



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:31 AM BST

PDB ID : 6JLM  
Title : XFEL structure of cyanobacterial photosystem II (dark state, dataset2)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
Resolution : 2.35 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

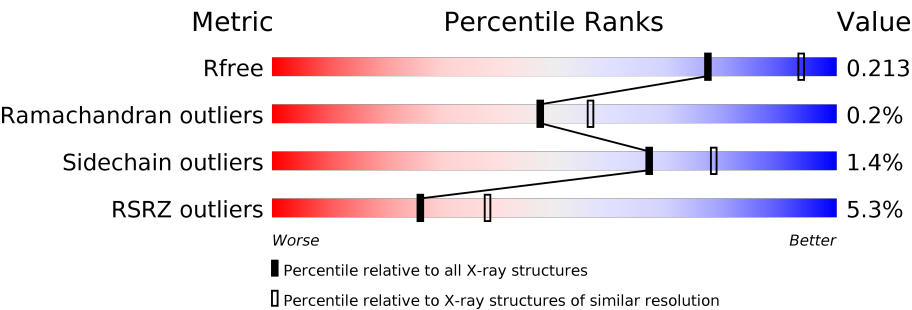
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

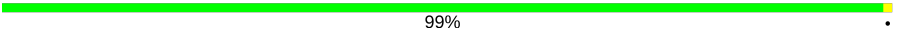
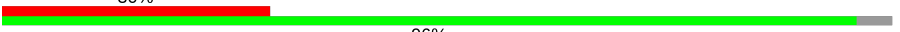

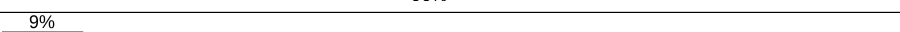
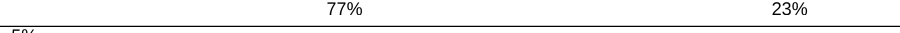

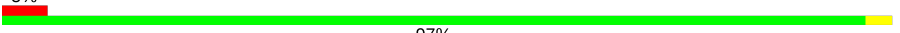

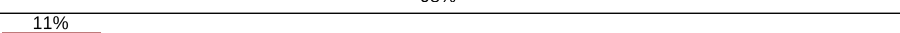
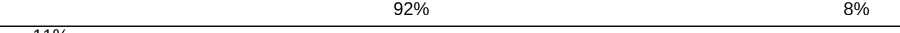

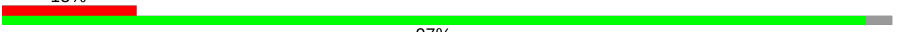

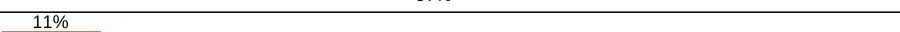
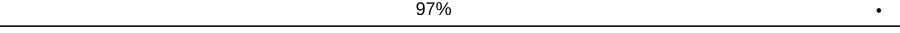
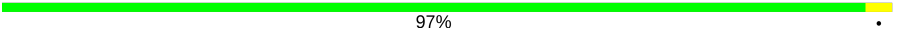
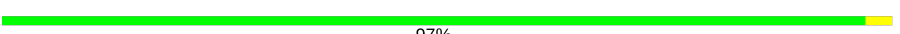

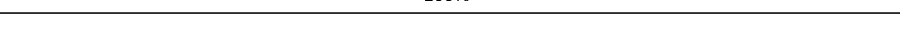


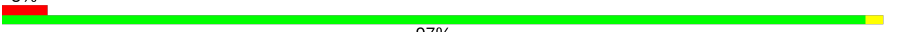

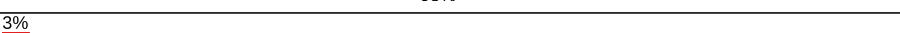

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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>0%</div><div>97%</div><div>..</div></div>
1	a	344	<div><div>4%</div><div>96%</div><div>..</div></div>
2	B	505	<div><div>3%</div><div>99%</div><div>.</div></div>
2	b	505	<div><div>6%</div><div>99%</div><div></div></div>
3	C	455	<div><div>4%</div><div>98%</div><div>..</div></div>
3	c	455	<div><div>2%</div><div>98%</div><div>.</div></div>
4	D	342	<div><div>0%</div><div>99%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
4	d	342	 99%
5	E	84	 30% 96%
5	e	84	 18% 96%
6	F	44	 9% 77% 23%
6	f	44	 5% 70% 27%
7	H	65	 5% 97%
7	h	65	 5% 98%
8	I	38	 11% 92% 8%
8	i	38	 11% 92% 8%
9	J	39	 15% 97%
9	j	39	 18% 97%
10	K	37	 11% 97%
10	k	37	 97%
11	L	37	 97%
11	l	37	 3% 100%
12	M	36	 89% 6% 6%
12	m	36	 94% 6%
13	O	244	 5% 97%
13	o	244	 2% 98%
14	T	32	 3% 91% 6%
14	t	32	 88% 6% 6%
15	U	104	 1% 89% 7%
15	u	104	 93% 7%
16	V	137	 1% 99%
16	v	137	 1% 100%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	407	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	405	X	-	-	-
24	CLA	a	406	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	c	902	X	-	-	-
24	CLA	c	903	X	-	-	-
24	CLA	c	904	X	-	-	-
24	CLA	c	905	X	-	-	-
24	CLA	c	906	X	-	-	-
24	CLA	c	907	X	-	-	-
24	CLA	c	908	X	-	-	-
24	CLA	c	909	X	-	-	-
24	CLA	c	910	X	-	-	-
24	CLA	c	911	X	-	-	-
24	CLA	c	912	X	-	-	-
24	CLA	c	913	X	-	-	-
24	CLA	c	914	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
24	CLA	d	406	X	-	-	-
28	GOL	V	204	-	-	-	X
29	LMT	F	101	-	-	-	X
37	DGD	e	101	-	-	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 54101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

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	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
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	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O		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		98	0	0
			239	163	41	35				

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

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

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

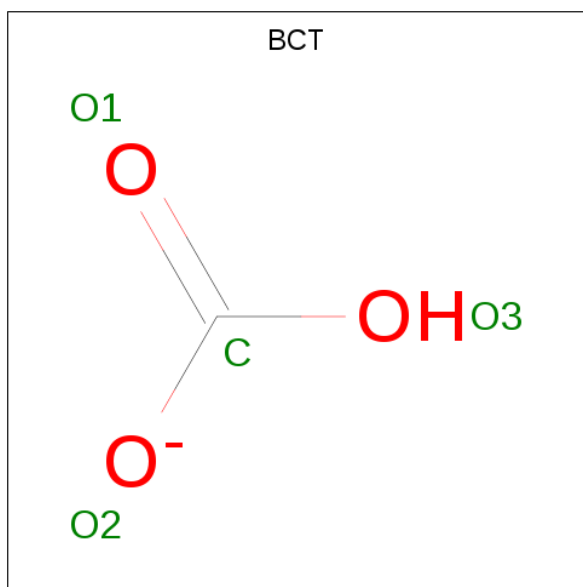
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

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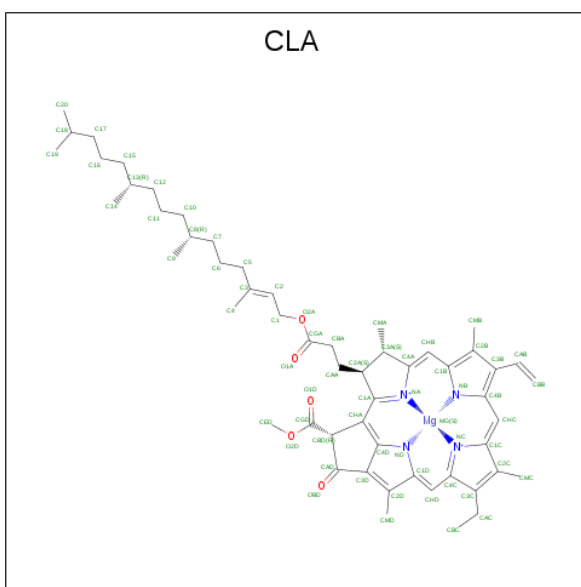
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

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



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

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

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

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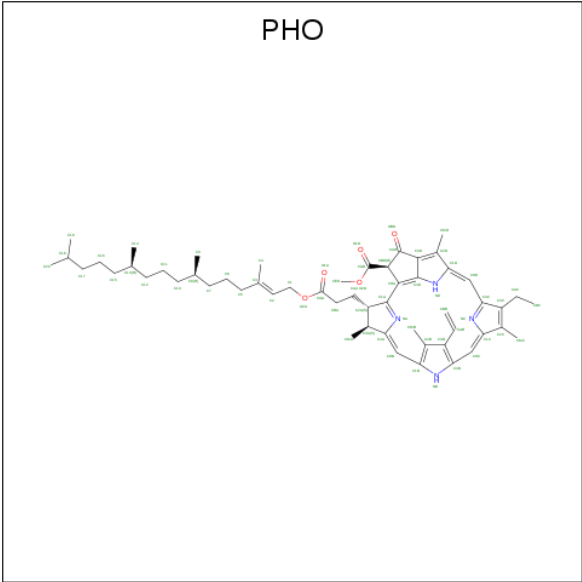
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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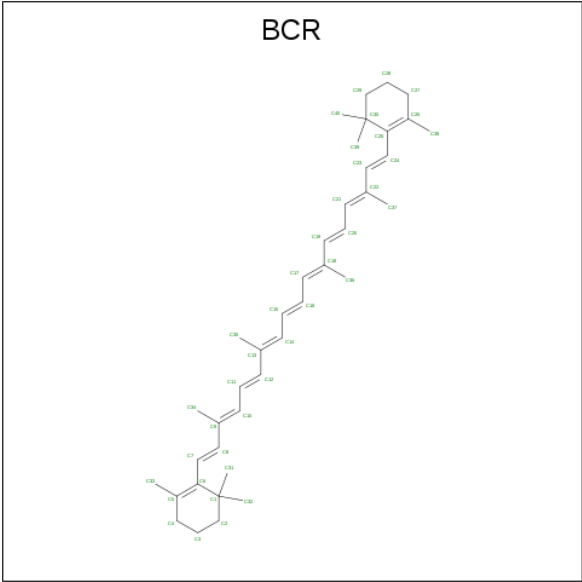
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



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

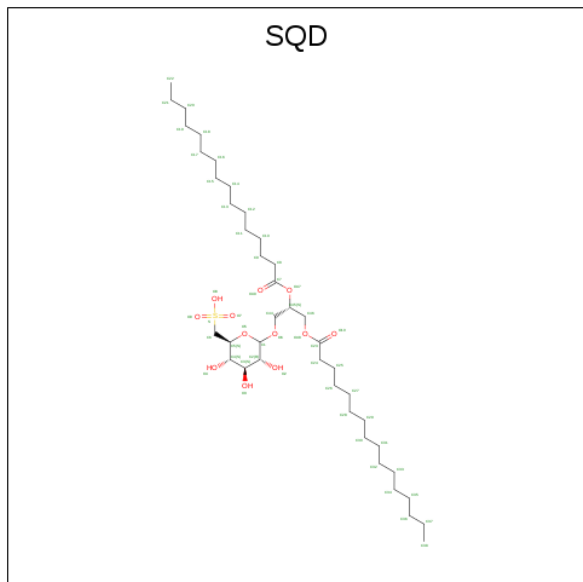
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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



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



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

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



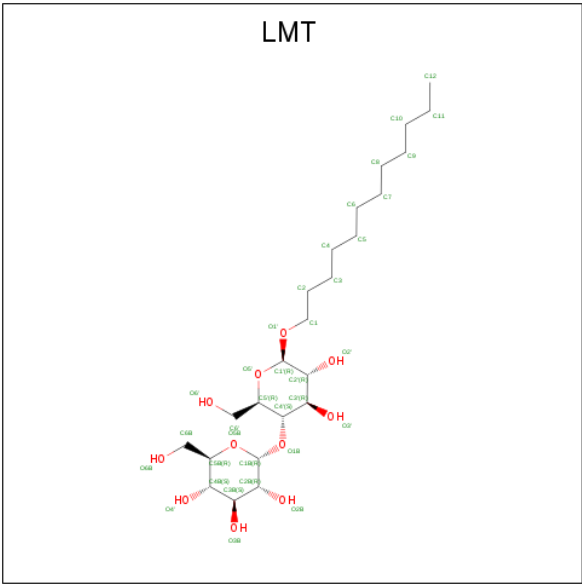
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

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

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



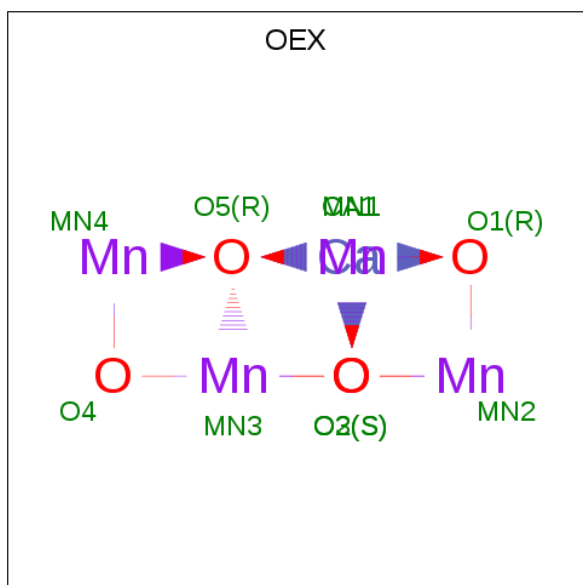
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total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

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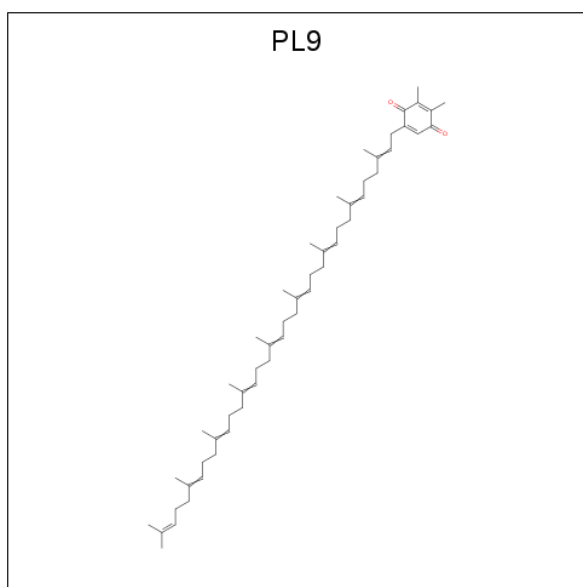
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	t	1	Total	C	O	0	0
			25	19	6		

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



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

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



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

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

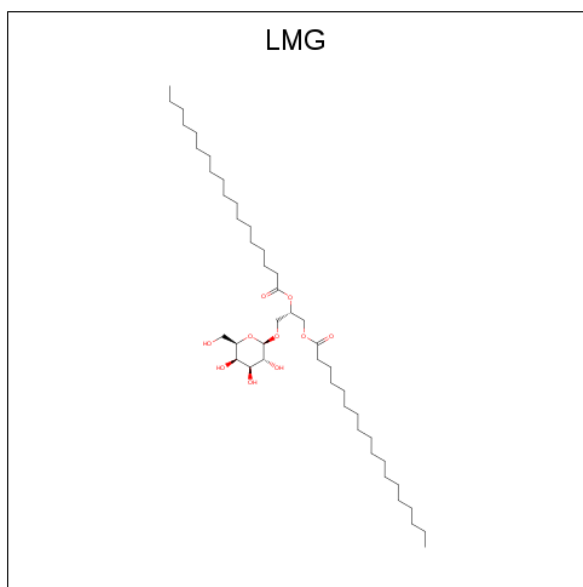
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	a	1	Total	C	O	0	0
			30	25	5		
32	c	1	Total	C	O	0	0
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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	x	1	Total C O 18 16 2	0	0
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	2	Total C O 53 47 6	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-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 51 41 10	0	0
33	B	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0

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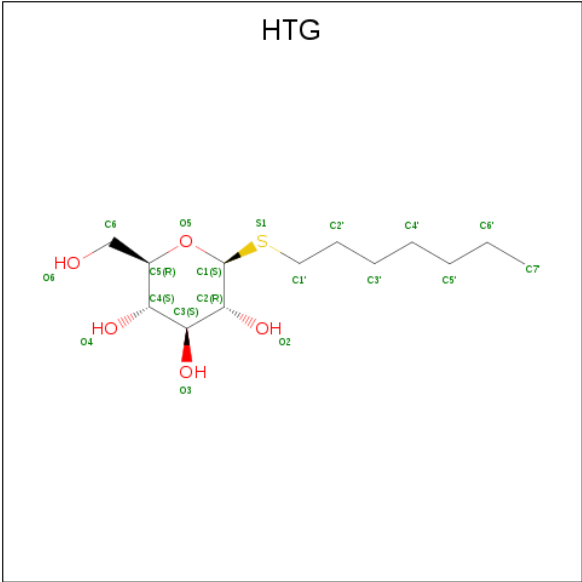
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	J	1	Total	C	O	0	0
			51	41	10		
33	Y	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total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

- 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).





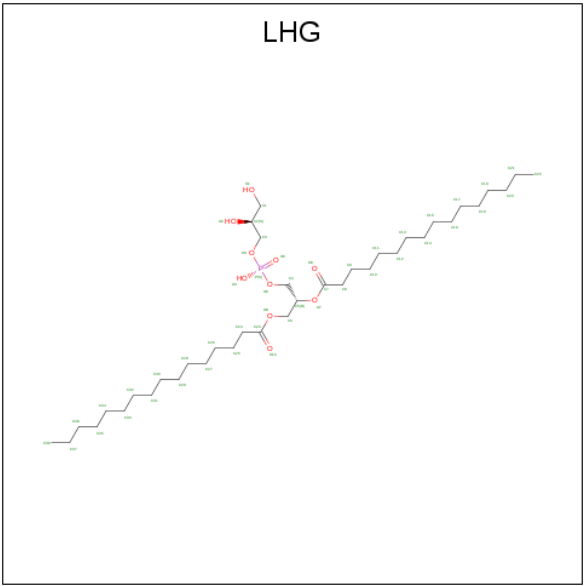
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	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-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



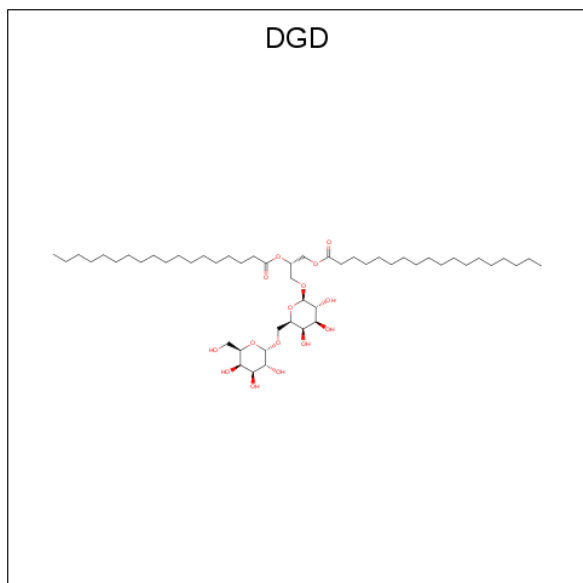
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			42	31	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	a	1	Total	C	O	P	0	0
			42	31	10	1		
36	b	1	Total	C	O	P	0	0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

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

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



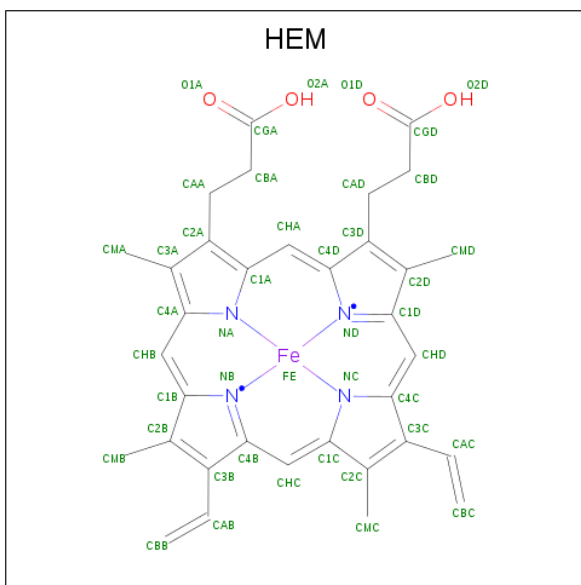
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total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

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

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



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	164	Total O 167 167	0	3
40	B	295	Total O 299 299	0	4
40	C	232	Total O 234 234	0	2
40	D	140	Total O 144 144	0	4
40	E	30	Total O 31 31	0	1
40	F	10	Total O 10 10	0	0
40	H	48	Total O 48 48	0	0
40	I	6	Total O 6 6	0	0
40	J	12	Total O 12 12	0	0
40	K	7	Total O 7 7	0	0
40	L	14	Total O 15 15	0	1
40	M	13	Total O 13 13	0	0
40	O	179	Total O 181 181	0	2
40	T	16	Total O 17 17	0	1
40	U	80	Total O 80 80	0	0
40	V	114	Total O 116 116	0	2
40	Y	4	Total O 4 4	0	0
40	X	9	Total O 9 9	0	0
40	Z	1	Total O 1 1	0	0
40	a	158	Total O 159 159	0	1
40	b	262	Total O 265 265	0	3
40	c	207	Total O 210 210	0	3

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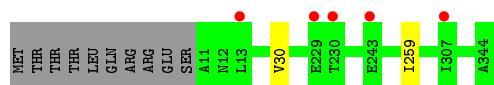
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	d	129	Total 132	O 132	0	3
40	e	19	Total 19	O 19	0	0
40	f	6	Total 6	O 6	0	0
40	h	40	Total 40	O 40	0	0
40	i	4	Total 4	O 4	0	0
40	j	6	Total 6	O 6	0	0
40	k	7	Total 7	O 7	0	0
40	l	10	Total 10	O 10	0	0
40	m	15	Total 15	O 15	0	0
40	o	155	Total 155	O 155	0	0
40	t	11	Total 11	O 11	0	0
40	u	97	Total 97	O 97	0	0
40	v	77	Total 78	O 78	0	1
40	y	2	Total 2	O 2	0	0
40	x	6	Total 6	O 6	0	0

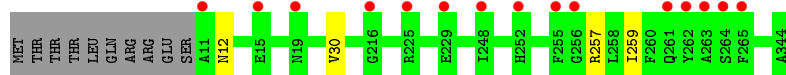
### 3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1



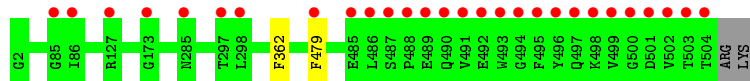
- Molecule 1: Photosystem II protein D1



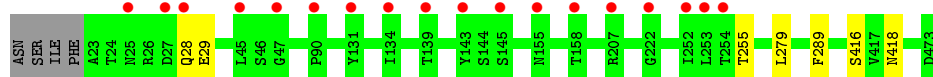
- Molecule 2: Photosystem II CP47 reaction center protein



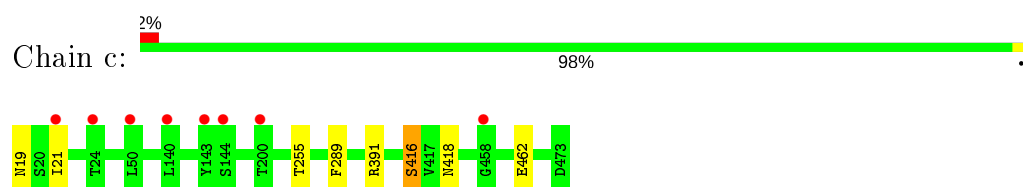
- Molecule 2: Photosystem II CP47 reaction center protein



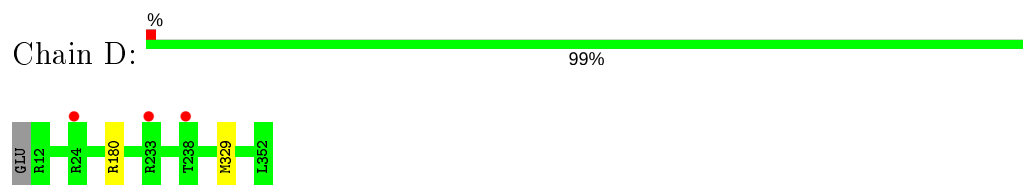
- Molecule 3: Photosystem II CP43 reaction center protein



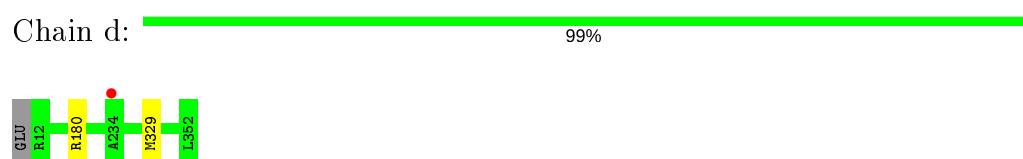
- Molecule 3: Photosystem II CP43 reaction center protein



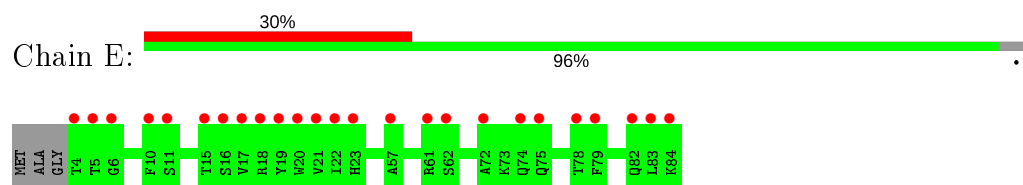
- Molecule 4: Photosystem II D2 protein



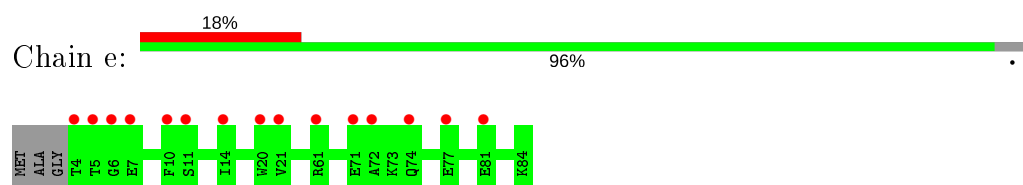
- Molecule 4: Photosystem II D2 protein



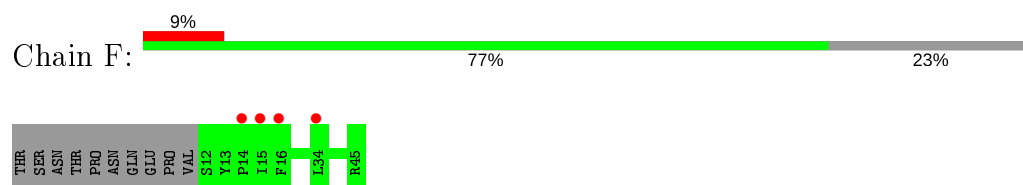
- Molecule 5: Cytochrome b559 subunit alpha



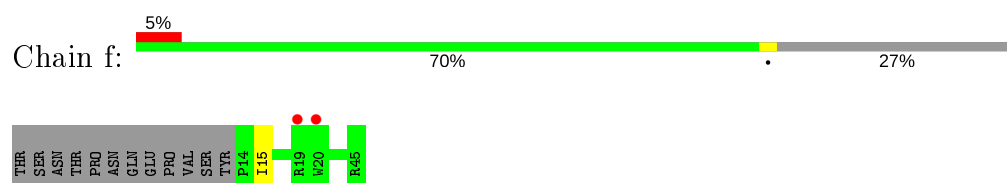
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

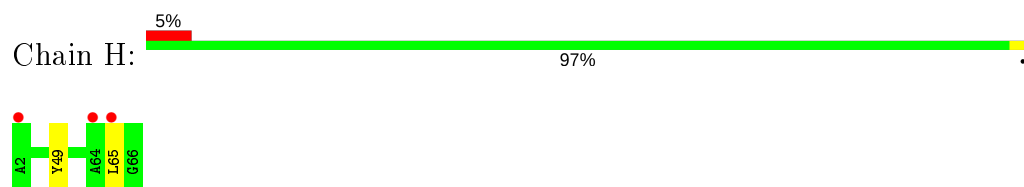


- Molecule 6: Cytochrome b559 subunit beta

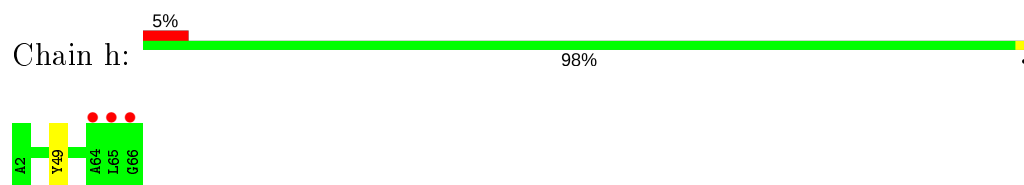




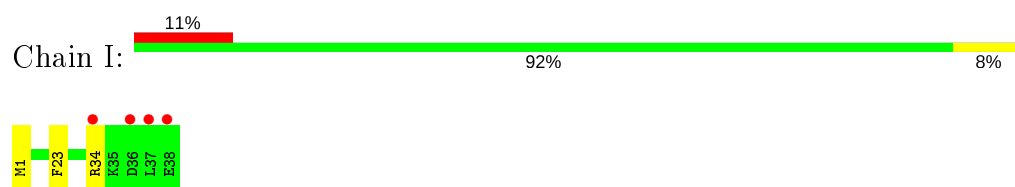
- Molecule 7: Photosystem II reaction center protein H



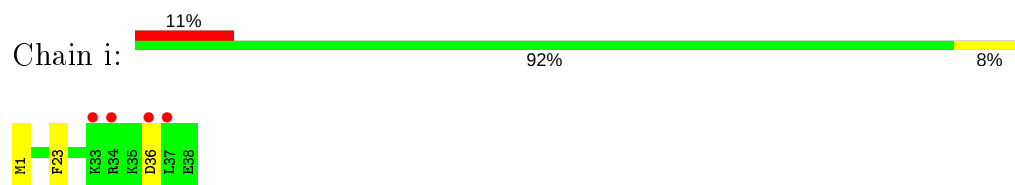
- Molecule 7: Photosystem II reaction center protein H



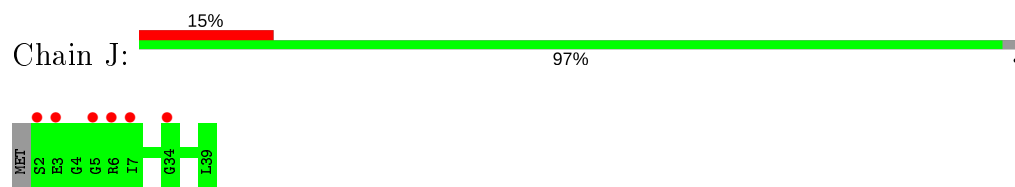
- Molecule 8: Photosystem II reaction center protein I



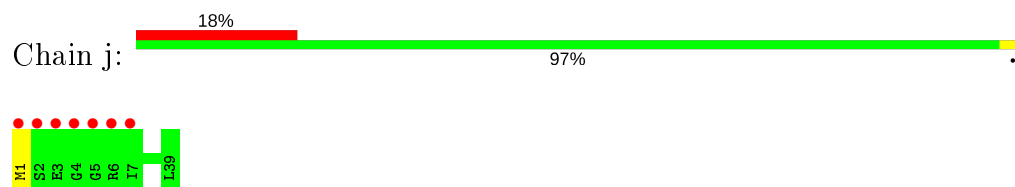
- Molecule 8: Photosystem II reaction center protein I



- 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: 97%



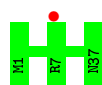
- Molecule 11: Photosystem II reaction center protein L

Chain L: 97%



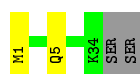
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%



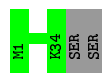
- Molecule 12: Photosystem II reaction center protein M

Chain M: 6% 6%



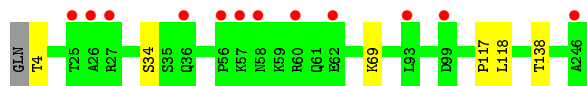
- Molecule 12: Photosystem II reaction center protein M

Chain m: 6%



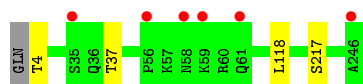
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 97%

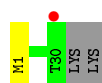
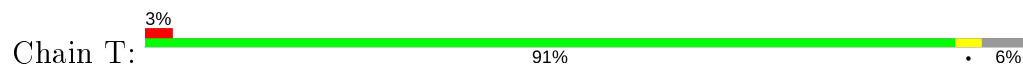


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

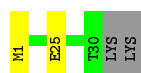
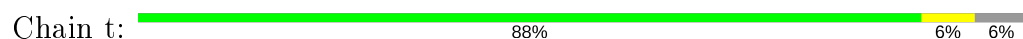
Chain o: 98%



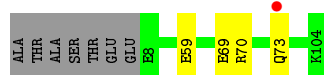
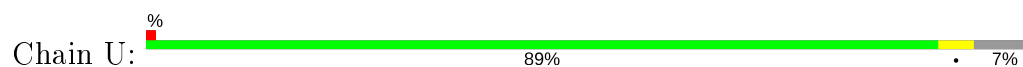
- Molecule 14: Photosystem II reaction center protein T



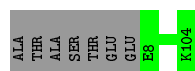
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



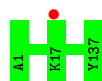
- Molecule 15: Photosystem II 12 kDa extrinsic protein



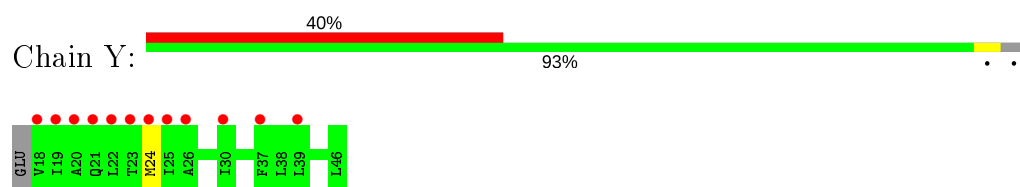
- Molecule 16: Cytochrome c-550



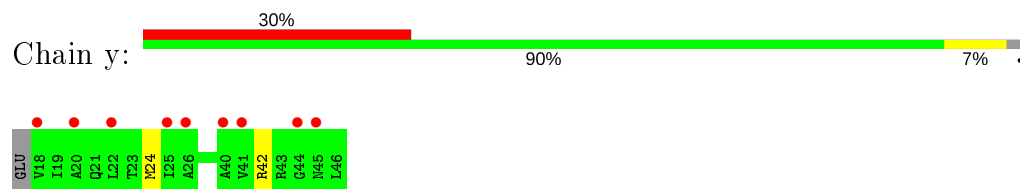
- Molecule 16: Cytochrome c-550



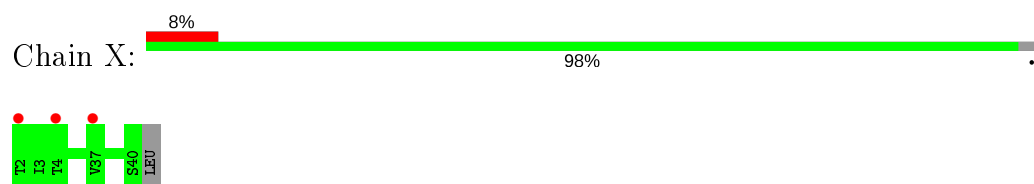
- Molecule 17: Photosystem II reaction center protein Ycf12



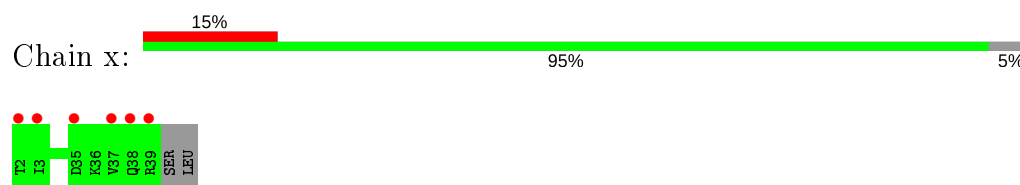
- Molecule 17: Photosystem II reaction center protein Ycf12



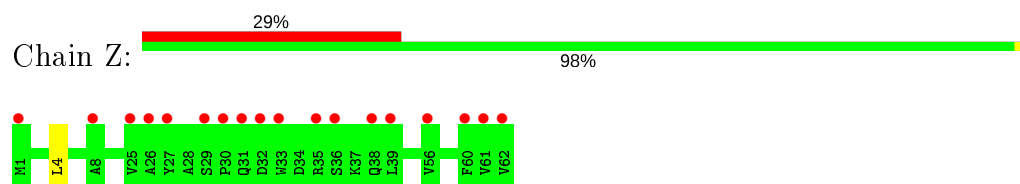
- Molecule 18: Photosystem II reaction center protein X



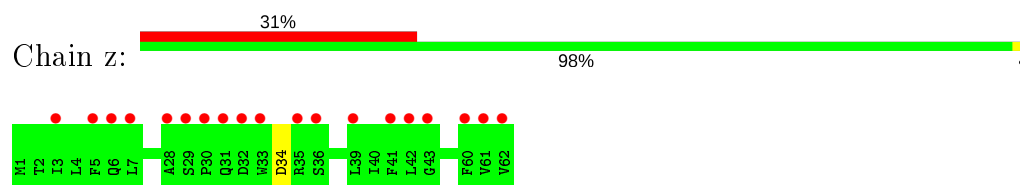
- Molecule 18: Photosystem II reaction center protein X



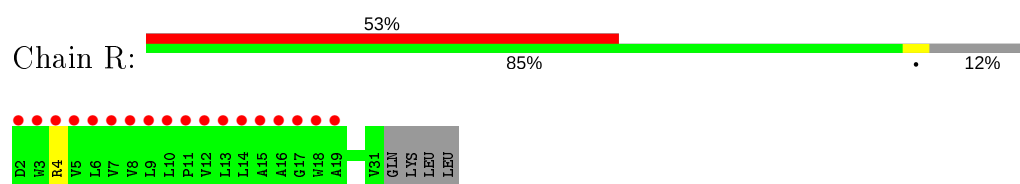
- Molecule 19: Photosystem II reaction center protein Z



- 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 – 2.35 121.57 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.35) 99.9 (121.57-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.153 , 0.209 0.160 , 0.213	Depositor DCC
$R_{free}$ test set	17809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 83.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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, FE2, SQD, BCT, HEM, FME, UNL, HTG, BCR, LMG

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	0.46	0/2728	0.56	0/3719
1	a	0.47	0/2748	0.57	0/3746
2	B	0.44	0/4191	0.54	0/5709
2	b	0.44	0/4198	0.54	0/5720
3	C	0.40	0/3626	0.52	0/4936
3	c	0.39	0/3676	0.52	0/5004
4	D	0.48	0/2818	0.56	0/3840
4	d	0.47	0/2818	0.56	0/3840
5	E	0.37	0/693	0.51	0/944
5	e	0.36	0/695	0.52	0/948
6	F	0.44	0/284	0.53	0/387
6	f	0.44	0/265	0.54	0/360
7	H	0.38	0/535	0.57	0/728
7	h	0.37	0/524	0.51	0/713
8	I	0.37	0/311	0.51	0/419
8	i	0.40	0/311	0.49	0/419
9	J	0.37	0/278	0.43	0/376
9	j	0.37	0/286	0.46	0/386
10	K	0.36	0/303	0.54	0/416
10	k	0.37	0/303	0.50	0/416
11	L	0.41	0/319	0.51	0/433
11	l	0.45	0/319	0.48	0/433
12	M	0.52	0/270	0.69	0/368
12	m	0.49	0/262	0.62	0/357
13	O	0.39	0/1958	0.56	0/2654
13	o	0.39	0/1937	0.57	0/2625
14	T	0.45	0/266	0.54	0/362
14	t	0.53	0/266	0.52	0/362
15	U	0.41	0/785	0.56	0/1064
15	u	0.41	0/785	0.56	0/1064
16	V	0.38	0/1096	0.52	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.37	0/1085	0.54	0/1473
17	Y	0.36	0/216	0.50	0/289
17	y	0.33	0/216	0.46	0/289
18	X	0.35	0/290	0.47	0/392
18	x	0.34	0/284	0.47	0/384
19	Z	0.32	0/490	0.48	0/669
19	z	0.29	0/490	0.50	0/669
20	R	0.24	0/245	0.39	0/338
All	All	0.42	0/43170	0.54	0/58738

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	328 (98%)	5 (2%)	2 (1%)	25	27
1	a	338/344 (98%)	331 (98%)	5 (2%)	2 (1%)	25	27
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	453/455 (100%)	442 (98%)	9 (2%)	2 (0%)	34	38
3	c	459/455 (101%)	448 (98%)	9 (2%)	2 (0%)	34	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	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%)	1 (3%)	1 (3%)	5	2
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	242 (97%)	6 (2%)	1 (0%)	34	38
13	o	246/244 (101%)	240 (98%)	6 (2%)	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%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5282/5384 (98%)	5151 (98%)	121 (2%)	10 (0%)	47	56

All (10) 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
8	I	34	ARG
1	a	259	ILE
13	O	138	THR
1	A	30	VAL
1	A	259	ILE
1	a	30	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	273 (99%)	2 (1%)	84	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	82
2	b	413/403 (102%)	411 (100%)	2 (0%)	88	94
3	C	356/356 (100%)	350 (98%)	6 (2%)	60	72
3	c	362/356 (102%)	352 (97%)	10 (3%)	43	53
4	D	277/277 (100%)	275 (99%)	2 (1%)	84	91
4	d	277/277 (100%)	275 (99%)	2 (1%)	84	91
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	74 (100%)	0	100	100

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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	41
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	43
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	68
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	52
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	22
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	42
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	46
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	46
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	53
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	30 (97%)	1 (3%)	39	47
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	61
13	o	211/207 (102%)	206 (98%)	5 (2%)	49	59
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	14
15	U	84/89 (94%)	81 (96%)	3 (4%)	35	43
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	117 (99%)	1 (1%)	81	89
16	v	117/117 (100%)	117 (100%)	0	100	100
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	33
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	8
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%)	51 (98%)	1 (2%)	57	68
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	68
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	39
All	All	4387/4403 (100%)	4324 (99%)	63 (1%)	67	78

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
2	B	472	ARG
2	B	479	PHE
2	B	492	GLU
2	B	505	ARG
3	C	28	GLN
3	C	29	GLU
3	C	255	THR
3	C	279	LEU
3	C	289	PHE
3	C	418	ASN
4	D	180	ARG
4	D	329	MET
7	H	49	TYR
7	H	65	LEU
8	I	23	PHE
10	K	17	ILE
11	L	13	ASN
12	M	5	GLN
13	O	4	THR
13	O	34	SER
13	O	69	LYS
13	O	117	PRO
13	O	118	LEU
15	U	59	GLU
15	U	70	ARG
15	U	73	GLN
16	V	85	GLU
17	Y	24	MET
19	Z	4	LEU
20	R	4	ARG
1	a	12	ASN
1	a	257	ARG
2	b	362	PHE
2	b	479	PHE
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

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Mol	Chain	Res	Type
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	180	ARG
4	d	329	MET
6	f	15	ILE
7	h	49	TYR
8	i	23	PHE
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
13	o	4	THR
13	o	37	THR
13	o	118	LEU
13	o	217[A]	SER
13	o	217[B]	SER
14	t	25[A]	GLU
14	t	25[B]	GLU
17	y	24	MET
17	y	42	ARG
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	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	130	GLN
13	O	147	ASN
16	V	118	HIS
19	Z	58	ASN
1	a	315	ASN
2	b	14	ASN
2	b	53	ASN
2	b	331	ASN

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Mol	Chain	Res	Type
3	c	201	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
15	u	78	ASN
15	u	81	HIS
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	$\# Z  > 2$
14	FME	T	1	14	8,9,10	0.69	0	7,9,11	1.44	1 (14%)
12	FME	m	1	12	8,9,10	0.67	0	7,9,11	1.08	0
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.26	1 (14%)
14	FME	t	1	14	8,9,10	0.80	0	7,9,11	2.51	5 (71%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.23	1 (14%)
12	FME	M	1	12	8,9,10	0.64	0	7,9,11	1.16	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
14	FME	T	1	14	-	3/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.15	116.44	122.82
14	t	1	FME	C-CA-N	3.05	115.23	109.73
14	T	1	FME	O-C-CA	-2.50	118.21	124.78
14	t	1	FME	O-C-CA	-2.47	118.31	124.78
14	t	1	FME	CE-SD-CG	-2.19	92.88	100.40
8	I	1	FME	O-C-CA	-2.15	119.14	124.78
14	t	1	FME	O1-CN-N	-2.10	119.73	125.27
12	M	1	FME	O-C-CA	-2.08	119.34	124.78
8	i	1	FME	CA-N-CN	-2.04	119.68	122.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 251 ligands modelled in this entry, 18 are unknown and 19 are monoatomic - leaving 214 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
28	GOL	V	204	-	5,5,5	0.38	0	5,5,5	0.37	0
31	PL9	A	417	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	23 (33%)
27	SQD	A	414	-	53,54,54	1.03	3 (5%)	62,65,65	1.12	6 (9%)
26	BCR	c	927	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)
30	OEX	A	416	1,3,40	0,15,15	0.00	-	-		
24	CLA	B	614	-	59,73,73	2.06	13 (22%)	67,113,113	2.16	25 (37%)
24	CLA	B	606	-	59,73,73	1.98	12 (20%)	67,113,113	2.24	20 (29%)
31	PL9	d	408	-	55,55,55	0.67	2 (3%)	68,69,69	1.69	16 (23%)
26	BCR	b	624	-	41,41,41	1.09	2 (4%)	56,56,56	1.21	4 (7%)
38	HEM	f	101	5,6	27,50,50	0.82	1 (3%)	17,82,82	2.15	3 (17%)
24	CLA	C	510	-	59,73,73	2.06	13 (22%)	67,113,113	2.18	21 (31%)
24	CLA	b	608	-	59,73,73	1.98	14 (23%)	67,113,113	2.29	21 (31%)
24	CLA	b	607	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	24 (35%)
36	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.11	4 (9%)
26	BCR	b	623	-	41,41,41	1.02	1 (2%)	56,56,56	1.29	7 (12%)
35	HTG	B	625	-	19,19,19	1.05	2 (10%)	23,24,24	1.64	2 (8%)
24	CLA	B	605	-	59,73,73	1.89	13 (22%)	67,113,113	2.20	22 (32%)
24	CLA	d	406	-	59,73,73	2.02	12 (20%)	67,113,113	2.14	20 (29%)
36	LHG	d	411	-	48,48,48	0.94	2 (4%)	51,54,54	1.08	3 (5%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.01	3 (5%)
29	LMT	C	520	-	36,36,36	0.48	0	47,47,47	1.17	4 (8%)
24	CLA	b	610	-	59,73,73	1.97	13 (22%)	67,113,113	2.22	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	a	405	-	59,73,73	2.00	13 (22%)	67,113,113	2.21	24 (35%)
28	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.35	0
26	BCR	A	410	-	41,41,41	1.11	1 (2%)	56,56,56	1.11	4 (7%)
24	CLA	A	409	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	23 (34%)
33	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
24	CLA	b	615	40	59,73,73	2.05	13 (22%)	67,113,113	2.17	24 (35%)
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.41	9 (16%)
28	GOL	V	206	-	5,5,5	0.43	0	5,5,5	0.32	0
24	CLA	B	602	40	59,73,73	2.03	14 (23%)	67,113,113	2.13	17 (25%)
28	GOL	v	205	-	5,5,5	0.33	0	5,5,5	0.47	0
33	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.10	4 (8%)
37	DGD	c	917	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	b	613	-	59,73,73	2.05	13 (22%)	67,113,113	2.24	25 (37%)
26	BCR	B	620	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	10 (17%)
24	CLA	c	913	-	59,73,73	2.03	12 (20%)	67,113,113	2.28	22 (32%)
29	LMT	a	401	-	36,36,36	0.51	1 (2%)	47,47,47	1.15	3 (6%)
36	LHG	a	418	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
25	PHO	A	408	-	67,69,69	2.16	17 (25%)	85,99,99	1.83	20 (23%)
24	CLA	c	904	-	59,73,73	1.99	12 (20%)	67,113,113	2.06	19 (28%)
23	BCT	d	402	21	0,3,3	0.00	-	0,3,3	0.00	-
29	LMT	m	103	-	36,36,36	0.49	0	47,47,47	1.08	3 (6%)
24	CLA	b	611	-	59,73,73	1.99	13 (22%)	67,113,113	2.22	21 (31%)
24	CLA	C	512	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	23 (34%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.57	11 (17%)
24	CLA	b	614	-	59,73,73	1.99	12 (20%)	67,113,113	2.20	21 (31%)
24	CLA	b	620	-	59,73,73	2.02	13 (22%)	67,113,113	2.20	24 (35%)
35	HTG	B	633	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	2 (8%)
24	CLA	A	406	40	59,73,73	2.07	13 (22%)	67,113,113	2.30	24 (35%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	13 (23%)
24	CLA	B	617	-	59,73,73	1.99	12 (20%)	67,113,113	2.19	21 (31%)
26	BCR	D	406	-	41,41,41	1.06	1 (2%)	56,56,56	1.74	10 (17%)
37	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	1.02	4 (5%)
24	CLA	b	616	-	59,73,73	1.95	13 (22%)	67,113,113	2.24	22 (32%)
24	CLA	B	612	-	59,73,73	1.94	13 (22%)	67,113,113	2.30	23 (34%)
29	LMT	M	101	-	36,36,36	0.46	0	47,47,47	0.92	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	611	40	59,73,73	2.00	14 (23%)	67,113,113	2.16	24 (35%)
24	CLA	c	910	-	59,73,73	2.10	13 (22%)	67,113,113	2.28	22 (32%)
37	DGD	c	918	-	63,63,67	0.90	2 (3%)	77,77,81	1.04	5 (6%)
26	BCR	d	407	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	15 (26%)
27	SQD	a	402	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	6 (9%)
27	SQD	L	102	-	53,54,54	1.04	3 (5%)	62,65,65	1.55	11 (17%)
25	PHO	a	407	-	67,69,69	2.11	17 (25%)	85,99,99	1.91	26 (30%)
29	LMT	a	417	-	36,36,36	0.42	0	47,47,47	0.79	1 (2%)
38	HEM	F	102	5,6	27,50,50	0.90	2 (7%)	17,82,82	2.32	3 (17%)
36	LHG	d	409	-	48,48,48	0.92	3 (6%)	51,54,54	1.11	6 (11%)
24	CLA	D	405	-	59,73,73	1.94	14 (23%)	67,113,113	2.17	22 (32%)
27	SQD	F	103	-	42,43,54	1.17	3 (7%)	51,54,65	1.58	9 (17%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.49	0
27	SQD	a	410	-	53,54,54	0.98	3 (5%)	62,65,65	1.64	11 (17%)
26	BCR	b	622	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	9 (16%)
28	GOL	c	928	-	5,5,5	0.41	0	5,5,5	0.25	0
24	CLA	b	619	-	59,73,73	2.03	13 (22%)	67,113,113	2.25	27 (40%)
36	LHG	D	409	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	3 (5%)
24	CLA	B	608	40	59,73,73	1.99	14 (23%)	67,113,113	2.11	21 (31%)
24	CLA	b	609	-	59,73,73	2.00	15 (25%)	67,113,113	2.25	19 (28%)
28	GOL	B	626	-	5,5,5	0.41	0	5,5,5	0.34	0
24	CLA	B	607	-	59,73,73	2.00	13 (22%)	67,113,113	2.25	23 (34%)
35	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.28	1 (4%)
24	CLA	d	404	40	59,73,73	2.04	12 (20%)	67,113,113	2.30	24 (35%)
24	CLA	C	509	-	59,73,73	2.09	13 (22%)	67,113,113	2.25	23 (34%)
24	CLA	d	405	-	59,73,73	1.98	14 (23%)	67,113,113	2.29	21 (31%)
28	GOL	v	203	-	5,5,5	0.35	0	5,5,5	0.27	0
27	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.45	6 (11%)
24	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	22 (32%)
29	LMT	t	101	-	25,25,36	0.50	0	30,30,47	0.77	1 (3%)
35	HTG	B	624	-	19,19,19	0.82	1 (5%)	23,24,24	1.74	4 (17%)
28	GOL	T	101	-	5,5,5	0.38	0	5,5,5	0.22	0
24	CLA	C	508	-	59,73,73	2.05	13 (22%)	67,113,113	2.19	21 (31%)
24	CLA	C	507	40	59,73,73	1.97	13 (22%)	67,113,113	2.15	21 (31%)
28	GOL	b	631	-	5,5,5	0.32	0	5,5,5	0.26	0
35	HTG	B	623	-	19,19,19	1.20	1 (5%)	23,24,24	1.28	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	DGD	D	408	-	52,52,67	1.04	3 (5%)	60,60,81	1.17	5 (8%)
28	GOL	B	631	-	5,5,5	0.33	0	5,5,5	0.43	0
26	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.53	10 (17%)
36	LHG	B	635	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
24	CLA	B	615	-	59,73,73	2.07	13 (22%)	67,113,113	2.13	22 (32%)
28	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.88	0
28	GOL	v	204	-	5,5,5	0.36	0	5,5,5	0.34	0
35	HTG	c	921	-	19,19,19	1.00	2 (10%)	23,24,24	1.56	1 (4%)
24	CLA	c	914	-	59,73,73	2.02	13 (22%)	67,113,113	2.12	21 (31%)
30	OEX	a	416	1,3,40	0,15,15	0.00	-	-	-	-
24	CLA	b	606	40	59,73,73	2.06	12 (20%)	67,113,113	2.23	18 (26%)
29	LMT	D	403	-	36,36,36	0.47	0	47,47,47	1.04	3 (6%)
28	GOL	V	201	34	5,5,5	0.34	0	5,5,5	0.26	0
28	GOL	b	629	-	5,5,5	0.38	0	5,5,5	0.49	0
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.85	1 (2%)
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	0.97	3 (5%)
36	LHG	d	410	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)
24	CLA	C	501	-	59,73,73	2.02	13 (22%)	67,113,113	2.20	22 (32%)
33	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.25	8 (13%)
28	GOL	c	924	-	5,5,5	0.37	0	5,5,5	0.61	0
28	GOL	A	413	-	5,5,5	0.38	0	5,5,5	0.22	0
35	HTG	d	414	-	16,16,19	1.14	2 (12%)	20,21,24	1.76	1 (5%)
38	HEM	V	202	16	27,50,50	0.84	1 (3%)	17,82,82	1.49	4 (23%)
33	LMG	A	419	-	51,51,55	0.96	2 (3%)	59,59,63	1.12	4 (6%)
24	CLA	B	603	-	59,73,73	1.99	13 (22%)	67,113,113	2.31	23 (34%)
24	CLA	c	907	-	59,73,73	1.97	14 (23%)	67,113,113	2.19	23 (34%)
35	HTG	V	203	-	19,19,19	1.02	2 (10%)	23,24,24	1.31	3 (13%)
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
29	LMT	F	101	-	36,36,36	0.46	0	47,47,47	0.90	1 (2%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
26	BCR	Y	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.67	11 (19%)
24	CLA	c	912	3	59,73,73	2.00	12 (20%)	67,113,113	2.03	19 (28%)
26	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	14 (25%)
26	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	8 (14%)
25	PHO	d	403	-	67,69,69	2.16	17 (25%)	85,99,99	2.05	23 (27%)
24	CLA	C	505	-	59,73,73	1.92	13 (22%)	67,113,113	2.18	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	PL9	a	415	-	55,55,55	0.64	2 (3%)	68,69,69	1.88	21 (30%)
28	GOL	l	101	-	5,5,5	0.47	0	5,5,5	0.24	0
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.12	6 (7%)
35	HTG	b	627	-	19,19,19	0.81	1 (5%)	23,24,24	1.54	3 (13%)
28	GOL	b	632	-	5,5,5	0.38	0	5,5,5	0.33	0
35	HTG	D	413	-	16,16,19	1.07	2 (12%)	20,21,24	1.52	1 (5%)
28	GOL	T	103	-	5,5,5	0.40	0	5,5,5	0.30	0
28	GOL	A	412	-	5,5,5	0.39	0	5,5,5	0.29	0
36	LHG	b	635	-	48,48,48	0.96	2 (4%)	51,54,54	1.12	3 (5%)
28	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.47	0
33	LMG	a	411	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	5 (8%)
24	CLA	c	908	40	59,73,73	1.99	13 (22%)	67,113,113	2.20	20 (29%)
24	CLA	C	506	-	59,73,73	2.00	13 (22%)	67,113,113	2.22	24 (35%)
24	CLA	B	610	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	22 (32%)
35	HTG	C	521	-	19,19,19	1.02	2 (10%)	23,24,24	1.76	3 (13%)
33	LMG	b	625	-	51,51,55	0.89	2 (3%)	59,59,63	1.11	5 (8%)
28	GOL	V	207	-	5,5,5	0.34	0	5,5,5	0.30	0
24	CLA	a	408	-	59,73,73	2.00	13 (22%)	67,113,113	2.23	25 (37%)
28	GOL	a	412	-	5,5,5	0.39	0	5,5,5	0.53	0
38	HEM	v	202	16	27,50,50	0.87	1 (3%)	17,82,82	1.39	2 (11%)
25	PHO	D	401	-	67,69,69	2.17	18 (26%)	85,99,99	1.95	21 (24%)
36	LHG	L	101	-	48,48,48	0.95	3 (6%)	51,54,54	1.13	5 (9%)
29	LMT	M	103	-	36,36,36	0.59	1 (2%)	47,47,47	1.08	4 (8%)
27	SQD	B	621	-	53,54,54	1.03	3 (5%)	62,65,65	1.44	8 (12%)
24	CLA	c	902	-	59,73,73	2.00	13 (22%)	67,113,113	2.17	24 (35%)
31	PL9	D	407	-	55,55,55	0.64	2 (3%)	68,69,69	1.89	22 (32%)
35	HTG	B	632	-	19,19,19	0.96	2 (10%)	23,24,24	1.37	2 (8%)
35	HTG	C	522	-	19,19,19	1.00	1 (5%)	23,24,24	1.71	4 (17%)
24	CLA	c	905	40	59,73,73	2.00	13 (22%)	67,113,113	2.21	25 (37%)
24	CLA	C	511	3	59,73,73	2.05	13 (22%)	67,113,113	2.12	21 (31%)
24	CLA	a	406	40	59,73,73	2.00	12 (20%)	67,113,113	2.18	22 (32%)
26	BCR	T	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.85	17 (30%)
29	LMT	e	102	-	36,36,36	0.48	0	47,47,47	0.86	1 (2%)
26	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
28	GOL	B	629	-	5,5,5	0.35	0	5,5,5	0.31	0
24	CLA	B	616	-	59,73,73	2.00	13 (22%)	67,113,113	2.12	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	A	405	-	59,73,73	2.05	13 (22%)	67,113,113	2.17	23 (34%)
24	CLA	b	621	-	59,73,73	2.03	13 (22%)	67,113,113	2.24	24 (35%)
24	CLA	D	404	-	59,73,73	1.97	14 (23%)	67,113,113	2.21	26 (38%)
28	GOL	c	923	-	5,5,5	0.37	0	5,5,5	0.22	0
28	GOL	O	302	-	5,5,5	0.33	0	5,5,5	0.39	0
35	HTG	b	628	-	19,19,19	1.21	2 (10%)	23,24,24	1.69	3 (13%)
24	CLA	B	604	-	59,73,73	2.05	13 (22%)	67,113,113	2.25	20 (29%)
29	LMT	b	626	-	25,25,36	0.47	0	30,30,47	0.58	0
37	DGD	c	916	-	63,63,67	0.84	2 (3%)	77,77,81	1.07	7 (9%)
28	GOL	B	630	-	5,5,5	0.39	0	5,5,5	0.21	0
35	HTG	b	603	-	19,19,19	1.00	2 (10%)	23,24,24	1.55	4 (17%)
28	GOL	a	413	-	5,5,5	0.41	0	5,5,5	0.26	0
26	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	9 (16%)
33	LMG	Z	101	-	37,37,55	0.97	2 (5%)	45,45,63	1.39	6 (13%)
35	HTG	c	922	-	19,19,19	1.00	2 (10%)	23,24,24	1.45	3 (13%)
24	CLA	C	504	40	59,73,73	2.06	13 (22%)	67,113,113	2.31	23 (34%)
28	GOL	b	633	-	5,5,5	0.37	0	5,5,5	0.41	0
26	BCR	a	409	-	41,41,41	1.05	1 (2%)	56,56,56	1.28	2 (3%)
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.47	12 (21%)
28	GOL	C	524	-	5,5,5	0.41	0	5,5,5	0.57	0
24	CLA	C	503	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	19 (28%)
24	CLA	A	407	40	59,73,73	1.99	13 (22%)	67,113,113	2.15	23 (34%)
28	GOL	a	419	34	5,5,5	0.31	0	5,5,5	0.40	0
24	CLA	b	617	-	59,73,73	2.02	12 (20%)	67,113,113	2.25	25 (37%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.02	6 (7%)
24	CLA	B	609	-	59,73,73	2.06	13 (22%)	67,113,113	2.10	21 (31%)
24	CLA	b	618	-	59,73,73	2.01	12 (20%)	67,113,113	2.25	21 (31%)
24	CLA	b	612	40	59,73,73	1.94	12 (20%)	67,113,113	2.15	22 (32%)
26	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.52	9 (16%)
24	CLA	C	513	-	59,73,73	1.99	12 (20%)	67,113,113	2.13	22 (32%)
36	LHG	D	410	-	48,48,48	0.97	2 (4%)	51,54,54	1.20	4 (7%)
29	LMT	A	415	-	36,36,36	0.67	1 (2%)	47,47,47	1.43	5 (10%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.47	0
24	CLA	c	911	-	59,73,73	2.02	13 (22%)	67,113,113	2.26	22 (32%)
37	DGD	C	517	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	7 (9%)
28	GOL	V	205	-	5,5,5	0.37	0	5,5,5	0.57	0
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMT	b	602	-	25,25,36	0.57	1 (4%)	30,30,47	1.12	2 (6%)
24	CLA	c	906	-	59,73,73	1.96	13 (22%)	67,113,113	2.19	19 (28%)
26	BCR	c	915	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	10 (17%)
24	CLA	B	613	-	59,73,73	2.00	13 (22%)	67,113,113	2.18	20 (29%)
24	CLA	c	909	-	59,73,73	2.04	13 (22%)	67,113,113	2.29	23 (34%)
24	CLA	c	903	-	59,73,73	2.04	13 (22%)	67,113,113	2.14	19 (28%)
33	LMG	Y	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.00	4 (6%)
35	HTG	b	604	-	19,19,19	0.99	2 (10%)	23,24,24	1.11	1 (4%)
28	GOL	b	630	-	5,5,5	0.40	0	5,5,5	0.14	0
33	LMG	c	920	-	51,51,55	0.95	2 (3%)	59,59,63	1.30	7 (11%)
33	LMG	c	919	-	51,51,55	0.88	2 (3%)	59,59,63	1.18	4 (6%)

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
28	GOL	V	204	-	-	2/4/4/4	-
31	PL9	A	417	-	-	13/53/73/73	0/1/1/1
27	SQD	A	414	-	-	13/49/69/69	0/1/1/1
24	CLA	c	913	-	3/3/20/25	12/37/135/135	-
24	CLA	B	614	-	3/3/20/25	8/37/135/135	-
24	CLA	B	606	-	3/3/20/25	6/37/135/135	-
31	PL9	d	408	-	-	3/53/73/73	0/1/1/1
26	BCR	b	624	-	-	0/29/63/63	0/2/2/2
38	HEM	f	101	5,6	-	1/6/54/54	-
24	CLA	C	510	-	3/3/20/25	8/37/135/135	-
24	CLA	b	608	-	2/2/20/25	5/37/135/135	-
24	CLA	b	607	-	2/2/20/25	5/37/135/135	-
36	LHG	E	101	-	-	19/46/46/53	-
26	BCR	b	623	-	-	1/29/63/63	0/2/2/2
35	HTG	B	625	-	-	5/10/30/30	0/1/1/1
24	CLA	B	605	-	3/3/20/25	4/37/135/135	-
24	CLA	d	406	-	3/3/20/25	6/37/135/135	-
36	LHG	d	411	-	-	12/53/53/53	-
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	C	520	-	-	6/21/61/61	0/2/2/2
24	CLA	b	610	-	3/3/20/25	4/37/135/135	-
24	CLA	a	405	-	3/3/20/25	4/37/135/135	-
28	GOL	D	402	-	-	4/4/4/4	-
26	BCR	A	410	-	-	4/29/63/63	0/2/2/2
24	CLA	A	409	-	3/3/20/25	10/37/135/135	-
33	LMG	B	622	-	-	8/46/66/70	0/1/1/1
24	CLA	b	615	40	3/3/20/25	5/37/135/135	-
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
28	GOL	V	206	-	-	2/4/4/4	-
24	CLA	B	602	40	3/3/20/25	14/37/135/135	-
28	GOL	v	205	-	-	2/4/4/4	-
33	LMG	z	101	-	-	11/34/54/70	0/1/1/1
37	DGD	c	917	-	-	18/51/91/95	0/2/2/2
24	CLA	b	613	-	2/2/20/25	1/37/135/135	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	BCR	c	927	-	-	0/29/63/63	0/2/2/2
29	LMT	a	401	-	-	7/21/61/61	0/2/2/2
36	LHG	a	418	-	-	15/46/46/53	-
25	PHO	A	408	-	-	2/53/103/103	0/5/6/6
24	CLA	c	904	-	3/3/20/25	6/37/135/135	-
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
24	CLA	b	611	-	3/3/20/25	14/37/135/135	-
24	CLA	C	512	-	3/3/20/25	9/37/135/135	-
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
24	CLA	b	614	-	2/2/20/25	3/37/135/135	-
24	CLA	b	620	-	3/3/20/25	7/37/135/135	-
24	CLA	c	910	-	3/3/20/25	15/37/135/135	-
24	CLA	A	406	40	3/3/20/25	4/37/135/135	-
26	BCR	t	102	-	-	5/29/63/63	0/2/2/2
24	CLA	B	617	-	3/3/20/25	8/37/135/135	-
26	BCR	D	406	-	-	8/29/63/63	0/2/2/2
37	DGD	h	102	-	-	9/51/91/95	0/2/2/2
24	CLA	b	616	-	3/3/20/25	3/37/135/135	-
24	CLA	B	612	-	3/3/20/25	1/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	M	101	-	-	6/21/61/61	0/2/2/2
24	CLA	B	611	40	3/3/20/25	4/37/135/135	-
37	DGD	c	918	-	-	13/51/91/95	0/2/2/2
26	BCR	d	407	-	-	4/29/63/63	0/2/2/2
27	SQD	a	402	-	-	10/49/69/69	0/1/1/1
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
27	SQD	L	102	-	-	22/49/69/69	0/1/1/1
25	PHO	a	407	-	-	5/53/103/103	0/5/6/6
29	LMT	a	417	-	-	4/21/61/61	0/2/2/2
38	HEM	F	102	5,6	-	0/6/54/54	-
36	LHG	d	409	-	-	18/53/53/53	-
24	CLA	D	405	-	3/3/20/25	4/37/135/135	-
27	SQD	F	103	-	-	15/38/58/69	0/1/1/1
28	GOL	B	627	-	-	2/4/4/4	-
27	SQD	a	410	-	-	14/49/69/69	0/1/1/1
26	BCR	b	622	-	-	2/29/63/63	0/2/2/2
28	GOL	c	928	-	-	2/4/4/4	-
24	CLA	b	619	-	3/3/20/25	20/37/135/135	-
24	CLA	B	608	40	3/3/20/25	4/37/135/135	-
24	CLA	b	609	-	3/3/20/25	3/37/135/135	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	B	607	-	3/3/20/25	5/37/135/135	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	d	404	40	3/3/20/25	6/37/135/135	-
24	CLA	C	509	-	3/3/20/25	14/37/135/135	-
24	CLA	d	405	-	1/1/20/25	5/37/135/135	-
28	GOL	v	203	-	-	2/4/4/4	-
35	HTG	b	604	-	-	1/10/30/30	0/1/1/1
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
24	CLA	C	502	-	3/3/20/25	8/37/135/135	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	C	508	-	3/3/20/25	5/37/135/135	-
24	CLA	C	507	40	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	b	631	-	-	4/4/4/4	-
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
37	DGD	D	408	-	-	18/47/67/95	0/1/1/2
28	GOL	B	631	-	-	1/4/4/4	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
36	LHG	B	635	-	-	13/53/53/53	-
24	CLA	B	615	-	3/3/20/25	18/37/135/135	-
28	GOL	C	523	-	-	2/4/4/4	-
28	GOL	v	204	-	-	2/4/4/4	-
35	HTG	c	921	-	-	4/10/30/30	0/1/1/1
24	CLA	b	606	40	3/3/20/25	16/37/135/135	-
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2
28	GOL	V	201	34	-	2/4/4/4	-
28	GOL	b	629	-	-	0/4/4/4	-
29	LMT	m	102	-	-	6/21/61/61	0/2/2/2
33	LMG	J	101	39	-	11/46/66/70	0/1/1/1
36	LHG	d	410	-	-	9/53/53/53	-
24	CLA	C	501	-	3/3/20/25	7/37/135/135	-
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
28	GOL	c	924	-	-	2/4/4/4	-
28	GOL	A	413	-	-	2/4/4/4	-
35	HTG	d	414	-	-	0/7/27/30	0/1/1/1
38	HEM	V	202	16	-	0/6/54/54	-
33	LMG	A	419	-	-	21/46/66/70	0/1/1/1
24	CLA	B	603	-	2/2/20/25	3/37/135/135	-
24	CLA	c	907	-	3/3/20/25	13/37/135/135	-
35	HTG	V	203	-	-	5/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMT	F	101	-	-	6/21/61/61	0/2/2/2
37	DGD	C	518	-	-	10/51/91/95	0/2/2/2
26	BCR	Y	102	-	-	4/29/63/63	0/2/2/2
24	CLA	c	912	3	3/3/20/25	6/37/135/135	-
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	2/29/63/63	0/2/2/2
25	PHO	d	403	-	-	4/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	505	-	1/1/20/25	6/37/135/135	-
31	PL9	a	415	-	-	15/53/73/73	0/1/1/1
28	GOL	l	101	-	-	0/4/4/4	-
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
35	HTG	b	627	-	-	2/10/30/30	0/1/1/1
28	GOL	b	632	-	-	2/4/4/4	-
35	HTG	D	413	-	-	0/7/27/30	0/1/1/1
28	GOL	T	103	-	-	2/4/4/4	-
28	GOL	A	412	-	-	0/4/4/4	-
36	LHG	b	635	-	-	20/53/53/53	-
28	GOL	B	628	-	-	2/4/4/4	-
33	LMG	a	411	-	-	14/46/66/70	0/1/1/1
24	CLA	c	908	40	3/3/20/25	4/37/135/135	-
24	CLA	C	506	-	3/3/20/25	6/37/135/135	-
24	CLA	B	610	-	2/2/20/25	3/37/135/135	-
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
33	LMG	b	625	-	-	8/46/66/70	0/1/1/1
28	GOL	V	207	-	-	4/4/4/4	-
24	CLA	a	408	-	3/3/20/25	10/37/135/135	-
28	GOL	a	412	-	-	4/4/4/4	-
38	HEM	v	202	16	-	0/6/54/54	-
25	PHO	D	401	-	-	5/53/103/103	0/5/6/6
24	CLA	c	914	-	2/2/20/25	5/37/135/135	-
29	LMT	M	103	-	-	11/21/61/61	0/2/2/2
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	c	902	-	3/3/20/25	5/37/135/135	-
31	PL9	D	407	-	-	9/53/73/73	0/1/1/1
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1
35	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	c	905	40	3/3/20/25	4/37/135/135	-
24	CLA	C	511	3	3/3/20/25	4/37/135/135	-
24	CLA	a	406	40	2/2/20/25	11/37/135/135	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
29	LMT	e	102	-	-	9/21/61/61	0/2/2/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	629	-	-	3/4/4/4	-
24	CLA	B	616	-	3/3/20/25	11/37/135/135	-
24	CLA	A	405	-	3/3/20/25	4/37/135/135	-
24	CLA	b	621	-	3/3/20/25	9/37/135/135	-
24	CLA	D	404	-	1/1/20/25	0/37/135/135	-
28	GOL	c	923	-	-	0/4/4/4	-
28	GOL	O	302	-	-	0/4/4/4	-
35	HTG	b	628	-	-	4/10/30/30	0/1/1/1
24	CLA	B	604	-	3/3/20/25	4/37/135/135	-
29	LMT	b	626	-	-	5/17/37/61	0/1/1/2
24	CLA	A	407	40	2/2/20/25	6/37/135/135	-
28	GOL	B	630	-	-	4/4/4/4	-
35	HTG	b	603	-	-	1/10/30/30	0/1/1/1
28	GOL	a	413	-	-	2/4/4/4	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	13/31/51/70	0/1/1/1
36	LHG	L	101	-	-	16/53/53/53	-
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
24	CLA	C	504	40	3/3/20/25	7/37/135/135	-
28	GOL	b	633	-	-	2/4/4/4	-
26	BCR	a	409	-	-	2/29/63/63	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	GOL	C	524	-	-	2/4/4/4	-
24	CLA	C	503	-	3/3/20/25	2/37/135/135	-
37	DGD	c	916	-	-	12/51/91/95	0/2/2/2
28	GOL	a	419	34	-	3/4/4/4	-
24	CLA	b	617	-	3/3/20/25	4/37/135/135	-
37	DGD	H	102	-	-	9/51/91/95	0/2/2/2
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-
24	CLA	b	618	-	3/3/20/25	3/37/135/135	-
24	CLA	b	612	40	3/3/20/25	1/37/135/135	-
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
36	LHG	D	409	-	-	11/53/53/53	-
36	LHG	D	410	-	-	18/53/53/53	-
29	LMT	A	415	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	636	-	-	2/4/4/4	-
24	CLA	c	911	-	3/3/20/25	7/37/135/135	-
37	DGD	C	517	-	-	19/51/91/95	0/2/2/2
28	GOL	V	205	-	-	0/4/4/4	-
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
29	LMT	b	602	-	-	7/17/37/61	0/1/1/2
24	CLA	c	906	-	2/2/20/25	8/37/135/135	-
26	BCR	c	915	-	-	4/29/63/63	0/2/2/2
24	CLA	B	613	-	3/3/20/25	5/37/135/135	-
24	CLA	c	909	-	3/3/20/25	7/37/135/135	-
24	CLA	c	903	-	2/2/20/25	5/37/135/135	-
33	LMG	Y	101	-	-	10/46/66/70	0/1/1/1
24	CLA	C	513	-	3/3/20/25	8/37/135/135	-
28	GOL	b	630	-	-	0/4/4/4	-
33	LMG	c	920	-	-	5/46/66/70	0/1/1/1
33	LMG	c	919	-	-	12/46/66/70	0/1/1/1

All (1137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	910	CLA	C3B-C2B	6.68	1.49	1.40
24	A	406	CLA	C3B-C2B	6.68	1.49	1.40
24	c	912	CLA	C3B-C2B	6.65	1.49	1.40
25	d	403	PHO	C3C-C2C	6.64	1.50	1.36
24	C	509	CLA	C3B-C2B	6.59	1.49	1.40
24	C	504	CLA	C3B-C2B	6.45	1.49	1.40
24	B	617	CLA	C3B-C2B	6.44	1.49	1.40
24	B	613	CLA	C3B-C2B	6.44	1.49	1.40
24	D	404	CLA	C3B-C2B	6.38	1.49	1.40
24	B	615	CLA	C3B-C2B	6.32	1.49	1.40
24	c	911	CLA	C3B-C2B	6.29	1.49	1.40
24	d	404	CLA	C3B-C2B	6.27	1.49	1.40
24	b	606	CLA	C3D-C2D	6.26	1.50	1.39
24	B	614	CLA	C3B-C2B	6.26	1.49	1.40
24	B	609	CLA	C3B-C2B	6.25	1.49	1.40
24	C	511	CLA	C3B-C2B	6.25	1.49	1.40
24	b	618	CLA	C3B-C2B	6.25	1.49	1.40
24	b	620	CLA	C3D-C2D	6.24	1.50	1.39
24	A	405	CLA	C3B-C2B	6.23	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C3B-C2B	6.21	1.49	1.40
24	c	909	CLA	C3B-C2B	6.20	1.49	1.40
24	B	610	CLA	C3D-C2D	6.19	1.50	1.39
24	b	619	CLA	C3B-C2B	6.19	1.49	1.40
24	C	504	CLA	C3D-C2D	6.19	1.50	1.39
24	b	615	CLA	C3B-C2B	6.11	1.48	1.40
24	A	407	CLA	C3D-C2D	6.11	1.50	1.39
24	B	616	CLA	C3D-C2D	6.10	1.50	1.39
24	c	905	CLA	C3B-C2B	6.10	1.48	1.40
24	b	616	CLA	C3B-C2B	6.10	1.48	1.40
24	B	605	CLA	C3B-C2B	6.06	1.48	1.40
24	B	614	CLA	C3D-C2D	6.05	1.50	1.39
24	d	404	CLA	C3D-C2D	6.05	1.50	1.39
24	d	405	CLA	C3B-C2B	6.03	1.48	1.40
24	B	608	CLA	C3B-C2B	6.02	1.48	1.40
24	B	604	CLA	C3B-C2B	5.99	1.48	1.40
24	b	613	CLA	C3D-C2D	5.99	1.50	1.39
25	A	408	PHO	C3C-C2C	5.99	1.49	1.36
24	C	511	CLA	C3D-C2D	5.98	1.50	1.39
24	A	406	CLA	C3D-C2D	5.97	1.50	1.39
24	b	617	CLA	C3B-C2B	5.97	1.48	1.40
24	c	903	CLA	C3D-C2D	5.96	1.50	1.39
24	c	907	CLA	C3B-C2B	5.96	1.48	1.40
24	B	602	CLA	C3B-C2B	5.95	1.48	1.40
24	b	606	CLA	C3B-C2B	5.93	1.48	1.40
24	C	510	CLA	C3B-C2B	5.91	1.48	1.40
24	C	508	CLA	C3D-C2D	5.91	1.50	1.39
24	a	405	CLA	C3B-C2B	5.90	1.48	1.40
24	b	607	CLA	C3B-C2B	5.88	1.48	1.40
25	D	401	PHO	C3C-C2C	5.87	1.49	1.36
24	b	617	CLA	C3D-C2D	5.87	1.50	1.39
24	b	620	CLA	C3B-C2B	5.86	1.48	1.40
24	C	506	CLA	C3D-C2D	5.85	1.49	1.39
24	A	409	CLA	C3D-C2D	5.85	1.49	1.39
24	c	909	CLA	C3D-C2D	5.85	1.49	1.39
24	C	506	CLA	C3B-C2B	5.84	1.48	1.40
24	C	509	CLA	C3D-C2D	5.83	1.49	1.39
24	c	902	CLA	C3B-C2B	5.82	1.48	1.40
24	c	903	CLA	C3B-C2B	5.80	1.48	1.40
24	C	508	CLA	C3B-C2B	5.80	1.48	1.40
24	c	904	CLA	C3B-C2B	5.80	1.48	1.40
25	d	403	PHO	C3B-C2B	5.79	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C3B-C2B	5.79	1.48	1.40
24	B	604	CLA	C3C-C2C	5.78	1.49	1.36
24	C	501	CLA	C3D-C2D	5.78	1.49	1.39
24	C	505	CLA	C3B-C2B	5.78	1.48	1.40
24	c	908	CLA	C3B-C2B	5.78	1.48	1.40
24	C	503	CLA	C3D-C2D	5.77	1.49	1.39
24	C	512	CLA	C3D-C2D	5.77	1.49	1.39
24	b	619	CLA	C3D-C2D	5.75	1.49	1.39
24	b	613	CLA	C3B-C2B	5.75	1.48	1.40
24	C	512	CLA	C3B-C2B	5.75	1.48	1.40
24	b	610	CLA	C3B-C2B	5.74	1.48	1.40
24	c	911	CLA	C3D-C2D	5.74	1.49	1.39
24	C	502	CLA	C3B-C2B	5.72	1.48	1.40
24	d	406	CLA	C3D-C2D	5.72	1.49	1.39
24	b	611	CLA	C3B-C2B	5.71	1.48	1.40
24	b	608	CLA	C3B-C2B	5.70	1.48	1.40
24	b	606	CLA	C3C-C2C	5.70	1.48	1.36
24	d	404	CLA	C3C-C2C	5.70	1.48	1.36
24	C	510	CLA	C3D-C2D	5.69	1.49	1.39
24	C	502	CLA	C3D-C2D	5.69	1.49	1.39
24	C	501	CLA	C3B-C2B	5.68	1.48	1.40
24	c	913	CLA	C3D-C2D	5.68	1.49	1.39
24	b	621	CLA	C3D-C2D	5.68	1.49	1.39
25	D	401	PHO	C3B-C2B	5.68	1.48	1.37
24	c	913	CLA	C3B-C2B	5.68	1.48	1.40
24	b	618	CLA	C3D-C2D	5.68	1.49	1.39
24	B	603	CLA	C3B-C2B	5.67	1.48	1.40
24	D	405	CLA	C3D-C2D	5.67	1.49	1.39
24	c	910	CLA	C3D-C2D	5.66	1.49	1.39
24	c	905	CLA	C3D-C2D	5.66	1.49	1.39
24	b	614	CLA	C3D-C2D	5.66	1.49	1.39
24	a	408	CLA	C3D-C2D	5.66	1.49	1.39
24	d	405	CLA	C3D-C2D	5.65	1.49	1.39
24	C	513	CLA	C3D-C2D	5.63	1.49	1.39
24	B	606	CLA	C3B-C2B	5.63	1.48	1.40
24	a	408	CLA	C3C-C2C	5.63	1.48	1.36
24	c	914	CLA	C3B-C2B	5.63	1.48	1.40
24	c	902	CLA	C3D-C2D	5.63	1.49	1.39
24	B	615	CLA	C3D-C2D	5.63	1.49	1.39
24	B	607	CLA	C3C-C2C	5.62	1.48	1.36
24	c	903	CLA	O2D-CGD	5.62	1.46	1.33
24	B	609	CLA	C3D-C2D	5.62	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3C-C2C	5.61	1.48	1.36
24	a	408	CLA	C3B-C2B	5.61	1.48	1.40
24	B	604	CLA	C3D-C2D	5.60	1.49	1.39
24	c	908	CLA	C3D-C2D	5.59	1.49	1.39
25	A	408	PHO	C3B-C2B	5.59	1.48	1.37
24	b	610	CLA	C3C-C2C	5.59	1.48	1.36
25	a	407	PHO	C3B-C2B	5.59	1.48	1.37
24	b	615	CLA	C3D-C2D	5.58	1.49	1.39
24	B	602	CLA	C3D-C2D	5.58	1.49	1.39
24	d	406	CLA	C3B-C2B	5.57	1.48	1.40
24	B	611	CLA	C3C-C2C	5.57	1.48	1.36
24	C	513	CLA	C3B-C2B	5.57	1.48	1.40
24	B	611	CLA	C3D-C2D	5.57	1.49	1.39
24	c	904	CLA	C3C-C2C	5.56	1.48	1.36
24	B	612	CLA	C3B-C2B	5.56	1.48	1.40
24	B	606	CLA	C3D-C2D	5.55	1.49	1.39
24	c	903	CLA	C3C-C2C	5.55	1.48	1.36
24	a	406	CLA	C3B-C2B	5.54	1.48	1.40
24	c	914	CLA	C3D-C2D	5.53	1.49	1.39
24	C	507	CLA	C3B-C2B	5.53	1.48	1.40
24	b	612	CLA	C3D-C2D	5.52	1.49	1.39
24	C	503	CLA	C3B-C2B	5.50	1.48	1.40
24	A	406	CLA	C3C-C2C	5.49	1.48	1.36
24	a	406	CLA	C3D-C2D	5.49	1.49	1.39
24	A	405	CLA	C3D-C2D	5.48	1.49	1.39
25	a	407	PHO	C3C-C2C	5.47	1.48	1.36
24	B	615	CLA	C3C-C2C	5.46	1.48	1.36
24	C	512	CLA	C3C-C2C	5.46	1.48	1.36
24	B	612	CLA	C3C-C2C	5.45	1.48	1.36
24	C	507	CLA	CHC-C1C	5.44	1.48	1.35
24	A	407	CLA	C3B-C2B	5.43	1.47	1.40
24	B	613	CLA	C3D-C2D	5.43	1.49	1.39
24	b	608	CLA	C3D-C2D	5.43	1.49	1.39
24	C	503	CLA	CHC-C1C	5.42	1.48	1.35
24	b	616	CLA	C3D-C2D	5.41	1.49	1.39
24	a	405	CLA	C3D-C2D	5.41	1.49	1.39
24	c	913	CLA	C3C-C2C	5.41	1.48	1.36
24	b	614	CLA	CHC-C1C	5.40	1.48	1.35
25	A	408	PHO	CHC-C1C	5.40	1.49	1.38
24	c	911	CLA	C3C-C2C	5.39	1.48	1.36
24	c	912	CLA	C3D-C2D	5.39	1.49	1.39
24	b	609	CLA	C3D-C2D	5.39	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C3D-C2D	5.39	1.49	1.39
24	C	509	CLA	C3C-C2C	5.38	1.48	1.36
25	d	403	PHO	CHC-C1C	5.38	1.49	1.38
24	C	501	CLA	CHC-C1C	5.37	1.48	1.35
24	c	914	CLA	C3C-C2C	5.37	1.48	1.36
24	B	602	CLA	C3C-C2C	5.36	1.48	1.36
24	C	503	CLA	C3C-C2C	5.36	1.48	1.36
24	b	611	CLA	C3D-C2D	5.36	1.49	1.39
25	A	408	PHO	CHB-C1B	5.35	1.49	1.38
24	B	611	CLA	C3B-C2B	5.35	1.47	1.40
24	B	603	CLA	C3C-C2C	5.34	1.48	1.36
24	B	612	CLA	C3D-C2D	5.34	1.49	1.39
24	A	407	CLA	C3C-C2C	5.33	1.48	1.36
24	b	607	CLA	C3C-C2C	5.33	1.48	1.36
24	b	619	CLA	C3C-C2C	5.33	1.48	1.36
24	b	618	CLA	O2D-CGD	5.33	1.46	1.33
24	A	409	CLA	CHC-C1C	5.33	1.48	1.35
24	b	617	CLA	C3C-C2C	5.33	1.48	1.36
24	b	618	CLA	C3C-C2C	5.32	1.48	1.36
24	a	405	CLA	C3C-C2C	5.32	1.48	1.36
24	C	513	CLA	C3C-C2C	5.32	1.48	1.36
24	C	508	CLA	C3C-C2C	5.31	1.48	1.36
24	c	906	CLA	C3C-C2C	5.31	1.48	1.36
24	c	904	CLA	C3D-C2D	5.31	1.48	1.39
24	B	607	CLA	C3B-C2B	5.31	1.47	1.40
24	B	607	CLA	CHC-C1C	5.31	1.48	1.35
24	b	611	CLA	C3C-C2C	5.30	1.48	1.36
24	c	906	CLA	C3B-C2B	5.30	1.47	1.40
24	C	507	CLA	C3C-C2C	5.29	1.48	1.36
24	b	607	CLA	CHC-C1C	5.28	1.48	1.35
24	d	406	CLA	O2D-CGD	5.27	1.46	1.33
24	a	406	CLA	CHC-C1C	5.27	1.48	1.35
25	D	401	PHO	O2D-CGD	5.26	1.46	1.33
24	c	904	CLA	CHC-C1C	5.25	1.48	1.35
24	b	614	CLA	C3B-C2B	5.25	1.47	1.40
24	b	615	CLA	CHC-C1C	5.25	1.48	1.35
24	b	610	CLA	CHC-C1C	5.25	1.48	1.35
25	d	403	PHO	CHB-C1B	5.25	1.48	1.38
24	c	909	CLA	O2D-CGD	5.25	1.46	1.33
24	C	512	CLA	CHC-C1C	5.25	1.48	1.35
26	b	624	BCR	C23-C22	-5.24	1.34	1.45
24	D	405	CLA	C3B-C2B	5.24	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	909	CLA	C3C-C2C	5.24	1.47	1.36
24	A	405	CLA	CHC-C1C	5.24	1.48	1.35
24	B	616	CLA	O2D-CGD	5.24	1.46	1.33
25	a	407	PHO	O2D-CGD	5.23	1.46	1.33
24	b	615	CLA	C3C-C2C	5.23	1.47	1.36
24	B	603	CLA	C3D-C2D	5.23	1.48	1.39
24	B	603	CLA	OBD-CAD	5.23	1.29	1.22
24	B	607	CLA	C3D-C2D	5.22	1.48	1.39
24	B	608	CLA	C3D-C2D	5.21	1.48	1.39
24	c	906	CLA	C3D-C2D	5.21	1.48	1.39
24	b	609	CLA	C3C-C2C	5.21	1.47	1.36
26	Y	102	BCR	C23-C22	-5.21	1.34	1.45
24	c	907	CLA	C3D-C2D	5.21	1.48	1.39
24	B	616	CLA	C3B-C2B	5.21	1.47	1.40
24	c	910	CLA	C3C-C2C	5.20	1.47	1.36
24	c	902	CLA	C3C-C2C	5.20	1.47	1.36
24	C	502	CLA	C3C-C2C	5.20	1.47	1.36
24	B	617	CLA	C3C-C2C	5.20	1.47	1.36
24	C	502	CLA	CHC-C1C	5.20	1.48	1.35
24	B	609	CLA	C3C-C2C	5.20	1.47	1.36
24	B	603	CLA	CHC-C1C	5.20	1.48	1.35
24	d	406	CLA	CHC-C1C	5.19	1.48	1.35
24	B	617	CLA	C3D-C2D	5.19	1.48	1.39
24	c	914	CLA	O2D-CGD	5.19	1.45	1.33
26	C	514	BCR	C23-C22	-5.19	1.34	1.45
24	b	613	CLA	C3C-C2C	5.19	1.47	1.36
24	B	608	CLA	C3C-C2C	5.19	1.47	1.36
24	C	511	CLA	CHC-C1C	5.18	1.48	1.35
24	B	606	CLA	C3C-C2C	5.18	1.47	1.36
26	k	101	BCR	C23-C22	-5.18	1.34	1.45
24	c	914	CLA	CHC-C1C	5.17	1.48	1.35
24	b	619	CLA	O2D-CGD	5.17	1.45	1.33
24	B	617	CLA	O2D-CGD	5.17	1.45	1.33
24	d	405	CLA	CHC-C1C	5.17	1.48	1.35
25	A	408	PHO	CHD-C1D	5.17	1.48	1.38
24	a	408	CLA	O2D-CGD	5.16	1.45	1.33
24	b	610	CLA	C3D-C2D	5.16	1.48	1.39
24	B	604	CLA	CHC-C1C	5.16	1.48	1.35
24	c	905	CLA	CHC-C1C	5.16	1.48	1.35
24	B	610	CLA	O2D-CGD	5.16	1.45	1.33
24	c	913	CLA	CHC-C1C	5.16	1.48	1.35
24	C	504	CLA	CHC-C1C	5.15	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	905	CLA	O2D-CGD	5.15	1.45	1.33
24	B	613	CLA	CHC-C1C	5.15	1.48	1.35
24	B	610	CLA	C3C-C2C	5.15	1.47	1.36
24	d	406	CLA	C3C-C2C	5.14	1.47	1.36
24	b	608	CLA	C3C-C2C	5.14	1.47	1.36
24	D	404	CLA	C3C-C2C	5.14	1.47	1.36
24	d	405	CLA	C3C-C2C	5.14	1.47	1.36
24	c	908	CLA	C3C-C2C	5.14	1.47	1.36
24	c	907	CLA	C3C-C2C	5.14	1.47	1.36
24	b	607	CLA	C3D-C2D	5.14	1.48	1.39
24	C	509	CLA	CHC-C1C	5.14	1.48	1.35
24	b	613	CLA	CHC-C1C	5.14	1.48	1.35
26	H	101	BCR	C23-C22	-5.13	1.34	1.45
24	c	910	CLA	CHC-C1C	5.13	1.48	1.35
24	c	907	CLA	O2D-CGD	5.12	1.45	1.33
25	D	401	PHO	CHB-C1B	5.12	1.48	1.38
24	b	621	CLA	CHC-C1C	5.12	1.48	1.35
24	D	404	CLA	C3D-C2D	5.12	1.48	1.39
24	B	605	CLA	C3D-C2D	5.11	1.48	1.39
24	B	610	CLA	CHC-C1C	5.11	1.48	1.35
24	C	513	CLA	CHC-C1C	5.11	1.48	1.35
24	b	619	CLA	CHC-C1C	5.11	1.48	1.35
24	b	616	CLA	O2D-CGD	5.11	1.45	1.33
24	C	505	CLA	C3D-C2D	5.10	1.48	1.39
24	C	501	CLA	C3C-C2C	5.10	1.47	1.36
24	A	409	CLA	C3C-C2C	5.10	1.47	1.36
24	b	614	CLA	C3C-C2C	5.10	1.47	1.36
24	C	510	CLA	O2D-CGD	5.10	1.45	1.33
24	B	617	CLA	CHC-C1C	5.10	1.48	1.35
24	b	621	CLA	O2D-CGD	5.09	1.45	1.33
24	b	620	CLA	C3C-C2C	5.09	1.47	1.36
24	C	505	CLA	C3C-C2C	5.09	1.47	1.36
25	d	403	PHO	O2D-CGD	5.08	1.45	1.33
26	t	102	BCR	C23-C22	-5.08	1.35	1.45
24	B	615	CLA	O2D-CGD	5.08	1.45	1.33
24	b	606	CLA	CHC-C1C	5.08	1.48	1.35
24	b	612	CLA	CHC-C1C	5.07	1.48	1.35
24	c	910	CLA	OBD-CAD	5.07	1.29	1.22
24	c	912	CLA	CHC-C1C	5.07	1.48	1.35
24	B	614	CLA	CHC-C1C	5.06	1.48	1.35
24	C	511	CLA	O2D-CGD	5.06	1.45	1.33
25	D	401	PHO	CHC-C1C	5.06	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608	CLA	CHC-C1C	5.06	1.47	1.35
24	C	508	CLA	O2D-CGD	5.06	1.45	1.33
24	B	616	CLA	CHC-C1C	5.05	1.47	1.35
24	A	409	CLA	O2D-CGD	5.05	1.45	1.33
24	b	614	CLA	O2D-CGD	5.05	1.45	1.33
24	B	602	CLA	O2D-CGD	5.05	1.45	1.33
24	c	906	CLA	CHC-C1C	5.04	1.47	1.35
24	B	614	CLA	O2D-CGD	5.04	1.45	1.33
24	C	512	CLA	O2D-CGD	5.04	1.45	1.33
24	B	605	CLA	C3C-C2C	5.04	1.47	1.36
24	C	513	CLA	O2D-CGD	5.03	1.45	1.33
24	c	913	CLA	OBD-CAD	5.03	1.29	1.22
24	b	621	CLA	C3C-C2C	5.03	1.47	1.36
24	B	615	CLA	OBD-CAD	5.03	1.29	1.22
24	a	405	CLA	CHC-C1C	5.03	1.47	1.35
24	b	613	CLA	O2D-CGD	5.03	1.45	1.33
24	c	908	CLA	CHC-C1C	5.02	1.47	1.35
24	A	407	CLA	CHC-C1C	5.02	1.47	1.35
24	c	909	CLA	CHC-C1C	5.02	1.47	1.35
24	A	409	CLA	C3B-C2B	5.02	1.47	1.40
24	c	905	CLA	C3C-C2C	5.01	1.47	1.36
24	b	617	CLA	CHC-C1C	5.01	1.47	1.35
24	B	612	CLA	O2D-CGD	5.00	1.45	1.33
24	C	510	CLA	CHC-C1C	5.00	1.47	1.35
24	C	504	CLA	C3C-C2C	5.00	1.47	1.36
24	b	606	CLA	O2D-CGD	5.00	1.45	1.33
24	B	607	CLA	O2D-CGD	4.99	1.45	1.33
24	c	910	CLA	O2D-CGD	4.99	1.45	1.33
24	c	902	CLA	O2D-CGD	4.99	1.45	1.33
24	B	606	CLA	CHC-C1C	4.99	1.47	1.35
24	A	406	CLA	OBD-CAD	4.99	1.29	1.22
24	a	408	CLA	CHC-C1C	4.99	1.47	1.35
24	a	406	CLA	OBD-CAD	4.98	1.29	1.22
24	c	903	CLA	CHC-C1C	4.98	1.47	1.35
24	C	505	CLA	CHC-C1C	4.98	1.47	1.35
24	B	609	CLA	OBD-CAD	4.97	1.29	1.22
24	C	511	CLA	C3C-C2C	4.97	1.47	1.36
24	b	612	CLA	O2D-CGD	4.96	1.45	1.33
24	b	616	CLA	C3C-C2C	4.96	1.47	1.36
25	a	407	PHO	CHB-C1B	4.96	1.48	1.38
24	C	502	CLA	O2D-CGD	4.96	1.45	1.33
24	c	911	CLA	OBD-CAD	4.95	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	OBD-CAD	4.95	1.29	1.22
24	C	509	CLA	O2D-CGD	4.95	1.45	1.33
24	B	609	CLA	CHC-C1C	4.95	1.47	1.35
24	B	606	CLA	O2D-CGD	4.95	1.45	1.33
24	C	510	CLA	OBD-CAD	4.95	1.29	1.22
24	A	405	CLA	OBD-CAD	4.95	1.29	1.22
26	K	101	BCR	C23-C22	-4.94	1.35	1.45
24	b	620	CLA	CHC-C1C	4.94	1.47	1.35
24	b	612	CLA	C3C-C2C	4.93	1.47	1.36
24	C	506	CLA	O2D-CGD	4.93	1.45	1.33
24	D	404	CLA	O2D-CGD	4.93	1.45	1.33
26	y	101	BCR	C23-C22	-4.93	1.35	1.45
24	b	611	CLA	CHC-C1C	4.93	1.47	1.35
24	B	602	CLA	CHC-C1C	4.92	1.47	1.35
24	C	506	CLA	CHC-C1C	4.92	1.47	1.35
24	C	506	CLA	C3C-C2C	4.92	1.47	1.36
24	c	912	CLA	C3C-C2C	4.91	1.47	1.36
24	c	913	CLA	O2D-CGD	4.91	1.45	1.33
24	D	405	CLA	CHC-C1C	4.90	1.47	1.35
24	b	609	CLA	O2D-CGD	4.90	1.45	1.33
24	b	610	CLA	O2D-CGD	4.89	1.45	1.33
24	B	609	CLA	O2D-CGD	4.89	1.45	1.33
24	B	611	CLA	CHC-C1C	4.89	1.47	1.35
24	D	405	CLA	C3C-C2C	4.89	1.47	1.36
24	c	907	CLA	CHC-C1C	4.88	1.47	1.35
26	b	623	BCR	C23-C22	-4.87	1.35	1.45
24	b	620	CLA	O2D-CGD	4.87	1.45	1.33
24	D	405	CLA	O2D-CGD	4.87	1.45	1.33
24	B	608	CLA	CHC-C1C	4.87	1.47	1.35
24	A	405	CLA	C3C-C2C	4.87	1.47	1.36
25	a	407	PHO	CHD-C1D	4.86	1.48	1.38
24	C	504	CLA	O2D-CGD	4.86	1.45	1.33
25	D	401	PHO	CHD-C1D	4.86	1.48	1.38
24	b	611	CLA	OBD-CAD	4.85	1.29	1.22
24	a	405	CLA	OBD-CAD	4.85	1.29	1.22
24	b	617	CLA	O2D-CGD	4.85	1.45	1.33
24	B	610	CLA	C3B-C2B	4.85	1.47	1.40
24	a	406	CLA	O2D-CGD	4.85	1.45	1.33
24	c	909	CLA	OBD-CAD	4.84	1.29	1.22
24	b	617	CLA	OBD-CAD	4.84	1.29	1.22
24	B	614	CLA	OBD-CAD	4.83	1.29	1.22
24	B	613	CLA	C3C-C2C	4.83	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	O2D-CGD	4.83	1.45	1.33
26	C	515	BCR	C23-C22	-4.82	1.35	1.45
24	c	906	CLA	O2D-CGD	4.82	1.45	1.33
24	C	508	CLA	CHC-C1C	4.82	1.47	1.35
24	B	616	CLA	C3C-C2C	4.81	1.47	1.36
24	A	407	CLA	O2D-CGD	4.81	1.44	1.33
24	b	615	CLA	O2D-CGD	4.81	1.44	1.33
24	A	409	CLA	OBD-CAD	4.81	1.29	1.22
26	a	409	BCR	C23-C22	-4.81	1.35	1.45
25	A	408	PHO	O2D-CGD	4.80	1.44	1.33
24	c	906	CLA	OBD-CAD	4.80	1.29	1.22
24	B	614	CLA	C3C-C2C	4.80	1.46	1.36
26	T	102	BCR	C23-C22	-4.79	1.35	1.45
24	c	908	CLA	O2D-CGD	4.79	1.44	1.33
24	a	406	CLA	C3C-C2C	4.79	1.46	1.36
24	c	911	CLA	CHC-C1C	4.78	1.47	1.35
24	b	609	CLA	CHC-C1C	4.78	1.47	1.35
26	A	410	BCR	C23-C22	-4.78	1.35	1.45
24	b	611	CLA	O2D-CGD	4.78	1.44	1.33
35	B	623	HTG	C1'-S1	-4.77	1.75	1.81
24	C	501	CLA	OBD-CAD	4.77	1.29	1.22
24	d	404	CLA	CHC-C1C	4.77	1.47	1.35
24	B	602	CLA	O2A-CGA	4.76	1.47	1.33
26	B	620	BCR	C23-C22	-4.76	1.35	1.45
24	A	407	CLA	OBD-CAD	4.75	1.28	1.22
24	B	611	CLA	O2D-CGD	4.75	1.44	1.33
24	b	608	CLA	O2D-CGD	4.74	1.44	1.33
26	d	407	BCR	C23-C22	-4.74	1.35	1.45
24	B	612	CLA	CHC-C1C	4.74	1.47	1.35
24	c	902	CLA	CHC-C1C	4.74	1.47	1.35
24	A	406	CLA	O2D-CGD	4.74	1.44	1.33
24	b	620	CLA	OBD-CAD	4.73	1.28	1.22
24	B	613	CLA	O2D-CGD	4.72	1.44	1.33
26	c	927	BCR	C23-C22	-4.72	1.35	1.45
24	b	614	CLA	OBD-CAD	4.71	1.28	1.22
24	C	501	CLA	O2D-CGD	4.71	1.44	1.33
26	h	101	BCR	C23-C22	-4.71	1.35	1.45
24	c	911	CLA	O2D-CGD	4.71	1.44	1.33
24	b	616	CLA	CHC-C1C	4.70	1.47	1.35
24	B	603	CLA	O2D-CGD	4.70	1.44	1.33
24	b	607	CLA	O2D-CGD	4.69	1.44	1.33
24	C	509	CLA	OBD-CAD	4.69	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHC-C1C	4.69	1.47	1.35
24	c	912	CLA	O2D-CGD	4.69	1.44	1.33
24	B	607	CLA	OBD-CAD	4.68	1.28	1.22
24	C	503	CLA	O2D-CGD	4.68	1.44	1.33
24	B	615	CLA	CHC-C1C	4.68	1.47	1.35
24	c	912	CLA	OBD-CAD	4.68	1.28	1.22
24	b	612	CLA	OBD-CAD	4.68	1.28	1.22
24	b	606	CLA	OBD-CAD	4.68	1.28	1.22
24	C	507	CLA	O2D-CGD	4.68	1.44	1.33
24	c	904	CLA	OBD-CAD	4.68	1.28	1.22
24	b	607	CLA	OBD-CAD	4.67	1.28	1.22
24	D	404	CLA	CHC-C1C	4.66	1.46	1.35
24	c	904	CLA	O2D-CGD	4.66	1.44	1.33
24	d	404	CLA	O2D-CGD	4.66	1.44	1.33
24	d	406	CLA	OBD-CAD	4.65	1.28	1.22
24	C	508	CLA	OBD-CAD	4.64	1.28	1.22
24	B	616	CLA	OBD-CAD	4.63	1.28	1.22
24	C	505	CLA	O2D-CGD	4.63	1.44	1.33
24	A	405	CLA	O2D-CGD	4.63	1.44	1.33
24	C	512	CLA	OBD-CAD	4.63	1.28	1.22
24	A	406	CLA	CHC-C1C	4.63	1.46	1.35
25	a	407	PHO	CHC-C1C	4.63	1.47	1.38
24	B	605	CLA	O2D-CGD	4.62	1.44	1.33
24	B	602	CLA	OBD-CAD	4.61	1.28	1.22
24	C	502	CLA	OBD-CAD	4.61	1.28	1.22
37	D	408	DGD	O1G-C1A	4.60	1.46	1.33
27	A	414	SQD	O48-C23	4.60	1.46	1.33
24	B	608	CLA	O2D-CGD	4.59	1.44	1.33
33	z	101	LMG	O8-C28	4.59	1.46	1.33
25	d	403	PHO	CHD-C1D	4.58	1.47	1.38
24	b	613	CLA	OBD-CAD	4.58	1.28	1.22
24	d	404	CLA	OBD-CAD	4.57	1.28	1.22
24	b	621	CLA	OBD-CAD	4.57	1.28	1.22
24	c	914	CLA	OBD-CAD	4.56	1.28	1.22
24	C	513	CLA	OBD-CAD	4.55	1.28	1.22
24	a	406	CLA	O2A-CGA	4.55	1.46	1.33
24	a	405	CLA	O2D-CGD	4.54	1.44	1.33
26	c	915	BCR	C23-C22	-4.53	1.36	1.45
27	a	402	SQD	O48-C23	4.53	1.46	1.33
24	c	908	CLA	OBD-CAD	4.53	1.28	1.22
27	f	102	SQD	O47-C7	4.52	1.47	1.34
24	C	503	CLA	OBD-CAD	4.52	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	OBD-CAD	4.51	1.28	1.22
24	c	910	CLA	O2A-CGA	4.51	1.46	1.33
24	b	609	CLA	O2A-CGA	4.51	1.46	1.33
24	C	508	CLA	O2A-CGA	4.51	1.46	1.33
37	e	101	DGD	O2G-C1B	4.50	1.47	1.34
24	b	618	CLA	CHC-C1C	4.49	1.46	1.35
24	C	509	CLA	O2A-CGA	4.48	1.46	1.33
37	D	408	DGD	O2G-C1B	4.48	1.46	1.34
24	C	511	CLA	OBD-CAD	4.47	1.28	1.22
24	C	504	CLA	OBD-CAD	4.47	1.28	1.22
24	B	610	CLA	O2A-CGA	4.47	1.46	1.33
24	b	608	CLA	OBD-CAD	4.46	1.28	1.22
24	c	907	CLA	OBD-CAD	4.45	1.28	1.22
27	F	103	SQD	O47-C7	4.45	1.46	1.34
26	b	622	BCR	C23-C22	-4.44	1.36	1.45
24	B	604	CLA	O2A-CGA	4.44	1.46	1.33
24	C	512	CLA	O2A-CGA	4.44	1.46	1.33
24	B	610	CLA	OBD-CAD	4.43	1.28	1.22
26	D	406	BCR	C23-C22	-4.42	1.36	1.45
24	B	617	CLA	OBD-CAD	4.42	1.28	1.22
24	b	612	CLA	C3B-C2B	4.42	1.46	1.40
24	b	621	CLA	O2A-CGA	4.42	1.46	1.33
33	Y	101	LMG	O8-C28	4.41	1.46	1.33
33	A	419	LMG	O7-C10	4.41	1.46	1.34
26	B	618	BCR	C23-C22	-4.40	1.36	1.45
36	a	418	LHG	O8-C23	4.39	1.46	1.33
36	D	410	LHG	O7-C7	4.38	1.46	1.34
24	c	902	CLA	OBD-CAD	4.38	1.28	1.22
24	B	608	CLA	OBD-CAD	4.38	1.28	1.22
24	A	406	CLA	O2A-CGA	4.38	1.46	1.33
24	b	606	CLA	O2A-CGA	4.37	1.46	1.33
27	f	102	SQD	O48-C23	4.37	1.46	1.33
36	L	101	LHG	O8-C23	4.37	1.46	1.33
24	d	405	CLA	O2D-CGD	4.37	1.43	1.33
24	B	609	CLA	O2A-CGA	4.35	1.46	1.33
33	B	622	LMG	O8-C28	4.35	1.46	1.33
33	C	519	LMG	O7-C10	4.34	1.46	1.34
24	c	912	CLA	O2A-CGA	4.34	1.46	1.33
24	B	615	CLA	O2A-CGA	4.34	1.46	1.33
24	d	404	CLA	O2A-CGA	4.33	1.46	1.33
33	A	419	LMG	O8-C28	4.32	1.46	1.33
24	c	908	CLA	O2A-CGA	4.32	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	E	101	LHG	O8-C23	4.31	1.45	1.33
24	C	506	CLA	O2A-CGA	4.31	1.45	1.33
24	c	909	CLA	O2A-CGA	4.30	1.45	1.33
24	B	616	CLA	O2A-CGA	4.30	1.45	1.33
27	L	102	SQD	O47-C7	4.30	1.46	1.34
24	C	507	CLA	OBD-CAD	4.29	1.28	1.22
33	a	411	LMG	O8-C28	4.29	1.45	1.33
37	e	101	DGD	O1G-C1A	4.29	1.45	1.33
24	b	612	CLA	O2A-CGA	4.29	1.45	1.33
37	c	918	DGD	O1G-C1A	4.29	1.45	1.33
24	b	620	CLA	O2A-CGA	4.28	1.45	1.33
36	b	635	LHG	O8-C23	4.28	1.45	1.33
27	a	402	SQD	O47-C7	4.28	1.46	1.34
27	B	621	SQD	O47-C7	4.28	1.46	1.34
24	C	510	CLA	O2A-CGA	4.27	1.45	1.33
24	B	606	CLA	OBD-CAD	4.27	1.28	1.22
24	d	406	CLA	O2A-CGA	4.26	1.45	1.33
24	b	618	CLA	OBD-CAD	4.26	1.28	1.22
35	b	628	HTG	C1'-S1	-4.26	1.76	1.81
37	c	917	DGD	O1G-C1A	4.25	1.45	1.33
24	B	613	CLA	OBD-CAD	4.25	1.28	1.22
24	b	619	CLA	O2A-CGA	4.25	1.45	1.33
24	c	913	CLA	O2A-CGA	4.25	1.45	1.33
24	c	903	CLA	OBD-CAD	4.25	1.28	1.22
37	C	518	DGD	O1G-C1A	4.24	1.45	1.33
24	B	607	CLA	O2A-CGA	4.24	1.45	1.33
26	B	619	BCR	C23-C22	-4.23	1.36	1.45
24	c	903	CLA	O2A-CGA	4.23	1.45	1.33
24	C	505	CLA	OBD-CAD	4.21	1.28	1.22
33	c	920	LMG	O7-C10	4.21	1.46	1.34
36	B	635	LHG	O8-C23	4.21	1.45	1.33
24	C	511	CLA	O2A-CGA	4.21	1.45	1.33
24	C	506	CLA	OBD-CAD	4.20	1.28	1.22
33	d	415	LMG	O7-C10	4.20	1.46	1.34
36	d	411	LHG	O7-C7	4.19	1.46	1.34
25	D	401	PHO	O2A-CGA	4.19	1.45	1.33
24	B	617	CLA	O2A-CGA	4.19	1.45	1.33
24	C	501	CLA	O2A-CGA	4.19	1.45	1.33
24	C	503	CLA	O2A-CGA	4.19	1.45	1.33
33	c	920	LMG	O8-C28	4.18	1.45	1.33
27	a	410	SQD	O48-C23	4.18	1.45	1.33
24	C	507	CLA	O2A-CGA	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	410	LHG	O8-C23	4.18	1.45	1.33
24	b	614	CLA	O2A-CGA	4.18	1.45	1.33
33	C	519	LMG	O8-C28	4.18	1.45	1.33
36	a	418	LHG	O7-C7	4.17	1.46	1.34
24	B	606	CLA	O2A-CGA	4.17	1.45	1.33
24	B	614	CLA	O2A-CGA	4.17	1.45	1.33
24	B	608	CLA	O2A-CGA	4.17	1.45	1.33
24	b	607	CLA	O2A-CGA	4.16	1.45	1.33
33	z	101	LMG	O7-C10	4.16	1.46	1.34
36	d	411	LHG	O8-C23	4.16	1.45	1.33
25	d	403	PHO	O2A-CGA	4.15	1.45	1.33
27	L	102	SQD	O48-C23	4.15	1.45	1.33
33	Z	101	LMG	O7-C10	4.15	1.46	1.34
24	b	609	CLA	OBD-CAD	4.15	1.28	1.22
27	B	621	SQD	O48-C23	4.14	1.45	1.33
24	C	513	CLA	O2A-CGA	4.13	1.45	1.33
24	c	906	CLA	O2A-CGA	4.13	1.45	1.33
24	b	611	CLA	O2A-CGA	4.13	1.45	1.33
37	C	517	DGD	O1G-C1A	4.13	1.45	1.33
24	c	914	CLA	O2A-CGA	4.12	1.45	1.33
33	d	415	LMG	O8-C28	4.12	1.45	1.33
25	A	408	PHO	O2A-CGA	4.12	1.45	1.33
24	d	405	CLA	OBD-CAD	4.12	1.28	1.22
24	B	613	CLA	O2A-CGA	4.12	1.45	1.33
37	C	516	DGD	O1G-C1A	4.12	1.45	1.33
24	a	408	CLA	O2A-CGA	4.12	1.45	1.33
37	h	102	DGD	O1G-C1A	4.11	1.45	1.33
37	C	516	DGD	O2G-C1B	4.10	1.45	1.34
24	B	604	CLA	OBD-CAD	4.10	1.28	1.22
24	D	405	CLA	O2A-CGA	4.10	1.45	1.33
24	a	408	CLA	OBD-CAD	4.08	1.28	1.22
37	H	102	DGD	O1G-C1A	4.08	1.45	1.33
36	E	101	LHG	O7-C7	4.07	1.45	1.34
24	b	613	CLA	O2A-CGA	4.07	1.45	1.33
36	b	635	LHG	O7-C7	4.07	1.45	1.34
24	A	409	CLA	O2A-CGA	4.07	1.45	1.33
24	c	911	CLA	O2A-CGA	4.06	1.45	1.33
27	F	103	SQD	O48-C23	4.06	1.45	1.33
24	B	611	CLA	O2A-CGA	4.06	1.45	1.33
24	b	616	CLA	OBD-CAD	4.05	1.28	1.22
24	b	616	CLA	O2A-CGA	4.05	1.45	1.33
33	c	919	LMG	O8-C28	4.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	404	CLA	O2A-CGA	4.02	1.45	1.33
24	b	619	CLA	OBD-CAD	4.02	1.27	1.22
24	c	905	CLA	OBD-CAD	4.02	1.27	1.22
24	d	405	CLA	O2A-CGA	4.02	1.45	1.33
24	D	404	CLA	OBD-CAD	4.02	1.27	1.22
36	d	409	LHG	O8-C23	4.01	1.45	1.33
24	D	405	CLA	OBD-CAD	4.01	1.27	1.22
33	B	622	LMG	O7-C10	4.01	1.45	1.34
24	b	618	CLA	O2A-CGA	4.01	1.45	1.33
24	C	504	CLA	O2A-CGA	4.00	1.45	1.33
27	a	410	SQD	O47-C7	4.00	1.45	1.34
27	A	411	SQD	O47-C7	4.00	1.45	1.34
24	b	617	CLA	O2A-CGA	3.99	1.45	1.33
25	a	407	PHO	OBD-CAD	3.99	1.29	1.22
24	C	502	CLA	O2A-CGA	3.99	1.45	1.33
24	A	407	CLA	O2A-CGA	3.99	1.45	1.33
37	c	916	DGD	O2G-C1B	3.99	1.45	1.34
24	b	610	CLA	OBD-CAD	3.98	1.27	1.22
33	Y	101	LMG	O7-C10	3.97	1.45	1.34
24	c	905	CLA	O2A-CGA	3.96	1.44	1.33
37	H	102	DGD	O2G-C1B	3.95	1.45	1.34
37	c	917	DGD	O2G-C1B	3.95	1.45	1.34
37	h	102	DGD	O2G-C1B	3.95	1.45	1.34
33	J	101	LMG	O8-C28	3.95	1.44	1.33
24	c	902	CLA	O2A-CGA	3.95	1.44	1.33
36	D	409	LHG	O8-C23	3.94	1.44	1.33
24	A	405	CLA	O2A-CGA	3.93	1.44	1.33
24	C	505	CLA	O2A-CGA	3.93	1.44	1.33
33	J	101	LMG	O7-C10	3.93	1.45	1.34
24	c	904	CLA	O2A-CGA	3.92	1.44	1.33
37	C	518	DGD	O2G-C1B	3.92	1.45	1.34
24	c	907	CLA	O2A-CGA	3.92	1.44	1.33
33	a	411	LMG	O7-C10	3.91	1.45	1.34
24	b	615	CLA	O2A-CGA	3.91	1.44	1.33
37	c	918	DGD	O2G-C1B	3.91	1.45	1.34
33	b	625	LMG	O8-C28	3.91	1.44	1.33
24	B	612	CLA	O2A-CGA	3.91	1.44	1.33
24	B	612	CLA	OBD-CAD	3.90	1.27	1.22
24	b	608	CLA	O2A-CGA	3.90	1.44	1.33
24	B	603	CLA	O2A-CGA	3.89	1.44	1.33
27	A	414	SQD	O47-C7	3.89	1.45	1.34
33	c	919	LMG	O7-C10	3.85	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	OBD-CAD	3.84	1.27	1.22
25	a	407	PHO	C3D-C2D	3.83	1.49	1.39
37	C	517	DGD	O2G-C1B	3.82	1.45	1.34
24	b	610	CLA	O2A-CGA	3.81	1.44	1.33
33	b	625	LMG	O7-C10	3.81	1.45	1.34
27	A	411	SQD	O48-C23	3.81	1.44	1.33
24	B	605	CLA	O2A-CGA	3.80	1.44	1.33
37	c	916	DGD	O1G-C1A	3.80	1.44	1.33
36	d	410	LHG	O7-C7	3.78	1.45	1.34
25	A	408	PHO	C3D-C2D	3.77	1.49	1.39
36	L	101	LHG	O7-C7	3.70	1.44	1.34
25	a	407	PHO	O2A-CGA	3.69	1.44	1.33
35	d	414	HTG	C1'-S1	-3.69	1.76	1.81
35	b	603	HTG	C1'-S1	-3.68	1.76	1.81
25	D	401	PHO	C3D-C2D	3.66	1.49	1.39
35	b	601	HTG	C1'-S1	-3.66	1.76	1.81
35	B	633	HTG	C1'-S1	-3.65	1.76	1.81
36	d	410	LHG	O8-C23	3.64	1.44	1.33
36	D	409	LHG	O7-C7	3.63	1.44	1.34
24	a	405	CLA	O2A-CGA	3.60	1.43	1.33
35	V	203	HTG	C1'-S1	-3.60	1.76	1.81
25	a	407	PHO	CHC-C4B	3.59	1.48	1.40
35	B	625	HTG	C1'-S1	-3.58	1.76	1.81
25	d	403	PHO	CHC-C4B	3.54	1.48	1.40
25	D	401	PHO	C4A-NA	-3.53	1.26	1.35
35	c	922	HTG	C1'-S1	-3.52	1.76	1.81
25	a	407	PHO	C4A-NA	-3.50	1.26	1.35
25	A	408	PHO	CHB-C4A	3.49	1.48	1.40
25	A	408	PHO	OBD-CAD	3.48	1.28	1.22
36	B	635	LHG	O7-C7	3.48	1.44	1.34
36	d	409	LHG	O7-C7	3.47	1.44	1.34
25	A	408	PHO	C4A-NA	-3.47	1.26	1.35
35	C	522	HTG	C1'-S1	-3.45	1.77	1.81
35	C	521	HTG	C1'-S1	-3.44	1.77	1.81
35	D	413	HTG	C1'-S1	-3.44	1.77	1.81
25	D	401	PHO	CHC-C4B	3.44	1.48	1.40
25	D	401	PHO	CHD-C4C	3.43	1.48	1.40
25	D	401	PHO	OBD-CAD	3.42	1.28	1.22
25	d	403	PHO	C3D-C2D	3.40	1.48	1.39
35	B	632	HTG	C1'-S1	-3.36	1.77	1.81
35	b	604	HTG	C1'-S1	-3.33	1.77	1.81
24	A	405	CLA	C4C-C3C	3.31	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	921	HTG	C1'-S1	-3.29	1.77	1.81
25	d	403	PHO	C4A-NA	-3.23	1.27	1.35
25	A	408	PHO	CHC-C4B	3.22	1.48	1.40
25	d	403	PHO	OBD-CAD	3.22	1.28	1.22
24	B	606	CLA	C1C-C2C	3.13	1.50	1.44
25	a	407	PHO	CHD-C4C	3.13	1.47	1.40
25	D	401	PHO	C3B-C4B	3.12	1.49	1.43
25	A	408	PHO	CHD-C4C	3.12	1.47	1.40
24	b	607	CLA	C1D-C2D	3.12	1.49	1.42
25	d	403	PHO	C3B-C4B	3.08	1.49	1.43
35	B	624	HTG	C1'-S1	-3.06	1.77	1.81
24	c	912	CLA	C1D-C2D	3.05	1.49	1.42
25	d	403	PHO	CHB-C4A	3.02	1.47	1.40
25	a	407	PHO	C3B-C4B	3.00	1.49	1.43
25	a	407	PHO	CHB-C4A	3.00	1.47	1.40
24	B	603	CLA	C1D-C2D	2.99	1.49	1.42
24	C	507	CLA	C1C-C2C	2.98	1.50	1.44
24	d	406	CLA	C1D-C2D	2.98	1.49	1.42
24	b	615	CLA	C1D-C2D	2.97	1.49	1.42
25	D	401	PHO	CHB-C4A	2.96	1.47	1.40
27	f	102	SQD	C6-S	-2.96	1.66	1.77
24	b	618	CLA	C4C-C3C	2.95	1.50	1.45
24	C	508	CLA	C4C-C3C	2.94	1.50	1.45
24	C	506	CLA	C1D-C2D	2.93	1.49	1.42
24	B	612	CLA	C1D-C2D	2.92	1.49	1.42
27	A	411	SQD	C6-S	-2.92	1.66	1.77
24	A	405	CLA	C1D-C2D	2.91	1.49	1.42
24	B	613	CLA	C1C-C2C	2.91	1.50	1.44
24	B	607	CLA	C1D-C2D	2.90	1.49	1.42
27	A	414	SQD	C6-S	-2.90	1.66	1.77
29	A	415	LMT	O1'-C1'	2.90	1.45	1.40
24	c	910	CLA	C1C-C2C	2.90	1.50	1.44
24	b	610	CLA	C1D-C2D	2.90	1.49	1.42
24	C	511	CLA	C4C-C3C	2.89	1.50	1.45
24	b	614	CLA	C1D-C2D	2.88	1.49	1.42
24	b	609	CLA	C1C-C2C	2.88	1.50	1.44
24	c	902	CLA	C4C-C3C	2.88	1.50	1.45
24	D	405	CLA	C1D-C2D	2.88	1.49	1.42
24	b	617	CLA	C1C-C2C	2.87	1.50	1.44
24	c	902	CLA	C1D-C2D	2.87	1.49	1.42
24	A	407	CLA	C1D-C2D	2.86	1.49	1.42
24	b	606	CLA	C1D-C2D	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	C1D-C2D	2.86	1.49	1.42
27	a	402	SQD	C6-S	-2.86	1.66	1.77
25	d	403	PHO	CHD-C4C	2.84	1.47	1.40
27	F	103	SQD	C6-S	-2.83	1.67	1.77
24	C	508	CLA	C1D-C2D	2.83	1.49	1.42
24	B	615	CLA	C1D-C2D	2.82	1.49	1.42
24	b	610	CLA	C1C-C2C	2.82	1.50	1.44
24	c	905	CLA	C1D-C2D	2.82	1.49	1.42
24	B	604	CLA	C1C-C2C	2.82	1.50	1.44
24	B	613	CLA	C1B-CHB	2.81	1.48	1.41
24	B	616	CLA	C1D-C2D	2.81	1.48	1.42
24	B	602	CLA	C1D-C2D	2.81	1.48	1.42
24	a	405	CLA	C1D-C2D	2.81	1.48	1.42
24	B	615	CLA	C4C-C3C	2.81	1.49	1.45
24	a	405	CLA	C4C-C3C	2.80	1.49	1.45
24	b	613	CLA	C1B-CHB	2.80	1.48	1.41
25	A	408	PHO	C3B-C4B	2.80	1.49	1.43
24	C	502	CLA	C1D-C2D	2.80	1.48	1.42
24	b	620	CLA	C1D-C2D	2.79	1.48	1.42
24	c	914	CLA	C1D-C2D	2.79	1.48	1.42
24	b	621	CLA	C1D-C2D	2.78	1.48	1.42
24	a	406	CLA	C1D-C2D	2.78	1.48	1.42
24	c	908	CLA	C1C-C2C	2.77	1.49	1.44
24	C	505	CLA	C1B-CHB	2.77	1.48	1.41
24	B	611	CLA	C1D-C2D	2.77	1.48	1.42
24	C	501	CLA	C1C-C2C	2.76	1.49	1.44
24	C	507	CLA	C4B-CHC	2.76	1.48	1.41
24	C	513	CLA	C1D-C2D	2.76	1.48	1.42
24	D	404	CLA	C1C-C2C	2.76	1.49	1.44
24	C	512	CLA	C1D-C2D	2.76	1.48	1.42
24	C	509	CLA	C1C-C2C	2.75	1.49	1.44
24	A	405	CLA	C1C-C2C	2.74	1.49	1.44
24	b	611	CLA	C1C-C2C	2.74	1.49	1.44
24	C	506	CLA	CHD-C4C	2.74	1.49	1.41
24	b	611	CLA	C1D-C2D	2.73	1.48	1.42
24	d	406	CLA	C4B-CHC	2.72	1.48	1.41
24	c	904	CLA	C1C-C2C	2.72	1.49	1.44
24	C	510	CLA	C1C-C2C	2.72	1.49	1.44
24	c	913	CLA	C1D-C2D	2.72	1.48	1.42
24	B	609	CLA	C1D-C2D	2.71	1.48	1.42
24	c	907	CLA	C1D-C2D	2.71	1.48	1.42
24	B	606	CLA	C4B-CHC	2.71	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	CHD-C4C	2.71	1.48	1.41
24	b	619	CLA	C1C-C2C	2.71	1.49	1.44
24	A	409	CLA	C1D-C2D	2.70	1.48	1.42
38	F	102	HEM	C3B-C2B	-2.70	1.36	1.40
24	C	504	CLA	C1B-CHB	2.70	1.48	1.41
24	B	608	CLA	C1D-C2D	2.70	1.48	1.42
24	C	507	CLA	C1D-C2D	2.70	1.48	1.42
33	Z	101	LMG	O8-C28	2.70	1.46	1.33
24	d	406	CLA	C1C-C2C	2.69	1.49	1.44
24	A	409	CLA	C4B-CHC	2.69	1.48	1.41
24	c	910	CLA	C1B-CHB	2.69	1.48	1.41
24	C	504	CLA	C1D-C2D	2.69	1.48	1.42
24	b	613	CLA	C4B-CHC	2.69	1.48	1.41
24	A	405	CLA	CHD-C4C	2.69	1.48	1.41
24	A	409	CLA	C4C-C3C	2.69	1.49	1.45
24	d	405	CLA	C1D-C2D	2.68	1.48	1.42
24	C	503	CLA	C1C-C2C	2.68	1.49	1.44
24	B	607	CLA	C1C-C2C	2.67	1.49	1.44
24	B	610	CLA	C1D-C2D	2.67	1.48	1.42
24	b	616	CLA	C1B-CHB	2.67	1.48	1.41
24	b	608	CLA	C1D-C2D	2.66	1.48	1.42
24	C	511	CLA	CHD-C4C	2.66	1.48	1.41
24	b	612	CLA	C1D-C2D	2.66	1.48	1.42
24	b	617	CLA	C1B-CHB	2.66	1.48	1.41
24	c	903	CLA	C1B-CHB	2.66	1.48	1.41
24	b	615	CLA	C1B-CHB	2.66	1.48	1.41
24	B	606	CLA	C1D-C2D	2.66	1.48	1.42
24	b	620	CLA	C1B-CHB	2.66	1.48	1.41
24	b	607	CLA	C1C-C2C	2.65	1.49	1.44
24	B	614	CLA	C1D-C2D	2.65	1.48	1.42
24	C	503	CLA	C1D-C2D	2.65	1.48	1.42
24	b	615	CLA	C4C-C3C	2.65	1.49	1.45
24	C	512	CLA	C1C-C2C	2.64	1.49	1.44
24	b	608	CLA	C1C-C2C	2.64	1.49	1.44
24	c	910	CLA	C1D-C2D	2.64	1.48	1.42
35	b	628	HTG	C1-S1	-2.64	1.76	1.80
27	L	102	SQD	C6-S	-2.64	1.67	1.77
24	C	501	CLA	CHD-C4C	2.63	1.48	1.41
24	C	502	CLA	C1C-C2C	2.63	1.49	1.44
24	C	510	CLA	C1B-CHB	2.63	1.48	1.41
24	c	914	CLA	C1C-C2C	2.63	1.49	1.44
24	C	509	CLA	C1D-C2D	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	CHD-C4C	2.63	1.48	1.41
24	c	902	CLA	CHD-C4C	2.62	1.48	1.41
24	c	906	CLA	C1B-CHB	2.62	1.48	1.41
27	B	621	SQD	C6-S	-2.62	1.67	1.77
24	C	503	CLA	C4B-CHC	2.62	1.48	1.41
24	C	506	CLA	C4C-C3C	2.62	1.49	1.45
24	B	615	CLA	C1C-C2C	2.62	1.49	1.44
35	b	627	HTG	C1'-S1	-2.62	1.78	1.81
24	C	504	CLA	C1C-C2C	2.62	1.49	1.44
24	C	501	CLA	C4B-CHC	2.62	1.48	1.41
24	b	618	CLA	C1B-CHB	2.61	1.48	1.41
31	A	417	PL9	C6-C5	2.61	1.48	1.35
24	c	911	CLA	CHD-C4C	2.61	1.48	1.41
24	B	615	CLA	C1B-CHB	2.60	1.48	1.41
24	C	510	CLA	C1D-C2D	2.60	1.48	1.42
24	D	404	CLA	C4C-C3C	2.60	1.49	1.45
24	c	904	CLA	C1D-C2D	2.60	1.48	1.42
24	c	911	CLA	C1D-C2D	2.59	1.48	1.42
24	B	614	CLA	C1C-C2C	2.59	1.49	1.44
24	C	513	CLA	CHD-C4C	2.59	1.48	1.41
24	c	911	CLA	C1B-CHB	2.59	1.48	1.41
24	b	613	CLA	C1D-C2D	2.59	1.48	1.42
24	b	613	CLA	C4C-C3C	2.59	1.49	1.45
24	C	504	CLA	CHD-C4C	2.58	1.48	1.41
24	b	615	CLA	CHD-C4C	2.58	1.48	1.41
24	C	503	CLA	CHD-C4C	2.58	1.48	1.41
24	c	908	CLA	C1D-C2D	2.58	1.48	1.42
24	C	502	CLA	C4C-C3C	2.58	1.49	1.45
24	B	611	CLA	CHD-C4C	2.58	1.48	1.41
24	A	409	CLA	C1C-C2C	2.57	1.49	1.44
24	c	904	CLA	C4B-CHC	2.57	1.48	1.41
31	a	415	PL9	C6-C5	2.57	1.48	1.35
24	A	407	CLA	CHD-C4C	2.57	1.48	1.41
24	a	405	CLA	CHD-C4C	2.57	1.48	1.41
24	C	508	CLA	CHD-C4C	2.57	1.48	1.41
24	A	406	CLA	C1D-C2D	2.57	1.48	1.42
24	c	914	CLA	CHD-C4C	2.56	1.48	1.41
24	b	621	CLA	C1B-CHB	2.56	1.48	1.41
24	C	509	CLA	C4C-C3C	2.56	1.49	1.45
24	c	906	CLA	C1C-C2C	2.56	1.49	1.44
24	C	511	CLA	C1B-CHB	2.56	1.48	1.41
24	c	913	CLA	CHD-C4C	2.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C4B-CHC	2.56	1.48	1.41
24	b	614	CLA	C1B-CHB	2.55	1.48	1.41
24	C	502	CLA	CHD-C4C	2.55	1.48	1.41
24	B	612	CLA	C1C-C2C	2.55	1.49	1.44
24	d	404	CLA	C1D-C2D	2.55	1.48	1.42
24	c	909	CLA	C1B-CHB	2.55	1.48	1.41
24	C	511	CLA	C1D-C2D	2.55	1.48	1.42
24	c	907	CLA	C1B-NB	-2.54	1.32	1.35
24	B	608	CLA	C1B-CHB	2.54	1.48	1.41
24	C	512	CLA	CHD-C4C	2.54	1.48	1.41
38	v	202	HEM	C3B-C2B	-2.54	1.36	1.40
24	C	512	CLA	C4B-CHC	2.54	1.48	1.41
24	c	902	CLA	C1B-CHB	2.54	1.48	1.41
24	b	619	CLA	C1B-CHB	2.54	1.48	1.41
24	A	409	CLA	CHD-C4C	2.53	1.48	1.41
24	c	914	CLA	C4B-CHC	2.53	1.48	1.41
24	C	510	CLA	CHD-C4C	2.53	1.48	1.41
27	a	410	SQD	C6-S	-2.53	1.68	1.77
24	b	617	CLA	C4B-CHC	2.53	1.48	1.41
24	c	910	CLA	CHD-C4C	2.53	1.48	1.41
24	B	608	CLA	C4B-CHC	2.52	1.48	1.41
24	B	616	CLA	C4B-CHC	2.52	1.48	1.41
24	B	614	CLA	C4C-C3C	2.52	1.49	1.45
24	B	610	CLA	C1B-CHB	2.52	1.48	1.41
24	B	609	CLA	CHD-C4C	2.52	1.48	1.41
24	c	913	CLA	C1C-C2C	2.52	1.49	1.44
24	B	613	CLA	C4C-C3C	2.52	1.49	1.45
24	b	619	CLA	C4B-CHC	2.52	1.48	1.41
24	d	404	CLA	CHD-C4C	2.52	1.48	1.41
24	b	613	CLA	C1C-C2C	2.52	1.49	1.44
31	d	408	PL9	C6-C5	2.51	1.48	1.35
24	B	615	CLA	CHD-C4C	2.51	1.48	1.41
24	B	609	CLA	C1C-C2C	2.51	1.49	1.44
24	a	408	CLA	C1D-C2D	2.51	1.48	1.42
24	C	504	CLA	C4B-CHC	2.51	1.48	1.41
24	B	608	CLA	CHD-C4C	2.51	1.48	1.41
24	b	610	CLA	C4B-CHC	2.51	1.48	1.41
24	b	621	CLA	C4B-CHC	2.50	1.47	1.41
24	B	605	CLA	C1D-C2D	2.50	1.48	1.42
24	C	505	CLA	C1C-C2C	2.50	1.49	1.44
24	B	608	CLA	C4C-C3C	2.50	1.49	1.45
24	b	614	CLA	CHD-C4C	2.50	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C1C-C2C	2.50	1.49	1.44
24	C	510	CLA	C4C-C3C	2.50	1.49	1.45
24	B	603	CLA	C4B-CHC	2.50	1.47	1.41
24	c	906	CLA	C4B-CHC	2.50	1.47	1.41
24	D	405	CLA	CHD-C4C	2.49	1.48	1.41
24	d	405	CLA	C4B-CHC	2.49	1.47	1.41
24	B	611	CLA	C4B-NB	-2.49	1.33	1.35
24	C	511	CLA	C1C-C2C	2.49	1.49	1.44
24	c	907	CLA	C1B-CHB	2.48	1.47	1.41
24	a	405	CLA	C4B-CHC	2.48	1.47	1.41
24	C	509	CLA	C4B-CHC	2.48	1.47	1.41
24	b	608	CLA	C4C-C3C	2.48	1.49	1.45
38	f	101	HEM	C3B-C2B	-2.48	1.36	1.40
24	b	609	CLA	C1B-CHB	2.48	1.47	1.41
24	b	613	CLA	CHD-C4C	2.48	1.48	1.41
24	B	603	CLA	C1C-C2C	2.47	1.49	1.44
24	b	607	CLA	C1B-CHB	2.47	1.47	1.41
24	C	509	CLA	C1B-CHB	2.47	1.47	1.41
24	C	510	CLA	C4B-CHC	2.47	1.47	1.41
24	b	620	CLA	C1C-C2C	2.47	1.49	1.44
24	C	509	CLA	CHD-C4C	2.47	1.48	1.41
24	C	502	CLA	C1B-CHB	2.47	1.47	1.41
24	B	616	CLA	CHD-C4C	2.47	1.48	1.41
35	c	921	HTG	C1-S1	-2.47	1.76	1.80
24	b	619	CLA	CHD-C4C	2.47	1.48	1.41
24	a	406	CLA	C4B-CHC	2.46	1.47	1.41
24	b	619	CLA	C1D-C2D	2.46	1.48	1.42
24	c	906	CLA	C4C-C3C	2.46	1.49	1.45
24	B	605	CLA	C1B-CHB	2.46	1.47	1.41
24	B	611	CLA	C1B-CHB	2.46	1.47	1.41
24	B	609	CLA	C4C-C3C	2.46	1.49	1.45
24	B	604	CLA	CHD-C4C	2.45	1.48	1.41
24	D	405	CLA	C4C-C3C	2.45	1.49	1.45
24	c	909	CLA	C1D-C2D	2.45	1.48	1.42
24	c	908	CLA	C4B-CHC	2.45	1.47	1.41
24	B	602	CLA	C1B-CHB	2.45	1.47	1.41
24	d	406	CLA	C1B-CHB	2.45	1.47	1.41
24	B	611	CLA	C4B-CHC	2.45	1.47	1.41
24	B	604	CLA	C1D-C2D	2.45	1.48	1.42
24	B	617	CLA	C4B-CHC	2.45	1.47	1.41
24	c	905	CLA	C1C-C2C	2.45	1.49	1.44
24	b	615	CLA	C4B-CHC	2.45	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	904	CLA	CHD-C4C	2.45	1.48	1.41
24	C	513	CLA	C4B-CHC	2.44	1.47	1.41
24	A	406	CLA	C1C-C2C	2.44	1.49	1.44
24	c	905	CLA	CHD-C4C	2.44	1.48	1.41
24	B	606	CLA	C1B-CHB	2.44	1.47	1.41
24	B	612	CLA	C1B-CHB	2.44	1.47	1.41
24	c	911	CLA	C4C-C3C	2.44	1.49	1.45
24	B	607	CLA	CHD-C4C	2.44	1.48	1.41
24	b	621	CLA	C4C-C3C	2.44	1.49	1.45
24	C	506	CLA	C1B-CHB	2.43	1.47	1.41
24	b	606	CLA	C4B-CHC	2.43	1.47	1.41
24	c	905	CLA	C4B-CHC	2.43	1.47	1.41
24	B	613	CLA	C4B-CHC	2.42	1.47	1.41
24	c	908	CLA	CHD-C4C	2.42	1.48	1.41
24	b	610	CLA	C1B-CHB	2.42	1.47	1.41
24	B	613	CLA	C1D-C2D	2.41	1.48	1.42
24	b	607	CLA	C4C-C3C	2.41	1.49	1.45
24	b	607	CLA	C4B-CHC	2.41	1.47	1.41
24	b	609	CLA	C4C-C3C	2.41	1.49	1.45
24	D	405	CLA	C1C-C2C	2.41	1.49	1.44
24	B	617	CLA	C1D-C2D	2.41	1.48	1.42
24	b	611	CLA	C1B-CHB	2.41	1.47	1.41
24	D	404	CLA	C1D-C2D	2.41	1.48	1.42
24	b	607	CLA	CHD-C4C	2.41	1.48	1.41
24	B	605	CLA	CHD-C4C	2.41	1.48	1.41
24	c	903	CLA	C1D-C2D	2.41	1.48	1.42
24	B	608	CLA	C1B-NB	-2.40	1.33	1.35
24	C	502	CLA	C4B-CHC	2.40	1.47	1.41
24	a	408	CLA	C4B-CHC	2.40	1.47	1.41
24	B	604	CLA	C1B-CHB	2.40	1.47	1.41
35	C	521	HTG	C1-S1	-2.40	1.77	1.80
24	B	607	CLA	C1B-CHB	2.40	1.47	1.41
24	B	611	CLA	C4C-C3C	2.40	1.49	1.45
24	d	405	CLA	C1C-C2C	2.40	1.49	1.44
24	B	602	CLA	C1C-C2C	2.40	1.49	1.44
24	b	615	CLA	C1C-C2C	2.39	1.49	1.44
24	b	620	CLA	C4B-CHC	2.39	1.47	1.41
24	B	607	CLA	C4C-C3C	2.39	1.49	1.45
24	c	913	CLA	C4B-CHC	2.38	1.47	1.41
24	c	910	CLA	C4B-CHC	2.38	1.47	1.41
24	C	504	CLA	C4C-C3C	2.38	1.49	1.45
24	C	508	CLA	C1B-CHB	2.38	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608	CLA	CHD-C4C	2.38	1.47	1.41
24	B	609	CLA	C1B-CHB	2.37	1.47	1.41
31	D	407	PL9	C6-C5	2.37	1.47	1.35
37	D	408	DGD	O3G-C1D	2.37	1.44	1.40
24	b	612	CLA	C1C-C2C	2.37	1.49	1.44
24	C	507	CLA	CHD-C4C	2.37	1.47	1.41
24	a	406	CLA	CHD-C4C	2.37	1.47	1.41
24	C	512	CLA	C1B-CHB	2.37	1.47	1.41
24	d	405	CLA	CHD-C4C	2.37	1.47	1.41
24	B	616	CLA	C1B-CHB	2.37	1.47	1.41
24	B	610	CLA	C4B-CHC	2.36	1.47	1.41
24	a	406	CLA	C1B-CHB	2.36	1.47	1.41
24	B	617	CLA	C1B-CHB	2.36	1.47	1.41
24	a	408	CLA	C1B-CHB	2.36	1.47	1.41
24	b	612	CLA	C1B-CHB	2.36	1.47	1.41
24	b	611	CLA	C4B-CHC	2.36	1.47	1.41
24	C	513	CLA	C1B-CHB	2.36	1.47	1.41
24	d	405	CLA	C4C-C3C	2.36	1.49	1.45
24	C	501	CLA	C4C-C3C	2.35	1.49	1.45
24	D	405	CLA	C1B-CHB	2.35	1.47	1.41
24	A	405	CLA	C1B-CHB	2.35	1.47	1.41
24	a	406	CLA	C1C-C2C	2.35	1.49	1.44
24	A	407	CLA	C4B-CHC	2.35	1.47	1.41
24	c	910	CLA	C4C-C3C	2.35	1.49	1.45
24	b	614	CLA	C1C-C2C	2.35	1.49	1.44
24	B	605	CLA	C1C-C2C	2.35	1.49	1.44
24	B	607	CLA	C4B-CHC	2.34	1.47	1.41
24	b	620	CLA	CHD-C4C	2.34	1.47	1.41
24	B	612	CLA	C4C-C3C	2.34	1.49	1.45
24	C	507	CLA	C1B-CHB	2.34	1.47	1.41
24	c	903	CLA	CHD-C4C	2.34	1.47	1.41
24	B	606	CLA	CHD-C4C	2.34	1.47	1.41
24	B	614	CLA	C4B-CHC	2.34	1.47	1.41
24	C	513	CLA	C1C-C2C	2.33	1.49	1.44
24	b	614	CLA	C4B-CHC	2.33	1.47	1.41
24	A	406	CLA	CHD-C4C	2.33	1.47	1.41
24	c	908	CLA	C1B-CHB	2.32	1.47	1.41
24	d	406	CLA	CHD-C4C	2.32	1.47	1.41
24	C	508	CLA	C1C-C2C	2.32	1.49	1.44
24	a	408	CLA	CHD-C4C	2.32	1.47	1.41
24	b	609	CLA	C1B-NB	-2.32	1.33	1.35
24	b	612	CLA	C4B-CHC	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C4C-C3C	2.31	1.49	1.45
24	c	908	CLA	C4C-C3C	2.31	1.49	1.45
24	b	612	CLA	CHD-C4C	2.31	1.47	1.41
24	b	609	CLA	CHD-C4C	2.31	1.47	1.41
24	b	619	CLA	C4C-C3C	2.31	1.49	1.45
24	b	609	CLA	C4B-CHC	2.31	1.47	1.41
24	B	602	CLA	CHD-C4C	2.30	1.47	1.41
24	B	604	CLA	C4B-CHC	2.30	1.47	1.41
24	C	503	CLA	C1B-CHB	2.30	1.47	1.41
24	c	905	CLA	C1B-CHB	2.30	1.47	1.41
25	d	403	PHO	C1A-NA	-2.30	1.33	1.37
24	b	609	CLA	C1D-C2D	2.30	1.47	1.42
24	B	602	CLA	C4B-CHC	2.30	1.47	1.41
24	B	616	CLA	C1C-C2C	2.30	1.49	1.44
24	c	907	CLA	CHD-C4C	2.30	1.47	1.41
24	c	909	CLA	CHD-C4C	2.30	1.47	1.41
25	A	408	PHO	C4D-CHA	2.30	1.50	1.43
24	D	404	CLA	CHD-C4C	2.29	1.47	1.41
24	a	405	CLA	C1C-C2C	2.29	1.49	1.44
35	B	625	HTG	C1-S1	-2.29	1.77	1.80
24	b	610	CLA	CHD-C4C	2.29	1.47	1.41
24	b	611	CLA	CHD-C4C	2.29	1.47	1.41
24	B	614	CLA	C1B-CHB	2.29	1.47	1.41
24	C	512	CLA	C4C-C3C	2.29	1.49	1.45
24	b	616	CLA	C4C-C3C	2.29	1.49	1.45
24	c	914	CLA	C1B-CHB	2.29	1.47	1.41
25	D	401	PHO	C4D-CHA	2.29	1.50	1.43
24	A	407	CLA	C1B-CHB	2.29	1.47	1.41
24	b	611	CLA	C4C-C3C	2.29	1.49	1.45
24	c	912	CLA	C1B-CHB	2.28	1.47	1.41
24	A	406	CLA	C4B-CHC	2.28	1.47	1.41
24	D	404	CLA	C4B-CHC	2.28	1.47	1.41
35	V	203	HTG	C1-S1	-2.28	1.77	1.80
24	b	618	CLA	CHD-C4C	2.28	1.47	1.41
24	c	903	CLA	C1C-C2C	2.28	1.49	1.44
24	B	605	CLA	C4C-C3C	2.28	1.49	1.45
24	c	904	CLA	C1B-CHB	2.28	1.47	1.41
24	c	912	CLA	CHD-C4C	2.28	1.47	1.41
37	h	102	DGD	O5D-C1E	2.27	1.44	1.40
24	D	404	CLA	C1B-NB	-2.27	1.33	1.35
24	a	405	CLA	C1B-CHB	2.27	1.47	1.41
24	c	913	CLA	C1B-CHB	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	CHD-C4C	2.26	1.47	1.41
24	B	610	CLA	CHD-C4C	2.26	1.47	1.41
24	c	907	CLA	C4B-CHC	2.26	1.47	1.41
24	b	616	CLA	C1C-C2C	2.26	1.48	1.44
25	A	408	PHO	C1A-NA	-2.25	1.33	1.37
24	D	404	CLA	C1B-CHB	2.25	1.47	1.41
35	d	414	HTG	C1-S1	-2.25	1.77	1.80
24	C	508	CLA	C4B-CHC	2.25	1.47	1.41
24	c	909	CLA	C4C-C3C	2.25	1.48	1.45
24	A	407	CLA	C1C-C2C	2.25	1.48	1.44
24	b	616	CLA	C1D-C2D	2.25	1.47	1.42
24	b	608	CLA	C4B-CHC	2.24	1.47	1.41
24	b	606	CLA	C1B-CHB	2.23	1.47	1.41
24	C	506	CLA	C4B-CHC	2.23	1.47	1.41
24	B	610	CLA	C1C-C2C	2.23	1.48	1.44
24	c	912	CLA	C1C-C2C	2.23	1.48	1.44
24	C	501	CLA	C1B-CHB	2.23	1.47	1.41
24	C	511	CLA	C4B-CHC	2.23	1.47	1.41
24	B	612	CLA	C4B-CHC	2.22	1.47	1.41
24	b	621	CLA	CHD-C4C	2.21	1.47	1.41
24	b	606	CLA	C1C-C2C	2.21	1.48	1.44
24	A	409	CLA	C1B-CHB	2.21	1.47	1.41
24	D	405	CLA	C4B-CHC	2.21	1.47	1.41
24	A	406	CLA	C4C-C3C	2.21	1.48	1.45
24	d	404	CLA	C1C-NC	-2.20	1.34	1.37
24	B	609	CLA	C4B-CHC	2.20	1.47	1.41
24	D	405	CLA	C1C-NC	-2.20	1.34	1.37
24	b	608	CLA	C1B-CHB	2.20	1.47	1.41
24	c	911	CLA	C4B-CHC	2.20	1.47	1.41
24	a	408	CLA	C1C-C2C	2.20	1.48	1.44
24	d	404	CLA	C1B-CHB	2.20	1.47	1.41
24	B	613	CLA	CHD-C4C	2.19	1.47	1.41
38	V	202	HEM	C3B-C2B	-2.19	1.37	1.40
24	B	602	CLA	C1C-NC	-2.19	1.34	1.37
24	b	618	CLA	C1C-C2C	2.19	1.48	1.44
24	A	407	CLA	C4C-C3C	2.19	1.48	1.45
29	M	103	LMT	O1'-C1'	2.19	1.43	1.40
25	a	407	PHO	C1A-NA	-2.18	1.33	1.37
25	D	401	PHO	C4C-C3C	2.18	1.49	1.45
35	c	922	HTG	C1-S1	-2.18	1.77	1.80
35	D	413	HTG	C1-S1	-2.18	1.77	1.80
24	B	610	CLA	C4C-C3C	2.17	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C1C-C2C	2.17	1.48	1.44
24	C	506	CLA	C1C-C2C	2.16	1.48	1.44
24	b	610	CLA	C4C-C3C	2.16	1.48	1.45
24	B	616	CLA	C4C-C3C	2.16	1.48	1.45
38	F	102	HEM	C4D-C3D	2.16	1.47	1.42
24	A	405	CLA	C4B-CHC	2.16	1.47	1.41
36	d	409	LHG	O7-C5	-2.16	1.41	1.46
26	b	624	BCR	C30-C25	-2.16	1.50	1.53
24	B	617	CLA	CHD-C4C	2.16	1.47	1.41
24	c	905	CLA	C1B-NB	-2.15	1.33	1.35
24	b	618	CLA	C1D-C2D	2.15	1.47	1.42
24	c	912	CLA	C4B-CHC	2.14	1.47	1.41
24	d	405	CLA	C1B-CHB	2.14	1.47	1.41
24	a	408	CLA	C4B-NB	-2.14	1.33	1.35
24	B	604	CLA	C1B-NB	-2.14	1.33	1.35
24	C	505	CLA	CHD-C4C	2.14	1.47	1.41
25	A	408	PHO	C4C-C3C	2.14	1.49	1.45
24	C	505	CLA	C1D-C2D	2.14	1.47	1.42
24	c	909	CLA	C1C-C2C	2.13	1.48	1.44
24	C	505	CLA	C4C-C3C	2.13	1.48	1.45
24	B	612	CLA	CHD-C4C	2.12	1.47	1.41
24	b	617	CLA	C1C-NC	-2.12	1.34	1.37
24	b	620	CLA	C4C-C3C	2.12	1.48	1.45
29	b	602	LMT	O1'-C1'	2.12	1.43	1.40
24	c	906	CLA	C1D-C2D	2.11	1.47	1.42
24	c	903	CLA	C4B-CHC	2.11	1.46	1.41
24	b	616	CLA	CHD-C4C	2.11	1.47	1.41
35	b	603	HTG	C1-S1	-2.11	1.77	1.80
29	a	401	LMT	O1'-C1'	2.11	1.43	1.40
35	b	604	HTG	C1-S1	-2.10	1.77	1.80
31	A	417	PL9	C2-C3	2.10	1.40	1.34
35	B	633	HTG	C1-S1	-2.10	1.77	1.80
24	C	503	CLA	C4C-C3C	2.10	1.48	1.45
25	a	407	PHO	C4D-CHA	2.09	1.49	1.43
24	c	902	CLA	C1C-C2C	2.09	1.48	1.44
24	b	617	CLA	C1D-C2D	2.09	1.47	1.42
24	c	907	CLA	C1C-C2C	2.09	1.48	1.44
24	d	404	CLA	C4B-CHC	2.09	1.46	1.41
25	D	401	PHO	C1A-NA	-2.09	1.33	1.37
24	B	615	CLA	C4B-CHC	2.09	1.46	1.41
25	d	403	PHO	C4D-CHA	2.09	1.49	1.43
24	B	605	CLA	C1A-CHA	2.08	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	403	PHO	C4C-C3C	2.08	1.49	1.45
24	b	608	CLA	C1B-NB	-2.08	1.33	1.35
24	c	909	CLA	C4B-CHC	2.08	1.46	1.41
31	a	415	PL9	C2-C3	2.07	1.40	1.34
24	c	914	CLA	C4C-C3C	2.06	1.48	1.45
24	c	903	CLA	C1C-NC	-2.06	1.34	1.37
24	c	902	CLA	C4B-CHC	2.06	1.46	1.41
24	b	616	CLA	C1B-NB	-2.05	1.33	1.35
37	C	517	DGD	O5D-C1E	2.04	1.43	1.40
25	D	401	PHO	C1B-NB	-2.04	1.34	1.38
24	B	617	CLA	C1C-C2C	2.04	1.48	1.44
24	c	911	CLA	C1C-C2C	2.04	1.48	1.44
24	c	906	CLA	CHD-C4C	2.04	1.46	1.41
25	a	407	PHO	C4C-C3C	2.04	1.49	1.45
24	A	406	CLA	C1B-CHB	2.04	1.46	1.41
24	B	603	CLA	C1B-NB	-2.03	1.33	1.35
35	B	632	HTG	C1-S1	-2.03	1.77	1.80
24	B	602	CLA	C4C-C3C	2.03	1.48	1.45
24	b	609	CLA	MG-NA	2.02	2.11	2.06
24	B	611	CLA	C1C-NC	-2.02	1.34	1.37
24	d	405	CLA	C1B-NB	-2.02	1.33	1.35
31	d	408	PL9	C2-C3	2.01	1.39	1.34
31	D	407	PL9	C2-C3	2.01	1.39	1.34
24	C	507	CLA	C4C-C3C	2.01	1.48	1.45
24	c	907	CLA	C4C-C3C	2.01	1.48	1.45
36	L	101	LHG	O7-C5	-2.00	1.41	1.46

All (2222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	405	CLA	C4A-NA-C1A	-7.75	103.22	106.71
25	d	403	PHO	CMD-C2D-C1D	7.30	136.30	125.06
24	b	608	CLA	C4A-NA-C1A	-7.14	103.50	106.71
24	B	606	CLA	CHD-C4C-C3C	-7.13	114.36	124.84
24	B	607	CLA	C4A-NA-C1A	-7.03	103.54	106.71
35	d	414	HTG	C1'-S1-C1	6.85	112.91	100.09
35	C	521	HTG	C1'-S1-C1	6.85	112.91	100.09
24	b	606	CLA	O2D-CGD-CBD	6.83	123.40	111.27
24	b	617	CLA	CHD-C4C-C3C	-6.80	114.84	124.84
24	b	618	CLA	C2C-C1C-NC	6.72	116.27	109.97
25	D	401	PHO	CMD-C2D-C1D	6.72	135.41	125.06
24	C	507	CLA	CHD-C4C-C3C	-6.69	115.00	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C4A-NA-C1A	-6.66	103.71	106.71
24	b	610	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
24	B	604	CLA	CHD-C4C-C3C	-6.52	115.26	124.84
24	b	620	CLA	CHD-C4C-C3C	-6.50	115.28	124.84
24	B	603	CLA	C4A-NA-C1A	-6.50	103.78	106.71
24	b	607	CLA	C4A-NA-C1A	-6.50	103.78	106.71
24	c	906	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
24	A	406	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
24	b	614	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	B	617	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
24	c	904	CLA	CHD-C4C-C3C	-6.36	115.48	124.84
38	F	102	HEM	CAD-CBD-CGD	6.35	123.32	112.67
24	C	504	CLA	O2D-CGD-CBD	6.35	122.54	111.27
24	B	602	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
24	c	908	CLA	CHD-C4C-C3C	-6.34	115.51	124.84
24	c	903	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
24	A	409	CLA	C4A-NA-C1A	-6.34	103.86	106.71
24	B	605	CLA	C2C-C1C-NC	6.32	115.90	109.97
24	b	613	CLA	C4A-NA-C1A	-6.31	103.87	106.71
24	C	503	CLA	CHD-C4C-C3C	-6.30	115.57	124.84
24	B	603	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
24	B	612	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
24	b	609	CLA	C4A-NA-C1A	-6.23	103.90	106.71
24	c	910	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
24	C	501	CLA	O2D-CGD-CBD	6.21	122.30	111.27
24	d	406	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
24	C	508	CLA	C4A-NA-C1A	-6.20	103.92	106.71
24	b	609	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	b	611	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
24	c	902	CLA	C2C-C1C-NC	6.19	115.77	109.97
24	C	505	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
24	B	617	CLA	O2D-CGD-CBD	6.18	122.26	111.27
24	b	616	CLA	C2C-C1C-NC	6.18	115.76	109.97
24	a	408	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
24	b	606	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
24	C	505	CLA	C4A-NA-C1A	-6.16	103.94	106.71
24	c	912	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
24	c	908	CLA	O2D-CGD-CBD	6.14	122.19	111.27
35	c	921	HTG	C1'-S1-C1	6.12	111.54	100.09
24	B	616	CLA	CHD-C4C-C3C	-6.12	115.85	124.84
24	a	406	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
24	c	913	CLA	O2D-CGD-CBD	6.09	122.09	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
24	b	614	CLA	C4A-NA-C1A	-6.05	103.98	106.71
24	c	911	CLA	C2C-C1C-NC	6.05	115.64	109.97
35	D	413	HTG	C1'-S1-C1	6.05	111.40	100.09
24	b	620	CLA	C4A-NA-C1A	-6.04	103.99	106.71
24	c	913	CLA	C4A-NA-C1A	-6.02	104.00	106.71
24	c	907	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
24	C	512	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
24	b	616	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
24	C	503	CLA	C4A-NA-C1A	-6.00	104.01	106.71
25	A	408	PHO	CMD-C2D-C1D	6.00	134.30	125.06
24	b	621	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	B	612	CLA	C4A-NA-C1A	-5.99	104.02	106.71
24	c	909	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
24	d	406	CLA	C4A-NA-C1A	-5.97	104.02	106.71
24	a	405	CLA	C2C-C1C-NC	5.96	115.55	109.97
24	c	913	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	C	504	CLA	C4A-NA-C1A	-5.94	104.03	106.71
24	C	510	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
24	b	619	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
24	c	909	CLA	C2C-C1C-NC	5.91	115.51	109.97
24	B	610	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	B	607	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
24	D	404	CLA	CHD-C4C-C3C	-5.89	116.17	124.84
24	B	602	CLA	O2D-CGD-CBD	5.89	121.74	111.27
24	D	404	CLA	C2C-C1C-NC	5.89	115.49	109.97
24	c	914	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
24	d	404	CLA	C2C-C1C-NC	5.85	115.45	109.97
24	D	404	CLA	C4A-NA-C1A	-5.85	104.08	106.71
24	b	609	CLA	O2D-CGD-CBD	5.84	121.65	111.27
24	C	509	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	C	513	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
24	C	506	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	b	609	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
24	B	614	CLA	C2C-C1C-NC	5.80	115.41	109.97
26	D	406	BCR	C7-C8-C9	-5.80	117.47	126.23
24	C	502	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
24	c	905	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
24	b	612	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
24	b	621	CLA	C4A-NA-C1A	-5.79	104.10	106.71
38	f	101	HEM	CAD-CBD-CGD	5.79	122.39	112.67
24	c	906	CLA	C2C-C1C-NC	5.79	115.39	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	O2D-CGD-CBD	5.78	121.55	111.27
24	B	610	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
24	b	611	CLA	C2C-C1C-NC	5.76	115.36	109.97
24	A	405	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	b	607	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
24	D	405	CLA	C4A-NA-C1A	-5.73	104.13	106.71
25	d	403	PHO	C3D-C2D-C1D	-5.72	97.53	105.87
24	b	619	CLA	O2D-CGD-CBD	5.72	121.42	111.27
24	b	606	CLA	C4A-NA-C1A	-5.71	104.14	106.71
24	b	621	CLA	O2D-CGD-CBD	5.71	121.42	111.27
24	B	605	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
24	d	405	CLA	C2C-C1C-NC	5.66	115.28	109.97
24	c	908	CLA	C2C-C1C-NC	5.66	115.27	109.97
24	c	907	CLA	C2C-C1C-NC	5.66	115.27	109.97
24	B	611	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
24	A	406	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	C	506	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	B	605	CLA	O2D-CGD-CBD	5.63	121.27	111.27
24	C	501	CLA	C4A-NA-C1A	-5.62	104.18	106.71
24	c	911	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	C	504	CLA	C2C-C1C-NC	5.60	115.22	109.97
35	B	624	HTG	C1'-S1-C1	5.60	110.56	100.09
24	C	507	CLA	O2D-CGD-CBD	5.60	121.21	111.27
24	C	505	CLA	C2C-C1C-NC	5.60	115.22	109.97
24	B	608	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
24	C	509	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	B	614	CLA	CHD-C4C-C3C	-5.59	116.63	124.84
24	B	606	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	B	611	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	b	618	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
24	b	610	CLA	O2D-CGD-CBD	5.56	121.14	111.27
27	f	102	SQD	O47-C7-C8	5.56	123.48	111.50
24	b	615	CLA	CHD-C4C-C3C	-5.55	116.67	124.84
24	d	404	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
24	C	510	CLA	O2D-CGD-CBD	5.54	121.11	111.27
24	c	909	CLA	O2D-CGD-CBD	5.53	121.10	111.27
24	b	612	CLA	C2C-C1C-NC	5.53	115.15	109.97
24	B	603	CLA	O2D-CGD-CBD	5.53	121.09	111.27
24	b	618	CLA	C4A-NA-C1A	-5.52	104.22	106.71
24	B	612	CLA	O2D-CGD-CBD	5.51	121.06	111.27
24	a	406	CLA	C4A-NA-C1A	-5.51	104.23	106.71
24	b	608	CLA	O2D-CGD-CBD	5.50	121.05	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	b	615	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	B	612	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	B	615	CLA	C2C-C1C-NC	5.48	115.11	109.97
24	B	615	CLA	O2D-CGD-CBD	5.47	120.99	111.27
24	c	914	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	b	608	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	B	614	CLA	C4A-NA-C1A	-5.45	104.25	106.71
24	C	501	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
35	B	633	HTG	C1'-S1-C1	5.45	110.28	100.09
24	C	511	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
24	c	902	CLA	O2D-CGD-CBD	5.44	120.94	111.27
24	B	609	CLA	C2C-C1C-NC	5.43	115.06	109.97
25	d	403	PHO	C1-C2-C3	-5.43	116.65	126.04
24	c	910	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	b	613	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
24	c	910	CLA	O2D-CGD-CBD	5.41	120.88	111.27
24	d	405	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
24	B	604	CLA	O2D-CGD-CBD	5.40	120.86	111.27
24	B	615	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
24	B	610	CLA	C2C-C1C-NC	5.40	115.03	109.97
25	a	407	PHO	CMD-C2D-C1D	5.39	133.36	125.06
24	B	608	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	a	406	CLA	O2D-CGD-CBD	5.38	120.83	111.27
24	B	609	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
24	b	611	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	A	407	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
24	c	906	CLA	C4A-NA-C1A	-5.36	104.30	106.71
25	D	401	PHO	C3D-C2D-C1D	-5.31	98.13	105.87
24	d	404	CLA	C4A-NA-C1A	-5.31	104.32	106.71
24	B	613	CLA	C2C-C1C-NC	5.30	114.94	109.97
24	A	407	CLA	O2D-CGD-CBD	5.29	120.68	111.27
24	C	504	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
25	a	407	PHO	C2D-C1D-ND	5.29	117.77	109.79
25	A	408	PHO	O2D-CGD-CBD	5.29	120.66	111.27
24	c	912	CLA	C4A-NA-C1A	-5.28	104.33	106.71
24	C	503	CLA	O2D-CGD-CBD	5.28	120.66	111.27
25	d	403	PHO	C2D-C1D-ND	5.28	117.76	109.79
24	C	508	CLA	C2C-C1C-NC	5.28	114.92	109.97
24	b	608	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
25	d	403	PHO	O2D-CGD-CBD	5.26	120.62	111.27
35	C	522	HTG	C1'-S1-C1	5.26	109.93	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	O2D-CGD-CBD	5.25	120.59	111.27
24	C	508	CLA	O2D-CGD-CBD	5.25	120.59	111.27
24	C	510	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	c	911	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	c	906	CLA	C3C-C4C-NC	5.24	116.45	110.57
27	L	102	SQD	O6-C1-C2	5.23	116.48	108.30
35	b	627	HTG	C1'-S1-C1	5.23	109.88	100.09
24	C	501	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	C	508	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
24	C	512	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	b	614	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	c	905	CLA	O2D-CGD-CBD	5.20	120.50	111.27
24	a	405	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
24	C	513	CLA	C2C-C1C-NC	5.19	114.83	109.97
24	B	617	CLA	C4A-NA-C1A	-5.18	104.38	106.71
27	a	410	SQD	O6-C1-C2	5.18	116.39	108.30
24	b	620	CLA	C2C-C1C-NC	5.18	114.82	109.97
26	Y	102	BCR	C33-C5-C6	-5.17	118.72	124.53
24	b	617	CLA	C3C-C4C-NC	5.17	116.37	110.57
24	b	613	CLA	C2C-C1C-NC	5.16	114.81	109.97
25	a	407	PHO	O2D-CGD-CBD	5.16	120.44	111.27
24	B	609	CLA	C4A-NA-C1A	-5.16	104.39	106.71
24	C	505	CLA	O2D-CGD-CBD	5.14	120.41	111.27
24	D	405	CLA	C2C-C1C-NC	5.14	114.78	109.97
24	c	904	CLA	C4A-NA-C1A	-5.13	104.40	106.71
29	A	415	LMT	C1'-O5'-C5'	5.13	123.75	113.69
24	C	509	CLA	C2C-C1C-NC	5.12	114.77	109.97
25	a	407	PHO	C3D-C2D-C1D	-5.12	98.41	105.87
24	A	409	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
24	c	905	CLA	C4A-NA-C1A	-5.12	104.41	106.71
24	B	603	CLA	C2C-C1C-NC	5.11	114.75	109.97
24	b	607	CLA	O2D-CGD-CBD	5.10	120.33	111.27
25	D	401	PHO	C2D-C1D-ND	5.10	117.49	109.79
24	B	608	CLA	O2D-CGD-CBD	5.09	120.32	111.27
24	d	405	CLA	O2D-CGD-CBD	5.09	120.32	111.27
24	b	611	CLA	O2D-CGD-CBD	5.09	120.31	111.27
24	D	405	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
24	a	405	CLA	C4A-NA-C1A	-5.08	104.42	106.71
25	D	401	PHO	C1-C2-C3	-5.07	117.27	126.04
27	F	103	SQD	O47-C7-C8	5.07	122.43	111.50
24	c	913	CLA	C2C-C1C-NC	5.06	114.71	109.97
24	B	604	CLA	C4A-NA-C1A	-5.06	104.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	C4A-NA-C1A	-5.05	104.44	106.71
24	C	512	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	C	511	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	b	612	CLA	C4A-NA-C1A	-5.03	104.44	106.71
35	B	625	HTG	C1'-S1-C1	5.03	109.49	100.09
24	A	405	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
24	C	507	CLA	C4A-NA-C1A	-5.01	104.45	106.71
24	b	615	CLA	C2C-C1C-NC	5.01	114.66	109.97
24	c	910	CLA	C4A-NA-C1A	-5.00	104.46	106.71
24	c	906	CLA	O2D-CGD-CBD	5.00	120.15	111.27
24	C	505	CLA	C3C-C4C-NC	5.00	116.18	110.57
24	B	607	CLA	C2C-C1C-NC	4.99	114.65	109.97
24	a	408	CLA	C4A-NA-C1A	-4.99	104.46	106.71
24	D	405	CLA	O2D-CGD-CBD	4.99	120.14	111.27
35	b	603	HTG	C1'-S1-C1	4.98	109.41	100.09
24	C	512	CLA	C4A-NA-C1A	-4.97	104.47	106.71
24	c	905	CLA	C2C-C1C-NC	4.96	114.62	109.97
24	C	503	CLA	C2C-C1C-NC	4.96	114.61	109.97
35	c	922	HTG	C1'-S1-C1	4.95	109.35	100.09
35	b	628	HTG	C1'-S1-C1	4.95	109.35	100.09
24	C	509	CLA	C1-C2-C3	-4.95	117.48	126.04
24	C	502	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	B	604	CLA	C2C-C1C-NC	4.95	114.61	109.97
24	A	406	CLA	O2D-CGD-CBD	4.94	120.05	111.27
27	A	411	SQD	O47-C7-C8	4.94	122.15	111.50
25	A	408	PHO	C2D-C1D-ND	4.93	117.23	109.79
25	A	408	PHO	C3D-C2D-C1D	-4.93	98.69	105.87
24	B	616	CLA	C2C-C1C-NC	4.91	114.57	109.97
24	b	619	CLA	C2C-C1C-NC	4.90	114.57	109.97
24	A	406	CLA	C4A-NA-C1A	-4.90	104.50	106.71
36	D	410	LHG	O7-C7-C8	4.89	122.04	111.50
35	B	632	HTG	C1'-S1-C1	4.88	109.21	100.09
38	F	102	HEM	CBA-CAA-C2A	-4.87	103.50	112.49
24	b	613	CLA	O2D-CGD-CBD	4.87	119.93	111.27
24	c	908	CLA	C3C-C4C-NC	4.86	116.02	110.57
24	C	510	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	C	506	CLA	O2D-CGD-CBD	4.85	119.89	111.27
24	b	617	CLA	C2C-C1C-NC	4.84	114.51	109.97
24	A	407	CLA	C4A-NA-C1A	-4.84	104.53	106.71
24	c	911	CLA	C1-C2-C3	-4.83	117.68	126.04
24	c	903	CLA	C2C-C1C-NC	4.81	114.48	109.97
24	C	513	CLA	C4A-NA-C1A	-4.81	104.55	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C2C-C1C-NC	4.80	114.47	109.97
24	B	613	CLA	C3C-C4C-NC	4.80	115.96	110.57
24	c	914	CLA	C2C-C1C-NC	4.80	114.47	109.97
38	f	101	HEM	CBD-CAD-C3D	-4.79	103.66	112.48
24	b	610	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	B	602	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	506	CLA	CHD-C4C-C3C	-4.78	117.81	124.84
24	C	509	CLA	O2D-CGD-CBD	4.77	119.75	111.27
27	L	102	SQD	O47-C7-C8	4.76	121.76	111.50
24	B	617	CLA	C2C-C1C-NC	4.75	114.42	109.97
24	b	614	CLA	C2C-C1C-NC	4.75	114.42	109.97
24	b	621	CLA	C2C-C1C-NC	4.74	114.42	109.97
24	c	902	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
24	B	606	CLA	C3C-C4C-NC	4.74	115.89	110.57
27	B	621	SQD	O47-C7-C8	4.74	121.71	111.50
24	b	606	CLA	C2C-C1C-NC	4.74	114.41	109.97
24	B	609	CLA	O2D-CGD-CBD	4.73	119.68	111.27
24	d	406	CLA	C2C-C1C-NC	4.73	114.40	109.97
24	d	404	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
24	a	408	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	A	407	CLA	C2C-C1C-NC	4.70	114.37	109.97
37	e	101	DGD	O2G-C1B-C2B	4.69	121.61	111.50
24	A	409	CLA	C2C-C1C-NC	4.68	114.36	109.97
24	C	502	CLA	C4A-NA-C1A	-4.68	104.60	106.71
27	B	621	SQD	O7-S-C6	4.68	112.50	106.94
27	a	410	SQD	O47-C7-C8	4.67	121.57	111.50
24	c	902	CLA	C4A-NA-C1A	-4.67	104.61	106.71
24	C	503	CLA	C1D-CHD-C4C	-4.67	116.40	122.56
24	b	616	CLA	C3C-C4C-NC	4.66	115.80	110.57
37	C	516	DGD	O2G-C1B-C2B	4.66	121.53	111.50
25	d	403	PHO	C4C-C3C-C2C	-4.65	101.64	106.78
24	b	607	CLA	C2C-C1C-NC	4.65	114.33	109.97
24	b	618	CLA	C3C-C4C-NC	4.64	115.78	110.57
24	C	507	CLA	C3C-C4C-NC	4.64	115.77	110.57
24	b	609	CLA	C3C-C4C-NC	4.63	115.77	110.57
24	B	611	CLA	C4A-NA-C1A	-4.62	104.63	106.71
24	a	408	CLA	O2D-CGD-CBD	4.61	119.47	111.27
26	t	102	BCR	C33-C5-C6	-4.61	119.35	124.53
27	B	621	SQD	O6-C1-C2	4.60	115.49	108.30
24	B	606	CLA	O2D-CGD-CBD	4.60	119.44	111.27
24	b	612	CLA	O2D-CGD-CBD	4.60	119.43	111.27
24	d	406	CLA	O2D-CGD-CBD	4.59	119.42	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	415	LMT	O5'-C5'-C4'	4.59	119.42	109.75
27	A	411	SQD	O6-C1-C2	4.58	115.46	108.30
24	C	511	CLA	CAC-C3C-C4C	4.57	130.74	124.81
33	a	411	LMG	O7-C10-C11	4.57	121.34	111.50
37	e	101	DGD	O6E-C5E-C4E	4.57	117.99	109.69
24	c	904	CLA	C2C-C1C-NC	4.56	114.25	109.97
26	B	618	BCR	C33-C5-C6	-4.56	119.40	124.53
24	b	621	CLA	CAC-C3C-C4C	4.56	130.72	124.81
24	B	605	CLA	C3C-C4C-NC	4.56	115.68	110.57
24	c	904	CLA	C3C-C4C-NC	4.56	115.68	110.57
24	B	612	CLA	C3C-C4C-NC	4.55	115.67	110.57
24	C	510	CLA	C1-C2-C3	-4.55	118.18	126.04
24	b	616	CLA	O2D-CGD-CBD	4.52	119.30	111.27
24	c	910	CLA	C1D-CHD-C4C	-4.52	116.59	122.56
24	C	507	CLA	C2C-C1C-NC	4.52	114.20	109.97
24	c	903	CLA	C4A-NA-C1A	-4.50	104.68	106.71
24	b	610	CLA	C3C-C4C-NC	4.49	115.61	110.57
37	c	918	DGD	O2G-C1B-C2B	4.49	121.17	111.50
33	c	920	LMG	O7-C10-C11	4.49	121.17	111.50
26	b	622	BCR	C15-C14-C13	-4.48	120.92	127.31
24	C	513	CLA	O2D-CGD-CBD	4.46	119.20	111.27
24	C	511	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	b	617	CLA	O2D-CGD-CBD	4.46	119.19	111.27
35	C	522	HTG	C1-O5-C5	4.45	120.79	112.58
24	a	405	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
24	a	406	CLA	C2C-C1C-NC	4.44	114.14	109.97
33	C	519	LMG	O7-C10-C11	4.44	121.06	111.50
24	B	606	CLA	C1D-CHD-C4C	-4.43	116.71	122.56
24	b	612	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	c	912	CLA	C2C-C1C-NC	4.43	114.12	109.97
24	b	621	CLA	C3C-C4C-NC	4.41	115.52	110.57
24	c	911	CLA	C4A-NA-C1A	-4.41	104.72	106.71
24	c	909	CLA	C4A-NA-C1A	-4.40	104.73	106.71
26	K	101	BCR	C7-C8-C9	-4.40	119.59	126.23
24	d	404	CLA	O2D-CGD-CBD	4.40	119.08	111.27
24	b	609	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
24	b	620	CLA	C1D-CHD-C4C	-4.38	116.78	122.56
35	b	628	HTG	O5-C1-C2	4.38	115.82	110.31
24	b	606	CLA	O2D-CGD-O1D	-4.36	115.32	123.84
27	A	411	SQD	C45-O47-C7	-4.36	107.06	117.79
24	c	903	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	A	409	CLA	O2D-CGD-CBD	4.35	119.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	C1-C2-C3	-4.35	118.51	126.04
24	b	611	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	B	603	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	C	502	CLA	O2D-CGD-CBD	4.33	118.97	111.27
25	D	401	PHO	O2D-CGD-CBD	4.33	118.97	111.27
26	b	622	BCR	C33-C5-C6	-4.33	119.67	124.53
37	D	408	DGD	O2G-C1B-C2B	4.33	120.83	111.50
35	B	625	HTG	O5-C1-C2	4.33	115.76	110.31
24	C	509	CLA	C3C-C4C-NC	4.33	115.42	110.57
24	c	909	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
24	A	406	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
33	c	920	LMG	C3-C4-C5	4.31	117.93	110.24
24	B	602	CLA	C3C-C4C-NC	4.31	115.40	110.57
24	b	611	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
24	b	610	CLA	O2D-CGD-O1D	-4.30	115.42	123.84
24	c	906	CLA	C1D-CHD-C4C	-4.30	116.88	122.56
24	B	607	CLA	C3C-C4C-NC	4.30	115.39	110.57
24	c	910	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	C	503	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	b	614	CLA	C3C-C4C-NC	4.29	115.38	110.57
24	B	611	CLA	O2D-CGD-CBD	4.28	118.88	111.27
24	b	615	CLA	O2D-CGD-CBD	4.28	118.88	111.27
24	c	904	CLA	C1-C2-C3	-4.28	118.64	126.04
24	b	620	CLA	C3C-C4C-NC	4.27	115.36	110.57
33	A	419	LMG	O7-C10-C11	4.26	120.69	111.50
24	b	616	CLA	C4A-NA-C1A	-4.26	104.79	106.71
24	B	617	CLA	C3C-C4C-NC	4.26	115.34	110.57
37	e	101	DGD	C3E-C4E-C5E	4.25	117.83	110.24
24	B	605	CLA	C3B-C4B-NB	4.25	114.70	109.21
24	B	603	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
24	c	907	CLA	C4A-NA-C1A	-4.23	104.80	106.71
26	H	101	BCR	C38-C26-C25	-4.23	119.78	124.53
24	b	618	CLA	C3B-C4B-NB	4.23	114.68	109.21
24	b	613	CLA	C3C-C4C-NC	4.22	115.31	110.57
24	B	617	CLA	C1D-CHD-C4C	-4.22	116.99	122.56
26	y	101	BCR	C33-C5-C6	-4.22	119.79	124.53
24	B	604	CLA	C3C-C4C-NC	4.22	115.30	110.57
24	B	608	CLA	C3C-C4C-NC	4.21	115.30	110.57
24	c	903	CLA	O2D-CGD-CBD	4.21	118.75	111.27
24	C	502	CLA	C1-C2-C3	-4.21	118.77	126.04
24	c	911	CLA	C4-C3-C5	4.19	122.32	115.27
26	b	622	BCR	C7-C8-C9	-4.19	119.91	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	407	PL9	C7-C8-C9	-4.19	119.82	126.79
24	C	512	CLA	C3C-C4C-NC	4.19	115.27	110.57
24	B	606	CLA	CMC-C2C-C1C	4.18	131.40	125.04
24	B	614	CLA	C3C-C4C-NC	4.17	115.25	110.57
31	a	415	PL9	C7-C3-C4	4.16	120.26	116.88
26	T	102	BCR	C11-C10-C9	-4.16	121.38	127.31
24	b	612	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
36	b	635	LHG	O7-C7-C8	4.15	120.44	111.50
24	D	404	CLA	C3C-C4C-NC	4.14	115.21	110.57
26	C	515	BCR	C7-C8-C9	-4.14	119.98	126.23
24	A	405	CLA	C3B-C4B-NB	4.12	114.54	109.21
24	d	405	CLA	C1C-C2C-C3C	-4.10	102.64	106.96
24	c	909	CLA	C3C-C4C-NC	4.10	115.17	110.57
24	C	513	CLA	C1D-CHD-C4C	-4.10	117.15	122.56
24	C	511	CLA	C4A-NA-C1A	-4.09	104.86	106.71
24	d	404	CLA	C3B-C4B-NB	4.09	114.50	109.21
24	d	405	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	d	406	CLA	C3C-C4C-NC	4.09	115.16	110.57
24	B	616	CLA	C3C-C4C-NC	4.08	115.15	110.57
24	c	907	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
24	A	409	CLA	CAC-C3C-C4C	4.07	130.09	124.81
24	B	605	CLA	C1C-C2C-C3C	-4.07	102.68	106.96
24	b	606	CLA	C1D-CHD-C4C	-4.06	117.19	122.56
24	C	504	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	B	614	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	c	902	CLA	CAC-C3C-C4C	4.05	130.07	124.81
24	B	610	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	C	510	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	C	506	CLA	CAC-C3C-C4C	4.05	130.06	124.81
24	a	408	CLA	C1-C2-C3	-4.05	119.05	126.04
24	c	909	CLA	C3B-C4B-NB	4.04	114.44	109.21
24	C	501	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	D	404	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	617	CLA	C4A-NA-C1A	-4.04	104.89	106.71
24	c	911	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	616	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	c	902	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	A	406	CLA	C1D-CHD-C4C	-4.03	117.24	122.56
29	D	403	LMT	O1B-C4'-C3'	4.03	118.00	107.28
24	b	619	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	b	607	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
24	C	511	CLA	C1D-CHD-C4C	-4.02	117.25	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C3C-C4C-NC	4.02	115.08	110.57
24	B	616	CLA	C1D-CHD-C4C	-4.02	117.26	122.56
25	A	408	PHO	C4C-C3C-C2C	-4.02	102.34	106.78
26	c	927	BCR	C15-C14-C13	-4.01	121.58	127.31
29	a	401	LMT	O5'-C5'-C4'	4.01	118.21	109.75
24	b	608	CLA	C1D-CHD-C4C	-4.01	117.26	122.56
24	c	903	CLA	C1D-CHD-C4C	-4.01	117.27	122.56
24	D	404	CLA	O2D-CGD-CBD	4.00	118.38	111.27
36	E	101	LHG	O7-C7-C8	4.00	120.12	111.50
24	c	902	CLA	O2D-CGD-O1D	-4.00	116.03	123.84
24	b	608	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
24	c	904	CLA	C1D-CHD-C4C	-3.99	117.29	122.56
24	A	405	CLA	C4A-NA-C1A	-3.99	104.91	106.71
24	c	913	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
24	B	602	CLA	C4A-NA-C1A	-3.97	104.92	106.71
24	b	616	CLA	C3B-C4B-NB	3.97	114.35	109.21
24	c	914	CLA	O2D-CGD-CBD	3.97	118.31	111.27
24	b	610	CLA	C1D-CHD-C4C	-3.96	117.33	122.56
24	A	405	CLA	C1D-CHD-C4C	-3.96	117.33	122.56
24	B	604	CLA	C1D-CHD-C4C	-3.96	117.33	122.56
24	C	513	CLA	C3C-C4C-NC	3.95	115.00	110.57
24	d	405	CLA	C1-C2-C3	-3.95	119.21	126.04
27	A	414	SQD	O48-C23-C24	3.95	124.31	111.91
24	B	615	CLA	C3C-C4C-NC	3.95	115.00	110.57
33	c	920	LMG	O6-C5-C4	3.95	116.86	109.69
24	b	615	CLA	C3C-C4C-NC	3.94	114.99	110.57
26	T	102	BCR	C15-C16-C17	-3.94	115.41	123.47
24	b	607	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	c	905	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	a	405	CLA	CAA-C2A-C3A	-3.93	102.00	112.78
24	B	604	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
24	c	909	CLA	C1-C2-C3	-3.93	119.24	126.04
24	C	501	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
24	c	911	CLA	C3B-C4B-NB	3.93	114.29	109.21
24	C	504	CLA	C3C-C4C-NC	3.92	114.97	110.57
29	b	602	LMT	C1'-O5'-C5'	3.92	121.39	113.69
24	b	621	CLA	C1D-CHD-C4C	-3.92	117.39	122.56
24	c	907	CLA	C3C-C4C-NC	3.92	114.97	110.57
24	d	405	CLA	O2D-CGD-O1D	-3.92	116.18	123.84
24	c	911	CLA	C1D-CHD-C4C	-3.92	117.39	122.56
24	a	408	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	A	405	CLA	C1C-C2C-C3C	-3.90	102.86	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	C1D-CHD-C4C	-3.90	117.41	122.56
26	a	409	BCR	C33-C5-C6	-3.90	120.15	124.53
24	c	907	CLA	O2D-CGD-CBD	3.89	118.18	111.27
26	t	102	BCR	C15-C14-C13	3.89	132.86	127.31
29	a	401	LMT	C1'-O5'-C5'	3.89	121.32	113.69
24	B	609	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
31	D	407	PL9	C37-C38-C39	-3.88	118.31	127.66
35	B	623	HTG	C1'-S1-C1	3.88	107.35	100.09
35	b	601	HTG	C1'-S1-C1	3.88	107.34	100.09
33	Z	101	LMG	O7-C10-C11	3.87	119.85	111.50
24	b	618	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	c	908	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
36	d	411	LHG	O7-C7-C8	3.87	119.84	111.50
24	b	611	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
24	C	502	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
24	a	408	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
24	b	617	CLA	C1-C2-C3	-3.87	119.35	126.04
24	A	405	CLA	CAC-C3C-C4C	3.87	129.82	124.81
24	c	902	CLA	C3B-C4B-NB	3.86	114.20	109.21
24	B	611	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
25	D	401	PHO	C4C-C3C-C2C	-3.85	102.52	106.78
24	a	406	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
24	B	607	CLA	C1D-CHD-C4C	-3.85	117.48	122.56
27	a	410	SQD	C1-C2-C3	-3.85	101.98	110.00
35	V	203	HTG	C1'-S1-C1	3.84	107.27	100.09
24	B	613	CLA	C4-C3-C5	3.84	121.73	115.27
26	t	102	BCR	C15-C16-C17	-3.84	115.62	123.47
24	A	406	CLA	C3C-C4C-NC	3.83	114.87	110.57
24	c	914	CLA	C1D-CHD-C4C	-3.83	117.51	122.56
24	B	603	CLA	C1D-CHD-C4C	-3.82	117.51	122.56
27	a	410	SQD	O8-S-C6	3.82	111.83	105.74
35	b	604	HTG	C1'-S1-C1	3.82	107.23	100.09
26	y	101	BCR	C15-C14-C13	-3.81	121.87	127.31
24	B	615	CLA	C4A-NA-C1A	-3.81	104.99	106.71
37	C	517	DGD	O2G-C1B-C2B	3.81	119.71	111.50
31	D	407	PL9	C42-C43-C44	-3.80	118.50	127.66
24	C	506	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	B	615	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	B	613	CLA	C4A-NA-C1A	-3.80	105.00	106.71
24	C	511	CLA	C1-C2-C3	-3.80	119.48	126.04
24	c	912	CLA	C3C-C4C-NC	3.79	114.82	110.57
24	c	914	CLA	C1C-C2C-C3C	-3.79	102.97	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C7-C8-C9	-3.78	120.53	126.23
24	b	618	CLA	C1D-CHD-C4C	-3.78	117.58	122.56
26	d	407	BCR	C24-C23-C22	-3.78	120.53	126.23
24	C	511	CLA	C3C-C4C-NC	3.77	114.80	110.57
37	H	102	DGD	O2G-C1B-C2B	3.77	119.62	111.50
24	b	609	CLA	CMC-C2C-C1C	3.77	130.78	125.04
26	H	101	BCR	C24-C23-C22	-3.77	120.55	126.23
37	c	917	DGD	O2G-C1B-C2B	3.77	119.62	111.50
31	a	415	PL9	C15-C14-C16	3.77	121.61	115.27
24	c	905	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	B	612	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	b	615	CLA	C1-C2-C3	-3.76	119.53	126.04
25	a	407	PHO	C4C-C3C-C2C	-3.76	102.62	106.78
24	b	609	CLA	C3B-C4B-NB	3.76	114.07	109.21
24	c	907	CLA	C3B-C4B-NB	3.74	114.04	109.21
24	C	505	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
24	C	511	CLA	C3B-C4B-NB	3.73	114.04	109.21
24	c	913	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
24	D	405	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	911	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	907	CLA	C1D-CHD-C4C	-3.73	117.64	122.56
29	C	520	LMT	O1B-C4'-C3'	3.73	117.20	107.28
25	D	401	PHO	CAC-C3C-C4C	3.73	129.29	125.22
24	c	908	CLA	CMC-C2C-C1C	3.73	130.71	125.04
26	D	406	BCR	C33-C5-C6	-3.73	120.34	124.53
24	C	508	CLA	C3C-C4C-NC	3.72	114.75	110.57
24	B	614	CLA	C3B-C4B-NB	3.72	114.02	109.21
37	D	408	DGD	C1D-C2D-C3D	3.72	117.74	110.00
33	c	919	LMG	O7-C10-C11	3.71	119.50	111.50
24	C	504	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
24	A	405	CLA	O2D-CGD-CBD	3.71	117.86	111.27
24	C	513	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
27	L	102	SQD	C3-C4-C5	3.71	116.85	110.24
24	c	910	CLA	C1-O2A-CGA	3.71	126.17	116.44
24	c	913	CLA	C1-C2-C3	-3.70	119.64	126.04
24	A	406	CLA	C3B-C4B-NB	3.70	113.99	109.21
24	A	406	CLA	CBC-CAC-C3C	-3.70	102.23	112.43
24	b	619	CLA	C1-C2-C3	-3.70	119.65	126.04
26	d	407	BCR	C38-C26-C25	-3.70	120.38	124.53
24	c	913	CLA	C3C-C4C-NC	3.70	114.72	110.57
24	b	619	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	b	617	CLA	C1D-CHD-C4C	-3.69	117.68	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	903	CLA	C1-C2-C3	-3.69	119.66	126.04
31	A	417	PL9	C20-C19-C21	3.69	121.48	115.27
24	C	501	CLA	C3C-C4C-NC	3.69	114.71	110.57
31	A	417	PL9	C37-C38-C39	-3.69	118.78	127.66
24	a	406	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	D	404	CLA	C1-C2-C3	-3.68	119.67	126.04
24	c	910	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	b	618	CLA	O2D-CGD-CBD	3.68	117.80	111.27
24	C	510	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	b	608	CLA	C3C-C4C-NC	3.68	114.69	110.57
24	C	502	CLA	CAC-C3C-C4C	3.67	129.58	124.81
36	B	635	LHG	O8-C23-C24	3.67	123.43	111.91
27	a	402	SQD	O47-C7-C8	3.67	119.41	111.50
24	B	615	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
24	B	616	CLA	CAC-C3C-C4C	3.66	129.56	124.81
24	C	504	CLA	C3B-C4B-NB	3.66	113.95	109.21
24	C	509	CLA	C1D-CHD-C4C	-3.66	117.72	122.56
24	B	616	CLA	O2D-CGD-CBD	3.66	117.77	111.27
24	C	512	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
24	B	611	CLA	CAA-C2A-C3A	-3.66	102.76	112.78
24	c	905	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
36	B	635	LHG	O7-C7-C8	3.65	119.37	111.50
24	B	612	CLA	C1-C2-C3	-3.65	119.73	126.04
26	T	102	BCR	C16-C17-C18	-3.65	122.10	127.31
24	B	610	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
24	b	613	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
24	A	407	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
24	c	902	CLA	C3C-C4C-NC	3.63	114.65	110.57
24	b	621	CLA	C4C-C3C-C2C	-3.63	101.60	106.90
24	c	914	CLA	C3C-C4C-NC	3.63	114.65	110.57
37	c	916	DGD	O2G-C1B-C2B	3.63	119.32	111.50
24	b	618	CLA	C1-C2-C3	-3.63	119.77	126.04
24	b	606	CLA	C3C-C4C-NC	3.63	114.64	110.57
24	B	610	CLA	O2D-CGD-CBD	3.62	117.71	111.27
24	d	404	CLA	CAA-C2A-C3A	-3.62	102.86	112.78
24	b	606	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
24	B	609	CLA	C3C-C4C-NC	3.62	114.63	110.57
26	h	101	BCR	C38-C26-C25	-3.62	120.46	124.53
26	T	102	BCR	C12-C13-C14	-3.62	113.39	118.94
24	B	608	CLA	C4A-NA-C1A	-3.61	105.08	106.71
24	c	907	CLA	C1-C2-C3	-3.61	119.80	126.04
24	D	405	CLA	CAC-C3C-C4C	3.61	129.50	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	615	CLA	CAC-C3C-C4C	3.61	129.49	124.81
24	c	904	CLA	O2D-CGD-CBD	3.61	117.68	111.27
33	b	625	LMG	O7-C10-C11	3.61	119.28	111.50
24	B	614	CLA	C1-C2-C3	-3.61	119.81	126.04
24	b	617	CLA	C4C-C3C-C2C	-3.60	101.65	106.90
24	C	504	CLA	C1D-CHD-C4C	-3.60	117.81	122.56
24	b	619	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
24	d	404	CLA	C1D-CHD-C4C	-3.59	117.82	122.56
24	b	621	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	b	608	CLA	CAA-C2A-C3A	-3.59	102.95	112.78
31	d	408	PL9	C10-C9-C11	3.59	121.31	115.27
38	F	102	HEM	CBD-CAD-C3D	-3.59	105.87	112.48
24	d	406	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
29	C	520	LMT	C1'-O5'-C5'	3.59	120.73	113.69
24	b	613	CLA	CAC-C3C-C4C	3.58	129.46	124.81
24	B	611	CLA	C3C-C4C-NC	3.57	114.58	110.57
24	a	406	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
24	c	909	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
35	B	624	HTG	C1-O5-C5	3.57	119.16	112.58
25	d	403	PHO	C4-C3-C5	3.57	121.27	115.27
24	c	906	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
26	T	102	BCR	C33-C5-C6	-3.56	120.53	124.53
24	b	620	CLA	O2D-CGD-CBD	3.56	117.60	111.27
24	c	910	CLA	C1-C2-C3	-3.56	119.88	126.04
24	D	405	CLA	C3B-C4B-NB	3.56	113.81	109.21
24	B	608	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
24	a	405	CLA	C3C-C4C-NC	3.56	114.56	110.57
24	C	505	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
24	d	406	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
24	A	405	CLA	O2A-CGA-CBA	3.56	123.07	111.91
24	A	409	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
26	B	618	BCR	C7-C8-C9	-3.56	120.86	126.23
24	a	405	CLA	C4-C3-C5	3.55	121.25	115.27
31	D	407	PL9	C10-C9-C11	3.55	121.25	115.27
33	C	519	LMG	C3-C4-C5	3.55	116.58	110.24
24	A	409	CLA	C3C-C4C-NC	3.55	114.55	110.57
33	Y	101	LMG	O7-C10-C11	3.55	119.15	111.50
33	z	101	LMG	O7-C10-C11	3.55	119.14	111.50
26	C	514	BCR	C33-C5-C6	-3.54	120.55	124.53
24	c	912	CLA	C1D-CHD-C4C	-3.54	117.88	122.56
24	A	407	CLA	C1C-C2C-C3C	-3.54	103.24	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	B	612	CLA	C3B-C4B-NB	3.53	113.78	109.21
24	C	508	CLA	C3B-C4B-NB	3.53	113.78	109.21
24	B	607	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
26	D	406	BCR	C29-C30-C25	3.53	115.91	110.48
31	a	415	PL9	C32-C33-C34	-3.53	119.17	127.66
24	B	613	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
36	d	410	LHG	O7-C7-C8	3.52	119.09	111.50
24	B	606	CLA	CHD-C4C-NC	3.52	129.75	124.20
33	B	622	LMG	O8-C28-C29	3.52	122.94	111.91
24	C	506	CLA	C3B-C4B-NB	3.51	113.75	109.21
24	C	505	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
26	C	514	BCR	C20-C21-C22	-3.51	122.30	127.31
33	J	101	LMG	O7-C10-C11	3.51	119.07	111.50
24	b	618	CLA	CHC-C1C-C2C	-3.51	117.01	126.72
24	b	608	CLA	C3B-C4B-NB	3.51	113.75	109.21
24	a	408	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	c	908	CLA	C4A-NA-C1A	-3.51	105.13	106.71
24	D	404	CLA	C3B-C4B-NB	3.50	113.74	109.21
24	B	613	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
31	d	408	PL9	C20-C19-C21	3.50	121.16	115.27
24	C	512	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	A	405	CLA	C3C-C4C-NC	3.50	114.50	110.57
24	B	617	CLA	C3B-C4B-NB	3.50	113.73	109.21
24	b	610	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	a	408	CLA	CHD-C4C-NC	3.50	129.71	124.20
24	a	405	CLA	C1D-CHD-C4C	-3.50	117.94	122.56
24	A	406	CLA	CHD-C4C-NC	3.49	129.71	124.20
24	b	608	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
26	d	407	BCR	C28-C27-C26	-3.48	107.86	114.08
24	B	602	CLA	C3B-C4B-NB	3.48	113.71	109.21
27	A	411	SQD	O8-S-C6	3.48	111.29	105.74
33	a	411	LMG	C8-O7-C10	-3.48	109.22	117.79
24	C	504	CLA	CMC-C2C-C1C	3.48	130.34	125.04
26	C	514	BCR	C15-C14-C13	-3.48	122.35	127.31
24	a	405	CLA	O2A-CGA-O1A	-3.47	114.82	123.59
24	B	610	CLA	C4D-C3D-CAD	-3.47	106.53	108.47
26	B	619	BCR	C28-C27-C26	-3.47	107.88	114.08
26	t	102	BCR	C11-C10-C9	-3.47	122.36	127.31
24	C	508	CLA	CAC-C3C-C4C	3.47	129.31	124.81
26	k	101	BCR	C20-C21-C22	-3.47	122.36	127.31
24	c	906	CLA	C1C-C2C-C3C	-3.47	103.31	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	CMC-C2C-C1C	3.47	130.32	125.04
24	A	406	CLA	CMB-C2B-C3B	3.47	131.16	124.68
24	C	510	CLA	C4-C3-C5	3.46	121.10	115.27
24	c	910	CLA	C3B-C4B-NB	3.46	113.68	109.21
24	B	602	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
24	C	510	CLA	C1D-CHD-C4C	-3.46	118.00	122.56
24	c	903	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
26	A	410	BCR	C33-C5-C6	-3.46	120.65	124.53
24	A	406	CLA	CAA-C2A-C3A	-3.45	103.33	112.78
24	B	608	CLA	C4-C3-C5	3.45	121.07	115.27
24	B	611	CLA	C3B-C4B-NB	3.45	113.67	109.21
31	a	415	PL9	C42-C43-C44	-3.45	119.36	127.66
27	F	103	SQD	O7-S-C6	3.45	111.03	106.94
31	a	415	PL9	C20-C19-C21	3.45	121.07	115.27
37	h	102	DGD	O2G-C1B-C2B	3.44	118.92	111.50
24	D	405	CLA	C4-C3-C5	3.44	121.06	115.27
24	B	615	CLA	C4-C3-C5	3.44	121.05	115.27
24	c	903	CLA	C4D-C3D-CAD	-3.44	106.55	108.47
31	A	417	PL9	C8-C7-C3	3.43	121.68	111.98
27	f	102	SQD	C1-O5-C5	3.43	120.42	113.69
24	C	501	CLA	CBC-CAC-C3C	-3.43	102.97	112.43
24	D	405	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
24	d	404	CLA	CBC-CAC-C3C	-3.43	102.98	112.43
24	A	405	CLA	CAA-C2A-C3A	-3.43	103.40	112.78
31	d	408	PL9	C42-C43-C44	-3.42	119.41	127.66
24	d	405	CLA	O2A-CGA-CBA	3.42	122.65	111.91
24	B	610	CLA	C3B-C4B-NB	3.42	113.63	109.21
24	C	507	CLA	C1D-CHD-C4C	-3.42	118.04	122.56
24	B	605	CLA	C1-C2-C3	-3.42	120.13	126.04
24	C	501	CLA	C1-C2-C3	-3.42	120.13	126.04
31	D	407	PL9	C40-C39-C41	3.42	121.02	115.27
24	c	908	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
24	c	912	CLA	O2D-CGD-CBD	3.41	117.34	111.27
24	b	606	CLA	CHD-C4C-NC	3.41	129.58	124.20
24	B	608	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	b	614	CLA	C1D-CHD-C4C	-3.41	118.06	122.56
24	C	506	CLA	C3C-C4C-NC	3.41	114.39	110.57
31	a	415	PL9	C22-C23-C24	-3.40	119.46	127.66
24	B	604	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
27	a	402	SQD	O48-C23-C24	3.40	122.59	111.91
24	A	407	CLA	C3C-C4C-NC	3.40	114.39	110.57
24	b	615	CLA	C1D-CHD-C4C	-3.40	118.07	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	415	PL9	C7-C8-C9	-3.40	121.14	126.79
26	c	927	BCR	C16-C17-C18	-3.40	122.46	127.31
24	c	902	CLA	CHC-C1C-C2C	-3.39	117.34	126.72
24	C	504	CLA	CBC-CAC-C3C	-3.38	103.11	112.43
24	b	612	CLA	CBC-CAC-C3C	-3.38	103.12	112.43
36	L	101	LHG	O7-C7-C8	3.38	118.78	111.50
24	d	404	CLA	C4D-C3D-CAD	-3.37	106.59	108.47
24	C	507	CLA	CMC-C2C-C1C	3.37	130.17	125.04
24	B	615	CLA	CAC-C3C-C4C	3.36	129.18	124.81
27	F	103	SQD	C1-O5-C5	3.36	120.29	113.69
24	c	904	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
24	B	613	CLA	C1-C2-C3	-3.35	120.24	126.04
24	C	503	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
26	B	619	BCR	C33-C5-C6	-3.34	120.77	124.53
24	b	617	CLA	C4-C3-C5	3.34	120.90	115.27
24	b	613	CLA	C1D-CHD-C4C	-3.34	118.14	122.56
24	a	405	CLA	C3B-C4B-NB	3.34	113.53	109.21
24	b	618	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	C	507	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
24	B	607	CLA	C1-C2-C3	-3.34	120.27	126.04
24	b	614	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
24	a	405	CLA	O2A-CGA-CBA	3.34	122.38	111.91
27	F	103	SQD	O5-C5-C4	3.34	115.75	109.69
26	D	406	BCR	C28-C27-C26	-3.34	108.12	114.08
24	b	611	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	C	505	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	b	616	CLA	C1D-CHD-C4C	-3.33	118.17	122.56
24	B	617	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
24	B	611	CLA	O2A-CGA-CBA	3.32	122.34	111.91
24	B	604	CLA	CHD-C4C-NC	3.32	129.44	124.20
24	C	509	CLA	C3B-C4B-NB	3.32	113.51	109.21
24	b	612	CLA	C3B-C4B-NB	3.32	113.51	109.21
24	a	406	CLA	C1D-CHD-C4C	-3.32	118.17	122.56
24	B	609	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	B	611	CLA	CHC-C1C-C2C	-3.32	117.55	126.72
24	B	607	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
31	d	408	PL9	C40-C39-C41	3.31	120.85	115.27
24	D	405	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
24	C	510	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	B	613	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	c	908	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
36	d	409	LHG	O7-C7-C8	3.31	118.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	CLA	CHD-C4C-NC	3.30	129.41	124.20
24	C	508	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
24	b	617	CLA	O2A-CGA-CBA	3.30	122.26	111.91
26	C	515	BCR	C24-C23-C22	-3.30	121.25	126.23
24	c	910	CLA	CMB-C2B-C3B	3.30	130.85	124.68
24	a	406	CLA	CMC-C2C-C1C	3.30	130.06	125.04
25	a	407	PHO	CMB-C2B-C1B	3.29	130.14	125.06
24	B	615	CLA	CHC-C1C-C2C	-3.29	117.61	126.72
26	c	915	BCR	C15-C14-C13	-3.29	122.61	127.31
31	a	415	PL9	C27-C28-C29	-3.29	119.74	127.66
24	B	612	CLA	C1D-CHD-C4C	-3.29	118.22	122.56
24	b	616	CLA	CHC-C1C-C2C	-3.29	117.63	126.72
26	D	406	BCR	C38-C26-C25	-3.29	120.84	124.53
24	a	408	CLA	C4-C3-C5	3.28	120.79	115.27
24	c	912	CLA	CHD-C4C-NC	3.28	129.38	124.20
24	B	617	CLA	CBC-CAC-C3C	-3.28	103.38	112.43
31	d	408	PL9	C27-C28-C29	-3.28	119.76	127.66
24	B	609	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
24	C	507	CLA	C1-C2-C3	-3.28	120.37	126.04
24	A	409	CLA	C4-C3-C5	3.27	120.78	115.27
24	d	404	CLA	C3C-C4C-NC	3.27	114.24	110.57
24	a	405	CLA	O2D-CGD-CBD	3.27	117.08	111.27
24	b	620	CLA	CHD-C4C-NC	3.27	129.36	124.20
24	B	606	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	b	621	CLA	O2A-CGA-CBA	3.27	122.17	111.91
24	b	617	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	A	407	CLA	C4-C3-C5	3.27	120.76	115.27
27	A	414	SQD	O47-C7-C8	3.26	118.53	111.50
24	B	610	CLA	C1-C2-C3	-3.26	120.40	126.04
24	b	613	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	b	610	CLA	C2A-C1A-CHA	-3.26	118.17	123.86
33	d	415	LMG	O7-C10-C11	3.25	118.52	111.50
31	A	417	PL9	C32-C33-C34	-3.25	119.83	127.66
24	C	509	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
24	c	912	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
24	b	612	CLA	CAA-C2A-C3A	-3.25	103.89	112.78
31	D	407	PL9	C53-C6-C1	3.24	121.62	114.99
24	B	611	CLA	C1D-CHD-C4C	-3.24	118.28	122.56
24	b	620	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
24	B	605	CLA	C4A-NA-C1A	-3.24	105.25	106.71
24	b	619	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	A	405	CLA	O2A-CGA-O1A	-3.24	115.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
27	a	402	SQD	O8-S-C6	3.24	110.90	105.74
24	c	911	CLA	CHC-C1C-C2C	-3.24	117.77	126.72
24	c	905	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	c	912	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	c	905	CLA	C4-C3-C5	3.23	120.70	115.27
24	d	404	CLA	CHC-C1C-C2C	-3.23	117.80	126.72
31	a	415	PL9	C35-C34-C36	3.23	120.70	115.27
24	b	614	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
24	C	509	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	b	613	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
24	b	610	CLA	CHD-C4C-NC	3.22	129.28	124.20
33	b	625	LMG	O8-C28-C29	3.22	122.01	111.91
24	B	614	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
26	Y	102	BCR	C15-C14-C13	-3.21	122.72	127.31
24	b	611	CLA	C4-C3-C5	3.21	120.67	115.27
24	a	408	CLA	C3B-C4B-NB	3.21	113.36	109.21
24	B	602	CLA	O2A-CGA-CBA	3.21	121.98	111.91
24	C	511	CLA	CMC-C2C-C1C	3.21	129.93	125.04
24	B	602	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
24	C	502	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	B	608	CLA	CAA-C2A-C3A	-3.20	104.00	112.78
24	B	605	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
24	c	913	CLA	C4-C3-C5	3.20	120.66	115.27
24	B	612	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	B	613	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
26	b	623	BCR	C24-C23-C22	-3.20	121.41	126.23
36	a	418	LHG	O7-C7-C8	3.20	118.39	111.50
24	D	405	CLA	C1D-CHD-C4C	-3.19	118.34	122.56
24	A	409	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
24	B	616	CLA	CMC-C2C-C1C	3.19	129.90	125.04
24	b	619	CLA	C1D-CHD-C4C	-3.19	118.35	122.56
24	C	504	CLA	CAC-C3C-C4C	3.19	128.95	124.81
24	b	610	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
26	Y	102	BCR	C16-C17-C18	-3.19	122.76	127.31
24	b	615	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	C	507	CLA	CHD-C4C-NC	3.18	129.22	124.20
24	C	509	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
27	f	102	SQD	O7-S-C6	3.18	110.72	106.94
24	C	504	CLA	CMB-C2B-C3B	3.18	130.63	124.68
24	B	610	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
24	B	617	CLA	CHD-C4C-NC	3.18	129.22	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	623	BCR	C15-C14-C13	-3.18	122.77	127.31
24	b	613	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	B	605	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
24	c	909	CLA	CHC-C1C-C2C	-3.18	117.93	126.72
25	A	408	PHO	C2A-C1A-NA	3.18	115.51	111.86
24	C	506	CLA	CBC-CAC-C3C	-3.18	103.67	112.43
24	a	405	CLA	CHC-C1C-C2C	-3.18	117.94	126.72
24	B	607	CLA	C3B-C4B-NB	3.17	113.31	109.21
24	c	907	CLA	CBC-CAC-C3C	-3.17	103.68	112.43
24	c	914	CLA	CMC-C2C-C1C	3.17	129.87	125.04
24	D	404	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	C	501	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	A	406	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
24	c	913	CLA	CHD-C4C-NC	3.17	129.19	124.20
26	Y	102	BCR	C24-C23-C22	-3.16	121.45	126.23
24	c	907	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
24	b	615	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
24	b	614	CLA	CHD-C4C-NC	3.16	129.18	124.20
24	b	611	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
24	B	604	CLA	C3B-C4B-NB	3.16	113.29	109.21
31	A	417	PL9	C7-C8-C9	-3.16	121.54	126.79
38	V	202	HEM	CBA-CAA-C2A	-3.15	106.67	112.49
36	D	410	LHG	O8-C23-C24	3.15	121.81	111.91
31	A	417	PL9	C22-C23-C24	-3.15	120.08	127.66
24	b	608	CLA	CAC-C3C-C4C	3.15	128.89	124.81
24	C	508	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
24	C	501	CLA	CMC-C2C-C1C	3.14	129.83	125.04
24	B	604	CLA	O2A-CGA-CBA	3.14	121.77	111.91
24	B	613	CLA	CAC-C3C-C4C	3.14	128.88	124.81
26	H	101	BCR	C16-C17-C18	-3.14	122.83	127.31
24	c	914	CLA	CHD-C4C-NC	3.14	129.15	124.20
24	b	614	CLA	C3B-C4B-NB	3.13	113.26	109.21
24	d	406	CLA	CMC-C2C-C1C	3.13	129.81	125.04
26	B	620	BCR	C28-C27-C26	-3.13	108.48	114.08
24	b	611	CLA	CMB-C2B-C3B	3.13	130.54	124.68
24	B	606	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	B	607	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	b	618	CLA	CAC-C3C-C4C	3.13	128.87	124.81
24	B	614	CLA	O2D-CGD-CBD	3.13	116.82	111.27
27	F	103	SQD	C3-C4-C5	3.13	115.81	110.24
24	B	604	CLA	C2A-C1A-CHA	-3.12	118.39	123.86
24	B	612	CLA	C4C-C3C-C2C	-3.12	102.34	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C11-C10-C9	-3.12	122.85	127.31
31	A	417	PL9	C7-C3-C4	3.12	119.41	116.88
24	c	903	CLA	C3B-C4B-NB	3.12	113.24	109.21
31	a	415	PL9	C17-C18-C19	-3.12	120.15	127.66
24	b	620	CLA	C3B-C4B-NB	3.12	113.24	109.21
24	b	615	CLA	O2A-CGA-CBA	3.12	121.69	111.91
26	b	624	BCR	C24-C23-C22	-3.12	121.52	126.23
26	c	915	BCR	C33-C5-C6	-3.12	121.03	124.53
24	d	406	CLA	CHD-C4C-NC	3.12	129.11	124.20
33	C	519	LMG	C4-C3-C2	3.11	116.26	110.82
26	D	406	BCR	C15-C14-C13	-3.11	122.87	127.31
24	b	617	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
24	C	503	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
24	b	615	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	C	506	CLA	CHC-C1C-C2C	-3.11	118.12	126.72
24	C	508	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	a	408	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
36	L	101	LHG	O8-C23-C24	3.10	121.65	111.91
24	A	407	CLA	C1-C2-C3	-3.10	120.68	126.04
24	A	409	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
33	Z	101	LMG	C1-O6-C5	3.10	119.78	113.69
24	B	604	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
24	b	619	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
31	D	407	PL9	C36-C37-C38	-3.10	101.69	111.88
24	B	602	CLA	CHD-C4C-NC	3.10	129.09	124.20
24	C	502	CLA	C3B-C4B-NB	3.10	113.22	109.21
33	Y	101	LMG	O8-C28-C29	3.09	121.62	111.91
24	d	404	CLA	CHD-C4C-NC	3.09	129.07	124.20
24	B	616	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
24	A	407	CLA	C3B-C4B-NB	3.09	113.20	109.21
24	B	610	CLA	CAC-C3C-C4C	3.09	128.82	124.81
24	A	405	CLA	CHC-C1C-C2C	-3.09	118.18	126.72
24	C	502	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	b	611	CLA	CMC-C2C-C1C	3.09	129.74	125.04
24	B	606	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
24	C	511	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
24	d	406	CLA	C3B-C4B-NB	3.08	113.19	109.21
24	B	616	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
26	Y	102	BCR	C40-C30-C25	-3.08	105.30	110.30
24	c	908	CLA	C4C-C3C-C2C	-3.08	102.42	106.90
24	b	616	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	B	608	CLA	CAC-C3C-C4C	3.07	128.80	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CMC-C2C-C1C	3.07	129.72	125.04
24	b	614	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	B	606	CLA	C2A-C1A-CHA	-3.07	118.49	123.86
31	a	415	PL9	C10-C9-C11	3.07	120.44	115.27
37	C	518	DGD	O1G-C1A-C2A	3.07	121.55	111.91
24	b	620	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	c	907	CLA	CHD-C4C-NC	3.07	129.04	124.20
35	b	603	HTG	O5-C5-C4	3.07	115.27	109.69
24	b	607	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
33	B	622	LMG	O7-C10-C11	3.06	118.11	111.50
31	A	417	PL9	C27-C28-C29	-3.06	120.28	127.66
24	C	503	CLA	CHD-C4C-NC	3.06	129.03	124.20
25	D	401	PHO	CHC-C1C-C2C	-3.06	118.03	125.73
24	C	503	CLA	C3B-C4B-NB	3.06	113.17	109.21
24	c	910	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	c	903	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	b	615	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
24	C	512	CLA	C3B-C4B-NB	3.06	113.16	109.21
25	a	407	PHO	O1D-CGD-CBD	-3.06	118.23	124.48
24	C	511	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	a	405	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	B	609	CLA	CMA-C3A-C4A	-3.05	103.56	111.77
26	B	619	BCR	C37-C22-C21	-3.05	118.65	122.92
24	B	603	CLA	CMA-C3A-C4A	-3.05	103.58	111.77
25	d	403	PHO	C2B-C1B-NB	3.05	114.39	109.79
24	B	608	CLA	C1D-CHD-C4C	-3.05	118.54	122.56
24	C	506	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	B	616	CLA	CHD-C4C-NC	3.05	129.00	124.20
24	d	405	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	b	606	CLA	C4-C3-C5	3.04	120.39	115.27
24	C	507	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
36	d	410	LHG	O8-C23-O10	-3.04	115.92	123.59
24	C	505	CLA	CMC-C2C-C1C	3.04	129.67	125.04
26	d	407	BCR	C7-C8-C9	-3.04	121.64	126.23
31	A	417	PL9	C45-C44-C46	3.04	120.38	115.27
24	B	603	CLA	OBD-CAD-C3D	-3.04	122.94	127.98
24	C	508	CLA	C4D-C3D-CAD	-3.03	106.78	108.47
24	B	605	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	a	406	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
24	B	615	CLA	O2A-CGA-CBA	3.03	121.42	111.91
24	b	617	CLA	C3B-C4B-NB	3.03	113.13	109.21
24	B	604	CLA	CMB-C2B-C3B	3.03	130.34	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	c	903	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
24	C	503	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
24	c	910	CLA	CMC-C2C-C1C	3.03	129.65	125.04
24	b	607	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
24	C	506	CLA	C1-C2-C3	-3.02	120.82	126.04
24	B	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	B	603	CLA	CHD-C4C-NC	3.02	128.96	124.20
26	d	407	BCR	C29-C30-C25	3.02	115.12	110.48
26	B	619	BCR	C29-C30-C25	3.02	115.12	110.48
24	C	512	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
37	C	518	DGD	O2G-C1B-C2B	3.01	117.99	111.50
24	C	509	CLA	C4-C3-C5	3.01	120.34	115.27
26	T	102	BCR	C15-C14-C13	3.01	131.60	127.31
24	b	611	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
24	b	612	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
24	B	612	CLA	CMC-C2C-C1C	3.01	129.62	125.04
24	B	604	CLA	C1-O2A-CGA	3.01	124.33	116.44
24	b	618	CLA	O2A-CGA-CBA	3.01	121.34	111.91
24	A	409	CLA	C3B-C4B-NB	3.01	113.10	109.21
37	D	408	DGD	O1G-C1A-C2A	3.00	121.33	111.91
24	b	620	CLA	C4-C3-C5	3.00	120.32	115.27
24	c	913	CLA	CBA-CAA-C2A	-3.00	105.01	113.86
24	C	506	CLA	C4-C3-C5	3.00	120.32	115.27
24	C	512	CLA	C1-C2-C3	-3.00	120.86	126.04
24	b	606	CLA	C3B-C4B-NB	3.00	113.08	109.21
24	C	511	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
24	B	616	CLA	C3B-C4B-NB	2.99	113.08	109.21
24	c	914	CLA	C1-C2-C3	-2.99	120.86	126.04
24	D	404	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
24	c	912	CLA	CMB-C2B-C3B	2.99	130.28	124.68
24	b	609	CLA	O2A-CGA-CBA	2.99	121.30	111.91
24	C	513	CLA	C1-C2-C3	-2.99	120.87	126.04
24	b	608	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	A	407	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
24	c	910	CLA	CHD-C4C-NC	2.99	128.91	124.20
26	C	515	BCR	C33-C5-C6	-2.99	121.17	124.53
24	C	508	CLA	C1D-CHD-C4C	-2.99	118.62	122.56
24	b	606	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
29	M	103	LMT	O1B-C1B-C2B	2.98	115.83	108.10
24	a	408	CLA	CMA-C3A-C2A	-2.98	101.80	113.83
24	a	408	CLA	O2D-CGD-O1D	-2.98	118.01	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	904	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
31	D	407	PL9	C45-C44-C46	2.98	120.28	115.27
26	D	406	BCR	C24-C23-C22	-2.98	121.73	126.23
37	c	918	DGD	O1G-C1A-C2A	2.98	121.25	111.91
24	b	607	CLA	C1D-CHD-C4C	-2.98	118.63	122.56
24	c	912	CLA	C3B-C4B-NB	2.97	113.06	109.21
36	B	635	LHG	O8-C23-O10	-2.97	116.09	123.59
24	D	405	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	B	614	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
24	B	611	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
36	E	101	LHG	O8-C23-C24	2.97	121.22	111.91
24	B	608	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
24	b	613	CLA	O2A-CGA-CBA	2.97	121.22	111.91
35	c	922	HTG	C1-O5-C5	2.96	118.05	112.58
24	d	405	CLA	O2A-CGA-O1A	-2.96	116.11	123.59
24	B	610	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
24	b	609	CLA	C1D-CHD-C4C	-2.96	118.65	122.56
24	c	912	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
24	a	406	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
24	a	405	CLA	C1-C2-C3	-2.96	120.92	126.04
24	B	612	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
24	B	611	CLA	CHD-C4C-NC	2.96	128.87	124.20
25	a	407	PHO	C3C-C4C-NC	2.96	114.86	110.28
24	c	913	CLA	C3B-C4B-NB	2.95	113.03	109.21
24	C	506	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
24	C	513	CLA	C3B-C4B-NB	2.95	113.03	109.21
24	C	504	CLA	C4-C3-C5	2.95	120.23	115.27
24	c	910	CLA	O2A-CGA-CBA	2.95	121.16	111.91
24	C	510	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
24	B	603	CLA	C3B-C4B-NB	2.95	113.02	109.21
31	d	408	PL9	C17-C18-C19	-2.95	120.56	127.66
24	C	505	CLA	CAC-C3C-C4C	2.94	128.63	124.81
25	a	407	PHO	CMC-C2C-C1C	2.94	129.59	125.06
24	B	605	CLA	C1D-CHD-C4C	-2.94	118.67	122.56
24	b	611	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
24	B	605	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	b	614	CLA	O2A-CGA-CBA	2.94	121.14	111.91
24	B	609	CLA	CMB-C2B-C3B	2.94	130.18	124.68
36	b	635	LHG	O8-C23-C24	2.94	121.13	111.91
26	b	623	BCR	C29-C30-C25	2.94	115.01	110.48
24	b	616	CLA	OBD-CAD-C3D	-2.94	123.10	127.98
24	c	904	CLA	CHD-C4C-NC	2.94	128.83	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	919	LMG	C8-O7-C10	-2.94	110.56	117.79
24	B	609	CLA	CAC-C3C-C4C	2.94	128.62	124.81
24	B	604	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
24	B	617	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
31	d	408	PL9	C12-C13-C14	-2.93	120.60	127.66
26	K	101	BCR	C20-C21-C22	-2.93	123.12	127.31
25	A	408	PHO	CAC-C3C-C4C	2.93	128.42	125.22
24	c	906	CLA	C1-C2-C3	-2.93	120.97	126.04
24	b	616	CLA	CAC-C3C-C4C	2.93	128.61	124.81
24	D	405	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
24	C	503	CLA	C1-C2-C3	-2.93	120.98	126.04
26	K	101	BCR	C33-C5-C6	-2.93	121.24	124.53
36	D	409	LHG	O7-C7-C8	2.93	117.81	111.50
24	b	613	CLA	C1-C2-C3	-2.93	120.98	126.04
24	C	507	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
24	b	611	CLA	CHD-C4C-NC	2.92	128.81	124.20
24	b	611	CLA	C1-O2A-CGA	2.92	124.11	116.44
27	L	102	SQD	O7-S-C6	2.92	110.41	106.94
24	c	906	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
27	a	410	SQD	C1-O5-C5	-2.92	107.96	113.69
24	b	607	CLA	C2A-C1A-CHA	-2.92	118.75	123.86
24	c	913	CLA	CBC-CAC-C3C	-2.92	104.39	112.43
24	A	405	CLA	CMB-C2B-C3B	2.92	130.14	124.68
27	A	414	SQD	O9-S-C6	2.92	110.41	106.94
24	b	608	CLA	CMB-C2B-C3B	2.92	130.13	124.68
24	c	912	CLA	C1-C2-C3	-2.92	121.00	126.04
24	A	409	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	d	404	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	C	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	b	617	CLA	CHD-C4C-NC	2.91	128.79	124.20
33	c	919	LMG	O8-C28-C29	2.91	121.04	111.91
24	B	602	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
24	b	607	CLA	C3B-C4B-NB	2.91	112.97	109.21
24	B	605	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	a	405	CLA	CAA-C2A-C1A	-2.91	102.44	111.97
24	b	619	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	C	501	CLA	CAC-C3C-C4C	2.91	128.58	124.81
31	d	408	PL9	C7-C8-C9	-2.90	121.96	126.79
24	c	906	CLA	C3B-C4B-NB	2.90	112.96	109.21
24	c	909	CLA	CHD-C4C-NC	2.90	128.78	124.20
24	b	619	CLA	C3B-C4B-NB	2.90	112.96	109.21
26	h	101	BCR	C7-C8-C9	-2.90	121.85	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	CHD-C4C-NC	2.90	128.78	124.20
25	a	407	PHO	CAC-C3C-C4C	2.90	128.38	125.22
24	a	408	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
24	B	606	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
24	C	509	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	B	610	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	b	621	CLA	C1-C2-C3	-2.89	121.04	126.04
24	c	910	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	b	621	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
24	B	609	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
24	B	617	CLA	O1D-CGD-CBD	-2.89	118.58	124.48
24	B	607	CLA	C4-C3-C5	2.89	120.13	115.27
24	c	914	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
24	B	608	CLA	C1-C2-C3	-2.88	121.06	126.04
24	B	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
24	C	512	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	c	905	CLA	C3B-C4B-NB	2.88	112.93	109.21
24	b	612	CLA	CMC-C2C-C1C	2.88	129.42	125.04
24	b	614	CLA	CBC-CAC-C3C	-2.88	104.50	112.43
24	c	912	CLA	CAC-C3C-C4C	2.88	128.54	124.81
24	A	407	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
27	L	102	SQD	O48-C23-C24	2.88	120.93	111.91
31	a	415	PL9	C53-C6-C1	2.87	120.86	114.99
24	C	513	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
25	D	401	PHO	C2A-C1A-NA	2.87	115.15	111.86
24	A	405	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	c	903	CLA	O2A-C1-C2	2.87	116.17	108.64
24	d	406	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
24	b	610	CLA	C4-C3-C5	2.87	120.09	115.27
24	B	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
24	b	619	CLA	O2A-CGA-CBA	2.87	120.90	111.91
24	A	407	CLA	CBC-CAC-C3C	-2.86	104.53	112.43
24	b	607	CLA	C4-C3-C5	2.86	120.09	115.27
37	C	517	DGD	C1E-O6E-C5E	-2.86	108.07	113.69
27	a	410	SQD	O9-S-C6	2.86	110.34	106.94
24	C	513	CLA	CHD-C4C-NC	2.86	128.71	124.20
24	C	506	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
24	B	606	CLA	OBD-CAD-C3D	-2.86	123.24	127.98
24	D	405	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
26	T	102	BCR	C35-C13-C12	2.85	122.57	118.08
26	C	514	BCR	C38-C26-C25	-2.85	121.33	124.53
31	A	417	PL9	C53-C6-C1	2.85	120.82	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
26	T	102	BCR	C21-C20-C19	-2.85	114.32	123.22
24	c	905	CLA	CHD-C4C-NC	2.85	128.69	124.20
36	d	409	LHG	O7-C7-O9	-2.85	116.81	123.70
24	c	907	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
24	c	903	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	B	612	CLA	CHD-C4C-NC	2.85	128.69	124.20
24	C	511	CLA	O2A-CGA-CBA	2.85	120.84	111.91
24	c	912	CLA	C4-C3-C5	2.85	120.06	115.27
26	C	515	BCR	C3-C4-C5	-2.85	109.00	114.08
24	c	903	CLA	O2A-CGA-CBA	2.84	120.83	111.91
24	c	912	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
24	B	604	CLA	CMC-C2C-C1C	2.84	129.37	125.04
31	a	415	PL9	C37-C38-C39	-2.84	120.82	127.66
24	b	608	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
25	D	401	PHO	CED-O2D-CGD	2.84	122.36	115.94
24	B	614	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
25	a	407	PHO	C2C-C1C-NC	2.84	114.08	109.79
24	a	406	CLA	C3B-C4B-NB	2.84	112.88	109.21
24	B	614	CLA	CMC-C2C-C1C	2.84	129.36	125.04
24	b	615	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
24	B	604	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	b	608	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
24	C	511	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
24	B	607	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
24	c	905	CLA	CMB-C2B-C3B	2.83	129.98	124.68
24	B	603	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
27	F	103	SQD	C44-O6-C1	-2.83	108.21	113.74
24	c	902	CLA	O2A-CGA-CBA	2.83	120.79	111.91
24	c	909	CLA	O2A-CGA-CBA	2.83	120.78	111.91
24	B	613	CLA	C2A-C1A-CHA	-2.83	118.92	123.86
24	a	408	CLA	O2A-CGA-CBA	2.83	120.78	111.91
31	D	407	PL9	C36-C34-C33	-2.83	115.40	121.12
24	B	603	CLA	C1-O2A-CGA	2.83	123.86	116.44
24	C	502	CLA	CMC-C2C-C1C	2.83	129.34	125.04
24	B	602	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
24	c	911	CLA	CHD-C4C-NC	2.82	128.65	124.20
24	c	902	CLA	C1D-CHD-C4C	-2.82	118.83	122.56
24	A	407	CLA	CHD-C4C-NC	2.82	128.65	124.20
27	A	411	SQD	O9-S-C6	2.82	110.29	106.94
24	B	605	CLA	CMC-C2C-C1C	2.82	129.33	125.04
26	C	514	BCR	C11-C10-C9	-2.82	123.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	905	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
24	C	506	CLA	C1D-CHD-C4C	-2.82	118.84	122.56
24	b	613	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
31	D	407	PL9	C12-C13-C14	-2.81	120.89	127.66
24	C	509	CLA	O2A-CGA-CBA	2.81	120.73	111.91
24	C	508	CLA	O2A-CGA-CBA	2.81	120.73	111.91
24	C	506	CLA	C4D-C3D-CAD	-2.81	106.90	108.47
33	Z	101	LMG	C9-O8-C28	2.81	124.17	117.10
24	B	609	CLA	CMC-C2C-C1C	2.81	129.32	125.04
24	b	606	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
31	A	417	PL9	C12-C13-C14	-2.81	120.90	127.66
25	a	407	PHO	CHD-C1D-C2D	-2.81	118.67	125.73
24	b	609	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	B	615	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
26	k	101	BCR	C24-C23-C22	-2.81	122.00	126.23
24	b	609	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
24	B	603	CLA	C1-C2-C3	-2.81	121.19	126.04
24	B	610	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
27	a	410	SQD	C44-O6-C1	-2.80	108.26	113.74
24	a	406	CLA	CAC-C3C-C4C	2.80	128.44	124.81
24	C	502	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
27	L	102	SQD	O8-S-C6	2.80	110.20	105.74
24	b	610	CLA	OBD-CAD-C3D	-2.80	123.33	127.98
24	B	606	CLA	O2A-CGA-CBA	2.80	120.69	111.91
35	V	203	HTG	C1-C2-C3	-2.80	105.06	110.59
24	b	610	CLA	C3B-C4B-NB	2.80	112.83	109.21
24	C	502	CLA	CHD-C4C-NC	2.80	128.61	124.20
31	D	407	PL9	C51-C49-C50	2.80	120.78	114.60
24	b	607	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	D	405	CLA	CHC-C1C-C2C	-2.80	118.99	126.72
26	y	101	BCR	C24-C23-C22	-2.79	122.01	126.23
24	B	608	CLA	C1-O2A-CGA	2.79	123.78	116.44
24	d	404	CLA	C4-C3-C5	2.79	119.97	115.27
24	D	404	CLA	CHD-C4C-NC	2.79	128.60	124.20
24	c	906	CLA	C4-C3-C5	2.79	119.97	115.27
27	A	414	SQD	O48-C23-O10	-2.79	116.55	123.59
24	c	907	CLA	OBD-CAD-C3D	-2.79	123.35	127.98
31	a	415	PL9	C7-C3-C2	-2.79	119.63	123.30
24	c	909	CLA	C4D-C3D-CAD	-2.79	106.91	108.47
26	c	927	BCR	C11-C10-C9	-2.79	123.33	127.31
26	C	515	BCR	C11-C10-C9	-2.79	123.33	127.31
24	c	909	CLA	CBC-CAC-C3C	-2.79	104.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	908	CLA	C1-C2-C3	-2.79	121.22	126.04
24	b	620	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	c	913	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	D	404	CLA	CMC-C2C-C1C	2.79	129.28	125.04
24	c	902	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
24	C	501	CLA	C3B-C4B-NB	2.79	112.81	109.21
24	C	502	CLA	O2A-CGA-CBA	2.79	120.65	111.91
33	Z	101	LMG	O6-C5-C4	2.78	114.75	109.69
24	d	406	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
27	f	102	SQD	O5-C5-C4	2.78	114.75	109.69
26	c	927	BCR	C28-C27-C26	-2.78	109.11	114.08
24	C	503	CLA	C4-C3-C5	2.78	119.95	115.27
24	A	407	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
24	B	612	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
24	B	608	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
24	d	405	CLA	C3B-C4B-NB	2.78	112.80	109.21
24	c	906	CLA	CAC-C3C-C4C	2.78	128.41	124.81
31	a	415	PL9	C40-C39-C41	2.78	119.94	115.27
24	c	908	CLA	C4-C3-C5	2.78	119.94	115.27
24	b	613	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	c	902	CLA	C4C-C3C-C2C	-2.77	102.85	106.90
37	C	517	DGD	O1G-C1A-C2A	2.77	120.61	111.91
24	B	617	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	B	608	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	c	905	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	d	404	CLA	CMA-C3A-C2A	-2.77	102.65	113.83
25	d	403	PHO	C3C-C4C-NC	2.77	114.58	110.28
24	b	608	CLA	O2A-CGA-CBA	2.77	120.61	111.91
27	a	410	SQD	O48-C23-C24	2.77	120.61	111.91
24	c	910	CLA	C4-C3-C5	2.77	119.93	115.27
24	C	509	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
24	C	509	CLA	C1-O2A-CGA	2.77	123.70	116.44
24	C	505	CLA	C3B-C4B-NB	2.76	112.78	109.21
26	B	620	BCR	C38-C26-C25	-2.76	121.43	124.53
29	M	103	LMT	O5'-C5'-C4'	2.76	115.57	109.75
24	B	607	CLA	CHC-C1C-C2C	-2.76	119.09	126.72
24	d	406	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
24	B	615	CLA	C1-O2A-CGA	2.76	123.68	116.44
24	b	621	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	614	CLA	CMB-C2B-C3B	2.75	129.83	124.68
24	C	513	CLA	CHC-C1C-C2C	-2.75	119.10	126.72
24	B	614	CLA	CAC-C3C-C4C	2.75	128.38	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C1D-CHD-C4C	-2.75	118.93	122.56
25	d	403	PHO	CHC-C1C-C2C	-2.75	118.81	125.73
27	a	402	SQD	C3-C4-C5	2.75	115.14	110.24
29	A	415	LMT	C4B-C3B-C2B	-2.75	106.02	110.82
24	c	909	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
35	C	521	HTG	C1-O5-C5	2.75	117.65	112.58
24	c	909	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	d	405	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
25	A	408	PHO	CHC-C1C-C2C	-2.75	118.83	125.73
27	F	103	SQD	O6-C1-C2	2.74	112.59	108.30
24	B	610	CLA	CHD-C4C-NC	2.74	128.53	124.20
24	b	620	CLA	CMC-C2C-C1C	2.74	129.22	125.04
24	b	619	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	B	607	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
24	b	614	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
24	B	607	CLA	O2A-CGA-CBA	2.74	120.51	111.91
24	C	504	CLA	CHC-C1C-C2C	-2.74	119.14	126.72
24	c	905	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	C	501	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
24	a	408	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
24	A	409	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
24	D	404	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	b	612	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	c	911	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
24	b	612	CLA	C1D-CHD-C4C	-2.73	118.95	122.56
24	B	606	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	A	405	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
24	C	512	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
36	d	409	LHG	O8-C23-C24	2.73	120.47	111.91
24	b	620	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
24	b	607	CLA	C1-C2-C3	-2.73	121.33	126.04
24	A	407	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	c	905	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	C	510	CLA	CMC-C2C-C1C	2.72	129.19	125.04
26	t	102	BCR	C12-C13-C14	-2.72	114.76	118.94
25	a	407	PHO	C1C-C2C-C3C	-2.72	103.38	106.51
27	L	102	SQD	O47-C7-O49	-2.72	117.13	123.70
25	D	401	PHO	C2B-C1B-NB	2.72	113.89	109.79
24	B	616	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
26	c	927	BCR	C33-C5-C6	-2.72	121.48	124.53
24	B	615	CLA	C1D-CHD-C4C	-2.72	118.97	122.56
24	c	910	CLA	CHC-C1C-C2C	-2.72	119.21	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	OBD-CAD-C3D	-2.71	123.47	127.98
24	B	609	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
24	b	619	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
24	C	513	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
26	b	624	BCR	C2-C1-C6	2.71	114.65	110.48
24	b	619	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	c	911	CLA	O2A-CGA-CBA	2.71	120.40	111.91
26	k	101	BCR	C34-C9-C8	2.71	122.34	118.08
24	c	905	CLA	CAA-C2A-C3A	-2.71	105.37	112.78
24	c	907	CLA	C4-C3-C5	2.71	119.82	115.27
24	c	914	CLA	CED-O2D-CGD	2.70	122.05	115.94
24	B	614	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	C	501	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	513	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	D	404	CLA	CAA-C2A-C3A	-2.70	105.38	112.78
37	h	102	DGD	O1G-C1A-C2A	2.70	120.39	111.91
24	c	914	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
24	c	905	CLA	OBD-CAD-C3D	-2.70	123.50	127.98
24	c	904	CLA	C4-C3-C5	2.70	119.81	115.27
24	C	507	CLA	O2A-CGA-CBA	2.70	120.38	111.91
26	c	915	BCR	C16-C17-C18	-2.70	123.46	127.31
25	a	407	PHO	C2B-C1B-NB	2.70	113.86	109.79
24	A	406	CLA	OBD-CAD-C3D	-2.70	123.50	127.98
24	b	621	CLA	CHD-C4C-NC	2.69	128.45	124.20
25	d	403	PHO	CHD-C1D-C2D	-2.69	118.95	125.73
24	c	908	CLA	CHD-C4C-NC	2.69	128.45	124.20
25	D	401	PHO	C4-C3-C5	2.69	119.80	115.27
25	d	403	PHO	C4D-ND-C1D	-2.69	101.92	106.76
24	c	910	CLA	CAC-C3C-C4C	2.69	128.30	124.81
24	C	508	CLA	CMB-C2B-C3B	2.69	129.71	124.68
25	A	408	PHO	C1-O2A-CGA	2.69	123.50	116.44
24	C	510	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
33	A	419	LMG	O1-C1-C2	2.69	112.50	108.30
24	C	507	CLA	OBD-CAD-C3D	-2.69	123.52	127.98
24	A	407	CLA	C1D-CHD-C4C	-2.69	119.01	122.56
24	B	607	CLA	CHD-C4C-NC	2.69	128.44	124.20
24	c	908	CLA	CAC-C3C-C4C	2.69	128.29	124.81
24	C	503	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
27	f	102	SQD	O47-C7-O49	-2.69	117.21	123.70
24	B	609	CLA	C4C-C3C-C2C	-2.68	102.98	106.90
24	D	404	CLA	C4D-C3D-CAD	-2.68	106.97	108.47
24	a	406	CLA	O2A-CGA-CBA	2.68	120.32	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	405	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
25	A	408	PHO	C3C-C4C-NC	2.68	114.44	110.28
24	d	405	CLA	C4-C3-C5	2.68	119.78	115.27
26	B	619	BCR	C31-C1-C6	-2.68	105.95	110.30
24	c	914	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	c	913	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
33	z	101	LMG	O8-C28-C29	2.68	120.30	111.91
24	B	613	CLA	O2A-CGA-CBA	2.67	120.30	111.91
24	B	609	CLA	CHD-C4C-NC	2.67	128.42	124.20
24	c	905	CLA	CHC-C1C-C2C	-2.67	119.32	126.72
35	C	522	HTG	O5-C5-C4	2.67	114.55	109.69
24	b	614	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
24	c	912	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
24	C	508	CLA	C1-C2-C3	-2.67	121.42	126.04
24	a	406	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
24	a	408	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
24	c	904	CLA	C3B-C4B-NB	2.67	112.66	109.21
24	b	612	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
24	d	404	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
24	A	409	CLA	C1-C2-C3	-2.67	121.43	126.04
24	C	505	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
25	A	408	PHO	C4D-CHA-C1A	-2.66	119.37	125.37
24	d	406	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
31	D	407	PL9	C35-C34-C36	2.66	119.75	115.27
26	K	101	BCR	C24-C23-C22	-2.66	122.22	126.23
26	b	623	BCR	C38-C26-C25	-2.66	121.54	124.53
31	D	407	PL9	C42-C41-C39	-2.66	104.24	112.98
24	b	616	CLA	O2A-CGA-CBA	2.65	120.24	111.91
24	b	609	CLA	CAC-C3C-C4C	2.65	128.25	124.81
33	b	625	LMG	O8-C28-O10	-2.65	116.89	123.59
24	B	606	CLA	C3B-C4B-NB	2.65	112.64	109.21
25	a	407	PHO	CHC-C1C-C2C	-2.65	119.06	125.73
36	D	410	LHG	O8-C23-O10	-2.65	116.90	123.59
24	C	509	CLA	CMC-C2C-C1C	2.65	129.07	125.04
24	c	914	CLA	C3B-C4B-NB	2.65	112.64	109.21
24	b	618	CLA	OBD-CAD-C3D	-2.65	123.58	127.98
24	C	504	CLA	C4D-C3D-CAD	-2.65	106.99	108.47
26	B	620	BCR	C32-C1-C6	-2.65	106.01	110.30
24	c	914	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
24	C	511	CLA	CHD-C4C-NC	2.64	128.37	124.20
24	b	618	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
24	b	606	CLA	C2A-C1A-CHA	-2.64	119.24	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	405	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
33	a	411	LMG	O8-C28-C29	2.64	120.19	111.91
29	M	103	LMT	O1'-C1'-C2'	2.64	112.42	108.30
24	C	503	CLA	O2A-CGA-CBA	2.64	120.18	111.91
24	d	406	CLA	O2A-CGA-CBA	2.63	120.17	111.91
24	c	907	CLA	CMC-C2C-C1C	2.63	129.05	125.04
26	B	620	BCR	C15-C14-C13	-2.63	123.56	127.31
24	C	509	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
24	C	512	CLA	C4-C3-C5	2.63	119.69	115.27
24	c	913	CLA	CMC-C2C-C1C	2.63	129.04	125.04
25	d	403	PHO	O2D-CGD-O1D	-2.63	118.70	123.84
24	b	620	CLA	C4D-C3D-CAD	-2.63	107.01	108.47
26	h	101	BCR	C24-C23-C22	-2.62	122.27	126.23
26	T	102	BCR	C34-C9-C10	-2.62	119.25	122.92
24	C	512	CLA	C1-O2A-CGA	2.62	123.33	116.44
25	a	407	PHO	C4D-ND-C1D	-2.62	102.05	106.76
26	y	101	BCR	C10-C11-C12	-2.62	115.03	123.22
24	b	615	CLA	CHD-C4C-NC	2.62	128.34	124.20
24	B	614	CLA	O2A-CGA-CBA	2.62	120.13	111.91
27	F	103	SQD	O48-C23-C24	2.62	120.13	111.91
24	C	513	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
26	B	619	BCR	C24-C23-C22	-2.62	122.28	126.23
25	D	401	PHO	C4D-ND-C1D	-2.62	102.05	106.76
24	B	611	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
24	b	607	CLA	CHC-C1C-C2C	-2.62	119.48	126.72
24	c	907	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	B	603	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
26	B	620	BCR	C10-C11-C12	-2.62	115.05	123.22
24	C	506	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
24	C	509	CLA	CHD-C4C-NC	2.62	128.33	124.20
26	h	101	BCR	C11-C10-C9	-2.62	123.58	127.31
31	D	407	PL9	C40-C39-C38	-2.62	116.97	123.68
24	d	405	CLA	CMC-C2C-C1C	2.61	129.02	125.04
24	A	407	CLA	CAC-C3C-C4C	2.61	128.20	124.81
24	A	409	CLA	CMC-C2C-C1C	2.61	129.02	125.04
24	A	406	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
24	C	512	CLA	O2A-CGA-CBA	2.61	120.10	111.91
24	c	912	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	D	404	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	a	406	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
36	L	101	LHG	O8-C23-O10	-2.61	117.01	123.59
24	b	613	CLA	O2A-CGA-O1A	-2.61	117.01	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4-C3-C5	2.61	119.66	115.27
24	A	406	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
33	Z	101	LMG	C1-C2-C3	2.61	115.42	110.00
26	B	620	BCR	C29-C30-C25	2.60	114.49	110.48
24	d	404	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
37	C	516	DGD	C3G-C2G-C1G	-2.60	105.63	111.79
24	b	607	CLA	CAC-C3C-C4C	2.60	128.19	124.81
24	a	406	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
24	d	406	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	B	616	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
37	c	916	DGD	C2G-O2G-C1B	-2.60	111.39	117.79
24	B	617	CLA	O2A-CGA-CBA	2.60	120.06	111.91
26	A	410	BCR	C8-C7-C6	-2.60	119.90	127.20
38	v	202	HEM	CAD-CBD-CGD	2.60	117.03	112.67
29	m	103	LMT	O5'-C5'-C4'	2.60	115.23	109.75
24	C	507	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
24	c	914	CLA	C4-C3-C5	2.60	119.64	115.27
24	c	909	CLA	C4-C3-C5	2.60	119.64	115.27
24	c	902	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
26	Y	102	BCR	C21-C20-C19	-2.59	115.12	123.22
26	d	407	BCR	C10-C11-C12	-2.59	115.12	123.22
25	A	408	PHO	C2C-C1C-NC	2.59	113.70	109.79
24	C	512	CLA	CMC-C2C-C1C	2.59	128.99	125.04
24	b	620	CLA	O2A-CGA-CBA	2.59	120.04	111.91
25	A	408	PHO	CHD-C1D-C2D	-2.59	119.21	125.73
24	c	913	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
35	B	624	HTG	O5-C1-C2	2.59	113.57	110.31
37	c	917	DGD	O1G-C1A-C2A	2.59	120.04	111.91
27	A	411	SQD	O48-C23-C24	2.59	120.04	111.91
24	b	614	CLA	C1-C2-C3	-2.59	121.56	126.04
24	C	503	CLA	CAC-C3C-C4C	2.59	128.17	124.81
27	A	411	SQD	C1-C2-C3	-2.59	104.61	110.00
24	d	405	CLA	CMB-C2B-C3B	2.59	129.52	124.68
24	a	408	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
37	c	918	DGD	C2G-O2G-C1B	-2.59	111.43	117.79
24	B	603	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	b	613	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	C	513	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
24	A	407	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
24	b	611	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
24	b	618	CLA	CMB-C2B-C3B	2.58	129.51	124.68
31	D	407	PL9	C27-C28-C29	-2.58	121.44	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	e	101	DGD	O5D-C1E-C2E	2.58	112.33	108.30
24	b	614	CLA	C4-C3-C5	2.58	119.61	115.27
37	C	516	DGD	O3G-C3G-C2G	-2.58	104.67	110.90
35	b	603	HTG	C1-O5-C5	2.58	117.33	112.58
26	b	624	BCR	C3-C4-C5	-2.58	109.48	114.08
24	c	908	CLA	C3B-C4B-NB	2.58	112.54	109.21
26	C	515	BCR	C28-C27-C26	-2.58	109.48	114.08
24	c	908	CLA	OBD-CAD-C3D	-2.58	123.70	127.98
24	d	406	CLA	C4-C3-C5	2.57	119.60	115.27
24	b	615	CLA	CMC-C2C-C1C	2.57	128.96	125.04
24	b	608	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
24	d	405	CLA	CAC-C3C-C4C	2.57	128.14	124.81
24	b	616	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
24	D	405	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
24	b	608	CLA	CBC-CAC-C3C	-2.57	105.35	112.43
24	C	513	CLA	C4-C3-C5	2.57	119.59	115.27
27	a	410	SQD	C45-O47-C7	-2.57	111.47	117.79
36	d	409	LHG	O8-C23-O10	-2.57	117.11	123.59
24	c	906	CLA	CHD-C4C-NC	2.57	128.25	124.20
24	C	513	CLA	O2A-CGA-CBA	2.57	119.96	111.91
24	b	615	CLA	CMA-C3A-C4A	-2.56	104.88	111.77
26	Y	102	BCR	C10-C11-C12	-2.56	115.22	123.22
24	A	405	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
35	C	522	HTG	O5-C1-C2	2.56	113.54	110.31
24	a	406	CLA	O2A-CGA-O1A	-2.56	117.12	123.59
36	L	101	LHG	C5-O7-C7	-2.56	111.48	117.79
27	A	414	SQD	O8-S-C6	2.56	109.82	105.74
24	c	909	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
24	C	502	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
24	D	405	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	A	405	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
33	A	419	LMG	C7-O1-C1	-2.55	108.75	113.74
24	A	409	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
24	c	908	CLA	CHC-C1C-C2C	-2.55	119.66	126.72
26	K	101	BCR	C10-C11-C12	-2.55	115.26	123.22
24	d	406	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
24	b	616	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
36	d	409	LHG	C5-O7-C7	-2.55	111.52	117.79
26	C	514	BCR	C16-C17-C18	-2.55	123.67	127.31
26	c	915	BCR	C7-C8-C9	-2.55	122.39	126.23
31	A	417	PL9	C30-C29-C31	2.55	119.56	115.27
31	A	417	PL9	C17-C18-C19	-2.55	121.53	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	t	101	LMT	C1'-O5'-C5'	2.55	118.68	113.69
24	B	611	CLA	C4-C3-C5	2.54	119.55	115.27
26	t	102	BCR	C29-C28-C27	-2.54	105.69	111.38
35	b	627	HTG	C1-C2-C3	2.54	115.61	110.59
24	B	612	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	b	616	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
24	b	616	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	c	913	CLA	O2A-CGA-CBA	2.54	119.88	111.91
24	b	608	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
24	b	608	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	B	602	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
27	B	621	SQD	O48-C23-C24	2.54	119.87	111.91
24	a	405	CLA	CHD-C4C-NC	2.54	128.20	124.20
25	A	408	PHO	O2D-CGD-O1D	-2.54	118.88	123.84
24	c	911	CLA	CAC-C3C-C4C	2.54	128.10	124.81
24	b	619	CLA	CHC-C1C-C2C	-2.53	119.71	126.72
24	C	503	CLA	C4D-C3D-CAD	-2.53	107.06	108.47
24	b	613	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
24	b	620	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
24	C	506	CLA	CMC-C2C-C1C	2.53	128.89	125.04
26	h	101	BCR	C10-C11-C12	-2.53	115.33	123.22
25	D	401	PHO	C4D-CHA-C1A	-2.53	119.69	125.37
27	L	102	SQD	C1-C2-C3	-2.52	104.74	110.00
24	d	406	CLA	O2A-CGA-O1A	-2.52	117.22	123.59
26	t	102	BCR	C1-C6-C7	2.52	122.91	115.78
31	A	417	PL9	C15-C14-C16	2.52	119.51	115.27
31	a	415	PL9	C30-C29-C31	2.52	119.51	115.27
24	B	612	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
26	B	619	BCR	C2-C1-C6	2.52	114.36	110.48
24	D	405	CLA	C4D-C3D-CAD	-2.52	107.07	108.47
24	b	617	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
24	b	609	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
24	b	607	CLA	OBD-CAD-C3D	-2.52	123.81	127.98
24	b	619	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
24	B	612	CLA	C4-C3-C5	2.51	119.50	115.27
24	b	610	CLA	CMC-C2C-C1C	2.51	128.86	125.04
24	C	513	CLA	CAC-C3C-C4C	2.51	128.07	124.81
31	a	415	PL9	C25-C24-C26	2.51	119.49	115.27
26	C	515	BCR	C21-C20-C19	-2.51	115.38	123.22
24	b	609	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
24	c	904	CLA	O2A-CGA-CBA	2.51	119.78	111.91
24	C	503	CLA	CMC-C2C-C1C	2.51	128.86	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
24	B	612	CLA	CBC-CAC-C3C	-2.51	105.52	112.43
24	c	907	CLA	CMB-C2B-C3B	2.51	129.37	124.68
24	C	512	CLA	CAC-C3C-C4C	2.51	128.06	124.81
24	B	613	CLA	CHC-C1C-C2C	-2.50	119.79	126.72
24	b	607	CLA	CMA-C3A-C2A	-2.50	103.74	113.83
24	c	905	CLA	CBC-CAC-C3C	-2.50	105.54	112.43
24	B	605	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	c	909	CLA	CMB-C2B-C3B	2.50	129.36	124.68
25	a	407	PHO	CBD-CHA-C1A	2.50	132.20	126.40
24	d	404	CLA	CMB-C2B-C3B	2.50	129.35	124.68
24	b	612	CLA	OBD-CAD-C3D	-2.50	123.83	127.98
36	D	409	LHG	O8-C23-O10	-2.50	117.29	123.59
24	B	612	CLA	C11-C12-C13	-2.50	107.85	115.92
24	A	406	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
38	V	202	HEM	C1D-C2D-C3D	-2.50	105.26	107.00
24	D	404	CLA	CMB-C2B-C3B	2.50	129.35	124.68
24	a	406	CLA	OBD-CAD-C3D	-2.49	123.84	127.98
37	C	516	DGD	O6D-C5D-C6D	2.49	111.70	106.67
26	C	515	BCR	C15-C16-C17	-2.49	118.37	123.47
24	C	510	CLA	CAC-C3C-C4C	2.49	128.04	124.81
24	A	409	CLA	CHD-C4C-NC	2.49	128.13	124.20
24	b	612	CLA	CHD-C4C-NC	2.49	128.13	124.20
24	B	614	CLA	OBD-CAD-C3D	-2.49	123.85	127.98
24	B	614	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	B	613	CLA	CHD-C4C-NC	2.49	128.12	124.20
38	v	202	HEM	CBA-CAA-C2A	-2.49	107.90	112.49
24	B	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	b	620	CLA	C11-C10-C8	-2.49	107.88	115.92
24	A	406	CLA	O2A-CGA-CBA	2.48	119.71	111.91
24	b	607	CLA	O2A-CGA-CBA	2.48	119.70	111.91
24	c	904	CLA	CMC-C2C-C1C	2.48	128.82	125.04
27	B	621	SQD	O47-C7-O49	-2.48	117.70	123.70
36	d	411	LHG	O8-C23-C24	2.48	119.70	111.91
31	A	417	PL9	C25-C24-C26	2.48	119.45	115.27
25	A	408	PHO	C1C-C2C-C3C	-2.48	103.66	106.51
24	C	504	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
24	D	404	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
37	H	102	DGD	O1G-C1A-C2A	2.48	119.69	111.91
36	a	418	LHG	O8-C23-C24	2.48	119.69	111.91
24	b	617	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
24	b	612	CLA	CAC-C3C-C4C	2.48	128.02	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	911	CLA	O1D-CGD-CBD	-2.47	119.42	124.48
24	c	914	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
24	B	617	CLA	C4-C3-C5	2.47	119.43	115.27
24	B	614	CLA	CMA-C3A-C4A	-2.47	105.12	111.77
36	d	410	LHG	O8-C23-C24	2.47	119.67	111.91
24	c	914	CLA	O2A-CGA-CBA	2.47	119.67	111.91
33	c	920	LMG	O8-C28-C29	2.47	119.66	111.91
24	b	610	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
24	B	604	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
24	C	508	CLA	CHD-C4C-NC	2.47	128.09	124.20
27	L	102	SQD	C44-O6-C1	-2.47	108.92	113.74
24	C	510	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
24	C	508	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
26	H	101	BCR	C16-C15-C14	-2.47	118.42	123.47
24	a	406	CLA	C4-C3-C5	2.46	119.42	115.27
24	c	905	CLA	C1-C2-C3	-2.46	121.78	126.04
26	c	927	BCR	C20-C21-C22	-2.46	123.80	127.31
24	C	505	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	B	608	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	a	405	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
37	D	408	DGD	O6D-C5D-C6D	2.46	111.63	106.67
24	B	615	CLA	CHD-C4C-NC	2.46	128.08	124.20
25	A	408	PHO	C4D-ND-C1D	-2.46	102.35	106.76
24	b	620	CLA	C1-C2-C3	-2.46	121.80	126.04
25	A	408	PHO	C2B-C1B-NB	2.46	113.50	109.79
24	A	405	CLA	CAA-C2A-C1A	-2.45	103.93	111.97
24	b	617	CLA	CMC-C2C-C1C	2.45	128.78	125.04
24	C	501	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
24	d	405	CLA	C1D-CHD-C4C	-2.45	119.33	122.56
37	e	101	DGD	C1E-O6E-C5E	2.45	118.49	113.69
24	b	621	CLA	C1C-C2C-C3C	-2.45	104.39	106.96
24	C	504	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	c	904	CLA	OBD-CAD-C3D	-2.44	123.92	127.98
25	a	407	PHO	C4D-CHA-C1A	-2.44	119.87	125.37
24	c	909	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
27	a	402	SQD	O48-C23-O10	-2.44	117.43	123.59
31	d	408	PL9	C36-C37-C38	-2.44	103.87	111.88
24	B	614	CLA	CED-O2D-CGD	2.44	121.45	115.94
25	d	403	PHO	C4D-CHA-C1A	-2.44	119.88	125.37
37	e	101	DGD	O1G-C1A-C2A	2.44	119.56	111.91
24	b	621	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
26	b	624	BCR	C38-C26-C25	-2.44	121.79	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	604	CLA	C4-C3-C5	2.44	119.37	115.27
24	c	907	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
38	V	202	HEM	CAD-CBD-CGD	2.43	116.75	112.67
24	c	903	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	c	902	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
25	a	407	PHO	CBA-CAA-C2A	-2.43	106.69	113.86
24	B	609	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	b	612	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
26	c	927	BCR	C38-C26-C25	-2.43	121.80	124.53
24	c	913	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
37	H	102	DGD	O6D-C5D-C6D	2.42	111.56	106.67
24	C	510	CLA	O2A-CGA-CBA	2.42	119.51	111.91
27	A	411	SQD	O47-C7-O49	-2.42	117.85	123.70
31	d	408	PL9	C30-C29-C31	2.42	119.35	115.27
26	C	515	BCR	C37-C22-C23	2.42	121.89	118.08
24	D	404	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
24	B	608	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
26	Y	102	BCR	C38-C26-C25	-2.42	121.81	124.53
26	K	101	BCR	C11-C10-C9	-2.42	123.86	127.31
24	C	510	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
24	c	907	CLA	CAC-C3C-C4C	2.42	127.95	124.81
26	y	101	BCR	C40-C30-C25	-2.42	106.38	110.30
24	A	409	CLA	O2A-CGA-CBA	2.42	119.50	111.91
24	c	911	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
24	B	611	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
37	h	102	DGD	O6E-C5E-C6E	2.41	112.44	106.44
31	a	415	PL9	C51-C49-C50	2.41	119.93	114.60
24	c	906	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
24	A	405	CLA	CHD-C4C-NC	2.41	128.00	124.20
37	C	517	DGD	O1G-C1A-O1A	-2.41	117.52	123.59
31	d	408	PL9	C45-C44-C46	2.41	119.32	115.27
31	D	407	PL9	C31-C32-C33	-2.40	103.98	111.88
24	b	617	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
24	b	613	CLA	CMB-C2B-C3B	2.40	129.17	124.68
35	b	627	HTG	O2-C2-C3	-2.40	104.80	110.35
24	b	615	CLA	CMB-C2B-C3B	2.40	129.16	124.68
24	b	615	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
33	d	415	LMG	O6-C5-C4	2.40	114.05	109.69
27	L	102	SQD	O5-C5-C4	2.40	114.05	109.69
24	c	910	CLA	OBD-CAD-C3D	-2.40	124.00	127.98
35	c	922	HTG	O5-C5-C4	2.40	114.04	109.69
24	B	614	CLA	C4-C3-C5	2.39	119.30	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	CHD-C4C-NC	2.39	127.97	124.20
24	b	612	CLA	CAA-CBA-CGA	2.39	120.24	113.25
24	b	619	CLA	C1-O2A-CGA	2.39	122.72	116.44
24	B	617	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
24	c	902	CLA	OBD-CAD-C3D	-2.39	124.02	127.98
31	d	408	PL9	C51-C49-C50	2.39	119.88	114.60
31	D	407	PL9	C7-C3-C4	2.39	118.82	116.88
24	C	506	CLA	C2A-C1A-CHA	-2.39	119.69	123.86
24	c	904	CLA	CAC-C3C-C4C	2.39	127.91	124.81
24	b	614	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
24	b	621	CLA	CMB-C2B-C3B	2.39	129.14	124.68
25	D	401	PHO	O2A-CGA-CBA	2.39	119.39	111.91
24	A	405	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	a	405	CLA	C4C-C3C-C2C	-2.38	103.42	106.90
24	b	617	CLA	CED-O2D-CGD	2.38	121.33	115.94
24	A	406	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
24	c	909	CLA	OBD-CAD-C3D	-2.38	124.03	127.98
31	d	408	PL9	C22-C23-C24	-2.38	121.93	127.66
37	h	102	DGD	O1G-C1A-O1A	-2.38	117.58	123.59
27	F	103	SQD	O47-C7-O49	-2.38	117.95	123.70
37	c	916	DGD	C3G-C2G-C1G	-2.38	106.16	111.79
36	D	410	LHG	C6-C5-C4	-2.38	106.16	111.79
24	d	404	CLA	C1-C2-C3	-2.38	121.93	126.04
27	f	102	SQD	O48-C23-C24	2.38	119.38	111.91
24	d	404	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
24	a	408	CLA	CMB-C2B-C3B	2.38	129.13	124.68
25	d	403	PHO	C2A-C1A-NA	2.38	114.59	111.86
33	J	101	LMG	O8-C28-O10	-2.38	117.59	123.59
26	c	915	BCR	C38-C26-C25	-2.38	121.86	124.53
24	B	603	CLA	C4-C3-C5	2.38	119.27	115.27
24	B	612	CLA	C1-O2A-CGA	2.37	122.67	116.44
24	A	406	CLA	CMA-C3A-C2A	-2.37	104.25	113.83
24	d	405	CLA	CHD-C4C-NC	2.37	127.94	124.20
24	a	408	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
24	B	616	CLA	C4-C3-C5	2.37	119.26	115.27
24	c	908	CLA	O2A-CGA-CBA	2.37	119.35	111.91
26	B	620	BCR	C37-C22-C23	2.37	121.81	118.08
24	B	609	CLA	O2A-CGA-CBA	2.37	119.35	111.91
26	T	102	BCR	C1-C6-C7	2.37	122.48	115.78
27	a	410	SQD	O47-C7-O49	-2.37	117.98	123.70
24	B	611	CLA	C1-C2-C3	-2.37	121.95	126.04
24	b	609	CLA	C1-C2-C3	-2.37	121.95	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	915	BCR	C3-C4-C5	-2.37	109.85	114.08
24	c	908	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	C	510	CLA	CMB-C2B-C3B	2.37	129.11	124.68
26	t	102	BCR	C21-C20-C19	-2.37	115.83	123.22
24	c	903	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	B	607	CLA	CAC-C3C-C4C	2.37	127.88	124.81
24	b	609	CLA	CHD-C4C-NC	2.37	127.93	124.20
31	A	417	PL9	C40-C39-C41	2.37	119.25	115.27
24	c	914	CLA	CAC-C3C-C4C	2.36	127.88	124.81
24	c	904	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
24	D	404	CLA	CAC-C3C-C4C	2.36	127.88	124.81
24	A	406	CLA	CED-O2D-CGD	2.36	121.28	115.94
24	A	407	CLA	CMC-C2C-C1C	2.36	128.63	125.04
24	B	610	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	b	619	CLA	CAC-C3C-C4C	2.36	127.87	124.81
24	c	904	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
26	b	622	BCR	C10-C11-C12	-2.36	115.86	123.22
24	C	504	CLA	C1-O2A-CGA	2.36	122.63	116.44
24	d	404	CLA	O2A-CGA-CBA	2.36	119.30	111.91
26	K	101	BCR	C29-C30-C25	2.36	114.11	110.48
24	B	605	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
31	A	417	PL9	C10-C9-C11	2.35	119.23	115.27
24	B	607	CLA	CMC-C2C-C1C	2.35	128.62	125.04
26	H	101	BCR	C10-C11-C12	-2.35	115.87	123.22
24	d	406	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
26	b	622	BCR	C36-C18-C17	-2.35	119.63	122.92
24	b	621	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
24	c	911	CLA	C4-C3-C2	-2.35	117.65	123.68
25	A	408	PHO	CBD-CHA-C1A	2.35	131.85	126.40
26	y	101	BCR	C38-C26-C25	-2.35	121.89	124.53
26	k	101	BCR	C7-C8-C9	-2.35	122.69	126.23
33	C	519	LMG	O8-C28-C29	2.35	119.27	111.91
26	d	407	BCR	C37-C22-C23	2.34	121.77	118.08
24	D	404	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
24	B	603	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	C	508	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
26	c	915	BCR	C37-C22-C23	2.34	121.77	118.08
27	A	411	SQD	C44-O6-C1	-2.34	109.17	113.74
25	D	401	PHO	C3C-C4C-NC	2.34	113.91	110.28
24	b	613	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
24	C	502	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
37	c	918	DGD	O1G-C1A-O1A	-2.34	117.70	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	902	CLA	C1-O2A-CGA	2.33	122.57	116.44
24	A	409	CLA	CHB-C4A-NA	2.33	127.74	124.51
24	B	616	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
26	B	618	BCR	C16-C17-C18	-2.33	123.98	127.31
24	D	405	CLA	CHD-C4C-NC	2.33	127.88	124.20
29	m	103	LMT	C1B-O5B-C5B	2.33	118.26	113.69
24	b	617	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
24	C	507	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
24	B	611	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
24	B	617	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
26	c	915	BCR	C21-C20-C19	-2.33	115.95	123.22
24	C	501	CLA	C4-C3-C5	2.33	119.19	115.27
24	b	608	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
27	A	411	SQD	O48-C23-O10	-2.33	117.72	123.59
24	b	607	CLA	CMB-C2B-C3B	2.32	129.03	124.68
24	b	613	CLA	CMA-C3A-C2A	-2.32	104.46	113.83
24	B	606	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
24	B	615	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
25	a	407	PHO	C2A-C1A-NA	2.32	114.52	111.86
31	D	407	PL9	C22-C23-C24	-2.32	122.08	127.66
26	D	406	BCR	C10-C11-C12	-2.32	115.99	123.22
24	c	906	CLA	CMC-C2C-C1C	2.32	128.56	125.04
24	C	502	CLA	C4D-C3D-CAD	-2.32	107.18	108.47
27	a	410	SQD	O5-C1-C2	-2.31	105.45	110.35
24	D	405	CLA	CHB-C4A-NA	2.31	127.71	124.51
26	C	514	BCR	C37-C22-C23	2.31	121.72	118.08
24	B	605	CLA	CHD-C4C-NC	2.31	127.85	124.20
33	c	920	LMG	C8-O7-C10	-2.31	112.10	117.79
26	c	927	BCR	C11-C12-C13	-2.31	119.92	126.42
31	A	417	PL9	C42-C43-C44	-2.31	122.10	127.66
24	C	512	CLA	O1D-CGD-CBD	-2.31	119.76	124.48
33	A	419	LMG	O8-C28-C29	2.31	119.15	111.91
37	C	518	DGD	O3G-C3G-C2G	-2.31	105.33	110.90
24	a	408	CLA	CMC-C2C-C1C	2.31	128.55	125.04
24	c	909	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	B	617	CLA	CMB-C2B-C3B	2.30	128.99	124.68
24	C	512	CLA	CHB-C4A-NA	2.30	127.70	124.51
26	d	407	BCR	C33-C5-C6	-2.30	121.94	124.53
24	D	404	CLA	CED-O2D-CGD	2.30	121.14	115.94
26	d	407	BCR	C15-C14-C13	-2.30	124.03	127.31
26	T	102	BCR	C37-C22-C23	2.30	121.70	118.08
26	b	622	BCR	C33-C5-C4	2.30	118.03	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	407	BCR	C39-C30-C25	-2.30	106.57	110.30
37	C	517	DGD	C2G-O2G-C1B	-2.30	112.14	117.79
37	H	102	DGD	C2G-O2G-C1B	-2.29	112.14	117.79
26	T	102	BCR	C3-C4-C5	-2.29	109.98	114.08
24	a	408	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
26	B	618	BCR	C38-C26-C25	-2.29	121.95	124.53
26	h	101	BCR	C16-C15-C14	-2.29	118.78	123.47
24	b	609	CLA	CMB-C2B-C3B	2.29	128.97	124.68
37	c	918	DGD	O2G-C1B-O1B	-2.29	118.16	123.70
24	C	506	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	C	508	CLA	C4-C3-C5	2.29	119.12	115.27
24	b	613	CLA	CHD-C4C-NC	2.29	127.81	124.20
24	B	610	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
24	C	510	CLA	C4-C3-C2	-2.29	117.81	123.68
33	B	622	LMG	O8-C28-O10	-2.29	117.82	123.59
24	C	505	CLA	O2A-CGA-CBA	2.29	119.08	111.91
24	C	507	CLA	C4-C3-C5	2.29	119.11	115.27
36	D	409	LHG	O8-C23-C24	2.28	119.07	111.91
26	b	622	BCR	C16-C17-C18	-2.28	124.05	127.31
24	B	603	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	C	506	CLA	CHD-C4C-NC	2.28	127.80	124.20
37	c	916	DGD	C4D-C3D-C2D	-2.28	106.84	110.82
27	B	621	SQD	C44-O6-C1	-2.28	109.28	113.74
35	b	628	HTG	C1-O5-C5	2.28	116.79	112.58
24	B	615	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
24	C	513	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
26	H	101	BCR	C7-C8-C9	-2.28	122.79	126.23
26	d	407	BCR	C21-C20-C19	-2.28	116.11	123.22
26	C	514	BCR	C23-C24-C25	-2.28	120.80	127.20
26	B	618	BCR	C37-C22-C21	-2.28	119.74	122.92
24	b	614	CLA	CMA-C3A-C4A	-2.27	105.66	111.77
33	J	101	LMG	O8-C28-C29	2.27	119.03	111.91
24	b	617	CLA	OBD-CAD-C3D	-2.27	124.21	127.98
24	C	505	CLA	C1-O2A-CGA	2.27	122.39	116.44
24	B	609	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	D	406	BCR	C39-C30-C25	-2.27	106.62	110.30
24	a	408	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	b	618	CLA	C4-C3-C5	2.26	119.08	115.27
24	b	607	CLA	CMC-C2C-C1C	2.26	128.49	125.04
31	D	407	PL9	C15-C14-C16	2.26	119.08	115.27
24	b	616	CLA	CMC-C2C-C1C	2.26	128.49	125.04
24	b	607	CLA	CBC-CAC-C3C	-2.26	106.19	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C4-C3-C5	2.26	119.08	115.27
24	B	611	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	A	409	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
26	B	618	BCR	C21-C20-C19	-2.26	116.16	123.22
33	Z	101	LMG	C8-O7-C10	-2.26	112.22	117.79
24	A	409	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	C	504	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	c	905	CLA	C4D-C3D-CAD	-2.26	107.21	108.47
26	d	407	BCR	C29-C28-C27	-2.26	106.33	111.38
37	c	916	DGD	O3G-C3G-C2G	-2.26	105.45	110.90
24	B	607	CLA	C11-C10-C8	-2.26	108.63	115.92
38	V	202	HEM	CBD-CAD-C3D	-2.26	108.32	112.48
26	c	927	BCR	C29-C30-C25	2.26	113.95	110.48
26	c	915	BCR	C35-C13-C14	-2.25	119.77	122.92
24	D	404	CLA	CMA-C3A-C4A	-2.25	105.71	111.77
24	b	621	CLA	C4-C3-C5	2.25	119.06	115.27
24	b	617	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
26	d	407	BCR	C38-C26-C27	2.25	117.94	113.62
24	C	507	CLA	C3B-C4B-NB	2.25	112.12	109.21
24	B	617	CLA	C1-O2A-CGA	2.25	122.35	116.44
24	C	505	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	A	405	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
26	B	619	BCR	C32-C1-C6	-2.25	106.65	110.30
24	b	615	CLA	C11-C12-C13	-2.25	108.65	115.92
36	B	635	LHG	C5-O7-C7	-2.25	112.25	117.79
26	c	927	BCR	C35-C13-C14	-2.25	119.77	122.92
24	C	510	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
26	B	619	BCR	C37-C22-C23	2.25	121.62	118.08
33	a	411	LMG	O7-C10-O9	-2.25	118.27	123.70
24	b	614	CLA	CMC-C2C-C1C	2.25	128.46	125.04
24	B	613	CLA	OBD-CAD-C3D	-2.24	124.25	127.98
24	B	614	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
37	C	517	DGD	C3G-O3G-C1D	-2.24	109.36	113.74
24	b	606	CLA	CMB-C2B-C3B	2.24	128.87	124.68
25	D	401	PHO	C2C-C1C-NC	2.24	113.17	109.79
26	k	101	BCR	C10-C11-C12	-2.24	116.22	123.22
33	Y	101	LMG	C8-O7-C10	-2.24	112.28	117.79
24	C	506	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
24	c	913	CLA	CMB-C2B-C3B	2.24	128.87	124.68
24	b	613	CLA	C4-C3-C5	2.24	119.04	115.27
24	c	913	CLA	C1-O2A-CGA	2.24	122.31	116.44
24	c	902	CLA	CMC-C2C-C1C	2.24	128.44	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	407	PHO	C1-O2A-CGA	2.24	122.31	116.44
24	C	501	CLA	O2A-CGA-CBA	2.23	118.92	111.91
24	B	606	CLA	CHC-C1C-C2C	-2.23	120.54	126.72
27	L	102	SQD	O48-C23-O10	-2.23	117.96	123.59
37	C	518	DGD	O6D-C5D-C6D	2.23	111.17	106.67
26	H	101	BCR	C31-C1-C6	-2.23	106.68	110.30
24	C	502	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
33	a	411	LMG	C7-O1-C1	-2.23	109.38	113.74
24	b	617	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	C	502	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	C	502	CLA	OBD-CAD-C3D	-2.23	124.28	127.98
24	c	903	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	a	417	LMT	C1B-O1B-C4'	-2.23	112.45	117.96
24	a	406	CLA	CMA-C3A-C2A	-2.23	104.84	113.83
25	d	403	PHO	CMB-C2B-C1B	2.23	128.49	125.06
24	C	504	CLA	OBD-CAD-C3D	-2.22	124.29	127.98
24	B	615	CLA	CMB-C2B-C3B	2.22	128.84	124.68
26	T	102	BCR	C37-C22-C21	-2.22	119.81	122.92
26	b	623	BCR	C28-C27-C26	-2.22	110.11	114.08
24	C	505	CLA	CMB-C2B-C1B	2.22	131.88	128.46
24	B	612	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	B	611	CLA	CAC-C3C-C4C	2.22	127.69	124.81
24	d	404	CLA	CAA-CBA-CGA	2.21	119.72	113.25
29	C	520	LMT	O5'-C5'-C4'	2.21	114.42	109.75
27	a	402	SQD	O5-C5-C4	2.21	113.71	109.69
38	f	101	HEM	CMA-C3A-C4A	-2.21	125.06	128.46
24	a	405	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
24	c	903	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
24	b	616	CLA	C4-C3-C5	2.21	118.99	115.27
24	b	607	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
26	T	102	BCR	C7-C8-C9	-2.21	122.89	126.23
24	b	610	CLA	O2A-CGA-CBA	2.21	118.84	111.91
25	A	408	PHO	C1-C2-C3	-2.21	122.22	126.04
25	a	407	PHO	CED-O2D-CGD	2.21	120.93	115.94
24	b	609	CLA	CHA-C1A-NA	-2.21	121.34	126.40
25	d	403	PHO	CAC-C3C-C2C	2.21	131.30	127.53
33	C	519	LMG	O6-C5-C4	2.20	113.70	109.69
24	b	619	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
29	A	415	LMT	C1B-O5B-C5B	2.20	118.01	113.69
37	C	517	DGD	O6E-C5E-C6E	2.20	111.91	106.44
24	b	618	CLA	CHA-C1A-NA	-2.20	121.36	126.40
26	t	102	BCR	C7-C6-C5	-2.20	116.13	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	409	LHG	O4-P-O5	2.20	123.12	112.24
29	a	401	LMT	O1B-C1B-C2B	2.20	113.80	108.10
24	c	908	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
24	c	902	CLA	C4-C3-C5	2.20	118.97	115.27
26	B	618	BCR	C11-C10-C9	-2.20	124.17	127.31
24	B	610	CLA	C1-O2A-CGA	2.20	122.21	116.44
24	C	509	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
24	d	405	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
24	B	616	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
25	d	403	PHO	CBD-CHA-C1A	2.19	131.48	126.40
33	Y	101	LMG	O8-C28-O10	-2.19	118.06	123.59
25	D	401	PHO	CHD-C1D-C2D	-2.19	120.22	125.73
33	d	415	LMG	C1-O6-C5	2.19	117.98	113.69
26	T	102	BCR	C2-C1-C6	2.19	113.85	110.48
25	D	401	PHO	C1C-C2C-C3C	-2.19	104.00	106.51
24	C	501	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	D	405	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
26	k	101	BCR	C38-C26-C25	-2.19	122.07	124.53
24	b	613	CLA	C11-C12-C13	-2.19	108.85	115.92
24	c	911	CLA	CMB-C2B-C3B	2.19	128.77	124.68
27	B	621	SQD	C3-C4-C5	2.19	114.14	110.24
24	c	909	CLA	C11-C10-C8	-2.19	108.86	115.92
24	B	602	CLA	CHB-C4A-NA	2.18	127.53	124.51
33	b	625	LMG	O7-C10-O9	-2.18	118.43	123.70
35	C	521	HTG	C4-C3-C2	-2.18	107.01	110.82
36	E	101	LHG	C5-O7-C7	-2.18	112.42	117.79
31	D	407	PL9	C30-C29-C31	2.18	118.94	115.27
24	c	902	CLA	CMB-C2B-C3B	2.18	128.76	124.68
26	B	620	BCR	C36-C18-C19	2.18	121.51	118.08
24	C	501	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	c	906	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
24	b	616	CLA	C4D-C3D-CAD	-2.18	107.26	108.47
25	a	407	PHO	C4-C3-C5	2.18	118.93	115.27
27	B	621	SQD	C1-C2-C3	-2.18	105.46	110.00
24	d	404	CLA	C1-O2A-CGA	2.18	122.15	116.44
24	c	914	CLA	CMB-C2B-C3B	2.18	128.75	124.68
24	C	511	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
24	c	904	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
26	y	101	BCR	C21-C20-C19	-2.17	116.43	123.22
24	b	621	CLA	CMC-C2C-C1C	2.17	128.35	125.04
25	d	403	PHO	C2C-C1C-NC	2.17	113.07	109.79
26	k	101	BCR	C3-C4-C5	-2.17	110.20	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	407	PHO	C1-C2-C3	-2.17	122.28	126.04
24	B	615	CLA	CMC-C2C-C1C	2.17	128.35	125.04
24	B	603	CLA	CMB-C2B-C3B	2.17	128.74	124.68
26	d	407	BCR	C16-C15-C14	-2.17	119.03	123.47
24	D	404	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
24	B	616	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
26	B	620	BCR	C37-C22-C21	-2.17	119.89	122.92
24	C	512	CLA	C11-C12-C13	-2.16	108.93	115.92
24	b	620	CLA	CED-O2D-CGD	2.16	120.83	115.94
33	c	919	LMG	O8-C28-O10	-2.16	118.14	123.59
35	B	632	HTG	C6-C5-C4	-2.16	107.94	113.00
24	b	615	CLA	CMA-C3A-C2A	-2.16	105.12	113.83
24	B	617	CLA	OBD-CAD-C3D	-2.16	124.40	127.98
25	D	401	PHO	CMB-C2B-C1B	2.16	128.39	125.06
24	b	619	CLA	C4-C3-C5	2.16	118.90	115.27
24	C	504	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
31	A	417	PL9	C47-C48-C49	-2.16	120.37	127.75
24	B	614	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
26	c	927	BCR	C37-C22-C21	-2.16	119.90	122.92
33	z	101	LMG	C7-O1-C1	-2.15	109.53	113.74
24	b	620	CLA	CHA-C1A-NA	-2.15	121.47	126.40
26	C	515	BCR	C15-C14-C13	-2.15	124.24	127.31
24	C	507	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
24	b	619	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
37	H	102	DGD	O1G-C1A-O1A	-2.15	118.17	123.59
24	C	509	CLA	OBD-CAD-C3D	-2.15	124.42	127.98
24	b	617	CLA	C11-C10-C8	-2.15	108.98	115.92
29	A	415	LMT	O5'-C5'-C6'	2.15	111.77	106.44
24	C	511	CLA	C4D-C3D-CAD	-2.14	107.27	108.47
24	C	509	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
24	c	907	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	b	620	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
26	T	102	BCR	C7-C6-C5	-2.14	116.27	121.46
24	B	611	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
24	B	611	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
36	L	101	LHG	O7-C7-O9	-2.14	118.53	123.70
24	a	405	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	b	621	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
24	b	612	CLA	O2A-CGA-CBA	2.14	118.61	111.91
26	k	101	BCR	C36-C18-C19	2.14	121.44	118.08
25	a	407	PHO	O2A-CGA-CBA	2.13	118.61	111.91
24	b	618	CLA	CHD-C4C-NC	2.13	127.57	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C16-C17-C18	-2.13	124.27	127.31
24	c	912	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
26	k	101	BCR	C34-C9-C10	-2.13	119.94	122.92
24	b	612	CLA	CMB-C2B-C1B	2.13	131.74	128.46
24	C	508	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	b	619	CLA	C4-C3-C2	-2.13	118.22	123.68
24	b	614	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
24	b	621	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
24	b	611	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
25	d	403	PHO	O2A-CGA-CBA	2.12	118.57	111.91
24	b	617	CLA	CAC-C3C-C2C	2.12	131.16	127.53
26	Y	102	BCR	C15-C16-C17	-2.12	119.13	123.47
31	d	408	PL9	C53-C6-C1	2.12	119.33	114.99
24	C	503	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
24	b	611	CLA	O2A-CGA-CBA	2.12	118.56	111.91
26	D	406	BCR	C38-C26-C27	2.12	117.69	113.62
35	B	624	HTG	C1-C2-C3	2.12	114.77	110.59
24	B	607	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
37	c	917	DGD	O6E-C1E-O5D	-2.12	104.96	109.97
24	C	502	CLA	C4-C3-C5	2.12	118.83	115.27
24	c	905	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	C	505	CLA	C4-C3-C5	2.12	118.83	115.27
26	y	101	BCR	C16-C17-C18	-2.12	124.29	127.31
31	d	408	PL9	C11-C9-C8	-2.12	116.83	121.12
24	a	405	CLA	CAC-C3C-C4C	2.12	127.56	124.81
25	d	403	PHO	C1C-C2C-C3C	-2.12	104.08	106.51
24	D	405	CLA	OBD-CAD-C3D	-2.12	124.47	127.98
24	B	605	CLA	C11-C10-C8	-2.11	109.08	115.92
36	b	635	LHG	O4-P-O5	2.11	122.69	112.24
24	D	404	CLA	C4-C3-C5	2.11	118.83	115.27
24	c	911	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
31	a	415	PL9	C45-C44-C46	2.11	118.83	115.27
25	A	408	PHO	CMB-C2B-C1B	2.11	128.32	125.06
37	D	408	DGD	C4D-C3D-C2D	2.11	114.51	110.82
24	C	501	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
26	H	101	BCR	C21-C20-C19	-2.11	116.63	123.22
24	C	511	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
24	b	615	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
26	T	102	BCR	C36-C18-C19	2.11	121.40	118.08
26	k	101	BCR	C2-C1-C6	2.11	113.72	110.48
24	B	616	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	A	417	PL9	C7-C3-C2	-2.11	120.53	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	415	PL9	C8-C7-C3	2.10	117.92	111.98
24	C	512	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
24	c	913	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
25	a	407	PHO	C16-C15-C13	-2.10	109.14	115.92
26	a	409	BCR	C8-C7-C6	-2.10	121.31	127.20
24	c	902	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
24	c	910	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
26	b	622	BCR	C29-C30-C25	2.09	113.70	110.48
26	Y	102	BCR	C37-C22-C23	2.09	121.37	118.08
24	B	610	CLA	CMB-C2B-C1B	2.09	131.68	128.46
24	B	607	CLA	OBD-CAD-C3D	-2.09	124.51	127.98
24	b	621	CLA	CBC-CAC-C3C	-2.09	106.67	112.43
24	A	407	CLA	CMA-C3A-C4A	-2.09	106.15	111.77
27	A	414	SQD	O6-C44-C45	-2.09	105.86	110.90
26	t	102	BCR	C28-C27-C26	-2.09	110.35	114.08
33	C	519	LMG	C8-O7-C10	-2.09	112.65	117.79
26	K	101	BCR	C31-C1-C6	-2.09	106.91	110.30
31	A	417	PL9	C16-C17-C18	-2.09	105.02	111.88
24	A	407	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	B	612	CLA	O2A-CGA-CBA	2.09	118.46	111.91
24	b	606	CLA	O2A-CGA-CBA	2.09	118.46	111.91
35	b	603	HTG	C6-C5-C4	-2.09	108.12	113.00
24	C	513	CLA	CHB-C4A-NA	2.09	127.40	124.51
24	B	609	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
24	C	511	CLA	C4-C3-C5	2.09	118.78	115.27
24	b	618	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
33	C	519	LMG	O7-C10-O9	-2.08	118.67	123.70
24	c	902	CLA	CHD-C4C-NC	2.08	127.48	124.20
26	b	623	BCR	C7-C8-C9	-2.08	123.09	126.23
24	C	507	CLA	CMB-C2B-C3B	2.08	128.57	124.68
33	c	920	LMG	O8-C28-O10	-2.08	118.34	123.59
24	b	618	CLA	CED-O2D-CGD	2.08	120.64	115.94
37	c	916	DGD	O1G-C1A-C2A	2.08	118.43	111.91
25	d	403	PHO	O2A-CGA-O1A	-2.08	118.35	123.59
29	D	403	LMT	O5B-C5B-C4B	2.08	113.47	109.69
37	c	917	DGD	O6E-C5E-C6E	2.08	111.60	106.44
24	B	611	CLA	CMB-C2B-C3B	2.08	128.56	124.68
26	d	407	BCR	C3-C4-C5	-2.08	110.37	114.08
24	C	509	CLA	C11-C12-C13	-2.08	109.21	115.92
37	e	101	DGD	O2G-C1B-O1B	-2.08	118.68	123.70
37	H	102	DGD	C3G-C2G-C1G	-2.07	106.88	111.79
37	c	917	DGD	O1G-C1A-O1A	-2.07	118.36	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C1-O2A-CGA	2.07	121.89	116.44
37	c	917	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
26	k	101	BCR	C15-C16-C17	-2.07	119.23	123.47
29	F	101	LMT	O5'-C5'-C4'	2.07	114.12	109.75
24	C	501	CLA	C2A-C3A-C4A	-2.07	98.52	101.87
24	c	907	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
24	c	905	CLA	C11-C10-C8	-2.07	109.23	115.92
37	C	516	DGD	O6E-C5E-C4E	2.07	113.45	109.69
24	b	611	CLA	C1-C2-C3	-2.07	122.47	126.04
33	b	625	LMG	O6-C5-C6	2.07	111.58	106.44
24	b	615	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
37	C	516	DGD	O2G-C1B-O1B	-2.07	118.71	123.70
26	k	101	BCR	C39-C30-C25	-2.07	106.95	110.30
24	b	613	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
24	a	405	CLA	CMC-C2C-C1C	2.06	128.18	125.04
31	D	407	PL9	C25-C24-C26	2.06	118.74	115.27
26	H	101	BCR	C15-C14-C13	-2.06	124.37	127.31
29	e	102	LMT	C1B-O5B-C5B	2.06	117.74	113.69
24	b	616	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
24	B	610	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
31	d	408	PL9	C40-C39-C38	-2.06	118.39	123.68
24	b	612	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
24	a	408	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
24	B	608	CLA	CMB-C2B-C3B	2.06	128.53	124.68
26	t	102	BCR	C35-C13-C12	2.06	121.32	118.08
31	A	417	PL9	C35-C34-C36	2.06	118.73	115.27
25	D	401	PHO	O2D-CGD-O1D	-2.06	119.81	123.84
24	B	614	CLA	CHA-C1A-NA	-2.06	121.69	126.40
24	B	613	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
26	K	101	BCR	C36-C18-C19	2.06	121.32	118.08
24	A	407	CLA	CMA-C3A-C2A	-2.06	105.54	113.83
24	C	513	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
33	C	519	LMG	C1-C2-C3	2.05	114.28	110.00
24	C	511	CLA	CMB-C2B-C3B	2.05	128.52	124.68
24	B	605	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
24	B	608	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
24	C	512	CLA	OBD-CAD-C3D	-2.05	124.58	127.98
26	b	622	BCR	C31-C1-C6	-2.05	106.97	110.30
35	B	633	HTG	C1-O5-C5	2.05	116.36	112.58
24	A	406	CLA	C1-C2-C3	-2.05	122.50	126.04
27	A	411	SQD	C1-O5-C5	-2.05	109.67	113.69
24	b	619	CLA	CHB-C4A-NA	2.05	127.34	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	CLA	CHB-C4A-NA	2.05	127.34	124.51
24	b	621	CLA	CMA-C3A-C2A	-2.05	105.58	113.83
26	B	618	BCR	C34-C9-C10	-2.05	120.06	122.92
24	B	606	CLA	C1-O2A-CGA	2.04	121.81	116.44
26	t	102	BCR	C3-C4-C5	-2.04	110.43	114.08
24	B	603	CLA	CAA-CBA-CGA	-2.04	107.28	113.25
24	c	911	CLA	CMC-C2C-C1C	2.04	128.15	125.04
24	A	406	CLA	CAC-C3C-C2C	2.04	131.02	127.53
24	B	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
24	b	620	CLA	C6-C7-C8	-2.04	109.33	115.92
29	C	520	LMT	C1B-O5B-C5B	2.04	117.69	113.69
24	b	606	CLA	CBC-CAC-C3C	-2.04	106.82	112.43
25	d	403	PHO	C4-C3-C2	-2.03	118.46	123.68
24	b	606	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
26	t	102	BCR	C34-C9-C10	-2.03	120.08	122.92
31	D	407	PL9	C17-C18-C19	-2.03	122.77	127.66
26	B	618	BCR	C37-C22-C23	2.03	121.28	118.08
29	D	403	LMT	C1B-O5B-C5B	2.03	117.67	113.69
24	C	505	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	b	620	CLA	C11-C12-C13	-2.03	109.37	115.92
26	K	101	BCR	C15-C14-C13	-2.03	124.42	127.31
36	E	101	LHG	O8-C23-O10	-2.03	118.48	123.59
24	B	617	CLA	CAC-C3C-C4C	2.03	127.44	124.81
24	B	615	CLA	CHC-C1C-NC	2.02	127.28	124.20
24	A	406	CLA	C4-C3-C5	2.02	118.68	115.27
33	c	920	LMG	O7-C10-O9	-2.02	118.81	123.70
33	z	101	LMG	C8-O7-C10	-2.02	112.81	117.79
24	B	610	CLA	C3D-CAD-CBD	2.02	110.27	107.61
26	K	101	BCR	C38-C26-C25	-2.02	122.26	124.53
37	C	518	DGD	O6E-C5E-C6E	2.02	111.47	106.44
36	B	635	LHG	O7-C7-O9	-2.02	118.81	123.70
35	V	203	HTG	O5-C1-C2	-2.02	107.77	110.31
24	B	607	CLA	C7-C6-C5	-2.02	107.87	113.36
26	h	101	BCR	C3-C2-C1	-2.02	107.38	114.60
26	b	623	BCR	C21-C20-C19	-2.02	116.91	123.22
36	d	410	LHG	O7-C7-O9	-2.02	118.82	123.70
31	A	417	PL9	C47-C46-C44	-2.02	106.33	112.98
24	b	611	CLA	O2A-CGA-O1A	-2.02	118.51	123.59
24	B	602	CLA	C4-C3-C5	2.01	118.66	115.27
26	c	915	BCR	C11-C10-C9	-2.01	124.44	127.31
37	c	916	DGD	O1G-C1A-O1A	-2.01	118.51	123.59
24	C	512	CLA	C4D-C3D-CAD	-2.01	107.35	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
24	c	905	CLA	O2A-CGA-CBA	2.01	118.22	111.91
26	k	101	BCR	C29-C30-C25	2.01	113.58	110.48
24	c	902	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
29	m	103	LMT	C1'-O5'-C5'	2.01	117.64	113.69
29	m	102	LMT	C1B-O5B-C5B	2.01	117.64	113.69
31	a	415	PL9	C35-C34-C33	-2.01	118.52	123.68
24	c	907	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
24	B	611	CLA	CHC-C1C-NC	2.01	127.25	124.20
29	M	103	LMT	C1B-O5B-C5B	2.01	117.63	113.69
24	C	507	CLA	CAC-C3C-C4C	2.01	127.41	124.81
36	d	411	LHG	O8-C23-O10	-2.01	118.53	123.59
24	c	906	CLA	C1-O2A-CGA	2.01	121.71	116.44
26	A	410	BCR	C7-C8-C9	-2.01	123.20	126.23
26	B	620	BCR	C16-C15-C14	-2.01	119.36	123.47
24	c	906	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
24	A	405	CLA	C7-C6-C5	-2.01	107.91	113.36
26	A	410	BCR	C3-C4-C5	-2.01	110.50	114.08
24	c	910	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	A	409	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
24	A	409	CLA	CED-O2D-CGD	2.00	120.47	115.94
26	Y	102	BCR	C35-C13-C12	2.00	121.23	118.08
29	b	602	LMT	C6'-C5'-C4'	-2.00	107.50	113.33
24	c	911	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
26	K	101	BCR	C3-C4-C5	-2.00	110.50	114.08
26	y	101	BCR	C32-C1-C6	-2.00	107.05	110.30

All (192) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	607	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	607	CLA	ND
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	d	406	CLA	NC
24	d	406	CLA	ND
24	d	406	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	a	405	CLA	NC
24	a	405	CLA	ND
24	a	405	CLA	NA
24	A	409	CLA	NC
24	A	409	CLA	ND
24	A	409	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	615	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	NA
24	c	913	CLA	NC
24	c	913	CLA	ND
24	c	913	CLA	NA
24	c	904	CLA	NC
24	c	904	CLA	ND
24	c	904	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	b	611	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	620	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	ND
24	c	910	CLA	NC

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Mol	Chain	Res	Type	Atom
24	c	910	CLA	ND
24	c	910	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	D	405	CLA	NC
24	D	405	CLA	ND
24	D	405	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	b	619	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	d	404	CLA	NC
24	d	404	CLA	ND
24	d	404	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	d	405	CLA	ND
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	C	501	CLA	NC
24	C	501	CLA	ND
24	C	501	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	c	907	CLA	NC
24	c	907	CLA	ND
24	c	907	CLA	NA
24	c	912	CLA	NC
24	c	912	CLA	ND
24	c	912	CLA	NA
24	C	505	CLA	ND
24	c	908	CLA	NC
24	c	908	CLA	ND
24	c	908	CLA	NA
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	a	408	CLA	NC
24	a	408	CLA	ND
24	a	408	CLA	NA
24	c	914	CLA	NC
24	c	914	CLA	NA
24	c	902	CLA	NC
24	c	902	CLA	ND
24	c	902	CLA	NA
24	c	905	CLA	NC
24	c	905	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	905	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	a	406	CLA	NC
24	a	406	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	b	621	CLA	NA
24	b	621	CLA	NC
24	b	621	CLA	ND
24	D	404	CLA	ND
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	A	407	CLA	NC
24	A	407	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	618	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	b	612	CLA	NA
24	c	911	CLA	NC
24	c	911	CLA	ND
24	c	911	CLA	NA
24	c	906	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	906	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	c	909	CLA	NC
24	c	909	CLA	ND
24	c	909	CLA	NA
24	c	903	CLA	NC
24	c	903	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA

All (1314) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	V	204	GOL	C1-C2-C3-O3
27	A	414	SQD	O6-C44-C45-O47
27	A	414	SQD	O5-C5-C6-S
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
36	E	101	LHG	C4-O6-P-O5
35	B	625	HTG	O5-C1-S1-C1'
29	C	520	LMT	C2'-C1'-O1'-C1
29	C	520	LMT	O5'-C1'-O1'-C1
24	b	610	CLA	C2-C3-C5-C6
24	b	610	CLA	C4-C3-C5-C6
28	D	402	GOL	C1-C2-C3-O3
28	D	402	GOL	O2-C2-C3-O3
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	C11-C10-C8-C9
28	v	205	GOL	O1-C1-C2-C3
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	O9-C10-O7-C8
33	z	101	LMG	C11-C10-O7-C8
26	Y	102	BCR	C1-C6-C7-C8
26	Y	102	BCR	C5-C6-C7-C8
29	a	401	LMT	C2'-C1'-O1'-C1
29	a	401	LMT	O5'-C1'-O1'-C1
36	a	418	LHG	C3-O3-P-O5
36	a	418	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
36	a	418	LHG	C4-O6-P-O3
36	a	418	LHG	C4-O6-P-O5
36	a	418	LHG	O10-C23-O8-C6
36	a	418	LHG	C24-C23-O8-C6
24	b	611	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	c	910	CLA	C2-C1-O2A-CGA
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C7-C8-C9-C34
26	D	406	BCR	C21-C22-C23-C24
26	D	406	BCR	C37-C22-C23-C24
28	b	633	GOL	O1-C1-C2-C3
26	d	407	BCR	C21-C22-C23-C24
26	d	407	BCR	C37-C22-C23-C24
27	a	402	SQD	O6-C44-C45-O47
27	a	402	SQD	O5-C5-C6-S
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
28	V	206	GOL	C1-C2-C3-O3
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
27	F	103	SQD	C5-C6-S-O8
27	F	103	SQD	C5-C6-S-O9
28	B	627	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-C3
24	b	619	CLA	CHA-CBD-CGD-O1D
24	b	619	CLA	CHA-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O1D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	C2-C3-C5-C6
24	b	619	CLA	C4-C3-C5-C6
37	e	101	DGD	C2B-C1B-O2G-C2G
37	e	101	DGD	O1B-C1B-O2G-C2G
37	e	101	DGD	C2D-C1D-O3G-C3G
37	e	101	DGD	O6D-C1D-O3G-C3G
37	e	101	DGD	O6E-C1E-O5D-C6D
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C2-C1-O2A-CGA
28	v	203	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
29	t	101	LMT	C2'-C1'-O1'-C1
29	t	101	LMT	O5'-C1'-O1'-C1
35	B	624	HTG	C2'-C1'-S1-C1
29	a	417	LMT	C2'-C1'-O1'-C1
29	a	417	LMT	O5'-C1'-O1'-C1
24	C	507	CLA	CHA-CBD-CGD-O2D
37	D	408	DGD	C2B-C1B-O2G-C2G
37	D	408	DGD	O1B-C1B-O2G-C2G
37	D	408	DGD	C2D-C1D-O3G-C3G
37	D	408	DGD	O6D-C1D-O3G-C3G
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
28	C	523	GOL	O1-C1-C2-C3
28	v	204	GOL	O1-C1-C2-C3
35	c	921	HTG	C2'-C1'-S1-C1
28	V	201	GOL	O1-C1-C2-C3
36	d	410	LHG	C3-O3-P-O4
33	C	519	LMG	C11-C10-O7-C8
28	c	924	GOL	O1-C1-C2-C3
28	A	413	GOL	C1-C2-C3-O3
29	F	101	LMT	C2'-C1'-O1'-C1
29	F	101	LMT	O5'-C1'-O1'-C1
31	a	415	PL9	C9-C11-C12-C13
31	a	415	PL9	C23-C24-C26-C27
31	a	415	PL9	C25-C24-C26-C27
28	b	632	GOL	O1-C1-C2-C3
28	T	103	GOL	O1-C1-C2-C3
36	L	101	LHG	C4-O6-P-O4
36	L	101	LHG	C4-O6-P-O5
28	B	628	GOL	O1-C1-C2-C3
28	V	207	GOL	C1-C2-C3-O3
28	a	412	GOL	C1-C2-C3-O3
28	a	412	GOL	O2-C2-C3-O3
29	M	103	LMT	O5'-C1'-O1'-C1
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	e	102	LMT	C2'-C1'-O1'-C1
29	e	102	LMT	O5'-C1'-O1'-C1
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C21-C22-C23-C24
26	y	101	BCR	C37-C22-C23-C24
28	B	630	GOL	C1-C2-C3-O3
28	B	630	GOL	O2-C2-C3-O3
33	Z	101	LMG	O6-C1-O1-C7
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
29	b	626	LMT	C2'-C1'-O1'-C1
29	b	626	LMT	O5'-C1'-O1'-C1
28	a	419	GOL	O1-C1-C2-C3
36	b	635	LHG	C4-O6-P-O4
36	b	635	LHG	C4-O6-P-O5
36	D	409	LHG	C3-O3-P-O6
36	D	409	LHG	C4-O6-P-O4
36	D	410	LHG	C4-O6-P-O4
29	A	415	LMT	C2'-C1'-O1'-C1
29	A	415	LMT	O5'-C1'-O1'-C1
29	b	602	LMT	C2'-C1'-O1'-C1
29	b	602	LMT	O5'-C1'-O1'-C1
24	c	909	CLA	CHA-CBD-CGD-O1D
24	c	909	CLA	CHA-CBD-CGD-O2D
29	D	403	LMT	C3'-C4'-O1B-C1B
29	C	520	LMT	C3'-C4'-O1B-C1B
24	C	509	CLA	CBD-CGD-O2D-CED
36	E	101	LHG	O10-C23-O8-C6
33	C	519	LMG	O9-C10-O7-C8
24	B	602	CLA	C3-C5-C6-C7
24	b	619	CLA	C3-C5-C6-C7
36	E	101	LHG	C24-C23-O8-C6
27	L	102	SQD	C8-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
37	e	101	DGD	O6E-C5E-C6E-O5E
24	A	409	CLA	C3-C5-C6-C7
24	c	907	CLA	C3-C5-C6-C7
36	D	410	LHG	C24-C23-O8-C6
35	b	628	HTG	S1-C1'-C2'-C3'
26	T	102	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
37	h	102	DGD	O6E-C5E-C6E-O5E
29	m	102	LMT	O5'-C5'-C6'-O6'
29	M	103	LMT	O5'-C5'-C6'-O6'
24	d	406	CLA	CBD-CGD-O2D-CED
24	c	912	CLA	CBD-CGD-O2D-CED
36	d	410	LHG	O2-C2-C3-O3
24	B	615	CLA	C3-C5-C6-C7
36	D	410	LHG	O10-C23-O8-C6
35	B	625	HTG	O5-C5-C6-O6
33	z	101	LMG	O6-C5-C6-O5
33	C	519	LMG	O6-C5-C6-O5
33	a	411	LMG	C17-C18-C19-C20
24	C	512	CLA	CBD-CGD-O2D-CED
29	m	102	LMT	C4'-C5'-C6'-O6'
29	M	101	LMT	O5B-C5B-C6B-O6B
31	A	417	PL9	C25-C24-C26-C27
31	a	415	PL9	C15-C14-C16-C17
31	a	415	PL9	C20-C19-C21-C22
31	a	415	PL9	C30-C29-C31-C32
31	A	417	PL9	C23-C24-C26-C27
31	a	415	PL9	C13-C14-C16-C17
31	a	415	PL9	C18-C19-C21-C22
24	B	607	CLA	C2A-CAA-CBA-CGA
31	A	417	PL9	C44-C46-C47-C48
31	d	408	PL9	C39-C41-C42-C43
31	D	407	PL9	C39-C41-C42-C43
29	M	103	LMT	C4'-C5'-C6'-O6'
29	e	102	LMT	C4'-C5'-C6'-O6'
36	E	101	LHG	C1-C2-C3-O3
33	z	101	LMG	C4-C5-C6-O5
24	C	509	CLA	O1A-CGA-O2A-C1
24	c	910	CLA	CBA-CGA-O2A-C1
37	e	101	DGD	C2A-C1A-O1G-C1G
24	C	509	CLA	CBA-CGA-O2A-C1
24	a	408	CLA	CBA-CGA-O2A-C1
37	h	102	DGD	C4E-C5E-C6E-O5E
33	d	415	LMG	C19-C20-C21-C22
24	B	614	CLA	C13-C15-C16-C17
37	e	101	DGD	C4E-C5E-C6E-O5E
27	a	402	SQD	C18-C19-C20-C21
24	C	506	CLA	C5-C6-C7-C8
37	e	101	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C2-C1-O1-C7
24	B	602	CLA	C14-C13-C15-C16
24	c	910	CLA	C11-C10-C8-C9
24	B	617	CLA	C6-C7-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	c	907	CLA	C6-C7-C8-C9
24	B	615	CLA	C10-C11-C12-C13
26	Y	102	BCR	C37-C22-C23-C24
26	c	915	BCR	C7-C8-C9-C34
24	A	407	CLA	C13-C15-C16-C17
24	B	617	CLA	C3-C5-C6-C7
24	c	913	CLA	C15-C16-C17-C18
24	C	508	CLA	C10-C11-C12-C13
24	B	616	CLA	C8-C10-C11-C12
29	C	520	LMT	O5B-C5B-C6B-O6B
33	J	101	LMG	O6-C5-C6-O5
37	c	918	DGD	C1A-C2A-C3A-C4A
35	b	628	HTG	C1'-C2'-C3'-C4'
24	A	409	CLA	C10-C11-C12-C13
24	B	617	CLA	C10-C11-C12-C13
24	C	509	CLA	C13-C15-C16-C17
24	b	606	CLA	C8-C10-C11-C12
28	B	626	GOL	O2-C2-C3-O3
28	c	924	GOL	O1-C1-C2-O2
28	a	419	GOL	O1-C1-C2-O2
27	A	414	SQD	C23-C24-C25-C26
33	C	519	LMG	C10-C11-C12-C13
33	Z	101	LMG	C10-C11-C12-C13
24	d	406	CLA	C15-C16-C17-C18
24	b	611	CLA	C10-C11-C12-C13
24	b	619	CLA	C5-C6-C7-C8
24	c	909	CLA	C15-C16-C17-C18
24	c	910	CLA	C3-C5-C6-C7
29	m	103	LMT	O5'-C5'-C6'-O6'
35	C	522	HTG	O5-C5-C6-O6
24	b	611	CLA	C15-C16-C17-C18
24	b	620	CLA	C10-C11-C12-C13
37	c	917	DGD	C3B-C4B-C5B-C6B
24	C	501	CLA	C15-C16-C17-C18
24	C	509	CLA	O1D-CGD-O2D-CED
24	B	614	CLA	C11-C10-C8-C7
24	b	611	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	505	CLA	C11-C12-C13-C15
24	b	621	CLA	C11-C12-C13-C15
37	e	101	DGD	O1A-C1A-O1G-C1G
24	a	408	CLA	O1A-CGA-O2A-C1
37	H	102	DGD	C3B-C4B-C5B-C6B
26	t	102	BCR	C13-C14-C15-C16
24	B	614	CLA	C8-C10-C11-C12
24	B	615	CLA	C8-C10-C11-C12
24	C	506	CLA	C13-C15-C16-C17
35	B	624	HTG	C1'-C2'-C3'-C4'
29	M	101	LMT	C4B-C5B-C6B-O6B
27	L	102	SQD	C31-C32-C33-C34
29	D	403	LMT	O1'-C1-C2-C3
24	c	910	CLA	O1A-CGA-O2A-C1
33	a	411	LMG	C10-C11-C12-C13
24	B	614	CLA	C15-C16-C17-C18
24	B	602	CLA	C10-C11-C12-C13
24	c	910	CLA	C15-C16-C17-C18
24	b	606	CLA	C10-C11-C12-C13
35	B	625	HTG	C4-C5-C6-O6
24	A	409	CLA	C13-C15-C16-C17
24	a	406	CLA	CBD-CGD-O2D-CED
33	c	919	LMG	C11-C10-O7-C8
33	d	415	LMG	C36-C37-C38-C39
24	a	408	CLA	C15-C16-C17-C18
36	E	101	LHG	C3-O3-P-O6
36	d	410	LHG	C3-O3-P-O6
36	L	101	LHG	C4-O6-P-O3
36	b	635	LHG	C4-O6-P-O3
33	C	519	LMG	C28-C29-C30-C31
24	D	405	CLA	C3-C5-C6-C7
24	A	409	CLA	CBA-CGA-O2A-C1
35	b	601	HTG	C1'-C2'-C3'-C4'
35	c	921	HTG	C1'-C2'-C3'-C4'
24	c	910	CLA	C13-C15-C16-C17
24	b	619	CLA	C13-C15-C16-C17
24	B	615	CLA	C4-C3-C5-C6
31	a	415	PL9	C12-C11-C9-C10
24	b	608	CLA	C5-C6-C7-C8
24	b	611	CLA	C2A-CAA-CBA-CGA
24	b	620	CLA	C16-C17-C18-C20
29	e	102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
24	b	609	CLA	C13-C15-C16-C17
36	a	418	LHG	C11-C12-C13-C14
27	A	411	SQD	C12-C13-C14-C15
33	A	419	LMG	C11-C10-O7-C8
24	B	605	CLA	C3-C5-C6-C7
37	e	101	DGD	C8B-C9B-CAB-CBB
37	D	408	DGD	C7A-C8A-C9A-CAA
37	C	516	DGD	C6A-C7A-C8A-C9A
33	a	411	LMG	C30-C31-C32-C33
29	b	602	LMT	C11-C10-C9-C8
33	d	415	LMG	C35-C36-C37-C38
27	a	402	SQD	C25-C26-C27-C28
33	A	419	LMG	O9-C10-O7-C8
33	c	919	LMG	O9-C10-O7-C8
24	C	513	CLA	CBD-CGD-O2D-CED
36	E	101	LHG	C24-C25-C26-C27
27	F	103	SQD	C26-C27-C28-C29
29	t	101	LMT	C3-C4-C5-C6
29	t	101	LMT	C7-C8-C9-C10
33	Y	101	LMG	C11-C12-C13-C14
27	L	102	SQD	C28-C29-C30-C31
27	F	103	SQD	C31-C32-C33-C34
36	E	101	LHG	O2-C2-C3-O3
37	C	517	DGD	C9A-CAA-CBA-CCA
37	C	517	DGD	CBB-CCB-CDB-CEB
24	C	509	CLA	C3-C5-C6-C7
24	a	408	CLA	C3-C5-C6-C7
27	B	621	SQD	C7-C8-C9-C10
37	c	917	DGD	C2E-C1E-O5D-C6D
37	C	517	DGD	C2E-C1E-O5D-C6D
33	B	622	LMG	C35-C36-C37-C38
37	c	918	DGD	C7A-C8A-C9A-CAA
37	c	916	DGD	C9A-CAA-CBA-CCA
24	A	409	CLA	O1A-CGA-O2A-C1
31	D	407	PL9	C45-C44-C46-C47
37	c	917	DGD	C9B-CAB-CBB-CCB
27	A	411	SQD	C9-C10-C11-C12
36	d	411	LHG	C29-C30-C31-C32
37	H	102	DGD	CBB-CCB-CDB-CEB
24	b	615	CLA	C11-C12-C13-C14
24	c	914	CLA	C11-C10-C8-C9
24	a	406	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C6-C7-C8-C9
24	c	909	CLA	C11-C10-C8-C9
24	a	405	CLA	C2C-C3C-CAC-CBC
27	a	410	SQD	C15-C16-C17-C18
33	C	519	LMG	C14-C15-C16-C17
37	H	102	DGD	C7A-C8A-C9A-CAA
33	c	919	LMG	C32-C33-C34-C35
24	C	504	CLA	C15-C16-C17-C18
29	b	626	LMT	C3'-C4'-O1B-C1B
33	B	622	LMG	C29-C30-C31-C32
36	a	418	LHG	C24-C25-C26-C27
37	c	918	DGD	C6A-C7A-C8A-C9A
36	b	635	LHG	C10-C11-C12-C13
28	B	626	GOL	C1-C2-C3-O3
28	b	631	GOL	O1-C1-C2-C3
28	b	631	GOL	C1-C2-C3-O3
36	B	635	LHG	O1-C1-C2-C3
36	d	411	LHG	O1-C1-C2-C3
28	B	629	GOL	O1-C1-C2-C3
28	B	631	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	a	413	GOL	O1-C1-C2-C3
28	B	636	GOL	O1-C1-C2-C3
24	c	912	CLA	O1D-CGD-O2D-CED
24	a	406	CLA	C10-C11-C12-C13
27	a	410	SQD	C30-C31-C32-C33
33	A	419	LMG	C11-C12-C13-C14
33	A	419	LMG	C13-C14-C15-C16
27	B	621	SQD	C34-C35-C36-C37
36	D	409	LHG	C32-C33-C34-C35
27	L	102	SQD	C12-C13-C14-C15
27	a	410	SQD	C11-C12-C13-C14
37	D	408	DGD	C2A-C3A-C4A-C5A
33	J	101	LMG	C19-C20-C21-C22
33	A	419	LMG	C14-C15-C16-C17
33	c	919	LMG	C36-C37-C38-C39
24	a	408	CLA	C16-C17-C18-C19
24	a	408	CLA	C16-C17-C18-C20
37	C	517	DGD	O6E-C1E-O5D-C6D
31	D	407	PL9	C9-C11-C12-C13
27	A	411	SQD	C13-C14-C15-C16
36	b	635	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
36	D	409	LHG	C13-C14-C15-C16
36	D	410	LHG	C29-C30-C31-C32
27	A	411	SQD	C15-C16-C17-C18
36	d	409	LHG	C16-C17-C18-C19
37	D	408	DGD	C8B-C9B-CAB-CBB
37	C	516	DGD	C4B-C5B-C6B-C7B
33	c	919	LMG	C39-C40-C41-C42
36	B	635	LHG	C23-C24-C25-C26
27	F	103	SQD	C34-C35-C36-C37
36	B	635	LHG	C24-C25-C26-C27
37	C	516	DGD	C7B-C8B-C9B-CAB
33	b	625	LMG	C30-C31-C32-C33
29	C	520	LMT	O5'-C5'-C6'-O6'
29	M	103	LMT	C2-C1-O1'-C1'
37	c	917	DGD	C9A-CAA-CBA-CCA
29	a	401	LMT	C7-C8-C9-C10
37	c	918	DGD	C6B-C7B-C8B-C9B
35	b	601	HTG	C3'-C4'-C5'-C6'
36	B	635	LHG	C28-C29-C30-C31
37	C	517	DGD	C4B-C5B-C6B-C7B
37	e	101	DGD	O6D-C5D-C6D-O5D
37	C	516	DGD	O6D-C5D-C6D-O5D
37	c	916	DGD	O6D-C5D-C6D-O5D
24	d	406	CLA	O1D-CGD-O2D-CED
25	a	407	PHO	C4-C3-C5-C6
25	a	407	PHO	C2-C3-C5-C6
24	B	615	CLA	C2-C3-C5-C6
31	a	415	PL9	C28-C29-C31-C32
31	D	407	PL9	C43-C44-C46-C47
36	L	101	LHG	C14-C15-C16-C17
29	b	602	LMT	C3-C4-C5-C6
28	V	204	GOL	O2-C2-C3-O3
28	v	205	GOL	O1-C1-C2-O2
28	b	633	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
28	V	201	GOL	O1-C1-C2-O2
28	A	413	GOL	O2-C2-C3-O3
28	b	632	GOL	O1-C1-C2-O2
28	T	103	GOL	O1-C1-C2-O2
28	B	628	GOL	O1-C1-C2-O2
28	V	207	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
28	B	630	GOL	O1-C1-C2-O2
37	C	517	DGD	CAB-CBB-CCB-CDB
33	c	919	LMG	C10-C11-C12-C13
36	d	410	LHG	C11-C10-C9-C8
36	d	409	LHG	O2-C2-C3-O3
24	d	404	CLA	C2C-C3C-CAC-CBC
33	J	101	LMG	C34-C35-C36-C37
33	B	622	LMG	C30-C31-C32-C33
36	d	409	LHG	C25-C26-C27-C28
29	b	602	LMT	C4-C5-C6-C7
24	B	617	CLA	C2-C1-O2A-CGA
36	b	635	LHG	C11-C12-C13-C14
37	c	916	DGD	C4D-C5D-C6D-O5D
33	z	101	LMG	C13-C14-C15-C16
27	F	103	SQD	C30-C31-C32-C33
37	e	101	DGD	C2A-C3A-C4A-C5A
33	A	419	LMG	C36-C37-C38-C39
26	t	102	BCR	C1-C6-C7-C8
26	t	102	BCR	C5-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
36	d	409	LHG	C32-C33-C34-C35
24	A	405	CLA	C13-C15-C16-C17
37	c	918	DGD	C5B-C6B-C7B-C8B
37	e	101	DGD	C2B-C3B-C4B-C5B
37	C	516	DGD	C1B-C2B-C3B-C4B
24	B	615	CLA	C5-C6-C7-C8
29	a	401	LMT	C2-C3-C4-C5
36	L	101	LHG	C10-C11-C12-C13
24	C	510	CLA	C4-C3-C5-C6
24	C	510	CLA	C2-C3-C5-C6
24	C	510	CLA	C6-C7-C8-C10
24	b	608	CLA	C6-C7-C8-C10
24	c	910	CLA	C6-C7-C8-C10
24	B	617	CLA	C6-C7-C8-C10
24	c	914	CLA	C11-C10-C8-C7
24	a	406	CLA	C6-C7-C8-C10
24	a	406	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C15
24	B	604	CLA	C6-C7-C8-C10
24	c	911	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	c	909	CLA	C11-C10-C8-C7
33	C	519	LMG	C13-C14-C15-C16
24	B	615	CLA	CBA-CGA-O2A-C1
33	A	419	LMG	C29-C28-O8-C9
27	a	402	SQD	C28-C29-C30-C31
36	E	101	LHG	C7-C8-C9-C10
24	C	512	CLA	O1D-CGD-O2D-CED
24	b	611	CLA	C8-C10-C11-C12
24	b	611	CLA	C13-C15-C16-C17
24	a	408	CLA	C10-C11-C12-C13
33	z	101	LMG	C12-C13-C14-C15
25	D	401	PHO	C2C-C3C-CAC-CBC
27	B	621	SQD	C31-C32-C33-C34
36	d	410	LHG	C32-C33-C34-C35
37	c	917	DGD	O6E-C1E-O5D-C6D
24	c	904	CLA	C8-C10-C11-C12
24	B	616	CLA	C5-C6-C7-C8
37	D	408	DGD	C6A-C7A-C8A-C9A
29	M	103	LMT	C11-C10-C9-C8
33	A	419	LMG	C10-C11-C12-C13
29	M	103	LMT	C2-C3-C4-C5
33	Z	101	LMG	O1-C7-C8-O7
36	D	410	LHG	O7-C5-C6-O8
29	t	101	LMT	C2-C3-C4-C5
37	C	517	DGD	C8B-C9B-CAB-CBB
24	b	620	CLA	C16-C17-C18-C19
37	D	408	DGD	C3B-C4B-C5B-C6B
29	e	102	LMT	C2-C3-C4-C5
37	c	916	DGD	O6E-C5E-C6E-O5E
24	c	911	CLA	C4-C3-C5-C6
37	H	102	DGD	C4E-C5E-C6E-O5E
24	B	610	CLA	C2-C3-C5-C6
31	A	417	PL9	C4-C3-C7-C8
31	a	415	PL9	C4-C3-C7-C8
24	B	614	CLA	C11-C10-C8-C9
24	C	510	CLA	C6-C7-C8-C9
24	b	608	CLA	C6-C7-C8-C9
24	c	910	CLA	C6-C7-C8-C9
24	b	619	CLA	C11-C12-C13-C14
24	B	615	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	a	406	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	a	406	CLA	C11-C12-C13-C14
24	b	621	CLA	C11-C12-C13-C14
29	M	103	LMT	O5B-C5B-C6B-O6B
27	A	414	SQD	C30-C31-C32-C33
37	c	916	DGD	CAB-CBB-CCB-CDB
24	c	914	CLA	C10-C11-C12-C13
27	A	414	SQD	C24-C25-C26-C27
37	c	918	DGD	C2A-C3A-C4A-C5A
24	B	615	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	C1A-C2A-CAA-CBA
24	c	909	CLA	C1A-C2A-CAA-CBA
24	B	611	CLA	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C20
37	c	917	DGD	C4A-C5A-C6A-C7A
24	c	905	CLA	C15-C16-C17-C18
36	D	410	LHG	C4-O6-P-O3
36	B	635	LHG	C26-C27-C28-C29
24	c	914	CLA	C3-C5-C6-C7
27	a	410	SQD	C34-C35-C36-C37
33	Y	101	LMG	C12-C13-C14-C15
33	d	415	LMG	C16-C17-C18-C19
29	b	602	LMT	C7-C8-C9-C10
29	C	520	LMT	O1'-C1-C2-C3
37	h	102	DGD	C5B-C6B-C7B-C8B
24	B	616	CLA	C15-C16-C17-C18
35	C	522	HTG	S1-C1'-C2'-C3'
24	C	510	CLA	CBA-CGA-O2A-C1
36	d	409	LHG	C1-C2-C3-O3
29	D	403	LMT	O5B-C5B-C6B-O6B
36	d	410	LHG	C1-C2-C3-O3
31	D	407	PL9	C15-C14-C16-C17
31	D	407	PL9	C13-C14-C16-C17
27	L	102	SQD	C27-C28-C29-C30
33	a	411	LMG	C14-C15-C16-C17
33	d	415	LMG	C14-C15-C16-C17
37	c	917	DGD	C5B-C6B-C7B-C8B
36	B	635	LHG	C34-C35-C36-C37
36	d	409	LHG	O10-C23-O8-C6
27	B	621	SQD	C11-C10-C9-C8
37	c	917	DGD	C2B-C3B-C4B-C5B
27	a	402	SQD	O6-C44-C45-C46
27	L	102	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
27	F	103	SQD	C44-C45-C46-O48
37	D	408	DGD	O1G-C1G-C2G-C3G
37	c	916	DGD	C2A-C3A-C4A-C5A
27	B	621	SQD	C44-C45-C46-O48
36	D	410	LHG	C4-C5-C6-O8
24	C	509	CLA	C5-C6-C7-C8
35	b	601	HTG	C2'-C3'-C4'-C5'
24	C	510	CLA	O1A-CGA-O2A-C1
33	A	419	LMG	O10-C28-O8-C9
37	c	917	DGD	C2G-C3G-O3G-C1D
37	c	917	DGD	C5D-C6D-O5D-C1E
33	C	519	LMG	C8-C7-O1-C1
33	A	419	LMG	C39-C40-C41-C42
33	Y	101	LMG	C31-C32-C33-C34
35	b	628	HTG	O5-C5-C6-O6
27	A	411	SQD	C7-C8-C9-C10
24	C	508	CLA	C5-C6-C7-C8
31	A	417	PL9	C19-C21-C22-C23
31	a	415	PL9	C14-C16-C17-C18
33	z	101	LMG	C16-C17-C18-C19
37	C	516	DGD	O6E-C5E-C6E-O5E
28	C	523	GOL	O1-C1-C2-O2
33	C	519	LMG	C4-C5-C6-O5
37	e	101	DGD	C9B-CAB-CBB-CCB
24	D	405	CLA	C8-C10-C11-C12
33	d	415	LMG	O6-C5-C6-O5
33	Z	101	LMG	O6-C5-C6-O5
27	B	621	SQD	C30-C31-C32-C33
37	C	517	DGD	C4A-C5A-C6A-C7A
36	d	409	LHG	C24-C23-O8-C6
24	C	511	CLA	CBA-CGA-O2A-C1
29	A	415	LMT	O5B-C5B-C6B-O6B
27	a	410	SQD	C9-C10-C11-C12
35	B	624	HTG	C4'-C5'-C6'-C7'
37	c	916	DGD	C8B-C9B-CAB-CBB
33	b	625	LMG	C40-C41-C42-C43
24	C	501	CLA	CBD-CGD-O2D-CED
36	D	410	LHG	C27-C28-C29-C30
24	a	408	CLA	C8-C10-C11-C12
24	b	606	CLA	C2-C1-O2A-CGA
24	C	513	CLA	C2-C1-O2A-CGA
37	e	101	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
37	c	917	DGD	C2A-C3A-C4A-C5A
29	A	415	LMT	O1'-C1-C2-C3
37	H	102	DGD	O6E-C5E-C6E-O5E
24	C	511	CLA	O1A-CGA-O2A-C1
36	d	409	LHG	C29-C30-C31-C32
29	M	103	LMT	C2'-C1'-O1'-C1
27	f	102	SQD	O6-C44-C45-O47
36	d	411	LHG	C31-C32-C33-C34
24	B	613	CLA	C8-C10-C11-C12
31	A	417	PL9	C45-C44-C46-C47
24	A	409	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C10-C8-C7
24	B	602	CLA	C12-C13-C15-C16
24	b	611	CLA	C11-C10-C8-C7
24	b	619	CLA	C11-C12-C13-C15
24	d	405	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	c	907	CLA	C6-C7-C8-C10
24	c	903	CLA	C11-C12-C13-C15
33	B	622	LMG	C38-C39-C40-C41
24	B	614	CLA	C11-C12-C13-C14
24	A	409	CLA	C6-C7-C8-C9
24	b	611	CLA	C11-C10-C8-C9
24	c	910	CLA	C14-C13-C15-C16
24	b	619	CLA	C11-C10-C8-C9
24	C	504	CLA	C11-C12-C13-C14
33	J	101	LMG	C13-C14-C15-C16
33	A	419	LMG	C32-C33-C34-C35
33	a	411	LMG	C12-C13-C14-C15
36	d	411	LHG	C24-C23-O8-C6
27	B	621	SQD	C24-C23-O48-C46
33	d	415	LMG	C17-C18-C19-C20
27	L	102	SQD	C32-C33-C34-C35
27	f	102	SQD	C25-C26-C27-C28
37	C	516	DGD	C4D-C5D-C6D-O5D
36	d	409	LHG	O1-C1-C2-C3
26	Y	102	BCR	C21-C22-C23-C24
29	D	403	LMT	C2-C3-C4-C5
37	C	517	DGD	C5A-C6A-C7A-C8A
24	A	409	CLA	C15-C16-C17-C18
27	L	102	SQD	C24-C23-O48-C46
24	c	907	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
36	d	409	LHG	C30-C31-C32-C33
29	m	103	LMT	O5'-C1'-O1'-C1
24	A	409	CLA	C8-C10-C11-C12
36	b	635	LHG	O6-C4-C5-C6
29	m	102	LMT	C5-C6-C7-C8
27	B	621	SQD	C16-C17-C18-C19
27	L	102	SQD	C7-C8-C9-C10
37	D	408	DGD	C1B-C2B-C3B-C4B
33	c	920	LMG	C10-C11-C12-C13
33	A	419	LMG	C20-C21-C22-C23
27	A	414	SQD	C24-C23-O48-C46
31	A	417	PL9	C43-C44-C46-C47
24	C	505	CLA	C2-C3-C5-C6
37	C	517	DGD	C1A-C2A-C3A-C4A
36	b	635	LHG	C31-C32-C33-C34
37	e	101	DGD	C4D-C5D-C6D-O5D
24	C	502	CLA	C16-C17-C18-C20
24	a	405	CLA	C4C-C3C-CAC-CBC
24	c	912	CLA	CBA-CGA-O2A-C1
33	B	622	LMG	C37-C38-C39-C40
37	h	102	DGD	CAA-CBA-CCA-CDA
27	L	102	SQD	C29-C30-C31-C32
24	b	614	CLA	C3A-C2A-CAA-CBA
24	B	608	CLA	C3A-C2A-CAA-CBA
35	B	624	HTG	C3'-C4'-C5'-C6'
33	A	419	LMG	C12-C13-C14-C15
33	Z	101	LMG	C13-C14-C15-C16
24	a	406	CLA	O1D-CGD-O2D-CED
36	d	409	LHG	C26-C27-C28-C29
24	b	619	CLA	C10-C11-C12-C13
27	A	414	SQD	O6-C44-C45-C46
36	E	101	LHG	C4-C5-C6-O8
27	a	410	SQD	O6-C44-C45-C46
37	e	101	DGD	O1G-C1G-C2G-C3G
33	A	419	LMG	C7-C8-C9-O8
33	a	411	LMG	C7-C8-C9-O8
33	Z	101	LMG	O1-C7-C8-C9
33	c	919	LMG	C7-C8-C9-O8
37	c	917	DGD	C6A-C7A-C8A-C9A
29	D	403	LMT	C5-C6-C7-C8
37	C	518	DGD	CBA-CCA-CDA-CEA
24	C	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
36	b	635	LHG	C28-C29-C30-C31
37	C	518	DGD	C8B-C9B-CAB-CBB
36	d	411	LHG	O10-C23-O8-C6
24	C	505	CLA	C4-C3-C5-C6
31	a	415	PL9	C12-C11-C9-C8
27	a	410	SQD	C27-C28-C29-C30
24	C	513	CLA	O1D-CGD-O2D-CED
24	B	604	CLA	C5-C6-C7-C8
36	E	101	LHG	C4-O6-P-O3
29	a	401	LMT	C9-C10-C11-C12
29	e	102	LMT	C9-C10-C11-C12
28	V	206	GOL	O2-C2-C3-O3
28	b	631	GOL	O1-C1-C2-O2
28	V	207	GOL	O1-C1-C2-O2
28	B	636	GOL	O1-C1-C2-O2
24	b	621	CLA	C10-C11-C12-C13
33	B	622	LMG	C16-C17-C18-C19
37	c	916	DGD	C7B-C8B-C9B-CAB
36	D	410	LHG	O6-C4-C5-O7
33	b	625	LMG	C17-C18-C19-C20
27	A	411	SQD	C16-C17-C18-C19
36	D	410	LHG	C12-C13-C14-C15
36	E	101	LHG	O7-C5-C6-O8
27	L	102	SQD	O47-C45-C46-O48
27	a	410	SQD	O6-C44-C45-O47
33	A	419	LMG	O7-C8-C9-O8
33	Z	101	LMG	O7-C8-C9-O8
33	c	920	LMG	O7-C8-C9-O8
27	L	102	SQD	C11-C10-C9-C8
27	f	102	SQD	C24-C25-C26-C27
37	c	916	DGD	O6E-C1E-O5D-C6D
24	A	405	CLA	C15-C16-C17-C18
37	h	102	DGD	CDA-CEA-CFA-CGA
27	A	411	SQD	C18-C19-C20-C21
37	C	516	DGD	C4A-C5A-C6A-C7A
36	b	635	LHG	C17-C18-C19-C20
24	C	512	CLA	C11-C10-C8-C9
24	b	606	CLA	C6-C7-C8-C9
24	c	903	CLA	C11-C12-C13-C14
33	b	625	LMG	C33-C34-C35-C36
36	D	410	LHG	C2-C3-O3-P
29	m	103	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
37	e	101	DGD	C4A-C5A-C6A-C7A
33	a	411	LMG	C32-C33-C34-C35
24	c	902	CLA	C2A-CAA-CBA-CGA
36	E	101	LHG	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	D	406	BCR	C5-C6-C7-C8
26	d	407	BCR	C23-C24-C25-C26
26	d	407	BCR	C23-C24-C25-C30
26	b	622	BCR	C1-C6-C7-C8
26	b	622	BCR	C5-C6-C7-C8
26	a	409	BCR	C1-C6-C7-C8
26	c	915	BCR	C1-C6-C7-C8
26	c	915	BCR	C5-C6-C7-C8
24	B	602	CLA	C8-C10-C11-C12
36	d	411	LHG	C35-C36-C37-C38
37	C	518	DGD	C6B-C7B-C8B-C9B
33	b	625	LMG	C36-C37-C38-C39
35	V	203	HTG	S1-C1'-C2'-C3'
36	d	410	LHG	C16-C17-C18-C19
37	H	102	DGD	CDB-CEB-CFB-CGB
27	A	411	SQD	C8-C7-O47-C45
25	d	403	PHO	C2C-C3C-CAC-CBC
37	H	102	DGD	CDA-CEA-CFA-CGA
24	C	506	CLA	C16-C17-C18-C20
36	a	418	LHG	C7-C8-C9-C10
27	a	410	SQD	C29-C30-C31-C32
27	B	621	SQD	C35-C36-C37-C38
27	f	102	SQD	C31-C32-C33-C34
27	B	621	SQD	O10-C23-O48-C46
33	A	419	LMG	C30-C31-C32-C33
24	B	602	CLA	C11-C12-C13-C15
24	c	913	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	c	910	CLA	C12-C13-C15-C16
24	b	606	CLA	C6-C7-C8-C10
24	a	406	CLA	C11-C10-C8-C7
24	b	621	CLA	C12-C13-C15-C16
24	d	404	CLA	C15-C16-C17-C18
24	c	910	CLA	CBD-CGD-O2D-CED
24	b	615	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	C12-C13-C14-C15
37	e	101	DGD	CCA-CDA-CEA-CFA
24	B	602	CLA	C2A-CAA-CBA-CGA
35	b	604	HTG	O5-C1-S1-C1'
35	V	203	HTG	O5-C1-S1-C1'
35	V	203	HTG	C2'-C1'-S1-C1
35	b	628	HTG	C2'-C1'-S1-C1
37	C	518	DGD	C2A-C1A-O1G-C1G
33	Y	101	LMG	C29-C28-O8-C9
37	H	102	DGD	O2G-C1B-C2B-C3B
33	A	419	LMG	C19-C20-C21-C22
27	B	621	SQD	C19-C20-C21-C22
33	Y	101	LMG	C30-C31-C32-C33
27	L	102	SQD	O10-C23-O48-C46
25	A	408	PHO	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
25	a	407	PHO	CAD-CBD-CGD-O2D
24	D	405	CLA	CAD-CBD-CGD-O2D
27	B	621	SQD	C46-C45-O47-C7
24	c	902	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O2D
36	L	101	LHG	C9-C10-C11-C12
24	c	913	CLA	CBA-CGA-O2A-C1
31	A	417	PL9	C15-C14-C16-C17
33	z	101	LMG	O1-C7-C8-C9
36	d	409	LHG	C4-C5-C6-O8
33	Z	101	LMG	C7-C8-C9-O8
24	c	912	CLA	O1A-CGA-O2A-C1
36	b	635	LHG	O6-C4-C5-O7
24	c	911	CLA	C13-C15-C16-C17
24	B	616	CLA	C10-C11-C12-C13
36	b	635	LHG	C9-C10-C11-C12
24	A	405	CLA	C16-C17-C18-C19
29	M	103	LMT	C2B-C1B-O1B-C4'
24	B	606	CLA	CHA-CBD-CGD-O1D
24	c	913	CLA	CHA-CBD-CGD-O1D
24	c	910	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	508	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	c	907	CLA	CHA-CBD-CGD-O1D
24	c	903	CLA	CHA-CBD-CGD-O1D
24	c	904	CLA	CBD-CGD-O2D-CED
27	A	414	SQD	O10-C23-O48-C46
29	D	403	LMT	C2'-C1'-O1'-C1
33	J	101	LMG	C30-C31-C32-C33
36	d	410	LHG	C34-C35-C36-C37
36	b	635	LHG	C33-C34-C35-C36
37	D	408	DGD	O1G-C1G-C2G-O2G
33	A	419	LMG	O1-C7-C8-O7
33	c	919	LMG	O7-C8-C9-O8
33	Y	101	LMG	O10-C28-O8-C9
27	a	402	SQD	C29-C30-C31-C32
24	c	907	CLA	C16-C17-C18-C19
28	D	402	GOL	O1-C1-C2-O2
28	B	629	GOL	O1-C1-C2-O2
24	B	610	CLA	C4-C3-C5-C6
24	c	913	CLA	O1A-CGA-O2A-C1
27	A	411	SQD	O49-C7-O47-C45
24	c	913	CLA	C11-C10-C8-C9
24	a	406	CLA	C11-C10-C8-C9
24	A	407	CLA	C11-C10-C8-C9
36	B	635	LHG	C33-C34-C35-C36
36	d	411	LHG	C9-C10-C11-C12
24	b	620	CLA	CBD-CGD-O2D-CED
37	h	102	DGD	O2G-C1B-C2B-C3B
24	c	911	CLA	C8-C10-C11-C12
36	a	418	LHG	C25-C26-C27-C28
36	d	409	LHG	C18-C19-C20-C21
26	t	102	BCR	C7-C8-C9-C34
28	D	402	GOL	O1-C1-C2-C3
37	c	917	DGD	C4B-C5B-C6B-C7B
26	c	915	BCR	C7-C8-C9-C10
24	C	502	CLA	C3-C5-C6-C7
24	C	501	CLA	C1A-C2A-CAA-CBA
24	b	616	CLA	C16-C17-C18-C20
36	L	101	LHG	C29-C30-C31-C32
33	b	625	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
37	C	517	DGD	C8A-C9A-CAA-CBA
33	Y	101	LMG	C16-C17-C18-C19
36	d	411	LHG	C28-C29-C30-C31
29	b	602	LMT	C2-C3-C4-C5
36	d	411	LHG	C2-C3-O3-P
36	E	101	LHG	C3-O3-P-O5
36	d	410	LHG	C3-O3-P-O5
36	D	410	LHG	C4-O6-P-O5
24	b	619	CLA	C16-C17-C18-C19
29	D	403	LMT	O5'-C1'-O1'-C1
24	b	617	CLA	C8-C10-C11-C12
36	L	101	LHG	O6-C4-C5-C6
24	C	508	CLA	C3-C5-C6-C7
37	c	917	DGD	C7A-C8A-C9A-CAA
35	b	603	HTG	C2'-C3'-C4'-C5'
37	C	518	DGD	O1A-C1A-O1G-C1G
24	d	406	CLA	C16-C17-C18-C19
24	B	606	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O1D
24	c	913	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	c	907	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	c	905	CLA	CAD-CBD-CGD-O1D
24	c	903	CLA	CAD-CBD-CGD-O1D
24	d	404	CLA	C4C-C3C-CAC-CBC
24	c	909	CLA	C10-C11-C12-C13
35	c	921	HTG	S1-C1'-C2'-C3'
24	A	406	CLA	C2C-C3C-CAC-CBC
27	a	410	SQD	C10-C11-C12-C13
37	C	517	DGD	CBA-CCA-CDA-CEA
37	C	517	DGD	C1B-C2B-C3B-C4B
35	B	625	HTG	C2-C1-S1-C1'
35	c	921	HTG	C2-C1-S1-C1'
24	c	907	CLA	C11-C10-C8-C7
35	V	203	HTG	C2-C1-S1-C1'
24	B	616	CLA	C12-C13-C15-C16
24	A	407	CLA	C11-C10-C8-C7
24	C	504	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	t	101	LMT	C11-C10-C9-C8
36	d	411	LHG	C33-C34-C35-C36
36	L	101	LHG	C17-C18-C19-C20
37	C	517	DGD	C3A-C4A-C5A-C6A
37	h	102	DGD	C6A-C7A-C8A-C9A
37	e	101	DGD	CAA-CBA-CCA-CDA
27	f	102	SQD	C26-C27-C28-C29
27	B	621	SQD	C14-C15-C16-C17
24	B	615	CLA	C16-C17-C18-C19
33	d	415	LMG	C38-C39-C40-C41
27	L	102	SQD	C18-C19-C20-C21
33	c	919	LMG	C17-C18-C19-C20
27	F	103	SQD	O47-C45-C46-O48
37	e	101	DGD	O1G-C1G-C2G-O2G
33	a	411	LMG	O7-C8-C9-O8
27	B	621	SQD	O47-C45-C46-O48
27	A	414	SQD	C17-C18-C19-C20
36	B	635	LHG	C25-C26-C27-C28
33	c	920	LMG	C37-C38-C39-C40
36	L	101	LHG	C32-C33-C34-C35
29	A	415	LMT	C5-C6-C7-C8
29	t	101	LMT	C4-C5-C6-C7
37	C	517	DGD	C5D-C6D-O5D-C1E
24	C	502	CLA	C16-C17-C18-C19
29	m	103	LMT	C2-C3-C4-C5
29	a	417	LMT	C7-C8-C9-C10
33	b	625	LMG	C34-C35-C36-C37
27	B	621	SQD	C17-C18-C19-C20
24	B	607	CLA	C10-C11-C12-C13
24	b	621	CLA	C4-C3-C5-C6
37	c	918	DGD	C4A-C5A-C6A-C7A
27	L	102	SQD	C10-C11-C12-C13
37	C	517	DGD	CAA-CBA-CCA-CDA
31	d	408	PL9	C13-C14-C16-C17
24	b	606	CLA	CAA-CBA-CGA-O2A
27	L	102	SQD	C11-C12-C13-C14
24	B	602	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	b	606	CLA	C11-C10-C8-C9
24	b	621	CLA	C14-C13-C15-C16
24	A	407	CLA	C6-C7-C8-C9
24	b	619	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
27	A	414	SQD	C25-C26-C27-C28
27	A	414	SQD	O5-C1-O6-C44
27	A	411	SQD	C14-C15-C16-C17
36	d	411	LHG	C11-C12-C13-C14
24	C	512	CLA	O1A-CGA-O2A-C1
36	B	635	LHG	O1-C1-C2-O2
28	a	413	GOL	O1-C1-C2-O2
28	C	524	GOL	O1-C1-C2-O2
28	a	419	GOL	O2-C2-C3-O3
29	a	401	LMT	C3-C4-C5-C6
37	e	101	DGD	C7B-C8B-C9B-CAB
33	A	419	LMG	C33-C34-C35-C36
27	a	402	SQD	C24-C25-C26-C27
27	a	410	SQD	C16-C17-C18-C19
31	d	408	PL9	C15-C14-C16-C17
37	H	102	DGD	CCA-CDA-CEA-CFA
29	M	101	LMT	C7-C8-C9-C10
27	a	410	SQD	C33-C34-C35-C36
36	D	410	LHG	C28-C29-C30-C31
27	L	102	SQD	C46-C45-O47-C7
24	b	607	CLA	C2A-CAA-CBA-CGA
24	B	603	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C8-C10-C11-C12
24	b	613	CLA	C13-C15-C16-C17
24	c	904	CLA	C2-C1-O2A-CGA
24	C	511	CLA	C2-C1-O2A-CGA
36	E	101	LHG	C19-C20-C21-C22
33	C	519	LMG	C29-C30-C31-C32
36	b	635	LHG	C5-C6-O8-C23
37	c	918	DGD	C7B-C8B-C9B-CAB
29	F	101	LMT	C2-C3-C4-C5
24	B	617	CLA	C16-C17-C18-C19
29	m	103	LMT	O1'-C1-C2-C3
24	b	620	CLA	O1D-CGD-O2D-CED
26	A	410	BCR	C1-C6-C7-C8
26	D	406	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	a	409	BCR	C5-C6-C7-C8
31	A	417	PL9	C13-C14-C16-C17
24	B	616	CLA	C13-C15-C16-C17
27	a	402	SQD	C31-C32-C33-C34
36	D	409	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	m	103	LMT	C11-C10-C9-C8
27	A	414	SQD	C2-C1-O6-C44
29	m	103	LMT	C2'-C1'-O1'-C1
37	c	916	DGD	C2E-C1E-O5D-C6D
37	h	102	DGD	C9B-CAB-CBB-CCB
33	z	101	LMG	O1-C7-C8-O7
27	f	102	SQD	O6-C44-C45-C46
33	c	920	LMG	C7-C8-C9-O8
24	A	407	CLA	C6-C7-C8-C10
24	C	504	CLA	C11-C12-C13-C15
24	d	405	CLA	C11-C12-C13-C14
29	D	403	LMT	O5B-C1B-O1B-C4'
24	c	906	CLA	C11-C12-C13-C14
24	b	616	CLA	C16-C17-C18-C19
36	B	635	LHG	C11-C10-C9-C8
29	e	102	LMT	C5-C6-C7-C8
29	e	102	LMT	C2B-C1B-O1B-C4'
37	C	518	DGD	C3B-C4B-C5B-C6B
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	907	CLA	C16-C17-C18-C20
37	C	518	DGD	C2A-C3A-C4A-C5A
28	c	928	GOL	C1-C2-C3-O3
36	D	410	LHG	C17-C18-C19-C20
24	C	501	CLA	O1D-CGD-O2D-CED
24	B	606	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	C16-C17-C18-C19
24	C	512	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	CBA-CGA-O2A-C1
24	C	513	CLA	CBA-CGA-O2A-C1
24	b	606	CLA	O1A-CGA-O2A-C1
25	D	401	PHO	C4C-C3C-CAC-CBC
24	B	602	CLA	CAA-CBA-CGA-O2A
33	d	415	LMG	C29-C30-C31-C32
24	b	616	CLA	C8-C10-C11-C12
24	B	611	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C16-C17-C18-C19
29	M	101	LMT	O5'-C1'-O1'-C1
27	B	621	SQD	C12-C13-C14-C15
24	C	513	CLA	C3-C5-C6-C7
36	a	418	LHG	C28-C29-C30-C31
27	A	414	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C13-C15-C16-C17
24	c	911	CLA	C3-C5-C6-C7
36	D	409	LHG	C9-C10-C11-C12
31	D	407	PL9	C28-C29-C31-C32
29	D	403	LMT	C2B-C1B-O1B-C4'
24	c	913	CLA	C2-C1-O2A-CGA
24	b	618	CLA	C2-C1-O2A-CGA
33	b	625	LMG	C32-C33-C34-C35
36	d	409	LHG	O7-C5-C6-O8
24	c	904	CLA	O1D-CGD-O2D-CED
24	c	912	CLA	C3-C5-C6-C7
29	m	102	LMT	C11-C10-C9-C8
24	a	408	CLA	C4-C3-C5-C6
24	b	621	CLA	C16-C17-C18-C19
37	e	101	DGD	C6A-C7A-C8A-C9A
29	F	101	LMT	C1-C2-C3-C4
33	B	622	LMG	C15-C16-C17-C18
24	C	509	CLA	C15-C16-C17-C18
37	c	916	DGD	C6A-C7A-C8A-C9A
24	d	406	CLA	C16-C17-C18-C20
24	B	617	CLA	C16-C17-C18-C20
37	C	516	DGD	O6E-C1E-O5D-C6D
26	A	410	BCR	C36-C18-C19-C20
36	d	409	LHG	C11-C10-C9-C8
27	a	410	SQD	C26-C27-C28-C29
24	A	406	CLA	C1A-C2A-CAA-CBA
24	d	404	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	c	902	CLA	C1A-C2A-CAA-CBA
24	b	611	CLA	C11-C12-C13-C15
24	a	406	CLA	C11-C12-C13-C15
24	c	911	CLA	C12-C13-C15-C16
29	M	101	LMT	O5'-C5'-C6'-O6'
26	h	101	BCR	C9-C10-C11-C12
33	a	411	LMG	C29-C30-C31-C32
37	c	916	DGD	C5B-C6B-C7B-C8B
36	B	635	LHG	C15-C16-C17-C18
37	D	408	DGD	C2B-C3B-C4B-C5B
24	b	619	CLA	C2A-CAA-CBA-CGA
24	c	913	CLA	C13-C15-C16-C17
24	b	619	CLA	C15-C16-C17-C18
37	D	408	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
29	b	626	LMT	C6-C7-C8-C9
36	D	410	LHG	C10-C11-C12-C13
36	L	101	LHG	O6-C4-C5-O7
37	c	918	DGD	CBA-CCA-CDA-CEA
37	c	917	DGD	C3A-C4A-C5A-C6A
31	a	415	PL9	C45-C44-C46-C47
33	a	411	LMG	C35-C36-C37-C38
24	b	620	CLA	C5-C6-C7-C8
29	M	101	LMT	C2'-C1'-O1'-C1
37	D	408	DGD	O2G-C2G-C3G-O3G
27	F	103	SQD	C24-C23-O48-C46
24	c	904	CLA	C5-C6-C7-C8
35	B	625	HTG	C3'-C4'-C5'-C6'
37	C	516	DGD	C9A-CAA-CBA-CCA
37	C	517	DGD	C6B-C7B-C8B-C9B
29	F	101	LMT	C4'-C5'-C6'-O6'
24	a	405	CLA	C2-C1-O2A-CGA
24	b	619	CLA	C2-C1-O2A-CGA
24	c	907	CLA	C2-C1-O2A-CGA
24	a	408	CLA	C2-C3-C5-C6
24	b	621	CLA	C2-C3-C5-C6
24	C	509	CLA	C8-C10-C11-C12
24	b	611	CLA	C14-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C14
33	J	101	LMG	C20-C21-C22-C23
29	M	103	LMT	O5B-C1B-O1B-C4'
24	A	405	CLA	C16-C17-C18-C20
27	F	103	SQD	O10-C23-O48-C46
26	A	410	BCR	C5-C6-C7-C8
26	D	406	BCR	C23-C24-C25-C26
26	D	406	BCR	C23-C24-C25-C30
26	h	101	BCR	C23-C24-C25-C30
26	C	514	BCR	C1-C6-C7-C8
24	C	513	CLA	C8-C10-C11-C12
33	A	419	LMG	O1-C7-C8-C9
36	D	409	LHG	C33-C34-C35-C36
33	Y	101	LMG	C35-C36-C37-C38
28	c	928	GOL	O1-C1-C2-C3
28	B	629	GOL	C1-C2-C3-O3
28	C	524	GOL	O1-C1-C2-C3
36	b	635	LHG	O1-C1-C2-C3
31	D	407	PL9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	C8-C7-O1-C1
37	C	516	DGD	C5D-C6D-O5D-C1E
37	C	517	DGD	C2G-C3G-O3G-C1D
27	a	410	SQD	C35-C36-C37-C38
33	B	622	LMG	O8-C28-C29-C30
29	m	102	LMT	C9-C10-C11-C12
24	b	609	CLA	C16-C17-C18-C19
38	f	101	HEM	C2A-CAA-CBA-CGA
24	C	507	CLA	C2A-CAA-CBA-CGA
24	C	501	CLA	C2A-CAA-CBA-CGA
24	c	907	CLA	C13-C15-C16-C17
27	F	103	SQD	C32-C33-C34-C35
33	c	919	LMG	C20-C21-C22-C23
36	D	410	LHG	O6-C4-C5-C6
31	A	417	PL9	C20-C19-C21-C22
24	b	606	CLA	C4-C3-C5-C6
24	B	612	CLA	C2-C3-C5-C6
24	c	906	CLA	C11-C12-C13-C15
24	b	620	CLA	C13-C15-C16-C17
24	B	609	CLA	C13-C15-C16-C17
28	b	631	GOL	O2-C2-C3-O3
36	b	635	LHG	O1-C1-C2-O2
33	Z	101	LMG	O7-C10-C11-C12
24	d	405	CLA	C16-C17-C18-C20
29	a	417	LMT	C6-C7-C8-C9
35	B	623	HTG	C4-C5-C6-O6
24	C	510	CLA	C8-C10-C11-C12
29	F	101	LMT	O1'-C1-C2-C3
33	d	415	LMG	C11-C12-C13-C14
37	c	917	DGD	C6B-C7B-C8B-C9B
36	L	101	LHG	C28-C29-C30-C31
35	B	623	HTG	C2'-C1'-S1-C1
37	C	518	DGD	C7A-C8A-C9A-CAA
37	c	917	DGD	O2G-C1B-C2B-C3B
24	C	512	CLA	CAA-CBA-CGA-O2A
27	f	102	SQD	O47-C7-C8-C9
35	B	623	HTG	C4'-C5'-C6'-C7'
31	A	417	PL9	C30-C29-C31-C32
31	A	417	PL9	C40-C39-C41-C42
24	B	607	CLA	C4-C3-C5-C6
24	c	914	CLA	C4-C3-C5-C6
24	B	616	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
37	C	516	DGD	O1A-C1A-O1G-C1G
31	a	415	PL9	C43-C44-C46-C47
24	c	907	CLA	C11-C10-C8-C9
24	B	616	CLA	C14-C13-C15-C16
24	C	504	CLA	C14-C13-C15-C16
27	a	402	SQD	C12-C13-C14-C15
24	A	409	CLA	C3A-C2A-CAA-CBA
24	B	613	CLA	O1A-CGA-O2A-C1
33	a	411	LMG	O8-C28-C29-C30
36	a	418	LHG	C14-C15-C16-C17
24	b	608	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	904	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	b	621	CLA	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	911	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
33	J	101	LMG	C15-C16-C17-C18
24	b	615	CLA	C2A-CAA-CBA-CGA
24	c	912	CLA	C2-C1-O2A-CGA
29	a	401	LMT	C6-C7-C8-C9
37	C	516	DGD	O2G-C1B-C2B-C3B
24	c	908	CLA	C5-C6-C7-C8
24	c	913	CLA	CAA-CBA-CGA-O2A
37	c	918	DGD	O1G-C1A-C2A-C3A
36	b	635	LHG	O7-C7-C8-C9
26	A	410	BCR	C17-C18-C19-C20
26	C	515	BCR	C7-C8-C9-C10
36	b	635	LHG	C34-C35-C36-C37
33	c	919	LMG	O1-C7-C8-C9
36	a	418	LHG	C18-C19-C20-C21
37	D	408	DGD	O1G-C1A-C2A-C3A
27	F	103	SQD	C33-C34-C35-C36
24	B	614	CLA	O2A-C1-C2-C3
24	B	605	CLA	O2A-C1-C2-C3
24	d	406	CLA	O2A-C1-C2-C3
25	A	408	PHO	O2A-C1-C2-C3
25	a	407	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C16-C17-C18-C19
27	L	102	SQD	C30-C31-C32-C33
27	f	102	SQD	C33-C34-C35-C36
25	a	407	PHO	C4B-C3B-CAB-CBB
24	B	606	CLA	C2A-CAA-CBA-CGA
24	c	908	CLA	C2A-CAA-CBA-CGA
33	a	411	LMG	C22-C23-C24-C25
36	D	410	LHG	C33-C34-C35-C36
36	a	418	LHG	O8-C23-C24-C25
36	D	410	LHG	C30-C31-C32-C33
37	c	918	DGD	C3A-C4A-C5A-C6A
24	b	607	CLA	CHA-CBD-CGD-O1D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	c	913	CLA	CHA-CBD-CGD-O2D
24	c	910	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	d	404	CLA	CHA-CBD-CGD-O1D
24	d	404	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	c	907	CLA	CHA-CBD-CGD-O2D
25	d	403	PHO	CHA-CBD-CGD-O1D
25	d	403	PHO	CHA-CBD-CGD-O2D
24	C	505	CLA	CHA-CBD-CGD-O2D
24	c	908	CLA	CHA-CBD-CGD-O1D
24	c	908	CLA	CHA-CBD-CGD-O2D
25	D	401	PHO	CHA-CBD-CGD-O2D
24	c	905	CLA	CHA-CBD-CGD-O1D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	c	906	CLA	CHA-CBD-CGD-O1D
24	c	906	CLA	CHA-CBD-CGD-O2D
24	c	903	CLA	CHA-CBD-CGD-O2D
36	B	635	LHG	C11-C12-C13-C14
24	B	616	CLA	C2-C3-C5-C6
36	B	635	LHG	C29-C30-C31-C32
29	D	403	LMT	C6-C7-C8-C9
24	b	606	CLA	C16-C17-C18-C20
31	A	417	PL9	C2-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
33	J	101	LMG	O1-C7-C8-O7
33	c	919	LMG	O1-C7-C8-O7
24	B	613	CLA	C13-C15-C16-C17
27	f	102	SQD	C35-C36-C37-C38
36	E	101	LHG	O8-C23-C24-C25
36	L	101	LHG	O7-C7-C8-C9
37	C	516	DGD	CAA-CBA-CCA-CDA
24	C	502	CLA	C11-C12-C13-C15
24	b	611	CLA	C11-C12-C13-C14
24	D	405	CLA	C11-C10-C8-C9
25	D	401	PHO	C14-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C14
29	m	103	LMT	C9-C10-C11-C12
33	a	411	LMG	C18-C19-C20-C21
36	b	635	LHG	C12-C13-C14-C15
37	C	516	DGD	C2A-C1A-O1G-C1G
24	b	607	CLA	C16-C17-C18-C20
24	d	405	CLA	C16-C17-C18-C19
24	b	617	CLA	O1A-CGA-O2A-C1
37	D	408	DGD	O1A-C1A-C2A-C3A
33	c	920	LMG	C12-C13-C14-C15
24	B	613	CLA	CBA-CGA-O2A-C1
24	C	509	CLA	C16-C17-C18-C19
37	C	518	DGD	CAB-CBB-CCB-CDB
28	V	207	GOL	O1-C1-C2-C3
28	a	412	GOL	O1-C1-C2-C3
24	C	510	CLA	CAA-CBA-CGA-O2A
37	D	408	DGD	C4B-C5B-C6B-C7B
24	b	614	CLA	C1A-C2A-CAA-CBA
24	d	405	CLA	C1A-C2A-CAA-CBA
36	d	409	LHG	C33-C34-C35-C36
24	C	512	CLA	CAA-CBA-CGA-O1A
27	A	411	SQD	C30-C31-C32-C33
24	b	608	CLA	C2A-CAA-CBA-CGA
24	a	405	CLA	C2A-CAA-CBA-CGA
24	c	902	CLA	CBD-CGD-O2D-CED
36	D	409	LHG	C4-O6-P-O3
29	e	102	LMT	O5B-C1B-O1B-C4'
33	Z	101	LMG	O9-C10-C11-C12
33	Y	101	LMG	C29-C30-C31-C32
36	E	101	LHG	O9-C7-O7-C5
33	a	411	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
37	c	918	DGD	O1A-C1A-C2A-C3A
27	f	102	SQD	O49-C7-C8-C9
37	C	516	DGD	C2E-C1E-O5D-C6D
24	c	905	CLA	C8-C10-C11-C12
27	L	102	SQD	C13-C14-C15-C16
36	D	409	LHG	C3-O3-P-O4
36	D	409	LHG	C4-O6-P-O5
24	c	913	CLA	CAA-CBA-CGA-O1A
24	C	503	CLA	C10-C11-C12-C13
26	b	623	BCR	C23-C24-C25-C30
24	C	513	CLA	C5-C6-C7-C8
37	e	101	DGD	C1A-C2A-C3A-C4A
36	L	101	LHG	O9-C7-C8-C9
36	d	409	LHG	O8-C23-C24-C25
37	e	101	DGD	O2G-C1B-C2B-C3B
24	b	611	CLA	C16-C17-C18-C19
36	b	635	LHG	O9-C7-C8-C9
35	b	627	HTG	C4'-C5'-C6'-C7'
36	E	101	LHG	C25-C26-C27-C28
37	C	518	DGD	CCB-CDB-CEB-CFB
33	J	101	LMG	C4-C5-C6-O5
33	z	101	LMG	C10-C11-C12-C13
37	c	917	DGD	O1B-C1B-C2B-C3B
36	a	418	LHG	O10-C23-C24-C25
36	d	409	LHG	O10-C23-C24-C25
24	b	614	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
27	B	621	SQD	C5-C6-S-O7
24	B	604	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	b	612	CLA	CAD-CBD-CGD-O1D
24	c	906	CLA	CAD-CBD-CGD-O1D
24	c	906	CLA	O1A-CGA-O2A-C1
24	b	618	CLA	CAA-CBA-CGA-O2A
37	c	918	DGD	O6D-C5D-C6D-O5D
24	B	605	CLA	C6-C7-C8-C9
28	a	412	GOL	O1-C1-C2-O2
36	D	409	LHG	C31-C32-C33-C34
24	C	505	CLA	CAA-CBA-CGA-O2A
29	b	626	LMT	C5-C6-C7-C8
35	C	522	HTG	C1'-C2'-C3'-C4'
36	d	411	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
24	c	906	CLA	CAA-CBA-CGA-O2A
36	E	101	LHG	C15-C16-C17-C18
24	A	407	CLA	C10-C11-C12-C13
24	c	910	CLA	C11-C10-C8-C7
24	b	619	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C10-C8-C7
25	D	401	PHO	C12-C13-C15-C16
24	c	902	CLA	C11-C12-C13-C15
37	h	102	DGD	C7B-C8B-C9B-CAB
37	C	517	DGD	O2G-C1B-C2B-C3B
33	Y	101	LMG	O7-C10-C11-C12
26	t	102	BCR	C7-C8-C9-C10
26	C	515	BCR	C21-C22-C23-C24
29	m	102	LMT	C2-C1-O1'-C1'
24	B	614	CLA	CAA-CBA-CGA-O2A
35	b	627	HTG	C2'-C3'-C4'-C5'
36	L	101	LHG	C16-C17-C18-C19
29	M	103	LMT	C3-C4-C5-C6
35	V	203	HTG	C4-C5-C6-O6
24	b	619	CLA	C8-C10-C11-C12
24	c	906	CLA	CAA-CBA-CGA-O1A
24	b	617	CLA	CBA-CGA-O2A-C1
31	D	407	PL9	C34-C36-C37-C38
36	L	101	LHG	C13-C14-C15-C16
33	A	419	LMG	O7-C10-C11-C12
25	d	403	PHO	C8-C10-C11-C12
36	E	101	LHG	O10-C23-C24-C25
24	B	615	CLA	CAA-CBA-CGA-O2A

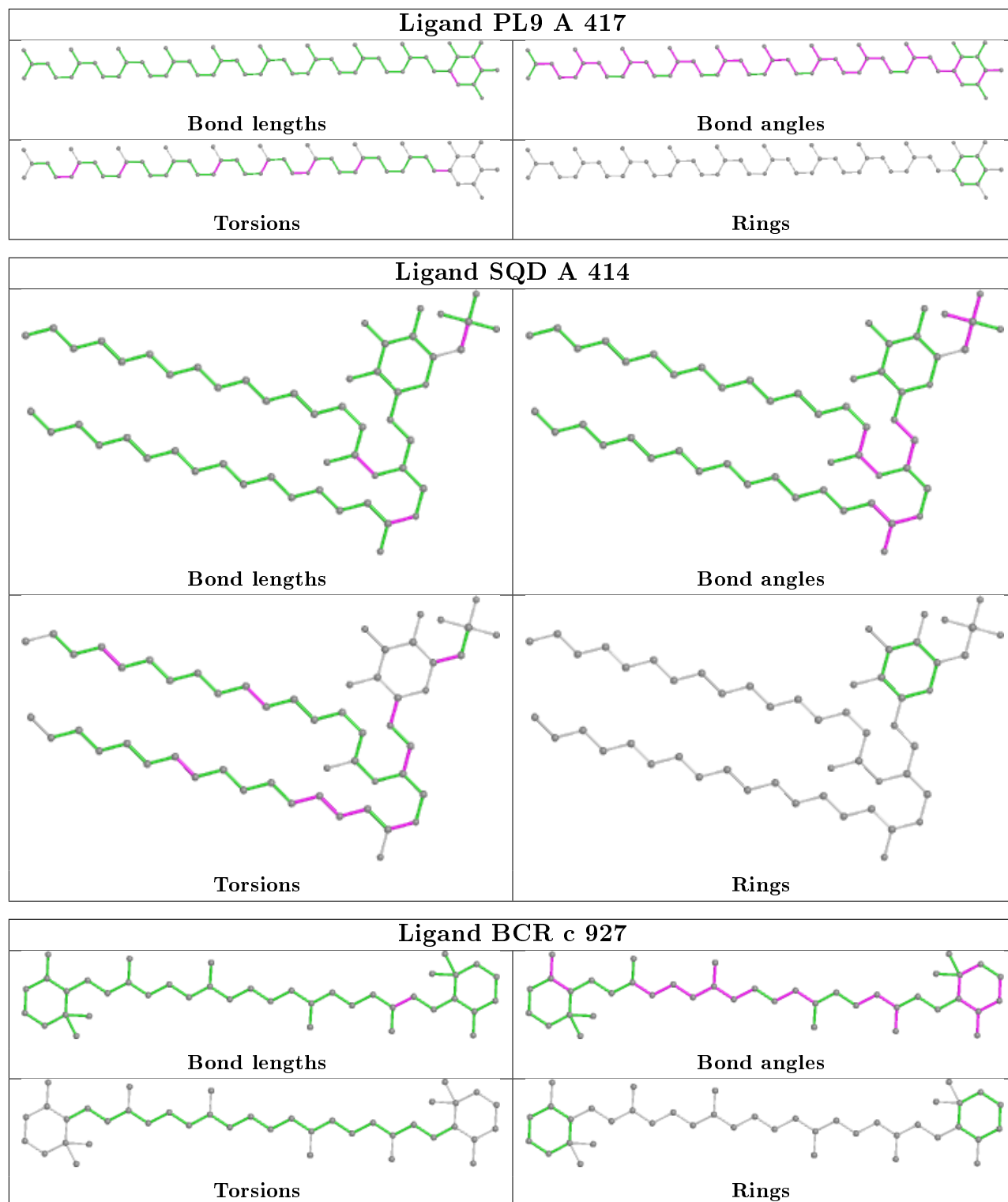
There are no ring outliers.

1 monomer is involved in 1 short contact:

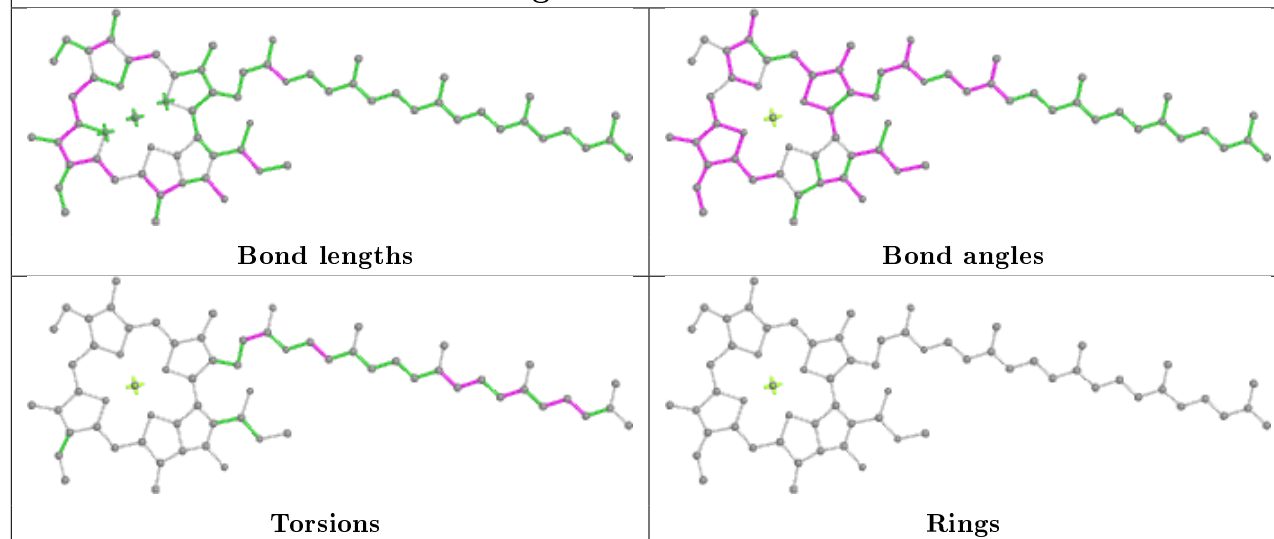
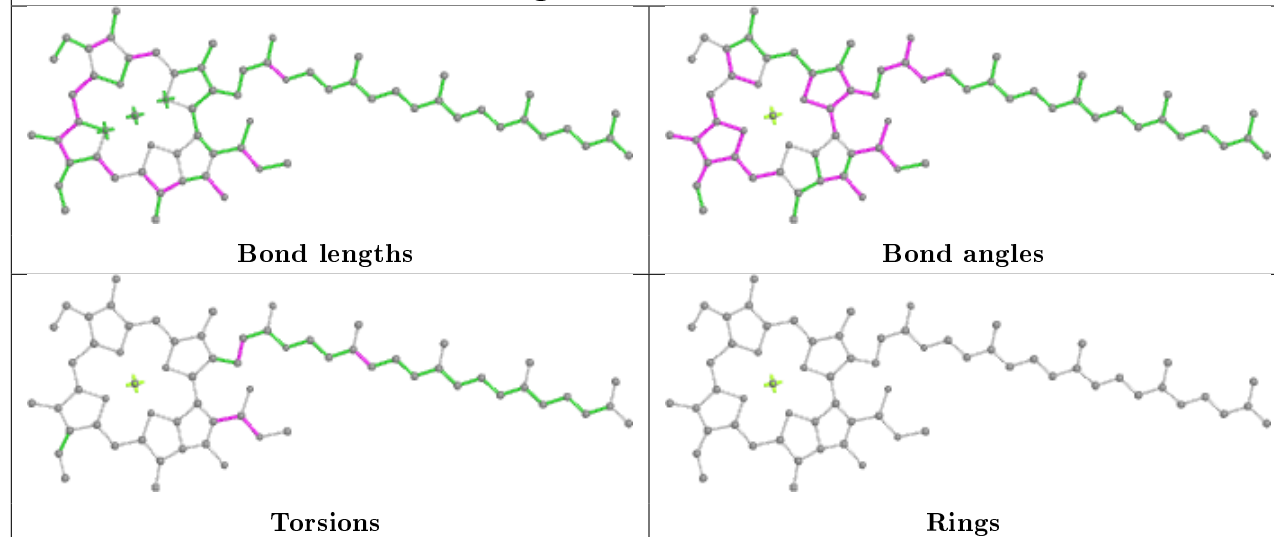
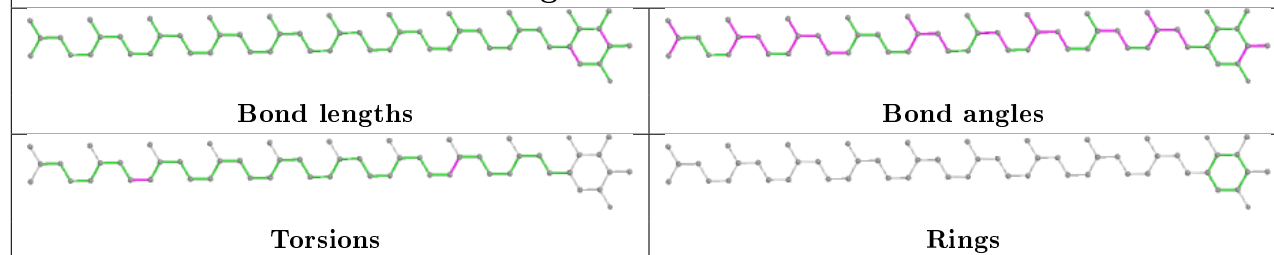
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	f	102	SQD	0	1

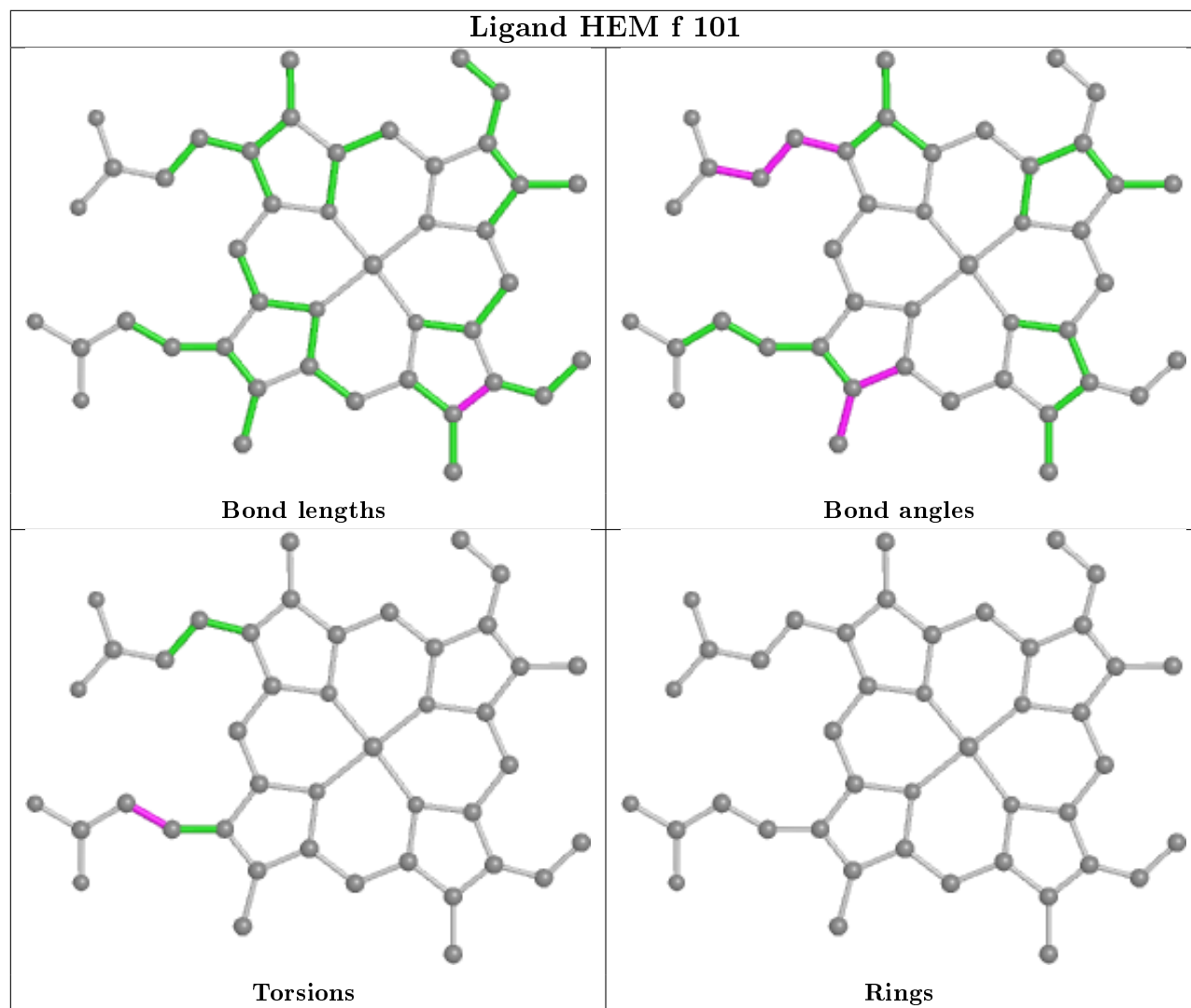
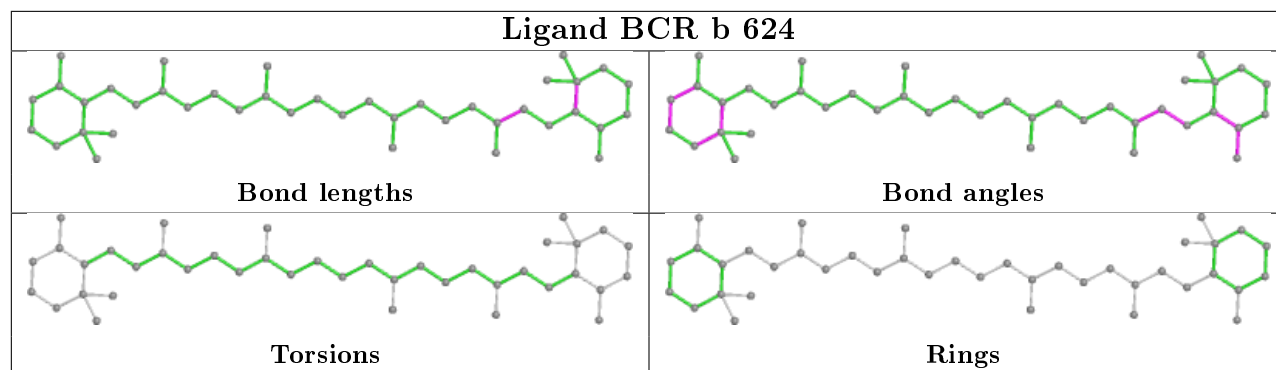
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

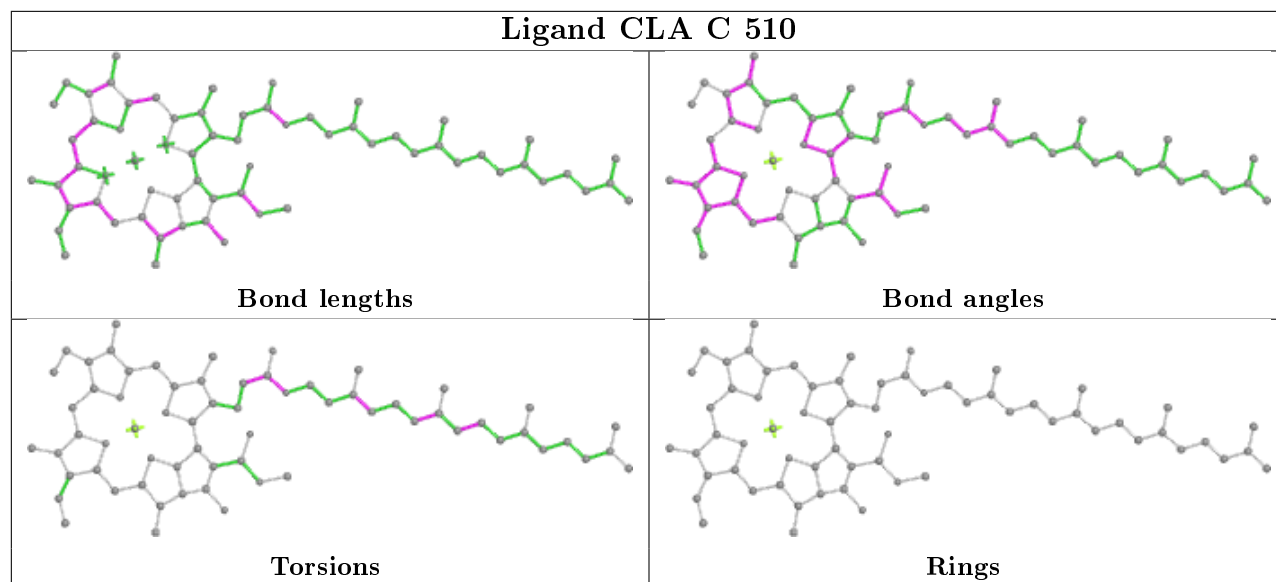




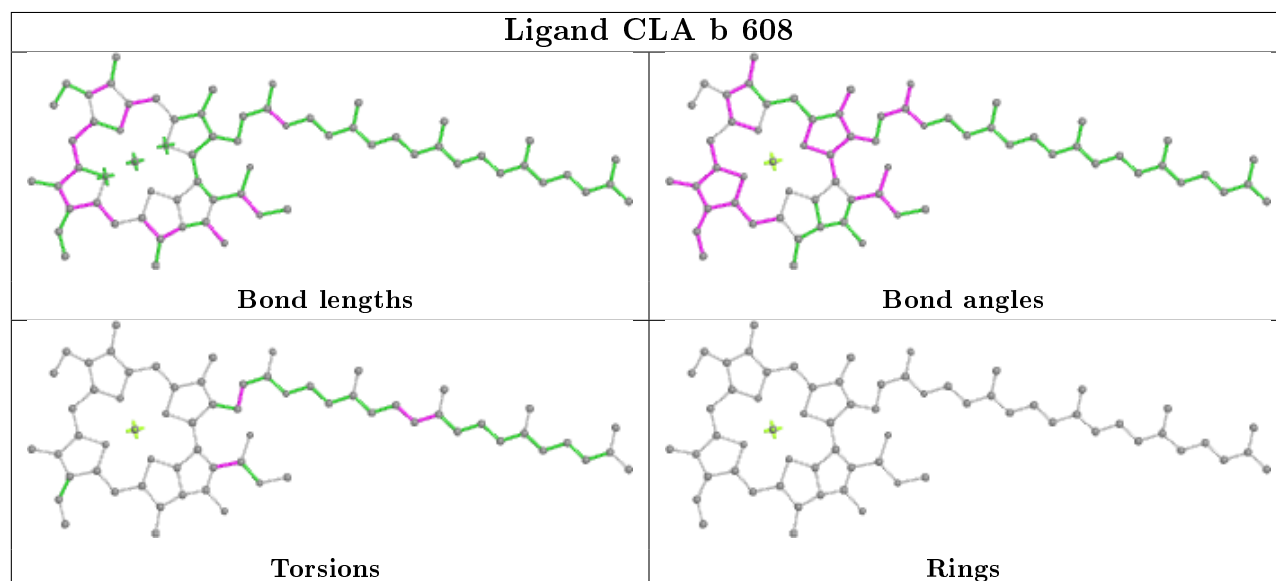
**Ligand CLA B 614****Ligand CLA B 606****Ligand PL9 d 408**



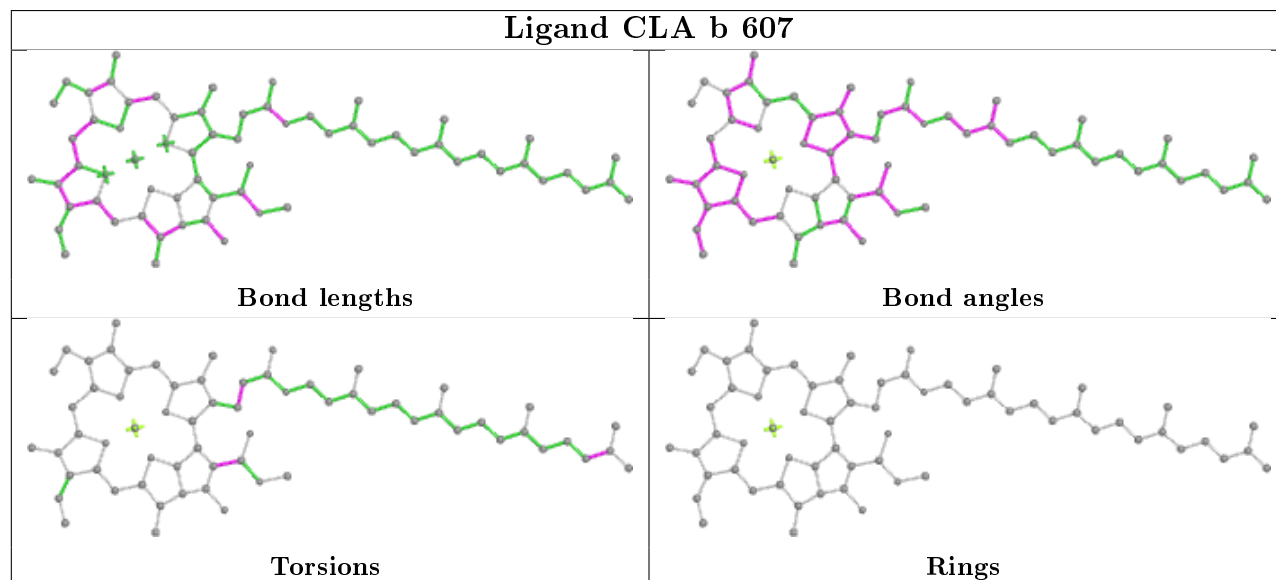
## Ligand CLA C 510

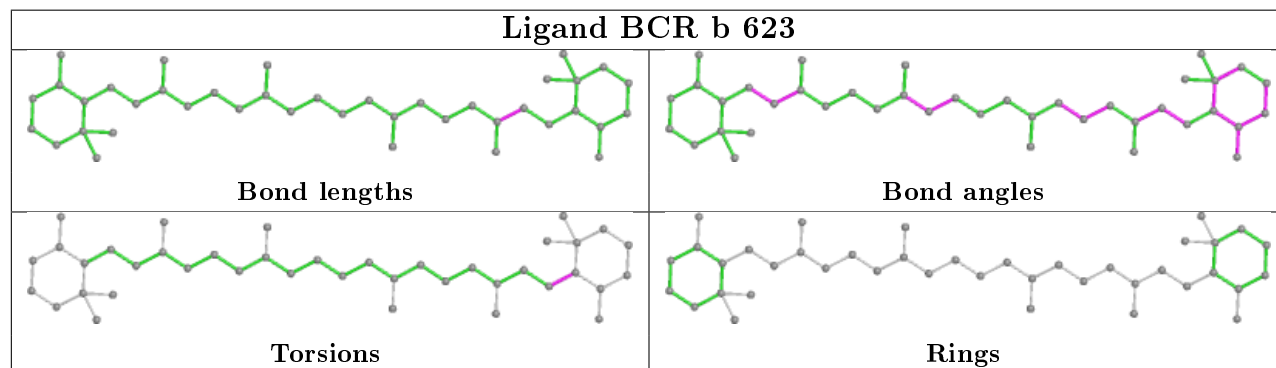
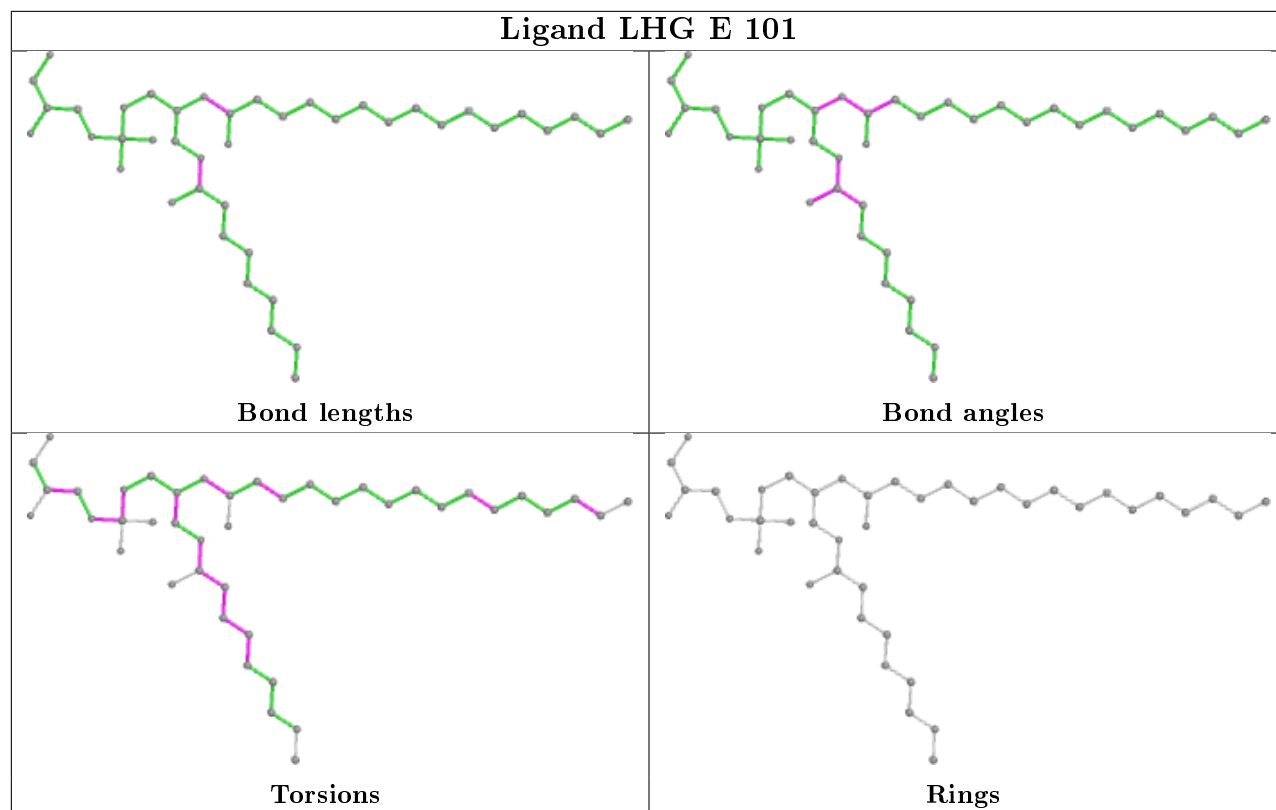


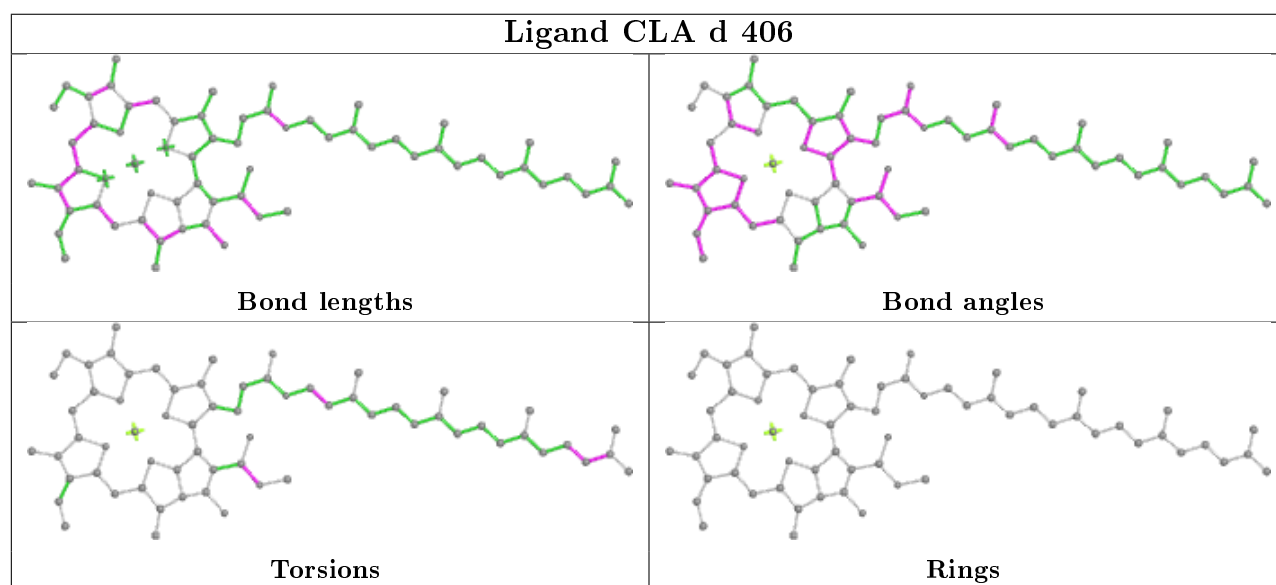
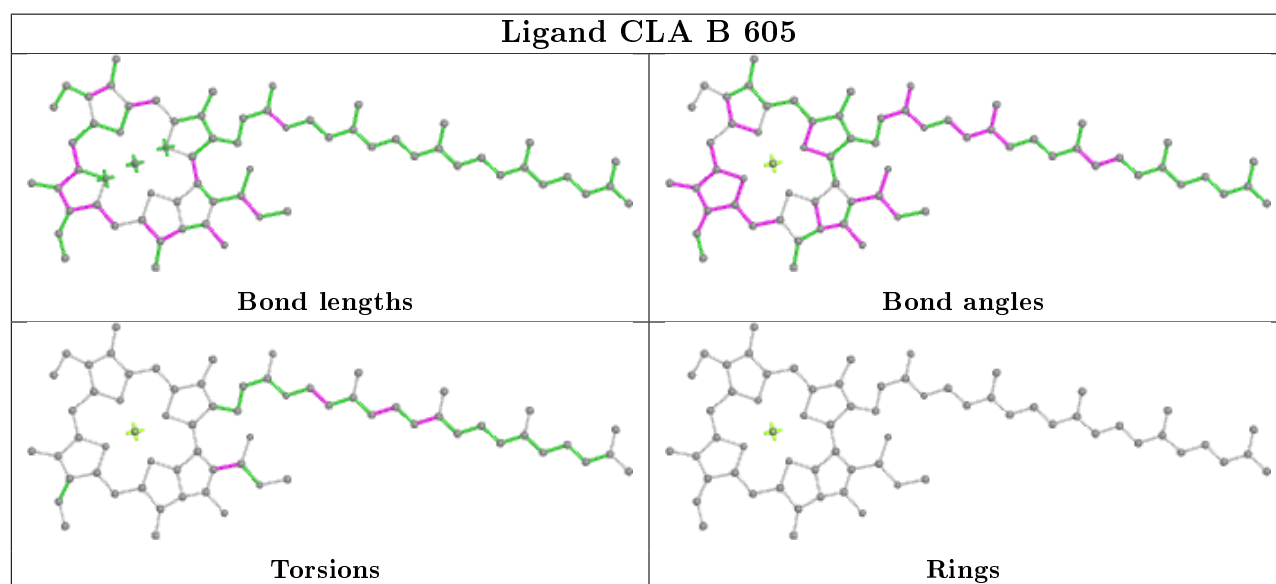
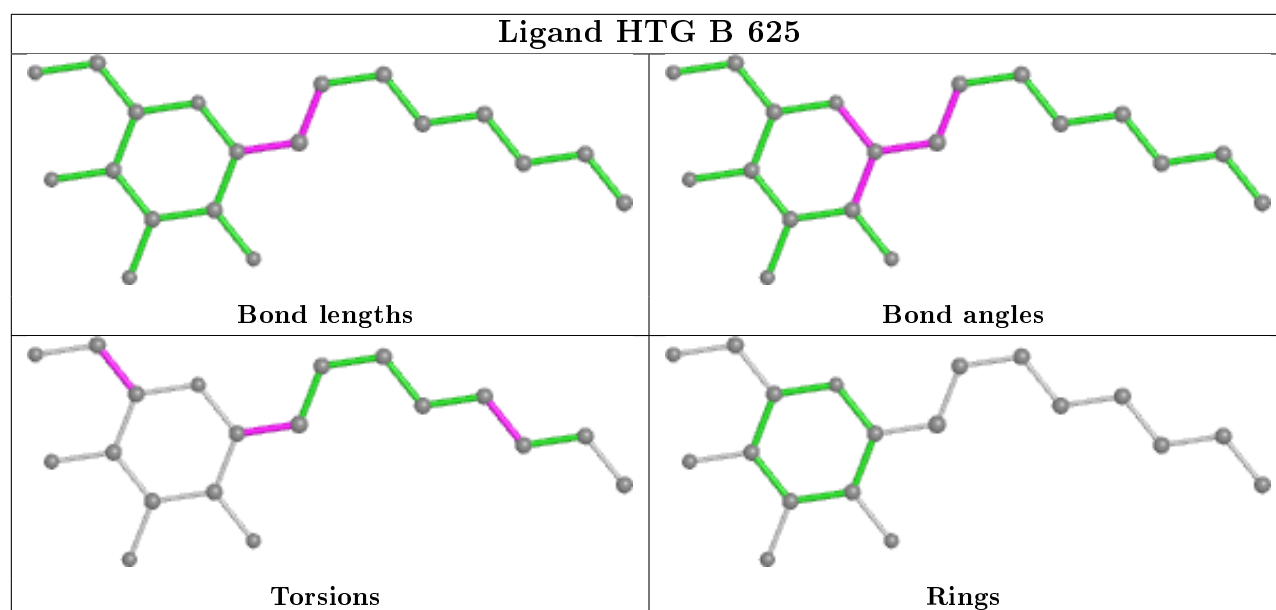
## Ligand CLA b 608

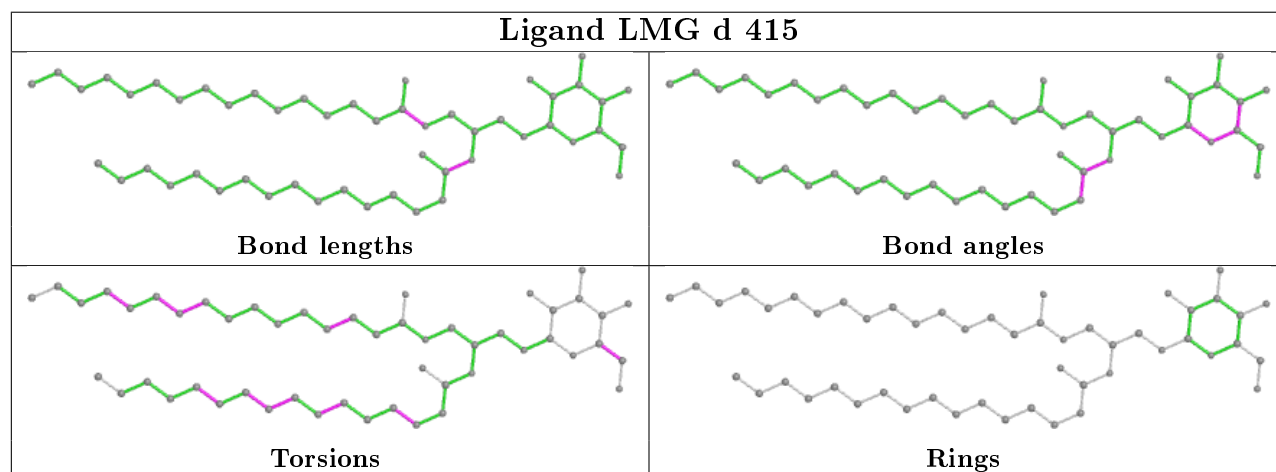
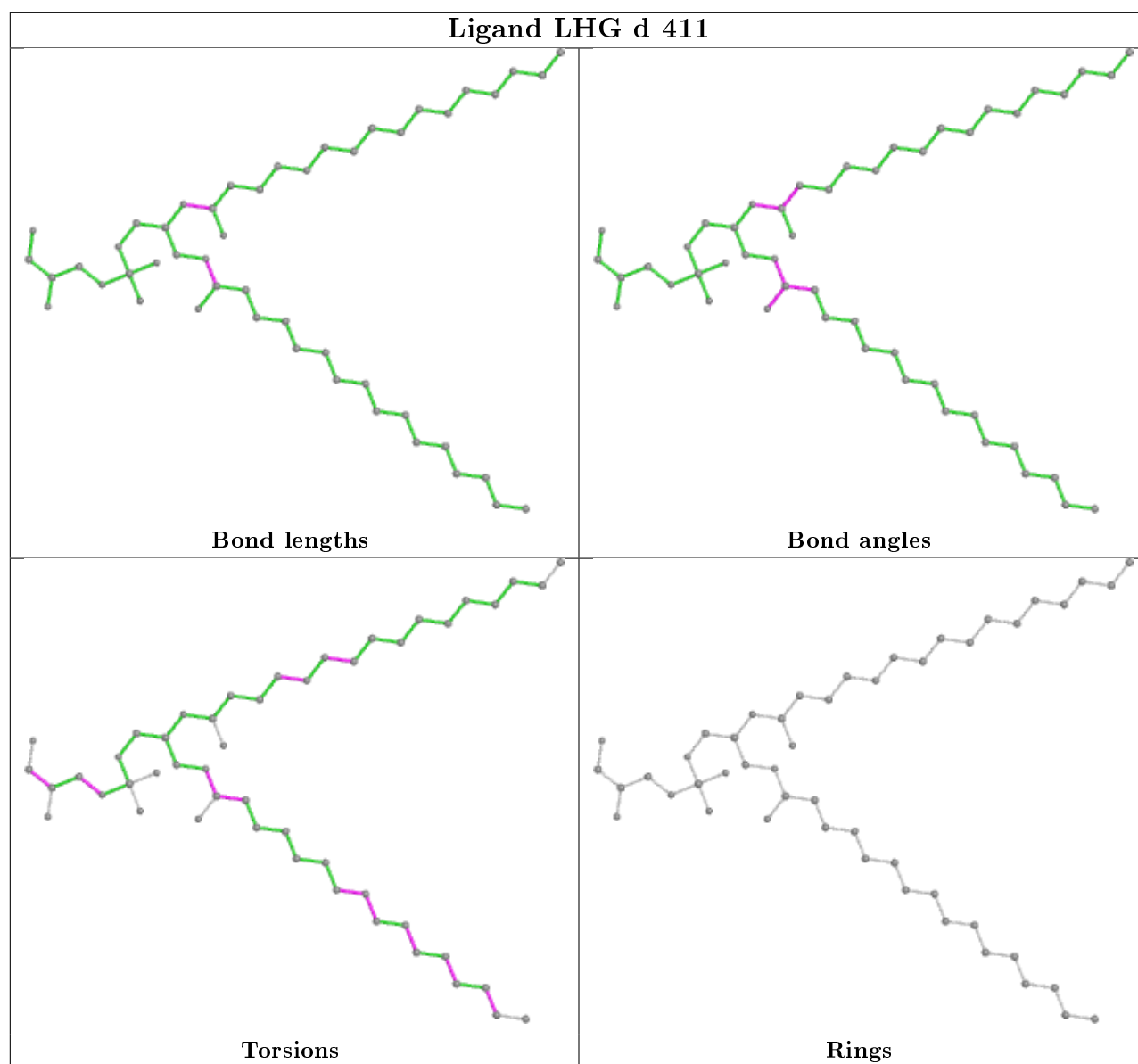


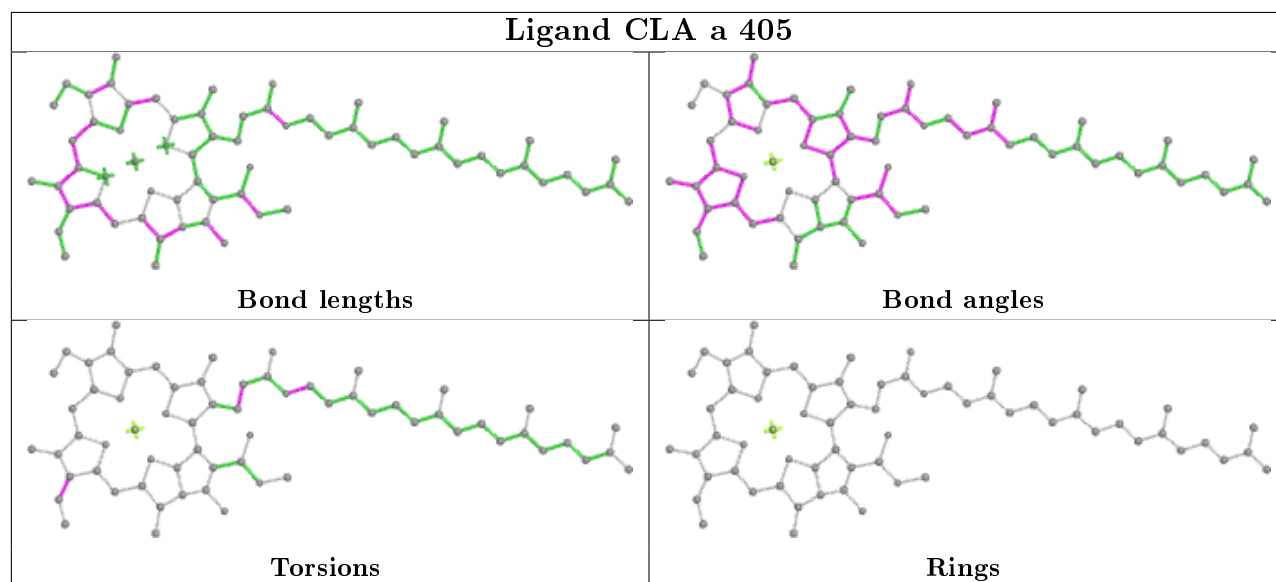
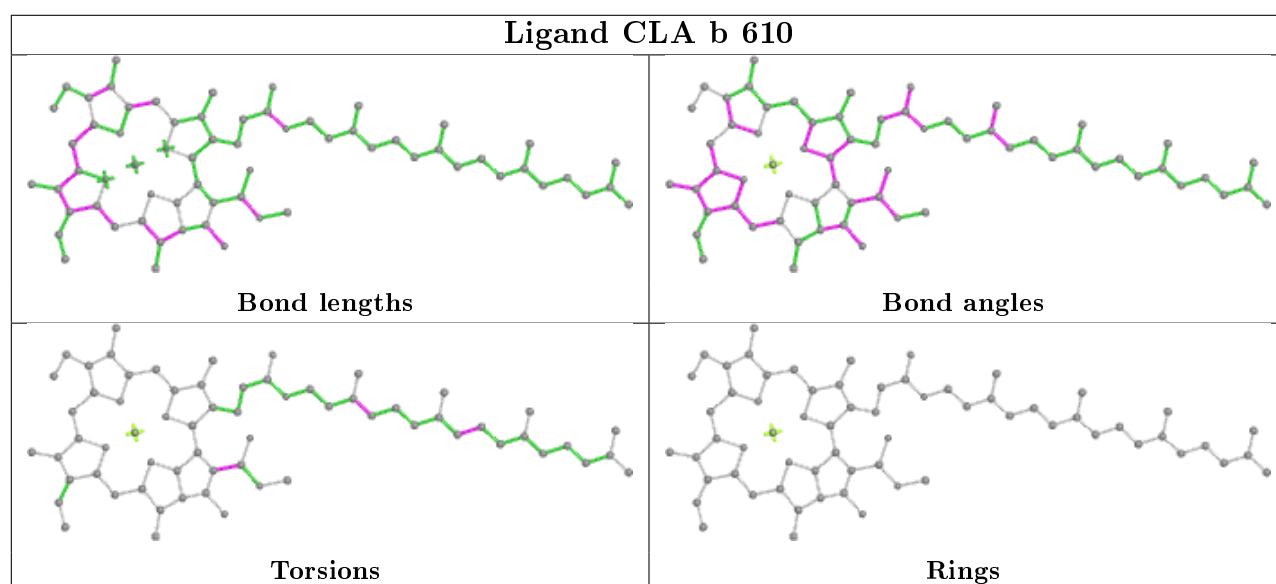
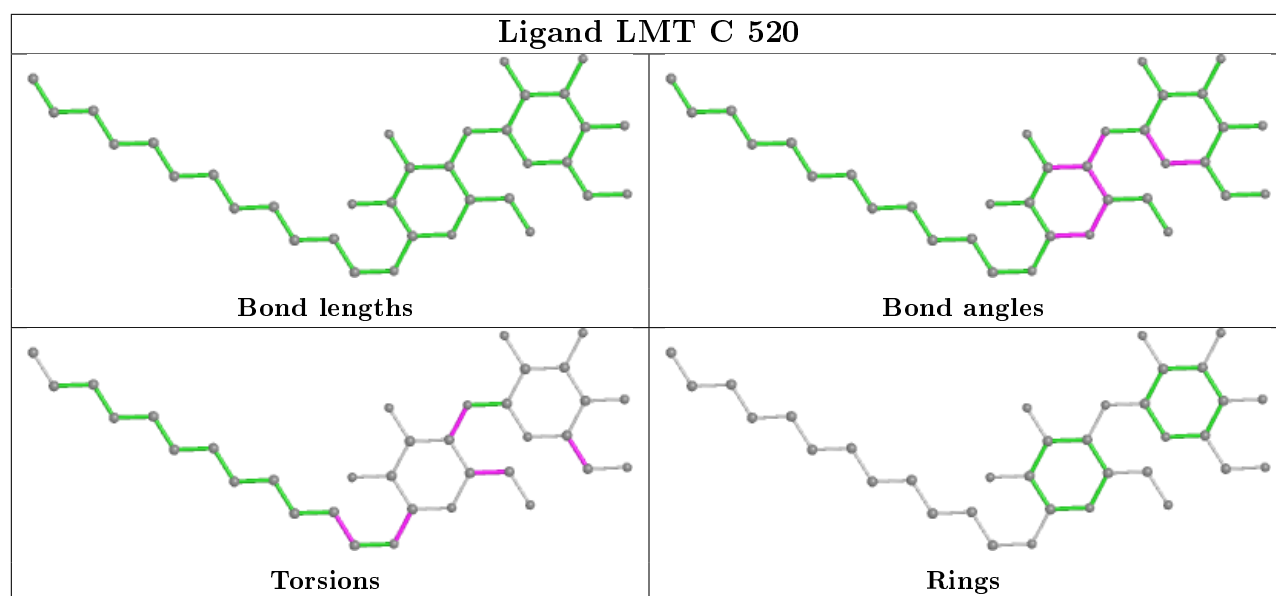
## Ligand CLA b 607

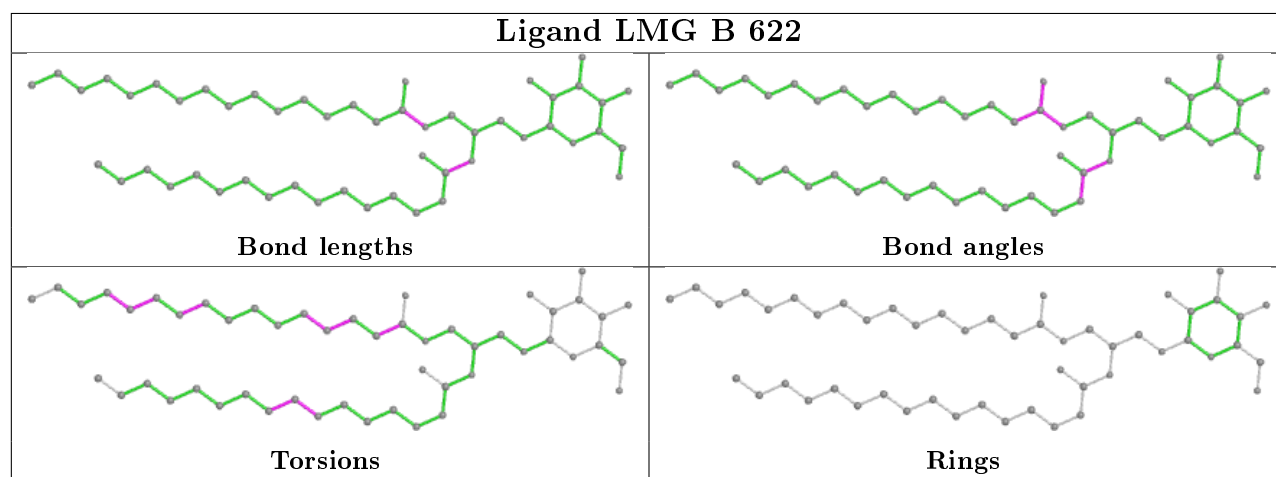
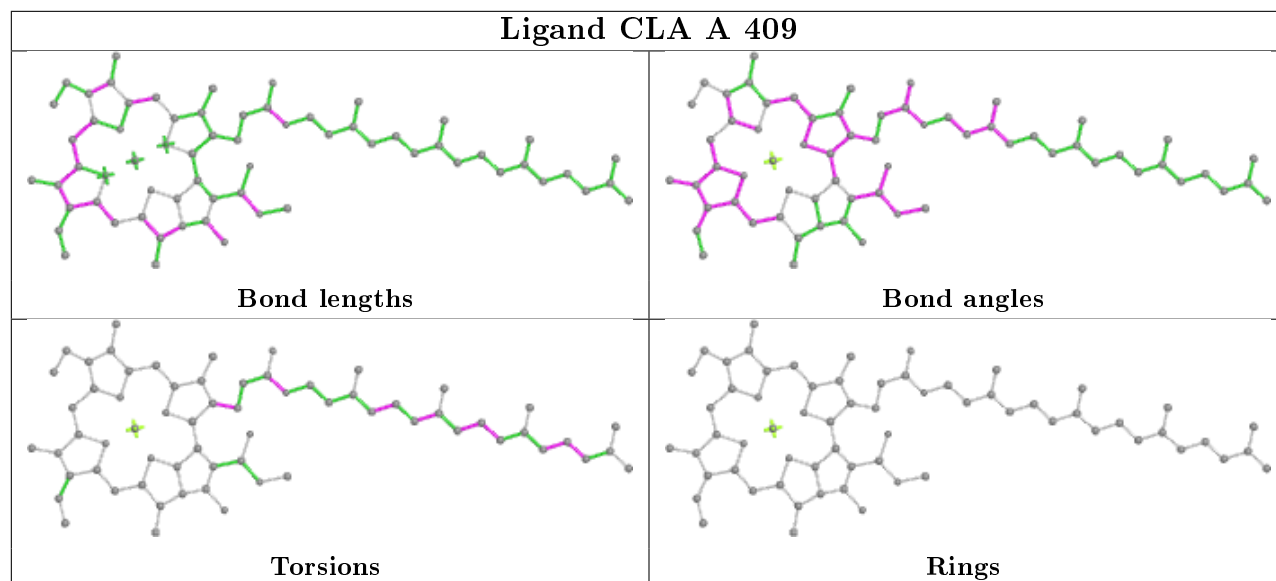
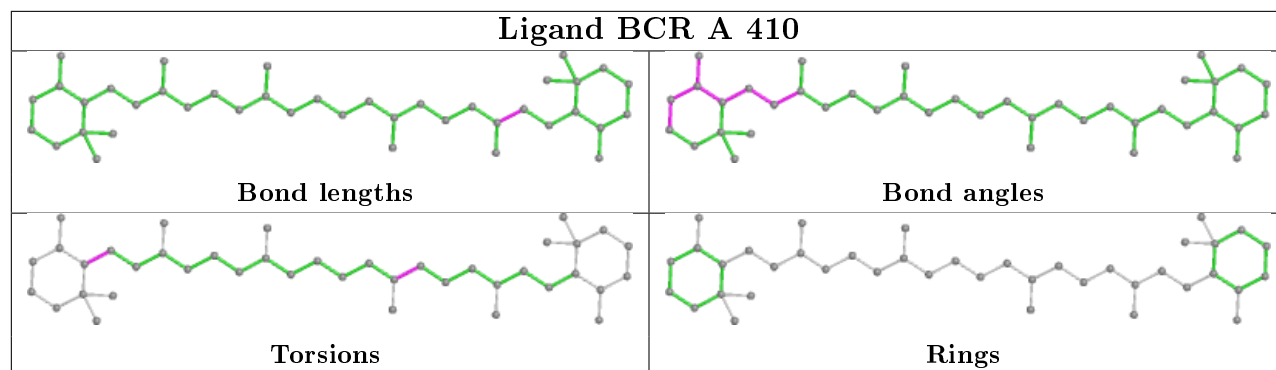




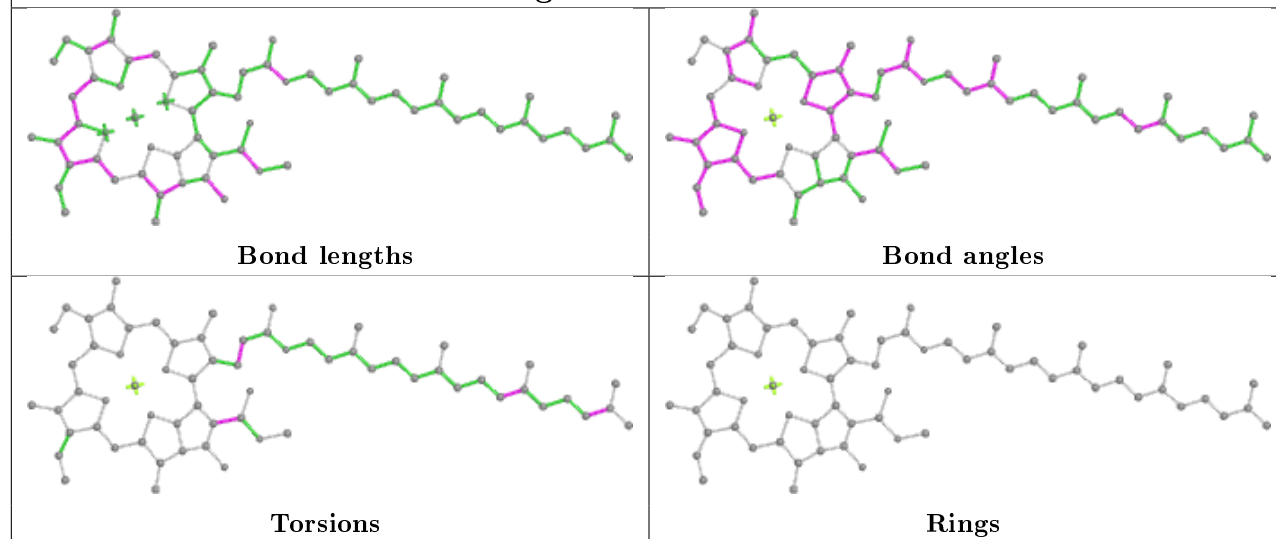
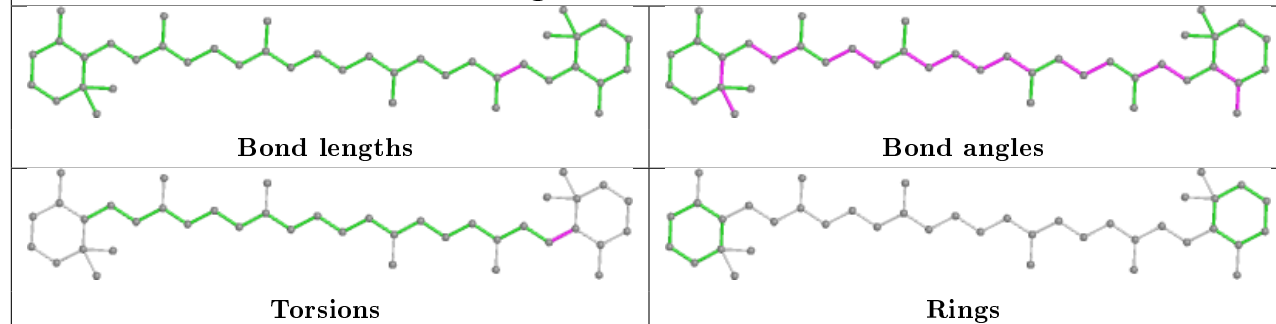
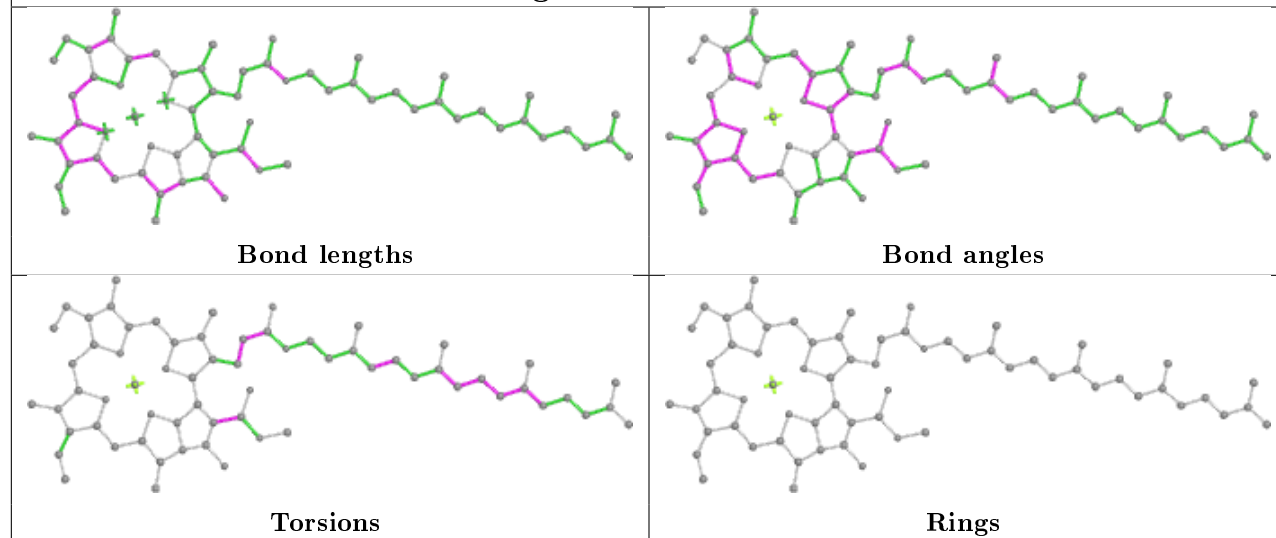


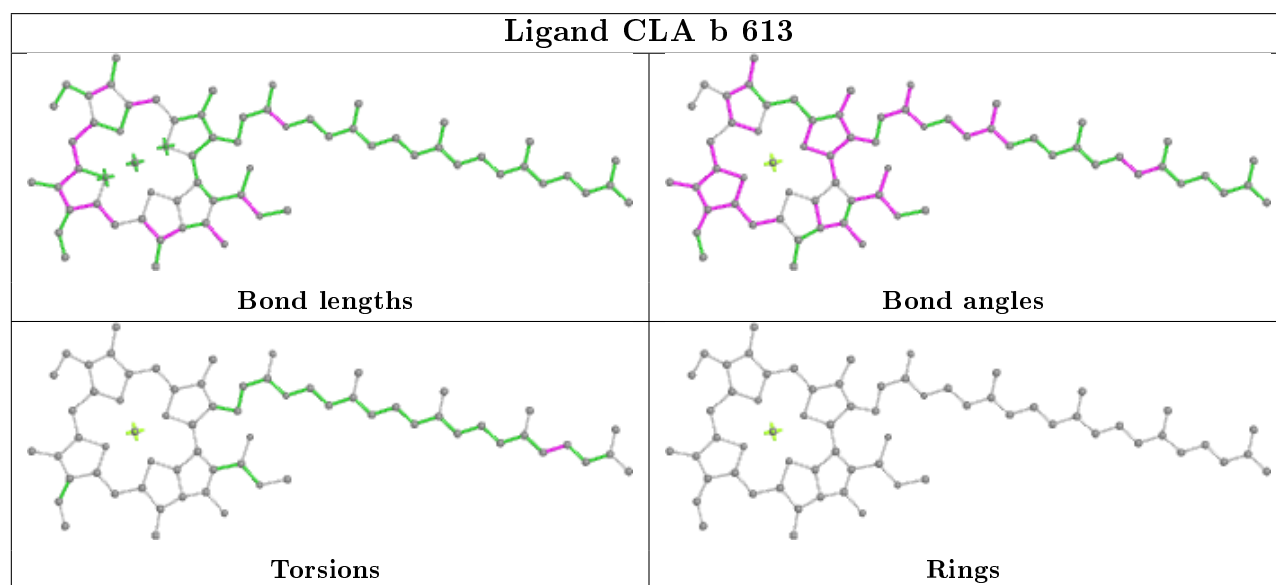
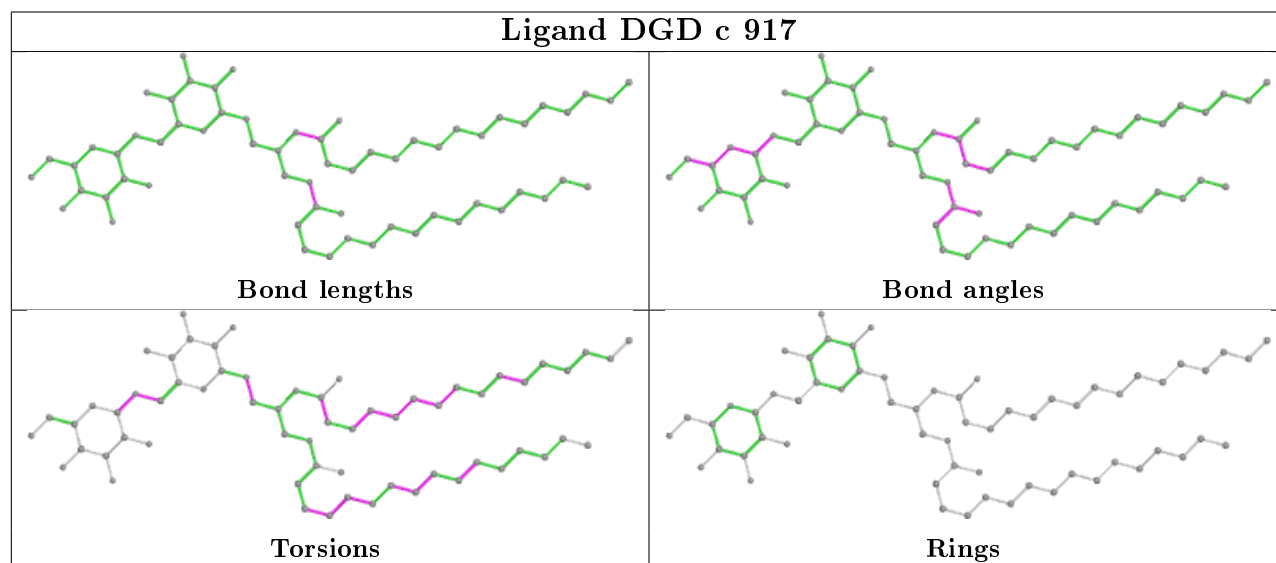
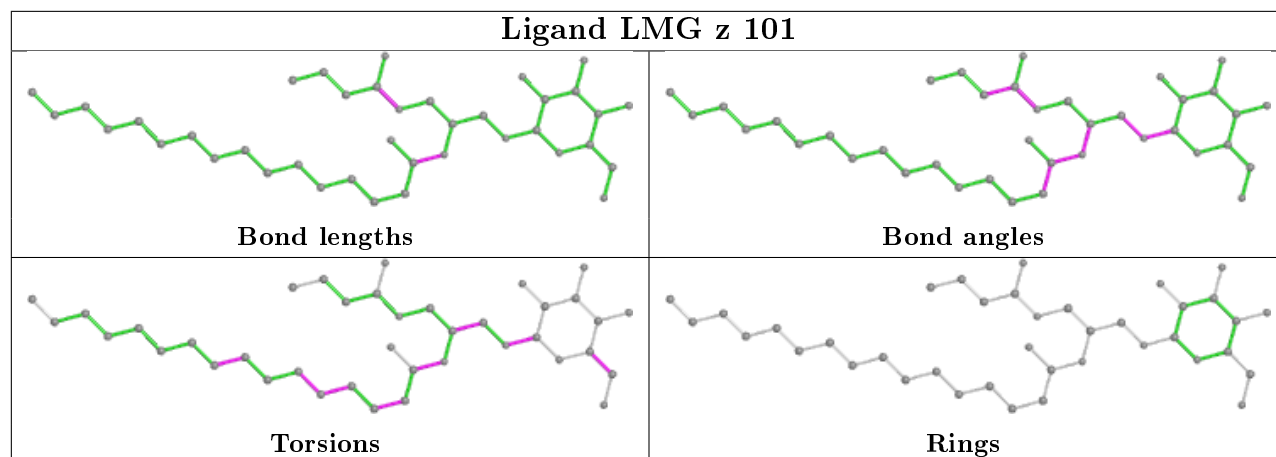


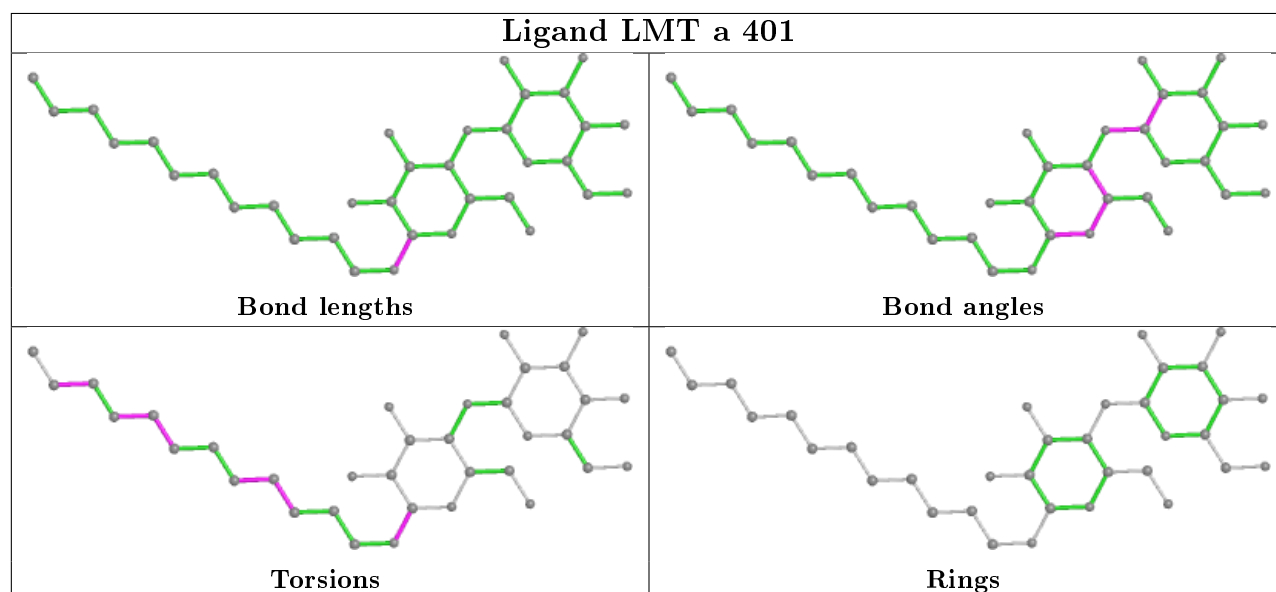
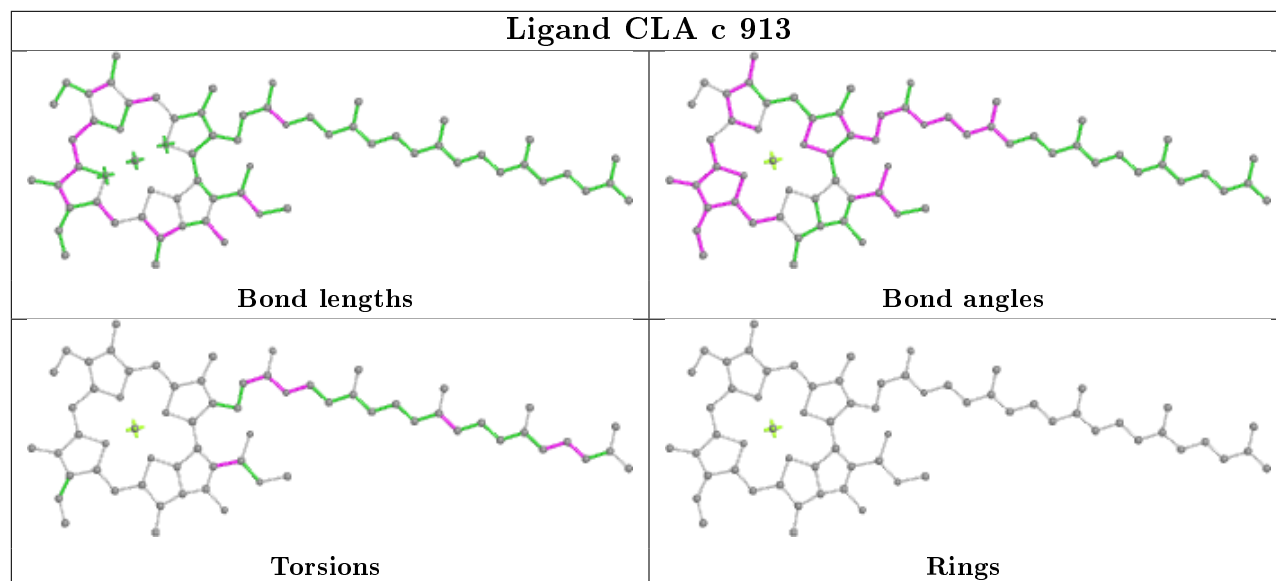
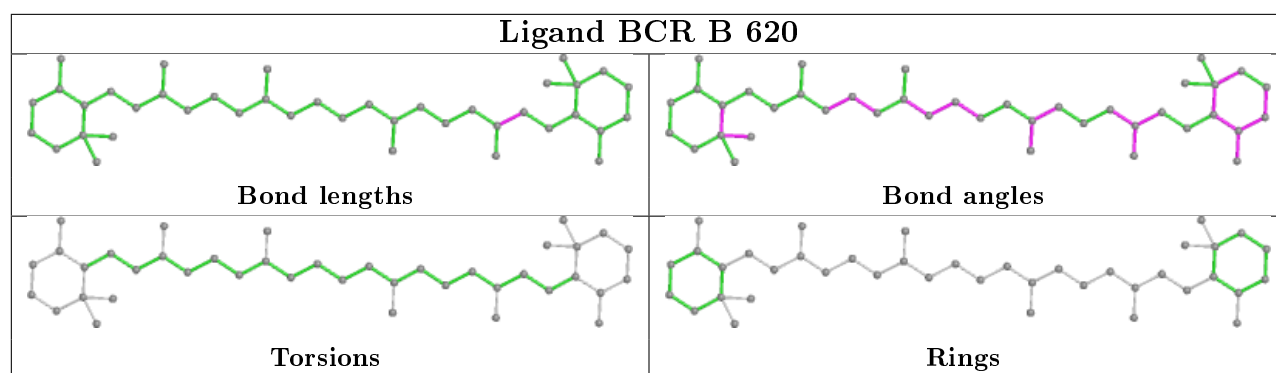


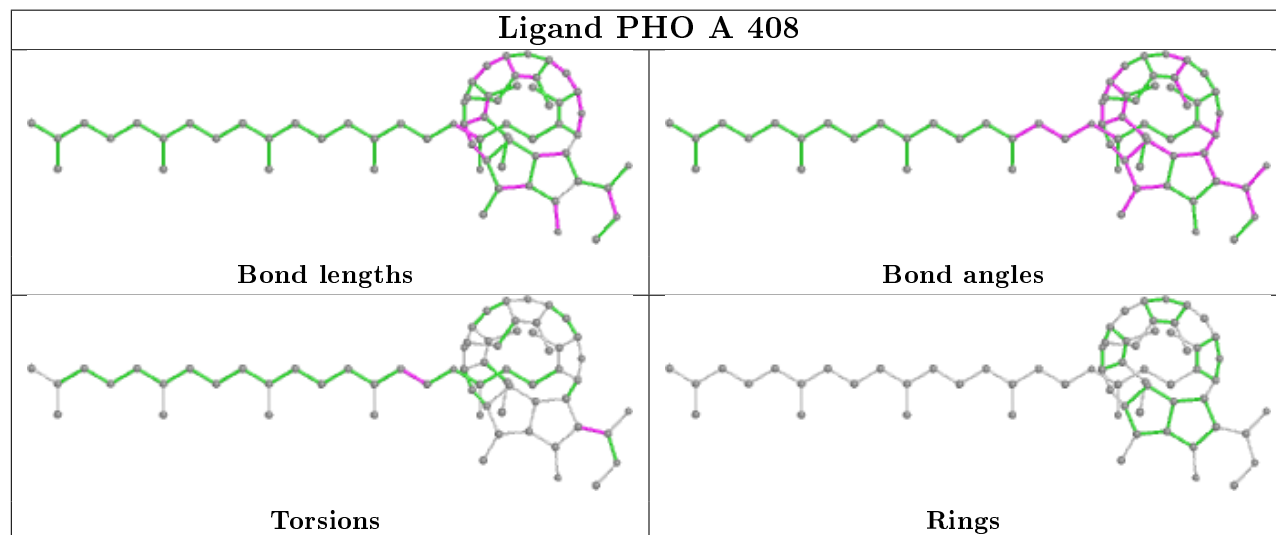
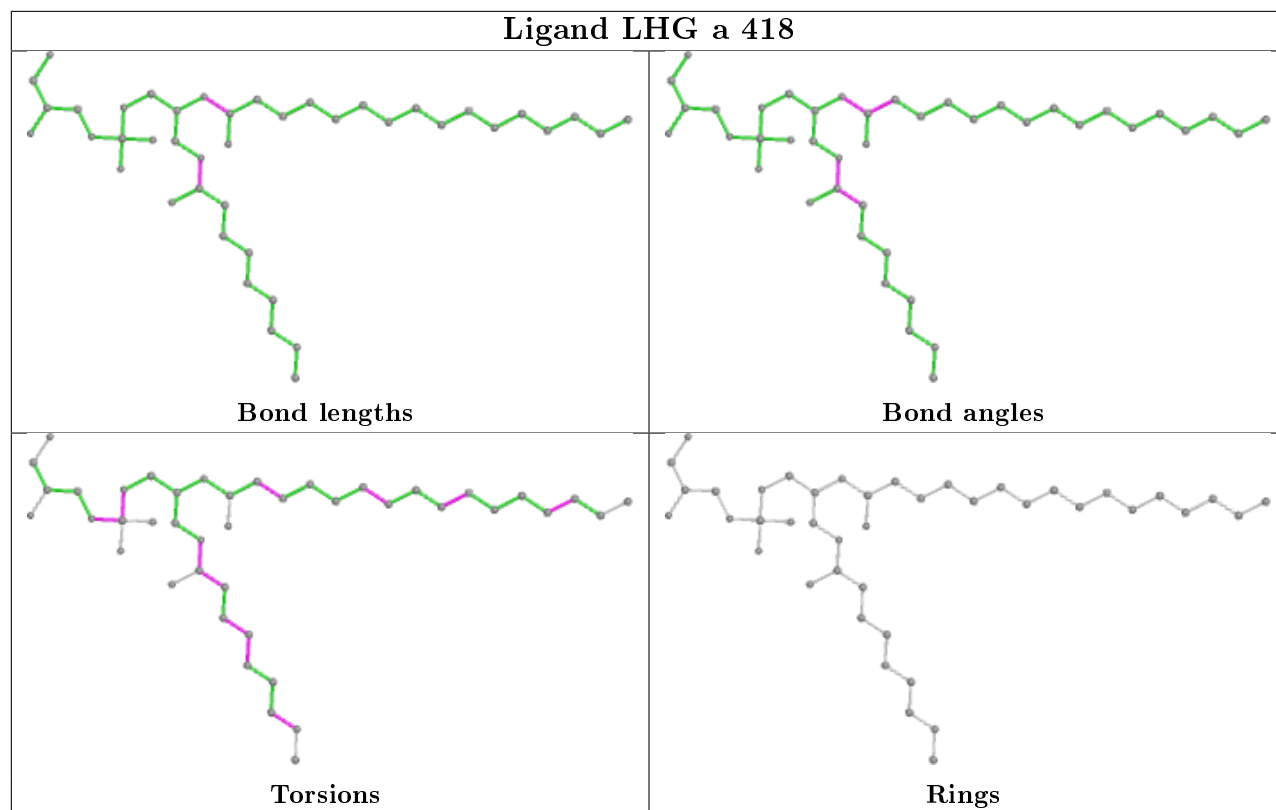




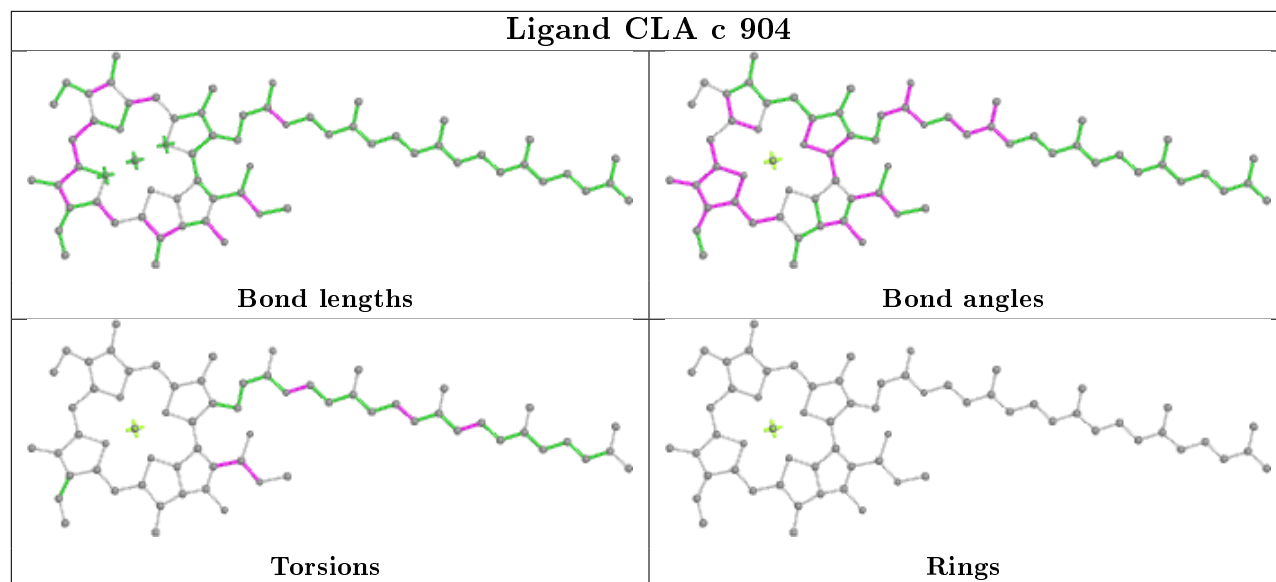
**Ligand CLA b 615****Ligand BCR H 101****Ligand CLA B 602**



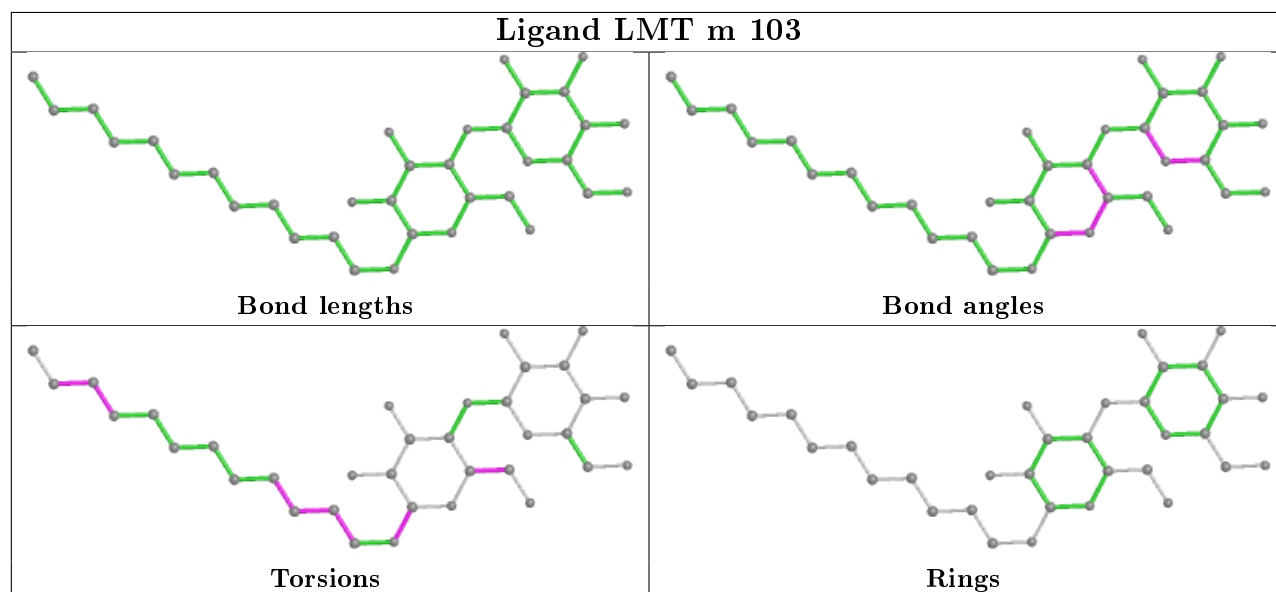




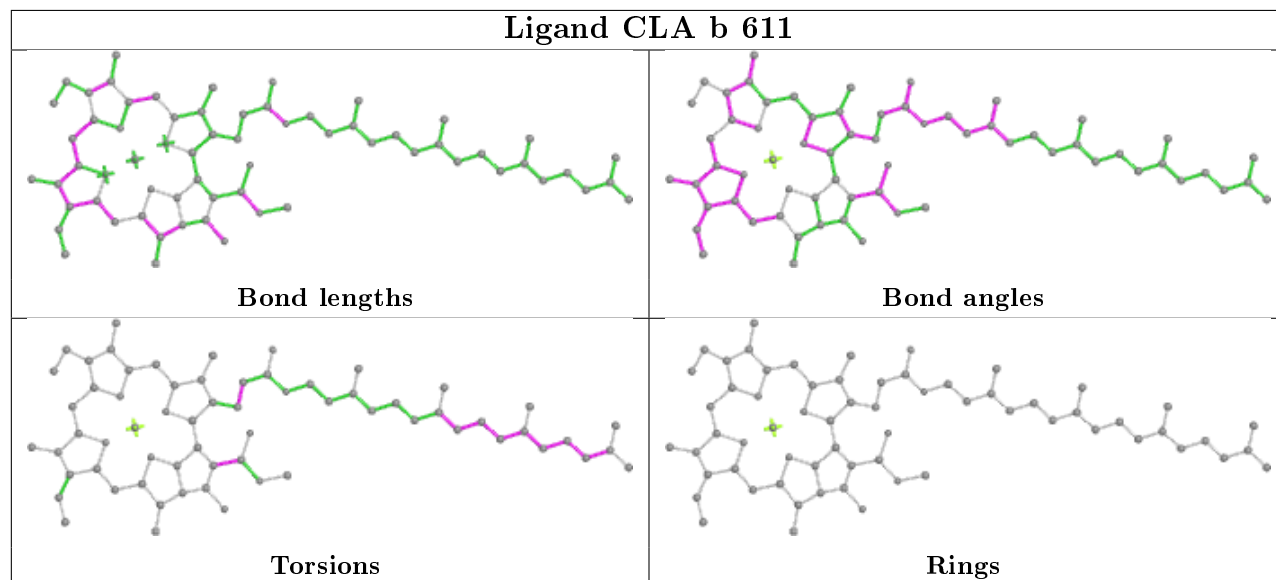
## Ligand CLA c 904



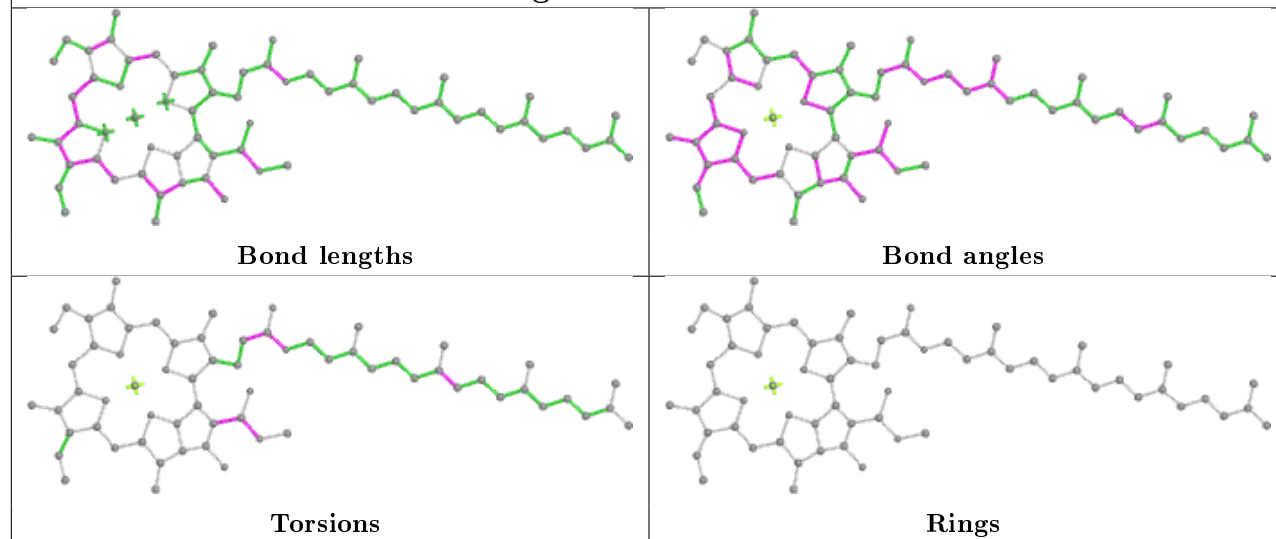
## Ligand LMT m 103



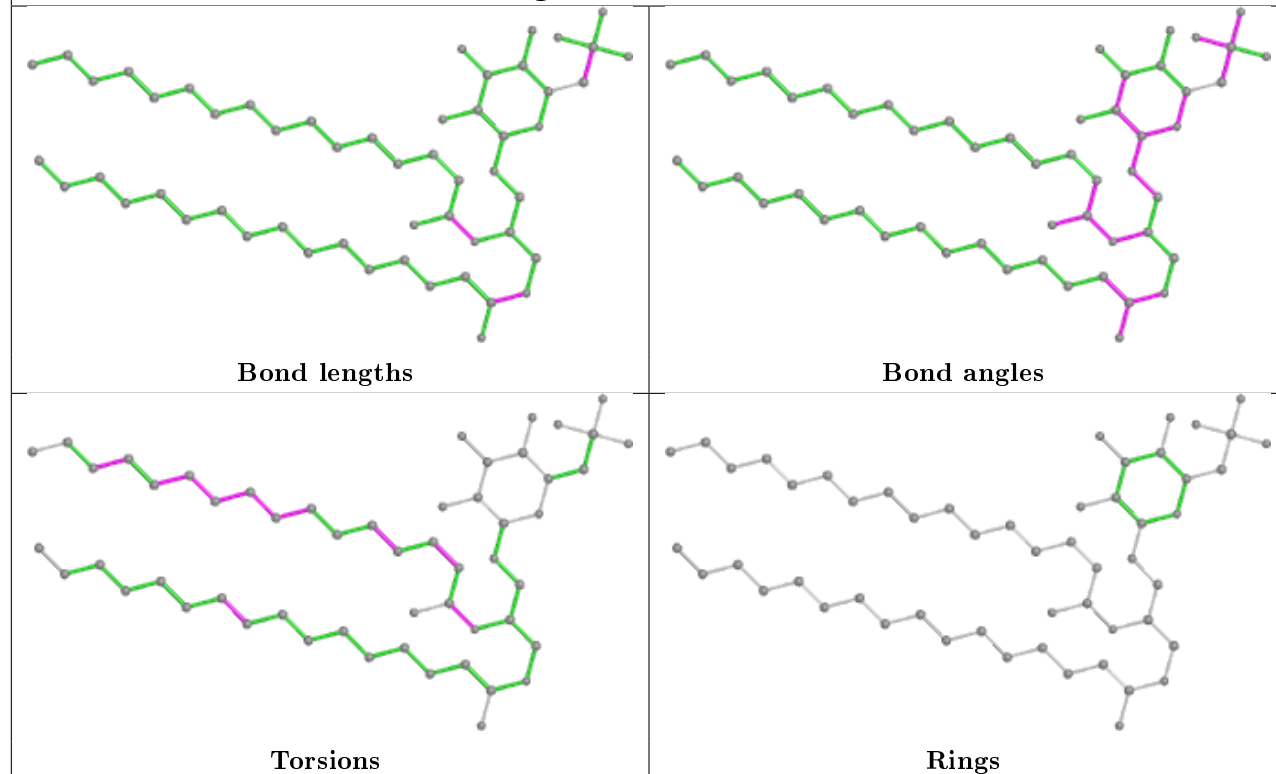
## Ligand CLA b 611



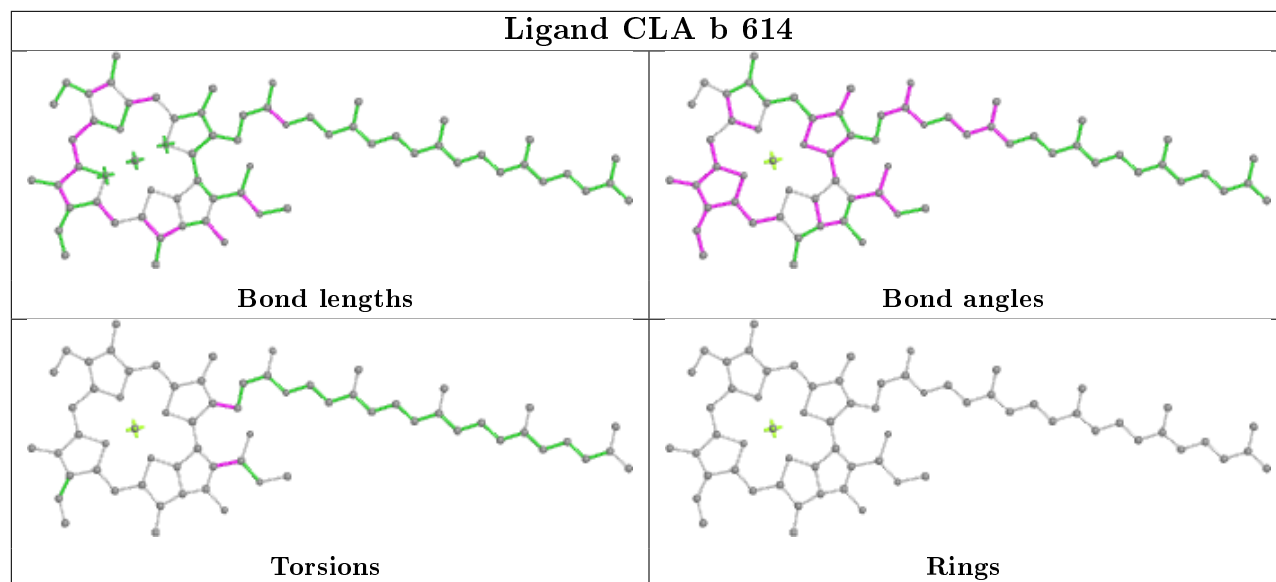
## Ligand CLA C 512



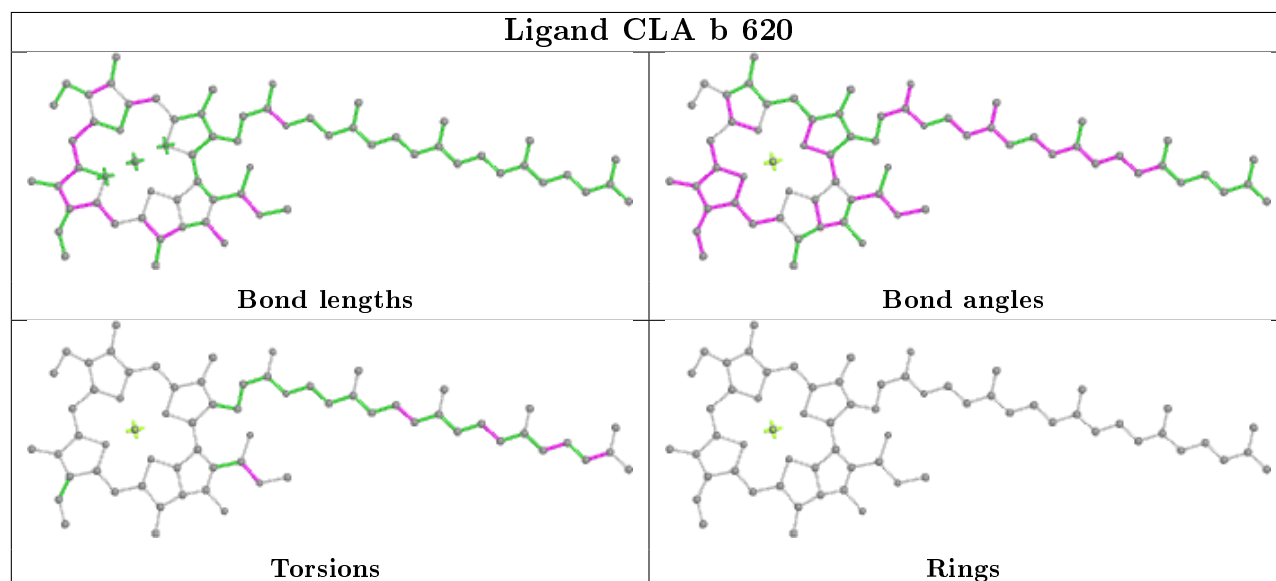
## Ligand SQD A 411



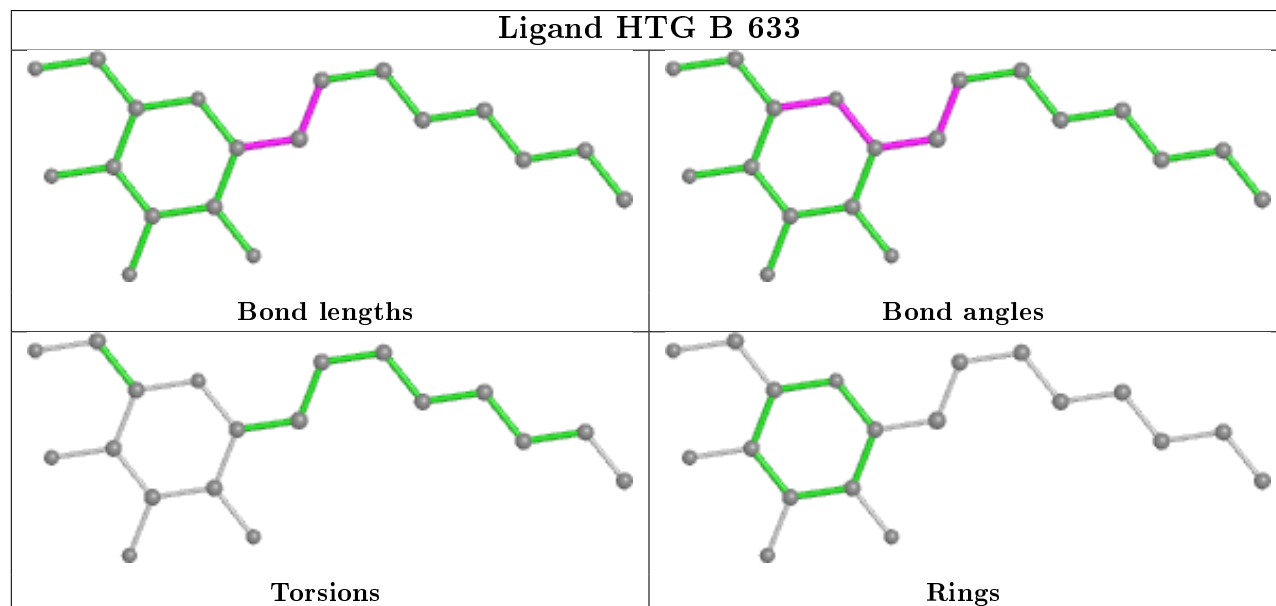
## Ligand CLA b 614

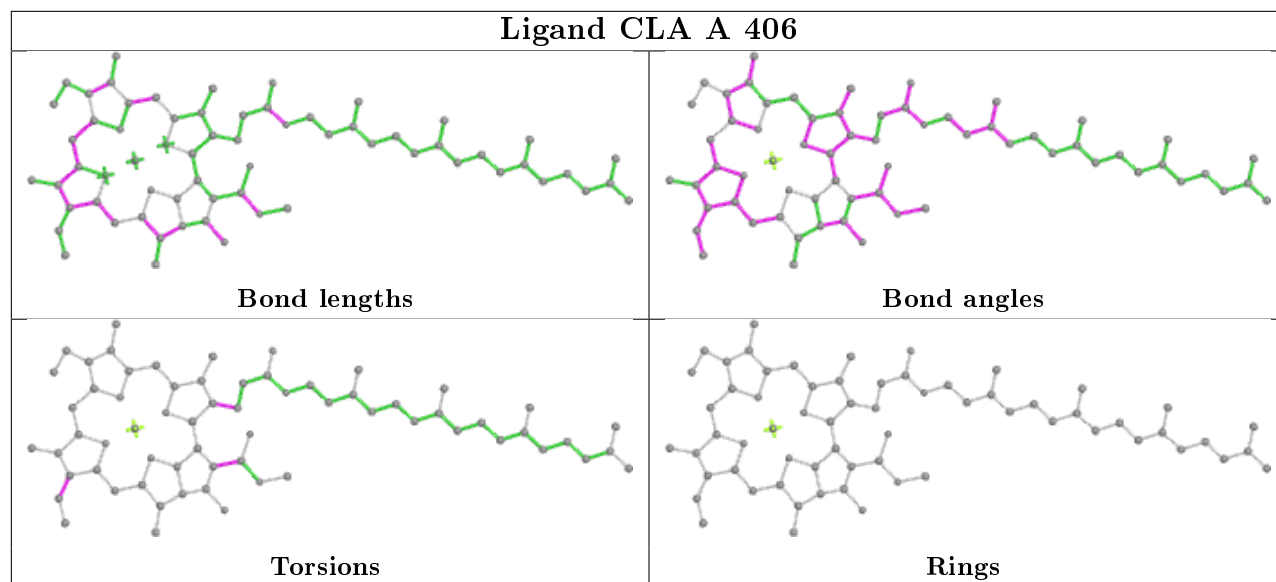
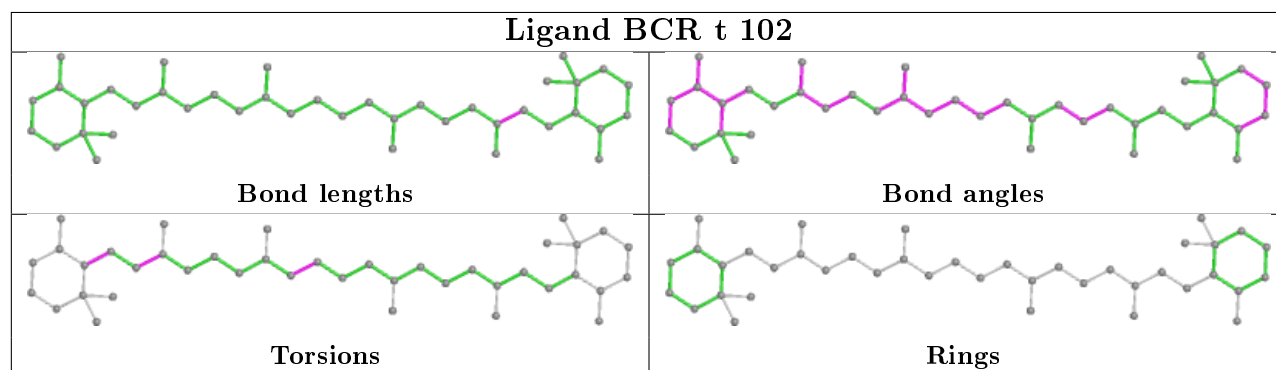
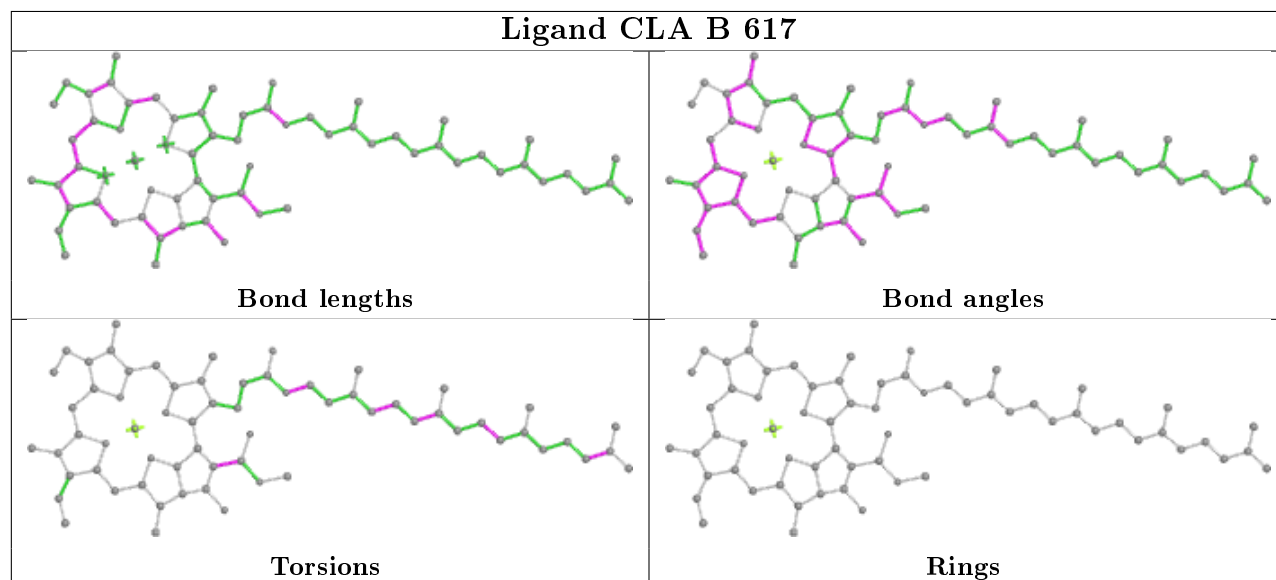


## Ligand CLA b 620

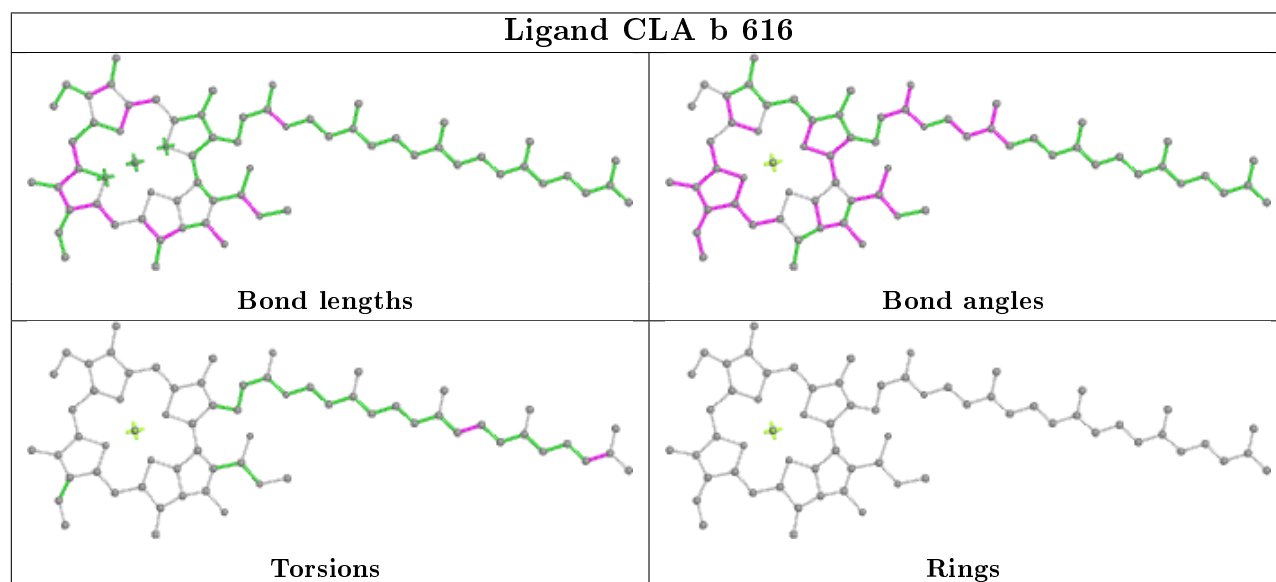
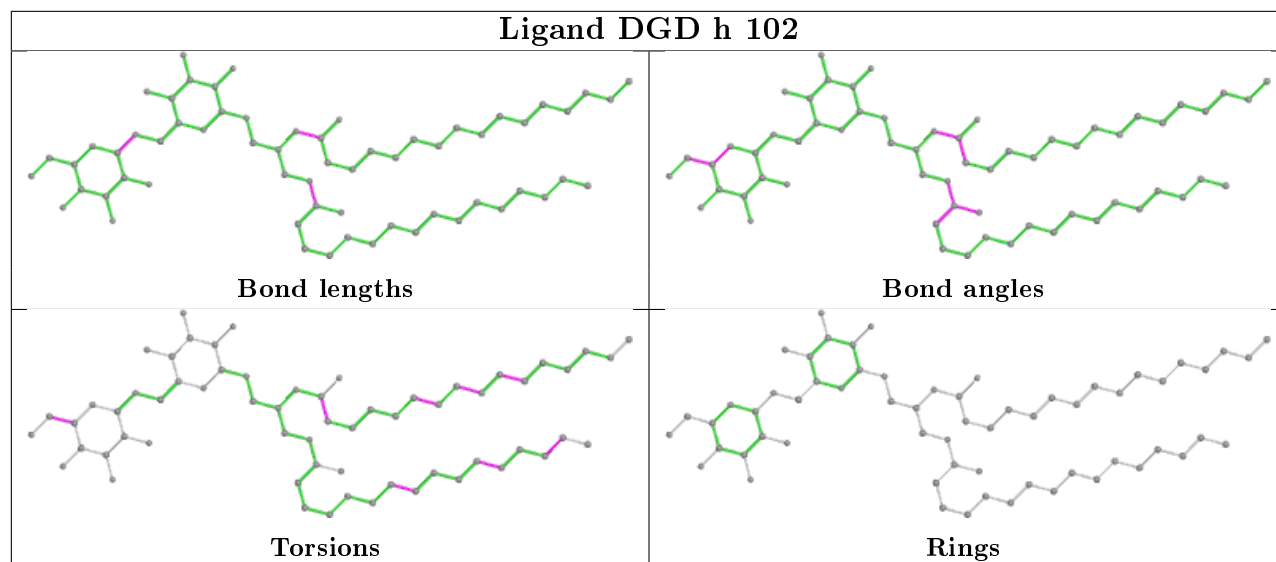
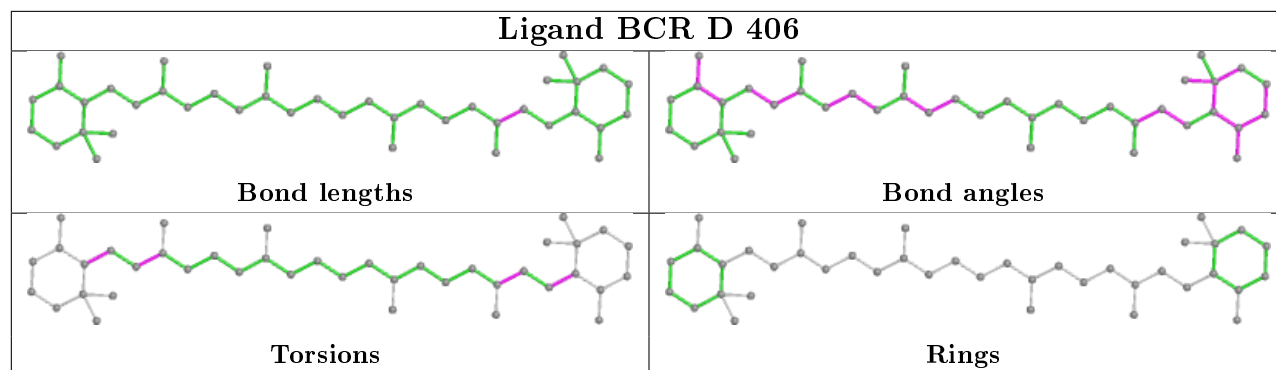


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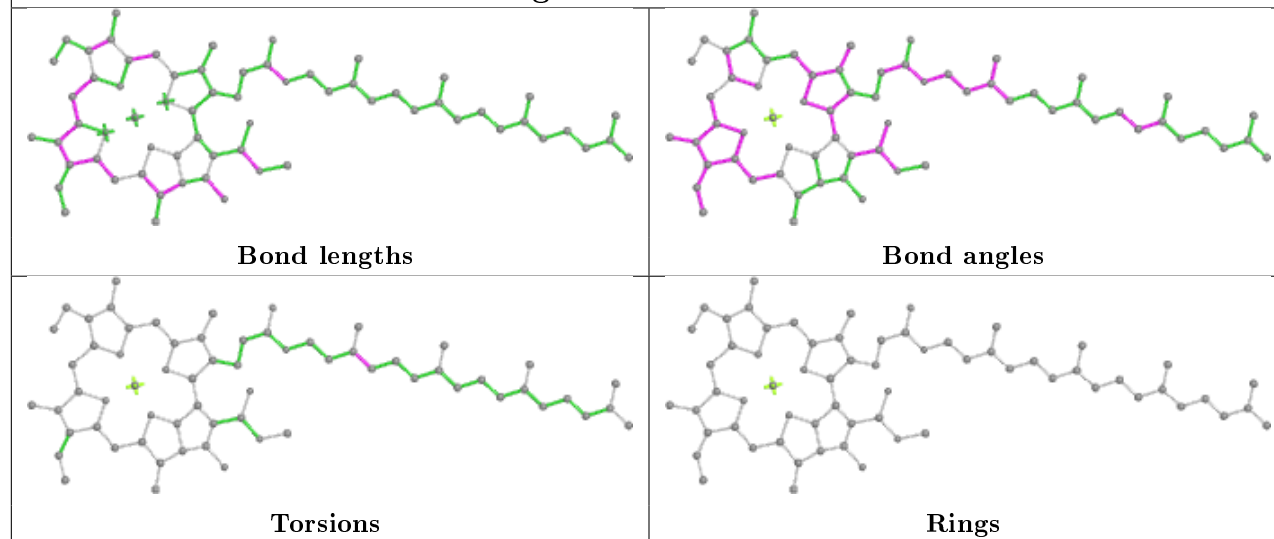


**Ligand CLA A 406****Ligand BCR t 102****Ligand CLA B 617**

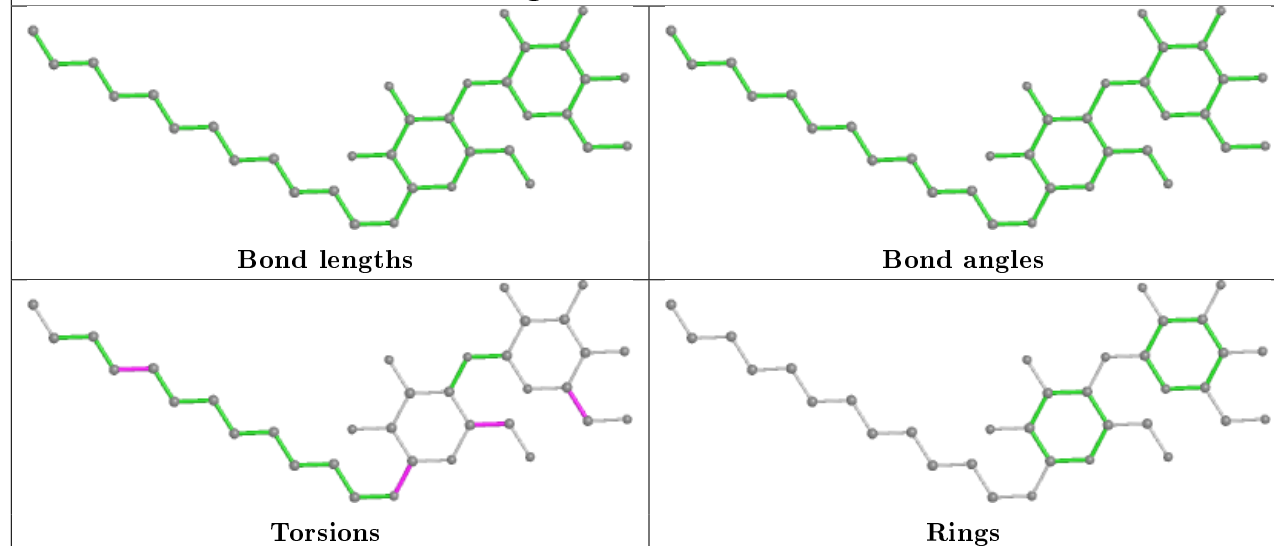




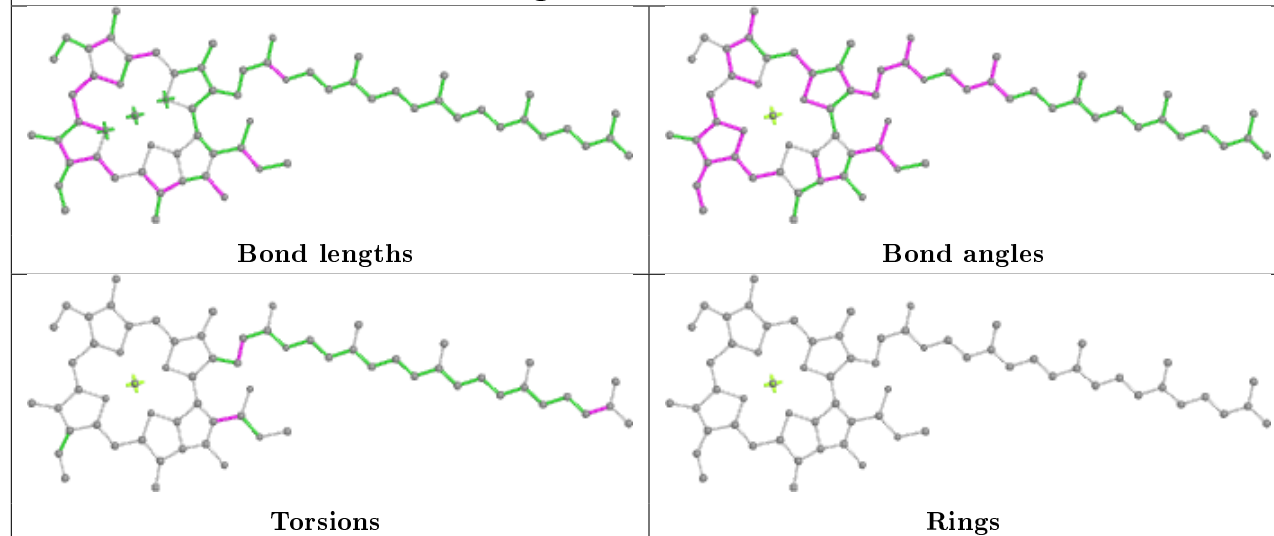
## Ligand CLA B 612



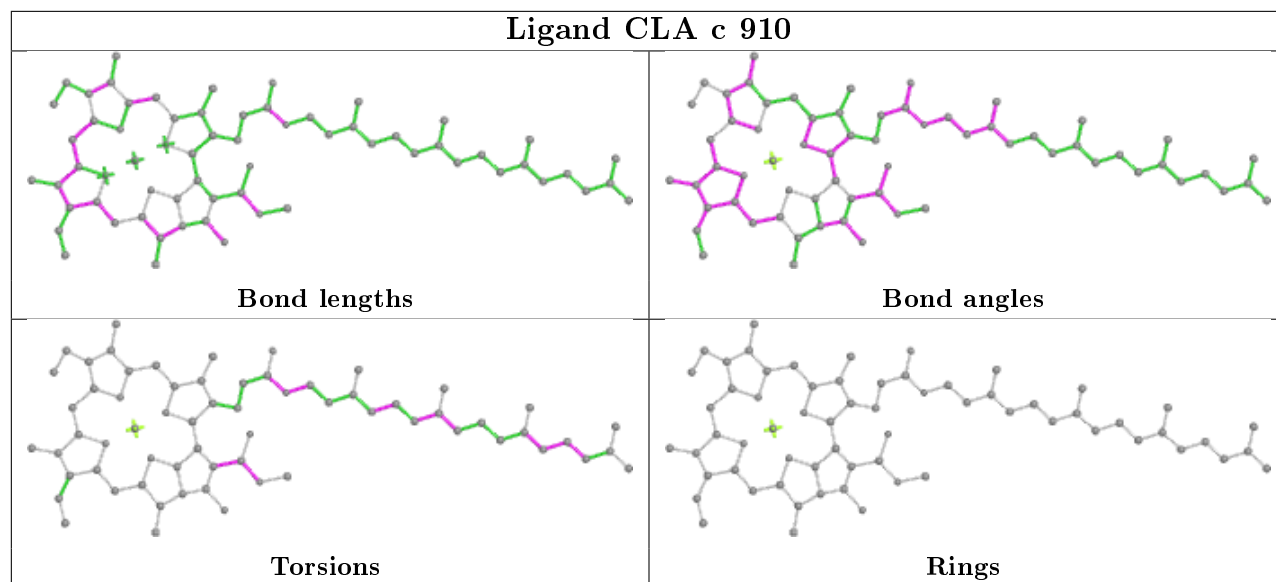
## Ligand LMT M 101



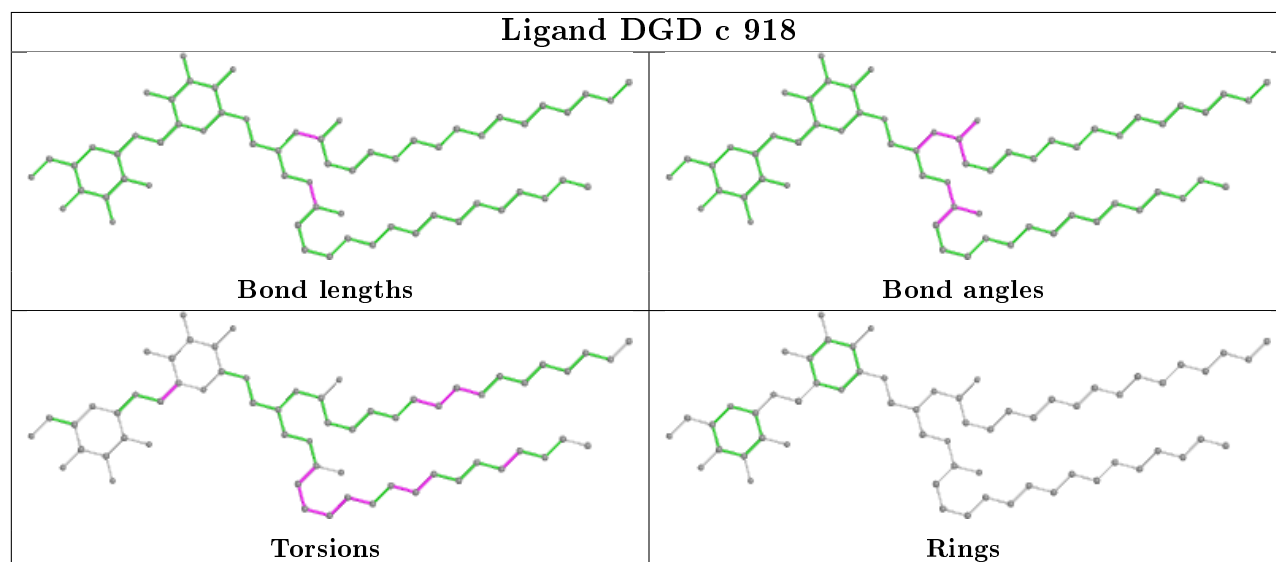
## Ligand CLA B 611



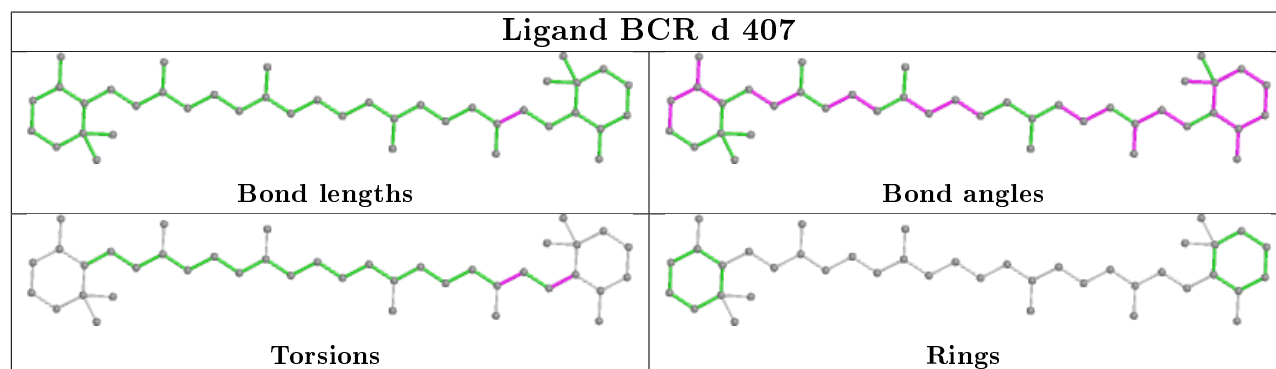
## Ligand CLA c 910

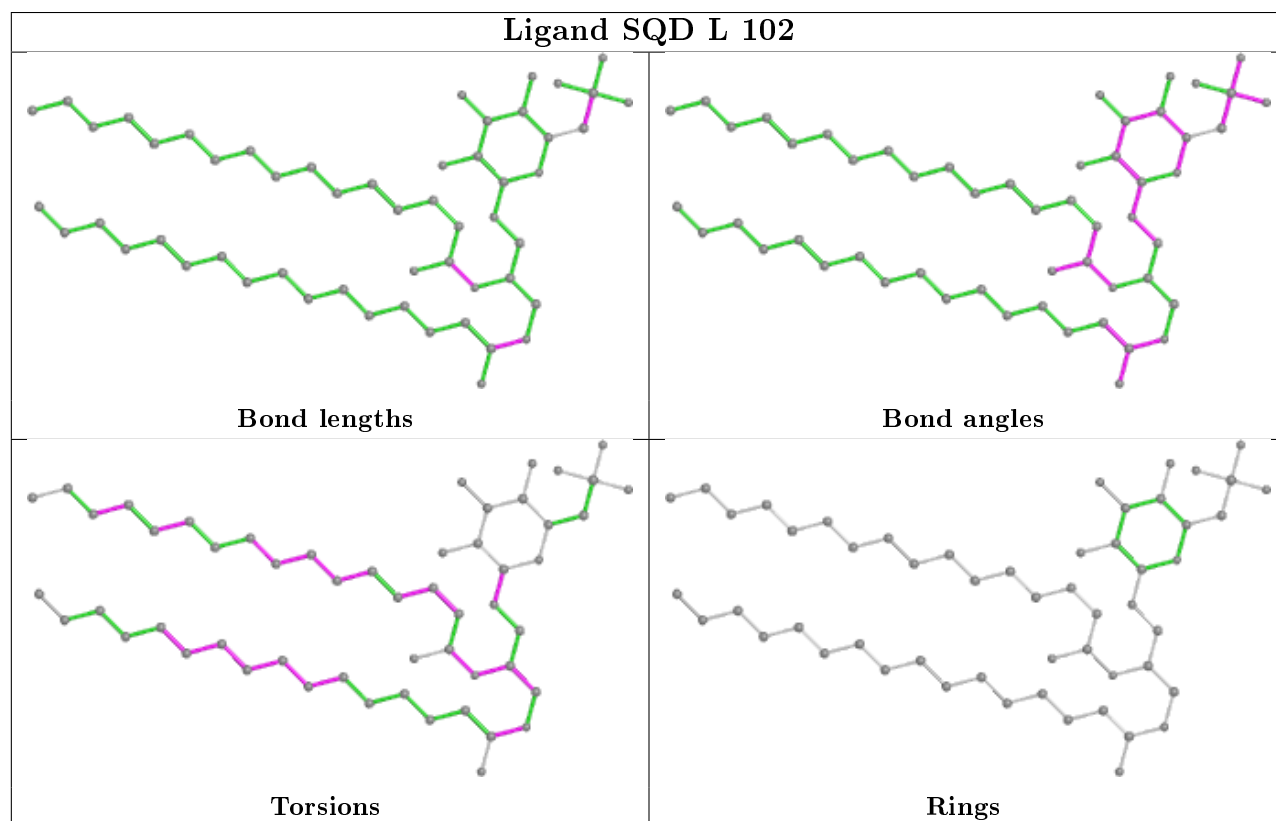
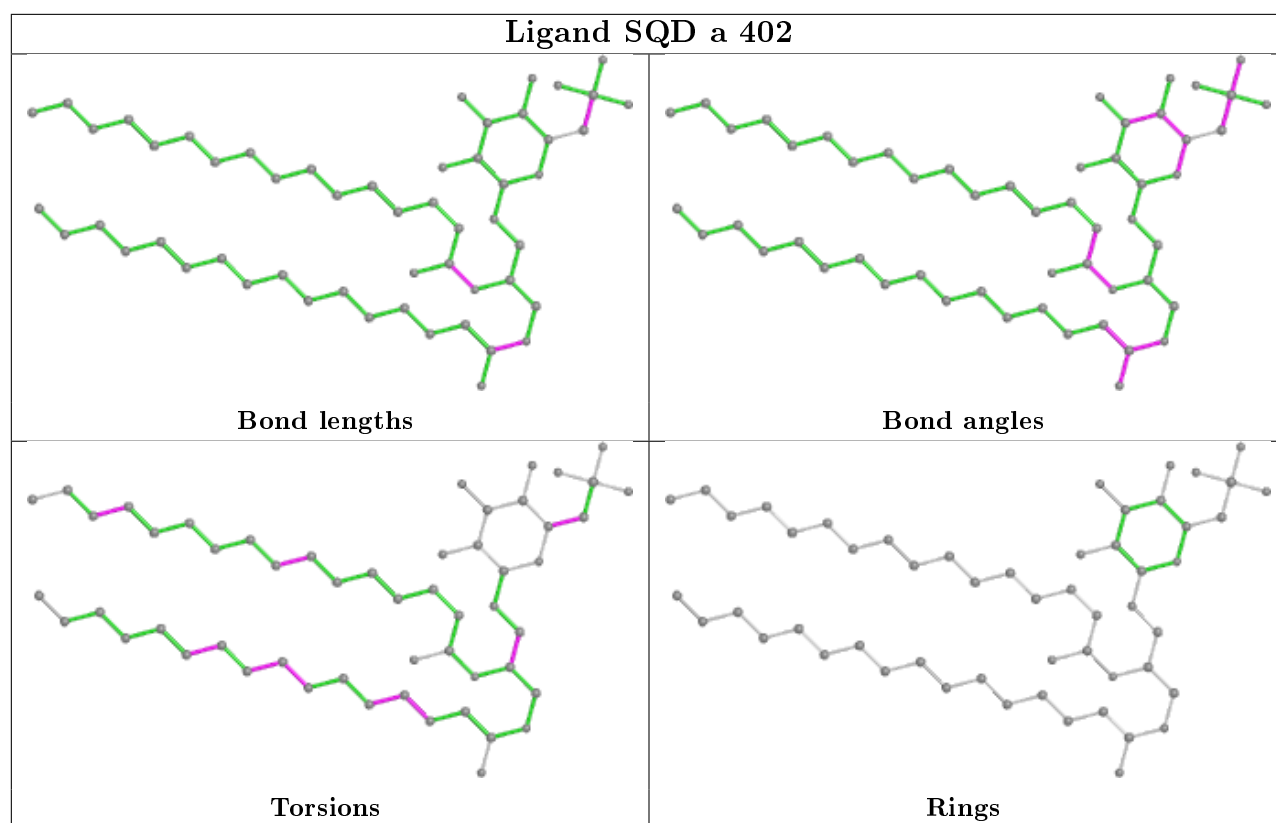


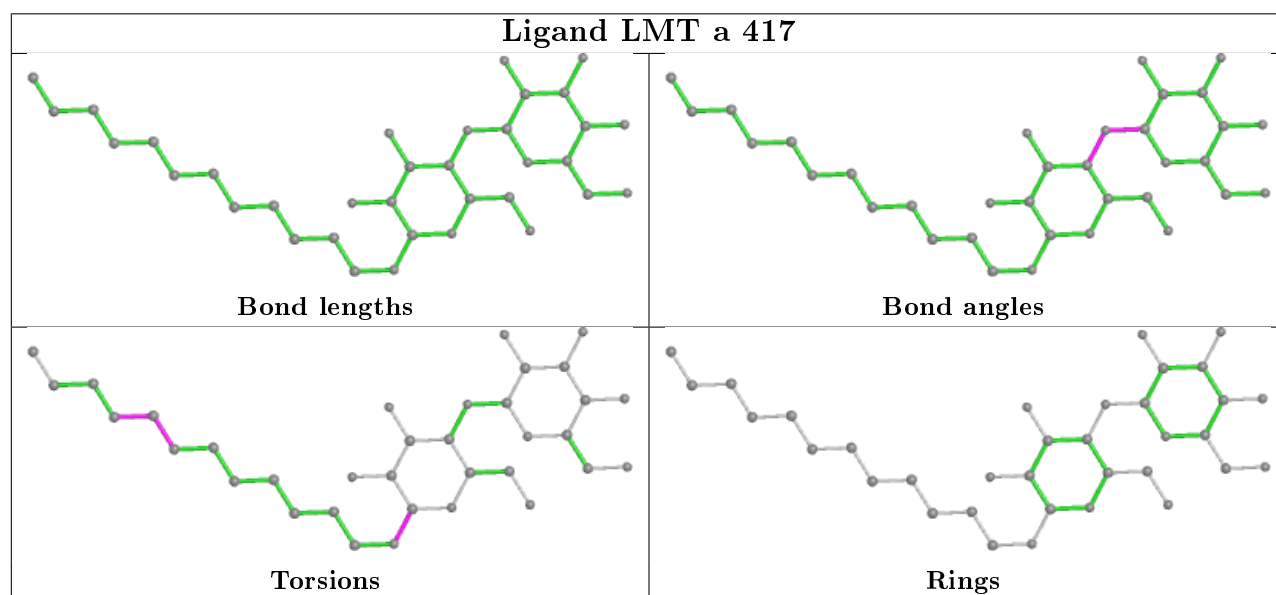
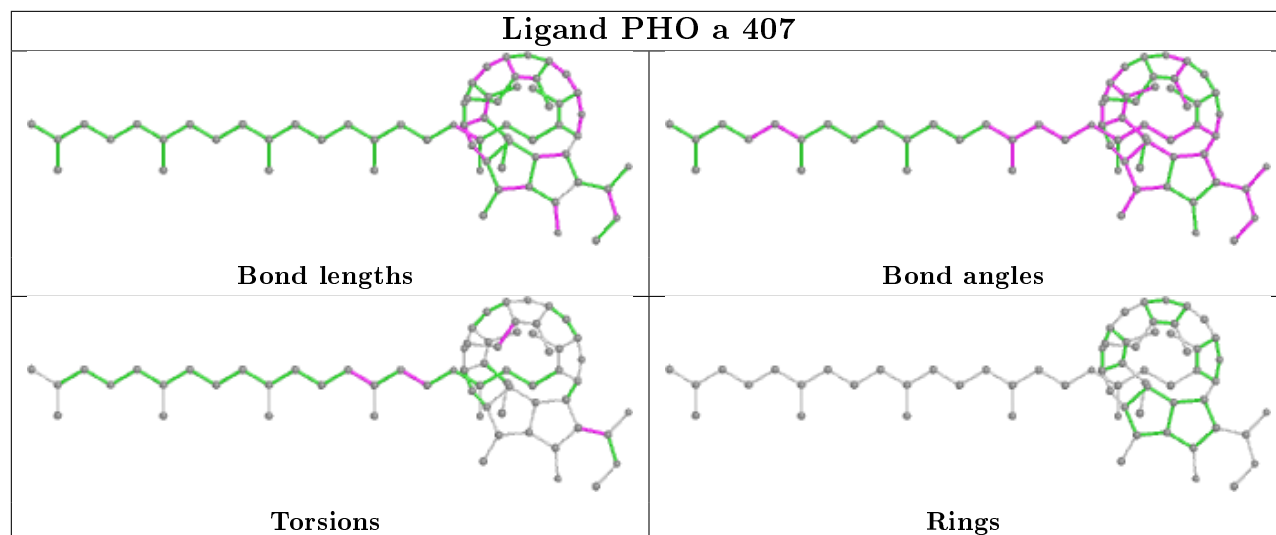
## Ligand DGD c 918

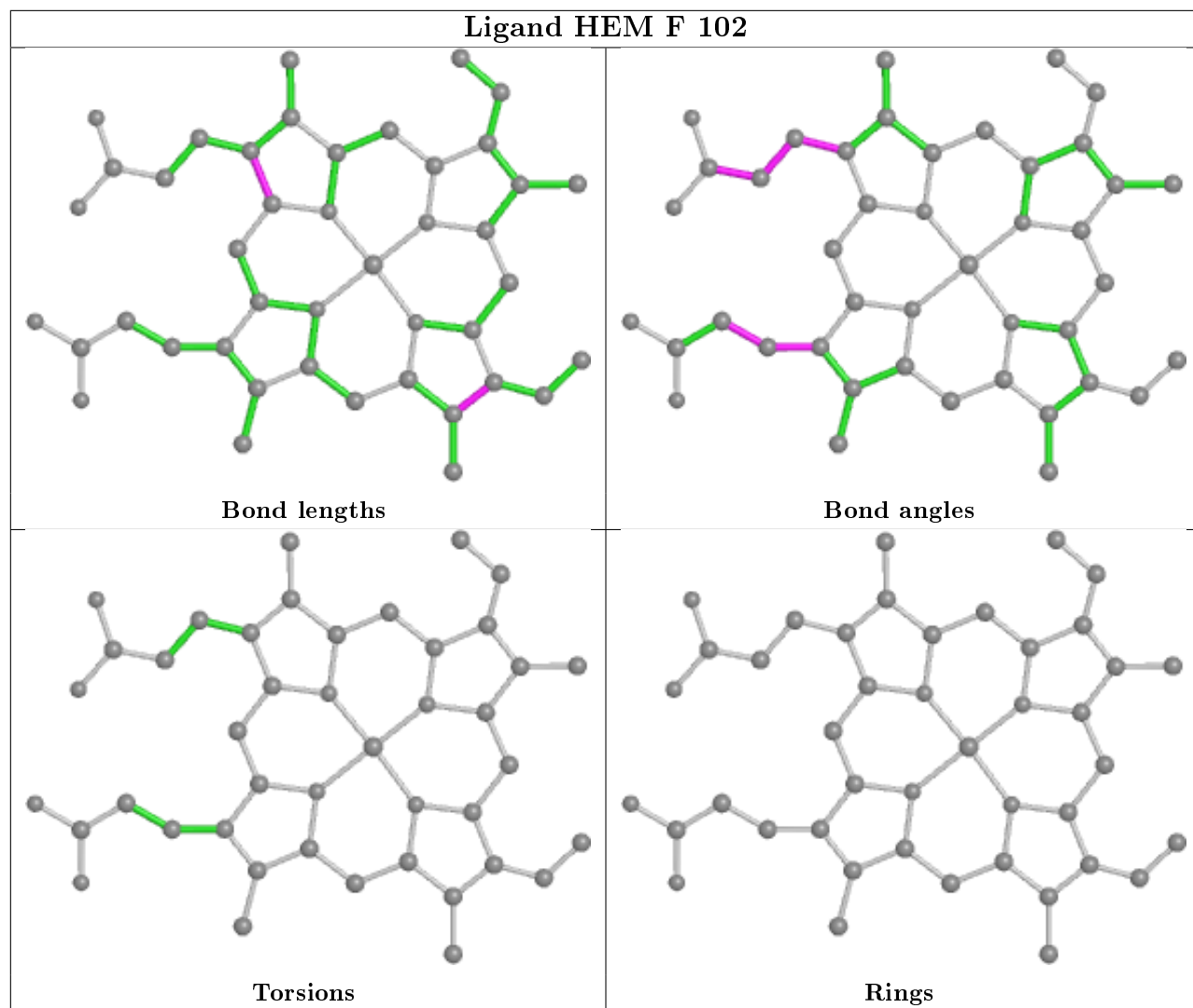


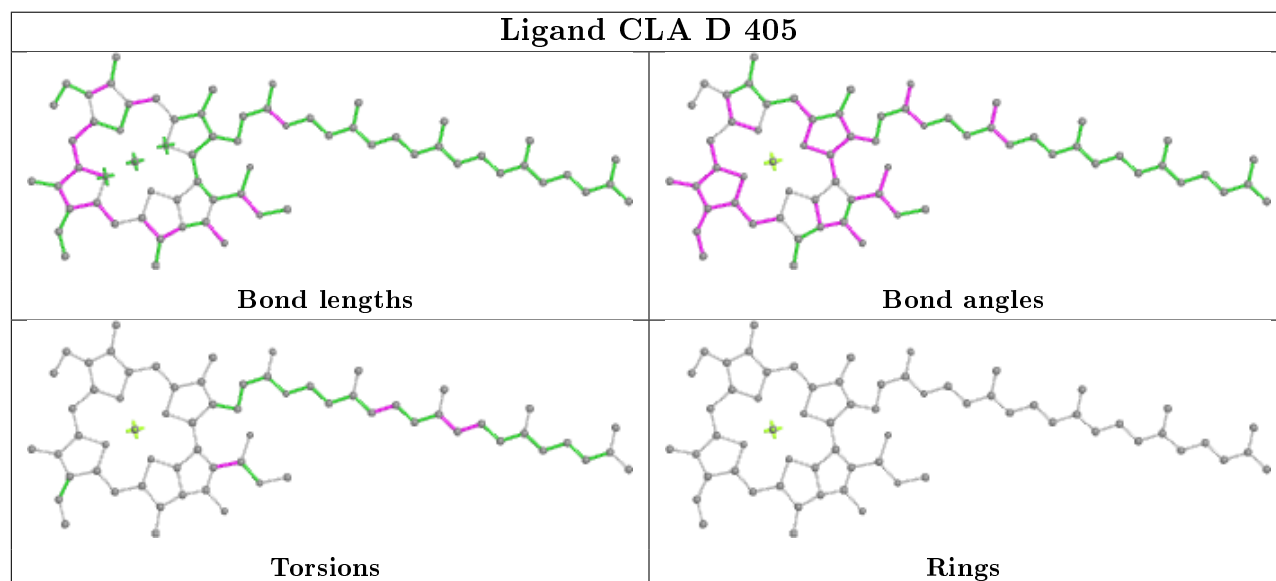
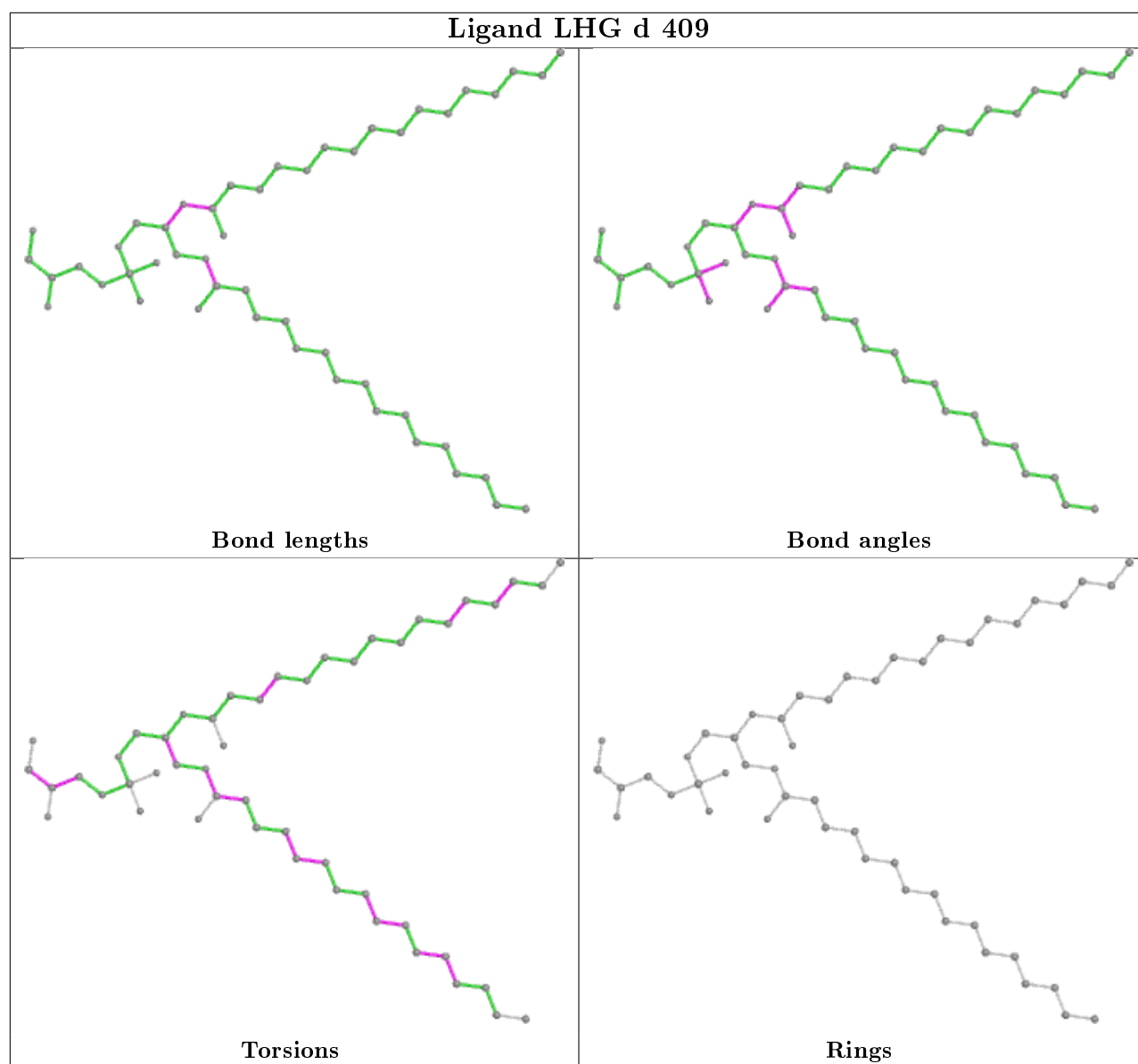
## Ligand BCR d 407

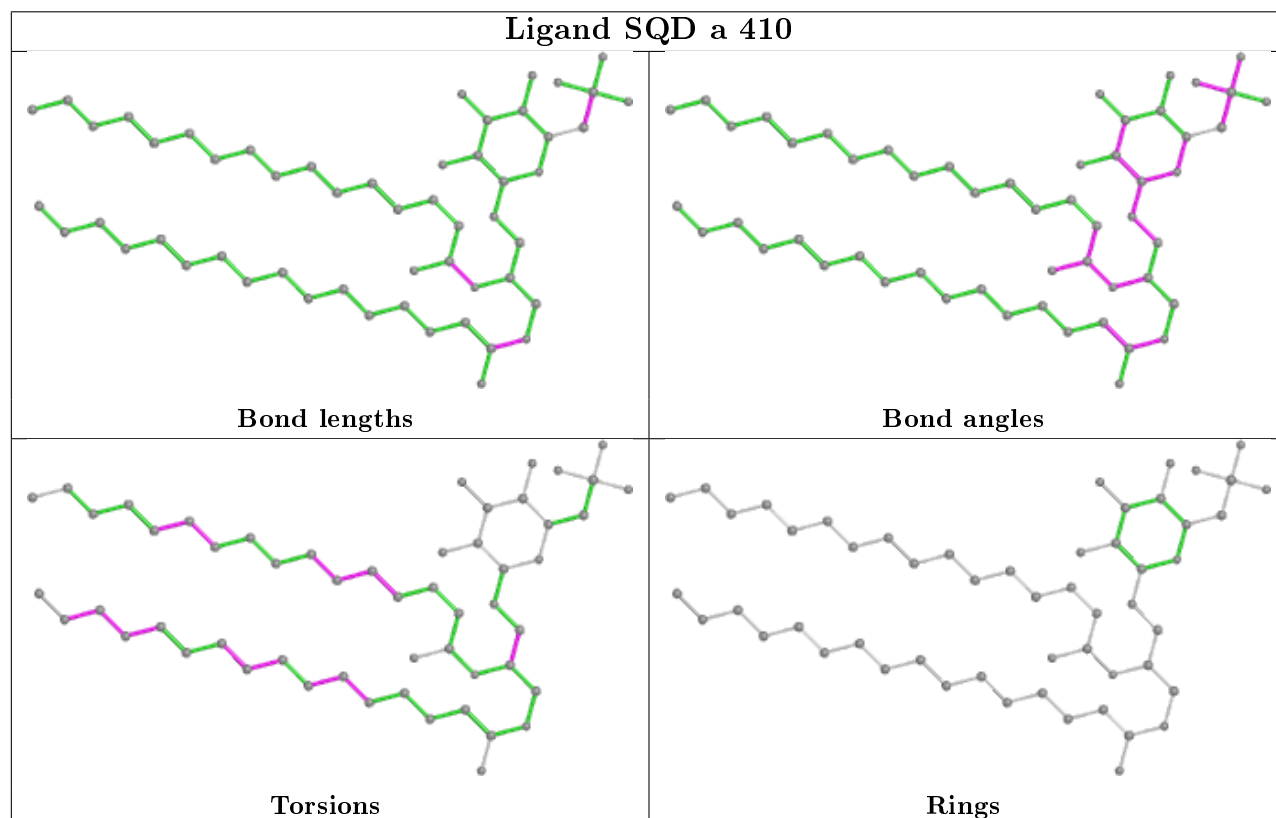
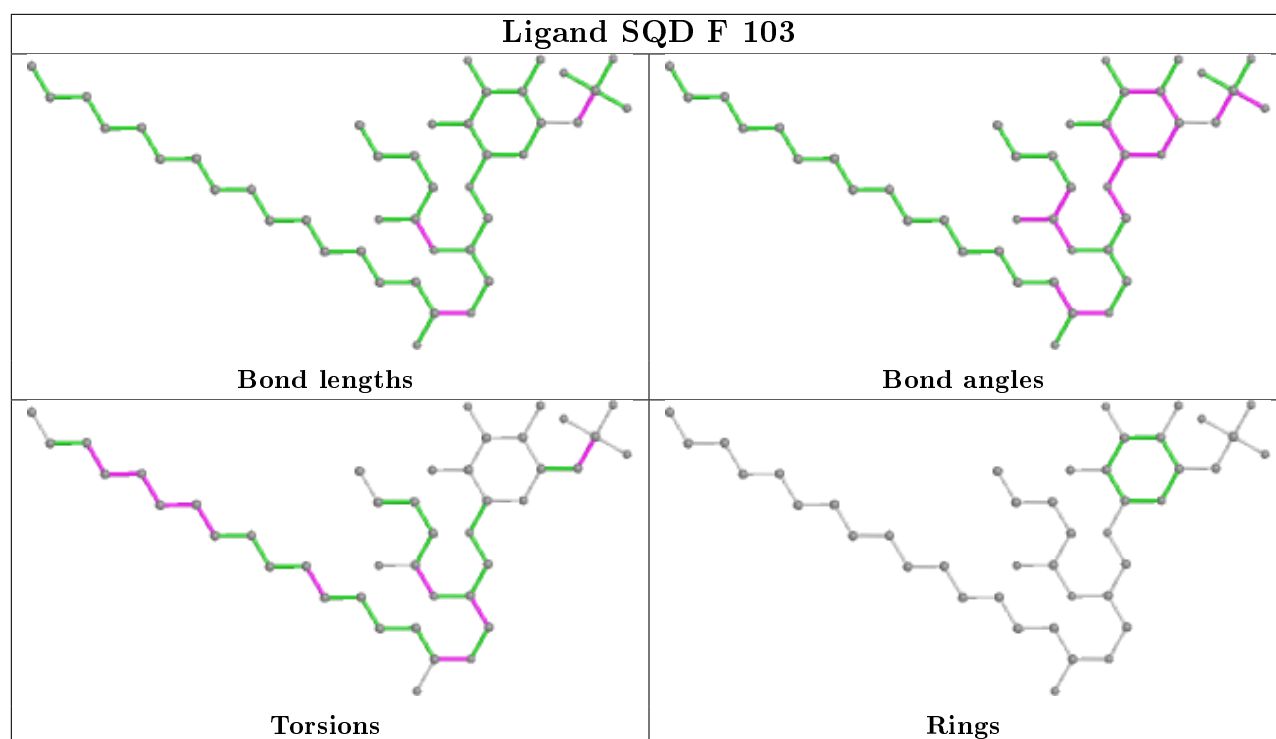




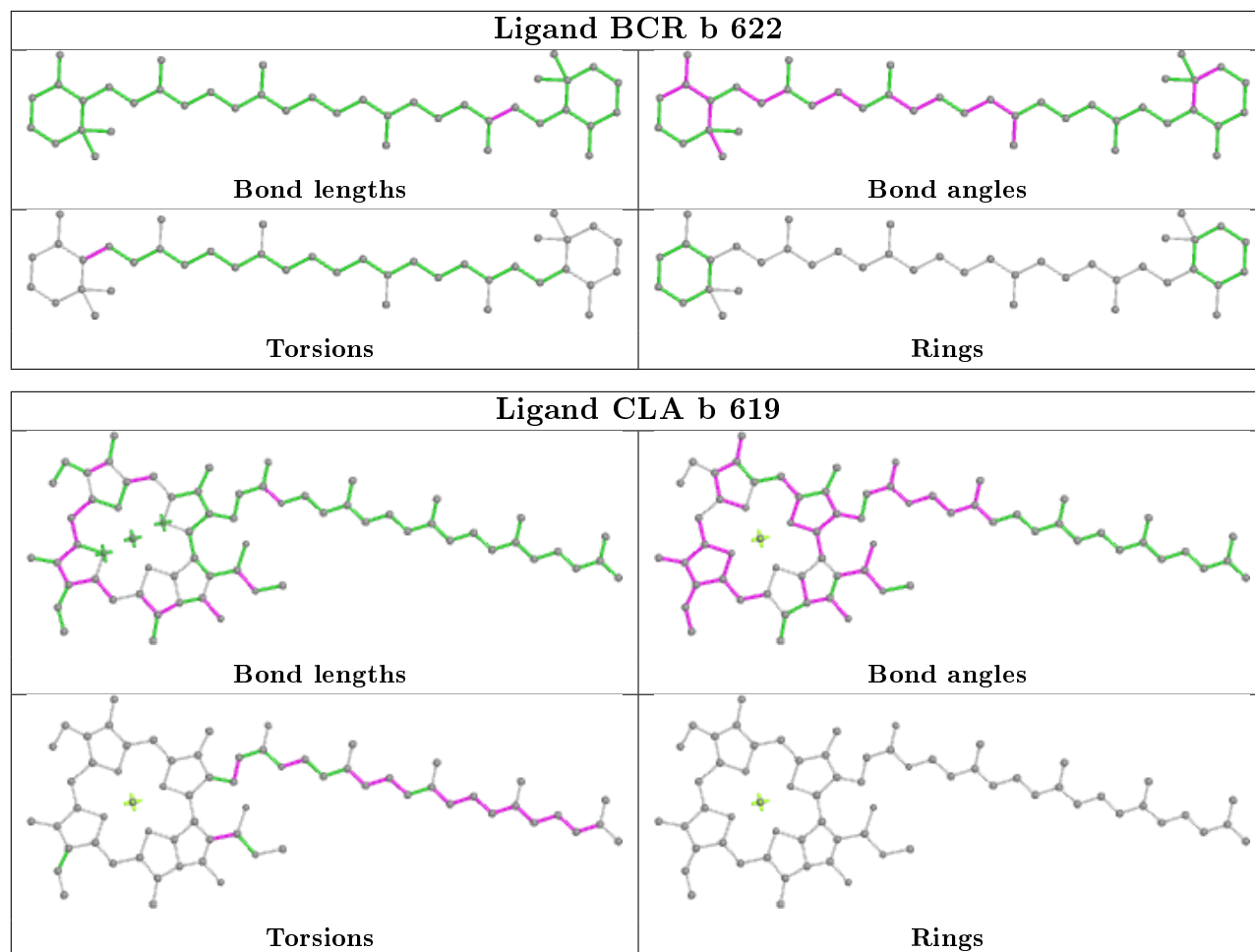


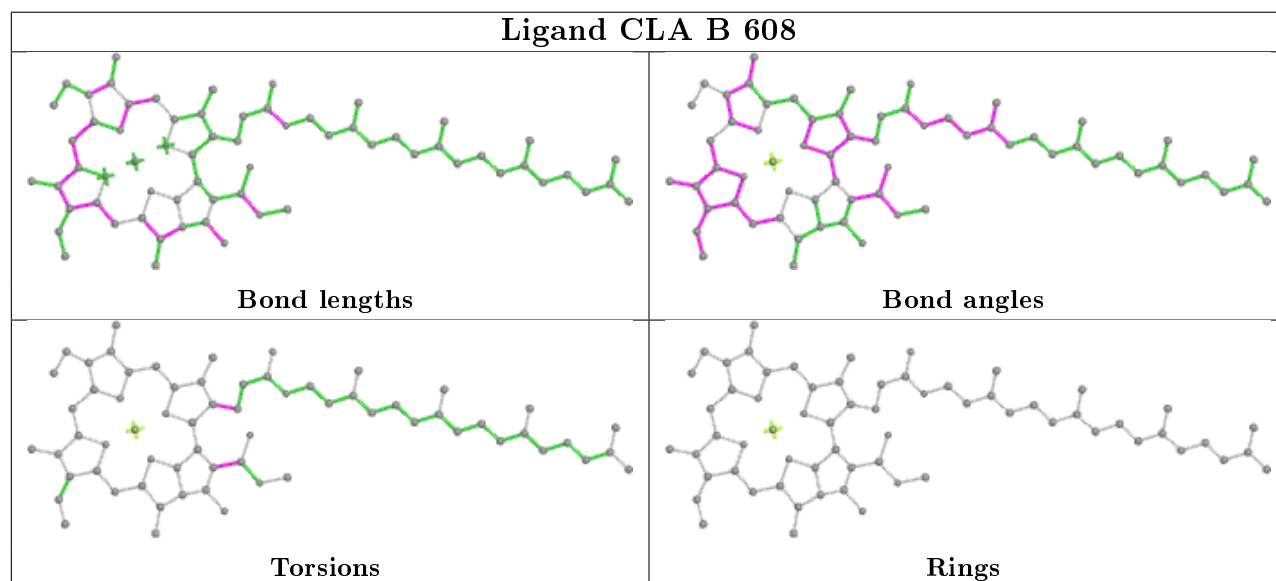
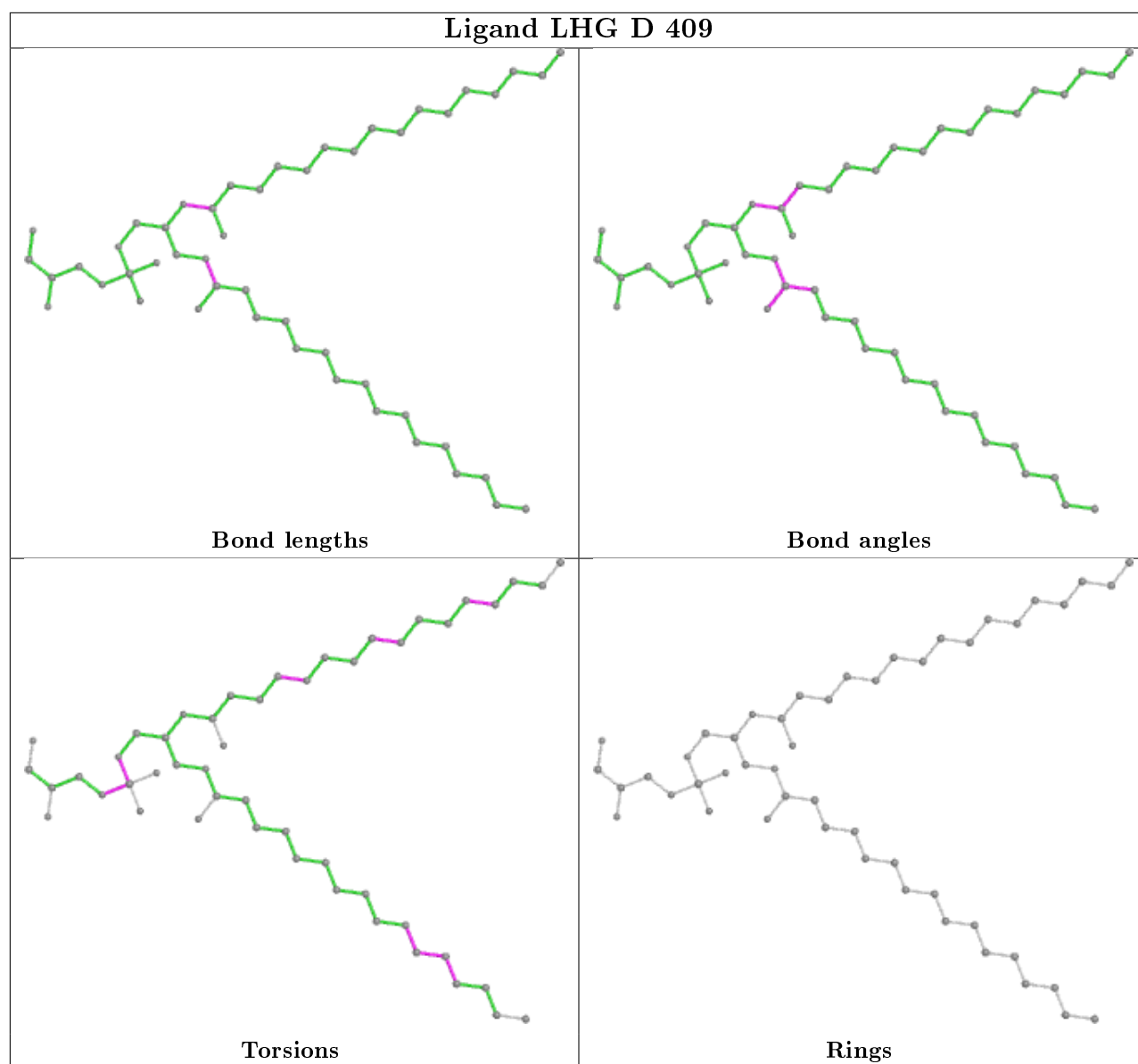




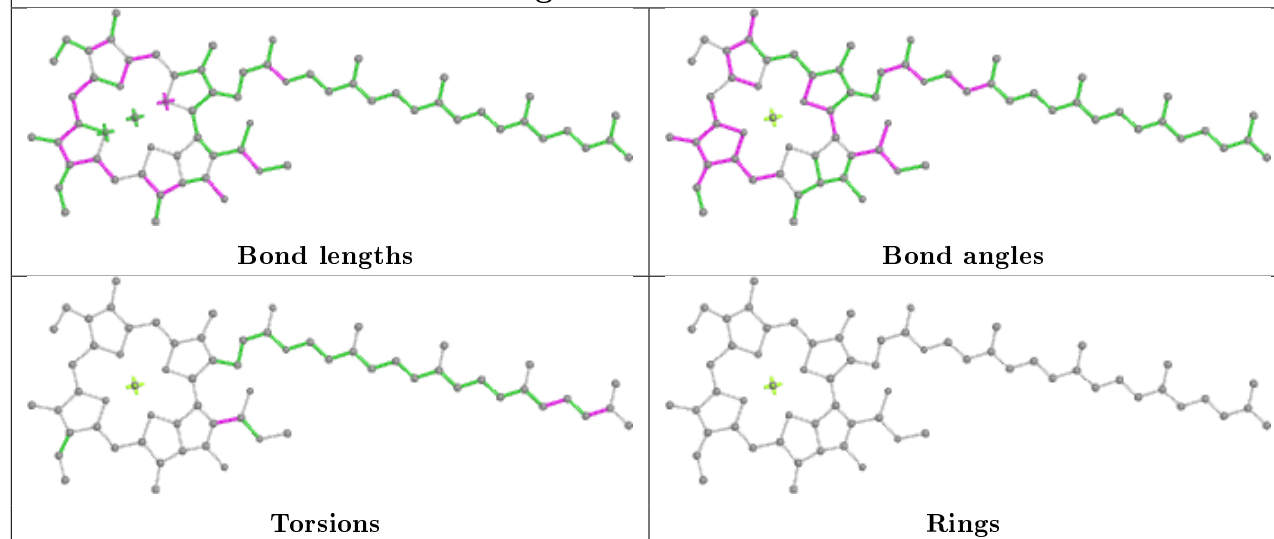




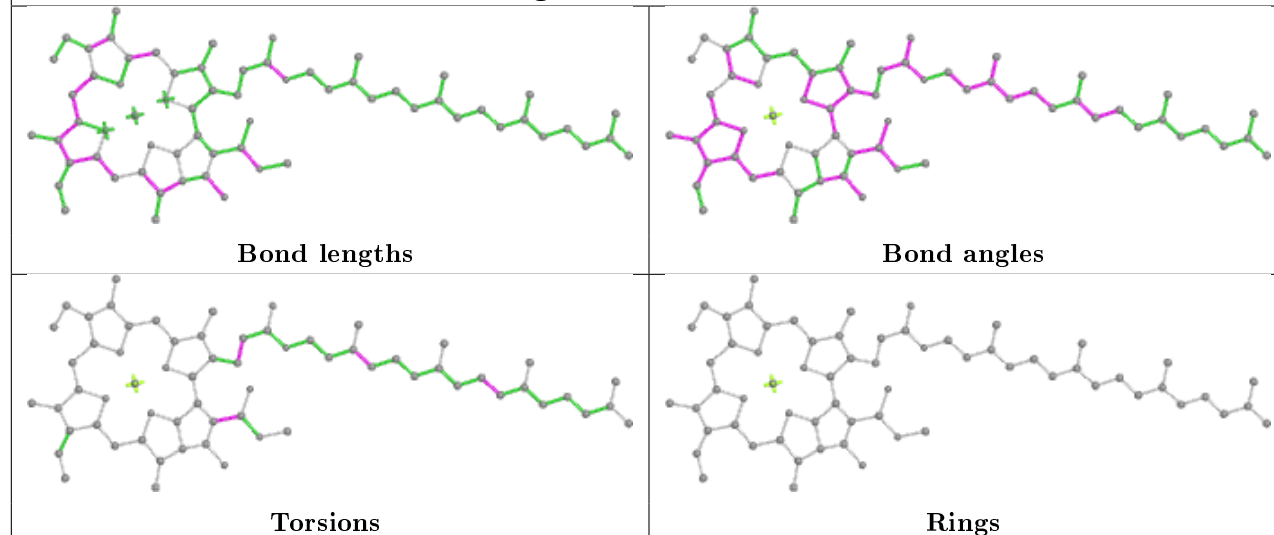




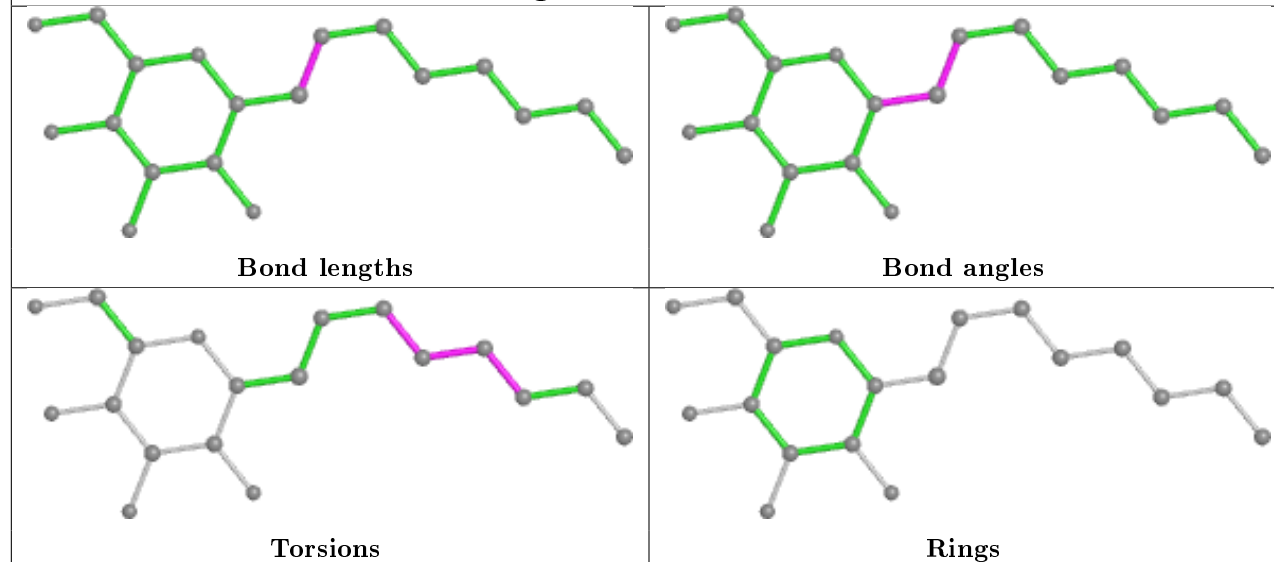
## Ligand CLA b 609



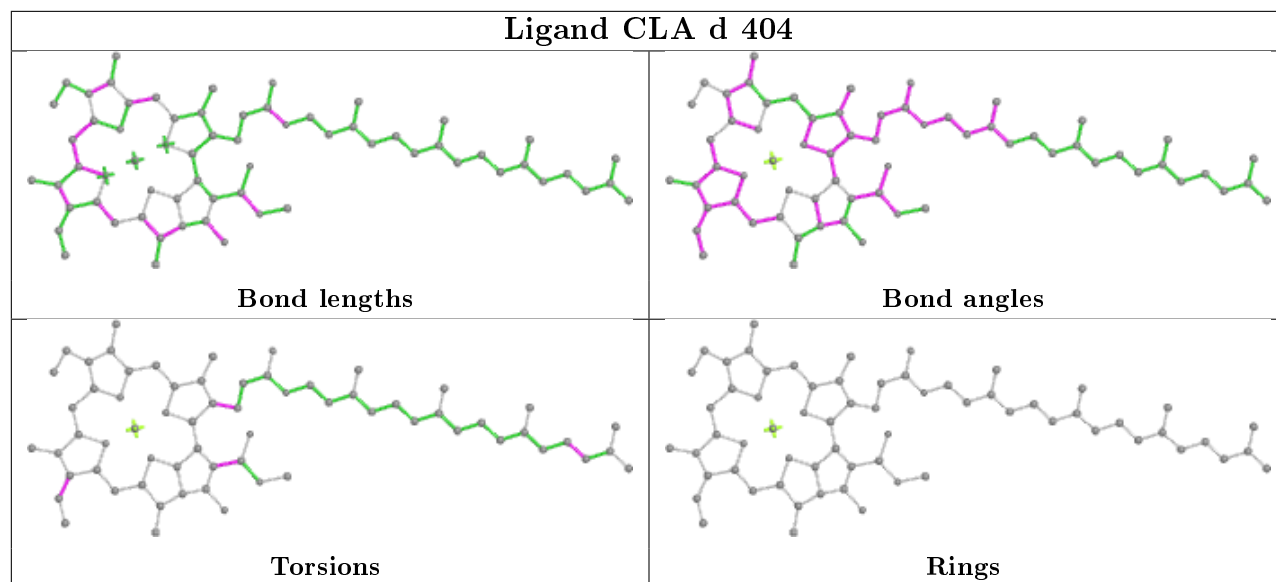
## Ligand CLA B 607



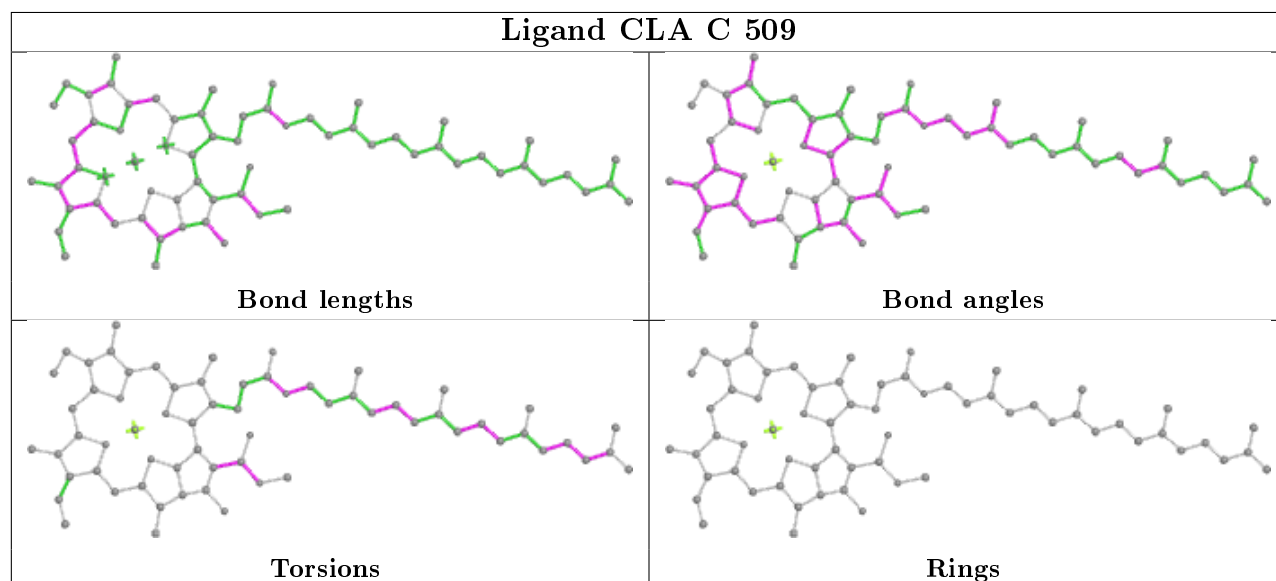
## Ligand HTG b 601



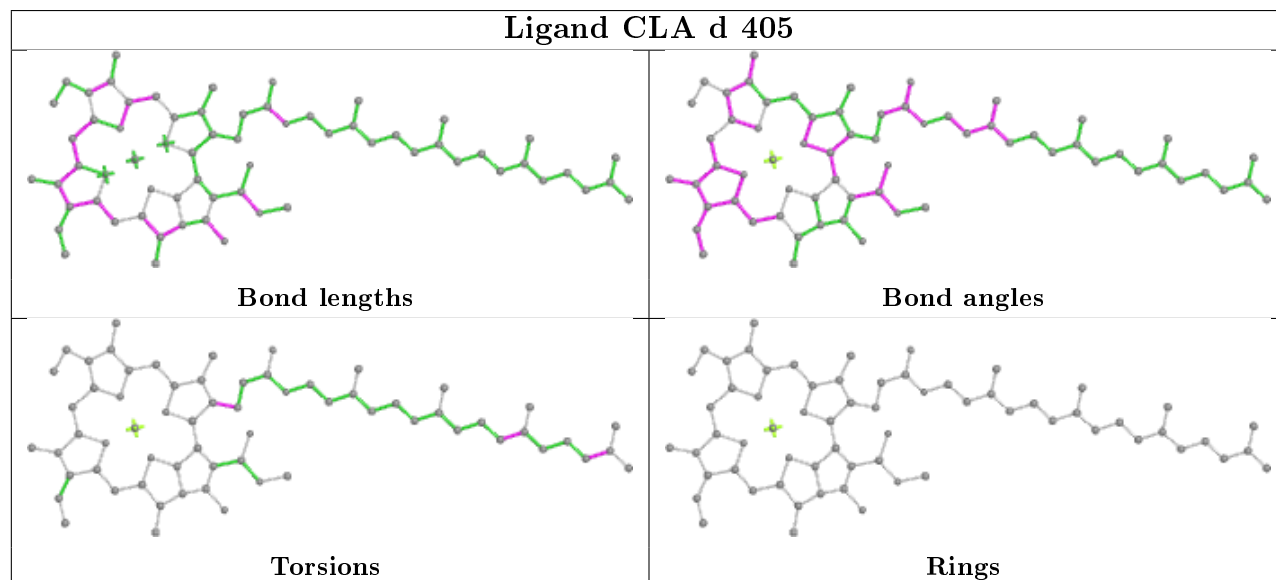
## Ligand CLA d 404

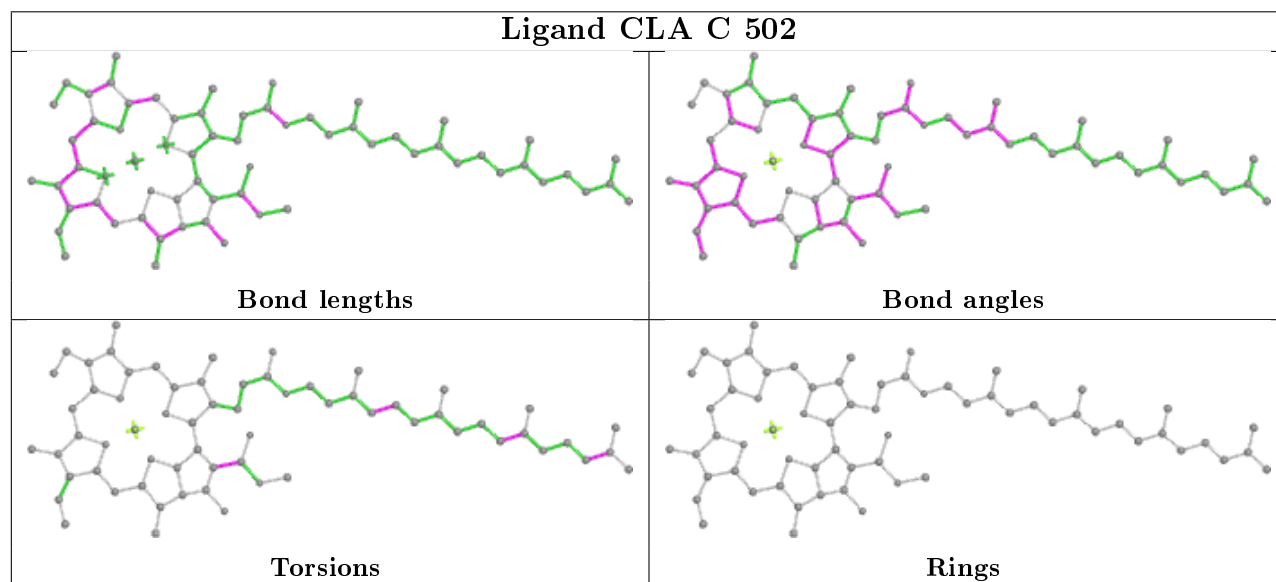
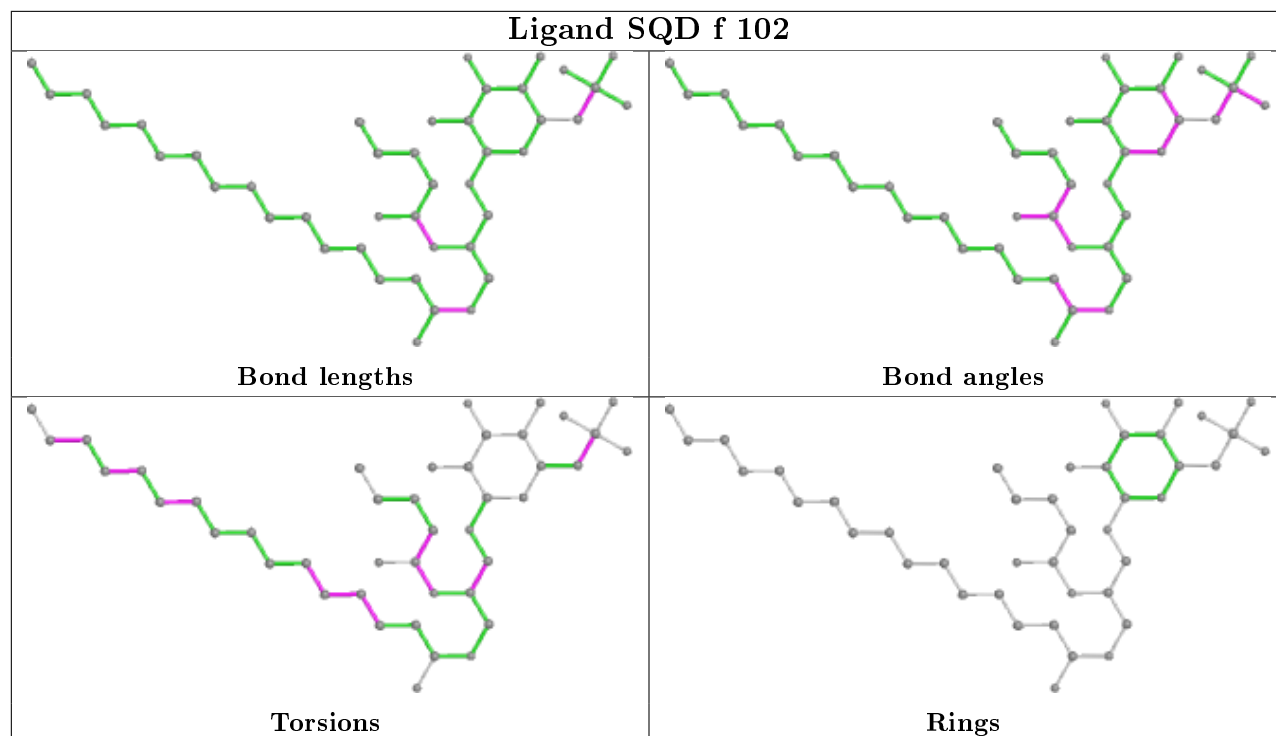


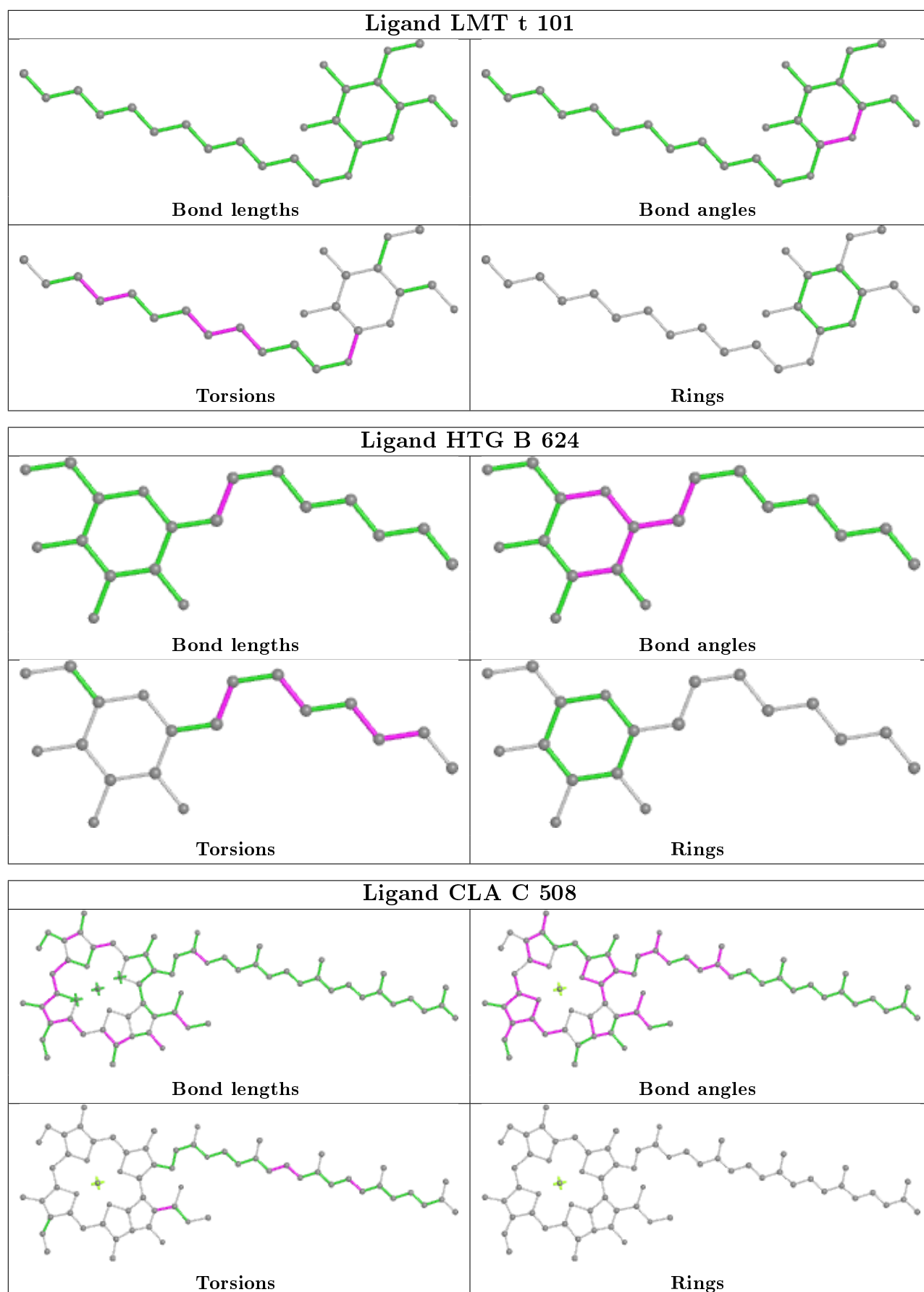
## Ligand CLA C 509



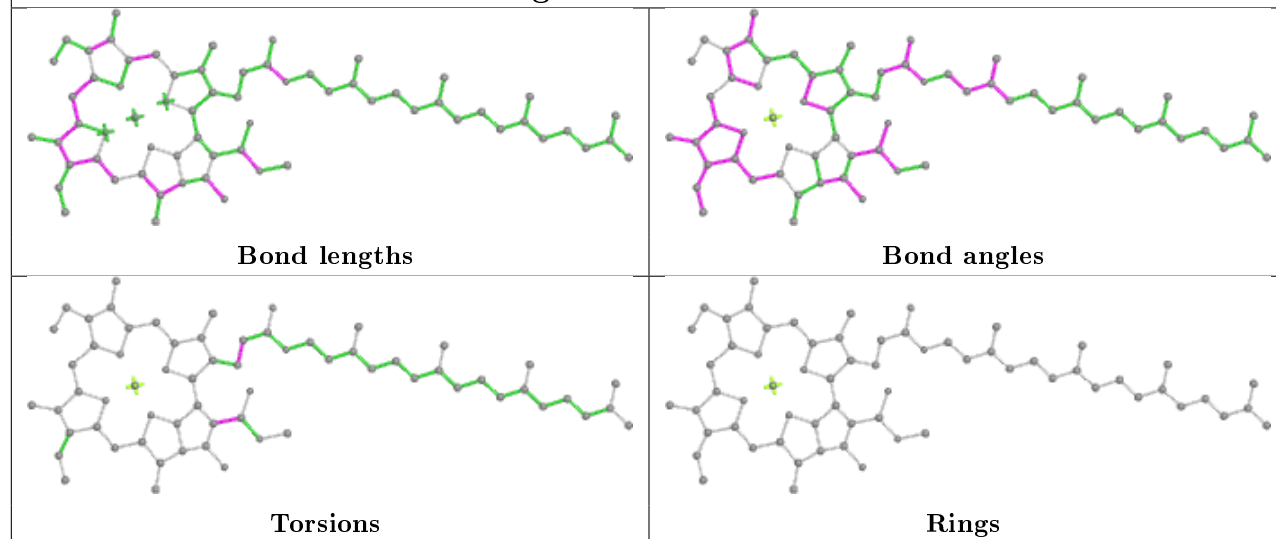
## Ligand CLA d 405



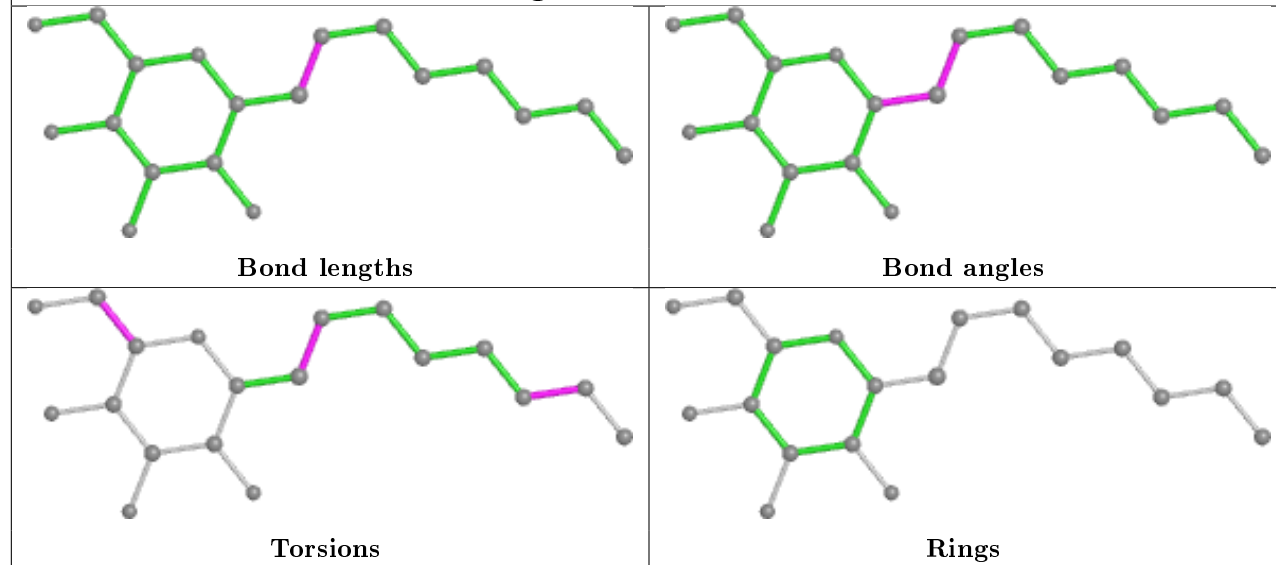


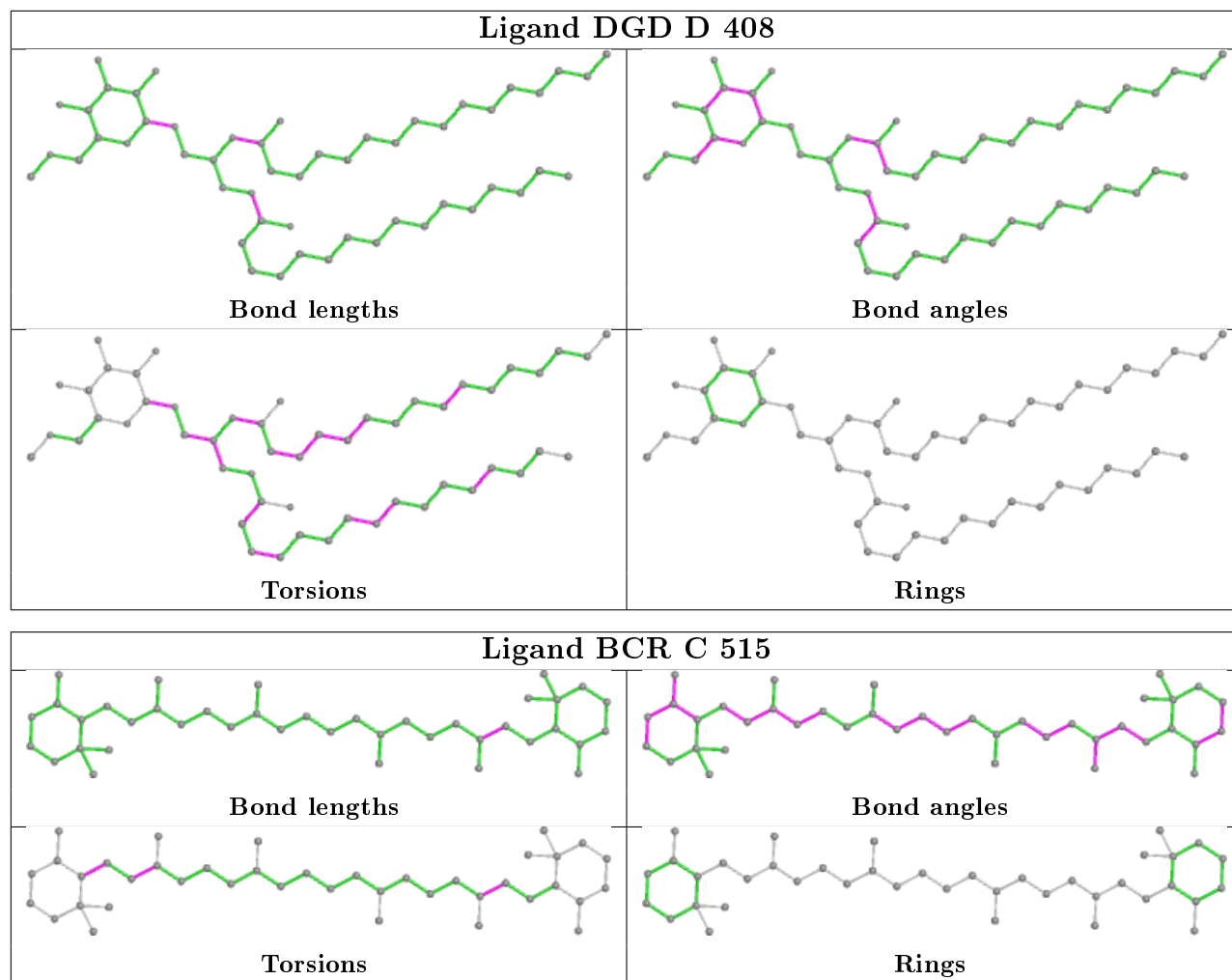


## Ligand CLA C 507

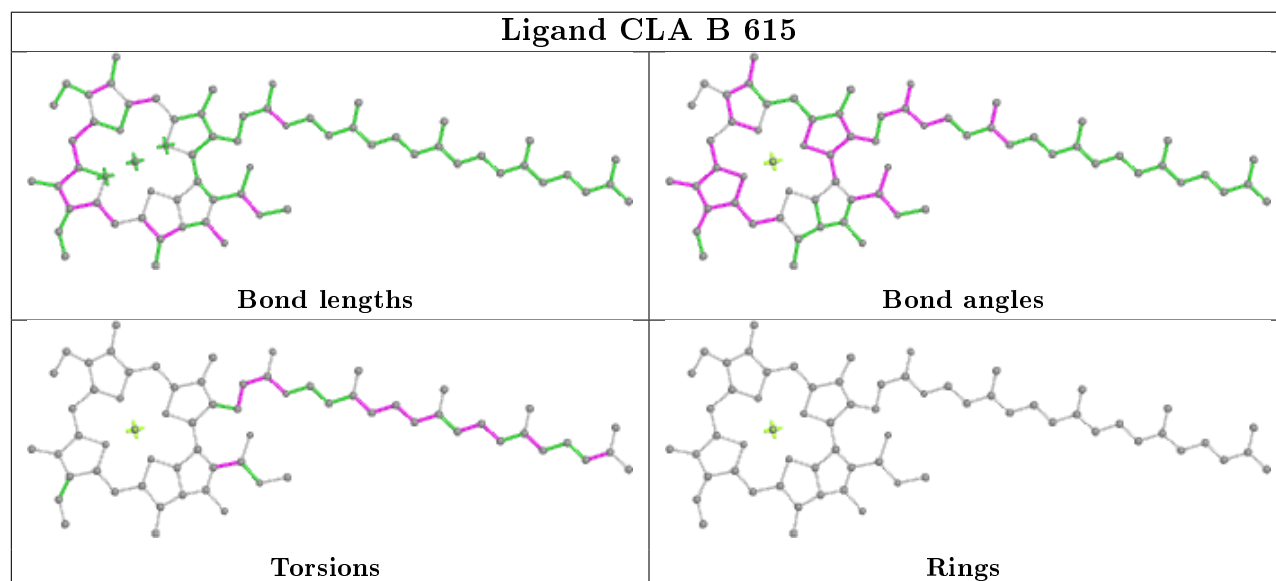
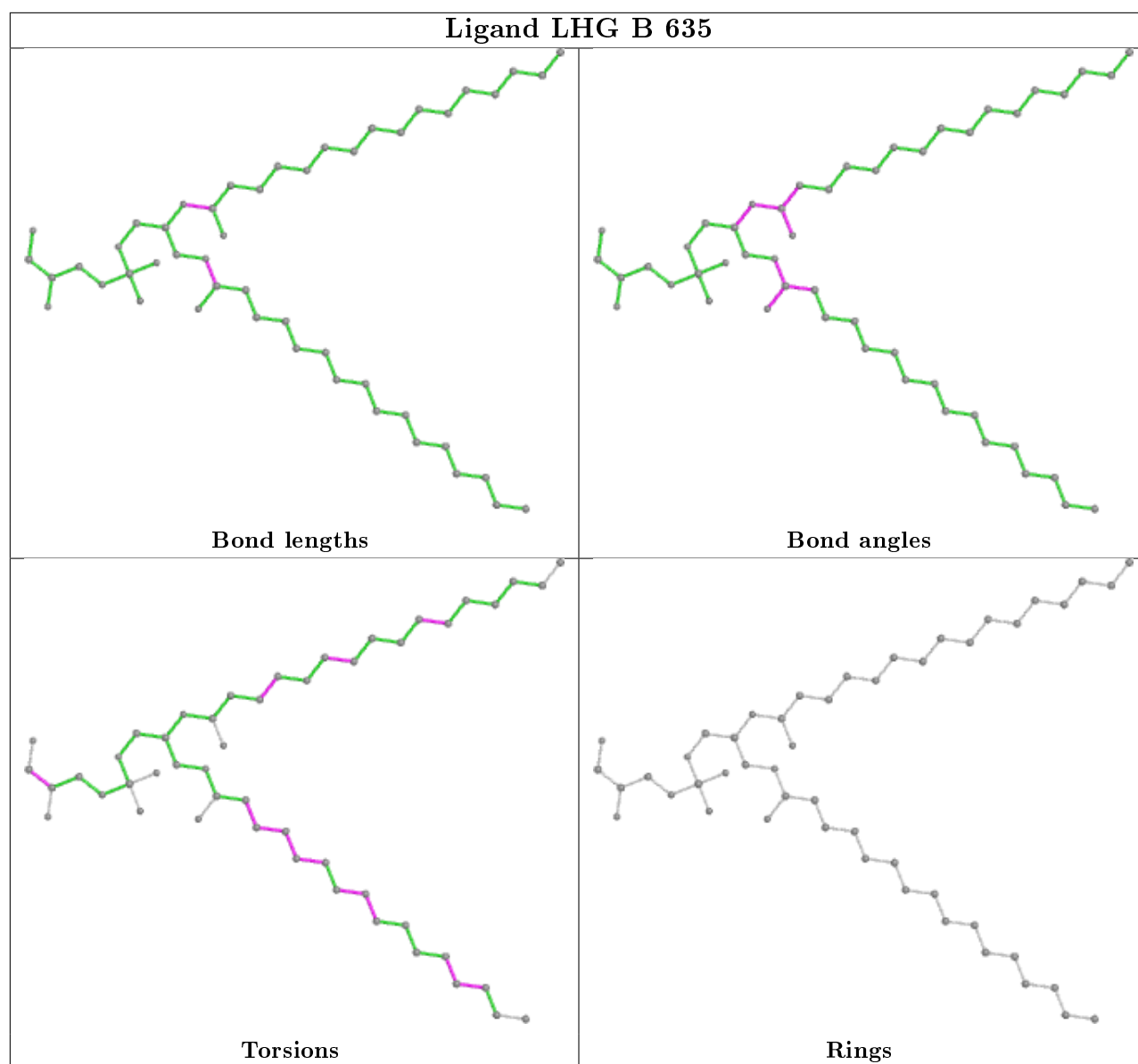


## Ligand HTG B 623

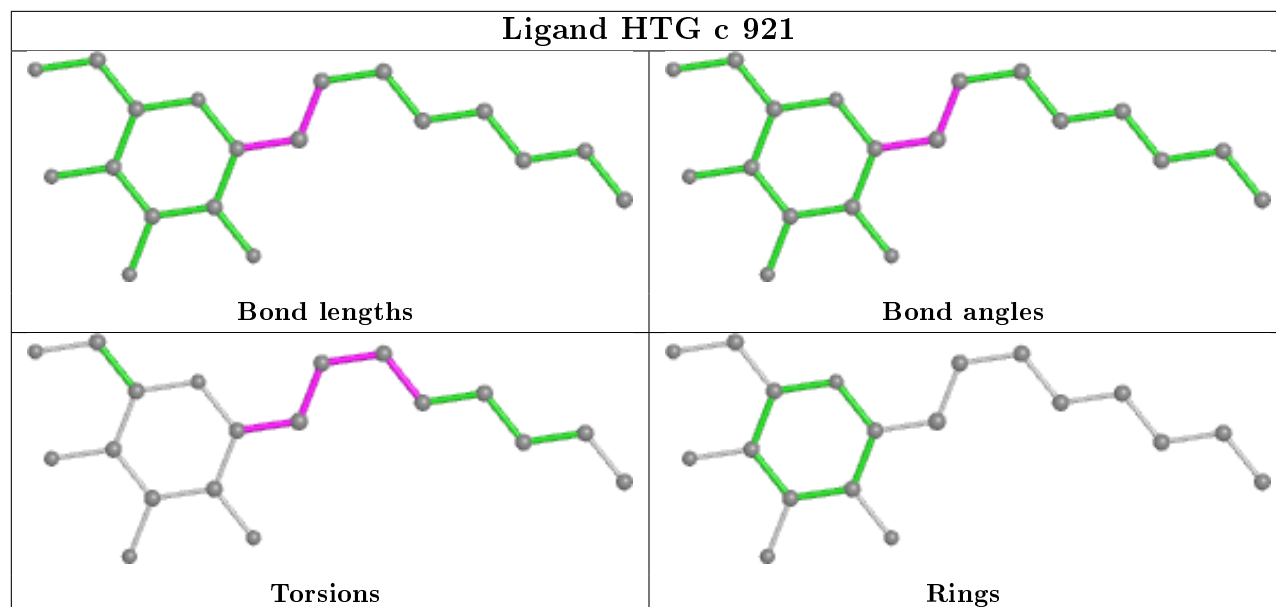




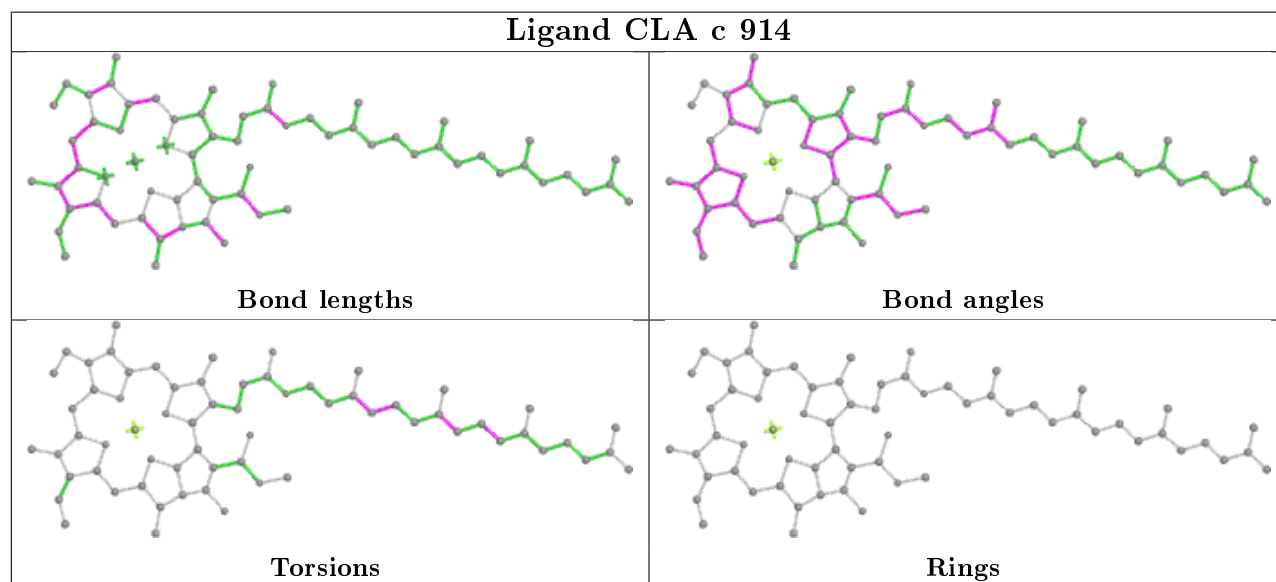




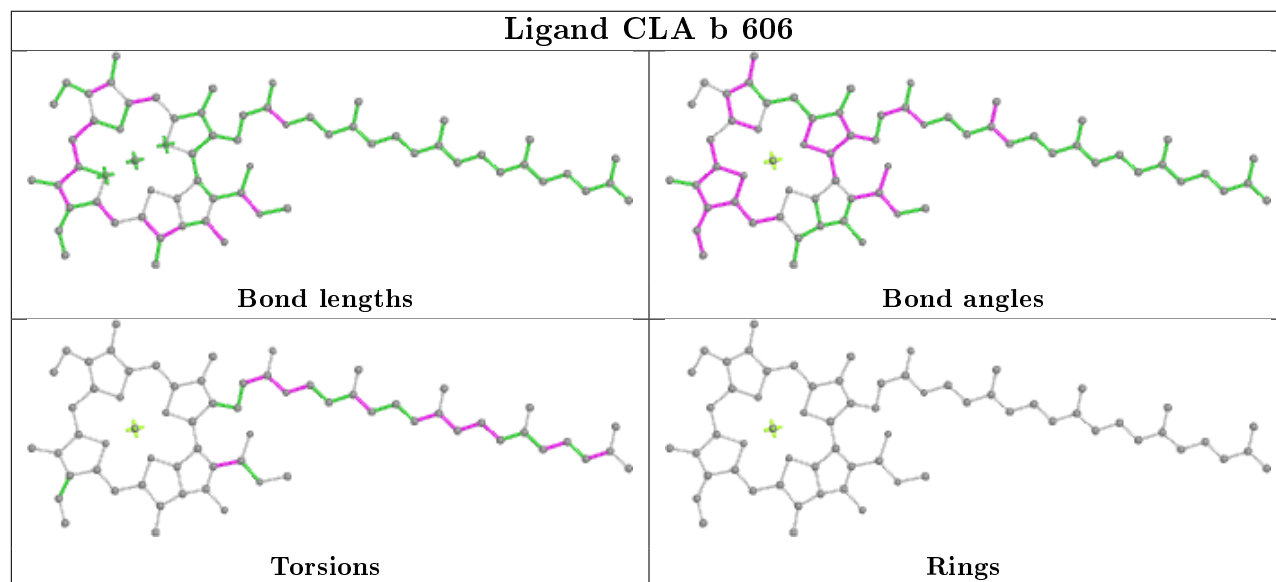
## Ligand HTG c 921

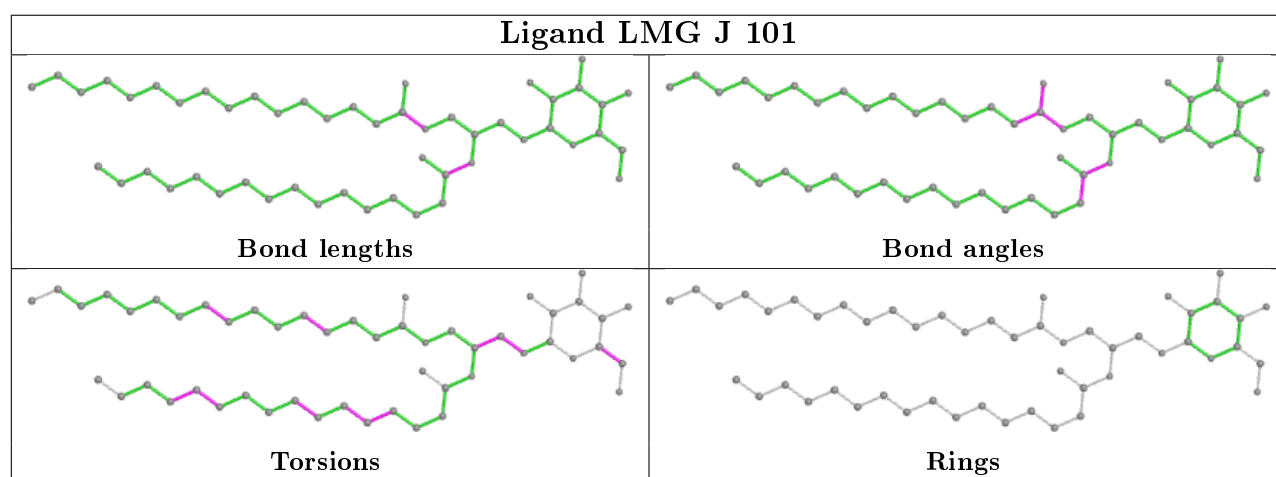
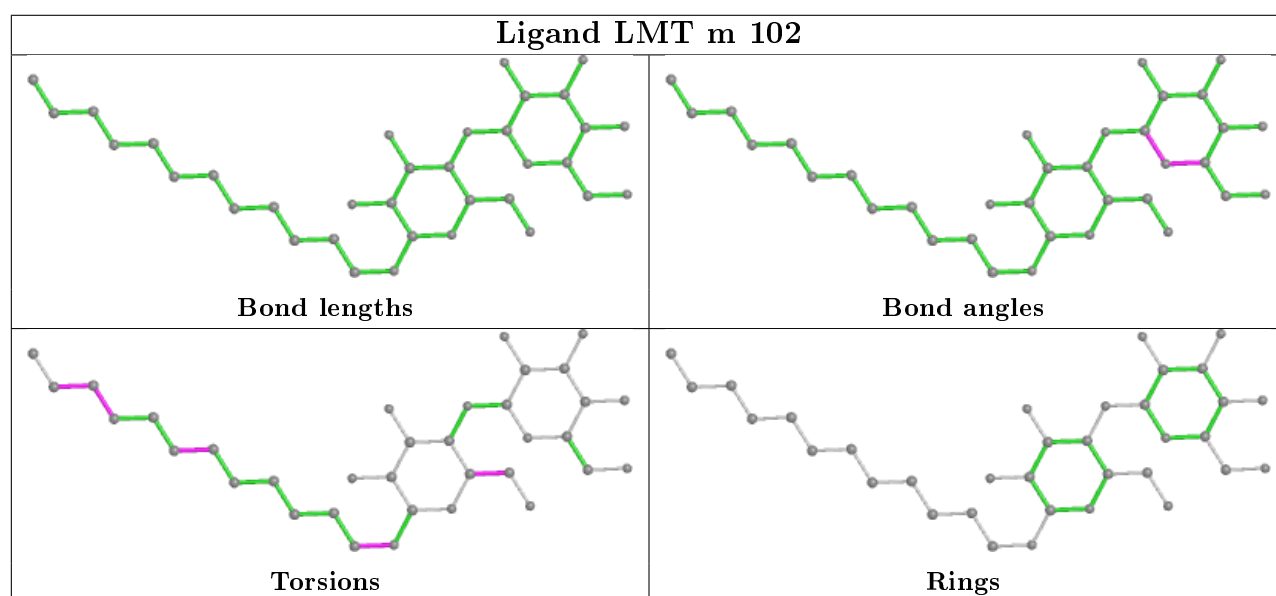
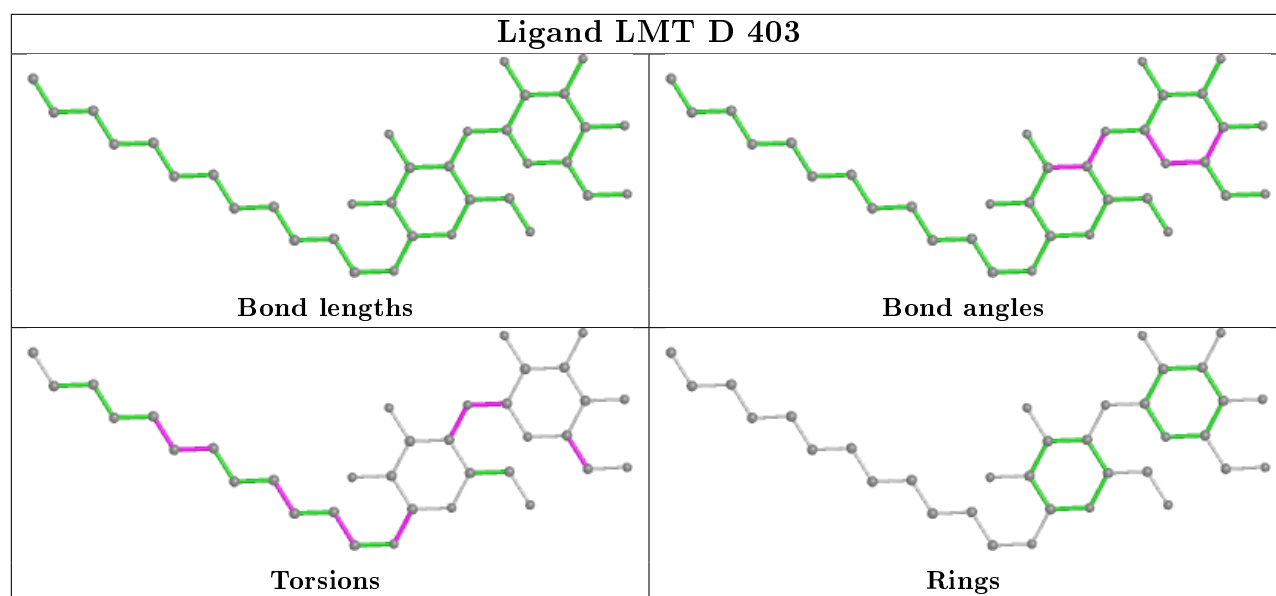


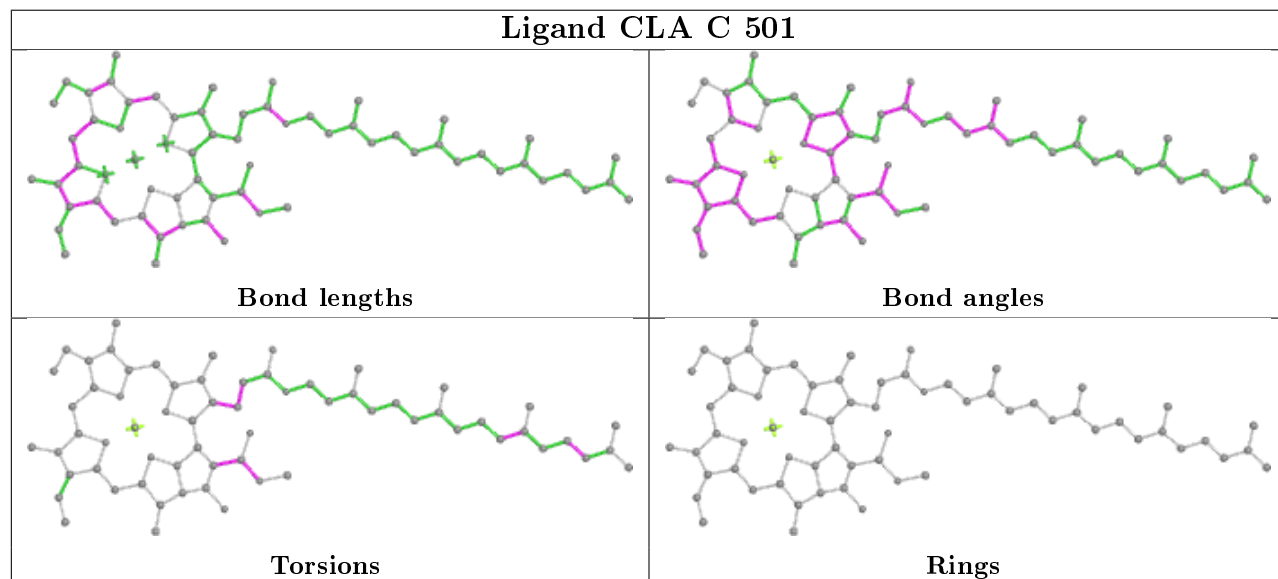
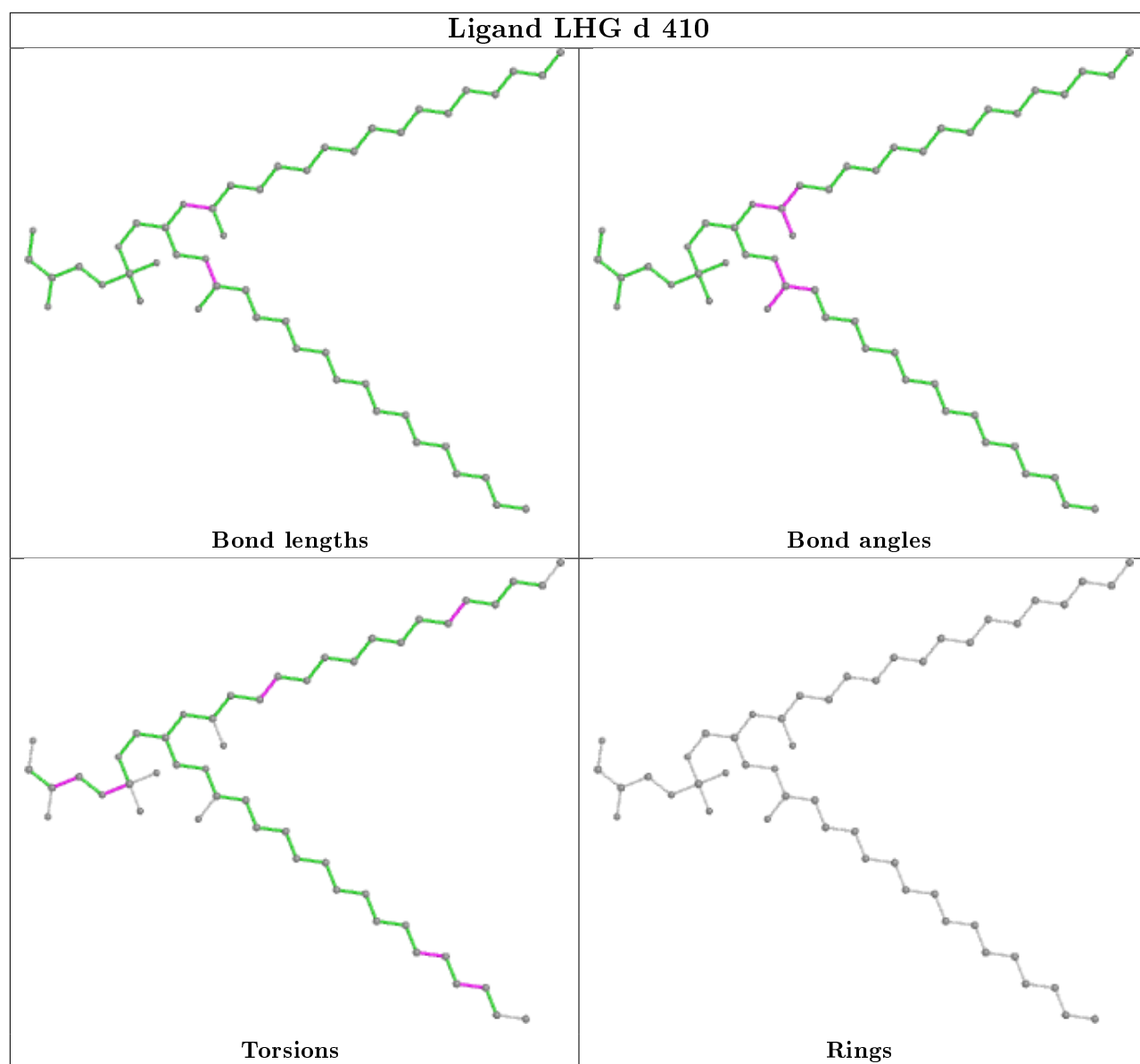
## Ligand CLA c 914

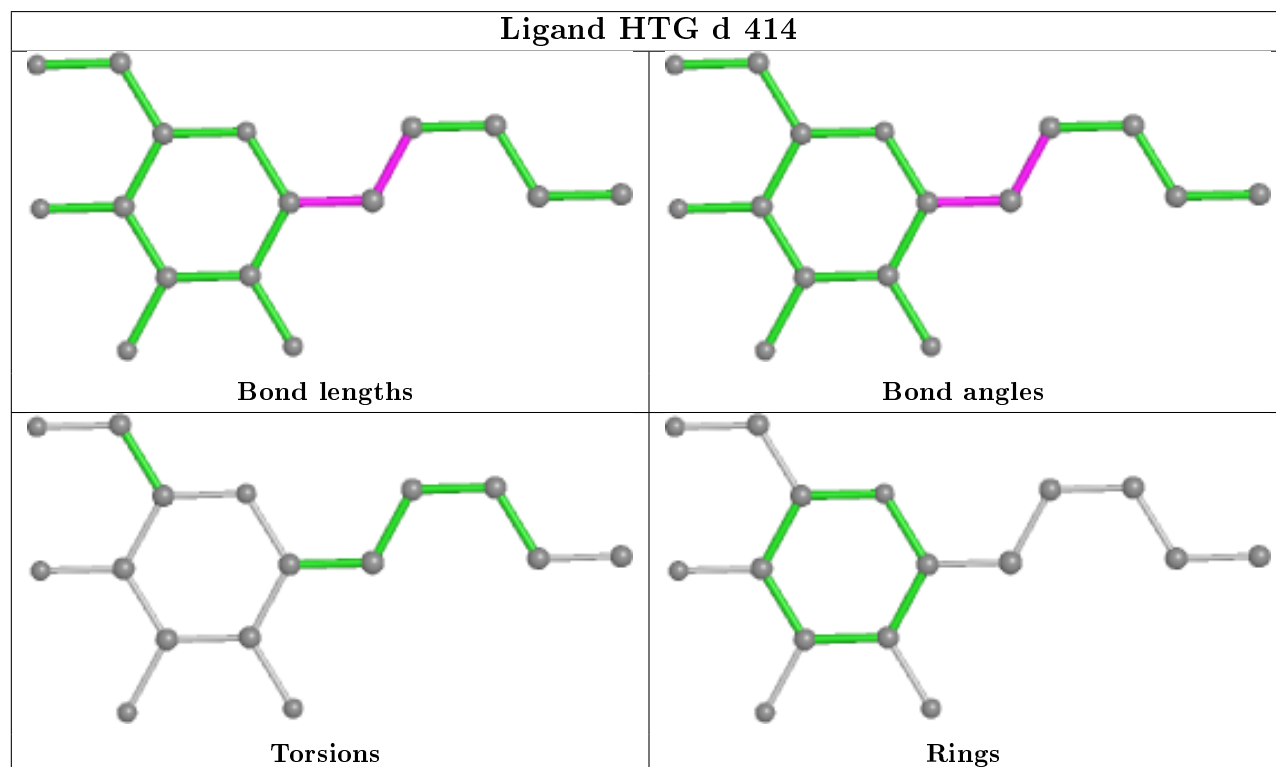
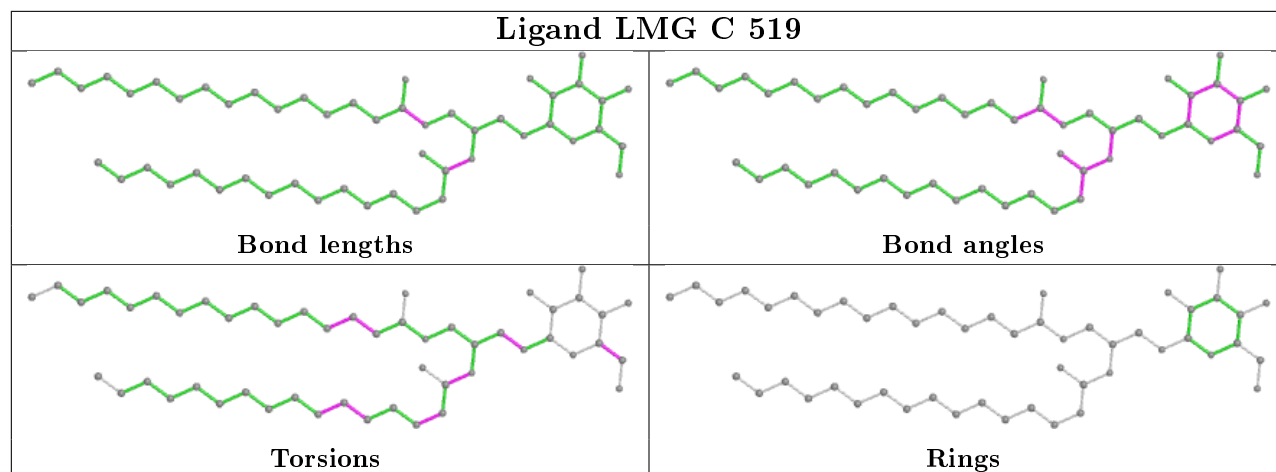


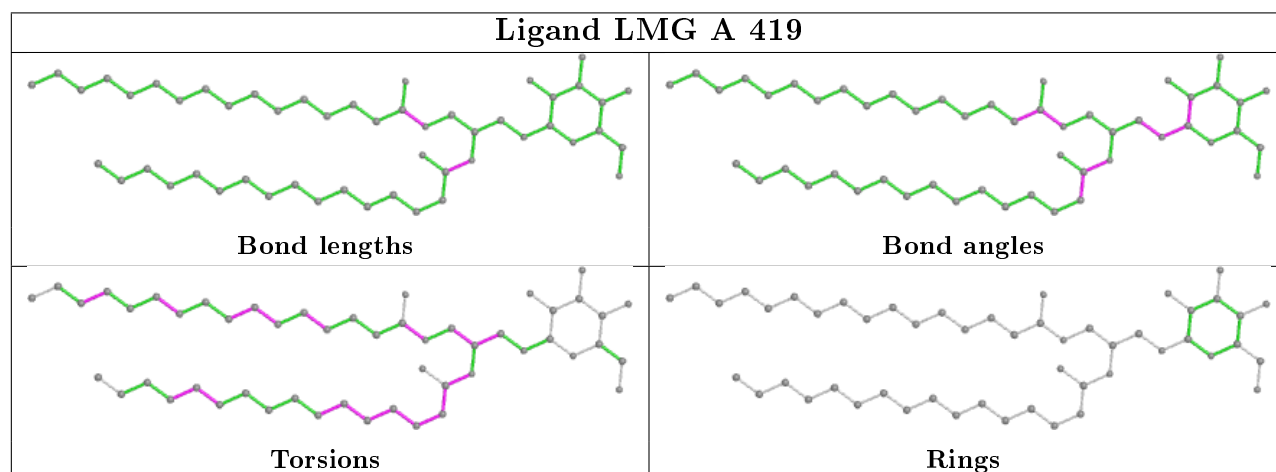
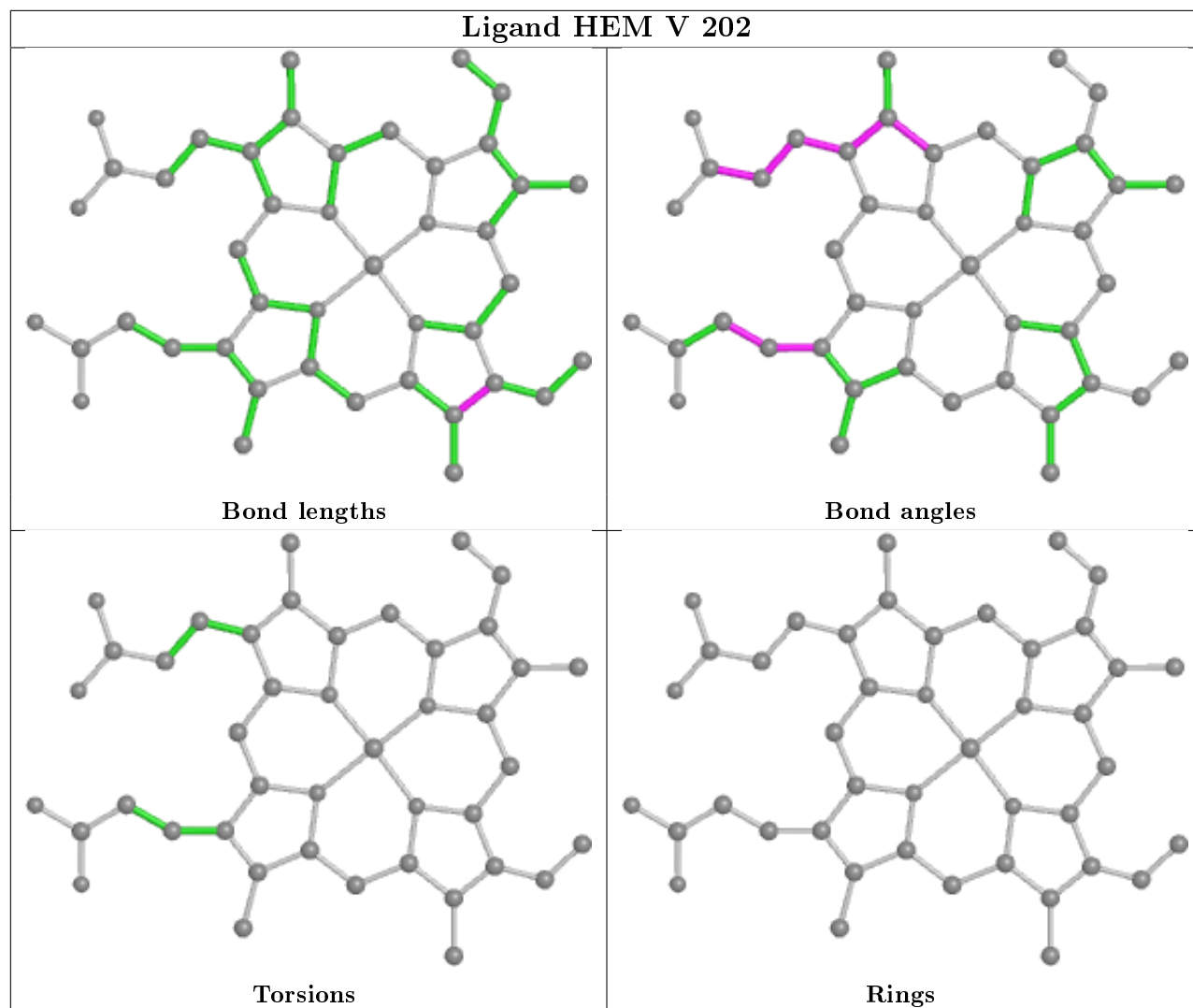
## Ligand CLA b 606



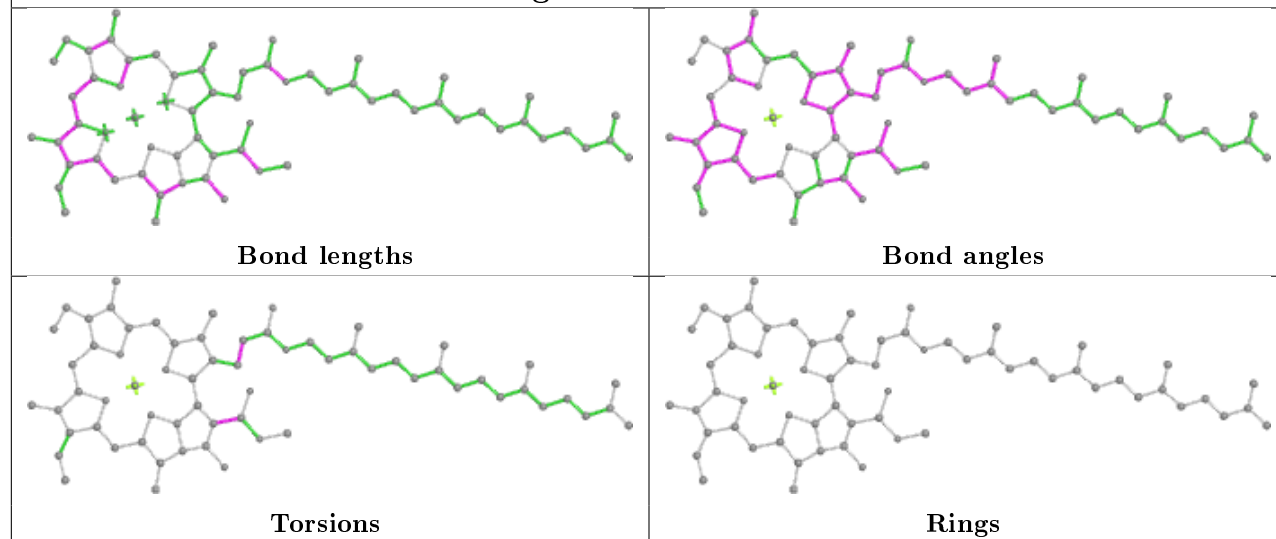




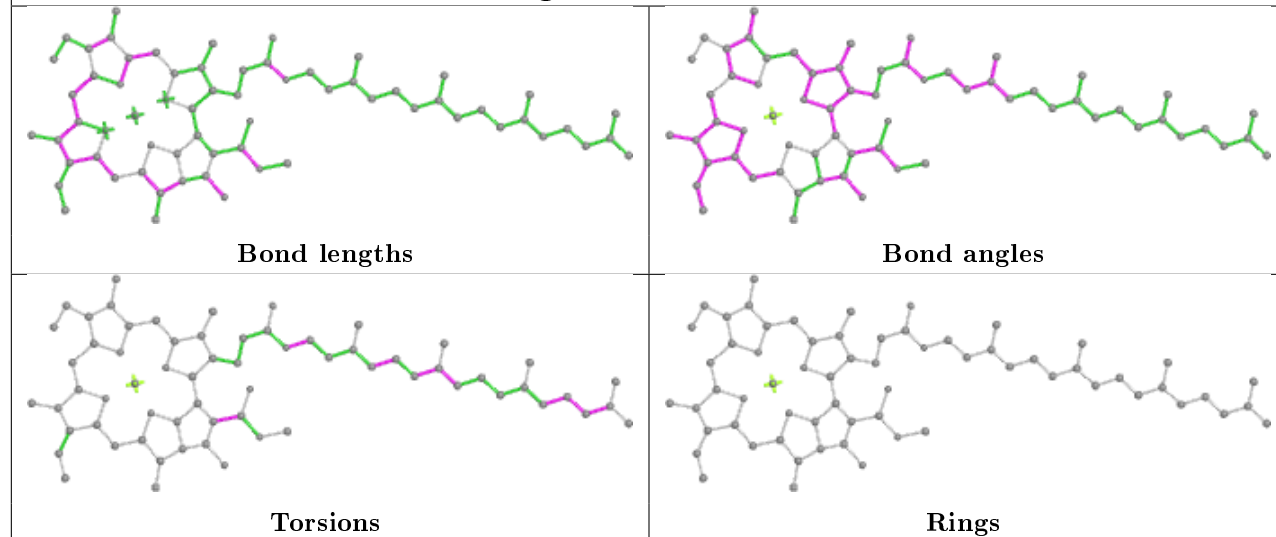




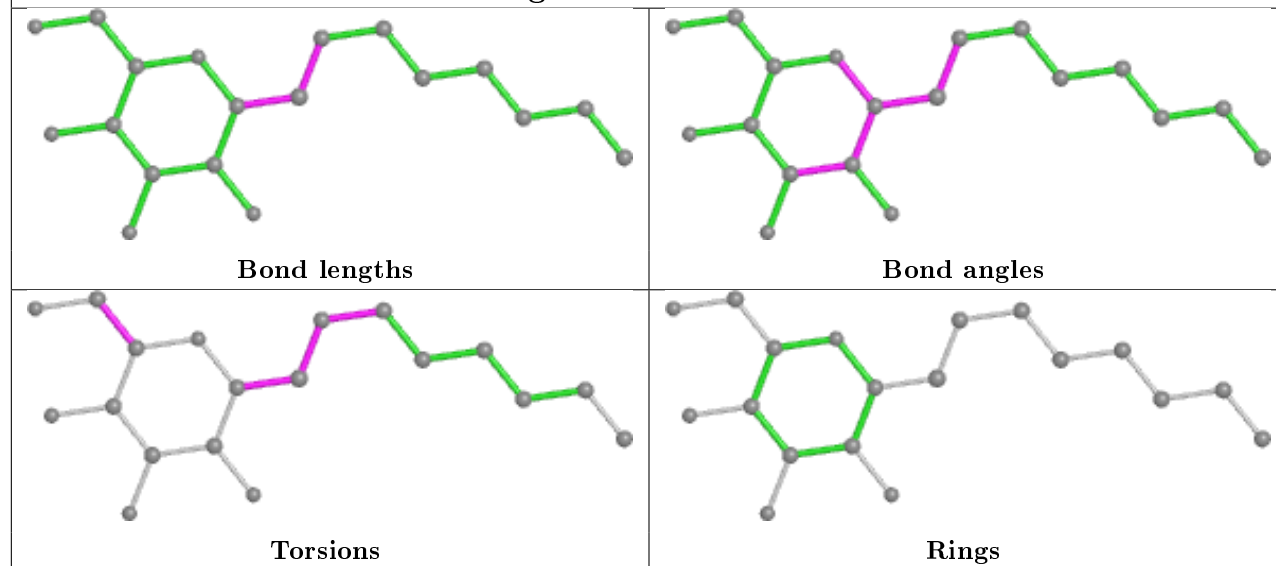
## Ligand CLA B 603

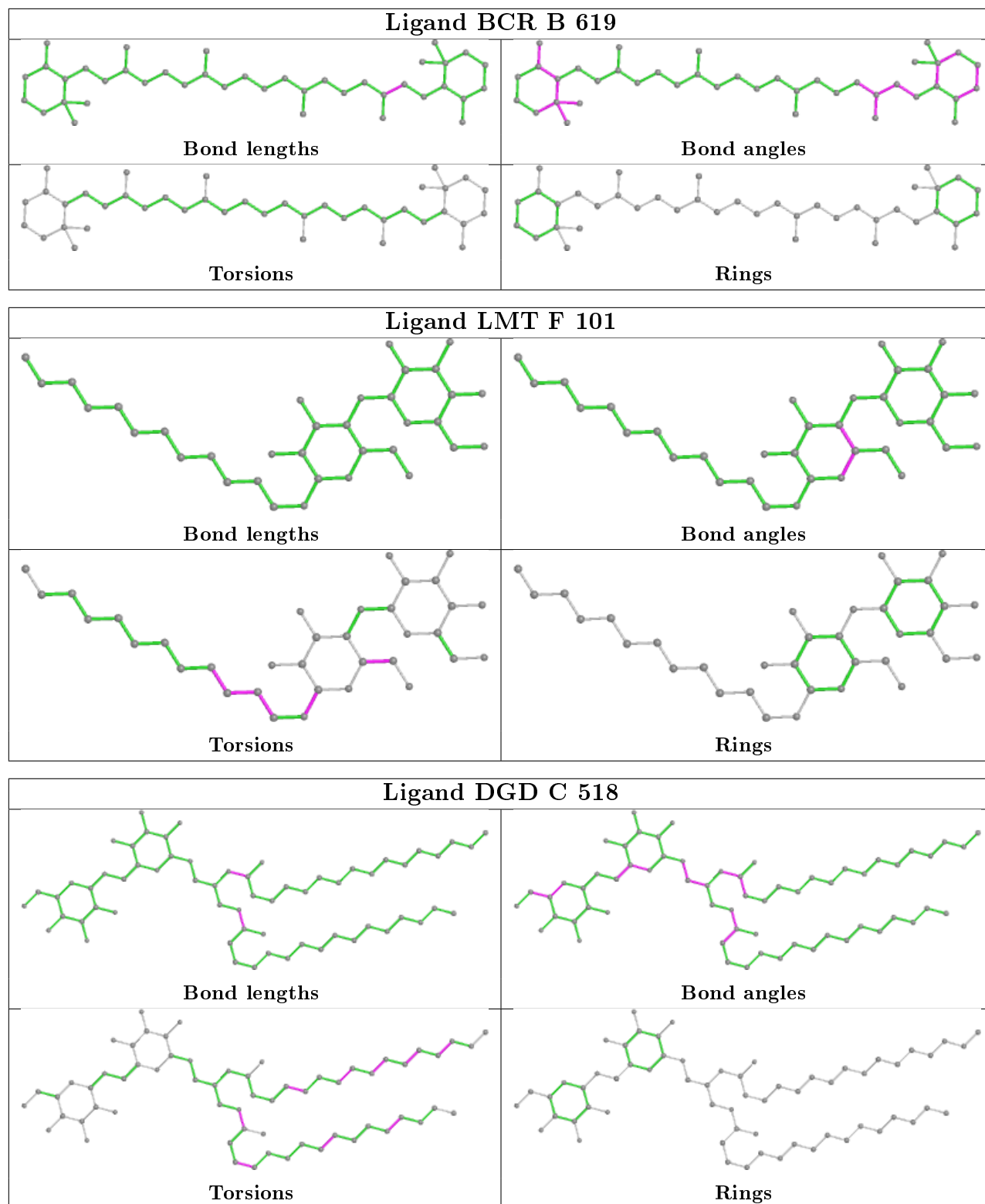


## Ligand CLA c 907

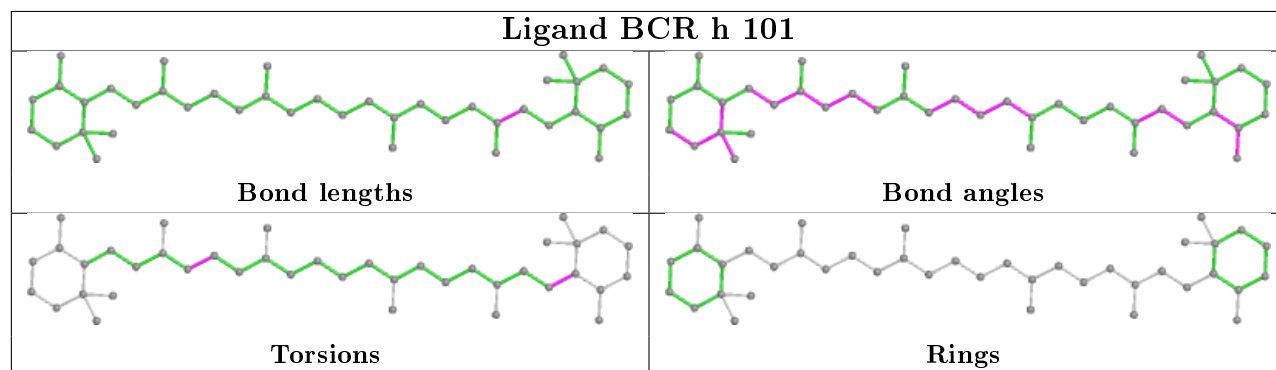
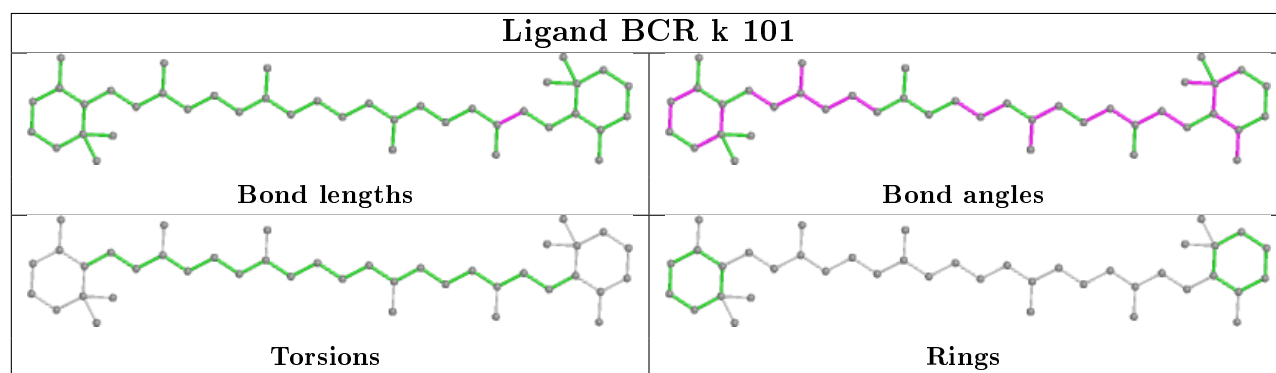
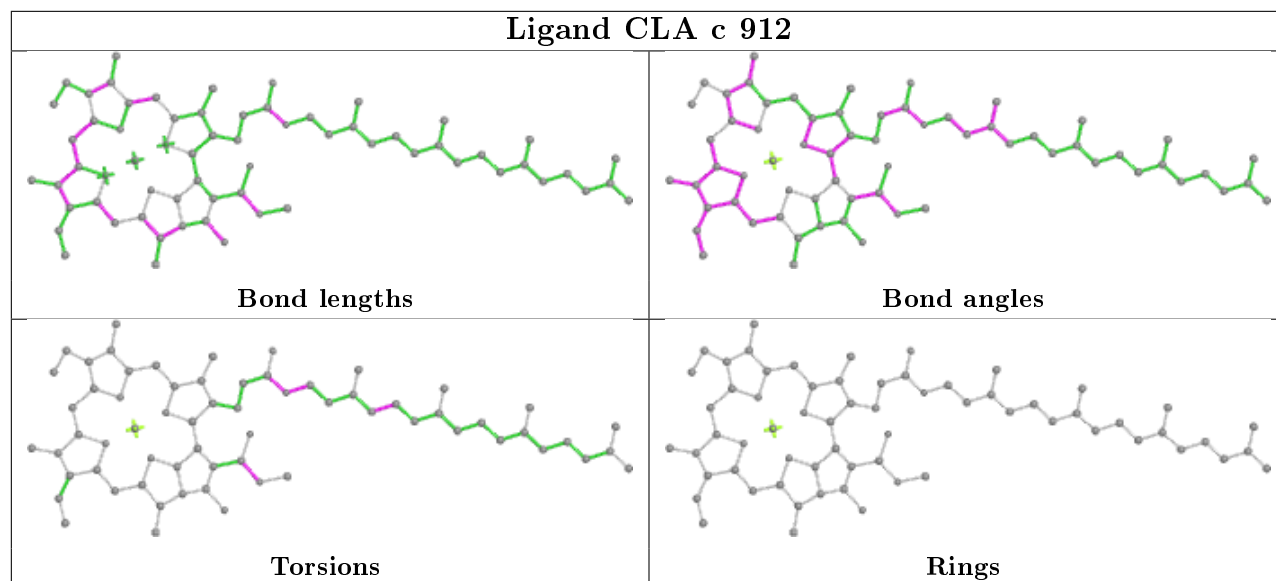
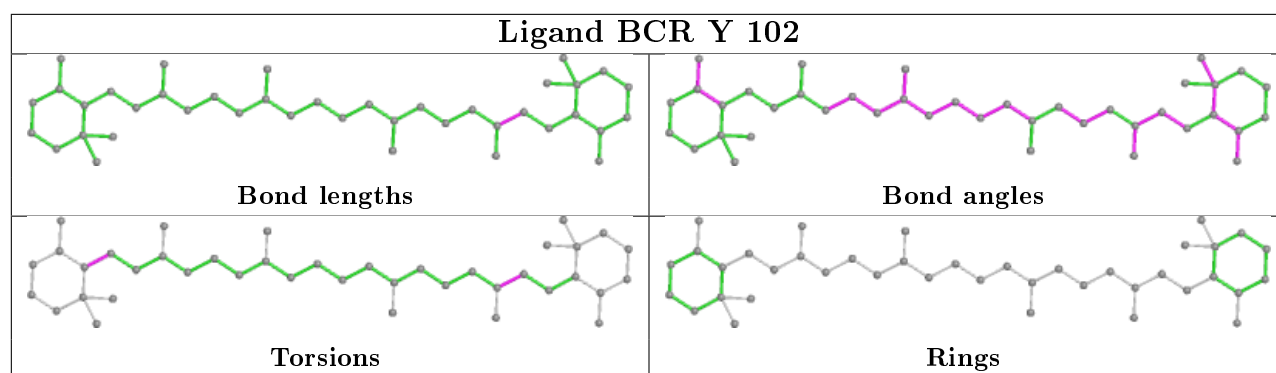


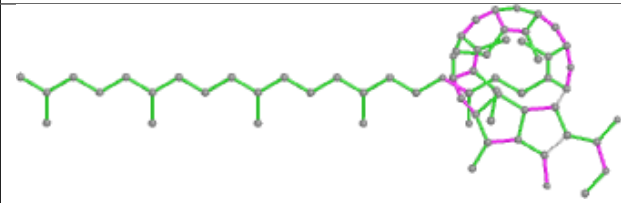
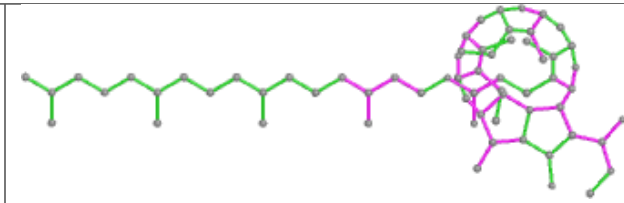
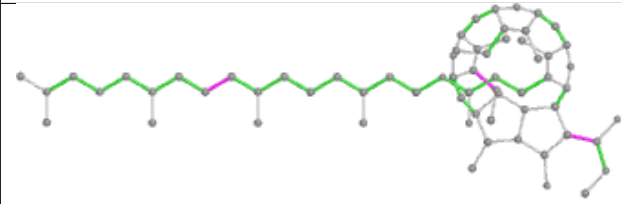
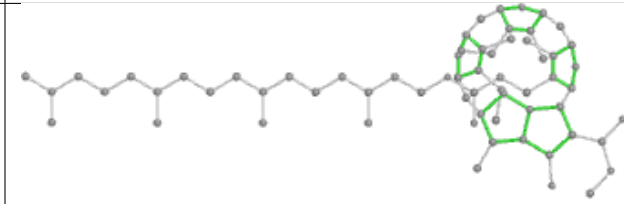
## Ligand HTG V 203

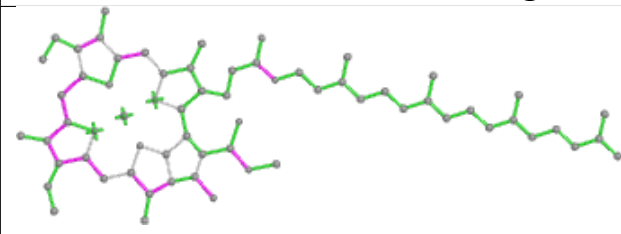
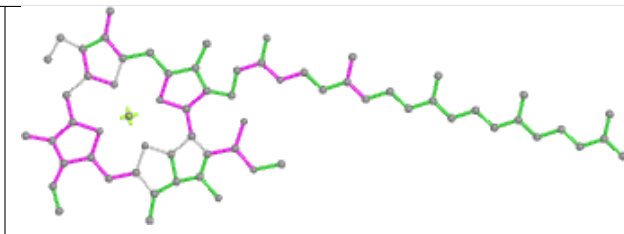
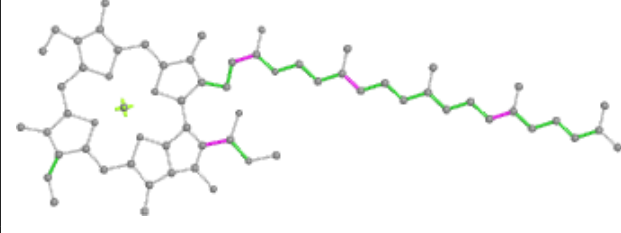
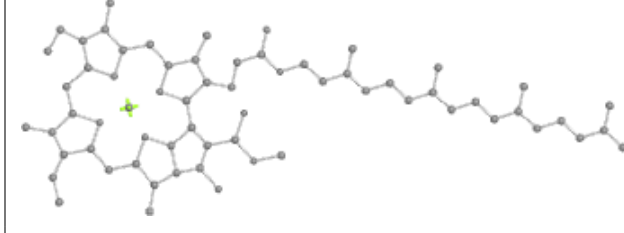


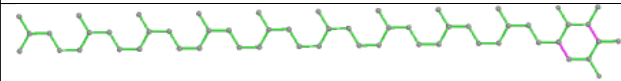
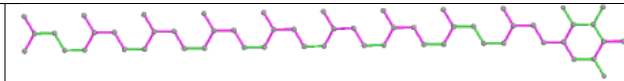
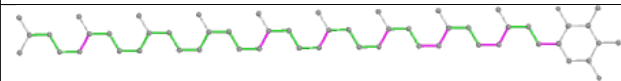
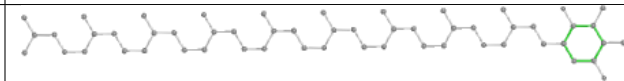


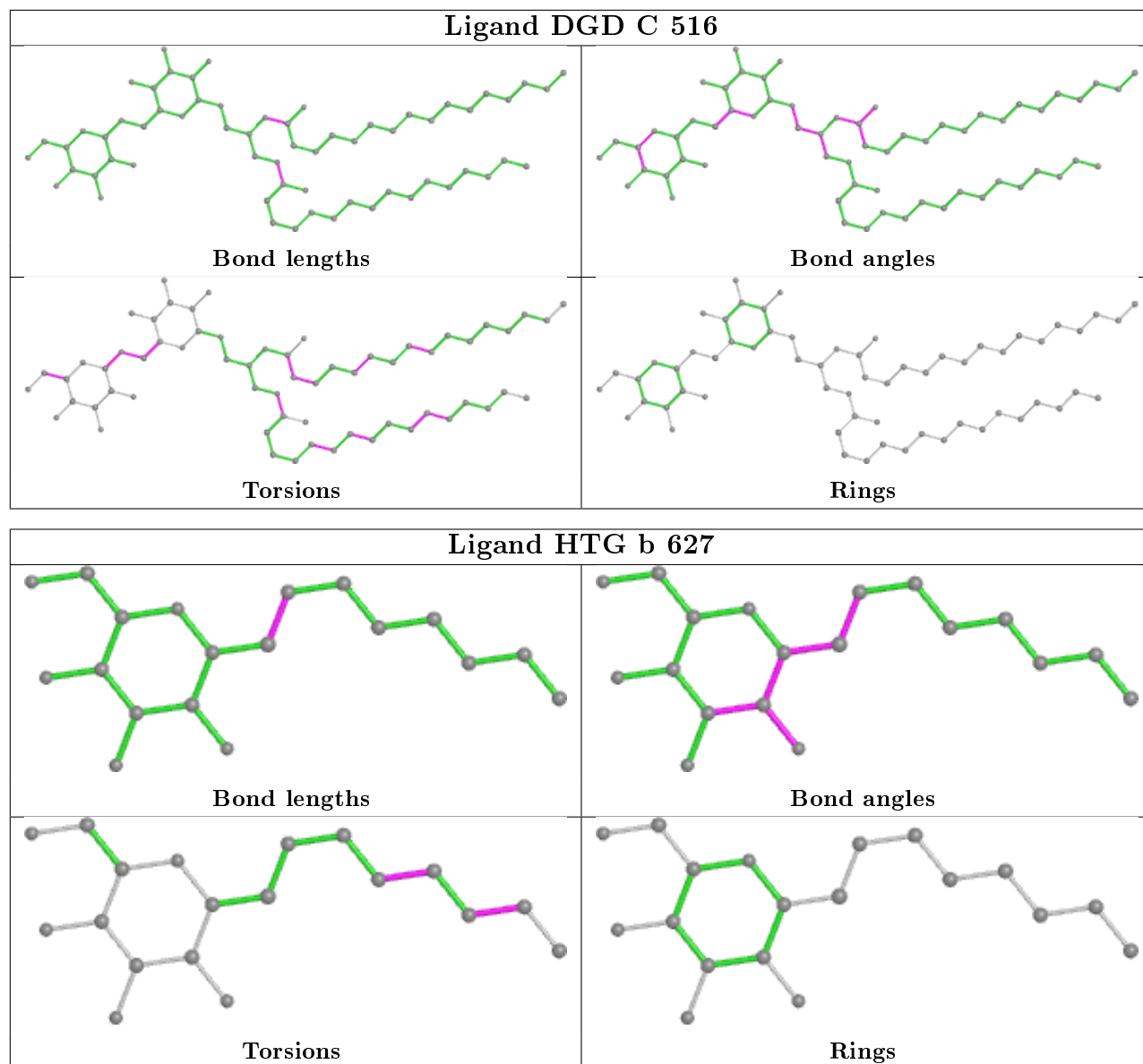


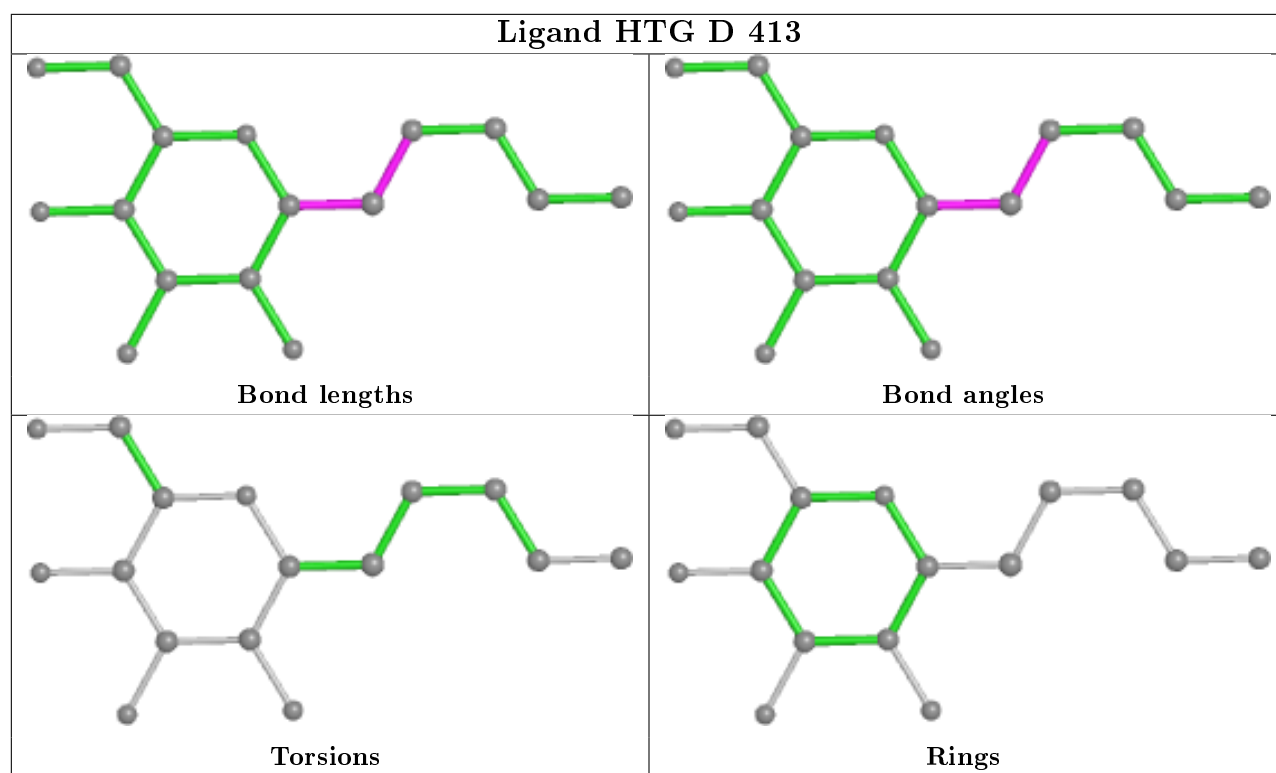


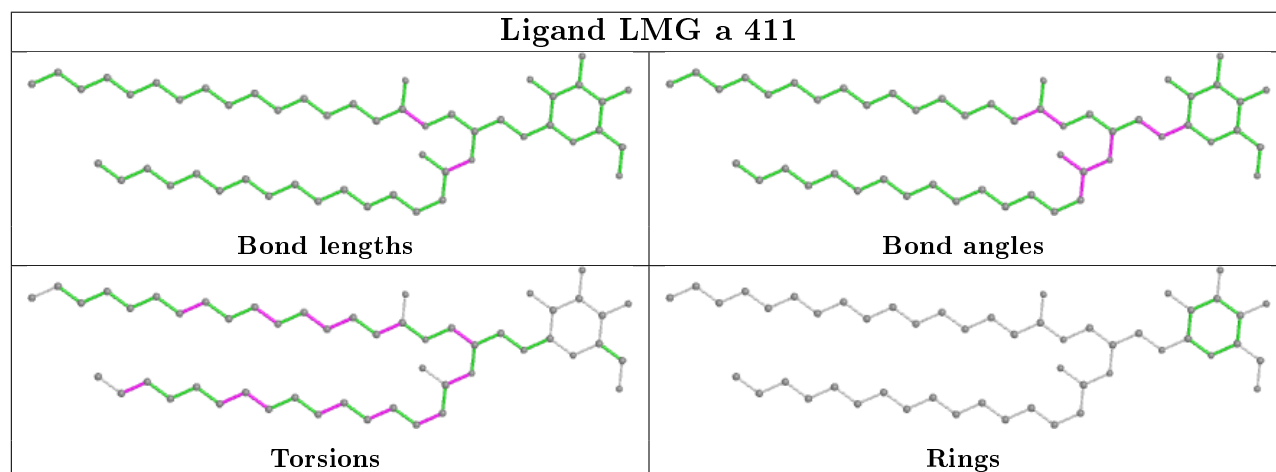
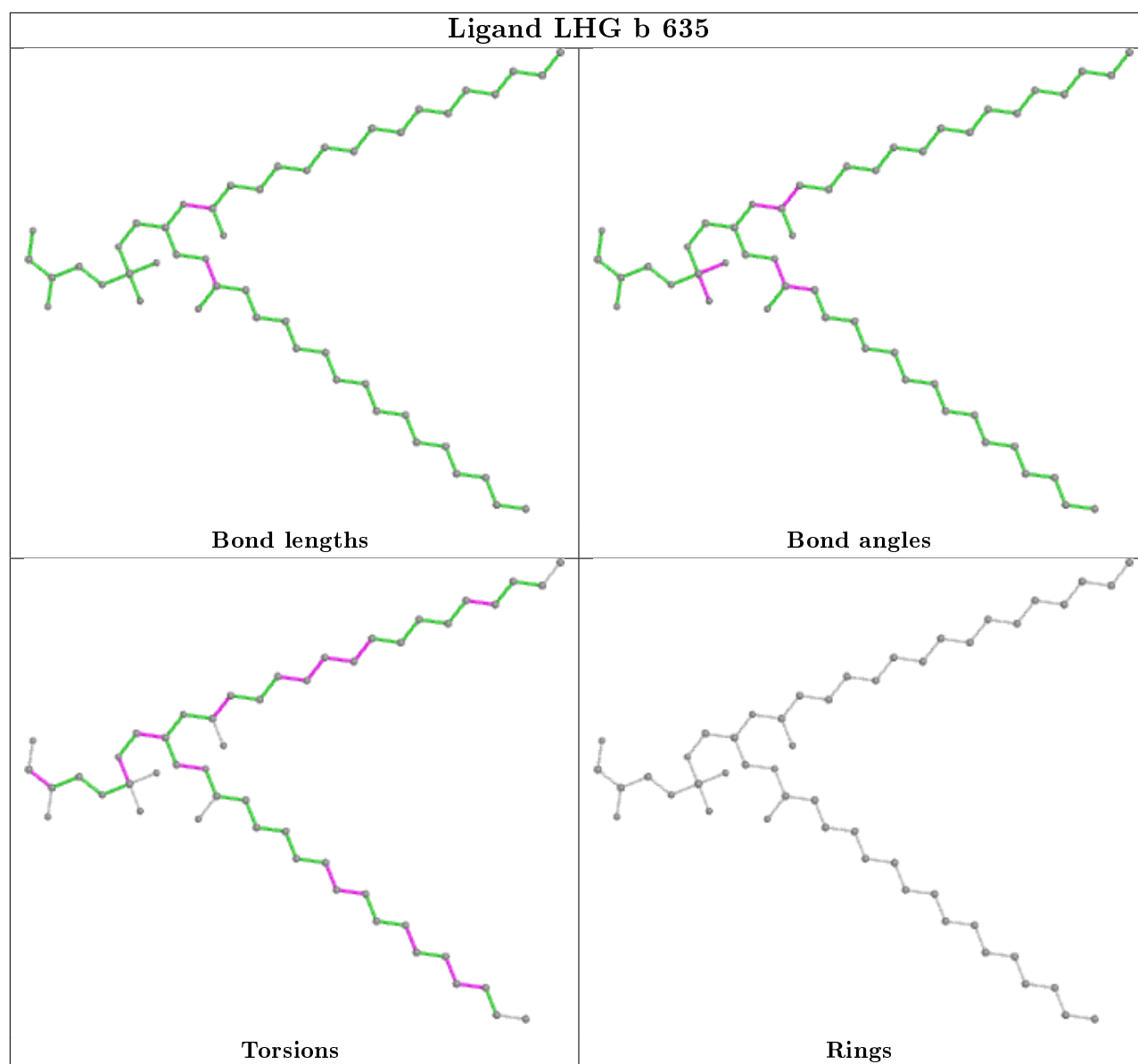
Ligand PHO d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

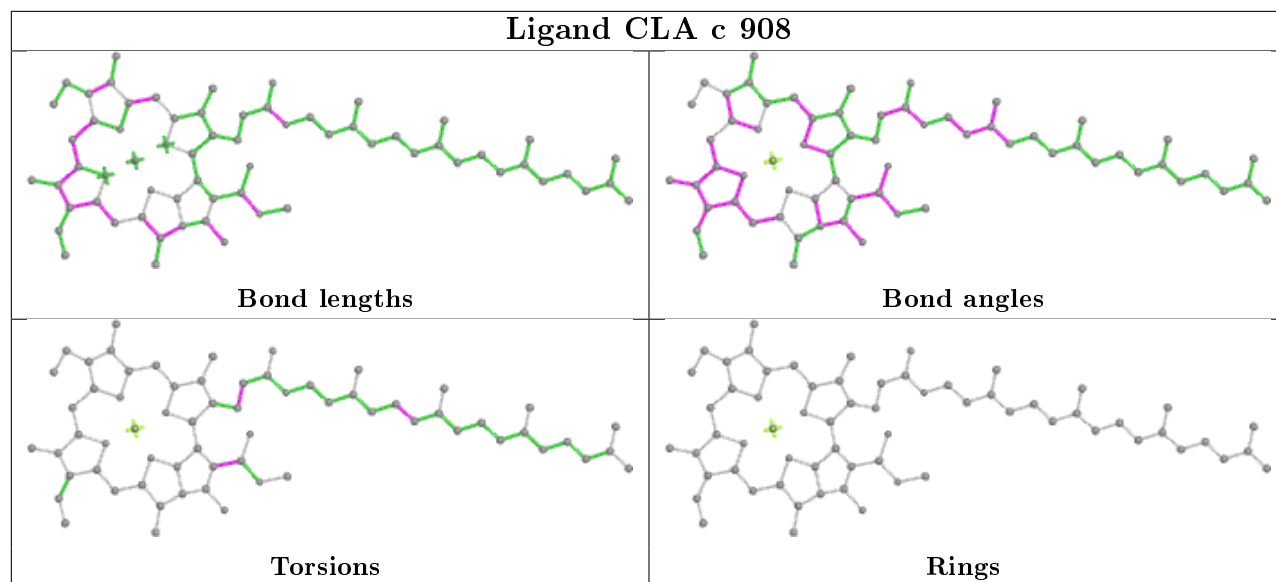
Ligand PL9 a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings



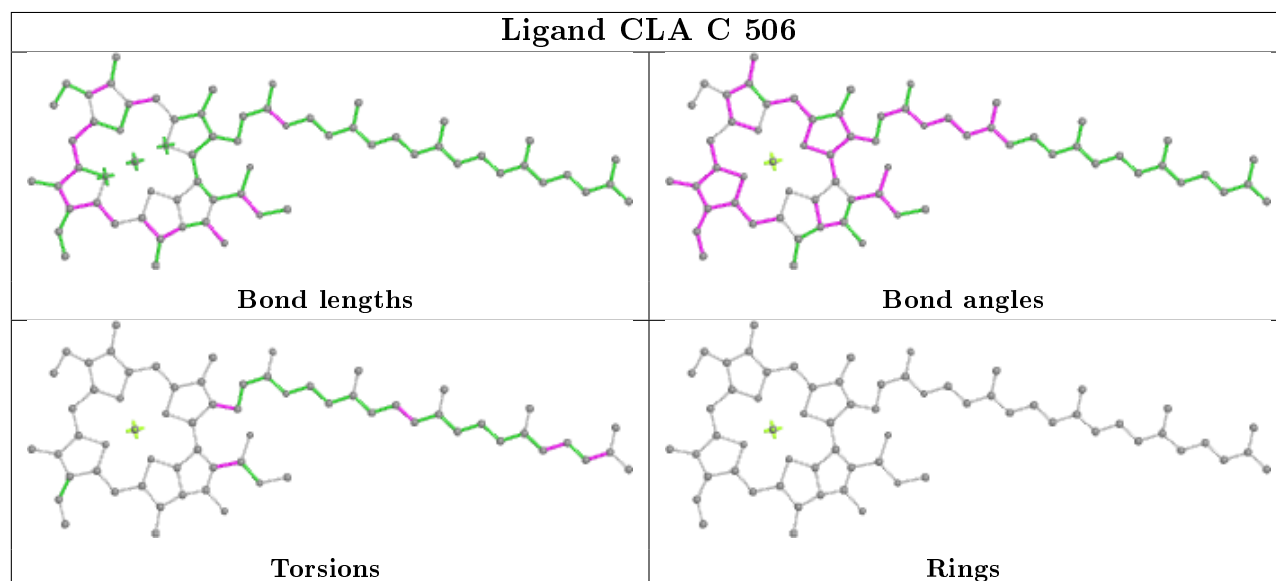




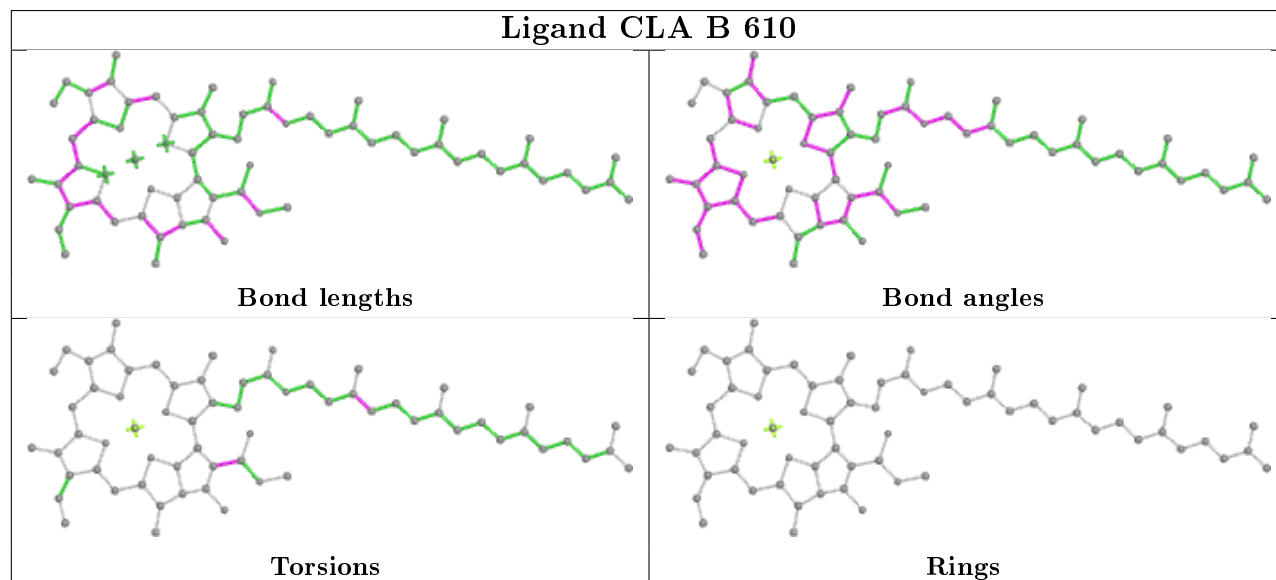
## Ligand CLA c 908

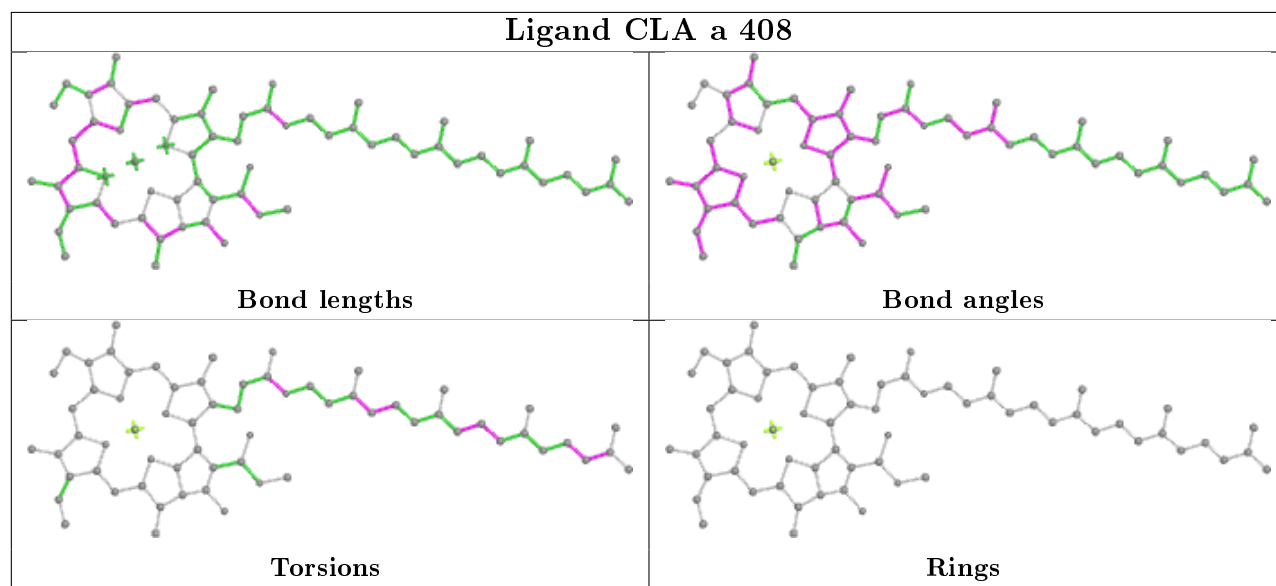
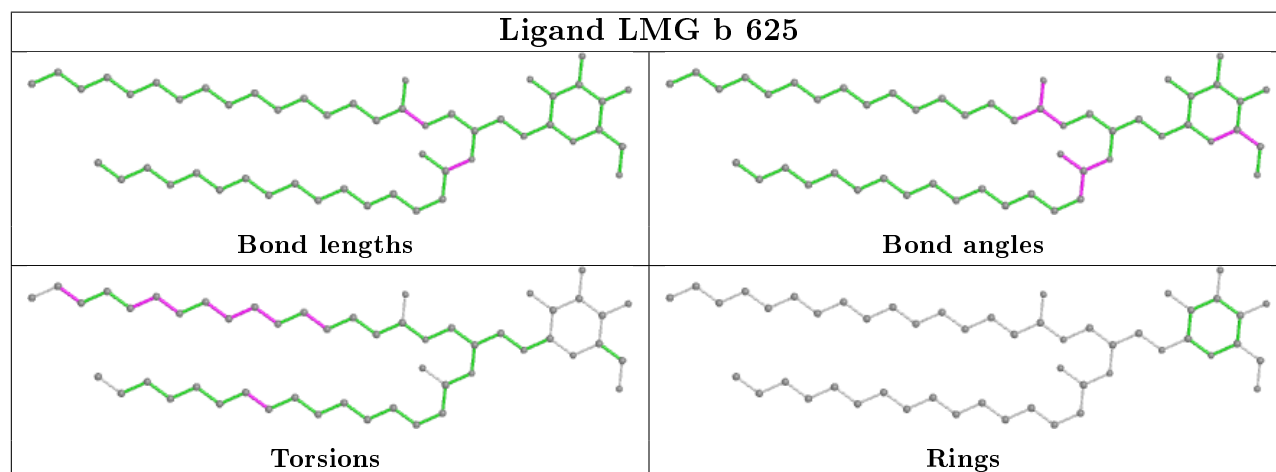
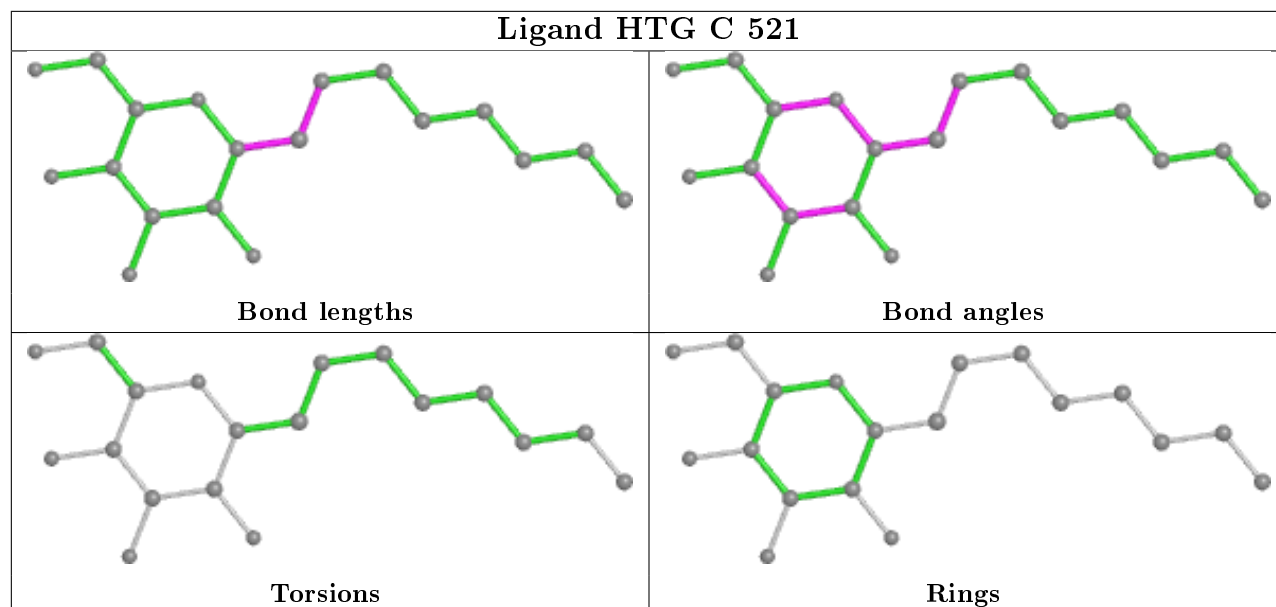


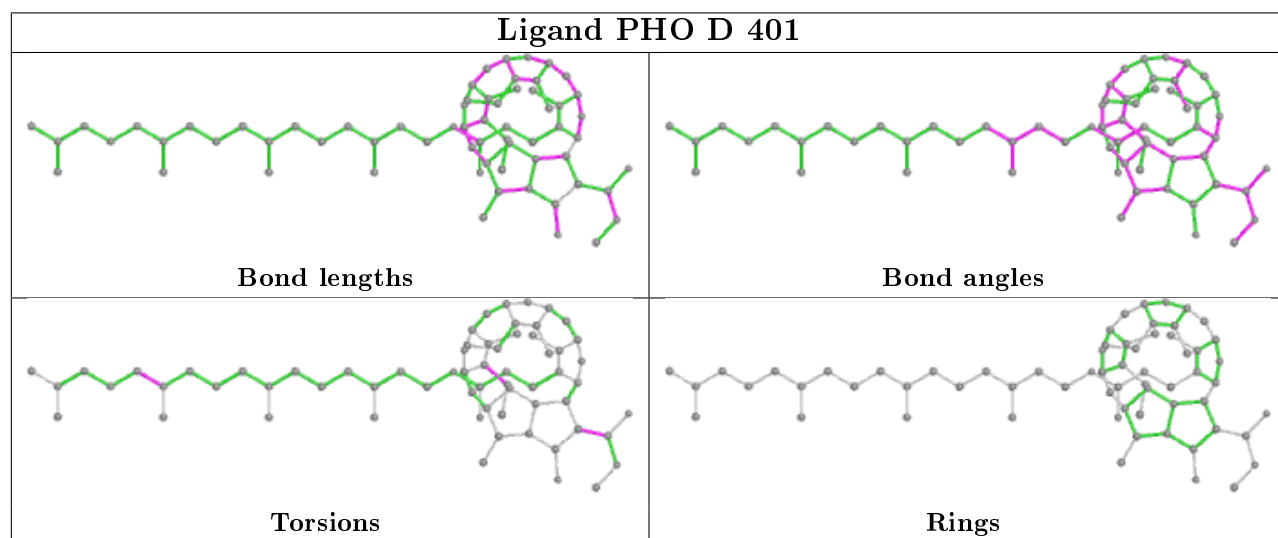
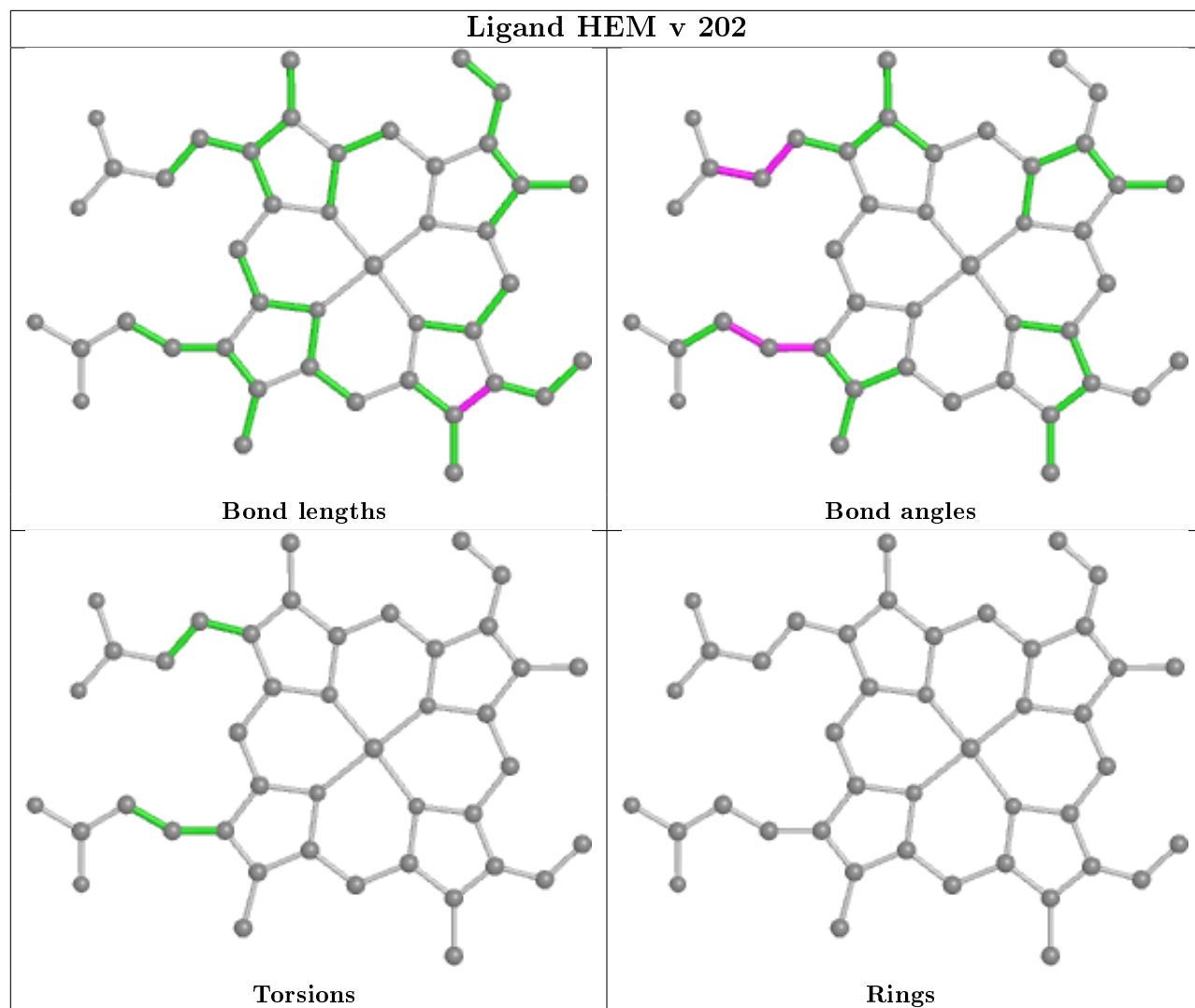
## Ligand CLA C 506



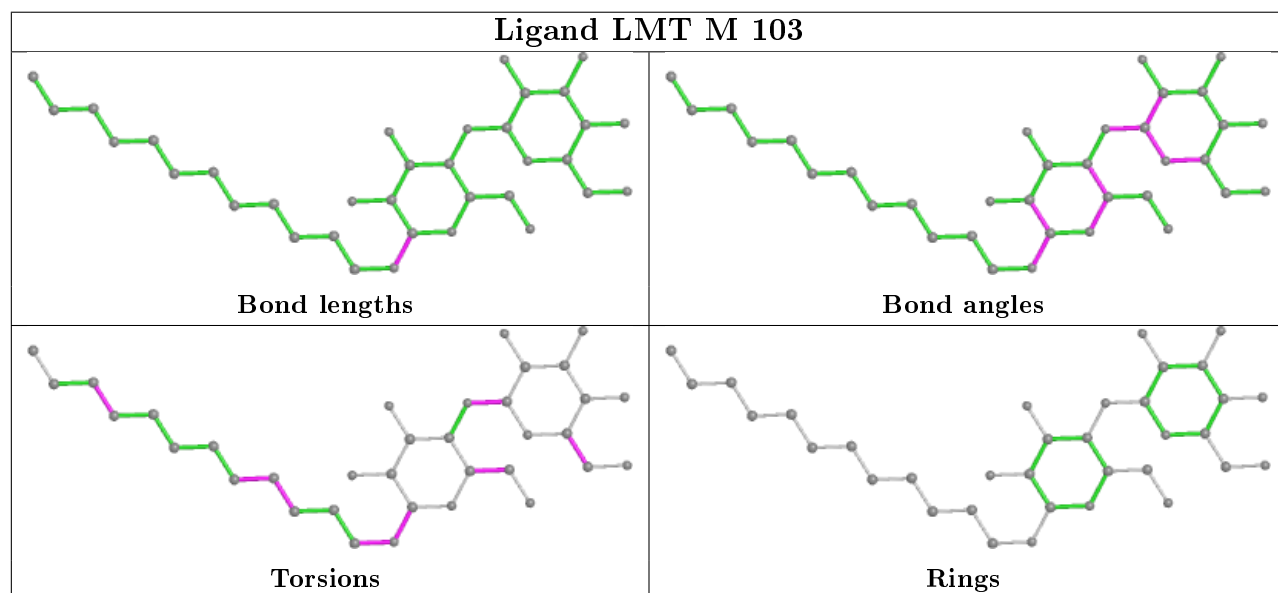
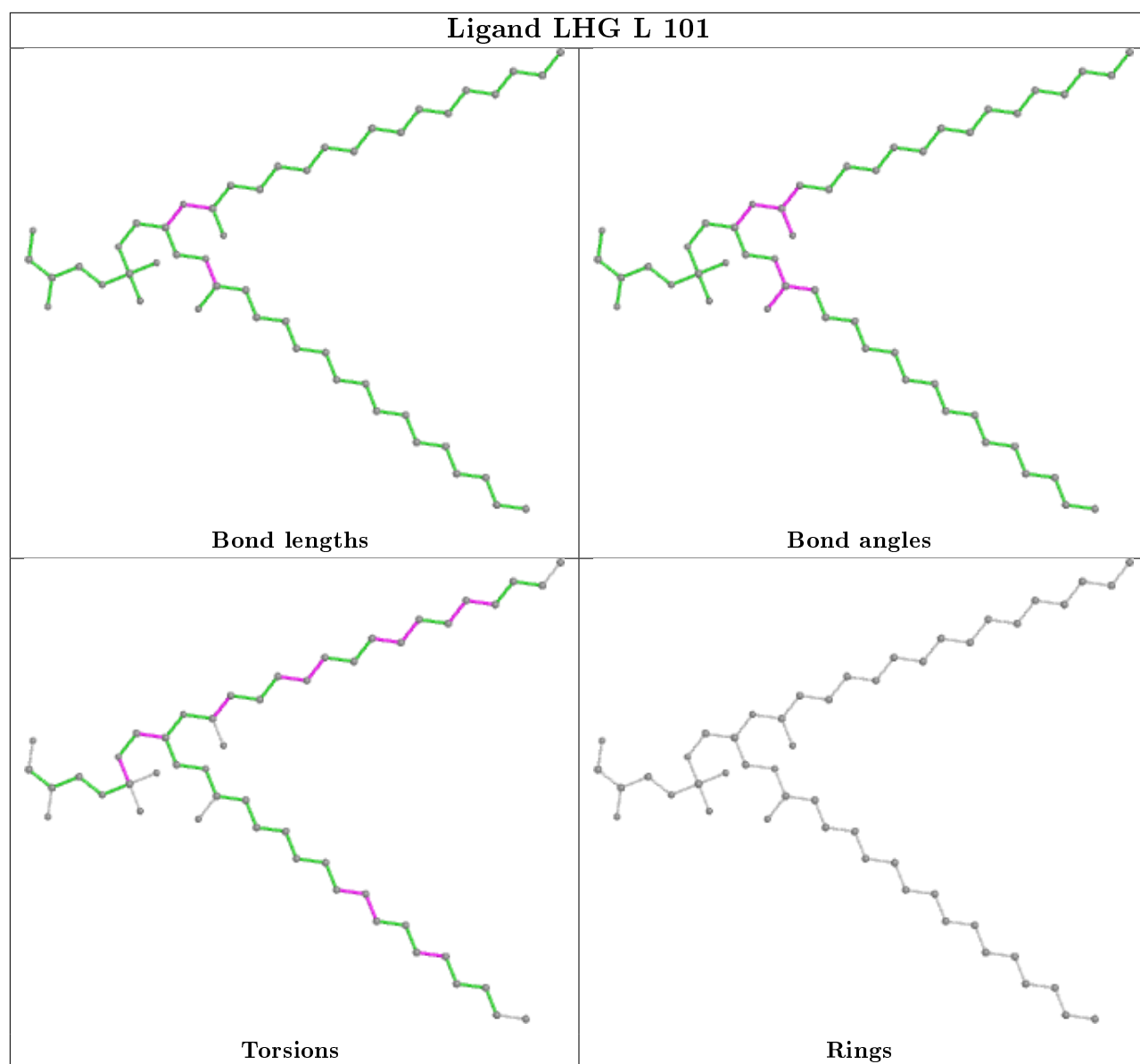
## Ligand CLA B 610

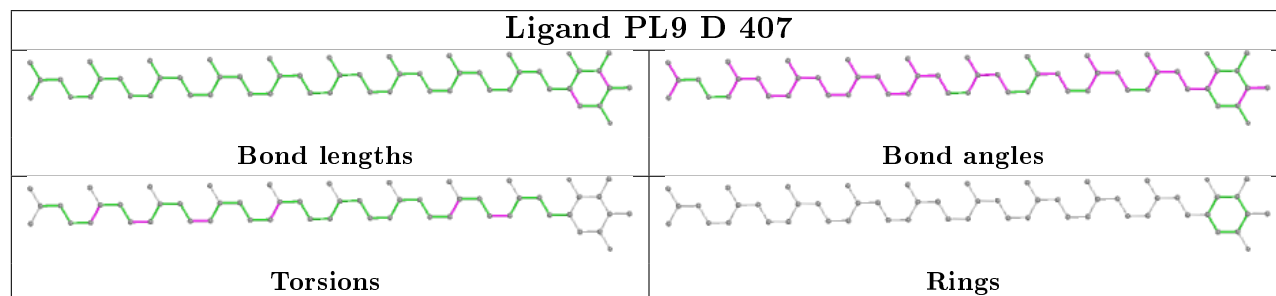
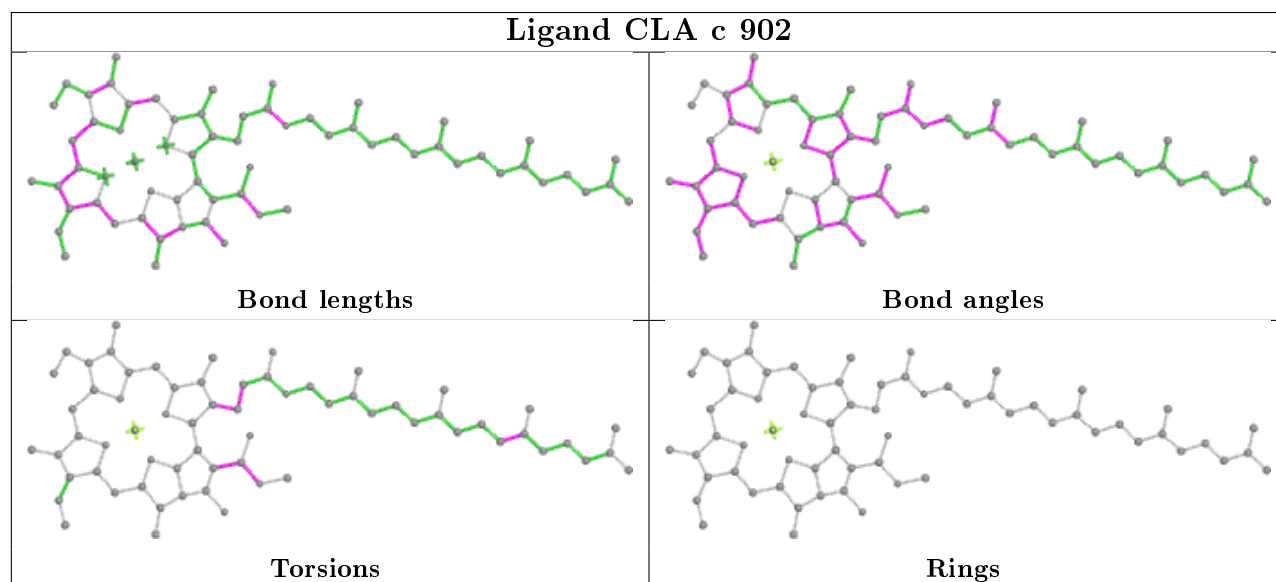
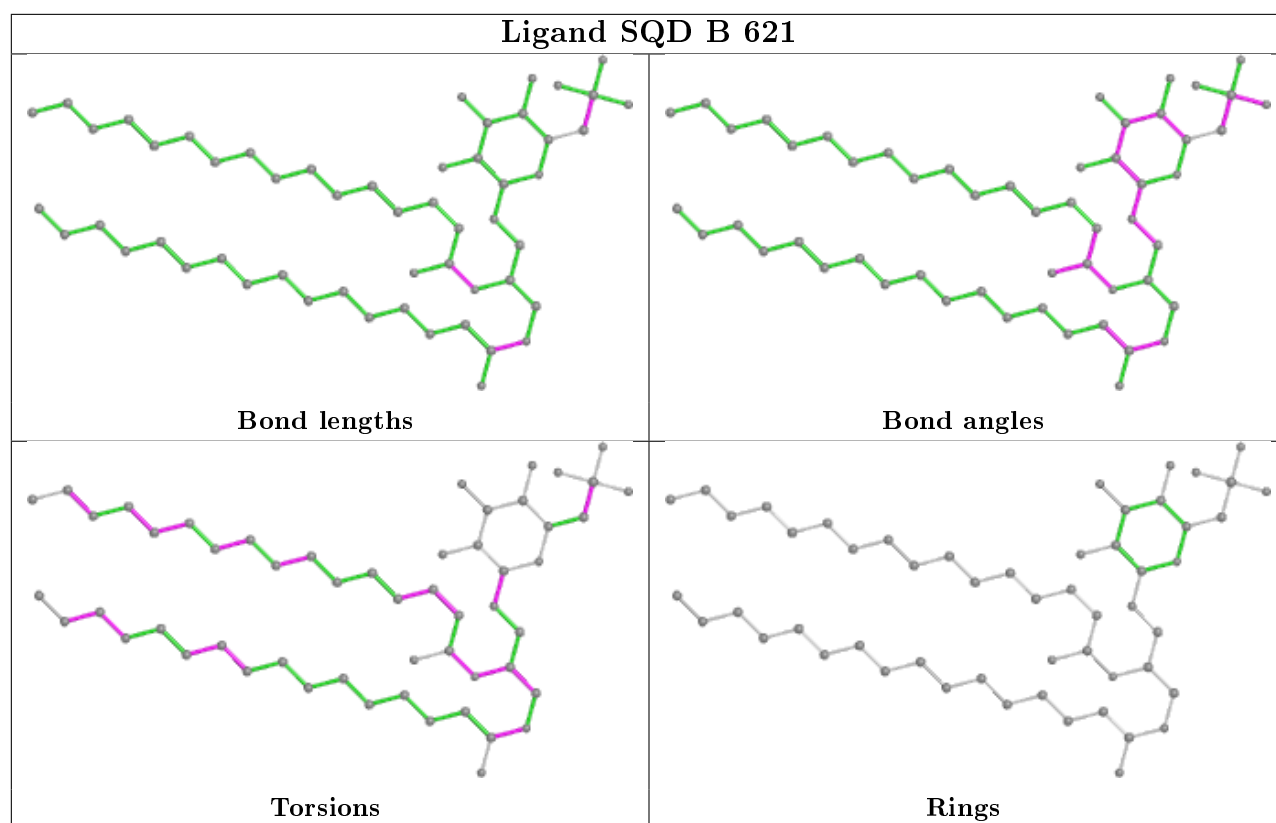


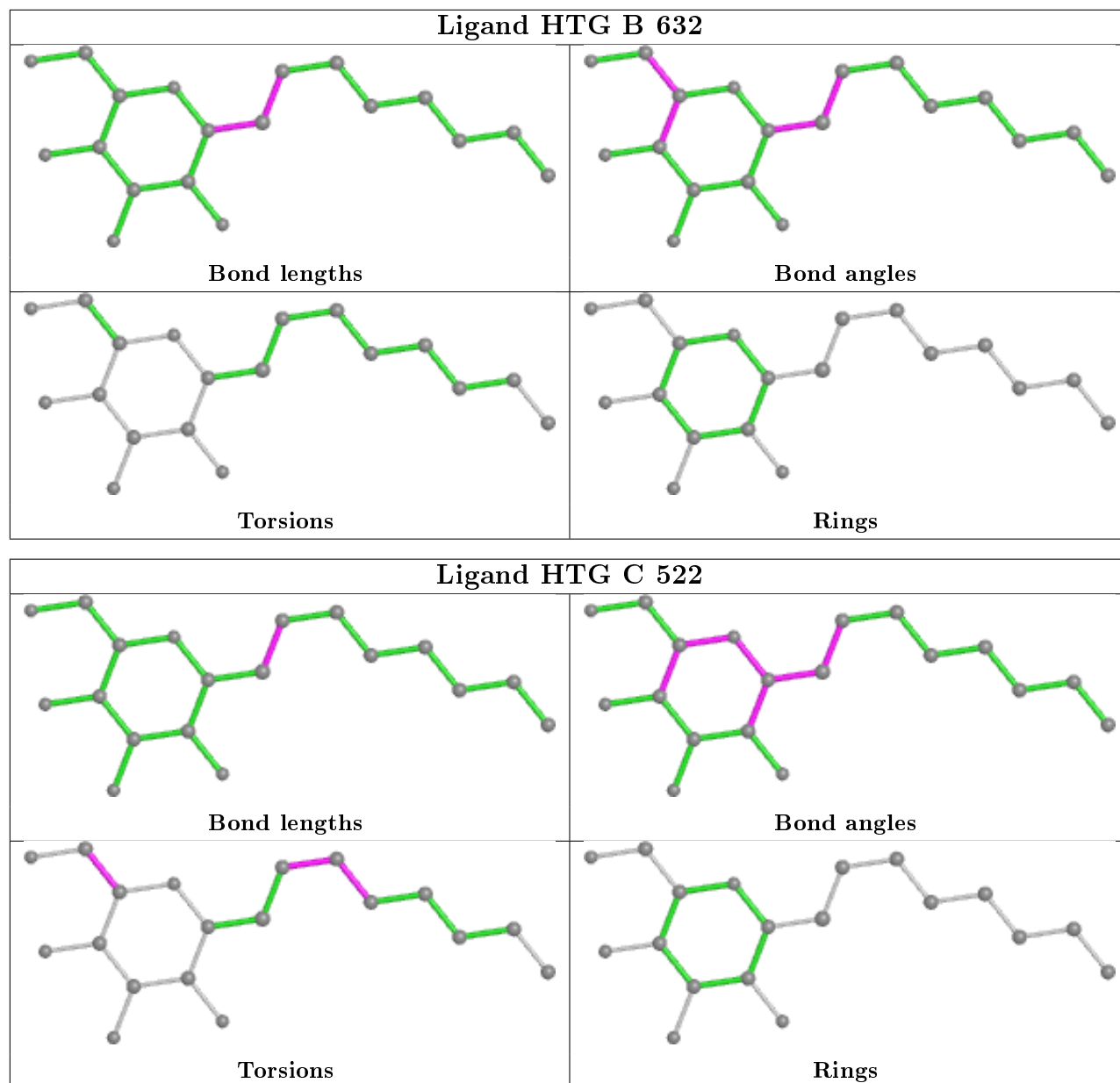




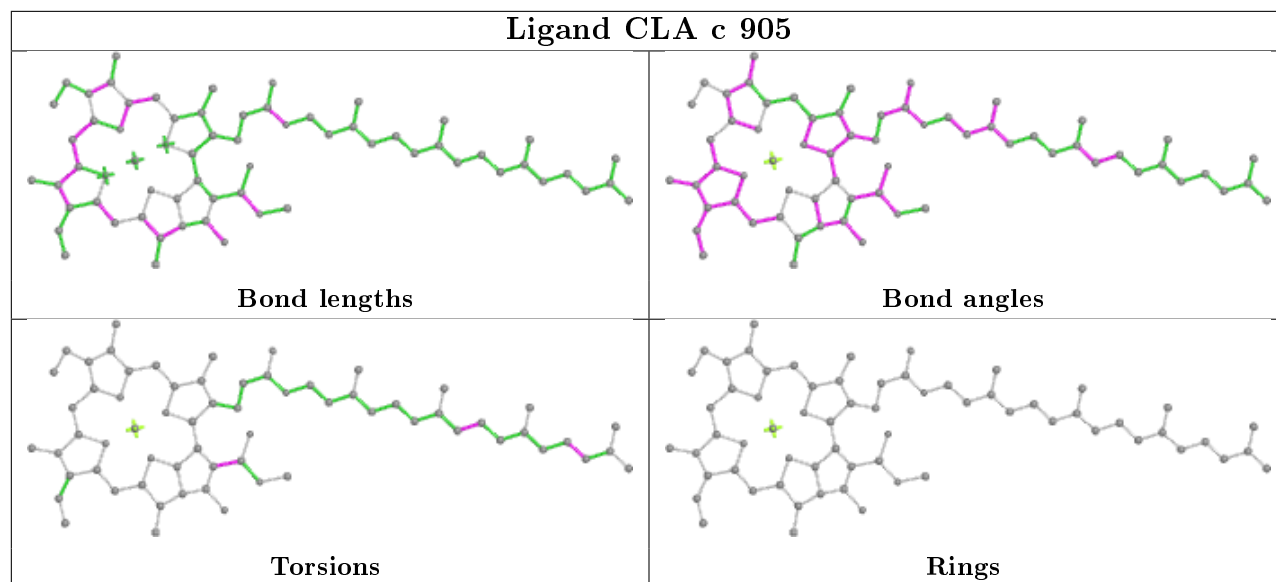




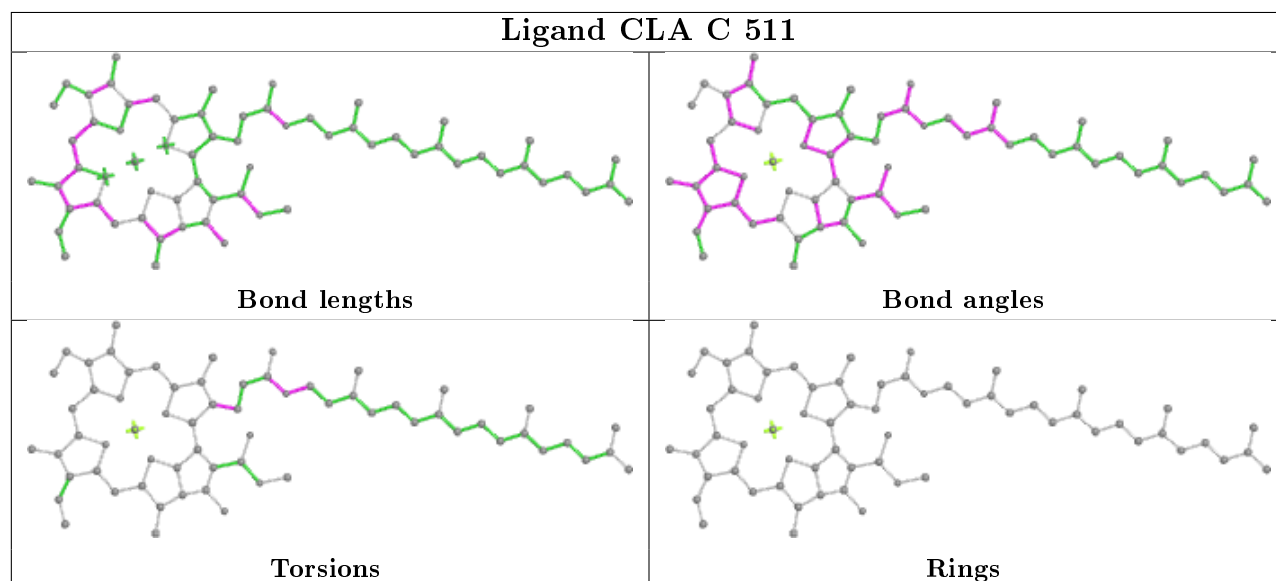




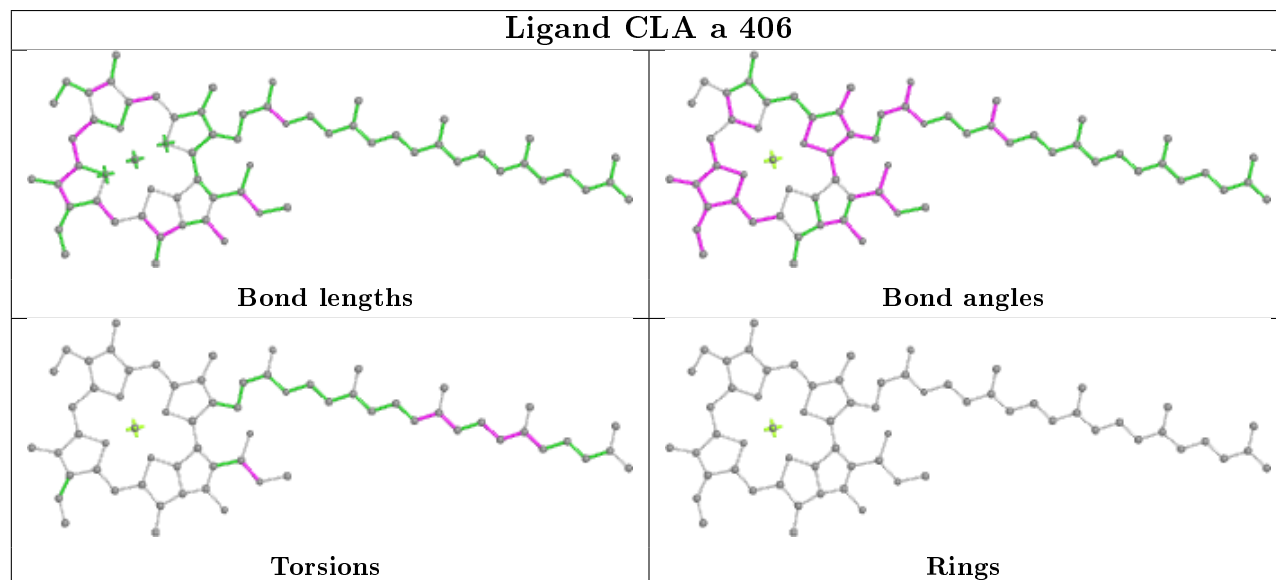
## Ligand CLA c 905

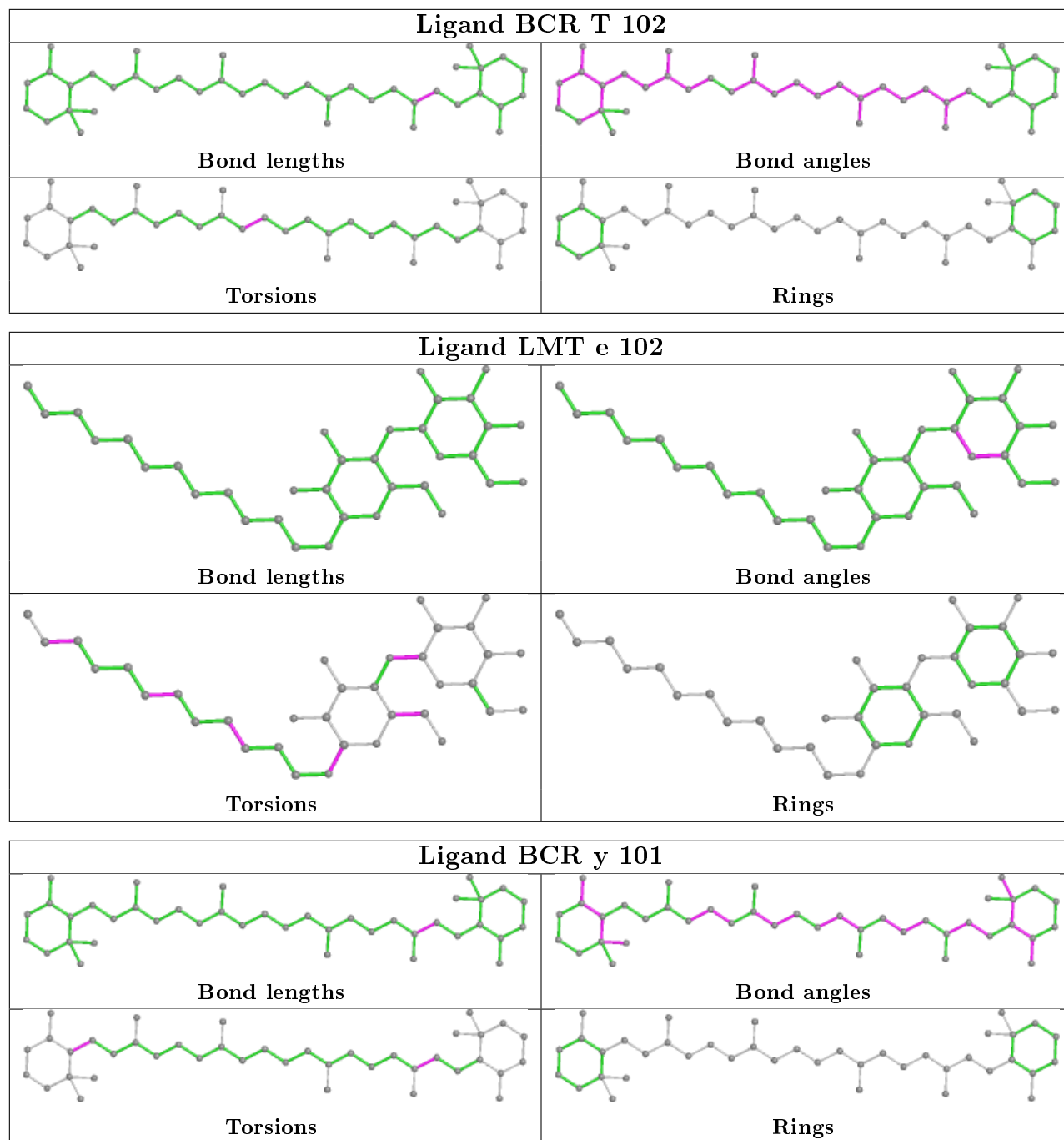


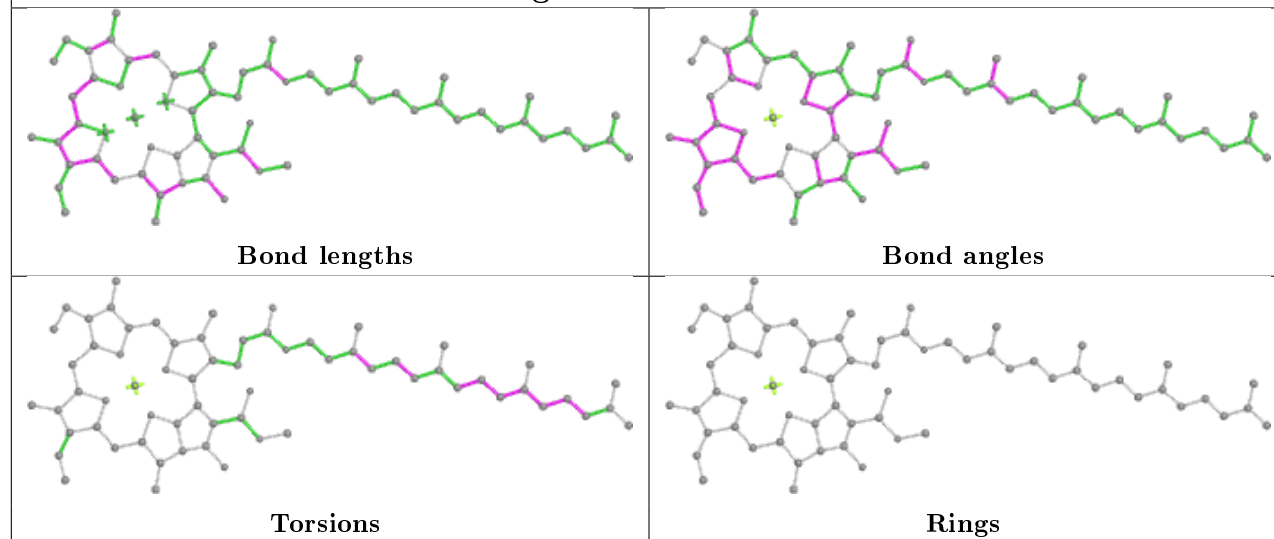
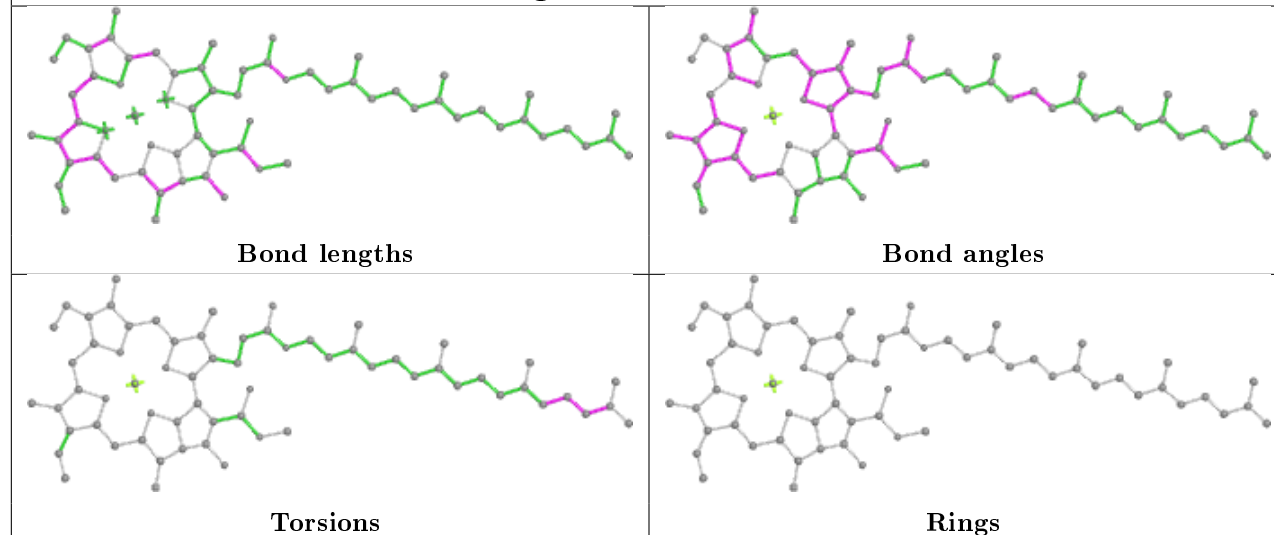
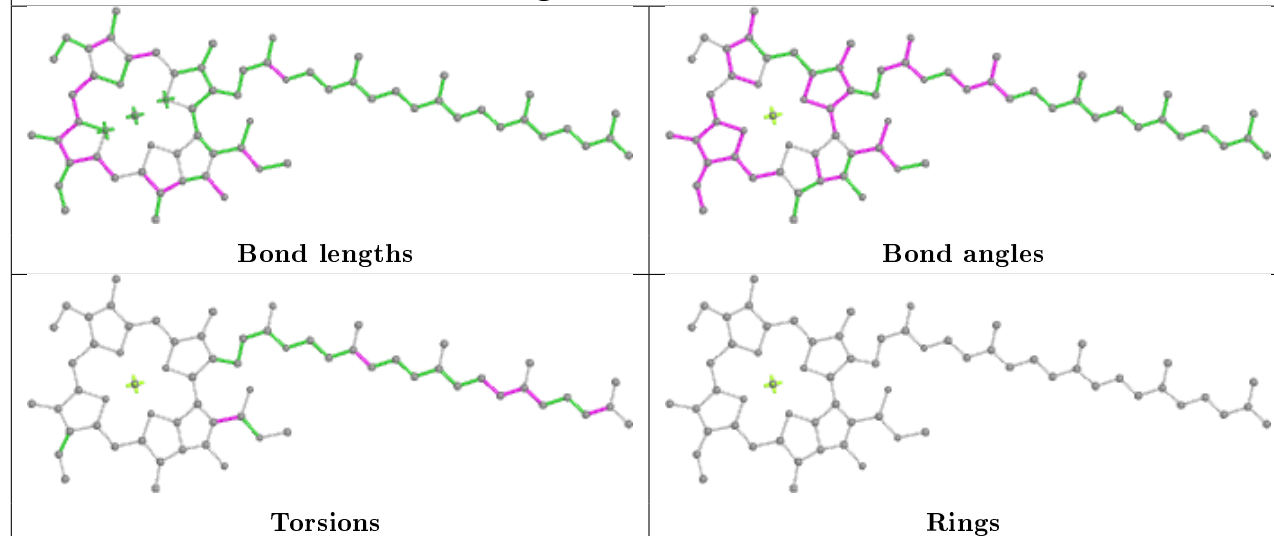
## Ligand CLA C 511



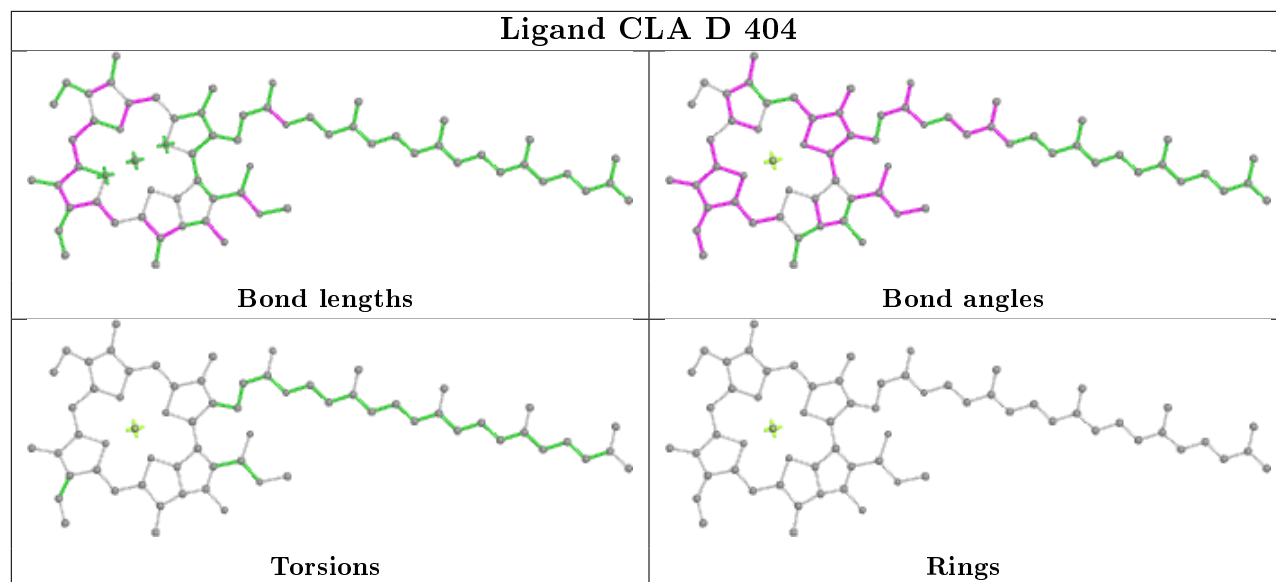
## Ligand CLA a 406



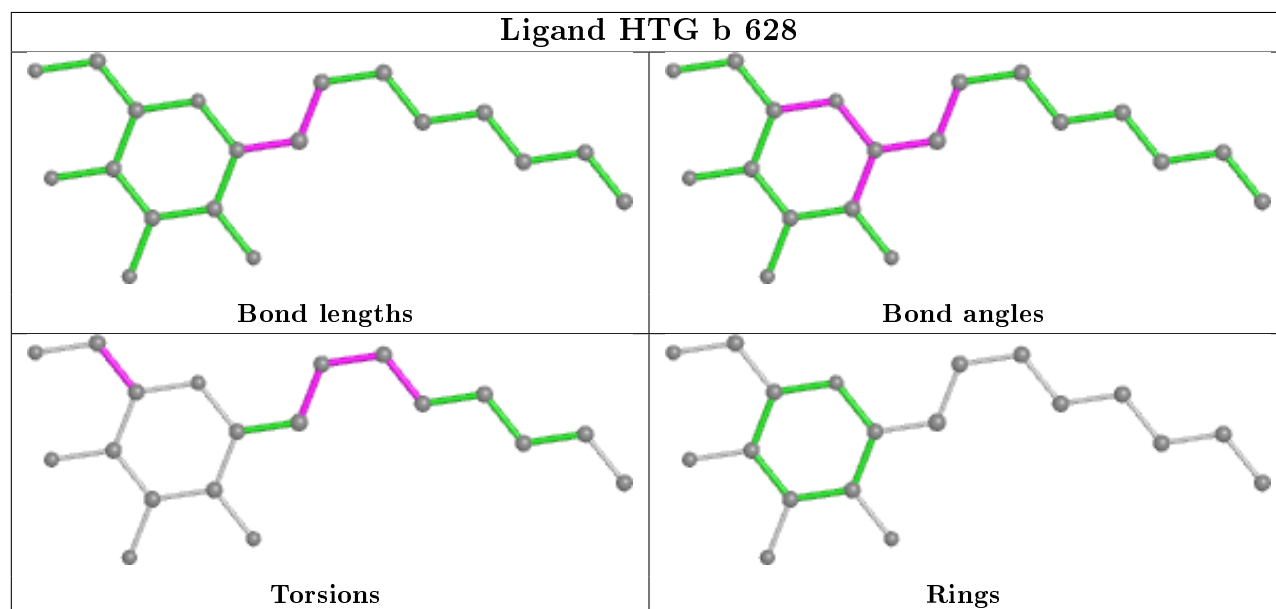


**Ligand CLA B 616****Ligand CLA A 405****Ligand CLA b 621**

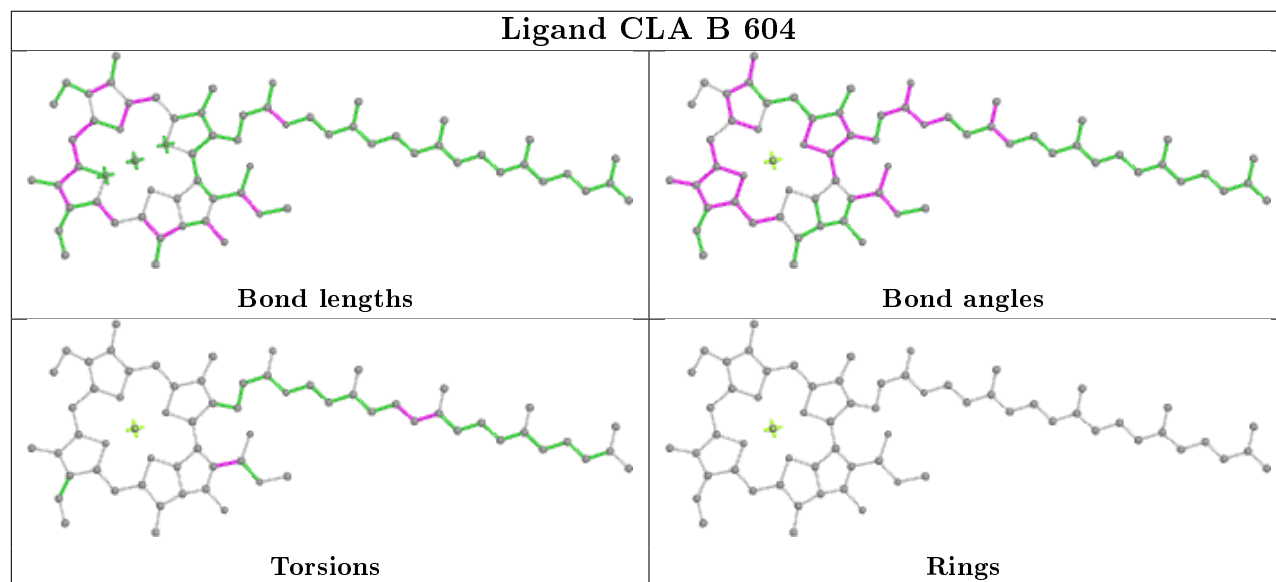
## Ligand CLA D 404

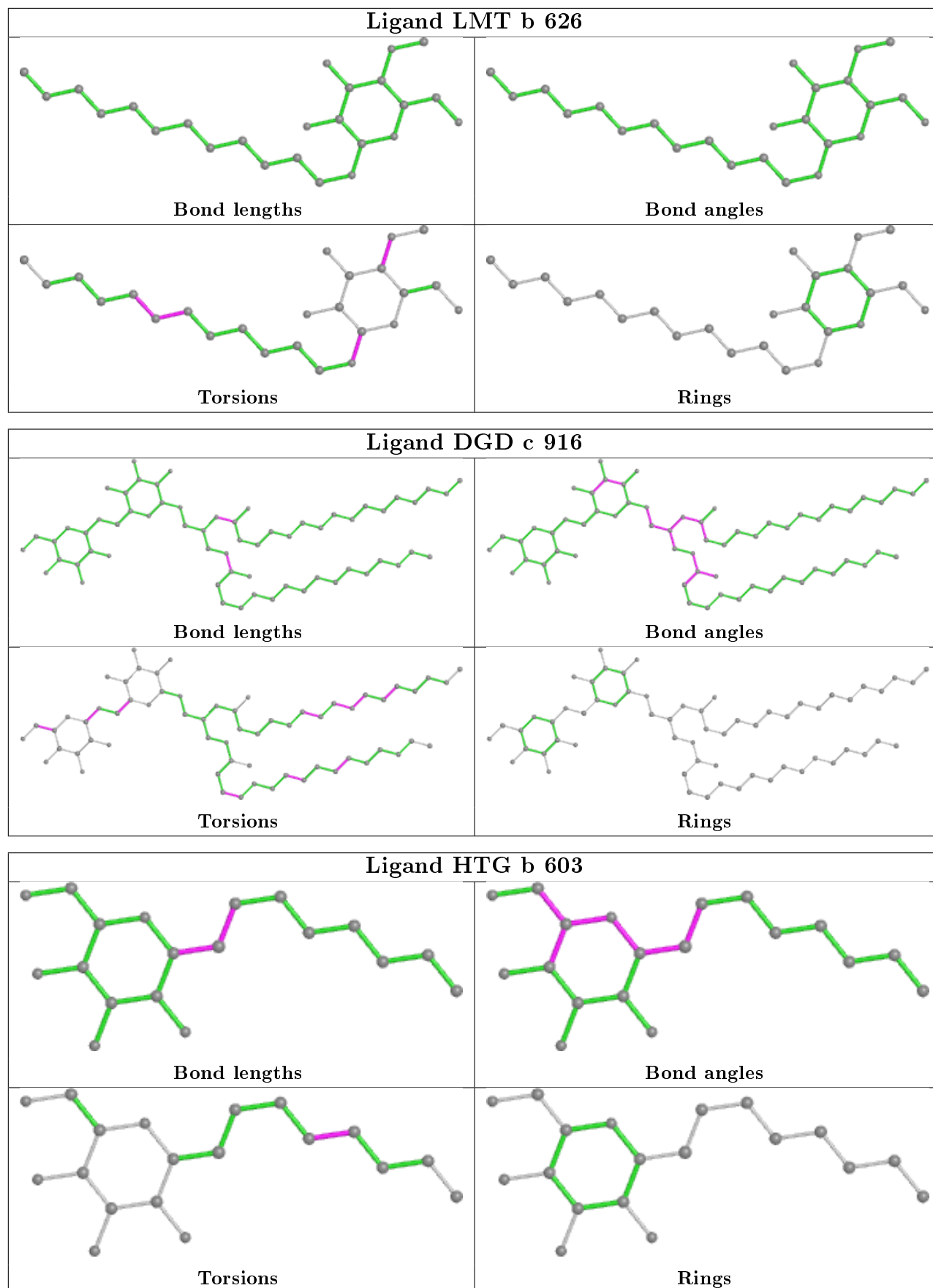


## Ligand HTG b 628

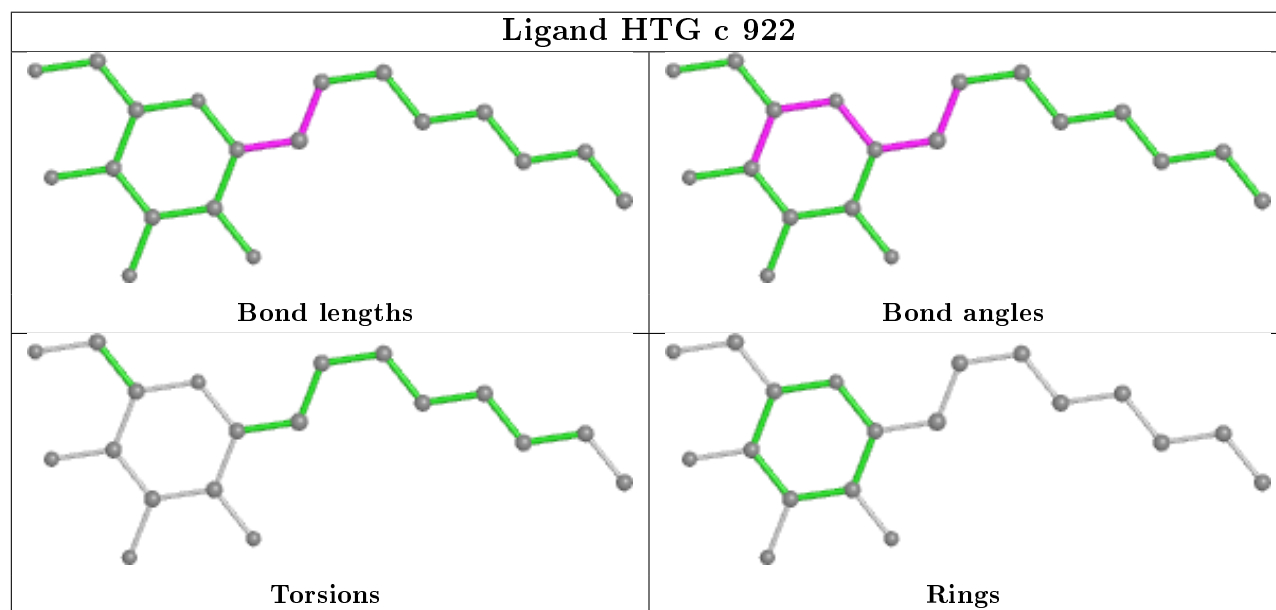
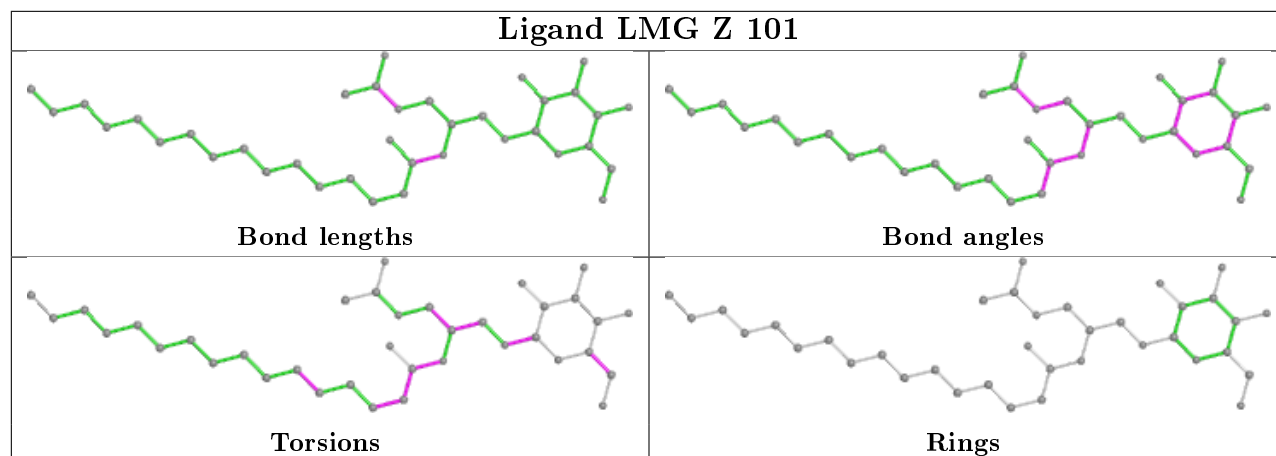
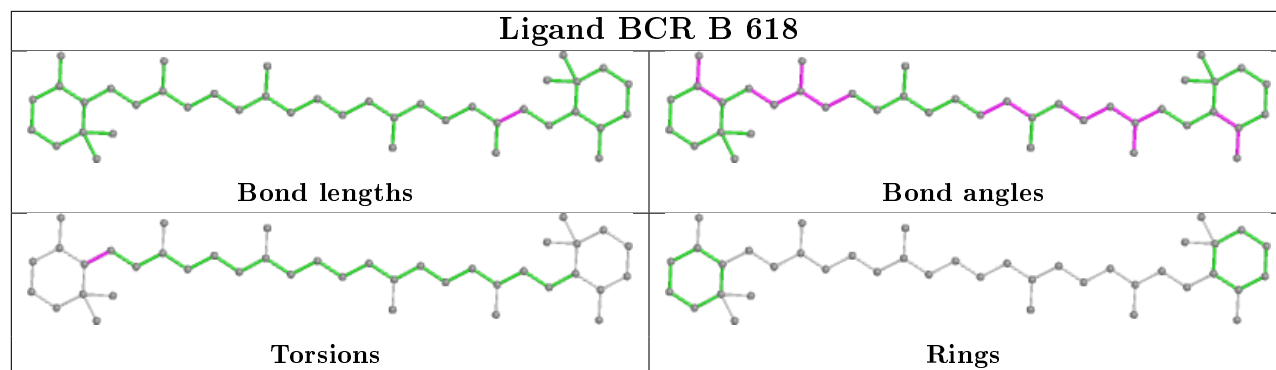


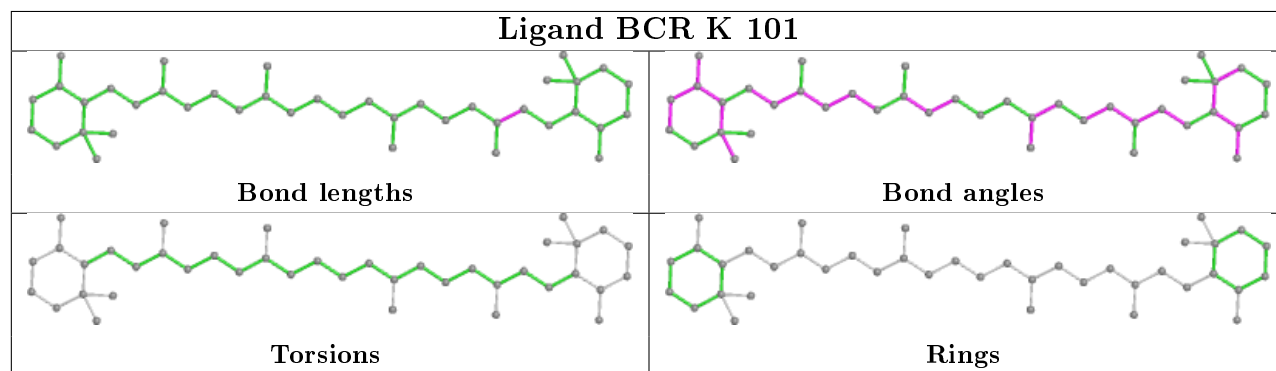
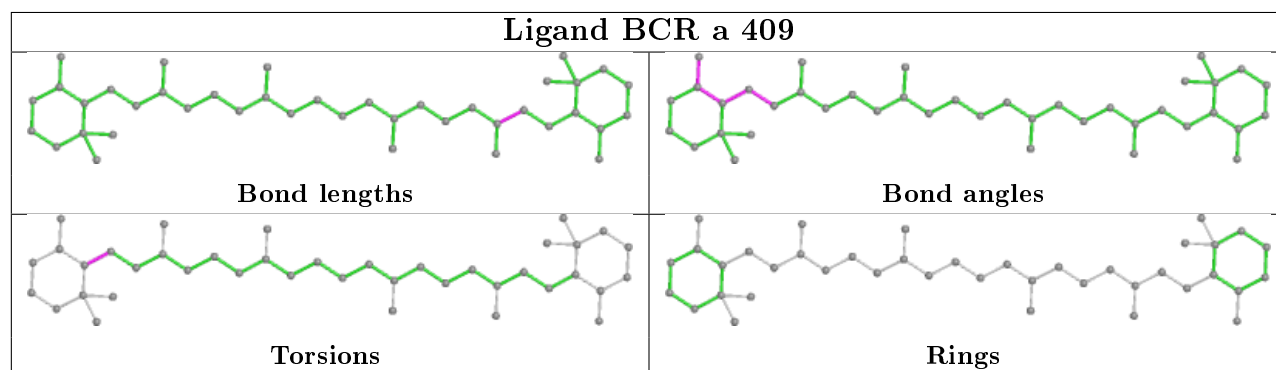
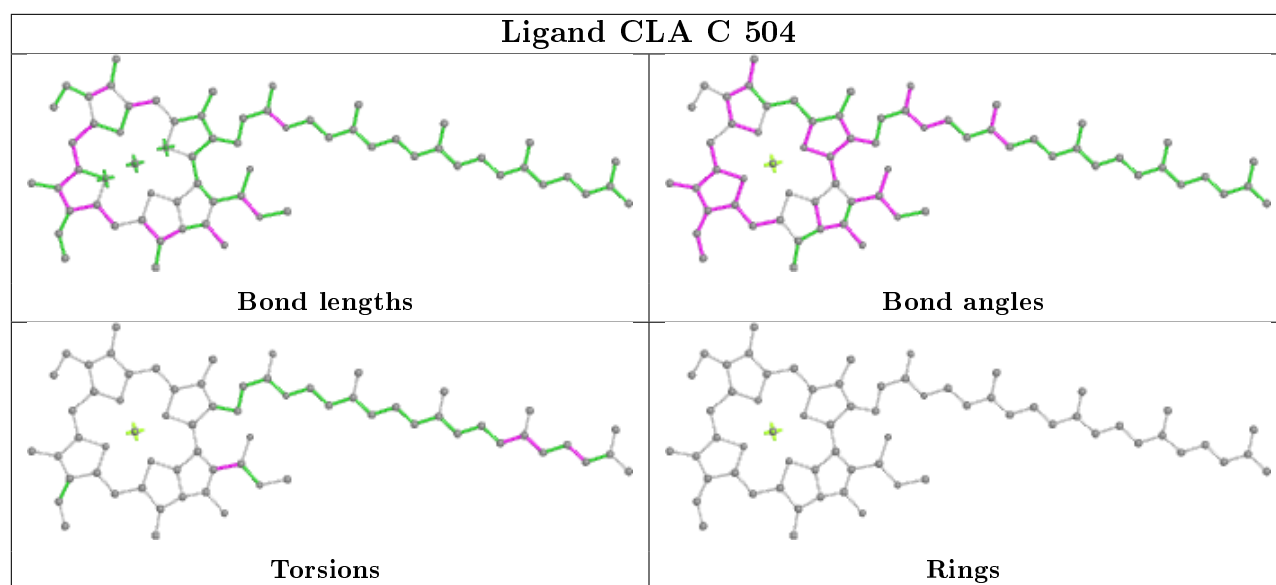
## Ligand CLA B 604



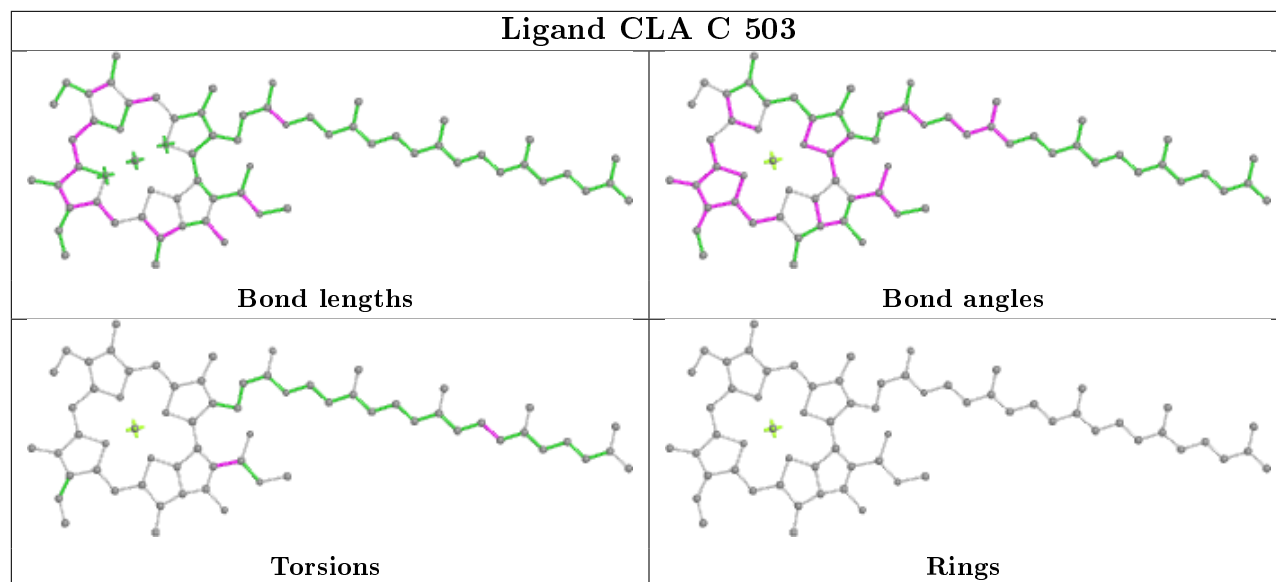




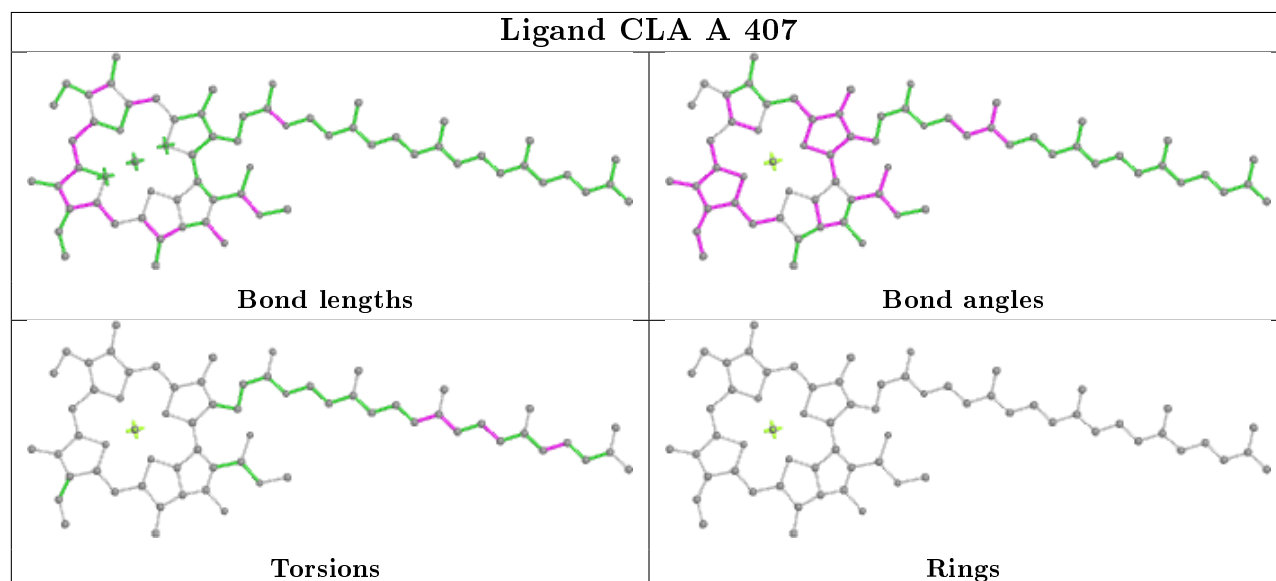




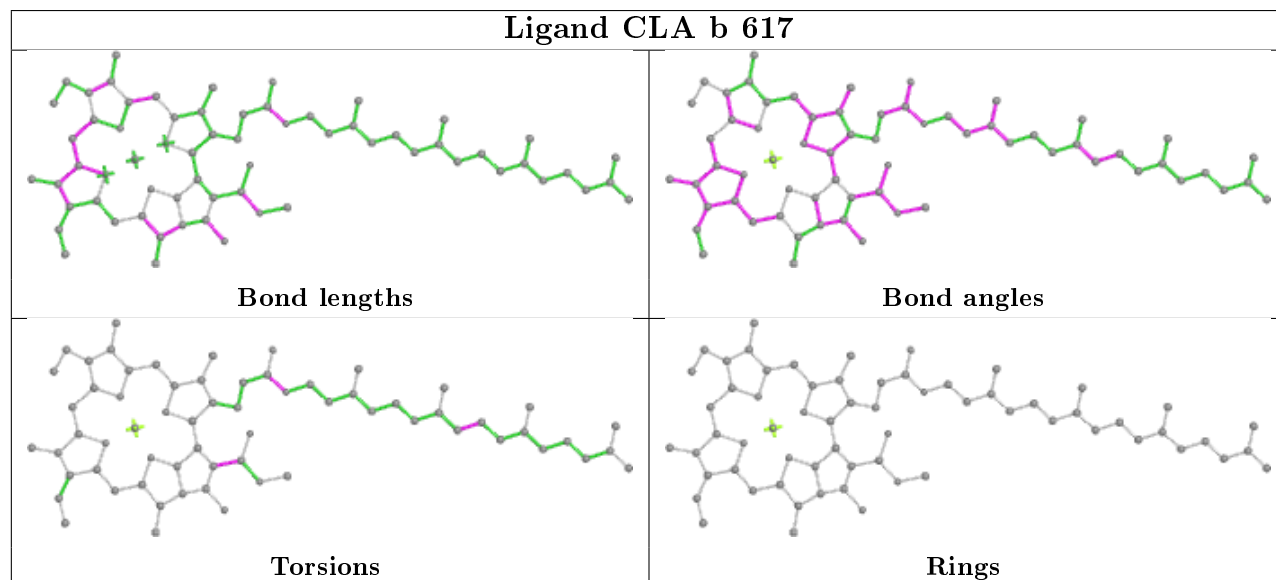
## Ligand CLA C 503

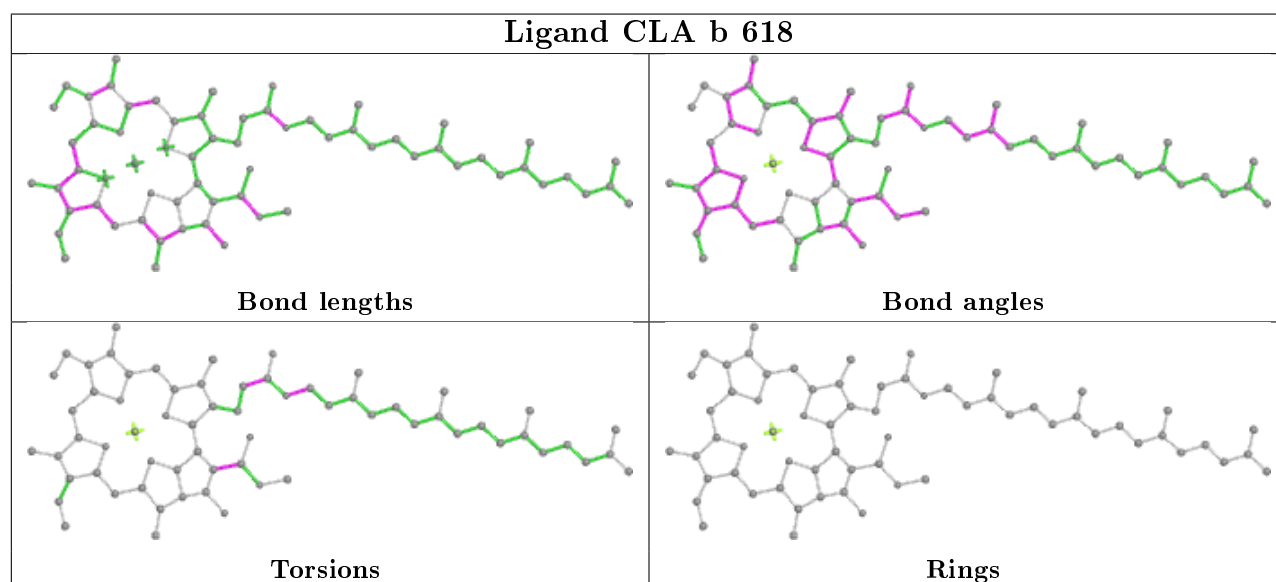
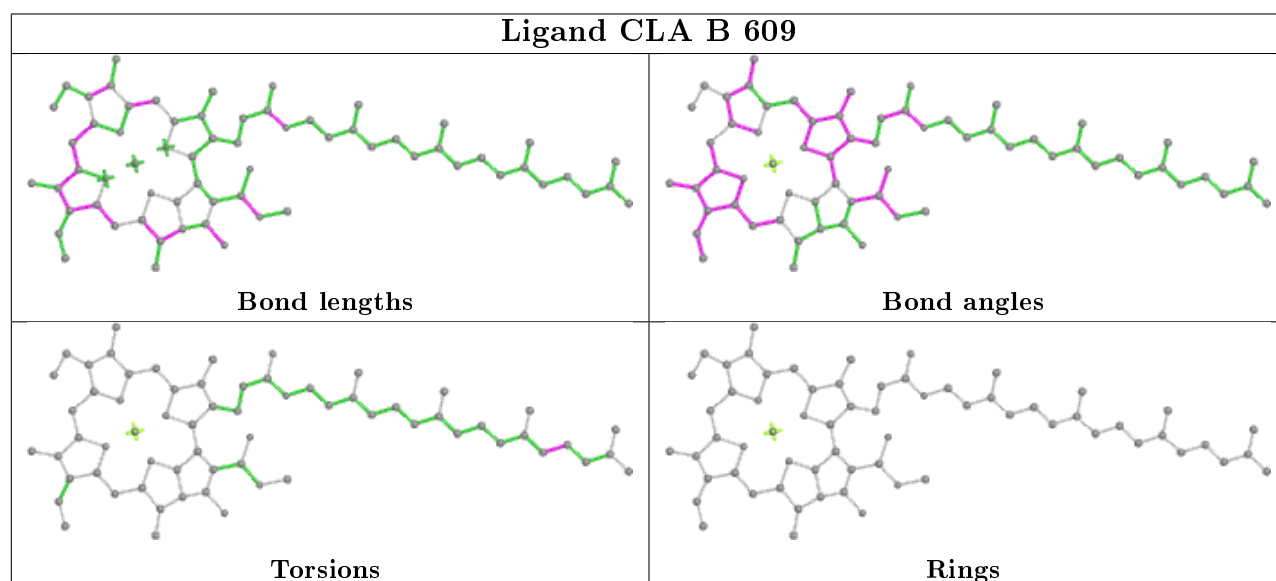
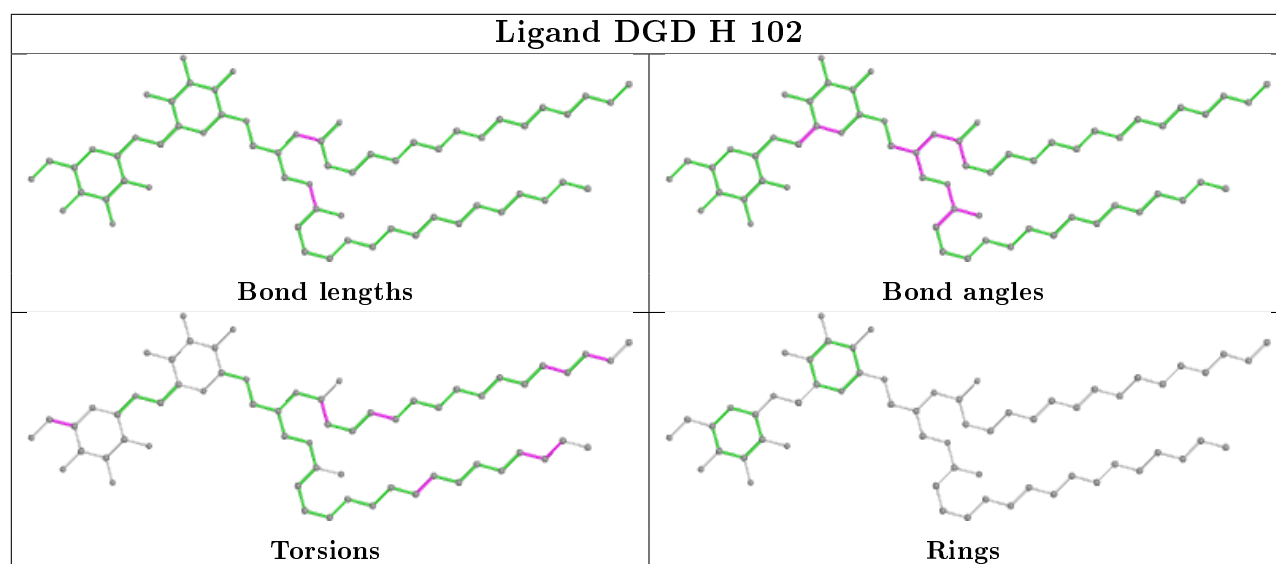


## Ligand CLA A 407

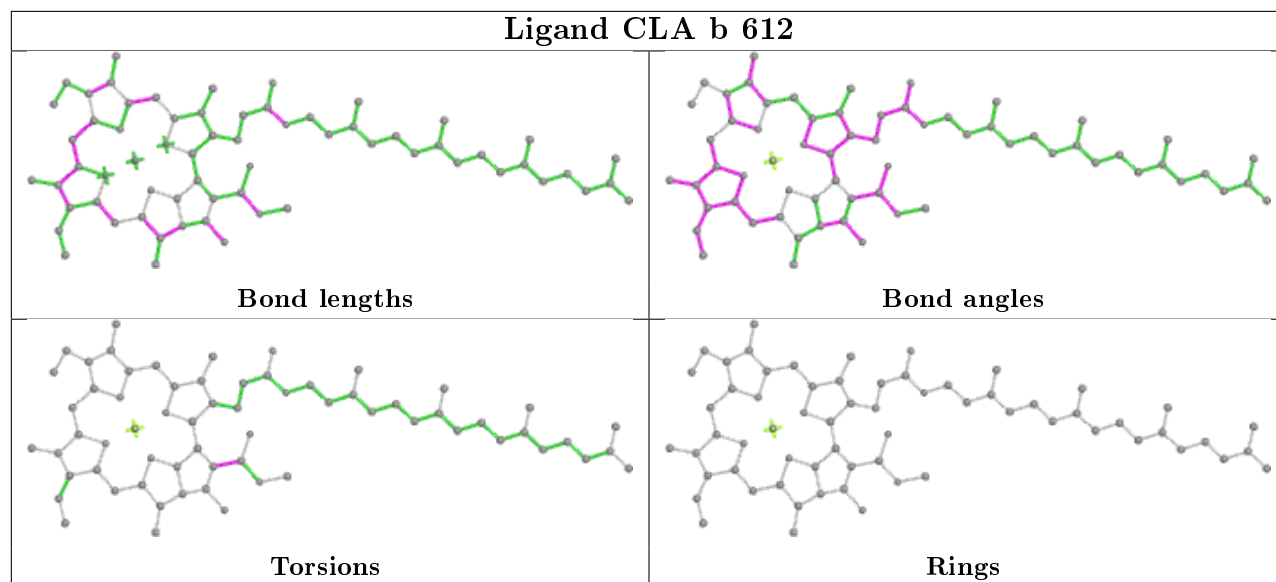


## Ligand CLA b 617

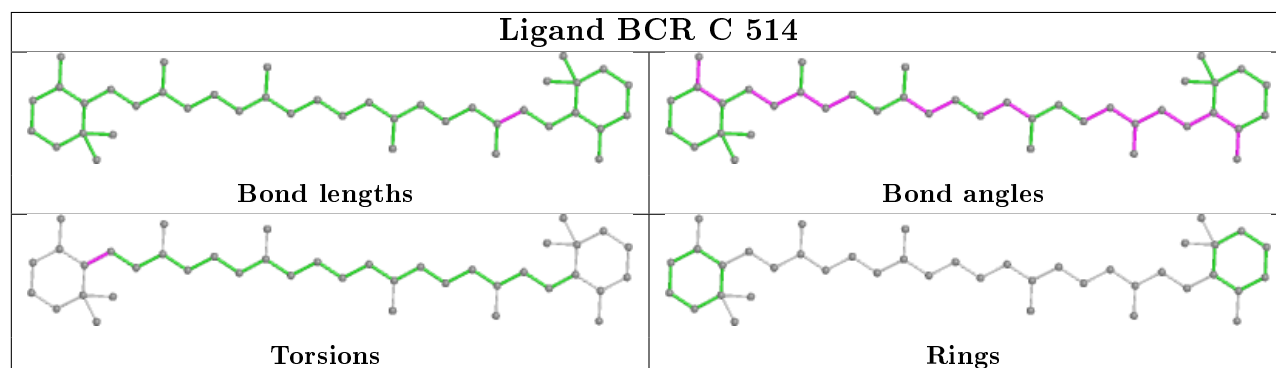




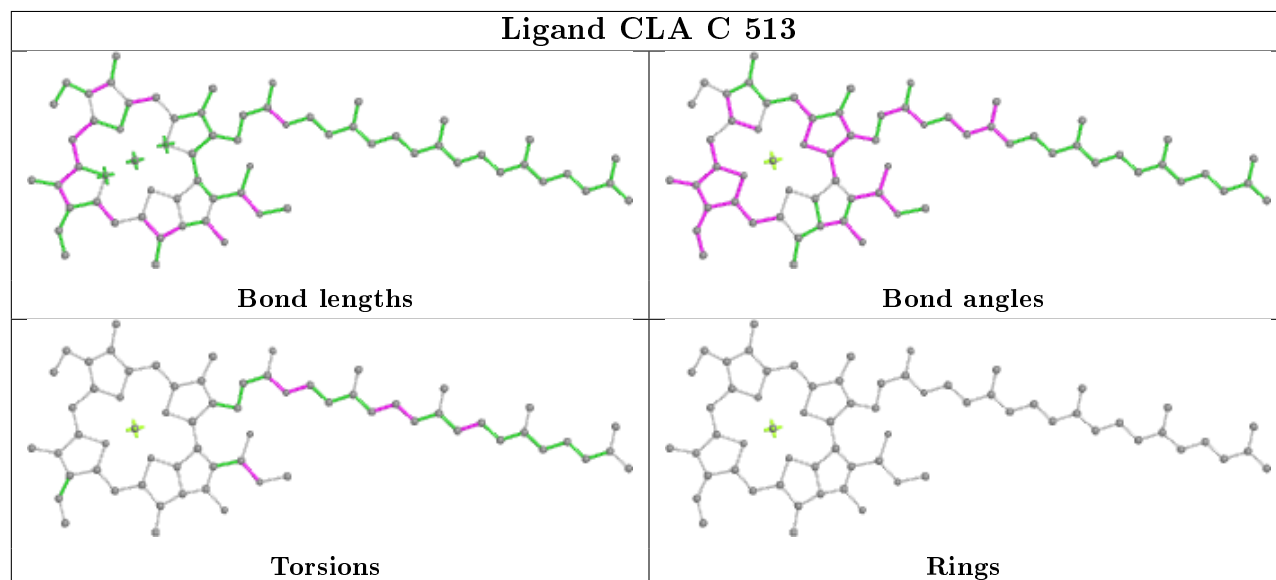
## Ligand CLA b 612

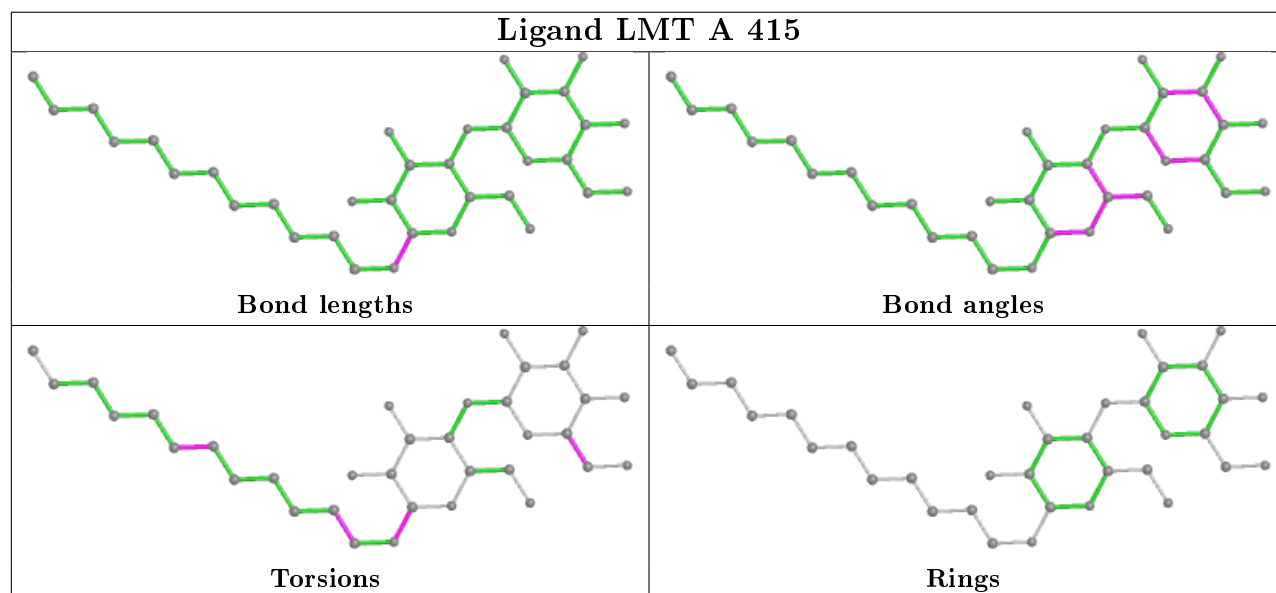
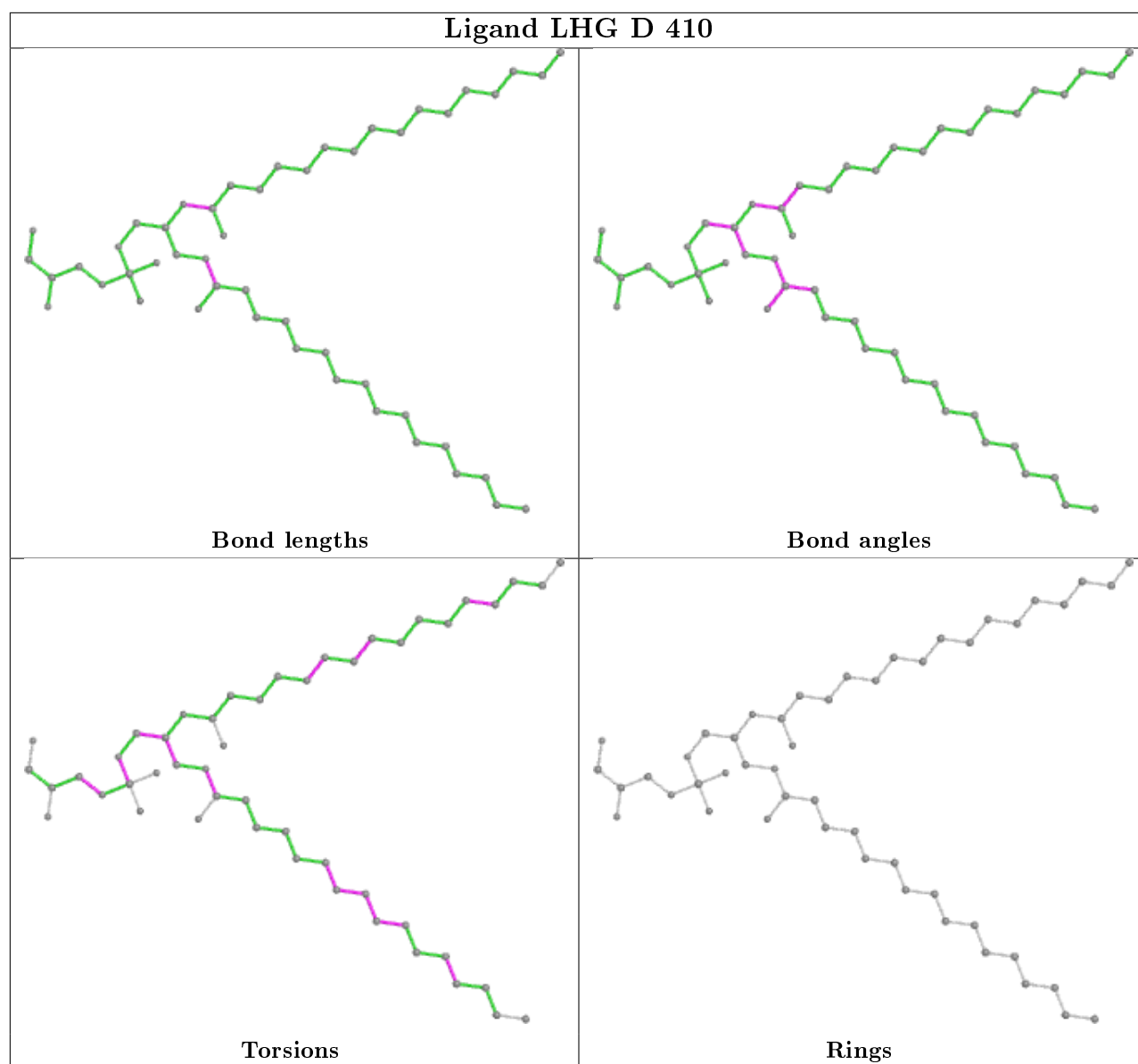


## Ligand BCR C 514

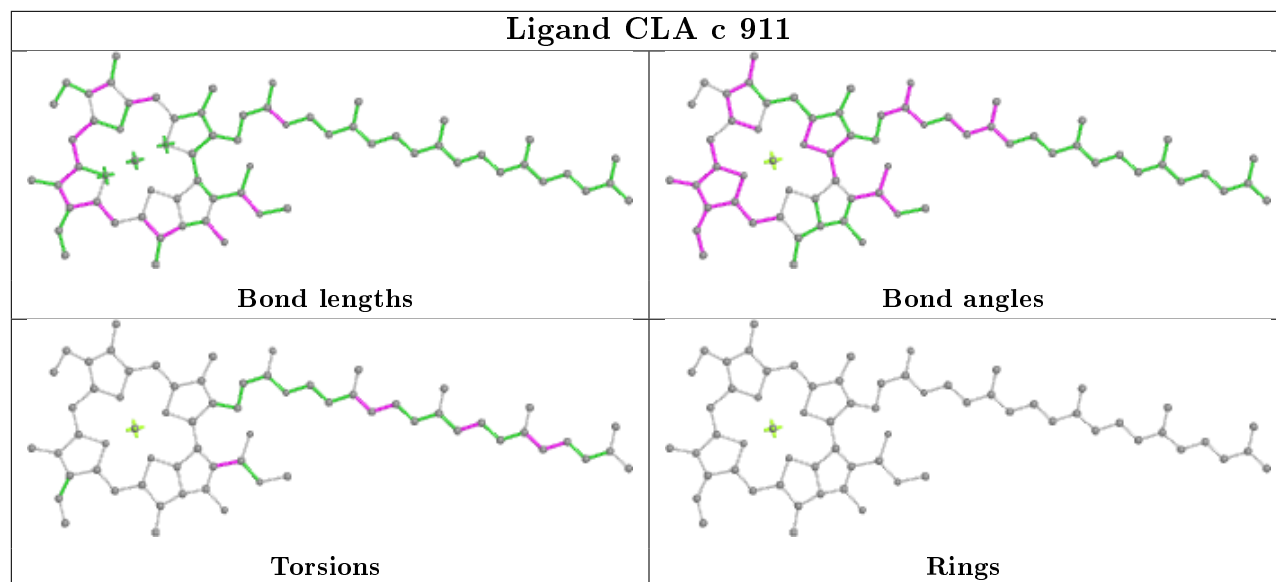


## Ligand CLA C 513

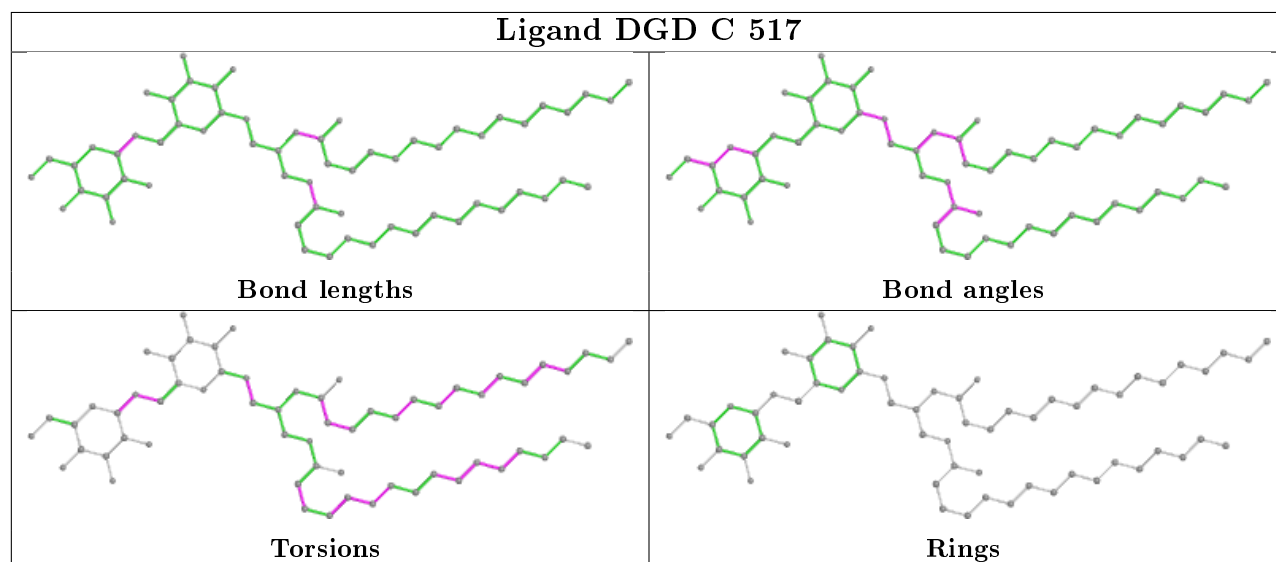




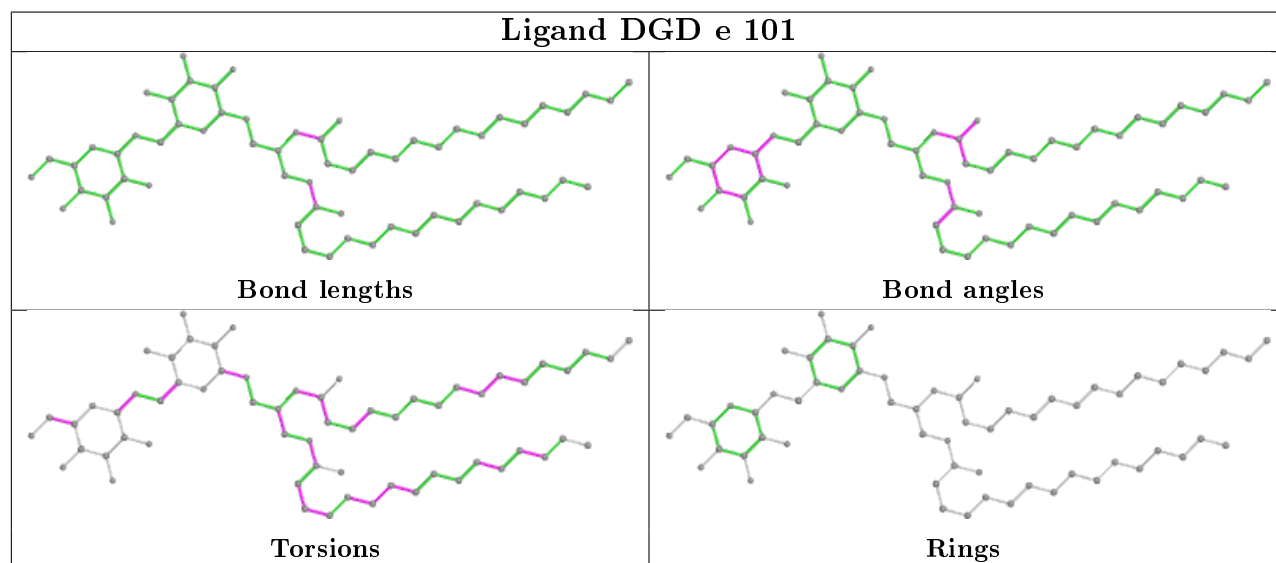
## Ligand CLA c 911

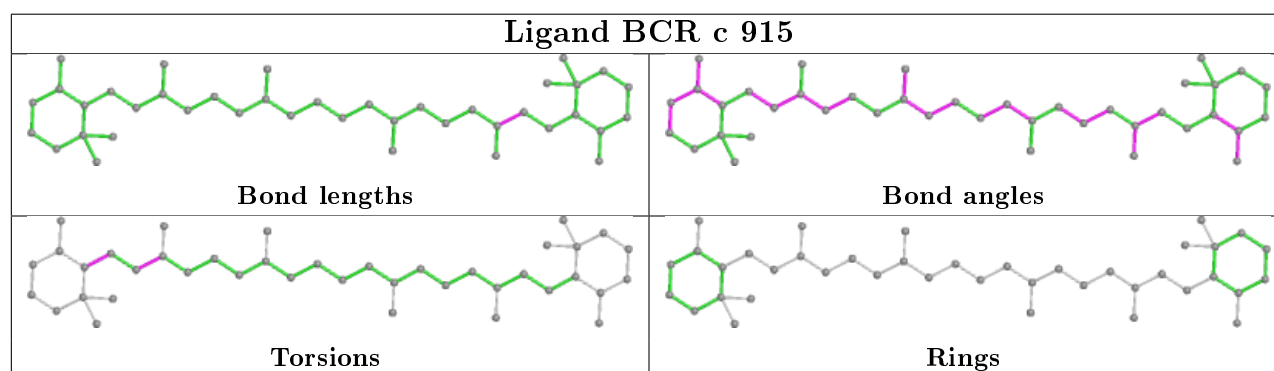
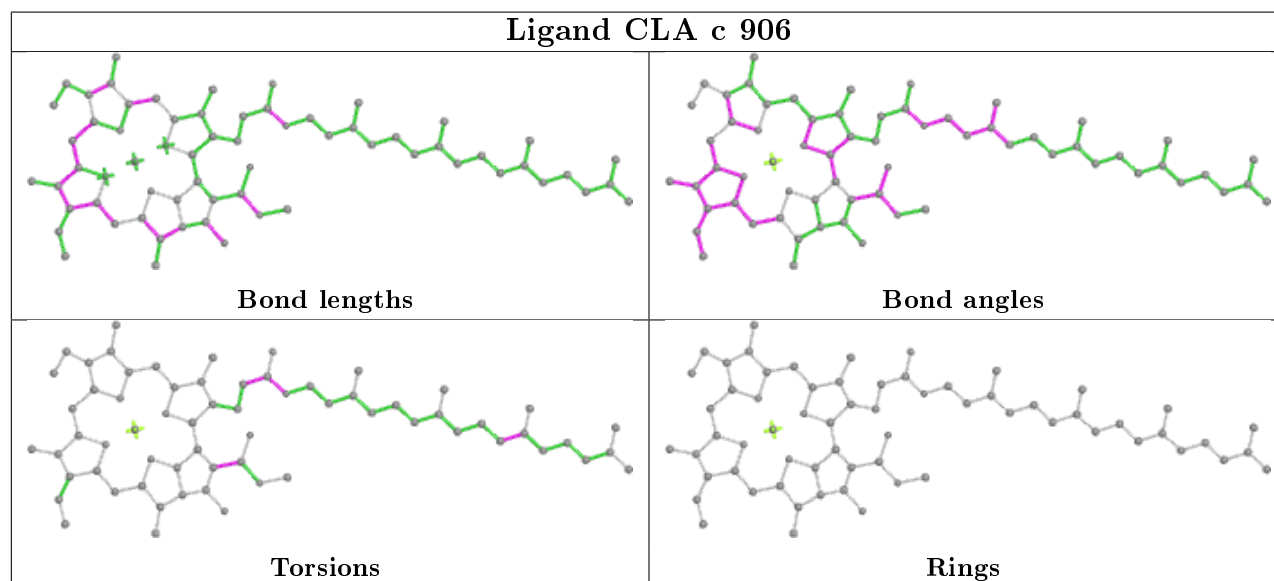
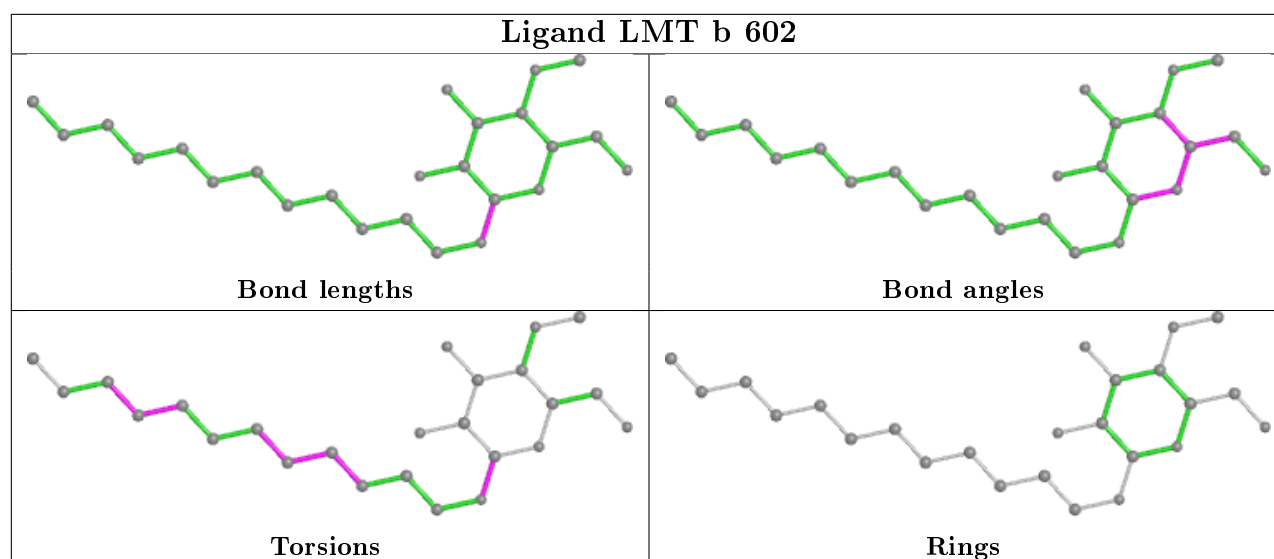


## Ligand DGD C 517

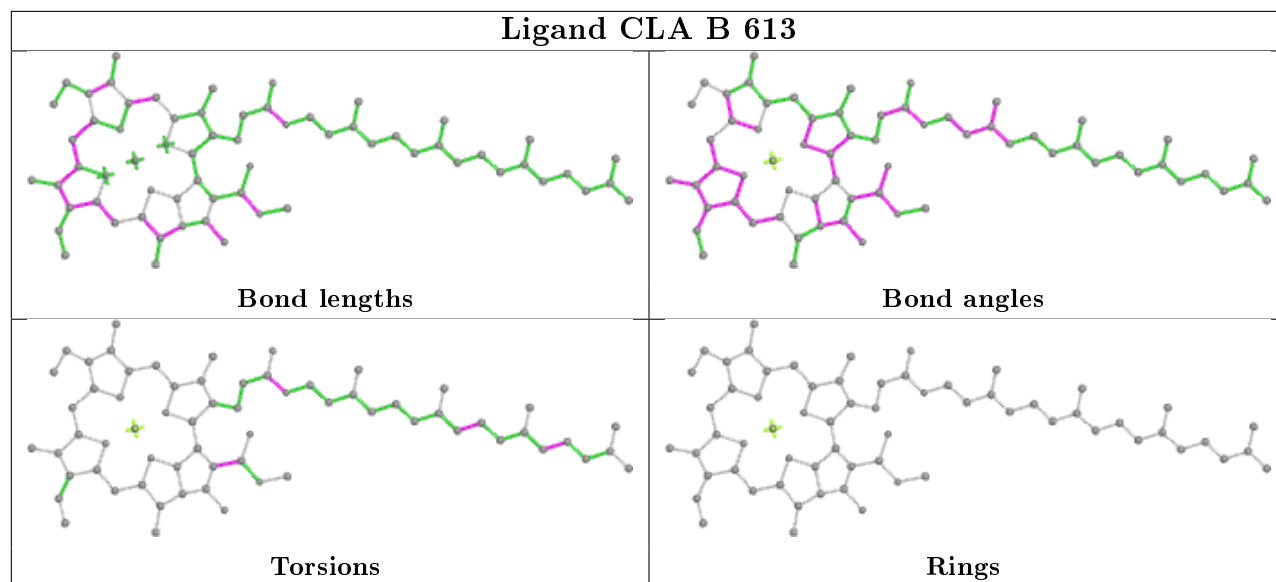
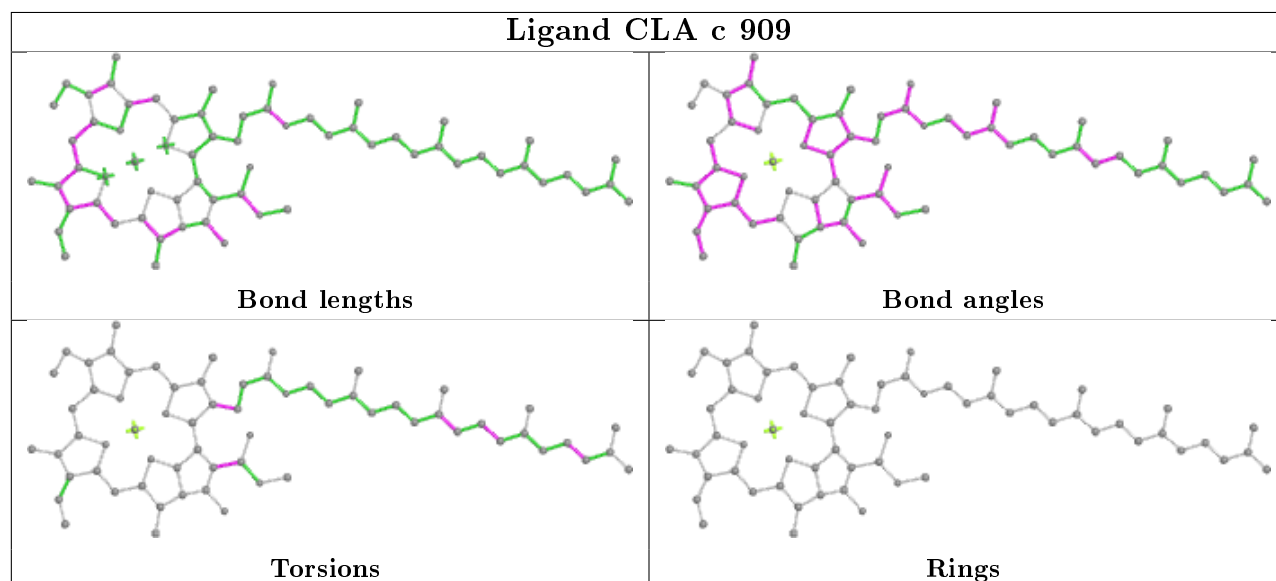
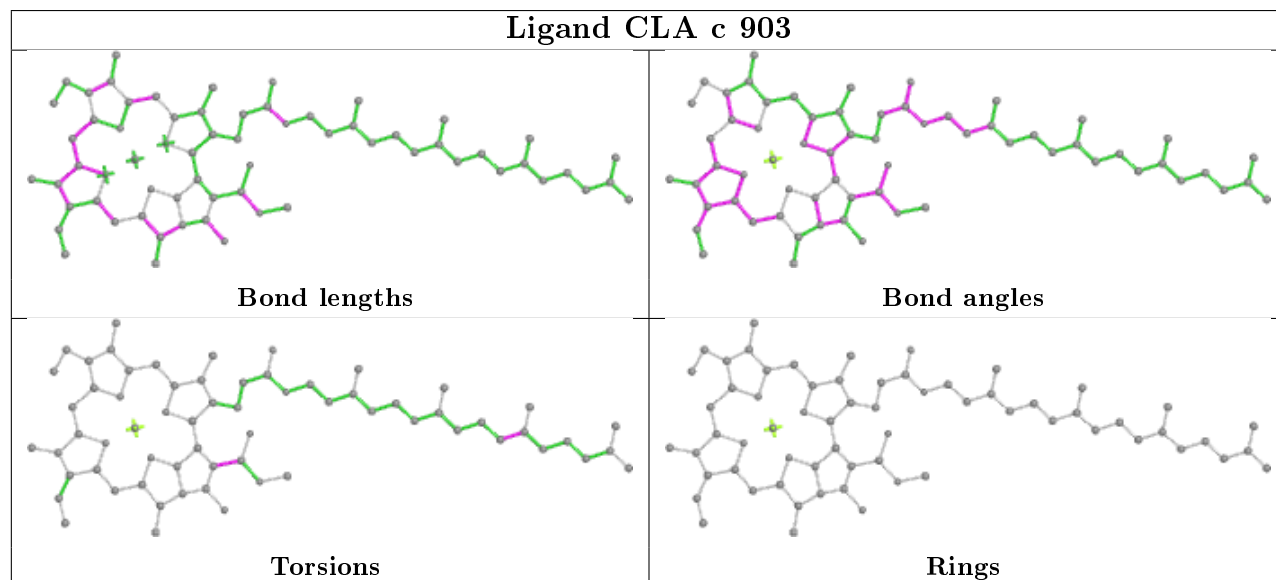


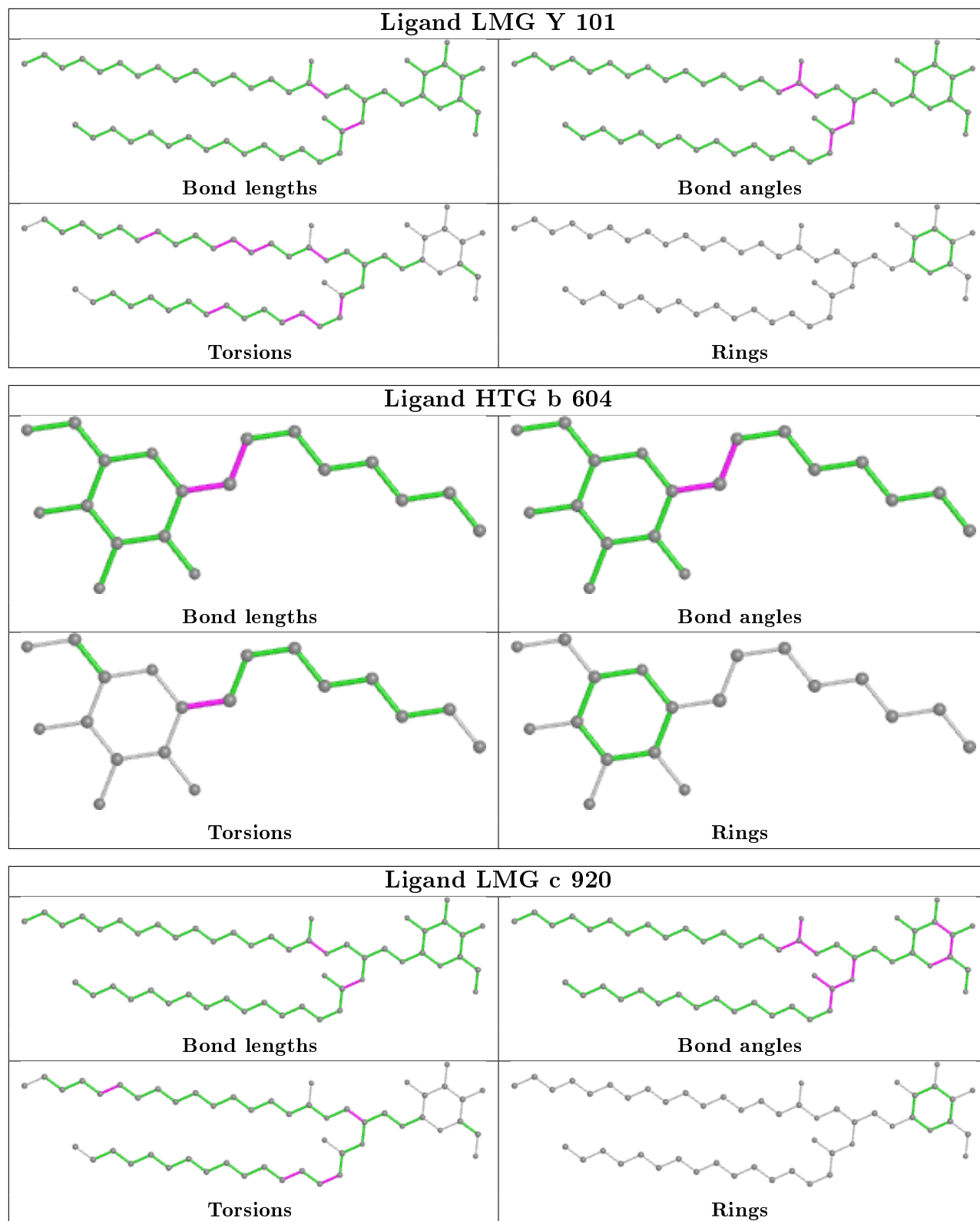
## Ligand DGD e 101

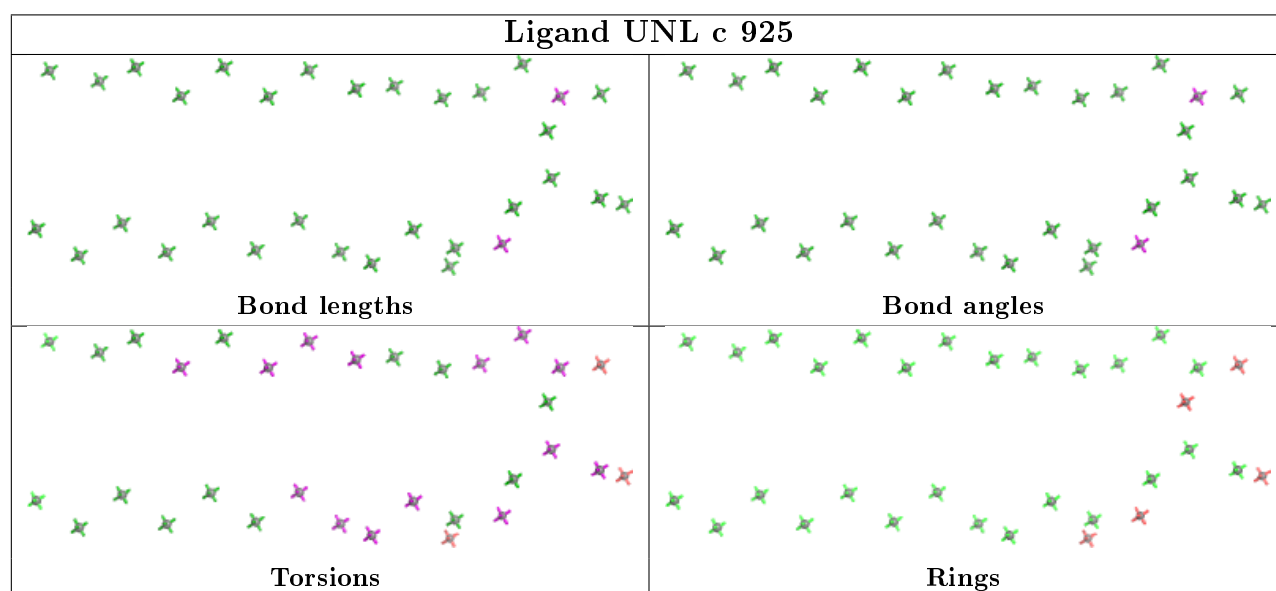
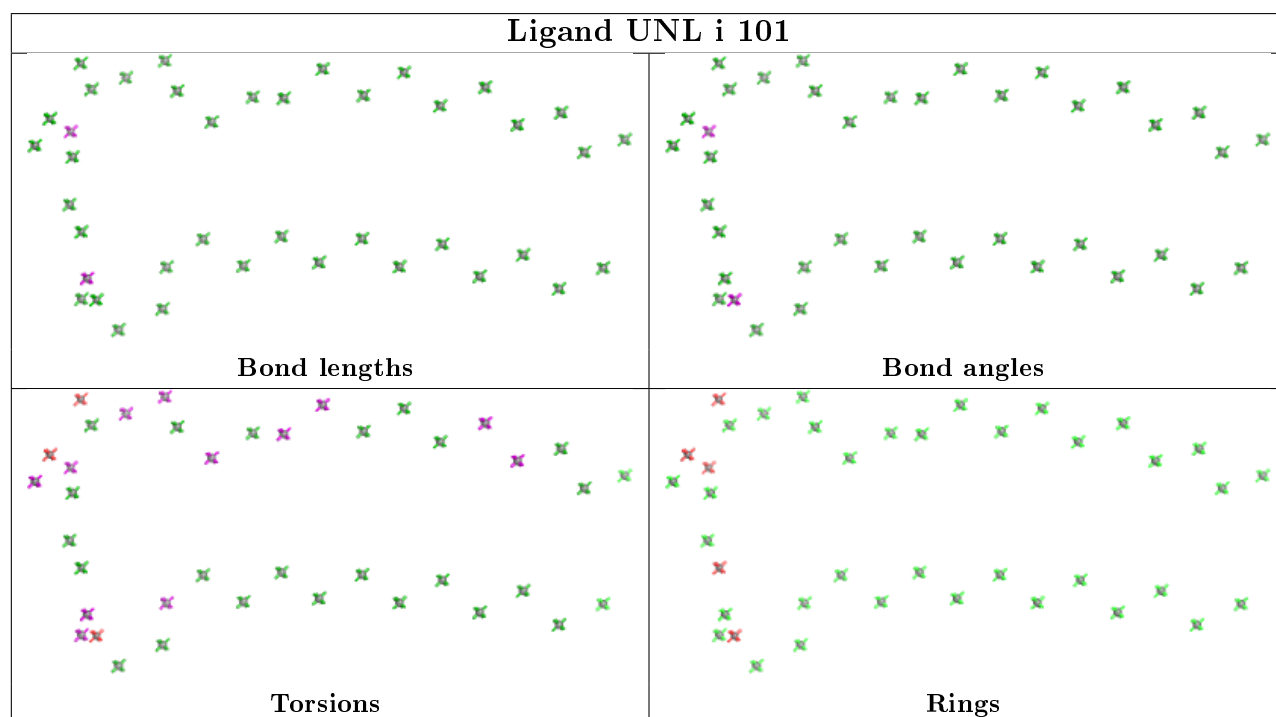
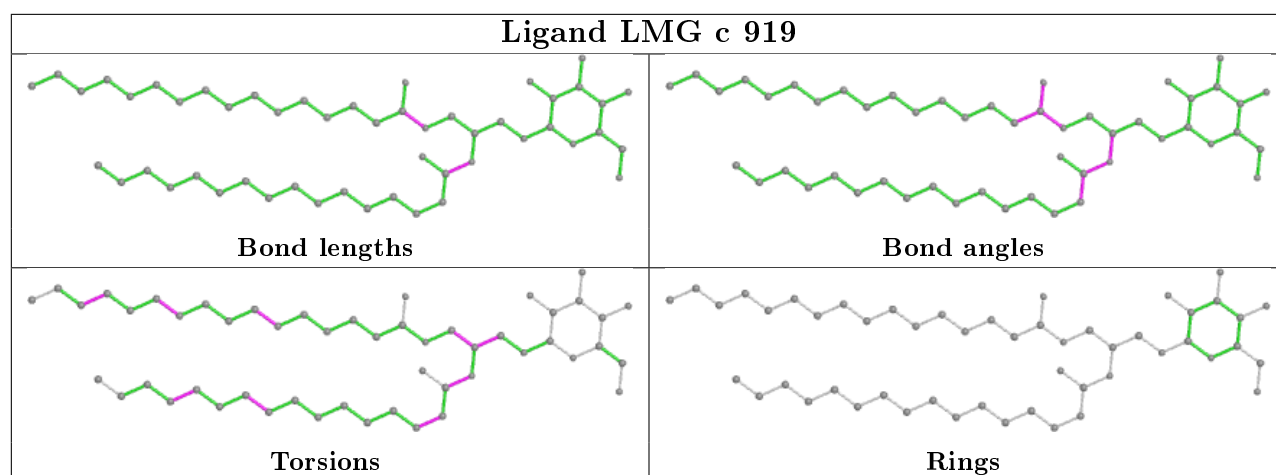


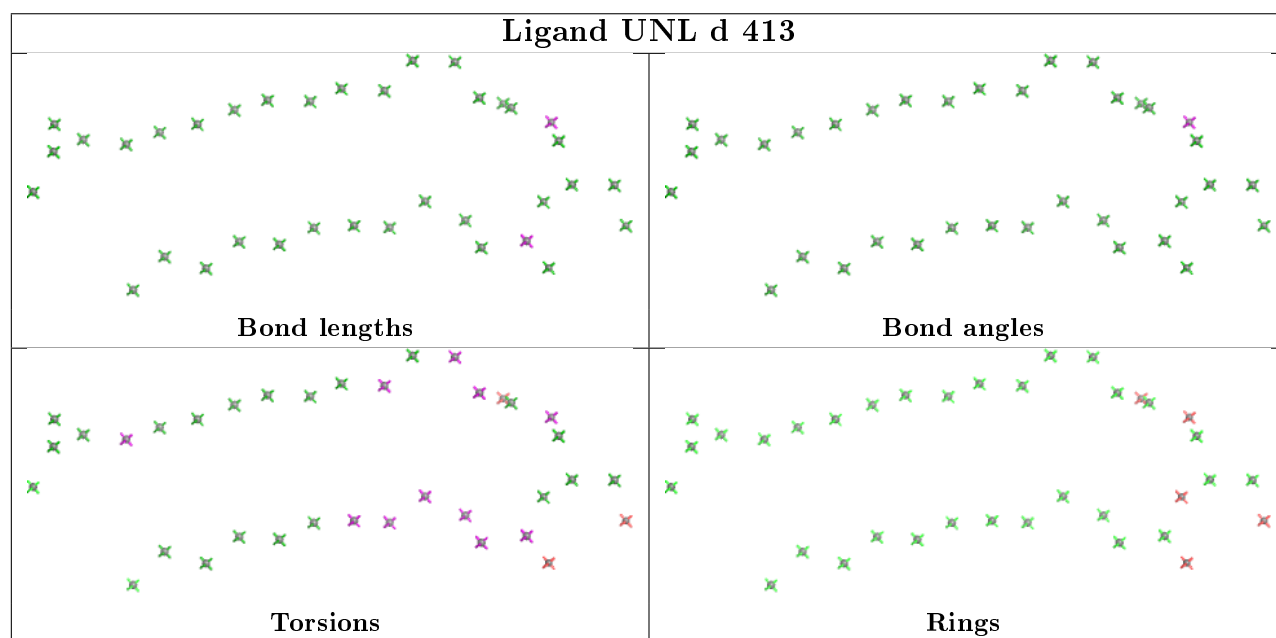
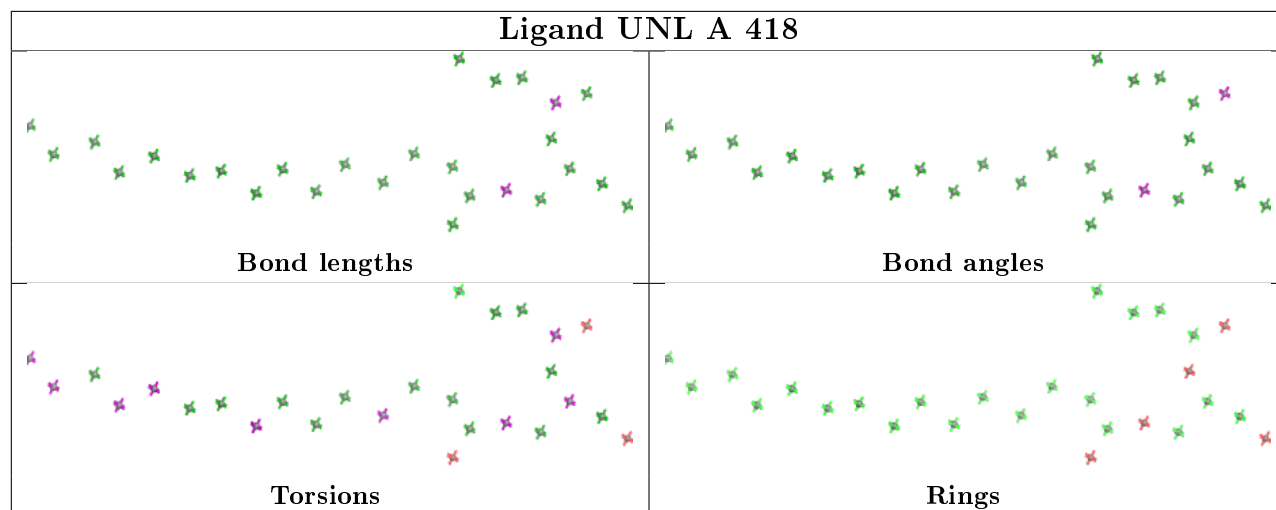


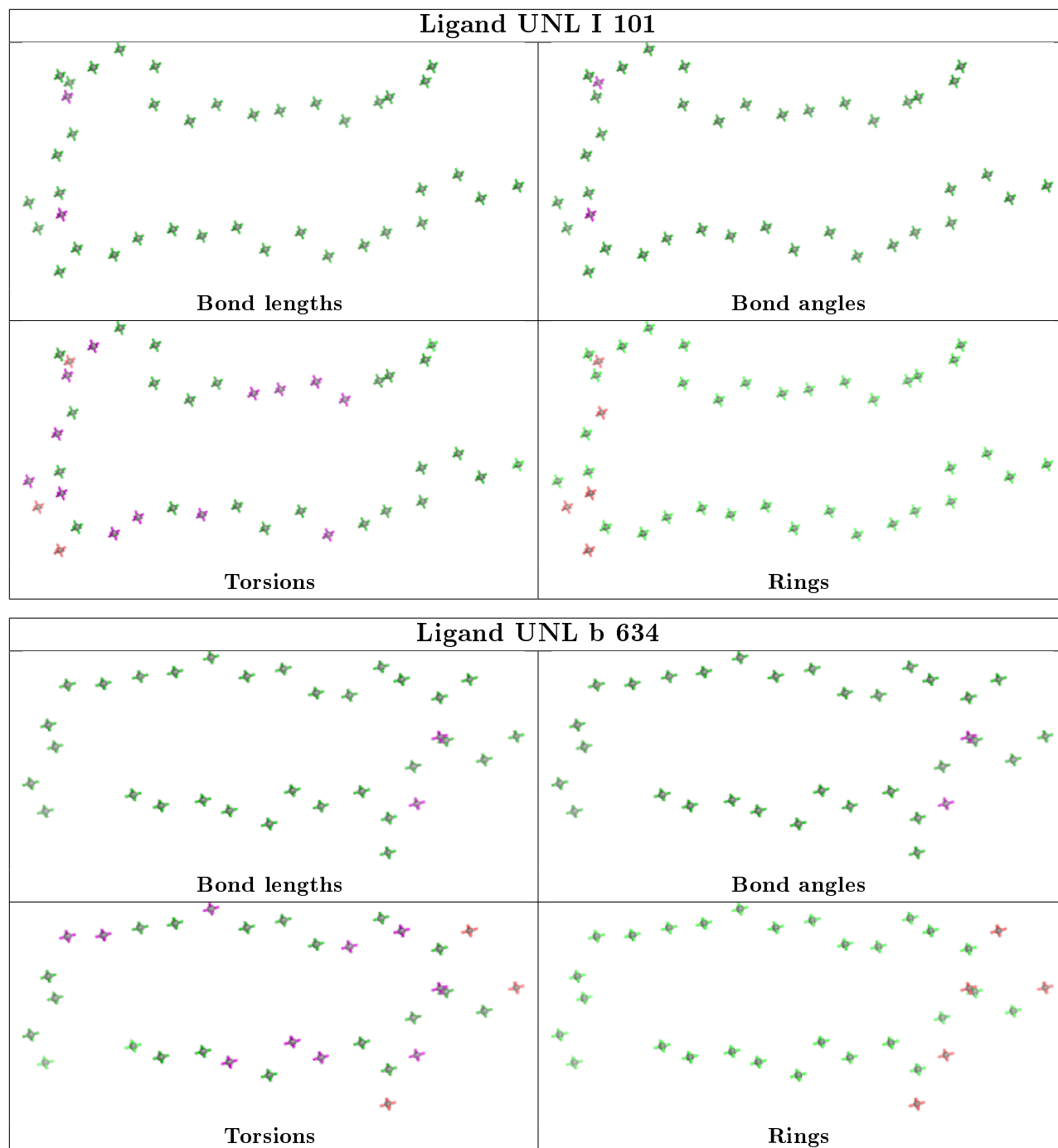


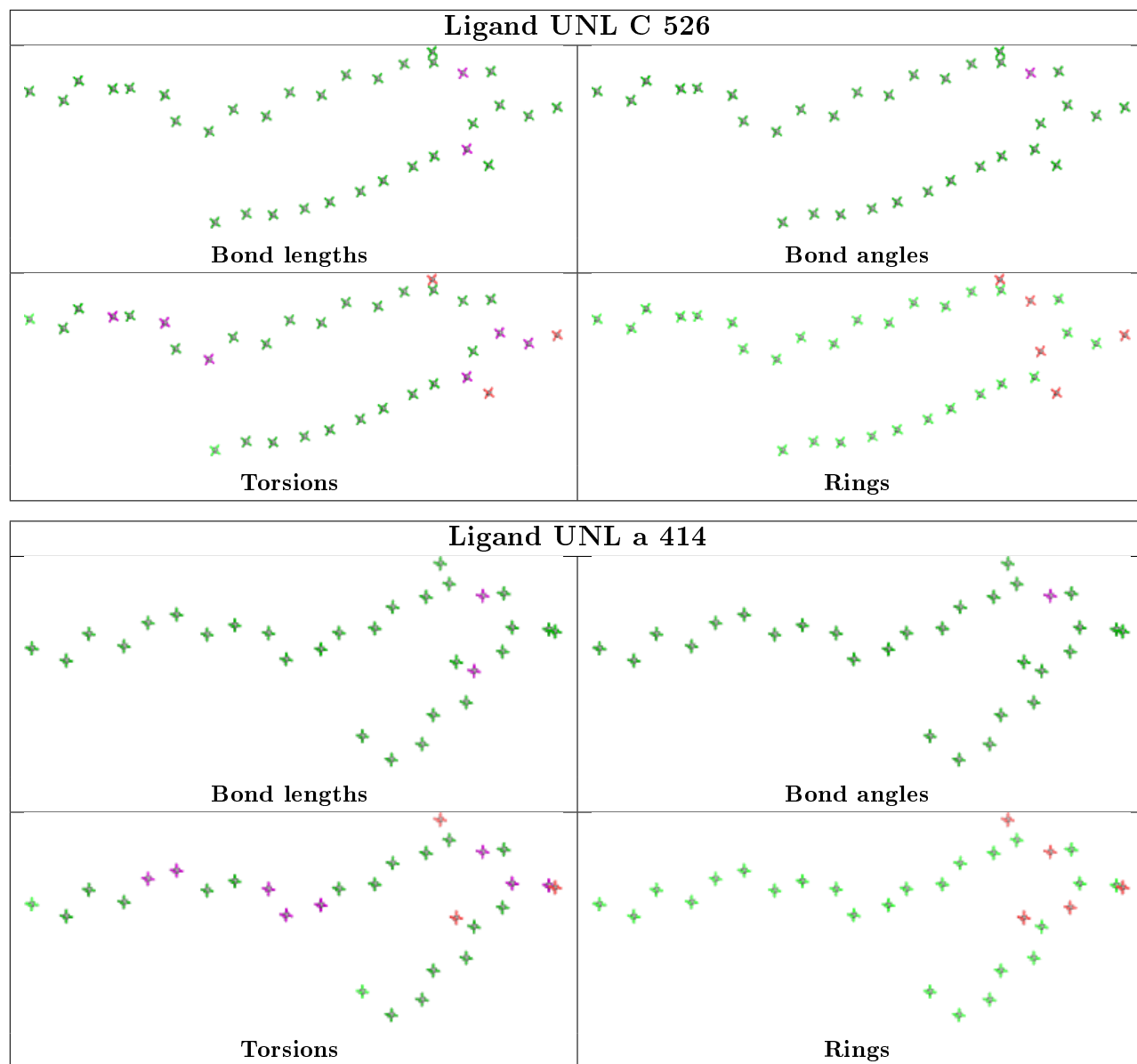
**Ligand CLA B 613****Ligand CLA c 909****Ligand CLA c 903**

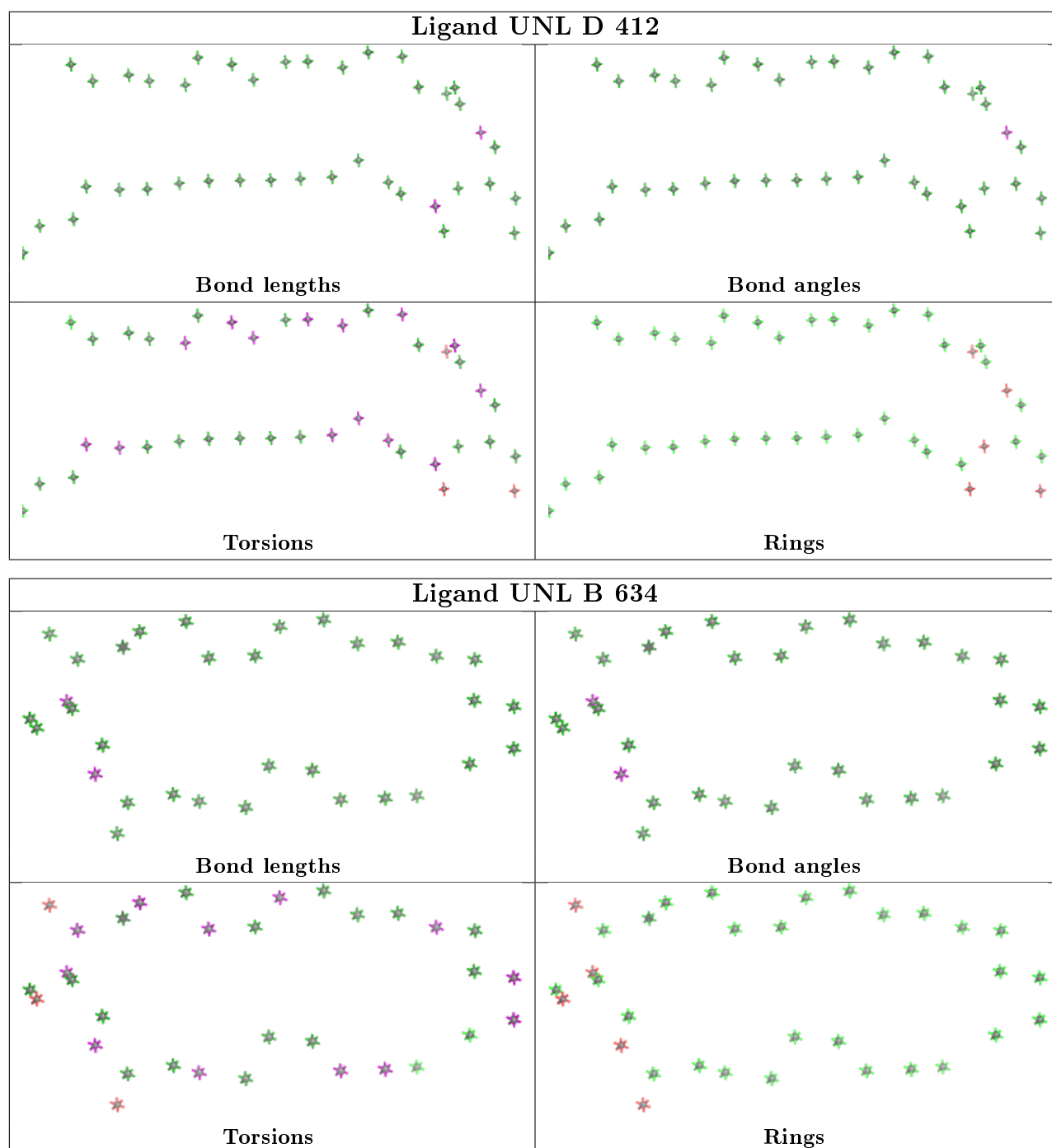












## 5.7 Other polymers [i](#)

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%)	0.28	5 (1%) 73 81	33, 43, 75, 139	0
1	a	334/344 (97%)	0.48	15 (4%) 33 46	31, 44, 84, 146	0
2	B	504/505 (99%)	0.38	14 (2%) 53 64	34, 48, 86, 137	0
2	b	503/505 (99%)	0.50	28 (5%) 24 35	34, 48, 93, 193	0
3	C	451/455 (99%)	0.42	18 (3%) 38 51	37, 56, 82, 134	0
3	c	455/455 (100%)	0.27	8 (1%) 68 77	39, 58, 83, 118	0
4	D	341/342 (99%)	0.29	3 (0%) 84 90	32, 45, 70, 129	0
4	d	341/342 (99%)	0.35	1 (0%) 94 97	34, 45, 69, 115	0
5	E	81/84 (96%)	1.37	25 (30%) 0 0	50, 73, 116, 150	0
5	e	81/84 (96%)	0.84	15 (18%) 1 2	51, 71, 125, 201	0
6	F	34/44 (77%)	0.48	4 (11%) 4 7	51, 62, 103, 104	0
6	f	32/44 (72%)	0.31	2 (6%) 20 29	50, 62, 118, 148	0
7	H	65/65 (100%)	0.30	3 (4%) 32 45	47, 57, 83, 145	0
7	h	65/65 (100%)	0.36	3 (4%) 32 45	47, 60, 83, 167	0
8	I	37/38 (97%)	0.57	4 (10%) 5 9	45, 58, 123, 187	0
8	i	37/38 (97%)	0.64	4 (10%) 5 9	44, 57, 116, 159	0
9	J	38/39 (97%)	0.99	6 (15%) 2 3	52, 68, 151, 185	0
9	j	39/39 (100%)	0.75	7 (17%) 1 2	52, 68, 140, 190	0
10	K	37/37 (100%)	0.71	4 (10%) 5 9	60, 68, 88, 112	0
10	k	37/37 (100%)	0.42	0 100 100	59, 67, 88, 112	0
11	L	37/37 (100%)	0.40	0 100 100	34, 39, 101, 132	0
11	l	37/37 (100%)	0.51	1 (2%) 54 64	34, 40, 105, 130	0
12	M	33/36 (91%)	0.64	0 100 100	29, 41, 75, 126	0
12	m	33/36 (91%)	0.55	0 100 100	35, 42, 78, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.42	12 (4%) 29 42	36, 54, 102, 146	0
13	o	243/244 (99%)	0.31	6 (2%) 57 67	36, 56, 112, 179	0
14	T	29/32 (90%)	0.57	1 (3%) 45 57	35, 40, 70, 142	0
14	t	29/32 (90%)	0.45	0 100 100	35, 39, 68, 141	0
15	U	97/104 (93%)	0.20	1 (1%) 82 88	39, 51, 82, 128	0
15	u	97/104 (93%)	0.17	0 100 100	42, 52, 76, 126	0
16	V	137/137 (100%)	0.36	1 (0%) 87 92	41, 54, 88, 123	0
16	v	137/137 (100%)	0.21	1 (0%) 87 92	43, 58, 89, 121	0
17	Y	29/30 (96%)	3.31	12 (41%) 0 0	73, 85, 162, 203	0
17	y	29/30 (96%)	1.50	9 (31%) 0 0	75, 85, 164, 202	0
18	X	39/40 (97%)	0.57	3 (7%) 13 20	52, 67, 135, 143	0
18	x	38/40 (95%)	0.94	6 (15%) 2 3	55, 67, 130, 140	0
19	Z	62/62 (100%)	1.44	18 (29%) 0 0	75, 89, 144, 191	0
19	z	62/62 (100%)	1.64	19 (30%) 0 0	75, 90, 144, 188	0
20	R	18/34 (52%)	5.55	18 (100%) 0 0	102, 135, 170, 172	0
All	All	5275/5384 (97%)	0.48	277 (5%) 26 38	29, 52, 103, 203	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	14.8
17	Y	20	ALA	13.7
2	b	494	GLY	12.3
17	Y	19	ILE	11.9
20	R	6	LEU	10.3
20	R	18	TRP	9.4
20	R	8	VAL	9.0
2	b	496	TYR	8.4
2	b	495	PHE	8.2
19	Z	61	VAL	8.1
19	z	3	ILE	8.0
18	x	2	THR	8.0
1	a	264	SER	7.9
17	Y	21	GLN	7.6
17	Y	23	THR	7.5
17	Y	22	LEU	7.5
20	R	15	ALA	7.4

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Mol	Chain	Res	Type	RSRZ
2	b	493	TRP	7.4
20	R	16	ALA	7.2
8	i	37	LEU	6.9
2	b	504	THR	6.6
5	e	5	THR	6.3
18	x	37	VAL	6.3
17	y	20	ALA	6.1
19	Z	31	GLN	6.1
9	j	1	MET	6.1
20	R	17	GLY	6.0
17	Y	26	ALA	5.9
13	O	62	GLU	5.9
19	Z	62	VAL	5.9
20	R	11	PRO	5.8
20	R	13	LEU	5.8
2	b	488	PRO	5.7
1	a	263	ALA	5.7
20	R	5	VAL	5.7
13	O	56	PRO	5.6
2	b	503	THR	5.6
19	z	5	PHE	5.5
18	x	38	GLN	5.4
3	c	140	LEU	5.3
20	R	9	LEU	5.3
5	E	84	LYS	5.2
8	I	36	ASP	5.1
1	a	11	ALA	5.1
2	b	497	GLN	5.1
2	B	496	TYR	5.0
5	E	79	PHE	5.0
2	b	489	GLU	4.9
5	E	19	TYR	4.9
2	b	487	SER	4.9
20	R	3	TRP	4.7
19	z	32	ASP	4.7
5	E	5	THR	4.7
19	Z	33	TRP	4.6
19	z	33	TRP	4.5
5	E	17	VAL	4.5
17	Y	25	ILE	4.5
9	j	2	SER	4.5
2	B	495	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
8	I	34	ARG	4.4
2	b	486	LEU	4.3
5	E	83	LEU	4.2
19	z	29	SER	4.2
20	R	2	ASP	4.2
2	B	481	GLY	4.2
17	y	41	VAL	4.2
3	C	131	TYR	4.1
1	a	256	GLY	4.1
18	x	39	ARG	4.0
19	z	62	VAL	4.0
5	E	82	GLN	3.9
3	c	143	TYR	3.9
10	K	16	ALA	3.9
19	Z	36	SER	3.9
19	z	35	ARG	3.9
2	b	86[A]	ILE	3.9
19	Z	30	PRO	3.9
3	C	25	ASN	3.8
19	Z	25	VAL	3.8
13	o	59	LYS	3.8
20	R	10	LEU	3.8
20	R	4	ARG	3.8
2	b	502	VAL	3.8
1	a	261	GLN	3.7
18	X	2	THR	3.7
19	z	41	PHE	3.7
2	b	499	VAL	3.7
9	j	4	GLY	3.7
17	y	44	GLY	3.6
5	E	4	THR	3.6
1	a	262	TYR	3.6
20	R	7	VAL	3.6
2	b	491	VAL	3.5
19	z	30	PRO	3.5
6	F	16	PHE	3.5
9	j	7	ILE	3.5
3	C	28	GLN	3.5
1	a	15	GLU	3.5
19	z	42	LEU	3.4
14	T	30	THR	3.4
19	z	43	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	b	485	GLU	3.3
19	Z	26	ALA	3.3
2	b	500	GLY	3.3
5	e	4	THR	3.3
5	E	11	SER	3.3
19	Z	29	SER	3.3
10	K	14	ALA	3.2
1	a	248	ILE	3.2
7	h	65	LEU	3.2
8	i	36	ASP	3.2
9	j	6	ARG	3.2
19	z	61	VAL	3.2
9	J	2	SER	3.2
3	C	207	ARG	3.2
3	c	24	THR	3.1
3	C	252	ILE	3.1
9	j	5	GLY	3.1
20	R	14	LEU	3.1
19	Z	39	LEU	3.1
13	o	58	ASN	3.1
3	C	253	LEU	3.0
3	C	222	GLY	3.0
5	E	78	THR	3.0
3	C	155	ASN	3.0
3	C	27	ASP	3.0
1	a	229	GLU	2.9
19	Z	32	ASP	2.9
1	a	19	ASN	2.9
19	z	7	LEU	2.9
2	b	490	GLN	2.9
3	C	145[A]	SER	2.9
5	e	7	GLU	2.9
16	V	71	GLY	2.8
5	e	21	VAL	2.8
5	E	15	THR	2.8
17	Y	30	ILE	2.8
2	B	479	PHE	2.8
17	Y	24	MET	2.8
7	h	66	GLY	2.8
13	O	25	THR	2.8
19	z	31	GLN	2.8
7	h	64	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
17	y	22	LEU	2.8
10	K	15	TYR	2.8
13	O	246	ALA	2.8
15	U	73	GLN	2.8
5	E	57	ALA	2.7
19	z	36	SER	2.7
5	e	20	TRP	2.7
20	R	12	VAL	2.7
8	I	37	LEU	2.7
4	D	24	ARG	2.7
3	C	139	THR	2.7
19	Z	1	MET	2.7
3	c	458	GLY	2.7
18	x	3	ILE	2.7
2	b	501	ASP	2.7
2	b	298	LEU	2.7
3	C	47	GLY	2.7
19	z	28	ALA	2.6
3	C	158	THR	2.6
1	a	265	PHE	2.6
19	Z	8	ALA	2.6
6	F	15	ILE	2.6
5	E	74	GLN	2.6
3	C	45	LEU	2.6
17	Y	37	PHE	2.6
19	z	39	LEU	2.6
9	J	3	GLU	2.6
2	B	295	GLY	2.6
2	b	85	GLY	2.6
5	e	6	GLY	2.6
17	y	40	ALA	2.6
3	c	144	SER	2.5
13	O	60	ARG	2.5
13	O	36	GLN	2.5
4	D	238	THR	2.5
9	J	7	ILE	2.5
1	a	252	HIS	2.5
2	B	293	ALA	2.5
5	E	20	TRP	2.5
1	A	230	THR	2.5
17	Y	39	LEU	2.5
19	z	60	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	134	ILE	2.5
9	J	6	ARG	2.4
2	B	290	ALA	2.4
19	Z	27	TYR	2.4
3	c	21	ILE	2.4
2	B	483	ASP	2.4
13	O	58	ASN	2.4
5	e	81	GLU	2.4
19	Z	35	ARG	2.4
2	b	285[A]	ASN	2.4
9	J	34	GLY	2.4
6	f	20	TRP	2.4
3	c	50	LEU	2.4
3	C	254	THR	2.4
5	E	61	ARG	2.4
2	B	504	THR	2.4
5	E	10	PHE	2.4
7	H	2	ALA	2.3
7	H	65	LEU	2.3
8	i	33	LYS	2.3
17	y	45	ASN	2.3
18	x	35	ASP	2.3
5	E	6	GLY	2.3
5	E	75	GLN	2.3
13	O	26	ALA	2.3
13	o	246	ALA	2.3
5	E	62[A]	SER	2.3
13	o	61	GLN	2.3
13	o	35	SER	2.3
2	B	494	GLY	2.3
5	e	74	GLN	2.3
9	J	5	GLY	2.3
5	E	21	VAL	2.3
8	I	38	GLU	2.3
2	B	296	ALA	2.3
5	e	71	GLU	2.3
3	C	90	PRO	2.3
20	R	19	ALA	2.3
9	j	3	GLU	2.2
1	a	255	PHE	2.2
5	e	10	PHE	2.2
4	d	234	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	72	ALA	2.2
13	O	93	LEU	2.2
8	i	34	ARG	2.2
16	v	17	LYS	2.2
1	A	13	LEU	2.2
10	K	10	LYS	2.2
5	E	16	SER	2.2
19	Z	60	PHE	2.2
5	E	22	ILE	2.2
18	X	4	THR	2.2
6	F	14	PRO	2.2
18	X	37	VAL	2.2
1	A	229	GLU	2.2
19	Z	38	GLN	2.2
5	e	14	ILE	2.2
13	o	56	PRO	2.2
13	O	99[A]	ASP	2.2
11	l	7	ARG	2.1
1	A	243	GLU	2.1
2	b	127	ARG	2.1
2	b	492	GLU	2.1
3	c	200	THR	2.1
2	B	239[A]	SER	2.1
2	b	173	GLY	2.1
5	e	72	ALA	2.1
17	y	26	ALA	2.1
17	y	25	ILE	2.1
1	a	225	ARG	2.1
5	e	61	ARG	2.1
7	H	64	ALA	2.1
17	y	18	VAL	2.1
2	b	479	PHE	2.1
3	C	143	TYR	2.1
2	b	498	LYS	2.1
1	A	307	ILE	2.0
4	D	233	ARG	2.0
2	b	297	THR	2.0
5	e	77	GLU	2.0
19	Z	56	VAL	2.0
5	E	18	ARG	2.0
2	B	284	ILE	2.0
1	a	216	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	129	GLY	2.0
5	e	11	SER	2.0
19	z	6	GLN	2.0
6	f	19	ARG	2.0
13	O	27	ARG	2.0
13	O	57	LYS	2.0
5	E	23	HIS	2.0
6	F	34	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.94	0.14	30,49,67,82	0
14	FME	t	1	10/11	0.94	0.14	26,36,47,88	0
12	FME	M	1	10/11	0.95	0.18	30,50,87,93	0
8	FME	i	1	10/11	0.95	0.15	43,60,73,75	0
12	FME	m	1	10/11	0.95	0.16	31,50,100,103	0
8	FME	I	1	10/11	0.96	0.12	28,49,62,64	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
29	LMT	F	101	35/35	0.33	0.53	102,149,179,184	0
37	DGD	e	101	62/66	0.41	0.43	72,118,208,212	0
35	HTG	d	414	16/19	0.47	0.25	68,115,134,134	0
32	UNL	j	101	10/-	0.50	0.28	56,83,95,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	LMT	a	417	35/35	0.53	0.38	95,123,147,148	0
37	DGD	D	408	52/66	0.54	0.36	58,108,151,171	0
28	GOL	V	204	6/6	0.55	0.60	75,90,97,100	0
36	LHG	a	418	42/49	0.55	0.32	69,131,187,193	0
32	UNL	C	526	34/-	0.58	0.24	76,120,132,136	0
22	CL	v	201	1/1	0.58	0.10	124,124,124,124	0
29	LMT	a	401	35/35	0.59	0.32	52,87,118,142	0
29	LMT	b	626	25/35	0.59	0.39	71,102,168,175	0
32	UNL	J	102	10/-	0.60	0.24	50,85,104,107	0
29	LMT	e	102	35/35	0.60	0.31	83,129,164,170	0
29	LMT	m	103	35/35	0.60	0.31	42,109,140,144	0
33	LMG	Z	101	37/55	0.62	0.31	55,121,146,154	0
29	LMT	C	520	35/35	0.62	0.36	88,135,162,175	0
29	LMT	A	415	35/35	0.65	0.25	41,84,115,119	0
27	SQD	f	102	43/54	0.67	0.29	97,116,175,182	0
33	LMG	Y	101	51/55	0.67	0.25	60,93,118,127	0
29	LMT	M	103	35/35	0.68	0.28	47,99,150,158	0
32	UNL	a	414	30/-	0.68	0.26	64,85,117,134	0
35	HTG	B	633	19/19	0.68	0.24	53,103,141,160	0
35	HTG	c	922	19/19	0.69	0.29	73,114,134,192	0
32	UNL	c	925	32/-	0.69	0.25	66,101,138,147	0
36	LHG	E	101	42/49	0.70	0.26	59,115,138,140	0
32	UNL	A	418	28/-	0.70	0.26	59,88,108,111	0
29	LMT	b	602	25/35	0.71	0.28	41,91,134,149	0
35	HTG	b	604	19/19	0.71	0.19	51,112,150,150	0
32	UNL	b	634	33/-	0.72	0.26	47,86,155,158	0
29	LMT	D	403	35/35	0.72	0.27	58,132,172,179	0
35	HTG	D	413	16/19	0.72	0.27	76,142,160,166	0
33	LMG	z	101	39/55	0.73	0.28	65,124,153,161	0
35	HTG	B	625	19/19	0.73	0.23	75,132,140,190	0
28	GOL	O	302	6/6	0.73	0.17	68,79,84,89	0
29	LMT	M	101	35/35	0.74	0.23	45,93,118,133	0
37	DGD	C	517	62/66	0.74	0.23	48,65,94,116	0
35	HTG	C	522	19/19	0.75	0.31	81,112,138,140	0
32	UNL	B	634	33/-	0.75	0.29	54,73,126,134	0
27	SQD	L	102	54/54	0.76	0.23	48,79,126,149	0
29	LMT	m	102	35/35	0.76	0.26	42,90,122,128	0
29	LMT	t	101	25/35	0.76	0.31	43,92,140,150	0
35	HTG	b	628	19/19	0.77	0.22	72,130,158,159	0
33	LMG	C	519	51/55	0.77	0.25	53,121,145,151	0
31	PL9	A	417	55/55	0.77	0.25	61,98,125,131	0
33	LMG	b	625	51/55	0.78	0.23	40,54,73,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	UNL	M	102	10/-	0.78	0.31	50,55,74,86	0
33	LMG	c	920	51/55	0.78	0.24	50,111,142,145	0
28	GOL	l	101	6/6	0.79	0.39	48,92,98,103	0
35	HTG	c	921	19/19	0.79	0.18	93,101,107,111	0
34	CA	f	103	1/1	0.79	0.09	126,126,126,126	0
27	SQD	a	402	54/54	0.79	0.22	45,75,125,133	0
27	SQD	F	103	43/54	0.80	0.25	77,120,145,149	0
27	SQD	B	621	54/54	0.80	0.25	53,88,137,156	0
22	CL	U	201	1/1	0.80	0.08	117,117,117,117	0
24	CLA	C	513	65/65	0.80	0.28	53,84,113,119	0
33	LMG	B	622	51/55	0.80	0.22	38,53,78,91	0
32	UNL	d	413	36/-	0.81	0.25	60,85,140,142	0
28	GOL	T	101	6/6	0.81	0.33	60,77,82,83	0
31	PL9	a	415	55/55	0.81	0.24	65,110,127,130	0
28	GOL	b	633	6/6	0.81	0.20	68,74,80,88	0
34	CA	B	601	1/1	0.81	0.06	138,138,138,138	0
35	HTG	b	601	19/19	0.81	0.20	42,57,82,87	0
35	HTG	b	603	19/19	0.81	0.19	47,75,92,93	0
32	UNL	D	412	40/-	0.82	0.20	51,88,141,144	0
32	UNL	m	101	10/-	0.82	0.34	58,66,81,81	0
35	HTG	b	627	19/19	0.82	0.25	55,73,94,109	0
24	CLA	C	504	65/65	0.82	0.20	36,57,79,95	0
37	DGD	h	102	62/66	0.82	0.21	34,52,71,82	0
28	GOL	V	207	6/6	0.82	0.18	81,86,89,98	0
28	GOL	v	204	6/6	0.82	0.22	84,87,94,112	0
33	LMG	c	919	51/55	0.82	0.20	51,89,123,128	0
33	LMG	A	419	51/55	0.83	0.19	54,88,107,128	0
35	HTG	B	632	19/19	0.83	0.17	48,84,110,115	0
37	DGD	H	102	62/66	0.83	0.21	31,51,88,102	0
28	GOL	v	203	6/6	0.83	0.21	72,88,91,94	0
37	DGD	C	518	62/66	0.83	0.18	39,58,92,100	0
27	SQD	A	414	54/54	0.83	0.22	49,75,134,141	0
27	SQD	a	410	54/54	0.84	0.18	51,81,110,114	0
32	UNL	i	101	40/-	0.84	0.24	48,77,140,147	0
35	HTG	V	203	19/19	0.84	0.33	73,95,125,231	0
32	UNL	I	101	40/-	0.84	0.24	42,88,155,156	0
35	HTG	B	624	19/19	0.84	0.23	50,73,82,92	0
33	LMG	a	411	51/55	0.84	0.22	51,84,96,105	0
32	UNL	X	101	18/-	0.85	0.17	53,73,112,114	0
28	GOL	C	523	6/6	0.85	0.34	74,80,89,92	0
28	GOL	T	103	6/6	0.85	0.47	103,108,112,114	0
28	GOL	a	419	6/6	0.85	0.17	73,85,94,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	DGD	c	917	62/66	0.85	0.20	35,60,112,137	0
28	GOL	c	924	6/6	0.85	0.34	81,87,97,102	0
24	CLA	c	914	65/65	0.85	0.20	68,84,105,115	0
27	SQD	A	411	54/54	0.86	0.20	43,87,114,116	0
24	CLA	B	602	65/65	0.87	0.19	43,67,119,143	0
37	DGD	c	918	62/66	0.87	0.19	41,56,90,110	0
24	CLA	b	607	65/65	0.87	0.20	30,50,60,63	0
34	CA	F	104	1/1	0.87	0.06	107,107,107,107	0
24	CLA	b	612	65/65	0.87	0.20	27,38,48,58	0
24	CLA	B	607	65/65	0.87	0.19	31,52,95,99	0
24	CLA	c	907	65/65	0.87	0.17	44,65,104,111	0
33	LMG	d	415	51/55	0.88	0.20	38,61,112,126	0
24	CLA	c	908	65/65	0.88	0.17	45,63,74,84	0
24	CLA	b	614	65/65	0.88	0.18	39,51,61,72	0
24	CLA	c	904	65/65	0.88	0.17	41,60,73,84	0
33	LMG	J	101	51/55	0.88	0.20	44,65,120,137	0
28	GOL	V	201	6/6	0.89	0.23	88,99,104,109	0
24	CLA	C	511	65/65	0.89	0.16	48,67,85,109	0
28	GOL	b	632	6/6	0.89	0.24	77,78,102,105	0
24	CLA	B	614	65/65	0.89	0.19	29,41,64,93	0
24	CLA	c	906	65/65	0.89	0.17	36,51,70,76	0
36	LHG	B	635	49/49	0.89	0.26	30,52,68,77	0
24	CLA	b	606	65/65	0.89	0.20	39,67,123,145	0
28	GOL	a	413	6/6	0.89	0.20	73,83,95,97	0
32	UNL	x	101	18/-	0.89	0.22	51,71,116,116	0
24	CLA	C	512	65/65	0.90	0.15	49,76,99,106	0
24	CLA	c	905	65/65	0.90	0.16	31,57,74,85	0
28	GOL	c	928	6/6	0.90	0.14	75,83,90,98	0
24	CLA	c	910	65/65	0.90	0.16	43,58,77,81	0
24	CLA	d	404	65/65	0.90	0.18	29,39,48,56	0
36	LHG	D	410	49/49	0.90	0.23	47,67,121,138	0
24	CLA	c	912	65/65	0.90	0.16	43,63,83,99	0
28	GOL	B	630	6/6	0.90	0.21	51,59,70,81	0
26	BCR	C	514	40/40	0.90	0.17	50,72,86,87	0
35	HTG	B	623	19/19	0.90	0.18	38,56,78,93	0
24	CLA	C	501	65/65	0.90	0.15	39,57,85,91	0
24	CLA	c	909	65/65	0.90	0.15	38,54,125,137	0
37	DGD	c	916	62/66	0.90	0.18	38,56,100,114	0
24	CLA	C	506	65/65	0.90	0.15	41,70,114,128	0
24	CLA	B	610	65/65	0.90	0.18	36,52,65,82	0
35	HTG	C	521	19/19	0.90	0.19	70,99,121,123	0
36	LHG	b	635	49/49	0.91	0.22	30,48,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	b	619	65/65	0.91	0.18	25,43,86,108	0
24	CLA	B	616	65/65	0.91	0.17	37,50,65,77	0
24	CLA	A	405	65/65	0.91	0.17	24,37,51,66	0
24	CLA	c	911	65/65	0.91	0.15	43,55,69,81	0
36	LHG	d	411	49/49	0.91	0.20	37,53,112,120	0
24	CLA	b	620	65/65	0.91	0.17	36,50,64,69	0
24	CLA	C	503	65/65	0.91	0.18	36,59,72,85	0
28	GOL	B	636	6/6	0.91	0.18	49,56,64,65	0
24	CLA	b	611	65/65	0.91	0.17	37,51,97,108	0
28	GOL	D	402	6/6	0.91	0.31	52,57,83,90	0
24	CLA	B	605	65/65	0.91	0.17	28,41,72,78	0
28	GOL	A	412	6/6	0.91	0.18	49,55,57,69	0
37	DGD	C	516	62/66	0.92	0.18	32,50,88,97	0
36	LHG	d	410	49/49	0.92	0.23	29,44,63,98	0
24	CLA	C	508	65/65	0.92	0.15	35,61,138,148	0
24	CLA	b	616	65/65	0.92	0.17	29,41,54,66	0
24	CLA	C	510	65/65	0.92	0.15	40,60,77,92	0
36	LHG	d	409	49/49	0.92	0.23	40,52,66,70	0
28	GOL	A	413	6/6	0.92	0.17	61,79,84,86	0
24	CLA	B	615	65/65	0.92	0.19	26,43,97,103	0
24	CLA	C	509	65/65	0.92	0.15	53,65,82,93	0
24	CLA	B	603	65/65	0.92	0.16	38,50,57,66	0
24	CLA	D	405	65/65	0.92	0.15	39,55,106,121	0
24	CLA	b	621	65/65	0.92	0.17	33,53,103,118	0
24	CLA	D	404	65/65	0.92	0.16	24,37,58,69	0
24	CLA	B	612	65/65	0.92	0.20	24,40,56,63	0
26	BCR	c	927	40/40	0.92	0.15	54,77,91,100	0
24	CLA	b	613	65/65	0.92	0.17	36,49,59,62	0
24	CLA	c	913	65/65	0.92	0.16	47,74,93,99	0
26	BCR	b	623	40/40	0.92	0.19	29,46,66,68	0
26	BCR	k	101	40/40	0.92	0.14	51,64,75,80	0
34	CA	o	301	1/1	0.92	0.05	97,97,97,97	0
24	CLA	a	405	65/65	0.92	0.19	24,38,53,67	0
26	BCR	H	101	40/40	0.92	0.17	33,57,78,85	0
24	CLA	d	406	65/65	0.93	0.19	40,54,106,124	0
24	CLA	d	405	65/65	0.93	0.17	24,40,55,69	0
32	UNL	D	411	17/-	0.93	0.22	40,71,92,94	0
24	CLA	b	615	65/65	0.93	0.18	35,47,61,67	0
24	CLA	C	507	65/65	0.93	0.16	41,66,77,86	0
24	CLA	B	608	65/65	0.93	0.17	25,41,51,61	0
24	CLA	a	408	65/65	0.93	0.20	32,53,122,130	0
26	BCR	y	101	40/40	0.93	0.15	47,63,74,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	GOL	B	626	6/6	0.93	0.19	44,53,66,87	0
34	CA	b	605	1/1	0.93	0.06	124,124,124,124	0
28	GOL	B	628	6/6	0.93	0.22	62,80,83,84	0
26	BCR	h	101	40/40	0.93	0.18	36,60,79,81	0
24	CLA	B	613	65/65	0.93	0.16	26,42,50,53	0
26	BCR	d	407	40/40	0.93	0.19	39,54,85,88	0
26	BCR	D	406	40/40	0.93	0.15	39,58,89,104	0
24	CLA	b	608	65/65	0.93	0.17	38,48,58,66	0
24	CLA	b	617	65/65	0.93	0.17	25,42,53,65	0
24	CLA	B	604	65/65	0.93	0.18	35,48,60,63	0
24	CLA	b	618	65/65	0.94	0.20	24,44,60,67	0
28	GOL	V	206	6/6	0.94	0.31	52,60,67,71	0
24	CLA	A	406	65/65	0.94	0.16	23,36,45,55	0
32	UNL	d	412	17/-	0.94	0.25	47,62,95,102	0
24	CLA	B	617	65/65	0.94	0.20	34,54,130,139	0
36	LHG	D	409	49/49	0.94	0.22	31,46,67,79	0
31	PL9	d	408	55/55	0.94	0.21	22,39,53,73	0
26	BCR	Y	102	40/40	0.94	0.14	51,71,90,107	0
36	LHG	L	101	49/49	0.94	0.22	36,47,56,62	0
25	PHO	A	408	64/64	0.94	0.16	26,39,46,54	0
25	PHO	d	403	64/64	0.94	0.17	27,44,54,62	0
24	CLA	C	505	65/65	0.94	0.15	41,54,71,89	0
26	BCR	K	101	40/40	0.94	0.15	43,63,79,82	0
24	CLA	B	606	65/65	0.94	0.16	28,40,55,57	0
28	GOL	B	627	6/6	0.94	0.25	54,64,88,102	0
24	CLA	c	902	65/65	0.94	0.16	44,60,72,81	0
24	CLA	c	903	65/65	0.94	0.15	39,52,76,80	0
31	PL9	D	407	55/55	0.94	0.21	29,42,52,60	0
24	CLA	b	610	65/65	0.94	0.17	31,43,53,61	0
28	GOL	b	630	6/6	0.94	0.17	50,82,94,95	0
24	CLA	A	407	65/65	0.94	0.15	28,43,106,119	0
24	CLA	B	609	65/65	0.94	0.18	32,46,59,67	0
28	GOL	v	205	6/6	0.95	0.21	48,59,69,78	0
26	BCR	A	410	40/40	0.95	0.18	32,42,54,54	0
28	GOL	b	631	6/6	0.95	0.19	58,70,81,100	0
24	CLA	C	502	65/65	0.95	0.14	42,56,69,85	0
28	GOL	V	205	6/6	0.95	0.17	45,51,58,72	0
26	BCR	b	622	40/40	0.95	0.18	32,44,56,60	0
34	CA	c	901	1/1	0.95	0.08	74,74,74,74	0
28	GOL	b	629	6/6	0.95	0.21	57,62,67,81	0
26	BCR	c	915	40/40	0.95	0.18	32,56,67,75	0
24	CLA	a	406	65/65	0.95	0.19	31,44,118,125	0

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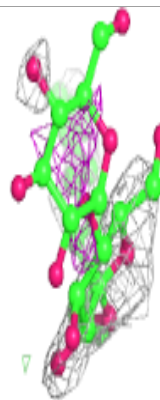
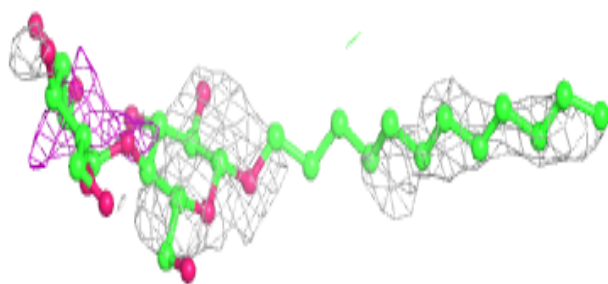
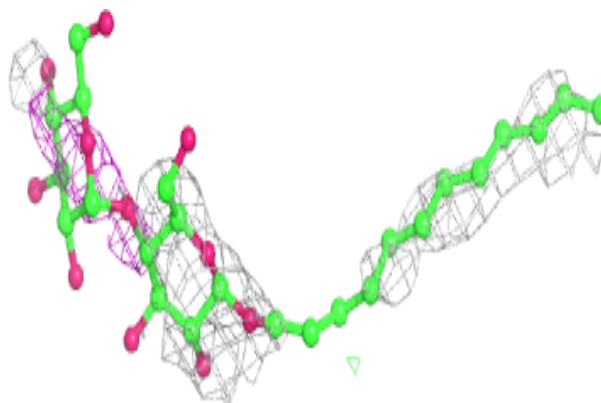
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	BCR	T	102	40/40	0.95	0.17	29,46,64,65	0
25	PHO	D	401	64/64	0.95	0.17	31,46,58,60	0
26	BCR	C	515	40/40	0.95	0.18	38,55,68,78	0
28	GOL	B	629	6/6	0.95	0.28	56,60,69,95	0
24	CLA	b	609	65/65	0.95	0.17	27,42,74,77	0
24	CLA	A	409	65/65	0.95	0.16	33,50,116,132	0
24	CLA	B	611	65/65	0.95	0.20	31,50,62,66	0
26	BCR	b	624	40/40	0.96	0.19	39,50,61,65	0
23	BCT	d	402	4/4	0.96	0.23	70,72,76,97	0
26	BCR	B	619	40/40	0.96	0.20	31,42,60,66	0
25	PHO	a	407	64/64	0.96	0.18	28,40,48,54	0
26	BCR	B	620	40/40	0.96	0.20	36,52,64,67	0
34	CA	O	301	1/1	0.96	0.06	89,89,89,89	0
38	HEM	f	101	43/43	0.96	0.16	51,85,128,152	0
26	BCR	B	618	40/40	0.96	0.21	29,40,51,54	0
22	CL	A	403	1/1	0.96	0.09	38,38,38,38	0
39	MG	j	102	1/1	0.96	0.13	61,61,61,61	0
38	HEM	V	202	43/43	0.96	0.14	31,45,54,59	0
26	BCR	a	409	40/40	0.96	0.19	28,43,54,59	0
23	BCT	A	404	4/4	0.96	0.21	59,62,74,108	0
28	GOL	a	412	6/6	0.96	0.24	54,61,67,72	0
26	BCR	t	102	40/40	0.96	0.19	33,46,62,64	0
38	HEM	v	202	43/43	0.97	0.14	46,58,65,70	0
34	CA	C	525	1/1	0.97	0.16	79,79,79,79	0
28	GOL	B	631	6/6	0.97	0.31	40,78,87,93	0
38	HEM	F	102	43/43	0.97	0.16	53,74,105,111	0
28	GOL	c	923	6/6	0.98	0.19	41,51,54,57	0
34	CA	c	926	1/1	0.98	0.11	77,77,77,77	0
39	MG	J	103	1/1	0.98	0.12	54,54,54,54	0
30	OEX	a	416	10/10	0.98	0.15	35,45,63,74	0
28	GOL	C	524	6/6	0.98	0.17	39,44,53,61	0
21	FE2	d	401	1/1	0.99	0.20	55,55,55,55	0
22	CL	a	403	1/1	0.99	0.17	37,37,37,37	0
21	FE2	A	401	1/1	0.99	0.16	56,56,56,56	0
30	OEX	A	416	10/10	0.99	0.14	39,45,61,77	0
22	CL	a	404	1/1	1.00	0.14	42,42,42,42	0
22	CL	A	402	1/1	1.00	0.16	35,35,35,35	0

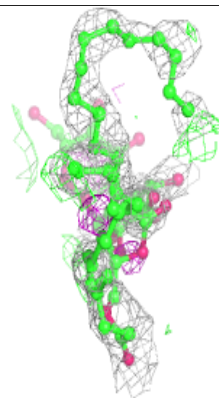
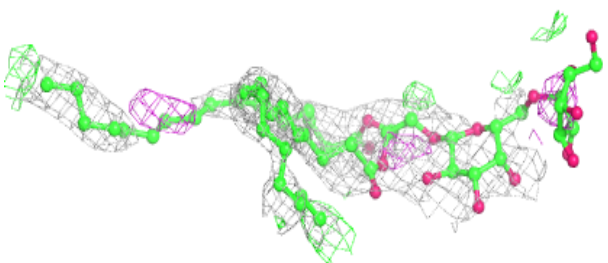
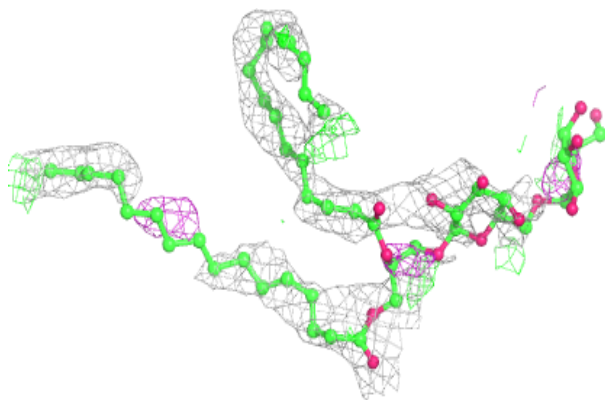
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around LMT F 101:**

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

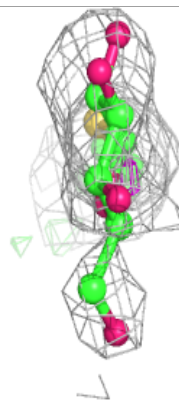
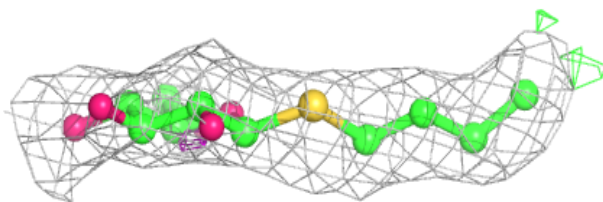
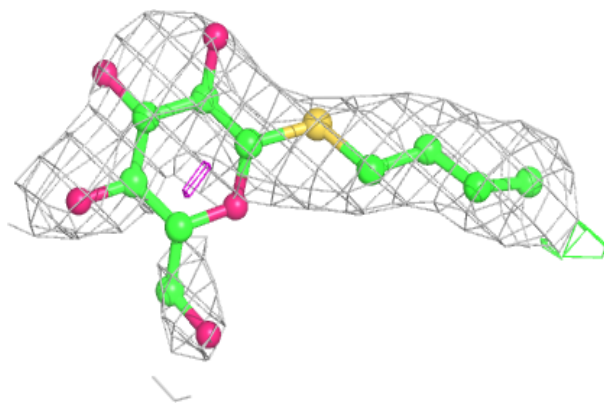
**Electron density around DGD e 101:**

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

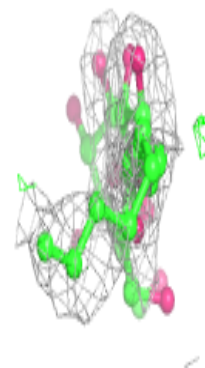
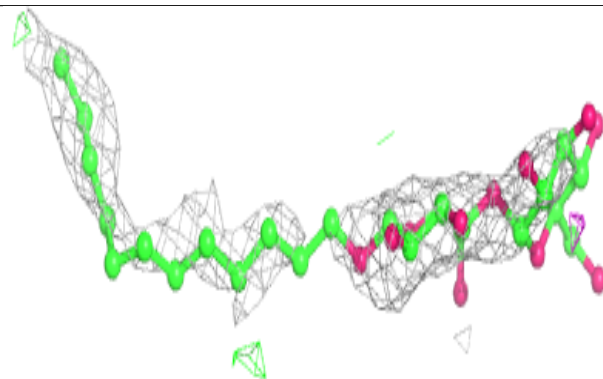
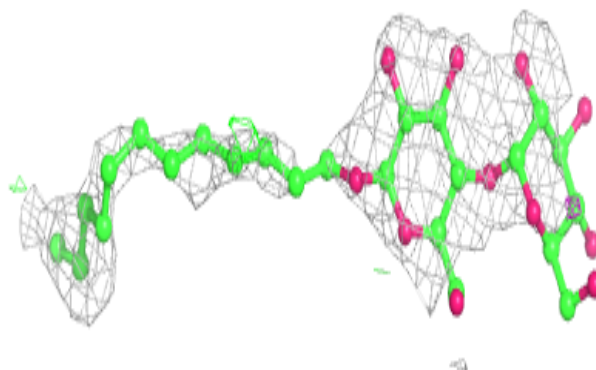


**Electron density around HTG d 414:**

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

**Electron density around LMT a 417:**

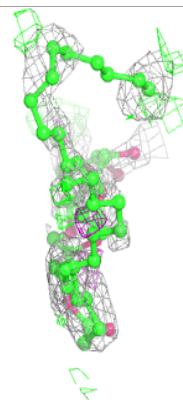
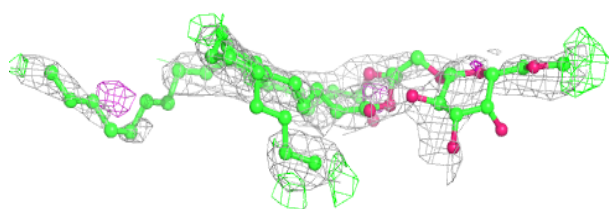
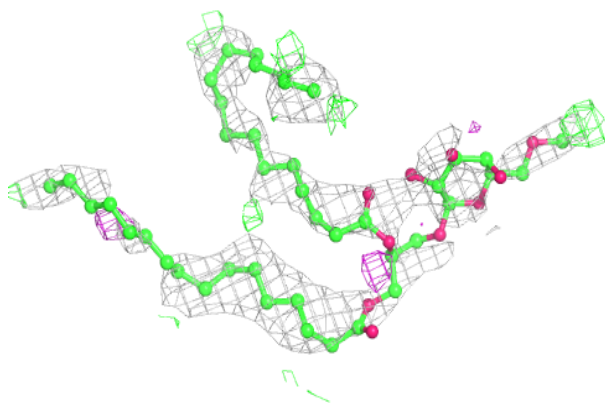
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



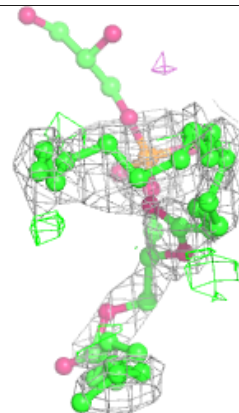
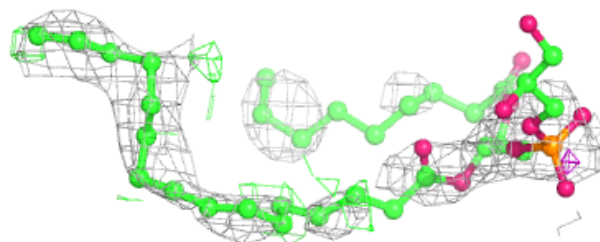
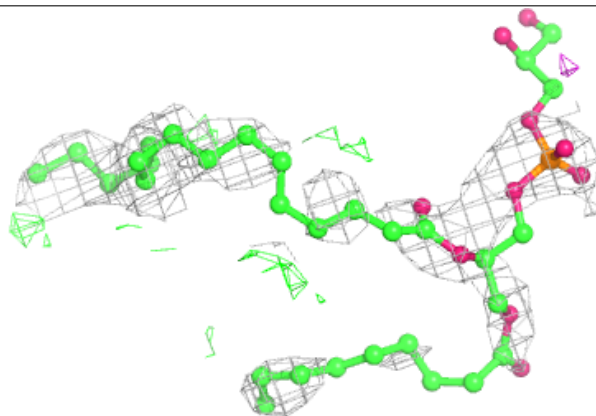


**Electron density around DGD D 408:**

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

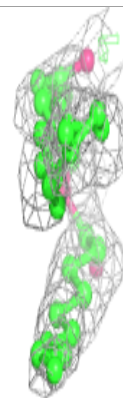
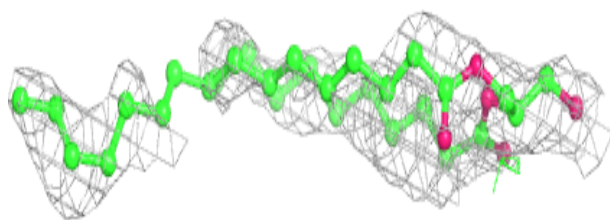
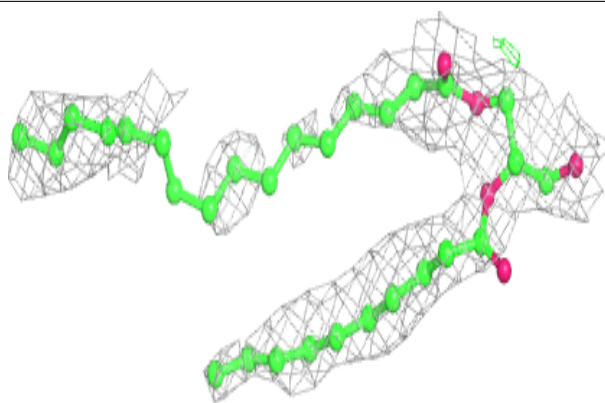
**Electron density around LHG a 418:**

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

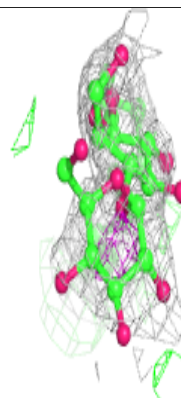
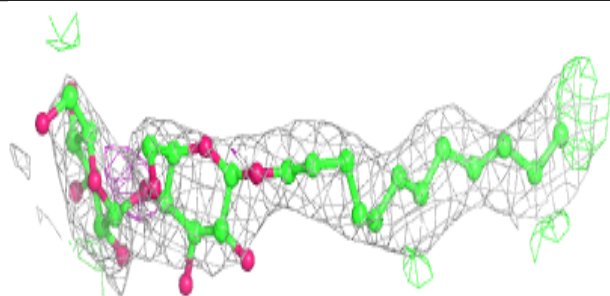
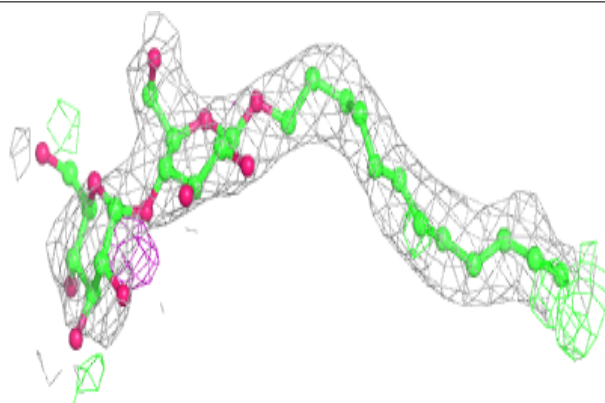


**Electron density around UNL C 526:**

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

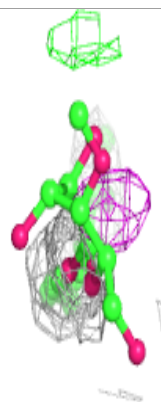
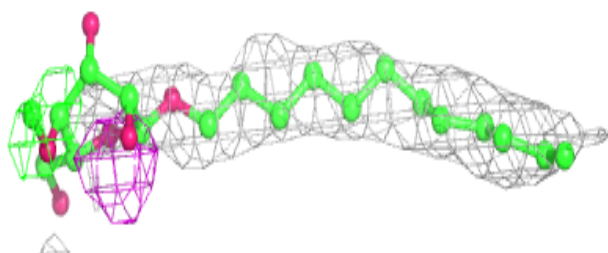
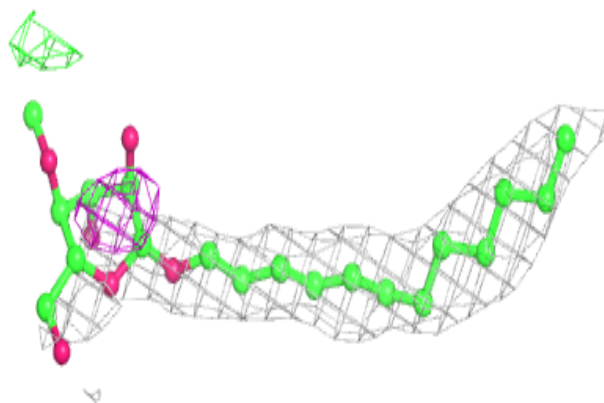
**Electron density around LMT a 401:**

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

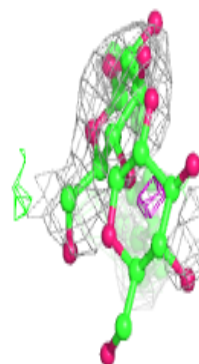
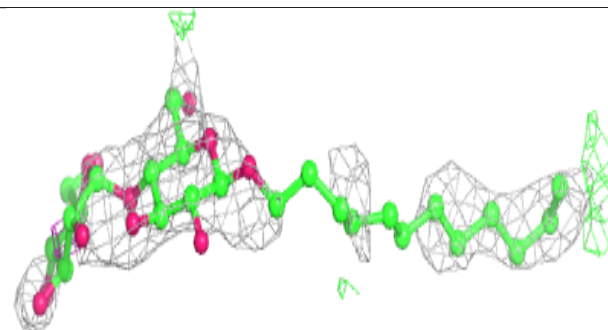
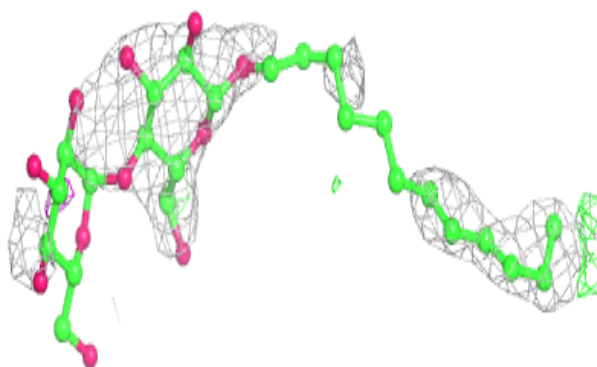


**Electron density around LMT b 626:**

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

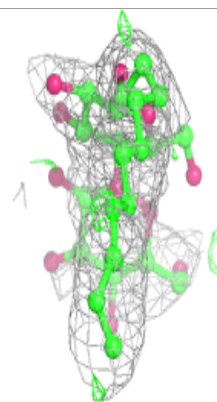
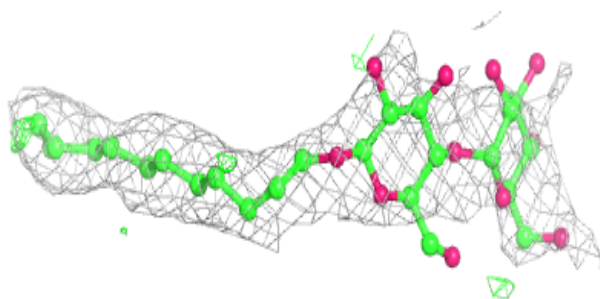
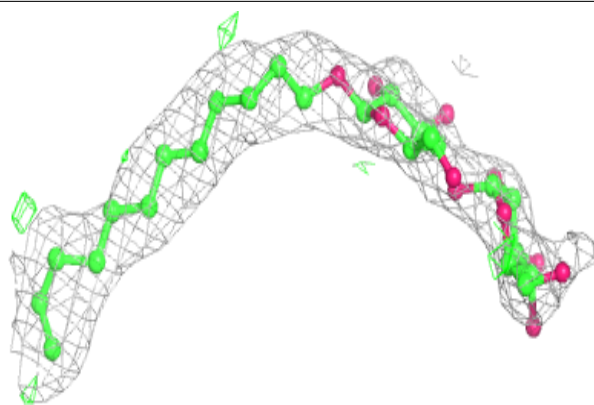
**Electron density around LMT e 102:**

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

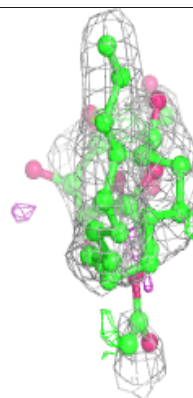
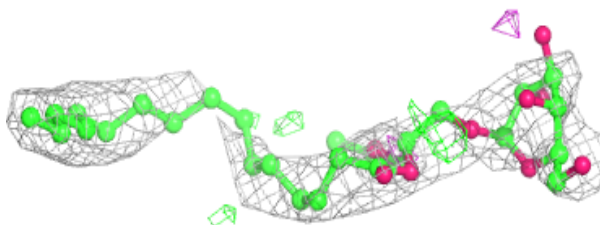
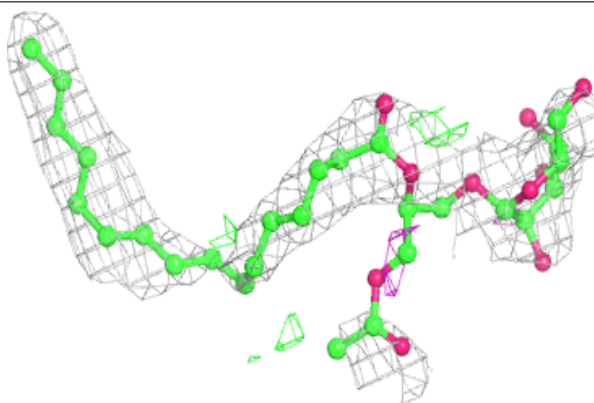


**Electron density around LMT m 103:**

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

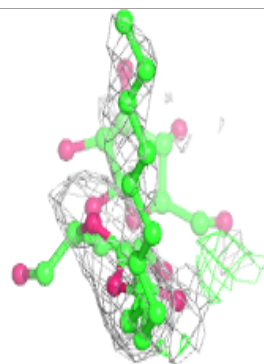
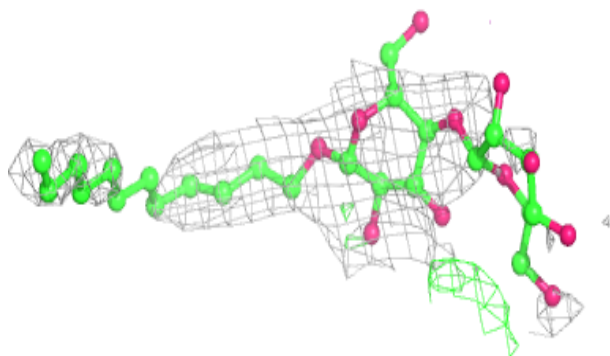
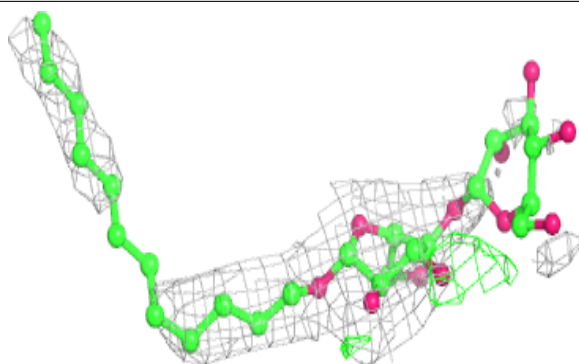
**Electron density around LMG Z 101:**

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

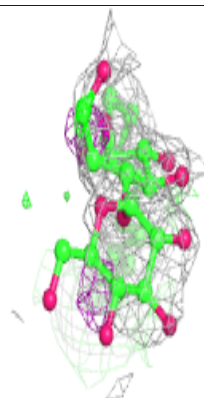
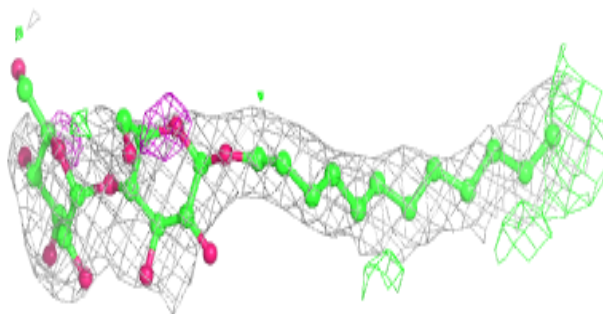
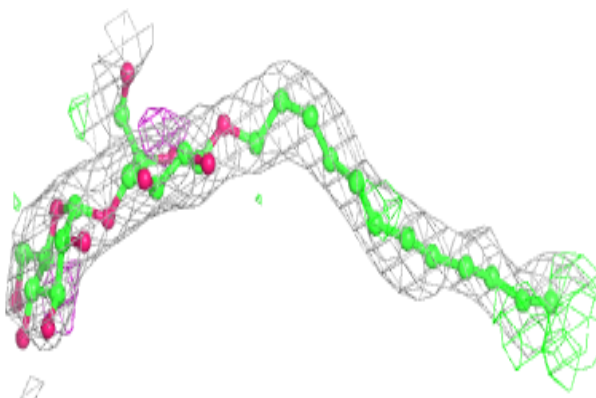


**Electron density around LMT C 520:**

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

**Electron density around LMT A 415:**

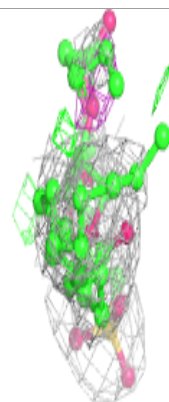
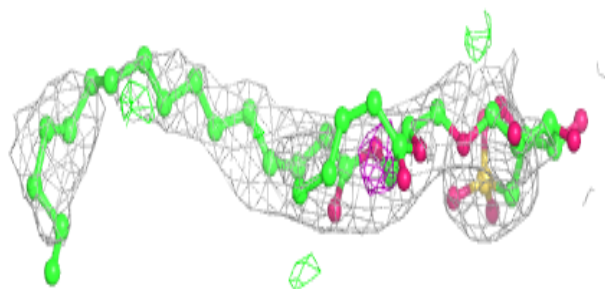
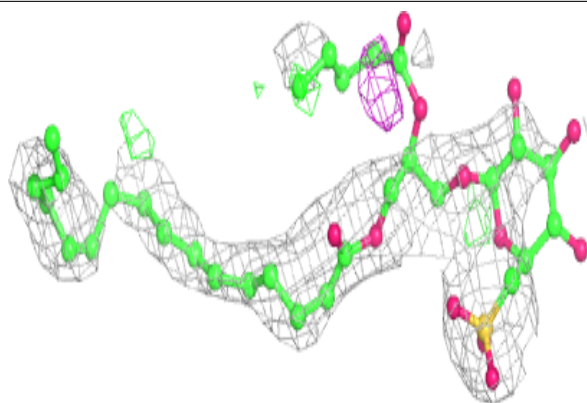
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



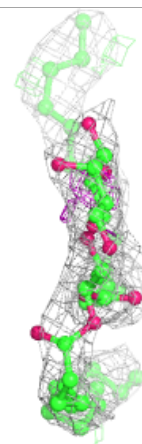
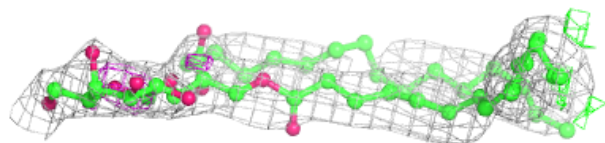
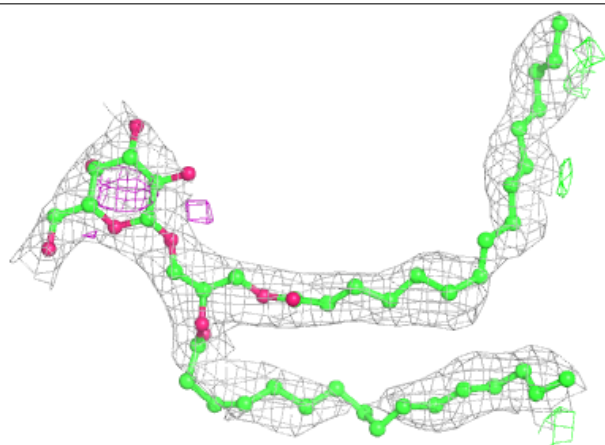


**Electron density around SQD f 102:**

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

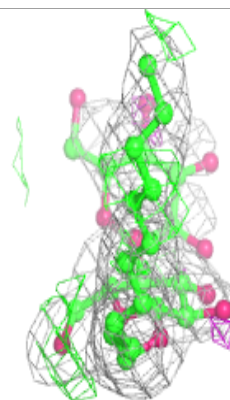
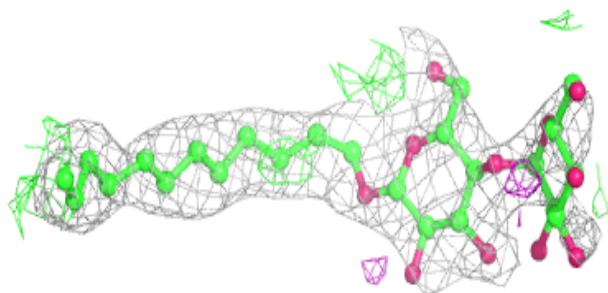
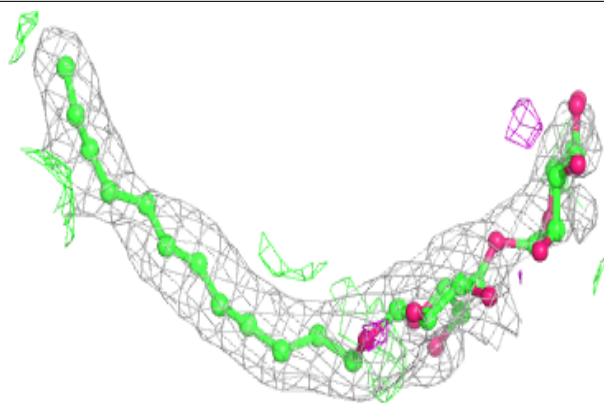
**Electron density around LMG Y 101:**

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

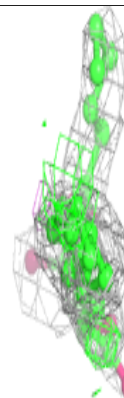
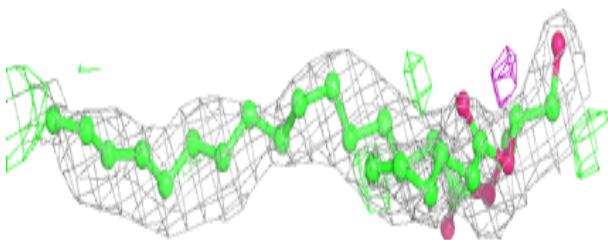
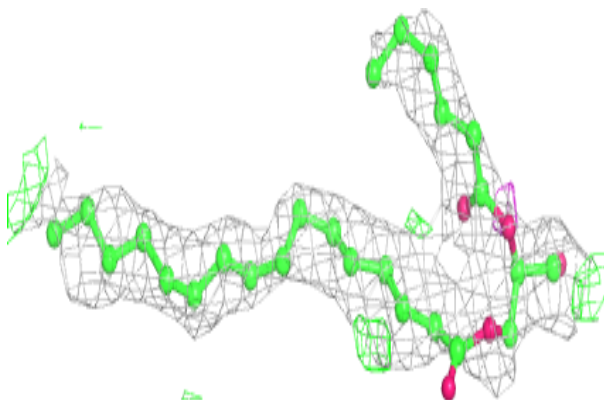


**Electron density around LMT M 103:**

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

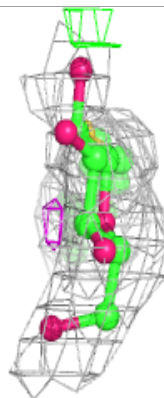
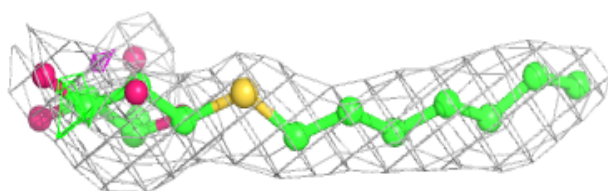
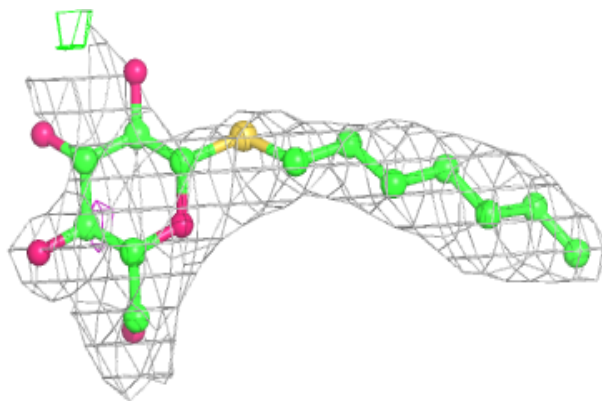
**Electron density around UNL a 414:**

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

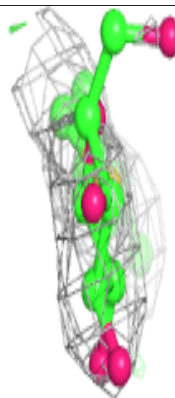
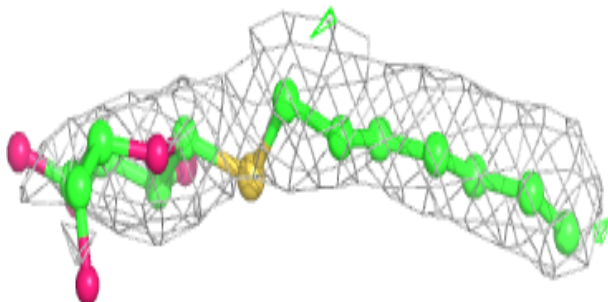
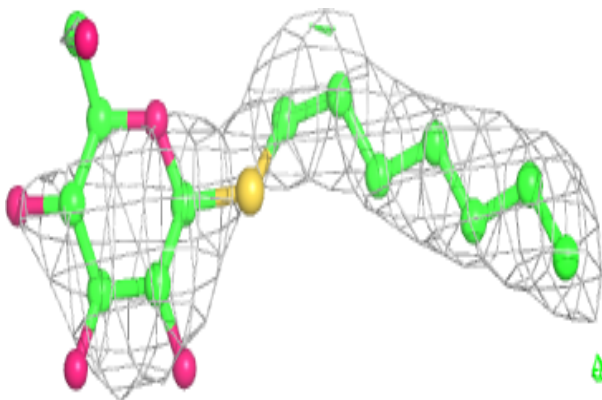


**Electron density around HTG B 633:**

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

**Electron density around HTG c 922:**

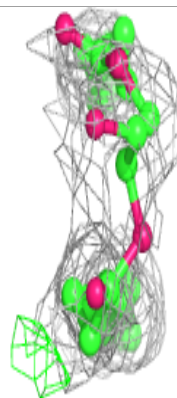
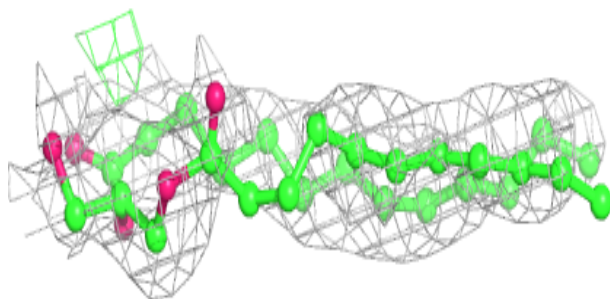
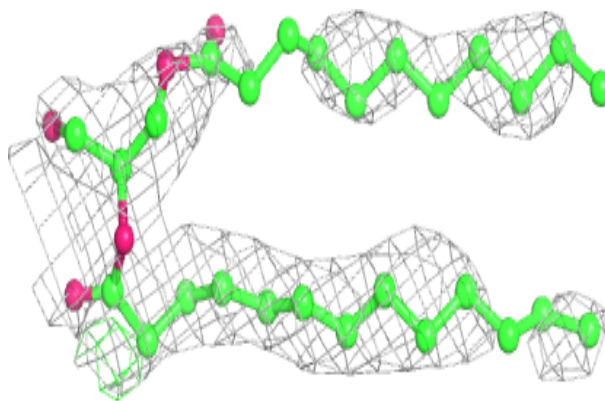
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





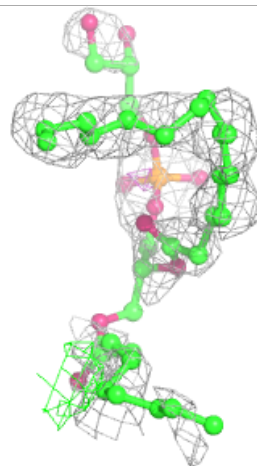
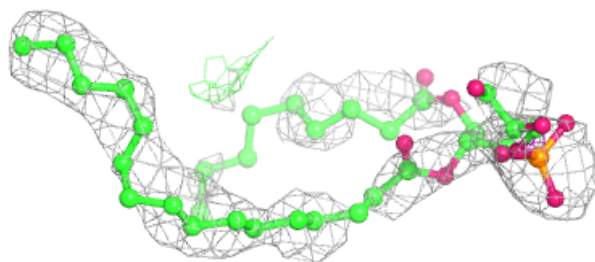
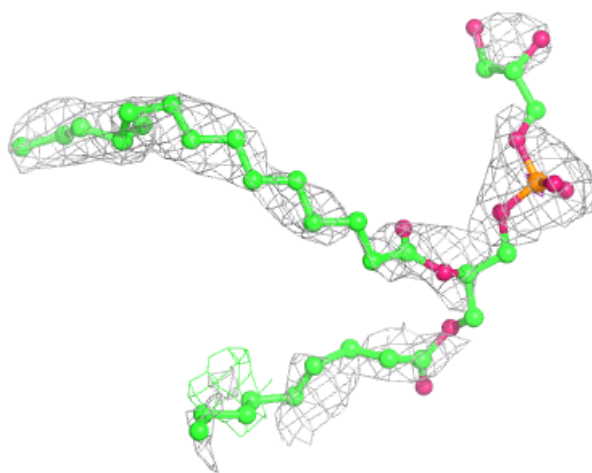
**Electron density around UNL c 925:**

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



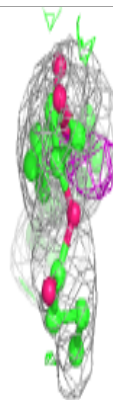
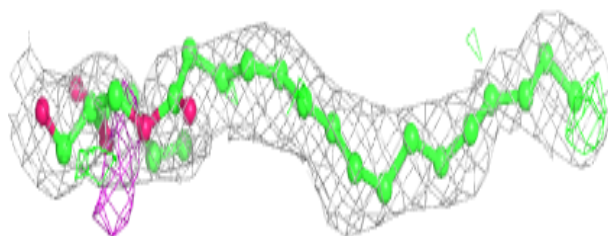
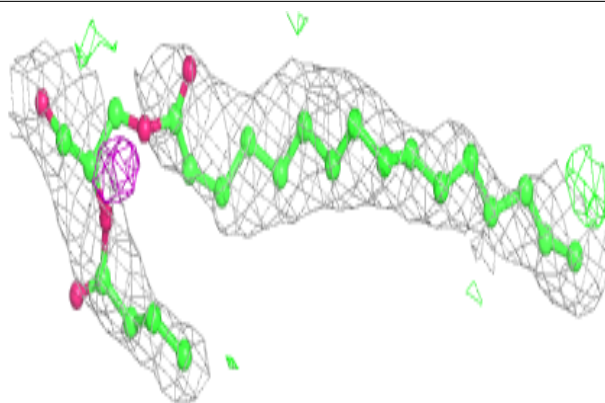
**Electron density around LHG E 101:**

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

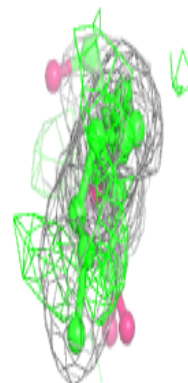
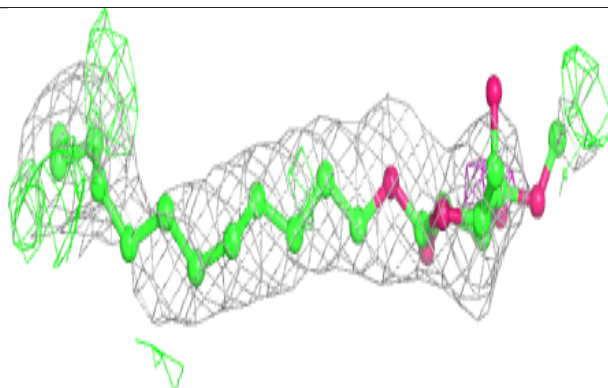
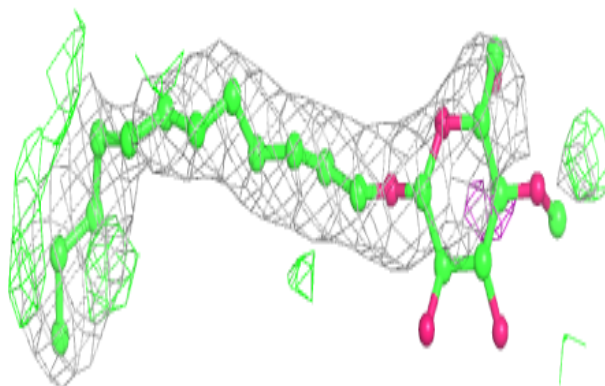


**Electron density around UNL A 418:**

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

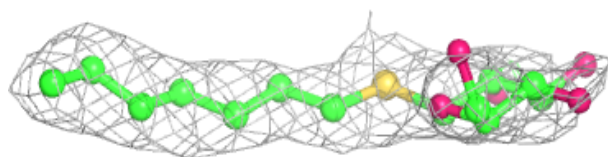
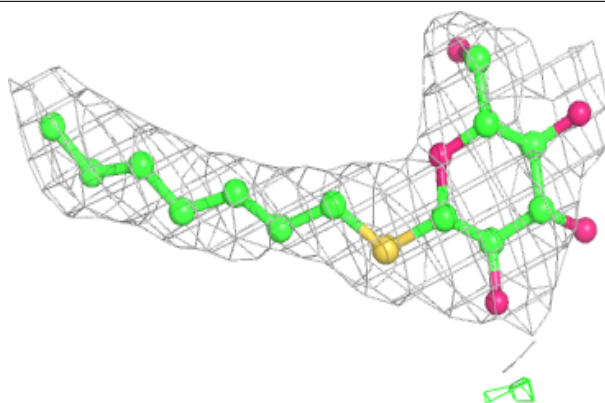
**Electron density around LMT b 602:**

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

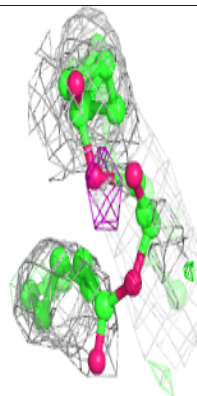
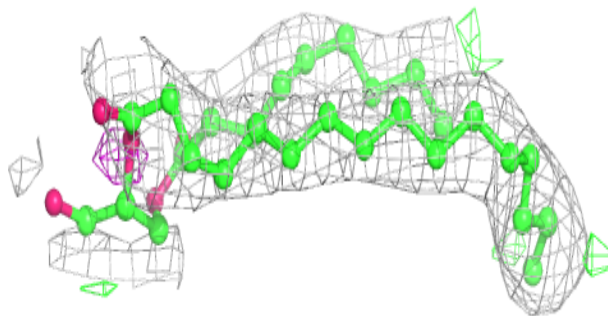
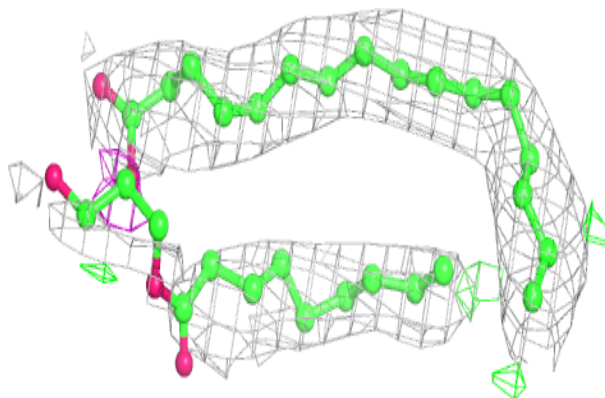


**Electron density around HTG b 604:**

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

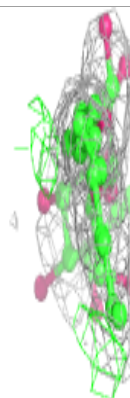
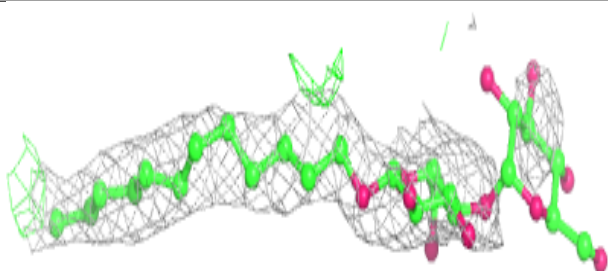
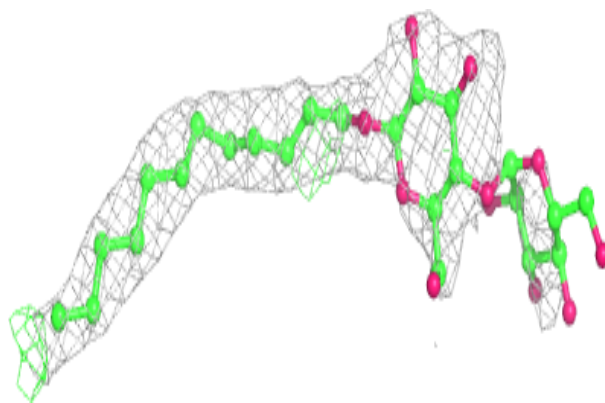
**Electron density around UNL b 634:**

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

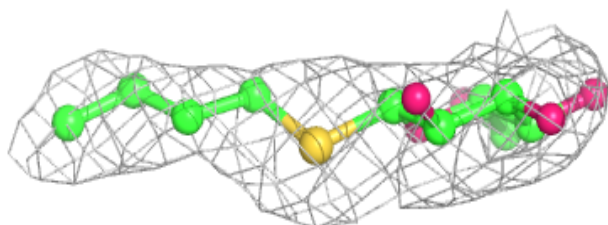
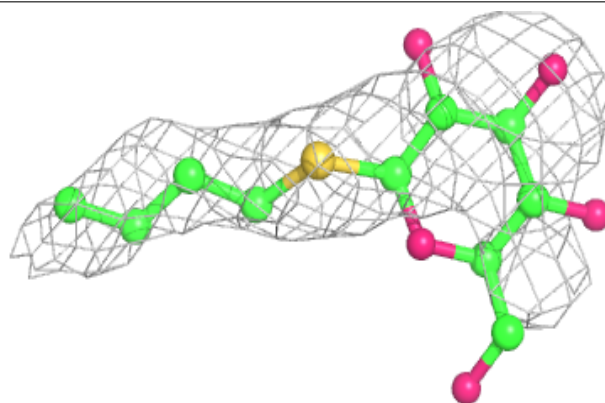


**Electron density around LMT D 403:**

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

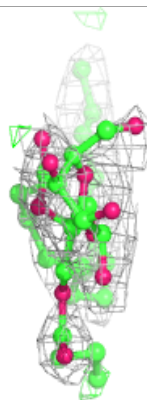
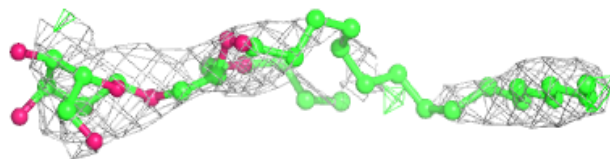
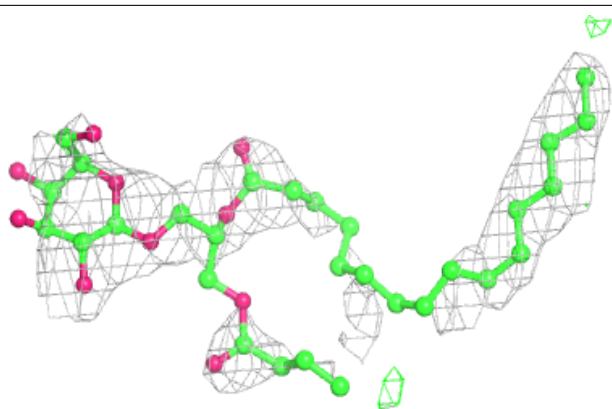
**Electron density around HTG D 413:**

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

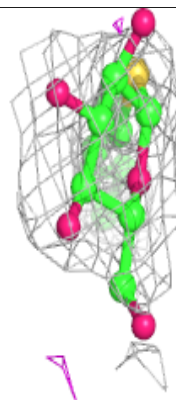
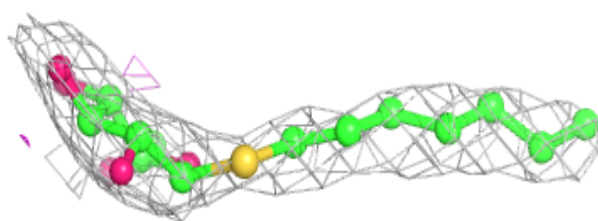
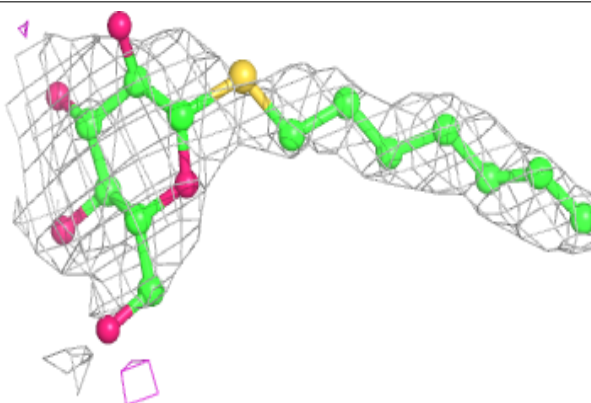


**Electron density around LMG z 101:**

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

**Electron density around HTG B 625:**

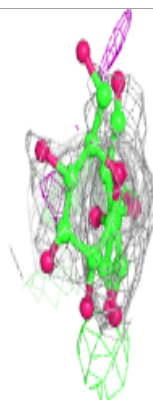
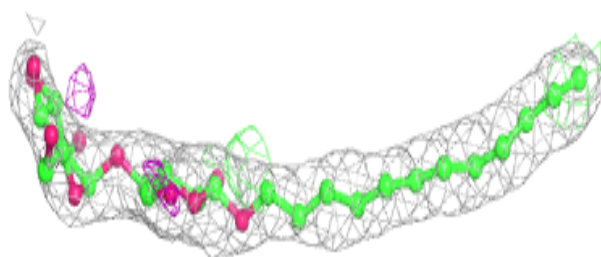
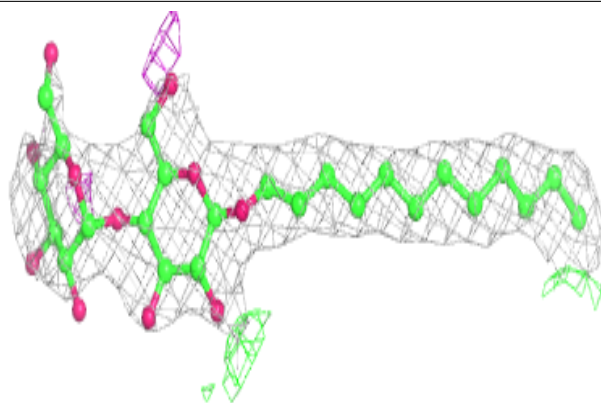
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



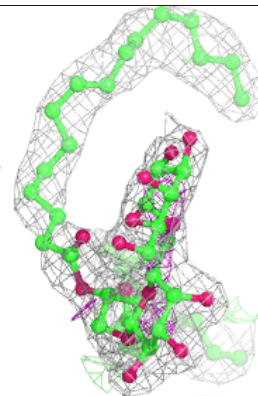
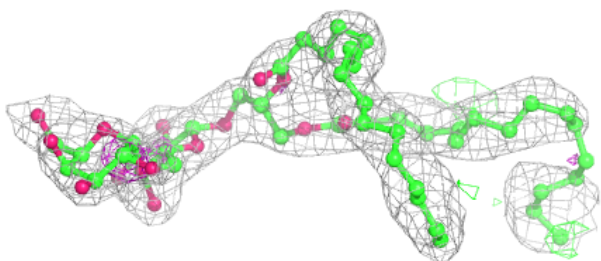
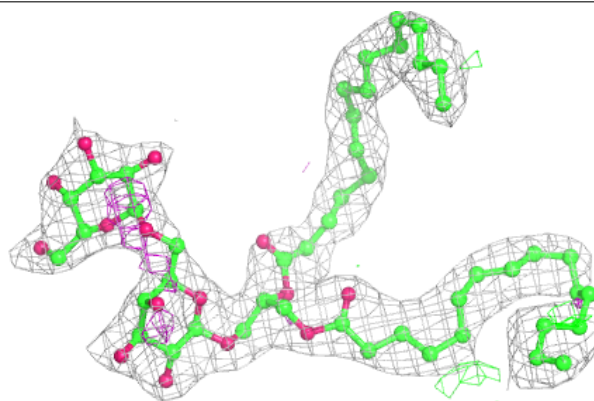


**Electron density around LMT M 101:**

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

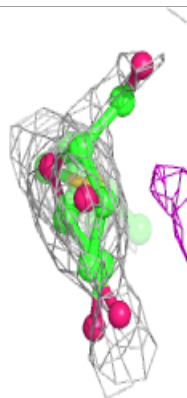
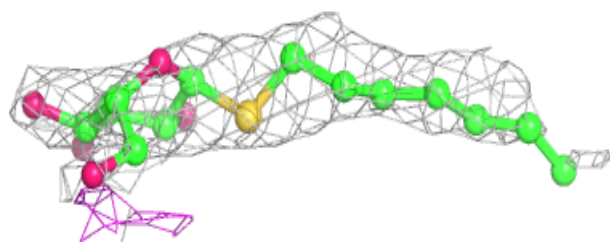
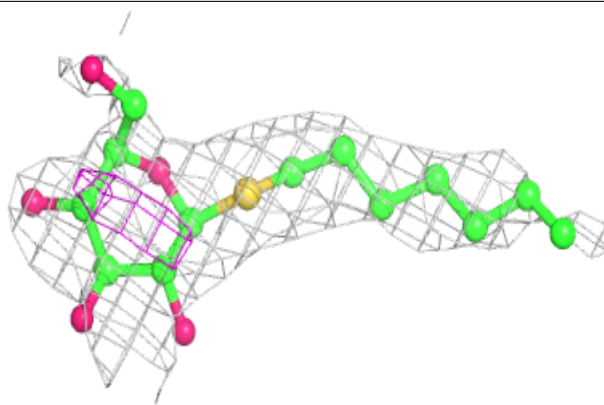
**Electron density around DGD C 517:**

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

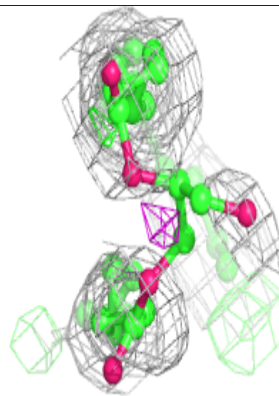
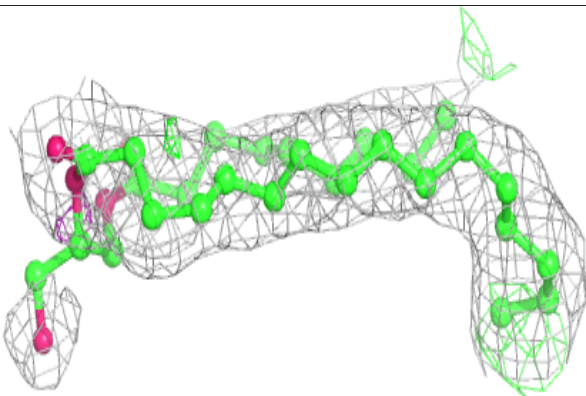
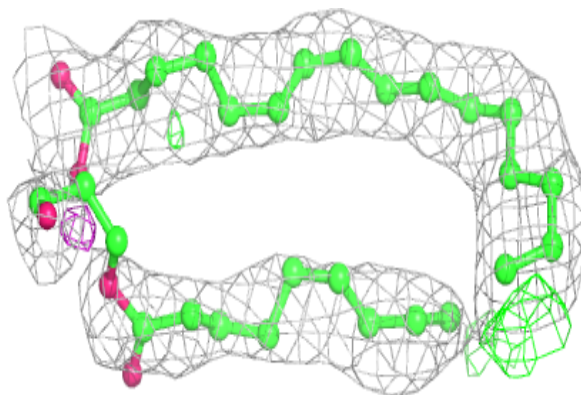


**Electron density around HTG C 522:**

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

**Electron density around UNL B 634:**

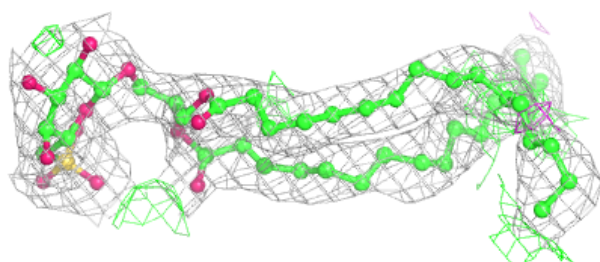
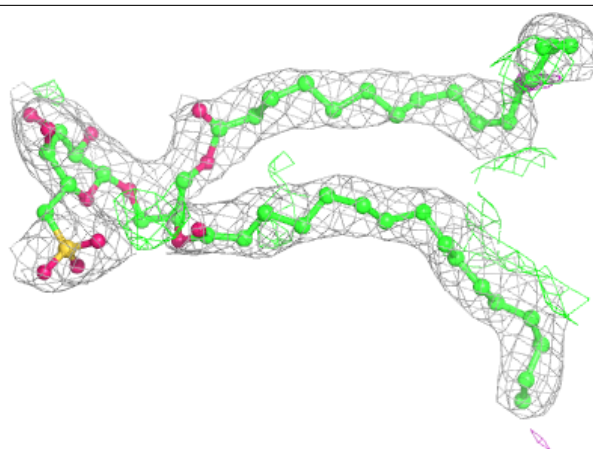
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



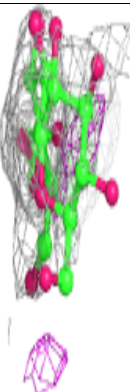
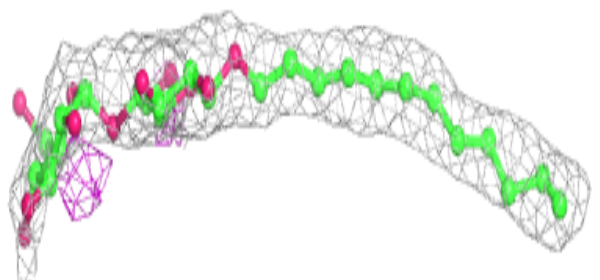
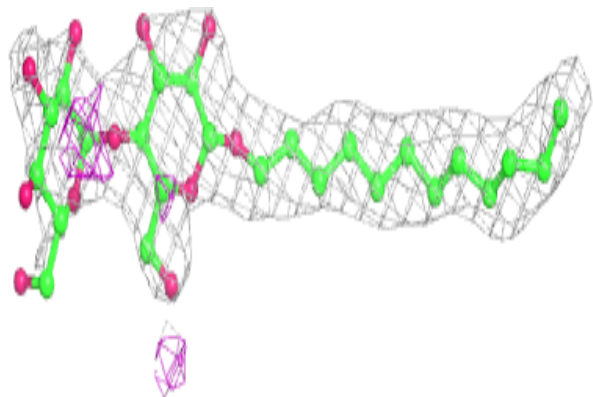


**Electron density around SQD L 102:**

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

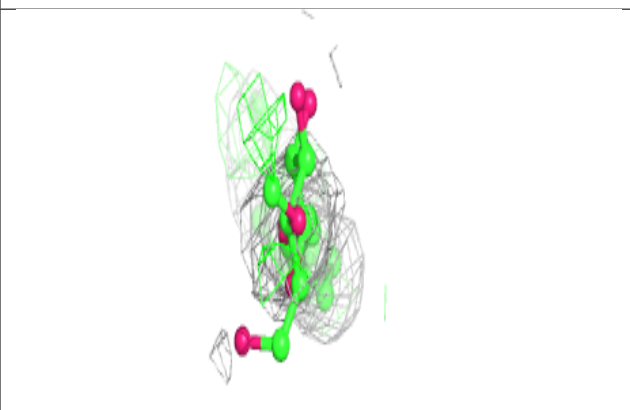
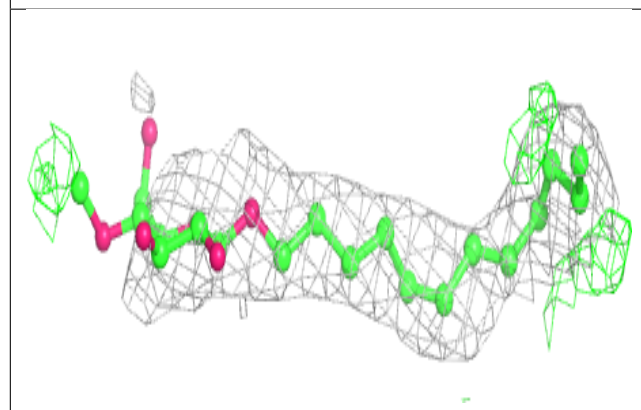
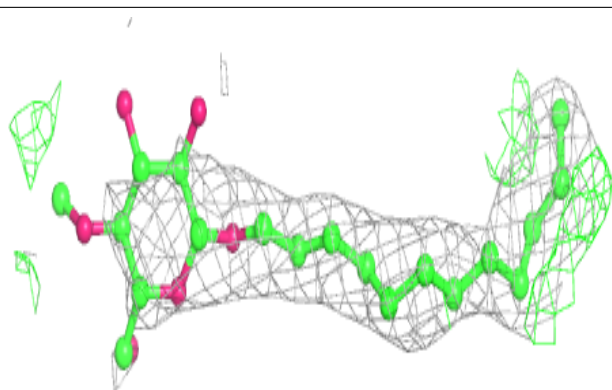
**Electron density around LMT m 102:**

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

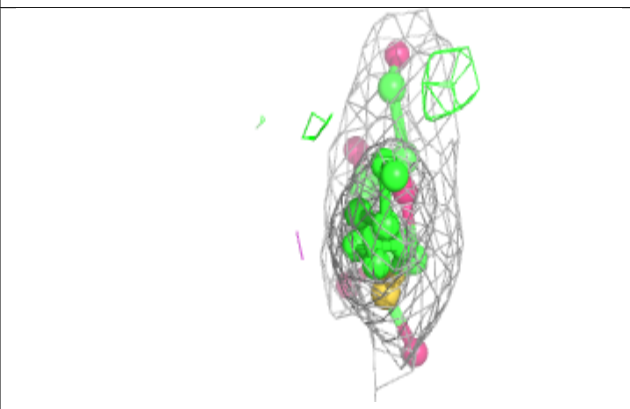
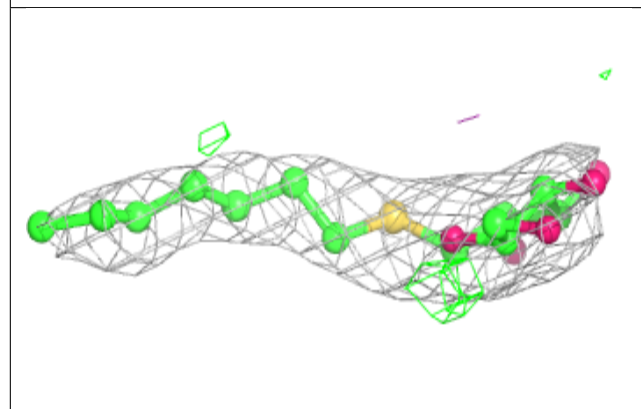
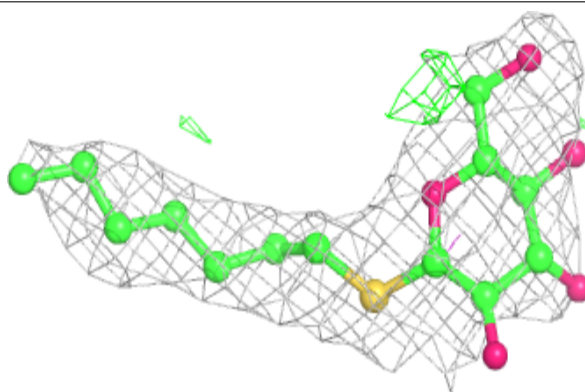


**Electron density around LMT t 101:**

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

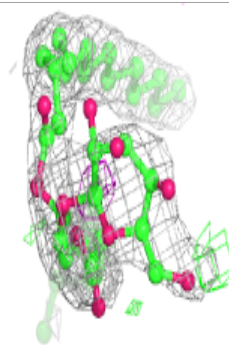
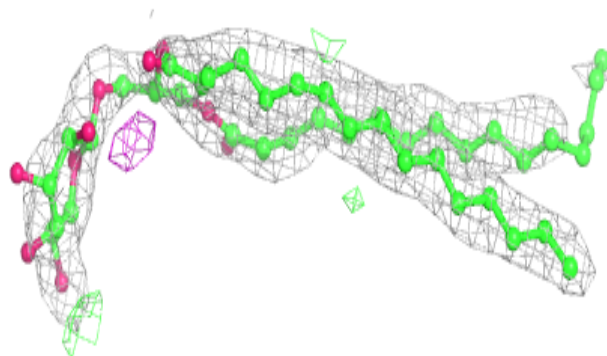
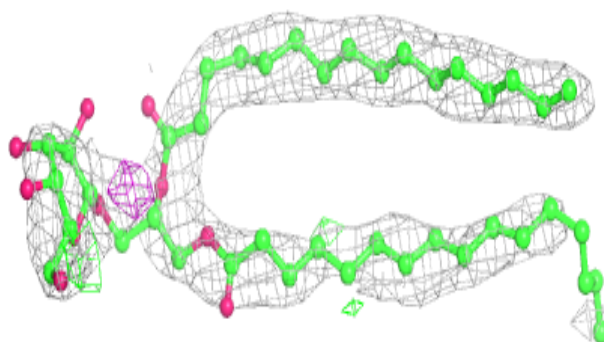
**Electron density around HTG b 628:**

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

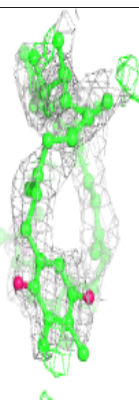
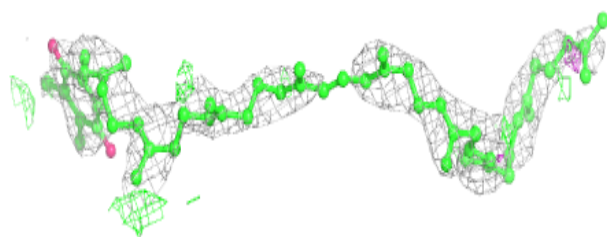
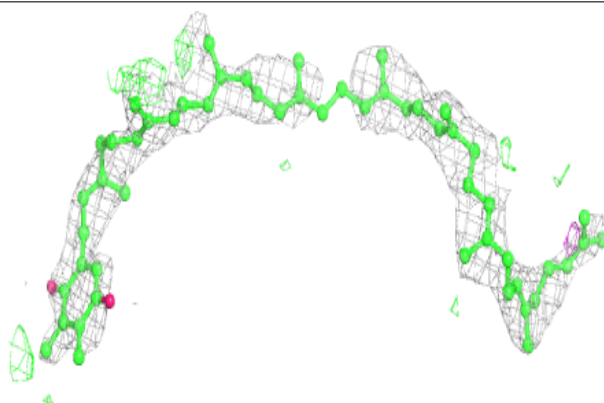


**Electron density around LMG C 519:**

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

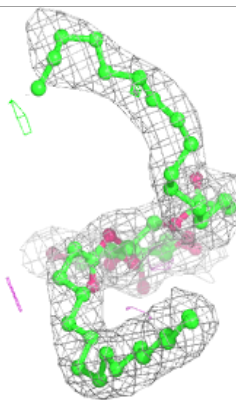
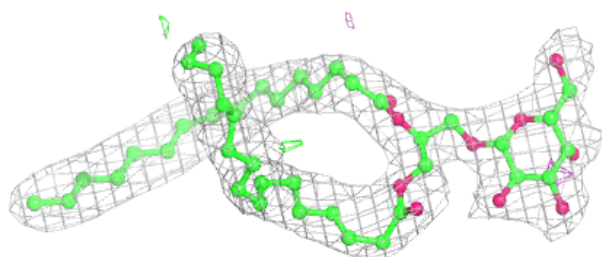
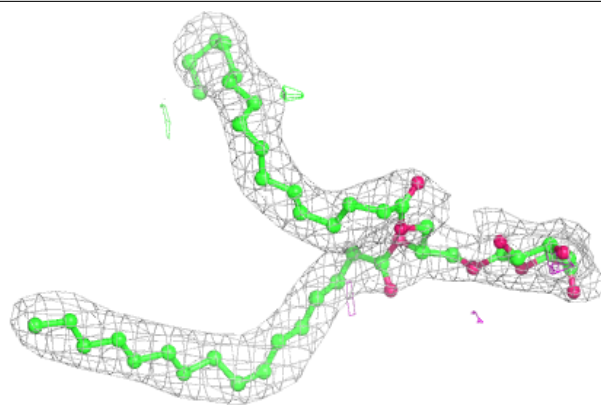
**Electron density around PL9 A 417:**

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

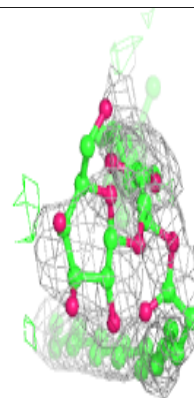
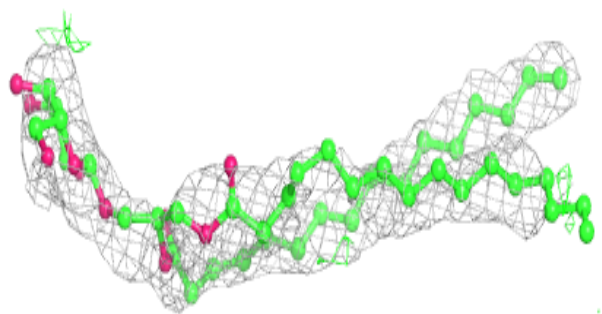
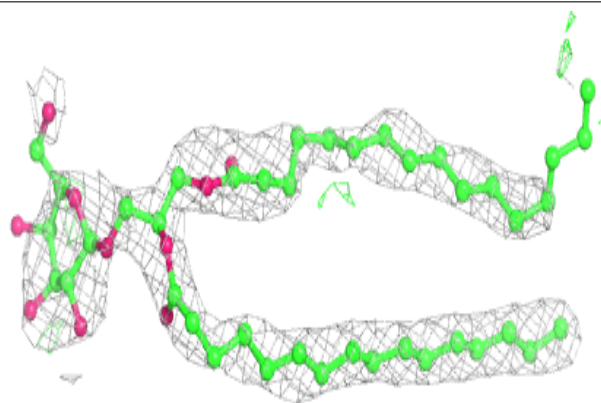


**Electron density around LMG b 625:**

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

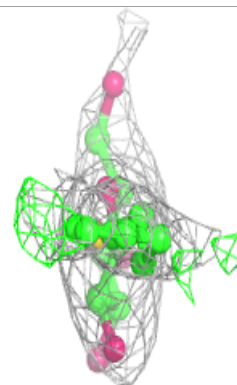
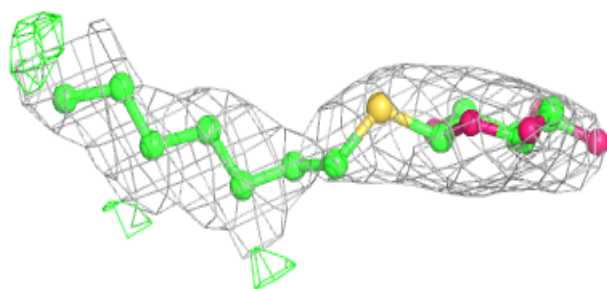
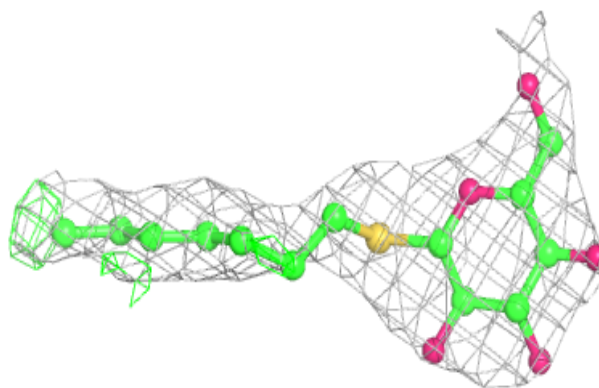
**Electron density around LMG c 920:**

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

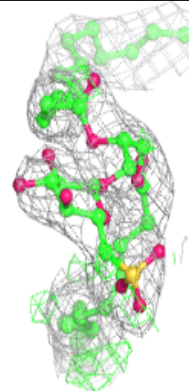
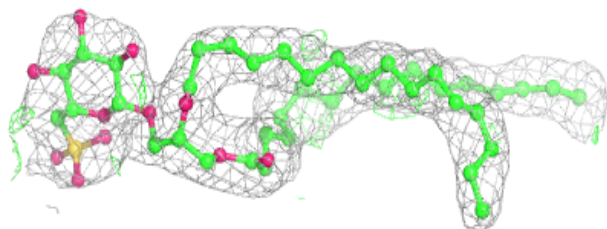
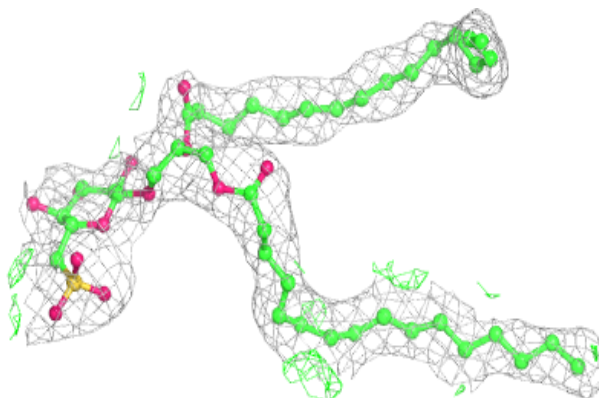


**Electron density around HTG c 921:**

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

**Electron density around SQD a 402:**

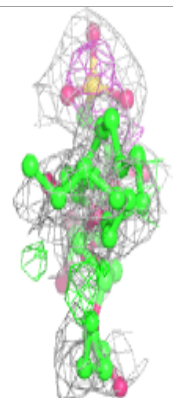
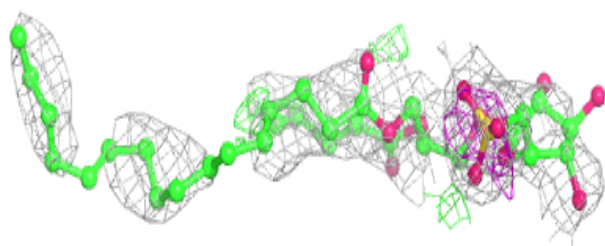
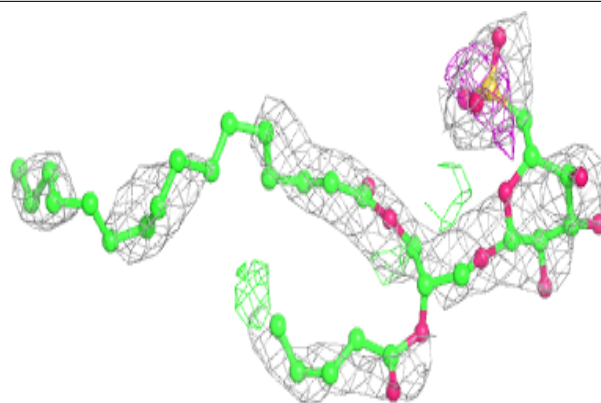
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



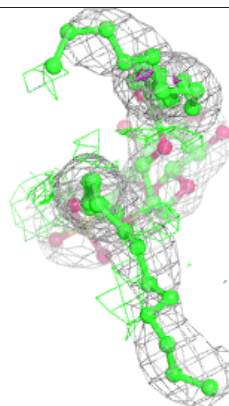
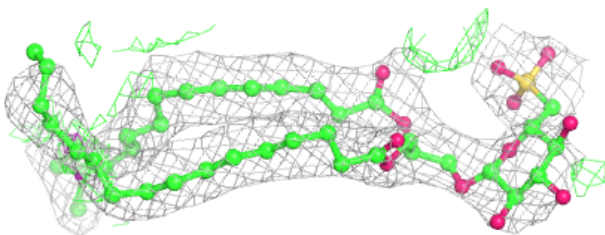
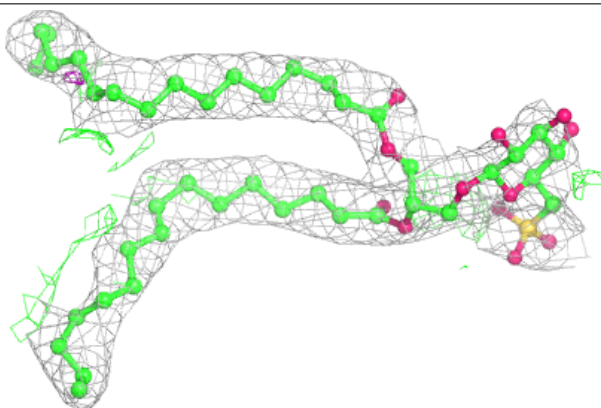


**Electron density around SQD F 103:**

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

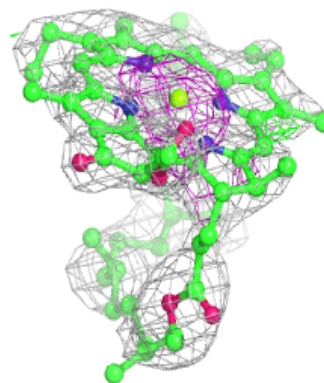
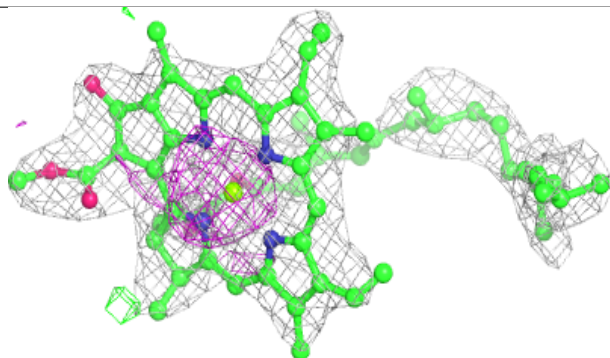
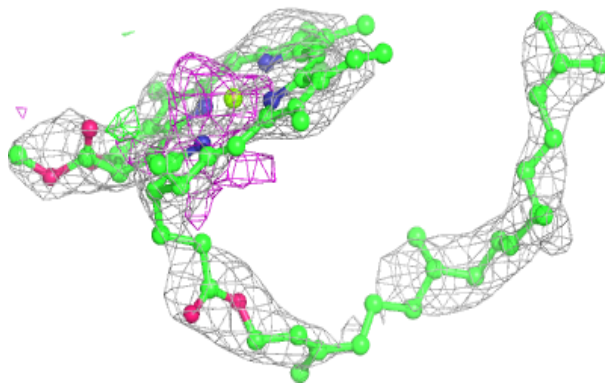
**Electron density around SQD B 621:**

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

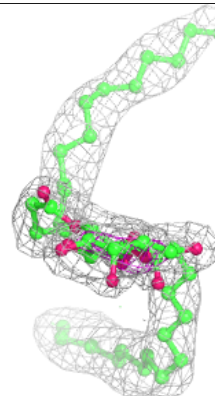
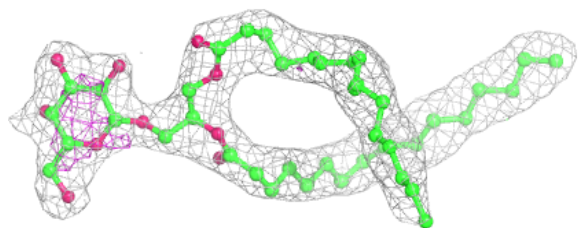
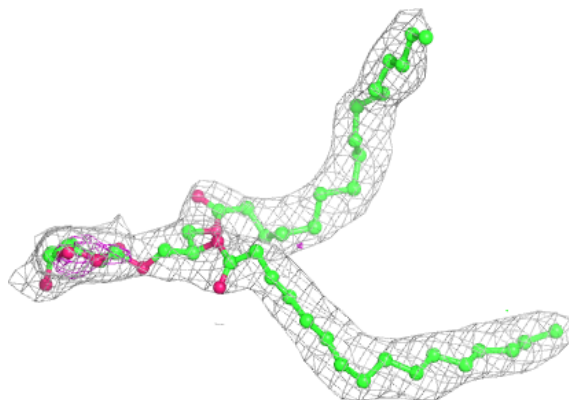


**Electron density around CLA C 513:**

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

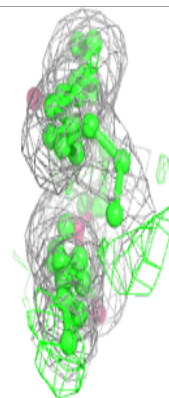
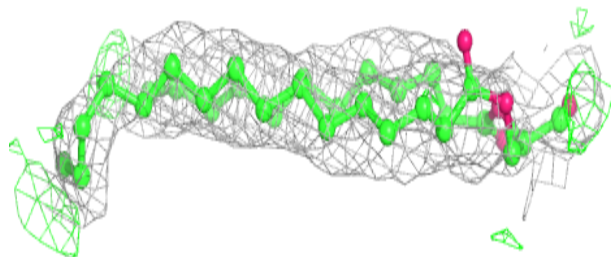
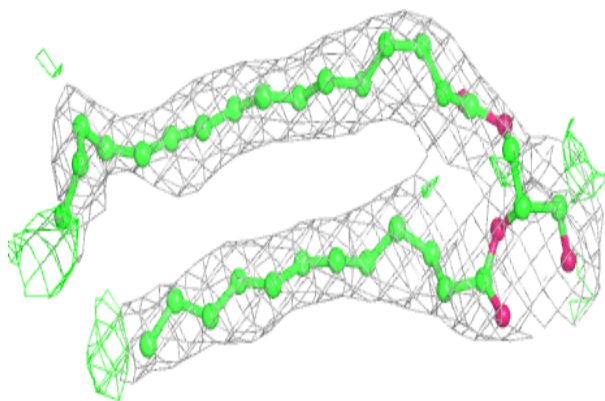
**Electron density around LMG B 622:**

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

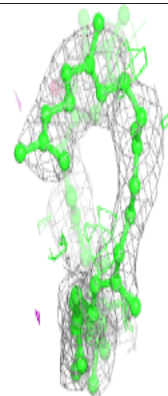
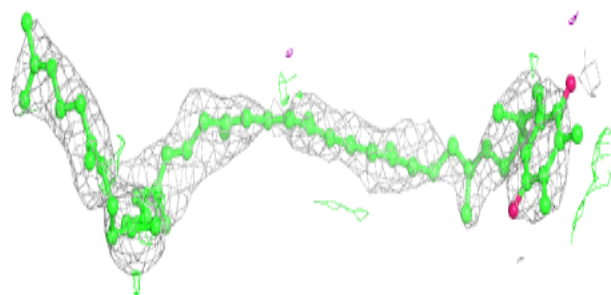
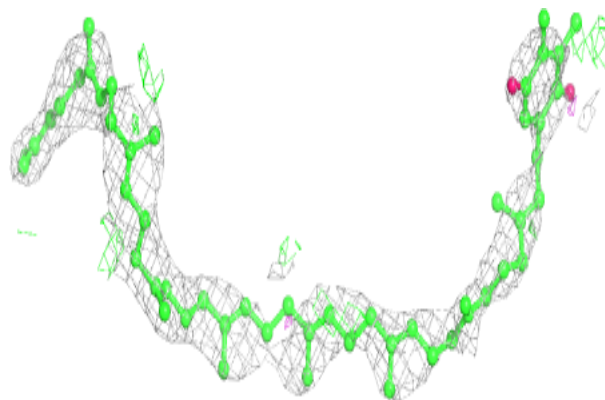


**Electron density around UNL d 413:**

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

**Electron density around PL9 a 415:**

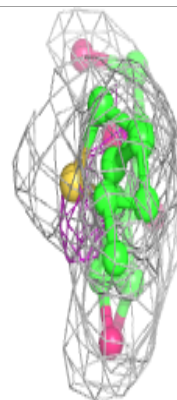
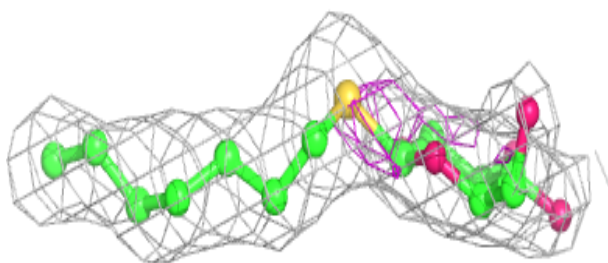
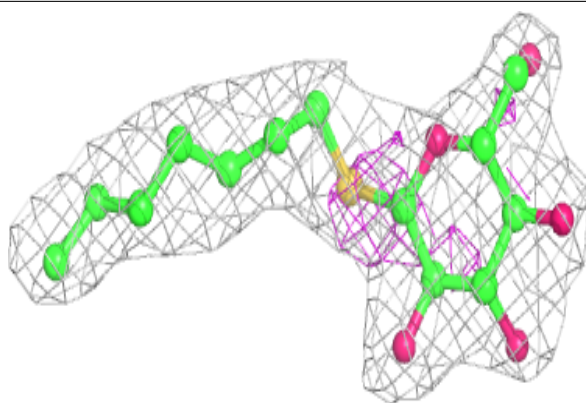
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



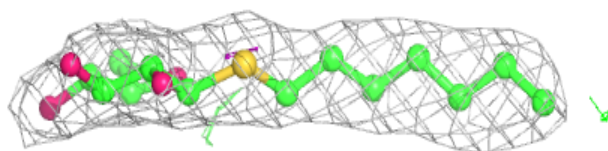
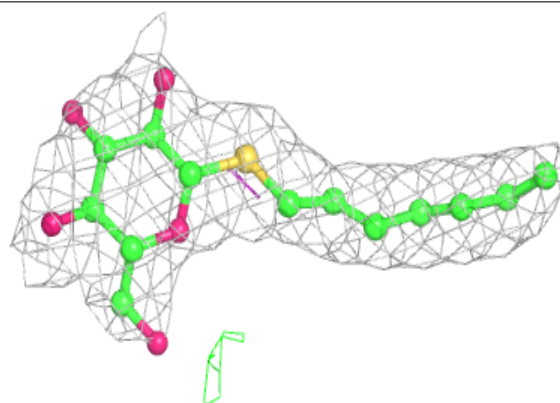


**Electron density around HTG b 601:**

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

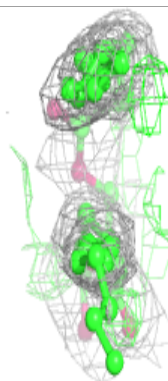
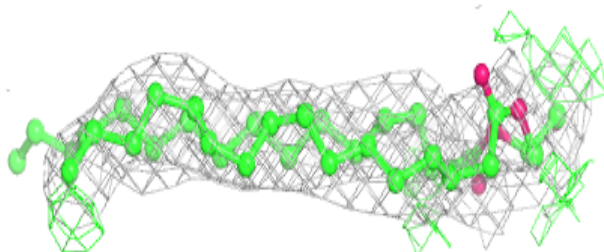
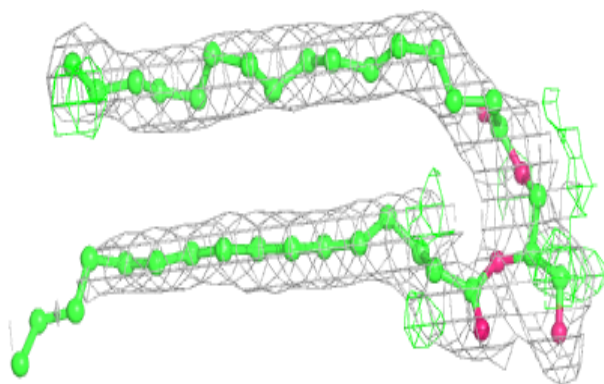
**Electron density around HTG b 603:**

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

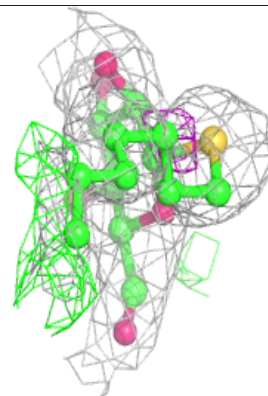
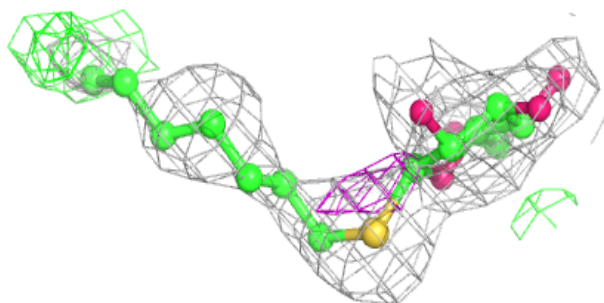
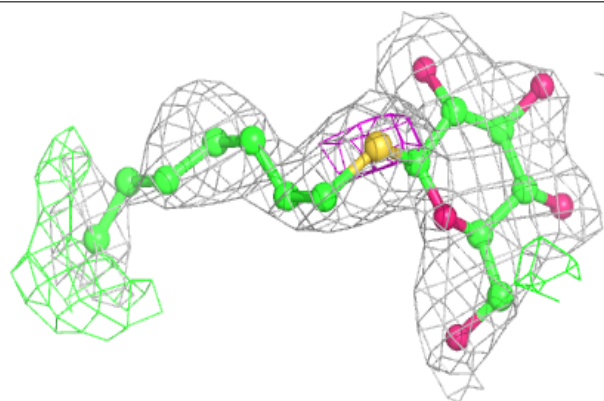


**Electron density around UNL D 412:**

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

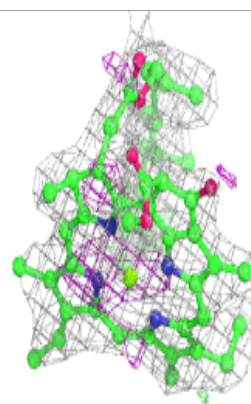
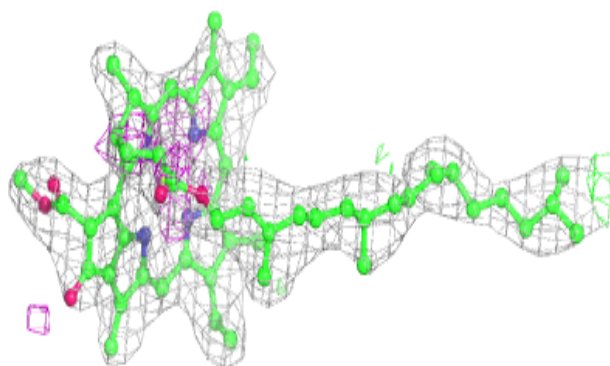
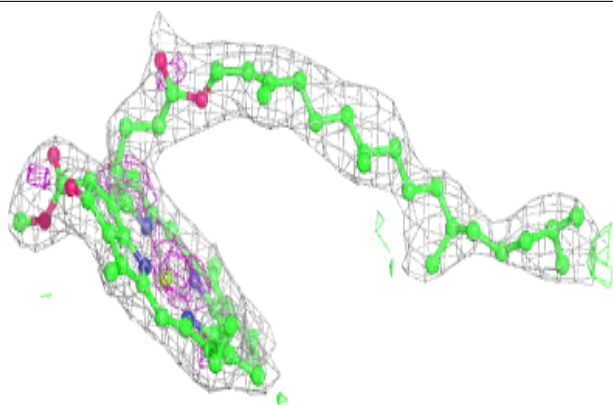
**Electron density around HTG b 627:**

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

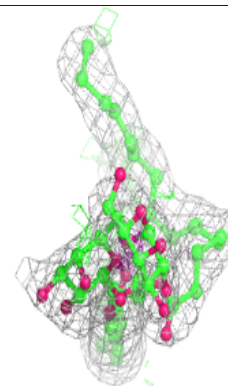
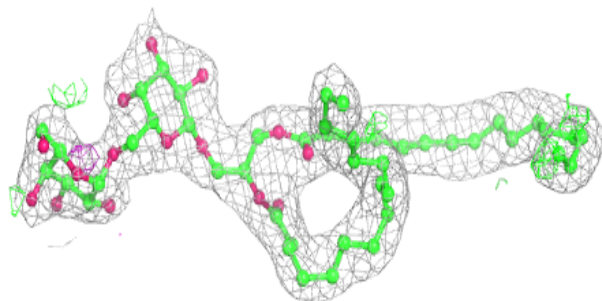
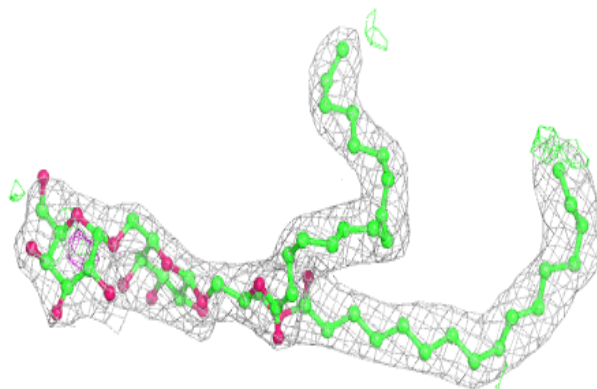


**Electron density around CLA C 504:**

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

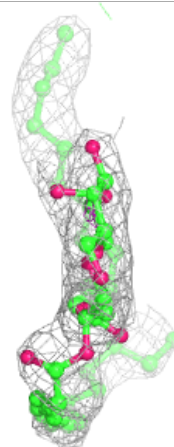
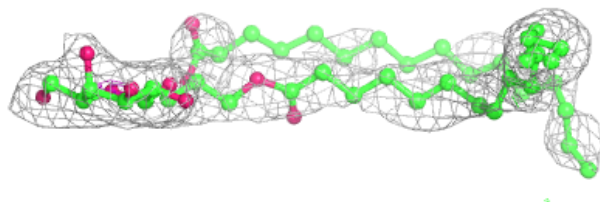
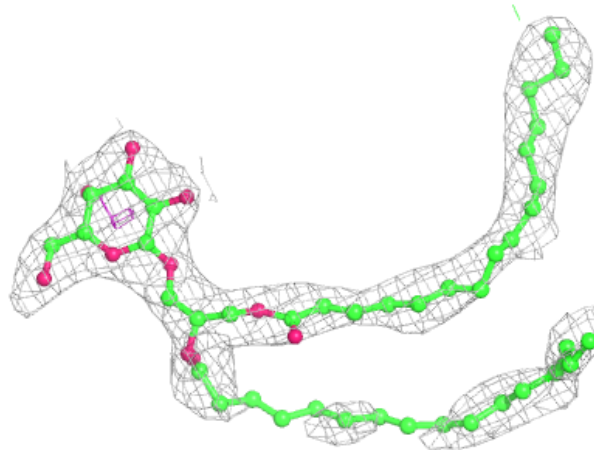
**Electron density around DGD h 102:**

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



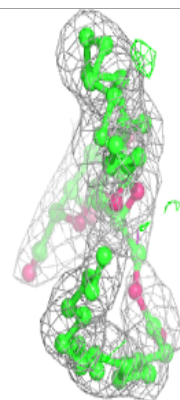
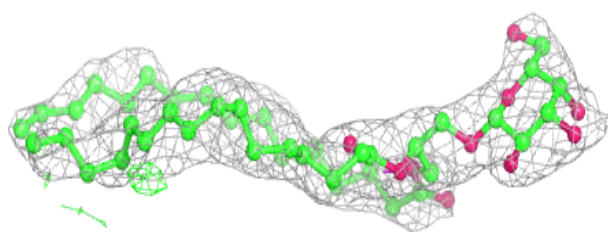
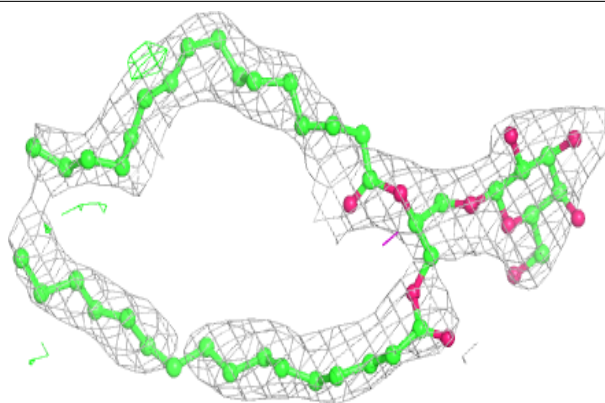
**Electron density around LMG c 919:**

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

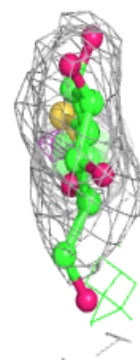
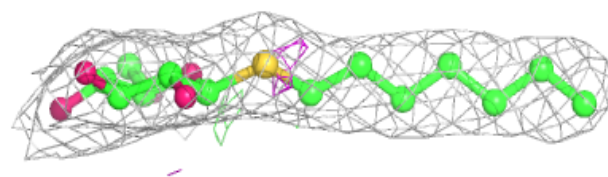
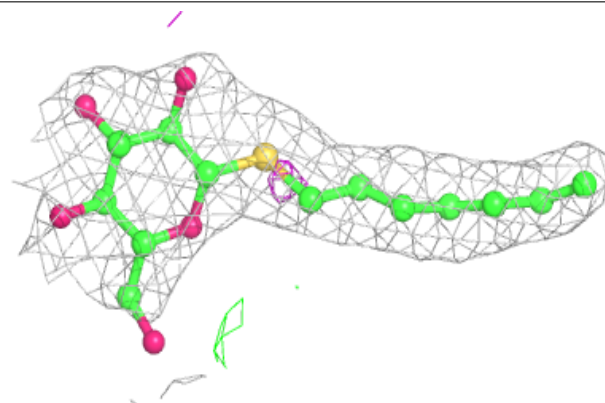


**Electron density around LMG A 419:**

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

**Electron density around HTG B 632:**

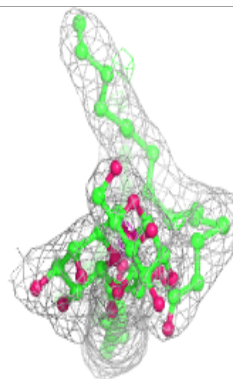
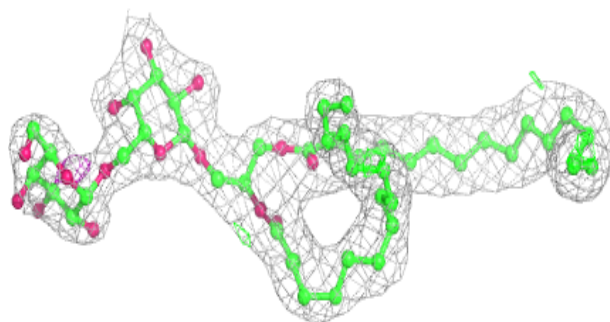
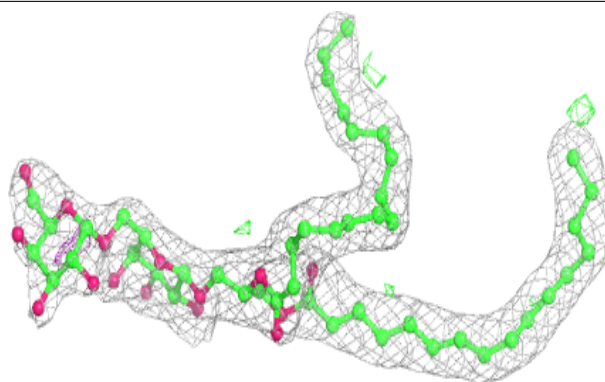
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



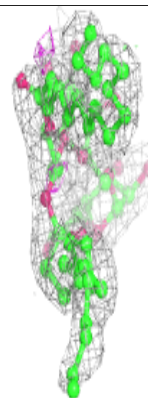
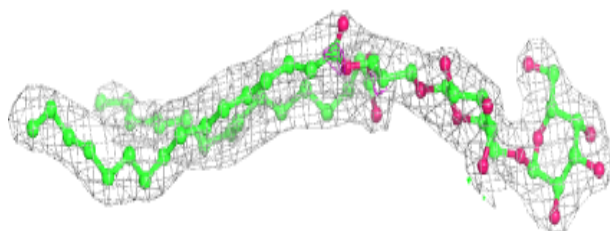
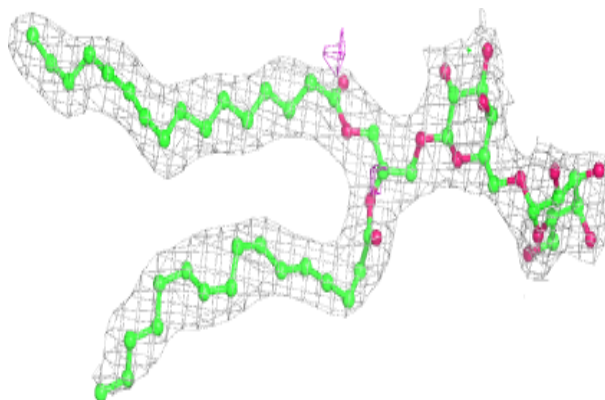


**Electron density around DGD H 102:**

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

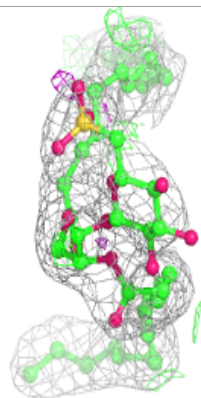
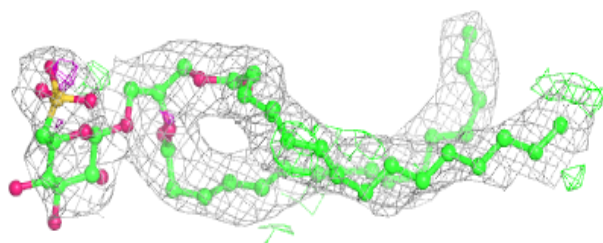
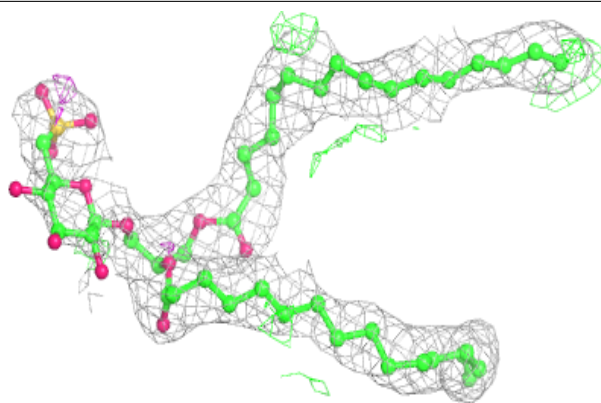
**Electron density around DGD C 518:**

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



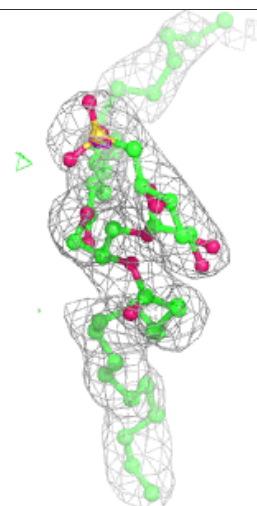
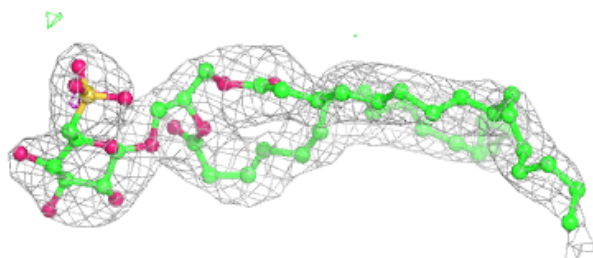
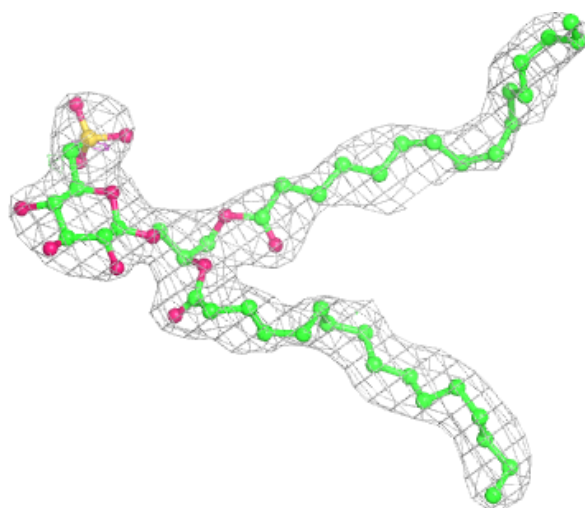
**Electron density around SQD A 414:**

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



**Electron density around SQD a 410:**

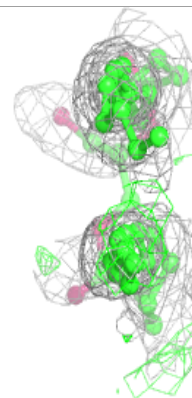
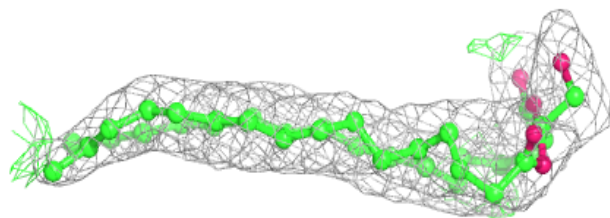
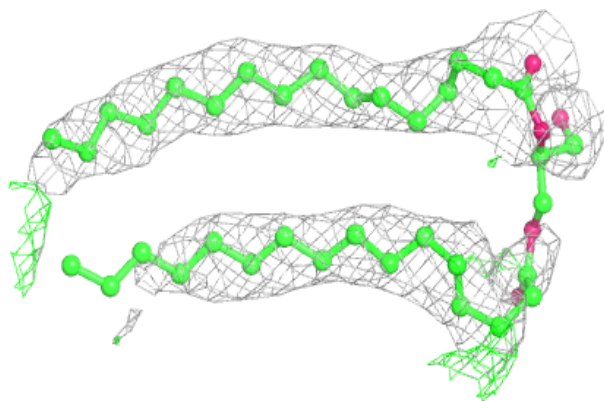
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



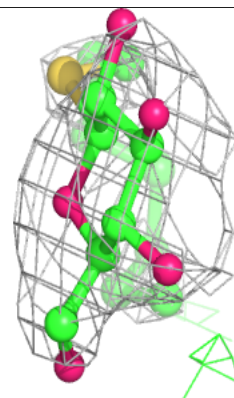
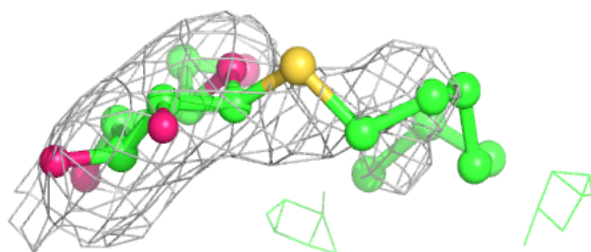
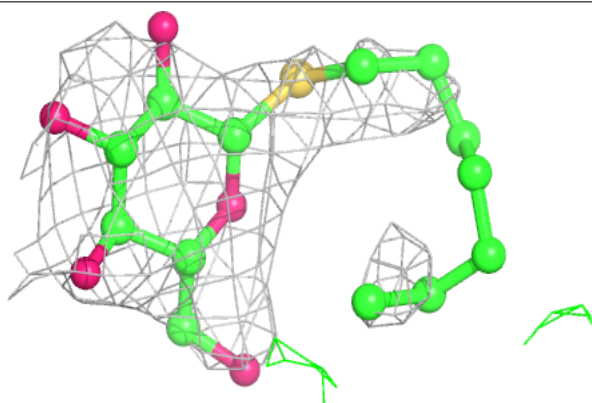


**Electron density around UNL i 101:**

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

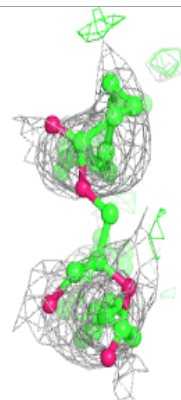
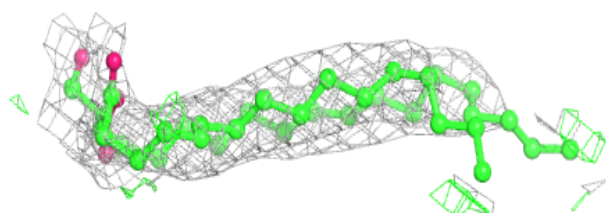
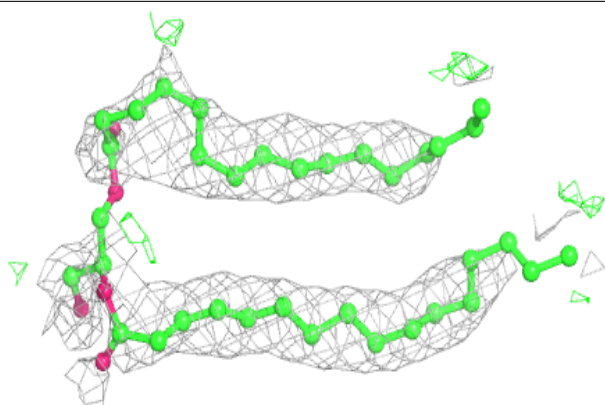
**Electron density around HTG V 203:**

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

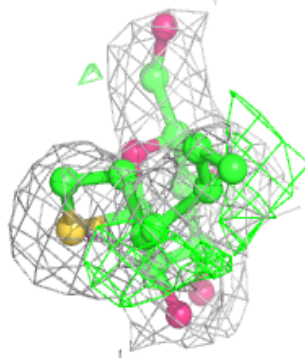
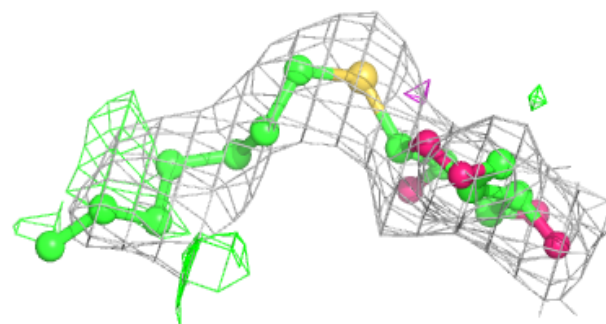
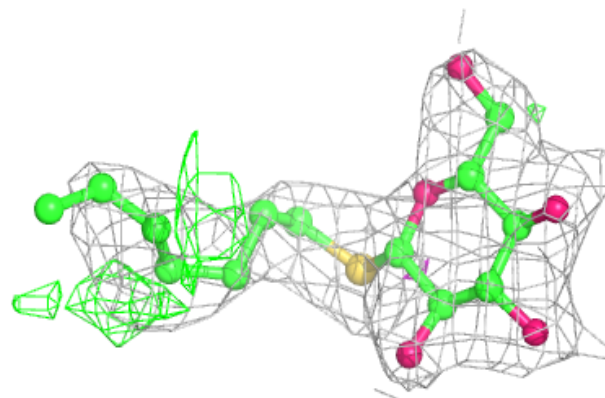


**Electron density around UNL I 101:**

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

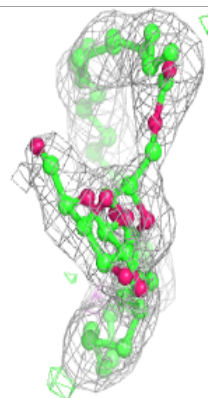
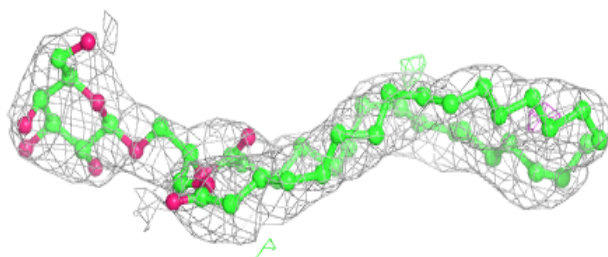
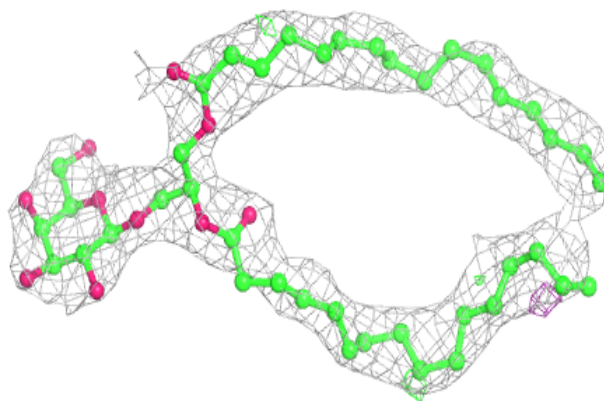
**Electron density around HTG B 624:**

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

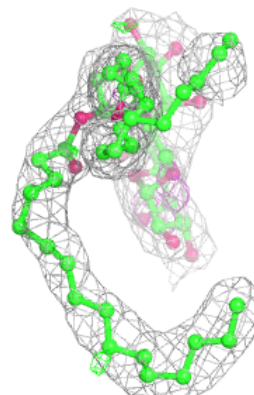
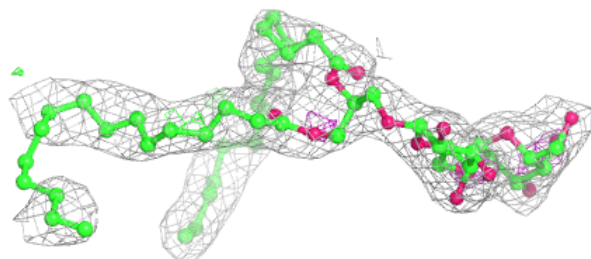
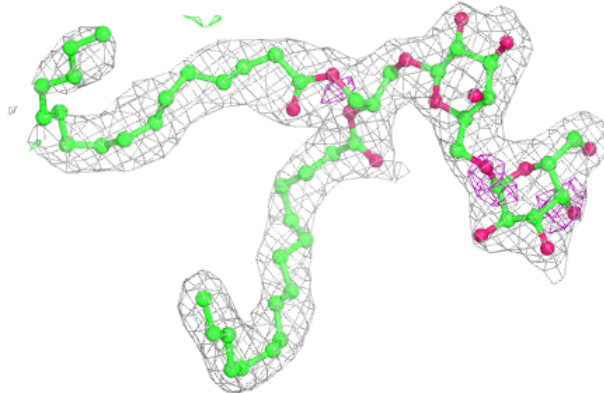


**Electron density around LMG a 411:**

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

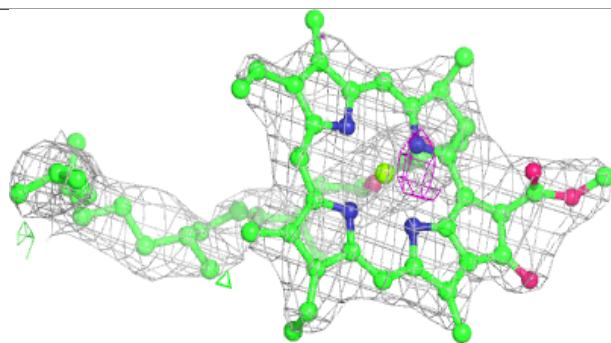
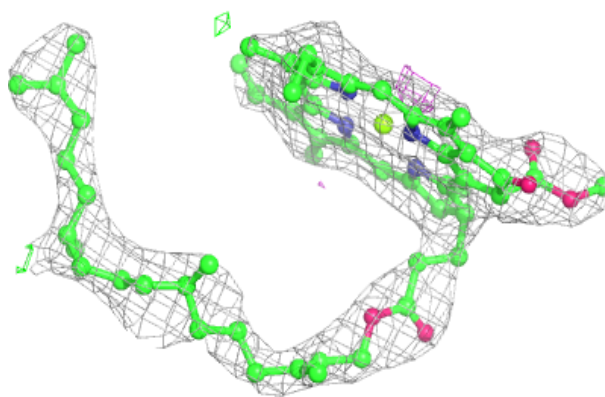
**Electron density around DGD c 917:**

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



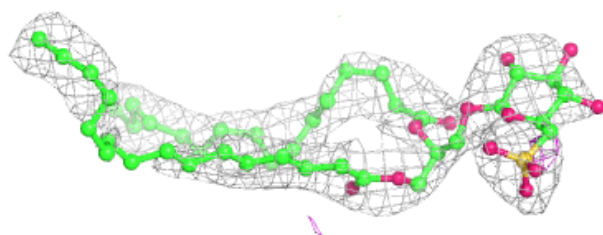
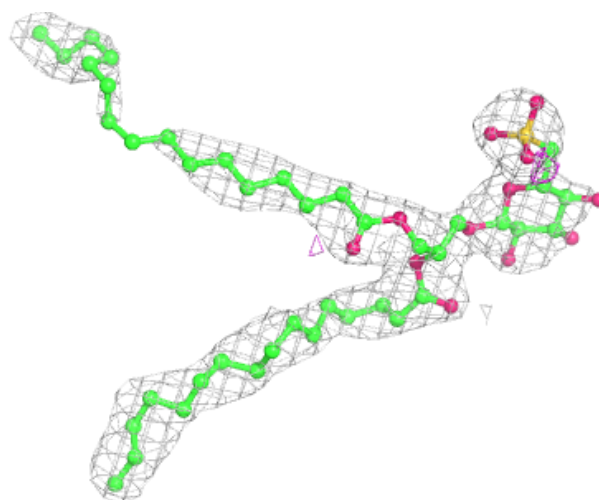
**Electron density around CLA c 914:**

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



**Electron density around SQD A 411:**

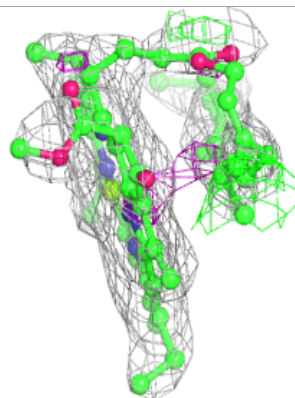
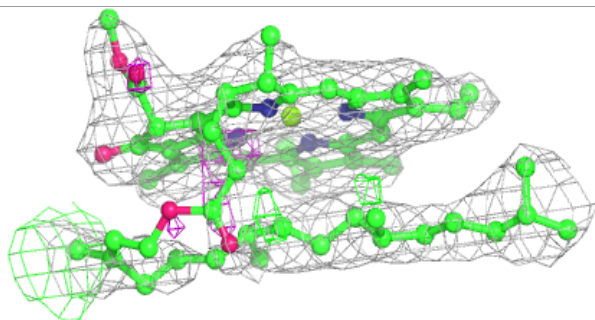
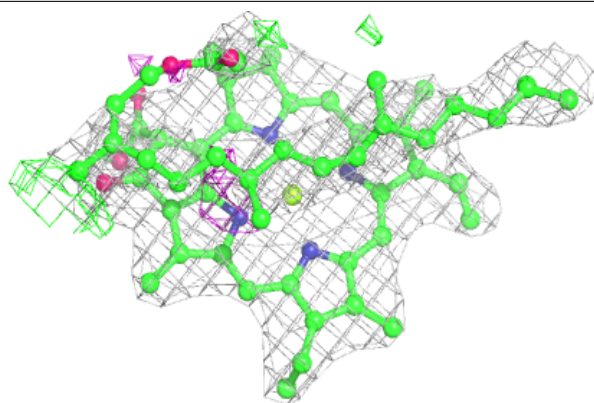
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



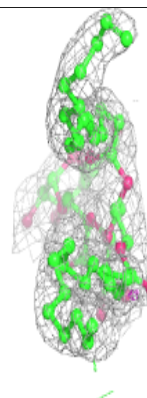
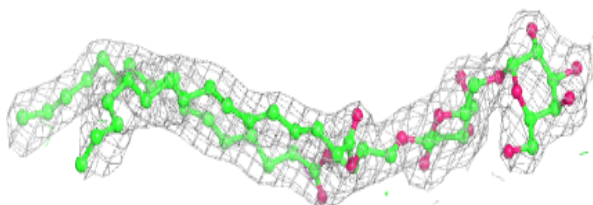
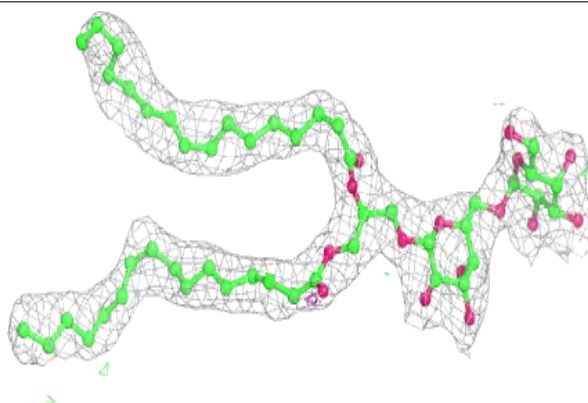


**Electron density around CLA B 602:**

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

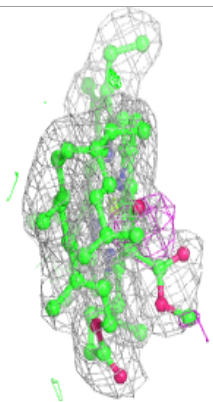
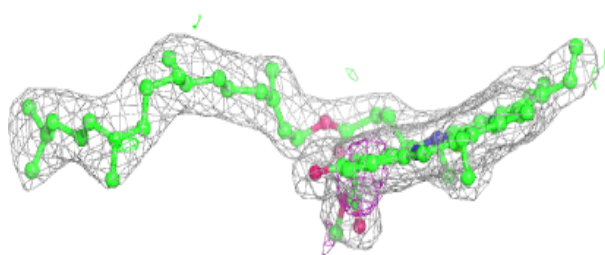
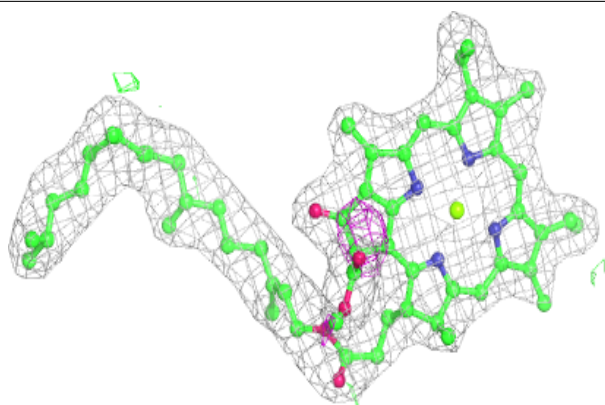
**Electron density around DGD c 918:**

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

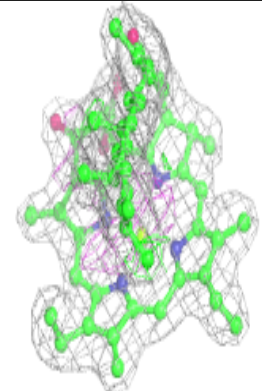
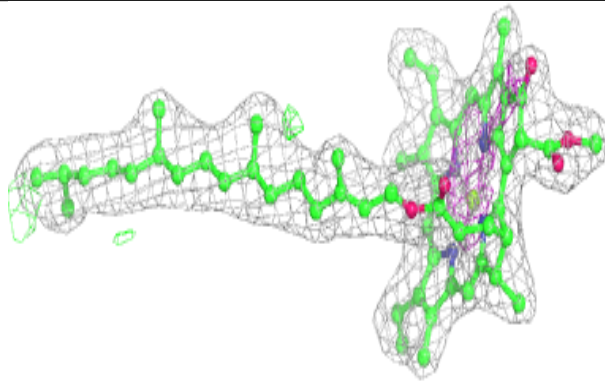
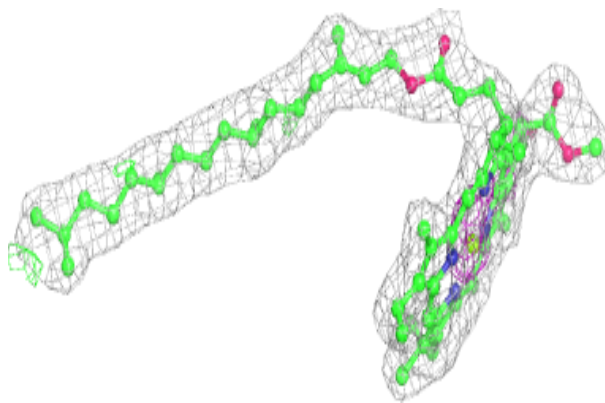


**Electron density around CLA b 607:**

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

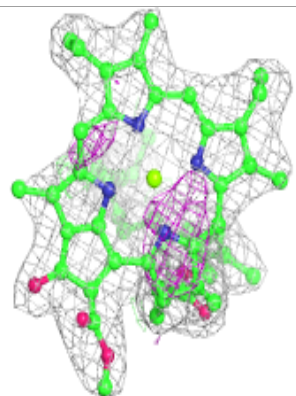
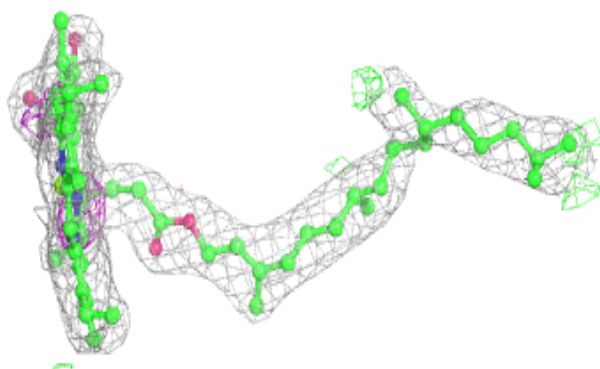
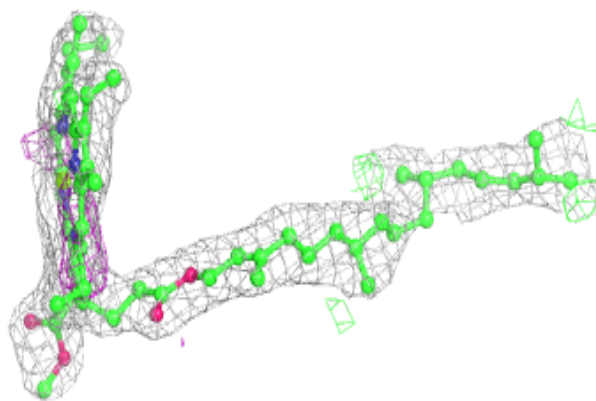
**Electron density around CLA b 612:**

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

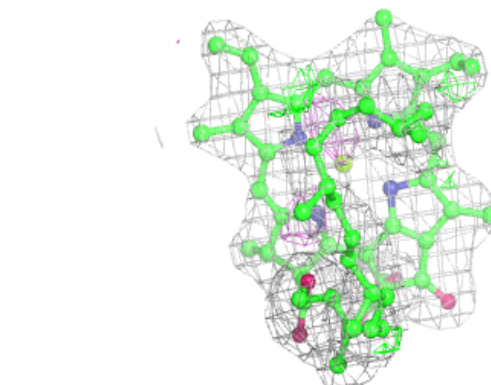
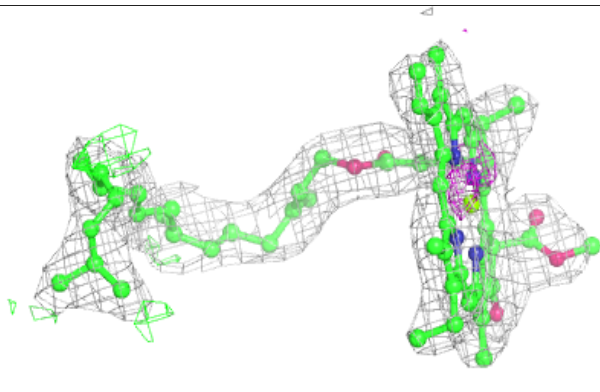
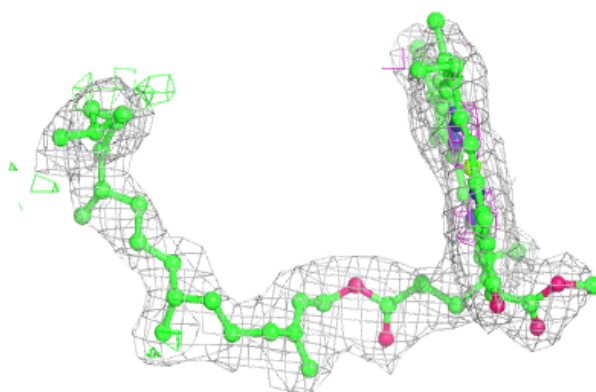


**Electron density around CLA B 607:**

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

**Electron density around CLA c 907:**

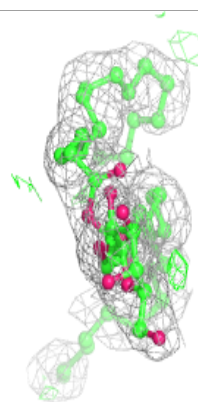
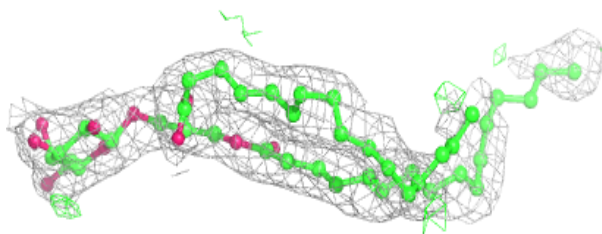
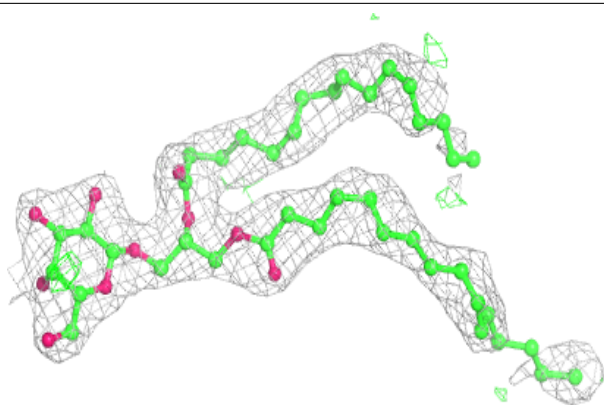
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





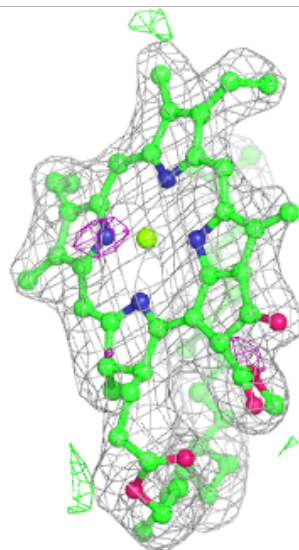
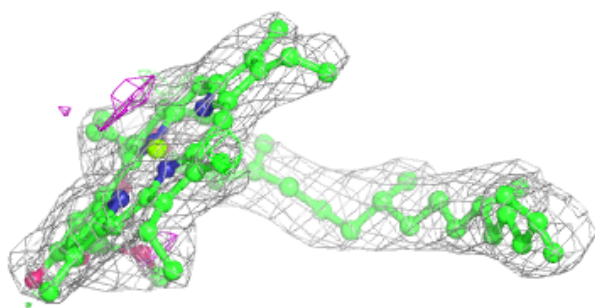
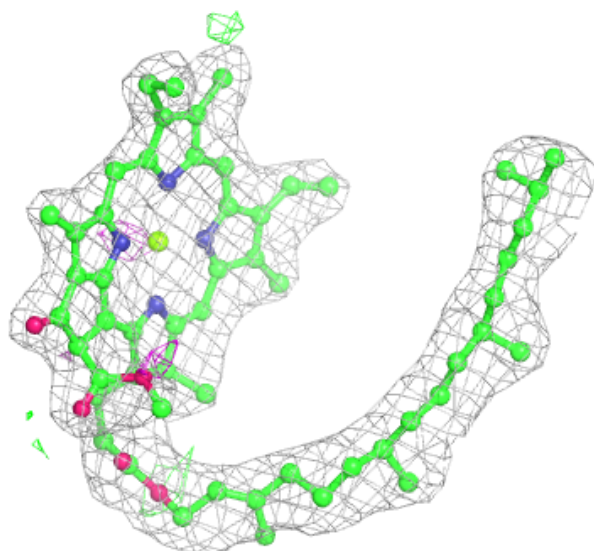
**Electron density around LMG d 415:**

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



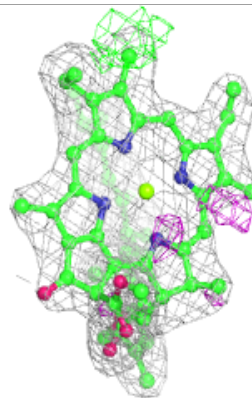
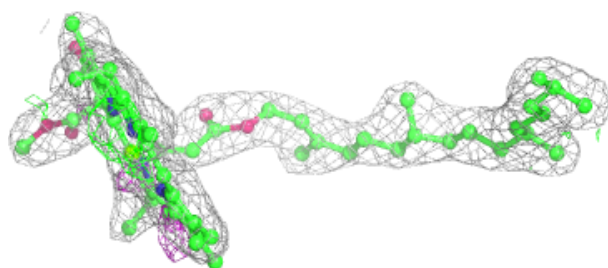
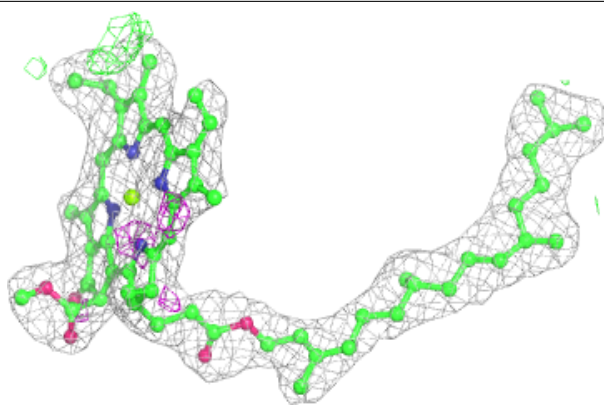
**Electron density around CLA c 908:**

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



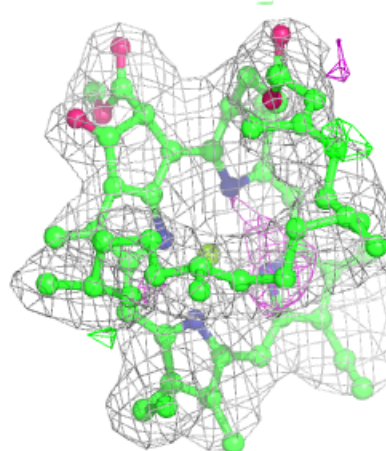
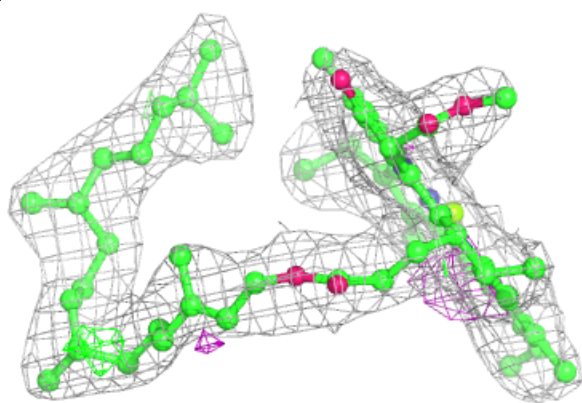
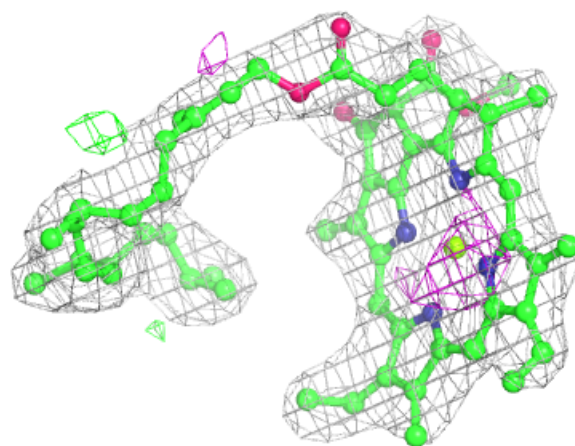
**Electron density around CLA b 614:**

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



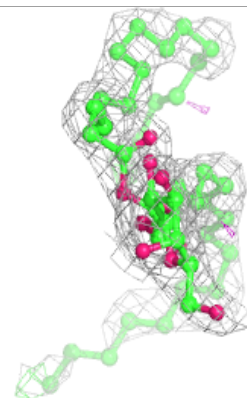
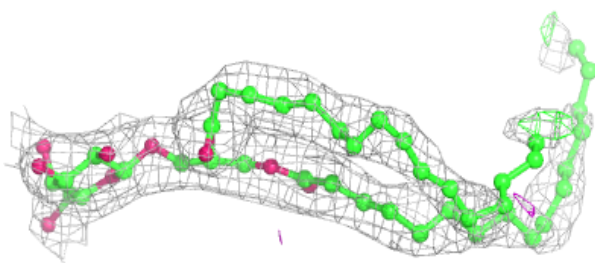
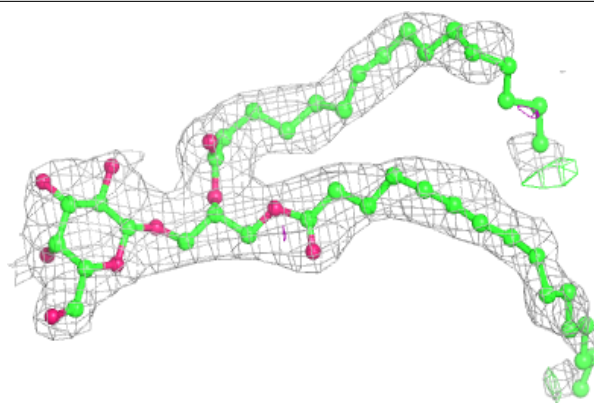
**Electron density around CLA c 904:**

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

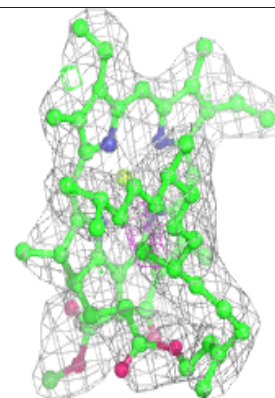
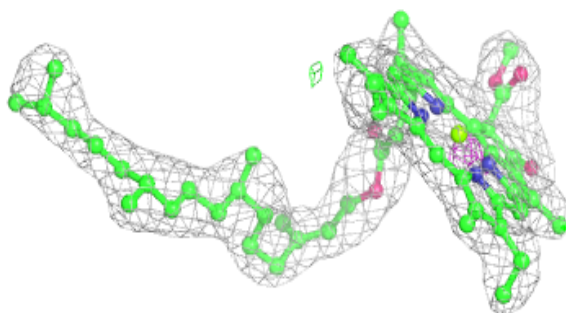
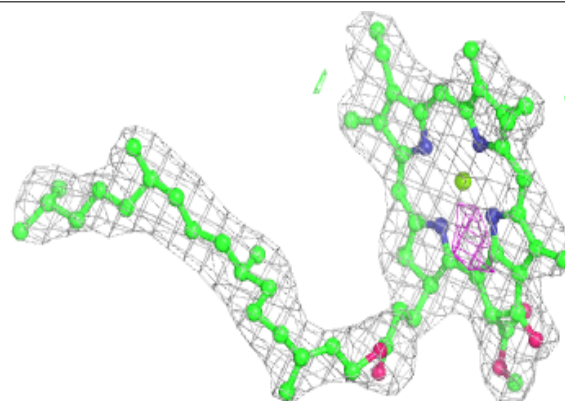


**Electron density around LMG J 101:**

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

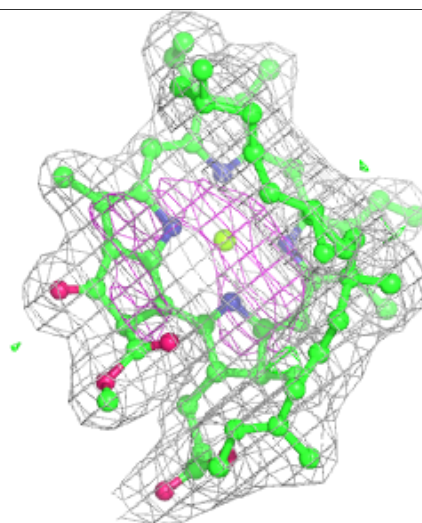
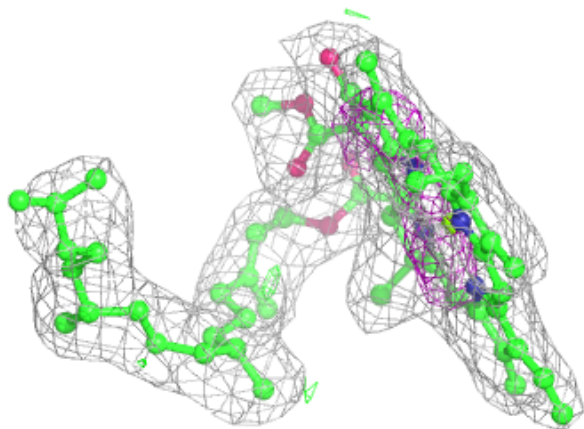
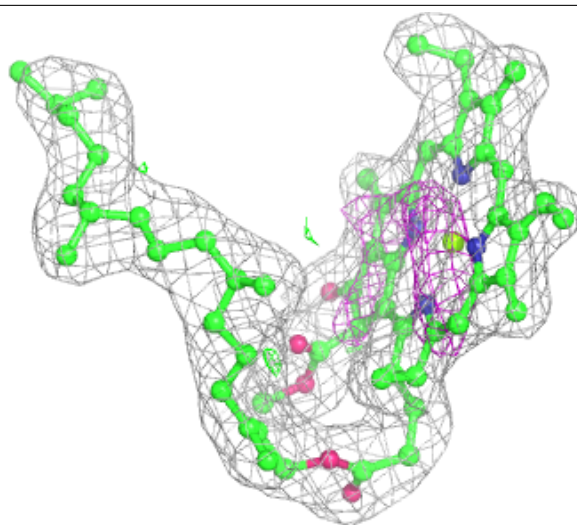
**Electron density around CLA C 511:**

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



**Electron density around CLA B 614:**

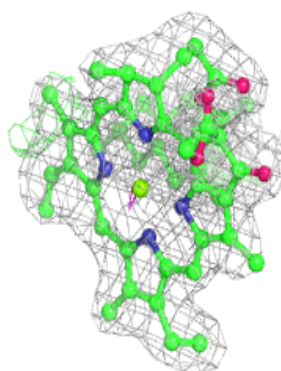
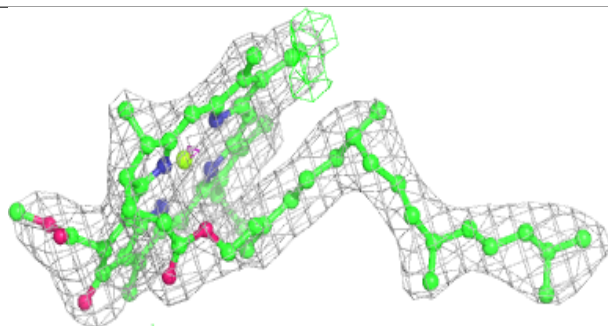
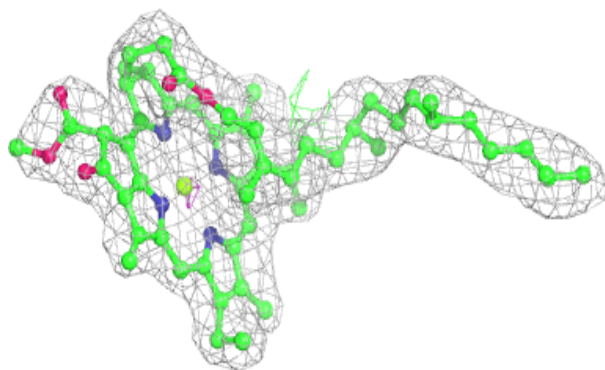
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



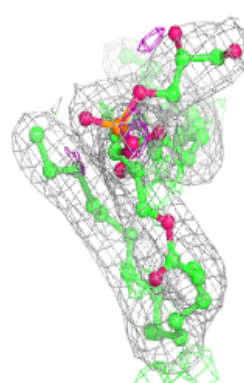
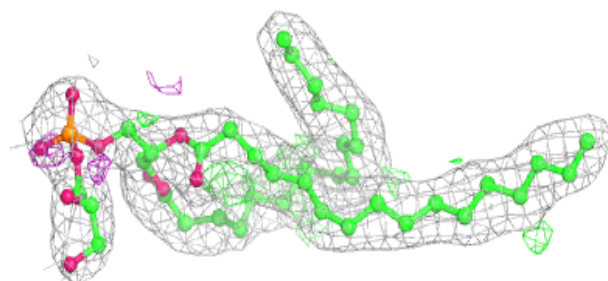
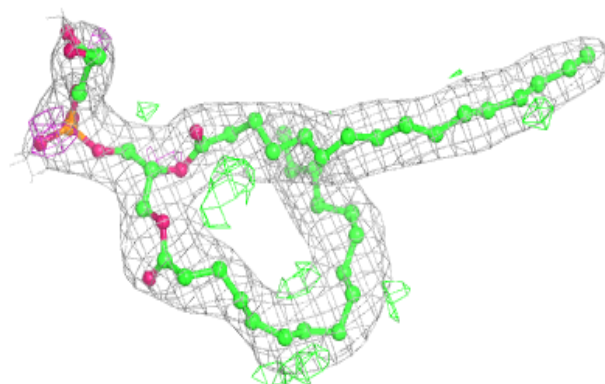


**Electron density around CLA c 906:**

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

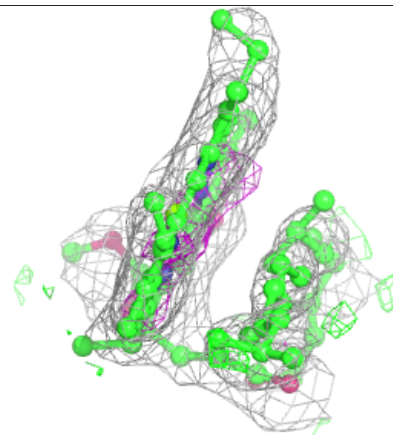
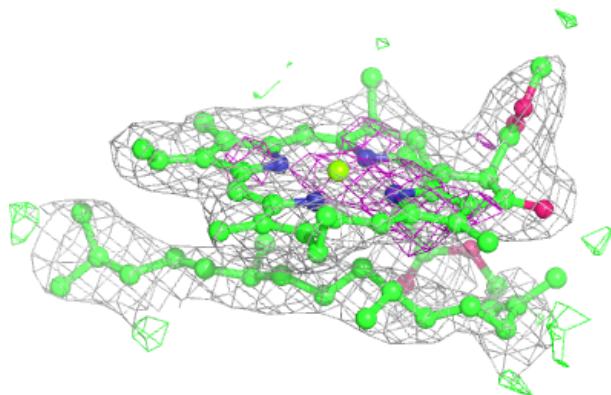
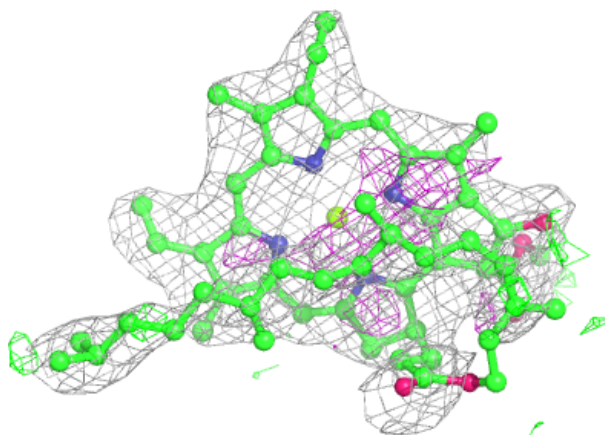
**Electron density around LHG B 635:**

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



**Electron density around CLA b 606:**

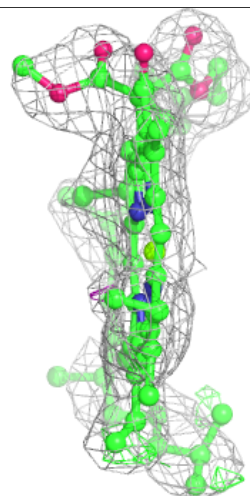
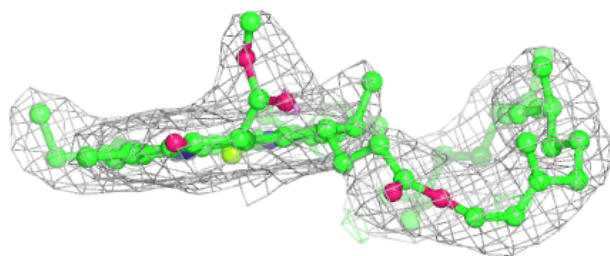
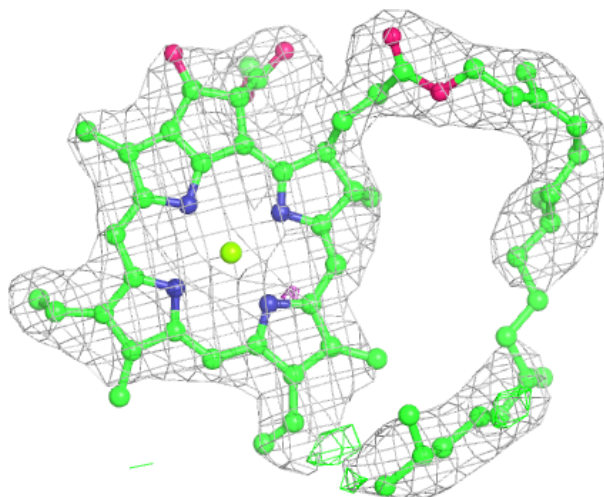
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





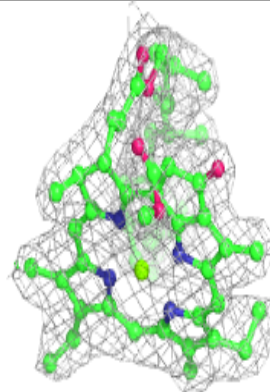
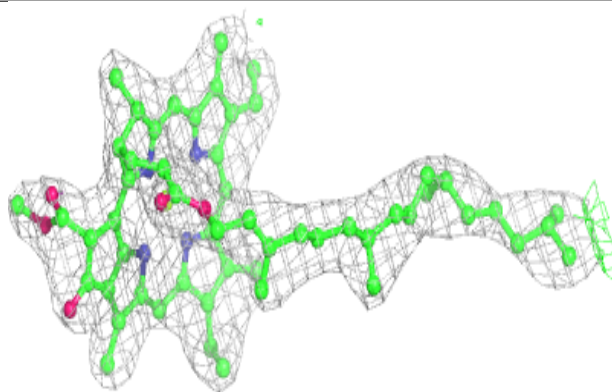
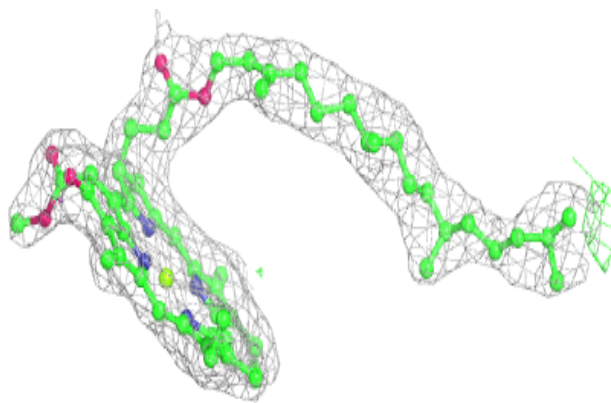
**Electron density around CLA C 512:**

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



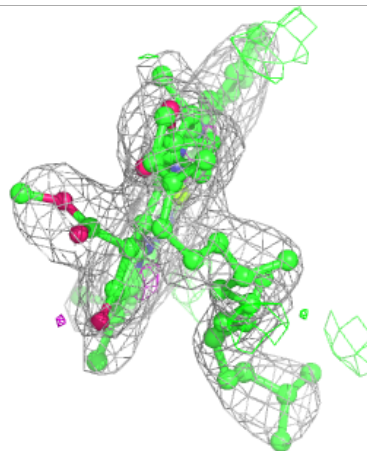
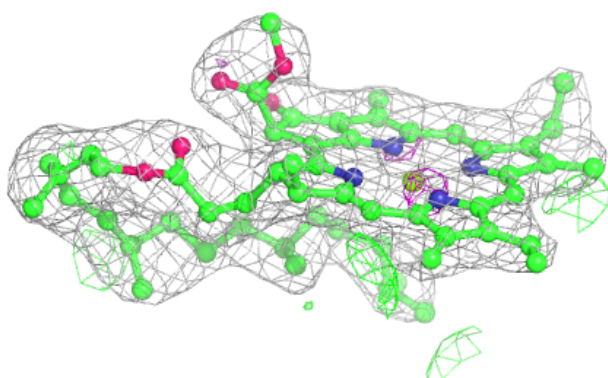
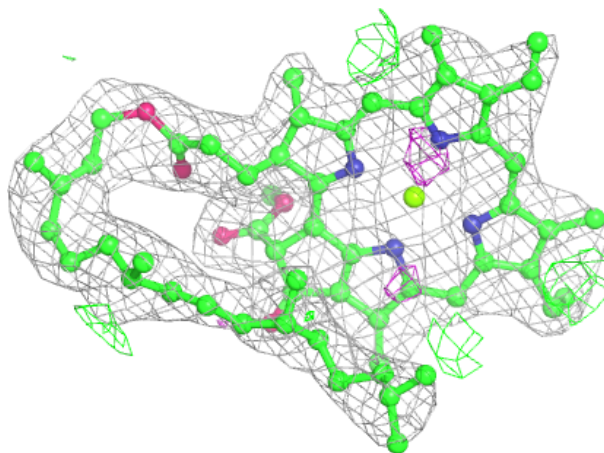
**Electron density around CLA c 905:**

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



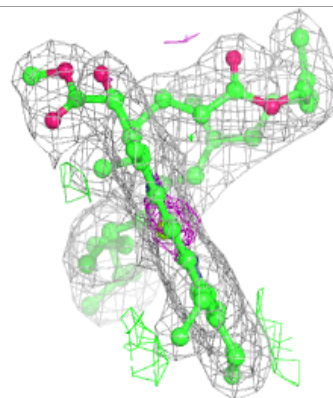
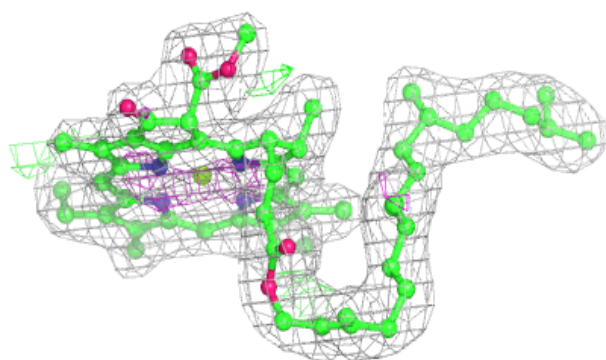
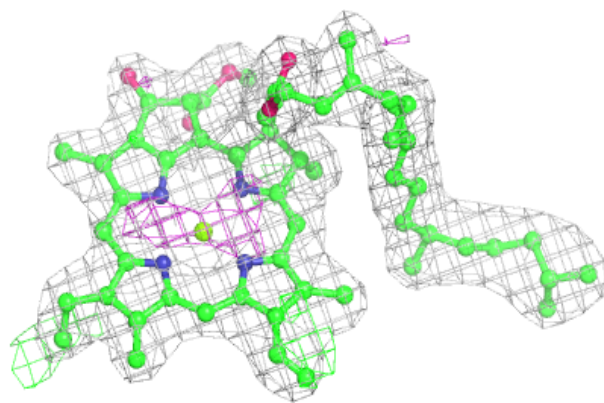
**Electron density around CLA c 910:**

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

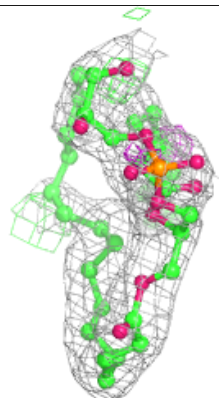
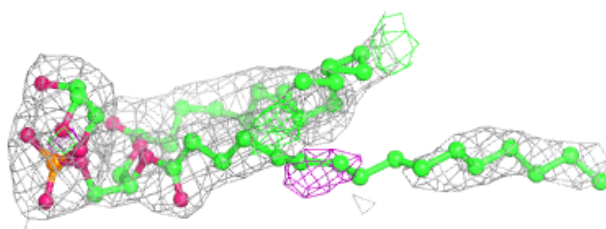
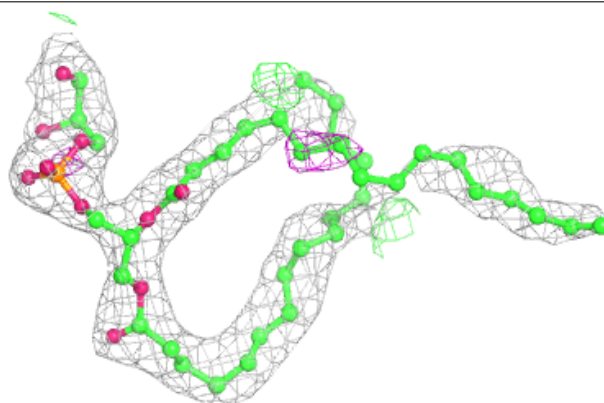


**Electron density around CLA d 404:**

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

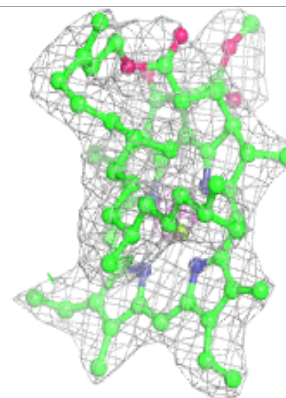
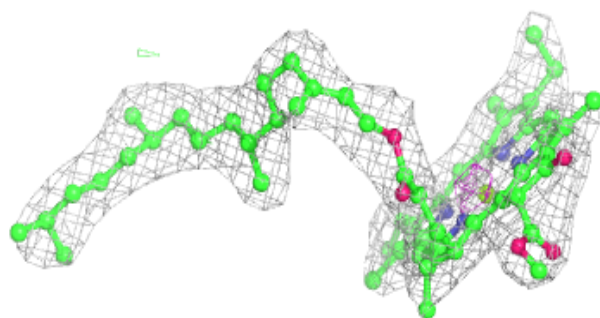
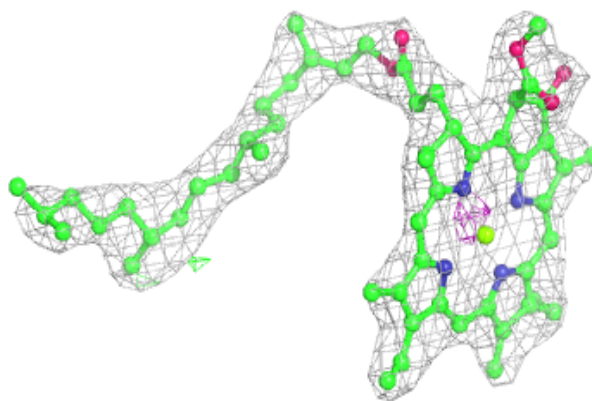
**Electron density around LHG D 410:**

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

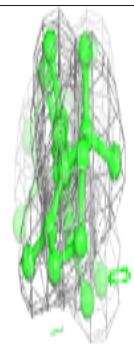
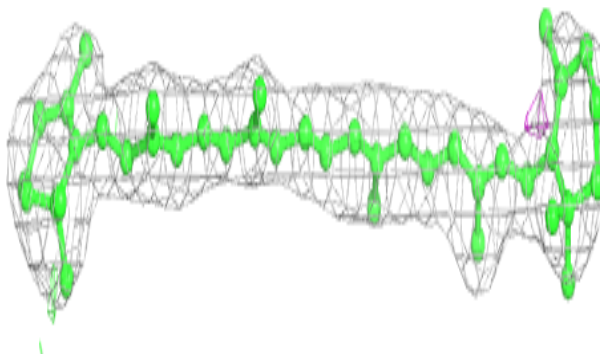
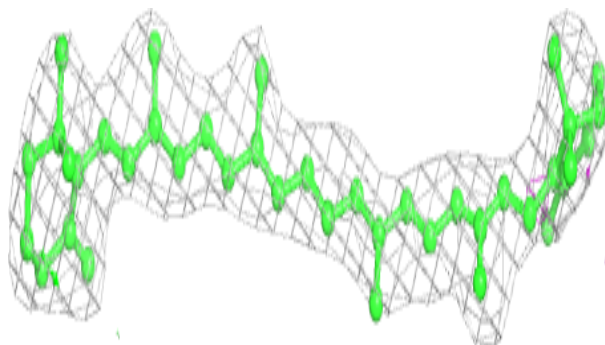


**Electron density around CLA c 912:**

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

**Electron density around BCR C 514:**

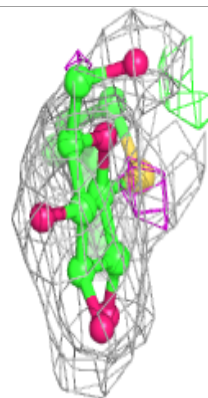
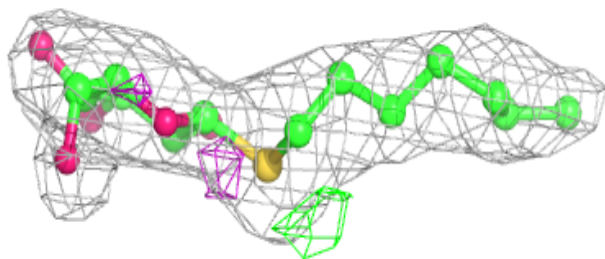
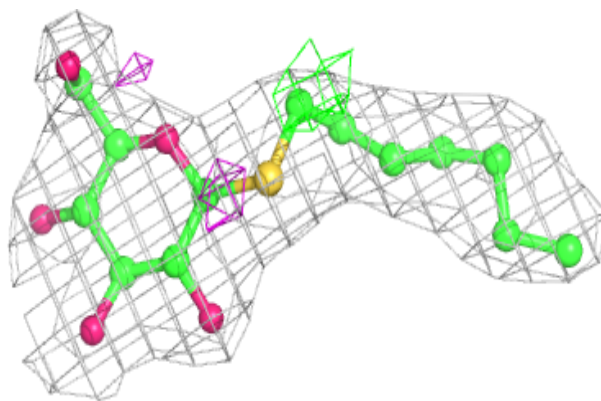
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



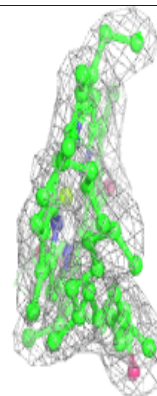
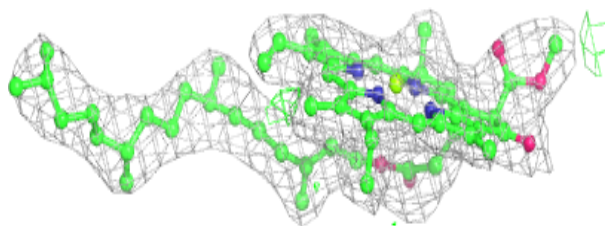
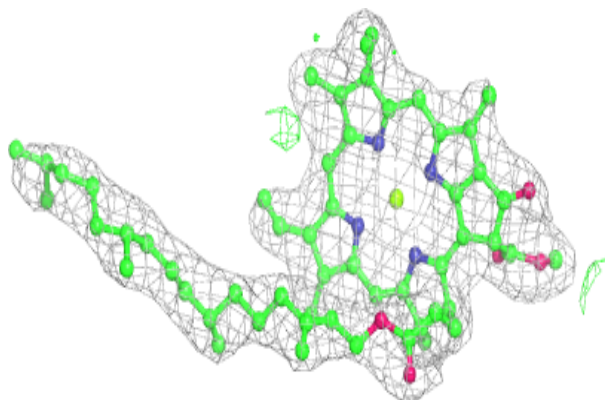


**Electron density around HTG B 623:**

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

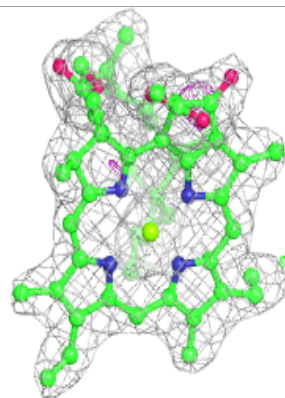
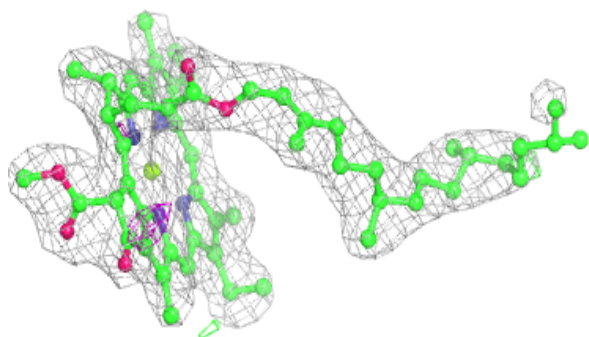
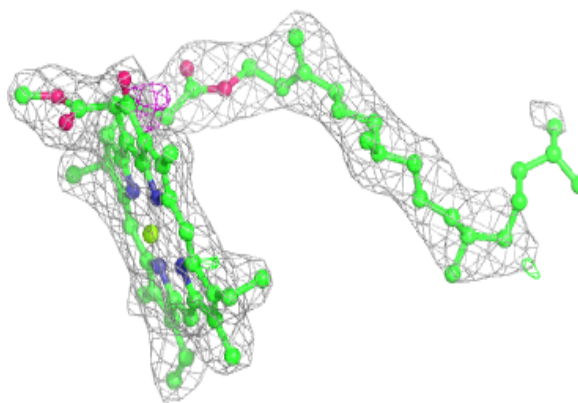
**Electron density around CLA C 501:**

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

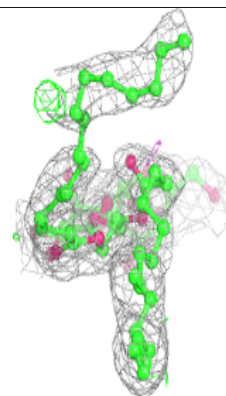
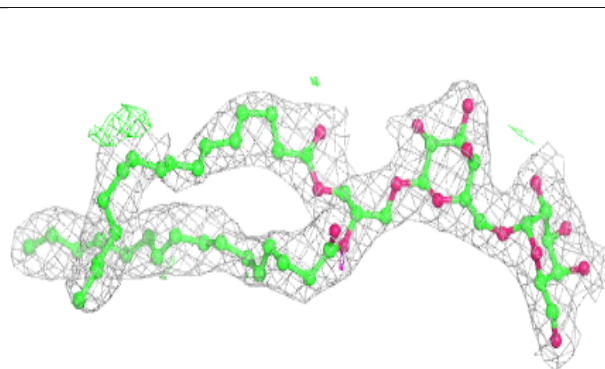
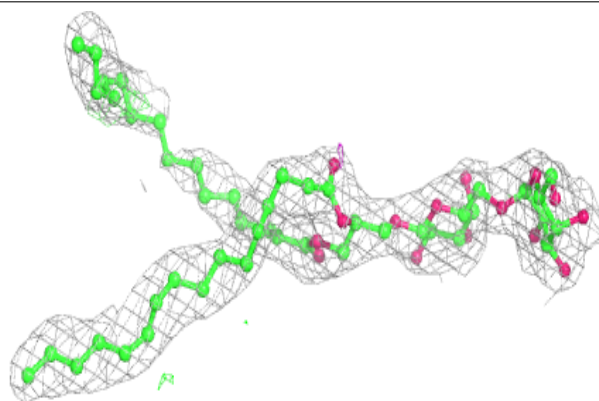


**Electron density around CLA c 909:**

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

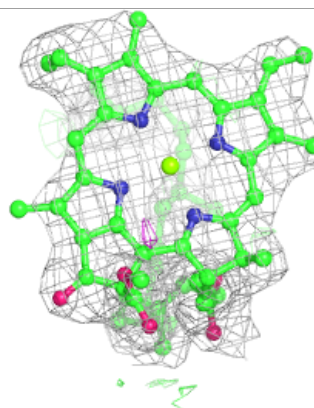
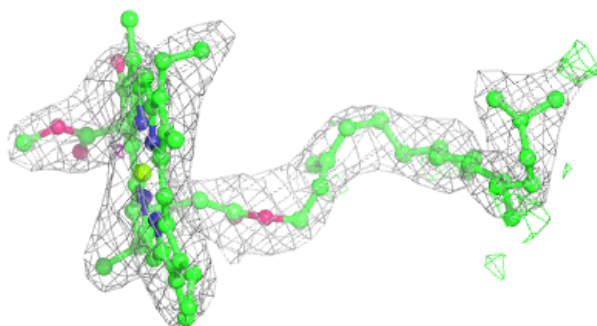
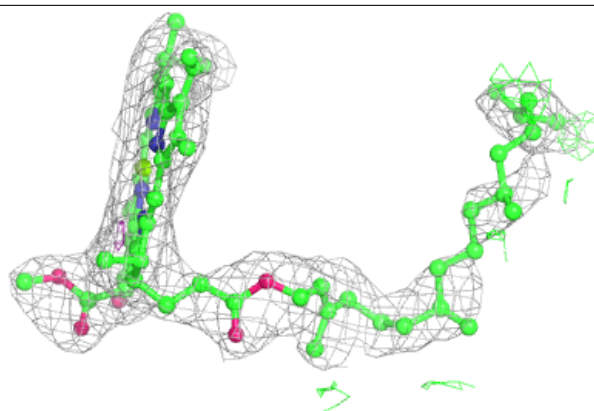
**Electron density around DGD c 916:**

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

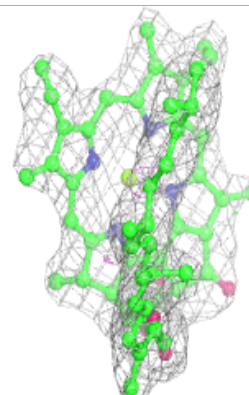
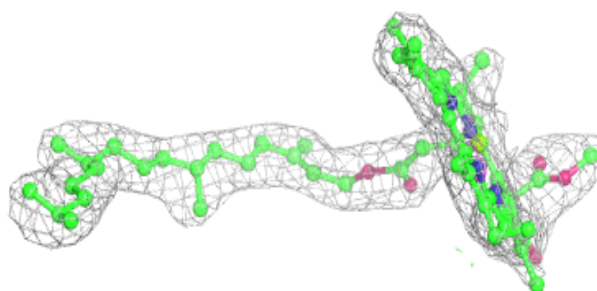
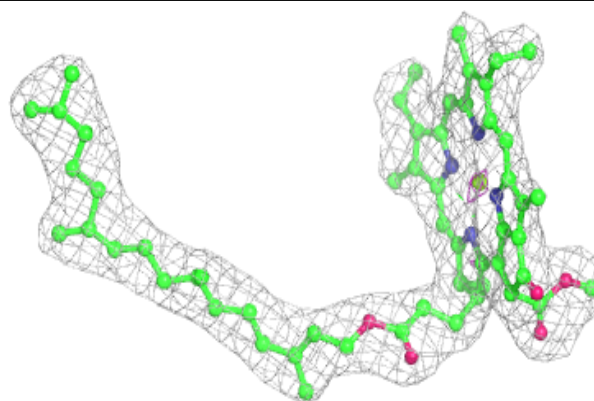


**Electron density around CLA C 506:**

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

**Electron density around CLA B 610:**

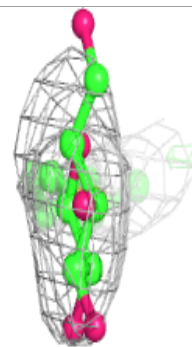
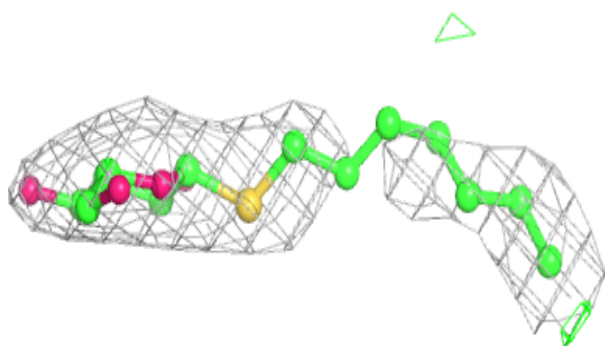
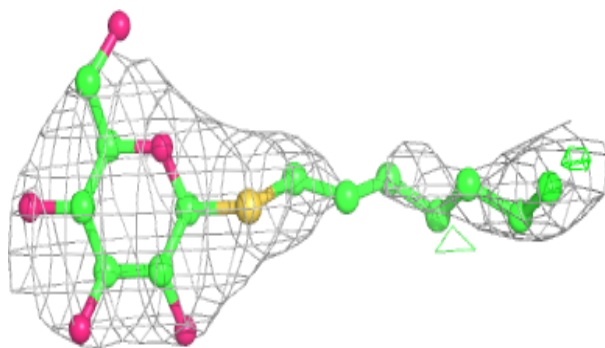
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





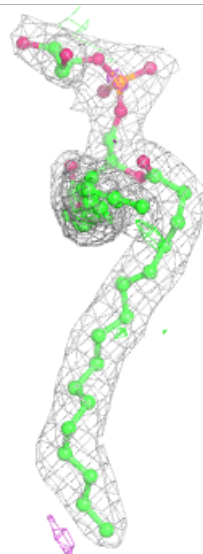
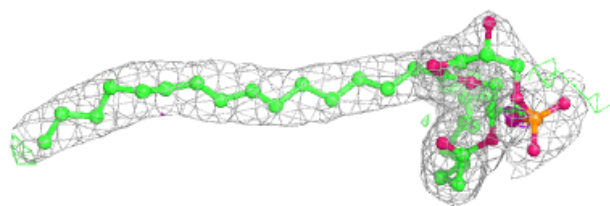
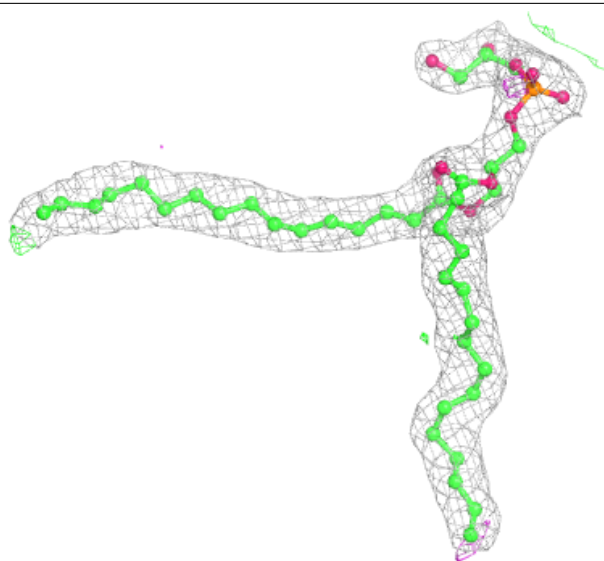
**Electron density around HTG C 521:**

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



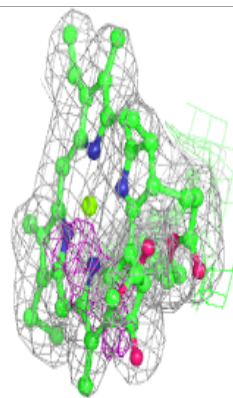
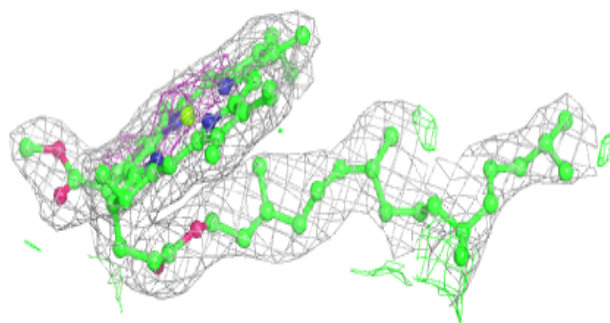
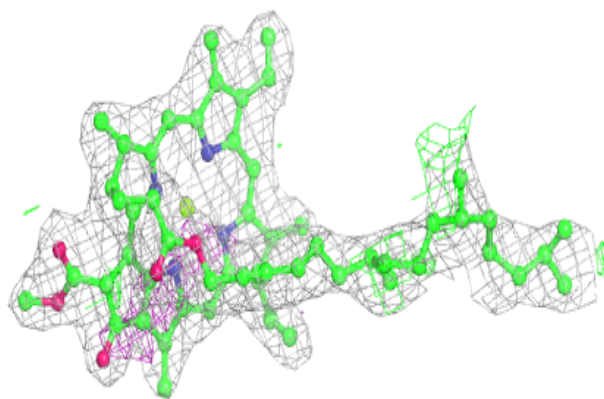
**Electron density around LHG b 635:**

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



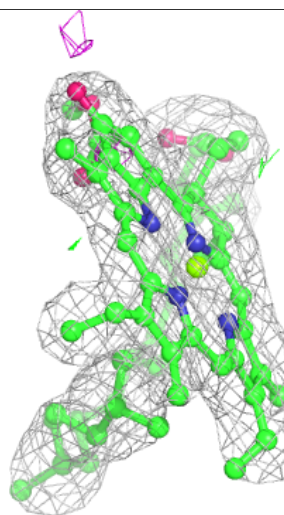
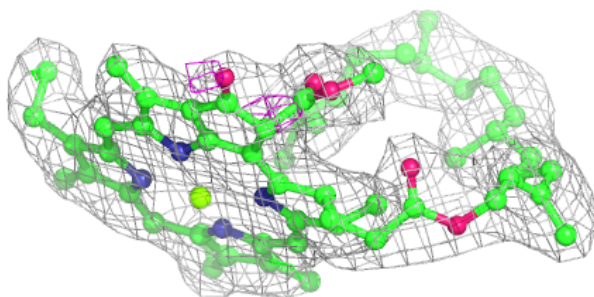
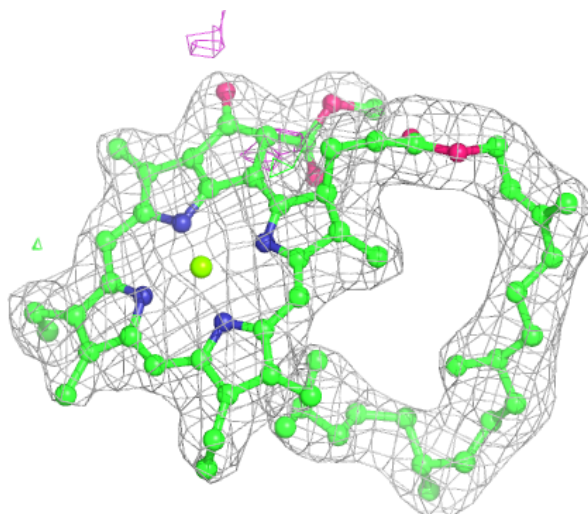
**Electron density around CLA b 619:**

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



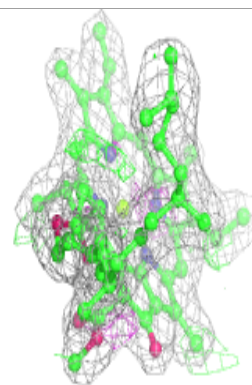
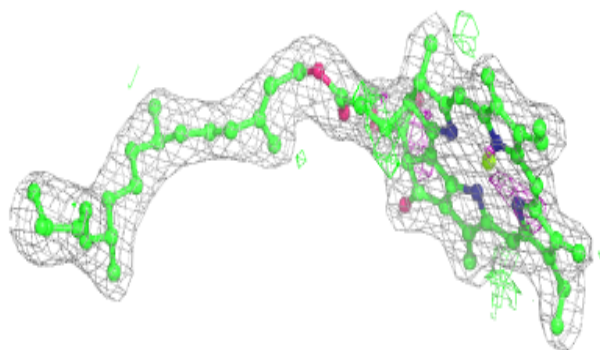
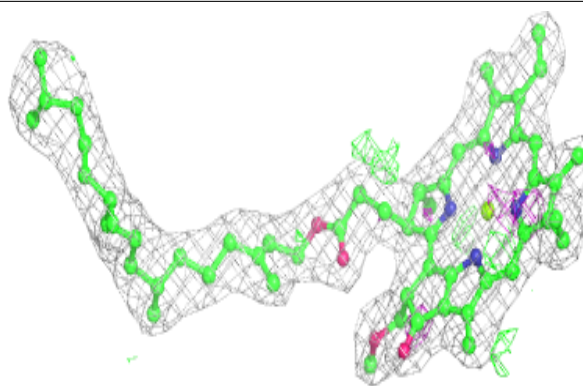
**Electron density around CLA B 616:**

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



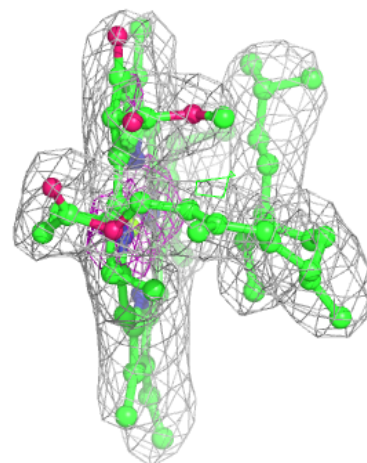
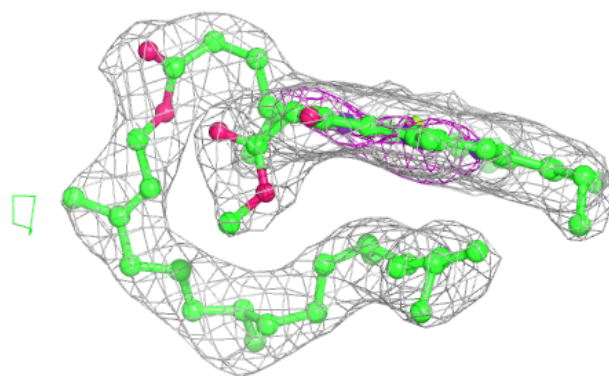
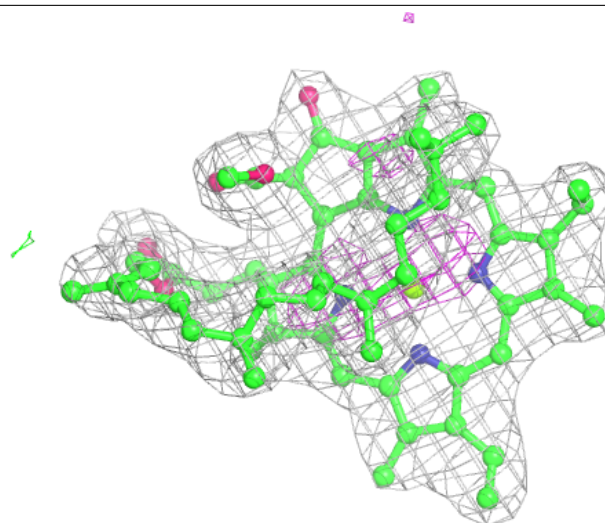
**Electron density around CLA A 405:**

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



**Electron density around CLA c 911:**

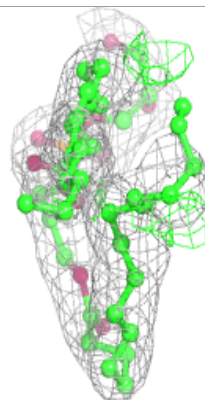
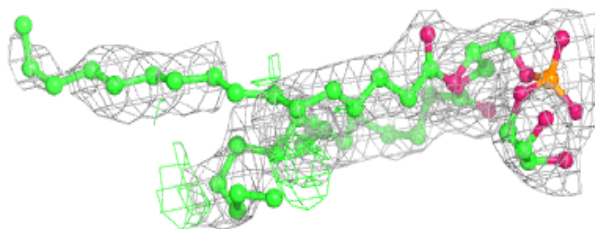
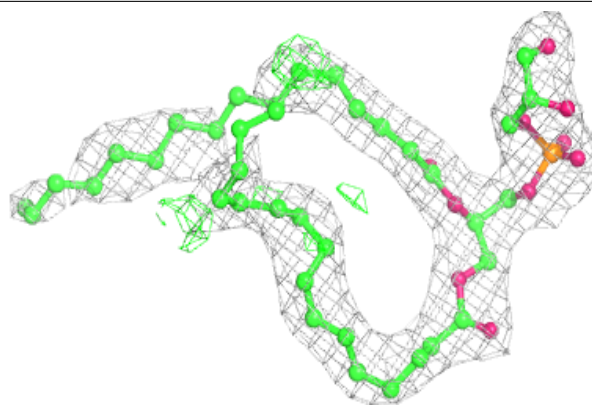
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



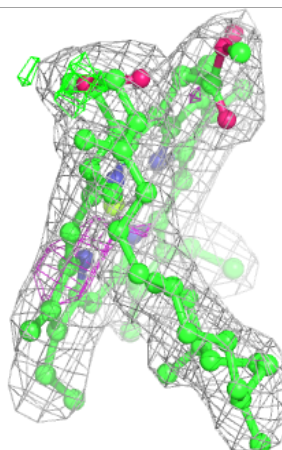
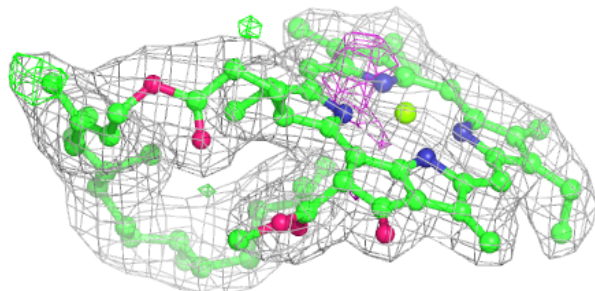
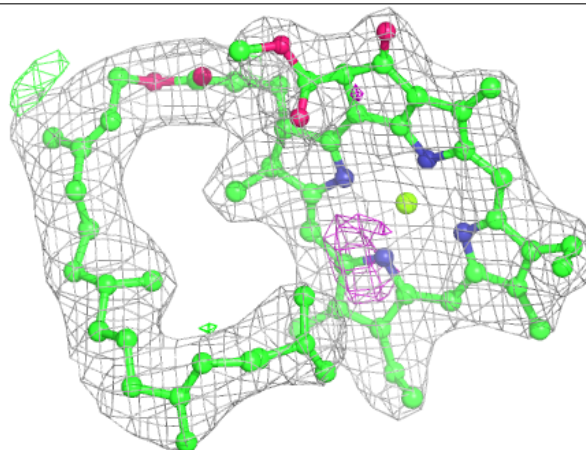


**Electron density around LHG d 411:**

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

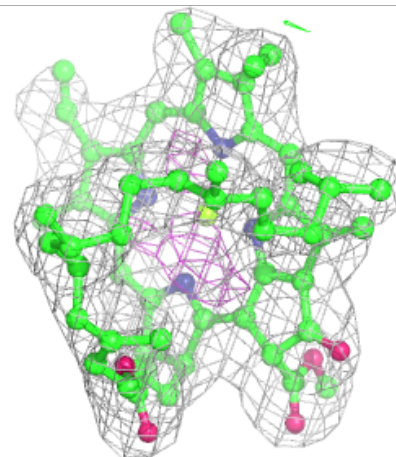
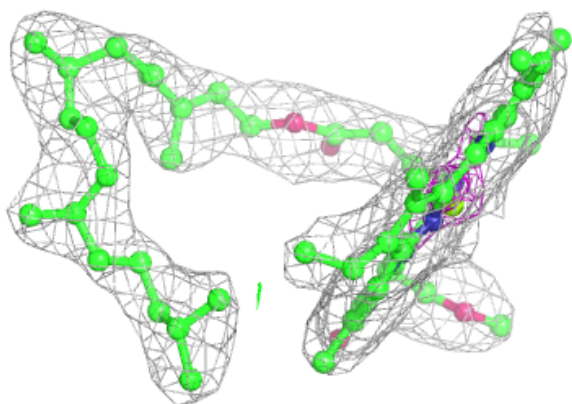
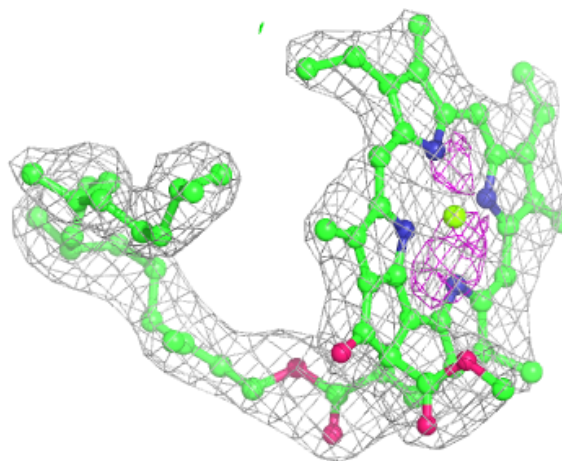
**Electron density around CLA b 620:**

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



**Electron density around CLA C 503:**

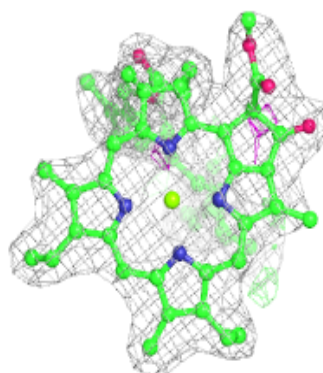
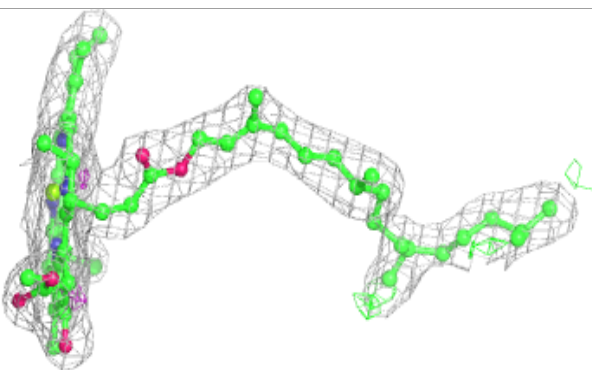
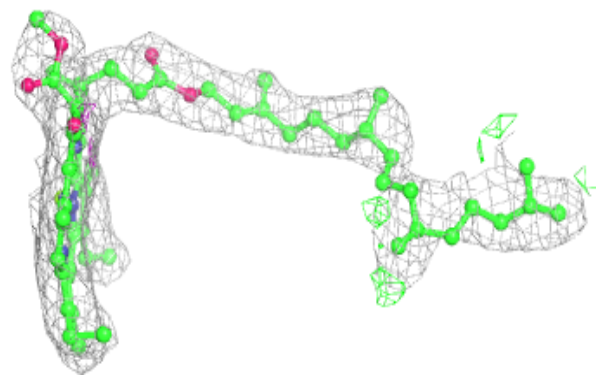
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



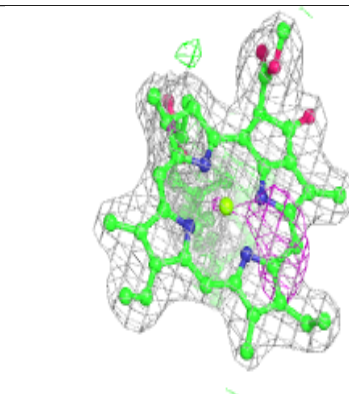
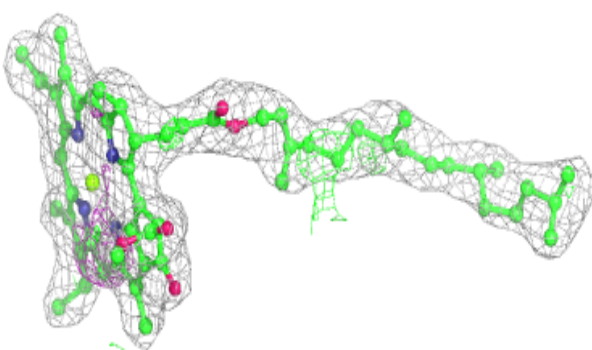
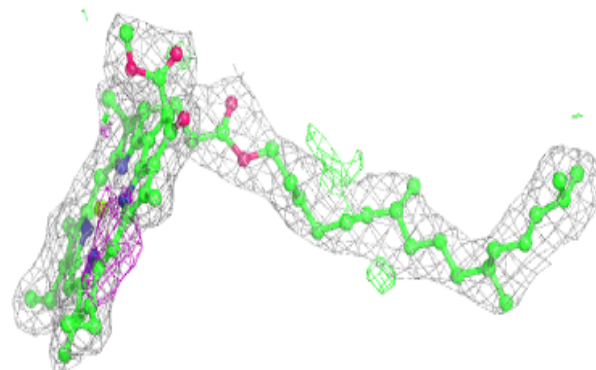


**Electron density around CLA b 611:**

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

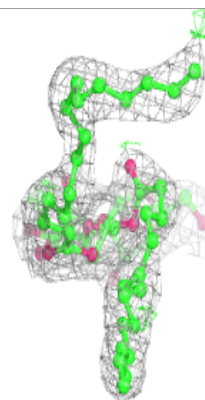
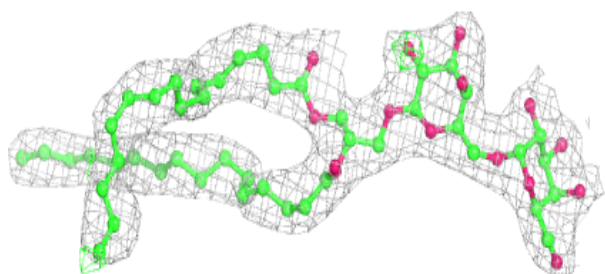
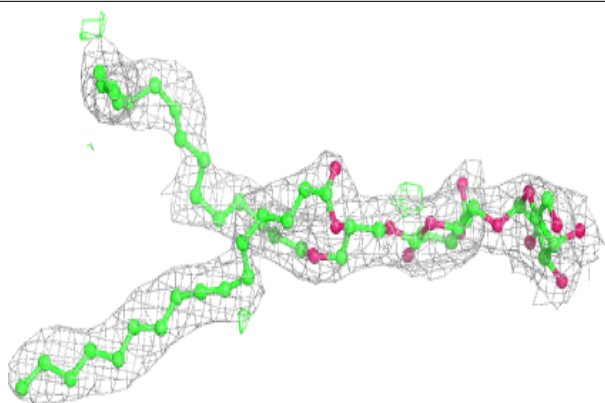
**Electron density around CLA B 605:**

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

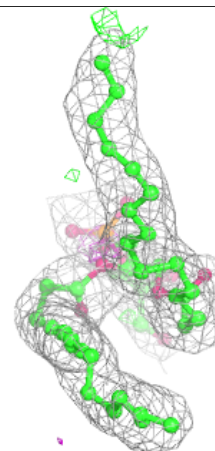
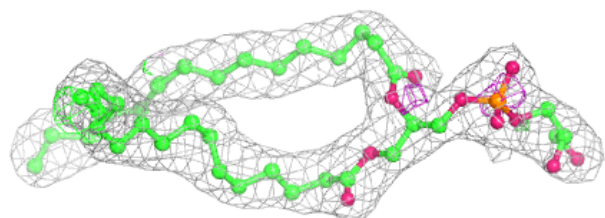
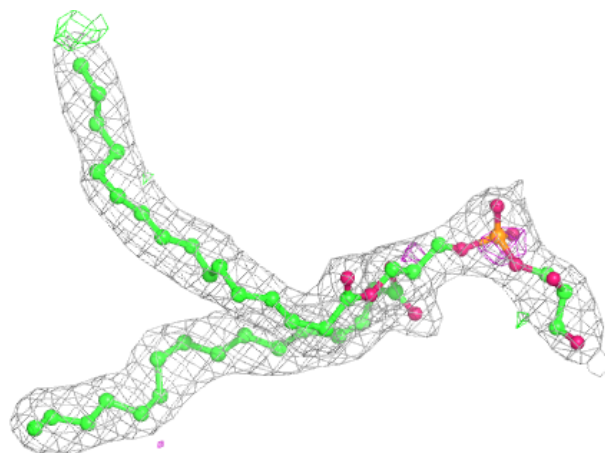


**Electron density around DGD C 516:**

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

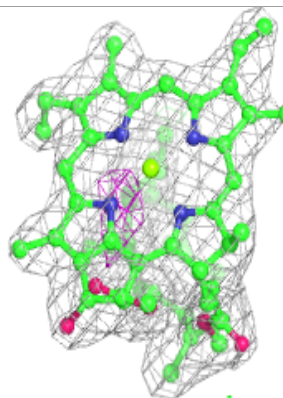
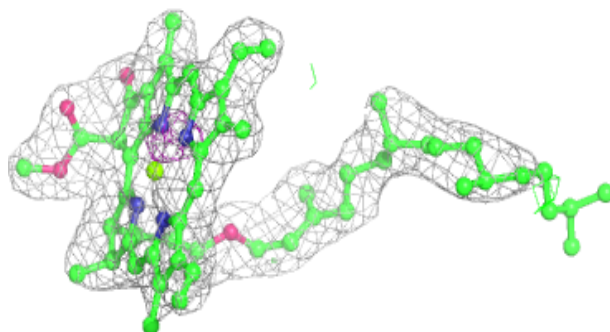
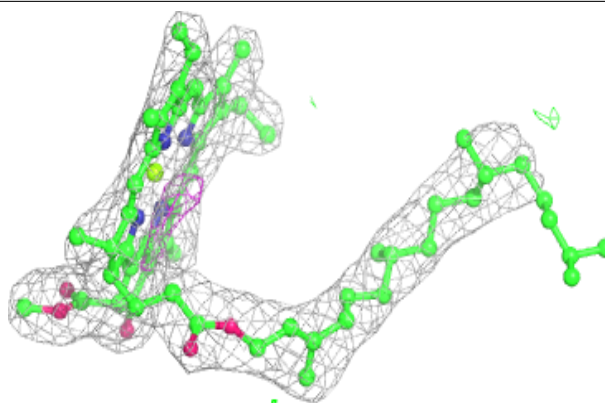
**Electron density around LHG d 410:**

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

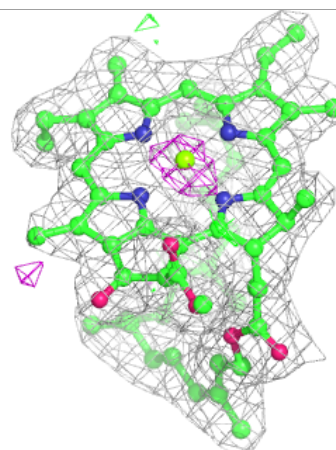
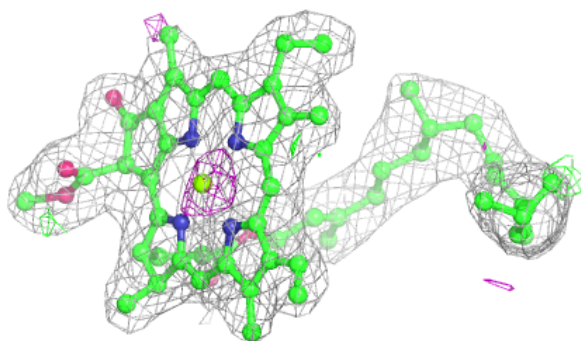
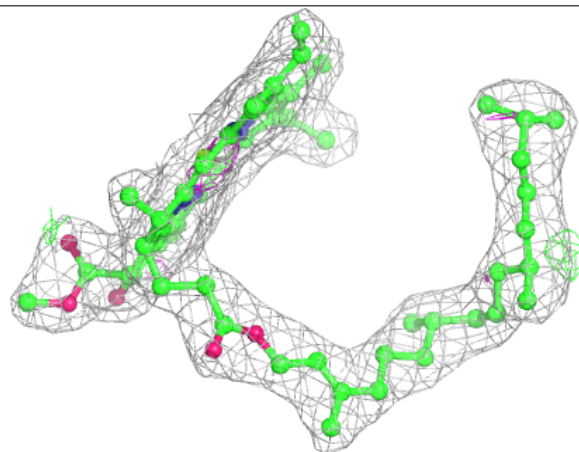


**Electron density around CLA C 508:**

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

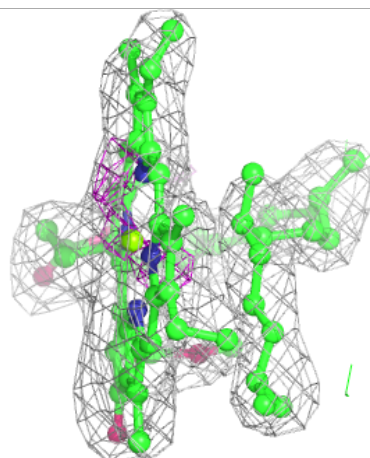
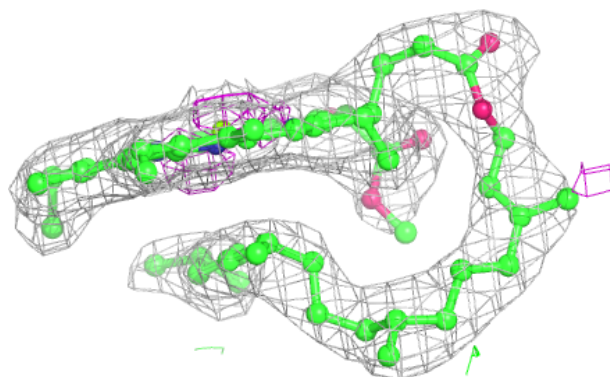
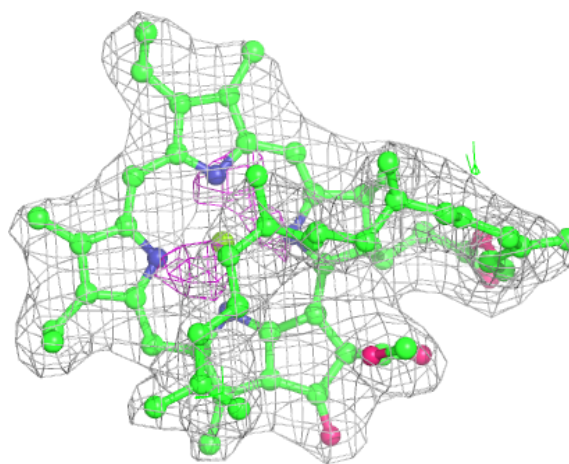
**Electron density around CLA b 616:**

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



**Electron density around CLA C 510:**

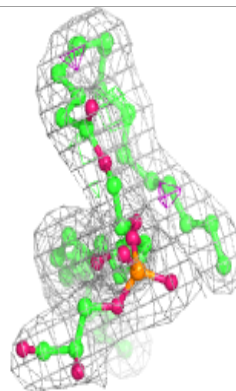
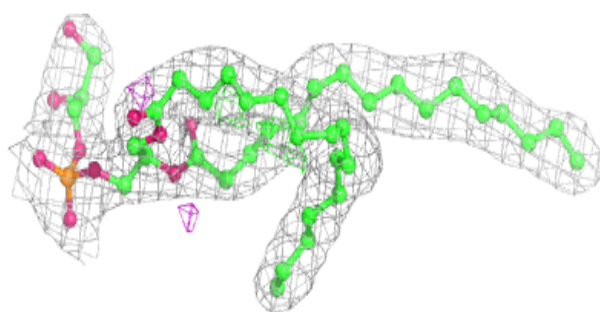
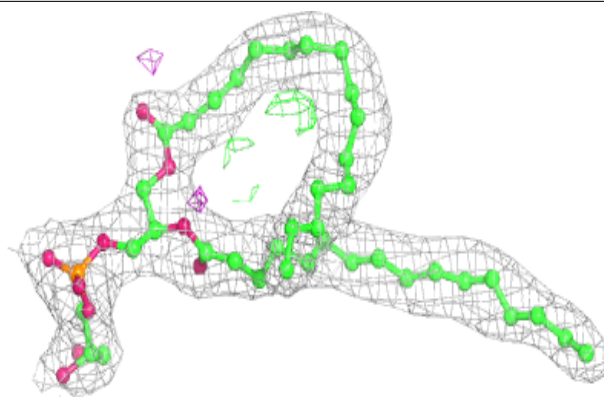
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



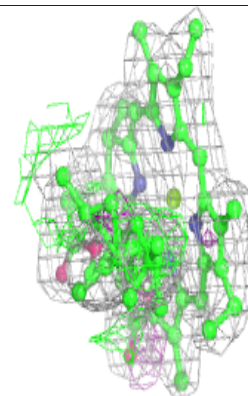
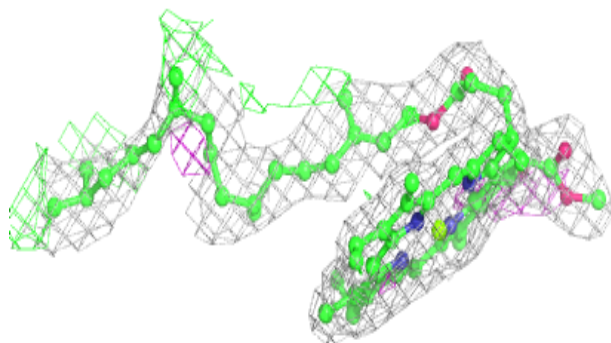
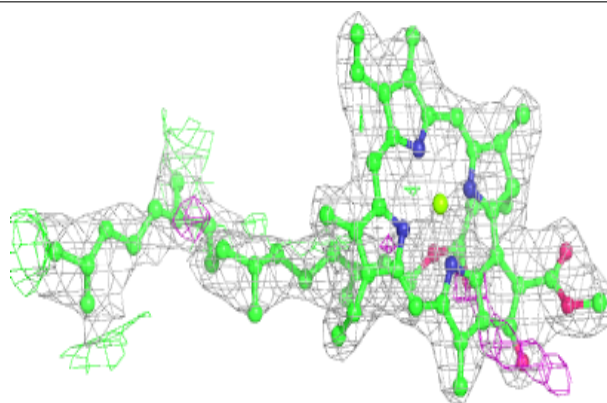


**Electron density around LHG d 409:**

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

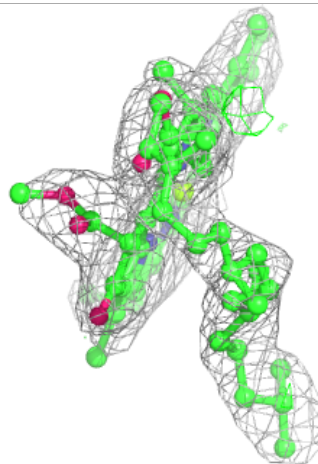
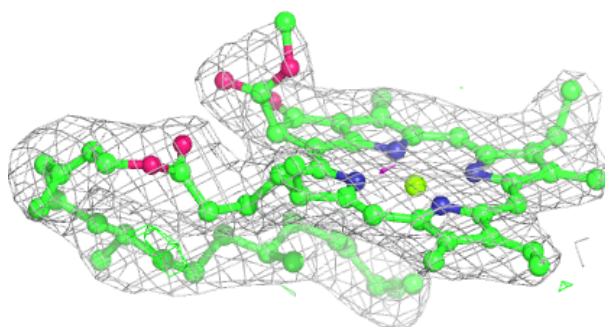
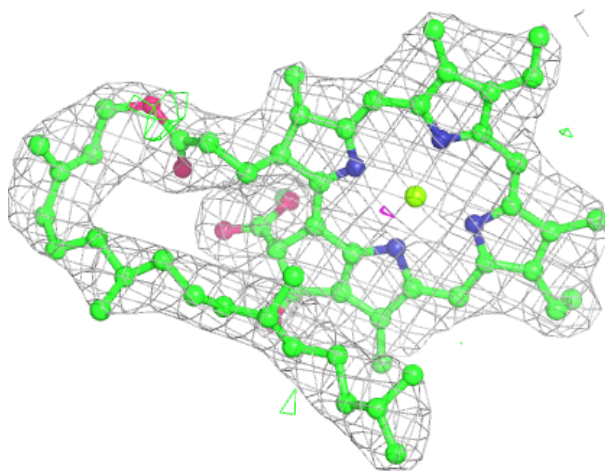
**Electron density around CLA B 615:**

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



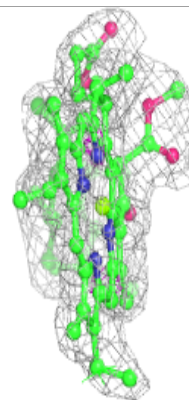
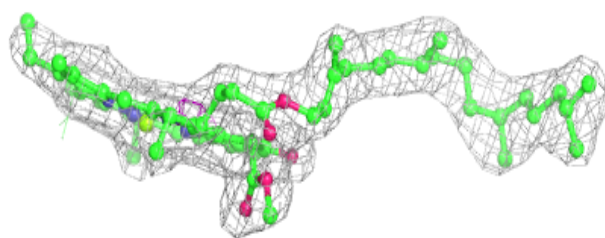
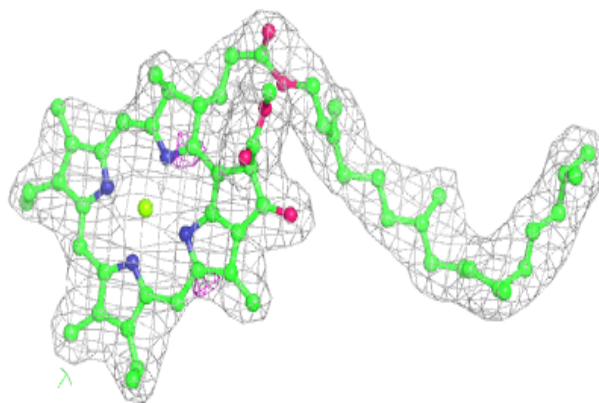
**Electron density around CLA C 509:**

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

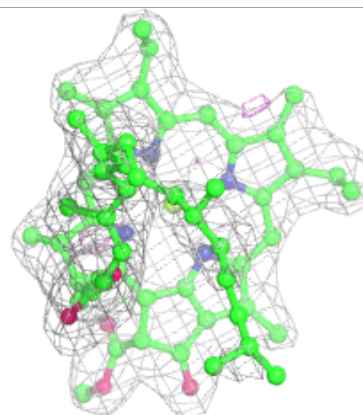
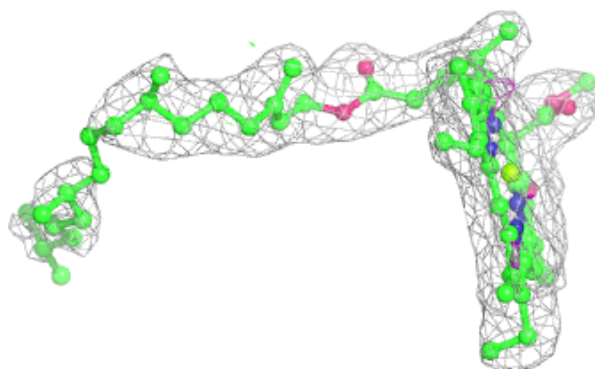
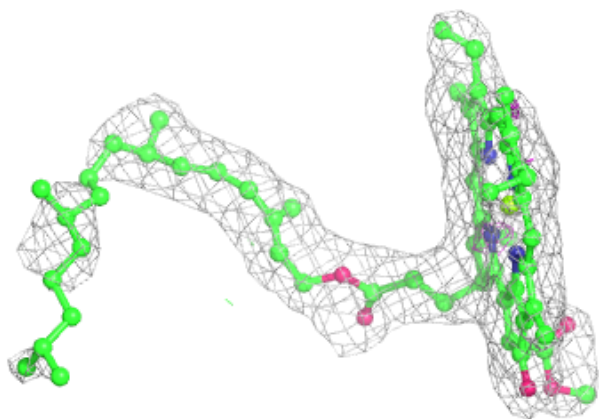


**Electron density around CLA B 603:**

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

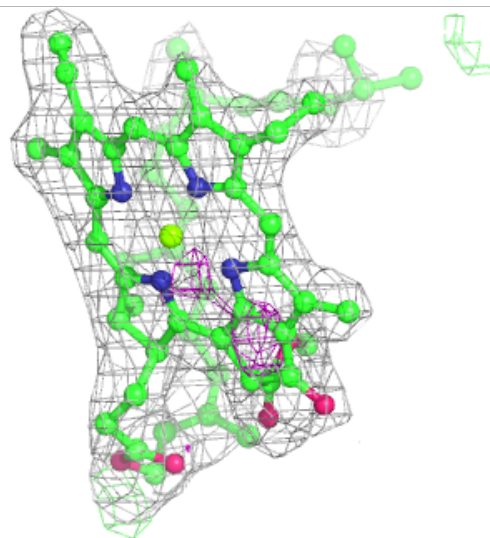
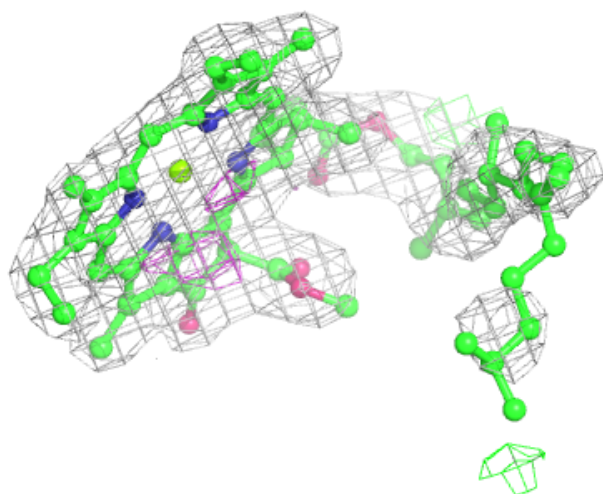
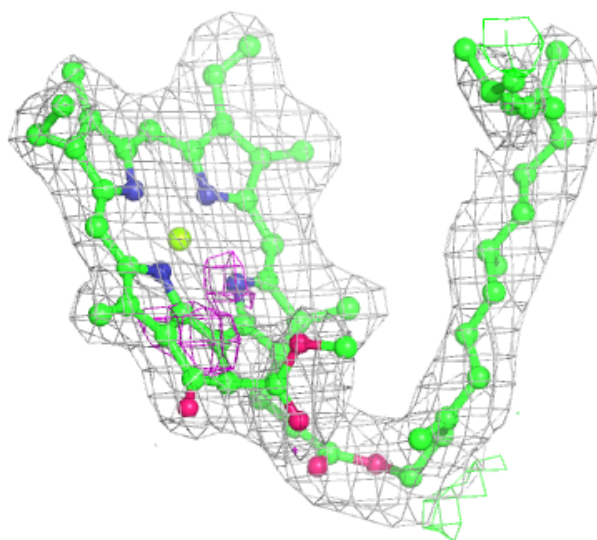
**Electron density around CLA D 405:**

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



**Electron density around CLA b 621:**

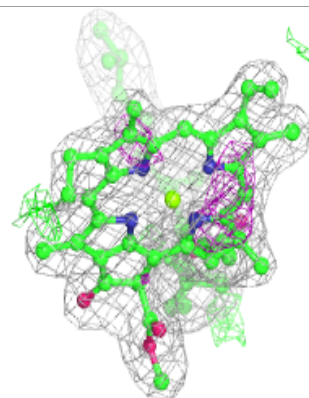
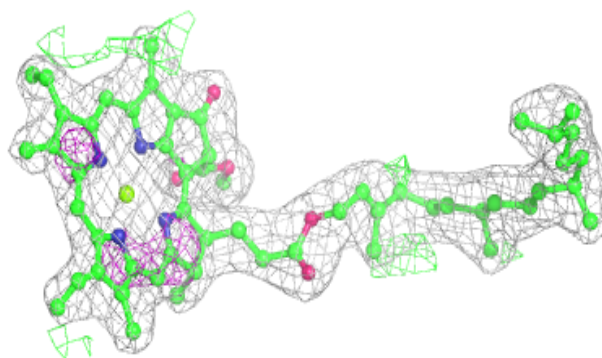
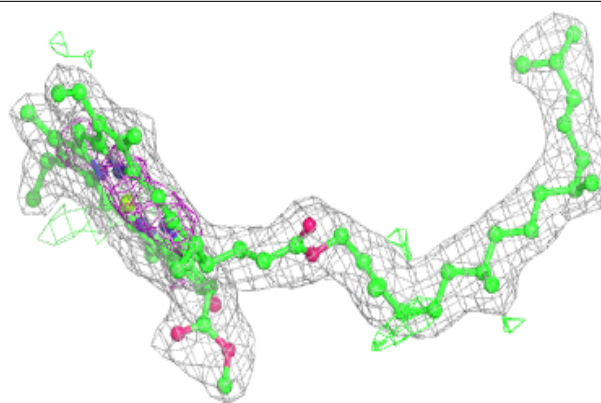
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





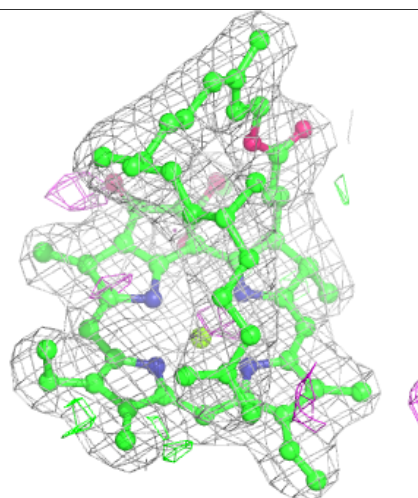
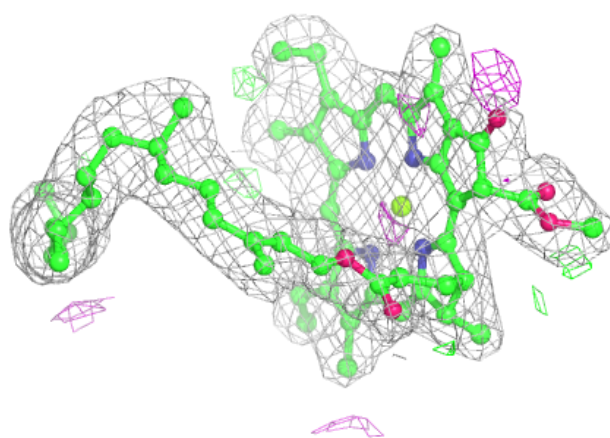
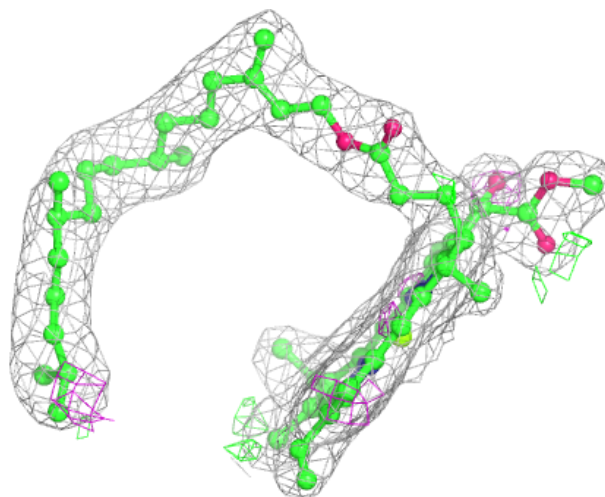
**Electron density around CLA D 404:**

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



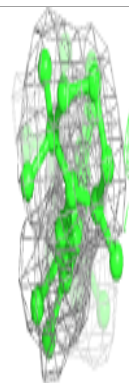
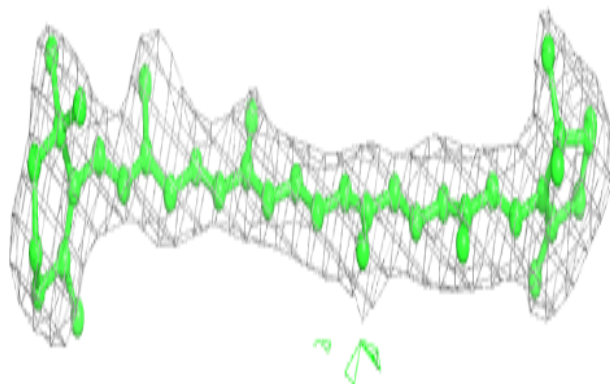
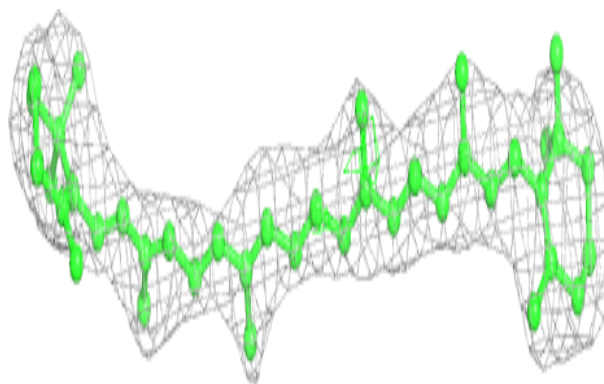
**Electron density around CLA B 612:**

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

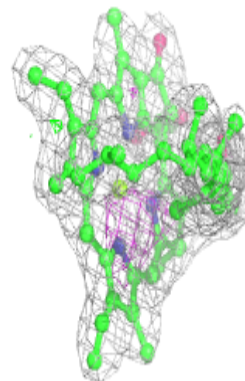
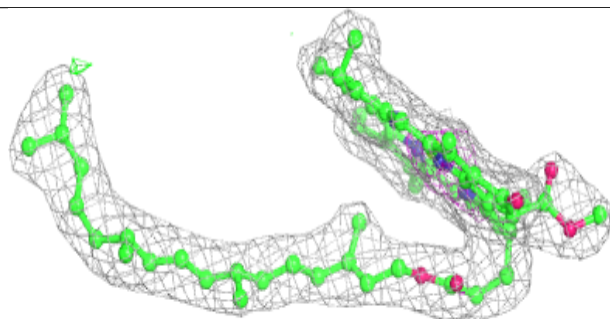
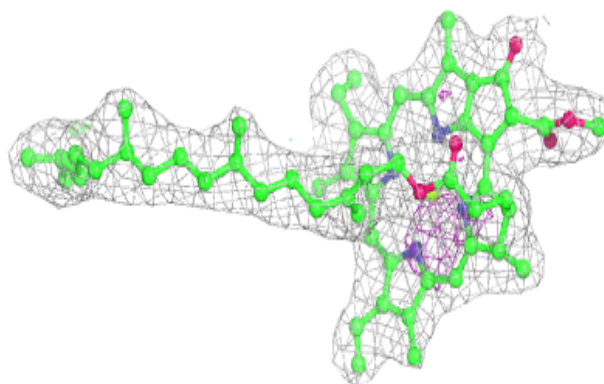


**Electron density around BCR c 927:**

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

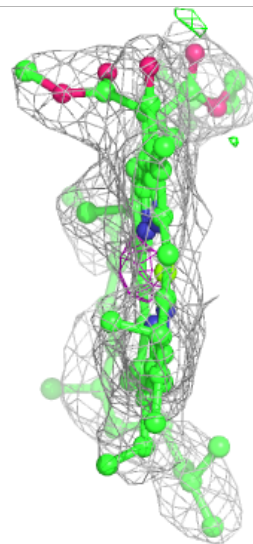
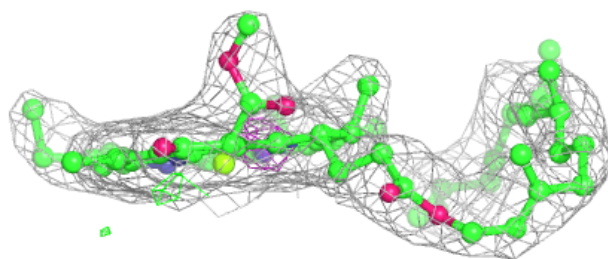
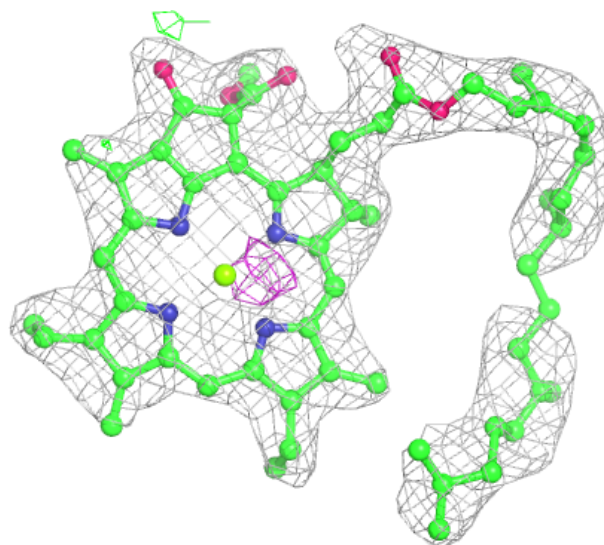
**Electron density around CLA b 613:**

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



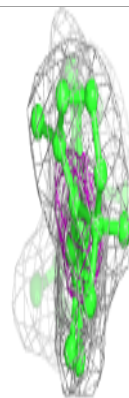
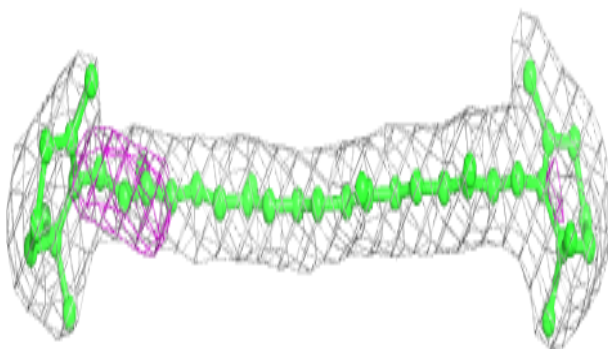
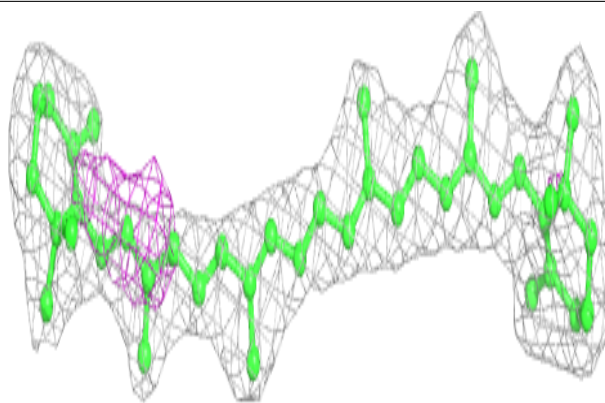
**Electron density around CLA c 913:**

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

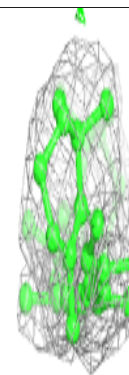
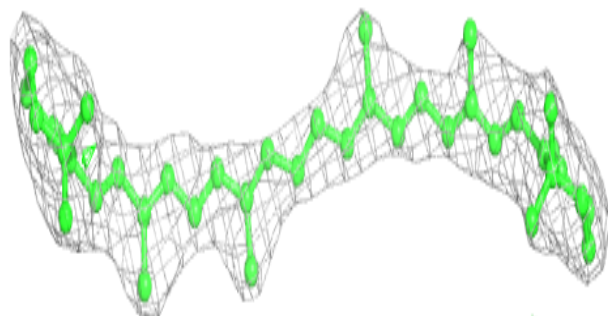
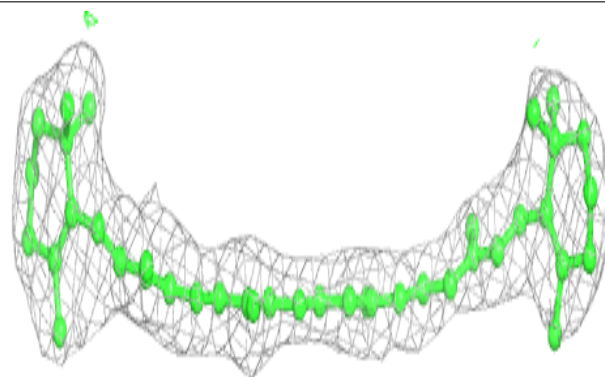


**Electron density around BCR b 623:**

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

**Electron density around BCR k 101:**

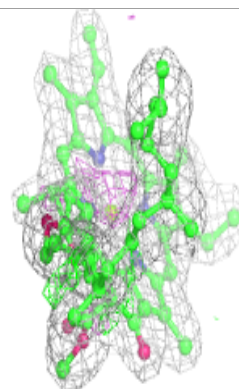
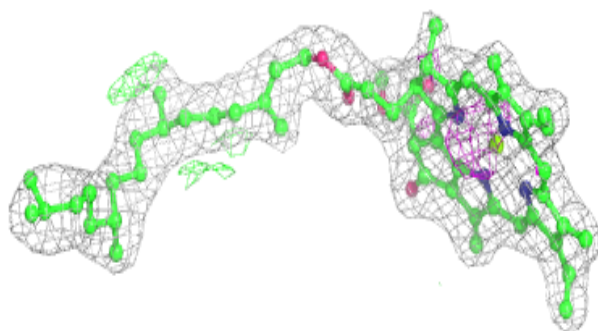
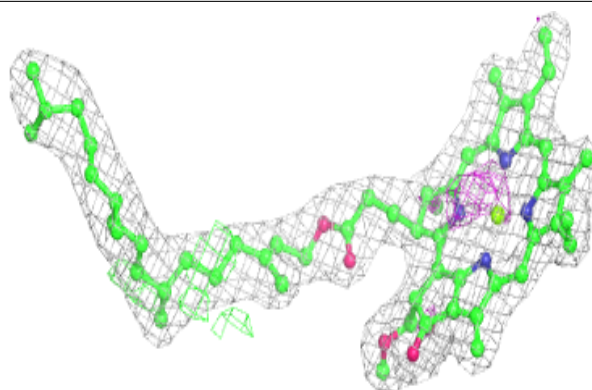
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



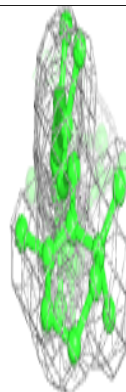
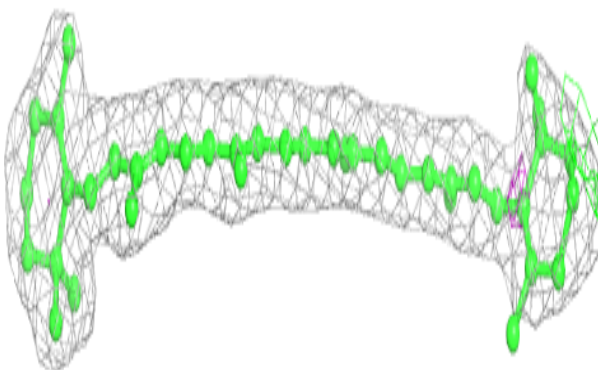
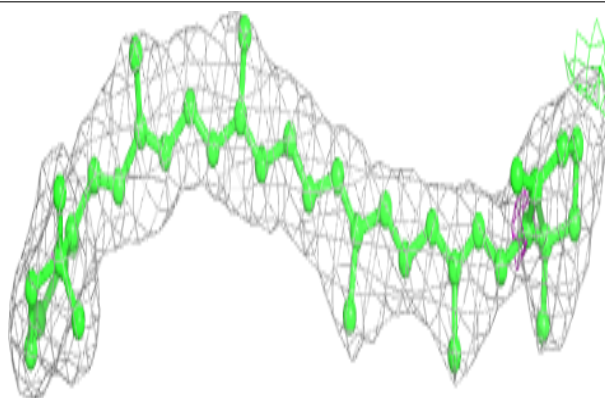


**Electron density around CLA a 405:**

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

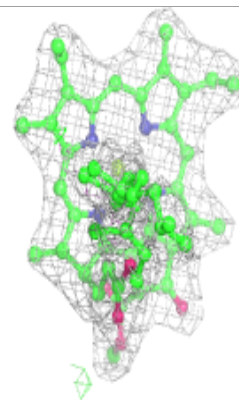
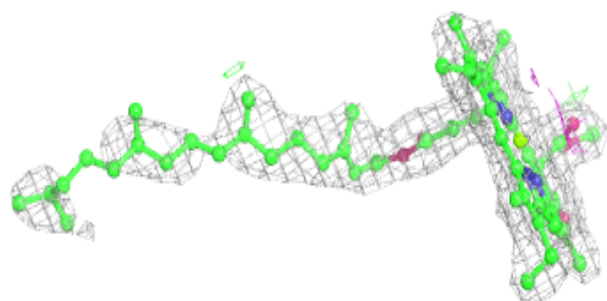
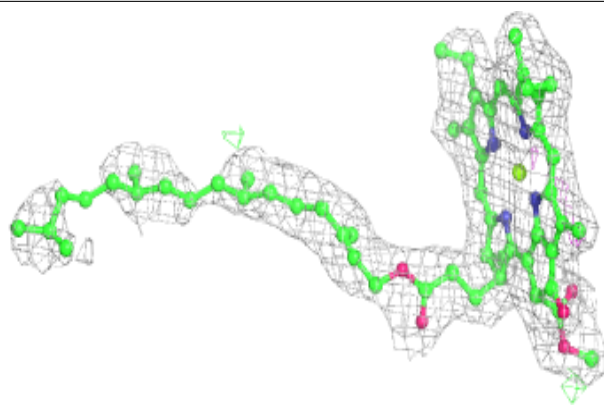
**Electron density around BCR H 101:**

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

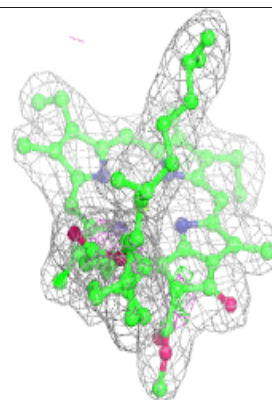
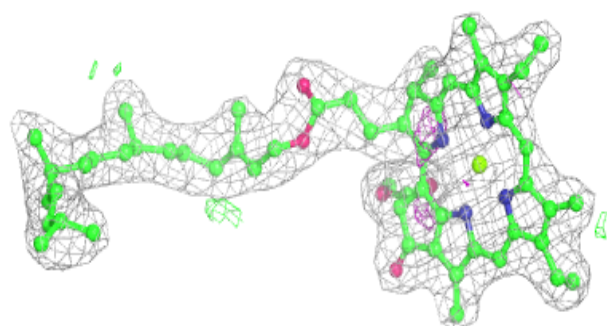
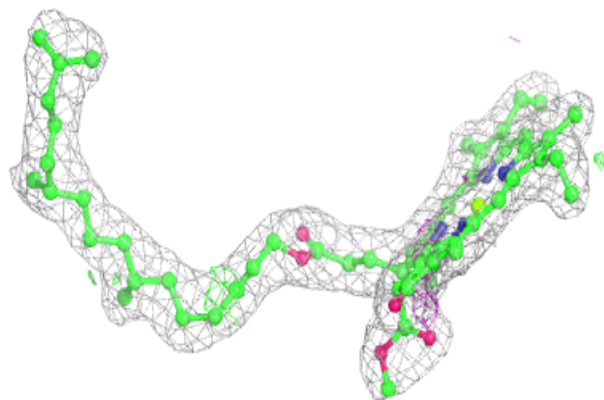


**Electron density around CLA d 406:**

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

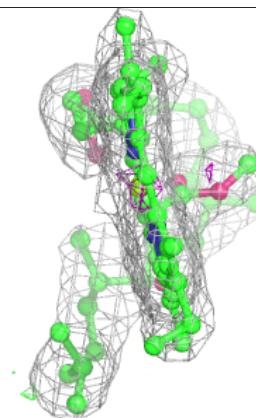
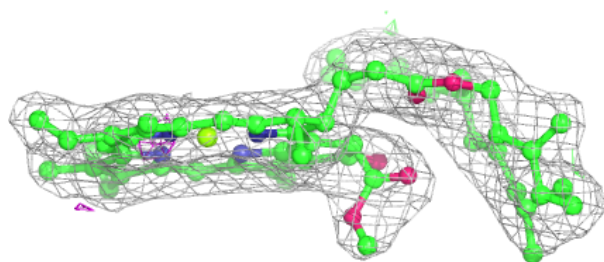
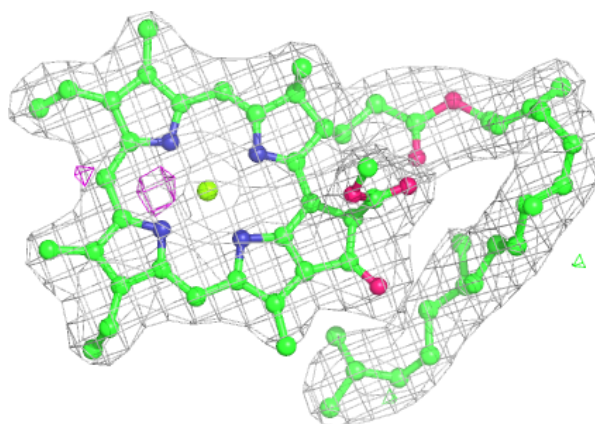
**Electron density around CLA d 405:**

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



**Electron density around CLA b 615:**

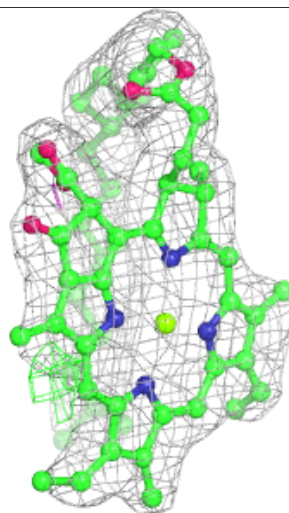
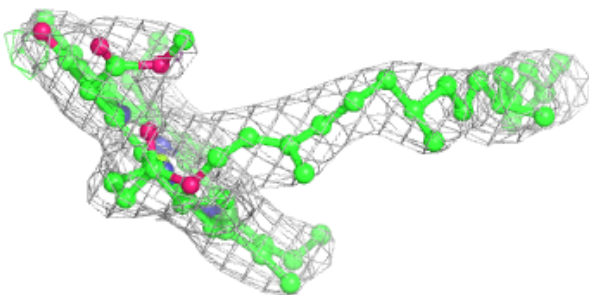
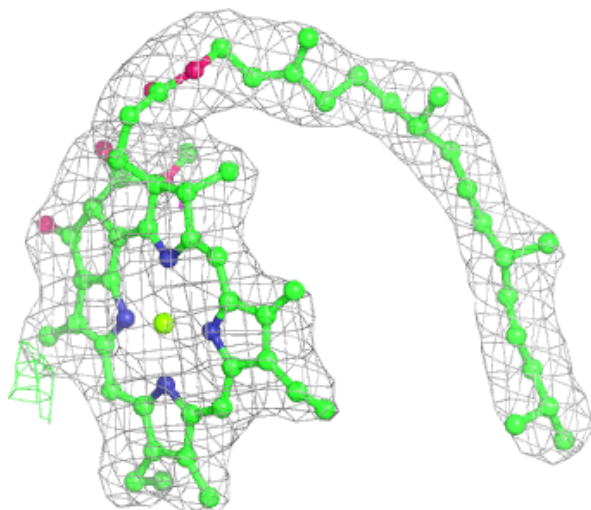
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





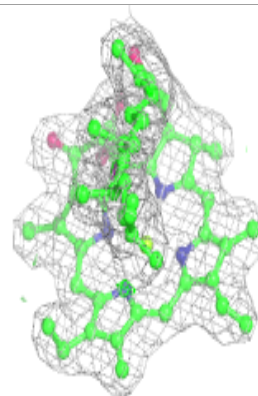
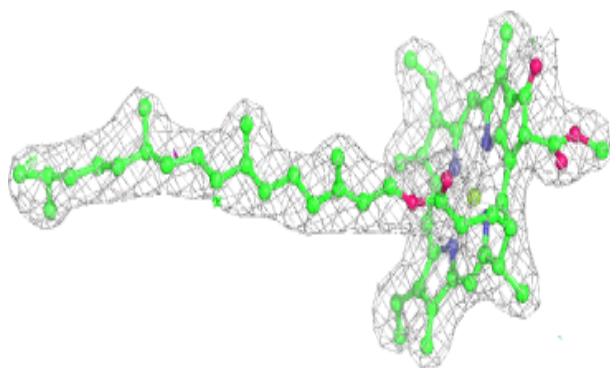
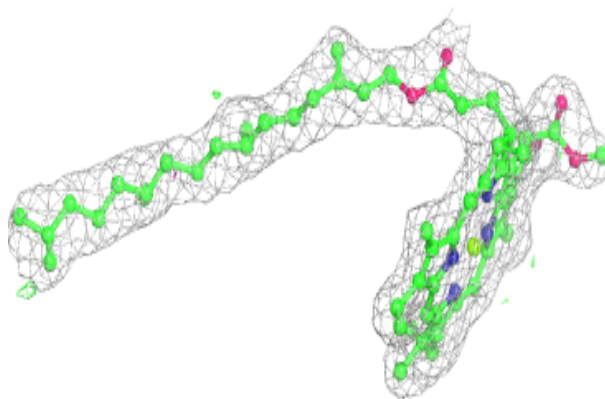
**Electron density around CLA C 507:**

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

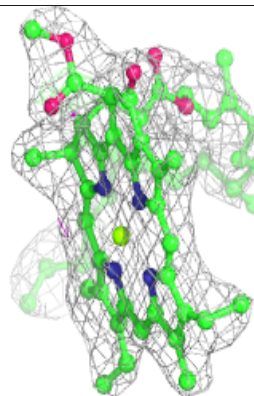
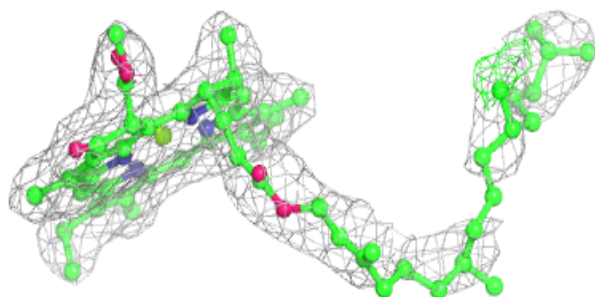
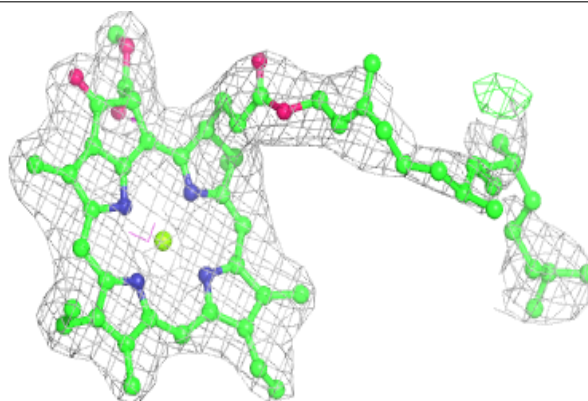


**Electron density around CLA B 608:**

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

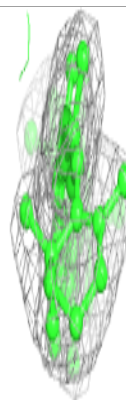
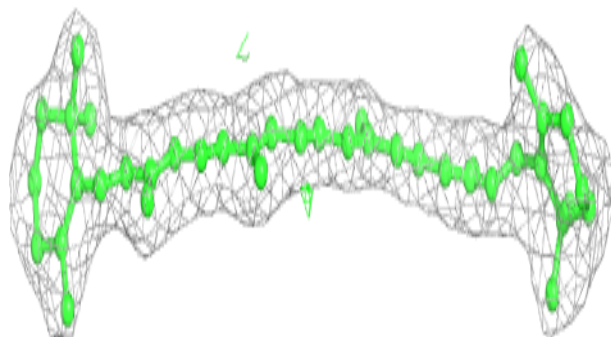
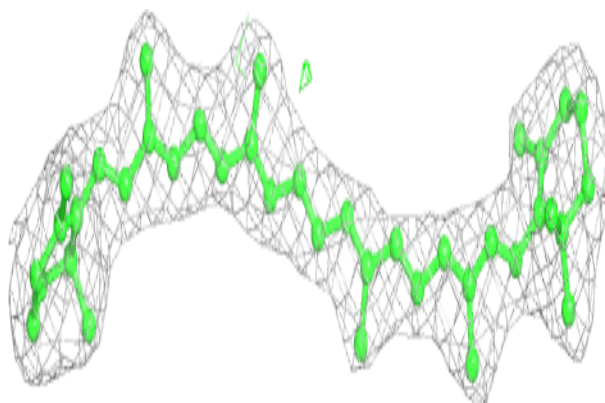
**Electron density around CLA a 408:**

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

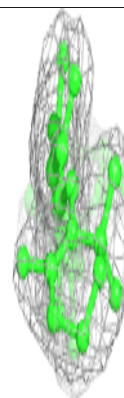
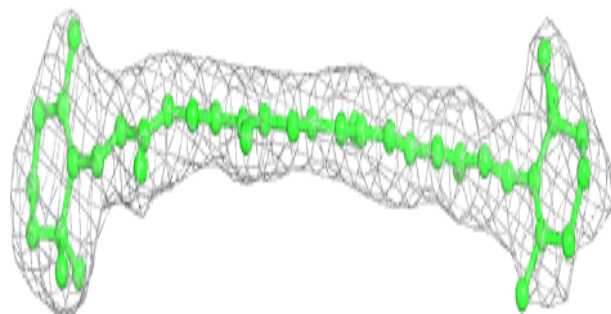
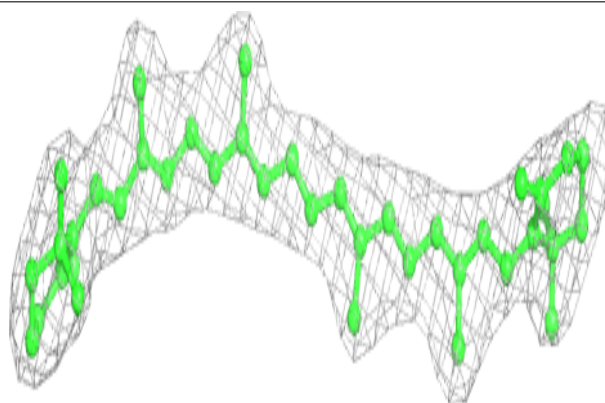


**Electron density around BCR y 101:**

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

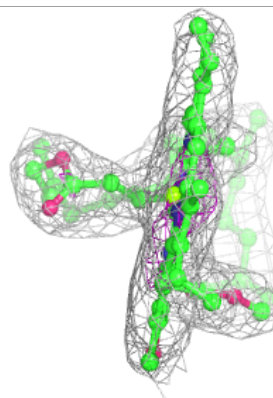
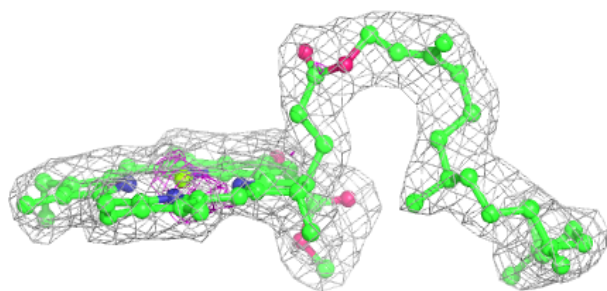
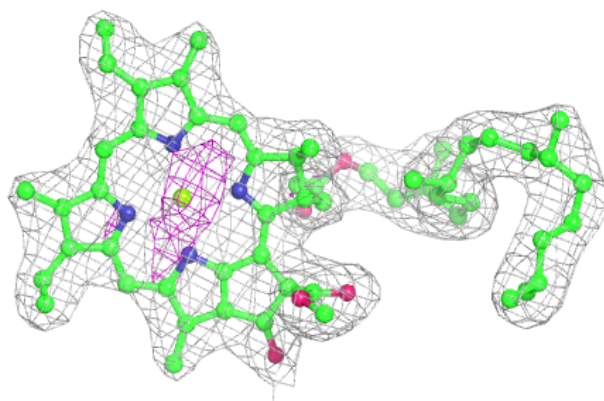
**Electron density around BCR h 101:**

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

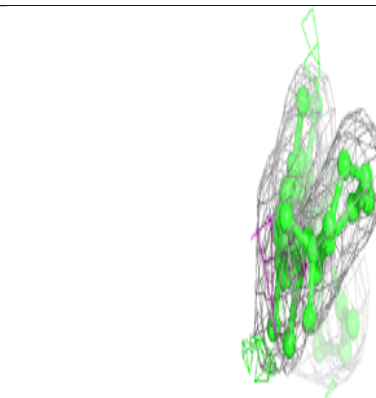
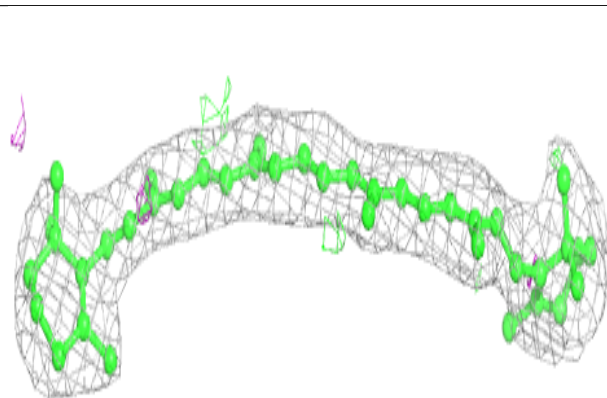
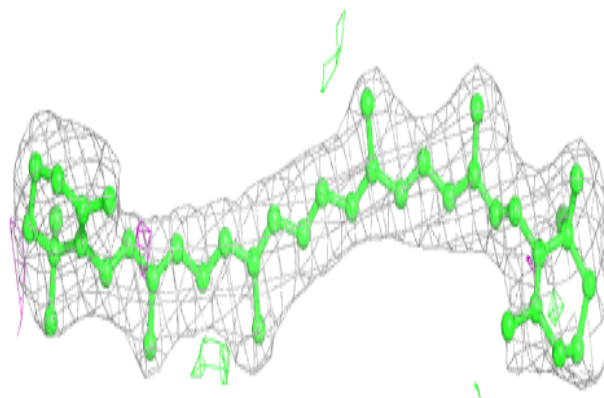


**Electron density around CLA B 613:**

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

**Electron density around BCR d 407:**

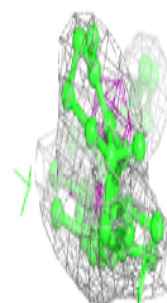
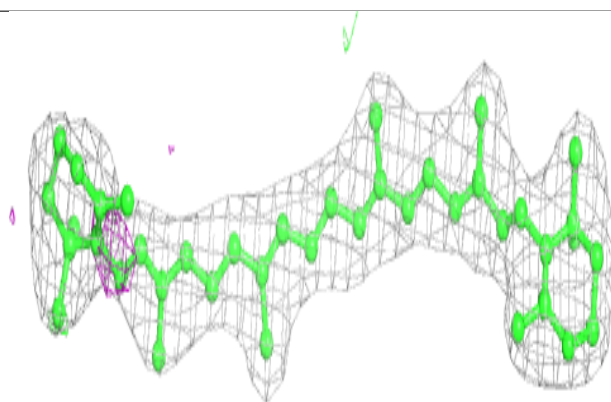
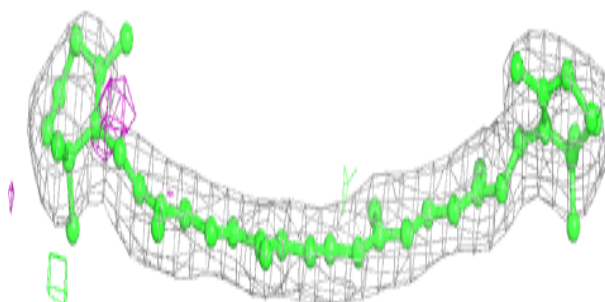
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



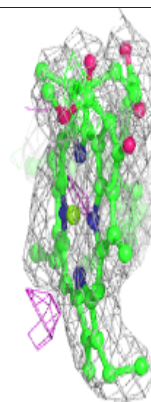
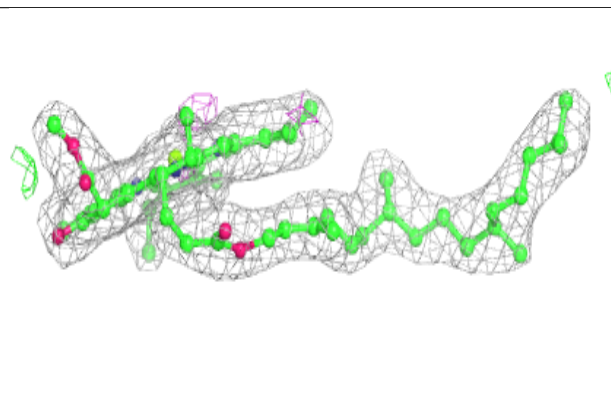
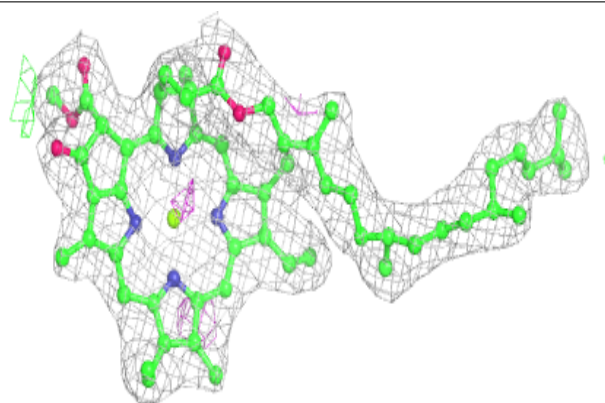


**Electron density around BCR D 406:**

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

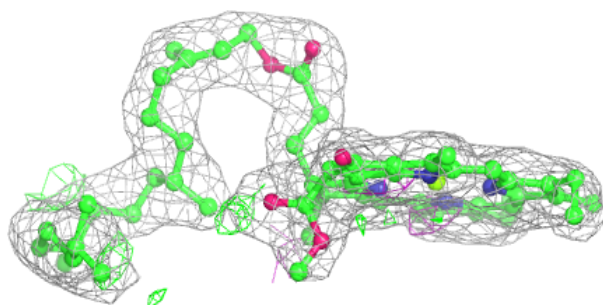
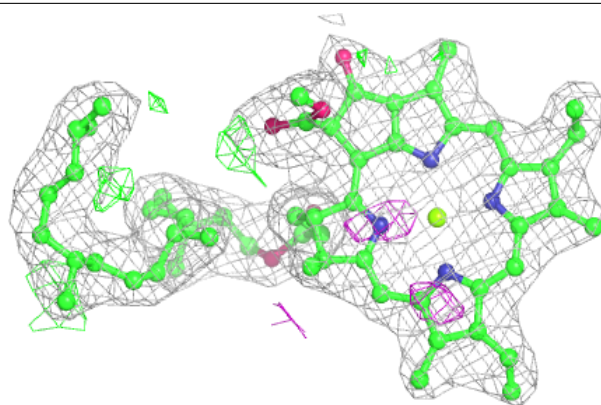
**Electron density around CLA b 608:**

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

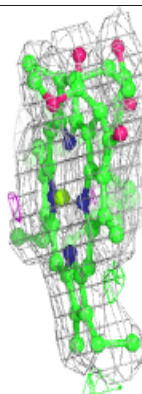
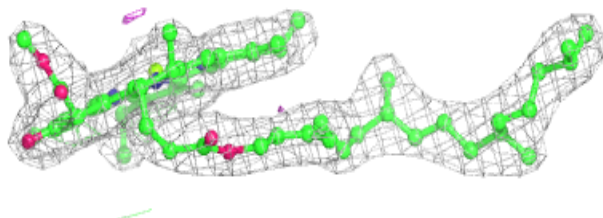
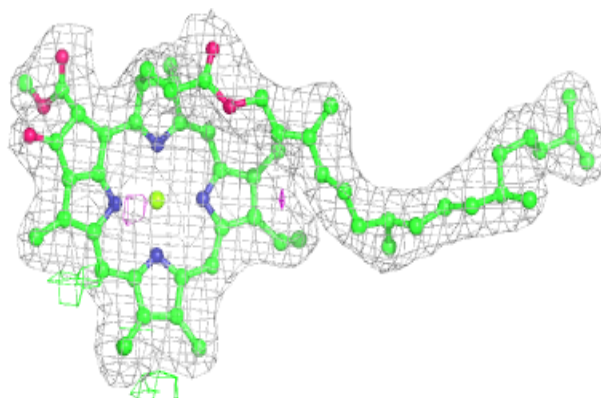


**Electron density around CLA b 617:**

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

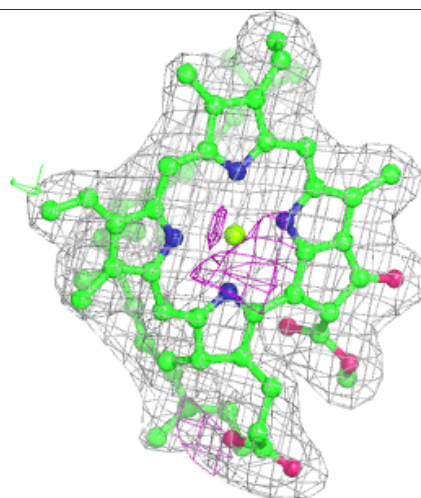
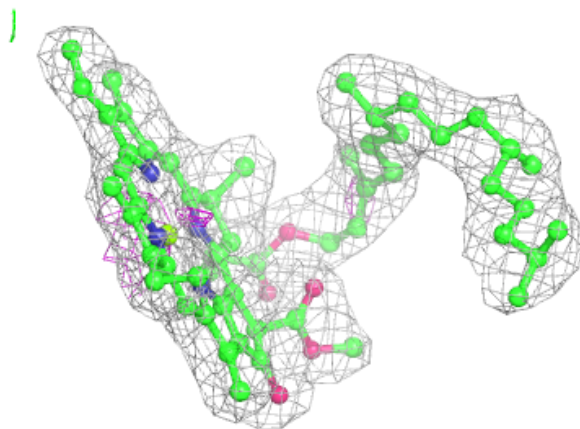
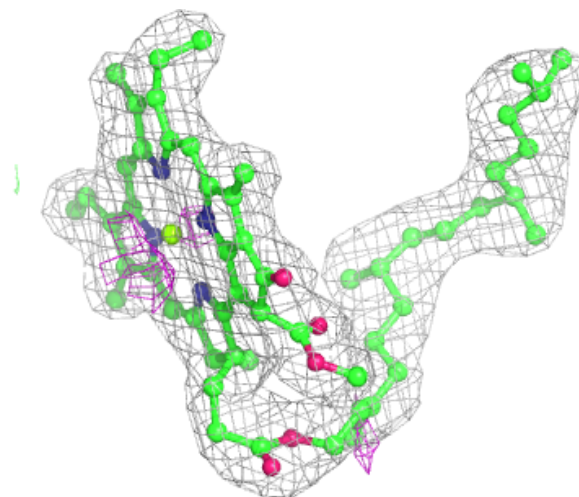
**Electron density around CLA B 604:**

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



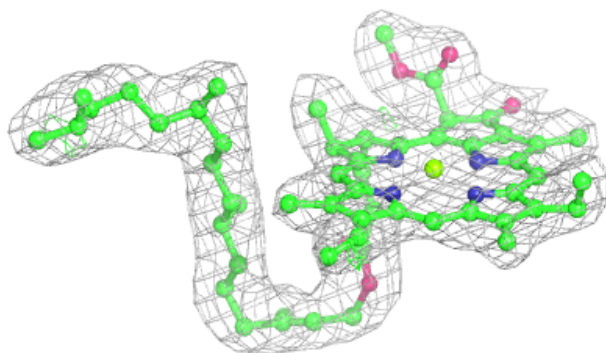
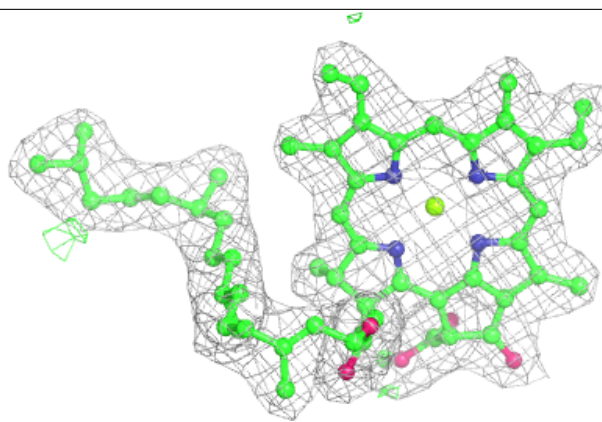
**Electron density around CLA b 618:**

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



**Electron density around CLA A 406:**

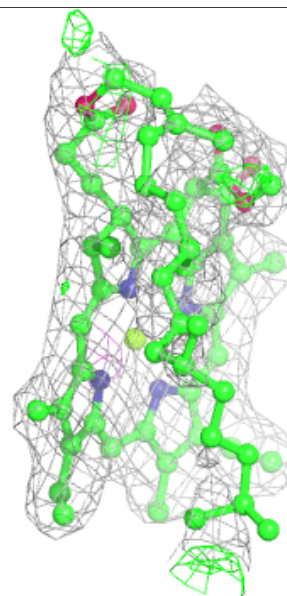
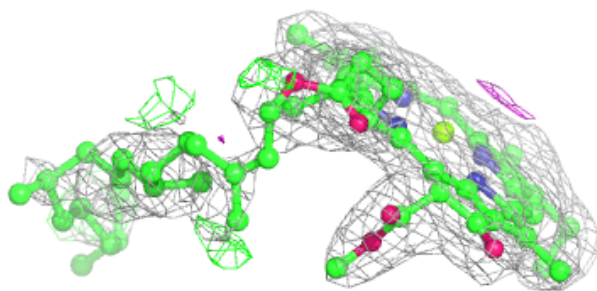
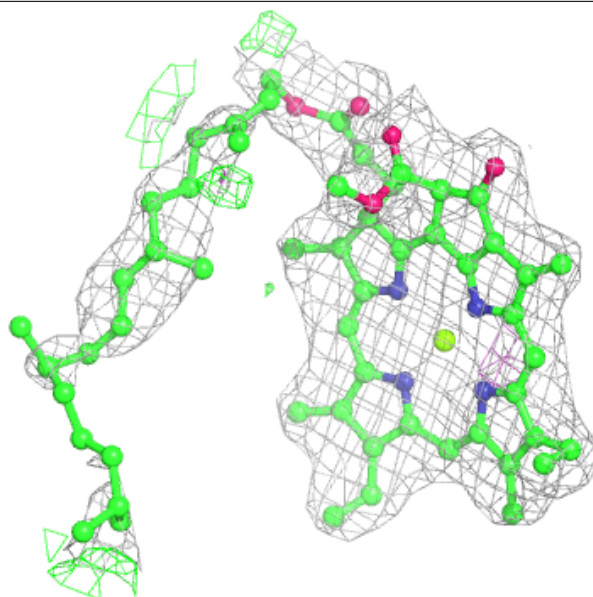
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





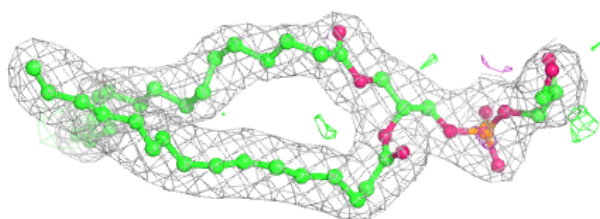
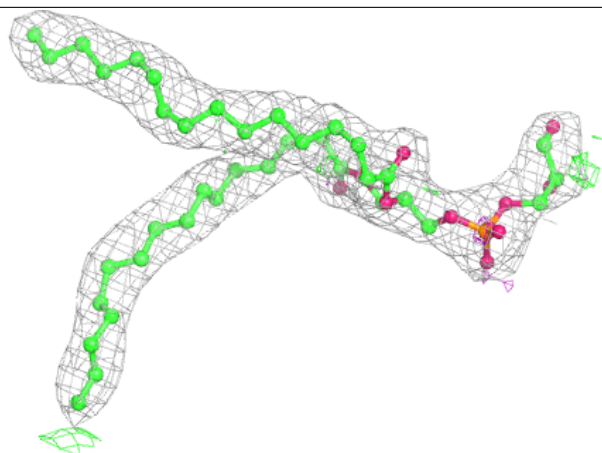
**Electron density around CLA B 617:**

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

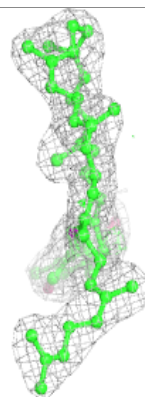
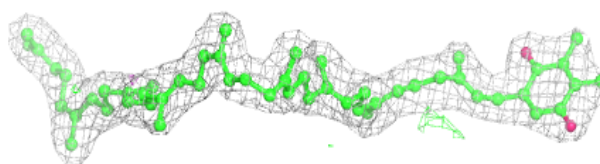
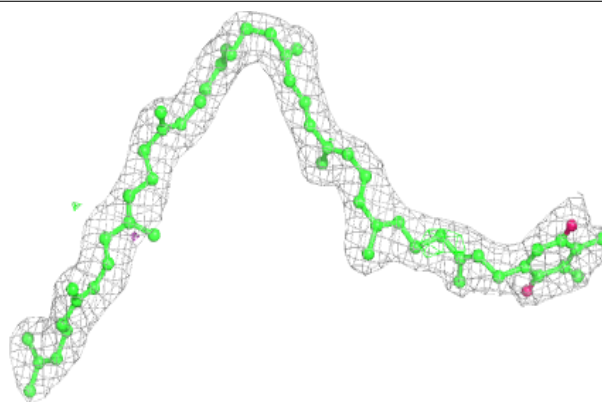


**Electron density around LHG D 409:**

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

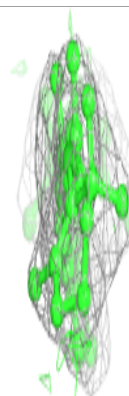
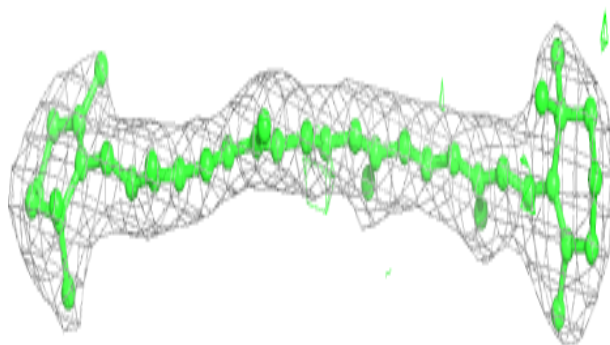
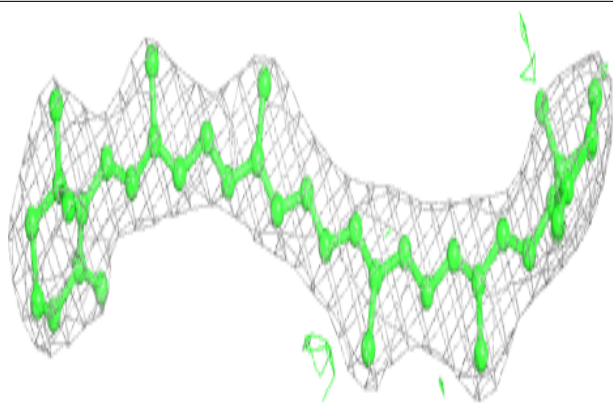
**Electron density around PL9 d 408:**

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



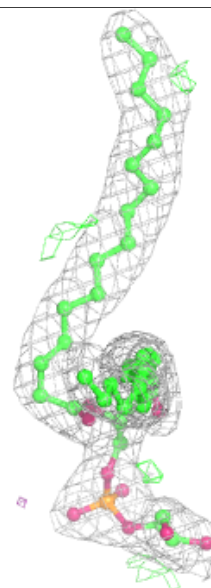
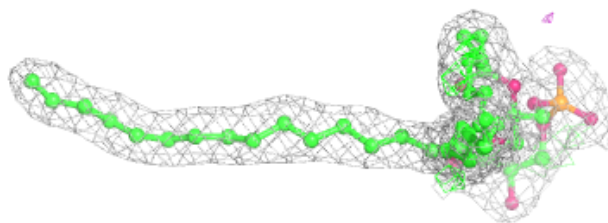
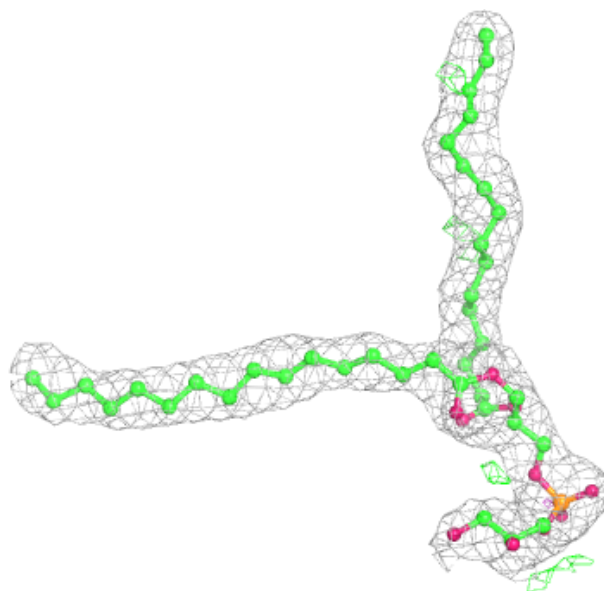
**Electron density around BCR Y 102:**

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



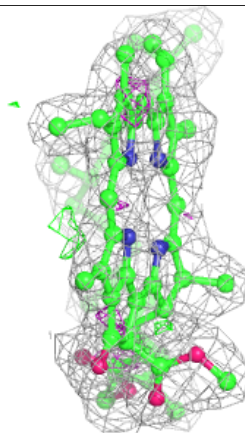
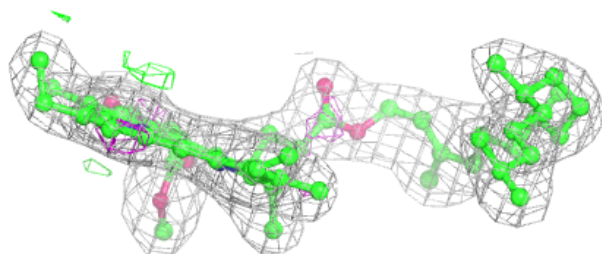
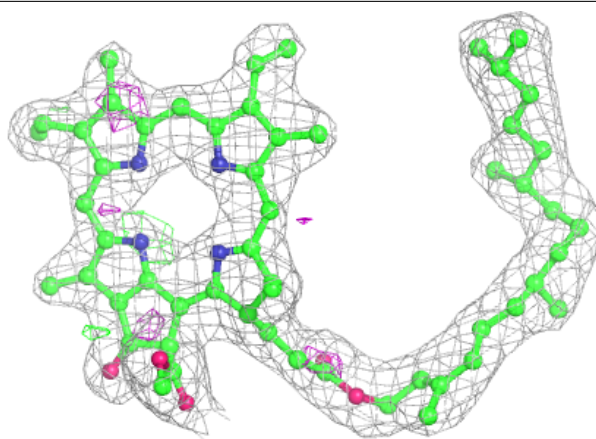
**Electron density around LHG L 101:**

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



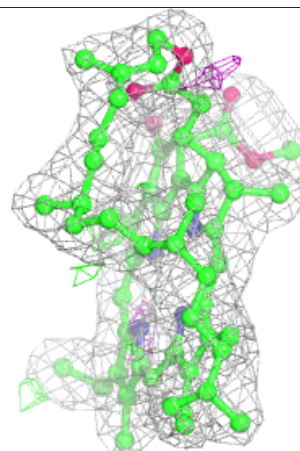
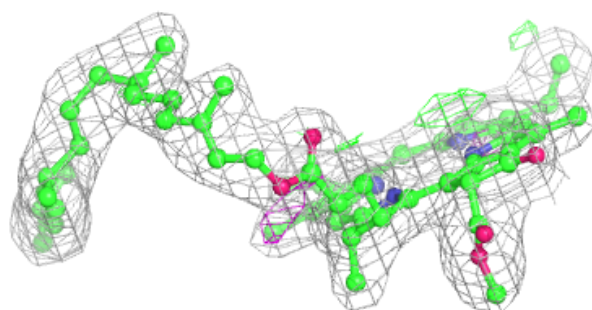
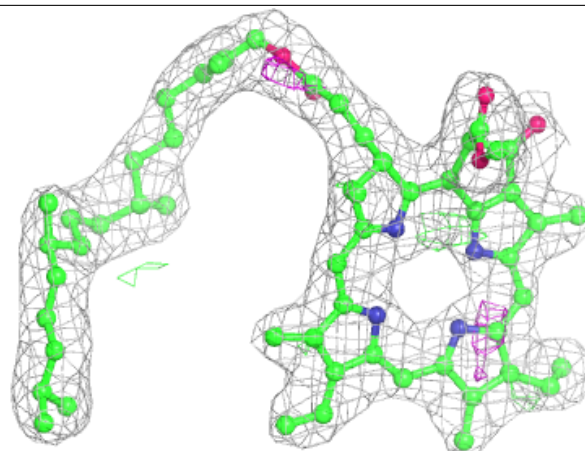
**Electron density around PHO A 408:**

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

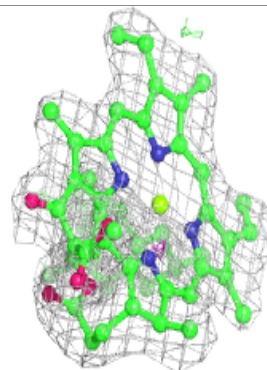
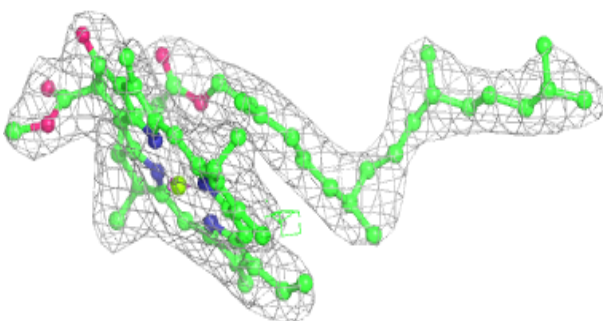
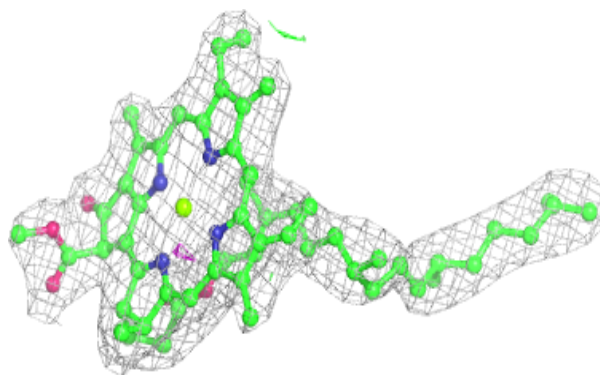


**Electron density around PHO d 403:**

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

**Electron density around CLA C 505:**

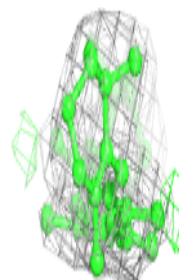
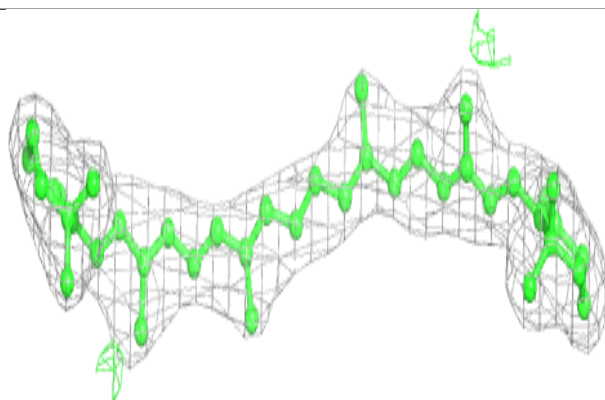
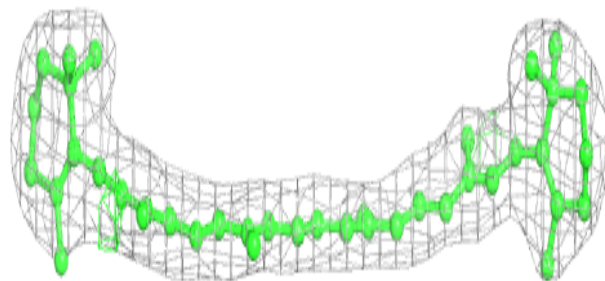
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



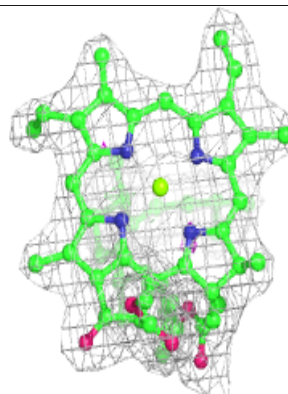
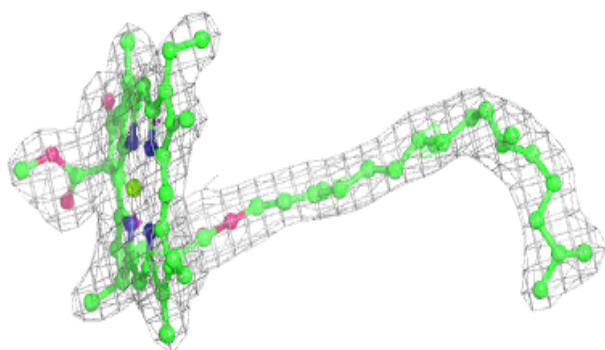
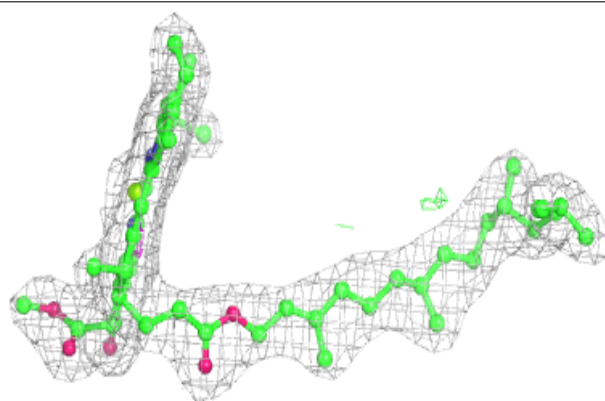


**Electron density around BCR K 101:**

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

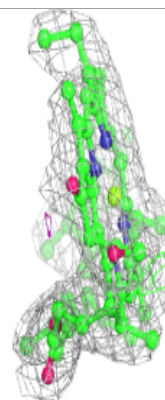
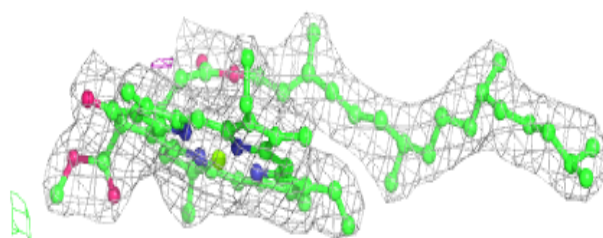
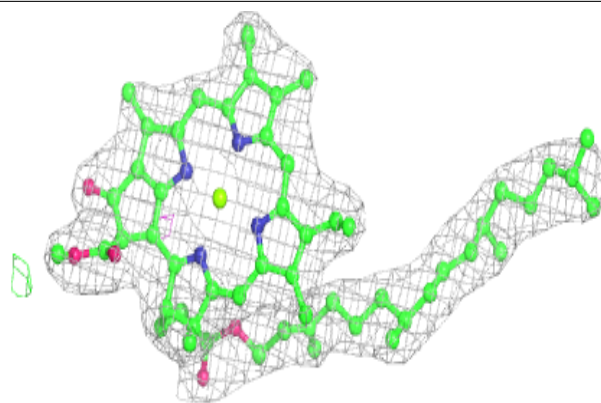
**Electron density around CLA B 606:**

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

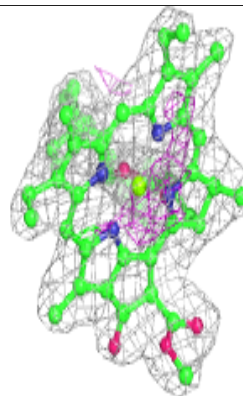
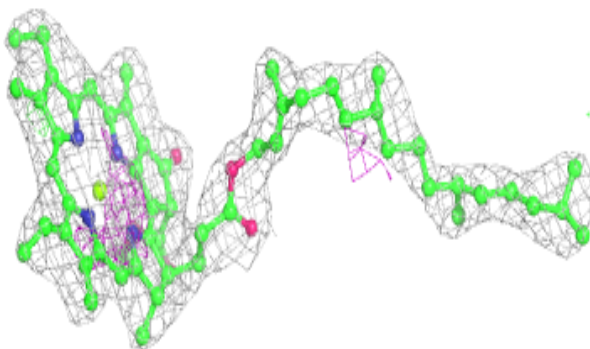
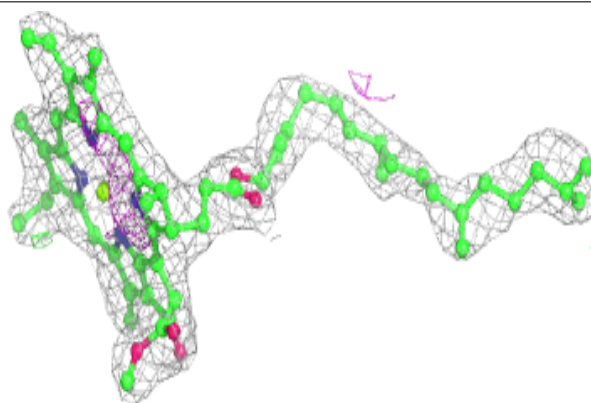


**Electron density around CLA c 902:**

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

**Electron density around CLA c 903:**

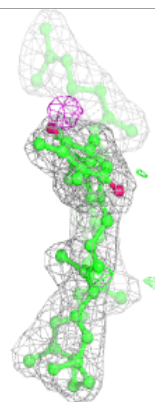
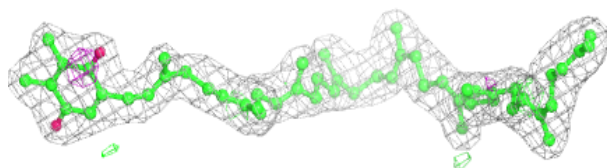
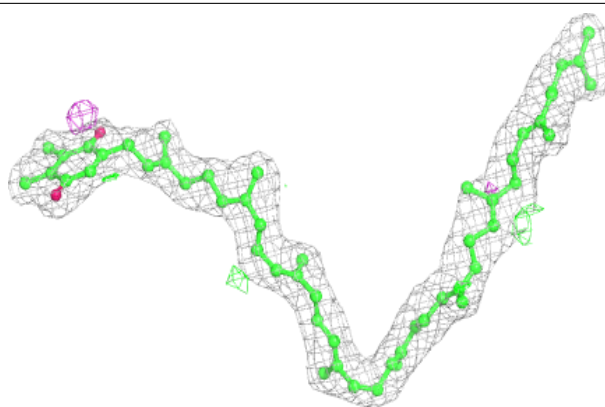
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



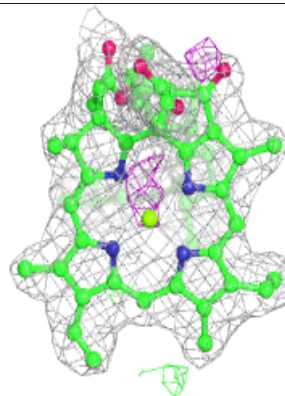
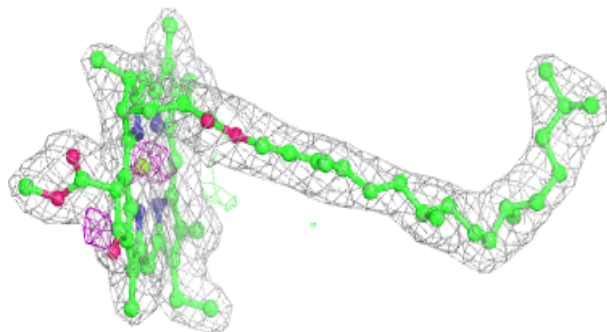
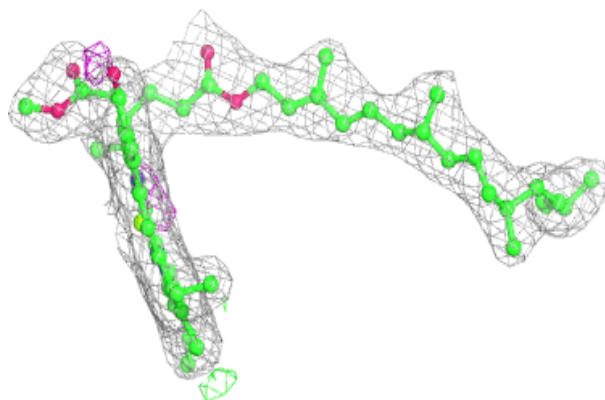


**Electron density around PL9 D 407:**

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

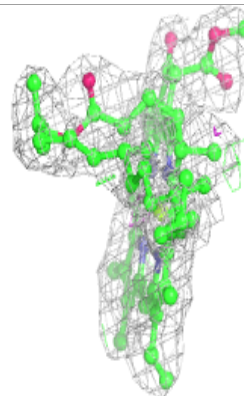
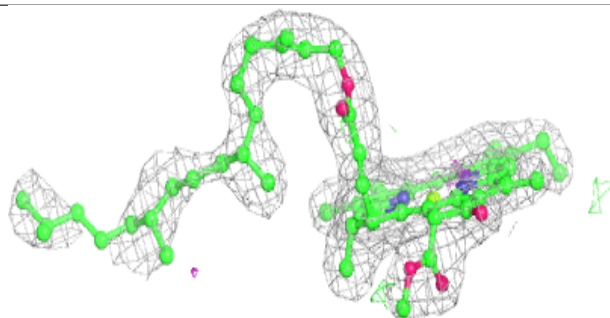
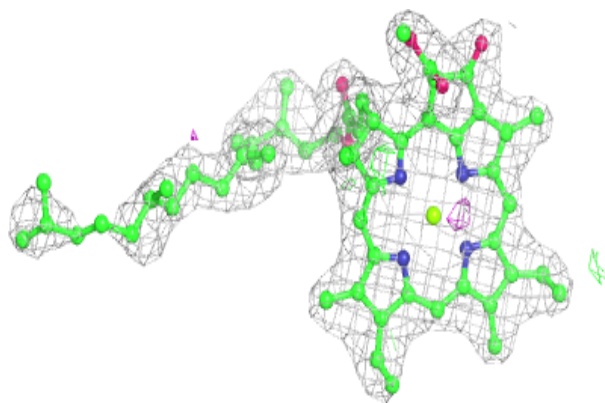
**Electron density around CLA b 610:**

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

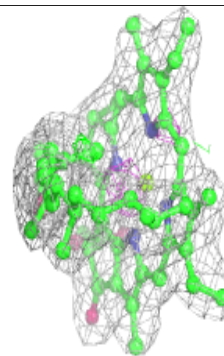
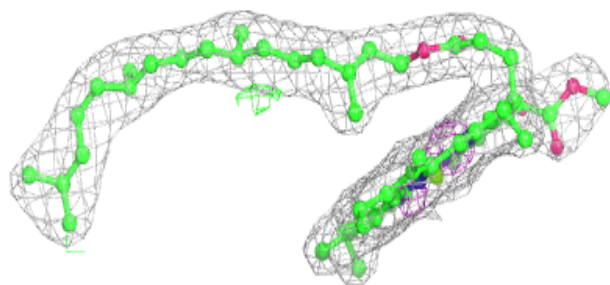
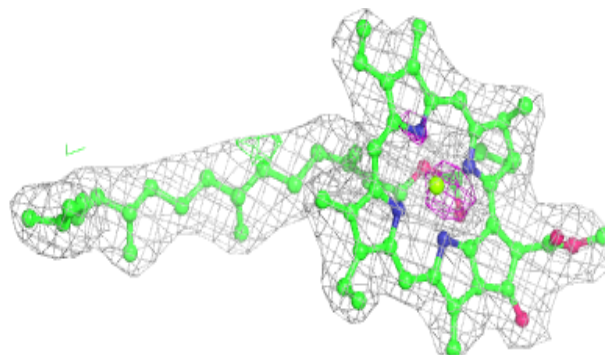


**Electron density around CLA A 407:**

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

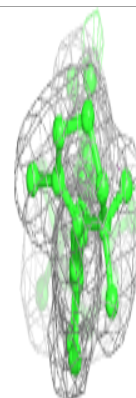
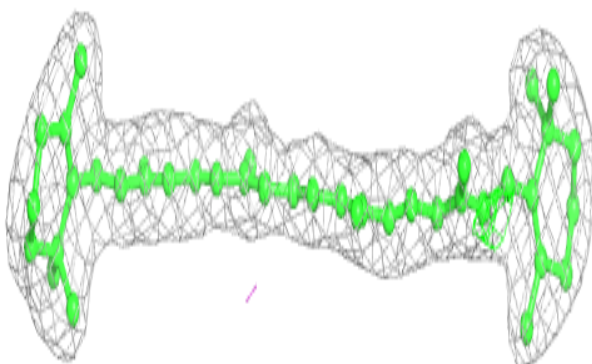
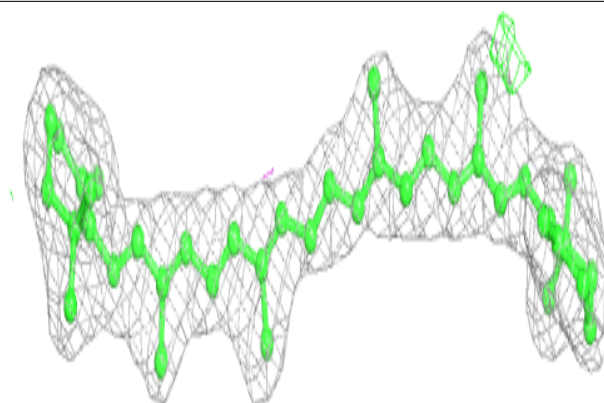
**Electron density around CLA B 609:**

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

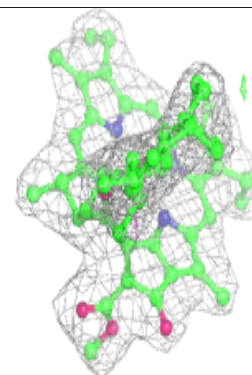
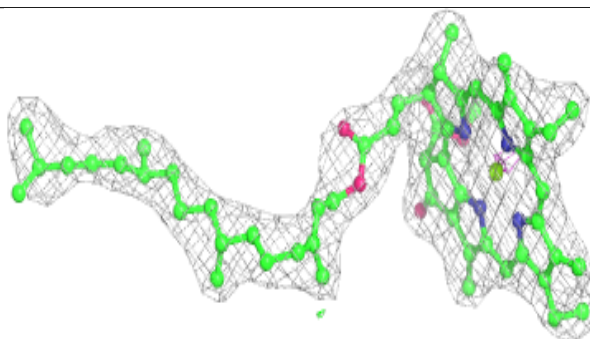
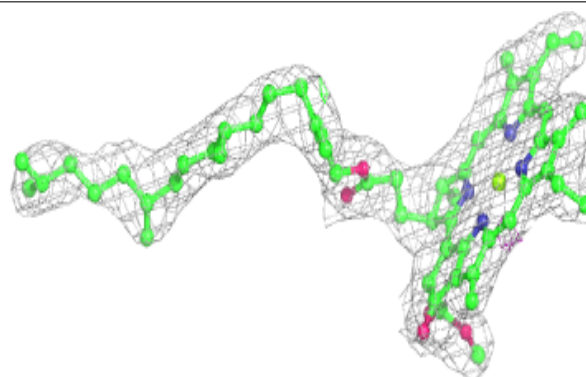


**Electron density around BCR A 410:**

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

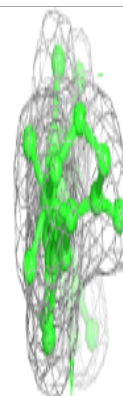
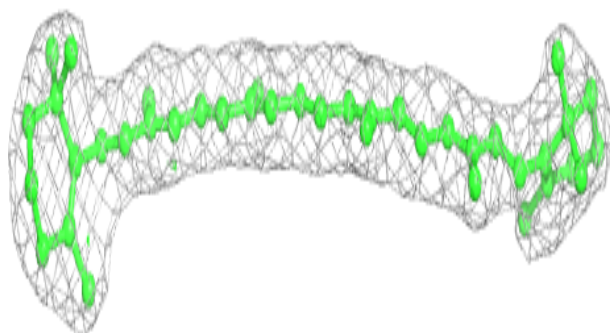
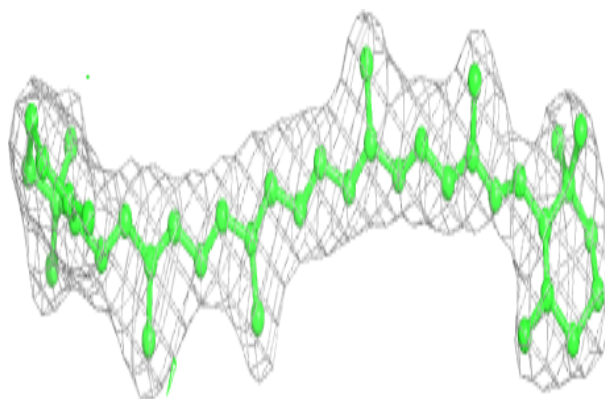
**Electron density around CLA C 502:**

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

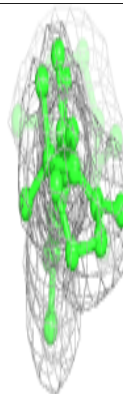
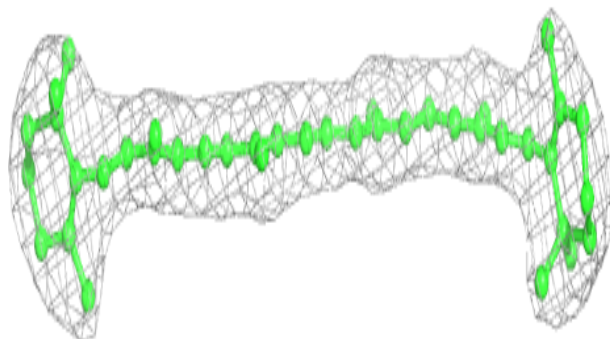
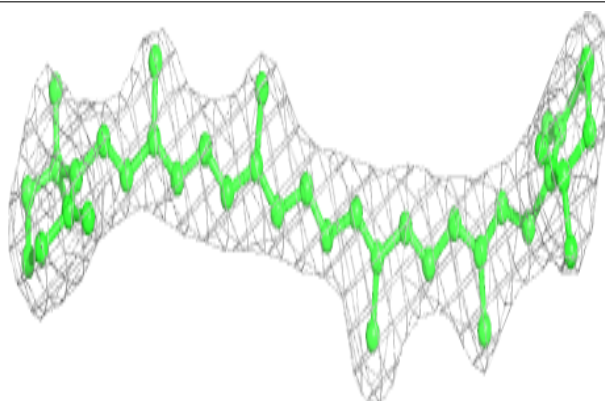


**Electron density around BCR b 622:**

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

**Electron density around BCR c 915:**

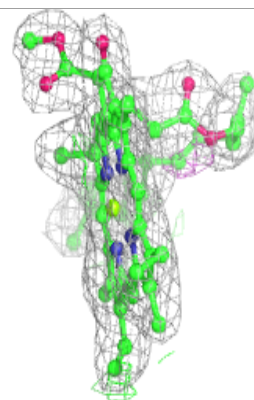
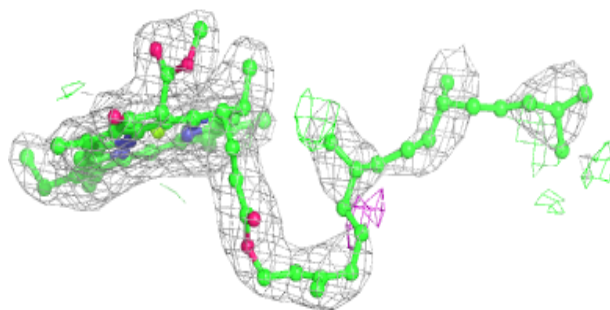
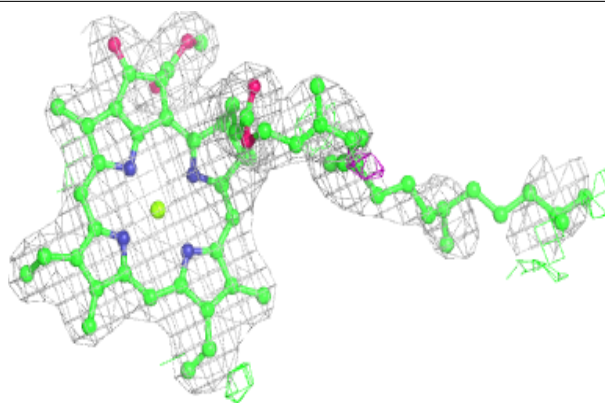
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



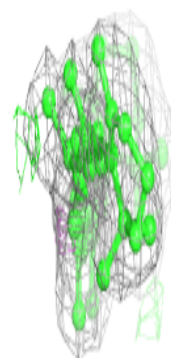
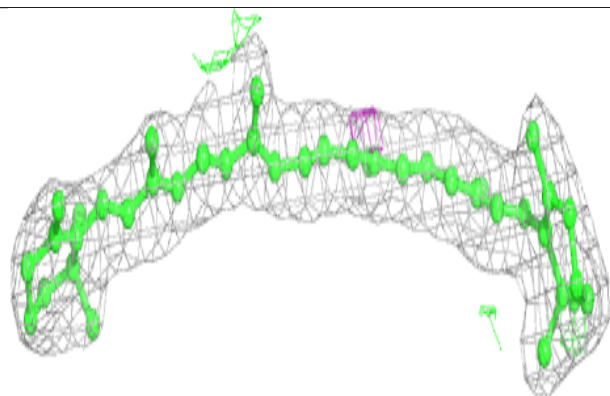
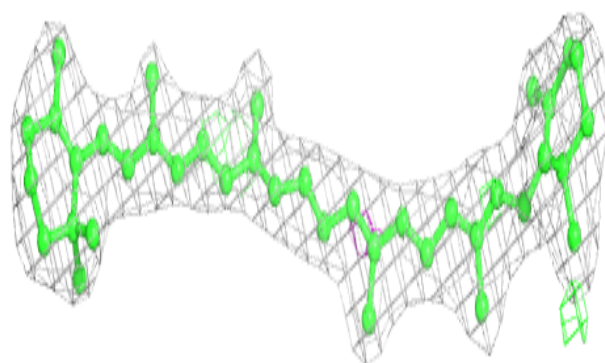


**Electron density around CLA a 406:**

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

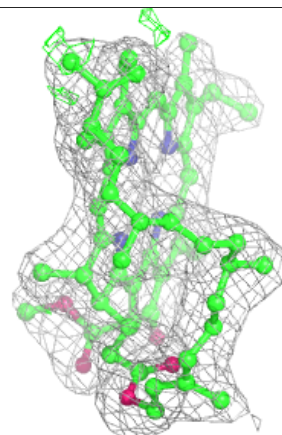
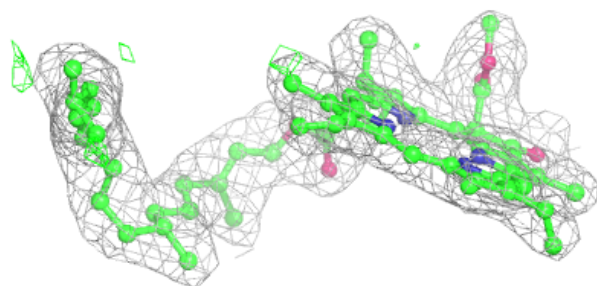
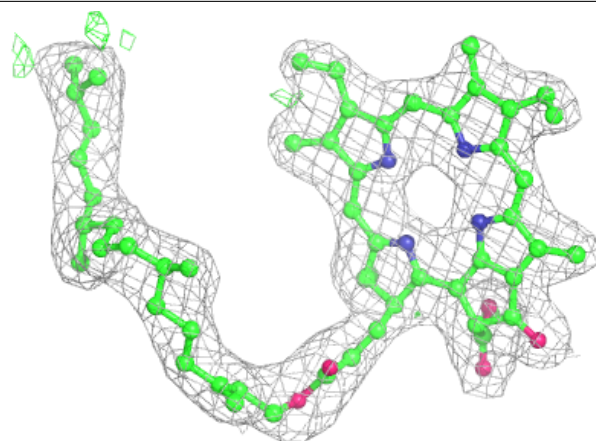
**Electron density around BCR T 102:**

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

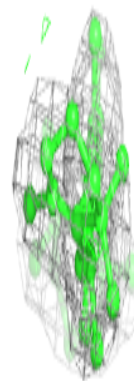
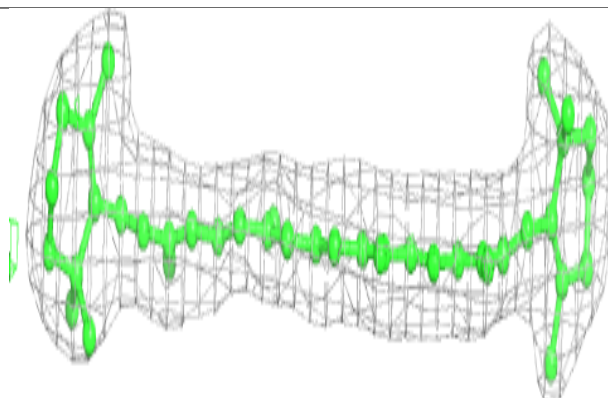
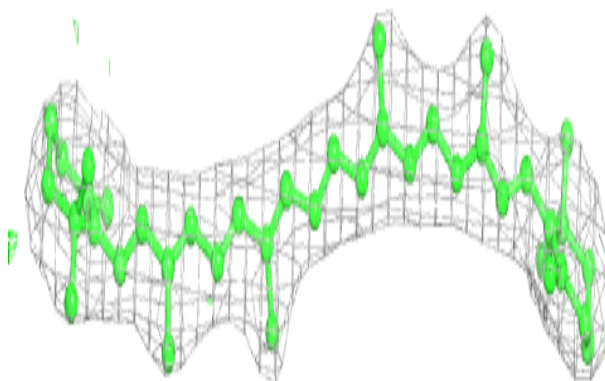


**Electron density around PHO D 401:**

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

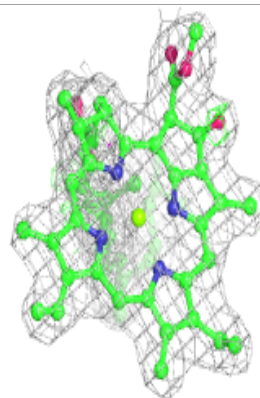
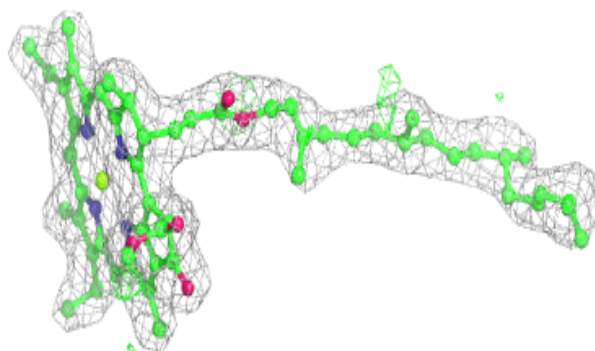
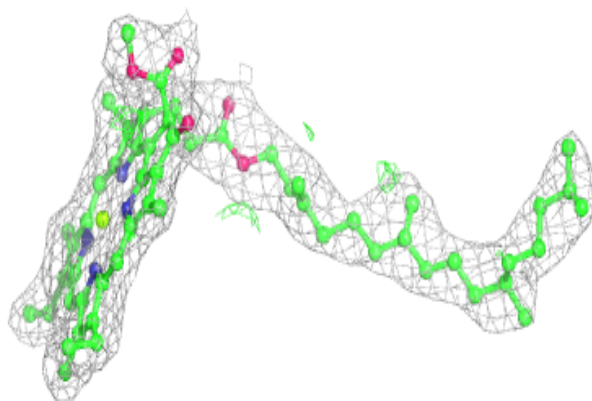
**Electron density around BCR C 515:**

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

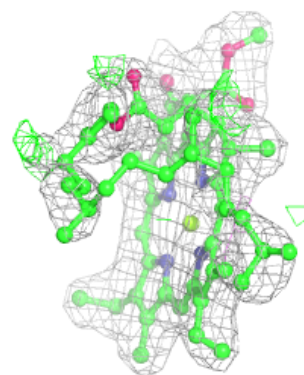
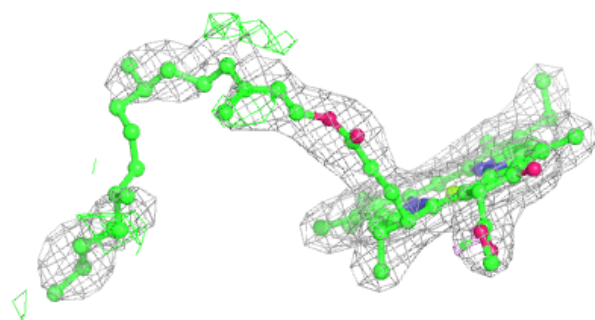
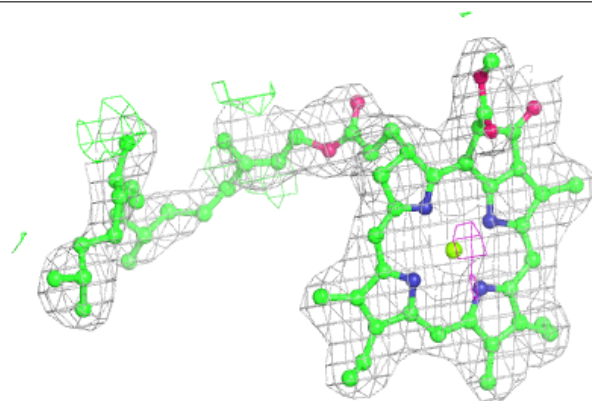


**Electron density around CLA b 609:**

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

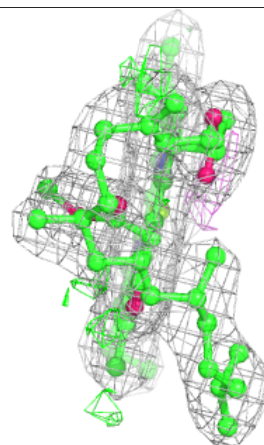
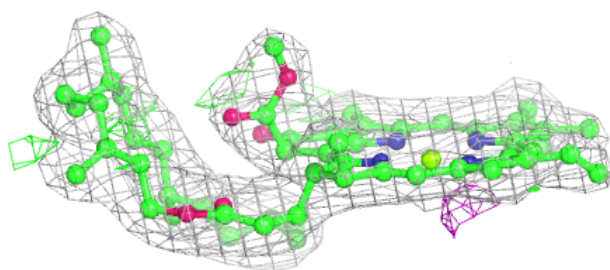
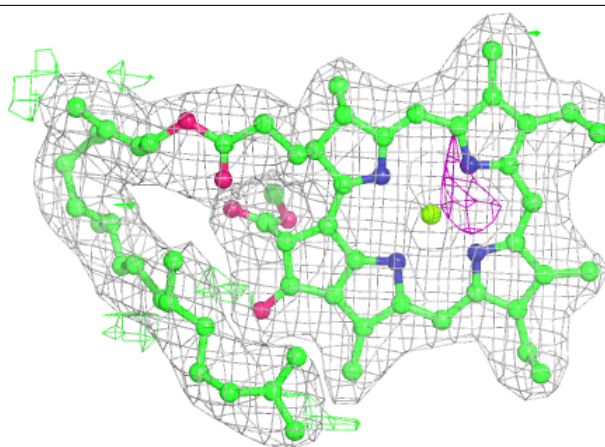
**Electron density around CLA A 409:**

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

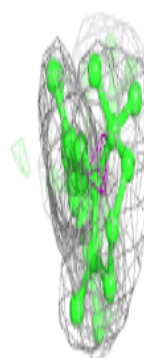
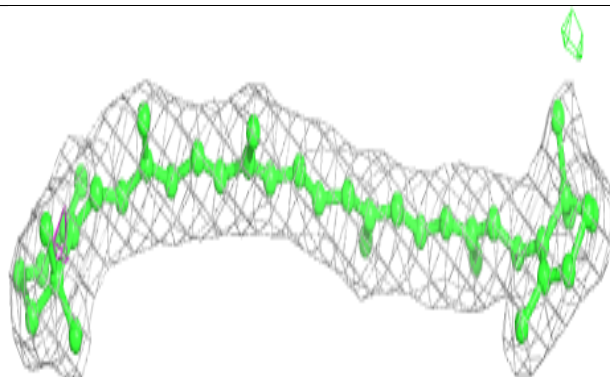
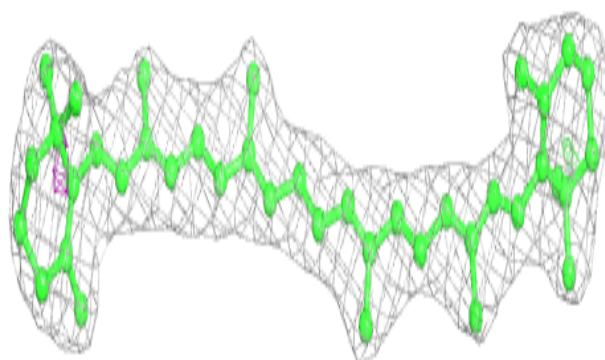


**Electron density around CLA B 611:**

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

**Electron density around BCR b 624:**

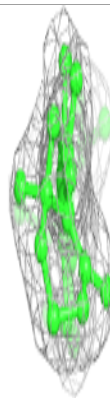
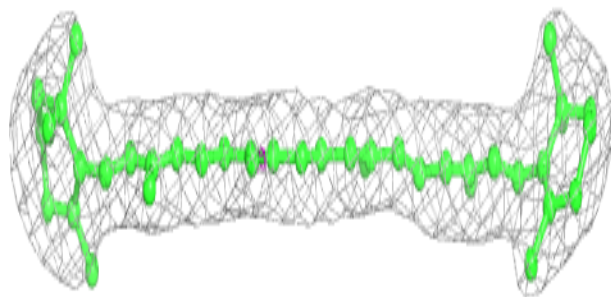
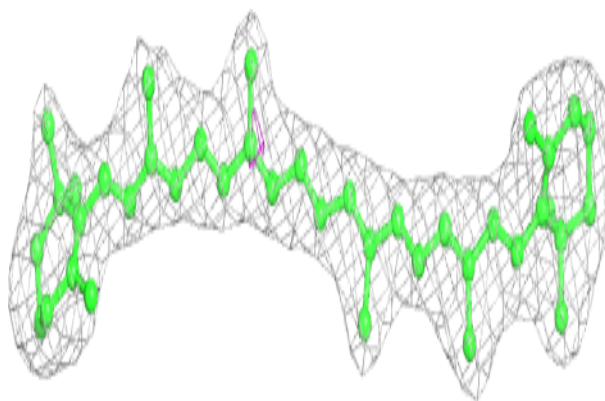
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





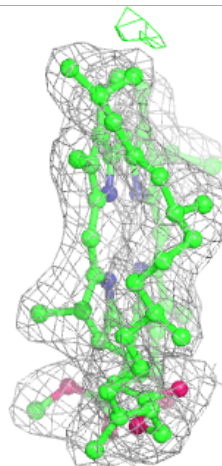
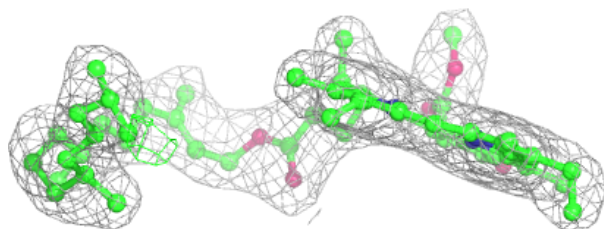
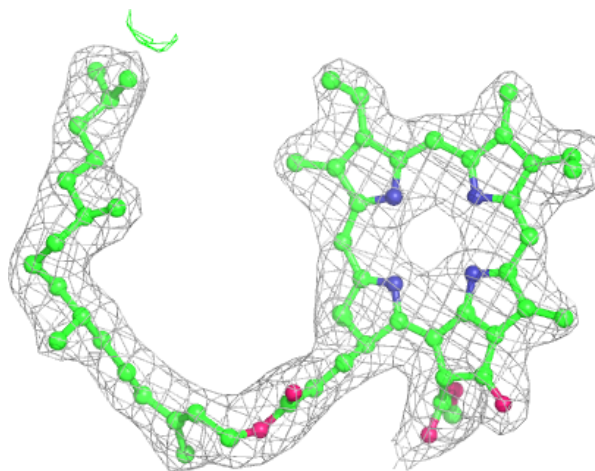
**Electron density around BCR B 619:**

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



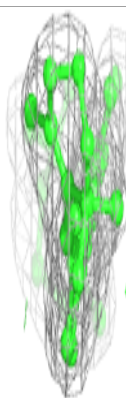
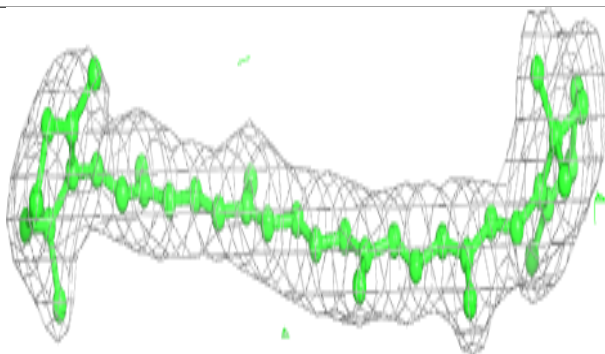
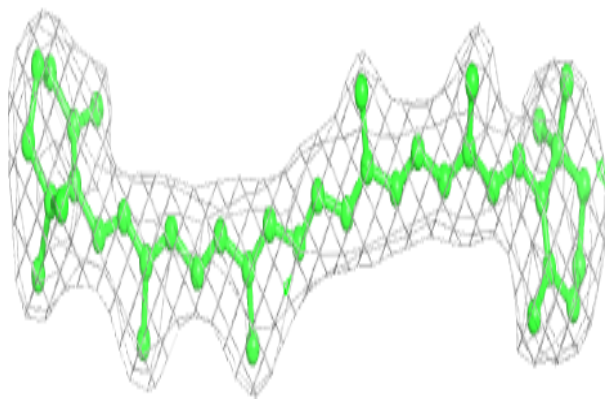
**Electron density around PHO a 407:**

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



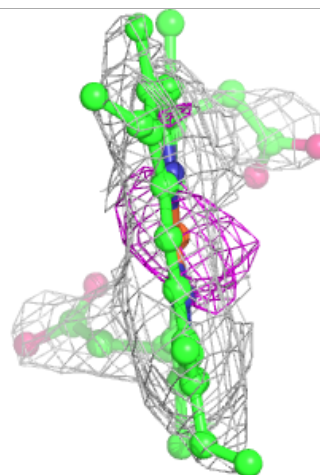
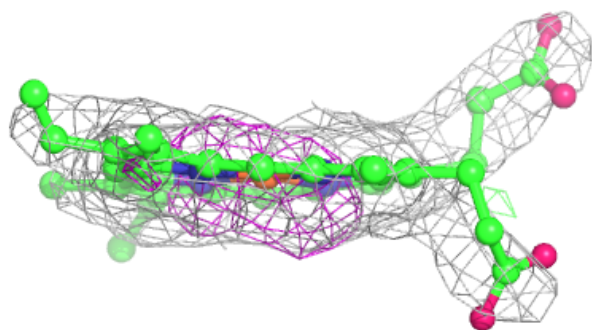
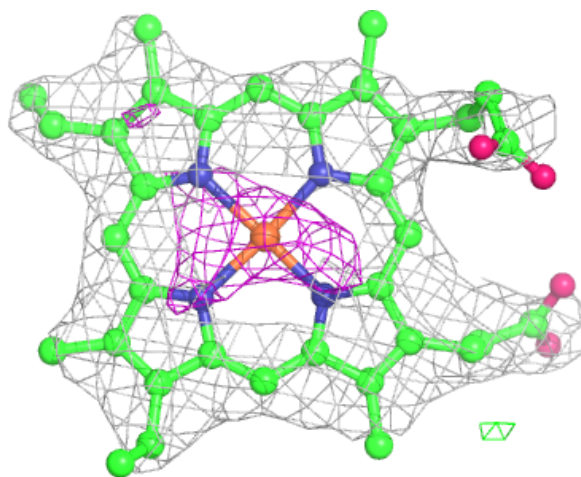
**Electron density around BCR B 620:**

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



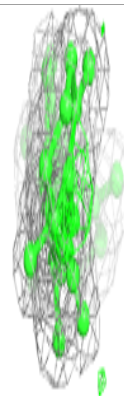
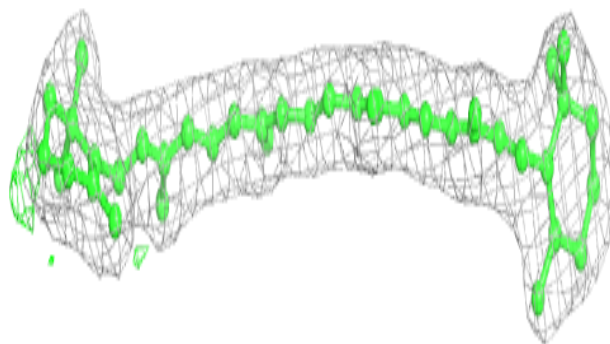
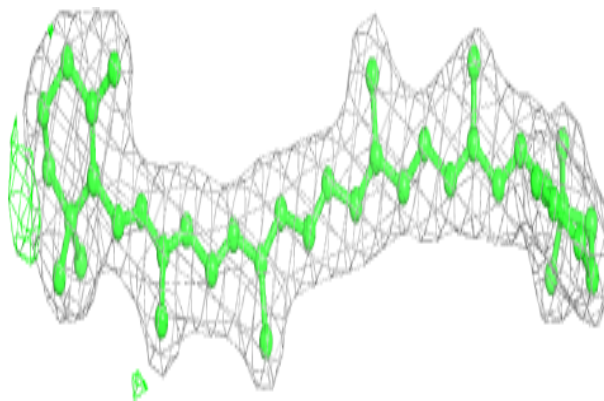
**Electron density around HEM f 101:**

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



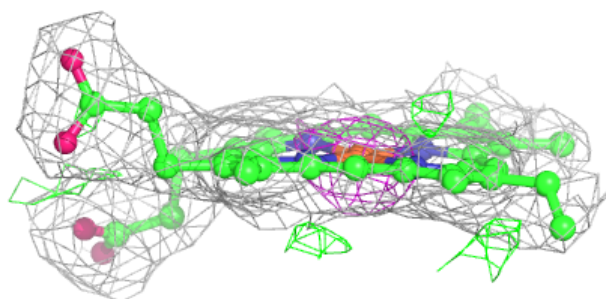
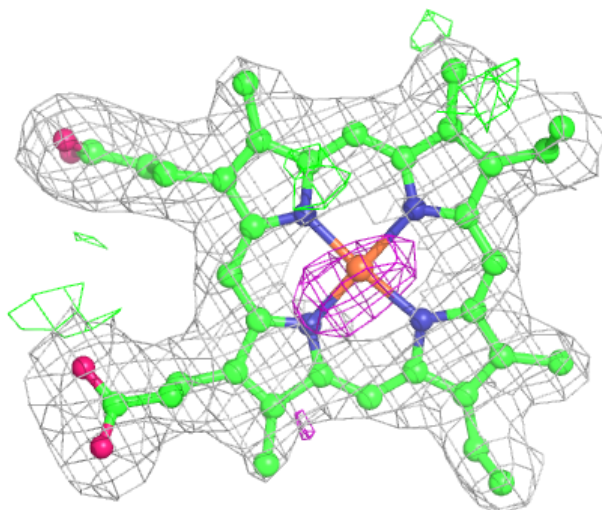
**Electron density around BCR B 618:**

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



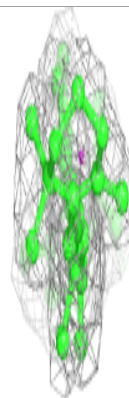
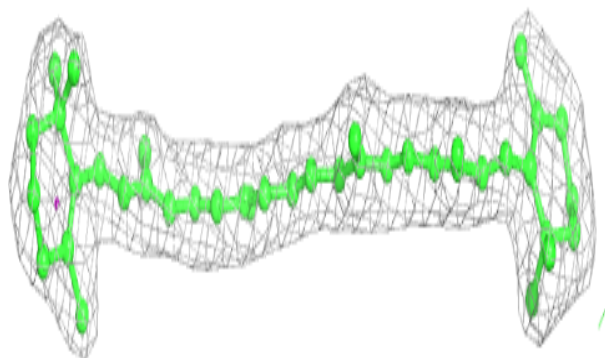
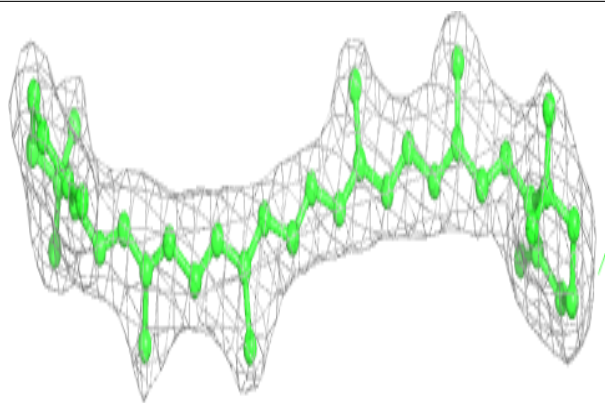
**Electron density around HEM V 202:**

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

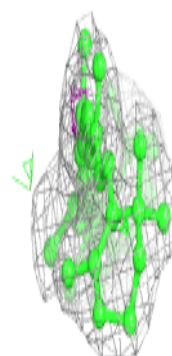
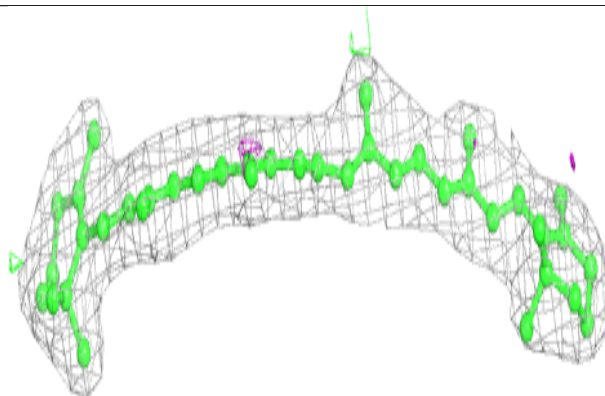
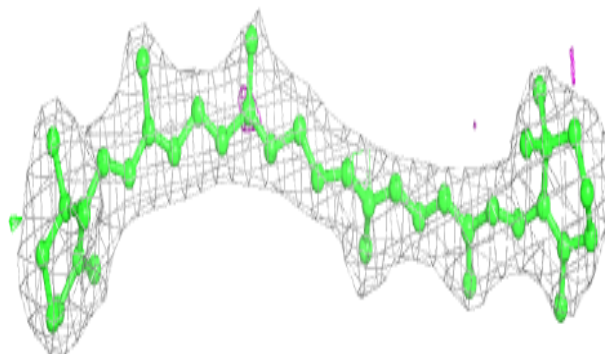


**Electron density around BCR a 409:**

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

**Electron density around BCR t 102:**

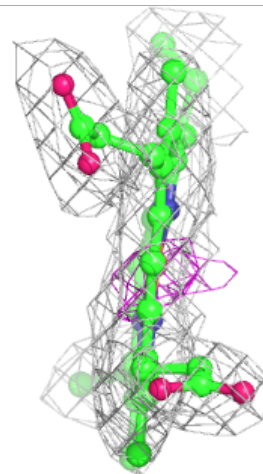
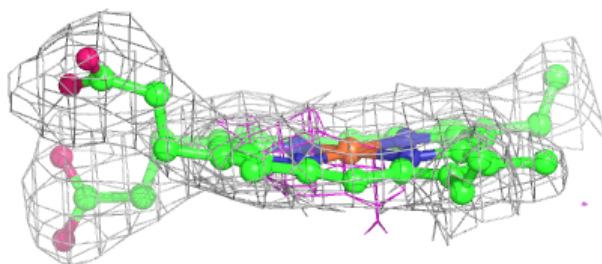
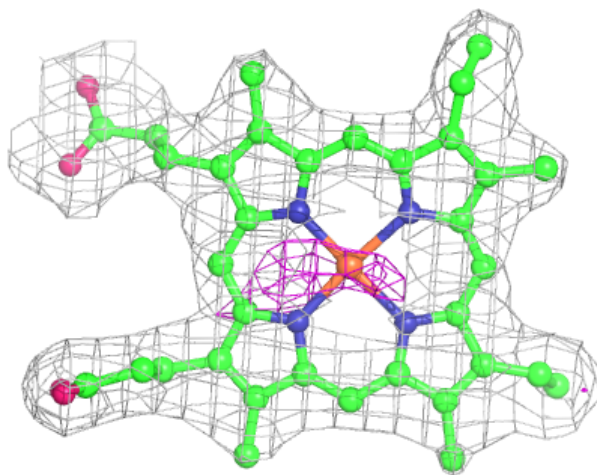
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM v 202:**

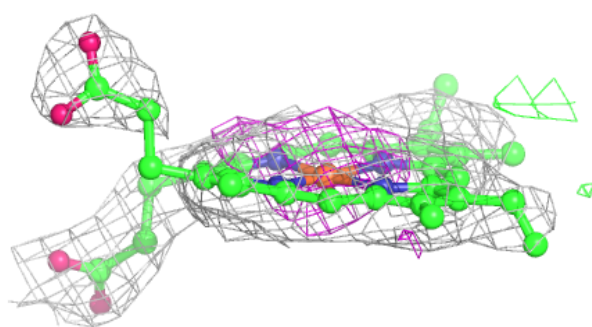
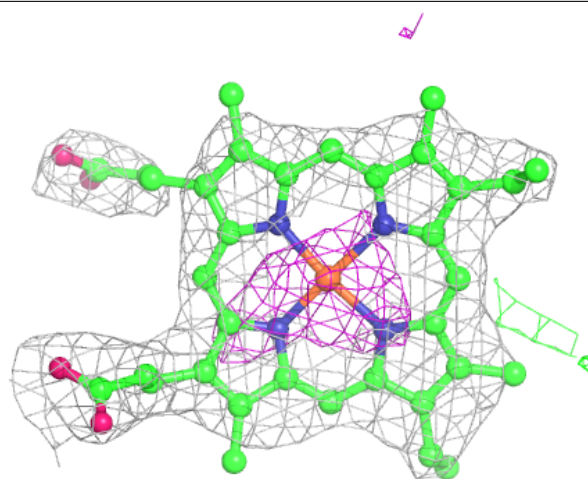
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.