612	CLA	CAA-C2A-C3A	-3.43	103.40	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	625	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
23	c	506	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
23	B	617	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
24	d	402[A]	PHO	O2D-CGD-O1D	-3.42	117.14	123.84
23	C	510	CLA	C3B-C4B-NB	3.42	113.64	109.21
23	a	409	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
23	b	622	CLA	O2D-CGD-CBD	3.42	117.35	111.27
23	A	405	CLA	CMB-C2B-C3B	3.42	131.07	124.68
31	D	408[B]	PL9	C36-C37-C38	-3.42	100.65	111.88
23	d	403	CLA	CHC-C1C-C2C	-3.41	117.28	126.72
23	d	405	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	B	608	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	C	505	CLA	CAC-C3C-C4C	3.41	129.24	124.81
23	a	411	CLA	C3C-C4C-NC	3.41	114.40	110.57
35	b	608	HTG	C1'-S1-C1	3.41	106.47	100.09
23	b	624	CLA	O2D-CGD-CBD	3.41	117.32	111.27
25	K	101	BCR	C15-C14-C13	-3.41	122.45	127.31
23	C	512	CLA	C1-C2-C3	-3.40	120.16	126.04
23	C	503	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
31	A	417[A]	PL9	C32-C33-C34	-3.40	119.47	127.66
23	c	513	CLA	CMC-C2C-C1C	3.40	130.22	125.04
25	b	626	BCR	C15-C14-C13	-3.40	122.46	127.31
23	C	507	CLA	C3C-C4C-NC	3.40	114.38	110.57
37	d	408	DGD	O5D-C1E-C2E	3.40	113.61	108.30
25	T	103	BCR	C12-C13-C14	-3.40	113.72	118.94
25	h	101	BCR	C7-C8-C9	-3.40	121.10	126.23
23	C	511	CLA	C3B-C4B-NB	3.39	113.60	109.21
23	A	405	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
23	a	411	CLA	C4A-NA-C1A	-3.39	105.18	106.71
23	A	406	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
23	c	512	CLA	CHC-C1C-C2C	-3.39	117.36	126.72
23	C	510	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	B	613	CLA	C1-C2-C3	-3.38	120.19	126.04
23	c	509	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
26	A	410	SQD	C45-O47-C7	-3.38	109.47	117.79
23	B	611	CLA	O2A-CGA-CBA	3.38	122.51	111.91
23	C	505	CLA	C4-C3-C5	3.38	120.95	115.27
25	b	628	BCR	C15-C14-C13	-3.37	122.50	127.31
23	B	614	CLA	CMC-C2C-C1C	3.37	130.17	125.04
26	f	102	SQD	C1-O5-C5	3.37	120.30	113.69
23	C	502	CLA	C1D-CHD-C4C	-3.37	118.12	122.56
23	c	510	CLA	C1D-CHD-C4C	-3.36	118.12	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	b	614	CLA	OBD-CAD-C3D	-3.36	122.40	127.98
39	F	102	HEM	CBD-CAD-C3D	-3.36	106.29	112.48
25	B	619	BCR	C2-C1-C6	3.36	115.65	110.48
31	d	407[A]	PL9	C42-C43-C44	-3.35	119.59	127.66
23	c	505	CLA	CAC-C3C-C4C	3.35	129.16	124.81
23	B	603	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
31	A	417[B]	PL9	C20-C19-C21	3.35	120.91	115.27
31	a	415[B]	PL9	C15-C14-C16	3.35	120.91	115.27
23	a	408	CLA	C1D-CHD-C4C	-3.35	118.14	122.56
23	C	505	CLA	CMC-C2C-C1C	3.35	130.14	125.04
23	b	614	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
28	T	104	LMT	C1'-O5'-C5'	3.35	120.26	113.69
25	T	103	BCR	C35-C13-C12	3.35	123.35	118.08
23	c	510	CLA	CBC-CAC-C3C	-3.34	103.22	112.43
25	c	526	BCR	C16-C17-C18	-3.34	122.54	127.31
23	C	506	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
25	d	406	BCR	C29-C30-C25	3.33	115.61	110.48
23	C	506	CLA	C3B-C4B-NB	3.33	113.52	109.21
23	D	405	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	b	619	CLA	C3B-C4B-NB	3.33	113.51	109.21
25	k	102	BCR	C24-C23-C22	-3.33	121.21	126.23
23	c	506	CLA	CAC-C3C-C4C	3.32	129.12	124.81
31	d	407[B]	PL9	C37-C38-C39	-3.32	119.66	127.66
23	A	408	CLA	C4-C3-C5	3.32	120.86	115.27
23	d	404	CLA	O2A-CGA-CBA	3.32	122.33	111.91
23	b	620	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
23	b	611	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
25	d	406	BCR	C16-C15-C14	-3.31	116.68	123.47
31	a	415[A]	PL9	C17-C18-C19	-3.31	119.68	127.66
23	C	504	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
23	b	620	CLA	CHC-C1C-C2C	-3.31	117.56	126.72
31	D	408[B]	PL9	C32-C33-C34	-3.31	119.68	127.66
23	c	515	CLA	CHD-C4C-NC	3.31	129.42	124.20
23	B	604	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
23	b	624	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
23	a	411	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
23	b	612	CLA	C3B-C4B-NB	3.30	113.48	109.21
23	b	610	CLA	C3B-C4B-NB	3.30	113.48	109.21
25	T	103	BCR	C15-C16-C17	-3.30	116.72	123.47
25	t	101	BCR	C15-C16-C17	-3.30	116.72	123.47
23	C	511	CLA	CAC-C3C-C4C	3.29	129.09	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	602	HTG	C1'-S1-C1	3.29	106.25	100.09
23	b	616	CLA	C3B-C4B-NB	3.28	113.45	109.21
23	a	409	CLA	C3B-C4B-NB	3.28	113.45	109.21
23	A	404	CLA	CAC-C3C-C4C	3.28	129.07	124.81
25	c	518	BCR	C7-C8-C9	-3.28	121.28	126.23
23	C	509	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
25	b	626	BCR	C16-C17-C18	-3.28	122.63	127.31
23	b	624	CLA	C4-C3-C5	3.28	120.78	115.27
23	c	515	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
23	b	611	CLA	C3B-C4B-NB	3.27	113.44	109.21
25	k	102	BCR	C20-C21-C22	-3.27	122.64	127.31
23	C	504	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
25	D	407	BCR	C29-C30-C25	3.27	115.51	110.48
23	C	507	CLA	CHC-C1C-C2C	-3.27	117.68	126.72
23	B	613	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	C	505	CLA	CMB-C2B-C3B	3.26	130.78	124.68
23	a	411	CLA	CHC-C1C-C2C	-3.26	117.70	126.72
23	B	606	CLA	C2A-C1A-CHA	-3.26	118.16	123.86
23	b	624	CLA	CAC-C3C-C4C	3.26	129.04	124.81
23	C	507	CLA	C3B-C4B-NB	3.26	113.42	109.21
23	B	617	CLA	CHD-C4C-NC	3.26	129.33	124.20
23	b	620	CLA	C1D-CHD-C4C	-3.26	118.26	122.56
35	c	524	HTG	C1-O5-C5	3.25	118.58	112.58
23	c	510	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
23	b	612	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
23	A	405	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
23	B	611	CLA	CHD-C4C-NC	3.25	129.32	124.20
24	D	402[A]	PHO	C4-C3-C5	3.25	120.74	115.27
23	a	408	CLA	O2D-CGD-CBD	3.25	117.04	111.27
23	d	405	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	B	607	CLA	C4-C3-C5	3.24	120.73	115.27
23	b	613	CLA	O2A-CGA-CBA	3.24	122.08	111.91
23	c	509	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
23	B	616	CLA	CMC-C2C-C1C	3.24	129.97	125.04
25	B	619	BCR	C28-C27-C26	-3.24	108.30	114.08
23	b	611	CLA	CAA-C2A-C3A	-3.24	103.92	112.78
23	B	611	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
31	A	417[A]	PL9	C20-C19-C21	3.23	120.71	115.27
23	B	603	CLA	C3B-C4B-NB	3.23	113.39	109.21
36	b	629	LMG	O8-C28-O10	-3.23	115.44	123.59
25	h	101	BCR	C16-C17-C18	-3.23	122.70	127.31
23	B	610	CLA	C1D-CHD-C4C	-3.23	118.30	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C4-C3-C5	3.23	120.70	115.27
23	b	619	CLA	O2A-CGA-CBA	3.23	122.03	111.91
23	c	513	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
24	A	407	PHO	C2A-C1A-NA	3.22	115.56	111.86
23	c	507	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
35	B	624	HTG	C1-C2-C3	3.22	116.95	110.59
23	D	406	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
23	B	615	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
31	A	417[B]	PL9	C7-C3-C2	-3.22	119.07	123.30
23	c	508	CLA	C3B-C4B-NB	3.21	113.37	109.21
23	B	608	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
23	C	505	CLA	C4D-C3D-CAD	-3.21	106.68	108.47
31	a	415[B]	PL9	C22-C23-C24	-3.21	119.94	127.66
23	a	411	CLA	C4-C3-C5	3.21	120.66	115.27
24	d	402[A]	PHO	C4-C3-C5	3.20	120.66	115.27
31	a	415[A]	PL9	C10-C9-C11	3.20	120.66	115.27
26	B	621	SQD	O6-C1-C2	3.20	113.30	108.30
23	b	618	CLA	C1D-CHD-C4C	-3.20	118.33	122.56
23	B	602	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
23	b	616	CLA	CMC-C2C-C1C	3.20	129.91	125.04
36	b	629	LMG	O7-C10-C11	3.20	118.40	111.50
31	D	408[A]	PL9	C42-C43-C44	-3.20	119.96	127.66
24	d	402[B]	PHO	C4-C3-C5	3.20	120.65	115.27
24	d	402[A]	PHO	C2B-C1B-NB	3.20	114.62	109.79
31	D	408[A]	PL9	C7-C8-C9	-3.19	121.48	126.79
23	B	614	CLA	C1-C2-C3	-3.19	120.52	126.04
23	C	507	CLA	C1D-CHD-C4C	-3.19	118.35	122.56
33	L	101	LHG	O7-C7-C8	3.19	118.38	111.50
23	c	514	CLA	CHC-C1C-C2C	-3.19	117.90	126.72
39	V	205	HEM	CAD-CBD-CGD	3.19	118.02	112.67
23	b	622	CLA	OBD-CAD-C3D	-3.19	122.69	127.98
23	B	612	CLA	CAC-C3C-C4C	3.18	128.94	124.81
25	K	101	BCR	C33-C5-C6	-3.18	120.95	124.53
23	B	608	CLA	CMC-C2C-C1C	3.18	129.89	125.04
23	c	512	CLA	C1-C2-C3	-3.18	120.54	126.04
23	B	602	CLA	O2A-CGA-CBA	3.18	121.89	111.91
23	C	503	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
25	A	409	BCR	C33-C5-C6	-3.18	120.95	124.53
31	a	415[A]	PL9	C37-C38-C39	-3.18	120.00	127.66
23	c	513	CLA	CMB-C2B-C3B	3.18	130.63	124.68
31	d	407[A]	PL9	C37-C38-C39	-3.18	120.01	127.66
23	b	611	CLA	C1C-C2C-C3C	-3.18	103.62	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	619	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
23	c	515	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	c	506	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	c	509	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
25	D	407	BCR	C15-C14-C13	-3.17	122.79	127.31
23	a	408	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
23	b	611	CLA	C1D-CHD-C4C	-3.17	118.38	122.56
23	B	617	CLA	CHC-C1C-C2C	-3.17	117.96	126.72
25	K	103	BCR	C33-C5-C6	-3.16	120.97	124.53
23	c	507	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
31	a	415[A]	PL9	C20-C19-C21	3.16	120.59	115.27
26	A	410	SQD	O8-S-C6	3.16	110.78	105.74
31	a	415[A]	PL9	C27-C28-C29	-3.16	120.05	127.66
23	D	406	CLA	CAC-C3C-C4C	3.16	128.91	124.81
31	A	417[A]	PL9	C37-C38-C39	-3.16	120.06	127.66
23	A	408	CLA	C1-C2-C3	-3.16	120.58	126.04
23	b	613	CLA	CMC-C2C-C1C	3.16	129.85	125.04
23	d	404	CLA	C4-C3-C5	3.15	120.58	115.27
23	c	516	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	b	623	CLA	O2A-CGA-CBA	3.15	121.79	111.91
23	d	403	CLA	CHD-C4C-NC	3.15	129.16	124.20
23	B	608	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
23	c	505	CLA	C1D-CHD-C4C	-3.15	118.41	122.56
23	C	506	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
23	C	513	CLA	CHD-C4C-NC	3.14	129.16	124.20
23	A	406	CLA	C3B-C4B-NB	3.14	113.28	109.21
23	c	509	CLA	C1-C2-C3	-3.14	120.61	126.04
31	D	408[A]	PL9	C37-C38-C39	-3.14	120.09	127.66
24	a	410	PHO	C3C-C4C-NC	3.14	115.15	110.28
23	c	515	CLA	C4-C3-C5	3.14	120.56	115.27
31	a	415[B]	PL9	C42-C43-C44	-3.14	120.10	127.66
26	F	104	SQD	C1-O5-C5	3.14	119.85	113.69
23	c	506	CLA	C1-C2-C3	-3.14	120.61	126.04
25	b	627	BCR	C15-C14-C13	-3.14	122.83	127.31
25	T	103	BCR	C21-C20-C19	-3.14	113.42	123.22
23	B	615	CLA	O2A-CGA-CBA	3.14	121.76	111.91
25	d	406	BCR	C15-C14-C13	-3.14	122.83	127.31
23	B	613	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
28	m	102	LMT	C1B-O5B-C5B	3.13	119.84	113.69
23	B	611	CLA	CMB-C2B-C3B	3.13	130.54	124.68
39	V	205	HEM	CBA-CAA-C2A	-3.13	106.71	112.49
23	B	617	CLA	C4C-C3C-C2C	-3.13	102.33	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	410	LHG	O7-C7-C8	3.13	118.25	111.50
23	b	625	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	A	408	CLA	CMC-C2C-C1C	3.13	129.81	125.04
31	D	408[A]	PL9	C10-C9-C11	3.13	120.53	115.27
31	A	417[B]	PL9	C22-C23-C24	-3.13	120.13	127.66
23	C	504	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
31	d	407[B]	PL9	C40-C39-C41	3.13	120.53	115.27
23	d	404	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	D	405	CLA	O2A-CGA-CBA	3.13	121.72	111.91
23	A	408	CLA	CHD-C4C-NC	3.12	129.13	124.20
23	c	508	CLA	CBC-CAC-C3C	-3.12	103.82	112.43
23	b	621	CLA	C3B-C4B-NB	3.12	113.25	109.21
23	C	506	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
25	B	620	BCR	C37-C22-C23	3.12	123.00	118.08
23	b	625	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	C	507	CLA	C4-C3-C5	3.12	120.52	115.27
23	b	611	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	A	406	CLA	C1D-CHD-C4C	-3.12	118.44	122.56
23	c	505	CLA	CMC-C2C-C1C	3.12	129.79	125.04
23	a	411	CLA	CAA-C2A-C3A	-3.12	104.25	112.78
31	A	417[A]	PL9	C7-C8-C9	-3.12	121.61	126.79
23	B	613	CLA	C3B-C4B-NB	3.12	113.24	109.21
23	b	615	CLA	C4-C3-C5	3.12	120.51	115.27
23	B	615	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
25	c	518	BCR	C15-C14-C13	-3.11	122.87	127.31
23	c	506	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
23	c	506	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	C	510	CLA	C1D-CHD-C4C	-3.11	118.45	122.56
23	C	509	CLA	C4D-C3D-CAD	-3.11	106.74	108.47
23	C	502	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
23	b	617	CLA	O2A-CGA-CBA	3.10	121.64	111.91
26	a	413	SQD	C45-O47-C7	-3.10	110.16	117.79
23	c	512	CLA	C4-C3-C5	3.10	120.48	115.27
23	B	616	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	B	612	CLA	CMA-C3A-C4A	-3.10	103.44	111.77
23	B	603	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
23	b	610	CLA	C4-C3-C5	3.10	120.48	115.27
23	B	610	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
23	b	621	CLA	C1C-C2C-C3C	-3.09	103.70	106.96
23	B	605	CLA	C1-C2-C3	-3.09	120.70	126.04
31	a	415[B]	PL9	C10-C9-C11	3.09	120.47	115.27
26	b	601	SQD	C3-C4-C5	3.09	115.75	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	B	607	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
25	H	101	BCR	C16-C17-C18	-3.09	122.90	127.31
23	b	612	CLA	CMC-C2C-C1C	3.09	129.74	125.04
31	a	415[A]	PL9	C7-C3-C2	-3.09	119.24	123.30
23	C	508	CLA	CHD-C4C-NC	3.09	129.06	124.20
23	b	625	CLA	CAC-C3C-C4C	3.09	128.81	124.81
23	B	613	CLA	C4-C3-C5	3.08	120.46	115.27
31	d	407[A]	PL9	C27-C28-C29	-3.08	120.24	127.66
23	b	624	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
23	A	404	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
31	A	417[B]	PL9	C32-C33-C34	-3.08	120.25	127.66
39	v	206	HEM	CBA-CAA-C2A	-3.08	106.81	112.49
23	D	406	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	A	408	CLA	CAA-C2A-C3A	-3.08	104.36	112.78
23	b	623	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
24	d	402[A]	PHO	C4D-CHA-C1A	-3.07	118.45	125.37
25	Y	101	BCR	C15-C16-C17	-3.07	117.18	123.47
23	b	619	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
31	a	415[A]	PL9	C42-C43-C44	-3.07	120.27	127.66
23	c	506	CLA	CHC-C1C-C2C	-3.07	118.23	126.72
31	D	408[B]	PL9	C10-C9-C11	3.07	120.43	115.27
23	C	510	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	A	406	CLA	CHD-C4C-NC	3.07	129.03	124.20
23	d	403	CLA	C1-C2-C3	-3.07	120.74	126.04
23	B	609	CLA	CMA-C3A-C4A	-3.07	103.53	111.77
23	a	409	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	c	505	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
23	b	622	CLA	C1-C2-C3	-3.06	120.75	126.04
23	B	612	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
23	b	617	CLA	C1D-CHD-C4C	-3.06	118.52	122.56
23	b	625	CLA	C3B-C4B-NB	3.06	113.16	109.21
23	C	503	CLA	CHD-C4C-NC	3.06	129.02	124.20
25	b	628	BCR	C3-C4-C5	-3.06	108.62	114.08
36	C	519	LMG	O8-C28-C29	3.06	121.50	111.91
23	C	503	CLA	C3B-C4B-NB	3.05	113.16	109.21
23	c	513	CLA	OBD-CAD-C3D	-3.05	122.91	127.98
23	A	405	CLA	CHD-C4C-NC	3.05	129.01	124.20
25	B	619	BCR	C29-C30-C25	3.05	115.18	110.48
23	b	610	CLA	CHD-C4C-NC	3.05	129.01	124.20
23	A	404	CLA	C4D-C3D-CAD	-3.05	106.77	108.47
24	D	402[B]	PHO	C4D-CHA-C1A	-3.05	118.50	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	624	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	b	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	A	405	CLA	C1-C2-C3	-3.05	120.77	126.04
26	b	601	SQD	C44-O6-C1	-3.05	107.78	113.74
23	B	613	CLA	C1D-CHD-C4C	-3.05	118.54	122.56
37	C	518	DGD	O2G-C1B-C2B	3.05	118.06	111.50
23	D	405	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
37	C	518	DGD	O1G-C1A-C2A	3.05	121.46	111.91
23	b	614	CLA	O2A-CGA-O1A	-3.05	115.91	123.59
23	C	510	CLA	CAC-C3C-C4C	3.04	128.76	124.81
36	M	101	LMG	O7-C10-C11	3.04	118.06	111.50
23	b	614	CLA	O2A-CGA-CBA	3.04	121.46	111.91
25	c	526	BCR	C11-C10-C9	-3.04	122.97	127.31
23	c	506	CLA	C1D-CHD-C4C	-3.04	118.55	122.56
23	C	511	CLA	C1D-CHD-C4C	-3.04	118.55	122.56
23	B	605	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
23	B	604	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	B	604	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	c	508	CLA	CAC-C3C-C4C	3.04	128.75	124.81
23	B	611	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	c	515	CLA	CAC-C3C-C4C	3.04	128.75	124.81
31	a	415[B]	PL9	C7-C3-C2	-3.03	119.31	123.30
23	a	409	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
31	A	417[A]	PL9	C7-C3-C2	-3.03	119.31	123.30
23	c	516	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	B	611	CLA	C1-C2-C3	-3.03	120.80	126.04
23	c	512	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
25	d	406	BCR	C7-C8-C9	-3.03	121.66	126.23
39	V	205	HEM	CBD-CAD-C3D	-3.03	106.90	112.48
33	d	409	LHG	O7-C7-C8	3.02	118.02	111.50
23	c	517	CLA	CMC-C2C-C1C	3.02	129.65	125.04
26	F	104	SQD	C3-C4-C5	3.02	115.63	110.24
31	a	415[B]	PL9	C17-C18-C19	-3.02	120.38	127.66
23	b	616	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
23	a	408	CLA	O2A-CGA-CBA	3.02	121.39	111.91
23	A	405	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	K	101	BCR	C38-C26-C25	-3.02	121.14	124.53
23	b	615	CLA	CHD-C4C-NC	3.02	128.96	124.20
23	c	507	CLA	CHD-C4C-NC	3.02	128.96	124.20
31	d	407[B]	PL9	C20-C19-C21	3.02	120.35	115.27
23	B	615	CLA	C2A-C1A-CHA	-3.02	118.58	123.86
23	d	403	CLA	C3C-C4C-NC	3.02	113.95	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	415[B]	PL9	C20-C19-C21	3.01	120.34	115.27
26	a	413	SQD	C1-O5-C5	-3.01	107.78	113.69
31	D	408[B]	PL9	C27-C28-C29	-3.01	120.41	127.66
35	V	206	HTG	C1-C2-C3	-3.01	104.65	110.59
23	a	411	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
23	B	602	CLA	CHC-C1C-C2C	-3.01	118.41	126.72
23	B	607	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
23	C	507	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
23	B	610	CLA	C1-C2-C3	-3.00	120.85	126.04
23	B	616	CLA	C3B-C4B-NB	3.00	113.09	109.21
23	B	606	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	c	517	CLA	CAC-C3C-C4C	3.00	128.70	124.81
23	c	510	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	b	623	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	b	621	CLA	O2A-CGA-CBA	2.99	121.30	111.91
35	C	523	HTG	O5-C5-C4	2.99	115.13	109.69
24	d	402[B]	PHO	C2B-C1B-NB	2.99	114.30	109.79
23	D	405	CLA	C3B-C4B-NB	2.99	113.07	109.21
23	C	507	CLA	C1-C2-C3	-2.99	120.88	126.04
23	C	504	CLA	O2A-CGA-CBA	2.98	121.26	111.91
23	c	515	CLA	C1-C2-C3	-2.98	120.89	126.04
23	B	605	CLA	C4-C3-C5	2.98	120.28	115.27
23	c	509	CLA	C3B-C4B-NB	2.98	113.06	109.21
23	a	409	CLA	CHC-C1C-C2C	-2.98	118.49	126.72
25	b	627	BCR	C38-C26-C25	-2.97	121.19	124.53
23	B	602	CLA	CHD-C4C-NC	2.97	128.89	124.20
23	b	621	CLA	CHD-C4C-NC	2.97	128.89	124.20
31	A	417[A]	PL9	C22-C23-C24	-2.97	120.50	127.66
23	c	513	CLA	CAC-C3C-C4C	2.97	128.67	124.81
23	B	611	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
23	B	617	CLA	O2A-CGA-CBA	2.97	121.23	111.91
23	b	622	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	C	506	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
23	D	406	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
23	b	620	CLA	O2A-CGA-CBA	2.97	121.22	111.91
23	c	512	CLA	CBC-CAC-C3C	-2.97	104.26	112.43
23	C	508	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
24	d	402[A]	PHO	CHC-C1C-C2C	-2.96	118.28	125.73
31	d	407[B]	PL9	C7-C8-C9	-2.96	121.86	126.79
23	B	608	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	b	616	CLA	C1D-CHD-C4C	-2.96	118.65	122.56
23	b	616	CLA	CHC-C1C-C2C	-2.96	118.53	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CHD-C4C-NC	2.96	128.87	124.20
23	B	607	CLA	C3B-C4B-NB	2.96	113.04	109.21
25	K	103	BCR	C10-C11-C12	-2.96	113.99	123.22
31	d	407[A]	PL9	C40-C39-C41	2.96	120.25	115.27
23	C	510	CLA	C1-O2A-CGA	2.96	124.20	116.44
23	b	610	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
23	B	614	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
25	B	620	BCR	C28-C27-C26	-2.95	108.80	114.08
24	D	402[A]	PHO	C2B-C1B-NB	2.95	114.25	109.79
23	b	610	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
23	C	513	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
23	b	620	CLA	C4D-C3D-CAD	-2.95	106.82	108.47
23	a	408	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	c	517	CLA	C1-C2-C3	-2.95	120.94	126.04
23	d	404	CLA	C4D-C3D-CAD	-2.95	106.83	108.47
23	D	405	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
31	a	415[B]	PL9	C27-C28-C29	-2.95	120.56	127.66
23	C	512	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
23	d	405	CLA	CAA-C2A-C3A	-2.95	104.71	112.78
23	c	513	CLA	O2A-CGA-CBA	2.95	121.15	111.91
23	b	618	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
23	b	625	CLA	O2A-CGA-CBA	2.94	121.14	111.91
25	Y	101	BCR	C10-C11-C12	-2.94	114.04	123.22
23	C	505	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
23	b	612	CLA	O2A-CGA-CBA	2.94	121.13	111.91
25	t	101	BCR	C20-C21-C22	-2.94	123.12	127.31
37	H	102	DGD	O2G-C1B-C2B	2.93	117.82	111.50
23	b	614	CLA	C2A-C1A-CHA	-2.93	118.73	123.86
23	B	615	CLA	C4-C3-C5	2.93	120.21	115.27
23	B	612	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
23	B	603	CLA	C4C-C3C-C2C	-2.93	102.62	106.90
23	b	623	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
36	Z	101	LMG	C1-O6-C5	2.93	119.44	113.69
23	B	604	CLA	O2A-CGA-CBA	2.93	121.10	111.91
23	a	411	CLA	CHD-C4C-NC	2.93	128.82	124.20
23	a	408	CLA	CAA-C2A-C3A	-2.93	104.76	112.78
23	c	517	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	B	609	CLA	CHD-C4C-NC	2.93	128.82	124.20
23	C	509	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
23	C	513	CLA	C3B-C4B-NB	2.93	112.99	109.21
23	b	614	CLA	C3B-C4B-NB	2.93	112.99	109.21
23	c	510	CLA	C1-C2-C3	-2.93	120.98	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	516	CLA	C1-C2-C3	-2.92	120.99	126.04
23	b	612	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	c	513	CLA	C1-O2A-CGA	2.92	124.11	116.44
23	b	625	CLA	C1-C2-C3	-2.92	120.99	126.04
23	A	404	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
23	B	617	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	B	608	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
23	b	619	CLA	CAC-C3C-C4C	2.91	128.59	124.81
31	A	417[A]	PL9	C27-C28-C29	-2.91	120.65	127.66
23	b	618	CLA	CHD-C4C-NC	2.91	128.79	124.20
23	b	613	CLA	CAC-C3C-C4C	2.91	128.59	124.81
25	K	101	BCR	C16-C17-C18	-2.91	123.16	127.31
26	b	601	SQD	C1-C2-C3	-2.91	103.94	110.00
23	b	614	CLA	CHD-C4C-NC	2.91	128.78	124.20
23	b	615	CLA	CMB-C2B-C3B	2.91	130.12	124.68
31	a	415[B]	PL9	C37-C38-C39	-2.91	120.66	127.66
23	B	609	CLA	CHC-C1C-C2C	-2.91	118.69	126.72
23	c	516	CLA	CMC-C2C-C1C	2.91	129.46	125.04
23	c	511	CLA	C3B-C4B-NB	2.90	112.96	109.21
25	t	101	BCR	C1-C6-C7	2.90	123.98	115.78
23	B	605	CLA	O2A-CGA-CBA	2.90	121.01	111.91
23	C	504	CLA	CMC-C2C-C1C	2.90	129.45	125.04
23	C	504	CLA	CHD-C4C-NC	2.90	128.77	124.20
25	T	103	BCR	C16-C17-C18	-2.90	123.18	127.31
23	B	613	CLA	CAC-C3C-C4C	2.90	128.57	124.81
23	B	602	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
23	C	512	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	C	504	CLA	CAC-C3C-C4C	2.89	128.56	124.81
23	B	615	CLA	CAC-C3C-C4C	2.89	128.56	124.81
23	d	403	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
31	A	417[B]	PL9	C7-C8-C9	-2.89	121.98	126.79
23	d	405	CLA	C3B-C4B-NB	2.89	112.94	109.21
23	c	512	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
23	A	408	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
33	b	634	LHG	O8-C23-C24	2.89	120.97	111.91
23	b	611	CLA	CMB-C2B-C3B	2.88	130.07	124.68
23	B	610	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	A	407	PHO	C4D-CHA-C1A	-2.88	118.89	125.37
33	D	412	LHG	O8-C23-C24	2.88	120.95	111.91
36	c	522	LMG	C8-O7-C10	-2.88	110.70	117.79
23	c	508	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	b	619	CLA	CHD-C4C-NC	2.88	128.74	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C24-C23-C22	-2.88	121.89	126.23
23	a	408	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
23	B	609	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	b	612	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
23	B	610	CLA	C4C-C3C-C2C	-2.88	102.71	106.90
23	B	604	CLA	CMB-C2B-C3B	2.88	130.06	124.68
23	d	404	CLA	CMC-C2C-C1C	2.88	129.42	125.04
23	c	507	CLA	C4-C3-C5	2.87	120.11	115.27
25	B	618	BCR	C29-C30-C25	2.87	114.91	110.48
23	B	607	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
31	A	417[A]	PL9	C42-C43-C44	-2.87	120.74	127.66
23	B	615	CLA	CHD-C4C-NC	2.87	128.73	124.20
23	B	611	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	A	406	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	B	617	CLA	OBD-CAD-C3D	-2.87	123.22	127.98
23	C	512	CLA	O2A-CGA-CBA	2.87	120.91	111.91
23	a	409	CLA	C1-C2-C3	-2.87	121.08	126.04
23	C	505	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
33	A	419	LHG	O8-C23-C24	2.87	120.90	111.91
23	a	408	CLA	C4-C3-C5	2.87	120.09	115.27
24	a	410	PHO	C2B-C1B-NB	2.87	114.11	109.79
23	a	408	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
24	a	410	PHO	CBA-CAA-C2A	-2.86	105.41	113.86
23	c	515	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
23	C	509	CLA	CHD-C4C-NC	2.86	128.71	124.20
25	t	101	BCR	C7-C6-C5	-2.86	114.53	121.46
23	C	513	CLA	C1-C2-C3	-2.86	121.10	126.04
31	A	417[B]	PL9	C53-C6-C1	2.86	120.84	114.99
31	a	415[A]	PL9	C35-C34-C36	2.86	120.08	115.27
24	A	407	PHO	C2B-C1B-NB	2.86	114.10	109.79
25	h	101	BCR	C38-C26-C25	-2.86	121.32	124.53
23	b	618	CLA	C3B-C4B-NB	2.86	112.90	109.21
24	A	407	PHO	C2C-C1C-NC	2.85	114.10	109.79
23	B	606	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
36	k	101	LMG	O8-C28-C29	2.85	120.86	111.91
23	b	620	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
31	D	408[A]	PL9	C40-C39-C41	2.85	120.07	115.27
23	D	405	CLA	CHD-C4C-NC	2.85	128.70	124.20
23	C	512	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
23	B	615	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
23	d	404	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
31	a	415[A]	PL9	C25-C24-C26	2.85	120.06	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4-C3-C5	2.85	120.06	115.27
37	D	409	DGD	O1G-C1A-C2A	2.84	120.83	111.91
23	d	404	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
23	b	621	CLA	O2A-CGA-O1A	-2.84	116.41	123.59
23	b	613	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
23	B	604	CLA	CHD-C4C-NC	2.84	128.68	124.20
33	L	101	LHG	O8-C23-C24	2.84	120.83	111.91
23	b	620	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
23	b	623	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
23	A	408	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	c	516	CLA	C4-C3-C5	2.84	120.05	115.27
23	b	623	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	a	409	CLA	C4-C3-C5	2.84	120.04	115.27
23	C	511	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
31	A	417[A]	PL9	C53-C6-C1	2.84	120.79	114.99
23	b	617	CLA	CHD-C4C-NC	2.84	128.67	124.20
25	c	526	BCR	C20-C21-C22	-2.83	123.26	127.31
31	a	415[A]	PL9	C53-C6-C1	2.83	120.79	114.99
23	B	609	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
23	b	615	CLA	CHC-C1C-C2C	-2.83	118.88	126.72
35	b	607	HTG	O5-C5-C4	2.83	114.84	109.69
23	c	510	CLA	O2A-CGA-CBA	2.83	120.80	111.91
31	a	415[B]	PL9	C25-C24-C26	2.83	120.03	115.27
23	c	515	CLA	O2A-CGA-CBA	2.83	120.79	111.91
24	D	402[A]	PHO	C4D-CHA-C1A	-2.83	119.00	125.37
23	C	514	CLA	CHD-C4C-NC	2.83	128.66	124.20
23	C	514	CLA	C3B-C4B-NB	2.83	112.86	109.21
24	d	402[A]	PHO	C2A-C1A-NA	2.83	115.11	111.86
23	b	617	CLA	C3B-C4B-NB	2.83	112.86	109.21
31	A	417[B]	PL9	C27-C28-C29	-2.83	120.86	127.66
31	A	417[B]	PL9	C45-C44-C46	2.83	120.03	115.27
23	C	514	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
23	B	612	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	D	408[B]	PL9	C53-C6-C1	2.82	120.77	114.99
23	B	605	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
23	b	611	CLA	C4-C3-C5	2.82	120.02	115.27
23	c	511	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
25	d	406	BCR	C37-C22-C23	2.82	122.53	118.08
23	C	502	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
23	c	511	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	b	612	CLA	C4-C3-C5	2.82	120.02	115.27
25	a	412	BCR	C33-C5-C6	-2.82	121.36	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	516	CLA	C3B-C4B-NB	2.82	112.86	109.21
25	K	101	BCR	C20-C21-C22	-2.82	123.29	127.31
23	A	406	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
37	c	519	DGD	C2G-O2G-C1B	-2.82	110.86	117.79
23	b	615	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
25	c	518	BCR	C16-C17-C18	-2.81	123.30	127.31
24	D	402[A]	PHO	C2A-C1A-NA	2.81	115.09	111.86
23	A	405	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
31	a	415[B]	PL9	C35-C34-C36	2.81	120.00	115.27
23	c	513	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	B	606	CLA	O2A-CGA-O1A	-2.81	116.50	123.59
23	b	616	CLA	CAC-C3C-C4C	2.81	128.46	124.81
25	b	628	BCR	C24-C23-C22	-2.81	121.99	126.23
25	b	626	BCR	C29-C30-C25	2.81	114.81	110.48
23	C	513	CLA	O2A-CGA-CBA	2.81	120.72	111.91
23	C	508	CLA	C1-C2-C3	-2.81	121.19	126.04
23	C	509	CLA	C1-C2-C3	-2.80	121.19	126.04
23	c	517	CLA	C2A-C1A-CHA	-2.80	118.96	123.86
23	C	514	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
23	b	624	CLA	C1-C2-C3	-2.80	121.20	126.04
24	A	407	PHO	C4C-C3C-C2C	-2.80	103.68	106.78
23	d	403	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
23	B	614	CLA	OBD-CAD-C3D	-2.80	123.33	127.98
23	d	403	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
23	b	624	CLA	CHD-C4C-NC	2.80	128.61	124.20
23	b	620	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	d	402[B]	PHO	CHC-C1C-C2C	-2.80	118.70	125.73
23	d	405	CLA	C4D-C3D-CAD	-2.79	106.91	108.47
23	C	504	CLA	C3B-C4B-NB	2.79	112.82	109.21
23	b	622	CLA	O2A-CGA-CBA	2.79	120.67	111.91
23	b	619	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
23	A	405	CLA	C4-C3-C5	2.79	119.97	115.27
23	b	621	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
23	B	616	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
36	a	414	LMG	C7-O1-C1	-2.79	108.28	113.74
23	a	408	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
31	D	408[A]	PL9	C22-C23-C24	-2.79	120.94	127.66
26	f	102	SQD	O5-C5-C4	2.79	114.76	109.69
23	B	615	CLA	CMC-C2C-C1C	2.79	129.28	125.04
23	b	616	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
26	b	601	SQD	O48-C23-C24	2.78	120.65	111.91
23	b	618	CLA	CHC-C1C-C2C	-2.78	119.02	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
23	b	621	CLA	OBD-CAD-C3D	-2.78	123.36	127.98
31	d	407[B]	PL9	C17-C18-C19	-2.78	120.97	127.66
31	D	408[A]	PL9	C27-C28-C29	-2.78	120.97	127.66
25	Y	101	BCR	C37-C22-C23	2.78	122.46	118.08
23	b	621	CLA	CAC-C3C-C4C	2.78	128.41	124.81
23	B	611	CLA	C3B-C4B-NB	2.77	112.80	109.21
23	c	507	CLA	CMC-C2C-C1C	2.77	129.26	125.04
24	d	402[A]	PHO	C3C-C4C-NC	2.77	114.58	110.28
23	C	503	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
25	B	620	BCR	C37-C22-C21	-2.77	119.04	122.92
23	D	405	CLA	C4-C3-C5	2.77	119.93	115.27
25	Y	101	BCR	C38-C26-C25	-2.77	121.42	124.53
23	B	612	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
31	d	407[A]	PL9	C53-C6-C1	2.77	120.65	114.99
23	B	614	CLA	O2A-CGA-CBA	2.77	120.60	111.91
31	D	408[A]	PL9	C25-C24-C26	2.77	119.93	115.27
23	C	508	CLA	CMC-C2C-C1C	2.77	129.25	125.04
23	B	617	CLA	CBC-CAC-C3C	-2.77	104.80	112.43
23	B	611	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
24	A	407	PHO	CBA-CAA-C2A	-2.77	105.70	113.86
37	H	102	DGD	C2G-O2G-C1B	-2.77	110.98	117.79
23	C	506	CLA	C1-O2A-CGA	2.77	123.70	116.44
23	C	502	CLA	C1-C2-C3	-2.76	121.27	126.04
23	c	514	CLA	CAC-C3C-C4C	2.76	128.39	124.81
23	B	604	CLA	O2A-CGA-O1A	-2.76	116.63	123.59
23	C	510	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	b	617	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
23	b	617	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
23	A	408	CLA	CAC-C3C-C4C	2.76	128.39	124.81
36	a	414	LMG	O8-C28-C29	2.75	120.55	111.91
24	d	402[B]	PHO	C4D-ND-C1D	-2.75	101.81	106.76
23	C	502	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	B	603	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	B	603	CLA	OBD-CAD-C3D	-2.75	123.41	127.98
25	A	409	BCR	C20-C21-C22	-2.75	123.39	127.31
23	b	625	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
23	b	610	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
31	d	407[A]	PL9	C15-C14-C16	2.75	119.89	115.27
37	C	516	DGD	O6D-C1D-O3G	-2.75	103.47	109.97
23	c	513	CLA	C4C-C3C-C2C	-2.75	102.90	106.90
24	D	402[A]	PHO	C4D-ND-C1D	-2.74	101.83	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
23	d	405	CLA	CAC-C3C-C4C	2.74	128.37	124.81
25	h	101	BCR	C10-C11-C12	-2.74	114.66	123.22
23	D	405	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
33	d	409	LHG	O8-C23-O10	-2.74	116.67	123.59
24	D	402[B]	PHO	C4-C3-C5	2.74	119.88	115.27
37	H	102	DGD	O1G-C1A-C2A	2.74	120.51	111.91
23	b	612	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	c	515	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
23	c	516	CLA	O2A-CGA-CBA	2.74	120.50	111.91
23	A	404	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
26	F	104	SQD	O48-C23-C24	2.74	120.50	111.91
23	d	405	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
23	B	610	CLA	CAC-C3C-C4C	2.74	128.36	124.81
31	a	415[A]	PL9	C40-C39-C41	2.73	119.87	115.27
25	b	628	BCR	C2-C1-C6	2.73	114.69	110.48
23	D	405	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
23	a	411	CLA	CHB-C4A-NA	2.73	128.29	124.51
23	c	508	CLA	OBD-CAD-C3D	-2.73	123.45	127.98
23	C	510	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
23	c	517	CLA	O2A-CGA-CBA	2.73	120.47	111.91
31	d	407[B]	PL9	C27-C28-C29	-2.73	121.09	127.66
23	C	513	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
23	b	612	CLA	CAC-C3C-C4C	2.73	128.35	124.81
23	B	608	CLA	C4-C3-C5	2.72	119.86	115.27
23	c	512	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
23	c	516	CLA	O1D-CGD-CBD	-2.72	118.91	124.48
25	t	101	BCR	C3-C4-C5	-2.72	109.22	114.08
23	B	602	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
23	C	503	CLA	C4D-C3D-CAD	-2.72	106.95	108.47
23	c	508	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
23	B	605	CLA	CAC-C3C-C4C	2.72	128.34	124.81
23	C	514	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
25	h	101	BCR	C11-C10-C9	-2.72	123.43	127.31
23	b	611	CLA	CHC-C1C-C2C	-2.72	119.21	126.72
23	C	503	CLA	CAC-C3C-C4C	2.72	128.33	124.81
23	B	614	CLA	C4-C3-C5	2.72	119.84	115.27
24	d	402[A]	PHO	CHD-C1D-C2D	-2.71	118.90	125.73
31	A	417[A]	PL9	C25-C24-C26	2.71	119.84	115.27
31	A	417[A]	PL9	C45-C44-C46	2.71	119.84	115.27
23	B	603	CLA	C4-C3-C5	2.71	119.83	115.27
23	b	612	CLA	C2A-C1A-CHA	-2.71	119.11	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	526	BCR	C38-C26-C25	-2.71	121.49	124.53
25	C	515	BCR	C16-C17-C18	-2.70	123.45	127.31
23	c	505	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	B	604	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
23	c	511	CLA	CAC-C3C-C4C	2.70	128.32	124.81
23	c	517	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	D	406	CLA	C1-C2-C3	-2.70	121.37	126.04
23	c	515	CLA	CMC-C2C-C1C	2.70	129.15	125.04
35	B	624	HTG	C1-O5-C5	2.70	117.56	112.58
26	a	413	SQD	O47-C7-O49	-2.70	117.18	123.70
23	C	502	CLA	C3B-C4B-NB	2.70	112.70	109.21
23	C	512	CLA	C4-C3-C5	2.70	119.81	115.27
23	a	409	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
23	c	506	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	C	511	CLA	CMC-C2C-C1C	2.70	129.15	125.04
36	z	101	LMG	O8-C28-C29	2.70	120.37	111.91
23	b	615	CLA	CMC-C2C-C1C	2.70	129.14	125.04
24	d	402[A]	PHO	C4D-ND-C1D	-2.70	101.92	106.76
31	A	417[A]	PL9	C15-C14-C16	2.69	119.80	115.27
26	a	413	SQD	O48-C23-C24	2.69	120.36	111.91
23	C	503	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	b	617	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
23	C	511	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
23	b	619	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
31	a	415[A]	PL9	C30-C29-C31	2.69	119.80	115.27
23	A	405	CLA	OBD-CAD-C3D	-2.69	123.52	127.98
35	C	523	HTG	O5-C1-C2	2.69	113.70	110.31
23	A	406	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
33	L	101	LHG	C5-O7-C7	-2.69	111.17	117.79
23	b	613	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	y	101	BCR	C16-C17-C18	-2.69	123.47	127.31
36	Z	101	LMG	O6-C5-C4	2.69	114.57	109.69
23	A	406	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
31	A	417[B]	PL9	C12-C13-C14	-2.68	121.20	127.66
24	A	407	PHO	C4D-ND-C1D	-2.68	101.94	106.76
23	B	614	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
23	B	613	CLA	O2A-CGA-CBA	2.68	120.32	111.91
31	a	415[B]	PL9	C53-C6-C1	2.68	120.47	114.99
25	B	619	BCR	C31-C1-C6	-2.68	105.95	110.30
23	B	607	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	c	516	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	c	514	CLA	O2A-CGA-CBA	2.68	120.31	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C6-C5-C3	-2.68	106.43	113.45
31	d	407[A]	PL9	C20-C19-C21	2.68	119.77	115.27
24	D	402[B]	PHO	CHC-C1C-C2C	-2.68	119.00	125.73
25	B	620	BCR	C10-C11-C12	-2.67	114.88	123.22
23	c	517	CLA	C3B-C4B-NB	2.67	112.66	109.21
23	C	506	CLA	C4-C3-C5	2.67	119.76	115.27
25	K	103	BCR	C3-C4-C5	-2.67	109.31	114.08
28	m	102	LMT	O5'-C5'-C4'	2.67	115.38	109.75
23	d	403	CLA	CMB-C2B-C3B	2.67	129.67	124.68
23	b	616	CLA	CHD-C4C-NC	2.67	128.41	124.20
31	d	407[A]	PL9	C10-C9-C11	2.67	119.76	115.27
23	d	405	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
24	D	402[A]	PHO	O2D-CGD-O1D	-2.66	118.63	123.84
23	D	406	CLA	CHD-C4C-NC	2.66	128.40	124.20
24	A	407	PHO	C1-C2-C3	-2.66	121.44	126.04
23	B	610	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
23	B	603	CLA	C1-O2A-CGA	2.66	123.43	116.44
23	b	615	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	A	410	SQD	O48-C23-C24	2.66	120.26	111.91
23	c	513	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
23	d	405	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
23	B	608	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
23	c	514	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	b	623	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
31	A	417[B]	PL9	C25-C24-C26	2.66	119.74	115.27
23	B	617	CLA	C1-O2A-CGA	2.66	123.41	116.44
23	c	511	CLA	C4-C3-C5	2.65	119.74	115.27
35	d	414	HTG	C1-O5-C5	2.65	117.47	112.58
23	c	505	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	B	605	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
31	a	415[B]	PL9	C40-C39-C41	2.65	119.73	115.27
23	b	610	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
26	F	104	SQD	O6-C1-C2	2.65	112.44	108.30
33	L	101	LHG	O8-C23-O10	-2.65	116.91	123.59
23	b	611	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	c	517	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
23	B	616	CLA	CBC-CAC-C3C	-2.65	105.13	112.43
23	c	514	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	A	405	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
31	d	407[B]	PL9	C25-C24-C26	2.65	119.72	115.27
23	B	607	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
23	c	515	CLA	O2D-CGD-O1D	-2.64	118.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CHD-C4C-NC	2.64	128.37	124.20
37	h	102	DGD	O1G-C1A-O1A	-2.64	116.92	123.59
25	Y	101	BCR	C40-C30-C25	-2.64	106.01	110.30
26	B	636	SQD	O48-C23-O10	-2.64	116.93	123.59
23	a	409	CLA	OBD-CAD-C3D	-2.64	123.60	127.98
23	c	511	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
25	a	412	BCR	C8-C7-C6	-2.64	119.80	127.20
25	d	406	BCR	C24-C23-C22	-2.64	122.25	126.23
23	c	508	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	c	507	CLA	O2A-CGA-CBA	2.64	120.18	111.91
33	d	409	LHG	O8-C23-C24	2.63	120.17	111.91
23	B	615	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
24	a	410	PHO	CBD-CHA-C1A	2.63	132.51	126.40
23	c	505	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	C	510	CLA	CMC-C2C-C1C	2.63	129.04	125.04
26	f	102	SQD	O47-C7-O49	-2.63	117.35	123.70
25	D	407	BCR	C10-C11-C12	-2.63	115.02	123.22
24	a	410	PHO	C1C-C2C-C3C	-2.63	103.49	106.51
25	Y	101	BCR	C24-C23-C22	-2.63	122.27	126.23
23	c	509	CLA	C4-C3-C5	2.63	119.69	115.27
24	d	402[A]	PHO	CAC-C3C-C4C	2.63	128.09	125.22
23	B	606	CLA	C3B-C4B-NB	2.63	112.61	109.21
24	D	402[B]	PHO	C4D-ND-C1D	-2.63	102.04	106.76
31	d	407[B]	PL9	C22-C23-C24	-2.63	121.34	127.66
23	c	505	CLA	C4D-C3D-CAD	-2.63	107.01	108.47
23	C	507	CLA	CMB-C2B-C3B	2.62	129.59	124.68
28	M	104	LMT	O1B-C1B-C2B	2.62	114.89	108.10
25	y	101	BCR	C10-C11-C12	-2.62	115.03	123.22
23	C	508	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
33	D	411	LHG	O8-C23-C24	2.62	120.13	111.91
24	D	402[A]	PHO	CHC-C1C-C2C	-2.62	119.14	125.73
23	C	508	CLA	C4-C3-C5	2.62	119.68	115.27
23	D	405	CLA	C1D-CHD-C4C	-2.62	119.10	122.56
31	d	407[A]	PL9	C12-C13-C14	-2.62	121.36	127.66
23	B	613	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
23	B	608	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	a	410	PHO	CAC-C3C-C4C	2.61	128.07	125.22
25	B	620	BCR	C32-C1-C6	-2.61	106.06	110.30
23	b	610	CLA	CMB-C2B-C3B	2.61	129.57	124.68
33	d	409	LHG	O7-C7-O9	-2.61	117.39	123.70
23	d	403	CLA	CMA-C3A-C2A	-2.61	103.30	113.83
31	A	417[A]	PL9	C30-C29-C31	2.61	119.66	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	CAA-C2A-C1A	-2.61	103.43	111.97
23	A	405	CLA	O2A-CGA-CBA	2.61	120.09	111.91
23	a	411	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
37	c	519	DGD	O3G-C3G-C2G	-2.61	104.61	110.90
23	C	512	CLA	CMB-C2B-C3B	2.61	129.55	124.68
23	B	608	CLA	C1-O2A-CGA	2.61	123.28	116.44
23	B	603	CLA	C4D-C3D-CAD	-2.61	107.02	108.47
26	f	102	SQD	O48-C23-C24	2.61	120.08	111.91
23	C	504	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
23	a	411	CLA	CMA-C3A-C2A	-2.60	103.32	113.83
23	B	605	CLA	CHD-C4C-NC	2.60	128.31	124.20
31	A	417[B]	PL9	C15-C14-C16	2.60	119.65	115.27
23	C	508	CLA	CHC-C1C-C2C	-2.60	119.52	126.72
23	b	611	CLA	C1-C2-C3	-2.60	121.54	126.04
23	C	509	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
23	b	625	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
23	b	623	CLA	CAC-C3C-C4C	2.60	128.19	124.81
23	c	511	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
23	b	619	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	b	625	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
23	c	516	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
23	b	618	CLA	C4-C3-C5	2.60	119.64	115.27
23	B	616	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
23	d	405	CLA	O2A-CGA-CBA	2.60	120.05	111.91
37	D	409	DGD	O6D-C5D-C6D	2.60	111.90	106.67
23	b	614	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
23	B	610	CLA	C4D-C3D-CAD	-2.59	107.02	108.47
36	C	519	LMG	C8-O7-C10	-2.59	111.41	117.79
23	C	510	CLA	C4-C3-C5	2.59	119.63	115.27
23	c	516	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
25	K	103	BCR	C2-C1-C6	2.59	114.47	110.48
24	a	410	PHO	C4D-CHA-C1A	-2.59	119.54	125.37
23	D	405	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
25	b	627	BCR	C29-C30-C25	2.59	114.47	110.48
23	B	613	CLA	CHD-C4C-NC	2.59	128.28	124.20
25	t	101	BCR	C35-C13-C12	2.59	122.16	118.08
23	B	609	CLA	CMC-C2C-C1C	2.59	128.98	125.04
25	y	101	BCR	C32-C1-C6	-2.58	106.11	110.30
23	B	610	CLA	CMB-C2B-C1B	2.58	132.44	128.46
31	A	417[A]	PL9	C12-C13-C14	-2.58	121.44	127.66
37	h	102	DGD	O1G-C1A-C2A	2.58	120.02	111.91
23	C	511	CLA	CBC-CAC-C3C	-2.58	105.31	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	PHO	C2C-C1C-NC	2.58	113.69	109.79
23	a	411	CLA	O2A-CGA-CBA	2.58	120.01	111.91
23	C	514	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
26	f	102	SQD	O7-S-C6	2.58	110.00	106.94
23	c	510	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
23	C	507	CLA	CMC-C2C-C1C	2.58	128.97	125.04
23	D	406	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
23	c	506	CLA	O2A-CGA-CBA	2.58	119.99	111.91
28	A	414	LMT	C1B-O5B-C5B	2.58	118.74	113.69
36	Z	101	LMG	C8-O7-C10	-2.57	111.45	117.79
31	D	408[A]	PL9	C53-C6-C1	2.57	120.25	114.99
24	a	410	PHO	CHD-C1D-C2D	-2.57	119.25	125.73
23	b	611	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	b	624	CLA	C11-C10-C8	-2.57	107.60	115.92
23	B	616	CLA	CAC-C3C-C4C	2.57	128.15	124.81
24	a	410	PHO	C4D-ND-C1D	-2.57	102.14	106.76
23	b	625	CLA	CMC-C2C-C1C	2.57	128.95	125.04
23	B	609	CLA	O2A-CGA-CBA	2.57	119.97	111.91
25	t	101	BCR	C37-C22-C23	2.57	122.12	118.08
23	A	408	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
25	c	518	BCR	C3-C4-C5	-2.57	109.50	114.08
23	c	510	CLA	OBD-CAD-C3D	-2.57	123.72	127.98
25	b	627	BCR	C37-C22-C21	-2.57	119.33	122.92
25	K	101	BCR	C23-C24-C25	-2.57	120.00	127.20
24	D	402[B]	PHO	CBD-CHA-C1A	2.56	132.35	126.40
23	d	404	CLA	CMB-C2B-C3B	2.56	129.47	124.68
33	d	410	LHG	O8-C23-O10	-2.56	117.12	123.59
23	B	614	CLA	CMB-C2B-C3B	2.56	129.47	124.68
23	c	512	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	a	410	PHO	CMC-C2C-C1C	2.56	129.01	125.06
23	C	509	CLA	O2A-CGA-CBA	2.56	119.95	111.91
36	C	520	LMG	O8-C28-C29	2.56	119.94	111.91
26	A	413	SQD	O9-S-C6	2.56	109.98	106.94
25	K	103	BCR	C15-C16-C17	-2.56	118.23	123.47
23	b	617	CLA	CMC-C2C-C1C	2.56	128.94	125.04
26	B	621	SQD	O48-C23-C24	2.56	119.94	111.91
37	C	516	DGD	O1G-C1A-C2A	2.56	119.93	111.91
24	D	402[B]	PHO	C2A-C1A-NA	2.56	114.80	111.86
23	d	405	CLA	C4-C3-C5	2.56	119.57	115.27
23	B	607	CLA	CHD-C4C-NC	2.55	128.23	124.20
23	C	507	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
23	C	502	CLA	CHD-C4C-NC	2.55	128.22	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	102	BCR	C3-C4-C5	-2.55	109.52	114.08
33	D	411	LHG	O7-C7-C8	2.55	116.99	111.50
25	B	620	BCR	C34-C9-C8	2.55	122.09	118.08
23	b	620	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	b	611	CLA	CMA-C3A-C2A	-2.55	103.56	113.83
23	B	609	CLA	CMB-C2B-C3B	2.55	129.44	124.68
23	A	404	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
31	A	417[B]	PL9	C30-C29-C31	2.54	119.55	115.27
23	b	611	CLA	CMC-C2C-C1C	2.54	128.91	125.04
23	C	511	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	B	605	CLA	OBD-CAD-C3D	-2.54	123.76	127.98
23	B	604	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
25	D	407	BCR	C33-C5-C6	-2.54	121.68	124.53
25	a	412	BCR	C20-C21-C22	-2.54	123.69	127.31
35	C	522	HTG	C1-O5-C5	2.54	117.26	112.58
37	C	517	DGD	O1G-C1A-C2A	2.54	119.87	111.91
23	c	508	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
24	d	402[B]	PHO	C4D-CHA-C1A	-2.54	119.66	125.37
25	t	101	BCR	C29-C28-C27	-2.54	105.71	111.38
37	c	521	DGD	C2G-O2G-C1B	-2.54	111.55	117.79
24	d	402[B]	PHO	C3C-C4C-NC	2.54	114.21	110.28
23	B	606	CLA	O2A-CGA-CBA	2.54	119.86	111.91
23	C	511	CLA	O2A-CGA-CBA	2.53	119.86	111.91
23	c	514	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
23	C	513	CLA	C4D-C3D-CAD	-2.53	107.06	108.47
31	a	415[A]	PL9	C51-C49-C50	2.53	120.20	114.60
23	c	517	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	C	509	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
25	T	103	BCR	C7-C8-C9	-2.53	122.41	126.23
31	A	417[A]	PL9	C17-C18-C19	-2.53	121.56	127.66
23	b	617	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
25	c	518	BCR	C11-C10-C9	-2.53	123.70	127.31
23	b	616	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	612	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	B	605	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	B	603	CLA	CMB-C2B-C3B	2.53	129.41	124.68
23	a	408	CLA	CMA-C3A-C4A	-2.53	104.98	111.77
26	A	410	SQD	O9-S-C6	2.53	109.94	106.94
25	t	101	BCR	C21-C20-C19	-2.52	115.35	123.22
23	a	409	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	b	625	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
24	D	402[A]	PHO	C1C-C2C-C3C	-2.52	103.61	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	406	BCR	C32-C1-C6	-2.52	106.21	110.30
31	D	408[B]	PL9	C45-C44-C46	2.52	119.51	115.27
23	A	406	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	c	510	CLA	CMC-C2C-C1C	2.52	128.87	125.04
31	A	417[B]	PL9	C17-C18-C19	-2.52	121.60	127.66
23	C	505	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
23	a	408	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	c	508	CLA	CMB-C2B-C3B	2.52	129.39	124.68
24	D	402[A]	PHO	C3C-C4C-NC	2.52	114.18	110.28
23	B	603	CLA	C11-C12-C13	-2.52	107.79	115.92
36	z	101	LMG	C8-O7-C10	-2.52	111.60	117.79
23	b	619	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	c	505	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	B	617	CLA	CMB-C2B-C3B	2.51	129.38	124.68
23	C	502	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
23	A	405	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
26	F	104	SQD	O47-C7-O49	-2.51	117.64	123.70
23	C	510	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	b	622	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	C	503	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	C	513	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
25	T	103	BCR	C1-C6-C7	2.51	122.87	115.78
23	B	612	CLA	CMC-C2C-C1C	2.51	128.85	125.04
31	d	407[B]	PL9	C10-C9-C11	2.51	119.49	115.27
31	D	408[A]	PL9	C20-C19-C21	2.50	119.48	115.27
23	C	506	CLA	CMC-C2C-C1C	2.50	128.85	125.04
25	B	619	BCR	C37-C22-C21	-2.50	119.42	122.92
24	A	407	PHO	CBD-CHA-C1A	2.50	132.20	126.40
23	d	405	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
37	C	516	DGD	O1G-C1A-O1A	-2.50	117.28	123.59
31	D	408[B]	PL9	C37-C38-C39	-2.50	121.64	127.66
23	B	607	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
25	c	518	BCR	C38-C26-C25	-2.50	121.73	124.53
23	c	515	CLA	CMB-C2B-C3B	2.49	129.34	124.68
25	C	515	BCR	C21-C20-C19	-2.49	115.44	123.22
23	B	612	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
25	k	102	BCR	C10-C11-C12	-2.49	115.44	123.22
24	D	402[B]	PHO	C1C-C2C-C3C	-2.49	103.65	106.51
24	D	402[A]	PHO	CHD-C1D-C2D	-2.49	119.46	125.73
25	d	406	BCR	C33-C5-C6	-2.49	121.73	124.53
23	C	507	CLA	CHD-C4C-NC	2.49	128.13	124.20
23	B	612	CLA	CHD-C4C-NC	2.49	128.13	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	520	DGD	C2G-O2G-C1B	-2.49	111.66	117.79
24	A	407	PHO	O2D-CGD-O1D	-2.49	118.97	123.84
25	a	412	BCR	C40-C30-C25	-2.49	106.26	110.30
23	c	512	CLA	CHD-C4C-NC	2.49	128.12	124.20
28	M	104	LMT	O1'-C1'-C2'	2.48	112.18	108.30
23	c	513	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
23	A	408	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
36	c	522	LMG	O8-C28-C29	2.48	119.70	111.91
25	H	101	BCR	C31-C1-C6	-2.48	106.28	110.30
25	K	103	BCR	C20-C21-C22	-2.48	123.77	127.31
23	c	514	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
23	b	613	CLA	CHD-C4C-NC	2.48	128.11	124.20
25	k	102	BCR	C7-C8-C9	-2.48	122.49	126.23
23	C	514	CLA	C4-C3-C5	2.48	119.44	115.27
26	a	413	SQD	O9-S-C6	2.48	109.88	106.94
23	D	406	CLA	O2A-CGA-CBA	2.48	119.68	111.91
23	b	615	CLA	O2A-CGA-CBA	2.47	119.67	111.91
37	C	517	DGD	O1G-C1A-O1A	-2.47	117.35	123.59
23	c	513	CLA	C4-C3-C5	2.47	119.43	115.27
23	c	507	CLA	C3B-C4B-NB	2.47	112.40	109.21
25	b	628	BCR	C21-C20-C19	-2.47	115.51	123.22
25	b	628	BCR	C16-C15-C14	-2.47	118.42	123.47
23	b	611	CLA	OBD-CAD-C3D	-2.47	123.88	127.98
23	B	616	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
23	C	503	CLA	C4-C3-C5	2.47	119.42	115.27
23	B	608	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
25	h	101	BCR	C24-C23-C22	-2.47	122.51	126.23
23	c	507	CLA	CAC-C3C-C4C	2.47	128.01	124.81
23	C	511	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	C	512	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
33	D	411	LHG	O8-C23-O10	-2.46	117.38	123.59
23	C	505	CLA	CHD-C4C-NC	2.46	128.08	124.20
23	d	404	CLA	C1D-CHD-C4C	-2.46	119.31	122.56
23	C	514	CLA	O2A-CGA-CBA	2.46	119.63	111.91
23	D	406	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
23	b	613	CLA	CMB-C2B-C3B	2.46	129.28	124.68
36	c	522	LMG	O7-C10-O9	-2.46	117.76	123.70
24	a	410	PHO	C4-C3-C5	2.46	119.41	115.27
23	B	613	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
36	C	520	LMG	C3-C4-C5	2.46	114.62	110.24
23	a	409	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
23	a	408	CLA	O2D-CGD-O1D	-2.46	119.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C4-C3-C5	2.46	119.40	115.27
31	d	407[B]	PL9	C45-C44-C46	2.46	119.40	115.27
23	B	616	CLA	C4D-C3D-CAD	-2.45	107.10	108.47
33	d	411	LHG	O8-C23-C24	2.45	119.61	111.91
23	a	408	CLA	C1-C2-C3	-2.45	121.80	126.04
24	D	402[B]	PHO	C2B-C1B-NB	2.45	113.49	109.79
31	A	417[B]	PL9	C10-C9-C11	2.45	119.40	115.27
31	A	417[B]	PL9	C42-C43-C44	-2.45	121.76	127.66
31	D	408[B]	PL9	C30-C29-C31	2.45	119.39	115.27
31	D	408[B]	PL9	C15-C14-C16	2.45	119.39	115.27
23	d	404	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
23	d	405	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
36	c	522	LMG	C3-C4-C5	2.44	114.60	110.24
33	a	419	LHG	O8-C23-C24	2.44	119.58	111.91
25	B	620	BCR	C20-C21-C22	-2.44	123.82	127.31
26	a	413	SQD	C44-O6-C1	-2.44	108.97	113.74
25	T	103	BCR	C2-C1-C6	2.44	114.23	110.48
36	Z	101	LMG	C1-C2-C3	2.44	115.07	110.00
23	d	404	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
37	d	408	DGD	O1G-C1A-C2A	2.44	119.56	111.91
25	d	406	BCR	C40-C30-C25	-2.43	106.35	110.30
23	b	623	CLA	CMB-C2B-C3B	2.43	129.23	124.68
23	b	622	CLA	CMA-C3A-C4A	-2.43	105.23	111.77
25	a	412	BCR	C15-C14-C13	-2.43	123.84	127.31
23	a	408	CLA	CMB-C2B-C3B	2.43	129.23	124.68
23	B	614	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
23	B	615	CLA	C1-O2A-CGA	2.43	122.83	116.44
23	B	607	CLA	OBD-CAD-C3D	-2.43	123.94	127.98
23	B	611	CLA	OBD-CAD-C3D	-2.43	123.94	127.98
25	T	103	BCR	C3-C4-C5	-2.43	109.73	114.08
23	B	614	CLA	C7-C6-C5	-2.43	106.76	113.36
36	Z	101	LMG	C9-O8-C28	2.43	123.21	117.10
37	c	519	DGD	O2G-C1B-O1B	-2.43	117.83	123.70
23	B	610	CLA	O2A-CGA-CBA	2.43	119.53	111.91
33	D	410	LHG	O7-C7-O9	-2.43	117.84	123.70
25	c	526	BCR	C35-C13-C14	-2.43	119.52	122.92
31	a	415[B]	PL9	C30-C29-C31	2.43	119.35	115.27
24	d	402[B]	PHO	C2A-C1A-NA	2.43	114.65	111.86
36	C	501	LMG	C7-O1-C1	-2.43	109.00	113.74
35	b	632	HTG	C1-O5-C5	2.42	117.05	112.58
25	c	518	BCR	C37-C22-C23	2.42	121.89	118.08
23	A	405	CLA	O2A-CGA-O1A	-2.42	117.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C38-C26-C25	-2.42	121.81	124.53
24	d	402[B]	PHO	O2D-CGD-O1D	-2.42	119.10	123.84
23	C	505	CLA	CAA-C2A-C3A	-2.42	106.15	112.78
23	c	506	CLA	O2A-C1-C2	2.42	114.99	108.64
31	D	408[A]	PL9	C12-C13-C14	-2.42	121.84	127.66
28	m	102	LMT	C1'-O5'-C5'	2.42	118.43	113.69
23	A	408	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
23	b	616	CLA	OBD-CAD-C3D	-2.42	123.97	127.98
23	B	604	CLA	C1-O2A-CGA	2.42	122.78	116.44
26	A	413	SQD	O6-C44-C45	-2.42	105.07	110.90
31	A	417[B]	PL9	C40-C39-C41	2.41	119.33	115.27
23	c	514	CLA	CBC-CAC-C3C	-2.41	105.78	112.43
25	y	101	BCR	C24-C23-C22	-2.41	122.59	126.23
26	A	413	SQD	O48-C23-O10	-2.41	117.50	123.59
33	D	412	LHG	O8-C23-O10	-2.41	117.50	123.59
28	A	414	LMT	C4B-C3B-C2B	-2.41	106.61	110.82
23	b	618	CLA	O2A-CGA-CBA	2.41	119.47	111.91
23	C	514	CLA	CAC-C3C-C4C	2.41	127.94	124.81
23	B	610	CLA	CMA-C3A-C4A	-2.41	105.30	111.77
31	D	408[A]	PL9	C15-C14-C16	2.41	119.32	115.27
25	c	526	BCR	C28-C27-C26	-2.41	109.78	114.08
26	b	601	SQD	C1-O5-C5	-2.41	108.96	113.69
23	B	607	CLA	CMC-C2C-C1C	2.41	128.70	125.04
23	D	405	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
23	c	507	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
23	b	613	CLA	O2A-CGA-O1A	-2.40	117.52	123.59
23	B	603	CLA	CAC-C3C-C4C	2.40	127.93	124.81
23	c	505	CLA	OBD-CAD-C3D	-2.40	123.99	127.98
25	c	526	BCR	C24-C23-C22	-2.40	122.60	126.23
23	A	408	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	A	404	CLA	CAA-CBA-CGA	-2.40	106.23	113.25
23	D	406	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	b	620	CLA	CHD-C4C-NC	2.40	127.99	124.20
26	A	410	SQD	O47-C7-O49	-2.40	117.90	123.70
24	d	402[B]	PHO	C1C-C2C-C3C	-2.40	103.75	106.51
23	b	624	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
24	D	402[B]	PHO	C3C-C4C-NC	2.40	114.00	110.28
25	t	101	BCR	C12-C13-C14	-2.40	115.26	118.94
23	b	613	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
23	c	506	CLA	CED-O2D-CGD	2.40	121.36	115.94
23	C	510	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
25	Y	101	BCR	C34-C9-C8	2.40	121.85	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	CAA-C2A-C3A	-2.40	106.21	112.78
28	M	104	LMT	O5'-C5'-C4'	2.40	114.81	109.75
23	b	622	CLA	CED-O2D-CGD	2.40	121.36	115.94
23	c	507	CLA	CHC-C1C-C2C	-2.39	120.10	126.72
25	T	103	BCR	C7-C6-C5	-2.39	115.67	121.46
31	A	417[A]	PL9	C10-C9-C11	2.39	119.29	115.27
31	D	408[B]	PL9	C12-C13-C14	-2.39	121.91	127.66
23	B	602	CLA	CAC-C3C-C4C	2.39	127.91	124.81
25	H	101	BCR	C10-C11-C12	-2.39	115.76	123.22
26	b	601	SQD	O7-S-C6	2.39	109.78	106.94
25	y	101	BCR	C21-C20-C19	-2.39	115.77	123.22
26	A	410	SQD	O48-C23-O10	-2.39	117.57	123.59
23	b	622	CLA	C4-C3-C5	2.39	119.28	115.27
37	C	517	DGD	C2G-O2G-C1B	-2.38	111.92	117.79
25	D	407	BCR	C38-C26-C27	2.38	118.20	113.62
25	C	515	BCR	C11-C10-C9	-2.38	123.91	127.31
23	b	625	CLA	C4-C3-C5	2.38	119.28	115.27
23	c	507	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
23	a	409	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
23	B	609	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	C	504	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	B	612	CLA	C4-C3-C5	2.38	119.27	115.27
23	C	504	CLA	C4-C3-C5	2.38	119.27	115.27
23	A	404	CLA	C4-C3-C5	2.38	119.27	115.27
23	d	404	CLA	CMA-C3A-C2A	-2.38	104.23	113.83
24	D	402[B]	PHO	CHD-C1D-C2D	-2.38	119.75	125.73
31	D	408[B]	PL9	C17-C18-C19	-2.38	121.94	127.66
23	c	517	CLA	C4-C3-C5	2.38	119.27	115.27
23	c	517	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	d	402[B]	PHO	O2A-CGA-CBA	2.37	119.36	111.91
31	D	408[A]	PL9	C45-C44-C46	2.37	119.26	115.27
23	A	406	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
31	d	407[B]	PL9	C15-C14-C16	2.37	119.26	115.27
23	C	510	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
24	d	402[A]	PHO	C2C-C1C-NC	2.37	113.37	109.79
23	B	606	CLA	C4-C3-C5	2.37	119.26	115.27
23	D	406	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
25	b	626	BCR	C36-C18-C17	-2.37	119.60	122.92
25	b	628	BCR	C10-C11-C12	-2.37	115.83	123.22
23	c	514	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
25	a	412	BCR	C38-C26-C25	-2.37	121.87	124.53
23	B	607	CLA	CAC-C3C-C4C	2.37	127.88	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CAC-C3C-C4C	2.36	127.88	124.81
23	B	607	CLA	O2A-CGA-CBA	2.36	119.33	111.91
37	c	521	DGD	O1G-C1A-C2A	2.36	119.32	111.91
31	D	408[A]	PL9	C17-C18-C19	-2.36	121.97	127.66
23	b	619	CLA	CMB-C2B-C3B	2.36	129.10	124.68
25	K	103	BCR	C28-C27-C26	-2.36	109.86	114.08
36	c	522	LMG	O6-C5-C4	2.36	113.98	109.69
23	b	618	CLA	CMC-C2C-C1C	2.36	128.63	125.04
23	b	618	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	B	614	CLA	CAC-C3C-C4C	2.36	127.87	124.81
31	a	415[B]	PL9	C45-C44-C46	2.36	119.24	115.27
23	B	609	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
23	a	409	CLA	O2A-CGA-CBA	2.35	119.30	111.91
24	d	402[A]	PHO	C4A-NA-C1A	-2.35	106.24	108.14
31	a	415[A]	PL9	C45-C44-C46	2.35	119.23	115.27
23	b	615	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
25	b	628	BCR	C11-C10-C9	-2.35	123.95	127.31
25	B	620	BCR	C36-C18-C19	2.35	121.78	118.08
37	C	516	DGD	O3G-C3G-C2G	-2.35	105.23	110.90
39	v	206	HEM	CAD-CBD-CGD	2.35	116.61	112.67
24	D	402[A]	PHO	CAC-C3C-C4C	2.35	127.78	125.22
31	d	407[B]	PL9	C12-C13-C14	-2.35	122.01	127.66
23	C	513	CLA	CMB-C2B-C3B	2.35	129.07	124.68
25	A	409	BCR	C38-C26-C25	-2.35	121.89	124.53
25	b	628	BCR	C8-C7-C6	-2.35	120.61	127.20
23	c	511	CLA	O2A-CGA-CBA	2.35	119.27	111.91
23	c	508	CLA	O1D-CGD-CBD	-2.35	119.69	124.48
25	H	101	BCR	C16-C15-C14	-2.35	118.67	123.47
23	C	503	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
23	B	614	CLA	CHD-C4C-NC	2.34	127.90	124.20
23	A	406	CLA	C1-C2-C3	-2.34	121.99	126.04
23	c	516	CLA	C11-C12-C13	-2.34	108.34	115.92
23	b	621	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
23	C	503	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	b	616	CLA	CED-O2D-CGD	2.34	121.23	115.94
26	B	621	SQD	O47-C7-O49	-2.34	118.05	123.70
23	c	512	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	b	623	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
23	d	405	CLA	C1-O2A-CGA	2.34	122.58	116.44
23	b	622	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
23	C	513	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
25	D	407	BCR	C30-C25-C24	2.34	122.39	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	O2A-CGA-CBA	2.33	119.23	111.91
23	b	623	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
23	C	509	CLA	CMB-C2B-C3B	2.33	129.04	124.68
23	B	604	CLA	C4-C3-C5	2.33	119.19	115.27
23	b	612	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
23	C	507	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
31	a	415[B]	PL9	C51-C49-C50	2.33	119.75	114.60
24	d	402[A]	PHO	CBD-CHA-C1A	2.33	131.81	126.40
23	A	404	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
31	D	408[A]	PL9	C35-C34-C36	2.33	119.19	115.27
23	A	404	CLA	CHB-C4A-NA	2.33	127.73	124.51
37	C	517	DGD	C1E-O6E-C5E	-2.33	109.12	113.69
23	a	409	CLA	CAA-CBA-CGA	2.33	120.05	113.25
31	D	408[B]	PL9	C25-C24-C26	2.33	119.19	115.27
23	b	617	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
36	C	501	LMG	O8-C28-C29	2.33	119.21	111.91
23	c	505	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
24	A	407	PHO	C4-C3-C5	2.32	119.18	115.27
23	B	608	CLA	OBD-CAD-C3D	-2.32	124.12	127.98
24	a	410	PHO	O1D-CGD-CBD	-2.32	119.73	124.48
23	c	509	CLA	C1-O2A-CGA	2.32	122.54	116.44
23	b	618	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
23	C	511	CLA	CMB-C2B-C3B	2.32	129.02	124.68
23	c	507	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	c	512	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	A	417[A]	PL9	C40-C39-C41	2.32	119.17	115.27
31	A	417[B]	PL9	C47-C48-C49	-2.32	119.83	127.75
37	d	408	DGD	C1E-O6E-C5E	2.32	118.24	113.69
31	D	408[B]	PL9	C7-C3-C4	2.32	118.76	116.88
23	c	510	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
23	b	625	CLA	CBC-CAC-C3C	-2.31	106.05	112.43
23	a	411	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
25	A	409	BCR	C8-C7-C6	-2.31	120.72	127.20
24	d	402[B]	PHO	CMB-C2B-C1B	2.31	128.62	125.06
31	A	417[B]	PL9	C35-C34-C36	2.31	119.15	115.27
23	C	506	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
23	d	403	CLA	O2A-CGA-CBA	2.31	119.15	111.91
23	c	507	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
23	d	403	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
23	B	606	CLA	C1-C2-C3	-2.30	122.06	126.04
23	d	405	CLA	CGD-CBD-CAD	-2.30	103.28	110.73
23	c	515	CLA	CBC-CAC-C3C	-2.30	106.10	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	407[B]	PL9	C51-C49-C50	2.30	119.67	114.60
28	m	102	LMT	O5B-C5B-C4B	2.30	113.86	109.69
23	c	510	CLA	CAA-C2A-C3A	-2.29	106.50	112.78
23	c	514	CLA	CMB-C2B-C3B	2.29	128.97	124.68
23	d	404	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
23	B	603	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
23	C	513	CLA	CMC-C2C-C1C	2.29	128.53	125.04
31	D	408[B]	PL9	C51-C49-C50	2.29	119.67	114.60
23	b	613	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
25	T	103	BCR	C34-C9-C10	-2.29	119.71	122.92
23	c	512	CLA	CAC-C3C-C4C	2.29	127.78	124.81
23	B	606	CLA	CAC-C3C-C4C	2.29	127.78	124.81
23	B	612	CLA	CMB-C2B-C3B	2.29	128.96	124.68
31	D	408[A]	PL9	C32-C33-C34	-2.29	122.15	127.66
23	A	408	CLA	CMA-C3A-C2A	-2.28	104.62	113.83
23	c	510	CLA	C4-C3-C5	2.28	119.11	115.27
26	A	410	SQD	C1-C2-C3	-2.28	105.24	110.00
31	d	407[A]	PL9	C45-C44-C46	2.28	119.11	115.27
23	c	506	CLA	C4-C3-C5	2.28	119.11	115.27
24	d	402[B]	PHO	CBD-CHA-C1A	2.28	131.69	126.40
36	d	416	LMG	O6-C5-C4	2.28	113.83	109.69
23	c	510	CLA	CMB-C2B-C3B	2.28	128.94	124.68
28	F	101	LMT	O5'-C5'-C4'	2.28	114.56	109.75
23	B	602	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	h	101	BCR	C31-C1-C6	-2.28	106.61	110.30
36	M	101	LMG	O8-C28-O10	-2.28	117.85	123.59
23	c	509	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
23	c	510	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	b	619	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
25	t	101	BCR	C15-C14-C13	2.27	130.55	127.31
23	c	511	CLA	C1-C2-C3	-2.27	122.11	126.04
23	A	404	CLA	CMA-C3A-C4A	-2.27	105.67	111.77
26	F	104	SQD	O7-S-C6	2.27	109.64	106.94
23	B	611	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
25	b	627	BCR	C3-C4-C5	-2.27	110.03	114.08
36	a	414	LMG	O7-C10-O9	-2.27	118.22	123.70
37	C	516	DGD	C2G-O2G-C1B	-2.27	112.21	117.79
23	b	616	CLA	CMA-C3A-C2A	-2.27	104.68	113.83
23	d	405	CLA	CMB-C2B-C3B	2.26	128.91	124.68
25	t	101	BCR	C7-C8-C9	-2.26	122.81	126.23
23	b	610	CLA	CAC-C3C-C4C	2.26	127.75	124.81
23	a	409	CLA	CAC-C3C-C4C	2.26	127.74	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	516	CLA	C11-C10-C8	-2.26	108.61	115.92
31	D	408[A]	PL9	C51-C49-C50	2.26	119.59	114.60
23	B	612	CLA	C4D-C3D-CAD	-2.26	107.21	108.47
23	B	610	CLA	CMC-C2C-C1C	2.26	128.48	125.04
23	c	517	CLA	CMB-C2B-C3B	2.26	128.90	124.68
23	C	510	CLA	O2A-CGA-CBA	2.26	118.99	111.91
24	D	402[A]	PHO	C2C-C1C-NC	2.26	113.19	109.79
23	B	606	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
24	D	402[A]	PHO	O2A-CGA-CBA	2.26	118.99	111.91
25	b	626	BCR	C10-C11-C12	-2.25	116.18	123.22
23	c	511	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
31	A	417[B]	PL9	C51-C49-C50	2.25	119.58	114.60
23	b	621	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	d	404	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
23	a	411	CLA	CAC-C3C-C4C	2.25	127.73	124.81
26	b	601	SQD	O47-C7-O49	-2.25	118.26	123.70
23	b	623	CLA	CMC-C2C-C1C	2.25	128.47	125.04
23	c	510	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	B	614	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	A	406	CLA	O2A-CGA-CBA	2.25	118.96	111.91
36	D	416	LMG	O8-C28-O10	-2.25	117.92	123.59
23	c	505	CLA	CMB-C2B-C3B	2.25	128.88	124.68
28	C	521	LMT	O5'-C5'-C4'	2.25	114.49	109.75
23	b	618	CLA	C1-O2A-CGA	2.25	122.34	116.44
23	b	624	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	d	406	BCR	C38-C26-C27	2.25	117.93	113.62
23	C	511	CLA	CED-O2D-CGD	2.25	121.02	115.94
25	c	526	BCR	C8-C7-C6	-2.24	120.90	127.20
23	B	616	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
25	t	101	BCR	C33-C5-C4	2.24	117.93	113.62
35	b	608	HTG	O5-C1-C2	2.24	113.14	110.31
23	C	513	CLA	C4-C3-C5	2.24	119.04	115.27
25	A	409	BCR	C15-C14-C13	-2.24	124.11	127.31
23	C	511	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
23	a	408	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	C	507	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
25	T	103	BCR	C37-C22-C23	2.24	121.61	118.08
23	C	513	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	c	507	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
23	b	624	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	c	511	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
23	B	617	CLA	CAA-C2A-C3A	-2.24	106.65	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	C4D-C3D-CAD	-2.24	107.22	108.47
23	A	408	CLA	CED-O2D-CGD	2.23	120.99	115.94
23	C	514	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
23	b	620	CLA	CMC-C2C-C1C	2.23	128.44	125.04
23	c	508	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
31	A	417[A]	PL9	C8-C7-C3	2.23	118.28	111.98
23	b	621	CLA	CED-O2D-CGD	2.23	120.98	115.94
23	c	507	CLA	CMB-C2B-C3B	2.23	128.85	124.68
23	d	404	CLA	O2A-C1-C2	2.23	114.50	108.64
24	d	402[B]	PHO	CHD-C1D-C2D	-2.23	120.12	125.73
23	b	611	CLA	C1-O2A-CGA	2.23	122.29	116.44
23	B	617	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
25	b	627	BCR	C37-C22-C23	2.23	121.59	118.08
24	d	402[B]	PHO	C2C-C1C-NC	2.23	113.15	109.79
31	D	408[B]	PL9	C22-C23-C24	-2.23	122.30	127.66
28	a	404	LMT	O1'-C1'-C2'	2.23	111.78	108.30
23	A	405	CLA	CMA-C3A-C2A	-2.23	104.85	113.83
23	b	622	CLA	C11-C10-C8	-2.23	108.72	115.92
25	K	103	BCR	C38-C26-C25	-2.22	122.03	124.53
23	B	603	CLA	C1-C2-C3	-2.22	122.20	126.04
25	K	101	BCR	C11-C10-C9	-2.22	124.14	127.31
23	C	506	CLA	C1-C2-C3	-2.22	122.20	126.04
35	b	602	HTG	C1-O5-C5	2.22	116.68	112.58
24	D	402[B]	PHO	C2C-C1C-NC	2.22	113.15	109.79
31	A	417[B]	PL9	C8-C7-C3	2.22	118.26	111.98
23	A	404	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
36	D	416	LMG	O8-C28-C29	2.22	118.88	111.91
25	B	618	BCR	C34-C9-C10	-2.22	119.81	122.92
23	b	619	CLA	CAA-CBA-CGA	-2.22	106.76	113.25
23	C	511	CLA	C6-C7-C8	-2.22	108.74	115.92
23	B	616	CLA	O2A-CGA-CBA	2.22	118.88	111.91
23	b	615	CLA	C1-O2A-CGA	2.22	122.27	116.44
23	B	602	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
31	D	408[B]	PL9	C20-C19-C21	2.22	119.00	115.27
23	b	624	CLA	O2A-CGA-CBA	2.22	118.87	111.91
23	b	616	CLA	C1-O2A-CGA	2.22	122.26	116.44
23	c	516	CLA	CBA-CAA-C2A	-2.22	107.32	113.86
23	b	615	CLA	CAA-C2A-C3A	-2.22	106.71	112.78
23	B	606	CLA	OBD-CAD-C3D	-2.22	124.30	127.98
24	A	407	PHO	C16-C15-C13	-2.22	108.76	115.92
23	c	515	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	c	517	CLA	CBC-CAC-C3C	-2.21	106.33	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
36	d	416	LMG	C6-C5-C4	-2.21	107.83	113.00
24	A	407	PHO	CBC-CAC-C3C	-2.21	106.34	112.43
23	b	621	CLA	C11-C10-C8	-2.21	108.78	115.92
23	B	603	CLA	C6-C7-C8	-2.21	108.78	115.92
23	b	614	CLA	CMC-C2C-C1C	2.21	128.40	125.04
26	F	104	SQD	C44-O6-C1	-2.21	109.43	113.74
35	B	631	HTG	C6-C5-C4	-2.21	107.83	113.00
25	B	620	BCR	C8-C9-C10	-2.21	115.55	118.94
23	b	611	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
23	A	408	CLA	OBD-CAD-C3D	-2.20	124.32	127.98
24	d	402[A]	PHO	O2A-CGA-CBA	2.20	118.82	111.91
23	B	610	CLA	C4-C3-C5	2.20	118.98	115.27
23	c	508	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	D	402[B]	PHO	O2D-CGD-O1D	-2.20	119.53	123.84
24	D	402[B]	PHO	O2A-CGA-CBA	2.20	118.82	111.91
28	C	521	LMT	O1B-C4'-C3'	2.20	113.14	107.28
23	c	512	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
31	A	417[A]	PL9	C35-C34-C36	2.20	118.97	115.27
23	b	615	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	C	508	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
23	C	507	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
25	k	102	BCR	C38-C26-C25	-2.20	122.06	124.53
23	B	605	CLA	CGD-CBD-CAD	-2.20	103.61	110.73
23	C	512	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
23	B	608	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
23	C	512	CLA	CED-O2D-CGD	2.20	120.91	115.94
23	d	404	CLA	CHD-C4C-NC	2.20	127.67	124.20
24	A	407	PHO	CMB-C2B-C1B	2.20	128.45	125.06
23	C	502	CLA	C4-C3-C5	2.20	118.96	115.27
23	B	609	CLA	CAC-C3C-C4C	2.20	127.66	124.81
23	b	620	CLA	C3D-CAD-CBD	2.19	110.50	107.61
23	B	613	CLA	CMB-C2B-C3B	2.19	128.78	124.68
23	A	404	CLA	CHD-C4C-NC	2.19	127.66	124.20
31	d	407[A]	PL9	C22-C23-C24	-2.19	122.38	127.66
23	b	610	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	C	511	CLA	C4-C3-C2	-2.19	118.06	123.68
25	K	103	BCR	C29-C30-C25	2.19	113.86	110.48
23	b	624	CLA	CMC-C2C-C1C	2.19	128.37	125.04
23	c	510	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
36	d	416	LMG	O8-C28-O10	-2.19	118.07	123.59
23	b	625	CLA	OBD-CAD-C3D	-2.19	124.35	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	627	BCR	C28-C27-C26	-2.19	110.17	114.08
23	d	403	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
23	A	404	CLA	CMC-C2C-C1C	2.19	128.37	125.04
35	b	607	HTG	C6-C5-C4	-2.19	107.89	113.00
23	b	625	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	B	608	CLA	C1-C2-C3	-2.18	122.27	126.04
25	C	515	BCR	C37-C22-C23	2.18	121.52	118.08
23	D	406	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
25	T	103	BCR	C36-C18-C19	2.18	121.52	118.08
25	K	103	BCR	C31-C1-C6	-2.18	106.76	110.30
23	d	405	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	a	410	PHO	CHC-C1C-C2C	-2.18	120.25	125.73
26	f	102	SQD	O8-S-C6	2.18	109.21	105.74
23	b	617	CLA	C4-C3-C5	2.18	118.94	115.27
23	C	514	CLA	CMB-C2B-C3B	2.18	128.75	124.68
23	C	509	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
23	b	619	CLA	CMA-C3A-C4A	-2.17	105.93	111.77
23	c	512	CLA	CMB-C2B-C3B	2.17	128.74	124.68
23	a	411	CLA	OBD-CAD-C3D	-2.17	124.38	127.98
25	Y	101	BCR	C28-C27-C26	-2.17	110.20	114.08
25	k	102	BCR	C36-C18-C19	2.17	121.50	118.08
37	H	102	DGD	O1G-C1A-O1A	-2.17	118.11	123.59
35	V	206	HTG	O5-C1-C2	-2.17	107.58	110.31
23	a	409	CLA	CMA-C3A-C2A	-2.17	105.08	113.83
25	h	101	BCR	C16-C15-C14	-2.17	119.03	123.47
25	Y	101	BCR	C21-C20-C19	-2.17	116.45	123.22
26	b	601	SQD	O6-C44-C45	2.17	116.12	110.90
25	B	620	BCR	C3-C4-C5	-2.17	110.21	114.08
23	b	622	CLA	CMB-C2B-C3B	2.17	128.73	124.68
23	A	404	CLA	OBD-CAD-C3D	-2.16	124.39	127.98
23	b	622	CLA	CHB-C4A-NA	2.16	127.50	124.51
36	c	522	LMG	O8-C28-O10	-2.16	118.13	123.59
23	C	502	CLA	O2A-CGA-CBA	2.16	118.69	111.91
23	C	509	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	A	407	PHO	C4A-NA-C1A	-2.16	106.39	108.14
36	k	101	LMG	C8-O7-C10	-2.16	112.47	117.79
25	d	406	BCR	C37-C22-C21	-2.16	119.90	122.92
39	e	101	HEM	CMC-C2C-C3C	2.16	128.72	124.68
23	B	616	CLA	C1-O2A-CGA	2.16	122.10	116.44
35	d	414	HTG	O5-C1-C2	2.16	113.03	110.31
23	C	514	CLA	CMC-C2C-C1C	2.15	128.32	125.04
23	C	508	CLA	C3B-C4B-NB	2.15	112.00	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
25	d	406	BCR	C21-C20-C19	-2.15	116.50	123.22
23	B	612	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	a	410	PHO	CAA-CBA-CGA	-2.15	106.97	113.25
23	b	615	CLA	C1-C2-C3	-2.15	122.32	126.04
24	a	410	PHO	C2A-C1A-NA	2.15	114.33	111.86
23	C	513	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	c	511	CLA	OBD-CAD-C3D	-2.15	124.42	127.98
23	c	505	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
23	B	605	CLA	CBC-CAC-C3C	-2.14	106.52	112.43
23	c	517	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
31	d	407[A]	PL9	C25-C24-C26	2.14	118.87	115.27
23	C	509	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
37	C	518	DGD	O3G-C3G-C2G	-2.14	105.73	110.90
25	y	101	BCR	C8-C7-C6	-2.14	121.19	127.20
23	B	608	CLA	O2A-CGA-CBA	2.14	118.62	111.91
23	b	612	CLA	CMB-C2B-C3B	2.14	128.68	124.68
28	B	634	LMT	C1'-O5'-C5'	2.14	117.88	113.69
24	d	402[B]	PHO	C3A-C4A-CHB	-2.14	118.14	121.83
23	d	405	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	d	406	BCR	C3-C4-C5	-2.13	110.27	114.08
23	c	506	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
36	C	501	LMG	C8-O7-C10	-2.13	112.54	117.79
23	B	615	CLA	CAA-C2A-C3A	-2.13	106.94	112.78
37	c	520	DGD	O1G-C1A-C2A	2.13	118.60	111.91
23	b	617	CLA	C11-C10-C8	-2.13	109.03	115.92
33	L	101	LHG	O4-P-O5	2.13	122.78	112.24
36	z	101	LMG	C7-O1-C1	-2.13	109.58	113.74
23	B	604	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
26	A	413	SQD	O8-S-C6	2.13	109.13	105.74
23	c	506	CLA	C3D-CAD-CBD	2.13	110.41	107.61
23	B	614	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
23	c	513	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
23	B	616	CLA	C1-C2-C3	-2.13	122.37	126.04
23	C	507	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
24	A	407	PHO	O1D-CGD-CBD	-2.12	120.14	124.48
23	B	616	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	C	507	CLA	O2A-CGA-CBA	2.12	118.57	111.91
23	b	617	CLA	CAC-C3C-C4C	2.12	127.56	124.81
35	C	522	HTG	C4-C3-C2	-2.12	107.12	110.82
35	b	607	HTG	C1-O5-C5	2.12	116.49	112.58
23	C	508	CLA	OBD-CAD-C3D	-2.12	124.46	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	OBD-CAD-C3D	-2.12	124.46	127.98
25	b	628	BCR	C37-C22-C23	2.12	121.42	118.08
24	D	402[A]	PHO	CBD-CHA-C1A	2.12	131.31	126.40
23	B	607	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
36	k	101	LMG	O8-C28-O10	-2.12	118.25	123.59
31	A	417[A]	PL9	C51-C49-C50	2.11	119.27	114.60
23	c	508	CLA	C1-O2A-CGA	2.11	121.99	116.44
23	B	602	CLA	C4-C3-C5	2.11	118.83	115.27
23	B	616	CLA	C4-C3-C5	2.11	118.83	115.27
31	a	415[A]	PL9	C12-C13-C14	-2.11	122.58	127.66
31	d	407[B]	PL9	C7-C3-C4	2.11	118.59	116.88
23	b	624	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
37	D	409	DGD	O6D-C1D-C2D	2.11	114.81	110.35
23	b	622	CLA	CHD-C4C-NC	2.11	127.53	124.20
37	c	521	DGD	O2G-C1B-O1B	-2.11	118.61	123.70
35	V	206	HTG	O5-C5-C4	2.11	113.52	109.69
23	D	406	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	b	618	CLA	C1-C2-C3	-2.11	122.40	126.04
23	C	503	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
23	d	403	CLA	CHB-C4A-NA	2.11	127.42	124.51
24	a	410	PHO	CED-O2D-CGD	2.11	120.70	115.94
23	B	609	CLA	C2A-C1A-CHA	-2.11	120.18	123.86
31	a	415[B]	PL9	C12-C13-C14	-2.10	122.59	127.66
23	B	609	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
24	d	402[A]	PHO	C1C-C2C-C3C	-2.10	104.09	106.51
25	b	626	BCR	C33-C5-C4	2.10	117.66	113.62
23	B	610	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
25	B	620	BCR	C2-C3-C4	-2.10	106.68	111.38
28	M	102	LMT	O5'-C1'-O1'	-2.10	105.00	109.97
23	C	509	CLA	CAC-C3C-C2C	2.10	131.12	127.53
23	A	406	CLA	CHB-C4A-NA	2.10	127.42	124.51
35	B	623	HTG	C1-O5-C5	2.10	116.45	112.58
25	k	102	BCR	C15-C14-C13	-2.10	124.31	127.31
23	C	512	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
23	D	405	CLA	CAC-C3C-C4C	2.10	127.53	124.81
23	b	616	CLA	CGD-CBD-CAD	-2.10	103.94	110.73
23	c	506	CLA	CMC-C2C-C1C	2.10	128.23	125.04
36	a	414	LMG	O8-C28-O10	-2.10	118.30	123.59
23	B	608	CLA	CHD-C4C-NC	2.10	127.51	124.20
25	c	518	BCR	C15-C16-C17	-2.09	119.18	123.47
23	b	619	CLA	C4-C3-C5	2.09	118.79	115.27
23	b	618	CLA	CAC-C3C-C4C	2.09	127.53	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	407[B]	PL9	C36-C37-C38	-2.09	105.00	111.88
23	c	515	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	610	CLA	C7-C6-C5	-2.09	107.67	113.36
23	b	622	CLA	CHA-C1A-NA	-2.09	121.61	126.40
25	K	101	BCR	C3-C4-C5	-2.09	110.34	114.08
24	D	402[B]	PHO	CAC-C3C-C4C	2.09	127.50	125.22
23	c	509	CLA	CHD-C4C-NC	2.09	127.49	124.20
23	B	610	CLA	C1-O2A-CGA	2.09	121.92	116.44
23	b	622	CLA	C4D-C3D-CAD	-2.09	107.31	108.47
23	B	617	CLA	C4D-C3D-CAD	-2.09	107.31	108.47
23	B	602	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
23	C	505	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
25	y	101	BCR	C40-C30-C25	-2.08	106.92	110.30
23	B	609	CLA	C4-C3-C5	2.08	118.78	115.27
23	C	503	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
23	a	411	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
37	d	408	DGD	O2G-C1B-O1B	-2.08	118.67	123.70
23	B	603	CLA	CMC-C2C-C1C	2.08	128.21	125.04
23	B	614	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
33	L	101	LHG	O7-C7-O9	-2.08	118.68	123.70
36	C	501	LMG	O7-C10-O9	-2.08	118.68	123.70
23	c	516	CLA	CHA-C1A-NA	-2.08	121.64	126.40
23	A	408	CLA	CBC-CAC-C3C	-2.08	106.70	112.43
23	c	508	CLA	O2A-CGA-CBA	2.08	118.43	111.91
23	c	508	CLA	C11-C10-C8	-2.08	109.21	115.92
35	B	622	HTG	O5-C5-C6	2.08	111.60	106.44
24	A	407	PHO	CHD-C1D-C2D	-2.07	120.51	125.73
23	C	509	CLA	CHB-C4A-NA	2.07	127.38	124.51
23	A	406	CLA	CMB-C2B-C1B	2.07	131.65	128.46
25	b	626	BCR	C3-C4-C5	-2.07	110.38	114.08
23	B	605	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
23	a	408	CLA	CHD-C4C-NC	2.07	127.47	124.20
23	B	615	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	B	603	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	b	614	CLA	CAC-C3C-C2C	2.07	131.07	127.53
23	C	514	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
31	d	407[B]	PL9	C47-C48-C49	-2.07	120.68	127.75
23	b	613	CLA	C6-C7-C8	-2.07	109.24	115.92
23	D	406	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
37	c	519	DGD	C3G-C2G-C1G	-2.07	106.90	111.79
23	b	620	CLA	CMB-C2B-C3B	2.07	128.54	124.68
24	A	407	PHO	C3A-C2A-C1A	-2.07	99.18	101.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	M	102	LMT	O6'-C6'-C5'	-2.07	104.20	111.29
35	B	623	HTG	C1-C2-C3	2.07	114.67	110.59
36	C	519	LMG	O8-C28-O10	-2.06	118.38	123.59
25	Y	101	BCR	C8-C7-C6	-2.06	121.41	127.20
23	B	616	CLA	CHA-C1A-NA	-2.06	121.67	126.40
23	C	505	CLA	C11-C10-C8	-2.06	109.25	115.92
23	b	610	CLA	CMC-C2C-C1C	2.06	128.18	125.04
25	b	626	BCR	C39-C30-C25	-2.06	106.96	110.30
23	c	509	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
23	B	603	CLA	C3D-CAD-CBD	2.06	110.32	107.61
23	b	620	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
23	b	618	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
31	D	408[B]	PL9	C7-C3-C2	-2.06	120.59	123.30
23	B	608	CLA	CMB-C2B-C3B	2.06	128.53	124.68
23	b	617	CLA	CHB-C4A-NA	2.06	127.36	124.51
31	d	407[A]	PL9	C35-C34-C36	2.06	118.73	115.27
23	c	509	CLA	O2A-CGA-CBA	2.06	118.36	111.91
23	a	408	CLA	CMC-C2C-C1C	2.06	128.17	125.04
23	b	615	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
33	A	419	LHG	O8-C23-O10	-2.05	118.41	123.59
31	D	408[A]	PL9	C7-C3-C4	2.05	118.55	116.88
25	b	626	BCR	C38-C26-C25	-2.05	122.22	124.53
25	y	101	BCR	C38-C26-C25	-2.05	122.22	124.53
35	c	524	HTG	O5-C5-C4	2.05	113.42	109.69
26	A	410	SQD	C44-O6-C1	-2.05	109.73	113.74
23	B	603	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
23	C	510	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	B	615	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
23	c	508	CLA	CED-O2D-CGD	2.05	120.58	115.94
26	f	102	SQD	O48-C23-O10	-2.05	118.42	123.59
37	C	516	DGD	C3G-C2G-C1G	-2.05	106.94	111.79
23	b	621	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	D	405	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	b	616	CLA	O2A-CGA-CBA	2.05	118.33	111.91
25	D	407	BCR	C3-C4-C5	-2.04	110.43	114.08
36	C	520	LMG	O6-C5-C4	2.04	113.41	109.69
23	c	512	CLA	OBD-CAD-C3D	-2.04	124.59	127.98
23	c	509	CLA	CED-O2D-CGD	2.04	120.56	115.94
26	b	601	SQD	O48-C23-O10	-2.04	118.44	123.59
24	d	402[A]	PHO	C3A-C4A-CHB	-2.04	118.30	121.83
24	D	402[B]	PHO	C6-C5-C3	-2.04	108.10	113.45
23	A	404	CLA	CED-O2D-CGD	2.04	120.55	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	621	SQD	O8-S-C6	2.04	108.99	105.74
23	B	612	CLA	O2A-CGA-CBA	2.04	118.31	111.91
25	D	407	BCR	C2-C3-C4	-2.04	106.82	111.38
23	C	510	CLA	C11-C12-C13	-2.04	109.33	115.92
23	c	509	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
23	d	403	CLA	C4-C3-C5	2.04	118.70	115.27
23	C	502	CLA	C1-O2A-CGA	2.04	121.78	116.44
36	C	519	LMG	O7-C10-O9	-2.04	118.78	123.70
25	B	619	BCR	C33-C5-C4	2.04	117.53	113.62
26	a	413	SQD	O48-C23-O10	-2.03	118.46	123.59
37	C	518	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
37	C	517	DGD	O2G-C1B-O1B	-2.03	118.79	123.70
25	A	409	BCR	C31-C1-C6	-2.03	107.00	110.30
23	b	613	CLA	CHA-C1A-NA	-2.03	121.75	126.40
25	h	101	BCR	C2-C3-C4	-2.03	106.84	111.38
37	c	519	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
31	a	415[B]	PL9	C10-C9-C8	-2.03	118.47	123.68
25	B	618	BCR	C15-C14-C13	-2.03	124.41	127.31
23	a	409	CLA	CHC-C1C-NC	2.03	127.28	124.20
23	B	604	CLA	OBD-CAD-C3D	-2.03	124.61	127.98
37	C	517	DGD	C3G-O3G-C1D	-2.03	109.78	113.74
23	B	617	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	C	511	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
23	C	512	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
23	b	611	CLA	O2A-CGA-CBA	2.02	118.26	111.91
23	B	611	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
23	c	517	CLA	C6-C7-C8	-2.02	109.38	115.92
23	D	405	CLA	CMB-C2B-C3B	2.02	128.47	124.68
33	A	419	LHG	C5-O7-C7	-2.02	112.81	117.79
23	C	503	CLA	OBD-CAD-C3D	-2.02	124.62	127.98
25	c	518	BCR	C23-C24-C25	-2.02	121.52	127.20
23	b	612	CLA	C7-C6-C5	-2.02	107.87	113.36
23	C	512	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
33	d	410	LHG	C6-C5-C4	-2.02	107.01	111.79
23	b	621	CLA	CMB-C2B-C3B	2.02	128.46	124.68
31	D	408[A]	PL9	C30-C29-C31	2.02	118.67	115.27
28	A	414	LMT	C6'-C5'-C4'	-2.02	107.45	113.33
23	b	615	CLA	CAC-C3C-C4C	2.02	127.43	124.81
23	C	513	CLA	CBC-CAC-C3C	-2.02	106.87	112.43
23	b	618	CLA	CAA-C2A-C3A	-2.01	107.26	112.78
25	y	101	BCR	C35-C13-C14	-2.01	120.10	122.92
23	C	512	CLA	O2A-CGA-O1A	-2.01	118.51	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	413	SQD	O5-C1-C2	-2.01	106.09	110.35
37	H	102	DGD	C3B-C2B-C1B	-2.01	106.30	113.62
37	c	519	DGD	O1G-C1A-C2A	2.01	118.22	111.91
25	c	518	BCR	C33-C5-C6	-2.01	122.27	124.53
23	c	505	CLA	C4-C3-C5	2.01	118.66	115.27
26	B	621	SQD	O48-C23-O10	-2.01	118.52	123.59
23	C	509	CLA	C4-C3-C5	2.01	118.65	115.27
31	D	408[A]	PL9	C7-C3-C2	-2.01	120.66	123.30
25	A	409	BCR	C24-C23-C22	-2.01	123.20	126.23
25	Y	101	BCR	C33-C5-C4	2.01	117.47	113.62
23	B	603	CLA	CHA-C1A-NA	-2.00	121.81	126.40
25	B	620	BCR	C15-C16-C17	-2.00	119.37	123.47
25	b	626	BCR	C36-C18-C19	2.00	121.23	118.08
23	C	504	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	c	517	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	c	508	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	b	625	CLA	C11-C10-C8	-2.00	109.45	115.92
31	d	407[A]	PL9	C30-C29-C31	2.00	118.64	115.27
23	B	613	CLA	OBD-CAD-C3D	-2.00	124.66	127.98

All (190) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	D	406	CLA	NC
23	D	406	CLA	ND
23	D	406	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	513	CLA	NA
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	a	408	CLA	NC
23	a	408	CLA	ND
23	a	408	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	c	517	CLA	NC
23	c	517	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	D	405	CLA	ND
23	B	616	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	b	621	CLA	NC
23	b	621	CLA	ND
23	b	621	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	612	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	c	514	CLA	NC
23	c	514	CLA	ND
23	c	514	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	c	515	CLA	NC
23	c	515	CLA	ND
23	c	515	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	c	516	CLA	NC
23	c	516	CLA	ND
23	c	516	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	c	509	CLA	ND
23	c	509	CLA	NA
23	a	411	CLA	NC
23	a	411	CLA	ND
23	a	411	CLA	NA
23	a	409	CLA	NC
23	a	409	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	512	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	b	624	CLA	NA
23	b	624	CLA	NC
23	b	624	CLA	ND
23	B	609	CLA	NC
23	B	609	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	b	618	CLA	NC
23	b	618	CLA	ND
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	b	622	CLA	NC
23	b	622	CLA	ND
23	b	622	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	NA
23	d	405	CLA	NC
23	d	405	CLA	ND
23	d	405	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	620	CLA	NC

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Mol	Chain	Res	Type	Atom
23	b	620	CLA	ND
23	b	620	CLA	NA
23	b	623	CLA	NC
23	b	623	CLA	ND
23	b	623	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	B	617	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	A	406	CLA	NC
23	A	406	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	C	512	CLA	NC
23	C	512	CLA	NA
23	C	506	CLA	ND
23	C	514	CLA	NC
23	C	514	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	b	625	CLA	NC
23	b	625	CLA	ND
23	b	625	CLA	NA
23	d	404	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA

All (1351) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	V	206	HTG	C2-C1-S1-C1'
35	V	206	HTG	O5-C1-S1-C1'
35	V	206	HTG	C2'-C1'-S1-C1
33	L	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	d	410	LHG	C3-O3-P-O6
28	T	104	LMT	C2'-C1'-O1'-C1
28	T	104	LMT	O5'-C1'-O1'-C1
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
26	f	102	SQD	C5-C6-S-O7
26	f	102	SQD	C5-C6-S-O8
26	f	102	SQD	C5-C6-S-O9
27	a	402	GOL	O1-C1-C2-C3
28	M	104	LMT	O5'-C1'-O1'-C1
23	c	513	CLA	C2-C1-O2A-CGA
27	b	606	GOL	O1-C1-C2-O2
27	b	606	GOL	O1-C1-C2-C3
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C21-C22-C23-C24
25	Y	101	BCR	C37-C22-C23-C24
27	a	401	GOL	C1-C2-C3-O3
27	a	401	GOL	O2-C2-C3-O3
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
23	B	615	CLA	C2-C3-C5-C6
25	d	406	BCR	C21-C22-C23-C24
25	d	406	BCR	C37-C22-C23-C24
27	B	627	GOL	O1-C1-C2-C3
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	v	202	GOL	O1-C1-C2-C3
33	D	410	LHG	C4-O6-P-O5
28	C	521	LMT	C2'-C1'-O1'-C1
28	C	521	LMT	O5'-C1'-O1'-C1
23	D	405	CLA	C12-C13-C15-C16
37	D	409	DGD	C2B-C1B-O2G-C2G
37	D	409	DGD	O1B-C1B-O2G-C2G
37	D	409	DGD	C2D-C1D-O3G-C3G
37	D	409	DGD	O6D-C1D-O3G-C3G
27	B	629	GOL	O1-C1-C2-C3
25	C	515	BCR	C1-C6-C7-C8
25	C	515	BCR	C7-C8-C9-C10
25	C	515	BCR	C7-C8-C9-C34
35	B	623	HTG	C2'-C1'-S1-C1
27	A	412	GOL	C1-C2-C3-O3
28	A	414	LMT	C2'-C1'-O1'-C1
28	A	414	LMT	O5'-C1'-O1'-C1
27	D	403	GOL	C1-C2-C3-O3
27	v	201	GOL	O1-C1-C2-C3
23	C	510	CLA	C2-C1-O2A-CGA
33	A	419	LHG	C4-O6-P-O5
26	F	104	SQD	O49-C7-O47-C45
26	F	104	SQD	C5-C6-S-O7
26	F	104	SQD	C5-C6-S-O8
26	F	104	SQD	C5-C6-S-O9
36	z	101	LMG	O9-C10-O7-C8
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
36	C	520	LMG	O9-C10-O7-C8
28	e	102	LMT	C2'-C1'-O1'-C1
28	e	102	LMT	O5'-C1'-O1'-C1
25	D	407	BCR	C7-C8-C9-C10
25	D	407	BCR	C7-C8-C9-C34
25	D	407	BCR	C21-C22-C23-C24
25	D	407	BCR	C37-C22-C23-C24
25	D	407	BCR	C23-C24-C25-C30
23	c	512	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O2D
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
26	b	601	SQD	O49-C7-O47-C45
28	F	101	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
28	F	101	LMT	O5'-C1'-O1'-C1
33	a	419	LHG	O1-C1-C2-C3
33	a	419	LHG	C4-O6-P-O3
33	a	419	LHG	C4-O6-P-O5
33	a	419	LHG	O10-C23-O8-C6
33	a	419	LHG	C24-C23-O8-C6
27	T	102	GOL	O1-C1-C2-O2
27	T	102	GOL	O1-C1-C2-C3
36	C	501	LMG	C11-C10-O7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
37	d	408	DGD	C2B-C1B-O2G-C2G
37	d	408	DGD	O1B-C1B-O2G-C2G
37	d	408	DGD	O6E-C1E-O5D-C6D
23	B	606	CLA	C2-C3-C5-C6
23	B	606	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
28	a	418	LMT	C2'-C1'-O1'-C1
28	a	418	LMT	O5'-C1'-O1'-C1
36	Z	101	LMG	O6-C1-O1-C7
36	Z	101	LMG	O9-C10-O7-C8
36	Z	101	LMG	C11-C10-O7-C8
35	c	523	HTG	C2'-C1'-S1-C1
27	v	203	GOL	O1-C1-C2-C3
28	b	630	LMT	C2'-C1'-O1'-C1
28	b	630	LMT	O5'-C1'-O1'-C1
23	b	623	CLA	CHA-CBD-CGD-O1D
23	b	623	CLA	CHA-CBD-CGD-O2D
23	b	623	CLA	CAD-CBD-CGD-O1D
23	b	623	CLA	C2-C3-C5-C6
23	b	623	CLA	C4-C3-C5-C6
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	C14-C13-C15-C16
23	C	508	CLA	CHA-CBD-CGD-O2D
28	a	404	LMT	C2'-C1'-O1'-C1
28	a	404	LMT	O5'-C1'-O1'-C1
28	B	634	LMT	C2'-C1'-O1'-C1
28	B	634	LMT	O5'-C1'-O1'-C1
27	V	201	GOL	O1-C1-C2-C3
27	V	201	GOL	C1-C2-C3-O3
23	c	510	CLA	C1A-C2A-CAA-CBA
23	c	510	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	a	415[A]	PL9	C12-C11-C9-C10
31	a	415[A]	PL9	C18-C19-C21-C22
31	a	415[A]	PL9	C20-C19-C21-C22
26	A	413	SQD	O6-C44-C45-O47
26	A	413	SQD	O5-C5-C6-S
27	f	101	GOL	O1-C1-C2-C3
33	b	634	LHG	O1-C1-C2-C3
33	b	634	LHG	C4-O6-P-O4
26	B	636	SQD	O6-C44-C45-O47
26	B	636	SQD	O5-C5-C6-S
26	B	636	SQD	C5-C6-S-O7
26	B	636	SQD	C5-C6-S-O8
27	b	605	GOL	O1-C1-C2-C3
26	B	621	SQD	O5-C1-O6-C44
26	B	621	SQD	O49-C7-O47-C45
26	B	621	SQD	C5-C6-S-O7
26	B	621	SQD	C5-C6-S-O8
26	B	621	SQD	C5-C6-S-O9
35	b	632	HTG	C2'-C1'-S1-C1
33	D	412	LHG	C4-O6-P-O4
27	c	502	GOL	O1-C1-C2-C3
28	C	521	LMT	O5B-C1B-O1B-C4'
28	D	404	LMT	C3'-C4'-O1B-C1B
23	C	510	CLA	CBD-CGD-O2D-CED
33	A	419	LHG	O10-C23-O8-C6
36	C	501	LMG	O9-C10-O7-C8
23	A	408	CLA	C3-C5-C6-C7
23	b	623	CLA	C3-C5-C6-C7
23	B	617	CLA	C3-C5-C6-C7
33	A	419	LHG	C24-C23-O8-C6
26	F	104	SQD	C8-C7-O47-C45
36	z	101	LMG	C11-C10-O7-C8
36	C	520	LMG	C11-C10-O7-C8
26	b	601	SQD	C8-C7-O47-C45
26	B	621	SQD	C8-C7-O47-C45
23	c	508	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
31	a	415[B]	PL9	C12-C11-C9-C10
23	B	607	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C3-C5-C6-C7
23	C	509	CLA	C3-C5-C6-C7
23	c	510	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
28	M	104	LMT	O5'-C5'-C6'-O6'
28	C	521	LMT	O5'-C5'-C6'-O6'
37	H	102	DGD	O6E-C5E-C6E-O5E
36	a	414	LMG	C17-C18-C19-C20
28	m	102	LMT	O5'-C5'-C6'-O6'
36	C	520	LMG	O6-C5-C6-O5
35	B	624	HTG	O5-C5-C6-O6
28	M	102	LMT	O5B-C5B-C6B-O6B
37	C	517	DGD	CBB-CCB-CDB-CEB
31	A	417[A]	PL9	C25-C24-C26-C27
31	A	417[B]	PL9	C25-C24-C26-C27
31	a	415[B]	PL9	C15-C14-C16-C17
31	a	415[B]	PL9	C20-C19-C21-C22
31	a	415[B]	PL9	C25-C24-C26-C27
31	a	415[A]	PL9	C15-C14-C16-C17
31	a	415[A]	PL9	C25-C24-C26-C27
31	A	417[A]	PL9	C23-C24-C26-C27
31	A	417[B]	PL9	C23-C24-C26-C27
23	b	614	CLA	C2-C3-C5-C6
31	a	415[B]	PL9	C13-C14-C16-C17
31	a	415[B]	PL9	C18-C19-C21-C22
31	a	415[B]	PL9	C23-C24-C26-C27
31	a	415[A]	PL9	C13-C14-C16-C17
31	a	415[A]	PL9	C23-C24-C26-C27
37	d	408	DGD	C4E-C5E-C6E-O5E
36	z	101	LMG	O6-C1-O1-C7
26	b	601	SQD	O5-C1-O6-C44
31	d	407[A]	PL9	C39-C41-C42-C43
31	D	408[B]	PL9	C39-C41-C42-C43
35	C	523	HTG	O5-C5-C6-O6
37	d	408	DGD	O6D-C5D-C6D-O5D
33	A	419	LHG	C1-C2-C3-O3
28	e	102	LMT	C4'-C5'-C6'-O6'
23	c	513	CLA	O1A-CGA-O2A-C1
23	a	411	CLA	C3-C5-C6-C7
23	c	513	CLA	CBA-CGA-O2A-C1
23	a	411	CLA	CBA-CGA-O2A-C1
33	D	412	LHG	C24-C23-O8-C6
36	z	101	LMG	O6-C5-C6-O5
23	A	404	CLA	CBD-CGD-O2D-CED
23	c	507	CLA	CBD-CGD-O2D-CED
36	Z	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	C	521	LMT	C5'-C4'-O1B-C1B
23	B	615	CLA	C10-C11-C12-C13
23	B	614	CLA	C15-C16-C17-C18
37	d	408	DGD	C2E-C1E-O5D-C6D
36	Z	101	LMG	C2-C1-O1-C7
33	D	412	LHG	O10-C23-O8-C6
23	c	508	CLA	C2-C3-C5-C6
23	B	603	CLA	C14-C13-C15-C16
23	C	502	CLA	C11-C12-C13-C14
23	B	617	CLA	C6-C7-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	b	615	CLA	C2A-CAA-CBA-CGA
25	C	515	BCR	C37-C22-C23-C24
25	T	103	BCR	C11-C12-C13-C35
35	b	632	HTG	S1-C1'-C2'-C3'
28	M	104	LMT	C4'-C5'-C6'-O6'
36	C	520	LMG	C10-C11-C12-C13
23	a	411	CLA	O1A-CGA-O2A-C1
28	M	105	LMT	O5'-C5'-C6'-O6'
37	H	102	DGD	C4E-C5E-C6E-O5E
23	C	507	CLA	C5-C6-C7-C8
23	A	408	CLA	C13-C15-C16-C17
23	b	624	CLA	C10-C11-C12-C13
23	C	502	CLA	C15-C16-C17-C18
28	C	521	LMT	O5B-C5B-C6B-O6B
37	C	517	DGD	C1A-C2A-C3A-C4A
23	B	615	CLA	C8-C10-C11-C12
23	b	610	CLA	C8-C10-C11-C12
23	B	616	CLA	C8-C10-C11-C12
23	b	612	CLA	C5-C6-C7-C8
27	f	101	GOL	O1-C1-C2-O2
33	A	419	LHG	C23-C24-C25-C26
36	a	414	LMG	C10-C11-C12-C13
36	d	416	LMG	C19-C20-C21-C22
23	C	507	CLA	C13-C15-C16-C17
23	c	513	CLA	C3-C5-C6-C7
37	C	516	DGD	O6D-C5D-C6D-O5D
23	B	617	CLA	C2-C1-O2A-CGA
23	b	623	CLA	C5-C6-C7-C8
37	d	408	DGD	C4D-C5D-C6D-O5D
36	k	101	LMG	C10-C11-C12-C13
26	A	413	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	c	505	CLA	CBD-CGD-O2D-CED
36	b	629	LMG	C30-C31-C32-C33
28	M	102	LMT	C4B-C5B-C6B-O6B
23	B	615	CLA	C5-C6-C7-C8
23	B	616	CLA	C11-C12-C13-C15
23	b	615	CLA	C12-C13-C15-C16
23	b	625	CLA	C11-C12-C13-C15
23	B	602	CLA	C3-C5-C6-C7
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	C10-C11-C12-C13
23	b	615	CLA	C13-C15-C16-C17
28	C	521	LMT	C3'-C4'-O1B-C1B
37	C	517	DGD	O6E-C1E-O5D-C6D
23	C	510	CLA	O1D-CGD-O2D-CED
31	d	407[B]	PL9	C39-C41-C42-C43
31	a	415[B]	PL9	C9-C11-C12-C13
31	a	415[B]	PL9	C14-C16-C17-C18
31	a	415[A]	PL9	C9-C11-C12-C13
28	T	104	LMT	O1'-C1-C2-C3
33	A	419	LHG	O2-C2-C3-O3
23	a	411	CLA	C15-C16-C17-C18
36	C	520	LMG	C4-C5-C6-O5
23	C	509	CLA	C10-C11-C12-C13
23	b	613	CLA	C13-C15-C16-C17
37	c	519	DGD	O6D-C5D-C6D-O5D
37	c	520	DGD	C3B-C4B-C5B-C6B
23	B	607	CLA	C10-C11-C12-C13
23	A	408	CLA	C8-C10-C11-C12
23	B	617	CLA	C10-C11-C12-C13
33	D	411	LHG	C3-O3-P-O6
33	D	410	LHG	C3-O3-P-O6
33	D	410	LHG	C4-O6-P-O3
33	A	419	LHG	C3-O3-P-O6
33	a	419	LHG	C3-O3-P-O6
33	b	634	LHG	C4-O6-P-O3
23	A	408	CLA	C10-C11-C12-C13
35	c	523	HTG	S1-C1'-C2'-C3'
37	C	516	DGD	C4D-C5D-C6D-O5D
23	b	612	CLA	C4-C3-C5-C6
35	B	624	HTG	C4-C5-C6-O6
36	k	101	LMG	C11-C10-O7-C8
26	A	410	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	k	101	LMG	C34-C35-C36-C37
37	H	102	DGD	C7A-C8A-C9A-CAA
36	M	101	LMG	C29-C30-C31-C32
36	C	501	LMG	C13-C14-C15-C16
37	d	408	DGD	C5A-C6A-C7A-C8A
28	B	634	LMT	C11-C10-C9-C8
37	C	517	DGD	C9A-CAA-CBA-CCA
37	C	517	DGD	C4B-C5B-C6B-C7B
36	C	519	LMG	C11-C12-C13-C14
36	C	519	LMG	C12-C13-C14-C15
33	a	419	LHG	C24-C25-C26-C27
36	C	501	LMG	C30-C31-C32-C33
37	d	408	DGD	C8B-C9B-CAB-CBB
37	C	516	DGD	C4B-C5B-C6B-C7B
37	c	519	DGD	C7B-C8B-C9B-CAB
26	a	413	SQD	C11-C12-C13-C14
37	C	517	DGD	CAB-CBB-CCB-CDB
36	k	101	LMG	O9-C10-O7-C8
28	T	104	LMT	C11-C10-C9-C8
36	d	416	LMG	C16-C17-C18-C19
35	B	623	HTG	C2'-C3'-C4'-C5'
37	C	518	DGD	CAA-CBA-CCA-CDA
36	C	501	LMG	C39-C40-C41-C42
37	d	408	DGD	C2A-C3A-C4A-C5A
37	c	520	DGD	C9A-CAA-CBA-CCA
37	c	519	DGD	C8A-C9A-CAA-CBA
33	d	409	LHG	C25-C26-C27-C28
23	B	604	CLA	C5-C6-C7-C8
33	D	411	LHG	O2-C2-C3-O3
26	b	601	SQD	C12-C13-C14-C15
28	M	104	LMT	C2'-C1'-O1'-C1
36	C	501	LMG	C2-C1-O1-C7
37	c	520	DGD	C2E-C1E-O5D-C6D
37	C	517	DGD	C2E-C1E-O5D-C6D
26	a	413	SQD	C15-C16-C17-C18
23	a	411	CLA	C16-C17-C18-C19
23	C	511	CLA	C4-C3-C5-C6
31	D	408[B]	PL9	C15-C14-C16-C17
24	A	407	PHO	C4-C3-C5-C6
36	M	101	LMG	C34-C35-C36-C37
36	a	414	LMG	C14-C15-C16-C17
35	B	631	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
33	b	634	LHG	C27-C28-C29-C30
31	d	407[A]	PL9	C13-C14-C16-C17
23	C	507	CLA	C6-C7-C8-C9
23	c	513	CLA	C11-C10-C8-C9
23	B	612	CLA	C14-C13-C15-C16
23	a	409	CLA	C6-C7-C8-C9
23	b	612	CLA	C6-C7-C8-C9
23	b	625	CLA	C11-C12-C13-C14
37	d	408	DGD	CAA-CBA-CCA-CDA
28	B	634	LMT	C3-C4-C5-C6
23	c	514	CLA	C8-C10-C11-C12
37	c	519	DGD	C4D-C5D-C6D-O5D
27	O	301	GOL	C1-C2-C3-O3
27	b	606	GOL	C1-C2-C3-O3
33	D	410	LHG	O1-C1-C2-C3
27	A	411	GOL	C1-C2-C3-O3
27	B	628	GOL	O1-C1-C2-C3
27	V	204	GOL	C1-C2-C3-O3
27	v	201	GOL	C1-C2-C3-O3
27	v	204	GOL	O1-C1-C2-C3
27	B	630	GOL	O1-C1-C2-C3
33	D	412	LHG	O1-C1-C2-C3
26	a	413	SQD	C9-C10-C11-C12
26	A	413	SQD	C11-C12-C13-C14
37	c	521	DGD	C5B-C6B-C7B-C8B
37	D	409	DGD	C8B-C9B-CAB-CBB
37	h	102	DGD	C5B-C6B-C7B-C8B
36	z	101	LMG	C12-C13-C14-C15
37	C	516	DGD	C5B-C6B-C7B-C8B
28	m	102	LMT	C2-C3-C4-C5
23	C	510	CLA	C16-C17-C18-C20
36	C	501	LMG	O6-C1-O1-C7
37	c	520	DGD	O6E-C1E-O5D-C6D
23	c	516	CLA	C15-C16-C17-C18
37	D	409	DGD	C3B-C4B-C5B-C6B
26	b	601	SQD	C32-C33-C34-C35
36	b	629	LMG	C36-C37-C38-C39
26	F	104	SQD	C34-C35-C36-C37
36	C	501	LMG	C11-C12-C13-C14
35	B	624	HTG	C3'-C4'-C5'-C6'
23	b	623	CLA	C13-C15-C16-C17
26	b	601	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	M	104	LMT	C2-C1-O1'-C1'
33	L	101	LHG	C12-C13-C14-C15
37	d	408	DGD	C9B-CAB-CBB-CCB
33	d	411	LHG	C29-C30-C31-C32
26	b	601	SQD	C29-C30-C31-C32
26	b	601	SQD	C33-C34-C35-C36
33	D	412	LHG	C29-C30-C31-C32
26	B	636	SQD	C23-C24-C25-C26
23	B	610	CLA	C4-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
28	M	105	LMT	C4'-C5'-C6'-O6'
31	d	407[A]	PL9	C43-C44-C46-C47
31	d	407[B]	PL9	C13-C14-C16-C17
23	B	610	CLA	C2-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
24	A	407	PHO	C2-C3-C5-C6
23	b	612	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
28	e	102	LMT	O5'-C5'-C6'-O6'
27	a	402	GOL	O1-C1-C2-O2
27	B	627	GOL	O1-C1-C2-O2
27	v	202	GOL	O1-C1-C2-O2
33	D	410	LHG	O1-C1-C2-O2
27	B	629	GOL	O1-C1-C2-O2
27	A	412	GOL	O2-C2-C3-O3
27	V	204	GOL	O2-C2-C3-O3
27	D	403	GOL	O2-C2-C3-O3
33	a	419	LHG	O1-C1-C2-O2
27	v	204	GOL	O1-C1-C2-O2
27	V	201	GOL	O2-C2-C3-O3
33	b	634	LHG	O1-C1-C2-O2
27	b	605	GOL	O1-C1-C2-O2
36	d	416	LMG	C38-C39-C40-C41
35	b	631	HTG	C3'-C4'-C5'-C6'
33	d	411	LHG	C31-C32-C33-C34
37	c	521	DGD	C2A-C3A-C4A-C5A
36	C	519	LMG	C31-C32-C33-C34
33	b	634	LHG	C10-C11-C12-C13
37	C	517	DGD	C1B-C2B-C3B-C4B
28	b	630	LMT	C3'-C4'-O1B-C1B
23	c	517	CLA	C10-C11-C12-C13
37	c	521	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
28	T	104	LMT	C1-C2-C3-C4
37	d	408	DGD	C2A-C1A-O1G-C1G
36	C	520	LMG	C29-C30-C31-C32
26	b	601	SQD	C28-C29-C30-C31
23	b	610	CLA	C2-C1-O2A-CGA
36	a	414	LMG	C29-C30-C31-C32
23	a	409	CLA	C10-C11-C12-C13
36	d	416	LMG	C14-C15-C16-C17
37	D	409	DGD	C6A-C7A-C8A-C9A
37	H	102	DGD	C6B-C7B-C8B-C9B
25	b	626	BCR	C1-C6-C7-C8
25	C	515	BCR	C5-C6-C7-C8
25	B	618	BCR	C1-C6-C7-C8
25	B	618	BCR	C5-C6-C7-C8
25	D	407	BCR	C23-C24-C25-C26
26	A	410	SQD	C14-C15-C16-C17
37	c	521	DGD	C2A-C1A-O1G-C1G
23	c	516	CLA	CBA-CGA-O2A-C1
26	f	102	SQD	C24-C25-C26-C27
28	A	414	LMT	C6-C7-C8-C9
26	a	413	SQD	C30-C31-C32-C33
36	c	522	LMG	C10-C11-C12-C13
37	D	409	DGD	C1B-C2B-C3B-C4B
26	F	104	SQD	C26-C27-C28-C29
23	c	513	CLA	C13-C15-C16-C17
23	B	616	CLA	C5-C6-C7-C8
36	z	101	LMG	C15-C16-C17-C18
31	d	407[A]	PL9	C45-C44-C46-C47
31	D	408[A]	PL9	C15-C14-C16-C17
31	d	407[B]	PL9	C15-C14-C16-C17
24	a	410	PHO	C4-C3-C5-C6
23	C	507	CLA	C6-C7-C8-C10
31	D	408[A]	PL9	C28-C29-C31-C32
23	B	604	CLA	C6-C7-C8-C10
23	c	514	CLA	C6-C7-C8-C10
23	B	603	CLA	C12-C13-C15-C16
23	b	623	CLA	C11-C12-C13-C15
23	C	502	CLA	C11-C10-C8-C7
23	b	612	CLA	C6-C7-C8-C10
24	a	410	PHO	C2-C3-C5-C6
37	c	521	DGD	C6B-C7B-C8B-C9B
37	c	521	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
36	C	501	LMG	C14-C15-C16-C17
23	C	513	CLA	CBA-CGA-O2A-C1
23	c	515	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
26	b	601	SQD	C35-C36-C37-C38
23	B	611	CLA	C2A-CAA-CBA-CGA
23	c	514	CLA	C13-C15-C16-C17
23	c	512	CLA	C15-C16-C17-C18
33	L	101	LHG	C14-C15-C16-C17
33	a	419	LHG	C11-C12-C13-C14
23	A	404	CLA	C13-C15-C16-C17
37	H	102	DGD	C7B-C8B-C9B-CAB
37	c	520	DGD	C9B-CAB-CBB-CCB
33	b	634	LHG	C28-C29-C30-C31
37	d	408	DGD	O1A-C1A-O1G-C1G
23	a	411	CLA	C16-C17-C18-C20
35	B	623	HTG	C4-C5-C6-O6
37	c	519	DGD	O6E-C1E-O5D-C6D
36	D	416	LMG	C19-C20-C21-C22
37	c	520	DGD	C4A-C5A-C6A-C7A
26	B	636	SQD	C25-C26-C27-C28
36	a	414	LMG	C11-C10-O7-C8
37	D	409	DGD	C7A-C8A-C9A-CAA
26	b	601	SQD	C14-C15-C16-C17
26	B	621	SQD	C34-C35-C36-C37
23	c	510	CLA	C15-C16-C17-C18
33	L	101	LHG	C13-C14-C15-C16
33	d	411	LHG	C11-C10-C9-C8
33	D	411	LHG	C32-C33-C34-C35
36	C	501	LMG	C32-C33-C34-C35
33	A	419	LHG	C16-C17-C18-C19
37	c	519	DGD	C2E-C1E-O5D-C6D
36	C	501	LMG	C36-C37-C38-C39
26	b	601	SQD	C31-C32-C33-C34
36	Z	101	LMG	C19-C20-C21-C22
37	d	408	DGD	O6E-C5E-C6E-O5E
31	d	407[A]	PL9	C15-C14-C16-C17
31	D	408[A]	PL9	C45-C44-C46-C47
28	C	521	LMT	C4'-C5'-C6'-O6'
31	a	415[A]	PL9	C12-C11-C9-C8
31	A	417[A]	PL9	C4-C3-C7-C8
31	A	417[B]	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
31	a	415[A]	PL9	C4-C3-C7-C8
36	d	416	LMG	C15-C16-C17-C18
23	B	604	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	a	409	CLA	C14-C13-C15-C16
23	b	623	CLA	C11-C12-C13-C14
23	B	613	CLA	CBD-CGD-O2D-CED
23	d	405	CLA	CBD-CGD-O2D-CED
28	B	634	LMT	C2-C3-C4-C5
33	D	412	LHG	C28-C29-C30-C31
23	C	513	CLA	C3-C5-C6-C7
37	h	102	DGD	CAA-CBA-CCA-CDA
36	C	520	LMG	C13-C14-C15-C16
37	C	516	DGD	C3B-C4B-C5B-C6B
36	Z	101	LMG	O6-C5-C6-O5
23	D	406	CLA	C8-C10-C11-C12
33	d	411	LHG	C33-C34-C35-C36
36	M	101	LMG	C36-C37-C38-C39
35	b	602	HTG	C2'-C3'-C4'-C5'
37	c	521	DGD	O1A-C1A-O1G-C1G
23	c	515	CLA	O1A-CGA-O2A-C1
23	c	516	CLA	O1A-CGA-O2A-C1
36	a	414	LMG	O9-C10-O7-C8
37	C	516	DGD	C1B-C2B-C3B-C4B
28	D	404	LMT	O5B-C5B-C6B-O6B
35	b	632	HTG	O5-C5-C6-O6
23	C	503	CLA	C3-C5-C6-C7
23	D	406	CLA	C3-C5-C6-C7
23	B	603	CLA	C3-C5-C6-C7
23	a	408	CLA	C2C-C3C-CAC-CBC
23	c	508	CLA	C8-C10-C11-C12
23	C	512	CLA	CBA-CGA-O2A-C1
36	C	520	LMG	C28-C29-C30-C31
23	c	507	CLA	O1D-CGD-O2D-CED
28	A	414	LMT	O5B-C5B-C6B-O6B
26	F	104	SQD	C32-C33-C34-C35
36	C	520	LMG	C37-C38-C39-C40
36	z	101	LMG	C4-C5-C6-O5
36	d	416	LMG	O6-C5-C6-O5
37	C	518	DGD	C8A-C9A-CAA-CBA
37	c	520	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	C	520	LMG	C14-C15-C16-C17
23	C	513	CLA	O1A-CGA-O2A-C1
28	e	102	LMT	C4-C5-C6-C7
33	A	419	LHG	C4-C5-C6-O8
26	F	104	SQD	C44-C45-C46-O48
36	a	414	LMG	C7-C8-C9-O8
26	a	413	SQD	O6-C44-C45-C46
36	Z	101	LMG	C7-C8-C9-O8
26	B	636	SQD	O6-C44-C45-C46
26	B	621	SQD	C44-C45-C46-O48
26	A	410	SQD	C15-C16-C17-C18
37	c	520	DGD	C2G-C3G-O3G-C1D
37	c	520	DGD	C5D-C6D-O5D-C1E
37	C	517	DGD	C2G-C3G-O3G-C1D
26	a	413	SQD	C19-C20-C21-C22
28	m	102	LMT	C1-C2-C3-C4
37	H	102	DGD	O2G-C1B-C2B-C3B
36	k	101	LMG	C39-C40-C41-C42
26	b	601	SQD	C27-C28-C29-C30
36	b	629	LMG	C40-C41-C42-C43
23	b	610	CLA	C10-C11-C12-C13
27	b	606	GOL	O2-C2-C3-O3
27	v	203	GOL	O1-C1-C2-O2
27	c	502	GOL	O1-C1-C2-O2
23	A	405	CLA	C2C-C3C-CAC-CBC
26	a	413	SQD	C17-C18-C19-C20
23	C	512	CLA	O1A-CGA-O2A-C1
26	F	104	SQD	C7-C8-C9-C10
33	d	411	LHG	C35-C36-C37-C38
28	a	404	LMT	C2-C3-C4-C5
28	M	104	LMT	O5B-C5B-C6B-O6B
37	C	516	DGD	O6E-C5E-C6E-O5E
37	c	519	DGD	O6E-C5E-C6E-O5E
23	c	514	CLA	C4-C3-C5-C6
31	D	408[B]	PL9	C35-C34-C36-C37
31	d	407[B]	PL9	C43-C44-C46-C47
26	B	621	SQD	C7-C8-C9-C10
23	A	408	CLA	CBA-CGA-O2A-C1
26	b	601	SQD	C10-C11-C12-C13
26	b	601	SQD	C46-C45-O47-C7
36	D	416	LMG	O6-C5-C6-O5
37	C	518	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	C8-C10-C11-C12
33	D	412	LHG	C12-C13-C14-C15
37	c	519	DGD	C6A-C7A-C8A-C9A
26	f	102	SQD	C25-C26-C27-C28
23	A	408	CLA	O1A-CGA-O2A-C1
37	D	409	DGD	C2A-C3A-C4A-C5A
36	k	101	LMG	O1-C7-C8-O7
36	Z	101	LMG	O1-C7-C8-O7
26	B	636	SQD	C31-C32-C33-C34
33	d	411	LHG	C7-C8-C9-C10
31	d	407[B]	PL9	C45-C44-C46-C47
23	c	513	CLA	C12-C13-C15-C16
31	D	408[A]	PL9	C13-C14-C16-C17
23	B	615	CLA	C12-C13-C15-C16
23	B	607	CLA	C11-C10-C8-C7
23	b	610	CLA	C6-C7-C8-C10
23	B	616	CLA	C12-C13-C15-C16
23	B	604	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C10-C8-C7
23	A	408	CLA	C6-C7-C8-C10
31	D	408[B]	PL9	C13-C14-C16-C17
23	b	623	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
37	h	102	DGD	O2G-C1B-C2B-C3B
37	c	519	DGD	C9A-CAA-CBA-CCA
23	c	513	CLA	C6-C7-C8-C9
23	c	513	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	B	607	CLA	C11-C10-C8-C9
23	b	610	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C10-C8-C9
23	A	408	CLA	C6-C7-C8-C9
23	c	509	CLA	C11-C12-C13-C14
23	B	602	CLA	C11-C10-C8-C9
23	C	506	CLA	C11-C12-C13-C14
23	b	625	CLA	C14-C13-C15-C16
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	C2A-CAA-CBA-CGA
37	h	102	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
36	D	416	LMG	C13-C14-C15-C16
37	h	102	DGD	CBB-CCB-CDB-CEB
23	A	404	CLA	O1D-CGD-O2D-CED
25	C	515	BCR	C21-C22-C23-C24
26	B	621	SQD	C33-C34-C35-C36
33	d	411	LHG	C24-C23-O8-C6
23	b	610	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	CBA-CGA-O2A-C1
26	B	621	SQD	C24-C23-O48-C46
36	z	101	LMG	C13-C14-C15-C16
36	a	414	LMG	C33-C34-C35-C36
33	L	101	LHG	C17-C18-C19-C20
28	M	102	LMT	O5'-C1'-O1'-C1
33	L	101	LHG	O6-C4-C5-C6
36	C	519	LMG	C28-C29-C30-C31
37	C	517	DGD	C7B-C8B-C9B-CAB
23	B	612	CLA	C13-C15-C16-C17
23	c	514	CLA	C2-C3-C5-C6
23	b	623	CLA	C10-C11-C12-C13
26	a	413	SQD	C33-C34-C35-C36
28	M	102	LMT	C5-C6-C7-C8
37	C	517	DGD	C4A-C5A-C6A-C7A
23	B	608	CLA	C16-C17-C18-C19
26	f	102	SQD	C31-C32-C33-C34
37	H	102	DGD	C5B-C6B-C7B-C8B
36	C	501	LMG	C12-C13-C14-C15
23	b	623	CLA	C15-C16-C17-C18
33	D	411	LHG	C24-C23-O8-C6
37	D	409	DGD	C4A-C5A-C6A-C7A
33	A	419	LHG	C24-C25-C26-C27
23	B	608	CLA	C3A-C2A-CAA-CBA
26	a	413	SQD	C27-C28-C29-C30
23	b	625	CLA	C10-C11-C12-C13
28	a	404	LMT	C6-C7-C8-C9
26	b	601	SQD	C24-C23-O48-C46
36	M	101	LMG	C15-C16-C17-C18
23	a	408	CLA	C13-C15-C16-C17
23	b	615	CLA	C10-C11-C12-C13
36	k	101	LMG	C7-C8-C9-O8
37	D	409	DGD	O1G-C1G-C2G-C3G
36	z	101	LMG	O1-C7-C8-C9
26	b	601	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
37	d	408	DGD	O1G-C1G-C2G-C3G
33	D	412	LHG	C4-C5-C6-O8
36	a	414	LMG	C35-C36-C37-C38
35	b	632	HTG	C1'-C2'-C3'-C4'
26	A	413	SQD	C30-C31-C32-C33
23	C	511	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	C16-C17-C18-C19
23	B	611	CLA	C16-C17-C18-C20
31	a	415[B]	PL9	C12-C11-C9-C8
37	c	520	DGD	C6A-C7A-C8A-C9A
33	A	419	LHG	C4-O6-P-O3
33	d	411	LHG	O10-C23-O8-C6
27	v	201	GOL	O1-C1-C2-O2
27	V	203	GOL	O2-C2-C3-O3
28	M	105	LMT	C11-C10-C9-C8
23	c	505	CLA	O1D-CGD-O2D-CED
37	h	102	DGD	CDB-CEB-CFB-CGB
23	b	614	CLA	O1A-CGA-O2A-C1
23	b	620	CLA	C16-C17-C18-C20
33	D	410	LHG	O8-C23-C24-C25
37	D	409	DGD	C2B-C3B-C4B-C5B
37	d	408	DGD	CCA-CDA-CEA-CFA
26	B	636	SQD	C28-C29-C30-C31
33	D	410	LHG	C34-C35-C36-C37
36	z	101	LMG	O1-C7-C8-O7
36	C	501	LMG	O1-C7-C8-O7
26	a	413	SQD	O6-C44-C45-O47
36	Z	101	LMG	O7-C8-C9-O8
33	D	412	LHG	O7-C5-C6-O8
35	B	622	HTG	C4'-C5'-C6'-C7'
33	D	410	LHG	C27-C28-C29-C30
33	d	409	LHG	C32-C33-C34-C35
37	d	408	DGD	O6D-C1D-O3G-C3G
31	D	408[A]	PL9	C9-C11-C12-C13
31	D	408[A]	PL9	C39-C41-C42-C43
36	b	629	LMG	C17-C18-C19-C20
26	A	413	SQD	C24-C25-C26-C27
23	C	510	CLA	C3-C5-C6-C7
23	c	515	CLA	C2-C1-O2A-CGA
23	b	617	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
36	k	101	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
36	a	414	LMG	C28-C29-C30-C31
23	B	615	CLA	C6-C7-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	B	611	CLA	C14-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C9
23	C	509	CLA	C6-C7-C8-C9
23	b	623	CLA	C11-C10-C8-C9
23	C	502	CLA	C11-C10-C8-C9
37	C	518	DGD	C9A-CAA-CBA-CCA
26	f	102	SQD	C26-C27-C28-C29
37	C	517	DGD	C8A-C9A-CAA-CBA
23	B	602	CLA	C10-C11-C12-C13
33	A	419	LHG	C25-C26-C27-C28
26	B	621	SQD	C12-C13-C14-C15
23	b	620	CLA	C16-C17-C18-C19
25	b	626	BCR	C5-C6-C7-C8
25	d	406	BCR	C23-C24-C25-C26
25	d	406	BCR	C23-C24-C25-C30
28	M	105	LMT	C9-C10-C11-C12
33	D	411	LHG	O10-C23-O8-C6
25	T	103	BCR	C11-C12-C13-C14
33	d	409	LHG	C33-C34-C35-C36
37	c	520	DGD	C2A-C3A-C4A-C5A
23	C	510	CLA	C16-C17-C18-C19
23	C	514	CLA	C5-C6-C7-C8
33	b	634	LHG	O6-C4-C5-C6
28	m	102	LMT	C4'-C5'-C6'-O6'
23	c	513	CLA	C6-C7-C8-C10
23	B	612	CLA	C11-C12-C13-C15
23	B	611	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C12-C13-C15
23	a	409	CLA	C12-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C10
23	B	602	CLA	C12-C13-C15-C16
23	b	625	CLA	C12-C13-C15-C16
26	B	636	SQD	C29-C30-C31-C32
25	t	101	BCR	C13-C14-C15-C16
37	d	408	DGD	C2B-C3B-C4B-C5B
23	a	411	CLA	C10-C11-C12-C13
35	b	608	HTG	O5-C1-S1-C1'
23	C	514	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	B	608	CLA	C16-C17-C18-C20
26	F	104	SQD	C24-C23-O48-C46
23	b	619	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	b	623	CLA	CAD-CBD-CGD-O2D
23	b	625	CLA	CAD-CBD-CGD-O2D
24	a	410	PHO	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	a	408	CLA	C4C-C3C-CAC-CBC
37	C	516	DGD	O6E-C1E-O5D-C6D
31	A	417[B]	PL9	C43-C44-C46-C47
33	d	411	LHG	C2-C3-O3-P
26	A	413	SQD	O6-C44-C45-C46
33	D	412	LHG	C2-C3-O3-P
26	B	621	SQD	O10-C23-O48-C46
26	B	621	SQD	C30-C31-C32-C33
33	b	634	LHG	C11-C12-C13-C14
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CHA-CBD-CGD-O1D
23	B	608	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O1D
24	d	402[B]	PHO	CHA-CBD-CGD-O1D
24	d	402[B]	PHO	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
24	D	402[B]	PHO	CHA-CBD-CGD-O1D
24	D	402[B]	PHO	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	c	506	CLA	CHA-CBD-CGD-O1D
28	D	404	LMT	C5-C6-C7-C8
23	b	610	CLA	C3-C5-C6-C7
23	b	610	CLA	O1A-CGA-O2A-C1
36	d	416	LMG	C17-C18-C19-C20
37	C	516	DGD	C2E-C1E-O5D-C6D
26	f	102	SQD	O6-C44-C45-O47
36	k	101	LMG	O7-C8-C9-O8
26	F	104	SQD	O47-C45-C46-O48
36	a	414	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
26	b	601	SQD	O47-C45-C46-O48
33	d	411	LHG	C25-C26-C27-C28
33	D	411	LHG	C34-C35-C36-C37
37	C	516	DGD	C4A-C5A-C6A-C7A
26	a	413	SQD	C29-C30-C31-C32
26	b	601	SQD	O10-C23-O48-C46
28	M	104	LMT	C2B-C1B-O1B-C4'
27	B	628	GOL	O1-C1-C2-O2
27	F	103	GOL	O1-C1-C2-O2
23	C	502	CLA	O1D-CGD-O2D-CED
37	d	408	DGD	C4A-C5A-C6A-C7A
31	A	417[A]	PL9	C15-C14-C16-C17
23	B	615	CLA	O1A-CGA-O2A-C1
31	d	407[A]	PL9	C28-C29-C31-C32
31	a	415[B]	PL9	C4-C3-C7-C8
23	D	405	CLA	C14-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C9
23	C	512	CLA	C6-C7-C8-C9
23	b	620	CLA	C8-C10-C11-C12
36	M	101	LMG	C16-C17-C18-C19
26	f	102	SQD	C33-C34-C35-C36
36	M	101	LMG	C31-C32-C33-C34
26	b	601	SQD	C13-C14-C15-C16
35	b	602	HTG	S1-C1'-C2'-C3'
37	D	409	DGD	C3A-C4A-C5A-C6A
37	h	102	DGD	C6A-C7A-C8A-C9A
23	c	517	CLA	C1A-C2A-CAA-CBA
23	c	515	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	d	403	CLA	C15-C16-C17-C18
37	h	102	DGD	C9B-CAB-CBB-CCB
37	c	519	DGD	C8B-C9B-CAB-CBB
23	B	615	CLA	CBA-CGA-O2A-C1
37	C	516	DGD	C3A-C4A-C5A-C6A
28	M	105	LMT	C3-C4-C5-C6
26	B	621	SQD	C11-C10-C9-C8
25	h	101	BCR	C9-C10-C11-C12
33	d	411	LHG	C30-C31-C32-C33
35	B	623	HTG	O5-C5-C6-O6
26	F	104	SQD	O10-C23-O48-C46
33	d	410	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
33	D	411	LHG	C3-O3-P-O4
33	D	410	LHG	C4-O6-P-O4
33	A	419	LHG	C3-O3-P-O5
33	a	419	LHG	C3-O3-P-O5
33	b	634	LHG	C4-O6-P-O5
23	b	611	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
33	d	409	LHG	C7-C8-C9-C10
37	C	518	DGD	C2A-C1A-O1G-C1G
26	B	636	SQD	C27-C28-C29-C30
23	d	405	CLA	C3-C5-C6-C7
36	b	629	LMG	C37-C38-C39-C40
36	a	414	LMG	C19-C20-C21-C22
23	c	508	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	b	616	CLA	CAD-CBD-CGD-O1D
23	B	610	CLA	CAD-CBD-CGD-O1D
23	B	608	CLA	CAD-CBD-CGD-O1D
23	b	618	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	B	602	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	c	510	CLA	CAD-CBD-CGD-O1D
26	B	636	SQD	C5-C6-S-O9
36	C	519	LMG	C10-C11-C12-C13
26	F	104	SQD	C31-C32-C33-C34
33	a	419	LHG	C25-C26-C27-C28
37	c	519	DGD	C4B-C5B-C6B-C7B
23	b	619	CLA	C16-C17-C18-C19
23	d	403	CLA	CBD-CGD-O2D-CED
33	L	101	LHG	O6-C4-C5-O7
23	c	516	CLA	C11-C10-C8-C7
23	a	409	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C15
23	C	502	CLA	C11-C12-C13-C15
23	B	617	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	A	406	CLA	C11-C10-C8-C7
23	B	602	CLA	CAA-CBA-CGA-O2A
37	c	521	DGD	C7A-C8A-C9A-CAA
33	D	410	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
26	a	413	SQD	C26-C27-C28-C29
23	A	406	CLA	C13-C15-C16-C17
23	B	602	CLA	C2A-CAA-CBA-CGA
35	B	622	HTG	S1-C1'-C2'-C3'
36	k	101	LMG	O1-C7-C8-C9
36	C	501	LMG	O1-C7-C8-C9
36	Z	101	LMG	O1-C7-C8-C9
26	B	621	SQD	C17-C18-C19-C20
37	D	409	DGD	O1G-C1G-C2G-O2G
33	A	419	LHG	O7-C5-C6-O8
23	c	511	CLA	C5-C6-C7-C8
37	c	521	DGD	CBA-CCA-CDA-CEA
37	C	518	DGD	C2A-C3A-C4A-C5A
36	C	520	LMG	C8-C7-O1-C1
23	B	611	CLA	C13-C15-C16-C17
23	b	615	CLA	C8-C10-C11-C12
37	c	520	DGD	CBB-CCB-CDB-CEB
26	B	636	SQD	C24-C25-C26-C27
23	b	619	CLA	C15-C16-C17-C18
23	C	511	CLA	C8-C10-C11-C12
23	b	624	CLA	C5-C6-C7-C8
23	b	619	CLA	C11-C12-C13-C14
23	B	616	CLA	C11-C12-C13-C14
23	B	612	CLA	C11-C12-C13-C14
23	C	505	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	B	613	CLA	C8-C10-C11-C12
31	a	415[A]	PL9	C14-C16-C17-C18
33	A	419	LHG	C9-C10-C11-C12
37	C	518	DGD	O1A-C1A-O1G-C1G
27	V	201	GOL	O1-C1-C2-O2
36	M	101	LMG	C35-C36-C37-C38
23	d	403	CLA	C2C-C3C-CAC-CBC
23	b	623	CLA	C16-C17-C18-C19
36	D	416	LMG	C12-C13-C14-C15
37	H	102	DGD	CDA-CEA-CFA-CGA
23	a	408	CLA	C15-C16-C17-C18
35	B	622	HTG	C1'-C2'-C3'-C4'
35	b	602	HTG	C1'-C2'-C3'-C4'
31	A	417[B]	PL9	C45-C44-C46-C47
37	c	519	DGD	C2A-C3A-C4A-C5A
23	c	513	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	C	520	LMG	C18-C19-C20-C21
23	B	616	CLA	C13-C15-C16-C17
23	B	613	CLA	O1D-CGD-O2D-CED
28	D	404	LMT	C2-C3-C4-C5
23	b	610	CLA	CAA-CBA-CGA-O2A
26	B	621	SQD	C46-C45-O47-C7
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
26	A	410	SQD	O49-C7-O47-C45
23	C	513	CLA	C2-C1-O2A-CGA
28	M	104	LMT	C2-C3-C4-C5
36	b	629	LMG	C34-C35-C36-C37
33	A	419	LHG	C15-C16-C17-C18
36	M	101	LMG	C33-C34-C35-C36
23	d	403	CLA	O1D-CGD-O2D-CED
24	a	410	PHO	CBA-CGA-O2A-C1
24	a	410	PHO	O1A-CGA-O2A-C1
28	a	418	LMT	C7-C8-C9-C10
23	a	408	CLA	C16-C17-C18-C19
23	C	508	CLA	C4-C3-C5-C6
25	c	526	BCR	C1-C6-C7-C8
25	b	627	BCR	C23-C24-C25-C30
33	a	419	LHG	O9-C7-O7-C5
35	b	631	HTG	C2'-C3'-C4'-C5'
35	B	624	HTG	C2'-C3'-C4'-C5'
28	T	104	LMT	C4-C5-C6-C7
28	e	102	LMT	C9-C10-C11-C12
37	c	520	DGD	C7A-C8A-C9A-CAA
35	B	623	HTG	C1'-C2'-C3'-C4'
23	b	619	CLA	C16-C17-C18-C20
35	B	622	HTG	C4-C5-C6-O6
26	A	410	SQD	C8-C7-O47-C45
33	a	419	LHG	C8-C7-O7-C5
28	D	404	LMT	C2'-C1'-O1'-C1
37	d	408	DGD	C2D-C1D-O3G-C3G
28	M	102	LMT	C2'-C1'-O1'-C1
26	A	410	SQD	C16-C17-C18-C19
26	F	104	SQD	O6-C44-C45-O47
26	B	621	SQD	O47-C45-C46-O48
35	b	607	HTG	C2'-C3'-C4'-C5'
33	a	419	LHG	C14-C15-C16-C17
23	C	510	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	z	101	LMG	C7-C8-C9-O8
31	A	417[B]	PL9	C15-C14-C16-C17
31	a	415[A]	PL9	C45-C44-C46-C47
37	H	102	DGD	C5A-C6A-C7A-C8A
23	a	409	CLA	C6-C7-C8-C10
23	C	512	CLA	C6-C7-C8-C10
23	d	404	CLA	C11-C12-C13-C15
36	D	416	LMG	C34-C35-C36-C37
33	b	634	LHG	C12-C13-C14-C15
23	B	604	CLA	C11-C10-C8-C9
25	T	103	BCR	C13-C14-C15-C16
36	D	416	LMG	C20-C21-C22-C23
26	b	601	SQD	C15-C16-C17-C18
26	A	413	SQD	C24-C23-O48-C46
33	d	409	LHG	C26-C27-C28-C29
37	C	518	DGD	C6B-C7B-C8B-C9B
23	C	514	CLA	CBA-CGA-O2A-C1
37	C	517	DGD	C8B-C9B-CAB-CBB
26	A	413	SQD	O10-C23-O48-C46
23	b	620	CLA	C13-C15-C16-C17
26	F	104	SQD	C30-C31-C32-C33
33	b	634	LHG	C32-C33-C34-C35
36	C	501	LMG	C10-C11-C12-C13
31	d	407[B]	PL9	C28-C29-C31-C32
26	a	413	SQD	C35-C36-C37-C38
23	b	623	CLA	C16-C17-C18-C20
37	c	520	DGD	C2B-C3B-C4B-C5B
23	b	611	CLA	C16-C17-C18-C20
28	D	404	LMT	O5'-C1'-O1'-C1
23	C	514	CLA	O1A-CGA-O2A-C1
36	k	101	LMG	C16-C17-C18-C19
37	C	518	DGD	C1B-C2B-C3B-C4B
26	F	104	SQD	C24-C25-C26-C27
28	a	418	LMT	C6-C7-C8-C9
33	b	634	LHG	C31-C32-C33-C34
28	m	102	LMT	C3-C4-C5-C6
23	b	625	CLA	C4-C3-C5-C6
26	A	413	SQD	C26-C27-C28-C29
31	A	417[A]	PL9	C13-C14-C16-C17
37	c	520	DGD	C4B-C5B-C6B-C7B
23	a	411	CLA	C8-C10-C11-C12
23	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	D	411	LHG	C13-C14-C15-C16
23	C	511	CLA	C2-C1-O2A-CGA
23	B	614	CLA	C2-C1-O2A-CGA
23	b	622	CLA	C2-C1-O2A-CGA
23	d	404	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C13-C15-C16-C17
23	B	614	CLA	C5-C6-C7-C8
36	c	522	LMG	O7-C8-C9-O8
23	b	619	CLA	C2A-CAA-CBA-CGA
37	d	408	DGD	O1G-C1G-C2G-O2G
37	H	102	DGD	O1B-C1B-C2B-C3B
23	A	405	CLA	C4C-C3C-CAC-CBC
23	b	624	CLA	C13-C15-C16-C17
23	A	406	CLA	C16-C17-C18-C20
28	T	104	LMT	C7-C8-C9-C10
31	d	407[A]	PL9	C30-C29-C31-C32
36	a	414	LMG	O6-C5-C6-O5
31	a	415[A]	PL9	C43-C44-C46-C47
23	d	405	CLA	O1D-CGD-O2D-CED
28	F	101	LMT	C4'-C5'-C6'-O6'
23	C	507	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C10-C8-C9
35	C	523	HTG	S1-C1'-C2'-C3'
33	D	411	LHG	C4-C5-C6-O8
28	M	104	LMT	O5B-C1B-O1B-C4'
35	B	623	HTG	C4'-C5'-C6'-C7'
37	C	518	DGD	C8B-C9B-CAB-CBB
37	H	102	DGD	CBB-CCB-CDB-CEB
37	C	518	DGD	CBA-CCA-CDA-CEA
28	F	101	LMT	C2-C3-C4-C5
28	M	105	LMT	O5'-C1'-O1'-C1
36	k	101	LMG	C36-C37-C38-C39
25	b	626	BCR	C36-C18-C19-C20
25	t	101	BCR	C11-C12-C13-C35
25	b	628	BCR	C11-C12-C13-C35
25	y	101	BCR	C37-C22-C23-C24
23	C	509	CLA	C13-C15-C16-C17
23	c	505	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C12-C13-C15-C16
23	b	616	CLA	C12-C13-C15-C16
23	B	615	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	O1A-CGA-O2A-C1
23	b	622	CLA	O1D-CGD-O2D-CED
37	D	409	DGD	C9B-CAB-CBB-CCB
23	a	408	CLA	C2A-CAA-CBA-CGA
23	b	623	CLA	C2A-CAA-CBA-CGA
26	A	413	SQD	C29-C30-C31-C32
33	b	634	LHG	O6-C4-C5-O7
23	A	408	CLA	C15-C16-C17-C18
23	a	411	CLA	C4-C3-C5-C6
23	b	617	CLA	C13-C15-C16-C17
26	A	413	SQD	C18-C19-C20-C21
23	B	614	CLA	C10-C11-C12-C13
23	C	502	CLA	C13-C15-C16-C17
36	d	416	LMG	C10-C11-C12-C13
28	B	634	LMT	C7-C8-C9-C10
36	z	101	LMG	O7-C8-C9-O8
23	B	609	CLA	C13-C15-C16-C17
35	C	523	HTG	C1'-C2'-C3'-C4'
23	A	406	CLA	C15-C16-C17-C18
23	C	503	CLA	C16-C17-C18-C20
23	c	513	CLA	C15-C16-C17-C18
23	b	614	CLA	C5-C6-C7-C8
23	c	514	CLA	O1A-CGA-O2A-C1
31	A	417[A]	PL9	C19-C21-C22-C23
31	a	415[A]	PL9	C39-C41-C42-C43
23	B	616	CLA	C4-C3-C5-C6
23	d	405	CLA	C4-C3-C5-C6
23	C	514	CLA	C4-C3-C5-C6
36	c	522	LMG	C32-C33-C34-C35
23	b	623	CLA	C2-C1-O2A-CGA
31	A	417[A]	PL9	C43-C44-C46-C47
31	A	417[B]	PL9	C13-C14-C16-C17
23	b	625	CLA	C2-C3-C5-C6
28	e	102	LMT	C2B-C1B-O1B-C4'
23	C	507	CLA	C16-C17-C18-C20
26	b	601	SQD	C30-C31-C32-C33
33	A	419	LHG	C11-C10-C9-C8
36	d	416	LMG	C35-C36-C37-C38
36	C	519	LMG	C35-C36-C37-C38
36	z	101	LMG	C16-C17-C18-C19
25	Y	101	BCR	C23-C24-C25-C26
25	Y	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	K	103	BCR	C1-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C30
25	c	518	BCR	C1-C6-C7-C8
25	b	627	BCR	C23-C24-C25-C26
25	K	101	BCR	C1-C6-C7-C8
33	d	411	LHG	O1-C1-C2-C3
27	F	103	GOL	O1-C1-C2-C3
25	c	526	BCR	C19-C20-C21-C22
23	B	607	CLA	C4-C3-C5-C6
31	D	408[B]	PL9	C45-C44-C46-C47
31	a	415[B]	PL9	C45-C44-C46-C47
25	y	101	BCR	C21-C22-C23-C24
23	c	510	CLA	C16-C17-C18-C20
31	D	408[B]	PL9	C33-C34-C36-C37
33	D	410	LHG	C11-C10-C9-C8
36	D	416	LMG	C8-C7-O1-C1
37	c	519	DGD	C5D-C6D-O5D-C1E
37	C	517	DGD	C5D-C6D-O5D-C1E
37	c	520	DGD	C3A-C4A-C5A-C6A
23	b	625	CLA	C16-C17-C18-C19
37	c	520	DGD	C5B-C6B-C7B-C8B
36	d	416	LMG	C29-C30-C31-C32
28	M	104	LMT	C11-C10-C9-C8
37	h	102	DGD	C3B-C4B-C5B-C6B
37	C	518	DGD	C3B-C4B-C5B-C6B
31	A	417[A]	PL9	C30-C29-C31-C32
23	c	514	CLA	C12-C13-C15-C16
23	C	504	CLA	CBD-CGD-O2D-CED
37	D	409	DGD	C5A-C6A-C7A-C8A
23	A	406	CLA	C2C-C3C-CAC-CBC
28	M	105	LMT	C5-C6-C7-C8
36	C	519	LMG	O10-C28-O8-C9
28	D	404	LMT	C2B-C1B-O1B-C4'
23	C	510	CLA	CBA-CGA-O2A-C1
33	a	419	LHG	C28-C29-C30-C31
35	B	624	HTG	O5-C1-S1-C1'
37	D	409	DGD	O1G-C1A-C2A-C3A
23	C	513	CLA	CAA-CBA-CGA-O2A
31	D	408[A]	PL9	C35-C34-C36-C37
23	c	517	CLA	C4-C3-C5-C6
23	b	610	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
36	k	101	LMG	C19-C20-C21-C22
33	a	419	LHG	O8-C23-C24-C25
37	c	520	DGD	O2G-C1B-C2B-C3B
23	b	616	CLA	C14-C13-C15-C16
23	c	516	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C10-C8-C9
23	A	406	CLA	C11-C10-C8-C9
23	d	404	CLA	C11-C12-C13-C14
23	b	616	CLA	C3A-C2A-CAA-CBA
23	B	610	CLA	C3A-C2A-CAA-CBA
23	b	618	CLA	C3A-C2A-CAA-CBA
23	C	514	CLA	C3A-C2A-CAA-CBA
26	a	413	SQD	C34-C35-C36-C37
23	B	604	CLA	C13-C15-C16-C17
26	f	102	SQD	O47-C7-C8-C9
23	C	511	CLA	CAA-CBA-CGA-O2A
23	C	504	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	611	CLA	CAD-CBD-CGD-O2D
23	c	516	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
23	B	617	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D
36	a	414	LMG	C34-C35-C36-C37
33	L	101	LHG	O7-C7-C8-C9
33	A	419	LHG	C19-C20-C21-C22
31	A	417[A]	PL9	C20-C19-C21-C22
31	A	417[A]	PL9	C45-C44-C46-C47
31	A	417[B]	PL9	C30-C29-C31-C32
31	A	417[B]	PL9	C35-C34-C36-C37
23	c	517	CLA	C2-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
23	B	616	CLA	C2-C3-C5-C6
23	a	411	CLA	C2-C3-C5-C6
23	b	620	CLA	C2-C3-C5-C6
31	a	415[B]	PL9	C43-C44-C46-C47
37	d	408	DGD	O2G-C1B-C2B-C3B
31	A	417[B]	PL9	C19-C21-C22-C23
37	C	516	DGD	C1G-C2G-C3G-O3G
35	V	206	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
36	k	101	LMG	O7-C10-C11-C12
33	b	634	LHG	O7-C7-C8-C9
37	h	102	DGD	C4E-C5E-C6E-O5E
37	h	102	DGD	O1B-C1B-C2B-C3B
35	b	607	HTG	C4'-C5'-C6'-C7'
23	B	614	CLA	O2A-C1-C2-C3
23	b	622	CLA	O2A-C1-C2-C3
23	d	405	CLA	O2A-C1-C2-C3
24	a	410	PHO	O2A-C1-C2-C3
28	A	414	LMT	O1'-C1-C2-C3
36	b	629	LMG	C16-C17-C18-C19
24	a	410	PHO	C4B-C3B-CAB-CBB
33	d	410	LHG	O10-C23-O8-C6
23	b	625	CLA	CBD-CGD-O2D-CED
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	513	CLA	CHA-CBD-CGD-O1D
23	c	513	CLA	CHA-CBD-CGD-O2D
24	D	402[A]	PHO	CHA-CBD-CGD-O1D
24	D	402[A]	PHO	CHA-CBD-CGD-O2D
25	d	406	BCR	C13-C14-C15-C16
23	c	511	CLA	CHA-CBD-CGD-O2D
23	B	608	CLA	CHA-CBD-CGD-O2D
24	d	402[A]	PHO	CHA-CBD-CGD-O1D
24	d	402[A]	PHO	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O2D
36	k	101	LMG	C29-C30-C31-C32
31	D	408[B]	PL9	C43-C44-C46-C47
33	A	419	LHG	C26-C27-C28-C29
35	B	632	HTG	S1-C1'-C2'-C3'
36	C	501	LMG	C31-C32-C33-C34
33	A	419	LHG	O8-C23-C24-C25
23	b	613	CLA	C2C-C3C-CAC-CBC
37	d	408	DGD	O2G-C2G-C3G-O3G
28	a	404	LMT	C3-C4-C5-C6
23	c	516	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	D	410	LHG	O10-C23-C24-C25
23	c	511	CLA	C2A-CAA-CBA-CGA
27	O	301	GOL	O2-C2-C3-O3
27	A	411	GOL	O2-C2-C3-O3
33	D	412	LHG	O1-C1-C2-O2
37	c	521	DGD	CCA-CDA-CEA-CFA
26	b	601	SQD	C11-C10-C9-C8
26	B	636	SQD	C24-C23-O48-C46
28	M	104	LMT	C3-C4-C5-C6
37	h	102	DGD	C9A-CAA-CBA-CCA
28	b	630	LMT	C6-C7-C8-C9
23	B	614	CLA	CAA-CBA-CGA-O2A
28	F	101	LMT	O1'-C1-C2-C3
23	C	508	CLA	C2-C3-C5-C6
23	b	612	CLA	C11-C10-C8-C7
35	B	631	HTG	C3'-C4'-C5'-C6'
23	c	508	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	a	409	CLA	C11-C12-C13-C14
23	b	612	CLA	C11-C10-C8-C9
37	D	409	DGD	O1A-C1A-C2A-C3A
28	D	404	LMT	O5B-C1B-O1B-C4'
37	C	516	DGD	C1A-C2A-C3A-C4A
23	c	514	CLA	CBA-CGA-O2A-C1
33	b	634	LHG	C9-C10-C11-C12
23	B	615	CLA	C2A-CAA-CBA-CGA
31	A	417[B]	PL9	C26-C27-C28-C29
31	a	415[B]	PL9	C11-C12-C13-C14
31	a	415[B]	PL9	C26-C27-C28-C29
36	k	101	LMG	C40-C41-C42-C43
36	Z	101	LMG	O7-C10-C11-C12
33	D	412	LHG	C9-C10-C11-C12
33	D	412	LHG	C13-C14-C15-C16
33	a	419	LHG	O10-C23-C24-C25
36	b	629	LMG	C15-C16-C17-C18
27	B	630	GOL	C1-C2-C3-O3
27	V	203	GOL	C1-C2-C3-O3
24	d	402[B]	PHO	C8-C10-C11-C12
26	f	102	SQD	O49-C7-C8-C9
36	k	101	LMG	O9-C10-C11-C12
37	c	520	DGD	O1B-C1B-C2B-C3B
36	M	101	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	O1D-CGD-O2D-CED
33	D	410	LHG	C28-C29-C30-C31
37	d	408	DGD	O1B-C1B-C2B-C3B
24	d	402[A]	PHO	C2C-C3C-CAC-CBC
23	d	403	CLA	C4C-C3C-CAC-CBC
23	b	613	CLA	C4C-C3C-CAC-CBC
23	b	621	CLA	O1A-CGA-O2A-C1
26	A	410	SQD	C13-C14-C15-C16
28	A	414	LMT	C4-C5-C6-C7
23	C	510	CLA	C8-C10-C11-C12
23	d	403	CLA	C13-C15-C16-C17
36	C	519	LMG	C29-C28-O8-C9
23	C	513	CLA	CAA-CBA-CGA-O1A
26	f	102	SQD	O6-C44-C45-C46
28	C	521	LMT	C4B-C5B-C6B-O6B
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C16-C17-C18-C19
33	L	101	LHG	O9-C7-C8-C9
23	A	404	CLA	C15-C16-C17-C18
37	d	408	DGD	C6A-C7A-C8A-C9A
36	Z	101	LMG	C13-C14-C15-C16
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	CAA-CBA-CGA-O1A
33	D	410	LHG	C3-O3-P-O5
33	D	412	LHG	C4-O6-P-O5
25	c	526	BCR	C5-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
23	c	508	CLA	C15-C16-C17-C18
33	b	634	LHG	O9-C7-C8-C9
26	A	410	SQD	C32-C33-C34-C35
26	B	636	SQD	O10-C23-O48-C46
36	C	520	LMG	O8-C28-C29-C30
26	b	601	SQD	O48-C23-C24-C25
23	b	622	CLA	CAA-CBA-CGA-O2A
26	A	413	SQD	C28-C29-C30-C31
36	C	519	LMG	O7-C10-C11-C12
33	L	101	LHG	C26-C27-C28-C29
31	d	407[B]	PL9	C11-C12-C13-C14
33	d	410	LHG	C24-C23-O8-C6
26	A	410	SQD	O5-C5-C6-S
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	CAD-CBD-CGD-O1D
23	c	509	CLA	CAD-CBD-CGD-O1D
26	b	601	SQD	O5-C5-C6-S
23	d	403	CLA	CAD-CBD-CGD-O1D
36	Z	101	LMG	O9-C10-C11-C12
23	C	509	CLA	C11-C12-C13-C14
23	C	502	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
37	d	408	DGD	CAB-CBB-CCB-CDB
27	B	630	GOL	O1-C1-C2-O2
27	B	630	GOL	O2-C2-C3-O3
33	d	410	LHG	C11-C10-C9-C8
37	c	519	DGD	CCA-CDA-CEA-CFA
23	B	612	CLA	C8-C10-C11-C12
37	c	521	DGD	O1G-C1A-C2A-C3A
23	c	514	CLA	CAA-CBA-CGA-O2A
23	c	509	CLA	CAA-CBA-CGA-O2A
36	C	501	LMG	O7-C10-C11-C12
37	C	516	DGD	O2G-C1B-C2B-C3B
35	c	523	HTG	C3'-C4'-C5'-C6'
36	C	519	LMG	C16-C17-C18-C19
36	D	416	LMG	O7-C10-C11-C12
28	C	521	LMT	C3-C4-C5-C6
37	h	102	DGD	C6B-C7B-C8B-C9B
23	d	404	CLA	C3-C5-C6-C7
23	c	516	CLA	CAA-CBA-CGA-O1A
31	D	408[A]	PL9	C30-C29-C31-C32
23	c	508	CLA	C12-C13-C15-C16
31	d	407[A]	PL9	C18-C19-C21-C22
23	C	511	CLA	C12-C13-C15-C16
23	A	408	CLA	C12-C13-C15-C16
23	b	618	CLA	C2-C3-C5-C6
23	d	405	CLA	C2-C3-C5-C6
33	A	419	LHG	O10-C23-C24-C25
23	B	614	CLA	CAA-CBA-CGA-O1A
36	M	101	LMG	O8-C28-C29-C30
37	d	408	DGD	C3A-C4A-C5A-C6A
26	B	621	SQD	C35-C36-C37-C38
25	b	626	BCR	C17-C18-C19-C20
25	t	101	BCR	C11-C12-C13-C14
33	d	411	LHG	O8-C23-C24-C25
36	z	101	LMG	O7-C10-C11-C12

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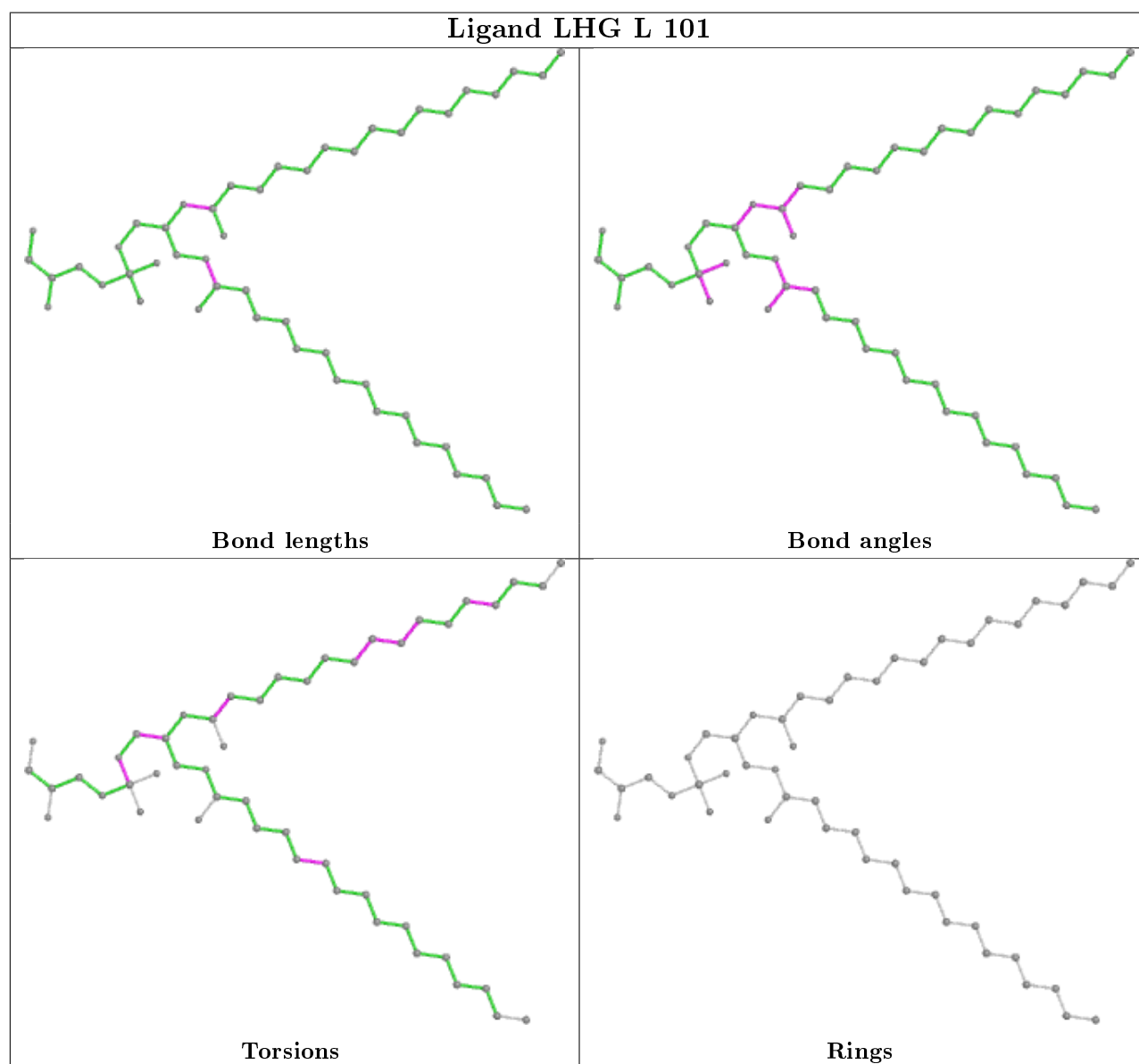
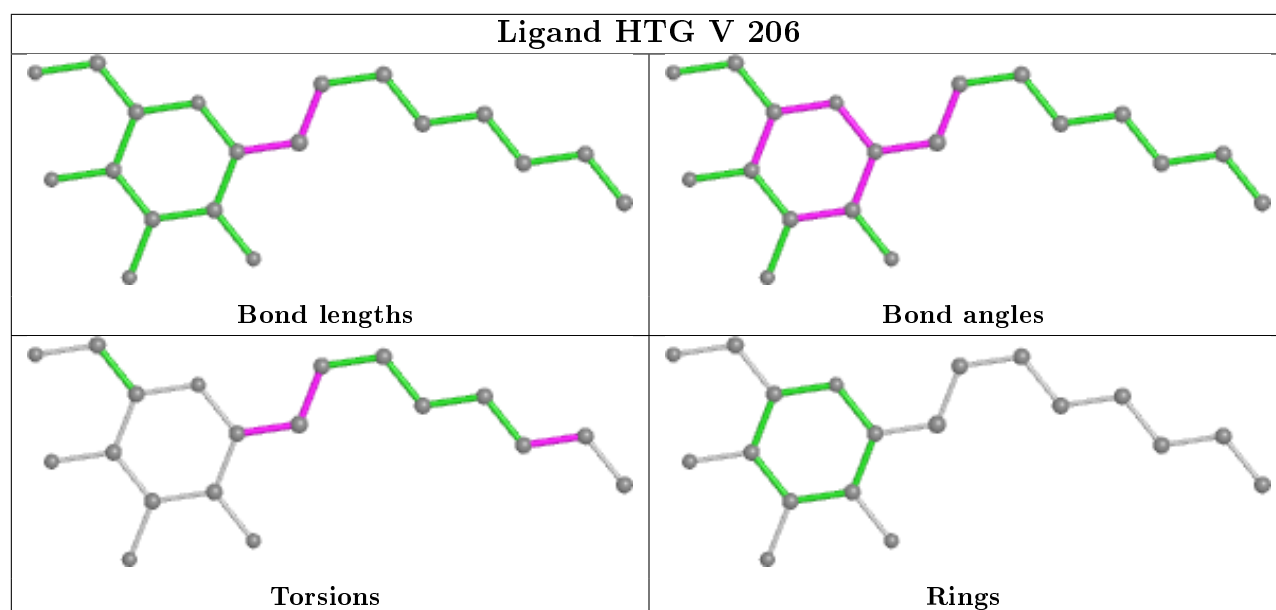
Mol	Chain	Res	Type	Atoms
37	c	521	DGD	O1A-C1A-C2A-C3A
36	z	101	LMG	O9-C10-C11-C12
36	C	519	LMG	O9-C10-C11-C12
23	b	622	CLA	CAA-CBA-CGA-O1A
33	D	412	LHG	O8-C23-C24-C25
23	b	621	CLA	C8-C10-C11-C12
23	B	614	CLA	C13-C15-C16-C17
36	D	416	LMG	O9-C10-C11-C12
26	A	413	SQD	C12-C13-C14-C15
36	c	522	LMG	C29-C30-C31-C32
26	B	621	SQD	C19-C20-C21-C22
37	C	517	DGD	C3A-C4A-C5A-C6A
33	D	412	LHG	C10-C11-C12-C13
23	d	404	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

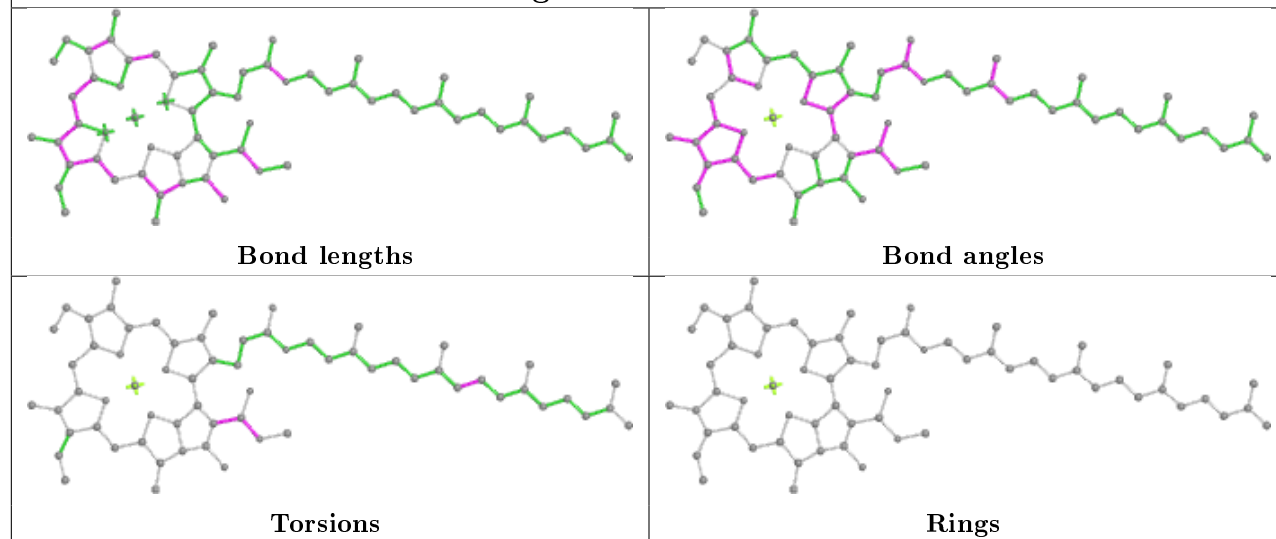
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	f	102	SQD	0	1

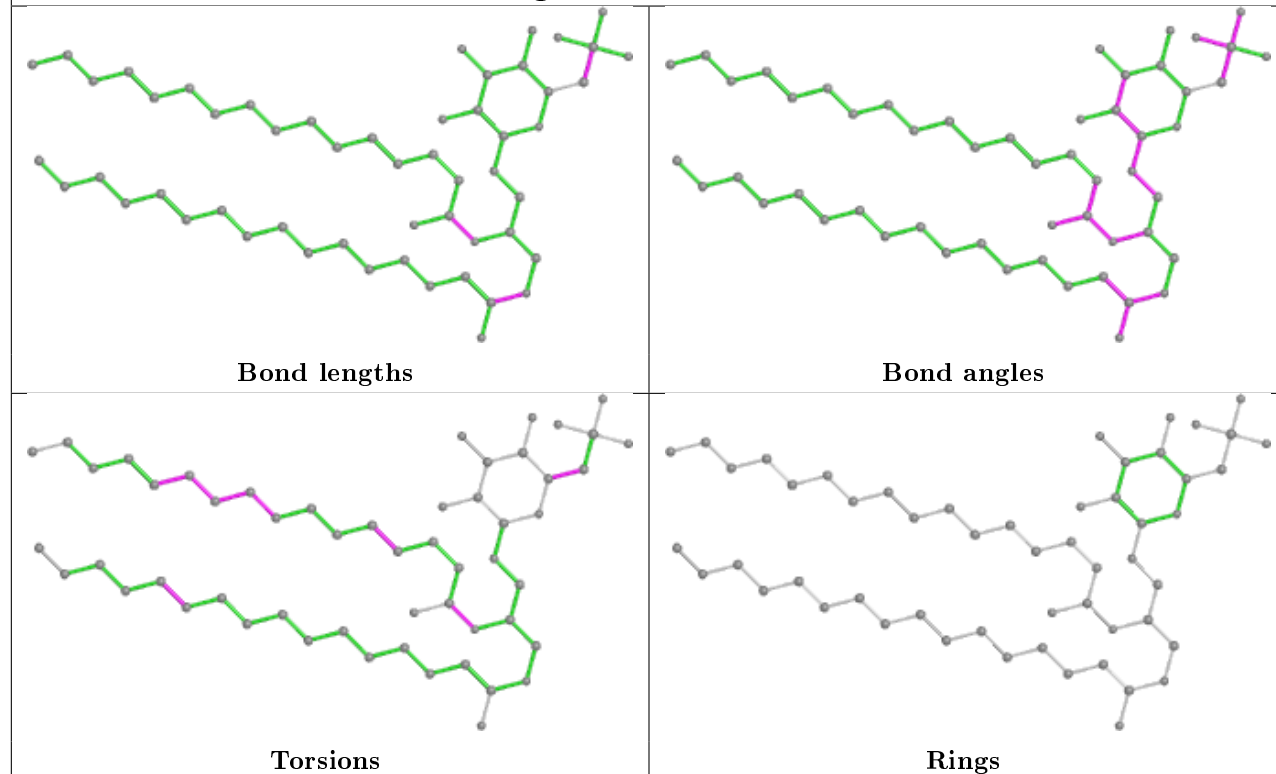
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



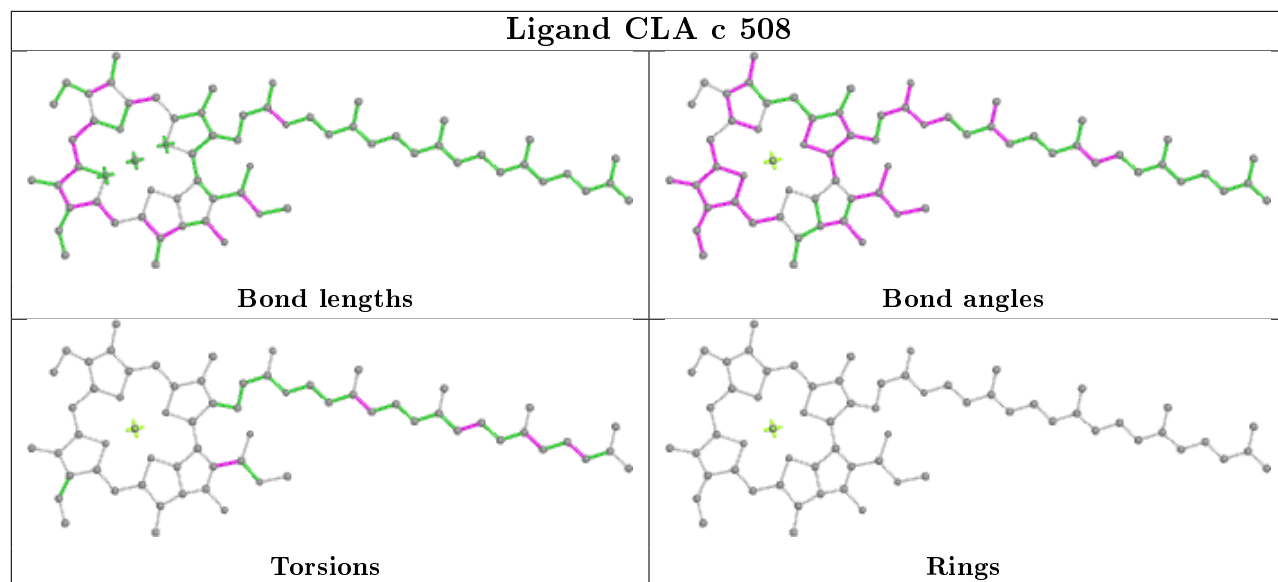
## Ligand CLA C 504



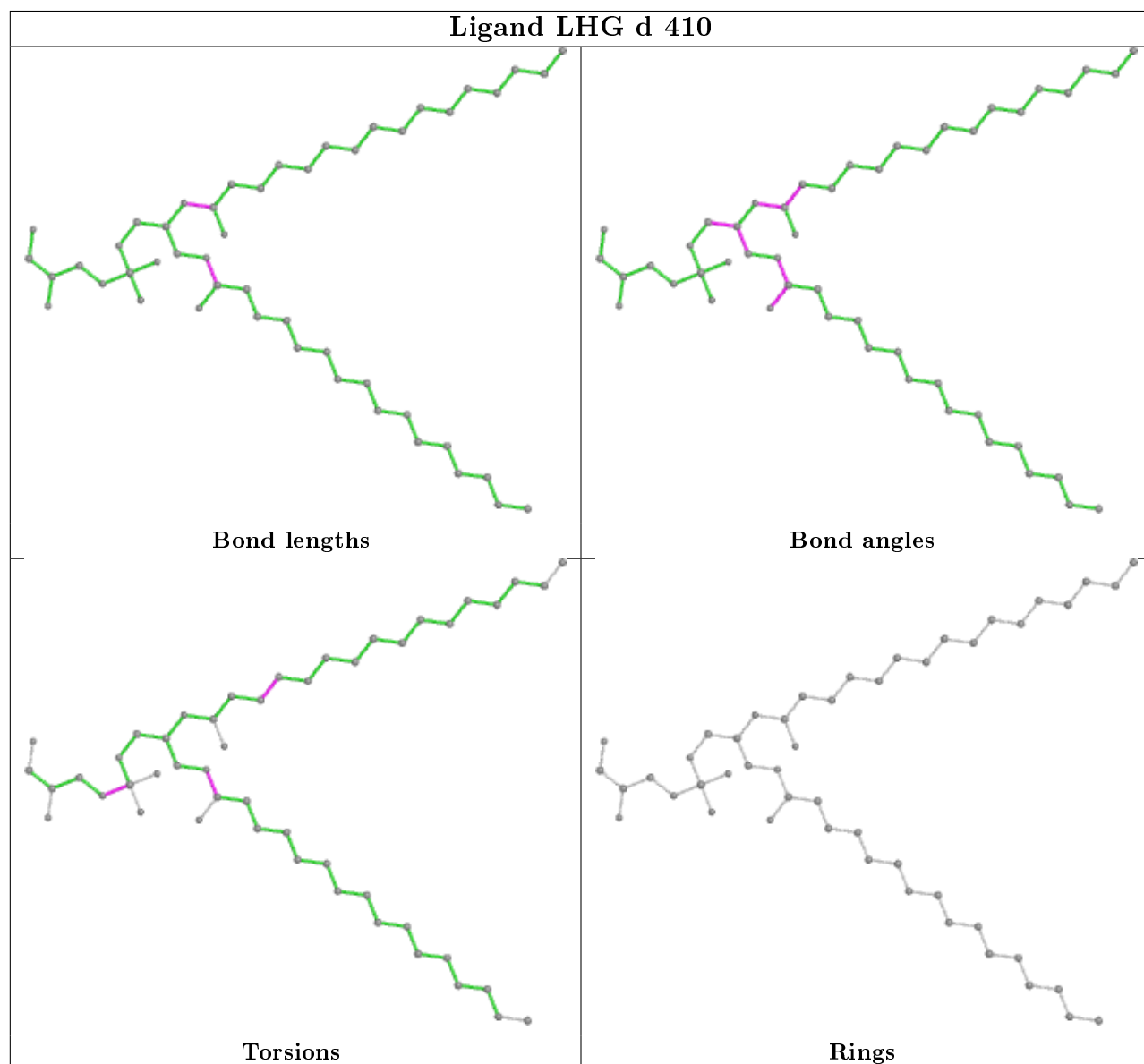
## Ligand SQD A 410



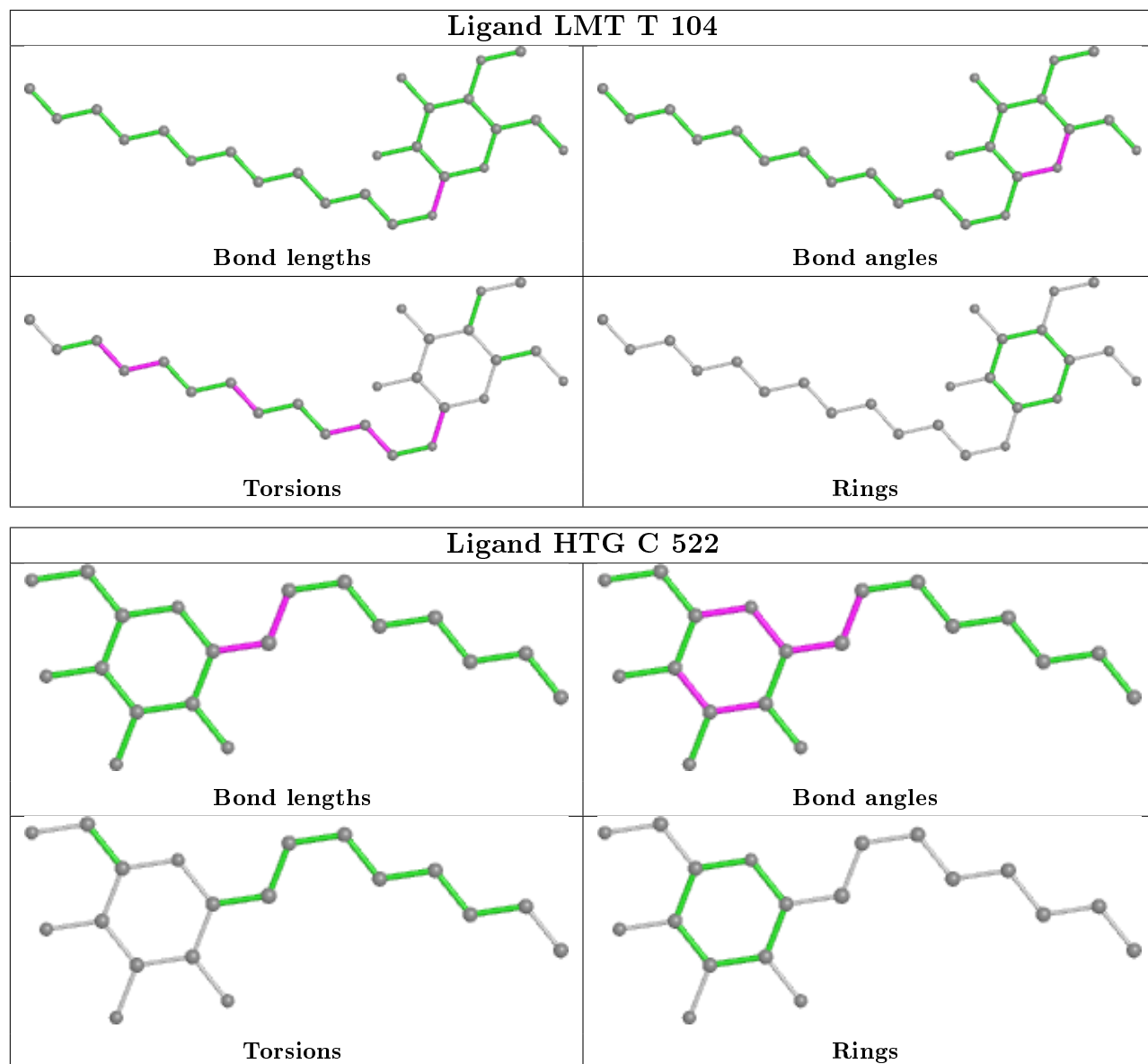
## Ligand CLA c 508

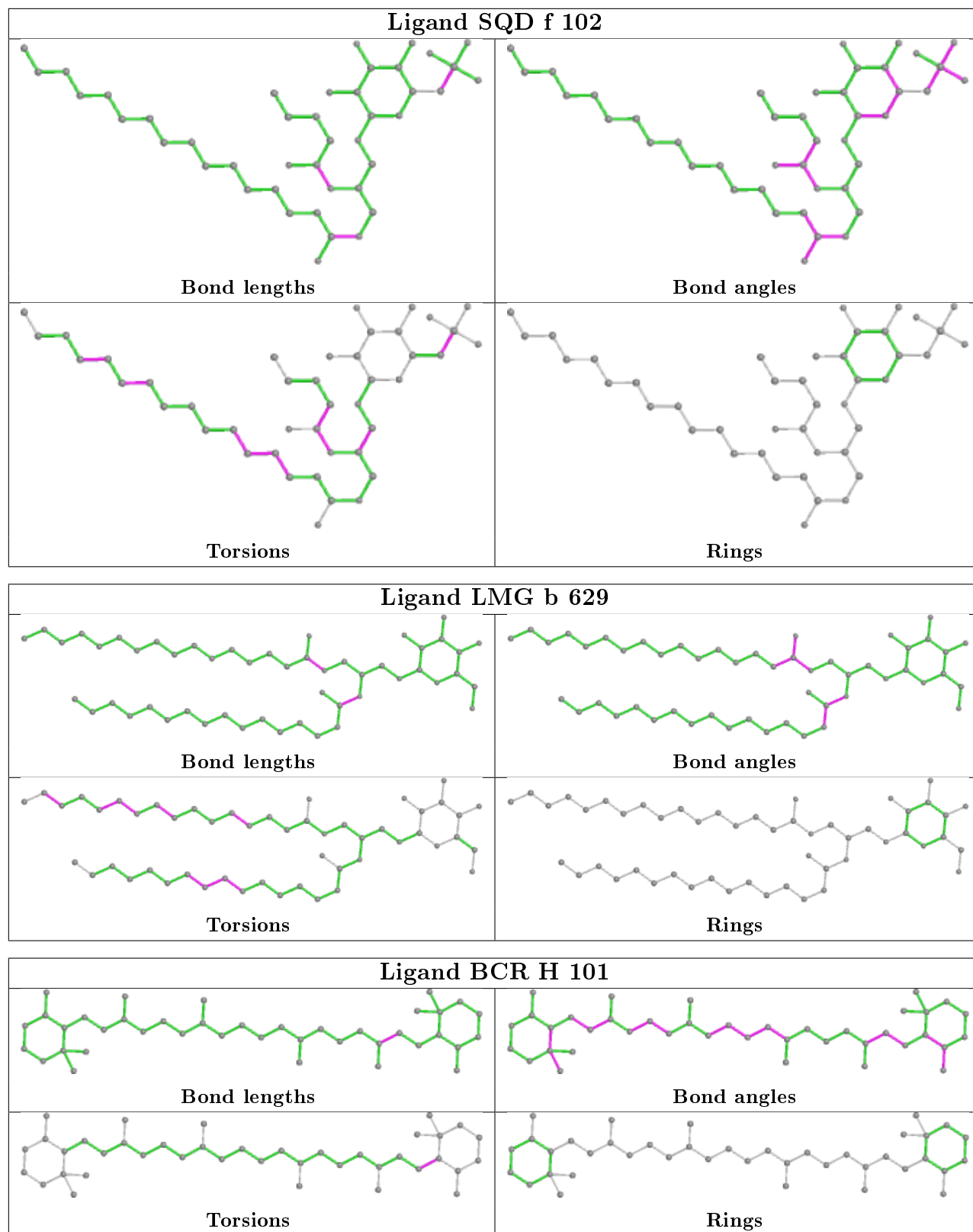


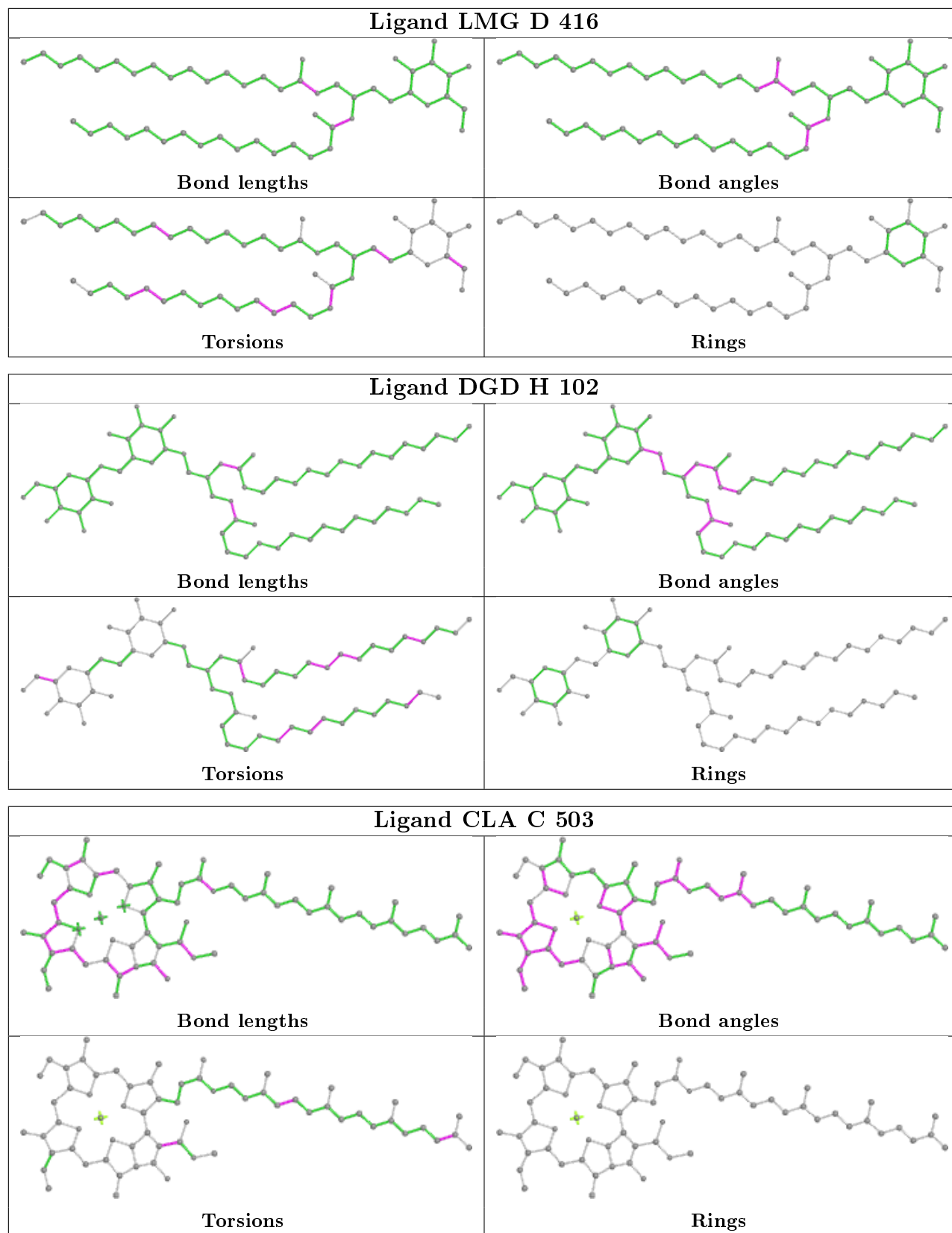
## Ligand LHG d 410



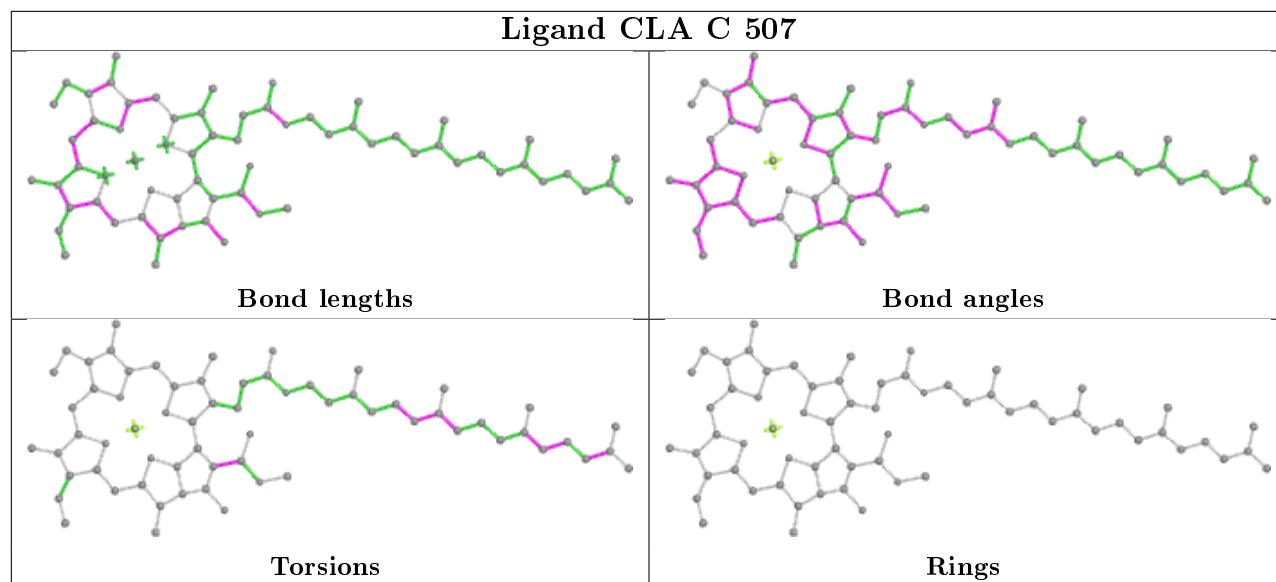




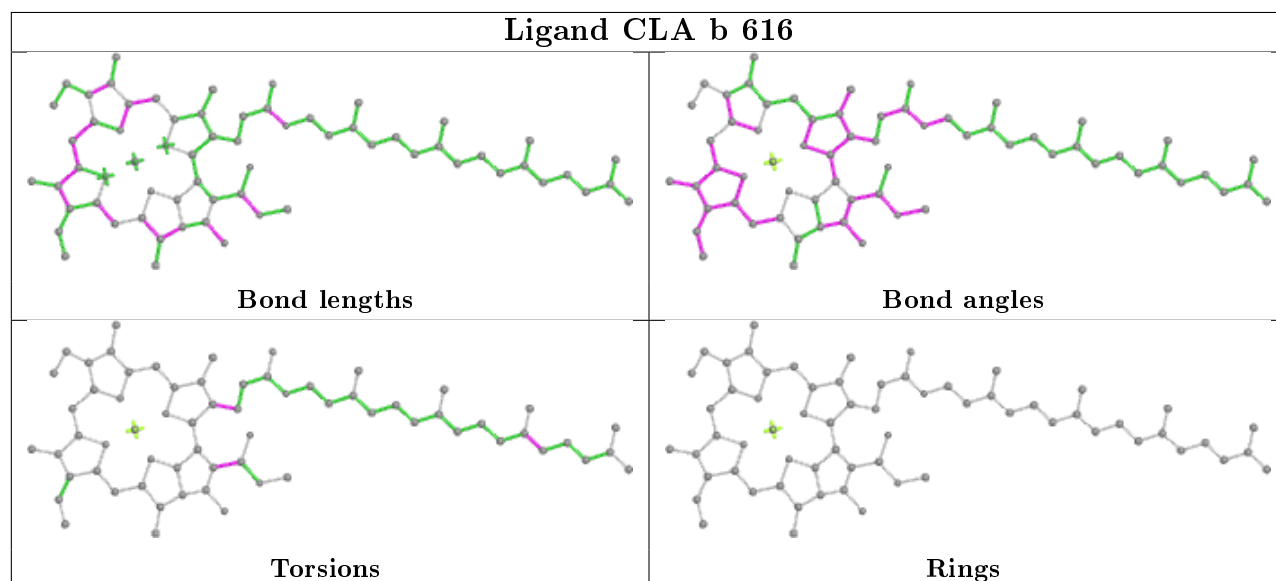




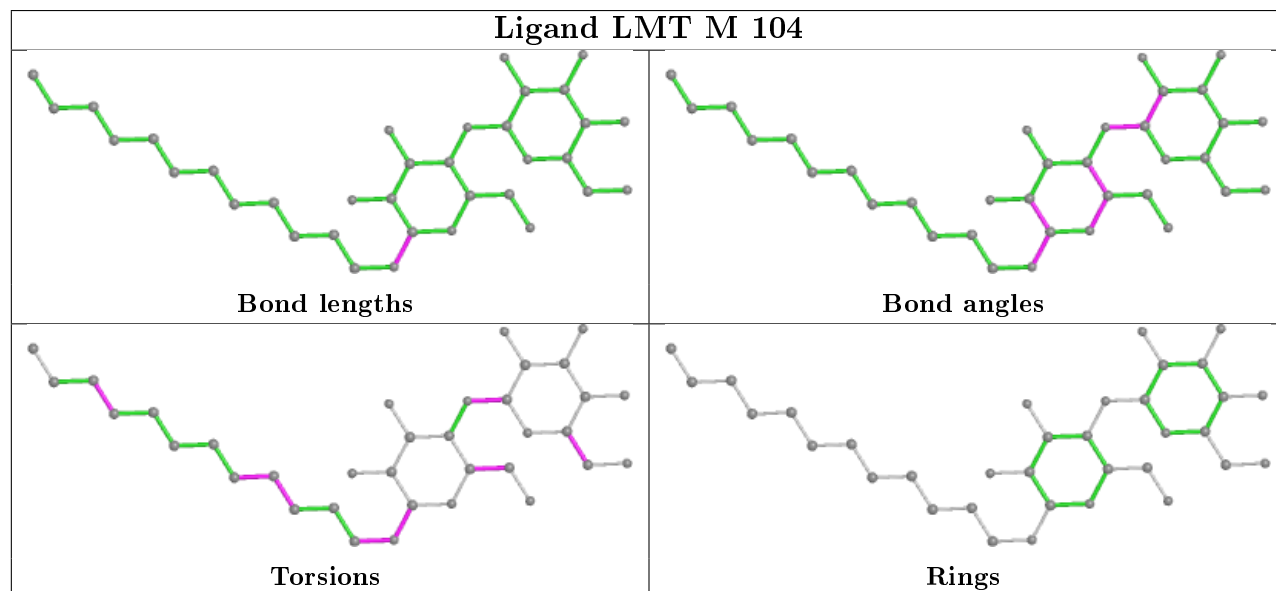
## Ligand CLA C 507



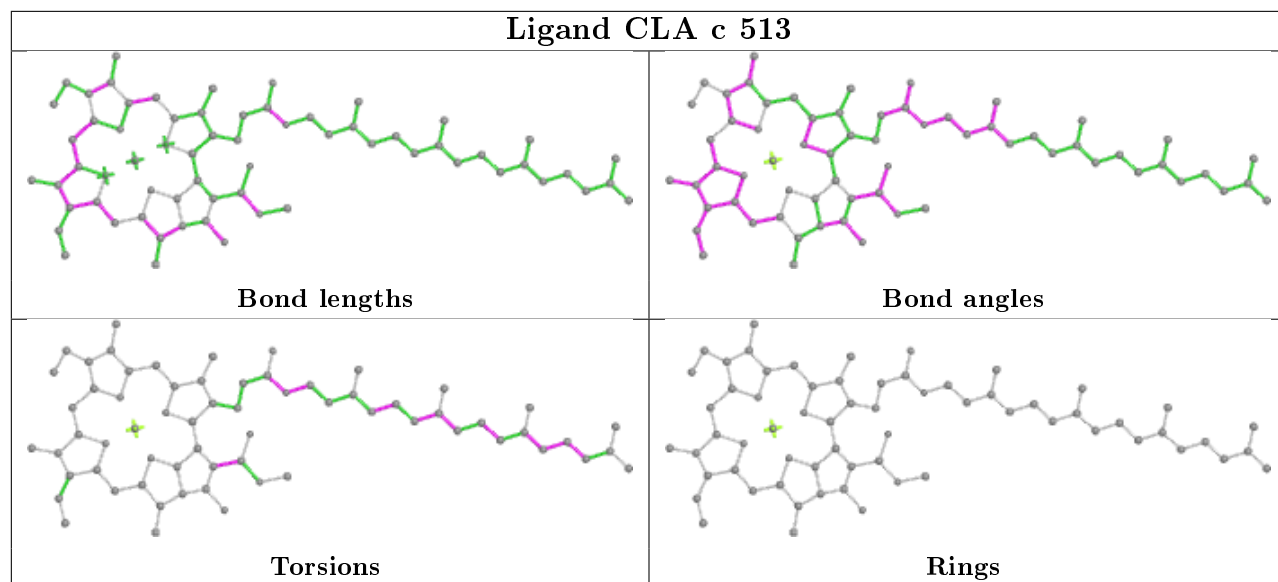
## Ligand CLA b 616



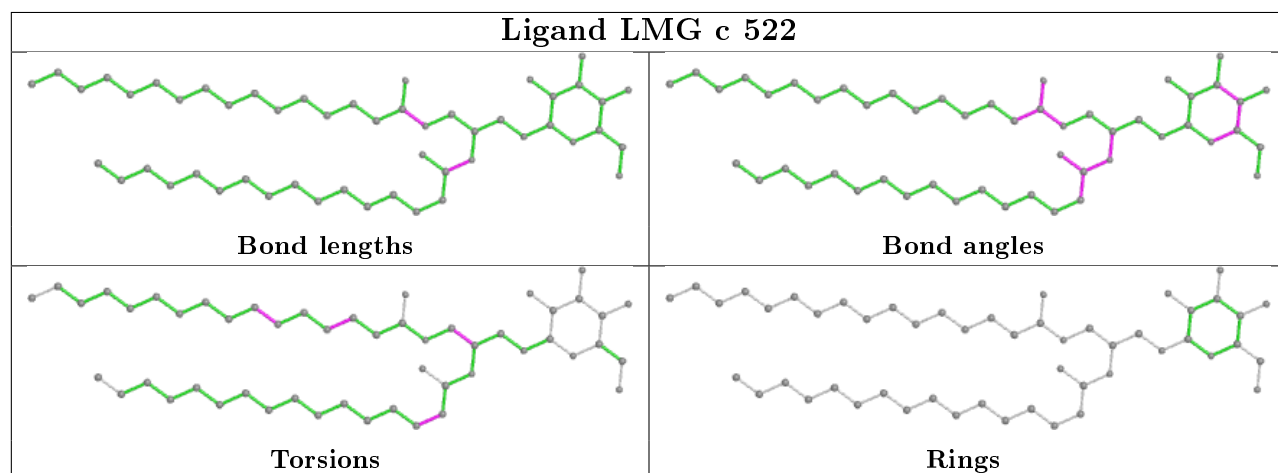
## Ligand LMT M 104



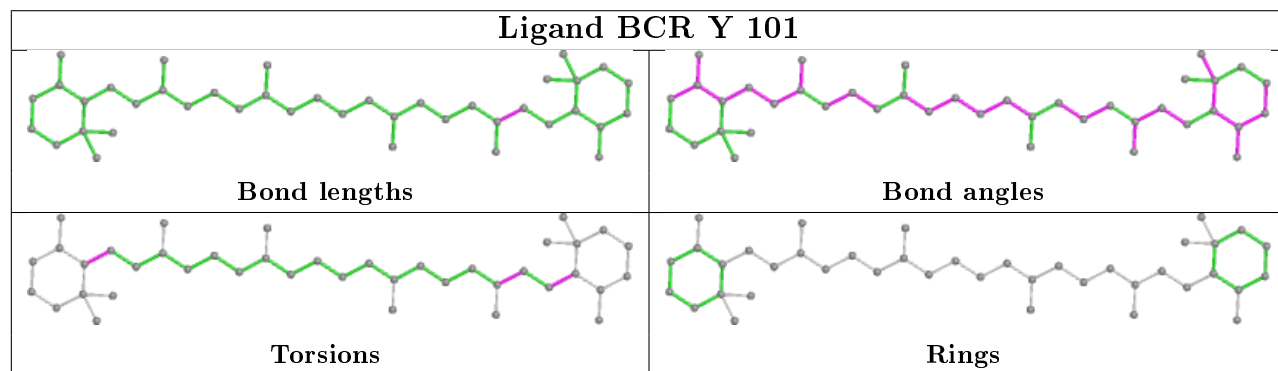
## Ligand CLA c 513



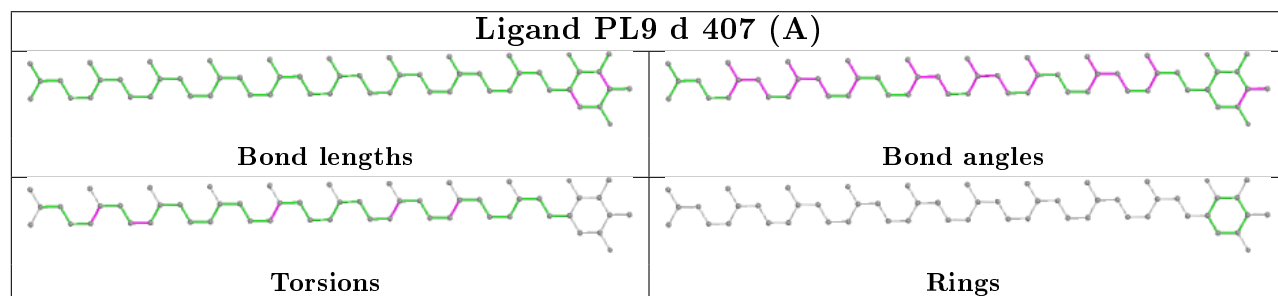
## Ligand LMG c 522

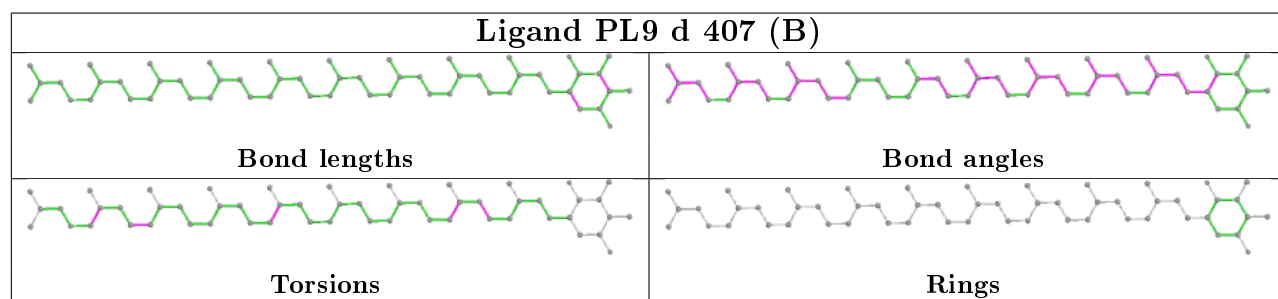
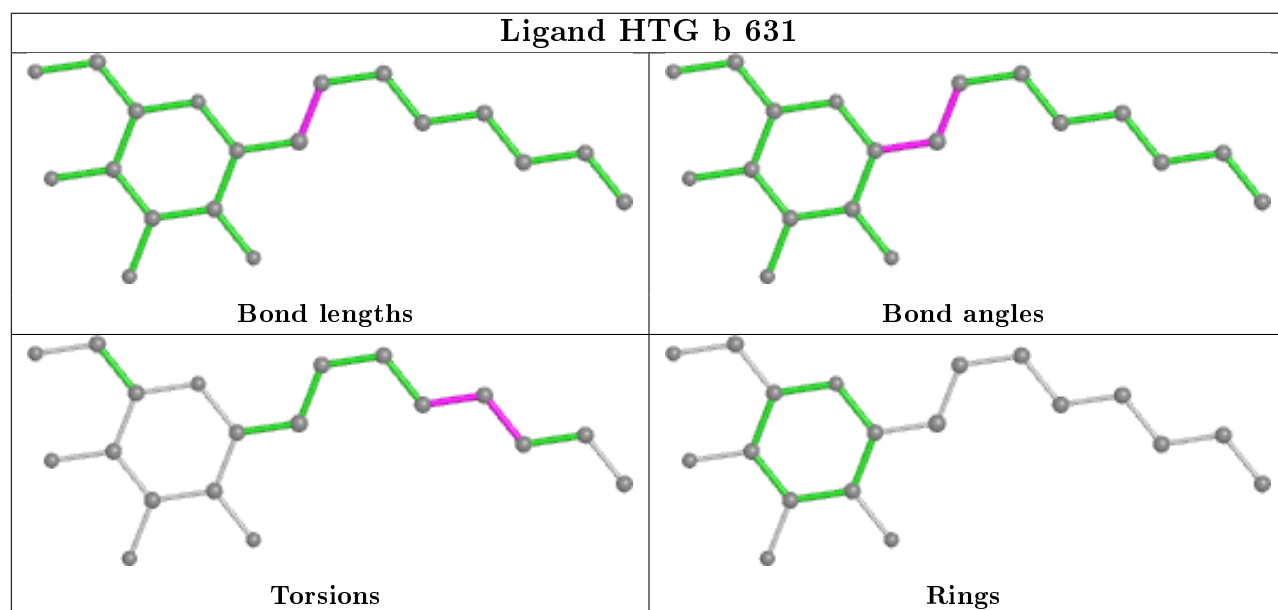
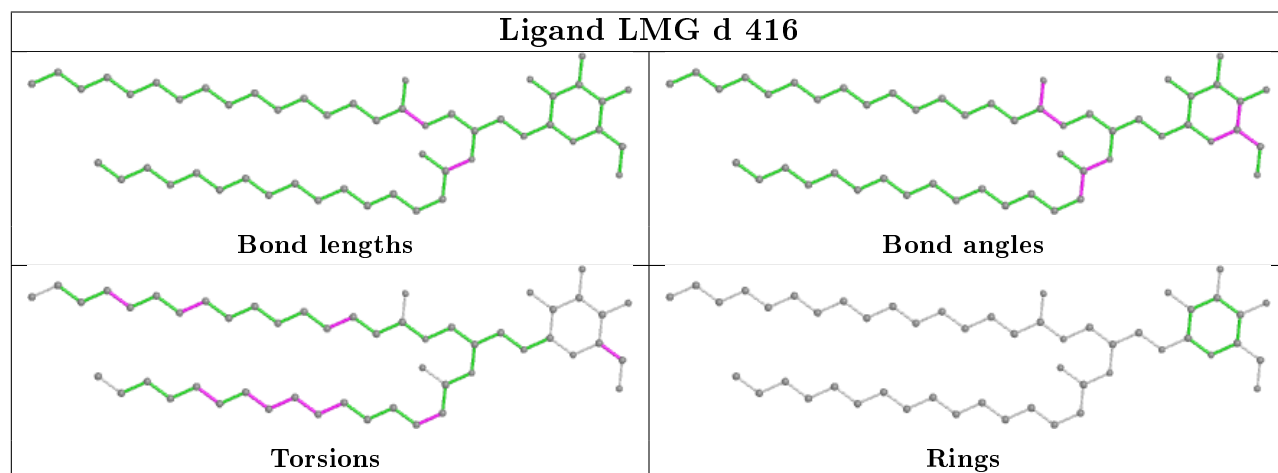
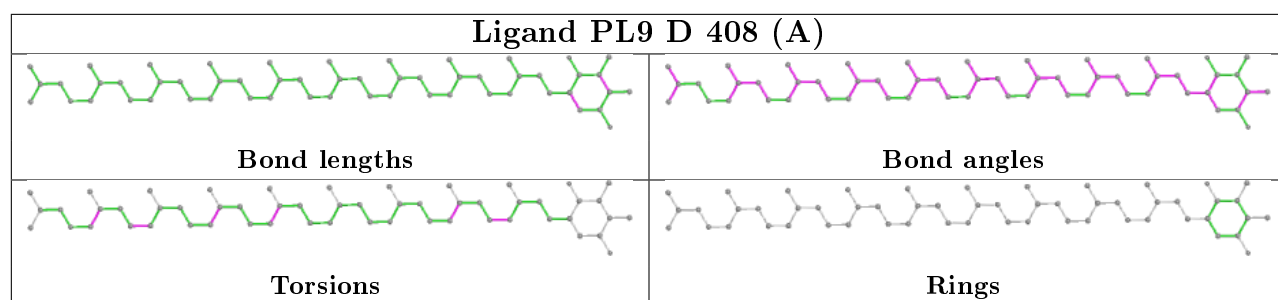


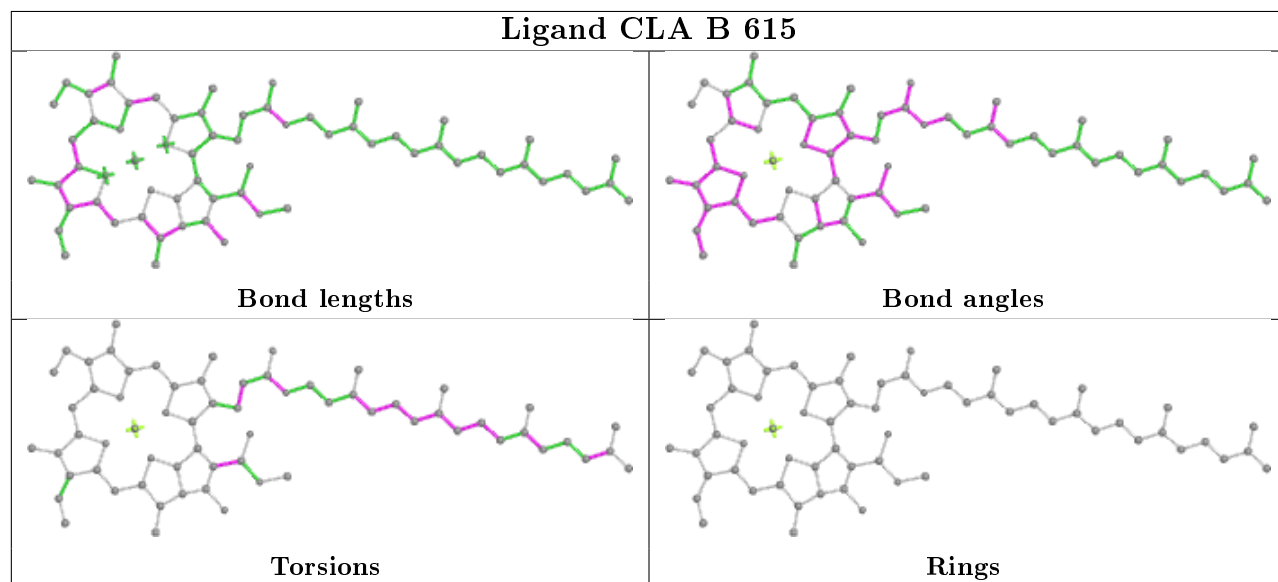
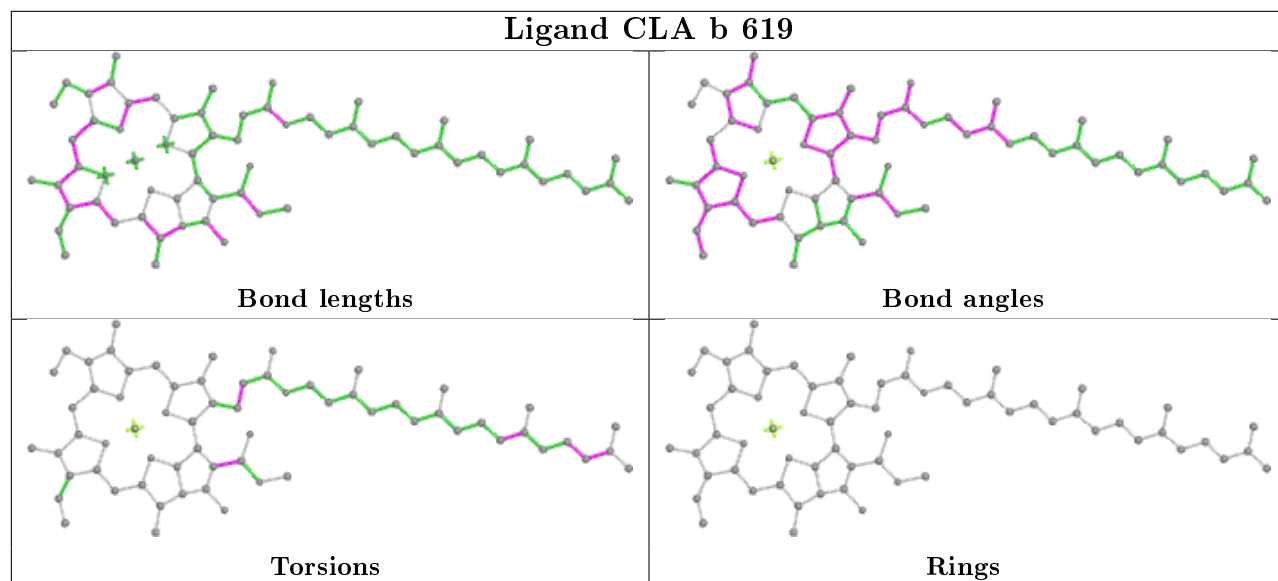
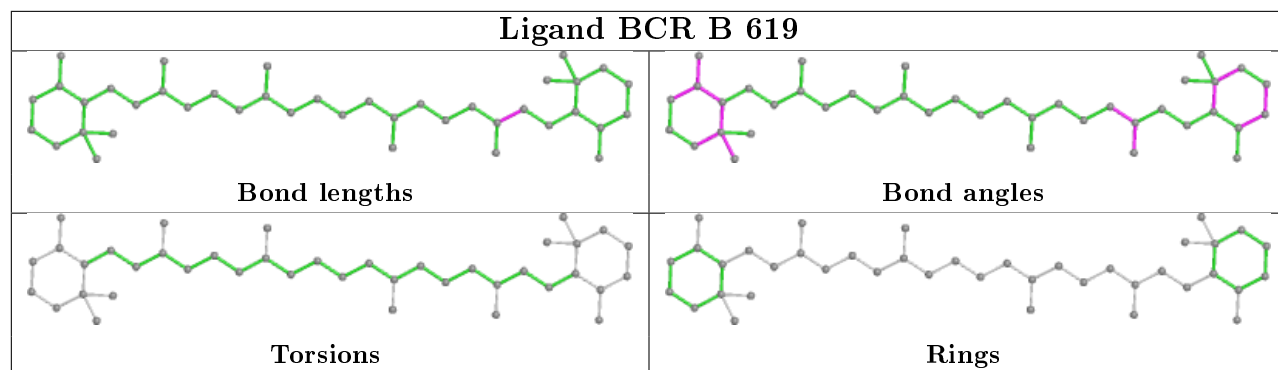
## Ligand BCR Y 101



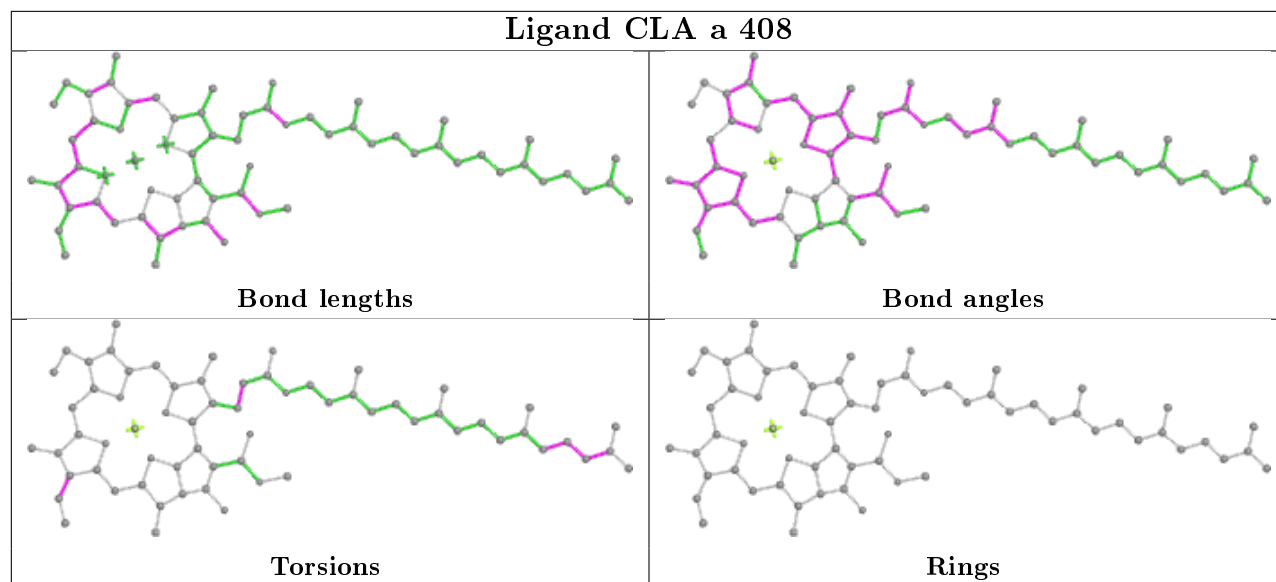
## Ligand PL9 d 407 (A)



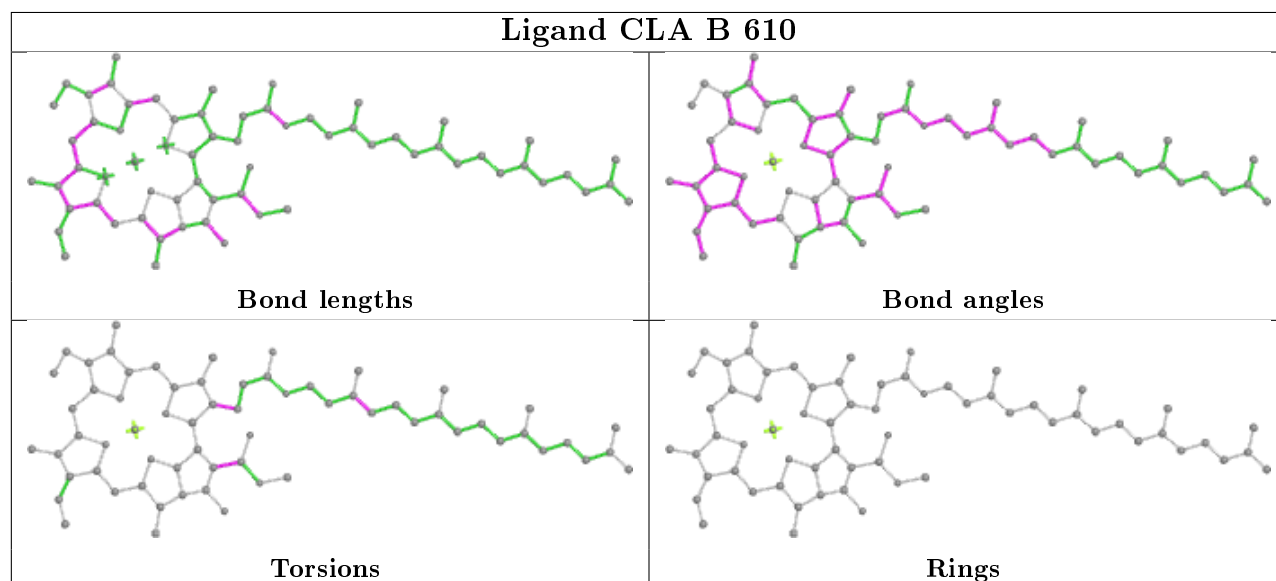




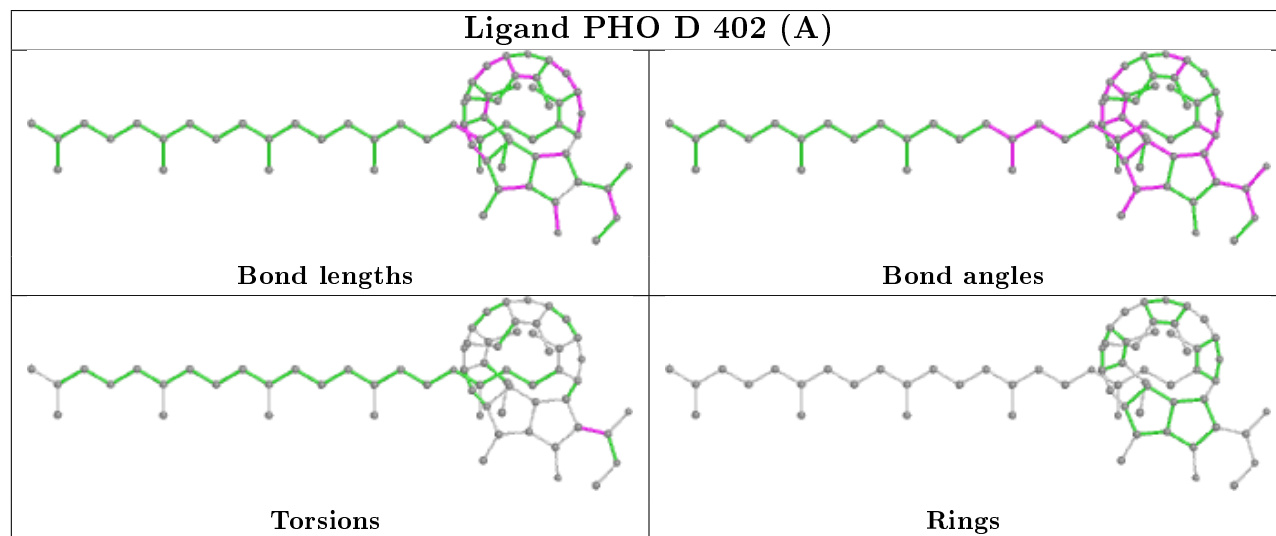
## Ligand CLA a 408



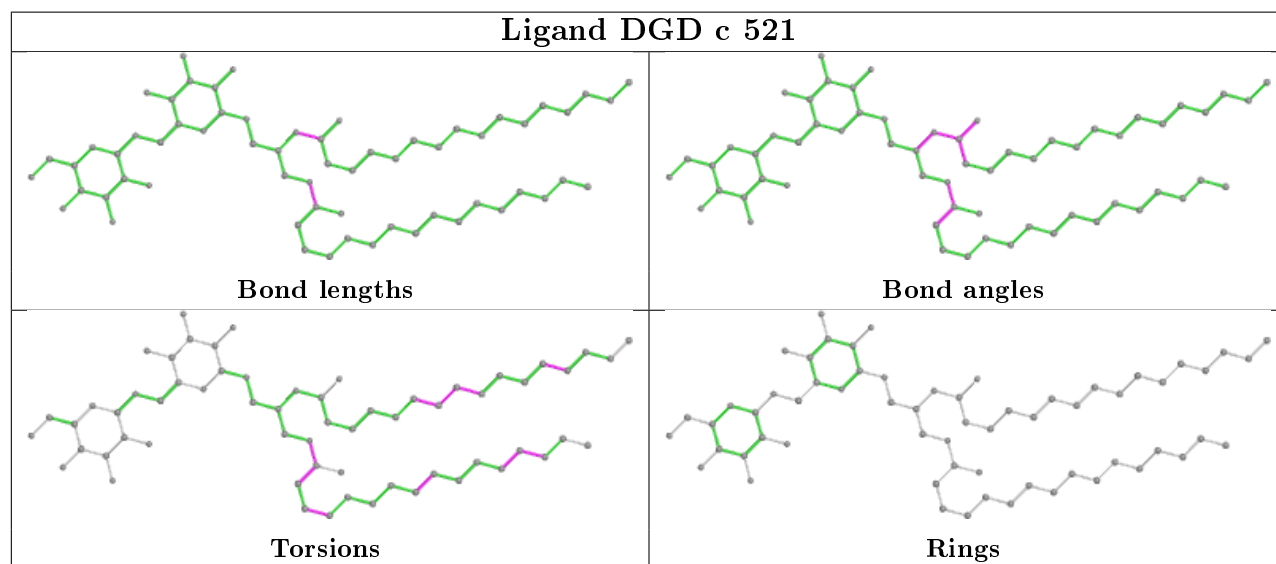
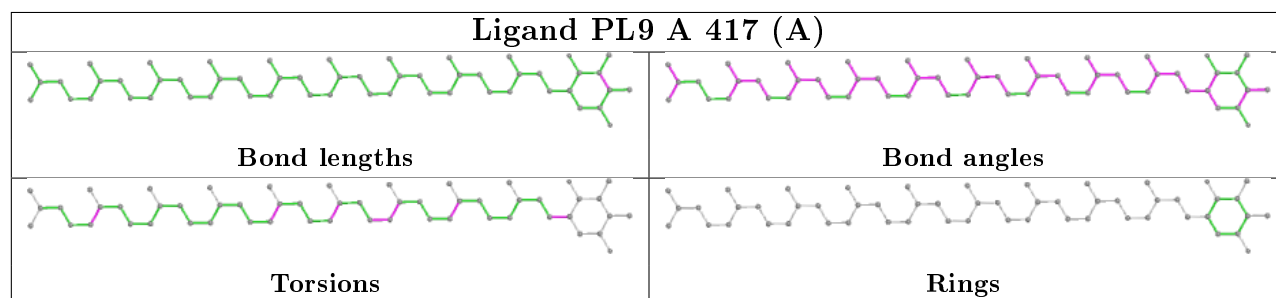
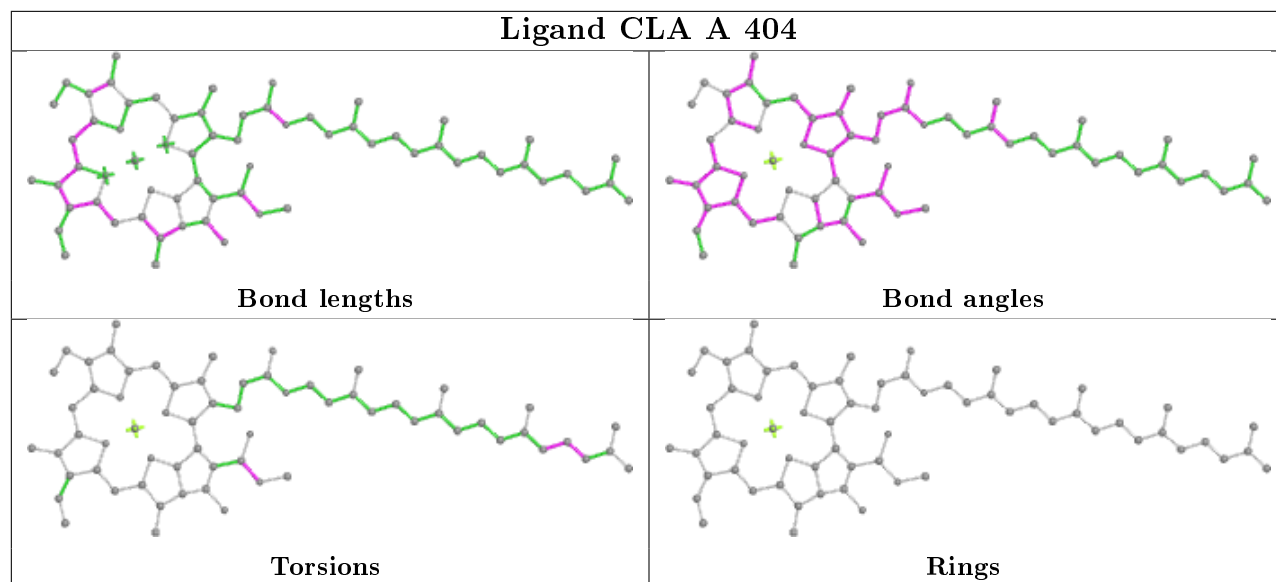
## Ligand CLA B 610



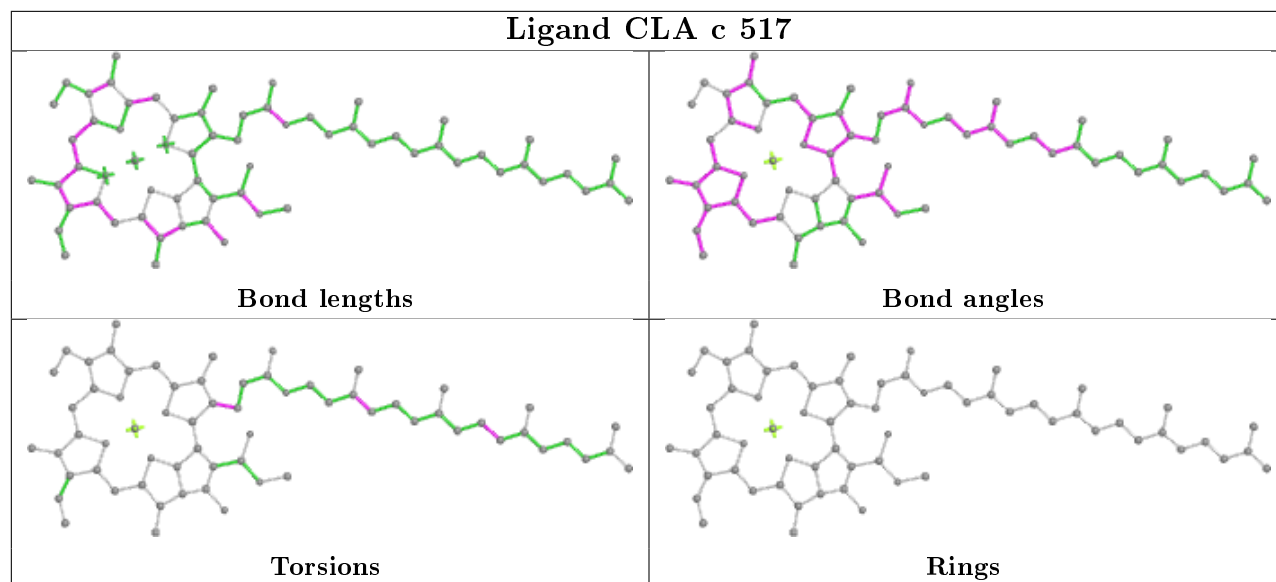
## Ligand PHO D 402 (A)



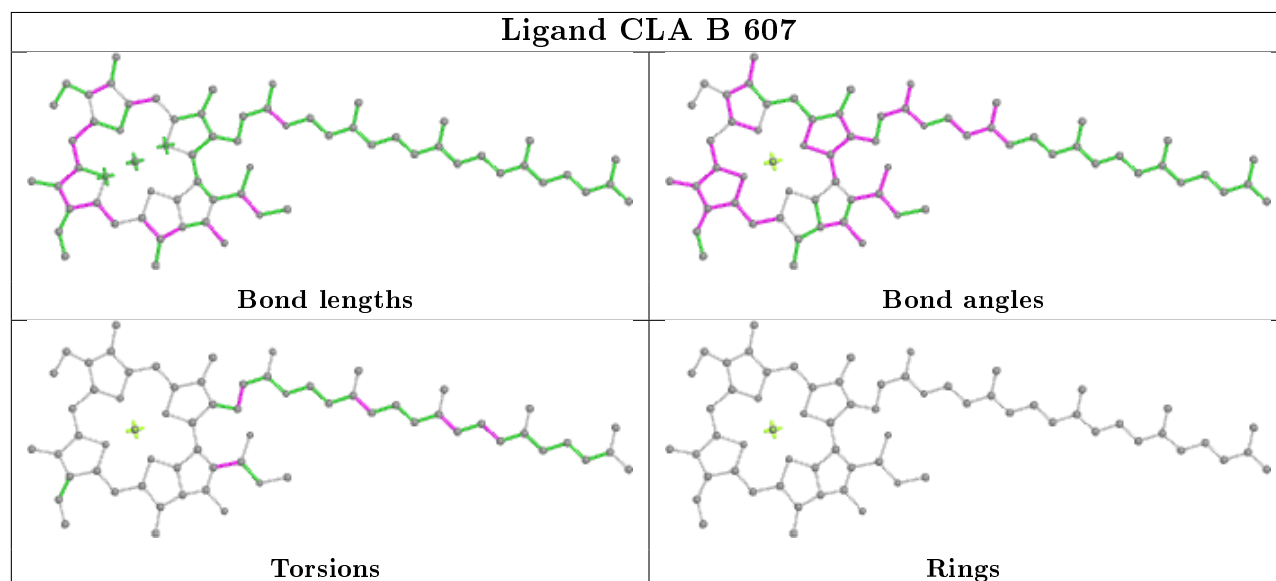




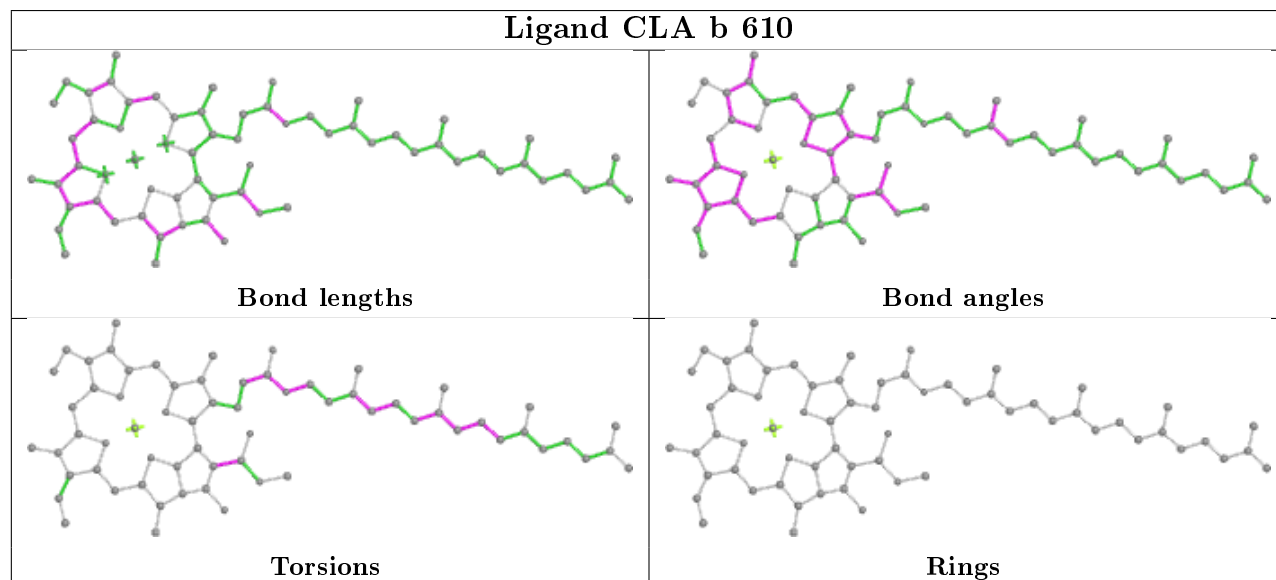
## Ligand CLA c 517

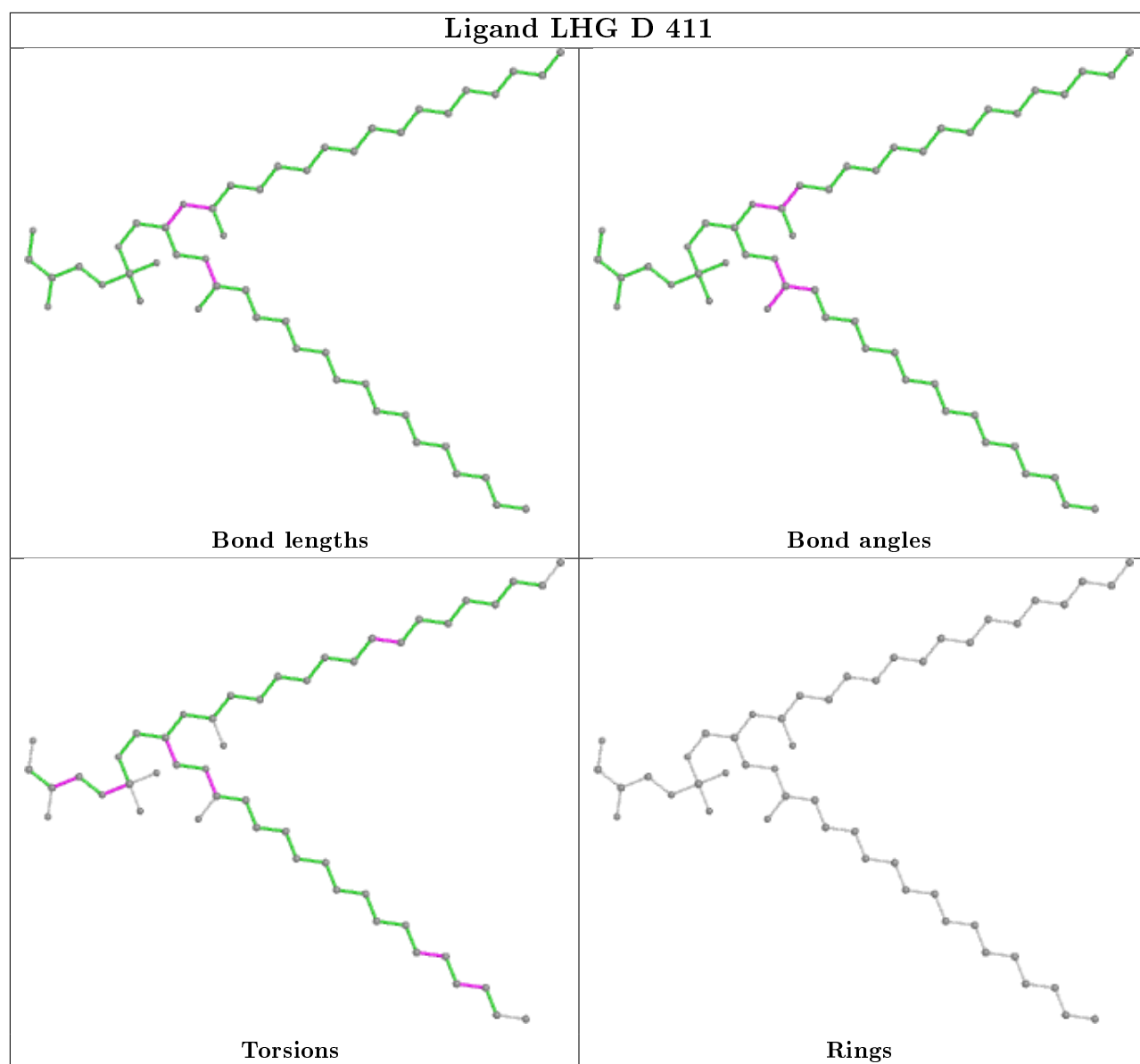


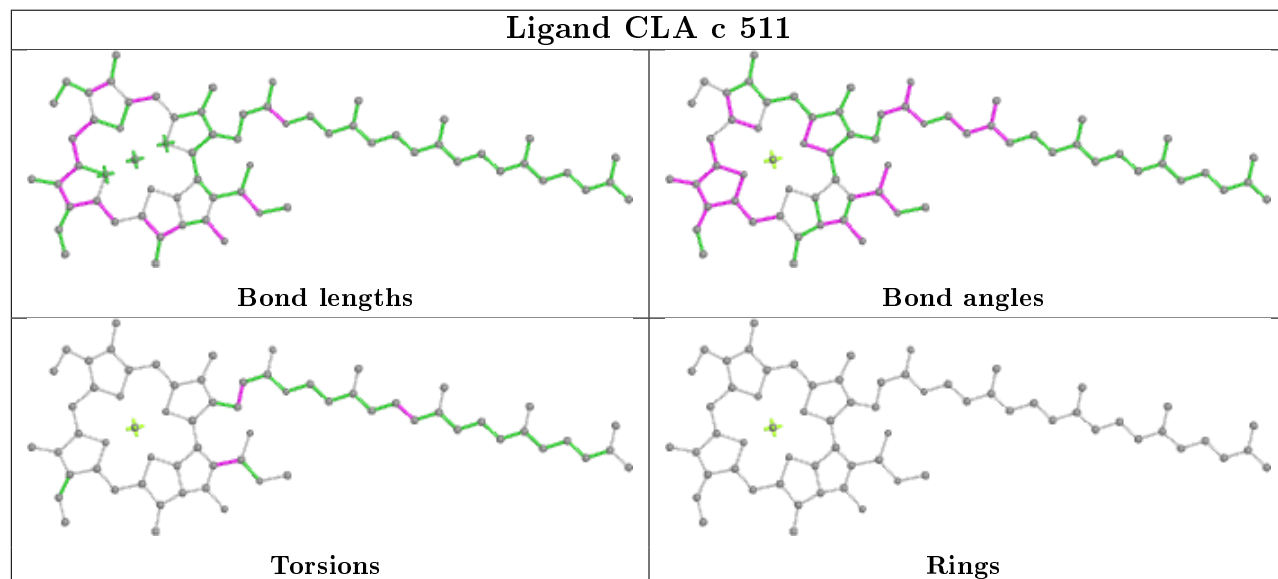
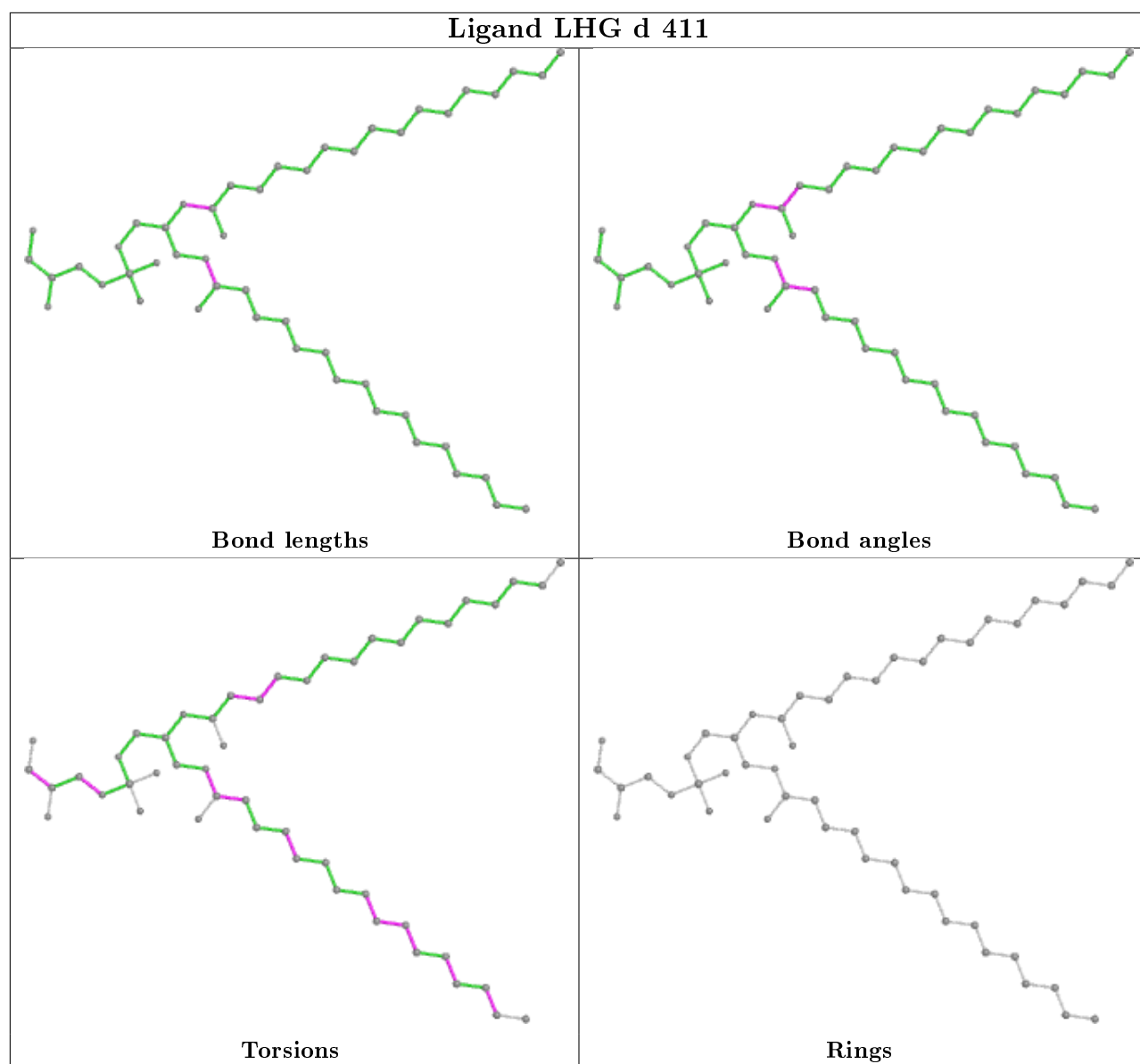
## Ligand CLA B 607

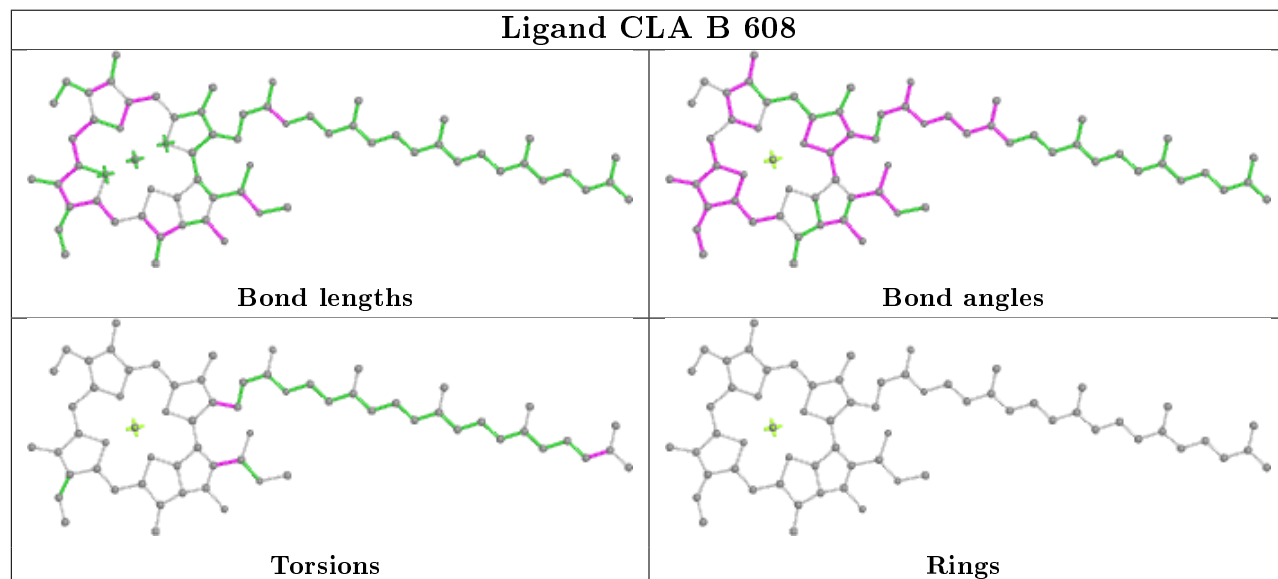
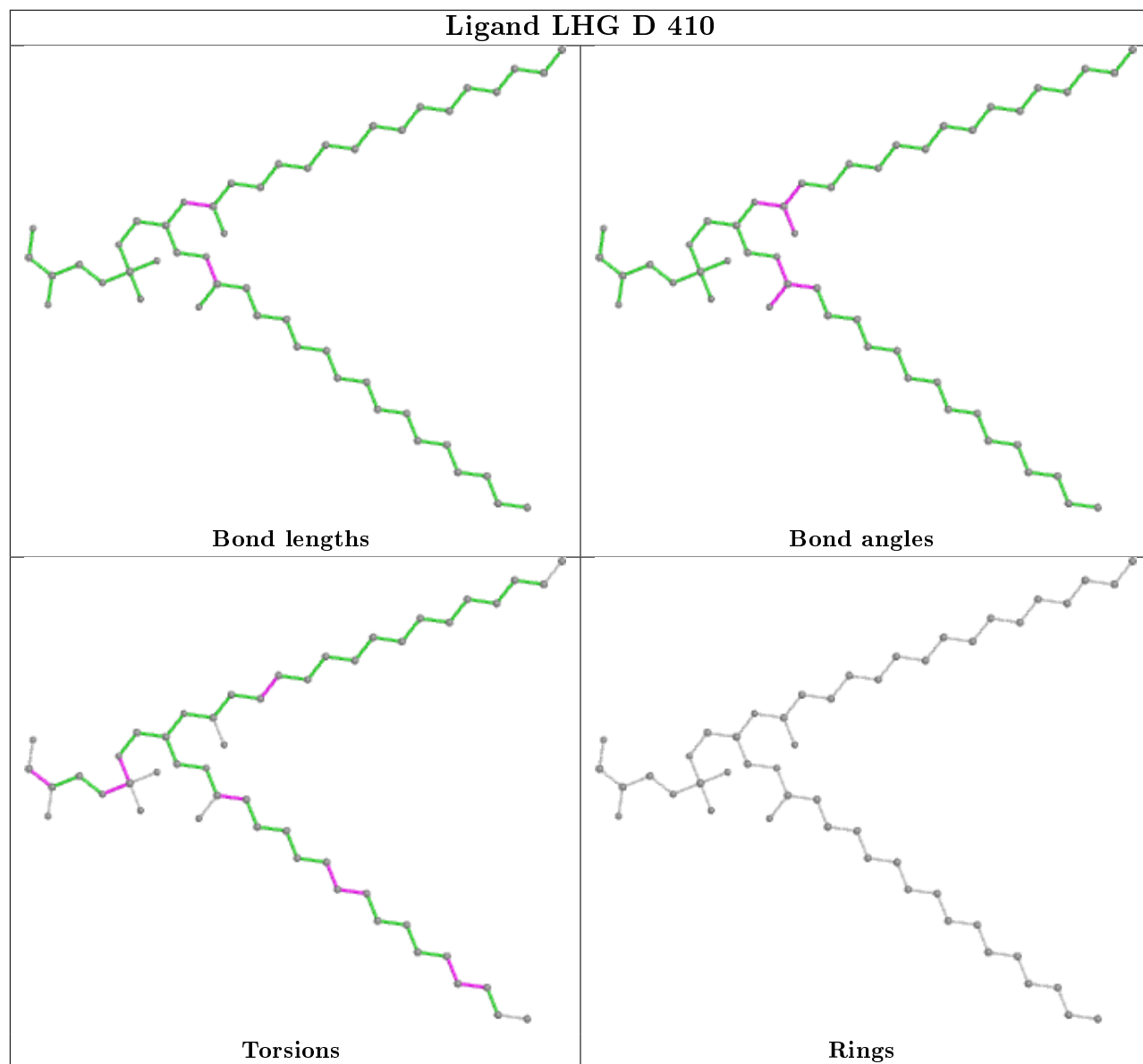


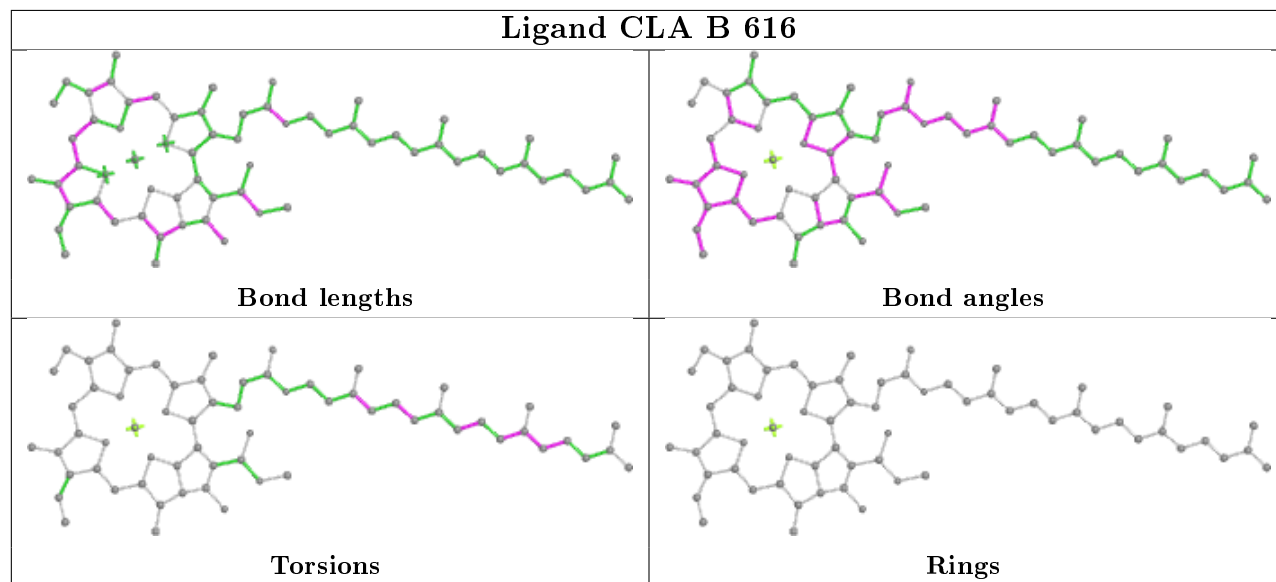
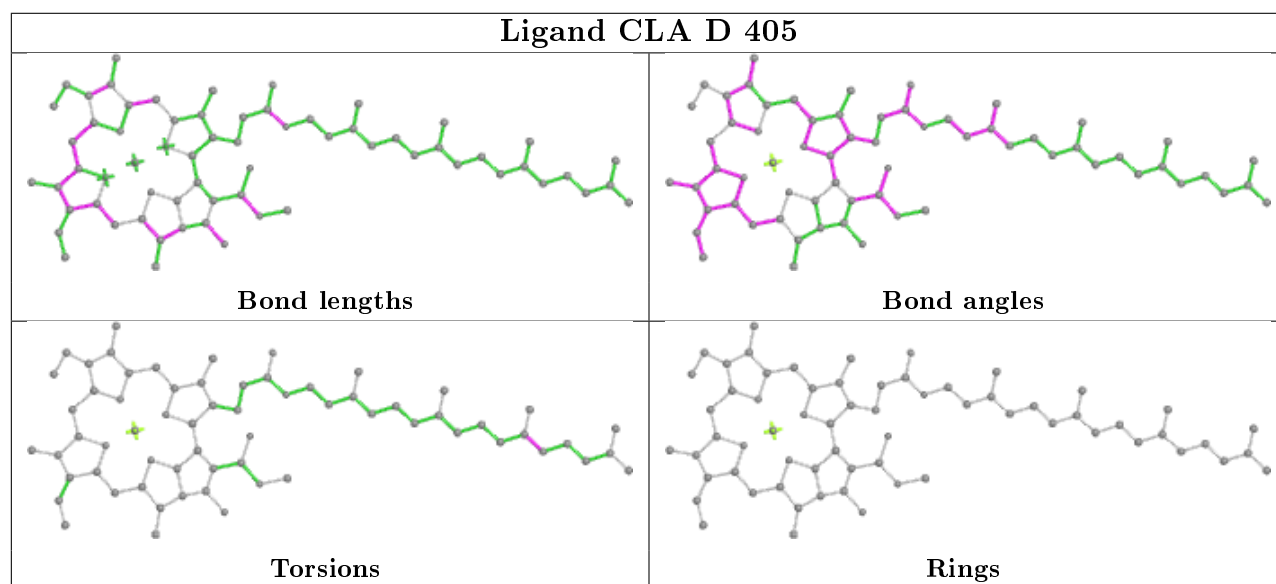
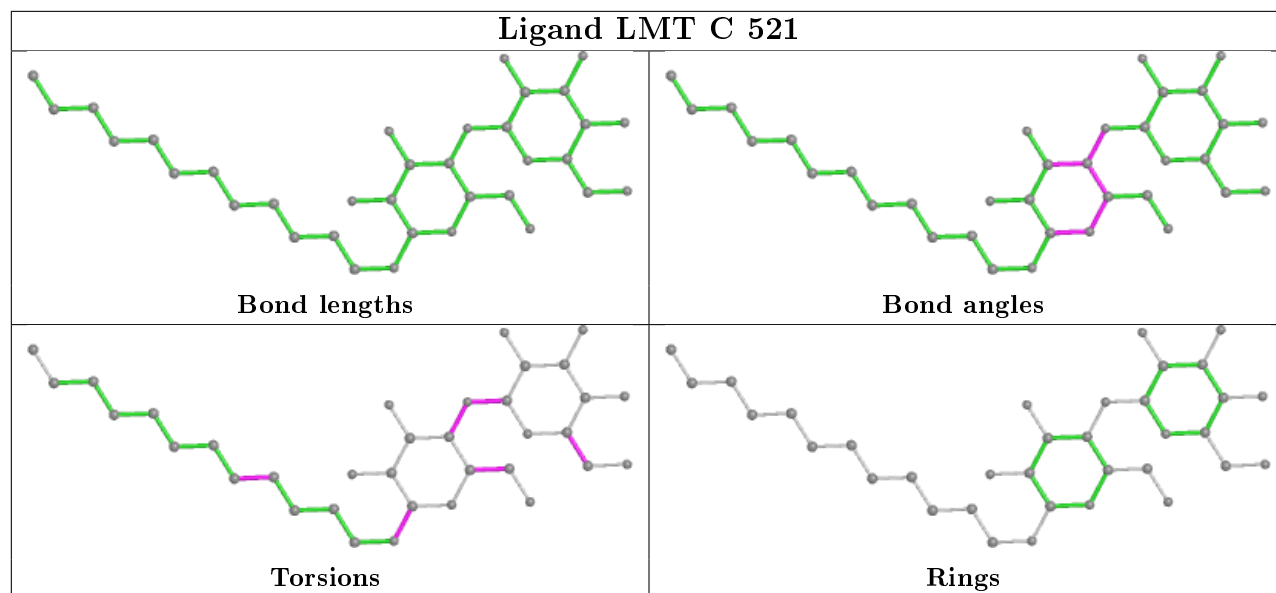
## Ligand CLA b 610

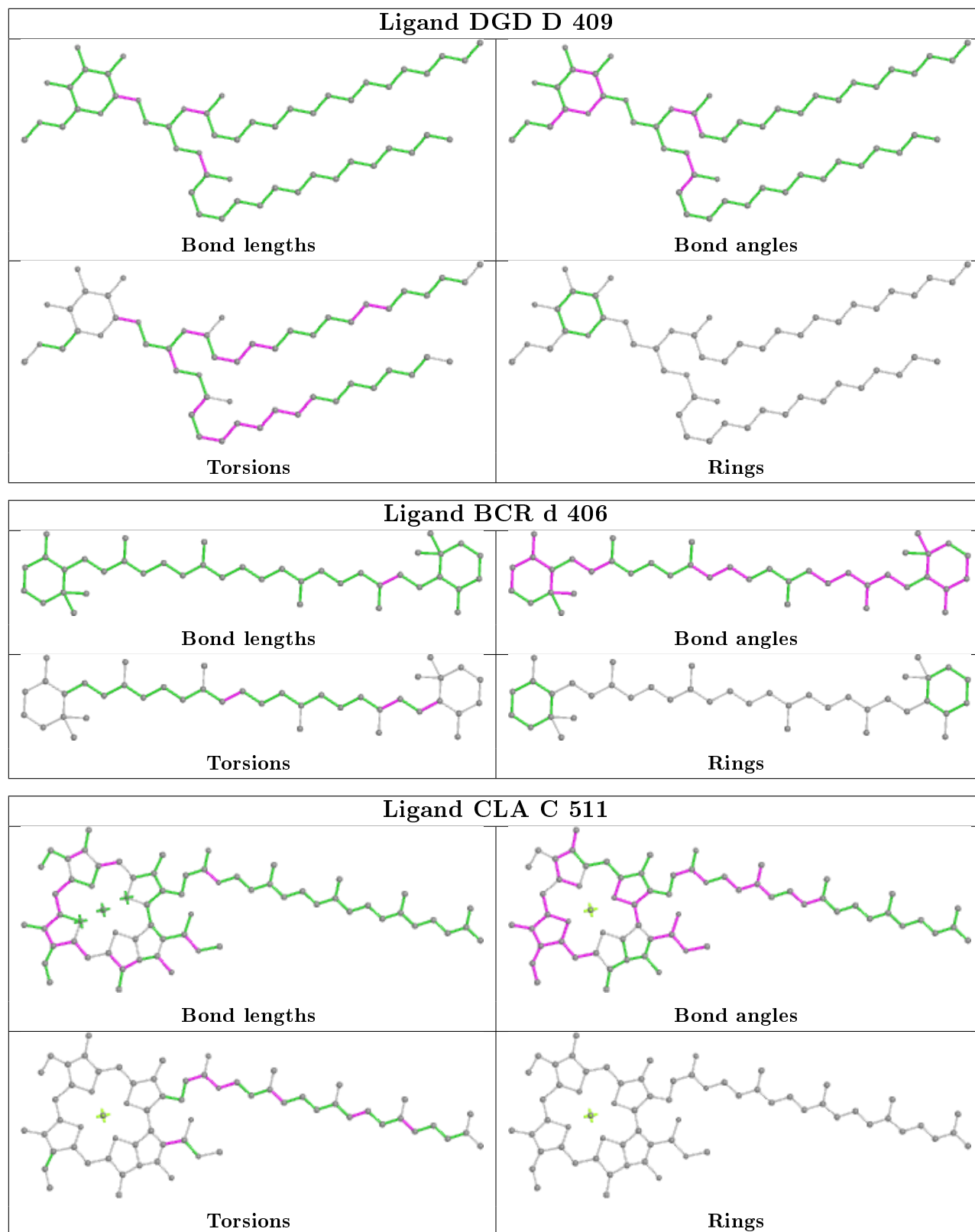


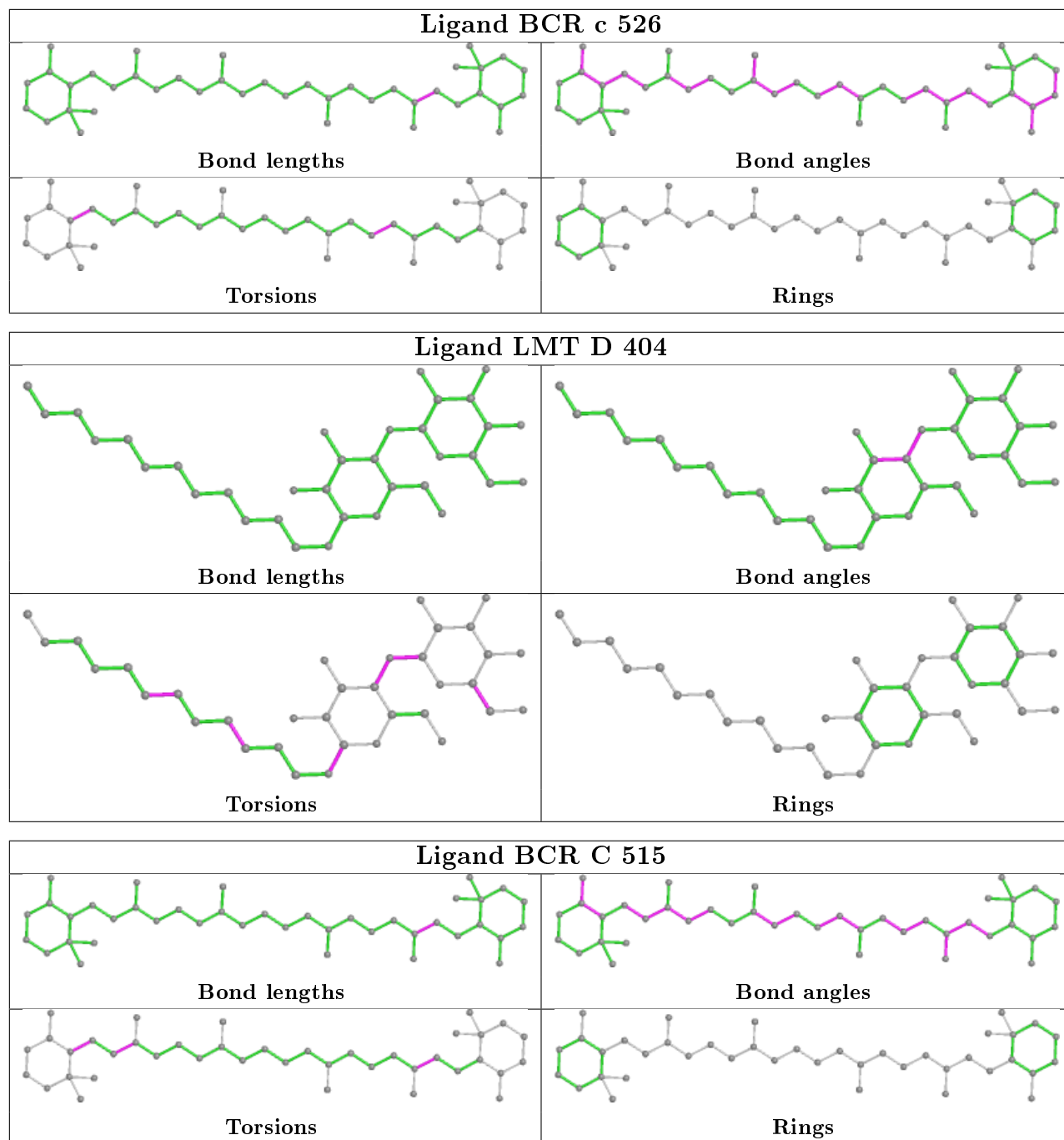




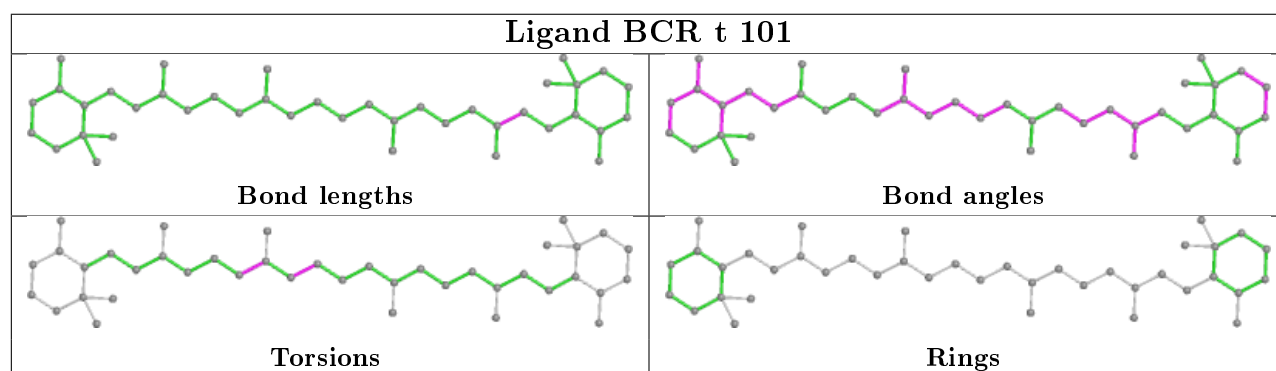
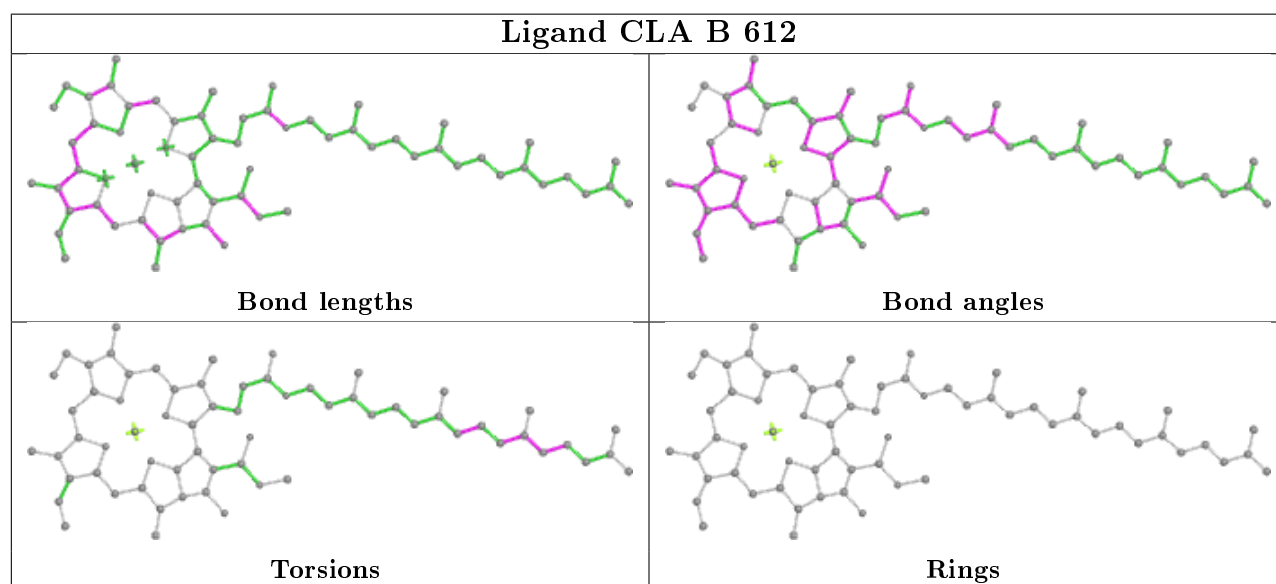
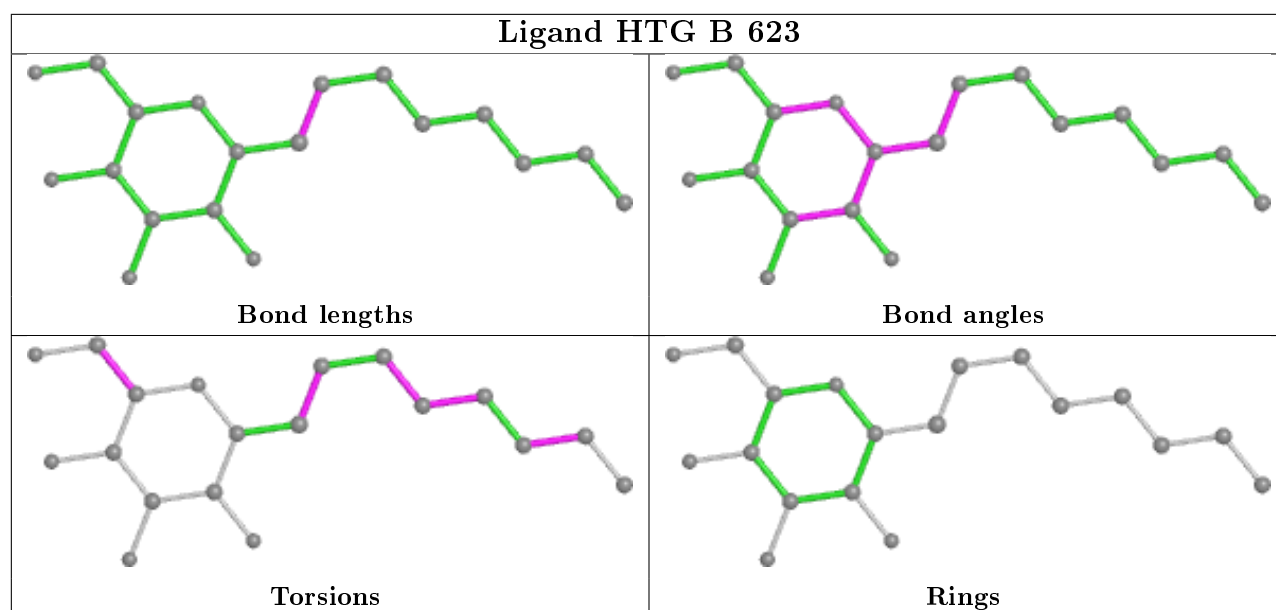


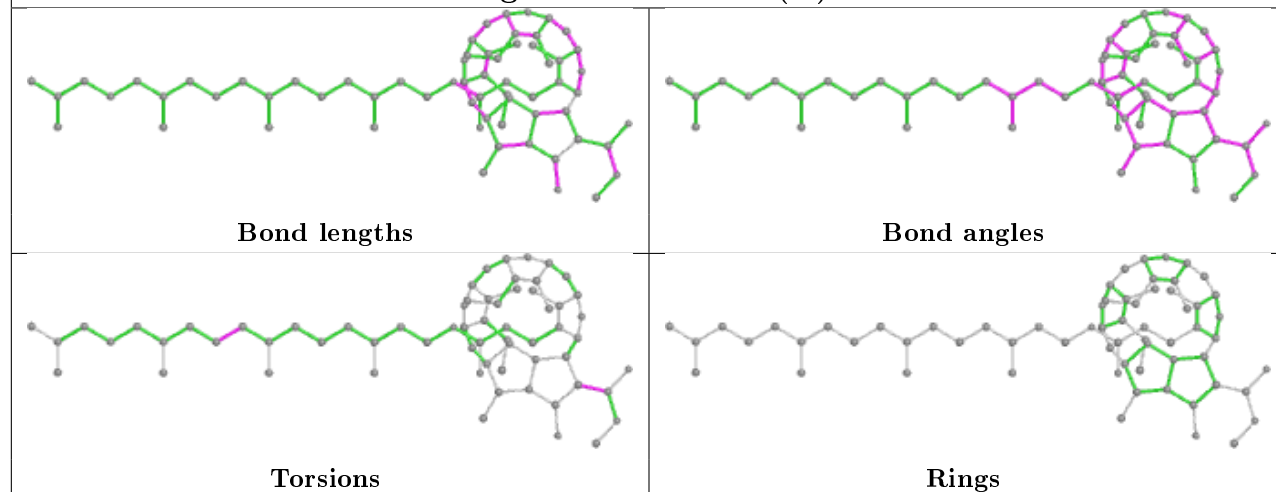
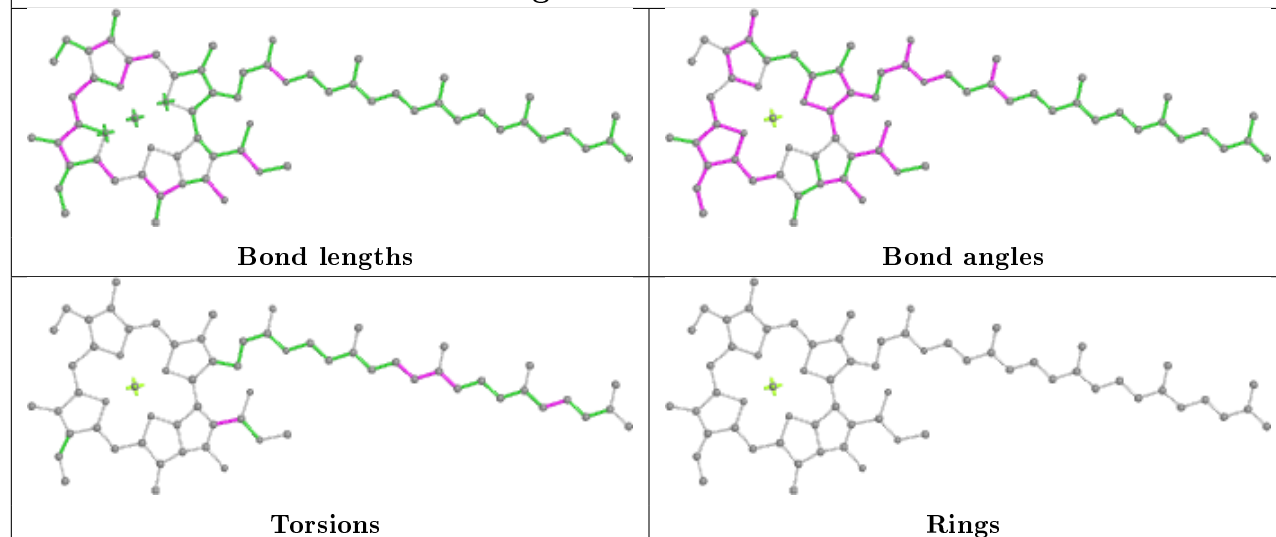
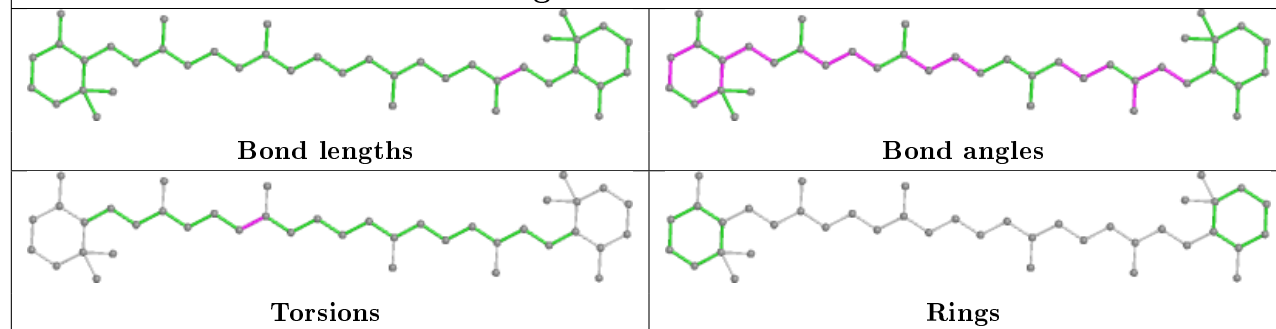


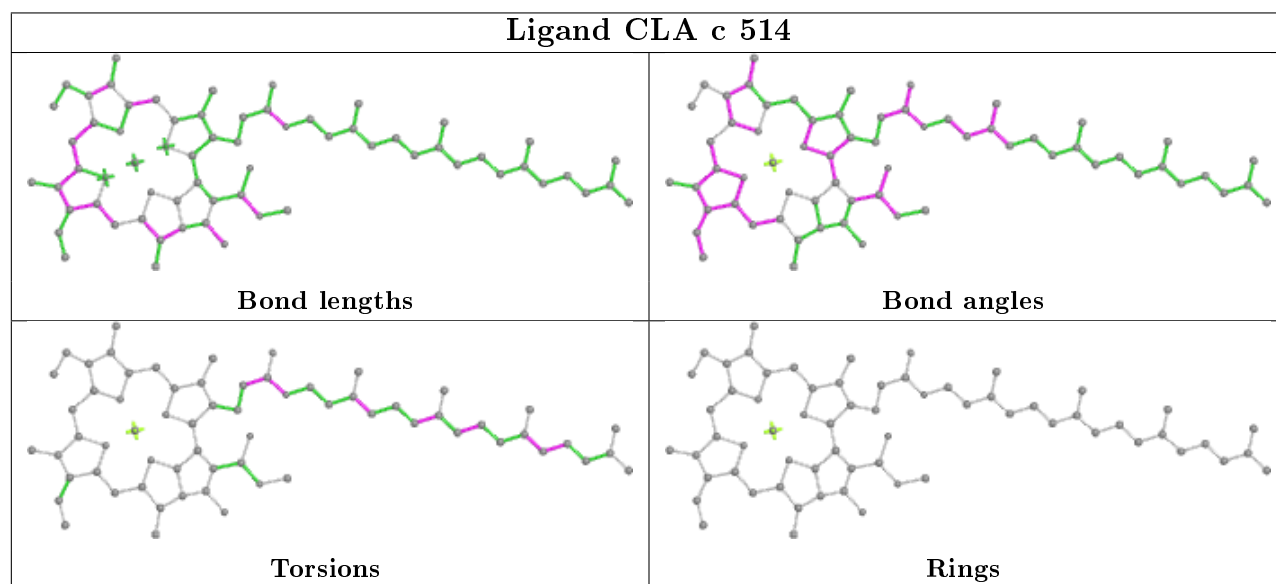
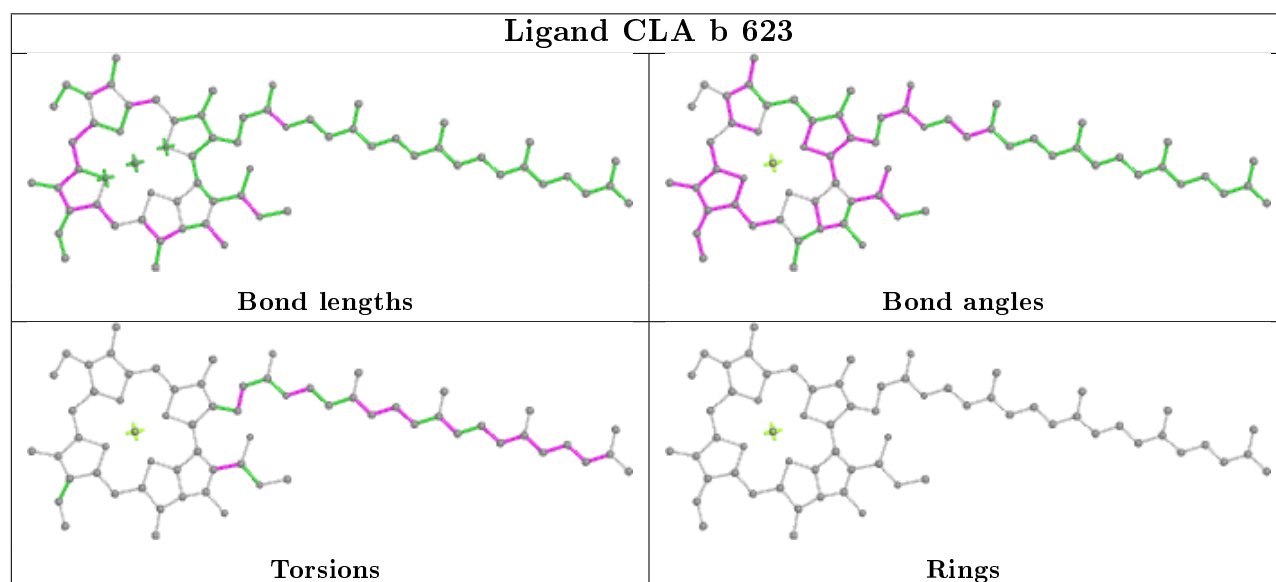
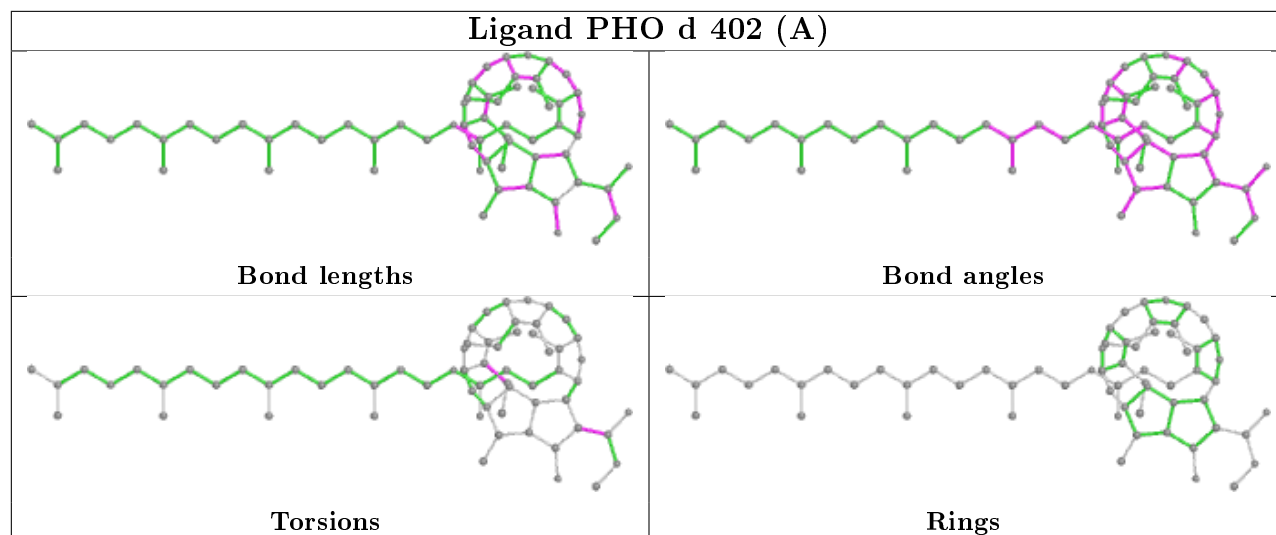




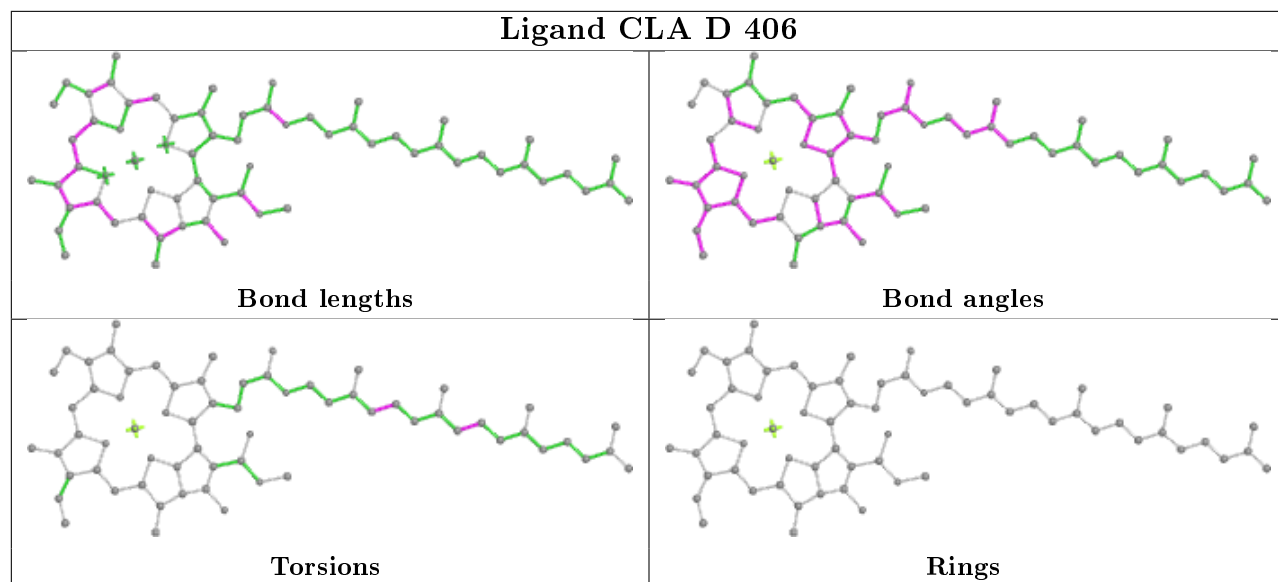




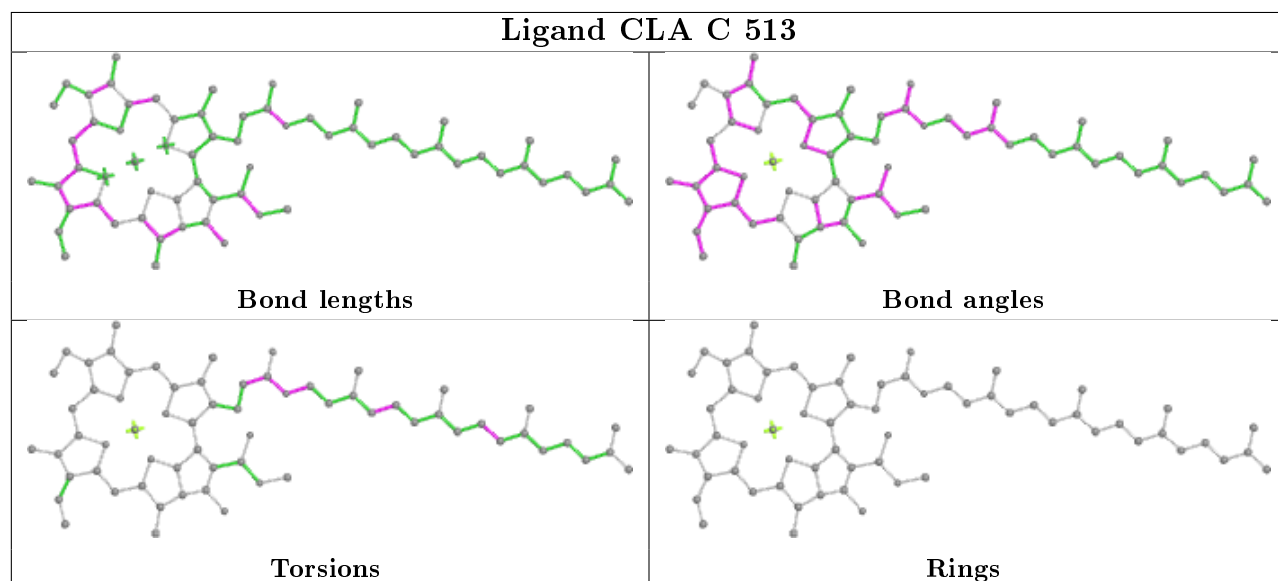
**Ligand PHO d 402 (B)****Ligand CLA B 604****Ligand BCR b 628**



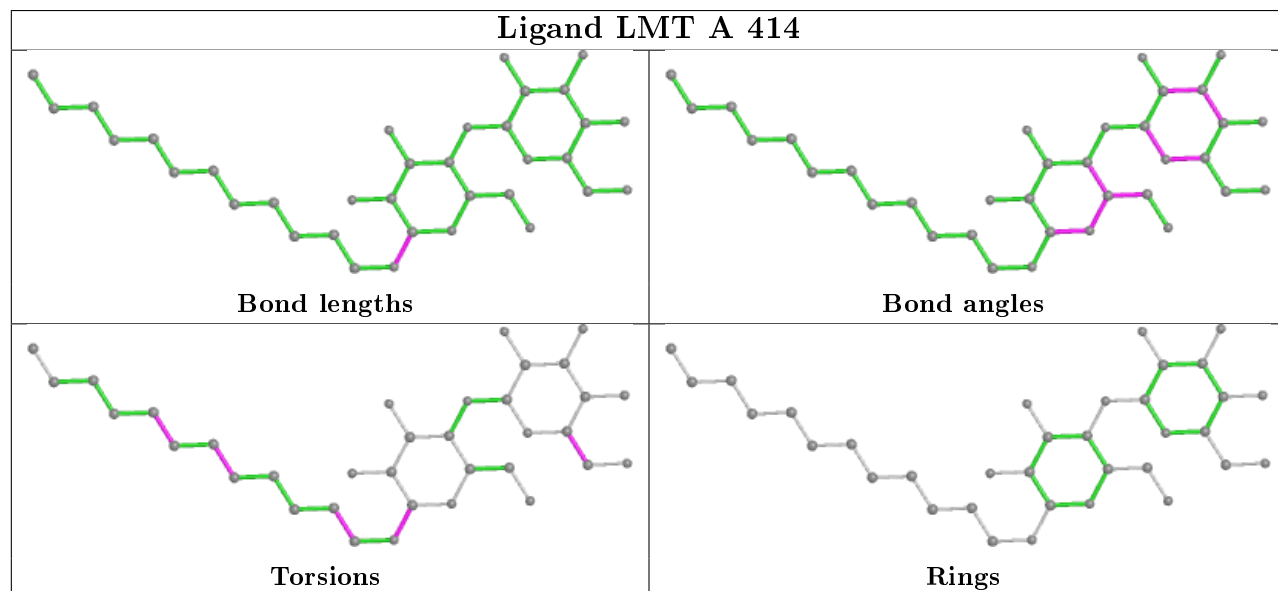
## Ligand CLA D 406

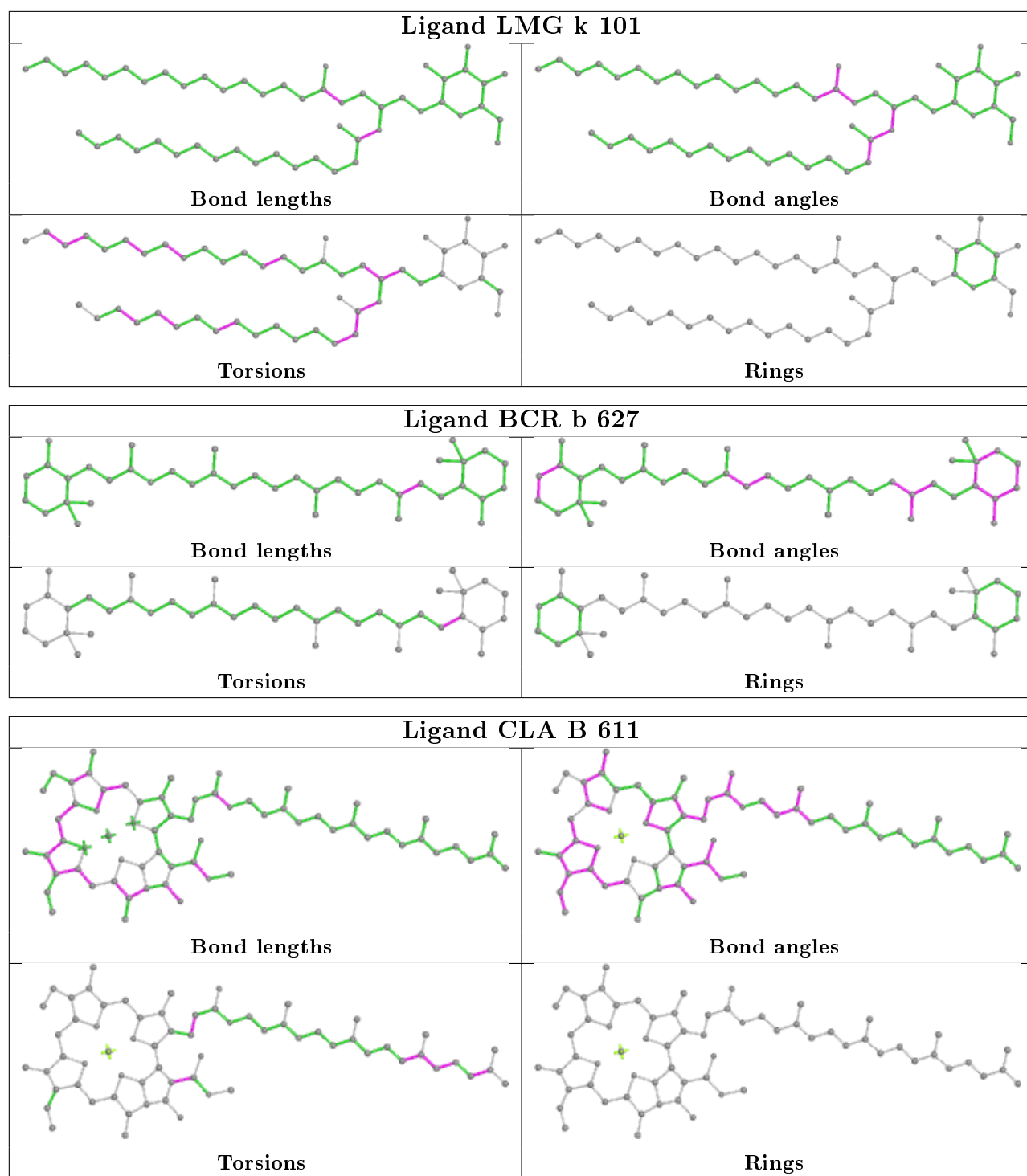


## Ligand CLA C 513

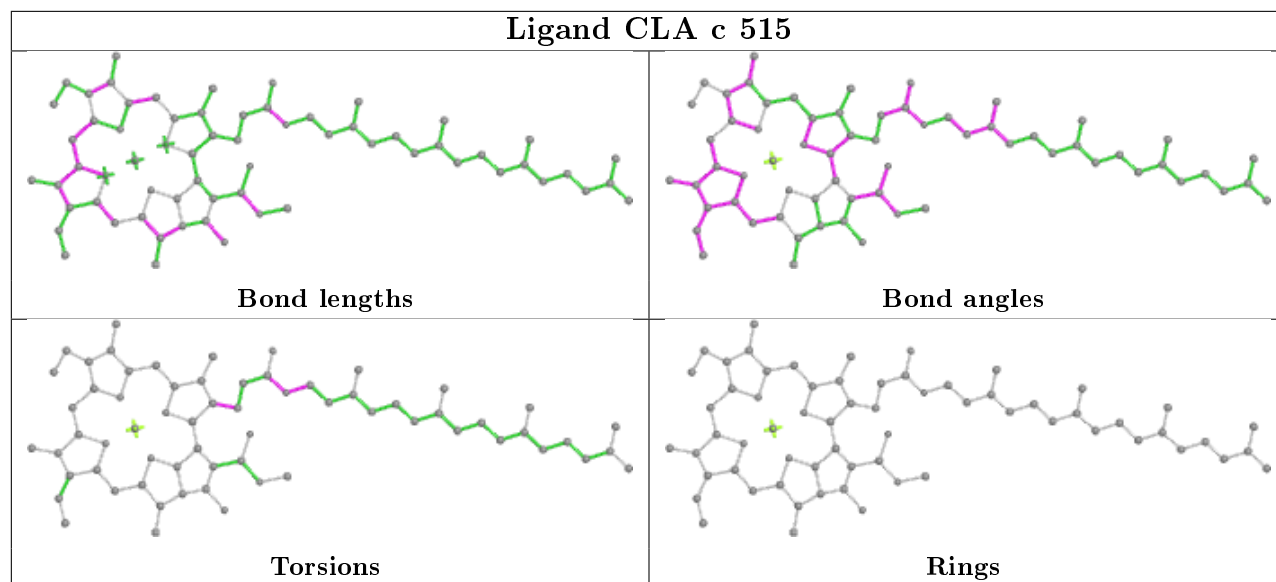


## Ligand LMT A 414

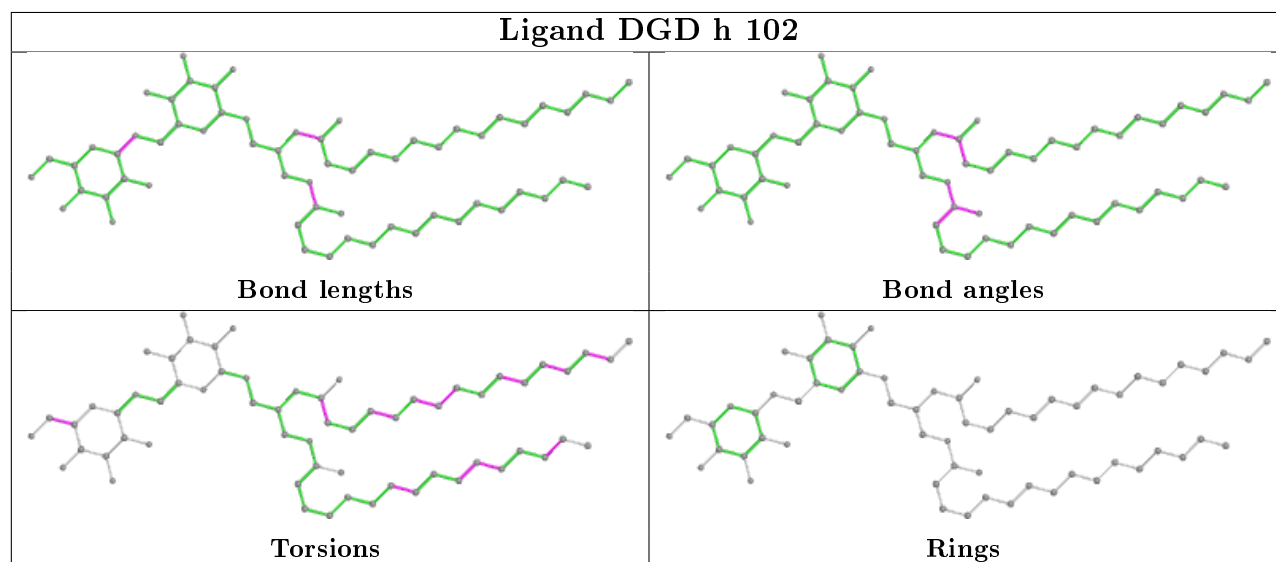




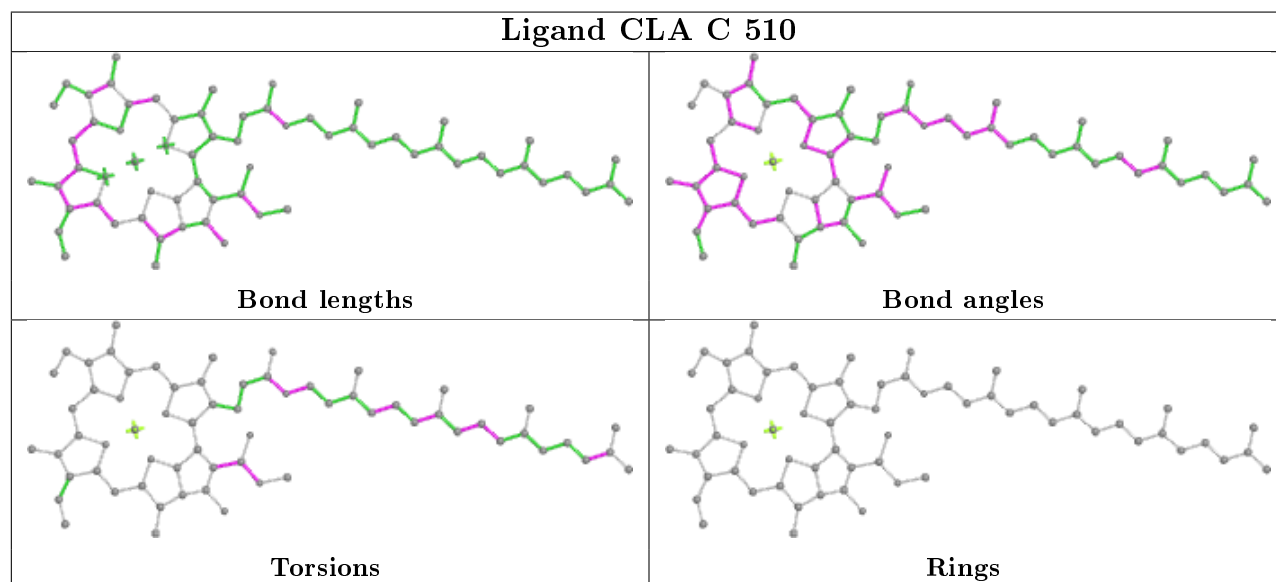
## Ligand CLA c 515

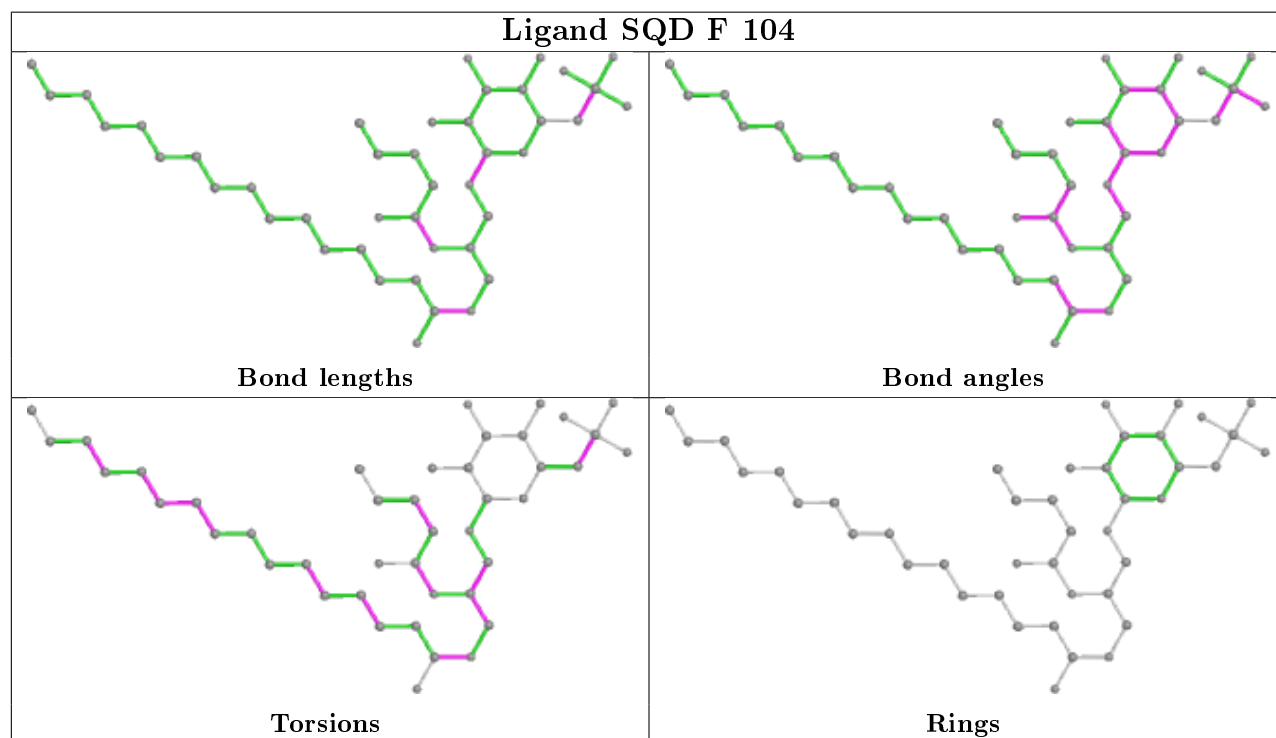
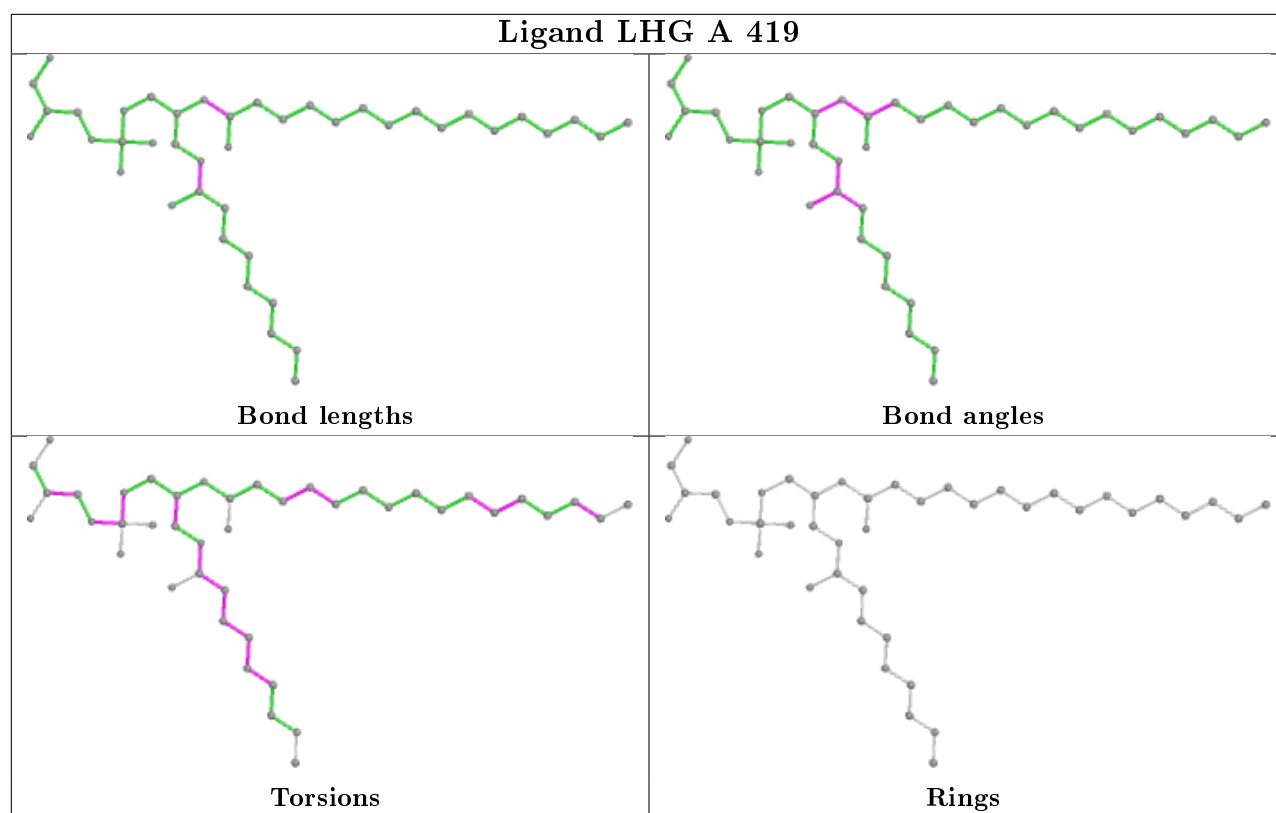


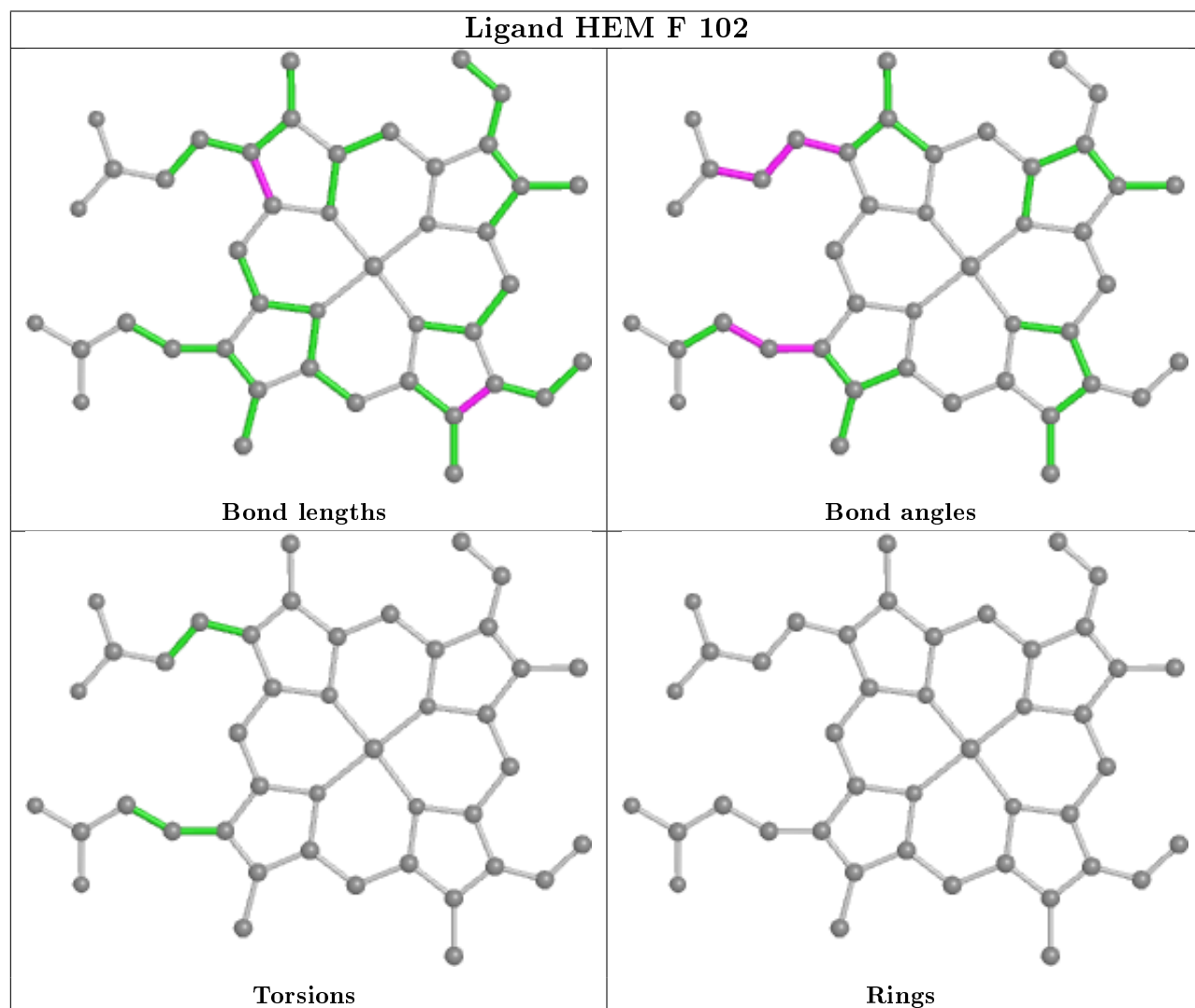
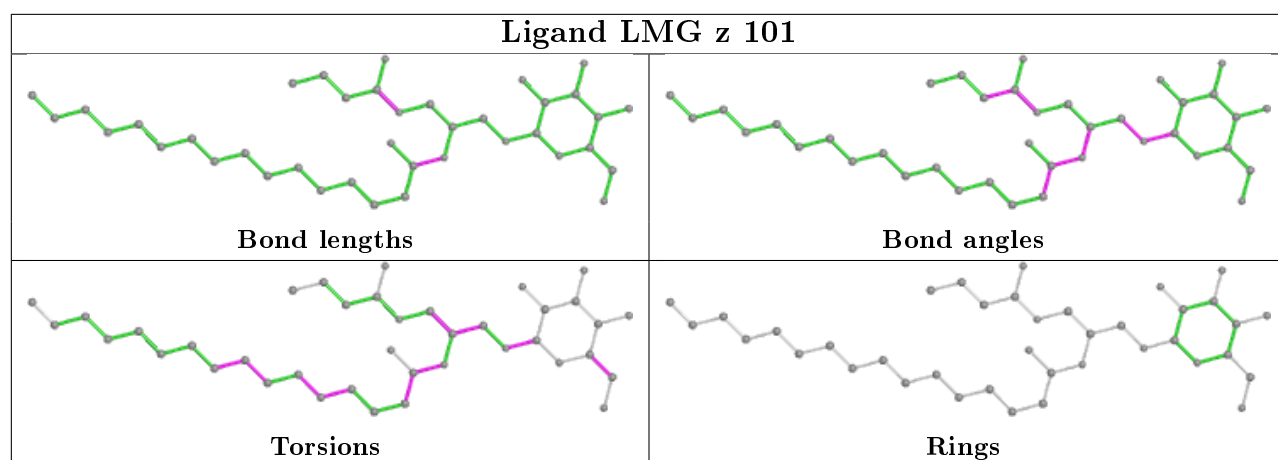
## Ligand DGD h 102



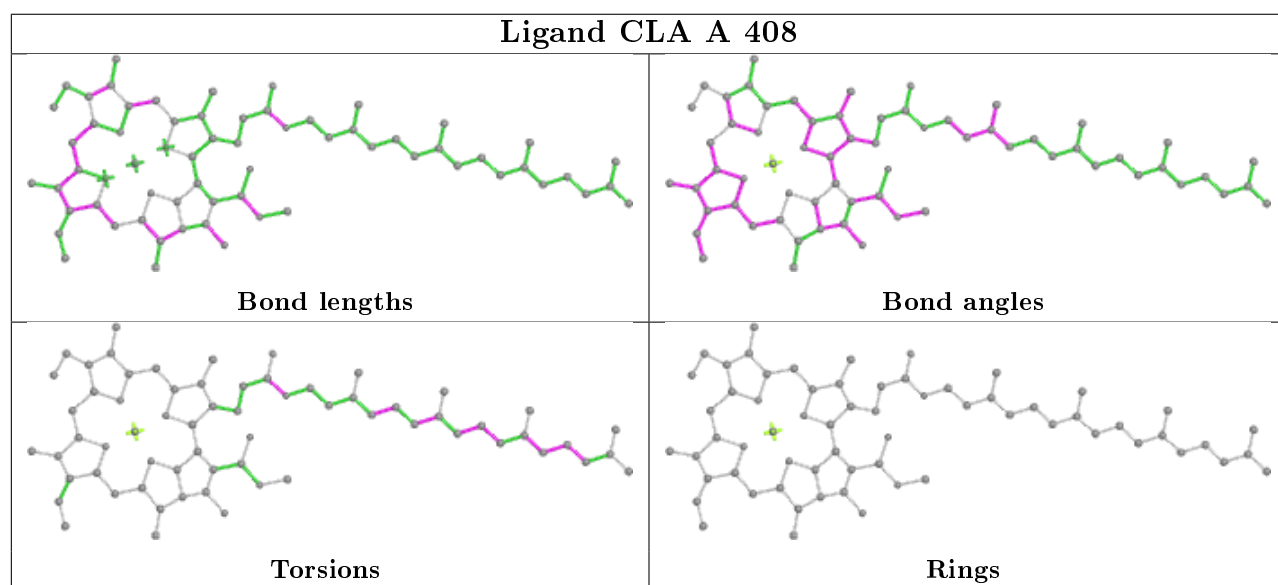
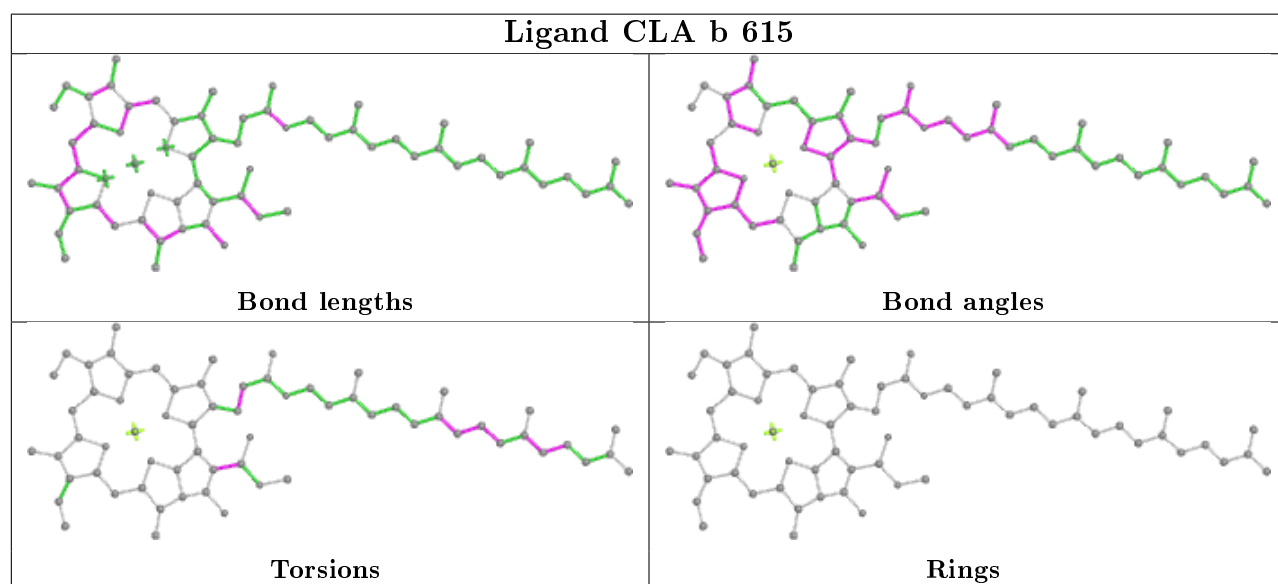
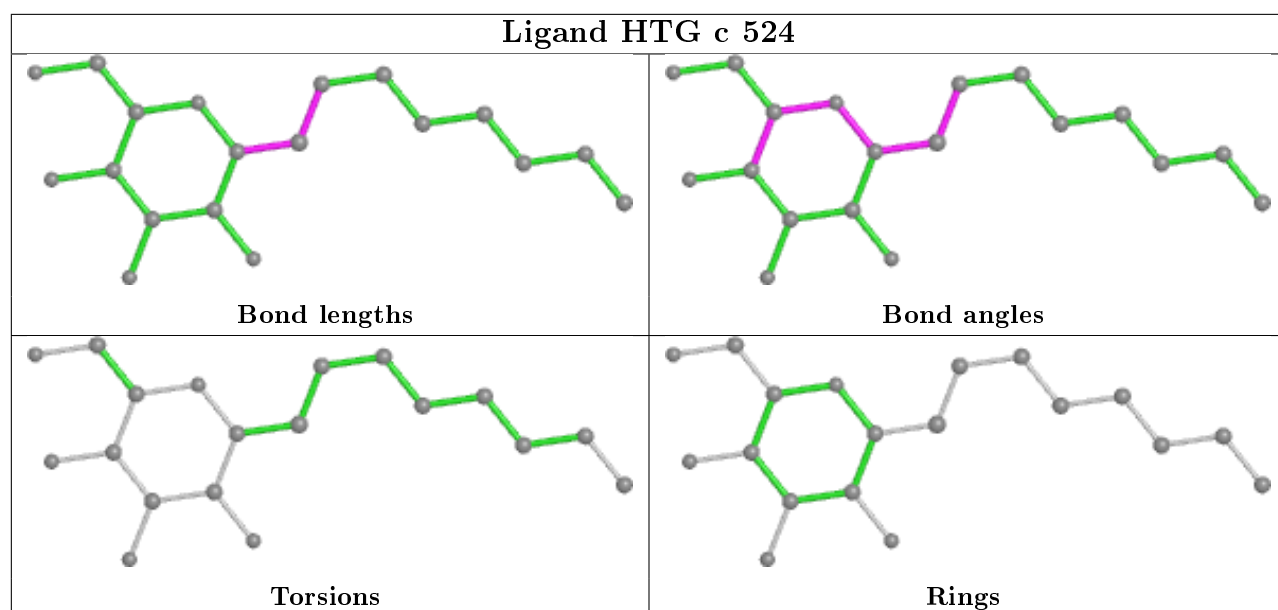
## Ligand CLA C 510

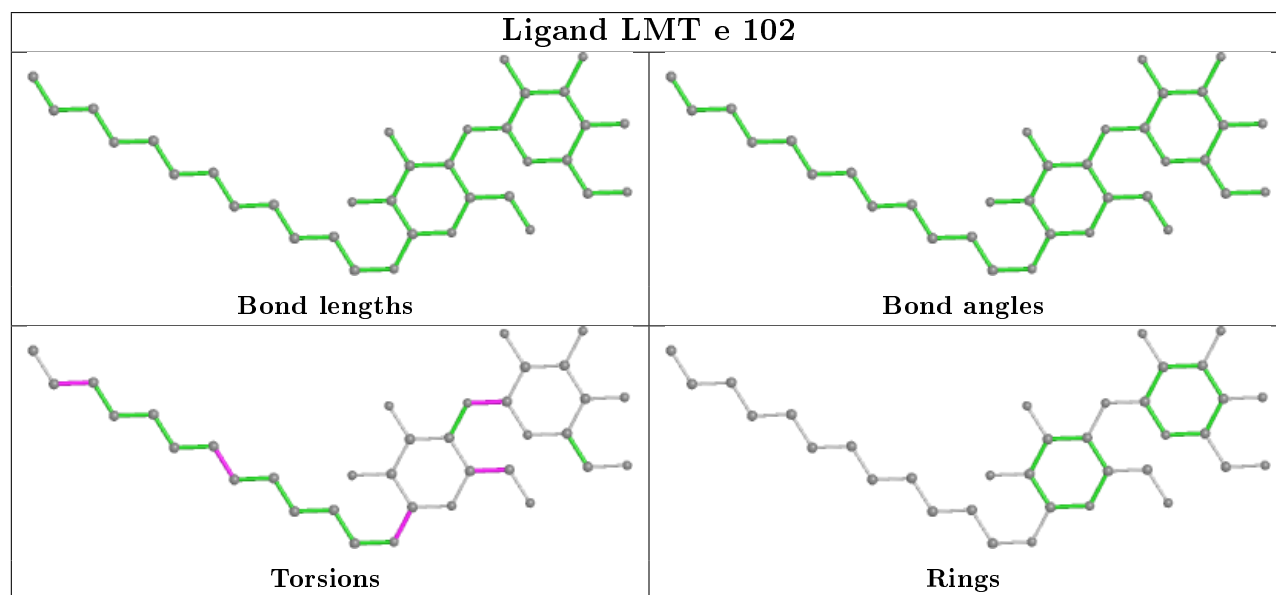
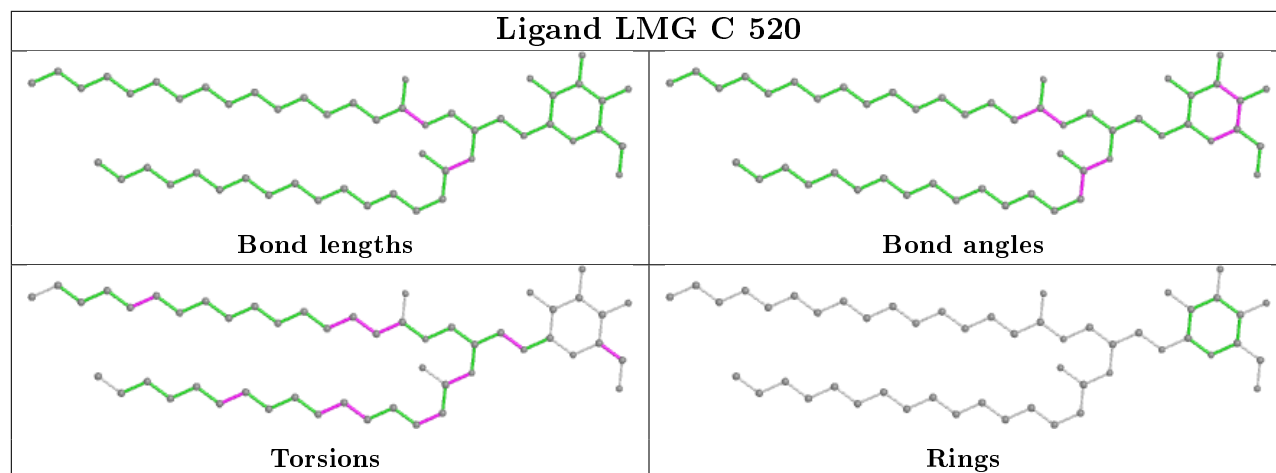
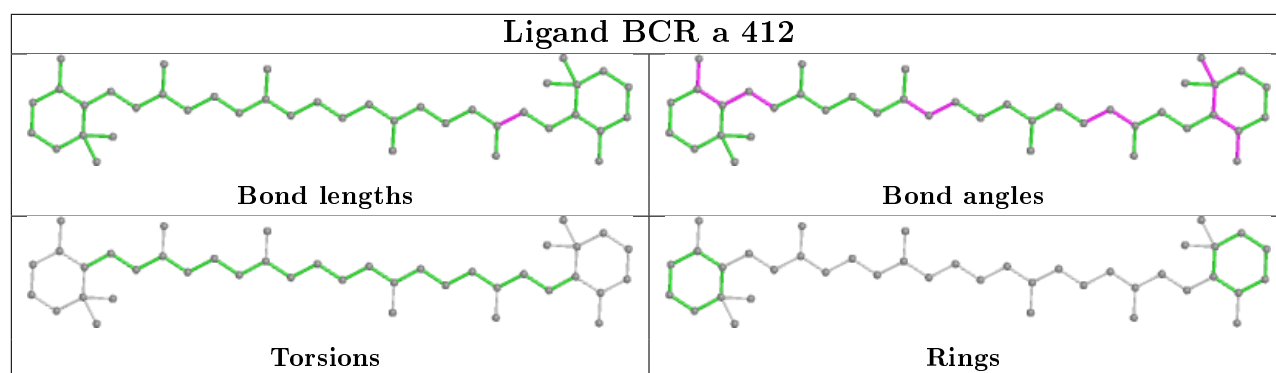


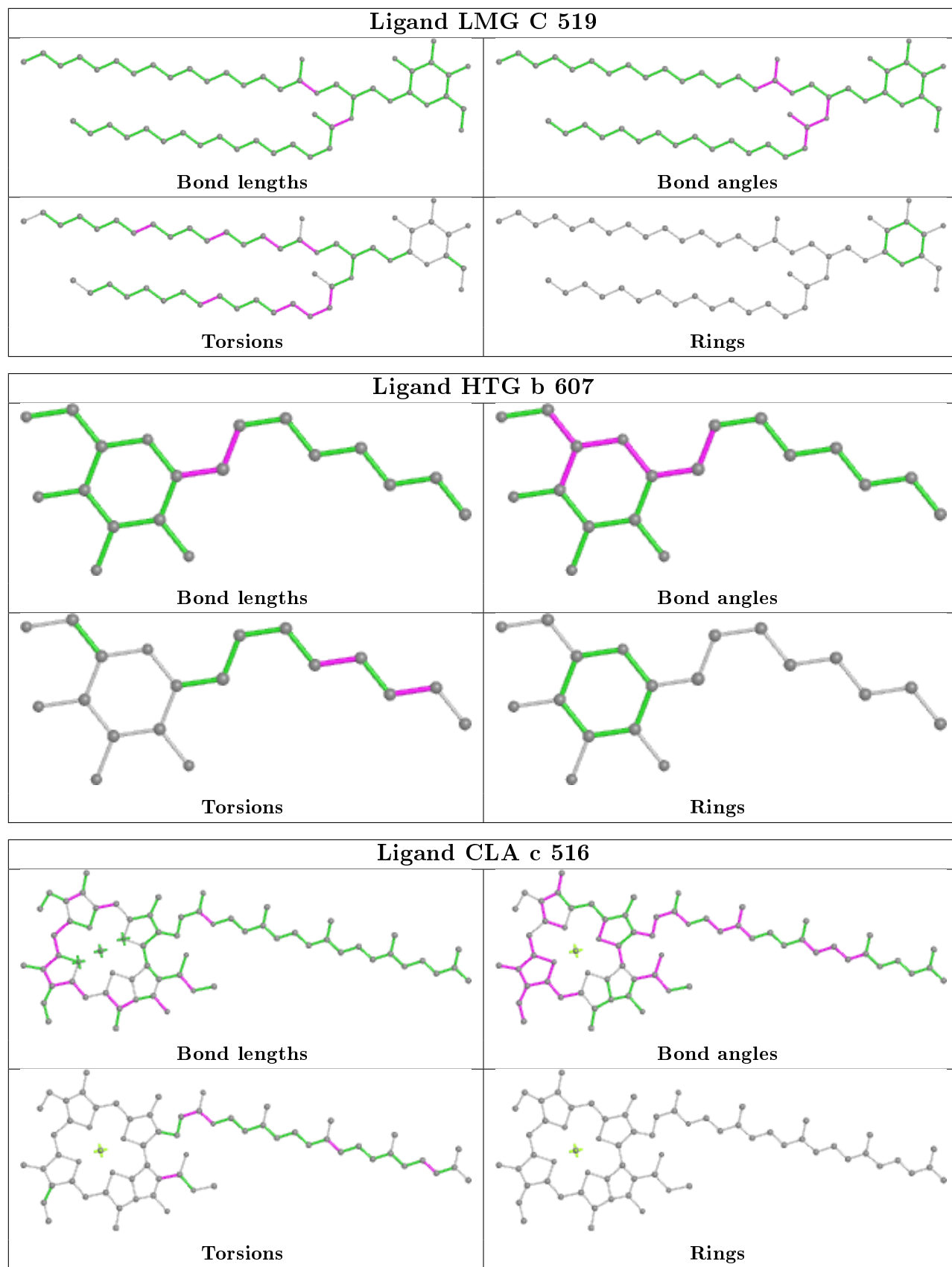


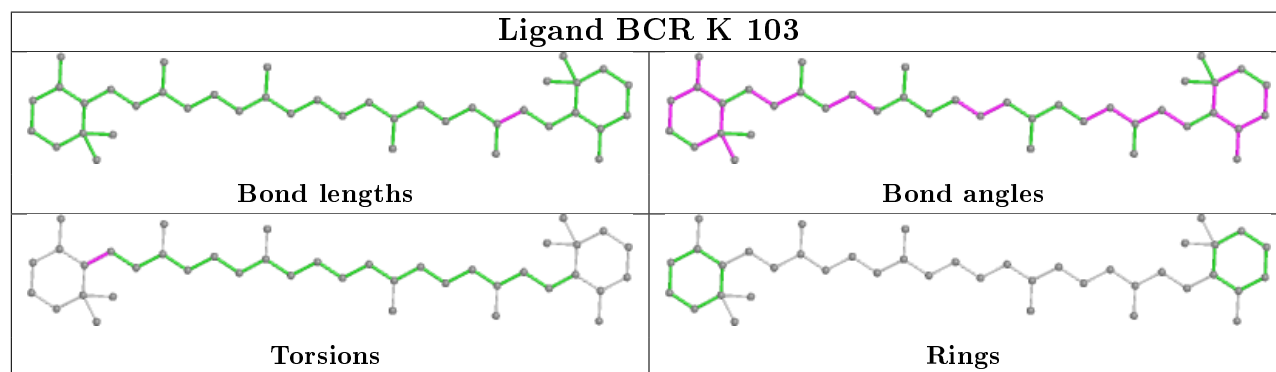
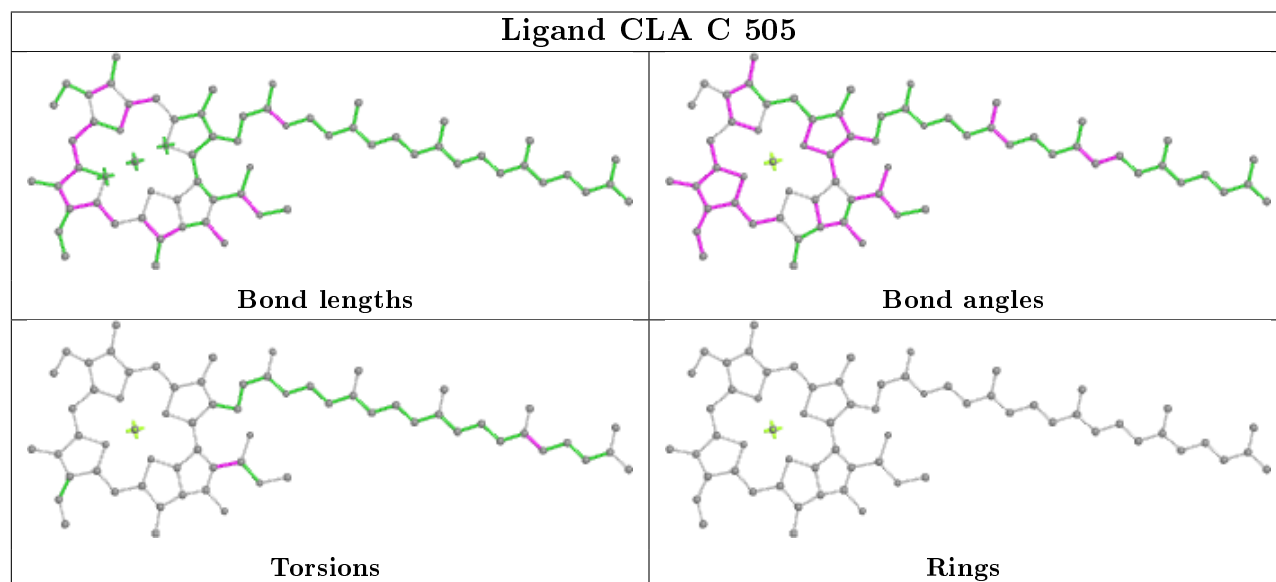
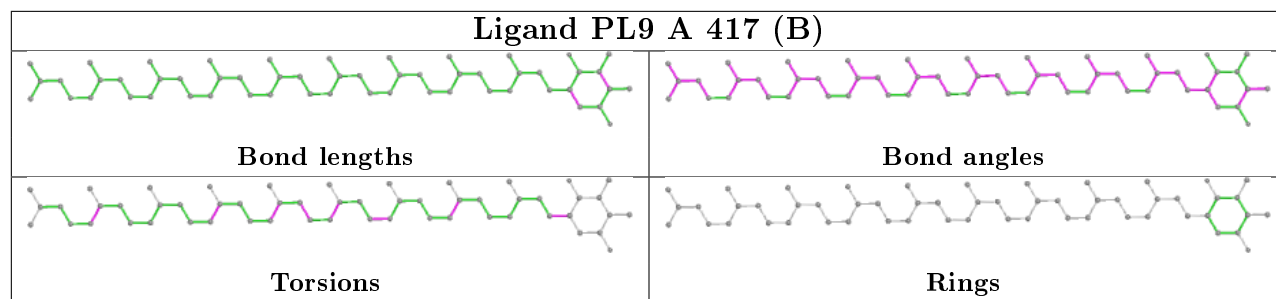




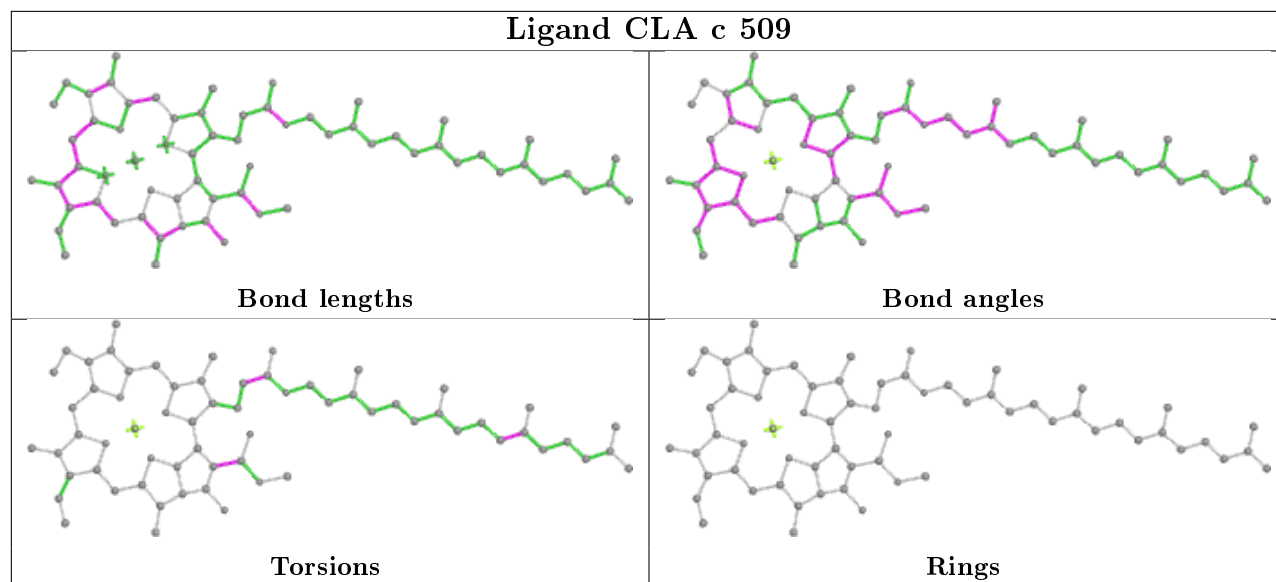




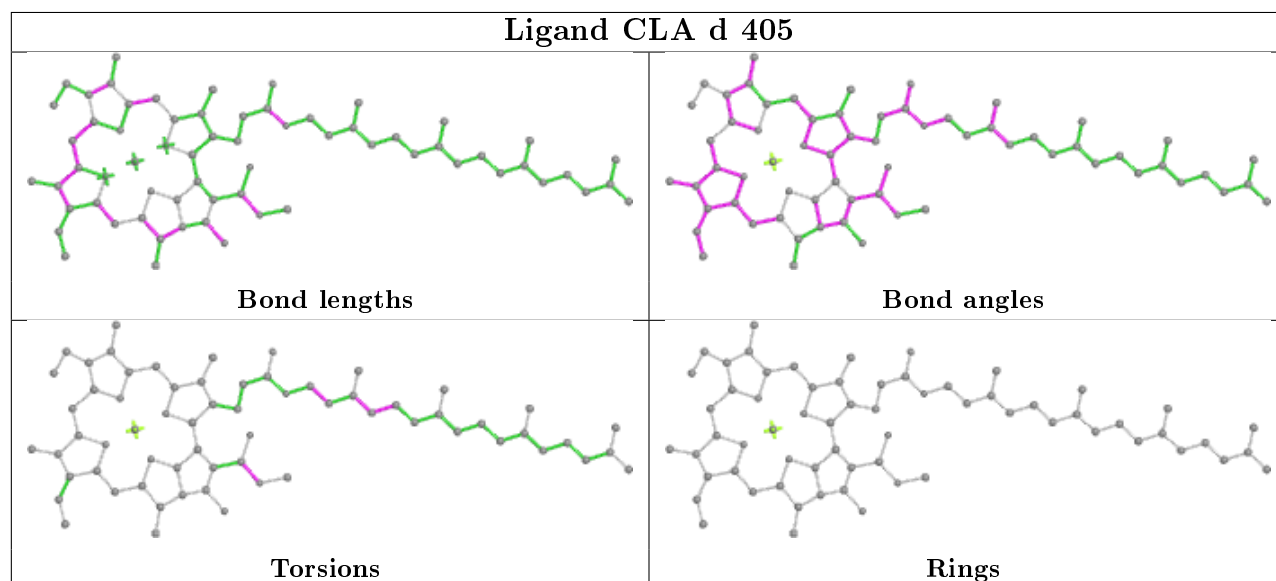




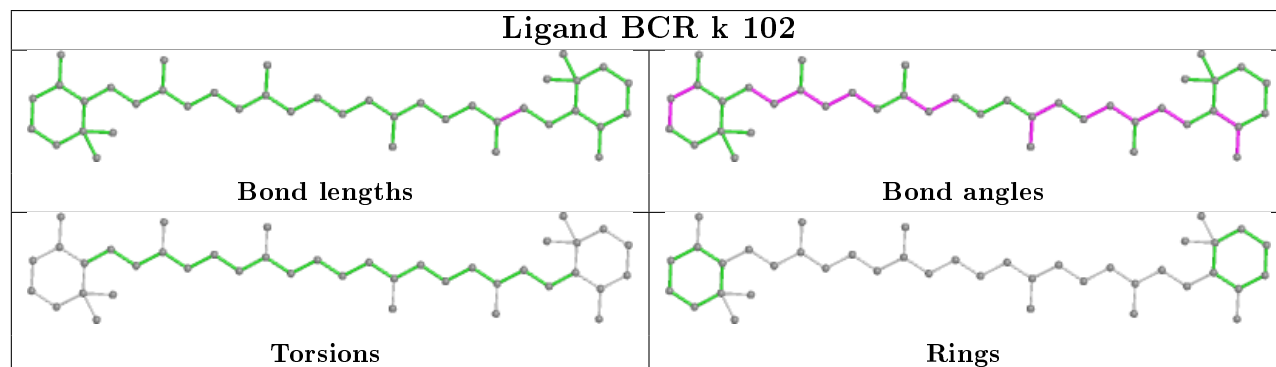
## Ligand CLA c 509



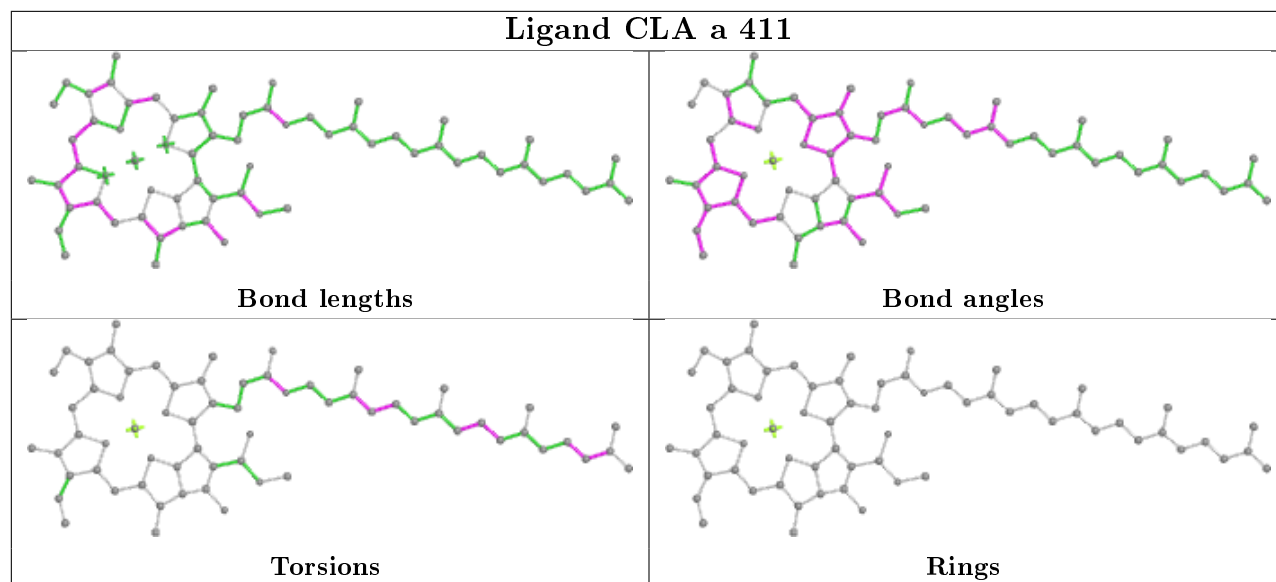
## Ligand CLA d 405



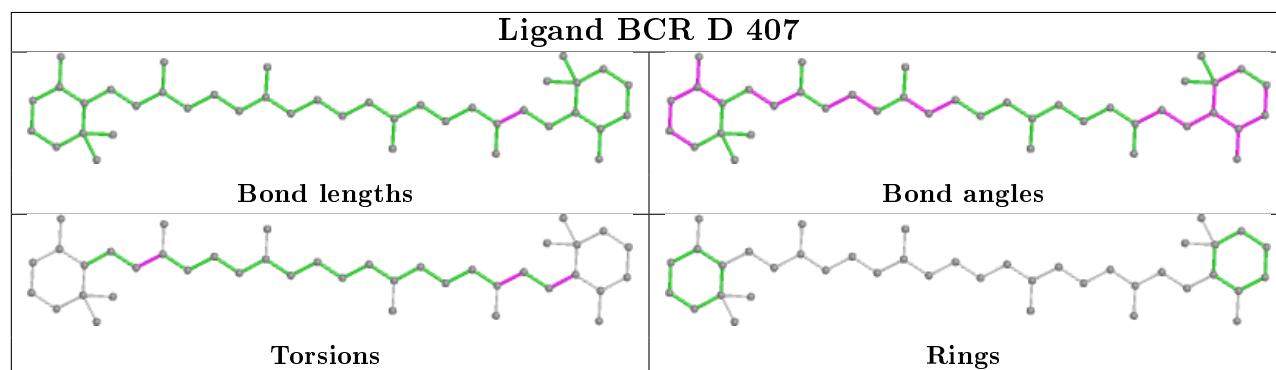
## Ligand BCR k 102



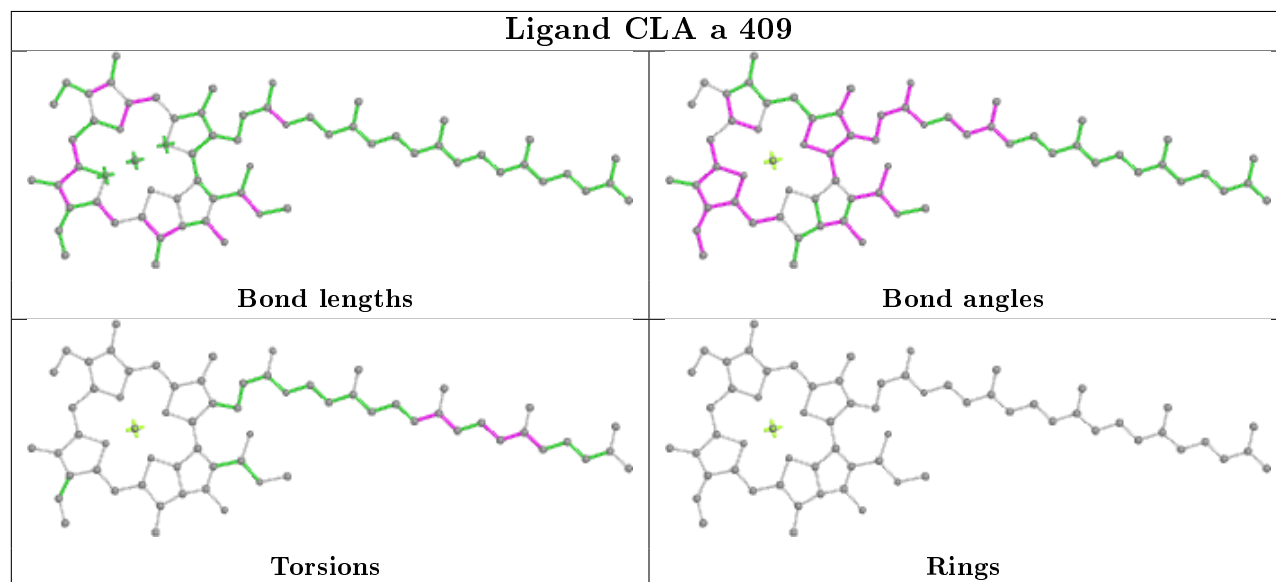
## Ligand CLA a 411

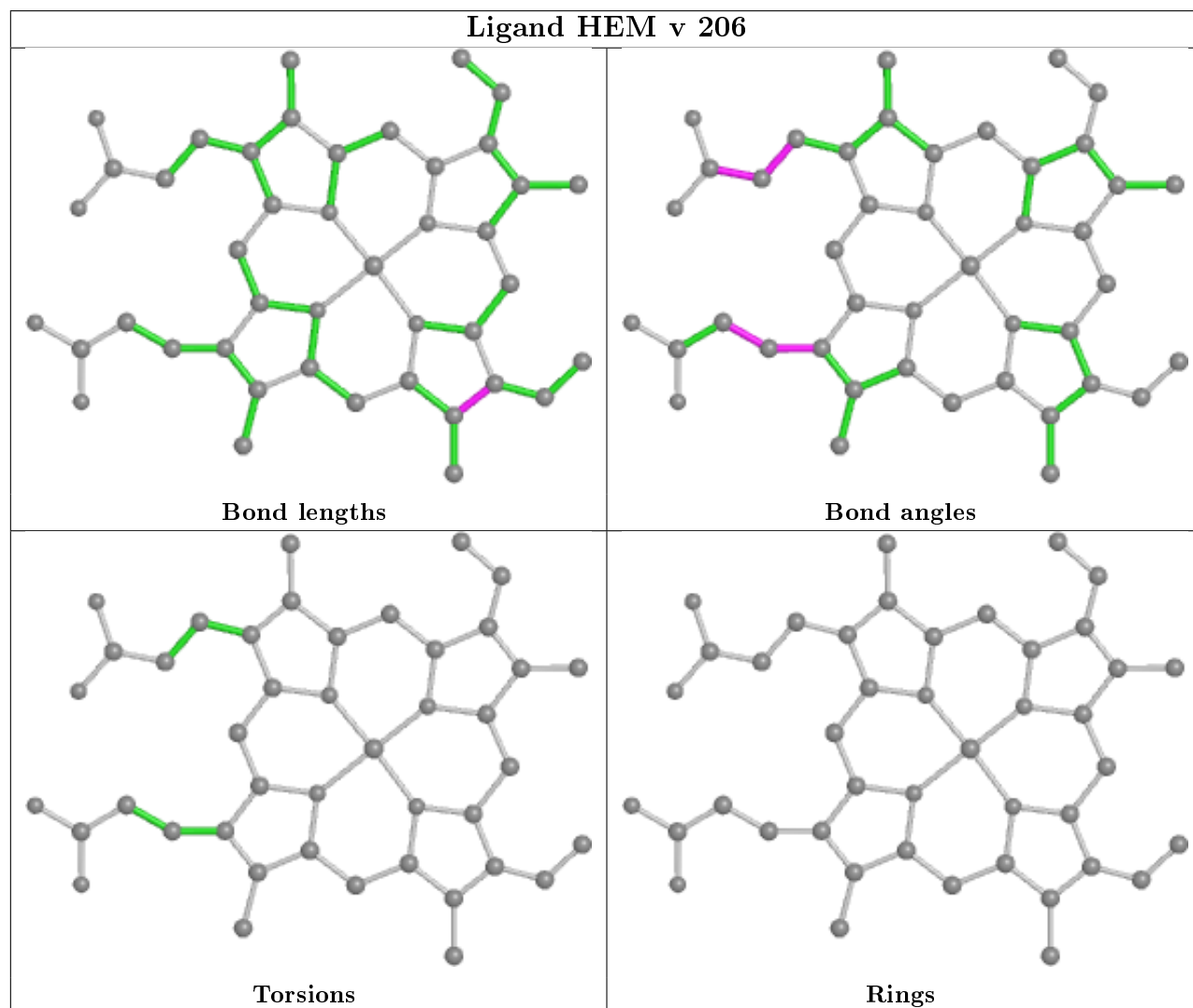
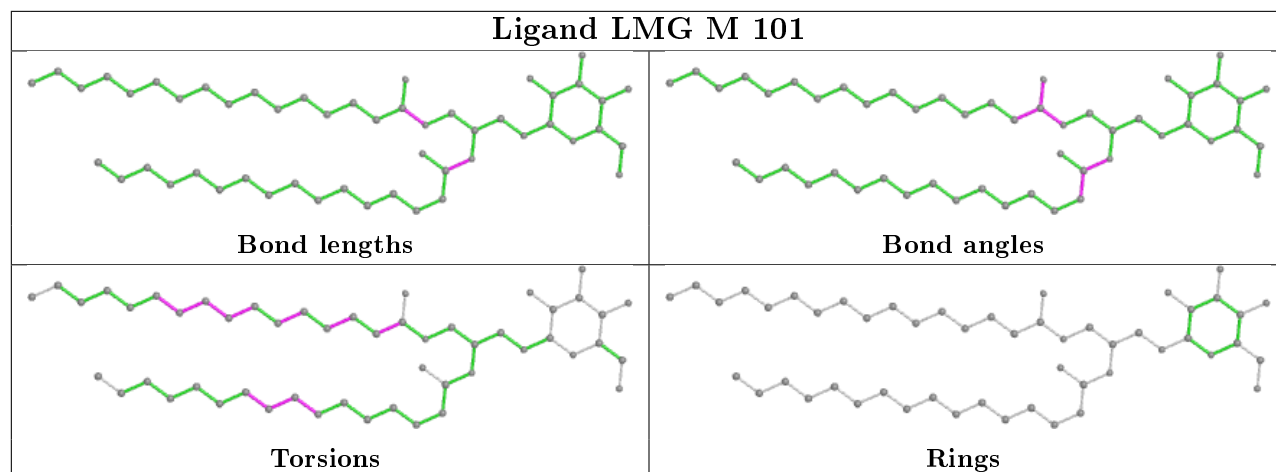


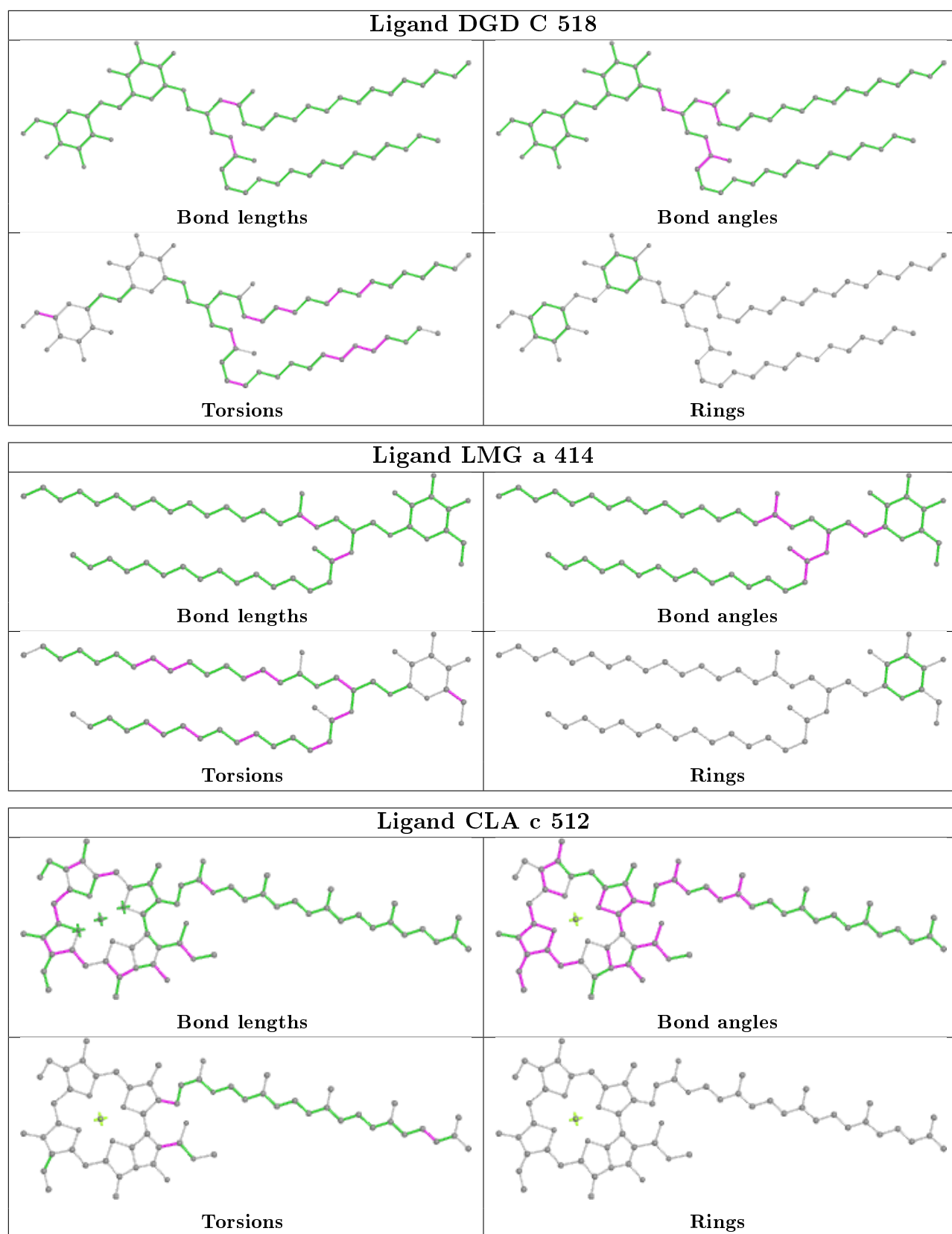
## Ligand BCR D 407



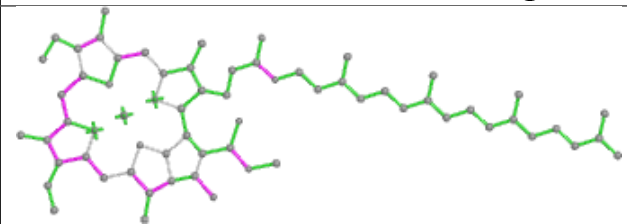
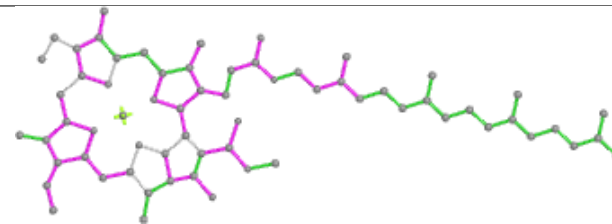
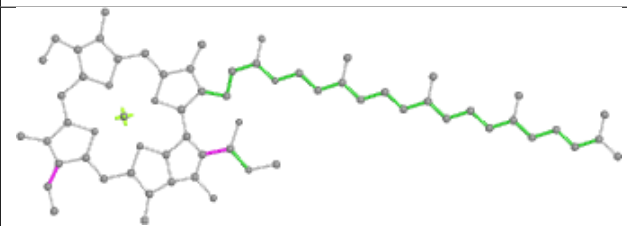
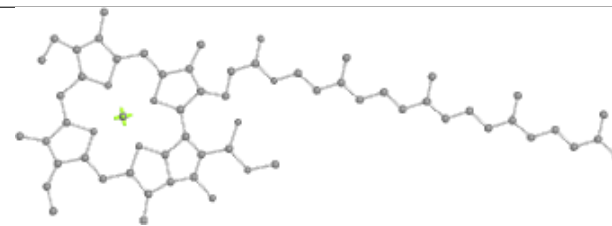
## Ligand CLA a 409

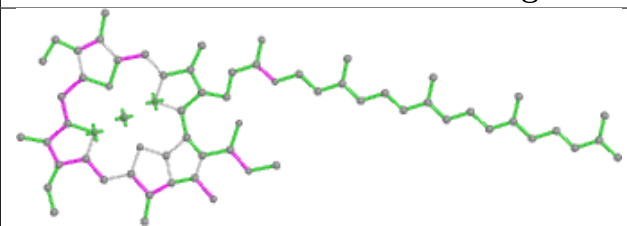
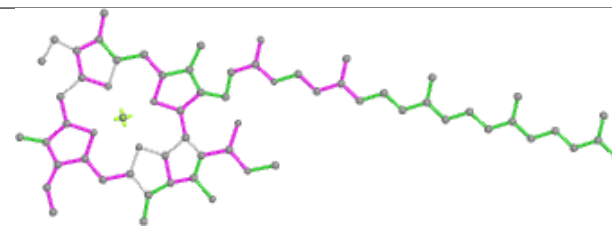
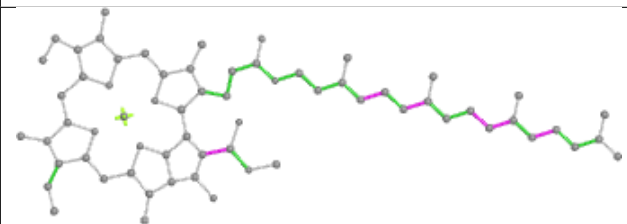
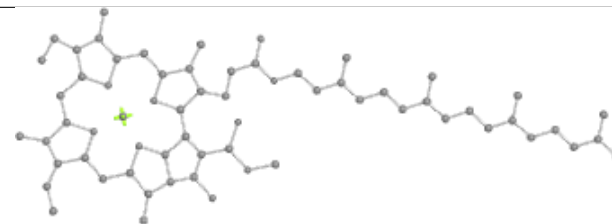


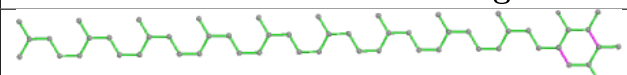
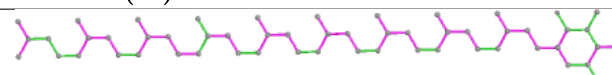
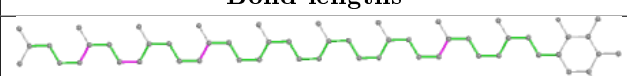
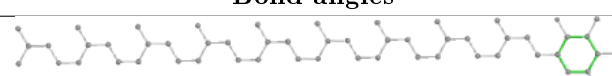


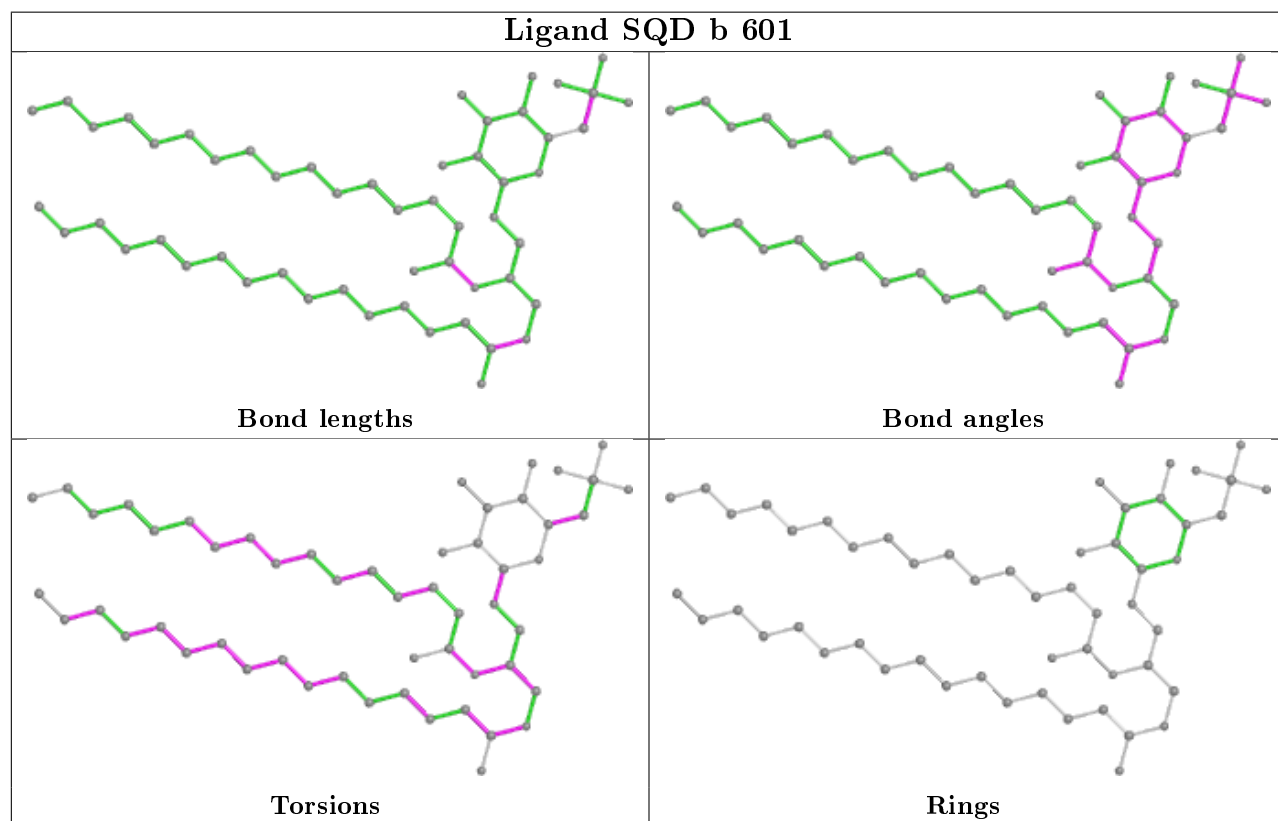
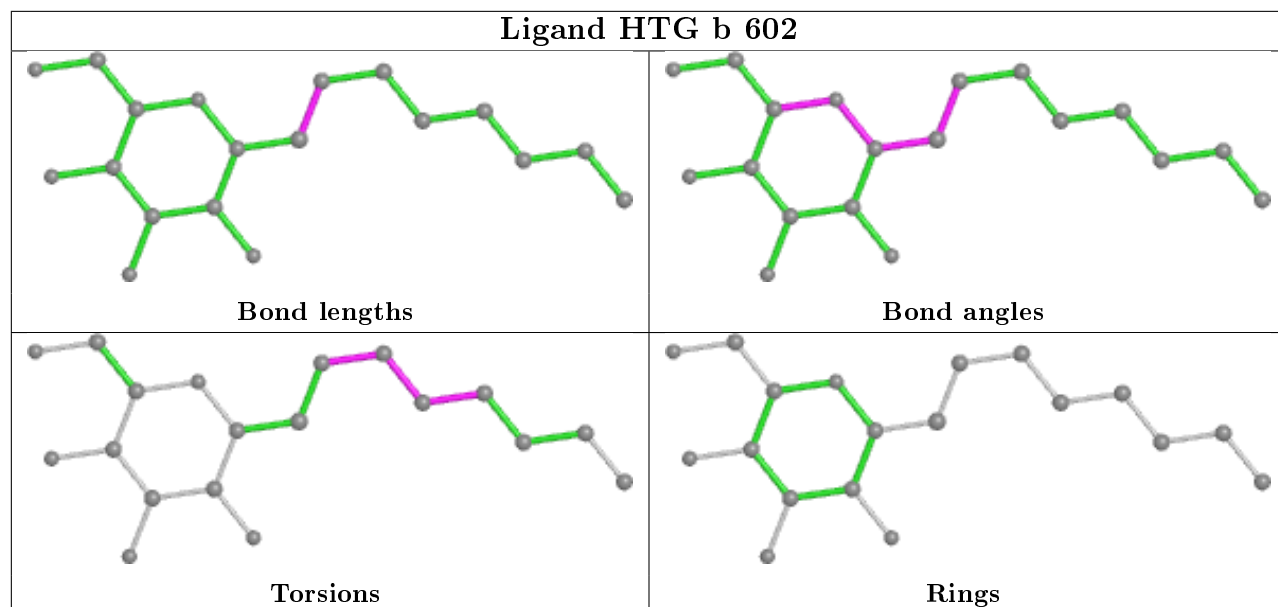


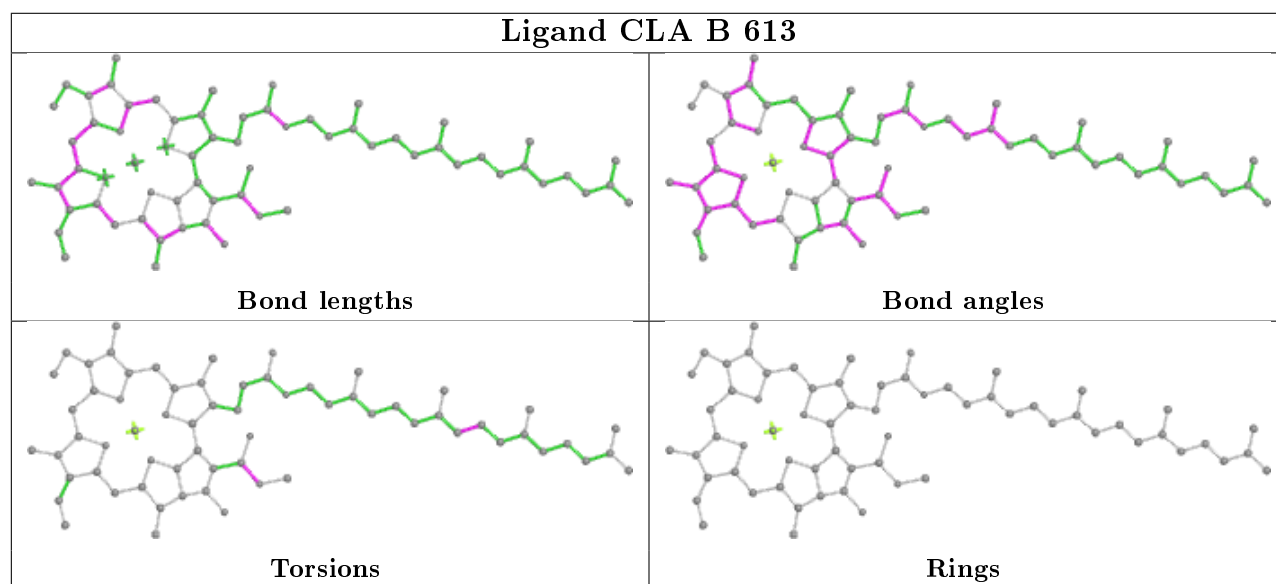
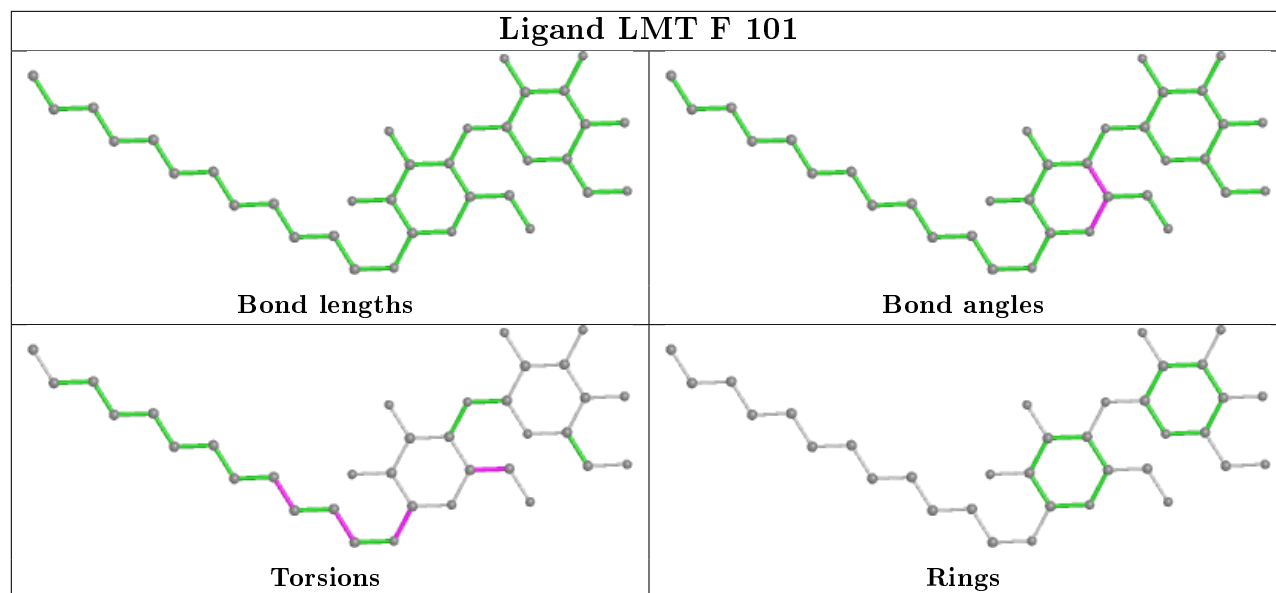


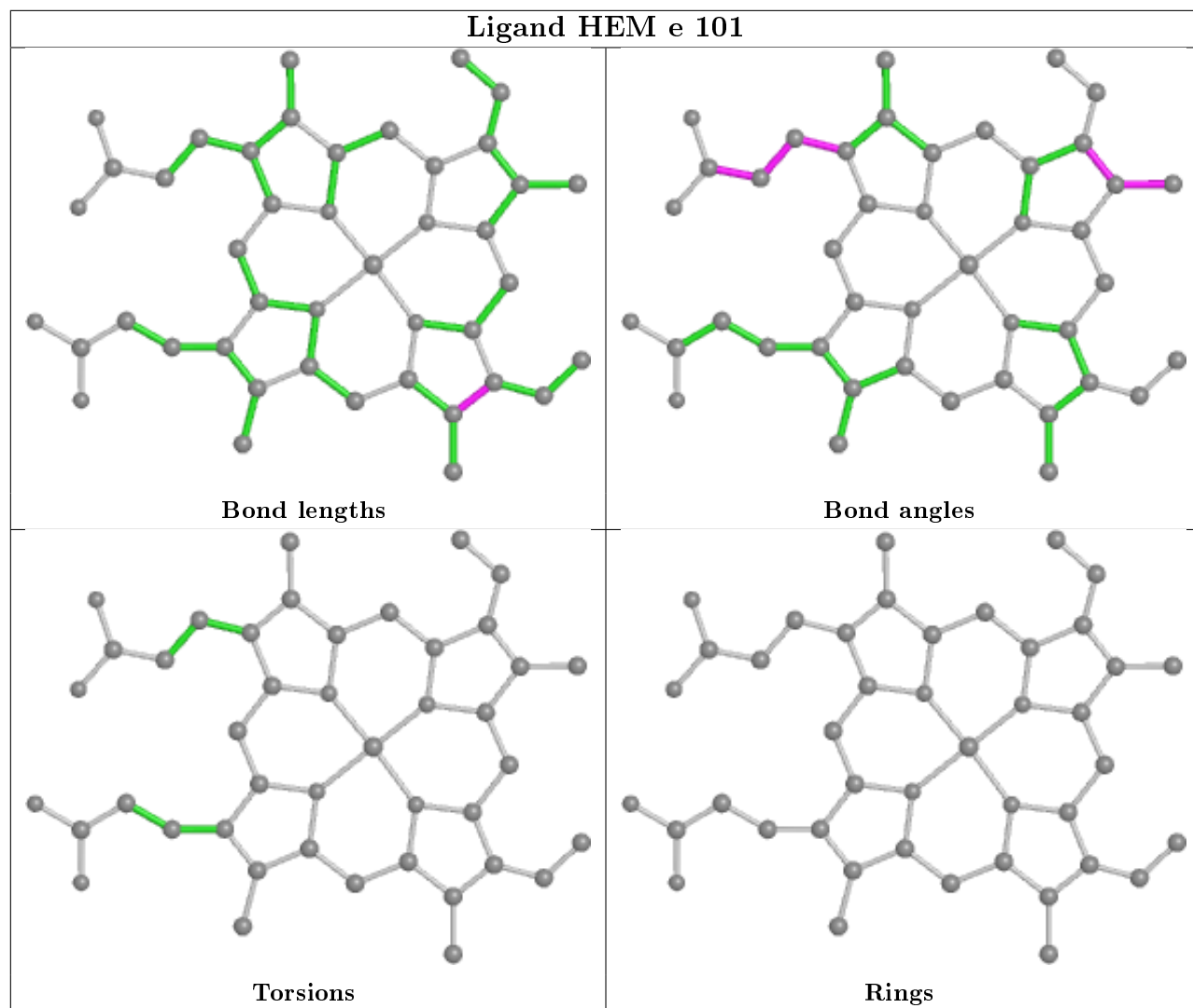
Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

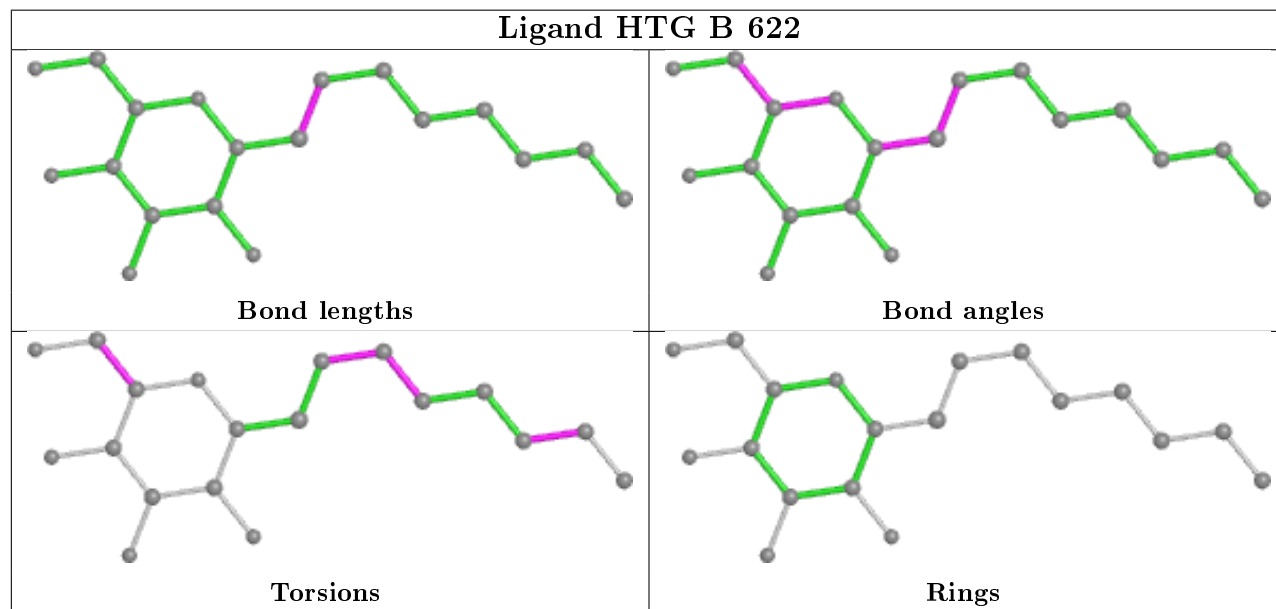
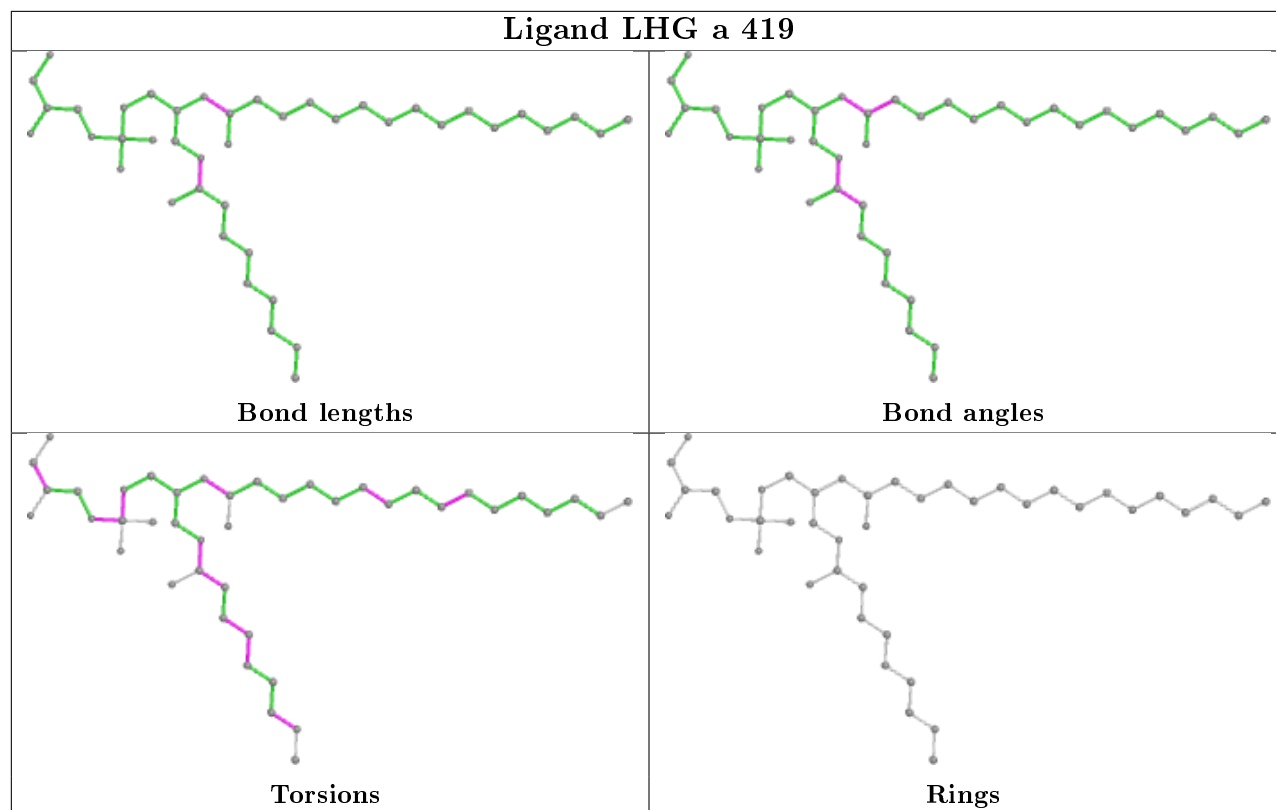
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 D 408 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

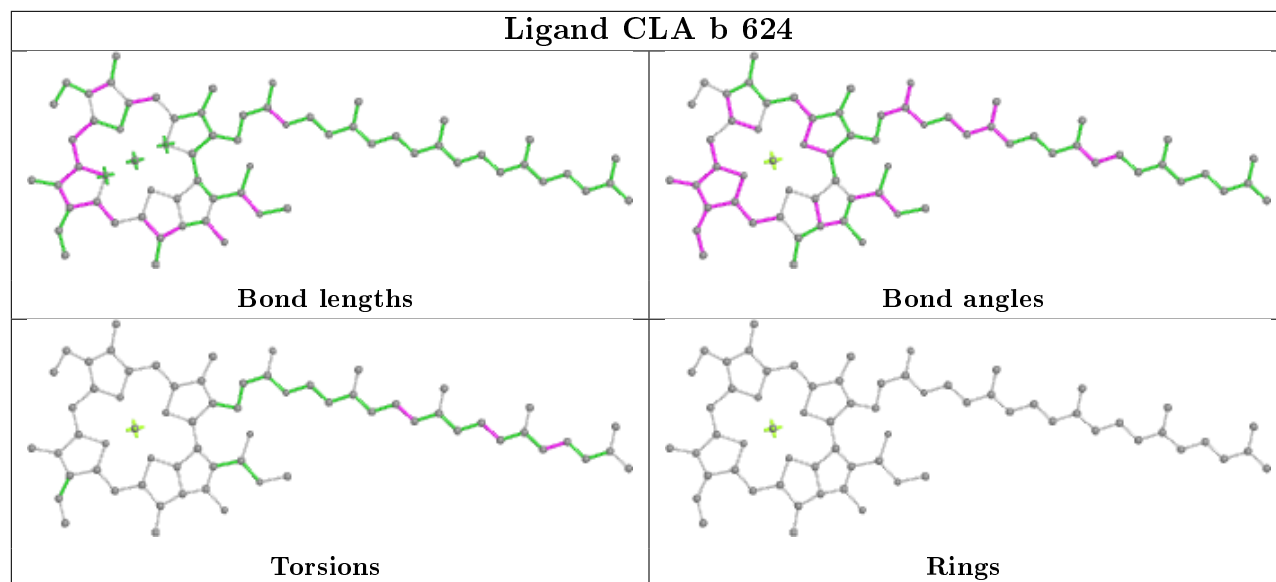




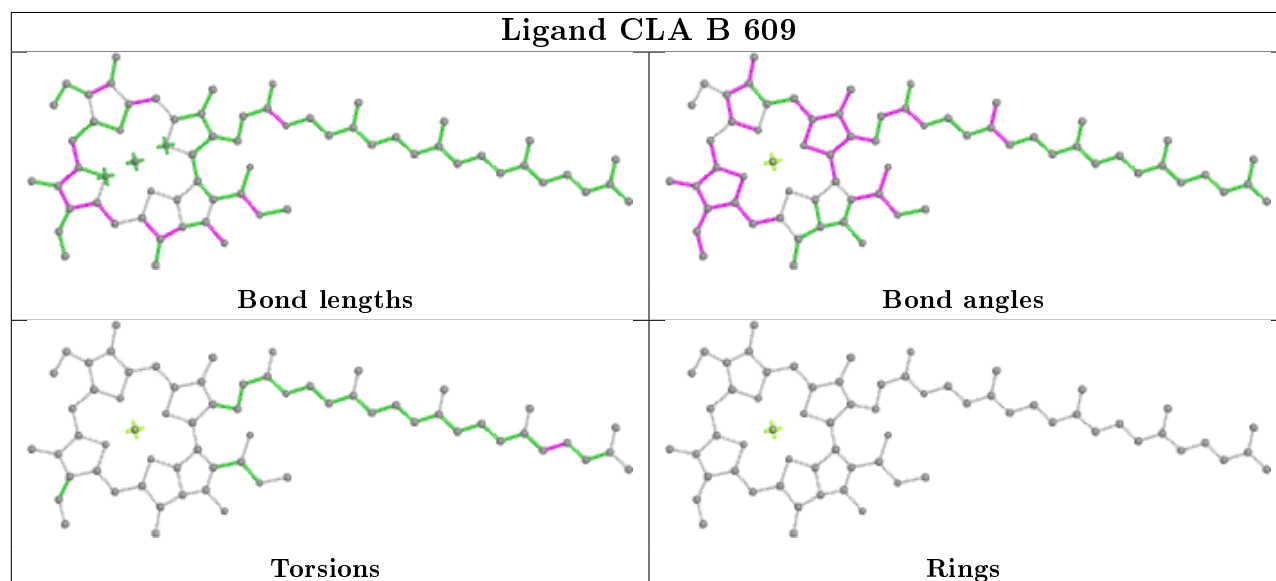




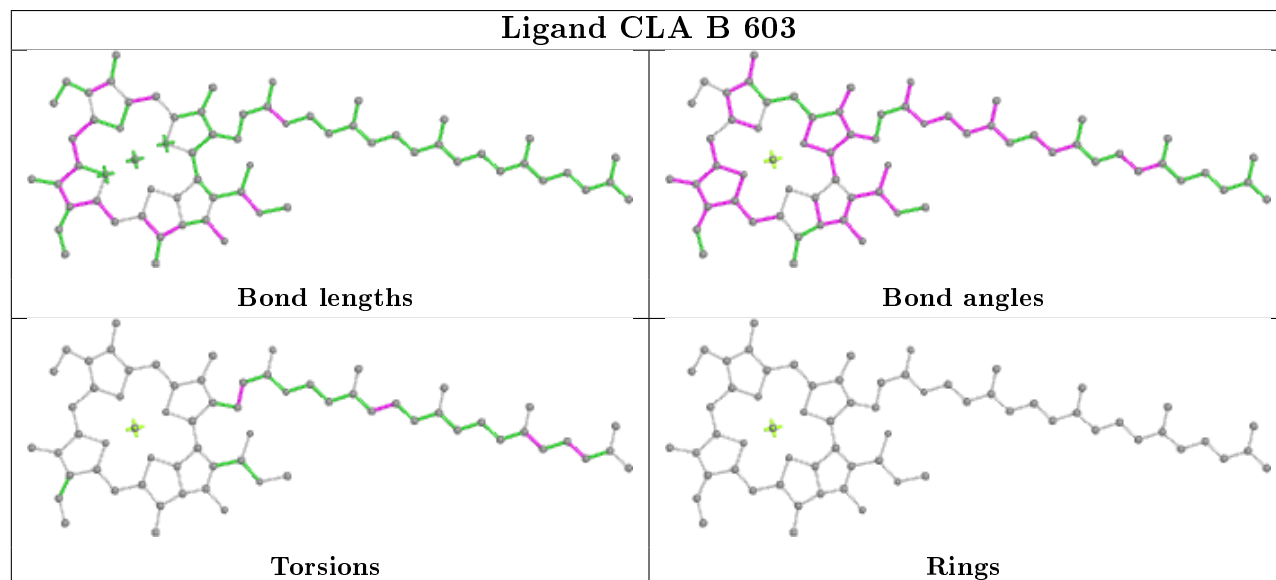
## Ligand CLA b 624

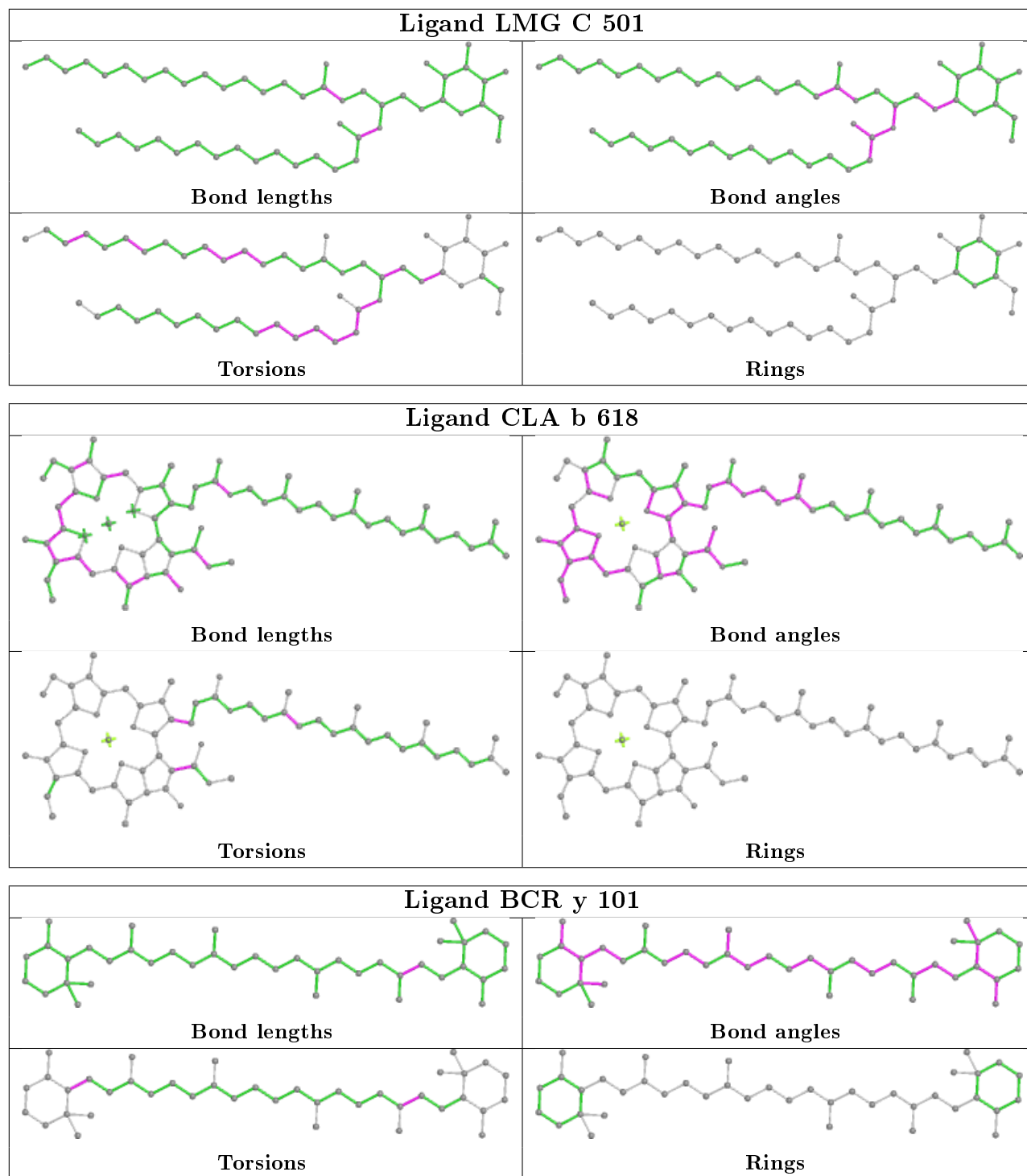


## Ligand CLA B 609

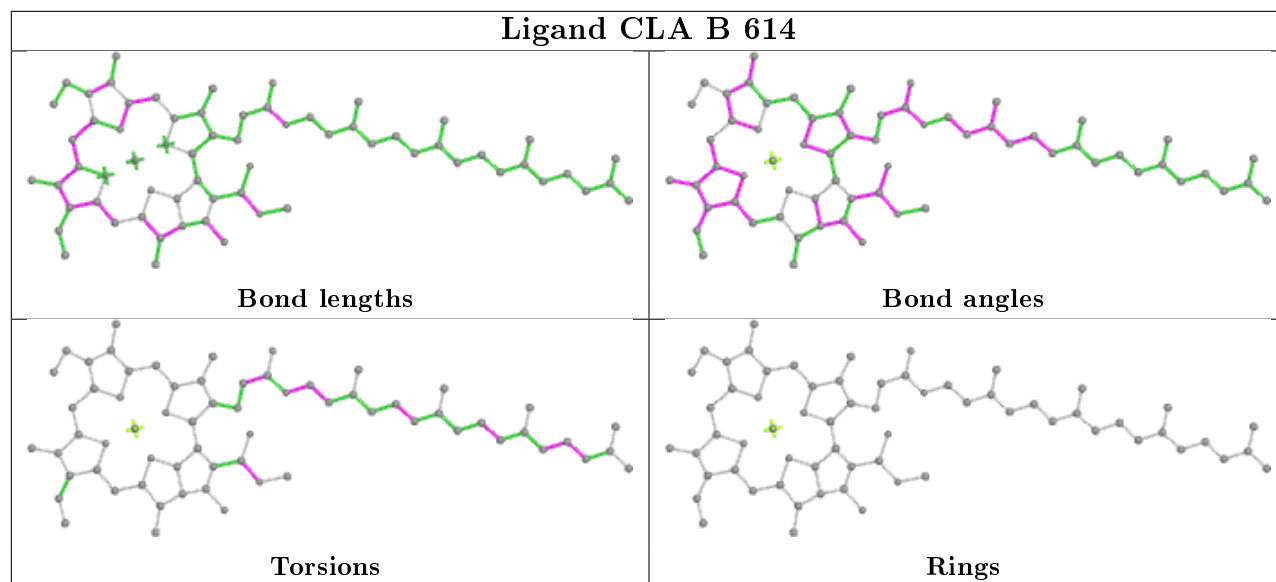


## Ligand CLA B 603

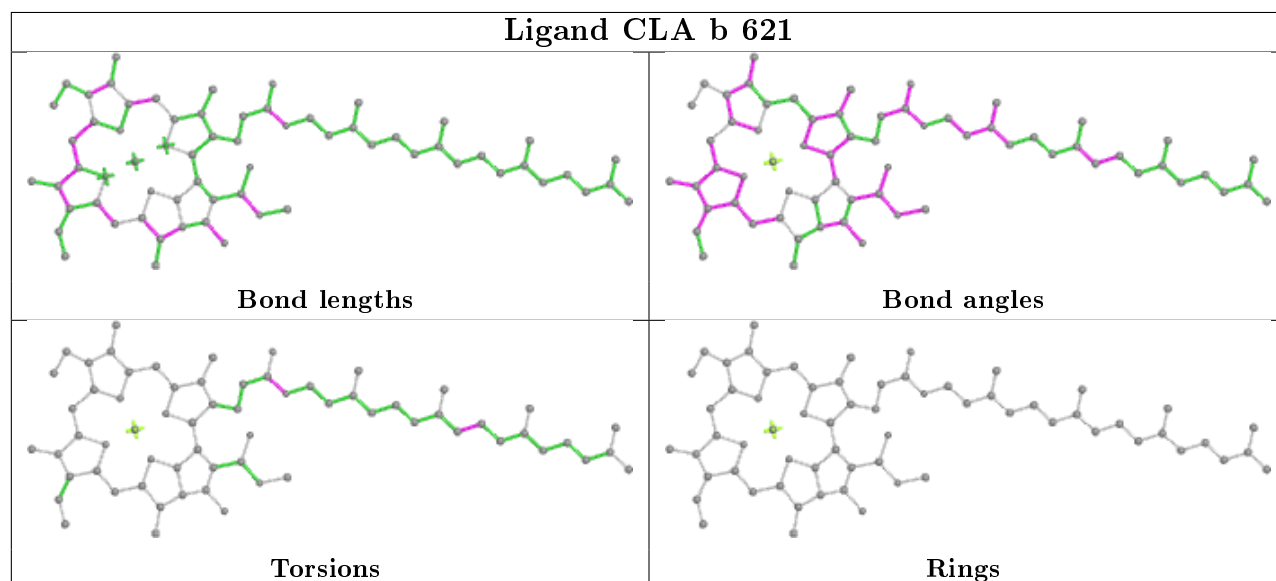




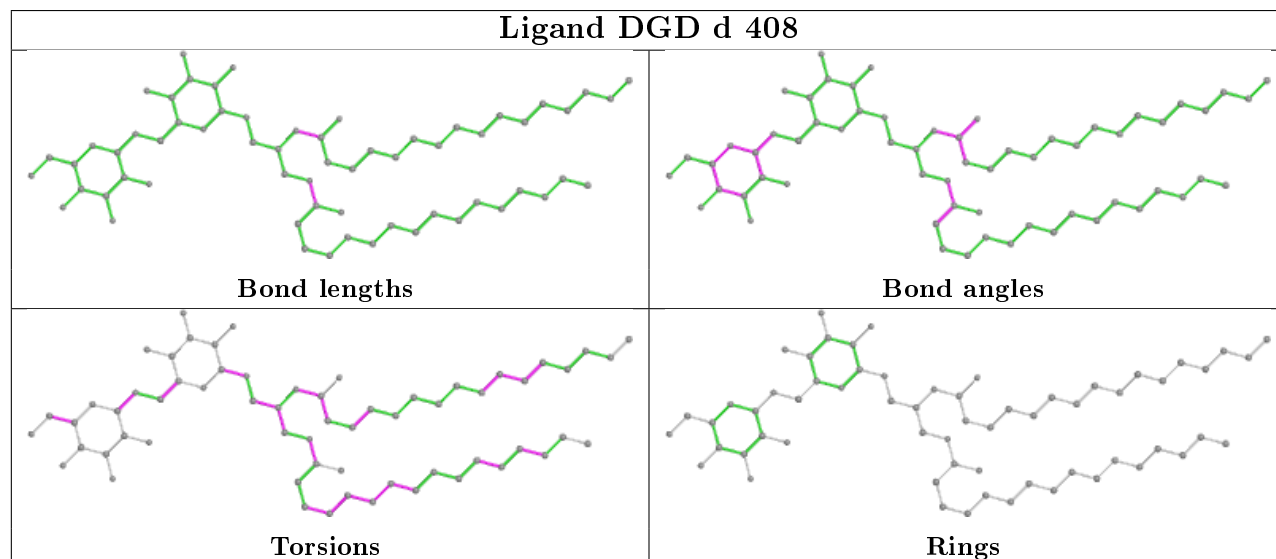
## Ligand CLA B 614



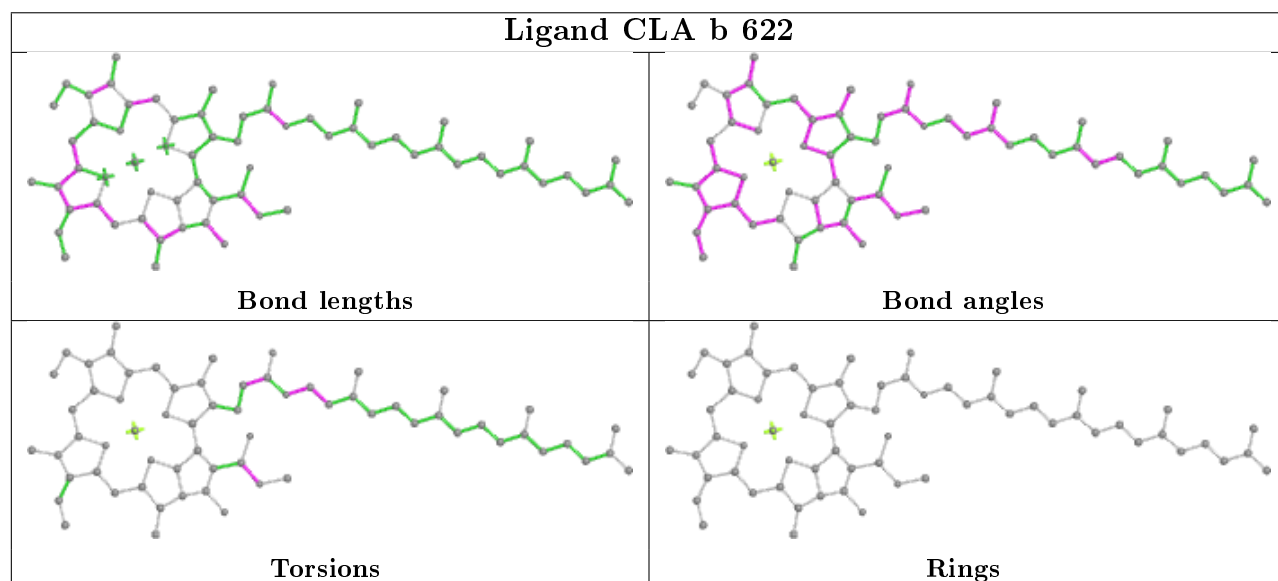
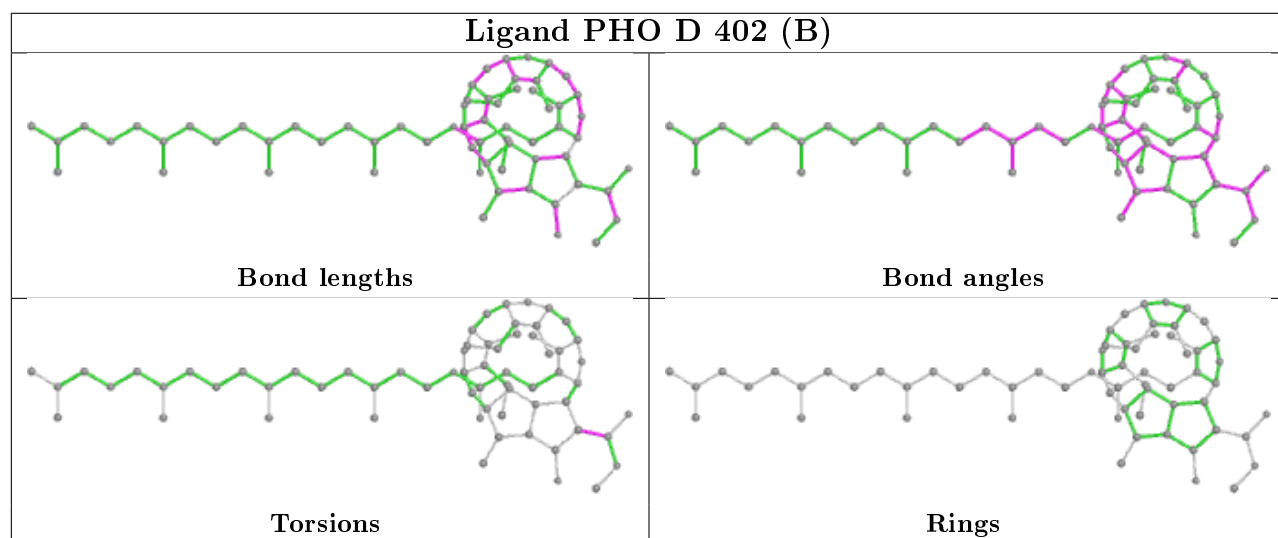
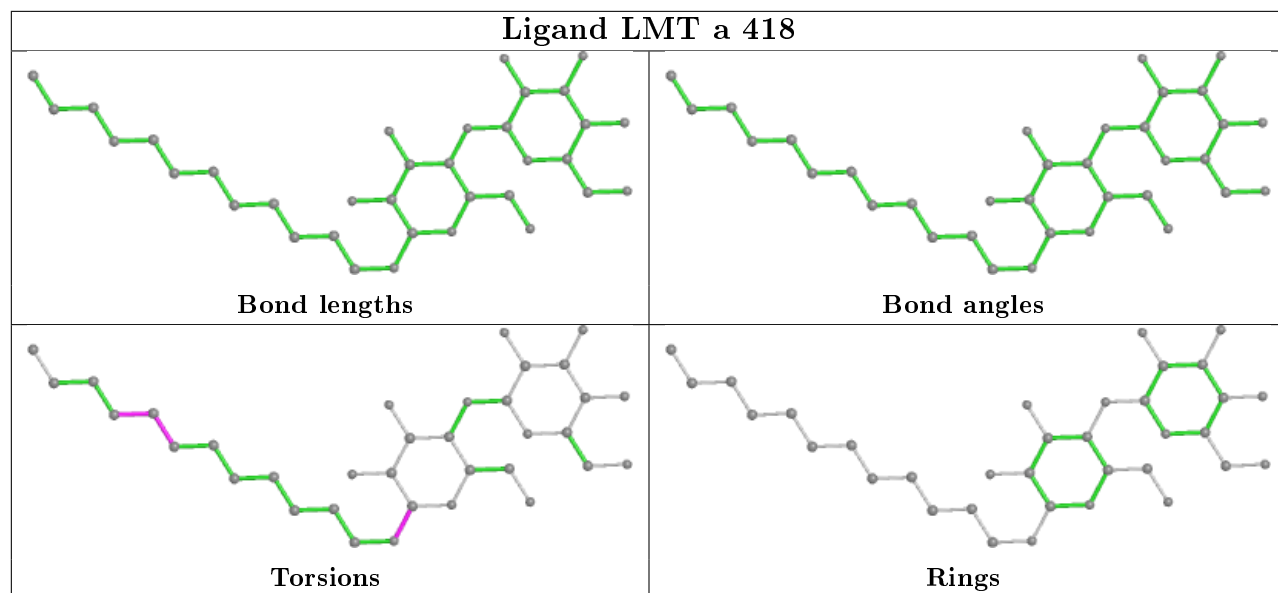
## Ligand CLA b 621

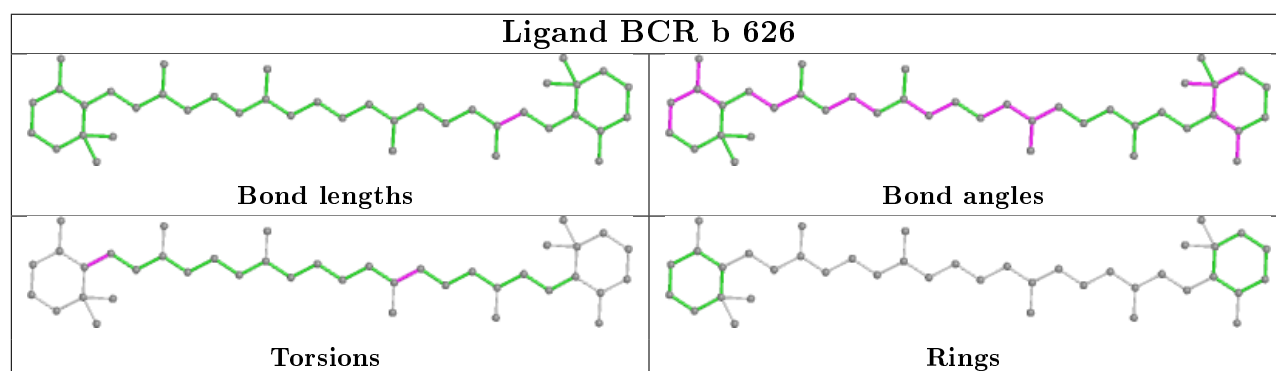
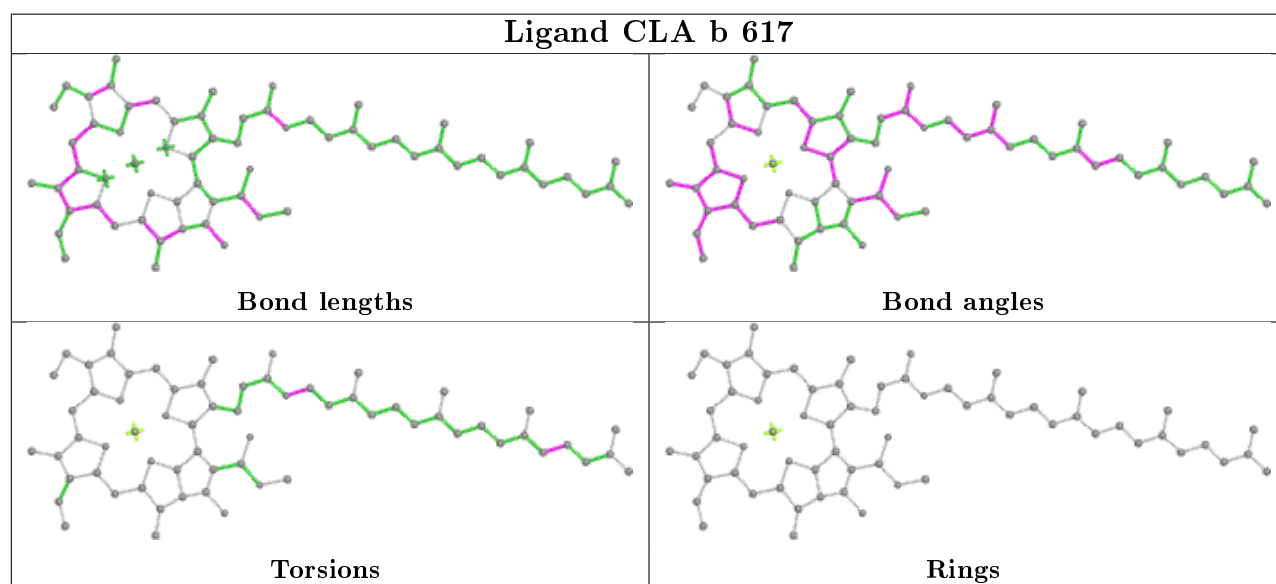
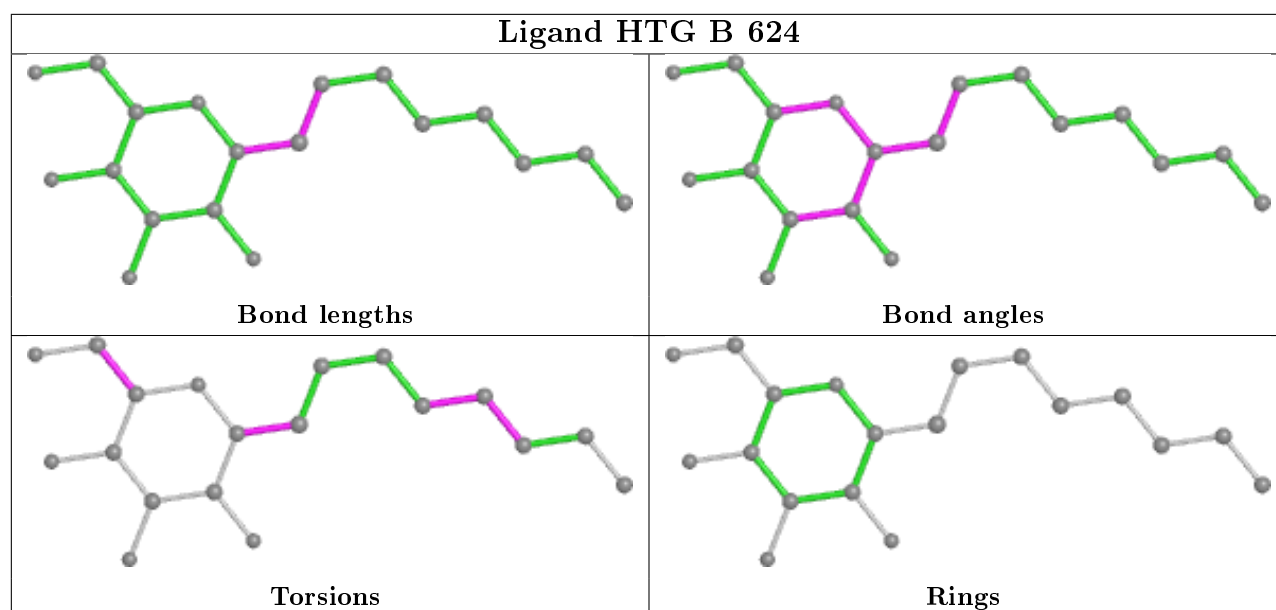


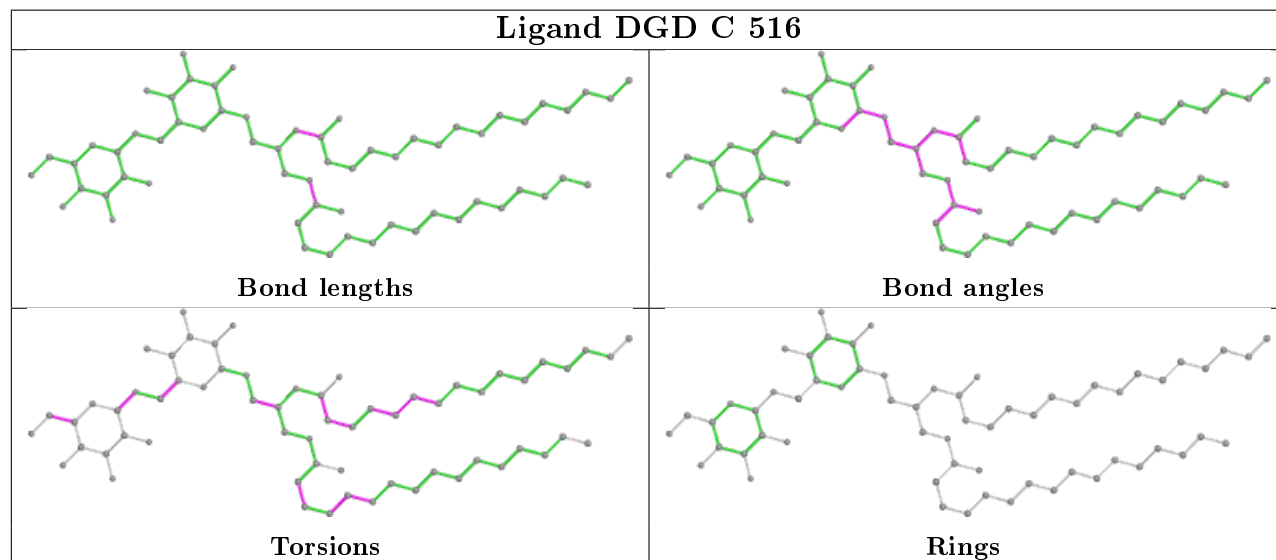
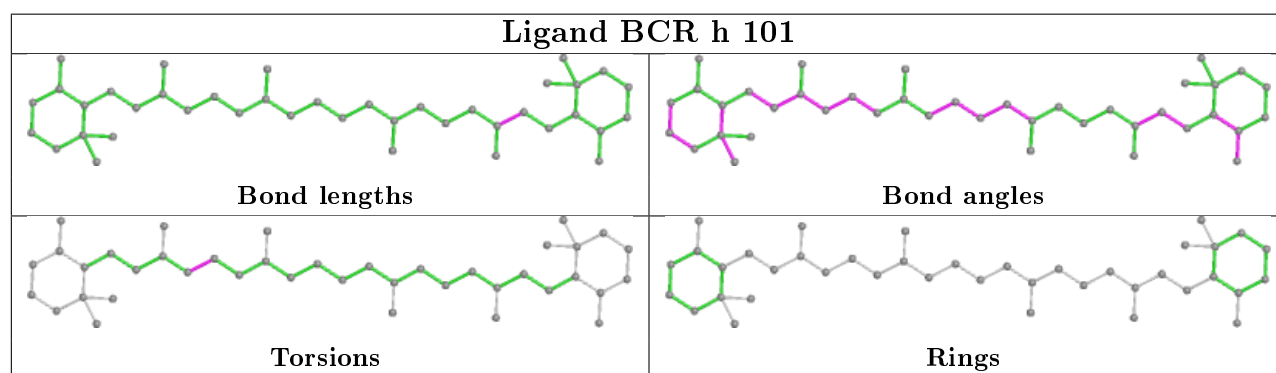
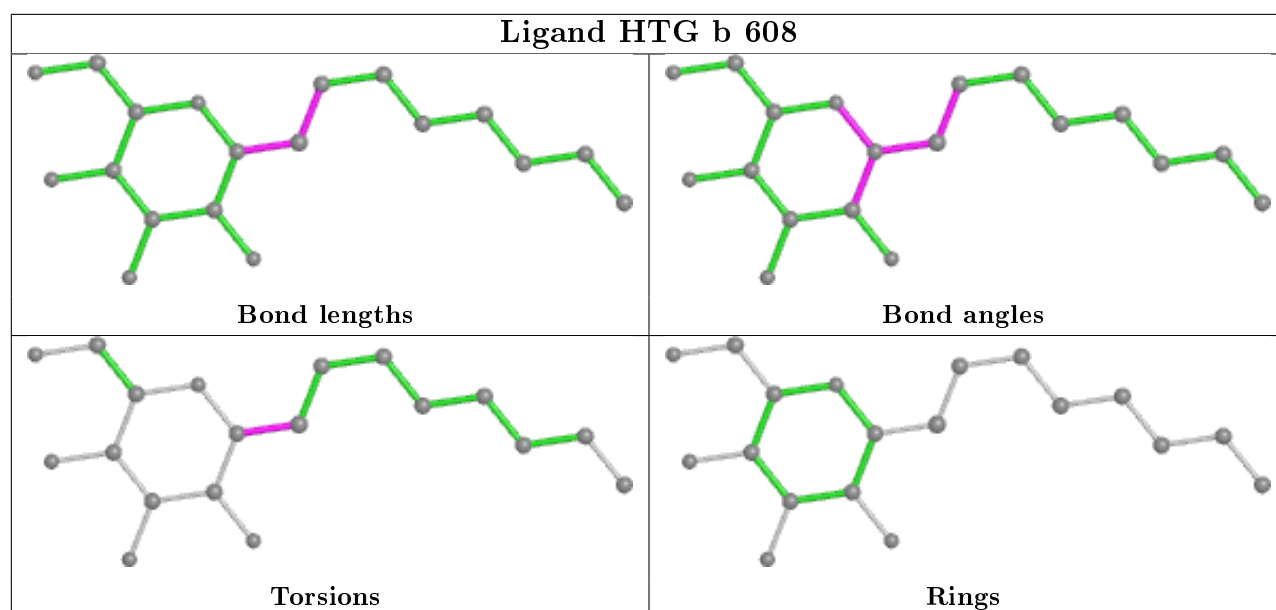
## Ligand DGD d 408

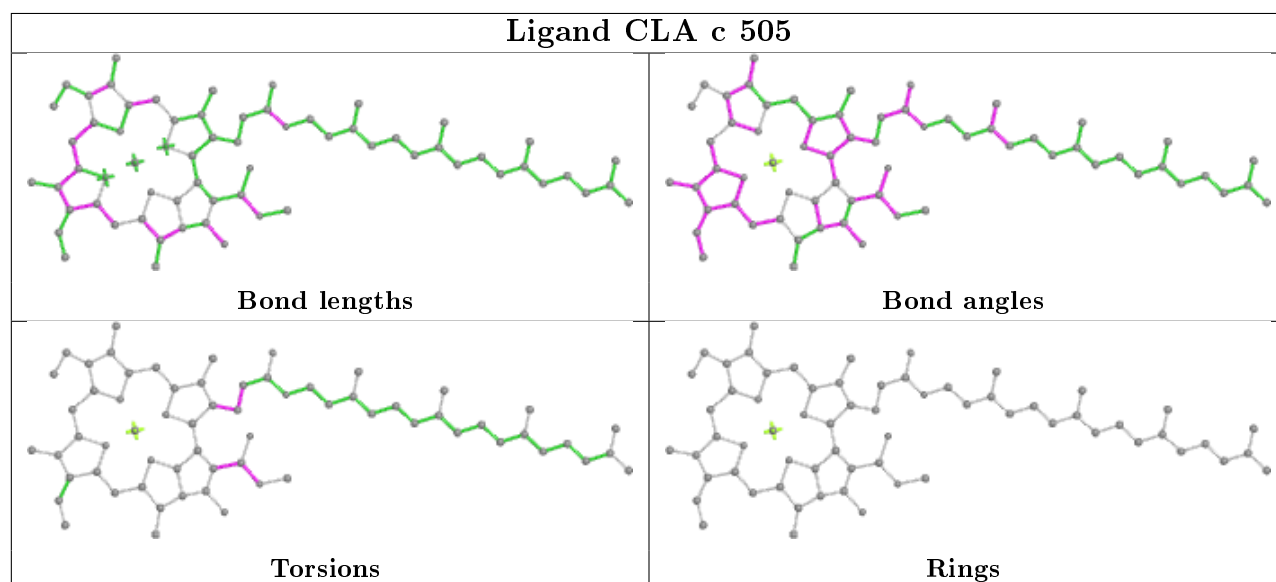
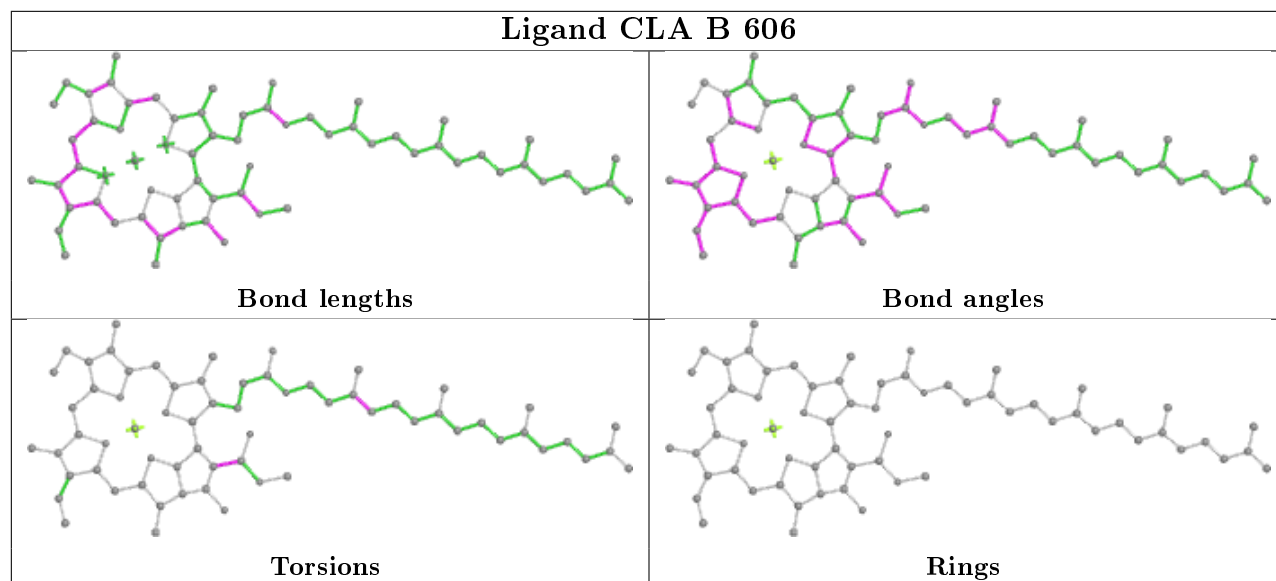
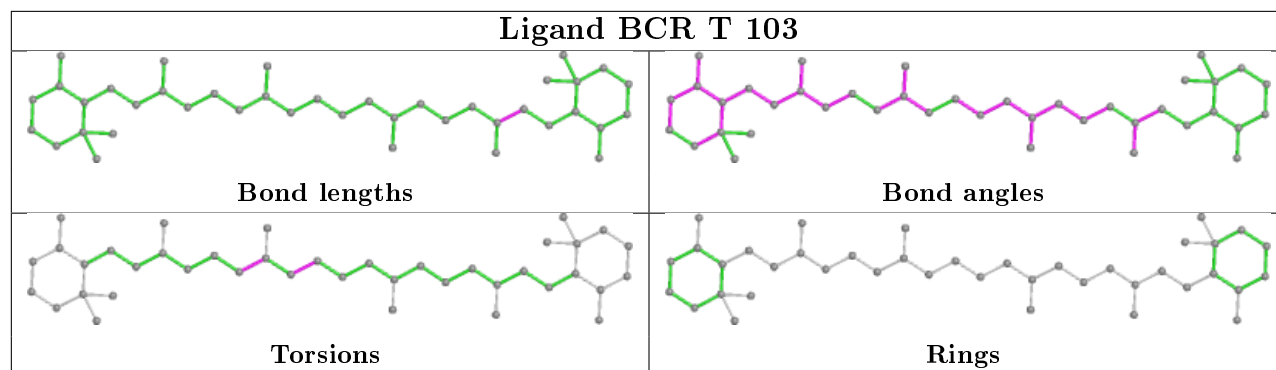




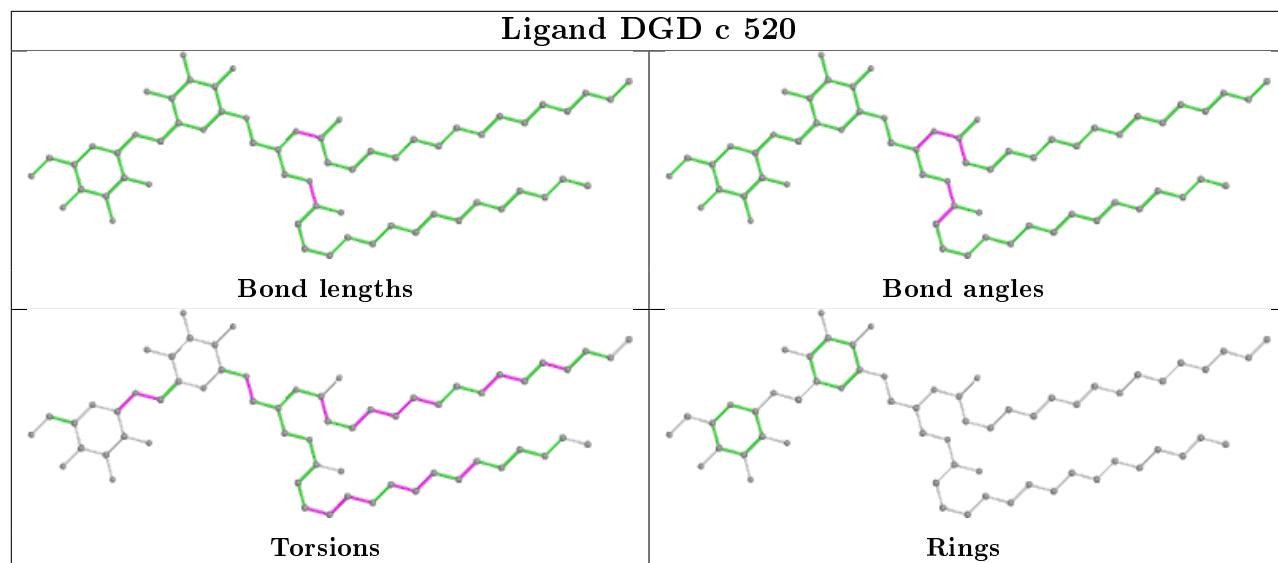




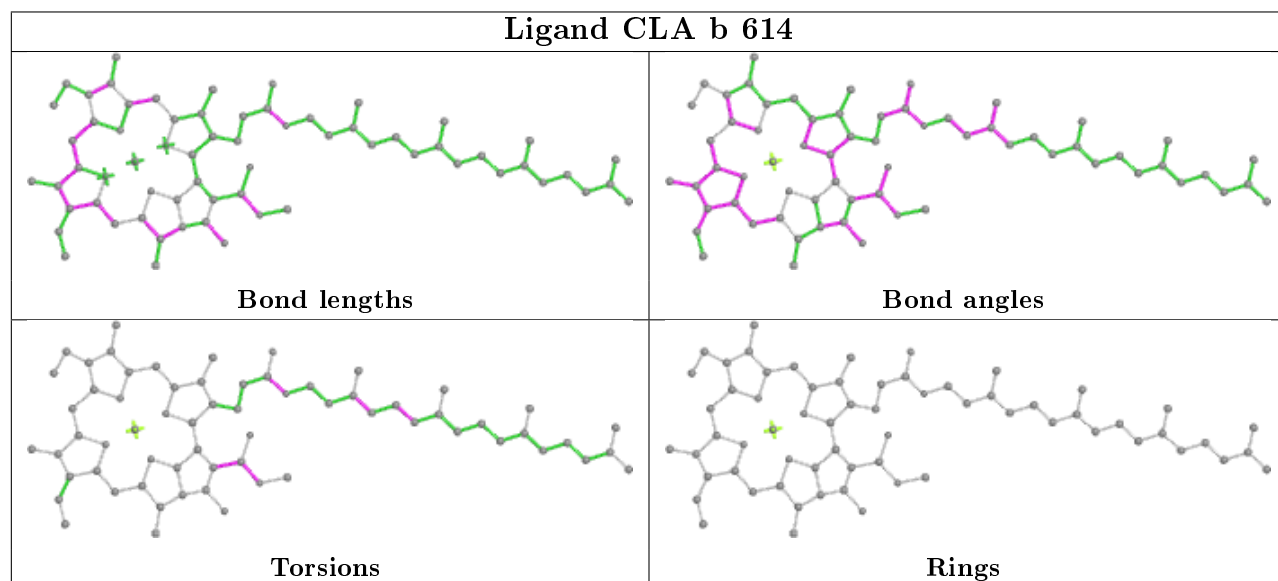




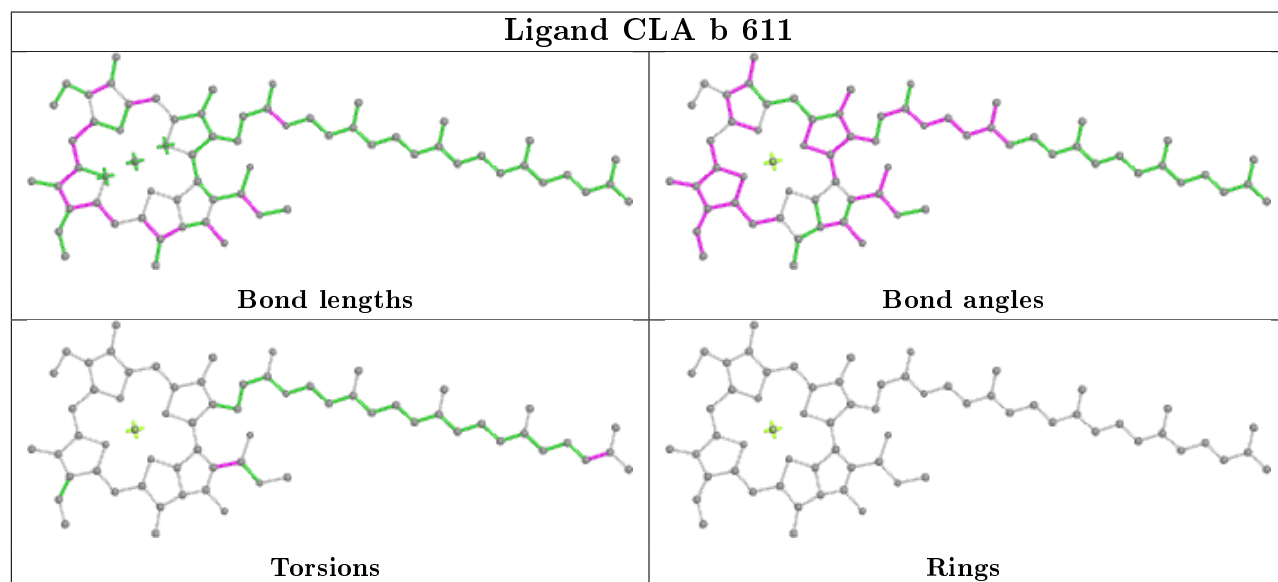
## Ligand DGD c 520

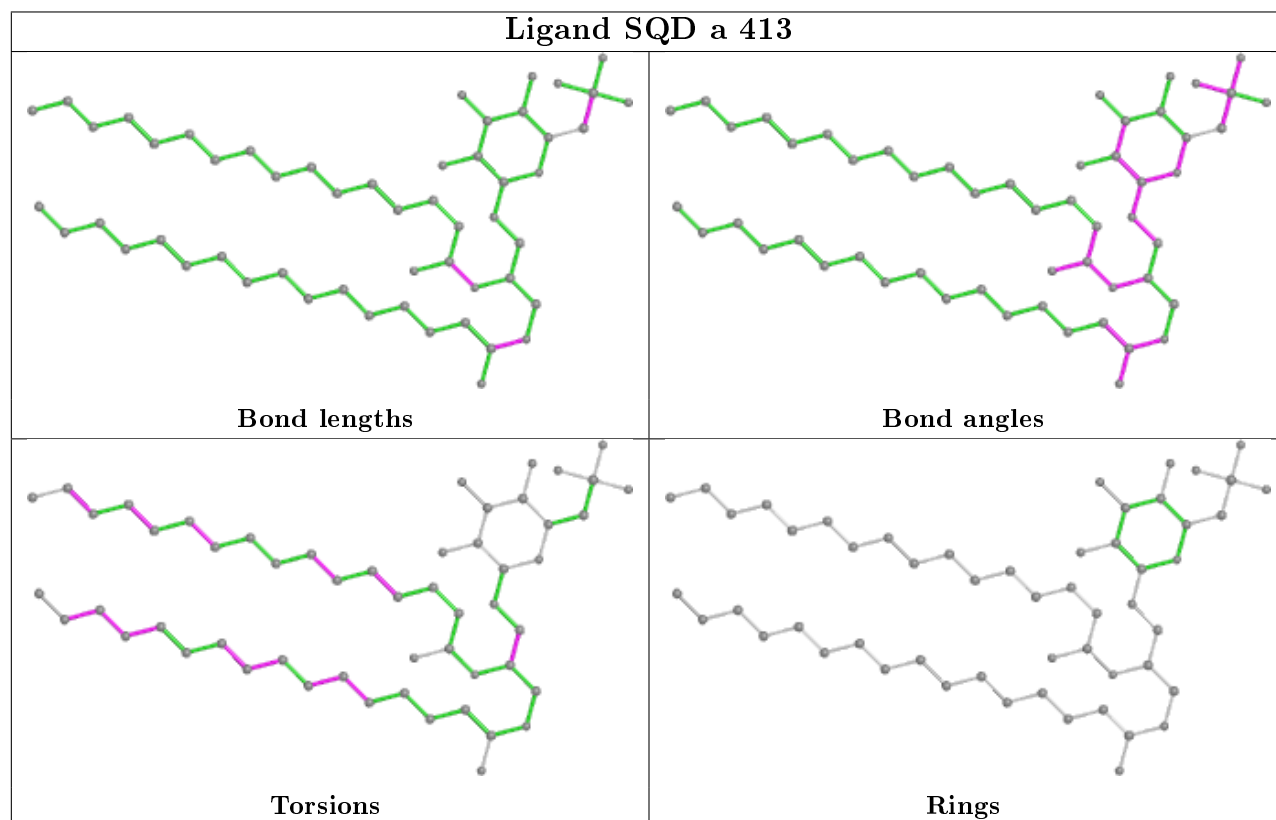
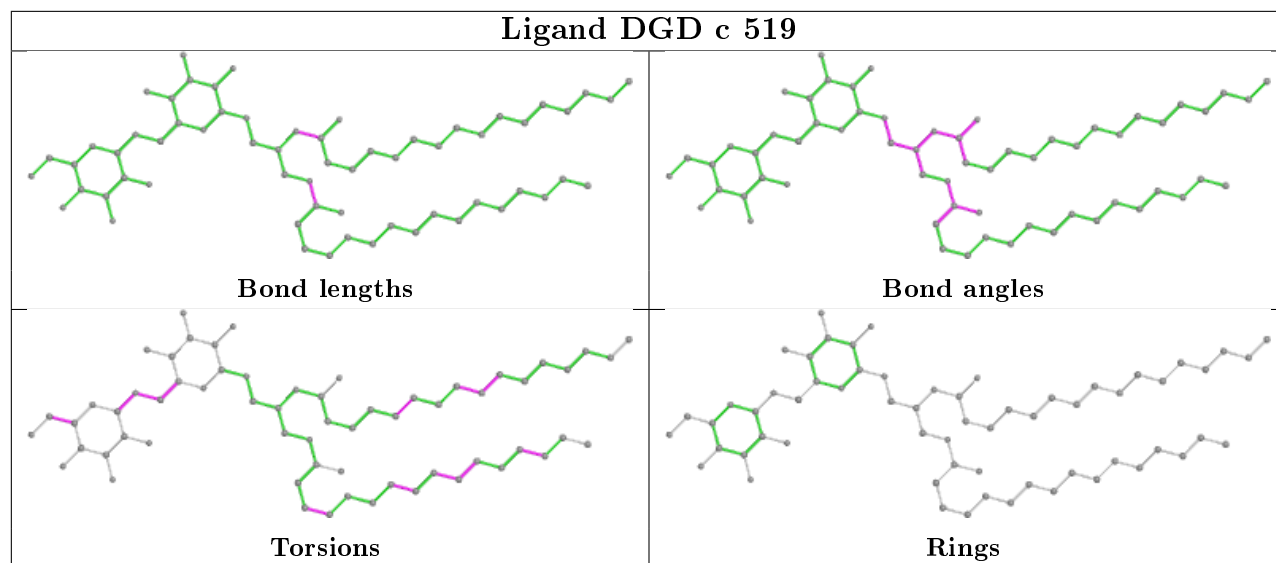


## Ligand CLA b 614

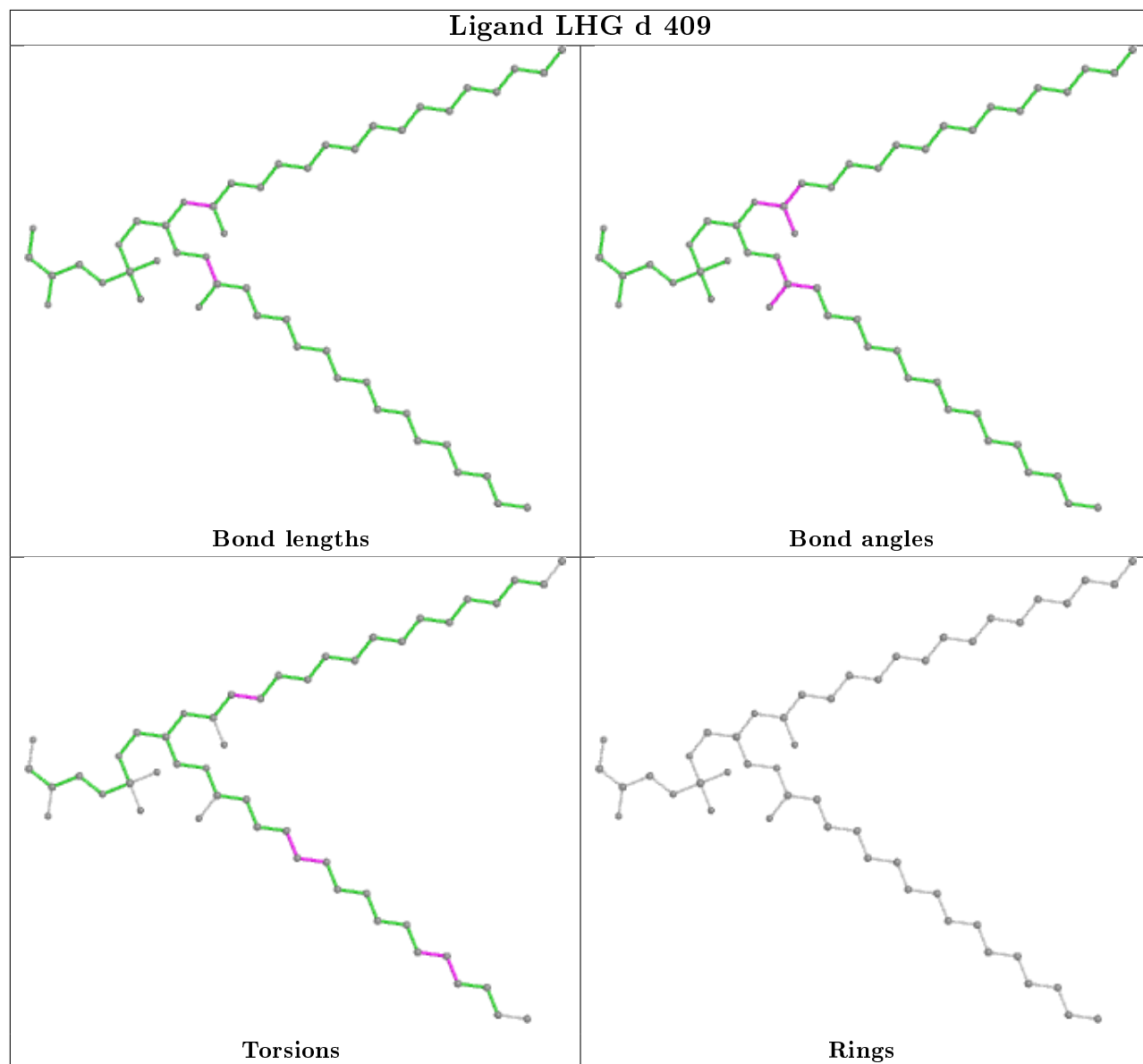


## Ligand CLA b 611

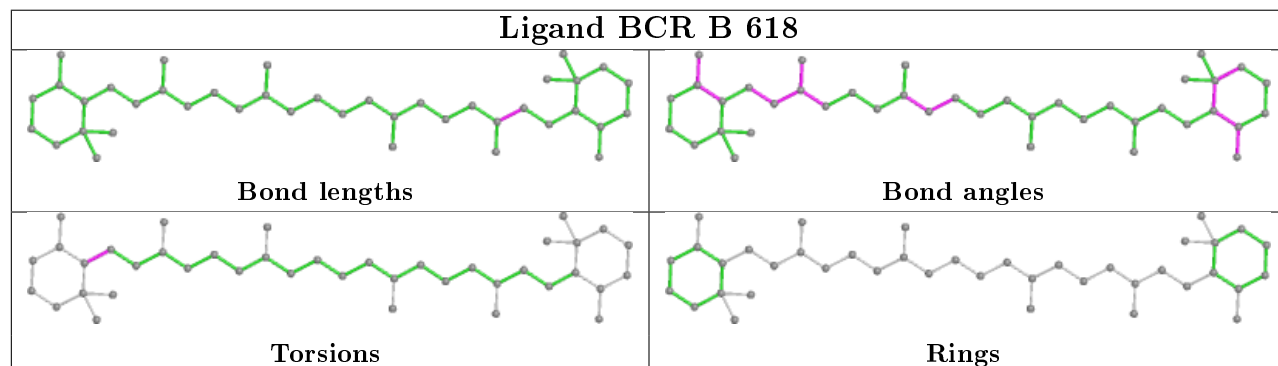




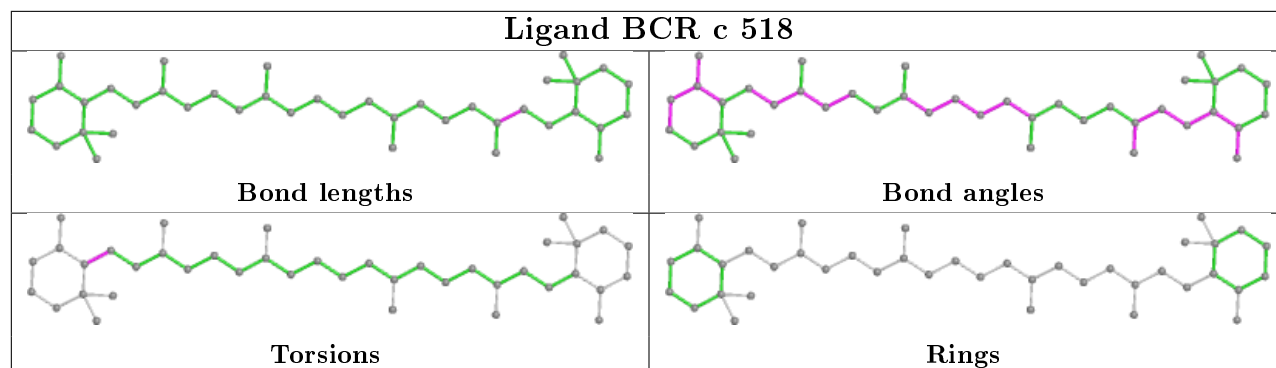
## Ligand LHG d 409



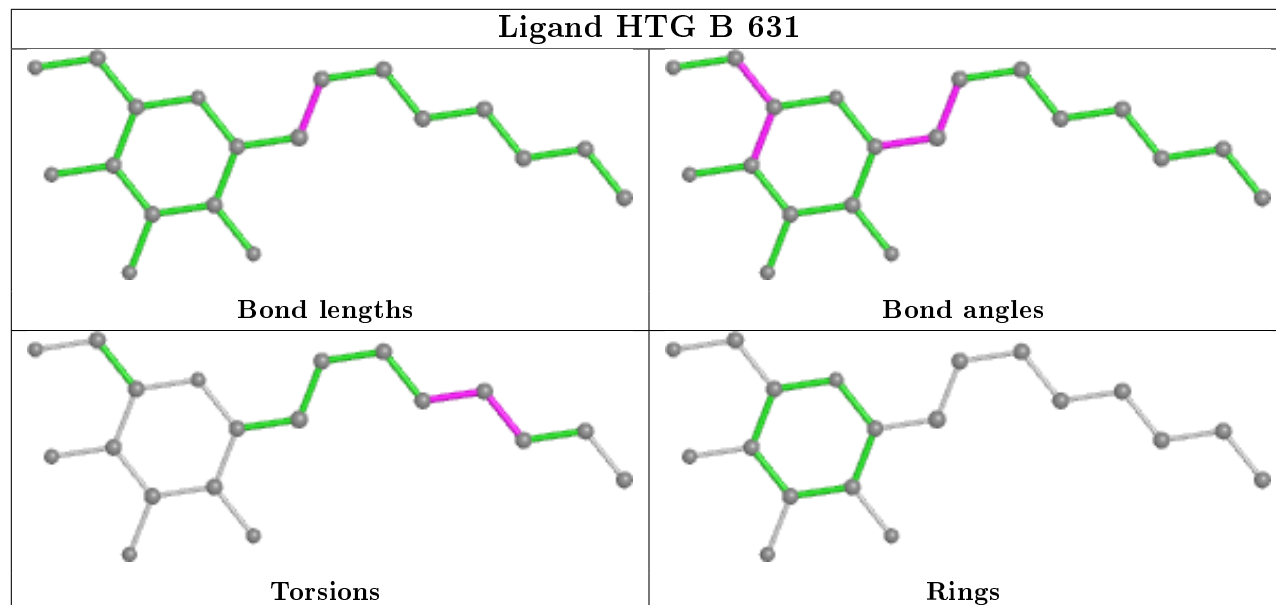
## Ligand BCR B 618



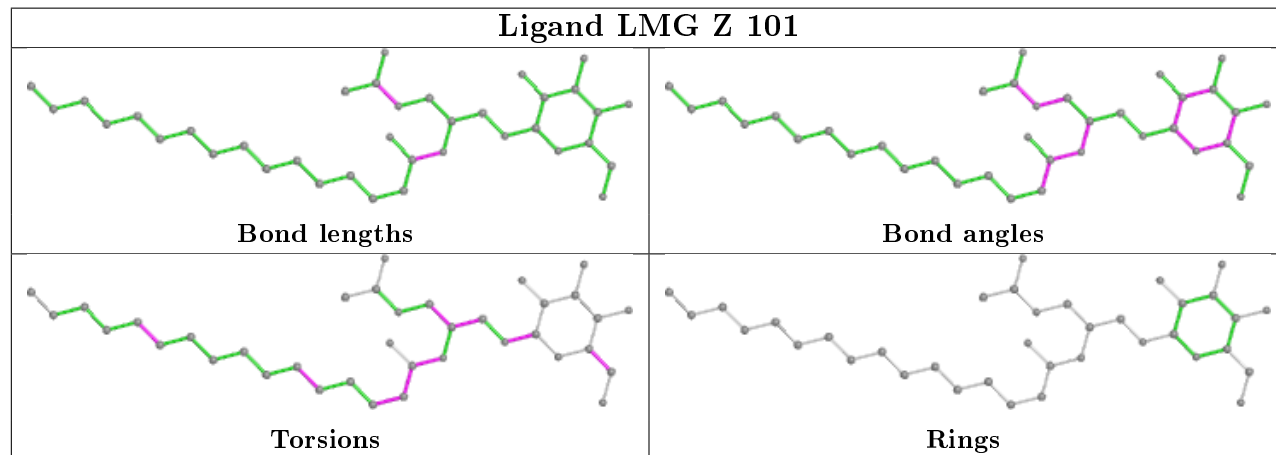
## Ligand BCR c 518



## Ligand HTG B 631

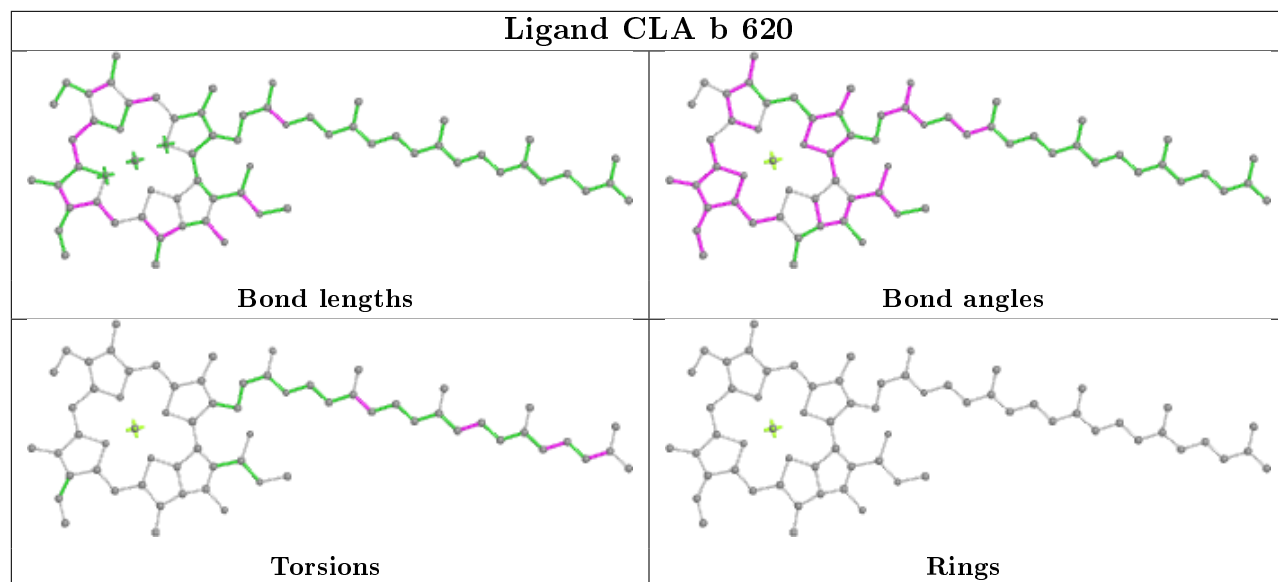


## Ligand LMG Z 101

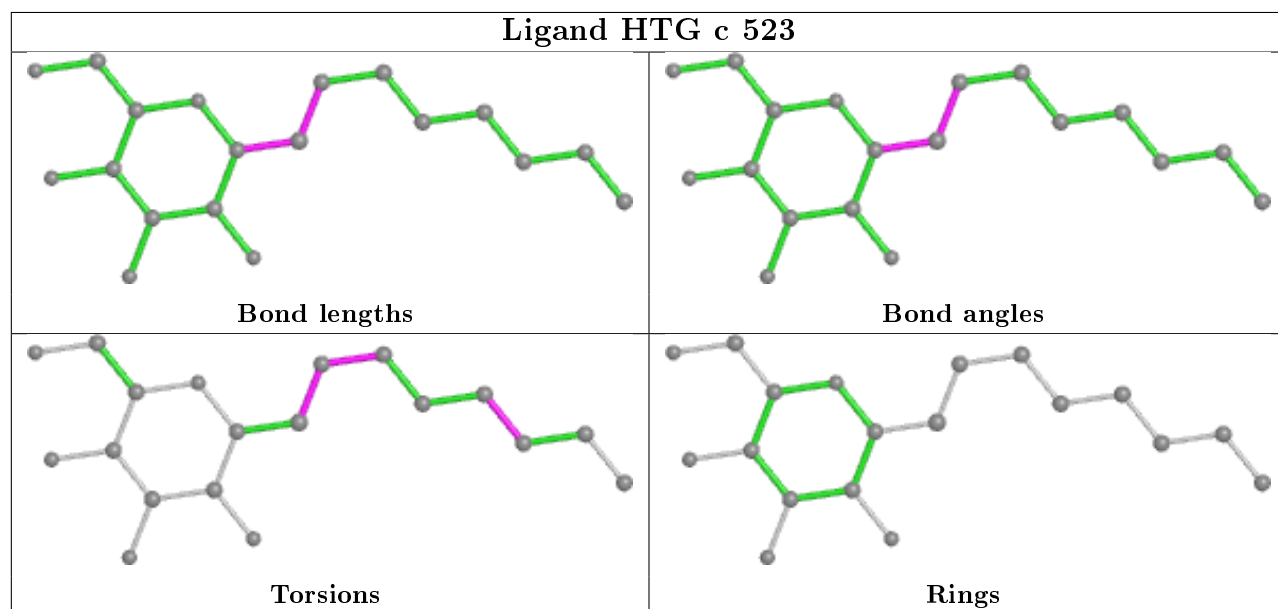




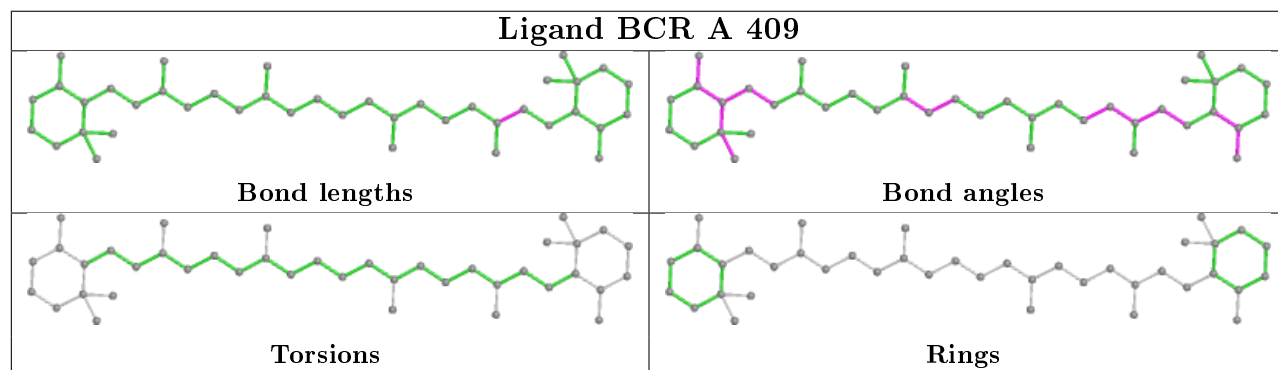
## Ligand CLA b 620

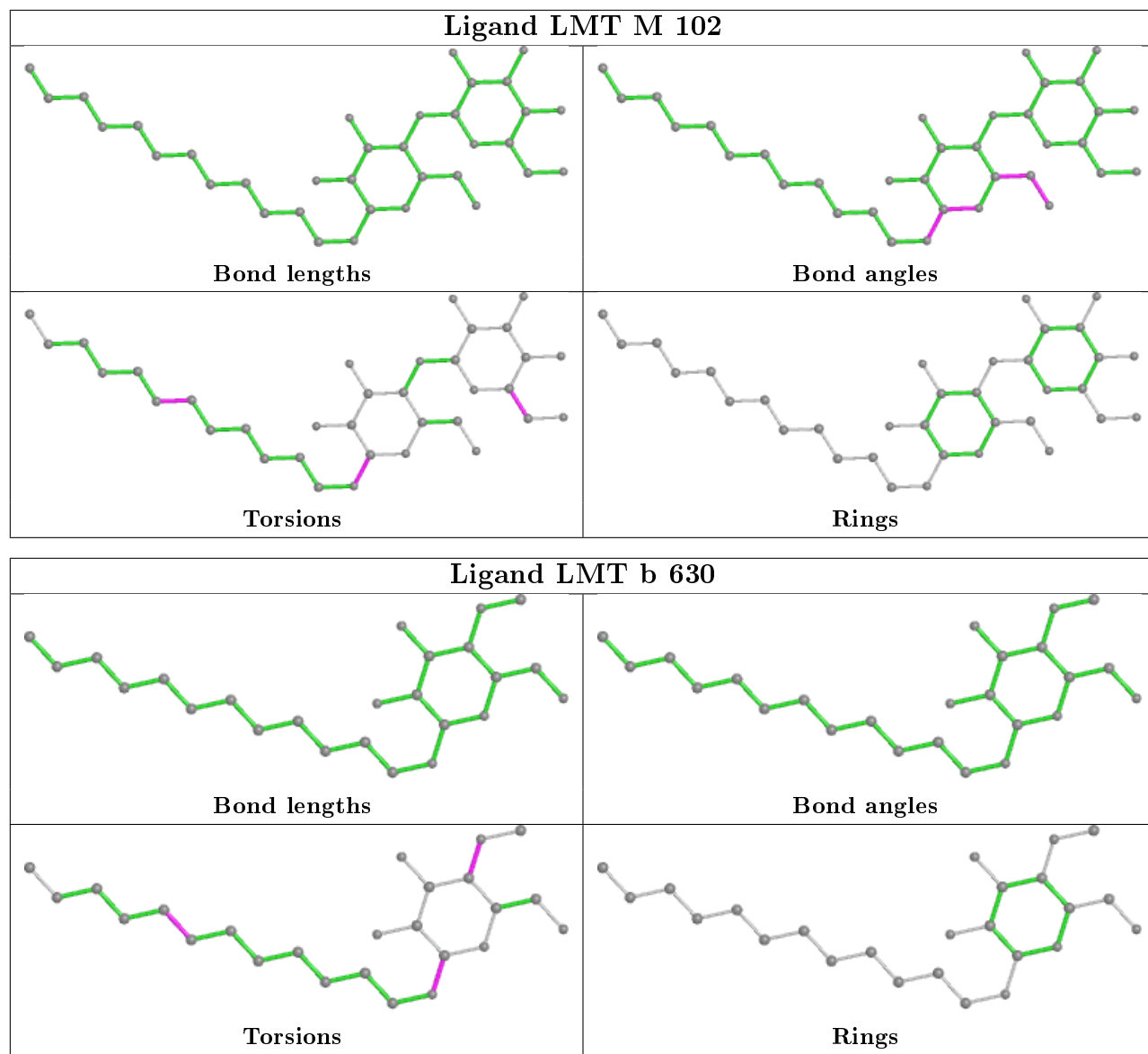


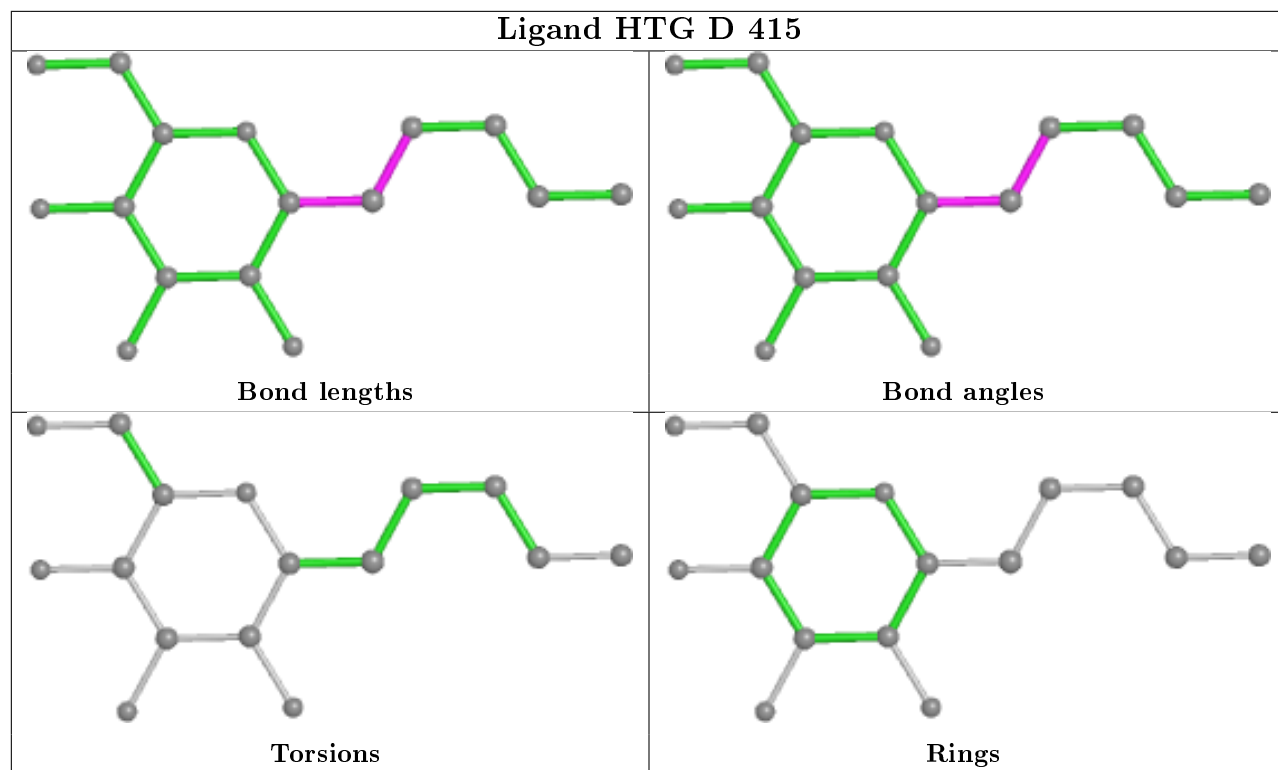
## Ligand HTG c 523

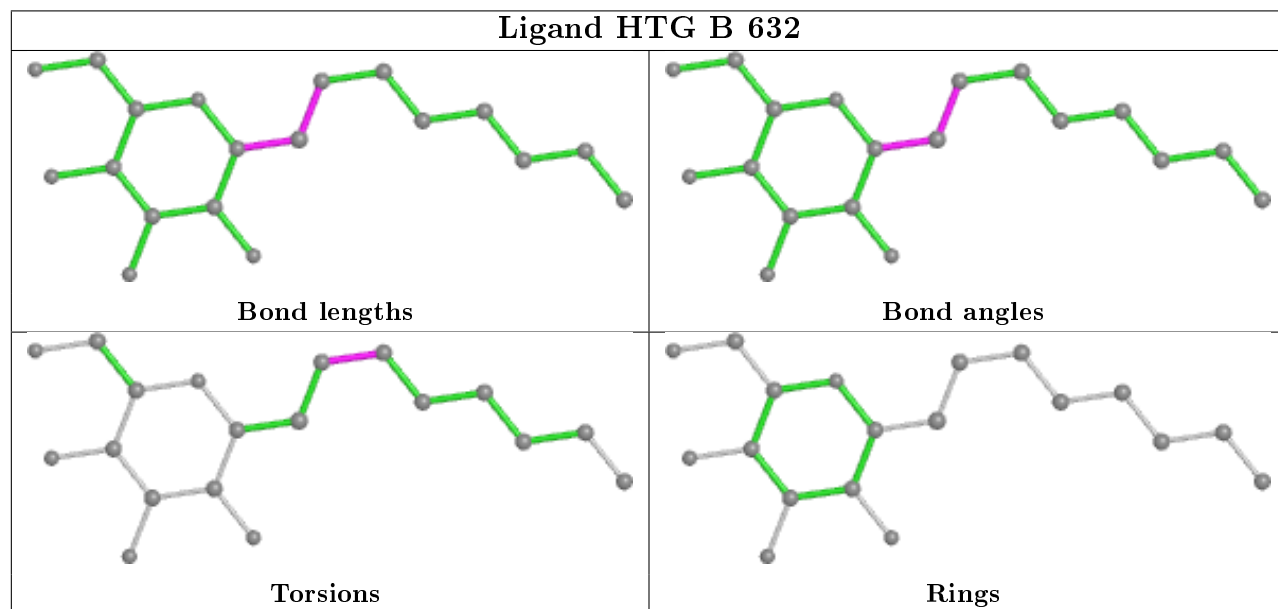
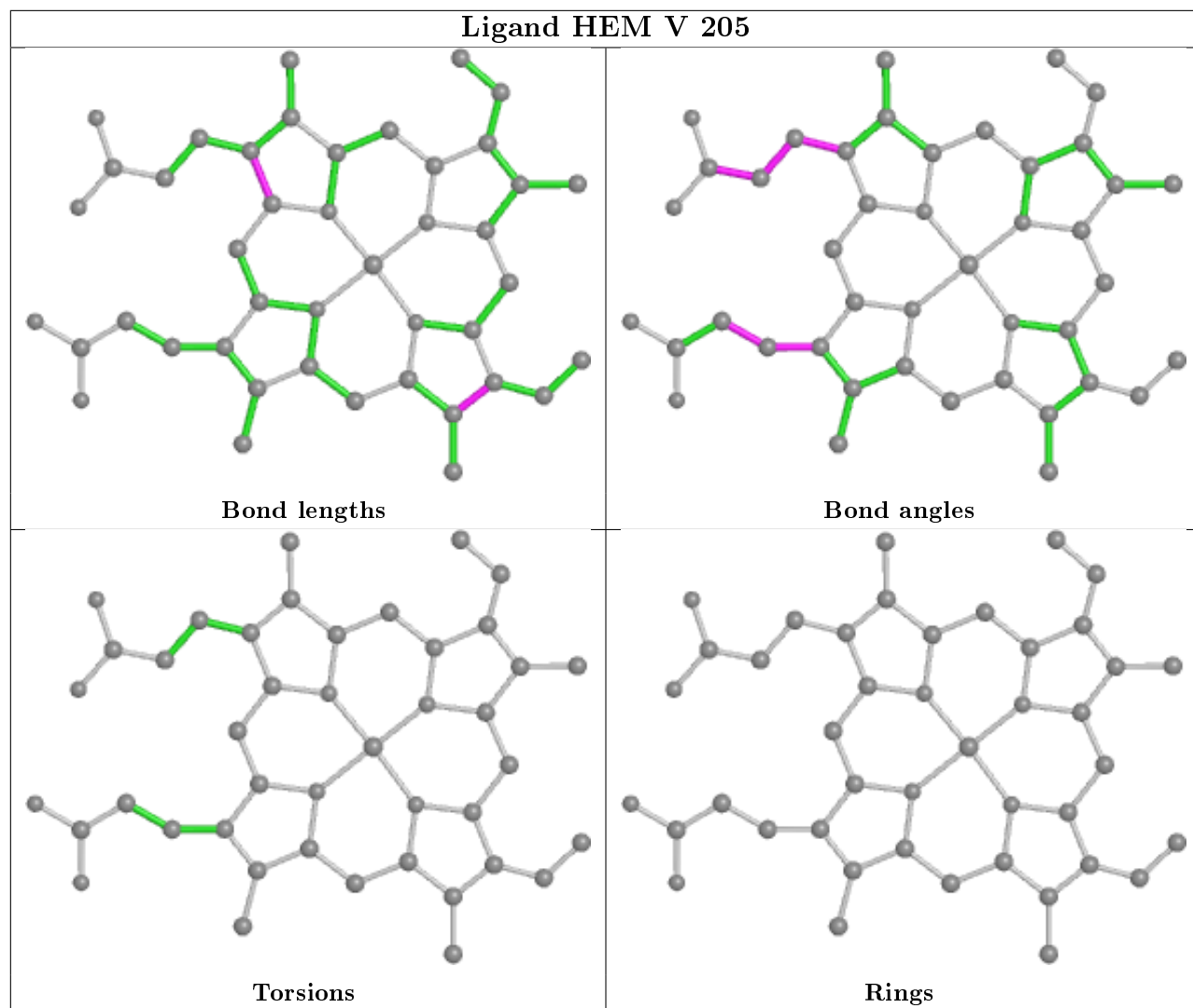


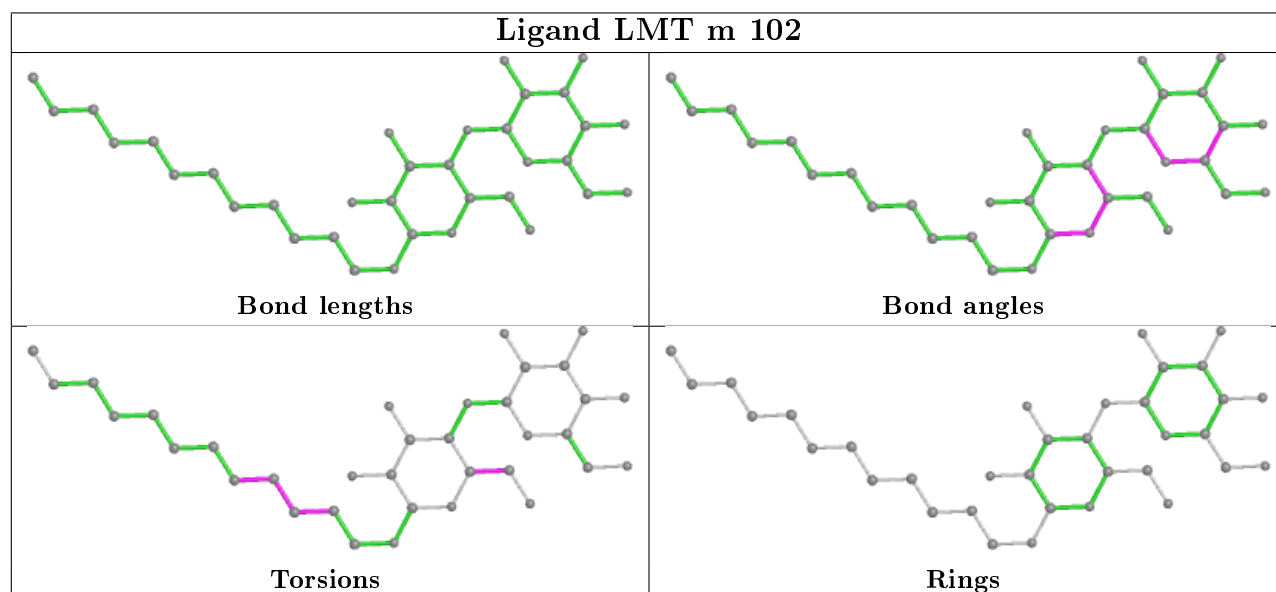
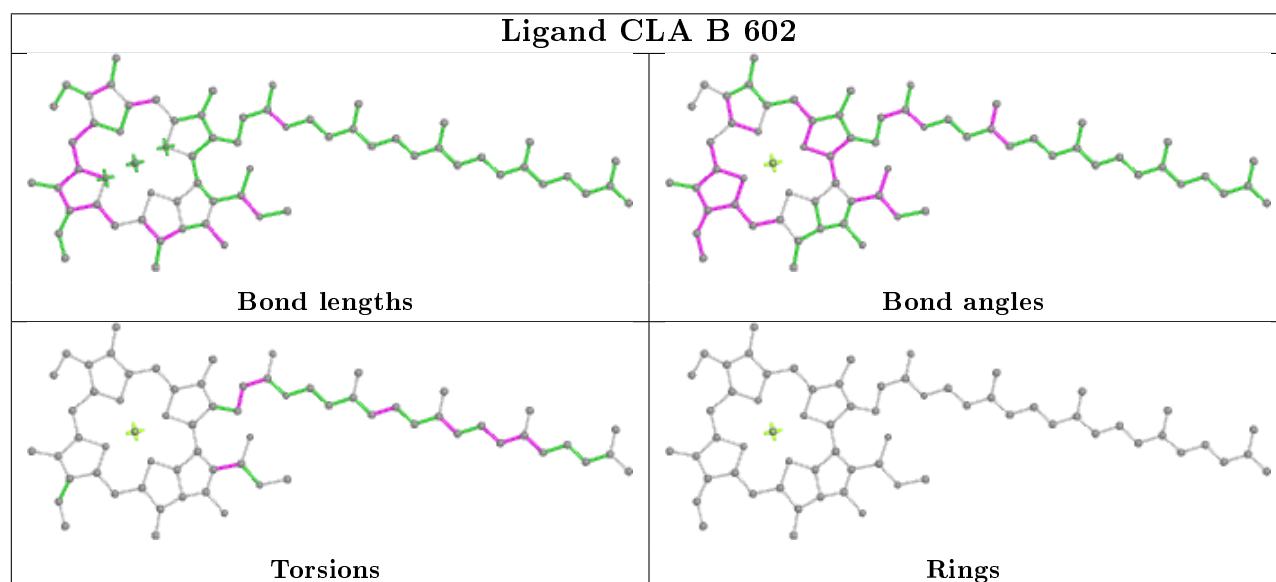
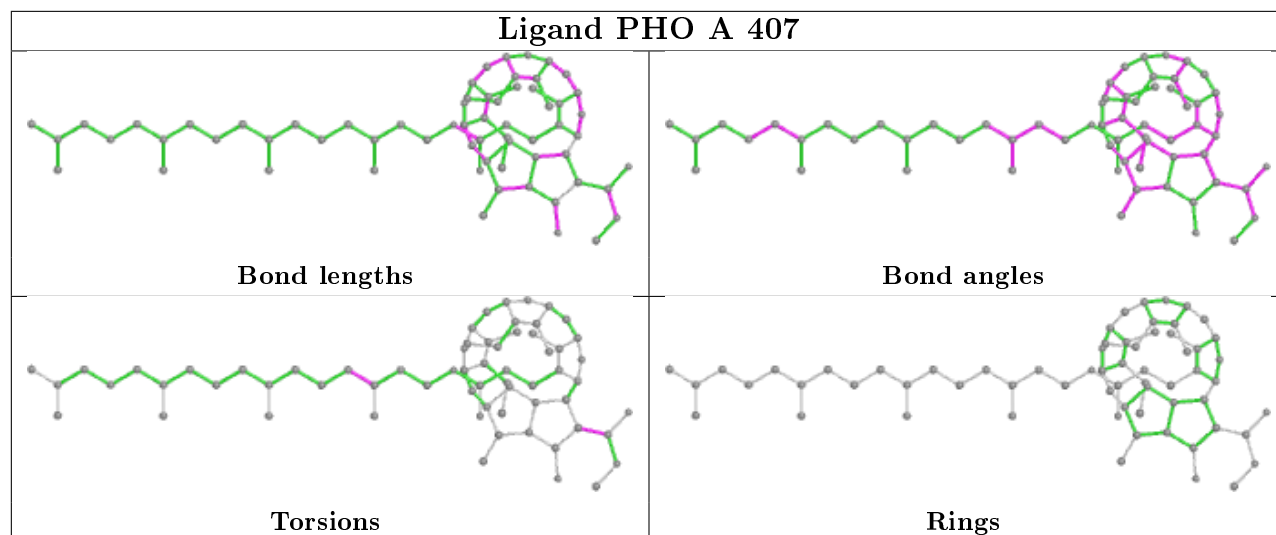
## Ligand BCR A 409



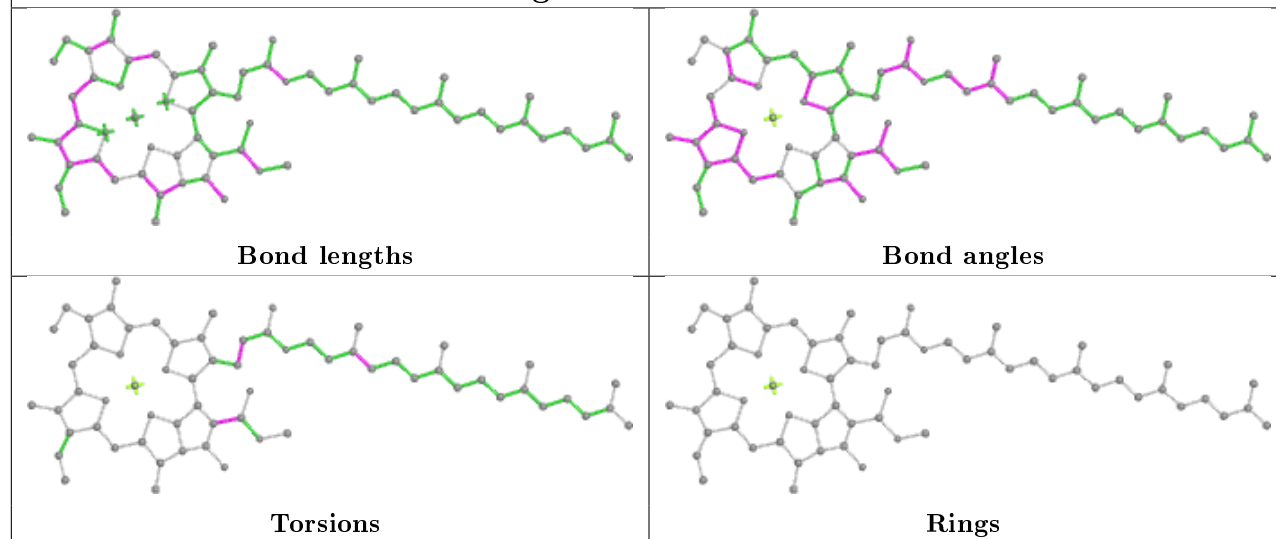




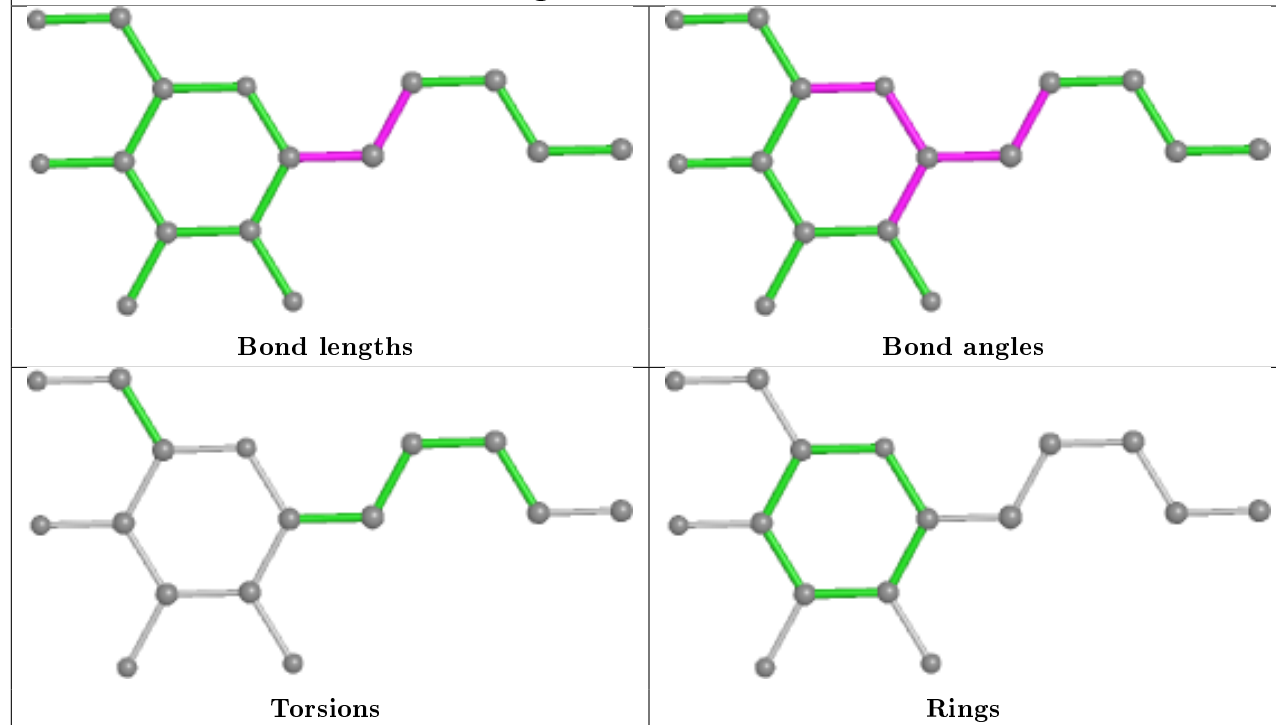




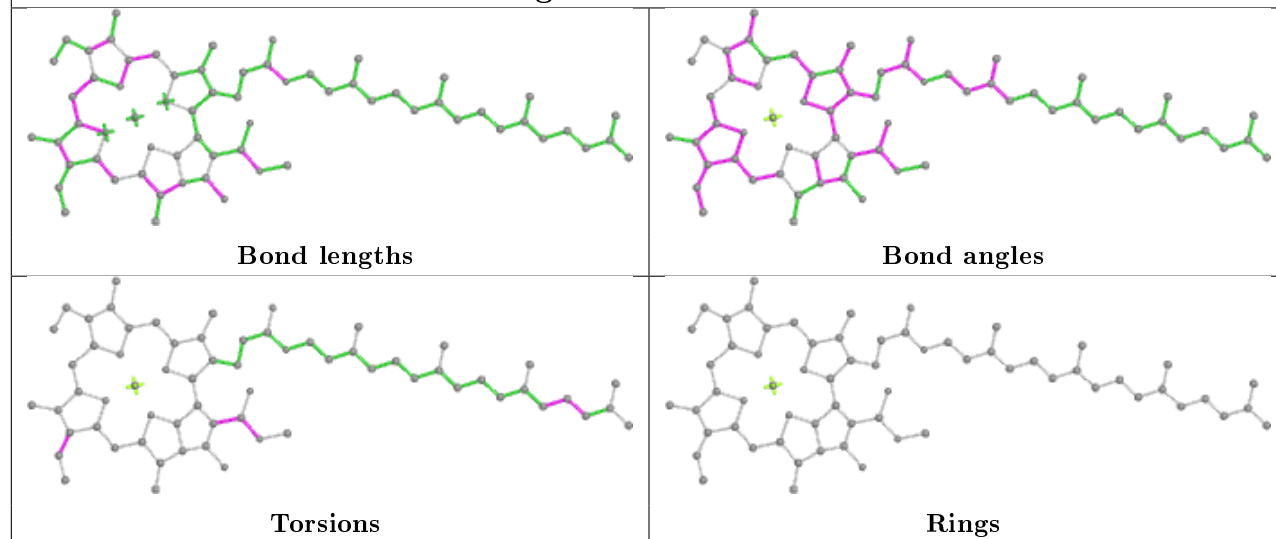
## Ligand CLA C 508



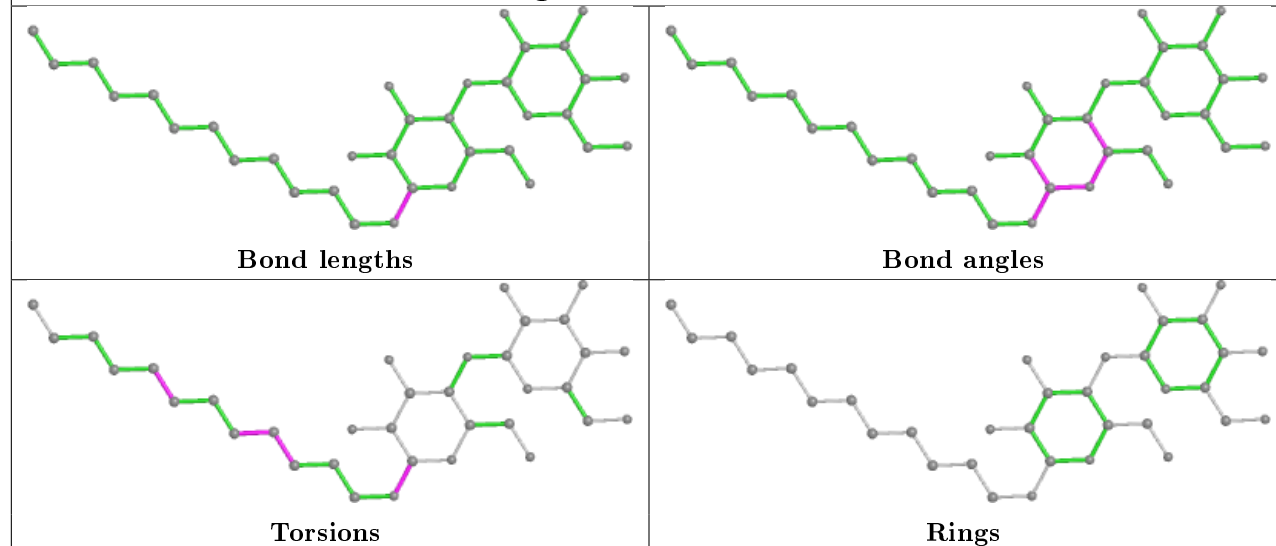
## Ligand HTG d 414



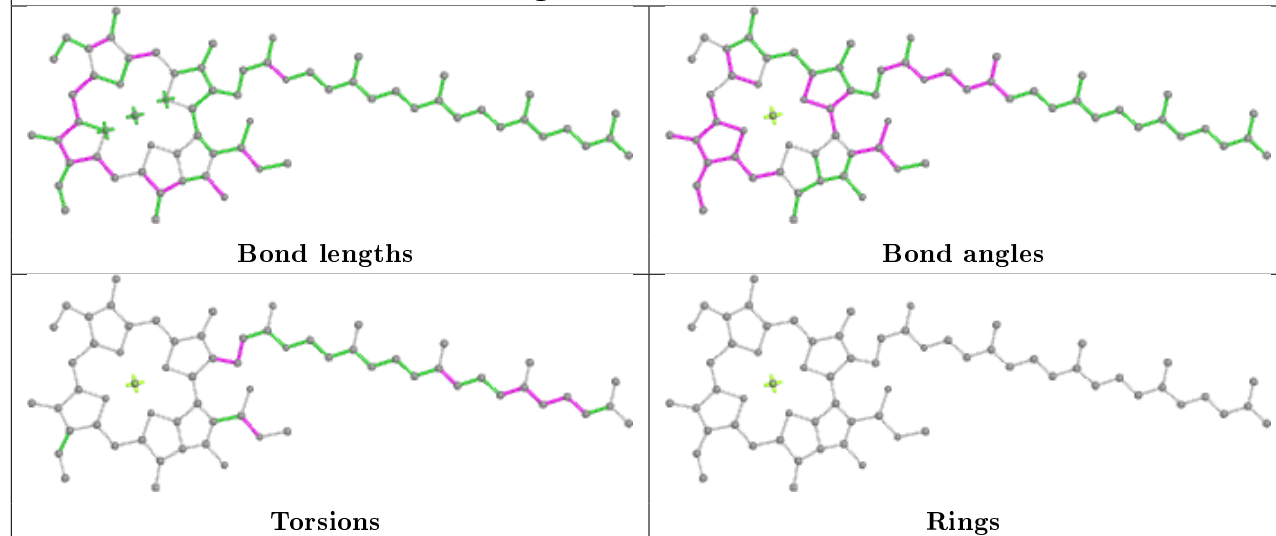
## Ligand CLA d 403

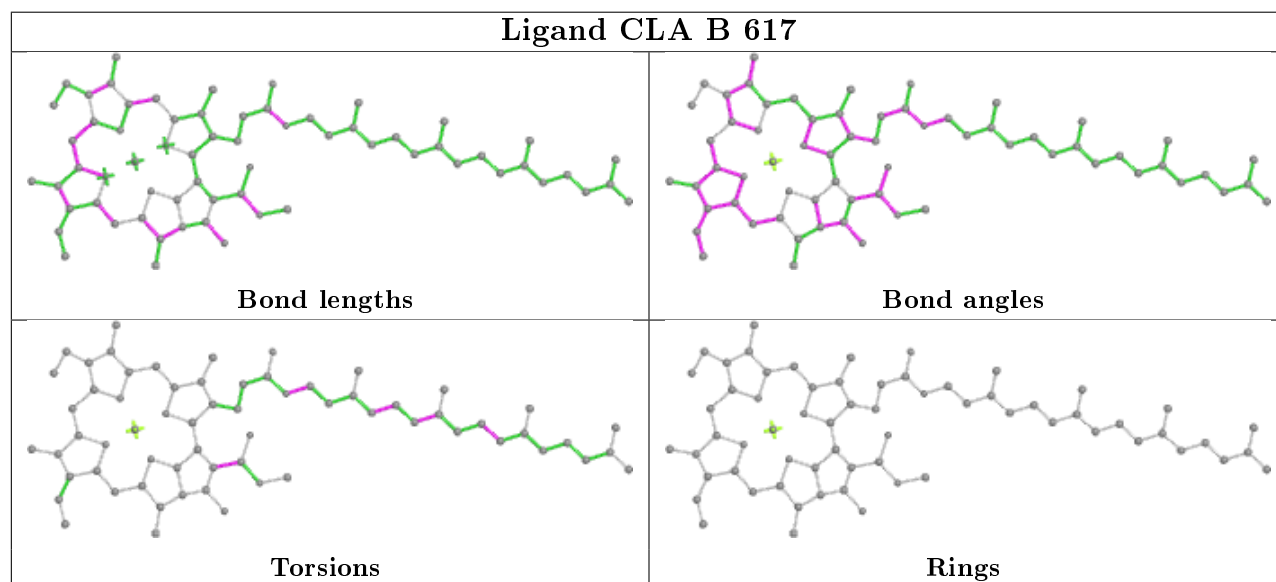
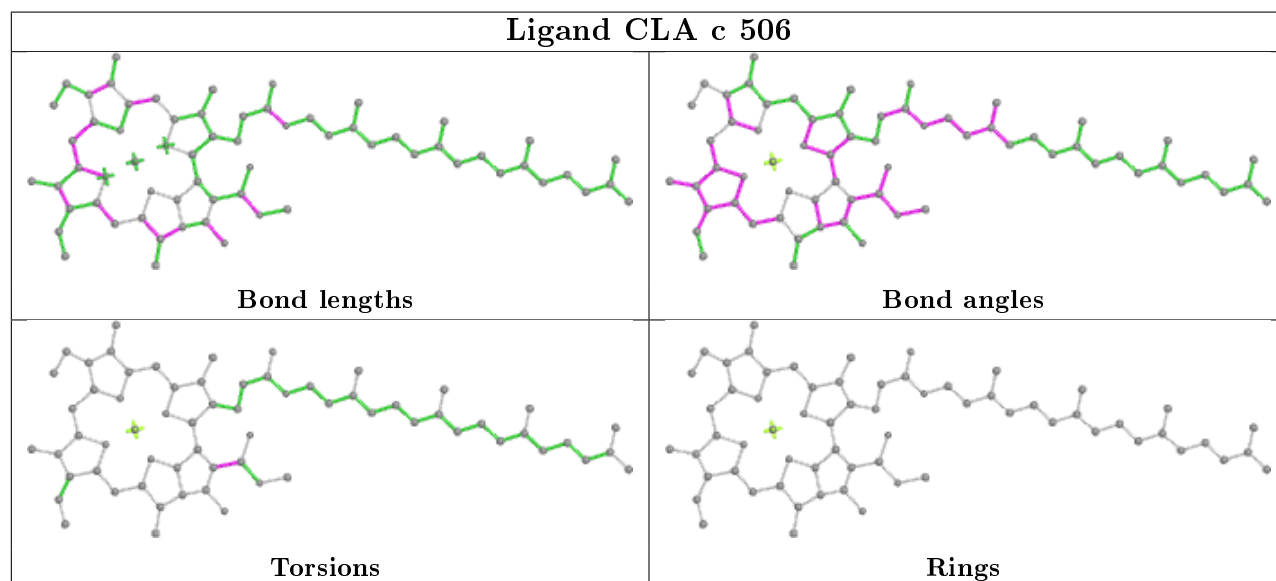
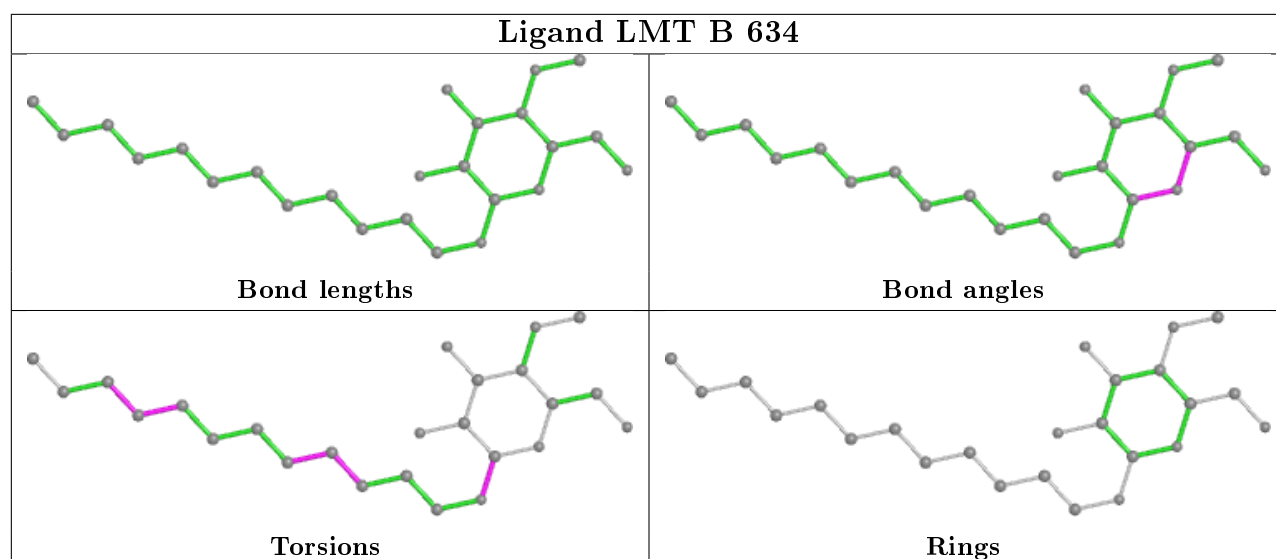


## Ligand LMT a 404

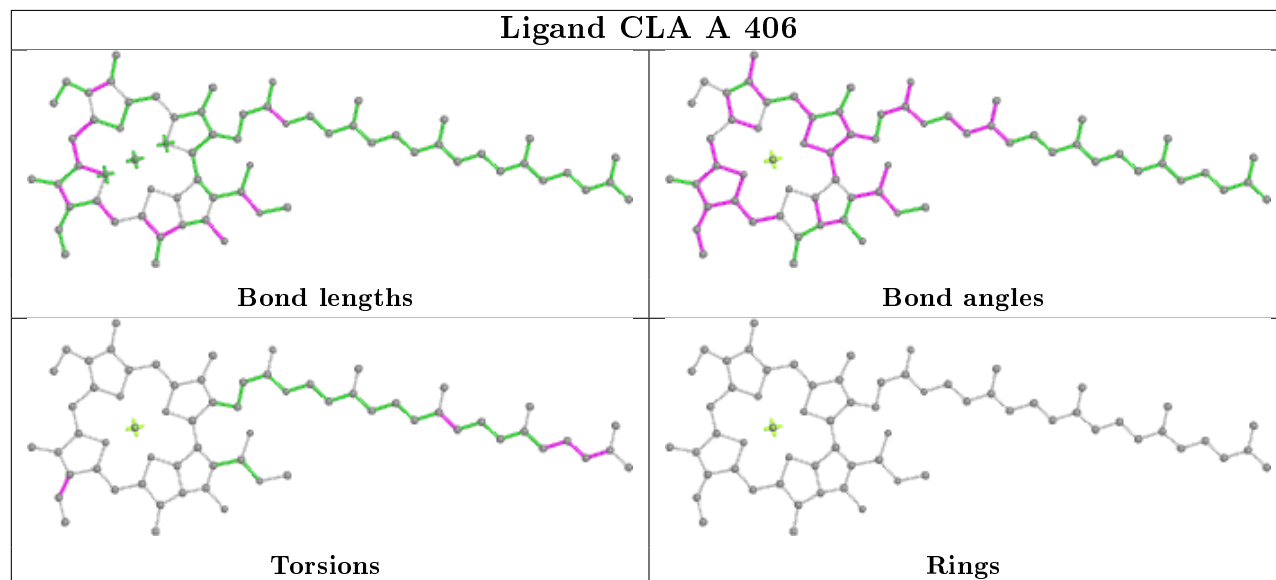
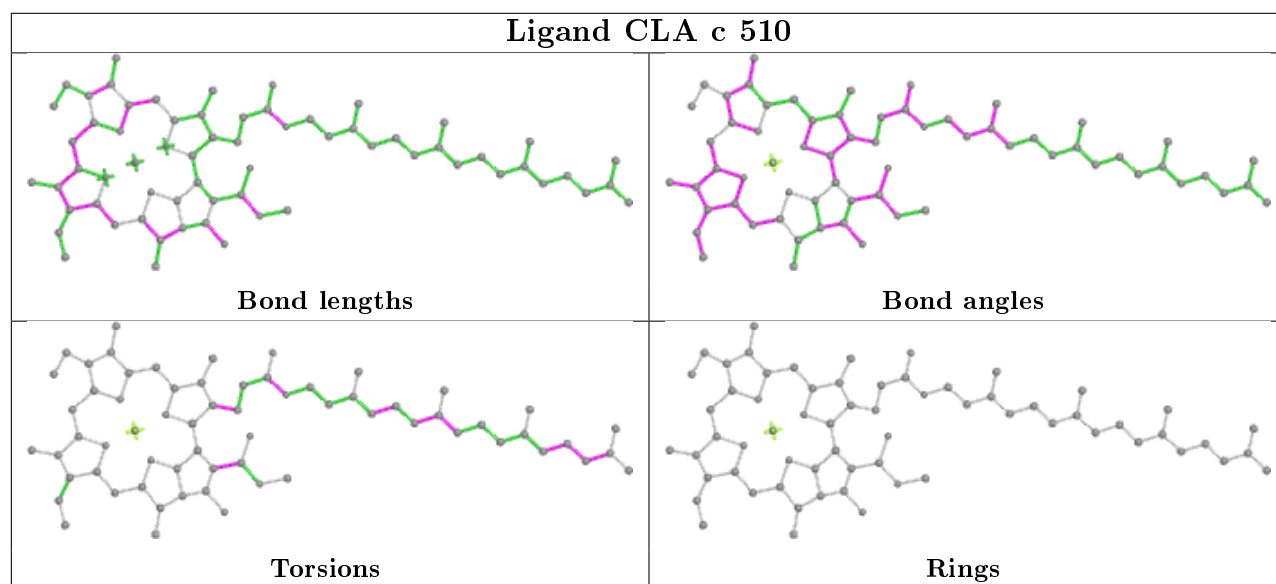
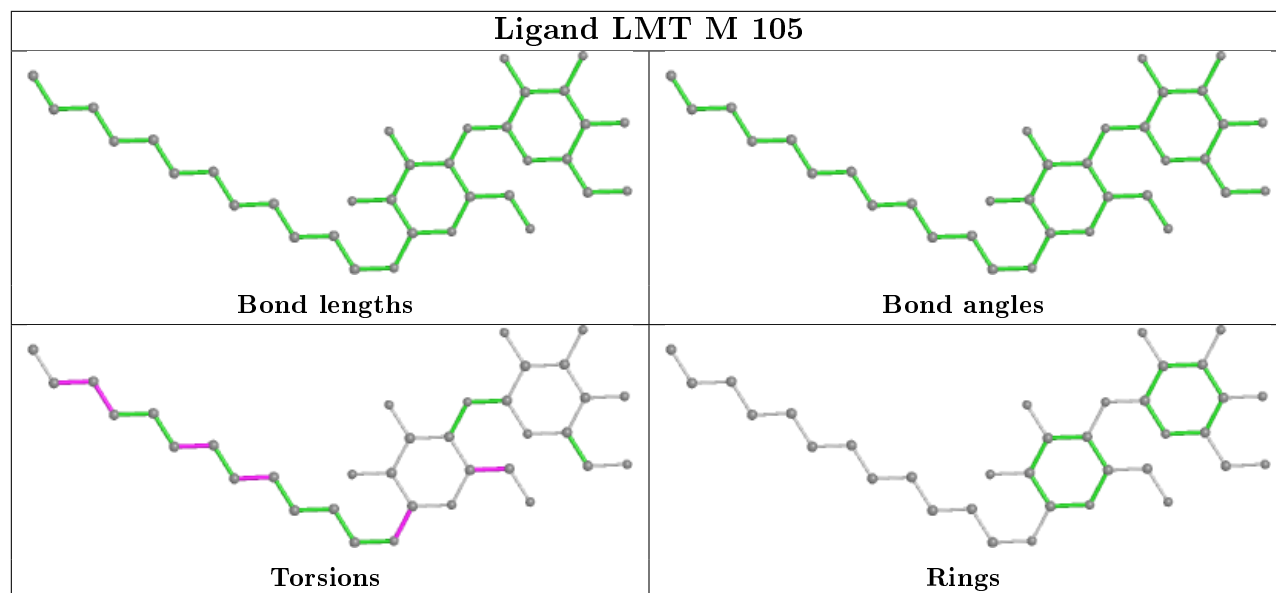


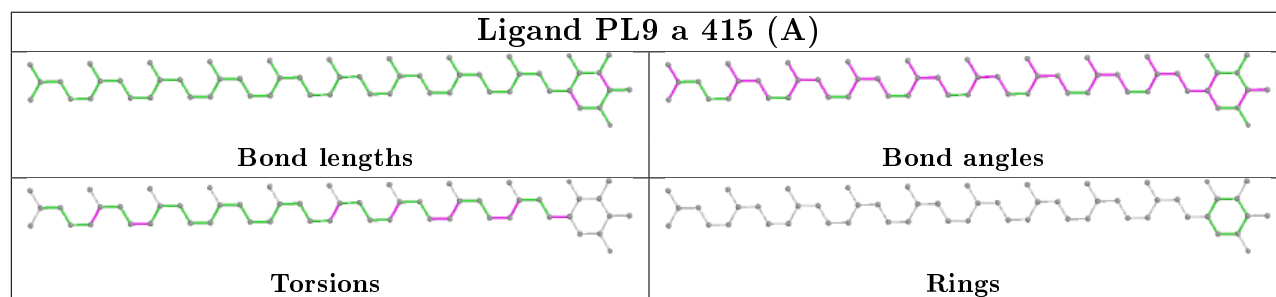
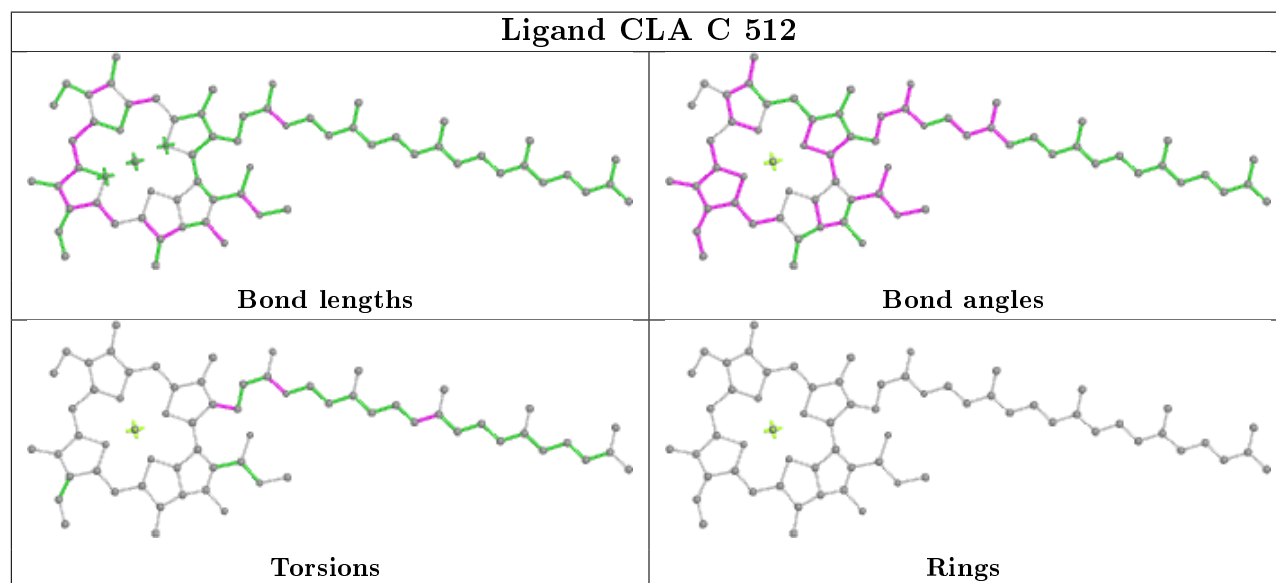
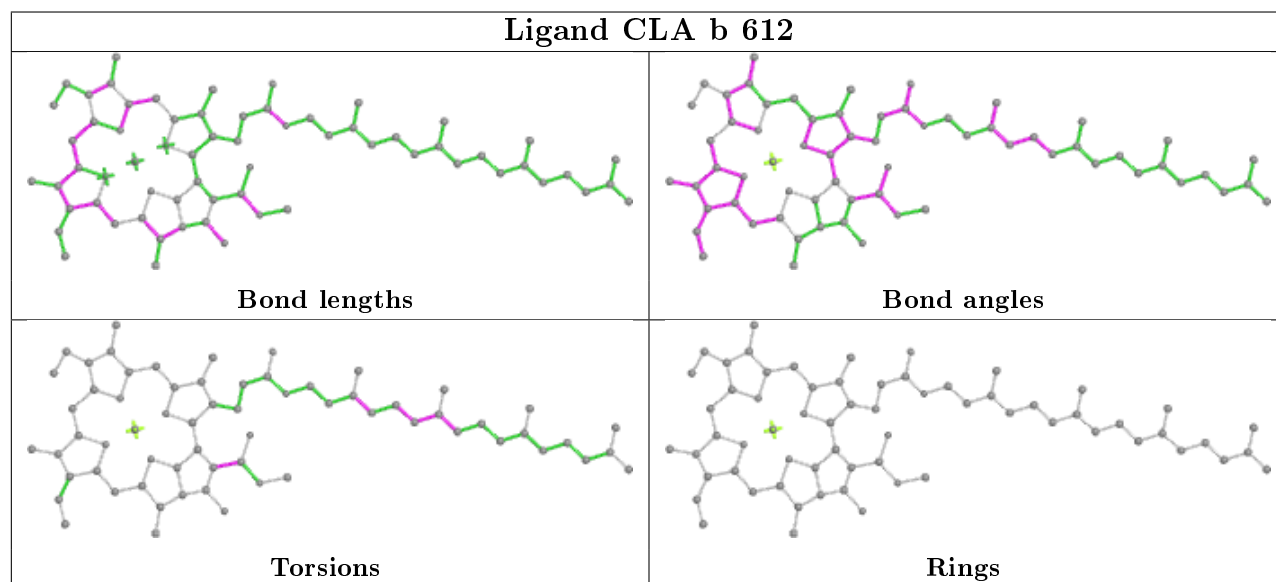
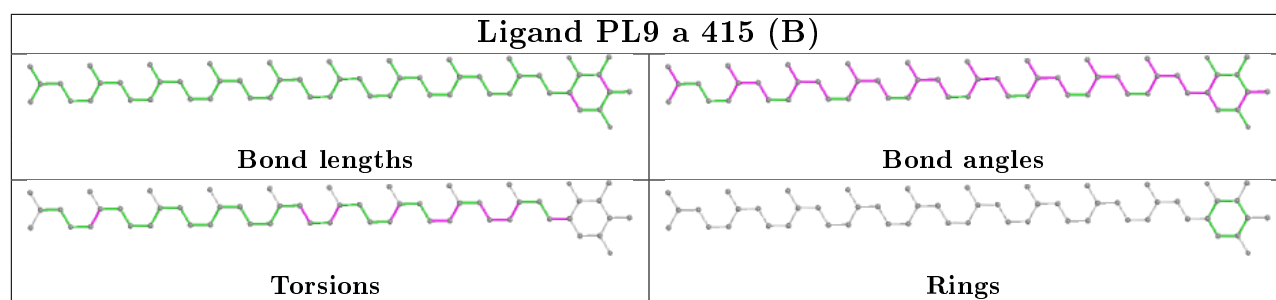
## Ligand CLA C 502

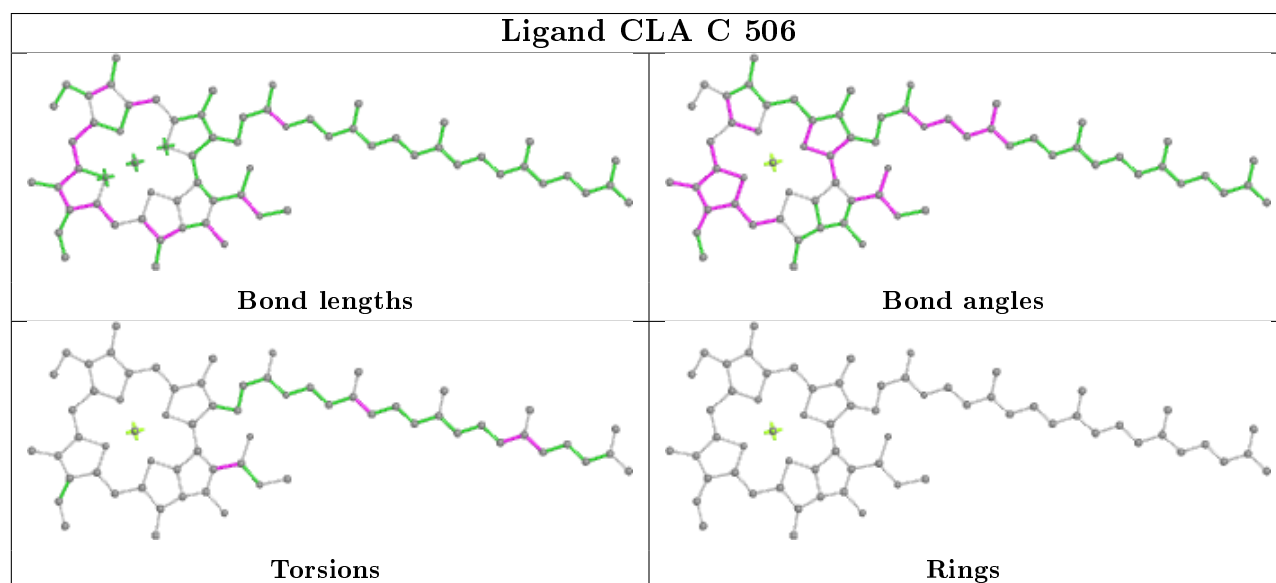
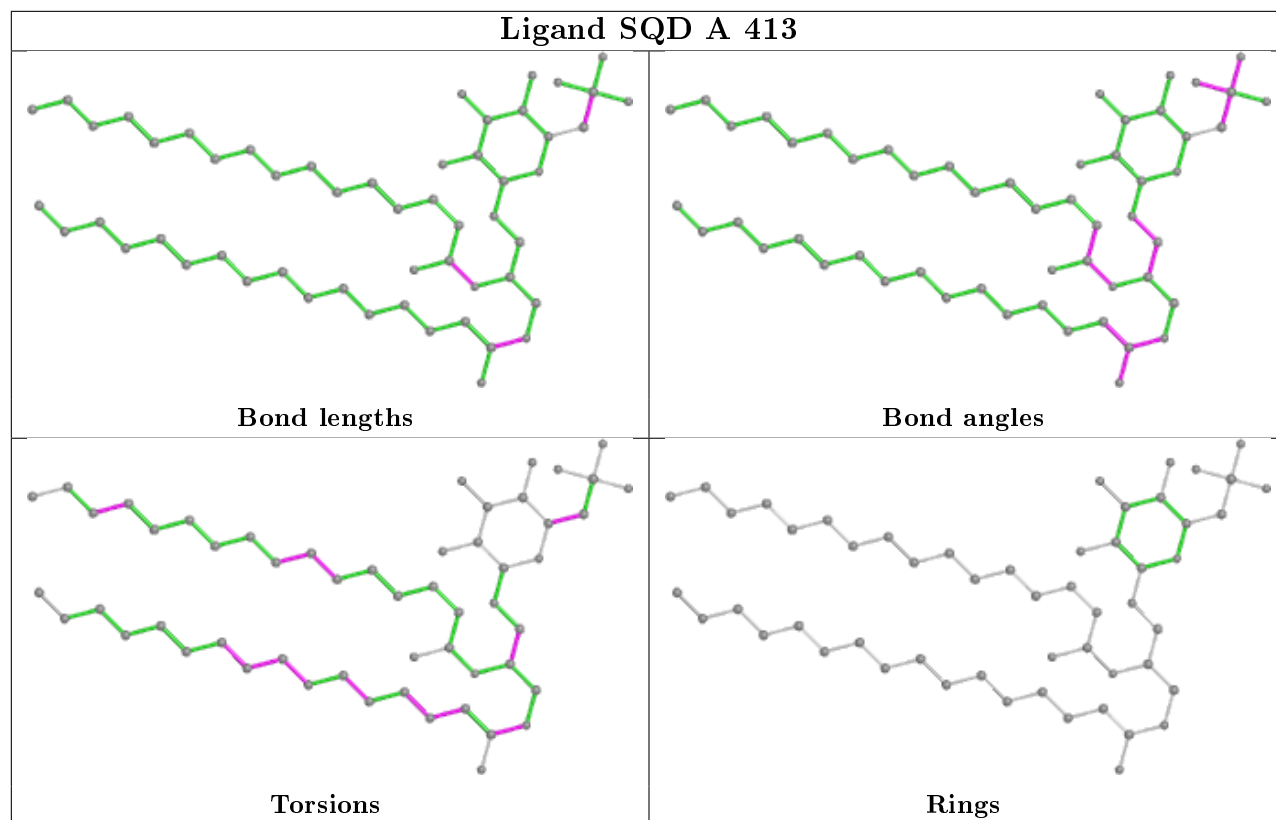
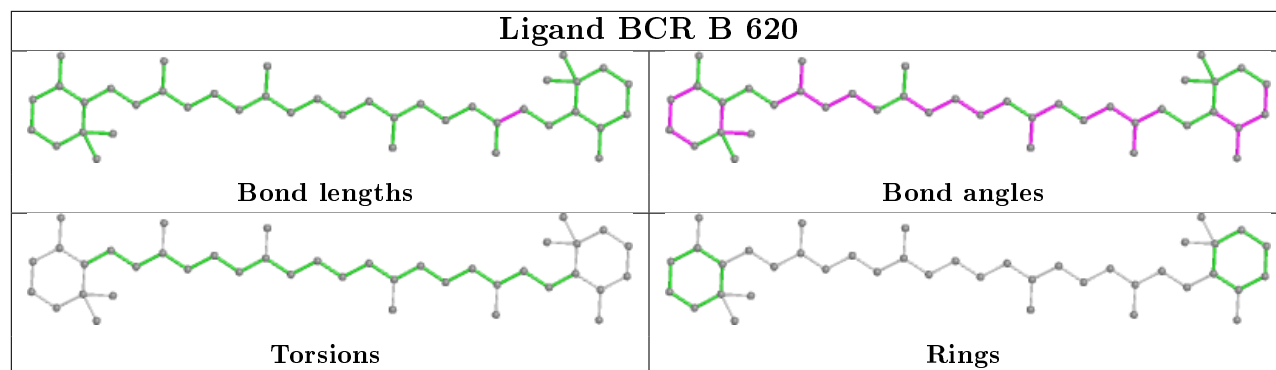


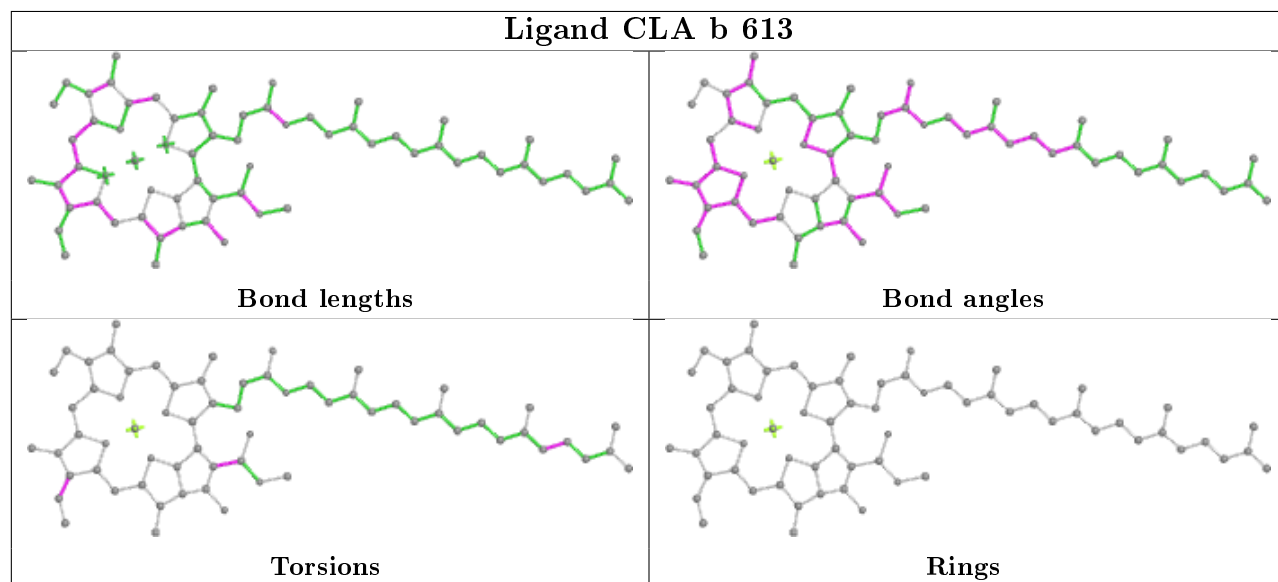
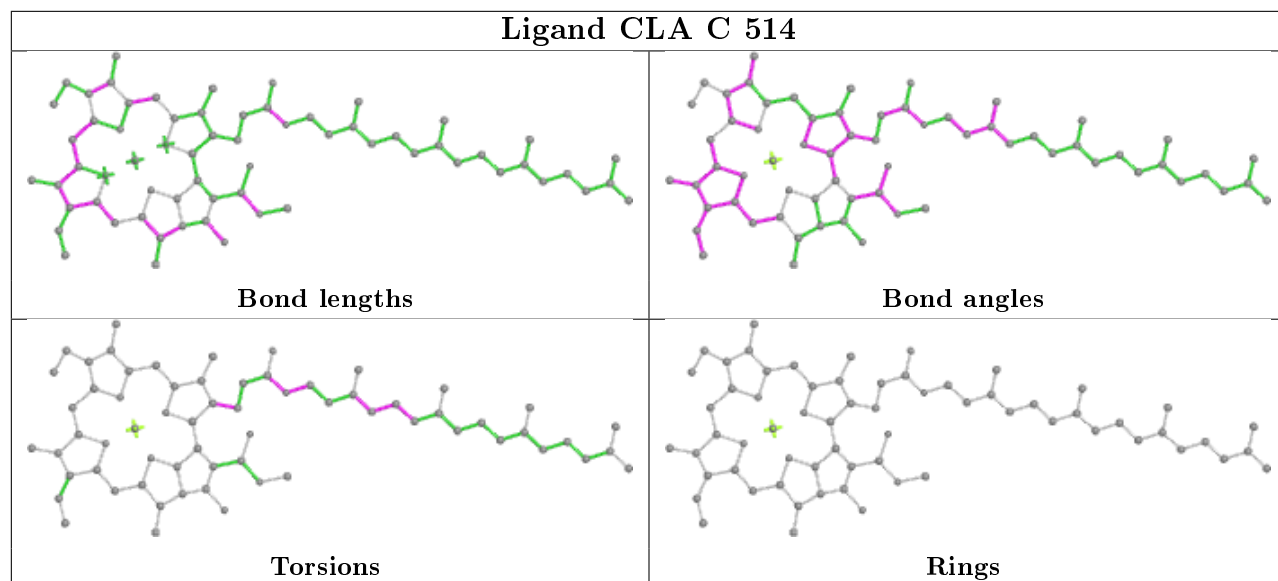
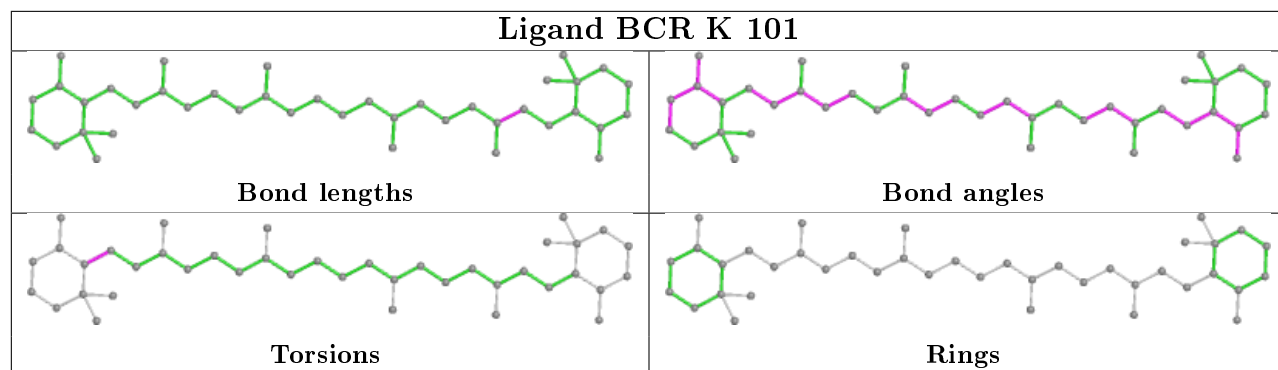


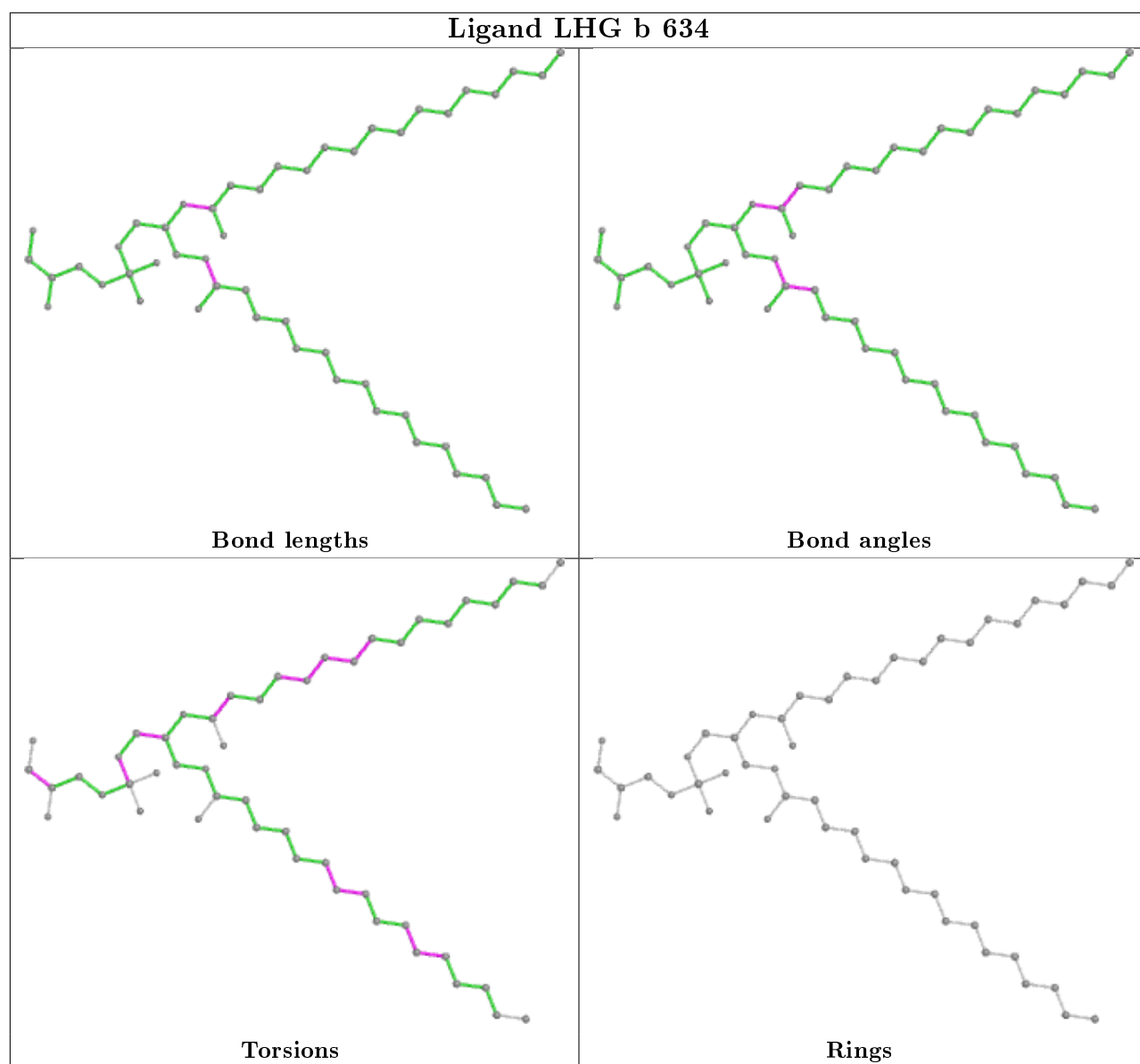


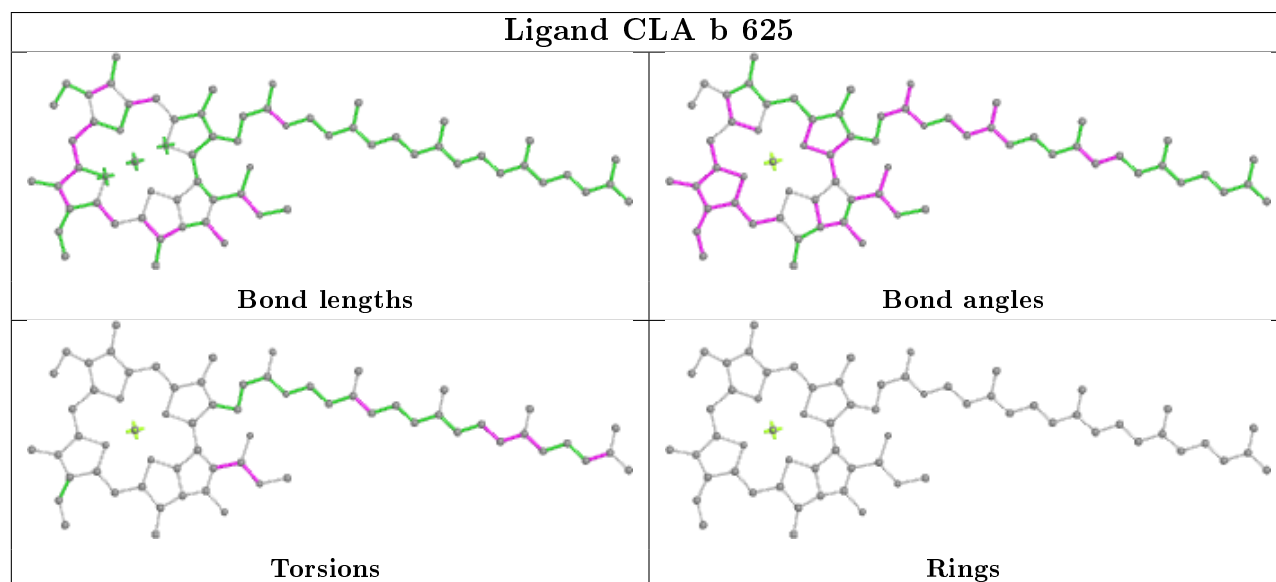
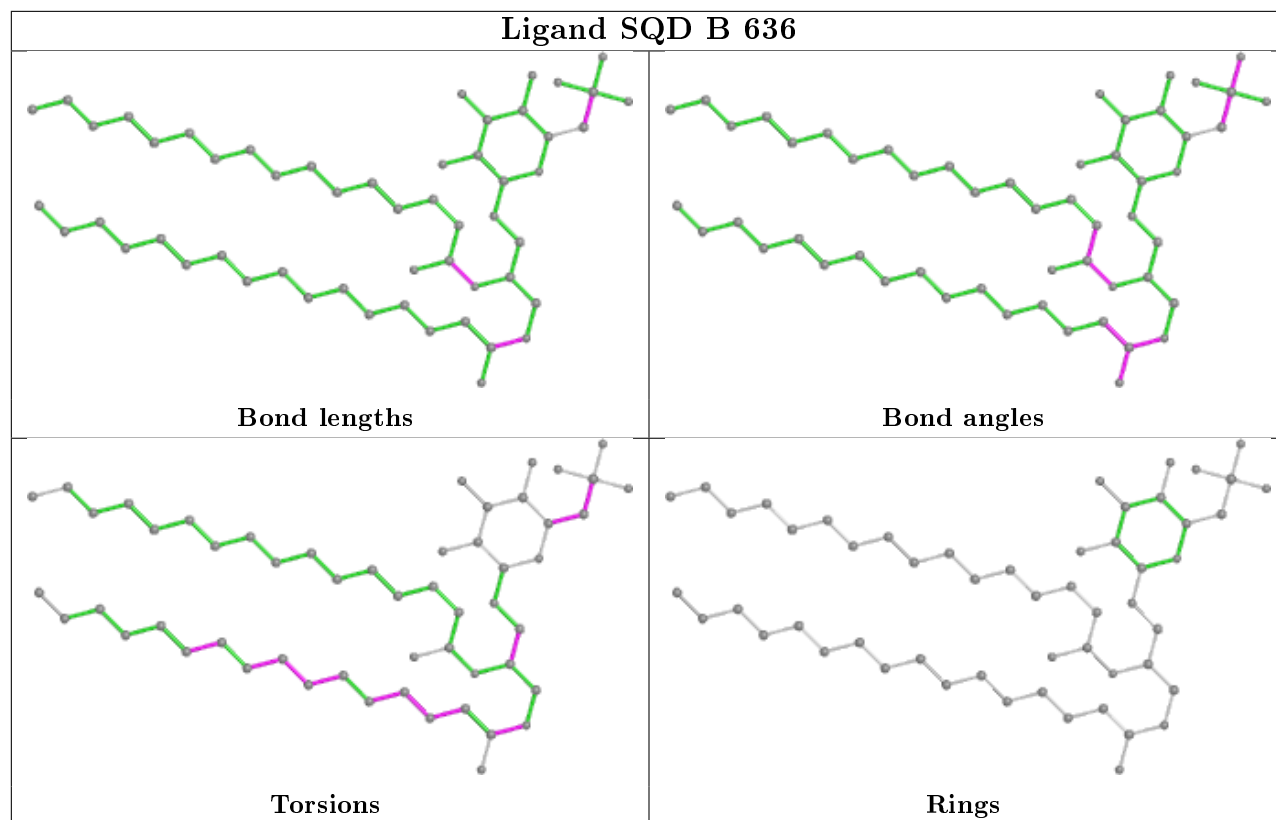


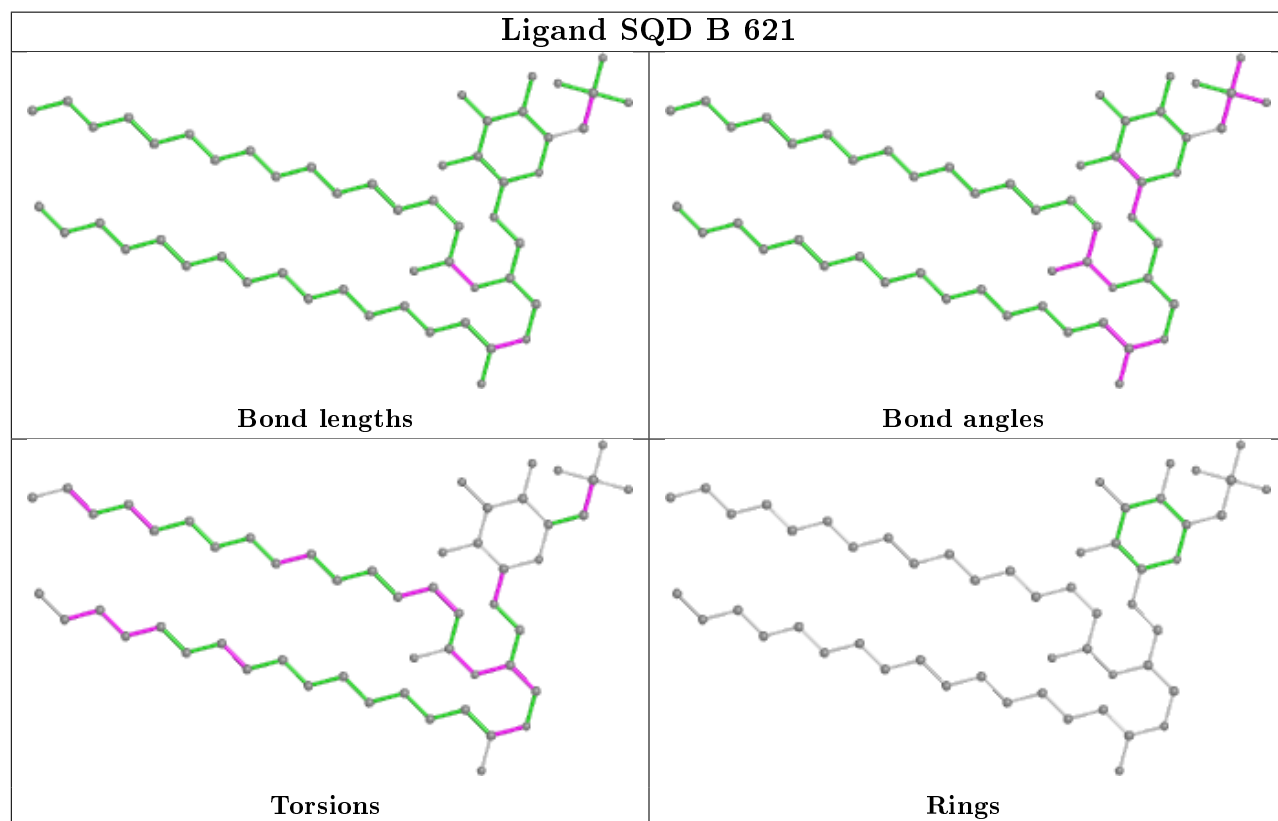
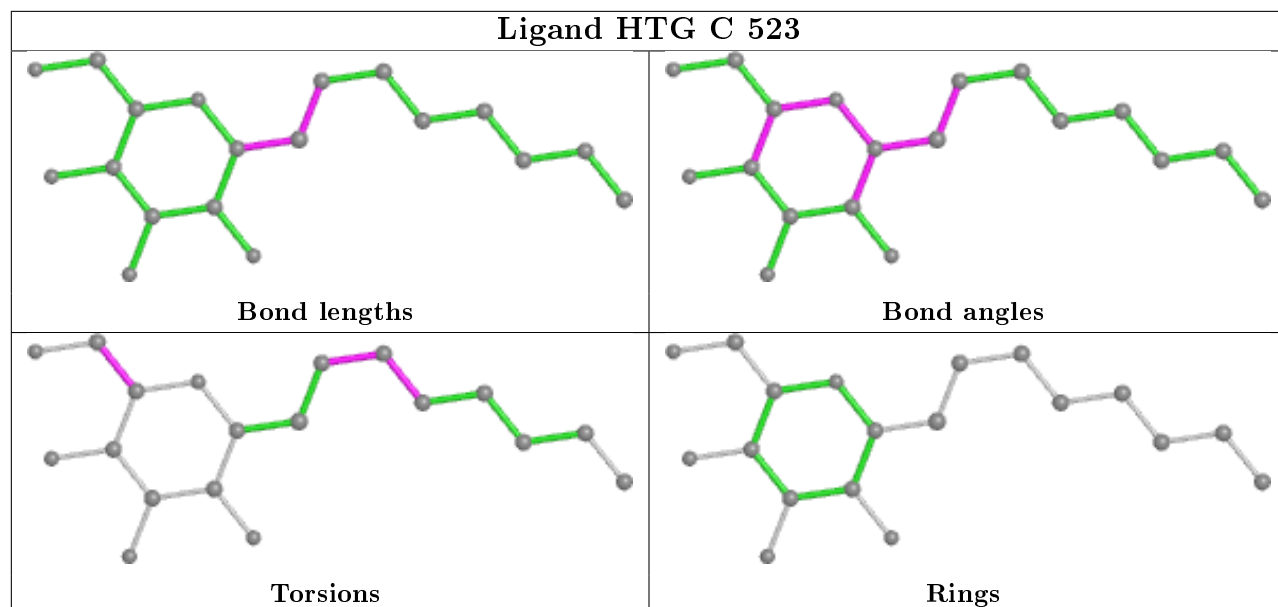


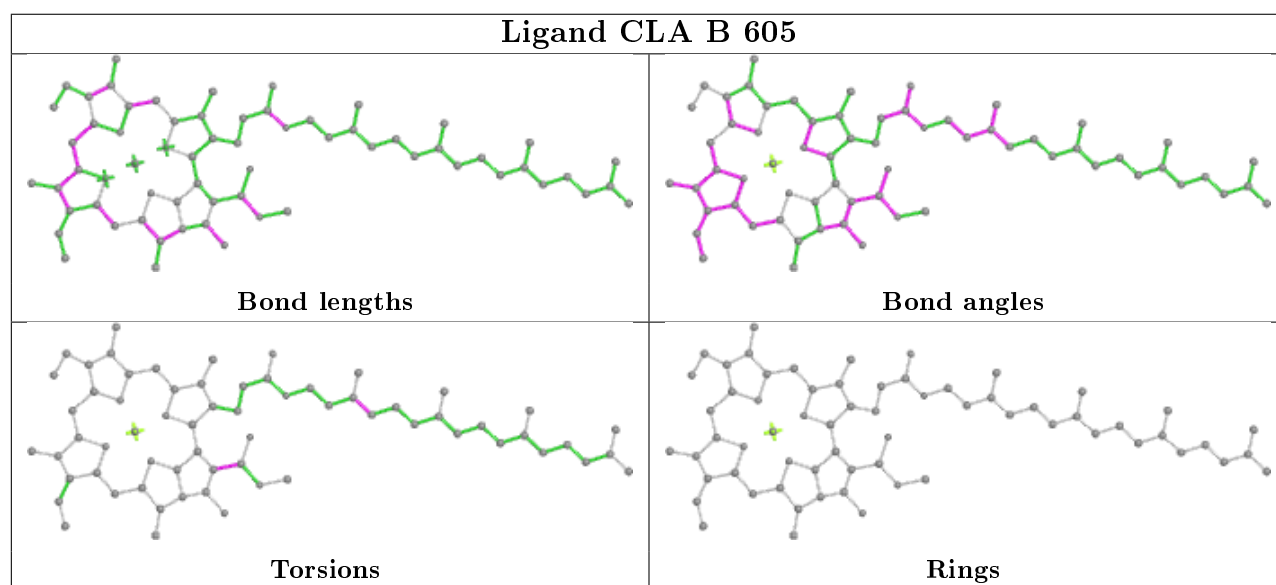
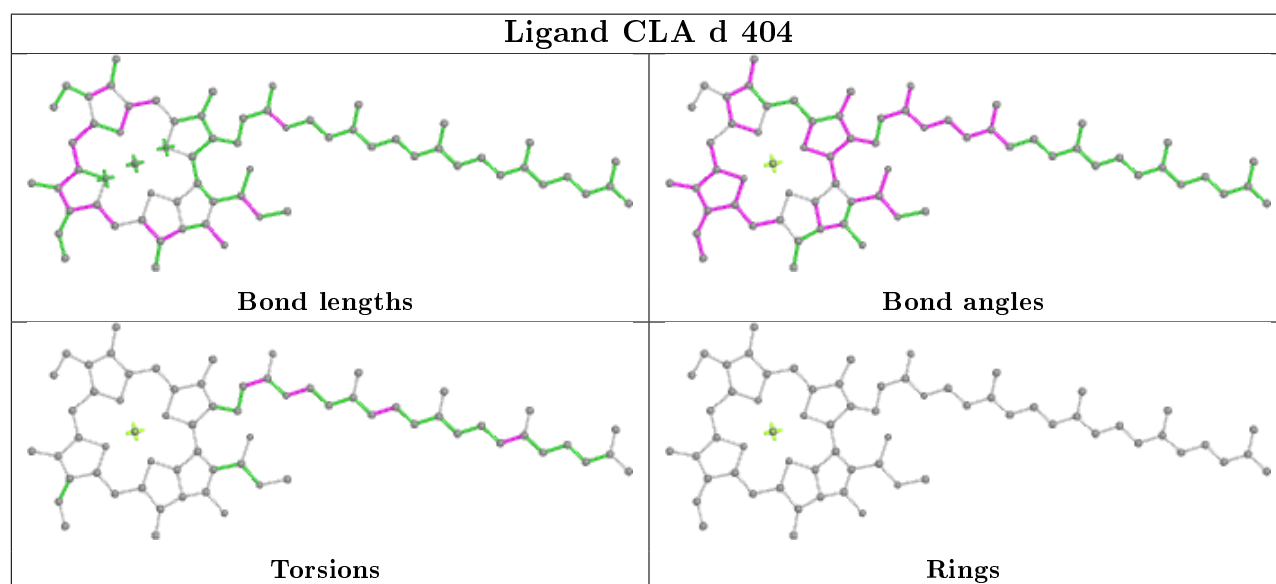
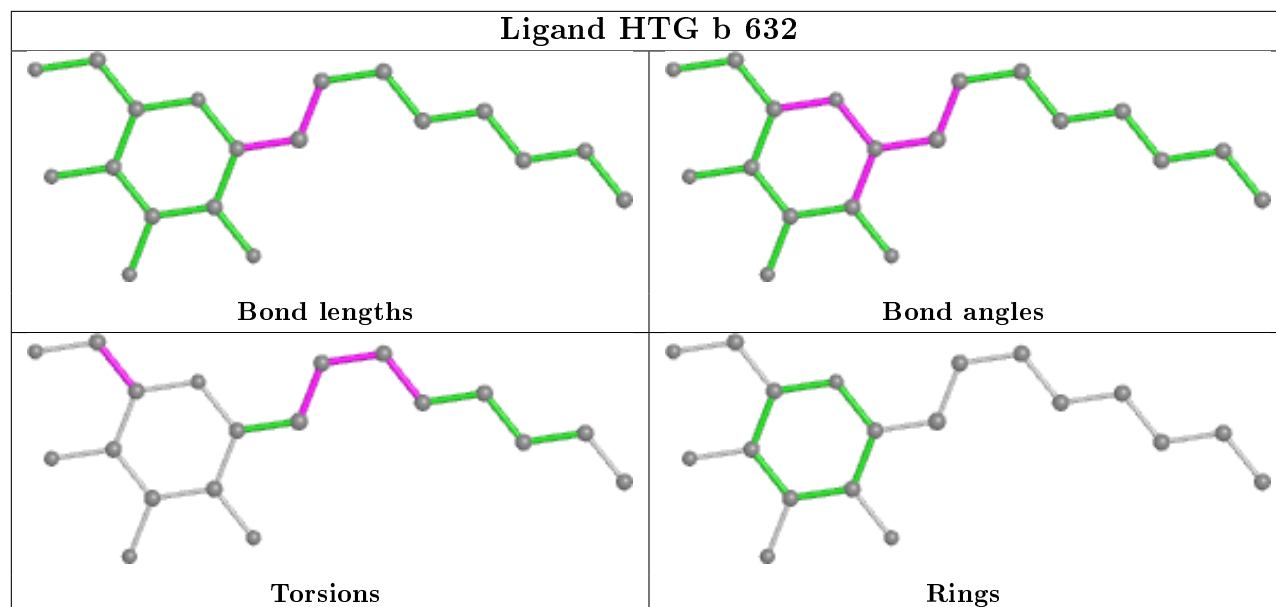




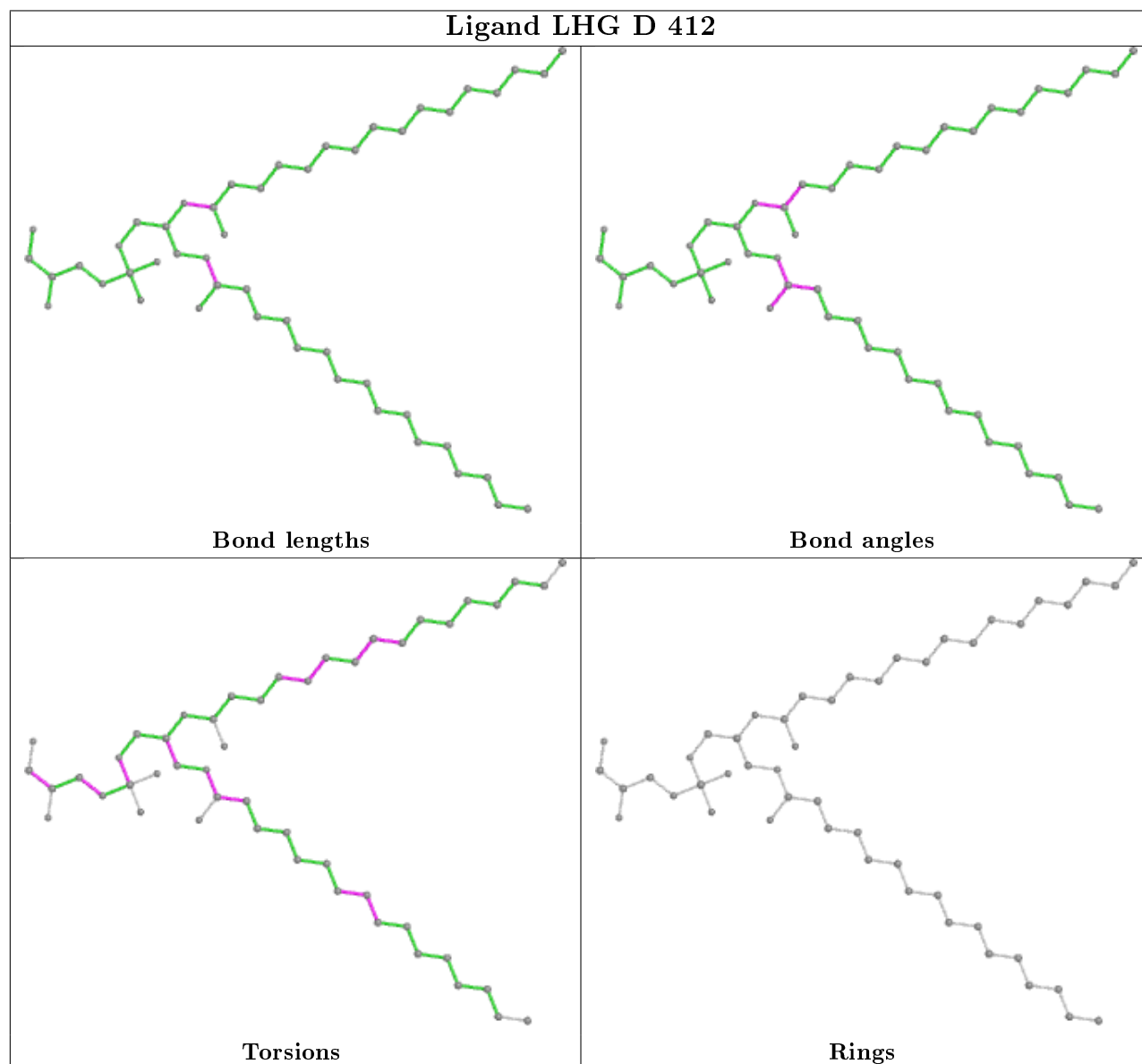
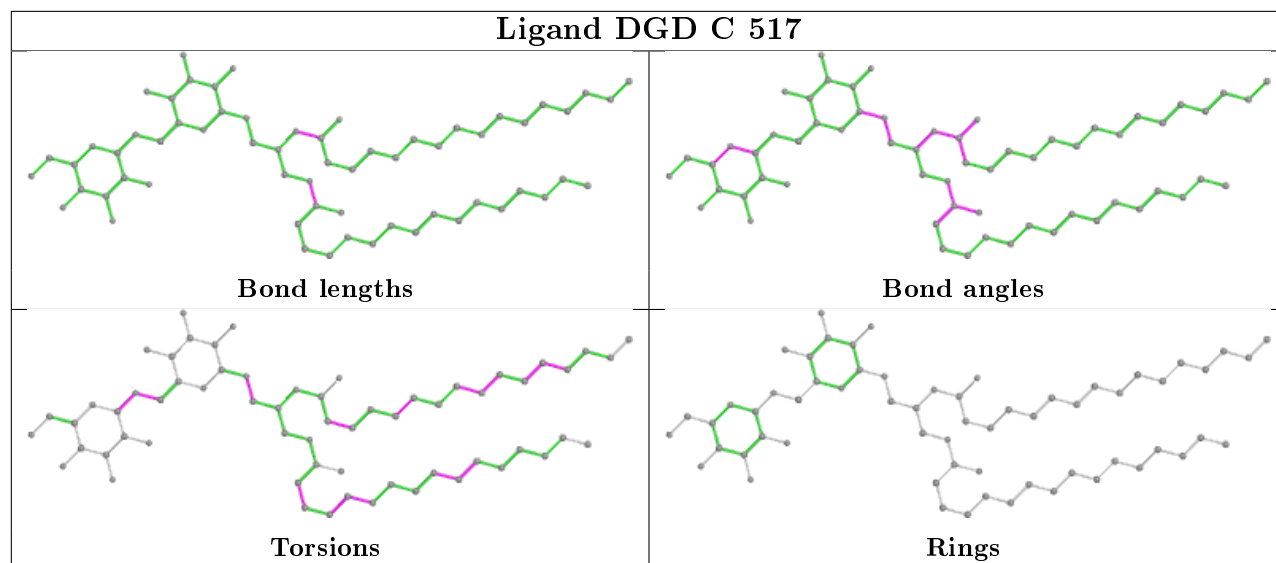


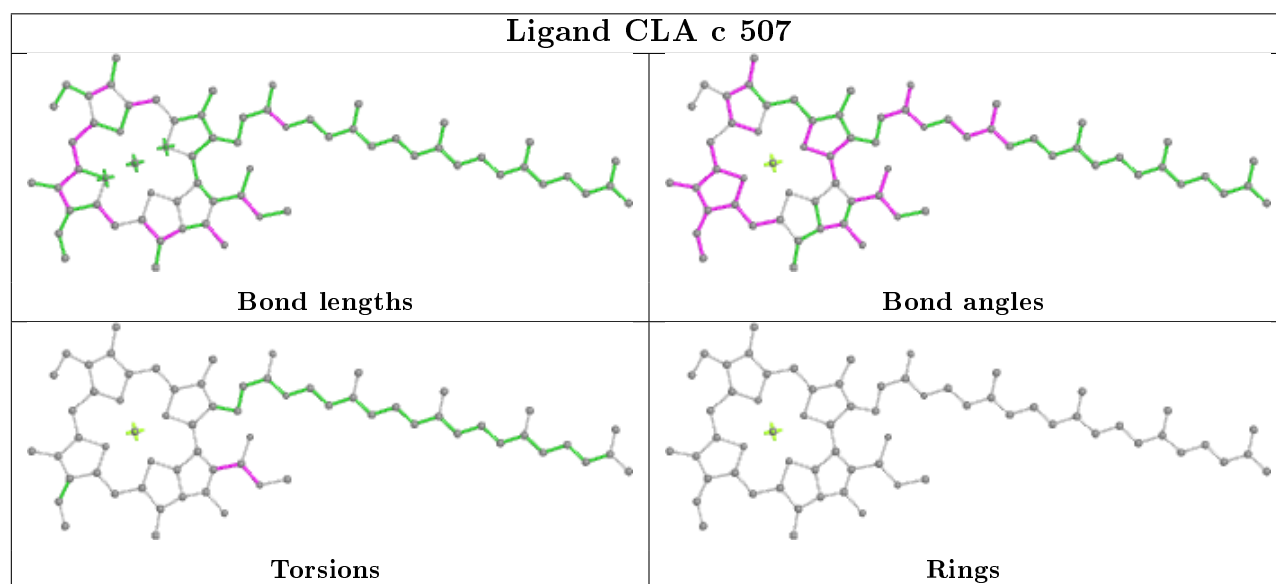
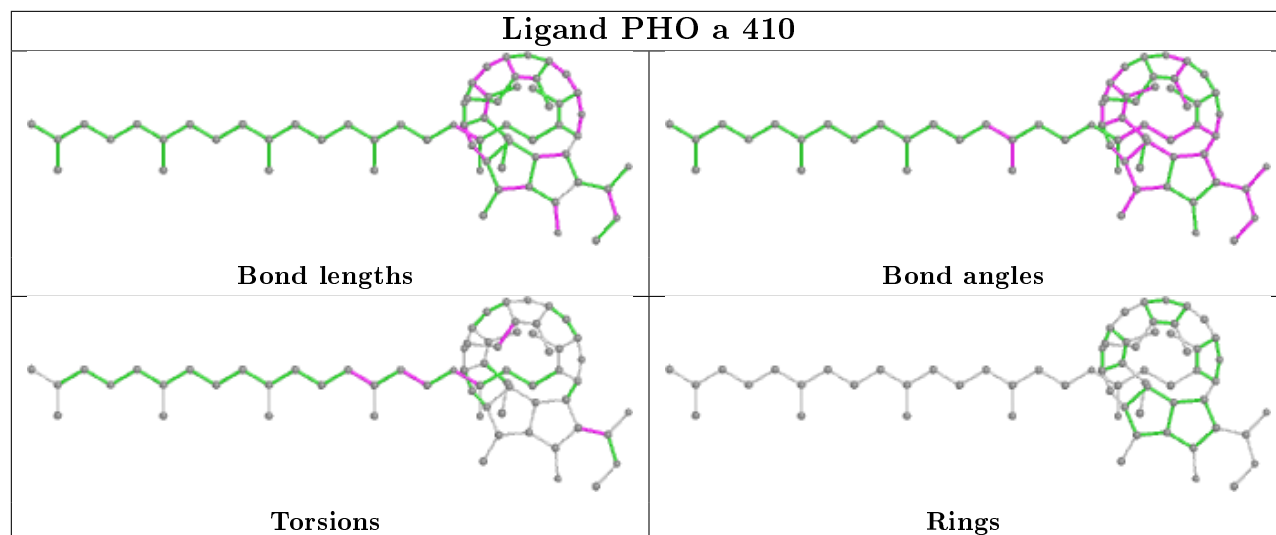


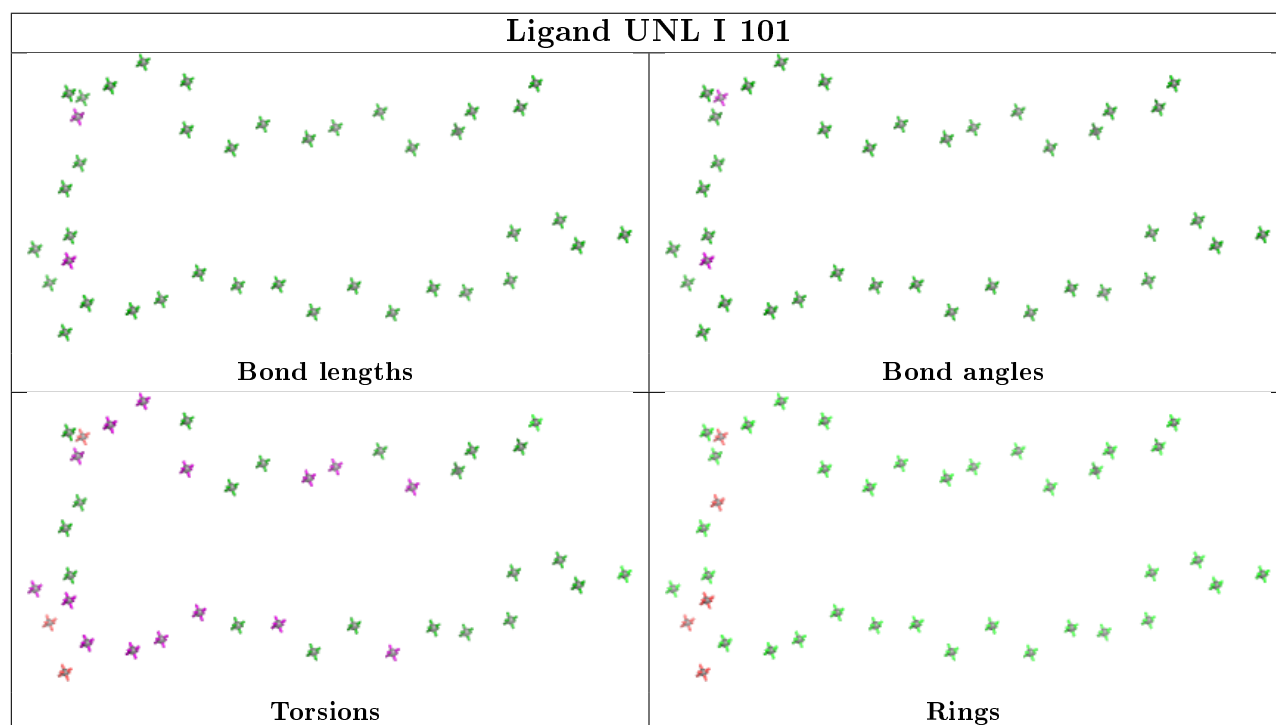
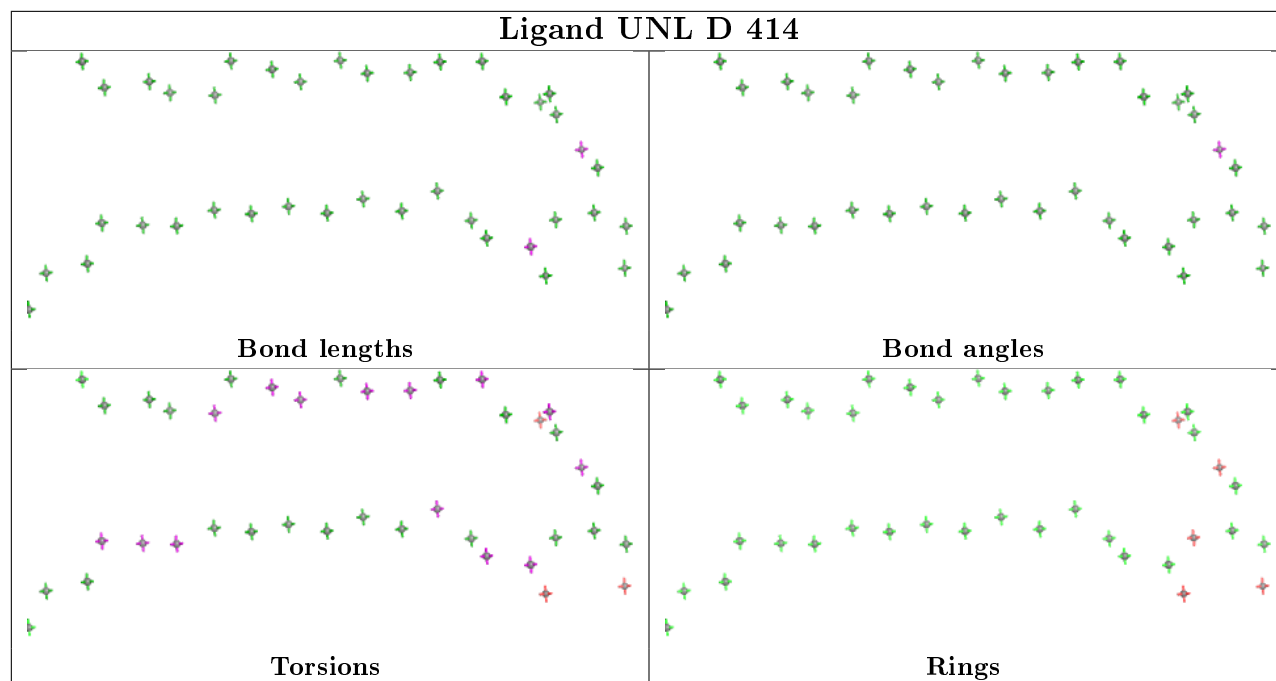


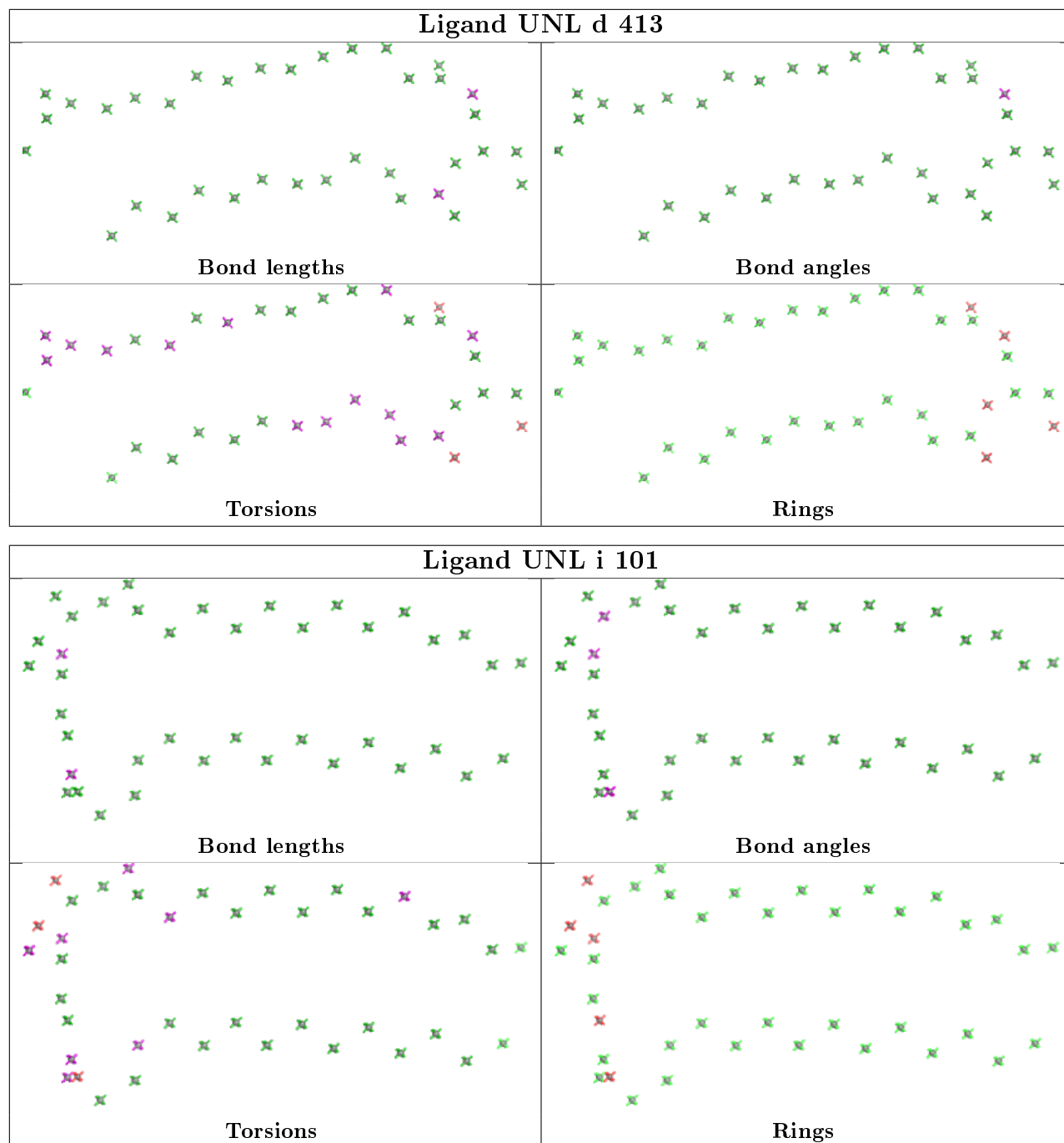


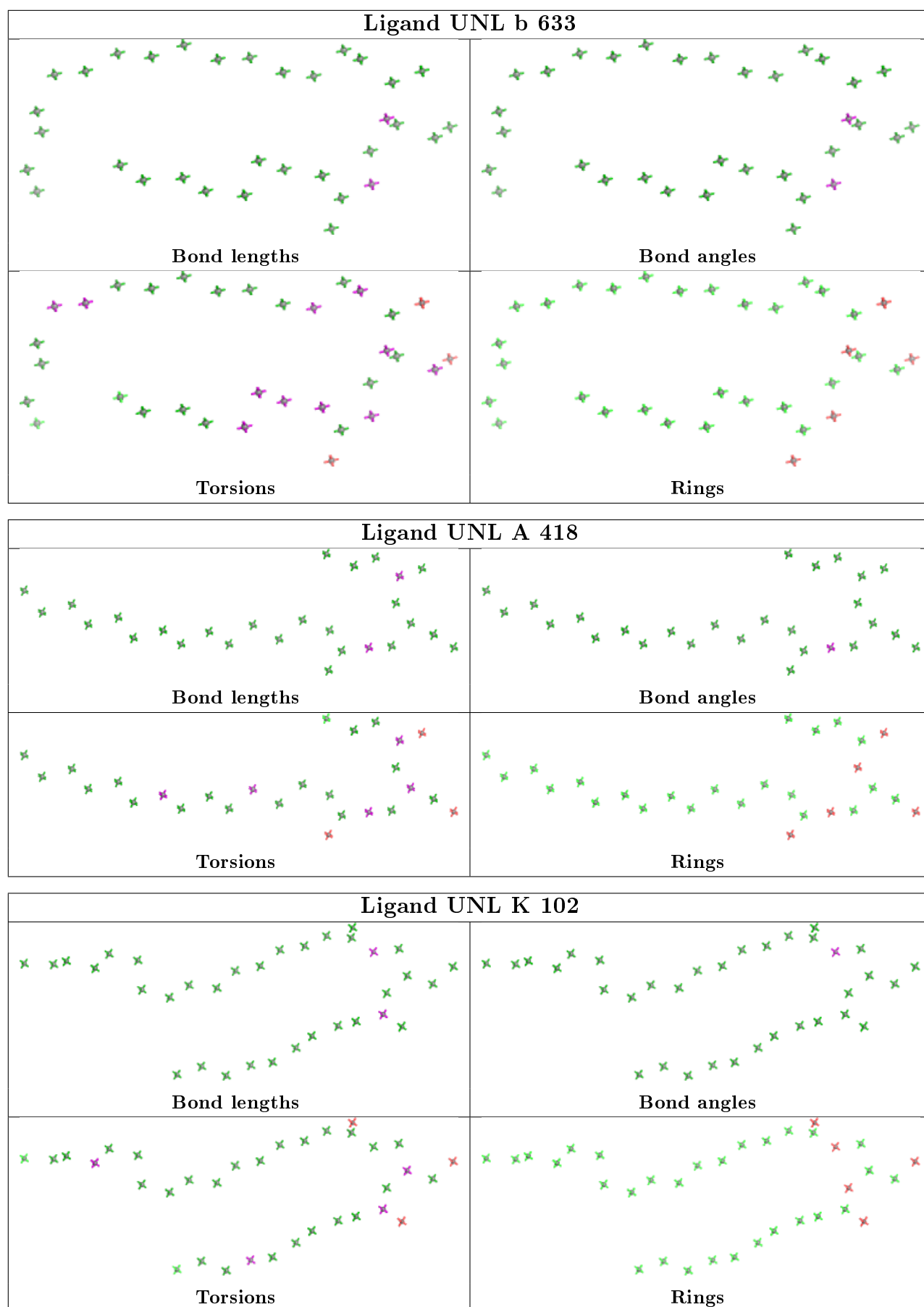


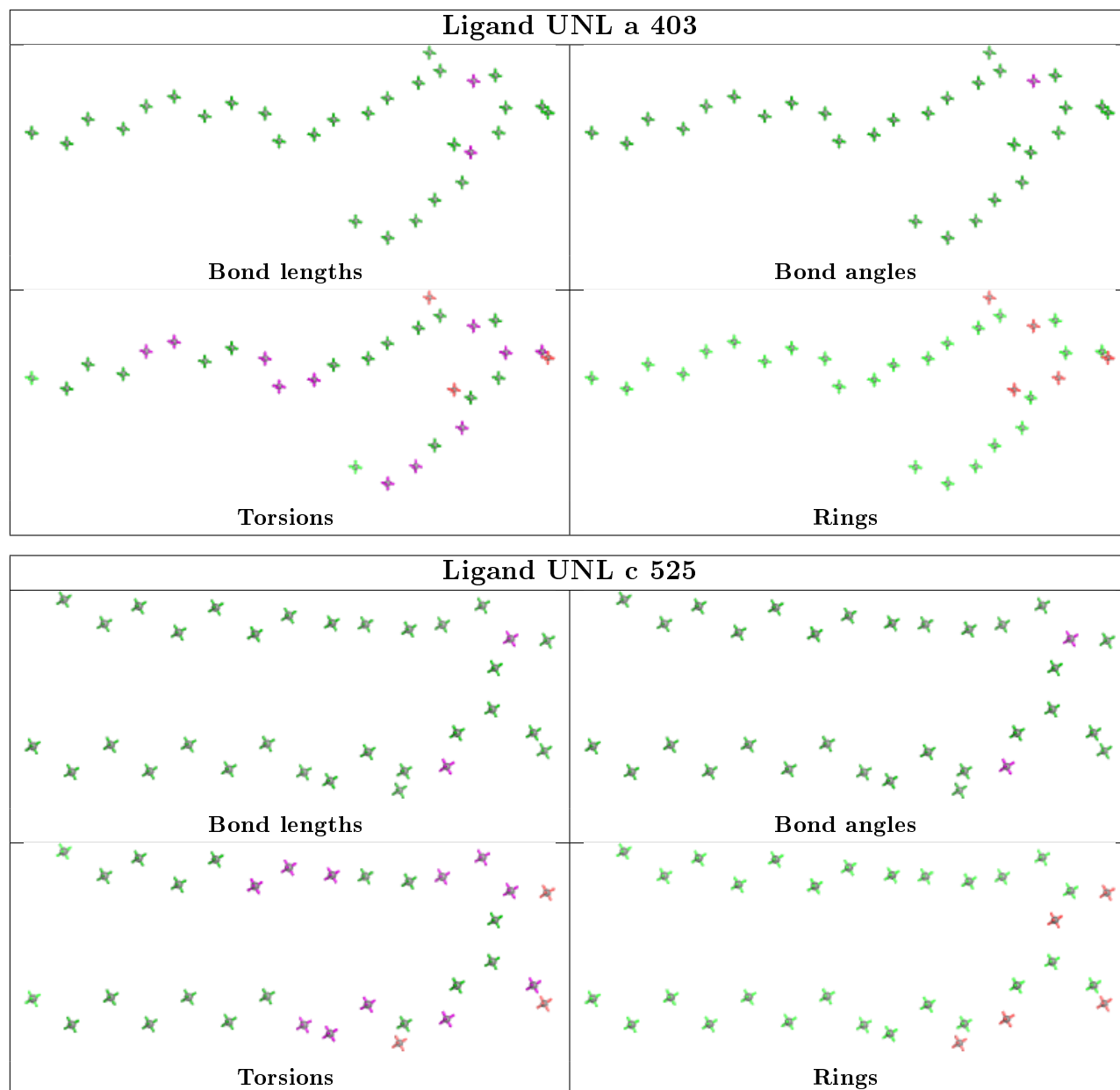


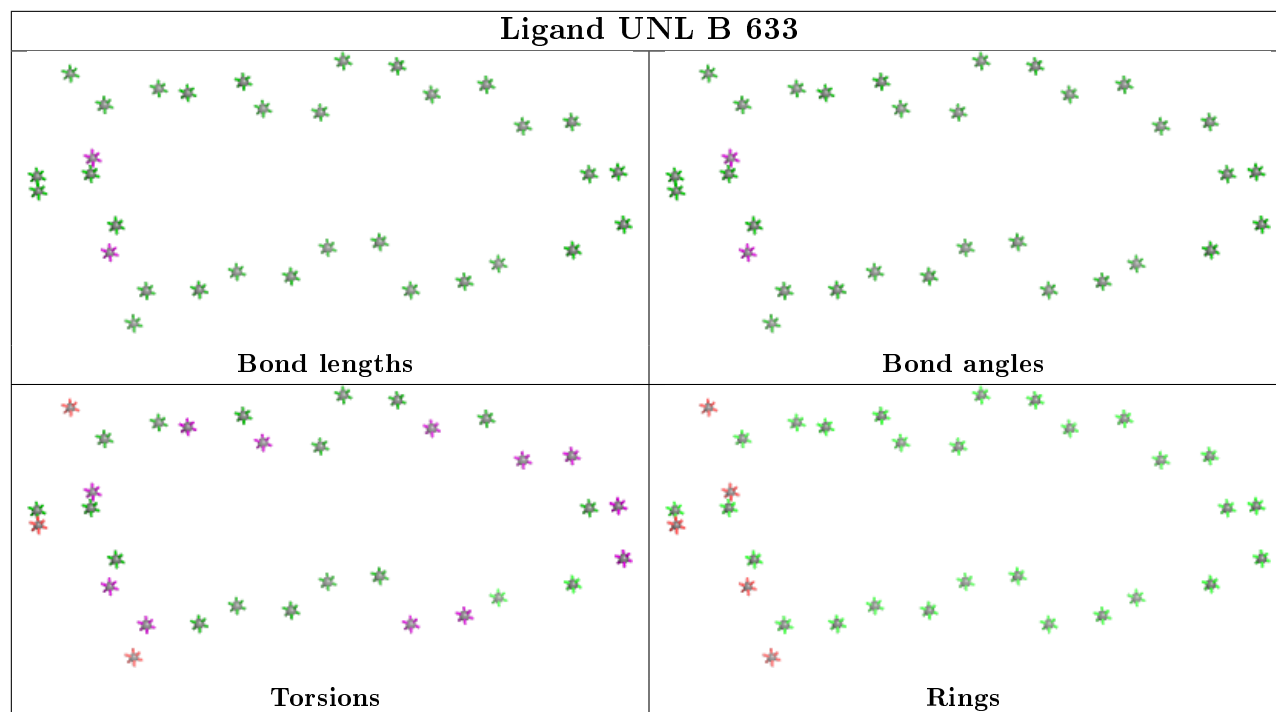












## 5.7 Other polymers [i](#)

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%)	-0.02	0 100 100	36, 48, 81, 127	0
1	a	334/344 (97%)	0.17	8 (2%) 59 57	37, 49, 86, 157	0
2	B	504/505 (99%)	0.03	6 (1%) 79 77	37, 53, 90, 153	0
2	b	503/505 (99%)	0.14	20 (3%) 38 37	40, 53, 102, 199	0
3	C	451/455 (99%)	0.09	14 (3%) 49 47	42, 63, 89, 152	0
3	c	455/455 (100%)	-0.01	3 (0%) 87 86	46, 66, 87, 137	0
4	D	341/342 (99%)	-0.03	1 (0%) 94 93	36, 49, 80, 132	0
4	d	341/342 (99%)	0.03	1 (0%) 94 93	36, 51, 81, 118	0
5	E	81/84 (96%)	1.17	19 (23%) 0 0	58, 84, 115, 160	0
5	e	81/84 (96%)	0.56	8 (9%) 7 6	60, 81, 131, 187	0
6	F	34/44 (77%)	0.43	4 (11%) 4 4	59, 72, 119, 124	0
6	f	32/44 (72%)	0.05	1 (3%) 49 47	59, 69, 132, 147	0
7	H	65/65 (100%)	-0.02	2 (3%) 49 47	54, 65, 89, 158	0
7	h	65/65 (100%)	-0.00	2 (3%) 49 47	53, 65, 84, 165	0
8	I	37/38 (97%)	0.30	4 (10%) 5 5	51, 65, 133, 192	0
8	i	37/38 (97%)	0.24	3 (8%) 12 11	52, 63, 125, 165	0
9	J	38/39 (97%)	0.76	5 (13%) 3 3	59, 78, 159, 185	0
9	j	39/39 (100%)	0.55	7 (17%) 1 1	58, 71, 156, 185	0
10	K	37/37 (100%)	0.47	4 (10%) 5 5	64, 78, 100, 110	0
10	k	37/37 (100%)	0.19	0 100 100	62, 77, 98, 117	0
11	L	37/37 (100%)	-0.01	0 100 100	37, 43, 99, 128	0
11	l	37/37 (100%)	0.05	0 100 100	39, 45, 105, 131	0
12	M	33/36 (91%)	0.07	0 100 100	35, 44, 74, 122	0
12	m	33/36 (91%)	0.28	0 100 100	35, 45, 82, 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%)	0.05	4 (1%) 72 70	39, 59, 106, 157	0
13	o	243/244 (99%)	-0.01	5 (2%) 63 61	40, 62, 116, 177	0
14	T	29/32 (90%)	0.13	1 (3%) 45 44	38, 45, 77, 142	0
14	t	29/32 (90%)	0.17	1 (3%) 45 44	39, 46, 72, 149	0
15	U	97/104 (93%)	-0.11	1 (1%) 82 80	44, 58, 91, 126	0
15	u	97/104 (93%)	-0.14	0 100 100	47, 61, 83, 126	0
16	V	137/137 (100%)	-0.01	1 (0%) 87 86	44, 59, 84, 114	0
16	v	137/137 (100%)	-0.02	1 (0%) 87 86	47, 69, 102, 141	0
17	Y	29/30 (96%)	3.53	11 (37%) 0 0	79, 96, 194, 213	0
17	y	29/30 (96%)	1.12	6 (20%) 1 0	79, 97, 147, 168	0
18	X	39/40 (97%)	0.13	0 100 100	63, 75, 126, 149	0
18	x	38/40 (95%)	0.44	3 (7%) 12 11	64, 72, 135, 162	0
19	Z	62/62 (100%)	1.23	16 (25%) 0 0	81, 99, 134, 146	0
19	z	62/62 (100%)	1.08	18 (29%) 0 0	80, 98, 144, 190	0
20	R	18/34 (52%)	5.70	18 (100%) 0 0	104, 152, 180, 185	0
All	All	5275/5384 (97%)	0.16	198 (3%) 40 39	35, 58, 110, 213	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	20.2
17	Y	19	ILE	14.8
17	Y	20	ALA	12.6
20	R	8	VAL	10.4
20	R	18	TRP	9.9
17	Y	21	GLN	9.2
20	R	6	LEU	9.2
20	R	16	ALA	8.2
20	R	15	ALA	8.0
2	b	494	GLY	8.0
2	b	496	TYR	7.7
17	Y	25	ILE	7.3
5	e	5	THR	7.3
17	Y	26	ALA	7.2
9	j	1	MET	6.9
17	Y	22	LEU	6.9
2	b	493	TRP	6.8

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Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	6.7
20	R	13	LEU	6.4
20	R	5	VAL	6.4
18	x	37	VAL	6.2
5	E	84	LYS	6.2
13	O	56	PRO	5.9
5	E	83	LEU	5.9
19	Z	31	GLN	5.9
20	R	12	VAL	5.8
8	i	37	LEU	5.6
5	e	4	THR	5.6
17	Y	23	THR	5.6
8	I	36	ASP	5.5
19	Z	61	VAL	5.5
2	b	504	THR	5.5
9	j	2	SER	5.3
3	c	140	LEU	5.3
20	R	11	PRO	5.2
9	j	4	GLY	5.2
17	y	20	ALA	5.2
2	b	503	THR	5.1
5	E	5	THR	5.1
5	E	79	PHE	5.0
5	E	82	GLN	4.9
1	a	264[A]	SER	4.9
5	E	19	TYR	4.8
18	x	2	THR	4.8
20	R	7	VAL	4.7
9	j	3	GLU	4.6
8	I	34	ARG	4.5
19	Z	36	SER	4.3
13	O	62	GLU	4.3
19	z	5	PHE	4.3
17	y	41	VAL	4.3
2	b	499	VAL	4.2
2	B	496	TYR	4.2
2	b	489	GLU	4.2
19	z	32	ASP	4.2
5	e	6	GLY	4.2
20	R	17	GLY	4.1
19	Z	30	PRO	4.1
2	b	502	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	b	497	GLN	4.1
7	h	66	GLY	4.1
2	b	487	SER	4.1
20	R	3	TRP	4.1
2	b	501	ASP	4.0
20	R	14	LEU	4.0
7	H	66	GLY	4.0
19	Z	62	VAL	4.0
5	E	17	VAL	3.9
19	Z	33	TRP	3.9
3	C	131	TYR	3.9
1	a	11	ALA	3.8
6	F	16	PHE	3.8
19	Z	29	SER	3.8
19	z	3	ILE	3.7
20	R	10	LEU	3.7
16	v	17	LYS	3.7
6	F	15	ILE	3.6
9	J	5	GLY	3.6
19	z	33	TRP	3.6
5	E	11	SER	3.6
2	b	486	LEU	3.6
3	c	143	TYR	3.6
18	x	38	GLN	3.6
20	R	9	LEU	3.5
10	K	14	ALA	3.5
1	a	263	ALA	3.5
1	a	262	TYR	3.4
19	z	30	PRO	3.4
20	R	2	ASP	3.4
2	b	491	VAL	3.3
9	j	7	ILE	3.3
2	b	488	PRO	3.2
1	a	248[A]	ILE	3.2
19	Z	26	ALA	3.2
19	Z	4	LEU	3.2
8	i	36	ASP	3.2
7	h	65	LEU	3.2
20	R	4	ARG	3.2
19	Z	32	ASP	3.1
3	C	28	GLN	3.1
19	Z	35	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	485	GLU	3.0
5	E	4	THR	3.0
5	E	78	THR	3.0
3	C	145[A]	SER	3.0
19	z	42	LEU	3.0
17	y	21	GLN	3.0
19	Z	3	ILE	3.0
17	Y	24	MET	2.9
2	B	495	PHE	2.9
13	o	59	LYS	2.9
2	B	479	PHE	2.9
19	z	41	PHE	2.9
5	e	10	PHE	2.8
19	Z	39	LEU	2.8
19	z	60	PHE	2.8
19	z	29	SER	2.8
19	z	35	ARG	2.8
13	o	58	ASN	2.7
17	y	25	ILE	2.7
13	o	61	GLN	2.7
1	a	15	GLU	2.7
4	D	238[A]	THR	2.7
4	d	234[A]	ALA	2.7
3	C	134	ILE	2.7
3	C	47	GLY	2.7
5	E	61	ARG	2.6
9	J	2	SER	2.6
5	E	6	GLY	2.6
19	z	39	LEU	2.6
2	B	501	ASP	2.6
10	K	16	ALA	2.6
19	Z	25	VAL	2.6
19	Z	56	VAL	2.6
5	E	21	VAL	2.6
1	a	265[A]	PHE	2.6
1	a	252[A]	HIS	2.6
3	c	21	ILE	2.5
13	O	60	ARG	2.5
19	Z	1	MET	2.5
19	z	61	VAL	2.5
2	b	500	GLY	2.5
5	E	15	THR	2.5

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Mol	Chain	Res	Type	RSRZ
14	t	30	THR	2.5
3	C	253	LEU	2.5
10	K	15	TYR	2.5
19	z	36	SER	2.5
7	H	64	ALA	2.5
20	R	19	ALA	2.5
6	f	20	TRP	2.4
13	o	132	ASN	2.4
19	z	31	GLN	2.4
3	C	23	ALA	2.4
5	E	23	HIS	2.4
17	Y	30	ILE	2.4
9	j	6	ARG	2.4
15	U	73	GLN	2.4
17	Y	41	VAL	2.4
2	b	294	SER	2.4
8	I	37	LEU	2.3
17	y	44	GLY	2.3
13	O	58	ASN	2.3
8	I	38	GLU	2.3
3	C	252	ILE	2.3
16	V	71	GLY	2.3
13	o	56	PRO	2.3
5	e	61	ARG	2.3
9	J	33	ALA	2.3
9	J	7	ILE	2.3
9	J	37	SER	2.3
19	z	62	VAL	2.2
3	C	254	THR	2.2
5	e	7	GLU	2.2
5	e	20	TRP	2.2
2	B	486	LEU	2.2
3	C	144	SER	2.2
3	C	155	ASN	2.2
9	j	5	GLY	2.2
6	F	13	TYR	2.1
5	e	21	VAL	2.1
19	z	7	LEU	2.1
5	E	16	SER	2.1
3	C	207	ARG	2.1
6	F	14	PRO	2.1
2	b	85	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	481	GLY	2.1
3	C	27	ASP	2.1
5	E	22	ILE	2.1
19	z	25	VAL	2.1
19	z	43	GLY	2.1
14	T	30	THR	2.0
3	C	25	ASN	2.0
10	K	10	LYS	2.0
8	i	34	ARG	2.0
2	b	492	GLU	2.0
5	E	10	PHE	2.0
5	E	20	TRP	2.0
17	y	26	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.91	0.15	38,51,69,90	0
8	FME	i	1	10/11	0.92	0.14	40,61,72,73	0
12	FME	m	1	10/11	0.95	0.16	35,51,99,110	0
14	FME	t	1	10/11	0.96	0.14	32,41,50,93	0
8	FME	I	1	10/11	0.97	0.15	42,55,62,63	0
12	FME	M	1	10/11	0.98	0.19	37,50,94,100	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	CA	b	609	1/1	0.23	0.07	147,147,147,147	0
28	LMT	F	101	35/35	0.24	0.57	133,168,178,179	0
37	DGD	d	408	62/66	0.31	0.47	83,130,177,185	0
32	UNL	J	101	10/-	0.36	0.27	80,97,103,105	0
28	LMT	b	630	25/35	0.46	0.44	84,108,161,164	0
33	LHG	a	419	42/49	0.54	0.33	83,141,183,185	0
28	LMT	a	418	35/35	0.54	0.40	97,135,160,164	0
37	DGD	D	409	52/66	0.55	0.36	75,108,154,165	0
32	UNL	K	102	34/-	0.56	0.25	91,128,136,139	0
26	SQD	f	102	43/54	0.57	0.33	102,125,159,165	0
28	LMT	C	521	35/35	0.58	0.36	102,138,166,166	0
28	LMT	m	102	35/35	0.60	0.25	50,108,132,133	0
32	UNL	a	403	30/-	0.61	0.30	75,97,125,131	0
33	LHG	A	419	42/49	0.61	0.29	77,120,144,148	0
32	UNL	c	525	32/-	0.62	0.24	80,99,140,150	0
28	LMT	a	404	35/35	0.62	0.30	57,98,122,147	0
35	HTG	d	414	16/19	0.64	0.22	83,103,113,126	0
36	LMG	C	519	51/55	0.65	0.24	61,104,123,126	0
36	LMG	Z	101	37/55	0.65	0.32	80,131,148,151	0
32	UNL	j	101	10/-	0.65	0.26	69,87,97,98	0
35	HTG	D	415	16/19	0.66	0.30	74,138,159,163	0
28	LMT	A	414	35/35	0.66	0.26	56,91,113,122	0
28	LMT	e	102	35/35	0.66	0.30	92,137,158,159	0
32	UNL	A	418	28/-	0.67	0.25	64,91,111,115	0
28	LMT	M	105	35/35	0.67	0.27	58,95,126,127	0
28	LMT	D	404	35/35	0.69	0.29	78,132,156,159	0
28	LMT	M	104	35/35	0.70	0.27	54,102,153,155	0
36	LMG	z	101	39/55	0.70	0.28	80,131,153,162	0
35	HTG	c	524	19/19	0.70	0.28	82,117,127,131	0
32	UNL	m	101	10/-	0.70	0.37	58,66,81,82	0
34	CA	B	601	1/1	0.71	0.07	123,123,123,123	0
28	LMT	B	634	25/35	0.71	0.32	56,85,147,154	0
28	LMT	T	104	25/35	0.71	0.31	47,81,132,142	0
32	UNL	B	633	33/-	0.72	0.29	60,86,131,134	0
27	GOL	v	202	6/6	0.73	0.22	86,100,101,109	0
32	UNL	b	633	33/-	0.73	0.27	56,92,143,145	0
35	HTG	B	624	19/19	0.73	0.26	74,126,137,186	0
37	DGD	C	517	62/66	0.73	0.23	52,73,103,110	0
27	GOL	V	201	6/6	0.74	0.48	83,92,94,96	0
35	HTG	C	523	19/19	0.74	0.28	87,108,129,139	0
35	HTG	b	632	19/19	0.76	0.22	84,140,154,155	0
31	PL9	A	417[B]	55/55	0.76	0.29	85,107,122,125	55
31	PL9	A	417[A]	55/55	0.76	0.29	85,107,123,125	55

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	LMG	C	520	51/55	0.77	0.31	67,119,131,134	0
31	PL9	a	415[A]	55/55	0.77	0.27	91,111,122,122	55
26	SQD	b	601	54/54	0.77	0.22	49,79,130,144	0
32	UNL	M	103	10/-	0.77	0.29	54,61,84,85	0
35	HTG	b	608	19/19	0.77	0.20	58,111,145,147	0
32	UNL	i	101	40/-	0.77	0.26	67,89,140,142	0
35	HTG	B	632	19/19	0.77	0.21	57,113,139,189	0
31	PL9	a	415[B]	55/55	0.77	0.27	92,111,122,123	55
32	UNL	d	413	36/-	0.78	0.26	60,91,132,138	0
27	GOL	b	606	6/6	0.78	0.21	79,90,98,98	0
36	LMG	b	629	51/55	0.78	0.21	43,57,75,87	0
26	SQD	F	104	43/54	0.78	0.24	90,122,138,144	0
27	GOL	O	301	6/6	0.79	0.23	83,92,94,97	0
26	SQD	B	636	54/54	0.79	0.23	45,81,130,132	0
27	GOL	t	102	6/6	0.80	0.41	71,91,105,109	0
36	LMG	M	101	51/55	0.80	0.21	40,60,77,89	0
36	LMG	c	522	51/55	0.80	0.24	64,114,125,127	0
23	CLA	C	514	65/65	0.80	0.28	64,87,119,126	0
32	UNL	I	101	40/-	0.80	0.26	51,88,154,155	0
28	LMT	M	102	35/35	0.81	0.21	44,94,118,130	0
26	SQD	A	413	54/54	0.81	0.23	56,80,130,138	0
21	CL	v	205	1/1	0.81	0.09	124,124,124,124	0
35	HTG	b	631	19/19	0.82	0.26	71,83,97,101	0
26	SQD	B	621	54/54	0.82	0.23	48,81,143,150	0
37	DGD	h	102	62/66	0.82	0.21	38,58,80,85	0
23	CLA	C	505	65/65	0.82	0.22	47,65,96,110	0
32	UNL	X	101	18/-	0.82	0.18	61,78,113,117	0
36	LMG	k	101	51/55	0.83	0.23	67,96,122,125	0
35	HTG	B	623	19/19	0.83	0.21	62,78,91,92	0
34	CA	F	105	1/1	0.83	0.04	112,112,112,112	0
23	CLA	c	517	65/65	0.84	0.22	85,97,108,112	0
35	HTG	b	607	19/19	0.84	0.20	49,81,95,101	0
36	LMG	C	501	51/55	0.84	0.20	58,91,106,111	0
37	DGD	H	102	62/66	0.84	0.20	42,58,97,102	0
37	DGD	C	518	62/66	0.84	0.19	49,66,88,97	0
32	UNL	D	414	40/-	0.84	0.21	59,87,128,135	0
34	CA	f	103	1/1	0.84	0.13	135,135,135,135	0
35	HTG	c	523	19/19	0.85	0.17	92,106,118,124	0
27	GOL	V	204	6/6	0.85	0.13	96,100,106,117	0
27	GOL	T	101	6/6	0.85	0.41	69,87,92,93	0
35	HTG	B	631	19/19	0.85	0.17	52,94,118,125	0
27	GOL	a	402	6/6	0.85	0.23	96,103,108,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	SQD	a	413	54/54	0.86	0.17	53,88,106,109	0
26	SQD	A	410	54/54	0.86	0.21	54,94,105,109	0
35	HTG	C	522	19/19	0.86	0.17	86,100,123,126	0
36	LMG	a	414	51/55	0.86	0.21	60,86,102,110	0
35	HTG	b	602	19/19	0.86	0.19	49,64,75,79	0
32	UNL	d	415	18/-	0.86	0.20	67,74,111,117	0
27	GOL	f	101	6/6	0.87	0.18	95,101,102,103	0
23	CLA	c	510	65/65	0.87	0.18	56,74,97,104	0
37	DGD	c	520	62/66	0.87	0.19	52,65,117,131	0
36	LMG	D	416	51/55	0.88	0.18	52,75,120,131	0
23	CLA	c	511	65/65	0.88	0.17	52,68,77,82	0
23	CLA	b	616	65/65	0.88	0.20	29,42,51,58	0
27	GOL	C	524	6/6	0.88	0.41	81,88,106,110	0
27	GOL	T	102	6/6	0.88	0.43	100,114,116,120	0
33	LHG	D	412	49/49	0.88	0.24	53,70,117,124	0
27	GOL	c	502	6/6	0.88	0.43	76,97,108,111	0
23	CLA	C	512	65/65	0.89	0.17	57,76,93,108	0
35	HTG	V	206	19/19	0.89	0.32	77,106,125,227	0
27	GOL	o	301	6/6	0.89	0.19	84,90,99,104	0
23	CLA	C	507	65/65	0.89	0.17	54,78,117,123	0
23	CLA	B	607	65/65	0.89	0.17	35,53,96,98	0
27	GOL	B	635	6/6	0.89	0.16	57,59,66,69	0
23	CLA	b	611	65/65	0.89	0.19	42,54,61,68	0
36	LMG	d	416	51/55	0.89	0.19	55,68,107,118	0
23	CLA	c	507	65/65	0.89	0.17	52,65,76,93	0
23	CLA	B	614	65/65	0.90	0.18	31,43,66,84	0
23	CLA	c	509	65/65	0.90	0.16	43,55,72,76	0
23	CLA	c	508	65/65	0.90	0.16	51,65,81,89	0
23	CLA	b	615	65/65	0.90	0.17	41,54,92,97	0
27	GOL	A	411	6/6	0.90	0.15	54,57,60,70	0
23	CLA	c	512	65/65	0.90	0.15	46,58,125,136	0
23	CLA	c	515	65/65	0.90	0.17	55,71,88,95	0
23	CLA	b	610	65/65	0.90	0.19	52,80,123,129	0
27	GOL	A	412	6/6	0.90	0.21	76,82,86,90	0
37	DGD	c	521	62/66	0.90	0.17	48,62,94,109	0
21	CL	U	201	1/1	0.90	0.07	116,116,116,116	0
35	HTG	B	622	19/19	0.90	0.18	48,68,85,91	0
33	LHG	D	410	49/49	0.90	0.23	40,53,65,67	0
23	CLA	b	618	65/65	0.90	0.18	46,55,65,68	0
23	CLA	C	513	65/65	0.90	0.17	61,83,93,101	0
27	GOL	v	203	6/6	0.91	0.23	93,105,109,120	0
25	BCR	K	101	40/40	0.91	0.15	62,87,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	LHG	d	411	49/49	0.91	0.20	49,64,116,122	0
23	CLA	C	511	65/65	0.91	0.15	54,71,81,84	0
25	BCR	c	526	40/40	0.91	0.16	68,87,98,99	0
25	BCR	H	101	40/40	0.91	0.18	43,64,79,81	0
27	GOL	F	103	6/6	0.91	0.31	104,108,111,111	0
23	CLA	C	504	65/65	0.91	0.20	50,66,79,84	0
23	CLA	B	602	65/65	0.91	0.19	52,74,118,137	0
23	CLA	C	509	65/65	0.91	0.15	49,66,130,139	0
23	CLA	b	624	65/65	0.91	0.16	43,53,73,79	0
23	CLA	B	610	65/65	0.91	0.18	45,54,62,68	0
23	CLA	C	502	65/65	0.91	0.15	50,63,78,92	0
37	DGD	C	516	62/66	0.92	0.17	42,55,89,91	0
23	CLA	c	513	65/65	0.92	0.17	54,68,82,91	0
23	CLA	B	616	65/65	0.92	0.17	40,54,71,78	0
33	LHG	b	634	49/49	0.92	0.21	38,52,68,85	0
33	LHG	d	410	49/49	0.92	0.23	37,48,64,91	0
23	CLA	b	625	65/65	0.92	0.17	44,61,111,117	0
23	CLA	c	516	65/65	0.92	0.17	62,77,93,97	0
37	DGD	c	519	62/66	0.92	0.18	41,60,100,103	0
23	CLA	c	514	65/65	0.92	0.15	51,63,72,82	0
25	BCR	y	101	40/40	0.92	0.16	56,72,84,92	0
22	BCT	A	403[B]	4/4	0.92	0.24	72,82,83,95	4
27	GOL	D	403	6/6	0.92	0.27	52,56,67,70	0
22	BCT	A	403[A]	4/4	0.92	0.24	76,81,81,92	4
23	CLA	D	406	65/65	0.92	0.15	45,61,114,119	0
25	BCR	Y	101	40/40	0.92	0.17	65,78,92,103	0
23	CLA	B	613	65/65	0.93	0.15	34,45,54,58	0
23	CLA	b	623	65/65	0.93	0.18	33,46,93,110	0
23	CLA	B	608	65/65	0.93	0.18	28,43,57,64	0
33	LHG	d	409	49/49	0.93	0.22	41,55,68,69	0
23	CLA	C	508	65/65	0.93	0.16	51,70,83,91	0
23	CLA	B	605	65/65	0.93	0.16	32,44,76,81	0
23	CLA	d	403	65/65	0.93	0.17	36,44,51,62	0
23	CLA	A	404	65/65	0.93	0.16	33,40,53,66	0
23	CLA	b	617	65/65	0.93	0.16	41,56,64,70	0
27	GOL	b	605	6/6	0.93	0.22	67,86,109,116	0
23	CLA	d	405	65/65	0.93	0.18	49,59,108,118	0
23	CLA	b	620	65/65	0.93	0.17	33,47,57,64	0
27	GOL	V	203	6/6	0.93	0.26	64,71,80,84	0
23	CLA	b	621	65/65	0.93	0.15	36,47,56,65	0
23	CLA	C	510	65/65	0.93	0.15	54,73,88,95	0
23	CLA	B	603	65/65	0.93	0.16	41,52,63,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	GOL	B	629	6/6	0.93	0.27	51,65,75,83	0
23	CLA	B	615	65/65	0.93	0.20	32,45,99,106	0
23	CLA	b	612	65/65	0.93	0.16	41,54,64,70	0
23	CLA	a	408	65/65	0.93	0.19	35,42,50,62	0
25	BCR	b	627	40/40	0.93	0.18	34,47,64,72	0
32	UNL	d	412	17/-	0.94	0.23	59,72,96,98	0
31	PL9	d	407[B]	55/55	0.94	0.21	34,44,54,60	55
23	CLA	B	612	65/65	0.94	0.18	32,44,55,60	0
25	BCR	h	101	40/40	0.94	0.17	52,67,77,78	0
33	LHG	D	411	49/49	0.94	0.21	32,49,73,81	0
23	CLA	C	506	65/65	0.94	0.14	48,58,74,83	0
27	GOL	V	202	6/6	0.94	0.20	54,67,81,83	0
23	CLA	b	619	65/65	0.94	0.17	42,54,63,70	0
27	GOL	B	627	6/6	0.94	0.22	71,79,86,91	0
23	CLA	c	505	65/65	0.94	0.15	52,66,75,79	0
32	UNL	D	413	17/-	0.94	0.19	50,76,96,100	0
25	BCR	d	406	40/40	0.94	0.20	51,64,84,86	0
25	BCR	k	102	40/40	0.94	0.16	59,75,87,90	0
23	CLA	a	411	65/65	0.94	0.19	39,57,122,128	0
23	CLA	B	609	65/65	0.94	0.19	41,51,67,70	0
25	BCR	D	407	40/40	0.94	0.17	51,65,105,115	0
23	CLA	D	405	65/65	0.94	0.17	31,42,64,67	0
27	GOL	B	626	6/6	0.94	0.23	53,67,81,92	0
23	CLA	B	617	65/65	0.94	0.20	43,58,134,136	0
33	LHG	L	101	49/49	0.94	0.21	41,50,59,62	0
27	GOL	C	525	6/6	0.94	0.20	56,58,70,72	0
22	BCT	d	401[A]	4/4	0.94	0.23	74,74,76,78	4
31	PL9	d	407[A]	55/55	0.94	0.21	33,44,54,60	55
22	BCT	d	401[B]	4/4	0.94	0.23	73,74,76,78	4
23	CLA	A	406	65/65	0.95	0.15	34,45,102,111	0
24	PHO	D	402[B]	64/64	0.95	0.17	36,48,58,63	64
23	CLA	b	622	65/65	0.95	0.19	34,47,60,67	0
31	PL9	D	408[A]	55/55	0.95	0.22	31,43,50,58	55
39	HEM	F	102	43/43	0.95	0.17	60,81,105,113	0
25	BCR	A	409	40/40	0.95	0.17	36,47,55,56	0
40	MG	J	102	1/1	0.95	0.12	64,64,64,64	0
25	BCR	K	103	40/40	0.95	0.16	59,74,89,92	0
23	CLA	C	503	65/65	0.95	0.15	45,65,72,76	0
23	CLA	A	408	65/65	0.95	0.15	38,56,120,128	0
25	BCR	T	103	40/40	0.95	0.15	30,50,64,66	0
39	HEM	e	101	43/43	0.95	0.19	72,91,130,138	0
23	CLA	B	611	65/65	0.95	0.19	40,57,67,70	0

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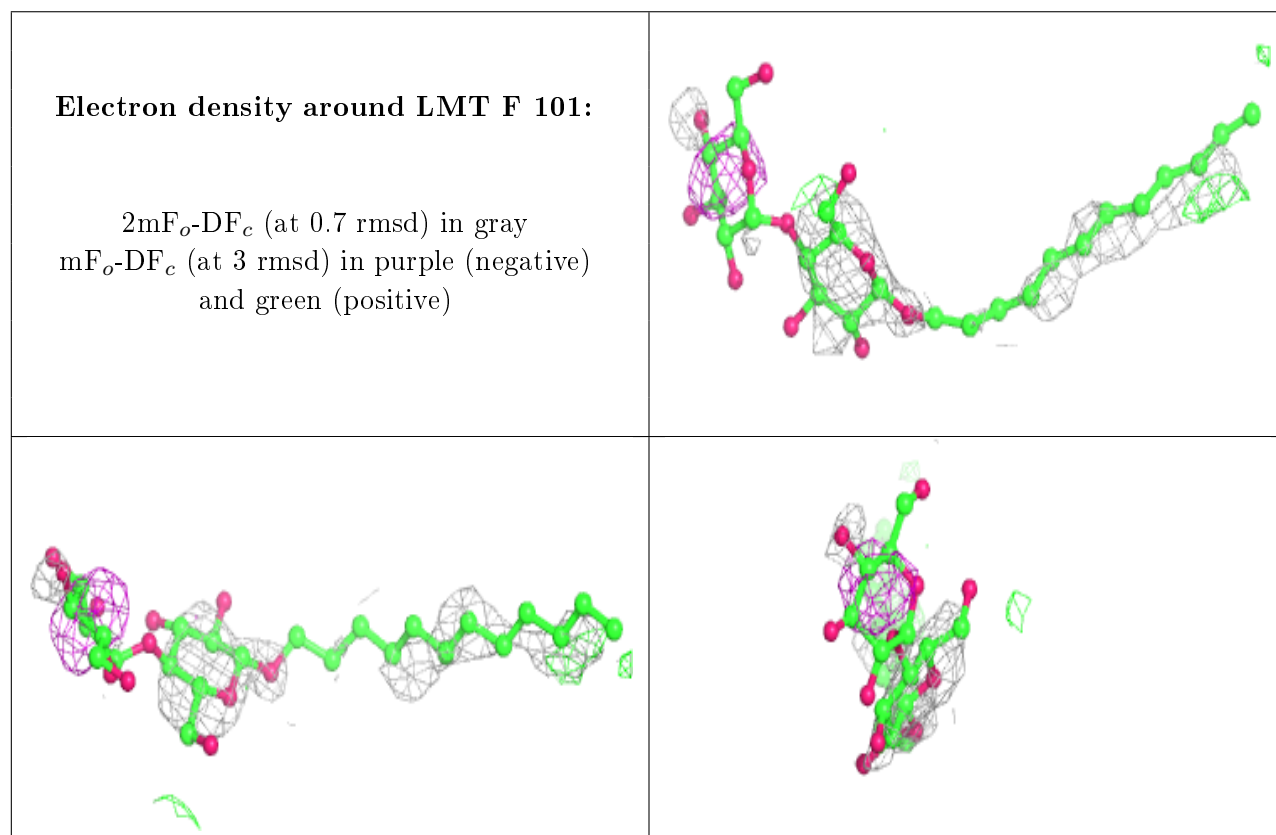
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	b	613	65/65	0.95	0.16	33,45,71,77	0
23	CLA	B	606	65/65	0.95	0.16	35,44,57,61	0
27	GOL	v	204	6/6	0.95	0.25	63,69,78,81	0
23	CLA	a	409	65/65	0.95	0.18	37,48,109,116	0
27	GOL	a	401	6/6	0.95	0.19	52,63,72,75	0
23	CLA	b	614	65/65	0.95	0.17	35,46,60,65	0
27	GOL	B	628	6/6	0.95	0.29	61,71,81,83	0
24	PHO	D	402[A]	64/64	0.95	0.17	37,49,59,63	64
24	PHO	A	407	64/64	0.95	0.16	30,41,50,55	0
25	BCR	C	515	40/40	0.95	0.17	50,64,76,78	0
23	CLA	d	404	65/65	0.95	0.17	35,43,58,69	0
24	PHO	d	402[B]	64/64	0.95	0.18	39,50,56,59	64
23	CLA	c	506	65/65	0.95	0.14	48,62,79,87	0
23	CLA	A	405	65/65	0.95	0.16	30,40,48,53	0
23	CLA	B	604	65/65	0.95	0.18	46,55,63,66	0
24	PHO	d	402[A]	64/64	0.95	0.18	37,51,57,59	64
31	PL9	D	408[B]	55/55	0.95	0.22	32,43,51,56	55
25	BCR	B	620	40/40	0.96	0.19	41,52,62,66	0
21	CL	A	402[A]	1/1	0.96	0.11	44,44,44,44	1
34	CA	c	504	1/1	0.96	0.07	85,85,85,85	0
25	BCR	a	412	40/40	0.96	0.18	37,47,54,57	0
25	BCR	b	628	40/40	0.96	0.18	40,59,69,70	0
25	BCR	B	619	40/40	0.96	0.18	36,48,61,67	0
25	BCR	c	518	40/40	0.96	0.19	52,64,77,80	0
25	BCR	t	101	40/40	0.96	0.19	33,52,66,68	0
27	GOL	b	604	6/6	0.96	0.15	63,68,80,82	0
25	BCR	B	618	40/40	0.96	0.20	34,45,56,58	0
24	PHO	a	410	64/64	0.96	0.19	36,44,50,53	0
21	CL	A	402[B]	1/1	0.96	0.11	46,46,46,46	1
27	GOL	v	201	6/6	0.96	0.18	72,80,88,97	0
34	CA	O	302	1/1	0.97	0.04	96,96,96,96	0
25	BCR	b	626	40/40	0.97	0.18	38,47,56,58	0
39	HEM	v	206	43/43	0.97	0.14	55,68,73,77	0
27	GOL	B	625	6/6	0.97	0.18	53,63,67,79	0
27	GOL	b	603	6/6	0.97	0.22	58,75,83,86	0
40	MG	j	102	1/1	0.97	0.15	71,71,71,71	0
27	GOL	B	630	6/6	0.97	0.35	50,85,91,96	0
39	HEM	V	205	43/43	0.97	0.13	46,53,60,62	0
34	CA	C	526	1/1	0.97	0.11	88,88,88,88	0
29	OEX	a	416[A]	10/10	0.98	0.15	41,48,53,56	10
34	CA	o	302	1/1	0.98	0.05	96,96,96,96	0
27	GOL	c	501	6/6	0.98	0.24	56,62,65,68	0

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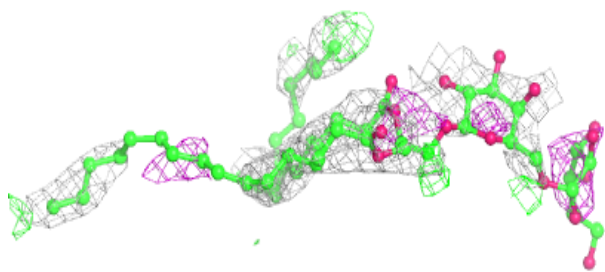
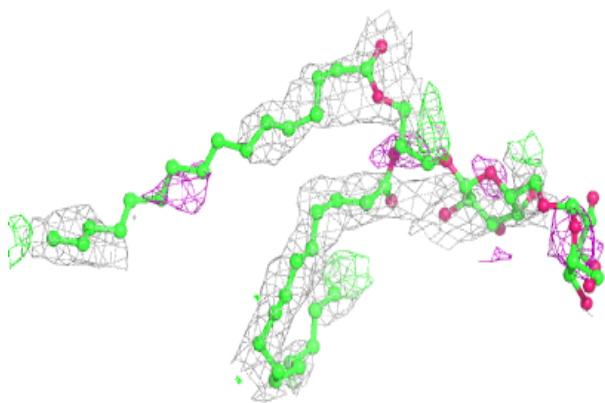
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	OEY	a	417[B]	11/11	0.98	0.16	40,48,57,78	11
30	OEY	A	416[B]	11/11	0.99	0.13	43,53,64,72	11
38	FE2	D	401[A]	1/1	0.99	0.08	70,70,70,70	1
34	CA	c	503	1/1	0.99	0.08	78,78,78,78	0
21	CL	a	406[A]	1/1	0.99	0.16	46,46,46,46	1
38	FE2	a	405[B]	1/1	0.99	0.10	62,62,62,62	0
21	CL	a	407[A]	1/1	0.99	0.13	52,52,52,52	1
29	OEX	A	415[A]	10/10	0.99	0.12	47,56,62,72	10
21	CL	a	407[B]	1/1	0.99	0.13	47,47,47,47	1
38	FE2	D	401[B]	1/1	0.99	0.08	69,69,69,69	1
21	CL	a	406[B]	1/1	0.99	0.16	47,47,47,47	1
21	CL	A	401[A]	1/1	1.00	0.17	42,42,42,42	1
21	CL	A	401[B]	1/1	1.00	0.17	39,39,39,39	1

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

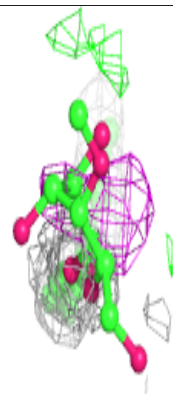
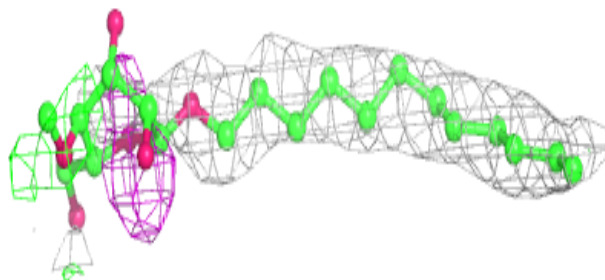
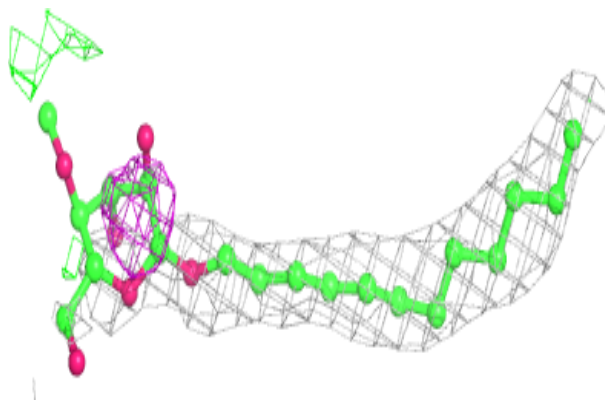


**Electron density around DGD d 408:**

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

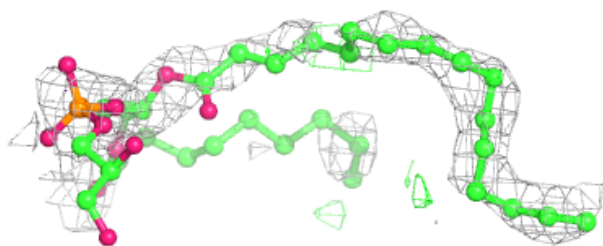
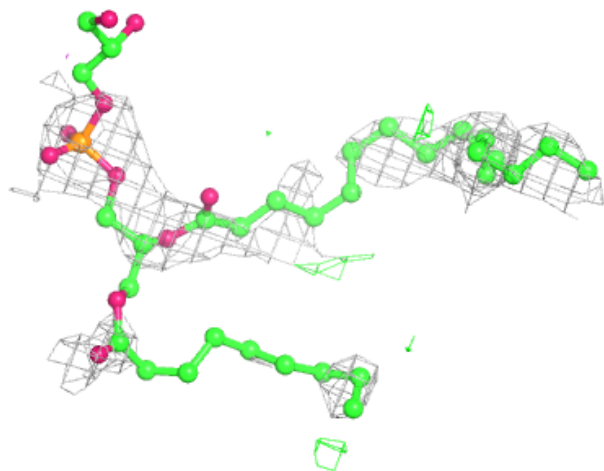
**Electron density around LMT b 630:**

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



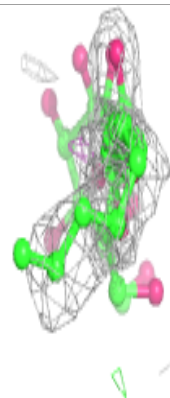
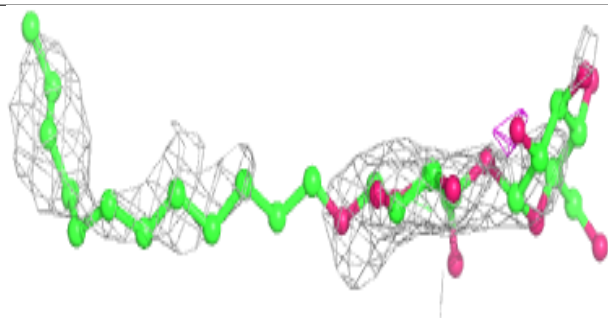
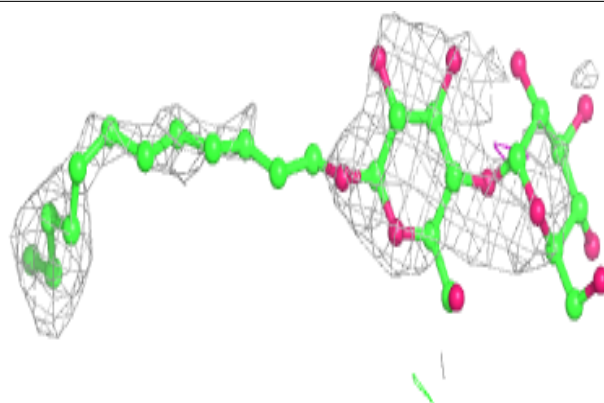
**Electron density around LHG a 419:**

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

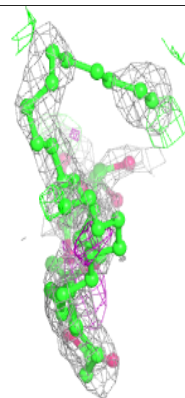
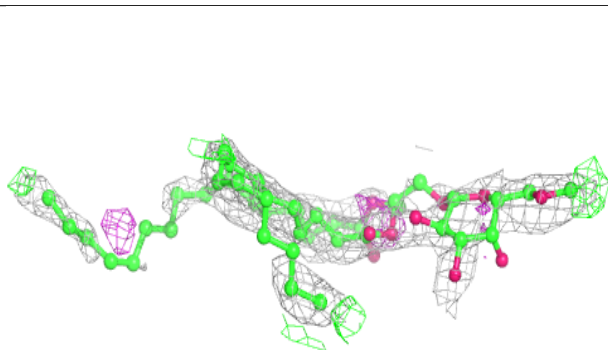
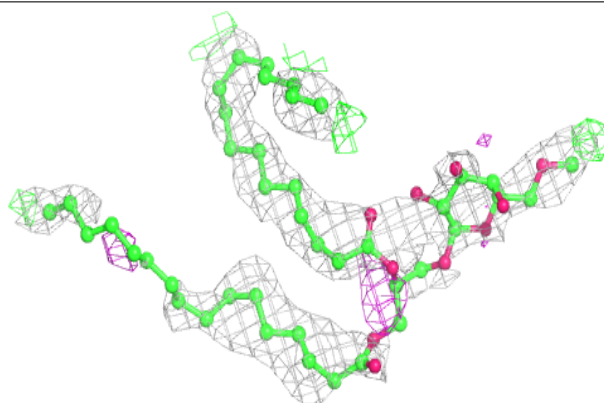


**Electron density around LMT a 418:**

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

**Electron density around DGD D 409:**

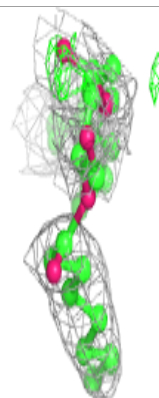
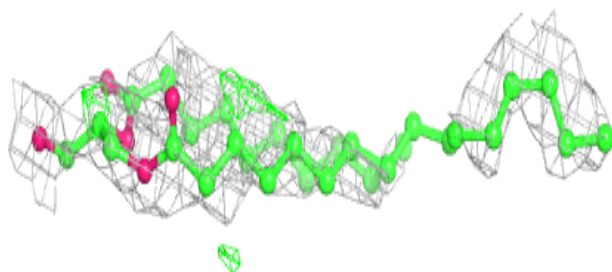
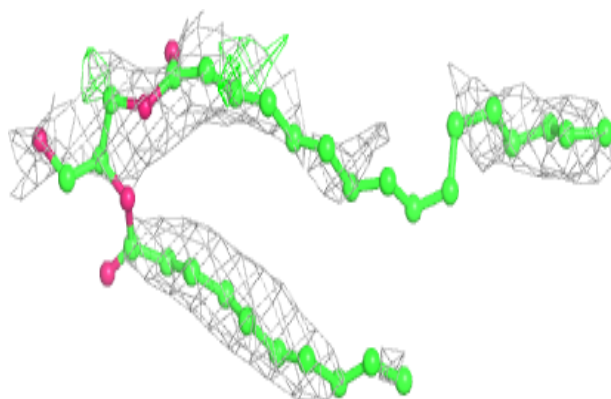
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



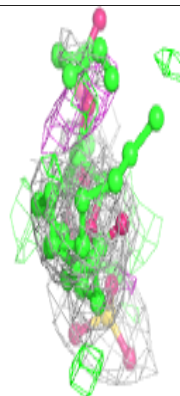
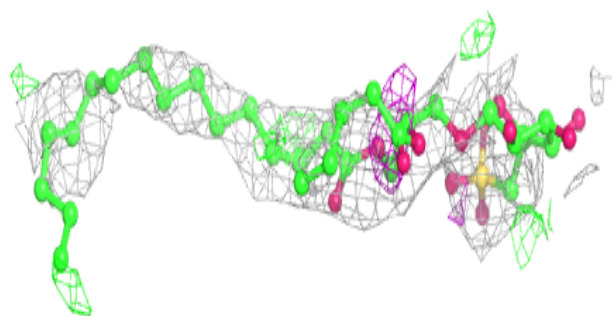
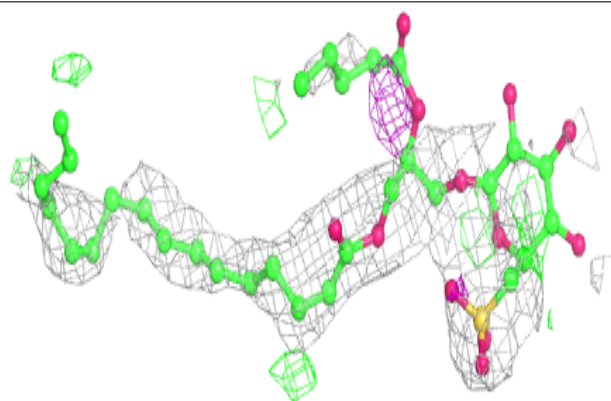


**Electron density around UNL K 102:**

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

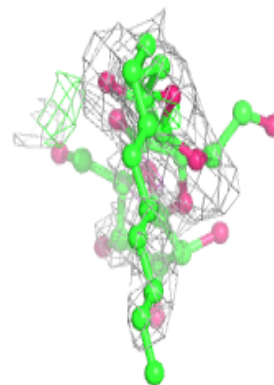
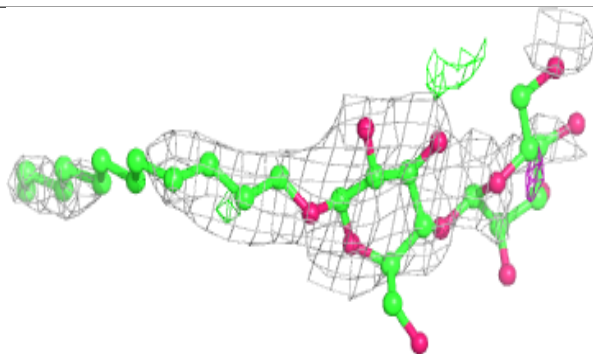
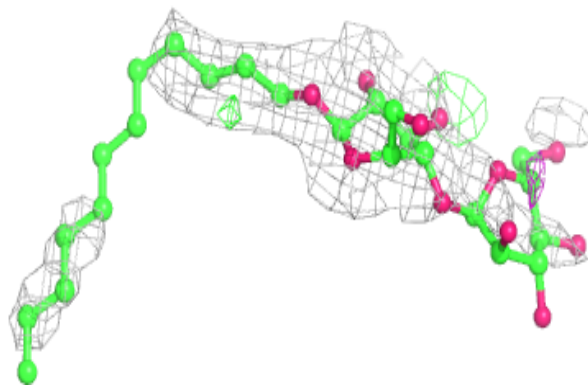
**Electron density around SQD f 102:**

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

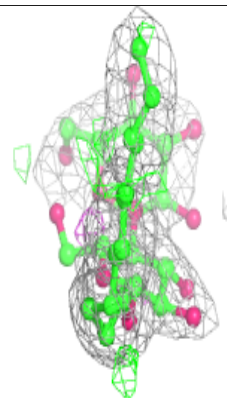
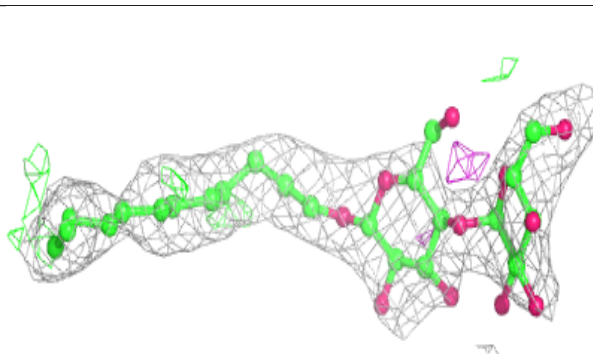
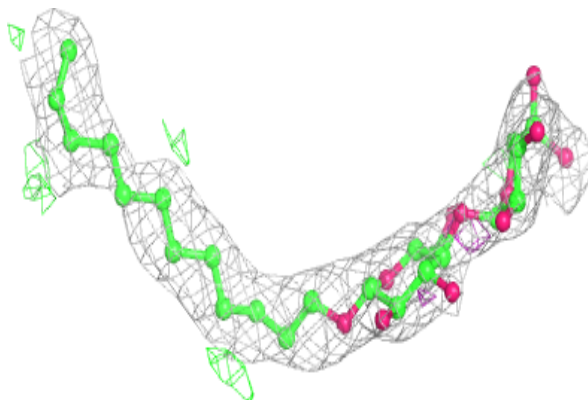


**Electron density around LMT C 521:**

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

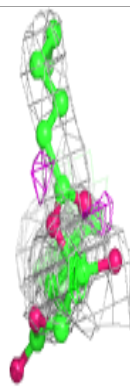
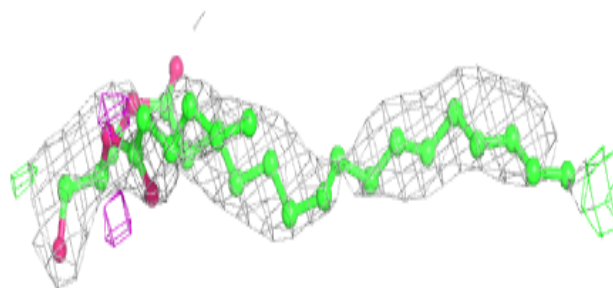
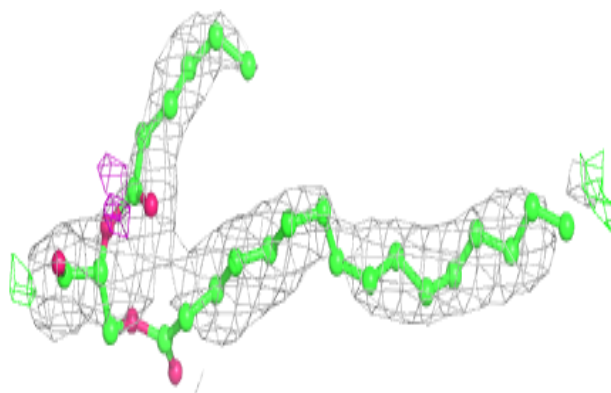
**Electron density around LMT m 102:**

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



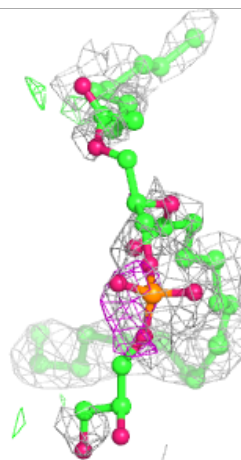
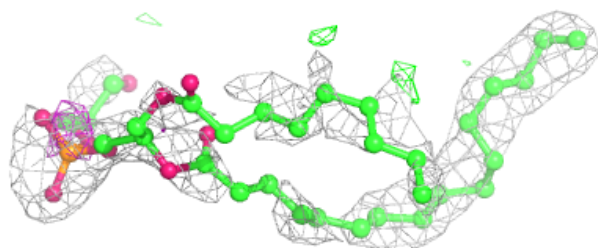
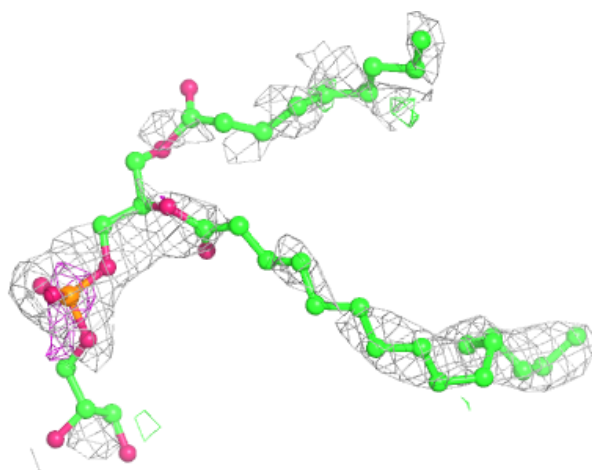
**Electron density around UNL a 403:**

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



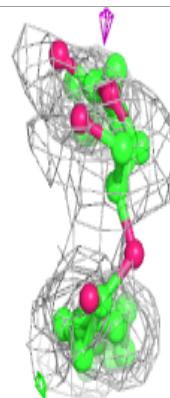
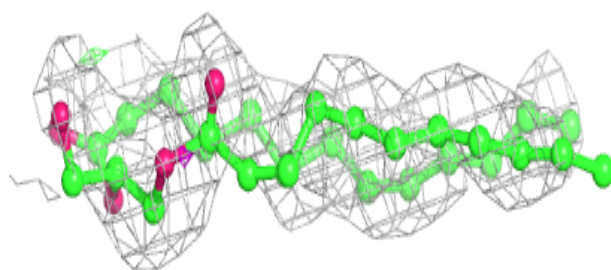
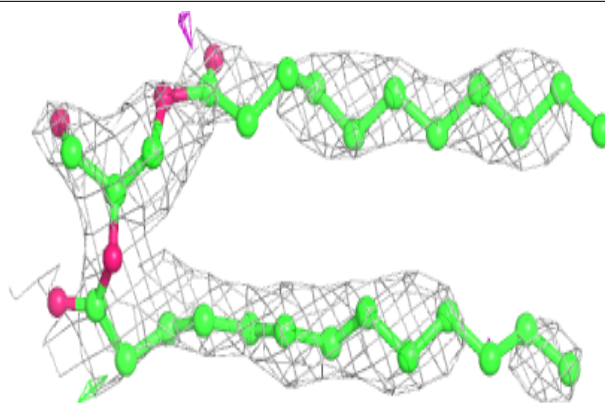
**Electron density around LHG A 419:**

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

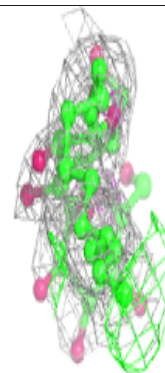
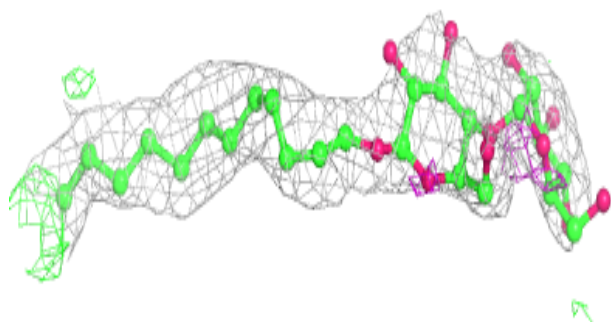
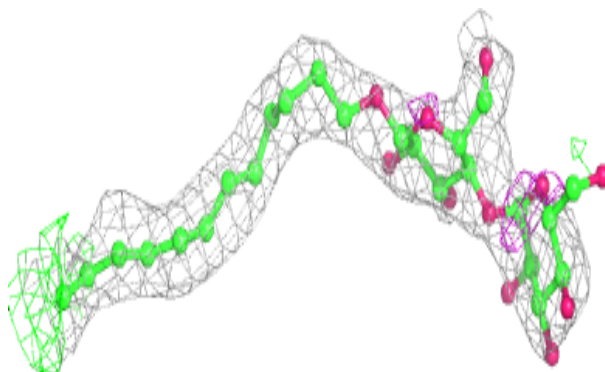


**Electron density around UNL c 525:**

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

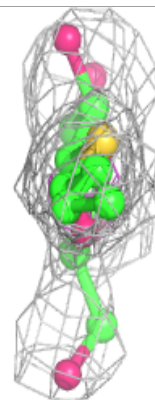
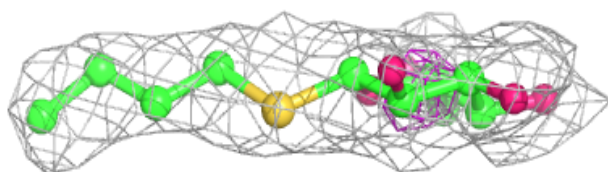
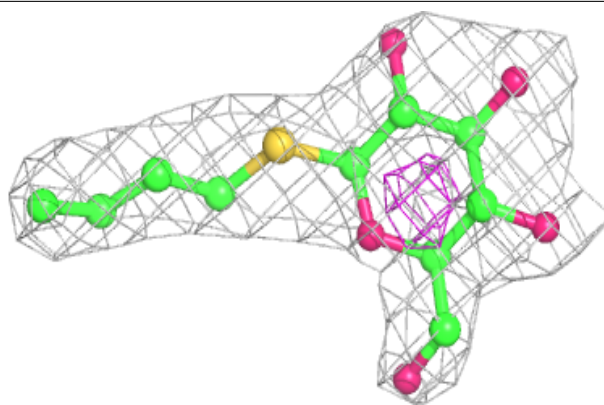
**Electron density around LMT a 404:**

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



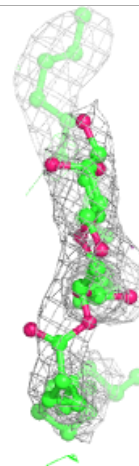
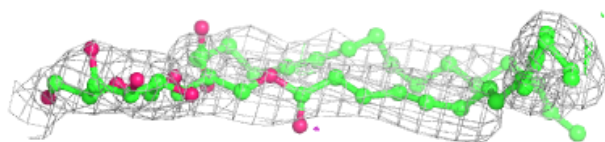
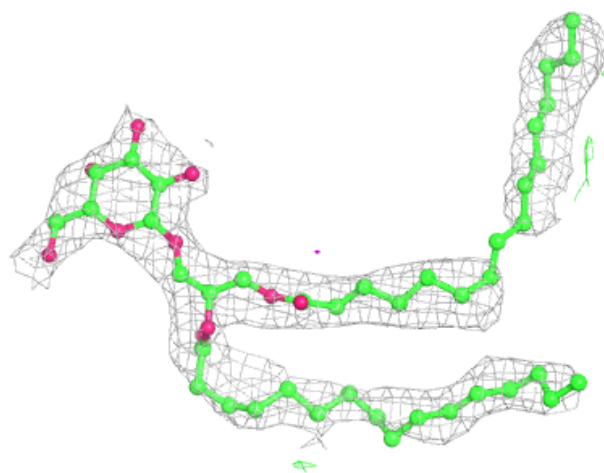
**Electron density around HTG d 414:**

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



**Electron density around LMG C 519:**

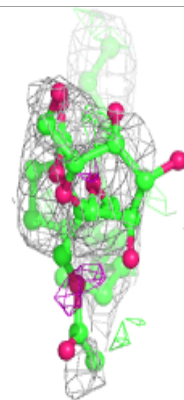
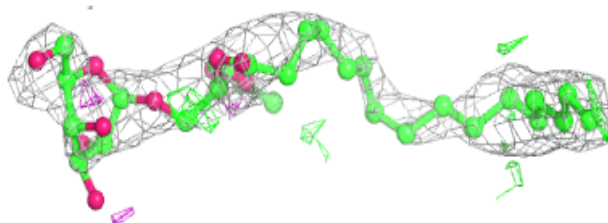
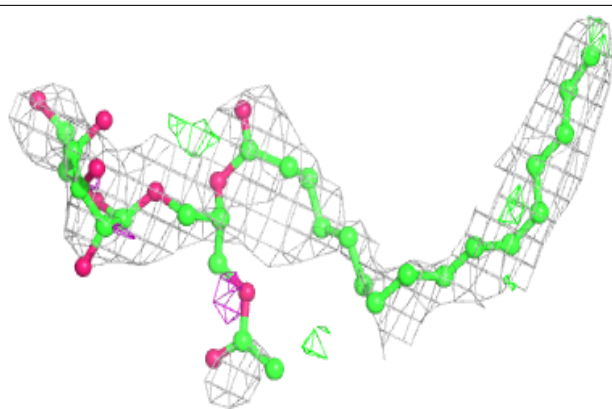
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



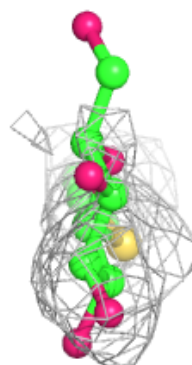
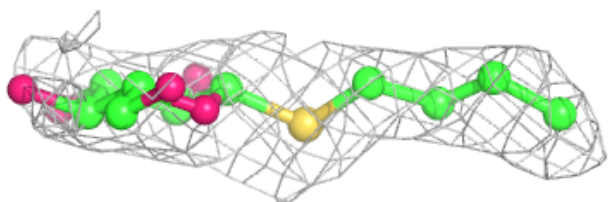
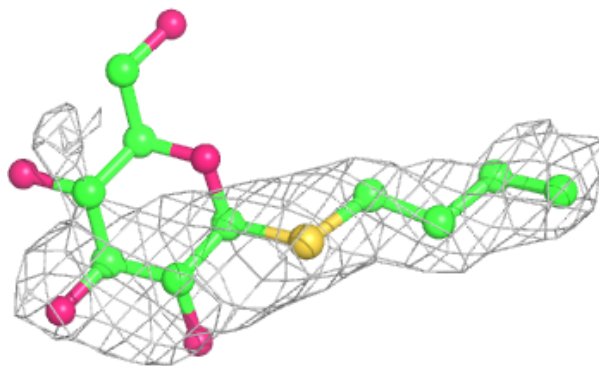


**Electron density around LMG Z 101:**

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

**Electron density around HTG D 415:**

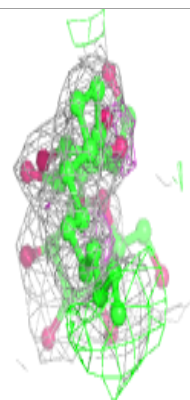
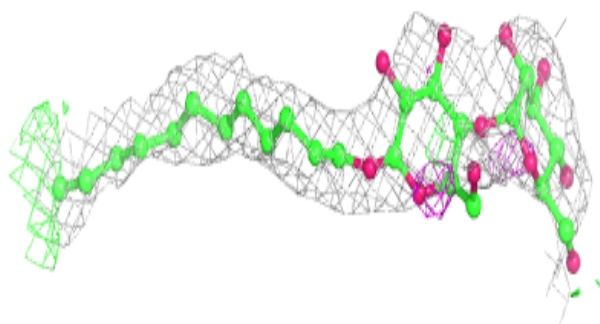
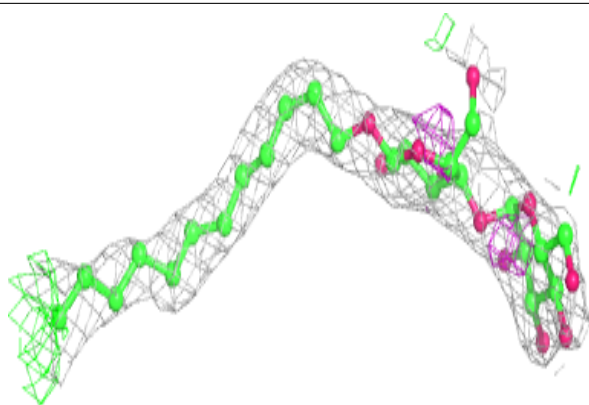
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



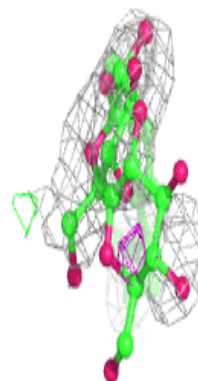
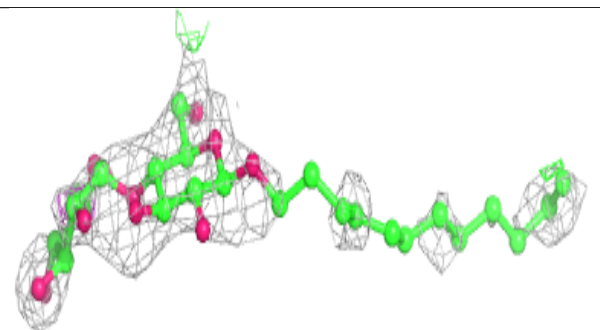
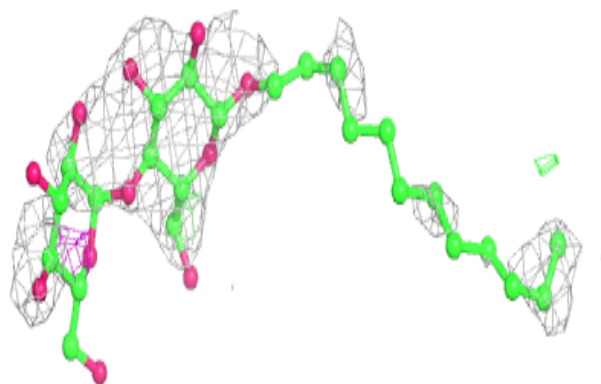


**Electron density around LMT A 414:**

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

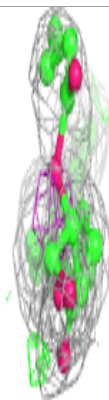
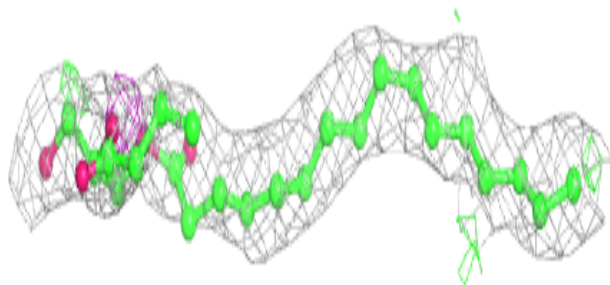
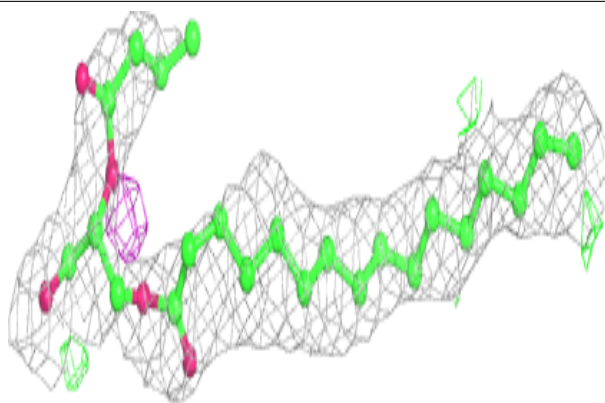
**Electron density around LMT e 102:**

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

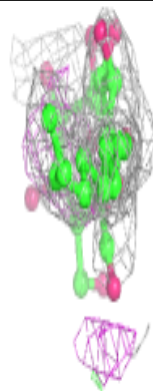
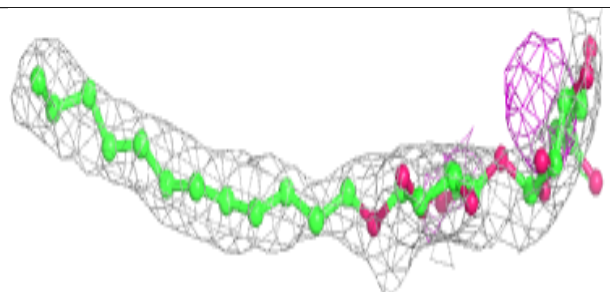
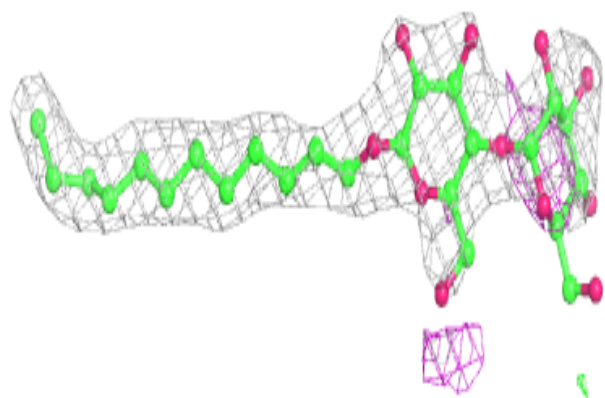


**Electron density around UNL A 418:**

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

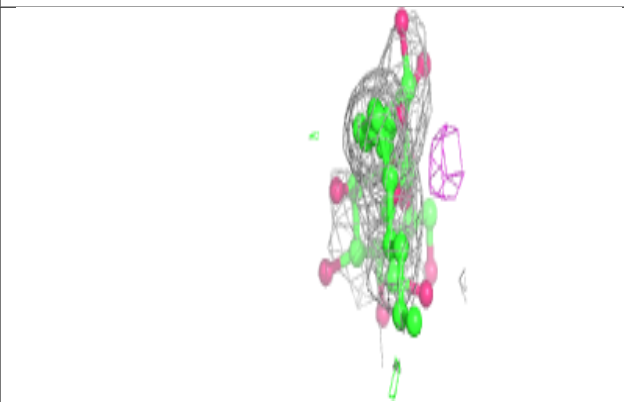
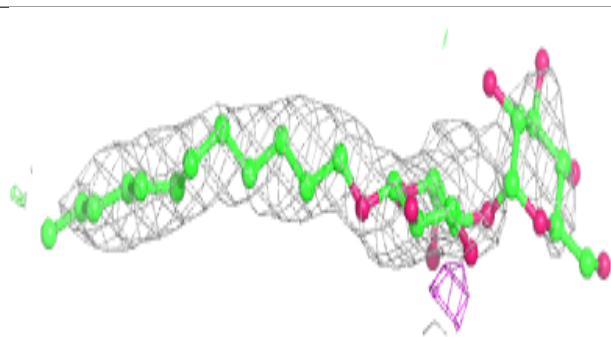
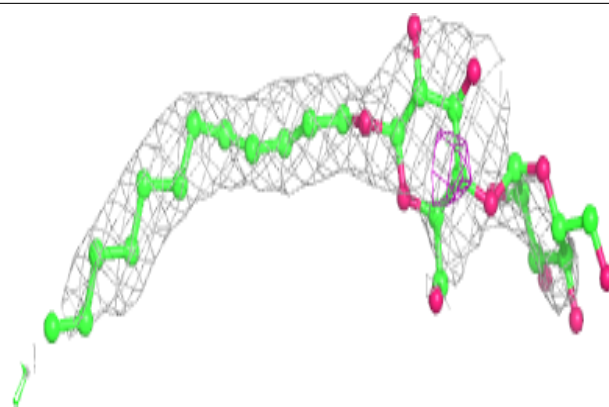
**Electron density around LMT M 105:**

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

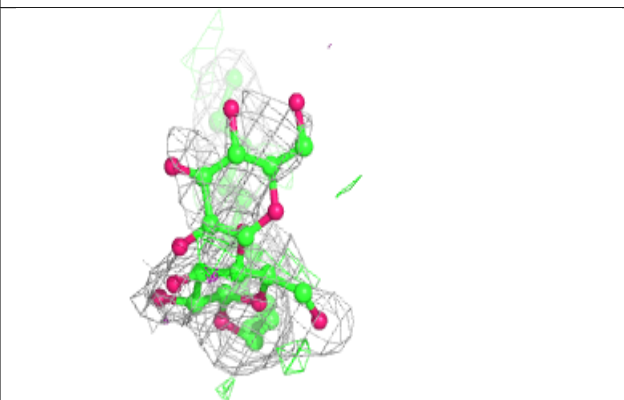
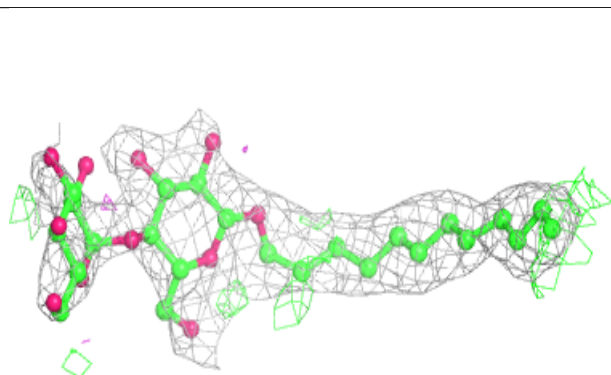
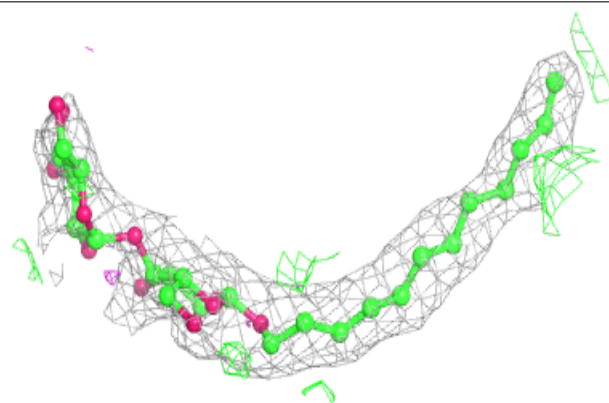


**Electron density around LMT D 404:**

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

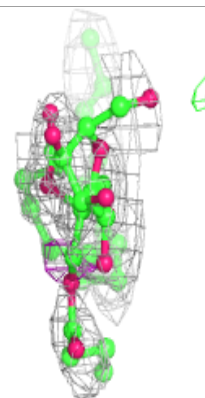
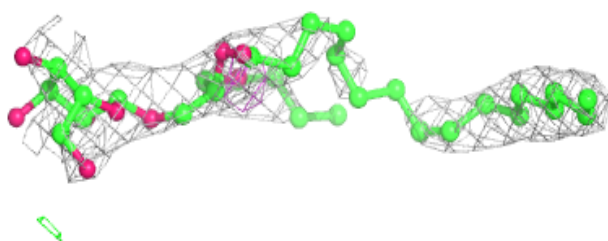
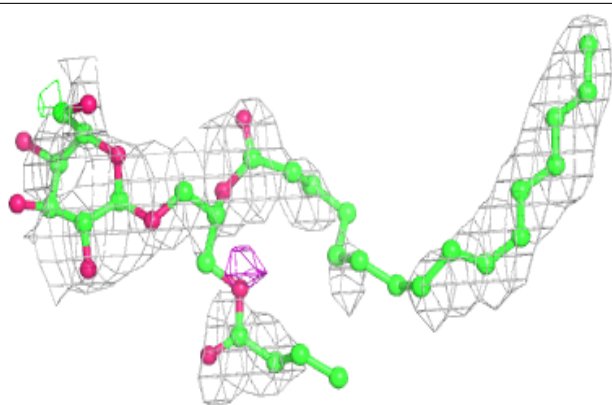
**Electron density around LMT M 104:**

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

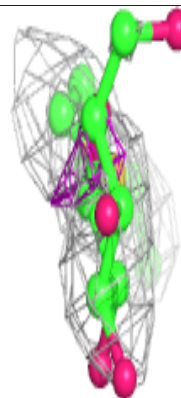
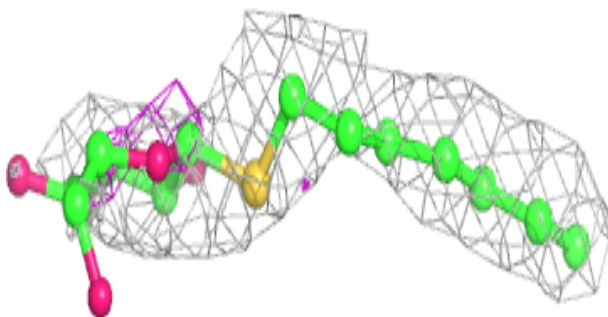
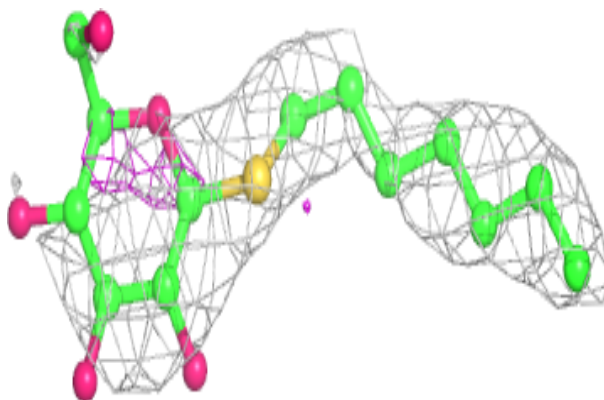


**Electron density around LMG z 101:**

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

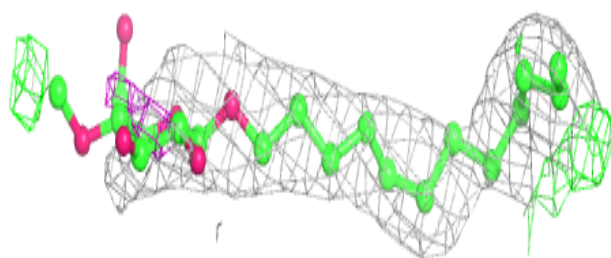
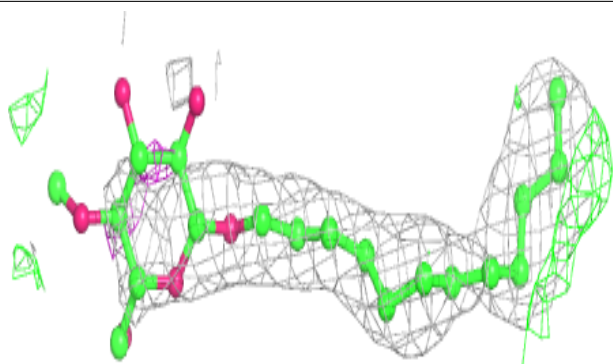
**Electron density around HTG c 524:**

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

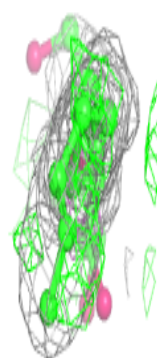
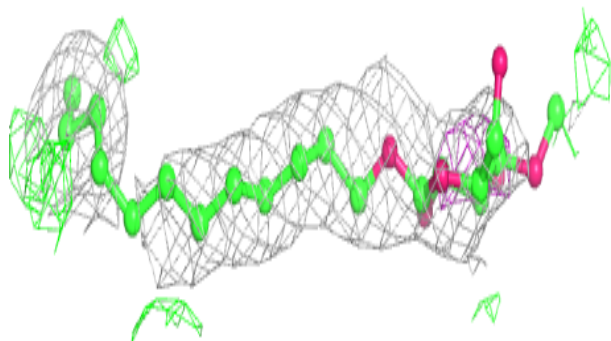
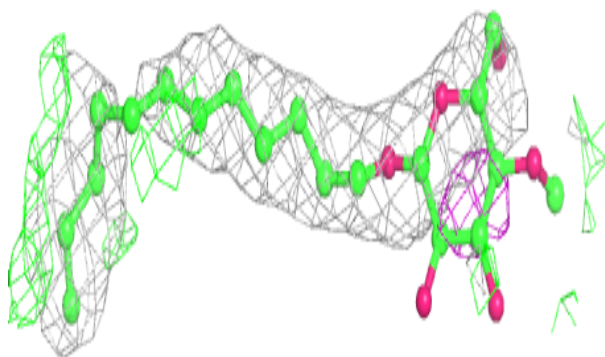


**Electron density around LMT B 634:**

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

**Electron density around LMT T 104:**

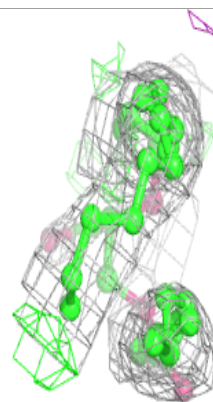
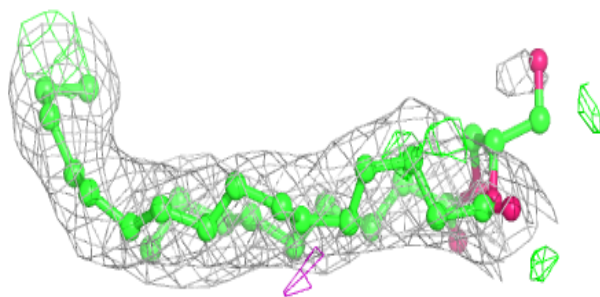
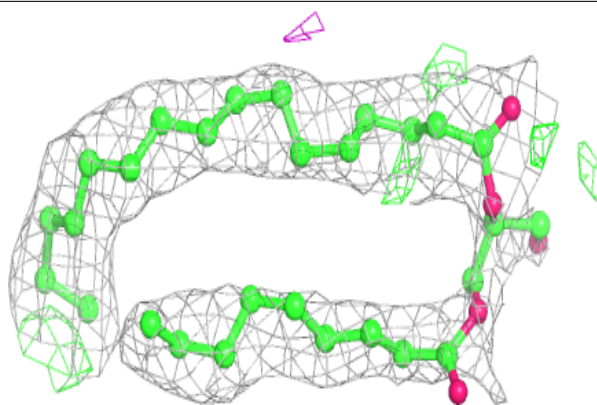
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



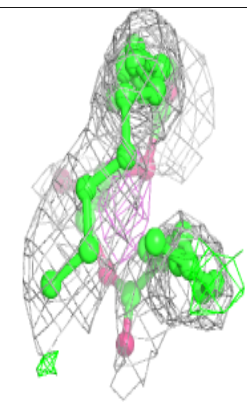
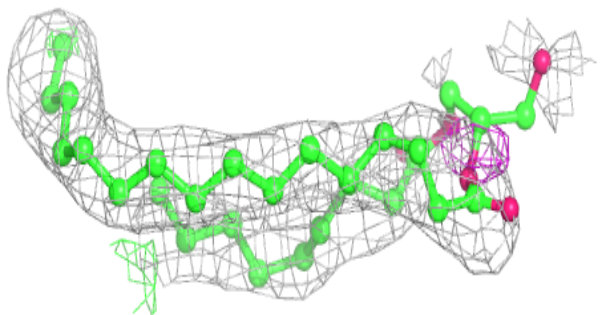
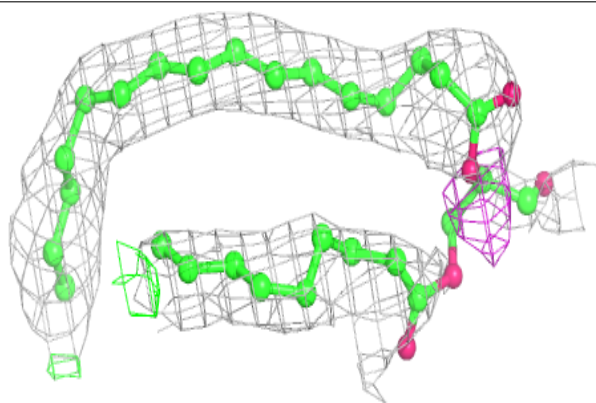


**Electron density around UNL B 633:**

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

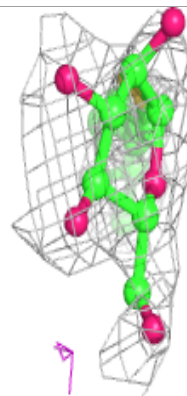
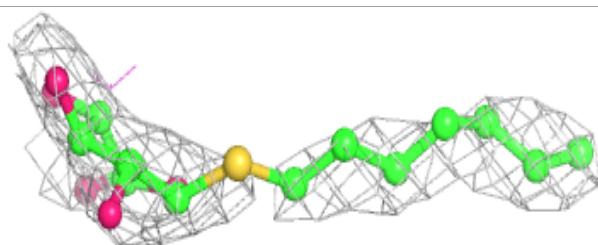
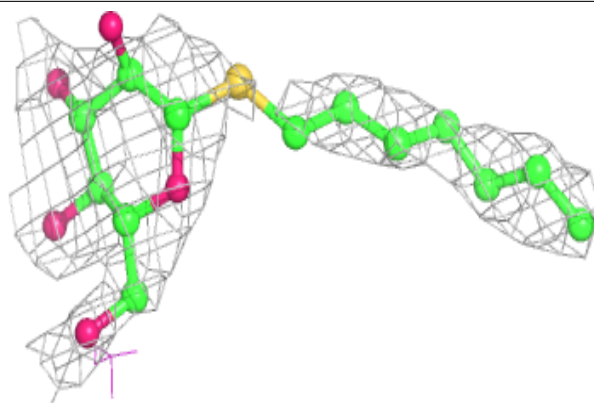
**Electron density around UNL b 633:**

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

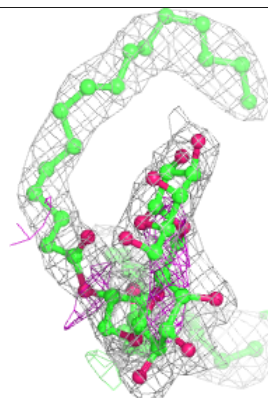
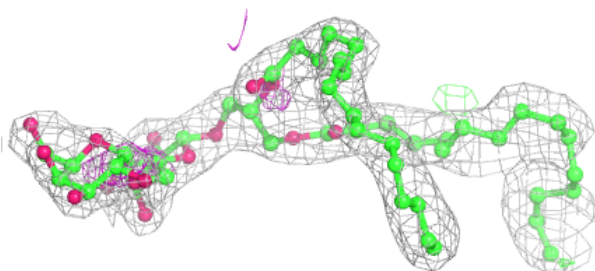
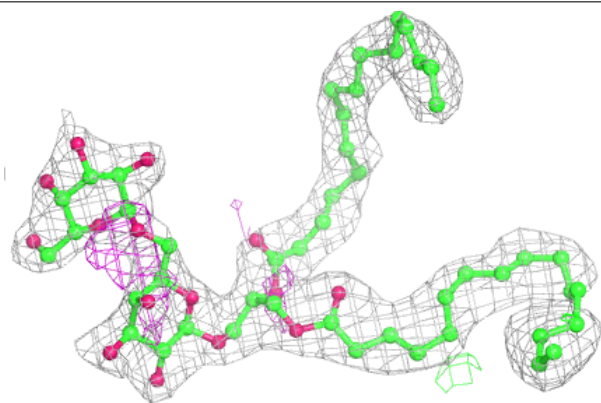


**Electron density around HTG B 624:**

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

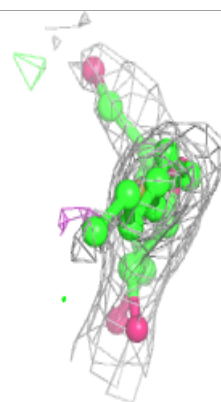
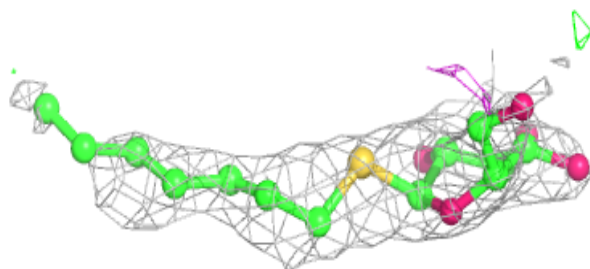
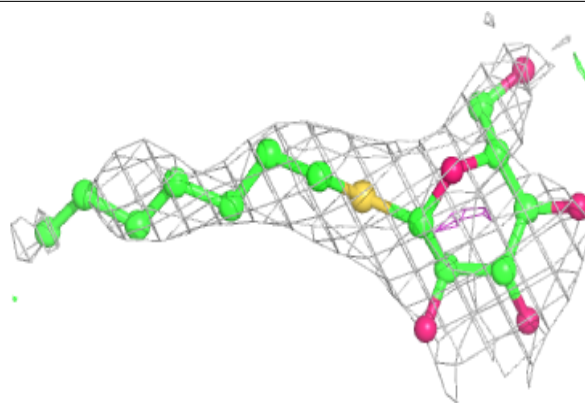
**Electron density around DGD C 517:**

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

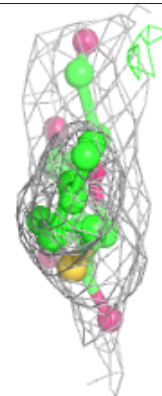
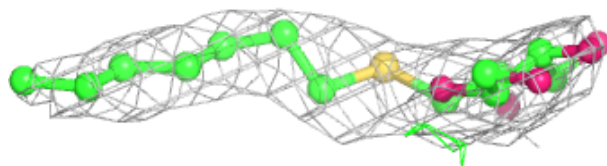
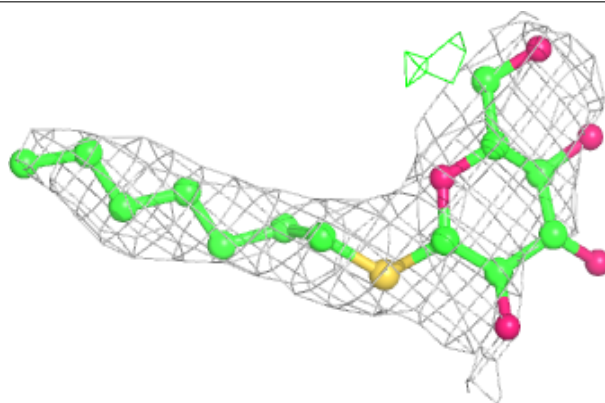


**Electron density around HTG C 523:**

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

**Electron density around HTG b 632:**

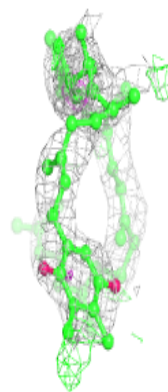
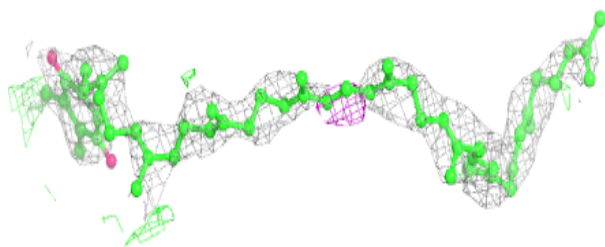
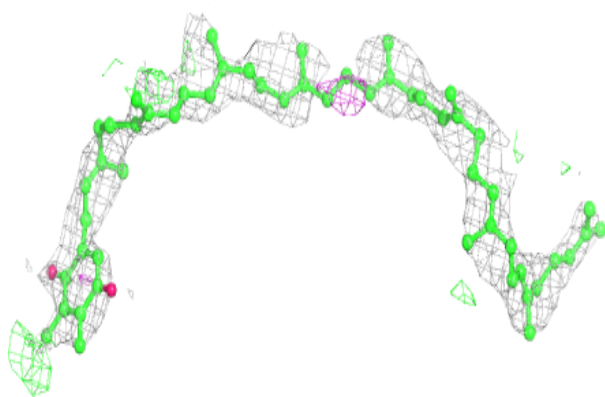
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



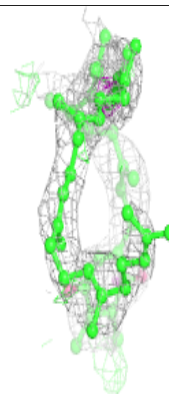
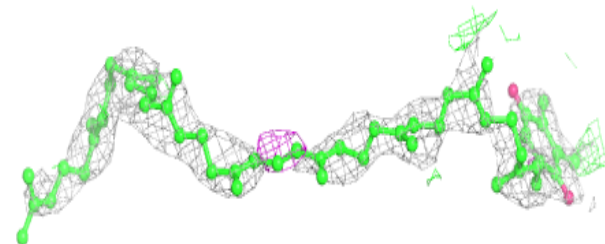
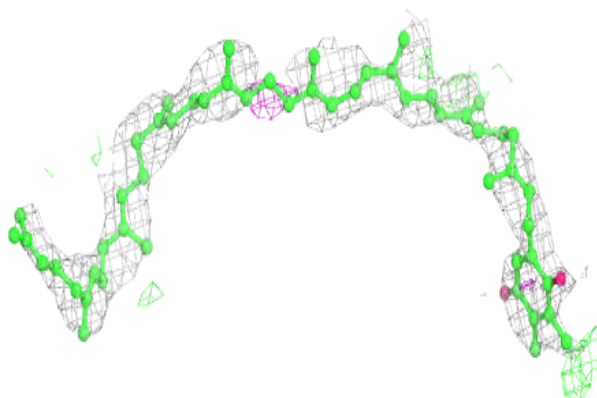


**Electron density around PL9 A 417 (B):**

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

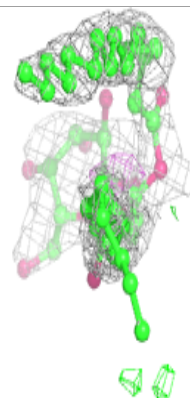
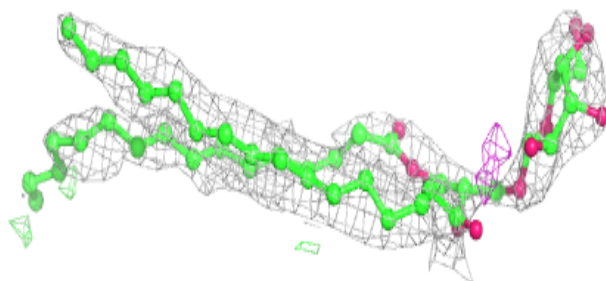
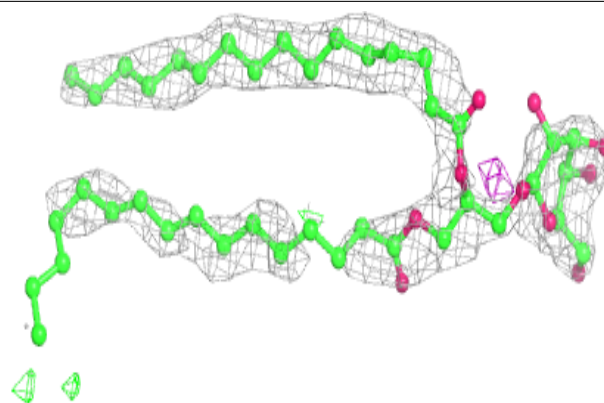
**Electron density around PL9 A 417 (A):**

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

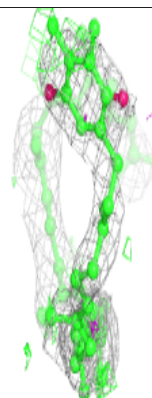
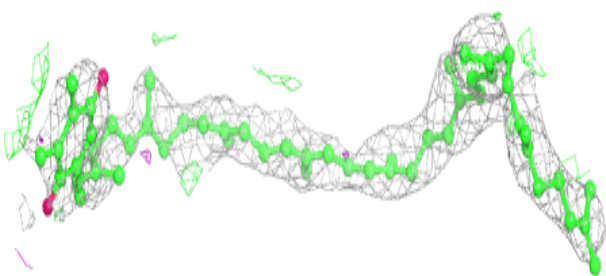
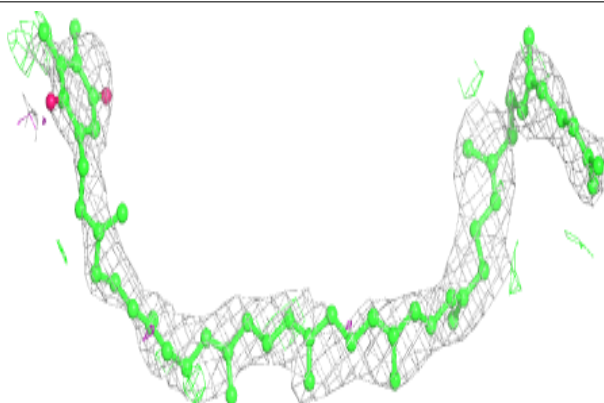


**Electron density around LMG C 520:**

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

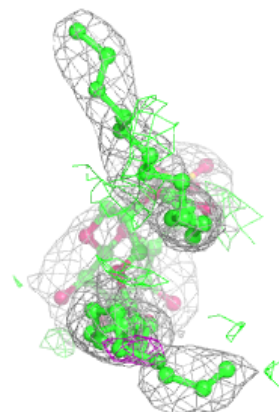
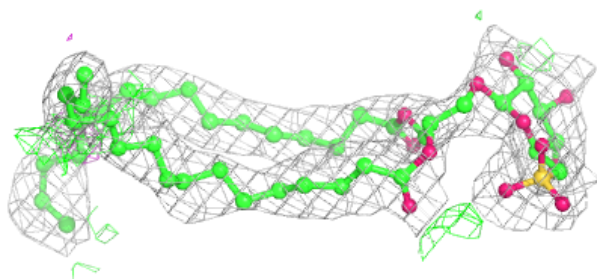
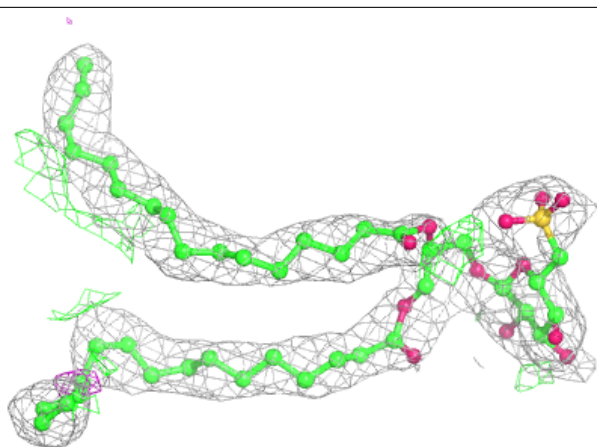
**Electron density around PL9 a 415 (A):**

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

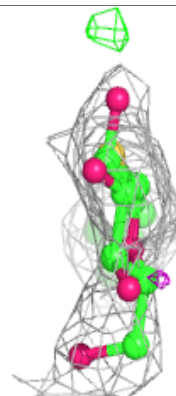
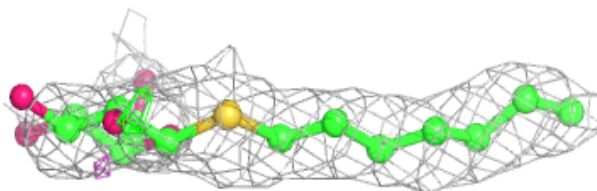
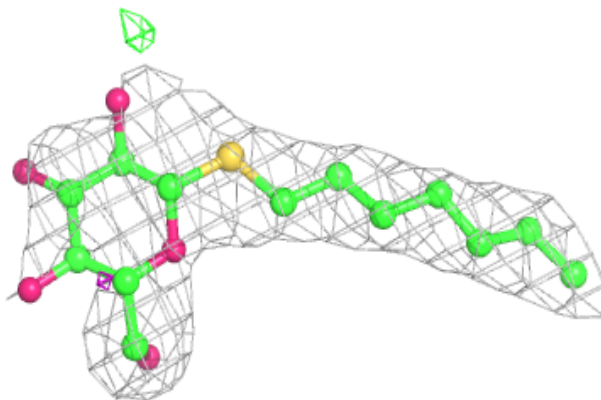


**Electron density around SQD b 601:**

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

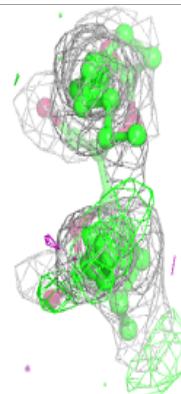
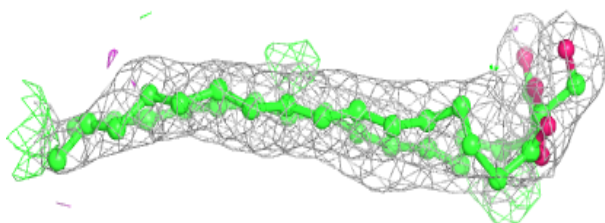
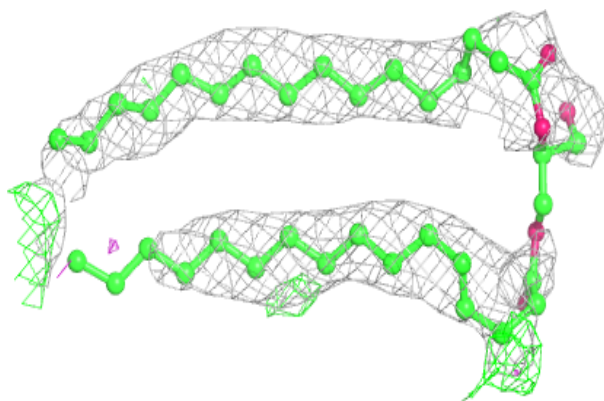
**Electron density around HTG b 608:**

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

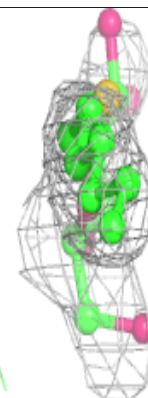
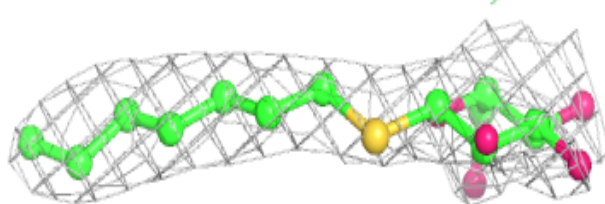
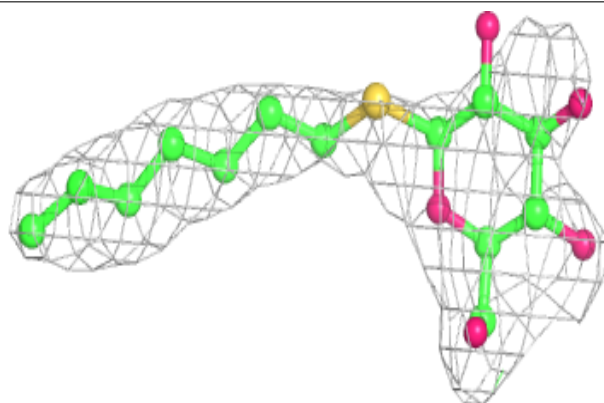


**Electron density around UNL i 101:**

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

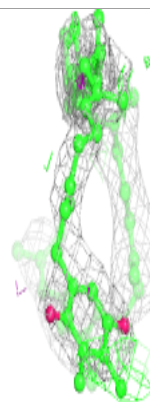
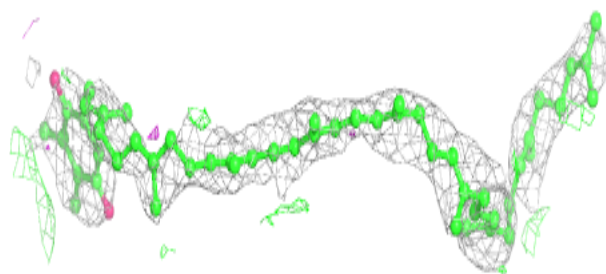
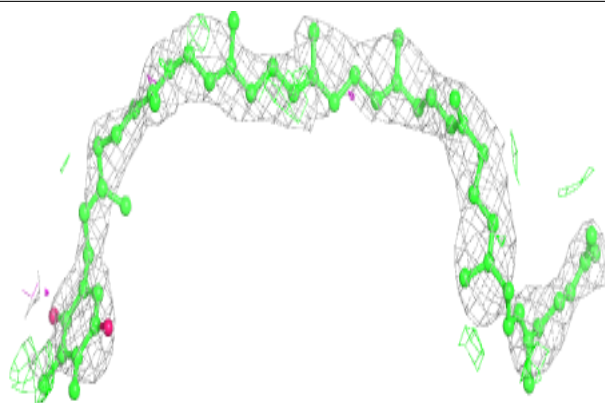
**Electron density around HTG B 632:**

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

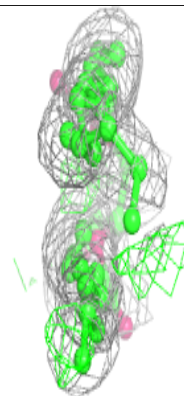
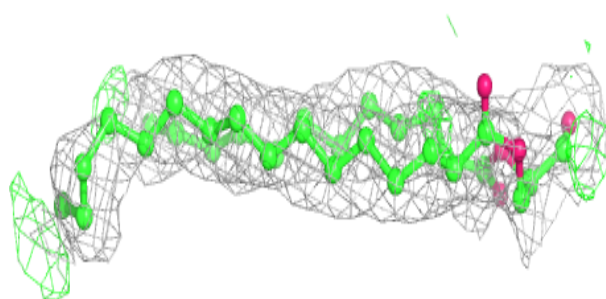
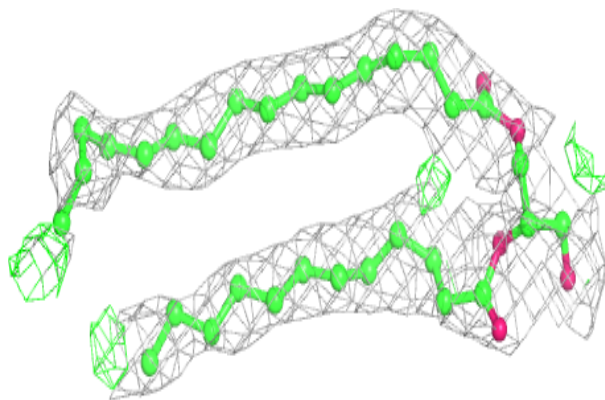


**Electron density around PL9 a 415 (B):**

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

**Electron density around UNL d 413:**

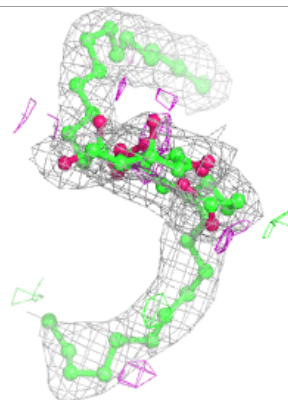
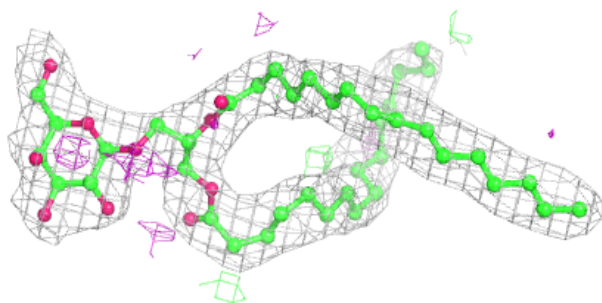
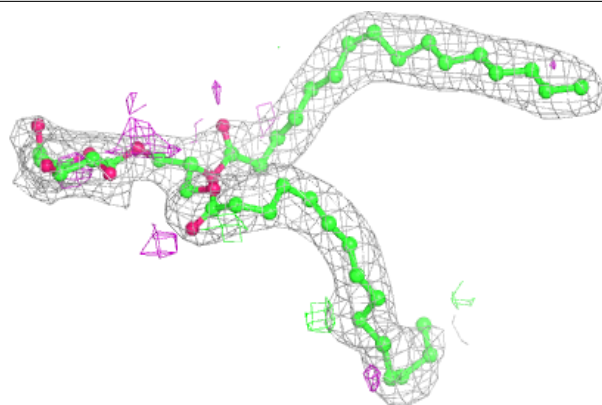
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



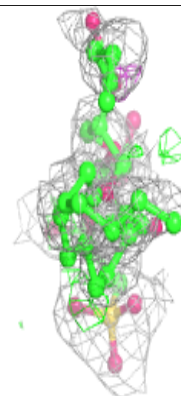
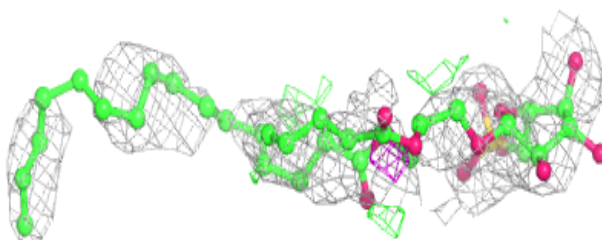
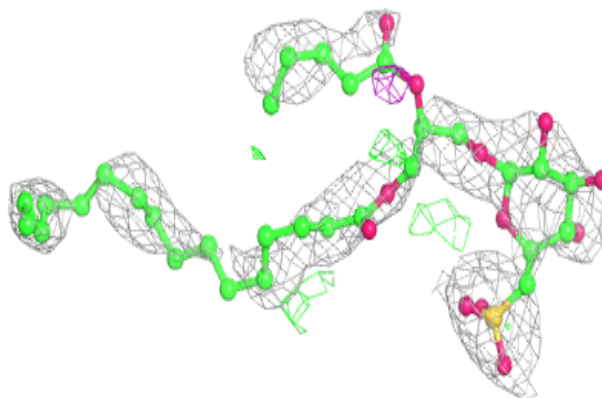


**Electron density around LMG b 629:**

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

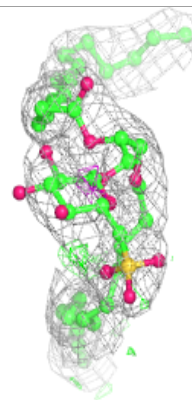
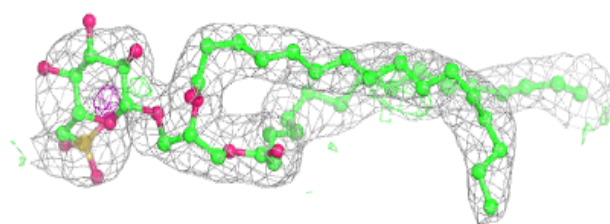
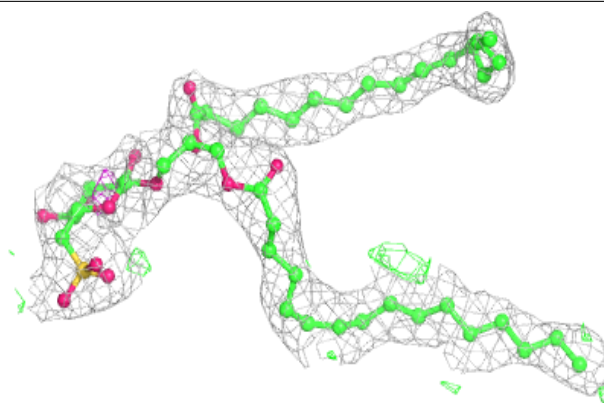
**Electron density around SQD F 104:**

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

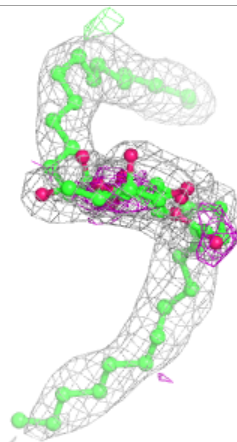
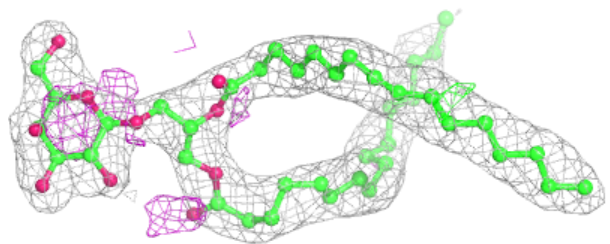
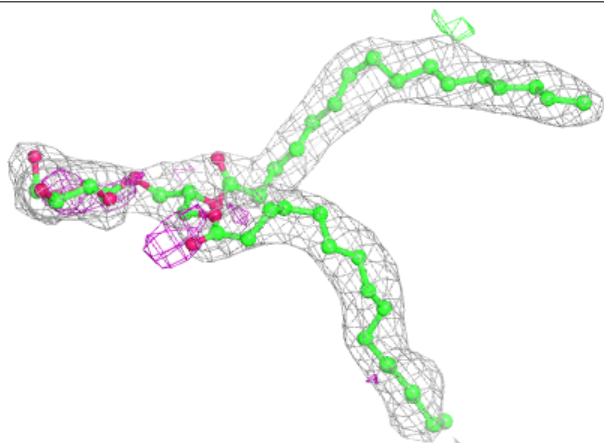


**Electron density around SQD B 636:**

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

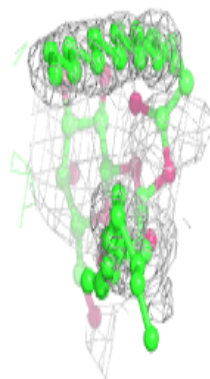
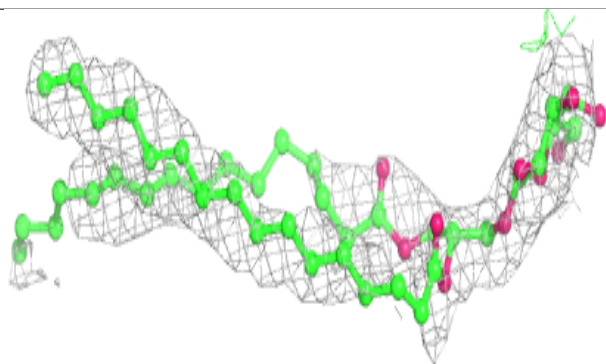
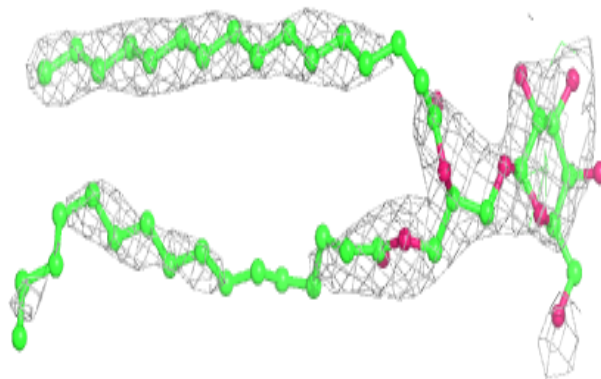
**Electron density around LMG M 101:**

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

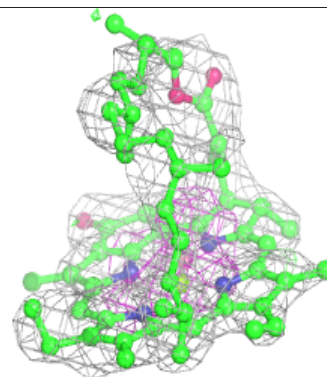
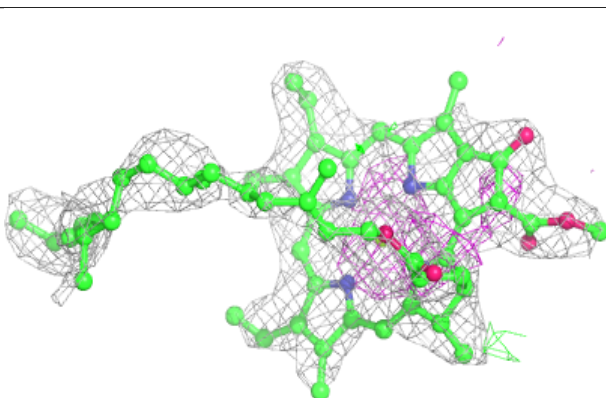
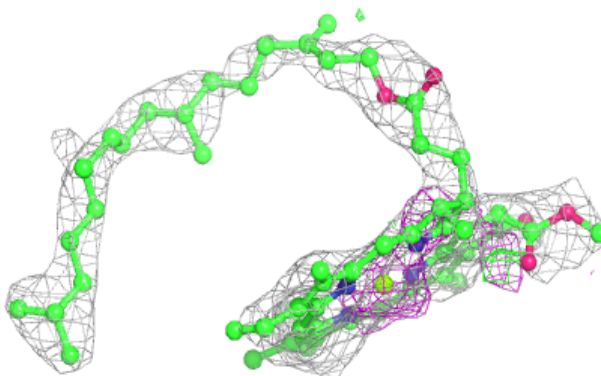


**Electron density around LMG c 522:**

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

**Electron density around CLA C 514:**

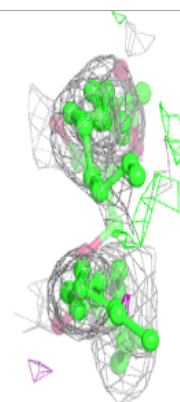
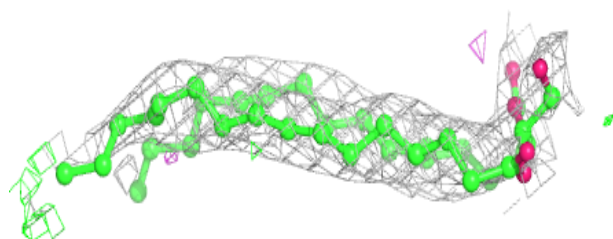
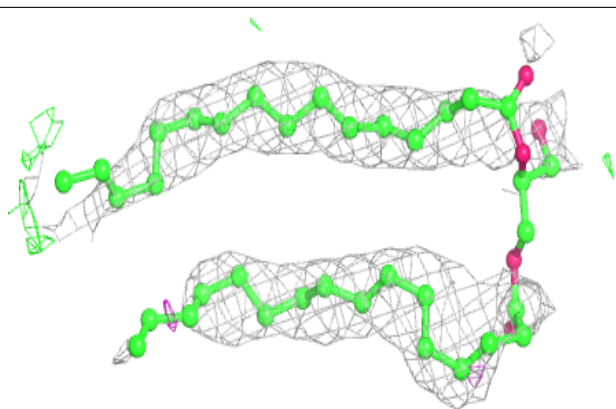
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



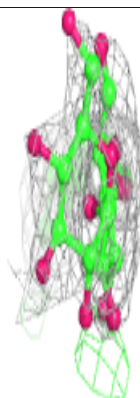
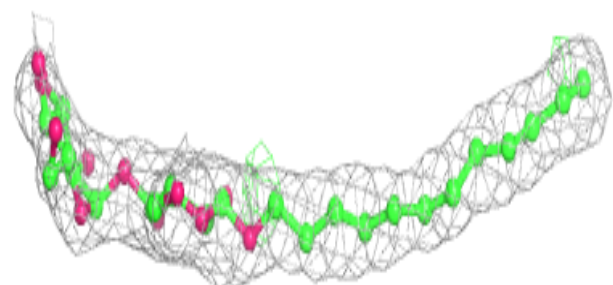
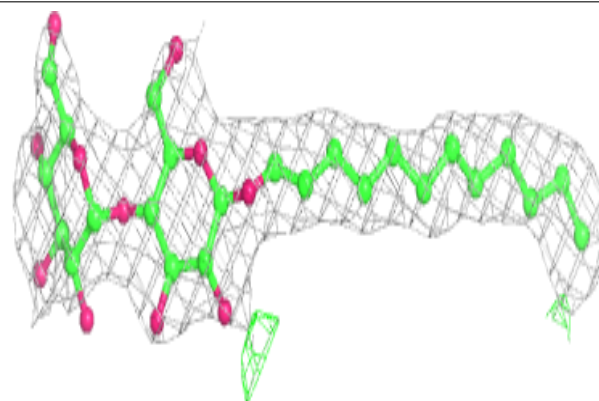


**Electron density around UNL I 101:**

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

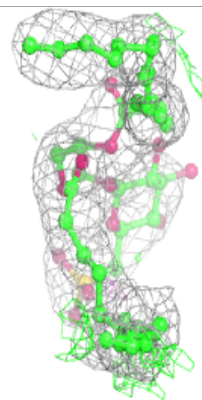
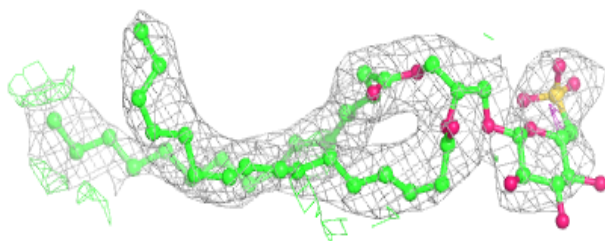
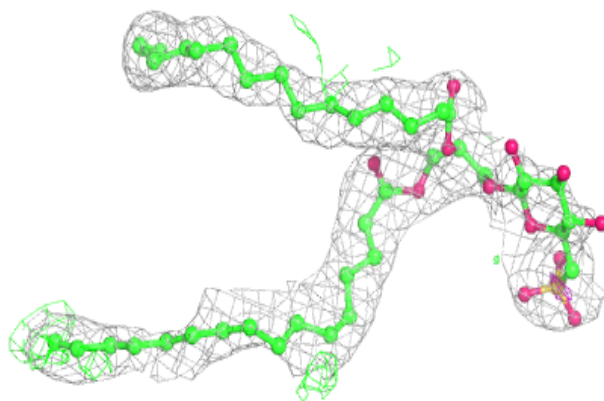
**Electron density around LMT M 102:**

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

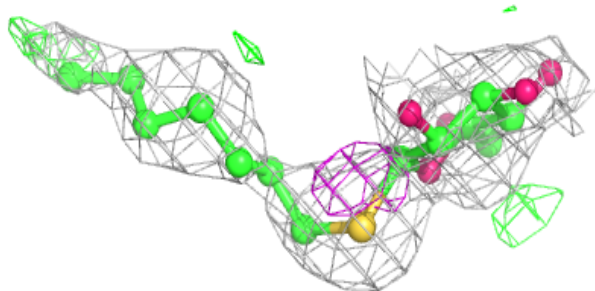
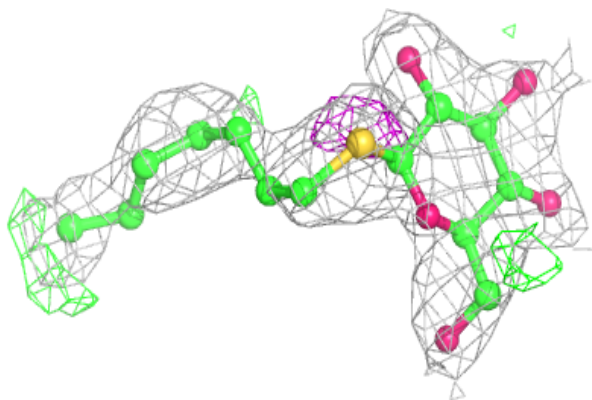


**Electron density around SQD A 413:**

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

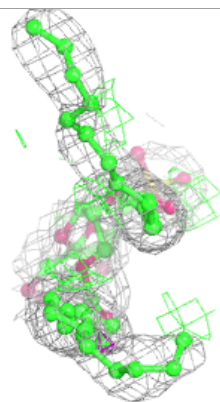
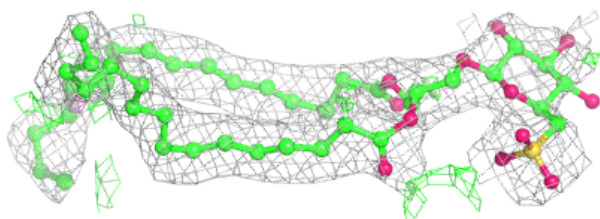
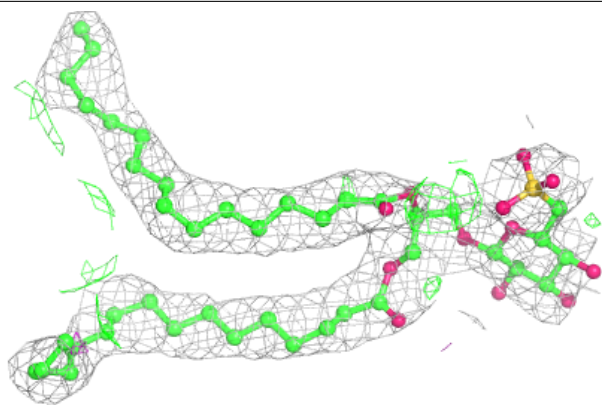
**Electron density around HTG b 631:**

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

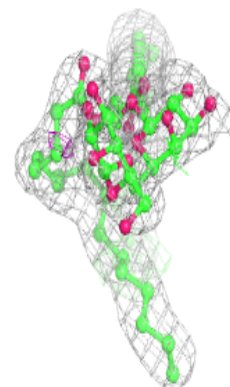
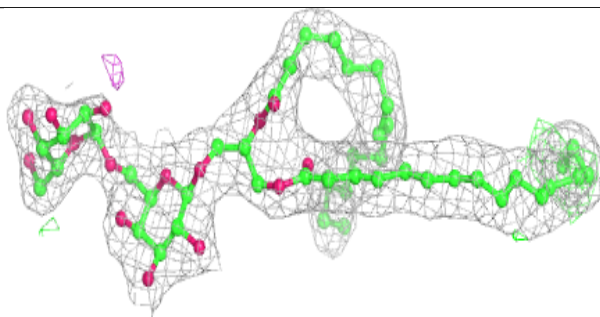
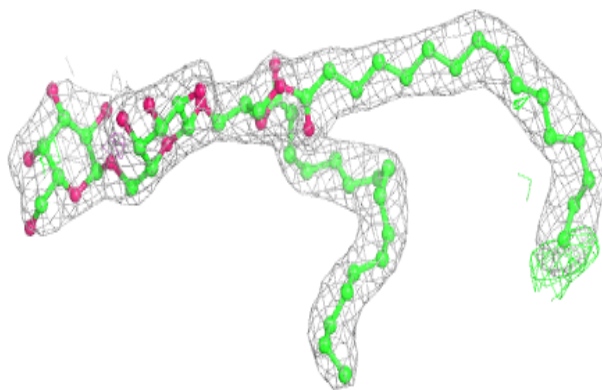


**Electron density around SQD B 621:**

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

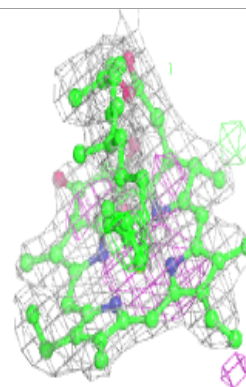
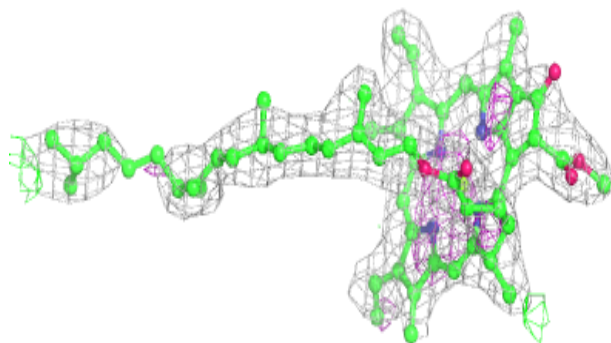
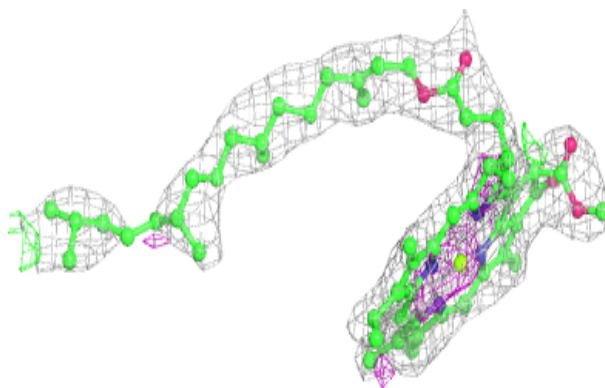
**Electron density around DGD h 102:**

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



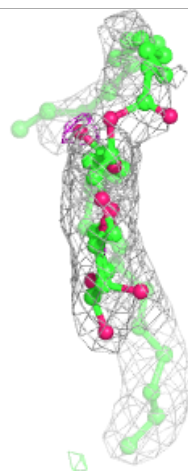
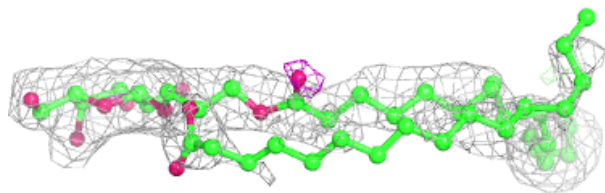
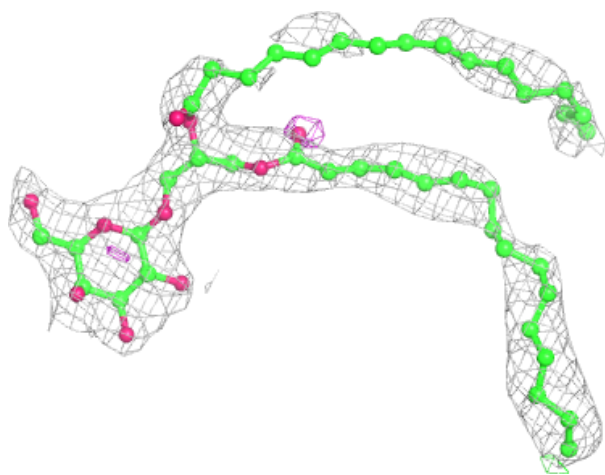
**Electron density around CLA C 505:**

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



**Electron density around LMG k 101:**

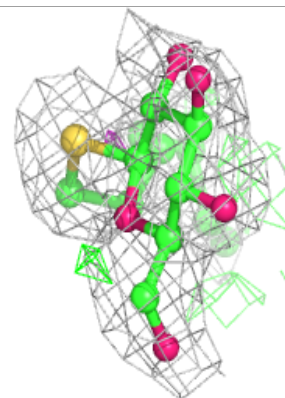
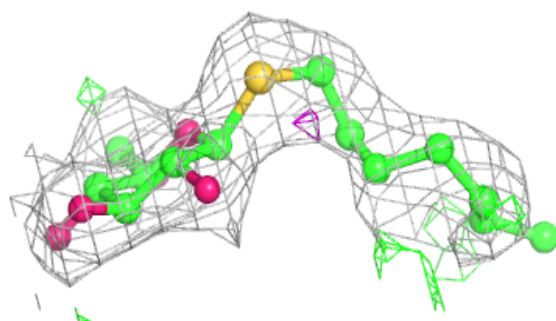
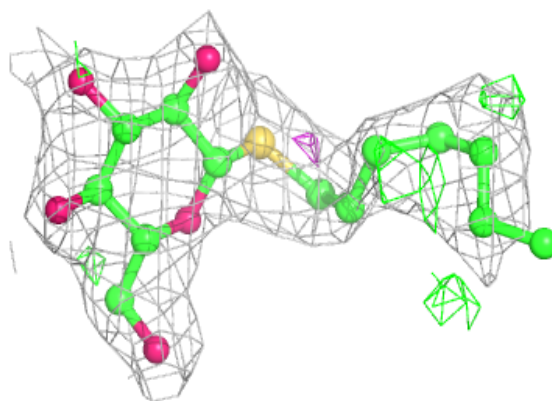
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



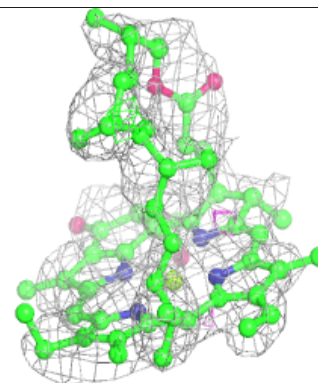
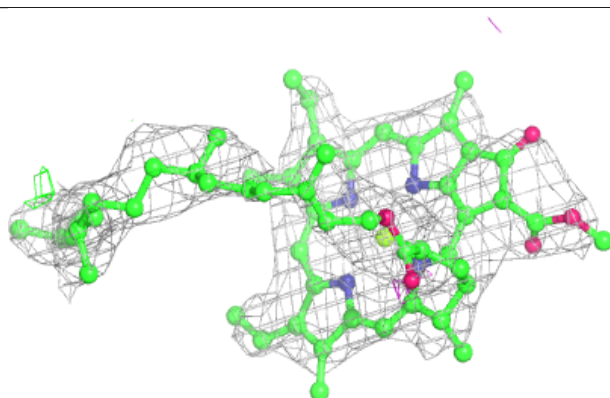
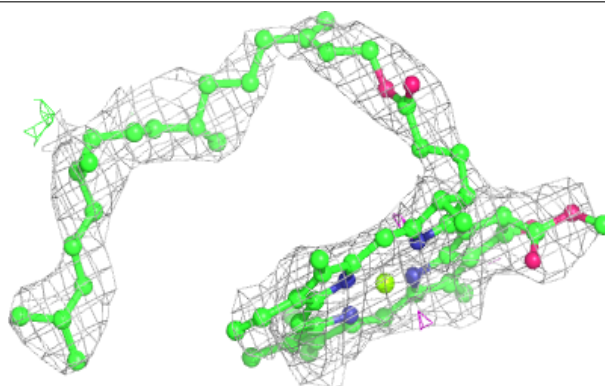


**Electron density around HTG B 623:**

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

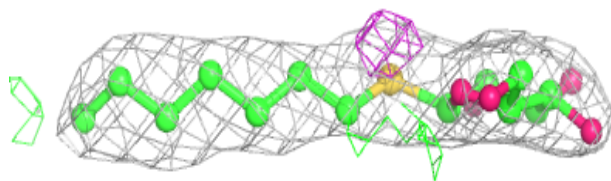
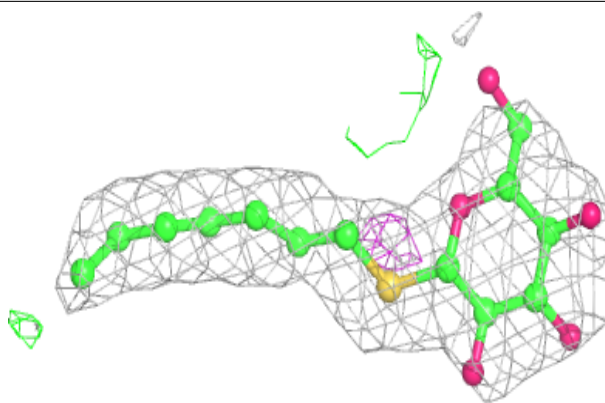
**Electron density around CLA c 517:**

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

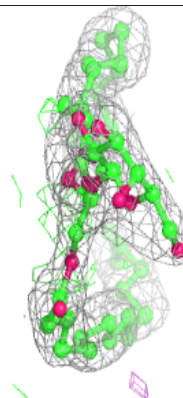
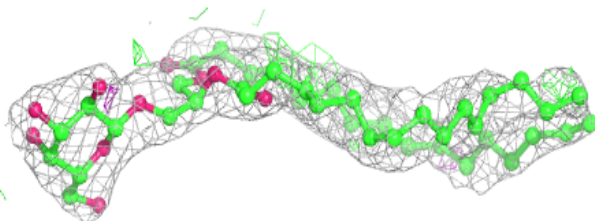
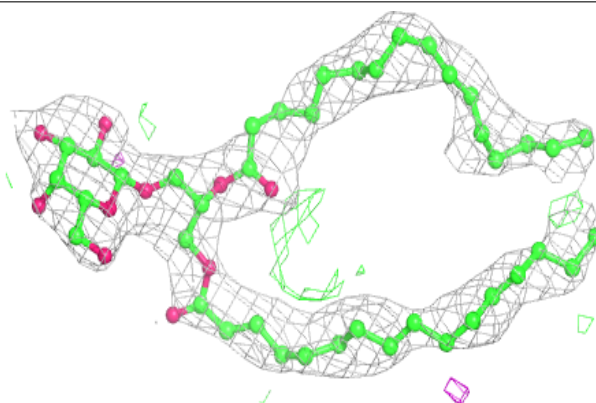


**Electron density around HTG b 607:**

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

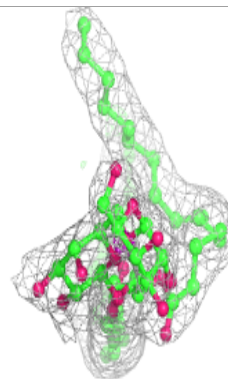
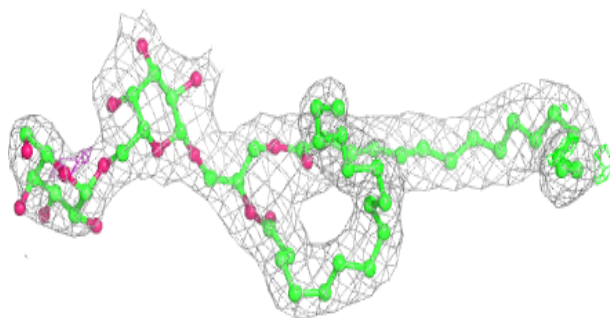
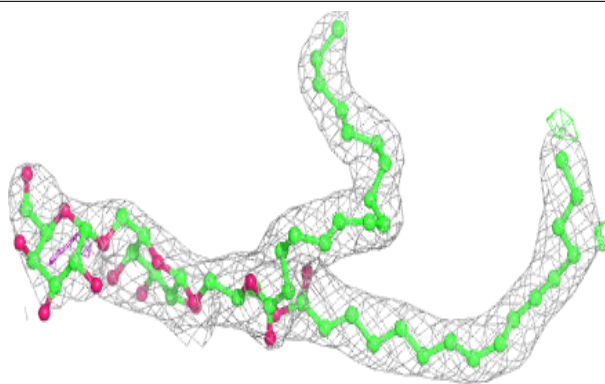
**Electron density around LMG C 501:**

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

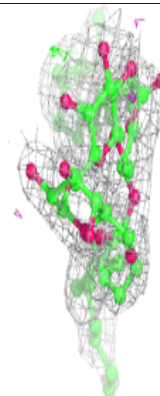
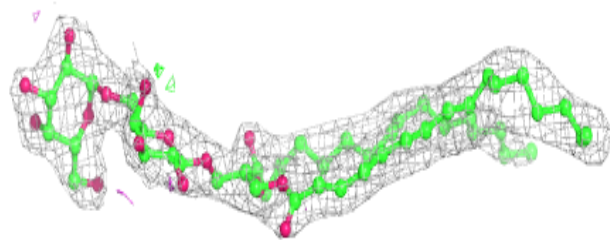
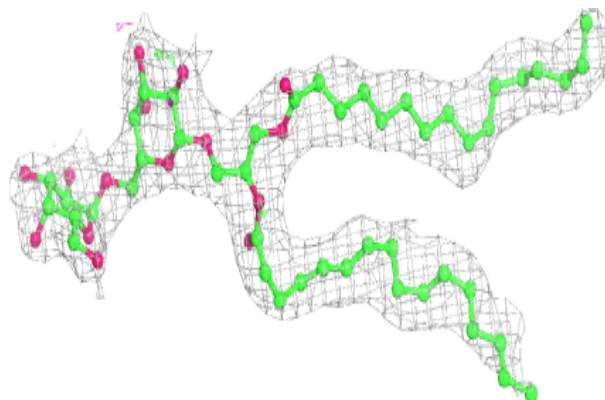


**Electron density around DGD H 102:**

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

**Electron density around DGD C 518:**

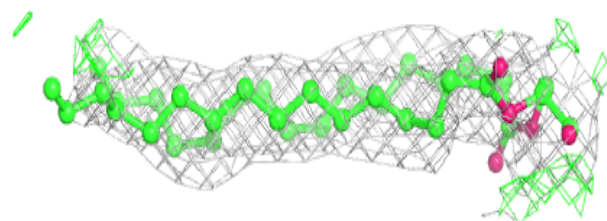
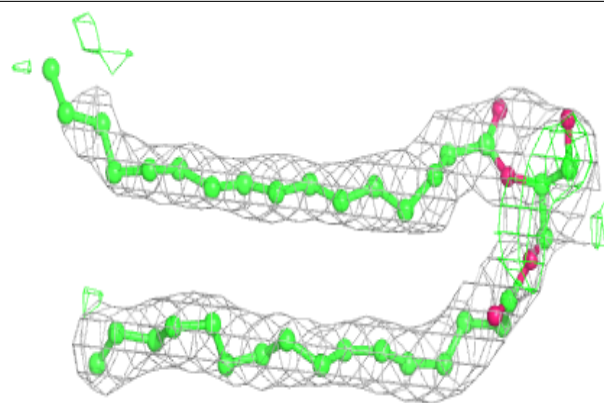
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



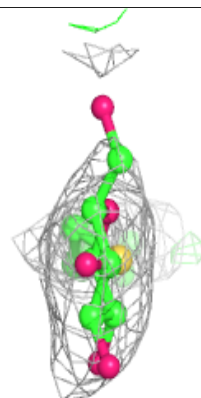
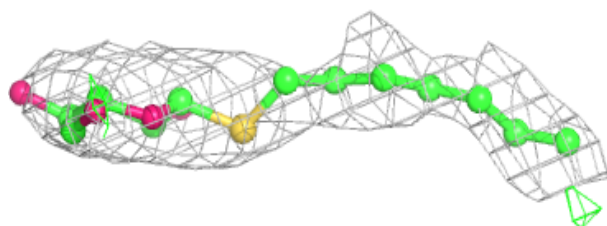
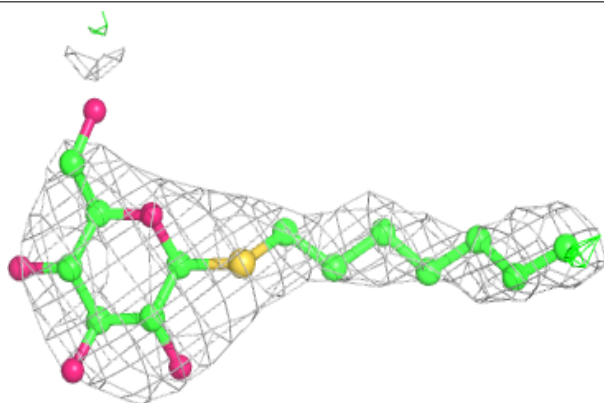


**Electron density around UNL D 414:**

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

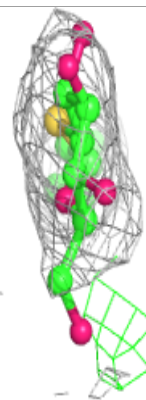
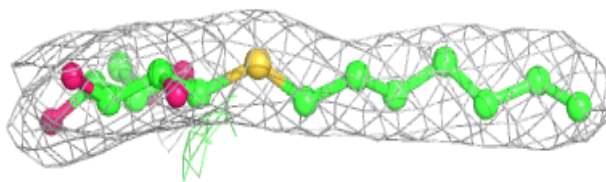
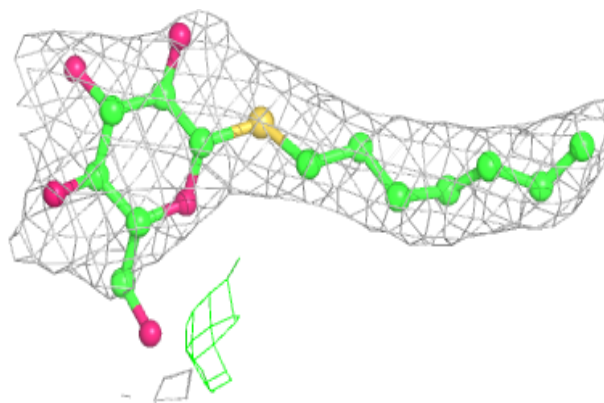
**Electron density around HTG c 523:**

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



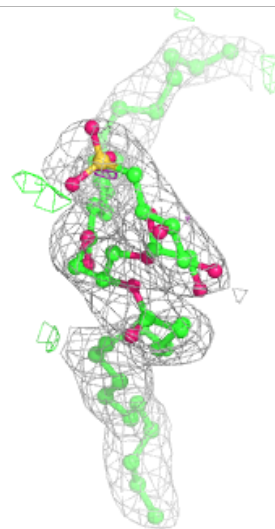
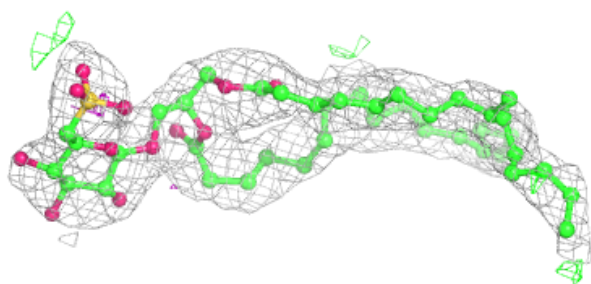
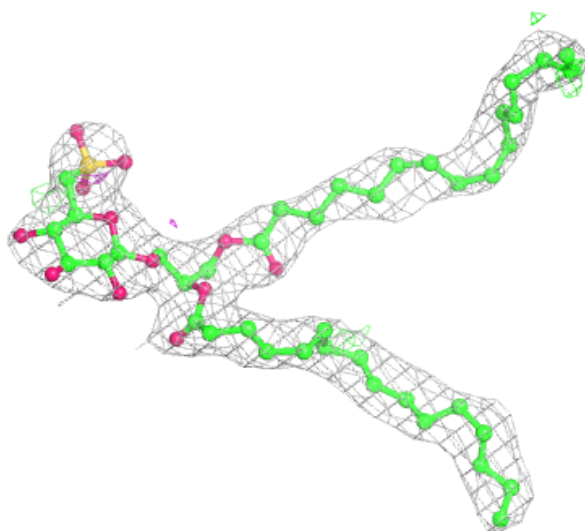
**Electron density around HTG B 631:**

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



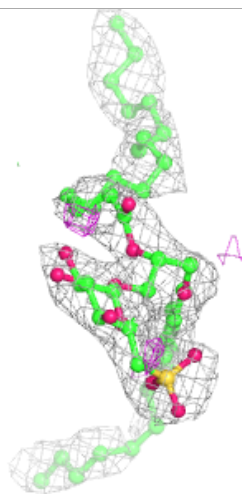
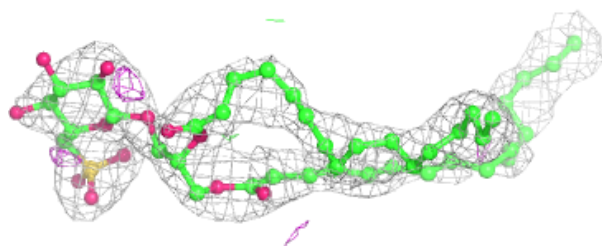
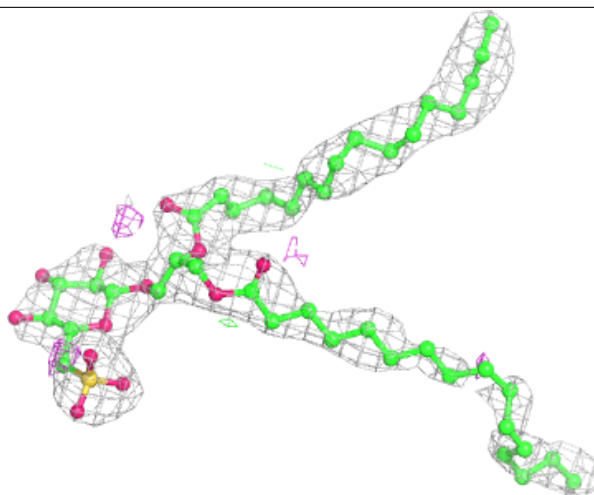
**Electron density around SQD a 413:**

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



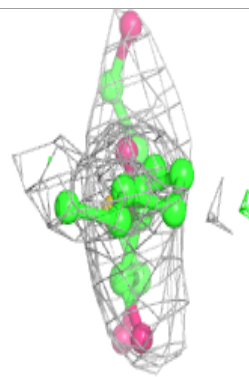
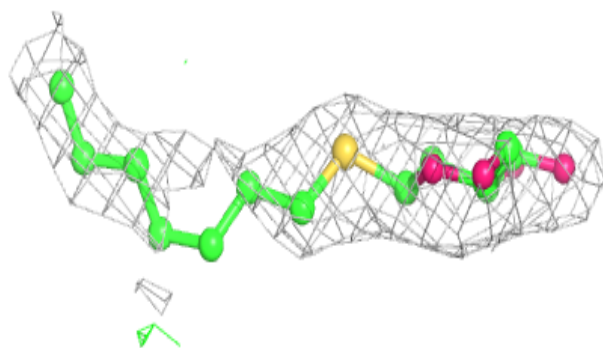
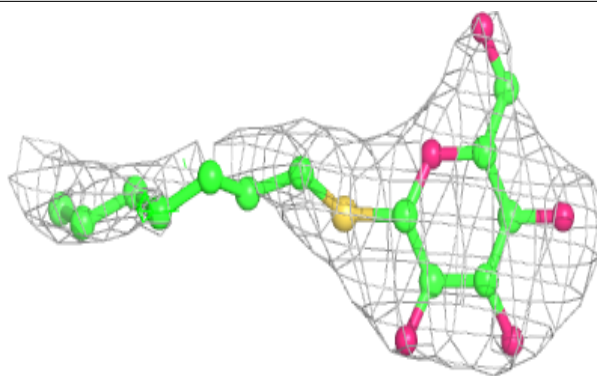
**Electron density around SQD A 410:**

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

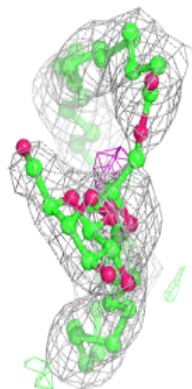
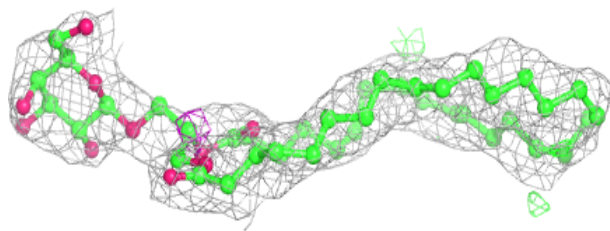
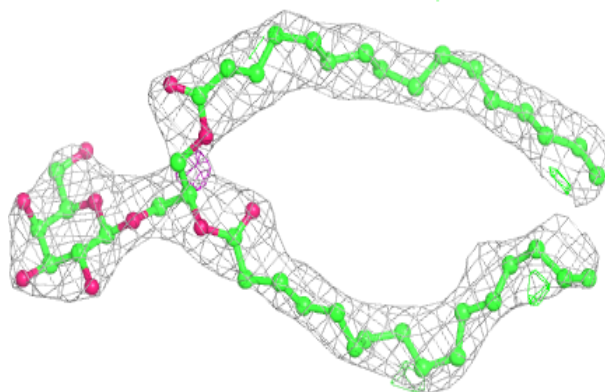


**Electron density around HTG C 522:**

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

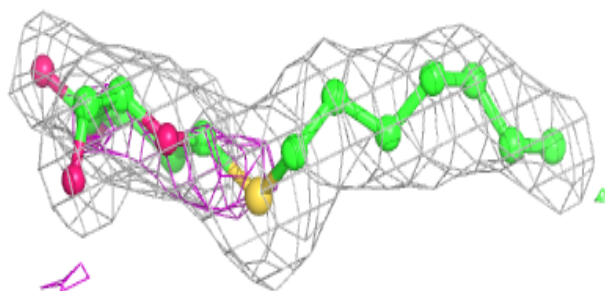
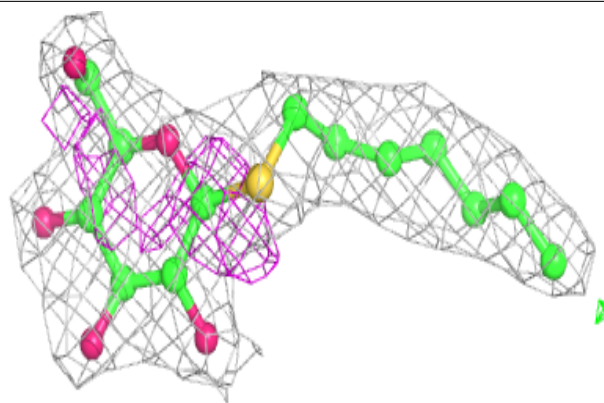
**Electron density around LMG a 414:**

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

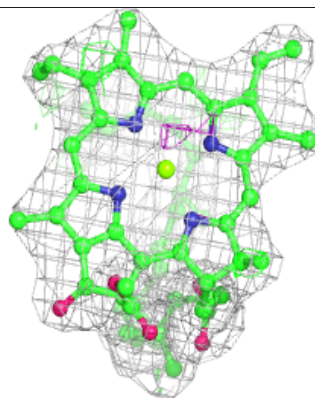
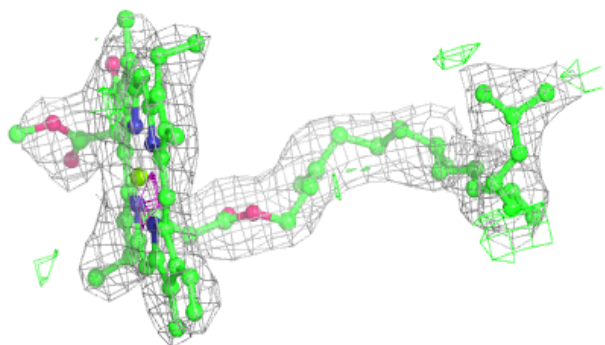
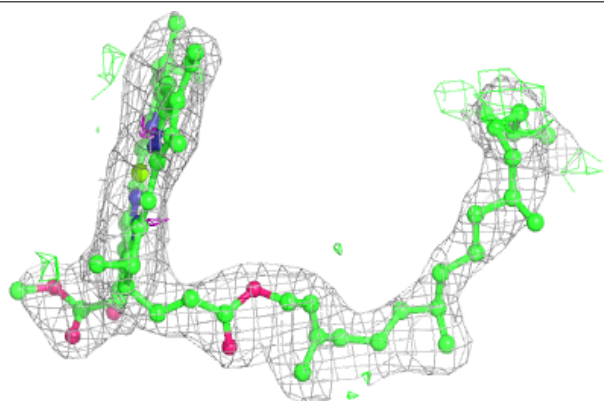


**Electron density around HTG b 602:**

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

**Electron density around CLA c 510:**

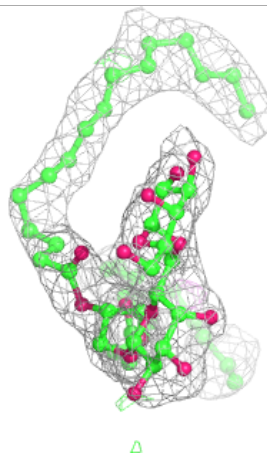
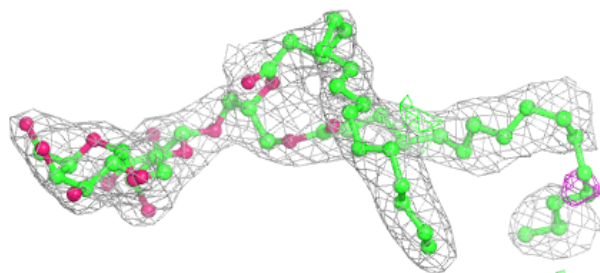
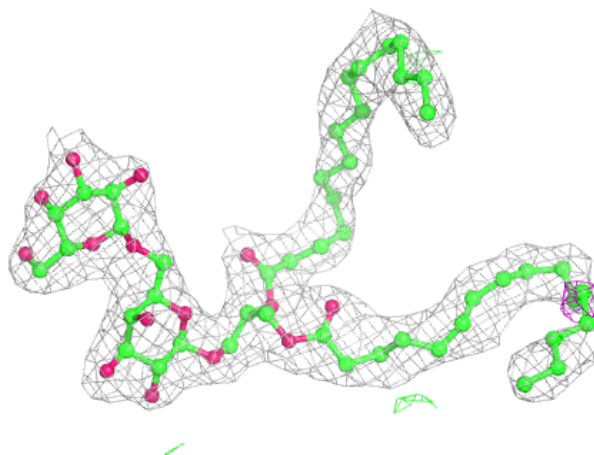
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



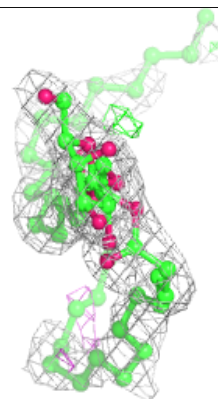
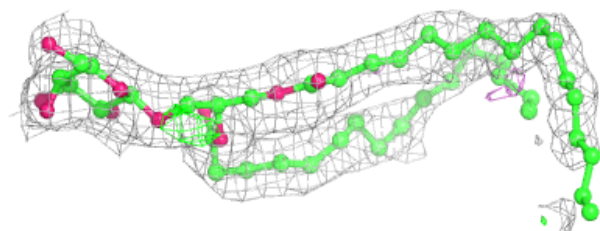
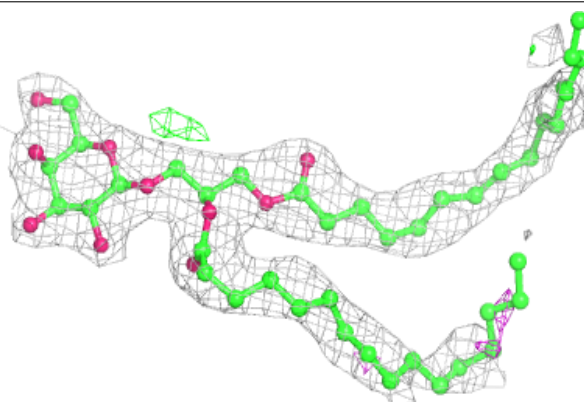


**Electron density around DGD c 520:**

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

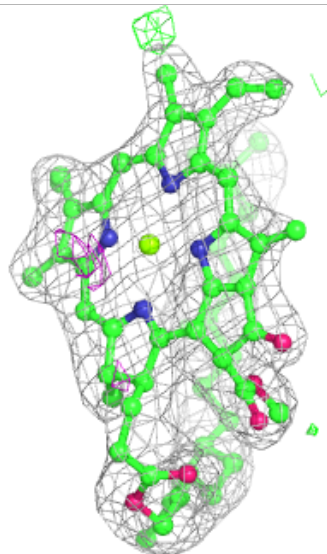
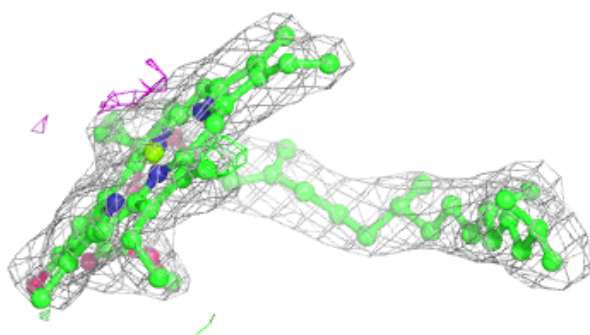
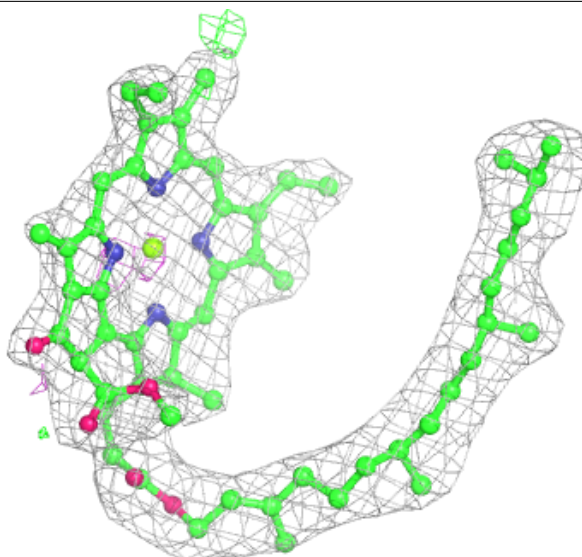
**Electron density around LMG D 416:**

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



**Electron density around CLA c 511:**

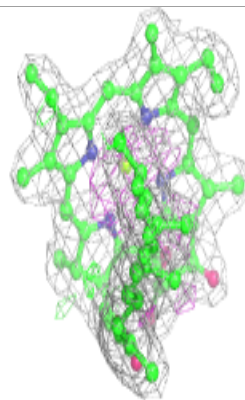
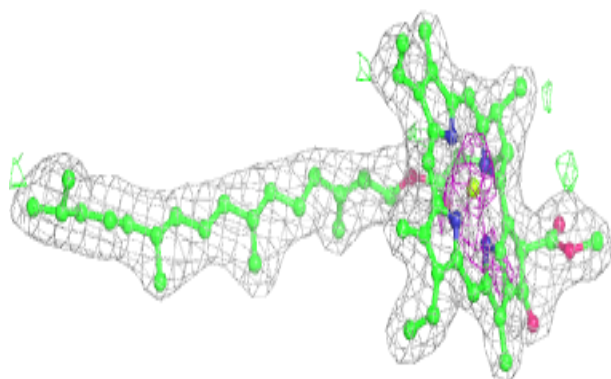
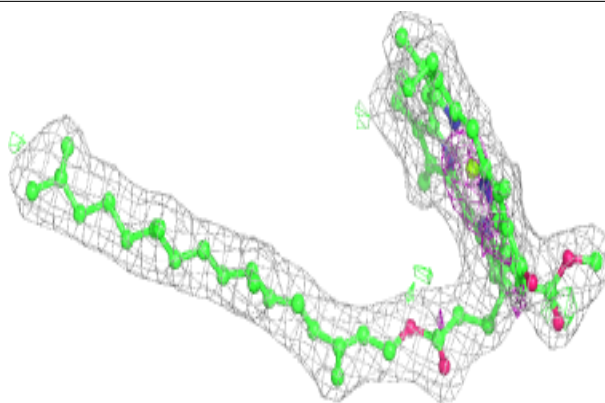
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



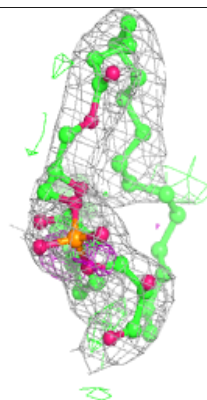
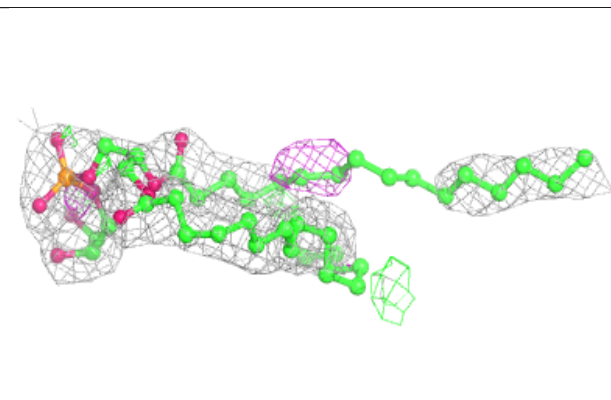
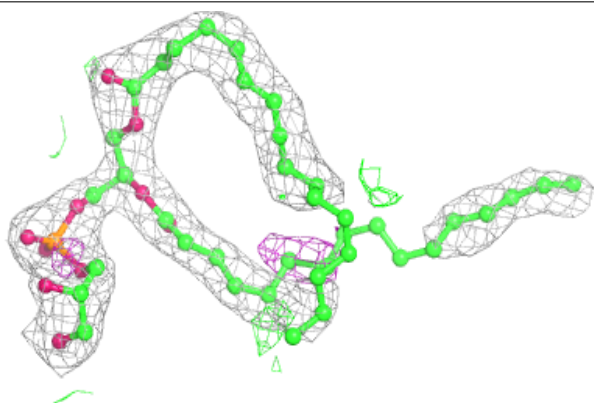


**Electron density around CLA b 616:**

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

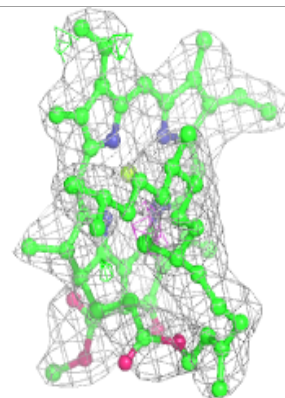
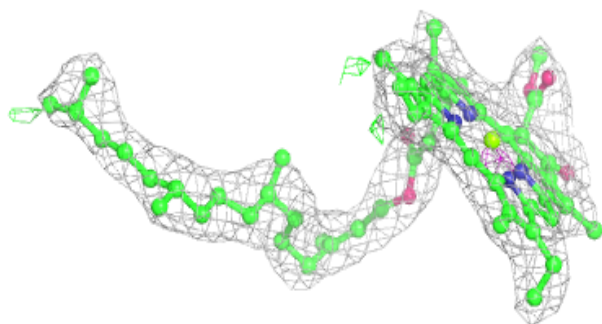
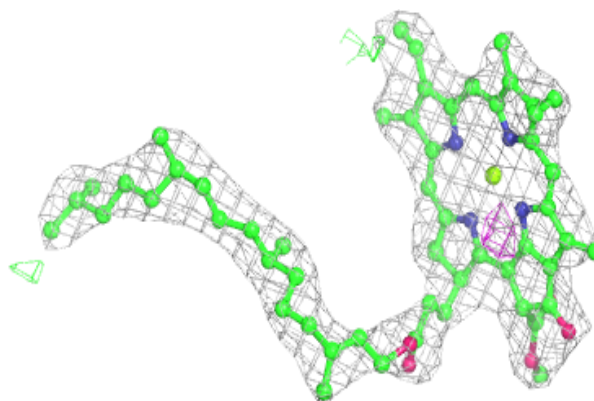
**Electron density around LHG D 412:**

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

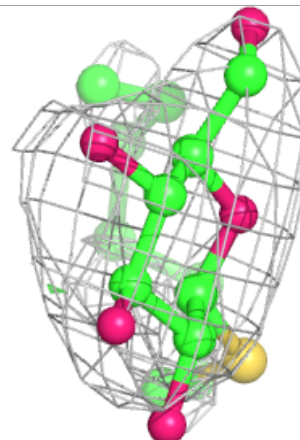
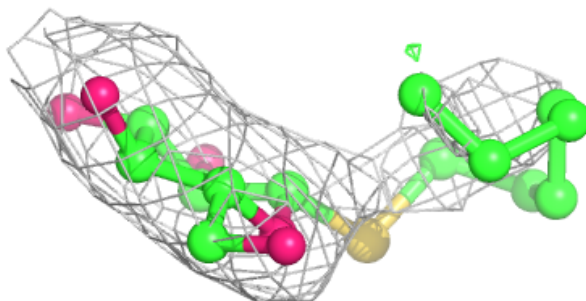
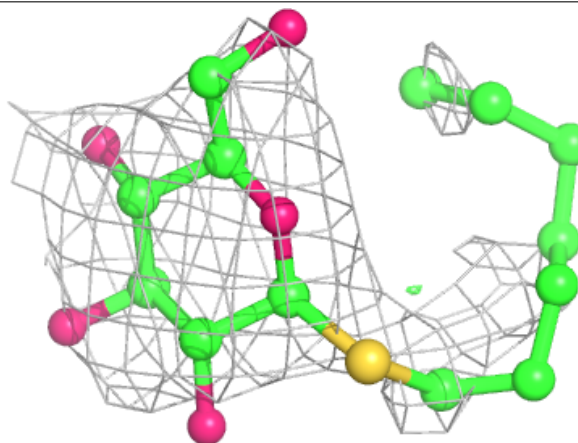


**Electron density around CLA C 512:**

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

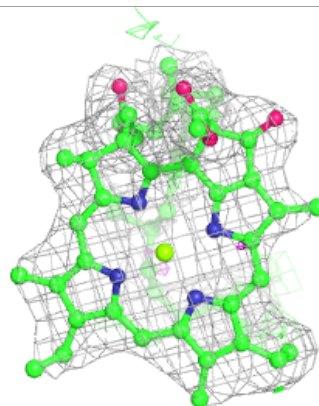
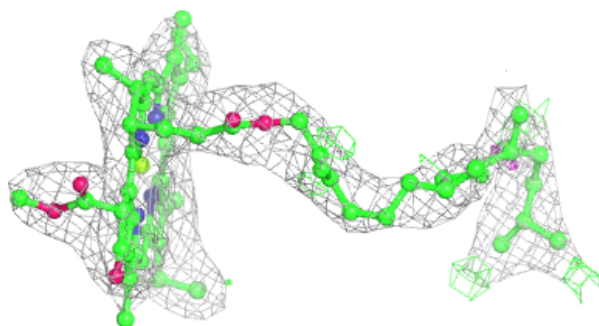
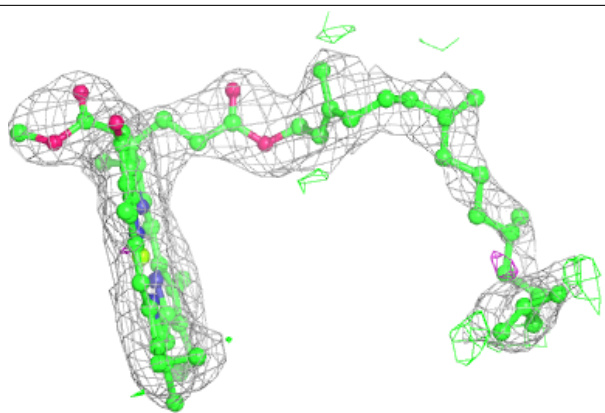
**Electron density around HTG V 206:**

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

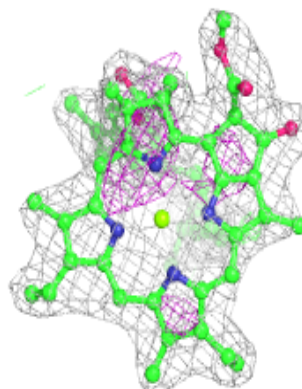
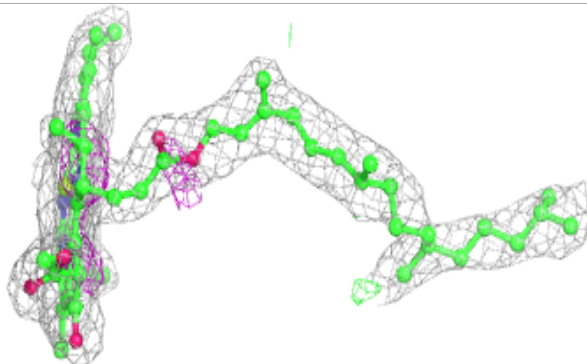
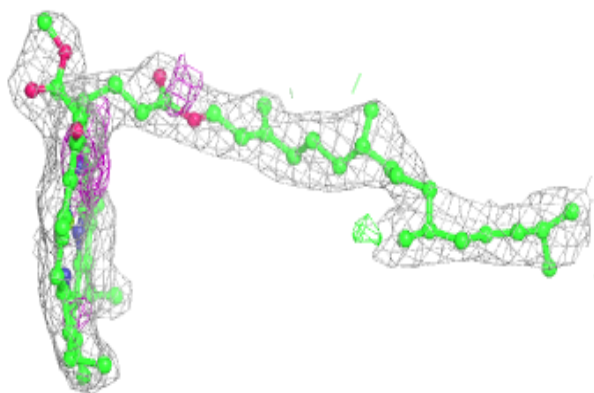


**Electron density around CLA C 507:**

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

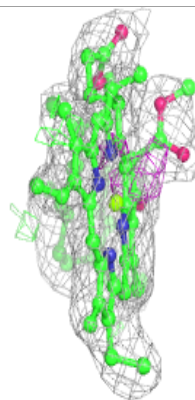
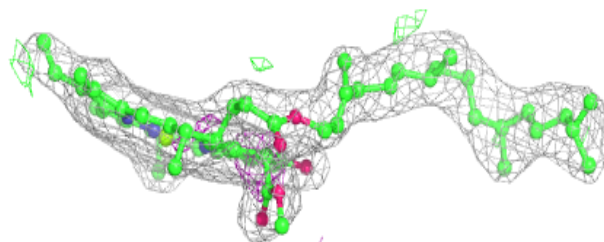
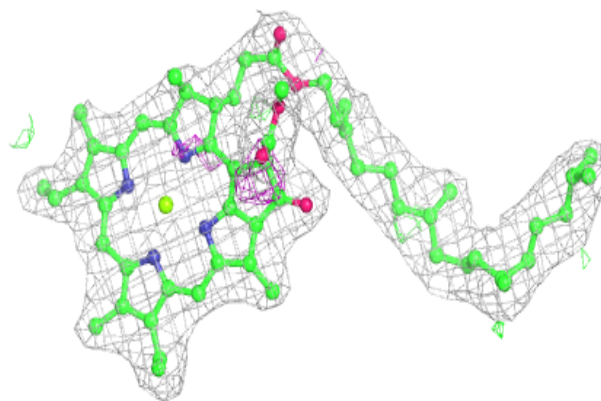
**Electron density around CLA B 607:**

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

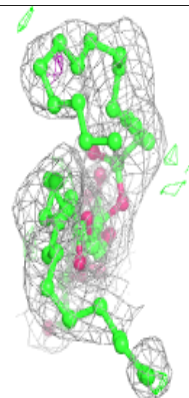
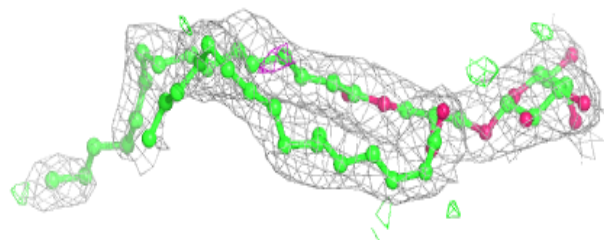
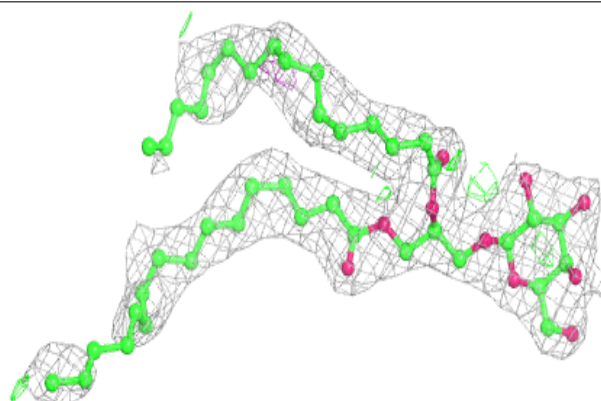


**Electron density around CLA b 611:**

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

**Electron density around LMG d 416:**

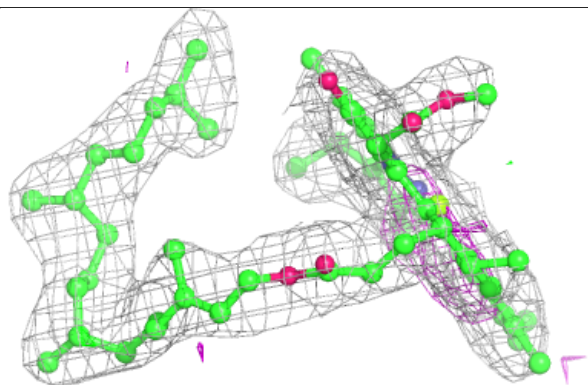
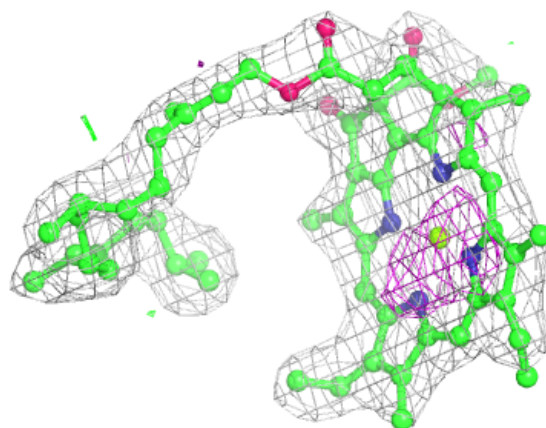
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





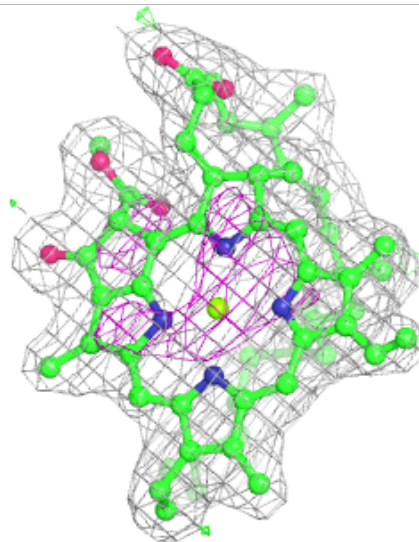
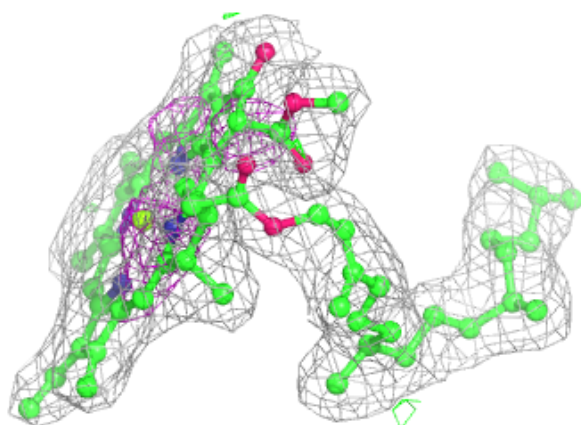
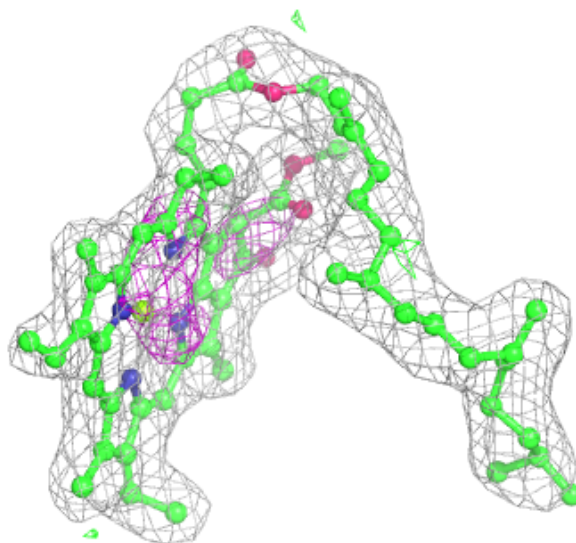
**Electron density around CLA c 507:**

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



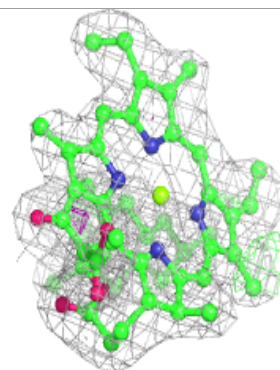
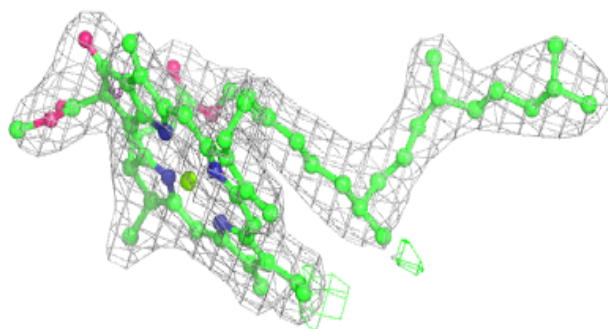
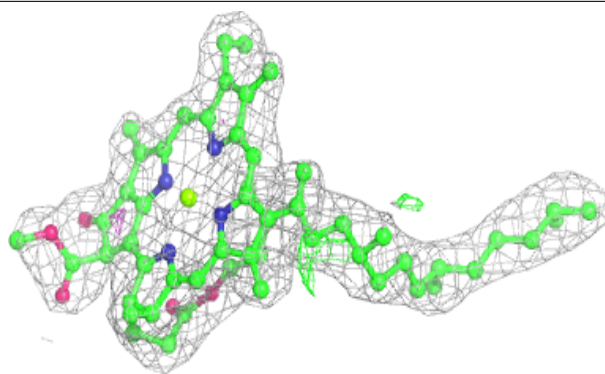
**Electron density around CLA B 614:**

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

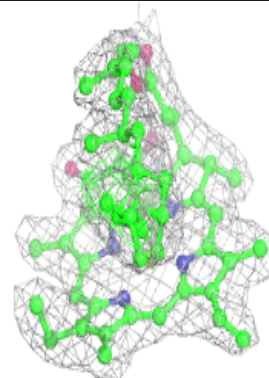
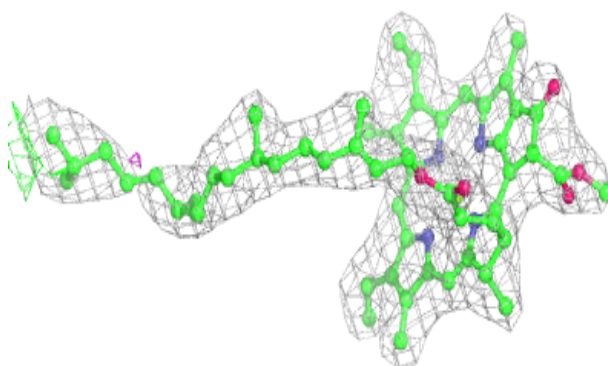
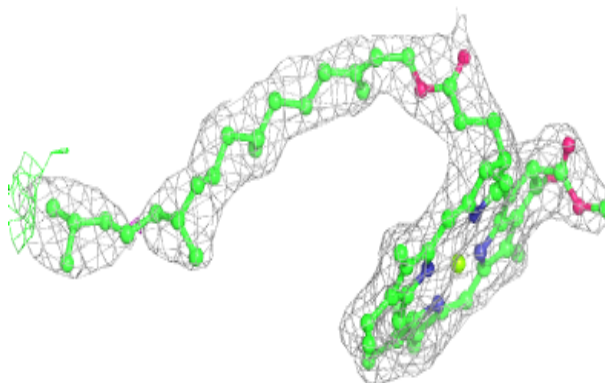


**Electron density around CLA c 509:**

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

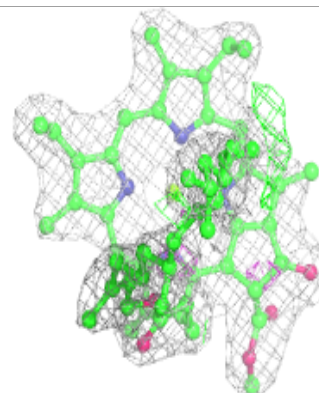
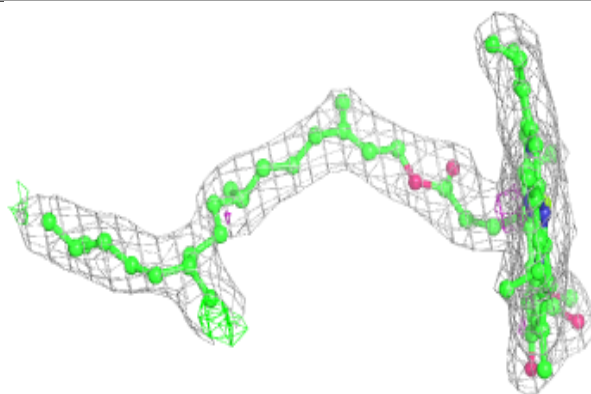
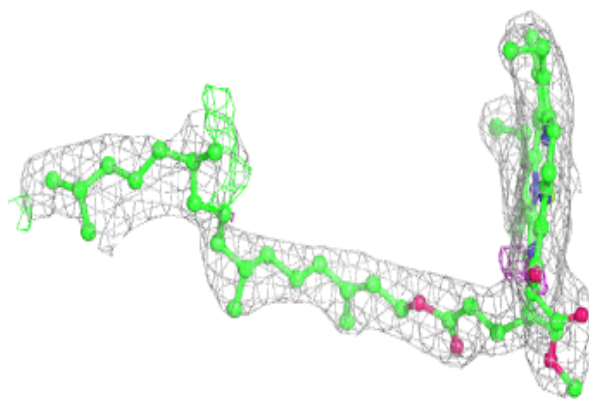
**Electron density around CLA c 508:**

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

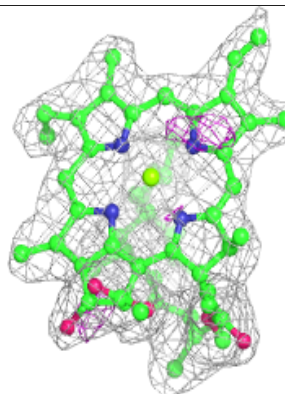
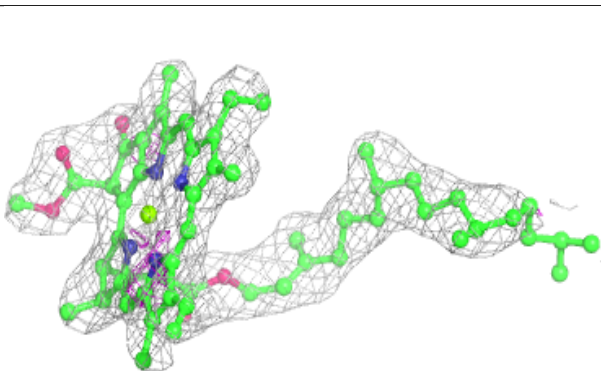
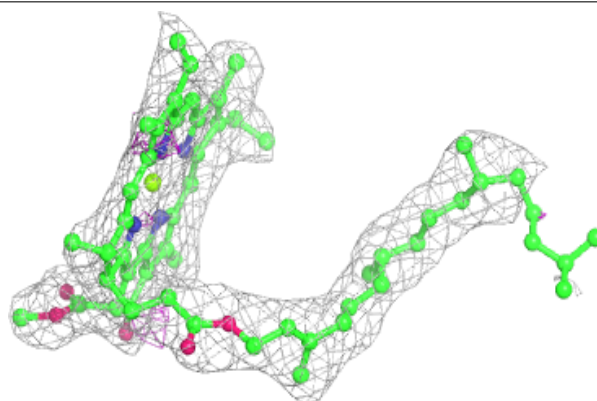


**Electron density around CLA b 615:**

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

**Electron density around CLA c 512:**

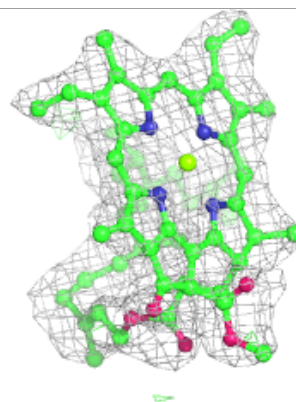
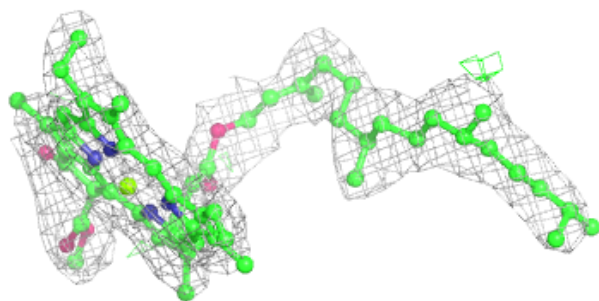
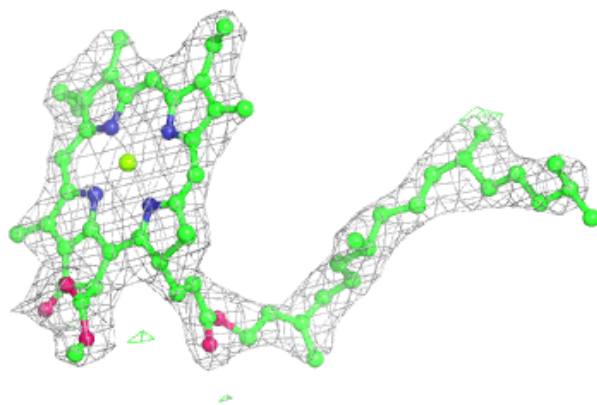
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



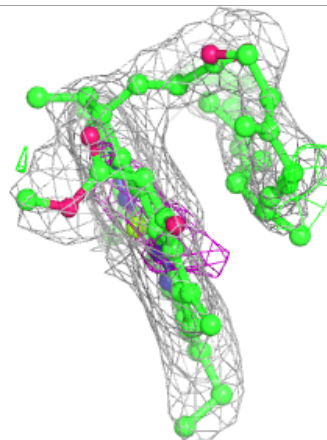
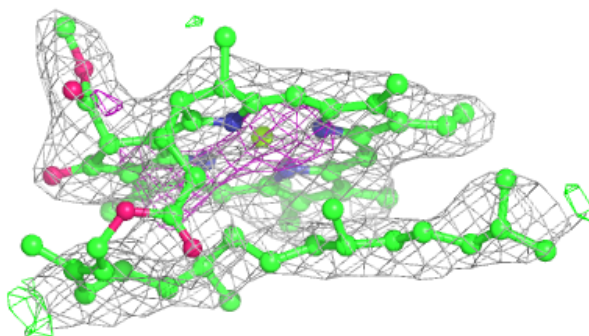
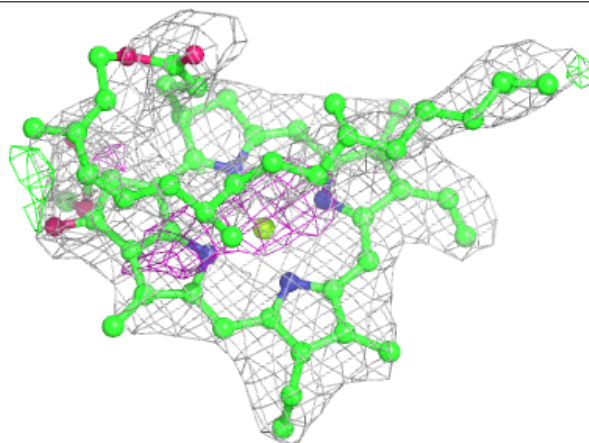


**Electron density around CLA c 515:**

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

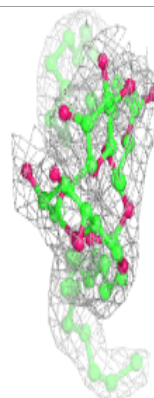
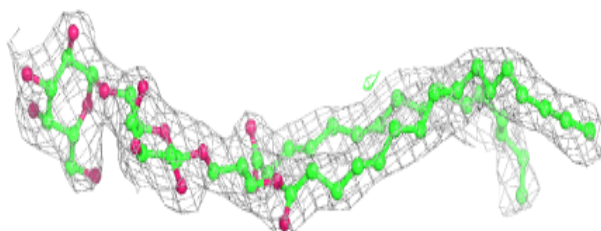
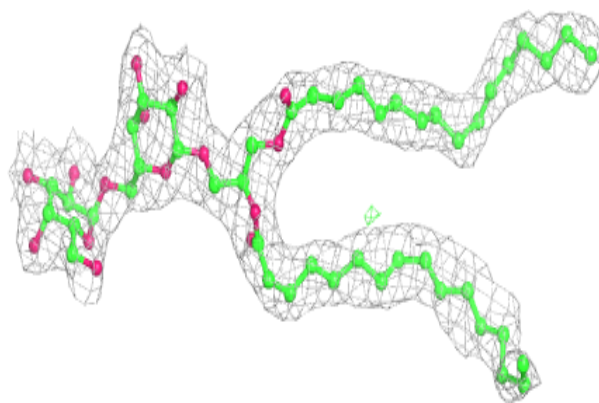
**Electron density around CLA b 610:**

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

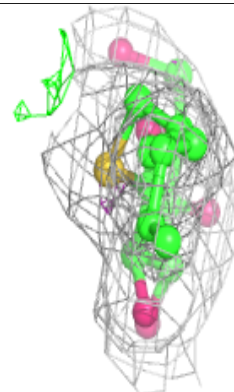
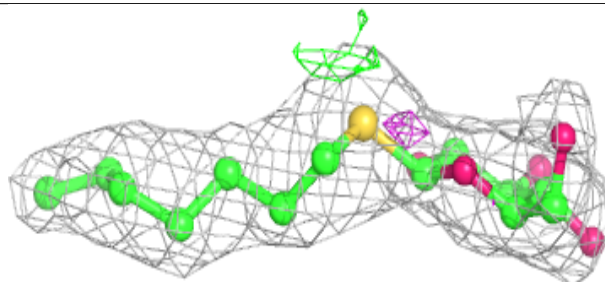
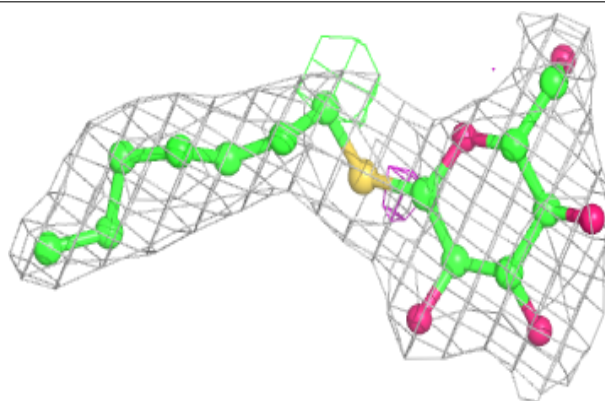


**Electron density around DGD c 521:**

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

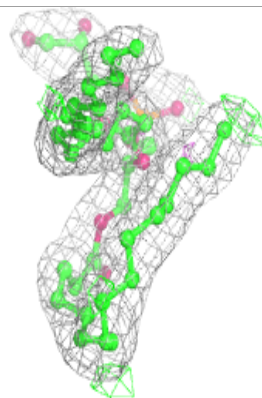
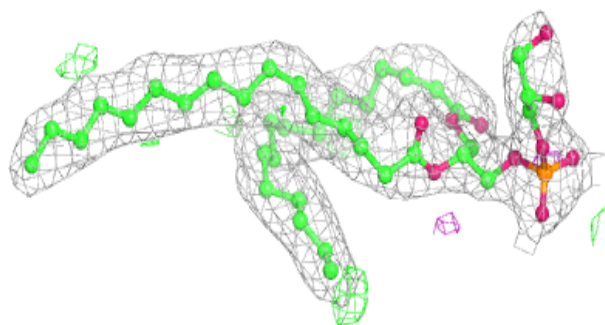
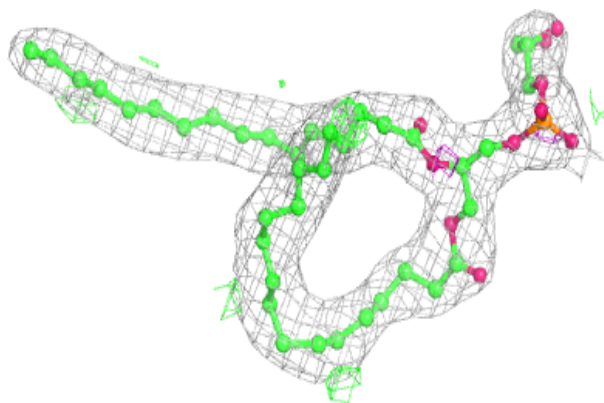
**Electron density around HTG B 622:**

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

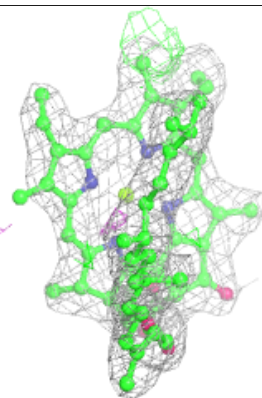
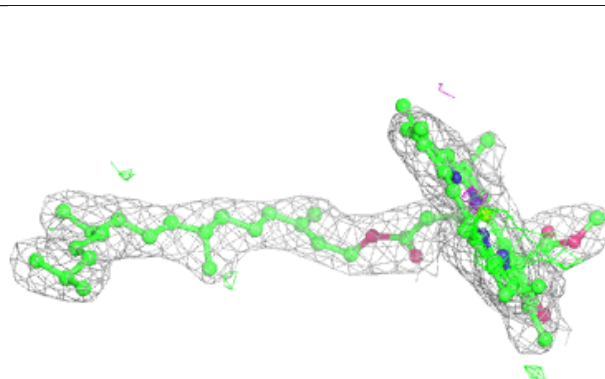
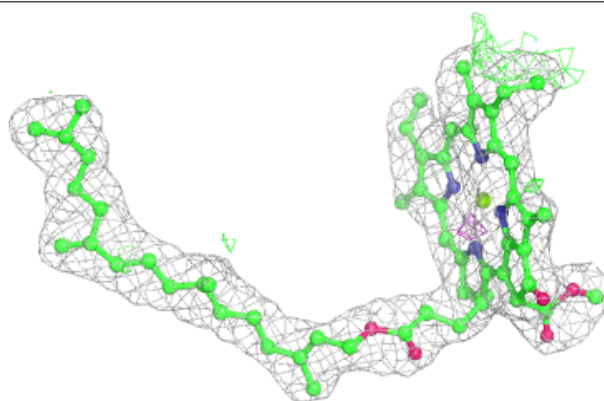


**Electron density around LHG D 410:**

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

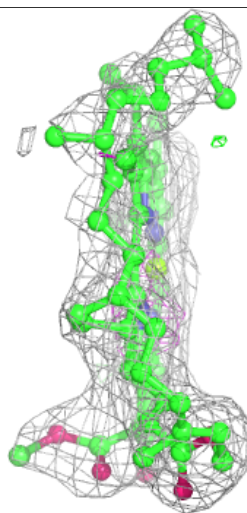
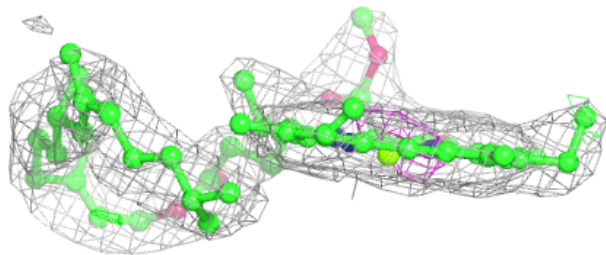
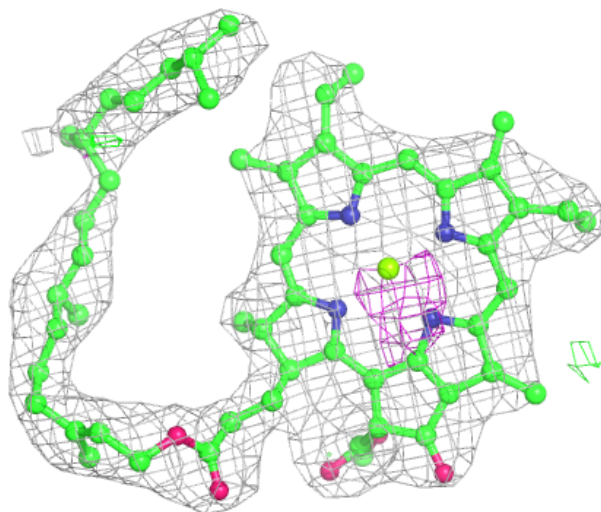
**Electron density around CLA b 618:**

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



**Electron density around CLA C 513:**

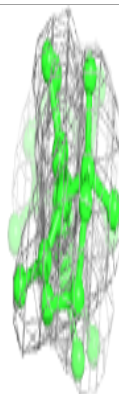
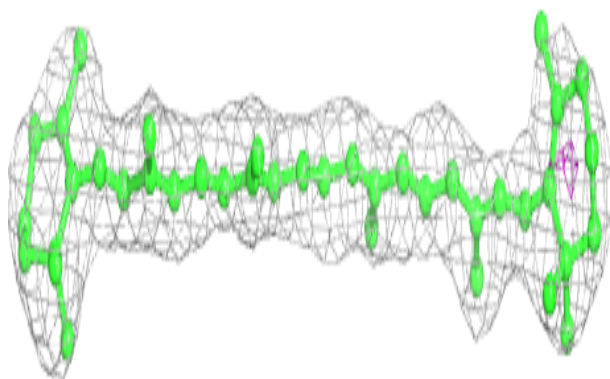
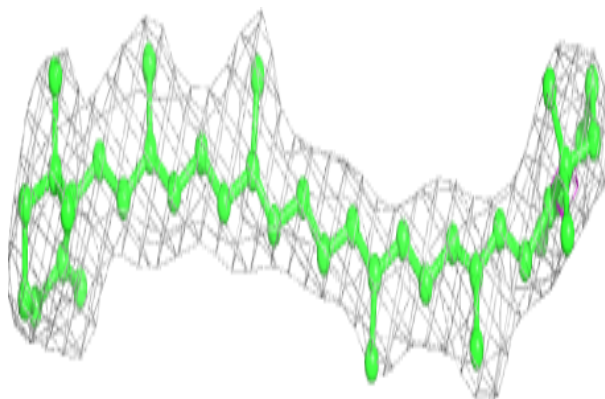
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



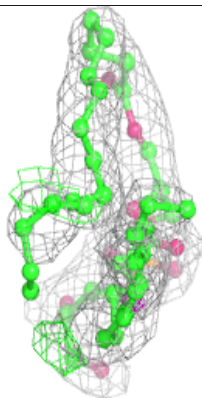
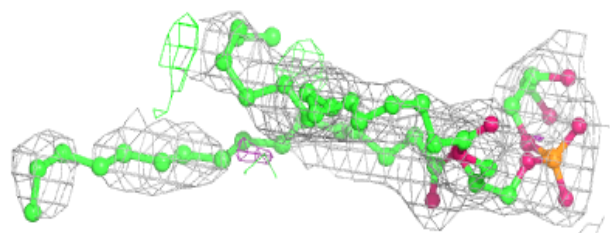
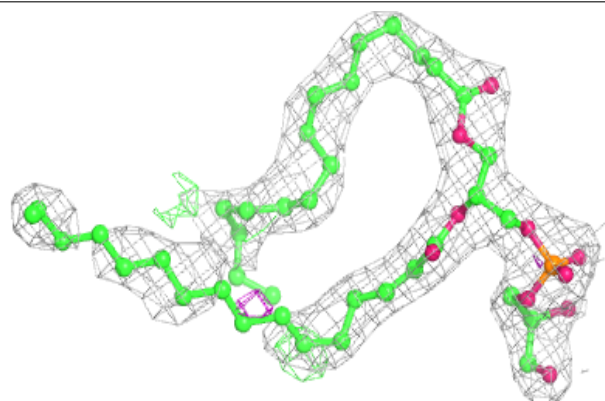


**Electron density around BCR K 101:**

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

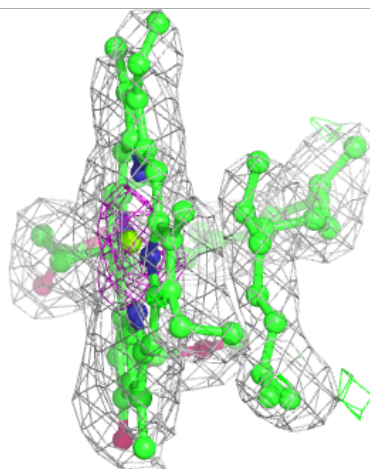
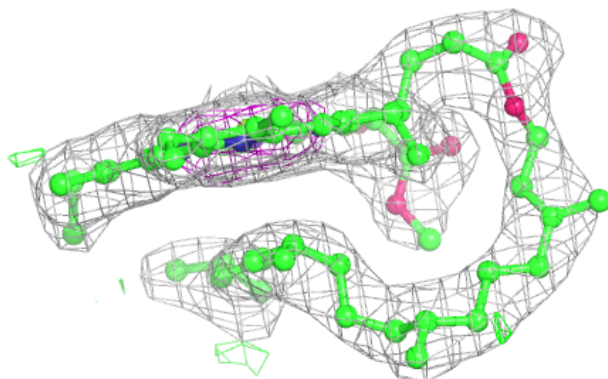
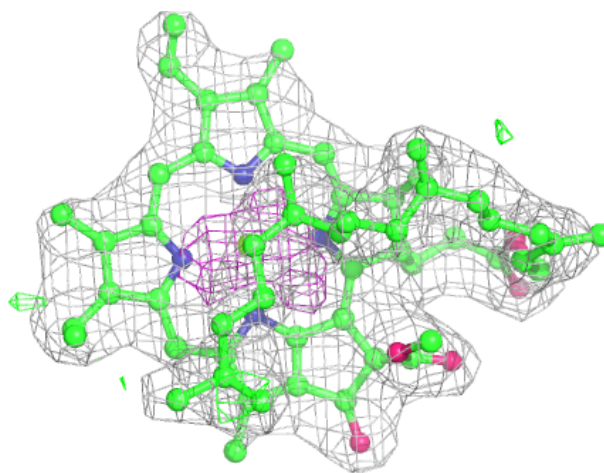
**Electron density around LHG d 411:**

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



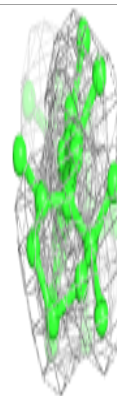
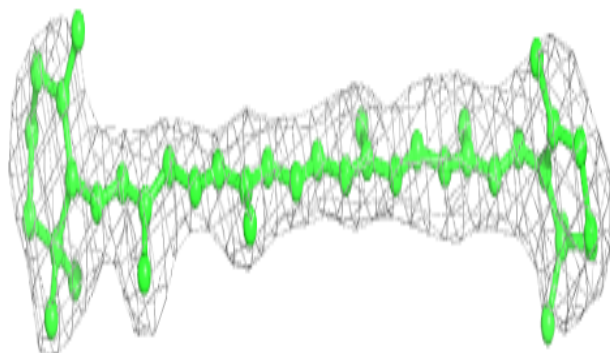
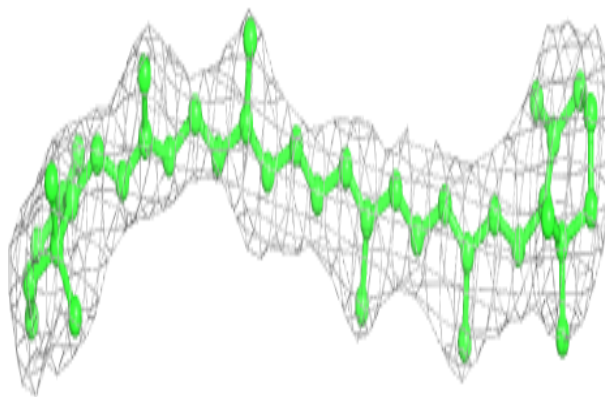
**Electron density around CLA C 511:**

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

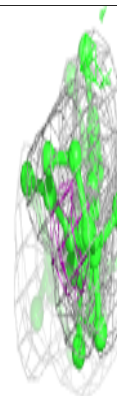
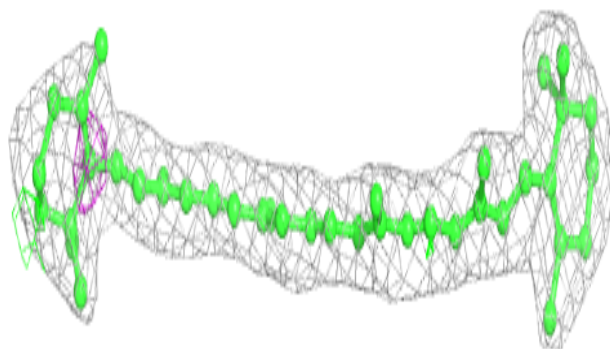
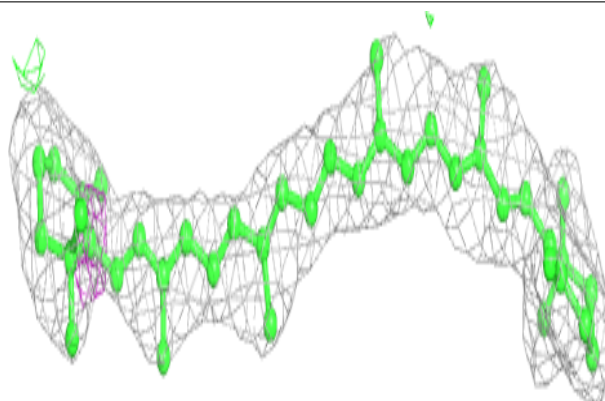


**Electron density around BCR c 526:**

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

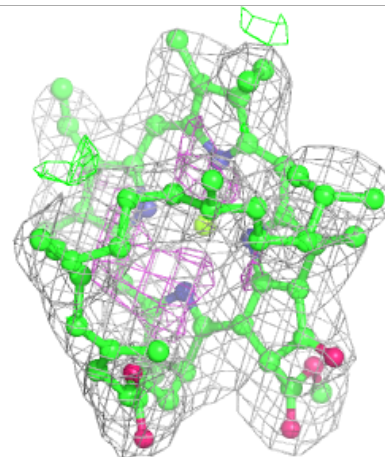
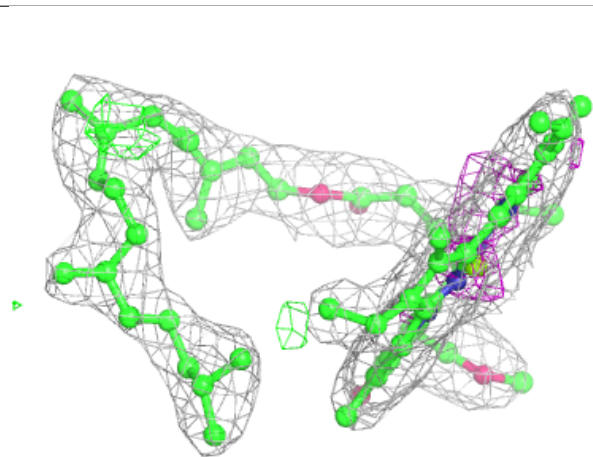
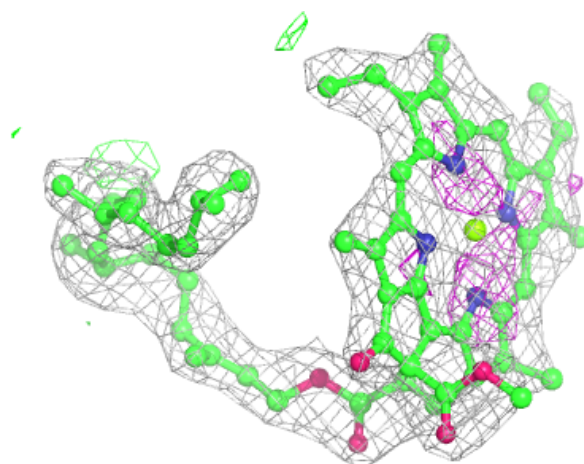
**Electron density around BCR H 101:**

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



**Electron density around CLA C 504:**

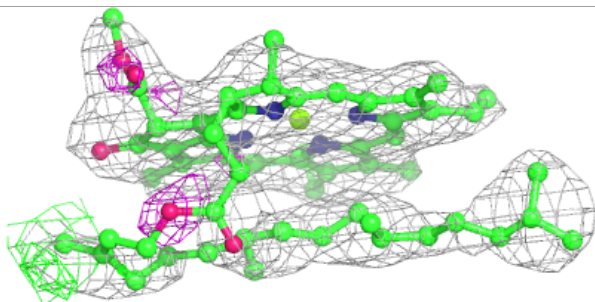
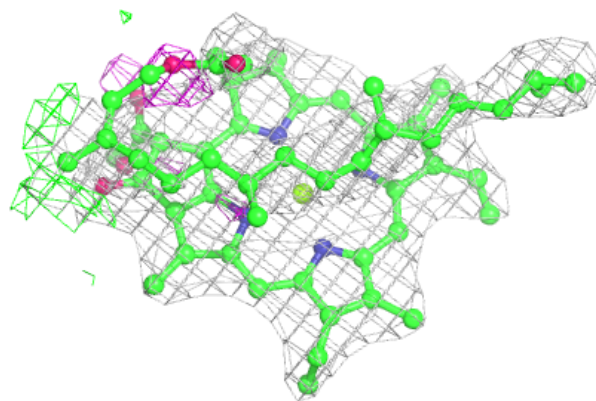
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



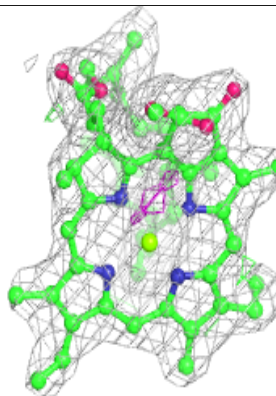
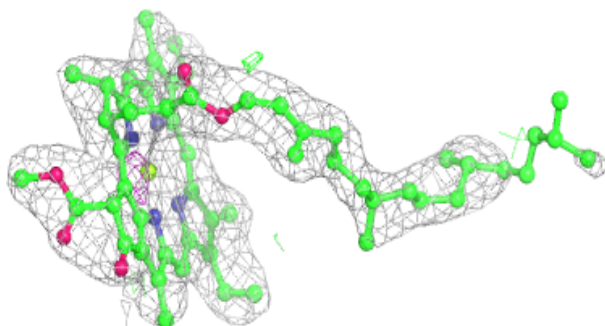
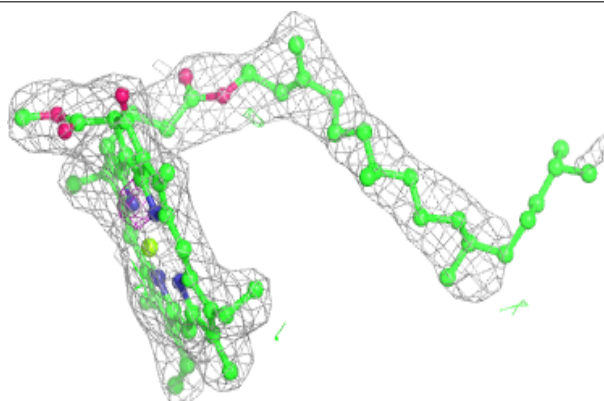


**Electron density around CLA B 602:**

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

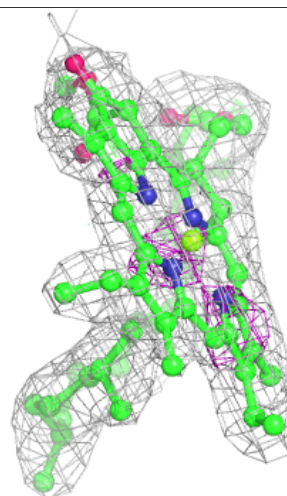
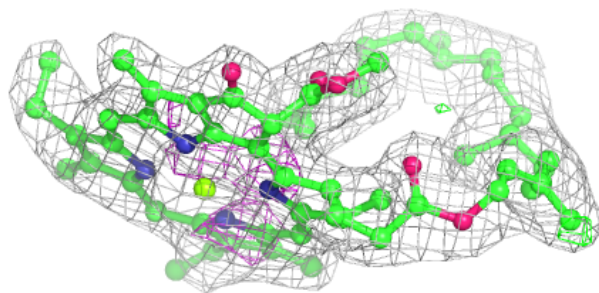
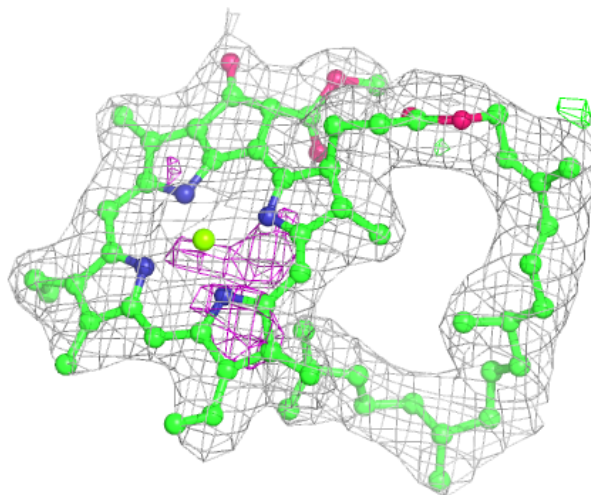
**Electron density around CLA C 509:**

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



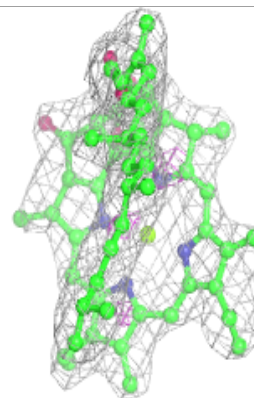
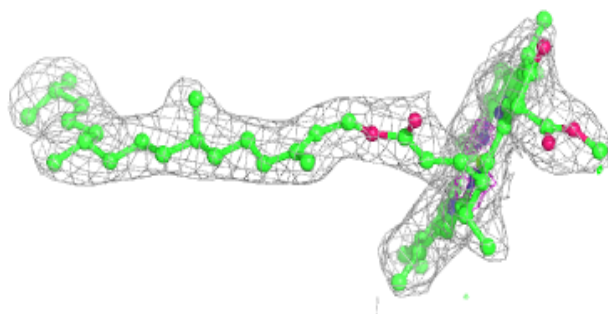
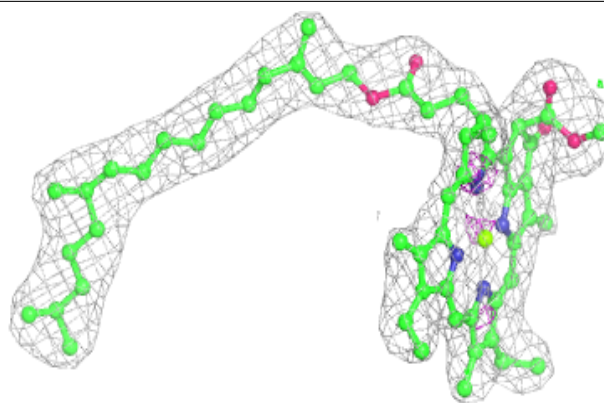
**Electron density around CLA b 624:**

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

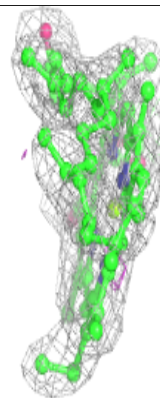
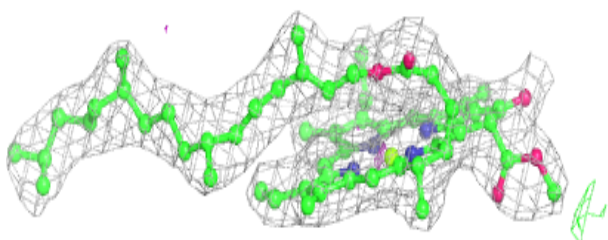
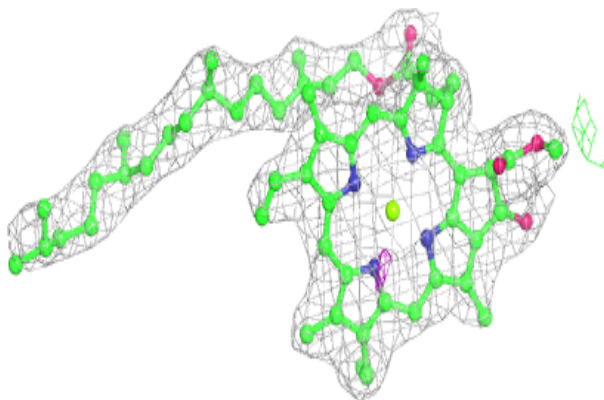


**Electron density around CLA B 610:**

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

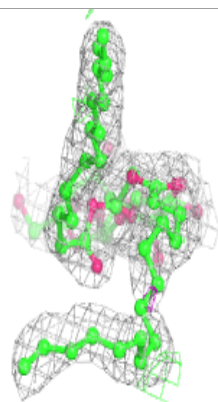
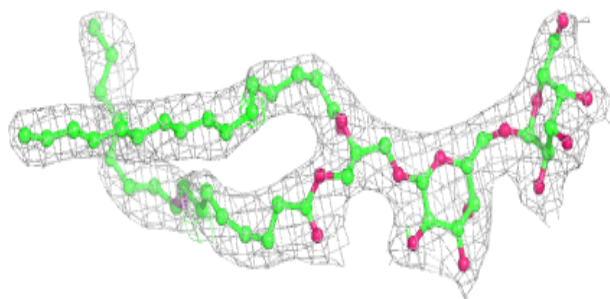
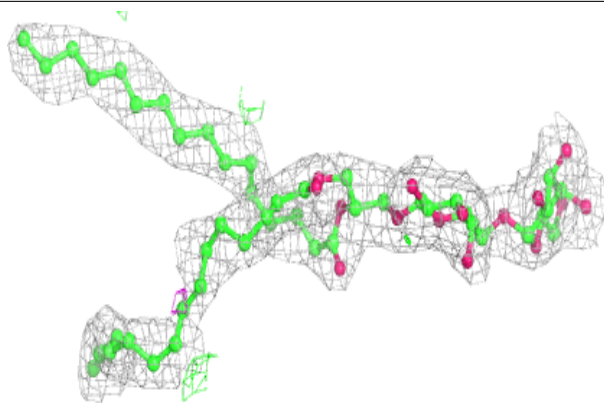
**Electron density around CLA C 502:**

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

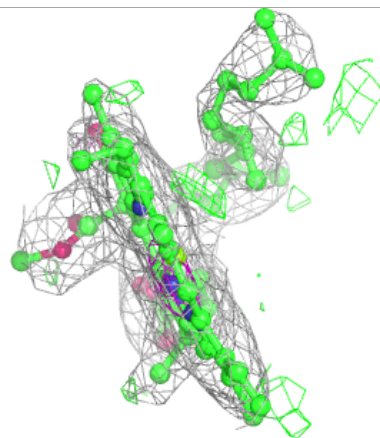
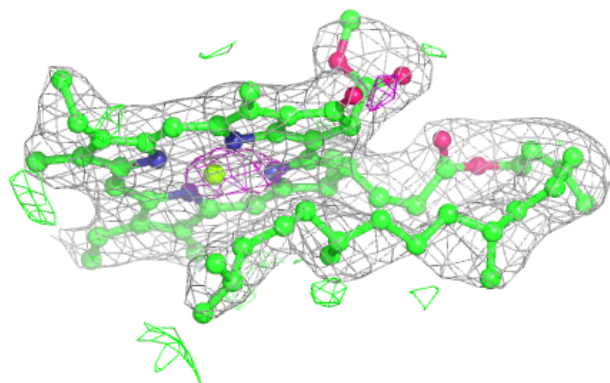
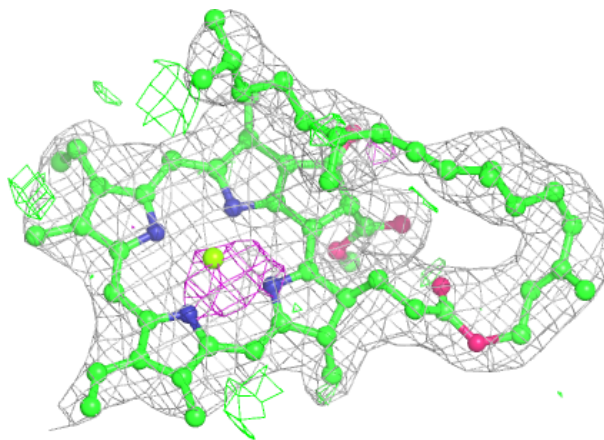


**Electron density around DGD C 516:**

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

**Electron density around CLA c 513:**

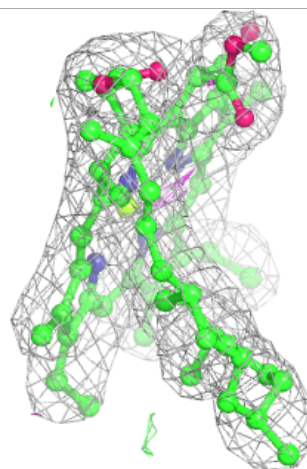
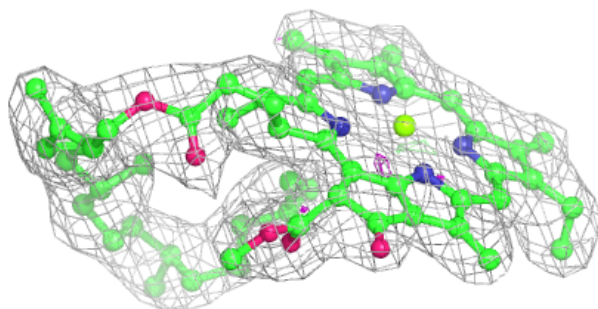
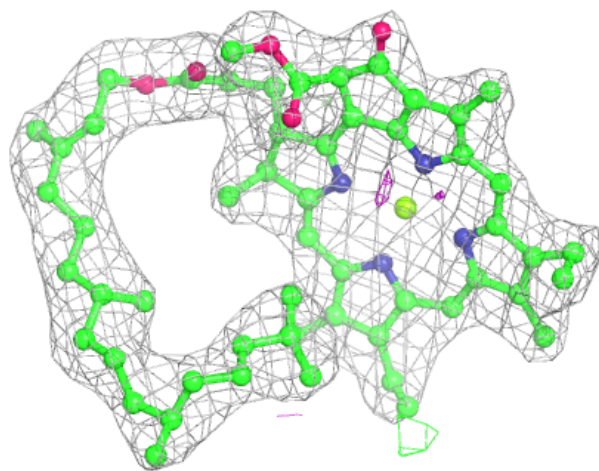
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





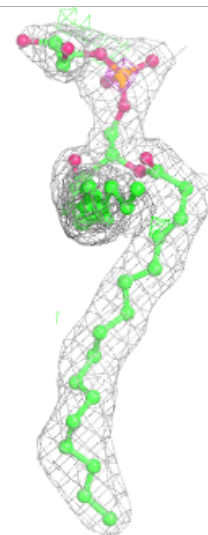
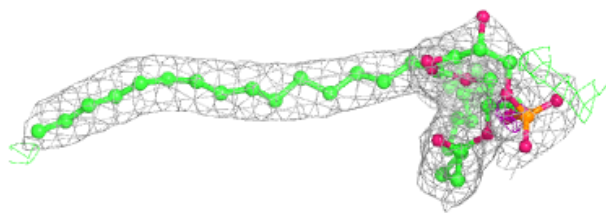
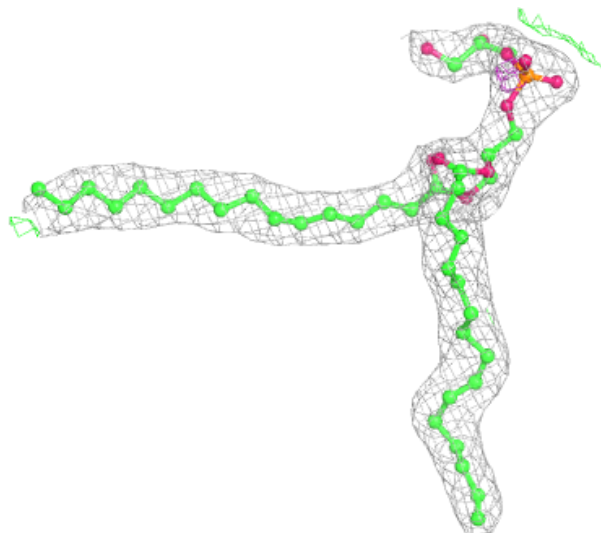
**Electron density around CLA B 616:**

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



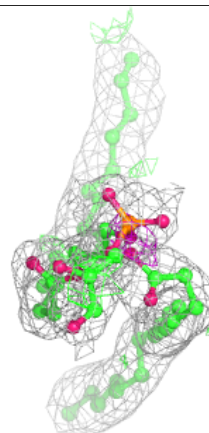
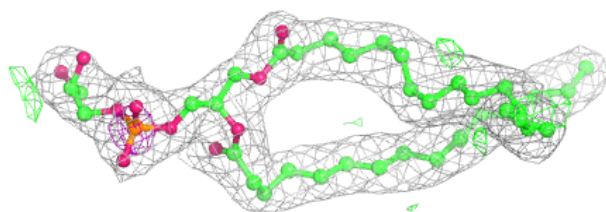
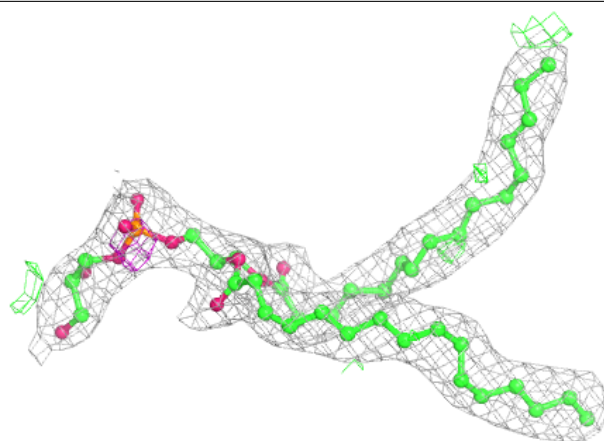
**Electron density around LHG b 634:**

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



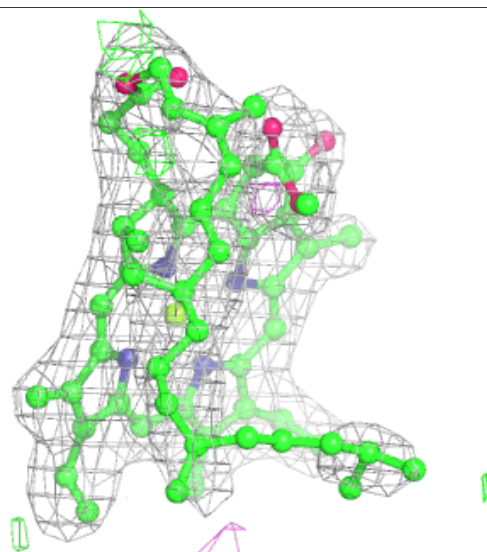
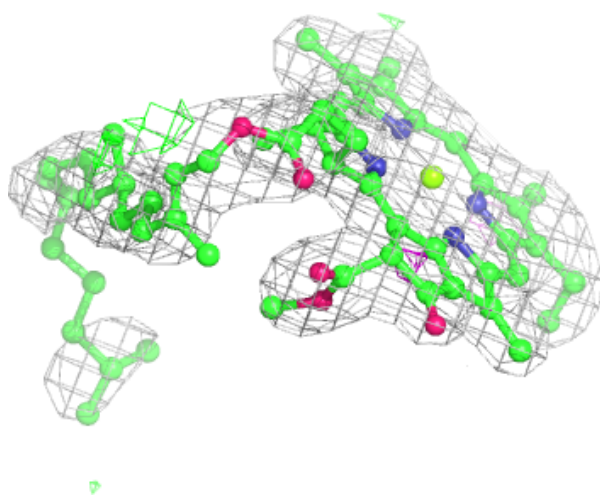
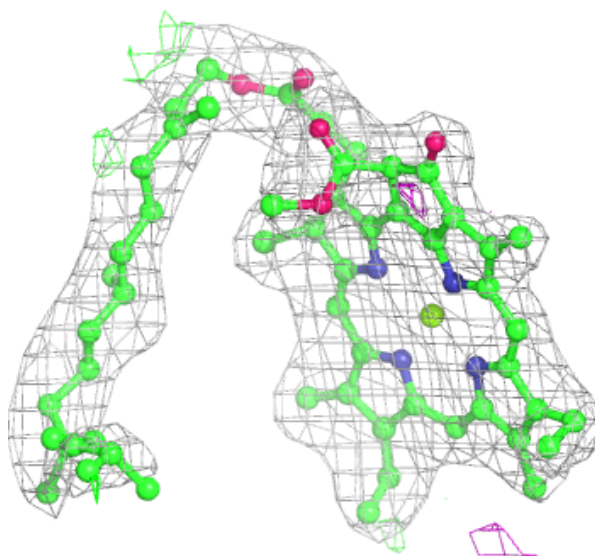
**Electron density around LHG d 410:**

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



**Electron density around CLA b 625:**

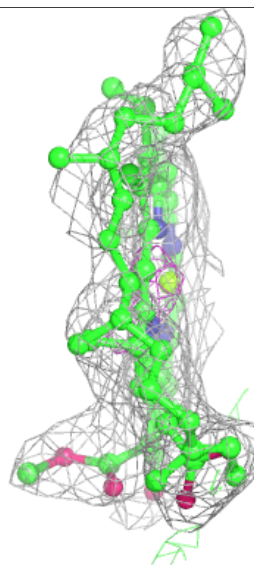
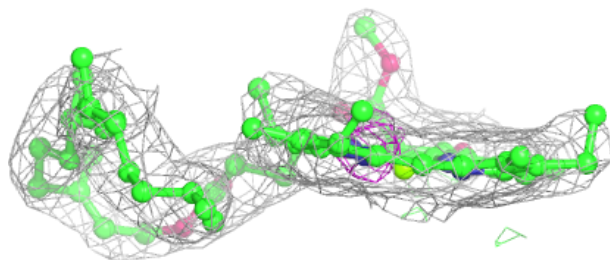
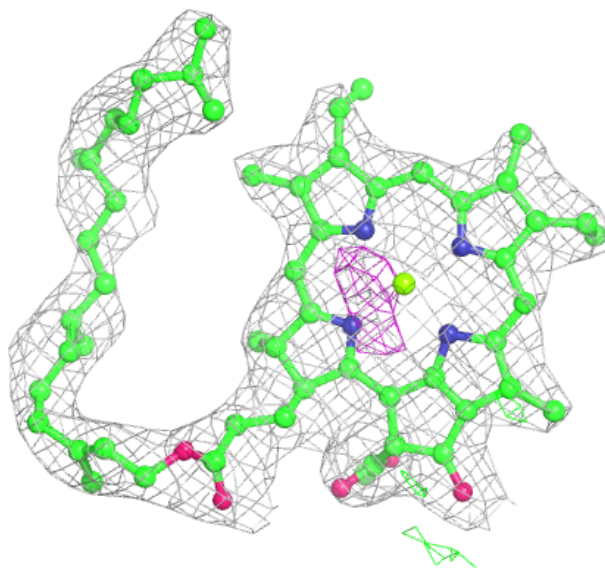
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





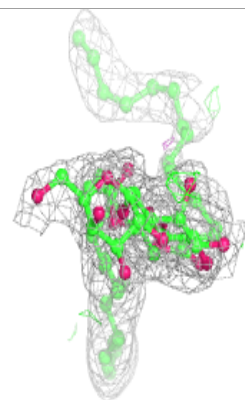
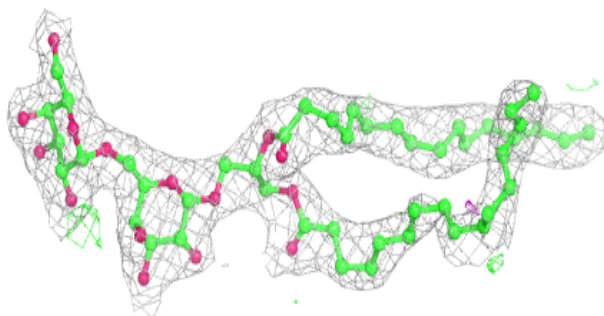
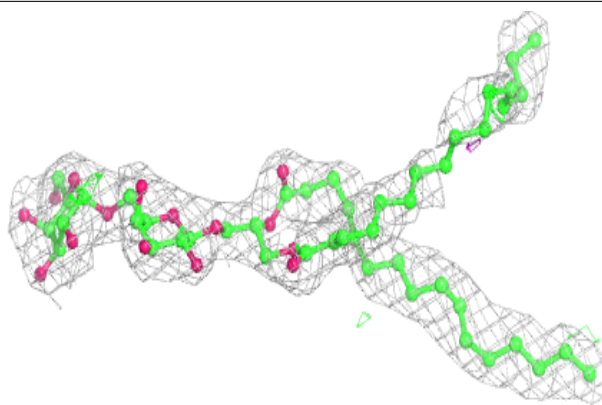
**Electron density around CLA c 516:**

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



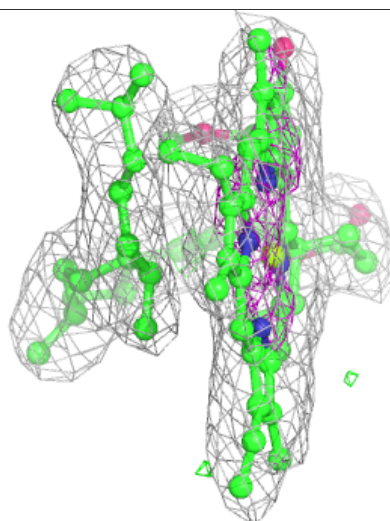
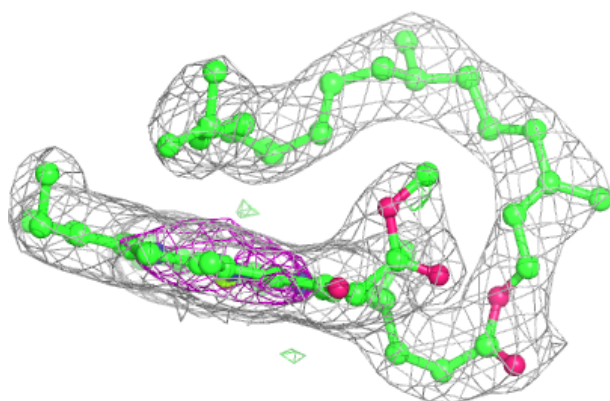
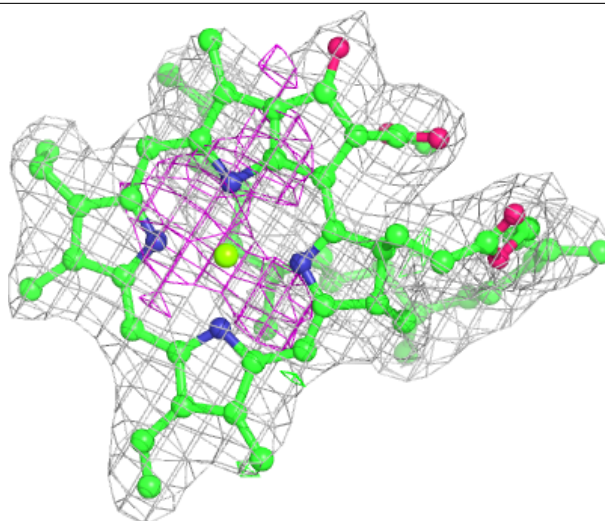
**Electron density around DGD c 519:**

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



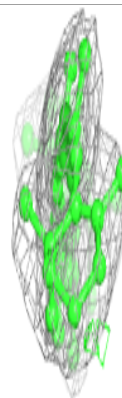
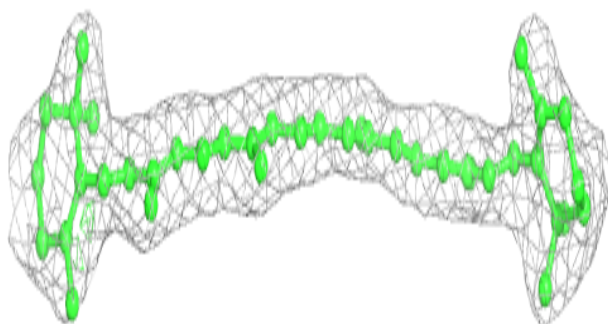
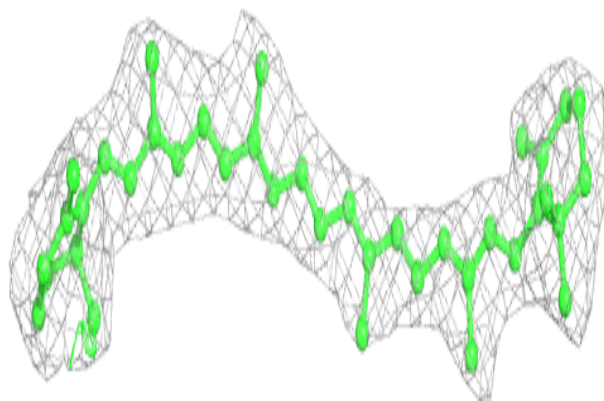
**Electron density around CLA c 514:**

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

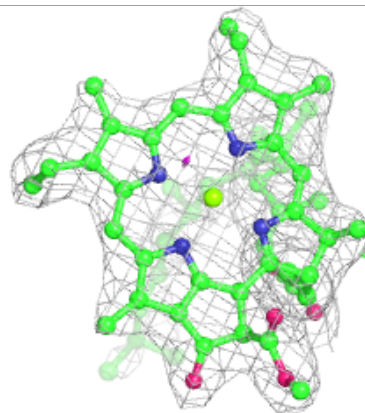
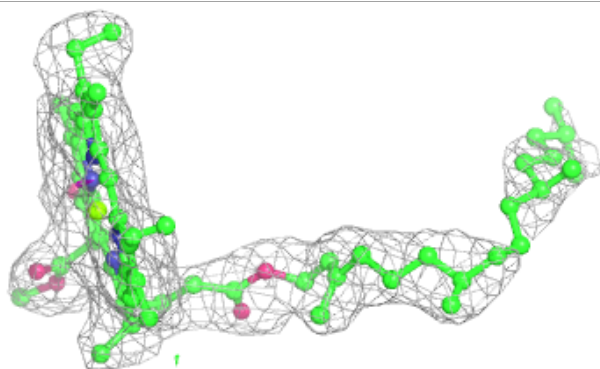
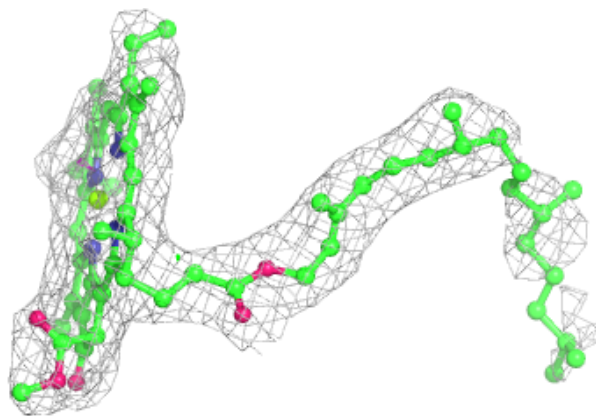


**Electron density around BCR y 101:**

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

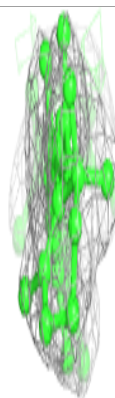
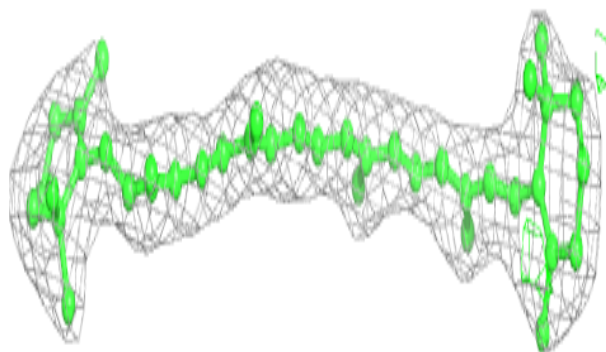
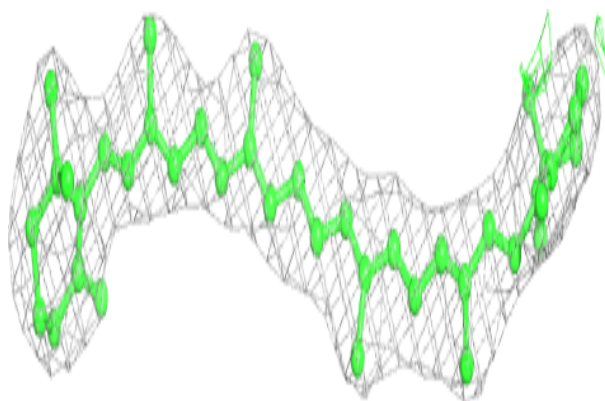
**Electron density around CLA D 406:**

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

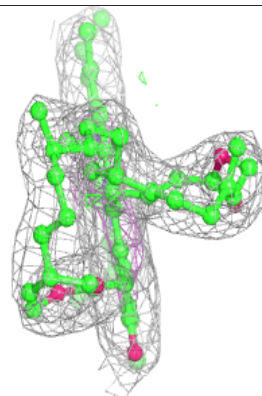
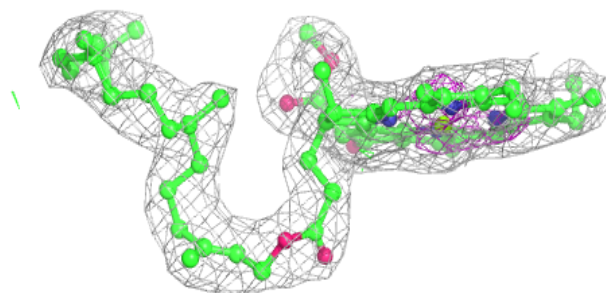
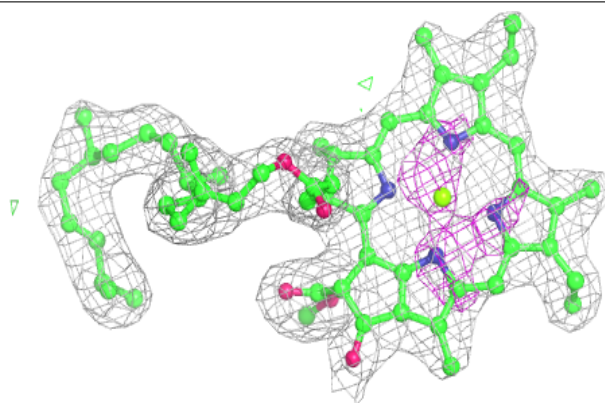


**Electron density around BCR Y 101:**

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

**Electron density around CLA B 613:**

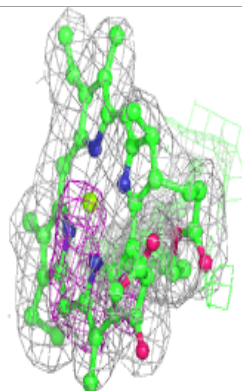
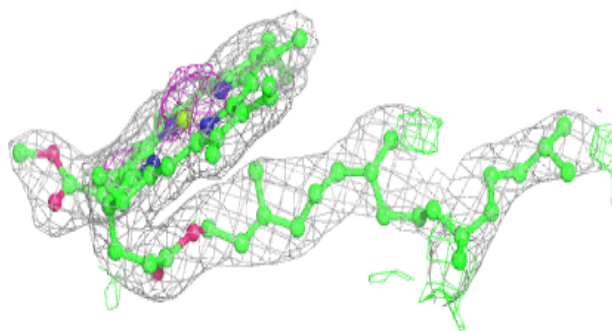
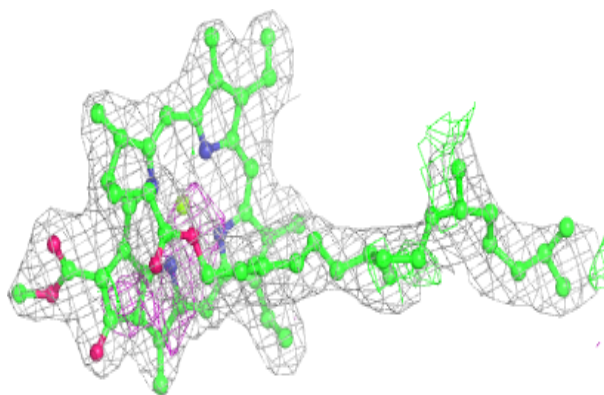
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



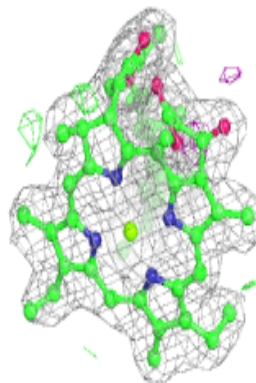
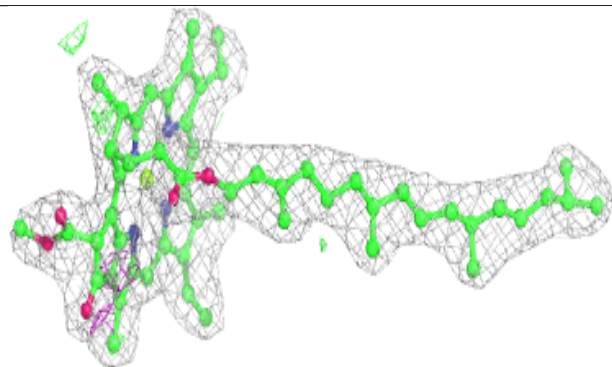
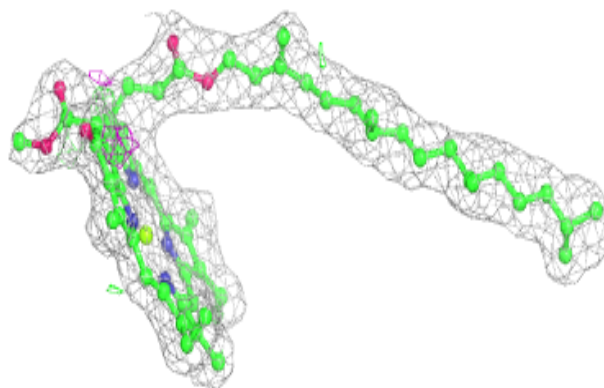


**Electron density around CLA b 623:**

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

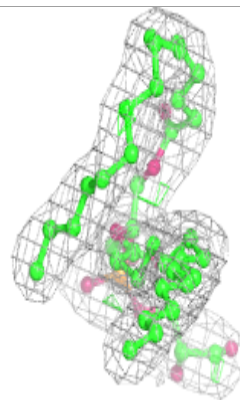
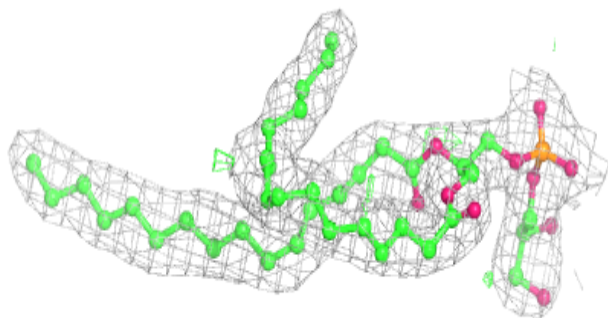
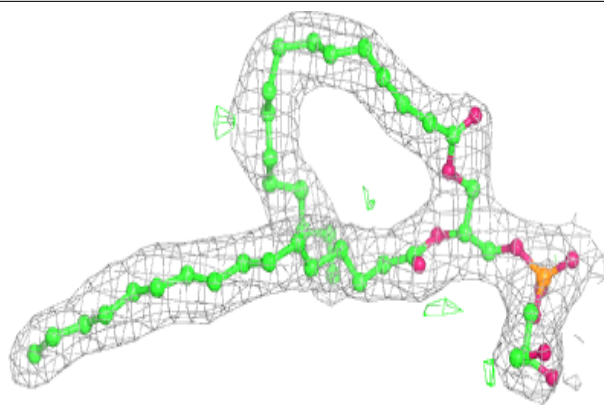
**Electron density around CLA B 608:**

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



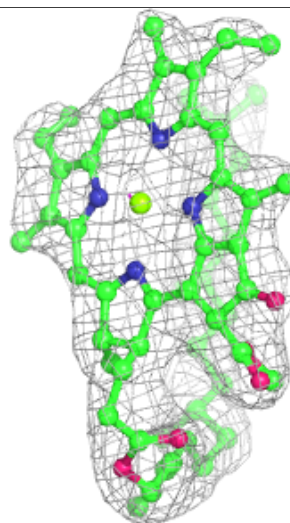
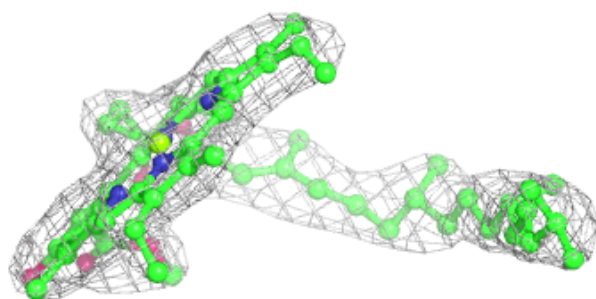
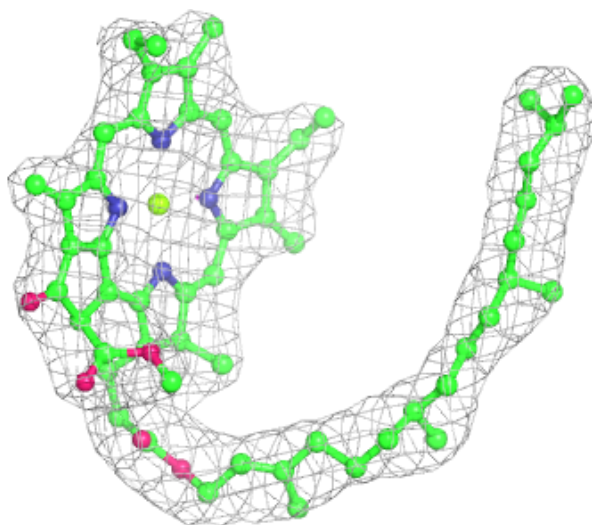
**Electron density around LHG d 409:**

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



**Electron density around CLA C 508:**

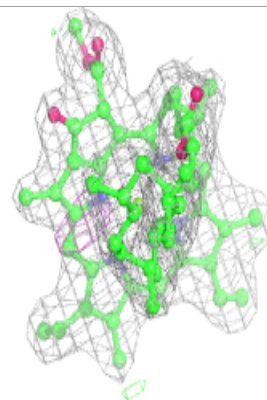
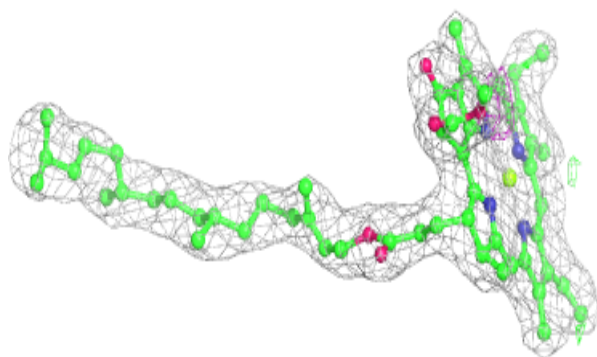
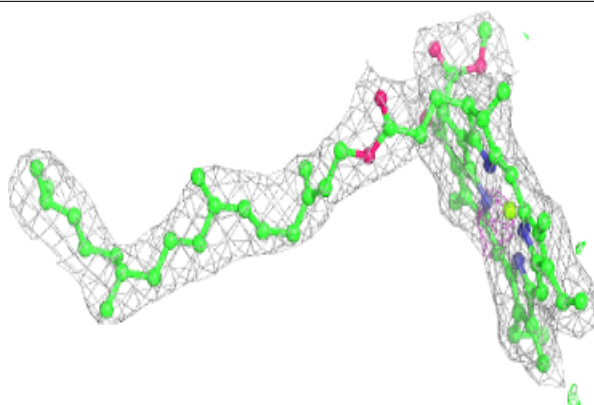
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



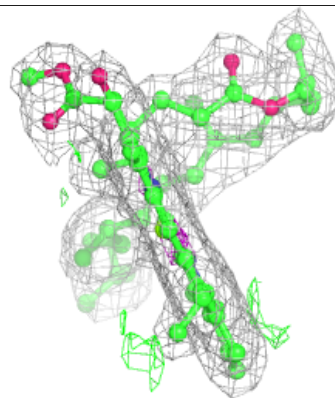
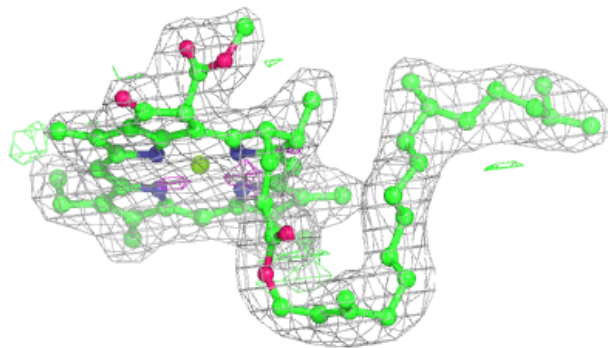
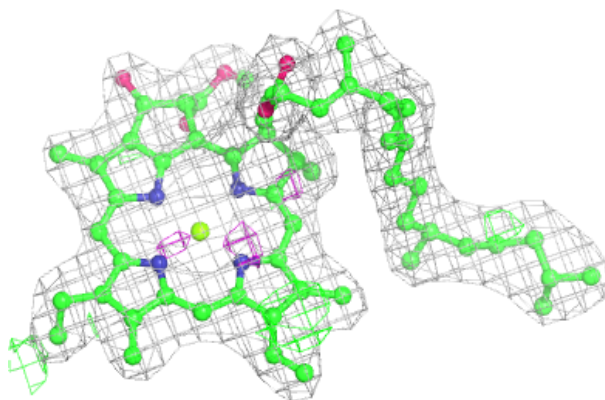


**Electron density around CLA B 605:**

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

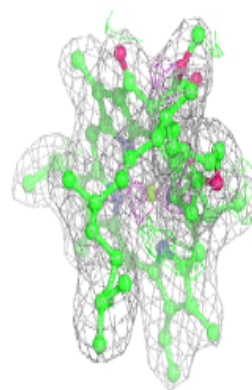
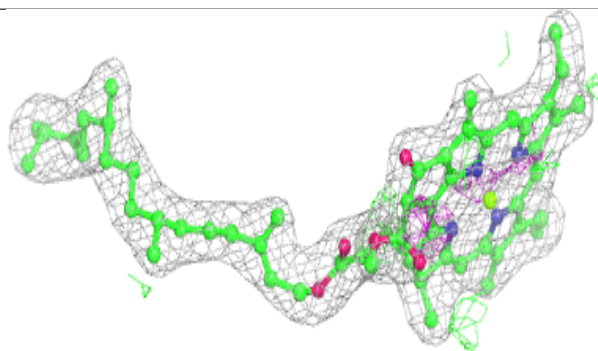
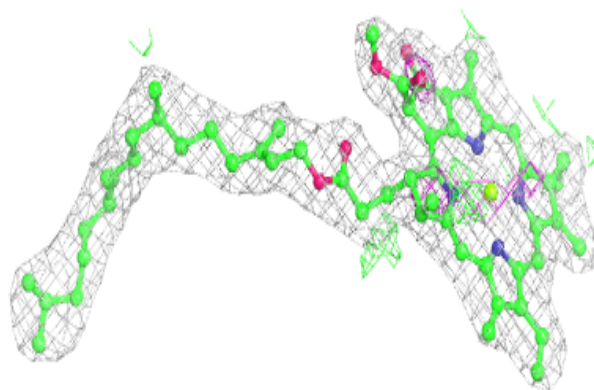
**Electron density around CLA d 403:**

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

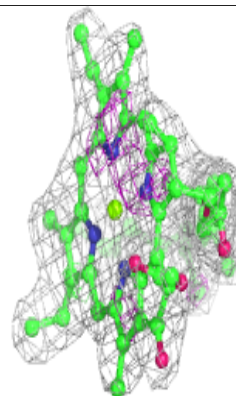
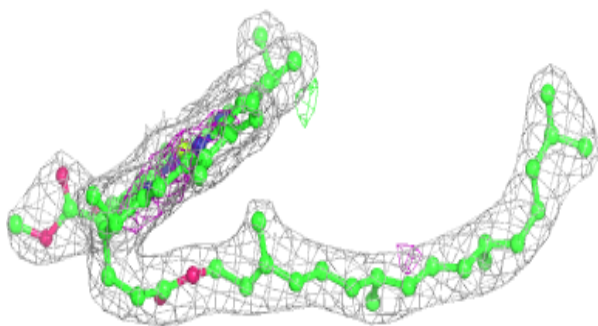
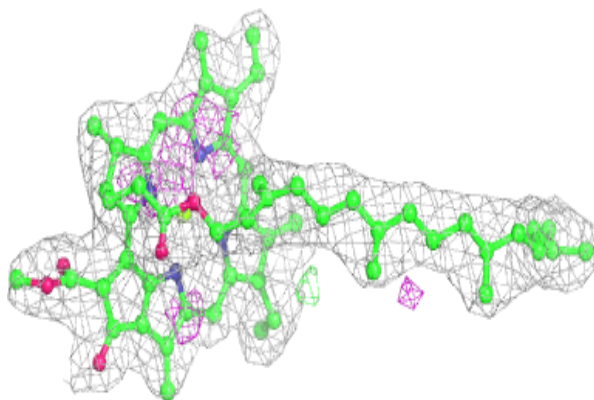


**Electron density around CLA A 404:**

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

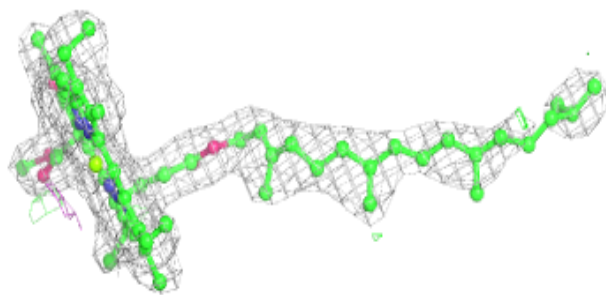
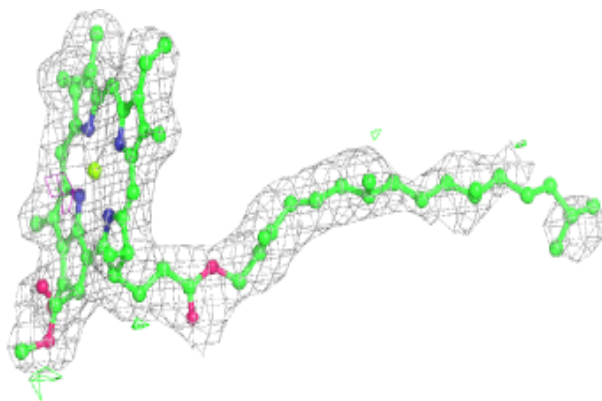
**Electron density around CLA b 617:**

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



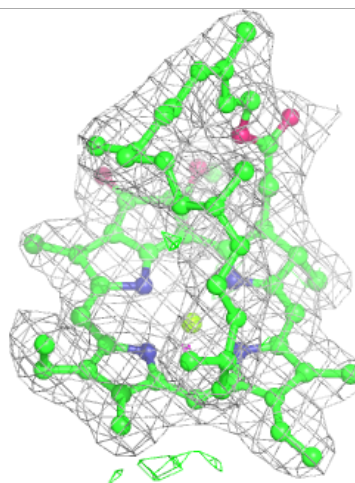
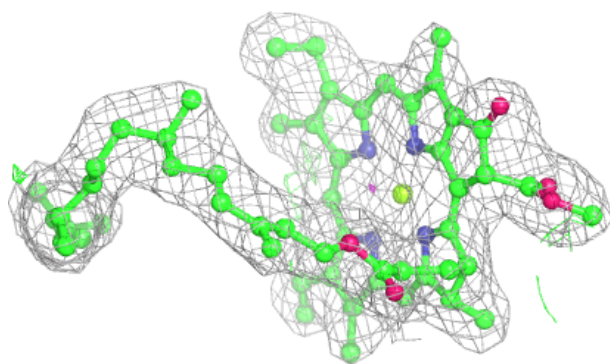
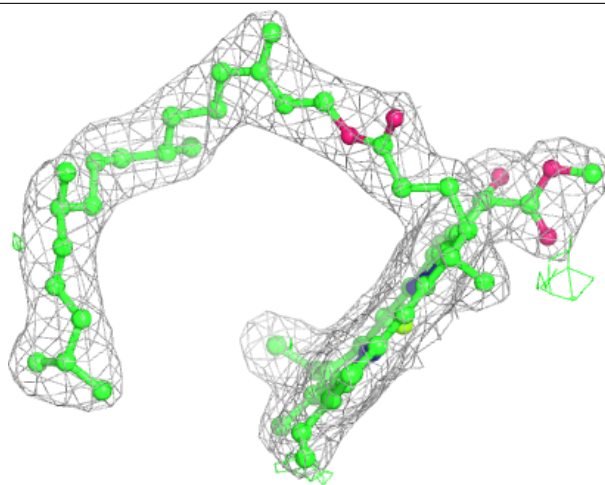
**Electron density around CLA d 405:**

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



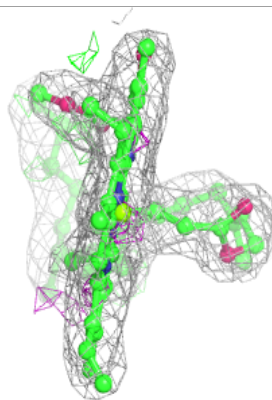
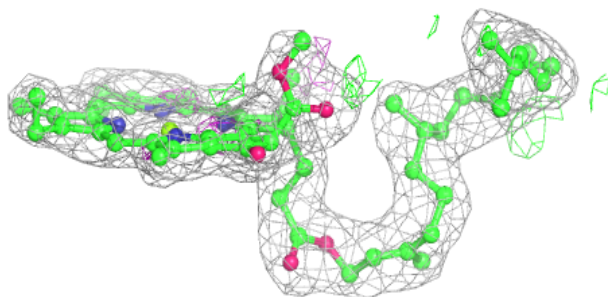
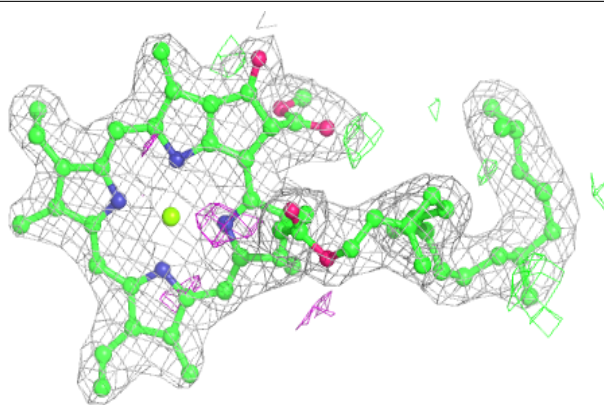
**Electron density around CLA b 620:**

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



**Electron density around CLA b 621:**

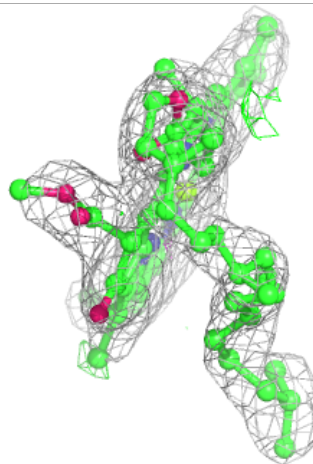
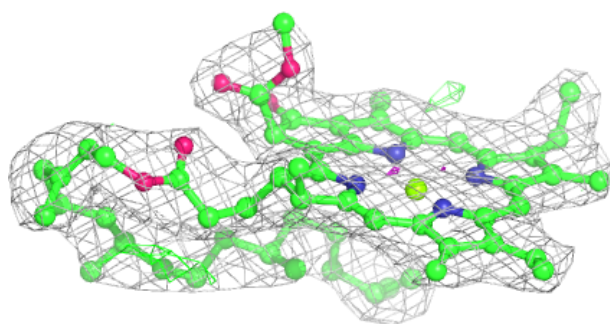
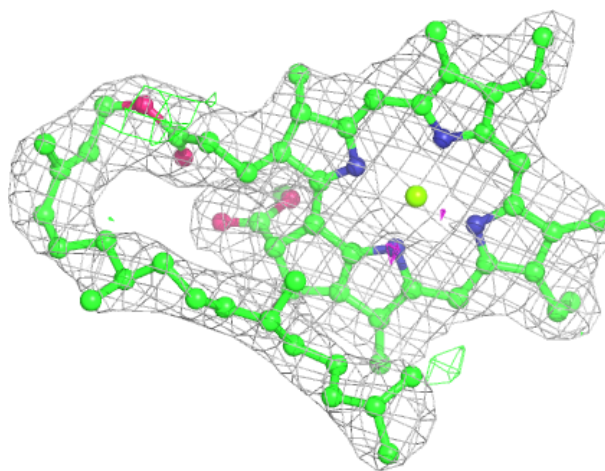
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





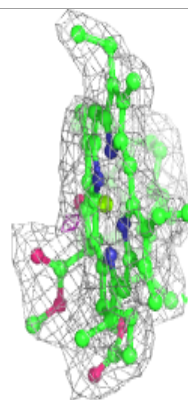
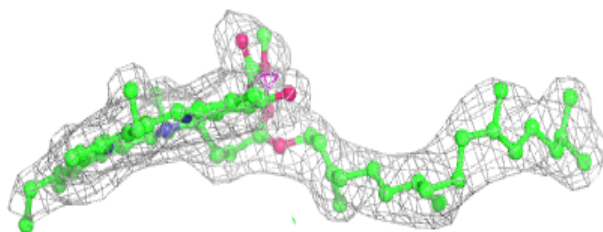
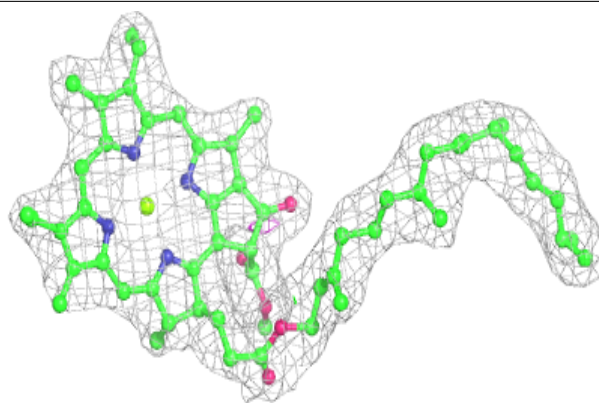
**Electron density around CLA C 510:**

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

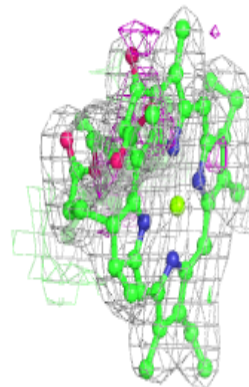
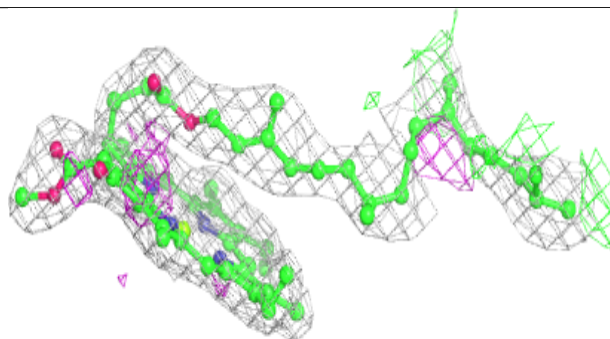
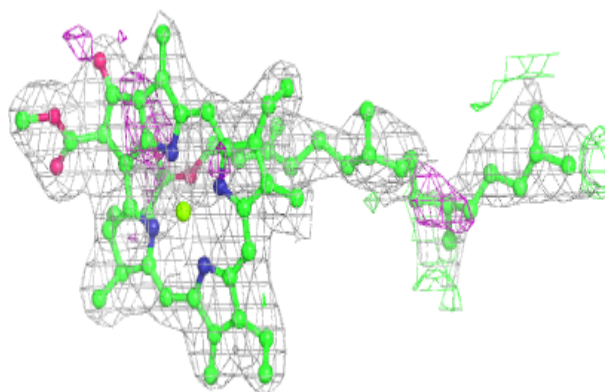


**Electron density around CLA B 603:**

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

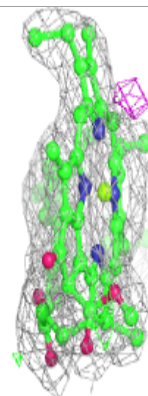
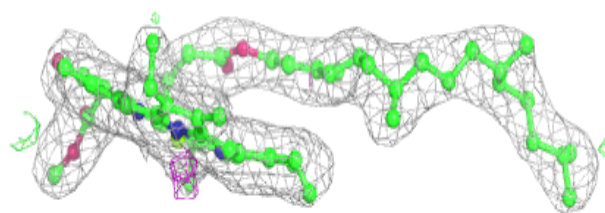
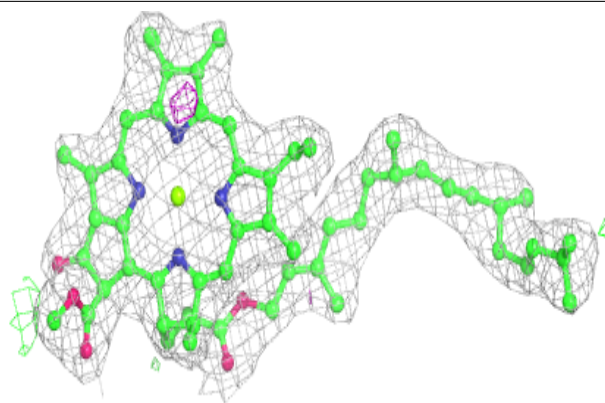
**Electron density around CLA B 615:**

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

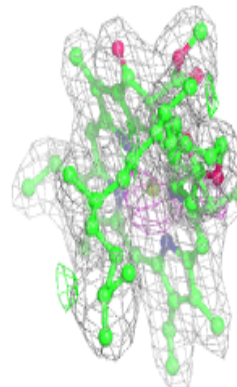
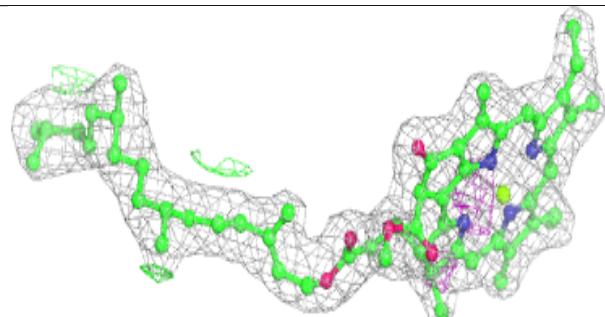
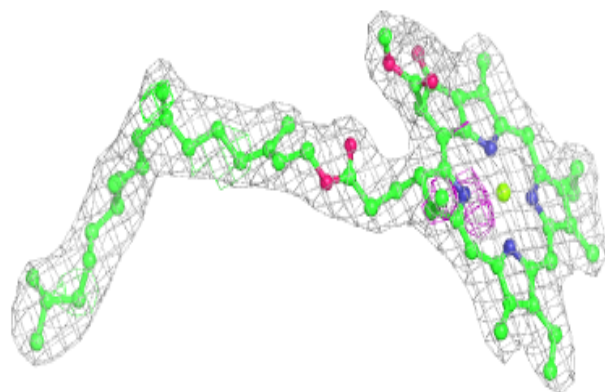


**Electron density around CLA b 612:**

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

**Electron density around CLA a 408:**

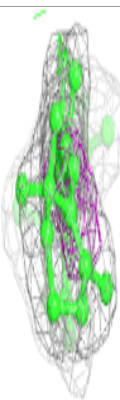
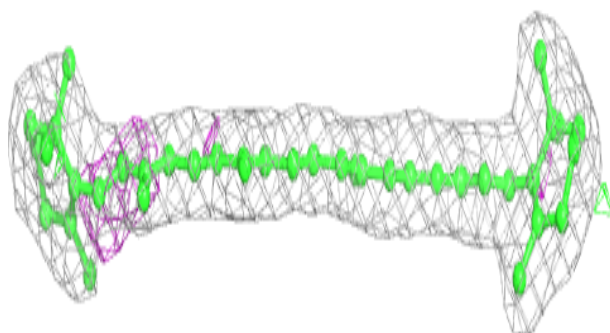
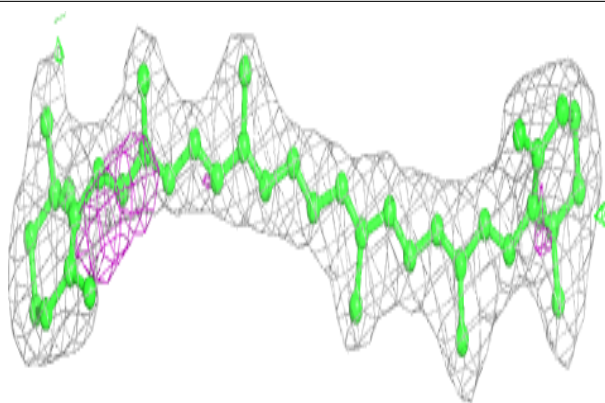
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



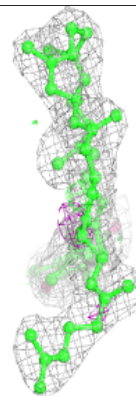
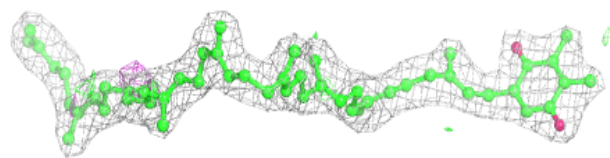
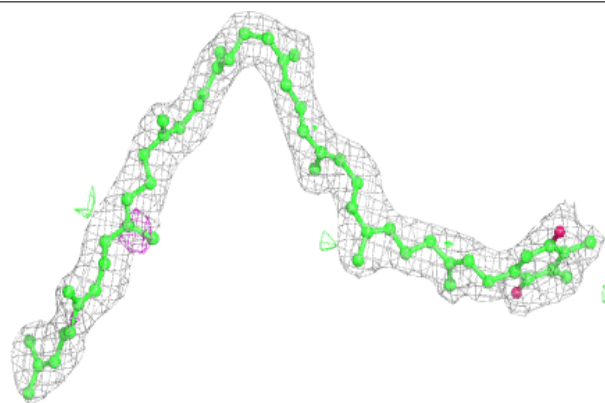


**Electron density around BCR b 627:**

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

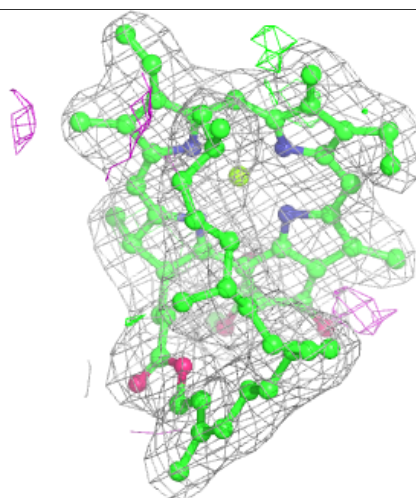
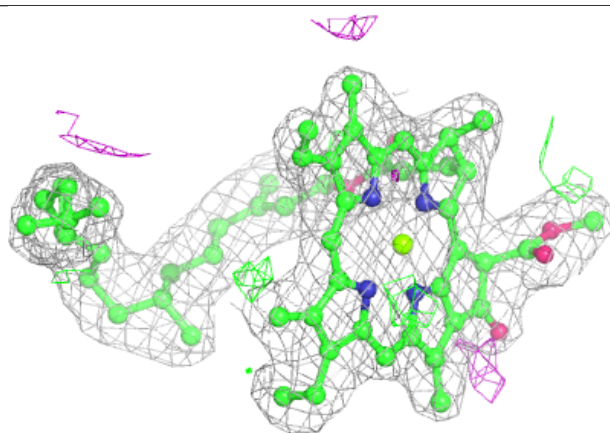
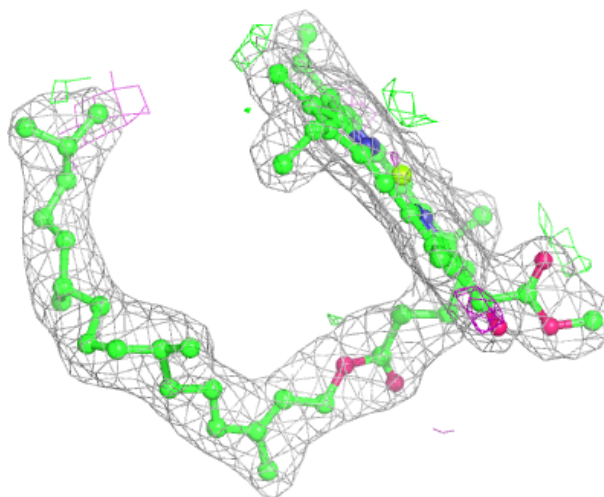
**Electron density around PL9 d 407 (B):**

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



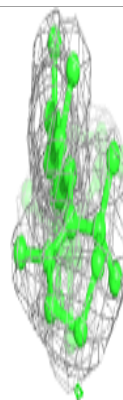
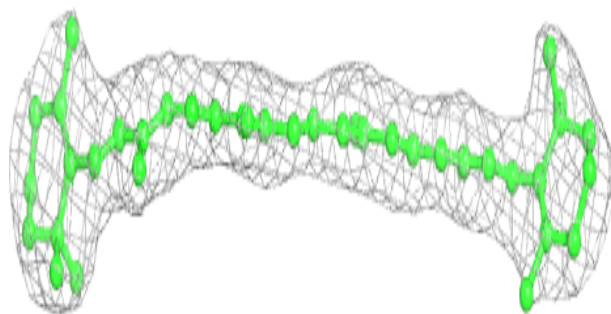
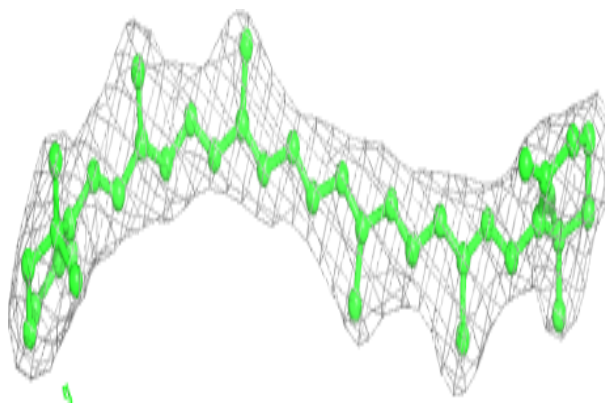
**Electron density around CLA B 612:**

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



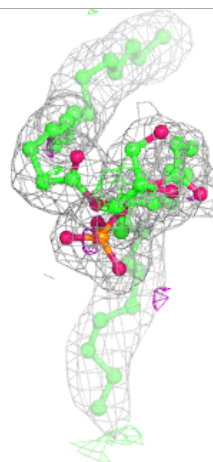
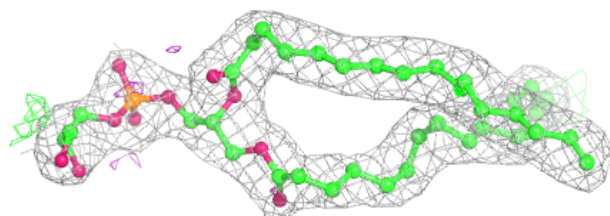
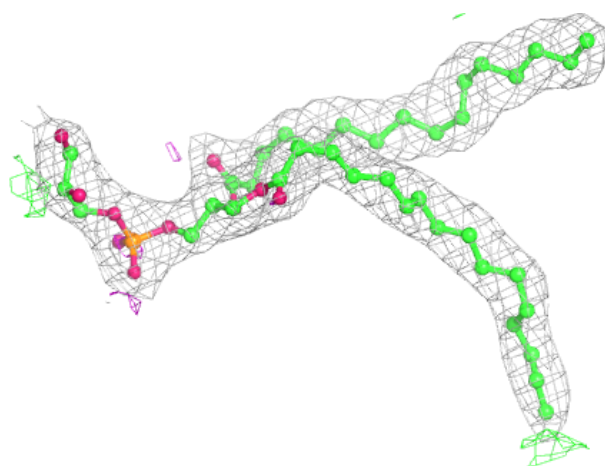
**Electron density around BCR h 101:**

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



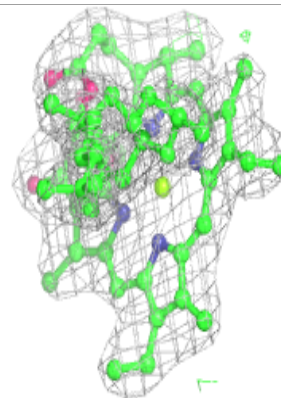
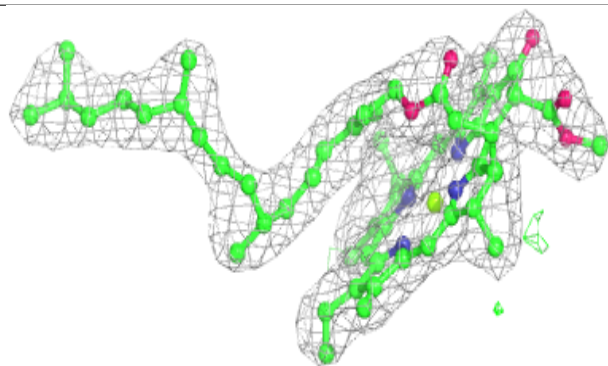
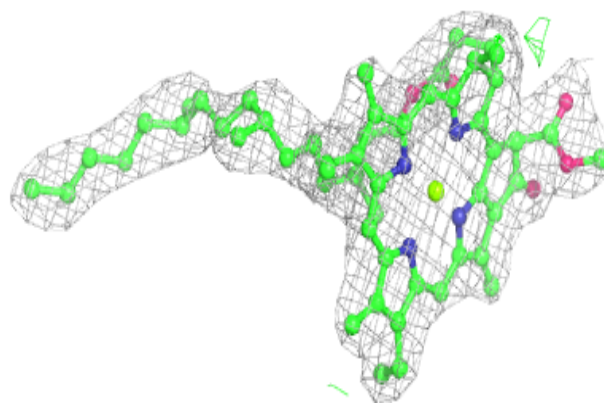
**Electron density around LHG D 411:**

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

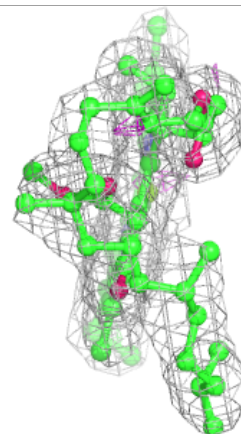
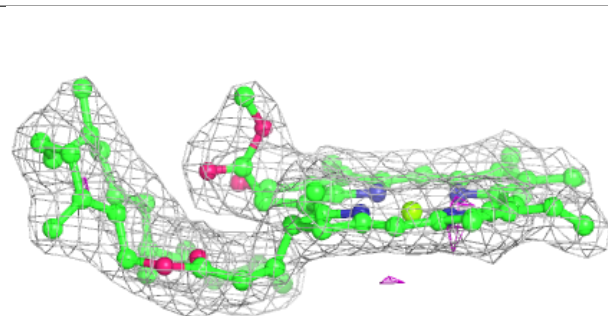
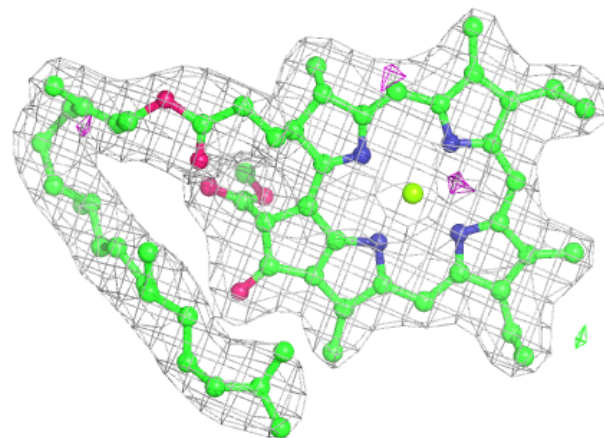


**Electron density around CLA C 506:**

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

**Electron density around CLA b 619:**

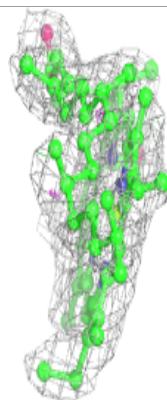
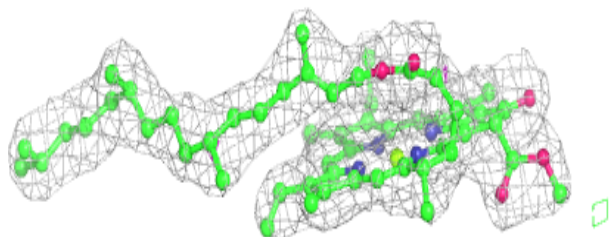
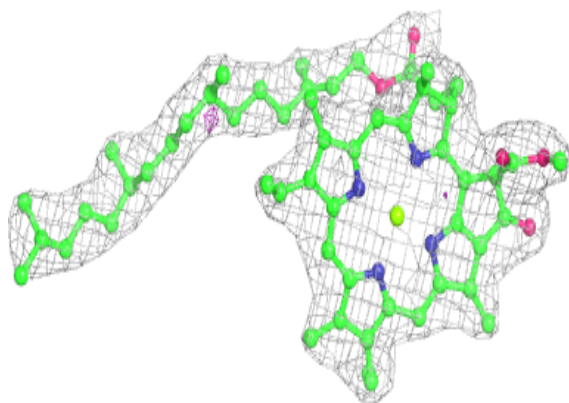
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



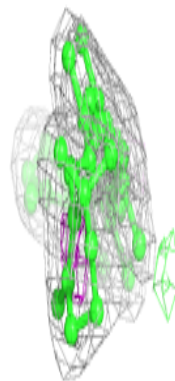
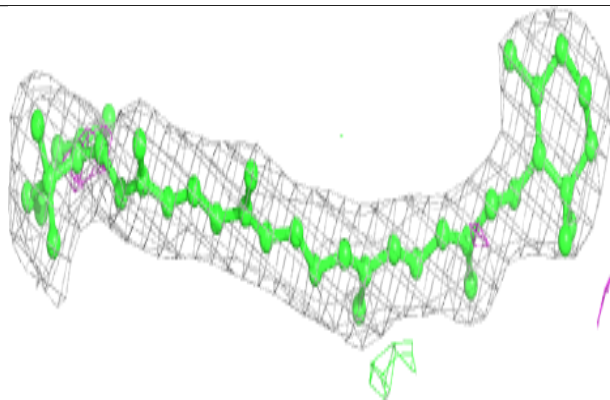
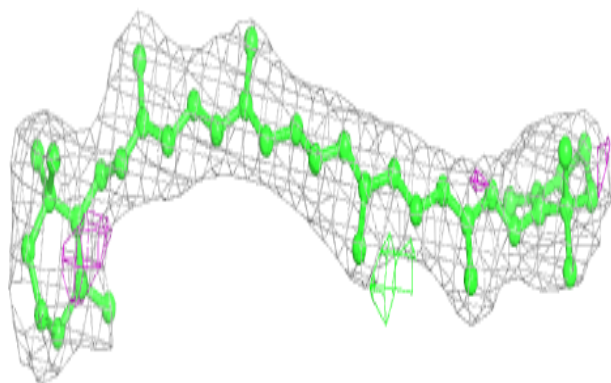


**Electron density around CLA c 505:**

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

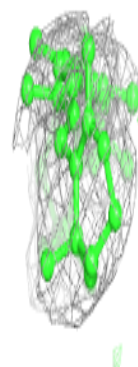
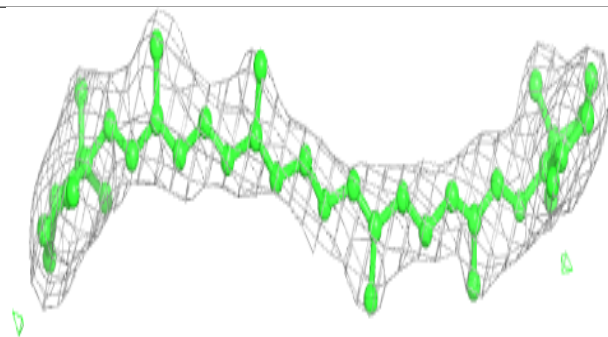
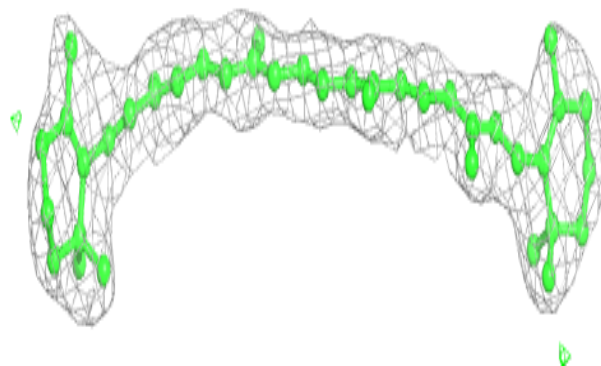
**Electron density around BCR d 406:**

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

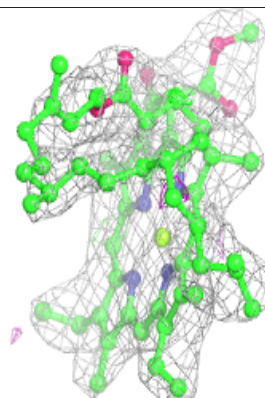
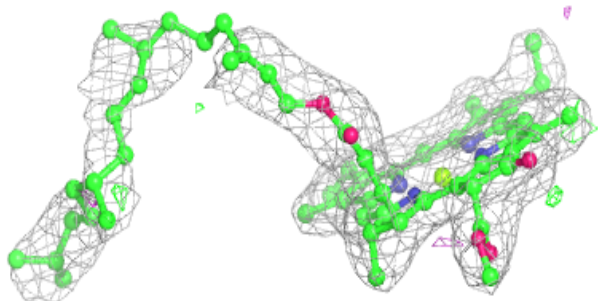
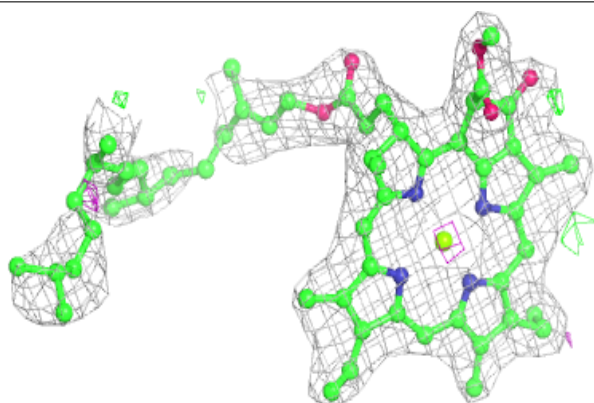


**Electron density around BCR k 102:**

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

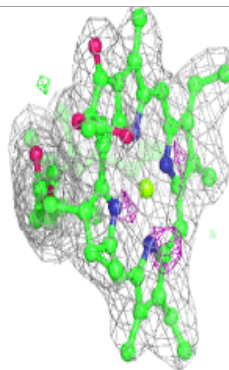
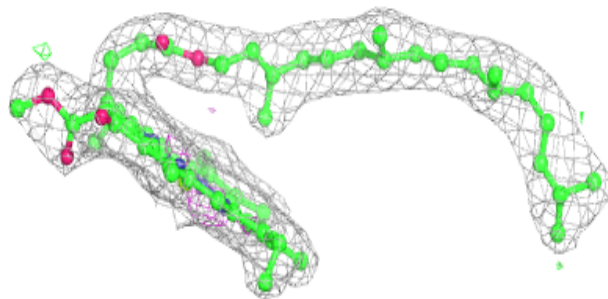
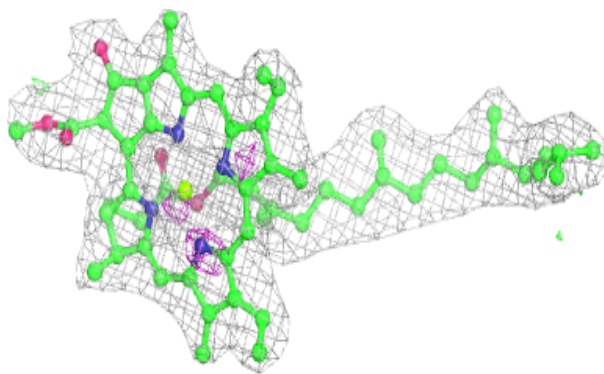
**Electron density around CLA a 411:**

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

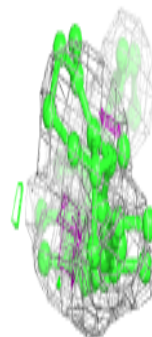
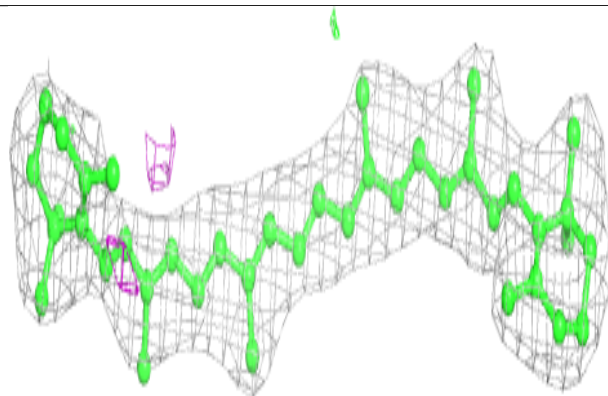
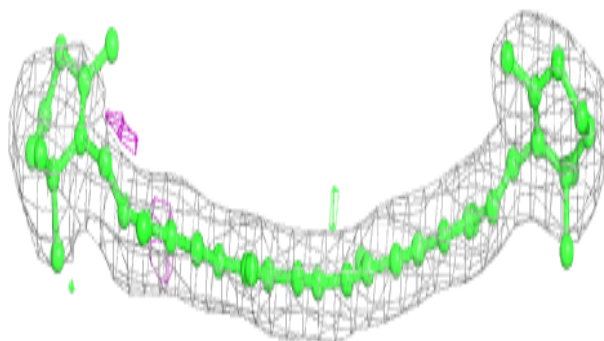


**Electron density around CLA B 609:**

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

**Electron density around BCR D 407:**

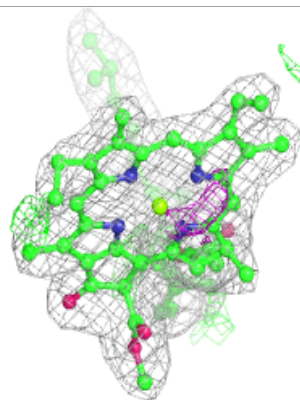
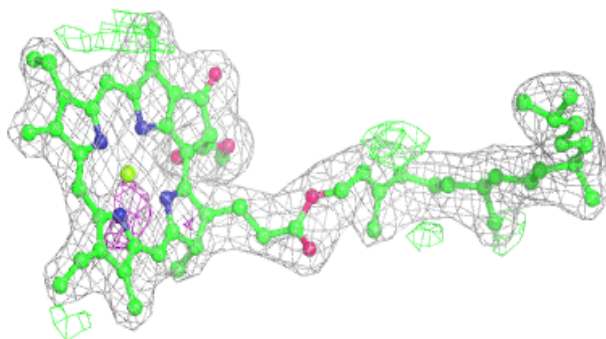
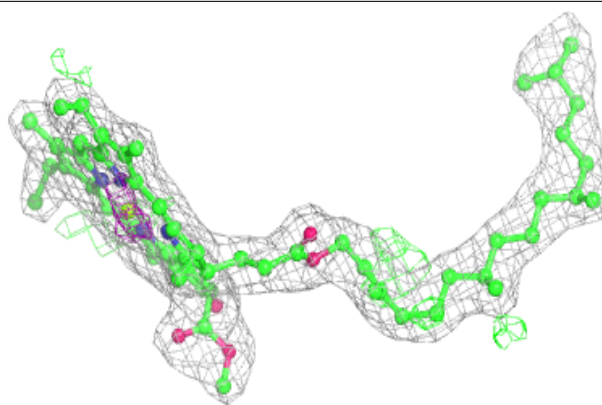
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





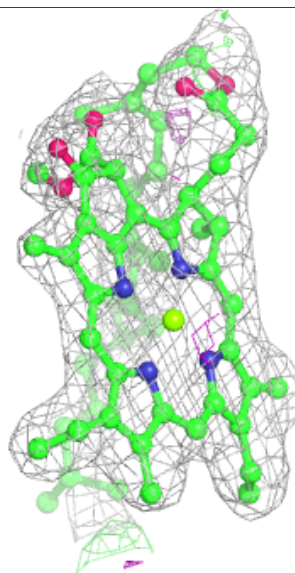
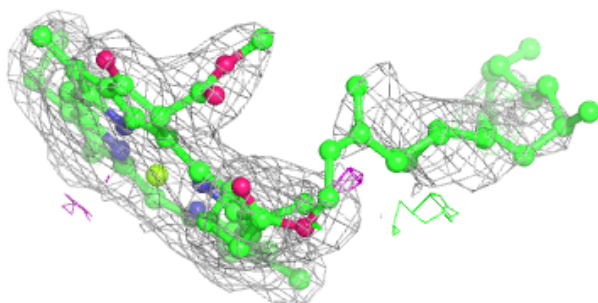
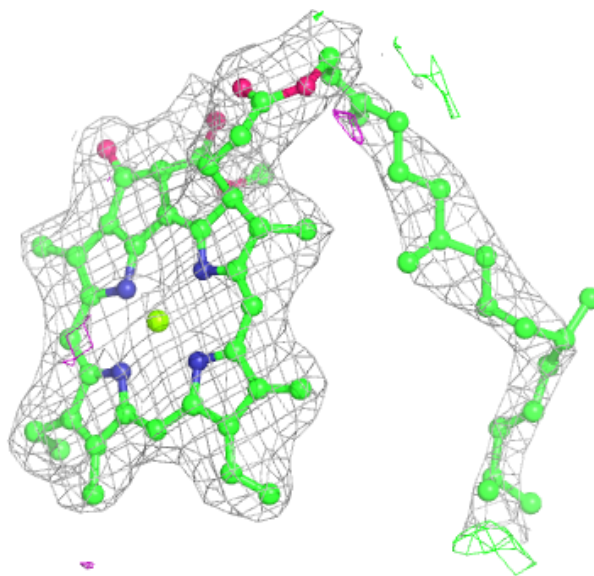
**Electron density around CLA D 405:**

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



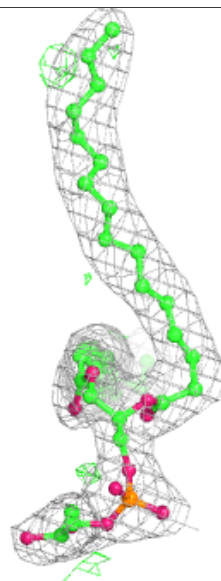
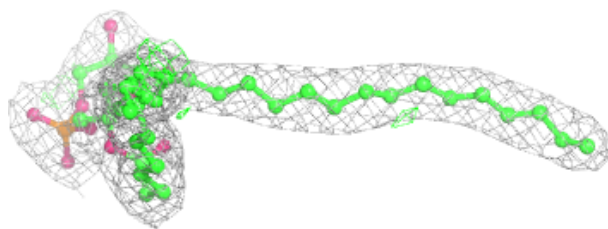
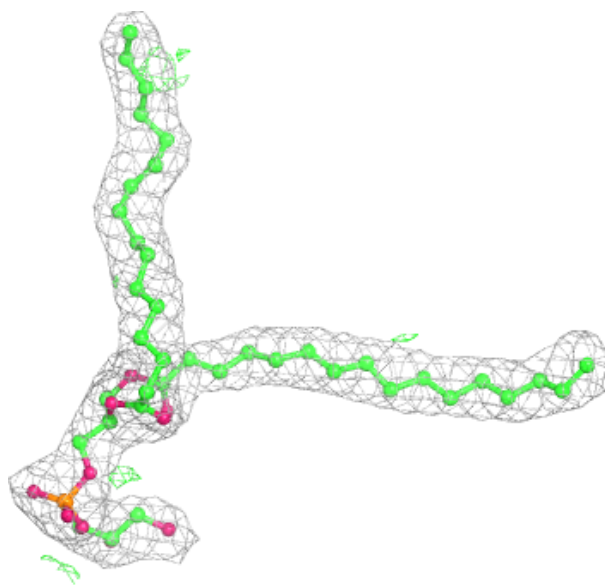
**Electron density around CLA B 617:**

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



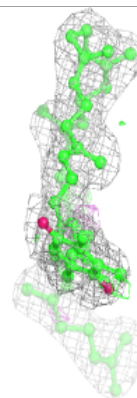
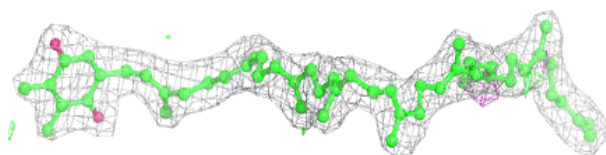
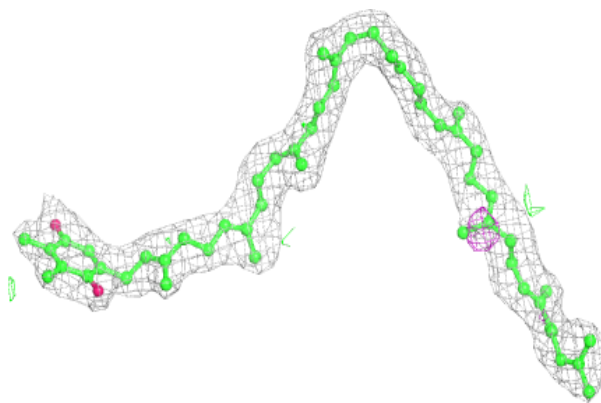
**Electron density around LHG L 101:**

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

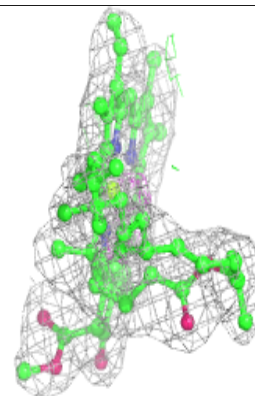
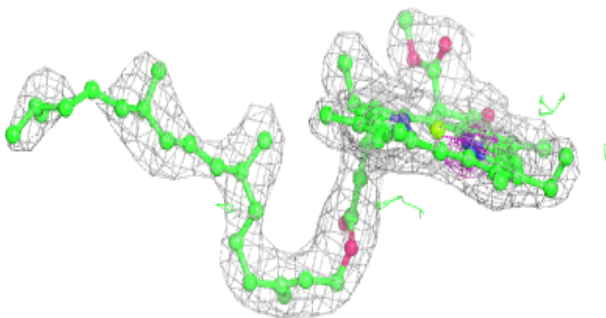
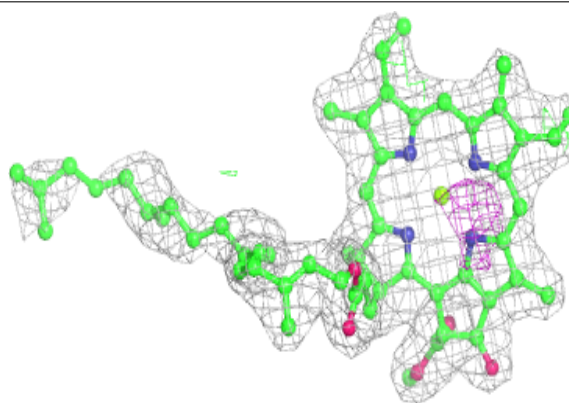


**Electron density around PL9 d 407 (A):**

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

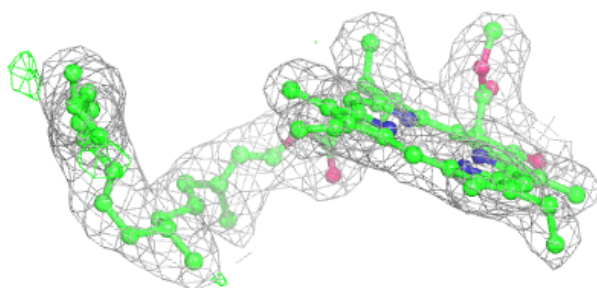
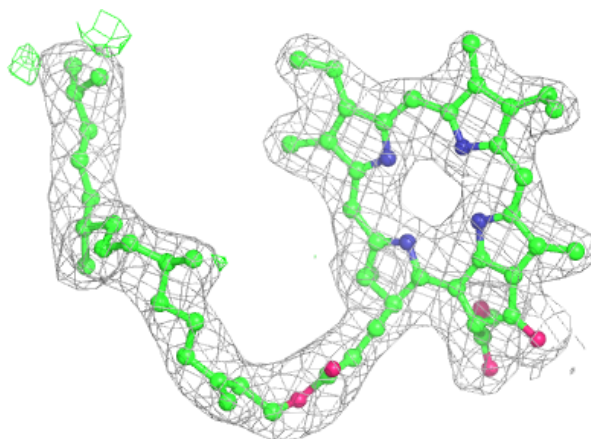
**Electron density around CLA A 406:**

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



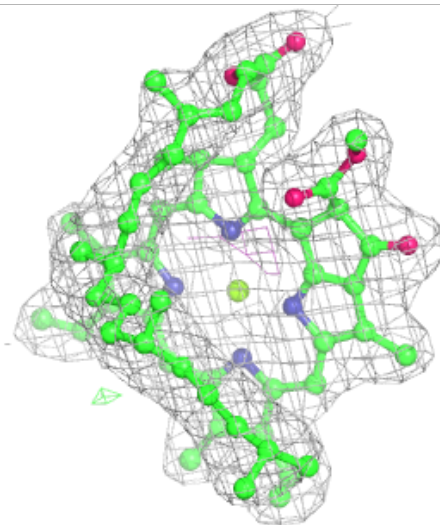
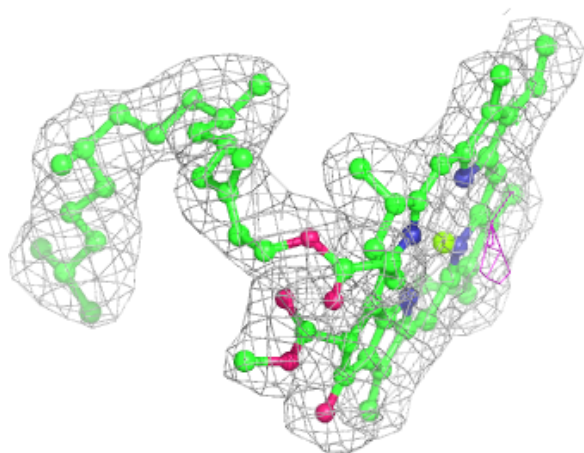
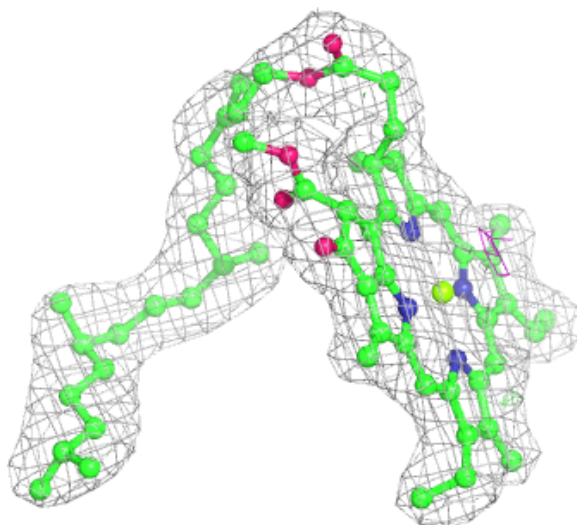
**Electron density around PHO D 402 (B):**

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



**Electron density around CLA b 622:**

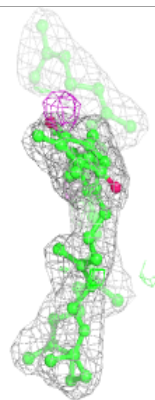
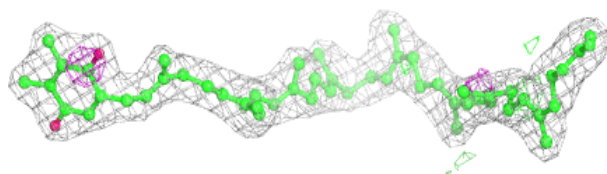
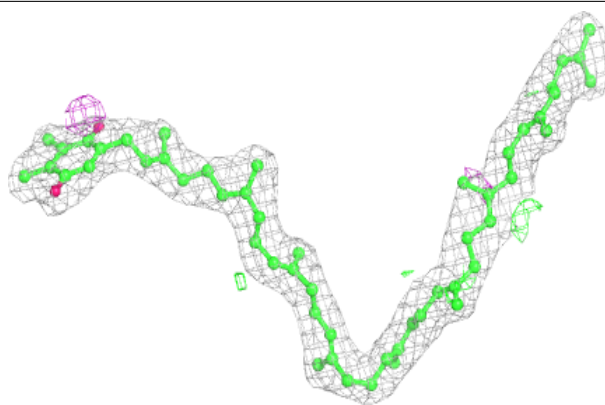
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



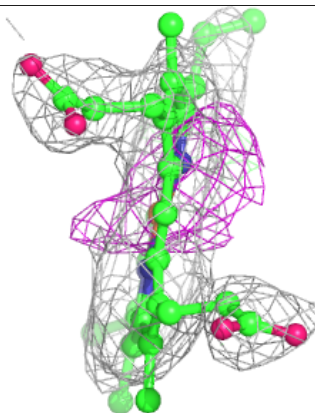
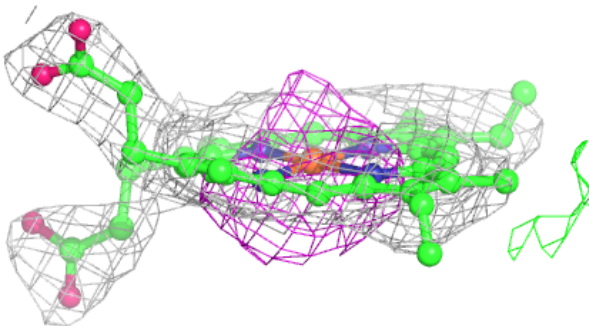
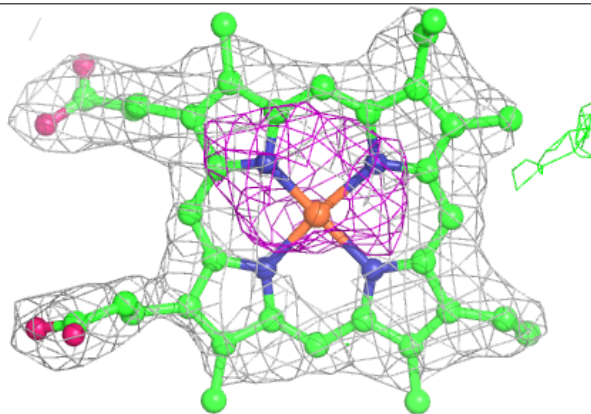


**Electron density around PL9 D 408 (A):**

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

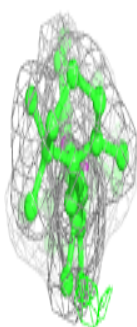
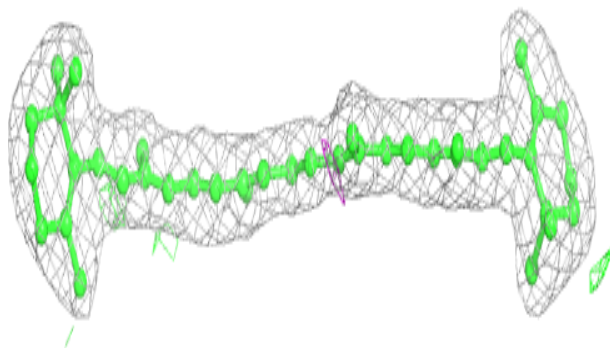
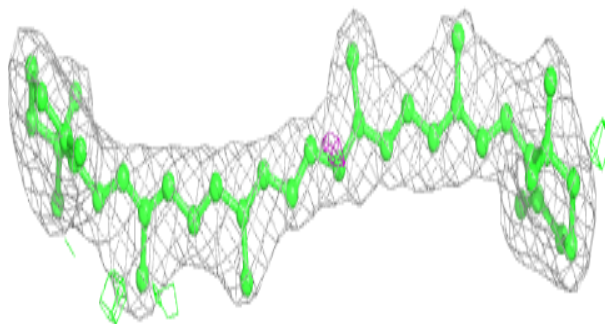
**Electron density around HEM F 102:**

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

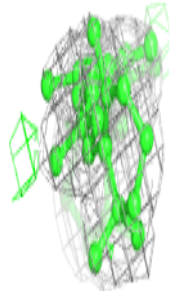
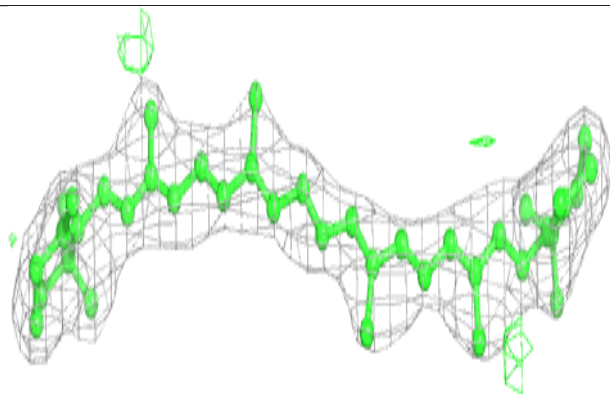
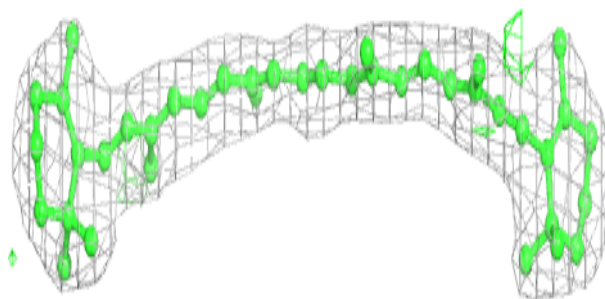


**Electron density around BCR A 409:**

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

**Electron density around BCR K 103:**

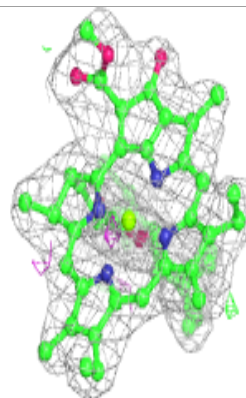
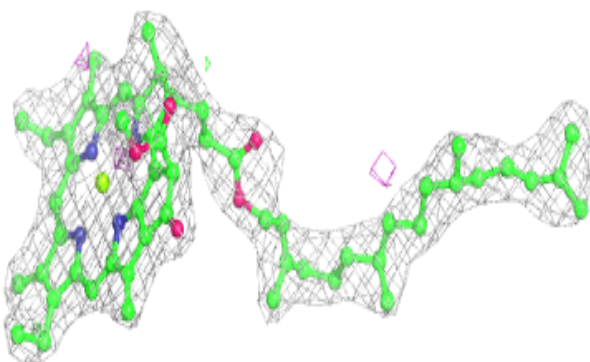
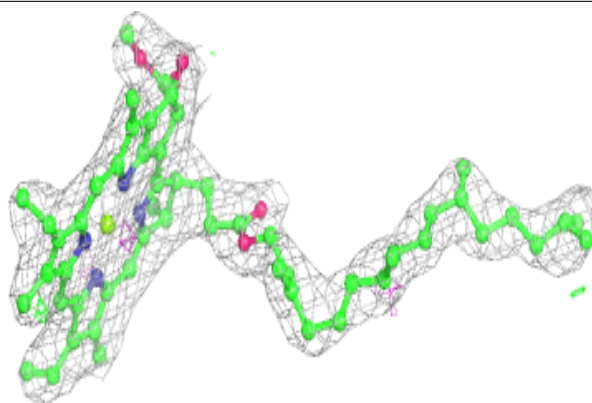
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



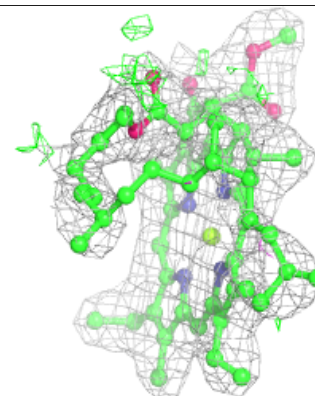
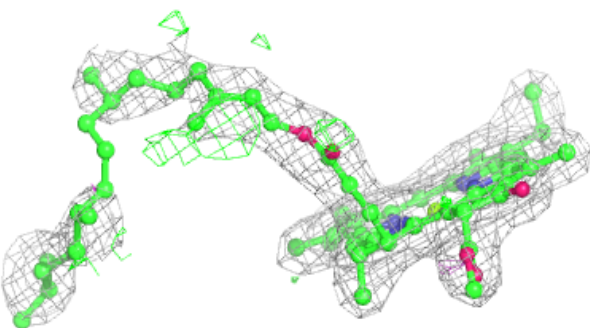
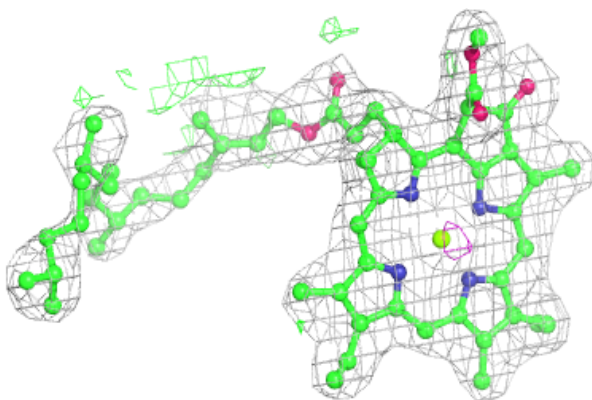


**Electron density around CLA C 503:**

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

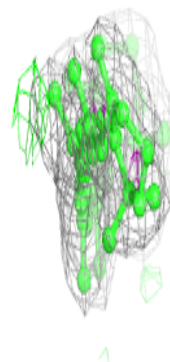
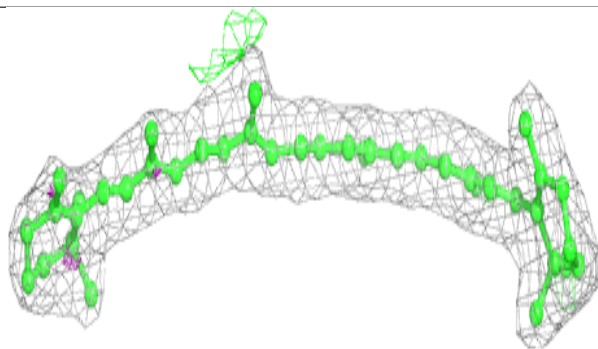
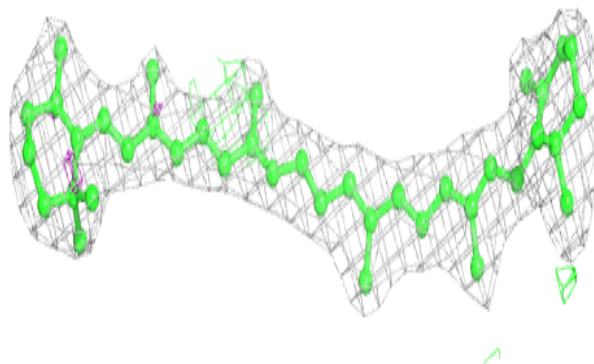
**Electron density around CLA A 408:**

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



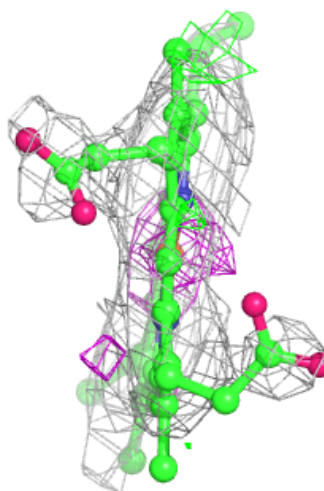
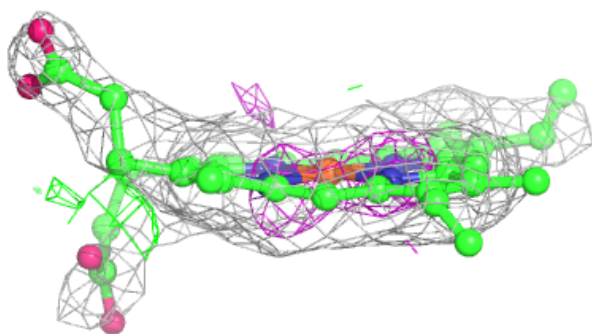
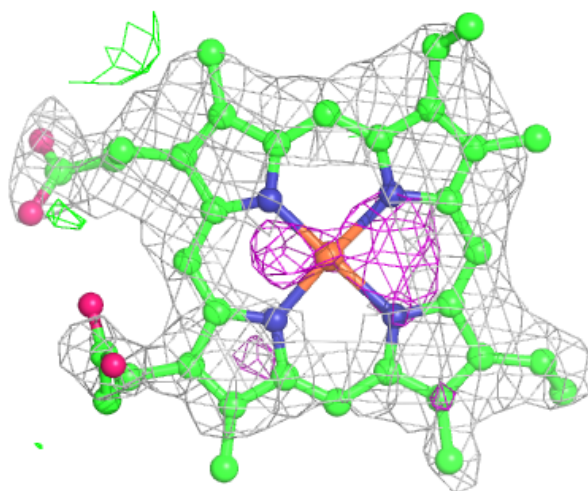
**Electron density around BCR T 103:**

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



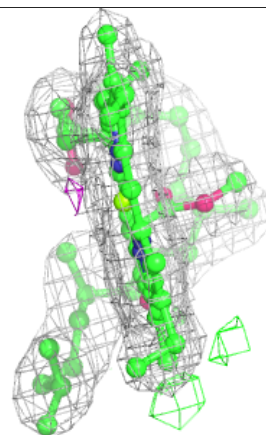
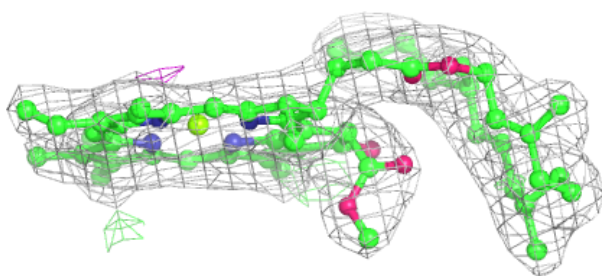
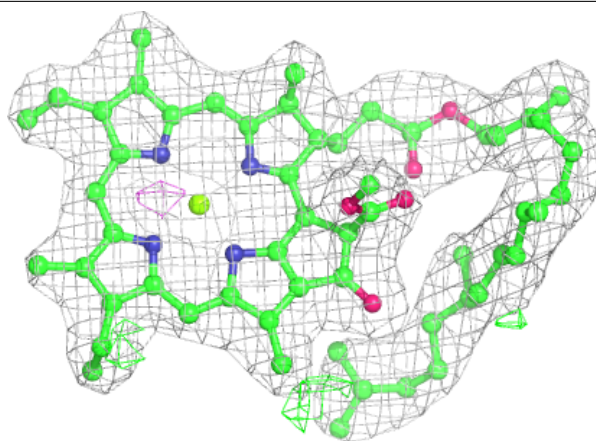
**Electron density around HEM e 101:**

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

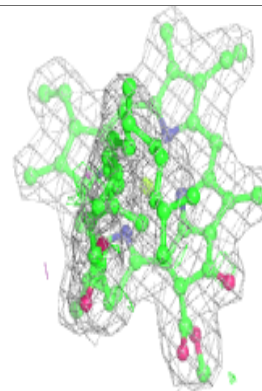
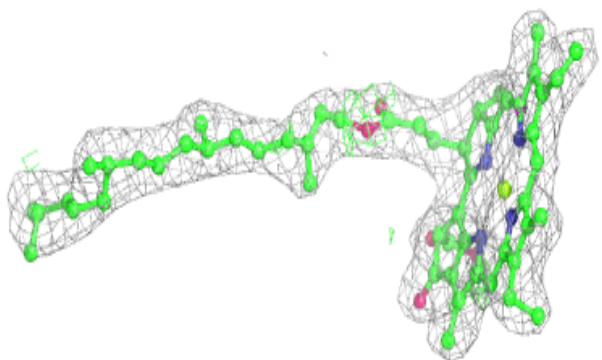
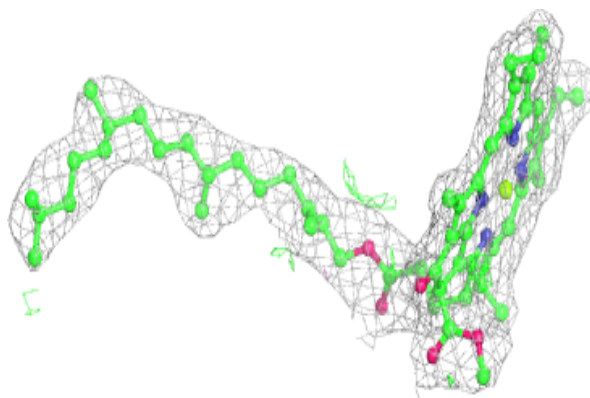


**Electron density around CLA B 611:**

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

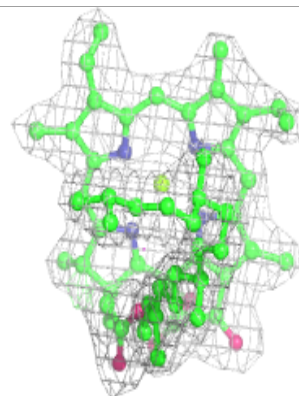
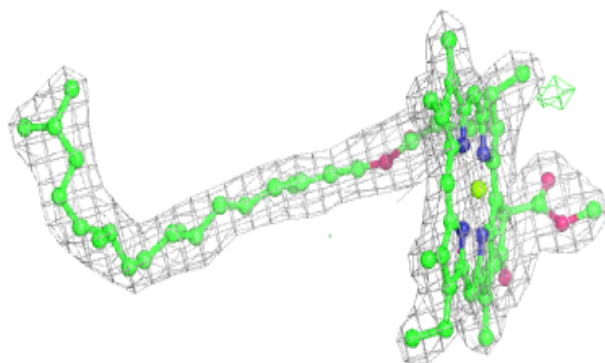
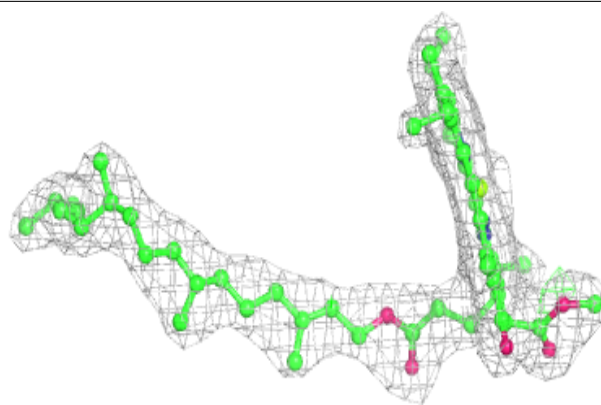
**Electron density around CLA b 613:**

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

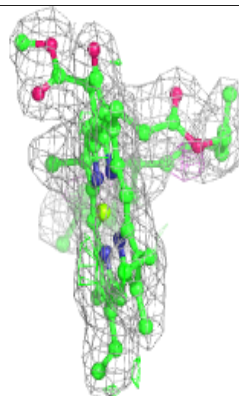
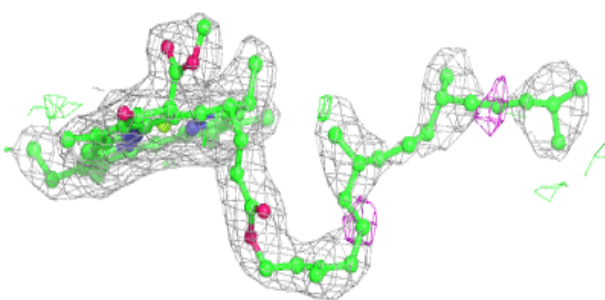
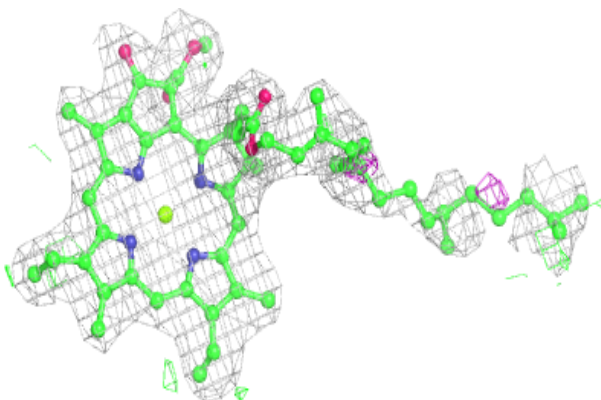


**Electron density around CLA B 606:**

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

**Electron density around CLA a 409:**

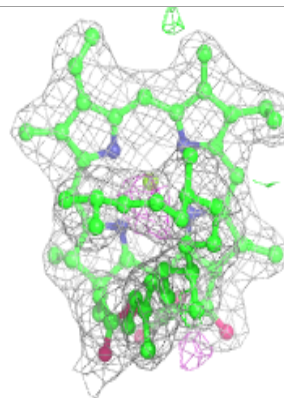
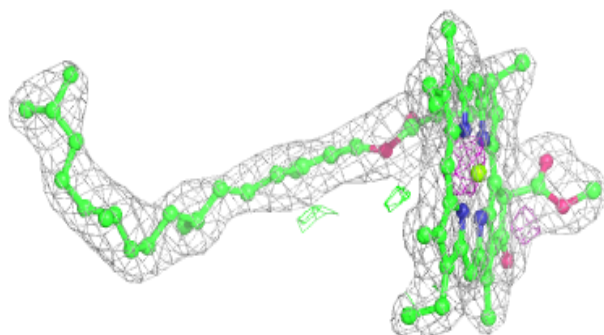
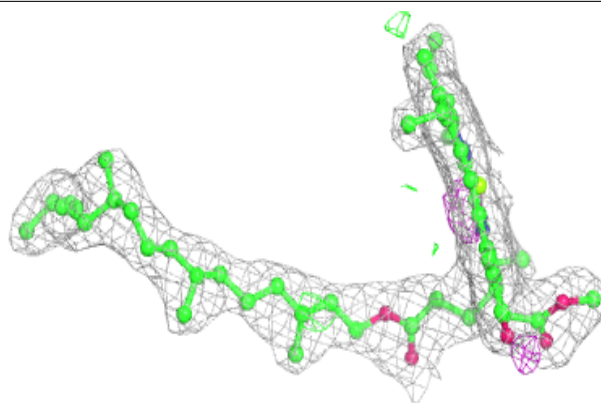
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



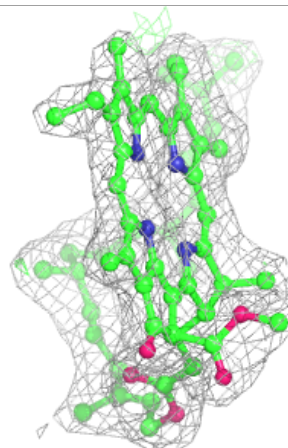
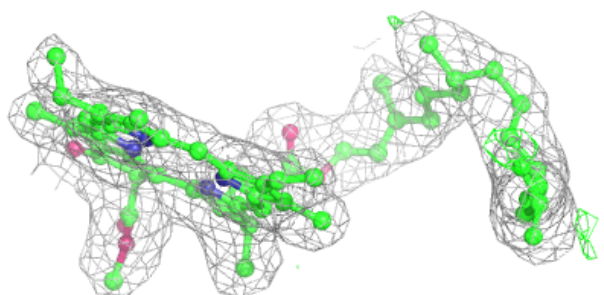
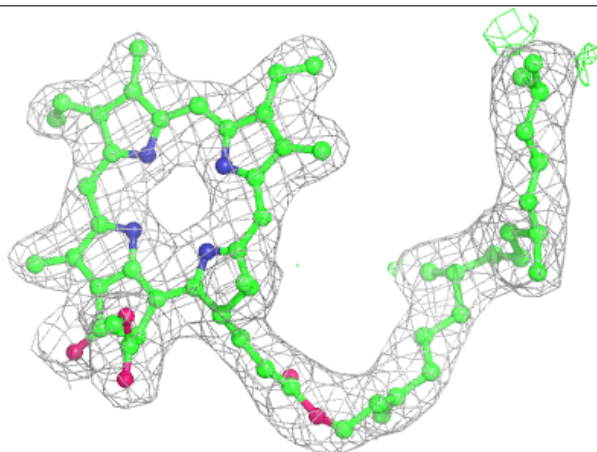


**Electron density around CLA b 614:**

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

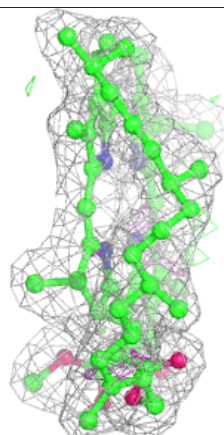
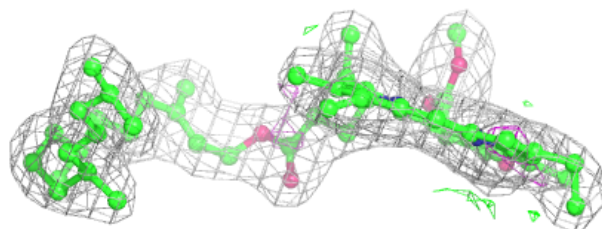
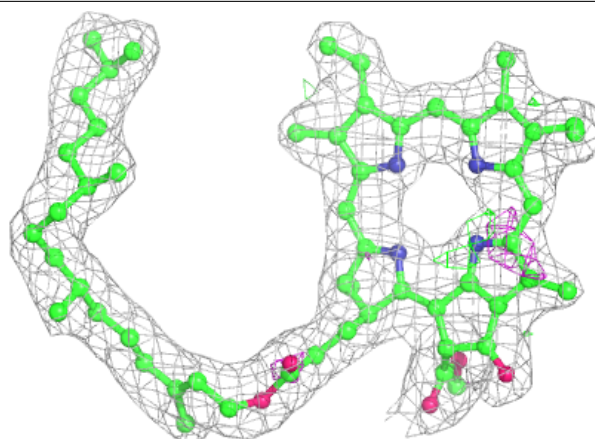
**Electron density around PHO D 402 (A):**

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

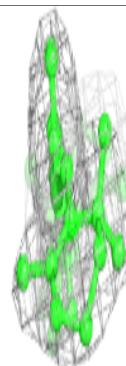
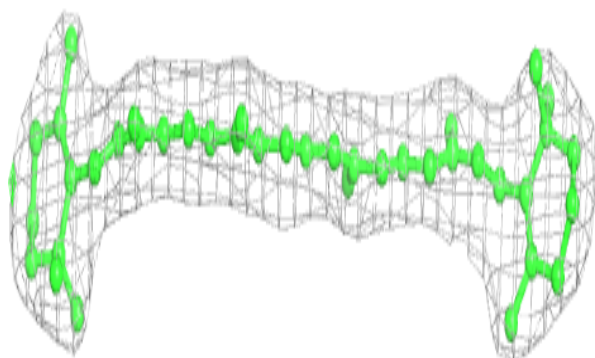
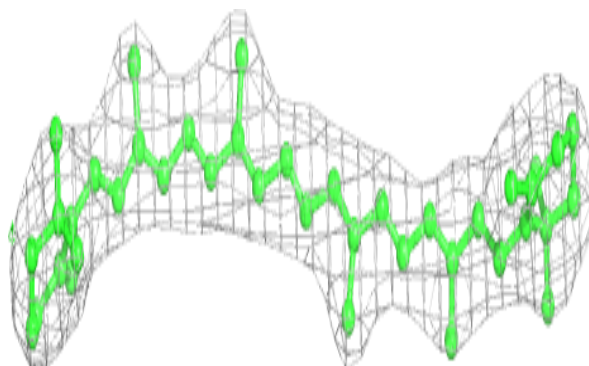


**Electron density around PHO A 407:**

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

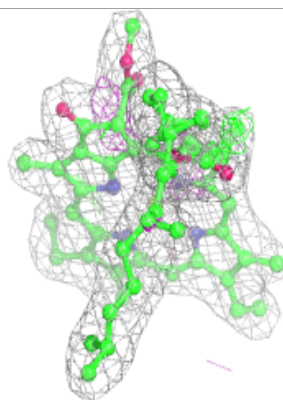
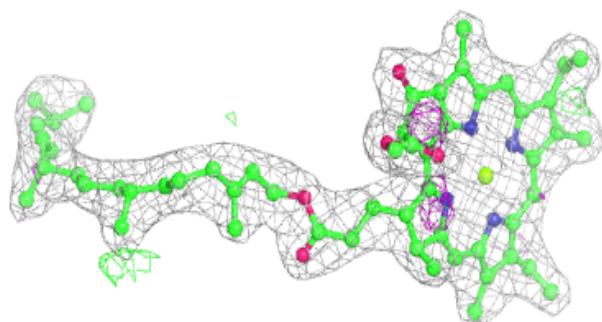
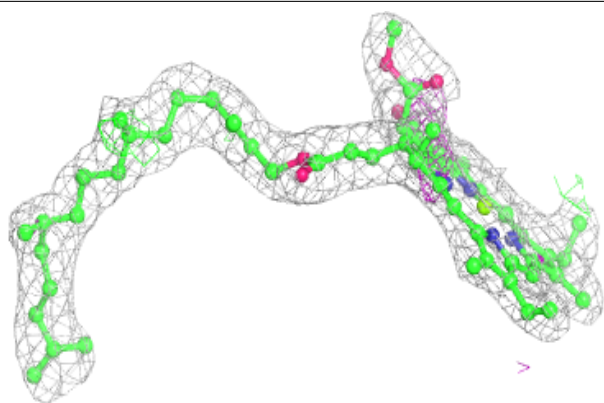
**Electron density around BCR C 515:**

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

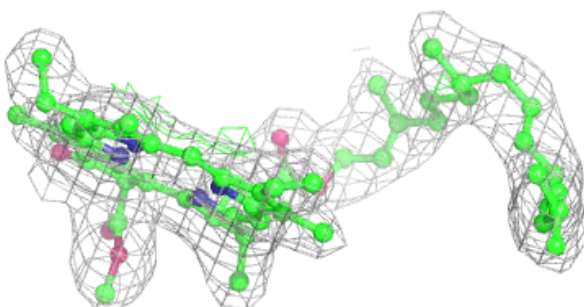
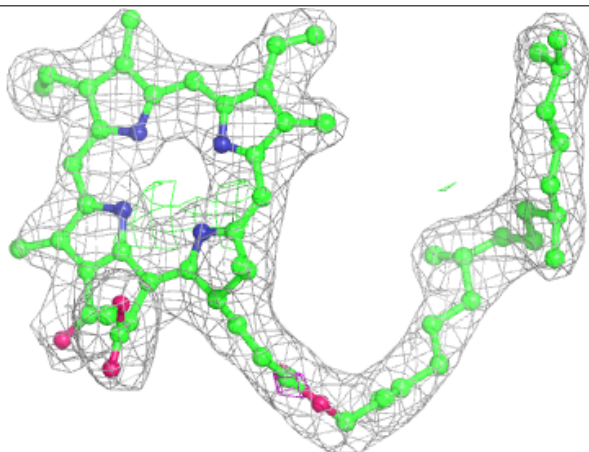


**Electron density around CLA d 404:**

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

**Electron density around PHO d 402 (B):**

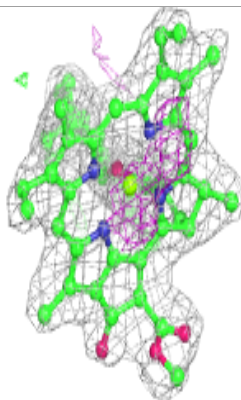
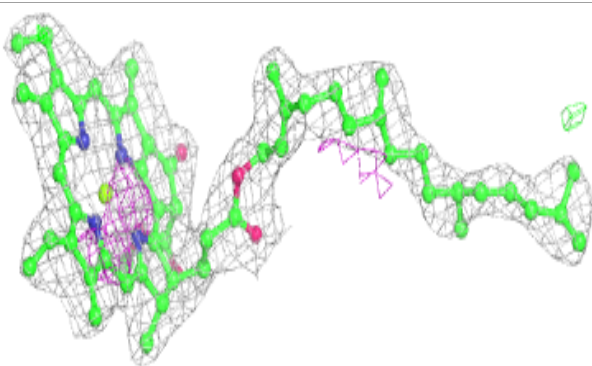
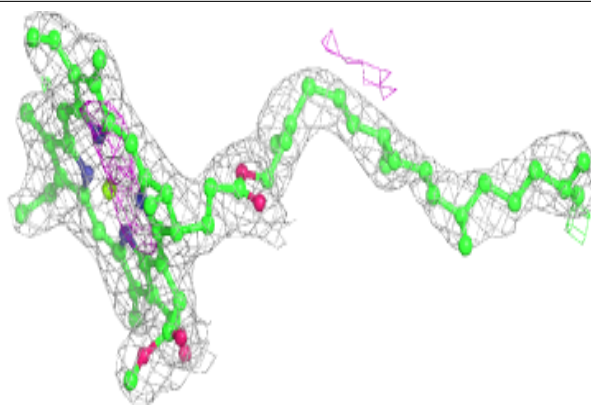
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



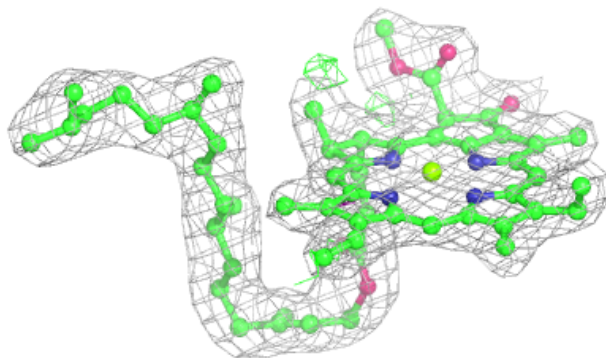
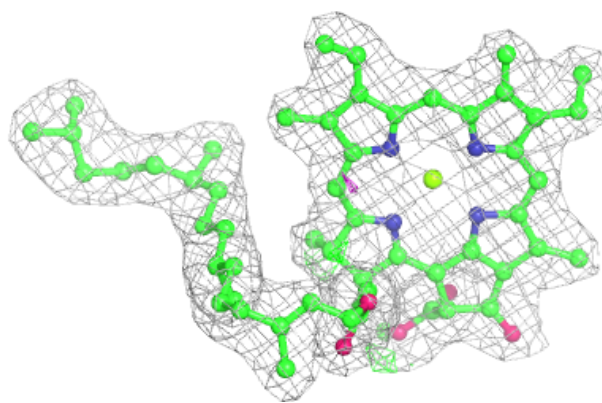


**Electron density around CLA c 506:**

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

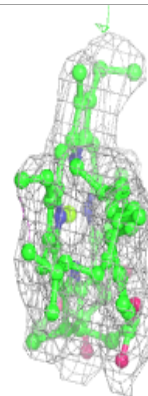
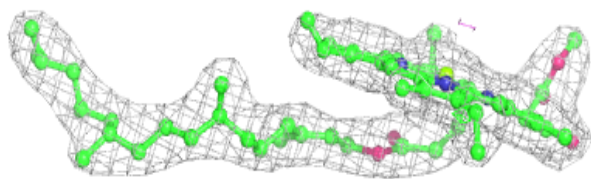
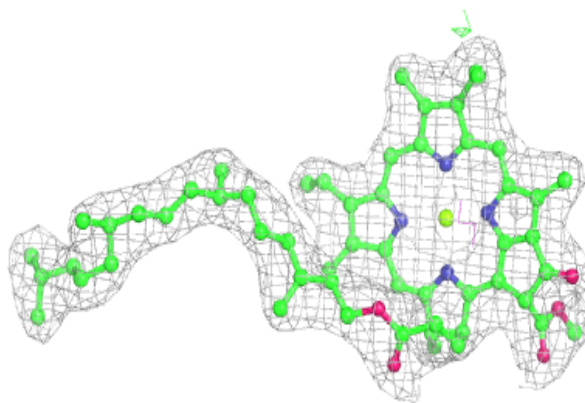
**Electron density around CLA A 405:**

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

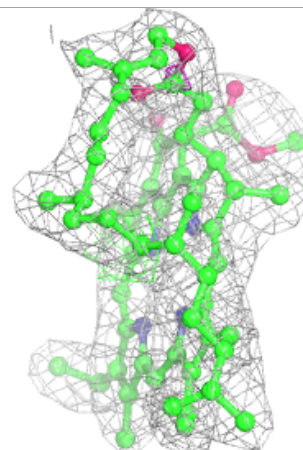
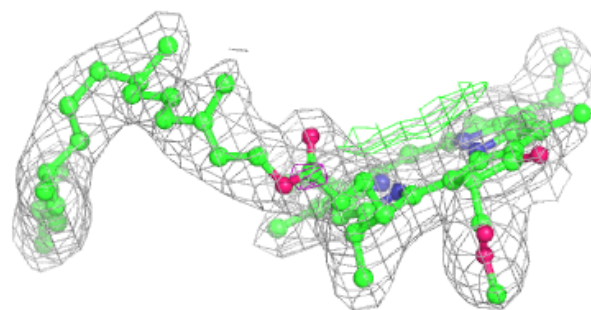
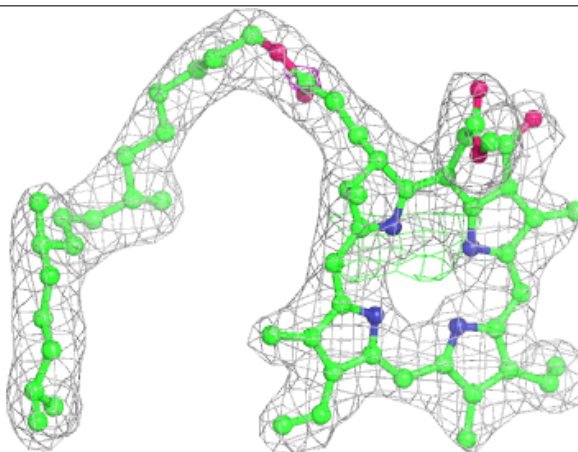


**Electron density around CLA B 604:**

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

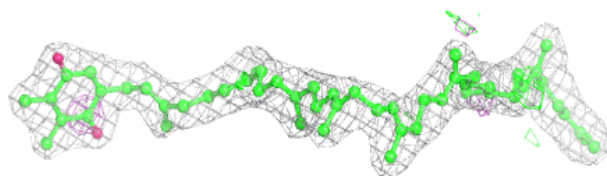
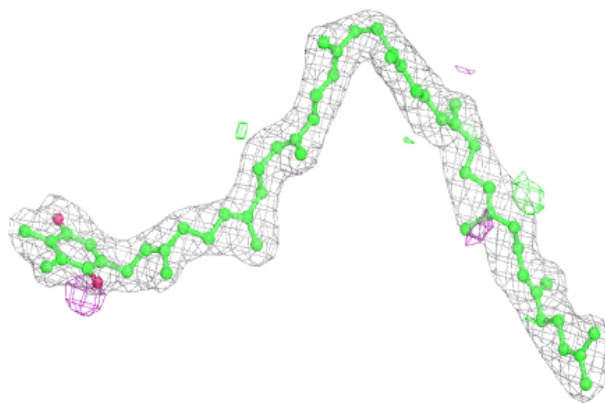
**Electron density around PHO d 402 (A):**

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

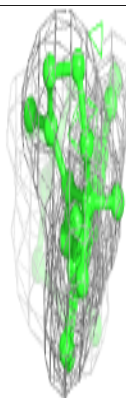
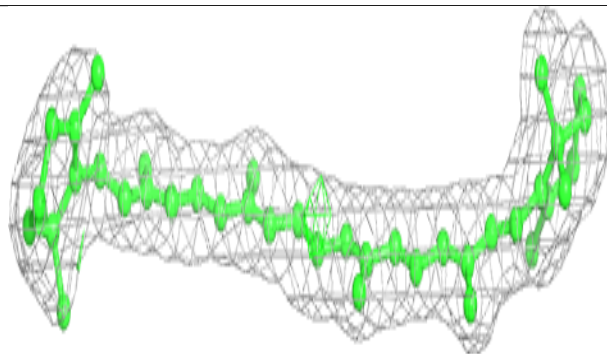
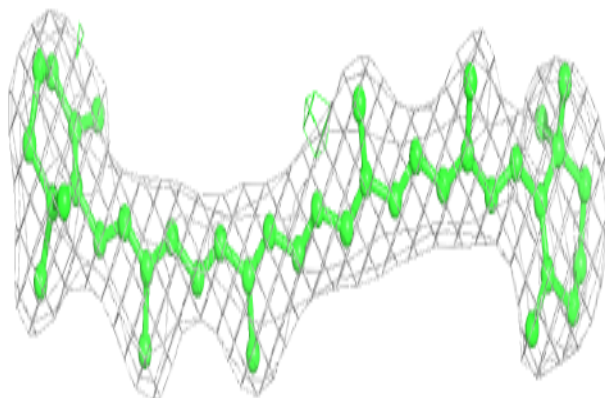


**Electron density around PL9 D 408 (B):**

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

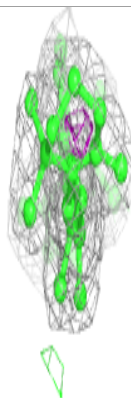
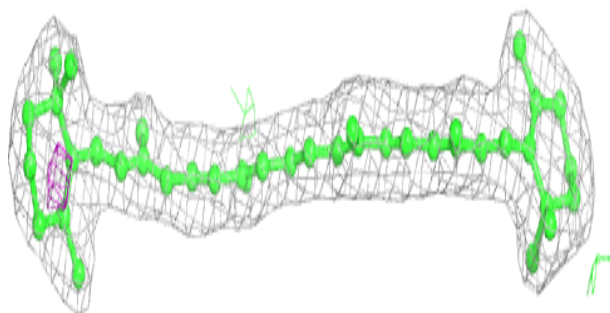
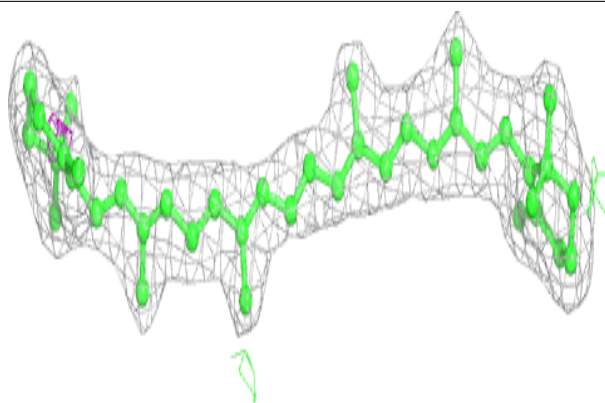
**Electron density around BCR B 620:**

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

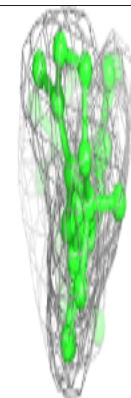
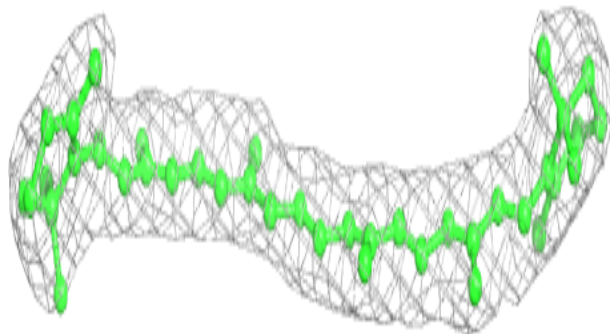
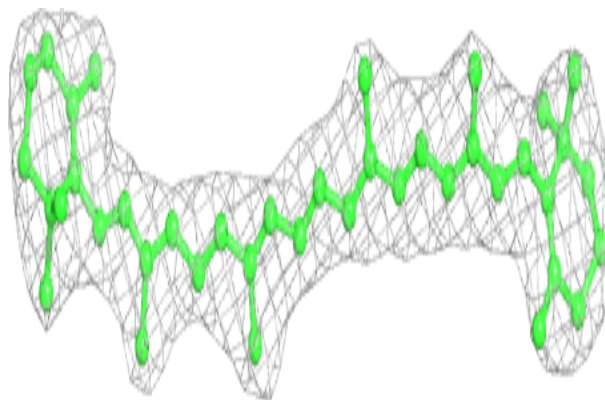


**Electron density around BCR a 412:**

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

**Electron density around BCR b 628:**

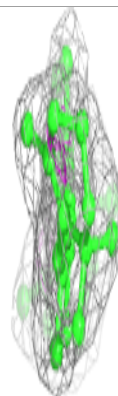
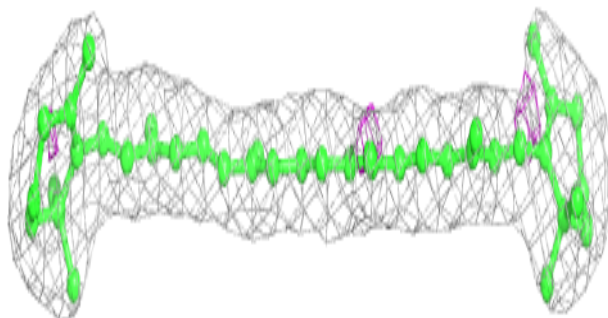
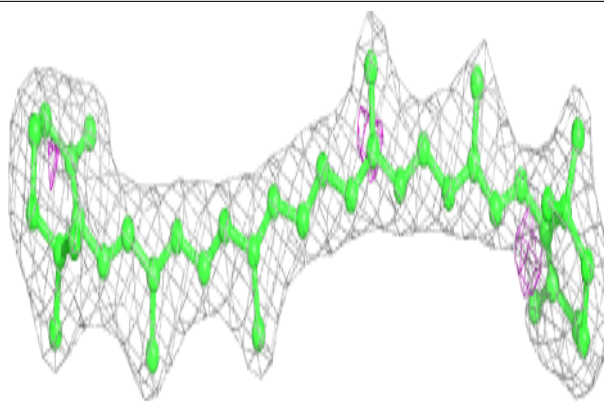
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



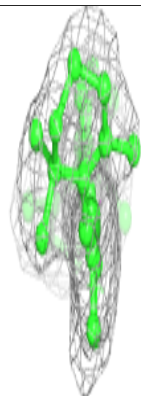
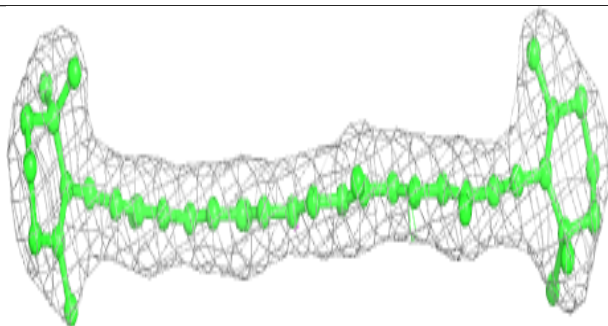
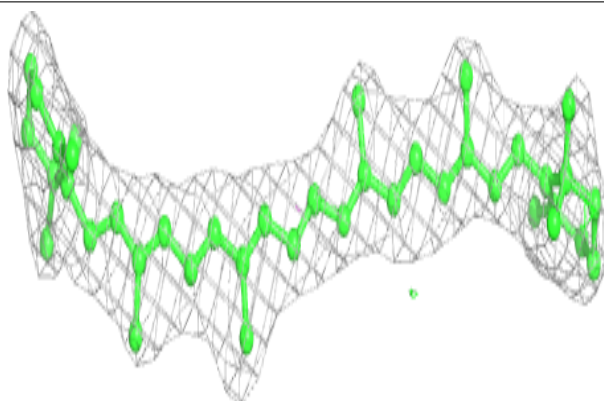


**Electron density around BCR B 619:**

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

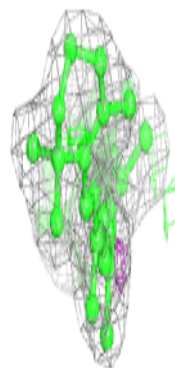
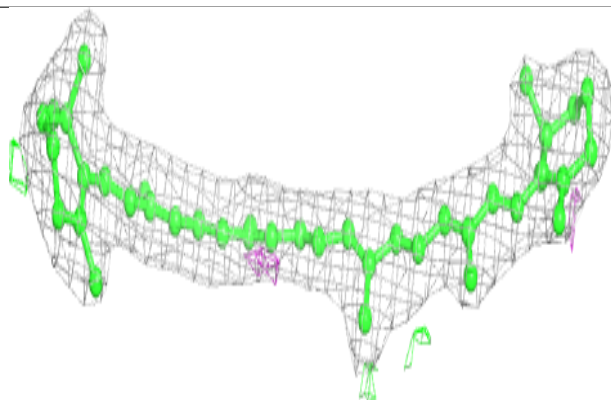
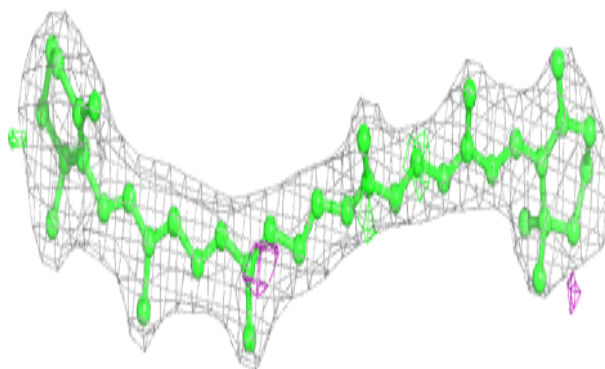
**Electron density around BCR c 518:**

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

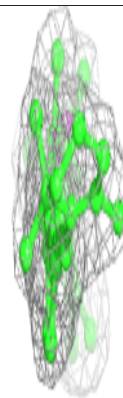
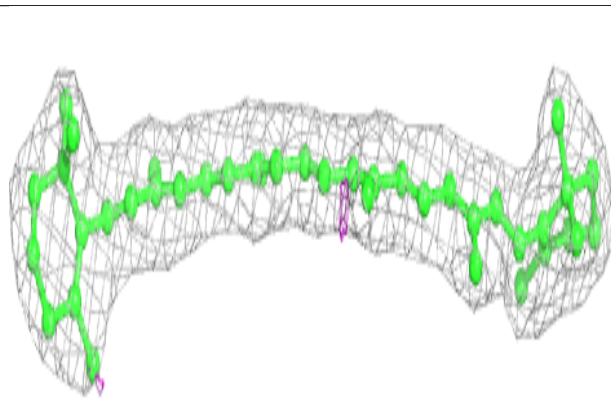
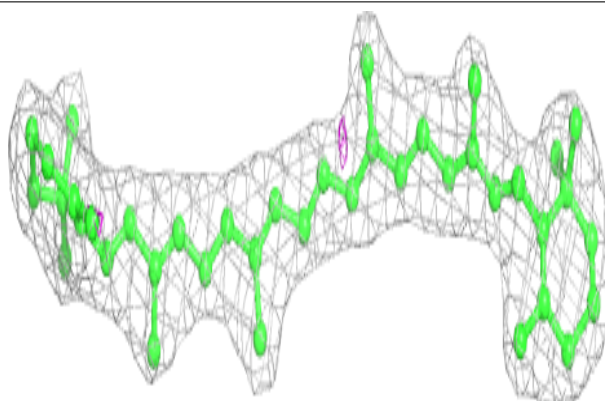


**Electron density around BCR t 101:**

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

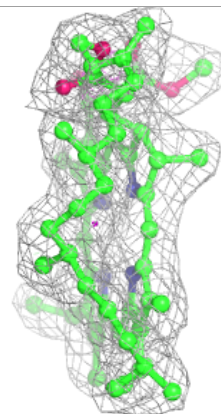
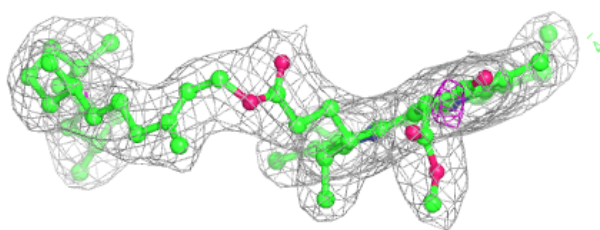
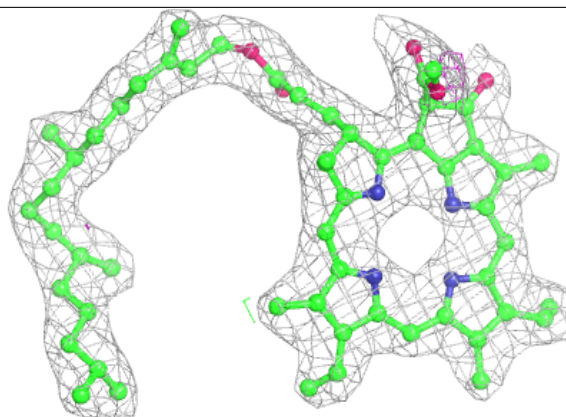
**Electron density around BCR B 618:**

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

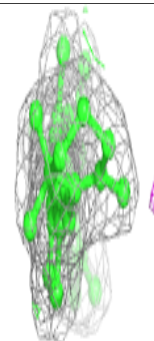
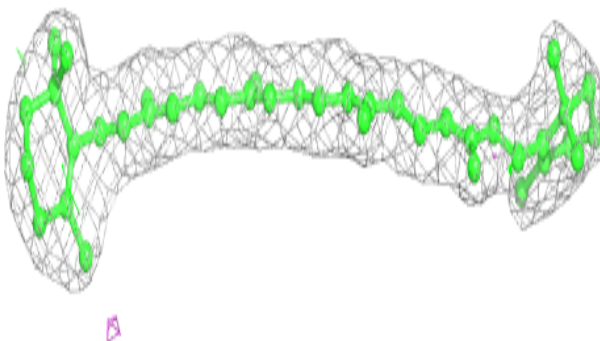
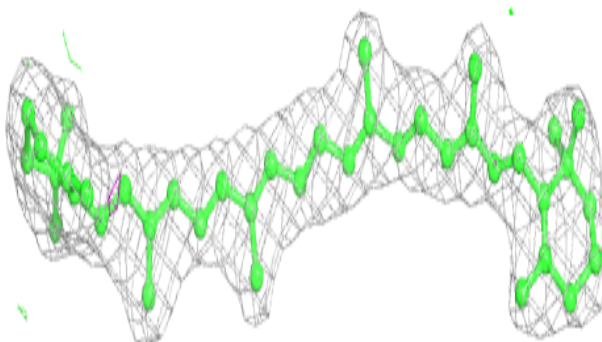


**Electron density around PHO a 410:**

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

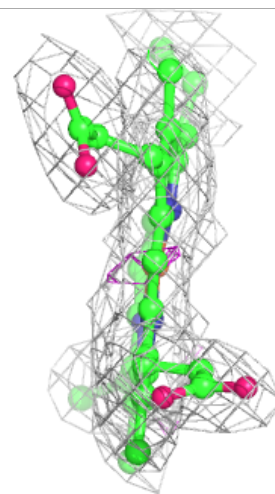
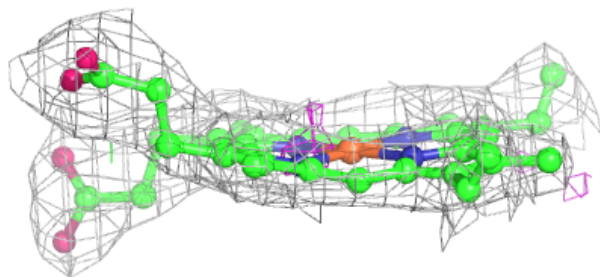
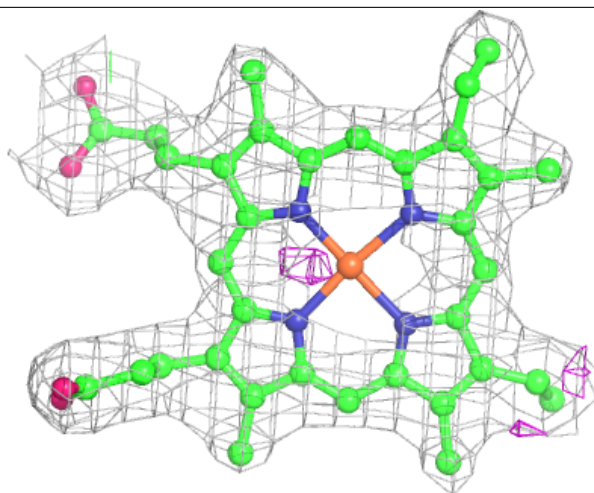
**Electron density around BCR b 626:**

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

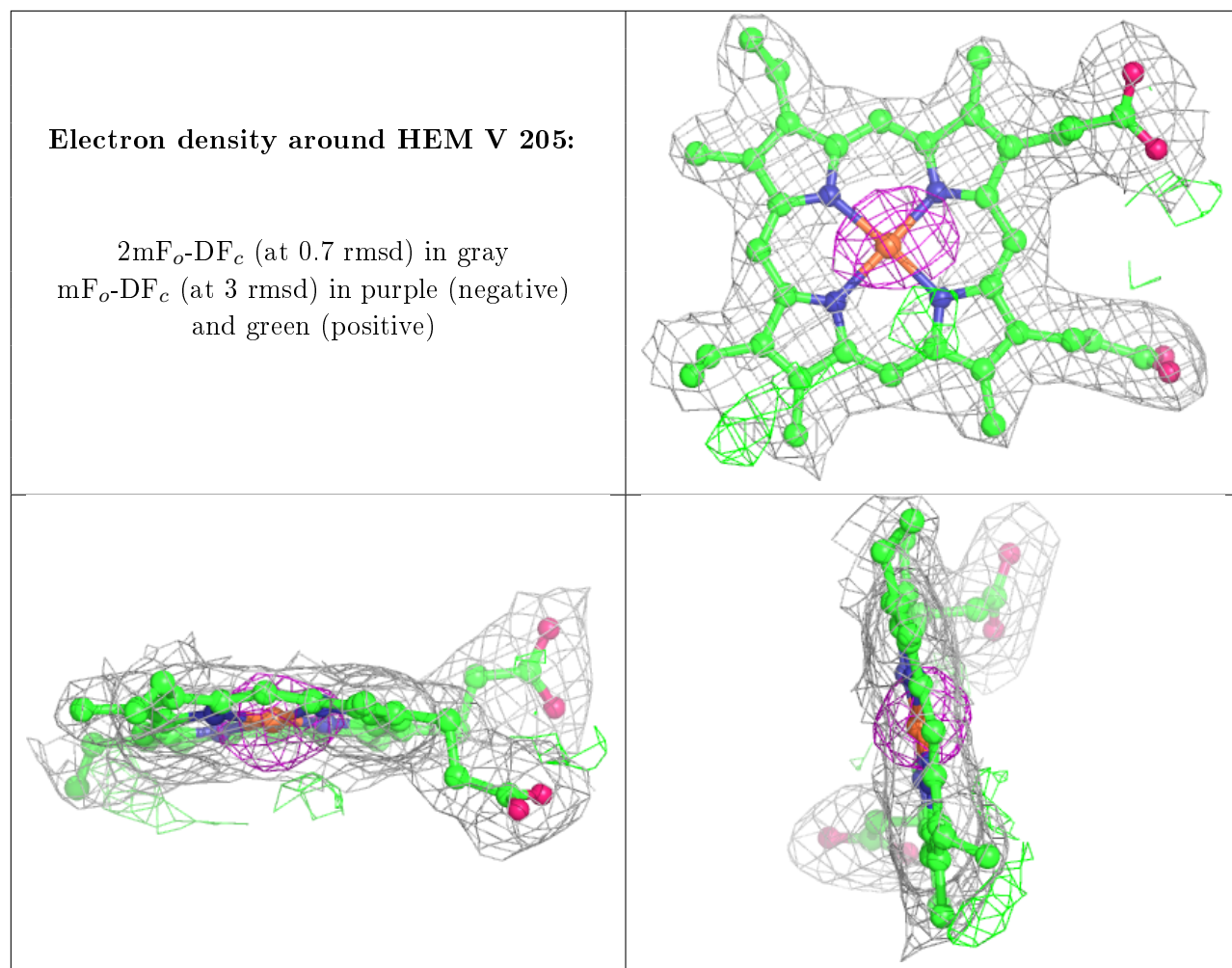


**Electron density around HEM v 206:**

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







## 6.5 Other polymers ⓘ

There are no such residues in this entry.