



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:59 PM BST

PDB ID : 6JLK  
Title : XFEL structure of cyanobacterial photosystem II (1F state, dataset1)  
Authors : Suga, M.; Shen, J.R.  
Deposited on : 2019-03-06  
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

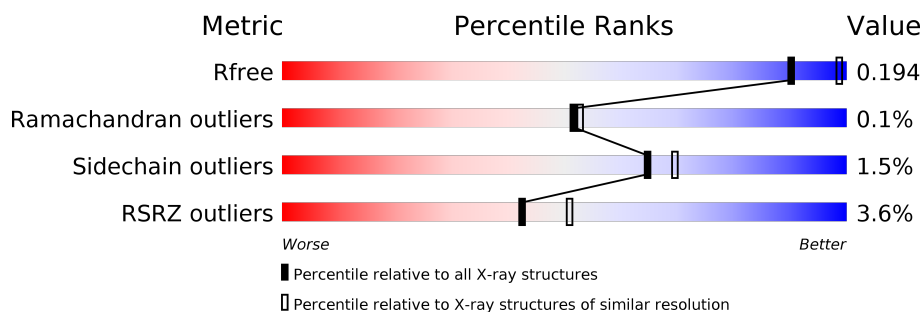
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 style="width: 97%;"></div> <div>97%</div> </div>
1	a	344	<div> <div style="width: 97%;"></div> <div>97%</div> </div>
2	B	505	<div> <div style="width: 99%;"></div> <div>99%</div> </div>
2	b	505	<div> <div style="width: 99%;"></div> <div>99%</div> </div>
3	C	455	<div> <div style="width: 98%;"></div> <div>98%</div> </div>
3	c	455	<div> <div style="width: 98%;"></div> <div>98%</div> </div>
4	D	342	<div> <div style="width: 99%;"></div> <div>99%</div> </div>

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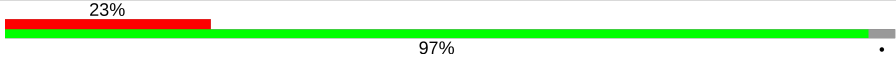
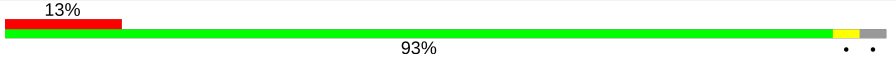
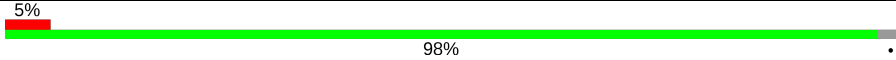
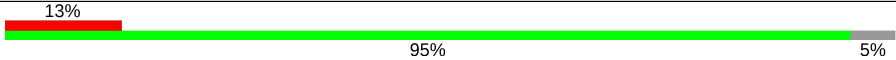
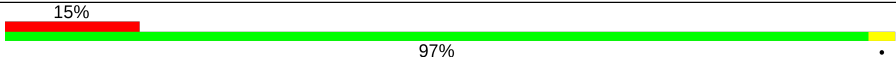
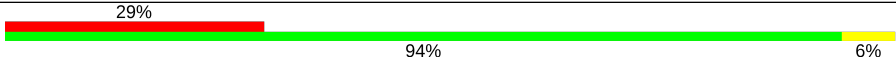



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Mol	Chain	Length	Quality of chain
4	d	342	 % 99%
5	E	84	 11% 95%
5	e	84	 14% 94%
6	F	44	 7% 77% 23%
6	f	44	 5% 70% 27%
7	H	65	 5% 97%
7	h	65	 3% 98%
8	I	38	 8% 97%
8	i	38	 3% 95% 5%
9	J	39	 8% 97%
9	j	39	 15% 97%
10	K	37	 97%
10	k	37	 95% 5%
11	L	37	 3% 97%
11	l	37	 5% 100%
12	M	36	 6% 86% 8% 6%
12	m	36	 3% 89% 6% 6%
13	O	244	 2% 98%
13	o	244	 2% 97%
14	T	32	 3% 88% 6% 6%
14	t	32	 88% 6% 6%
15	U	104	 91% 7%
15	u	104	 93% 7%
16	V	137	 100%
16	v	137	 2% 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	410	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	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	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	410	X	-	-	-
24	CLA	a	412	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	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
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	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	c	517	X	-	-	-
24	CLA	c	518	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 55631 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	53	0
			3019	1966	498	537	18			
1	a	334	Total	C	N	O	S	0	55	0
			3027	1973	498	538	18			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	7	0
			3518	2300	587	618	13			
3	c	455	Total	C	N	O	S	0	13	0
			3598	2356	599	629	14			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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



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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		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	1
			2	2		
21	a	1	Total	Fe	0	1
			2	2		

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

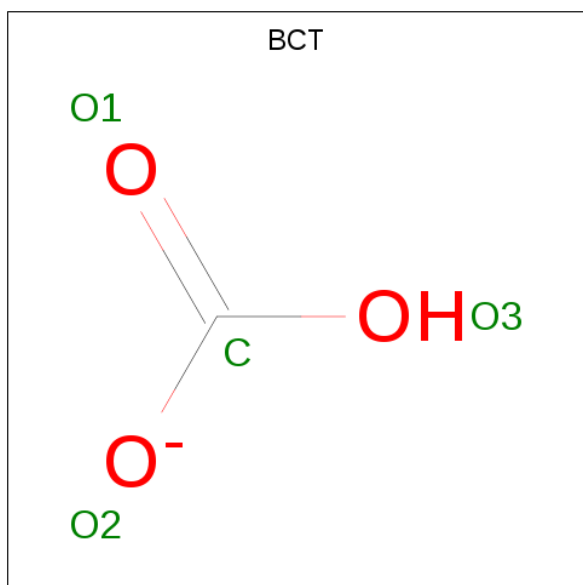
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

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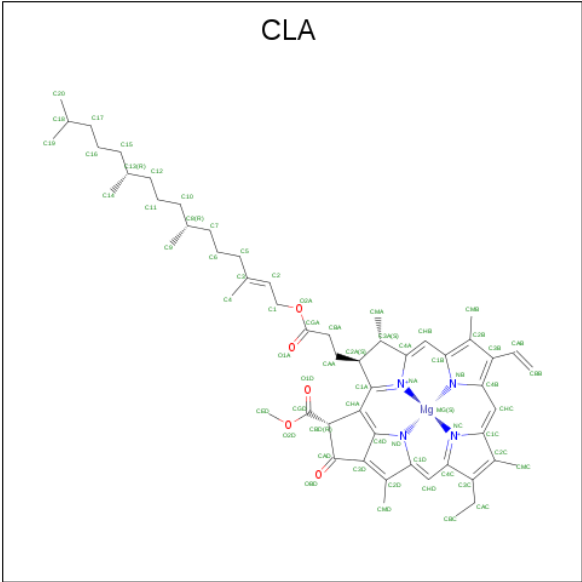
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

- 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	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

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



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

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

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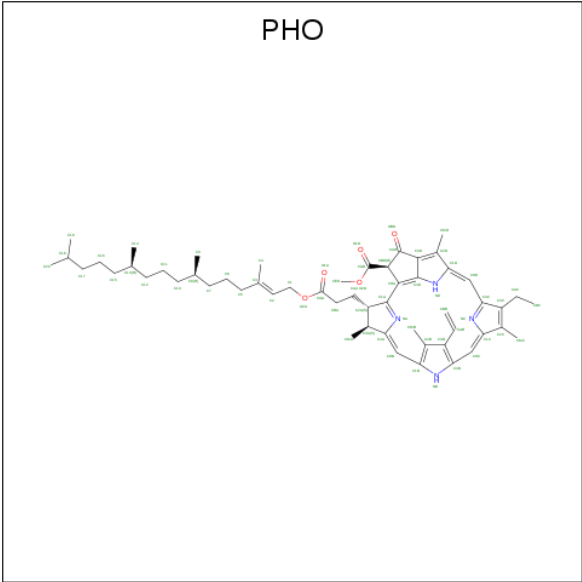
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

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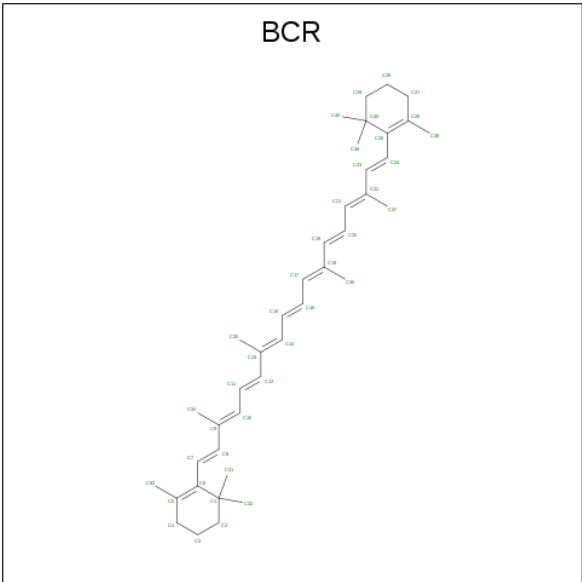
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	1
			128	110	8	10		

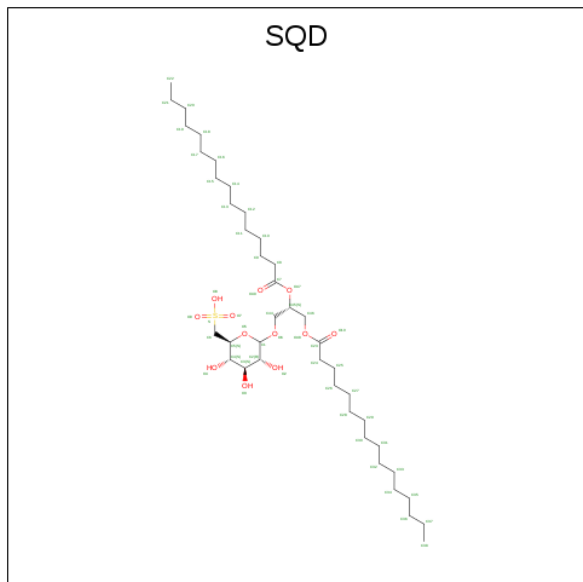
- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



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

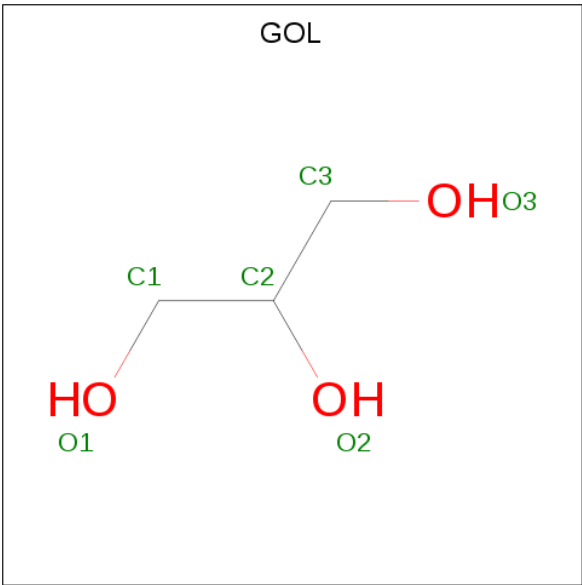


- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



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:  $C_3H_8O_3$ ).



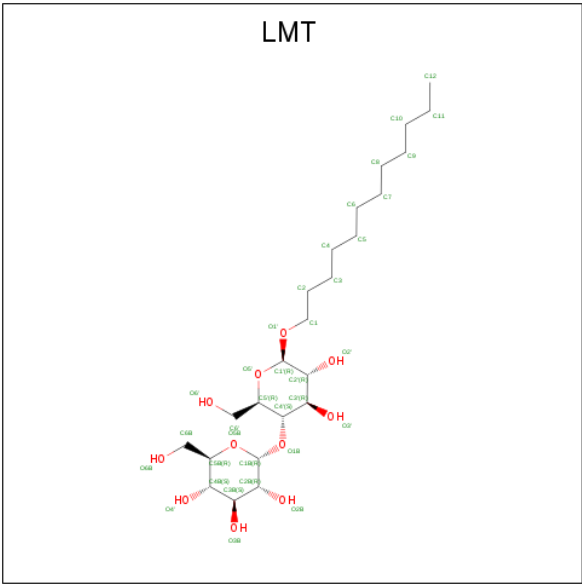
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

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

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



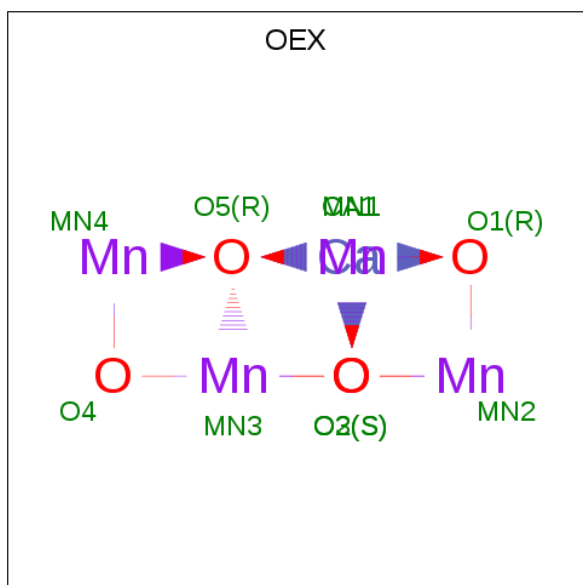
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			25	19	6		
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	f	1	Total	C	O	0	0
			35	24	11		

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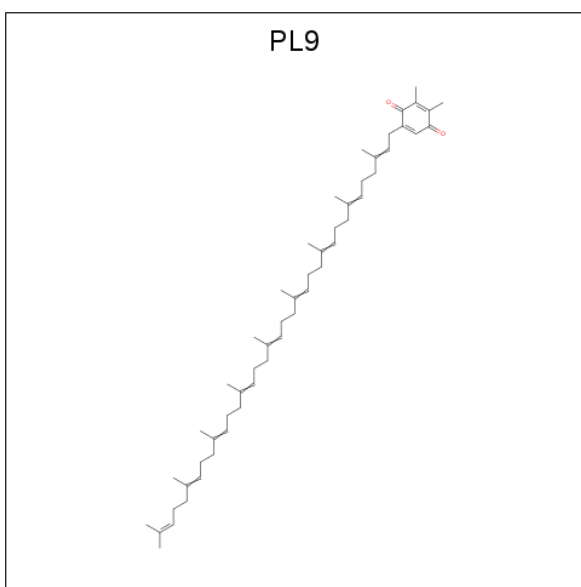
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
30	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

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



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

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

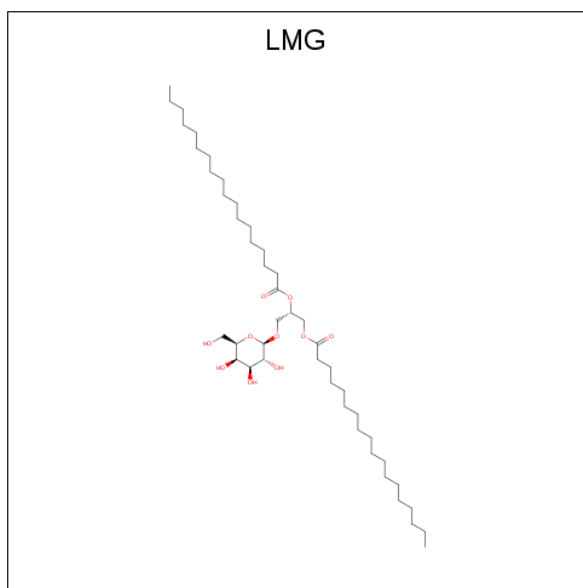
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	B	1	Total	C	O	0	0
			33	28	5		
32	I	1	Total	C	O	0	0
			40	35	5		
32	C	1	Total	C	O	0	0
			34	29	5		
32	a	1	Total	C	O	0	0
			30	25	5		
32	c	1	Total	C	O	0	0
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

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

- Molecule 33 is 1,2-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
33	C	1	Total C O 51 41 10	0	0

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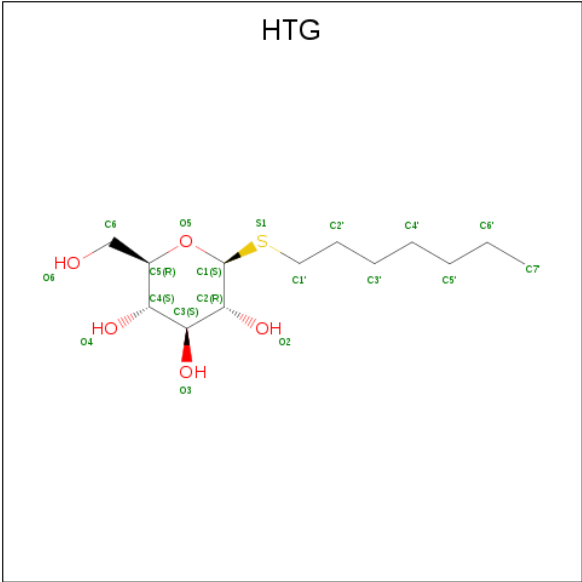
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	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).





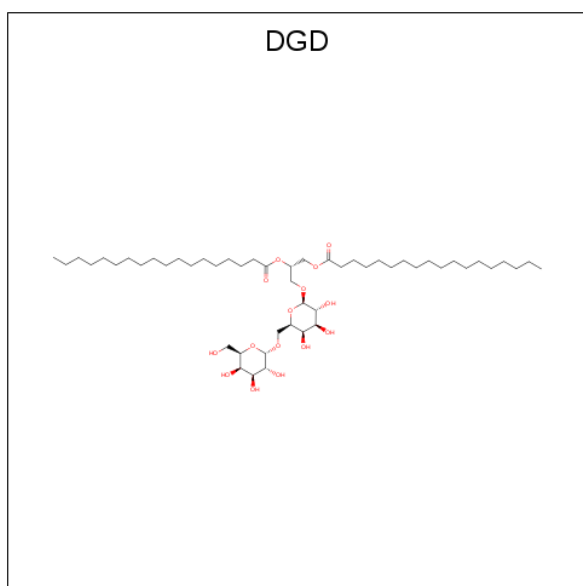
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



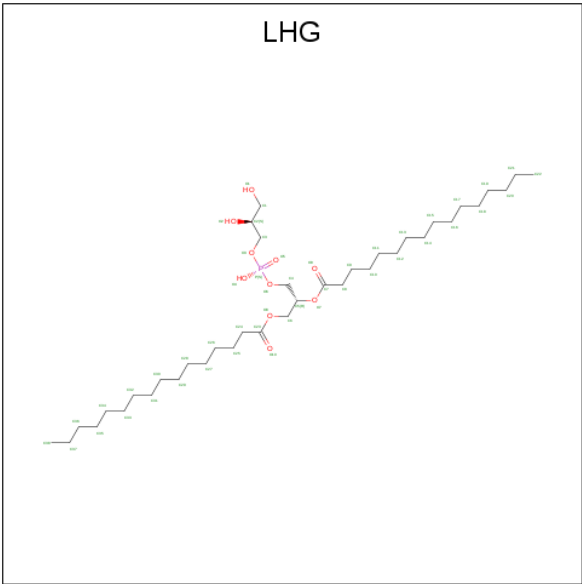
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	D	1	Total	C	O		0	0
			52	42	10			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

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

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



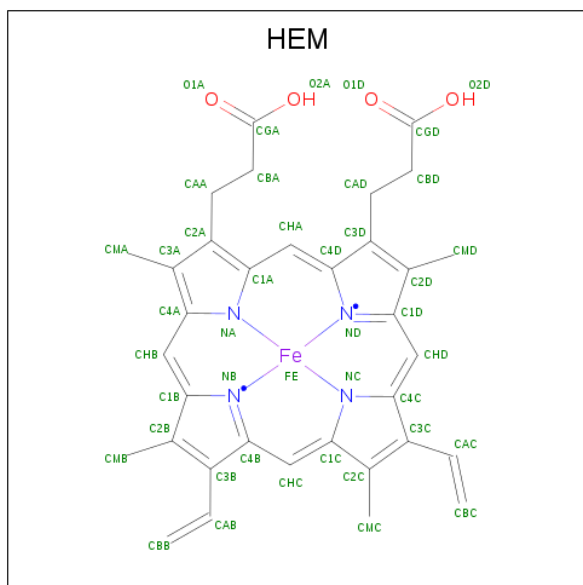
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	b	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	e	1	Total	C	O	P	0	0
			42	31	10	1		

- 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
40	A	166	Total O 179 179	0	15
40	B	289	Total O 293 293	0	4
40	C	229	Total O 233 233	0	6
40	D	146	Total O 151 151	0	5
40	E	32	Total O 33 33	0	1
40	F	8	Total O 8 8	0	0
40	H	44	Total O 44 44	0	0
40	I	5	Total O 5 5	0	0
40	J	12	Total O 12 12	0	0
40	K	8	Total O 8 8	0	0
40	L	18	Total O 19 19	0	1
40	M	19	Total O 19 19	0	0
40	O	175	Total O 177 177	0	2
40	T	16	Total O 17 17	0	1
40	U	82	Total O 82 82	0	0
40	V	113	Total O 115 115	0	2
40	Y	5	Total O 5 5	0	0
40	X	8	Total O 8 8	0	0
40	Z	1	Total O 1 1	0	0
40	a	155	Total O 167 167	0	14
40	b	259	Total O 262 262	0	3
40	c	202	Total O 207 207	0	7

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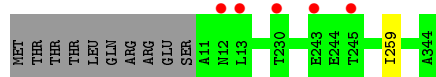
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	d	134	Total 137	O 137	0	3
40	e	16	Total 16	O 16	0	0
40	f	7	Total 7	O 7	0	0
40	h	42	Total 42	O 42	0	0
40	i	5	Total 5	O 5	0	0
40	j	7	Total 7	O 7	0	0
40	k	7	Total 7	O 7	0	0
40	l	9	Total 9	O 9	0	0
40	m	16	Total 16	O 16	0	0
40	o	157	Total 157	O 157	0	0
40	t	11	Total 11	O 11	0	0
40	u	93	Total 93	O 93	0	0
40	v	81	Total 82	O 82	0	1
40	y	2	Total 2	O 2	0	0
40	x	6	Total 6	O 6	0	0

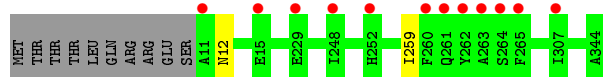
### 3 Residue-property plots [i](#)

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.

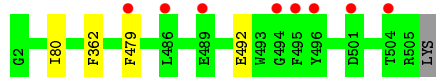
- Molecule 1: Photosystem II protein D1



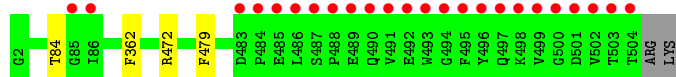
- Molecule 1: Photosystem II protein D1



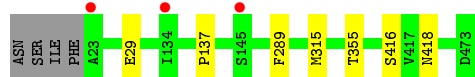
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



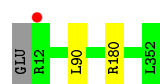
- Molecule 3: Photosystem II CP43 reaction center protein



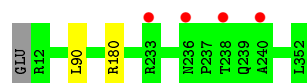
- Molecule 3: Photosystem II CP43 reaction center protein



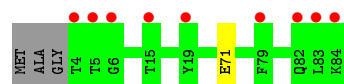
- Molecule 4: Photosystem II D2 protein



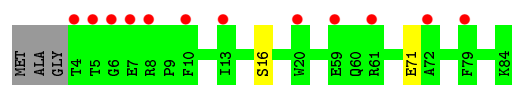
- Molecule 4: Photosystem II D2 protein



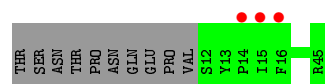
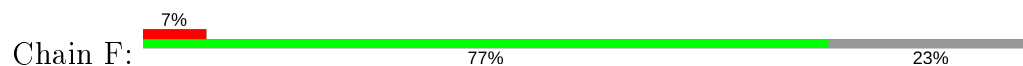
- Molecule 5: Cytochrome b559 subunit alpha



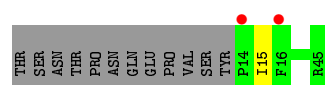
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta

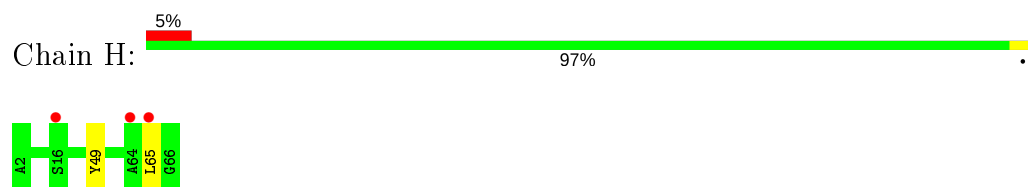


- Molecule 6: Cytochrome b559 subunit beta

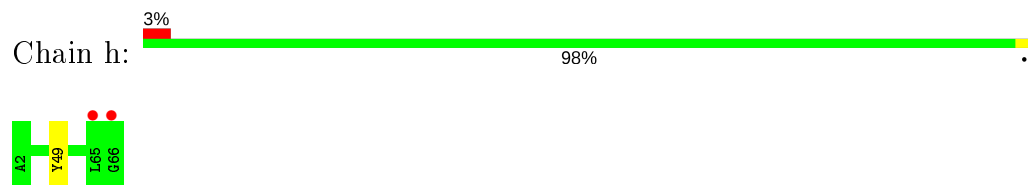




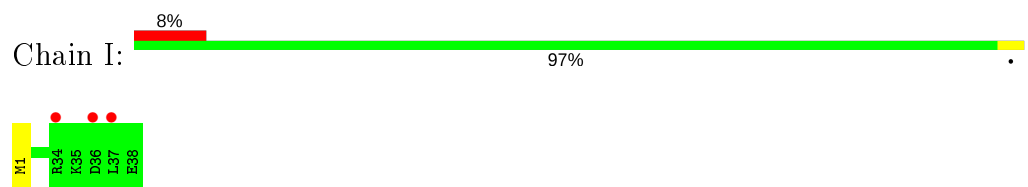
- Molecule 7: Photosystem II reaction center protein H



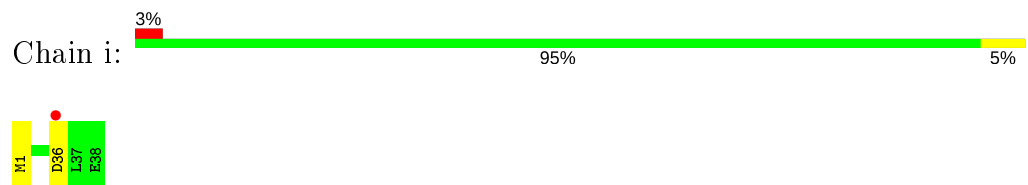
- Molecule 7: Photosystem II reaction center protein H



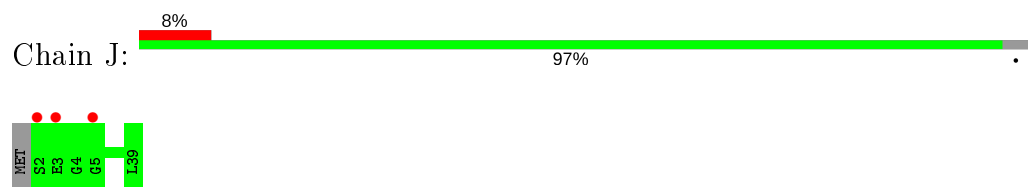
- Molecule 8: Photosystem II reaction center protein I



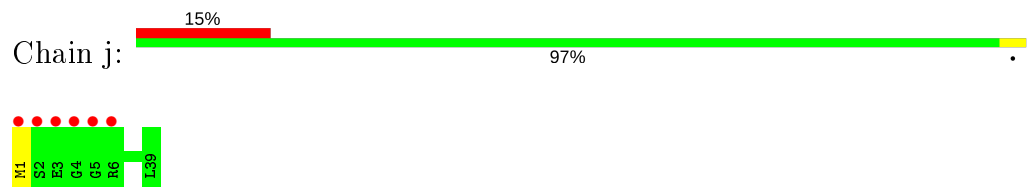
- Molecule 8: Photosystem II reaction center protein I



- 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: 95% 5%



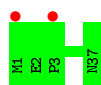
- Molecule 11: Photosystem II reaction center protein L

Chain L: 3% 97% .



- Molecule 11: Photosystem II reaction center protein L

Chain l: 5% 100%



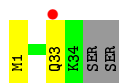
- Molecule 12: Photosystem II reaction center protein M

Chain M: 6% 86% 8% 6%



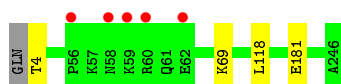
- Molecule 12: Photosystem II reaction center protein M

Chain m: 3% 89% 6% 6%

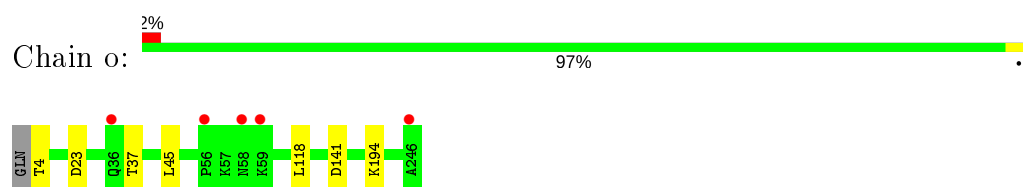


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

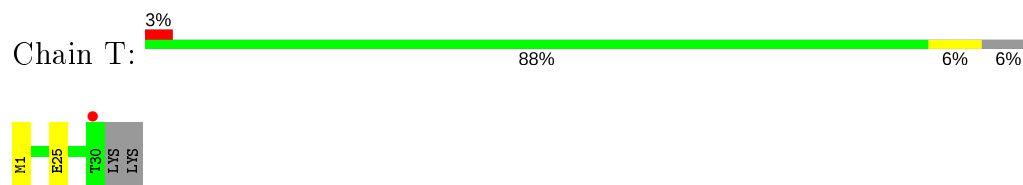
Chain O: 2% 98% .



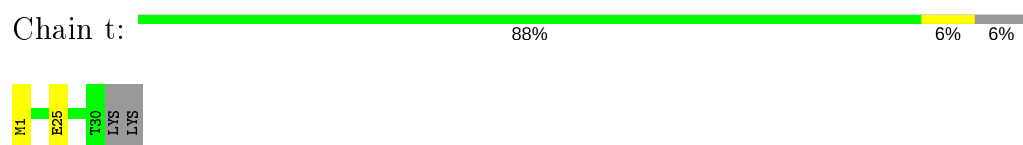
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



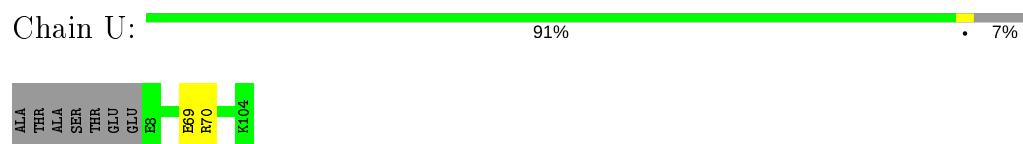
- Molecule 14: Photosystem II reaction center protein T



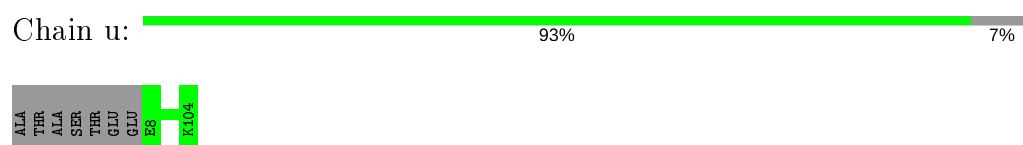
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

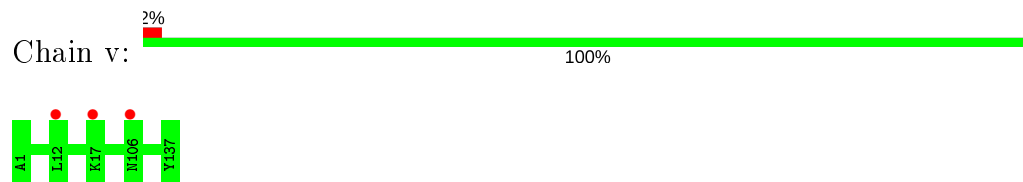


- Molecule 16: Cytochrome c-550



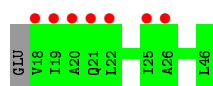
There are no outlier residues recorded for this chain.

- Molecule 16: Cytochrome c-550

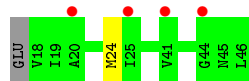


- Molecule 17: Photosystem II reaction center protein Ycf12





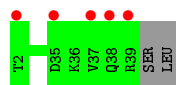
- Molecule 17: Photosystem II reaction center protein Ycf12



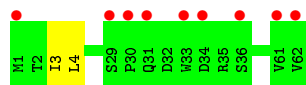
- Molecule 18: Photosystem II reaction center protein X



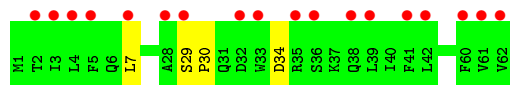
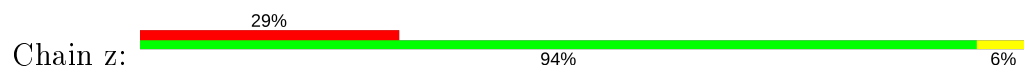
- Molecule 18: Photosystem II reaction center protein X



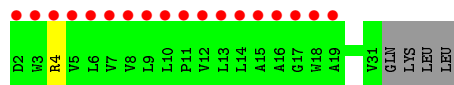
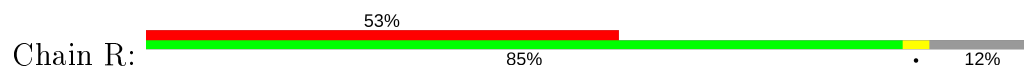
- Molecule 19: Photosystem II reaction center protein Z



- 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, $\alpha$ , $\beta$ , $\gamma$	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 178.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.15) 99.9 (178.86-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.149 , 0.193 0.151 , 0.194	Depositor DCC
$R_{free}$ test set	26831 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 79.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55631	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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	0.47	0/3121	0.56	0/4250
1	a	0.46	0/3135	0.55	0/4269
2	B	0.45	0/4191	0.53	0/5709
2	b	0.43	0/4198	0.52	0/5720
3	C	0.40	0/3643	0.50	0/4958
3	c	0.39	0/3731	0.51	0/5076
4	D	0.50	0/2952	0.56	0/4021
4	d	0.48	0/2952	0.53	0/4021
5	E	0.36	0/693	0.49	0/944
5	e	0.34	0/695	0.49	0/948
6	F	0.44	0/284	0.51	0/387
6	f	0.42	0/265	0.50	0/360
7	H	0.36	0/535	0.54	0/728
7	h	0.37	0/524	0.50	0/713
8	I	0.35	0/311	0.48	0/419
8	i	0.36	0/311	0.47	0/419
9	J	0.35	0/278	0.43	0/376
9	j	0.36	0/286	0.46	0/386
10	K	0.36	0/303	0.49	0/416
10	k	0.35	0/303	0.51	0/416
11	L	0.47	0/319	0.46	0/433
11	l	0.48	0/319	0.46	0/433
12	M	0.46	0/270	0.59	0/368
12	m	0.43	0/262	0.53	0/357
13	O	0.39	0/1958	0.55	0/2654
13	o	0.36	0/1937	0.52	0/2625
14	T	0.48	0/266	0.53	0/362
14	t	0.52	0/266	0.52	0/362
15	U	0.40	0/785	0.53	0/1064
15	u	0.40	0/785	0.53	0/1064
16	V	0.40	0/1109	0.51	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.35	0/1098	0.50	0/1488
17	Y	0.36	0/216	0.49	0/289
17	y	0.30	0/216	0.44	0/289
18	X	0.33	0/290	0.46	0/392
18	x	0.31	0/284	0.45	0/384
19	Z	0.30	0/490	0.42	0/669
19	z	0.28	0/490	0.44	0/669
20	R	0.23	0/245	0.37	0/338
All	All	0.42	0/44316	0.52	0/60278

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	384/344 (112%)	375 (98%)	8 (2%)	1 (0%)	41	37
1	a	386/344 (112%)	377 (98%)	8 (2%)	1 (0%)	41	37
2	B	512/505 (101%)	509 (99%)	3 (1%)	0	100	100
2	b	513/505 (102%)	504 (98%)	9 (2%)	0	100	100
3	C	456/455 (100%)	448 (98%)	6 (1%)	2 (0%)	34	29
3	c	466/455 (102%)	454 (97%)	10 (2%)	2 (0%)	34	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	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%)	59 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
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%)	92 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	36 (100%)	0	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%)	1 (2%)	1 (2%)	9	3
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5419/5384 (101%)	5300 (98%)	112 (2%)	7 (0%)	51	53

All (7) 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
1	a	259	ILE
19	z	30	PRO
1	A	259	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/279 (112%)	312 (100%)	0	100	100
1	a	314/279 (112%)	313 (100%)	1 (0%)	92	95
2	B	412/403 (102%)	408 (99%)	4 (1%)	76	81
2	b	413/403 (102%)	409 (99%)	4 (1%)	76	81
3	C	357/356 (100%)	351 (98%)	6 (2%)	60	65
3	c	367/356 (103%)	357 (97%)	10 (3%)	44	46
4	D	290/277 (105%)	288 (99%)	2 (1%)	84	89
4	d	290/277 (105%)	288 (99%)	2 (1%)	84	89
5	E	74/73 (101%)	73 (99%)	1 (1%)	67	72
5	e	74/73 (101%)	72 (97%)	2 (3%)	44	46
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	33
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	61
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	42
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	32
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	37
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	11
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	44
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	29 (94%)	2 (6%)	17	12
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	37
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	53
13	o	211/207 (102%)	204 (97%)	7 (3%)	38	37
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	9
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	9
15	U	84/89 (94%)	83 (99%)	1 (1%)	71	76
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	22/23 (96%)	22 (100%)	0	100	100
17	y	22/23 (96%)	21 (96%)	1 (4%)	27	24
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%)	50 (96%)	2 (4%)	33	31
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	15
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	29
All	All	4500/4403 (102%)	4431 (98%)	69 (2%)	65	69

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	80	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	362	PHE
2	B	479	PHE
2	B	492	GLU
3	C	29	GLU
3	C	137	PRO
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	418	ASN
4	D	90	LEU
4	D	180	ARG
5	E	71	GLU
7	H	49	TYR
7	H	65	LEU
10	K	17	ILE
11	L	13	ASN
12	M	5	GLN
12	M	9	ILE
13	O	4	THR
13	O	69	LYS
13	O	118	LEU
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
19	Z	3	ILE
19	Z	4	LEU
20	R	4	ARG
1	a	12	ASN
2	b	84	THR
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
3	c	19	ASN
3	c	79	LYS
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	90	LEU
4	d	180	ARG
5	e	16	SER
5	e	71	GLU
6	f	15	ILE
7	h	49	TYR
8	i	36	ASP
9	j	1	MET
10	k	10	LYS
10	k	17	ILE
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	37	THR
13	o	45	LEU
13	o	118	LEU
13	o	141	ASP
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
17	y	24	MET
19	z	7	LEU
19	z	29	SER
19	z	34	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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
3	C	201	ASN
3	C	418	ASN
4	D	61	HIS
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN

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Mol	Chain	Res	Type
19	Z	58	ASN
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
13	o	130	GLN
19	z	58	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
12	FME	M	1	12	8,9,10	0.68	0	7,9,11	1.31	1 (14%)
12	FME	m	1	12	8,9,10	0.64	0	7,9,11	1.52	3 (42%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.28	1 (14%)
14	FME	t	1	14	8,9,10	0.80	0	7,9,11	2.19	4 (57%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.09	1 (14%)
14	FME	T	1	14	8,9,10	0.68	0	7,9,11	1.31	1 (14%)

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

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

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.45	117.52	122.82
14	t	1	FME	C-CA-N	2.48	114.20	109.73
14	t	1	FME	O-C-CA	-2.44	118.37	124.78
14	T	1	FME	O-C-CA	-2.44	118.38	124.78
12	m	1	FME	CA-N-CN	-2.29	119.30	122.82
12	m	1	FME	O-C-CA	-2.22	118.97	124.78
12	m	1	FME	O1-CN-N	-2.17	119.56	125.27
8	I	1	FME	O-C-CA	-2.16	119.13	124.78
8	i	1	FME	O-C-CA	-2.11	119.25	124.78
14	t	1	FME	CE-SD-CG	-2.04	93.40	100.40
12	M	1	FME	CA-N-CN	-2.01	119.73	122.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

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 267 ligands modelled in this entry, 18 are unknown and 25 are monoatomic - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	OEX	A	418[A]	1,3,40	0,15,15	0.00	-	-		
24	CLA	C	503	-	59,73,73	2.02	13 (22%)	67,113,113	2.02	18 (26%)
31	PL9	d	405[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.55	13 (19%)
24	CLA	c	513	-	59,73,73	2.09	13 (22%)	67,113,113	2.23	21 (31%)
36	DGD	c	521	-	63,63,67	0.88	2 (3%)	77,77,81	0.94	5 (6%)
28	GOL	v	203	-	5,5,5	0.39	0	5,5,5	0.23	0
26	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.45	9 (16%)
24	CLA	c	516	3	59,73,73	2.00	13 (22%)	67,113,113	2.03	23 (34%)
38	HEM	e	103	5,6	27,50,50	0.78	2 (7%)	17,82,82	1.70	2 (11%)
33	LMG	A	421	-	51,51,55	0.93	2 (3%)	59,59,63	1.10	4 (6%)
24	CLA	B	614	-	59,73,73	2.04	13 (22%)	67,113,113	2.08	25 (37%)
28	GOL	V	201	-	5,5,5	0.39	0	5,5,5	0.32	0
24	CLA	C	502	-	59,73,73	1.97	13 (22%)	67,113,113	2.11	22 (32%)
36	DGD	C	517	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	6 (7%)
24	CLA	b	624	-	59,73,73	1.97	13 (22%)	67,113,113	2.18	21 (31%)
26	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	7 (12%)
24	CLA	c	508	-	59,73,73	2.00	13 (22%)	67,113,113	2.10	18 (26%)
36	DGD	C	518	-	63,63,67	0.87	2 (3%)	77,77,81	0.90	4 (5%)
37	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	5 (9%)
33	LMG	d	413	39	51,51,55	0.92	2 (3%)	59,59,63	0.94	3 (5%)
28	GOL	A	422	34	5,5,5	0.35	0	5,5,5	0.22	0
33	LMG	c	524	-	51,51,55	0.96	2 (3%)	59,59,63	1.24	7 (11%)
37	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	0.86	3 (5%)
29	LMT	a	419	-	36,36,36	0.45	0	47,47,47	0.77	0
38	HEM	v	205	16	27,50,50	0.78	0	17,82,82	1.21	2 (11%)
24	CLA	c	506	-	59,73,73	1.96	13 (22%)	67,113,113	2.17	21 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	GOL	B	636	-	5,5,5	0.40	0	5,5,5	0.46	0
26	BCR	t	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	15 (26%)
24	CLA	A	405	-	59,73,73	2.03	13 (22%)	67,113,113	2.25	23 (34%)
24	CLA	B	603	-	59,73,73	2.04	13 (22%)	67,113,113	2.27	23 (34%)
35	HTG	b	601	-	19,19,19	0.97	1 (5%)	23,24,24	1.09	2 (8%)
28	GOL	O	301	-	5,5,5	0.35	0	5,5,5	0.39	0
33	LMG	D	413	39	51,51,55	0.87	2 (3%)	59,59,63	1.00	5 (8%)
24	CLA	b	616	40	59,73,73	1.92	13 (22%)	67,113,113	2.16	20 (29%)
26	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	8 (14%)
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.32	0
28	GOL	t	102	-	5,5,5	0.48	0	5,5,5	0.11	0
33	LMG	b	629	-	51,51,55	0.90	2 (3%)	59,59,63	1.07	5 (8%)
24	CLA	C	511	3	59,73,73	2.03	12 (20%)	67,113,113	2.13	23 (34%)
28	GOL	a	420	34	5,5,5	0.33	0	5,5,5	0.41	0
29	LMT	A	417	-	36,36,36	0.59	1 (2%)	47,47,47	1.25	4 (8%)
36	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.16	8 (10%)
26	BCR	c	528	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	7 (12%)
24	CLA	B	604	-	59,73,73	2.04	13 (22%)	67,113,113	2.34	23 (34%)
24	CLA	C	512	-	59,73,73	2.01	13 (22%)	67,113,113	2.23	22 (32%)
24	CLA	B	616	-	59,73,73	1.93	12 (20%)	67,113,113	2.09	20 (29%)
28	GOL	A	413	-	5,5,5	0.29	0	5,5,5	0.40	0
26	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	8 (14%)
24	CLA	A	406	40	59,73,73	1.95	15 (25%)	67,113,113	2.32	28 (41%)
29	LMT	f	102	-	36,36,36	0.47	0	47,47,47	0.91	1 (2%)
25	PHO	a	411	-	67,69,69	2.13	17 (25%)	85,99,99	1.88	23 (27%)
28	GOL	v	201	-	5,5,5	0.32	0	5,5,5	0.24	0
28	GOL	A	414	-	5,5,5	0.44	0	5,5,5	0.48	0
26	BCR	C	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.48	10 (17%)
24	CLA	C	509	-	59,73,73	2.10	13 (22%)	67,113,113	2.21	22 (32%)
29	LMT	F	101	-	36,36,36	0.47	0	47,47,47	0.93	1 (2%)
38	HEM	V	205	16	27,50,50	0.88	1 (3%)	17,82,82	1.43	2 (11%)
24	CLA	b	610	40	59,73,73	2.03	13 (22%)	67,113,113	2.23	20 (29%)
24	CLA	A	410	-	59,73,73	2.02	13 (22%)	67,113,113	2.16	26 (38%)
26	BCR	D	404	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	9 (16%)
28	GOL	T	101	-	5,5,5	0.45	0	5,5,5	0.13	0
35	HTG	B	624	-	19,19,19	0.78	1 (5%)	23,24,24	1.64	3 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	C	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.50	9 (16%)
24	CLA	D	403	-	59,73,73	1.99	13 (22%)	67,113,113	2.21	23 (34%)
25	PHO	A	409[A]	-	67,69,69	2.13	17 (25%)	85,99,99	1.94	20 (23%)
24	CLA	b	625	-	59,73,73	2.00	12 (20%)	67,113,113	2.28	24 (35%)
37	LHG	b	634	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	4 (7%)
28	GOL	B	631	-	5,5,5	0.40	0	5,5,5	0.28	0
24	CLA	b	618	-	59,73,73	1.97	13 (22%)	67,113,113	2.17	23 (34%)
31	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.65	20 (29%)
25	PHO	A	409[B]	-	67,69,69	2.15	16 (23%)	85,99,99	1.94	20 (23%)
24	CLA	B	612	-	59,73,73	1.97	13 (22%)	67,113,113	2.28	21 (31%)
24	CLA	C	505	-	59,73,73	1.93	13 (22%)	67,113,113	2.14	18 (26%)
24	CLA	C	501	-	59,73,73	1.98	13 (22%)	67,113,113	2.13	20 (29%)
24	CLA	B	605	-	59,73,73	1.95	14 (23%)	67,113,113	2.16	22 (32%)
35	HTG	B	625	-	19,19,19	1.06	2 (10%)	23,24,24	1.85	4 (17%)
29	LMT	B	635	-	25,25,36	0.52	0	30,30,47	0.83	1 (3%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.10	3 (6%)
24	CLA	d	402	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	22 (32%)
26	BCR	c	519	-	41,41,41	1.02	1 (2%)	56,56,56	1.44	7 (12%)
24	CLA	d	403	-	59,73,73	2.00	14 (23%)	67,113,113	2.16	23 (34%)
24	CLA	B	602	40	59,73,73	2.03	12 (20%)	67,113,113	2.17	20 (29%)
28	GOL	B	626	-	5,5,5	0.43	0	5,5,5	0.36	0
24	CLA	b	622	-	59,73,73	2.01	12 (20%)	67,113,113	2.12	22 (32%)
28	GOL	o	301	-	5,5,5	0.38	0	5,5,5	0.22	0
30	OEX	a	416[A]	1,3,40	0,15,15	0.00	-	-		
27	SQD	a	414	-	53,54,54	0.96	3 (5%)	62,65,65	1.63	13 (20%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.96	1 (3%)
37	LHG	d	407	-	48,48,48	0.88	2 (4%)	51,54,54	0.99	4 (7%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
28	GOL	c	502	-	5,5,5	0.27	0	5,5,5	0.47	0
37	LHG	d	406	-	48,48,48	0.90	3 (6%)	51,54,54	1.04	4 (7%)
31	PL9	A	419[B]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
24	CLA	b	621	-	59,73,73	2.06	14 (23%)	67,113,113	2.27	25 (37%)
29	LMT	M	103	-	36,36,36	0.53	1 (2%)	47,47,47	0.96	3 (6%)
30	OEX	a	416[B]	1,3,40	0,15,15	0.00	-	-		
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.26	0
35	HTG	B	623	-	19,19,19	1.03	1 (5%)	23,24,24	1.18	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LMT	b	630	-	25,25,36	0.51	0	30,30,47	0.67	0
26	BCR	k	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.41	8 (14%)
26	BCR	A	411	-	41,41,41	0.99	1 (2%)	56,56,56	1.14	6 (10%)
24	CLA	C	504	40	59,73,73	2.07	14 (23%)	67,113,113	2.21	22 (32%)
24	CLA	b	615	-	59,73,73	1.97	12 (20%)	67,113,113	2.30	22 (32%)
24	CLA	c	510	-	59,73,73	1.94	13 (22%)	67,113,113	2.27	19 (28%)
24	CLA	B	606	-	59,73,73	2.01	13 (22%)	67,113,113	2.25	21 (31%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.21	3 (6%)
24	CLA	B	607	-	59,73,73	1.97	14 (23%)	67,113,113	2.31	24 (35%)
27	SQD	B	621	-	53,54,54	1.02	3 (5%)	62,65,65	1.48	9 (14%)
29	LMT	m	103	-	36,36,36	0.47	0	47,47,47	0.99	3 (6%)
29	LMT	a	404	-	36,36,36	0.46	0	47,47,47	1.08	3 (6%)
24	CLA	c	507	-	59,73,73	2.03	14 (23%)	67,113,113	2.15	20 (29%)
35	HTG	D	412	-	16,16,19	1.13	2 (12%)	20,21,24	1.50	1 (5%)
24	CLA	b	612	-	59,73,73	2.03	13 (22%)	67,113,113	2.30	24 (35%)
24	CLA	c	512	40	59,73,73	1.98	13 (22%)	67,113,113	2.28	20 (29%)
36	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	0.97	4 (5%)
27	SQD	f	101	-	42,43,54	1.19	3 (7%)	51,54,65	1.46	9 (17%)
31	PL9	d	405[A]	-	55,55,55	0.70	2 (3%)	68,69,69	1.54	16 (23%)
24	CLA	B	611	40	59,73,73	2.05	15 (25%)	67,113,113	2.18	25 (37%)
35	HTG	c	526	-	19,19,19	1.02	2 (10%)	23,24,24	1.47	2 (8%)
35	HTG	b	607	-	19,19,19	1.00	2 (10%)	23,24,24	1.22	1 (4%)
37	LHG	e	102	-	41,41,48	1.02	2 (4%)	44,47,54	0.95	2 (4%)
24	CLA	b	619	40	59,73,73	2.03	14 (23%)	67,113,113	2.16	22 (32%)
28	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.76	0
35	HTG	c	525	-	19,19,19	1.05	2 (10%)	23,24,24	1.55	2 (8%)
28	GOL	C	525	-	5,5,5	0.34	0	5,5,5	0.48	0
31	PL9	A	419[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.77	22 (32%)
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	1.04	1 (2%)
24	CLA	c	509	40	59,73,73	2.01	13 (22%)	67,113,113	2.27	24 (35%)
33	LMG	B	622	-	51,51,55	0.92	2 (3%)	59,59,63	1.07	5 (8%)
35	HTG	C	523	-	19,19,19	1.00	1 (5%)	23,24,24	1.78	4 (17%)
24	CLA	B	609	-	59,73,73	1.98	13 (22%)	67,113,113	2.15	24 (35%)
24	CLA	a	410	40	59,73,73	1.99	13 (22%)	67,113,113	2.17	23 (34%)
23	BCT	A	404[A]	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	BCR	b	628	-	41,41,41	1.08	1 (2%)	56,56,56	1.24	6 (10%)
23	BCT	A	404[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	b	606	-	5,5,5	0.36	0	5,5,5	0.28	0
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.08	4 (9%)
27	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.56	10 (16%)
28	GOL	b	604	-	5,5,5	0.38	0	5,5,5	0.24	0
36	DGD	D	406	-	52,52,67	1.02	3 (5%)	60,60,81	1.18	5 (8%)
27	SQD	A	412	-	53,54,54	0.97	3 (5%)	62,65,65	1.53	11 (17%)
35	HTG	B	632	-	19,19,19	1.06	2 (10%)	23,24,24	1.40	3 (13%)
28	GOL	A	415	-	5,5,5	0.41	0	5,5,5	0.22	0
37	LHG	D	409	-	48,48,48	0.97	2 (4%)	51,54,54	1.03	3 (5%)
31	PL9	a	415[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	20 (29%)
35	HTG	V	206	-	19,19,19	1.02	2 (10%)	23,24,24	1.32	3 (13%)
31	PL9	a	415[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.91	20 (29%)
27	SQD	F	103	-	42,43,54	1.16	3 (7%)	51,54,65	1.59	11 (21%)
26	BCR	b	626	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	6 (10%)
35	HTG	b	632	-	19,19,19	1.13	2 (10%)	23,24,24	1.75	3 (13%)
28	GOL	c	503	-	5,5,5	0.39	0	5,5,5	0.61	0
23	BCT	a	417[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	b	603	-	5,5,5	0.33	0	5,5,5	0.12	0
24	CLA	C	507	40	59,73,73	1.99	13 (22%)	67,113,113	2.06	22 (32%)
24	CLA	B	608	40	59,73,73	1.89	13 (22%)	67,113,113	2.13	27 (40%)
25	PHO	A	408	-	67,69,69	2.13	17 (25%)	85,99,99	1.87	20 (23%)
35	HTG	b	608	-	19,19,19	1.06	2 (10%)	23,24,24	1.28	3 (13%)
33	LMG	c	501	-	51,51,55	0.89	2 (3%)	59,59,63	1.17	4 (6%)
28	GOL	B	627	-	5,5,5	0.33	0	5,5,5	0.47	0
26	BCR	T	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.54	12 (21%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.25	0
24	CLA	b	611	-	59,73,73	1.98	13 (22%)	67,113,113	2.24	23 (34%)
24	CLA	d	401	40	59,73,73	2.04	14 (23%)	67,113,113	2.29	27 (40%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.26	0
29	LMT	M	101	-	36,36,36	0.40	0	47,47,47	0.90	0
24	CLA	c	511	-	59,73,73	2.00	14 (23%)	67,113,113	2.20	26 (38%)
24	CLA	b	614	-	59,73,73	1.97	12 (20%)	67,113,113	2.28	19 (28%)
24	CLA	C	510	-	59,73,73	2.01	13 (22%)	67,113,113	2.11	23 (34%)
24	CLA	B	613	-	59,73,73	2.02	12 (20%)	67,113,113	2.18	23 (34%)
36	DGD	c	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	SQD	A	416	-	53,54,54	1.04	3 (5%)	62,65,65	1.14	4 (6%)
24	CLA	b	617	-	59,73,73	2.03	13 (22%)	67,113,113	2.13	22 (32%)
36	DGD	c	522	-	63,63,67	0.90	2 (3%)	77,77,81	1.01	4 (5%)
24	CLA	C	508	-	59,73,73	2.08	13 (22%)	67,113,113	2.14	20 (29%)
33	LMG	Z	101	-	37,37,55	0.96	2 (5%)	45,45,63	1.39	6 (13%)
28	GOL	a	401	-	5,5,5	0.44	0	5,5,5	0.48	0
28	GOL	B	629	-	5,5,5	0.33	0	5,5,5	0.36	0
36	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.01	8 (10%)
35	HTG	b	631	-	19,19,19	0.81	1 (5%)	23,24,24	1.41	2 (8%)
24	CLA	c	517	-	59,73,73	2.04	13 (22%)	67,113,113	2.30	23 (34%)
28	GOL	b	605	-	5,5,5	0.36	0	5,5,5	0.30	0
33	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	0.99	4 (6%)
35	HTG	C	522	-	19,19,19	1.03	2 (10%)	23,24,24	1.59	2 (8%)
36	DGD	e	101	-	63,63,67	0.92	2 (3%)	77,77,81	1.18	7 (9%)
24	CLA	B	615	-	59,73,73	1.98	13 (22%)	67,113,113	2.24	21 (31%)
24	CLA	C	506	-	59,73,73	2.01	14 (23%)	67,113,113	2.18	24 (35%)
24	CLA	D	402	-	59,73,73	1.98	14 (23%)	67,113,113	2.30	24 (35%)
26	BCR	B	620	-	41,41,41	1.06	1 (2%)	56,56,56	1.43	6 (10%)
35	HTG	d	411	-	16,16,19	1.14	2 (12%)	20,21,24	1.72	2 (10%)
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	9 (16%)
27	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.20	5 (8%)
30	OEX	A	418[B]	1,3,40	0,15,15	0.00	-	-	-	-
24	CLA	b	623	-	59,73,73	2.02	13 (22%)	67,113,113	2.25	24 (35%)
33	LMG	c	523	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)
28	GOL	V	203	-	5,5,5	0.38	0	5,5,5	0.29	0
31	PL9	D	405[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.74	20 (29%)
28	GOL	b	602	-	5,5,5	0.43	0	5,5,5	0.48	0
37	LHG	D	407	-	48,48,48	0.84	2 (4%)	51,54,54	1.14	5 (9%)
24	CLA	B	610	-	59,73,73	2.00	13 (22%)	67,113,113	2.15	22 (32%)
26	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.69	13 (23%)
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.31	6 (10%)
28	GOL	B	628	-	5,5,5	0.34	0	5,5,5	0.54	0
26	BCR	Y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	10 (17%)
28	GOL	V	202	-	5,5,5	0.39	0	5,5,5	0.37	0
28	GOL	v	202	-	5,5,5	0.34	0	5,5,5	0.25	0
24	CLA	a	412	-	59,73,73	1.99	14 (23%)	67,113,113	2.24	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	a	409	-	59,73,73	1.99	13 (22%)	67,113,113	2.19	24 (35%)
26	BCR	a	413	-	41,41,41	1.03	1 (2%)	56,56,56	1.14	6 (10%)
29	LMT	m	102	-	36,36,36	0.47	0	47,47,47	0.83	0
24	CLA	A	407	40	59,73,73	2.03	13 (22%)	67,113,113	2.14	23 (34%)
24	CLA	c	518	-	59,73,73	2.01	13 (22%)	67,113,113	2.15	21 (31%)
24	CLA	b	620	-	59,73,73	1.96	12 (20%)	67,113,113	2.13	22 (32%)
35	HTG	B	633	-	19,19,19	1.01	2 (10%)	23,24,24	1.44	1 (4%)
24	CLA	b	613	-	59,73,73	1.95	12 (20%)	67,113,113	2.24	21 (31%)
24	CLA	C	513	-	59,73,73	2.01	13 (22%)	67,113,113	2.07	23 (34%)
25	PHO	a	418[B]	-	67,69,69	2.13	16 (23%)	85,99,99	2.01	22 (25%)
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.25	4 (7%)
25	PHO	a	418[A]	-	67,69,69	2.11	17 (25%)	85,99,99	2.07	22 (25%)
24	CLA	B	617	-	59,73,73	1.99	13 (22%)	67,113,113	2.28	21 (31%)
24	CLA	c	514	-	59,73,73	2.05	13 (22%)	67,113,113	2.20	21 (31%)
38	HEM	F	102	5,6	27,50,50	0.90	2 (7%)	17,82,82	2.26	3 (17%)
24	CLA	c	515	-	59,73,73	2.01	13 (22%)	67,113,113	2.19	23 (34%)
37	LHG	d	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	2 (3%)
23	BCT	a	417[A]	21	0,3,3	0.00	-	0,3,3	0.00	-

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
24	CLA	C	503	-	3/3/20/25	2/37/135/135	-
31	PL9	d	405[B]	-	-	8/53/73/73	0/1/1/1
24	CLA	c	513	-	3/3/20/25	5/37/135/135	-
36	DGD	c	521	-	-	16/51/91/95	0/2/2/2
28	GOL	v	203	-	-	2/4/4/4	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	516	3	3/3/20/25	5/37/135/135	-
38	HEM	e	103	5,6	-	2/6/54/54	-
33	LMG	A	421	-	-	18/46/66/70	0/1/1/1
24	CLA	B	614	-	3/3/20/25	5/37/135/135	-
28	GOL	V	201	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	502	-	2/2/20/25	5/37/135/135	-
36	DGD	C	517	-	-	16/51/91/95	0/2/2/2
24	CLA	b	624	-	3/3/20/25	3/37/135/135	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
28	GOL	b	602	-	-	0/4/4/4	-
24	CLA	c	508	-	2/2/20/25	2/37/135/135	-
36	DGD	C	518	-	-	10/51/91/95	0/2/2/2
37	LHG	L	101	-	-	14/53/53/53	-
33	LMG	d	413	39	-	11/46/66/70	0/1/1/1
28	GOL	A	422	34	-	2/4/4/4	-
33	LMG	c	524	-	-	4/46/66/70	0/1/1/1
37	LHG	D	408	-	-	8/53/53/53	-
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
38	HEM	v	205	16	-	0/6/54/54	-
24	CLA	c	506	-	3/3/20/25	2/37/135/135	-
28	GOL	B	636	-	-	0/4/4/4	-
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
24	CLA	A	405	-	3/3/20/25	4/37/135/135	-
24	CLA	B	603	-	2/2/20/25	4/37/135/135	-
35	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	c	510	-	2/2/20/25	3/37/135/135	-
33	LMG	D	413	39	-	9/46/66/70	0/1/1/1
24	CLA	b	616	40	3/3/20/25	1/37/135/135	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
28	GOL	V	204	-	-	0/4/4/4	-
28	GOL	t	102	-	-	0/4/4/4	-
38	HEM	V	205	16	-	0/6/54/54	-
24	CLA	C	511	3	3/3/20/25	3/37/135/135	-
28	GOL	a	420	34	-	3/4/4/4	-
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
36	DGD	C	516	-	-	12/51/91/95	0/2/2/2
24	CLA	c	514	-	3/3/20/25	12/37/135/135	-
24	CLA	B	604	-	3/3/20/25	4/37/135/135	-
24	CLA	C	512	-	3/3/20/25	10/37/135/135	-
24	CLA	B	616	-	3/3/20/25	11/37/135/135	-
28	GOL	A	413	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	H	101	-	-	1/29/63/63	0/2/2/2
24	CLA	A	406	40	3/3/20/25	4/37/135/135	-
29	LMT	f	102	-	-	10/21/61/61	0/2/2/2
25	PHO	a	411	-	-	5/53/103/103	0/5/6/6
28	GOL	v	201	-	-	2/4/4/4	-
28	GOL	A	414	-	-	2/4/4/4	-
28	GOL	V	202	-	-	2/4/4/4	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	C	509	-	3/3/20/25	11/37/135/135	-
29	LMT	F	101	-	-	5/21/61/61	0/2/2/2
24	CLA	b	610	40	3/3/20/25	19/37/135/135	-
24	CLA	A	410	-	3/3/20/25	8/37/135/135	-
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
28	GOL	T	101	-	-	0/4/4/4	-
35	HTG	B	624	-	-	5/10/30/30	0/1/1/1
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
24	CLA	D	403	-	3/3/20/25	5/37/135/135	-
25	PHO	A	409[A]	-	-	2/53/103/103	0/5/6/6
24	CLA	b	625	-	3/3/20/25	8/37/135/135	-
37	LHG	b	634	-	-	16/53/53/53	-
28	GOL	B	631	-	-	0/4/4/4	-
24	CLA	b	618	-	2/2/20/25	4/37/135/135	-
31	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
25	PHO	A	409[B]	-	-	2/53/103/103	0/5/6/6
24	CLA	B	612	-	2/2/20/25	4/37/135/135	-
24	CLA	C	505	-	1/1/20/25	5/37/135/135	-
24	CLA	C	501	-	3/3/20/25	6/37/135/135	-
24	CLA	B	605	-	3/3/20/25	4/37/135/135	-
35	HTG	B	625	-	-	4/10/30/30	0/1/1/1
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
33	LMG	z	101	-	-	14/34/54/70	0/1/1/1
24	CLA	d	402	-	1/1/20/25	2/37/135/135	-
26	BCR	c	519	-	-	2/29/63/63	0/2/2/2
24	CLA	d	403	-	3/3/20/25	2/37/135/135	-
24	CLA	B	602	40	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	b	622	-	3/3/20/25	3/37/135/135	-
31	PL9	A	419[A]	-	-	14/53/73/73	0/1/1/1
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
37	LHG	d	407	-	-	7/53/53/53	-
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
28	GOL	c	502	-	-	0/4/4/4	-
37	LHG	d	406	-	-	11/53/53/53	-
31	PL9	A	419[B]	-	-	10/53/73/73	0/1/1/1
24	CLA	b	621	-	3/3/20/25	3/37/135/135	-
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
28	GOL	a	402	-	-	2/4/4/4	-
35	HTG	B	623	-	-	3/10/30/30	0/1/1/1
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
33	LMG	B	622	-	-	6/46/66/70	0/1/1/1
24	CLA	b	615	-	2/2/20/25	10/37/135/135	-
24	CLA	B	606	-	3/3/20/25	4/37/135/135	-
24	CLA	c	518	-	2/2/20/25	5/37/135/135	-
24	CLA	B	607	-	3/3/20/25	4/37/135/135	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
24	CLA	c	507	-	3/3/20/25	7/37/135/135	-
35	HTG	D	412	-	-	0/7/27/30	0/1/1/1
24	CLA	b	612	-	2/2/20/25	4/37/135/135	-
24	CLA	c	512	40	3/3/20/25	5/37/135/135	-
36	DGD	h	102	-	-	12/51/91/95	0/2/2/2
27	SQD	f	101	-	-	12/38/58/69	0/1/1/1
31	PL9	d	405[A]	-	-	5/53/73/73	0/1/1/1
24	CLA	B	611	40	3/3/20/25	4/37/135/135	-
35	HTG	c	526	-	-	0/10/30/30	0/1/1/1
35	HTG	b	607	-	-	1/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	e	102	-	-	17/46/46/53	-
24	CLA	b	619	40	3/3/20/25	8/37/135/135	-
28	GOL	C	524	-	-	2/4/4/4	-
35	HTG	c	525	-	-	3/10/30/30	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	-
24	CLA	C	510	-	3/3/20/25	9/37/135/135	-
29	LMT	D	401	-	-	9/21/61/61	0/2/2/2
24	CLA	c	509	40	3/3/20/25	4/37/135/135	-
24	CLA	C	504	40	3/3/20/25	5/37/135/135	-
35	HTG	C	523	-	-	2/10/30/30	0/1/1/1
28	GOL	B	629	-	-	2/4/4/4	-
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-
24	CLA	a	410	40	2/2/20/25	9/37/135/135	-
28	GOL	b	606	-	-	2/4/4/4	-
37	LHG	E	101	-	-	25/46/46/53	-
27	SQD	L	102	-	-	23/49/69/69	0/1/1/1
28	GOL	b	604	-	-	2/4/4/4	-
36	DGD	D	406	-	-	22/47/67/95	0/1/1/2
27	SQD	A	412	-	-	11/49/69/69	0/1/1/1
35	HTG	B	632	-	-	3/10/30/30	0/1/1/1
28	GOL	A	415	-	-	2/4/4/4	-
37	LHG	D	409	-	-	10/53/53/53	-
28	GOL	o	301	-	-	4/4/4/4	-
29	LMT	m	102	-	-	8/21/61/61	0/2/2/2
35	HTG	V	206	-	-	4/10/30/30	0/1/1/1
31	PL9	a	415[B]	-	-	14/53/73/73	0/1/1/1
27	SQD	F	103	-	-	15/38/58/69	0/1/1/1
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
35	HTG	b	632	-	-	6/10/30/30	0/1/1/1
28	GOL	c	503	-	-	1/4/4/4	-
28	GOL	b	603	-	-	0/4/4/4	-
24	CLA	C	507	40	3/3/20/25	6/37/135/135	-
24	CLA	B	608	40	3/3/20/25	4/37/135/135	-
25	PHO	A	408	-	-	3/53/103/103	0/5/6/6
35	HTG	b	608	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	501	-	-	15/46/66/70	0/1/1/1
28	GOL	B	627	-	-	2/4/4/4	-
26	BCR	T	103	-	-	1/29/63/63	0/2/2/2
28	GOL	B	630	-	-	4/4/4/4	-
24	CLA	b	611	-	2/2/20/25	3/37/135/135	-
24	CLA	d	401	40	3/3/20/25	6/37/135/135	-
28	GOL	T	102	-	-	2/4/4/4	-
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	CLA	c	511	-	3/3/20/25	10/37/135/135	-
24	CLA	b	614	-	2/2/20/25	4/37/135/135	-
24	CLA	B	613	-	3/3/20/25	3/37/135/135	-
36	DGD	c	520	-	-	13/51/91/95	0/2/2/2
27	SQD	A	416	-	-	16/49/69/69	0/1/1/1
24	CLA	b	617	-	2/2/20/25	2/37/135/135	-
36	DGD	c	522	-	-	14/51/91/95	0/2/2/2
24	CLA	C	508	-	3/3/20/25	4/37/135/135	-
33	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
28	GOL	a	401	-	-	2/4/4/4	-
28	GOL	O	301	-	-	2/4/4/4	-
36	DGD	H	102	-	-	11/51/91/95	0/2/2/2
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
24	CLA	c	517	-	3/3/20/25	10/37/135/135	-
28	GOL	b	605	-	-	2/4/4/4	-
33	LMG	C	519	-	-	10/46/66/70	0/1/1/1
24	CLA	b	623	-	3/3/20/25	22/37/135/135	-
36	DGD	e	101	-	-	27/51/91/95	0/2/2/2
24	CLA	B	615	-	3/3/20/25	14/37/135/135	-
24	CLA	C	506	-	3/3/20/25	7/37/135/135	-
24	CLA	D	402	-	2/2/20/25	0/37/135/135	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
35	HTG	d	411	-	-	1/7/27/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	a	405	-	-	15/49/69/69	0/1/1/1
24	CLA	B	617	-	3/3/20/25	6/37/135/135	-
29	LMT	C	521	-	-	9/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	c	523	-	-	13/46/66/70	0/1/1/1
28	GOL	V	203	-	-	1/4/4/4	-
31	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1
26	BCR	c	528	-	-	0/29/63/63	0/2/2/2
37	LHG	D	407	-	-	10/53/53/53	-
24	CLA	B	610	-	2/2/20/25	4/37/135/135	-
26	BCR	d	404	-	-	6/29/63/63	0/2/2/2
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
26	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
28	GOL	v	202	-	-	2/4/4/4	-
24	CLA	a	412	-	3/3/20/25	9/37/135/135	-
24	CLA	a	409	-	3/3/20/25	4/37/135/135	-
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
31	PL9	a	415[A]	-	-	18/53/73/73	0/1/1/1
24	CLA	A	407	40	2/2/20/25	3/37/135/135	-
26	BCR	b	628	-	-	0/29/63/63	0/2/2/2
24	CLA	b	620	-	3/3/20/25	3/37/135/135	-
35	HTG	B	633	-	-	0/10/30/30	0/1/1/1
24	CLA	b	613	-	3/3/20/25	5/37/135/135	-
24	CLA	C	513	-	3/3/20/25	7/37/135/135	-
25	PHO	a	418[B]	-	-	3/53/103/103	0/5/6/6
26	BCR	b	627	-	-	1/29/63/63	0/2/2/2
25	PHO	a	418[A]	-	-	1/53/103/103	0/5/6/6
37	LHG	d	408	-	-	10/53/53/53	-
38	HEM	F	102	5,6	-	0/6/54/54	-
24	CLA	c	515	-	3/3/20/25	9/37/135/135	-
33	LMG	b	629	-	-	11/46/66/70	0/1/1/1

All (1180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C3B-C2B	6.67	1.49	1.40
24	B	605	CLA	C3B-C2B	6.67	1.49	1.40
24	C	504	CLA	C3B-C2B	6.43	1.49	1.40
24	C	509	CLA	C3B-C2B	6.40	1.49	1.40
24	c	513	CLA	C3B-C2B	6.39	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C3B-C2B	6.34	1.49	1.40
24	B	613	CLA	C3B-C2B	6.31	1.49	1.40
24	c	511	CLA	C3B-C2B	6.29	1.49	1.40
24	B	614	CLA	C3B-C2B	6.28	1.49	1.40
24	c	513	CLA	C3D-C2D	6.26	1.50	1.39
24	c	515	CLA	C3B-C2B	6.24	1.49	1.40
24	b	619	CLA	C3B-C2B	6.23	1.49	1.40
24	B	610	CLA	C3D-C2D	6.20	1.50	1.39
24	C	509	CLA	C3D-C2D	6.20	1.50	1.39
24	A	405	CLA	C3B-C2B	6.19	1.49	1.40
24	C	508	CLA	C3B-C2B	6.19	1.49	1.40
24	a	409	CLA	C3B-C2B	6.13	1.48	1.40
24	D	402	CLA	C3B-C2B	6.13	1.48	1.40
24	b	622	CLA	C3B-C2B	6.13	1.48	1.40
24	b	617	CLA	C3B-C2B	6.12	1.48	1.40
24	b	625	CLA	C3D-C2D	6.08	1.50	1.39
24	b	615	CLA	C3B-C2B	6.08	1.48	1.40
24	C	511	CLA	C3D-C2D	6.07	1.50	1.39
24	b	623	CLA	C3D-C2D	6.07	1.50	1.39
24	c	512	CLA	C3B-C2B	6.04	1.48	1.40
24	c	514	CLA	C3B-C2B	6.03	1.48	1.40
24	b	625	CLA	C3B-C2B	6.03	1.48	1.40
24	c	509	CLA	C3B-C2B	6.01	1.48	1.40
24	C	506	CLA	C3D-C2D	6.00	1.50	1.39
24	A	406	CLA	C3B-C2B	6.00	1.48	1.40
24	d	401	CLA	C3B-C2B	6.00	1.48	1.40
24	c	516	CLA	C3D-C2D	5.99	1.50	1.39
24	B	612	CLA	C3D-C2D	5.99	1.50	1.39
24	C	510	CLA	C3B-C2B	5.98	1.48	1.40
24	C	504	CLA	C3D-C2D	5.98	1.50	1.39
24	b	610	CLA	C3D-C2D	5.97	1.50	1.39
24	c	507	CLA	C3D-C2D	5.97	1.50	1.39
24	b	612	CLA	C3B-C2B	5.97	1.48	1.40
24	b	620	CLA	C3B-C2B	5.97	1.48	1.40
24	c	506	CLA	C3B-C2B	5.95	1.48	1.40
25	A	409[B]	PHO	C3B-C2B	5.95	1.49	1.37
24	c	516	CLA	C3B-C2B	5.95	1.48	1.40
24	b	624	CLA	C3D-C2D	5.92	1.50	1.39
24	B	607	CLA	C3B-C2B	5.91	1.48	1.40
24	B	603	CLA	C3B-C2B	5.91	1.48	1.40
24	A	406	CLA	C3D-C2D	5.90	1.50	1.39
24	b	610	CLA	C3B-C2B	5.89	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C3B-C2B	5.89	1.48	1.40
24	d	401	CLA	C3D-C2D	5.89	1.50	1.39
25	A	409[A]	PHO	C3B-C2B	5.88	1.49	1.37
24	C	512	CLA	C3D-C2D	5.87	1.50	1.39
24	B	611	CLA	C3D-C2D	5.87	1.50	1.39
24	D	403	CLA	C3D-C2D	5.86	1.49	1.39
24	c	517	CLA	C3D-C2D	5.86	1.49	1.39
24	D	403	CLA	C3B-C2B	5.86	1.48	1.40
24	B	602	CLA	C3B-C2B	5.84	1.48	1.40
24	A	410	CLA	C3B-C2B	5.84	1.48	1.40
24	b	621	CLA	C3D-C2D	5.84	1.49	1.39
24	C	502	CLA	C3B-C2B	5.84	1.48	1.40
24	C	507	CLA	C3B-C2B	5.83	1.48	1.40
25	a	418[B]	PHO	C3C-C2C	5.83	1.49	1.36
24	a	412	CLA	C3D-C2D	5.83	1.49	1.39
25	a	418[A]	PHO	C3C-C2C	5.82	1.49	1.36
25	A	409[B]	PHO	C3C-C2C	5.82	1.49	1.36
24	C	503	CLA	C3D-C2D	5.81	1.49	1.39
24	c	517	CLA	C3B-C2B	5.81	1.48	1.40
24	B	604	CLA	C3B-C2B	5.81	1.48	1.40
24	b	623	CLA	C3B-C2B	5.78	1.48	1.40
24	c	514	CLA	C3D-C2D	5.77	1.49	1.39
24	C	511	CLA	C3B-C2B	5.75	1.48	1.40
24	A	407	CLA	C3B-C2B	5.75	1.48	1.40
24	c	512	CLA	C3D-C2D	5.75	1.49	1.39
25	A	408	PHO	C3B-C2B	5.74	1.48	1.37
24	B	602	CLA	C3D-C2D	5.74	1.49	1.39
24	C	508	CLA	C3D-C2D	5.73	1.49	1.39
24	b	614	CLA	C3B-C2B	5.72	1.48	1.40
24	b	617	CLA	C3D-C2D	5.72	1.49	1.39
25	A	408	PHO	C3C-C2C	5.72	1.48	1.36
25	a	411	PHO	C3B-C2B	5.71	1.48	1.37
24	c	509	CLA	C3D-C2D	5.71	1.49	1.39
24	c	507	CLA	C3B-C2B	5.70	1.48	1.40
24	c	510	CLA	C3B-C2B	5.70	1.48	1.40
24	D	402	CLA	C3D-C2D	5.70	1.49	1.39
25	a	418[B]	PHO	C3B-C2B	5.70	1.48	1.37
24	d	403	CLA	C3B-C2B	5.70	1.48	1.40
24	C	508	CLA	C3C-C2C	5.69	1.48	1.36
24	A	410	CLA	C3D-C2D	5.69	1.49	1.39
24	B	609	CLA	C3D-C2D	5.68	1.49	1.39
24	C	507	CLA	C3D-C2D	5.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3D-C2D	5.68	1.49	1.39
24	A	407	CLA	C3D-C2D	5.67	1.49	1.39
24	B	606	CLA	C3D-C2D	5.66	1.49	1.39
24	C	512	CLA	C3B-C2B	5.65	1.48	1.40
24	C	513	CLA	C3B-C2B	5.65	1.48	1.40
24	B	612	CLA	C3B-C2B	5.64	1.48	1.40
24	b	610	CLA	C3C-C2C	5.63	1.48	1.36
24	b	611	CLA	C3B-C2B	5.63	1.48	1.40
24	B	604	CLA	C3D-C2D	5.62	1.49	1.39
24	C	505	CLA	C3B-C2B	5.61	1.48	1.40
24	b	622	CLA	C3D-C2D	5.60	1.49	1.39
24	c	518	CLA	C3D-C2D	5.60	1.49	1.39
24	b	613	CLA	C3D-C2D	5.60	1.49	1.39
24	C	502	CLA	C3D-C2D	5.59	1.49	1.39
24	c	511	CLA	C3D-C2D	5.59	1.49	1.39
25	a	411	PHO	C3C-C2C	5.58	1.48	1.36
24	C	501	CLA	C3D-C2D	5.58	1.49	1.39
24	B	603	CLA	C3D-C2D	5.57	1.49	1.39
24	d	402	CLA	C3B-C2B	5.57	1.48	1.40
24	b	614	CLA	C3C-C2C	5.56	1.48	1.36
24	b	615	CLA	C3D-C2D	5.55	1.49	1.39
24	B	608	CLA	C3B-C2B	5.54	1.48	1.40
24	C	513	CLA	C3D-C2D	5.52	1.49	1.39
24	a	410	CLA	C3B-C2B	5.52	1.48	1.40
24	c	506	CLA	C3D-C2D	5.51	1.49	1.39
24	B	611	CLA	C3C-C2C	5.50	1.48	1.36
24	d	402	CLA	C3D-C2D	5.50	1.49	1.39
24	b	619	CLA	C3C-C2C	5.50	1.48	1.36
24	C	506	CLA	C3B-C2B	5.49	1.48	1.40
24	B	617	CLA	C3D-C2D	5.49	1.49	1.39
24	b	624	CLA	C3B-C2B	5.48	1.48	1.40
24	b	618	CLA	C3D-C2D	5.48	1.49	1.39
24	B	609	CLA	C3B-C2B	5.46	1.47	1.40
24	C	503	CLA	C3B-C2B	5.46	1.47	1.40
24	B	611	CLA	C3B-C2B	5.46	1.47	1.40
24	B	606	CLA	O2D-CGD	5.45	1.46	1.33
25	a	418[A]	PHO	C3B-C2B	5.45	1.48	1.37
25	A	409[A]	PHO	C3C-C2C	5.44	1.48	1.36
24	C	510	CLA	C3C-C2C	5.44	1.48	1.36
24	C	513	CLA	C3C-C2C	5.44	1.48	1.36
24	B	604	CLA	C3C-C2C	5.43	1.48	1.36
24	C	509	CLA	C3C-C2C	5.43	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C3D-C2D	5.43	1.49	1.39
25	a	418[A]	PHO	CHC-C1C	5.42	1.49	1.38
24	c	518	CLA	C3C-C2C	5.42	1.48	1.36
24	B	615	CLA	C3B-C2B	5.42	1.47	1.40
24	B	613	CLA	C3D-C2D	5.42	1.49	1.39
24	b	623	CLA	C3C-C2C	5.42	1.48	1.36
24	c	508	CLA	CHC-C1C	5.41	1.48	1.35
24	B	603	CLA	C3C-C2C	5.41	1.48	1.36
24	D	402	CLA	C3C-C2C	5.41	1.48	1.36
24	A	407	CLA	C3C-C2C	5.39	1.48	1.36
24	c	515	CLA	C3D-C2D	5.38	1.49	1.39
24	b	622	CLA	C3C-C2C	5.38	1.48	1.36
24	B	615	CLA	C3D-C2D	5.37	1.49	1.39
24	C	503	CLA	C3C-C2C	5.37	1.48	1.36
24	D	403	CLA	C3C-C2C	5.36	1.48	1.36
24	b	611	CLA	C3C-C2C	5.36	1.48	1.36
24	C	512	CLA	C3C-C2C	5.36	1.48	1.36
24	b	611	CLA	C3D-C2D	5.36	1.49	1.39
24	c	513	CLA	C3C-C2C	5.36	1.48	1.36
24	C	503	CLA	CHC-C1C	5.35	1.48	1.35
24	C	510	CLA	C3D-C2D	5.35	1.49	1.39
24	c	508	CLA	C3B-C2B	5.35	1.47	1.40
24	c	518	CLA	C3B-C2B	5.35	1.47	1.40
24	b	620	CLA	C3D-C2D	5.34	1.49	1.39
24	d	403	CLA	C3D-C2D	5.33	1.49	1.39
24	B	603	CLA	CHC-C1C	5.33	1.48	1.35
24	c	515	CLA	C3C-C2C	5.33	1.48	1.36
24	b	617	CLA	C3C-C2C	5.32	1.48	1.36
24	b	621	CLA	C3C-C2C	5.31	1.48	1.36
24	a	412	CLA	C3C-C2C	5.31	1.48	1.36
24	B	604	CLA	CHC-C1C	5.31	1.48	1.35
24	a	410	CLA	C3D-C2D	5.30	1.48	1.39
24	d	401	CLA	C3C-C2C	5.30	1.48	1.36
24	B	616	CLA	C3D-C2D	5.29	1.48	1.39
24	b	616	CLA	C3D-C2D	5.29	1.48	1.39
25	a	418[B]	PHO	CHC-C1C	5.28	1.48	1.38
24	c	507	CLA	C3C-C2C	5.28	1.48	1.36
24	B	602	CLA	C3C-C2C	5.28	1.48	1.36
24	B	615	CLA	C3C-C2C	5.27	1.47	1.36
24	B	608	CLA	C3D-C2D	5.27	1.48	1.39
24	c	517	CLA	CHC-C1C	5.26	1.48	1.35
24	B	611	CLA	OBD-CAD	5.26	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C3D-C2D	5.26	1.48	1.39
24	C	501	CLA	CHC-C1C	5.25	1.48	1.35
24	b	615	CLA	C3C-C2C	5.25	1.47	1.36
24	A	405	CLA	C3D-C2D	5.25	1.48	1.39
24	b	619	CLA	C3D-C2D	5.25	1.48	1.39
24	b	612	CLA	C3D-C2D	5.25	1.48	1.39
24	C	507	CLA	C3C-C2C	5.24	1.47	1.36
24	B	606	CLA	CHC-C1C	5.24	1.48	1.35
24	d	403	CLA	C3C-C2C	5.23	1.47	1.36
24	B	610	CLA	C3C-C2C	5.23	1.47	1.36
24	a	409	CLA	C3C-C2C	5.23	1.47	1.36
24	c	511	CLA	C3C-C2C	5.23	1.47	1.36
24	c	517	CLA	C3C-C2C	5.23	1.47	1.36
24	b	623	CLA	O2D-CGD	5.22	1.45	1.33
25	a	411	PHO	O2D-CGD	5.22	1.45	1.33
24	C	505	CLA	CHC-C1C	5.22	1.48	1.35
24	A	407	CLA	CHC-C1C	5.21	1.48	1.35
24	b	616	CLA	C3C-C2C	5.21	1.47	1.36
24	c	509	CLA	O2D-CGD	5.21	1.45	1.33
24	C	504	CLA	CHC-C1C	5.20	1.48	1.35
24	a	412	CLA	C3B-C2B	5.20	1.47	1.40
24	d	402	CLA	CHC-C1C	5.20	1.48	1.35
25	A	409[B]	PHO	CHC-C1C	5.20	1.48	1.38
24	C	508	CLA	CHC-C1C	5.20	1.48	1.35
24	C	513	CLA	CHC-C1C	5.20	1.48	1.35
24	A	405	CLA	CHC-C1C	5.19	1.48	1.35
24	b	616	CLA	C3B-C2B	5.19	1.47	1.40
24	B	603	CLA	O2D-CGD	5.18	1.45	1.33
26	b	628	BCR	C23-C22	-5.18	1.34	1.45
24	d	403	CLA	CHC-C1C	5.17	1.48	1.35
24	c	508	CLA	C3D-C2D	5.17	1.48	1.39
26	B	620	BCR	C23-C22	-5.17	1.34	1.45
24	a	410	CLA	CHC-C1C	5.17	1.48	1.35
24	C	502	CLA	C3C-C2C	5.17	1.47	1.36
24	B	612	CLA	C3C-C2C	5.16	1.47	1.36
24	c	508	CLA	C3C-C2C	5.16	1.47	1.36
24	c	512	CLA	C3C-C2C	5.16	1.47	1.36
24	c	513	CLA	O2D-CGD	5.16	1.45	1.33
24	b	618	CLA	C3B-C2B	5.16	1.47	1.40
24	C	502	CLA	CHC-C1C	5.16	1.48	1.35
24	b	620	CLA	C3C-C2C	5.15	1.47	1.36
24	C	505	CLA	C3C-C2C	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	CHC-C1C	5.14	1.48	1.35
24	C	507	CLA	CHC-C1C	5.13	1.48	1.35
24	b	622	CLA	O2D-CGD	5.13	1.45	1.33
25	a	418[A]	PHO	CHB-C1B	5.13	1.48	1.38
24	b	613	CLA	C3C-C2C	5.13	1.47	1.36
24	B	607	CLA	C3C-C2C	5.13	1.47	1.36
24	c	514	CLA	C3C-C2C	5.12	1.47	1.36
24	B	608	CLA	C3C-C2C	5.12	1.47	1.36
24	B	616	CLA	C3B-C2B	5.12	1.47	1.40
24	a	409	CLA	C3D-C2D	5.12	1.48	1.39
24	C	509	CLA	CHC-C1C	5.12	1.48	1.35
24	A	407	CLA	OBD-CAD	5.12	1.29	1.22
24	a	410	CLA	OBD-CAD	5.12	1.29	1.22
24	B	616	CLA	CHC-C1C	5.12	1.48	1.35
24	b	614	CLA	CHC-C1C	5.12	1.48	1.35
24	B	607	CLA	C3D-C2D	5.11	1.48	1.39
25	A	409[B]	PHO	O2D-CGD	5.11	1.45	1.33
24	B	609	CLA	C3C-C2C	5.11	1.47	1.36
24	b	618	CLA	C3C-C2C	5.11	1.47	1.36
24	C	511	CLA	C3C-C2C	5.11	1.47	1.36
24	B	607	CLA	O2D-CGD	5.11	1.45	1.33
24	b	611	CLA	CHC-C1C	5.11	1.48	1.35
24	c	514	CLA	OBD-CAD	5.10	1.29	1.22
24	A	406	CLA	C3C-C2C	5.10	1.47	1.36
24	b	612	CLA	OBD-CAD	5.10	1.29	1.22
24	d	401	CLA	O2D-CGD	5.10	1.45	1.33
24	c	508	CLA	OBD-CAD	5.10	1.29	1.22
24	B	614	CLA	C3C-C2C	5.10	1.47	1.36
24	c	509	CLA	C3C-C2C	5.09	1.47	1.36
26	k	101	BCR	C23-C22	-5.09	1.35	1.45
24	c	506	CLA	C3C-C2C	5.09	1.47	1.36
24	c	516	CLA	C3C-C2C	5.09	1.47	1.36
24	B	615	CLA	CHC-C1C	5.09	1.48	1.35
24	C	512	CLA	CHC-C1C	5.08	1.48	1.35
25	A	408	PHO	CHB-C1B	5.08	1.48	1.38
24	c	517	CLA	O2D-CGD	5.08	1.45	1.33
24	C	504	CLA	C3C-C2C	5.08	1.47	1.36
24	C	506	CLA	C3C-C2C	5.08	1.47	1.36
24	c	507	CLA	O2D-CGD	5.07	1.45	1.33
24	B	610	CLA	CHC-C1C	5.07	1.48	1.35
24	b	623	CLA	CHC-C1C	5.07	1.48	1.35
24	B	606	CLA	C3B-C2B	5.07	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	C3B-C2B	5.07	1.47	1.40
24	c	507	CLA	CHC-C1C	5.07	1.48	1.35
24	B	602	CLA	CHC-C1C	5.06	1.48	1.35
24	b	621	CLA	O2D-CGD	5.06	1.45	1.33
24	c	509	CLA	CHC-C1C	5.06	1.47	1.35
24	c	518	CLA	CHC-C1C	5.06	1.47	1.35
24	b	625	CLA	O2D-CGD	5.05	1.45	1.33
24	B	606	CLA	C3C-C2C	5.05	1.47	1.36
24	B	605	CLA	CHC-C1C	5.05	1.47	1.35
24	d	403	CLA	O2D-CGD	5.05	1.45	1.33
24	b	624	CLA	C3C-C2C	5.05	1.47	1.36
24	b	612	CLA	CHC-C1C	5.05	1.47	1.35
24	C	508	CLA	O2D-CGD	5.05	1.45	1.33
24	c	516	CLA	CHC-C1C	5.04	1.47	1.35
24	b	616	CLA	CHC-C1C	5.04	1.47	1.35
24	c	514	CLA	O2D-CGD	5.04	1.45	1.33
24	b	618	CLA	O2D-CGD	5.04	1.45	1.33
24	b	612	CLA	O2D-CGD	5.04	1.45	1.33
24	b	617	CLA	CHC-C1C	5.03	1.47	1.35
24	B	617	CLA	CHC-C1C	5.03	1.47	1.35
24	c	518	CLA	O2D-CGD	5.03	1.45	1.33
24	b	618	CLA	CHC-C1C	5.03	1.47	1.35
24	A	410	CLA	C3C-C2C	5.03	1.47	1.36
25	A	409[A]	PHO	O2D-CGD	5.02	1.45	1.33
26	T	103	BCR	C23-C22	-5.02	1.35	1.45
24	C	504	CLA	OBD-CAD	5.02	1.29	1.22
24	B	616	CLA	O2D-CGD	5.02	1.45	1.33
24	C	513	CLA	O2D-CGD	5.01	1.45	1.33
24	C	509	CLA	O2D-CGD	5.01	1.45	1.33
24	A	405	CLA	OBD-CAD	5.00	1.29	1.22
24	B	614	CLA	O2D-CGD	5.00	1.45	1.33
24	b	610	CLA	CHC-C1C	5.00	1.47	1.35
24	b	612	CLA	C3C-C2C	5.00	1.47	1.36
24	c	510	CLA	C3C-C2C	4.99	1.47	1.36
24	B	614	CLA	OBD-CAD	4.99	1.29	1.22
25	a	418[B]	PHO	O2D-CGD	4.99	1.45	1.33
24	c	513	CLA	OBD-CAD	4.98	1.29	1.22
24	B	602	CLA	O2D-CGD	4.98	1.45	1.33
24	C	510	CLA	CHC-C1C	4.98	1.47	1.35
24	B	617	CLA	O2D-CGD	4.98	1.45	1.33
24	b	616	CLA	O2D-CGD	4.98	1.45	1.33
24	A	410	CLA	CHC-C1C	4.98	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	O2D-CGD	4.98	1.45	1.33
25	a	411	PHO	CHD-C1D	4.98	1.48	1.38
24	C	506	CLA	CHC-C1C	4.97	1.47	1.35
24	b	610	CLA	O2D-CGD	4.97	1.45	1.33
24	b	614	CLA	O2D-CGD	4.97	1.45	1.33
25	A	408	PHO	CHD-C1D	4.96	1.48	1.38
24	b	618	CLA	OBD-CAD	4.96	1.29	1.22
24	B	607	CLA	CHC-C1C	4.96	1.47	1.35
24	c	514	CLA	CHC-C1C	4.96	1.47	1.35
24	B	605	CLA	C3D-C2D	4.96	1.48	1.39
24	b	620	CLA	O2D-CGD	4.96	1.45	1.33
24	C	510	CLA	O2D-CGD	4.95	1.45	1.33
24	c	517	CLA	OBD-CAD	4.95	1.29	1.22
24	d	402	CLA	C3C-C2C	4.95	1.47	1.36
24	C	506	CLA	O2D-CGD	4.95	1.45	1.33
25	A	409[A]	PHO	CHC-C1C	4.94	1.48	1.38
24	A	407	CLA	O2D-CGD	4.94	1.45	1.33
25	A	409[B]	PHO	CHB-C1B	4.94	1.48	1.38
24	D	403	CLA	CHC-C1C	4.94	1.47	1.35
25	A	409[A]	PHO	CHD-C1D	4.93	1.48	1.38
24	B	606	CLA	OBD-CAD	4.93	1.29	1.22
24	c	512	CLA	CHC-C1C	4.92	1.47	1.35
24	B	610	CLA	OBD-CAD	4.92	1.29	1.22
24	c	515	CLA	OBD-CAD	4.92	1.29	1.22
24	b	613	CLA	CHC-C1C	4.92	1.47	1.35
24	C	501	CLA	C3C-C2C	4.92	1.47	1.36
24	B	605	CLA	C3C-C2C	4.92	1.47	1.36
24	C	505	CLA	C3D-C2D	4.92	1.48	1.39
24	B	603	CLA	OBD-CAD	4.91	1.29	1.22
26	C	514	BCR	C23-C22	-4.91	1.35	1.45
24	C	512	CLA	O2D-CGD	4.90	1.45	1.33
24	C	501	CLA	OBD-CAD	4.90	1.29	1.22
24	A	410	CLA	OBD-CAD	4.90	1.29	1.22
24	c	511	CLA	CHC-C1C	4.89	1.47	1.35
24	B	612	CLA	O2D-CGD	4.89	1.45	1.33
26	d	404	BCR	C23-C22	-4.88	1.35	1.45
24	b	615	CLA	CHC-C1C	4.88	1.47	1.35
24	B	612	CLA	CHC-C1C	4.88	1.47	1.35
24	A	410	CLA	O2D-CGD	4.87	1.45	1.33
24	b	619	CLA	O2D-CGD	4.87	1.45	1.33
24	b	622	CLA	CHC-C1C	4.87	1.47	1.35
24	a	412	CLA	O2D-CGD	4.86	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	CLA	OBD-CAD	4.86	1.29	1.22
24	A	405	CLA	C3C-C2C	4.86	1.47	1.36
25	A	409[A]	PHO	CHB-C1B	4.86	1.48	1.38
25	a	418[B]	PHO	CHB-C1B	4.85	1.48	1.38
24	b	624	CLA	O2D-CGD	4.85	1.45	1.33
24	c	515	CLA	CHC-C1C	4.85	1.47	1.35
24	b	621	CLA	CHC-C1C	4.85	1.47	1.35
24	a	412	CLA	CHC-C1C	4.85	1.47	1.35
24	B	610	CLA	C3B-C2B	4.84	1.47	1.40
24	D	403	CLA	O2D-CGD	4.84	1.45	1.33
24	B	608	CLA	CHC-C1C	4.83	1.47	1.35
26	h	101	BCR	C23-C22	-4.83	1.35	1.45
24	c	515	CLA	O2D-CGD	4.82	1.45	1.33
24	B	613	CLA	CHC-C1C	4.82	1.47	1.35
24	B	617	CLA	C3C-C2C	4.82	1.47	1.36
24	C	511	CLA	O2D-CGD	4.82	1.45	1.33
24	a	410	CLA	C3C-C2C	4.82	1.47	1.36
24	b	624	CLA	CHC-C1C	4.82	1.47	1.35
24	b	615	CLA	O2D-CGD	4.81	1.44	1.33
24	a	409	CLA	O2D-CGD	4.81	1.44	1.33
24	b	625	CLA	CHC-C1C	4.80	1.47	1.35
26	K	101	BCR	C23-C22	-4.80	1.35	1.45
24	C	511	CLA	CHC-C1C	4.79	1.47	1.35
24	A	405	CLA	O2D-CGD	4.79	1.44	1.33
24	B	602	CLA	O2A-CGA	4.79	1.47	1.33
25	a	418[B]	PHO	CHD-C1D	4.79	1.48	1.38
24	b	617	CLA	OBD-CAD	4.79	1.29	1.22
24	C	501	CLA	O2D-CGD	4.79	1.44	1.33
24	c	513	CLA	CHC-C1C	4.79	1.47	1.35
24	B	614	CLA	CHC-C1C	4.79	1.47	1.35
24	B	611	CLA	CHC-C1C	4.78	1.47	1.35
24	b	620	CLA	CHC-C1C	4.78	1.47	1.35
24	b	619	CLA	CHC-C1C	4.78	1.47	1.35
24	B	613	CLA	O2D-CGD	4.78	1.44	1.33
26	H	101	BCR	C23-C22	-4.77	1.35	1.45
25	A	408	PHO	CHC-C1C	4.77	1.47	1.38
26	C	515	BCR	C23-C22	-4.77	1.35	1.45
25	a	418[A]	PHO	O2D-CGD	4.77	1.44	1.33
26	y	101	BCR	C23-C22	-4.76	1.35	1.45
25	a	411	PHO	CHB-C1B	4.76	1.47	1.38
24	B	616	CLA	C3C-C2C	4.76	1.46	1.36
24	C	512	CLA	OBD-CAD	4.76	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	O2D-CGD	4.75	1.44	1.33
24	B	609	CLA	OBD-CAD	4.75	1.28	1.22
24	b	611	CLA	OBD-CAD	4.75	1.28	1.22
24	B	610	CLA	O2D-CGD	4.74	1.44	1.33
24	c	506	CLA	CHC-C1C	4.74	1.47	1.35
24	c	506	CLA	O2D-CGD	4.74	1.44	1.33
24	B	613	CLA	OBD-CAD	4.74	1.28	1.22
24	B	613	CLA	C3C-C2C	4.73	1.46	1.36
24	B	609	CLA	O2D-CGD	4.71	1.44	1.33
24	c	508	CLA	O2D-CGD	4.71	1.44	1.33
24	b	619	CLA	OBD-CAD	4.71	1.28	1.22
24	b	621	CLA	OBD-CAD	4.70	1.28	1.22
24	C	508	CLA	OBD-CAD	4.69	1.28	1.22
24	c	510	CLA	O2D-CGD	4.69	1.44	1.33
25	a	418[A]	PHO	CHD-C1D	4.68	1.47	1.38
24	b	625	CLA	C3C-C2C	4.68	1.46	1.36
24	d	402	CLA	OBD-CAD	4.68	1.28	1.22
24	a	409	CLA	CHC-C1C	4.68	1.47	1.35
24	B	604	CLA	OBD-CAD	4.68	1.28	1.22
24	B	611	CLA	O2D-CGD	4.67	1.44	1.33
24	C	511	CLA	OBD-CAD	4.66	1.28	1.22
24	b	611	CLA	O2D-CGD	4.66	1.44	1.33
24	b	623	CLA	OBD-CAD	4.66	1.28	1.22
27	a	405	SQD	O48-C23	4.66	1.47	1.33
24	C	507	CLA	O2D-CGD	4.66	1.44	1.33
26	c	528	BCR	C23-C22	-4.65	1.36	1.45
25	A	409[B]	PHO	CHD-C1D	4.64	1.47	1.38
26	Y	101	BCR	C23-C22	-4.64	1.36	1.45
24	c	513	CLA	O2A-CGA	4.64	1.46	1.33
24	B	609	CLA	CHC-C1C	4.64	1.46	1.35
24	d	401	CLA	CHC-C1C	4.64	1.46	1.35
24	D	402	CLA	O2D-CGD	4.64	1.44	1.33
24	B	608	CLA	O2D-CGD	4.63	1.44	1.33
24	D	402	CLA	CHC-C1C	4.63	1.46	1.35
25	A	408	PHO	O2D-CGD	4.63	1.44	1.33
26	t	101	BCR	C23-C22	-4.62	1.36	1.45
24	c	516	CLA	OBD-CAD	4.62	1.28	1.22
24	C	504	CLA	O2D-CGD	4.62	1.44	1.33
24	a	410	CLA	O2D-CGD	4.61	1.44	1.33
24	c	512	CLA	O2D-CGD	4.61	1.44	1.33
24	C	505	CLA	O2D-CGD	4.60	1.44	1.33
27	A	416	SQD	O48-C23	4.60	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	518	CLA	OBD-CAD	4.60	1.28	1.22
24	C	502	CLA	O2D-CGD	4.59	1.44	1.33
25	a	411	PHO	CHC-C1C	4.59	1.47	1.38
24	B	616	CLA	OBD-CAD	4.58	1.28	1.22
24	B	615	CLA	O2D-CGD	4.57	1.44	1.33
24	B	605	CLA	O2D-CGD	4.57	1.44	1.33
24	b	620	CLA	OBD-CAD	4.57	1.28	1.22
27	f	101	SQD	O47-C7	4.56	1.47	1.34
24	c	516	CLA	O2D-CGD	4.56	1.44	1.33
24	C	503	CLA	OBD-CAD	4.56	1.28	1.22
24	b	613	CLA	O2D-CGD	4.56	1.44	1.33
24	c	507	CLA	OBD-CAD	4.54	1.28	1.22
24	B	610	CLA	O2A-CGA	4.54	1.46	1.33
36	D	406	DGD	O1G-C1A	4.54	1.46	1.33
26	D	404	BCR	C23-C22	-4.53	1.36	1.45
26	a	413	BCR	C23-C22	-4.53	1.36	1.45
24	C	509	CLA	OBD-CAD	4.52	1.28	1.22
24	a	409	CLA	OBD-CAD	4.51	1.28	1.22
24	b	624	CLA	OBD-CAD	4.50	1.28	1.22
26	b	626	BCR	C23-C22	-4.50	1.36	1.45
24	d	402	CLA	O2D-CGD	4.50	1.44	1.33
24	C	503	CLA	O2D-CGD	4.49	1.44	1.33
27	F	103	SQD	O47-C7	4.48	1.46	1.34
24	C	509	CLA	O2A-CGA	4.47	1.46	1.33
24	B	604	CLA	O2D-CGD	4.47	1.44	1.33
24	d	403	CLA	OBD-CAD	4.47	1.28	1.22
26	B	618	BCR	C23-C22	-4.47	1.36	1.45
33	C	519	LMG	O8-C28	4.46	1.46	1.33
24	B	615	CLA	OBD-CAD	4.46	1.28	1.22
33	z	101	LMG	O8-C28	4.45	1.46	1.33
26	c	519	BCR	C23-C22	-4.45	1.36	1.45
24	A	406	CLA	CHC-C1C	4.43	1.46	1.35
24	d	401	CLA	OBD-CAD	4.42	1.28	1.22
24	C	507	CLA	OBD-CAD	4.42	1.28	1.22
24	b	622	CLA	OBD-CAD	4.42	1.28	1.22
24	C	513	CLA	OBD-CAD	4.42	1.28	1.22
24	d	402	CLA	O2A-CGA	4.41	1.46	1.33
24	C	512	CLA	O2A-CGA	4.41	1.46	1.33
24	C	508	CLA	O2A-CGA	4.41	1.46	1.33
36	D	406	DGD	O2G-C1B	4.40	1.46	1.34
24	C	506	CLA	O2A-CGA	4.40	1.46	1.33
24	C	503	CLA	O2A-CGA	4.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	OBD-CAD	4.40	1.28	1.22
24	C	510	CLA	OBD-CAD	4.40	1.28	1.22
24	D	403	CLA	OBD-CAD	4.38	1.28	1.22
26	A	411	BCR	C23-C22	-4.38	1.36	1.45
24	b	625	CLA	OBD-CAD	4.38	1.28	1.22
24	b	610	CLA	O2A-CGA	4.38	1.46	1.33
24	b	624	CLA	O2A-CGA	4.38	1.46	1.33
24	B	602	CLA	OBD-CAD	4.37	1.28	1.22
24	c	516	CLA	O2A-CGA	4.37	1.46	1.33
37	E	101	LHG	O8-C23	4.37	1.46	1.33
36	e	101	DGD	O2G-C1B	4.37	1.46	1.34
24	c	514	CLA	O2A-CGA	4.37	1.46	1.33
24	B	617	CLA	OBD-CAD	4.36	1.28	1.22
24	B	612	CLA	OBD-CAD	4.36	1.28	1.22
26	b	627	BCR	C23-C22	-4.35	1.36	1.45
24	a	410	CLA	O2A-CGA	4.34	1.46	1.33
33	A	421	LMG	O7-C10	4.33	1.46	1.34
27	a	405	SQD	O47-C7	4.33	1.46	1.34
33	C	520	LMG	O7-C10	4.32	1.46	1.34
27	B	621	SQD	O47-C7	4.31	1.46	1.34
37	D	409	LHG	O7-C7	4.31	1.46	1.34
36	e	101	DGD	O1G-C1A	4.30	1.45	1.33
24	C	507	CLA	O2A-CGA	4.30	1.45	1.33
24	C	511	CLA	O2A-CGA	4.28	1.45	1.33
33	c	524	LMG	O7-C10	4.27	1.46	1.34
24	c	512	CLA	OBD-CAD	4.27	1.28	1.22
24	b	612	CLA	O2A-CGA	4.27	1.45	1.33
37	e	102	LHG	O8-C23	4.26	1.45	1.33
36	H	102	DGD	O1G-C1A	4.26	1.45	1.33
37	b	634	LHG	O8-C23	4.26	1.45	1.33
24	d	401	CLA	O2A-CGA	4.26	1.45	1.33
24	C	502	CLA	OBD-CAD	4.26	1.28	1.22
24	c	510	CLA	OBD-CAD	4.26	1.28	1.22
24	C	501	CLA	O2A-CGA	4.25	1.45	1.33
24	c	511	CLA	OBD-CAD	4.25	1.28	1.22
24	B	609	CLA	O2A-CGA	4.25	1.45	1.33
24	b	610	CLA	OBD-CAD	4.24	1.28	1.22
25	a	418[B]	PHO	O2A-CGA	4.24	1.45	1.33
24	b	615	CLA	OBD-CAD	4.23	1.28	1.22
24	c	512	CLA	O2A-CGA	4.23	1.45	1.33
24	A	406	CLA	O2D-CGD	4.23	1.43	1.33
27	f	101	SQD	O48-C23	4.23	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	518	CLA	O2A-CGA	4.22	1.45	1.33
27	L	102	SQD	O47-C7	4.22	1.46	1.34
33	B	622	LMG	O8-C28	4.22	1.45	1.33
33	A	421	LMG	O8-C28	4.22	1.45	1.33
33	C	520	LMG	O8-C28	4.21	1.45	1.33
24	B	616	CLA	O2A-CGA	4.20	1.45	1.33
24	c	506	CLA	OBD-CAD	4.20	1.28	1.22
33	c	524	LMG	O8-C28	4.20	1.45	1.33
24	c	517	CLA	O2A-CGA	4.20	1.45	1.33
24	C	506	CLA	OBD-CAD	4.20	1.28	1.22
24	C	513	CLA	O2A-CGA	4.19	1.45	1.33
24	B	606	CLA	O2A-CGA	4.19	1.45	1.33
37	d	408	LHG	O8-C23	4.18	1.45	1.33
36	c	522	DGD	O1G-C1A	4.18	1.45	1.33
24	b	618	CLA	O2A-CGA	4.17	1.45	1.33
24	B	617	CLA	O2A-CGA	4.16	1.45	1.33
37	e	102	LHG	O7-C7	4.16	1.46	1.34
33	b	629	LMG	O8-C28	4.16	1.45	1.33
24	B	615	CLA	O2A-CGA	4.15	1.45	1.33
24	b	617	CLA	O2A-CGA	4.15	1.45	1.33
33	d	413	LMG	O7-C10	4.15	1.46	1.34
36	C	518	DGD	O1G-C1A	4.15	1.45	1.33
33	c	501	LMG	O8-C28	4.14	1.45	1.33
37	d	408	LHG	O7-C7	4.13	1.46	1.34
27	L	102	SQD	O48-C23	4.13	1.45	1.33
33	c	523	LMG	O8-C28	4.13	1.45	1.33
24	b	611	CLA	O2A-CGA	4.13	1.45	1.33
27	a	414	SQD	O48-C23	4.13	1.45	1.33
25	a	418[A]	PHO	O2A-CGA	4.13	1.45	1.33
24	B	607	CLA	O2A-CGA	4.12	1.45	1.33
24	b	623	CLA	O2A-CGA	4.12	1.45	1.33
36	C	517	DGD	O1G-C1A	4.12	1.45	1.33
33	Z	101	LMG	O7-C10	4.12	1.45	1.34
37	E	101	LHG	O7-C7	4.12	1.45	1.34
25	A	409[B]	PHO	O2A-CGA	4.12	1.45	1.33
24	A	410	CLA	O2A-CGA	4.11	1.45	1.33
24	c	508	CLA	O2A-CGA	4.11	1.45	1.33
24	A	406	CLA	O2A-CGA	4.10	1.45	1.33
24	b	625	CLA	O2A-CGA	4.10	1.45	1.33
36	c	521	DGD	O1G-C1A	4.10	1.45	1.33
36	h	102	DGD	O1G-C1A	4.10	1.45	1.33
24	C	510	CLA	O2A-CGA	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	z	101	LMG	O7-C10	4.09	1.45	1.34
37	D	408	LHG	O7-C7	4.09	1.45	1.34
27	F	103	SQD	O48-C23	4.07	1.45	1.33
24	c	506	CLA	O2A-CGA	4.07	1.45	1.33
24	d	403	CLA	O2A-CGA	4.05	1.45	1.33
27	A	416	SQD	O47-C7	4.05	1.45	1.34
26	B	619	BCR	C23-C22	-4.05	1.37	1.45
24	b	616	CLA	OBD-CAD	4.05	1.28	1.22
24	A	407	CLA	O2A-CGA	4.05	1.45	1.33
37	D	409	LHG	O8-C23	4.04	1.45	1.33
25	A	408	PHO	O2A-CGA	4.04	1.45	1.33
27	B	621	SQD	O48-C23	4.04	1.45	1.33
24	b	619	CLA	O2A-CGA	4.04	1.45	1.33
36	c	522	DGD	O2G-C1B	4.04	1.45	1.34
24	b	614	CLA	OBD-CAD	4.04	1.27	1.22
24	C	505	CLA	O2A-CGA	4.03	1.45	1.33
36	c	520	DGD	O1G-C1A	4.03	1.45	1.33
24	B	604	CLA	O2A-CGA	4.03	1.45	1.33
24	B	613	CLA	O2A-CGA	4.03	1.45	1.33
24	b	613	CLA	OBD-CAD	4.03	1.27	1.22
37	L	101	LHG	O8-C23	4.03	1.45	1.33
24	B	607	CLA	OBD-CAD	4.02	1.27	1.22
24	C	504	CLA	O2A-CGA	4.01	1.45	1.33
33	d	413	LMG	O8-C28	4.01	1.45	1.33
24	a	412	CLA	O2A-CGA	4.01	1.45	1.33
37	D	408	LHG	O8-C23	4.01	1.45	1.33
24	c	507	CLA	O2A-CGA	4.00	1.45	1.33
24	C	505	CLA	OBD-CAD	4.00	1.27	1.22
24	B	614	CLA	O2A-CGA	3.98	1.45	1.33
27	A	412	SQD	O47-C7	3.98	1.45	1.34
35	b	632	HTG	C1'-S1	-3.97	1.76	1.81
24	b	620	CLA	O2A-CGA	3.97	1.44	1.33
36	H	102	DGD	O2G-C1B	3.96	1.45	1.34
33	c	523	LMG	O7-C10	3.96	1.45	1.34
24	A	405	CLA	O2A-CGA	3.96	1.44	1.33
24	D	402	CLA	O2A-CGA	3.96	1.44	1.33
24	b	621	CLA	O2A-CGA	3.95	1.44	1.33
25	A	409[A]	PHO	O2A-CGA	3.95	1.44	1.33
33	D	413	LMG	O8-C28	3.95	1.44	1.33
33	B	622	LMG	O7-C10	3.94	1.45	1.34
24	c	511	CLA	O2A-CGA	3.94	1.44	1.33
33	C	519	LMG	O7-C10	3.93	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	623	HTG	C1'-S1	-3.93	1.76	1.81
24	A	406	CLA	OBD-CAD	3.93	1.27	1.22
24	B	611	CLA	O2A-CGA	3.92	1.44	1.33
36	C	516	DGD	O1G-C1A	3.92	1.44	1.33
24	b	615	CLA	O2A-CGA	3.92	1.44	1.33
24	B	605	CLA	O2A-CGA	3.92	1.44	1.33
25	a	411	PHO	OBD-CAD	3.91	1.29	1.22
24	c	509	CLA	O2A-CGA	3.89	1.44	1.33
24	C	502	CLA	O2A-CGA	3.87	1.44	1.33
24	D	403	CLA	O2A-CGA	3.87	1.44	1.33
27	A	412	SQD	O48-C23	3.87	1.44	1.33
25	A	409[A]	PHO	C3D-C2D	3.87	1.49	1.39
24	B	603	CLA	O2A-CGA	3.87	1.44	1.33
36	h	102	DGD	O2G-C1B	3.87	1.45	1.34
24	b	614	CLA	O2A-CGA	3.86	1.44	1.33
33	b	629	LMG	O7-C10	3.86	1.45	1.34
24	B	608	CLA	O2A-CGA	3.85	1.44	1.33
37	d	407	LHG	O7-C7	3.85	1.45	1.34
35	B	632	HTG	C1'-S1	-3.84	1.76	1.81
24	b	613	CLA	O2A-CGA	3.83	1.44	1.33
25	A	408	PHO	OBD-CAD	3.83	1.29	1.22
33	c	501	LMG	O7-C10	3.83	1.45	1.34
37	D	407	LHG	O8-C23	3.82	1.44	1.33
25	a	418[A]	PHO	C3D-C2D	3.82	1.49	1.39
36	C	518	DGD	O2G-C1B	3.82	1.45	1.34
36	C	516	DGD	O2G-C1B	3.81	1.45	1.34
37	b	634	LHG	O7-C7	3.81	1.45	1.34
24	b	622	CLA	O2A-CGA	3.80	1.44	1.33
27	a	414	SQD	O47-C7	3.80	1.45	1.34
36	c	521	DGD	O2G-C1B	3.77	1.44	1.34
25	a	418[B]	PHO	C3D-C2D	3.77	1.49	1.39
24	B	612	CLA	O2A-CGA	3.77	1.44	1.33
36	C	517	DGD	O2G-C1B	3.77	1.44	1.34
24	c	515	CLA	O2A-CGA	3.76	1.44	1.33
37	d	406	LHG	O8-C23	3.75	1.44	1.33
24	c	510	CLA	O2A-CGA	3.75	1.44	1.33
37	L	101	LHG	O7-C7	3.70	1.44	1.34
25	a	411	PHO	C3D-C2D	3.70	1.49	1.39
35	V	206	HTG	C1'-S1	-3.70	1.76	1.81
24	b	616	CLA	O2A-CGA	3.70	1.44	1.33
36	c	520	DGD	O2G-C1B	3.69	1.44	1.34
35	d	411	HTG	C1'-S1	-3.68	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	413	LMG	O7-C10	3.67	1.44	1.34
35	B	625	HTG	C1'-S1	-3.67	1.76	1.81
35	D	412	HTG	C1'-S1	-3.66	1.76	1.81
37	d	407	LHG	O8-C23	3.65	1.44	1.33
35	b	608	HTG	C1'-S1	-3.64	1.76	1.81
25	A	408	PHO	C3D-C2D	3.64	1.49	1.39
25	A	409[B]	PHO	C3D-C2D	3.64	1.49	1.39
37	d	406	LHG	O7-C7	3.62	1.44	1.34
35	c	525	HTG	C1'-S1	-3.61	1.76	1.81
25	A	409[B]	PHO	C4A-NA	-3.60	1.26	1.35
25	a	418[B]	PHO	CHC-C4B	3.58	1.48	1.40
25	A	409[A]	PHO	CHC-C4B	3.57	1.48	1.40
24	B	608	CLA	OBD-CAD	3.57	1.27	1.22
24	a	409	CLA	O2A-CGA	3.56	1.43	1.33
24	D	402	CLA	OBD-CAD	3.56	1.27	1.22
35	c	526	HTG	C1'-S1	-3.55	1.76	1.81
25	a	411	PHO	C4A-NA	-3.54	1.26	1.35
35	B	633	HTG	C1'-S1	-3.53	1.76	1.81
25	A	409[B]	PHO	CHC-C4B	3.52	1.48	1.40
35	C	522	HTG	C1'-S1	-3.52	1.76	1.81
25	A	408	PHO	CHD-C4C	3.51	1.48	1.40
25	a	411	PHO	CHC-C4B	3.50	1.48	1.40
24	B	605	CLA	OBD-CAD	3.48	1.27	1.22
35	C	523	HTG	C1'-S1	-3.48	1.77	1.81
35	b	601	HTG	C1'-S1	-3.46	1.77	1.81
25	A	409[A]	PHO	C4A-NA	-3.46	1.26	1.35
35	b	607	HTG	C1'-S1	-3.45	1.77	1.81
25	A	408	PHO	C4A-NA	-3.44	1.26	1.35
25	a	411	PHO	CHD-C4C	3.39	1.48	1.40
25	A	408	PHO	CHB-C4A	3.38	1.48	1.40
24	B	613	CLA	C1C-C2C	3.37	1.51	1.44
25	A	409[B]	PHO	OBD-CAD	3.32	1.28	1.22
25	A	409[A]	PHO	OBD-CAD	3.31	1.28	1.22
25	a	418[B]	PHO	C4A-NA	-3.29	1.27	1.35
37	D	407	LHG	O7-C7	3.25	1.43	1.34
25	a	418[A]	PHO	CHC-C4B	3.25	1.48	1.40
25	a	418[B]	PHO	OBD-CAD	3.25	1.28	1.22
25	A	409[A]	PHO	CHD-C4C	3.21	1.47	1.40
25	A	409[B]	PHO	CHD-C4C	3.21	1.47	1.40
25	a	411	PHO	O2A-CGA	3.19	1.42	1.33
25	a	411	PHO	C3B-C4B	3.17	1.49	1.43
24	C	508	CLA	C4C-C3C	3.16	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C1C-C2C	3.15	1.50	1.44
25	A	409[A]	PHO	C3B-C4B	3.14	1.49	1.43
25	A	409[B]	PHO	C3B-C4B	3.11	1.49	1.43
25	a	418[B]	PHO	CHD-C4C	3.10	1.47	1.40
25	a	418[A]	PHO	C3B-C4B	3.10	1.49	1.43
24	A	405	CLA	C4C-C3C	3.08	1.50	1.45
25	a	418[A]	PHO	OBD-CAD	3.06	1.27	1.22
24	B	606	CLA	C1C-C2C	3.06	1.50	1.44
24	B	613	CLA	C1B-NB	-3.06	1.32	1.35
24	B	602	CLA	C1D-C2D	3.06	1.49	1.42
25	a	418[B]	PHO	C3B-C4B	3.05	1.49	1.43
25	a	418[A]	PHO	C4A-NA	-3.05	1.27	1.35
25	A	408	PHO	CHC-C4B	3.04	1.47	1.40
25	a	418[A]	PHO	CHD-C4C	3.02	1.47	1.40
27	f	101	SQD	C6-S	-2.98	1.66	1.77
24	b	619	CLA	C1D-C2D	2.97	1.49	1.42
27	A	416	SQD	C6-S	-2.97	1.66	1.77
24	d	403	CLA	C1D-C2D	2.97	1.49	1.42
35	b	631	HTG	C1'-S1	-2.97	1.77	1.81
24	B	611	CLA	C1D-C2D	2.96	1.49	1.42
24	B	610	CLA	C1D-C2D	2.94	1.49	1.42
24	C	511	CLA	C4C-C3C	2.94	1.50	1.45
24	a	409	CLA	C4C-C3C	2.93	1.50	1.45
24	C	513	CLA	C1D-C2D	2.92	1.49	1.42
25	a	418[A]	PHO	CHB-C4A	2.92	1.47	1.40
24	d	402	CLA	C1D-C2D	2.92	1.49	1.42
24	C	501	CLA	C1D-C2D	2.91	1.49	1.42
24	b	616	CLA	C1D-C2D	2.90	1.49	1.42
35	B	624	HTG	C1'-S1	-2.90	1.77	1.81
24	c	518	CLA	C1D-C2D	2.89	1.49	1.42
24	B	604	CLA	C1C-C2C	2.89	1.50	1.44
24	C	503	CLA	C1D-C2D	2.88	1.49	1.42
24	a	409	CLA	C1D-C2D	2.88	1.49	1.42
24	b	625	CLA	C1D-C2D	2.88	1.49	1.42
25	a	418[B]	PHO	CHB-C4A	2.88	1.47	1.40
24	C	510	CLA	C1B-CHB	2.88	1.49	1.41
24	C	507	CLA	C1C-C2C	2.87	1.50	1.44
24	b	611	CLA	C1D-C2D	2.86	1.49	1.42
25	a	411	PHO	CHB-C4A	2.86	1.47	1.40
24	c	514	CLA	C1B-CHB	2.86	1.48	1.41
24	C	508	CLA	C1D-C2D	2.86	1.49	1.42
24	b	612	CLA	C1C-C2C	2.84	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C1D-C2D	2.84	1.49	1.42
24	A	407	CLA	C1D-C2D	2.83	1.49	1.42
24	B	614	CLA	C1C-C2C	2.83	1.50	1.44
24	c	518	CLA	C1C-C2C	2.82	1.50	1.44
24	D	403	CLA	C1D-C2D	2.81	1.48	1.42
24	B	603	CLA	C1D-C2D	2.80	1.48	1.42
24	B	608	CLA	C1D-C2D	2.80	1.48	1.42
24	B	607	CLA	C1C-C2C	2.80	1.50	1.44
24	b	622	CLA	C4C-C3C	2.80	1.49	1.45
27	a	405	SQD	C6-S	-2.79	1.67	1.77
24	c	511	CLA	C1D-C2D	2.79	1.48	1.42
24	b	615	CLA	C1D-C2D	2.79	1.48	1.42
24	B	614	CLA	C4C-C3C	2.79	1.49	1.45
24	D	402	CLA	C1C-C2C	2.78	1.50	1.44
24	B	616	CLA	C4B-CHC	2.78	1.48	1.41
24	b	610	CLA	C1D-C2D	2.78	1.48	1.42
24	C	503	CLA	C1C-C2C	2.78	1.49	1.44
24	b	618	CLA	C1D-C2D	2.78	1.48	1.42
24	c	516	CLA	C1D-C2D	2.77	1.48	1.42
24	A	407	CLA	C4B-CHC	2.77	1.48	1.41
24	C	504	CLA	C1C-C2C	2.76	1.49	1.44
24	B	605	CLA	C1D-C2D	2.76	1.48	1.42
24	a	410	CLA	C1D-C2D	2.76	1.48	1.42
27	F	103	SQD	C6-S	-2.75	1.67	1.77
38	F	102	HEM	C3B-C2B	-2.75	1.36	1.40
24	c	509	CLA	C1D-C2D	2.75	1.48	1.42
25	A	409[B]	PHO	CHB-C4A	2.75	1.46	1.40
24	B	612	CLA	C1B-CHB	2.75	1.48	1.41
24	b	617	CLA	C1B-CHB	2.75	1.48	1.41
24	C	505	CLA	C4B-CHC	2.74	1.48	1.41
24	d	401	CLA	C1D-C2D	2.74	1.48	1.42
24	c	509	CLA	C1C-C2C	2.74	1.49	1.44
24	B	615	CLA	C1B-CHB	2.73	1.48	1.41
24	C	503	CLA	C4B-CHC	2.73	1.48	1.41
24	c	515	CLA	C1B-CHB	2.72	1.48	1.41
24	D	402	CLA	C1B-NB	-2.72	1.32	1.35
24	C	511	CLA	C1B-CHB	2.71	1.48	1.41
24	d	403	CLA	C1C-C2C	2.71	1.49	1.44
24	A	410	CLA	C1C-C2C	2.71	1.49	1.44
24	B	609	CLA	C1D-C2D	2.70	1.48	1.42
24	C	505	CLA	C1C-C2C	2.70	1.49	1.44
24	C	509	CLA	C1D-C2D	2.70	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C1C-C2C	2.70	1.49	1.44
24	B	606	CLA	C4B-CHC	2.70	1.48	1.41
24	B	614	CLA	C1B-CHB	2.70	1.48	1.41
24	B	616	CLA	C1D-C2D	2.69	1.48	1.42
24	c	517	CLA	C1C-C2C	2.68	1.49	1.44
24	b	625	CLA	C1B-CHB	2.68	1.48	1.41
24	c	508	CLA	C4B-CHC	2.68	1.48	1.41
24	b	617	CLA	C1C-C2C	2.68	1.49	1.44
29	A	417	LMT	O1'-C1'	2.68	1.44	1.40
24	B	613	CLA	C1B-CHB	2.68	1.48	1.41
24	b	624	CLA	C1D-C2D	2.67	1.48	1.42
24	C	504	CLA	C1B-CHB	2.67	1.48	1.41
24	c	512	CLA	C1C-C2C	2.67	1.49	1.44
24	B	612	CLA	C1D-C2D	2.67	1.48	1.42
24	a	410	CLA	C1C-C2C	2.67	1.49	1.44
24	b	614	CLA	C1B-CHB	2.66	1.48	1.41
24	B	615	CLA	C1C-C2C	2.66	1.49	1.44
24	a	412	CLA	CHD-C4C	2.66	1.48	1.41
24	C	509	CLA	C1C-C2C	2.66	1.49	1.44
27	B	621	SQD	C6-S	-2.66	1.67	1.77
24	C	506	CLA	CHD-C4C	2.66	1.48	1.41
24	C	510	CLA	C1D-C2D	2.66	1.48	1.42
24	c	506	CLA	C4C-C3C	2.65	1.49	1.45
24	b	615	CLA	C1C-C2C	2.65	1.49	1.44
24	b	612	CLA	C1B-CHB	2.65	1.48	1.41
24	b	615	CLA	C1B-CHB	2.64	1.48	1.41
24	b	613	CLA	C1B-CHB	2.64	1.48	1.41
24	D	403	CLA	C4C-C3C	2.64	1.49	1.45
24	C	511	CLA	C1D-C2D	2.64	1.48	1.42
24	C	503	CLA	CHD-C4C	2.63	1.48	1.41
24	c	508	CLA	C1D-C2D	2.63	1.48	1.42
24	C	507	CLA	C1D-C2D	2.63	1.48	1.42
24	c	506	CLA	C1D-C2D	2.63	1.48	1.42
24	C	504	CLA	C1D-C2D	2.62	1.48	1.42
27	A	412	SQD	C6-S	-2.62	1.67	1.77
24	b	614	CLA	C1D-C2D	2.62	1.48	1.42
24	c	510	CLA	C1B-CHB	2.62	1.48	1.41
24	a	412	CLA	C1D-C2D	2.62	1.48	1.42
24	c	515	CLA	C1D-C2D	2.62	1.48	1.42
24	B	607	CLA	C1D-C2D	2.62	1.48	1.42
24	B	615	CLA	C1D-C2D	2.61	1.48	1.42
24	C	502	CLA	C1C-C2C	2.61	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	C1D-C2D	2.61	1.48	1.42
24	A	410	CLA	C1D-C2D	2.61	1.48	1.42
24	c	518	CLA	CHD-C4C	2.61	1.48	1.41
24	b	620	CLA	C4C-C3C	2.61	1.49	1.45
24	C	508	CLA	C1C-C2C	2.61	1.49	1.44
27	a	414	SQD	C6-S	-2.60	1.67	1.77
24	C	501	CLA	CHD-C4C	2.60	1.48	1.41
24	c	513	CLA	C1D-C2D	2.60	1.48	1.42
27	L	102	SQD	C6-S	-2.60	1.67	1.77
24	c	518	CLA	C4C-C3C	2.60	1.49	1.45
24	C	513	CLA	C4B-CHC	2.60	1.48	1.41
25	A	409[A]	PHO	CHB-C4A	2.60	1.46	1.40
33	Z	101	LMG	O8-C28	2.60	1.46	1.33
24	C	509	CLA	C4C-C3C	2.60	1.49	1.45
24	B	613	CLA	C1D-C2D	2.60	1.48	1.42
24	B	602	CLA	C4B-CHC	2.60	1.48	1.41
24	b	617	CLA	C1D-C2D	2.60	1.48	1.42
24	b	617	CLA	CHD-C4C	2.59	1.48	1.41
24	A	407	CLA	CHD-C4C	2.59	1.48	1.41
24	d	403	CLA	C4B-CHC	2.59	1.48	1.41
24	a	410	CLA	C1B-CHB	2.59	1.48	1.41
24	B	603	CLA	C4C-C3C	2.59	1.49	1.45
24	c	509	CLA	C1B-CHB	2.59	1.48	1.41
24	B	617	CLA	C1B-CHB	2.59	1.48	1.41
24	C	510	CLA	CHD-C4C	2.59	1.48	1.41
24	A	407	CLA	C1C-C2C	2.59	1.49	1.44
24	B	616	CLA	C1C-C2C	2.58	1.49	1.44
24	B	605	CLA	C1B-CHB	2.58	1.48	1.41
31	a	415[B]	PL9	C6-C5	2.58	1.48	1.35
24	B	604	CLA	C1B-CHB	2.58	1.48	1.41
24	b	616	CLA	C4B-CHC	2.58	1.48	1.41
24	d	402	CLA	CHD-C4C	2.58	1.48	1.41
24	c	507	CLA	CHD-C4C	2.58	1.48	1.41
31	a	415[A]	PL9	C6-C5	2.58	1.48	1.35
24	b	622	CLA	C1C-C2C	2.57	1.49	1.44
24	B	614	CLA	C1D-C2D	2.57	1.48	1.42
24	C	512	CLA	C1C-C2C	2.57	1.49	1.44
24	b	622	CLA	C1B-CHB	2.57	1.48	1.41
24	c	510	CLA	C1C-C2C	2.57	1.49	1.44
24	A	410	CLA	C4B-CHC	2.56	1.48	1.41
24	C	511	CLA	CHD-C4C	2.56	1.48	1.41
24	b	619	CLA	C1B-CHB	2.56	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	405[B]	PL9	C6-C5	2.56	1.48	1.35
24	a	409	CLA	CHD-C4C	2.56	1.48	1.41
24	B	604	CLA	C4B-CHC	2.56	1.48	1.41
24	A	410	CLA	C1B-CHB	2.55	1.48	1.41
31	A	419[B]	PL9	C6-C5	2.55	1.48	1.35
24	d	401	CLA	CHD-C4C	2.55	1.48	1.41
24	B	612	CLA	C1C-C2C	2.55	1.49	1.44
24	c	517	CLA	C4B-CHC	2.54	1.48	1.41
24	B	609	CLA	C4C-C3C	2.54	1.49	1.45
31	A	419[A]	PL9	C6-C5	2.54	1.48	1.35
24	B	617	CLA	C4C-C3C	2.54	1.49	1.45
24	b	617	CLA	C4B-CHC	2.54	1.48	1.41
24	C	509	CLA	CHD-C4C	2.54	1.48	1.41
31	d	405[A]	PL9	C6-C5	2.53	1.48	1.35
24	C	502	CLA	C1D-C2D	2.53	1.48	1.42
31	d	405[B]	PL9	C6-C5	2.53	1.48	1.35
24	d	401	CLA	C1B-CHB	2.53	1.48	1.41
24	B	603	CLA	C4B-CHC	2.53	1.48	1.41
24	B	602	CLA	CHD-C4C	2.53	1.48	1.41
24	c	510	CLA	C4C-C3C	2.53	1.49	1.45
24	b	619	CLA	C4B-CHC	2.52	1.48	1.41
24	C	508	CLA	CHD-C4C	2.52	1.48	1.41
24	b	610	CLA	C4B-CHC	2.51	1.48	1.41
24	c	506	CLA	C1B-CHB	2.51	1.48	1.41
24	a	409	CLA	C1C-C2C	2.51	1.49	1.44
24	C	506	CLA	C4C-C3C	2.51	1.49	1.45
24	A	405	CLA	C1C-C2C	2.51	1.49	1.44
24	C	502	CLA	C1B-CHB	2.51	1.48	1.41
24	C	510	CLA	C4C-C3C	2.51	1.49	1.45
24	C	507	CLA	C4B-CHC	2.51	1.48	1.41
24	C	513	CLA	CHD-C4C	2.51	1.48	1.41
24	c	512	CLA	C1D-C2D	2.50	1.48	1.42
24	b	613	CLA	C1D-C2D	2.50	1.48	1.42
24	B	606	CLA	C1B-CHB	2.50	1.47	1.41
24	C	512	CLA	C1D-C2D	2.50	1.48	1.42
24	c	509	CLA	C4B-CHC	2.50	1.47	1.41
24	c	507	CLA	C1D-C2D	2.50	1.48	1.42
24	c	518	CLA	C4B-CHC	2.50	1.47	1.41
24	D	403	CLA	CHD-C4C	2.49	1.48	1.41
24	b	618	CLA	C1B-CHB	2.49	1.47	1.41
24	b	614	CLA	C4B-CHC	2.49	1.47	1.41
25	a	411	PHO	C1A-NA	-2.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C4C-C3C	2.49	1.49	1.45
24	C	510	CLA	C1C-C2C	2.48	1.49	1.44
24	b	621	CLA	C1B-CHB	2.48	1.47	1.41
24	c	517	CLA	CHD-C4C	2.48	1.48	1.41
24	d	403	CLA	C1B-CHB	2.48	1.47	1.41
24	C	504	CLA	CHD-C4C	2.48	1.48	1.41
24	b	623	CLA	C1D-C2D	2.48	1.48	1.42
24	C	501	CLA	C1C-C2C	2.48	1.49	1.44
24	c	515	CLA	CHD-C4C	2.48	1.48	1.41
24	c	511	CLA	CHD-C4C	2.47	1.48	1.41
24	B	614	CLA	C4B-CHC	2.47	1.47	1.41
24	c	508	CLA	CHD-C4C	2.47	1.48	1.41
24	b	623	CLA	CHD-C4C	2.47	1.48	1.41
24	D	403	CLA	C1B-CHB	2.47	1.47	1.41
24	B	602	CLA	C1B-CHB	2.47	1.47	1.41
24	b	620	CLA	C1B-CHB	2.47	1.47	1.41
24	c	514	CLA	C1D-C2D	2.47	1.48	1.42
24	b	610	CLA	CHD-C4C	2.47	1.48	1.41
24	B	603	CLA	C1C-C2C	2.46	1.49	1.44
25	A	408	PHO	C1A-NA	-2.46	1.32	1.37
24	b	621	CLA	C1C-C2C	2.46	1.49	1.44
24	c	517	CLA	C1D-C2D	2.46	1.48	1.42
24	c	515	CLA	C4C-C3C	2.46	1.49	1.45
24	c	510	CLA	C1D-C2D	2.46	1.48	1.42
24	A	410	CLA	C4C-C3C	2.46	1.49	1.45
24	a	412	CLA	C1B-CHB	2.46	1.47	1.41
24	A	406	CLA	C1D-C2D	2.46	1.48	1.42
24	B	603	CLA	CHD-C4C	2.46	1.48	1.41
24	c	510	CLA	C4B-CHC	2.46	1.47	1.41
24	C	509	CLA	C1B-CHB	2.45	1.47	1.41
24	b	615	CLA	CHD-C4C	2.45	1.48	1.41
24	C	505	CLA	C1B-CHB	2.45	1.47	1.41
24	d	403	CLA	C4C-C3C	2.45	1.49	1.45
24	C	501	CLA	C4B-CHC	2.45	1.47	1.41
24	B	610	CLA	C1B-CHB	2.45	1.47	1.41
24	c	506	CLA	CHD-C4C	2.45	1.48	1.41
24	c	511	CLA	C1B-CHB	2.45	1.47	1.41
24	B	607	CLA	C4B-CHC	2.45	1.47	1.41
24	B	609	CLA	CHD-C4C	2.45	1.48	1.41
24	C	512	CLA	C4B-CHC	2.45	1.47	1.41
24	c	514	CLA	CHD-C4C	2.44	1.48	1.41
24	C	512	CLA	C1B-CHB	2.44	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CHD-C4C	2.44	1.48	1.41
24	c	507	CLA	C1C-C2C	2.44	1.49	1.44
24	B	606	CLA	CHD-C4C	2.44	1.48	1.41
24	A	405	CLA	CHD-C4C	2.44	1.48	1.41
24	B	606	CLA	C1D-C2D	2.44	1.48	1.42
24	b	625	CLA	C1C-NC	-2.44	1.34	1.37
24	b	612	CLA	C4B-CHC	2.44	1.47	1.41
24	C	506	CLA	C1B-CHB	2.44	1.47	1.41
24	A	405	CLA	C1D-C2D	2.44	1.48	1.42
24	c	513	CLA	C1B-CHB	2.44	1.47	1.41
24	c	509	CLA	CHD-C4C	2.44	1.48	1.41
25	A	409[B]	PHO	C1A-NA	-2.44	1.32	1.37
24	B	613	CLA	C4B-CHC	2.44	1.47	1.41
24	b	620	CLA	C1D-C2D	2.44	1.48	1.42
24	C	504	CLA	C4B-CHC	2.43	1.47	1.41
24	A	406	CLA	C1B-NB	-2.43	1.33	1.35
24	B	611	CLA	C1B-CHB	2.43	1.47	1.41
24	a	410	CLA	CHD-C4C	2.43	1.48	1.41
35	b	607	HTG	C1-S1	-2.43	1.77	1.80
24	B	609	CLA	C1C-C2C	2.43	1.49	1.44
24	B	615	CLA	C4B-CHC	2.43	1.47	1.41
24	B	611	CLA	C4B-CHC	2.43	1.47	1.41
24	B	609	CLA	C1B-CHB	2.42	1.47	1.41
24	a	409	CLA	C4B-CHC	2.42	1.47	1.41
31	D	405[A]	PL9	C6-C5	2.42	1.47	1.35
24	D	403	CLA	C1C-C2C	2.42	1.49	1.44
24	c	515	CLA	C1C-C2C	2.42	1.49	1.44
25	A	409[A]	PHO	C4D-CHA	2.42	1.50	1.43
24	C	513	CLA	C1C-C2C	2.42	1.49	1.44
24	b	611	CLA	C1C-C2C	2.41	1.49	1.44
24	D	402	CLA	C1B-CHB	2.41	1.47	1.41
24	b	621	CLA	C4B-CHC	2.41	1.47	1.41
24	C	511	CLA	C1C-C2C	2.41	1.49	1.44
24	d	402	CLA	C1B-CHB	2.41	1.47	1.41
24	C	510	CLA	C4B-CHC	2.41	1.47	1.41
24	B	604	CLA	C1D-C2D	2.41	1.48	1.42
24	a	412	CLA	C4B-NB	-2.41	1.33	1.35
24	b	616	CLA	C1C-C2C	2.41	1.49	1.44
24	c	513	CLA	CHD-C4C	2.41	1.48	1.41
24	C	507	CLA	C1B-CHB	2.41	1.47	1.41
24	B	611	CLA	C4C-C3C	2.41	1.49	1.45
24	C	501	CLA	C1B-CHB	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	C4B-CHC	2.41	1.47	1.41
24	c	507	CLA	C1B-CHB	2.40	1.47	1.41
35	c	525	HTG	C1-S1	-2.40	1.77	1.80
24	b	621	CLA	C1C-NC	-2.40	1.34	1.37
24	B	605	CLA	C1C-C2C	2.40	1.49	1.44
24	C	509	CLA	C4B-CHC	2.39	1.47	1.41
24	B	607	CLA	C1B-NB	-2.39	1.33	1.35
24	B	608	CLA	C4B-CHC	2.39	1.47	1.41
24	c	512	CLA	C1B-CHB	2.39	1.47	1.41
24	B	612	CLA	C4B-CHC	2.39	1.47	1.41
24	B	608	CLA	C1C-C2C	2.39	1.49	1.44
24	b	622	CLA	C1D-C2D	2.39	1.48	1.42
24	b	613	CLA	C1C-C2C	2.39	1.49	1.44
24	C	507	CLA	CHD-C4C	2.39	1.47	1.41
24	c	514	CLA	C1C-C2C	2.38	1.49	1.44
24	C	504	CLA	C4C-C3C	2.38	1.49	1.45
35	D	412	HTG	C1-S1	-2.38	1.77	1.80
24	b	624	CLA	C1B-CHB	2.38	1.47	1.41
24	b	618	CLA	CHD-C4C	2.37	1.47	1.41
24	b	614	CLA	CHD-C4C	2.37	1.47	1.41
35	b	632	HTG	C1-S1	-2.37	1.77	1.80
24	B	607	CLA	C4C-C3C	2.37	1.49	1.45
24	B	604	CLA	CHD-C4C	2.37	1.47	1.41
24	d	403	CLA	CHD-C4C	2.37	1.47	1.41
24	b	624	CLA	CHD-C4C	2.37	1.47	1.41
25	a	411	PHO	C4C-C3C	2.37	1.49	1.45
24	C	502	CLA	CHD-C4C	2.37	1.47	1.41
25	A	409[A]	PHO	C1A-NA	-2.37	1.32	1.37
24	C	502	CLA	C4B-CHC	2.37	1.47	1.41
24	B	605	CLA	C4B-CHC	2.36	1.47	1.41
25	A	408	PHO	C4C-C3C	2.36	1.49	1.45
24	c	507	CLA	C4C-C3C	2.36	1.49	1.45
24	B	616	CLA	C1B-CHB	2.36	1.47	1.41
35	d	411	HTG	C1-S1	-2.36	1.77	1.80
24	C	505	CLA	CHD-C4C	2.36	1.47	1.41
24	B	602	CLA	C1C-C2C	2.36	1.49	1.44
24	B	608	CLA	C4C-C3C	2.36	1.49	1.45
24	a	412	CLA	C4B-CHC	2.35	1.47	1.41
24	B	611	CLA	C1C-NC	-2.35	1.34	1.37
24	b	610	CLA	C1C-C2C	2.35	1.49	1.44
24	D	402	CLA	C4B-CHC	2.35	1.47	1.41
24	d	402	CLA	C1B-NB	-2.35	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	CHD-C4C	2.35	1.47	1.41
24	c	508	CLA	C4C-C3C	2.34	1.49	1.45
24	B	607	CLA	CHD-C4C	2.34	1.47	1.41
24	b	618	CLA	C1C-C2C	2.34	1.49	1.44
35	b	608	HTG	C1-S1	-2.34	1.77	1.80
24	B	612	CLA	CHD-C4C	2.34	1.47	1.41
35	C	522	HTG	C1-S1	-2.34	1.77	1.80
24	B	617	CLA	C4B-CHC	2.34	1.47	1.41
36	D	406	DGD	O3G-C1D	2.34	1.44	1.40
24	c	516	CLA	C4B-CHC	2.34	1.47	1.41
24	b	616	CLA	CHD-C4C	2.33	1.47	1.41
24	b	620	CLA	CHD-C4C	2.33	1.47	1.41
24	C	513	CLA	C4C-C3C	2.32	1.49	1.45
24	B	608	CLA	C1B-CHB	2.32	1.47	1.41
24	b	617	CLA	C4C-C3C	2.32	1.49	1.45
24	b	619	CLA	CHD-C4C	2.32	1.47	1.41
24	b	611	CLA	C4C-C3C	2.31	1.49	1.45
24	B	610	CLA	C4B-CHC	2.31	1.47	1.41
24	b	613	CLA	C4B-CHC	2.31	1.47	1.41
24	C	502	CLA	C4C-C3C	2.31	1.49	1.45
24	A	405	CLA	C4B-CHC	2.31	1.47	1.41
24	B	615	CLA	C4C-C3C	2.31	1.49	1.45
38	V	205	HEM	C4D-C3D	2.31	1.47	1.42
24	d	402	CLA	C4C-C3C	2.30	1.49	1.45
24	B	610	CLA	C4C-C3C	2.30	1.49	1.45
24	b	611	CLA	CHD-C4C	2.30	1.47	1.41
24	C	512	CLA	CHD-C4C	2.30	1.47	1.41
24	b	618	CLA	C4B-CHC	2.30	1.47	1.41
24	A	406	CLA	CHD-C4C	2.30	1.47	1.41
24	c	512	CLA	C4C-C3C	2.30	1.49	1.45
24	a	412	CLA	C1C-C2C	2.30	1.49	1.44
24	B	617	CLA	CHD-C4C	2.29	1.47	1.41
24	C	503	CLA	C1B-CHB	2.29	1.47	1.41
24	b	623	CLA	C4C-C3C	2.29	1.49	1.45
25	A	408	PHO	C3B-C4B	2.29	1.48	1.43
24	B	604	CLA	C4C-C3C	2.29	1.49	1.45
24	c	507	CLA	C4B-CHC	2.28	1.47	1.41
24	A	405	CLA	C1B-CHB	2.28	1.47	1.41
24	b	625	CLA	CHD-C4C	2.28	1.47	1.41
24	B	607	CLA	C1B-CHB	2.28	1.47	1.41
24	B	603	CLA	C1B-CHB	2.28	1.47	1.41
24	b	611	CLA	C4B-CHC	2.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C4B-CHC	2.28	1.47	1.41
24	b	624	CLA	C1C-C2C	2.28	1.49	1.44
24	B	610	CLA	CHD-C4C	2.28	1.47	1.41
24	C	505	CLA	C4C-C3C	2.27	1.49	1.45
25	A	409[B]	PHO	C4D-CHA	2.27	1.49	1.43
35	c	526	HTG	C1-S1	-2.27	1.77	1.80
24	c	514	CLA	C4C-C3C	2.27	1.48	1.45
36	h	102	DGD	O5D-C1E	2.27	1.44	1.40
24	b	613	CLA	C4C-C3C	2.27	1.48	1.45
24	c	516	CLA	C1B-CHB	2.27	1.47	1.41
24	c	508	CLA	C1B-CHB	2.27	1.47	1.41
24	c	512	CLA	CHD-C4C	2.26	1.47	1.41
24	C	501	CLA	C4C-C3C	2.26	1.48	1.45
24	C	503	CLA	C4C-C3C	2.26	1.48	1.45
25	A	408	PHO	C4D-CHA	2.26	1.49	1.43
24	b	624	CLA	C4C-C3C	2.26	1.48	1.45
24	B	608	CLA	CHD-C4C	2.26	1.47	1.41
24	C	507	CLA	C4C-C3C	2.25	1.48	1.45
24	b	624	CLA	C4B-CHC	2.25	1.47	1.41
24	c	510	CLA	CHD-C4C	2.24	1.47	1.41
24	d	401	CLA	C4B-CHC	2.24	1.47	1.41
24	A	410	CLA	CHD-C4C	2.24	1.47	1.41
24	b	616	CLA	C1B-CHB	2.24	1.47	1.41
24	c	518	CLA	C1B-CHB	2.24	1.47	1.41
24	d	401	CLA	C1C-NC	-2.24	1.34	1.37
24	B	615	CLA	CHD-C4C	2.24	1.47	1.41
24	b	619	CLA	C4C-C3C	2.24	1.48	1.45
24	C	513	CLA	C1B-CHB	2.23	1.47	1.41
24	c	517	CLA	C4C-C3C	2.23	1.48	1.45
24	b	623	CLA	C1C-C2C	2.23	1.48	1.44
24	d	402	CLA	C4B-CHC	2.23	1.47	1.41
24	B	617	CLA	C1D-C2D	2.23	1.47	1.42
35	B	632	HTG	C1-S1	-2.23	1.77	1.80
24	d	401	CLA	C4B-NB	-2.23	1.33	1.35
24	B	611	CLA	C1C-C2C	2.23	1.48	1.44
24	c	514	CLA	C4B-CHC	2.23	1.47	1.41
25	a	418[A]	PHO	C1A-NA	-2.23	1.33	1.37
35	V	206	HTG	C1-S1	-2.23	1.77	1.80
24	c	515	CLA	C4B-CHC	2.23	1.47	1.41
24	b	623	CLA	C4B-CHC	2.22	1.47	1.41
24	c	516	CLA	C4C-C3C	2.22	1.48	1.45
24	A	406	CLA	C1C-C2C	2.22	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	CLA	CHD-C4C	2.22	1.47	1.41
24	B	605	CLA	CHD-C4C	2.22	1.47	1.41
24	b	611	CLA	C1B-CHB	2.22	1.47	1.41
24	d	401	CLA	C1C-C2C	2.21	1.48	1.44
24	c	512	CLA	C4B-CHC	2.21	1.47	1.41
24	a	412	CLA	C4C-C3C	2.21	1.48	1.45
24	A	406	CLA	C4B-CHC	2.21	1.47	1.41
24	B	605	CLA	C4C-C3C	2.20	1.48	1.45
25	a	418[B]	PHO	C4D-CHA	2.20	1.49	1.43
24	c	513	CLA	C1C-C2C	2.20	1.48	1.44
24	b	619	CLA	C1C-C2C	2.20	1.48	1.44
24	C	506	CLA	C1C-C2C	2.20	1.48	1.44
24	B	614	CLA	CHD-C4C	2.20	1.47	1.41
24	b	623	CLA	C1B-CHB	2.20	1.47	1.41
24	d	403	CLA	C1B-NB	-2.19	1.33	1.35
24	a	410	CLA	C4C-C3C	2.18	1.48	1.45
24	c	516	CLA	CHD-C4C	2.18	1.47	1.41
24	b	625	CLA	C4B-CHC	2.18	1.47	1.41
24	A	407	CLA	C4C-C3C	2.18	1.48	1.45
24	c	506	CLA	C1C-C2C	2.18	1.48	1.44
24	b	621	CLA	CHD-C4C	2.17	1.47	1.41
24	c	516	CLA	C1C-C2C	2.17	1.48	1.44
24	c	511	CLA	C4B-CHC	2.16	1.47	1.41
24	c	511	CLA	C1C-C2C	2.16	1.48	1.44
24	B	617	CLA	C1C-C2C	2.16	1.48	1.44
24	c	511	CLA	C4C-C3C	2.16	1.48	1.45
25	a	418[B]	PHO	C1A-NA	-2.16	1.33	1.37
24	b	619	CLA	C1C-NC	-2.16	1.34	1.37
24	b	612	CLA	C4C-C3C	2.15	1.48	1.45
24	a	409	CLA	C1B-CHB	2.15	1.47	1.41
24	C	508	CLA	C4B-CHC	2.15	1.47	1.41
24	C	506	CLA	C4B-CHC	2.15	1.47	1.41
24	b	610	CLA	C1B-CHB	2.15	1.47	1.41
24	A	406	CLA	C1B-CHB	2.15	1.47	1.41
24	B	616	CLA	CHD-C4C	2.15	1.47	1.41
24	c	511	CLA	C1B-NB	-2.15	1.33	1.35
24	b	621	CLA	C4C-C3C	2.14	1.48	1.45
37	d	406	LHG	O7-C5	-2.14	1.41	1.46
35	B	633	HTG	C1-S1	-2.14	1.77	1.80
35	B	625	HTG	C1-S1	-2.14	1.77	1.80
24	b	612	CLA	CHD-C4C	2.13	1.47	1.41
24	c	506	CLA	C4B-CHC	2.13	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C1B-NB	-2.13	1.33	1.35
24	B	612	CLA	C4C-C3C	2.13	1.48	1.45
25	a	411	PHO	C4D-CHA	2.13	1.49	1.43
24	D	402	CLA	C1D-C2D	2.13	1.47	1.42
24	c	513	CLA	C4C-C3C	2.12	1.48	1.45
24	C	505	CLA	C1D-C2D	2.12	1.47	1.42
24	a	410	CLA	C4B-CHC	2.12	1.46	1.41
24	C	508	CLA	C1B-CHB	2.11	1.46	1.41
38	e	103	HEM	C4D-C3D	2.11	1.47	1.42
24	B	610	CLA	C1C-C2C	2.11	1.48	1.44
24	c	507	CLA	C1C-NC	-2.10	1.34	1.37
24	B	605	CLA	C1A-CHA	2.10	1.51	1.43
31	d	405[A]	PL9	C2-C3	2.10	1.40	1.34
25	a	418[A]	PHO	C1C-NC	-2.10	1.34	1.38
24	b	621	CLA	C1D-C2D	2.10	1.47	1.42
24	A	407	CLA	C1B-CHB	2.10	1.46	1.41
24	B	609	CLA	C4B-CHC	2.10	1.46	1.41
31	a	415[A]	PL9	C2-C3	2.09	1.40	1.34
25	a	418[A]	PHO	C4D-CHA	2.09	1.49	1.43
38	F	102	HEM	C4D-C3D	2.09	1.47	1.42
24	c	517	CLA	C1B-CHB	2.09	1.46	1.41
24	c	513	CLA	C4B-CHC	2.08	1.46	1.41
24	b	618	CLA	C4C-C3C	2.08	1.48	1.45
24	b	610	CLA	C4C-C3C	2.07	1.48	1.45
24	C	506	CLA	C1B-NB	-2.07	1.33	1.35
29	M	103	LMT	O1'-C1'	2.07	1.43	1.40
31	D	405[B]	PL9	C2-C3	2.06	1.40	1.34
24	C	512	CLA	C4C-C3C	2.05	1.48	1.45
31	A	419[A]	PL9	C2-C3	2.05	1.40	1.34
24	b	615	CLA	C4B-CHC	2.05	1.46	1.41
24	c	509	CLA	C4C-C3C	2.05	1.48	1.45
31	d	405[B]	PL9	C2-C3	2.05	1.40	1.34
24	b	616	CLA	C1B-NB	-2.04	1.33	1.35
36	H	102	DGD	O5D-C1E	2.04	1.43	1.40
38	e	103	HEM	C3B-C2B	-2.04	1.37	1.40
31	a	415[B]	PL9	C2-C3	2.03	1.40	1.34
24	B	611	CLA	C1B-NB	-2.03	1.33	1.35
24	A	406	CLA	C4C-C3C	2.01	1.48	1.45
24	B	606	CLA	C4C-C3C	2.01	1.48	1.45
25	A	409[A]	PHO	C1B-NB	-2.00	1.34	1.38
24	A	406	CLA	C1C-NC	-2.00	1.34	1.37

All (2311) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CHD-C4C-C3C	-7.17	114.30	124.84
24	c	517	CLA	C4A-NA-C1A	-7.02	103.55	106.71
24	b	614	CLA	CHD-C4C-C3C	-6.89	114.71	124.84
25	A	408	PHO	CMD-C2D-C1D	6.83	135.59	125.06
24	B	603	CLA	C4A-NA-C1A	-6.82	103.64	106.71
24	b	614	CLA	C4A-NA-C1A	-6.79	103.66	106.71
38	F	102	HEM	CAD-CBD-CGD	6.77	124.03	112.67
24	c	512	CLA	O2D-CGD-CBD	6.76	123.28	111.27
25	A	409[B]	PHO	CMD-C2D-C1D	6.75	135.46	125.06
24	B	613	CLA	CHD-C4C-C3C	-6.72	114.96	124.84
24	d	402	CLA	C4A-NA-C1A	-6.71	103.69	106.71
24	b	610	CLA	O2D-CGD-CBD	6.63	123.06	111.27
25	A	409[A]	PHO	CMD-C2D-C1D	6.61	135.25	125.06
25	a	418[B]	PHO	CMD-C2D-C1D	6.58	135.20	125.06
24	B	612	CLA	CHD-C4C-C3C	-6.57	115.17	124.84
25	a	411	PHO	CMD-C2D-C1D	6.53	135.12	125.06
24	c	510	CLA	C4A-NA-C1A	-6.49	103.79	106.71
35	d	411	HTG	C1'-S1-C1	6.46	112.18	100.09
24	c	508	CLA	CHD-C4C-C3C	-6.44	115.38	124.84
24	B	616	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
24	c	512	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
35	C	522	HTG	C1'-S1-C1	6.39	112.04	100.09
24	b	613	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	B	604	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
24	b	611	CLA	C4A-NA-C1A	-6.35	103.85	106.71
25	a	418[A]	PHO	CMD-C2D-C1D	6.34	134.83	125.06
24	c	508	CLA	C4A-NA-C1A	-6.34	103.85	106.71
24	C	512	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
24	B	604	CLA	O2D-CGD-CBD	6.32	122.50	111.27
24	C	503	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
24	C	505	CLA	C4A-NA-C1A	-6.32	103.86	106.71
24	b	623	CLA	O2D-CGD-CBD	6.31	122.48	111.27
24	B	617	CLA	O2D-CGD-CBD	6.30	122.46	111.27
24	C	505	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
24	D	402	CLA	C4A-NA-C1A	-6.24	103.90	106.71
24	b	615	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
24	b	621	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
24	b	612	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
24	b	616	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
24	a	409	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	C	511	CLA	C2C-C1C-NC	6.19	115.77	109.97
24	b	615	CLA	C4A-NA-C1A	-6.17	103.93	106.71
24	d	401	CLA	C2C-C1C-NC	6.17	115.75	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	O2D-CGD-CBD	6.17	122.23	111.27
24	d	403	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
24	b	618	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
24	B	605	CLA	C2C-C1C-NC	6.14	115.72	109.97
24	c	510	CLA	CHD-C4C-C3C	-6.13	115.82	124.84
24	C	507	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
24	b	624	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
24	a	410	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
24	b	610	CLA	CHD-C4C-C3C	-6.10	115.88	124.84
24	b	624	CLA	C4A-NA-C1A	-6.09	103.97	106.71
24	B	609	CLA	C2C-C1C-NC	6.08	115.67	109.97
24	c	509	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
24	c	517	CLA	O2D-CGD-CBD	6.06	122.04	111.27
24	b	625	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
24	c	512	CLA	C2C-C1C-NC	6.04	115.63	109.97
24	b	613	CLA	O2D-CGD-CBD	6.02	121.96	111.27
24	B	602	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
24	B	607	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
24	B	617	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	D	402	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	c	506	CLA	C2C-C1C-NC	5.99	115.59	109.97
24	A	407	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
24	b	622	CLA	C2C-C1C-NC	5.99	115.58	109.97
24	b	625	CLA	O2D-CGD-CBD	5.99	121.91	111.27
24	c	510	CLA	C2C-C1C-NC	5.98	115.58	109.97
24	D	402	CLA	C2C-C1C-NC	5.97	115.56	109.97
24	d	401	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
24	C	510	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	B	610	CLA	C4A-NA-C1A	-5.96	104.03	106.71
24	c	514	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	A	406	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
24	C	502	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
24	c	518	CLA	C4A-NA-C1A	-5.93	104.04	106.71
24	B	614	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
24	c	507	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
24	B	610	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
24	B	616	CLA	C4A-NA-C1A	-5.91	104.05	106.71
35	c	525	HTG	C1'-S1-C1	5.91	111.14	100.09
24	B	615	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
24	c	515	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	b	618	CLA	C4A-NA-C1A	-5.88	104.06	106.71
24	A	406	CLA	C2C-C1C-NC	5.88	115.48	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C2C-C1C-NC	5.87	115.47	109.97
24	b	611	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	C	506	CLA	C2C-C1C-NC	5.84	115.44	109.97
24	A	410	CLA	CHD-C4C-C3C	-5.83	116.26	124.84
24	B	615	CLA	O2D-CGD-CBD	5.83	121.62	111.27
24	B	602	CLA	O2D-CGD-CBD	5.83	121.62	111.27
24	d	402	CLA	C2C-C1C-NC	5.83	115.43	109.97
24	b	617	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	c	517	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	b	620	CLA	C2C-C1C-NC	5.81	115.42	109.97
24	B	617	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	C	512	CLA	O2D-CGD-CBD	5.80	121.57	111.27
24	c	510	CLA	O2D-CGD-CBD	5.80	121.57	111.27
35	B	633	HTG	C1'-S1-C1	5.79	110.93	100.09
24	A	405	CLA	C2C-C1C-NC	5.79	115.40	109.97
24	b	616	CLA	C2C-C1C-NC	5.79	115.40	109.97
24	B	605	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
24	b	619	CLA	CHD-C4C-C3C	-5.78	116.33	124.84
24	A	405	CLA	C4A-NA-C1A	-5.78	104.11	106.71
24	a	412	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
24	c	511	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	b	610	CLA	C4A-NA-C1A	-5.75	104.12	106.71
24	B	603	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
24	A	407	CLA	C4A-NA-C1A	-5.74	104.12	106.71
24	a	412	CLA	C2C-C1C-NC	5.74	115.35	109.97
24	D	403	CLA	C2C-C1C-NC	5.73	115.34	109.97
24	c	516	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
24	c	518	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
24	b	620	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
24	b	617	CLA	C4A-NA-C1A	-5.70	104.14	106.71
24	D	403	CLA	C4A-NA-C1A	-5.69	104.15	106.71
35	D	412	HTG	C1'-S1-C1	5.68	110.72	100.09
24	c	509	CLA	C2C-C1C-NC	5.68	115.29	109.97
24	C	511	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
24	B	608	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	B	607	CLA	C4A-NA-C1A	-5.65	104.16	106.71
24	c	513	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	C	509	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
24	C	503	CLA	C4A-NA-C1A	-5.63	104.17	106.71
24	c	513	CLA	C2C-C1C-NC	5.63	115.24	109.97
24	c	511	CLA	CHD-C4C-C3C	-5.62	116.57	124.84
24	B	607	CLA	C2C-C1C-NC	5.62	115.24	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C4A-NA-C1A	-5.62	104.18	106.71
24	B	614	CLA	C2C-C1C-NC	5.61	115.23	109.97
24	d	403	CLA	C4A-NA-C1A	-5.61	104.18	106.71
24	c	515	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
24	b	612	CLA	O2D-CGD-CBD	5.58	121.19	111.27
24	b	623	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
35	B	625	HTG	C1'-S1-C1	5.57	110.51	100.09
24	C	504	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
24	C	508	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	b	624	CLA	C2C-C1C-NC	5.54	115.17	109.97
24	b	613	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
24	c	514	CLA	C2C-C1C-NC	5.54	115.16	109.97
24	b	615	CLA	C2C-C1C-NC	5.54	115.16	109.97
24	B	610	CLA	C2C-C1C-NC	5.53	115.16	109.97
24	b	623	CLA	C2C-C1C-NC	5.52	115.15	109.97
24	B	617	CLA	C2C-C1C-NC	5.49	115.12	109.97
24	C	513	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
24	C	508	CLA	O2D-CGD-CBD	5.48	121.01	111.27
24	a	410	CLA	C4A-NA-C1A	-5.48	104.24	106.71
24	B	611	CLA	C2C-C1C-NC	5.48	115.10	109.97
24	B	611	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
24	b	619	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	b	622	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
24	B	609	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
24	B	607	CLA	O2D-CGD-CBD	5.44	120.94	111.27
24	C	504	CLA	C2C-C1C-NC	5.44	115.06	109.97
24	b	625	CLA	C4A-NA-C1A	-5.43	104.27	106.71
26	Y	101	BCR	C33-C5-C6	-5.43	118.44	124.53
25	A	409[A]	PHO	C3D-C2D-C1D	-5.42	97.97	105.87
24	B	604	CLA	C2C-C1C-NC	5.41	115.04	109.97
24	C	509	CLA	C2C-C1C-NC	5.41	115.04	109.97
24	B	604	CLA	C4A-NA-C1A	-5.41	104.28	106.71
24	C	501	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
24	A	410	CLA	C2C-C1C-NC	5.38	115.02	109.97
27	f	101	SQD	O47-C7-C8	5.38	123.10	111.50
24	C	505	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	b	612	CLA	C4A-NA-C1A	-5.37	104.29	106.71
35	B	624	HTG	C1'-S1-C1	5.37	110.13	100.09
24	b	618	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	c	506	CLA	O2D-CGD-CBD	5.36	120.80	111.27
24	D	403	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
25	a	418[A]	PHO	O2D-CGD-CBD	5.34	120.76	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	CLA	C2C-C1C-NC	5.34	114.97	109.97
24	B	613	CLA	C3C-C4C-NC	5.34	116.56	110.57
24	b	612	CLA	C2C-C1C-NC	5.34	114.97	109.97
24	b	617	CLA	C2C-C1C-NC	5.34	114.97	109.97
25	a	418[B]	PHO	O2D-CGD-CBD	5.33	120.74	111.27
24	C	507	CLA	O2D-CGD-CBD	5.32	120.72	111.27
24	c	506	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
35	c	526	HTG	C1'-S1-C1	5.31	110.02	100.09
35	b	632	HTG	C1'-S1-C1	5.31	110.02	100.09
25	A	409[B]	PHO	C3D-C2D-C1D	-5.31	98.14	105.87
24	C	506	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
24	C	510	CLA	C2C-C1C-NC	5.30	114.94	109.97
24	B	613	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	C	508	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
26	D	404	BCR	C7-C8-C9	-5.30	118.23	126.23
24	c	509	CLA	O2D-CGD-CBD	5.29	120.67	111.27
35	b	631	HTG	C1'-S1-C1	5.27	109.95	100.09
24	C	501	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	c	507	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	B	603	CLA	O2D-CGD-CBD	5.26	120.62	111.27
27	L	102	SQD	O6-C1-C2	5.25	116.50	108.30
24	a	412	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	B	606	CLA	C4A-NA-C1A	-5.24	104.35	106.71
24	b	621	CLA	C2C-C1C-NC	5.24	114.88	109.97
25	a	411	PHO	O2D-CGD-CBD	5.24	120.58	111.27
24	A	406	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	b	615	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	c	518	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	B	608	CLA	C2C-C1C-NC	5.22	114.86	109.97
24	c	513	CLA	C4A-NA-C1A	-5.22	104.36	106.71
24	c	513	CLA	O2D-CGD-CBD	5.20	120.51	111.27
24	A	407	CLA	O2D-CGD-CBD	5.17	120.46	111.27
24	b	613	CLA	C4A-NA-C1A	-5.16	104.39	106.71
25	a	418[A]	PHO	C3D-C2D-C1D	-5.16	98.35	105.87
24	C	512	CLA	C4A-NA-C1A	-5.16	104.39	106.71
24	B	603	CLA	C2C-C1C-NC	5.15	114.79	109.97
25	A	409[B]	PHO	C2D-C1D-ND	5.14	117.55	109.79
27	F	103	SQD	O47-C7-C8	5.13	122.56	111.50
24	a	409	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
27	a	414	SQD	O6-C1-C2	5.11	116.28	108.30
24	C	509	CLA	C1-C2-C3	-5.10	117.22	126.04
24	b	611	CLA	O2D-CGD-CBD	5.10	120.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	418[A]	PHO	C1-C2-C3	-5.10	117.22	126.04
24	a	409	CLA	C4A-NA-C1A	-5.09	104.42	106.71
35	C	523	HTG	C1'-S1-C1	5.09	109.62	100.09
25	A	409[A]	PHO	C2D-C1D-ND	5.09	117.47	109.79
24	c	510	CLA	C3C-C4C-NC	5.09	116.28	110.57
25	a	418[B]	PHO	C3D-C2D-C1D	-5.08	98.47	105.87
24	B	615	CLA	C2C-C1C-NC	5.07	114.72	109.97
24	b	621	CLA	C3C-C4C-NC	5.06	116.25	110.57
24	B	602	CLA	C4A-NA-C1A	-5.06	104.43	106.71
24	b	614	CLA	C2C-C1C-NC	5.06	114.71	109.97
24	C	510	CLA	O2D-CGD-CBD	5.04	120.22	111.27
24	B	611	CLA	C4A-NA-C1A	-5.04	104.44	106.71
24	C	513	CLA	C2C-C1C-NC	5.04	114.69	109.97
25	A	408	PHO	C2D-C1D-ND	5.04	117.39	109.79
25	A	408	PHO	C3D-C2D-C1D	-5.03	98.54	105.87
24	C	502	CLA	C2C-C1C-NC	5.03	114.68	109.97
25	A	409[A]	PHO	C1-C2-C3	-5.03	117.34	126.04
24	B	602	CLA	C2C-C1C-NC	5.03	114.68	109.97
24	C	513	CLA	C4A-NA-C1A	-5.02	104.45	106.71
24	C	503	CLA	C2C-C1C-NC	5.02	114.68	109.97
24	b	619	CLA	O2D-CGD-CBD	5.02	120.19	111.27
24	C	512	CLA	C2C-C1C-NC	5.02	114.68	109.97
24	c	516	CLA	C2C-C1C-NC	5.01	114.67	109.97
35	B	625	HTG	O5-C1-C2	5.01	116.61	110.31
24	C	505	CLA	O2D-CGD-CBD	5.00	120.16	111.27
24	a	410	CLA	C2C-C1C-NC	5.00	114.66	109.97
24	C	504	CLA	O2D-CGD-CBD	4.98	120.12	111.27
24	D	403	CLA	O2D-CGD-CBD	4.97	120.11	111.27
24	C	505	CLA	C3C-C4C-NC	4.97	116.15	110.57
25	a	418[A]	PHO	C2D-C1D-ND	4.97	117.29	109.79
25	A	409[B]	PHO	C1-C2-C3	-4.97	117.45	126.04
24	b	616	CLA	O2D-CGD-CBD	4.97	120.09	111.27
27	B	621	SQD	O47-C7-C8	4.96	122.18	111.50
27	B	621	SQD	O6-C1-C2	4.95	116.03	108.30
24	b	611	CLA	C2C-C1C-NC	4.94	114.60	109.97
25	a	418[B]	PHO	C2D-C1D-ND	4.93	117.24	109.79
35	C	523	HTG	C1-O5-C5	4.90	121.62	112.58
24	B	616	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	d	403	CLA	C2C-C1C-NC	4.89	114.55	109.97
24	D	402	CLA	C3C-C4C-NC	4.89	116.05	110.57
24	d	401	CLA	C4A-NA-C1A	-4.88	104.51	106.71
24	c	517	CLA	C2C-C1C-NC	4.88	114.55	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	411	PHO	C3D-C2D-C1D	-4.88	98.76	105.87
24	b	610	CLA	C2C-C1C-NC	4.87	114.54	109.97
24	b	623	CLA	C4A-NA-C1A	-4.87	104.52	106.71
24	c	514	CLA	O2D-CGD-CBD	4.87	119.91	111.27
24	B	605	CLA	C4A-NA-C1A	-4.86	104.52	106.71
36	C	516	DGD	O2G-C1B-C2B	4.85	121.94	111.50
24	B	609	CLA	O2D-CGD-CBD	4.83	119.84	111.27
24	B	615	CLA	C4A-NA-C1A	-4.81	104.54	106.71
24	B	608	CLA	O2D-CGD-CBD	4.81	119.82	111.27
27	A	412	SQD	O47-C7-C8	4.80	121.86	111.50
24	A	405	CLA	CAC-C3C-C4C	4.78	131.02	124.81
25	a	418[B]	PHO	C1-C2-C3	-4.78	117.78	126.04
24	B	606	CLA	O2D-CGD-CBD	4.78	119.76	111.27
24	B	605	CLA	O2D-CGD-CBD	4.78	119.76	111.27
24	c	512	CLA	C3C-C4C-NC	4.76	115.91	110.57
24	b	625	CLA	C2C-C1C-NC	4.75	114.42	109.97
24	B	606	CLA	C3C-C4C-NC	4.75	115.90	110.57
26	b	626	BCR	C33-C5-C6	-4.74	119.20	124.53
24	C	506	CLA	C4A-NA-C1A	-4.74	104.58	106.71
24	B	606	CLA	C2C-C1C-NC	4.73	114.41	109.97
24	C	509	CLA	C4A-NA-C1A	-4.73	104.58	106.71
24	d	402	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
24	b	620	CLA	C4A-NA-C1A	-4.72	104.58	106.71
24	a	410	CLA	O2D-CGD-CBD	4.72	119.65	111.27
24	b	613	CLA	C3C-C4C-NC	4.72	115.86	110.57
29	A	417	LMT	C1'-O5'-C5'	4.71	122.94	113.69
24	c	509	CLA	C4A-NA-C1A	-4.70	104.59	106.71
24	d	403	CLA	O2D-CGD-CBD	4.70	119.63	111.27
24	b	621	CLA	O2D-CGD-CBD	4.69	119.60	111.27
25	a	418[A]	PHO	C4C-C3C-C2C	-4.69	101.60	106.78
24	c	508	CLA	C3C-C4C-NC	4.68	115.82	110.57
24	b	615	CLA	C3C-C4C-NC	4.68	115.82	110.57
25	a	411	PHO	C2D-C1D-ND	4.68	116.84	109.79
24	B	614	CLA	C3C-C4C-NC	4.67	115.81	110.57
26	t	101	BCR	C33-C5-C6	-4.67	119.28	124.53
27	L	102	SQD	O47-C7-C8	4.67	121.56	111.50
24	c	506	CLA	C4A-NA-C1A	-4.66	104.61	106.71
24	B	612	CLA	O2D-CGD-CBD	4.65	119.53	111.27
24	b	614	CLA	O2D-CGD-CBD	4.64	119.52	111.27
24	C	508	CLA	C4A-NA-C1A	-4.64	104.62	106.71
24	c	515	CLA	O2D-CGD-CBD	4.63	119.50	111.27
24	B	605	CLA	C3C-C4C-NC	4.63	115.76	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
38	F	102	HEM	CBD-CAD-C3D	-4.60	103.99	112.48
24	C	507	CLA	C4A-NA-C1A	-4.60	104.64	106.71
33	c	524	LMG	O7-C10-C11	4.60	121.41	111.50
24	b	612	CLA	C3C-C4C-NC	4.59	115.72	110.57
24	c	509	CLA	C3C-C4C-NC	4.59	115.72	110.57
33	A	421	LMG	O7-C10-C11	4.58	121.38	111.50
24	b	621	CLA	C4A-NA-C1A	-4.58	104.65	106.71
24	C	507	CLA	C2C-C1C-NC	4.58	114.26	109.97
24	A	405	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
24	A	410	CLA	C3C-C4C-NC	4.57	115.70	110.57
24	B	612	CLA	C4A-NA-C1A	-4.57	104.65	106.71
24	B	613	CLA	C2C-C1C-NC	4.57	114.25	109.97
24	B	604	CLA	C3C-C4C-NC	4.57	115.69	110.57
26	B	620	BCR	C15-C14-C13	-4.56	120.80	127.31
24	B	604	CLA	O2D-CGD-O1D	-4.55	114.95	123.84
24	c	511	CLA	C4A-NA-C1A	-4.55	104.66	106.71
24	B	612	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	a	412	CLA	C4A-NA-C1A	-4.53	104.67	106.71
24	B	615	CLA	C3C-C4C-NC	4.53	115.65	110.57
24	C	506	CLA	O2D-CGD-CBD	4.50	119.26	111.27
36	e	101	DGD	O2G-C1B-C2B	4.50	121.19	111.50
24	A	407	CLA	C2C-C1C-NC	4.49	114.18	109.97
24	C	503	CLA	C3C-C4C-NC	4.49	115.60	110.57
24	B	617	CLA	C1D-CHD-C4C	-4.49	116.64	122.56
24	c	513	CLA	C3C-C4C-NC	4.48	115.60	110.57
24	C	502	CLA	C1-C2-C3	-4.48	118.29	126.04
24	b	616	CLA	C3C-C4C-NC	4.48	115.60	110.57
33	C	520	LMG	O7-C10-C11	4.48	121.16	111.50
24	C	504	CLA	C4A-NA-C1A	-4.48	104.69	106.71
24	C	509	CLA	O2D-CGD-CBD	4.48	119.22	111.27
25	A	409[B]	PHO	O2D-CGD-CBD	4.47	119.22	111.27
24	A	406	CLA	CBC-CAC-C3C	-4.47	100.11	112.43
24	C	512	CLA	C3C-C4C-NC	4.47	115.58	110.57
24	b	616	CLA	C1C-C2C-C3C	-4.46	102.27	106.96
24	b	622	CLA	C3C-C4C-NC	4.46	115.57	110.57
24	b	618	CLA	O2D-CGD-CBD	4.46	119.19	111.27
24	d	402	CLA	O2D-CGD-CBD	4.45	119.18	111.27
35	B	632	HTG	C1'-S1-C1	4.45	108.41	100.09
24	c	514	CLA	C4A-NA-C1A	-4.44	104.71	106.71
24	a	412	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
25	A	409[A]	PHO	O2D-CGD-CBD	4.43	119.14	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C3C-C4C-NC	4.43	115.53	110.57
24	b	614	CLA	C3C-C4C-NC	4.42	115.52	110.57
35	b	632	HTG	O5-C1-C2	4.40	115.85	110.31
24	C	502	CLA	C4A-NA-C1A	-4.39	104.73	106.71
24	A	410	CLA	O2D-CGD-CBD	4.39	119.07	111.27
24	c	508	CLA	C2C-C1C-NC	4.39	114.08	109.97
24	b	618	CLA	C3C-C4C-NC	4.38	115.48	110.57
24	d	401	CLA	C1D-CHD-C4C	-4.37	116.79	122.56
25	a	418[B]	PHO	C4C-C3C-C2C	-4.35	101.96	106.78
24	c	511	CLA	O2D-CGD-CBD	4.35	119.00	111.27
24	C	510	CLA	C4A-NA-C1A	-4.35	104.75	106.71
24	c	515	CLA	C4A-NA-C1A	-4.35	104.75	106.71
24	c	507	CLA	C3C-C4C-NC	4.35	115.45	110.57
25	A	408	PHO	O2D-CGD-CBD	4.35	118.99	111.27
24	c	514	CLA	C1D-CHD-C4C	-4.34	116.83	122.56
24	B	607	CLA	C3C-C4C-NC	4.34	115.43	110.57
24	C	502	CLA	O2D-CGD-CBD	4.33	118.97	111.27
26	B	618	BCR	C33-C5-C6	-4.33	119.67	124.53
24	C	511	CLA	C3B-C4B-NB	4.32	114.80	109.21
24	B	611	CLA	O2D-CGD-CBD	4.32	118.94	111.27
35	b	607	HTG	C1'-S1-C1	4.31	108.15	100.09
24	b	625	CLA	C1D-CHD-C4C	-4.31	116.87	122.56
24	A	406	CLA	C3B-C4B-NB	4.31	114.78	109.21
33	c	501	LMG	O7-C10-C11	4.31	120.78	111.50
24	a	410	CLA	C3C-C4C-NC	4.30	115.40	110.57
24	B	612	CLA	CMC-C2C-C1C	4.30	131.58	125.04
24	d	401	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
24	C	513	CLA	O2D-CGD-CBD	4.29	118.89	111.27
24	b	620	CLA	O2D-CGD-CBD	4.28	118.88	111.27
24	b	624	CLA	C3C-C4C-NC	4.28	115.37	110.57
24	d	401	CLA	C3B-C4B-NB	4.28	114.74	109.21
24	c	508	CLA	O2D-CGD-CBD	4.27	118.86	111.27
24	B	606	CLA	C1D-CHD-C4C	-4.26	116.94	122.56
24	B	615	CLA	O2D-CGD-O1D	-4.25	115.52	123.84
36	c	522	DGD	O2G-C1B-C2B	4.25	120.67	111.50
36	e	101	DGD	O6E-C5E-C4E	4.25	117.41	109.69
24	b	613	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
26	d	404	BCR	C24-C23-C22	-4.24	119.82	126.23
27	A	412	SQD	O6-C1-C2	4.24	114.92	108.30
27	a	414	SQD	O47-C7-C8	4.24	120.64	111.50
24	c	516	CLA	C4A-NA-C1A	-4.23	104.80	106.71
24	B	609	CLA	C1C-C2C-C3C	-4.23	102.51	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	C3C-C4C-NC	4.22	115.30	110.57
24	B	608	CLA	C3C-C4C-NC	4.22	115.30	110.57
24	c	508	CLA	C1D-CHD-C4C	-4.22	116.99	122.56
24	C	507	CLA	C3C-C4C-NC	4.22	115.30	110.57
25	a	418[A]	PHO	O2D-CGD-O1D	-4.21	115.62	123.84
24	c	511	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
24	a	409	CLA	C1C-C2C-C3C	-4.20	102.54	106.96
24	C	511	CLA	O2D-CGD-CBD	4.19	118.72	111.27
24	B	617	CLA	C3C-C4C-NC	4.19	115.27	110.57
24	c	507	CLA	O2D-CGD-CBD	4.19	118.71	111.27
24	b	612	CLA	CAA-C2A-C3A	-4.18	101.33	112.78
24	c	512	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
27	a	414	SQD	O9-S-C6	4.17	111.90	106.94
24	B	606	CLA	CMC-C2C-C1C	4.17	131.38	125.04
24	C	501	CLA	C4A-NA-C1A	-4.16	104.84	106.71
26	C	514	BCR	C7-C8-C9	-4.16	119.95	126.23
24	C	510	CLA	C3C-C4C-NC	4.15	115.23	110.57
24	b	625	CLA	CAC-C3C-C4C	4.15	130.19	124.81
24	D	402	CLA	O2D-CGD-CBD	4.15	118.64	111.27
26	y	101	BCR	C33-C5-C6	-4.15	119.87	124.53
24	C	502	CLA	C3C-C4C-NC	4.14	115.22	110.57
26	c	519	BCR	C7-C8-C9	-4.14	119.97	126.23
24	C	509	CLA	C3C-C4C-NC	4.14	115.22	110.57
24	b	622	CLA	C4A-NA-C1A	-4.14	104.84	106.71
24	b	625	CLA	C3C-C4C-NC	4.13	115.21	110.57
24	c	514	CLA	C3C-C4C-NC	4.13	115.20	110.57
26	d	404	BCR	C38-C26-C25	-4.13	119.89	124.53
24	B	607	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
24	b	619	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	d	401	CLA	O2D-CGD-CBD	4.12	118.59	111.27
36	D	406	DGD	O2G-C1B-C2B	4.12	120.37	111.50
24	b	612	CLA	C1D-CHD-C4C	-4.12	117.13	122.56
24	c	515	CLA	C1-C2-C3	-4.11	118.93	126.04
24	B	612	CLA	C1D-CHD-C4C	-4.11	117.13	122.56
24	c	509	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
24	c	512	CLA	C4A-NA-C1A	-4.09	104.86	106.71
24	B	610	CLA	C3C-C4C-NC	4.09	115.16	110.57
38	e	103	HEM	CAD-CBD-CGD	4.09	119.53	112.67
24	c	514	CLA	C3B-C4B-NB	4.09	114.49	109.21
24	B	609	CLA	C4A-NA-C1A	-4.08	104.87	106.71
24	b	623	CLA	C3C-C4C-NC	4.07	115.14	110.57
24	c	506	CLA	C3C-C4C-NC	4.06	115.12	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	CAA-C2A-C3A	-4.06	101.67	112.78
24	D	403	CLA	C3C-C4C-NC	4.06	115.12	110.57
24	B	603	CLA	C3C-C4C-NC	4.05	115.11	110.57
24	c	512	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
26	b	626	BCR	C7-C8-C9	-4.05	120.12	126.23
33	Z	101	LMG	O7-C10-C11	4.04	120.21	111.50
24	c	518	CLA	O2D-CGD-CBD	4.04	118.45	111.27
24	C	504	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	D	402	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
26	k	101	BCR	C24-C23-C22	-4.04	120.14	126.23
24	A	405	CLA	C1D-CHD-C4C	-4.04	117.23	122.56
24	c	506	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
24	B	614	CLA	C4A-NA-C1A	-4.03	104.89	106.71
24	c	515	CLA	C3B-C4B-NB	4.03	114.42	109.21
24	c	515	CLA	C3C-C4C-NC	4.03	115.08	110.57
24	b	613	CLA	C3B-C4B-NB	4.02	114.41	109.21
24	C	511	CLA	C3C-C4C-NC	4.02	115.08	110.57
26	H	101	BCR	C38-C26-C25	-4.02	120.01	124.53
29	C	521	LMT	O1B-C4'-C3'	4.02	117.97	107.28
24	b	610	CLA	C1D-CHD-C4C	-4.02	117.25	122.56
24	C	504	CLA	C3C-C4C-NC	4.02	115.08	110.57
24	b	610	CLA	C3C-C4C-NC	4.01	115.07	110.57
29	A	417	LMT	O5'-C5'-C4'	4.01	118.22	109.75
26	D	404	BCR	C33-C5-C6	-4.00	120.03	124.53
24	C	503	CLA	C1D-CHD-C4C	-4.00	117.27	122.56
24	b	625	CLA	C3B-C4B-NB	4.00	114.39	109.21
24	c	509	CLA	C1D-CHD-C4C	-3.99	117.30	122.56
24	B	615	CLA	CAC-C3C-C4C	3.99	129.98	124.81
24	C	511	CLA	C1D-CHD-C4C	-3.98	117.31	122.56
24	B	604	CLA	C1D-CHD-C4C	-3.98	117.31	122.56
24	c	511	CLA	C3B-C4B-NB	3.98	114.35	109.21
24	B	611	CLA	C3C-C4C-NC	3.98	115.03	110.57
24	A	405	CLA	C3C-C4C-NC	3.98	115.03	110.57
24	d	402	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
27	a	405	SQD	O47-C7-C8	3.97	120.06	111.50
24	B	609	CLA	C3C-C4C-NC	3.97	115.03	110.57
24	b	610	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
24	b	614	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	b	615	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
27	a	414	SQD	O8-S-C6	3.97	112.06	105.74
24	C	508	CLA	C3C-C4C-NC	3.97	115.02	110.57
26	y	101	BCR	C15-C14-C13	-3.96	121.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	C3C-C4C-NC	3.96	115.01	110.57
24	a	412	CLA	C3C-C4C-NC	3.96	115.01	110.57
24	c	510	CLA	C1D-CHD-C4C	-3.96	117.33	122.56
24	c	518	CLA	C1D-CHD-C4C	-3.96	117.33	122.56
24	b	621	CLA	C1D-CHD-C4C	-3.96	117.34	122.56
27	L	102	SQD	C3-C4-C5	3.95	117.29	110.24
24	c	514	CLA	C1-C2-C3	-3.95	119.21	126.04
24	B	604	CLA	CAA-C2A-C3A	-3.95	101.96	112.78
24	d	401	CLA	CBC-CAC-C3C	-3.95	101.55	112.43
37	D	409	LHG	O7-C7-C8	3.94	120.00	111.50
24	b	622	CLA	C3B-C4B-NB	3.94	114.31	109.21
24	b	611	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	b	623	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
24	b	623	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
31	a	415[A]	PL9	C22-C23-C24	-3.94	118.19	127.66
29	D	401	LMT	O1B-C4'-C3'	3.93	117.74	107.28
27	B	621	SQD	O7-S-C6	3.93	111.61	106.94
24	C	510	CLA	C1-C2-C3	-3.93	119.25	126.04
24	B	612	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	b	615	CLA	C3B-C4B-NB	3.92	114.28	109.21
24	c	515	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
24	b	615	CLA	C1D-CHD-C4C	-3.92	117.38	122.56
26	H	101	BCR	C16-C17-C18	-3.92	121.71	127.31
24	b	623	CLA	C1-C2-C3	-3.92	119.27	126.04
33	b	629	LMG	O7-C10-C11	3.92	119.95	111.50
31	a	415[A]	PL9	C15-C14-C16	3.92	121.86	115.27
24	C	501	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
25	a	411	PHO	CAC-C3C-C4C	3.91	129.49	125.22
24	c	512	CLA	C1D-CHD-C4C	-3.91	117.40	122.56
24	B	602	CLA	C3C-C4C-NC	3.90	114.95	110.57
24	B	602	CLA	C1D-CHD-C4C	-3.90	117.41	122.56
24	c	515	CLA	C4-C3-C5	3.90	121.83	115.27
24	B	604	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
26	D	404	BCR	C24-C23-C22	-3.89	120.36	126.23
25	A	409[A]	PHO	C4C-C3C-C2C	-3.89	102.48	106.78
24	B	607	CLA	C1D-CHD-C4C	-3.89	117.43	122.56
24	c	513	CLA	C3B-C4B-NB	3.88	114.23	109.21
24	b	624	CLA	C1D-CHD-C4C	-3.88	117.44	122.56
24	A	405	CLA	C3B-C4B-NB	3.88	114.22	109.21
31	a	415[A]	PL9	C32-C33-C34	-3.87	118.33	127.66
24	B	605	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
37	D	407	LHG	O7-C7-C8	3.87	119.85	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	d	403	CLA	C3C-C4C-NC	3.86	114.90	110.57
24	b	621	CLA	C4C-C3C-C2C	-3.86	101.28	106.90
25	A	409[B]	PHO	C4C-C3C-C2C	-3.86	102.52	106.78
24	C	505	CLA	C1D-CHD-C4C	-3.86	117.47	122.56
24	c	507	CLA	C1D-CHD-C4C	-3.85	117.47	122.56
24	c	518	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	c	517	CLA	C3C-C4C-NC	3.85	114.89	110.57
31	a	415[B]	PL9	C22-C23-C24	-3.85	118.39	127.66
36	c	520	DGD	O2G-C1B-C2B	3.85	119.80	111.50
27	A	416	SQD	O47-C7-C8	3.85	119.80	111.50
36	D	406	DGD	C1D-C2D-C3D	3.85	118.00	110.00
33	C	519	LMG	O7-C10-C11	3.84	119.78	111.50
24	b	620	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	b	624	CLA	O2D-CGD-CBD	3.84	118.08	111.27
31	a	415[A]	PL9	C7-C3-C4	3.83	119.99	116.88
24	b	620	CLA	C3C-C4C-NC	3.83	114.86	110.57
24	D	402	CLA	C3B-C4B-NB	3.82	114.16	109.21
31	a	415[B]	PL9	C32-C33-C34	-3.82	118.45	127.66
36	c	521	DGD	O2G-C1B-C2B	3.82	119.74	111.50
24	C	506	CLA	C3C-C4C-NC	3.82	114.85	110.57
24	c	506	CLA	CAC-C3C-C4C	3.82	129.76	124.81
24	b	611	CLA	CAA-C2A-C3A	-3.82	102.33	112.78
24	c	511	CLA	C3C-C4C-NC	3.81	114.85	110.57
24	d	402	CLA	C3B-C4B-NB	3.81	114.14	109.21
24	b	614	CLA	C1D-CHD-C4C	-3.81	117.53	122.56
24	B	604	CLA	CMC-C2C-C1C	3.81	130.84	125.04
35	B	623	HTG	C1'-S1-C1	3.81	107.21	100.09
24	c	506	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
24	B	610	CLA	O2D-CGD-CBD	3.80	118.03	111.27
24	C	504	CLA	CBC-CAC-C3C	-3.80	101.96	112.43
24	b	616	CLA	C4A-NA-C1A	-3.80	105.00	106.71
24	a	409	CLA	C3C-C4C-NC	3.80	114.83	110.57
24	b	622	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
36	C	517	DGD	O2G-C1B-C2B	3.79	119.67	111.50
24	B	612	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	C	513	CLA	C3C-C4C-NC	3.79	114.82	110.57
24	C	512	CLA	C1-C2-C3	-3.79	119.49	126.04
27	A	412	SQD	C45-O47-C7	-3.79	108.47	117.79
24	B	605	CLA	C3B-C4B-NB	3.78	114.10	109.21
36	e	101	DGD	C3E-C4E-C5E	3.78	116.98	110.24
24	b	620	CLA	C1-C2-C3	-3.78	119.51	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	516	CLA	C3C-C4C-NC	3.78	114.81	110.57
24	A	405	CLA	CAA-C2A-C3A	-3.77	102.45	112.78
24	A	407	CLA	C3C-C4C-NC	3.77	114.80	110.57
24	B	602	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
26	h	101	BCR	C16-C17-C18	-3.77	121.93	127.31
24	B	612	CLA	CAC-C3C-C4C	3.77	129.70	124.81
24	D	403	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	c	517	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
24	C	504	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	c	506	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	a	409	CLA	C1-C2-C3	-3.75	119.56	126.04
24	D	402	CLA	C1-C2-C3	-3.75	119.56	126.04
37	E	101	LHG	O7-C7-C8	3.75	119.57	111.50
31	a	415[B]	PL9	C7-C3-C4	3.75	119.92	116.88
24	a	412	CLA	C1-C2-C3	-3.74	119.57	126.04
24	A	410	CLA	CAC-C3C-C4C	3.74	129.66	124.81
24	C	511	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
26	t	101	BCR	C15-C16-C17	-3.72	115.84	123.47
24	c	518	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
31	A	419[B]	PL9	C7-C3-C4	3.72	119.90	116.88
33	c	524	LMG	O6-C5-C4	3.71	116.44	109.69
27	a	405	SQD	O8-S-C6	3.71	111.66	105.74
24	d	403	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
24	d	402	CLA	C3C-C4C-NC	3.70	114.72	110.57
24	C	509	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
27	A	416	SQD	O48-C23-C24	3.70	123.51	111.91
24	C	504	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
24	b	617	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	a	412	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
26	T	103	BCR	C33-C5-C6	-3.69	120.39	124.53
24	b	621	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	a	409	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
24	A	405	CLA	O2D-CGD-CBD	3.68	117.80	111.27
24	B	608	CLA	C4A-NA-C1A	-3.68	105.05	106.71
24	b	612	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
29	a	404	LMT	C1'-O5'-C5'	3.68	120.90	113.69
24	B	607	CLA	CMC-C2C-C1C	3.68	130.64	125.04
24	C	506	CLA	CAC-C3C-C4C	3.67	129.58	124.81
24	b	619	CLA	C1-C2-C3	-3.67	119.70	126.04
24	B	613	CLA	C4A-NA-C1A	-3.66	105.06	106.71
27	a	405	SQD	O48-C23-C24	3.66	123.40	111.91
31	d	405[A]	PL9	C42-C43-C44	-3.66	118.84	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	A	406	CLA	C3C-C4C-NC	3.66	114.67	110.57
24	b	617	CLA	O2D-CGD-CBD	3.66	117.77	111.27
24	c	513	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	c	509	CLA	C4-C3-C5	3.65	121.42	115.27
24	B	616	CLA	C1D-CHD-C4C	-3.65	117.74	122.56
24	c	507	CLA	C4D-C3D-CAD	-3.65	106.44	108.47
24	c	510	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
24	C	508	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	b	620	CLA	C1D-CHD-C4C	-3.64	117.75	122.56
24	b	612	CLA	CMC-C2C-C1C	3.64	130.59	125.04
24	C	501	CLA	C3C-C4C-NC	3.64	114.65	110.57
24	d	402	CLA	C1-C2-C3	-3.64	119.75	126.04
24	D	402	CLA	C4D-C3D-CAD	-3.63	106.44	108.47
24	C	511	CLA	CAC-C3C-C4C	3.63	129.53	124.81
31	a	415[B]	PL9	C15-C14-C16	3.63	121.39	115.27
24	B	609	CLA	C3B-C4B-NB	3.63	113.90	109.21
31	a	415[B]	PL9	C7-C8-C9	-3.63	120.75	126.79
24	D	403	CLA	CAC-C3C-C4C	3.61	129.50	124.81
24	c	514	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
37	L	101	LHG	O7-C7-C8	3.61	119.29	111.50
24	B	611	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	C	513	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	B	616	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
27	a	414	SQD	C1-C2-C3	-3.61	102.48	110.00
26	C	514	BCR	C33-C5-C6	-3.61	120.48	124.53
24	a	410	CLA	CMC-C2C-C1C	3.60	130.53	125.04
24	B	610	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	b	618	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
33	z	101	LMG	O7-C10-C11	3.59	119.24	111.50
24	B	602	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
24	b	618	CLA	C1D-CHD-C4C	-3.59	117.82	122.56
24	C	501	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
24	B	610	CLA	C3B-C4B-NB	3.58	113.84	109.21
33	c	524	LMG	C3-C4-C5	3.58	116.63	110.24
24	B	610	CLA	C1D-CHD-C4C	-3.58	117.83	122.56
24	C	512	CLA	C1D-CHD-C4C	-3.58	117.84	122.56
24	C	502	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
24	B	616	CLA	CMC-C2C-C1C	3.58	130.48	125.04
24	B	603	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
29	a	404	LMT	O5'-C5'-C4'	3.56	117.25	109.75
24	B	615	CLA	C1C-C2C-C3C	-3.55	103.22	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	C1D-CHD-C4C	-3.55	117.87	122.56
24	B	606	CLA	CHD-C4C-NC	3.55	129.80	124.20
24	B	603	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
24	c	517	CLA	C1D-CHD-C4C	-3.54	117.88	122.56
24	C	506	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	c	511	CLA	CBC-CAC-C3C	-3.54	102.67	112.43
31	D	405[A]	PL9	C40-C39-C41	3.54	121.23	115.27
24	C	503	CLA	O2D-CGD-CBD	3.54	117.56	111.27
24	c	516	CLA	O2D-CGD-CBD	3.54	117.55	111.27
33	c	523	LMG	O7-C10-C11	3.54	119.12	111.50
24	B	614	CLA	C3B-C4B-NB	3.53	113.78	109.21
26	c	519	BCR	C33-C5-C6	-3.53	120.56	124.53
24	B	608	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	C	509	CLA	C3B-C4B-NB	3.53	113.77	109.21
35	b	608	HTG	C1'-S1-C1	3.53	106.69	100.09
26	D	404	BCR	C38-C26-C25	-3.53	120.57	124.53
24	b	614	CLA	CHD-C4C-NC	3.53	129.76	124.20
24	c	510	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
24	D	403	CLA	C3B-C4B-NB	3.52	113.76	109.21
31	D	405[A]	PL9	C42-C43-C44	-3.52	119.18	127.66
24	B	606	CLA	C4-C3-C5	3.52	121.19	115.27
24	A	405	CLA	O2A-CGA-CBA	3.52	122.94	111.91
29	C	521	LMT	C1'-O5'-C5'	3.52	120.59	113.69
24	C	508	CLA	C3B-C4B-NB	3.52	113.75	109.21
24	b	621	CLA	O2A-CGA-CBA	3.51	122.94	111.91
24	c	511	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
24	A	406	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
24	B	607	CLA	C3B-C4B-NB	3.51	113.74	109.21
25	a	418[A]	PHO	C4-C3-C5	3.51	121.17	115.27
24	D	403	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
24	A	405	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	a	410	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
24	A	407	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
26	b	626	BCR	C15-C14-C13	-3.50	122.32	127.31
24	b	611	CLA	C1C-C2C-C3C	-3.49	103.28	106.96
24	B	607	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
24	b	612	CLA	C3B-C4B-NB	3.49	113.73	109.21
24	c	510	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
24	B	613	CLA	C3B-C4B-NB	3.49	113.72	109.21
27	A	412	SQD	O8-S-C6	3.49	111.30	105.74
24	B	614	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
24	A	407	CLA	C4-C3-C5	3.48	121.13	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	411	PHO	C4C-C3C-C2C	-3.48	102.93	106.78
24	b	625	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
24	B	608	CLA	C3B-C4B-NB	3.48	113.71	109.21
24	c	508	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
24	c	516	CLA	C1D-CHD-C4C	-3.48	117.97	122.56
24	A	406	CLA	C4D-C3D-CAD	-3.48	106.53	108.47
26	k	101	BCR	C7-C8-C9	-3.47	120.98	126.23
24	C	510	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
31	a	415[A]	PL9	C7-C8-C9	-3.47	121.01	126.79
25	a	411	PHO	O1D-CGD-CBD	-3.47	117.38	124.48
24	c	513	CLA	C1D-CHD-C4C	-3.47	117.98	122.56
25	A	408	PHO	C4C-C3C-C2C	-3.47	102.94	106.78
24	b	611	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
27	F	103	SQD	O6-C1-C2	3.47	113.72	108.30
24	A	406	CLA	C4A-NA-C1A	-3.47	105.15	106.71
24	B	617	CLA	C3B-C4B-NB	3.46	113.69	109.21
26	T	103	BCR	C11-C10-C9	-3.46	122.37	127.31
26	d	404	BCR	C7-C8-C9	-3.46	121.01	126.23
33	c	523	LMG	O8-C28-C29	3.46	122.76	111.91
37	d	407	LHG	O7-C7-C8	3.46	118.95	111.50
24	c	516	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
24	d	403	CLA	CMC-C2C-C1C	3.45	130.30	125.04
24	C	513	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
25	a	418[B]	PHO	O2D-CGD-O1D	-3.45	117.09	123.84
24	b	624	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	A	410	CLA	C4A-NA-C1A	-3.45	105.16	106.71
24	b	614	CLA	C4-C3-C5	3.45	121.07	115.27
24	A	410	CLA	C1D-CHD-C4C	-3.45	118.01	122.56
26	H	101	BCR	C24-C23-C22	-3.44	121.03	126.23
24	C	512	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	b	623	CLA	C3B-C4B-NB	3.44	113.66	109.21
36	h	102	DGD	O2G-C1B-C2B	3.44	118.91	111.50
24	C	501	CLA	CMC-C2C-C1C	3.44	130.28	125.04
24	C	505	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
24	B	603	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
24	B	613	CLA	CMC-C2C-C1C	3.43	130.27	125.04
26	B	619	BCR	C28-C27-C26	-3.43	107.96	114.08
24	b	614	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
24	b	622	CLA	C1-C2-C3	-3.42	120.13	126.04
24	B	603	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
26	b	627	BCR	C29-C30-C25	3.42	115.75	110.48
27	A	412	SQD	O9-S-C6	3.42	111.00	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	412	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
31	A	419[A]	PL9	C7-C3-C4	3.41	119.65	116.88
24	b	617	CLA	C1D-CHD-C4C	-3.41	118.05	122.56
31	A	419[A]	PL9	C37-C38-C39	-3.41	119.44	127.66
27	f	101	SQD	C1-O5-C5	3.41	120.37	113.69
31	A	419[B]	PL9	C32-C33-C34	-3.41	119.46	127.66
35	B	624	HTG	C1-O5-C5	3.40	118.86	112.58
26	c	528	BCR	C15-C14-C13	-3.40	122.46	127.31
24	b	611	CLA	C1D-CHD-C4C	-3.40	118.07	122.56
26	C	515	BCR	C33-C5-C6	-3.39	120.72	124.53
24	B	615	CLA	C3B-C4B-NB	3.39	113.60	109.21
24	B	613	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
24	B	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
24	b	610	CLA	C1C-C2C-C3C	-3.39	103.40	106.96
26	C	515	BCR	C7-C8-C9	-3.38	121.12	126.23
24	B	614	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
31	A	419[A]	PL9	C20-C19-C21	3.38	120.96	115.27
29	T	104	LMT	C1'-O5'-C5'	3.38	120.33	113.69
24	b	620	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	D	403	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
24	C	502	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	C	510	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
24	C	507	CLA	CMC-C2C-C1C	3.37	130.18	125.04
24	b	615	CLA	C4-C3-C5	3.37	120.94	115.27
24	b	614	CLA	C2A-C1A-CHA	-3.37	117.97	123.86
24	a	409	CLA	CAA-C2A-C3A	-3.37	103.56	112.78
24	c	518	CLA	CMC-C2C-C1C	3.37	130.16	125.04
24	c	507	CLA	C4C-C3C-C2C	-3.36	102.01	106.90
24	b	624	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
24	c	508	CLA	CMC-C2C-C1C	3.35	130.15	125.04
24	A	410	CLA	C1C-C2C-C3C	-3.35	103.43	106.96
24	B	604	CLA	O2A-CGA-O1A	-3.35	115.13	123.59
24	C	511	CLA	C4A-NA-C1A	-3.35	105.20	106.71
26	A	411	BCR	C33-C5-C6	-3.34	120.77	124.53
31	D	405[A]	PL9	C7-C8-C9	-3.34	121.23	126.79
24	B	605	CLA	C1-C2-C3	-3.34	120.26	126.04
24	b	619	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
24	c	507	CLA	C3B-C4B-NB	3.34	113.53	109.21
24	c	516	CLA	C3B-C4B-NB	3.34	113.53	109.21
26	C	514	BCR	C15-C14-C13	-3.34	122.55	127.31
31	d	405[B]	PL9	C42-C43-C44	-3.33	119.63	127.66
24	C	504	CLA	C1D-CHD-C4C	-3.33	118.16	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	SQD	C44-O6-C1	-3.33	107.23	113.74
24	b	619	CLA	C1C-C2C-C3C	-3.33	103.45	106.96
24	B	605	CLA	C1D-CHD-C4C	-3.32	118.17	122.56
24	c	507	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
24	b	619	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	B	615	CLA	O2A-CGA-O1A	-3.31	115.24	123.59
24	A	410	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	C	501	CLA	C1-C2-C3	-3.31	120.32	126.04
31	a	415[B]	PL9	C17-C18-C19	-3.31	119.69	127.66
24	c	508	CLA	CAC-C3C-C4C	3.31	129.10	124.81
27	F	103	SQD	O7-S-C6	3.30	110.86	106.94
24	A	410	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
24	d	402	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
24	C	503	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
24	C	501	CLA	CBC-CAC-C3C	-3.29	103.36	112.43
35	V	206	HTG	C1'-S1-C1	3.29	106.25	100.09
31	A	419[A]	PL9	C32-C33-C34	-3.29	119.75	127.66
24	C	512	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	c	509	CLA	CMC-C2C-C1C	3.28	130.03	125.04
31	a	415[A]	PL9	C17-C18-C19	-3.28	119.76	127.66
24	a	409	CLA	CMB-C2B-C3B	3.28	130.81	124.68
24	B	617	CLA	CAC-C3C-C4C	3.28	129.06	124.81
24	d	403	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
24	b	616	CLA	C3B-C4B-NB	3.27	113.44	109.21
24	A	407	CLA	CBC-CAC-C3C	-3.27	103.41	112.43
24	b	621	CLA	O2A-CGA-O1A	-3.27	115.34	123.59
24	B	602	CLA	O2A-CGA-CBA	3.27	122.17	111.91
24	a	410	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
24	B	617	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
31	D	405[A]	PL9	C10-C9-C11	3.26	120.76	115.27
25	A	409[A]	PHO	C4-C3-C5	3.26	120.76	115.27
25	A	408	PHO	C4D-CHA-C1A	-3.26	118.03	125.37
24	a	412	CLA	C3B-C4B-NB	3.26	113.42	109.21
24	b	624	CLA	CAC-C3C-C4C	3.26	129.04	124.81
24	B	606	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
24	b	610	CLA	C3B-C4B-NB	3.26	113.42	109.21
24	c	509	CLA	C1-C2-C3	-3.26	120.41	126.04
24	d	401	CLA	CAA-C2A-C3A	-3.25	103.86	112.78
24	c	513	CLA	CAC-C3C-C4C	3.25	129.03	124.81
24	c	513	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
24	c	514	CLA	CAC-C3C-C4C	3.25	129.02	124.81
24	d	403	CLA	CHD-C4C-NC	3.24	129.31	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
24	C	509	CLA	CAC-C3C-C4C	3.24	129.01	124.81
24	b	615	CLA	CMC-C2C-C1C	3.24	129.97	125.04
25	A	409[B]	PHO	C4-C3-C5	3.24	120.72	115.27
24	b	613	CLA	C1D-CHD-C4C	-3.24	118.28	122.56
38	V	205	HEM	CAD-CBD-CGD	3.24	118.10	112.67
24	C	507	CLA	C1C-C2C-C3C	-3.24	103.56	106.96
24	a	409	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	B	610	CLA	CHC-C1C-C2C	-3.23	117.78	126.72
24	C	501	CLA	C3B-C4B-NB	3.23	113.38	109.21
24	B	608	CLA	C1D-CHD-C4C	-3.23	118.30	122.56
24	C	505	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
24	C	506	CLA	C1D-CHD-C4C	-3.23	118.30	122.56
24	B	605	CLA	CAC-C3C-C4C	3.23	129.00	124.81
24	d	402	CLA	CAC-C3C-C4C	3.22	128.99	124.81
24	b	617	CLA	OBD-CAD-C3D	-3.22	122.63	127.98
24	b	619	CLA	C3B-C4B-NB	3.22	113.38	109.21
33	c	501	LMG	C8-O7-C10	-3.22	109.86	117.79
24	B	607	CLA	CBC-CAC-C3C	-3.22	103.55	112.43
24	b	619	CLA	CAC-C3C-C4C	3.22	128.99	124.81
37	d	408	LHG	O7-C7-C8	3.22	118.44	111.50
24	A	410	CLA	C4-C3-C5	3.22	120.69	115.27
24	C	506	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
24	B	617	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
24	C	508	CLA	CMB-C2B-C3B	3.22	130.70	124.68
25	a	418[B]	PHO	C2B-C1B-NB	3.21	114.64	109.79
33	D	413	LMG	O7-C10-C11	3.21	118.42	111.50
24	C	501	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
24	C	512	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
31	a	415[A]	PL9	C20-C19-C21	3.21	120.67	115.27
24	A	406	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
26	B	619	BCR	C29-C30-C25	3.21	115.42	110.48
31	D	405[B]	PL9	C42-C43-C44	-3.20	119.94	127.66
24	b	622	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
25	a	418[B]	PHO	C4-C3-C5	3.20	120.66	115.27
24	B	608	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
24	c	510	CLA	CAC-C3C-C4C	3.20	128.96	124.81
26	c	528	BCR	C11-C10-C9	-3.20	122.74	127.31
33	B	622	LMG	O8-C28-C29	3.20	121.95	111.91
31	A	419[B]	PL9	C20-C19-C21	3.20	120.66	115.27
24	C	511	CLA	CHC-C1C-C2C	-3.20	117.87	126.72
31	a	415[A]	PL9	C42-C43-C44	-3.20	119.95	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	415[A]	PL9	C10-C9-C11	3.20	120.65	115.27
31	D	405[B]	PL9	C7-C8-C9	-3.20	121.47	126.79
24	B	606	CLA	C2A-C1A-CHA	-3.19	118.27	123.86
24	D	402	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	B	614	CLA	C1-C2-C3	-3.19	120.52	126.04
24	B	606	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
24	B	612	CLA	C4D-C3D-CAD	-3.19	106.69	108.47
24	c	513	CLA	C1-C2-C3	-3.19	120.52	126.04
24	b	625	CLA	O2A-CGA-CBA	3.19	121.92	111.91
24	b	624	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
24	c	509	CLA	C3B-C4B-NB	3.19	113.33	109.21
31	a	415[B]	PL9	C37-C38-C39	-3.19	119.98	127.66
25	A	409[A]	PHO	CHC-C1C-C2C	-3.19	117.71	125.73
24	A	406	CLA	CHD-C4C-NC	3.19	129.23	124.20
25	a	418[A]	PHO	C4D-CHA-C1A	-3.19	118.20	125.37
24	B	607	CLA	CAC-C3C-C4C	3.19	128.94	124.81
24	B	613	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	C	510	CLA	C4-C3-C5	3.18	120.62	115.27
31	a	415[B]	PL9	C10-C9-C11	3.18	120.62	115.27
26	B	618	BCR	C7-C8-C9	-3.18	121.43	126.23
24	b	613	CLA	CAC-C3C-C4C	3.18	128.93	124.81
24	b	623	CLA	C1D-CHD-C4C	-3.18	118.37	122.56
35	b	601	HTG	C1'-S1-C1	3.18	106.03	100.09
24	b	617	CLA	C3B-C4B-NB	3.17	113.31	109.21
37	b	634	LHG	O7-C7-C8	3.17	118.34	111.50
24	B	611	CLA	C3B-C4B-NB	3.17	113.31	109.21
24	b	622	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	c	515	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	C	509	CLA	C1D-CHD-C4C	-3.17	118.38	122.56
24	b	622	CLA	CAC-C3C-C4C	3.17	128.92	124.81
31	a	415[B]	PL9	C27-C28-C29	-3.17	120.03	127.66
31	d	405[B]	PL9	C37-C38-C39	-3.17	120.04	127.66
24	C	506	CLA	CBC-CAC-C3C	-3.16	103.71	112.43
24	A	405	CLA	CMB-C2B-C3B	3.16	130.59	124.68
35	C	523	HTG	O5-C5-C4	3.16	115.43	109.69
31	a	415[B]	PL9	C20-C19-C21	3.16	120.58	115.27
31	A	419[B]	PL9	C37-C38-C39	-3.15	120.06	127.66
24	A	407	CLA	CHD-C4C-NC	3.15	129.17	124.20
24	b	611	CLA	C3B-C4B-NB	3.15	113.28	109.21
24	b	622	CLA	CHC-C1C-C2C	-3.15	118.01	126.72
24	C	505	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
26	K	101	BCR	C24-C23-C22	-3.15	121.48	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C4D-C3D-CAD	-3.15	106.72	108.47
24	C	510	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	B	612	CLA	CHD-C4C-NC	3.14	129.16	124.20
24	B	615	CLA	CMC-C2C-C1C	3.14	129.83	125.04
24	c	511	CLA	C1-C2-C3	-3.14	120.61	126.04
31	D	405[B]	PL9	C37-C38-C39	-3.14	120.10	127.66
24	C	502	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
24	c	512	CLA	CMC-C2C-C1C	3.14	129.82	125.04
24	a	409	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
31	A	419[B]	PL9	C7-C8-C9	-3.14	121.57	126.79
24	C	504	CLA	CAC-C3C-C4C	3.13	128.88	124.81
24	b	610	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
24	C	502	CLA	C1D-CHD-C4C	-3.13	118.43	122.56
24	C	512	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	B	615	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	C	508	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
24	b	621	CLA	CAC-C3C-C4C	3.12	128.86	124.81
31	d	405[A]	PL9	C40-C39-C41	3.12	120.52	115.27
24	B	604	CLA	O2A-CGA-CBA	3.12	121.70	111.91
24	B	608	CLA	CAC-C3C-C4C	3.12	128.86	124.81
31	D	405[B]	PL9	C10-C9-C11	3.12	120.52	115.27
24	B	615	CLA	O2A-CGA-CBA	3.12	121.69	111.91
24	C	503	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
24	b	613	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
24	c	513	CLA	C4D-C3D-CAD	-3.11	106.73	108.47
24	d	402	CLA	C2A-C1A-CHA	-3.11	118.41	123.86
33	Z	101	LMG	O6-C5-C4	3.11	115.35	109.69
24	c	517	CLA	CMC-C2C-C1C	3.11	129.78	125.04
26	T	103	BCR	C15-C16-C17	-3.11	117.10	123.47
24	C	508	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
24	B	611	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	c	511	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
24	b	616	CLA	CMC-C2C-C1C	3.10	129.76	125.04
31	A	419[A]	PL9	C53-C6-C1	3.10	121.33	114.99
24	C	506	CLA	C4-C3-C5	3.10	120.49	115.27
24	B	611	CLA	O2A-CGA-CBA	3.10	121.64	111.91
36	C	518	DGD	O2G-C1B-C2B	3.10	118.18	111.50
24	B	614	CLA	O2D-CGD-CBD	3.10	116.78	111.27
24	b	620	CLA	CHC-C1C-C2C	-3.10	118.15	126.72
24	c	506	CLA	OBD-CAD-C3D	-3.10	122.84	127.98
24	d	403	CLA	C3B-C4B-NB	3.10	113.22	109.21
33	C	519	LMG	O8-C28-C29	3.10	121.63	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	404	BCR	C33-C5-C6	-3.10	121.05	124.53
24	C	504	CLA	C4-C3-C5	3.10	120.48	115.27
25	a	418[B]	PHO	C4D-CHA-C1A	-3.10	118.40	125.37
24	B	608	CLA	C1-C2-C3	-3.10	120.69	126.04
24	B	616	CLA	CHD-C4C-NC	3.09	129.07	124.20
36	H	102	DGD	O1G-C1A-C2A	3.09	121.60	111.91
24	B	604	CLA	C3B-C4B-NB	3.09	113.20	109.21
24	B	617	CLA	CBC-CAC-C3C	-3.09	103.92	112.43
26	c	528	BCR	C33-C5-C6	-3.08	121.06	124.53
24	c	516	CLA	CAC-C3C-C4C	3.08	128.81	124.81
31	D	405[A]	PL9	C36-C37-C38	-3.08	101.75	111.88
24	B	603	CLA	C3B-C4B-NB	3.08	113.19	109.21
26	D	404	BCR	C28-C27-C26	-3.08	108.58	114.08
26	C	514	BCR	C16-C17-C18	-3.08	122.91	127.31
24	b	613	CLA	CMC-C2C-C1C	3.08	129.73	125.04
24	c	517	CLA	C4-C3-C5	3.08	120.45	115.27
31	a	415[A]	PL9	C27-C28-C29	-3.08	120.25	127.66
37	D	407	LHG	O8-C23-C24	3.08	121.56	111.91
24	b	610	CLA	CHD-C4C-NC	3.08	129.05	124.20
24	B	609	CLA	C1-C2-C3	-3.08	120.72	126.04
27	F	103	SQD	O5-C5-C4	3.08	115.28	109.69
37	D	407	LHG	O8-C23-O10	-3.08	115.83	123.59
31	a	415[B]	PL9	C7-C3-C2	-3.08	119.26	123.30
24	b	611	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
24	B	602	CLA	CHD-C4C-NC	3.07	129.05	124.20
24	B	614	CLA	OBD-CAD-C3D	-3.07	122.88	127.98
31	a	415[B]	PL9	C42-C43-C44	-3.07	120.26	127.66
31	A	419[B]	PL9	C7-C3-C2	-3.07	119.26	123.30
24	B	617	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
24	B	617	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
36	H	102	DGD	O2G-C1B-C2B	3.07	118.12	111.50
24	B	616	CLA	O2D-CGD-CBD	3.07	116.72	111.27
25	a	411	PHO	C2B-C1B-NB	3.07	114.42	109.79
24	c	506	CLA	CHC-C1C-C2C	-3.06	118.24	126.72
24	b	615	CLA	O2A-CGA-O1A	-3.06	115.86	123.59
24	c	515	CLA	CHC-C1C-C2C	-3.06	118.25	126.72
37	b	634	LHG	O8-C23-C24	3.06	121.52	111.91
24	B	616	CLA	C3B-C4B-NB	3.06	113.17	109.21
26	K	101	BCR	C15-C14-C13	-3.06	122.94	127.31
31	d	405[B]	PL9	C27-C28-C29	-3.06	120.29	127.66
24	c	513	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
26	D	404	BCR	C29-C30-C25	3.06	115.19	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	CAA-C2A-C1A	-3.05	101.97	111.97
25	A	408	PHO	C2C-C1C-NC	3.05	114.39	109.79
24	b	625	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
24	B	608	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	A	405	CLA	CHC-C1C-C2C	-3.05	118.29	126.72
24	C	513	CLA	C1-C2-C3	-3.05	120.77	126.04
31	A	419[A]	PL9	C45-C44-C46	3.05	120.39	115.27
26	b	627	BCR	C38-C26-C25	-3.04	121.11	124.53
24	d	401	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
38	e	103	HEM	CBD-CAD-C3D	-3.04	106.88	112.48
24	C	511	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
24	b	617	CLA	CMC-C2C-C1C	3.04	129.67	125.04
31	A	419[A]	PL9	C22-C23-C24	-3.04	120.34	127.66
24	B	613	CLA	C4-C3-C5	3.04	120.38	115.27
24	B	602	CLA	C3B-C4B-NB	3.04	113.14	109.21
24	d	401	CLA	CHC-C1C-C2C	-3.04	118.32	126.72
24	C	504	CLA	CMC-C2C-C1C	3.03	129.66	125.04
24	c	511	CLA	CAA-C2A-C3A	-3.03	104.47	112.78
24	A	406	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
26	h	101	BCR	C38-C26-C25	-3.03	121.12	124.53
24	C	505	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	A	405	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	B	609	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
25	a	418[A]	PHO	C2B-C1B-NB	3.03	114.36	109.79
24	b	620	CLA	CAC-C3C-C4C	3.03	128.74	124.81
24	A	407	CLA	C2A-C1A-CHA	-3.02	118.57	123.86
24	a	410	CLA	O2A-CGA-O1A	-3.02	115.96	123.59
25	A	408	PHO	CMB-C2B-C1B	3.02	129.72	125.06
24	c	508	CLA	C1-C2-C3	-3.02	120.81	126.04
31	D	405[A]	PL9	C15-C14-C16	3.02	120.36	115.27
24	b	624	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
24	B	607	CLA	CMB-C2B-C3B	3.02	130.32	124.68
24	b	615	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
24	a	410	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
37	D	408	LHG	O7-C7-C8	3.01	118.00	111.50
25	a	418[A]	PHO	CHD-C1D-C2D	-3.01	118.15	125.73
25	a	411	PHO	CHC-C1C-C2C	-3.01	118.16	125.73
24	C	509	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
24	b	616	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
24	c	518	CLA	CAC-C3C-C4C	3.01	128.71	124.81
24	c	512	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	a	412	CLA	C4-C3-C5	3.01	120.33	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	409	LHG	O8-C23-C24	3.00	121.34	111.91
33	B	622	LMG	O7-C10-C11	3.00	117.98	111.50
24	D	403	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
37	E	101	LHG	O8-C23-C24	3.00	121.33	111.91
24	b	610	CLA	C4-C3-C5	3.00	120.32	115.27
24	c	506	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
25	A	408	PHO	CHC-C1C-C2C	-3.00	118.18	125.73
26	b	628	BCR	C38-C26-C25	-3.00	121.16	124.53
24	B	611	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
24	B	608	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
24	D	402	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
24	b	616	CLA	CAA-C2A-C3A	-3.00	104.58	112.78
24	c	507	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
27	f	101	SQD	O5-C5-C4	2.99	115.13	109.69
25	A	408	PHO	C1C-C2C-C3C	-2.99	103.07	106.51
24	B	613	CLA	C2A-C1A-CHA	-2.99	118.63	123.86
31	a	415[A]	PL9	C35-C34-C36	2.99	120.30	115.27
24	B	609	CLA	C1D-CHD-C4C	-2.99	118.61	122.56
24	d	401	CLA	CHD-C4C-NC	2.99	128.91	124.20
25	a	418[A]	PHO	CAC-C3C-C4C	2.99	128.48	125.22
24	c	514	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	B	605	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
26	C	515	BCR	C24-C23-C22	-2.99	121.72	126.23
27	L	102	SQD	O8-S-C6	2.99	110.50	105.74
24	B	610	CLA	CAC-C3C-C4C	2.99	128.68	124.81
24	b	618	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
26	B	620	BCR	C38-C26-C25	-2.98	121.18	124.53
24	b	621	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
24	b	612	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	C	506	CLA	C1-C2-C3	-2.98	120.88	126.04
24	B	603	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
31	d	405[A]	PL9	C10-C9-C11	2.98	120.29	115.27
24	C	509	CLA	C1-O2A-CGA	2.98	124.27	116.44
24	B	613	CLA	CAC-C3C-C4C	2.98	128.68	124.81
24	C	512	CLA	CHD-C4C-NC	2.98	128.90	124.20
24	C	509	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
25	A	409[B]	PHO	C2B-C1B-NB	2.98	114.28	109.79
24	C	509	CLA	CMB-C2B-C3B	2.97	130.24	124.68
24	C	508	CLA	CAC-C3C-C4C	2.97	128.67	124.81
24	A	407	CLA	C1D-CHD-C4C	-2.97	118.64	122.56
24	B	603	CLA	CHC-C1C-C2C	-2.97	118.51	126.72
24	D	403	CLA	C4-C3-C5	2.97	120.26	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	624	CLA	C4-C3-C5	2.97	120.26	115.27
24	C	506	CLA	C4D-C3D-CAD	-2.97	106.82	108.47
26	d	404	BCR	C15-C14-C13	-2.96	123.08	127.31
24	b	622	CLA	CED-O2D-CGD	2.96	122.64	115.94
24	b	615	CLA	CMB-C2B-C3B	2.96	130.22	124.68
24	B	605	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
31	A	419[B]	PL9	C22-C23-C24	-2.96	120.53	127.66
24	C	501	CLA	CAC-C3C-C4C	2.96	128.65	124.81
24	C	507	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	a	410	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
24	B	613	CLA	C1-C2-C3	-2.95	120.93	126.04
24	C	504	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
24	A	405	CLA	O2A-CGA-O1A	-2.95	116.14	123.59
24	a	412	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
24	b	614	CLA	O2A-CGA-O1A	-2.95	116.14	123.59
24	c	515	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
35	b	608	HTG	O5-C1-C2	2.95	114.03	110.31
24	A	410	CLA	C1-C2-C3	-2.95	120.94	126.04
24	b	625	CLA	CHD-C4C-NC	2.95	128.85	124.20
24	D	402	CLA	CMC-C2C-C1C	2.95	129.53	125.04
37	e	102	LHG	O7-C7-C8	2.95	117.86	111.50
24	b	621	CLA	C4-C3-C5	2.95	120.23	115.27
24	C	507	CLA	CHD-C4C-NC	2.95	128.85	124.20
24	b	616	CLA	C4-C3-C5	2.95	120.23	115.27
24	c	517	CLA	C1-C2-C3	-2.95	120.94	126.04
26	K	101	BCR	C7-C8-C9	-2.95	121.78	126.23
24	d	402	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
24	C	503	CLA	CHD-C4C-NC	2.95	128.84	124.20
31	a	415[A]	PL9	C53-C6-C1	2.95	121.01	114.99
25	A	409[A]	PHO	C2B-C1B-NB	2.94	114.23	109.79
25	a	418[B]	PHO	CHC-C1C-C2C	-2.94	118.33	125.73
38	F	102	HEM	CBA-CAA-C2A	-2.94	107.06	112.49
24	C	508	CLA	C1D-CHD-C4C	-2.94	118.67	122.56
24	c	514	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	a	409	CLA	O2A-CGA-CBA	2.94	121.14	111.91
27	F	103	SQD	O48-C23-C24	2.94	121.13	111.91
31	A	419[A]	PL9	C7-C8-C9	-2.94	121.90	126.79
24	B	604	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	B	605	CLA	CMC-C2C-C1C	2.93	129.51	125.04
31	A	419[A]	PL9	C8-C7-C3	2.93	120.27	111.98
24	c	517	CLA	CHD-C4C-NC	2.93	128.83	124.20
24	B	610	CLA	C4C-C3C-C2C	-2.93	102.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CMC-C2C-C1C	2.93	129.50	125.04
24	C	508	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	C	511	CLA	C4-C3-C5	2.93	120.20	115.27
25	a	418[A]	PHO	C3C-C4C-NC	2.93	114.82	110.28
24	A	406	CLA	C4-C3-C5	2.93	120.19	115.27
31	d	405[B]	PL9	C40-C39-C41	2.92	120.19	115.27
24	b	623	CLA	CHC-C1C-C2C	-2.92	118.64	126.72
35	b	608	HTG	C1-O5-C5	2.92	117.97	112.58
24	a	412	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
24	B	604	CLA	CHD-C4C-NC	2.92	128.81	124.20
26	c	528	BCR	C16-C17-C18	-2.92	123.14	127.31
24	c	518	CLA	C1-C2-C3	-2.92	120.99	126.04
31	a	415[A]	PL9	C40-C39-C41	2.92	120.18	115.27
24	c	513	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	y	101	BCR	C16-C17-C18	-2.92	123.15	127.31
24	c	508	CLA	CHD-C4C-NC	2.92	128.80	124.20
24	d	403	CLA	C2A-C1A-CHA	-2.92	118.76	123.86
31	d	405[A]	PL9	C37-C38-C39	-2.92	120.64	127.66
31	A	419[B]	PL9	C27-C28-C29	-2.91	120.64	127.66
24	c	512	CLA	C3B-C4B-NB	2.91	112.98	109.21
24	C	511	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	c	506	CLA	C1D-CHD-C4C	-2.91	118.71	122.56
26	h	101	BCR	C11-C10-C9	-2.91	123.15	127.31
24	a	410	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
36	c	520	DGD	C2G-O2G-C1B	-2.91	110.62	117.79
24	b	625	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	D	403	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
26	B	619	BCR	C33-C5-C6	-2.91	121.26	124.53
26	Y	101	BCR	C37-C22-C23	2.90	122.65	118.08
26	B	619	BCR	C37-C22-C21	-2.90	118.86	122.92
24	B	615	CLA	C4-C3-C5	2.90	120.16	115.27
24	C	502	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
25	a	411	PHO	CMB-C2B-C1B	2.90	129.53	125.06
24	c	516	CLA	C1-C2-C3	-2.90	121.02	126.04
24	b	614	CLA	C3B-C4B-NB	2.90	112.96	109.21
24	b	622	CLA	C4-C3-C5	2.90	120.15	115.27
24	c	516	CLA	CMB-C2B-C3B	2.90	130.10	124.68
25	a	411	PHO	C1-O2A-CGA	2.90	124.05	116.44
24	c	516	CLA	CHD-C4C-NC	2.90	128.77	124.20
24	B	616	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
24	b	620	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
24	c	506	CLA	CMC-C2C-C1C	2.90	129.45	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C11-C10-C9	-2.90	123.18	127.31
24	b	614	CLA	C4C-C3C-C2C	-2.90	102.68	106.90
36	C	517	DGD	C2G-O2G-C1B	-2.89	110.67	117.79
24	b	624	CLA	CHD-C4C-NC	2.89	128.76	124.20
36	D	406	DGD	O1G-C1A-C2A	2.89	120.99	111.91
24	C	505	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	a	410	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	c	517	CLA	C3B-C4B-NB	2.89	112.95	109.21
24	b	611	CLA	CHD-C4C-NC	2.89	128.76	124.20
24	A	407	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	B	615	CLA	C1D-CHD-C4C	-2.89	118.75	122.56
31	A	419[B]	PL9	C42-C43-C44	-2.89	120.70	127.66
36	C	517	DGD	O1G-C1A-C2A	2.89	120.97	111.91
24	C	504	CLA	CMB-C2B-C3B	2.89	130.08	124.68
24	b	618	CLA	C3B-C4B-NB	2.89	112.94	109.21
24	c	510	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
24	c	510	CLA	C3B-C4B-NB	2.88	112.94	109.21
25	a	418[A]	PHO	C2A-C1A-NA	2.88	115.17	111.86
24	b	612	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	C	501	CLA	C1-O2A-CGA	2.88	124.00	116.44
24	B	614	CLA	CAC-C3C-C4C	2.88	128.54	124.81
24	c	507	CLA	C1-C2-C3	-2.88	121.07	126.04
24	A	410	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
24	b	610	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
31	a	415[A]	PL9	C37-C38-C39	-2.87	120.74	127.66
24	b	618	CLA	CHD-C4C-NC	2.87	128.73	124.20
24	b	615	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	a	410	CLA	CHD-C4C-NC	2.87	128.73	124.20
37	d	406	LHG	O8-C23-O10	-2.87	116.35	123.59
26	d	404	BCR	C29-C30-C25	2.87	114.90	110.48
24	b	623	CLA	CMC-C2C-C1C	2.87	129.41	125.04
37	D	409	LHG	O8-C23-O10	-2.87	116.36	123.59
24	b	621	CLA	C1-C2-C3	-2.87	121.08	126.04
36	h	102	DGD	O1G-C1A-C2A	2.87	120.90	111.91
25	A	409[B]	PHO	C2A-C1A-NA	2.86	115.15	111.86
24	B	607	CLA	CHC-C1C-C2C	-2.86	118.80	126.72
24	C	513	CLA	C4C-C3C-C2C	-2.86	102.72	106.90
24	B	617	CLA	CHD-C4C-NC	2.86	128.71	124.20
31	a	415[B]	PL9	C35-C34-C36	2.86	120.08	115.27
24	c	514	CLA	CHD-C4C-NC	2.86	128.71	124.20
24	c	516	CLA	CMC-C2C-C1C	2.86	129.39	125.04
37	d	406	LHG	O8-C23-C24	2.86	120.88	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	519	BCR	C38-C26-C25	-2.86	121.32	124.53
24	A	406	CLA	CMB-C2B-C3B	2.86	130.03	124.68
24	b	612	CLA	CAC-C3C-C4C	2.86	128.52	124.81
24	C	506	CLA	CAA-C2A-C3A	-2.86	104.95	112.78
24	d	403	CLA	C4-C3-C5	2.86	120.08	115.27
31	D	405[A]	PL9	C53-C6-C1	2.86	120.83	114.99
24	b	613	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
24	C	510	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	b	611	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
24	A	406	CLA	CAA-C2A-C3A	-2.85	104.97	112.78
31	A	419[A]	PL9	C12-C13-C14	-2.85	120.80	127.66
24	B	602	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	b	622	CLA	O2D-CGD-CBD	2.85	116.33	111.27
24	b	625	CLA	C1-C2-C3	-2.85	121.11	126.04
24	b	616	CLA	CHD-C4C-NC	2.85	128.69	124.20
24	c	518	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
24	B	612	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	b	621	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
31	a	415[B]	PL9	C53-C6-C1	2.85	120.81	114.99
24	B	607	CLA	C1-C2-C3	-2.85	121.12	126.04
24	c	518	CLA	CHD-C4C-NC	2.85	128.69	124.20
24	B	610	CLA	CHD-C4C-NC	2.84	128.69	124.20
25	A	408	PHO	CBD-CHA-C1A	2.84	133.00	126.40
24	D	403	CLA	C4D-C3D-CAD	-2.84	106.88	108.47
24	b	620	CLA	CHD-C4C-NC	2.84	128.69	124.20
31	A	419[B]	PL9	C53-C6-C1	2.84	120.80	114.99
31	a	415[B]	PL9	C25-C24-C26	2.84	120.05	115.27
27	L	102	SQD	C44-O6-C1	-2.84	108.19	113.74
26	Y	101	BCR	C10-C11-C12	-2.84	114.36	123.22
24	c	507	CLA	CAC-C3C-C4C	2.84	128.49	124.81
24	C	513	CLA	C3B-C4B-NB	2.84	112.88	109.21
31	D	405[B]	PL9	C40-C39-C41	2.84	120.04	115.27
24	c	511	CLA	C4-C3-C5	2.83	120.04	115.27
24	C	503	CLA	O2A-CGA-CBA	2.83	120.80	111.91
24	C	502	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
24	b	623	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
24	c	512	CLA	CHD-C4C-NC	2.83	128.66	124.20
31	A	419[A]	PL9	C27-C28-C29	-2.83	120.84	127.66
24	C	512	CLA	CHC-C1C-C2C	-2.83	118.90	126.72
24	C	502	CLA	CHD-C4C-NC	2.83	128.66	124.20
24	a	410	CLA	CAC-C3C-C4C	2.83	128.48	124.81
26	k	101	BCR	C20-C21-C22	-2.83	123.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	O2A-CGA-O1A	-2.83	116.46	123.59
24	b	617	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
24	a	410	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
24	c	515	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	B	603	CLA	CAC-C3C-C4C	2.82	128.47	124.81
24	d	402	CLA	O2A-CGA-CBA	2.82	120.76	111.91
36	c	522	DGD	O1G-C1A-C2A	2.82	120.76	111.91
24	c	511	CLA	CMB-C2B-C3B	2.82	129.95	124.68
24	D	402	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
24	b	612	CLA	O2A-CGA-CBA	2.82	120.74	111.91
24	a	412	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
31	a	415[A]	PL9	C25-C24-C26	2.81	120.00	115.27
24	B	615	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
24	c	509	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
25	A	409[B]	PHO	C4D-CHA-C1A	-2.81	119.04	125.37
35	V	206	HTG	C1-C2-C3	-2.81	105.04	110.59
24	b	623	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
33	d	413	LMG	O7-C10-C11	2.81	117.56	111.50
24	B	616	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	C	510	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	c	511	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
27	L	102	SQD	O7-S-C6	2.81	110.27	106.94
24	B	609	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	a	418[B]	PHO	C2A-C1A-NA	2.80	115.08	111.86
24	B	607	CLA	OBD-CAD-C3D	-2.80	123.33	127.98
24	a	412	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	c	515	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	b	611	CLA	C4-C3-C5	2.79	119.97	115.27
24	d	402	CLA	C4-C3-C5	2.79	119.97	115.27
25	a	418[A]	PHO	C4D-ND-C1D	-2.79	101.74	106.76
24	a	409	CLA	O2D-CGD-CBD	2.79	116.23	111.27
31	D	405[B]	PL9	C22-C23-C24	-2.79	120.94	127.66
24	b	618	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
24	D	402	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	b	618	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
24	C	505	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	c	516	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	b	620	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	b	618	CLA	C4-C3-C5	2.79	119.96	115.27
24	b	621	CLA	CMB-C2B-C3B	2.78	129.89	124.68
24	C	506	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	B	607	CLA	C4-C3-C5	2.78	119.95	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C1D-CHD-C4C	-2.78	118.89	122.56
31	D	405[B]	PL9	C27-C28-C29	-2.78	120.96	127.66
24	b	617	CLA	CBC-CAC-C3C	-2.78	104.77	112.43
26	Y	101	BCR	C15-C14-C13	-2.78	123.35	127.31
24	c	511	CLA	CHD-C4C-NC	2.78	128.58	124.20
24	A	407	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
25	a	418[A]	PHO	CHC-C1C-C2C	-2.78	118.75	125.73
24	B	610	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
24	c	517	CLA	O2A-CGA-CBA	2.78	120.62	111.91
24	B	609	CLA	O2A-CGA-CBA	2.77	120.61	111.91
24	c	518	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
24	b	619	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	B	608	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
24	b	612	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	d	401	CLA	CMA-C3A-C2A	-2.77	102.64	113.83
26	c	519	BCR	C15-C14-C13	-2.77	123.35	127.31
24	c	510	CLA	C1-C2-C3	-2.77	121.25	126.04
24	b	615	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
24	B	603	CLA	C1-C2-C3	-2.77	121.25	126.04
26	K	101	BCR	C3-C4-C5	-2.77	109.13	114.08
24	B	607	CLA	CHD-C4C-NC	2.77	128.57	124.20
24	C	504	CLA	OBD-CAD-C3D	-2.77	123.39	127.98
24	B	608	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
24	b	617	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
24	c	512	CLA	C4-C3-C5	2.76	119.92	115.27
24	C	509	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	B	609	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
31	d	405[B]	PL9	C53-C6-C1	2.76	120.64	114.99
24	b	617	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	D	405[B]	PL9	C25-C24-C26	2.76	119.91	115.27
24	d	403	CLA	CAC-C3C-C4C	2.76	128.39	124.81
26	t	101	BCR	C11-C10-C9	-2.76	123.37	127.31
24	C	507	CLA	O2A-CGA-CBA	2.76	120.57	111.91
24	D	402	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
25	A	408	PHO	C4D-ND-C1D	-2.76	101.80	106.76
24	B	613	CLA	CBC-CAC-C3C	-2.76	104.83	112.43
24	b	613	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	604	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
31	D	405[A]	PL9	C7-C3-C4	2.75	119.11	116.88
24	C	507	CLA	CAC-C3C-C4C	2.75	128.38	124.81
31	d	405[B]	PL9	C15-C14-C16	2.75	119.90	115.27
24	a	410	CLA	O2A-CGA-CBA	2.75	120.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	412	CLA	CMA-C3A-C2A	-2.75	102.72	113.83
24	A	410	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
24	c	516	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
24	B	613	CLA	C1D-CHD-C4C	-2.75	118.93	122.56
25	A	409[B]	PHO	C4D-ND-C1D	-2.75	101.82	106.76
24	c	516	CLA	O2A-CGA-CBA	2.75	120.54	111.91
24	B	602	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
24	c	509	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
31	d	405[A]	PL9	C27-C28-C29	-2.75	121.04	127.66
24	C	508	CLA	C1-C2-C3	-2.75	121.29	126.04
24	A	410	CLA	CMA-C3A-C4A	-2.75	104.39	111.77
24	b	619	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	B	615	CLA	OBD-CAD-C3D	-2.75	123.42	127.98
31	a	415[B]	PL9	C40-C39-C41	2.75	119.89	115.27
24	b	616	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
24	c	507	CLA	O2A-CGA-CBA	2.74	120.52	111.91
24	C	513	CLA	CHC-C1C-C2C	-2.74	119.13	126.72
27	F	103	SQD	O9-S-C6	2.74	110.20	106.94
24	a	412	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
24	C	513	CLA	O2A-CGA-CBA	2.74	120.51	111.91
24	B	606	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
24	B	612	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
24	b	610	CLA	CMB-C2B-C3B	2.74	129.80	124.68
26	B	619	BCR	C2-C1-C6	2.74	114.69	110.48
24	c	518	CLA	O2A-CGA-CBA	2.74	120.50	111.91
25	a	418[B]	PHO	C3C-C4C-NC	2.74	114.52	110.28
24	c	514	CLA	O2A-CGA-CBA	2.74	120.49	111.91
33	z	101	LMG	O8-C28-C29	2.73	120.49	111.91
35	B	625	HTG	C1-O5-C5	2.73	117.62	112.58
24	b	615	CLA	CHD-C4C-NC	2.73	128.51	124.20
24	c	517	CLA	CMB-C2B-C3B	2.73	129.79	124.68
24	c	516	CLA	C4-C3-C5	2.73	119.86	115.27
36	C	516	DGD	C3G-C2G-C1G	-2.73	105.34	111.79
27	B	621	SQD	C3-C4-C5	2.72	115.10	110.24
24	C	509	CLA	O2A-CGA-CBA	2.72	120.46	111.91
24	b	612	CLA	CMA-C3A-C2A	-2.72	102.84	113.83
26	b	628	BCR	C2-C1-C6	2.72	114.67	110.48
24	c	518	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
31	d	405[A]	PL9	C20-C19-C21	2.72	119.85	115.27
24	B	615	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
25	A	409[A]	PHO	O2D-CGD-O1D	-2.72	118.52	123.84
24	A	410	CLA	CHB-C4A-NA	2.72	128.27	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CHD-C4C-NC	2.72	128.49	124.20
24	c	517	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
25	a	418[B]	PHO	CHD-C1D-C2D	-2.72	118.89	125.73
24	b	616	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
24	c	512	CLA	CHC-C1C-C2C	-2.72	119.20	126.72
33	b	629	LMG	O8-C28-C29	2.71	120.42	111.91
24	D	403	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
31	A	419[B]	PL9	C45-C44-C46	2.71	119.83	115.27
25	a	418[B]	PHO	C4D-ND-C1D	-2.71	101.89	106.76
24	C	502	CLA	CHC-C1C-C2C	-2.71	119.22	126.72
24	B	606	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
24	b	623	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
35	b	632	HTG	C1-O5-C5	2.71	117.58	112.58
24	D	402	CLA	CAA-C2A-C3A	-2.71	105.36	112.78
24	B	606	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	c	518	CLA	C3B-C4B-NB	2.71	112.71	109.21
24	b	619	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	B	613	CLA	CHD-C4C-NC	2.71	128.47	124.20
26	b	628	BCR	C24-C23-C22	-2.71	122.15	126.23
31	A	419[B]	PL9	C15-C14-C16	2.71	119.82	115.27
31	d	405[B]	PL9	C20-C19-C21	2.70	119.82	115.27
27	a	414	SQD	C45-O47-C7	-2.70	111.14	117.79
26	B	620	BCR	C10-C11-C12	-2.70	114.78	123.22
29	f	102	LMT	C1B-O5B-C5B	2.70	118.99	113.69
31	a	415[B]	PL9	C30-C29-C31	2.70	119.81	115.27
27	L	102	SQD	O48-C23-C24	2.70	120.37	111.91
24	C	503	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	C	501	CLA	CHD-C4C-NC	2.70	128.45	124.20
25	a	418[A]	PHO	C4A-NA-C1A	-2.70	105.96	108.14
31	A	419[B]	PL9	C25-C24-C26	2.70	119.81	115.27
24	b	616	CLA	C1D-CHD-C4C	-2.70	119.00	122.56
24	C	506	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	c	510	CLA	C4-C3-C5	2.69	119.80	115.27
25	a	411	PHO	C2C-C1C-NC	2.69	113.85	109.79
25	A	409[A]	PHO	C3C-C4C-NC	2.69	114.45	110.28
24	a	409	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
24	b	611	CLA	CAC-C3C-C4C	2.69	128.30	124.81
24	d	403	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
24	d	402	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
24	b	621	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
24	b	618	CLA	O2A-CGA-O1A	-2.68	116.82	123.59
24	d	401	CLA	C4C-C3C-C2C	-2.68	102.99	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
26	h	101	BCR	C7-C8-C9	-2.68	122.19	126.23
27	A	412	SQD	O48-C23-C24	2.68	120.32	111.91
24	d	403	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	B	602	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
24	a	412	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	B	609	CLA	CBC-CAC-C3C	-2.68	105.05	112.43
24	C	511	CLA	CHD-C4C-NC	2.68	128.42	124.20
24	b	625	CLA	C4D-C3D-CAD	-2.68	106.98	108.47
26	C	514	BCR	C20-C21-C22	-2.68	123.49	127.31
24	c	514	CLA	CMC-C2C-C1C	2.67	129.11	125.04
24	c	507	CLA	CHD-C4C-NC	2.67	128.42	124.20
35	c	526	HTG	C1-O5-C5	2.67	117.51	112.58
24	b	617	CLA	CHD-C4C-NC	2.67	128.41	124.20
24	B	607	CLA	O2A-CGA-CBA	2.67	120.29	111.91
24	C	505	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
24	A	407	CLA	CMC-C2C-C1C	2.67	129.10	125.04
31	d	405[B]	PL9	C10-C9-C11	2.67	119.76	115.27
36	C	516	DGD	O1G-C1A-O1A	-2.67	116.86	123.59
24	C	513	CLA	CHD-C4C-NC	2.67	128.41	124.20
24	b	615	CLA	O2A-CGA-CBA	2.67	120.28	111.91
24	c	508	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
36	h	102	DGD	O1G-C1A-O1A	-2.67	116.86	123.59
24	c	512	CLA	C4D-C3D-CAD	-2.66	106.98	108.47
24	A	405	CLA	CAA-C2A-C1A	-2.66	103.25	111.97
24	B	614	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
24	C	504	CLA	C2A-C1A-CHA	-2.66	119.20	123.86
26	Y	101	BCR	C16-C17-C18	-2.66	123.51	127.31
33	c	501	LMG	O8-C28-C29	2.66	120.26	111.91
24	C	506	CLA	CMC-C2C-C1C	2.66	129.09	125.04
26	t	101	BCR	C1-C6-C7	2.66	123.31	115.78
24	c	517	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
24	B	611	CLA	CMA-C3A-C4A	-2.66	104.63	111.77
31	A	419[A]	PL9	C25-C24-C26	2.66	119.74	115.27
24	B	606	CLA	CAC-C3C-C4C	2.66	128.26	124.81
25	a	411	PHO	C1C-C2C-C3C	-2.66	103.45	106.51
24	b	611	CLA	O2A-CGA-CBA	2.66	120.25	111.91
31	D	405[A]	PL9	C25-C24-C26	2.66	119.74	115.27
25	A	409[B]	PHO	O2D-CGD-O1D	-2.66	118.65	123.84
37	e	102	LHG	O8-C23-C24	2.65	120.24	111.91
24	C	501	CLA	CHC-C1C-C2C	-2.65	119.38	126.72
27	F	103	SQD	C44-O6-C1	-2.65	108.56	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	CBC-CAC-C3C	-2.65	105.12	112.43
24	B	609	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
35	V	206	HTG	O5-C1-C2	-2.65	106.98	110.31
24	b	616	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
27	F	103	SQD	C3-C4-C5	2.65	114.96	110.24
26	c	519	BCR	C3-C4-C5	-2.65	109.35	114.08
25	A	409[A]	PHO	C2A-C1A-NA	2.65	114.90	111.86
24	c	512	CLA	OBD-CAD-C3D	-2.65	123.59	127.98
24	C	504	CLA	C1-O2A-CGA	2.64	123.38	116.44
24	c	509	CLA	CHD-C4C-NC	2.64	128.36	124.20
24	d	403	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
31	A	419[A]	PL9	C30-C29-C31	2.64	119.71	115.27
24	b	618	CLA	CMC-C2C-C1C	2.64	129.06	125.04
24	b	614	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
24	B	605	CLA	OBD-CAD-C3D	-2.64	123.60	127.98
24	B	607	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
26	B	620	BCR	C2-C1-C6	2.64	114.54	110.48
24	B	616	CLA	CAC-C3C-C4C	2.63	128.23	124.81
25	A	409[A]	PHO	CAC-C3C-C4C	2.63	128.09	125.22
24	C	507	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
33	Z	101	LMG	C1-O6-C5	2.63	118.85	113.69
27	A	412	SQD	O48-C23-O10	-2.63	116.95	123.59
36	C	518	DGD	O1G-C1A-C2A	2.63	120.16	111.91
26	t	101	BCR	C15-C14-C13	2.63	131.06	127.31
24	b	613	CLA	O2A-CGA-CBA	2.63	120.16	111.91
31	d	405[A]	PL9	C53-C6-C1	2.63	120.36	114.99
24	c	506	CLA	C4D-C3D-CAD	-2.63	107.00	108.47
27	A	416	SQD	O48-C23-O10	-2.63	116.96	123.59
24	C	501	CLA	C4-C3-C5	2.63	119.69	115.27
24	c	511	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
24	c	517	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
36	H	102	DGD	O1G-C1A-O1A	-2.63	116.97	123.59
27	B	621	SQD	O48-C23-C24	2.63	120.15	111.91
24	a	412	CLA	CMC-C2C-C1C	2.63	129.04	125.04
24	D	402	CLA	CMB-C2B-C3B	2.62	129.59	124.68
24	b	619	CLA	C4-C3-C5	2.62	119.68	115.27
24	C	503	CLA	C3B-C4B-NB	2.62	112.60	109.21
26	B	619	BCR	C31-C1-C6	-2.62	106.05	110.30
24	B	609	CLA	CAC-C3C-C4C	2.62	128.21	124.81
24	b	613	CLA	C1-C2-C3	-2.62	121.52	126.04
24	B	605	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
24	A	410	CLA	CMC-C2C-C1C	2.62	129.02	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	CHB-C4A-NA	2.61	128.13	124.51
26	T	103	BCR	C35-C13-C12	2.61	122.20	118.08
36	e	101	DGD	C1E-O6E-C5E	2.61	118.82	113.69
31	D	405[A]	PL9	C37-C38-C39	-2.61	121.37	127.66
24	A	407	CLA	C3B-C4B-NB	2.61	112.59	109.21
24	B	617	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
24	c	512	CLA	C1-C2-C3	-2.61	121.52	126.04
26	b	627	BCR	C37-C22-C21	-2.61	119.26	122.92
24	B	607	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
24	c	515	CLA	CHD-C4C-NC	2.61	128.32	124.20
24	c	518	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
24	C	508	CLA	C4-C3-C5	2.61	119.66	115.27
24	c	509	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
31	D	405[A]	PL9	C22-C23-C24	-2.61	121.37	127.66
31	A	419[B]	PL9	C30-C29-C31	2.61	119.66	115.27
25	A	409[B]	PHO	CHC-C1C-C2C	-2.61	119.17	125.73
24	B	614	CLA	CMC-C2C-C1C	2.61	129.01	125.04
33	c	501	LMG	C7-O1-C1	-2.61	108.64	113.74
24	c	513	CLA	CMB-C2B-C3B	2.61	129.56	124.68
24	b	623	CLA	O2A-CGA-CBA	2.61	120.09	111.91
24	b	614	CLA	OBD-CAD-C3D	-2.61	123.65	127.98
24	D	403	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
31	d	405[B]	PL9	C12-C13-C14	-2.61	121.38	127.66
26	t	101	BCR	C20-C21-C22	-2.60	123.59	127.31
26	y	101	BCR	C10-C11-C12	-2.60	115.09	123.22
24	C	513	CLA	C4-C3-C5	2.60	119.65	115.27
24	b	620	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
26	T	103	BCR	C34-C9-C10	-2.60	119.28	122.92
31	A	419[A]	PL9	C15-C14-C16	2.60	119.65	115.27
24	b	612	CLA	CMB-C2B-C3B	2.60	129.54	124.68
24	c	518	CLA	C4-C3-C5	2.60	119.64	115.27
26	t	101	BCR	C3-C4-C5	-2.60	109.44	114.08
31	a	415[A]	PL9	C30-C29-C31	2.60	119.64	115.27
24	b	615	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	D	402	CLA	C4-C3-C5	2.60	119.64	115.27
24	B	606	CLA	C1-C2-C3	-2.60	121.55	126.04
26	h	101	BCR	C16-C15-C14	-2.60	118.16	123.47
25	a	418[B]	PHO	CAC-C3C-C4C	2.59	128.05	125.22
26	d	404	BCR	C28-C27-C26	-2.59	109.44	114.08
24	B	612	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
37	d	408	LHG	O8-C23-C24	2.59	120.05	111.91
24	a	410	CLA	C4-C3-C5	2.59	119.63	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	407	LHG	C5-O7-C7	-2.59	111.41	117.79
24	b	617	CLA	O2A-CGA-CBA	2.59	120.04	111.91
24	a	409	CLA	CAC-C3C-C4C	2.59	128.17	124.81
24	C	511	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
24	b	625	CLA	C4-C3-C5	2.59	119.63	115.27
24	C	502	CLA	CMC-C2C-C1C	2.59	128.98	125.04
36	C	516	DGD	O3G-C3G-C2G	-2.59	104.65	110.90
24	c	517	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
31	A	419[B]	PL9	C12-C13-C14	-2.59	121.43	127.66
24	B	610	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
24	a	412	CLA	OBD-CAD-C3D	-2.59	123.69	127.98
24	A	407	CLA	CAA-C2A-C3A	-2.59	105.70	112.78
24	C	503	CLA	CHC-C1C-C2C	-2.58	119.57	126.72
24	b	618	CLA	O2A-CGA-CBA	2.58	120.01	111.91
24	c	506	CLA	CBC-CAC-C3C	-2.58	105.31	112.43
24	C	511	CLA	O2A-CGA-CBA	2.58	120.01	111.91
24	C	513	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	B	609	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	B	608	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
24	C	504	CLA	CHD-C4C-NC	2.58	128.26	124.20
24	c	508	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
33	c	523	LMG	C8-O7-C10	-2.58	111.45	117.79
24	b	616	CLA	OBD-CAD-C3D	-2.57	123.71	127.98
24	B	614	CLA	C4-C3-C5	2.57	119.60	115.27
24	C	505	CLA	CHD-C4C-NC	2.57	128.26	124.20
35	C	523	HTG	O5-C1-C2	2.57	113.55	110.31
24	c	509	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
24	b	623	CLA	CAC-C3C-C4C	2.57	128.15	124.81
36	c	520	DGD	O2G-C1B-O1B	-2.57	117.49	123.70
36	C	517	DGD	O1G-C1A-O1A	-2.57	117.11	123.59
26	H	101	BCR	C10-C11-C12	-2.57	115.20	123.22
27	A	416	SQD	O8-S-C6	2.57	109.83	105.74
27	L	102	SQD	O47-C7-O49	-2.57	117.50	123.70
27	f	101	SQD	O7-S-C6	2.57	109.99	106.94
24	c	513	CLA	C4-C3-C5	2.57	119.59	115.27
24	C	510	CLA	CAC-C3C-C4C	2.57	128.14	124.81
25	a	411	PHO	C2A-C1A-NA	2.57	114.81	111.86
24	b	621	CLA	OBD-CAD-C3D	-2.57	123.72	127.98
33	C	520	LMG	O8-C28-C29	2.56	119.95	111.91
27	f	101	SQD	O47-C7-O49	-2.56	117.51	123.70
26	h	101	BCR	C10-C11-C12	-2.56	115.22	123.22
24	b	614	CLA	O2A-CGA-CBA	2.56	119.94	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
24	C	504	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
24	b	618	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
31	D	405[B]	PL9	C53-C6-C1	2.56	120.22	114.99
24	d	403	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
24	c	509	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
33	D	413	LMG	C7-O1-C1	-2.56	108.74	113.74
27	a	414	SQD	O48-C23-C24	2.56	119.93	111.91
24	b	617	CLA	CAC-C3C-C4C	2.56	128.13	124.81
24	C	509	CLA	CHD-C4C-NC	2.56	128.23	124.20
36	e	101	DGD	O1G-C1A-C2A	2.55	119.92	111.91
31	a	415[A]	PL9	C51-C49-C50	2.55	120.25	114.60
26	B	618	BCR	C15-C14-C13	-2.55	123.67	127.31
24	b	623	CLA	CHD-C4C-NC	2.55	128.23	124.20
24	B	608	CLA	C4-C3-C5	2.55	119.57	115.27
24	b	624	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
24	b	612	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
25	A	408	PHO	C2A-C1A-NA	2.55	114.79	111.86
31	D	405[A]	PL9	C27-C28-C29	-2.55	121.52	127.66
31	a	415[B]	PL9	C51-C49-C50	2.55	120.23	114.60
24	C	502	CLA	C4-C3-C5	2.55	119.56	115.27
37	L	101	LHG	O8-C23-C24	2.55	119.90	111.91
24	b	620	CLA	O2A-CGA-CBA	2.54	119.89	111.91
24	c	510	CLA	CMC-C2C-C1C	2.54	128.91	125.04
24	C	509	CLA	C4-C3-C5	2.54	119.55	115.27
24	b	619	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
26	y	101	BCR	C24-C23-C22	-2.54	122.39	126.23
24	c	509	CLA	CAC-C3C-C4C	2.54	128.11	124.81
24	B	606	CLA	C3B-C4B-NB	2.54	112.50	109.21
24	A	407	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
24	b	612	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
24	b	619	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
24	b	617	CLA	CMB-C2B-C3B	2.54	129.42	124.68
31	A	419[B]	PL9	C17-C18-C19	-2.54	121.56	127.66
25	A	409[B]	PHO	C3C-C4C-NC	2.53	114.21	110.28
24	b	625	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
24	B	617	CLA	C1-O2A-CGA	2.53	123.09	116.44
24	C	513	CLA	CAC-C3C-C4C	2.53	128.09	124.81
25	A	409[A]	PHO	C1C-C2C-C3C	-2.53	103.60	106.51
31	D	405[B]	PL9	C20-C19-C21	2.53	119.53	115.27
27	f	101	SQD	O48-C23-C24	2.53	119.85	111.91
24	B	608	CLA	CHD-C4C-NC	2.53	128.19	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C4-C3-C5	2.53	119.53	115.27
26	K	101	BCR	C20-C21-C22	-2.53	123.70	127.31
24	c	506	CLA	CMB-C2B-C3B	2.53	129.41	124.68
24	B	615	CLA	CMB-C2B-C3B	2.53	129.40	124.68
24	d	403	CLA	CMB-C2B-C3B	2.52	129.40	124.68
24	C	501	CLA	C4C-C3C-C2C	-2.52	103.22	106.90
24	C	502	CLA	CAC-C3C-C4C	2.52	128.08	124.81
24	C	511	CLA	CMC-C2C-C1C	2.52	128.88	125.04
36	C	516	DGD	C2G-O2G-C1B	-2.52	111.58	117.79
24	c	517	CLA	CBA-CAA-C2A	-2.52	106.42	113.86
24	b	614	CLA	CAC-C3C-C2C	2.52	131.84	127.53
24	B	611	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
24	B	611	CLA	CHD-C4C-NC	2.52	128.17	124.20
24	C	512	CLA	CMC-C2C-C1C	2.52	128.88	125.04
25	A	408	PHO	C4-C3-C5	2.52	119.50	115.27
24	B	613	CLA	CMB-C2B-C3B	2.52	129.38	124.68
26	H	101	BCR	C7-C8-C9	-2.51	122.44	126.23
24	B	603	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
24	d	402	CLA	C1D-CHD-C4C	-2.51	119.24	122.56
24	B	609	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	B	615	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	b	620	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
35	B	624	HTG	C1-C2-C3	2.51	115.54	110.59
25	A	409[A]	PHO	C2C-C1C-NC	2.51	113.57	109.79
24	A	406	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
24	b	620	CLA	CMC-C2C-C1C	2.50	128.85	125.04
33	c	524	LMG	O8-C28-C29	2.50	119.77	111.91
26	h	101	BCR	C20-C21-C22	-2.50	123.74	127.31
25	A	409[B]	PHO	C1C-C2C-C3C	-2.50	103.63	106.51
24	c	512	CLA	O2A-CGA-CBA	2.50	119.76	111.91
24	C	502	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
26	k	101	BCR	C11-C10-C9	-2.50	123.74	127.31
27	A	412	SQD	C1-C2-C3	-2.50	104.79	110.00
24	a	410	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
24	c	507	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	c	514	CLA	C4-C3-C5	2.50	119.47	115.27
31	a	415[A]	PL9	C7-C3-C2	-2.50	120.01	123.30
26	t	101	BCR	C7-C6-C5	-2.50	115.41	121.46
24	B	614	CLA	C1D-CHD-C4C	-2.50	119.26	122.56
24	C	507	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
26	K	101	BCR	C2-C1-C6	2.50	114.32	110.48
24	C	513	CLA	CMC-C2C-C1C	2.50	128.84	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	419[A]	PL9	C42-C43-C44	-2.50	121.65	127.66
29	m	103	LMT	O5'-C5'-C4'	2.49	115.01	109.75
24	A	405	CLA	CMA-C3A-C4A	-2.49	105.07	111.77
24	B	617	CLA	O2A-CGA-CBA	2.49	119.73	111.91
24	c	513	CLA	CAA-C2A-C3A	-2.49	105.95	112.78
24	b	624	CLA	CMC-C2C-C1C	2.49	128.83	125.04
24	D	402	CLA	C1D-CHD-C4C	-2.49	119.27	122.56
24	A	405	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
24	d	402	CLA	CMC-C2C-C1C	2.49	128.83	125.04
26	C	515	BCR	C21-C20-C19	-2.48	115.48	123.22
26	T	103	BCR	C21-C20-C19	-2.48	115.48	123.22
24	C	506	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	C	511	CLA	C1-C2-C3	-2.48	121.76	126.04
25	A	409[B]	PHO	CHD-C1D-C2D	-2.48	119.50	125.73
31	D	405[A]	PL9	C42-C41-C39	-2.48	104.83	112.98
24	B	609	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
24	B	610	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	b	615	CLA	CAA-C2A-C3A	-2.47	106.01	112.78
24	B	604	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
26	K	101	BCR	C33-C5-C6	-2.47	121.76	124.53
24	c	513	CLA	O2A-CGA-CBA	2.47	119.65	111.91
31	A	419[A]	PL9	C10-C9-C11	2.47	119.42	115.27
24	c	515	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	c	517	CLA	O1D-CGD-CBD	-2.47	119.44	124.48
24	B	614	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	c	507	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
24	B	616	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
24	C	512	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
26	a	413	BCR	C33-C5-C6	-2.46	121.76	124.53
37	d	406	LHG	O7-C7-C8	2.46	116.81	111.50
24	c	514	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
24	C	509	CLA	C4D-C3D-CAD	-2.46	107.10	108.47
24	A	410	CLA	CED-O2D-CGD	2.46	121.50	115.94
24	B	614	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	B	613	CLA	O2A-CGA-CBA	2.46	119.61	111.91
25	A	409[A]	PHO	C4D-ND-C1D	-2.46	102.35	106.76
26	T	103	BCR	C2-C1-C6	2.45	114.26	110.48
24	b	622	CLA	O2A-CGA-CBA	2.45	119.61	111.91
26	T	103	BCR	C29-C28-C27	-2.45	105.89	111.38
29	M	103	LMT	O1B-C1B-C2B	2.45	114.45	108.10
24	b	619	CLA	CMB-C2B-C3B	2.45	129.26	124.68
26	b	627	BCR	C28-C27-C26	-2.45	109.70	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	CHD-C4C-NC	2.45	128.06	124.20
24	C	506	CLA	OBD-CAD-C3D	-2.45	123.92	127.98
26	d	404	BCR	C3-C4-C5	-2.45	109.71	114.08
24	b	625	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
24	C	513	CLA	CAA-C2A-C3A	-2.44	106.09	112.78
24	b	613	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
24	C	502	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	A	405	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	C	510	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	b	616	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
26	y	101	BCR	C21-C20-C19	-2.44	115.61	123.22
24	c	511	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	b	621	CLA	CHD-C4C-NC	2.44	128.04	124.20
24	a	410	CLA	CBC-CAC-C3C	-2.44	105.72	112.43
31	D	405[A]	PL9	C51-C49-C50	2.44	119.98	114.60
24	b	611	CLA	C1-C2-C3	-2.44	121.83	126.04
31	D	405[A]	PL9	C12-C13-C14	-2.44	121.80	127.66
25	A	408	PHO	CAC-C3C-C4C	2.44	127.88	125.22
24	C	507	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
26	H	101	BCR	C29-C30-C25	2.43	114.23	110.48
24	b	621	CLA	CED-O2D-CGD	2.43	121.44	115.94
24	b	622	CLA	CMA-C3A-C4A	-2.43	105.23	111.77
24	d	402	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
24	B	603	CLA	CMB-C2B-C3B	2.43	129.23	124.68
24	C	507	CLA	C3B-C4B-NB	2.43	112.35	109.21
24	A	410	CLA	CHD-C4C-NC	2.43	128.03	124.20
24	b	617	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
24	c	508	CLA	O2A-CGA-CBA	2.43	119.53	111.91
33	C	520	LMG	C8-O7-C10	-2.43	111.81	117.79
24	B	604	CLA	CAC-C3C-C4C	2.43	127.96	124.81
26	t	101	BCR	C21-C20-C19	-2.43	115.64	123.22
31	A	419[B]	PL9	C10-C9-C11	2.43	119.35	115.27
24	B	602	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
24	A	407	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
24	d	401	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
24	a	412	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	d	404	BCR	C2-C1-C6	2.42	114.21	110.48
24	C	513	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
24	c	511	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
24	b	618	CLA	CAC-C3C-C4C	2.42	127.95	124.81
24	b	621	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
24	D	403	CLA	CMC-C2C-C1C	2.42	128.72	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
24	C	512	CLA	CAC-C3C-C4C	2.41	127.94	124.81
31	D	405[B]	PL9	C12-C13-C14	-2.41	121.85	127.66
25	A	408	PHO	C2B-C1B-NB	2.41	113.43	109.79
24	c	509	CLA	OBD-CAD-C3D	-2.41	123.98	127.98
24	b	613	CLA	OBD-CAD-C3D	-2.41	123.98	127.98
24	D	403	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
24	c	515	CLA	CAC-C3C-C4C	2.41	127.93	124.81
33	c	524	LMG	C8-O7-C10	-2.41	111.87	117.79
24	B	611	CLA	CMB-C2B-C3B	2.40	129.17	124.68
27	a	414	SQD	O47-C7-O49	-2.40	117.90	123.70
24	b	623	CLA	CHB-C4A-NA	2.40	127.83	124.51
24	C	503	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	D	405[B]	PL9	C15-C14-C16	2.40	119.31	115.27
26	C	514	BCR	C37-C22-C23	2.40	121.85	118.08
24	B	603	CLA	C1-O2A-CGA	2.40	122.73	116.44
24	b	623	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
37	D	407	LHG	O7-C7-O9	-2.39	117.93	123.70
37	L	101	LHG	C5-O7-C7	-2.39	111.91	117.79
24	B	605	CLA	C4-C3-C5	2.39	119.29	115.27
24	b	618	CLA	CMB-C2B-C1B	2.39	132.13	128.46
26	C	515	BCR	C15-C16-C17	-2.39	118.58	123.47
24	C	505	CLA	C1-O2A-CGA	2.39	122.71	116.44
24	C	502	CLA	O2A-CGA-CBA	2.39	119.40	111.91
24	C	508	CLA	O2A-CGA-CBA	2.38	119.39	111.91
24	c	516	CLA	CED-O2D-CGD	2.38	121.33	115.94
24	d	403	CLA	O2A-CGA-CBA	2.38	119.39	111.91
27	a	405	SQD	O48-C23-O10	-2.38	117.57	123.59
24	c	511	CLA	OBD-CAD-C3D	-2.38	124.02	127.98
26	Y	101	BCR	C34-C9-C8	2.38	121.83	118.08
25	a	418[A]	PHO	CMB-C2B-C1B	2.38	128.73	125.06
24	c	506	CLA	O2A-CGA-CBA	2.38	119.38	111.91
24	c	517	CLA	CAC-C3C-C4C	2.38	127.90	124.81
24	B	605	CLA	O2A-CGA-CBA	2.38	119.38	111.91
25	A	408	PHO	O2D-CGD-O1D	-2.38	119.19	123.84
24	b	624	CLA	C11-C10-C8	-2.38	108.23	115.92
36	D	406	DGD	C4D-C3D-C2D	2.38	114.97	110.82
24	A	410	CLA	O2A-CGA-CBA	2.38	119.37	111.91
33	Z	101	LMG	C1-C2-C3	2.38	114.94	110.00
27	L	102	SQD	C1-C2-C3	-2.38	105.05	110.00
24	b	617	CLA	C1-C2-C3	-2.37	121.94	126.04
31	D	405[B]	PL9	C45-C44-C46	2.37	119.26	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	401	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	B	612	CLA	C1-C2-C3	-2.37	121.94	126.04
24	c	508	CLA	C3B-C4B-NB	2.37	112.28	109.21
24	B	613	CLA	OBD-CAD-C3D	-2.37	124.04	127.98
31	D	405[B]	PL9	C17-C18-C19	-2.37	121.95	127.66
38	V	205	HEM	CBA-CAA-C2A	-2.37	108.11	112.49
33	c	523	LMG	O8-C28-O10	-2.37	117.61	123.59
27	A	412	SQD	O47-C7-O49	-2.37	117.97	123.70
24	B	610	CLA	CMB-C2B-C1B	2.37	132.10	128.46
25	a	411	PHO	C4D-ND-C1D	-2.37	102.50	106.76
36	H	102	DGD	C3G-O3G-C1D	-2.37	109.11	113.74
33	Z	101	LMG	C9-O8-C28	2.37	123.05	117.10
24	c	513	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	b	610	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	b	612	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
36	c	521	DGD	O1G-C1A-C2A	2.37	119.33	111.91
24	B	609	CLA	OBD-CAD-C3D	-2.37	124.05	127.98
26	k	101	BCR	C10-C11-C12	-2.36	115.84	123.22
24	c	511	CLA	O2A-CGA-CBA	2.36	119.33	111.91
24	b	615	CLA	CBC-CAC-C3C	-2.36	105.91	112.43
24	b	616	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
24	C	508	CLA	CHD-C4C-NC	2.36	127.93	124.20
24	D	402	CLA	CHD-C4C-NC	2.36	127.93	124.20
24	C	503	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
26	t	101	BCR	C16-C15-C14	2.36	128.31	123.47
36	e	101	DGD	O5D-C1E-C2E	2.36	111.99	108.30
24	C	510	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	B	611	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	D	403	CLA	CHD-C4C-NC	2.36	127.92	124.20
26	C	515	BCR	C15-C14-C13	-2.35	123.95	127.31
24	C	512	CLA	C1-O2A-CGA	2.35	122.62	116.44
24	B	607	CLA	C1-O2A-CGA	2.35	122.62	116.44
24	c	516	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
25	a	418[B]	PHO	CBD-CHA-C1A	2.35	131.86	126.40
24	c	516	CLA	C1-O2A-CGA	2.35	122.61	116.44
25	A	409[B]	PHO	CAC-C3C-C4C	2.35	127.78	125.22
24	b	623	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
24	B	605	CLA	CHD-C4C-NC	2.35	127.91	124.20
31	d	405[A]	PL9	C12-C13-C14	-2.35	122.00	127.66
24	b	622	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
24	A	406	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
26	B	620	BCR	C32-C1-C6	-2.35	106.49	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	CHD-C4C-NC	2.35	127.90	124.20
24	a	409	CLA	CMC-C2C-C1C	2.35	128.61	125.04
24	d	402	CLA	CMA-C3A-C2A	-2.34	104.37	113.83
24	c	509	CLA	O2A-CGA-CBA	2.34	119.27	111.91
31	D	405[A]	PL9	C40-C39-C38	-2.34	117.67	123.68
31	D	405[A]	PL9	C32-C33-C34	-2.34	122.02	127.66
27	a	414	SQD	O48-C23-O10	-2.34	117.68	123.59
24	b	625	CLA	C2A-C1A-CHA	-2.34	119.76	123.86
24	B	604	CLA	C4-C3-C5	2.34	119.21	115.27
29	M	103	LMT	O5'-C5'-C4'	2.34	114.69	109.75
24	c	511	CLA	CMC-C2C-C1C	2.34	128.60	125.04
24	b	615	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
24	C	503	CLA	C4-C3-C5	2.34	119.21	115.27
36	C	517	DGD	O2G-C1B-O1B	-2.34	118.05	123.70
24	D	402	CLA	CAC-C3C-C4C	2.34	127.84	124.81
24	C	512	CLA	O2A-CGA-CBA	2.34	119.24	111.91
25	a	418[B]	PHO	C2C-C1C-NC	2.34	113.31	109.79
24	B	617	CLA	OBD-CAD-C3D	-2.34	124.10	127.98
31	a	415[B]	PL9	C45-C44-C46	2.34	119.20	115.27
33	B	622	LMG	O6-C5-C4	2.33	113.93	109.69
24	C	513	CLA	CMB-C2B-C3B	2.33	129.04	124.68
24	B	611	CLA	CAA-CBA-CGA	-2.33	106.43	113.25
33	D	413	LMG	O8-C28-O10	-2.33	117.70	123.59
24	B	616	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
24	C	509	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
24	a	412	CLA	O2A-CGA-CBA	2.33	119.22	111.91
24	B	608	CLA	OBD-CAD-C3D	-2.33	124.11	127.98
31	D	405[B]	PL9	C35-C34-C36	2.33	119.19	115.27
31	A	419[B]	PL9	C40-C39-C41	2.33	119.19	115.27
24	b	612	CLA	C4-C3-C5	2.33	119.19	115.27
24	B	607	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
24	c	506	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
24	A	407	CLA	C1-C2-C3	-2.33	122.02	126.04
24	c	515	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
24	B	616	CLA	CMB-C2B-C1B	2.33	132.04	128.46
24	B	614	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
24	C	510	CLA	CMC-C2C-C1C	2.32	128.58	125.04
24	B	609	CLA	CMB-C2B-C3B	2.32	129.03	124.68
24	A	410	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
24	c	516	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
24	D	402	CLA	CED-O2D-CGD	2.32	121.19	115.94
31	d	405[A]	PL9	C25-C24-C26	2.32	119.17	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	CHD-C4C-NC	2.32	127.86	124.20
24	b	619	CLA	CMC-C2C-C1C	2.32	128.57	125.04
24	a	409	CLA	CHD-C4C-NC	2.32	127.86	124.20
25	a	411	PHO	C3C-C4C-NC	2.32	113.87	110.28
24	D	403	CLA	OBD-CAD-C3D	-2.32	124.13	127.98
37	D	408	LHG	O8-C23-O10	-2.32	117.75	123.59
31	d	405[A]	PL9	C15-C14-C16	2.32	119.17	115.27
27	F	103	SQD	O47-C7-O49	-2.32	118.11	123.70
24	c	506	CLA	CHD-C4C-NC	2.32	127.85	124.20
29	C	521	LMT	O5'-C5'-C4'	2.32	114.63	109.75
24	B	612	CLA	O2A-CGA-CBA	2.31	119.17	111.91
24	c	508	CLA	C4-C3-C5	2.31	119.16	115.27
24	B	603	CLA	C4-C3-C5	2.31	119.16	115.27
24	b	616	CLA	CED-O2D-CGD	2.31	121.16	115.94
31	d	405[B]	PL9	C45-C44-C46	2.31	119.16	115.27
33	d	413	LMG	O6-C5-C4	2.31	113.89	109.69
24	B	603	CLA	CMC-C2C-C1C	2.31	128.56	125.04
29	B	635	LMT	C1'-O5'-C5'	2.31	118.22	113.69
25	a	411	PHO	CBA-CAA-C2A	-2.31	107.05	113.86
24	c	515	CLA	CMB-C2B-C3B	2.31	129.00	124.68
27	A	412	SQD	C1-O5-C5	-2.30	109.17	113.69
24	b	624	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
26	b	628	BCR	C15-C14-C13	-2.30	124.02	127.31
24	B	612	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
24	B	612	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	C	501	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
24	b	621	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
26	K	101	BCR	C16-C17-C18	-2.30	124.03	127.31
24	c	510	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
25	a	418[A]	PHO	C2C-C1C-NC	2.30	113.26	109.79
24	d	401	CLA	C4-C3-C5	2.30	119.14	115.27
27	A	412	SQD	C44-O6-C1	-2.30	109.25	113.74
33	A	421	LMG	C8-O7-C10	-2.30	112.14	117.79
27	a	414	SQD	C1-O5-C5	-2.30	109.18	113.69
24	d	401	CLA	C1-C2-C3	-2.30	122.07	126.04
26	t	101	BCR	C29-C28-C27	-2.29	106.25	111.38
27	F	103	SQD	C1-C2-C3	-2.29	105.22	110.00
24	B	603	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
24	b	611	CLA	CMC-C2C-C1C	2.29	128.53	125.04
31	D	405[B]	PL9	C32-C33-C34	-2.29	122.14	127.66
24	A	410	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
31	A	419[A]	PL9	C17-C18-C19	-2.29	122.14	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C39-C30-C25	-2.29	106.58	110.30
24	A	406	CLA	CED-O2D-CGD	2.29	121.12	115.94
24	c	514	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
24	B	606	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
24	C	503	CLA	CAC-C3C-C4C	2.29	127.78	124.81
37	d	407	LHG	O8-C23-C24	2.29	119.09	111.91
25	a	418[B]	PHO	C4A-NA-C1A	-2.29	106.29	108.14
24	c	515	CLA	CMC-C2C-C1C	2.29	128.52	125.04
24	A	410	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
24	C	508	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
35	B	632	HTG	C6-C5-C4	-2.29	107.65	113.00
26	C	515	BCR	C28-C27-C26	-2.29	110.00	114.08
24	B	611	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
25	a	418[A]	PHO	CBD-CHA-C1A	2.28	131.70	126.40
24	B	610	CLA	C1-O2A-CGA	2.28	122.44	116.44
26	D	404	BCR	C10-C11-C12	-2.28	116.09	123.22
26	B	618	BCR	C34-C9-C10	-2.28	119.72	122.92
24	b	623	CLA	CMB-C2B-C3B	2.28	128.95	124.68
24	A	410	CLA	CMB-C2B-C3B	2.28	128.94	124.68
24	A	405	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
27	B	621	SQD	O47-C7-O49	-2.28	118.19	123.70
24	b	625	CLA	CBC-CAC-C3C	-2.28	106.15	112.43
26	T	103	BCR	C16-C17-C18	-2.28	124.06	127.31
36	C	516	DGD	O1G-C1A-C2A	2.28	119.06	111.91
35	B	625	HTG	C1-C2-C3	2.28	115.09	110.59
24	D	402	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
24	b	620	CLA	CMA-C3A-C4A	-2.27	105.66	111.77
24	b	624	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
24	c	511	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
24	b	622	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
24	b	611	CLA	CMB-C2B-C3B	2.27	128.93	124.68
24	B	616	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
36	c	521	DGD	C3B-C2B-C1B	-2.27	105.36	113.62
24	A	406	CLA	CAC-C3C-C4C	2.27	127.76	124.81
25	a	411	PHO	CMC-C2C-C1C	2.27	128.56	125.06
37	D	408	LHG	O8-C23-C24	2.27	119.03	111.91
24	b	611	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
24	a	409	CLA	OBD-CAD-C3D	-2.27	124.22	127.98
33	A	421	LMG	O8-C28-C29	2.27	119.02	111.91
24	B	612	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
24	d	401	CLA	CAC-C3C-C4C	2.26	127.75	124.81
24	C	513	CLA	C2A-C1A-CHA	-2.26	119.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
26	B	620	BCR	C28-C27-C26	-2.26	110.04	114.08
26	c	528	BCR	C29-C30-C25	2.26	113.96	110.48
25	A	409[B]	PHO	O2A-CGA-CBA	2.26	119.00	111.91
24	b	611	CLA	C1-O2A-CGA	2.26	122.37	116.44
24	C	511	CLA	C4D-C3D-CAD	-2.26	107.21	108.47
24	B	614	CLA	CMA-C3A-C2A	-2.26	104.73	113.83
24	c	511	CLA	CGD-CBD-CAD	-2.26	103.43	110.73
24	b	618	CLA	C1-O2A-CGA	2.26	122.36	116.44
24	b	624	CLA	C1-C2-C3	-2.25	122.14	126.04
37	d	407	LHG	C6-C5-C4	-2.25	106.46	111.79
24	b	625	CLA	CMB-C2B-C3B	2.25	128.89	124.68
31	D	405[B]	PL9	C51-C49-C50	2.25	119.58	114.60
35	B	632	HTG	C3-C4-C5	2.25	114.26	110.24
24	b	618	CLA	CMA-C3A-C4A	-2.25	105.72	111.77
36	C	518	DGD	O3G-C3G-C2G	-2.25	105.47	110.90
36	C	518	DGD	C3G-C2G-C1G	-2.25	106.47	111.79
24	b	613	CLA	CHA-C1A-NA	-2.25	121.25	126.40
26	B	618	BCR	C11-C10-C9	-2.25	124.10	127.31
25	a	411	PHO	CAA-CBA-CGA	-2.25	106.68	113.25
24	c	518	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
24	b	612	CLA	C7-C6-C5	-2.25	107.25	113.36
26	k	101	BCR	C2-C1-C6	2.25	113.94	110.48
26	c	528	BCR	C34-C9-C10	-2.24	119.78	122.92
25	A	409[B]	PHO	C2C-C1C-NC	2.24	113.18	109.79
33	b	629	LMG	O7-C10-O9	-2.24	118.28	123.70
24	C	508	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
24	c	507	CLA	O2A-C1-C2	2.24	114.53	108.64
26	T	103	BCR	C1-C6-C7	2.24	122.12	115.78
24	B	603	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
24	A	410	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
31	A	419[B]	PL9	C8-C7-C3	2.24	118.31	111.98
24	B	602	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	a	409	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
24	B	605	CLA	C11-C10-C8	-2.24	108.69	115.92
24	B	616	CLA	C1-C2-C3	-2.24	122.18	126.04
24	B	611	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
24	C	504	CLA	C4D-C3D-CAD	-2.23	107.22	108.47
24	C	510	CLA	OBD-CAD-C3D	-2.23	124.27	127.98
25	A	409[A]	PHO	C4D-CHA-C1A	-2.23	120.34	125.37
24	b	610	CLA	CAC-C3C-C4C	2.23	127.71	124.81
24	C	511	CLA	O2A-CGA-O1A	-2.23	117.96	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	C4-C3-C5	2.23	119.02	115.27
36	c	522	DGD	C2G-O2G-C1B	-2.23	112.30	117.79
24	C	512	CLA	C4-C3-C5	2.23	119.02	115.27
24	a	409	CLA	C4-C3-C5	2.23	119.02	115.27
24	C	513	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
29	m	103	LMT	C1'-O5'-C5'	2.23	118.06	113.69
25	a	411	PHO	C4D-CHA-C1A	-2.23	120.36	125.37
24	B	610	CLA	O2A-CGA-CBA	2.23	118.90	111.91
24	d	401	CLA	CMB-C2B-C3B	2.23	128.84	124.68
24	b	610	CLA	C4D-C3D-CAD	-2.23	107.23	108.47
24	C	507	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
24	c	510	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
31	A	419[A]	PL9	C7-C3-C2	-2.22	120.38	123.30
24	d	401	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
24	C	508	CLA	OBD-CAD-C3D	-2.22	124.30	127.98
36	c	521	DGD	C2G-O2G-C1B	-2.22	112.33	117.79
24	d	402	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
37	L	101	LHG	O7-C7-O9	-2.22	118.34	123.70
24	b	625	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
26	a	413	BCR	C7-C8-C9	-2.22	122.88	126.23
25	A	408	PHO	C3C-C4C-NC	2.22	113.72	110.28
33	Z	101	LMG	C8-O7-C10	-2.22	112.33	117.79
24	b	622	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
24	D	402	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
24	C	511	CLA	CMB-C2B-C3B	2.21	128.82	124.68
36	C	516	DGD	O2G-C1B-O1B	-2.21	118.35	123.70
24	C	507	CLA	C4-C3-C5	2.21	118.99	115.27
24	c	511	CLA	CAC-C3C-C4C	2.21	127.68	124.81
24	B	610	CLA	C7-C6-C5	-2.21	107.35	113.36
24	c	509	CLA	C11-C10-C8	-2.21	108.77	115.92
25	a	418[B]	PHO	O2A-CGA-CBA	2.21	118.84	111.91
24	C	505	CLA	C4-C3-C5	2.21	118.99	115.27
24	B	604	CLA	CMA-C3A-C2A	-2.21	104.91	113.83
24	C	510	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	B	614	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
29	A	417	LMT	C4B-C3B-C2B	-2.21	106.97	110.82
24	b	619	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
31	d	405[B]	PL9	C22-C23-C24	-2.21	122.35	127.66
31	A	419[B]	PL9	C35-C34-C36	2.21	118.98	115.27
24	c	508	CLA	CHC-C1C-C2C	-2.21	120.62	126.72
24	B	602	CLA	CMC-C2C-C1C	2.21	128.40	125.04
24	b	621	CLA	C2A-C1A-CHA	-2.21	120.00	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	103	BCR	C12-C13-C14	-2.20	115.56	118.94
26	B	619	BCR	C30-C25-C26	-2.20	119.51	122.61
24	b	624	CLA	O2A-CGA-CBA	2.20	118.82	111.91
24	c	514	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
24	A	406	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	A	406	CLA	CAA-CBA-CGA	2.20	119.68	113.25
36	H	102	DGD	C2G-O2G-C1B	-2.20	112.38	117.79
24	B	617	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
24	d	403	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
26	B	619	BCR	C37-C22-C23	2.20	121.54	118.08
26	d	404	BCR	C38-C26-C27	2.20	117.84	113.62
24	B	608	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	b	614	CLA	CMC-C2C-C1C	2.20	128.38	125.04
24	c	510	CLA	CED-O2D-CGD	2.19	120.90	115.94
26	h	101	BCR	C37-C22-C21	-2.19	119.85	122.92
33	D	413	LMG	O8-C28-C29	2.19	118.79	111.91
24	a	410	CLA	C1-C2-C3	-2.19	122.25	126.04
24	d	403	CLA	OBD-CAD-C3D	-2.19	124.34	127.98
24	d	403	CLA	C1-C2-C3	-2.19	122.25	126.04
36	D	406	DGD	O6D-C5D-C6D	2.19	111.09	106.67
37	d	407	LHG	O8-C23-O10	-2.19	118.06	123.59
24	b	610	CLA	O2A-CGA-CBA	2.19	118.78	111.91
24	b	615	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
35	d	411	HTG	C1-O5-C5	2.19	116.61	112.58
26	d	404	BCR	C10-C11-C12	-2.19	116.39	123.22
24	B	608	CLA	CMB-C2B-C3B	2.19	128.77	124.68
24	A	405	CLA	CMA-C3A-C2A	-2.19	105.01	113.83
24	B	610	CLA	CMC-C2C-C1C	2.18	128.36	125.04
24	C	513	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
26	C	515	BCR	C38-C26-C25	-2.18	122.08	124.53
24	C	506	CLA	CED-O2D-CGD	2.18	120.87	115.94
24	B	614	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	b	617	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
26	t	101	BCR	C37-C22-C23	2.18	121.51	118.08
24	d	401	CLA	O2A-CGA-CBA	2.18	118.75	111.91
24	c	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
24	d	401	CLA	CMC-C2C-C1C	2.18	128.36	125.04
27	B	621	SQD	C44-O6-C1	-2.18	109.48	113.74
26	Y	101	BCR	C21-C20-C19	-2.18	116.43	123.22
24	c	515	CLA	C4-C3-C2	-2.17	118.10	123.68
24	B	610	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
24	B	616	CLA	O2A-CGA-O1A	-2.17	118.11	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C38-C26-C25	-2.17	122.09	124.53
24	b	613	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	b	622	CLA	CHD-C4C-NC	2.17	127.62	124.20
36	h	102	DGD	C2G-O2G-C1B	-2.17	112.45	117.79
24	A	405	CLA	CMC-C2C-C1C	2.17	128.34	125.04
37	L	101	LHG	O8-C23-O10	-2.17	118.12	123.59
24	C	510	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
33	A	421	LMG	C7-O1-C1	-2.17	109.51	113.74
24	D	403	CLA	CHB-C4A-NA	2.16	127.50	124.51
24	A	410	CLA	CBC-CAC-C3C	-2.16	106.47	112.43
25	a	411	PHO	O2A-CGA-CBA	2.16	118.69	111.91
24	b	624	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	d	405[B]	PL9	C25-C24-C26	2.16	118.91	115.27
26	t	101	BCR	C12-C13-C14	-2.16	115.62	118.94
24	B	609	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	B	616	CLA	O2A-CGA-CBA	2.16	118.69	111.91
24	c	506	CLA	C4-C3-C5	2.16	118.91	115.27
24	B	606	CLA	OBD-CAD-C3D	-2.16	124.39	127.98
24	b	620	CLA	CHB-C4A-NA	2.16	127.50	124.51
24	d	403	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
29	a	404	LMT	C1B-O1B-C4'	-2.16	112.63	117.96
24	b	619	CLA	CMA-C3A-C2A	-2.15	105.14	113.83
24	B	604	CLA	CBC-CAC-C3C	-2.15	106.50	112.43
24	c	508	CLA	C1-O2A-CGA	2.15	122.09	116.44
24	b	617	CLA	CMA-C3A-C2A	-2.15	105.15	113.83
24	C	507	CLA	C1-C2-C3	-2.15	122.33	126.04
25	A	408	PHO	C1-C2-C3	-2.15	122.33	126.04
26	Y	101	BCR	C15-C16-C17	-2.15	119.07	123.47
31	d	405[A]	PL9	C40-C39-C38	-2.15	118.17	123.68
25	a	411	PHO	CHD-C1D-C2D	-2.15	120.33	125.73
25	a	411	PHO	CBD-CHA-C1A	2.15	131.38	126.40
31	a	415[A]	PL9	C8-C7-C3	2.15	118.05	111.98
24	c	518	CLA	O2A-CGA-O1A	-2.14	118.18	123.59
24	b	621	CLA	CMC-C2C-C1C	2.14	128.31	125.04
24	b	618	CLA	OBD-CAD-C3D	-2.14	124.42	127.98
24	A	407	CLA	CMA-C3A-C2A	-2.14	105.18	113.83
24	B	613	CLA	CHC-C1C-C2C	-2.14	120.79	126.72
24	b	620	CLA	OBD-CAD-C3D	-2.14	124.42	127.98
26	D	404	BCR	C3-C4-C5	-2.14	110.25	114.08
31	D	405[A]	PL9	C35-C34-C36	2.14	118.87	115.27
35	b	631	HTG	C1-C2-C3	2.14	114.81	110.59
24	B	613	CLA	CMA-C3A-C2A	-2.14	105.20	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	402	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
26	H	101	BCR	C15-C14-C13	-2.14	124.26	127.31
33	z	101	LMG	C8-O7-C10	-2.14	112.53	117.79
24	A	407	CLA	CAA-CBA-CGA	2.14	119.49	113.25
27	a	414	SQD	O9-S-O7	-2.13	106.56	113.95
37	E	101	LHG	C5-O7-C7	-2.13	112.53	117.79
37	b	634	LHG	O8-C23-O10	-2.13	118.20	123.59
24	b	618	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
36	C	516	DGD	O6D-C5D-C6D	2.13	110.97	106.67
35	b	601	HTG	C1-O5-C5	2.13	116.52	112.58
31	a	415[A]	PL9	C45-C44-C46	2.13	118.86	115.27
27	f	101	SQD	O48-C23-O10	-2.13	118.21	123.59
26	H	101	BCR	C39-C30-C25	-2.13	106.84	110.30
24	b	621	CLA	CHB-C4A-NA	2.13	127.46	124.51
24	d	401	CLA	CED-O2D-CGD	2.13	120.76	115.94
24	B	608	CLA	C1-O2A-CGA	2.13	122.03	116.44
24	a	409	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
26	b	628	BCR	C16-C17-C18	-2.13	124.27	127.31
24	C	511	CLA	C1-O2A-CGA	2.13	122.03	116.44
26	c	519	BCR	C21-C20-C19	-2.13	116.58	123.22
24	C	505	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
25	A	408	PHO	CHD-C1D-C2D	-2.13	120.38	125.73
25	A	409[A]	PHO	O2A-CGA-CBA	2.13	118.58	111.91
36	C	517	DGD	C3G-O3G-C1D	-2.13	109.59	113.74
24	b	619	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
31	A	419[B]	PL9	C51-C49-C50	2.12	119.29	114.60
24	B	614	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
31	D	405[A]	PL9	C20-C19-C21	2.12	118.84	115.27
24	B	604	CLA	CBA-CAA-C2A	2.12	120.12	113.86
26	C	514	BCR	C38-C26-C25	-2.12	122.15	124.53
31	d	405[A]	PL9	C36-C37-C38	-2.12	104.92	111.88
24	b	623	CLA	C4-C3-C5	2.12	118.83	115.27
36	e	101	DGD	O2G-C1B-O1B	-2.12	118.59	123.70
24	c	512	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	B	606	CLA	CMB-C2B-C1B	2.12	131.72	128.46
24	b	610	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
29	m	103	LMT	C1B-O1B-C4'	-2.12	112.73	117.96
26	d	404	BCR	C39-C30-C25	-2.12	106.87	110.30
27	B	621	SQD	O9-S-C6	2.11	109.45	106.94
24	B	615	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
24	b	611	CLA	OBD-CAD-C3D	-2.11	124.47	127.98
24	A	406	CLA	CMA-C3A-C2A	-2.11	105.30	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	514	BCR	C23-C24-C25	-2.11	121.27	127.20
36	c	521	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
36	c	520	DGD	O1G-C1A-C2A	2.11	118.53	111.91
24	c	514	CLA	CMB-C2B-C3B	2.11	128.63	124.68
24	c	507	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
24	C	505	CLA	CHA-C1A-NA	-2.11	121.57	126.40
25	A	409[B]	PHO	CBD-CHA-C1A	2.11	131.29	126.40
24	A	406	CLA	CMC-C2C-C1C	2.11	128.25	125.04
24	B	602	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
24	B	611	CLA	CGD-CBD-CAD	-2.11	103.91	110.73
24	C	510	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
26	A	411	BCR	C3-C4-C5	-2.11	110.32	114.08
33	B	622	LMG	O8-C28-O10	-2.11	118.28	123.59
26	T	103	BCR	C28-C27-C26	-2.10	110.32	114.08
24	a	410	CLA	CAA-CBA-CGA	2.10	119.40	113.25
31	a	415[B]	PL9	C12-C13-C14	-2.10	122.59	127.66
24	B	610	CLA	CED-O2D-CGD	2.10	120.69	115.94
24	B	611	CLA	C1-C2-C3	-2.10	122.41	126.04
24	A	405	CLA	CHB-C4A-NA	2.10	127.42	124.51
27	a	405	SQD	C3-C4-C5	2.10	113.99	110.24
31	A	419[A]	PL9	C47-C46-C44	-2.10	106.06	112.98
26	a	413	BCR	C38-C26-C25	-2.10	122.17	124.53
33	C	519	LMG	O7-C10-O9	-2.10	118.63	123.70
33	b	629	LMG	O8-C28-O10	-2.10	118.30	123.59
27	B	621	SQD	O8-S-C6	2.10	109.08	105.74
24	b	613	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
24	B	612	CLA	CED-O2D-CGD	2.10	120.68	115.94
24	C	507	CLA	O1D-CGD-CBD	-2.10	120.20	124.48
31	D	405[A]	PL9	C47-C48-C49	-2.10	120.59	127.75
24	A	406	CLA	C3D-CAD-CBD	2.09	110.36	107.61
24	b	610	CLA	C1-O2A-CGA	2.09	121.93	116.44
24	c	509	CLA	CMB-C2B-C3B	2.09	128.59	124.68
29	M	103	LMT	O5B-C5B-C4B	2.09	113.49	109.69
26	a	413	BCR	C8-C7-C6	-2.09	121.33	127.20
36	c	520	DGD	O6D-C5D-C6D	2.09	110.88	106.67
31	A	419[A]	PL9	C51-C49-C50	2.09	119.21	114.60
24	b	620	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
24	c	517	CLA	C1-O2A-CGA	2.09	121.92	116.44
24	B	604	CLA	CMB-C2B-C3B	2.09	128.58	124.68
31	A	419[A]	PL9	C40-C39-C41	2.09	118.78	115.27
24	A	406	CLA	OBD-CAD-C3D	-2.09	124.52	127.98
24	B	608	CLA	C1B-CHB-C4A	-2.08	125.99	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	522	DGD	O1G-C1A-O1A	-2.08	118.34	123.59
24	A	406	CLA	O2A-CGA-CBA	2.08	118.44	111.91
24	B	607	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
25	a	418[A]	PHO	C1C-C2C-C3C	-2.08	104.12	106.51
33	d	413	LMG	C1-O6-C5	2.08	117.77	113.69
24	C	502	CLA	OBD-CAD-C3D	-2.08	124.53	127.98
24	B	611	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	Y	101	BCR	C40-C30-C25	-2.08	106.93	110.30
26	B	619	BCR	C8-C7-C6	-2.08	121.37	127.20
24	a	412	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
36	H	102	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
24	C	506	CLA	CMB-C2B-C3B	2.07	128.56	124.68
24	d	401	CLA	C1-O2A-CGA	2.07	121.88	116.44
24	C	512	CLA	OBD-CAD-C3D	-2.07	124.54	127.98
26	A	411	BCR	C8-C7-C6	-2.07	121.38	127.20
24	c	517	CLA	CMA-C3A-C4A	-2.07	106.21	111.77
26	b	626	BCR	C29-C30-C25	2.07	113.67	110.48
35	c	525	HTG	C6-C5-C4	-2.07	108.16	113.00
24	C	511	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
38	v	205	HEM	CBA-CAA-C2A	-2.07	108.67	112.49
26	Y	101	BCR	C28-C27-C26	-2.07	110.39	114.08
31	d	405[A]	PL9	C22-C23-C24	-2.06	122.69	127.66
24	b	622	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
24	D	403	CLA	O2A-CGA-CBA	2.06	118.38	111.91
24	B	602	CLA	CAC-C3C-C4C	2.06	127.49	124.81
24	C	503	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
27	L	102	SQD	O5-C5-C4	2.06	113.44	109.69
29	A	417	LMT	C6'-C5'-C4'	-2.06	107.33	113.33
26	b	628	BCR	C21-C20-C19	-2.06	116.79	123.22
27	f	101	SQD	O9-S-C6	2.06	109.39	106.94
26	c	519	BCR	C16-C17-C18	-2.06	124.37	127.31
26	t	101	BCR	C2-C1-C6	2.06	113.65	110.48
31	d	405[B]	PL9	C35-C34-C36	2.06	118.73	115.27
24	b	623	CLA	C4-C3-C2	-2.06	118.40	123.68
24	A	407	CLA	O2A-CGA-CBA	2.06	118.36	111.91
24	b	611	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
27	f	101	SQD	C4-C3-C2	-2.06	107.23	110.82
33	c	524	LMG	O7-C10-O9	-2.06	118.73	123.70
24	b	613	CLA	CHD-C4C-NC	2.06	127.44	124.20
24	c	509	CLA	C6-C7-C8	-2.06	109.28	115.92
25	a	418[A]	PHO	C3A-C4A-CHB	-2.05	118.28	121.83
25	a	418[B]	PHO	C1C-C2C-C3C	-2.05	104.15	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	626	BCR	C16-C17-C18	-2.05	124.38	127.31
24	c	514	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
24	B	608	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
24	c	516	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
24	C	512	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
27	F	103	SQD	O48-C23-O10	-2.05	118.41	123.59
24	C	509	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
26	A	411	BCR	C24-C23-C22	-2.05	123.14	126.23
25	a	418[B]	PHO	C3A-C4A-CHB	-2.05	118.29	121.83
24	B	603	CLA	O2A-CGA-CBA	2.05	118.34	111.91
31	d	405[A]	PL9	C35-C34-C36	2.05	118.72	115.27
26	A	411	BCR	C38-C26-C25	-2.05	122.23	124.53
35	C	522	HTG	C1-O5-C5	2.05	116.36	112.58
26	a	413	BCR	C3-C4-C5	-2.05	110.42	114.08
26	K	101	BCR	C36-C18-C19	2.05	121.30	118.08
24	B	609	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
24	a	410	CLA	CMA-C3A-C2A	-2.05	105.57	113.83
26	b	626	BCR	C10-C11-C12	-2.05	116.83	123.22
24	c	518	CLA	CMB-C2B-C3B	2.05	128.51	124.68
24	B	602	CLA	CMB-C2B-C3B	2.05	128.50	124.68
24	C	507	CLA	CMB-C2B-C3B	2.04	128.50	124.68
24	B	605	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
33	D	413	LMG	O7-C10-O9	-2.04	118.76	123.70
33	b	629	LMG	C9-C8-C7	-2.04	106.96	111.79
36	H	102	DGD	O6E-C5E-C6E	2.04	111.51	106.44
31	D	405[B]	PL9	C7-C3-C4	2.04	118.53	116.88
33	B	622	LMG	C9-C8-C7	-2.04	106.96	111.79
24	c	516	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
26	d	404	BCR	C21-C20-C19	-2.04	116.86	123.22
24	B	614	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
37	E	101	LHG	O8-C23-O10	-2.04	118.45	123.59
24	C	506	CLA	O2A-CGA-CBA	2.04	118.30	111.91
37	d	406	LHG	O7-C7-O9	-2.03	118.79	123.70
24	b	625	CLA	CHC-C1C-NC	2.03	127.29	124.20
24	b	622	CLA	CMB-C2B-C3B	2.03	128.48	124.68
24	c	507	CLA	CMB-C2B-C3B	2.03	128.48	124.68
24	B	608	CLA	CED-O2D-CGD	2.03	120.53	115.94
24	c	511	CLA	CHB-C4A-NA	2.03	127.32	124.51
33	c	524	LMG	O8-C28-O10	-2.03	118.48	123.59
24	B	605	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
25	A	409[A]	PHO	C3A-C4A-NA	2.02	116.50	113.05
24	A	407	CLA	CAC-C3C-C4C	2.02	127.44	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	CMB-C2B-C3B	2.02	128.46	124.68
24	d	401	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
38	v	205	HEM	C3C-C4C-NC	-2.02	107.12	110.94
24	b	625	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
24	C	512	CLA	CHB-C4A-NA	2.02	127.31	124.51
31	d	405[A]	PL9	O1-C4-C3	-2.02	118.49	120.72
24	B	613	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	b	612	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
27	a	414	SQD	O6-C44-C45	-2.02	106.03	110.90
25	A	409[A]	PHO	CHD-C1D-C2D	-2.02	120.65	125.73
33	C	519	LMG	O8-C28-O10	-2.02	118.50	123.59
24	B	608	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
24	B	605	CLA	CHA-C1A-NA	-2.02	121.78	126.40
26	a	413	BCR	C15-C14-C13	-2.02	124.43	127.31
26	k	101	BCR	C38-C26-C25	-2.02	122.26	124.53
31	D	405[B]	PL9	C30-C29-C31	2.02	118.66	115.27
26	D	404	BCR	C38-C26-C27	2.02	117.49	113.62
24	d	402	CLA	CHD-C4C-NC	2.01	127.38	124.20
24	c	515	CLA	OBD-CAD-C3D	-2.01	124.64	127.98
24	C	501	CLA	C6-C7-C8	-2.01	109.41	115.92
24	C	507	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	C	510	CLA	C4-C3-C2	-2.01	118.51	123.68
37	b	634	LHG	O4-P-O5	2.01	122.19	112.24
24	c	515	CLA	C6-C7-C8	-2.01	109.42	115.92
26	A	411	BCR	C7-C8-C9	-2.01	123.19	126.23
24	c	512	CLA	CHB-C4A-NA	2.01	127.29	124.51
24	B	617	CLA	CMB-C2B-C3B	2.01	128.44	124.68
24	C	506	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
26	t	101	BCR	C37-C22-C21	-2.01	120.11	122.92
24	B	608	CLA	CHB-C4A-NA	2.01	127.29	124.51
29	F	101	LMT	C1B-O5B-C5B	2.01	117.63	113.69
31	D	405[B]	PL9	C7-C3-C2	-2.01	120.66	123.30
26	C	514	BCR	C11-C10-C9	-2.01	124.45	127.31
26	B	618	BCR	C29-C30-C25	2.01	113.57	110.48
26	c	528	BCR	C28-C27-C26	-2.00	110.50	114.08
24	D	403	CLA	CMB-C2B-C3B	2.00	128.43	124.68
26	C	515	BCR	C40-C30-C25	-2.00	107.05	110.30
33	C	520	LMG	C3-C4-C5	2.00	113.81	110.24
24	C	510	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
31	d	405[A]	PL9	C45-C44-C46	2.00	118.64	115.27
36	H	102	DGD	C3E-C4E-C5E	-2.00	106.67	110.24
31	A	419[A]	PL9	C16-C17-C18	-2.00	105.31	111.88

All (189) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA
24	c	516	CLA	NC
24	c	516	CLA	ND
24	c	516	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	624	CLA	NA
24	b	624	CLA	NC
24	b	624	CLA	ND
24	c	508	CLA	NC
24	c	508	CLA	NA
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	c	510	CLA	ND
24	c	510	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	d	402	CLA	ND
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	c	514	CLA	NC
24	c	514	CLA	ND
24	c	514	CLA	NA
24	B	604	CLA	NC

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Mol	Chain	Res	Type	Atom
24	B	604	CLA	ND
24	B	604	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	A	410	CLA	NC
24	A	410	CLA	ND
24	A	410	CLA	NA
24	D	403	CLA	NC
24	D	403	CLA	ND
24	D	403	CLA	NA
24	b	625	CLA	NA
24	b	625	CLA	NC
24	b	625	CLA	ND
24	B	612	CLA	NC
24	B	612	CLA	ND
24	C	505	CLA	ND
24	C	501	CLA	NC
24	C	501	CLA	ND
24	C	501	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	d	403	CLA	NC
24	d	403	CLA	ND
24	d	403	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	b	622	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	622	CLA	ND
24	b	622	CLA	NA
24	b	621	CLA	NC
24	b	621	CLA	ND
24	b	621	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	c	518	CLA	NC
24	c	518	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	b	619	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	NA
24	a	410	CLA	NC
24	a	410	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	d	401	CLA	NC
24	d	401	CLA	ND
24	d	401	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	c	517	CLA	NC
24	c	517	CLA	ND
24	c	517	CLA	NA
24	b	623	CLA	NC
24	b	623	CLA	ND
24	b	623	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	D	402	CLA	ND
24	D	402	CLA	NA
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	B	610	CLA	NC

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Mol	Chain	Res	Type	Atom
24	B	610	CLA	ND
24	a	412	CLA	NC
24	a	412	CLA	ND
24	a	412	CLA	NA
24	a	409	CLA	NC
24	a	409	CLA	ND
24	a	409	CLA	NA
24	A	407	CLA	NC
24	A	407	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	ND
24	b	620	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	c	515	CLA	NC
24	c	515	CLA	ND
24	c	515	CLA	NA

All (1276) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	c	513	CLA	CHA-CBD-CGD-O1D
24	c	513	CLA	CHA-CBD-CGD-O2D
38	e	103	HEM	C2A-CAA-CBA-CGA
38	e	103	HEM	C3D-CAD-CBD-CGD
28	V	201	GOL	C1-C2-C3-O3
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
37	L	101	LHG	C4-O6-P-O4
37	L	101	LHG	C4-O6-P-O5
28	A	422	GOL	O1-C1-C2-C3
37	D	408	LHG	C4-O6-P-O4
24	B	603	CLA	C14-C13-C15-C16
29	A	417	LMT	C2'-C1'-O1'-C1
29	A	417	LMT	O5'-C1'-O1'-C1
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
29	f	102	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
29	f	102	LMT	O5'-C1'-O1'-C1
28	A	414	GOL	C1-C2-C3-O3
24	C	509	CLA	C2-C1-O2A-CGA
28	a	420	GOL	O1-C1-C2-C3
29	F	101	LMT	C2'-C1'-O1'-C1
29	F	101	LMT	O5'-C1'-O1'-C1
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
37	b	634	LHG	C4-O6-P-O4
35	B	625	HTG	O5-C1-S1-C1'
29	B	635	LMT	C2'-C1'-O1'-C1
29	B	635	LMT	O5'-C1'-O1'-C1
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	O9-C10-O7-C8
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CAD-CBD-CGD-O1D
29	T	104	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
37	d	407	LHG	C3-O3-P-O4
29	C	521	LMT	C2'-C1'-O1'-C1
29	C	521	LMT	O5'-C1'-O1'-C1
29	M	103	LMT	O5'-C1'-O1'-C1
28	a	402	GOL	O1-C1-C2-C3
29	b	630	LMT	C2'-C1'-O1'-C1
29	b	630	LMT	O5'-C1'-O1'-C1
24	b	615	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O9
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
27	f	101	SQD	O49-C7-O47-C45
27	f	101	SQD	C8-C7-O47-C45
27	f	101	SQD	C5-C6-S-O7
27	f	101	SQD	C5-C6-S-O8
27	f	101	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
29	a	419	LMT	C2'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
37	e	102	LHG	C3-O3-P-O5
37	e	102	LHG	C3-O3-P-O6
28	C	524	GOL	O1-C1-C2-C3
35	c	525	HTG	C2'-C1'-S1-C1
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O5
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
28	b	604	GOL	O1-C1-C2-C3
36	D	406	DGD	C2B-C1B-O2G-C2G
36	D	406	DGD	C2D-C1D-O3G-C3G
36	D	406	DGD	O6D-C1D-O3G-C3G
28	A	415	GOL	C1-C2-C3-O3
31	a	415[B]	PL9	C12-C11-C9-C10
31	a	415[B]	PL9	C18-C19-C21-C22
31	a	415[B]	PL9	C20-C19-C21-C22
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
26	b	626	BCR	C1-C6-C7-C8
28	B	627	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
28	T	102	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-C3
24	b	614	CLA	C2-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
27	A	416	SQD	O6-C44-C45-O47
24	C	508	CLA	CHA-CBD-CGD-O1D
24	b	623	CLA	CHA-CBD-CGD-O1D
24	b	623	CLA	CHA-CBD-CGD-O2D
24	b	623	CLA	CAD-CBD-CGD-O1D
24	b	623	CLA	C2-C3-C5-C6
24	b	623	CLA	C4-C3-C5-C6
36	e	101	DGD	C2B-C1B-O2G-C2G
36	e	101	DGD	O1B-C1B-O2G-C2G
36	e	101	DGD	O6E-C1E-O5D-C6D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
33	C	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O6-C1-O1-C7
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
28	B	628	GOL	O1-C1-C2-C3
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
35	B	624	HTG	C2'-C1'-S1-C1
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
35	b	632	HTG	O5-C1-S1-C1'
35	b	632	HTG	C2'-C1'-S1-C1
37	e	102	LHG	O10-C23-O8-C6
29	C	521	LMT	C3'-C4'-O1B-C1B
29	D	401	LMT	C3'-C4'-O1B-C1B
37	E	101	LHG	O10-C23-O8-C6
24	c	516	CLA	CBD-CGD-O2D-CED
36	D	406	DGD	O1B-C1B-O2G-C2G
33	C	520	LMG	O9-C10-O7-C8
24	A	410	CLA	C3-C5-C6-C7
24	b	623	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
37	e	102	LHG	C24-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
33	z	101	LMG	C11-C10-O7-C8
27	B	621	SQD	C8-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
31	a	415[A]	PL9	C12-C11-C9-C10
31	a	415[A]	PL9	C20-C19-C21-C22
36	C	516	DGD	C2A-C3A-C4A-C5A
24	c	511	CLA	C3-C5-C6-C7
24	B	615	CLA	C3-C5-C6-C7
35	b	632	HTG	S1-C1'-C2'-C3'
33	z	101	LMG	O6-C5-C6-O5
37	d	407	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
37	E	101	LHG	O2-C2-C3-O3
29	M	103	LMT	O5'-C5'-C6'-O6'
33	A	421	LMG	C11-C10-O7-C8
29	f	102	LMT	C4'-C5'-C6'-O6'
29	f	102	LMT	O5'-C5'-C6'-O6'
29	M	103	LMT	O5B-C5B-C6B-O6B
24	B	602	CLA	C3-C5-C6-C7
35	V	206	HTG	S1-C1'-C2'-C3'
33	C	520	LMG	O6-C5-C6-O5
29	M	101	LMT	O5B-C5B-C6B-O6B
31	A	419[A]	PL9	C25-C24-C26-C27
31	A	419[B]	PL9	C25-C24-C26-C27
31	a	415[A]	PL9	C15-C14-C16-C17
31	a	415[A]	PL9	C25-C24-C26-C27
31	a	415[B]	PL9	C15-C14-C16-C17
31	a	415[B]	PL9	C25-C24-C26-C27
31	A	419[A]	PL9	C23-C24-C26-C27
31	A	419[B]	PL9	C23-C24-C26-C27
31	a	415[A]	PL9	C13-C14-C16-C17
31	a	415[A]	PL9	C23-C24-C26-C27
31	a	415[B]	PL9	C13-C14-C16-C17
31	a	415[B]	PL9	C23-C24-C26-C27
24	b	615	CLA	C2A-CAA-CBA-CGA
24	B	607	CLA	C2A-CAA-CBA-CGA
33	z	101	LMG	C4-C5-C6-O5
27	B	621	SQD	O5-C1-O6-C44
31	d	405[B]	PL9	C39-C41-C42-C43
31	d	405[A]	PL9	C39-C41-C42-C43
31	D	405[A]	PL9	C39-C41-C42-C43
24	C	509	CLA	C3-C5-C6-C7
29	M	103	LMT	C4'-C5'-C6'-O6'
29	m	103	LMT	O5'-C5'-C6'-O6'
33	A	421	LMG	O9-C10-O7-C8
24	C	509	CLA	O1A-CGA-O2A-C1
24	C	509	CLA	CBA-CGA-O2A-C1
24	B	615	CLA	C5-C6-C7-C8
29	D	401	LMT	O5B-C5B-C6B-O6B
33	c	501	LMG	C17-C18-C19-C20
24	B	602	CLA	C10-C11-C12-C13
24	B	615	CLA	C8-C10-C11-C12
33	Z	101	LMG	C10-C11-C12-C13
36	e	101	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C2-C1-O1-C7
31	a	415[A]	PL9	C12-C11-C9-C8
24	c	514	CLA	C11-C10-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	B	602	CLA	C11-C10-C8-C9
24	b	619	CLA	C11-C12-C13-C14
24	c	511	CLA	C6-C7-C8-C9
24	B	617	CLA	C6-C7-C8-C9
33	B	622	LMG	C15-C16-C17-C18
24	B	616	CLA	C8-C10-C11-C12
26	D	404	BCR	C7-C8-C9-C34
27	B	621	SQD	C7-C8-C9-C10
24	b	624	CLA	C10-C11-C12-C13
24	C	501	CLA	C15-C16-C17-C18
35	B	625	HTG	O5-C5-C6-O6
33	C	520	LMG	C28-C29-C30-C31
35	b	601	HTG	C1'-C2'-C3'-C4'
35	c	525	HTG	C1'-C2'-C3'-C4'
24	c	513	CLA	C15-C16-C17-C18
24	A	410	CLA	C13-C15-C16-C17
24	C	508	CLA	C10-C11-C12-C13
24	B	615	CLA	C10-C11-C12-C13
28	v	203	GOL	O1-C1-C2-O2
28	a	420	GOL	O1-C1-C2-O2
28	a	402	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-O2
28	b	605	GOL	O1-C1-C2-O2
28	V	202	GOL	O1-C1-C2-O2
27	A	416	SQD	C23-C24-C25-C26
36	c	522	DGD	C1A-C2A-C3A-C4A
33	c	523	LMG	C10-C11-C12-C13
29	A	417	LMT	O5B-C5B-C6B-O6B
24	b	610	CLA	C2-C1-O2A-CGA
29	M	101	LMT	C4B-C5B-C6B-O6B
33	c	501	LMG	C10-C11-C12-C13
24	c	516	CLA	O1D-CGD-O2D-CED
24	c	514	CLA	C12-C13-C15-C16
24	b	615	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	C	508	CLA	C5-C6-C7-C8
24	b	623	CLA	C5-C6-C7-C8
29	T	104	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
36	e	101	DGD	O6D-C1D-O3G-C3G
24	a	412	CLA	C8-C10-C11-C12
31	a	415[A]	PL9	C9-C11-C12-C13
31	a	415[B]	PL9	C9-C11-C12-C13
37	e	102	LHG	C11-C12-C13-C14
27	A	416	SQD	C26-C27-C28-C29
24	c	514	CLA	C13-C15-C16-C17
24	C	506	CLA	C13-C15-C16-C17
24	C	504	CLA	C15-C16-C17-C18
24	b	623	CLA	C13-C15-C16-C17
24	C	506	CLA	C5-C6-C7-C8
29	M	103	LMT	C4B-C5B-C6B-O6B
33	C	520	LMG	C4-C5-C6-O5
27	F	103	SQD	C26-C27-C28-C29
24	b	610	CLA	C8-C10-C11-C12
24	b	615	CLA	C13-C15-C16-C17
24	B	617	CLA	C10-C11-C12-C13
37	L	101	LHG	C4-O6-P-O3
37	b	634	LHG	C4-O6-P-O3
37	d	407	LHG	C3-O3-P-O6
37	D	407	LHG	C23-C24-C25-C26
35	b	632	HTG	C1'-C2'-C3'-C4'
35	c	525	HTG	S1-C1'-C2'-C3'
37	E	101	LHG	C1-C2-C3-O3
35	b	632	HTG	O5-C5-C6-O6
31	a	415[A]	PL9	C30-C29-C31-C32
24	c	515	CLA	C4-C3-C5-C6
24	c	514	CLA	C15-C16-C17-C18
37	D	408	LHG	C32-C33-C34-C35
35	C	523	HTG	O5-C5-C6-O6
24	D	403	CLA	C3-C5-C6-C7
24	c	509	CLA	C15-C16-C17-C18
33	A	421	LMG	C14-C15-C16-C17
29	M	103	LMT	C2-C3-C4-C5
27	A	416	SQD	C30-C31-C32-C33
33	c	523	LMG	C11-C10-O7-C8
29	m	102	LMT	O5'-C5'-C6'-O6'
29	T	104	LMT	C11-C10-C9-C8
37	e	102	LHG	C24-C25-C26-C27
36	D	406	DGD	C6A-C7A-C8A-C9A
27	A	412	SQD	C9-C10-C11-C12
36	H	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
35	B	624	HTG	C2'-C3'-C4'-C5'
24	b	623	CLA	C16-C17-C18-C19
24	a	412	CLA	C16-C17-C18-C19
36	c	521	DGD	C9A-CAA-CBA-CCA
33	d	413	LMG	C17-C18-C19-C20
36	C	516	DGD	C4B-C5B-C6B-C7B
36	C	517	DGD	C9A-CAA-CBA-CCA
36	C	518	DGD	CAA-CBA-CCA-CDA
33	c	501	LMG	C21-C22-C23-C24
33	c	523	LMG	O9-C10-O7-C8
24	c	518	CLA	C10-C11-C12-C13
24	a	412	CLA	C10-C11-C12-C13
29	B	635	LMT	C3-C4-C5-C6
33	B	622	LMG	C29-C30-C31-C32
27	B	621	SQD	C30-C31-C32-C33
27	L	102	SQD	C27-C28-C29-C30
29	T	104	LMT	C4-C5-C6-C7
36	c	521	DGD	C2E-C1E-O5D-C6D
36	C	517	DGD	C2E-C1E-O5D-C6D
29	D	401	LMT	C2'-C1'-O1'-C1
27	A	416	SQD	C2-C1-O6-C44
36	e	101	DGD	C2D-C1D-O3G-C3G
29	m	102	LMT	C2'-C1'-O1'-C1
36	e	101	DGD	CCA-CDA-CEA-CFA
33	c	523	LMG	C34-C35-C36-C37
33	d	413	LMG	O6-C5-C6-O5
31	d	405[A]	PL9	C45-C44-C46-C47
27	L	102	SQD	C12-C13-C14-C15
36	c	522	DGD	C6A-C7A-C8A-C9A
31	d	405[B]	PL9	C13-C14-C16-C17
24	b	610	CLA	C11-C10-C8-C9
24	C	505	CLA	C11-C12-C13-C14
24	b	612	CLA	C6-C7-C8-C9
24	a	410	CLA	C11-C12-C13-C14
36	c	520	DGD	O6D-C5D-C6D-O5D
36	c	521	DGD	C4A-C5A-C6A-C7A
37	D	409	LHG	C29-C30-C31-C32
36	e	101	DGD	C8B-C9B-CAB-CBB
33	z	101	LMG	C12-C13-C14-C15
37	d	406	LHG	C32-C33-C34-C35
36	h	102	DGD	CAA-CBA-CCA-CDA
37	D	407	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
28	v	203	GOL	O1-C1-C2-C3
28	v	201	GOL	O1-C1-C2-C3
28	B	626	GOL	C1-C2-C3-O3
28	o	301	GOL	O1-C1-C2-C3
28	o	301	GOL	C1-C2-C3-O3
28	B	629	GOL	O1-C1-C2-C3
28	b	605	GOL	O1-C1-C2-C3
37	D	407	LHG	O1-C1-C2-C3
28	V	202	GOL	O1-C1-C2-C3
28	v	202	GOL	O1-C1-C2-C3
36	C	516	DGD	C3B-C4B-C5B-C6B
36	c	520	DGD	C5A-C6A-C7A-C8A
29	a	404	LMT	C4B-C5B-C6B-O6B
37	e	102	LHG	C23-C24-C25-C26
33	A	421	LMG	C11-C12-C13-C14
37	L	101	LHG	C14-C15-C16-C17
36	C	516	DGD	C5B-C6B-C7B-C8B
27	a	414	SQD	C11-C12-C13-C14
36	c	522	DGD	C7A-C8A-C9A-CAA
36	c	522	DGD	C6B-C7B-C8B-C9B
33	b	629	LMG	C38-C39-C40-C41
24	b	620	CLA	C16-C17-C18-C19
35	B	632	HTG	C4-C5-C6-O6
29	m	102	LMT	O5'-C1'-O1'-C1
24	B	614	CLA	C13-C15-C16-C17
36	c	522	DGD	C7B-C8B-C9B-CAB
33	C	519	LMG	C11-C12-C13-C14
29	A	417	LMT	C6-C7-C8-C9
37	E	101	LHG	C24-C25-C26-C27
36	c	520	DGD	C9A-CAA-CBA-CCA
37	D	407	LHG	C24-C25-C26-C27
36	c	520	DGD	C8B-C9B-CAB-CBB
36	c	522	DGD	CBA-CCA-CDA-CEA
37	d	408	LHG	C29-C30-C31-C32
24	c	514	CLA	C3-C5-C6-C7
27	L	102	SQD	C24-C23-O48-C46
29	M	103	LMT	C2-C1-O1'-C1'
33	d	413	LMG	C36-C37-C38-C39
37	D	409	LHG	C24-C25-C26-C27
33	b	629	LMG	C32-C33-C34-C35
33	z	101	LMG	C15-C16-C17-C18
35	b	631	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
29	C	521	LMT	O5B-C5B-C6B-O6B
27	B	621	SQD	C31-C32-C33-C34
36	D	406	DGD	C2A-C3A-C4A-C5A
33	c	501	LMG	C14-C15-C16-C17
29	T	104	LMT	C1-C2-C3-C4
25	A	408	PHO	C4-C3-C5-C6
31	D	405[A]	PL9	C15-C14-C16-C17
31	d	405[B]	PL9	C43-C44-C46-C47
24	C	510	CLA	C2-C3-C5-C6
31	a	415[A]	PL9	C18-C19-C21-C22
25	A	408	PHO	C2-C3-C5-C6
24	c	515	CLA	C2-C3-C5-C6
27	a	405	SQD	C25-C26-C27-C28
28	v	201	GOL	O1-C1-C2-O2
28	A	414	GOL	O2-C2-C3-O3
28	B	630	GOL	O1-C1-C2-O2
28	B	630	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
33	A	421	LMG	C30-C31-C32-C33
27	a	414	SQD	C29-C30-C31-C32
29	a	404	LMT	C2-C3-C4-C5
24	b	624	CLA	C16-C17-C18-C19
24	a	412	CLA	C16-C17-C18-C20
33	Z	101	LMG	C19-C20-C21-C22
24	c	511	CLA	C15-C16-C17-C18
33	D	413	LMG	C19-C20-C21-C22
29	T	104	LMT	C7-C8-C9-C10
36	h	102	DGD	C4E-C5E-C6E-O5E
33	B	622	LMG	C31-C32-C33-C34
24	c	514	CLA	C2-C1-O2A-CGA
24	B	617	CLA	C2-C1-O2A-CGA
36	c	520	DGD	CAB-CBB-CCB-CDB
36	H	102	DGD	C7A-C8A-C9A-CAA
27	a	405	SQD	C31-C32-C33-C34
26	b	626	BCR	C5-C6-C7-C8
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C26
26	d	404	BCR	C23-C24-C25-C30
33	d	413	LMG	C19-C20-C21-C22
37	b	634	LHG	C27-C28-C29-C30
35	B	632	HTG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
27	a	414	SQD	C9-C10-C11-C12
36	e	101	DGD	C2A-C3A-C4A-C5A
29	C	521	LMT	O5'-C5'-C6'-O6'
24	B	602	CLA	C8-C10-C11-C12
27	A	412	SQD	C13-C14-C15-C16
36	e	101	DGD	C5A-C6A-C7A-C8A
31	d	405[B]	PL9	C45-C44-C46-C47
31	D	405[B]	PL9	C15-C14-C16-C17
24	B	603	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C15
24	b	625	CLA	C11-C12-C13-C15
31	D	405[B]	PL9	C28-C29-C31-C32
24	C	505	CLA	C11-C12-C13-C15
24	b	612	CLA	C6-C7-C8-C10
31	d	405[A]	PL9	C43-C44-C46-C47
24	a	410	CLA	C11-C12-C13-C15
31	D	405[A]	PL9	C13-C14-C16-C17
35	C	523	HTG	S1-C1'-C2'-C3'
24	C	511	CLA	O1A-CGA-O2A-C1
27	L	102	SQD	O10-C23-O48-C46
27	L	102	SQD	C31-C32-C33-C34
24	B	616	CLA	C5-C6-C7-C8
24	c	515	CLA	C8-C10-C11-C12
26	t	101	BCR	C13-C14-C15-C16
24	b	623	CLA	C16-C17-C18-C20
36	e	101	DGD	O6D-C5D-C6D-O5D
24	C	511	CLA	CBA-CGA-O2A-C1
36	e	101	DGD	C2A-C1A-O1G-C1G
37	d	406	LHG	C29-C30-C31-C32
27	A	412	SQD	C14-C15-C16-C17
33	B	622	LMG	C36-C37-C38-C39
35	b	631	HTG	C3'-C4'-C5'-C6'
36	C	517	DGD	C4B-C5B-C6B-C7B
27	B	621	SQD	C24-C23-O48-C46
36	c	520	DGD	C4D-C5D-C6D-O5D
36	c	521	DGD	O6E-C1E-O5D-C6D
36	C	517	DGD	O6E-C1E-O5D-C6D
29	D	401	LMT	O5'-C1'-O1'-C1
27	A	416	SQD	O5-C1-O6-C44
24	a	412	CLA	C15-C16-C17-C18
29	f	102	LMT	C5-C6-C7-C8
29	B	635	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
29	B	635	LMT	C7-C8-C9-C10
29	a	419	LMT	C6-C7-C8-C9
27	L	102	SQD	C29-C30-C31-C32
33	b	629	LMG	C33-C34-C35-C36
33	c	501	LMG	C29-C30-C31-C32
36	C	517	DGD	C8A-C9A-CAA-CBA
27	F	103	SQD	C2-C1-O6-C44
24	b	620	CLA	C16-C17-C18-C20
33	d	413	LMG	C35-C36-C37-C38
36	D	406	DGD	C8B-C9B-CAB-CBB
24	c	517	CLA	C15-C16-C17-C18
24	b	613	CLA	C13-C15-C16-C17
31	d	405[B]	PL9	C15-C14-C16-C17
31	D	405[B]	PL9	C45-C44-C46-C47
24	C	510	CLA	C4-C3-C5-C6
31	D	405[A]	PL9	C45-C44-C46-C47
31	a	415[B]	PL9	C12-C11-C9-C8
31	A	419[A]	PL9	C4-C3-C7-C8
31	A	419[B]	PL9	C4-C3-C7-C8
31	a	415[A]	PL9	C4-C3-C7-C8
31	a	415[B]	PL9	C4-C3-C7-C8
33	c	501	LMG	C33-C34-C35-C36
24	c	514	CLA	C14-C13-C15-C16
24	b	610	CLA	C6-C7-C8-C9
24	b	625	CLA	C11-C12-C13-C14
24	a	410	CLA	C14-C13-C15-C16
24	b	623	CLA	C11-C12-C13-C14
24	C	506	CLA	C6-C7-C8-C9
36	c	520	DGD	O6E-C5E-C6E-O5E
27	L	102	SQD	C30-C31-C32-C33
24	c	517	CLA	CBA-CGA-O2A-C1
37	d	408	LHG	C31-C32-C33-C34
24	C	506	CLA	C1A-C2A-CAA-CBA
24	b	624	CLA	C16-C17-C18-C20
37	b	634	LHG	C33-C34-C35-C36
27	a	414	SQD	C15-C16-C17-C18
36	h	102	DGD	C6A-C7A-C8A-C9A
37	D	407	LHG	C25-C26-C27-C28
37	D	408	LHG	C4-O6-P-O3
33	A	421	LMG	C10-C11-C12-C13
24	b	623	CLA	CBD-CGD-O2D-CED
24	C	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	635	LMT	C11-C10-C9-C8
36	c	520	DGD	C7B-C8B-C9B-CAB
36	h	102	DGD	C5B-C6B-C7B-C8B
27	L	102	SQD	C32-C33-C34-C35
27	L	102	SQD	C24-C25-C26-C27
27	A	416	SQD	C11-C12-C13-C14
36	D	406	DGD	C1B-C2B-C3B-C4B
35	b	601	HTG	C2'-C3'-C4'-C5'
36	C	516	DGD	O6E-C5E-C6E-O5E
27	B	621	SQD	C35-C36-C37-C38
27	F	103	SQD	C31-C32-C33-C34
33	Z	101	LMG	O6-C5-C6-O5
33	A	421	LMG	C7-C8-C9-O8
27	B	621	SQD	C44-C45-C46-O48
37	E	101	LHG	C4-C5-C6-O8
36	D	406	DGD	O1G-C1G-C2G-C3G
27	A	412	SQD	C18-C19-C20-C21
27	F	103	SQD	C44-C45-C46-O48
33	c	501	LMG	C7-C8-C9-O8
27	A	416	SQD	O6-C44-C45-C46
36	e	101	DGD	O1G-C1G-C2G-C3G
27	a	405	SQD	O6-C44-C45-C46
37	d	406	LHG	C25-C26-C27-C28
36	c	521	DGD	C2G-C3G-O3G-C1D
36	c	521	DGD	C5D-C6D-O5D-C1E
33	C	520	LMG	C8-C7-O1-C1
29	a	404	LMT	C3-C4-C5-C6
27	a	405	SQD	C28-C29-C30-C31
29	a	404	LMT	O5B-C5B-C6B-O6B
37	E	101	LHG	C10-C11-C12-C13
24	C	512	CLA	O1A-CGA-O2A-C1
24	c	517	CLA	O1A-CGA-O2A-C1
36	e	101	DGD	O1A-C1A-O1G-C1G
33	b	629	LMG	C40-C41-C42-C43
24	b	619	CLA	C16-C17-C18-C20
37	E	101	LHG	C19-C20-C21-C22
36	H	102	DGD	CDA-CEA-CFA-CGA
28	V	201	GOL	O2-C2-C3-O3
28	A	422	GOL	O1-C1-C2-O2
28	C	524	GOL	O1-C1-C2-O2
28	A	415	GOL	O2-C2-C3-O3
29	b	630	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
29	a	404	LMT	C7-C8-C9-C10
37	L	101	LHG	C13-C14-C15-C16
27	L	102	SQD	C28-C29-C30-C31
36	H	102	DGD	CDB-CEB-CFB-CGB
24	B	602	CLA	CBA-CGA-O2A-C1
27	L	102	SQD	C35-C36-C37-C38
33	C	519	LMG	C14-C15-C16-C17
24	B	604	CLA	C5-C6-C7-C8
24	c	512	CLA	C5-C6-C7-C8
33	d	413	LMG	C38-C39-C40-C41
36	C	517	DGD	CAB-CBB-CCB-CDB
29	C	521	LMT	C9-C10-C11-C12
37	D	409	LHG	C12-C13-C14-C15
33	D	413	LMG	O6-C5-C6-O5
24	b	612	CLA	C5-C6-C7-C8
36	C	516	DGD	O6D-C5D-C6D-O5D
24	C	513	CLA	C2-C1-O2A-CGA
27	B	621	SQD	C11-C10-C9-C8
36	D	406	DGD	C7A-C8A-C9A-CAA
36	c	521	DGD	C2B-C3B-C4B-C5B
29	A	417	LMT	O1'-C1-C2-C3
27	F	103	SQD	C30-C31-C32-C33
27	B	621	SQD	O10-C23-O48-C46
33	A	421	LMG	C13-C14-C15-C16
33	A	421	LMG	C36-C37-C38-C39
24	a	410	CLA	C10-C11-C12-C13
24	b	623	CLA	C10-C11-C12-C13
27	f	101	SQD	O6-C44-C45-O47
33	Z	101	LMG	O1-C7-C8-O7
33	C	520	LMG	C11-C12-C13-C14
33	c	501	LMG	C35-C36-C37-C38
24	c	509	CLA	C4-C3-C5-C6
24	C	512	CLA	C11-C10-C8-C7
24	b	610	CLA	C6-C7-C8-C10
31	D	405[B]	PL9	C13-C14-C16-C17
24	B	602	CLA	C11-C10-C8-C7
24	c	511	CLA	C6-C7-C8-C10
24	b	623	CLA	C11-C12-C13-C15
24	B	615	CLA	C12-C13-C15-C16
24	B	602	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C14-C13-C15-C16
24	D	403	CLA	C11-C10-C8-C9
24	b	615	CLA	C14-C13-C15-C16
24	c	511	CLA	C11-C10-C8-C9
24	B	615	CLA	C14-C13-C15-C16
37	D	409	LHG	C28-C29-C30-C31
24	b	610	CLA	CBA-CGA-O2A-C1
26	d	404	BCR	C7-C8-C9-C34
24	b	619	CLA	C16-C17-C18-C19
37	D	408	LHG	C26-C27-C28-C29
26	D	404	BCR	C7-C8-C9-C10
24	C	512	CLA	C3-C5-C6-C7
37	d	407	LHG	C1-C2-C3-O3
33	z	101	LMG	C13-C14-C15-C16
33	C	519	LMG	C31-C32-C33-C34
24	c	516	CLA	CBA-CGA-O2A-C1
24	a	412	CLA	CBA-CGA-O2A-C1
29	m	102	LMT	C1-C2-C3-C4
27	a	405	SQD	C23-C24-C25-C26
35	B	625	HTG	C3'-C4'-C5'-C6'
33	b	629	LMG	C39-C40-C41-C42
33	d	413	LMG	C13-C14-C15-C16
24	B	611	CLA	C16-C17-C18-C20
37	e	102	LHG	O6-C4-C5-C6
31	a	415[A]	PL9	C39-C41-C42-C43
33	C	519	LMG	C30-C31-C32-C33
36	c	522	DGD	C2A-C1A-O1G-C1G
33	d	413	LMG	C29-C30-C31-C32
31	a	415[A]	PL9	C28-C29-C31-C32
24	B	612	CLA	C15-C16-C17-C18
36	C	517	DGD	C5A-C6A-C7A-C8A
36	h	102	DGD	O2G-C1B-C2B-C3B
27	F	103	SQD	C34-C35-C36-C37
24	b	613	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C3A-C2A-CAA-CBA
29	B	635	LMT	C4-C5-C6-C7
36	e	101	DGD	CAA-CBA-CCA-CDA
27	A	416	SQD	C24-C25-C26-C27
36	h	102	DGD	O6E-C5E-C6E-O5E
37	D	409	LHG	C24-C23-O8-C6
27	A	416	SQD	C24-C23-O48-C46
29	D	401	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	C10-C11-C12-C13
27	a	414	SQD	O6-C44-C45-C46
37	e	102	LHG	C4-C5-C6-O8
27	L	102	SQD	C44-C45-C46-O48
33	Z	101	LMG	C7-C8-C9-O8
33	c	523	LMG	O1-C7-C8-C9
33	c	523	LMG	C7-C8-C9-O8
33	d	413	LMG	C14-C15-C16-C17
36	e	101	DGD	C4D-C5D-C6D-O5D
29	F	101	LMT	O1'-C1-C2-C3
36	c	521	DGD	C3B-C4B-C5B-C6B
36	e	101	DGD	C4A-C5A-C6A-C7A
31	a	415[A]	PL9	C45-C44-C46-C47
33	b	629	LMG	C37-C38-C39-C40
36	C	517	DGD	C4A-C5A-C6A-C7A
28	o	301	GOL	O1-C1-C2-O2
28	b	604	GOL	O1-C1-C2-O2
28	c	503	GOL	O1-C1-C2-O2
27	a	414	SQD	C34-C35-C36-C37
33	c	501	LMG	C12-C13-C14-C15
37	e	102	LHG	O6-C4-C5-O7
36	C	518	DGD	C2A-C1A-O1G-C1G
33	C	519	LMG	C29-C28-O8-C9
37	d	407	LHG	C34-C35-C36-C37
29	a	404	LMT	C6-C7-C8-C9
24	c	516	CLA	O1A-CGA-O2A-C1
24	a	412	CLA	O1A-CGA-O2A-C1
37	d	406	LHG	C11-C10-C9-C8
35	b	607	HTG	C4'-C5'-C6'-C7'
27	f	101	SQD	C24-C25-C26-C27
27	L	102	SQD	C11-C12-C13-C14
27	A	412	SQD	C15-C16-C17-C18
27	a	414	SQD	O6-C44-C45-O47
36	D	406	DGD	O2G-C2G-C3G-O3G
33	Z	101	LMG	O7-C8-C9-O8
25	a	411	PHO	C2C-C3C-CAC-CBC
24	B	611	CLA	C16-C17-C18-C19
31	D	405[B]	PL9	C9-C11-C12-C13
31	D	405[B]	PL9	C39-C41-C42-C43
35	b	601	HTG	C3'-C4'-C5'-C6'
33	c	523	LMG	C40-C41-C42-C43
24	c	516	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
24	c	514	CLA	C11-C12-C13-C14
24	B	604	CLA	C6-C7-C8-C9
24	b	623	CLA	C11-C10-C8-C9
24	A	410	CLA	CBA-CGA-O2A-C1
31	A	419[A]	PL9	C2-C3-C7-C8
27	F	103	SQD	C32-C33-C34-C35
36	c	520	DGD	CBA-CCA-CDA-CEA
24	B	614	CLA	C15-C16-C17-C18
24	A	405	CLA	C13-C15-C16-C17
24	b	610	CLA	O1A-CGA-O2A-C1
36	c	521	DGD	C6A-C7A-C8A-C9A
36	e	101	DGD	C2B-C3B-C4B-C5B
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	404	BCR	C1-C6-C7-C8
26	D	404	BCR	C5-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	C	514	BCR	C1-C6-C7-C8
26	C	514	BCR	C5-C6-C7-C8
36	C	518	DGD	CDA-CEA-CFA-CGA
36	H	102	DGD	O2G-C1B-C2B-C3B
33	C	519	LMG	C29-C30-C31-C32
26	d	404	BCR	C7-C8-C9-C10
36	C	516	DGD	C4D-C5D-C6D-O5D
33	b	629	LMG	C30-C31-C32-C33
24	b	625	CLA	C10-C11-C12-C13
36	h	102	DGD	CDB-CEB-CFB-CGB
24	C	509	CLA	C16-C17-C18-C19
24	C	513	CLA	C3-C5-C6-C7
27	F	103	SQD	C7-C8-C9-C10
35	B	625	HTG	C4-C5-C6-O6
36	C	518	DGD	C8A-C9A-CAA-CBA
33	A	421	LMG	C12-C13-C14-C15
24	b	610	CLA	CAA-CBA-CGA-O2A
37	D	408	LHG	O2-C2-C3-O3
36	c	522	DGD	C5B-C6B-C7B-C8B
24	c	514	CLA	C6-C7-C8-C10
24	B	616	CLA	C12-C13-C15-C16
24	B	612	CLA	C12-C13-C15-C16
24	c	509	CLA	C2-C3-C5-C6
24	a	410	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	a	415[A]	PL9	C43-C44-C46-C47
24	c	511	CLA	C11-C10-C8-C7
24	c	517	CLA	C11-C10-C8-C7
24	B	617	CLA	C6-C7-C8-C10
24	C	503	CLA	C8-C10-C11-C12
24	c	508	CLA	C8-C10-C11-C12
26	T	103	BCR	C13-C14-C15-C16
27	a	414	SQD	C27-C28-C29-C30
24	b	610	CLA	C10-C11-C12-C13
37	E	101	LHG	C8-C7-O7-C5
29	f	102	LMT	C4-C5-C6-C7
33	c	524	LMG	C10-C11-C12-C13
24	d	403	CLA	C15-C16-C17-C18
24	C	510	CLA	CBA-CGA-O2A-C1
33	d	413	LMG	C16-C17-C18-C19
35	d	411	HTG	C4-C5-C6-O6
29	C	521	LMT	O1'-C1-C2-C3
27	f	101	SQD	C31-C32-C33-C34
37	D	409	LHG	C25-C26-C27-C28
27	a	405	SQD	C19-C20-C21-C22
24	C	509	CLA	CBD-CGD-O2D-CED
33	A	421	LMG	C32-C33-C34-C35
24	c	508	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	D	403	CLA	CAD-CBD-CGD-O2D
24	b	625	CLA	CAD-CBD-CGD-O2D
24	C	505	CLA	CAD-CBD-CGD-O2D
24	B	602	CLA	CAD-CBD-CGD-O2D
24	c	518	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	b	623	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
29	m	103	LMT	C1-C2-C3-C4
37	e	102	LHG	C14-C15-C16-C17
31	A	419[A]	PL9	C15-C14-C16-C17
24	b	625	CLA	C4-C3-C5-C6
27	F	103	SQD	O5-C1-O6-C44
24	D	403	CLA	C8-C10-C11-C12
24	b	623	CLA	C15-C16-C17-C18
24	b	625	CLA	C2-C3-C5-C6
24	B	610	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	D	405[A]	PL9	C9-C11-C12-C13
37	L	101	LHG	C7-C8-C9-C10
36	C	516	DGD	C1B-C2B-C3B-C4B
33	A	421	LMG	O1-C7-C8-C9
33	z	101	LMG	O1-C7-C8-C9
37	D	409	LHG	C2-C3-O3-P
37	d	408	LHG	C2-C3-O3-P
37	D	409	LHG	O10-C23-O8-C6
24	b	614	CLA	C8-C10-C11-C12
33	C	520	LMG	C16-C17-C18-C19
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	A	410	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
36	c	522	DGD	O1A-C1A-O1G-C1G
33	C	519	LMG	O10-C28-O8-C9
36	h	102	DGD	C9B-CAB-CBB-CCB
37	E	101	LHG	C15-C16-C17-C18
37	e	102	LHG	O7-C5-C6-O8
37	E	101	LHG	O7-C5-C6-O8
27	L	102	SQD	O47-C45-C46-O48
36	D	406	DGD	O1G-C1G-C2G-O2G
33	c	501	LMG	O7-C8-C9-O8
33	c	523	LMG	O1-C7-C8-O7
33	c	523	LMG	O7-C8-C9-O8
27	A	416	SQD	O10-C23-O48-C46
28	a	401	GOL	O2-C2-C3-O3
37	D	407	LHG	O1-C1-C2-O2
28	v	202	GOL	O1-C1-C2-O2
27	a	414	SQD	C35-C36-C37-C38
37	d	406	LHG	C33-C34-C35-C36
36	c	520	DGD	C3A-C4A-C5A-C6A
31	A	419[B]	PL9	C15-C14-C16-C17
33	B	622	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
36	C	518	DGD	O1A-C1A-O1G-C1G
31	d	405[B]	PL9	C28-C29-C31-C32
31	A	419[A]	PL9	C13-C14-C16-C17
37	E	101	LHG	O9-C7-O7-C5
24	B	612	CLA	C14-C13-C15-C16
24	c	517	CLA	C11-C10-C8-C9
36	c	522	DGD	C2A-C3A-C4A-C5A
33	c	523	LMG	C39-C40-C41-C42
27	B	621	SQD	C5-C6-S-O8
27	F	103	SQD	C5-C6-S-O8
33	c	524	LMG	O6-C5-C6-O5
35	B	632	HTG	O5-C5-C6-O6
27	a	414	SQD	C19-C20-C21-C22
36	H	102	DGD	C3B-C4B-C5B-C6B
28	O	301	GOL	O1-C1-C2-C3
29	C	521	LMT	C1-C2-C3-C4
24	c	513	CLA	C1A-C2A-CAA-CBA
37	E	101	LHG	C23-C24-C25-C26
24	c	507	CLA	C16-C17-C18-C19
37	D	408	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O3
27	B	621	SQD	C17-C18-C19-C20
29	m	103	LMT	C11-C10-C9-C8
24	c	512	CLA	C4-C3-C5-C6
24	b	617	CLA	C13-C15-C16-C17
31	D	405[A]	PL9	C43-C44-C46-C47
37	d	406	LHG	C30-C31-C32-C33
37	E	101	LHG	C25-C26-C27-C28
36	e	101	DGD	C6A-C7A-C8A-C9A
27	a	405	SQD	C29-C30-C31-C32
37	D	408	LHG	C4-O6-P-O5
37	b	634	LHG	C4-O6-P-O5
24	B	616	CLA	C16-C17-C18-C20
33	D	413	LMG	C13-C14-C15-C16
36	C	517	DGD	CBB-CCB-CDB-CEB
31	a	415[A]	PL9	C14-C16-C17-C18
33	c	523	LMG	C36-C37-C38-C39
36	C	518	DGD	C9A-CAA-CBA-CCA
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	c	507	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	511	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
27	A	416	SQD	O5-C5-C6-S
24	B	610	CLA	CAD-CBD-CGD-O1D
29	D	401	LMT	C2B-C1B-O1B-C4'
24	c	515	CLA	CBA-CGA-O2A-C1
37	b	634	LHG	C10-C11-C12-C13
24	d	402	CLA	C11-C12-C13-C15
24	a	410	CLA	C11-C10-C8-C7
37	E	101	LHG	C7-C8-C9-C10
35	V	206	HTG	C2-C1-S1-C1'
24	A	407	CLA	C11-C10-C8-C7
29	m	102	LMT	C5-C6-C7-C8
33	c	501	LMG	C31-C32-C33-C34
27	B	621	SQD	C12-C13-C14-C15
35	V	206	HTG	C2'-C3'-C4'-C5'
24	a	409	CLA	C2C-C3C-CAC-CBC
27	a	414	SQD	C30-C31-C32-C33
27	L	102	SQD	C11-C10-C9-C8
29	D	401	LMT	C4B-C5B-C6B-O6B
37	d	408	LHG	C30-C31-C32-C33
24	C	509	CLA	C10-C11-C12-C13
27	f	101	SQD	O6-C44-C45-C46
36	e	101	DGD	C7B-C8B-C9B-CAB
33	Z	101	LMG	O1-C7-C8-C9
27	a	405	SQD	C27-C28-C29-C30
33	A	421	LMG	O1-C7-C8-O7
33	z	101	LMG	O1-C7-C8-O7
27	F	103	SQD	O47-C45-C46-O48
36	e	101	DGD	O1G-C1G-C2G-O2G
29	m	103	LMT	C2-C3-C4-C5
29	f	102	LMT	C2B-C1B-O1B-C4'
27	A	412	SQD	C16-C17-C18-C19
36	H	102	DGD	CCA-CDA-CEA-CFA
36	D	406	DGD	C3B-C4B-C5B-C6B
27	a	405	SQD	C24-C25-C26-C27
25	a	411	PHO	C2-C3-C5-C6
33	C	520	LMG	C15-C16-C17-C18
24	b	621	CLA	C8-C10-C11-C12
24	B	613	CLA	C8-C10-C11-C12
24	a	410	CLA	C6-C7-C8-C9
37	D	407	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C16-C17-C18-C19
31	a	415[B]	PL9	C14-C16-C17-C18
37	b	634	LHG	C17-C18-C19-C20
24	c	515	CLA	O1A-CGA-O2A-C1
28	O	301	GOL	O1-C1-C2-O2
27	a	405	SQD	C35-C36-C37-C38
33	A	421	LMG	C17-C18-C19-C20
24	d	401	CLA	C2C-C3C-CAC-CBC
36	c	521	DGD	C1A-C2A-C3A-C4A
37	d	407	LHG	O10-C23-O8-C6
29	m	103	LMT	C4'-C5'-C6'-O6'
27	A	412	SQD	C7-C8-C9-C10
24	A	405	CLA	C16-C17-C18-C19
37	d	408	LHG	C33-C34-C35-C36
36	c	522	DGD	C4A-C5A-C6A-C7A
24	C	502	CLA	C3-C5-C6-C7
27	B	621	SQD	C46-C45-O47-C7
27	L	102	SQD	C46-C45-O47-C7
24	b	619	CLA	C2A-CAA-CBA-CGA
24	C	511	CLA	C2-C1-O2A-CGA
24	B	602	CLA	C2-C1-O2A-CGA
24	b	623	CLA	C2-C1-O2A-CGA
36	C	518	DGD	C2A-C3A-C4A-C5A
27	L	102	SQD	C33-C34-C35-C36
36	D	406	DGD	C4B-C5B-C6B-C7B
36	e	101	DGD	C9B-CAB-CBB-CCB
24	C	509	CLA	C8-C10-C11-C12
25	a	411	PHO	C4-C3-C5-C6
26	c	519	BCR	C1-C6-C7-C8
26	c	519	BCR	C5-C6-C7-C8
24	b	618	CLA	C2-C3-C5-C6
24	C	509	CLA	C13-C15-C16-C17
24	a	409	CLA	C4C-C3C-CAC-CBC
24	b	610	CLA	C16-C17-C18-C20
29	m	103	LMT	O5'-C1'-O1'-C1
36	c	520	DGD	O6E-C1E-O5D-C6D
33	c	501	LMG	C22-C23-C24-C25
27	B	621	SQD	O47-C45-C46-O48
33	A	421	LMG	C18-C19-C20-C21
37	e	102	LHG	C13-C14-C15-C16
37	e	102	LHG	C4-O6-P-O3
37	b	634	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	A	405	CLA	C15-C16-C17-C18
36	D	406	DGD	C2B-C3B-C4B-C5B
24	B	607	CLA	C10-C11-C12-C13
36	D	406	DGD	C1G-C2G-C3G-O3G
31	a	415[B]	PL9	C45-C44-C46-C47
33	b	629	LMG	C20-C21-C22-C23
24	c	514	CLA	C11-C10-C8-C7
24	B	604	CLA	C6-C7-C8-C10
24	b	610	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
24	b	619	CLA	C12-C13-C15-C16
33	D	413	LMG	C34-C35-C36-C37
24	B	616	CLA	C11-C12-C13-C14
24	b	619	CLA	C14-C13-C15-C16
24	a	410	CLA	C11-C10-C8-C9
24	A	407	CLA	C11-C10-C8-C9
36	C	517	DGD	C1A-C2A-C3A-C4A
37	d	407	LHG	C24-C23-O8-C6
37	D	407	LHG	C33-C34-C35-C36
29	M	101	LMT	C3-C4-C5-C6
36	c	522	DGD	O6D-C5D-C6D-O5D
29	a	419	LMT	C7-C8-C9-C10
24	B	610	CLA	C4-C3-C5-C6
24	a	412	CLA	C4-C3-C5-C6
27	L	102	SQD	C7-C8-C9-C10
28	a	420	GOL	O2-C2-C3-O3
28	B	626	GOL	O2-C2-C3-O3
28	o	301	GOL	O2-C2-C3-O3
28	B	629	GOL	O1-C1-C2-O2
24	c	507	CLA	C16-C17-C18-C20
35	B	623	HTG	C4-C5-C6-O6
35	B	624	HTG	C1'-C2'-C3'-C4'
24	B	605	CLA	CBD-CGD-O2D-CED
29	m	102	LMT	C4'-C5'-C6'-O6'
26	h	101	BCR	C9-C10-C11-C12
31	A	419[A]	PL9	C19-C21-C22-C23
24	b	615	CLA	C8-C10-C11-C12
33	c	501	LMG	C30-C31-C32-C33
24	b	618	CLA	C4-C3-C5-C6
24	B	616	CLA	C4-C3-C5-C6
31	d	405[A]	PL9	C30-C29-C31-C32
24	B	616	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	A	419[B]	PL9	C13-C14-C16-C17
31	d	405[A]	PL9	C28-C29-C31-C32
24	C	513	CLA	O1A-CGA-O2A-C1
27	a	414	SQD	C17-C18-C19-C20
37	b	634	LHG	C34-C35-C36-C37
24	b	622	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C2-C1-O2A-CGA
29	M	103	LMT	C2'-C1'-O1'-C1
36	c	520	DGD	C2E-C1E-O5D-C6D
24	A	406	CLA	C2C-C3C-CAC-CBC
36	C	518	DGD	C6B-C7B-C8B-C9B
36	D	406	DGD	C1A-C2A-C3A-C4A
36	e	101	DGD	CAB-CBB-CCB-CDB
24	b	618	CLA	C3A-C2A-CAA-CBA
31	d	405[B]	PL9	C30-C29-C31-C32
31	A	419[A]	PL9	C45-C44-C46-C47
37	D	407	LHG	C11-C10-C9-C8
31	a	415[B]	PL9	C43-C44-C46-C47
33	D	413	LMG	C20-C21-C22-C23
36	c	520	DGD	C2A-C3A-C4A-C5A
24	B	608	CLA	C6-C7-C8-C9
24	B	615	CLA	C6-C7-C8-C9
36	C	517	DGD	C3A-C4A-C5A-C6A
24	C	504	CLA	C13-C15-C16-C17
27	a	414	SQD	C12-C13-C14-C15
37	E	101	LHG	C14-C15-C16-C17
24	c	511	CLA	C10-C11-C12-C13
36	h	102	DGD	O1G-C1G-C2G-C3G
33	d	413	LMG	C18-C19-C20-C21
36	H	102	DGD	C5B-C6B-C7B-C8B
33	C	519	LMG	C16-C17-C18-C19
24	b	621	CLA	C1A-C2A-CAA-CBA
24	c	511	CLA	C1A-C2A-CAA-CBA
24	C	504	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	b	623	CLA	C12-C13-C15-C16
24	c	515	CLA	C12-C13-C15-C16
28	b	606	GOL	O1-C1-C2-O2
24	b	615	CLA	C10-C11-C12-C13
36	c	521	DGD	C2A-C3A-C4A-C5A
27	A	412	SQD	O49-C7-O47-C45
24	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
37	L	101	LHG	O6-C4-C5-C6
37	b	634	LHG	O6-C4-C5-C6
27	A	416	SQD	C17-C18-C19-C20
24	c	518	CLA	C4-C3-C5-C6
36	c	521	DGD	C3A-C4A-C5A-C6A
29	D	401	LMT	C5-C6-C7-C8
33	C	519	LMG	C12-C13-C14-C15
36	H	102	DGD	C4E-C5E-C6E-O5E
24	a	412	CLA	C2-C3-C5-C6
33	c	523	LMG	C20-C21-C22-C23
24	b	610	CLA	C13-C15-C16-C17
24	C	501	CLA	C13-C15-C16-C17
33	D	413	LMG	C16-C17-C18-C19
33	c	523	LMG	C17-C18-C19-C20
37	d	408	LHG	C28-C29-C30-C31
24	B	609	CLA	C13-C15-C16-C17
24	b	610	CLA	C16-C17-C18-C19
36	c	521	DGD	C7A-C8A-C9A-CAA
29	b	630	LMT	C6-C7-C8-C9
37	d	408	LHG	C9-C10-C11-C12
31	A	419[B]	PL9	C19-C21-C22-C23
31	a	415[B]	PL9	C39-C41-C42-C43
37	D	408	LHG	C13-C14-C15-C16
35	B	623	HTG	C3'-C4'-C5'-C6'
24	A	406	CLA	C15-C16-C17-C18
24	b	623	CLA	O1D-CGD-O2D-CED
37	D	409	LHG	C9-C10-C11-C12
24	c	518	CLA	C2-C1-O2A-CGA
31	A	419[A]	PL9	C43-C44-C46-C47
24	B	616	CLA	C2-C3-C5-C6
31	A	419[B]	PL9	C43-C44-C46-C47
29	f	102	LMT	C9-C10-C11-C12
24	B	602	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	C26-C27-C28-C29
36	D	406	DGD	CBA-CCA-CDA-CEA
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C16-C17-C18-C19
26	H	101	BCR	C23-C24-C25-C30
26	b	627	BCR	C23-C24-C25-C30
27	A	416	SQD	C25-C26-C27-C28
28	b	606	GOL	O1-C1-C2-C3
28	a	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	A	412	SQD	C12-C13-C14-C15
24	B	605	CLA	C4-C3-C5-C6
33	B	622	LMG	O8-C28-C29-C30
36	C	517	DGD	C2G-C3G-O3G-C1D
36	C	517	DGD	C5D-C6D-O5D-C1E
36	D	406	DGD	C2G-C3G-O3G-C1D
33	Z	101	LMG	C8-C7-O1-C1
36	h	102	DGD	CDA-CEA-CFA-CGA
24	b	620	CLA	C8-C10-C11-C12
36	C	516	DGD	O2G-C1B-C2B-C3B
29	M	101	LMT	O5'-C1'-O1'-C1
29	D	401	LMT	O1'-C1-C2-C3
31	A	419[A]	PL9	C20-C19-C21-C22
31	A	419[A]	PL9	C40-C39-C41-C42
24	b	610	CLA	C4-C3-C5-C6
24	d	403	CLA	C4-C3-C5-C6
31	A	419[B]	PL9	C30-C29-C31-C32
27	A	412	SQD	C8-C7-O47-C45
31	A	419[A]	PL9	C9-C11-C12-C13
27	A	416	SQD	C12-C13-C14-C15
24	b	625	CLA	C12-C13-C15-C16
24	c	507	CLA	C11-C12-C13-C15
24	a	410	CLA	C6-C7-C8-C10
36	C	516	DGD	CAA-CBA-CCA-CDA
37	b	634	LHG	C13-C14-C15-C16
37	L	101	LHG	C33-C34-C35-C36
37	d	406	LHG	C34-C35-C36-C37
33	A	421	LMG	O7-C8-C9-O8
33	c	524	LMG	O7-C8-C9-O8
24	d	401	CLA	C15-C16-C17-C18
35	V	206	HTG	O5-C1-S1-C1'
37	e	102	LHG	O8-C23-C24-C25
29	a	404	LMT	C1-C2-C3-C4
31	A	419[A]	PL9	C30-C29-C31-C32
31	D	405[B]	PL9	C35-C34-C36-C37
24	c	512	CLA	C2-C3-C5-C6
37	b	634	LHG	C7-C8-C9-C10
37	d	406	LHG	C26-C27-C28-C29
33	z	101	LMG	O7-C10-C11-C12
33	C	519	LMG	C21-C22-C23-C24
29	m	102	LMT	C9-C10-C11-C12
24	c	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	d	402	CLA	C11-C12-C13-C14
24	b	625	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C10-C8-C9
24	C	507	CLA	C11-C10-C8-C9
24	c	515	CLA	C11-C12-C13-C14
36	e	101	DGD	C3A-C4A-C5A-C6A
33	A	421	LMG	C37-C38-C39-C40
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	610	CLA	C3A-C2A-CAA-CBA
24	C	512	CLA	CAA-CBA-CGA-O2A
37	d	406	LHG	O8-C23-C24-C25
27	f	101	SQD	O47-C7-C8-C9
24	C	510	CLA	CAA-CBA-CGA-O2A
33	z	101	LMG	C11-C12-C13-C14
27	B	621	SQD	C19-C20-C21-C22
27	A	416	SQD	C29-C30-C31-C32
24	C	503	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	C	501	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	b	621	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
25	a	411	PHO	CAD-CBD-CGD-O2D
24	c	517	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C16-C17-C18-C19
33	D	413	LMG	C30-C31-C32-C33
29	f	102	LMT	C1-C2-C3-C4
33	c	524	LMG	C32-C33-C34-C35
33	Z	101	LMG	O7-C10-C11-C12
27	a	405	SQD	C24-C23-O48-C46
31	A	419[B]	PL9	C20-C19-C21-C22
31	A	419[B]	PL9	C45-C44-C46-C47
31	D	405[A]	PL9	C35-C34-C36-C37
24	b	613	CLA	C3-C5-C6-C7
24	c	518	CLA	C2-C3-C5-C6
24	c	517	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	C30-C31-C32-C33
33	c	501	LMG	C18-C19-C20-C21
26	K	101	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	Y	101	BCR	C21-C22-C23-C24
27	a	405	SQD	O10-C23-O48-C46
35	B	624	HTG	C3'-C4'-C5'-C6'
24	B	614	CLA	O2A-C1-C2-C3
25	a	411	PHO	O2A-C1-C2-C3
24	b	613	CLA	O2A-C1-C2-C3
37	d	408	LHG	C11-C12-C13-C14
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	CHA-CBD-CGD-O1D
25	A	409[A]	PHO	CHA-CBD-CGD-O1D
25	A	409[A]	PHO	CHA-CBD-CGD-O2D
25	A	409[B]	PHO	CHA-CBD-CGD-O1D
25	A	409[B]	PHO	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O1D
24	d	401	CLA	CHA-CBD-CGD-O2D
25	a	418[B]	PHO	CHA-CBD-CGD-O1D
25	a	418[B]	PHO	CHA-CBD-CGD-O2D
25	a	418[A]	PHO	CHA-CBD-CGD-O2D
36	C	517	DGD	C6B-C7B-C8B-C9B
37	e	102	LHG	C28-C29-C30-C31
24	B	612	CLA	C2-C3-C5-C6
24	b	610	CLA	C3-C5-C6-C7
24	C	509	CLA	C16-C17-C18-C20
37	L	101	LHG	O7-C7-C8-C9
36	c	522	DGD	O1G-C1A-C2A-C3A
36	e	101	DGD	O2G-C1B-C2B-C3B
24	c	515	CLA	CAA-CBA-CGA-O2A
27	A	412	SQD	O6-C44-C45-O47
27	a	414	SQD	C7-C8-C9-C10
37	L	101	LHG	C18-C19-C20-C21
29	F	101	LMT	C1-C2-C3-C4
24	C	513	CLA	C5-C6-C7-C8
37	E	101	LHG	O8-C23-C24-C25
36	D	406	DGD	O1G-C1A-C2A-C3A
28	V	203	GOL	O2-C2-C3-O3
24	d	401	CLA	C4C-C3C-CAC-CBC
24	c	517	CLA	C3-C5-C6-C7
35	B	624	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
29	f	102	LMT	O5B-C1B-O1B-C4'
31	A	419[A]	PL9	C28-C29-C31-C32
24	A	407	CLA	C12-C13-C15-C16
37	D	409	LHG	C33-C34-C35-C36
35	b	632	HTG	C4-C5-C6-O6
24	B	614	CLA	CAA-CBA-CGA-O2A
24	B	613	CLA	CAA-CBA-CGA-O2A
33	c	501	LMG	C13-C14-C15-C16
24	c	510	CLA	C11-C12-C13-C14
24	b	615	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C12-C13-C14
36	h	102	DGD	O1B-C1B-C2B-C3B
26	k	101	BCR	C9-C10-C11-C12
29	M	103	LMT	C2B-C1B-O1B-C4'
33	b	629	LMG	C29-C28-O8-C9
35	B	623	HTG	C4'-C5'-C6'-C7'
24	a	409	CLA	C2A-CAA-CBA-CGA
27	a	405	SQD	C12-C13-C14-C15
37	d	408	LHG	C25-C26-C27-C28
37	b	634	LHG	C14-C15-C16-C17
33	z	101	LMG	C16-C17-C18-C19
26	K	101	BCR	C7-C8-C9-C34
33	z	101	LMG	O9-C10-C11-C12
37	d	406	LHG	O10-C23-C24-C25
24	b	615	CLA	C15-C16-C17-C18
36	C	518	DGD	C8B-C9B-CAB-CBB
29	m	103	LMT	C5-C6-C7-C8
24	C	506	CLA	C4-C3-C5-C6
37	b	634	LHG	O1-C1-C2-C3
37	D	407	LHG	C26-C27-C28-C29
25	a	418[B]	PHO	C2C-C3C-CAC-CBC
24	C	513	CLA	C1A-C2A-CAA-CBA
37	L	101	LHG	C16-C17-C18-C19
27	B	621	SQD	C14-C15-C16-C17
24	C	509	CLA	O1D-CGD-O2D-CED
24	B	614	CLA	C2-C1-O2A-CGA
24	C	510	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA
37	e	102	LHG	O10-C23-C24-C25
37	b	634	LHG	O7-C7-C8-C9
24	c	506	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	b	623	CLA	C2A-CAA-CBA-CGA
24	c	510	CLA	CBD-CGD-O2D-CED
31	a	415[A]	PL9	C2-C3-C7-C8
24	C	512	CLA	CAA-CBA-CGA-O1A
27	f	101	SQD	O49-C7-C8-C9
24	B	605	CLA	C13-C15-C16-C17
24	a	409	CLA	C15-C16-C17-C18
29	C	521	LMT	C3-C4-C5-C6
36	C	518	DGD	CBB-CCB-CDB-CEB
36	H	102	DGD	C8A-C9A-CAA-CBA
24	C	510	CLA	CAA-CBA-CGA-O1A
36	c	522	DGD	O1A-C1A-C2A-C3A
29	m	103	LMT	C2'-C1'-O1'-C1
24	C	502	CLA	C13-C15-C16-C17
31	a	415[A]	PL9	C3-C7-C8-C9
24	b	611	CLA	C16-C17-C18-C20
24	b	622	CLA	CAA-CBA-CGA-O2A
33	C	520	LMG	C13-C14-C15-C16
36	D	406	DGD	C5B-C6B-C7B-C8B
36	D	406	DGD	O1A-C1A-C2A-C3A
24	c	517	CLA	CAA-CBA-CGA-O1A
36	e	101	DGD	O1B-C1B-C2B-C3B
33	A	421	LMG	O6-C5-C6-O5
24	A	405	CLA	C2A-CAA-CBA-CGA
24	C	507	CLA	C2A-CAA-CBA-CGA
27	F	103	SQD	C33-C34-C35-C36
24	C	510	CLA	C8-C10-C11-C12
29	F	101	LMT	C2-C3-C4-C5
36	h	102	DGD	CBB-CCB-CDB-CEB
27	L	102	SQD	C23-C24-C25-C26
24	b	610	CLA	CAA-CBA-CGA-O1A
33	Z	101	LMG	O9-C10-C11-C12
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
27	L	102	SQD	O5-C5-C6-S
24	B	608	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
37	d	406	LHG	C7-C8-C9-C10
36	c	521	DGD	CCB-CDB-CEB-CFB
27	f	101	SQD	C30-C31-C32-C33

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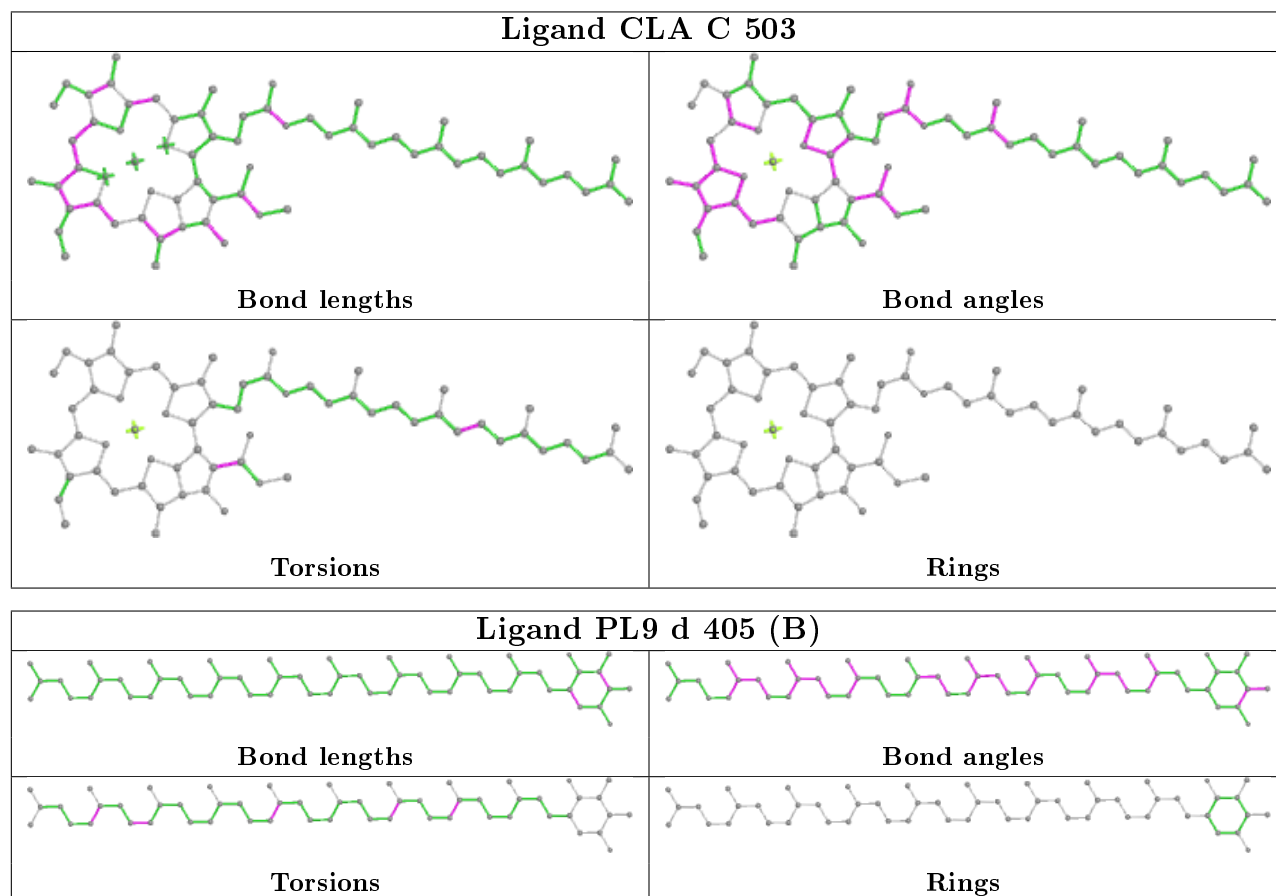
Mol	Chain	Res	Type	Atoms
24	C	512	CLA	C6-C7-C8-C9
24	C	504	CLA	C14-C13-C15-C16
36	C	516	DGD	C6A-C7A-C8A-C9A
37	L	101	LHG	O9-C7-C8-C9
36	H	102	DGD	O1B-C1B-C2B-C3B
36	c	521	DGD	O2G-C1B-C2B-C3B
33	b	629	LMG	O8-C28-C29-C30
24	d	401	CLA	C13-C15-C16-C17
24	C	507	CLA	C5-C6-C7-C8
33	D	413	LMG	C12-C13-C14-C15
27	a	414	SQD	C10-C11-C12-C13
24	c	506	CLA	CAA-CBA-CGA-O2A
33	D	413	LMG	O7-C10-C11-C12
24	C	505	CLA	CAA-CBA-CGA-O2A
37	d	408	LHG	O8-C23-C24-C25
24	c	511	CLA	C13-C15-C16-C17
37	E	101	LHG	O10-C23-C24-C25
31	D	405[B]	PL9	C30-C29-C31-C32
31	d	405[B]	PL9	C18-C19-C21-C22
24	A	410	CLA	C6-C7-C8-C10
24	A	410	CLA	C12-C13-C15-C16
24	C	501	CLA	C11-C12-C13-C15
24	b	619	CLA	C11-C12-C13-C15
36	C	517	DGD	CAA-CBA-CCA-CDA
37	E	101	LHG	O7-C7-C8-C9
36	e	101	DGD	C6B-C7B-C8B-C9B
37	E	101	LHG	O9-C7-C8-C9
24	B	613	CLA	CAA-CBA-CGA-O1A
24	c	515	CLA	CAA-CBA-CGA-O1A
29	m	102	LMT	O1'-C1-C2-C3
36	C	517	DGD	O2G-C1B-C2B-C3B
36	C	516	DGD	O6E-C1E-O5D-C6D
24	A	410	CLA	C8-C10-C11-C12
24	A	410	CLA	C15-C16-C17-C18
33	b	629	LMG	O10-C28-O8-C9
37	b	634	LHG	C11-C12-C13-C14
24	c	510	CLA	CAA-CBA-CGA-O2A
24	C	501	CLA	CAA-CBA-CGA-O2A
24	b	622	CLA	CAA-CBA-CGA-O1A
24	b	623	CLA	C8-C10-C11-C12
36	c	521	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

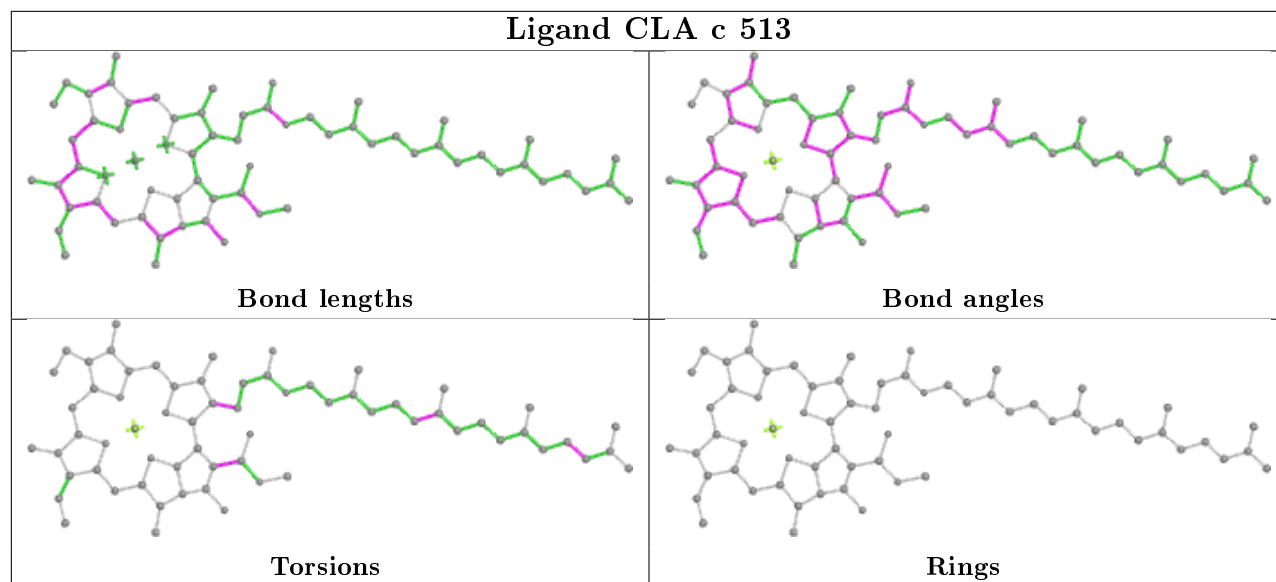
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	f	101	SQD	0	1

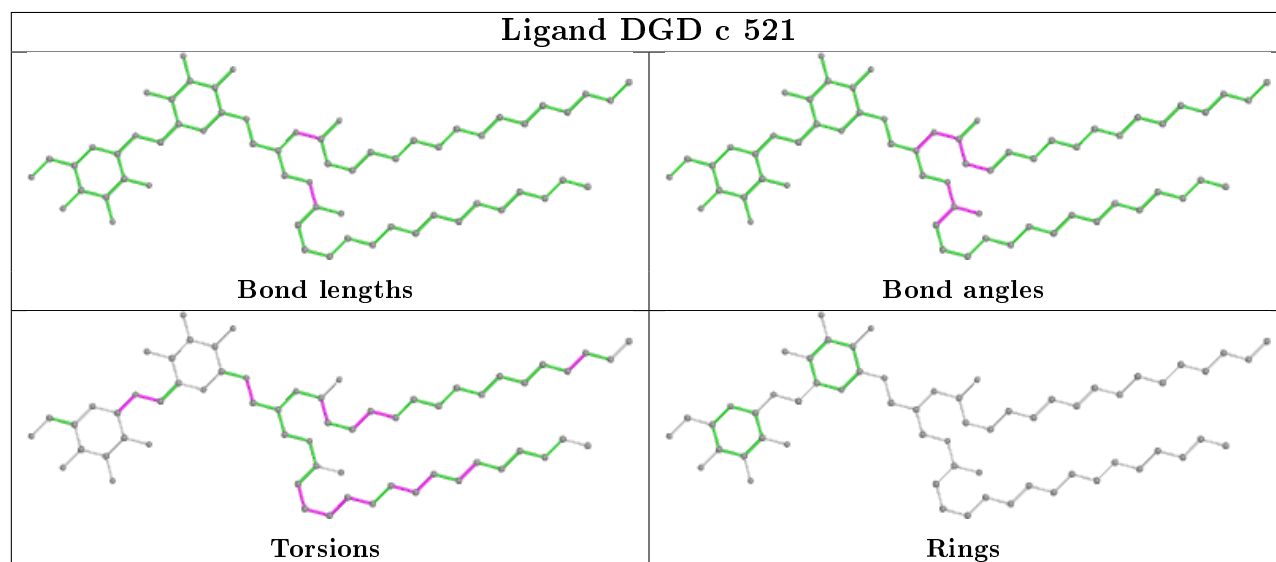
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



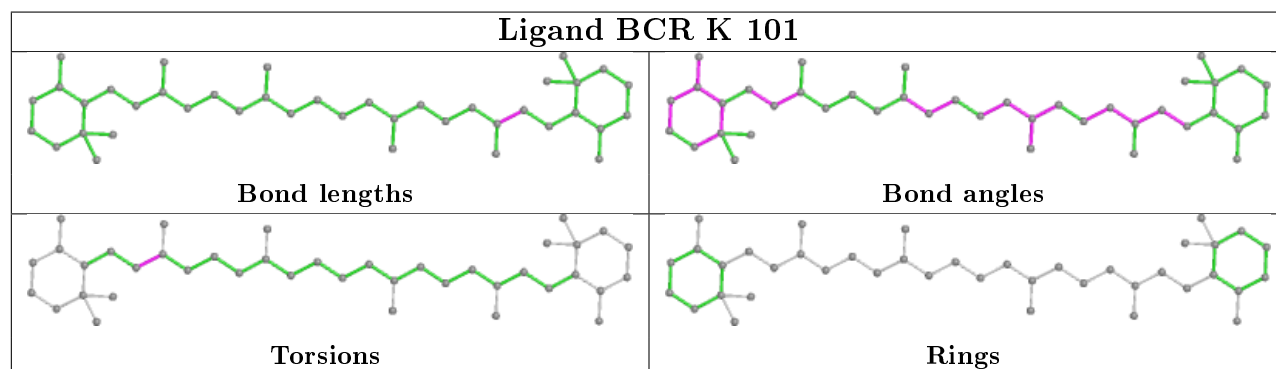
## Ligand CLA c 513



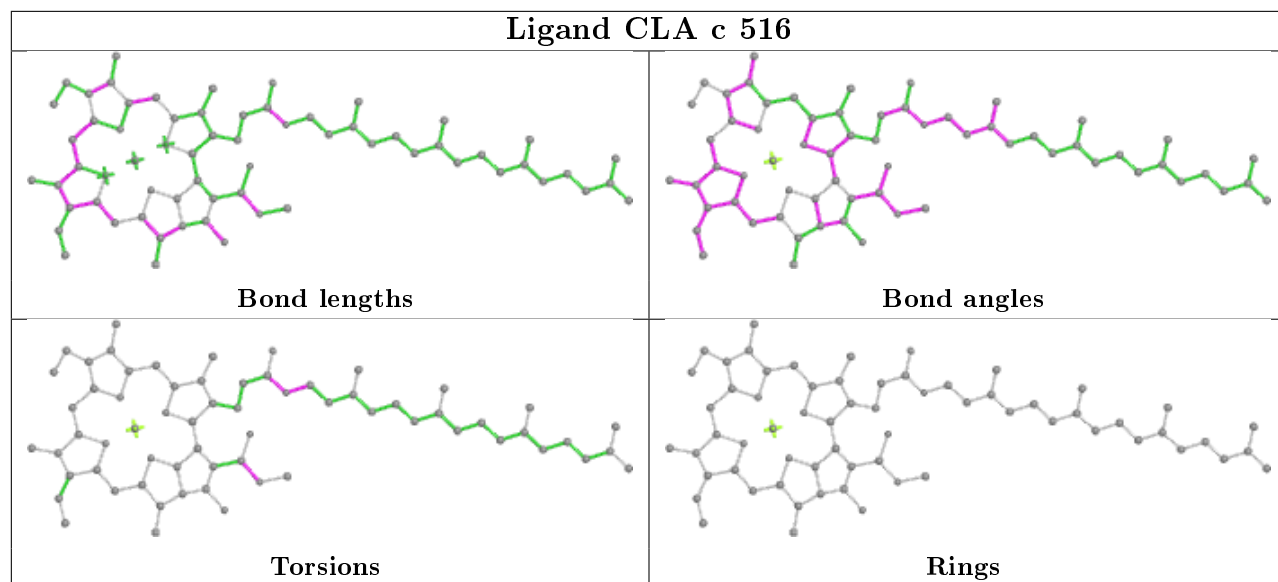
## Ligand DGD c 521



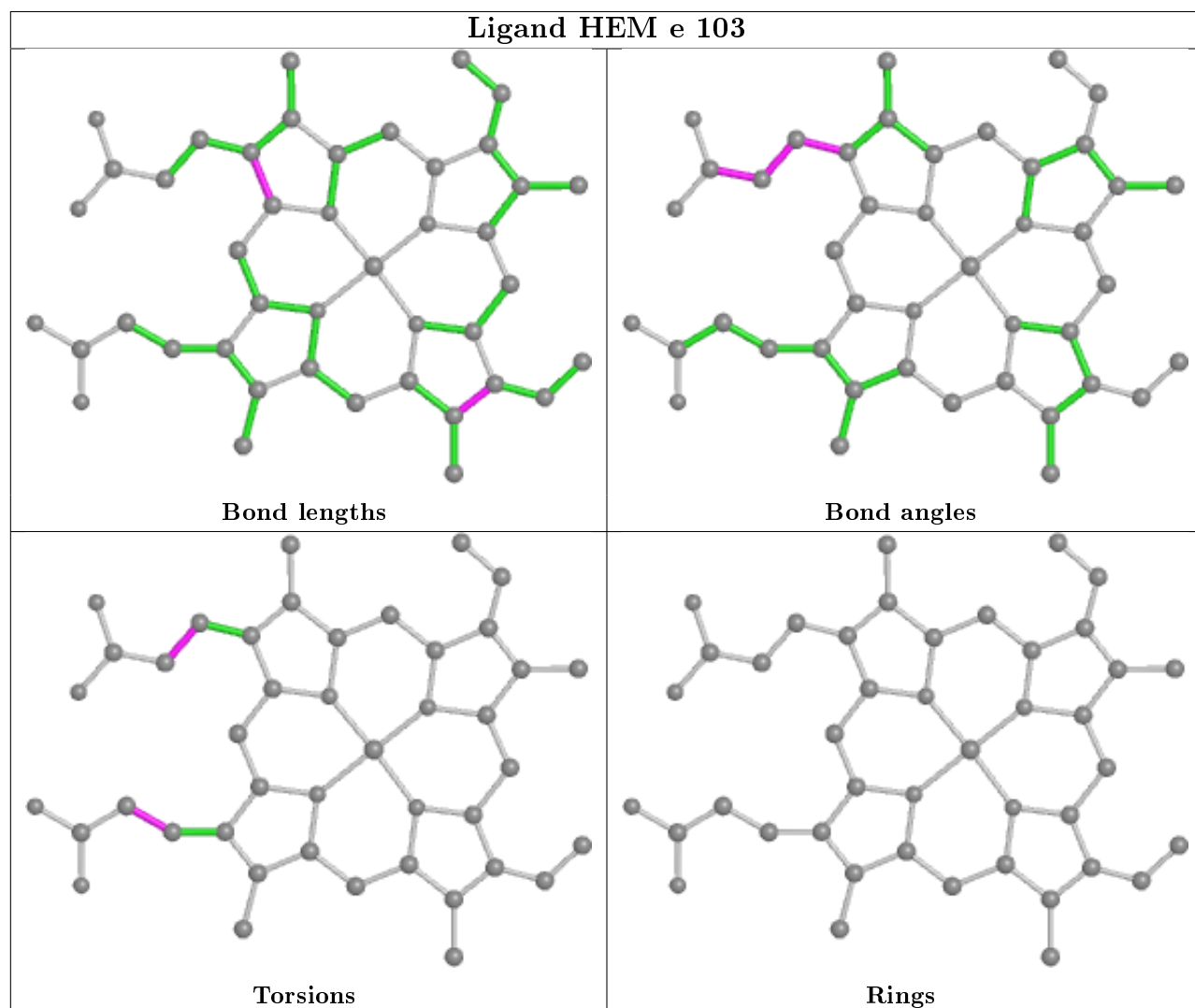
## Ligand BCR K 101

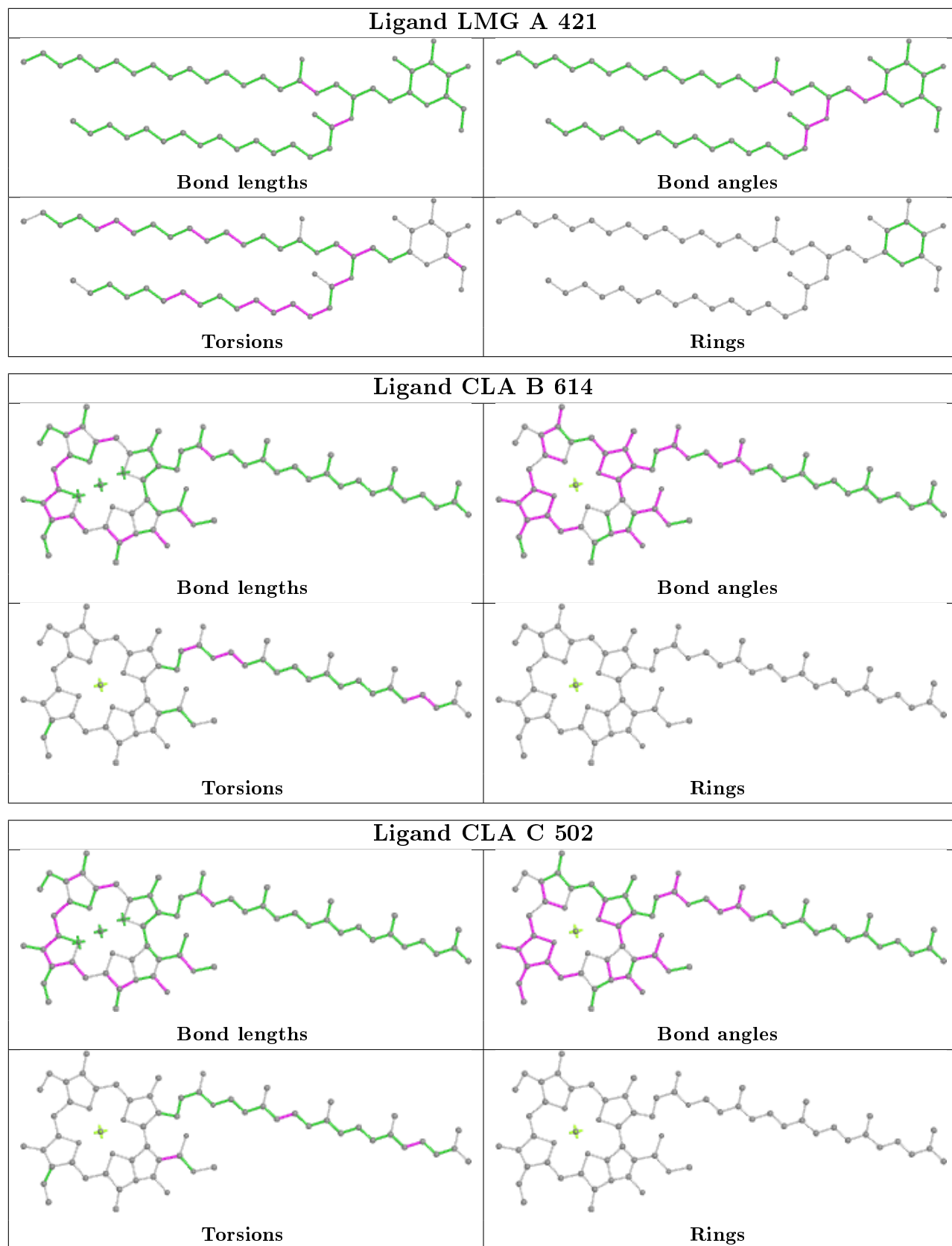


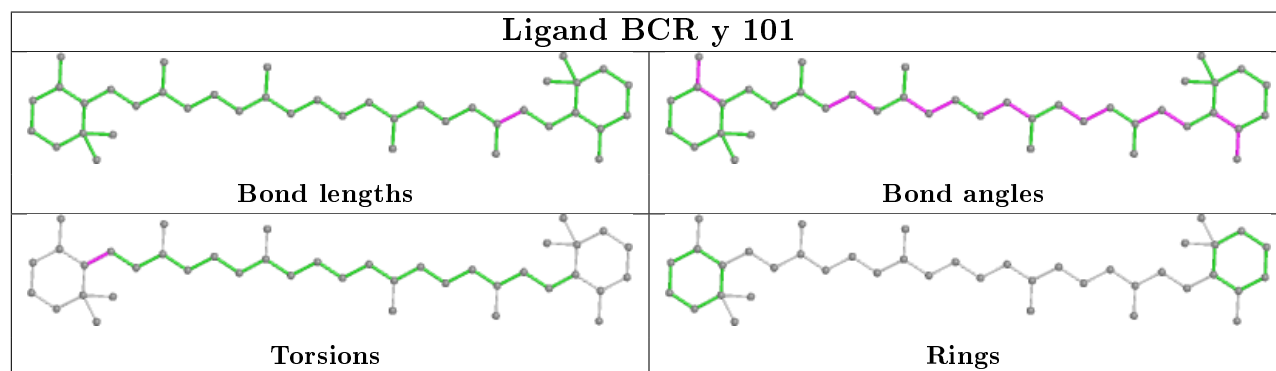
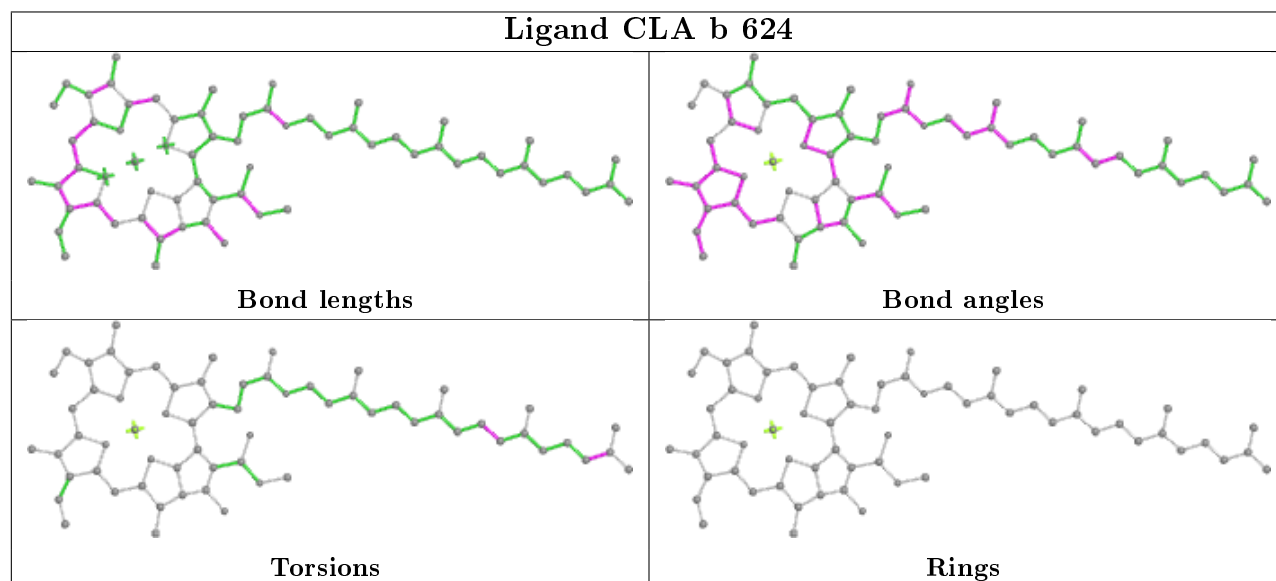
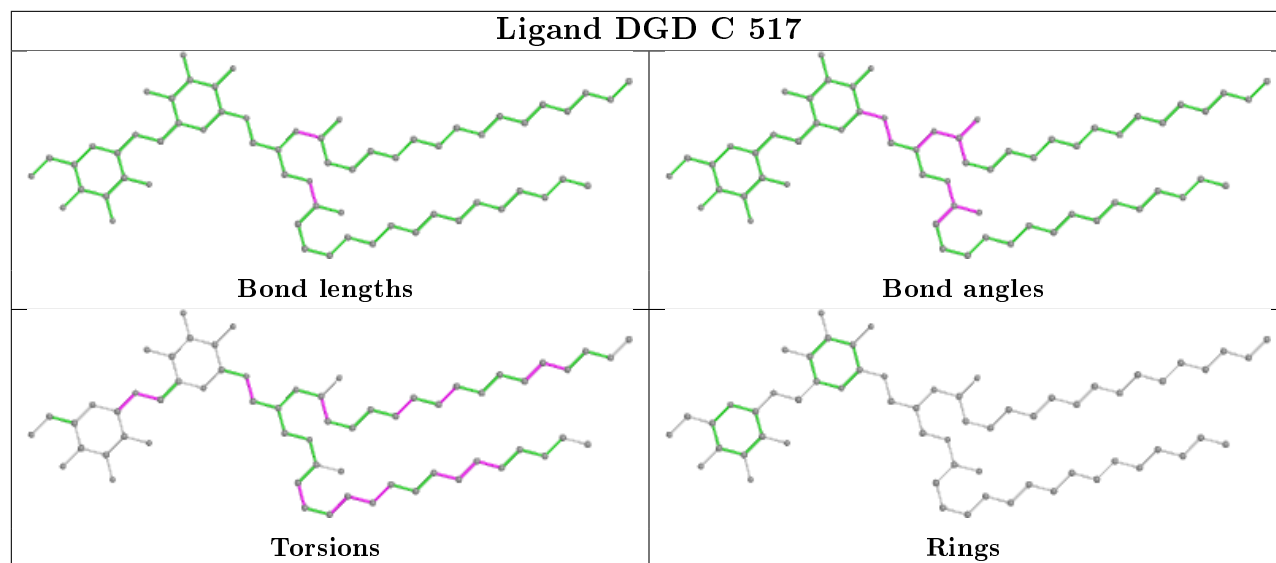
## Ligand CLA c 516

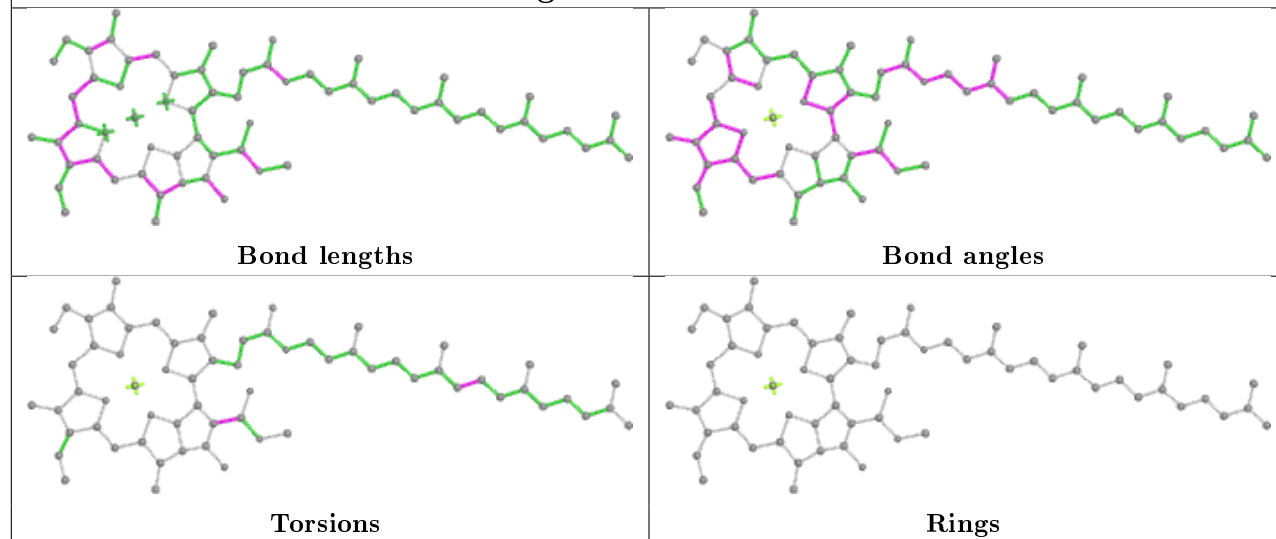
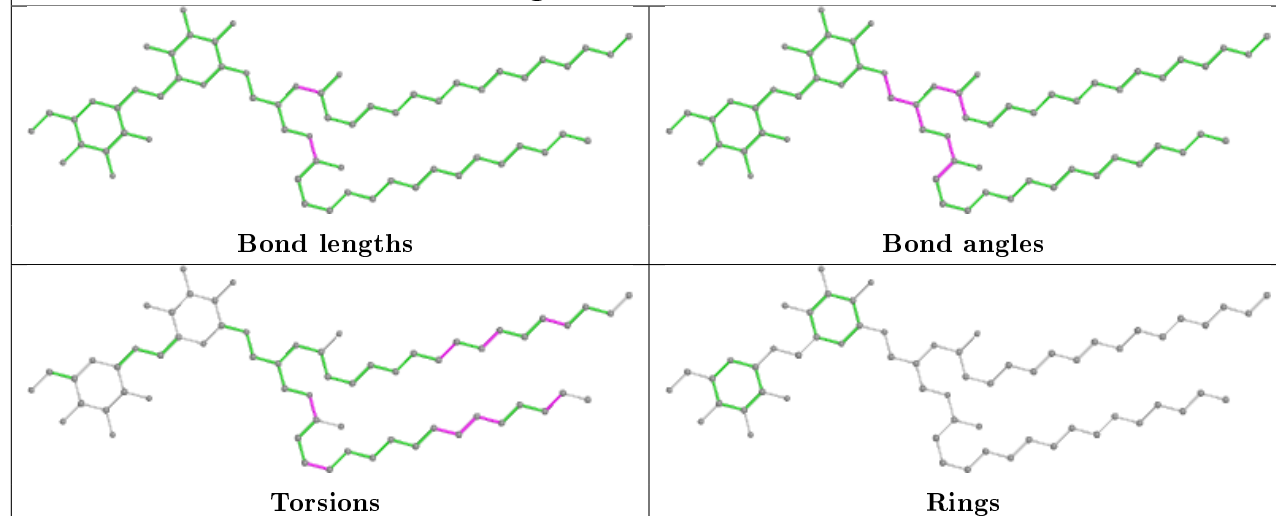


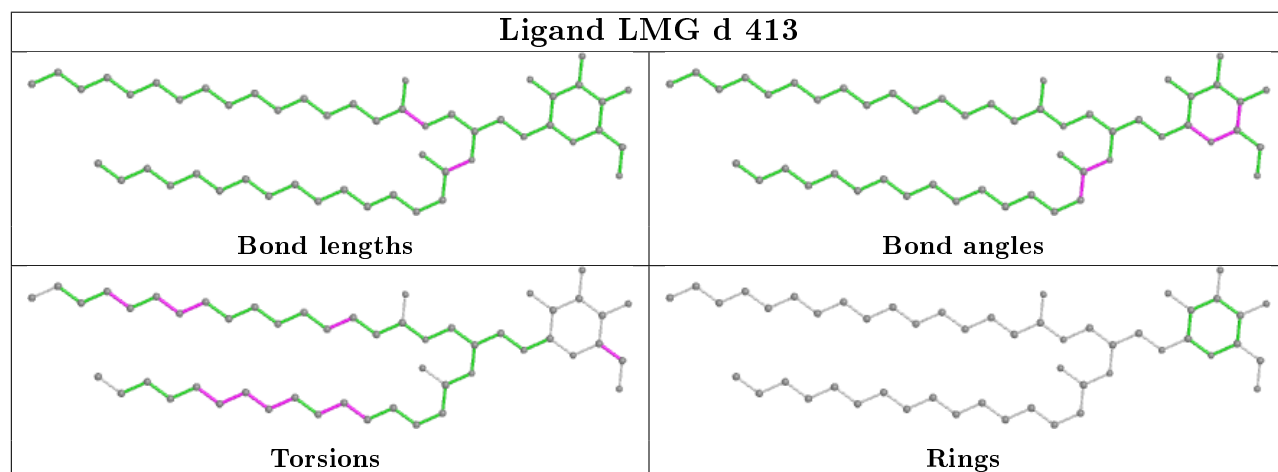
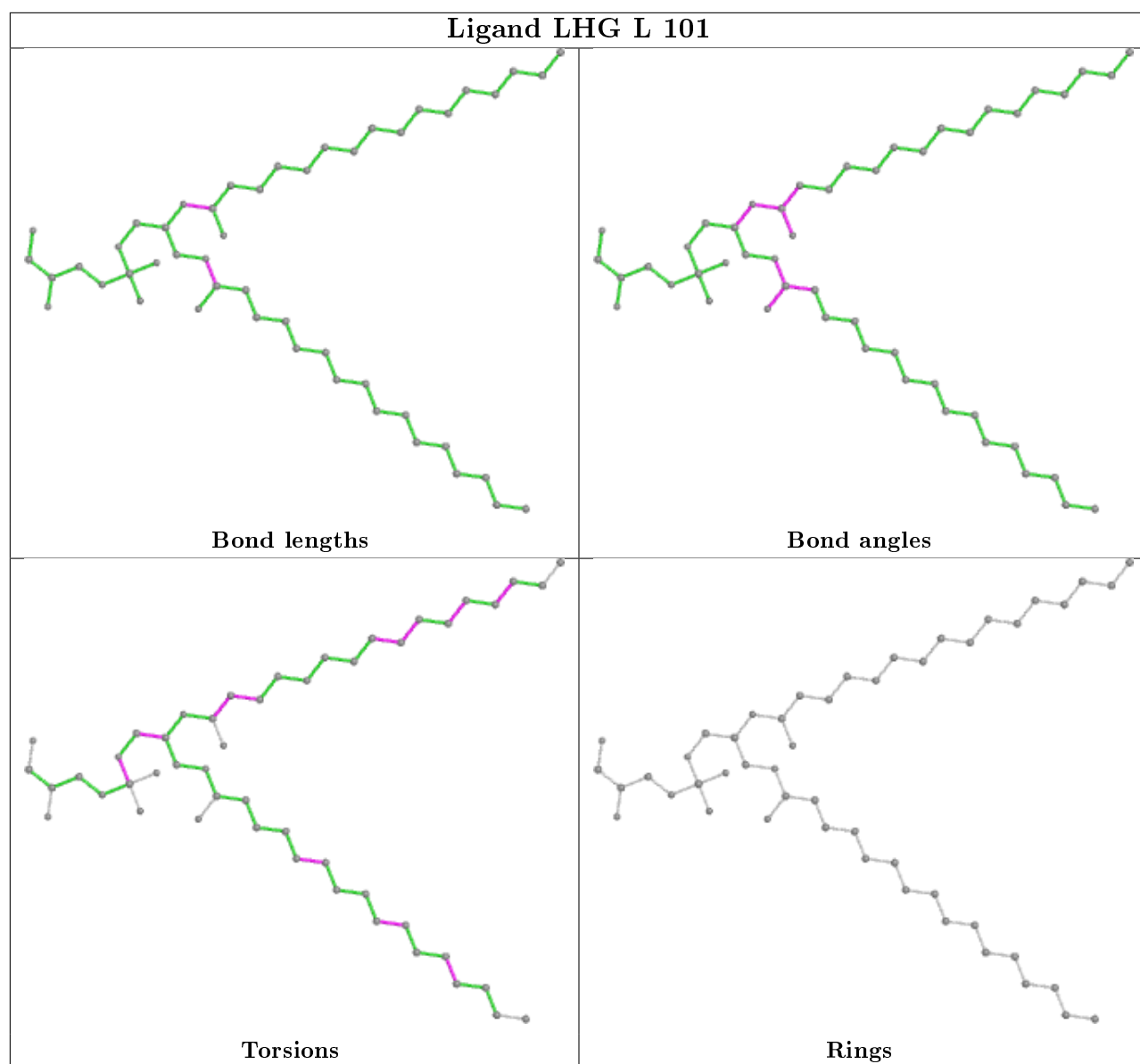
## Ligand HEM e 103



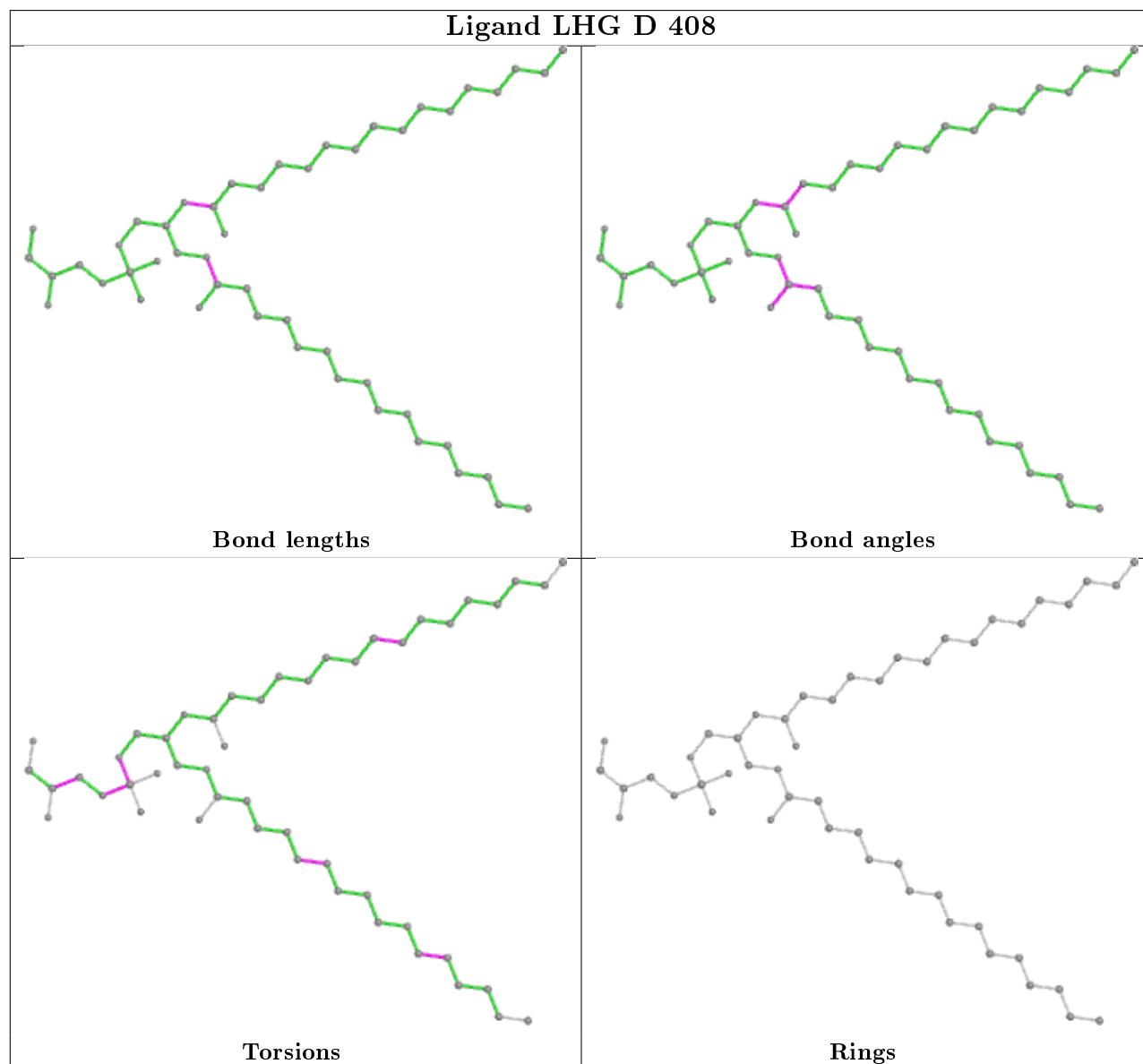
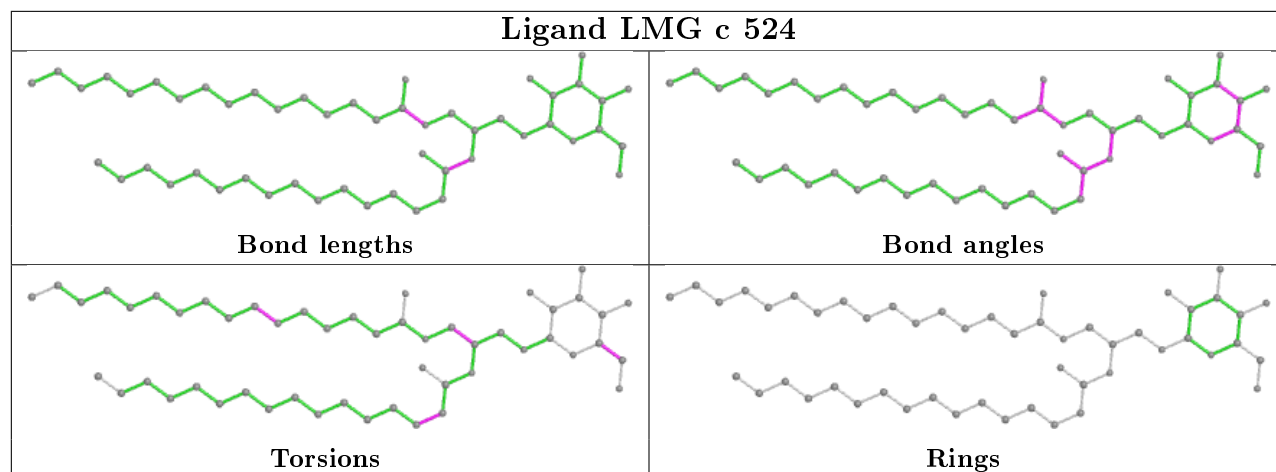


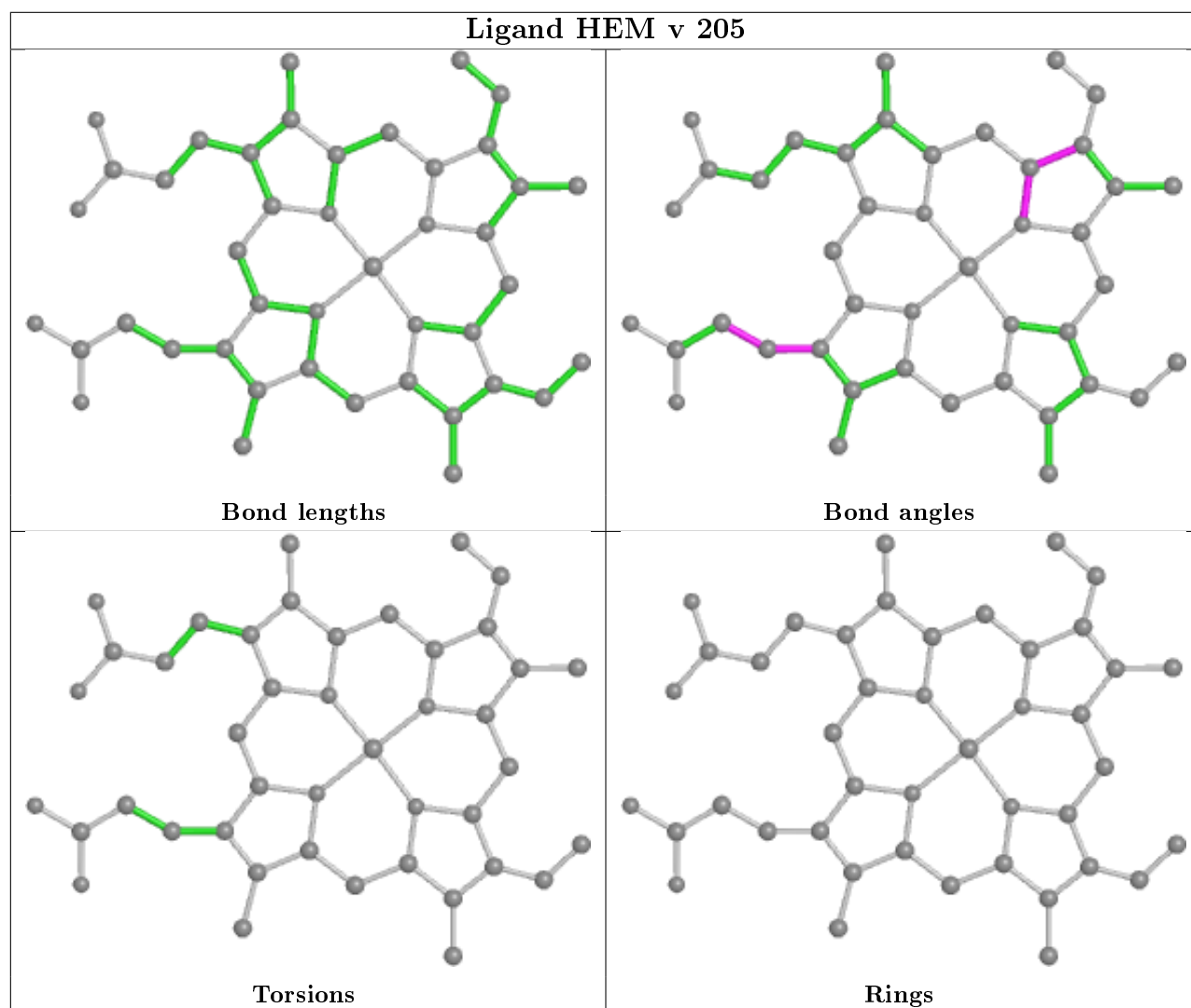
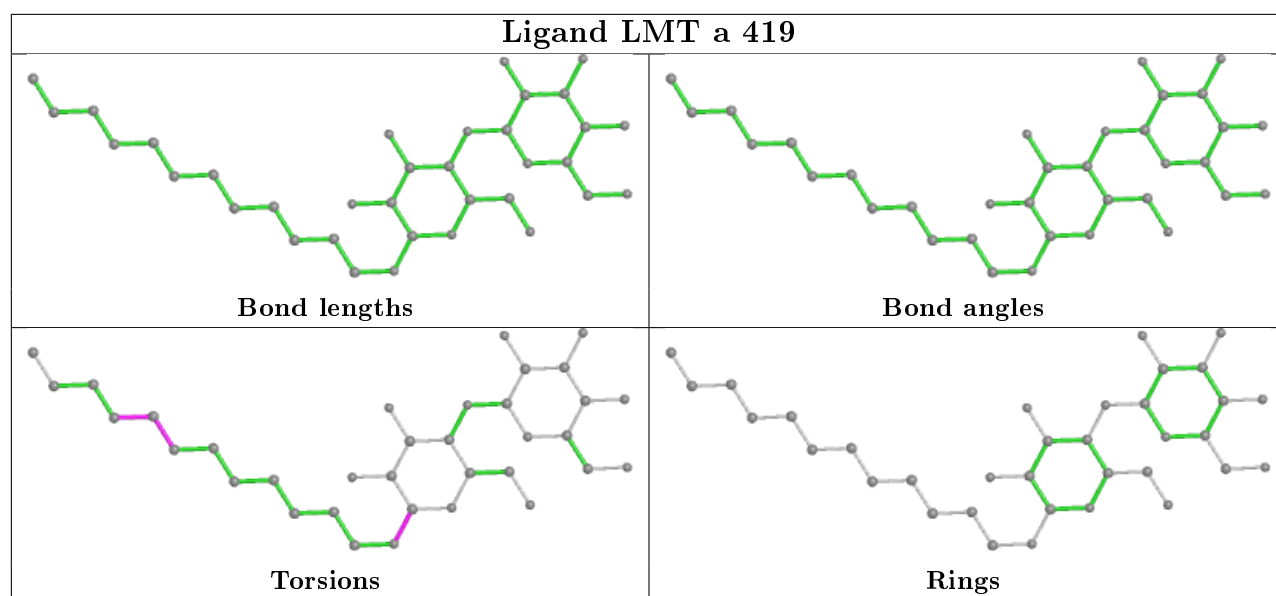


**Ligand CLA c 508****Ligand DGD C 518**

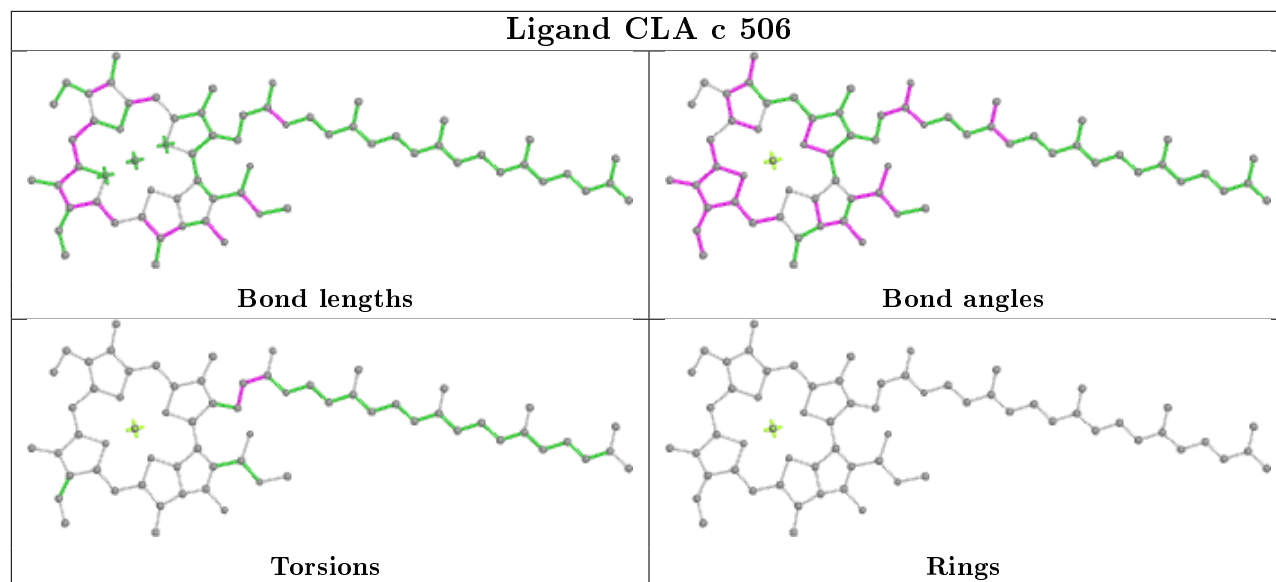




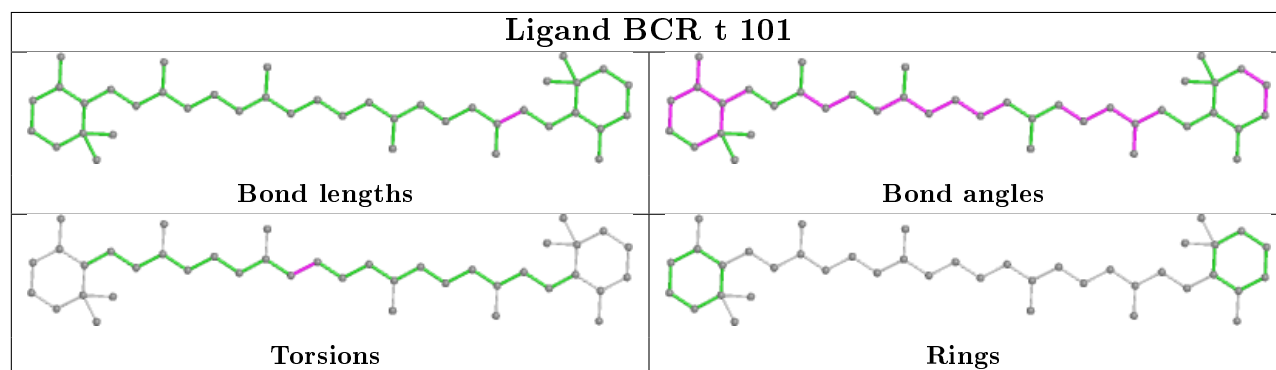




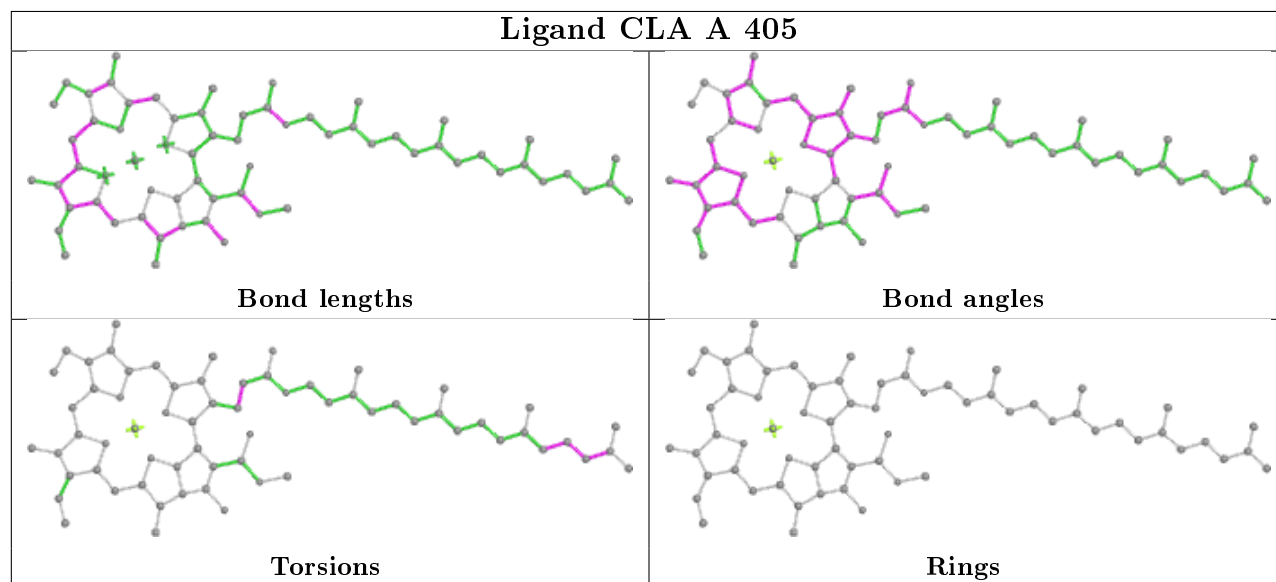
## Ligand CLA c 506



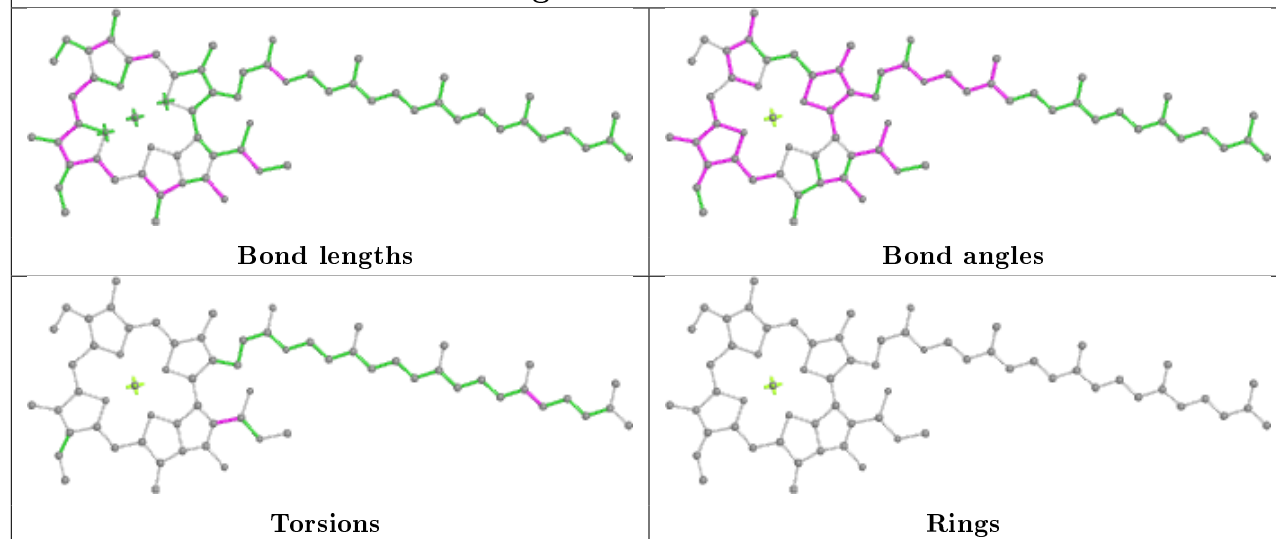
## Ligand BCR t 101



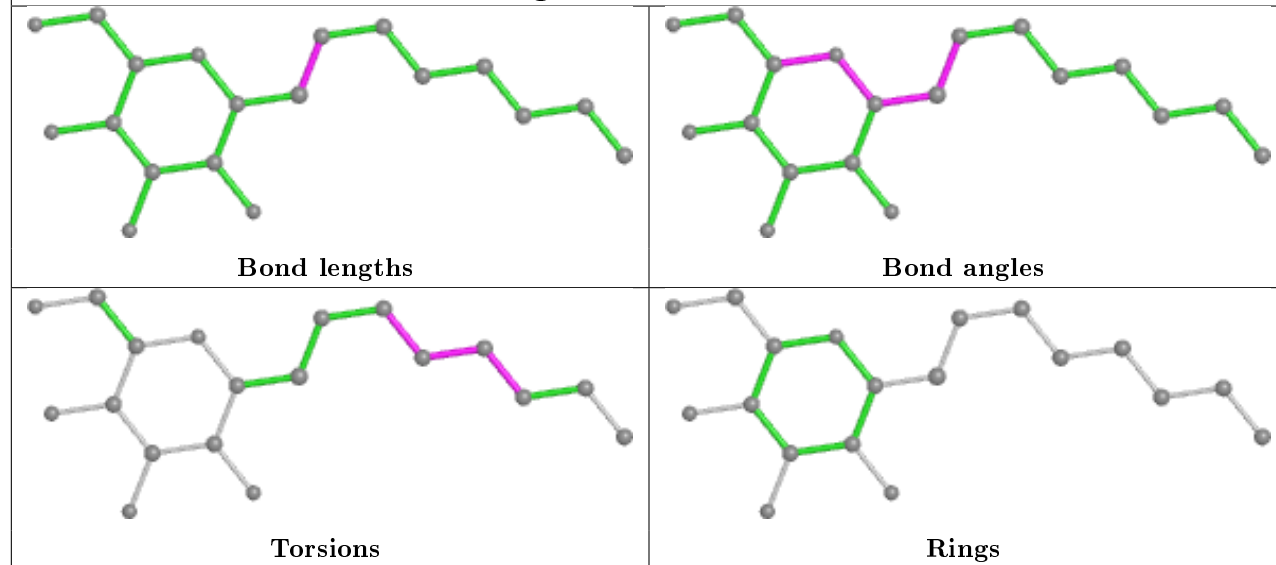
## Ligand CLA A 405



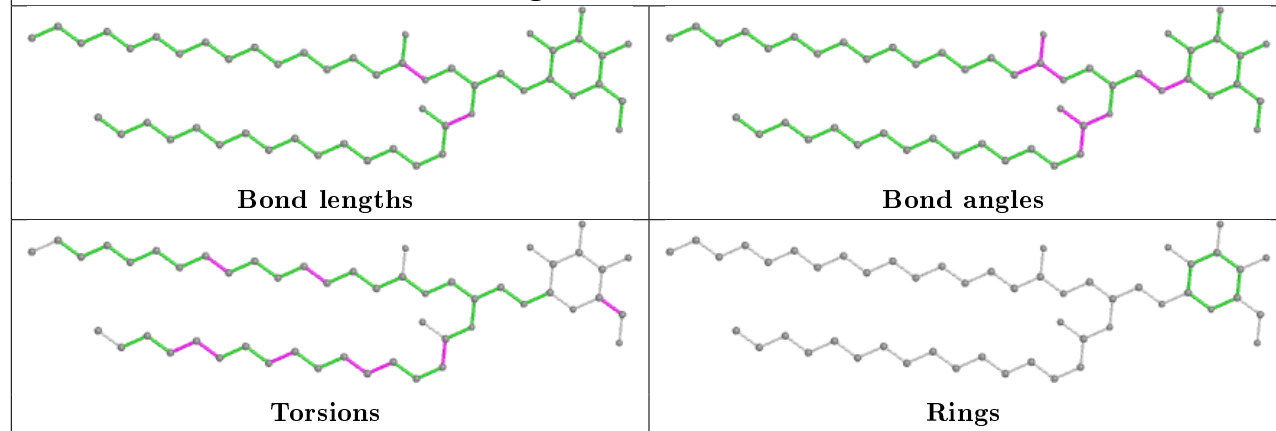
## Ligand CLA B 603



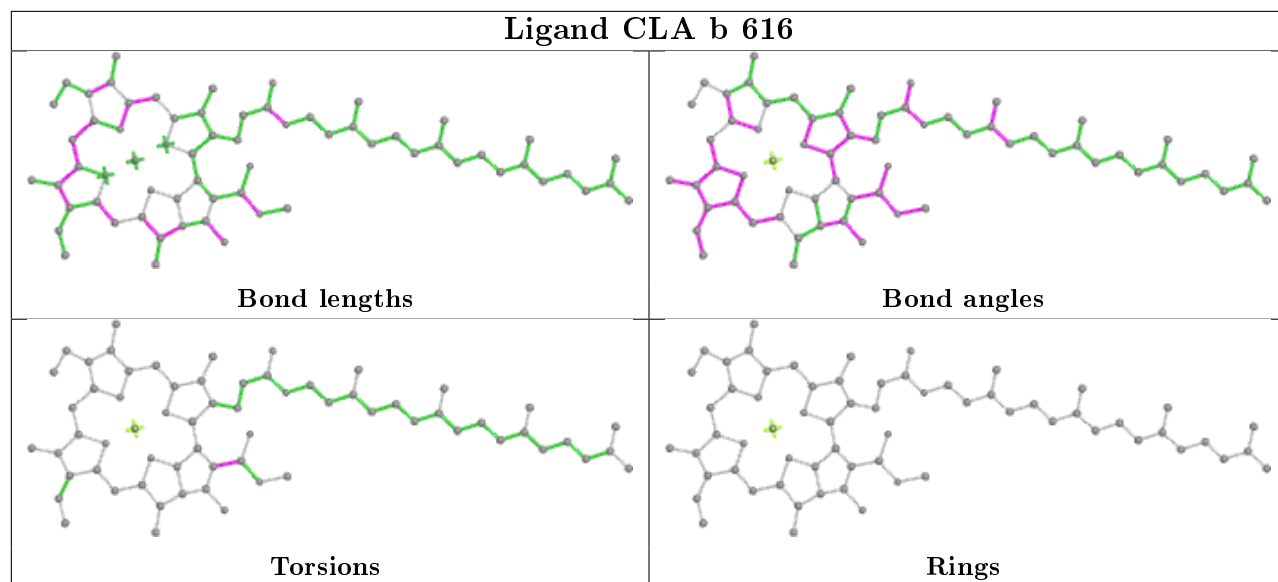
## Ligand HTG b 601



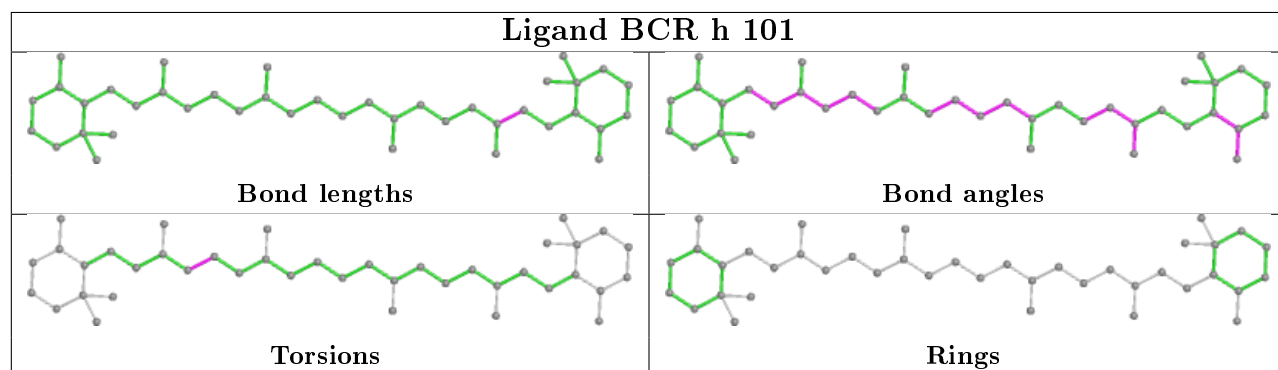
## Ligand LMG D 413



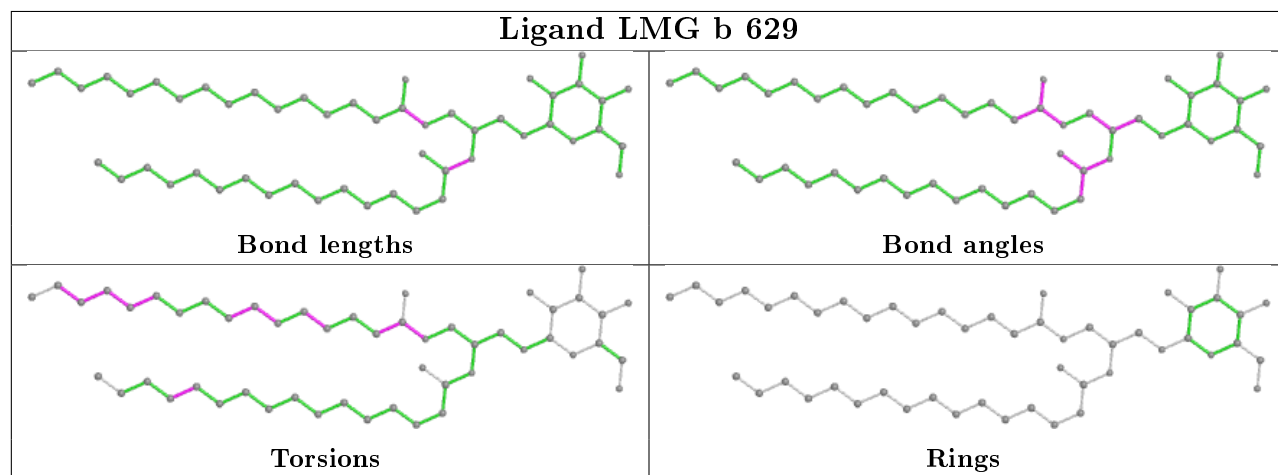
## Ligand CLA b 616



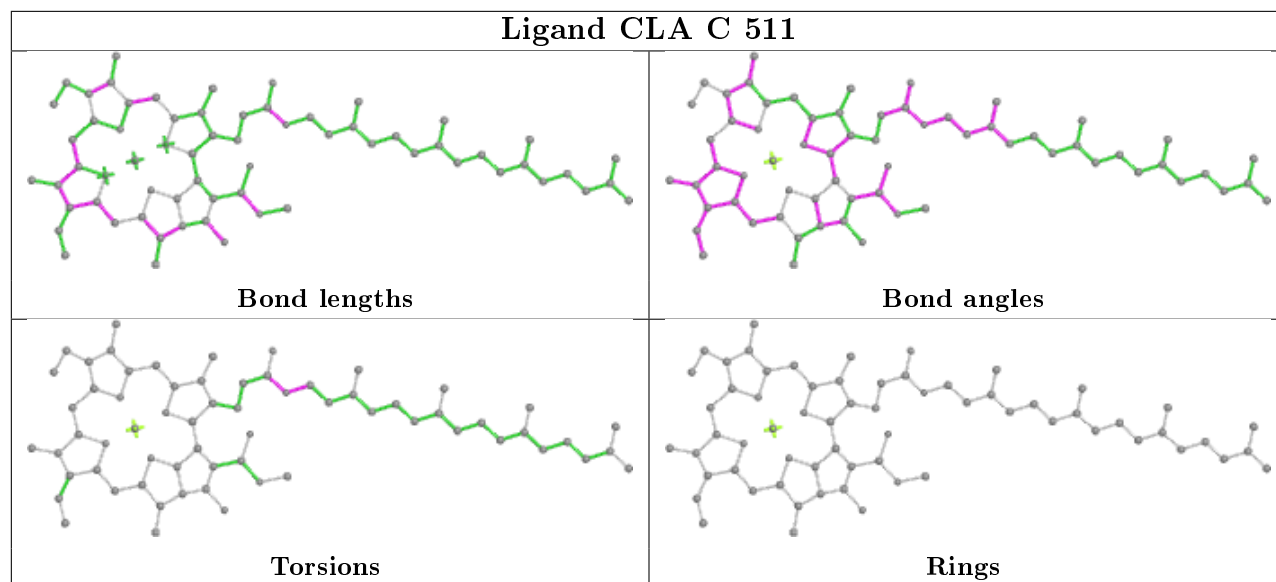
## Ligand BCR h 101



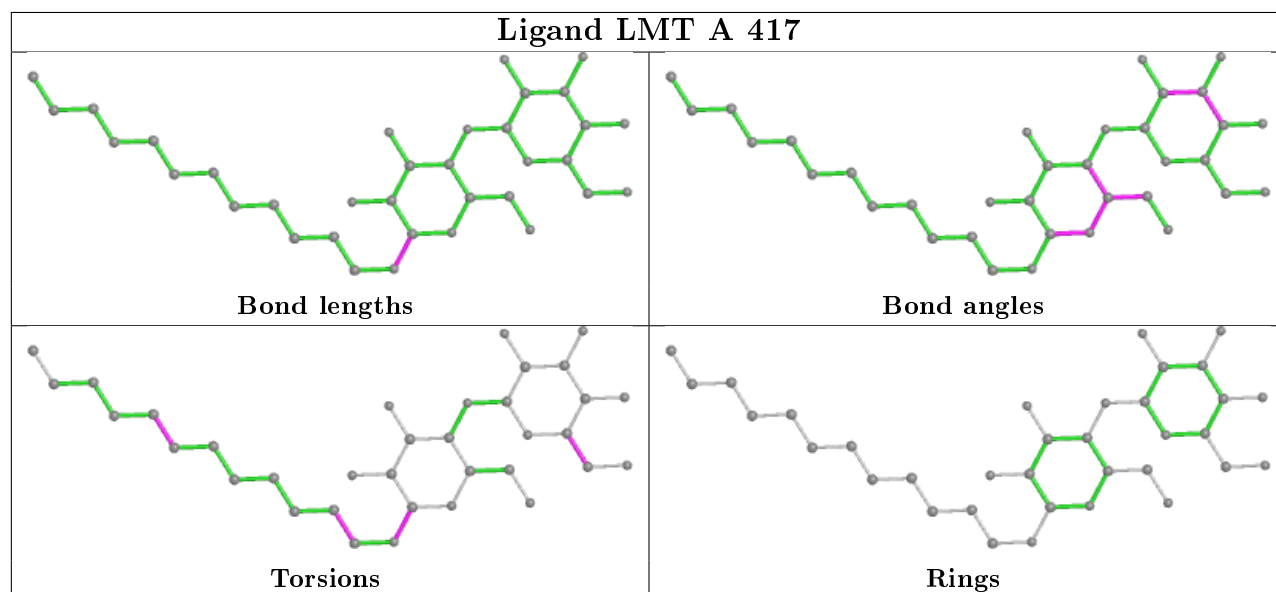
## Ligand LMG b 629



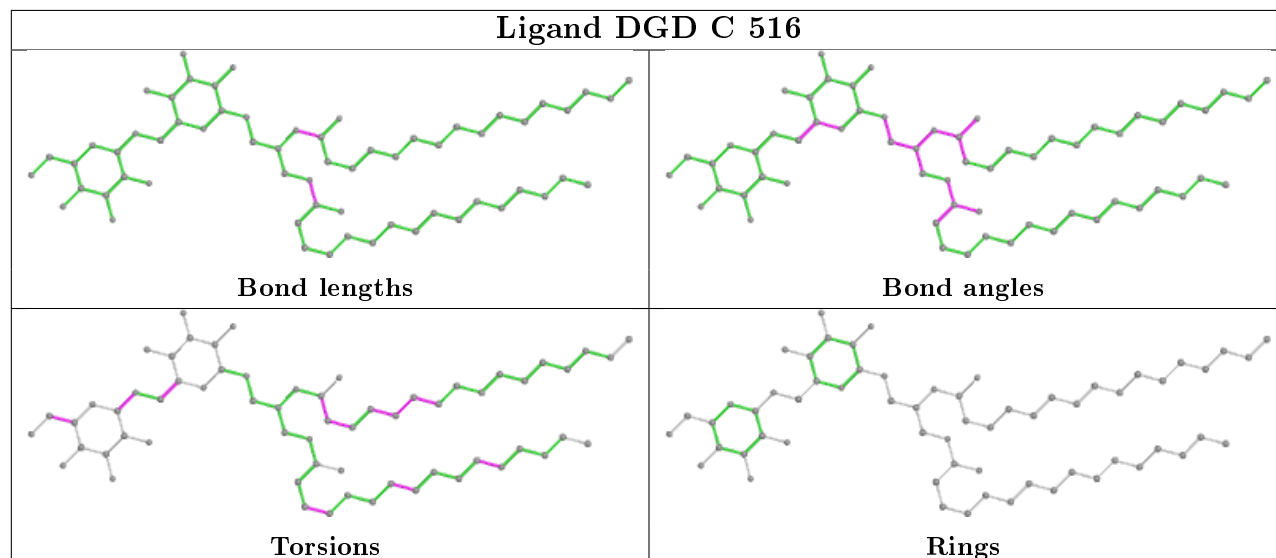
## Ligand CLA C 511

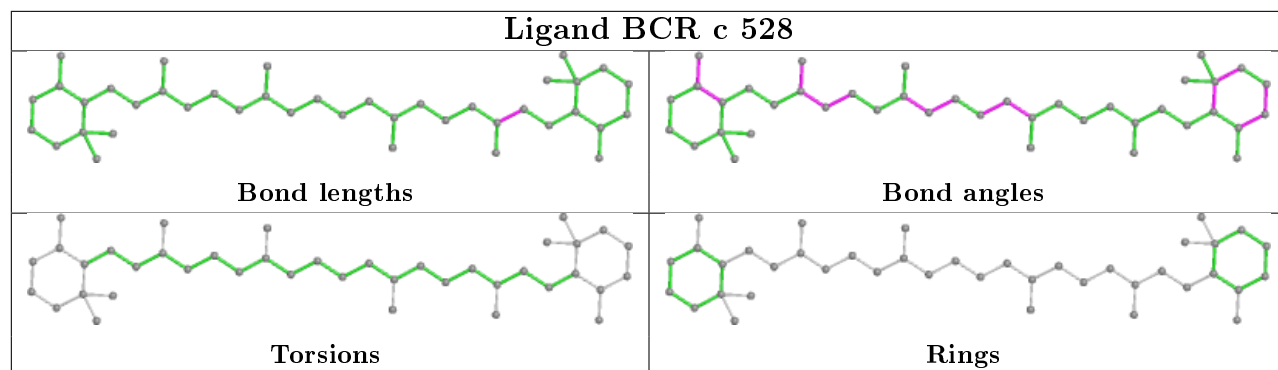
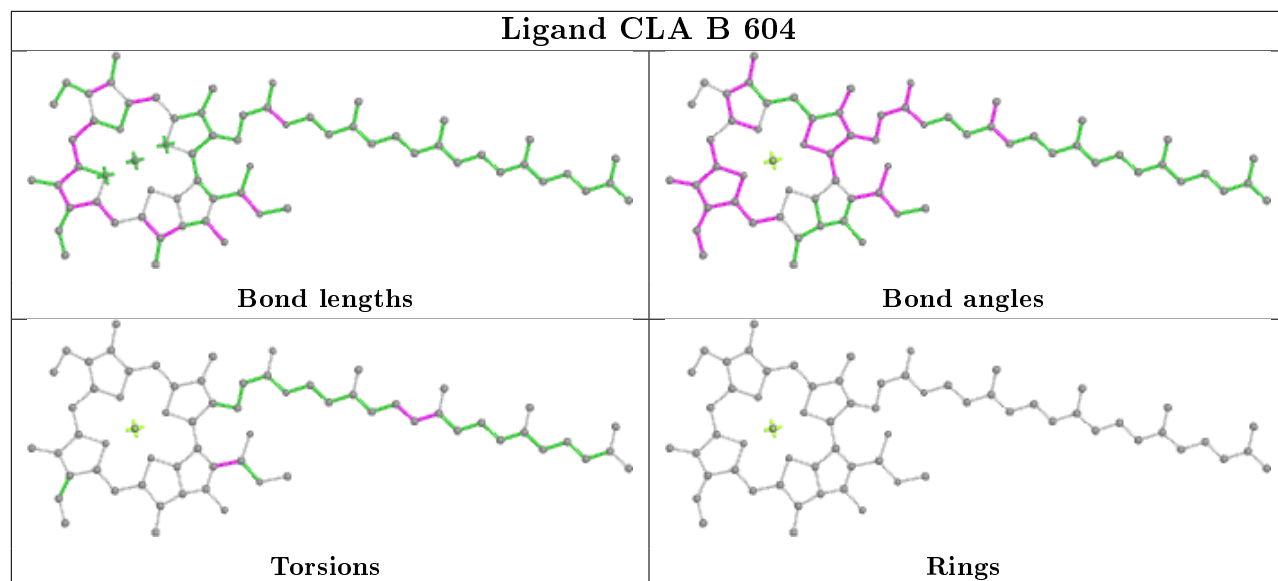
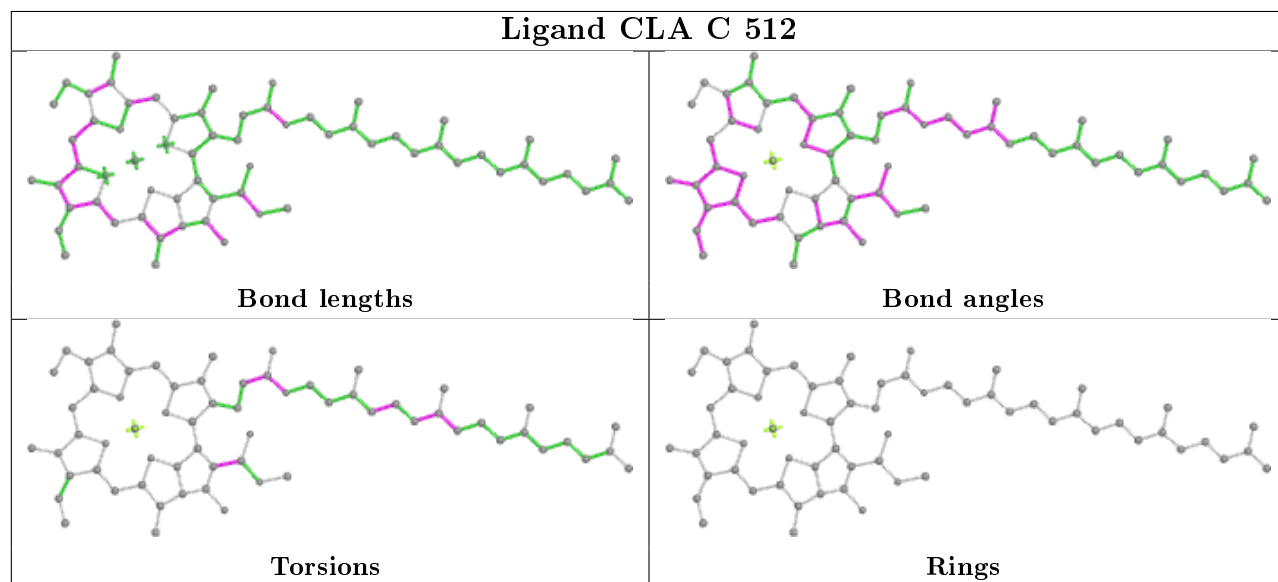


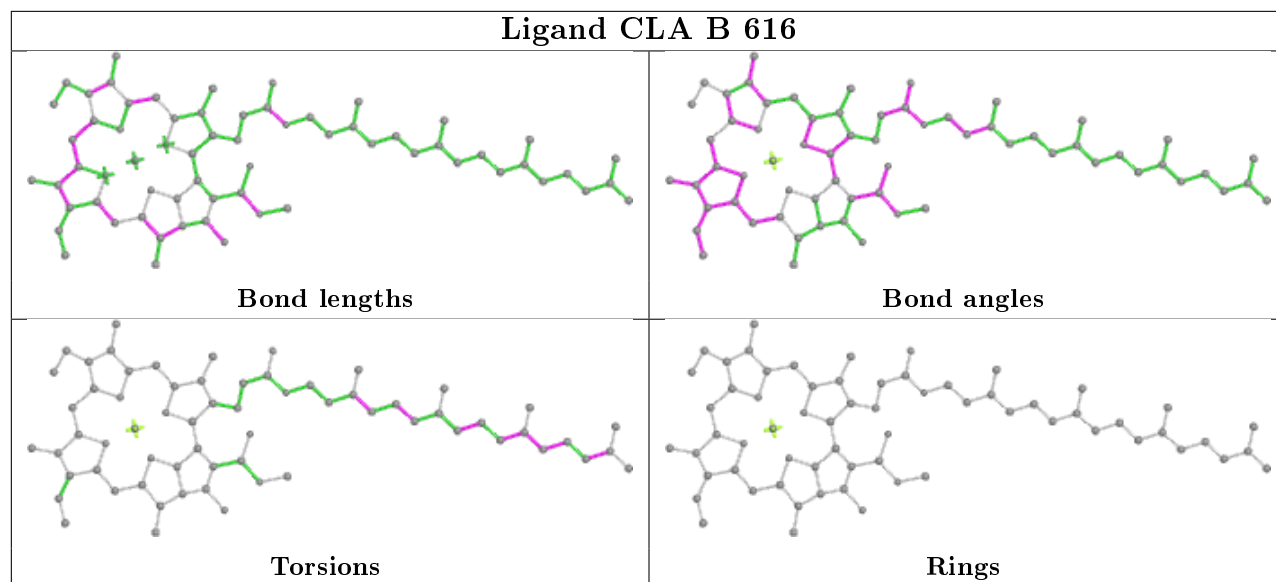
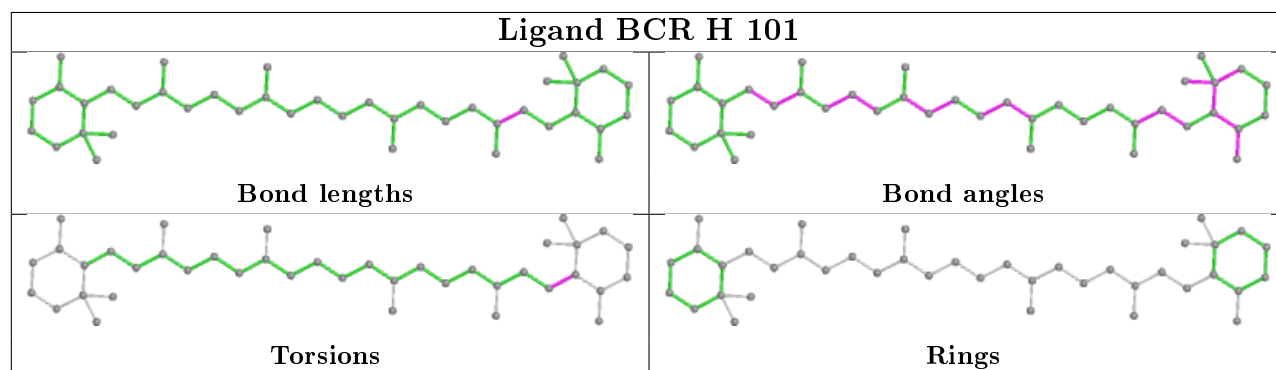
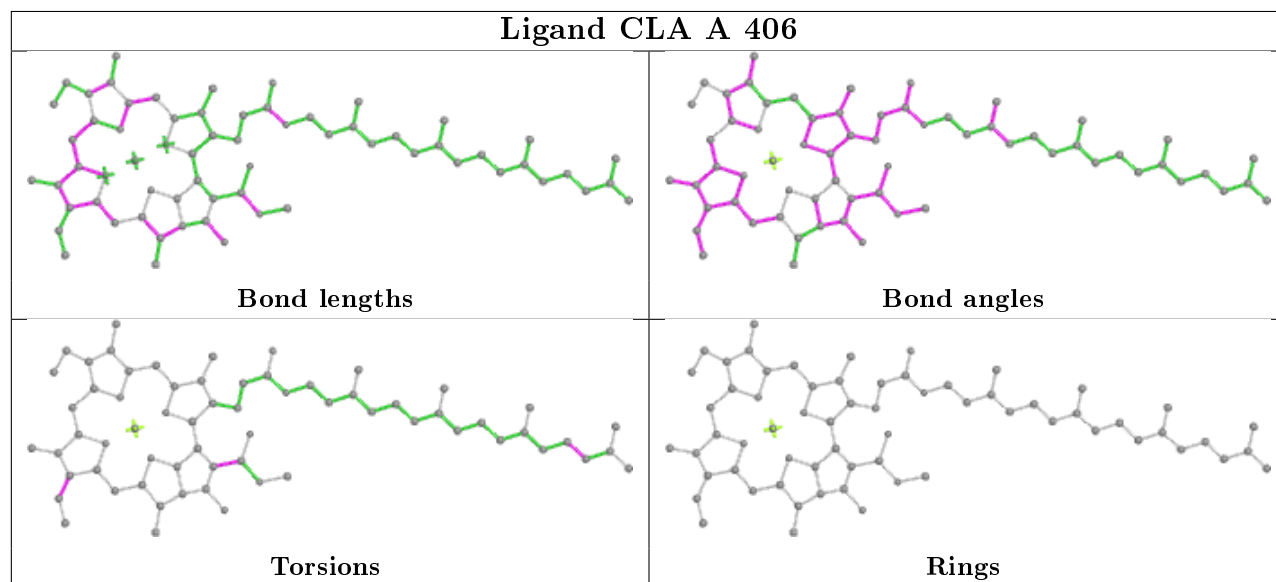
## Ligand LMT A 417



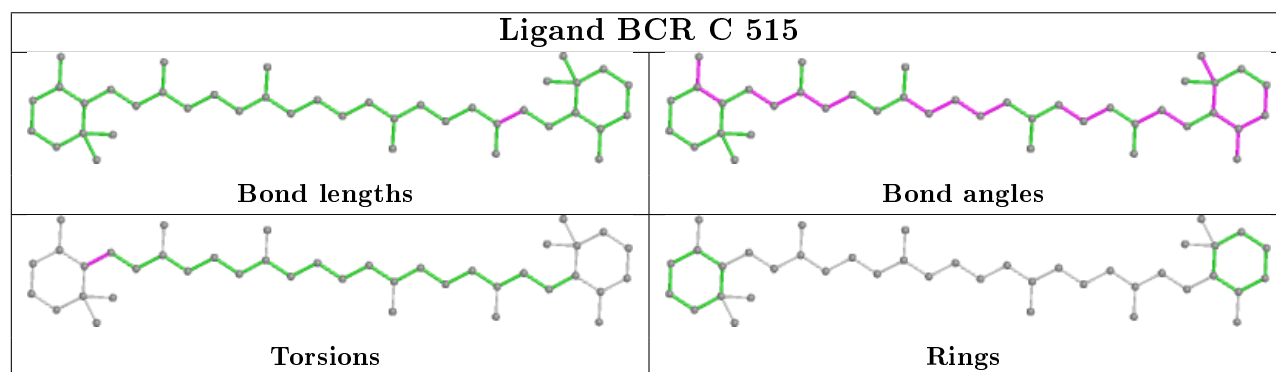
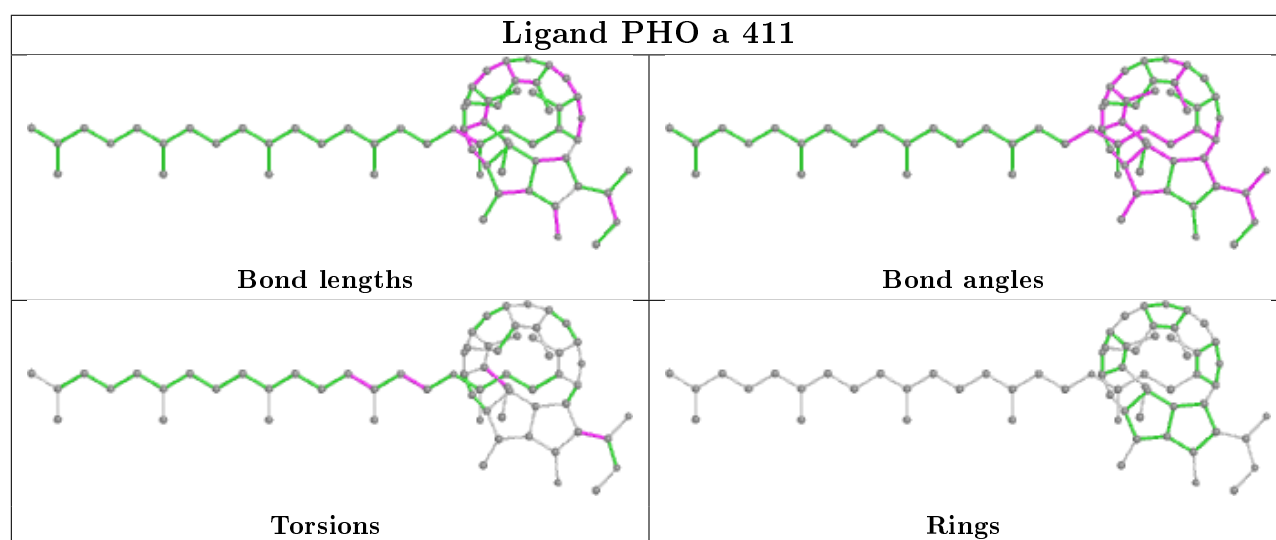
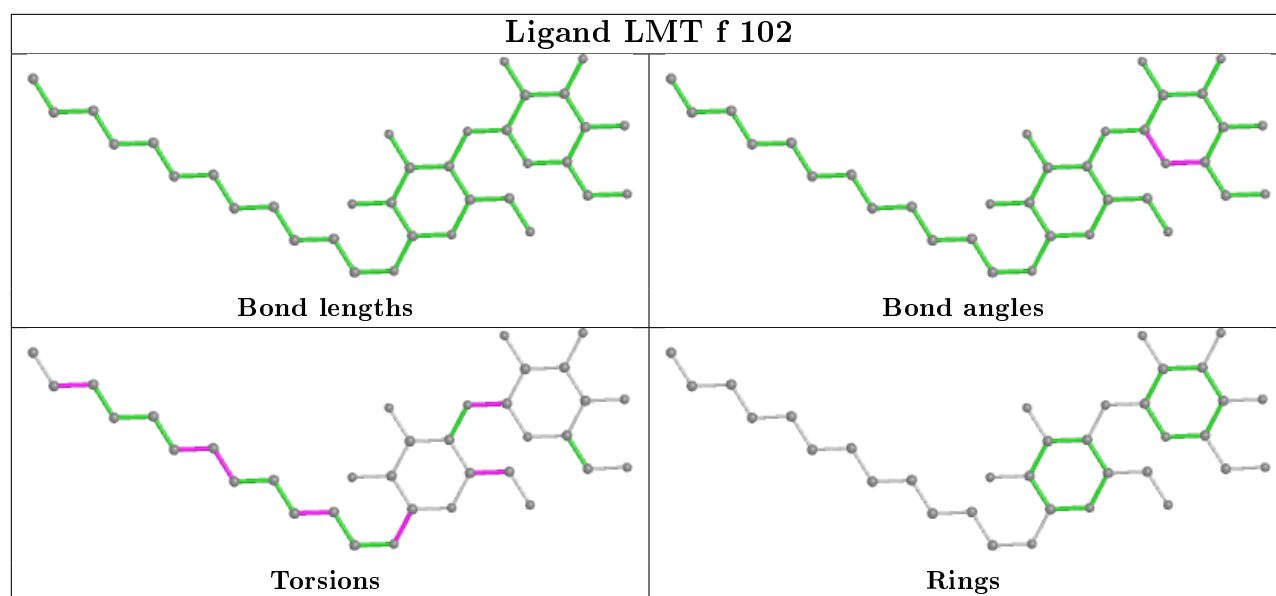
## Ligand DGD C 516



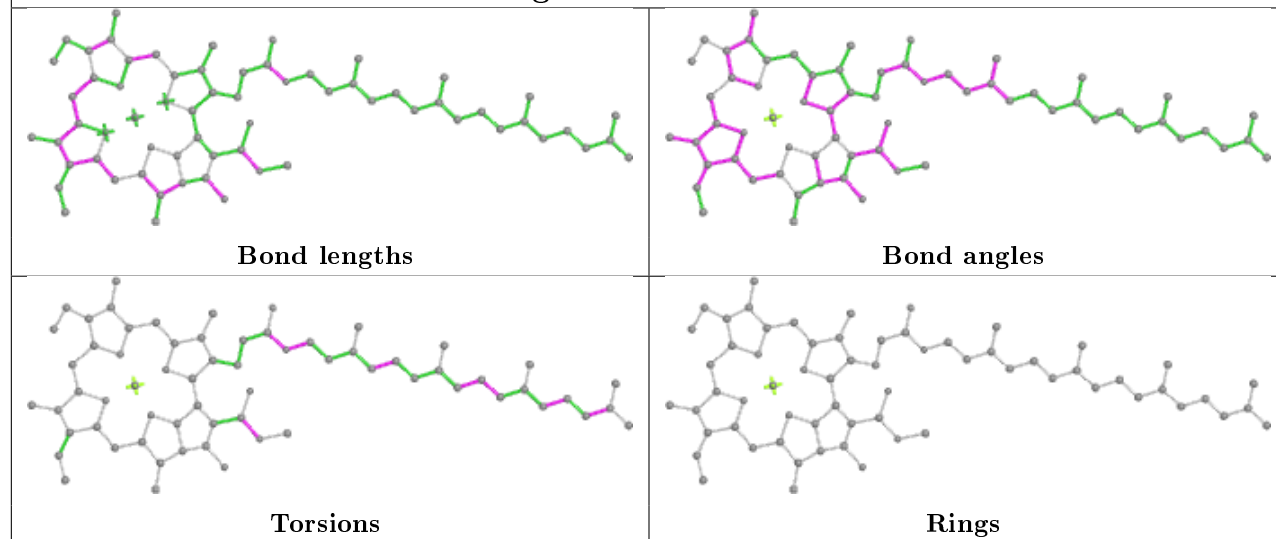
**Ligand BCR c 528****Ligand CLA B 604****Ligand CLA C 512**

**Ligand CLA B 616****Ligand BCR H 101****Ligand CLA A 406**

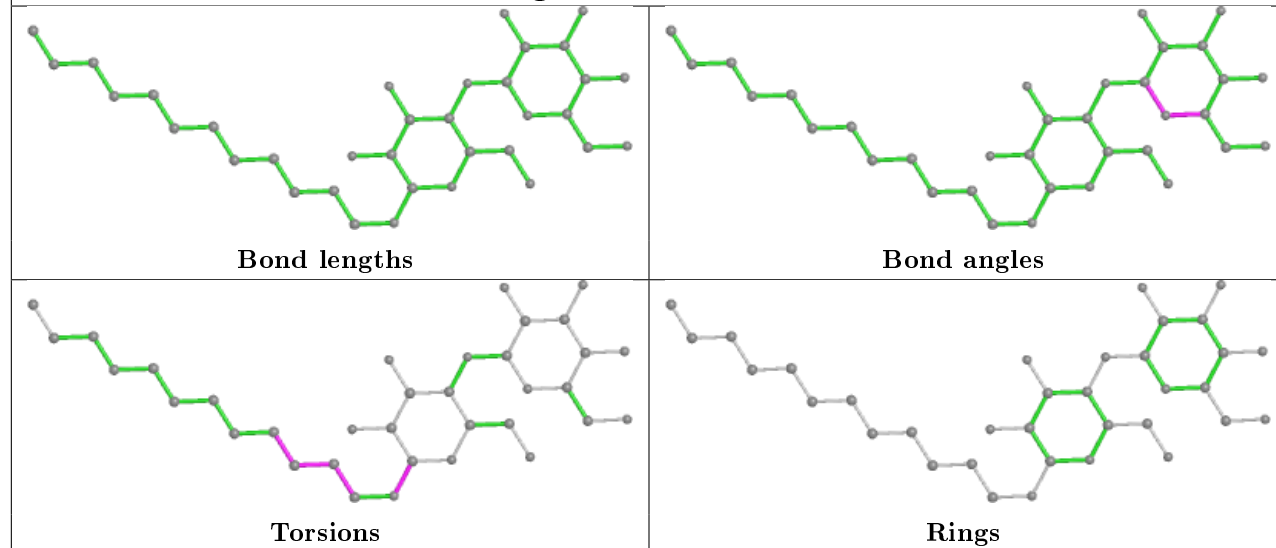




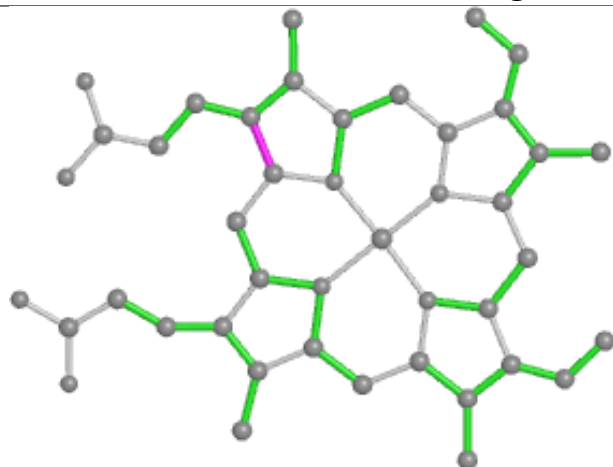
## Ligand CLA C 509



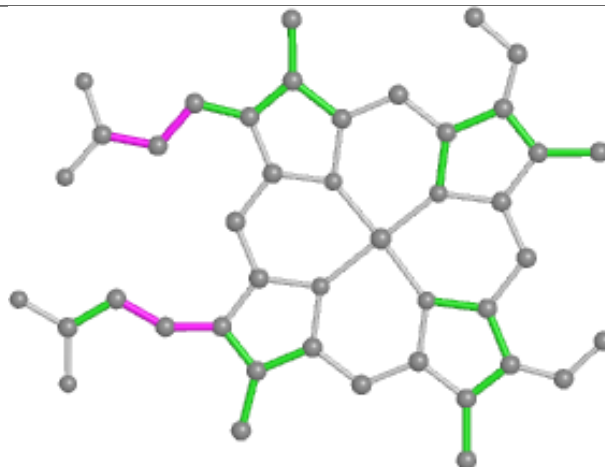
## Ligand LMT F 101



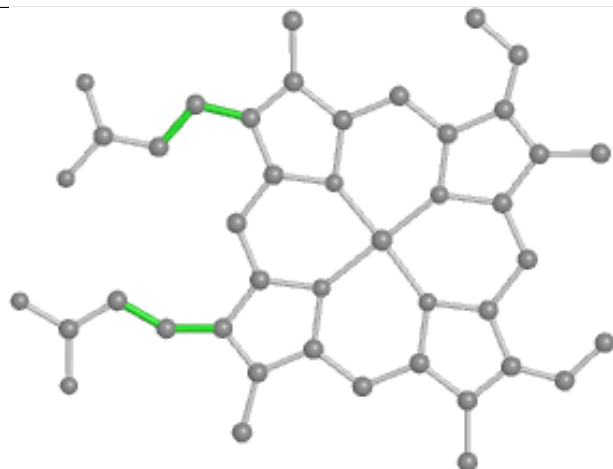
## Ligand HEM V 205



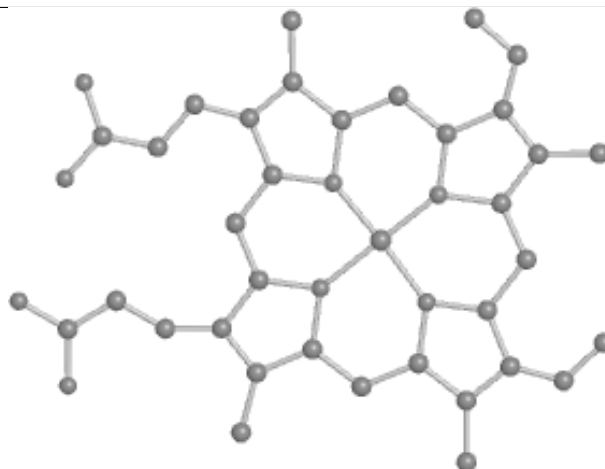
Bond lengths



Bond angles

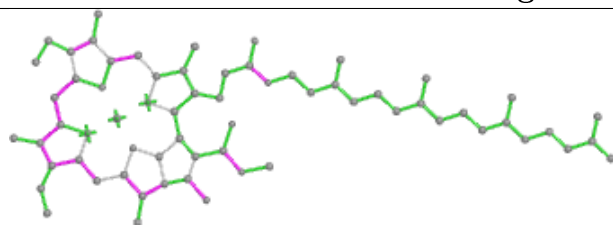


Torsions

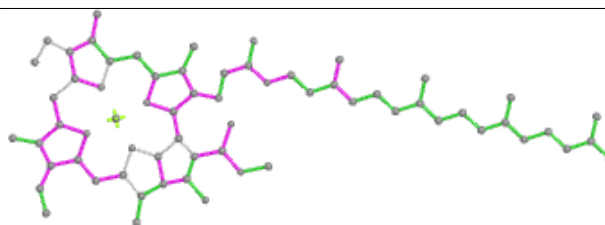


Rings

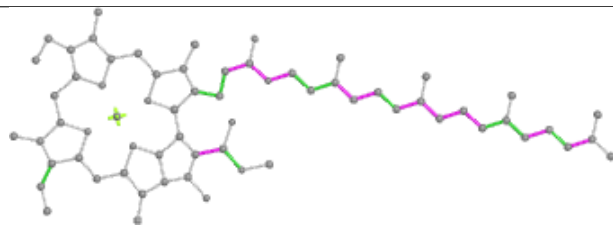
## Ligand CLA b 610



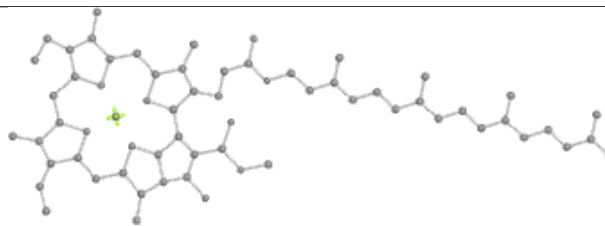
Bond lengths



Bond angles

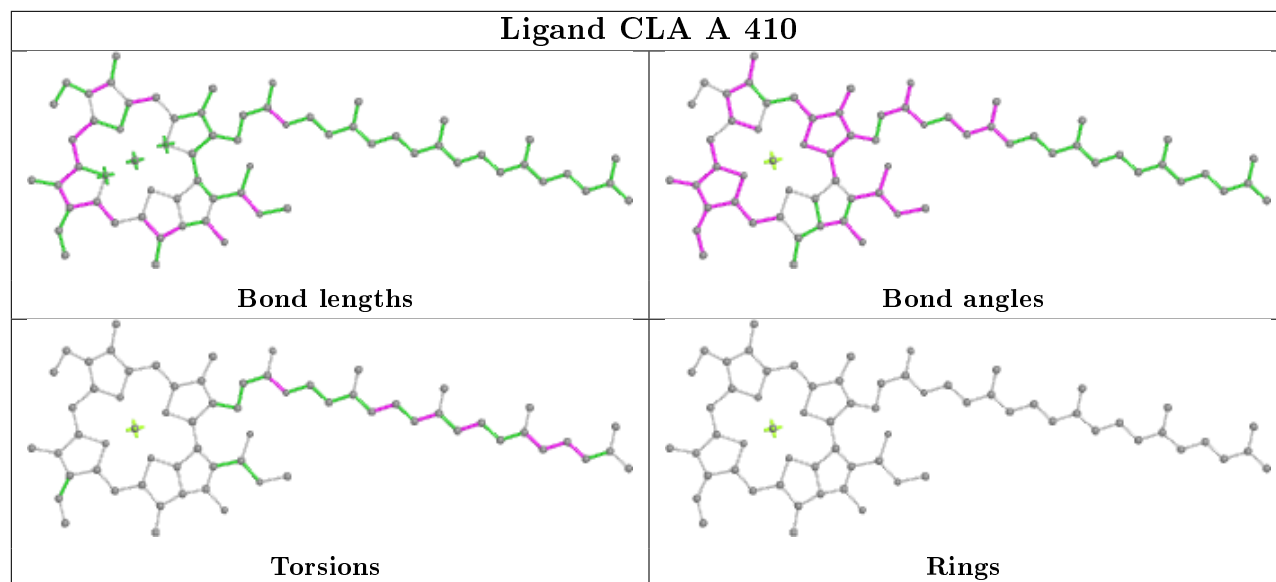


Torsions

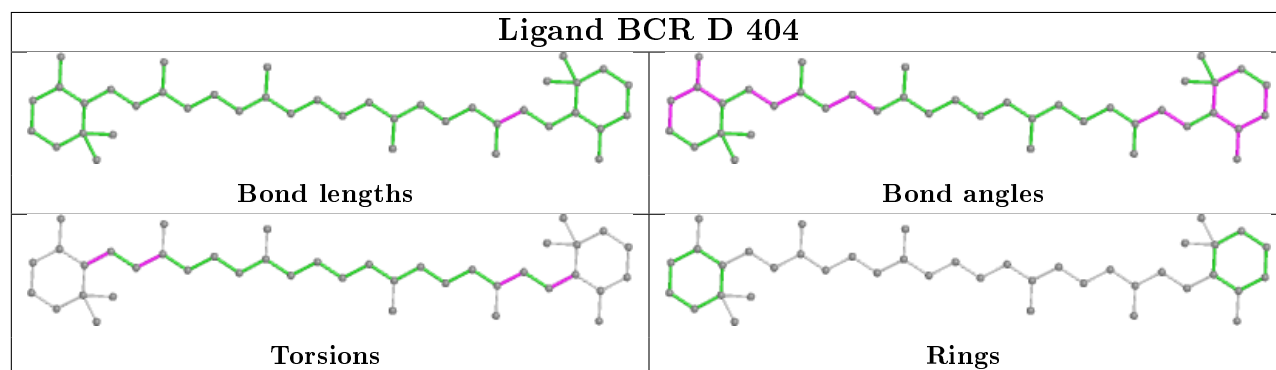


Rings

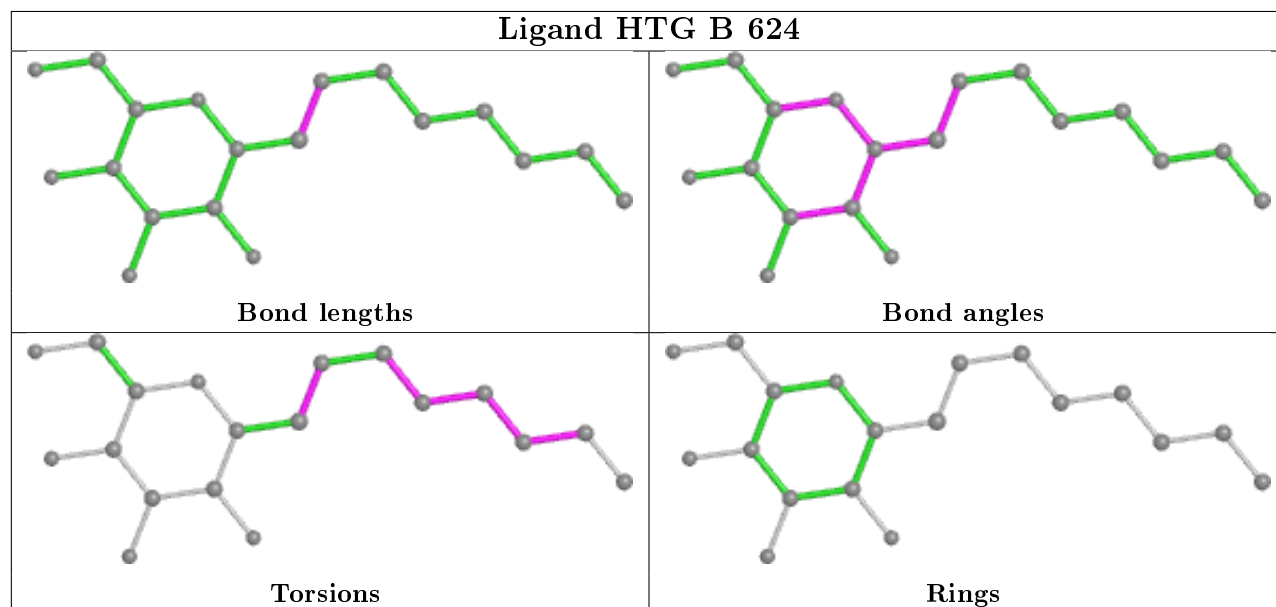
## Ligand CLA A 410

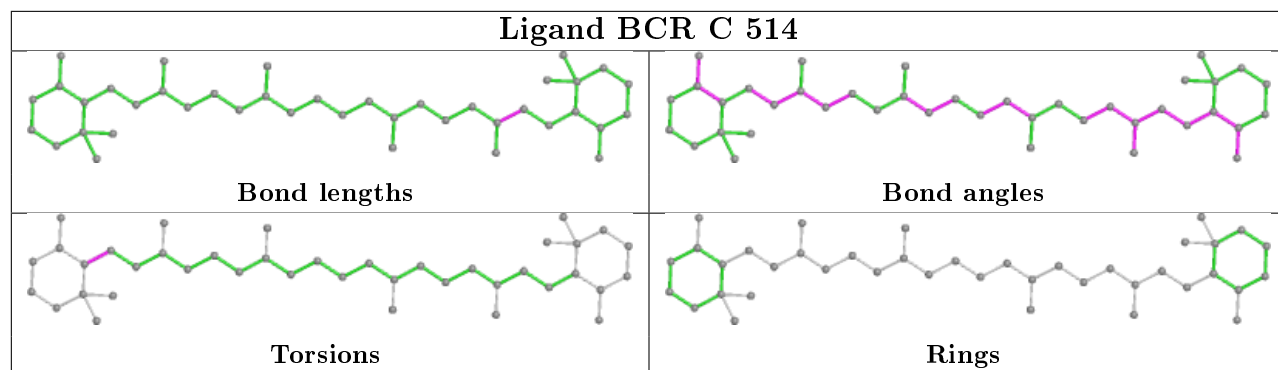
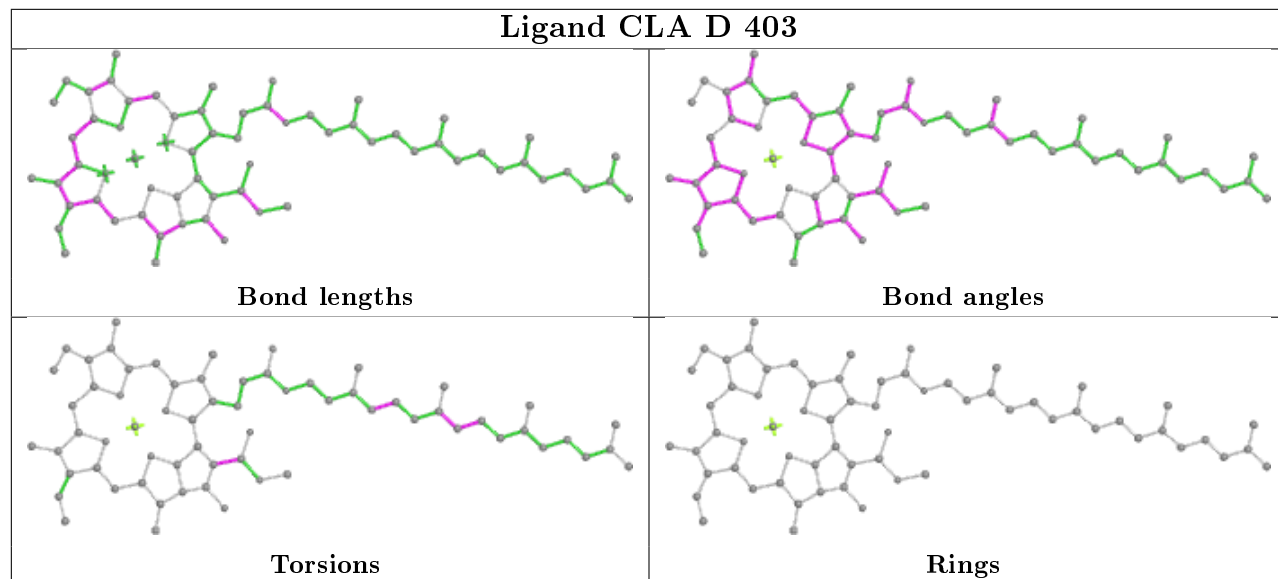
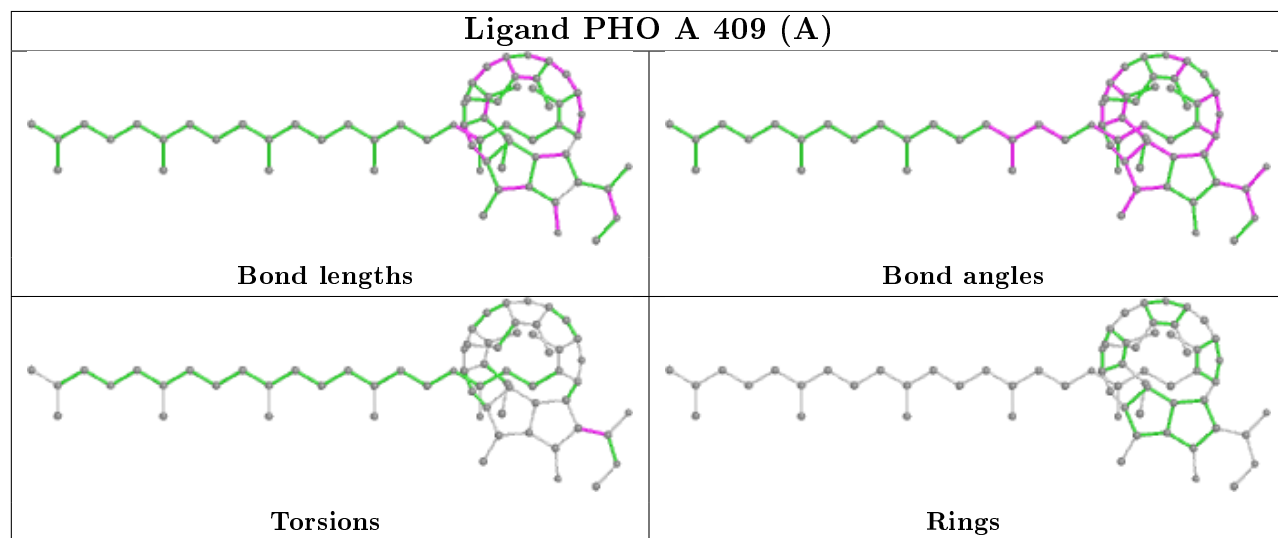


## Ligand BCR D 404

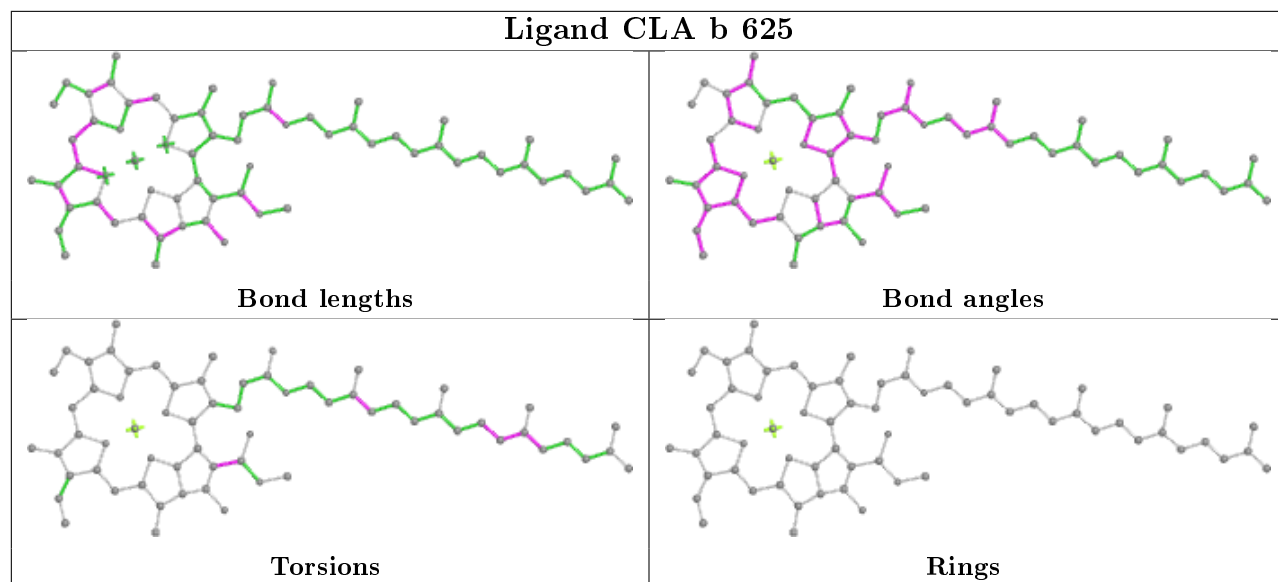


## Ligand HTG B 624

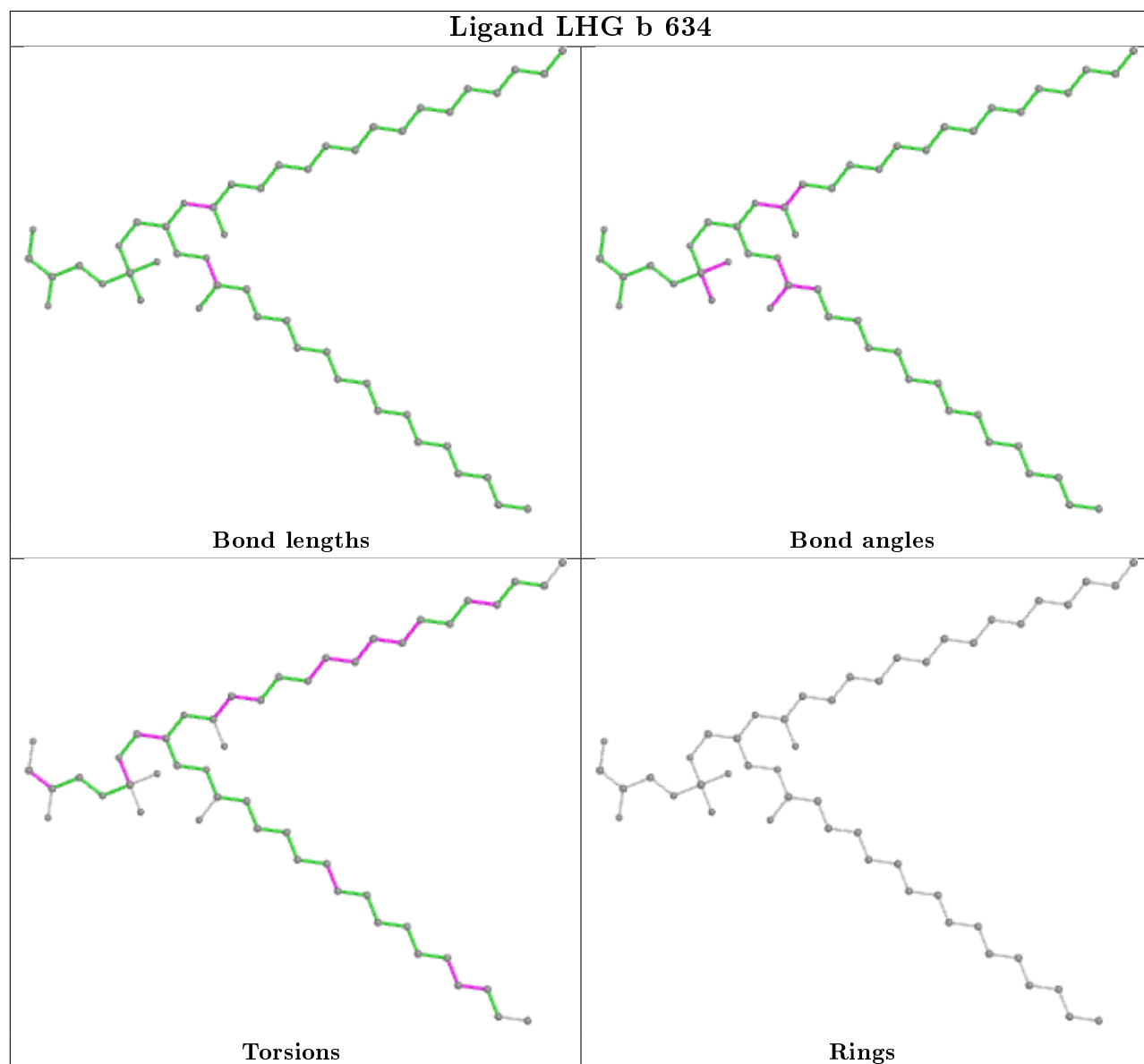


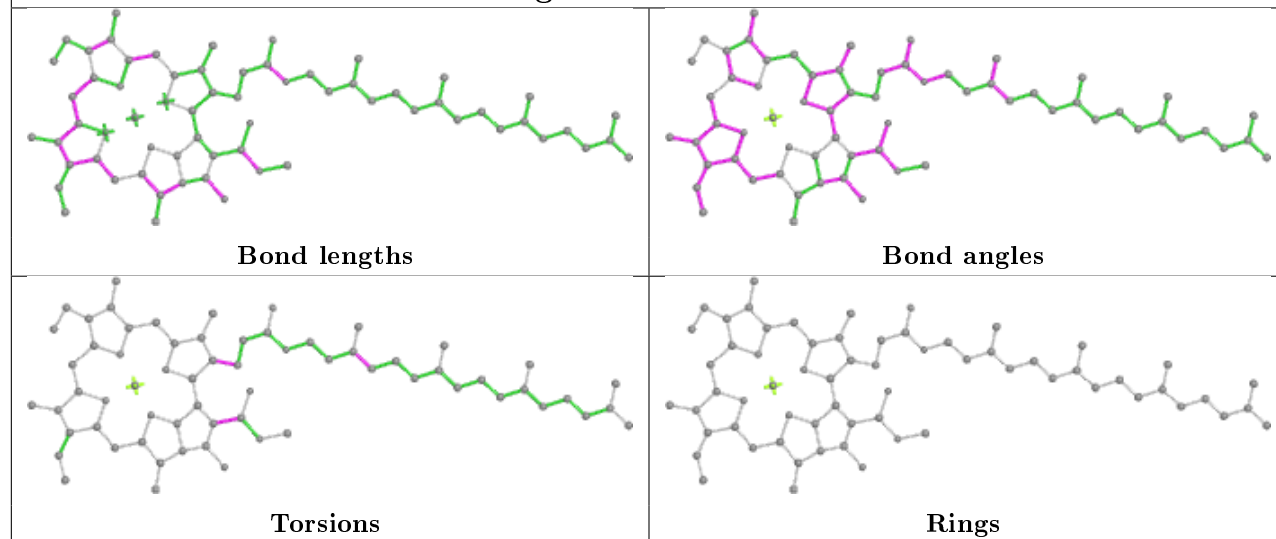
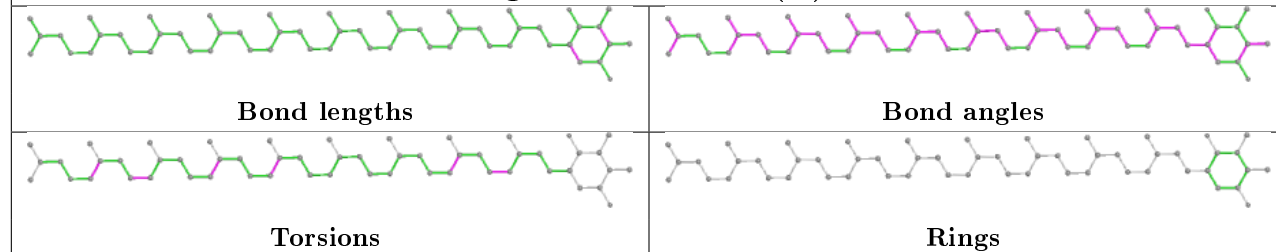
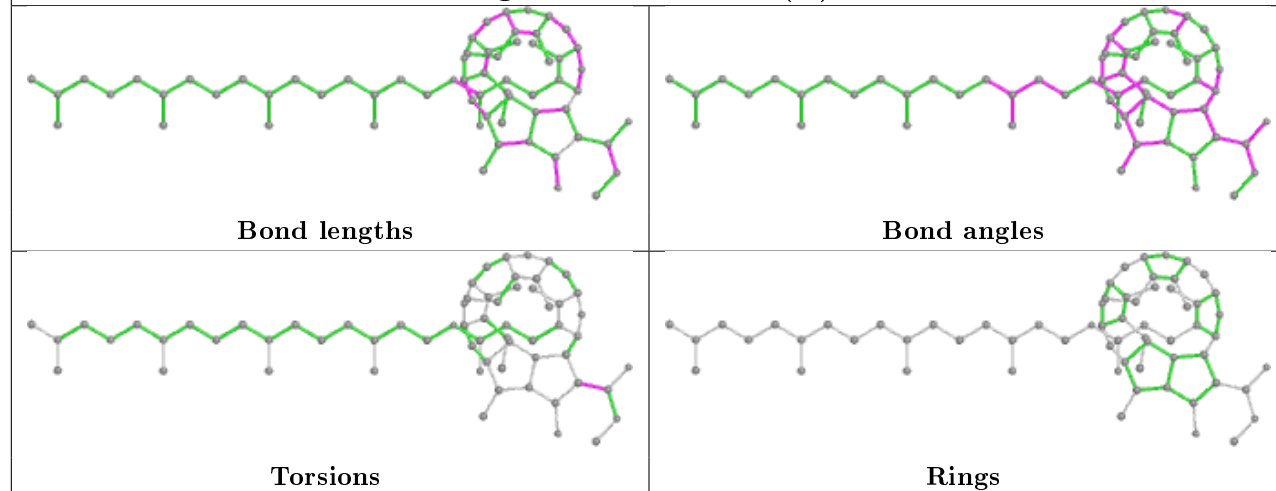
**Ligand BCR C 514****Ligand CLA D 403****Ligand PHO A 409 (A)**

## Ligand CLA b 625

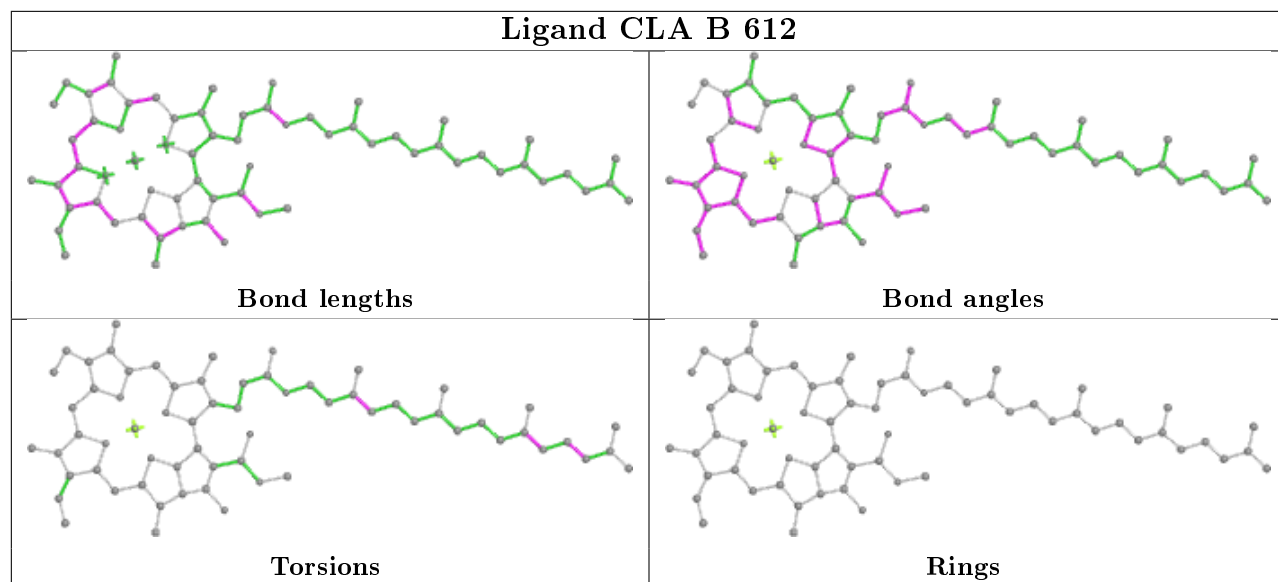


## Ligand LHG b 634

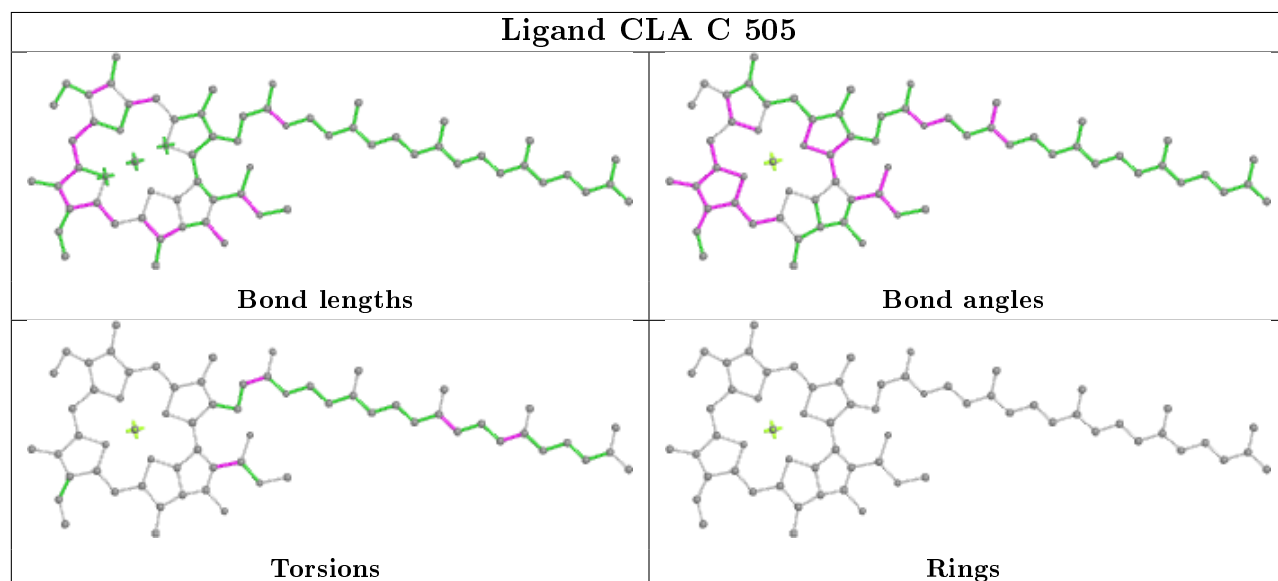


**Ligand CLA b 618****Ligand PL9 D 405 (B)****Ligand PHO A 409 (B)**

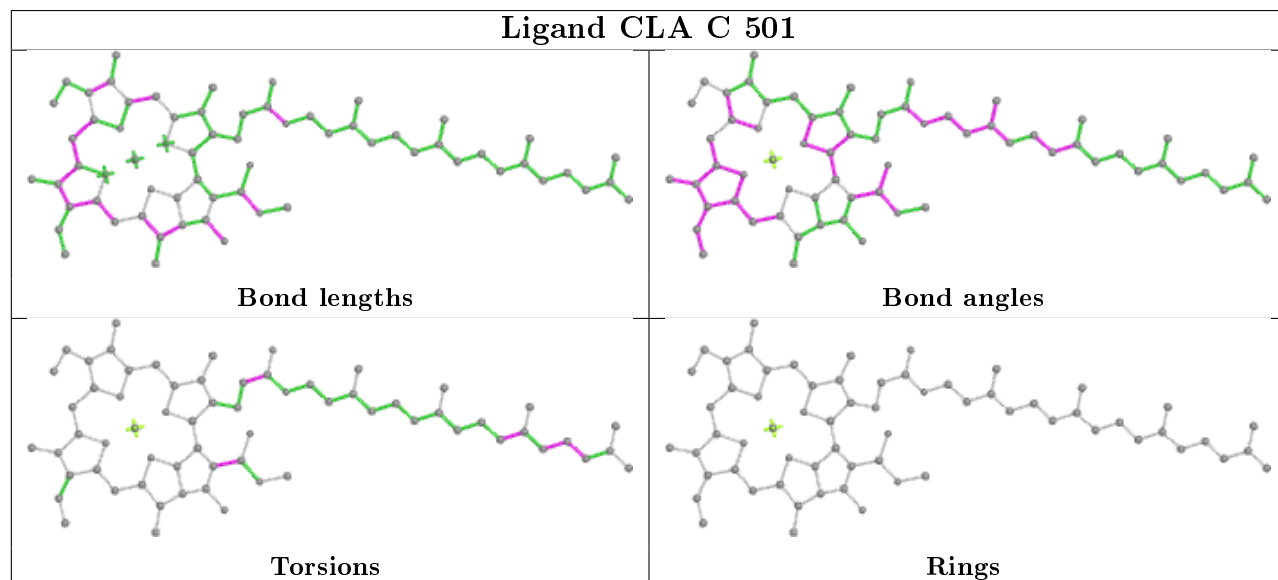
## Ligand CLA B 612



## Ligand CLA C 505

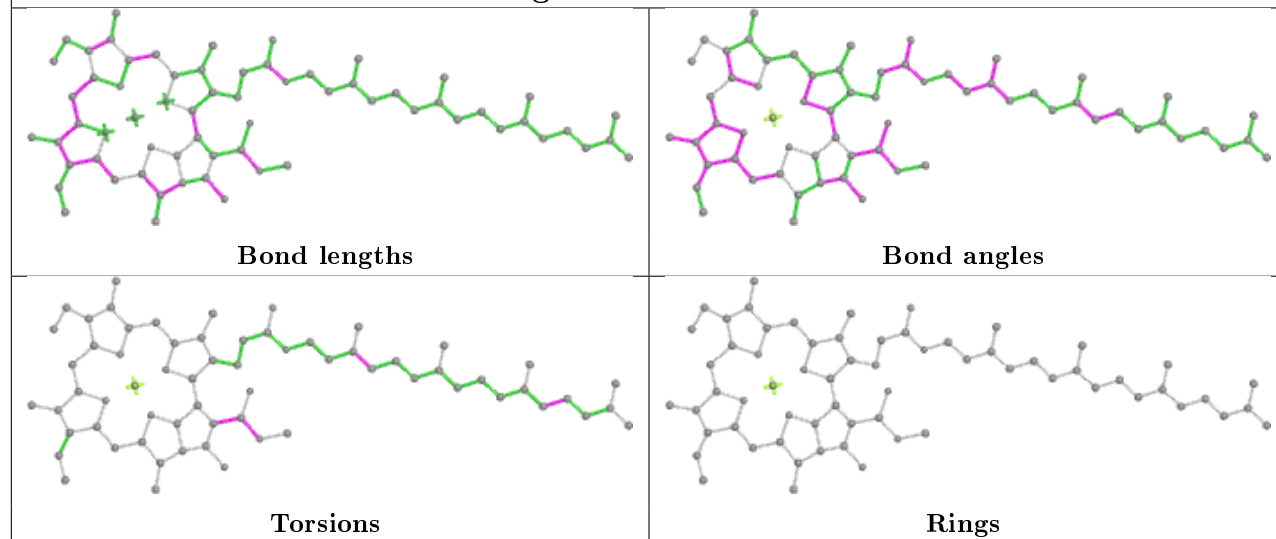


## Ligand CLA C 501

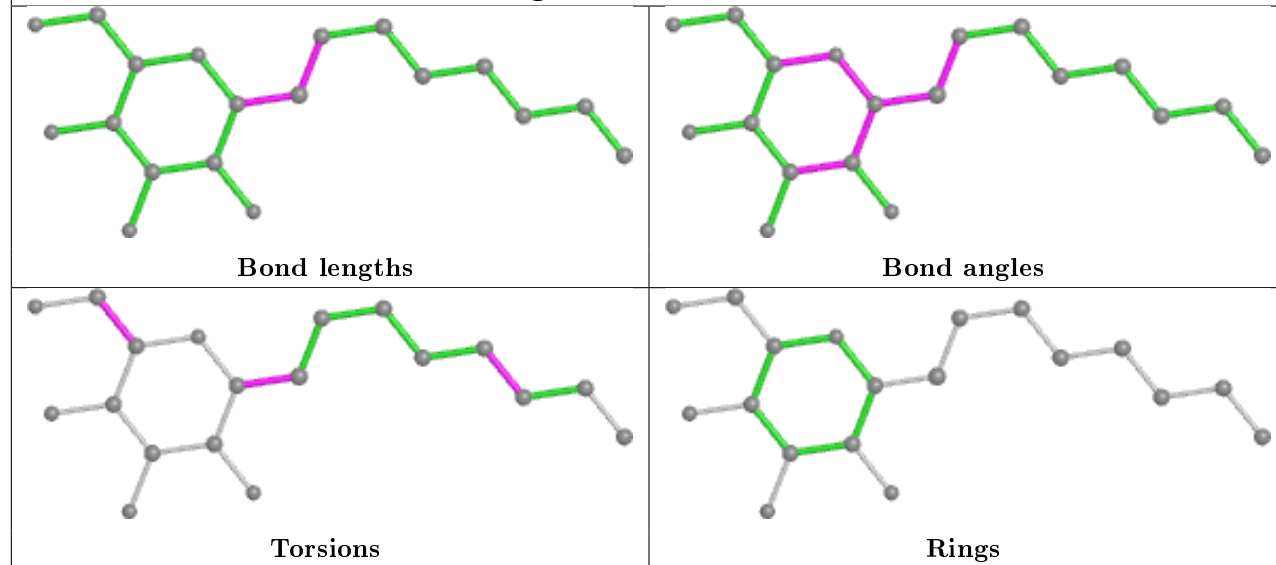




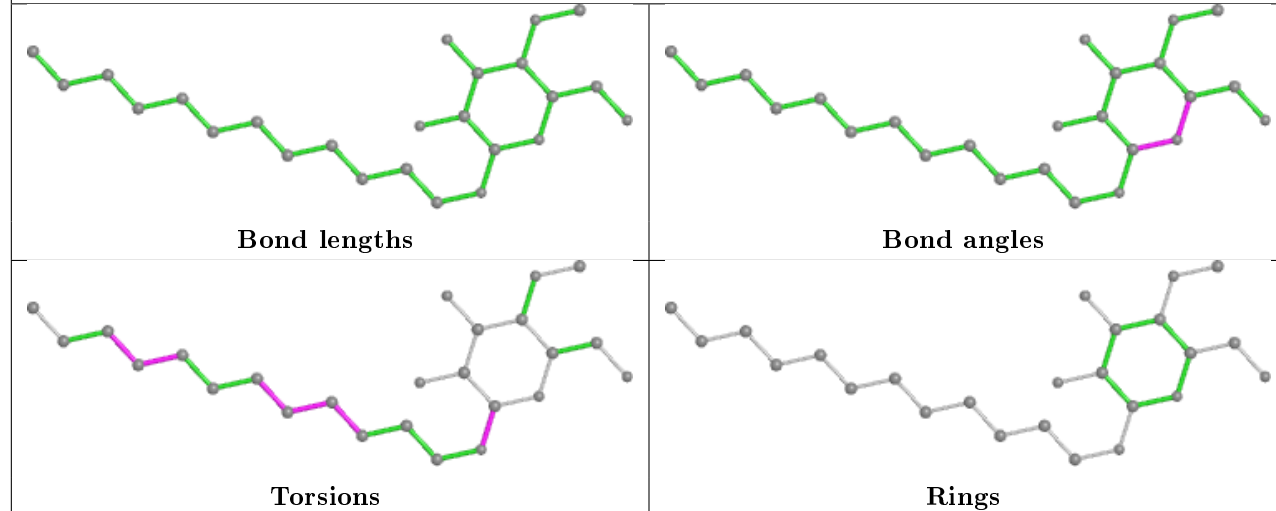
## Ligand CLA B 605

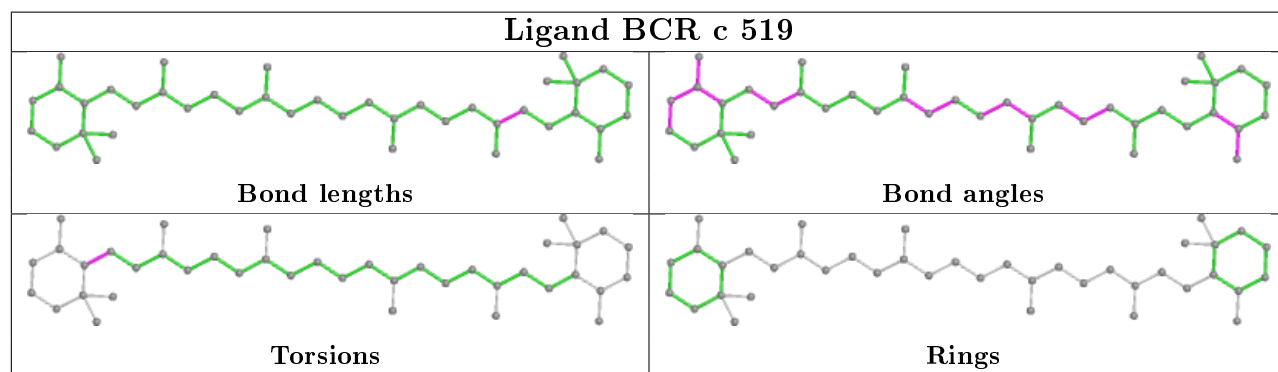
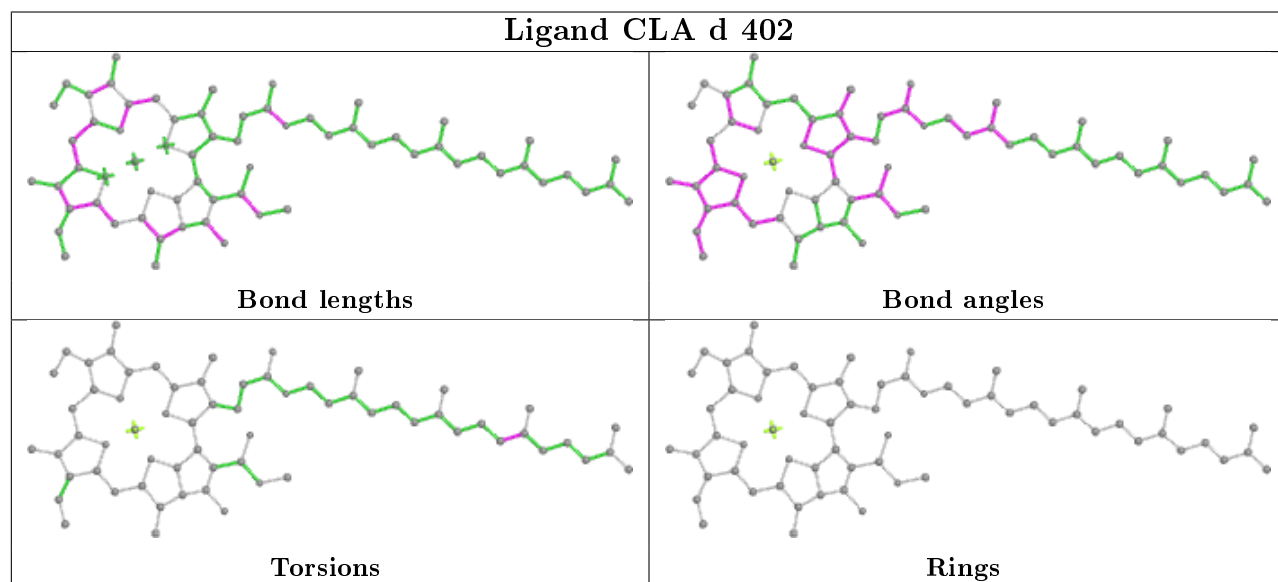
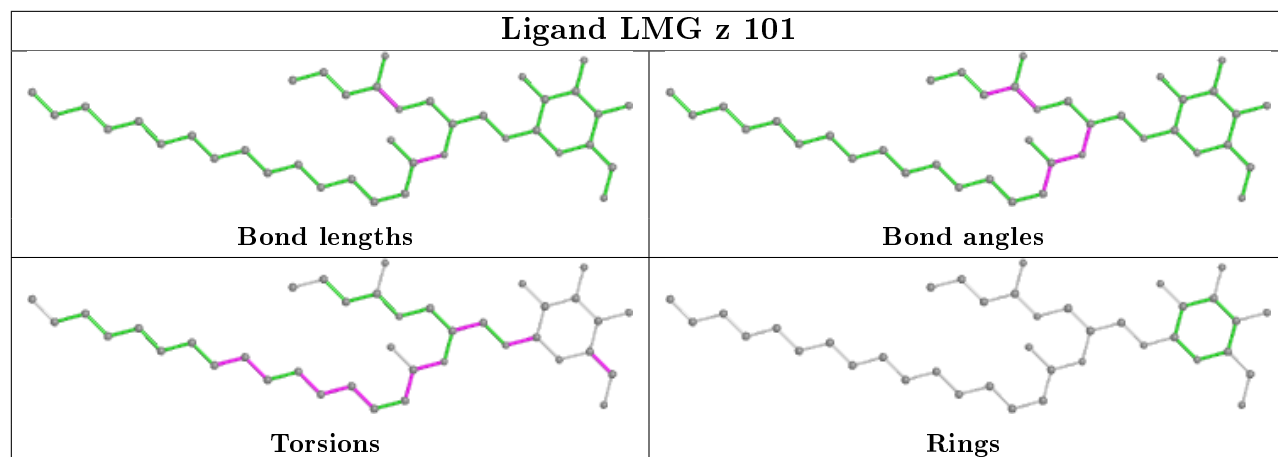


## Ligand HTG B 625

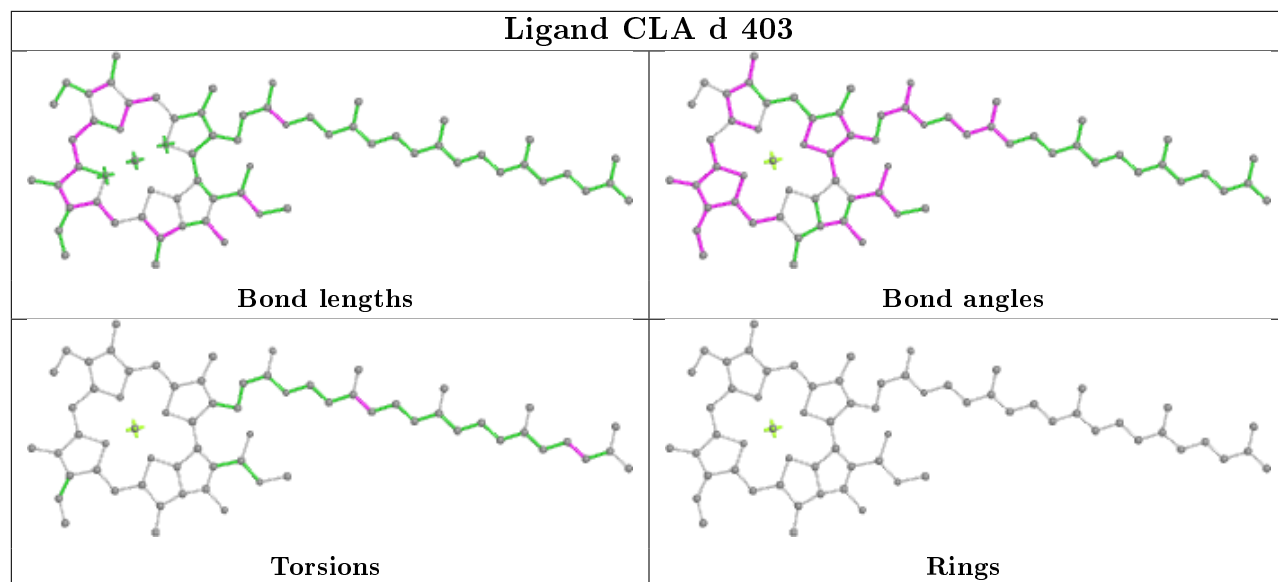


## Ligand LMT B 635

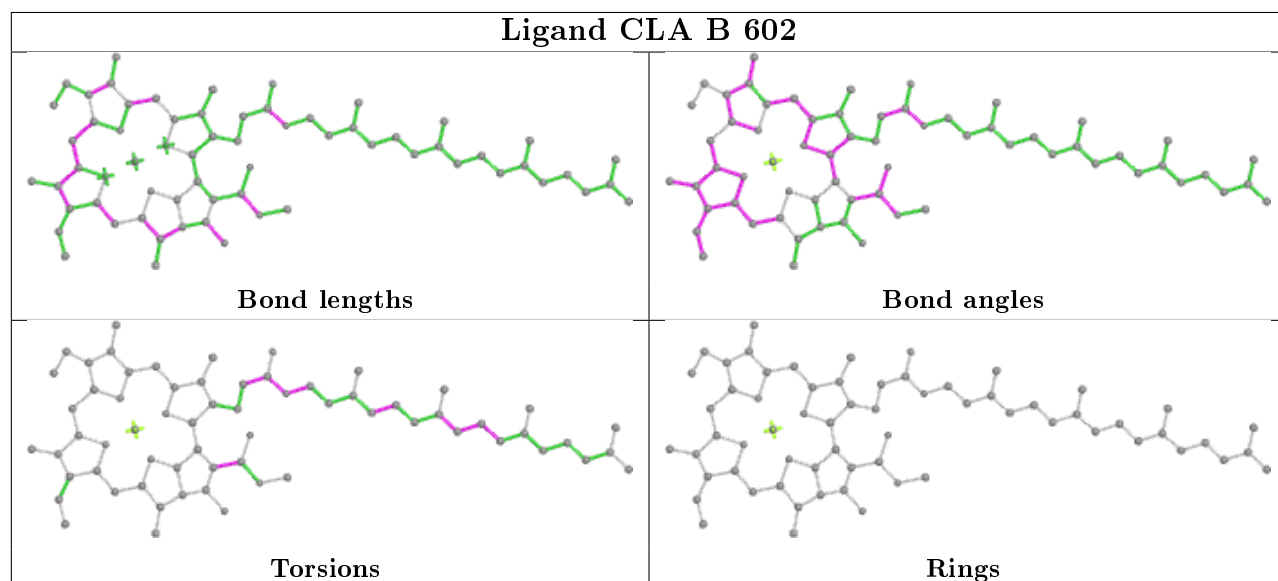




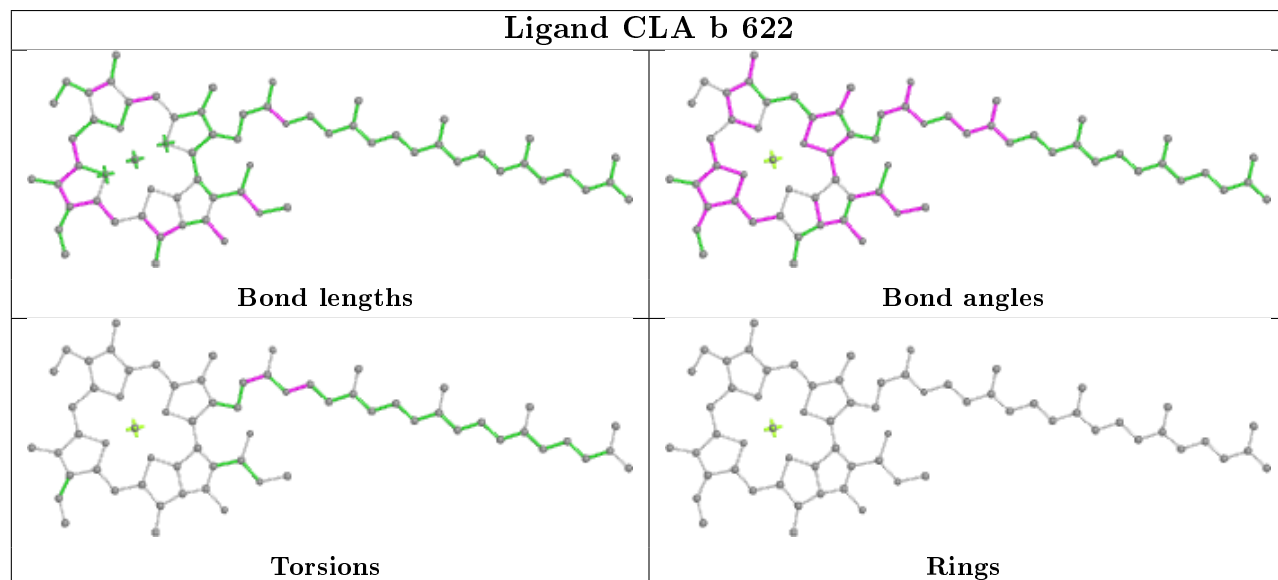
## Ligand CLA d 403

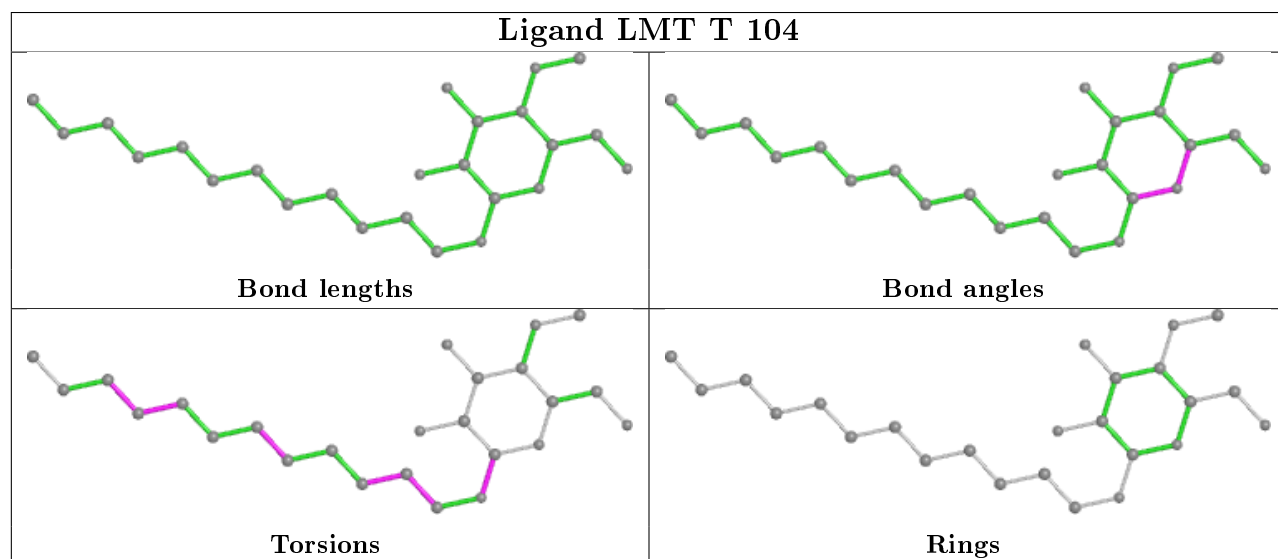
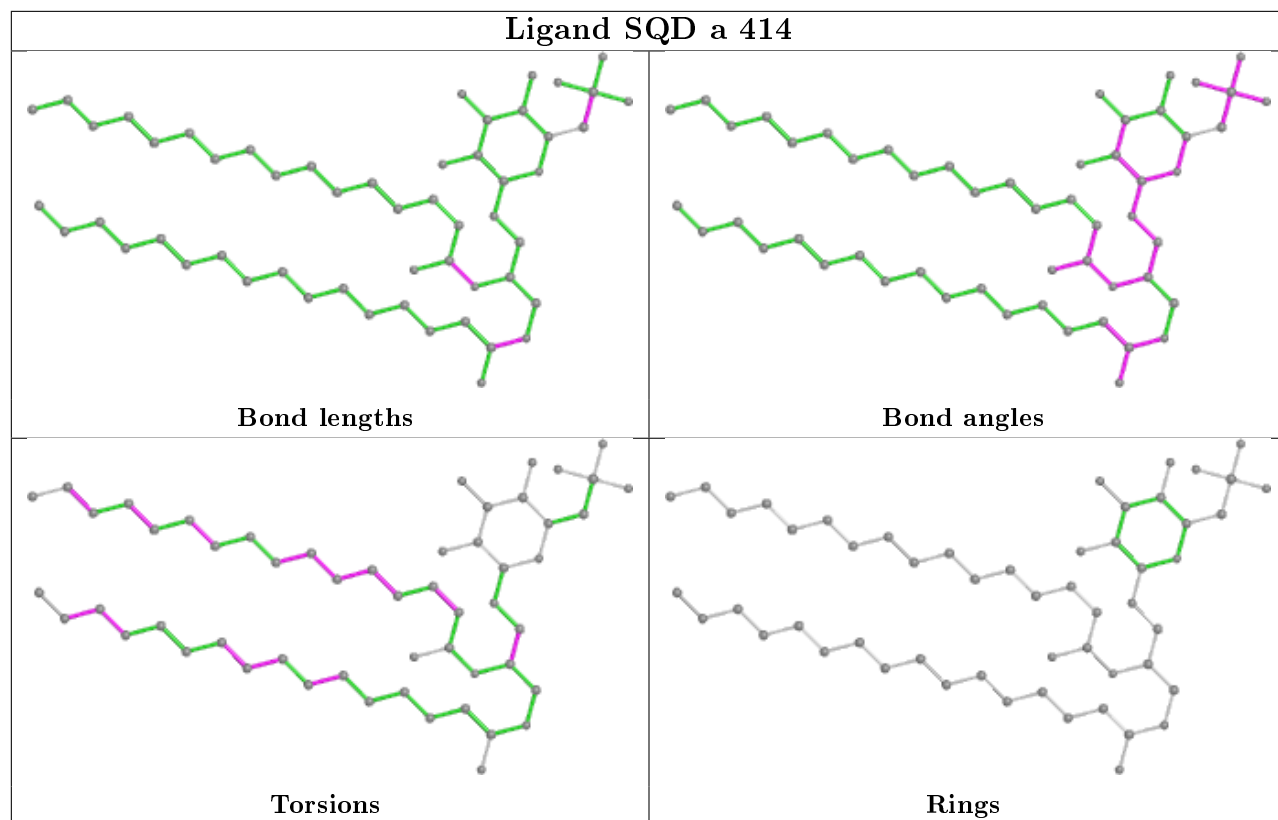


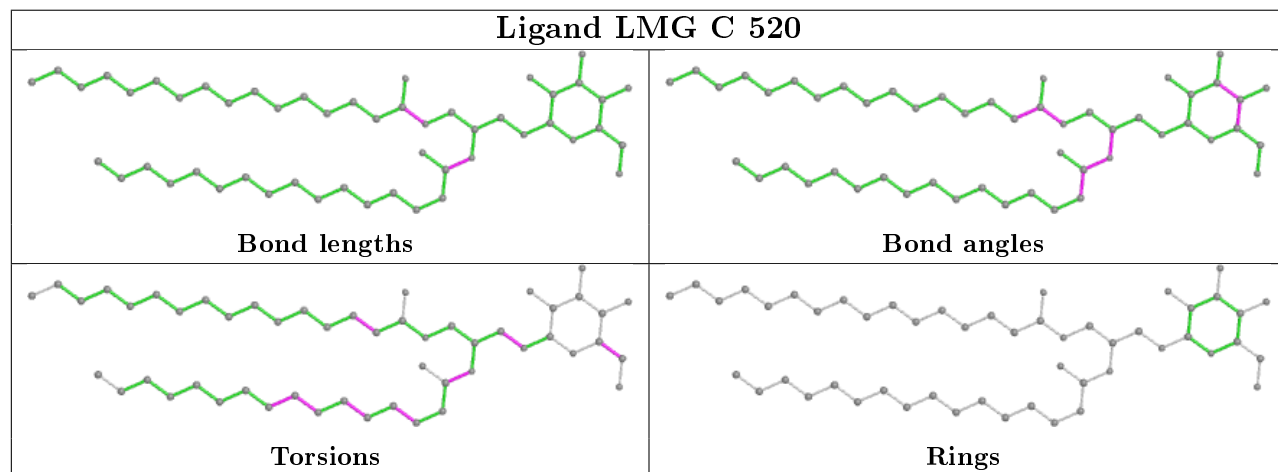
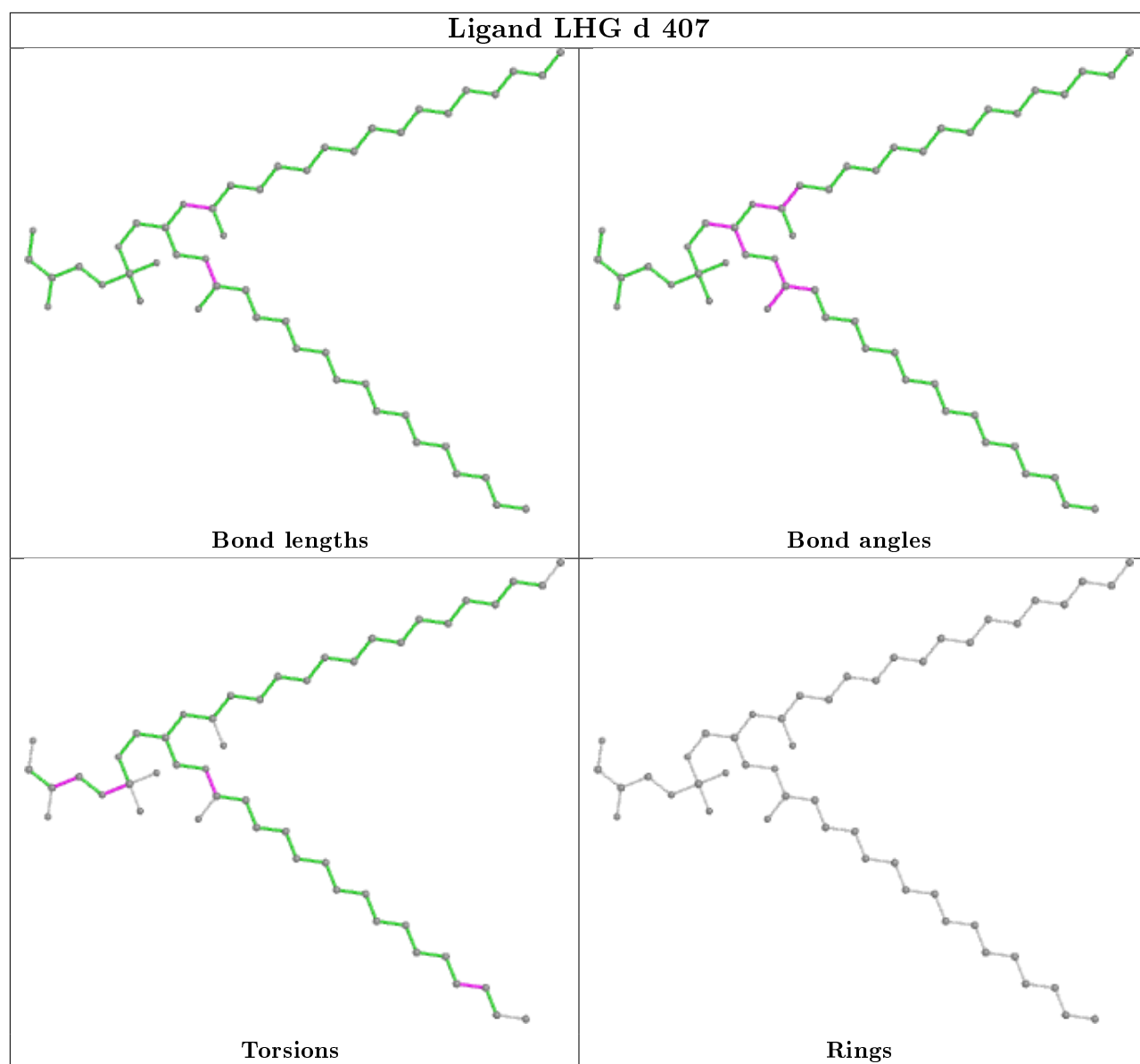
## Ligand CLA B 602

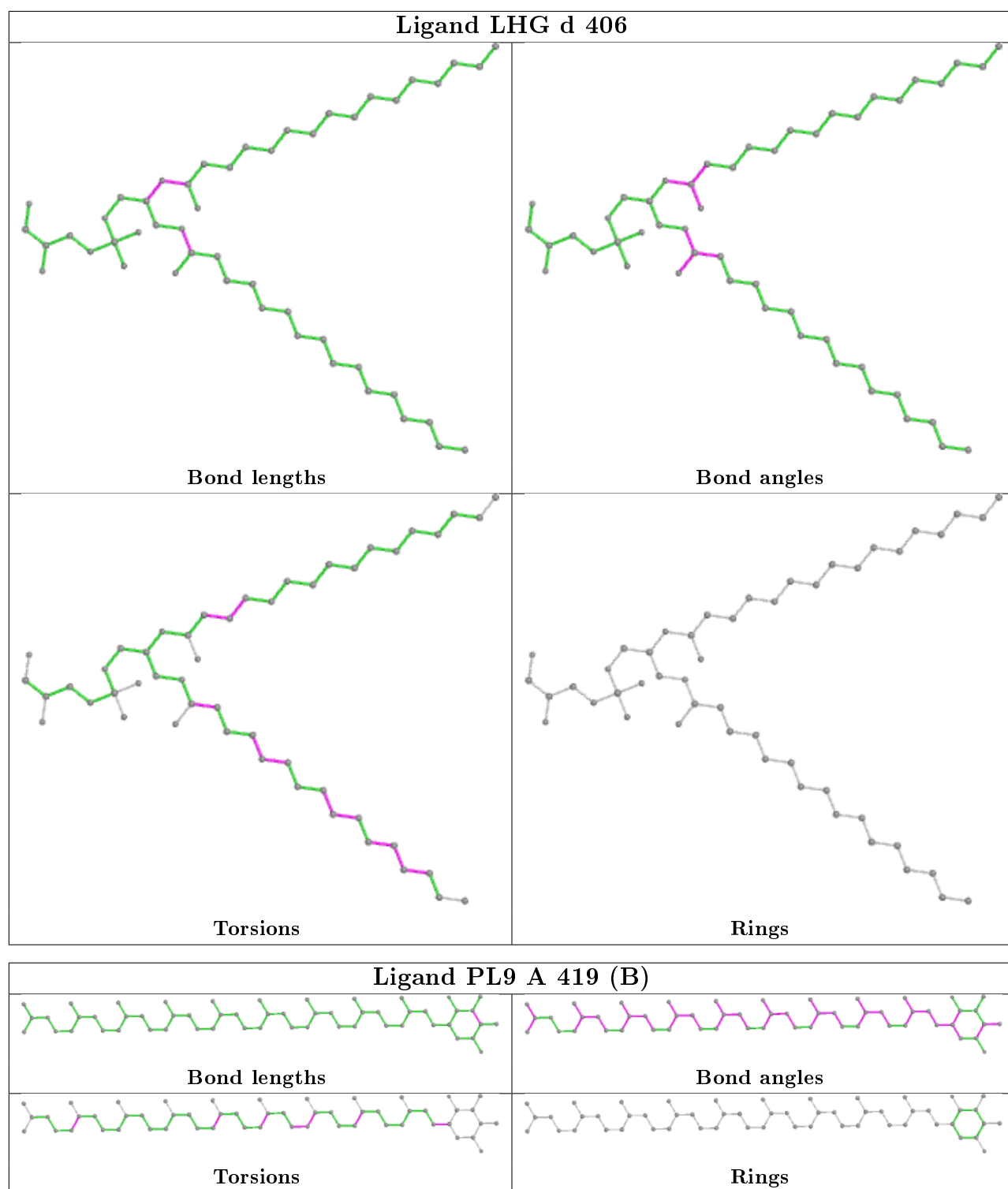


## Ligand CLA b 622

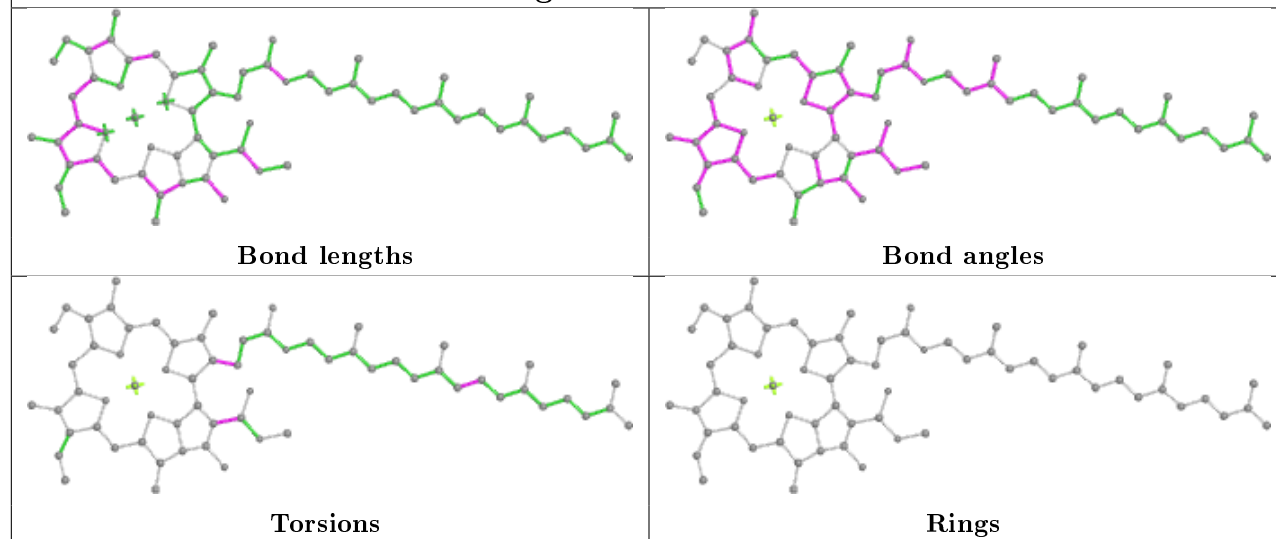




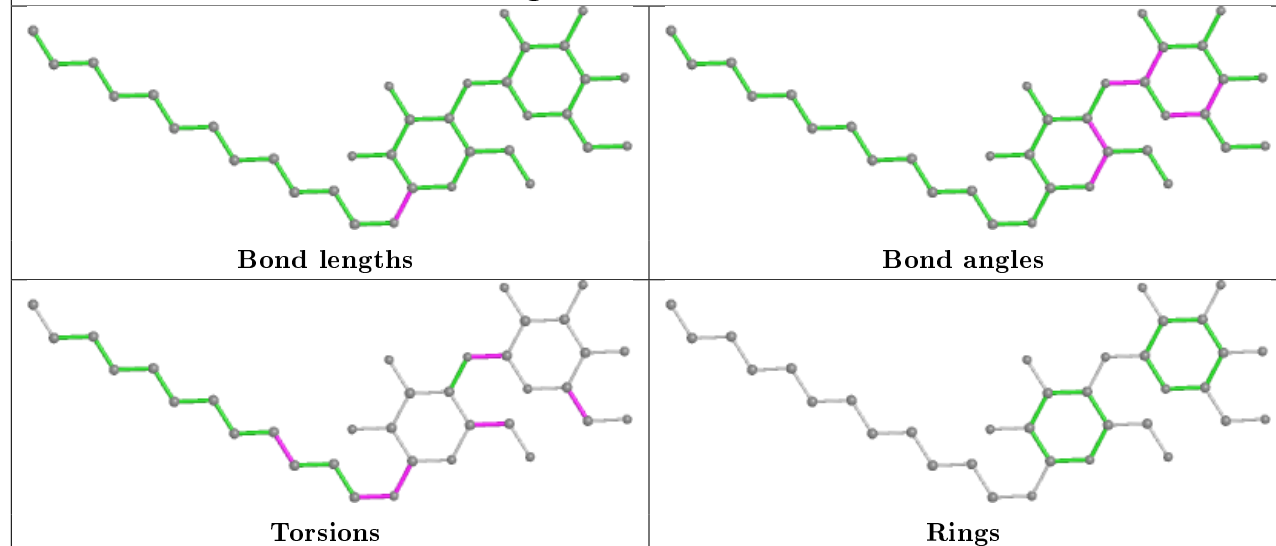




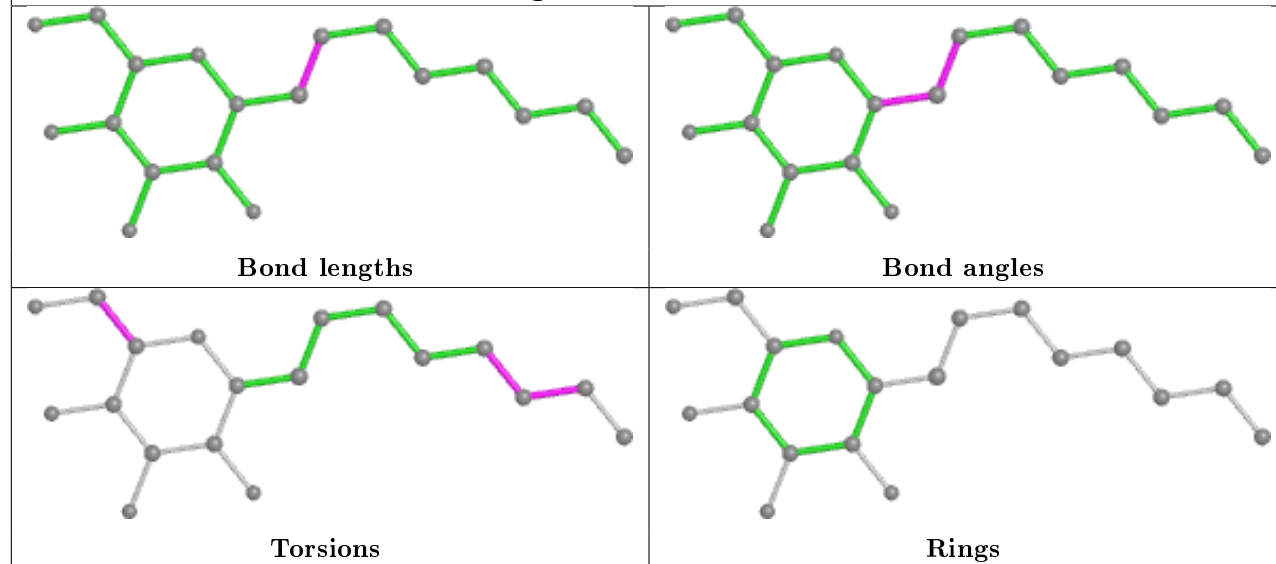
## Ligand CLA b 621

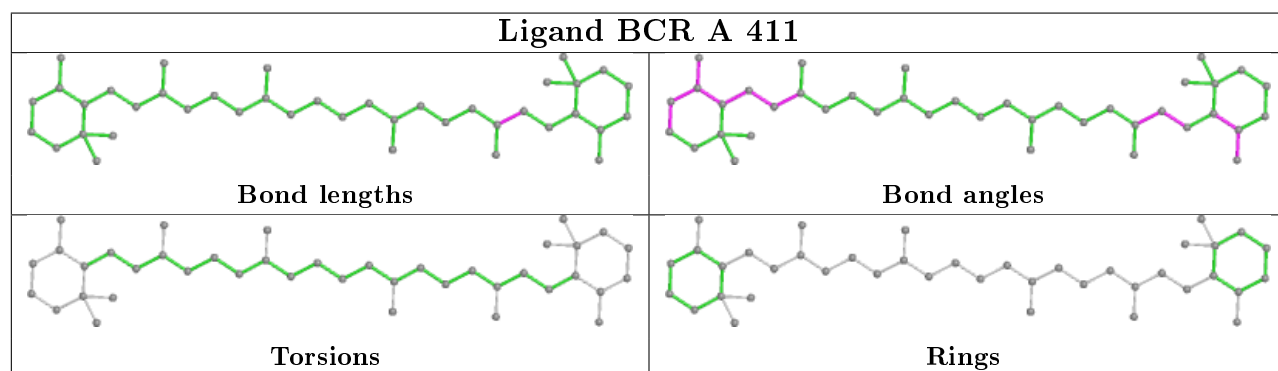
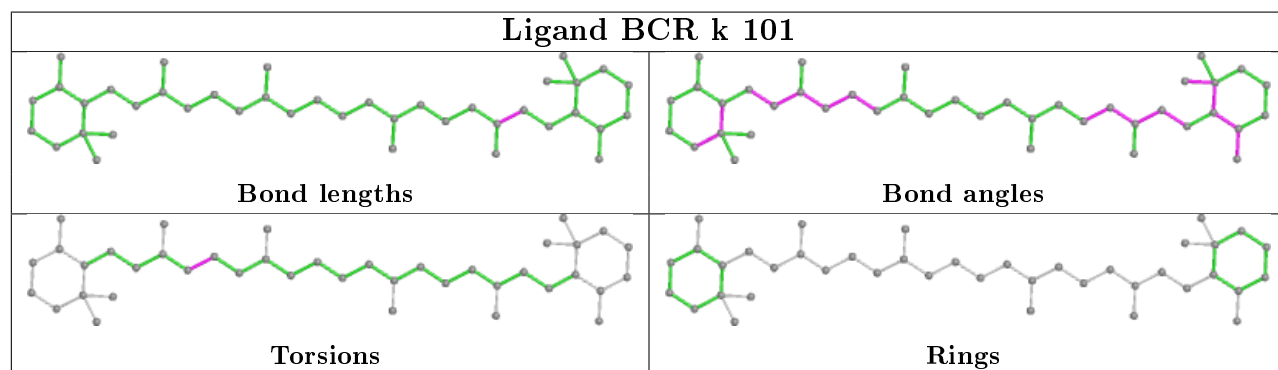
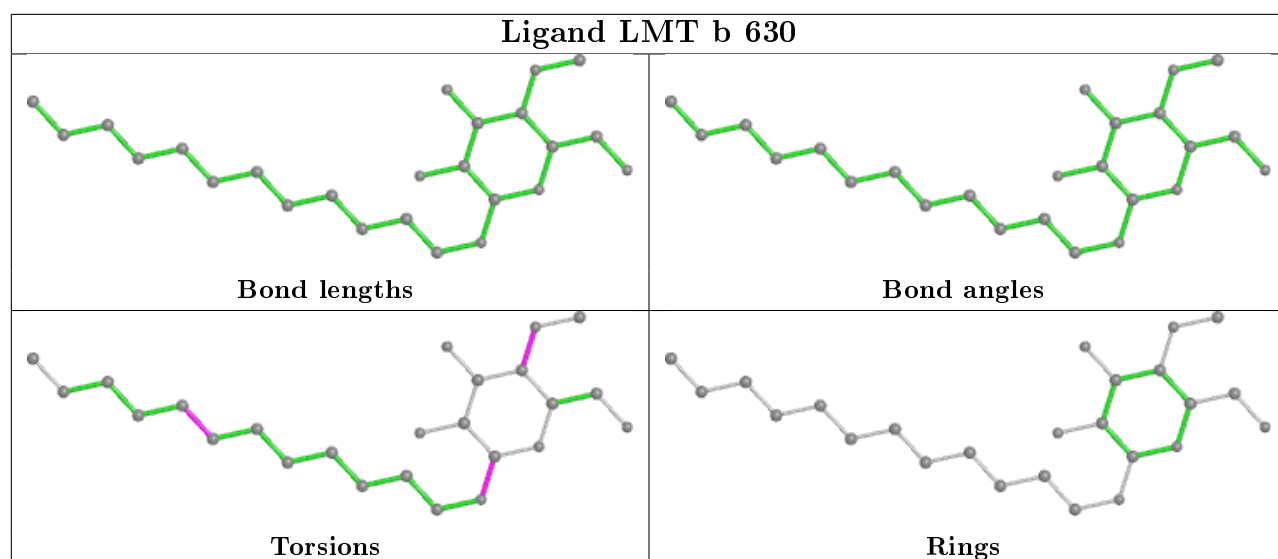


## Ligand LMT M 103



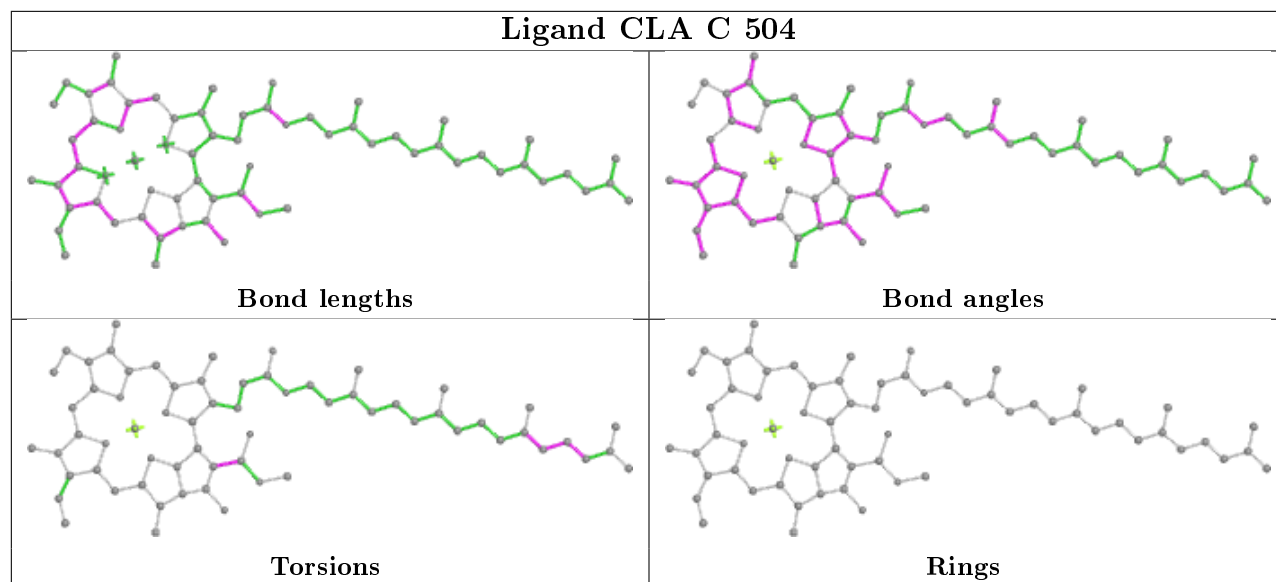
## Ligand HTG B 623



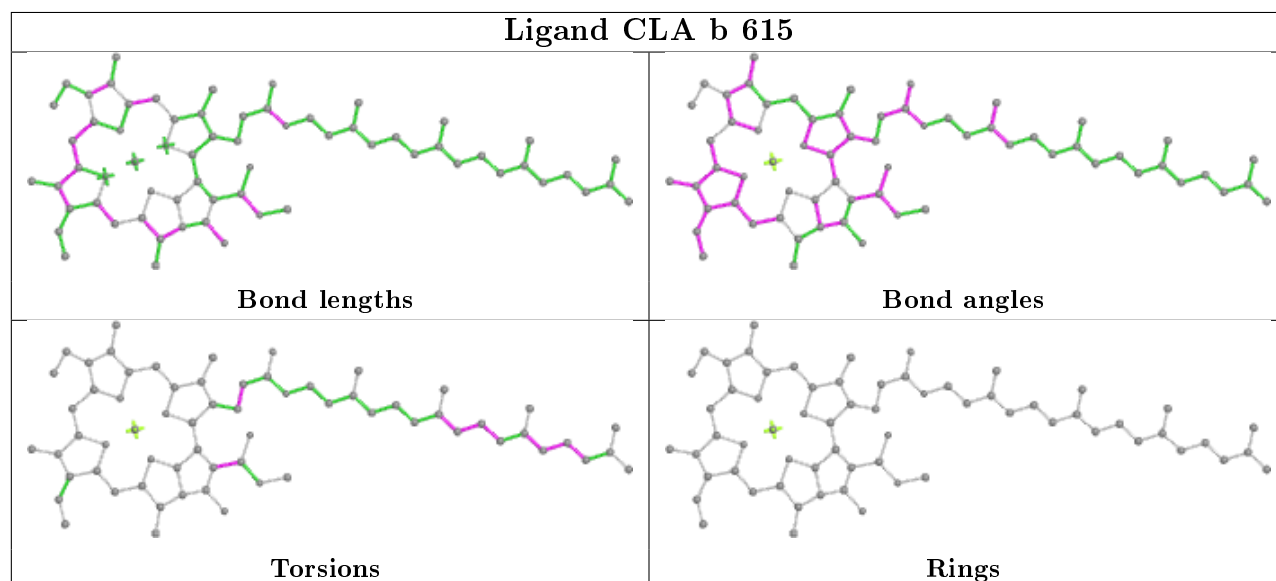




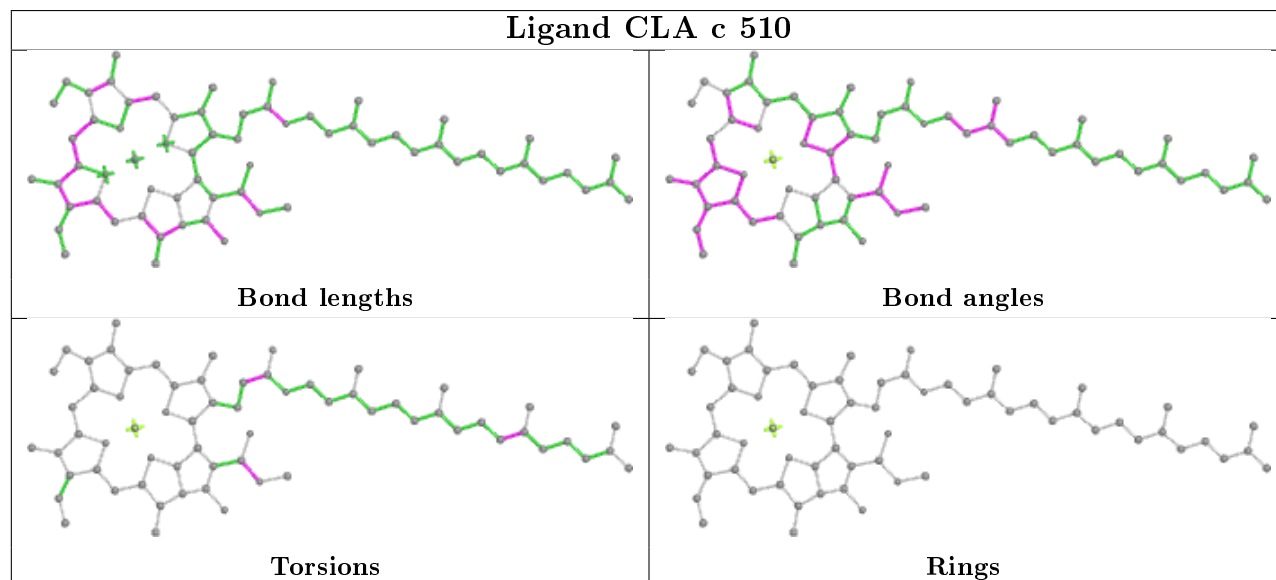
## Ligand CLA C 504



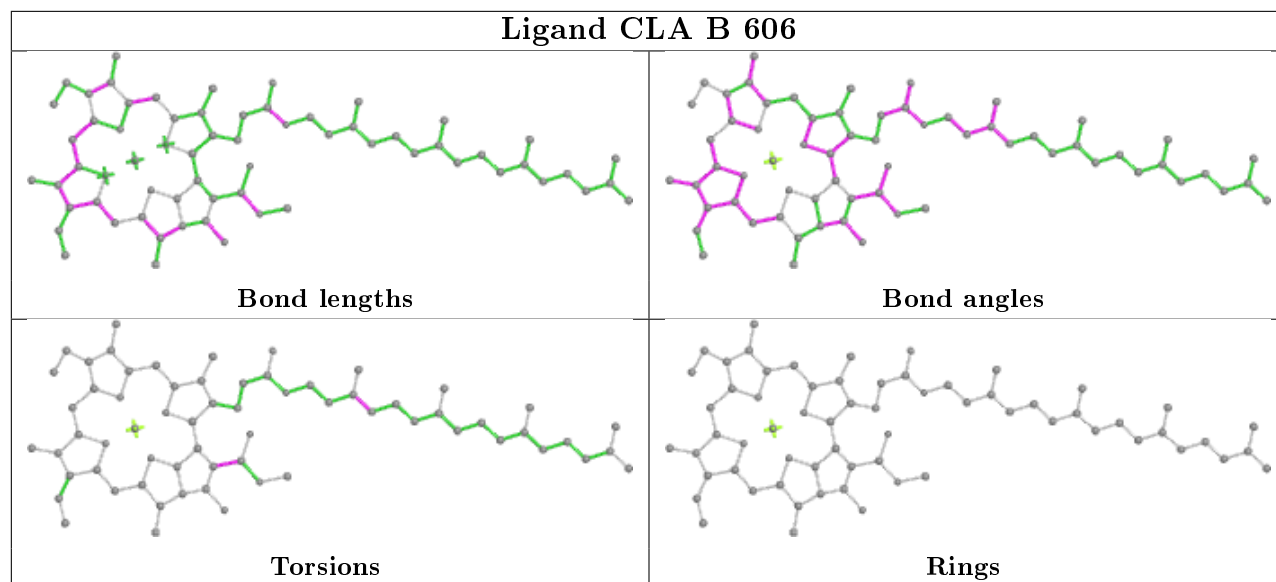
## Ligand CLA b 615



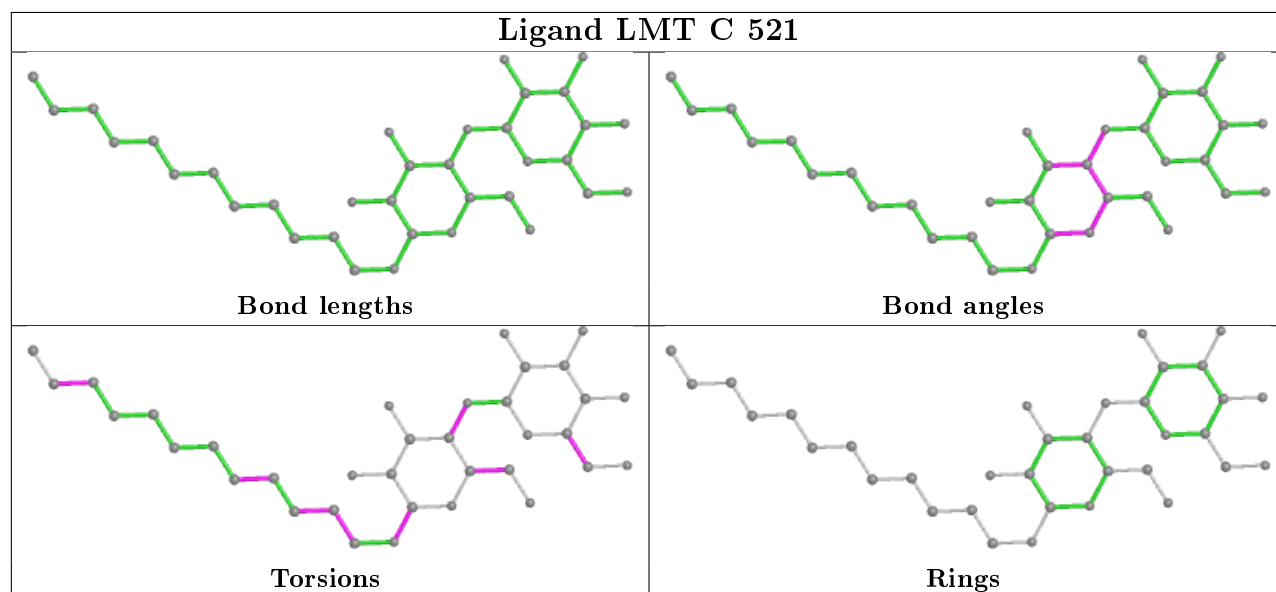
## Ligand CLA c 510



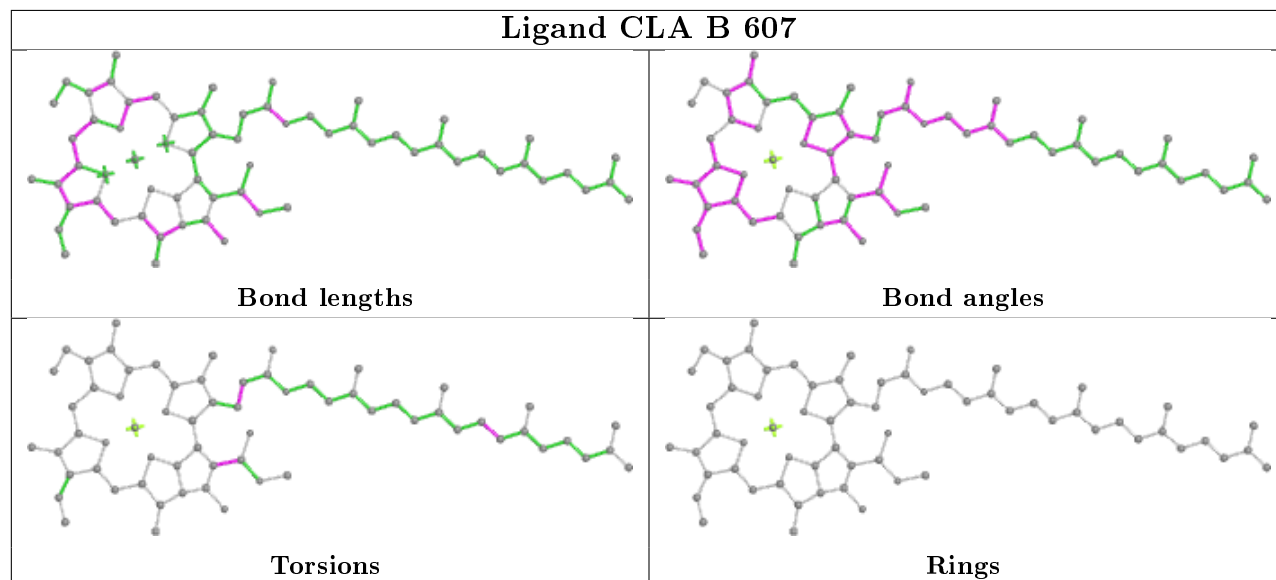
## Ligand CLA B 606

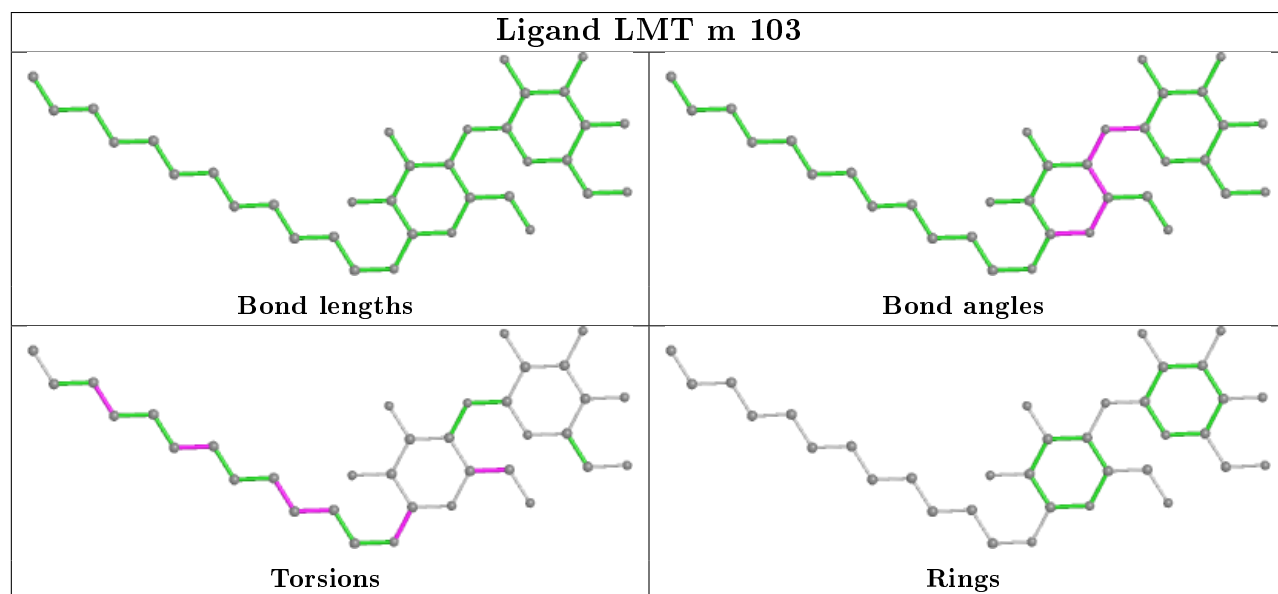
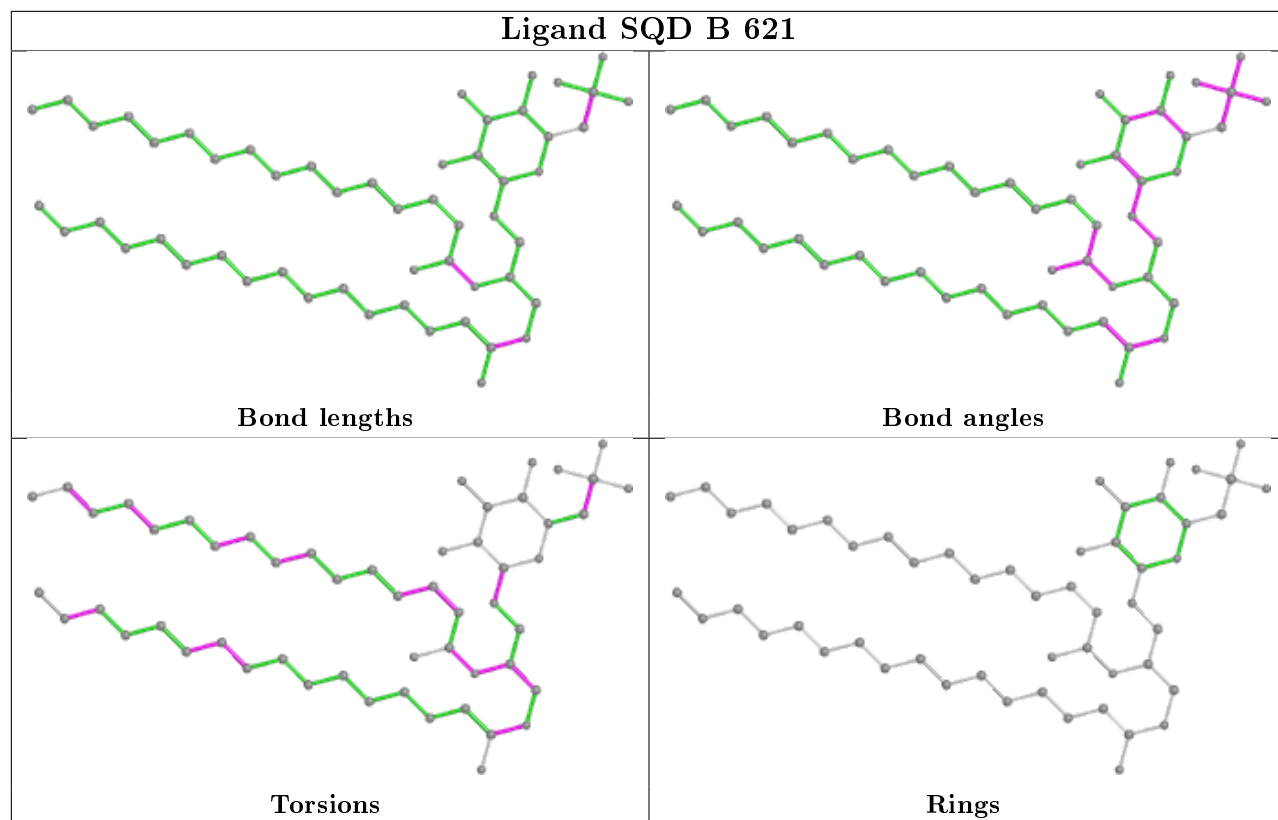


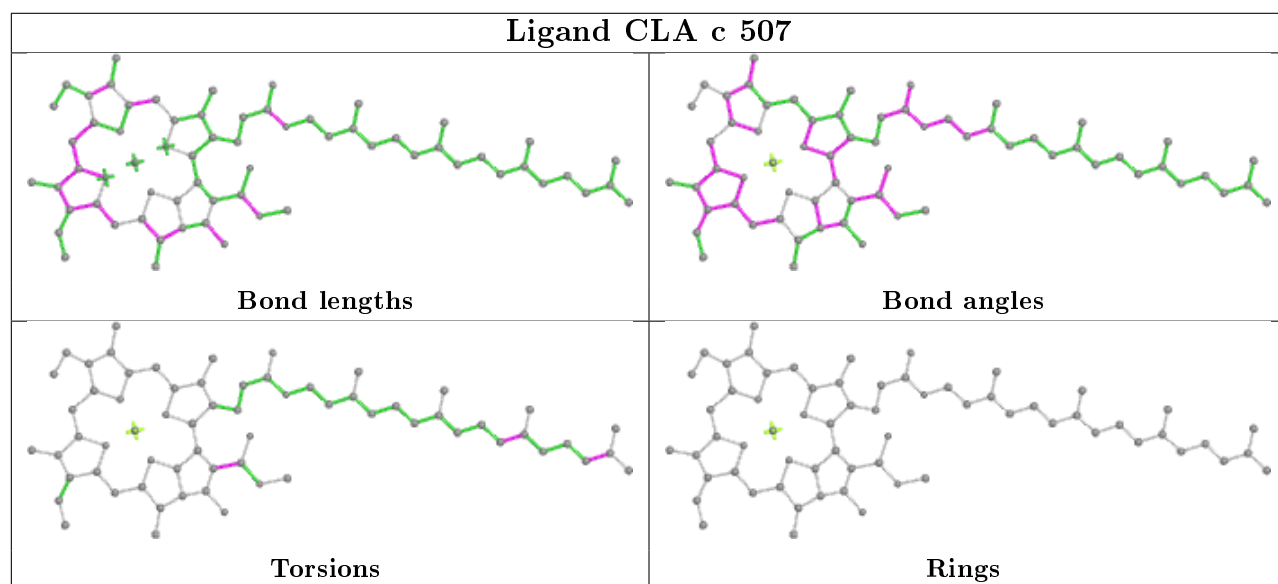
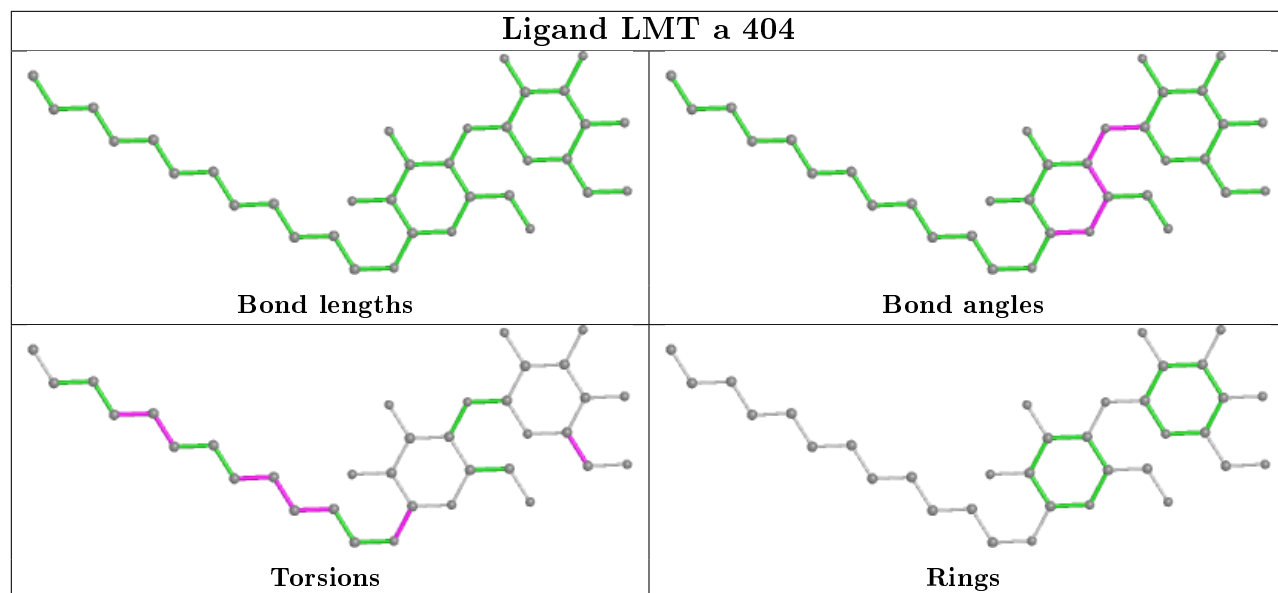
## Ligand LMT C 521

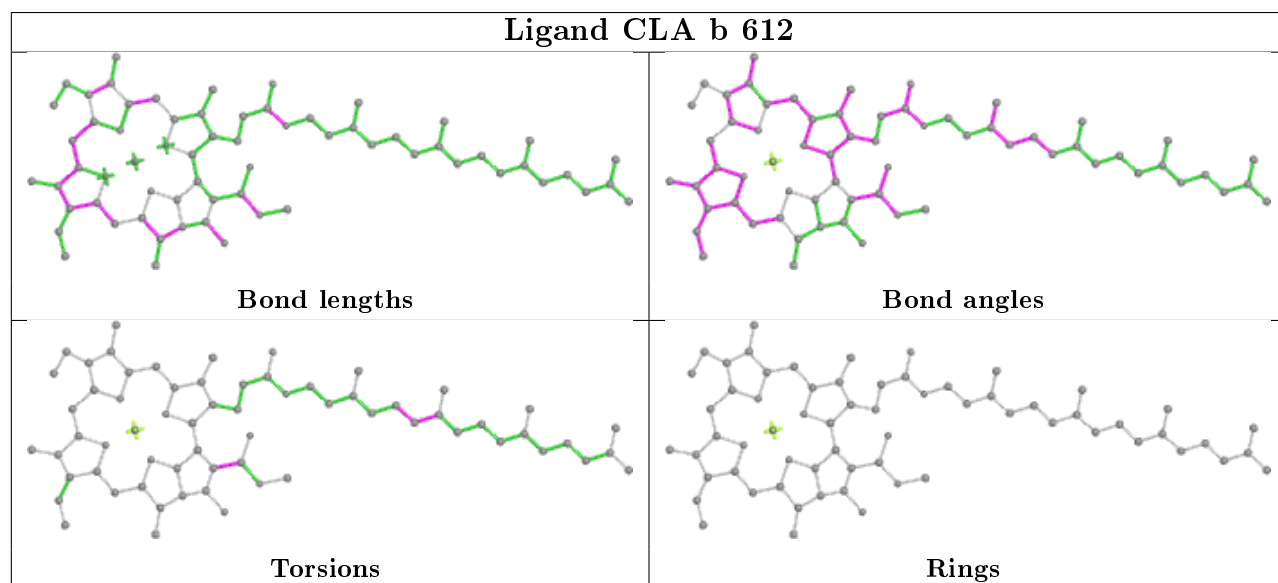
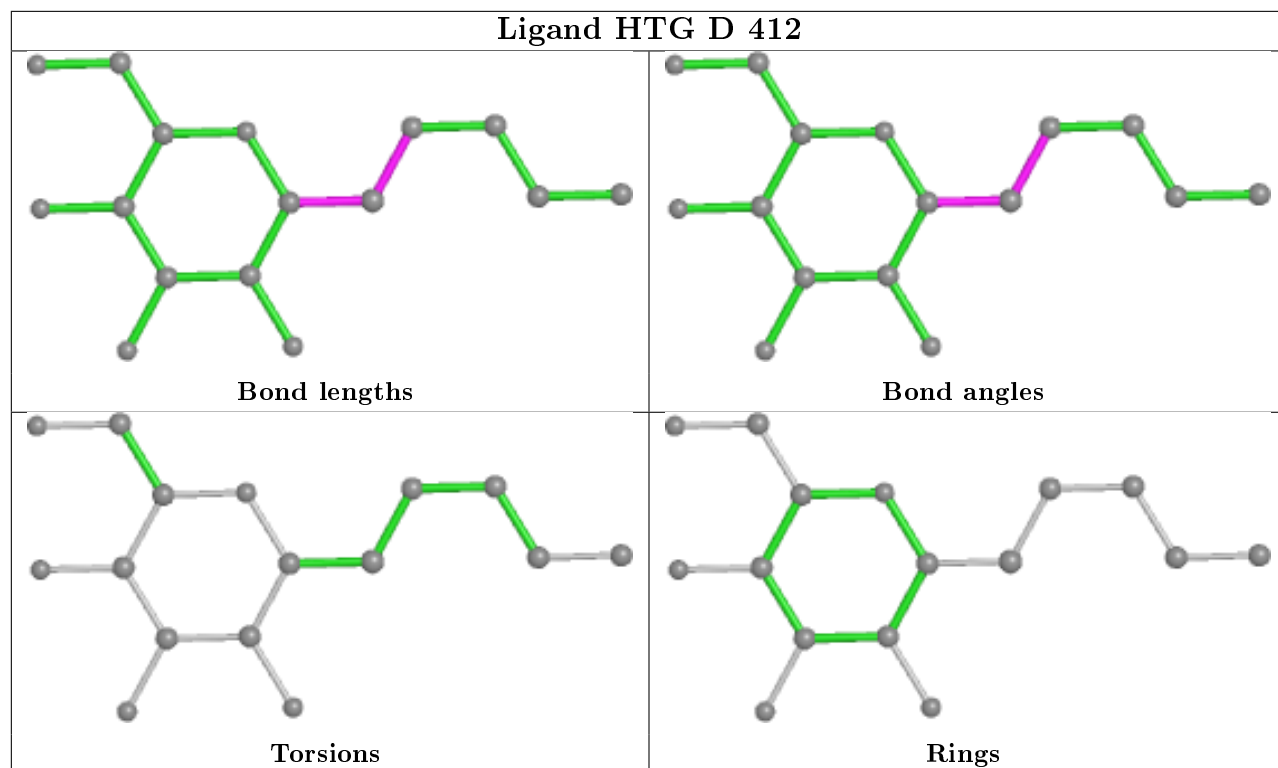


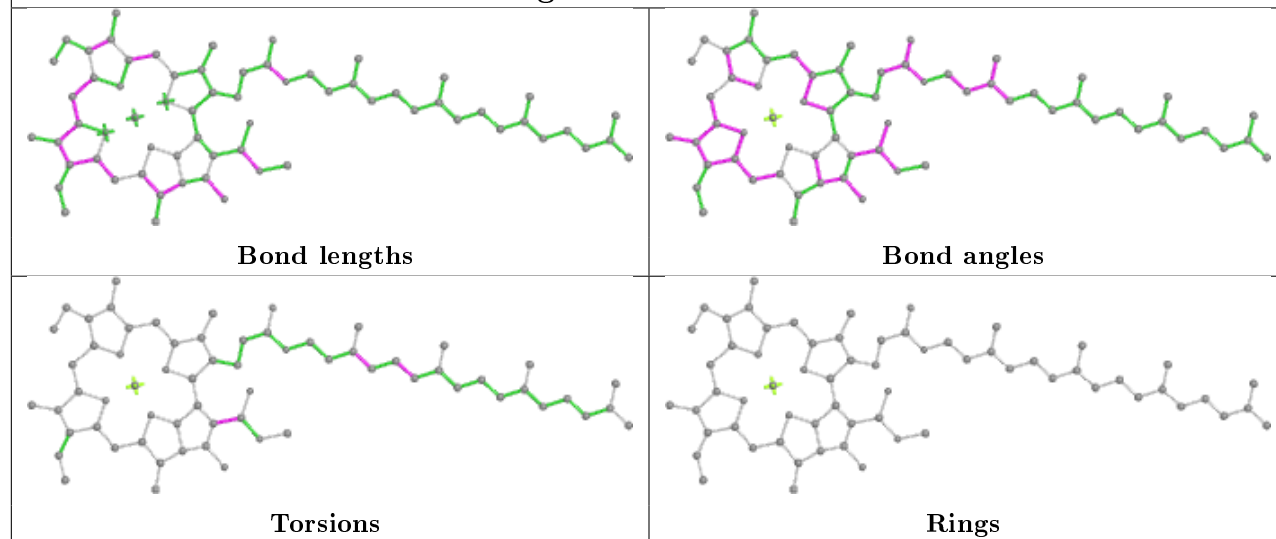
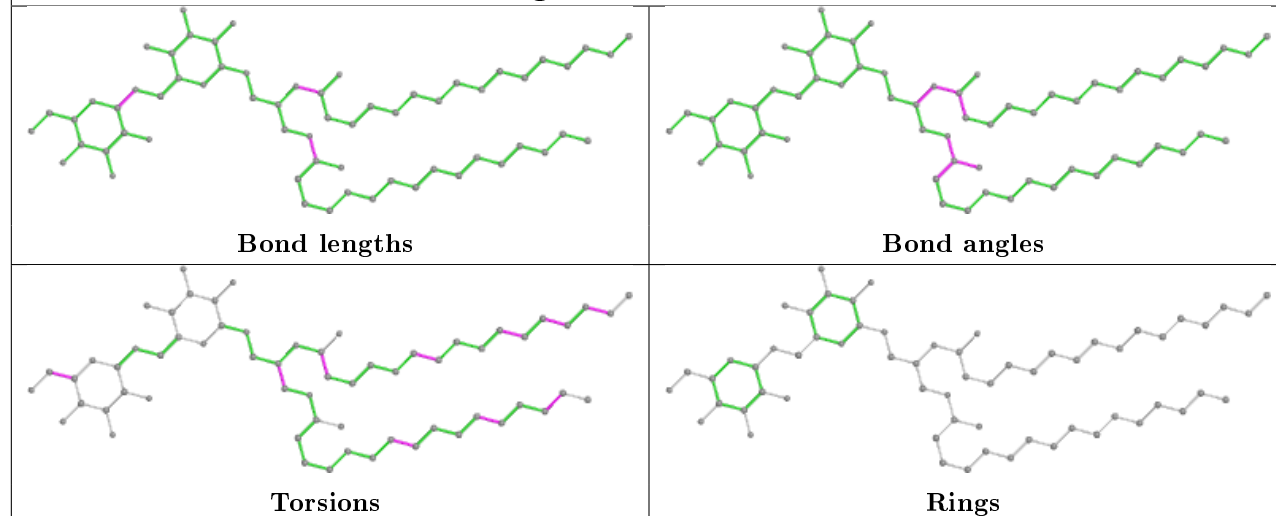
## Ligand CLA B 607

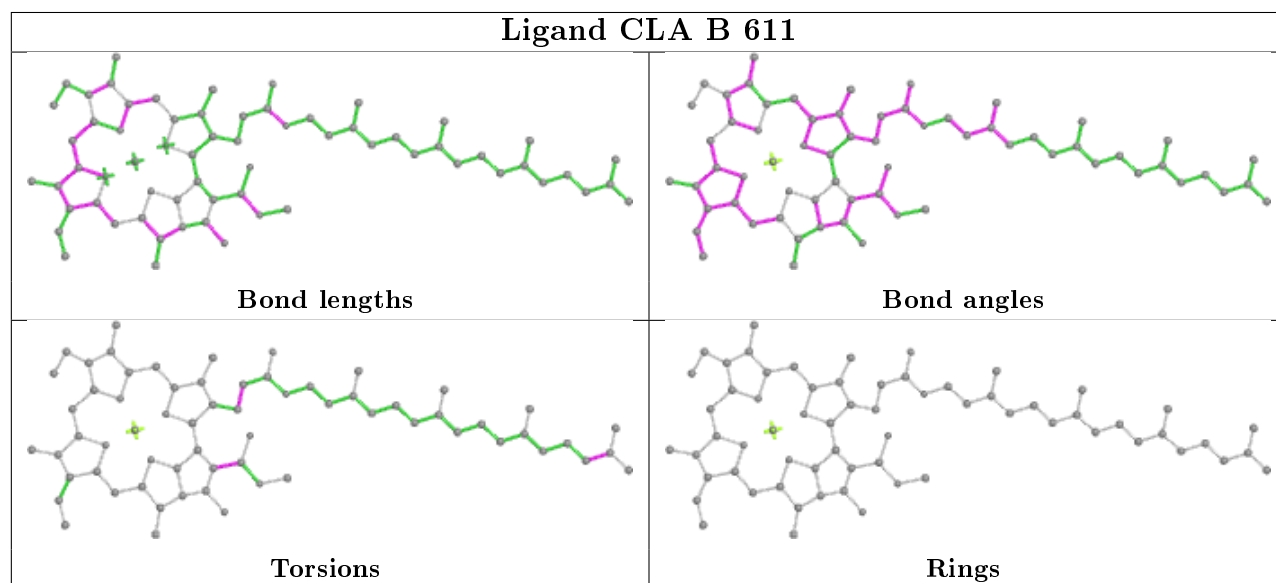
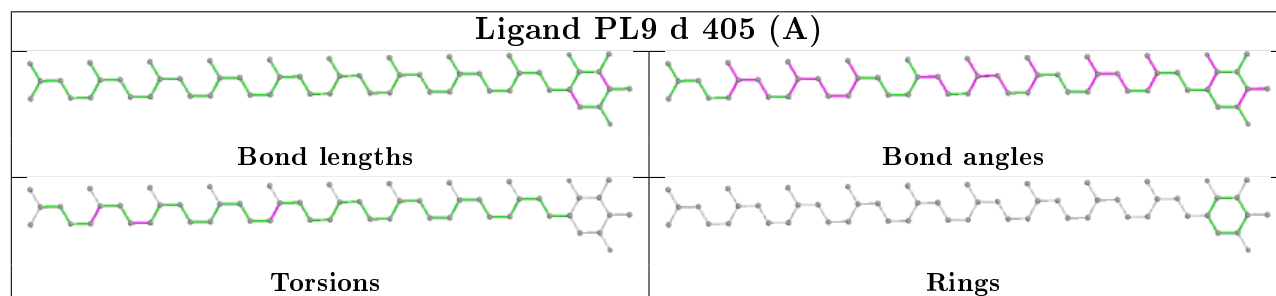
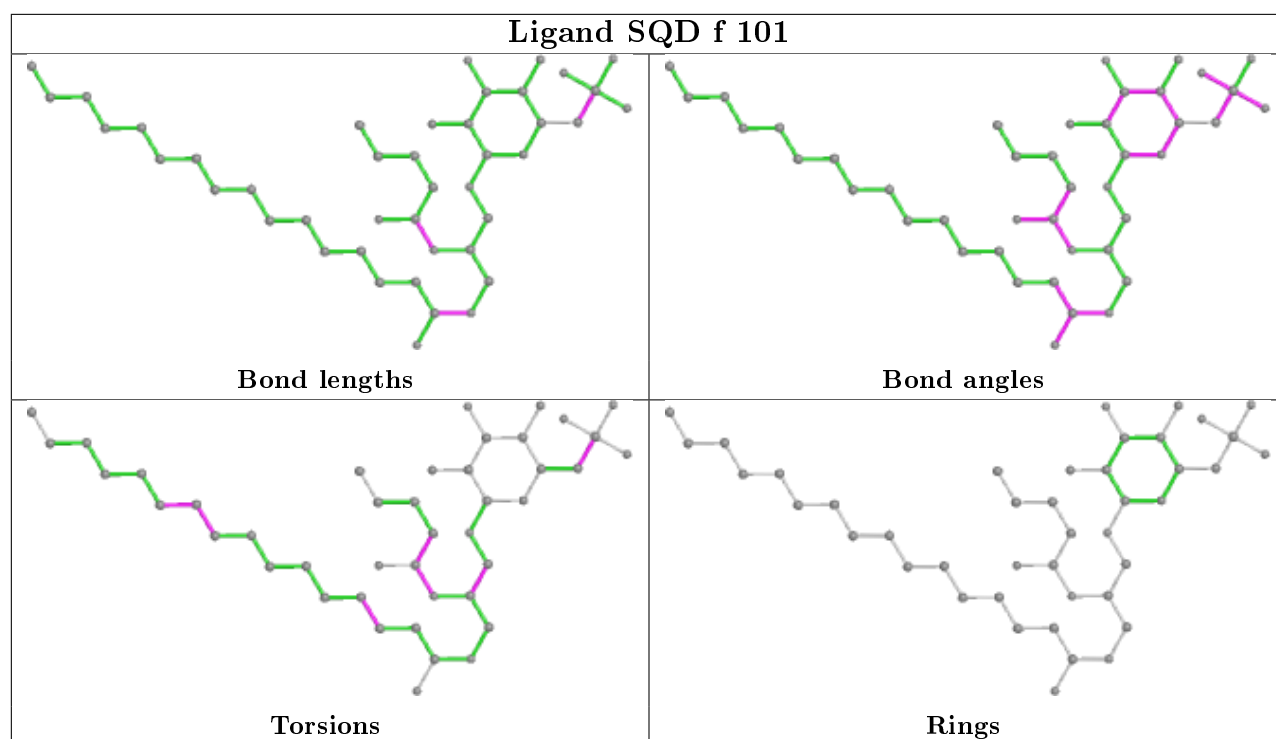


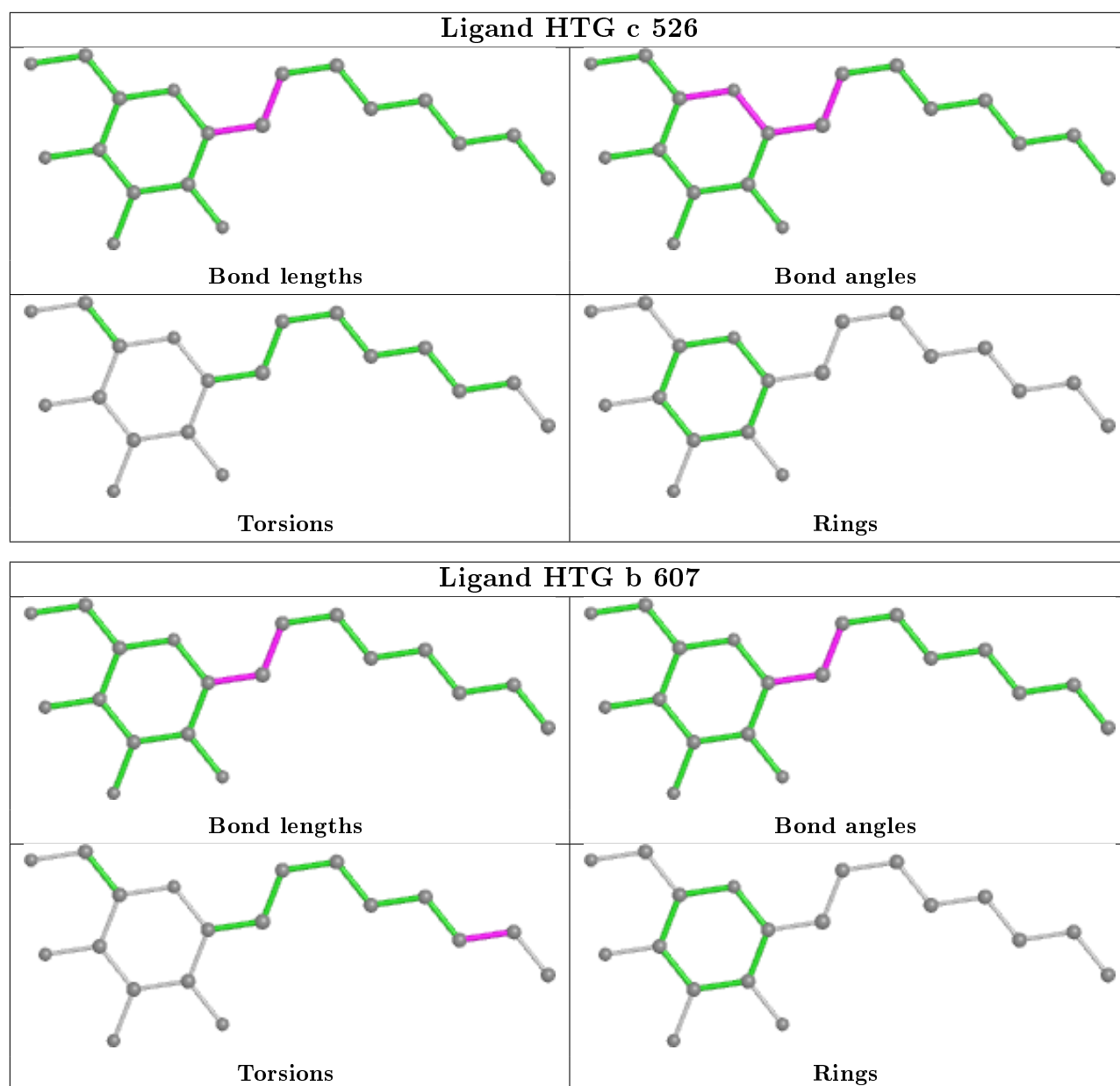




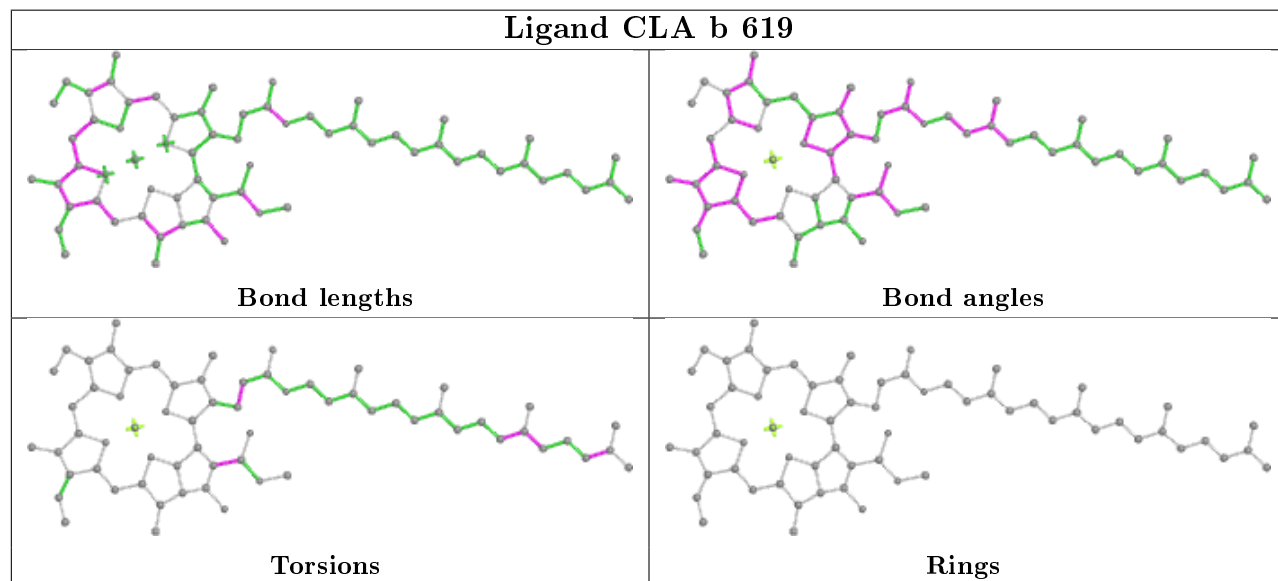
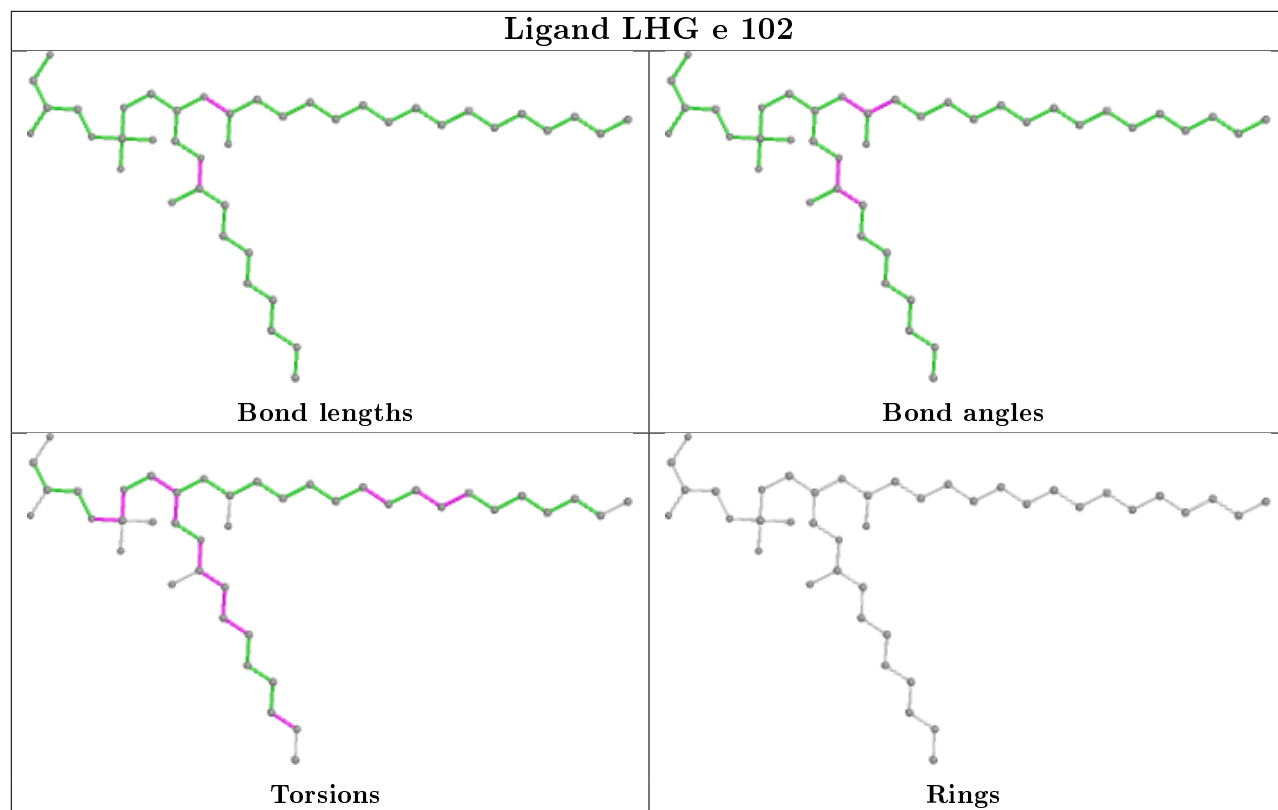


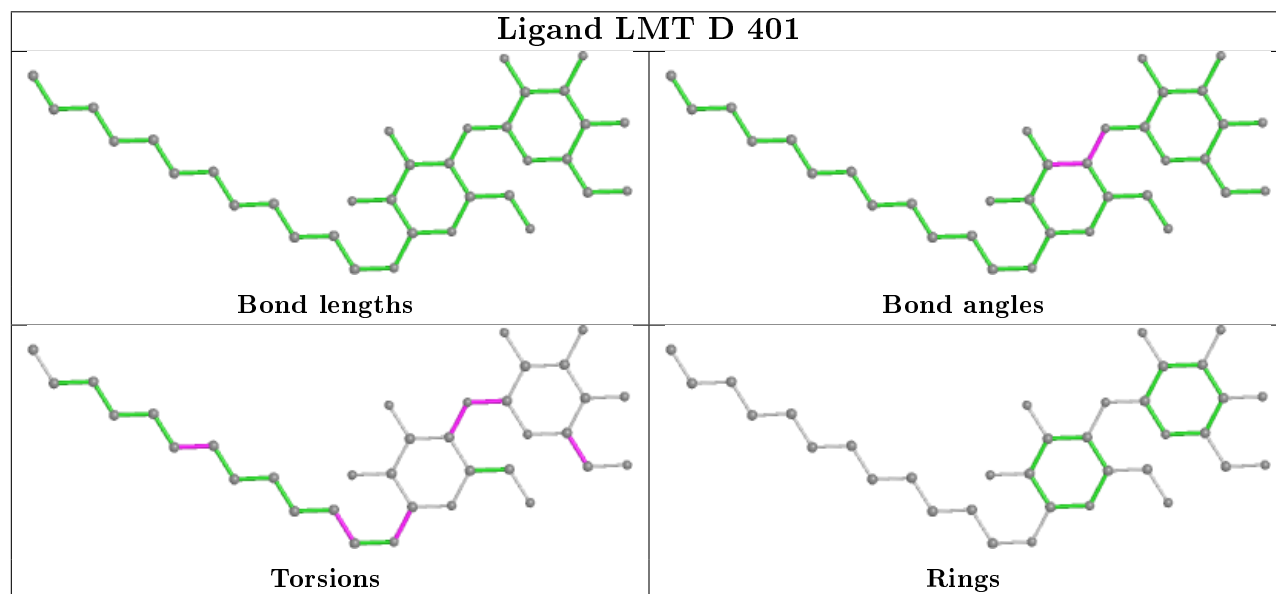
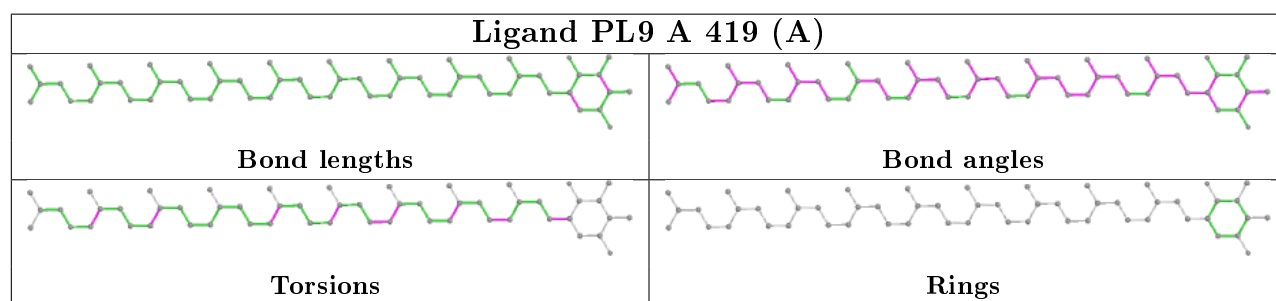
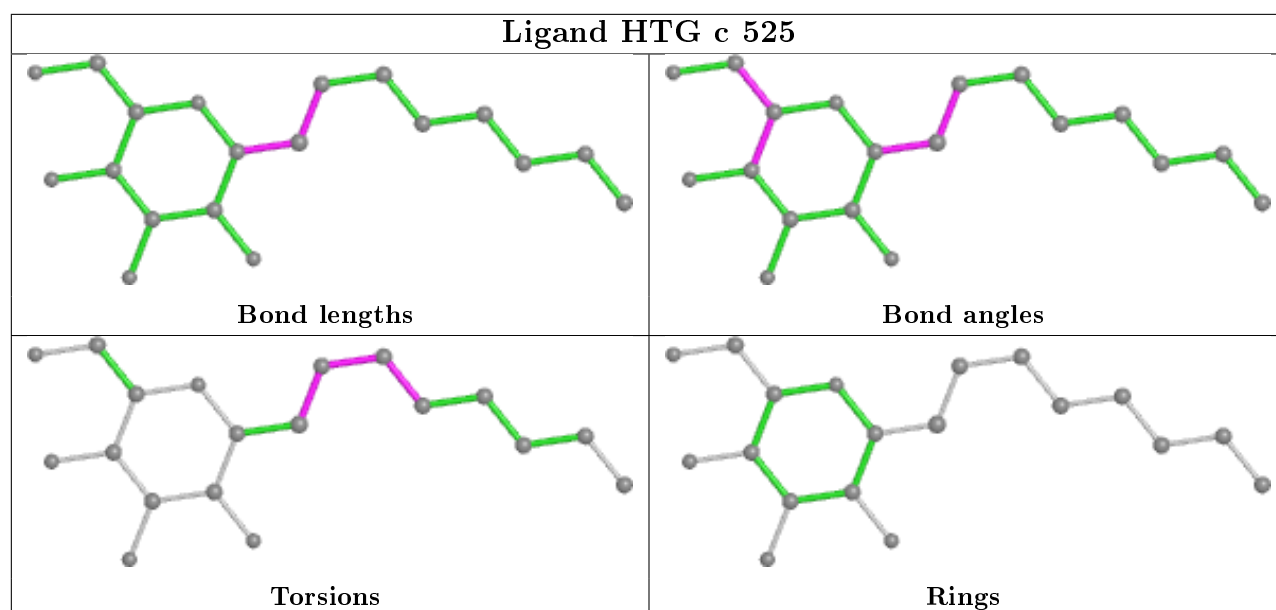
**Ligand CLA c 512****Ligand DGD h 102**



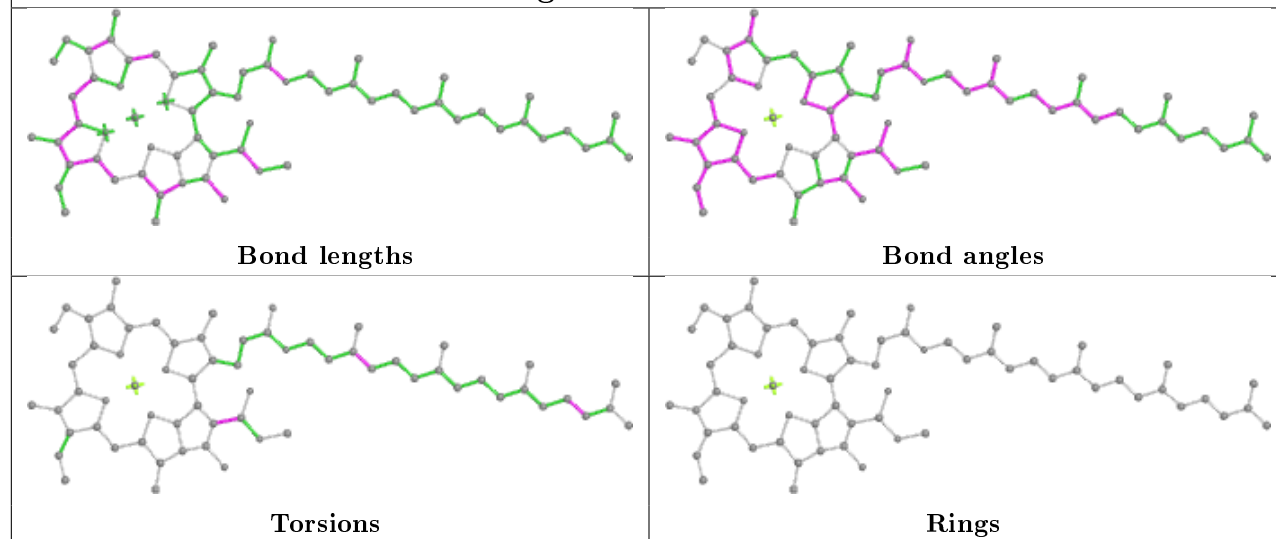




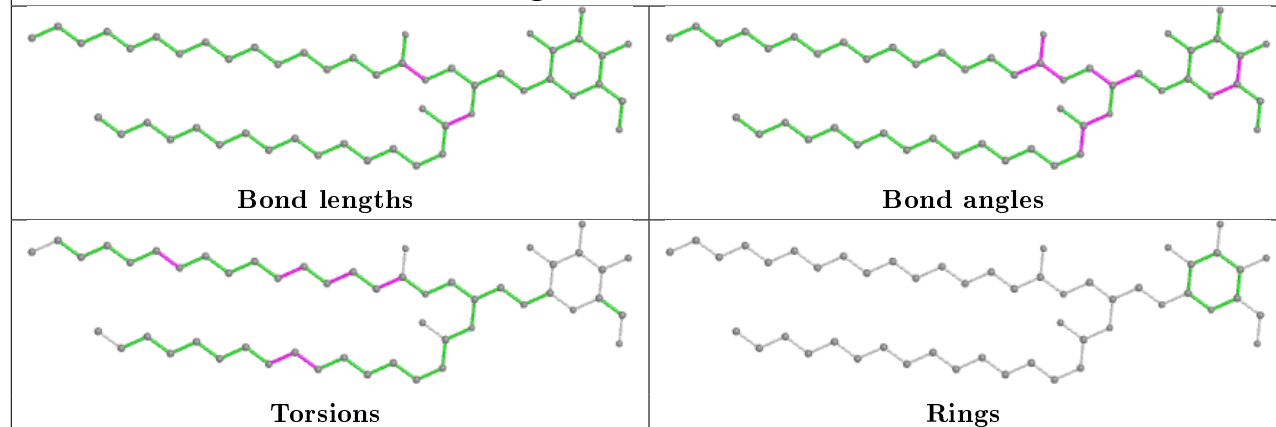




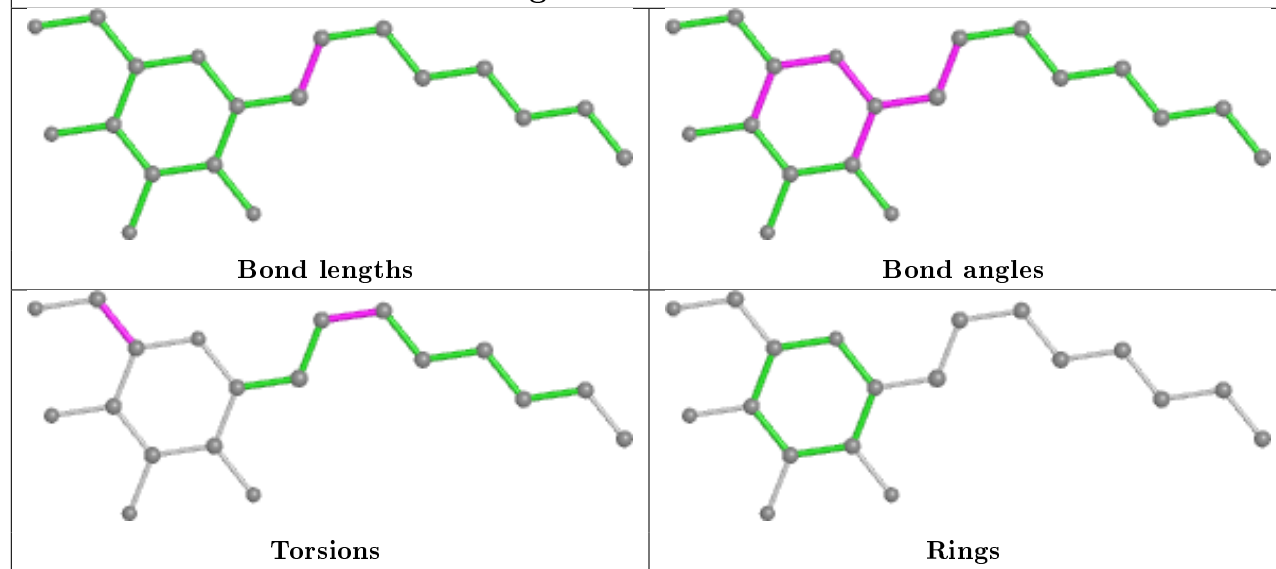
## Ligand CLA c 509



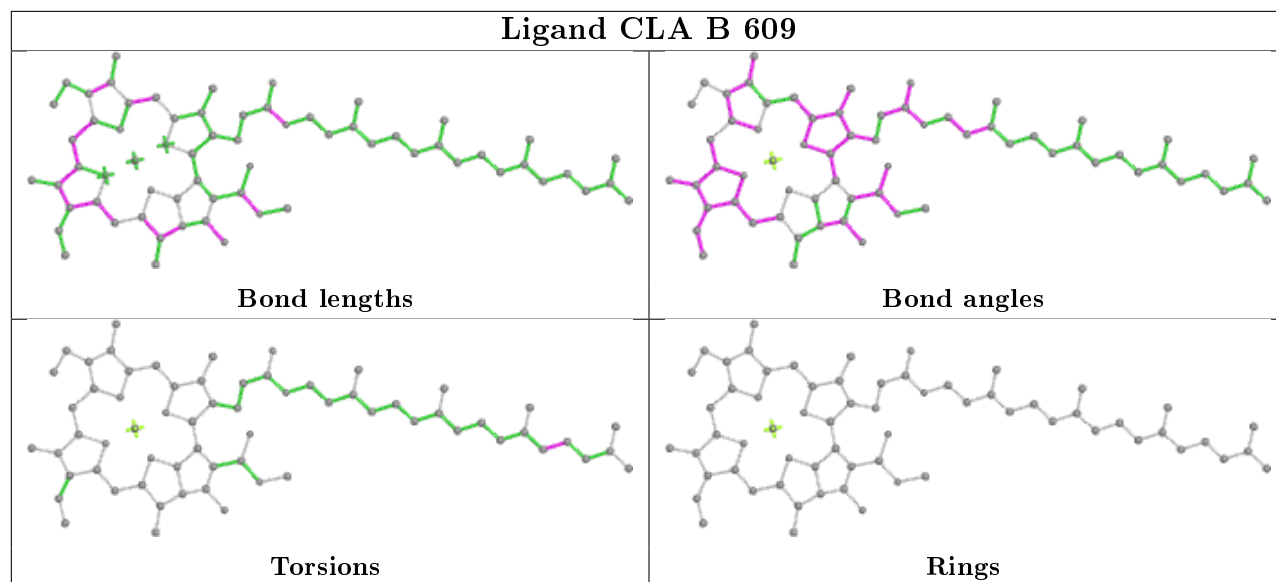
## Ligand LMG B 622



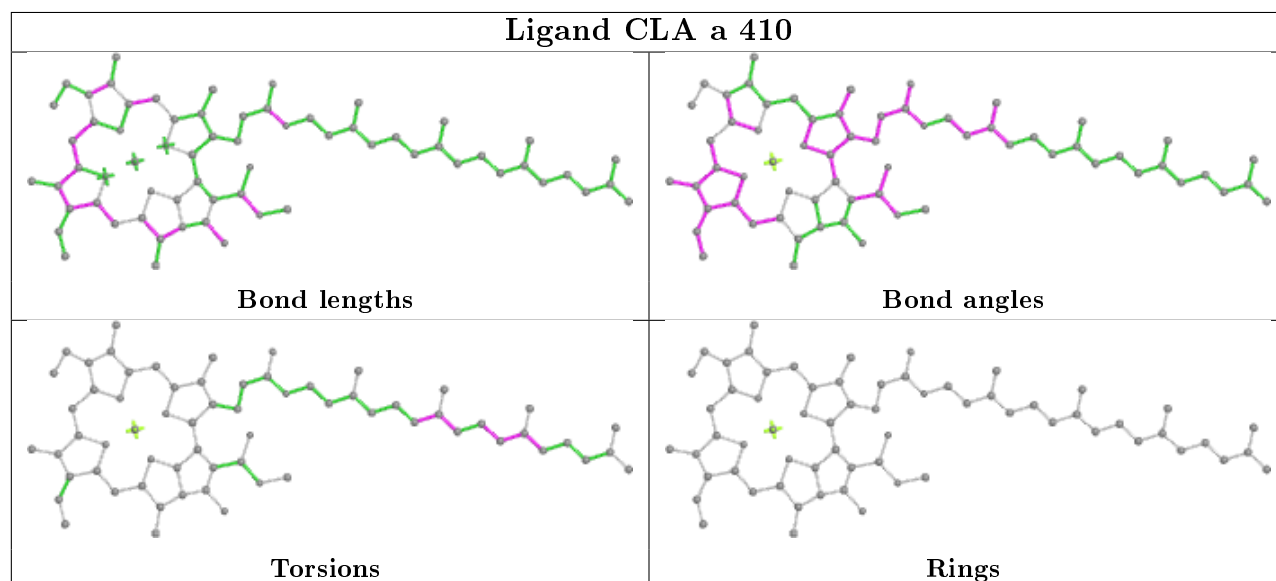
## Ligand HTG C 523



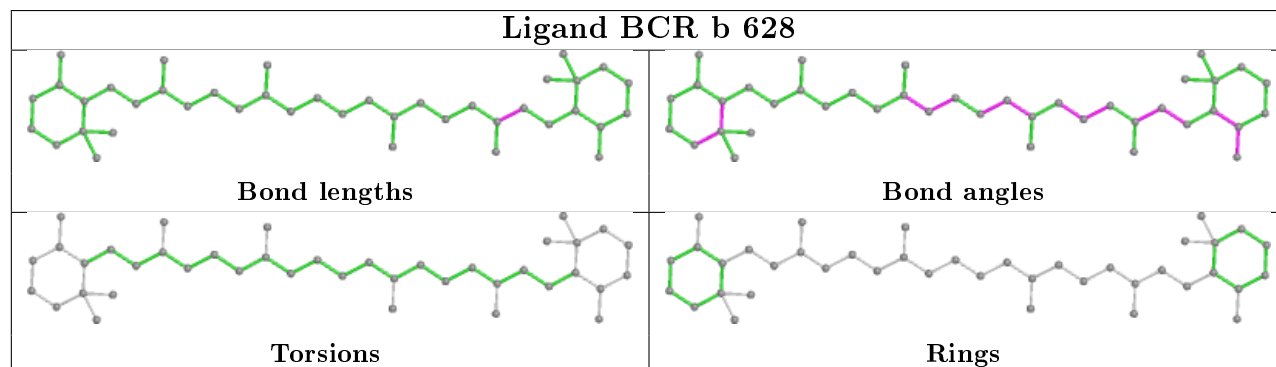
## Ligand CLA B 609

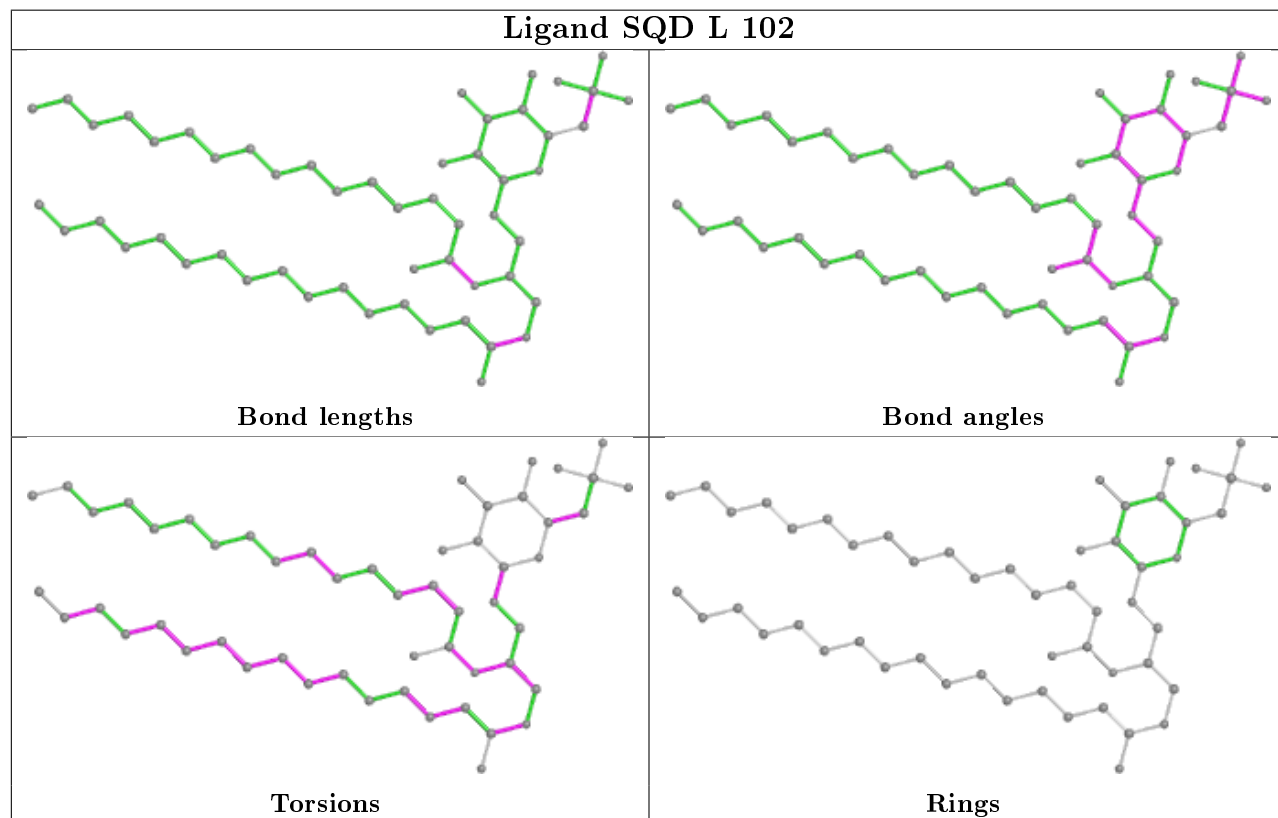
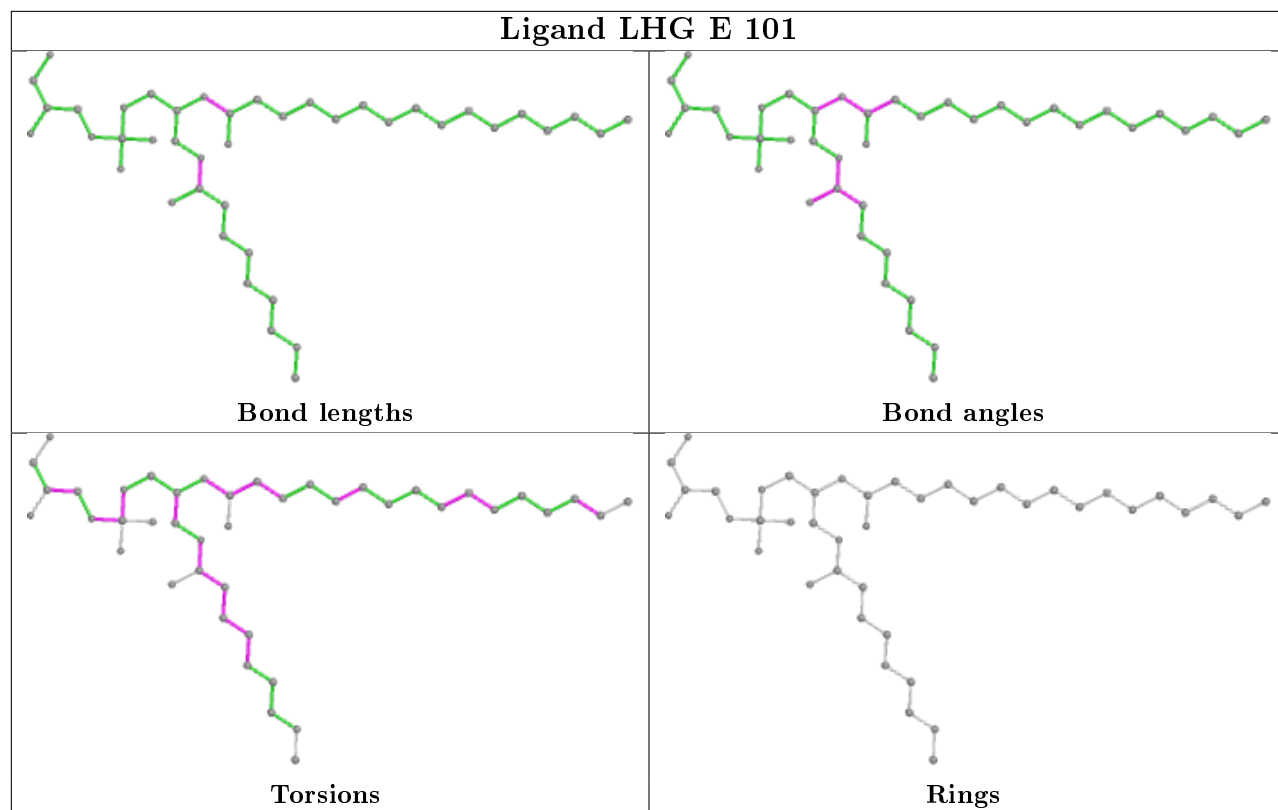


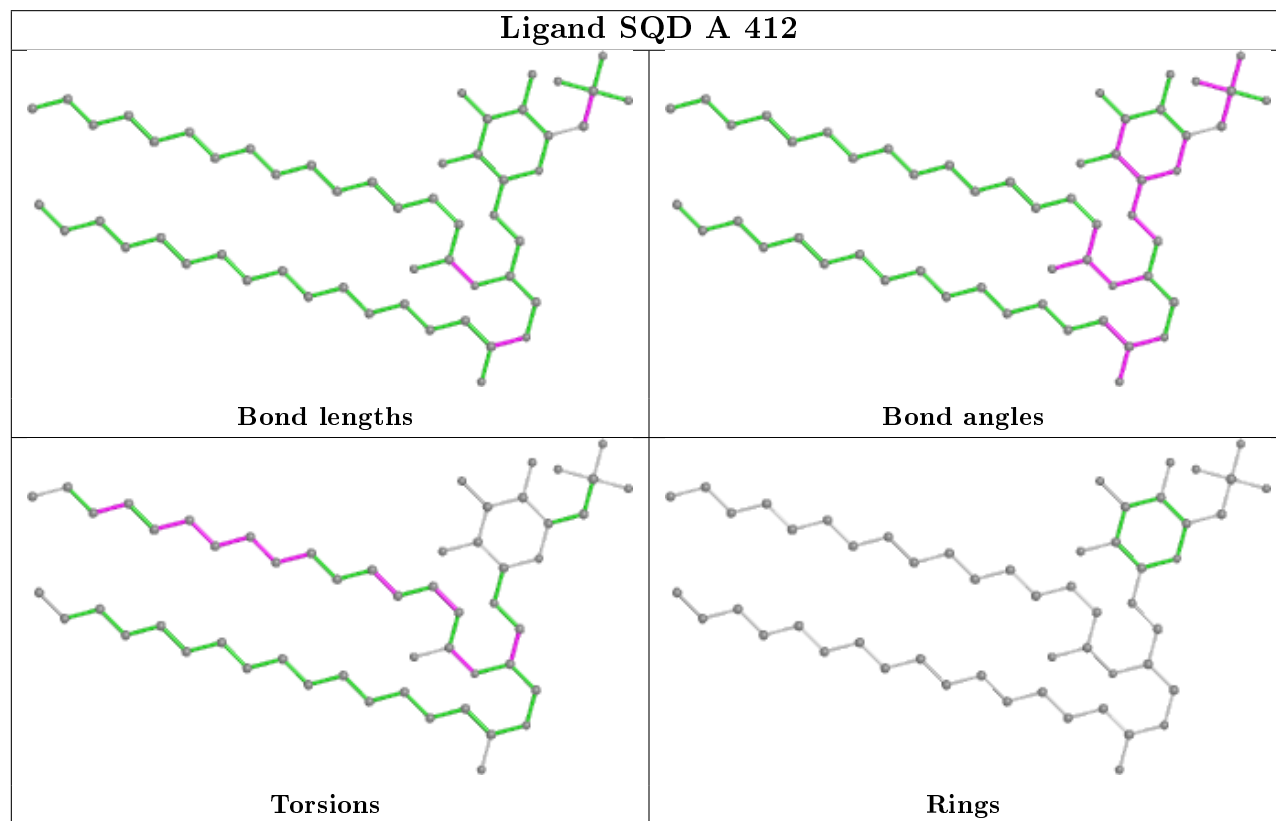
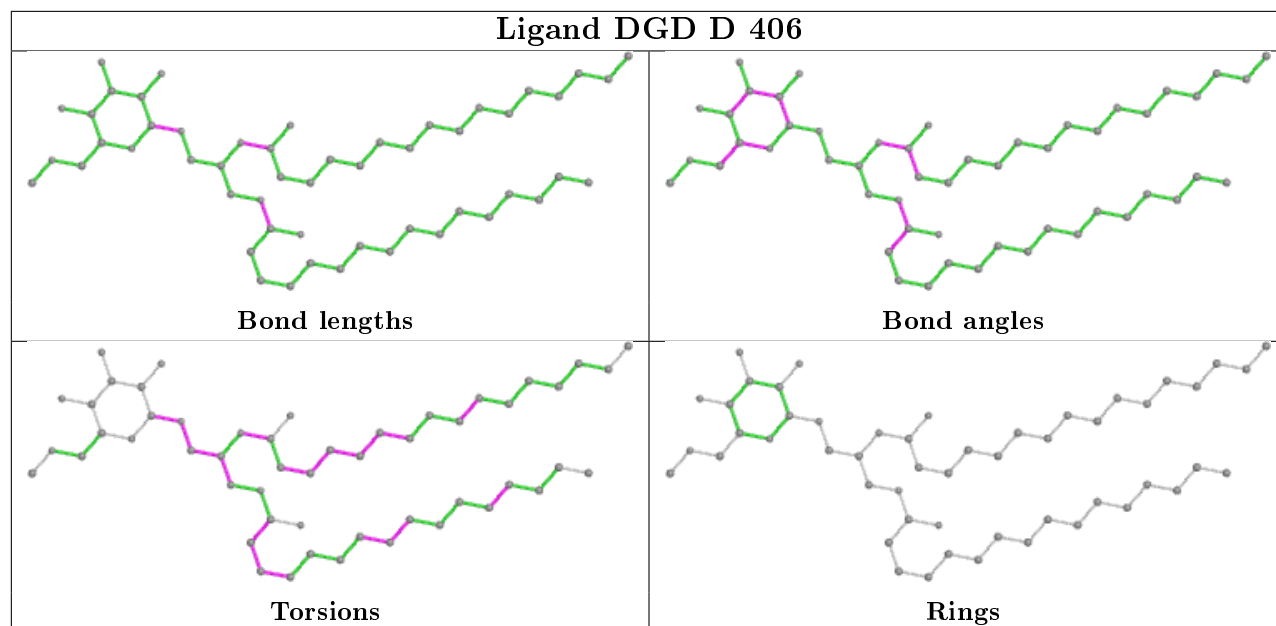
## Ligand CLA a 410

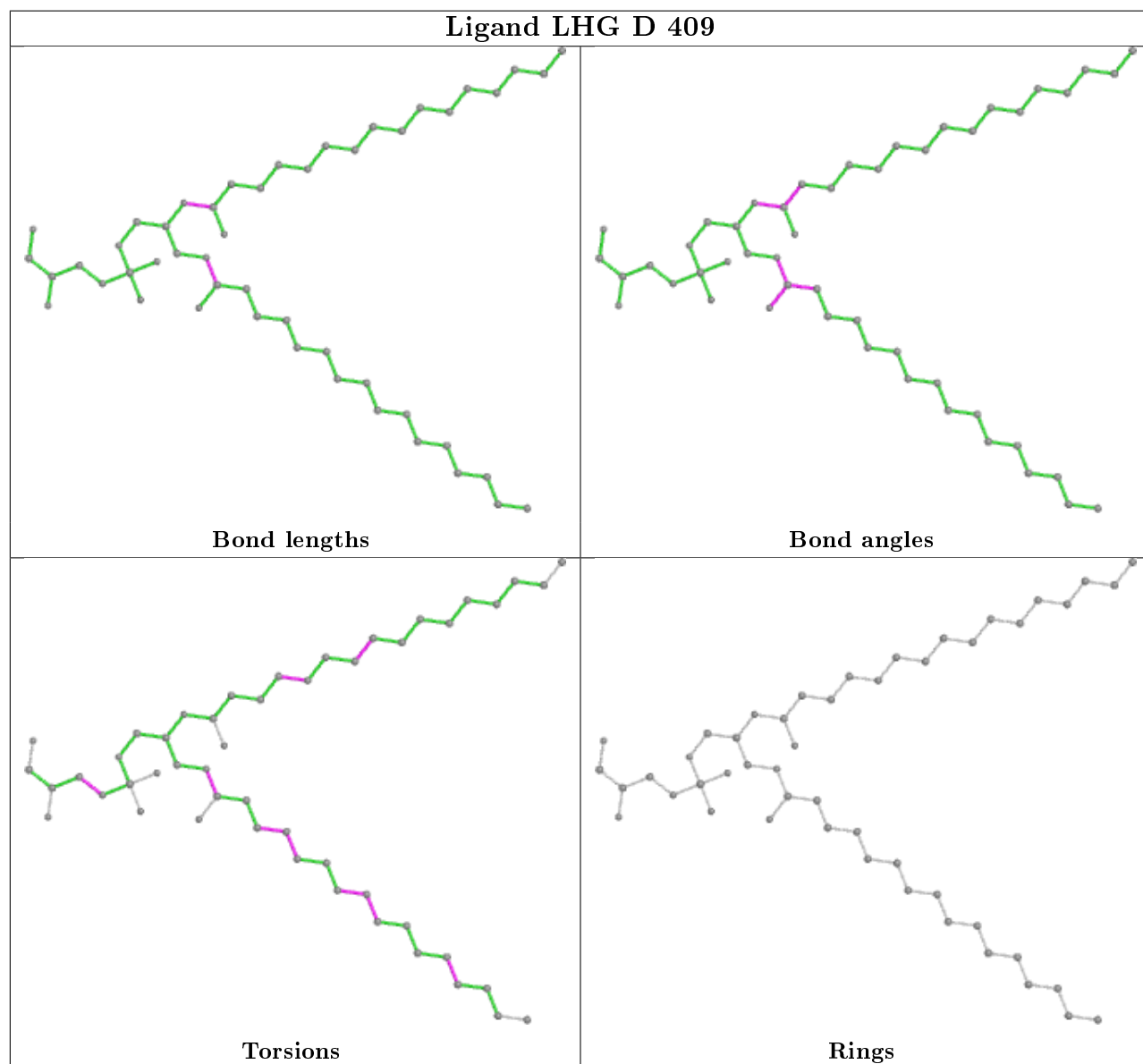
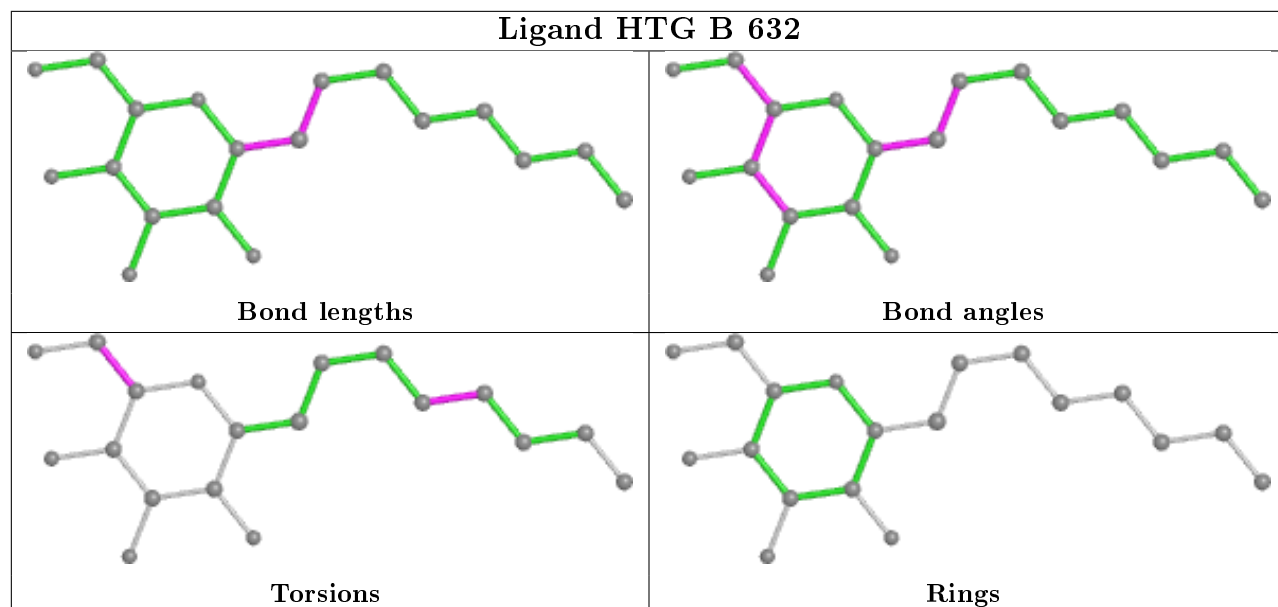


## Ligand BCR b 628







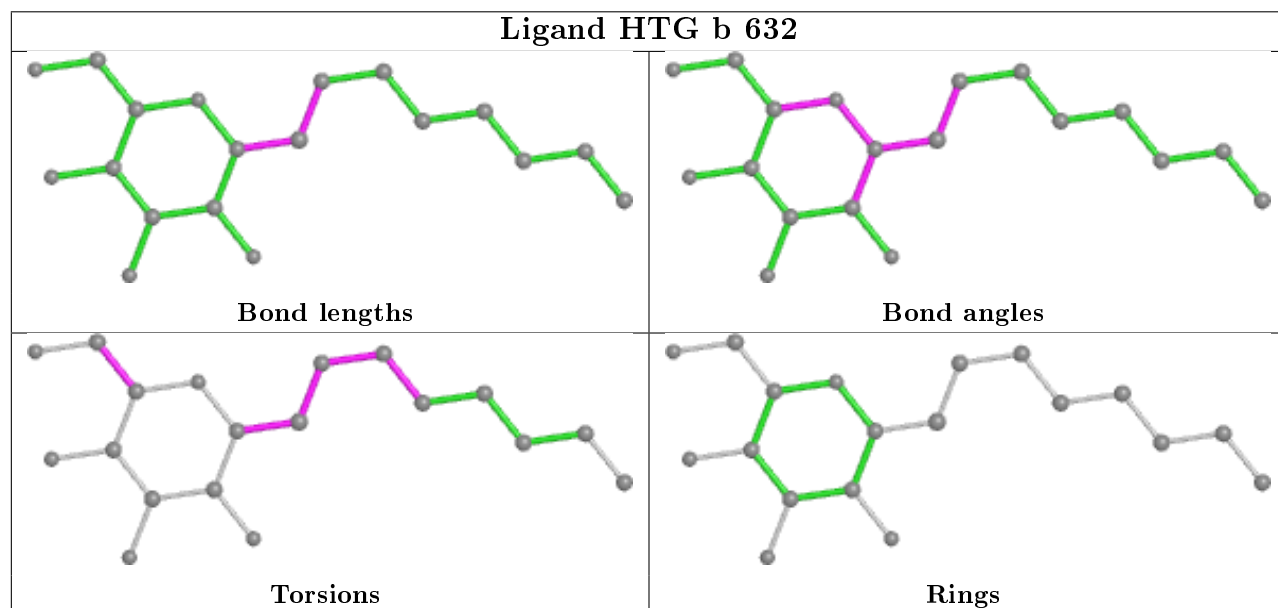
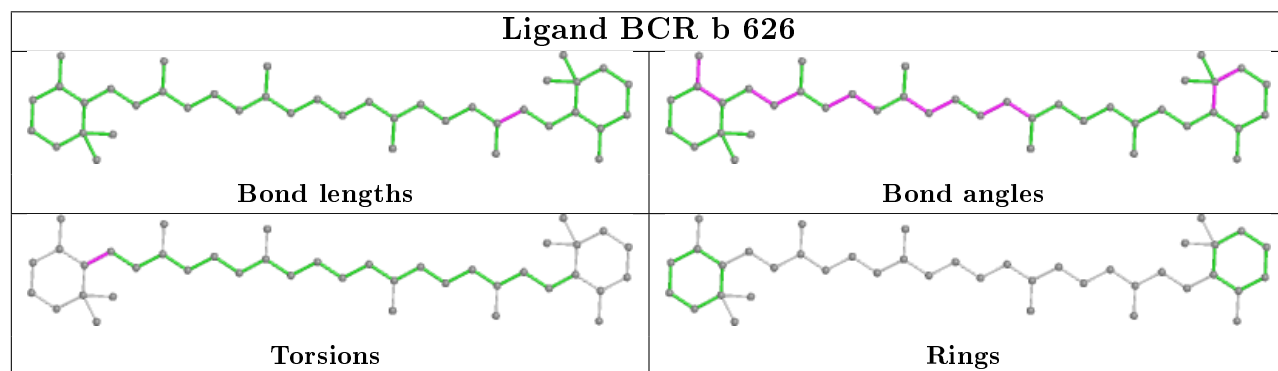
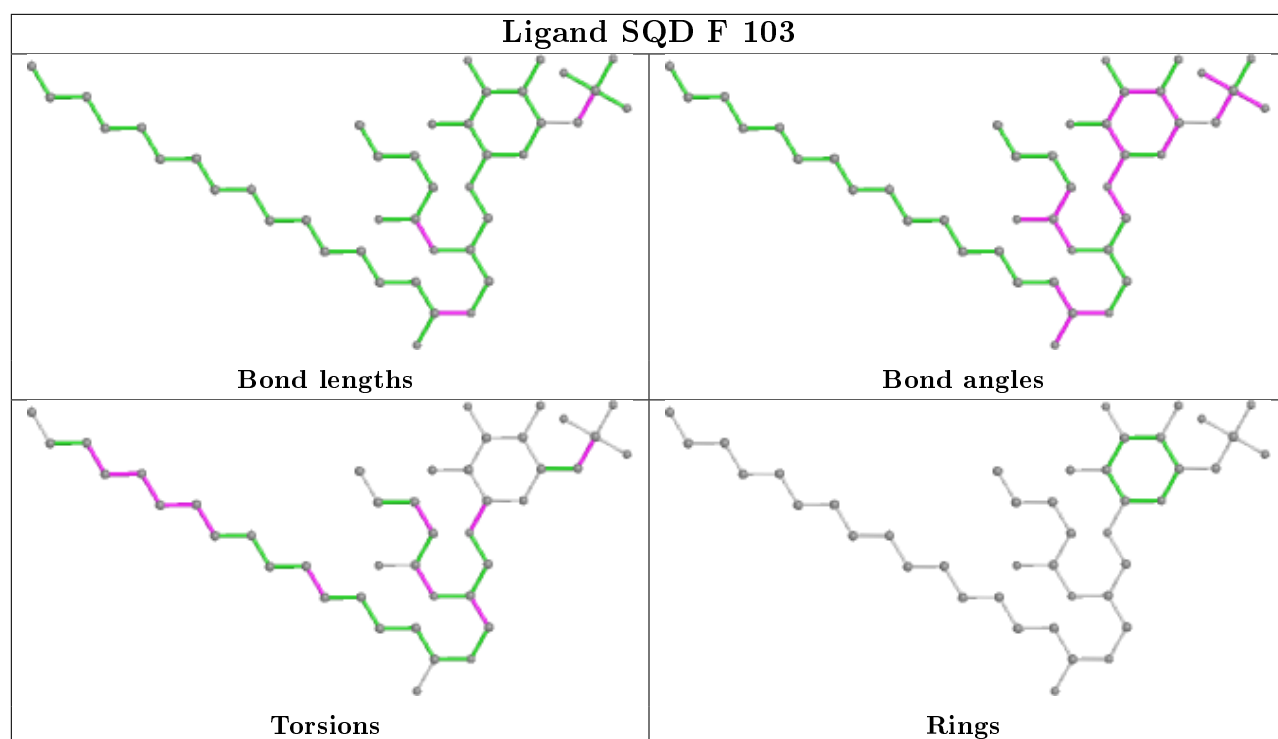


Ligand PL9 a 415 (A)	
<p>Bond lengths</p>	<p>Bond angles</p>
<p>Torsions</p>	<p>Rings</p>

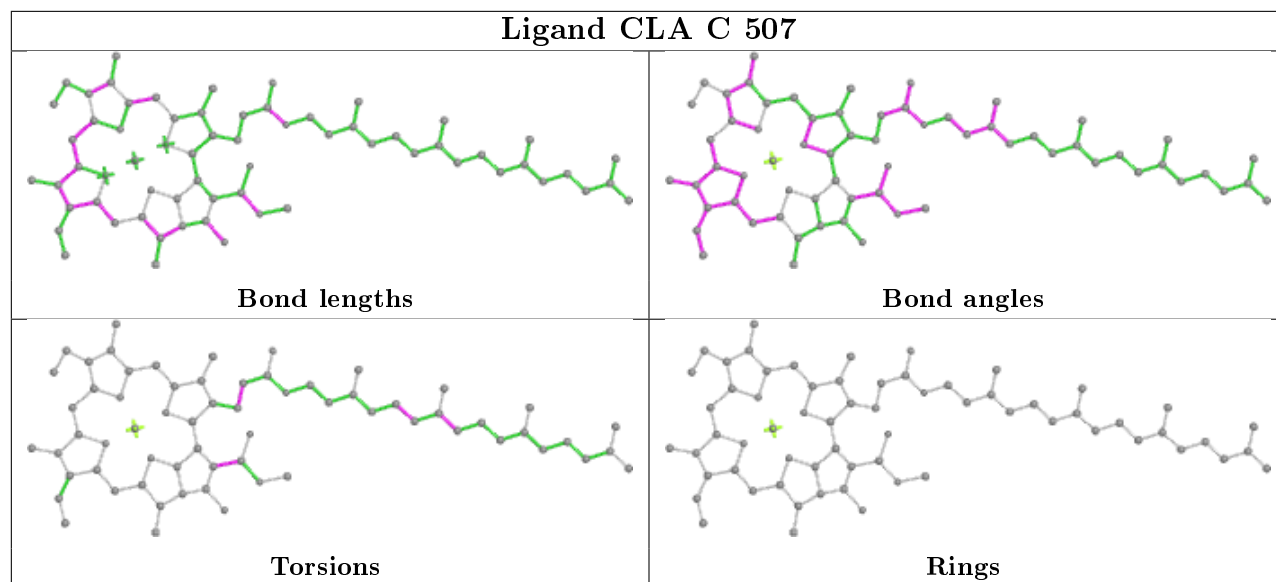
Ligand HTG V 206	
<p>Bond lengths</p>	<p>Bond angles</p>
<p>Torsions</p>	<p>Rings</p>

Ligand PL9 a 415 (B)	
<p>Bond lengths</p>	<p>Bond angles</p>
<p>Torsions</p>	<p>Rings</p>

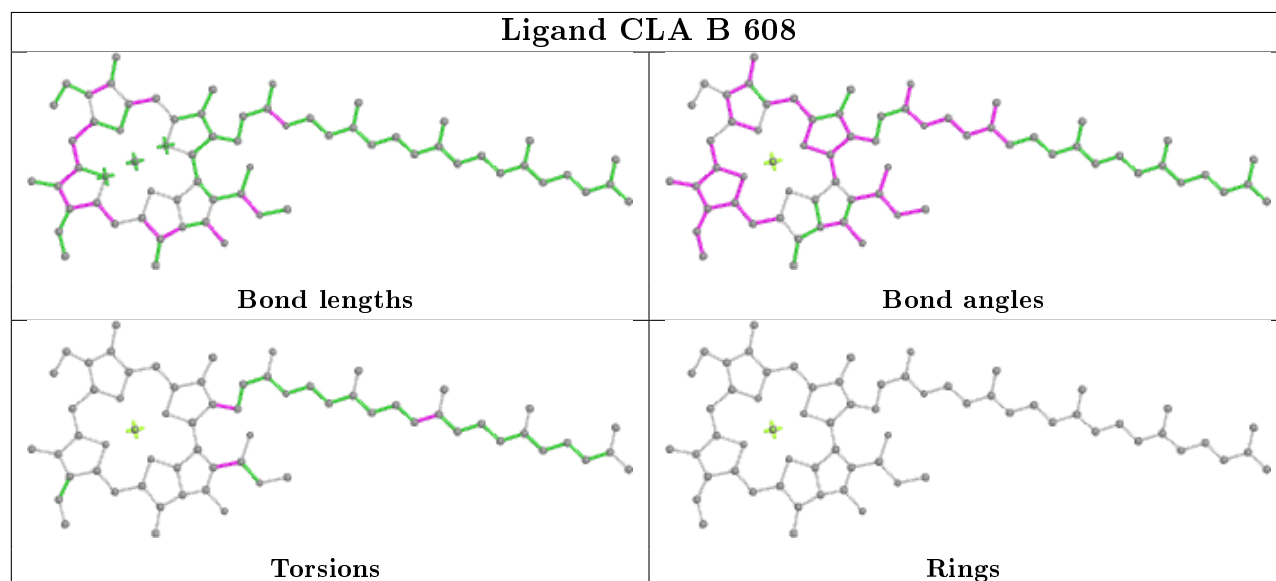




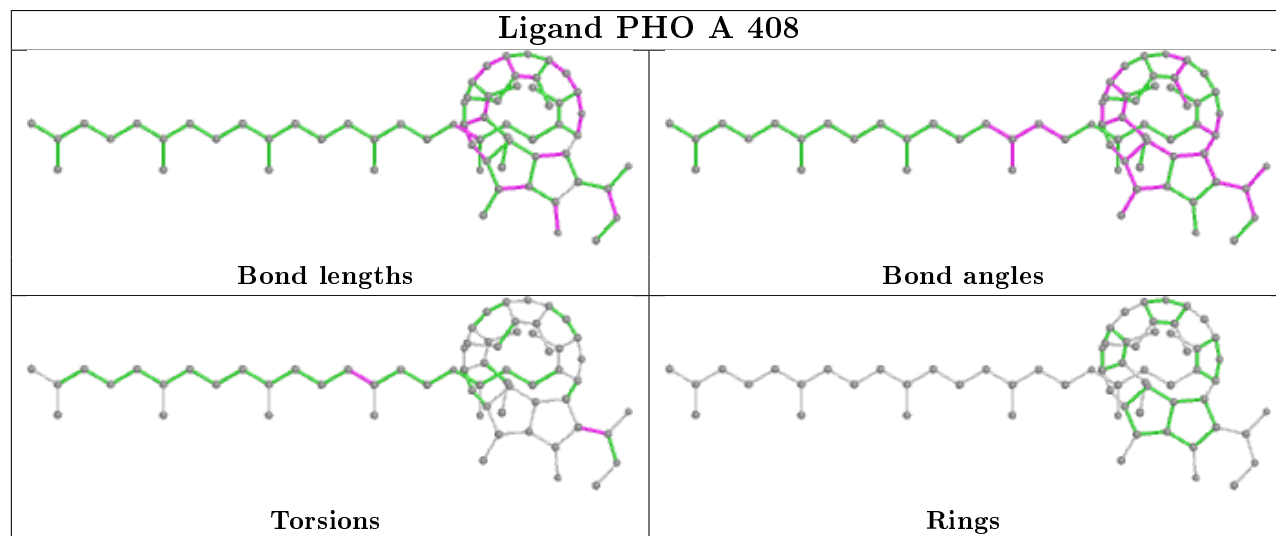
## Ligand CLA C 507

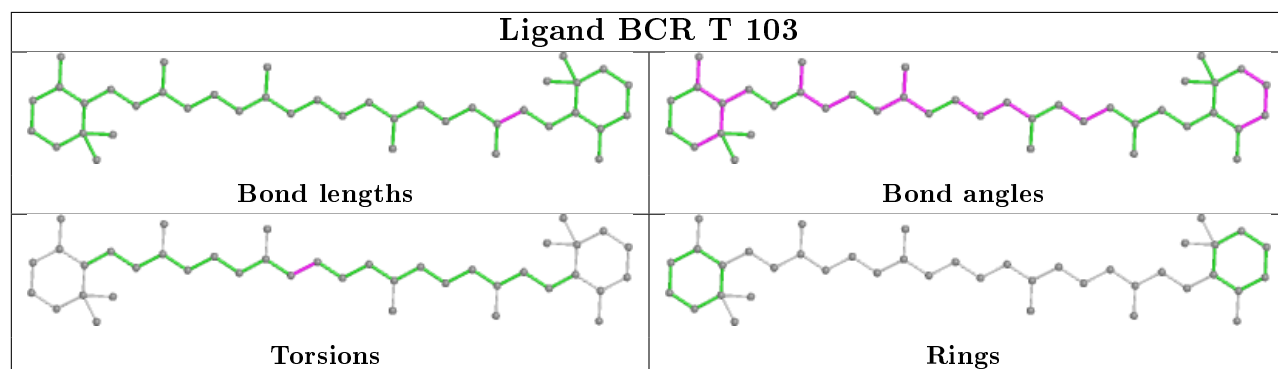
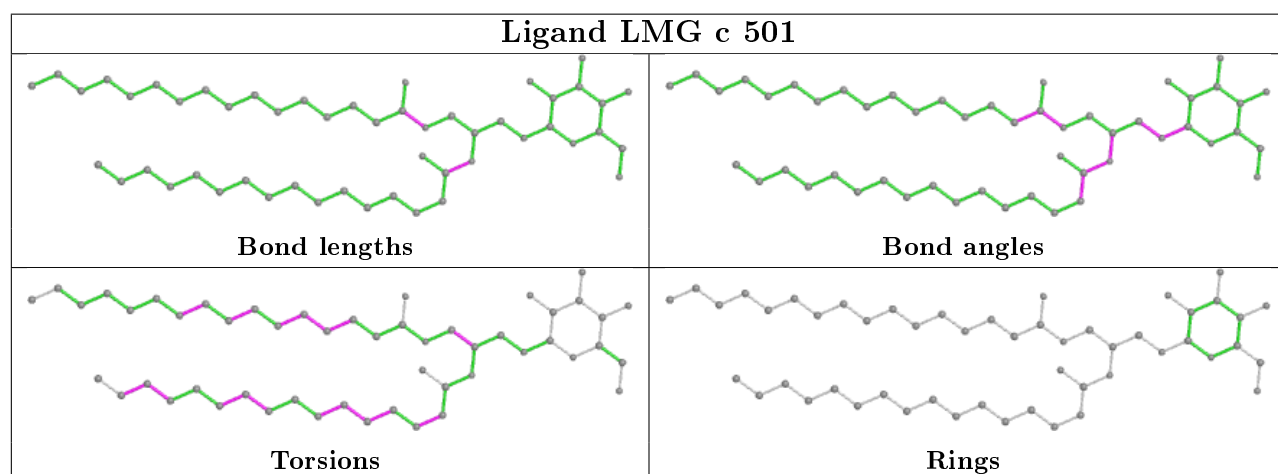
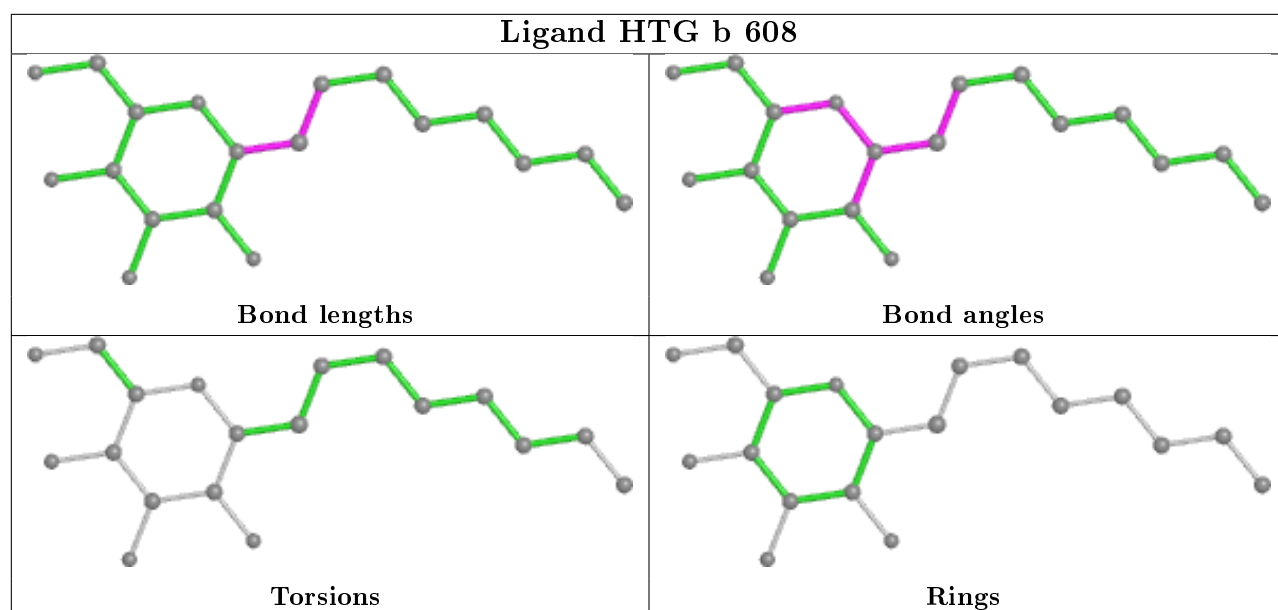


## Ligand CLA B 608

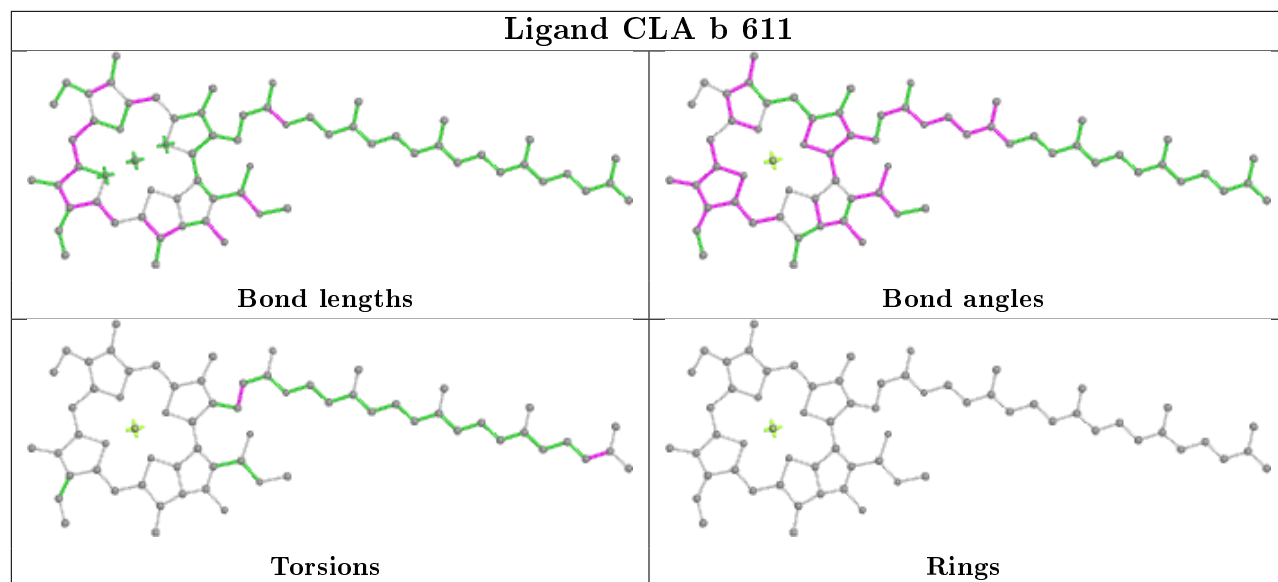


## Ligand PHO A 408

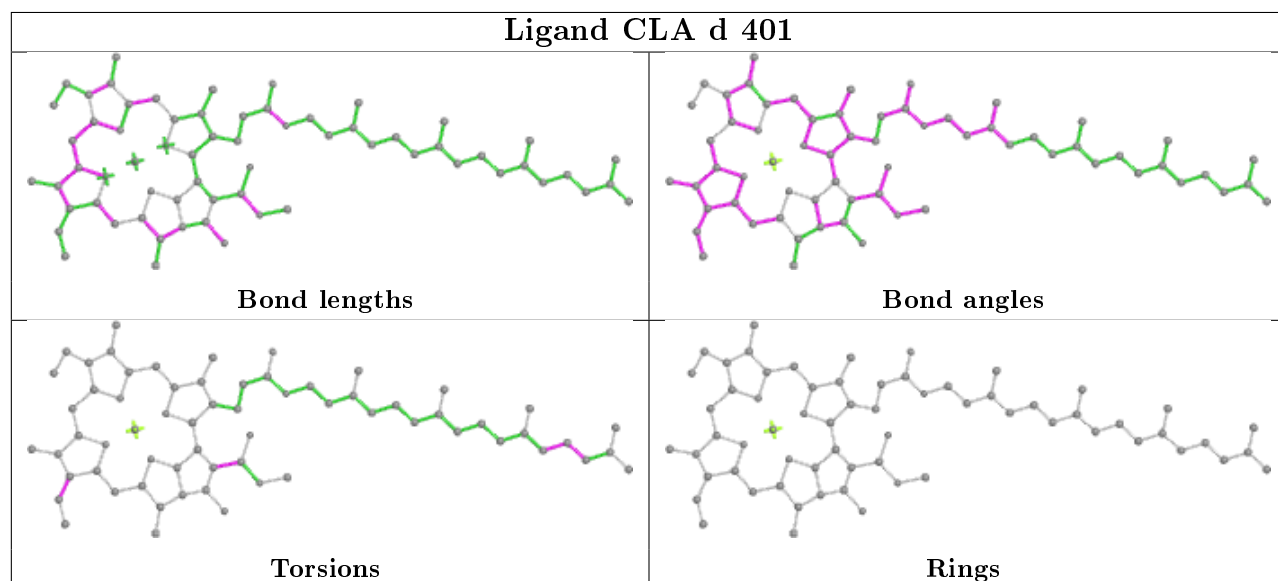




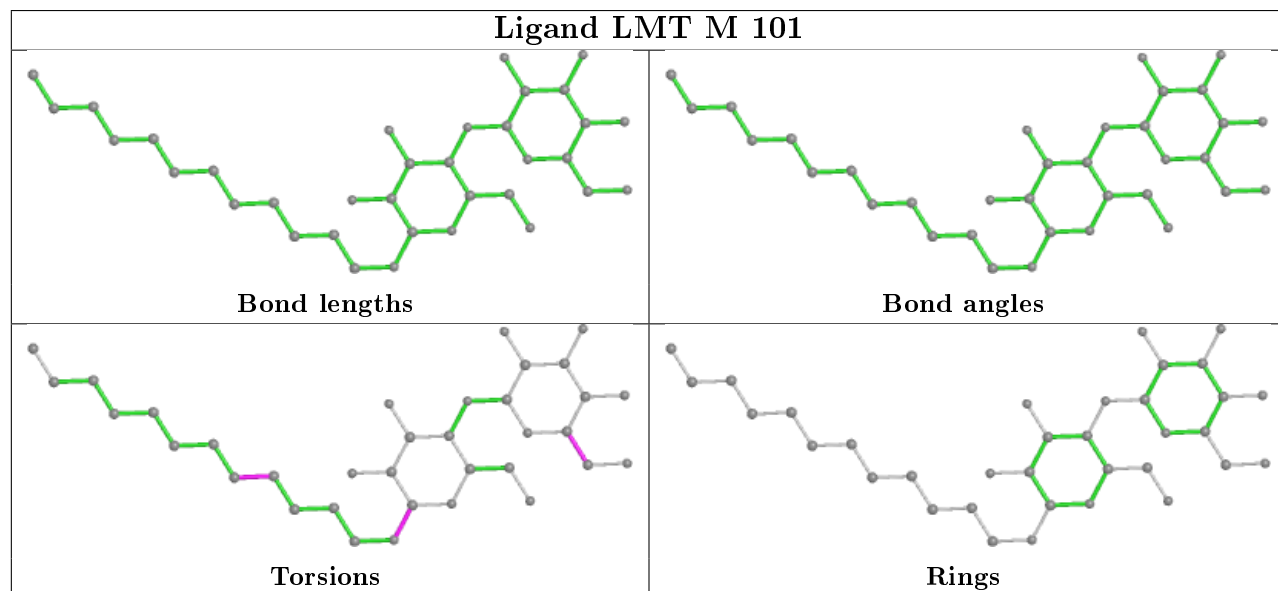
## Ligand CLA b 611



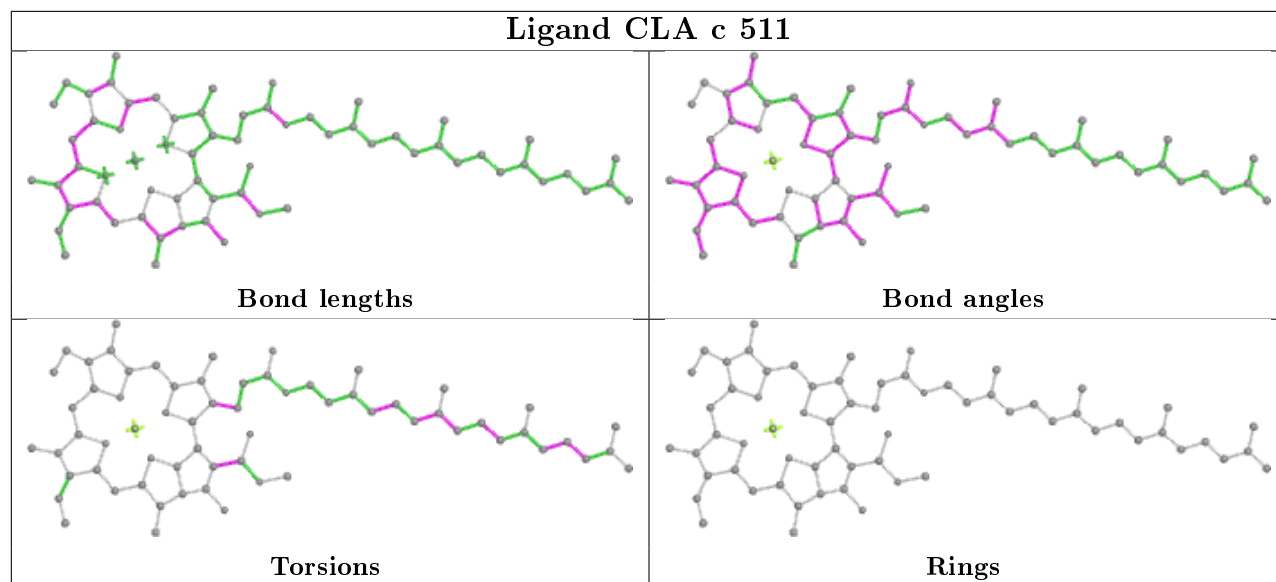
## Ligand CLA d 401



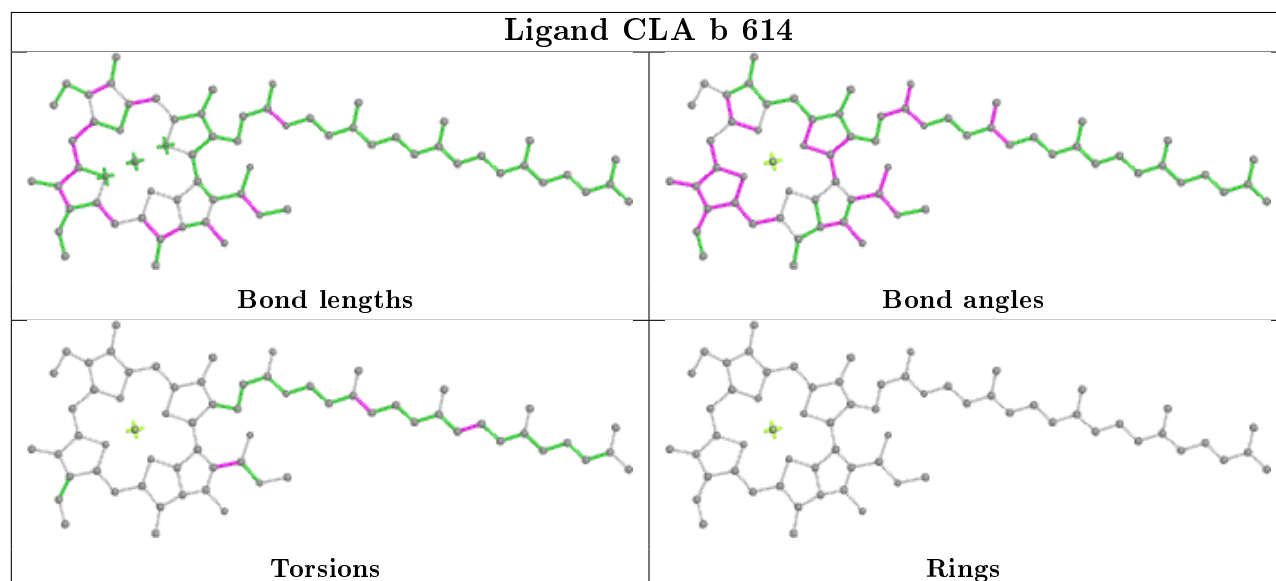
## Ligand LMT M 101



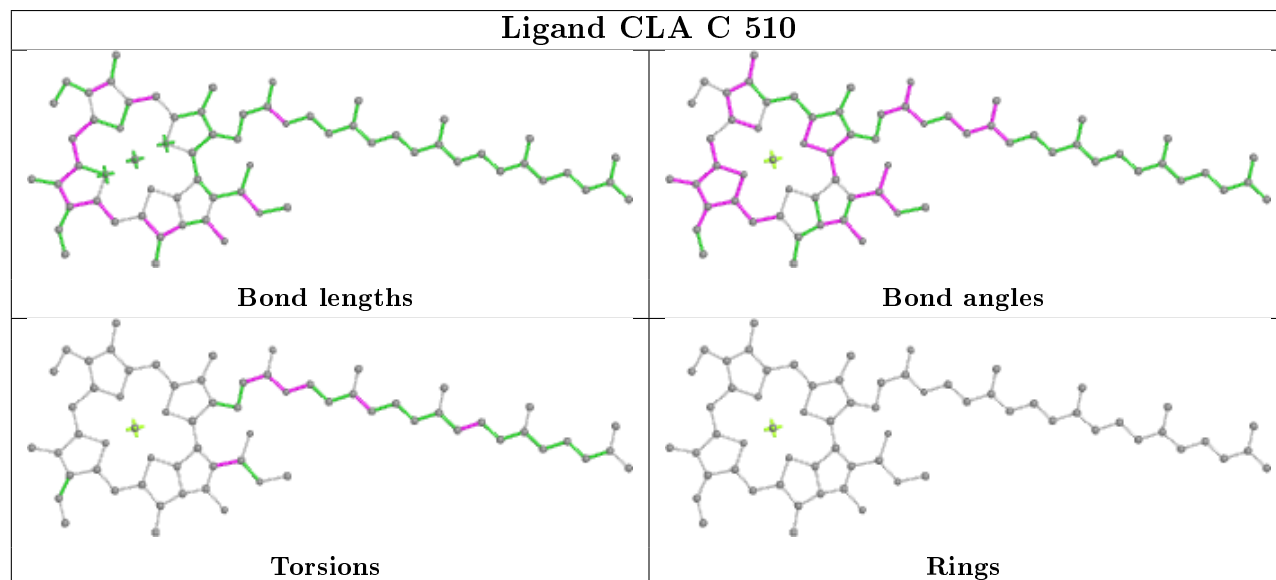
## Ligand CLA c 511

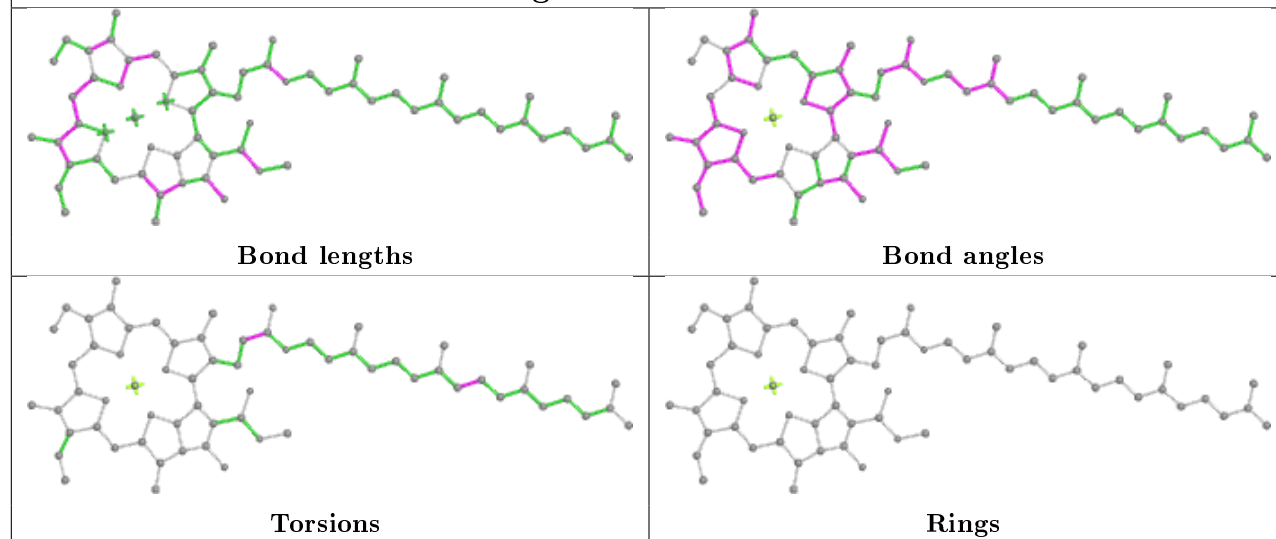
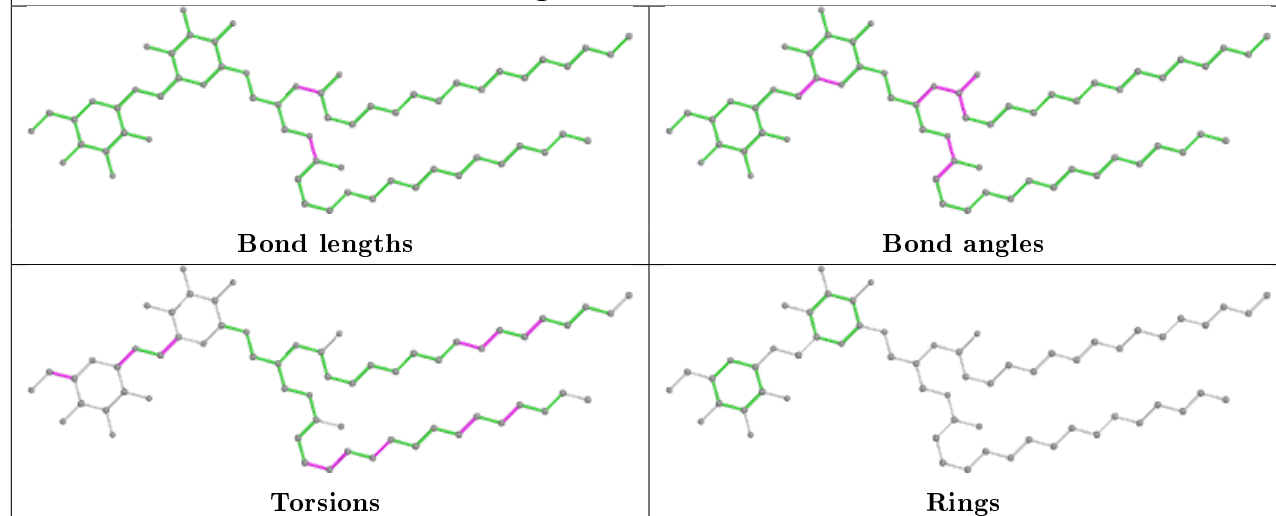


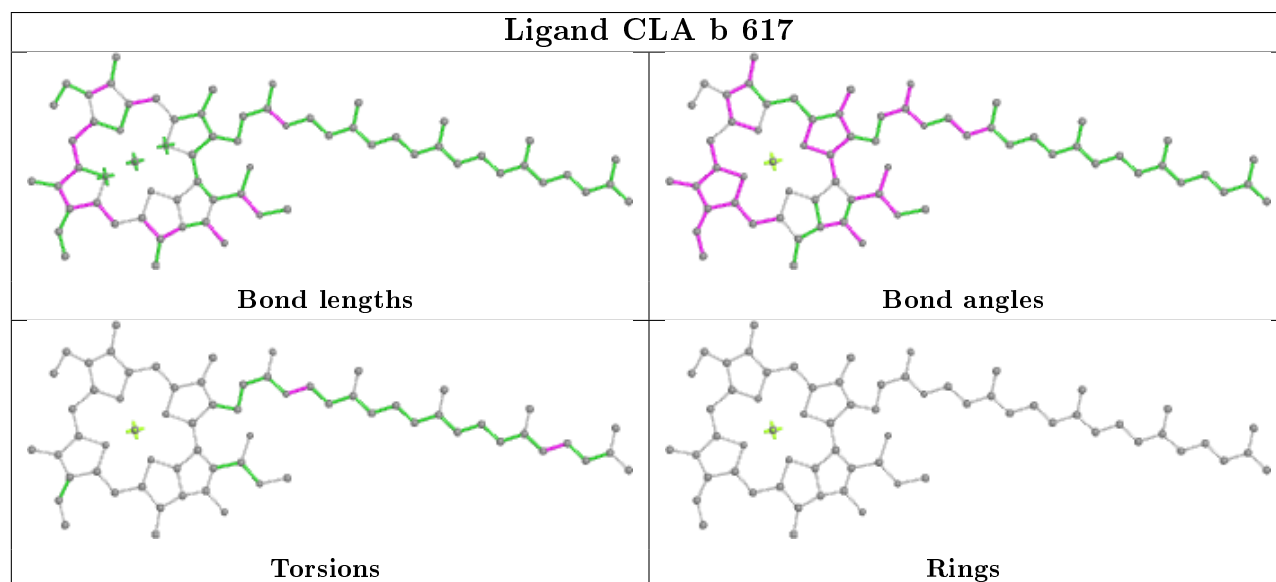
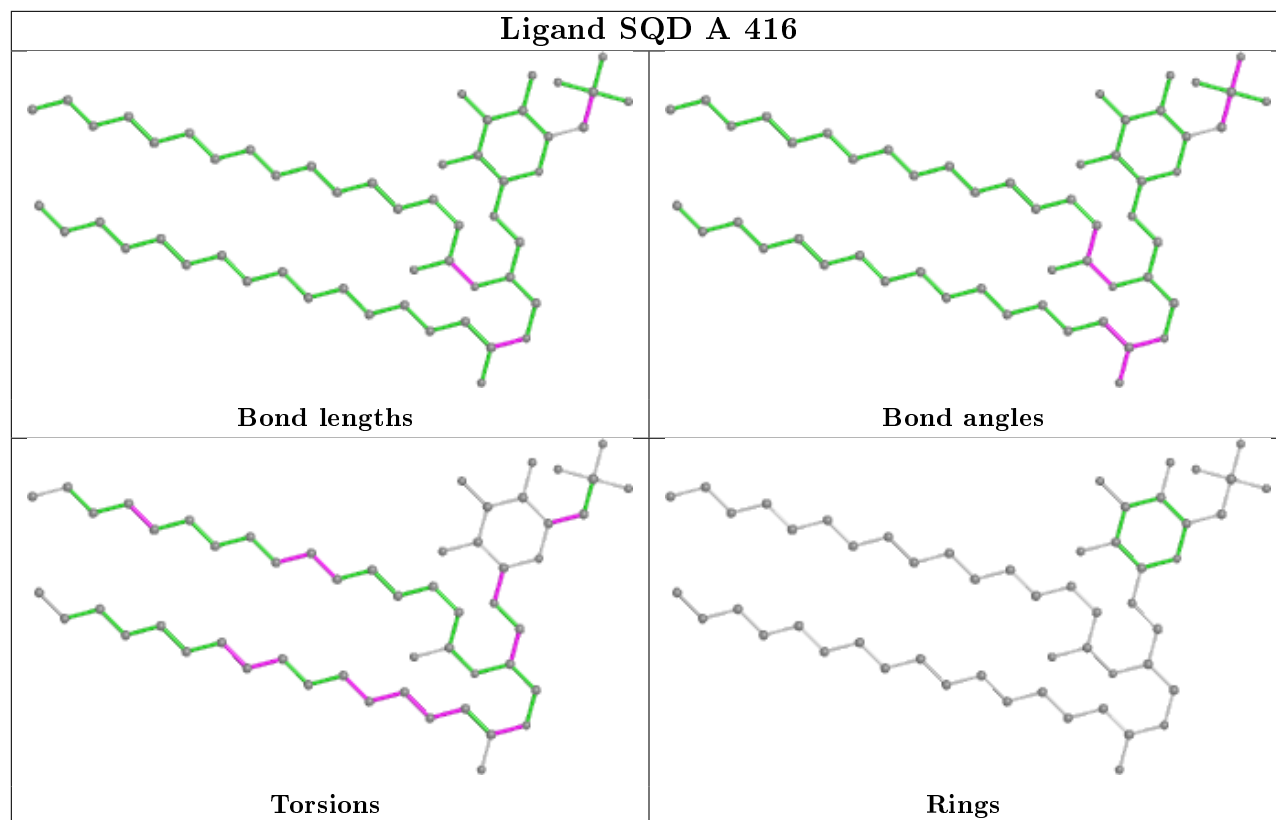
## Ligand CLA b 614



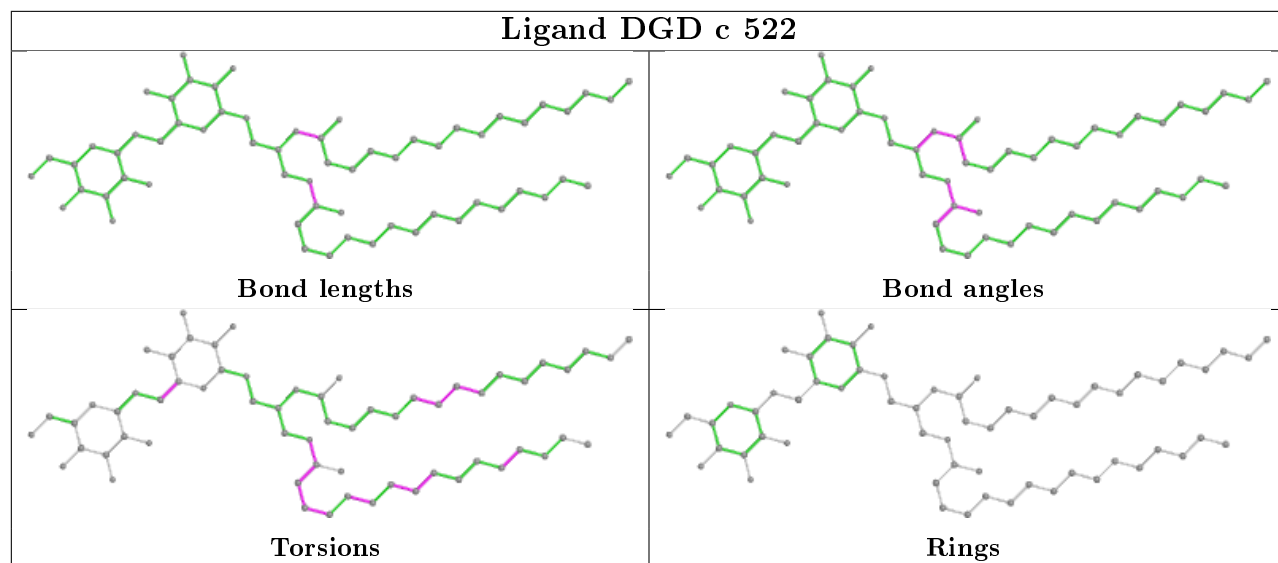
## Ligand CLA C 510



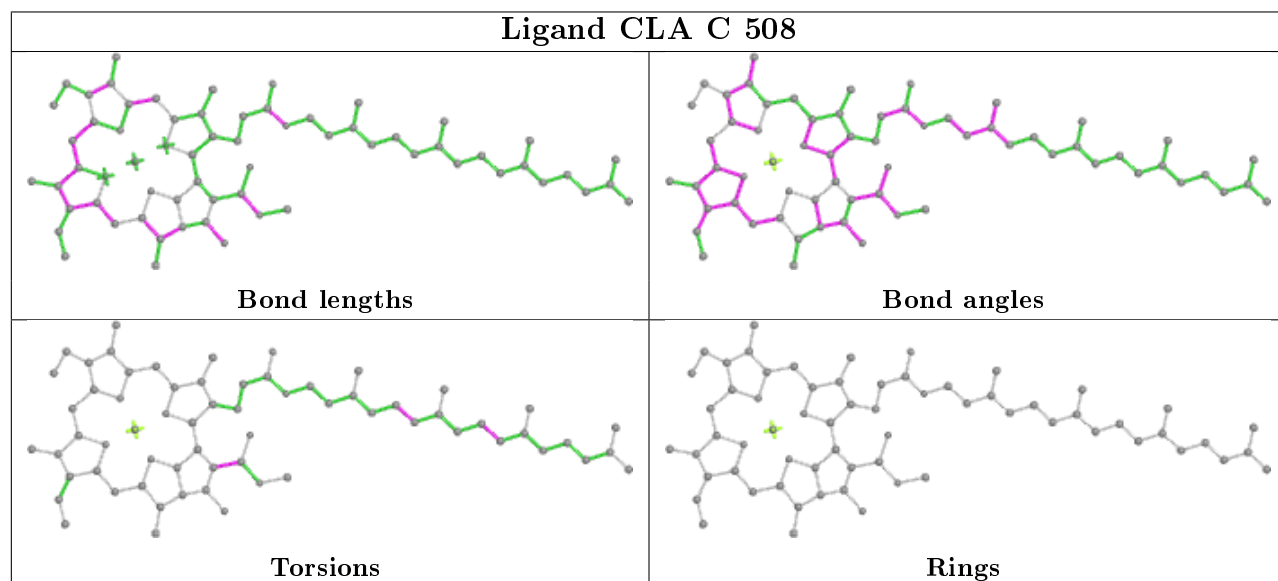
**Ligand CLA B 613****Ligand DGD c 520**



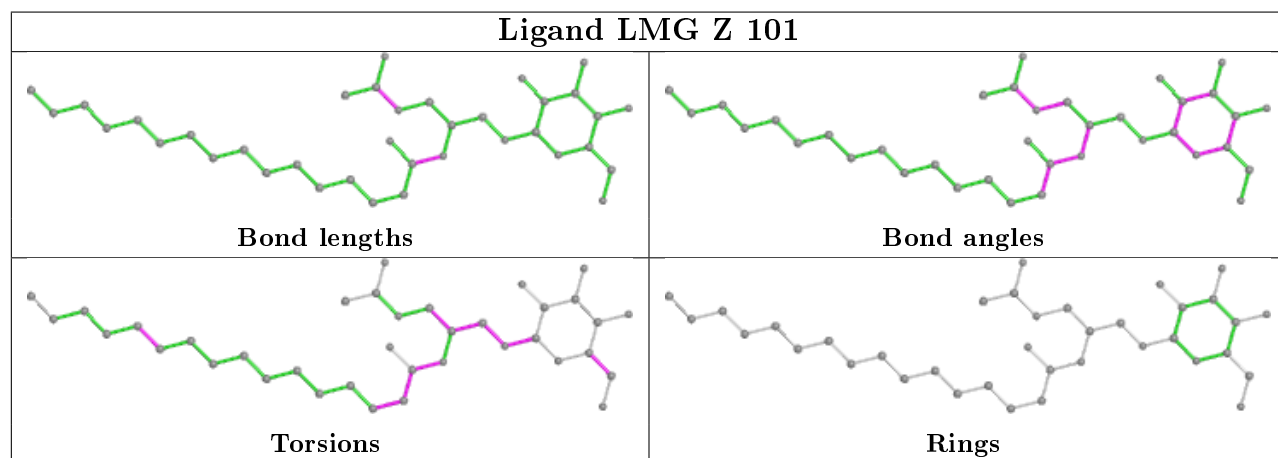
## Ligand DGD c 522



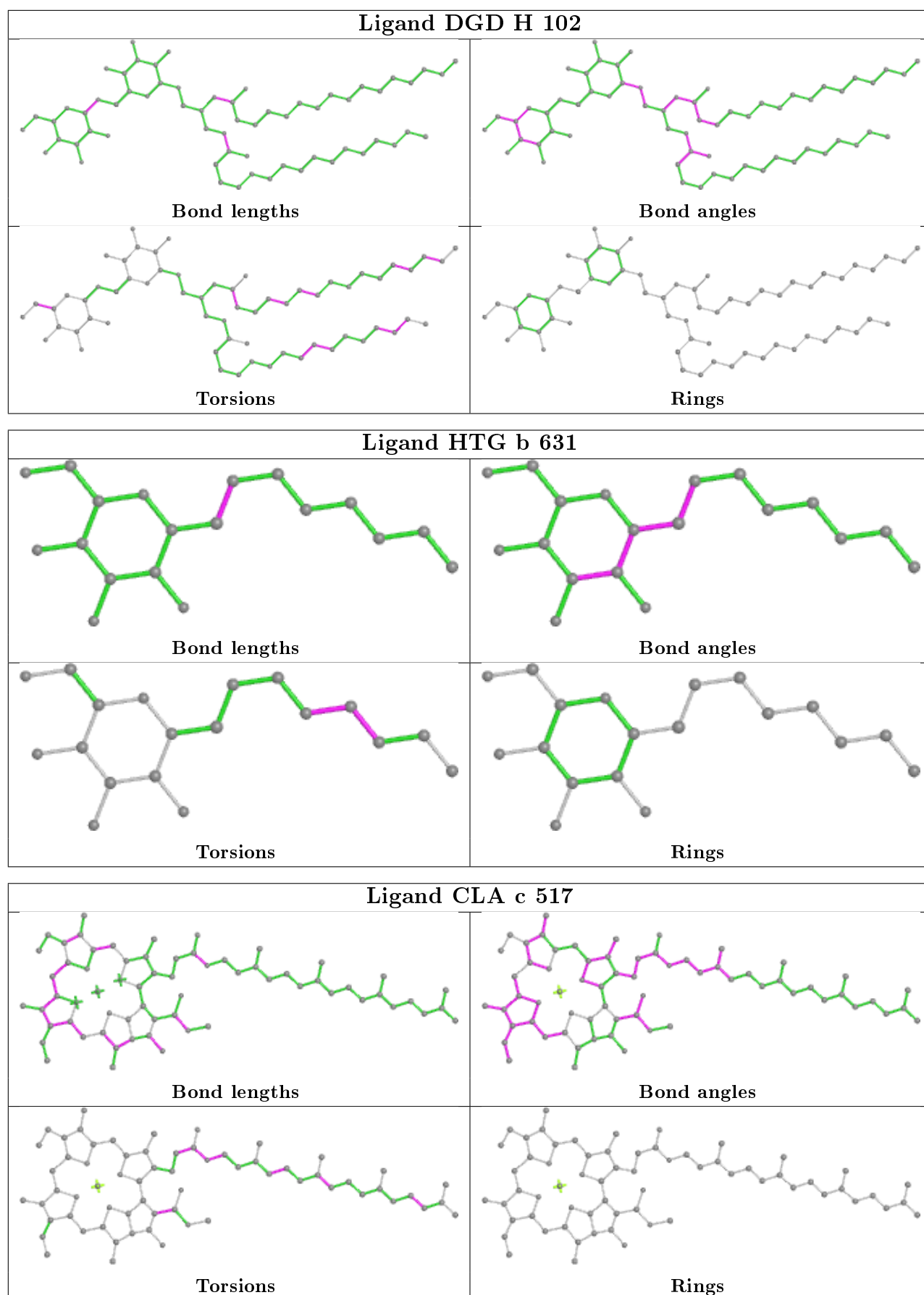
## Ligand CLA C 508

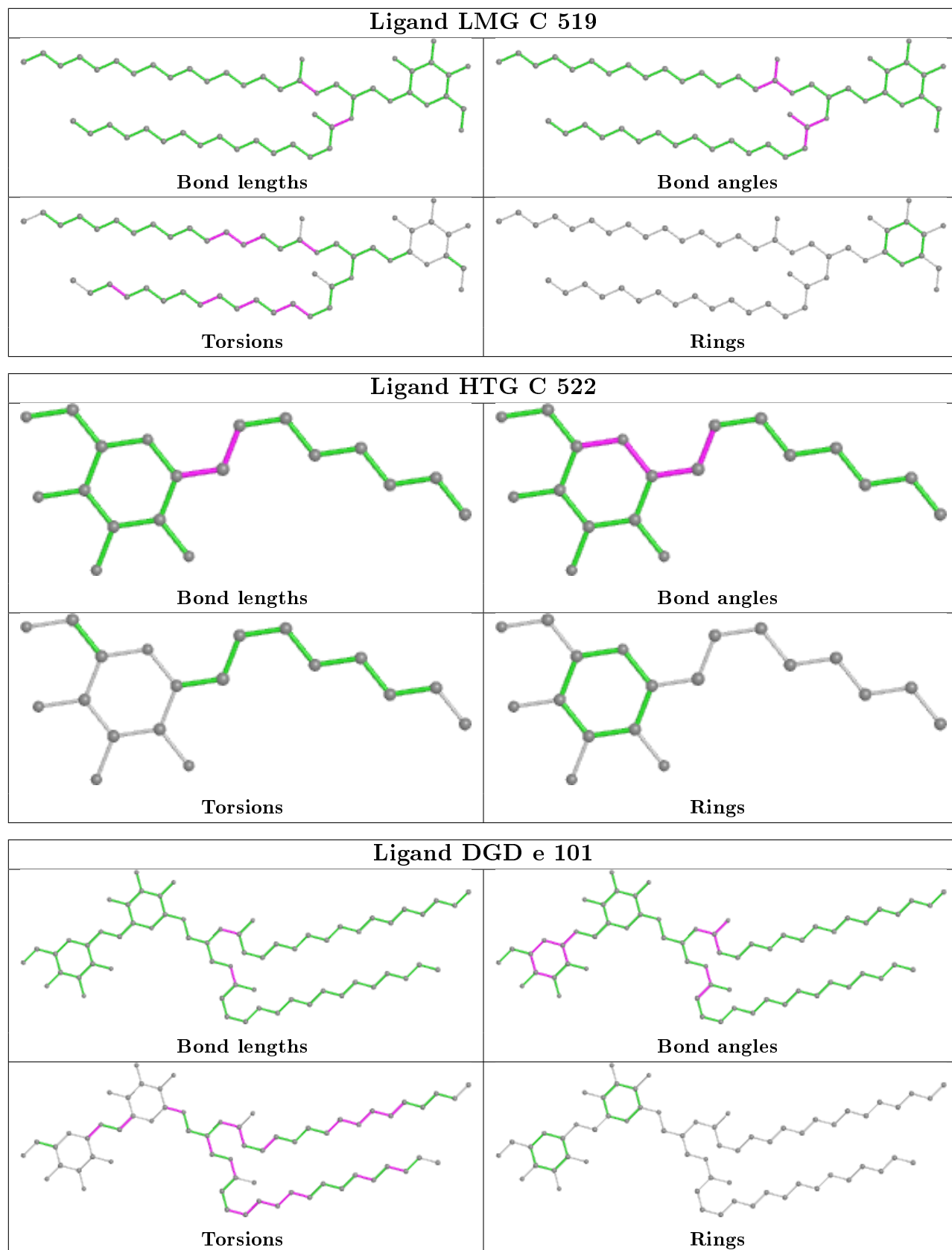


## Ligand LMG Z 101

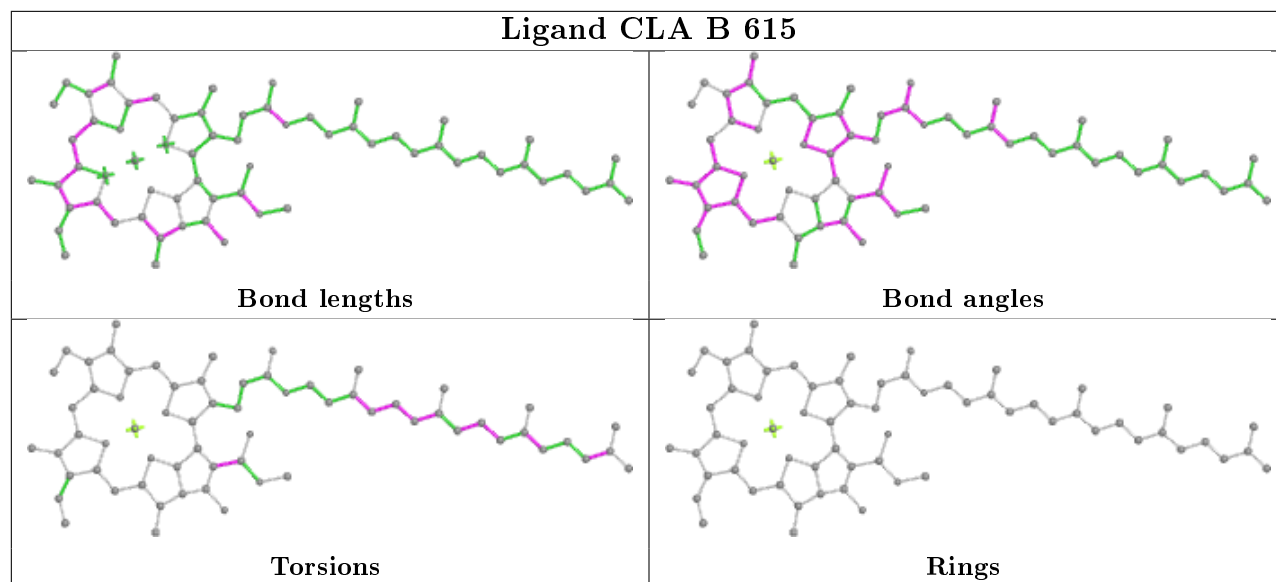




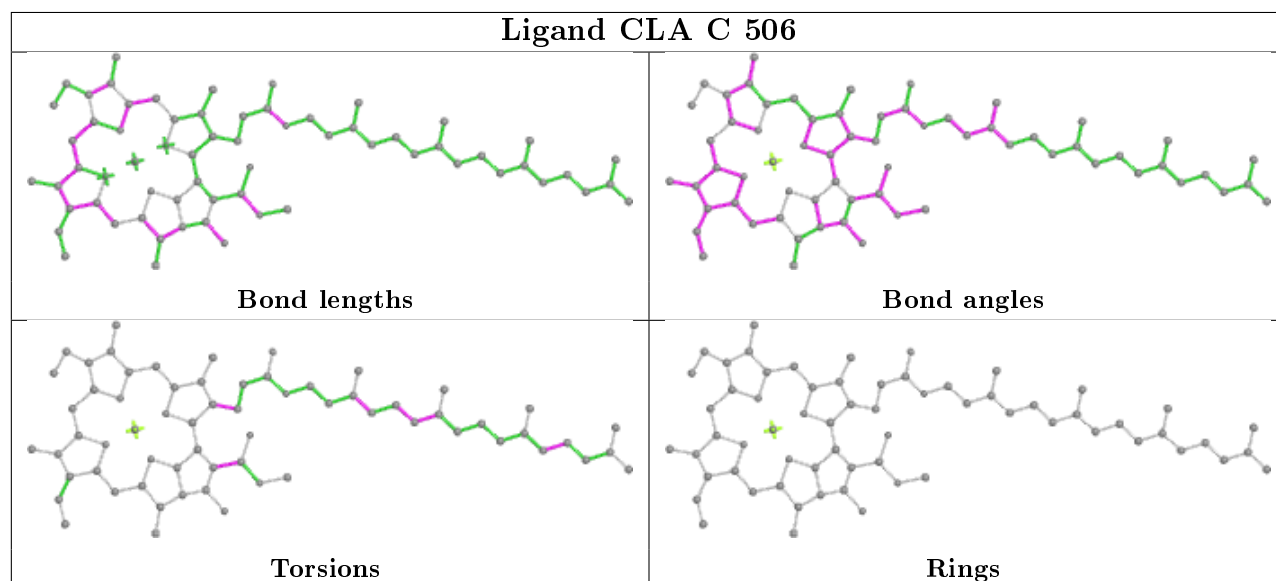




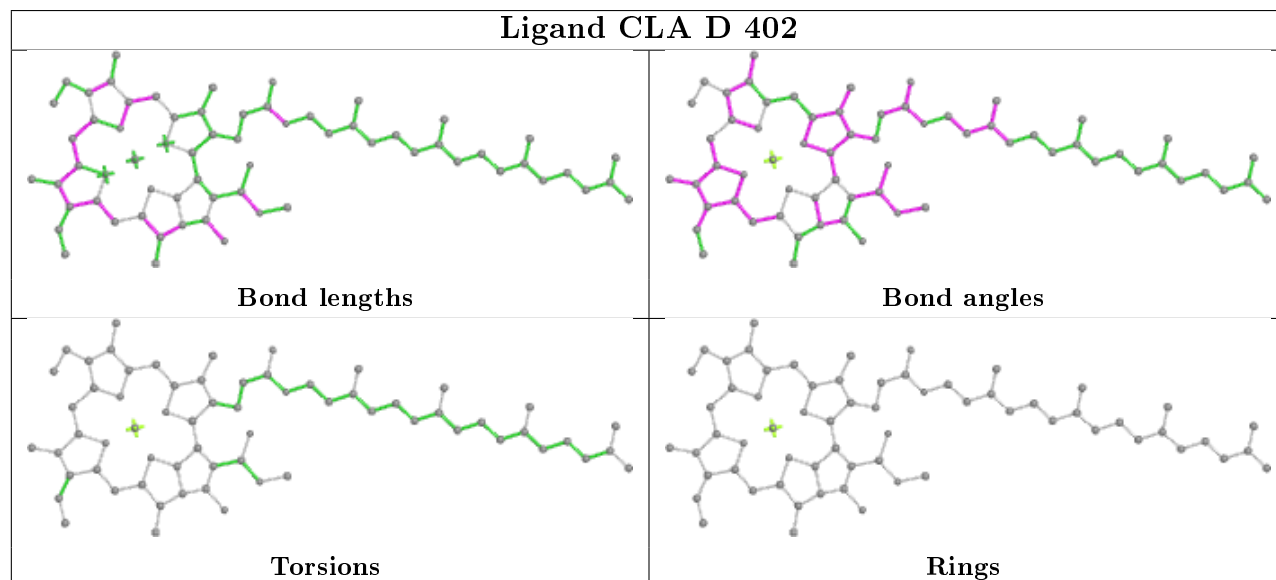
## Ligand CLA B 615

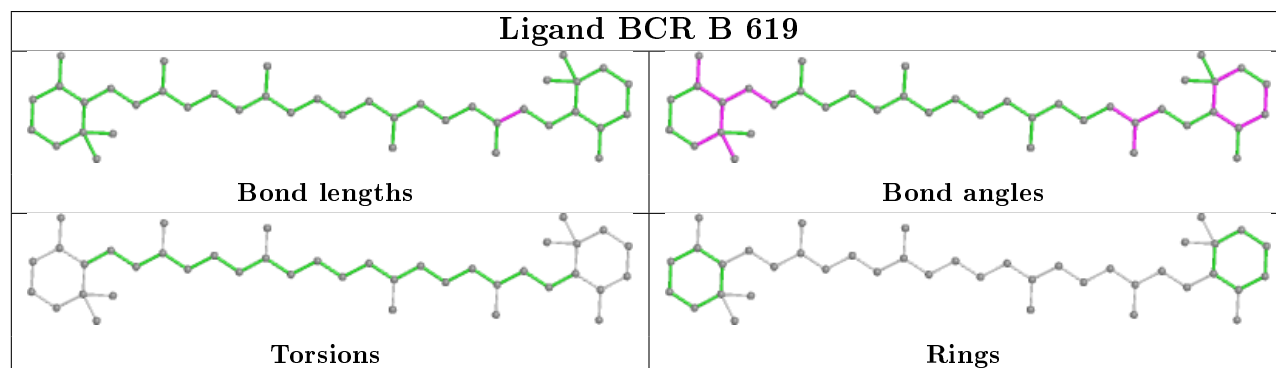
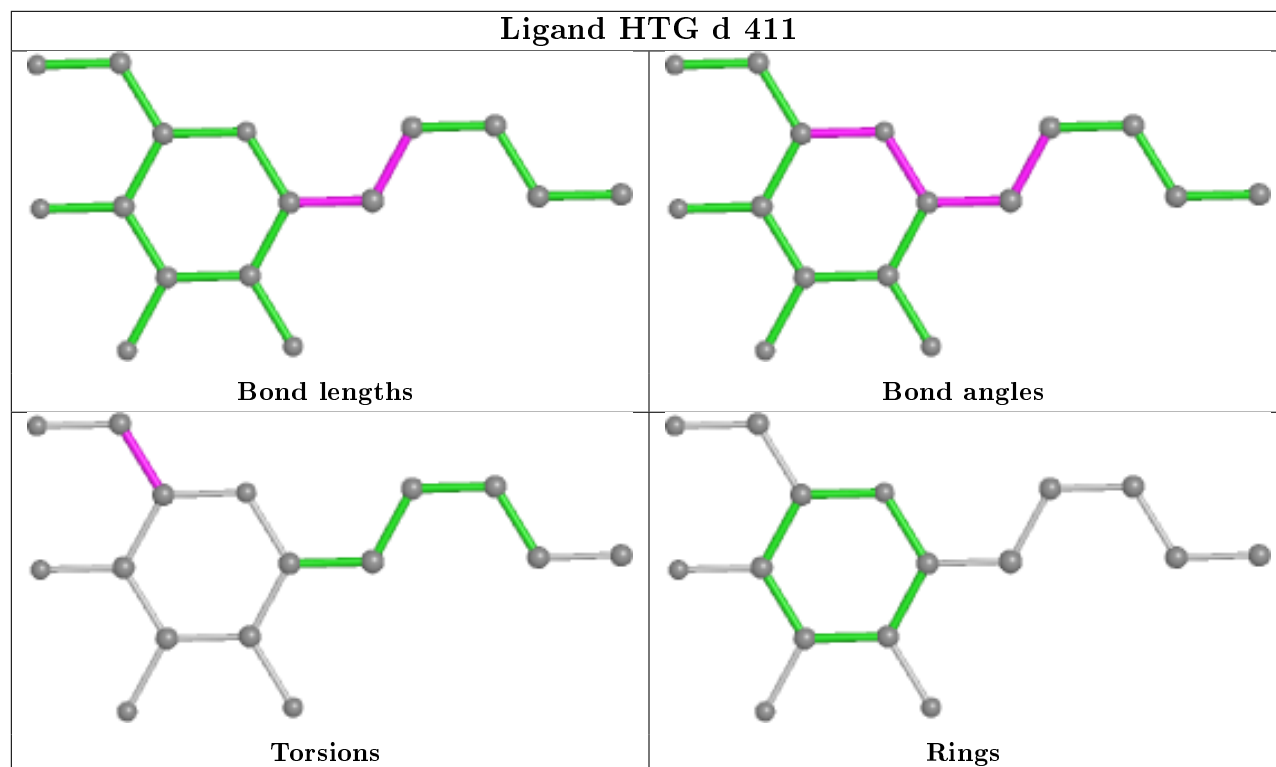
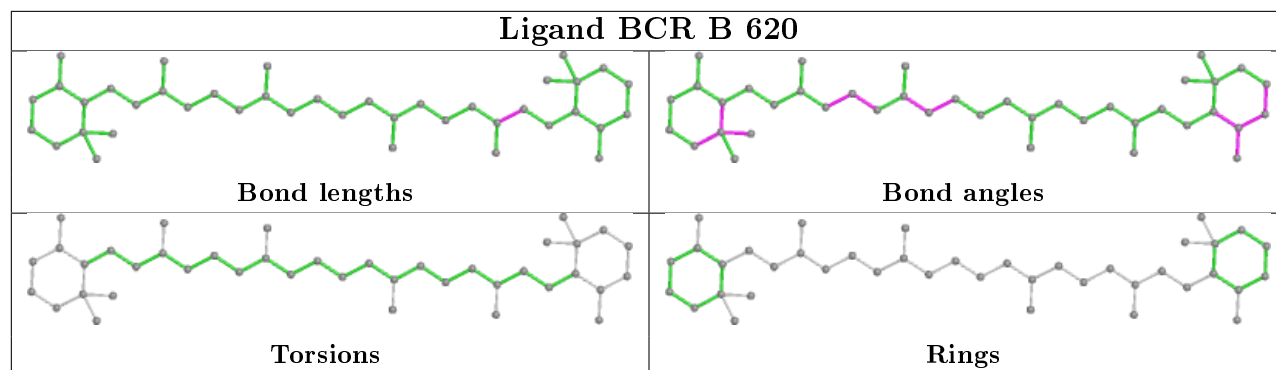


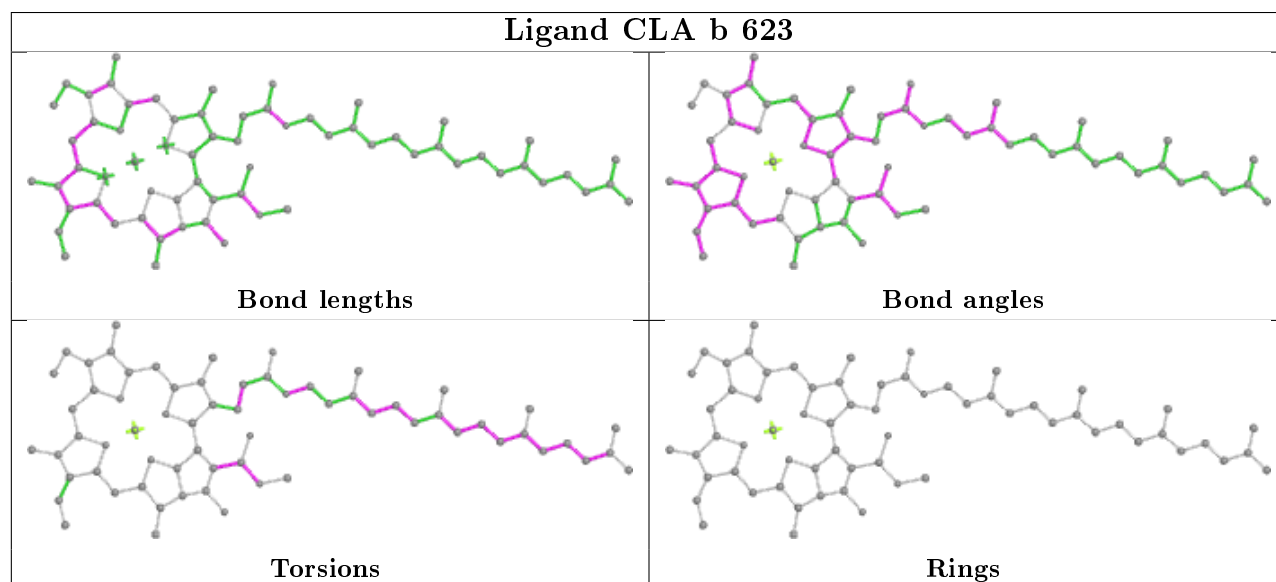
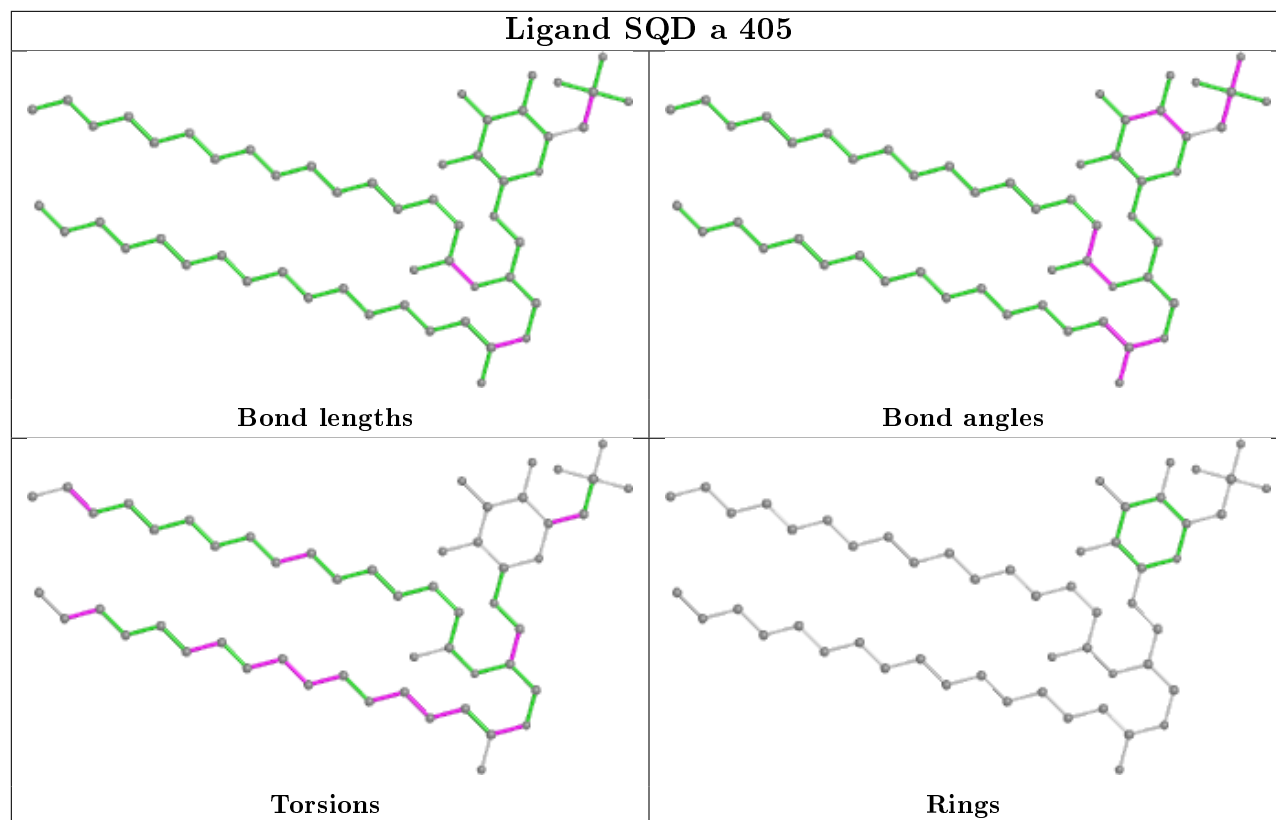
## Ligand CLA C 506

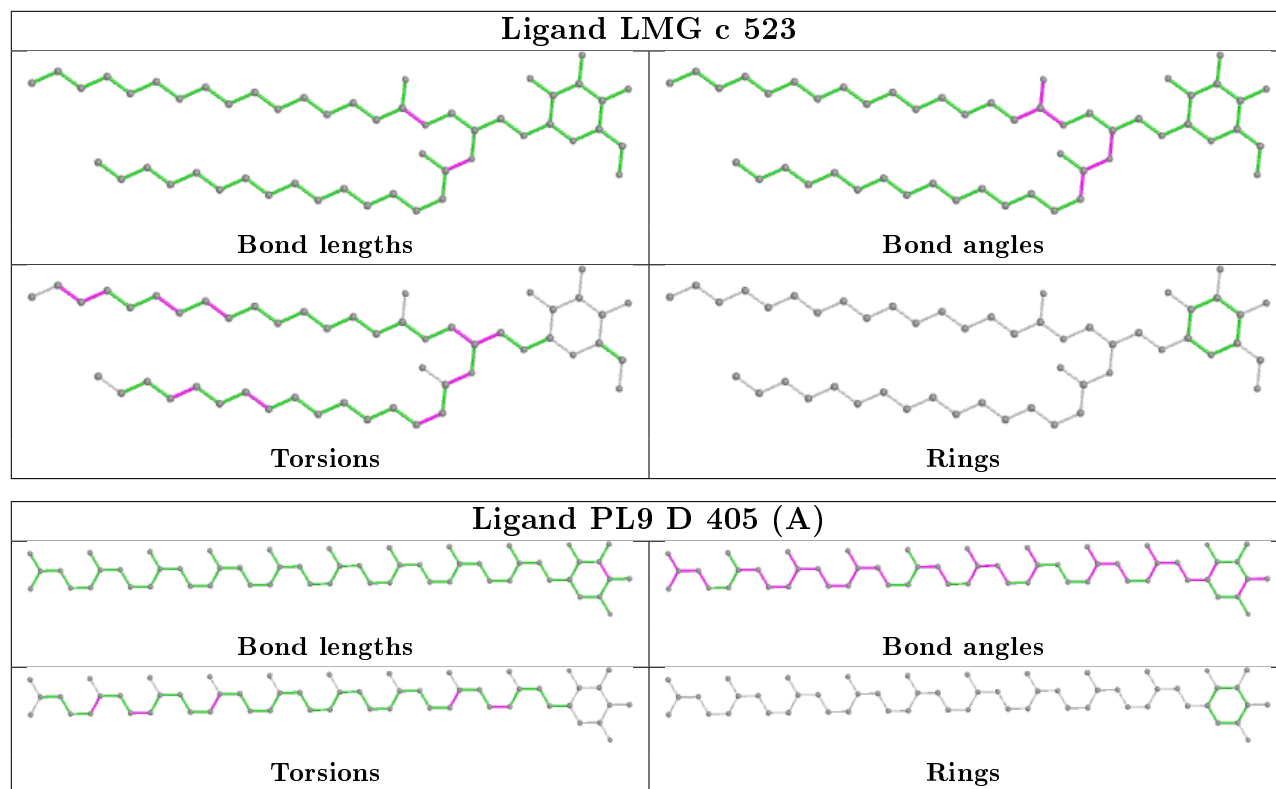


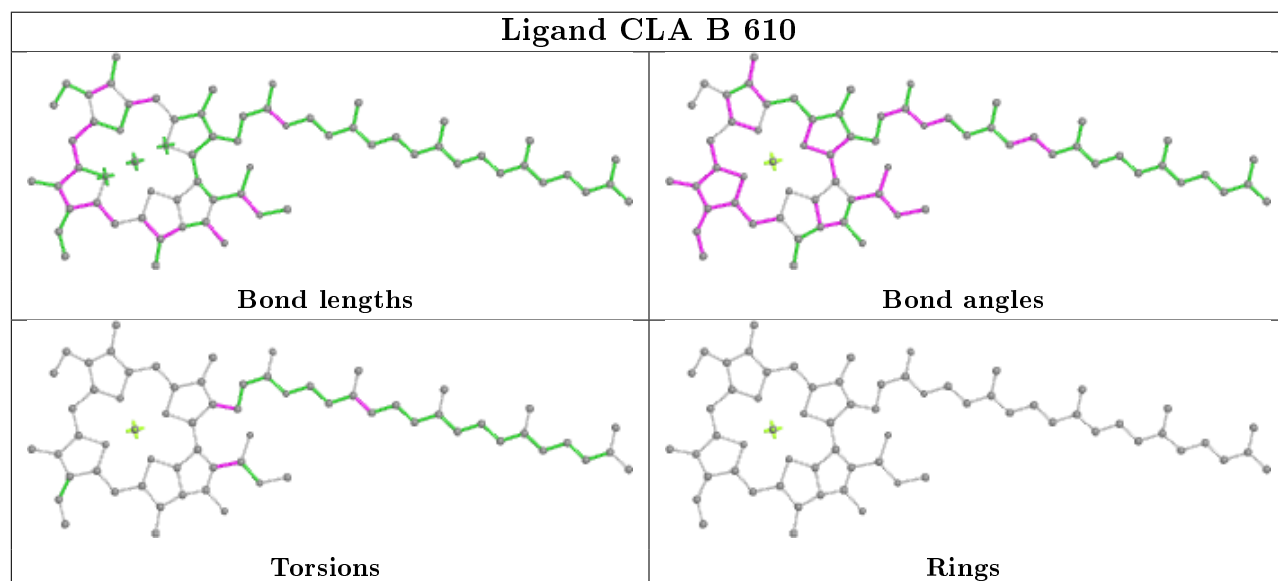
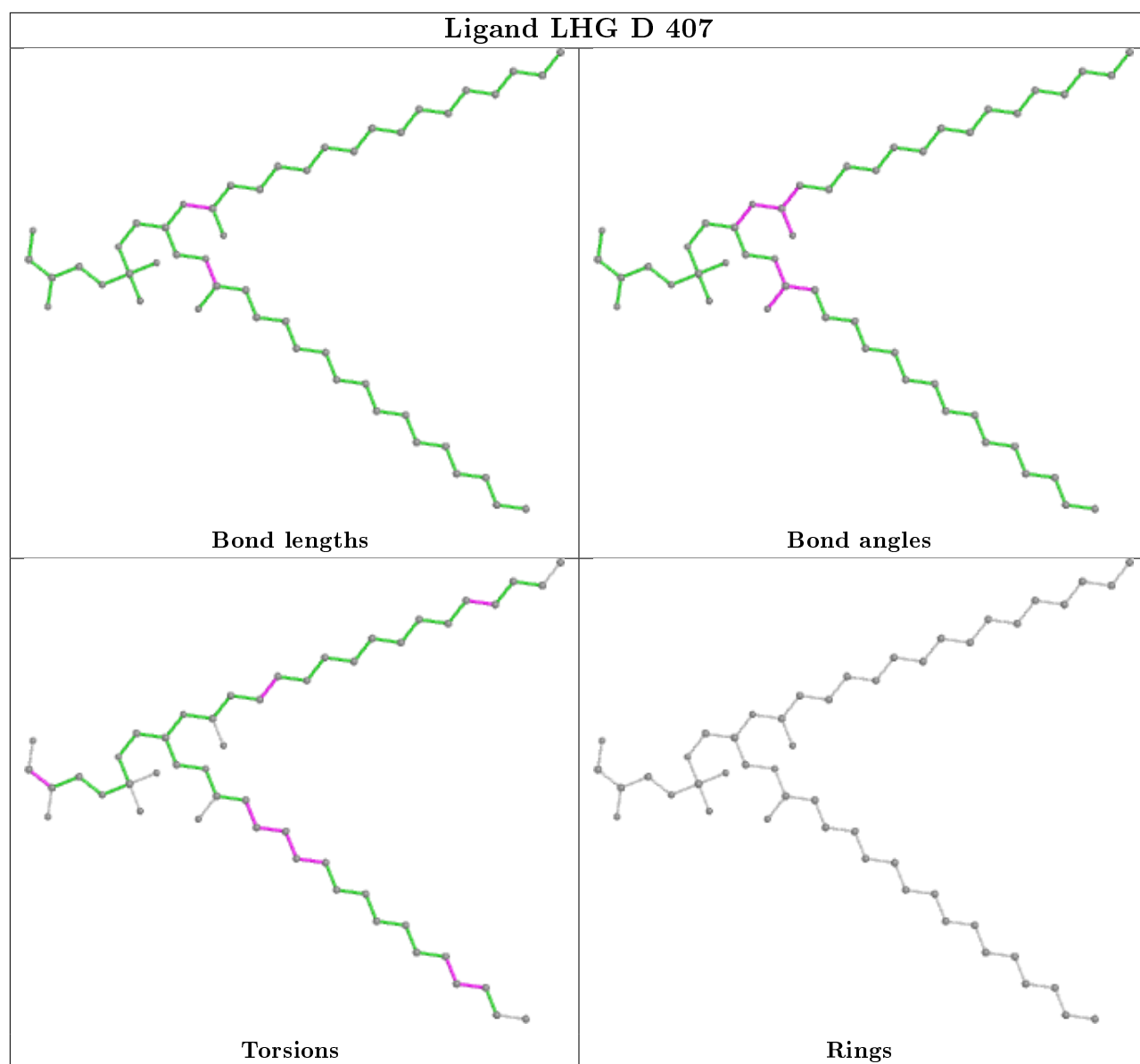
## Ligand CLA D 402

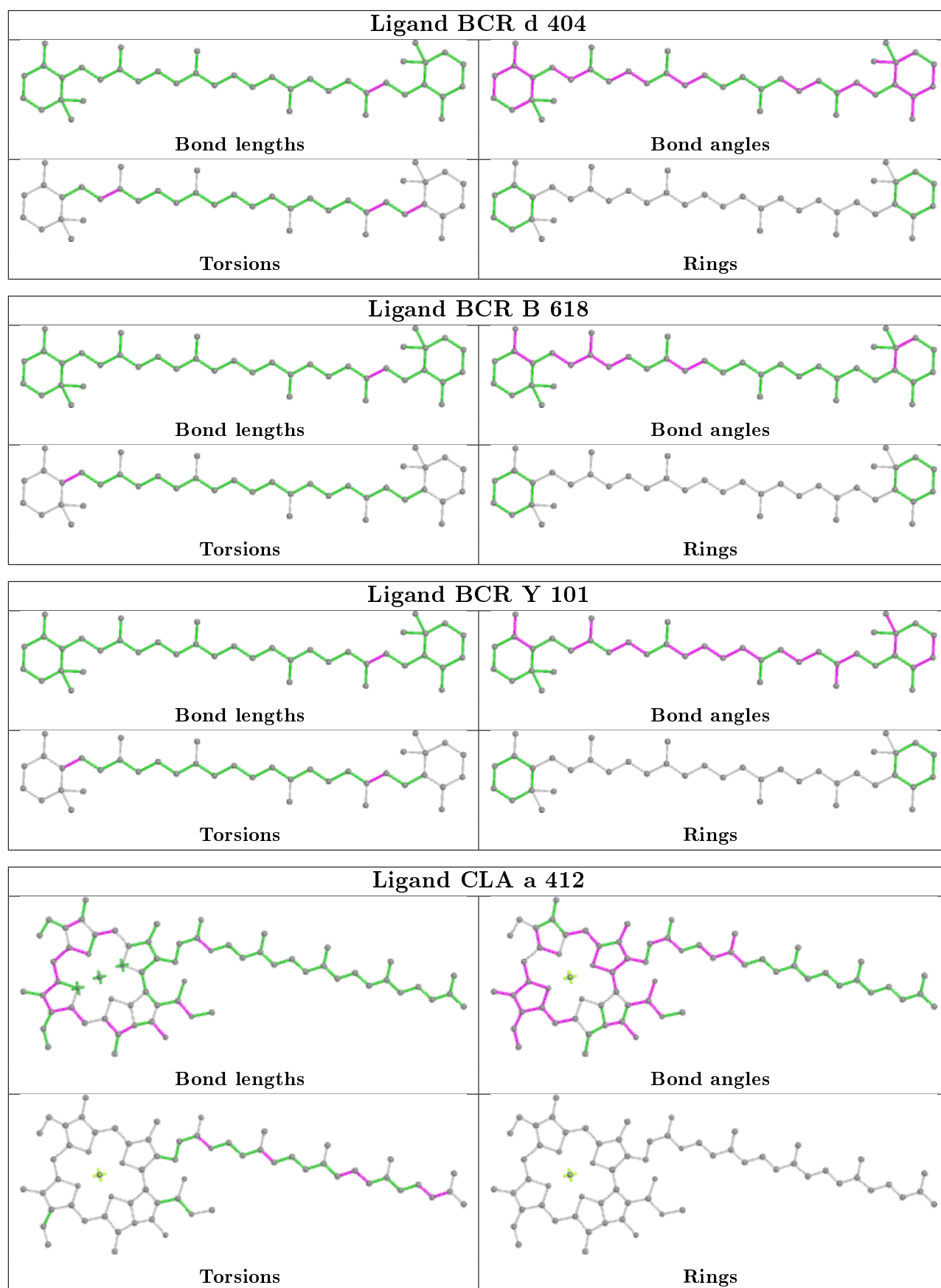




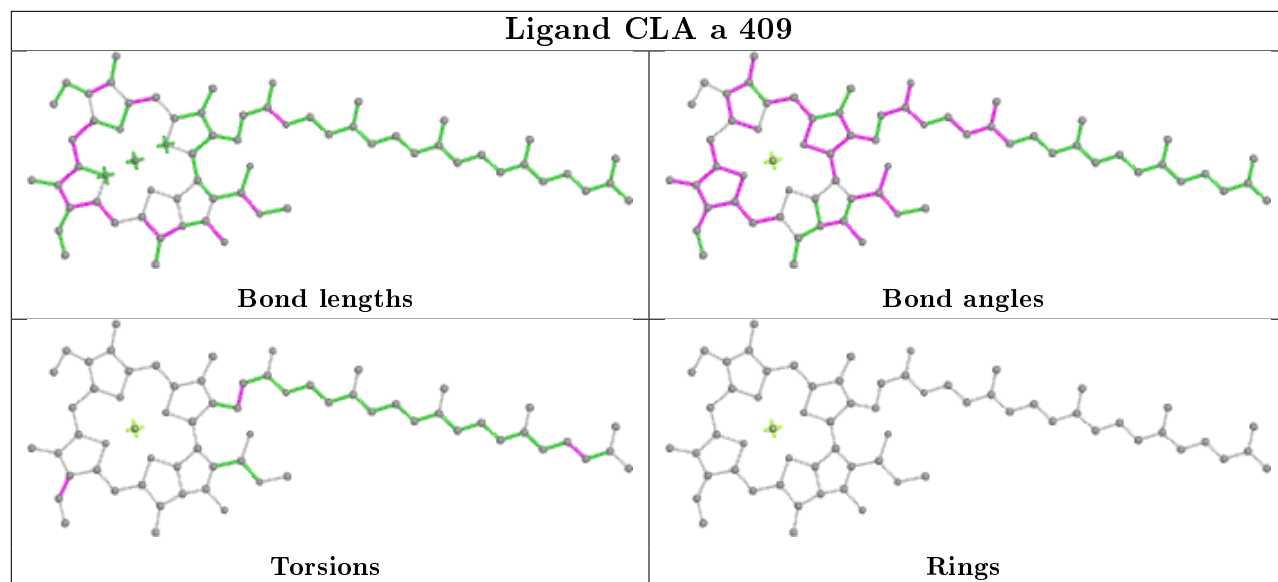
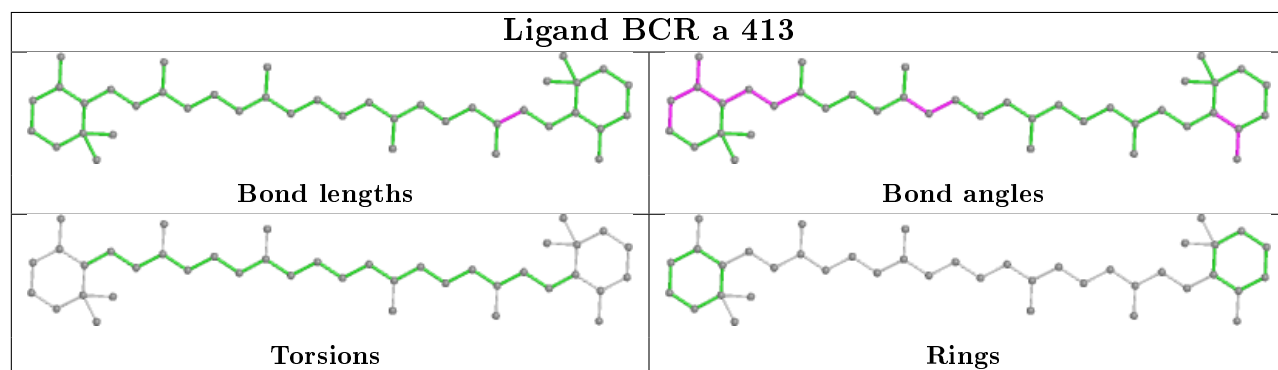
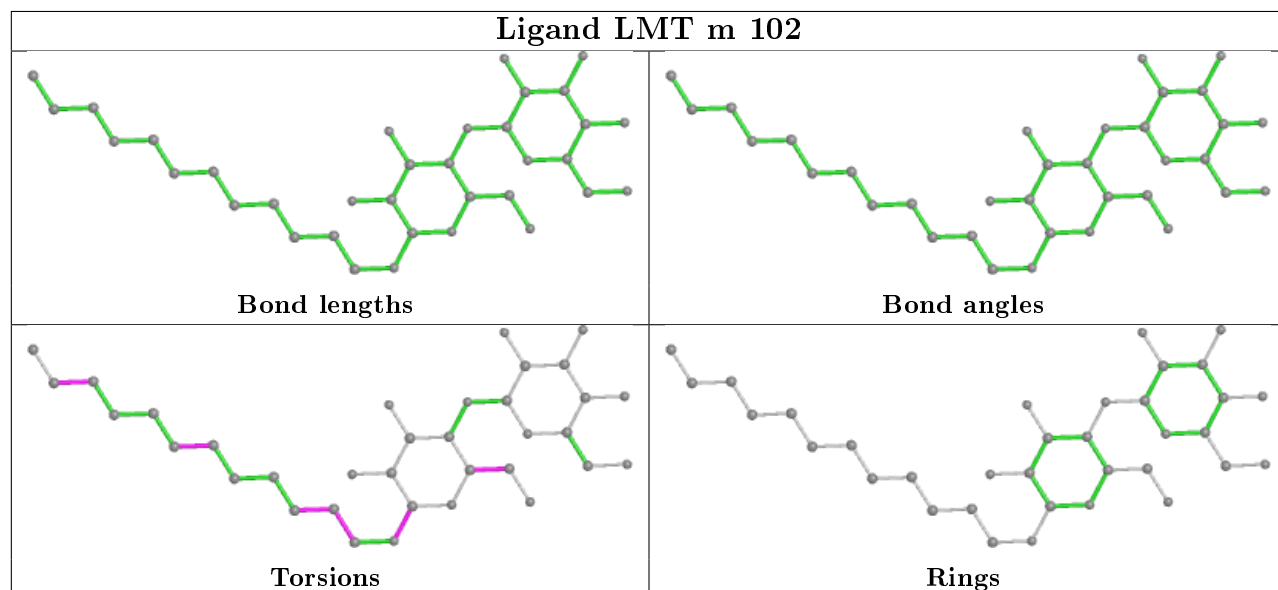




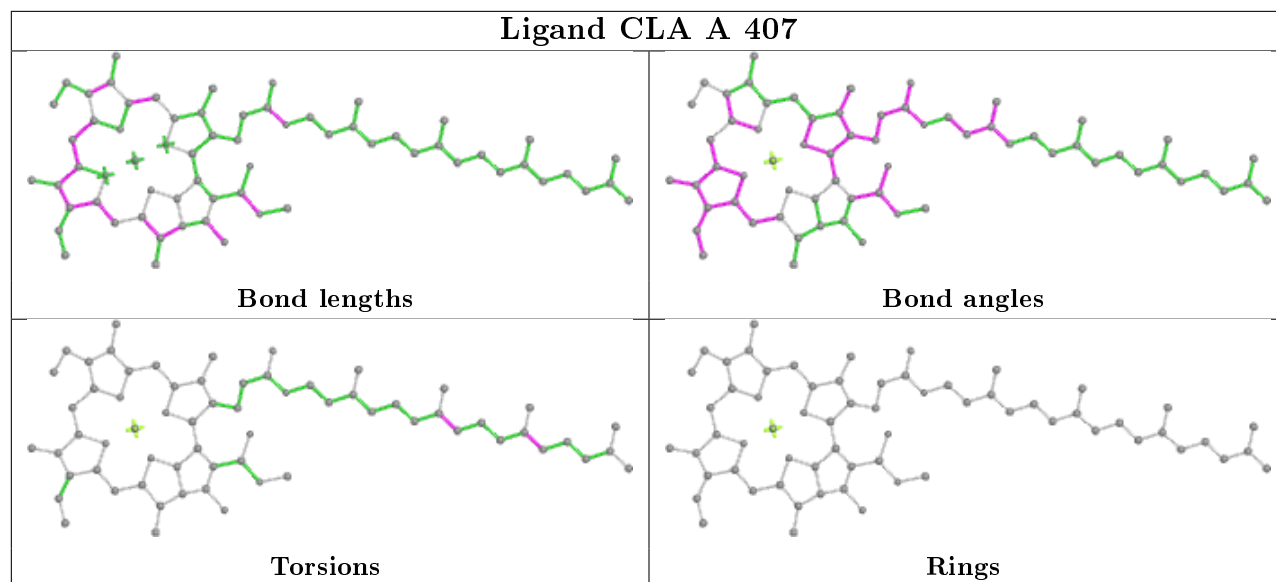




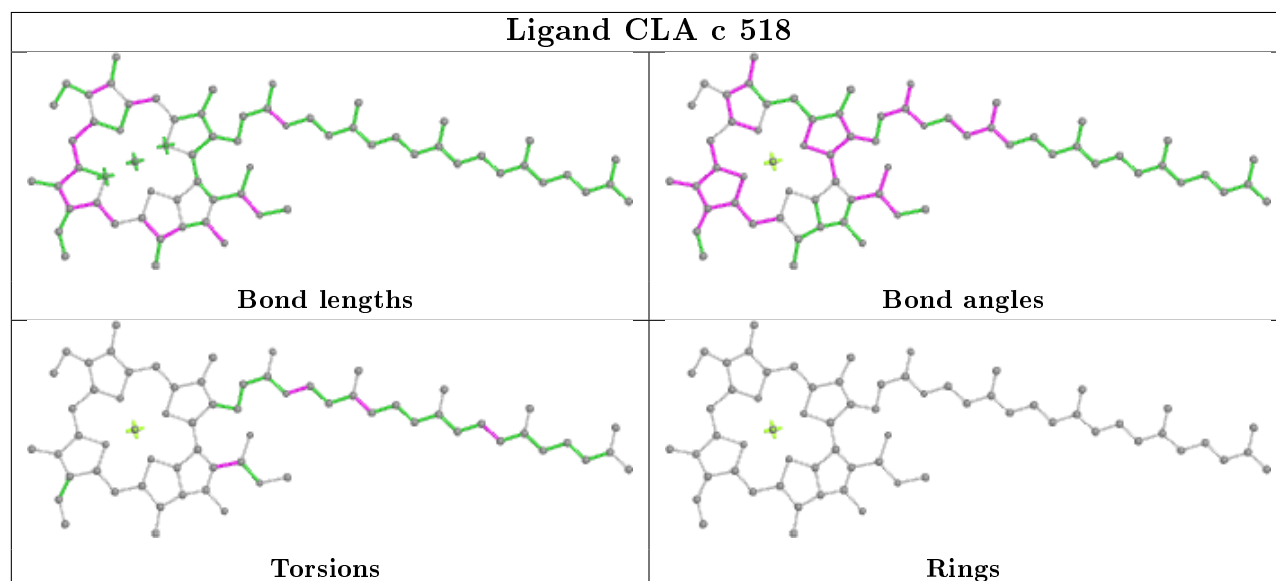


**Ligand CLA a 409****Ligand BCR a 413****Ligand LMT m 102**

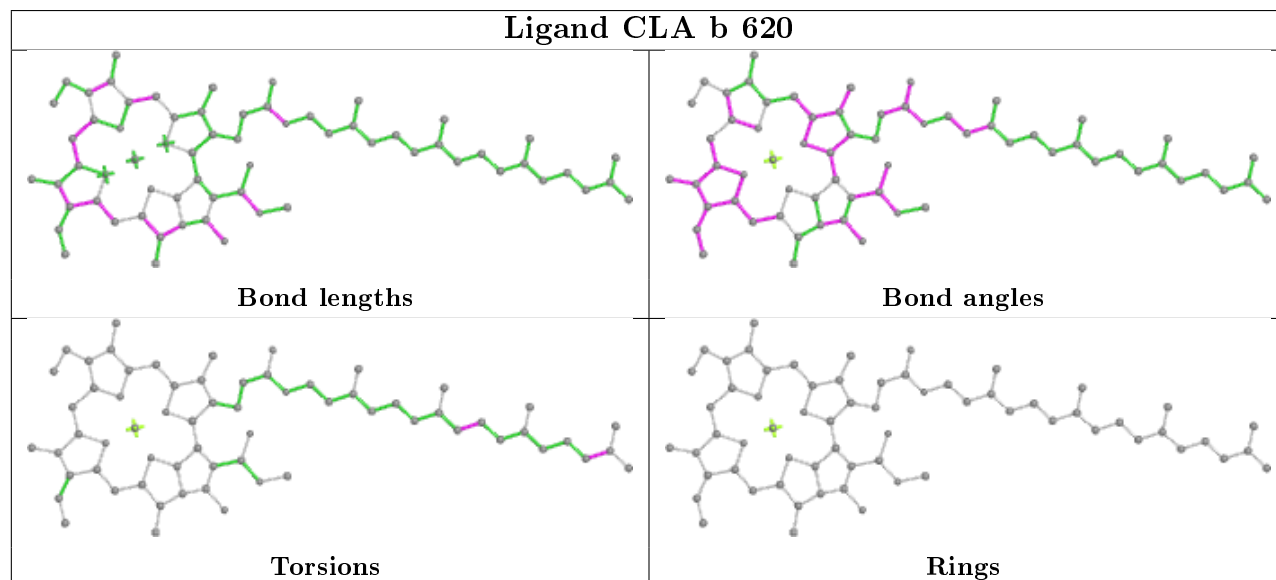
## Ligand CLA A 407

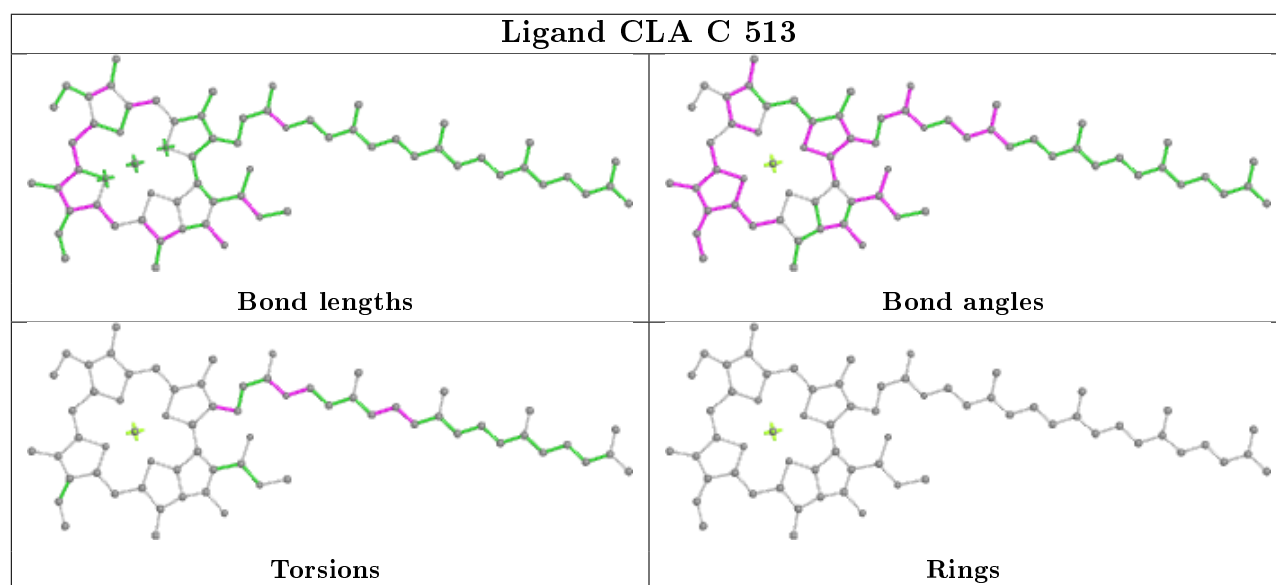
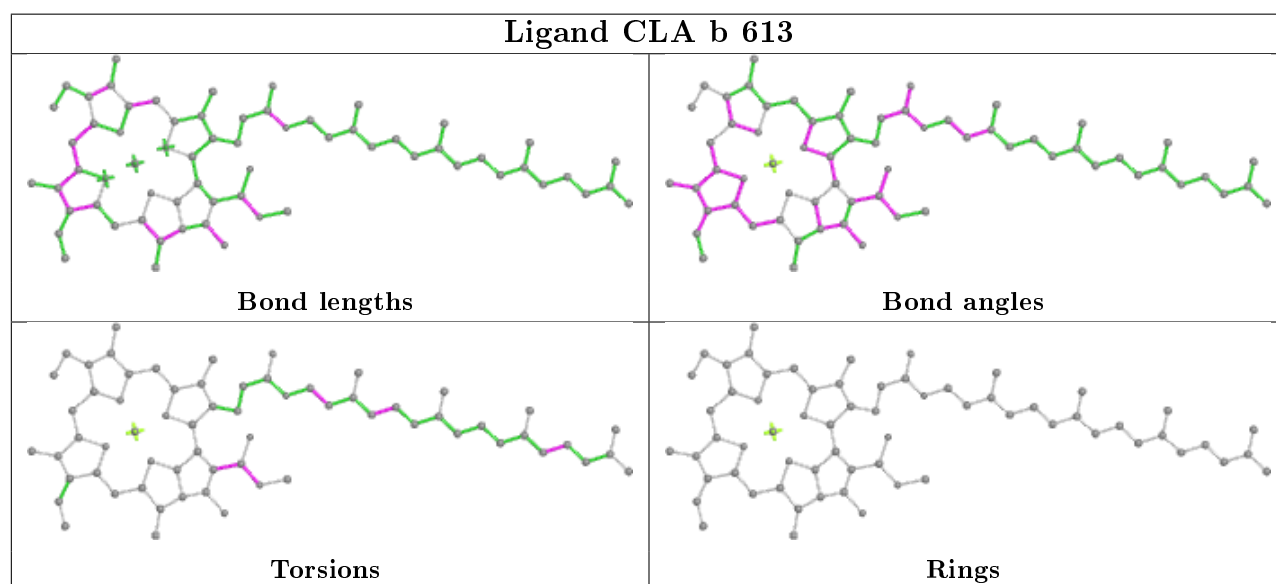
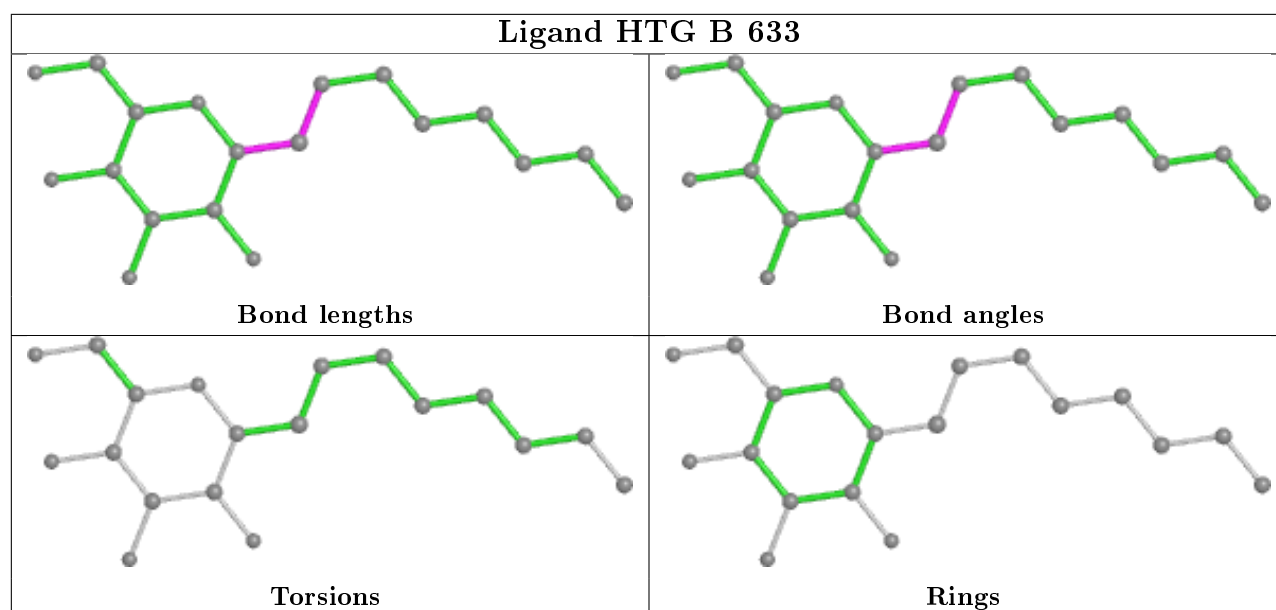


## Ligand CLA c 518

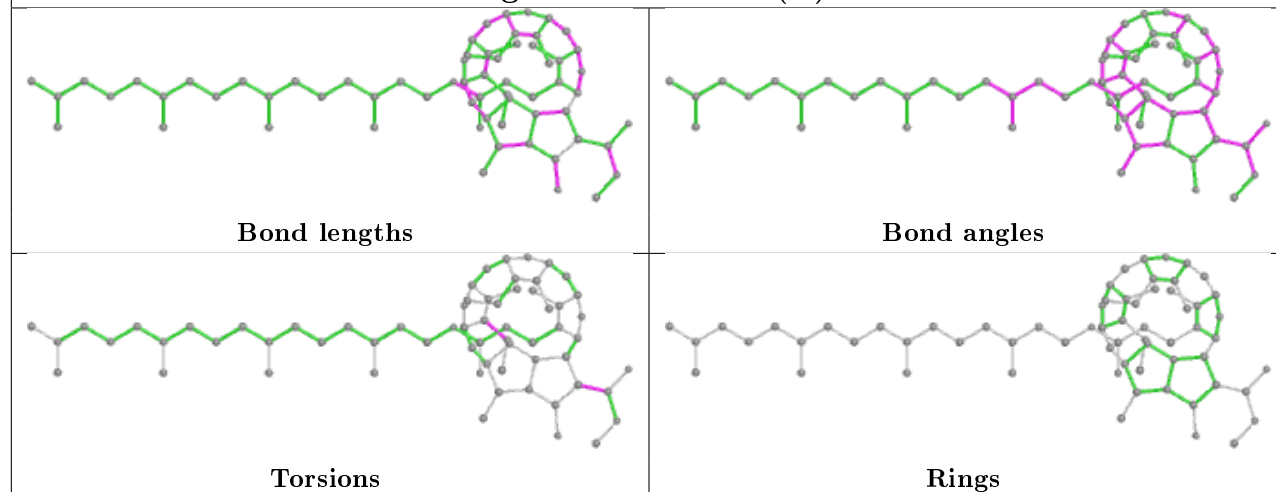


## Ligand CLA b 620

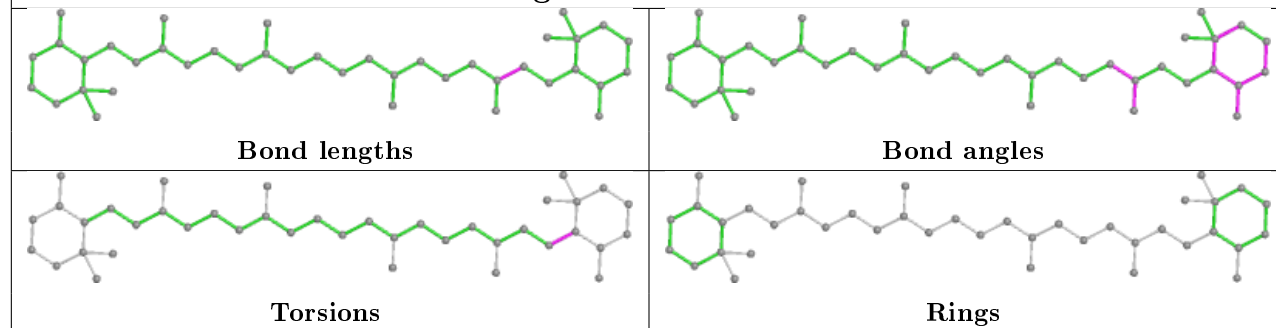




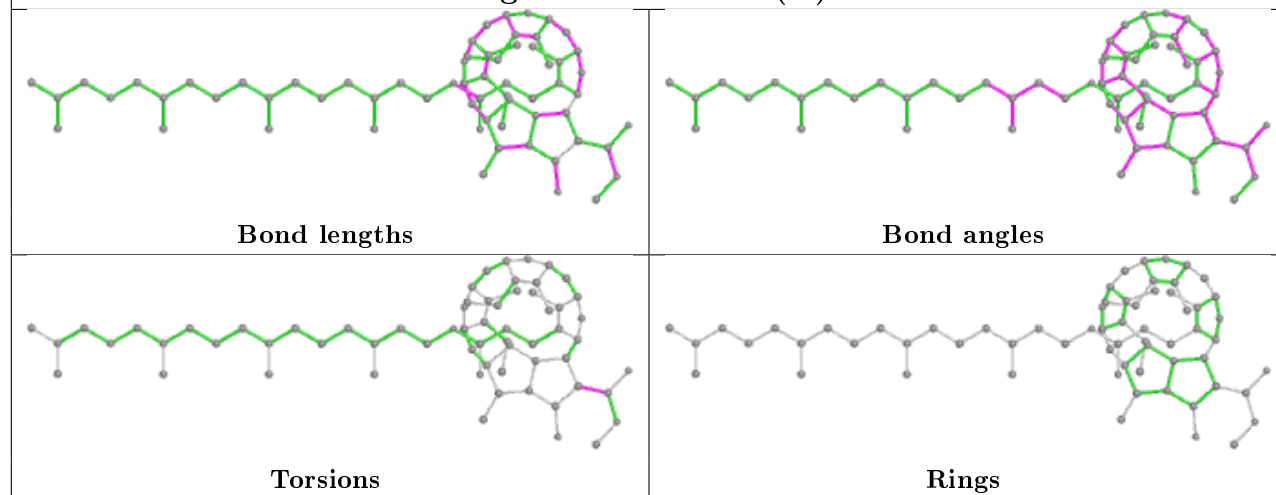
## Ligand PHO a 418 (B)



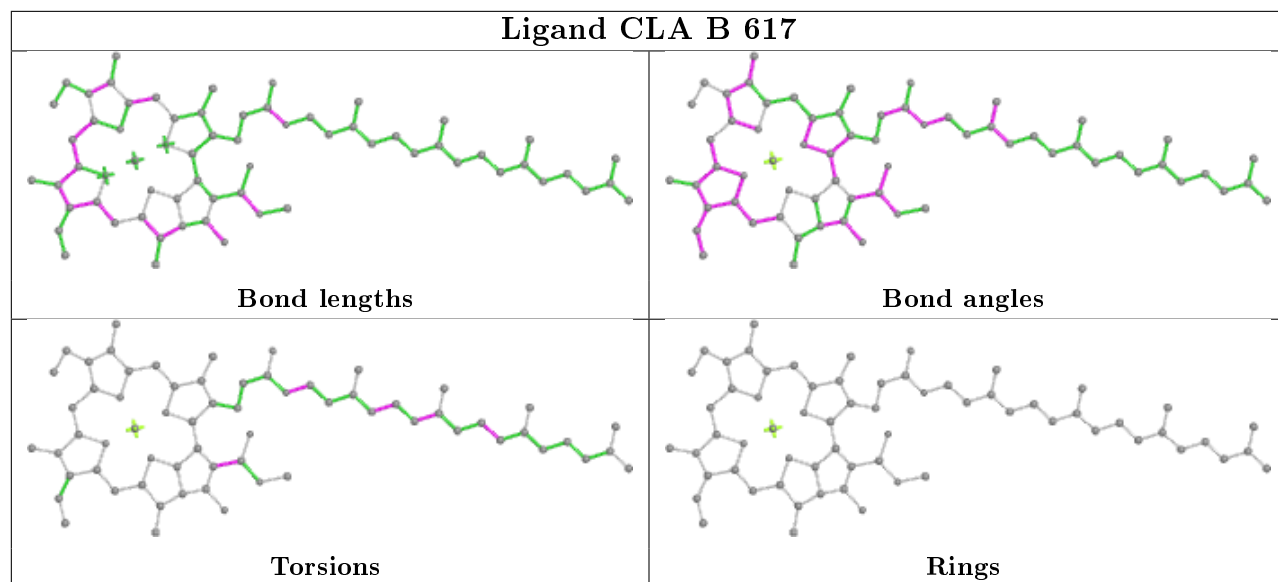
## Ligand BCR b 627



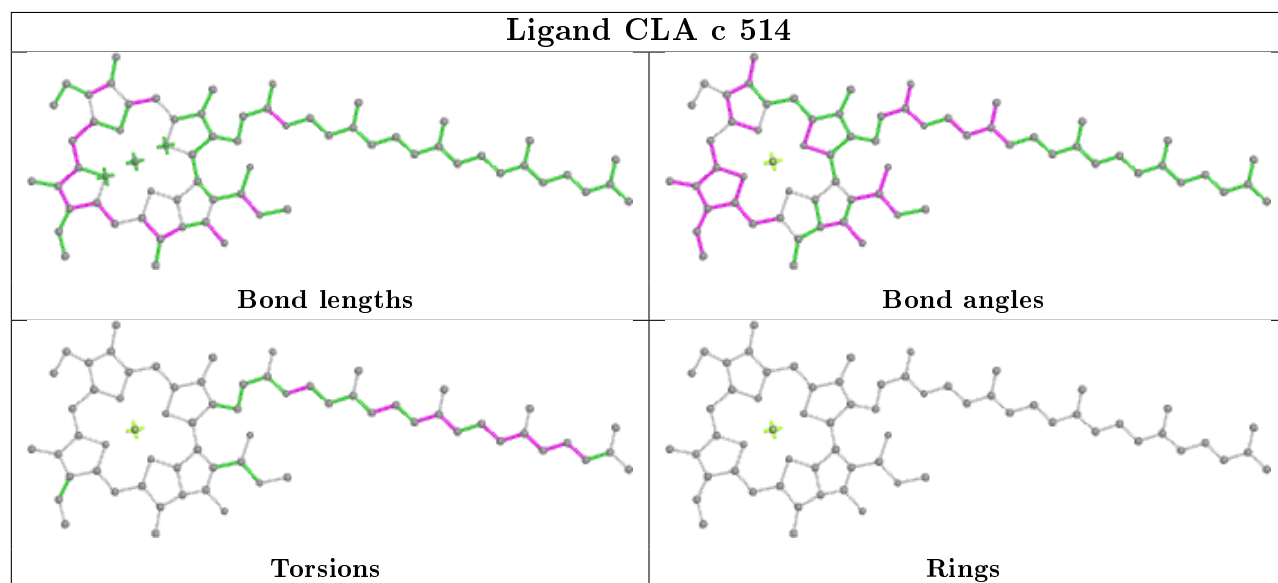
## Ligand PHO a 418 (A)

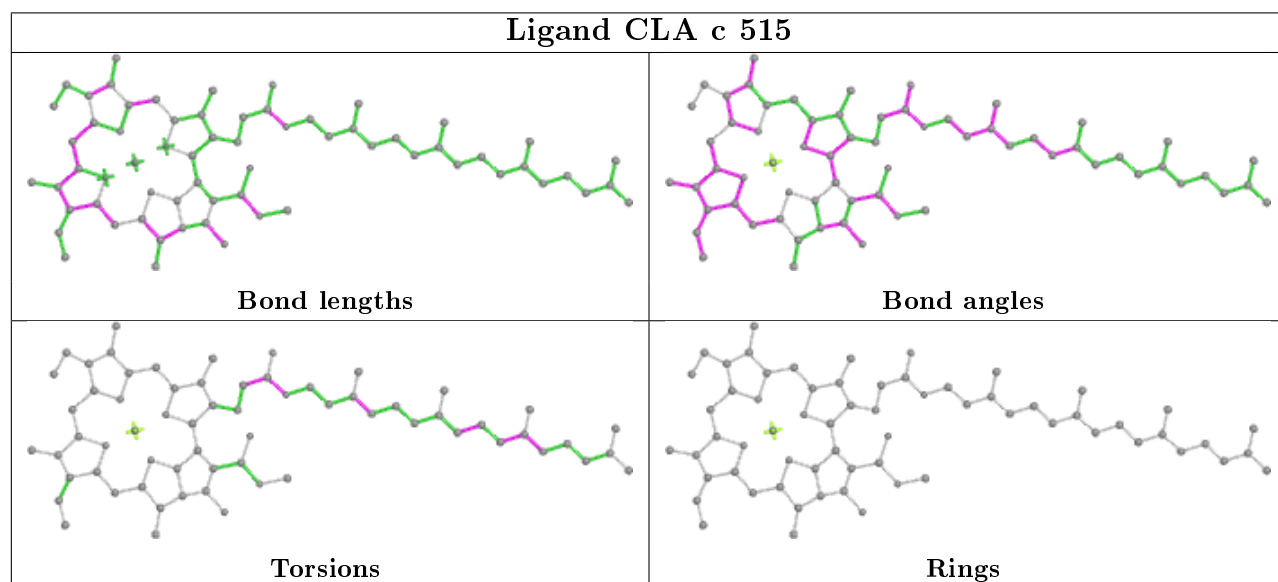
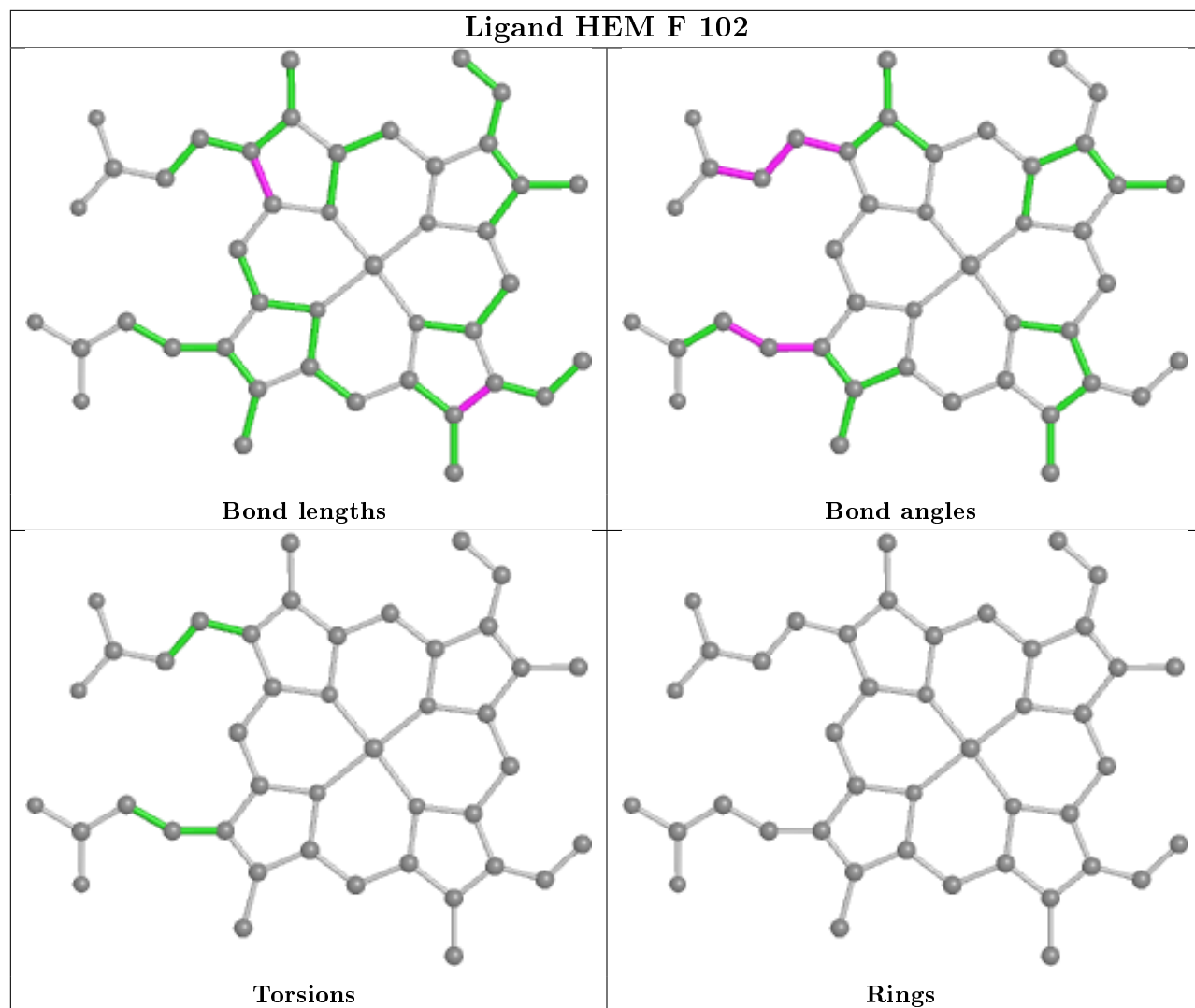


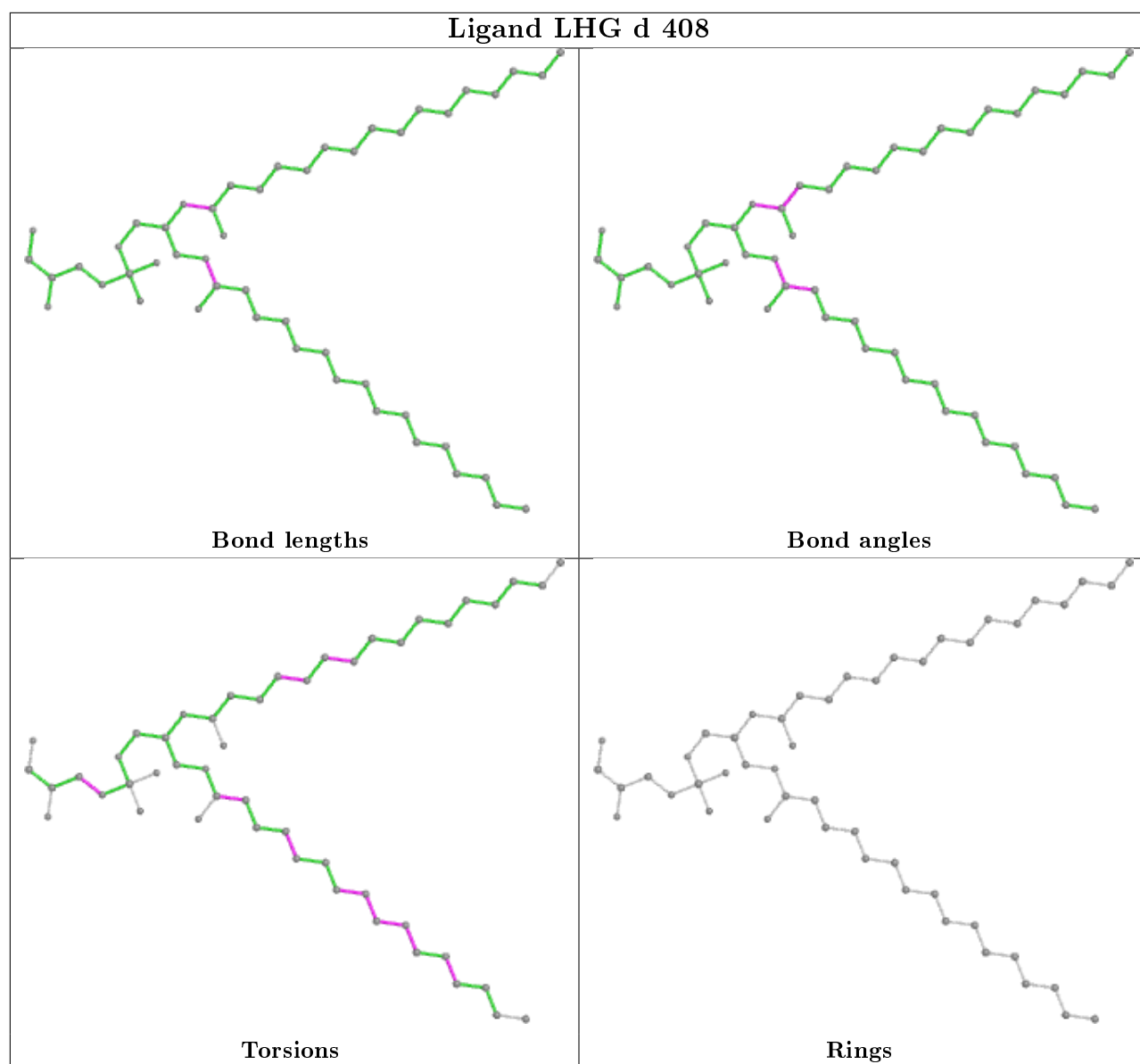
## Ligand CLA B 617

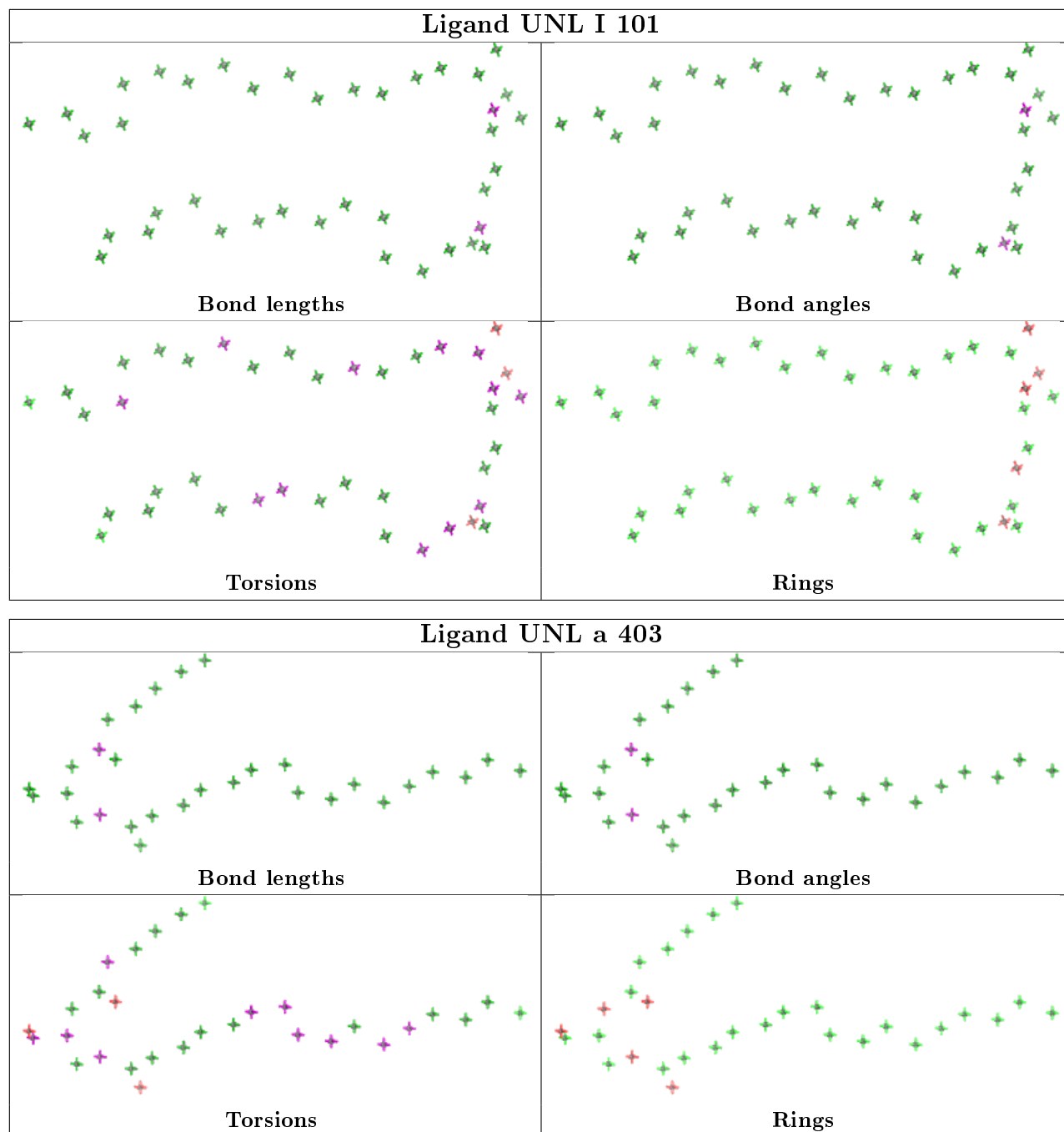


## Ligand CLA c 514

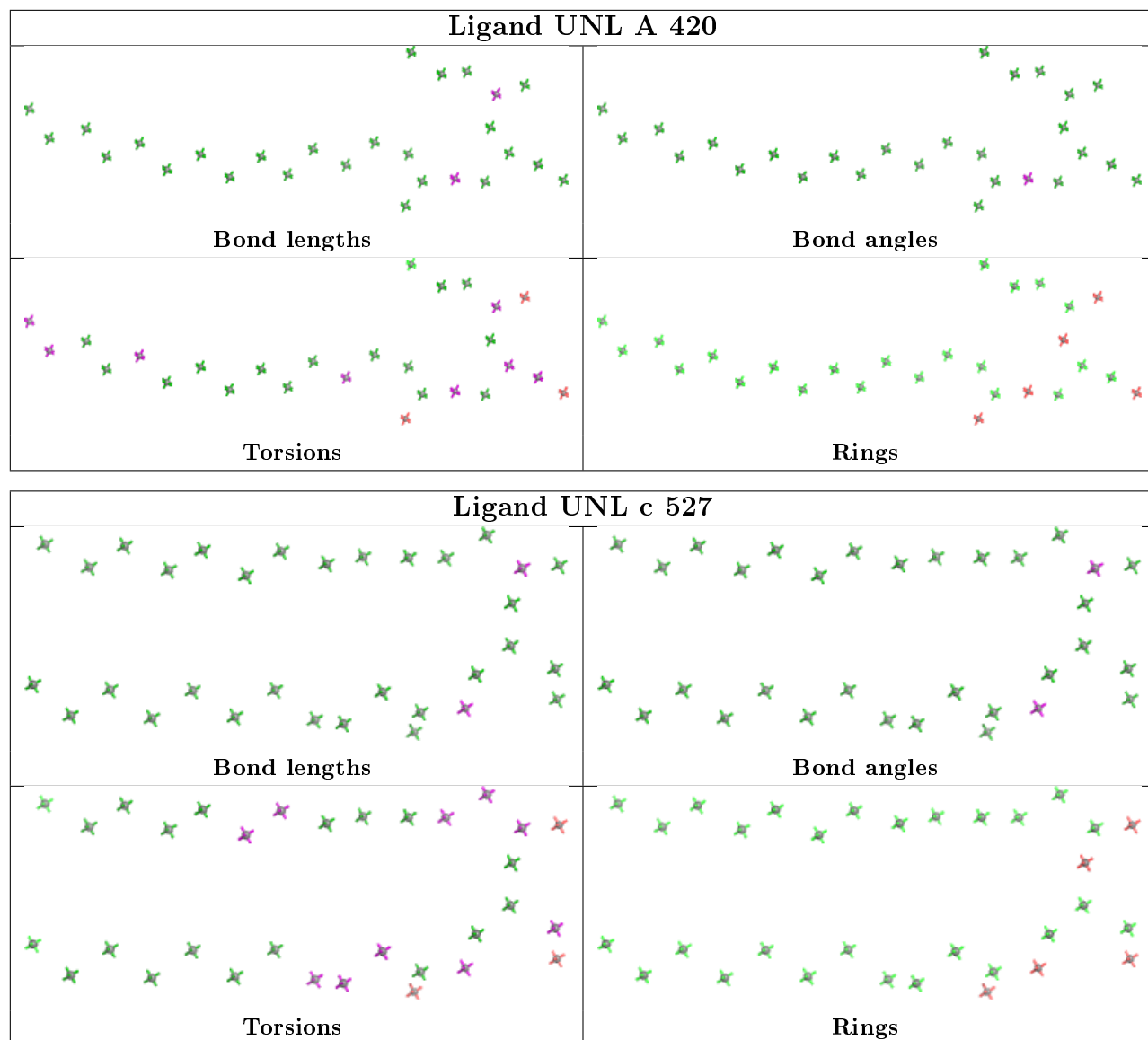


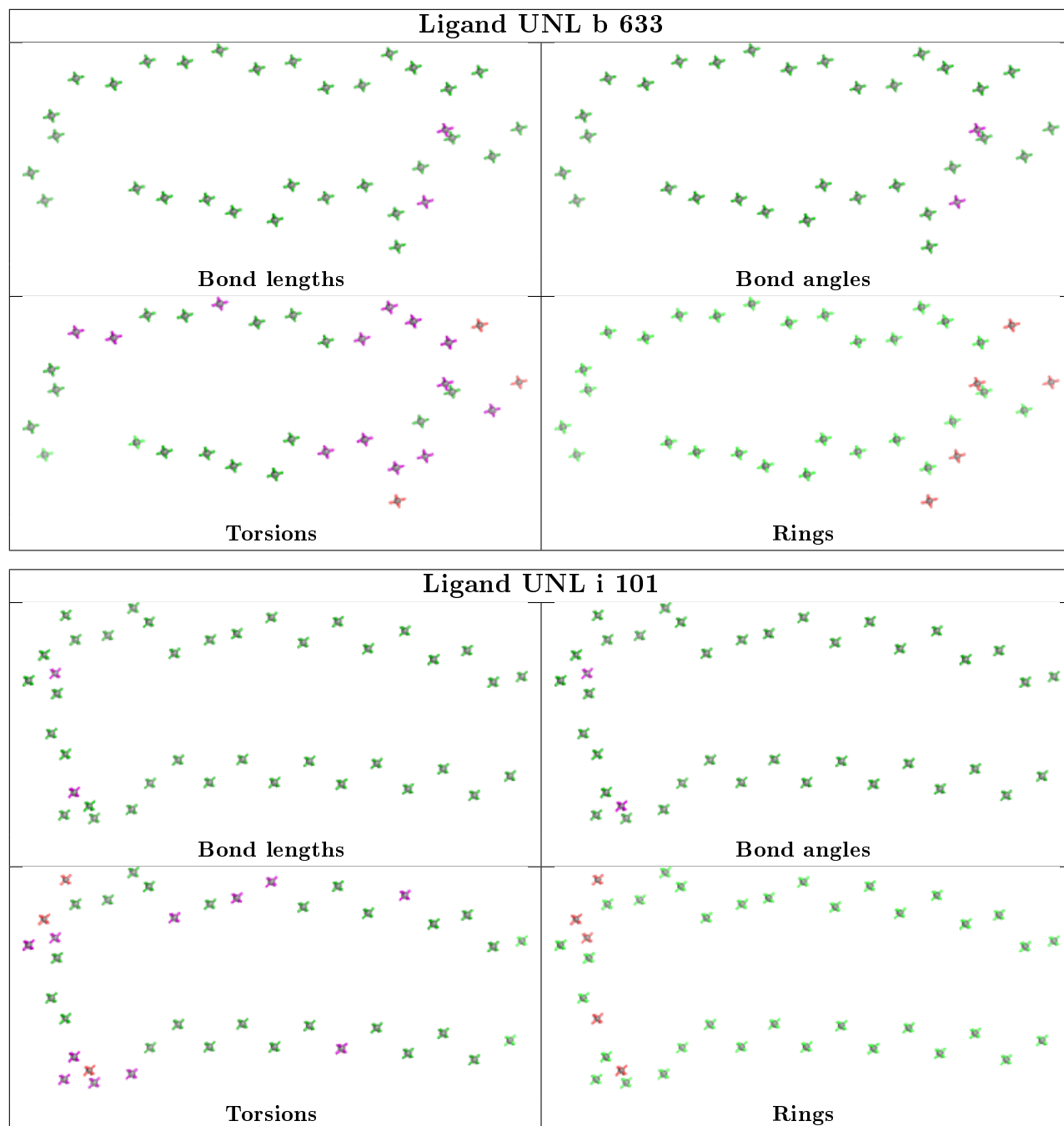


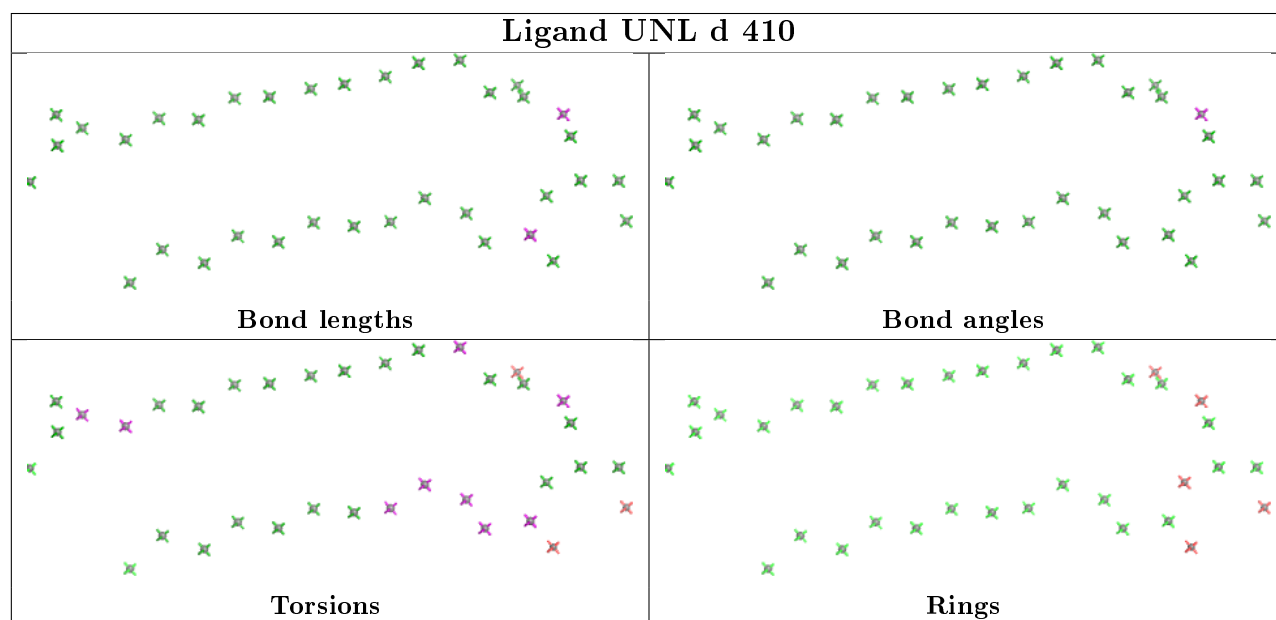
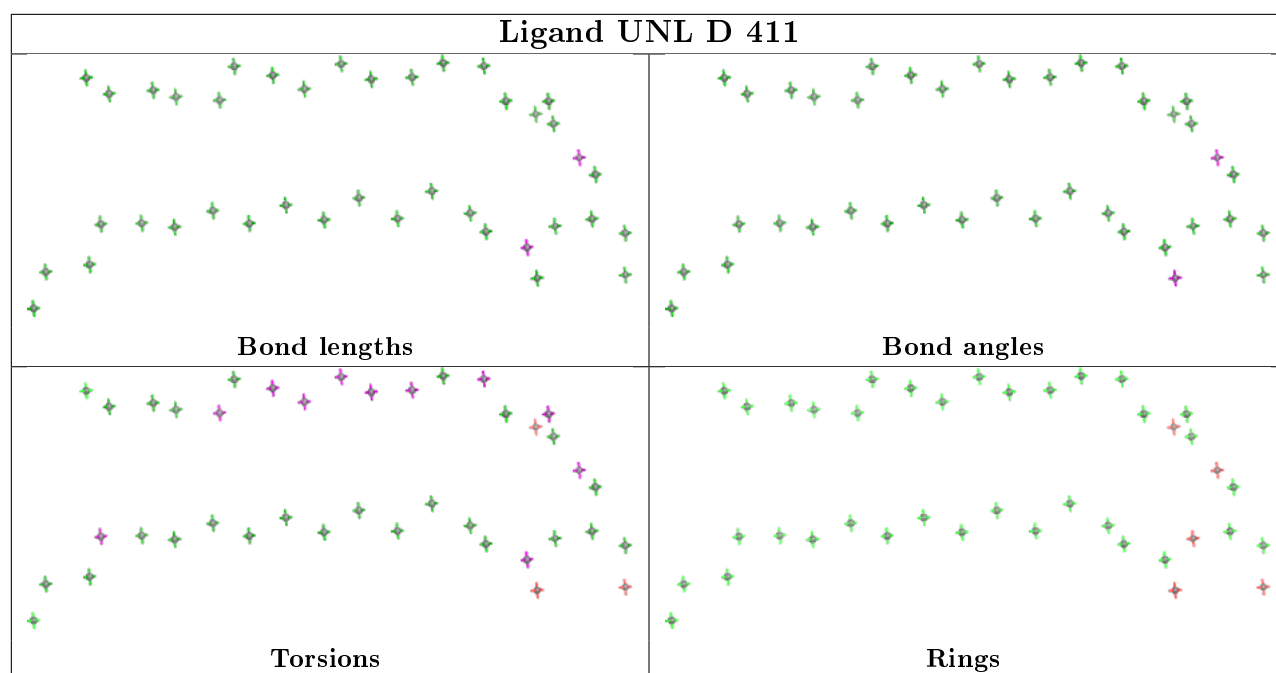


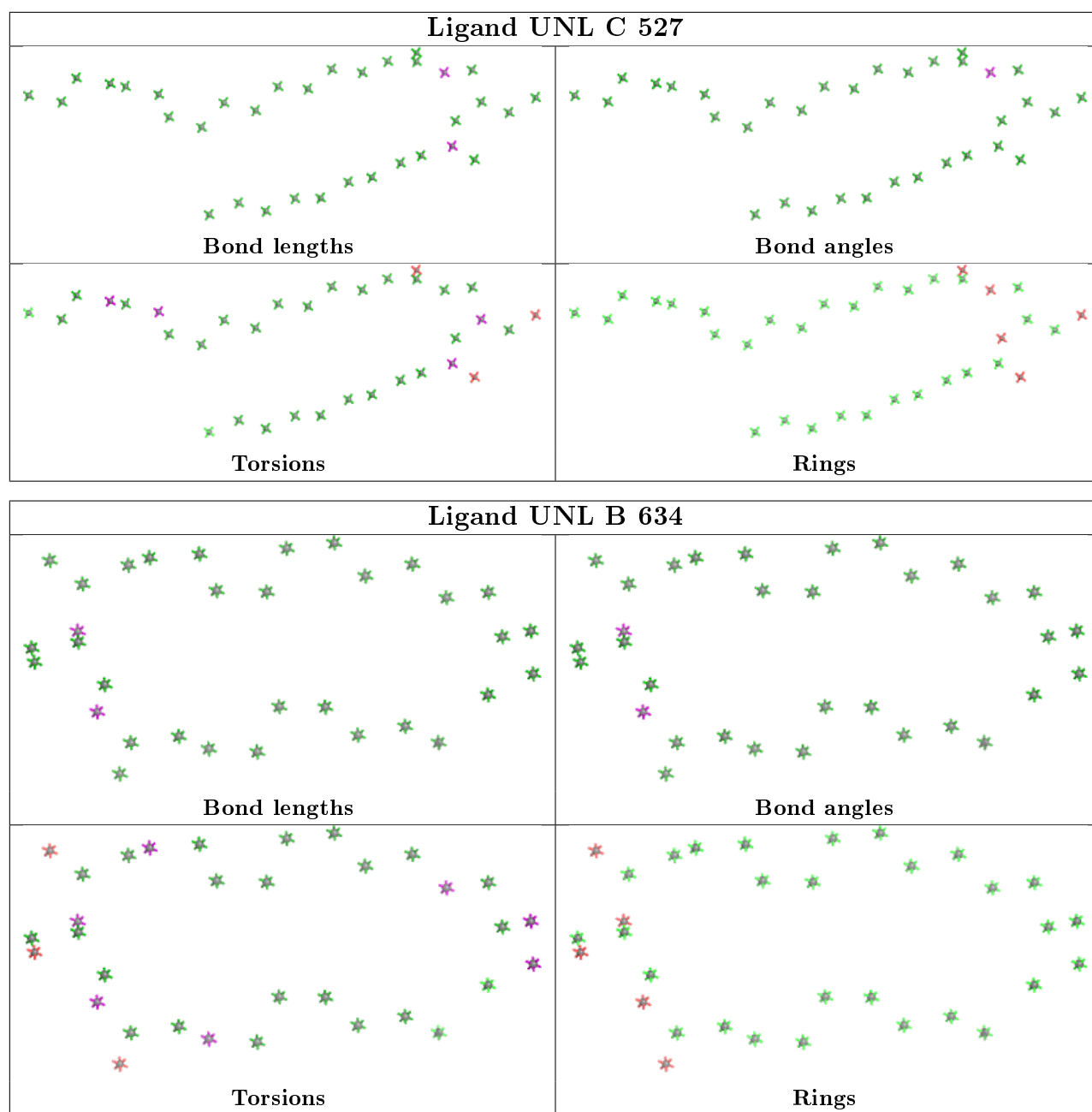












## 5.7 Other polymers [i](#)

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%)	0.09	5 (1%) 73 79	29, 39, 69, 117	0
1	a	334/344 (97%)	0.18	12 (3%) 42 51	31, 39, 74, 152	0
2	B	504/505 (99%)	0.11	8 (1%) 72 77	31, 43, 77, 123	0
2	b	503/505 (99%)	0.21	24 (4%) 30 39	31, 44, 81, 180	0
3	C	451/455 (99%)	0.09	3 (0%) 87 91	34, 51, 70, 116	0
3	c	455/455 (100%)	0.05	6 (1%) 77 82	38, 53, 70, 115	0
4	D	341/342 (99%)	0.07	1 (0%) 94 95	28, 40, 65, 131	0
4	d	341/342 (99%)	0.03	4 (1%) 79 83	29, 41, 66, 122	0
5	E	81/84 (96%)	0.66	9 (11%) 5 7	46, 64, 94, 130	0
5	e	81/84 (96%)	0.91	12 (14%) 2 3	47, 65, 115, 176	0
6	F	34/44 (77%)	0.35	3 (8%) 10 14	46, 56, 90, 105	0
6	f	32/44 (72%)	0.32	2 (6%) 20 27	47, 57, 116, 141	0
7	H	65/65 (100%)	0.20	3 (4%) 32 42	40, 53, 72, 150	0
7	h	65/65 (100%)	0.09	2 (3%) 49 58	42, 55, 75, 163	0
8	I	37/38 (97%)	0.18	3 (8%) 12 16	43, 54, 108, 151	0
8	i	37/38 (97%)	0.17	1 (2%) 54 63	42, 52, 98, 131	0
9	J	38/39 (97%)	0.50	3 (7%) 12 17	46, 61, 135, 169	0
9	j	39/39 (100%)	0.68	6 (15%) 2 2	47, 61, 131, 171	0
10	K	37/37 (100%)	0.08	0 100 100	51, 61, 77, 101	0
10	k	37/37 (100%)	0.24	0 100 100	52, 61, 77, 102	0
11	L	37/37 (100%)	0.14	1 (2%) 54 63	29, 35, 100, 120	0
11	l	37/37 (100%)	0.25	2 (5%) 25 34	31, 35, 99, 120	0
12	M	33/36 (91%)	0.25	2 (6%) 21 28	30, 37, 63, 113	0
12	m	33/36 (91%)	0.22	1 (3%) 50 59	32, 38, 68, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.06	5 (2%) 63 71	31, 49, 91, 137	0
13	o	243/244 (99%)	0.09	5 (2%) 63 71	33, 51, 104, 170	0
14	T	29/32 (90%)	0.18	1 (3%) 45 53	31, 37, 64, 133	0
14	t	29/32 (90%)	0.12	0 100 100	31, 38, 64, 133	0
15	U	97/104 (93%)	-0.06	0 100 100	37, 48, 77, 116	0
15	u	97/104 (93%)	-0.06	0 100 100	39, 49, 71, 116	0
16	V	137/137 (100%)	0.07	0 100 100	35, 49, 78, 116	0
16	v	137/137 (100%)	0.09	3 (2%) 62 69	40, 55, 84, 118	0
17	Y	29/30 (96%)	2.04	7 (24%) 0 0	66, 80, 141, 149	0
17	y	29/30 (96%)	0.85	4 (13%) 2 3	66, 81, 142, 149	0
18	X	39/40 (97%)	0.34	2 (5%) 28 36	51, 61, 115, 136	0
18	x	38/40 (95%)	0.72	5 (13%) 3 4	53, 62, 116, 137	0
19	Z	62/62 (100%)	0.72	9 (14%) 2 3	66, 78, 125, 165	0
19	z	62/62 (100%)	1.27	18 (29%) 0 0	68, 80, 126, 166	0
20	R	18/34 (52%)	7.20	18 (100%) 0 0	107, 137, 177, 178	0
All	All	5275/5384 (97%)	0.20	190 (3%) 42 51	28, 48, 91, 180	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	18.4
20	R	15	ALA	13.6
20	R	18	TRP	13.0
5	e	5	THR	12.4
2	b	496	TYR	11.3
20	R	6	LEU	9.5
20	R	9	LEU	8.9
20	R	16	ALA	8.8
19	z	3	ILE	8.8
2	b	495	PHE	8.8
20	R	17	GLY	8.4
20	R	8	VAL	8.4
9	j	1	MET	8.3
17	Y	19	ILE	8.3
2	b	494	GLY	8.1
20	R	5	VAL	7.7
20	R	3	TRP	7.7

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Mol	Chain	Res	Type	RSRZ
1	a	264[A]	SER	7.7
20	R	14	LEU	7.5
2	b	499	VAL	7.3
2	b	486	LEU	7.2
18	x	2	THR	6.9
2	b	489	GLU	6.6
20	R	12	VAL	6.6
17	Y	20	ALA	6.5
5	e	6	GLY	5.9
18	x	37	VAL	5.9
7	h	65	LEU	5.9
20	R	11	PRO	5.7
13	O	56	PRO	5.7
19	Z	62	VAL	5.6
20	R	13	LEU	5.3
2	B	479	PHE	5.2
3	C	23	ALA	5.2
5	e	4	THR	5.1
13	o	58	ASN	5.1
5	E	6	GLY	5.0
17	Y	21	GLN	5.0
2	b	493	TRP	5.0
19	Z	31	GLN	5.0
17	y	20	ALA	4.9
1	a	262	TYR	4.8
18	x	38	GLN	4.7
19	z	62	VAL	4.7
19	z	5	PHE	4.6
2	b	487	SER	4.6
7	h	66	GLY	4.6
9	j	4	GLY	4.6
2	B	495	PHE	4.5
19	Z	33	TRP	4.5
17	Y	22	LEU	4.4
2	b	504	THR	4.3
5	E	5	THR	4.3
20	R	10	LEU	4.3
2	b	488	PRO	4.2
20	R	19	ALA	4.2
19	Z	61	VAL	4.1
1	a	263	ALA	4.1
2	b	485	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
17	Y	26	ALA	4.0
2	B	496	TYR	3.9
20	R	4	ARG	3.9
5	E	4	THR	3.9
9	j	3	GLU	3.9
2	B	494	GLY	3.9
2	b	498	LYS	3.9
9	J	5	GLY	3.9
2	b	484	PRO	3.8
2	b	497	GLN	3.8
19	z	32	ASP	3.7
19	z	61	VAL	3.7
5	E	19	TYR	3.6
2	b	500	GLY	3.6
6	F	16	PHE	3.6
1	a	261	GLN	3.5
5	e	7	GLU	3.5
2	B	501	ASP	3.5
5	e	10	PHE	3.4
13	O	60	ARG	3.4
13	o	246	ALA	3.3
8	I	37	LEU	3.3
5	E	84	LYS	3.2
1	a	248[A]	ILE	3.2
19	z	35	ARG	3.2
20	R	7	VAL	3.2
19	z	33	TRP	3.2
13	o	59	LYS	3.2
11	l	3	PRO	3.1
18	x	39	ARG	3.1
9	J	2	SER	3.0
2	B	504	THR	3.0
13	O	62	GLU	3.0
2	b	503	THR	3.0
4	D	12	ARG	3.0
2	b	502	VAL	3.0
5	e	61	ARG	3.0
2	b	491	VAL	2.9
2	b	501	ASP	2.9
19	z	2	THR	2.9
2	b	490	GLN	2.9
7	H	64	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
20	R	2	ASP	2.9
6	f	14	PRO	2.9
1	a	265[A]	PHE	2.8
17	Y	25	ILE	2.8
2	b	86[A]	ILE	2.8
19	z	38	GLN	2.8
17	y	25	ILE	2.7
1	a	11	ALA	2.7
18	X	37	VAL	2.7
19	Z	30	PRO	2.7
1	a	260	PHE	2.7
6	F	15	ILE	2.7
5	E	15	THR	2.7
1	A	12	ASN	2.7
5	e	72	ALA	2.7
13	o	56	PRO	2.6
16	v	106	ASN	2.6
5	E	83	LEU	2.6
18	X	40	SER	2.6
19	z	42	LEU	2.6
9	J	3	GLU	2.6
1	A	13	LEU	2.6
2	b	85	GLY	2.5
8	I	36	ASP	2.5
5	E	79	PHE	2.5
19	z	41	PHE	2.5
3	c	143	TYR	2.5
1	a	229	GLU	2.5
14	T	30	THR	2.5
6	F	14	PRO	2.5
17	y	41	VAL	2.4
5	e	13	ILE	2.4
5	E	82	GLN	2.4
7	H	65	LEU	2.4
6	f	16	PHE	2.4
8	I	34	ARG	2.4
5	e	20	TRP	2.4
16	v	17	LYS	2.4
9	j	5	GLY	2.4
1	a	252[A]	HIS	2.4
19	z	28	ALA	2.4
3	C	145[A]	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	483	ASP	2.4
18	x	35	ASP	2.4
4	d	240[A]	ALA	2.3
7	H	16	SER	2.3
3	c	200	THR	2.3
5	e	8	ARG	2.3
1	A	243[A]	GLU	2.3
19	z	29	SER	2.3
4	d	236[A]	ASN	2.3
3	c	207	ARG	2.3
2	B	489	GLU	2.3
5	e	59	GLU	2.3
9	j	2	SER	2.3
2	b	492	GLU	2.3
3	c	257	PHE	2.2
19	Z	29	SER	2.2
12	M	33	GLN	2.2
19	Z	34	ASP	2.2
9	j	6	ARG	2.2
19	z	60	PHE	2.1
1	a	15	GLU	2.1
8	i	36	ASP	2.1
13	O	59	LYS	2.1
2	B	486	LEU	2.1
19	z	7	LEU	2.1
11	l	1	MET	2.1
1	A	230	THR	2.1
19	z	4	LEU	2.1
19	z	36	SER	2.1
5	e	79	PHE	2.1
17	y	44	GLY	2.1
3	c	20	SER	2.1
11	L	1	MET	2.1
12	M	34	LYS	2.1
1	a	307[A]	ILE	2.0
3	C	134	ILE	2.0
12	m	33	GLN	2.0
13	o	36	GLN	2.0
19	Z	1	MET	2.0
13	O	58	ASN	2.0
19	Z	36	SER	2.0
16	v	12	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
19	z	39	LEU	2.0
1	A	245[A]	THR	2.0
4	d	238[A]	THR	2.0
4	d	233[A]	ARG	2.0
3	c	21	ILE	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	0.95	0.11	35,38,64,74	0
12	FME	m	1	10/11	0.97	0.15	34,43,98,115	0
8	FME	i	1	10/11	0.97	0.13	41,51,56,58	0
8	FME	I	1	10/11	0.97	0.12	37,45,52,53	0
12	FME	M	1	10/11	0.97	0.12	31,47,81,85	0
14	FME	t	1	10/11	0.98	0.13	28,38,44,87	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
36	DGD	e	101	62/66	0.45	0.39	70,118,175,181	0
29	LMT	F	101	35/35	0.50	0.34	86,125,152,156	0
29	LMT	b	630	25/35	0.59	0.30	72,92,147,149	0
32	UNL	C	527	34/-	0.59	0.23	73,108,129,134	0
37	LHG	e	102	42/49	0.61	0.32	69,134,167,172	0
32	UNL	j	101	10/-	0.63	0.25	70,82,96,99	0
36	DGD	D	406	52/66	0.64	0.28	65,108,147,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	LMT	C	521	35/35	0.64	0.31	90,123,152,162	0
29	LMT	M	103	35/35	0.64	0.25	41,102,141,150	0
29	LMT	D	401	35/35	0.67	0.27	67,118,146,155	0
35	HTG	d	411	16/19	0.67	0.19	65,109,124,127	0
29	LMT	a	419	35/35	0.68	0.35	87,111,130,134	0
32	UNL	a	403	30/-	0.68	0.26	69,91,126,131	0
29	LMT	f	102	35/35	0.69	0.29	72,121,149,154	0
35	HTG	D	412	16/19	0.70	0.29	75,142,157,157	0
32	UNL	c	527	32/-	0.71	0.22	67,100,136,144	0
33	LMG	Z	101	37/55	0.71	0.27	54,111,132,135	0
32	UNL	A	420	28/-	0.71	0.21	61,86,104,106	0
32	UNL	J	101	10/-	0.71	0.20	47,72,89,101	0
35	HTG	c	526	19/19	0.72	0.30	66,105,123,137	0
27	SQD	f	101	43/54	0.73	0.26	86,120,144,145	0
37	LHG	E	101	42/49	0.73	0.23	67,101,123,128	0
35	HTG	B	633	19/19	0.74	0.20	56,109,139,175	0
29	LMT	m	103	35/35	0.74	0.23	40,96,125,132	0
35	HTG	b	608	19/19	0.76	0.21	56,108,148,148	0
31	PL9	a	415[B]	55/55	0.77	0.26	73,103,117,120	55
29	LMT	a	404	35/35	0.77	0.23	47,82,112,131	0
32	UNL	B	634	33/-	0.77	0.22	56,87,134,138	0
32	UNL	b	633	33/-	0.77	0.24	50,94,155,158	0
31	PL9	a	415[A]	55/55	0.77	0.26	75,104,117,119	55
32	UNL	m	101	10/-	0.78	0.23	49,60,85,88	0
35	HTG	B	625	19/19	0.78	0.21	70,112,141,147	0
33	LMG	C	519	51/55	0.79	0.21	49,83,108,117	0
31	PL9	A	419[B]	55/55	0.79	0.23	69,94,108,111	55
27	SQD	L	102	54/54	0.79	0.19	50,77,123,141	0
31	PL9	A	419[A]	55/55	0.79	0.23	68,94,108,110	55
29	LMT	m	102	35/35	0.80	0.22	42,81,100,107	0
34	CA	b	609	1/1	0.80	0.14	134,134,134,134	0
29	LMT	A	417	35/35	0.80	0.20	40,80,108,129	0
35	HTG	C	523	19/19	0.80	0.21	79,91,124,126	0
27	SQD	A	416	54/54	0.81	0.18	52,73,111,128	0
27	SQD	B	621	54/54	0.81	0.20	51,88,147,155	0
34	CA	B	601	1/1	0.82	0.12	130,130,130,130	0
29	LMT	M	101	35/35	0.82	0.20	41,80,99,100	0
33	LMG	C	520	51/55	0.83	0.20	56,109,125,129	0
32	UNL	I	101	40/-	0.83	0.23	41,84,142,153	0
28	GOL	V	201	6/6	0.83	0.38	64,77,86,93	0
33	LMG	c	524	51/55	0.83	0.22	49,106,129,132	0
27	SQD	a	405	54/54	0.84	0.17	47,77,116,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	DGD	C	517	62/66	0.84	0.16	42,54,96,112	0
32	UNL	i	101	40/-	0.84	0.22	48,78,138,141	0
32	UNL	d	410	36/-	0.84	0.19	51,76,129,142	0
33	LMG	c	501	51/55	0.84	0.19	57,79,98,99	0
29	LMT	B	635	25/35	0.84	0.23	40,80,134,138	0
29	LMT	T	104	25/35	0.84	0.23	37,79,133,138	0
28	GOL	T	102	6/6	0.85	0.26	94,108,113,115	0
28	GOL	v	201	6/6	0.85	0.25	68,88,90,92	0
33	LMG	A	421	51/55	0.85	0.17	57,82,106,115	0
33	LMG	z	101	39/55	0.85	0.22	67,115,138,158	0
35	HTG	b	632	19/19	0.85	0.22	66,118,148,149	0
33	LMG	c	523	51/55	0.86	0.18	48,86,111,115	0
32	UNL	M	102	10/-	0.86	0.19	47,64,75,75	0
35	HTG	B	624	19/19	0.86	0.18	48,64,89,93	0
27	SQD	F	103	43/54	0.86	0.20	76,102,119,129	0
33	LMG	b	629	51/55	0.86	0.17	42,51,72,94	0
32	UNL	D	411	40/-	0.87	0.17	52,79,130,139	0
28	GOL	b	606	6/6	0.88	0.17	64,79,86,86	0
33	LMG	B	622	51/55	0.88	0.17	33,50,74,90	0
27	SQD	A	412	54/54	0.88	0.18	45,78,95,98	0
28	GOL	c	503	6/6	0.88	0.40	76,80,97,101	0
28	GOL	O	301	6/6	0.89	0.11	64,79,82,85	0
28	GOL	v	202	6/6	0.89	0.20	70,79,96,112	0
35	HTG	c	525	19/19	0.89	0.13	87,92,102,120	0
24	CLA	c	518	65/65	0.89	0.17	56,80,99,108	0
32	UNL	X	101	18/-	0.89	0.15	54,73,97,100	0
35	HTG	B	632	19/19	0.89	0.14	45,72,101,109	0
38	HEM	F	102	43/43	0.89	0.17	44,66,89,137	0
24	CLA	C	513	65/65	0.89	0.18	52,66,102,109	0
28	GOL	A	415	6/6	0.89	0.18	52,75,79,82	0
36	DGD	H	102	62/66	0.89	0.17	35,48,66,78	0
36	DGD	h	102	62/66	0.89	0.16	39,50,67,79	0
28	GOL	T	101	6/6	0.90	0.30	58,74,93,97	0
27	SQD	a	414	54/54	0.90	0.15	57,80,103,109	0
28	GOL	a	402	6/6	0.90	0.16	70,93,94,94	0
36	DGD	c	521	62/66	0.90	0.15	41,52,105,128	0
35	HTG	b	631	19/19	0.90	0.21	56,71,84,96	0
37	LHG	D	407	49/49	0.90	0.18	31,49,62,73	0
35	HTG	b	607	19/19	0.90	0.15	47,71,80,81	0
35	HTG	V	206	19/19	0.90	0.25	66,94,116,209	0
32	UNL	d	412	18/-	0.90	0.15	60,72,112,113	0
36	DGD	c	522	62/66	0.91	0.15	38,52,87,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
28	GOL	A	413	6/6	0.91	0.14	45,49,54,58	0
36	DGD	C	518	62/66	0.91	0.14	35,51,74,87	0
28	GOL	B	636	6/6	0.91	0.12	48,56,62,62	0
24	CLA	c	512	65/65	0.91	0.13	42,54,67,72	0
33	LMG	d	413	51/55	0.91	0.15	45,58,100,110	0
28	GOL	A	414	6/6	0.91	0.24	49,59,62,64	0
28	GOL	a	420	6/6	0.91	0.20	78,80,91,92	0
28	GOL	B	628	6/6	0.92	0.15	54,73,79,84	0
33	LMG	D	413	51/55	0.92	0.17	38,60,105,128	0
24	CLA	c	508	65/65	0.92	0.14	41,52,62,86	0
22	CL	v	204	1/1	0.92	0.09	95,95,95,95	0
34	CA	F	104	1/1	0.92	0.05	84,84,84,84	0
24	CLA	b	611	65/65	0.92	0.15	32,46,52,57	0
35	HTG	C	522	19/19	0.92	0.15	72,85,101,107	0
24	CLA	C	504	65/65	0.92	0.16	34,47,81,94	0
35	HTG	B	623	19/19	0.92	0.16	40,56,72,76	0
24	CLA	b	616	65/65	0.92	0.14	24,35,44,54	0
28	GOL	V	204	6/6	0.92	0.18	72,78,80,89	0
24	CLA	b	618	65/65	0.92	0.15	37,49,58,71	0
35	HTG	b	601	19/19	0.92	0.12	40,47,70,71	0
28	GOL	o	301	6/6	0.93	0.14	65,78,89,107	0
24	CLA	b	610	65/65	0.93	0.16	44,68,104,134	0
26	BCR	c	528	40/40	0.93	0.13	60,73,83,85	0
28	GOL	A	422	6/6	0.93	0.23	68,73,74,82	0
24	CLA	B	610	65/65	0.93	0.14	34,46,55,64	0
24	CLA	c	511	65/65	0.93	0.13	43,63,91,107	0
28	GOL	C	524	6/6	0.93	0.28	59,63,76,80	0
37	LHG	D	409	49/49	0.93	0.19	39,55,116,129	0
24	CLA	b	615	65/65	0.93	0.13	32,44,88,106	0
24	CLA	c	513	65/65	0.93	0.13	35,48,113,129	0
24	CLA	C	501	65/65	0.93	0.13	38,50,73,81	0
28	GOL	v	203	6/6	0.93	0.17	48,49,57,59	0
24	CLA	c	516	65/65	0.93	0.14	43,55,75,88	0
28	GOL	t	102	6/6	0.93	0.40	51,80,90,96	0
24	CLA	B	602	65/65	0.93	0.16	41,62,95,124	0
24	CLA	C	506	65/65	0.93	0.13	46,62,105,114	0
28	GOL	B	626	6/6	0.93	0.17	44,54,59,80	0
24	CLA	c	515	65/65	0.93	0.12	39,52,65,71	0
24	CLA	C	511	65/65	0.93	0.12	41,58,69,83	0
28	GOL	B	630	6/6	0.93	0.23	48,59,72,76	0
24	CLA	C	509	65/65	0.94	0.14	43,55,74,81	0
24	CLA	B	615	65/65	0.94	0.14	26,40,90,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	B	614	65/65	0.94	0.14	27,36,66,74	0
32	UNL	D	410	17/-	0.94	0.15	40,70,83,89	0
24	CLA	c	506	65/65	0.94	0.12	41,55,65,70	0
24	CLA	C	507	65/65	0.94	0.14	41,56,68,70	0
24	CLA	c	509	65/65	0.94	0.12	38,53,74,79	0
37	LHG	L	101	49/49	0.94	0.16	33,45,56,59	0
24	CLA	C	512	65/65	0.94	0.11	48,64,81,92	0
24	CLA	B	607	65/65	0.94	0.14	32,44,93,103	0
36	DGD	C	516	62/66	0.94	0.14	33,47,88,96	0
26	BCR	C	514	40/40	0.94	0.13	49,67,81,84	0
37	LHG	d	407	49/49	0.94	0.17	32,42,57,88	0
24	CLA	b	625	65/65	0.94	0.13	35,52,101,109	0
36	DGD	c	520	62/66	0.94	0.13	36,48,94,107	0
37	LHG	d	406	49/49	0.94	0.17	37,51,59,74	0
37	LHG	b	634	49/49	0.94	0.16	36,45,58,64	0
32	UNL	d	409	17/-	0.94	0.18	47,69,97,101	0
24	CLA	C	508	65/65	0.94	0.12	36,48,114,125	0
24	CLA	B	603	65/65	0.94	0.13	35,43,50,53	0
24	CLA	C	503	65/65	0.94	0.13	40,50,61,64	0
24	CLA	c	517	65/65	0.94	0.13	49,63,82,86	0
26	BCR	b	627	40/40	0.94	0.15	31,42,60,67	0
28	GOL	b	605	6/6	0.94	0.20	70,80,101,103	0
24	CLA	c	510	65/65	0.94	0.13	36,48,67,78	0
26	BCR	y	101	40/40	0.94	0.14	43,63,72,80	0
24	CLA	b	623	65/65	0.94	0.14	26,40,88,115	0
26	BCR	T	103	40/40	0.95	0.13	31,46,61,62	0
37	LHG	D	408	49/49	0.95	0.17	33,43,61,89	0
26	BCR	B	619	40/40	0.95	0.15	27,40,56,63	0
24	CLA	B	612	65/65	0.95	0.15	26,38,50,57	0
24	CLA	B	617	65/65	0.95	0.15	36,49,116,118	0
24	CLA	d	401	65/65	0.95	0.13	26,33,43,52	0
24	CLA	C	505	65/65	0.95	0.13	38,47,68,78	0
24	CLA	B	616	65/65	0.95	0.13	34,45,65,77	0
24	CLA	b	612	65/65	0.95	0.13	33,44,54,59	0
26	BCR	K	101	40/40	0.95	0.14	43,57,65,68	0
24	CLA	b	621	65/65	0.95	0.13	28,40,49,52	0
24	CLA	b	624	65/65	0.95	0.13	33,46,62,70	0
24	CLA	A	405	65/65	0.95	0.15	25,33,45,67	0
28	GOL	V	202	6/6	0.95	0.14	39,47,52,62	0
24	CLA	b	617	65/65	0.95	0.13	32,45,53,60	0
24	CLA	d	403	65/65	0.95	0.13	41,51,103,111	0
26	BCR	D	404	40/40	0.95	0.14	41,50,92,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	CLA	a	409	65/65	0.95	0.14	27,35,49,58	0
24	CLA	b	619	65/65	0.95	0.13	36,45,53,62	0
24	CLA	b	620	65/65	0.95	0.13	29,39,49,55	0
26	BCR	d	404	40/40	0.95	0.14	40,52,79,83	0
26	BCR	H	101	40/40	0.95	0.13	35,51,65,67	0
34	CA	f	103	1/1	0.95	0.06	106,106,106,106	0
26	BCR	k	101	40/40	0.95	0.14	44,59,73,75	0
26	BCR	h	101	40/40	0.95	0.12	38,55,66,68	0
24	CLA	C	510	65/65	0.95	0.12	39,51,62,71	0
24	CLA	D	403	65/65	0.95	0.14	38,51,101,119	0
37	LHG	d	408	49/49	0.95	0.17	34,53,104,109	0
24	CLA	c	514	65/65	0.95	0.13	43,54,74,85	0
24	CLA	B	604	65/65	0.95	0.13	34,43,49,63	0
28	GOL	B	631	6/6	0.95	0.27	43,76,84,87	0
28	GOL	B	627	6/6	0.95	0.19	52,62,79,94	0
26	BCR	B	620	40/40	0.96	0.14	35,46,58,60	0
26	BCR	C	515	40/40	0.96	0.16	39,54,63,65	0
24	CLA	b	614	65/65	0.96	0.14	28,39,52,55	0
28	GOL	V	203	6/6	0.96	0.13	54,59,59,63	0
31	PL9	D	405[A]	55/55	0.96	0.16	26,37,44,57	55
26	BCR	t	101	40/40	0.96	0.14	34,47,64,65	0
24	CLA	B	613	65/65	0.96	0.12	27,37,46,54	0
24	CLA	B	605	65/65	0.96	0.13	27,36,71,75	0
24	CLA	B	606	65/65	0.96	0.13	29,39,54,58	0
38	HEM	e	103	43/43	0.96	0.17	55,81,121,150	0
25	PHO	A	409[A]	64/64	0.96	0.14	33,40,47,49	64
26	BCR	Y	101	40/40	0.96	0.11	47,60,71,80	0
24	CLA	A	406	65/65	0.96	0.14	25,32,42,51	0
26	BCR	c	519	40/40	0.96	0.14	39,54,66,70	0
24	CLA	a	412	65/65	0.96	0.14	31,46,114,124	0
28	GOL	a	401	6/6	0.96	0.23	49,63,68,76	0
28	GOL	B	629	6/6	0.96	0.12	50,52,55,60	0
31	PL9	d	405[B]	55/55	0.96	0.16	24,38,46,57	55
28	GOL	b	603	6/6	0.96	0.14	45,63,75,80	0
24	CLA	A	407	65/65	0.96	0.12	28,39,101,116	0
24	CLA	c	507	65/65	0.96	0.12	40,51,66,73	0
24	CLA	d	402	65/65	0.96	0.14	26,36,60,71	0
24	CLA	B	608	65/65	0.96	0.14	24,35,47,52	0
25	PHO	A	408	64/64	0.96	0.13	28,34,40,40	0
24	CLA	b	613	65/65	0.96	0.13	27,38,73,79	0
24	CLA	A	410	65/65	0.96	0.13	30,45,122,130	0
24	CLA	B	609	65/65	0.96	0.15	35,43,56,60	0

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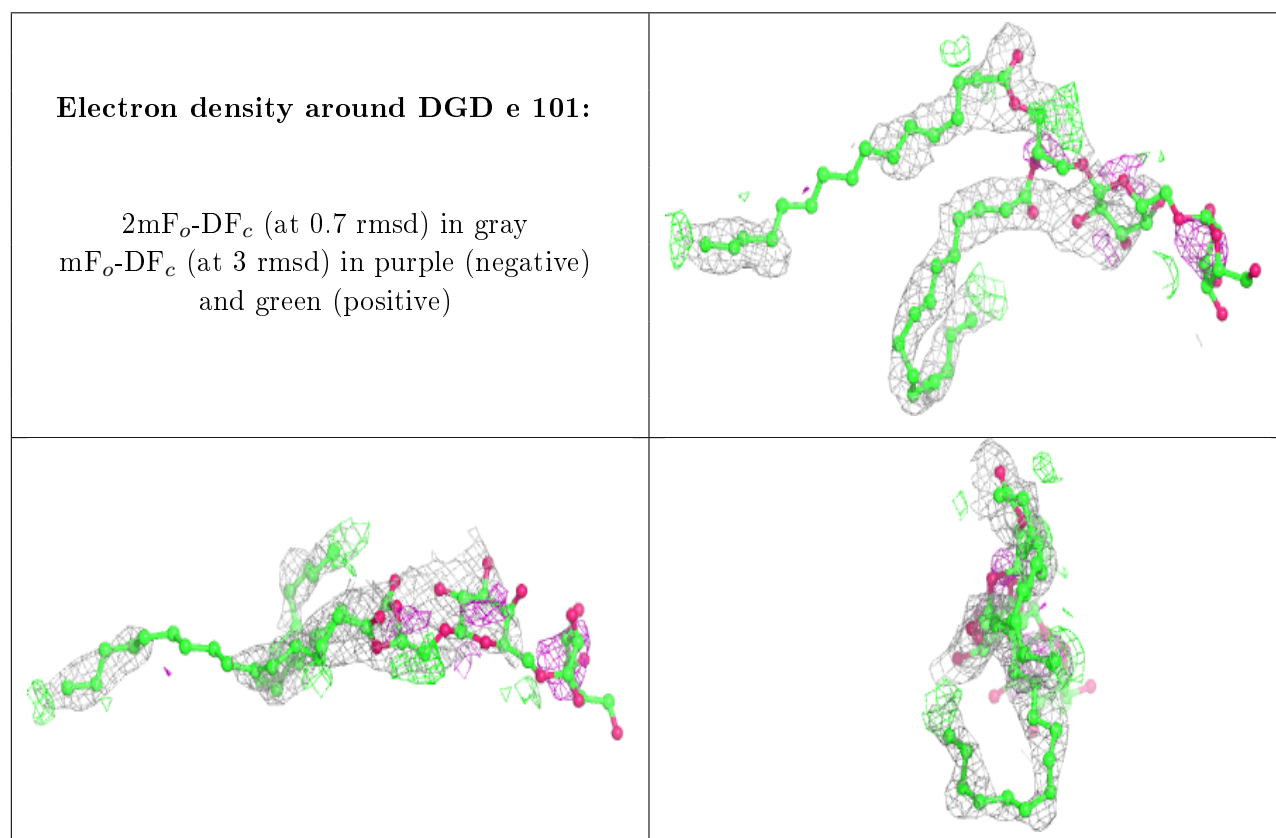
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	PL9	D	405[B]	55/55	0.96	0.16	28,36,45,62	55
25	PHO	a	418[B]	64/64	0.96	0.14	28,41,48,51	64
24	CLA	b	622	65/65	0.96	0.15	27,39,56,62	0
25	PHO	a	418[A]	64/64	0.96	0.14	28,41,47,50	64
24	CLA	D	402	65/65	0.96	0.14	24,34,55,61	0
25	PHO	A	409[B]	64/64	0.96	0.14	27,40,48,49	64
31	PL9	d	405[A]	55/55	0.96	0.16	27,37,46,57	55
28	GOL	b	604	6/6	0.96	0.23	58,63,68,86	0
24	CLA	B	611	65/65	0.96	0.14	36,46,54,69	0
23	BCT	A	404[B]	4/4	0.97	0.12	47,48,62,72	4
26	BCR	B	618	40/40	0.97	0.14	27,39,46,48	0
28	GOL	b	602	6/6	0.97	0.18	56,58,65,89	0
39	MG	j	102	1/1	0.97	0.19	57,57,57,57	0
22	CL	U	201	1/1	0.97	0.17	92,92,92,92	0
23	BCT	a	417[A]	4/4	0.97	0.13	59,60,62,70	4
26	BCR	A	411	40/40	0.97	0.14	28,39,46,48	0
24	CLA	C	502	65/65	0.97	0.13	36,46,61,78	0
26	BCR	b	626	40/40	0.97	0.15	32,41,47,49	0
24	CLA	a	410	65/65	0.97	0.14	31,41,105,114	0
23	BCT	a	417[B]	4/4	0.97	0.13	50,59,61,66	4
26	BCR	a	413	40/40	0.97	0.13	28,39,48,56	0
23	BCT	A	404[A]	4/4	0.97	0.12	47,55,60,72	4
26	BCR	b	628	40/40	0.97	0.14	35,50,62,66	0
25	PHO	a	411	64/64	0.97	0.14	28,36,41,47	0
34	CA	c	505	1/1	0.98	0.06	75,75,75,75	0
38	HEM	v	205	43/43	0.98	0.12	41,52,56,60	0
22	CL	A	403[A]	1/1	0.98	0.13	33,33,33,33	1
34	CA	c	504	1/1	0.98	0.07	67,67,67,67	0
34	CA	o	302	1/1	0.98	0.07	90,90,90,90	0
34	CA	O	302	1/1	0.98	0.04	81,81,81,81	0
22	CL	A	403[B]	1/1	0.98	0.13	35,35,35,35	1
39	MG	J	102	1/1	0.98	0.08	52,52,52,52	0
34	CA	C	526	1/1	0.98	0.09	70,70,70,70	0
38	HEM	V	205	43/43	0.98	0.12	34,40,51,56	0
28	GOL	c	502	6/6	0.99	0.13	38,44,46,48	0
21	FE2	a	406[B]	1/1	0.99	0.15	48,48,48,48	1
28	GOL	C	525	6/6	0.99	0.12	32,42,44,45	0
22	CL	A	402[A]	1/1	0.99	0.15	32,32,32,32	1
30	OEX	a	416[B]	10/10	0.99	0.12	32,38,43,46	10
30	OEX	A	418[B]	10/10	0.99	0.14	33,37,39,39	10
21	FE2	a	406[A]	1/1	0.99	0.15	48,48,48,48	1
30	OEX	A	418[A]	10/10	0.99	0.14	30,36,43,56	10

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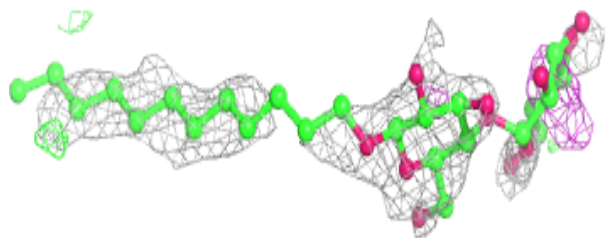
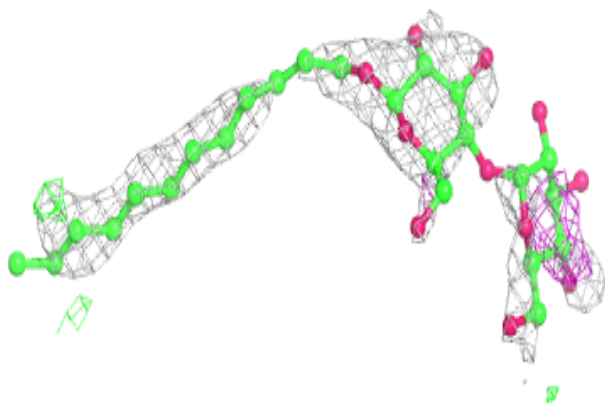
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CL	A	402[B]	1/1	0.99	0.15	32,32,32,32	1
30	OEX	a	416[A]	10/10	0.99	0.12	34,37,40,52	10
22	CL	a	408[B]	1/1	1.00	0.13	40,40,40,40	1
22	CL	a	407[B]	1/1	1.00	0.10	37,37,37,37	1
21	FE2	A	401[B]	1/1	1.00	0.12	50,50,50,50	1
22	CL	a	408[A]	1/1	1.00	0.13	40,40,40,40	1
21	FE2	A	401[A]	1/1	1.00	0.12	47,47,47,47	1
22	CL	a	407[A]	1/1	1.00	0.10	36,36,36,36	1

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

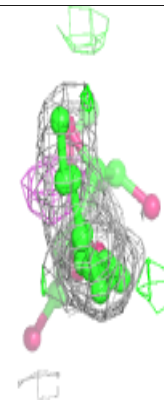
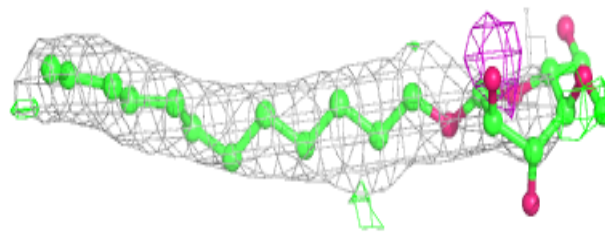
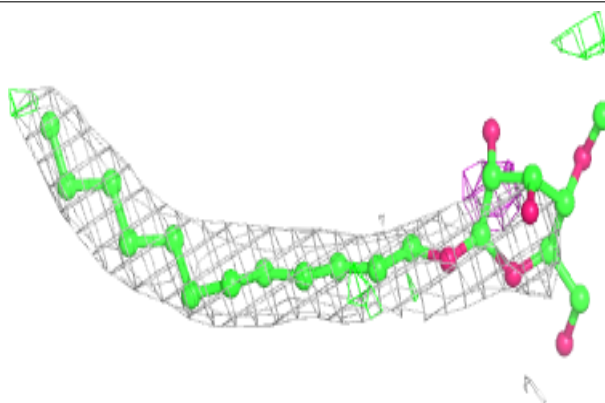


**Electron density around LMT F 101:**

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

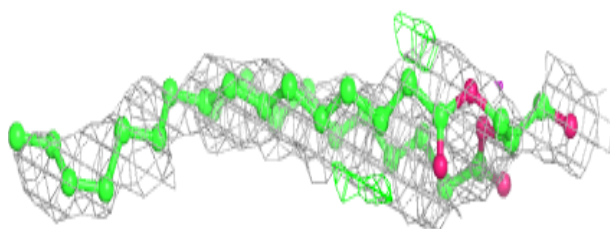
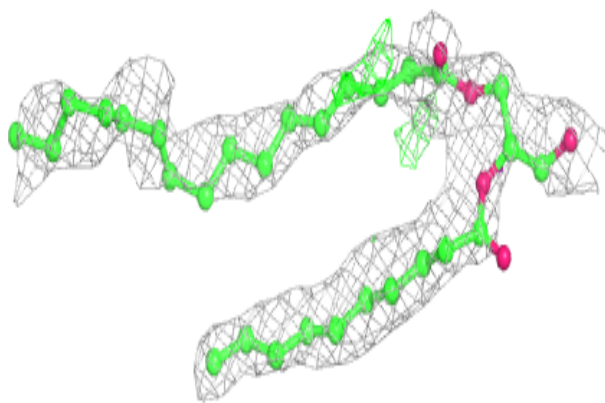
**Electron density around LMT b 630:**

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



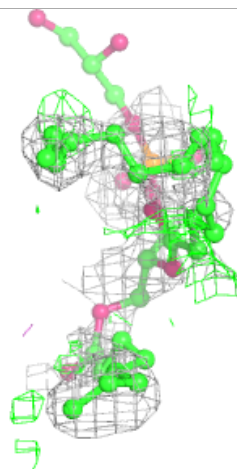
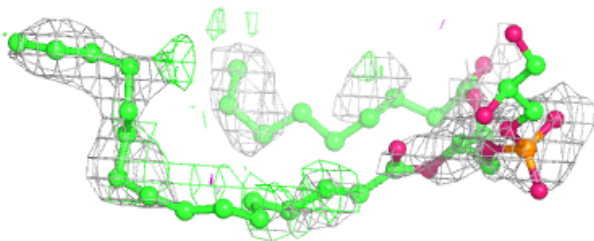
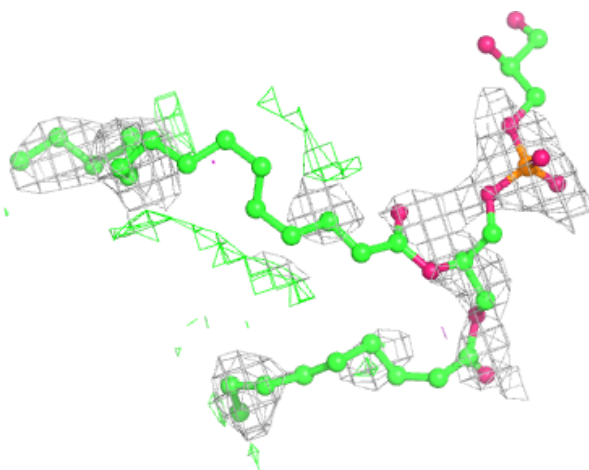
**Electron density around UNL C 527:**

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



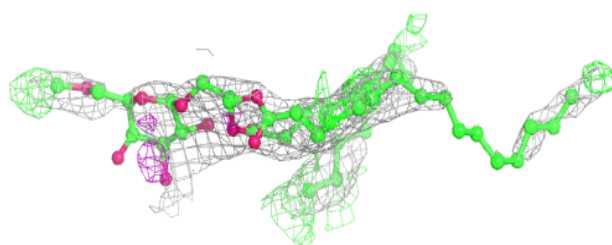
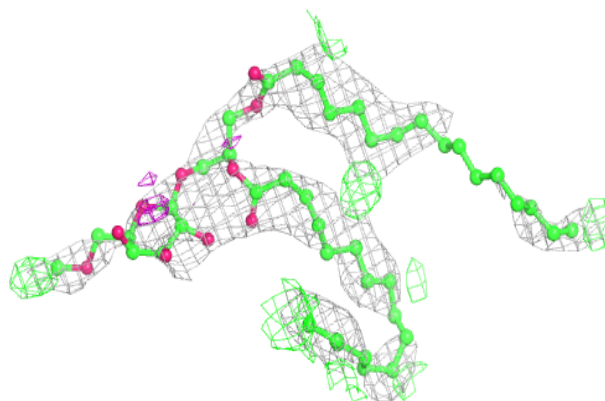
**Electron density around LHG e 102:**

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

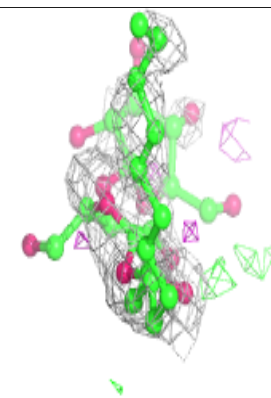
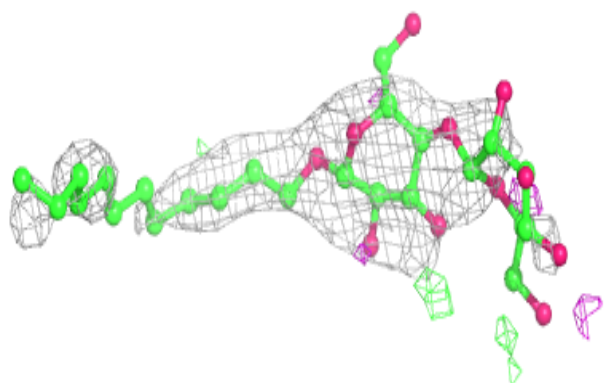
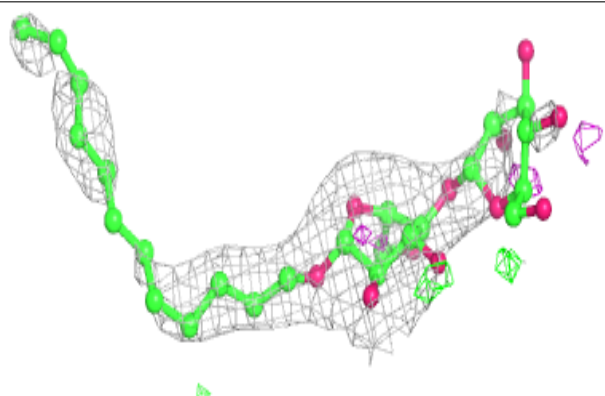


**Electron density around DGD D 406:**

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

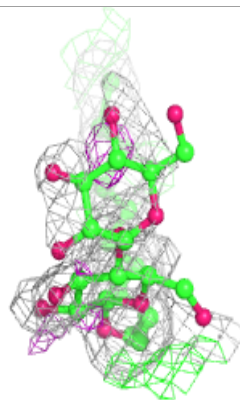
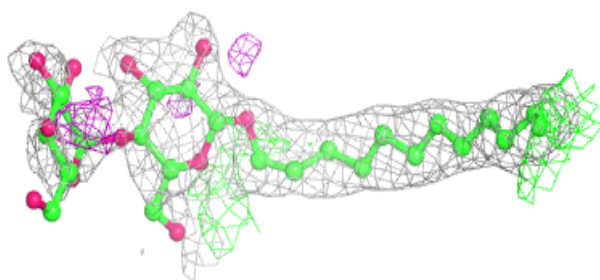
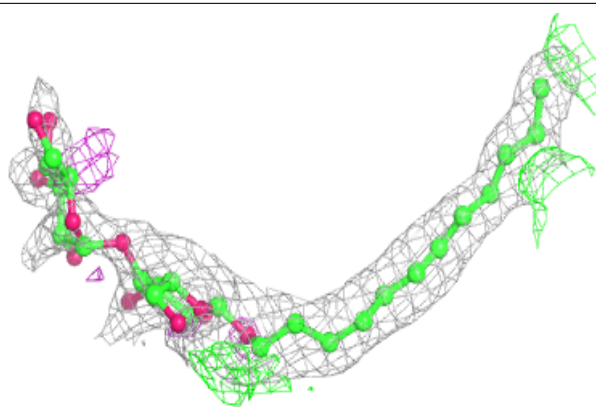
**Electron density around LMT C 521:**

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

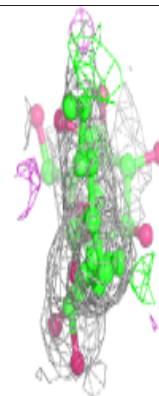
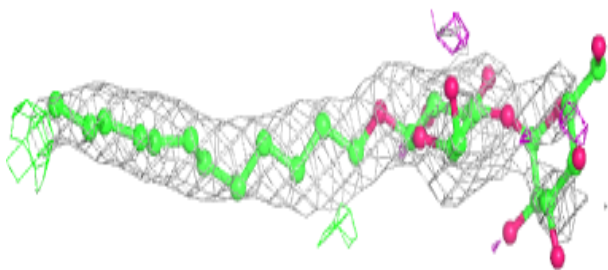
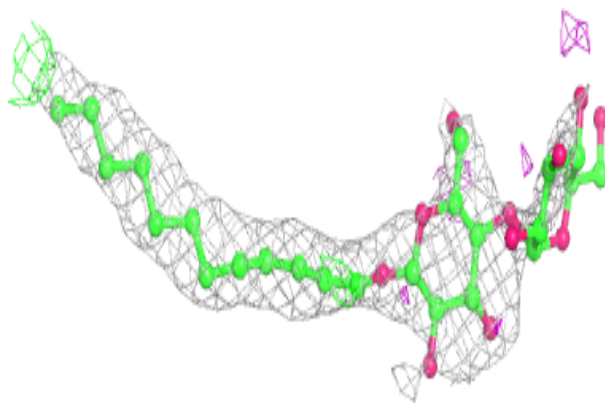


**Electron density around LMT M 103:**

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

**Electron density around LMT D 401:**

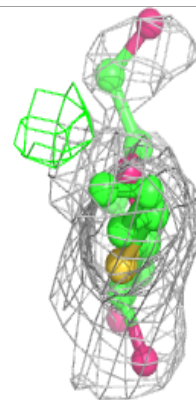
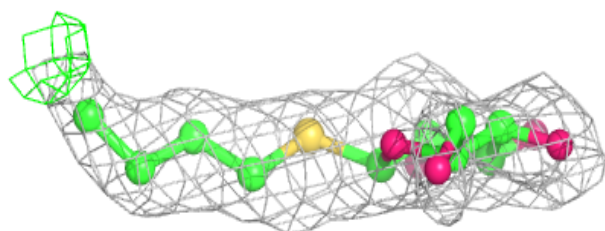
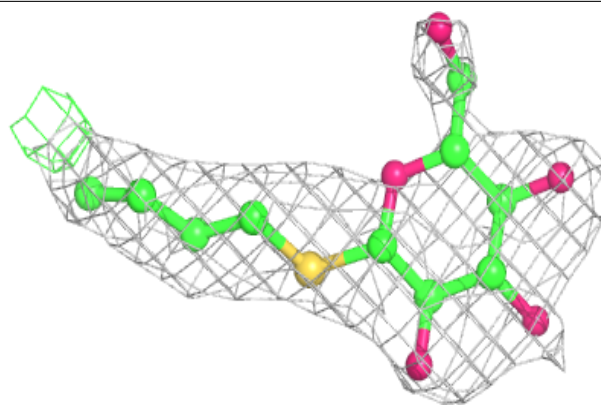
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



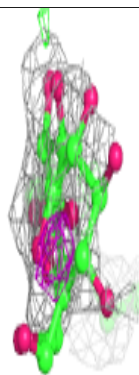
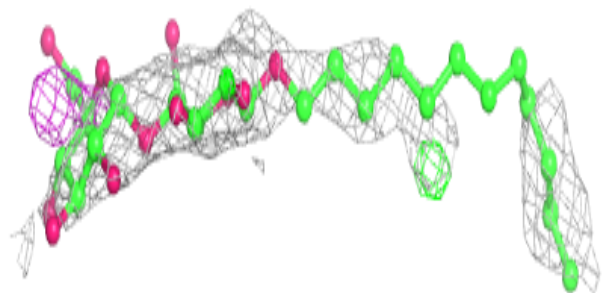
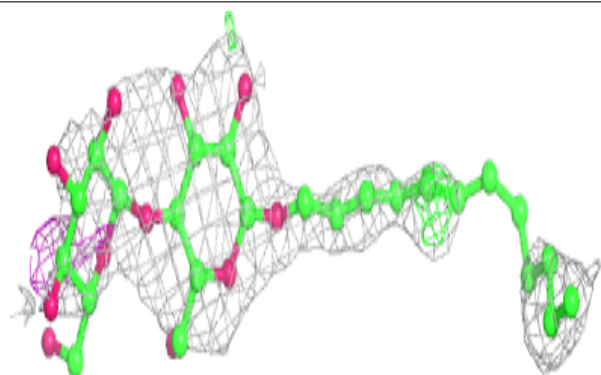


**Electron density around HTG d 411:**

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

**Electron density around LMT a 419:**

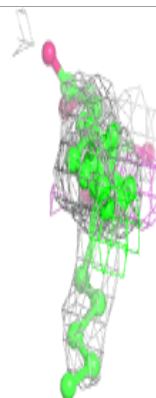
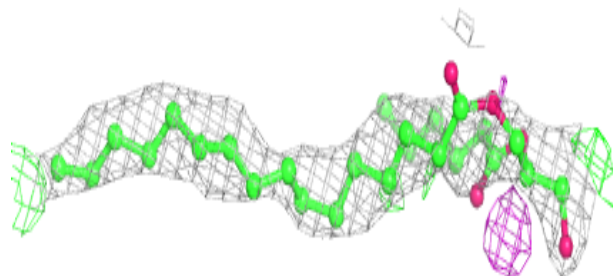
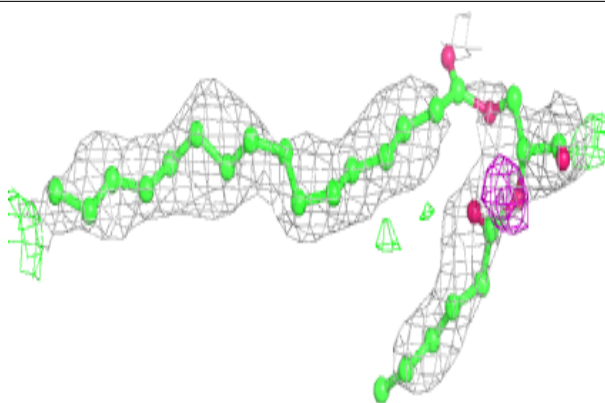
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



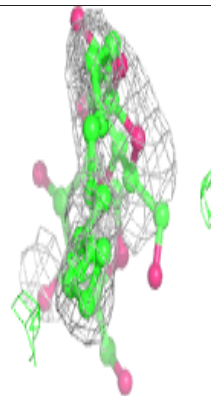
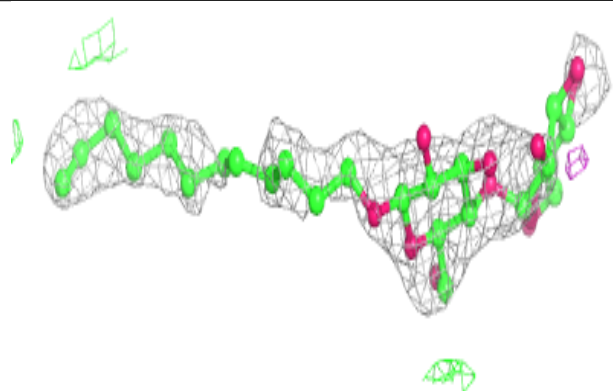
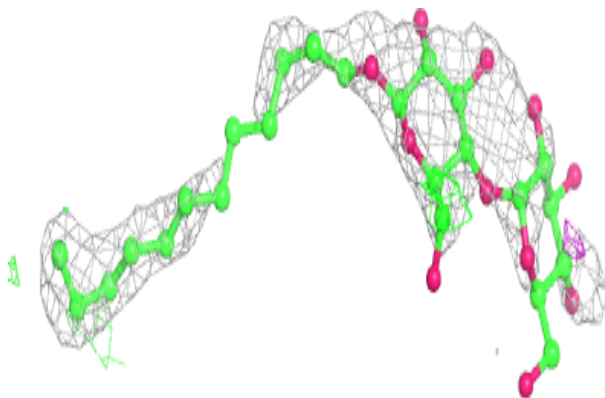


**Electron density around UNL a 403:**

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

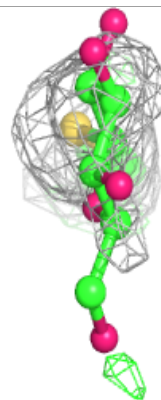
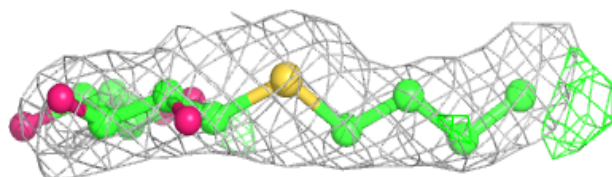
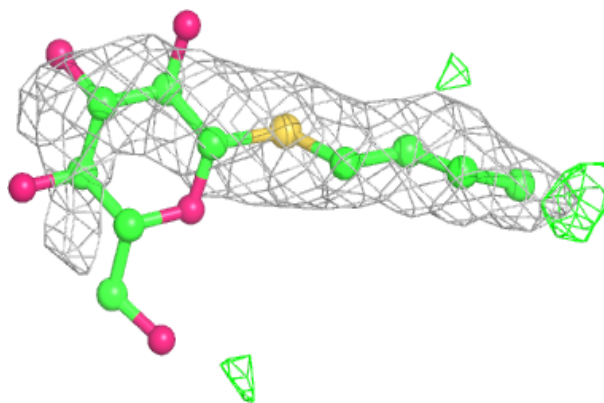
**Electron density around LMT f 102:**

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

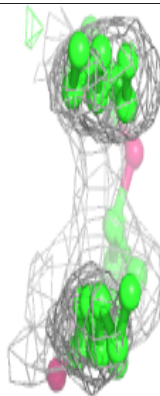
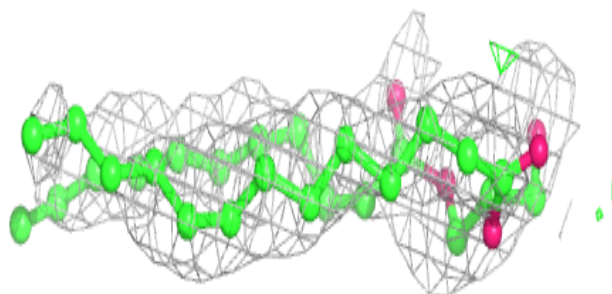
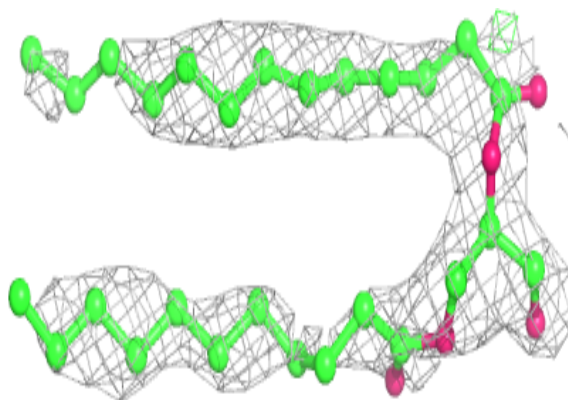


**Electron density around HTG D 412:**

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

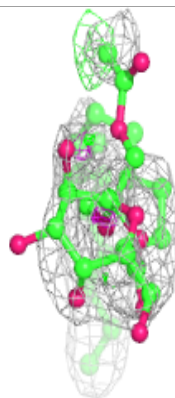
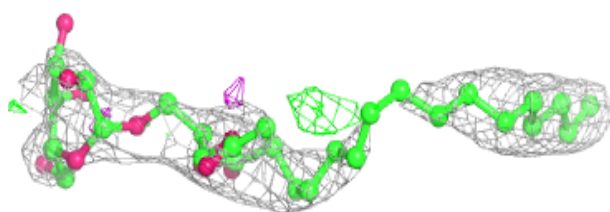
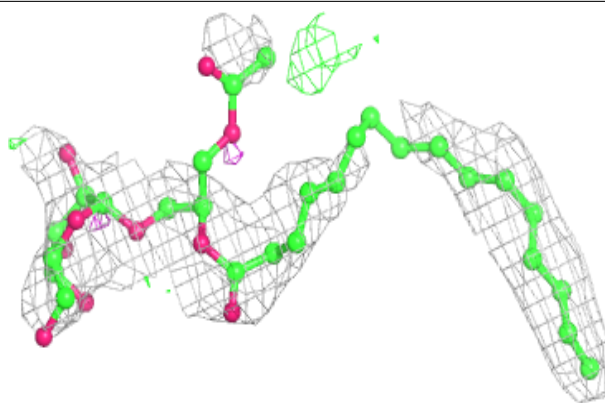
**Electron density around UNL c 527:**

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

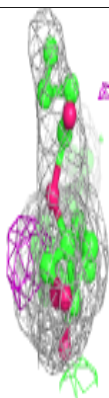
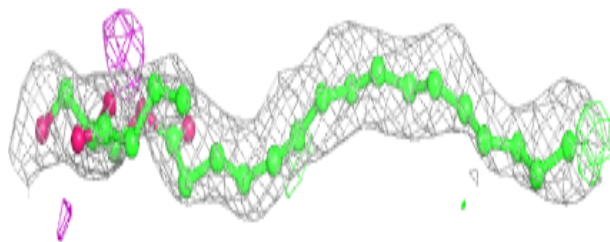
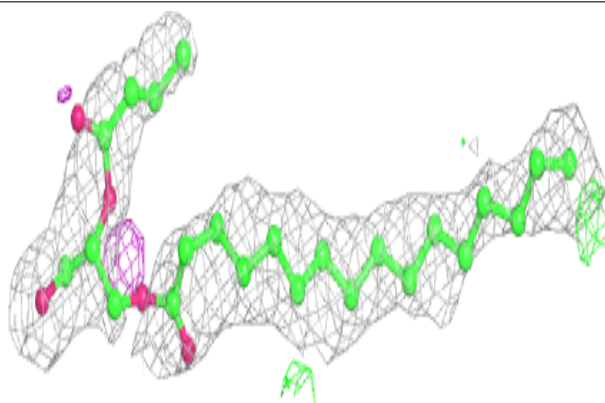


**Electron density around LMG Z 101:**

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

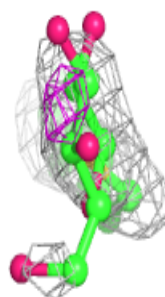
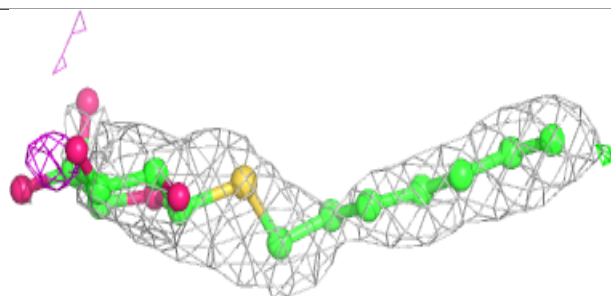
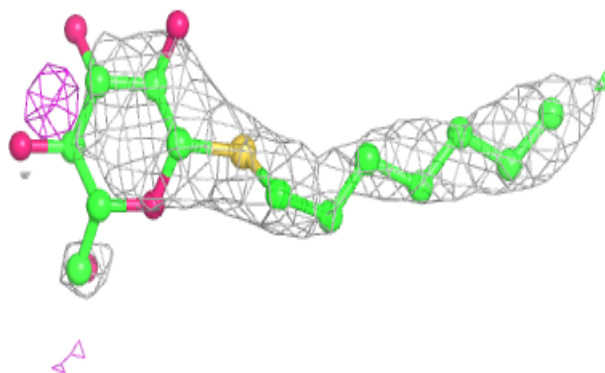
**Electron density around UNL A 420:**

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

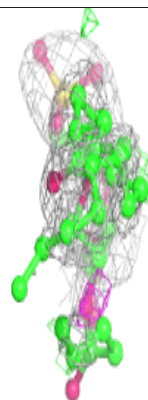
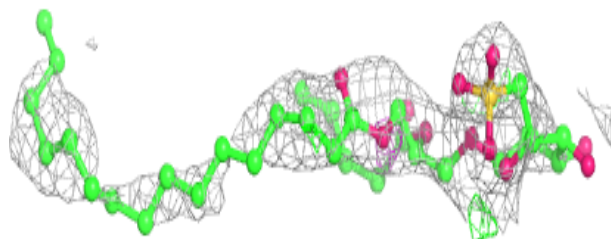
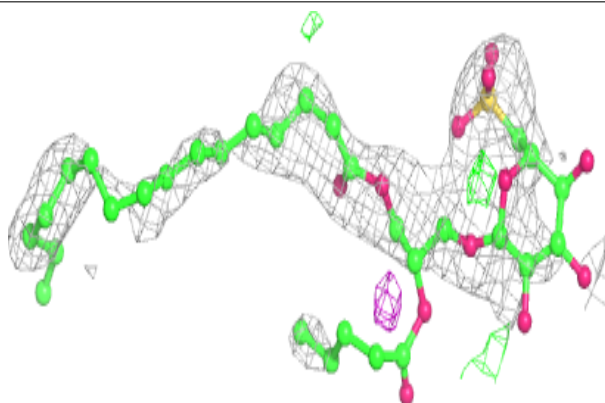


**Electron density around HTG c 526:**

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

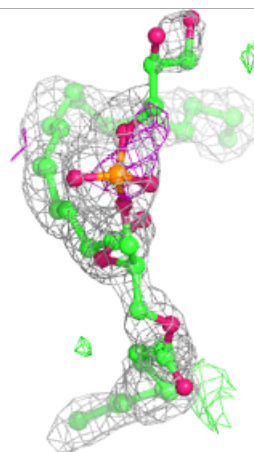
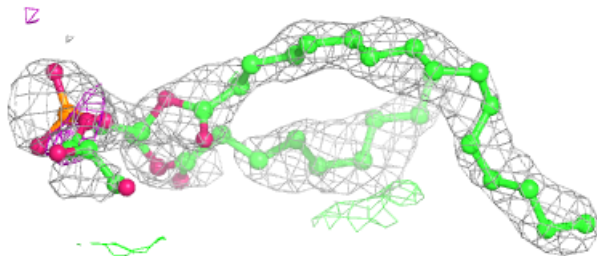
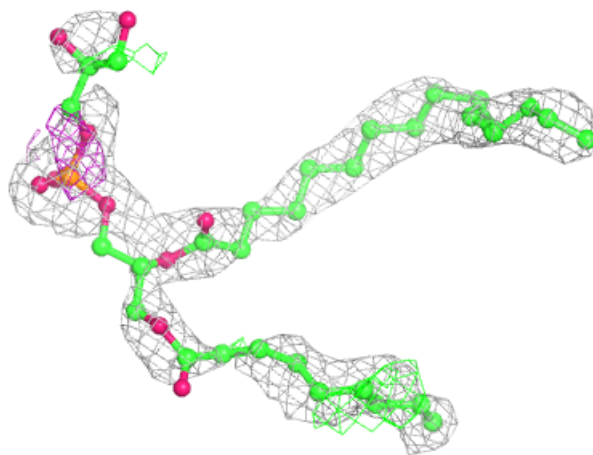
**Electron density around SQD f 101:**

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



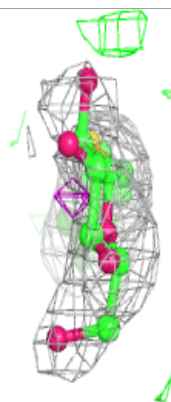
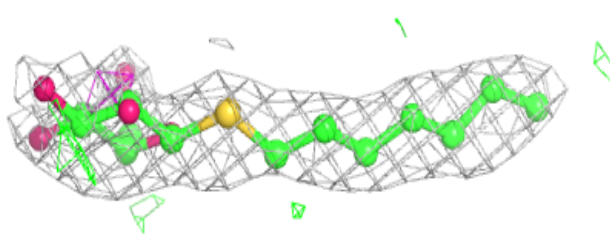
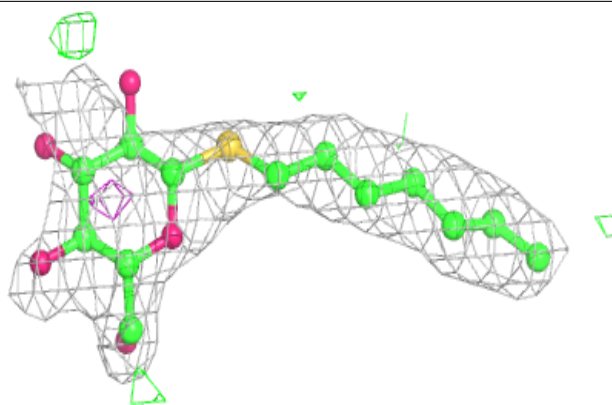
**Electron density around LHG E 101:**

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

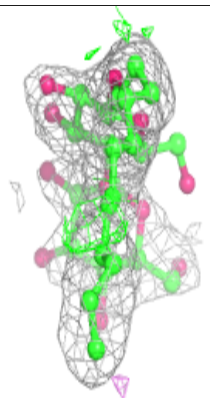
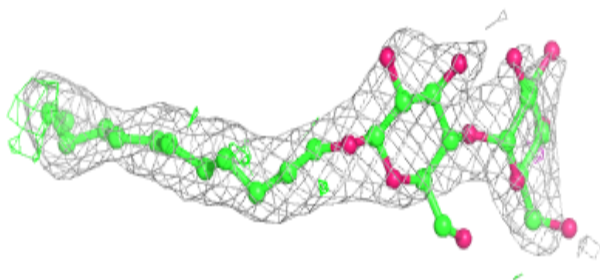
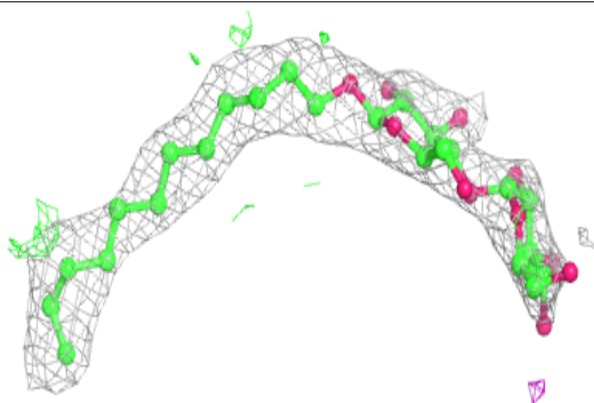


**Electron density around HTG B 633:**

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

**Electron density around LMT m 103:**

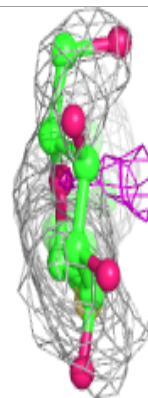
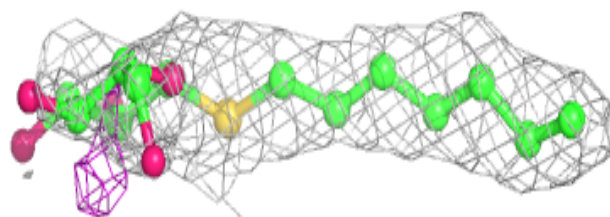
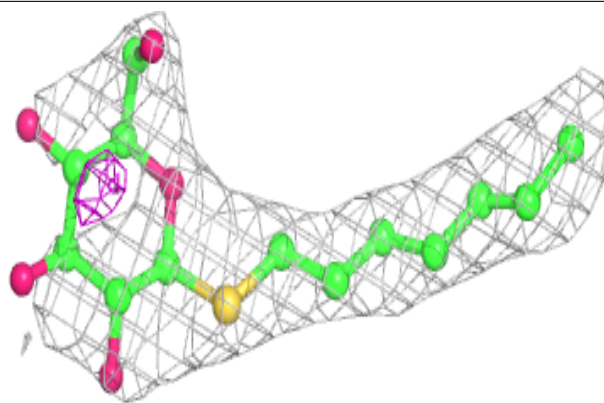
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



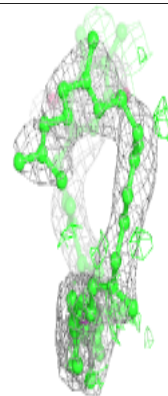
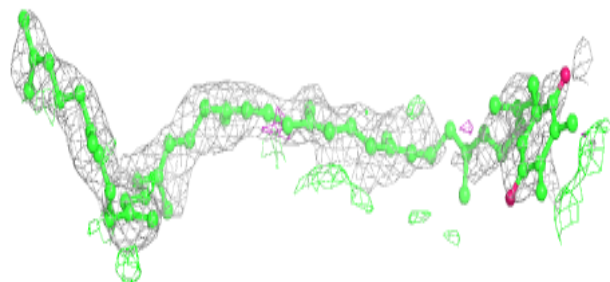
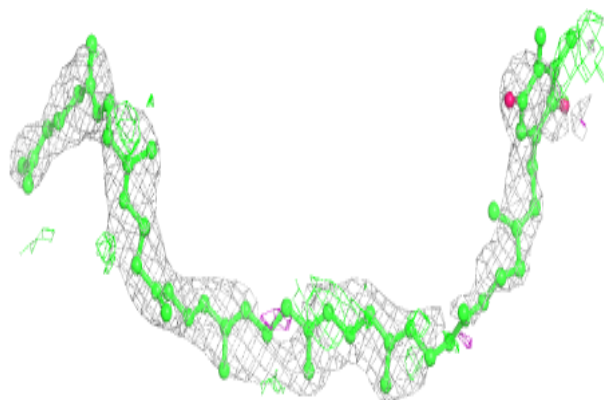


**Electron density around HTG b 608:**

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

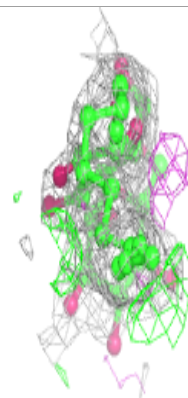
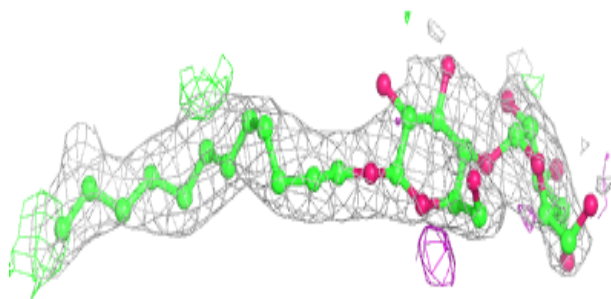
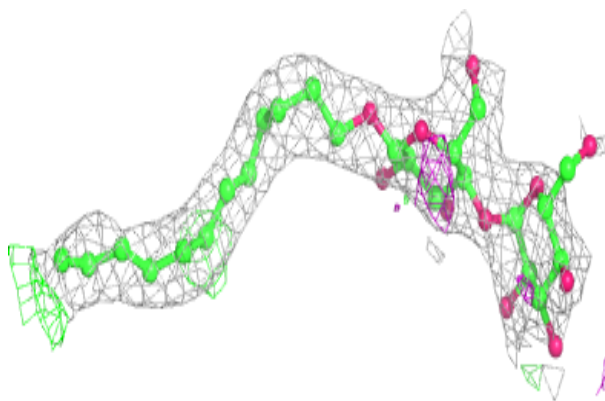
**Electron density around PL9 a 415 (B):**

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

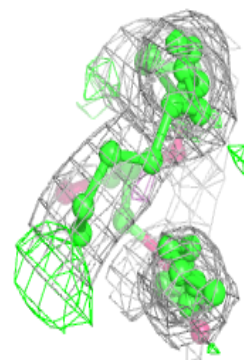
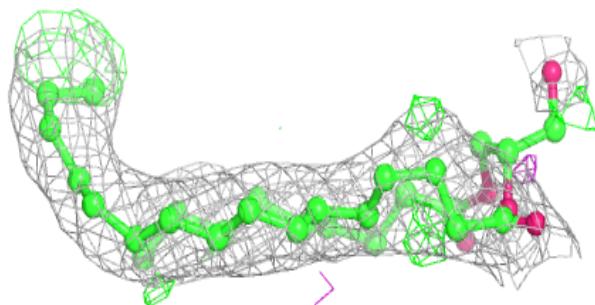
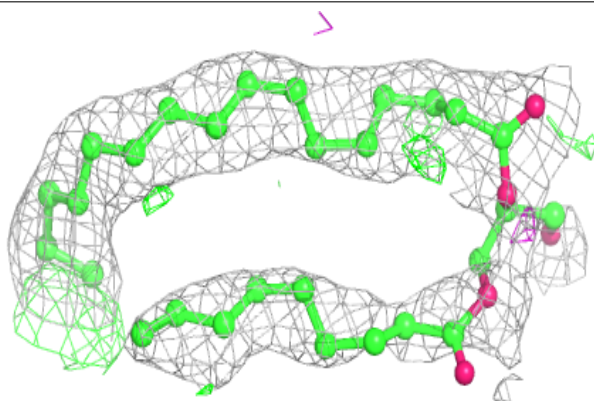


**Electron density around LMT a 404:**

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

**Electron density around UNL B 634:**

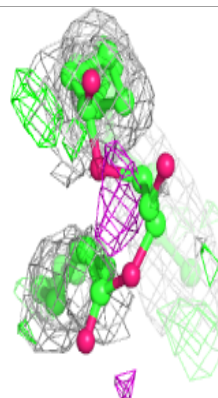
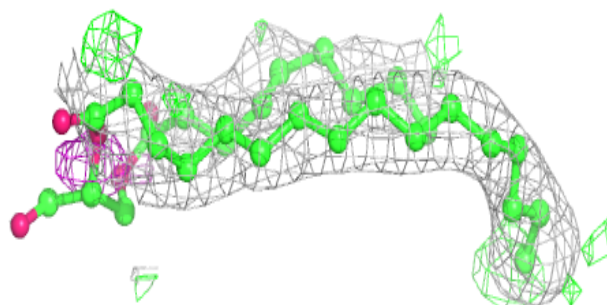
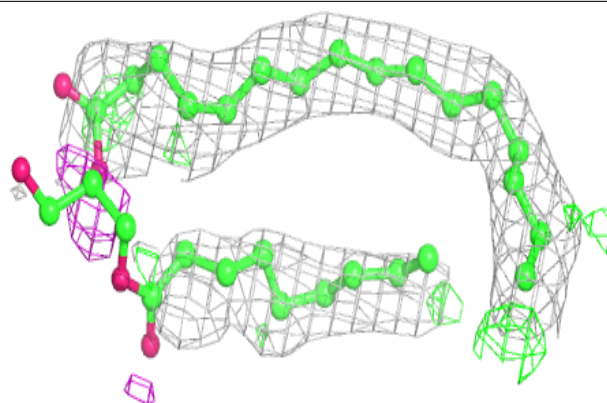
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



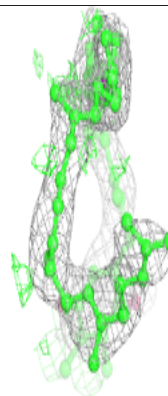
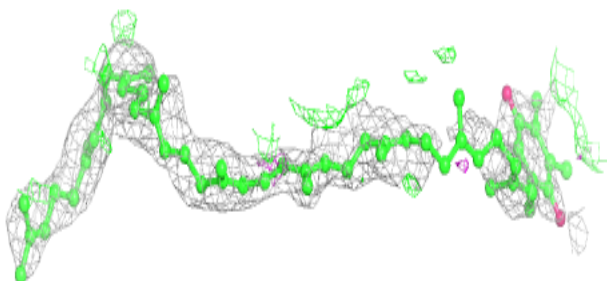
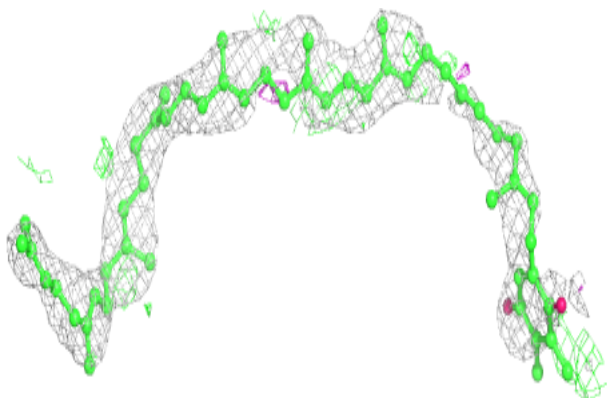


**Electron density around UNL b 633:**

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

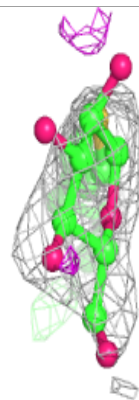
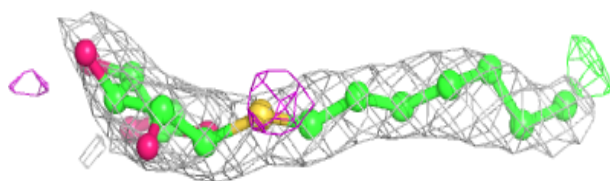
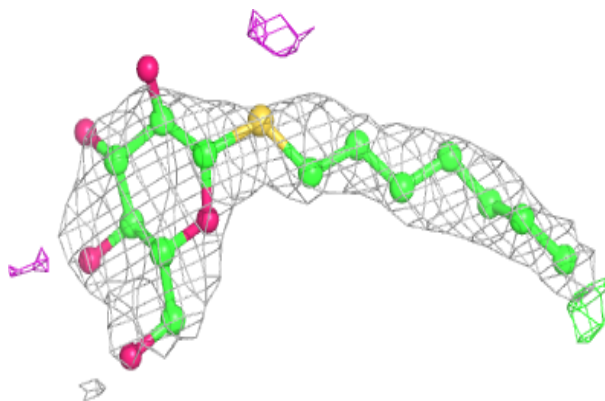
**Electron density around PL9 a 415 (A):**

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

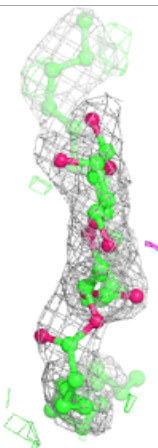
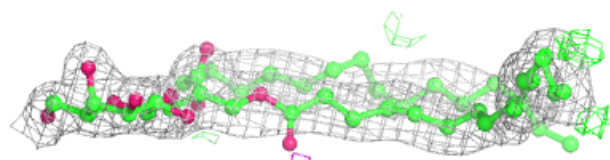
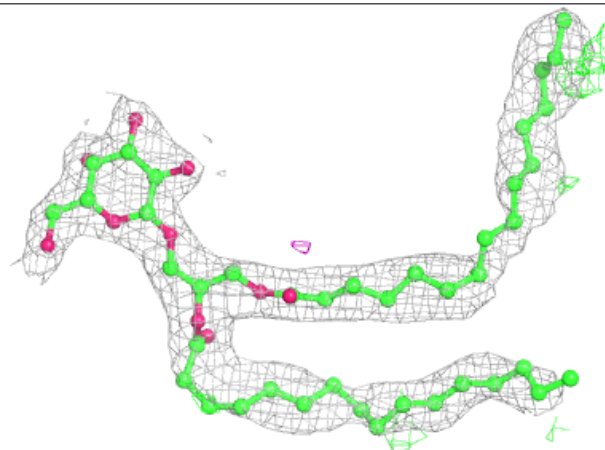


**Electron density around HTG B 625:**

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

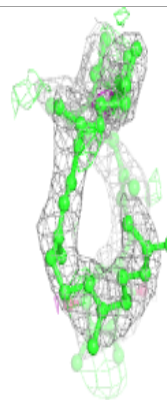
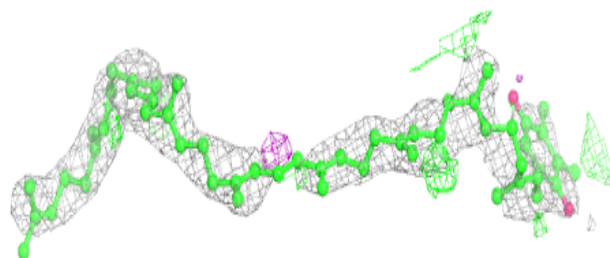
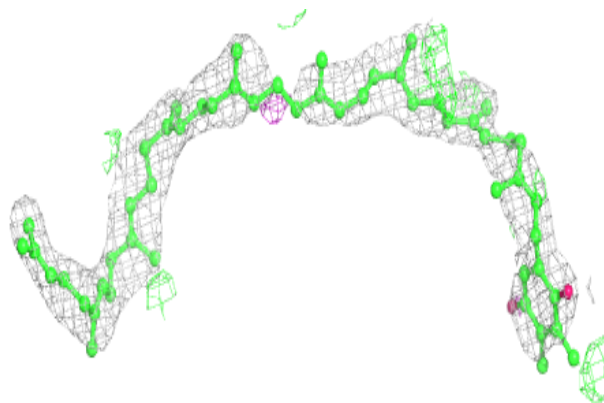
**Electron density around LMG C 519:**

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

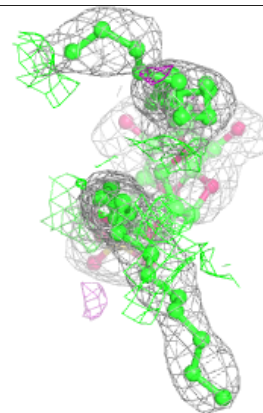
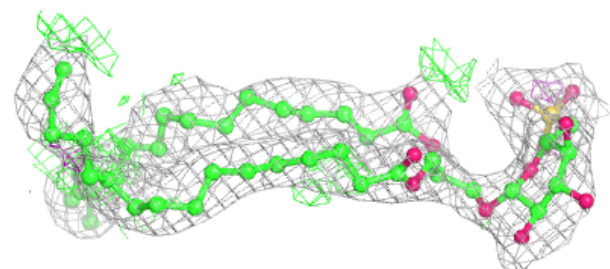
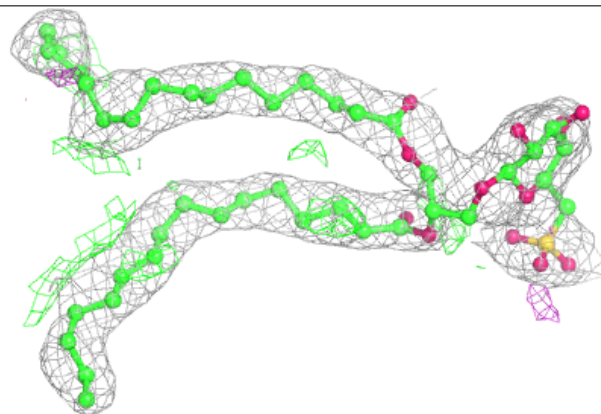


**Electron density around PL9 A 419 (B):**

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

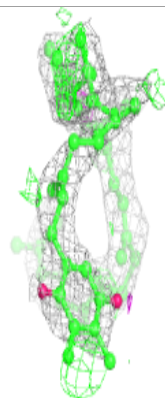
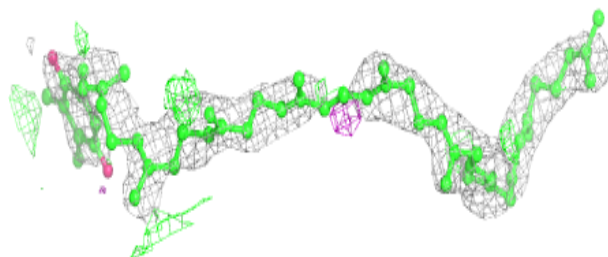
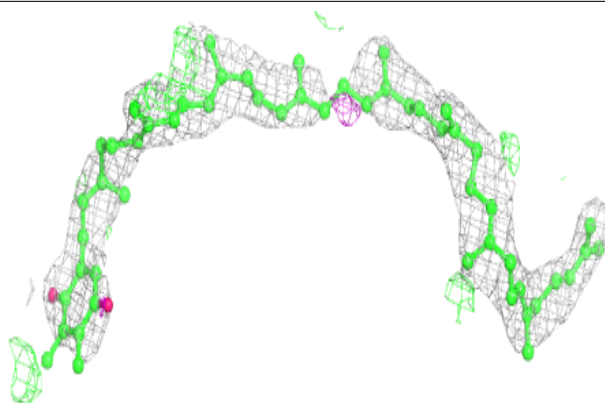
**Electron density around SQD L 102:**

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

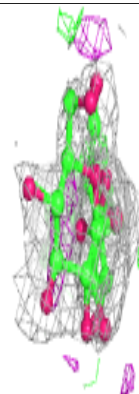
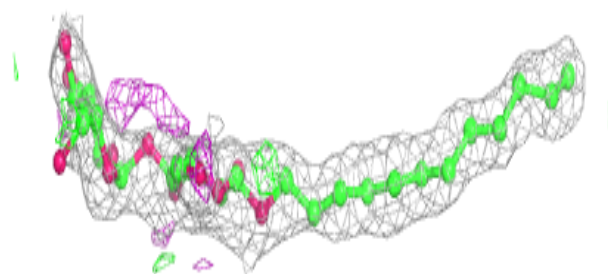
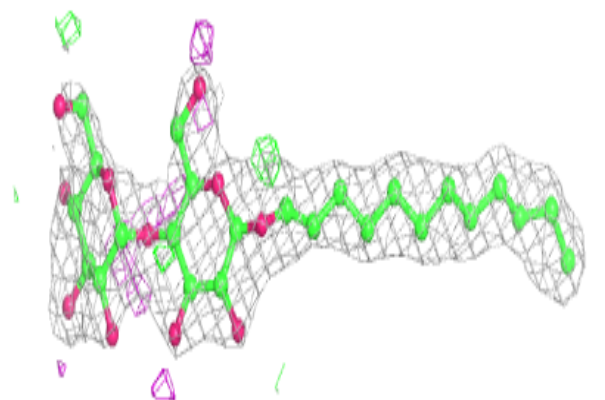


**Electron density around PL9 A 419 (A):**

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

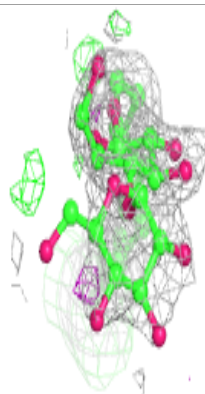
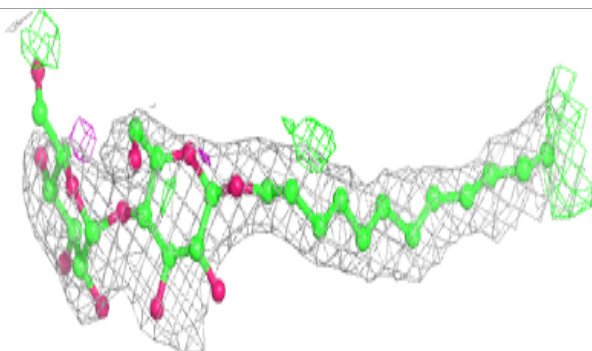
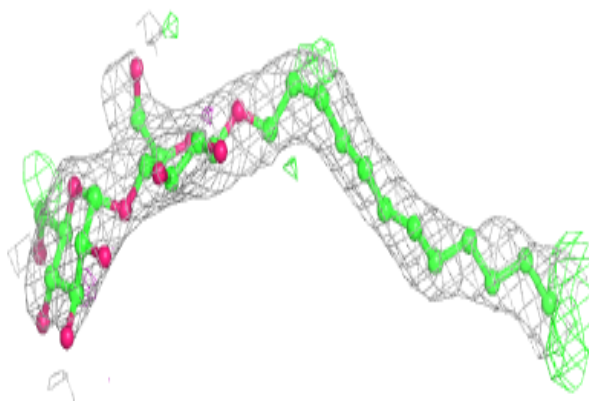
**Electron density around LMT m 102:**

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

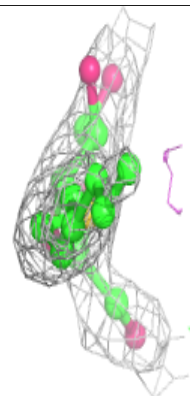
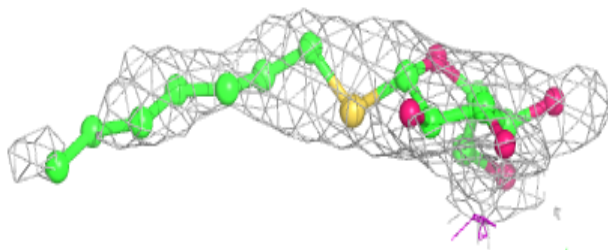
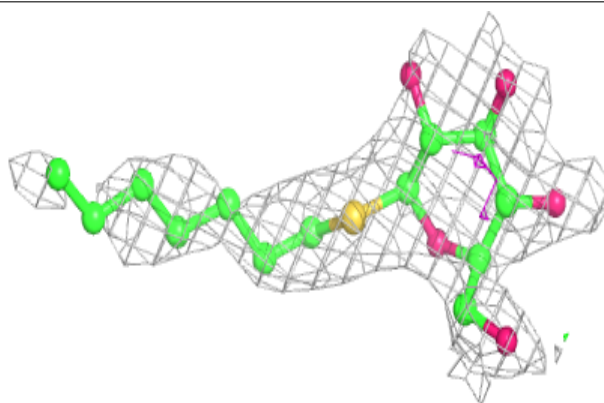


**Electron density around LMT A 417:**

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

**Electron density around HTG C 523:**

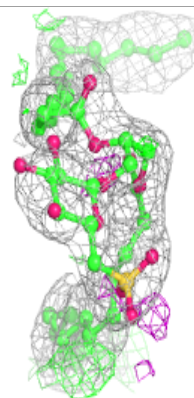
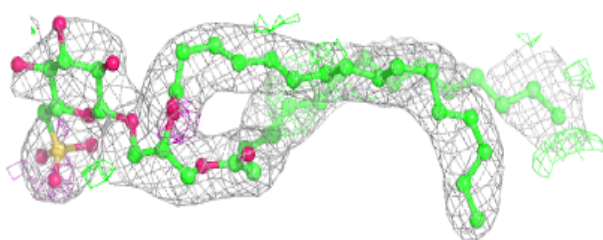
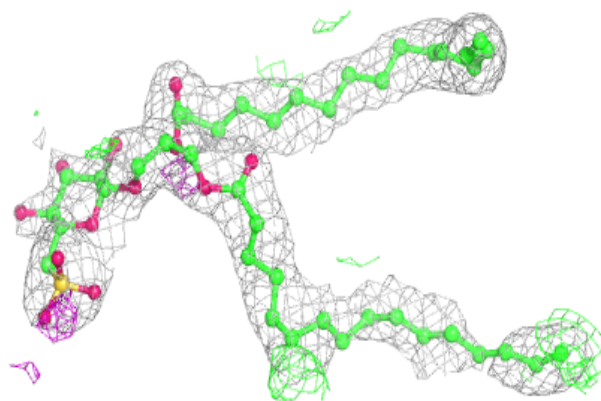
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



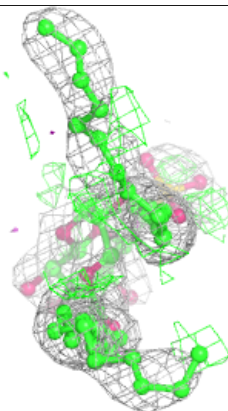
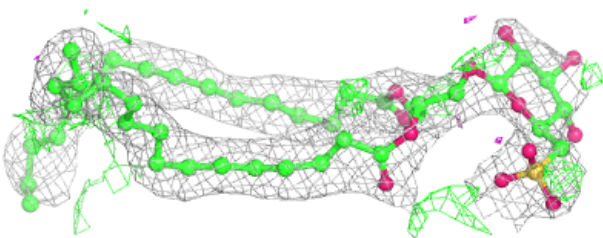
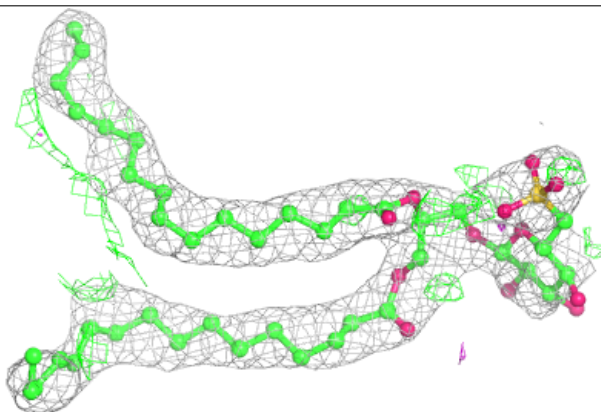


**Electron density around SQD A 416:**

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

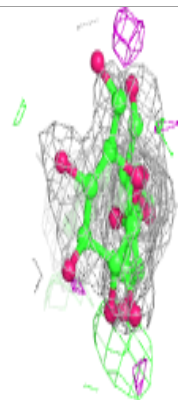
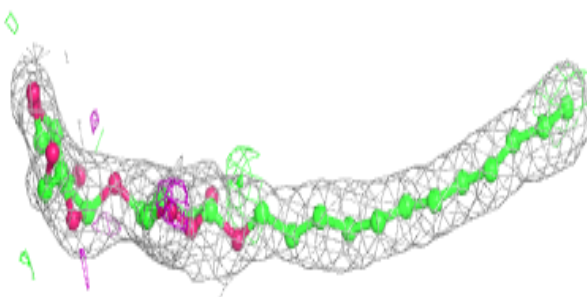
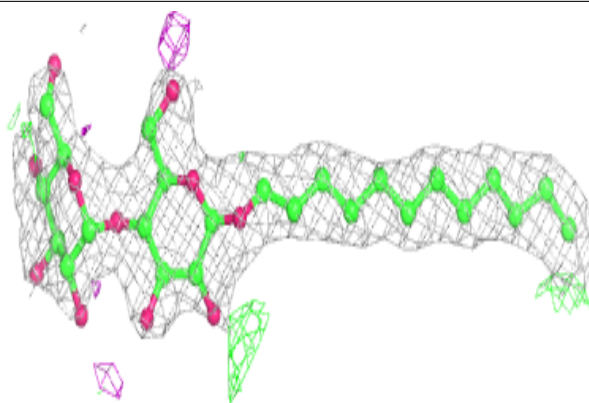
**Electron density around SQD B 621:**

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

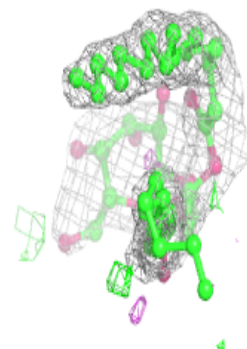
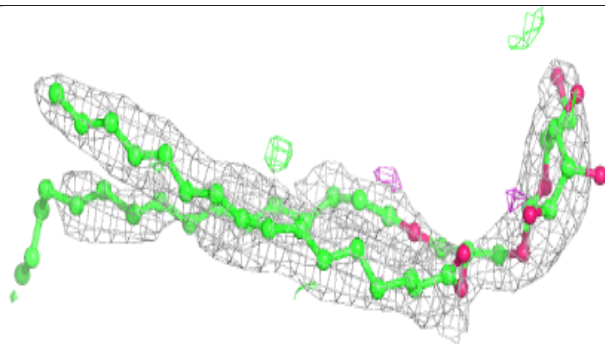
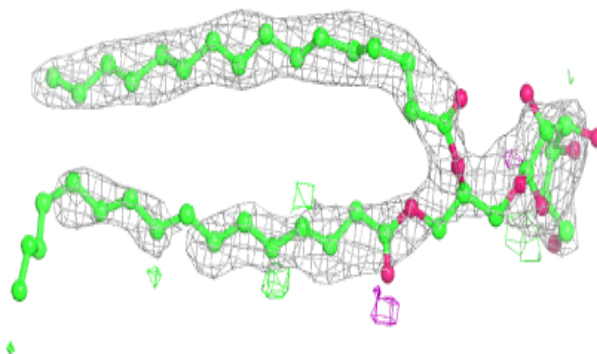


**Electron density around LMT M 101:**

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

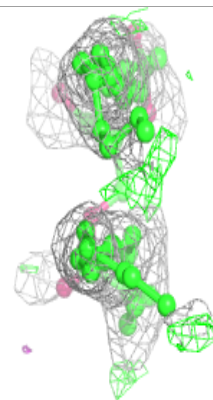
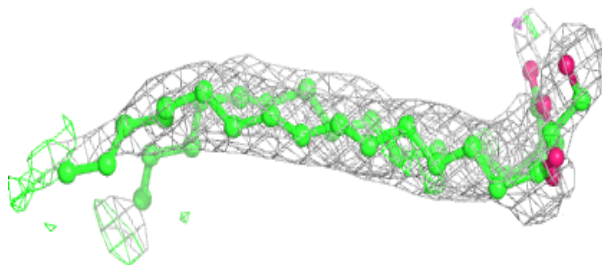
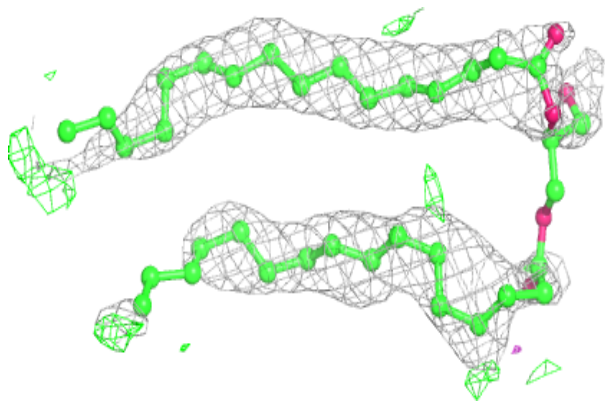
**Electron density around LMG C 520:**

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

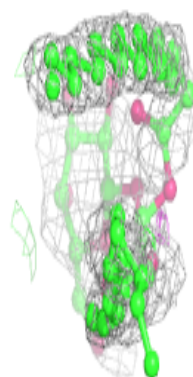
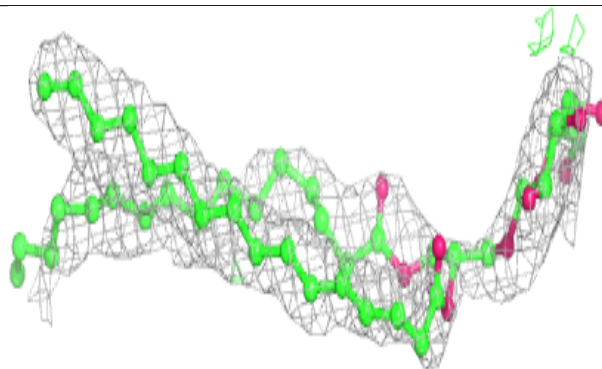
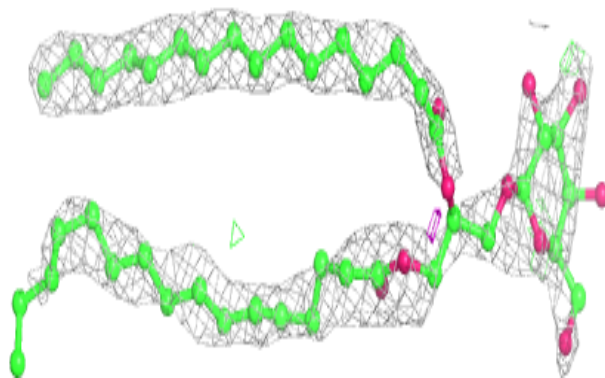


**Electron density around UNL I 101:**

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

**Electron density around LMG c 524:**

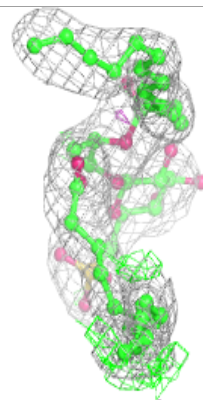
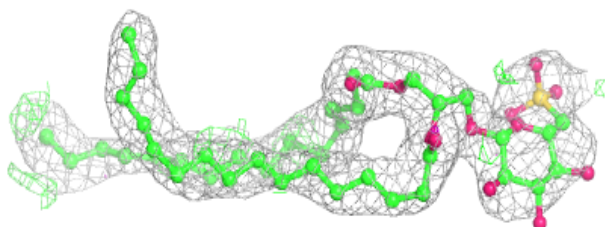
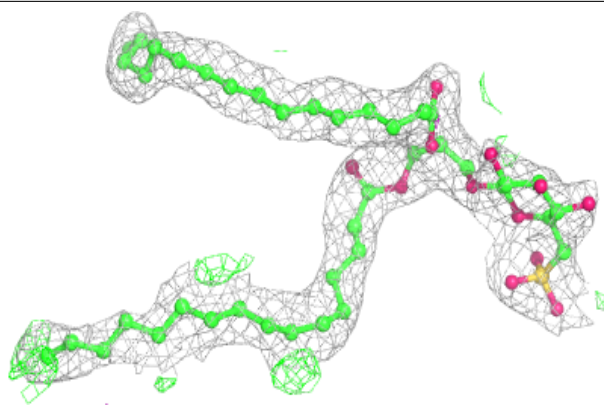
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



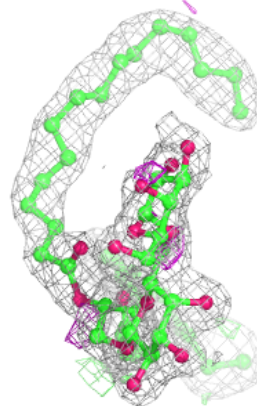
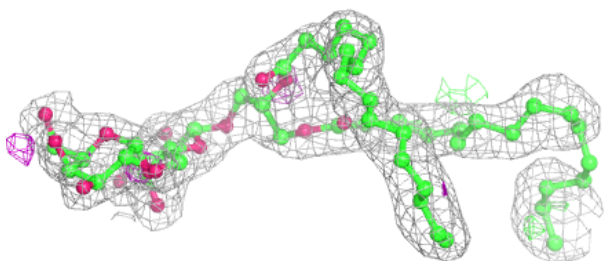
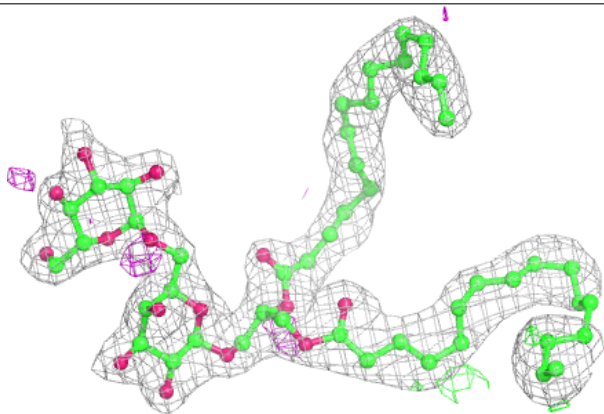


**Electron density around SQD a 405:**

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

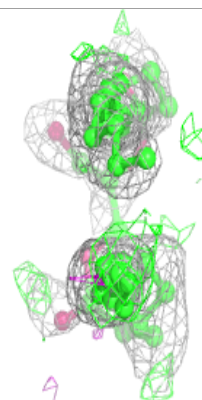
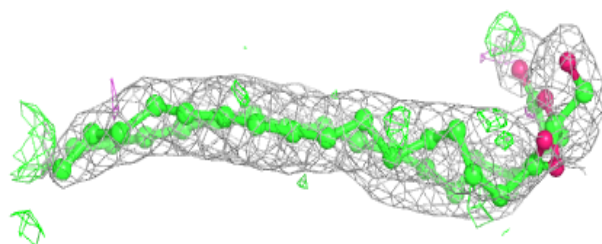
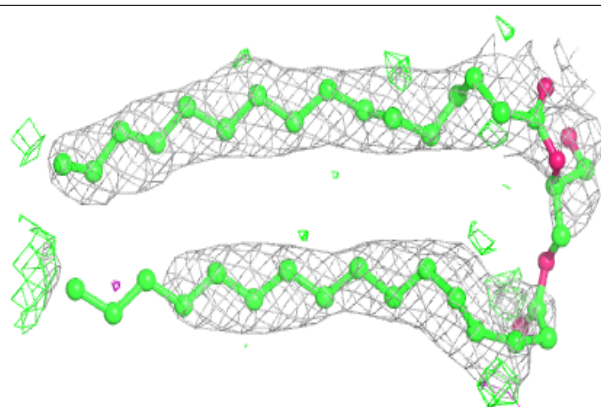
**Electron density around DGD C 517:**

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

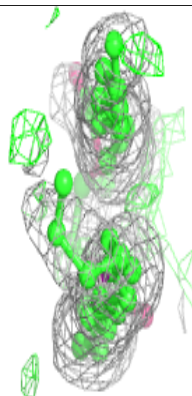
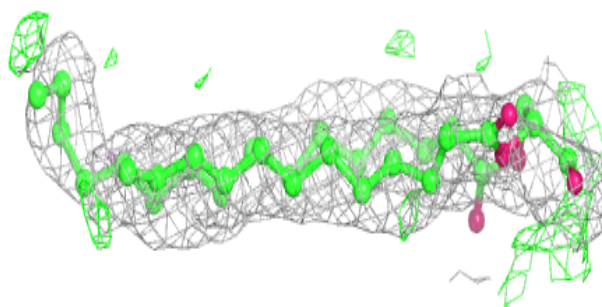
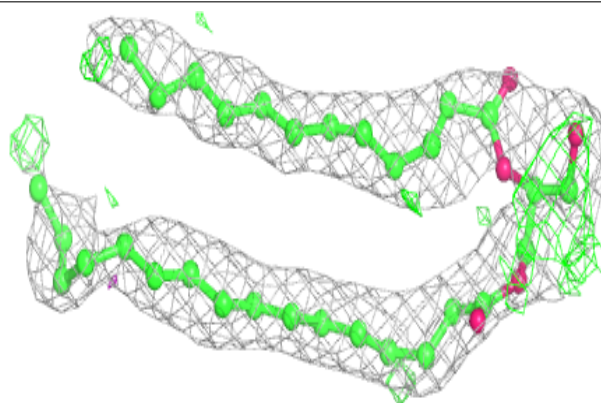


**Electron density around UNL i 101:**

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

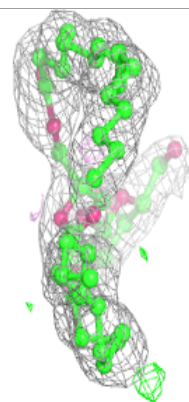
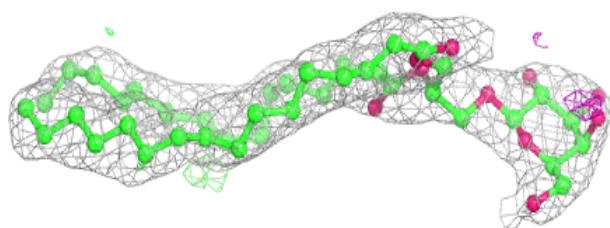
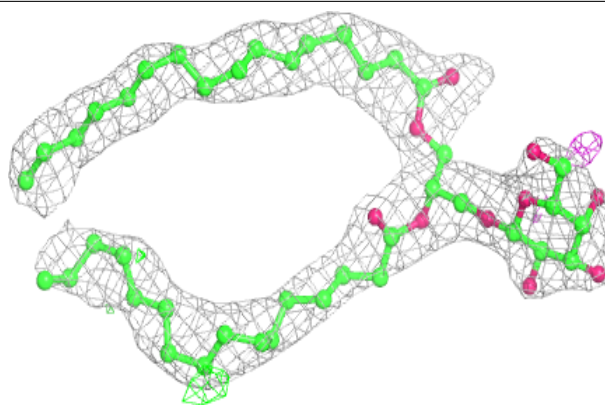
**Electron density around UNL d 410:**

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

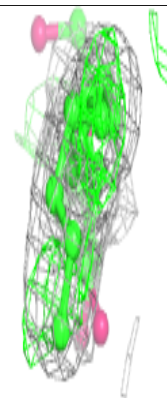
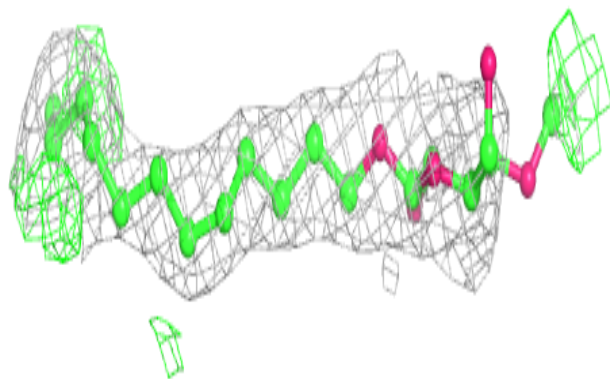
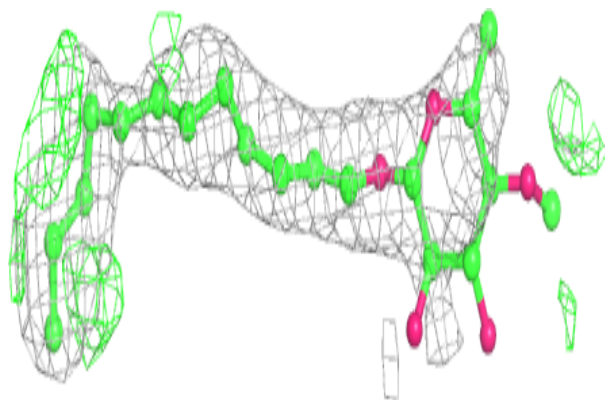


**Electron density around LMG c 501:**

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

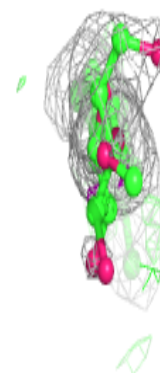
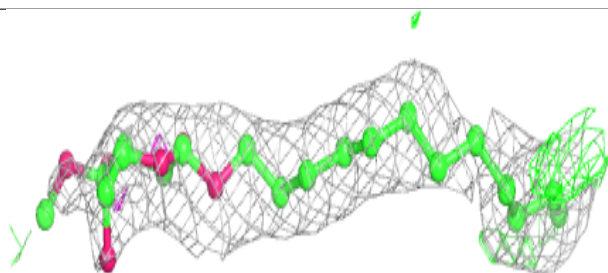
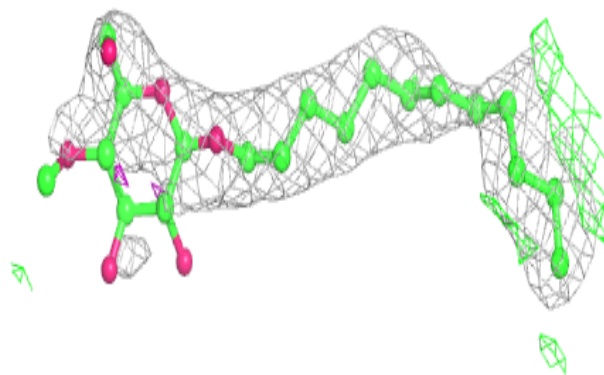
**Electron density around LMT B 635:**

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

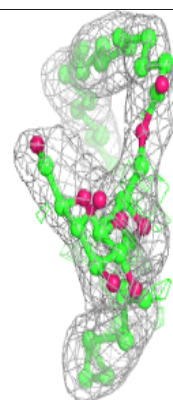
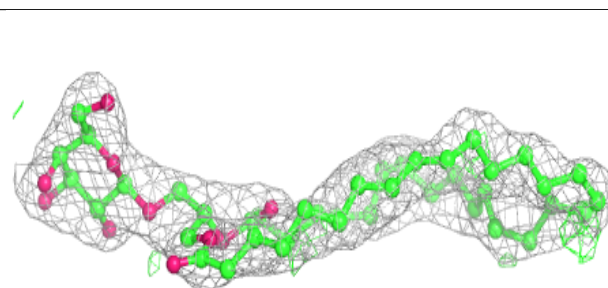
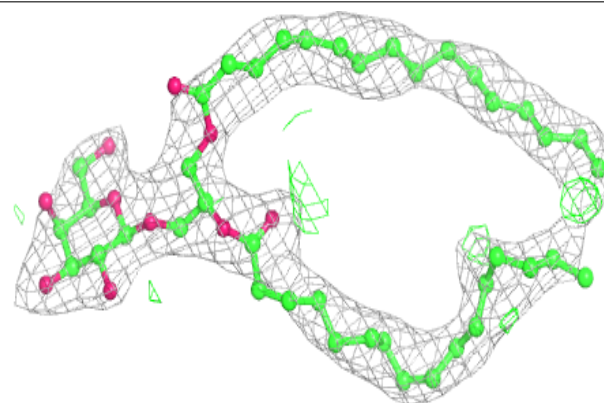


**Electron density around LMT T 104:**

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

**Electron density around LMG A 421:**

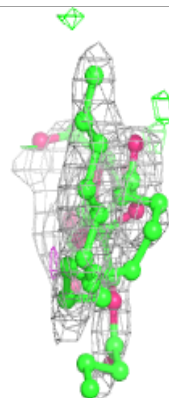
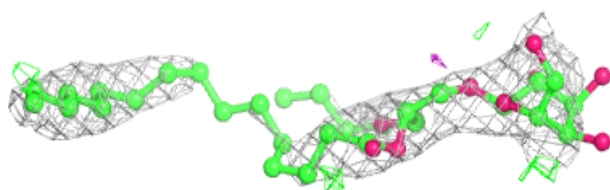
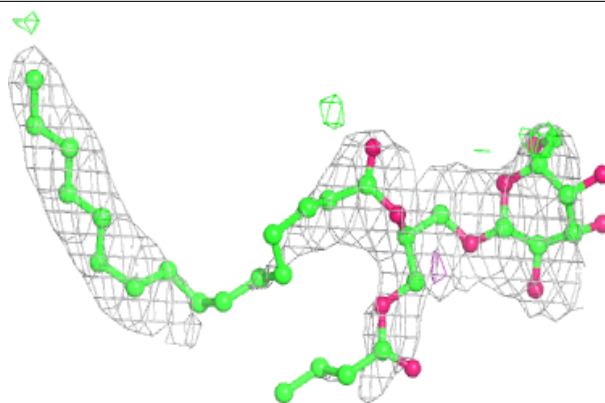
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



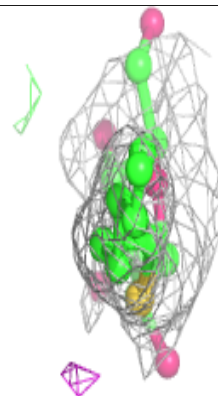
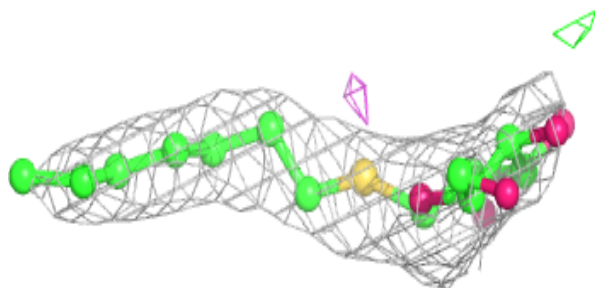
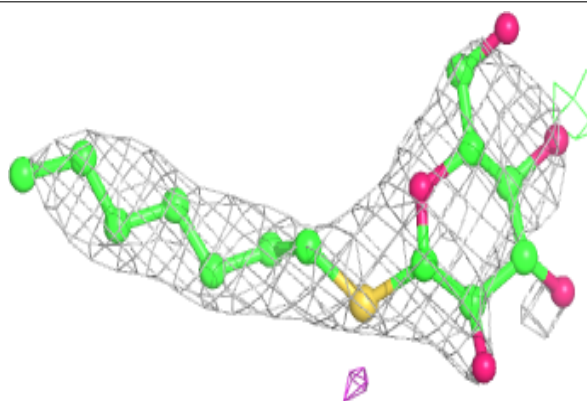


**Electron density around LMG z 101:**

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

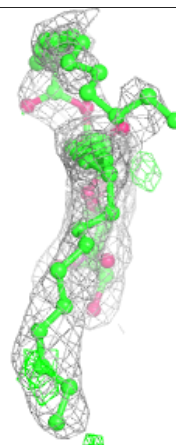
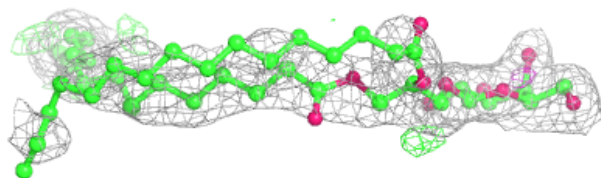
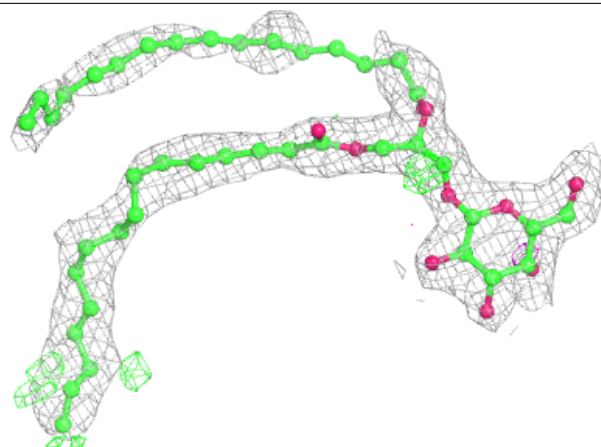
**Electron density around HTG b 632:**

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

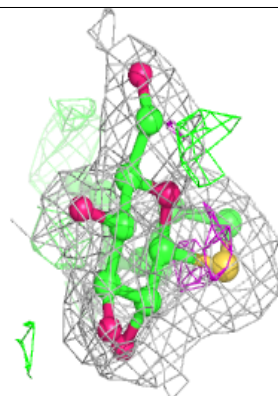
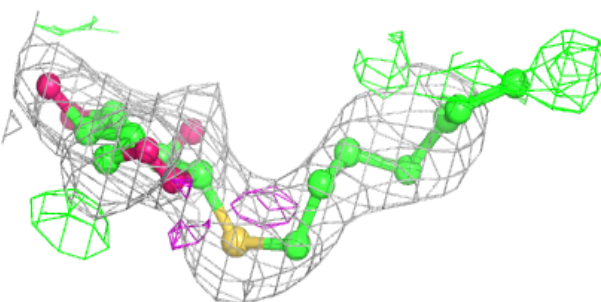
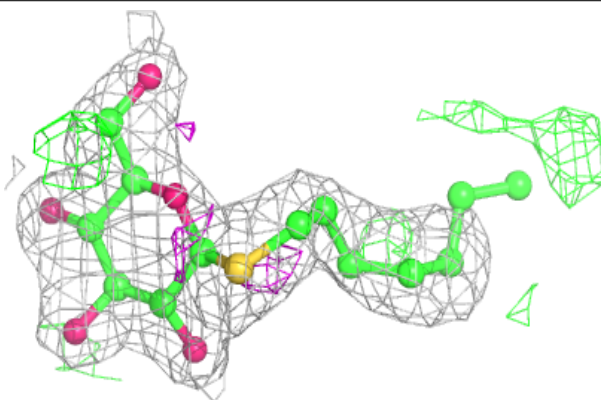


**Electron density around LMG c 523:**

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

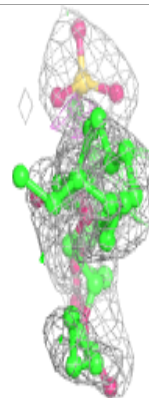
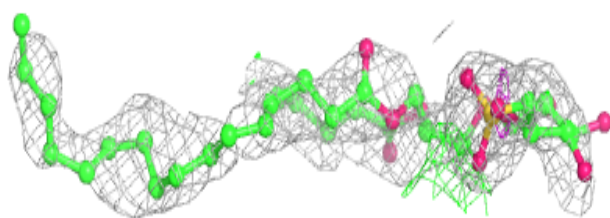
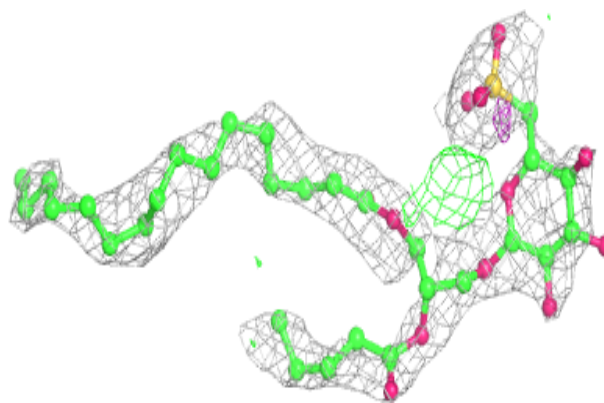
**Electron density around HTG B 624:**

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

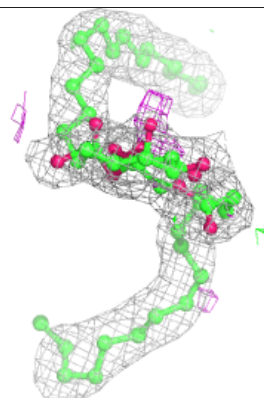
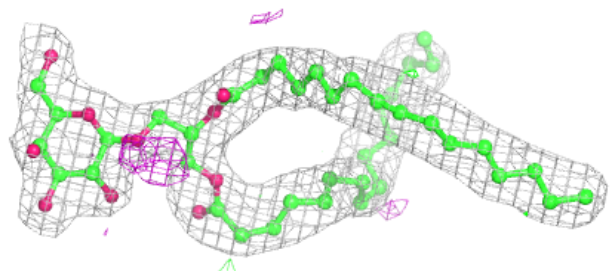
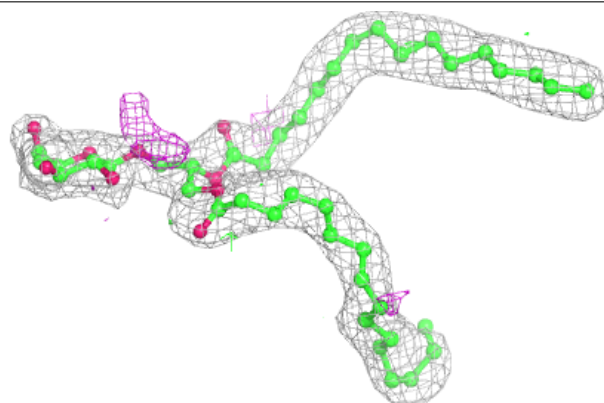


**Electron density around SQD F 103:**

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

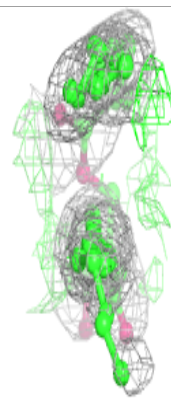
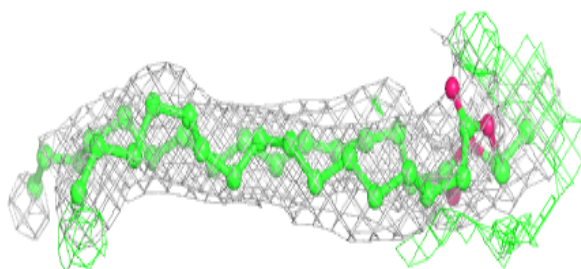
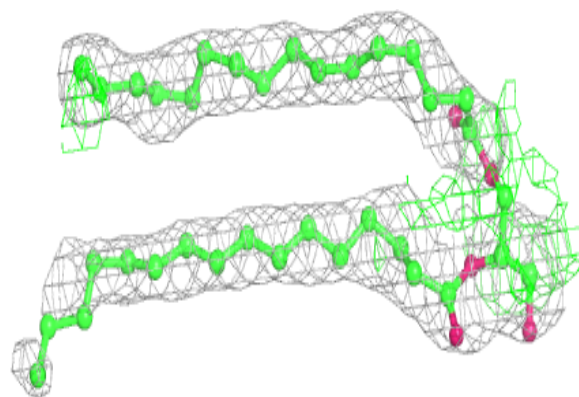
**Electron density around LMG b 629:**

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

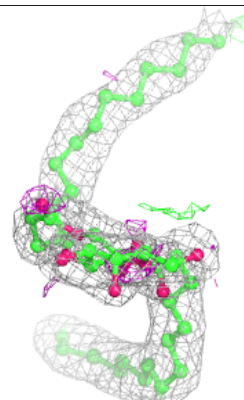
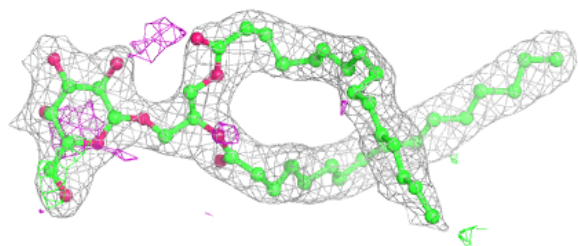
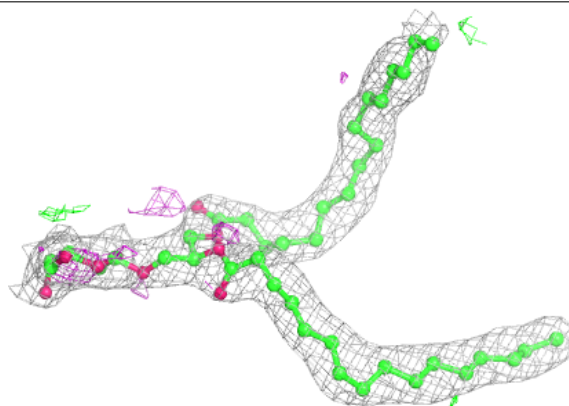


**Electron density around UNL D 411:**

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

**Electron density around LMG B 622:**

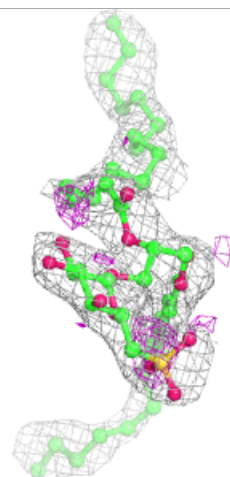
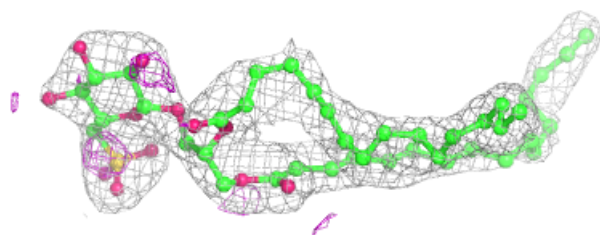
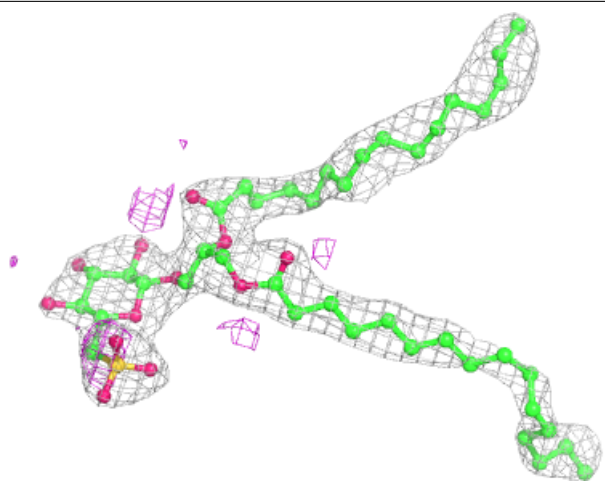
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





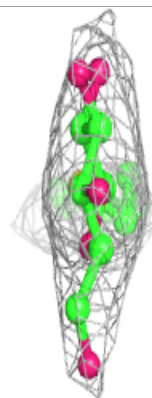
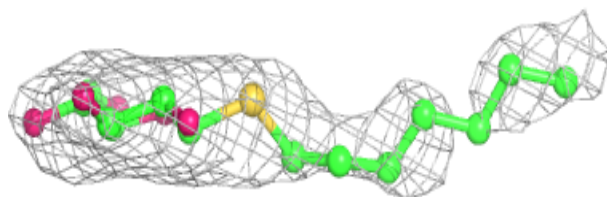
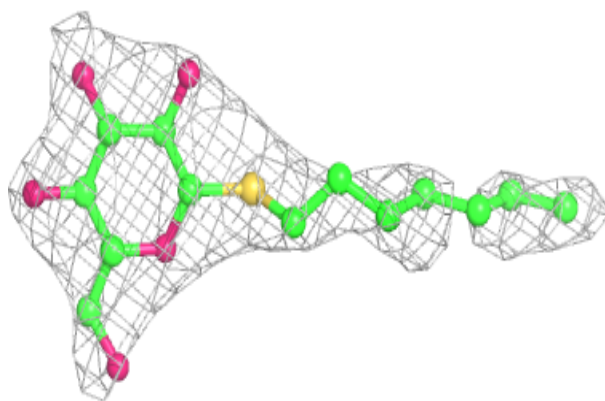
**Electron density around SQD A 412:**

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

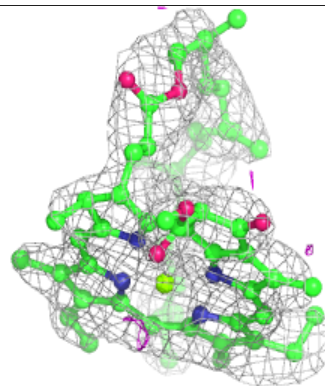
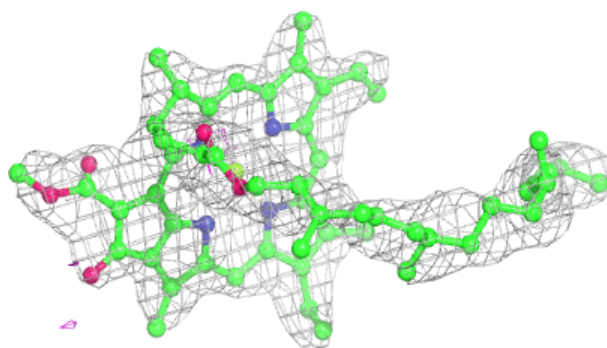
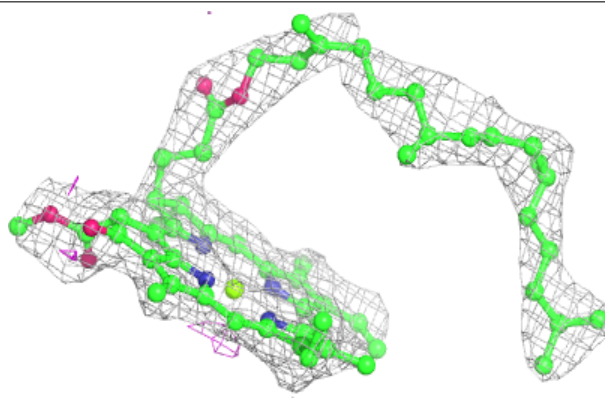


**Electron density around HTG c 525:**

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

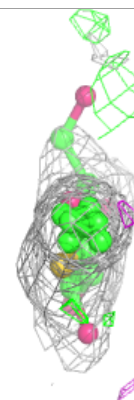
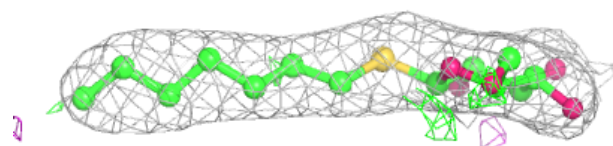
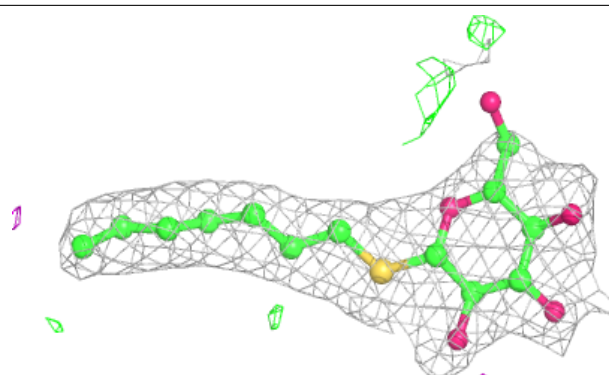
**Electron density around CLA c 518:**

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

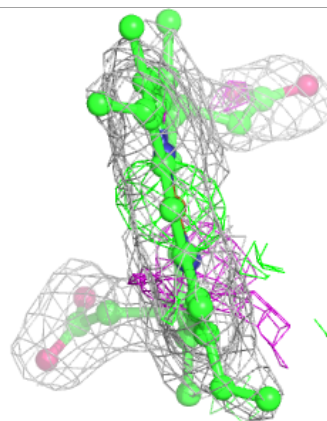
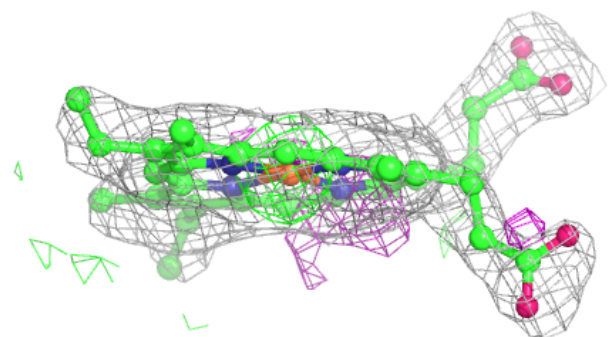
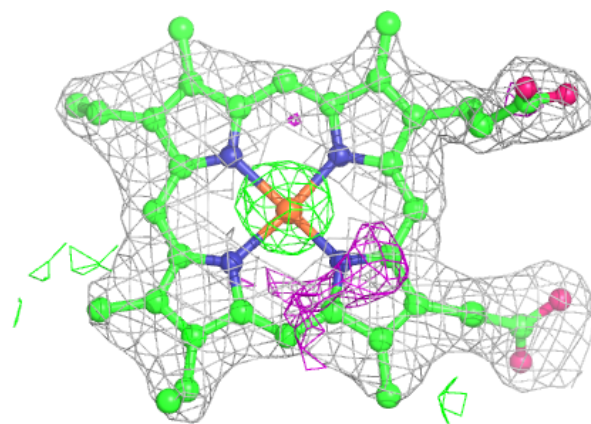


**Electron density around HTG B 632:**

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

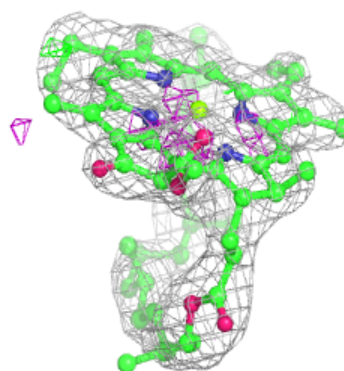
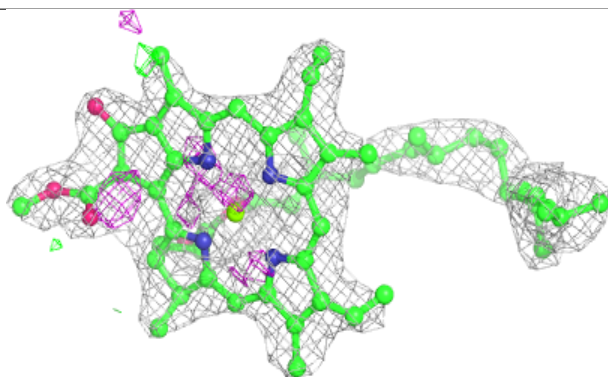
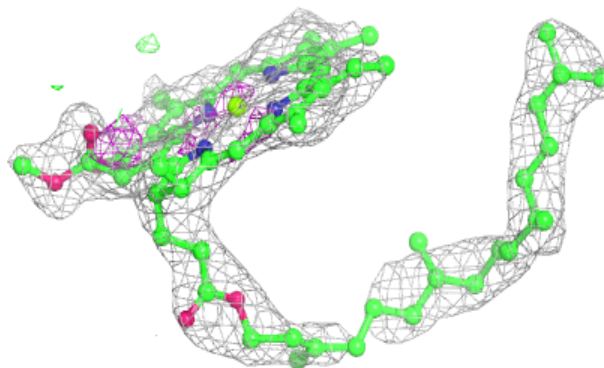
**Electron density around HEM F 102:**

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

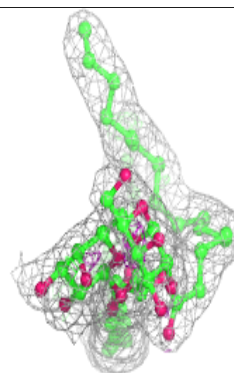
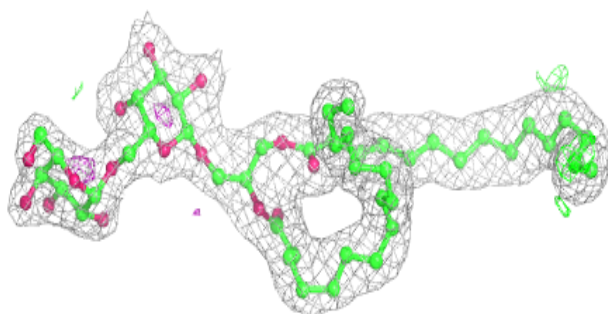
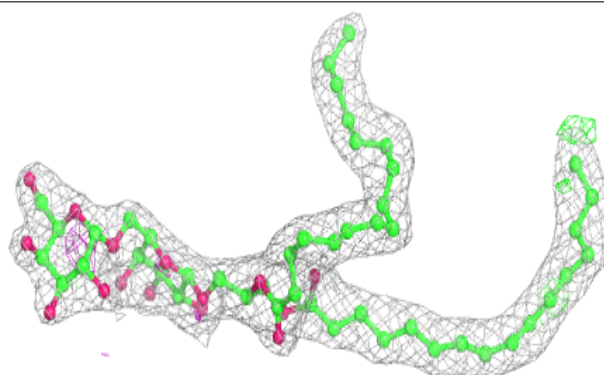


**Electron density around CLA C 513:**

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

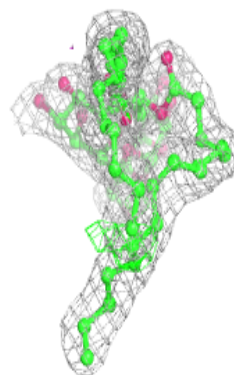
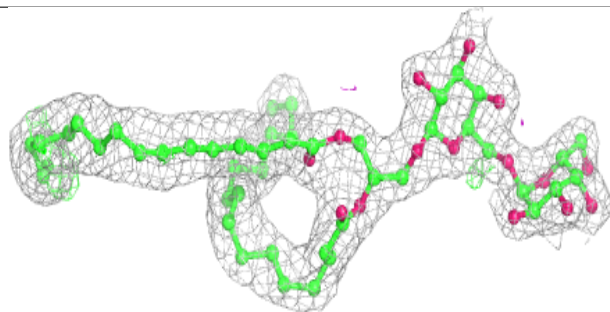
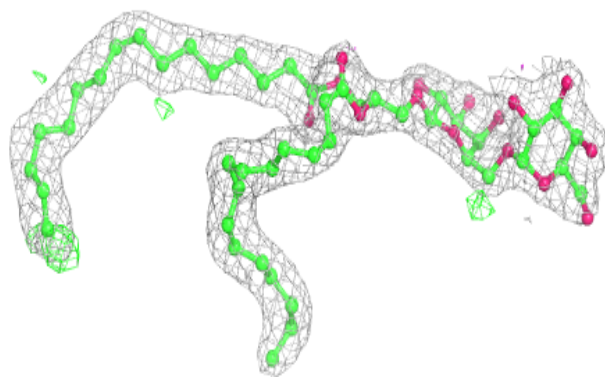
**Electron density around DGD H 102:**

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



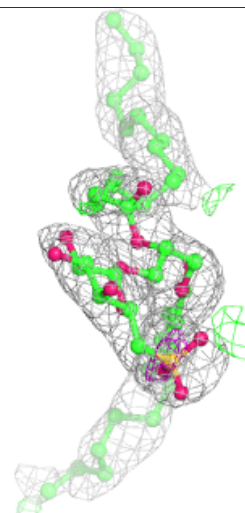
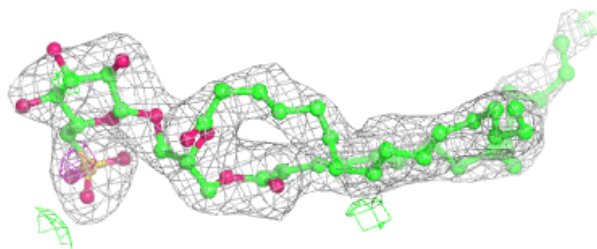
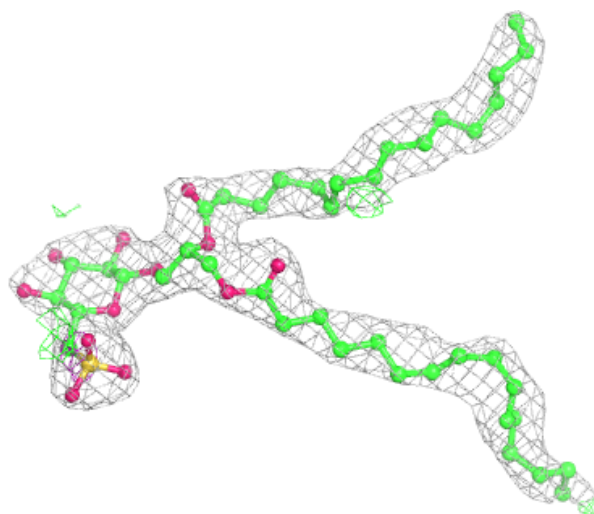
**Electron density around DGD h 102:**

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



**Electron density around SQD a 414:**

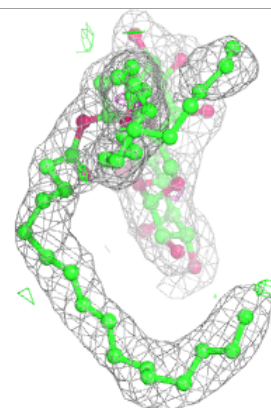
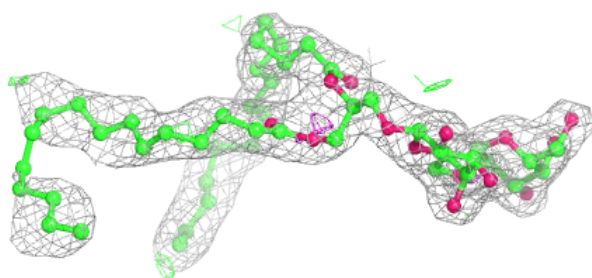
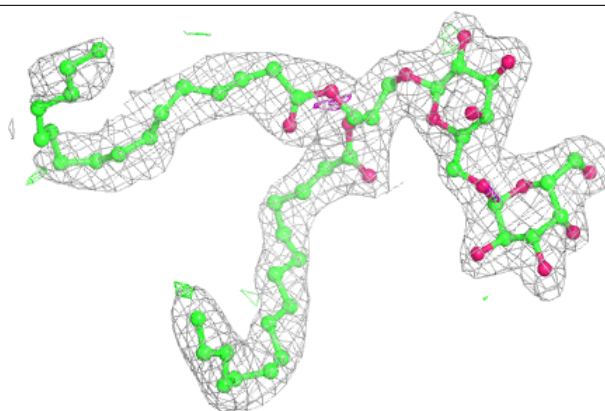
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



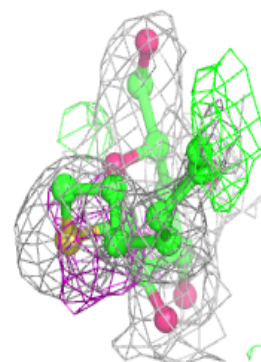
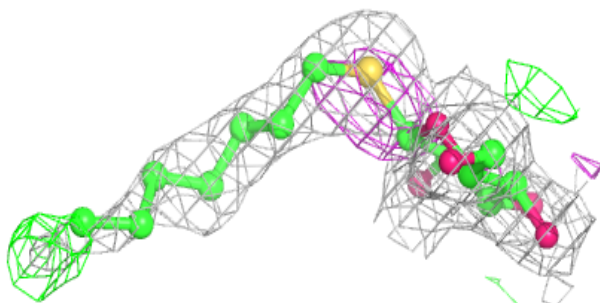
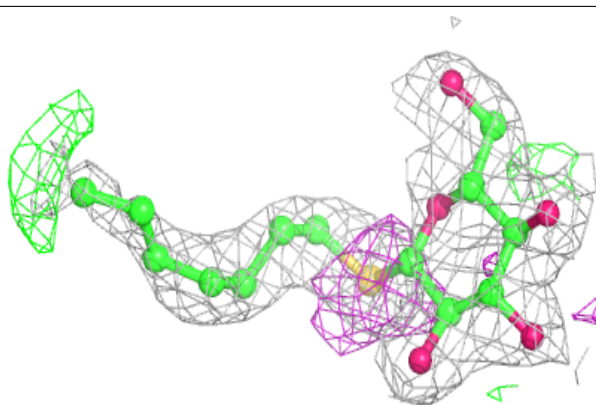


**Electron density around DGD c 521:**

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

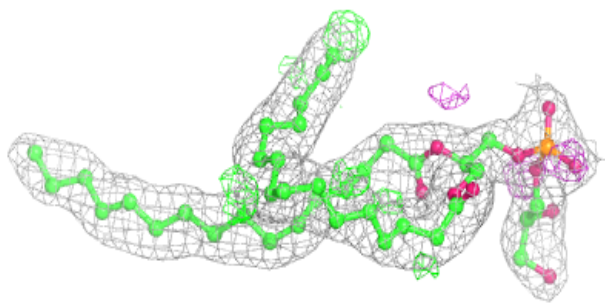
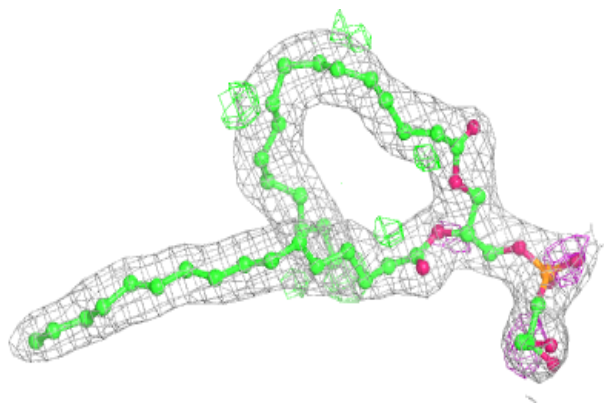
**Electron density around HTG b 631:**

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

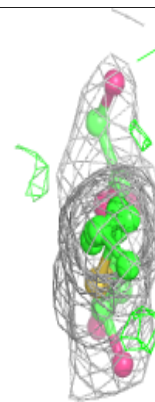
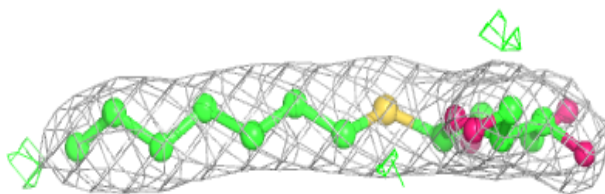
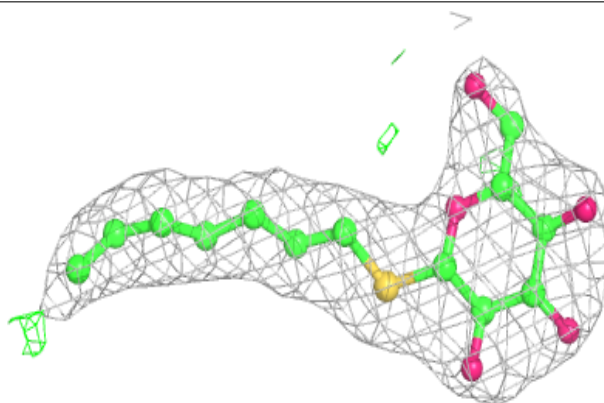


**Electron density around LHG D 407:**

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

**Electron density around HTG b 607:**

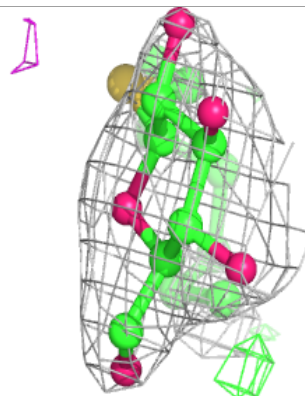
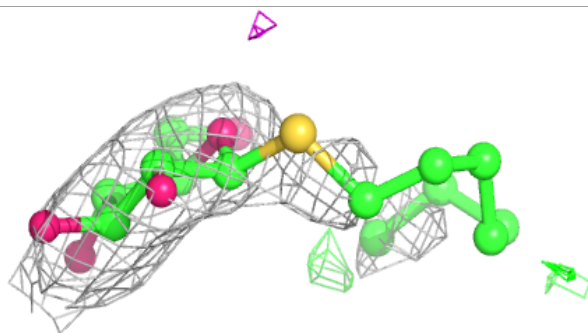
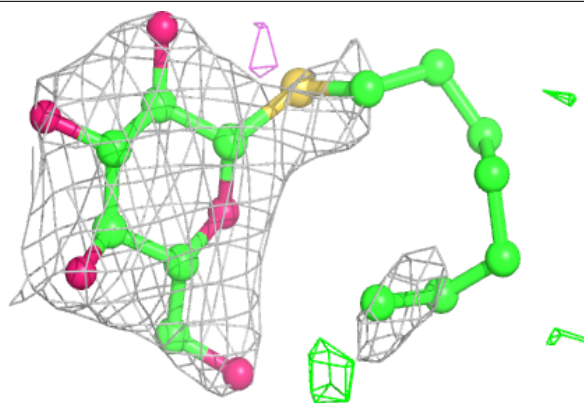
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



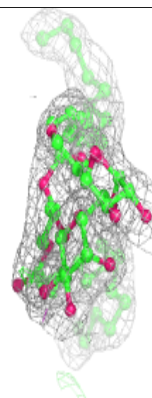
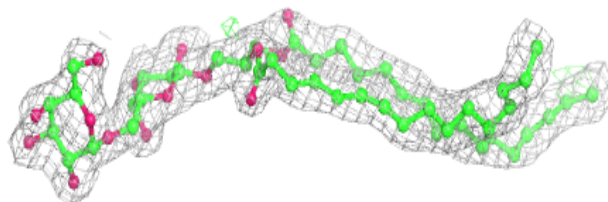
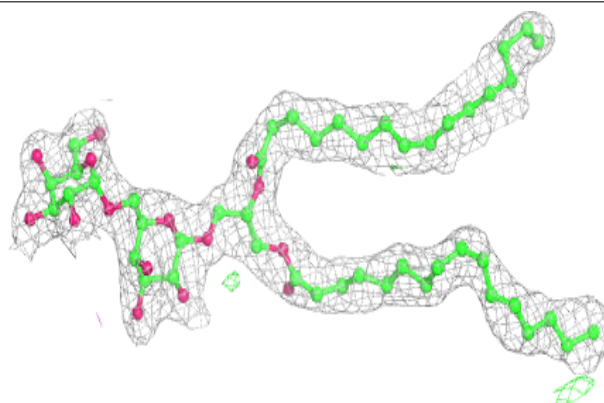


**Electron density around HTG V 206:**

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

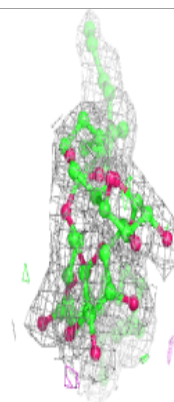
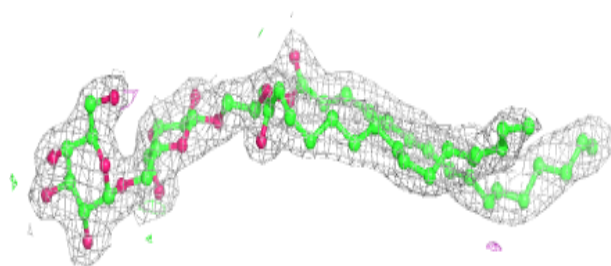
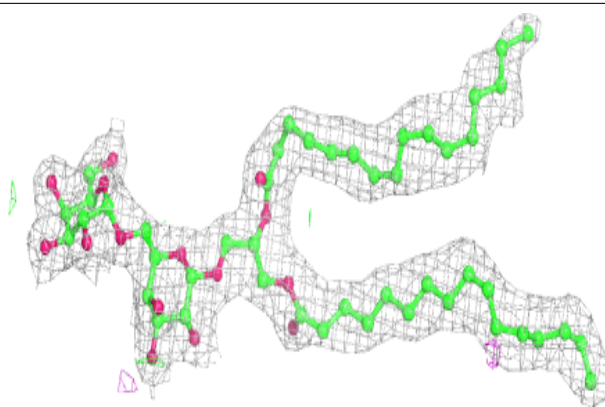
**Electron density around DGD c 522:**

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



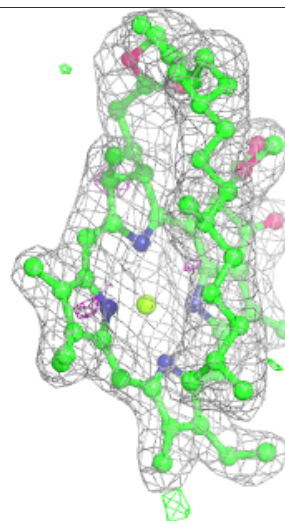
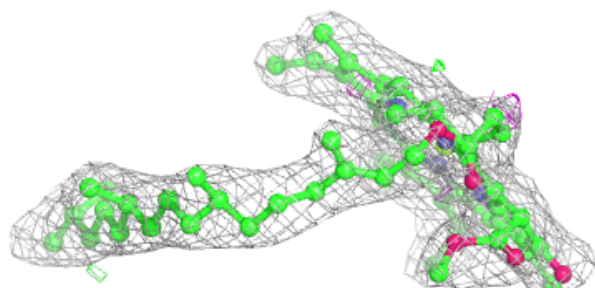
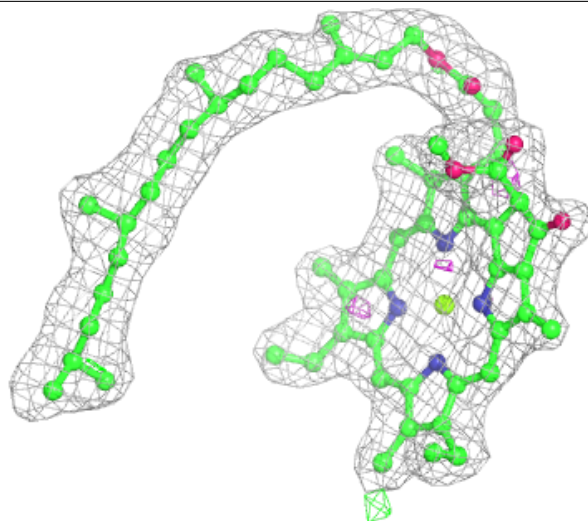
**Electron density around DGD C 518:**

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



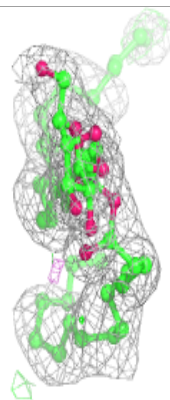
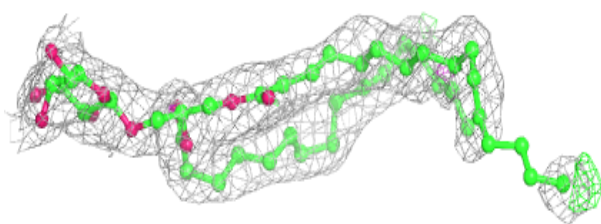
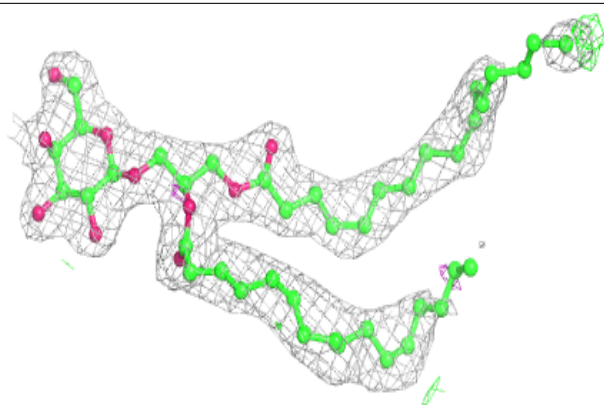
**Electron density around CLA c 512:**

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

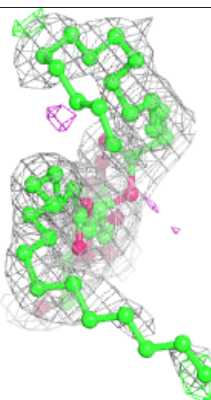
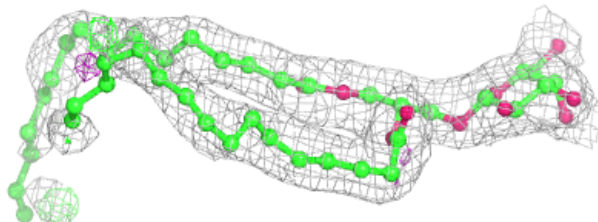
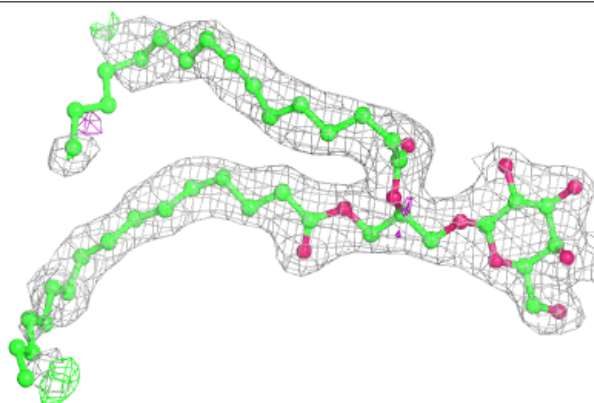


**Electron density around LMG d 413:**

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

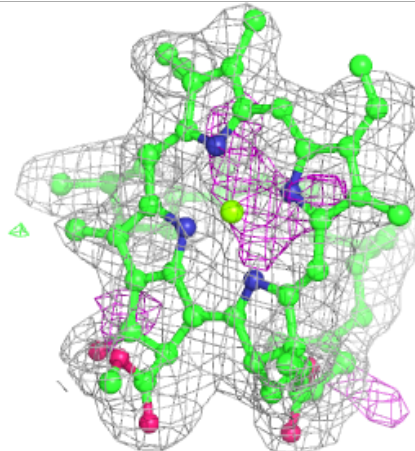
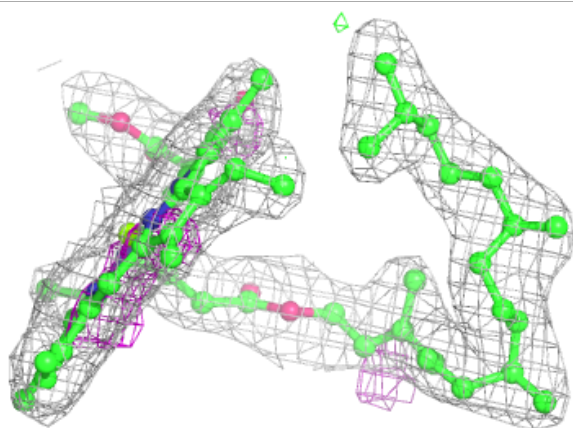
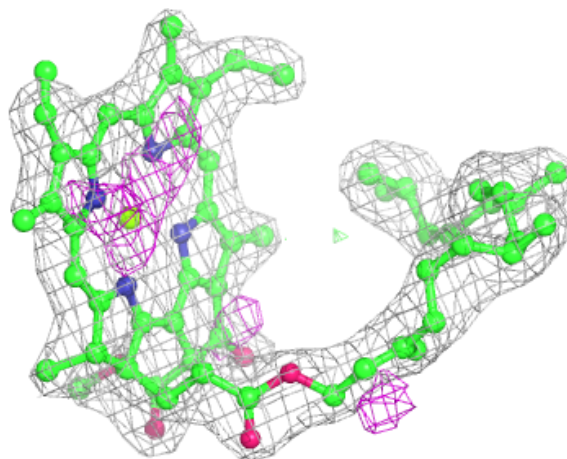
**Electron density around LMG D 413:**

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



**Electron density around CLA c 508:**

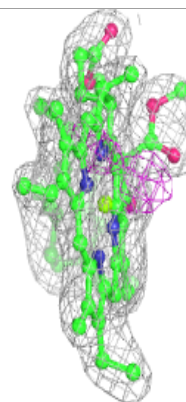
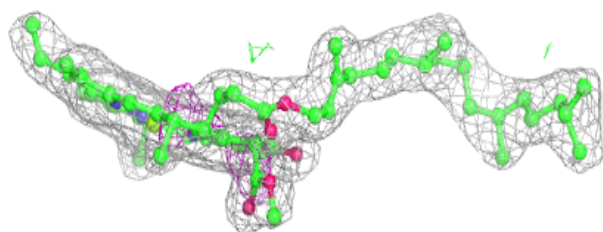
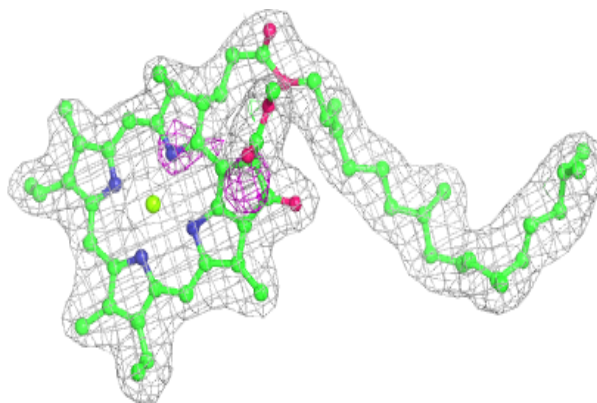
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



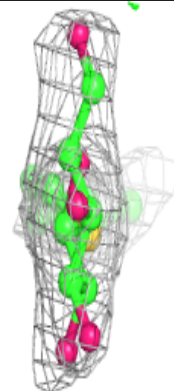
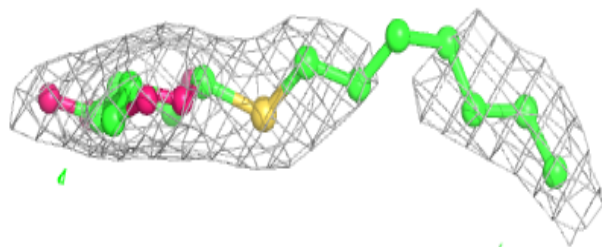
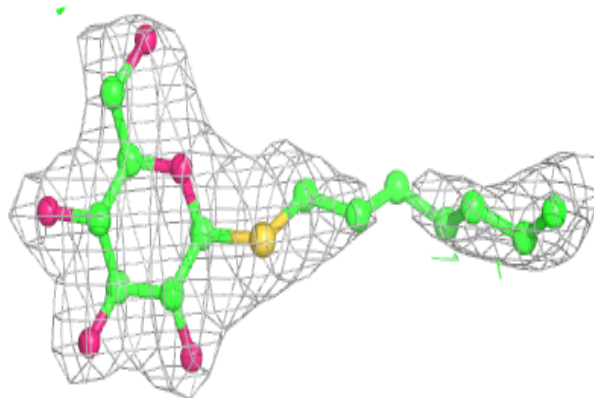


**Electron density around CLA b 611:**

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

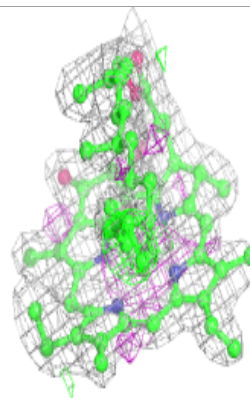
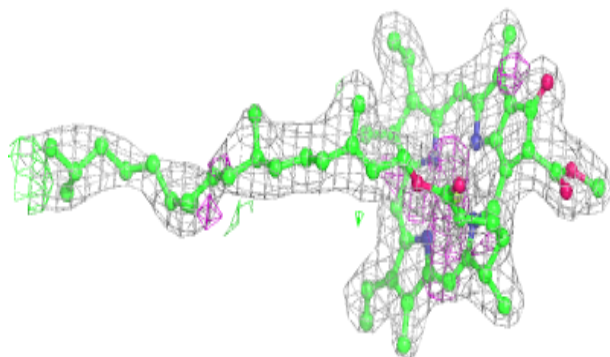
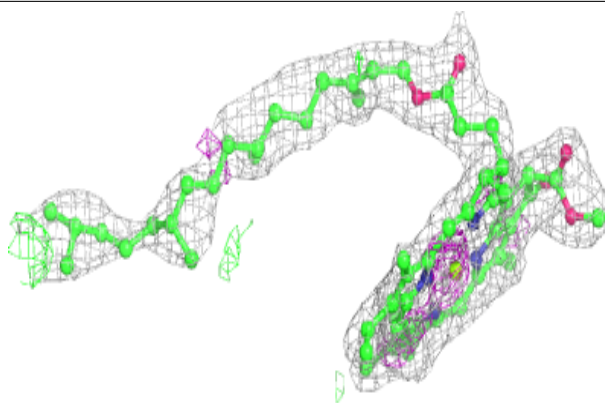
**Electron density around HTG C 522:**

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

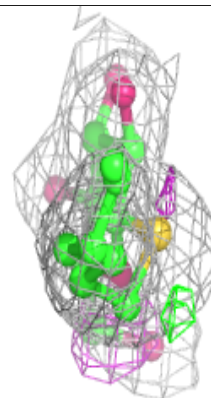
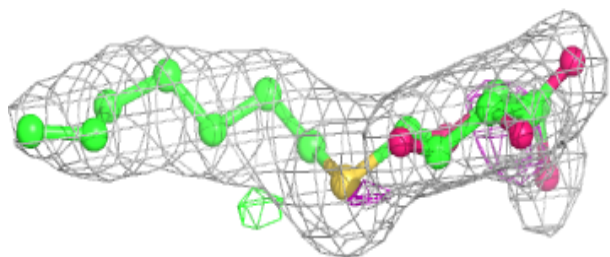
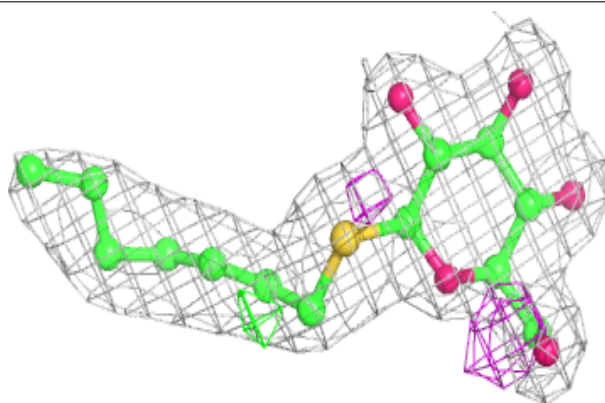


**Electron density around CLA C 504:**

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

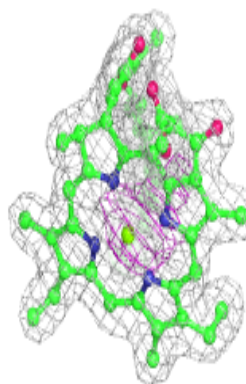
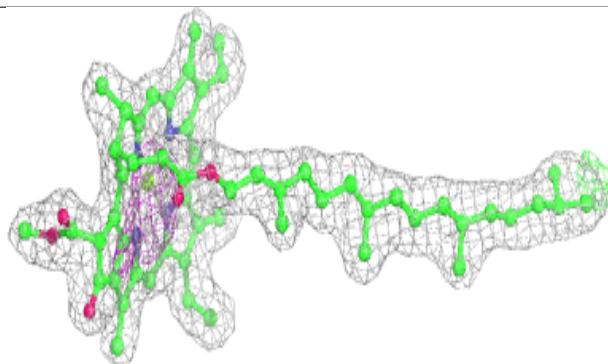
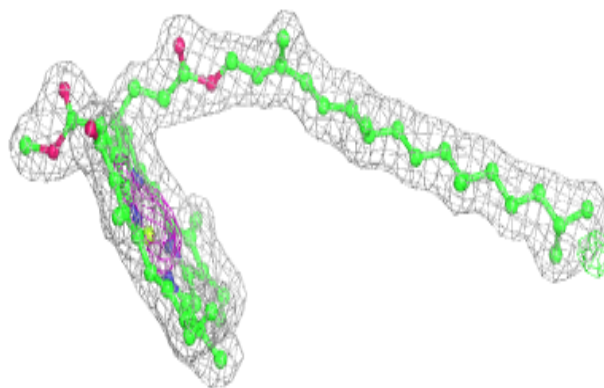
**Electron density around HTG B 623:**

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

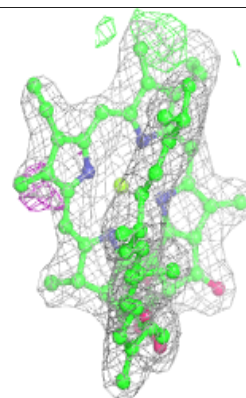
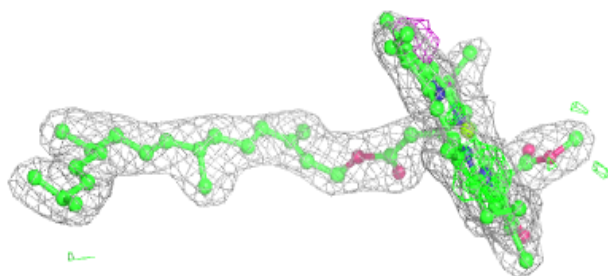
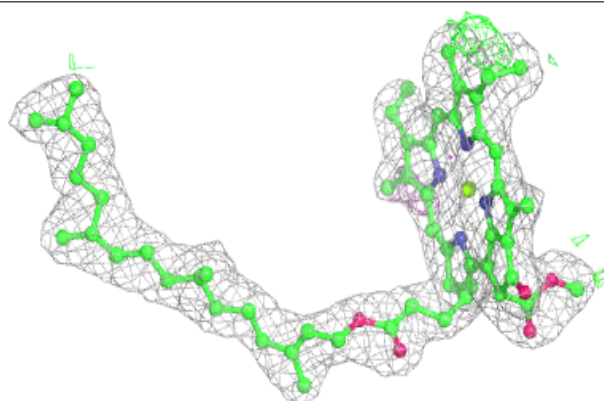


**Electron density around CLA b 616:**

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

**Electron density around CLA b 618:**

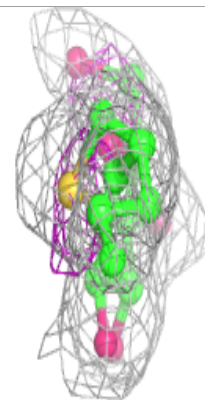
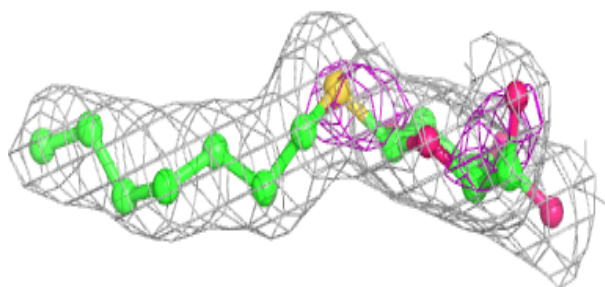
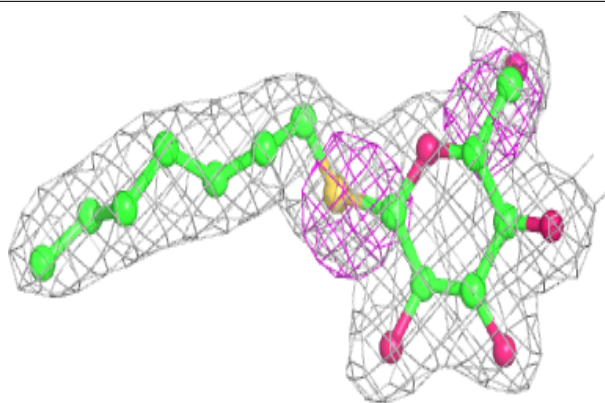
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



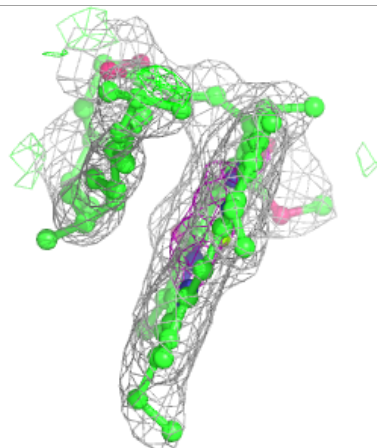
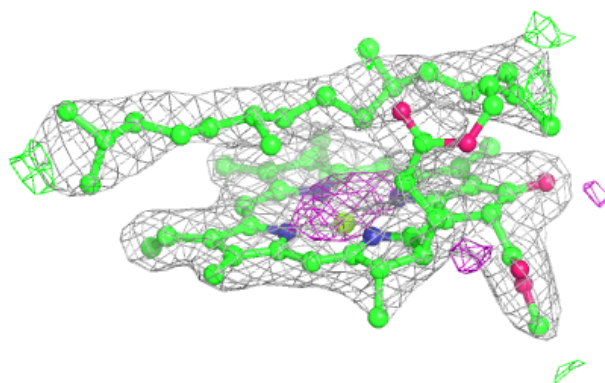
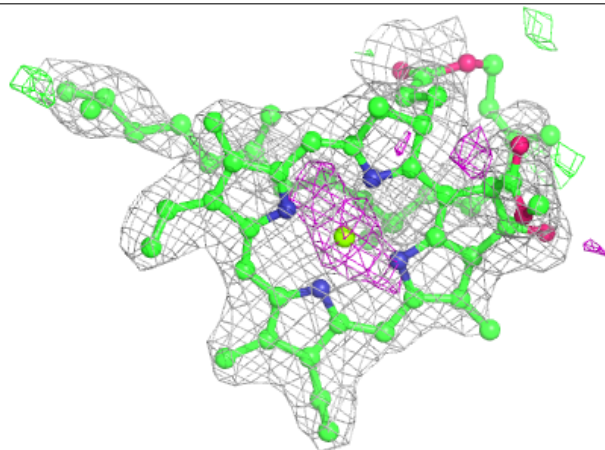


**Electron density around HTG b 601:**

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

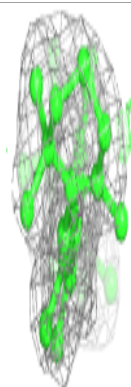
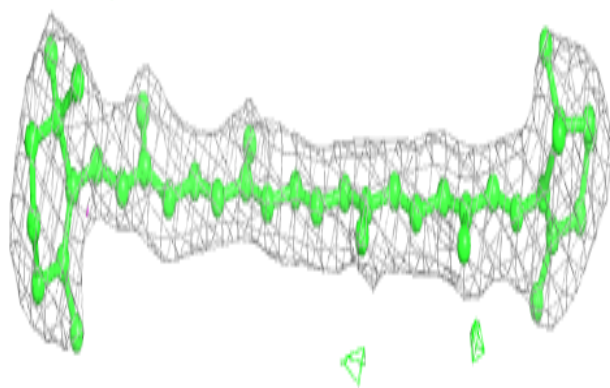
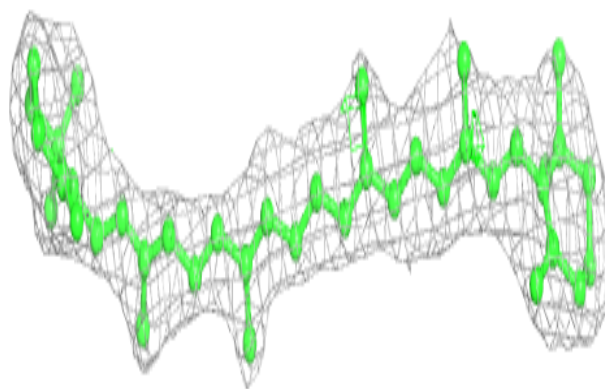
**Electron density around CLA b 610:**

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

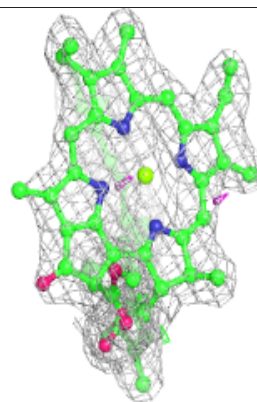
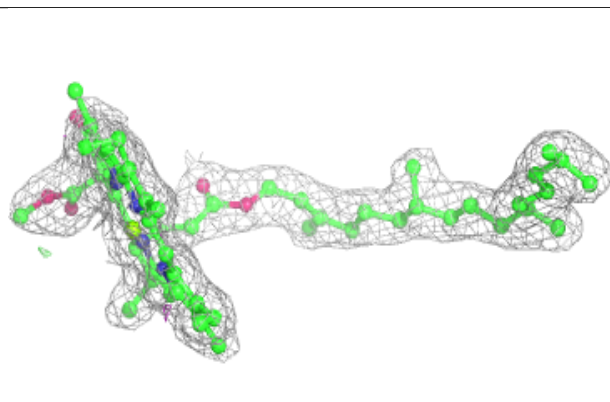
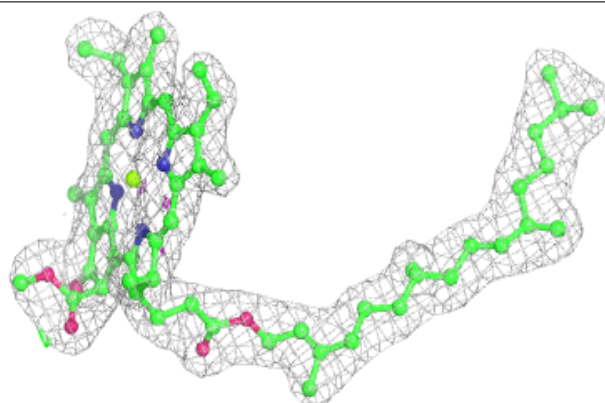


**Electron density around BCR c 528:**

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

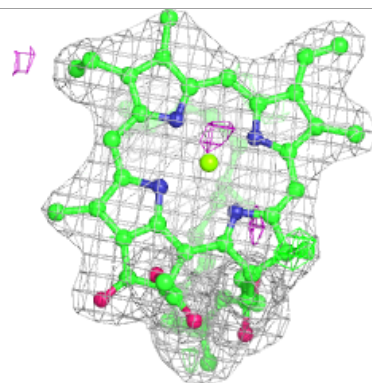
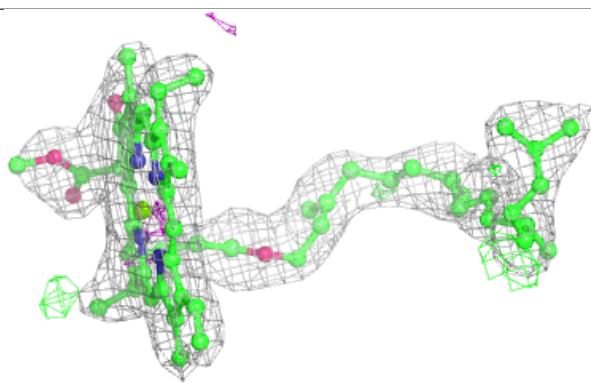
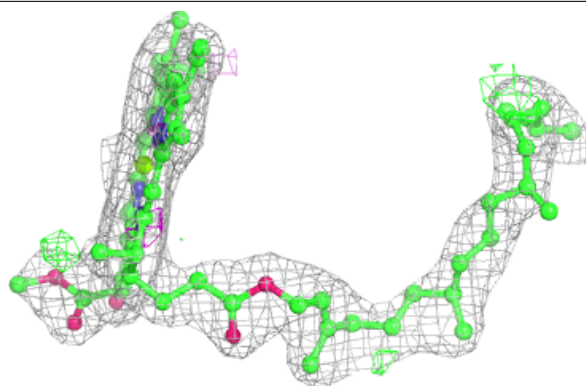
**Electron density around CLA B 610:**

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

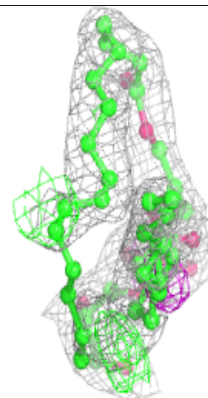
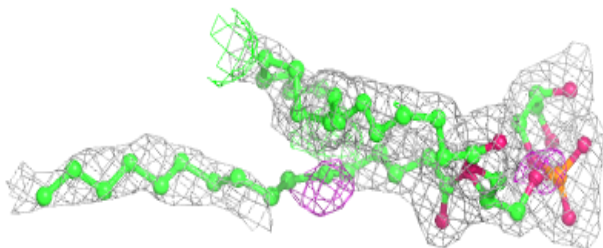
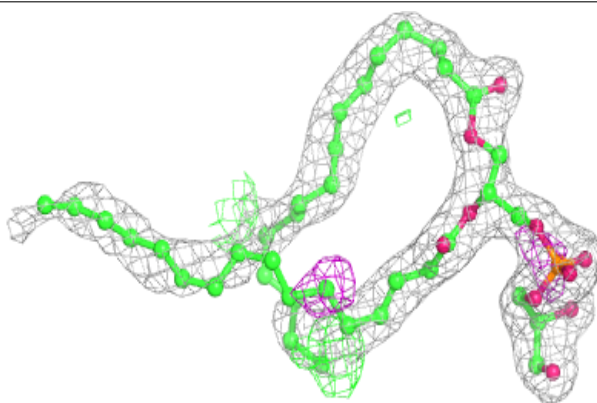


**Electron density around CLA c 511:**

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

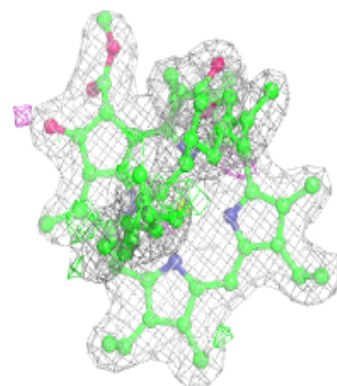
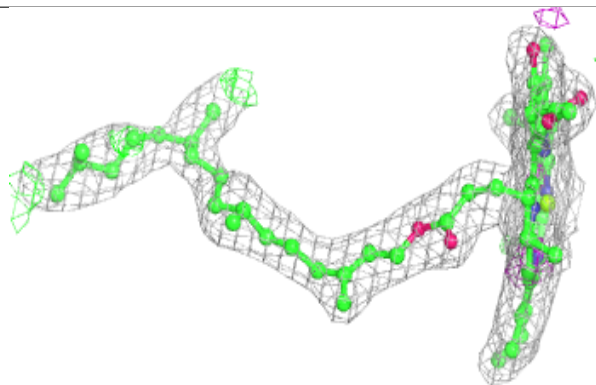
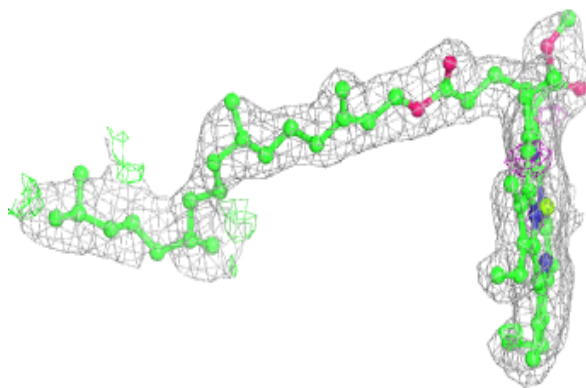
**Electron density around LHG D 409:**

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

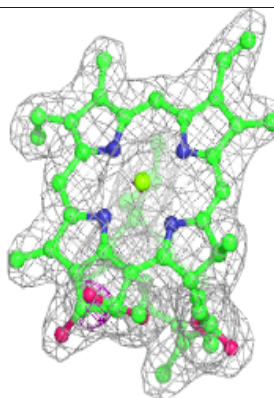
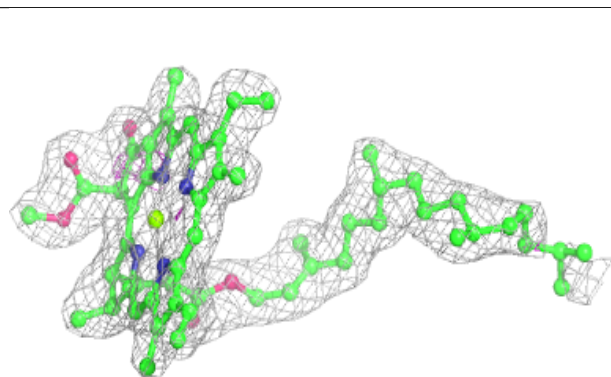
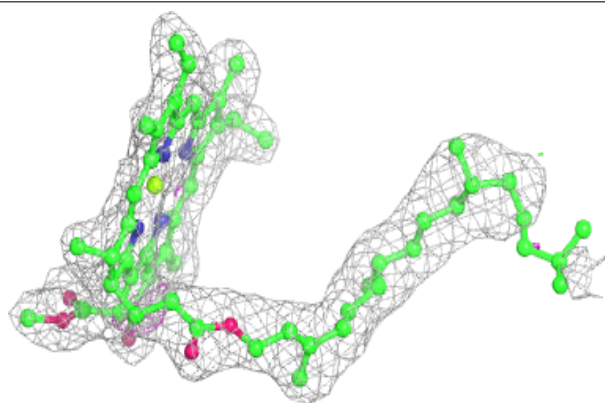


**Electron density around CLA b 615:**

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

**Electron density around CLA c 513:**

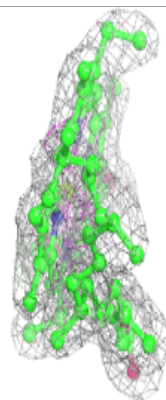
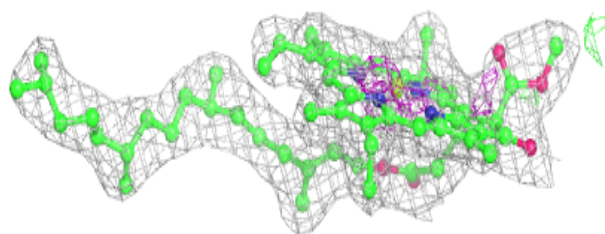
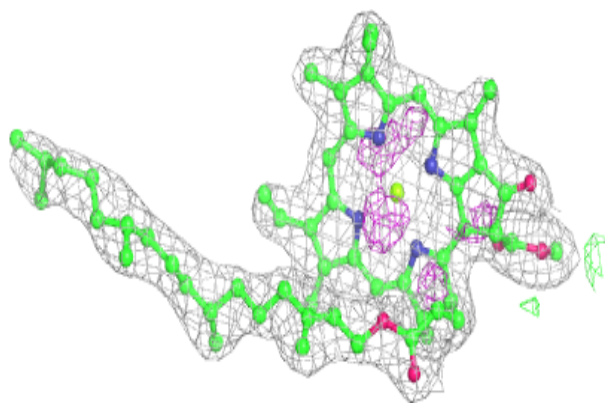
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



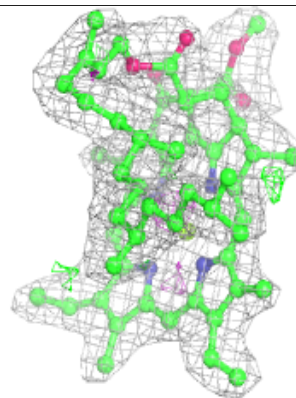
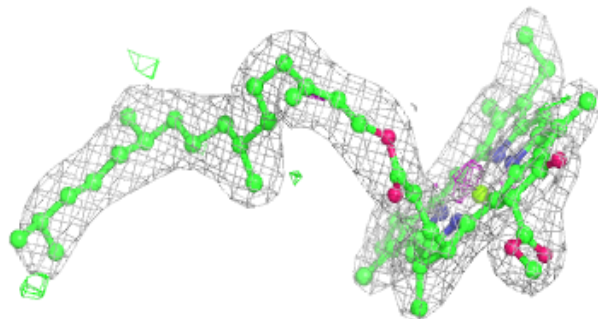
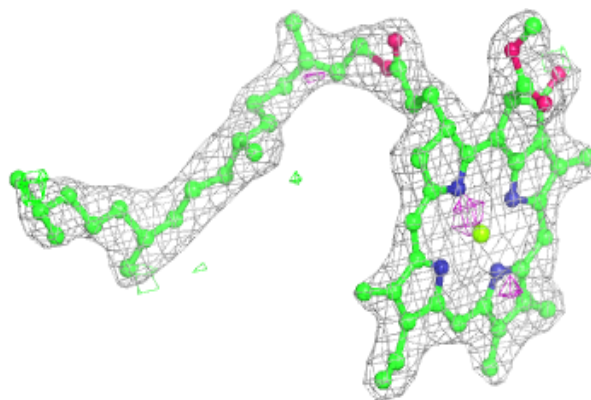


**Electron density around CLA C 501:**

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

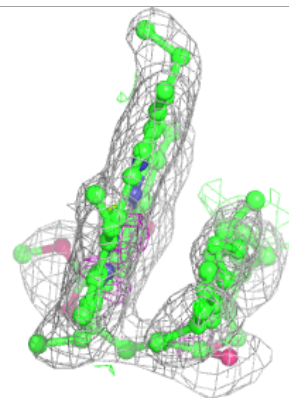
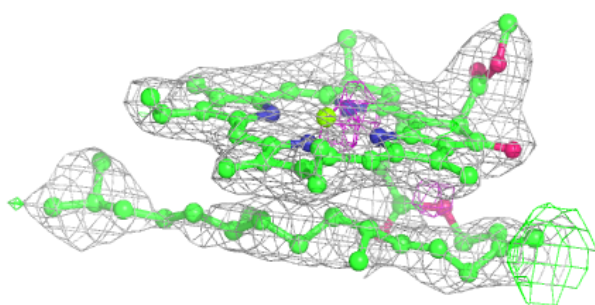
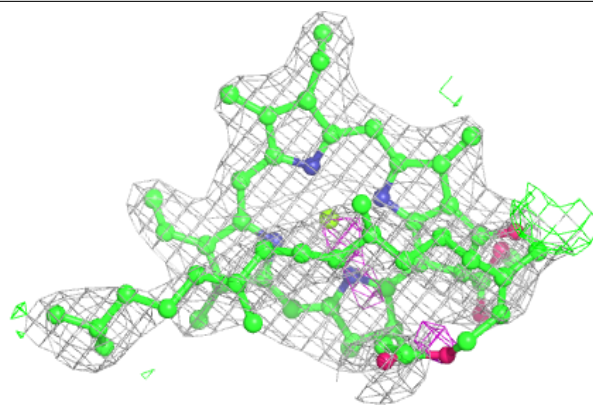
**Electron density around CLA c 516:**

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

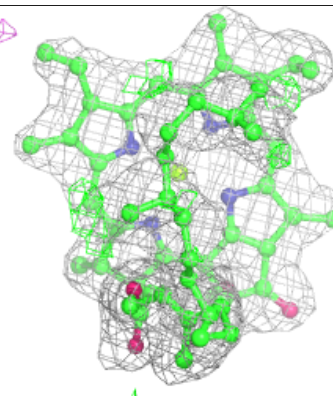
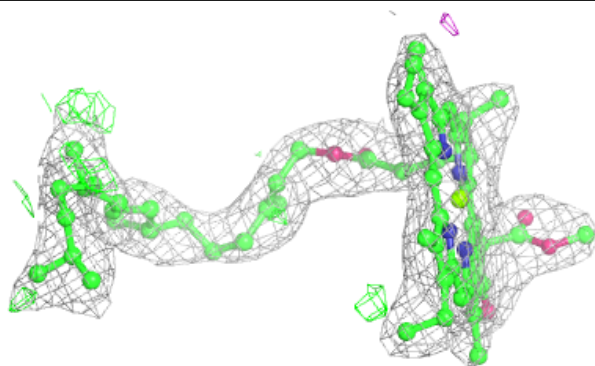
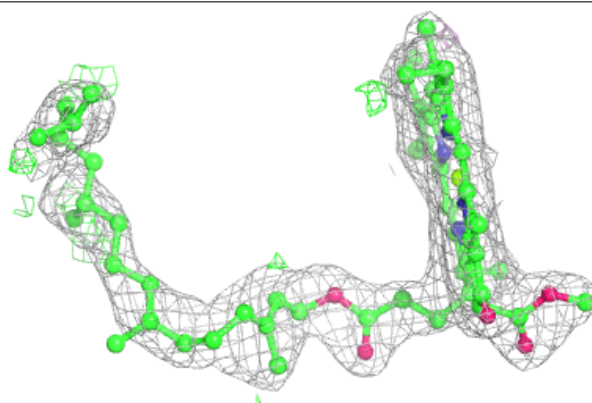


**Electron density around CLA B 602:**

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

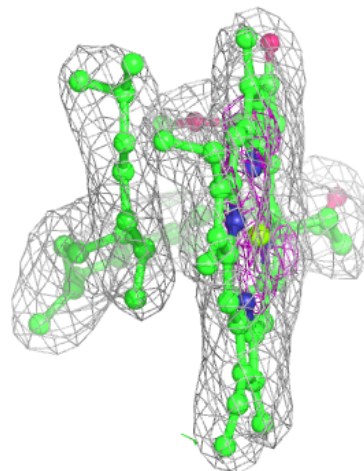
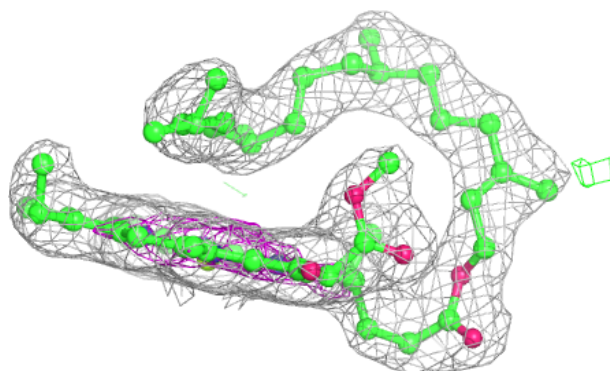
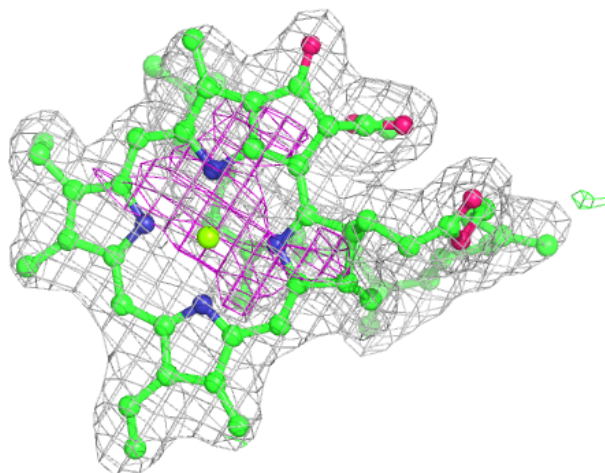
**Electron density around CLA C 506:**

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



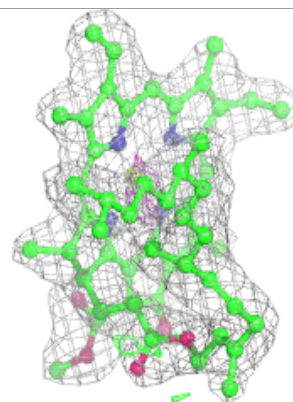
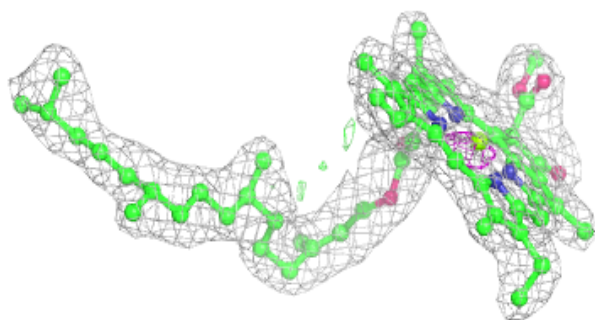
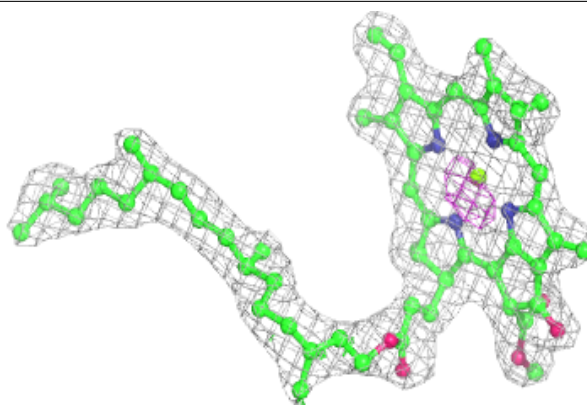
**Electron density around CLA c 515:**

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



**Electron density around CLA C 511:**

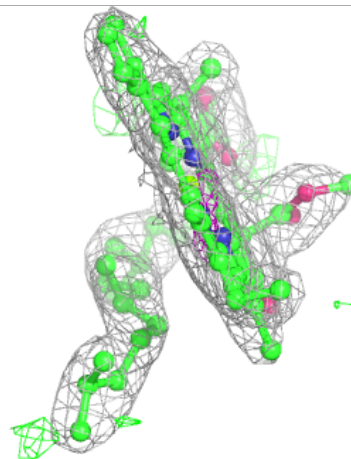
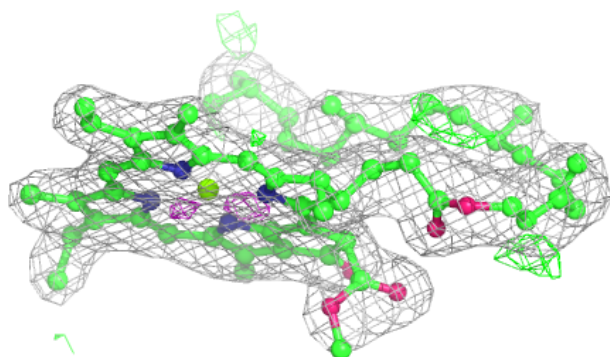
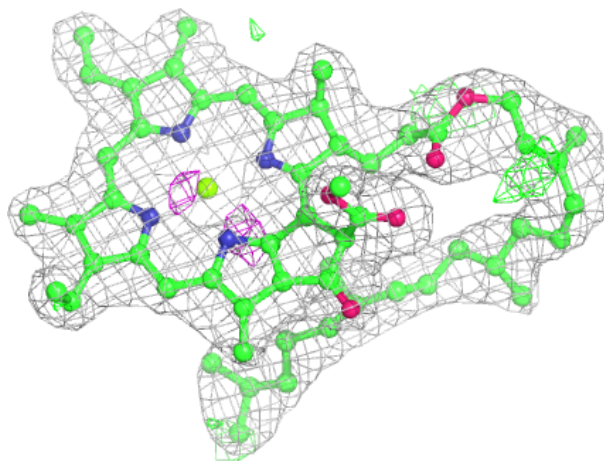
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





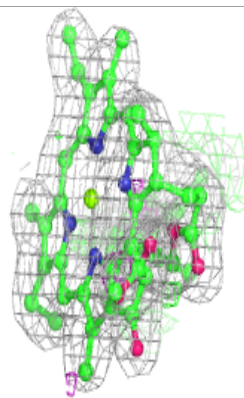
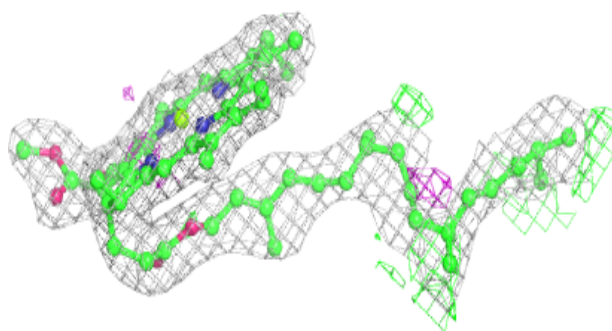
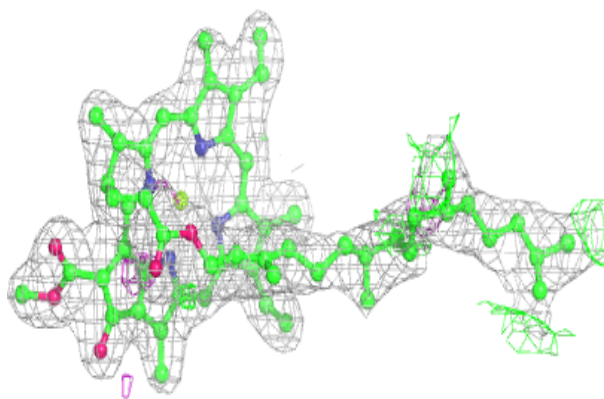
**Electron density around CLA C 509:**

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



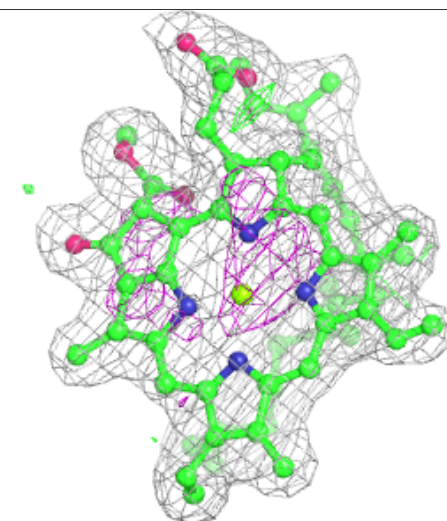
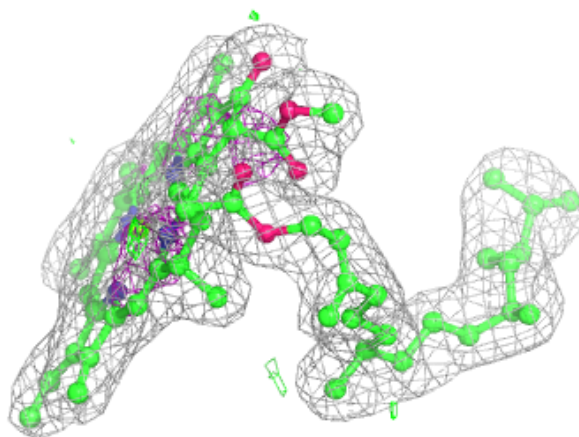
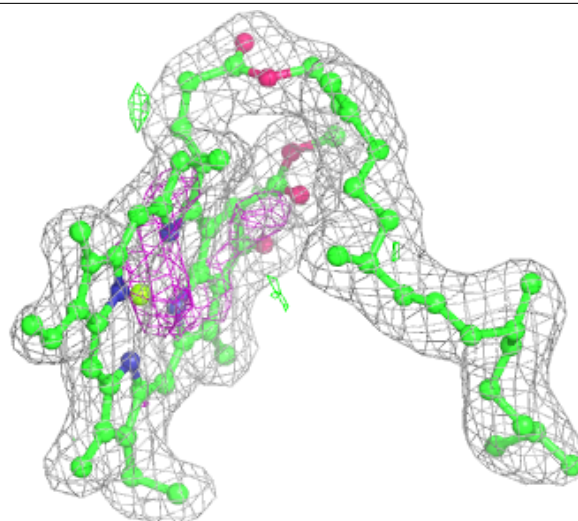
**Electron density around CLA B 615:**

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



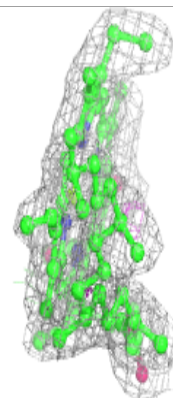
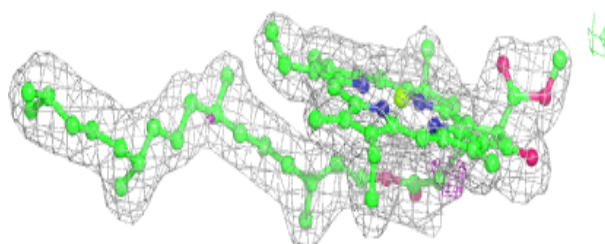
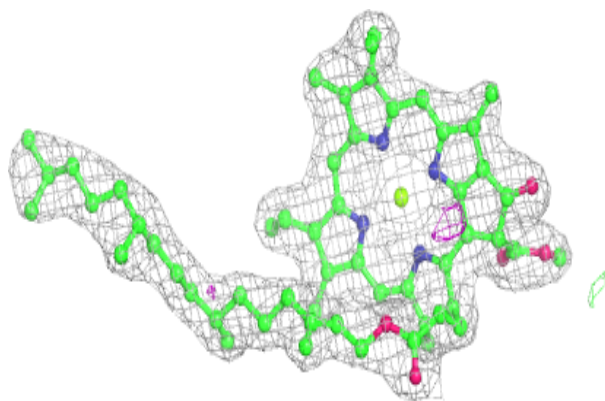
**Electron density around CLA B 614:**

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



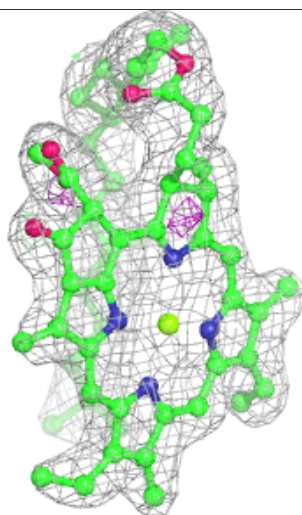
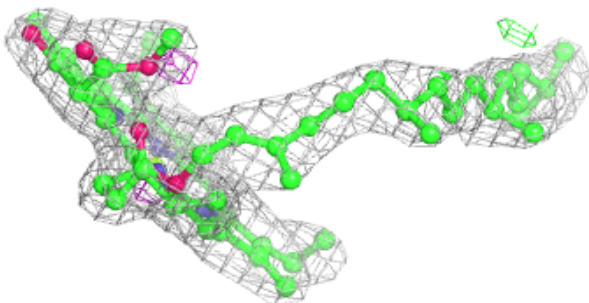
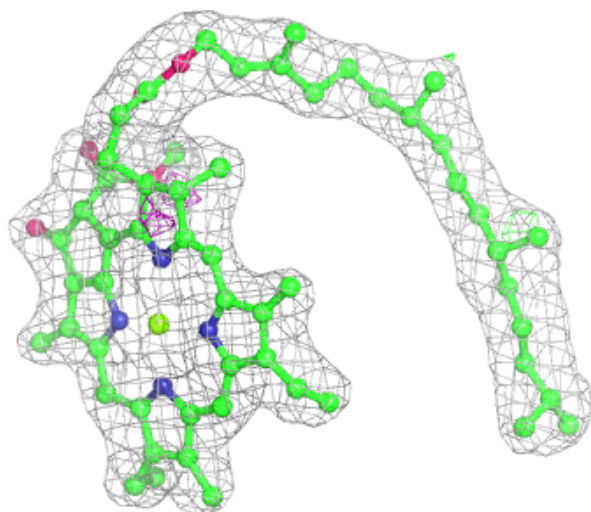
**Electron density around CLA c 506:**

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



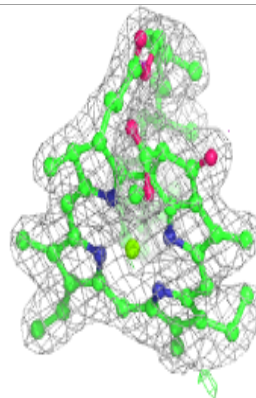
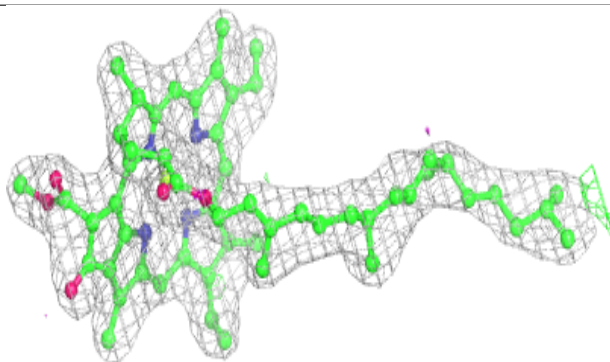
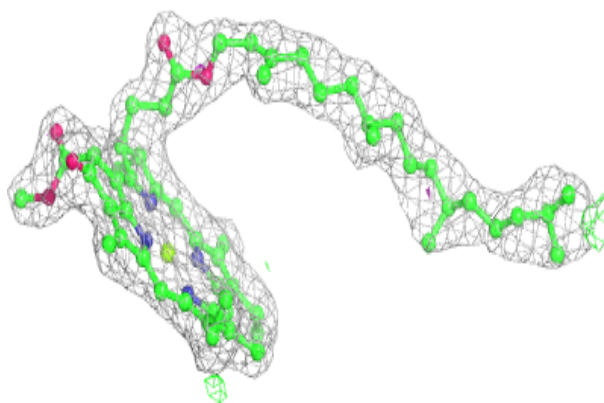
**Electron density around CLA C 507:**

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



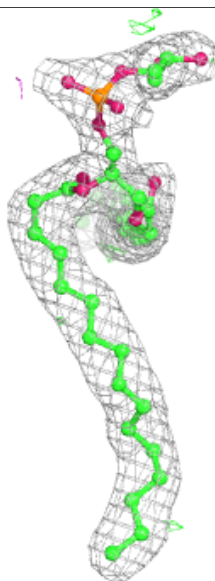
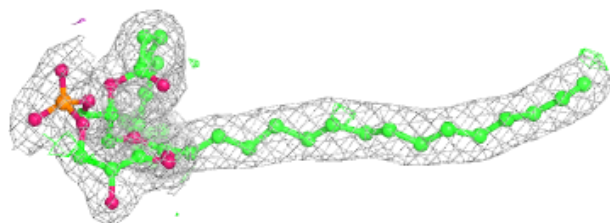
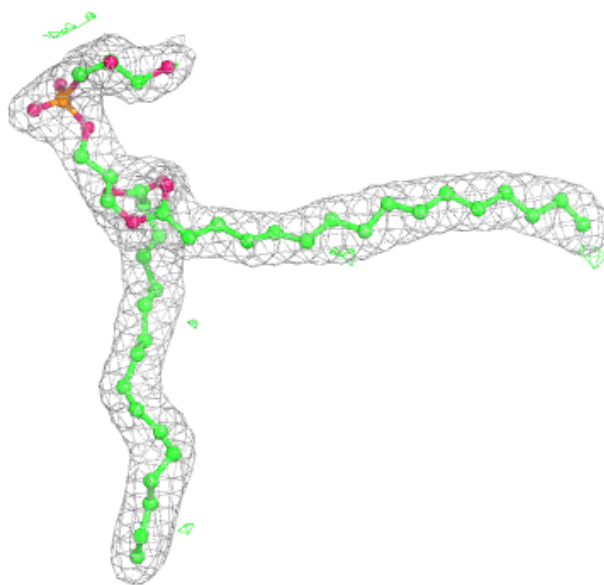
**Electron density around CLA c 509:**

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



**Electron density around LHG L 101:**

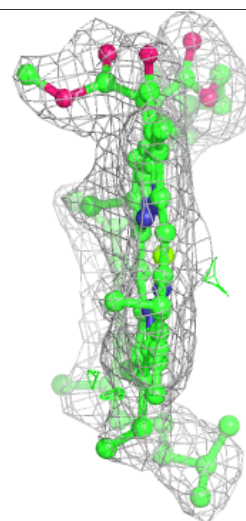
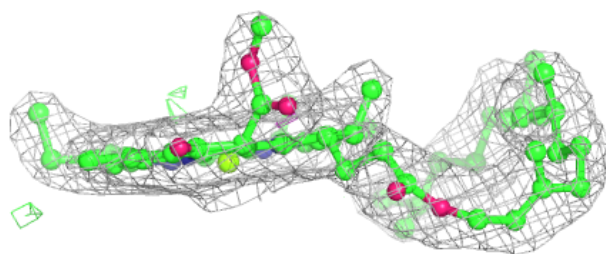
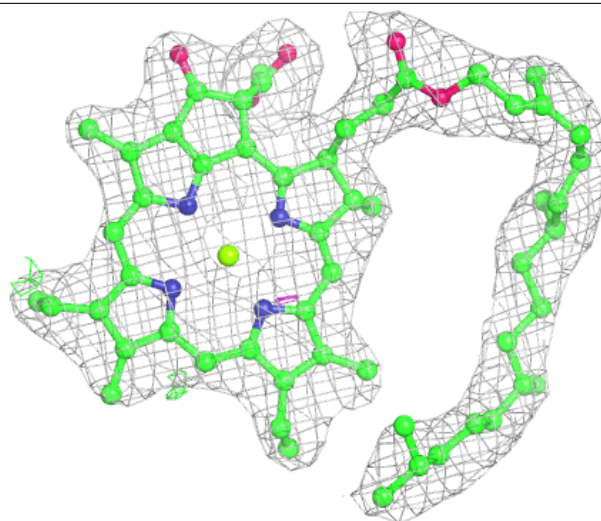
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CLA C 512:**

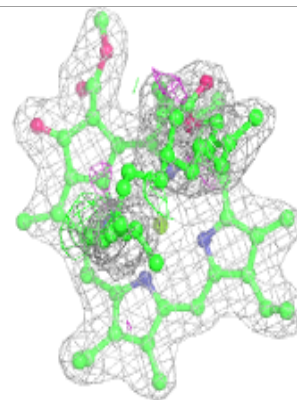
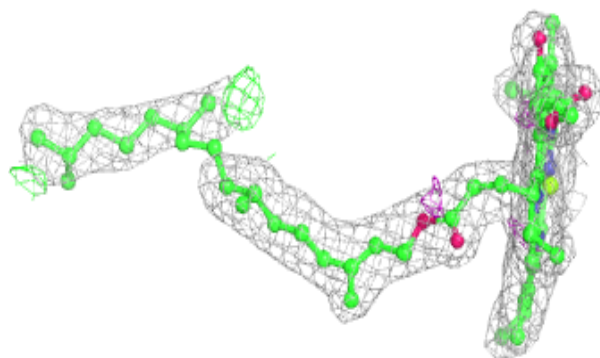
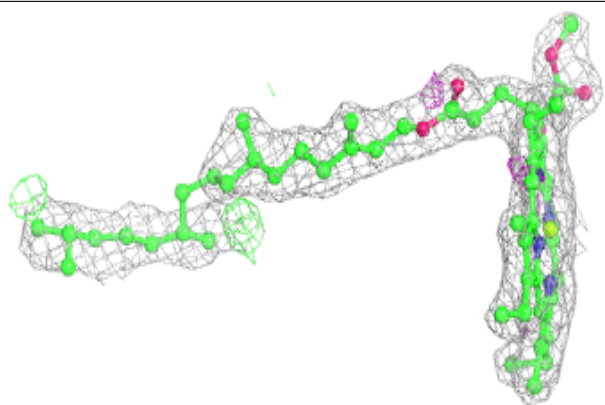
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



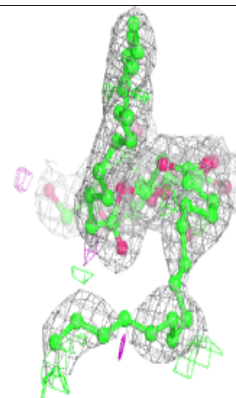
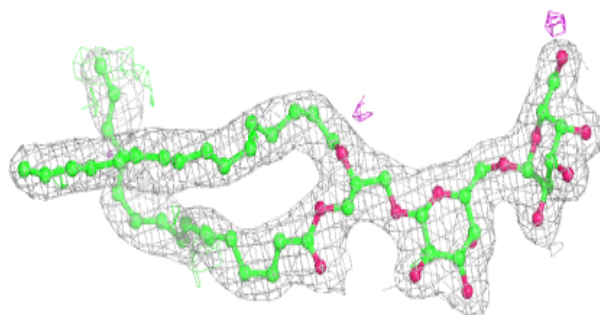
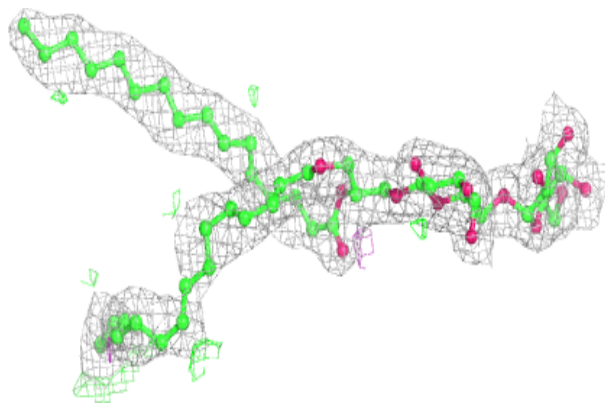


**Electron density around CLA B 607:**

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

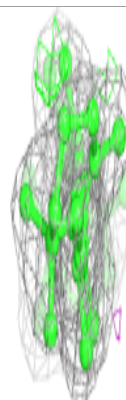
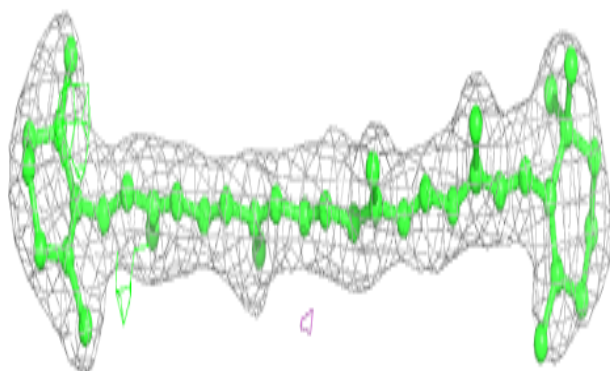
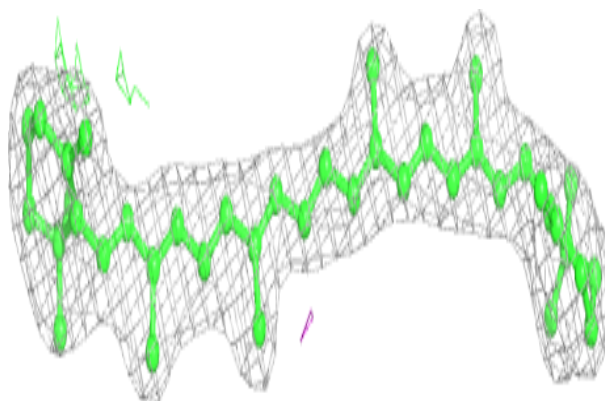
**Electron density around DGD C 516:**

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

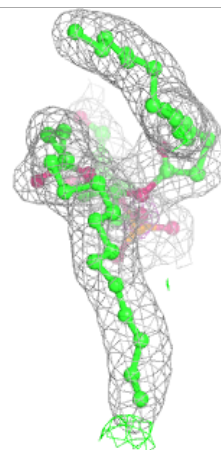
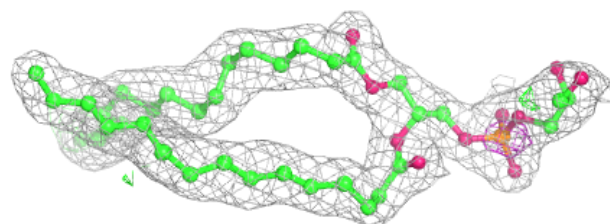
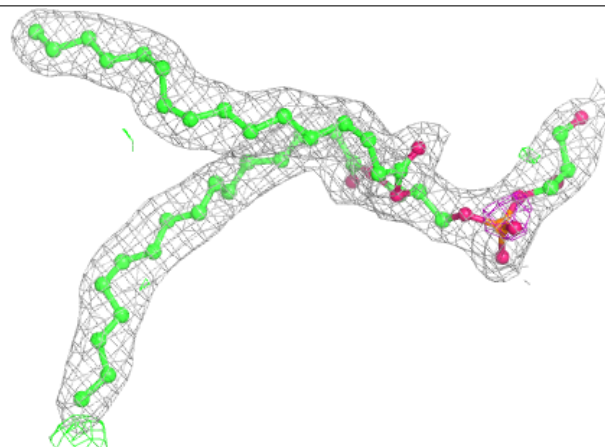


**Electron density around BCR C 514:**

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

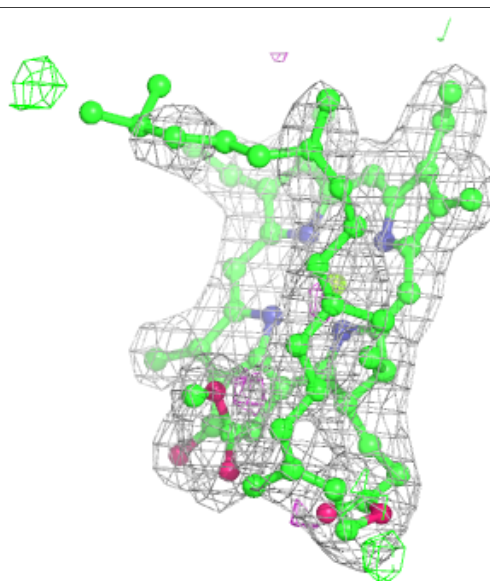
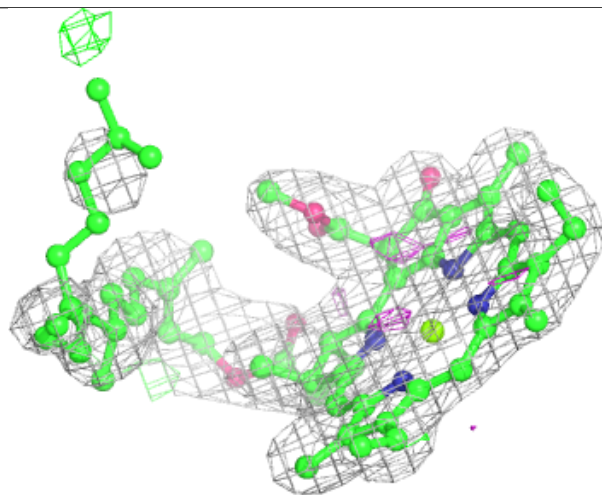
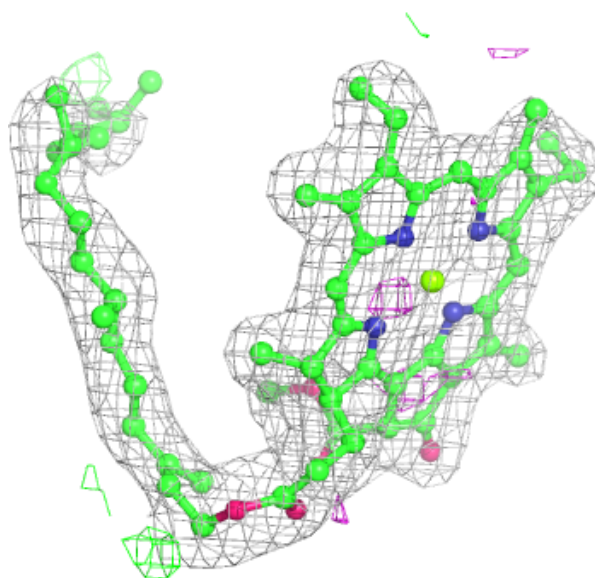
**Electron density around LHG d 407:**

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



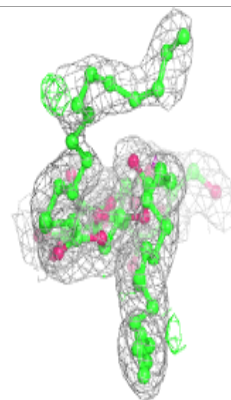
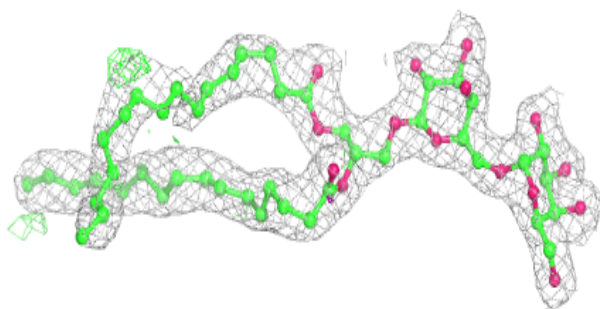
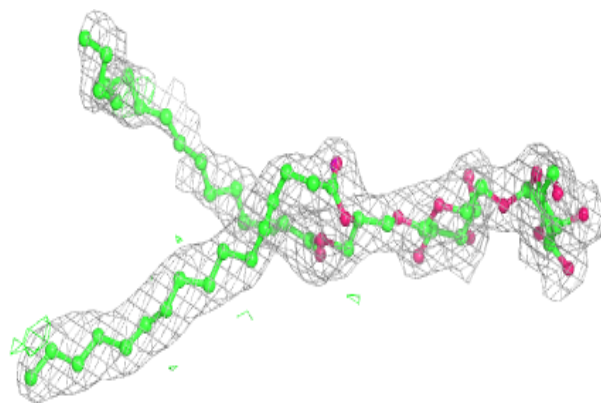
**Electron density around CLA b 625:**

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

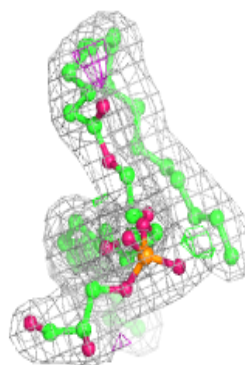
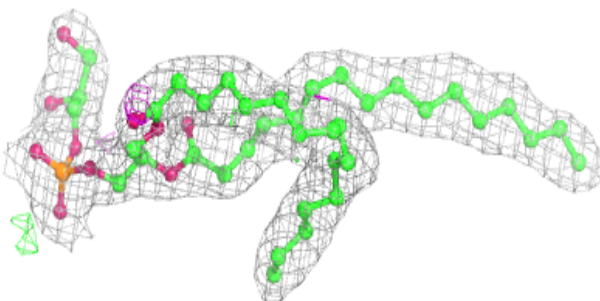
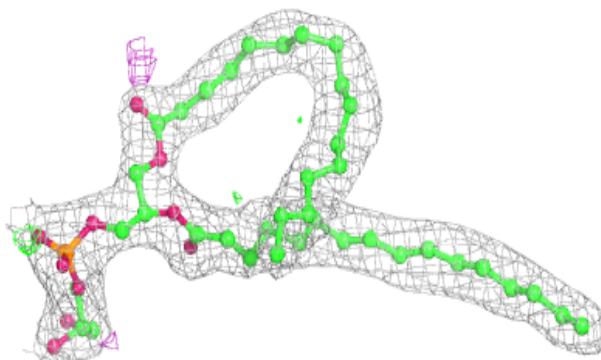


**Electron density around DGD c 520:**

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

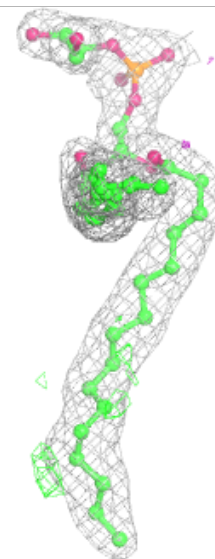
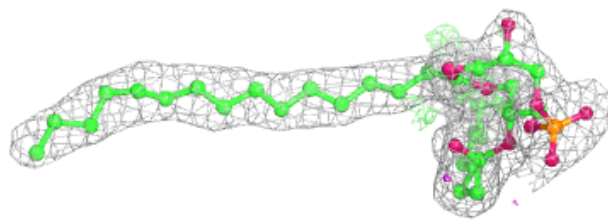
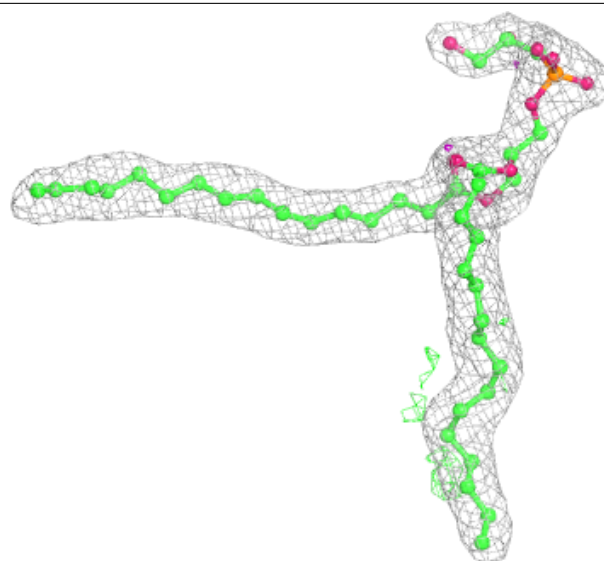
**Electron density around LHG d 406:**

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



**Electron density around LHG b 634:**

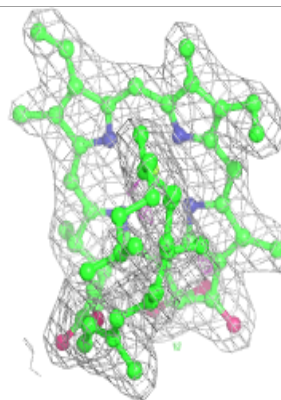
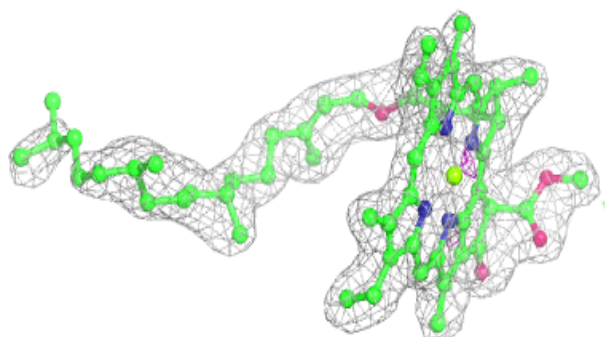
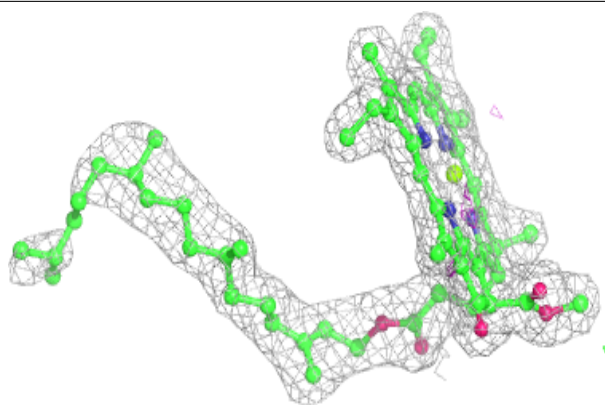
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



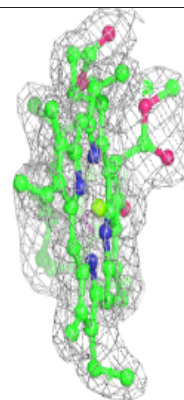
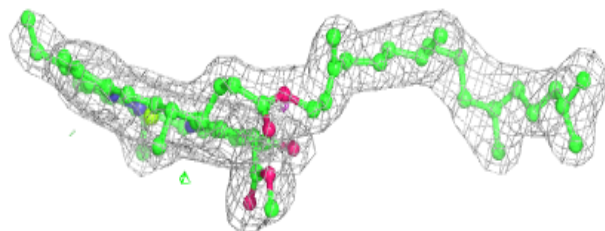
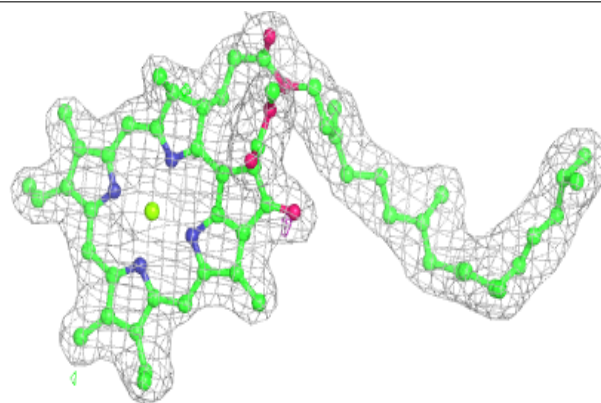


**Electron density around CLA C 508:**

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

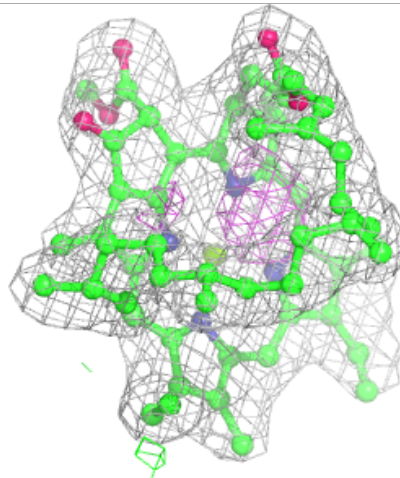
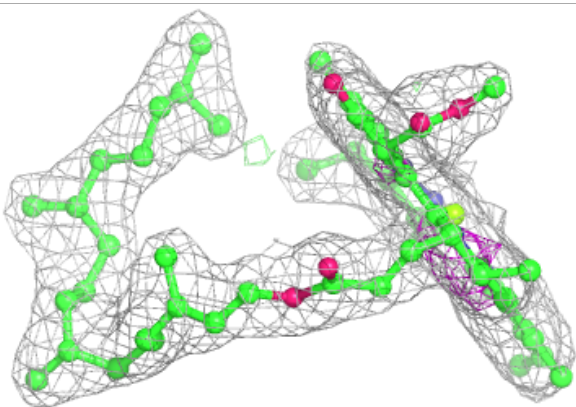
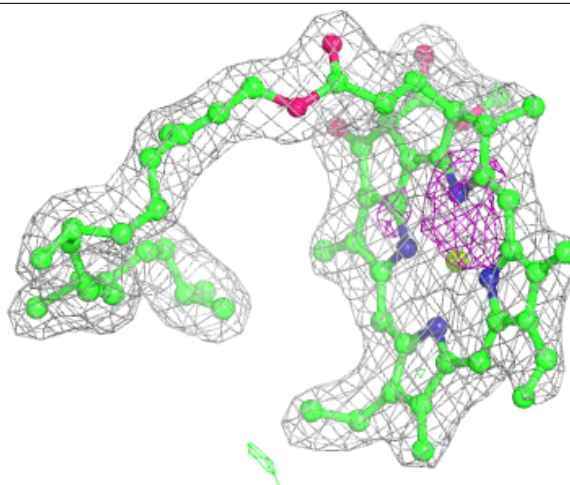
**Electron density around CLA B 603:**

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



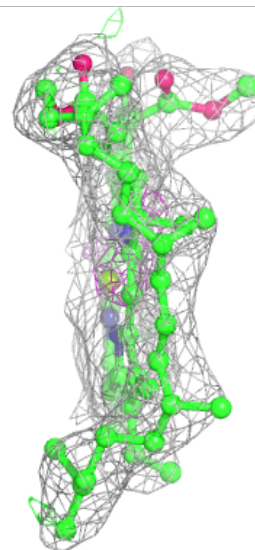
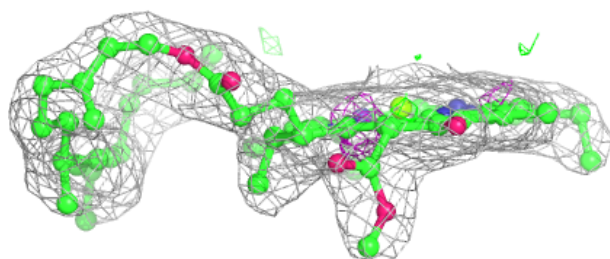
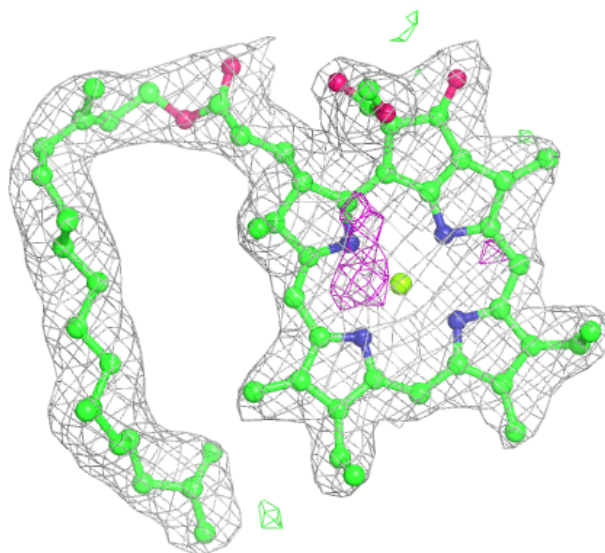
**Electron density around CLA C 503:**

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



**Electron density around CLA c 517:**

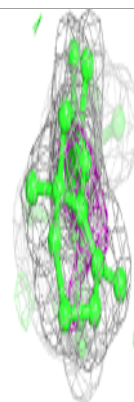
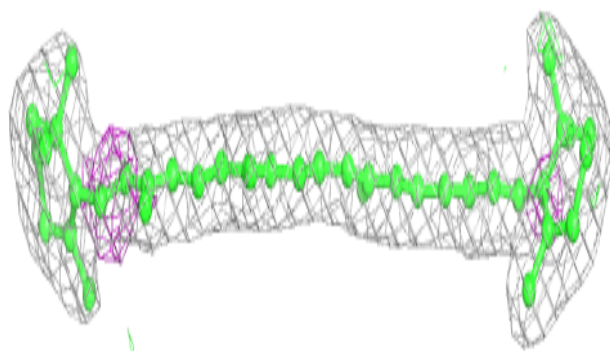
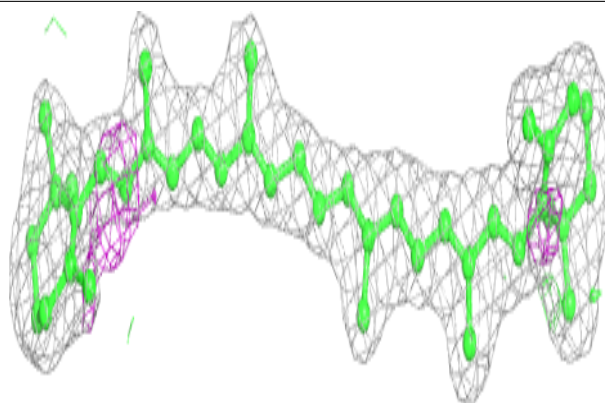
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



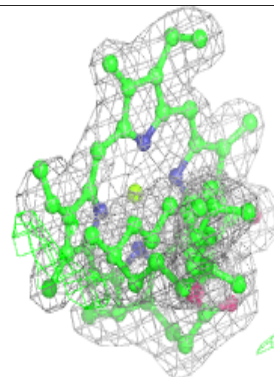
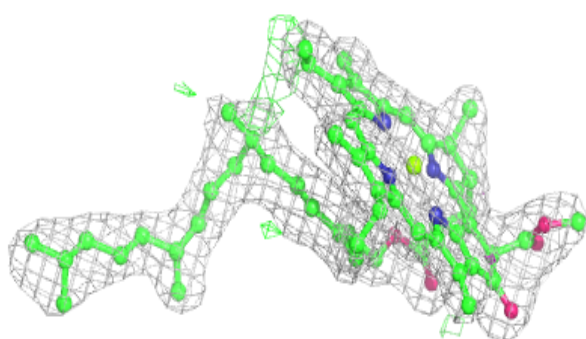
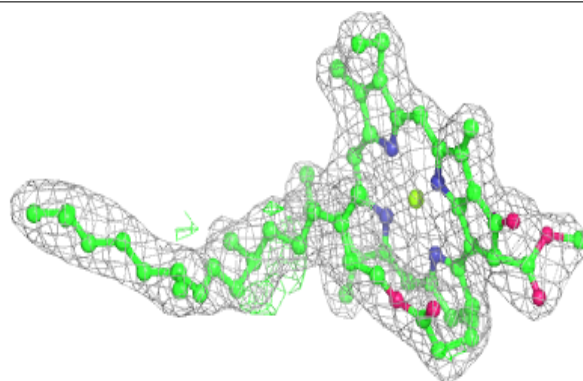


**Electron density around BCR b 627:**

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

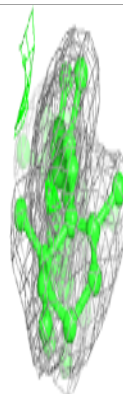
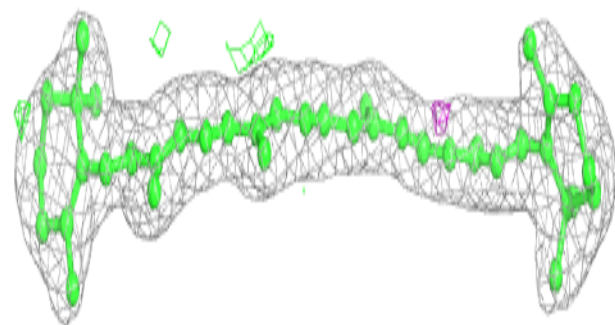
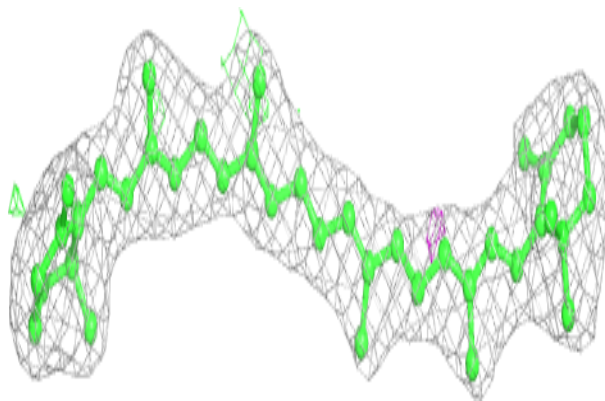
**Electron density around CLA c 510:**

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

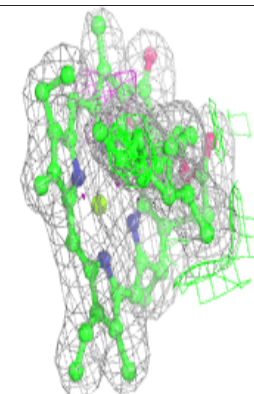
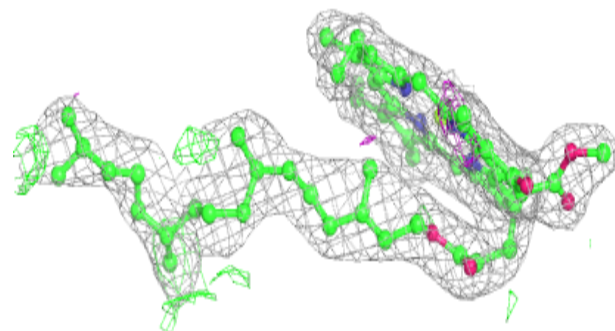
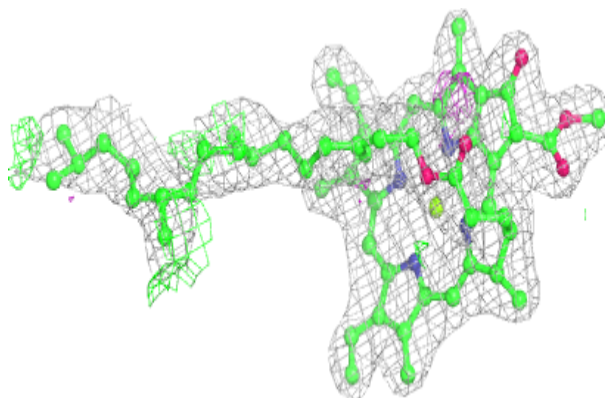


**Electron density around BCR y 101:**

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

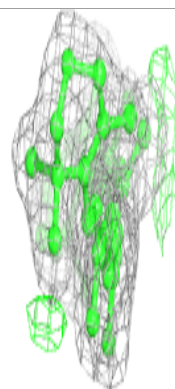
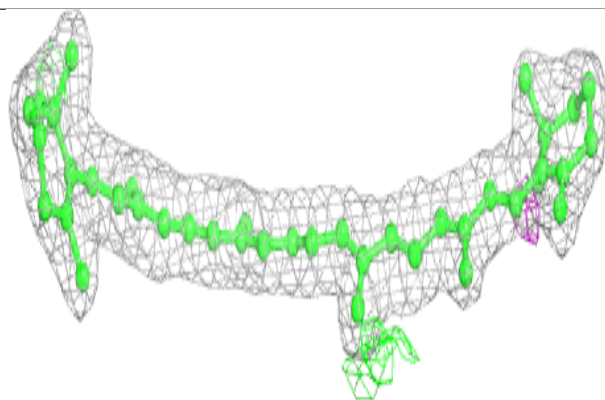
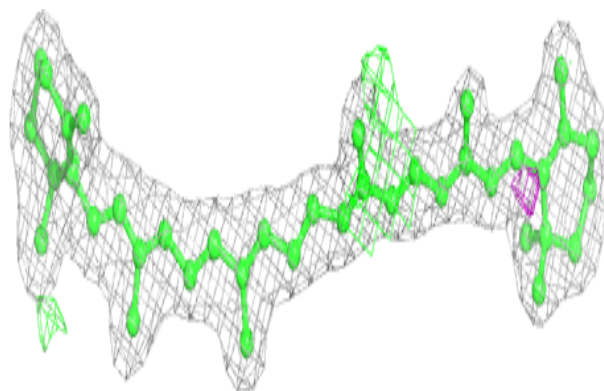
**Electron density around CLA b 623:**

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

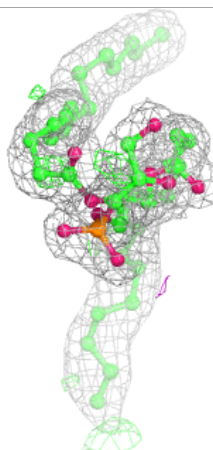
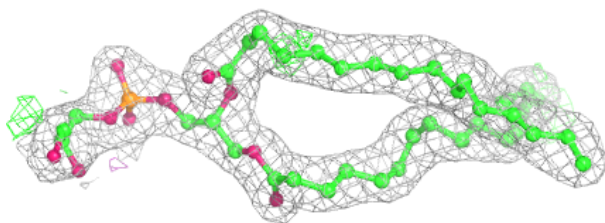
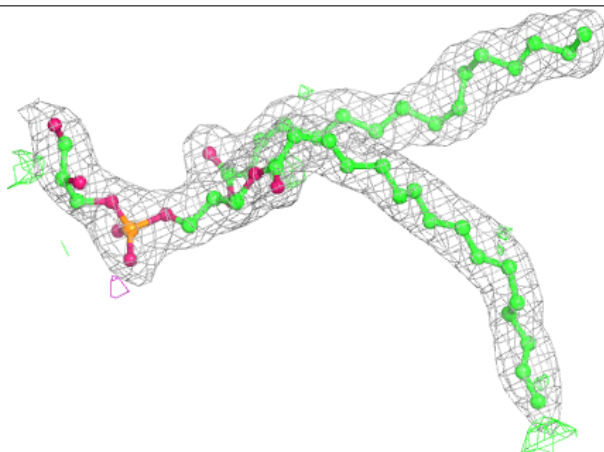


**Electron density around BCR T 103:**

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

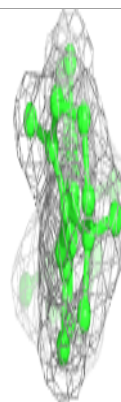
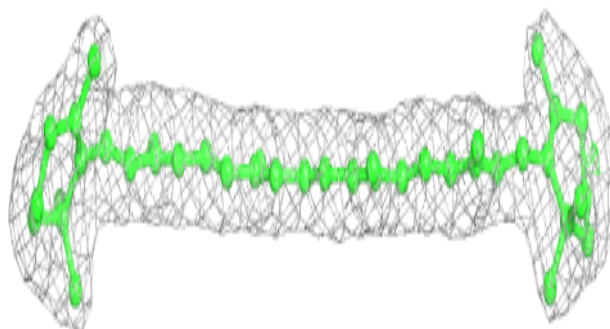
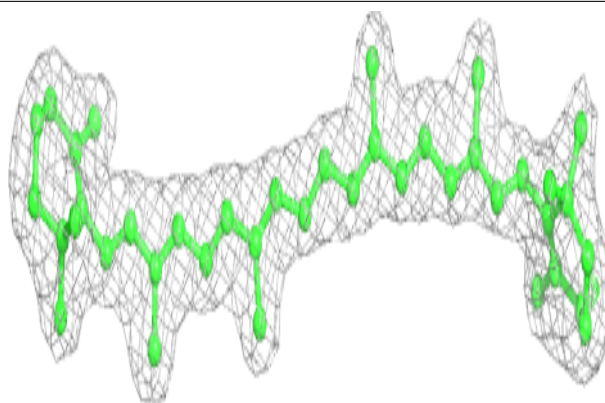
**Electron density around LHG D 408:**

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



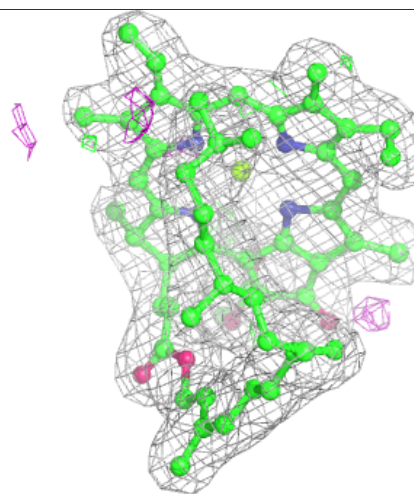
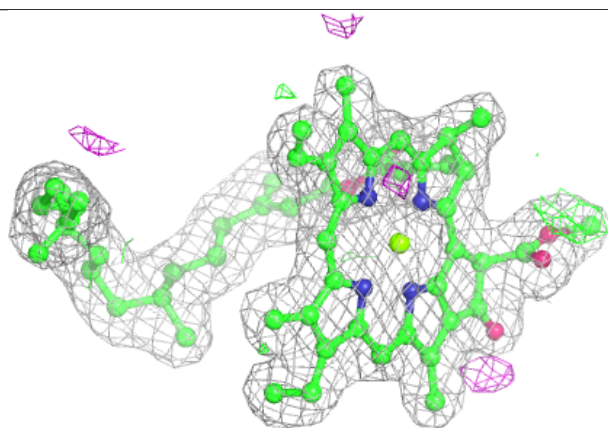
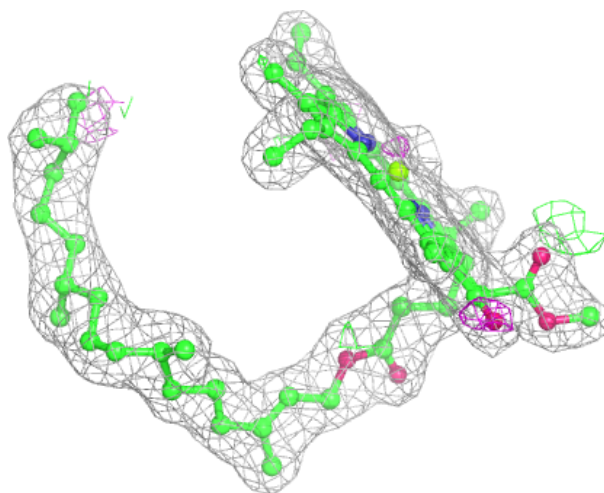
**Electron density around BCR B 619:**

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



**Electron density around CLA B 612:**

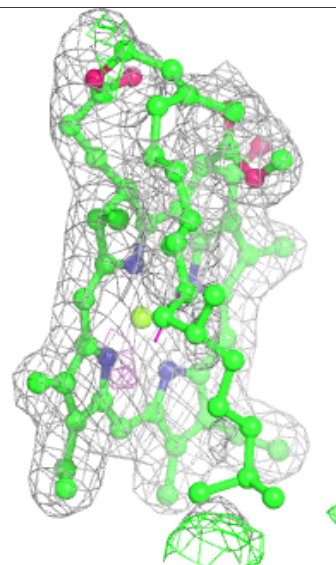
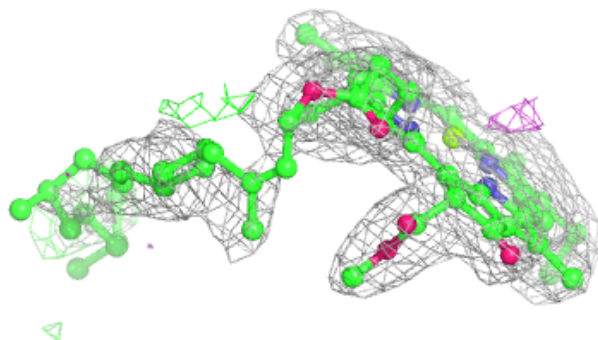
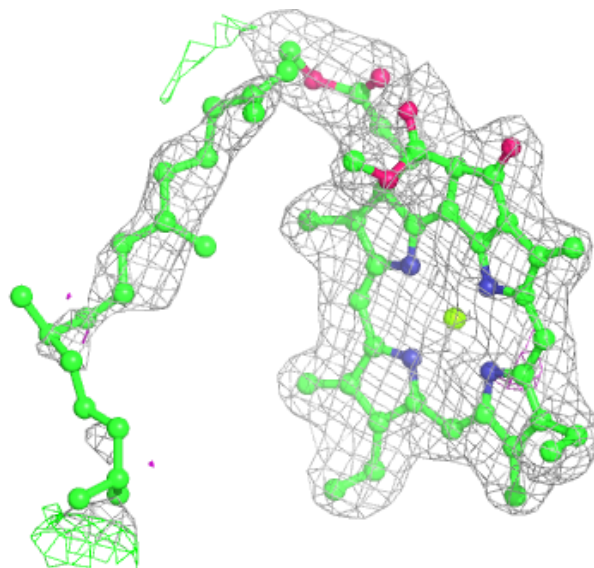
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





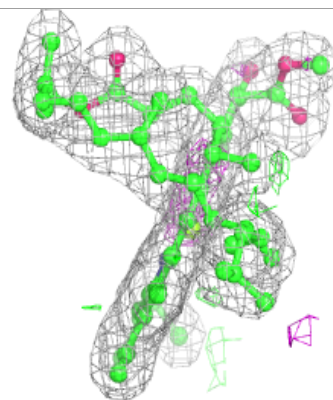
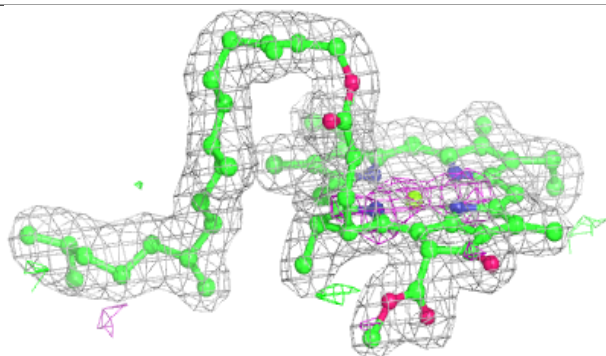
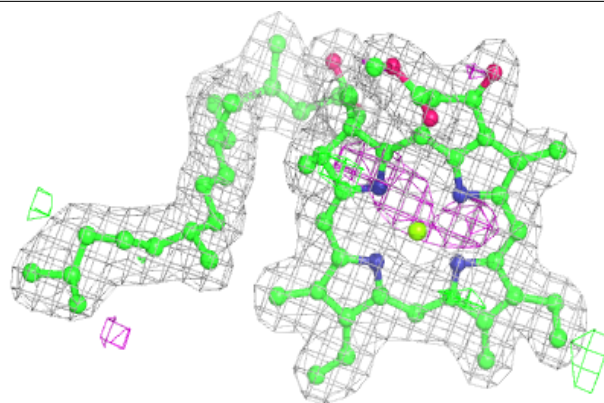
**Electron density around CLA B 617:**

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

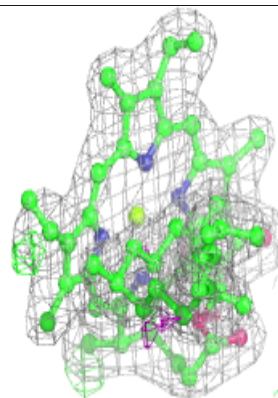
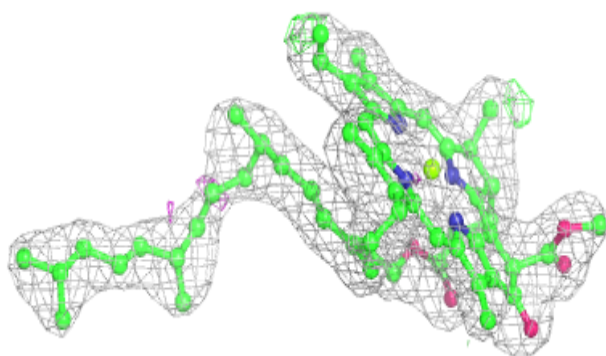
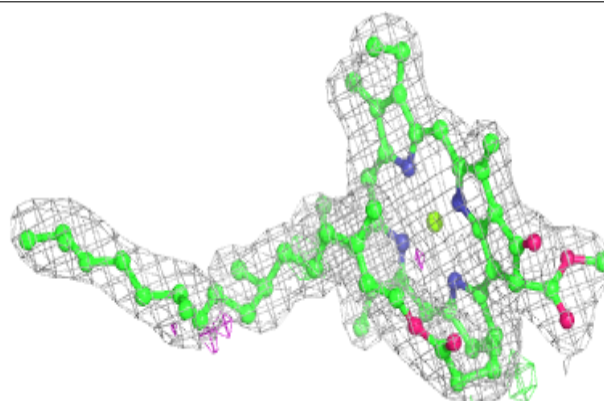


**Electron density around CLA d 401:**

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

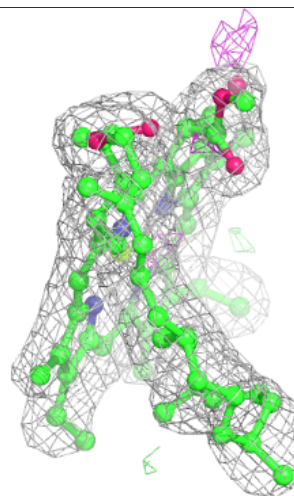
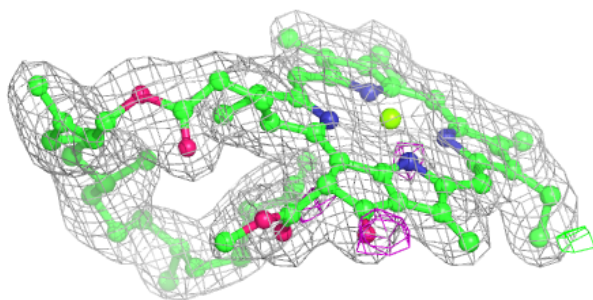
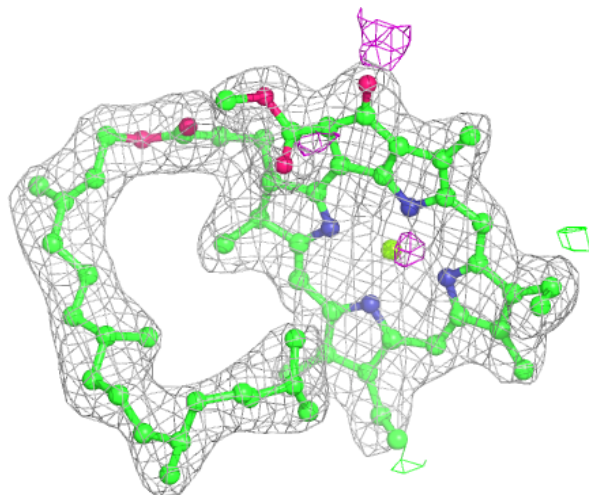
**Electron density around CLA C 505:**

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



**Electron density around CLA B 616:**

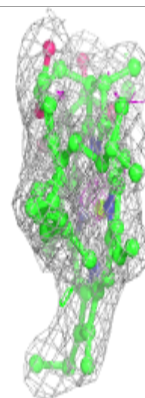
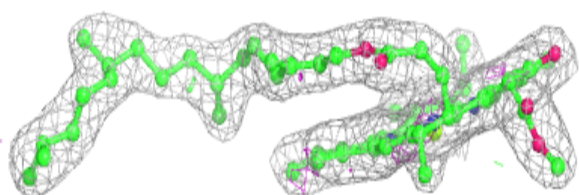
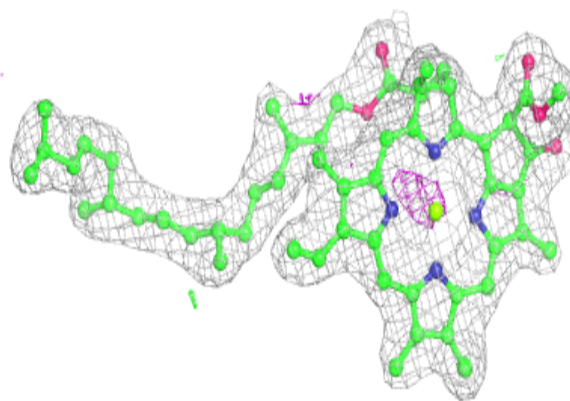
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



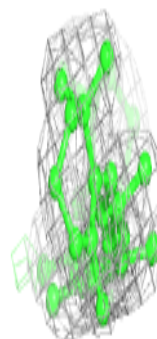
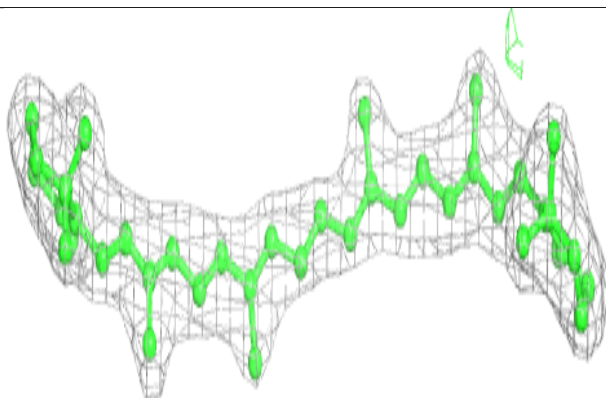
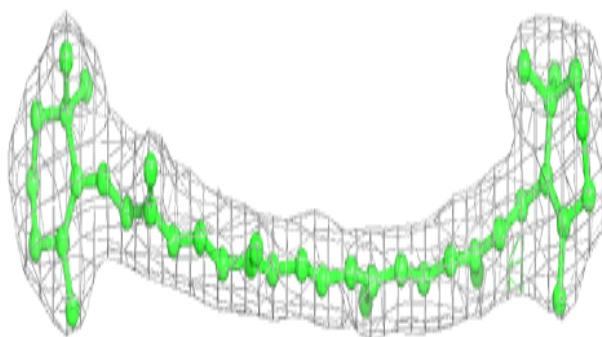


**Electron density around CLA b 612:**

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

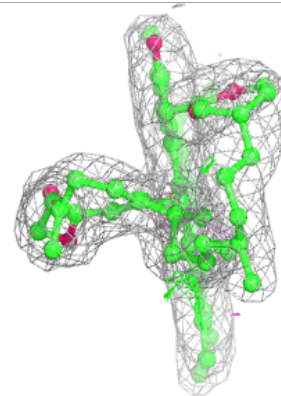
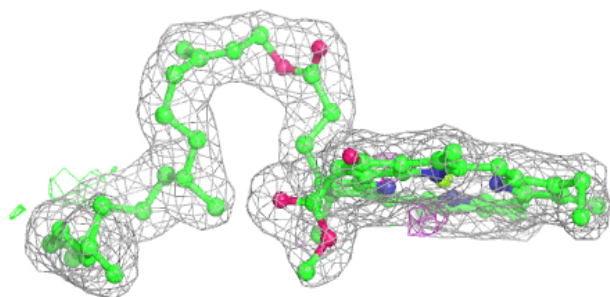
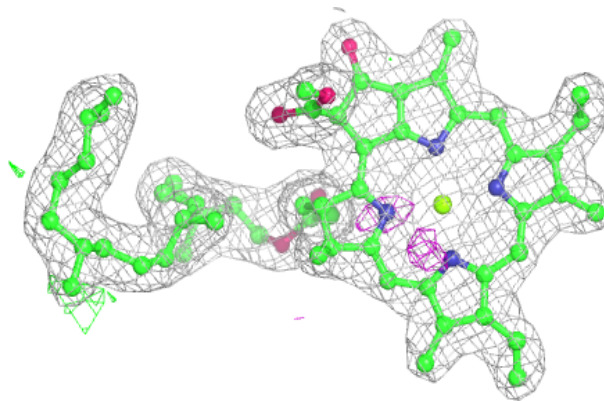
**Electron density around BCR K 101:**

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



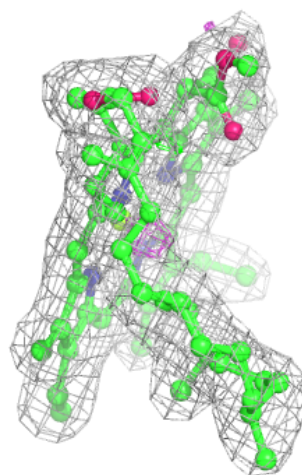
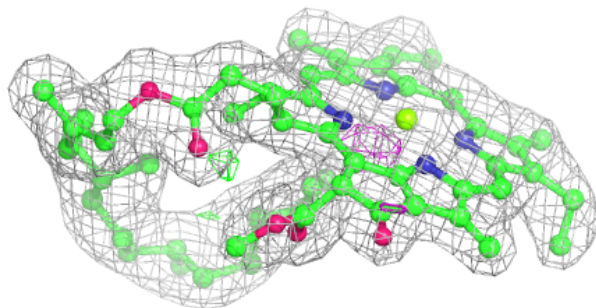
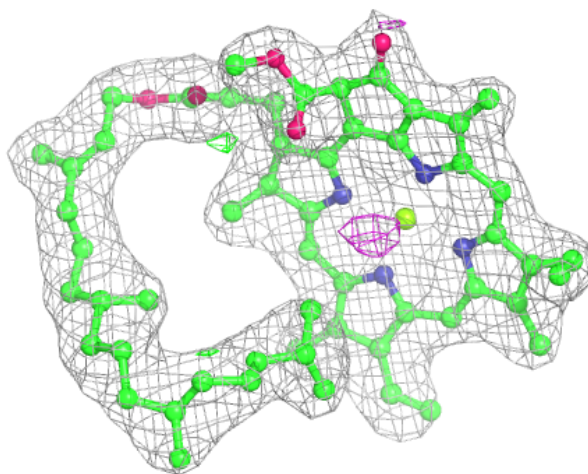
**Electron density around CLA b 621:**

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



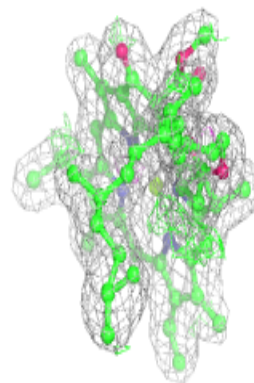
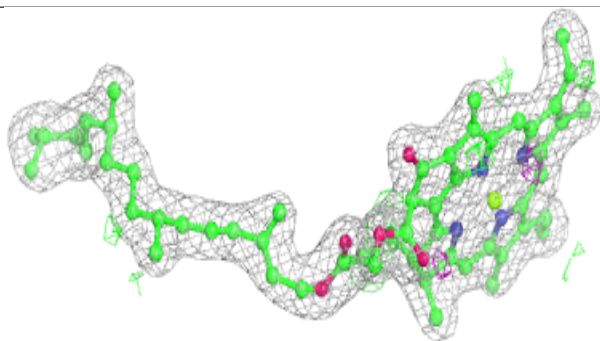
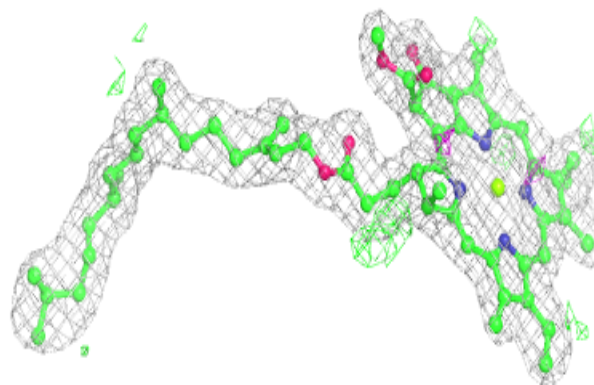
**Electron density around CLA b 624:**

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

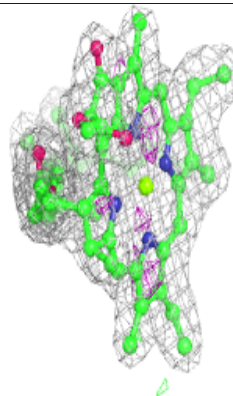
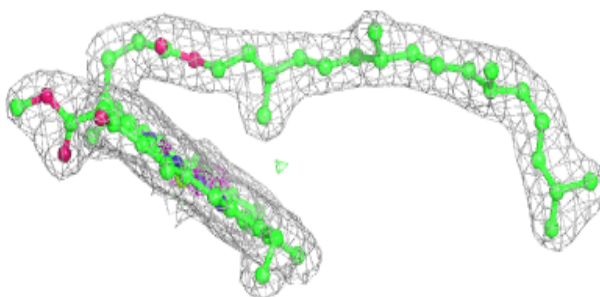
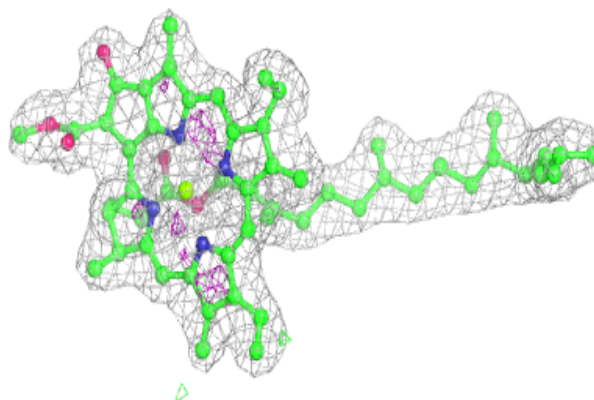


**Electron density around CLA A 405:**

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

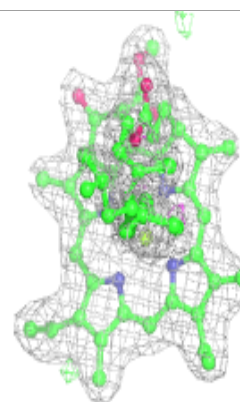
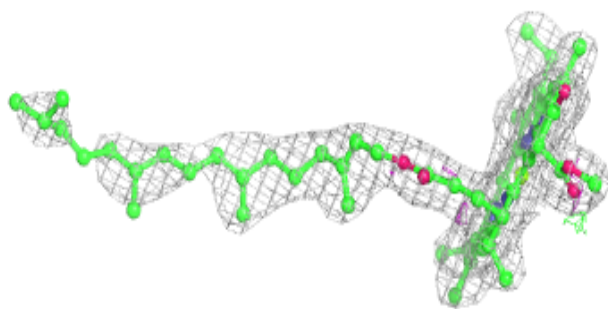
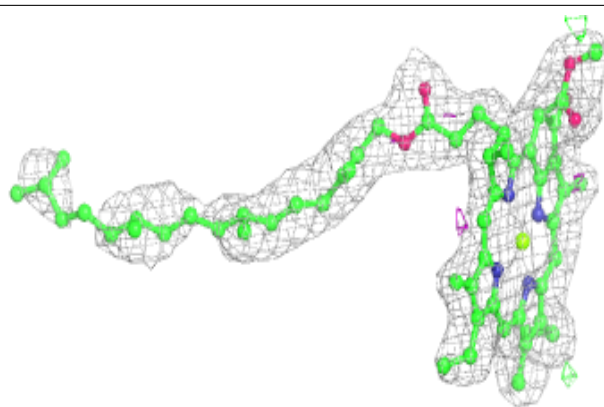
**Electron density around CLA b 617:**

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

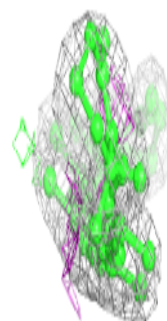
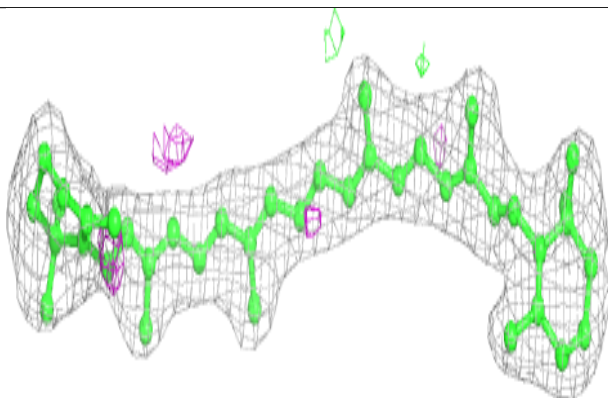
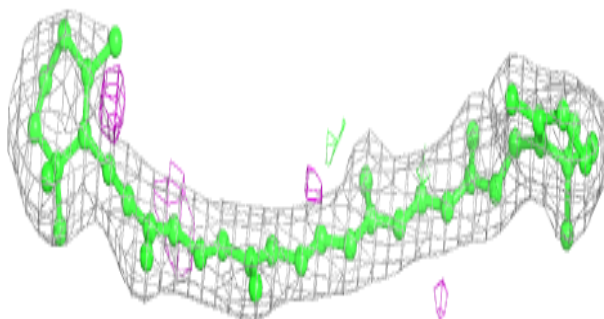


**Electron density around CLA d 403:**

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

**Electron density around BCR D 404:**

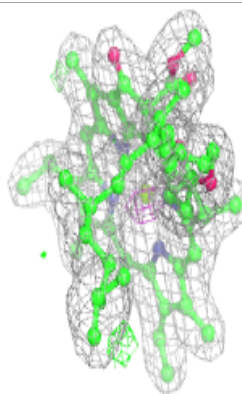
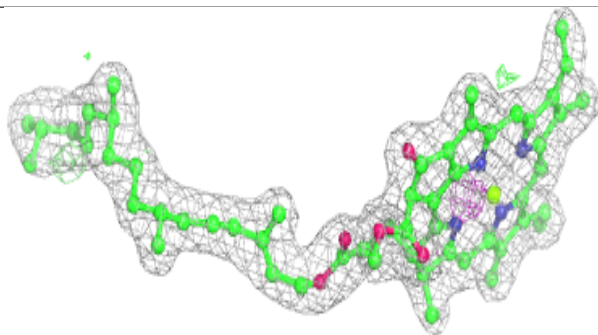
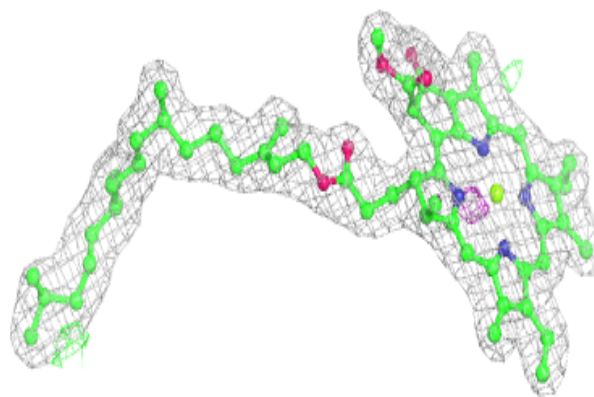
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



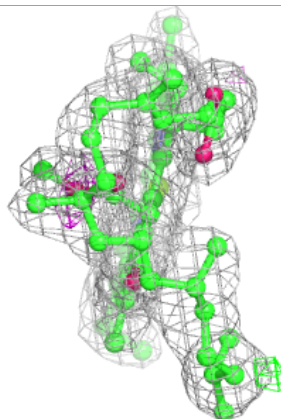
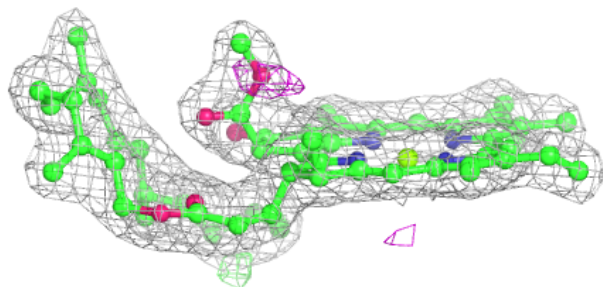
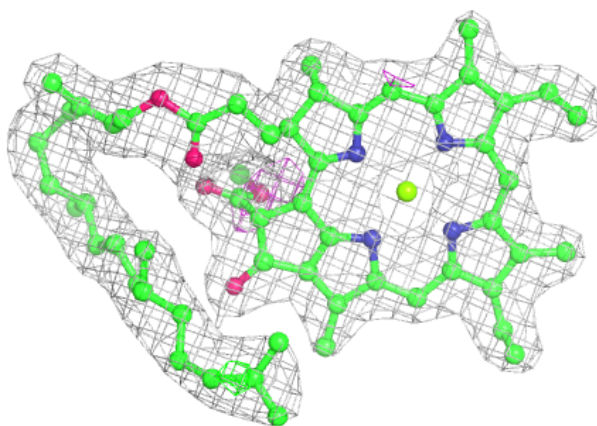


**Electron density around CLA a 409:**

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

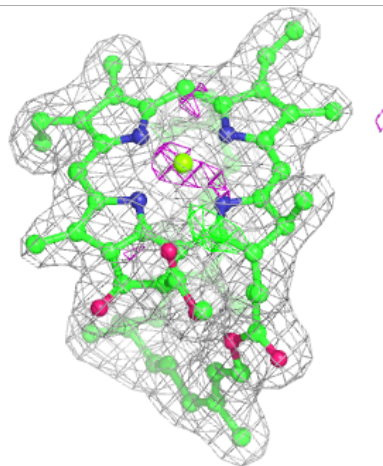
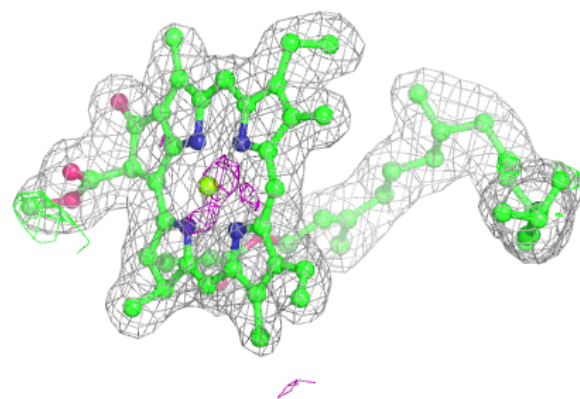
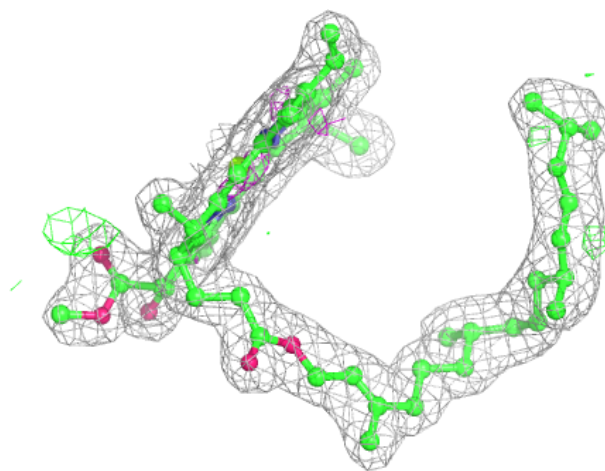
**Electron density around CLA b 619:**

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



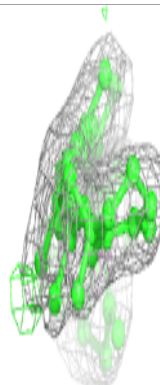
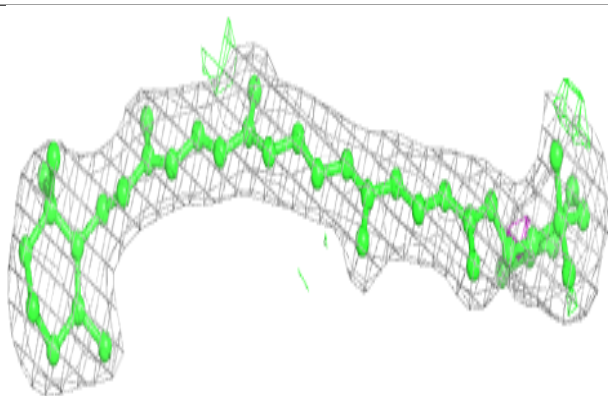
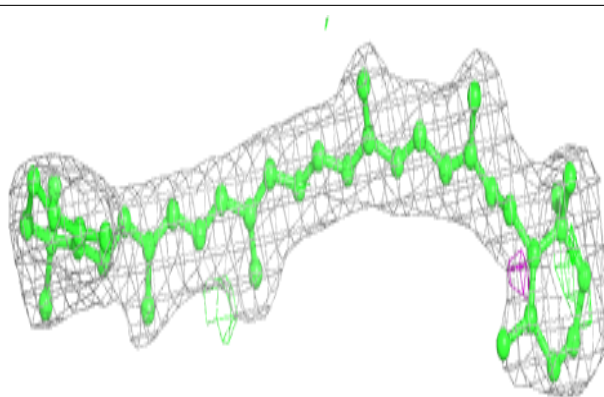
**Electron density around CLA b 620:**

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

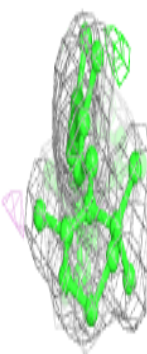
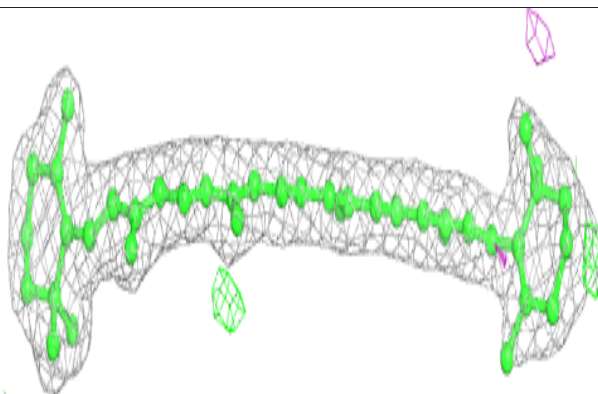
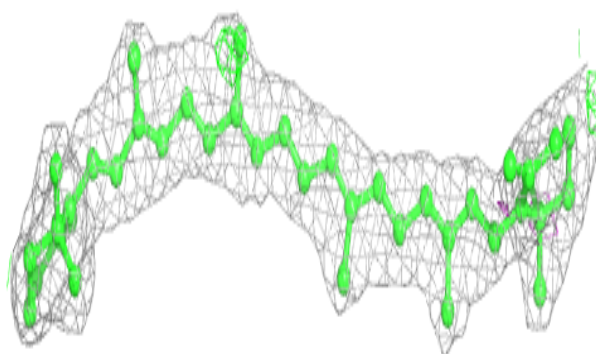


**Electron density around BCR d 404:**

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

**Electron density around BCR H 101:**

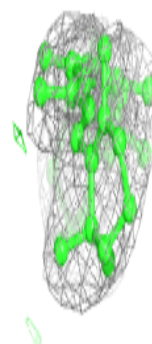
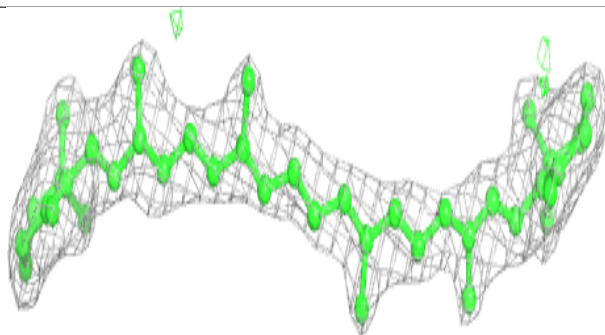
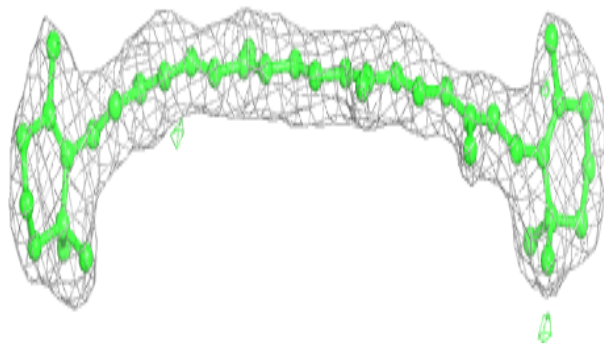
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



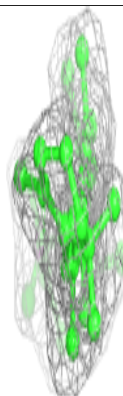
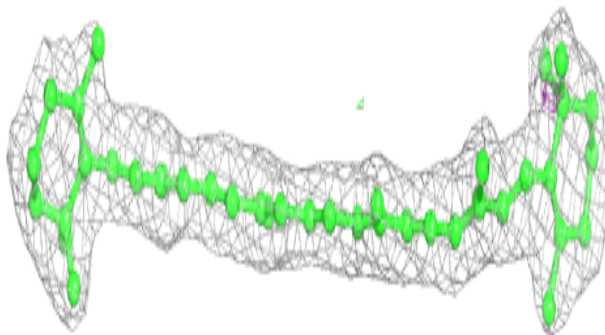
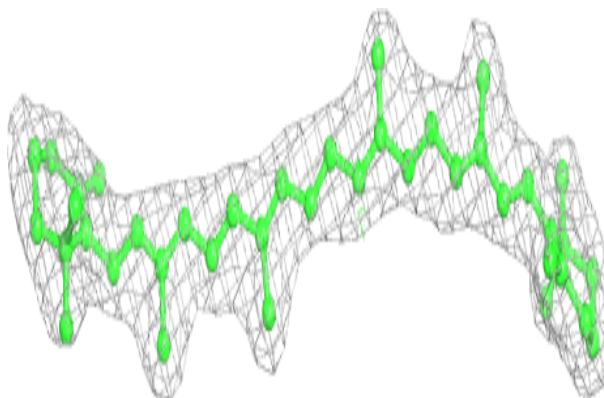


**Electron density around BCR k 101:**

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

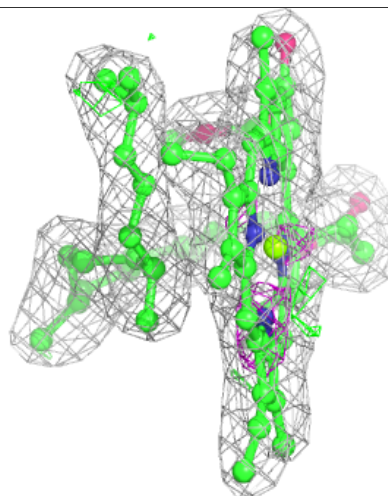
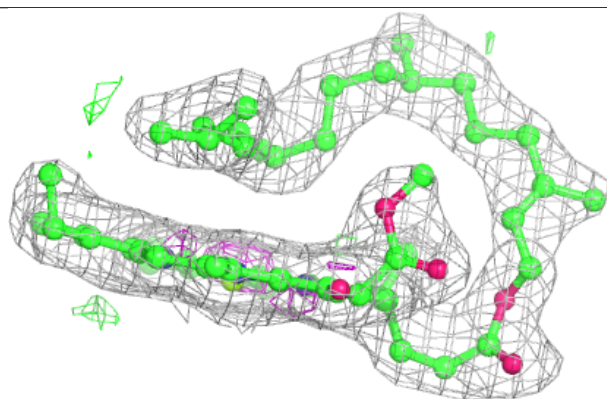
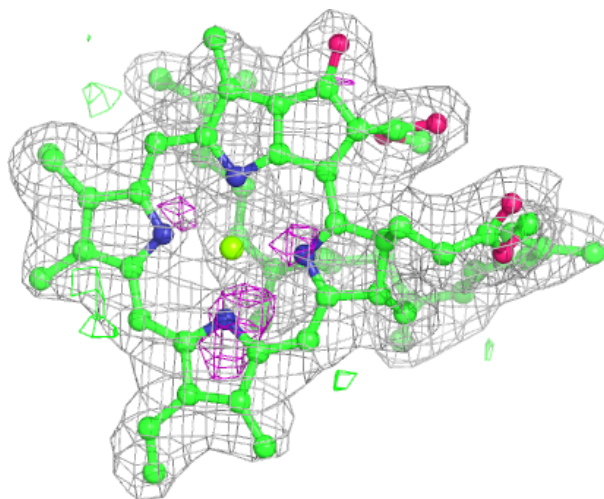
**Electron density around BCR h 101:**

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



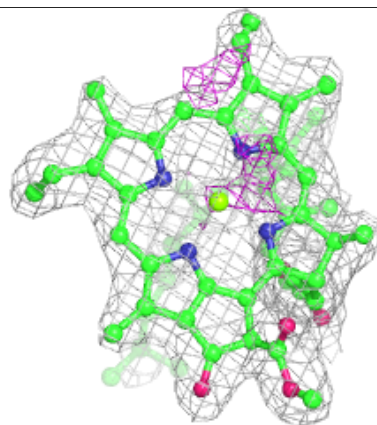
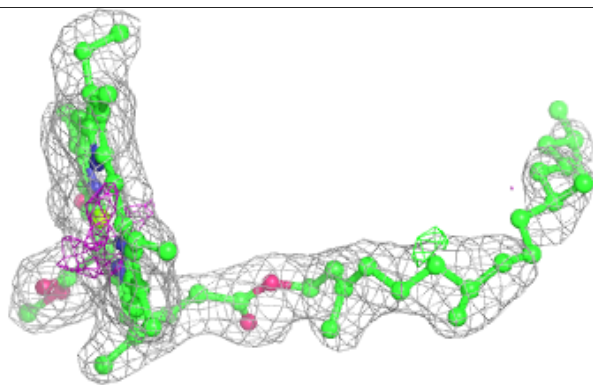
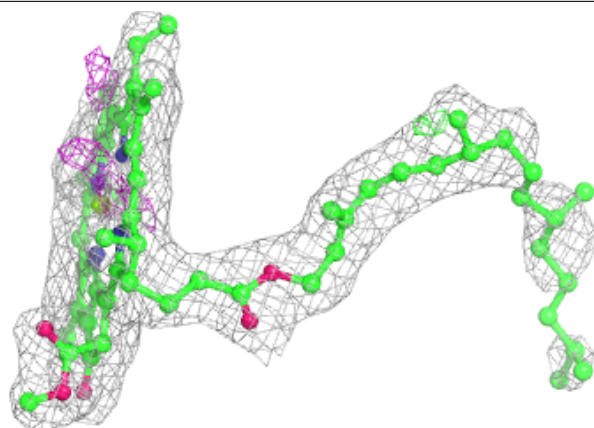
**Electron density around CLA C 510:**

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

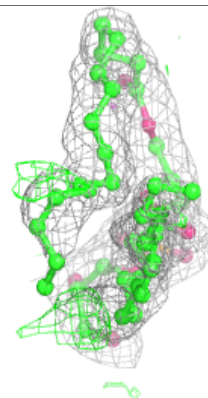
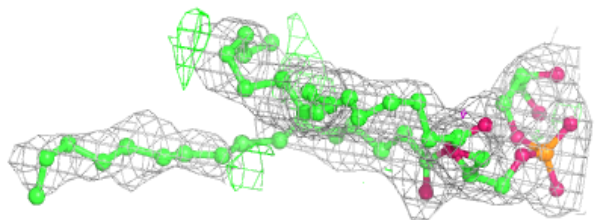
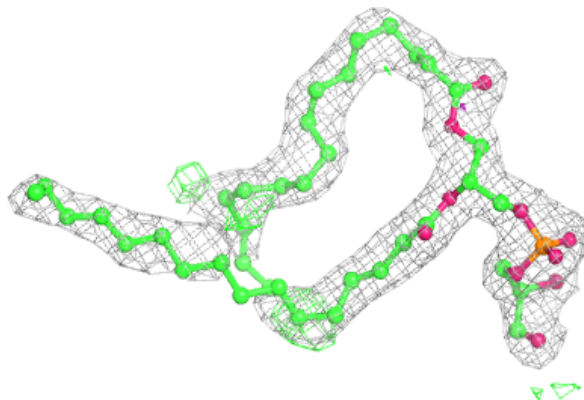


**Electron density around CLA D 403:**

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

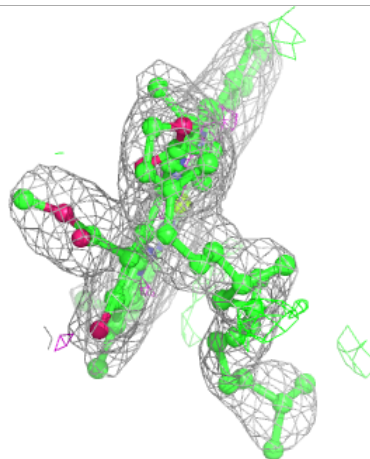
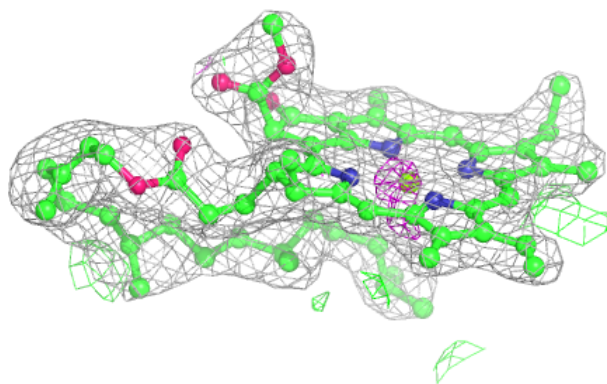
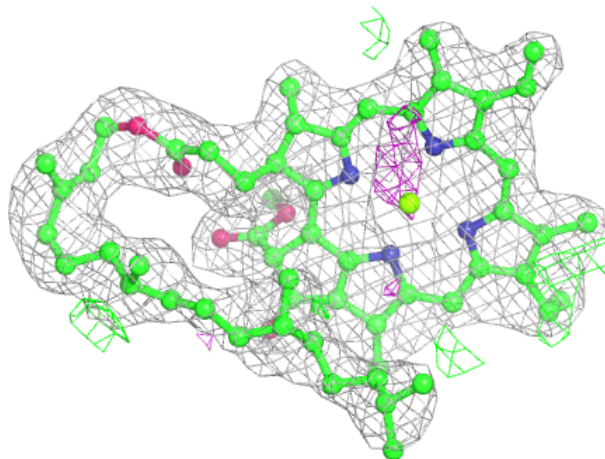
**Electron density around LHG d 408:**

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



**Electron density around CLA c 514:**

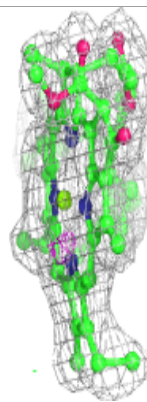
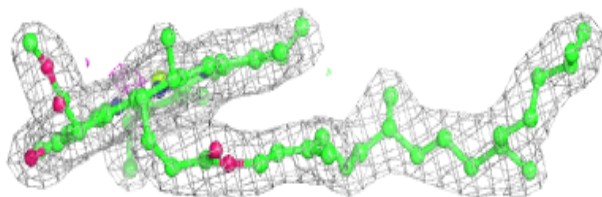
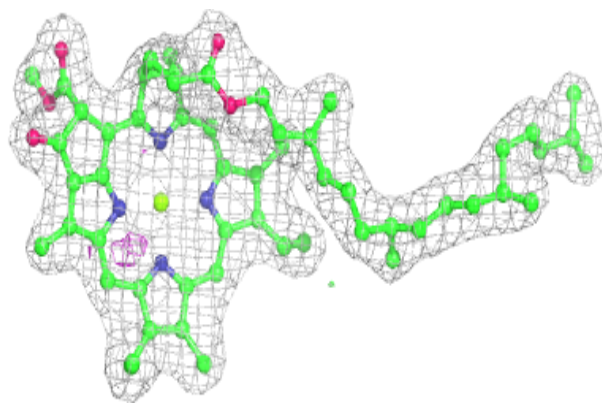
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



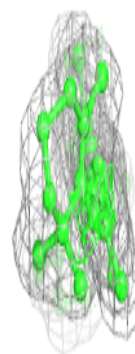
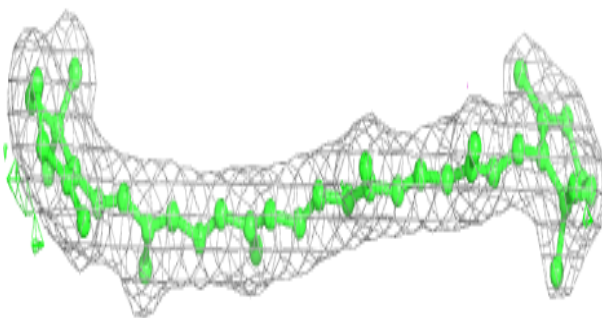
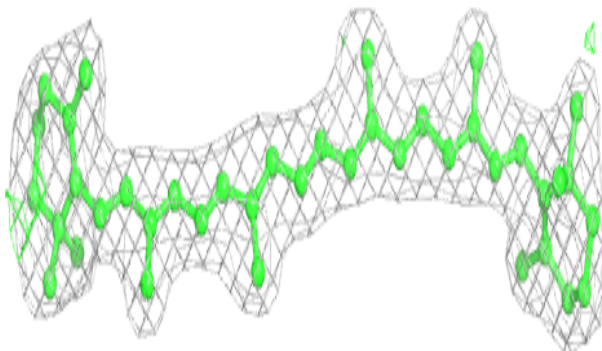


**Electron density around CLA B 604:**

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

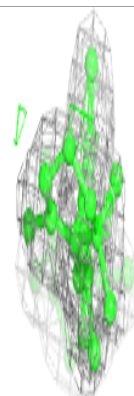
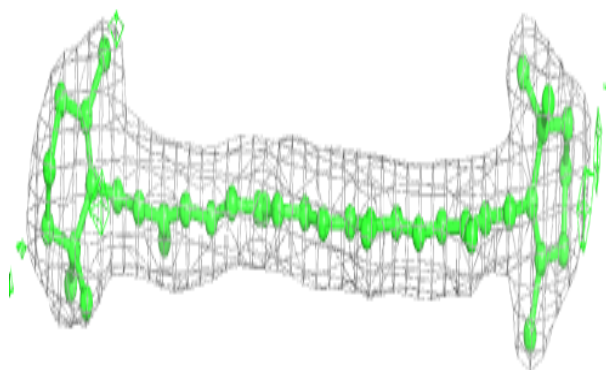
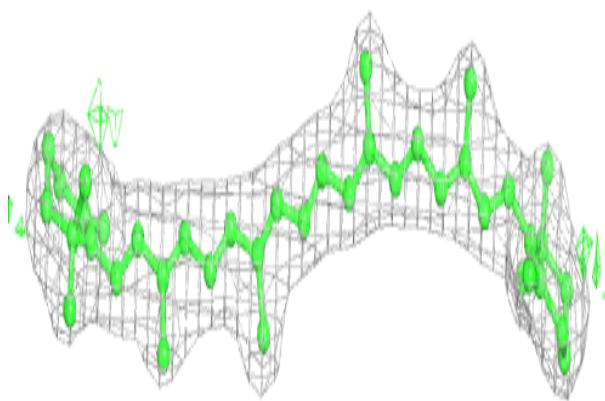
**Electron density around BCR B 620:**

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

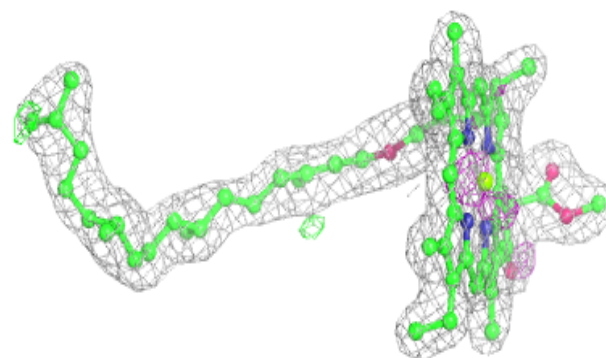
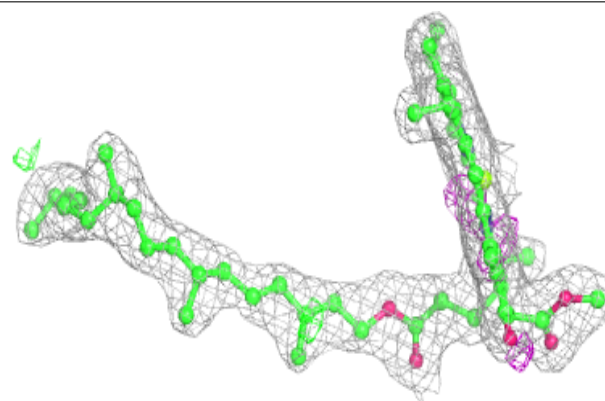


**Electron density around BCR C 515:**

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

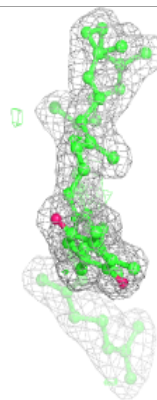
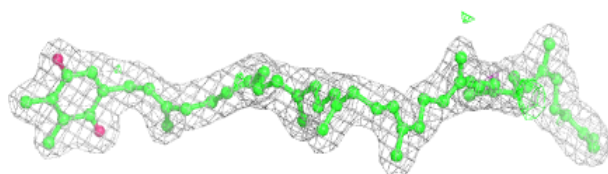
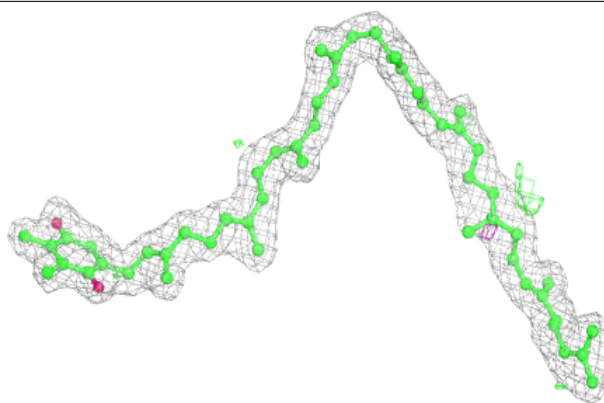
**Electron density around CLA b 614:**

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

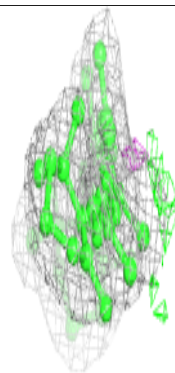
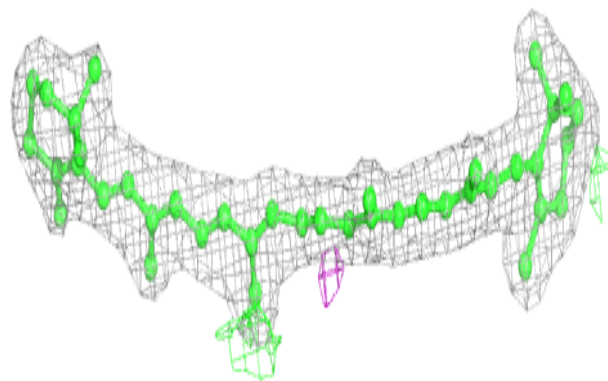
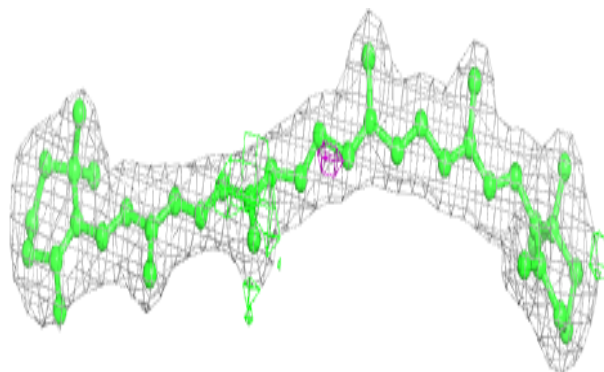


**Electron density around PL9 D 405 (A):**

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

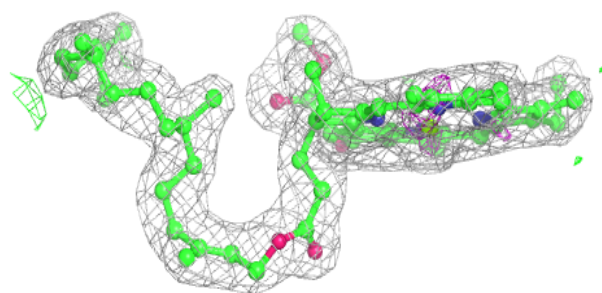
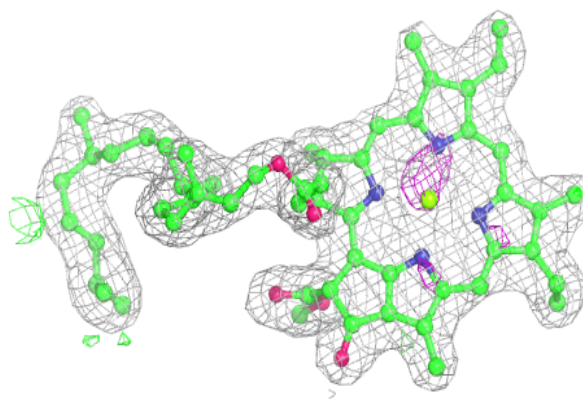
**Electron density around BCR t 101:**

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

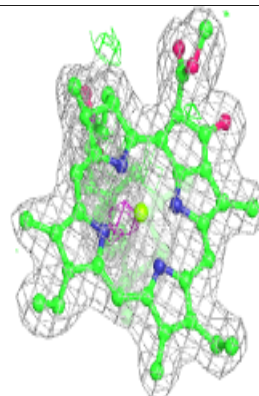
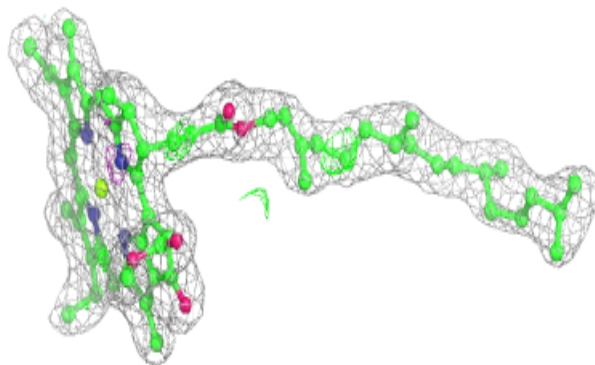
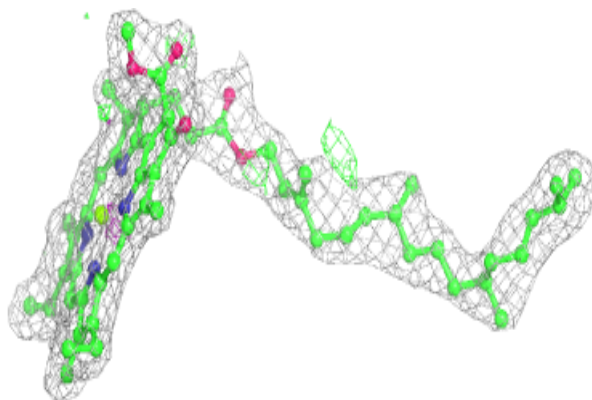


**Electron density around CLA B 613:**

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

**Electron density around CLA B 605:**

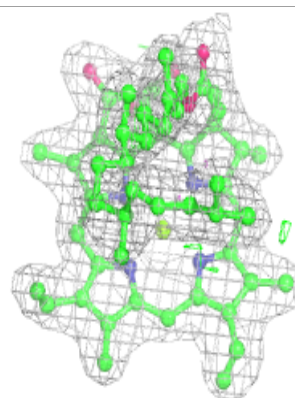
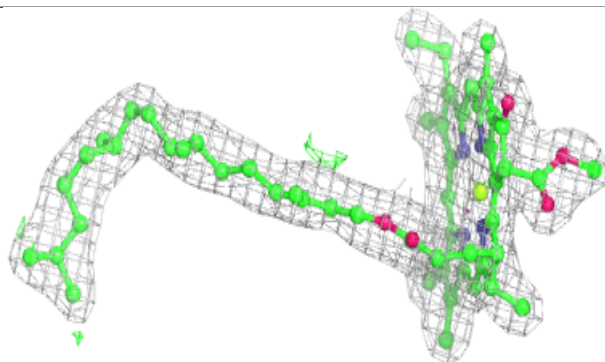
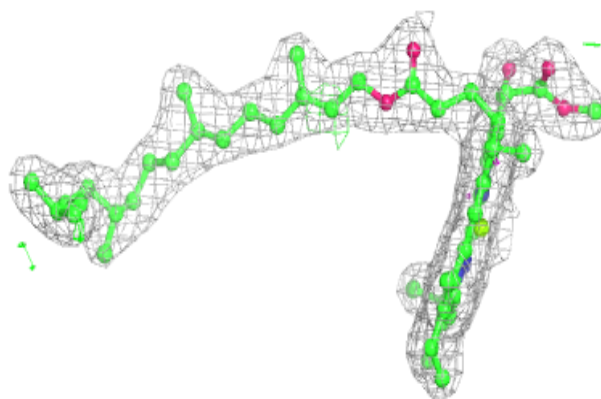
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





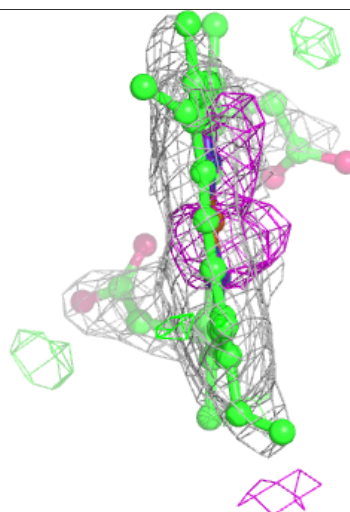
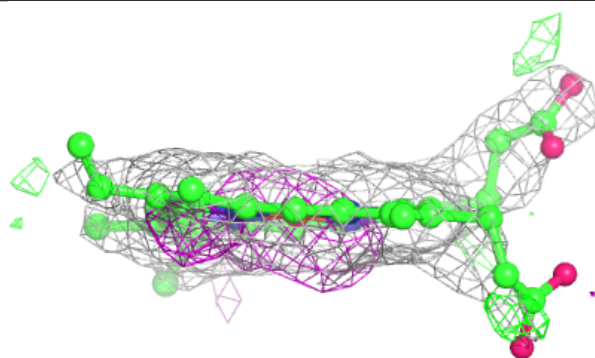
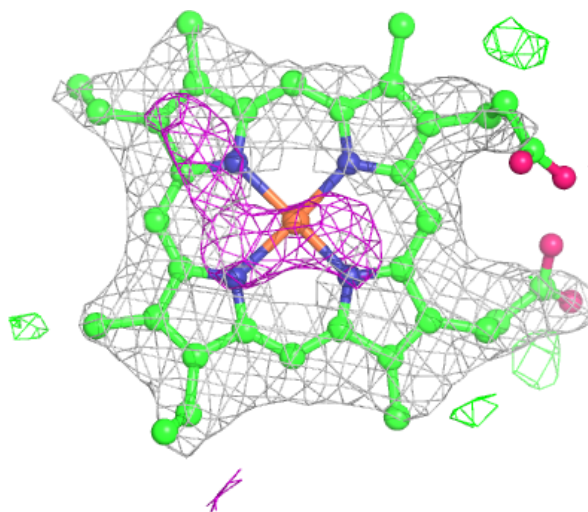
**Electron density around CLA B 606:**

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



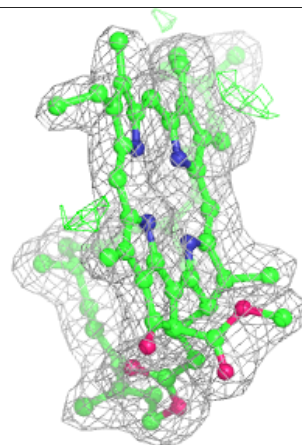
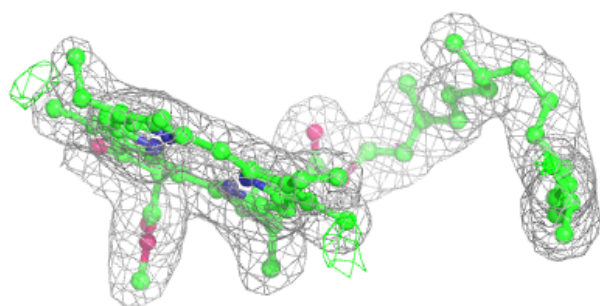
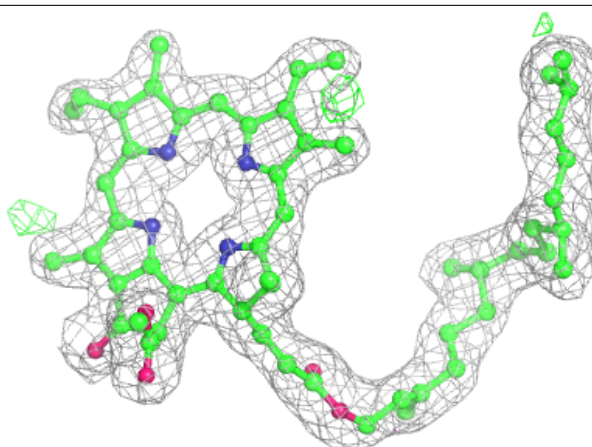
**Electron density around HEM e 103:**

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

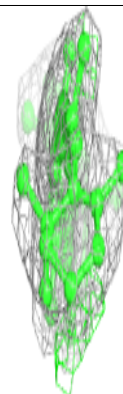
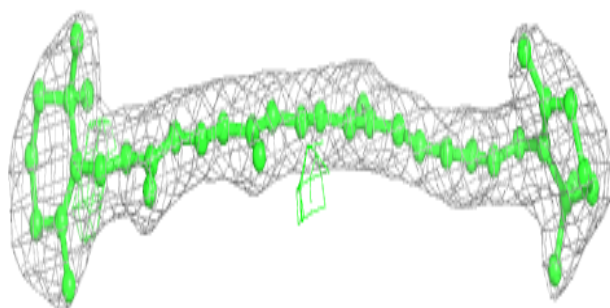
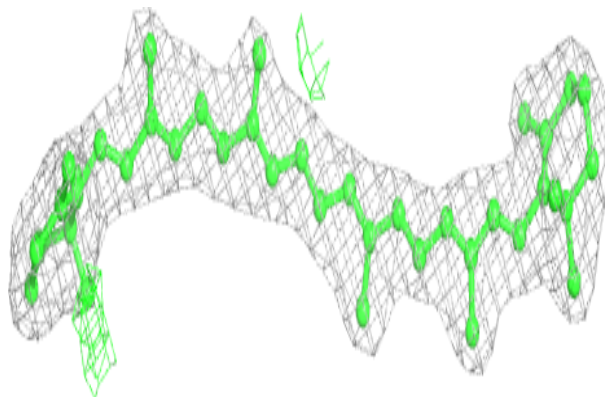


**Electron density around PHO A 409 (A):**

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

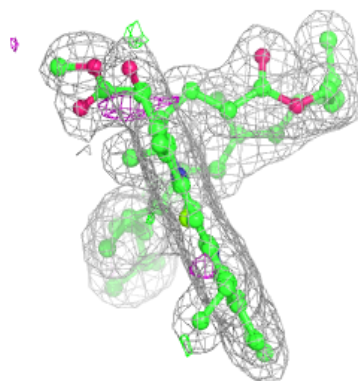
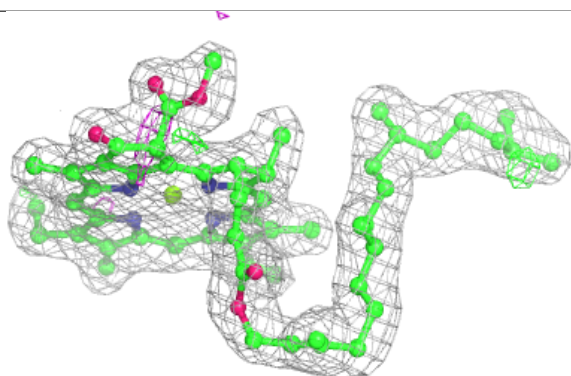
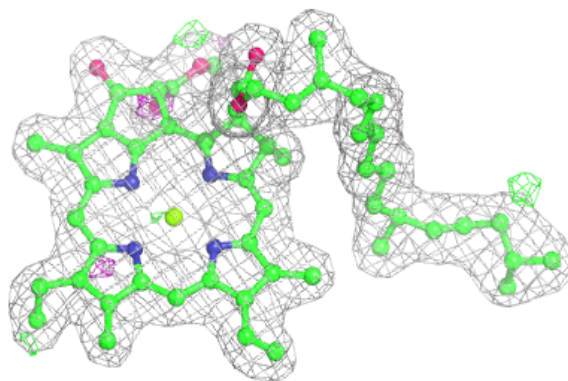
**Electron density around BCR Y 101:**

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

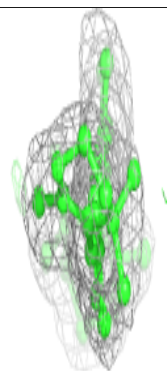
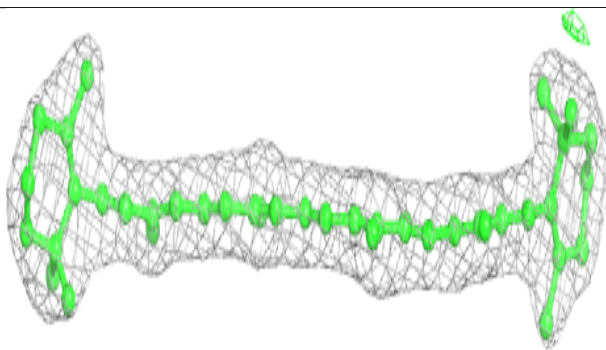
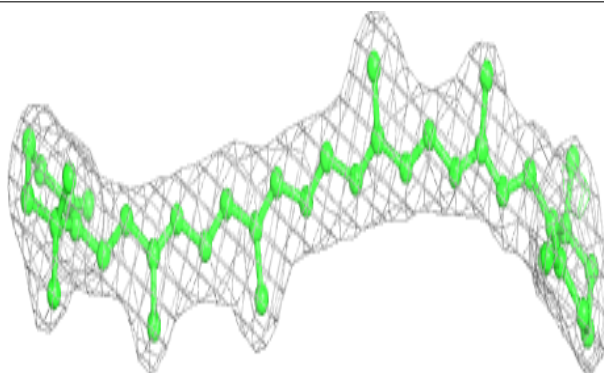


**Electron density around CLA A 406:**

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

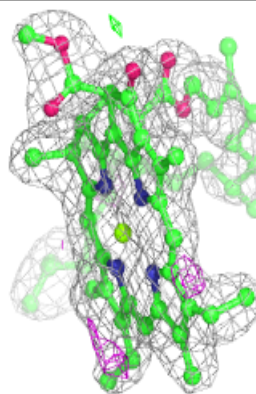
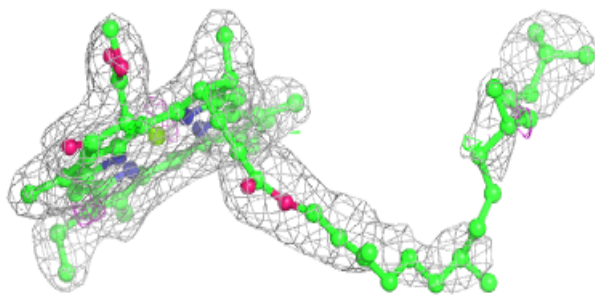
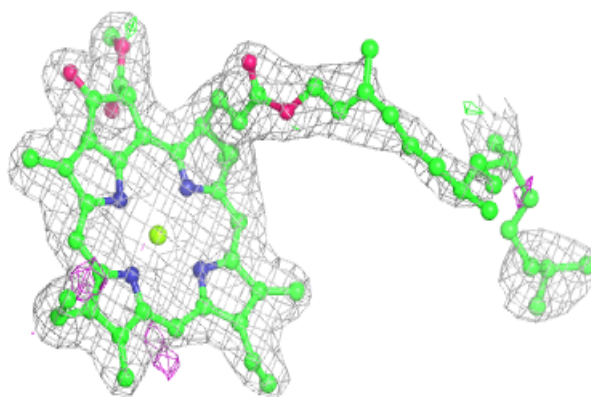
**Electron density around BCR c 519:**

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

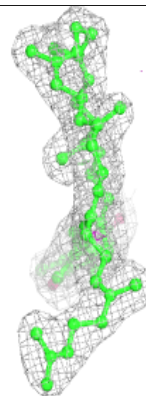
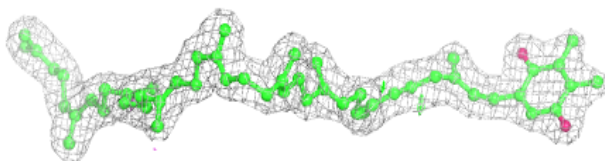
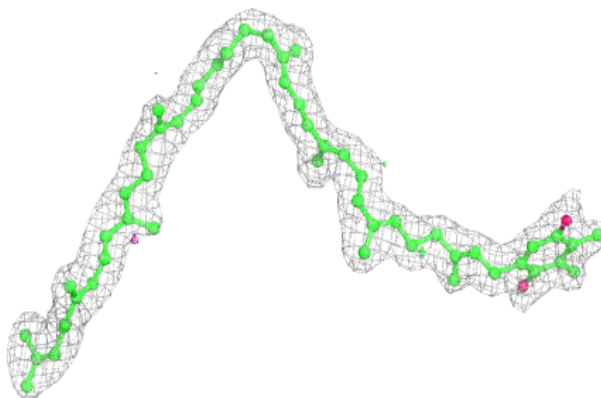


**Electron density around CLA a 412:**

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

**Electron density around PL9 d 405 (B):**

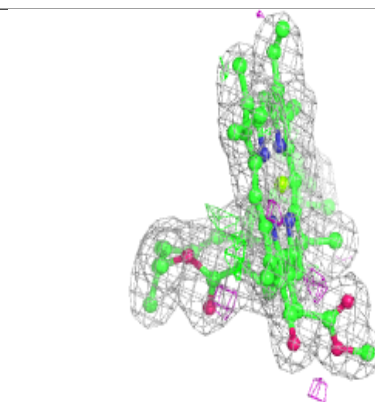
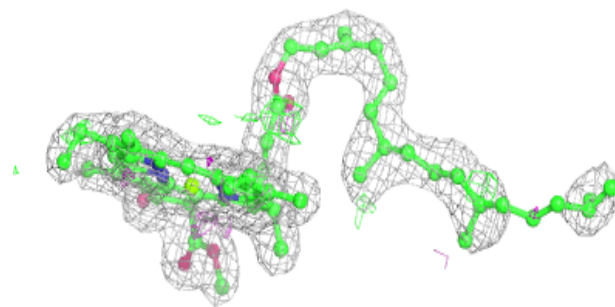
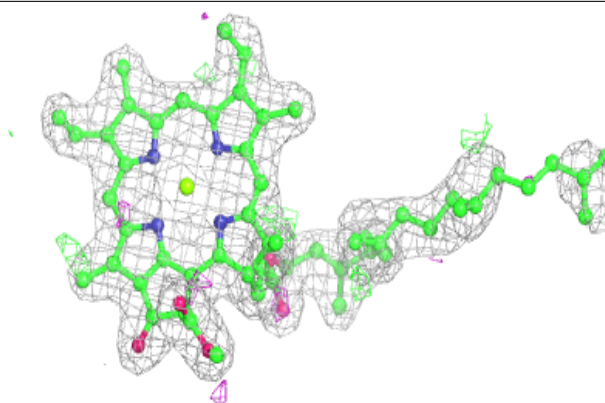
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



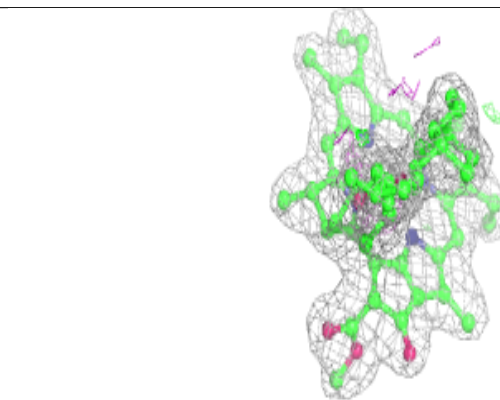
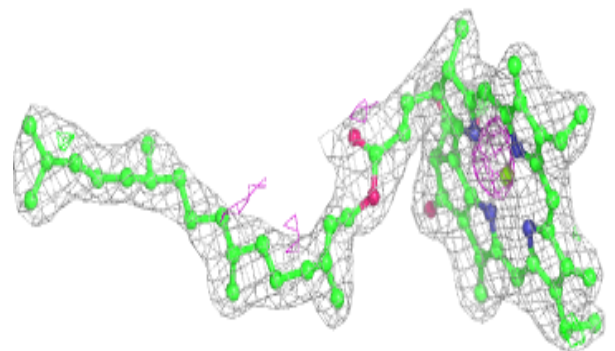
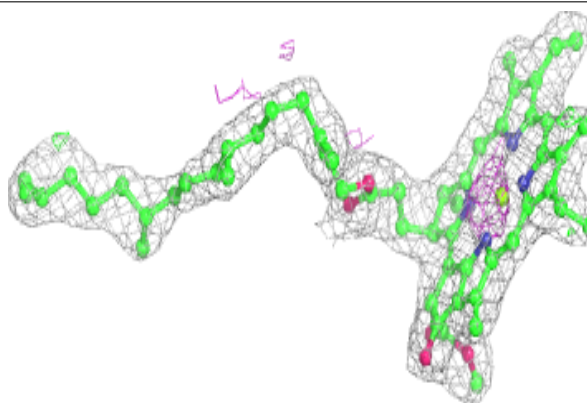


**Electron density around CLA A 407:**

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

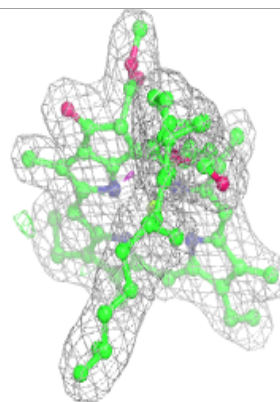
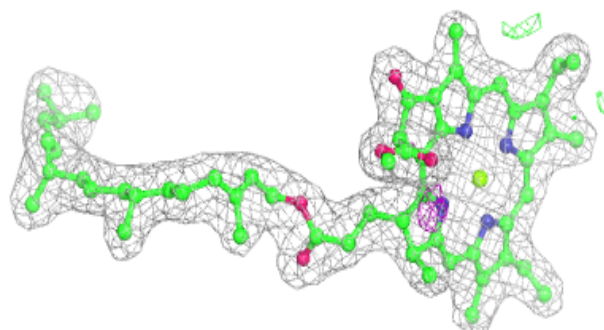
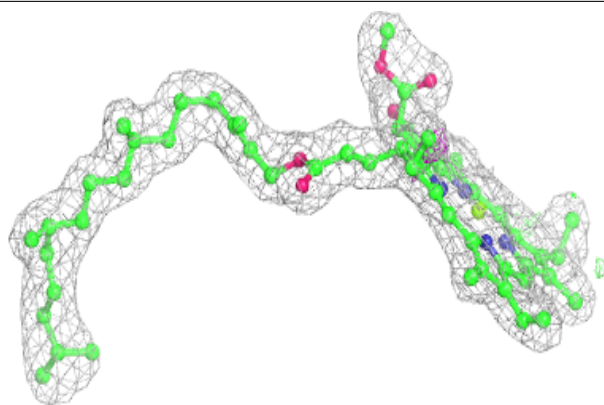
**Electron density around CLA c 507:**

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

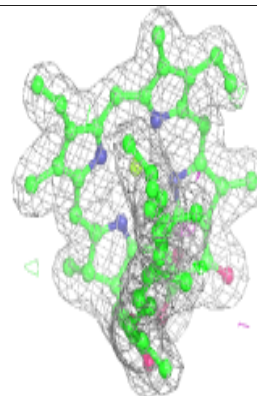
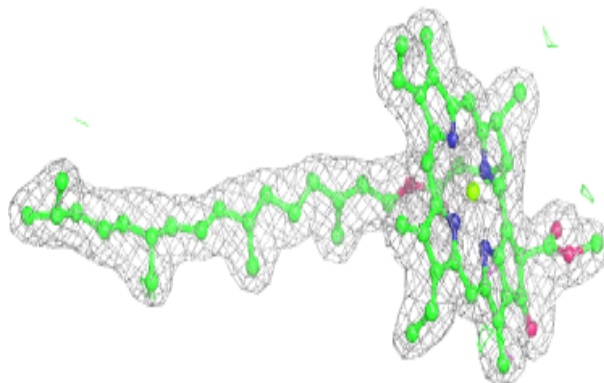
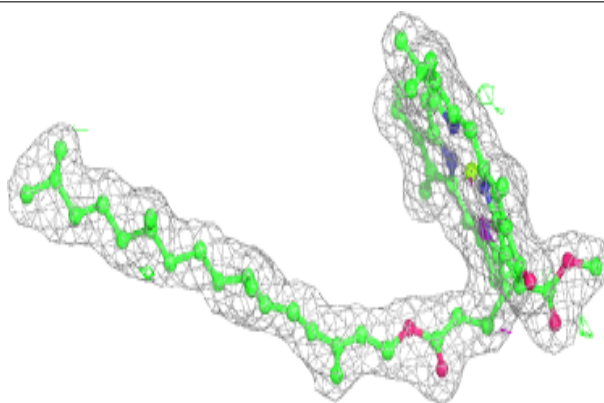


**Electron density around CLA d 402:**

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

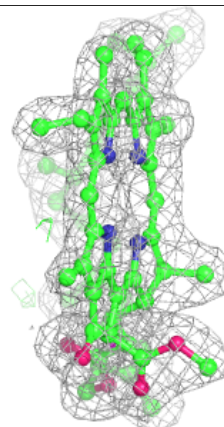
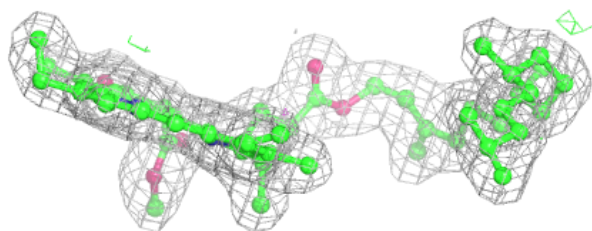
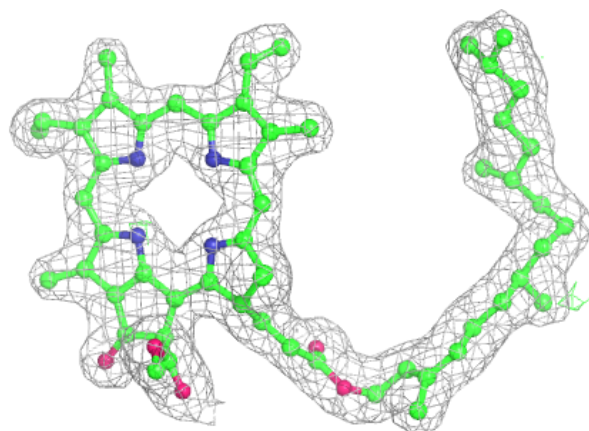
**Electron density around CLA B 608:**

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

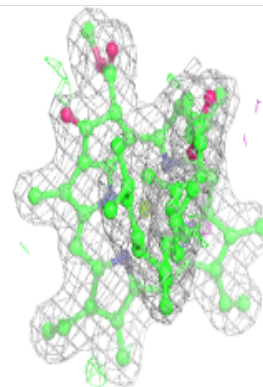
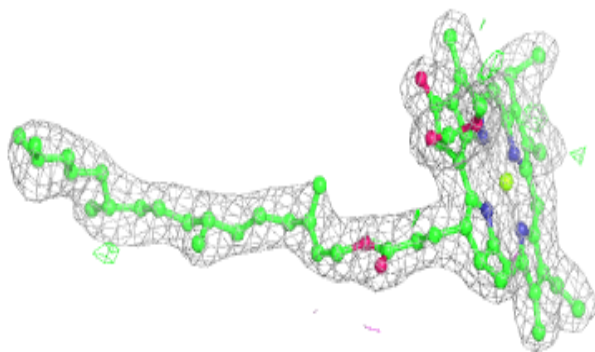
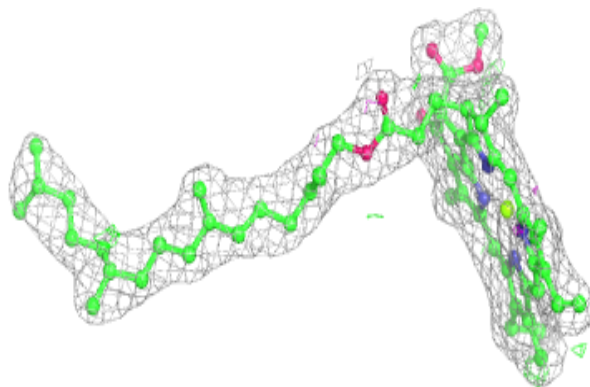


**Electron density around PHO A 408:**

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

**Electron density around CLA b 613:**

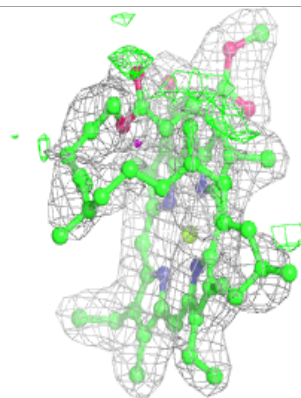
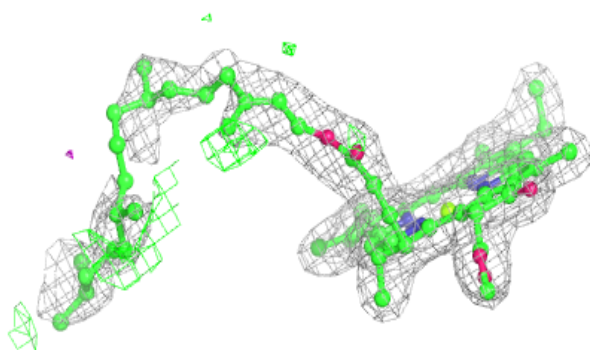
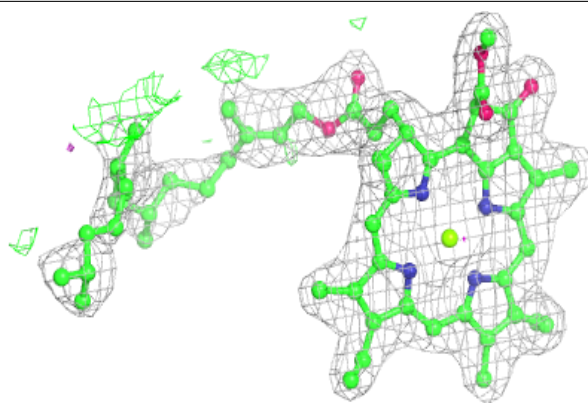
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



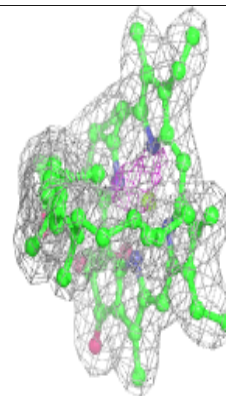
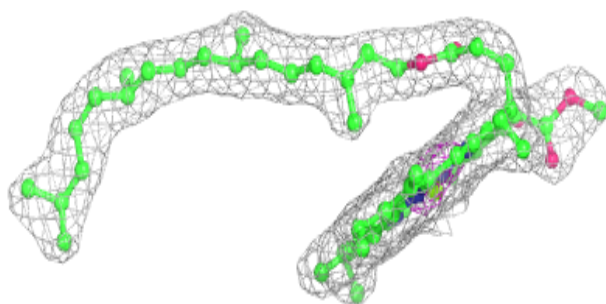
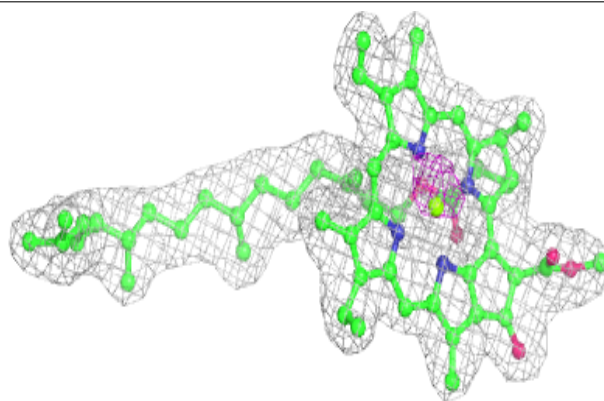


**Electron density around CLA A 410:**

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

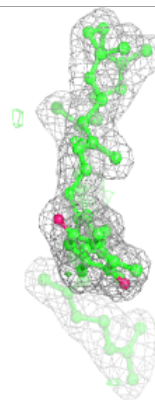
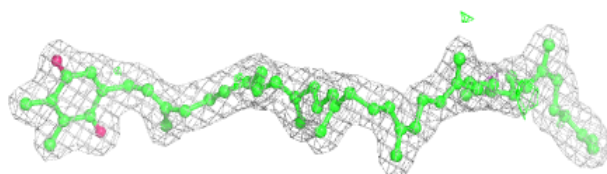
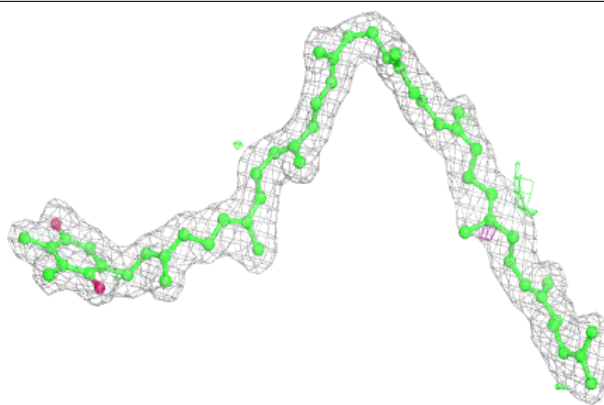
**Electron density around CLA B 609:**

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



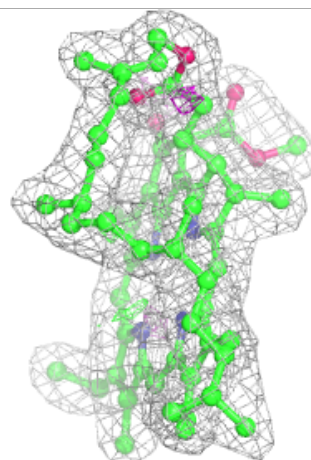
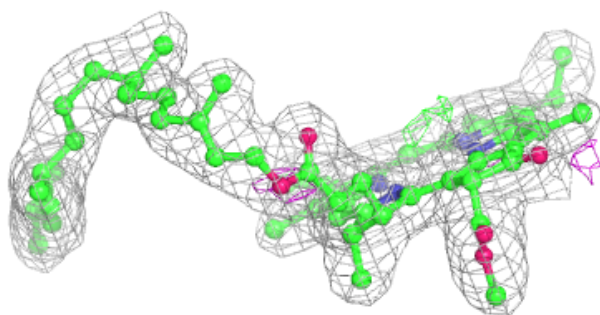
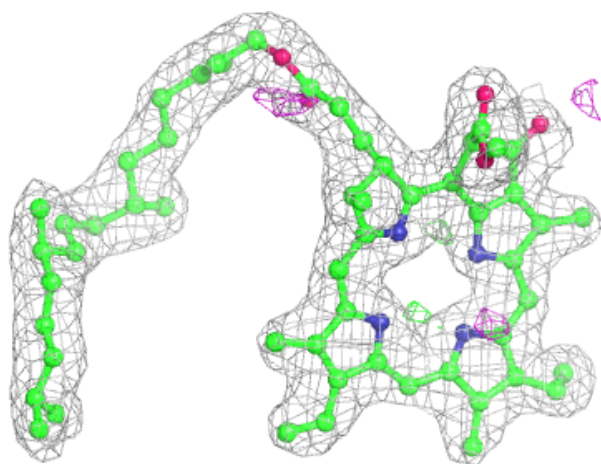
**Electron density around PL9 D 405 (B):**

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



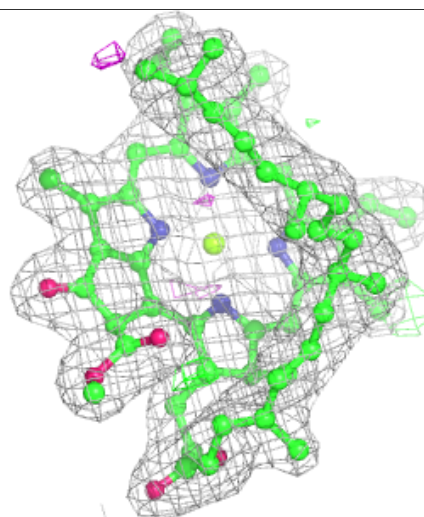
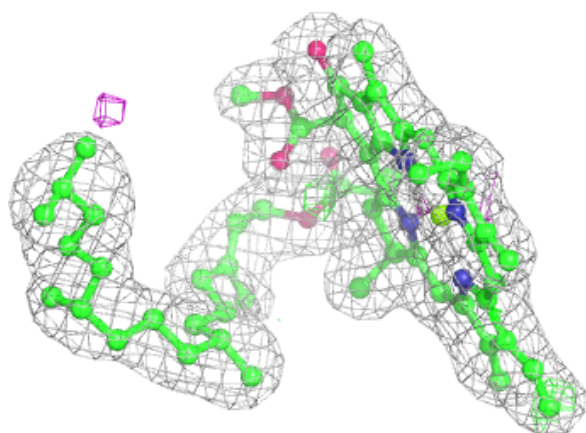
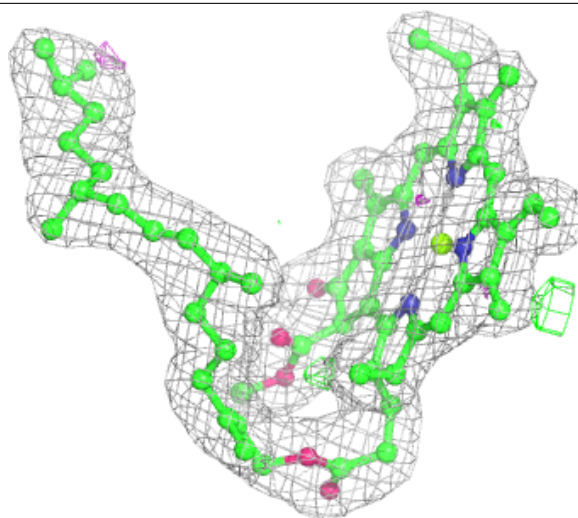
**Electron density around PHO a 418 (B):**

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



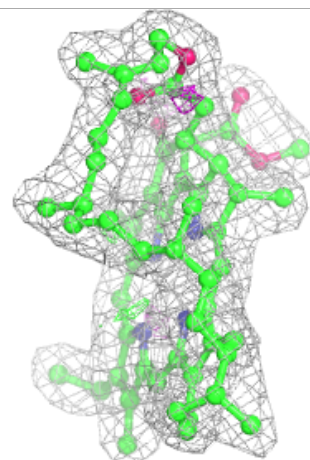
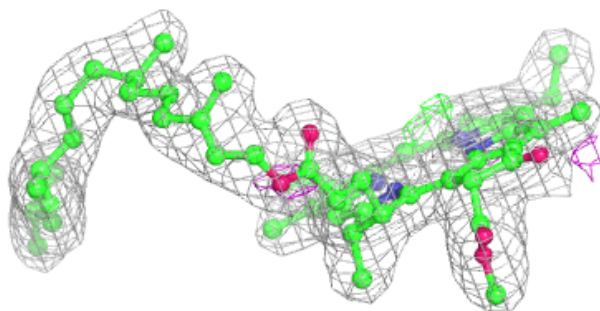
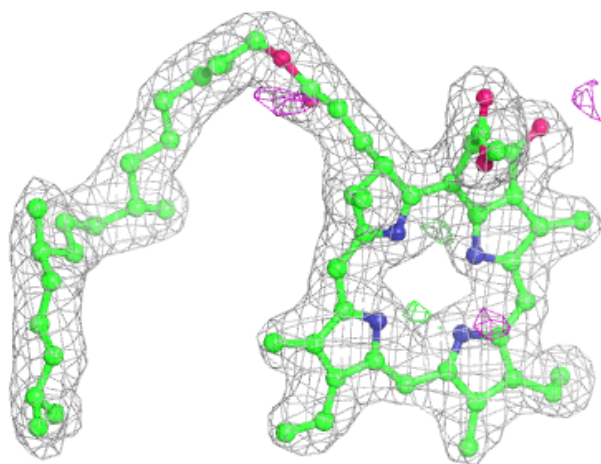
**Electron density around CLA b 622:**

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



**Electron density around PHO a 418 (A):**

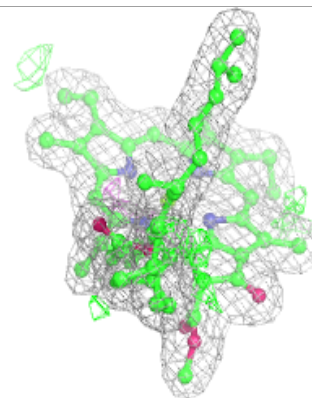
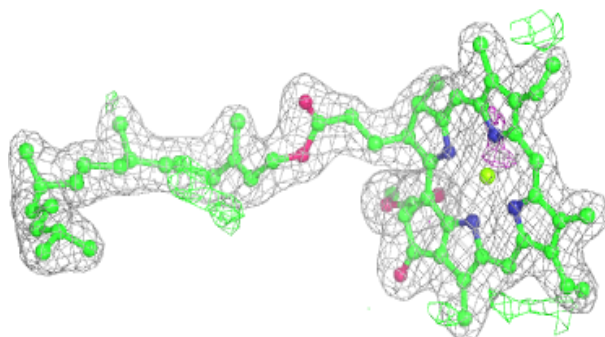
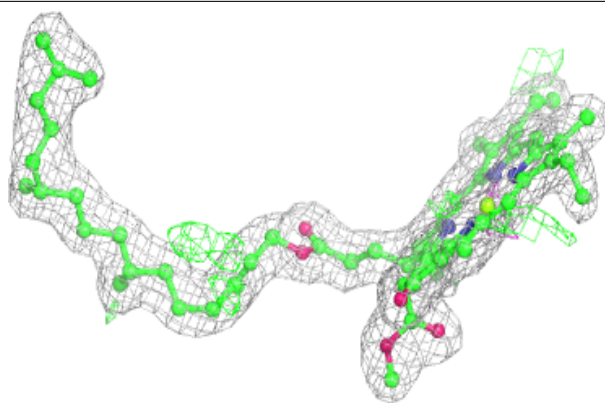
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



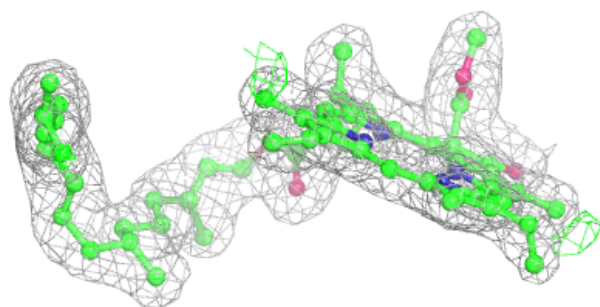
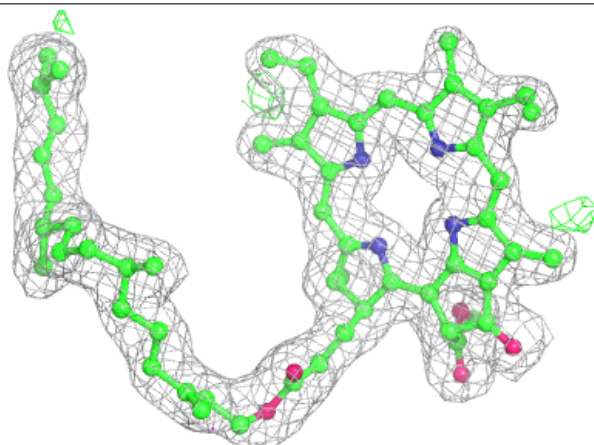


**Electron density around CLA D 402:**

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

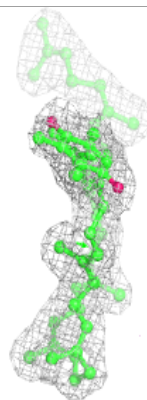
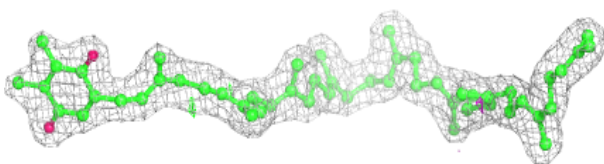
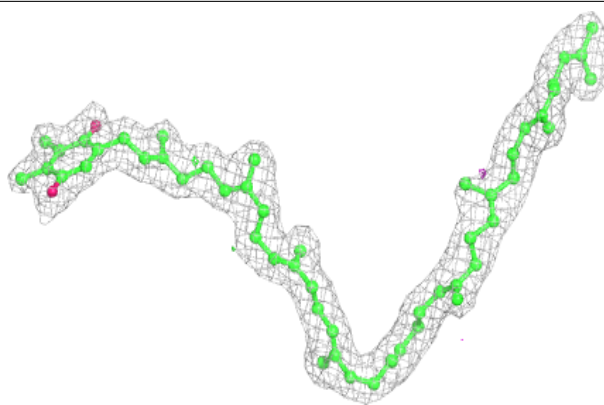
**Electron density around PHO A 409 (B):**

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

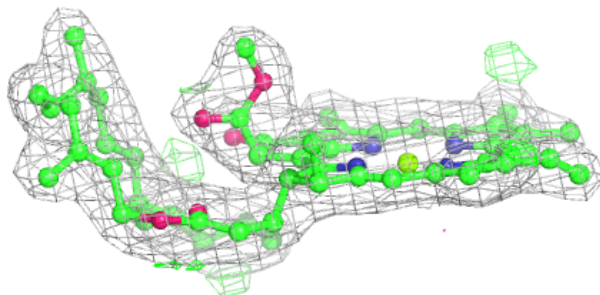
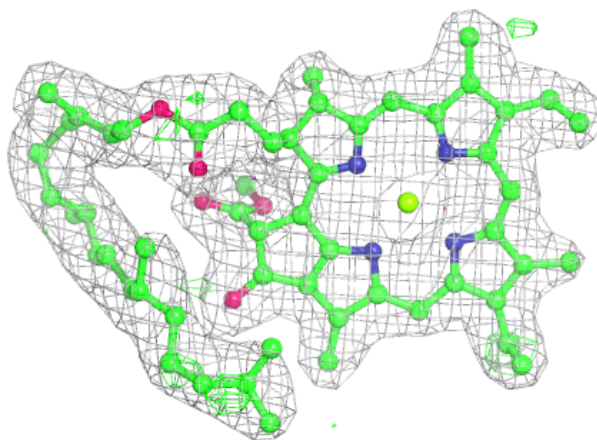


**Electron density around PL9 d 405 (A):**

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

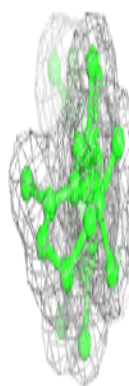
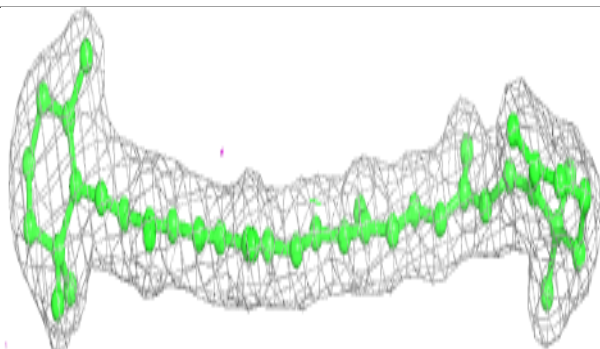
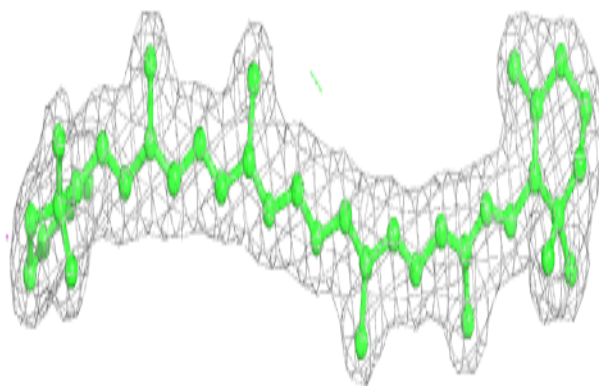
**Electron density around CLA B 611:**

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

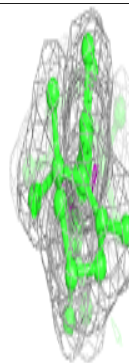
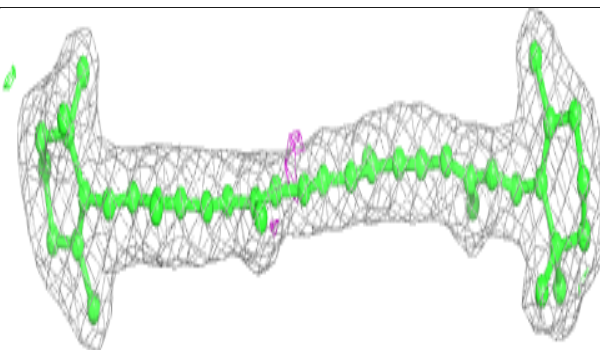
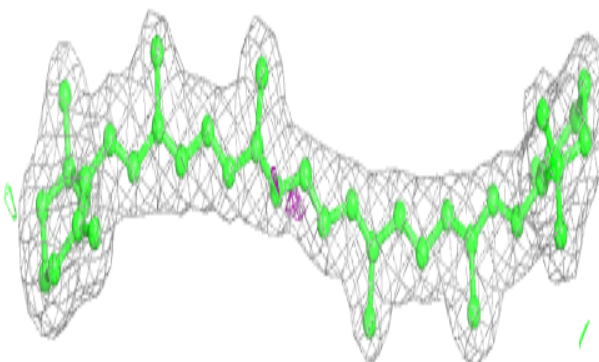


**Electron density around BCR B 618:**

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

**Electron density around BCR A 411:**

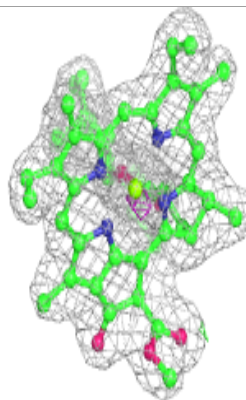
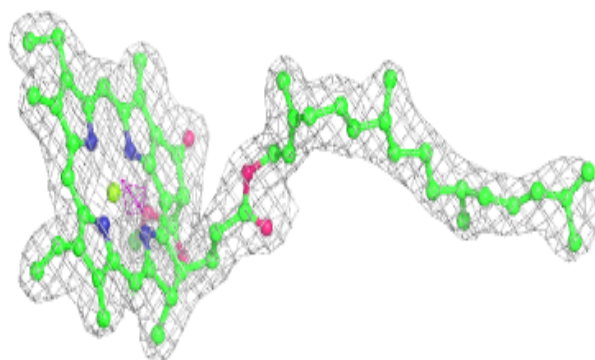
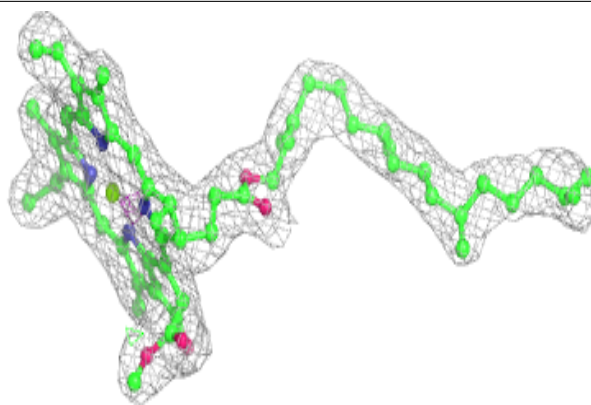
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



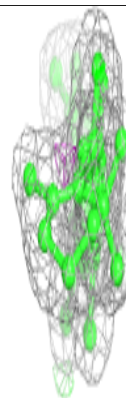
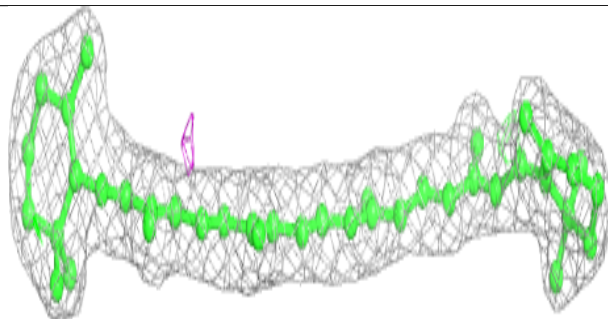
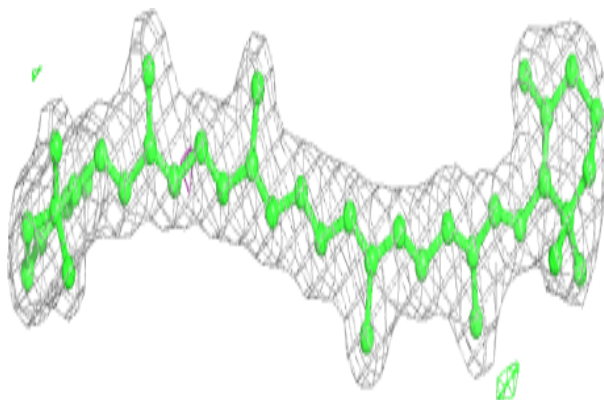


**Electron density around CLA C 502:**

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

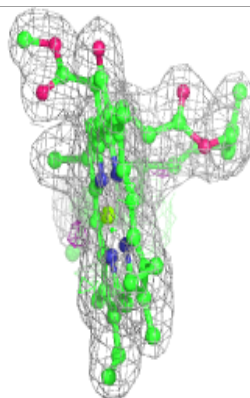
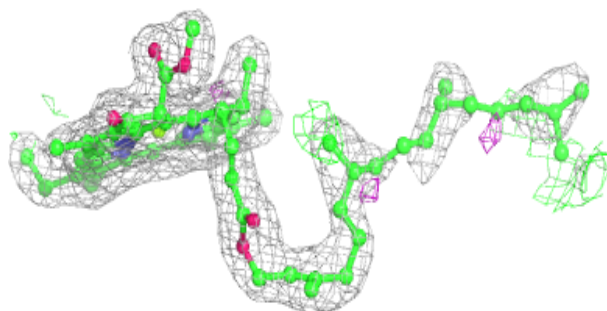
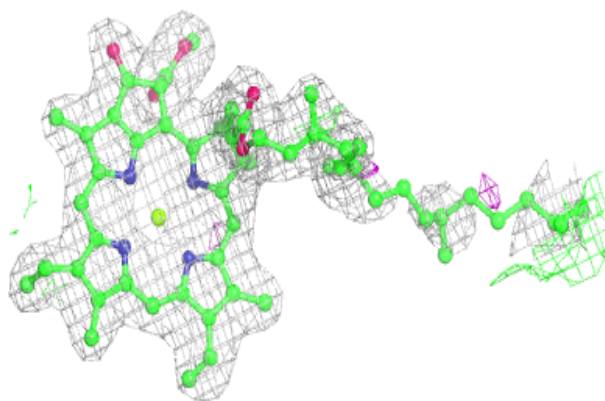
**Electron density around BCR b 626:**

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

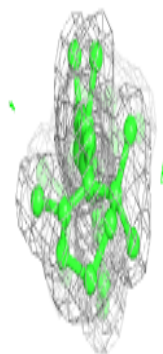
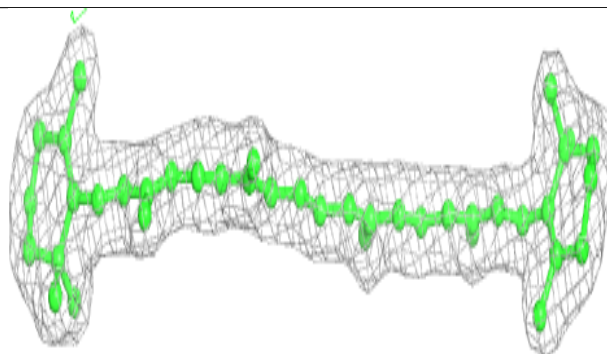
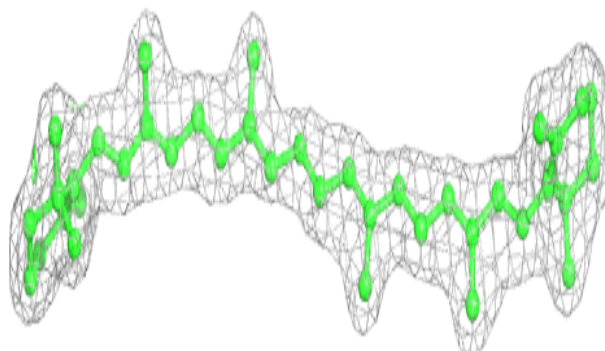


**Electron density around CLA a 410:**

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

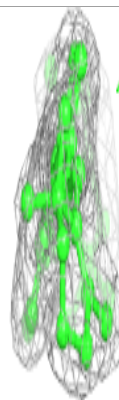
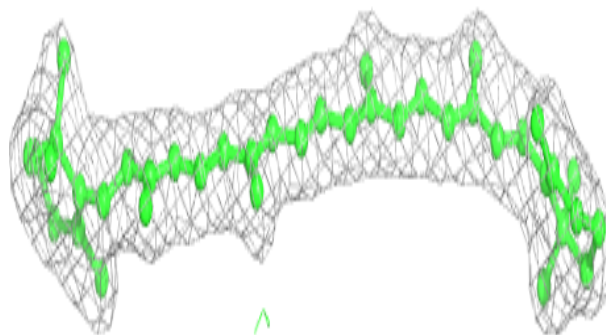
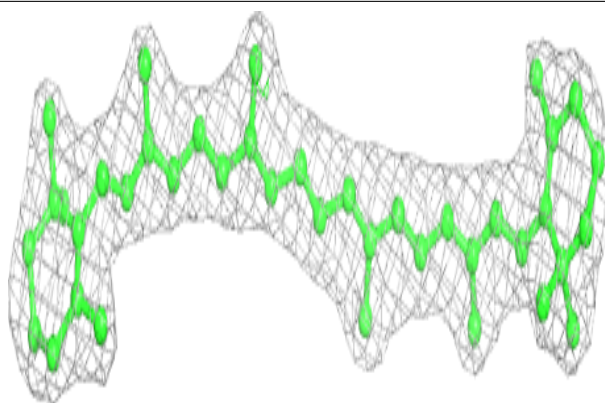
**Electron density around BCR a 413:**

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

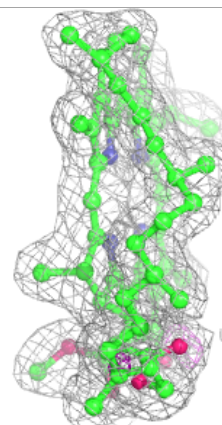
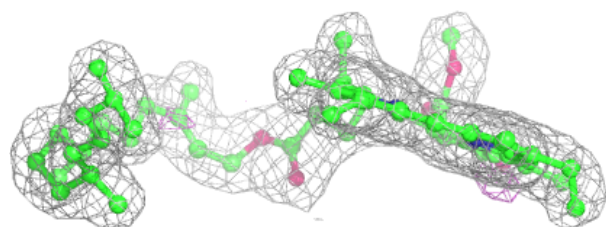
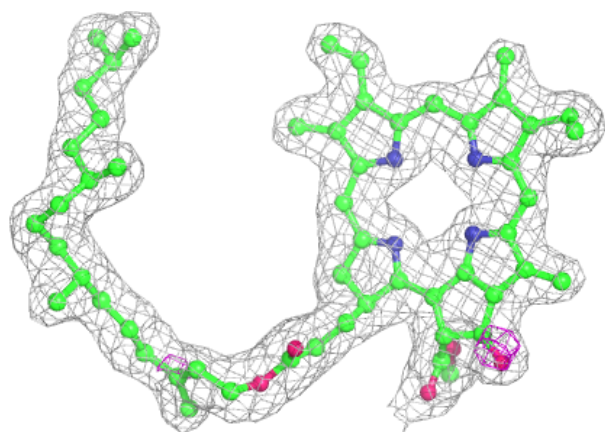


**Electron density around BCR b 628:**

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

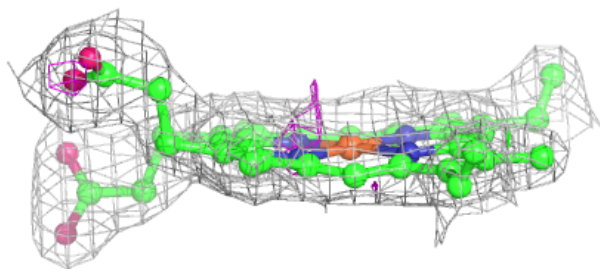
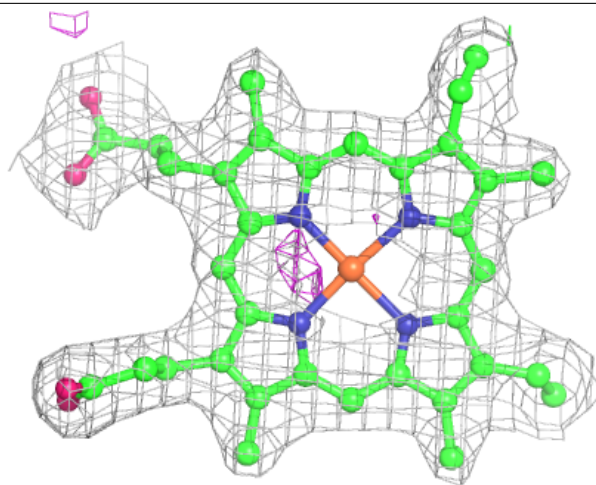
**Electron density around PHO a 411:**

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



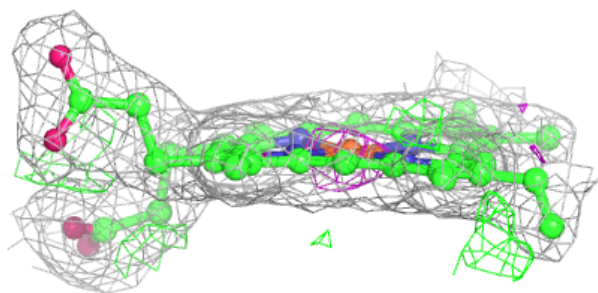
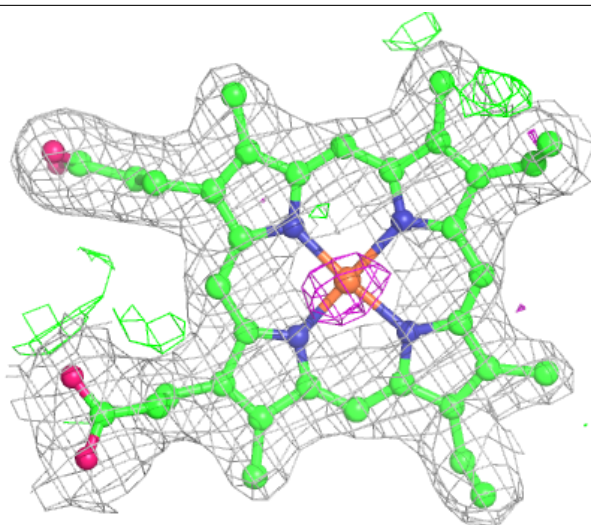
**Electron density around HEM v 205:**

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



**Electron density around HEM V 205:**

$2mF_o-DF_c$  (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.