



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:18 PM BST

PDB ID : 6JLN
Title : XFEL structure of cyanobacterial photosystem II (1F state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

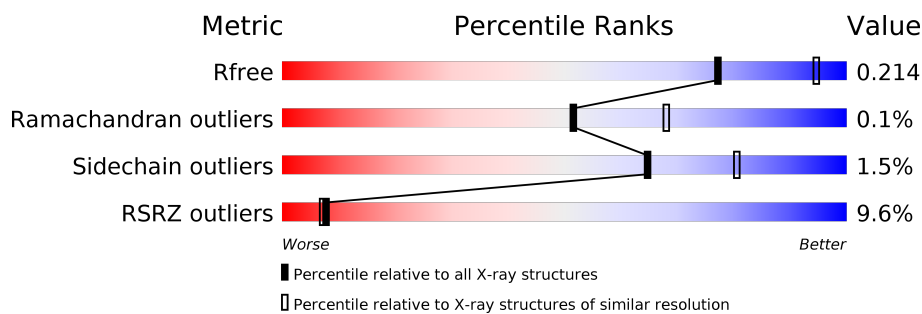
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
1	a	344	<div> <div>3%</div> <div>97%</div> <div>..</div> </div>
2	B	505	<div> <div>5%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>8%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>7%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>8%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div>4%</div> <div>99%</div> <div>.</div> </div>

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	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	505	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
27	SQD	B	621	-	-	-	X
28	GOL	V	201	-	-	-	X
29	LMT	E	102	-	-	-	X
29	LMT	M	104	-	-	-	X
29	LMT	T	104	-	-	-	X
29	LMT	a	419	-	-	-	X
29	LMT	m	103	-	-	-	X
29	LMT	t	101	-	-	-	X
33	UNL	M	103	-	-	-	X
33	UNL	c	525	-	-	-	X
33	UNL	j	101	-	-	-	X
33	UNL	m	101	-	-	-	X
34	LMG	z	101	-	-	-	X
36	HTG	C	523	-	-	-	X
36	HTG	b	632	-	-	-	X
36	HTG	c	524	-	-	-	X
37	DGD	D	408	-	-	-	X
37	DGD	e	101	-	-	-	X

2 Entry composition

There are 41 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	S	0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

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

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

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

- Molecule 21 is 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).

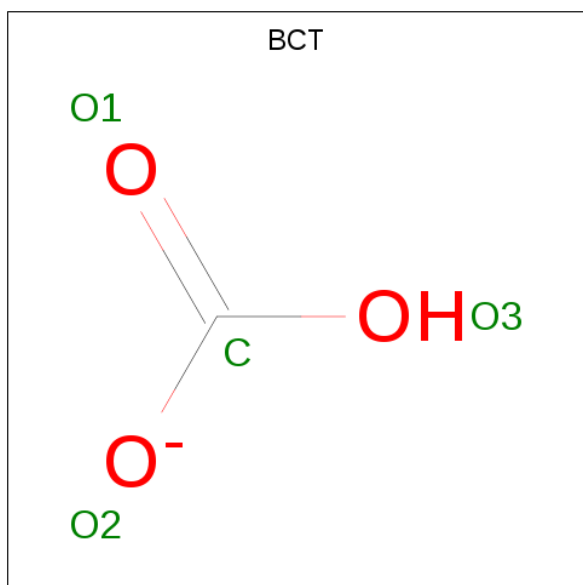
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

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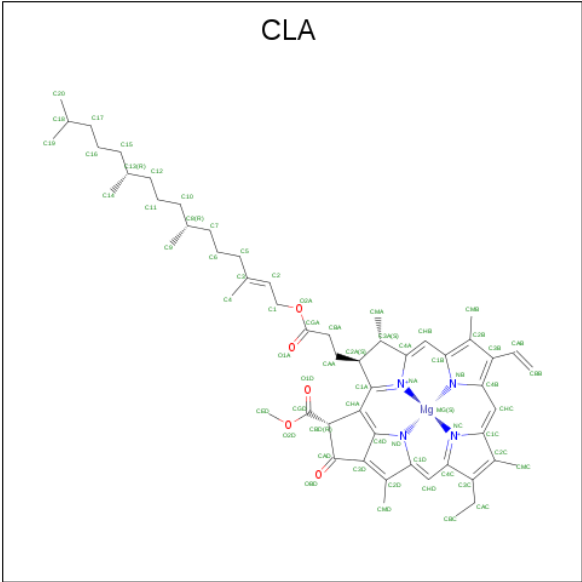
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	d	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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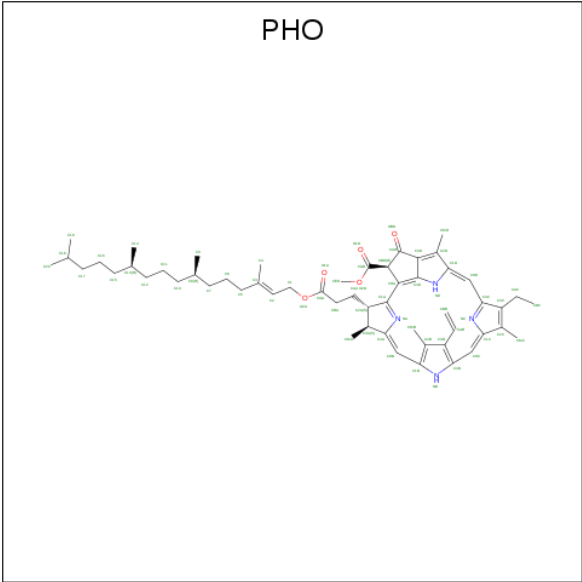
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 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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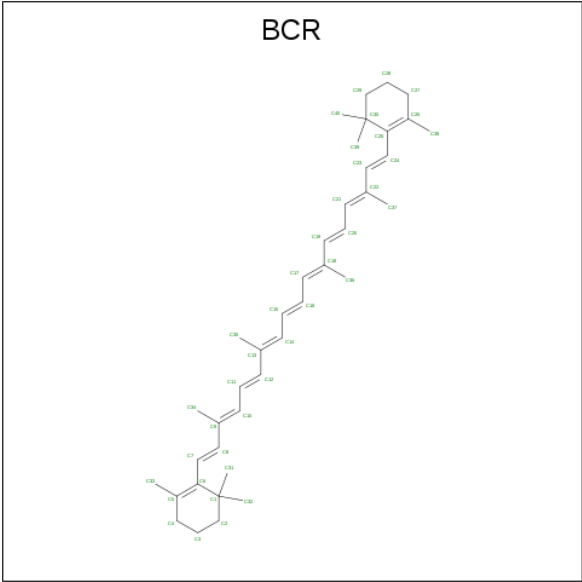
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: C₅₅H₇₄N₄O₅).



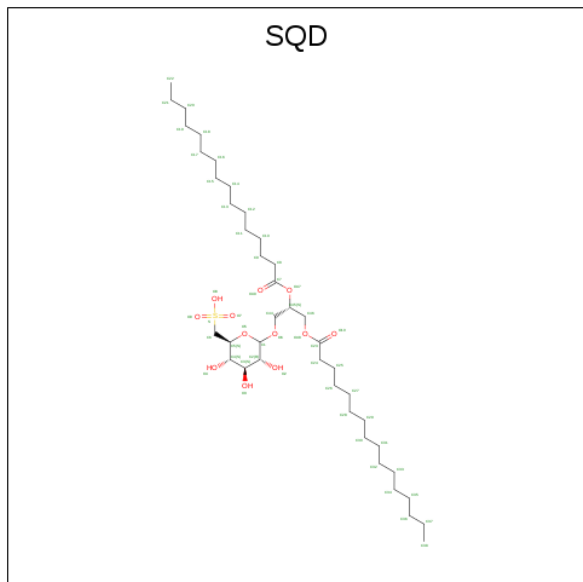
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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: $C_3H_8O_3$).



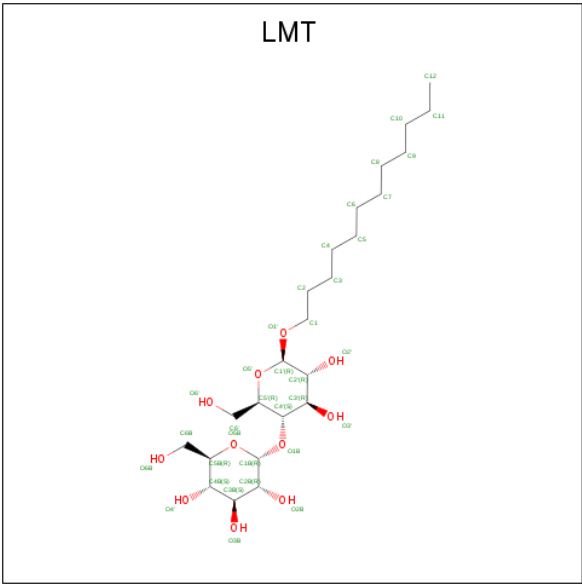
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28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

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

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



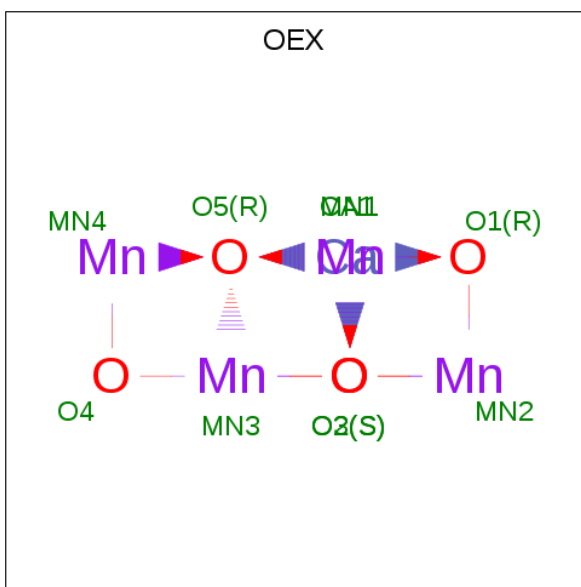
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	E	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			25	19	6		
29	a	1	Total	C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

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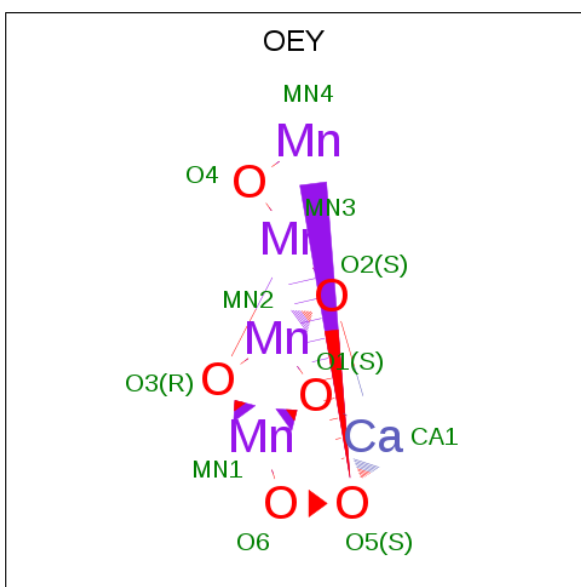
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		
29	t	1	Total	C	O	0	0
			25	19	6		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



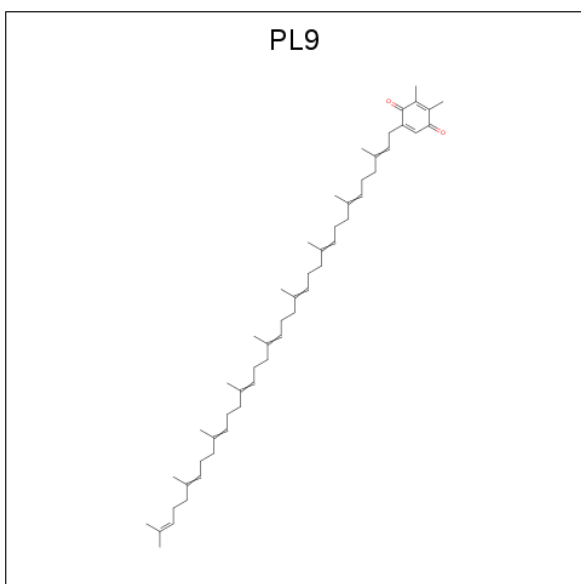
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 31 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

- Molecule 32 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: $C_{53}H_{80}O_2$).



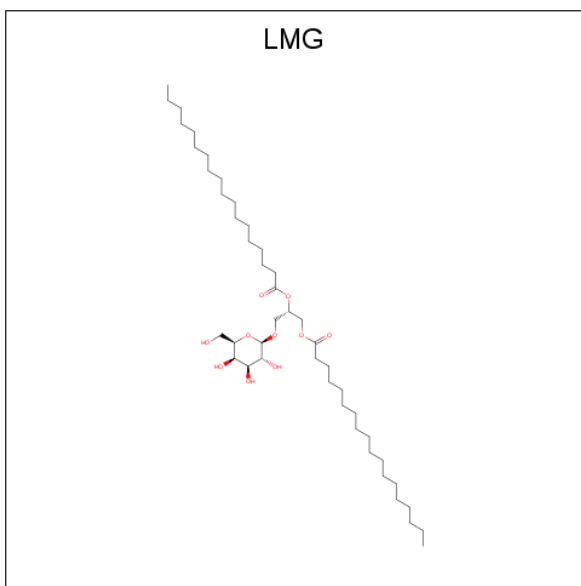
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			110	106	4		
32	D	1	Total	C	O	0	1
			110	106	4		
32	a	1	Total	C	O	0	1
			110	106	4		
32	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 33 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	J	1	Total	C		0	0
			10	10			
33	i	1	Total	C	O	0	0
			40	35	5		
33	D	2	Total	C	O	0	0
			57	51	6		
33	B	1	Total	C	O	0	0
			33	28	5		
33	I	1	Total	C	O	0	0
			40	35	5		
33	C	1	Total	C	O	0	0
			34	29	5		
33	a	1	Total	C	O	0	0
			30	25	5		
33	c	1	Total	C	O	0	0
			32	27	5		
33	A	1	Total	C	O	0	0
			28	23	5		
33	j	1	Total	C		0	0
			10	10			
33	X	1	Total	C	O	0	0
			18	16	2		
33	d	3	Total	C	O	0	0
			71	63	8		
33	m	1	Total	C		0	0
			10	10			
33	b	1	Total	C	O	0	0
			33	28	5		
33	M	1	Total	C		0	0
			10	10			

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C₄₅H₈₆O₁₀).

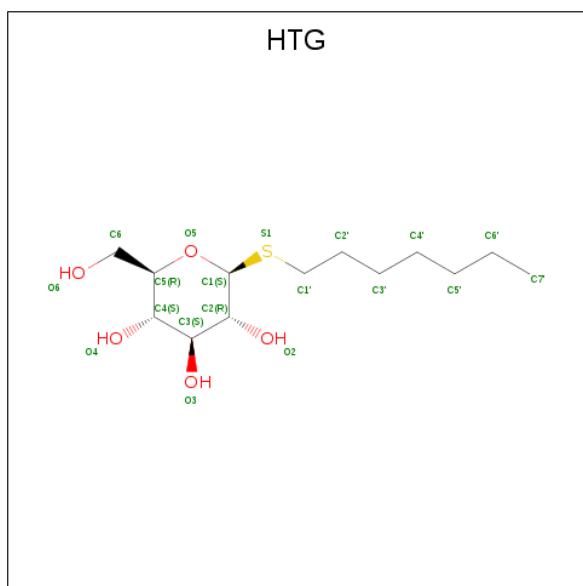


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	M	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	b	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	k	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 36 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



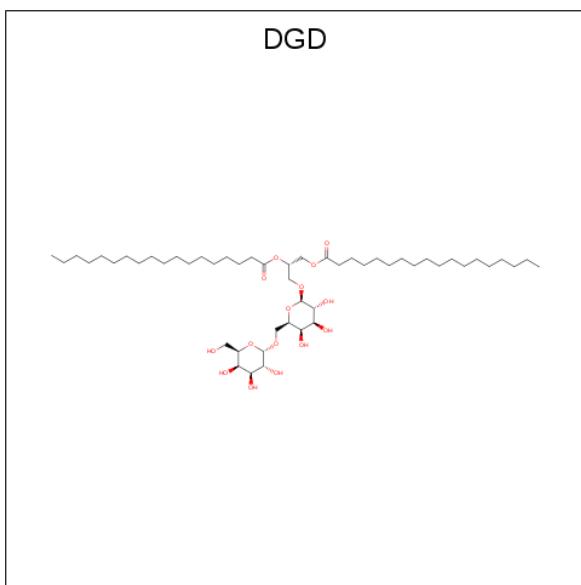
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0

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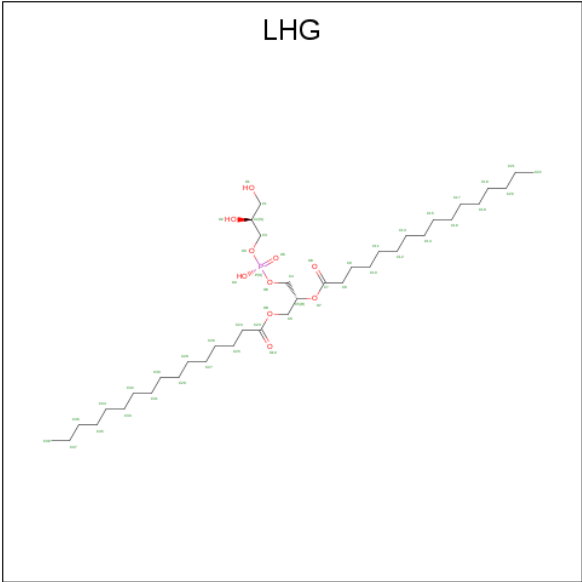
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19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

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 38 is 1,3-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
39	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	
39	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
39	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
39	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	162	Total	O		
			175	175	0	15
41	B	284	Total	O		
			288	288	0	4
41	C	232	Total	O		
			236	236	0	6

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	D	144	Total 149	O 149	0	5
41	E	36	Total 37	O 37	0	1
41	F	7	Total 7	O 7	0	0
41	H	41	Total 41	O 41	0	0
41	I	4	Total 4	O 4	0	0
41	J	10	Total 10	O 10	0	0
41	K	8	Total 8	O 8	0	0
41	L	16	Total 17	O 17	0	1
41	M	23	Total 23	O 23	0	0
41	O	177	Total 179	O 179	0	2
41	T	15	Total 16	O 16	0	1
41	U	83	Total 83	O 83	0	0
41	V	114	Total 116	O 116	0	2
41	Y	4	Total 4	O 4	0	0
41	X	8	Total 8	O 8	0	0
41	Z	1	Total 1	O 1	0	0
41	a	157	Total 168	O 168	0	13
41	b	261	Total 264	O 264	0	3
41	c	200	Total 206	O 206	0	8
41	d	134	Total 137	O 137	0	3
41	e	20	Total 20	O 20	0	0

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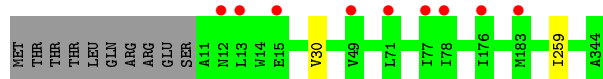
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	f	6	Total 6	O 6	0	0
41	h	42	Total 42	O 42	0	0
41	i	5	Total 5	O 5	0	0
41	j	7	Total 7	O 7	0	0
41	k	8	Total 8	O 8	0	0
41	l	7	Total 7	O 7	0	0
41	m	15	Total 15	O 15	0	0
41	o	152	Total 152	O 152	0	0
41	t	14	Total 14	O 14	0	0
41	u	95	Total 95	O 95	0	0
41	v	85	Total 86	O 86	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

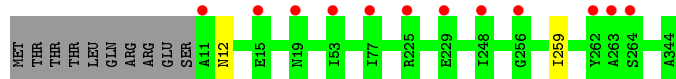
3 Residue-property plots [i](#)

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.

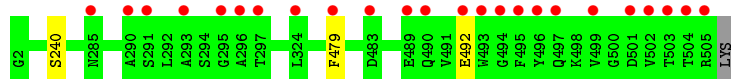
- Molecule 1: Photosystem II protein D1



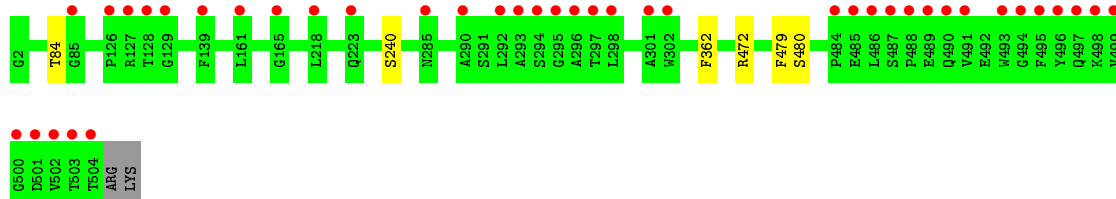
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

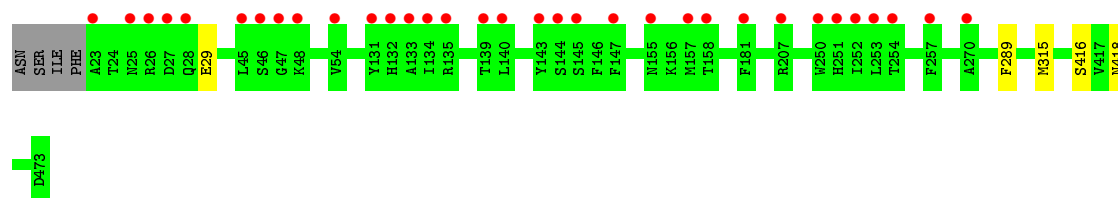


- Molecule 2: Photosystem II CP47 reaction center protein

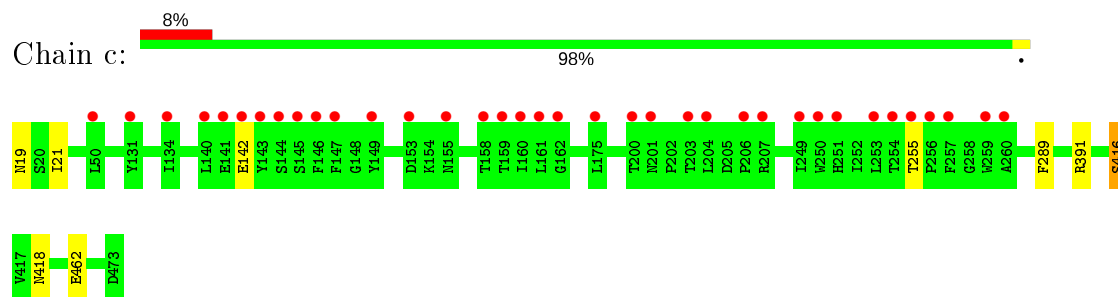


- Molecule 3: Photosystem II CP43 reaction center protein

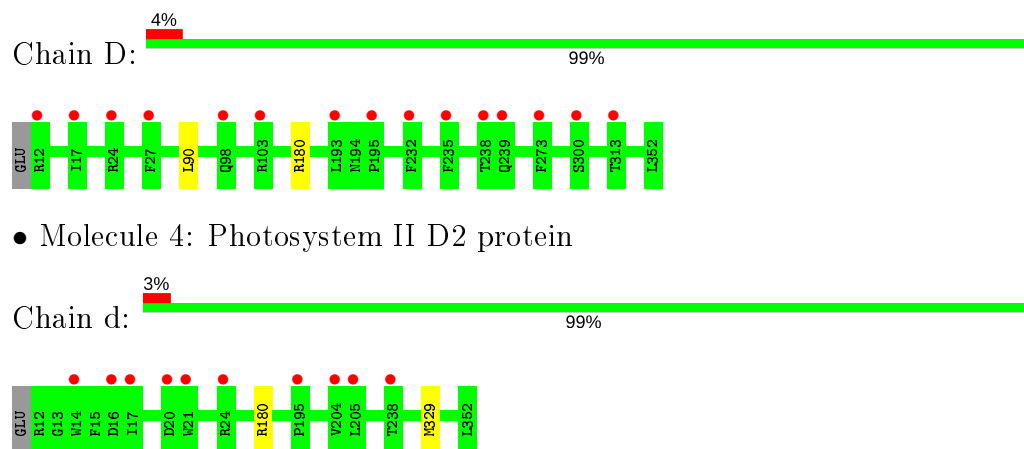




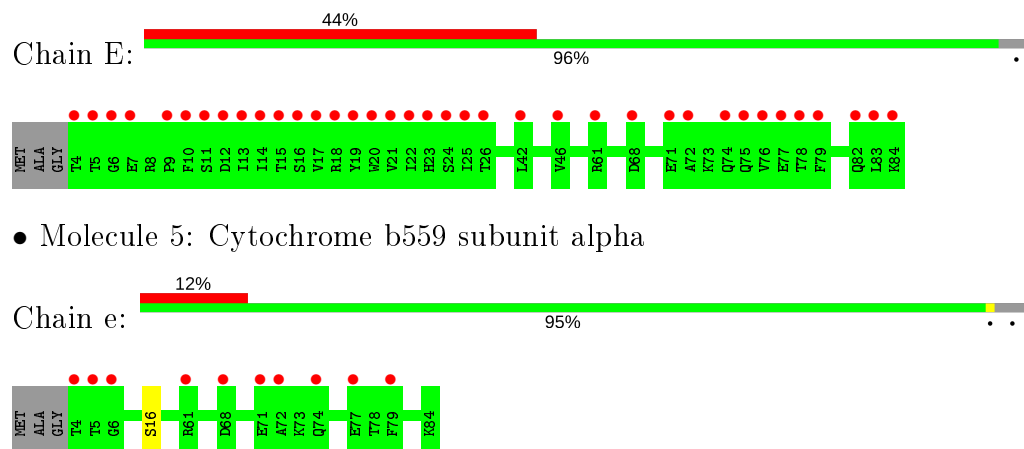
- Molecule 3: Photosystem II CP43 reaction center protein



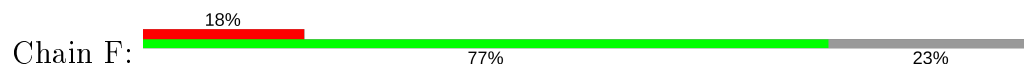
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

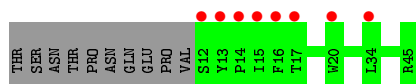


- Molecule 5: Cytochrome b559 subunit alpha

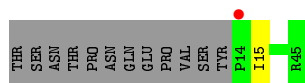


- Molecule 6: Cytochrome b559 subunit beta

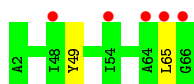




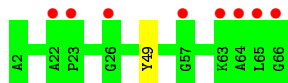
- Molecule 6: Cytochrome b559 subunit beta



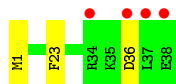
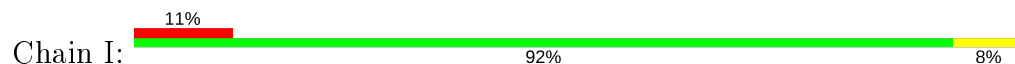
- Molecule 7: Photosystem II reaction center protein H



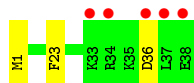
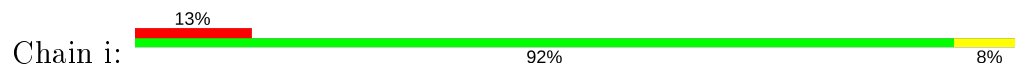
- Molecule 7: Photosystem II reaction center protein H



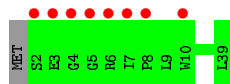
- Molecule 8: Photosystem II reaction center protein I



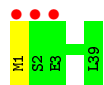
- Molecule 8: Photosystem II reaction center protein I



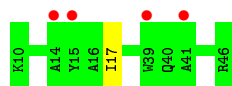
- Molecule 9: Photosystem II reaction center protein J



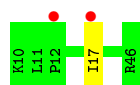
- Molecule 9: Photosystem II reaction center protein J



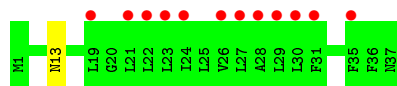
- Molecule 10: Photosystem II reaction center protein K



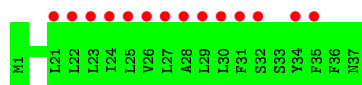
- Molecule 10: Photosystem II reaction center protein K



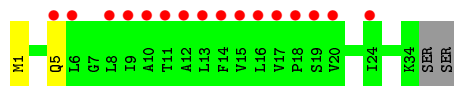
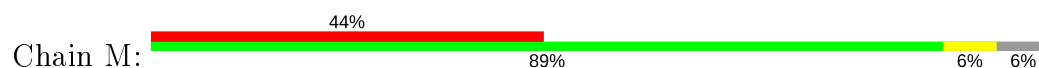
- Molecule 11: Photosystem II reaction center protein L



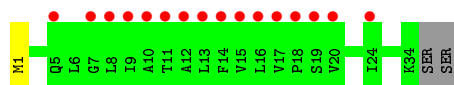
- Molecule 11: Photosystem II reaction center protein L



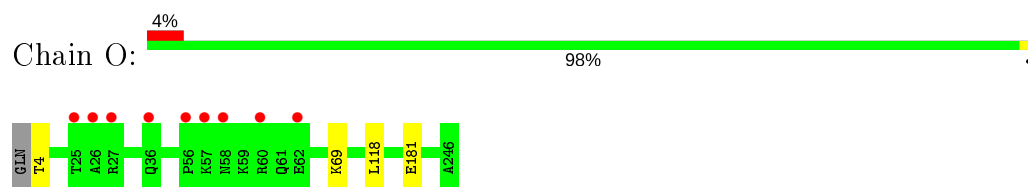
- Molecule 12: Photosystem II reaction center protein M



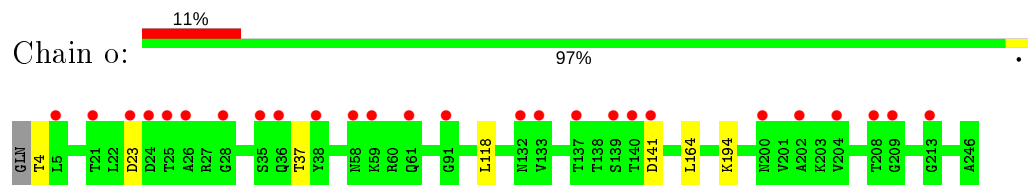
- Molecule 12: Photosystem II reaction center protein M



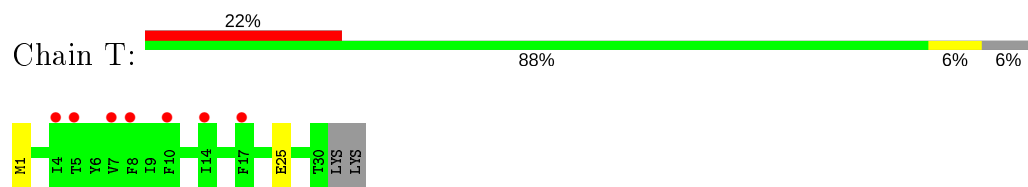
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



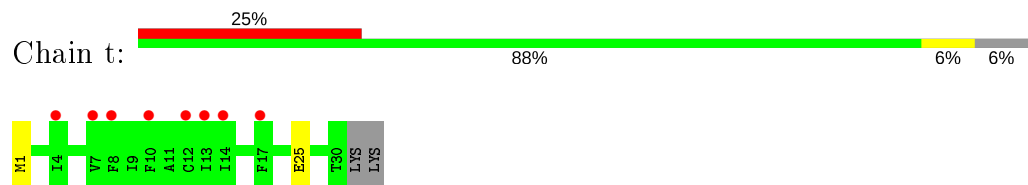
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



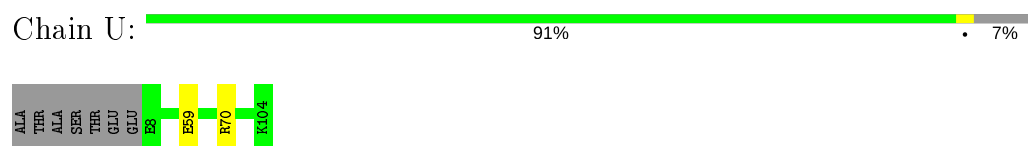
- Molecule 14: Photosystem II reaction center protein T



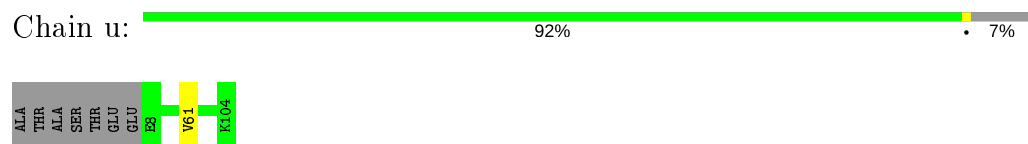
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

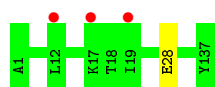


- Molecule 16: Cytochrome c-550

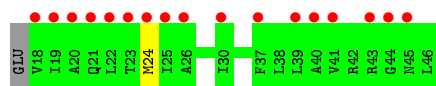


There are no outlier residues recorded for this chain.

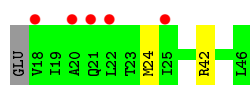
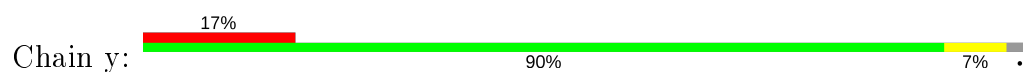
- Molecule 16: Cytochrome c-550



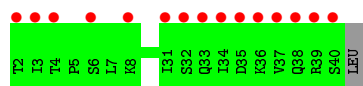
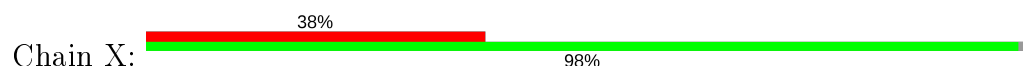
- Molecule 17: Photosystem II reaction center protein Ycf12



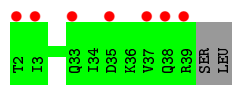
- Molecule 17: Photosystem II reaction center protein Ycf12



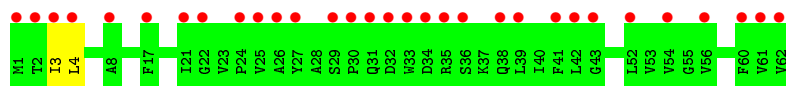
- Molecule 18: Photosystem II reaction center protein X



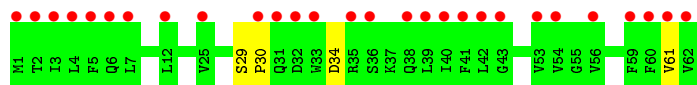
- Molecule 18: Photosystem II reaction center protein X



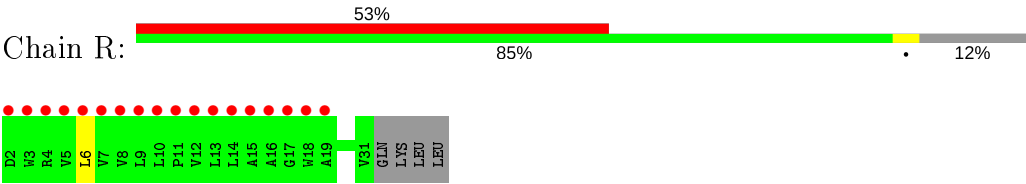
- Molecule 19: Photosystem II reaction center protein Z



- 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, α , β , γ	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 92.96 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.40) 99.2 (92.96-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.154 , 0.212 0.158 , 0.214	Depositor DCC
R_{free} test set	17838 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55631	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, OEY, LMG, FE2, BCT, HEM, FME, UNL, HTG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/3121	0.56	0/4250
1	a	0.44	0/3135	0.56	0/4269
2	B	0.42	0/4191	0.54	0/5709
2	b	0.43	0/4198	0.54	0/5720
3	C	0.38	0/3643	0.49	0/4958
3	c	0.38	0/3731	0.51	0/5076
4	D	0.46	0/2952	0.54	0/4021
4	d	0.46	0/2952	0.55	0/4021
5	E	0.34	0/693	0.49	0/944
5	e	0.33	0/695	0.50	0/948
6	F	0.38	0/284	0.52	0/387
6	f	0.39	0/265	0.51	0/360
7	H	0.36	0/535	0.53	0/728
7	h	0.35	0/524	0.51	0/713
8	I	0.37	0/311	0.49	0/419
8	i	0.35	0/311	0.48	0/419
9	J	0.38	0/278	0.42	0/376
9	j	0.33	0/286	0.45	0/386
10	K	0.33	0/303	0.51	0/416
10	k	0.36	0/303	0.49	0/416
11	L	0.44	0/319	0.51	0/433
11	l	0.42	0/319	0.46	0/433
12	M	0.47	0/270	0.57	0/368
12	m	0.44	0/262	0.59	0/357
13	O	0.38	0/1958	0.56	0/2654
13	o	0.38	0/1937	0.55	0/2625
14	T	0.45	0/266	0.53	0/362
14	t	0.51	0/266	0.54	0/362
15	U	0.38	0/785	0.54	0/1064
15	u	0.38	0/785	0.55	0/1064
16	V	0.37	0/1109	0.51	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.37	0/1098	0.52	0/1488
17	Y	0.35	0/216	0.49	0/289
17	y	0.32	0/216	0.47	0/289
18	X	0.34	0/290	0.45	0/392
18	x	0.33	0/284	0.49	0/384
19	Z	0.30	0/490	0.43	0/669
19	z	0.29	0/490	0.45	0/669
20	R	0.26	0/245	0.38	0/338
All	All	0.41	0/44316	0.53	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 ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	377 (98%)	5 (1%)	2 (0%)	29	41
1	a	386/344 (112%)	378 (98%)	7 (2%)	1 (0%)	41	55
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	456/455 (100%)	446 (98%)	8 (2%)	2 (0%)	34	48
3	c	466/455 (102%)	450 (97%)	14 (3%)	2 (0%)	34	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	343 (97%)	12 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	34 (92%)	3 (8%)	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%)	241 (97%)	8 (3%)	0	100	100
13	o	246/244 (101%)	235 (96%)	11 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	4	3
20	R	28/34 (82%)	28 (100%)	0	0	100	100
All	All	5419/5384 (101%)	5272 (97%)	138 (2%)	9 (0%)	51	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	a	259	ILE
19	z	30	PRO
1	A	259	ILE
1	A	30	VAL
19	z	61	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/279 (112%)	312 (100%)	0	100	100
1	a	314/279 (112%)	313 (100%)	1 (0%)	92	97
2	B	412/403 (102%)	409 (99%)	3 (1%)	84	92
2	b	413/403 (102%)	407 (98%)	6 (2%)	65	80
3	C	357/356 (100%)	353 (99%)	4 (1%)	73	87
3	c	367/356 (103%)	356 (97%)	11 (3%)	41	61
4	D	290/277 (105%)	288 (99%)	2 (1%)	84	92
4	d	290/277 (105%)	288 (99%)	2 (1%)	84	92
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	51
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	54
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	75
8	I	34/34 (100%)	32 (94%)	2 (6%)	19	32
8	i	34/34 (100%)	32 (94%)	2 (6%)	19	32
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	53
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	57
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	57
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	63
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	30 (97%)	1 (3%)	39	59
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	209 (98%)	5 (2%)	50	70
13	o	211/207 (102%)	204 (97%)	7 (3%)	38	57
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	22
15	U	84/89 (94%)	82 (98%)	2 (2%)	49	68
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	85
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	117 (99%)	1 (1%)	81	91
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	44
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	14
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	51
19	z	52/52 (100%)	50 (96%)	2 (4%)	33	51
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	49
All	All	4500/4403 (102%)	4429 (98%)	71 (2%)	65	79

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	240	SER
2	B	479	PHE
2	B	492	GLU
3	C	29	GLU
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	90	LEU
4	D	180	ARG
7	H	49	TYR
7	H	65	LEU
8	I	23	PHE
8	I	36	ASP
10	K	17	ILE
11	L	13	ASN
12	M	5	GLN
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	59	GLU
15	U	70	ARG
17	Y	24	MET
19	Z	3	ILE
19	Z	4	LEU
20	R	6	LEU
1	a	12	ASN
2	b	84	THR
2	b	240	SER
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	21	ILE
3	c	142	GLU
3	c	255	THR
3	c	289	PHE
3	c	391	ARG
3	c	416[A]	SER

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Mol	Chain	Res	Type
3	c	416[B]	SER
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	180	ARG
4	d	329	MET
5	e	16	SER
6	f	15	ILE
7	h	49	TYR
8	i	23	PHE
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
13	o	4	THR
13	o	23	ASP
13	o	37	THR
13	o	118	LEU
13	o	141	ASP
13	o	164	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	61	VAL
16	v	28	GLU
17	y	24	MET
17	y	42	ARG
19	z	29	SER
19	z	34	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	53	ASN
2	B	331	ASN
2	B	490	GLN
2	B	497	GLN
4	D	61	HIS
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN

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Mol	Chain	Res	Type
13	O	147	ASN
15	U	81	HIS
16	V	118	HIS
19	Z	58	ASN
1	a	12	ASN
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
2	b	490	GLN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
13	o	124	ASN
13	o	130	GLN
13	o	147	ASN
16	v	86	GLN
19	z	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	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.44	2 (28%)
12	FME	M	1	12	8,9,10	0.70	0	7,9,11	1.36	2 (28%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.22	1 (14%)
14	FME	T	1	14	8,9,10	0.70	0	7,9,11	1.32	1 (14%)
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.37	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	FME	t	1	14	8,9,10	0.79	0	7,9,11	2.10	3 (42%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	C-CA-N	3.25	115.61	109.73
14	t	1	FME	CA-N-CN	-2.77	118.57	122.82
8	I	1	FME	CA-N-CN	-2.50	118.97	122.82
14	T	1	FME	O-C-CA	-2.41	118.45	124.78
14	t	1	FME	O-C-CA	-2.37	118.57	124.78
12	M	1	FME	CA-N-CN	-2.32	119.25	122.82
8	i	1	FME	O-C-CA	-2.19	119.04	124.78
12	M	1	FME	O-C-CA	-2.09	119.30	124.78
8	I	1	FME	O-C-CA	-2.08	119.33	124.78
12	m	1	FME	CA-N-CN	-2.04	119.69	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
12	m	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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$
24	CLA	C	513	-	59,73,73	2.01	13 (22%)	67,113,113	2.08	21 (31%)
26	BCR	c	526	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	9 (16%)
36	HTG	b	632	-	19,19,19	1.19	2 (10%)	23,24,24	1.68	3 (13%)
24	CLA	c	517	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	21 (31%)
26	BCR	T	103	-	41,41,41	1.01	1 (2%)	56,56,56	1.77	14 (25%)
28	GOL	A	412	-	5,5,5	0.40	0	5,5,5	0.15	0
28	GOL	B	630	-	5,5,5	0.37	0	5,5,5	0.28	0
34	LMG	M	101	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
24	CLA	d	404	-	59,73,73	1.99	14 (23%)	67,113,113	2.28	23 (34%)
24	CLA	C	507	41	59,73,73	1.99	13 (22%)	67,113,113	2.04	19 (28%)
26	BCR	d	406	-	41,41,41	1.08	1 (2%)	56,56,56	1.66	15 (26%)
24	CLA	A	405	-	59,73,73	2.10	13 (22%)	67,113,113	2.28	22 (32%)
24	CLA	B	606	-	59,73,73	2.00	13 (22%)	67,113,113	2.11	19 (28%)
26	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	8 (14%)
24	CLA	B	614	-	59,73,73	2.08	13 (22%)	67,113,113	2.18	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PHO	a	411	-	67,69,69	2.19	17 (25%)	85,99,99	1.90	22 (25%)
39	HEM	V	205	16	27,50,50	0.88	2 (7%)	17,82,82	1.57	4 (23%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.13	4 (8%)
28	GOL	b	601	-	5,5,5	0.38	0	5,5,5	0.44	0
32	PL9	d	407[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.64	17 (25%)
32	PL9	A	417[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.77	22 (32%)
24	CLA	b	622	-	59,73,73	1.99	12 (20%)	67,113,113	2.20	19 (28%)
28	GOL	D	402	-	5,5,5	0.42	0	5,5,5	0.29	0
24	CLA	D	404	-	59,73,73	1.96	13 (22%)	67,113,113	2.31	23 (34%)
24	CLA	d	403	41	59,73,73	1.99	12 (20%)	67,113,113	2.28	23 (34%)
26	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.53	10 (17%)
28	GOL	v	202	-	5,5,5	0.36	0	5,5,5	0.32	0
30	OEX	a	417[A]	1,3,41	0,15,15	0.00	-	-		
36	HTG	c	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.46	2 (8%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.04	6 (7%)
24	CLA	b	615	-	59,73,73	2.02	13 (22%)	67,113,113	2.19	23 (34%)
26	BCR	y	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	10 (17%)
34	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	3 (5%)
38	LHG	d	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
28	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.22	0
28	GOL	V	203	-	5,5,5	0.42	0	5,5,5	0.24	0
24	CLA	B	609	-	59,73,73	2.02	13 (22%)	67,113,113	2.10	21 (31%)
38	LHG	D	409	-	48,48,48	0.86	2 (4%)	51,54,54	1.00	3 (5%)
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.40	7 (12%)
28	GOL	F	103	35	5,5,5	0.36	0	5,5,5	0.24	0
26	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.56	7 (12%)
28	GOL	v	201	-	5,5,5	0.33	0	5,5,5	0.32	0
24	CLA	C	511	3	59,73,73	2.08	13 (22%)	67,113,113	2.16	22 (32%)
24	CLA	A	406	41	59,73,73	2.06	15 (25%)	67,113,113	2.30	24 (35%)
38	LHG	D	411	-	48,48,48	0.99	2 (4%)	51,54,54	1.12	3 (5%)
37	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.96	3 (3%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.29	0
24	CLA	D	405	-	59,73,73	1.97	14 (23%)	67,113,113	2.16	23 (34%)
38	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	0.73	2 (3%)
24	CLA	b	612	-	59,73,73	1.99	13 (22%)	67,113,113	2.32	23 (34%)
32	PL9	a	416[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.84	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HTG	B	622	-	19,19,19	1.10	1 (5%)	23,24,24	1.35	1 (4%)
24	CLA	a	409	-	59,73,73	2.04	13 (22%)	67,113,113	2.22	24 (35%)
26	BCR	b	628	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	10 (17%)
26	BCR	a	413	-	41,41,41	1.03	1 (2%)	56,56,56	1.48	9 (16%)
36	HTG	c	524	-	19,19,19	1.02	2 (10%)	23,24,24	1.50	2 (8%)
25	PHO	D	401[A]	-	67,69,69	2.13	16 (23%)	85,99,99	1.94	20 (23%)
26	BCR	C	514	-	41,41,41	1.06	1 (2%)	56,56,56	1.42	8 (14%)
34	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	5 (8%)
24	CLA	c	505	-	59,73,73	1.99	14 (23%)	67,113,113	2.14	22 (32%)
25	PHO	D	401[B]	-	67,69,69	2.18	17 (25%)	85,99,99	1.94	22 (25%)
28	GOL	B	627	-	5,5,5	0.36	0	5,5,5	0.51	0
24	CLA	B	604	-	59,73,73	2.00	14 (23%)	67,113,113	2.22	22 (32%)
24	CLA	B	616	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	20 (29%)
24	CLA	C	509	-	59,73,73	2.06	13 (22%)	67,113,113	2.20	24 (35%)
37	DGD	D	408	-	52,52,67	1.03	3 (5%)	60,60,81	1.19	5 (8%)
39	HEM	v	206	16	27,50,50	0.91	1 (3%)	17,82,82	1.40	2 (11%)
24	CLA	b	621	-	59,73,73	2.05	13 (22%)	67,113,113	2.27	21 (31%)
25	PHO	A	408	-	67,69,69	2.14	17 (25%)	85,99,99	1.93	22 (25%)
29	LMT	D	403	-	36,36,36	0.43	0	47,47,47	1.00	1 (2%)
29	LMT	a	419	-	36,36,36	0.43	0	47,47,47	0.78	1 (2%)
24	CLA	B	615	-	59,73,73	2.04	12 (20%)	67,113,113	2.24	24 (35%)
36	HTG	D	414	-	16,16,19	1.07	2 (12%)	20,21,24	1.32	1 (5%)
37	DGD	c	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.03	6 (7%)
29	LMT	M	102	-	36,36,36	0.42	0	47,47,47	0.87	1 (2%)
34	LMG	k	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
23	BCT	A	404[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	a	421	35	5,5,5	0.33	0	5,5,5	0.43	0
36	HTG	B	631	-	19,19,19	1.03	2 (10%)	23,24,24	1.36	2 (8%)
24	CLA	c	510	-	59,73,73	2.00	13 (22%)	67,113,113	2.15	23 (34%)
31	OXY	A	416[B]	1,3,41	0,14,16	0.00	-	-	-	-
24	CLA	b	613	-	59,73,73	1.97	13 (22%)	67,113,113	2.32	20 (29%)
24	CLA	C	503	-	59,73,73	2.04	13 (22%)	67,113,113	2.19	19 (28%)
26	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.70	15 (26%)
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.87	0
29	LMT	b	630	-	25,25,36	0.50	0	30,30,47	0.66	0
24	CLA	B	603	-	59,73,73	2.07	14 (23%)	67,113,113	2.28	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HTG	b	602	-	19,19,19	0.95	1 (5%)	23,24,24	1.07	2 (8%)
24	CLA	b	614	-	59,73,73	2.00	14 (23%)	67,113,113	2.25	22 (32%)
28	GOL	O	301	-	5,5,5	0.36	0	5,5,5	0.36	0
24	CLA	c	512	-	59,73,73	2.03	13 (22%)	67,113,113	2.27	23 (34%)
29	LMT	m	103	-	36,36,36	0.51	0	47,47,47	1.06	4 (8%)
24	CLA	B	612	-	59,73,73	2.00	13 (22%)	67,113,113	2.25	24 (35%)
25	PHO	d	402[A]	-	67,69,69	2.11	17 (25%)	85,99,99	2.07	22 (25%)
24	CLA	b	618	-	59,73,73	2.01	13 (22%)	67,113,113	2.19	23 (34%)
28	GOL	B	626	-	5,5,5	0.33	0	5,5,5	0.37	0
24	CLA	c	514	-	59,73,73	2.03	13 (22%)	67,113,113	2.21	23 (34%)
24	CLA	a	412	-	59,73,73	1.99	14 (23%)	67,113,113	2.19	22 (32%)
24	CLA	c	506	-	59,73,73	2.01	14 (23%)	67,113,113	2.15	20 (29%)
24	CLA	B	611	41	59,73,73	2.06	12 (20%)	67,113,113	2.15	26 (38%)
27	SQD	A	411	-	53,54,54	0.98	3 (5%)	62,65,65	1.53	11 (17%)
28	GOL	B	628	-	5,5,5	0.34	0	5,5,5	0.39	0
36	HTG	b	608	-	19,19,19	1.05	2 (10%)	23,24,24	1.11	3 (13%)
27	SQD	L	102	-	53,54,54	1.05	3 (5%)	62,65,65	1.59	12 (19%)
38	LHG	a	420	-	41,41,48	1.03	2 (4%)	44,47,54	0.93	2 (4%)
30	OEX	A	415[A]	1,3,41	0,15,15	0.00	-	-	-	-
28	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.23	0
24	CLA	c	509	-	59,73,73	1.99	13 (22%)	67,113,113	2.13	19 (28%)
23	BCT	d	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
29	LMT	a	404	-	36,36,36	0.47	1 (2%)	47,47,47	1.16	3 (6%)
37	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	6 (7%)
27	SQD	F	101	-	42,43,54	1.17	3 (7%)	51,54,65	1.69	11 (21%)
28	GOL	B	629	-	5,5,5	0.44	0	5,5,5	0.30	0
24	CLA	B	608	41	59,73,73	2.00	14 (23%)	67,113,113	2.12	22 (32%)
26	BCR	k	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.52	11 (19%)
37	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.98	4 (5%)
24	CLA	b	610	41	59,73,73	2.08	12 (20%)	67,113,113	2.17	22 (32%)
24	CLA	b	611	-	59,73,73	2.04	13 (22%)	67,113,113	2.23	24 (35%)
29	LMT	t	101	-	25,25,36	0.52	0	30,30,47	0.76	1 (3%)
24	CLA	C	502	-	59,73,73	2.02	13 (22%)	67,113,113	2.19	23 (34%)
24	CLA	b	623	-	59,73,73	1.99	14 (23%)	67,113,113	2.25	22 (32%)
24	CLA	b	617	-	59,73,73	2.04	13 (22%)	67,113,113	2.22	24 (35%)
26	BCR	b	626	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	516	-	59,73,73	2.06	13 (22%)	67,113,113	2.31	22 (32%)
26	BCR	B	620	-	41,41,41	1.01	1 (2%)	56,56,56	1.59	12 (21%)
26	BCR	c	518	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	11 (19%)
29	LMT	e	102	-	36,36,36	0.49	0	47,47,47	0.84	1 (2%)
24	CLA	C	508	-	59,73,73	2.05	13 (22%)	67,113,113	2.18	25 (37%)
29	LMT	A	414	-	36,36,36	0.57	1 (2%)	47,47,47	1.27	4 (8%)
28	GOL	V	202	-	5,5,5	0.33	0	5,5,5	0.36	0
24	CLA	b	625	-	59,73,73	2.01	12 (20%)	67,113,113	2.23	24 (35%)
34	LMG	d	415	40	51,51,55	0.94	2 (3%)	59,59,63	1.12	7 (11%)
28	GOL	B	625	-	5,5,5	0.40	0	5,5,5	0.15	0
24	CLA	c	511	41	59,73,73	2.02	13 (22%)	67,113,113	2.22	21 (31%)
24	CLA	c	515	3	59,73,73	1.97	13 (22%)	67,113,113	2.04	21 (31%)
32	PL9	d	407[A]	-	55,55,55	0.69	2 (3%)	68,69,69	1.54	15 (22%)
26	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	11 (19%)
38	LHG	d	408	-	48,48,48	0.90	3 (6%)	51,54,54	1.06	5 (9%)
32	PL9	A	417[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.80	22 (32%)
28	GOL	a	401	-	5,5,5	0.39	0	5,5,5	0.24	0
28	GOL	C	525	-	5,5,5	0.42	0	5,5,5	0.41	0
38	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.15	4 (9%)
26	BCR	D	406	-	41,41,41	1.05	1 (2%)	56,56,56	1.76	13 (23%)
34	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	3 (5%)
24	CLA	b	620	-	59,73,73	1.95	12 (20%)	67,113,113	2.16	21 (31%)
24	CLA	B	617	-	59,73,73	2.01	12 (20%)	67,113,113	2.19	21 (31%)
28	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.31	0
28	GOL	T	101	-	5,5,5	0.39	0	5,5,5	0.28	0
24	CLA	d	405	-	59,73,73	2.01	12 (20%)	67,113,113	2.20	21 (31%)
24	CLA	C	504	41	59,73,73	2.04	13 (22%)	67,113,113	2.25	21 (31%)
39	HEM	f	101	5,6	27,50,50	0.86	1 (3%)	17,82,82	1.96	4 (23%)
28	GOL	v	204	-	5,5,5	0.37	0	5,5,5	0.24	0
36	HTG	b	631	-	19,19,19	0.80	1 (5%)	23,24,24	1.35	1 (4%)
26	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.37	9 (16%)
37	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	3 (3%)
38	LHG	d	409	-	48,48,48	0.88	2 (4%)	51,54,54	1.01	5 (9%)
37	DGD	C	517	-	63,63,67	0.88	2 (3%)	77,77,81	1.05	9 (11%)
24	CLA	A	407	41	59,73,73	1.97	13 (22%)	67,113,113	2.12	23 (34%)
24	CLA	B	605	-	59,73,73	1.90	13 (22%)	67,113,113	2.21	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	512	-	59,73,73	2.04	13 (22%)	67,113,113	2.23	23 (34%)
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.33	0
24	CLA	c	513	-	59,73,73	2.07	13 (22%)	67,113,113	2.19	23 (34%)
24	CLA	C	501	-	59,73,73	2.02	13 (22%)	67,113,113	2.17	20 (29%)
36	HTG	C	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.74	4 (17%)
28	GOL	t	103	-	5,5,5	0.41	0	5,5,5	0.23	0
24	CLA	c	507	-	59,73,73	1.99	13 (22%)	67,113,113	2.14	21 (31%)
26	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	13 (23%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.14	5 (10%)
32	PL9	a	416[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.91	20 (29%)
24	CLA	C	510	-	59,73,73	2.07	13 (22%)	67,113,113	2.17	24 (35%)
24	CLA	a	410	41	59,73,73	2.00	13 (22%)	67,113,113	2.20	22 (32%)
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.45	7 (13%)
27	SQD	a	414	-	53,54,54	0.95	3 (5%)	62,65,65	1.57	11 (17%)
32	PL9	D	407[A]	-	55,55,55	0.66	1 (1%)	68,69,69	1.74	20 (29%)
29	LMT	T	104	-	25,25,36	0.55	1 (4%)	30,30,47	1.06	2 (6%)
39	HEM	E	103	5,6	27,50,50	0.89	2 (7%)	17,82,82	2.31	3 (17%)
36	HTG	C	522	-	19,19,19	1.03	2 (10%)	23,24,24	1.67	1 (4%)
37	DGD	e	101	-	63,63,67	0.95	3 (4%)	77,77,81	1.28	7 (9%)
32	PL9	D	407[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.81	22 (32%)
27	SQD	A	413	-	53,54,54	1.02	3 (5%)	62,65,65	1.15	6 (9%)
24	CLA	A	409	-	59,73,73	1.98	13 (22%)	67,113,113	2.14	23 (34%)
27	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.41	5 (8%)
24	CLA	B	613	-	59,73,73	2.02	12 (20%)	67,113,113	2.19	20 (29%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.10	5 (9%)
28	GOL	b	604	-	5,5,5	0.33	0	5,5,5	0.26	0
34	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	5 (8%)
24	CLA	b	624	-	59,73,73	2.00	13 (22%)	67,113,113	2.10	18 (26%)
24	CLA	b	619	41	59,73,73	2.04	14 (23%)	67,113,113	2.21	24 (35%)
34	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.36	7 (15%)
24	CLA	C	505	-	59,73,73	1.98	14 (23%)	67,113,113	2.16	18 (26%)
24	CLA	B	607	-	59,73,73	2.00	13 (22%)	67,113,113	2.21	22 (32%)
31	OEY	a	418[B]	1,3,41	0,14,16	0.00	-	-	-	-
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.28	0
24	CLA	b	616	41	59,73,73	2.00	13 (22%)	67,113,113	2.14	21 (31%)
29	LMT	E	102	-	36,36,36	0.49	0	47,47,47	0.94	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCT	A	404[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	b	603	-	5,5,5	0.40	0	5,5,5	0.37	0
34	LMG	D	415	40	51,51,55	0.89	2 (3%)	59,59,63	0.96	3 (5%)
25	PHO	d	402[B]	-	67,69,69	2.13	17 (25%)	85,99,99	2.04	22 (25%)
29	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.11	3 (6%)
28	GOL	o	301	-	5,5,5	0.41	0	5,5,5	0.34	0
36	HTG	b	607	-	19,19,19	1.00	1 (5%)	23,24,24	1.39	4 (17%)
28	GOL	B	634	-	5,5,5	0.45	0	5,5,5	0.45	0
28	GOL	c	502	-	5,5,5	0.39	0	5,5,5	0.37	0
24	CLA	B	602	41	59,73,73	2.07	14 (23%)	67,113,113	2.11	19 (28%)
36	HTG	V	206	-	19,19,19	1.02	2 (10%)	23,24,24	1.44	4 (17%)
34	LMG	c	522	-	51,51,55	0.95	2 (3%)	59,59,63	1.17	7 (11%)
36	HTG	B	623	-	19,19,19	0.85	1 (5%)	23,24,24	1.48	1 (4%)
26	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	8 (14%)
24	CLA	B	610	-	59,73,73	1.95	13 (22%)	67,113,113	2.17	22 (32%)
36	HTG	B	624	-	19,19,19	1.05	2 (10%)	23,24,24	2.06	4 (17%)
27	SQD	a	405	-	53,54,54	1.08	3 (5%)	62,65,65	1.19	4 (6%)
36	HTG	B	632	-	19,19,19	1.05	2 (10%)	23,24,24	1.43	2 (8%)
28	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.75	0
28	GOL	v	203	-	5,5,5	0.33	0	5,5,5	0.47	0
28	GOL	b	605	-	5,5,5	0.38	0	5,5,5	0.32	0
36	HTG	d	413	-	16,16,19	1.23	2 (12%)	20,21,24	1.81	2 (10%)
24	CLA	c	508	41	59,73,73	2.01	14 (23%)	67,113,113	2.16	24 (35%)
23	BCT	d	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
26	BCR	A	410	-	41,41,41	1.07	1 (2%)	56,56,56	1.15	3 (5%)
24	CLA	C	506	-	59,73,73	1.98	14 (23%)	67,113,113	2.19	23 (34%)
38	LHG	b	634	-	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
37	DGD	H	102	-	63,63,67	0.90	2 (3%)	77,77,81	1.03	5 (6%)
34	LMG	b	629	-	51,51,55	0.91	3 (5%)	59,59,63	1.07	5 (8%)

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	513	-	3/3/20/25	7/37/135/135	-
26	BCR	c	526	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	HTG	b	632	-	-	4/10/30/30	0/1/1/1
24	CLA	c	517	-	2/2/20/25	5/37/135/135	-
26	BCR	T	103	-	-	2/29/63/63	0/2/2/2
28	GOL	A	412	-	-	1/4/4/4	-
28	GOL	B	630	-	-	0/4/4/4	-
34	LMG	M	101	-	-	12/46/66/70	0/1/1/1
24	CLA	d	404	-	1/1/20/25	3/37/135/135	-
24	CLA	C	507	41	3/3/20/25	4/37/135/135	-
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
24	CLA	A	405	-	3/3/20/25	4/37/135/135	-
24	CLA	B	606	-	3/3/20/25	7/37/135/135	-
24	CLA	c	510	-	3/3/20/25	13/37/135/135	-
24	CLA	B	614	-	3/3/20/25	8/37/135/135	-
25	PHO	a	411	-	-	5/53/103/103	0/5/6/6
39	HEM	V	205	16	-	0/6/54/54	-
34	LMG	z	101	-	-	12/34/54/70	0/1/1/1
28	GOL	b	601	-	-	0/4/4/4	-
32	PL9	d	407[B]	-	-	8/53/73/73	0/1/1/1
32	PL9	A	417[A]	-	-	14/53/73/73	0/1/1/1
24	CLA	b	622	-	3/3/20/25	11/37/135/135	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
24	CLA	D	404	-	1/1/20/25	2/37/135/135	-
37	DGD	C	516	-	-	14/51/91/95	0/2/2/2
24	CLA	d	403	41	2/2/20/25	8/37/135/135	-
26	BCR	C	515	-	-	6/29/63/63	0/2/2/2
28	GOL	v	202	-	-	2/4/4/4	-
28	GOL	o	301	-	-	2/4/4/4	-
36	HTG	c	523	-	-	3/10/30/30	0/1/1/1
37	DGD	c	519	-	-	15/51/91/95	0/2/2/2
24	CLA	b	615	-	3/3/20/25	11/37/135/135	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
34	LMG	C	520	-	-	13/46/66/70	0/1/1/1
38	LHG	d	410	-	-	16/53/53/53	-
28	GOL	b	606	-	-	2/4/4/4	-
28	GOL	V	203	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	609	-	2/2/20/25	0/37/135/135	-
38	LHG	D	409	-	-	14/53/53/53	-
26	BCR	b	627	-	-	1/29/63/63	0/2/2/2
28	GOL	F	103	35	-	1/4/4/4	-
26	BCR	H	101	-	-	6/29/63/63	0/2/2/2
28	GOL	v	201	-	-	1/4/4/4	-
34	LMG	D	415	40	-	8/46/66/70	0/1/1/1
24	CLA	A	406	41	3/3/20/25	5/37/135/135	-
38	LHG	D	411	-	-	12/53/53/53	-
37	DGD	h	102	-	-	10/51/91/95	0/2/2/2
28	GOL	T	102	-	-	2/4/4/4	-
24	CLA	D	405	-	3/3/20/25	4/37/135/135	-
38	LHG	D	410	-	-	6/53/53/53	-
24	CLA	b	612	-	2/2/20/25	10/37/135/135	-
32	PL9	a	416[B]	-	-	15/53/73/73	0/1/1/1
36	HTG	B	622	-	-	2/10/30/30	0/1/1/1
24	CLA	a	409	-	3/3/20/25	6/37/135/135	-
24	CLA	B	603	-	3/3/20/25	3/37/135/135	-
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
36	HTG	c	524	-	-	2/10/30/30	0/1/1/1
25	PHO	D	401[A]	-	-	2/53/103/103	0/5/6/6
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
34	LMG	C	519	-	-	8/46/66/70	0/1/1/1
24	CLA	c	505	-	3/3/20/25	3/37/135/135	-
36	HTG	V	206	-	-	4/10/30/30	0/1/1/1
25	PHO	D	401[B]	-	-	2/53/103/103	0/5/6/6
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	B	604	-	3/3/20/25	5/37/135/135	-
24	CLA	B	616	-	3/3/20/25	9/37/135/135	-
24	CLA	C	509	-	3/3/20/25	14/37/135/135	-
37	DGD	D	408	-	-	21/47/67/95	0/1/1/2
39	HEM	v	206	16	-	0/6/54/54	-
24	CLA	b	621	-	3/3/20/25	1/37/135/135	-
25	PHO	A	408	-	-	3/53/103/103	0/5/6/6
29	LMT	D	403	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
24	CLA	B	615	-	2/2/20/25	17/37/135/135	-
36	HTG	D	414	-	-	0/7/27/30	0/1/1/1
37	DGD	c	520	-	-	18/51/91/95	0/2/2/2
29	LMT	M	102	-	-	10/21/61/61	0/2/2/2
34	LMG	k	101	-	-	14/46/66/70	0/1/1/1
37	DGD	C	518	-	-	12/51/91/95	0/2/2/2
28	GOL	a	421	35	-	2/4/4/4	-
36	HTG	B	631	-	-	1/10/30/30	0/1/1/1
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	CLA	b	613	-	3/3/20/25	5/37/135/135	-
24	CLA	C	503	-	3/3/20/25	3/37/135/135	-
32	PL9	a	416[A]	-	-	18/53/73/73	0/1/1/1
29	LMT	m	102	-	-	10/21/61/61	0/2/2/2
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
24	CLA	b	614	-	3/3/20/25	7/37/135/135	-
28	GOL	O	301	-	-	3/4/4/4	-
24	CLA	c	512	-	3/3/20/25	4/37/135/135	-
29	LMT	m	103	-	-	8/21/61/61	0/2/2/2
24	CLA	B	612	-	3/3/20/25	1/37/135/135	-
25	PHO	d	402[A]	-	-	1/53/103/103	0/5/6/6
27	SQD	a	405	-	-	12/49/69/69	0/1/1/1
24	CLA	b	618	-	3/3/20/25	3/37/135/135	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	c	514	-	3/3/20/25	8/37/135/135	-
24	CLA	a	412	-	3/3/20/25	10/37/135/135	-
24	CLA	c	506	-	2/2/20/25	4/37/135/135	-
24	CLA	B	611	41	3/3/20/25	4/37/135/135	-
27	SQD	A	411	-	-	12/49/69/69	0/1/1/1
28	GOL	B	628	-	-	2/4/4/4	-
36	HTG	b	608	-	-	0/10/30/30	0/1/1/1
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
38	LHG	a	420	-	-	18/46/46/53	-
28	GOL	c	501	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	509	-	2/2/20/25	3/37/135/135	-
29	LMT	a	404	-	-	7/21/61/61	0/2/2/2
24	CLA	B	607	-	3/3/20/25	5/37/135/135	-
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
28	GOL	B	629	-	-	4/4/4/4	-
24	CLA	B	608	41	3/3/20/25	5/37/135/135	-
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
24	CLA	B	602	41	3/3/20/25	15/37/135/135	-
24	CLA	b	610	41	3/3/20/25	15/37/135/135	-
24	CLA	b	611	-	2/2/20/25	4/37/135/135	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
24	CLA	C	502	-	3/3/20/25	5/37/135/135	-
24	CLA	b	623	-	3/3/20/25	21/37/135/135	-
24	CLA	b	617	-	2/2/20/25	2/37/135/135	-
26	BCR	b	626	-	-	3/29/63/63	0/2/2/2
24	CLA	c	516	-	3/3/20/25	8/37/135/135	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LMT	e	102	-	-	10/21/61/61	0/2/2/2
24	CLA	C	508	-	3/3/20/25	7/37/135/135	-
29	LMT	A	414	-	-	6/21/61/61	0/2/2/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	b	625	-	3/3/20/25	11/37/135/135	-
34	LMG	d	415	40	-	10/46/66/70	0/1/1/1
28	GOL	B	625	-	-	0/4/4/4	-
24	CLA	c	511	41	3/3/20/25	3/37/135/135	-
24	CLA	c	515	3	3/3/20/25	6/37/135/135	-
32	PL9	d	407[A]	-	-	5/53/73/73	0/1/1/1
26	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
38	LHG	d	408	-	-	13/53/53/53	-
32	PL9	A	417[B]	-	-	10/53/73/73	0/1/1/1
28	GOL	a	401	-	-	2/4/4/4	-
28	GOL	C	525	-	-	2/4/4/4	-
38	LHG	E	101	-	-	23/46/46/53	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
34	LMG	A	419	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	620	-	3/3/20/25	7/37/135/135	-
24	CLA	B	617	-	3/3/20/25	6/37/135/135	-
28	GOL	V	201	-	-	2/4/4/4	-
28	GOL	D	402	-	-	4/4/4/4	-
28	GOL	T	101	-	-	0/4/4/4	-
24	CLA	d	405	-	3/3/20/25	6/37/135/135	-
24	CLA	C	504	41	3/3/20/25	6/37/135/135	-
39	HEM	f	101	5,6	-	0/6/54/54	-
28	GOL	v	204	-	-	2/4/4/4	-
36	HTG	b	631	-	-	2/10/30/30	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
37	DGD	c	521	-	-	14/51/91/95	0/2/2/2
38	LHG	d	409	-	-	10/53/53/53	-
37	DGD	C	517	-	-	20/51/91/95	0/2/2/2
24	CLA	A	407	41	2/2/20/25	5/37/135/135	-
24	CLA	B	605	-	3/3/20/25	5/37/135/135	-
24	CLA	C	512	-	3/3/20/25	6/37/135/135	-
28	GOL	a	402	-	-	2/4/4/4	-
24	CLA	c	513	-	3/3/20/25	15/37/135/135	-
24	CLA	C	501	-	3/3/20/25	12/37/135/135	-
36	HTG	C	523	-	-	3/10/30/30	0/1/1/1
28	GOL	t	103	-	-	0/4/4/4	-
24	CLA	c	507	-	3/3/20/25	6/37/135/135	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2
24	CLA	b	619	41	3/3/20/25	7/37/135/135	-
24	CLA	a	410	41	2/2/20/25	10/37/135/135	-
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
32	PL9	D	407[A]	-	-	7/53/73/73	0/1/1/1
29	LMT	T	104	-	-	9/17/37/61	0/1/1/2
39	HEM	E	103	5,6	-	0/6/54/54	-
36	HTG	C	522	-	-	1/10/30/30	0/1/1/1
37	DGD	e	101	-	-	26/51/91/95	0/2/2/2
32	PL9	D	407[B]	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	413	-	-	17/49/69/69	0/1/1/1
24	CLA	A	409	-	2/2/20/25	10/37/135/135	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
24	CLA	B	613	-	3/3/20/25	3/37/135/135	-
38	LHG	L	101	-	-	13/53/53/53	-
28	GOL	b	604	-	-	2/4/4/4	-
34	LMG	a	415	-	-	17/46/66/70	0/1/1/1
24	CLA	b	624	-	3/3/20/25	5/37/135/135	-
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
24	CLA	C	505	-	1/1/20/25	6/37/135/135	-
28	GOL	c	502	-	-	2/4/4/4	-
28	GOL	V	204	-	-	4/4/4/4	-
24	CLA	b	616	41	3/3/20/25	1/37/135/135	-
29	LMT	E	102	-	-	4/21/61/61	0/2/2/2
28	GOL	b	603	-	-	0/4/4/4	-
24	CLA	C	511	3	2/2/20/25	2/37/135/135	-
25	PHO	d	402[B]	-	-	4/53/103/103	0/5/6/6
29	LMT	C	521	-	-	9/21/61/61	0/2/2/2
36	HTG	b	607	-	-	3/10/30/30	0/1/1/1
28	GOL	B	634	-	-	0/4/4/4	-
26	BCR	c	518	-	-	4/29/63/63	0/2/2/2
24	CLA	C	510	-	3/3/20/25	11/37/135/135	-
34	LMG	c	522	-	-	7/46/66/70	0/1/1/1
36	HTG	B	623	-	-	6/10/30/30	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
24	CLA	B	610	-	3/3/20/25	6/37/135/135	-
36	HTG	B	624	-	-	4/10/30/30	0/1/1/1
26	BCR	t	102	-	-	7/29/63/63	0/2/2/2
36	HTG	B	632	-	-	0/10/30/30	0/1/1/1
28	GOL	C	524	-	-	1/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
28	GOL	b	605	-	-	2/4/4/4	-
36	HTG	d	413	-	-	1/7/27/30	0/1/1/1
24	CLA	c	508	41	3/3/20/25	9/37/135/135	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	506	-	3/3/20/25	10/37/135/135	-
38	LHG	b	634	-	-	15/53/53/53	-
37	DGD	H	102	-	-	10/51/91/95	0/2/2/2
34	LMG	b	629	-	-	11/46/66/70	0/1/1/1

All (1185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-C2B	6.56	1.49	1.40
24	B	613	CLA	C3B-C2B	6.55	1.49	1.40
24	c	513	CLA	C3B-C2B	6.49	1.49	1.40
24	C	511	CLA	C3B-C2B	6.48	1.49	1.40
24	D	404	CLA	C3B-C2B	6.47	1.49	1.40
24	C	509	CLA	C3B-C2B	6.47	1.49	1.40
24	B	605	CLA	C3B-C2B	6.33	1.49	1.40
24	B	603	CLA	C3B-C2B	6.31	1.49	1.40
24	A	406	CLA	C3B-C2B	6.30	1.49	1.40
24	b	621	CLA	C3B-C2B	6.30	1.49	1.40
24	B	616	CLA	C3D-C2D	6.28	1.50	1.39
24	b	613	CLA	C3B-C2B	6.25	1.49	1.40
24	b	619	CLA	C3B-C2B	6.23	1.49	1.40
24	c	514	CLA	C3B-C2B	6.23	1.49	1.40
24	C	504	CLA	C3B-C2B	6.21	1.49	1.40
24	B	615	CLA	C3B-C2B	6.21	1.49	1.40
24	b	611	CLA	C3B-C2B	6.21	1.49	1.40
24	b	610	CLA	C3D-C2D	6.20	1.50	1.39
24	b	610	CLA	C3B-C2B	6.19	1.49	1.40
24	c	511	CLA	C3B-C2B	6.16	1.48	1.40
24	A	405	CLA	C3B-C2B	6.16	1.48	1.40
24	C	511	CLA	C3D-C2D	6.15	1.50	1.39
24	C	510	CLA	C3B-C2B	6.14	1.48	1.40
24	a	409	CLA	C3B-C2B	6.14	1.48	1.40
24	c	508	CLA	C3B-C2B	6.13	1.48	1.40
24	b	620	CLA	C3B-C2B	6.12	1.48	1.40
24	b	623	CLA	C3B-C2B	6.12	1.48	1.40
24	b	622	CLA	C3B-C2B	6.10	1.48	1.40
24	C	508	CLA	C3B-C2B	6.10	1.48	1.40
24	b	624	CLA	C3D-C2D	6.10	1.50	1.39
24	A	405	CLA	C3D-C2D	6.10	1.50	1.39
24	C	512	CLA	C3D-C2D	6.09	1.50	1.39
24	c	512	CLA	C3B-C2B	6.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3D-C2D	6.08	1.50	1.39
24	B	609	CLA	C3B-C2B	6.07	1.48	1.40
24	C	504	CLA	C3D-C2D	6.06	1.50	1.39
24	b	612	CLA	C3B-C2B	6.06	1.48	1.40
24	c	516	CLA	C3D-C2D	6.05	1.50	1.39
24	B	617	CLA	C3B-C2B	6.05	1.48	1.40
24	d	405	CLA	C3D-C2D	6.01	1.50	1.39
24	C	502	CLA	C3B-C2B	6.01	1.48	1.40
24	B	612	CLA	C3B-C2B	6.00	1.48	1.40
24	B	611	CLA	C3B-C2B	5.99	1.48	1.40
24	c	506	CLA	C3B-C2B	5.99	1.48	1.40
24	C	502	CLA	C3D-C2D	5.98	1.50	1.39
24	b	615	CLA	C3B-C2B	5.97	1.48	1.40
24	d	403	CLA	C3B-C2B	5.96	1.48	1.40
25	D	401[B]	PHO	C3C-C2C	5.95	1.49	1.36
24	c	515	CLA	C3B-C2B	5.95	1.48	1.40
25	d	402[B]	PHO	C3B-C2B	5.94	1.49	1.37
25	d	402[B]	PHO	C3C-C2C	5.94	1.49	1.36
24	c	505	CLA	C3B-C2B	5.94	1.48	1.40
24	C	506	CLA	C3D-C2D	5.93	1.50	1.39
24	c	510	CLA	C3B-C2B	5.93	1.48	1.40
24	C	513	CLA	C3B-C2B	5.90	1.48	1.40
24	c	512	CLA	C3D-C2D	5.87	1.50	1.39
24	b	625	CLA	C3B-C2B	5.87	1.48	1.40
24	A	406	CLA	C3D-C2D	5.87	1.50	1.39
24	b	617	CLA	C3D-C2D	5.87	1.50	1.39
25	D	401[A]	PHO	C3B-C2B	5.86	1.49	1.37
24	B	612	CLA	C3D-C2D	5.85	1.49	1.39
24	a	410	CLA	C3B-C2B	5.84	1.48	1.40
24	B	602	CLA	C3B-C2B	5.84	1.48	1.40
24	B	615	CLA	C3D-C2D	5.82	1.49	1.39
25	d	402[A]	PHO	C3C-C2C	5.82	1.49	1.36
25	A	408	PHO	C3B-C2B	5.82	1.49	1.37
24	a	409	CLA	C3D-C2D	5.81	1.49	1.39
24	b	625	CLA	C3D-C2D	5.81	1.49	1.39
24	b	617	CLA	C3B-C2B	5.81	1.48	1.40
24	b	614	CLA	C3B-C2B	5.81	1.48	1.40
24	b	613	CLA	C3D-C2D	5.81	1.49	1.39
24	b	624	CLA	C3B-C2B	5.80	1.48	1.40
24	d	404	CLA	C3D-C2D	5.79	1.49	1.39
24	C	503	CLA	C3D-C2D	5.79	1.49	1.39
24	C	510	CLA	C3D-C2D	5.78	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C3D-C2D	5.78	1.49	1.39
24	c	506	CLA	C3D-C2D	5.77	1.49	1.39
25	D	401[B]	PHO	C3B-C2B	5.77	1.49	1.37
24	B	603	CLA	C3C-C2C	5.76	1.49	1.36
24	C	512	CLA	C3B-C2B	5.76	1.48	1.40
24	B	611	CLA	C3C-C2C	5.76	1.49	1.36
24	B	607	CLA	C3B-C2B	5.76	1.48	1.40
24	B	608	CLA	C3B-C2B	5.75	1.48	1.40
24	C	501	CLA	C3D-C2D	5.75	1.49	1.39
24	c	508	CLA	C3D-C2D	5.73	1.49	1.39
24	c	511	CLA	C3D-C2D	5.72	1.49	1.39
25	A	408	PHO	C3C-C2C	5.69	1.48	1.36
24	B	604	CLA	C3C-C2C	5.69	1.48	1.36
24	B	613	CLA	C3D-C2D	5.69	1.49	1.39
24	c	517	CLA	C3D-C2D	5.67	1.49	1.39
24	b	614	CLA	C3D-C2D	5.67	1.49	1.39
24	c	507	CLA	C3B-C2B	5.66	1.48	1.40
25	a	411	PHO	C3B-C2B	5.66	1.48	1.37
24	C	501	CLA	C3B-C2B	5.66	1.48	1.40
24	b	618	CLA	C3D-C2D	5.66	1.49	1.39
24	b	612	CLA	C3D-C2D	5.65	1.49	1.39
24	C	508	CLA	C3C-C2C	5.65	1.48	1.36
24	C	509	CLA	C3D-C2D	5.65	1.49	1.39
24	B	604	CLA	C3B-C2B	5.65	1.48	1.40
24	b	623	CLA	C3D-C2D	5.64	1.49	1.39
24	c	513	CLA	C3D-C2D	5.64	1.49	1.39
24	b	610	CLA	C3C-C2C	5.63	1.48	1.36
24	d	403	CLA	C3D-C2D	5.63	1.49	1.39
24	c	516	CLA	C3B-C2B	5.62	1.48	1.40
24	C	507	CLA	C3D-C2D	5.62	1.49	1.39
25	a	411	PHO	C3C-C2C	5.61	1.48	1.36
24	b	615	CLA	C3D-C2D	5.61	1.49	1.39
24	C	508	CLA	C3D-C2D	5.61	1.49	1.39
24	C	513	CLA	C3D-C2D	5.60	1.49	1.39
24	D	405	CLA	C3D-C2D	5.60	1.49	1.39
24	c	507	CLA	C3D-C2D	5.59	1.49	1.39
24	B	602	CLA	C3D-C2D	5.57	1.49	1.39
24	B	603	CLA	C3D-C2D	5.57	1.49	1.39
24	b	621	CLA	C3D-C2D	5.57	1.49	1.39
24	B	609	CLA	C3D-C2D	5.57	1.49	1.39
24	b	616	CLA	C3D-C2D	5.56	1.49	1.39
24	C	505	CLA	C3B-C2B	5.56	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C3D-C2D	5.56	1.49	1.39
24	C	507	CLA	C3B-C2B	5.56	1.48	1.40
24	B	602	CLA	C3C-C2C	5.55	1.48	1.36
24	A	407	CLA	C3D-C2D	5.55	1.49	1.39
24	C	503	CLA	C3B-C2B	5.53	1.48	1.40
24	a	412	CLA	C3D-C2D	5.53	1.49	1.39
24	d	404	CLA	C3B-C2B	5.52	1.48	1.40
24	B	617	CLA	C3D-C2D	5.52	1.49	1.39
24	c	505	CLA	C3D-C2D	5.52	1.49	1.39
24	c	517	CLA	C3B-C2B	5.51	1.48	1.40
24	c	515	CLA	C3D-C2D	5.50	1.49	1.39
24	c	509	CLA	C3B-C2B	5.50	1.48	1.40
24	A	407	CLA	C3B-C2B	5.50	1.48	1.40
24	B	611	CLA	C3D-C2D	5.49	1.49	1.39
24	d	405	CLA	C3B-C2B	5.49	1.48	1.40
24	A	406	CLA	C3C-C2C	5.48	1.48	1.36
24	c	516	CLA	C3C-C2C	5.48	1.48	1.36
24	C	503	CLA	CHC-C1C	5.46	1.49	1.35
24	C	512	CLA	C3C-C2C	5.46	1.48	1.36
24	C	510	CLA	C3C-C2C	5.46	1.48	1.36
24	b	622	CLA	C3D-C2D	5.45	1.49	1.39
24	b	611	CLA	C3C-C2C	5.45	1.48	1.36
24	b	620	CLA	C3D-C2D	5.45	1.49	1.39
24	C	506	CLA	C3B-C2B	5.44	1.47	1.40
25	d	402[A]	PHO	CHC-C1C	5.44	1.49	1.38
24	a	412	CLA	C3B-C2B	5.44	1.47	1.40
25	D	401[A]	PHO	C3C-C2C	5.44	1.48	1.36
25	d	402[A]	PHO	C3B-C2B	5.43	1.48	1.37
24	C	503	CLA	C3C-C2C	5.43	1.48	1.36
24	B	616	CLA	O2D-CGD	5.42	1.46	1.33
24	D	404	CLA	C3D-C2D	5.42	1.49	1.39
24	A	405	CLA	C3C-C2C	5.41	1.48	1.36
24	C	501	CLA	CHC-C1C	5.40	1.48	1.35
24	c	517	CLA	C3C-C2C	5.39	1.48	1.36
24	b	621	CLA	C3C-C2C	5.39	1.48	1.36
24	c	514	CLA	C3D-C2D	5.39	1.49	1.39
24	c	514	CLA	C3C-C2C	5.39	1.48	1.36
24	B	607	CLA	C3C-C2C	5.39	1.48	1.36
24	D	405	CLA	C3B-C2B	5.38	1.47	1.40
24	B	615	CLA	C3C-C2C	5.38	1.48	1.36
24	A	405	CLA	CHC-C1C	5.38	1.48	1.35
24	b	616	CLA	C3B-C2B	5.38	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C3C-C2C	5.37	1.48	1.36
24	C	501	CLA	C3C-C2C	5.37	1.48	1.36
24	b	615	CLA	C3C-C2C	5.37	1.48	1.36
24	a	412	CLA	C3C-C2C	5.37	1.48	1.36
24	a	409	CLA	C3C-C2C	5.37	1.48	1.36
24	B	606	CLA	C3B-C2B	5.36	1.47	1.40
24	c	507	CLA	C3C-C2C	5.35	1.48	1.36
24	b	611	CLA	C3D-C2D	5.35	1.49	1.39
24	b	618	CLA	C3B-C2B	5.35	1.47	1.40
24	c	516	CLA	CHC-C1C	5.35	1.48	1.35
24	B	606	CLA	O2D-CGD	5.34	1.46	1.33
24	B	617	CLA	C3C-C2C	5.34	1.48	1.36
24	B	616	CLA	CHC-C1C	5.33	1.48	1.35
24	b	619	CLA	C3C-C2C	5.33	1.48	1.36
24	b	622	CLA	C3C-C2C	5.32	1.48	1.36
25	a	411	PHO	CHB-C1B	5.32	1.49	1.38
24	B	611	CLA	CHC-C1C	5.31	1.48	1.35
24	C	513	CLA	C3C-C2C	5.31	1.48	1.36
24	C	505	CLA	C3D-C2D	5.31	1.48	1.39
25	a	411	PHO	O2D-CGD	5.30	1.46	1.33
24	a	410	CLA	C3D-C2D	5.30	1.48	1.39
24	D	404	CLA	C3C-C2C	5.30	1.48	1.36
24	c	511	CLA	CHC-C1C	5.30	1.48	1.35
24	a	412	CLA	O2D-CGD	5.30	1.46	1.33
24	B	616	CLA	C3B-C2B	5.29	1.47	1.40
24	B	608	CLA	CHC-C1C	5.29	1.48	1.35
24	B	608	CLA	C3D-C2D	5.29	1.48	1.39
24	C	504	CLA	CHC-C1C	5.29	1.48	1.35
24	b	617	CLA	C3C-C2C	5.29	1.48	1.36
24	b	618	CLA	O2D-CGD	5.28	1.46	1.33
24	b	617	CLA	CHC-C1C	5.28	1.48	1.35
24	b	624	CLA	C3C-C2C	5.28	1.47	1.36
24	C	509	CLA	C3C-C2C	5.27	1.47	1.36
24	b	618	CLA	OBD-CAD	5.27	1.29	1.22
24	A	407	CLA	C3C-C2C	5.26	1.47	1.36
24	c	506	CLA	C3C-C2C	5.26	1.47	1.36
24	b	619	CLA	C3D-C2D	5.26	1.48	1.39
24	D	405	CLA	C3C-C2C	5.25	1.47	1.36
24	b	625	CLA	CHC-C1C	5.25	1.48	1.35
24	d	403	CLA	C3C-C2C	5.25	1.47	1.36
24	B	615	CLA	O2D-CGD	5.25	1.46	1.33
24	c	513	CLA	C3C-C2C	5.25	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	CHC-C1C	5.25	1.48	1.35
24	b	622	CLA	O2D-CGD	5.24	1.46	1.33
24	b	611	CLA	CHC-C1C	5.24	1.48	1.35
26	C	514	BCR	C23-C22	-5.24	1.34	1.45
24	b	620	CLA	O2D-CGD	5.24	1.46	1.33
24	B	613	CLA	CHC-C1C	5.24	1.48	1.35
24	C	505	CLA	C3C-C2C	5.23	1.47	1.36
24	c	510	CLA	C3D-C2D	5.23	1.48	1.39
24	c	509	CLA	C3C-C2C	5.23	1.47	1.36
24	c	509	CLA	CHC-C1C	5.22	1.48	1.35
24	B	603	CLA	OBD-CAD	5.22	1.29	1.22
24	b	614	CLA	C3C-C2C	5.22	1.47	1.36
26	k	102	BCR	C23-C22	-5.22	1.34	1.45
24	c	506	CLA	O2D-CGD	5.21	1.45	1.33
24	B	604	CLA	C3D-C2D	5.21	1.48	1.39
24	d	405	CLA	CHC-C1C	5.21	1.48	1.35
24	d	405	CLA	O2D-CGD	5.20	1.45	1.33
24	B	610	CLA	C3C-C2C	5.20	1.47	1.36
24	B	612	CLA	C3C-C2C	5.20	1.47	1.36
24	c	510	CLA	O2D-CGD	5.20	1.45	1.33
24	A	407	CLA	CHC-C1C	5.20	1.48	1.35
24	B	603	CLA	CHC-C1C	5.20	1.48	1.35
24	B	602	CLA	O2D-CGD	5.20	1.45	1.33
25	D	401[B]	PHO	CHB-C1B	5.20	1.48	1.38
25	a	411	PHO	CHD-C1D	5.18	1.48	1.38
24	B	609	CLA	C3C-C2C	5.18	1.47	1.36
25	D	401[B]	PHO	O2D-CGD	5.18	1.45	1.33
24	B	607	CLA	O2D-CGD	5.18	1.45	1.33
24	B	607	CLA	CHC-C1C	5.18	1.48	1.35
24	B	606	CLA	C3D-C2D	5.18	1.48	1.39
24	c	512	CLA	C3C-C2C	5.17	1.47	1.36
24	C	504	CLA	C3C-C2C	5.17	1.47	1.36
24	C	505	CLA	CHC-C1C	5.16	1.48	1.35
24	b	610	CLA	CHC-C1C	5.16	1.48	1.35
24	c	512	CLA	CHC-C1C	5.15	1.48	1.35
25	A	408	PHO	CHD-C1D	5.15	1.48	1.38
25	d	402[A]	PHO	CHB-C1B	5.14	1.48	1.38
24	B	604	CLA	CHC-C1C	5.14	1.48	1.35
24	B	617	CLA	O2D-CGD	5.14	1.45	1.33
24	A	409	CLA	C3B-C2B	5.14	1.47	1.40
24	b	621	CLA	OBD-CAD	5.13	1.29	1.22
24	c	507	CLA	CHC-C1C	5.13	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	O2D-CGD	5.13	1.45	1.33
24	C	507	CLA	CHC-C1C	5.12	1.48	1.35
25	a	411	PHO	CHC-C1C	5.12	1.48	1.38
24	A	409	CLA	CHC-C1C	5.12	1.48	1.35
26	Y	101	BCR	C23-C22	-5.11	1.35	1.45
24	B	602	CLA	CHC-C1C	5.11	1.48	1.35
24	C	508	CLA	CHC-C1C	5.10	1.48	1.35
24	d	405	CLA	C3C-C2C	5.10	1.47	1.36
24	b	618	CLA	CHC-C1C	5.10	1.48	1.35
24	c	509	CLA	C3D-C2D	5.10	1.48	1.39
24	B	614	CLA	O2D-CGD	5.10	1.45	1.33
24	b	616	CLA	CHC-C1C	5.10	1.48	1.35
24	A	409	CLA	O2D-CGD	5.09	1.45	1.33
24	d	404	CLA	C3C-C2C	5.09	1.47	1.36
24	C	508	CLA	O2D-CGD	5.08	1.45	1.33
24	a	410	CLA	CHC-C1C	5.08	1.48	1.35
24	B	610	CLA	O2D-CGD	5.08	1.45	1.33
24	C	502	CLA	CHC-C1C	5.08	1.48	1.35
24	b	621	CLA	O2D-CGD	5.08	1.45	1.33
24	C	510	CLA	O2D-CGD	5.07	1.45	1.33
24	B	605	CLA	C3D-C2D	5.07	1.48	1.39
24	c	510	CLA	C3C-C2C	5.07	1.47	1.36
24	B	617	CLA	CHC-C1C	5.07	1.48	1.35
24	B	606	CLA	C3C-C2C	5.07	1.47	1.36
25	D	401[B]	PHO	CHC-C1C	5.07	1.48	1.38
24	a	410	CLA	OBD-CAD	5.06	1.29	1.22
24	c	505	CLA	C3C-C2C	5.06	1.47	1.36
24	b	612	CLA	C3C-C2C	5.06	1.47	1.36
24	c	511	CLA	C3C-C2C	5.05	1.47	1.36
24	C	511	CLA	C3C-C2C	5.05	1.47	1.36
24	b	617	CLA	O2D-CGD	5.05	1.45	1.33
24	c	513	CLA	CHC-C1C	5.05	1.47	1.35
24	b	619	CLA	CHC-C1C	5.05	1.47	1.35
24	c	515	CLA	C3C-C2C	5.04	1.47	1.36
24	B	605	CLA	C3C-C2C	5.04	1.47	1.36
24	c	507	CLA	O2D-CGD	5.04	1.45	1.33
24	C	502	CLA	O2D-CGD	5.04	1.45	1.33
24	b	623	CLA	O2D-CGD	5.04	1.45	1.33
24	a	410	CLA	C3C-C2C	5.04	1.47	1.36
24	C	511	CLA	CHC-C1C	5.04	1.47	1.35
26	t	102	BCR	C23-C22	-5.04	1.35	1.45
24	b	614	CLA	CHC-C1C	5.04	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	623	CLA	C3C-C2C	5.04	1.47	1.36
24	C	511	CLA	O2D-CGD	5.04	1.45	1.33
24	C	513	CLA	CHC-C1C	5.03	1.47	1.35
24	b	611	CLA	OBD-CAD	5.03	1.29	1.22
25	d	402[B]	PHO	O2D-CGD	5.03	1.45	1.33
24	b	623	CLA	CHC-C1C	5.03	1.47	1.35
26	h	101	BCR	C23-C22	-5.03	1.35	1.45
25	D	401[A]	PHO	O2D-CGD	5.03	1.45	1.33
25	A	408	PHO	CHC-C1C	5.03	1.48	1.38
24	b	625	CLA	C3C-C2C	5.02	1.47	1.36
24	A	409	CLA	C3C-C2C	5.02	1.47	1.36
24	C	509	CLA	O2D-CGD	5.02	1.45	1.33
24	c	505	CLA	O2D-CGD	5.02	1.45	1.33
25	A	408	PHO	CHB-C1B	5.02	1.48	1.38
24	C	509	CLA	CHC-C1C	5.02	1.47	1.35
26	b	628	BCR	C23-C22	-5.02	1.35	1.45
24	c	508	CLA	CHC-C1C	5.02	1.47	1.35
24	b	625	CLA	O2D-CGD	5.01	1.45	1.33
24	B	607	CLA	C3D-C2D	5.01	1.48	1.39
24	b	614	CLA	O2D-CGD	5.01	1.45	1.33
24	C	504	CLA	O2D-CGD	5.00	1.45	1.33
26	K	101	BCR	C23-C22	-5.00	1.35	1.45
26	A	410	BCR	C23-C22	-5.00	1.35	1.45
24	c	517	CLA	CHC-C1C	5.00	1.47	1.35
24	C	512	CLA	O2D-CGD	5.00	1.45	1.33
24	C	506	CLA	O2D-CGD	5.00	1.45	1.33
24	c	505	CLA	CHC-C1C	5.00	1.47	1.35
24	C	502	CLA	C3C-C2C	5.00	1.47	1.36
24	B	614	CLA	OBD-CAD	4.99	1.29	1.22
24	B	613	CLA	C3C-C2C	4.99	1.47	1.36
24	b	610	CLA	O2D-CGD	4.99	1.45	1.33
24	c	515	CLA	CHC-C1C	4.99	1.47	1.35
24	c	513	CLA	O2D-CGD	4.99	1.45	1.33
24	B	611	CLA	OBD-CAD	4.98	1.29	1.22
24	A	405	CLA	O2D-CGD	4.98	1.45	1.33
24	b	612	CLA	CHC-C1C	4.97	1.47	1.35
24	c	514	CLA	CHC-C1C	4.97	1.47	1.35
24	c	508	CLA	O2D-CGD	4.97	1.45	1.33
24	b	624	CLA	CHC-C1C	4.97	1.47	1.35
24	a	412	CLA	CHC-C1C	4.97	1.47	1.35
24	b	612	CLA	O2D-CGD	4.97	1.45	1.33
25	D	401[A]	PHO	CHC-C1C	4.97	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	O2D-CGD	4.96	1.45	1.33
25	d	402[B]	PHO	CHB-C1B	4.96	1.48	1.38
24	B	615	CLA	CHC-C1C	4.96	1.47	1.35
24	A	407	CLA	O2D-CGD	4.96	1.45	1.33
24	d	404	CLA	CHC-C1C	4.96	1.47	1.35
24	c	517	CLA	O2D-CGD	4.95	1.45	1.33
24	b	620	CLA	C3C-C2C	4.95	1.47	1.36
24	B	614	CLA	C3C-C2C	4.95	1.47	1.36
24	b	619	CLA	OBD-CAD	4.94	1.29	1.22
24	a	409	CLA	CHC-C1C	4.93	1.47	1.35
25	A	408	PHO	O2D-CGD	4.93	1.45	1.33
26	c	526	BCR	C23-C22	-4.93	1.35	1.45
24	B	608	CLA	C3C-C2C	4.93	1.47	1.36
24	B	614	CLA	CHC-C1C	4.93	1.47	1.35
25	D	401[A]	PHO	CHD-C1D	4.92	1.48	1.38
26	C	515	BCR	C23-C22	-4.92	1.35	1.45
24	B	606	CLA	CHC-C1C	4.92	1.47	1.35
24	B	612	CLA	O2D-CGD	4.91	1.45	1.33
24	b	619	CLA	O2D-CGD	4.91	1.45	1.33
24	B	613	CLA	OBD-CAD	4.91	1.29	1.22
24	c	516	CLA	O2D-CGD	4.91	1.45	1.33
24	C	506	CLA	CHC-C1C	4.91	1.47	1.35
24	B	609	CLA	O2D-CGD	4.90	1.45	1.33
24	C	513	CLA	O2D-CGD	4.90	1.45	1.33
24	c	508	CLA	C3C-C2C	4.90	1.47	1.36
24	b	613	CLA	C3C-C2C	4.90	1.47	1.36
24	c	516	CLA	OBD-CAD	4.89	1.29	1.22
24	D	405	CLA	CHC-C1C	4.89	1.47	1.35
24	b	618	CLA	C3C-C2C	4.89	1.47	1.36
24	b	615	CLA	CHC-C1C	4.89	1.47	1.35
24	b	613	CLA	CHC-C1C	4.88	1.47	1.35
24	c	513	CLA	OBD-CAD	4.88	1.29	1.22
25	d	402[B]	PHO	CHC-C1C	4.88	1.48	1.38
25	D	401[A]	PHO	CHB-C1B	4.87	1.48	1.38
24	C	506	CLA	C3C-C2C	4.87	1.47	1.36
24	b	621	CLA	CHC-C1C	4.86	1.47	1.35
26	c	518	BCR	C23-C22	-4.86	1.35	1.45
24	C	510	CLA	CHC-C1C	4.86	1.47	1.35
24	c	506	CLA	CHC-C1C	4.86	1.47	1.35
26	y	101	BCR	C23-C22	-4.86	1.35	1.45
24	C	505	CLA	O2D-CGD	4.85	1.45	1.33
24	b	616	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	OBD-CAD	4.85	1.29	1.22
24	b	617	CLA	OBD-CAD	4.85	1.29	1.22
26	D	406	BCR	C23-C22	-4.85	1.35	1.45
24	B	616	CLA	C3C-C2C	4.85	1.47	1.36
24	B	608	CLA	O2D-CGD	4.83	1.45	1.33
26	H	101	BCR	C23-C22	-4.83	1.35	1.45
24	B	610	CLA	CHC-C1C	4.83	1.47	1.35
24	A	406	CLA	OBD-CAD	4.83	1.29	1.22
24	c	510	CLA	CHC-C1C	4.82	1.47	1.35
26	T	103	BCR	C23-C22	-4.82	1.35	1.45
24	B	602	CLA	O2A-CGA	4.81	1.47	1.33
24	c	512	CLA	O2D-CGD	4.81	1.44	1.33
24	c	511	CLA	O2D-CGD	4.81	1.44	1.33
24	B	605	CLA	CHC-C1C	4.81	1.47	1.35
24	c	509	CLA	O2D-CGD	4.81	1.44	1.33
26	d	406	BCR	C23-C22	-4.81	1.35	1.45
25	D	401[B]	PHO	CHD-C1D	4.80	1.48	1.38
24	c	509	CLA	OBD-CAD	4.80	1.29	1.22
24	B	603	CLA	O2D-CGD	4.79	1.44	1.33
24	c	514	CLA	O2D-CGD	4.79	1.44	1.33
24	d	403	CLA	O2D-CGD	4.79	1.44	1.33
24	d	404	CLA	O2D-CGD	4.79	1.44	1.33
25	d	402[A]	PHO	O2D-CGD	4.78	1.44	1.33
24	A	406	CLA	O2D-CGD	4.78	1.44	1.33
24	b	611	CLA	O2D-CGD	4.77	1.44	1.33
24	b	622	CLA	CHC-C1C	4.76	1.47	1.35
24	C	501	CLA	OBD-CAD	4.75	1.28	1.22
24	B	604	CLA	O2D-CGD	4.75	1.44	1.33
24	c	514	CLA	OBD-CAD	4.75	1.28	1.22
24	D	405	CLA	O2D-CGD	4.74	1.44	1.33
26	B	620	BCR	C23-C22	-4.74	1.35	1.45
24	B	615	CLA	OBD-CAD	4.74	1.28	1.22
24	B	613	CLA	O2D-CGD	4.73	1.44	1.33
24	B	610	CLA	C3B-C2B	4.73	1.46	1.40
24	C	511	CLA	OBD-CAD	4.73	1.28	1.22
24	b	615	CLA	OBD-CAD	4.73	1.28	1.22
24	B	611	CLA	O2D-CGD	4.72	1.44	1.33
24	C	501	CLA	O2D-CGD	4.71	1.44	1.33
24	b	613	CLA	O2D-CGD	4.70	1.44	1.33
24	B	602	CLA	OBD-CAD	4.70	1.28	1.22
24	C	503	CLA	OBD-CAD	4.70	1.28	1.22
25	d	402[B]	PHO	CHD-C1D	4.70	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	618	BCR	C23-C22	-4.69	1.35	1.45
24	b	624	CLA	O2D-CGD	4.68	1.44	1.33
24	d	403	CLA	CHC-C1C	4.68	1.47	1.35
24	C	510	CLA	OBD-CAD	4.67	1.28	1.22
24	b	616	CLA	OBD-CAD	4.67	1.28	1.22
25	d	402[A]	PHO	CHD-C1D	4.67	1.47	1.38
24	c	515	CLA	O2D-CGD	4.67	1.44	1.33
24	b	610	CLA	OBD-CAD	4.67	1.28	1.22
24	C	513	CLA	OBD-CAD	4.66	1.28	1.22
24	c	512	CLA	OBD-CAD	4.66	1.28	1.22
24	a	409	CLA	O2D-CGD	4.65	1.44	1.33
24	B	609	CLA	OBD-CAD	4.65	1.28	1.22
24	c	511	CLA	OBD-CAD	4.65	1.28	1.22
24	C	507	CLA	OBD-CAD	4.65	1.28	1.22
24	B	612	CLA	CHC-C1C	4.64	1.46	1.35
24	C	509	CLA	OBD-CAD	4.64	1.28	1.22
24	a	410	CLA	O2D-CGD	4.64	1.44	1.33
24	c	517	CLA	OBD-CAD	4.63	1.28	1.22
24	D	405	CLA	OBD-CAD	4.63	1.28	1.22
24	A	406	CLA	CHC-C1C	4.61	1.46	1.35
24	b	620	CLA	CHC-C1C	4.60	1.46	1.35
26	b	627	BCR	C23-C22	-4.59	1.36	1.45
24	d	405	CLA	OBD-CAD	4.59	1.28	1.22
24	B	607	CLA	OBD-CAD	4.58	1.28	1.22
24	b	614	CLA	OBD-CAD	4.57	1.28	1.22
24	C	502	CLA	OBD-CAD	4.56	1.28	1.22
24	b	624	CLA	OBD-CAD	4.56	1.28	1.22
24	B	610	CLA	OBD-CAD	4.56	1.28	1.22
26	a	413	BCR	C23-C22	-4.56	1.36	1.45
24	C	507	CLA	O2D-CGD	4.55	1.44	1.33
24	B	606	CLA	OBD-CAD	4.55	1.28	1.22
27	f	102	SQD	O47-C7	4.55	1.47	1.34
24	A	407	CLA	OBD-CAD	4.54	1.28	1.22
37	D	408	DGD	O1G-C1A	4.53	1.46	1.33
24	b	616	CLA	O2A-CGA	4.53	1.46	1.33
26	b	626	BCR	C23-C22	-4.53	1.36	1.45
34	z	101	LMG	O8-C28	4.53	1.46	1.33
24	C	508	CLA	OBD-CAD	4.53	1.28	1.22
24	C	512	CLA	OBD-CAD	4.52	1.28	1.22
24	B	617	CLA	OBD-CAD	4.52	1.28	1.22
24	a	409	CLA	OBD-CAD	4.52	1.28	1.22
27	a	405	SQD	O48-C23	4.51	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	O2D-CGD	4.50	1.44	1.33
24	C	505	CLA	OBD-CAD	4.49	1.28	1.22
24	b	610	CLA	O2A-CGA	4.49	1.46	1.33
24	c	515	CLA	OBD-CAD	4.49	1.28	1.22
24	c	507	CLA	OBD-CAD	4.48	1.28	1.22
24	b	625	CLA	OBD-CAD	4.48	1.28	1.22
27	A	413	SQD	O48-C23	4.48	1.46	1.33
24	B	616	CLA	OBD-CAD	4.47	1.28	1.22
24	C	508	CLA	O2A-CGA	4.47	1.46	1.33
37	e	101	DGD	O2G-C1B	4.46	1.46	1.34
24	B	609	CLA	CHC-C1C	4.45	1.46	1.35
27	F	101	SQD	O47-C7	4.45	1.46	1.34
24	C	509	CLA	O2A-CGA	4.45	1.46	1.33
24	c	512	CLA	O2A-CGA	4.44	1.46	1.33
26	B	619	BCR	C23-C22	-4.44	1.36	1.45
24	d	405	CLA	O2A-CGA	4.43	1.46	1.33
24	c	513	CLA	O2A-CGA	4.42	1.46	1.33
27	a	405	SQD	O47-C7	4.42	1.46	1.34
24	d	403	CLA	O2A-CGA	4.41	1.46	1.33
24	B	608	CLA	OBD-CAD	4.41	1.28	1.22
24	a	412	CLA	OBD-CAD	4.40	1.28	1.22
24	D	404	CLA	CHC-C1C	4.39	1.46	1.35
24	C	504	CLA	OBD-CAD	4.39	1.28	1.22
38	D	411	LHG	O7-C7	4.39	1.46	1.34
37	D	408	DGD	O2G-C1B	4.39	1.46	1.34
24	D	404	CLA	O2D-CGD	4.38	1.43	1.33
24	d	403	CLA	OBD-CAD	4.38	1.28	1.22
34	C	519	LMG	O8-C28	4.38	1.46	1.33
24	b	624	CLA	O2A-CGA	4.38	1.46	1.33
24	c	506	CLA	OBD-CAD	4.37	1.28	1.22
24	B	615	CLA	O2A-CGA	4.36	1.46	1.33
24	D	404	CLA	OBD-CAD	4.36	1.28	1.22
24	c	510	CLA	OBD-CAD	4.36	1.28	1.22
36	B	622	HTG	C1'-S1	-4.36	1.75	1.81
24	B	604	CLA	O2A-CGA	4.35	1.46	1.33
24	a	410	CLA	O2A-CGA	4.34	1.46	1.33
24	D	404	CLA	O2A-CGA	4.34	1.46	1.33
24	c	508	CLA	OBD-CAD	4.34	1.28	1.22
25	a	411	PHO	OBD-CAD	4.34	1.30	1.22
38	a	420	LHG	O8-C23	4.34	1.46	1.33
24	b	615	CLA	O2A-CGA	4.34	1.46	1.33
38	D	411	LHG	O8-C23	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	101	LHG	O8-C23	4.33	1.46	1.33
37	e	101	DGD	O1G-C1A	4.33	1.46	1.33
34	C	520	LMG	O7-C10	4.33	1.46	1.34
37	C	518	DGD	O1G-C1A	4.31	1.45	1.33
24	A	409	CLA	OBD-CAD	4.31	1.28	1.22
24	B	607	CLA	O2A-CGA	4.31	1.45	1.33
24	B	605	CLA	O2D-CGD	4.30	1.43	1.33
27	f	102	SQD	O48-C23	4.30	1.45	1.33
24	B	606	CLA	O2A-CGA	4.29	1.45	1.33
37	c	521	DGD	O1G-C1A	4.29	1.45	1.33
24	B	612	CLA	OBD-CAD	4.29	1.28	1.22
24	b	620	CLA	O2A-CGA	4.29	1.45	1.33
24	b	625	CLA	O2A-CGA	4.29	1.45	1.33
24	B	609	CLA	O2A-CGA	4.28	1.45	1.33
27	B	621	SQD	O47-C7	4.28	1.46	1.34
24	B	617	CLA	O2A-CGA	4.28	1.45	1.33
24	C	506	CLA	O2A-CGA	4.28	1.45	1.33
27	L	102	SQD	O47-C7	4.28	1.46	1.34
24	c	511	CLA	O2A-CGA	4.27	1.45	1.33
24	C	512	CLA	O2A-CGA	4.27	1.45	1.33
24	C	510	CLA	O2A-CGA	4.27	1.45	1.33
24	C	506	CLA	OBD-CAD	4.27	1.28	1.22
24	c	517	CLA	O2A-CGA	4.26	1.45	1.33
34	d	415	LMG	O8-C28	4.26	1.45	1.33
24	A	406	CLA	O2A-CGA	4.25	1.45	1.33
24	C	507	CLA	O2A-CGA	4.25	1.45	1.33
25	d	402[B]	PHO	O2A-CGA	4.24	1.45	1.33
37	H	102	DGD	O1G-C1A	4.24	1.45	1.33
34	M	101	LMG	O8-C28	4.23	1.45	1.33
24	C	503	CLA	O2A-CGA	4.23	1.45	1.33
24	B	610	CLA	O2A-CGA	4.23	1.45	1.33
24	d	404	CLA	O2A-CGA	4.23	1.45	1.33
24	c	516	CLA	O2A-CGA	4.22	1.45	1.33
34	c	522	LMG	O8-C28	4.22	1.45	1.33
24	c	515	CLA	O2A-CGA	4.22	1.45	1.33
24	b	612	CLA	O2A-CGA	4.21	1.45	1.33
27	L	102	SQD	O48-C23	4.21	1.45	1.33
24	b	618	CLA	O2A-CGA	4.21	1.45	1.33
24	c	509	CLA	O2A-CGA	4.21	1.45	1.33
34	A	419	LMG	O7-C10	4.21	1.46	1.34
24	B	608	CLA	O2A-CGA	4.20	1.45	1.33
38	E	101	LHG	O7-C7	4.20	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	O2A-CGA	4.19	1.45	1.33
24	c	506	CLA	O2A-CGA	4.18	1.45	1.33
37	C	518	DGD	O2G-C1B	4.18	1.46	1.34
34	A	419	LMG	O8-C28	4.18	1.45	1.33
34	a	415	LMG	O8-C28	4.17	1.45	1.33
37	H	102	DGD	O2G-C1B	4.17	1.46	1.34
24	D	405	CLA	O2A-CGA	4.17	1.45	1.33
38	L	101	LHG	O8-C23	4.16	1.45	1.33
24	a	412	CLA	O2A-CGA	4.16	1.45	1.33
36	b	632	HTG	C1'-S1	-4.16	1.76	1.81
38	a	420	LHG	O7-C7	4.16	1.46	1.34
34	c	522	LMG	O7-C10	4.15	1.46	1.34
34	C	520	LMG	O8-C28	4.15	1.45	1.33
24	C	504	CLA	O2A-CGA	4.14	1.45	1.33
34	d	415	LMG	O7-C10	4.14	1.46	1.34
24	C	513	CLA	O2A-CGA	4.13	1.45	1.33
24	c	510	CLA	O2A-CGA	4.13	1.45	1.33
37	c	520	DGD	O1G-C1A	4.13	1.45	1.33
25	d	402[A]	PHO	O2A-CGA	4.12	1.45	1.33
27	F	101	SQD	O48-C23	4.12	1.45	1.33
24	c	505	CLA	O2A-CGA	4.11	1.45	1.33
34	z	101	LMG	O7-C10	4.11	1.45	1.34
37	h	102	DGD	O2G-C1B	4.10	1.45	1.34
24	b	613	CLA	O2A-CGA	4.10	1.45	1.33
24	b	623	CLA	O2A-CGA	4.10	1.45	1.33
38	b	634	LHG	O7-C7	4.10	1.45	1.34
24	b	623	CLA	OBD-CAD	4.10	1.28	1.22
34	M	101	LMG	O7-C10	4.09	1.45	1.34
25	D	401[B]	PHO	O2A-CGA	4.08	1.45	1.33
24	c	505	CLA	OBD-CAD	4.08	1.28	1.22
24	C	511	CLA	O2A-CGA	4.08	1.45	1.33
34	Z	101	LMG	O7-C10	4.08	1.45	1.34
24	b	617	CLA	O2A-CGA	4.08	1.45	1.33
24	b	611	CLA	O2A-CGA	4.07	1.45	1.33
38	D	409	LHG	O8-C23	4.07	1.45	1.33
24	B	612	CLA	O2A-CGA	4.06	1.45	1.33
24	A	409	CLA	O2A-CGA	4.06	1.45	1.33
24	d	404	CLA	OBD-CAD	4.05	1.28	1.22
38	b	634	LHG	O8-C23	4.05	1.45	1.33
24	c	514	CLA	O2A-CGA	4.04	1.45	1.33
34	k	101	LMG	O8-C28	4.03	1.45	1.33
24	C	502	CLA	O2A-CGA	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	411	SQD	O48-C23	4.02	1.45	1.33
38	d	410	LHG	O7-C7	4.02	1.45	1.34
37	C	517	DGD	O1G-C1A	4.02	1.45	1.33
24	b	613	CLA	OBD-CAD	4.02	1.27	1.22
27	a	414	SQD	O48-C23	4.01	1.45	1.33
24	c	508	CLA	O2A-CGA	4.01	1.45	1.33
38	D	410	LHG	O7-C7	4.01	1.45	1.34
24	B	616	CLA	O2A-CGA	4.00	1.45	1.33
27	B	621	SQD	O48-C23	4.00	1.45	1.33
27	A	413	SQD	O47-C7	4.00	1.45	1.34
37	h	102	DGD	O1G-C1A	3.99	1.45	1.33
37	C	516	DGD	O2G-C1B	3.99	1.45	1.34
34	D	415	LMG	O7-C10	3.99	1.45	1.34
38	d	409	LHG	O7-C7	3.99	1.45	1.34
34	b	629	LMG	O7-C10	3.99	1.45	1.34
24	A	405	CLA	O2A-CGA	3.98	1.45	1.33
38	d	410	LHG	O8-C23	3.98	1.45	1.33
36	d	413	HTG	C1'-S1	-3.97	1.76	1.81
38	D	410	LHG	O8-C23	3.97	1.44	1.33
24	B	603	CLA	O2A-CGA	3.97	1.44	1.33
24	c	507	CLA	O2A-CGA	3.97	1.44	1.33
24	b	622	CLA	OBD-CAD	3.96	1.27	1.22
24	b	621	CLA	O2A-CGA	3.96	1.44	1.33
25	D	401[A]	PHO	O2A-CGA	3.95	1.44	1.33
27	A	411	SQD	O47-C7	3.95	1.45	1.34
24	B	605	CLA	OBD-CAD	3.94	1.27	1.22
37	c	519	DGD	O2G-C1B	3.94	1.45	1.34
24	B	614	CLA	O2A-CGA	3.93	1.44	1.33
24	B	613	CLA	O2A-CGA	3.93	1.44	1.33
24	C	505	CLA	O2A-CGA	3.92	1.44	1.33
34	a	415	LMG	O7-C10	3.91	1.45	1.34
34	D	415	LMG	O8-C28	3.91	1.44	1.33
37	C	516	DGD	O1G-C1A	3.90	1.44	1.33
24	B	611	CLA	O2A-CGA	3.89	1.44	1.33
34	C	519	LMG	O7-C10	3.88	1.45	1.34
24	B	604	CLA	OBD-CAD	3.87	1.27	1.22
37	C	517	DGD	O2G-C1B	3.87	1.45	1.34
25	D	401[A]	PHO	C3D-C2D	3.87	1.49	1.39
25	A	408	PHO	O2A-CGA	3.86	1.44	1.33
37	c	521	DGD	O2G-C1B	3.86	1.45	1.34
25	a	411	PHO	C3D-C2D	3.86	1.49	1.39
24	b	612	CLA	OBD-CAD	3.86	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	520	DGD	O2G-C1B	3.85	1.45	1.34
34	b	629	LMG	O8-C28	3.85	1.44	1.33
25	a	411	PHO	O2A-CGA	3.85	1.44	1.33
25	d	402[A]	PHO	C3D-C2D	3.84	1.49	1.39
24	b	614	CLA	O2A-CGA	3.84	1.44	1.33
37	c	519	DGD	O1G-C1A	3.84	1.44	1.33
24	B	605	CLA	O2A-CGA	3.83	1.44	1.33
24	b	622	CLA	O2A-CGA	3.80	1.44	1.33
38	L	101	LHG	O7-C7	3.79	1.45	1.34
34	k	101	LMG	O7-C10	3.79	1.45	1.34
38	d	408	LHG	O8-C23	3.78	1.44	1.33
27	a	414	SQD	O47-C7	3.78	1.45	1.34
36	b	607	HTG	C1'-S1	-3.75	1.76	1.81
24	b	619	CLA	O2A-CGA	3.75	1.44	1.33
24	b	620	CLA	OBD-CAD	3.75	1.27	1.22
24	a	409	CLA	O2A-CGA	3.75	1.44	1.33
24	A	407	CLA	O2A-CGA	3.75	1.44	1.33
36	B	631	HTG	C1'-S1	-3.69	1.76	1.81
25	D	401[B]	PHO	OBD-CAD	3.69	1.28	1.22
36	B	632	HTG	C1'-S1	-3.66	1.76	1.81
25	d	402[B]	PHO	OBD-CAD	3.65	1.28	1.22
36	V	206	HTG	C1'-S1	-3.64	1.76	1.81
25	A	408	PHO	C3D-C2D	3.62	1.49	1.39
25	A	408	PHO	C4A-NA	-3.62	1.26	1.35
25	D	401[B]	PHO	CHC-C4B	3.59	1.48	1.40
36	c	524	HTG	C1'-S1	-3.58	1.76	1.81
25	D	401[B]	PHO	C3D-C2D	3.58	1.48	1.39
25	D	401[A]	PHO	CHC-C4B	3.56	1.48	1.40
36	B	624	HTG	C1'-S1	-3.56	1.76	1.81
25	D	401[B]	PHO	C4A-NA	-3.56	1.26	1.35
36	b	608	HTG	C1'-S1	-3.53	1.76	1.81
25	a	411	PHO	CHC-C4B	3.52	1.48	1.40
38	d	408	LHG	O7-C7	3.51	1.44	1.34
25	A	408	PHO	CHD-C4C	3.50	1.48	1.40
25	D	401[A]	PHO	C4A-NA	-3.44	1.26	1.35
38	d	409	LHG	O8-C23	3.44	1.43	1.33
25	d	402[B]	PHO	CHC-C4B	3.44	1.48	1.40
36	C	522	HTG	C1'-S1	-3.43	1.77	1.81
25	d	402[B]	PHO	C4A-NA	-3.42	1.27	1.35
36	b	602	HTG	C1'-S1	-3.36	1.77	1.81
36	c	523	HTG	C1'-S1	-3.36	1.77	1.81
25	D	401[B]	PHO	CHD-C4C	3.35	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	414	HTG	C1'-S1	-3.34	1.77	1.81
25	A	408	PHO	CHC-C4B	3.33	1.48	1.40
25	D	401[A]	PHO	OBD-CAD	3.32	1.28	1.22
36	C	523	HTG	C1'-S1	-3.31	1.77	1.81
25	d	402[B]	PHO	C3D-C2D	3.29	1.48	1.39
24	b	622	CLA	C4C-C3C	3.27	1.50	1.45
25	a	411	PHO	CHD-C4C	3.26	1.48	1.40
38	D	409	LHG	O7-C7	3.25	1.43	1.34
25	d	402[A]	PHO	CHC-C4B	3.24	1.48	1.40
25	A	408	PHO	CHB-C4A	3.23	1.48	1.40
25	a	411	PHO	C4A-NA	-3.23	1.27	1.35
25	D	401[A]	PHO	CHD-C4C	3.20	1.47	1.40
25	a	411	PHO	CHB-C4A	3.18	1.47	1.40
25	d	402[B]	PHO	CHD-C4C	3.16	1.47	1.40
25	D	401[A]	PHO	C3B-C4B	3.16	1.49	1.43
36	B	623	HTG	C1'-S1	-3.13	1.77	1.81
25	A	408	PHO	OBD-CAD	3.13	1.27	1.22
24	A	405	CLA	C4C-C3C	3.12	1.50	1.45
25	d	402[A]	PHO	C3B-C4B	3.12	1.49	1.43
25	D	401[B]	PHO	CHB-C4A	3.12	1.47	1.40
24	B	606	CLA	C1D-C2D	3.06	1.49	1.42
24	b	611	CLA	C1D-C2D	3.06	1.49	1.42
25	d	402[A]	PHO	C4A-NA	-3.05	1.27	1.35
24	c	515	CLA	C1D-C2D	3.05	1.49	1.42
25	d	402[A]	PHO	CHD-C4C	3.05	1.47	1.40
25	d	402[B]	PHO	CHB-C4A	3.04	1.47	1.40
25	d	402[A]	PHO	OBD-CAD	3.04	1.27	1.22
25	D	401[B]	PHO	C3B-C4B	3.04	1.49	1.43
24	B	611	CLA	C1D-C2D	3.03	1.49	1.42
24	C	501	CLA	C1C-C2C	3.02	1.50	1.44
24	b	619	CLA	C1D-C2D	3.02	1.49	1.42
25	A	408	PHO	C3B-C4B	3.02	1.49	1.43
24	B	602	CLA	C1D-C2D	3.01	1.49	1.42
24	B	606	CLA	C1C-C2C	3.00	1.50	1.44
24	A	409	CLA	C1D-C2D	2.99	1.49	1.42
24	b	624	CLA	C1D-C2D	2.99	1.49	1.42
24	C	513	CLA	C1D-C2D	2.96	1.49	1.42
24	C	504	CLA	C1D-C2D	2.95	1.49	1.42
24	C	503	CLA	C1C-C2C	2.95	1.50	1.44
24	b	610	CLA	C1D-C2D	2.95	1.49	1.42
25	d	402[A]	PHO	CHB-C4A	2.94	1.47	1.40
24	b	618	CLA	C1D-C2D	2.94	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C1D-C2D	2.93	1.49	1.42
24	B	603	CLA	C1D-C2D	2.93	1.49	1.42
36	b	631	HTG	C1'-S1	-2.92	1.77	1.81
24	a	409	CLA	C1D-C2D	2.92	1.49	1.42
25	a	411	PHO	C3B-C4B	2.91	1.49	1.43
24	C	510	CLA	C4C-C3C	2.91	1.50	1.45
24	b	621	CLA	C1B-CHB	2.91	1.49	1.41
24	B	608	CLA	C1D-C2D	2.91	1.49	1.42
24	A	407	CLA	C1D-C2D	2.90	1.49	1.42
24	D	405	CLA	C1D-C2D	2.90	1.49	1.42
24	c	511	CLA	C1C-C2C	2.89	1.50	1.44
24	C	508	CLA	C1D-C2D	2.89	1.49	1.42
27	f	102	SQD	C6-S	-2.87	1.66	1.77
24	a	409	CLA	C4C-C3C	2.87	1.50	1.45
24	B	616	CLA	C4B-CHC	2.87	1.49	1.41
24	d	405	CLA	C1D-C2D	2.87	1.49	1.42
27	F	101	SQD	C6-S	-2.87	1.66	1.77
25	d	402[B]	PHO	C3B-C4B	2.86	1.49	1.43
24	B	610	CLA	C1D-C2D	2.85	1.49	1.42
24	b	614	CLA	C1C-C2C	2.85	1.50	1.44
24	B	614	CLA	C4C-C3C	2.84	1.49	1.45
24	b	614	CLA	C1D-C2D	2.84	1.49	1.42
24	C	509	CLA	C1D-C2D	2.83	1.49	1.42
27	A	413	SQD	C6-S	-2.82	1.67	1.77
24	B	607	CLA	C1C-C2C	2.81	1.50	1.44
24	b	621	CLA	C1C-C2C	2.80	1.50	1.44
24	d	403	CLA	C1D-C2D	2.80	1.48	1.42
24	A	406	CLA	C1D-C2D	2.80	1.48	1.42
24	C	512	CLA	C1C-C2C	2.79	1.50	1.44
24	C	510	CLA	C1D-C2D	2.78	1.48	1.42
24	B	613	CLA	C1C-C2C	2.78	1.49	1.44
24	B	609	CLA	C1D-C2D	2.78	1.48	1.42
27	a	405	SQD	C6-S	-2.77	1.67	1.77
24	C	503	CLA	C4B-CHC	2.77	1.48	1.41
24	B	608	CLA	C1C-C2C	2.76	1.49	1.44
24	c	514	CLA	C1B-CHB	2.76	1.48	1.41
24	C	511	CLA	CHD-C4C	2.76	1.49	1.41
24	C	503	CLA	C1D-C2D	2.76	1.48	1.42
24	B	611	CLA	C4B-CHC	2.74	1.48	1.41
24	b	616	CLA	C1D-C2D	2.74	1.48	1.42
24	c	512	CLA	C1C-C2C	2.74	1.49	1.44
24	A	409	CLA	C4C-C3C	2.74	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	C1D-C2D	2.74	1.48	1.42
24	B	609	CLA	C4C-C3C	2.74	1.49	1.45
24	B	606	CLA	C4C-C3C	2.73	1.49	1.45
24	c	517	CLA	C1C-C2C	2.73	1.49	1.44
24	c	514	CLA	C1D-C2D	2.73	1.48	1.42
24	a	410	CLA	C1D-C2D	2.73	1.48	1.42
24	c	516	CLA	C1D-C2D	2.72	1.48	1.42
24	c	513	CLA	C1D-C2D	2.72	1.48	1.42
24	C	513	CLA	CHD-C4C	2.72	1.48	1.41
24	d	403	CLA	CHD-C4C	2.72	1.48	1.41
24	C	507	CLA	C1D-C2D	2.72	1.48	1.42
36	b	632	HTG	C1-S1	-2.72	1.76	1.80
27	A	411	SQD	C6-S	-2.72	1.67	1.77
24	A	405	CLA	C1C-C2C	2.71	1.49	1.44
24	c	505	CLA	C1D-C2D	2.71	1.48	1.42
24	d	404	CLA	C1B-NB	-2.71	1.32	1.35
39	v	206	HEM	C3B-C2B	-2.71	1.36	1.40
24	c	517	CLA	C1D-C2D	2.71	1.48	1.42
24	b	622	CLA	C1D-C2D	2.71	1.48	1.42
24	B	607	CLA	C1D-C2D	2.71	1.48	1.42
24	a	410	CLA	C1C-C2C	2.70	1.49	1.44
24	C	506	CLA	C1D-C2D	2.70	1.48	1.42
24	B	611	CLA	CHD-C4C	2.70	1.48	1.41
39	E	103	HEM	C3B-C2B	-2.70	1.36	1.40
24	B	614	CLA	C1D-C2D	2.70	1.48	1.42
24	b	623	CLA	C1D-C2D	2.70	1.48	1.42
39	f	101	HEM	C3B-C2B	-2.70	1.36	1.40
24	c	516	CLA	CHD-C4C	2.69	1.48	1.41
24	b	623	CLA	CHD-C4C	2.69	1.48	1.41
34	Z	101	LMG	O8-C28	2.69	1.46	1.33
24	B	612	CLA	C4C-C3C	2.69	1.49	1.45
24	b	618	CLA	C1B-CHB	2.69	1.48	1.41
24	b	625	CLA	C1D-C2D	2.68	1.48	1.42
24	b	617	CLA	C4B-CHC	2.68	1.48	1.41
24	c	509	CLA	C4C-C3C	2.68	1.49	1.45
24	c	509	CLA	C1D-C2D	2.67	1.48	1.42
24	C	510	CLA	CHD-C4C	2.67	1.48	1.41
24	C	501	CLA	C1D-C2D	2.67	1.48	1.42
24	b	622	CLA	CHD-C4C	2.67	1.48	1.41
24	C	504	CLA	CHD-C4C	2.66	1.48	1.41
24	C	501	CLA	C4B-CHC	2.66	1.48	1.41
27	L	102	SQD	C6-S	-2.66	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	C4C-C3C	2.66	1.49	1.45
24	C	502	CLA	C1C-C2C	2.66	1.49	1.44
24	B	616	CLA	C1C-C2C	2.65	1.49	1.44
24	C	511	CLA	C1B-CHB	2.65	1.48	1.41
24	c	509	CLA	C1B-CHB	2.65	1.48	1.41
24	C	507	CLA	C4B-CHC	2.65	1.48	1.41
24	b	622	CLA	C1B-CHB	2.64	1.48	1.41
24	B	614	CLA	C1C-C2C	2.64	1.49	1.44
27	a	414	SQD	C6-S	-2.64	1.67	1.77
24	c	514	CLA	CHD-C4C	2.64	1.48	1.41
24	a	409	CLA	CHD-C4C	2.63	1.48	1.41
24	A	405	CLA	CHD-C4C	2.63	1.48	1.41
24	b	615	CLA	C1C-C2C	2.63	1.49	1.44
24	B	615	CLA	C1C-C2C	2.63	1.49	1.44
24	c	510	CLA	CHD-C4C	2.63	1.48	1.41
24	C	511	CLA	C4C-C3C	2.62	1.49	1.45
24	b	610	CLA	CHD-C4C	2.62	1.48	1.41
24	B	603	CLA	C1C-C2C	2.62	1.49	1.44
24	b	617	CLA	C1D-C2D	2.61	1.48	1.42
24	A	407	CLA	C1C-C2C	2.61	1.49	1.44
24	C	503	CLA	CHD-C4C	2.61	1.48	1.41
27	B	621	SQD	C6-S	-2.61	1.67	1.77
32	a	416[B]	PL9	C6-C5	2.61	1.48	1.35
24	B	604	CLA	C1D-C2D	2.61	1.48	1.42
24	B	616	CLA	C1D-C2D	2.61	1.48	1.42
24	C	502	CLA	C1D-C2D	2.61	1.48	1.42
32	A	417[B]	PL9	C6-C5	2.60	1.48	1.35
32	d	407[B]	PL9	C6-C5	2.60	1.48	1.35
24	b	625	CLA	C1B-CHB	2.60	1.48	1.41
24	c	513	CLA	C1C-C2C	2.60	1.49	1.44
24	B	608	CLA	CHD-C4C	2.60	1.48	1.41
24	D	404	CLA	C4C-C3C	2.60	1.49	1.45
24	c	513	CLA	CHD-C4C	2.60	1.48	1.41
24	c	508	CLA	C1D-C2D	2.60	1.48	1.42
24	b	613	CLA	C1C-C2C	2.60	1.49	1.44
24	c	511	CLA	C1D-C2D	2.59	1.48	1.42
25	D	401[A]	PHO	CHB-C4A	2.59	1.46	1.40
24	c	507	CLA	C1C-C2C	2.59	1.49	1.44
24	C	509	CLA	C1B-CHB	2.59	1.48	1.41
24	d	404	CLA	C1D-C2D	2.59	1.48	1.42
32	a	416[A]	PL9	C6-C5	2.58	1.48	1.35
24	c	516	CLA	C1C-C2C	2.58	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	522	HTG	C1-S1	-2.58	1.76	1.80
24	b	615	CLA	C1D-C2D	2.58	1.48	1.42
24	B	606	CLA	C1B-CHB	2.57	1.48	1.41
24	c	514	CLA	C4C-C3C	2.57	1.49	1.45
24	C	509	CLA	CHD-C4C	2.57	1.48	1.41
24	B	604	CLA	C1C-C2C	2.57	1.49	1.44
24	C	510	CLA	C1B-CHB	2.57	1.48	1.41
24	B	612	CLA	C1C-C2C	2.57	1.49	1.44
24	C	512	CLA	C1D-C2D	2.57	1.48	1.42
24	c	509	CLA	C4B-CHC	2.57	1.48	1.41
24	C	511	CLA	C1D-C2D	2.57	1.48	1.42
24	c	507	CLA	C1D-C2D	2.57	1.48	1.42
24	b	620	CLA	C1B-CHB	2.56	1.48	1.41
24	c	512	CLA	C1B-CHB	2.56	1.48	1.41
32	D	407[B]	PL9	C6-C5	2.56	1.48	1.35
24	B	607	CLA	C4B-CHC	2.55	1.48	1.41
24	C	502	CLA	C1B-CHB	2.55	1.48	1.41
32	A	417[A]	PL9	C6-C5	2.55	1.48	1.35
24	B	602	CLA	C1B-CHB	2.55	1.48	1.41
24	B	610	CLA	C1B-CHB	2.55	1.48	1.41
24	b	612	CLA	C1C-C2C	2.55	1.49	1.44
24	A	409	CLA	CHD-C4C	2.54	1.48	1.41
24	c	515	CLA	CHD-C4C	2.54	1.48	1.41
32	d	407[A]	PL9	C6-C5	2.54	1.48	1.35
24	b	619	CLA	CHD-C4C	2.54	1.48	1.41
24	B	609	CLA	CHD-C4C	2.54	1.48	1.41
24	b	617	CLA	C1C-C2C	2.54	1.49	1.44
24	B	608	CLA	C4B-CHC	2.54	1.48	1.41
24	c	508	CLA	C1C-C2C	2.53	1.49	1.44
24	A	407	CLA	CHD-C4C	2.53	1.48	1.41
24	c	505	CLA	C1B-CHB	2.53	1.48	1.41
24	c	511	CLA	C4B-CHC	2.53	1.48	1.41
24	C	507	CLA	CHD-C4C	2.53	1.48	1.41
24	B	603	CLA	C4B-CHC	2.52	1.48	1.41
24	B	610	CLA	C4C-C3C	2.52	1.49	1.45
24	c	505	CLA	CHD-C4C	2.52	1.48	1.41
24	b	619	CLA	C1B-NB	-2.52	1.33	1.35
24	c	517	CLA	CHD-C4C	2.52	1.48	1.41
24	C	507	CLA	C1C-C2C	2.52	1.49	1.44
24	B	606	CLA	C4B-CHC	2.52	1.48	1.41
24	b	611	CLA	C1C-C2C	2.52	1.49	1.44
24	C	513	CLA	C4B-CHC	2.52	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C4B-CHC	2.52	1.48	1.41
24	c	505	CLA	C4C-C3C	2.52	1.49	1.45
24	b	617	CLA	C1B-CHB	2.52	1.48	1.41
24	b	618	CLA	CHD-C4C	2.51	1.48	1.41
24	B	613	CLA	C1B-CHB	2.51	1.48	1.41
24	b	611	CLA	CHD-C4C	2.51	1.48	1.41
24	b	623	CLA	C1B-CHB	2.51	1.48	1.41
24	b	613	CLA	C1B-CHB	2.51	1.48	1.41
24	c	505	CLA	C1C-C2C	2.51	1.49	1.44
24	C	508	CLA	CHD-C4C	2.51	1.48	1.41
24	B	604	CLA	C4B-CHC	2.51	1.48	1.41
24	B	606	CLA	CHD-C4C	2.50	1.48	1.41
24	c	506	CLA	CHD-C4C	2.50	1.48	1.41
24	c	513	CLA	C1B-CHB	2.50	1.47	1.41
24	C	509	CLA	C4C-C3C	2.50	1.49	1.45
24	B	614	CLA	CHD-C4C	2.50	1.48	1.41
24	b	618	CLA	C1C-C2C	2.50	1.49	1.44
24	a	412	CLA	C1D-C2D	2.50	1.48	1.42
24	C	512	CLA	C4B-CHC	2.50	1.47	1.41
36	d	413	HTG	C1-S1	-2.50	1.76	1.80
24	B	612	CLA	C1D-C2D	2.49	1.48	1.42
24	C	510	CLA	C4B-CHC	2.49	1.47	1.41
24	B	611	CLA	C1B-CHB	2.49	1.47	1.41
24	C	513	CLA	C4C-C3C	2.49	1.49	1.45
24	B	605	CLA	C4C-C3C	2.49	1.49	1.45
24	b	624	CLA	CHD-C4C	2.49	1.48	1.41
24	B	613	CLA	C1D-C2D	2.49	1.48	1.42
24	a	409	CLA	C1C-C2C	2.49	1.49	1.44
24	B	609	CLA	C1C-NC	-2.48	1.34	1.37
24	C	505	CLA	C1C-C2C	2.48	1.49	1.44
25	A	408	PHO	C1A-NA	-2.48	1.32	1.37
24	B	602	CLA	CHD-C4C	2.48	1.48	1.41
24	b	625	CLA	C4B-CHC	2.48	1.47	1.41
24	a	412	CLA	CHD-C4C	2.48	1.48	1.41
24	B	608	CLA	C4C-C3C	2.47	1.49	1.45
24	D	405	CLA	C1B-CHB	2.47	1.47	1.41
39	V	205	HEM	C3B-C2B	-2.47	1.36	1.40
24	B	604	CLA	CHD-C4C	2.47	1.48	1.41
24	b	625	CLA	CHD-C4C	2.47	1.48	1.41
24	c	508	CLA	CHD-C4C	2.46	1.48	1.41
24	C	505	CLA	C1B-CHB	2.46	1.47	1.41
24	A	407	CLA	C4B-CHC	2.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C1D-C2D	2.46	1.48	1.42
24	C	509	CLA	C4B-CHC	2.46	1.47	1.41
24	c	517	CLA	C4B-CHC	2.46	1.47	1.41
24	B	617	CLA	CHD-C4C	2.46	1.48	1.41
24	A	409	CLA	C4B-CHC	2.45	1.47	1.41
24	B	615	CLA	C1D-C2D	2.45	1.48	1.42
24	B	614	CLA	C1B-CHB	2.45	1.47	1.41
37	D	408	DGD	O3G-C1D	2.45	1.44	1.40
24	C	506	CLA	C4C-C3C	2.45	1.49	1.45
24	C	506	CLA	CHD-C4C	2.45	1.48	1.41
24	c	506	CLA	C1D-C2D	2.45	1.48	1.42
24	d	404	CLA	C4B-CHC	2.45	1.47	1.41
24	b	619	CLA	C4B-CHC	2.45	1.47	1.41
24	C	512	CLA	CHD-C4C	2.45	1.48	1.41
24	a	410	CLA	C1B-CHB	2.44	1.47	1.41
24	C	505	CLA	C1D-C2D	2.44	1.48	1.42
24	B	602	CLA	C4B-CHC	2.44	1.47	1.41
24	B	617	CLA	C1D-C2D	2.44	1.48	1.42
24	b	617	CLA	CHD-C4C	2.44	1.48	1.41
24	b	612	CLA	C4C-C3C	2.44	1.49	1.45
24	C	504	CLA	C1C-C2C	2.44	1.49	1.44
24	B	616	CLA	C1B-CHB	2.44	1.47	1.41
24	C	505	CLA	C4B-CHC	2.44	1.47	1.41
24	C	501	CLA	C1B-CHB	2.44	1.47	1.41
24	B	604	CLA	C1B-NB	-2.44	1.33	1.35
24	C	505	CLA	C4C-C3C	2.43	1.49	1.45
24	d	405	CLA	C4B-CHC	2.43	1.47	1.41
25	D	401[A]	PHO	C4D-CHA	2.43	1.50	1.43
24	b	610	CLA	C1C-C2C	2.43	1.49	1.44
24	c	516	CLA	C4B-CHC	2.43	1.47	1.41
24	b	615	CLA	C1B-CHB	2.43	1.47	1.41
24	d	404	CLA	C4C-C3C	2.43	1.49	1.45
32	D	407[A]	PL9	C6-C5	2.42	1.48	1.35
24	b	610	CLA	C4B-CHC	2.42	1.47	1.41
24	b	620	CLA	C1D-C2D	2.42	1.48	1.42
24	b	624	CLA	C1B-CHB	2.42	1.47	1.41
24	B	608	CLA	C1B-CHB	2.42	1.47	1.41
24	A	409	CLA	C1C-C2C	2.42	1.49	1.44
24	b	612	CLA	C1B-CHB	2.41	1.47	1.41
24	C	508	CLA	C4C-C3C	2.41	1.49	1.45
24	c	506	CLA	C1B-CHB	2.41	1.47	1.41
24	c	509	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C4C-C3C	2.41	1.49	1.45
24	c	513	CLA	C4C-C3C	2.41	1.49	1.45
24	c	510	CLA	C1B-CHB	2.41	1.47	1.41
24	b	613	CLA	C1D-C2D	2.40	1.48	1.42
24	b	614	CLA	C1B-CHB	2.40	1.47	1.41
24	b	621	CLA	C4B-CHC	2.40	1.47	1.41
24	b	616	CLA	C1B-CHB	2.40	1.47	1.41
24	c	509	CLA	CHD-C4C	2.40	1.48	1.41
24	d	403	CLA	C1C-NC	-2.40	1.34	1.37
24	B	610	CLA	CHD-C4C	2.40	1.48	1.41
24	C	503	CLA	C4C-C3C	2.40	1.49	1.45
24	c	515	CLA	C1B-CHB	2.40	1.47	1.41
24	D	405	CLA	CHD-C4C	2.40	1.48	1.41
24	b	616	CLA	C4B-CHC	2.39	1.47	1.41
24	C	505	CLA	CHD-C4C	2.39	1.48	1.41
24	C	501	CLA	CHD-C4C	2.39	1.48	1.41
29	A	414	LMT	O1'-C1'	2.39	1.44	1.40
24	c	511	CLA	CHD-C4C	2.39	1.48	1.41
24	A	406	CLA	CHD-C4C	2.39	1.48	1.41
24	b	612	CLA	C1D-C2D	2.39	1.48	1.42
24	c	507	CLA	C4B-CHC	2.39	1.47	1.41
24	b	616	CLA	C1C-C2C	2.39	1.49	1.44
24	B	612	CLA	CHD-C4C	2.38	1.47	1.41
24	b	620	CLA	C4C-C3C	2.38	1.49	1.45
24	C	509	CLA	C1C-C2C	2.38	1.49	1.44
24	d	404	CLA	CHD-C4C	2.38	1.47	1.41
24	B	615	CLA	C1B-CHB	2.38	1.47	1.41
24	a	409	CLA	C4B-CHC	2.38	1.47	1.41
24	A	406	CLA	C4B-NB	-2.38	1.33	1.35
24	d	404	CLA	C1C-C2C	2.37	1.49	1.44
24	C	502	CLA	CHD-C4C	2.37	1.47	1.41
24	C	502	CLA	C4B-CHC	2.37	1.47	1.41
24	B	602	CLA	C1C-C2C	2.36	1.49	1.44
24	c	511	CLA	C1B-CHB	2.36	1.47	1.41
24	D	404	CLA	CHD-C4C	2.36	1.47	1.41
24	A	409	CLA	C1B-CHB	2.36	1.47	1.41
24	C	510	CLA	C1C-C2C	2.35	1.49	1.44
24	C	503	CLA	C1B-CHB	2.35	1.47	1.41
25	D	401[A]	PHO	C1A-NA	-2.35	1.32	1.37
24	b	611	CLA	C1B-CHB	2.35	1.47	1.41
24	C	507	CLA	C4C-C3C	2.35	1.49	1.45
24	b	614	CLA	CHD-C4C	2.35	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	517	CLA	C1B-CHB	2.35	1.47	1.41
36	D	414	HTG	C1-S1	-2.34	1.77	1.80
24	a	412	CLA	C1B-CHB	2.34	1.47	1.41
24	b	612	CLA	C4B-CHC	2.34	1.47	1.41
24	C	511	CLA	C1C-C2C	2.34	1.49	1.44
24	c	510	CLA	C4B-CHC	2.34	1.47	1.41
24	B	617	CLA	C1B-CHB	2.34	1.47	1.41
24	B	612	CLA	C4B-CHC	2.34	1.47	1.41
24	a	410	CLA	CHD-C4C	2.33	1.47	1.41
24	b	611	CLA	C4B-CHC	2.33	1.47	1.41
24	B	603	CLA	CHD-C4C	2.33	1.47	1.41
24	C	513	CLA	C1B-CHB	2.33	1.47	1.41
24	C	512	CLA	C4C-C3C	2.33	1.49	1.45
24	C	506	CLA	C1B-NB	-2.33	1.33	1.35
24	d	405	CLA	C1C-C2C	2.33	1.49	1.44
24	c	508	CLA	C4B-CHC	2.32	1.47	1.41
24	c	513	CLA	C4B-CHC	2.32	1.47	1.41
36	b	608	HTG	C1-S1	-2.31	1.77	1.80
24	B	605	CLA	C1D-C2D	2.31	1.47	1.42
25	A	408	PHO	C4D-CHA	2.30	1.50	1.43
24	D	405	CLA	C4C-C3C	2.30	1.49	1.45
24	C	504	CLA	C4C-C3C	2.30	1.49	1.45
24	C	504	CLA	C4B-CHC	2.29	1.47	1.41
24	B	605	CLA	CHD-C4C	2.29	1.47	1.41
24	c	512	CLA	C4B-CHC	2.29	1.47	1.41
36	c	523	HTG	C1-S1	-2.29	1.77	1.80
24	b	615	CLA	C1B-NB	-2.29	1.33	1.35
24	B	614	CLA	C4B-CHC	2.29	1.47	1.41
24	B	607	CLA	C1B-CHB	2.29	1.47	1.41
24	C	506	CLA	C1B-CHB	2.29	1.47	1.41
24	C	512	CLA	C1B-CHB	2.29	1.47	1.41
24	c	508	CLA	C1B-CHB	2.29	1.47	1.41
24	b	620	CLA	C4B-CHC	2.28	1.47	1.41
24	B	617	CLA	C4B-CHC	2.28	1.47	1.41
24	b	615	CLA	CHD-C4C	2.28	1.47	1.41
24	D	404	CLA	C1C-C2C	2.28	1.49	1.44
24	d	405	CLA	C1B-CHB	2.27	1.47	1.41
25	d	402[B]	PHO	C4C-C3C	2.27	1.49	1.45
24	C	504	CLA	C1B-CHB	2.27	1.47	1.41
24	c	507	CLA	C1B-CHB	2.27	1.47	1.41
24	B	605	CLA	C1B-CHB	2.27	1.47	1.41
24	d	405	CLA	CHD-C4C	2.27	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C4B-CHC	2.26	1.47	1.41
24	c	505	CLA	C1B-NB	-2.26	1.33	1.35
24	B	612	CLA	C1B-CHB	2.26	1.47	1.41
24	c	511	CLA	C4C-C3C	2.26	1.48	1.45
24	b	618	CLA	C4B-CHC	2.26	1.47	1.41
24	b	613	CLA	CHD-C4C	2.26	1.47	1.41
39	E	103	HEM	C4D-C3D	2.26	1.47	1.42
24	D	404	CLA	C1D-C2D	2.26	1.47	1.42
24	B	613	CLA	C4B-CHC	2.26	1.47	1.41
24	c	512	CLA	CHD-C4C	2.26	1.47	1.41
24	c	514	CLA	C1C-C2C	2.26	1.48	1.44
24	b	623	CLA	C1C-C2C	2.26	1.48	1.44
24	B	607	CLA	C4C-C3C	2.26	1.48	1.45
24	a	409	CLA	C1B-CHB	2.26	1.47	1.41
24	b	613	CLA	C4B-CHC	2.26	1.47	1.41
25	a	411	PHO	C4D-CHA	2.25	1.49	1.43
24	d	403	CLA	C1B-CHB	2.25	1.47	1.41
25	d	402[A]	PHO	C1A-NA	-2.25	1.33	1.37
24	b	623	CLA	C4C-C3C	2.25	1.48	1.45
24	B	609	CLA	C1B-CHB	2.24	1.47	1.41
24	D	404	CLA	C4B-CHC	2.24	1.47	1.41
25	a	411	PHO	C1A-NA	-2.24	1.33	1.37
24	C	508	CLA	C4B-CHC	2.24	1.47	1.41
24	C	513	CLA	C1C-C2C	2.24	1.48	1.44
24	c	517	CLA	C4C-C3C	2.23	1.48	1.45
24	b	620	CLA	CHD-C4C	2.23	1.47	1.41
38	d	408	LHG	O7-C5	-2.23	1.41	1.46
24	C	506	CLA	C1C-C2C	2.23	1.48	1.44
24	D	405	CLA	C4B-CHC	2.23	1.47	1.41
36	c	524	HTG	C1-S1	-2.22	1.77	1.80
36	V	206	HTG	C1-S1	-2.22	1.77	1.80
25	d	402[B]	PHO	C1A-NA	-2.22	1.33	1.37
24	D	404	CLA	C1B-CHB	2.22	1.47	1.41
24	c	506	CLA	C4C-C3C	2.22	1.48	1.45
24	C	502	CLA	C4C-C3C	2.22	1.48	1.45
24	c	510	CLA	C4C-C3C	2.22	1.48	1.45
24	A	406	CLA	C1C-NC	-2.21	1.34	1.37
24	a	410	CLA	C4C-C3C	2.21	1.48	1.45
24	a	410	CLA	C4B-CHC	2.21	1.47	1.41
24	c	507	CLA	CHD-C4C	2.21	1.47	1.41
24	c	507	CLA	C4C-C3C	2.20	1.48	1.45
24	c	508	CLA	C4C-C3C	2.20	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	624	CLA	C4B-CHC	2.20	1.47	1.41
24	B	617	CLA	C4C-C3C	2.20	1.48	1.45
24	C	508	CLA	C1B-CHB	2.20	1.47	1.41
24	B	604	CLA	C1B-CHB	2.20	1.47	1.41
24	b	617	CLA	C4C-C3C	2.20	1.48	1.45
24	b	614	CLA	C4B-CHC	2.20	1.47	1.41
24	B	607	CLA	CHD-C4C	2.20	1.47	1.41
24	c	505	CLA	C4B-CHC	2.19	1.47	1.41
24	a	412	CLA	C4C-C3C	2.19	1.48	1.45
24	A	405	CLA	C1B-NB	-2.19	1.33	1.35
37	h	102	DGD	O5D-C1E	2.19	1.43	1.40
24	b	612	CLA	CHD-C4C	2.18	1.47	1.41
25	D	401[B]	PHO	C4D-CHA	2.18	1.49	1.43
24	A	407	CLA	C4C-C3C	2.18	1.48	1.45
39	V	205	HEM	C4D-C3D	2.18	1.47	1.42
24	B	611	CLA	C4C-C3C	2.18	1.48	1.45
24	c	506	CLA	C4B-CHC	2.18	1.47	1.41
24	a	412	CLA	C4B-CHC	2.18	1.47	1.41
24	b	616	CLA	CHD-C4C	2.18	1.47	1.41
24	B	605	CLA	C1C-C2C	2.18	1.48	1.44
24	C	506	CLA	C4B-CHC	2.17	1.47	1.41
24	C	508	CLA	C1C-C2C	2.17	1.48	1.44
24	b	619	CLA	C1B-CHB	2.17	1.47	1.41
24	B	603	CLA	C4C-C3C	2.17	1.48	1.45
24	c	515	CLA	C1C-C2C	2.17	1.48	1.44
24	B	616	CLA	CHD-C4C	2.16	1.47	1.41
24	c	512	CLA	C4C-C3C	2.16	1.48	1.45
36	B	632	HTG	C1-S1	-2.16	1.77	1.80
24	C	511	CLA	C4B-CHC	2.16	1.47	1.41
25	A	408	PHO	C4C-C3C	2.16	1.49	1.45
24	b	623	CLA	C4B-CHC	2.15	1.47	1.41
24	b	616	CLA	C1B-NB	-2.15	1.33	1.35
24	B	604	CLA	C4C-C3C	2.15	1.48	1.45
24	C	501	CLA	C4C-C3C	2.15	1.48	1.45
24	C	507	CLA	C1B-CHB	2.15	1.47	1.41
24	b	611	CLA	C4C-C3C	2.15	1.48	1.45
24	C	505	CLA	C1B-NB	-2.14	1.33	1.35
24	B	615	CLA	CHD-C4C	2.14	1.47	1.41
24	c	515	CLA	C4B-CHC	2.14	1.46	1.41
24	c	516	CLA	C1B-CHB	2.14	1.46	1.41
24	b	622	CLA	C1C-C2C	2.13	1.48	1.44
24	B	613	CLA	CHD-C4C	2.13	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C4C-C3C	2.13	1.48	1.45
24	D	405	CLA	C1C-C2C	2.13	1.48	1.44
24	B	610	CLA	C4B-CHC	2.12	1.46	1.41
24	b	621	CLA	CHD-C4C	2.12	1.47	1.41
24	A	405	CLA	C4B-CHC	2.12	1.46	1.41
24	D	405	CLA	C1C-NC	-2.12	1.34	1.37
25	D	401[B]	PHO	C1A-NA	-2.12	1.33	1.37
24	a	412	CLA	C1C-C2C	2.11	1.48	1.44
24	c	508	CLA	C4B-NB	-2.11	1.33	1.35
25	d	402[A]	PHO	C1C-NC	-2.11	1.34	1.38
32	d	407[A]	PL9	C2-C3	2.11	1.40	1.34
24	B	603	CLA	C1B-CHB	2.11	1.46	1.41
24	b	619	CLA	C1C-C2C	2.11	1.48	1.44
24	c	516	CLA	C4C-C3C	2.10	1.48	1.45
24	b	614	CLA	C4C-C3C	2.10	1.48	1.45
34	b	629	LMG	O1-C1	2.10	1.43	1.40
24	d	403	CLA	C4C-C3C	2.10	1.48	1.45
25	D	401[B]	PHO	C1B-NB	-2.10	1.34	1.38
25	d	402[B]	PHO	C4D-CHA	2.10	1.49	1.43
24	B	608	CLA	C1B-NB	-2.09	1.33	1.35
24	A	406	CLA	C4C-C3C	2.09	1.48	1.45
25	d	402[A]	PHO	C4D-CHA	2.09	1.49	1.43
32	a	416[B]	PL9	C2-C3	2.09	1.40	1.34
24	A	406	CLA	C1B-CHB	2.09	1.46	1.41
24	B	602	CLA	C1C-NC	-2.09	1.34	1.37
24	A	406	CLA	C4B-CHC	2.08	1.46	1.41
32	a	416[A]	PL9	C2-C3	2.08	1.40	1.34
24	B	605	CLA	C4B-CHC	2.08	1.46	1.41
24	b	623	CLA	C1B-NB	-2.08	1.33	1.35
36	B	631	HTG	C1-S1	-2.08	1.77	1.80
24	b	621	CLA	C4C-C3C	2.08	1.48	1.45
36	B	624	HTG	C1-S1	-2.08	1.77	1.80
24	c	515	CLA	C4C-C3C	2.08	1.48	1.45
24	b	625	CLA	C4C-C3C	2.08	1.48	1.45
24	b	624	CLA	C4C-C3C	2.08	1.48	1.45
24	d	404	CLA	C1B-CHB	2.08	1.46	1.41
24	B	610	CLA	C1C-C2C	2.07	1.48	1.44
24	c	510	CLA	C1B-NB	-2.07	1.33	1.35
24	c	506	CLA	C1C-NC	-2.07	1.34	1.37
24	b	610	CLA	C1B-CHB	2.06	1.46	1.41
24	b	624	CLA	C1C-C2C	2.06	1.48	1.44
24	B	602	CLA	C4C-C3C	2.05	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	404	LMT	O1'-C1'	2.05	1.43	1.40
24	B	609	CLA	C1C-C2C	2.05	1.48	1.44
32	A	417[B]	PL9	C2-C3	2.04	1.40	1.34
24	A	406	CLA	C1C-C2C	2.04	1.48	1.44
24	A	407	CLA	C1B-CHB	2.04	1.46	1.41
32	A	417[A]	PL9	C2-C3	2.04	1.40	1.34
24	b	614	CLA	C1C-NC	-2.04	1.34	1.37
37	c	520	DGD	O5D-C1E	2.03	1.43	1.40
24	b	615	CLA	C4B-CHC	2.03	1.46	1.41
29	T	104	LMT	O1'-C1'	2.03	1.43	1.40
37	e	101	DGD	O5D-C1E	2.03	1.43	1.40
34	Z	101	LMG	O1-C1	2.03	1.43	1.40
24	c	506	CLA	C1C-C2C	2.02	1.48	1.44
25	a	411	PHO	C1B-NB	-2.01	1.34	1.38
24	a	412	CLA	C1B-NB	-2.01	1.33	1.35
29	M	104	LMT	O1'-C1'	2.01	1.43	1.40
24	c	512	CLA	C1D-C2D	2.00	1.47	1.42
24	B	603	CLA	C1B-NB	-2.00	1.33	1.35

All (2340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	C4A-NA-C1A	-7.55	103.31	106.71
24	c	516	CLA	C4A-NA-C1A	-7.43	103.37	106.71
25	D	401[B]	PHO	CMD-C2D-C1D	7.25	136.23	125.06
25	d	402[B]	PHO	CMD-C2D-C1D	7.24	136.21	125.06
24	A	405	CLA	C4A-NA-C1A	-7.18	103.48	106.71
24	C	503	CLA	C4A-NA-C1A	-7.18	103.48	106.71
25	A	408	PHO	CMD-C2D-C1D	7.16	136.09	125.06
39	E	103	HEM	CAD-CBD-CGD	7.07	124.53	112.67
36	C	522	HTG	C1'-S1-C1	6.97	113.13	100.09
24	b	621	CLA	CHD-C4C-C3C	-6.84	114.79	124.84
36	d	413	HTG	C1'-S1-C1	6.81	112.83	100.09
24	a	409	CLA	C4A-NA-C1A	-6.75	103.67	106.71
24	c	511	CLA	O2D-CGD-CBD	6.73	123.23	111.27
24	d	403	CLA	C2C-C1C-NC	6.71	116.26	109.97
24	B	616	CLA	C4A-NA-C1A	-6.70	103.70	106.71
25	a	411	PHO	CMD-C2D-C1D	6.67	135.34	125.06
24	c	516	CLA	O2D-CGD-CBD	6.65	123.09	111.27
24	B	616	CLA	CHD-C4C-C3C	-6.65	115.06	124.84
24	B	603	CLA	C4A-NA-C1A	-6.65	103.72	106.71
24	b	622	CLA	C2C-C1C-NC	6.63	116.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	CLA	O2D-CGD-CBD	6.62	123.04	111.27
24	B	615	CLA	CHD-C4C-C3C	-6.61	115.13	124.84
25	D	401[A]	PHO	CMD-C2D-C1D	6.60	135.24	125.06
24	b	614	CLA	CHD-C4C-C3C	-6.60	115.14	124.84
24	D	404	CLA	C2C-C1C-NC	6.59	116.15	109.97
24	b	619	CLA	C4A-NA-C1A	-6.58	103.75	106.71
24	B	609	CLA	C2C-C1C-NC	6.47	116.03	109.97
24	c	511	CLA	CHD-C4C-C3C	-6.43	115.38	124.84
24	B	613	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
25	d	402[A]	PHO	CMD-C2D-C1D	6.36	134.87	125.06
24	b	620	CLA	C2C-C1C-NC	6.32	115.89	109.97
24	c	507	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
24	b	613	CLA	C2C-C1C-NC	6.28	115.86	109.97
24	B	607	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
24	C	504	CLA	O2D-CGD-CBD	6.24	122.35	111.27
24	c	512	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
24	b	625	CLA	O2D-CGD-CBD	6.22	122.31	111.27
24	b	613	CLA	C4A-NA-C1A	-6.21	103.91	106.71
24	C	503	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
24	B	605	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	B	606	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
24	C	512	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
24	b	625	CLA	C4A-NA-C1A	-6.20	103.92	106.71
24	B	607	CLA	C4A-NA-C1A	-6.20	103.92	106.71
24	B	603	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
24	b	615	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
24	b	611	CLA	C4A-NA-C1A	-6.17	103.93	106.71
24	b	610	CLA	O2D-CGD-CBD	6.17	122.22	111.27
24	a	410	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
24	d	405	CLA	CHD-C4C-C3C	-6.13	115.82	124.84
24	b	617	CLA	C4A-NA-C1A	-6.12	103.96	106.71
24	B	612	CLA	C4A-NA-C1A	-6.11	103.96	106.71
24	b	624	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	C	502	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
24	b	618	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
24	B	612	CLA	C2C-C1C-NC	6.04	115.63	109.97
24	B	614	CLA	C2C-C1C-NC	6.02	115.61	109.97
24	C	501	CLA	O2D-CGD-CBD	6.01	121.95	111.27
24	b	612	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
24	C	501	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
24	c	509	CLA	C4A-NA-C1A	-6.01	104.01	106.71
24	B	602	CLA	CHD-C4C-C3C	-5.99	116.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CHD-C4C-C3C	-5.98	116.04	124.84
24	a	409	CLA	C2C-C1C-NC	5.98	115.58	109.97
24	b	625	CLA	CHD-C4C-C3C	-5.98	116.04	124.84
24	B	614	CLA	C4A-NA-C1A	-5.97	104.02	106.71
36	B	624	HTG	O5-C1-C2	5.95	117.80	110.31
24	C	507	CLA	CHD-C4C-C3C	-5.94	116.10	124.84
24	b	612	CLA	C4A-NA-C1A	-5.94	104.03	106.71
24	C	505	CLA	C4A-NA-C1A	-5.93	104.04	106.71
24	B	613	CLA	O2D-CGD-CBD	5.93	121.80	111.27
24	B	610	CLA	C2C-C1C-NC	5.92	115.52	109.97
24	B	611	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
24	b	611	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
24	d	404	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	b	610	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
24	C	512	CLA	O2D-CGD-CBD	5.86	121.69	111.27
24	B	604	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
24	C	504	CLA	C4A-NA-C1A	-5.86	104.07	106.71
24	B	602	CLA	O2D-CGD-CBD	5.86	121.67	111.27
24	B	617	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	c	517	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	C	505	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
24	c	514	CLA	C2C-C1C-NC	5.84	115.44	109.97
24	A	406	CLA	C2C-C1C-NC	5.83	115.44	109.97
24	A	407	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	b	613	CLA	O2D-CGD-CBD	5.82	121.61	111.27
36	B	624	HTG	C1'-S1-C1	5.81	110.96	100.09
24	C	510	CLA	C2C-C1C-NC	5.80	115.41	109.97
24	D	404	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
24	b	617	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
24	B	617	CLA	O2D-CGD-CBD	5.77	121.53	111.27
24	c	510	CLA	C2C-C1C-NC	5.77	115.38	109.97
24	A	409	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	c	515	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
24	C	506	CLA	C2C-C1C-NC	5.74	115.35	109.97
24	A	406	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
24	c	509	CLA	CHD-C4C-C3C	-5.72	116.42	124.84
24	C	508	CLA	O2D-CGD-CBD	5.72	121.44	111.27
24	B	615	CLA	O2D-CGD-CBD	5.72	121.43	111.27
24	D	404	CLA	C4A-NA-C1A	-5.69	104.15	106.71
36	B	623	HTG	C1'-S1-C1	5.68	110.71	100.09
27	L	102	SQD	O6-C1-C2	5.66	117.13	108.30
24	c	508	CLA	CHD-C4C-C3C	-5.65	116.53	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	617	CLA	C4A-NA-C1A	-5.65	104.17	106.71
24	d	405	CLA	C4A-NA-C1A	-5.64	104.17	106.71
24	c	512	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	c	506	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
24	c	505	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
24	b	621	CLA	O2D-CGD-CBD	5.62	121.25	111.27
24	c	513	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
24	c	509	CLA	C2C-C1C-NC	5.61	115.22	109.97
24	b	612	CLA	C2C-C1C-NC	5.58	115.20	109.97
24	b	613	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	B	605	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
25	D	401[B]	PHO	C3D-C2D-C1D	-5.57	97.75	105.87
24	c	513	CLA	C2C-C1C-NC	5.57	115.19	109.97
24	b	623	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
24	c	516	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
24	a	412	CLA	O2D-CGD-CBD	5.57	121.16	111.27
24	B	612	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
24	a	412	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
24	D	405	CLA	C2C-C1C-NC	5.55	115.17	109.97
24	b	615	CLA	C2C-C1C-NC	5.54	115.17	109.97
24	a	412	CLA	C2C-C1C-NC	5.54	115.17	109.97
24	C	505	CLA	O2D-CGD-CBD	5.53	121.10	111.27
36	c	523	HTG	C1'-S1-C1	5.51	110.40	100.09
26	Y	101	BCR	C33-C5-C6	-5.51	118.34	124.53
24	c	514	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
24	b	623	CLA	C2C-C1C-NC	5.50	115.13	109.97
24	c	505	CLA	O2D-CGD-CBD	5.50	121.04	111.27
24	b	618	CLA	O2D-CGD-CBD	5.49	121.03	111.27
24	B	604	CLA	O2D-CGD-CBD	5.48	121.01	111.27
24	b	624	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	b	618	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	c	517	CLA	C4A-NA-C1A	-5.44	104.26	106.71
25	d	402[B]	PHO	C3D-C2D-C1D	-5.43	97.96	105.87
24	C	511	CLA	C2C-C1C-NC	5.43	115.06	109.97
24	C	509	CLA	CHD-C4C-C3C	-5.42	116.86	124.84
24	c	509	CLA	O2D-CGD-CBD	5.42	120.91	111.27
24	b	612	CLA	O2D-CGD-CBD	5.42	120.90	111.27
25	D	401[A]	PHO	C3D-C2D-C1D	-5.42	97.98	105.87
24	b	614	CLA	O2D-CGD-CBD	5.41	120.89	111.27
24	B	614	CLA	CHD-C4C-C3C	-5.41	116.88	124.84
24	C	513	CLA	C2C-C1C-NC	5.41	115.04	109.97
24	B	610	CLA	CHD-C4C-C3C	-5.41	116.89	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	411	PHO	C3D-C2D-C1D	-5.40	98.00	105.87
24	b	610	CLA	C4A-NA-C1A	-5.40	104.28	106.71
24	C	509	CLA	C2C-C1C-NC	5.39	115.02	109.97
24	C	512	CLA	C4A-NA-C1A	-5.39	104.28	106.71
27	f	102	SQD	O47-C7-C8	5.39	123.12	111.50
24	B	608	CLA	C2C-C1C-NC	5.38	115.02	109.97
24	B	608	CLA	C4A-NA-C1A	-5.36	104.30	106.71
24	c	507	CLA	C2C-C1C-NC	5.36	114.99	109.97
25	d	402[B]	PHO	C2D-C1D-ND	5.36	117.87	109.79
24	b	624	CLA	C2C-C1C-NC	5.35	114.99	109.97
25	d	402[A]	PHO	O2D-CGD-CBD	5.34	120.76	111.27
24	C	508	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
24	c	508	CLA	O2D-CGD-CBD	5.34	120.75	111.27
36	B	632	HTG	C1'-S1-C1	5.34	110.07	100.09
24	C	511	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
24	B	611	CLA	C4A-NA-C1A	-5.32	104.31	106.71
24	B	604	CLA	C4A-NA-C1A	-5.32	104.31	106.71
24	C	504	CLA	C2C-C1C-NC	5.32	114.96	109.97
24	B	605	CLA	O2D-CGD-CBD	5.30	120.69	111.27
24	b	619	CLA	CHD-C4C-C3C	-5.30	117.04	124.84
24	C	508	CLA	C4A-NA-C1A	-5.30	104.32	106.71
26	C	515	BCR	C7-C8-C9	-5.30	118.22	126.23
24	C	504	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
24	d	403	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
24	c	505	CLA	C2C-C1C-NC	5.30	114.93	109.97
24	c	506	CLA	C4A-NA-C1A	-5.29	104.33	106.71
24	B	617	CLA	C2C-C1C-NC	5.29	114.93	109.97
24	d	404	CLA	CHD-C4C-C3C	-5.29	117.07	124.84
25	A	408	PHO	C3D-C2D-C1D	-5.28	98.18	105.87
24	b	619	CLA	C2C-C1C-NC	5.27	114.91	109.97
24	b	614	CLA	C4A-NA-C1A	-5.26	104.34	106.71
24	A	407	CLA	O2D-CGD-CBD	5.25	120.60	111.27
24	C	505	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	c	510	CLA	C4A-NA-C1A	-5.24	104.35	106.71
36	b	632	HTG	C1'-S1-C1	5.23	109.88	100.09
24	c	506	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	A	405	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	510	CLA	O2D-CGD-CBD	5.22	120.54	111.27
24	D	405	CLA	CHD-C4C-C3C	-5.21	117.18	124.84
24	B	607	CLA	C2C-C1C-NC	5.20	114.85	109.97
36	c	524	HTG	C1'-S1-C1	5.20	109.82	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	O2D-CGD-CBD	5.20	120.51	111.27
24	b	620	CLA	CHD-C4C-C3C	-5.19	117.20	124.84
25	D	401[B]	PHO	C2D-C1D-ND	5.19	117.63	109.79
24	C	506	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
25	d	402[A]	PHO	C3D-C2D-C1D	-5.18	98.33	105.87
24	c	510	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
24	C	510	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
24	b	616	CLA	O2D-CGD-CBD	5.16	120.43	111.27
24	c	514	CLA	O2D-CGD-CBD	5.15	120.43	111.27
24	C	503	CLA	O2D-CGD-CBD	5.15	120.42	111.27
24	C	513	CLA	CHD-C4C-C3C	-5.15	117.27	124.84
24	d	405	CLA	O2D-CGD-CBD	5.14	120.40	111.27
24	B	608	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
24	c	511	CLA	C2C-C1C-NC	5.13	114.78	109.97
24	C	501	CLA	C4A-NA-C1A	-5.12	104.41	106.71
24	b	618	CLA	C4A-NA-C1A	-5.10	104.41	106.71
24	a	410	CLA	C4A-NA-C1A	-5.10	104.41	106.71
24	b	621	CLA	C2C-C1C-NC	5.10	114.75	109.97
36	C	523	HTG	C1'-S1-C1	5.10	109.62	100.09
24	a	410	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	b	616	CLA	C2C-C1C-NC	5.09	114.74	109.97
25	D	401[A]	PHO	C2D-C1D-ND	5.09	117.47	109.79
24	B	606	CLA	O2D-CGD-CBD	5.09	120.31	111.27
25	d	402[A]	PHO	C1-C2-C3	-5.08	117.25	126.04
24	c	513	CLA	O2D-CGD-CBD	5.08	120.30	111.27
24	b	617	CLA	O2D-CGD-CBD	5.08	120.29	111.27
24	c	513	CLA	C4A-NA-C1A	-5.08	104.42	106.71
24	c	512	CLA	O2D-CGD-CBD	5.07	120.27	111.27
24	b	615	CLA	C4A-NA-C1A	-5.06	104.43	106.71
24	B	606	CLA	C2C-C1C-NC	5.06	114.71	109.97
25	d	402[B]	PHO	O2D-CGD-CBD	5.06	120.25	111.27
24	B	603	CLA	O2D-CGD-CBD	5.05	120.25	111.27
24	c	517	CLA	C2C-C1C-NC	5.05	114.70	109.97
24	b	622	CLA	C3B-C4B-NB	5.04	115.73	109.21
24	B	612	CLA	O2D-CGD-CBD	5.04	120.23	111.27
24	b	614	CLA	C2C-C1C-NC	5.04	114.69	109.97
24	B	603	CLA	C2C-C1C-NC	5.04	114.69	109.97
36	b	631	HTG	C1'-S1-C1	5.03	109.50	100.09
24	C	507	CLA	C4A-NA-C1A	-5.03	104.44	106.71
25	D	401[A]	PHO	C1-C2-C3	-5.03	117.35	126.04
24	C	507	CLA	C2C-C1C-NC	5.02	114.68	109.97
24	C	502	CLA	C2C-C1C-NC	5.02	114.68	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402[A]	PHO	C2D-C1D-ND	5.01	117.36	109.79
24	B	615	CLA	C2C-C1C-NC	5.01	114.67	109.97
24	c	508	CLA	C2C-C1C-NC	5.01	114.67	109.97
24	C	509	CLA	O2D-CGD-CBD	5.01	120.17	111.27
25	A	408	PHO	C2D-C1D-ND	5.01	117.35	109.79
24	c	512	CLA	C4A-NA-C1A	-5.00	104.46	106.71
27	F	101	SQD	O47-C7-C8	4.99	122.25	111.50
26	D	406	BCR	C7-C8-C9	-4.98	118.71	126.23
24	A	406	CLA	C4A-NA-C1A	-4.98	104.47	106.71
25	a	411	PHO	C2D-C1D-ND	4.98	117.30	109.79
24	b	620	CLA	O2D-CGD-CBD	4.98	120.11	111.27
24	C	506	CLA	C4A-NA-C1A	-4.98	104.47	106.71
24	A	409	CLA	CHD-C4C-C3C	-4.98	117.52	124.84
24	c	512	CLA	C3C-C4C-NC	4.97	116.15	110.57
24	B	602	CLA	C2C-C1C-NC	4.97	114.63	109.97
24	b	621	CLA	C3C-C4C-NC	4.97	116.14	110.57
26	H	101	BCR	C7-C8-C9	-4.97	118.73	126.23
24	B	608	CLA	O2D-CGD-CBD	4.96	120.09	111.27
24	B	609	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
25	d	402[B]	PHO	C1-C2-C3	-4.95	117.48	126.04
24	C	512	CLA	C2C-C1C-NC	4.95	114.61	109.97
36	D	414	HTG	C1'-S1-C1	4.95	109.34	100.09
24	D	405	CLA	O2D-CGD-CBD	4.93	120.04	111.27
24	C	503	CLA	C2C-C1C-NC	4.93	114.59	109.97
24	C	501	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	b	615	CLA	O2D-CGD-CBD	4.91	120.00	111.27
26	T	103	BCR	C33-C5-C6	-4.90	119.03	124.53
27	B	621	SQD	O47-C7-C8	4.89	122.04	111.50
24	A	406	CLA	O2D-CGD-CBD	4.89	119.95	111.27
24	d	403	CLA	C1C-C2C-C3C	-4.88	101.82	106.96
24	B	605	CLA	C4A-NA-C1A	-4.87	104.52	106.71
39	f	101	HEM	CAD-CBD-CGD	4.87	120.84	112.67
24	B	604	CLA	C2C-C1C-NC	4.87	114.53	109.97
24	B	613	CLA	C2C-C1C-NC	4.87	114.53	109.97
24	c	515	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	b	610	CLA	C2C-C1C-NC	4.86	114.53	109.97
24	C	510	CLA	C4A-NA-C1A	-4.86	104.52	106.71
24	B	615	CLA	C4A-NA-C1A	-4.85	104.53	106.71
36	B	622	HTG	C1'-S1-C1	4.85	109.16	100.09
24	A	405	CLA	CHD-C4C-C3C	-4.84	117.72	124.84
24	b	611	CLA	O2D-CGD-CBD	4.84	119.86	111.27
24	a	409	CLA	CHD-C4C-C3C	-4.83	117.74	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	CLA	O2D-CGD-CBD	4.82	119.84	111.27
36	B	631	HTG	C1'-S1-C1	4.82	109.10	100.09
24	b	612	CLA	C1D-CHD-C4C	-4.82	116.20	122.56
24	d	405	CLA	C2C-C1C-NC	4.81	114.48	109.97
24	c	507	CLA	C3C-C4C-NC	4.81	115.97	110.57
24	C	511	CLA	C4A-NA-C1A	-4.80	104.55	106.71
24	C	507	CLA	O2D-CGD-CBD	4.80	119.80	111.27
26	k	102	BCR	C20-C21-C22	-4.79	120.47	127.31
24	B	615	CLA	C3C-C4C-NC	4.78	115.93	110.57
37	e	101	DGD	O2G-C1B-C2B	4.77	121.79	111.50
24	c	511	CLA	C3C-C4C-NC	4.77	115.92	110.57
24	D	405	CLA	C4A-NA-C1A	-4.77	104.56	106.71
24	B	611	CLA	C2C-C1C-NC	4.76	114.43	109.97
27	A	411	SQD	O47-C7-C8	4.74	121.72	111.50
24	C	505	CLA	C3C-C4C-NC	4.74	115.88	110.57
24	B	607	CLA	O2D-CGD-CBD	4.74	119.69	111.27
24	D	404	CLA	C1C-C2C-C3C	-4.74	101.98	106.96
24	A	409	CLA	C4A-NA-C1A	-4.73	104.58	106.71
24	A	407	CLA	C2C-C1C-NC	4.73	114.40	109.97
37	e	101	DGD	O6E-C5E-C4E	4.72	118.27	109.69
27	B	621	SQD	O7-S-C6	4.72	112.55	106.94
24	B	613	CLA	C3C-C4C-NC	4.72	115.86	110.57
24	B	610	CLA	C4A-NA-C1A	-4.72	104.58	106.71
25	a	411	PHO	O2D-CGD-CBD	4.72	119.65	111.27
24	B	616	CLA	C3C-C4C-NC	4.72	115.86	110.57
24	C	508	CLA	C2C-C1C-NC	4.71	114.39	109.97
24	b	613	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
27	a	414	SQD	O47-C7-C8	4.71	121.65	111.50
24	d	403	CLA	C3B-C4B-NB	4.71	115.30	109.21
24	B	606	CLA	C4A-NA-C1A	-4.71	104.59	106.71
24	B	605	CLA	C3C-C4C-NC	4.70	115.84	110.57
27	A	411	SQD	O6-C1-C2	4.70	115.64	108.30
24	b	614	CLA	C3C-C4C-NC	4.70	115.84	110.57
24	B	616	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	b	622	CLA	C4A-NA-C1A	-4.69	104.60	106.71
24	b	617	CLA	C2C-C1C-NC	4.69	114.37	109.97
24	b	623	CLA	C4A-NA-C1A	-4.69	104.60	106.71
24	C	506	CLA	O2D-CGD-CBD	4.67	119.57	111.27
25	d	402[A]	PHO	C4C-C3C-C2C	-4.67	101.61	106.78
26	y	101	BCR	C33-C5-C6	-4.66	119.30	124.53
24	b	622	CLA	CHD-C4C-C3C	-4.65	118.00	124.84
27	a	414	SQD	O6-C1-C2	4.65	115.56	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	C4A-NA-C1A	-4.64	104.62	106.71
24	c	515	CLA	C2C-C1C-NC	4.63	114.31	109.97
32	D	407[B]	PL9	C7-C8-C9	-4.62	119.09	126.79
36	C	523	HTG	C1-O5-C5	4.62	121.10	112.58
24	C	509	CLA	C1-C2-C3	-4.62	118.06	126.04
24	C	502	CLA	C4A-NA-C1A	-4.60	104.64	106.71
24	c	507	CLA	C4A-NA-C1A	-4.60	104.64	106.71
24	C	503	CLA	C3C-C4C-NC	4.58	115.71	110.57
27	F	101	SQD	O5-C5-C4	4.58	118.00	109.69
25	D	401[B]	PHO	C1-C2-C3	-4.57	118.14	126.04
24	B	607	CLA	C3C-C4C-NC	4.57	115.70	110.57
24	c	507	CLA	C1D-CHD-C4C	-4.56	116.54	122.56
24	A	407	CLA	C4A-NA-C1A	-4.56	104.66	106.71
26	K	101	BCR	C7-C8-C9	-4.51	119.42	126.23
34	a	415	LMG	O7-C10-C11	4.50	121.21	111.50
24	C	502	CLA	C1-C2-C3	-4.49	118.27	126.04
24	b	611	CLA	C2C-C1C-NC	4.49	114.18	109.97
24	A	406	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
24	c	506	CLA	O2D-CGD-CBD	4.47	119.21	111.27
38	D	411	LHG	O7-C7-C8	4.47	121.14	111.50
26	B	618	BCR	C33-C5-C6	-4.47	119.51	124.53
24	c	514	CLA	C4A-NA-C1A	-4.46	104.70	106.71
24	d	404	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	d	403	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	C	512	CLA	C3C-C4C-NC	4.44	115.56	110.57
24	D	404	CLA	C1-C2-C3	-4.43	118.37	126.04
25	D	401[A]	PHO	O2D-CGD-CBD	4.43	119.14	111.27
24	c	509	CLA	C3C-C4C-NC	4.42	115.53	110.57
24	C	502	CLA	O2D-CGD-CBD	4.42	119.13	111.27
24	c	516	CLA	C2C-C1C-NC	4.42	114.11	109.97
24	A	409	CLA	O2D-CGD-CBD	4.41	119.11	111.27
24	B	602	CLA	C4A-NA-C1A	-4.41	104.72	106.71
24	b	625	CLA	C2C-C1C-NC	4.40	114.09	109.97
24	B	609	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	B	612	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	b	616	CLA	C4A-NA-C1A	-4.39	104.73	106.71
34	C	520	LMG	O7-C10-C11	4.38	120.94	111.50
34	c	522	LMG	O7-C10-C11	4.38	120.93	111.50
24	B	610	CLA	O2D-CGD-CBD	4.37	119.04	111.27
24	b	618	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	C	511	CLA	C1-C2-C3	-4.35	118.52	126.04
24	c	508	CLA	C4A-NA-C1A	-4.34	104.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C3C-C4C-NC	4.34	115.44	110.57
26	D	406	BCR	C24-C23-C22	-4.34	119.67	126.23
36	b	607	HTG	C1'-S1-C1	4.34	108.21	100.09
24	B	609	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
24	C	511	CLA	O2D-CGD-CBD	4.31	118.92	111.27
34	A	419	LMG	O7-C10-C11	4.30	120.78	111.50
24	b	619	CLA	O2D-CGD-CBD	4.30	118.90	111.27
24	B	613	CLA	CMC-C2C-C1C	4.28	131.56	125.04
24	B	611	CLA	O2D-CGD-CBD	4.27	118.86	111.27
24	c	510	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
24	b	612	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	B	609	CLA	O2D-CGD-CBD	4.27	118.85	111.27
24	c	514	CLA	C1-C2-C3	-4.27	118.66	126.04
27	L	102	SQD	O47-C7-C8	4.26	120.69	111.50
24	B	606	CLA	C3C-C4C-NC	4.26	115.35	110.57
37	C	516	DGD	O2G-C1B-C2B	4.26	120.68	111.50
24	a	412	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
27	B	621	SQD	O6-C1-C2	4.25	114.93	108.30
24	C	502	CLA	C3C-C4C-NC	4.24	115.33	110.57
24	a	409	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
29	A	414	LMT	C1'-O5'-C5'	4.23	122.00	113.69
32	D	407[B]	PL9	C42-C43-C44	-4.23	117.47	127.66
26	T	103	BCR	C11-C10-C9	-4.23	121.28	127.31
27	a	405	SQD	O47-C7-C8	4.21	120.58	111.50
24	b	613	CLA	C3C-C4C-NC	4.21	115.29	110.57
24	c	517	CLA	O2D-CGD-CBD	4.20	118.74	111.27
25	d	402[A]	PHO	O2D-CGD-O1D	-4.20	115.62	123.84
24	b	616	CLA	C3C-C4C-NC	4.20	115.28	110.57
29	D	403	LMT	O1B-C4'-C3'	4.19	118.43	107.28
24	C	510	CLA	C1-C2-C3	-4.19	118.80	126.04
24	b	620	CLA	C4A-NA-C1A	-4.19	104.82	106.71
26	b	626	BCR	C15-C14-C13	-4.19	121.34	127.31
24	A	409	CLA	CAC-C3C-C4C	4.18	130.24	124.81
24	B	603	CLA	C3C-C4C-NC	4.18	115.26	110.57
27	L	102	SQD	C3-C4-C5	4.18	117.69	110.24
24	B	614	CLA	C3C-C4C-NC	4.18	115.26	110.57
24	d	404	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
39	f	101	HEM	CBD-CAD-C3D	-4.17	104.79	112.48
24	b	615	CLA	C1D-CHD-C4C	-4.15	117.08	122.56
24	c	505	CLA	C4A-NA-C1A	-4.15	104.84	106.71
24	c	517	CLA	C3C-C4C-NC	4.15	115.22	110.57
26	H	101	BCR	C38-C26-C25	-4.14	119.88	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	102	BCR	C33-C5-C6	-4.14	119.88	124.53
24	b	625	CLA	C1D-CHD-C4C	-4.13	117.11	122.56
24	a	410	CLA	C3C-C4C-NC	4.12	115.19	110.57
37	D	408	DGD	O2G-C1B-C2B	4.12	120.38	111.50
24	b	623	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
24	b	620	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
27	a	405	SQD	O8-S-C6	4.10	112.27	105.74
24	c	511	CLA	C4A-NA-C1A	-4.10	104.86	106.71
36	V	206	HTG	C1'-S1-C1	4.09	107.75	100.09
24	c	506	CLA	C3C-C4C-NC	4.09	115.16	110.57
29	A	414	LMT	O5'-C5'-C4'	4.08	118.36	109.75
24	A	405	CLA	CAC-C3C-C4C	4.07	130.09	124.81
24	b	620	CLA	C3C-C4C-NC	4.07	115.14	110.57
24	D	404	CLA	O2D-CGD-CBD	4.07	118.50	111.27
24	B	616	CLA	C1D-CHD-C4C	-4.07	117.19	122.56
26	C	515	BCR	C33-C5-C6	-4.07	119.96	124.53
24	c	507	CLA	O2D-CGD-CBD	4.07	118.50	111.27
37	e	101	DGD	C3E-C4E-C5E	4.07	117.50	110.24
24	a	412	CLA	C3B-C4B-NB	4.06	114.46	109.21
38	E	101	LHG	O7-C7-C8	4.06	120.25	111.50
24	b	615	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	b	611	CLA	C3C-C4C-NC	4.06	115.12	110.57
24	A	406	CLA	CBC-CAC-C3C	-4.06	101.25	112.43
24	B	612	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
24	b	625	CLA	C3C-C4C-NC	4.06	115.12	110.57
24	B	614	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
36	b	632	HTG	O5-C1-C2	4.04	115.40	110.31
37	D	408	DGD	C1D-C2D-C3D	4.04	118.41	110.00
37	c	519	DGD	O2G-C1B-C2B	4.04	120.20	111.50
24	d	404	CLA	C3C-C4C-NC	4.03	115.10	110.57
24	B	604	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	c	505	CLA	C3C-C4C-NC	4.03	115.09	110.57
24	A	405	CLA	C1D-CHD-C4C	-4.03	117.24	122.56
29	a	404	LMT	C1'-O5'-C5'	4.02	121.59	113.69
24	A	405	CLA	CMB-C2B-C3B	4.02	132.21	124.68
24	C	506	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	C	507	CLA	C3C-C4C-NC	4.02	115.08	110.57
26	y	101	BCR	C15-C14-C13	-4.01	121.58	127.31
24	C	511	CLA	C3B-C4B-NB	4.00	114.39	109.21
37	c	521	DGD	O2G-C1B-C2B	4.00	120.13	111.50
26	B	620	BCR	C15-C14-C13	-4.00	121.60	127.31
24	C	511	CLA	CAC-C3C-C4C	4.00	130.00	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C3C-C4C-NC	4.00	115.05	110.57
24	b	619	CLA	C3C-C4C-NC	4.00	115.05	110.57
24	B	606	CLA	C1D-CHD-C4C	-4.00	117.28	122.56
24	b	624	CLA	C3C-C4C-NC	3.99	115.05	110.57
24	B	609	CLA	C3B-C4B-NB	3.99	114.37	109.21
24	c	511	CLA	C1D-CHD-C4C	-3.99	117.29	122.56
24	b	619	CLA	C1-C2-C3	-3.99	119.15	126.04
25	d	402[B]	PHO	C4C-C3C-C2C	-3.98	102.37	106.78
24	b	622	CLA	CAC-C3C-C4C	3.98	129.98	124.81
26	c	526	BCR	C15-C14-C13	-3.98	121.62	127.31
24	C	504	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
24	C	502	CLA	C1D-CHD-C4C	-3.97	117.31	122.56
24	D	405	CLA	C3C-C4C-NC	3.97	115.03	110.57
24	C	503	CLA	C1D-CHD-C4C	-3.97	117.32	122.56
24	b	614	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
32	d	407[B]	PL9	C42-C43-C44	-3.97	118.11	127.66
24	B	617	CLA	C1D-CHD-C4C	-3.97	117.33	122.56
24	D	404	CLA	C3C-C4C-NC	3.96	115.02	110.57
24	d	405	CLA	C3C-C4C-NC	3.96	115.01	110.57
24	C	513	CLA	O2D-CGD-CBD	3.96	118.30	111.27
24	b	613	CLA	CMC-C2C-C1C	3.95	131.06	125.04
24	B	617	CLA	C3C-C4C-NC	3.95	115.00	110.57
24	c	508	CLA	C3C-C4C-NC	3.95	115.00	110.57
24	c	513	CLA	C3C-C4C-NC	3.94	114.99	110.57
26	Y	101	BCR	C15-C14-C13	-3.94	121.68	127.31
26	b	628	BCR	C24-C23-C22	-3.94	120.28	126.23
24	B	610	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
32	a	416[A]	PL9	C22-C23-C24	-3.94	118.18	127.66
24	b	617	CLA	C3C-C4C-NC	3.94	114.98	110.57
24	b	621	CLA	C1D-CHD-C4C	-3.94	117.36	122.56
26	b	627	BCR	C15-C14-C13	-3.93	121.70	127.31
24	c	514	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
24	c	515	CLA	O2D-CGD-CBD	3.93	118.25	111.27
24	A	405	CLA	CAA-C2A-C3A	-3.92	102.03	112.78
32	a	416[A]	PL9	C15-C14-C16	3.92	121.87	115.27
24	b	622	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
25	a	411	PHO	CAC-C3C-C4C	3.92	129.50	125.22
24	A	406	CLA	CMB-C2B-C3B	3.91	132.00	124.68
24	B	602	CLA	C3C-C4C-NC	3.91	114.96	110.57
24	B	603	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
24	B	605	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
27	A	413	SQD	O47-C7-C8	3.91	119.92	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	C1-C2-C3	-3.91	119.29	126.04
24	B	607	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
24	b	610	CLA	C1D-CHD-C4C	-3.90	117.41	122.56
24	b	611	CLA	O2D-CGD-O1D	-3.89	116.22	123.84
25	D	401[A]	PHO	C4C-C3C-C2C	-3.89	102.47	106.78
39	E	103	HEM	CBD-CAD-C3D	-3.89	105.31	112.48
24	B	615	CLA	O2D-CGD-O1D	-3.89	116.23	123.84
24	d	405	CLA	C1D-CHD-C4C	-3.88	117.43	122.56
24	c	505	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
27	F	101	SQD	O6-C1-C2	3.88	114.36	108.30
32	a	416[A]	PL9	C32-C33-C34	-3.88	118.32	127.66
24	C	501	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
38	d	410	LHG	O7-C7-C8	3.87	119.85	111.50
29	a	404	LMT	O5'-C5'-C4'	3.87	117.92	109.75
24	A	405	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	b	617	CLA	C1-C2-C3	-3.87	119.35	126.04
24	C	511	CLA	C1D-CHD-C4C	-3.87	117.46	122.56
24	b	621	CLA	C4A-NA-C1A	-3.86	104.97	106.71
24	c	513	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
32	A	417[B]	PL9	C7-C3-C4	3.85	120.01	116.88
24	A	409	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	B	605	CLA	C1-C2-C3	-3.84	119.40	126.04
24	b	623	CLA	C3C-C4C-NC	3.84	114.88	110.57
24	b	616	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	B	603	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
32	d	407[B]	PL9	C7-C8-C9	-3.83	120.42	126.79
24	C	504	CLA	C1D-CHD-C4C	-3.83	117.51	122.56
24	b	610	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
26	c	518	BCR	C15-C14-C13	-3.83	121.85	127.31
24	A	405	CLA	C3B-C4B-NB	3.82	114.16	109.21
24	c	513	CLA	C1D-CHD-C4C	-3.82	117.52	122.56
25	a	411	PHO	C4C-C3C-C2C	-3.81	102.56	106.78
34	C	519	LMG	O7-C10-C11	3.81	119.72	111.50
26	D	406	BCR	C38-C26-C25	-3.81	120.25	124.53
24	C	503	CLA	O2D-CGD-O1D	-3.80	116.40	123.84
24	C	510	CLA	C3C-C4C-NC	3.80	114.83	110.57
24	B	613	CLA	C4A-NA-C1A	-3.80	105.00	106.71
26	t	102	BCR	C3-C4-C5	-3.80	107.30	114.08
24	B	602	CLA	C1D-CHD-C4C	-3.80	117.55	122.56
32	a	416[A]	PL9	C7-C3-C4	3.79	119.96	116.88
24	B	610	CLA	C3C-C4C-NC	3.79	114.82	110.57
24	C	513	CLA	C1C-C2C-C3C	-3.79	102.98	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
24	C	509	CLA	C3C-C4C-NC	3.78	114.81	110.57
24	B	608	CLA	C3C-C4C-NC	3.78	114.81	110.57
24	B	605	CLA	C3B-C4B-NB	3.78	114.10	109.21
24	b	623	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
24	C	501	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
24	C	501	CLA	CMC-C2C-C1C	3.77	130.77	125.04
24	c	512	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	b	618	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	A	407	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
24	C	510	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	c	517	CLA	C1D-CHD-C4C	-3.76	117.60	122.56
24	b	624	CLA	C1D-CHD-C4C	-3.76	117.60	122.56
24	b	612	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
26	b	626	BCR	C7-C8-C9	-3.75	120.57	126.23
24	d	403	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
24	c	510	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	a	410	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
24	c	514	CLA	C4-C3-C5	3.73	121.55	115.27
24	C	506	CLA	CBC-CAC-C3C	-3.72	102.17	112.43
32	A	417[B]	PL9	C37-C38-C39	-3.72	118.70	127.66
34	Z	101	LMG	O7-C10-C11	3.72	119.52	111.50
24	C	506	CLA	CAC-C3C-C4C	3.72	129.63	124.81
26	d	406	BCR	C28-C27-C26	-3.72	107.44	114.08
24	b	619	CLA	CAC-C3C-C4C	3.71	129.62	124.81
24	b	622	CLA	C3C-C4C-NC	3.71	114.73	110.57
24	B	604	CLA	C1D-CHD-C4C	-3.71	117.67	122.56
24	c	510	CLA	O2D-CGD-CBD	3.71	117.85	111.27
24	C	508	CLA	C3C-C4C-NC	3.70	114.72	110.57
27	A	413	SQD	O48-C23-C24	3.70	123.53	111.91
24	c	514	CLA	C3C-C4C-NC	3.70	114.72	110.57
24	A	406	CLA	C3B-C4B-NB	3.70	113.99	109.21
27	A	411	SQD	O8-S-C6	3.70	111.64	105.74
37	c	520	DGD	O2G-C1B-C2B	3.69	119.46	111.50
24	C	501	CLA	C1D-CHD-C4C	-3.69	117.68	122.56
24	c	508	CLA	C1D-CHD-C4C	-3.69	117.69	122.56
24	C	508	CLA	C3B-C4B-NB	3.69	113.98	109.21
24	a	410	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
24	B	615	CLA	C1D-CHD-C4C	-3.68	117.70	122.56
34	a	415	LMG	C8-O7-C10	-3.68	108.74	117.79
24	A	407	CLA	C3C-C4C-NC	3.68	114.69	110.57
24	C	506	CLA	C3C-C4C-NC	3.67	114.69	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	622	CLA	CHC-C1C-C2C	-3.67	116.58	126.72
32	d	407[A]	PL9	C42-C43-C44	-3.66	118.84	127.66
24	d	403	CLA	CBC-CAC-C3C	-3.66	102.33	112.43
24	c	513	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	C	507	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	C	509	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
24	D	405	CLA	C3B-C4B-NB	3.65	113.94	109.21
24	c	508	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
24	b	617	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
27	a	414	SQD	O8-S-C6	3.65	111.55	105.74
26	b	626	BCR	C33-C5-C6	-3.65	120.43	124.53
29	T	104	LMT	C1'-O5'-C5'	3.65	120.84	113.69
24	a	409	CLA	C3B-C4B-NB	3.64	113.92	109.21
32	a	416[B]	PL9	C7-C3-C4	3.64	119.84	116.88
24	B	604	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
24	C	512	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
24	b	620	CLA	C3B-C4B-NB	3.64	113.91	109.21
24	c	512	CLA	C4D-C3D-CAD	-3.63	106.44	108.47
24	b	623	CLA	C1-C2-C3	-3.63	119.76	126.04
24	B	617	CLA	C3B-C4B-NB	3.63	113.91	109.21
24	d	403	CLA	CHC-C1C-C2C	-3.63	116.68	126.72
24	A	409	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	C	505	CLA	C1D-CHD-C4C	-3.62	117.78	122.56
24	C	510	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	B	610	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	C	511	CLA	C3C-C4C-NC	3.62	114.63	110.57
24	d	403	CLA	C4A-NA-C1A	-3.61	105.08	106.71
24	B	613	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	C	513	CLA	C1D-CHD-C4C	-3.61	117.79	122.56
24	D	405	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
25	D	401[B]	PHO	C4C-C3C-C2C	-3.61	102.79	106.78
26	c	518	BCR	C16-C17-C18	-3.61	122.16	127.31
24	A	407	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
26	C	514	BCR	C7-C8-C9	-3.61	120.78	126.23
24	C	509	CLA	C3B-C4B-NB	3.61	113.87	109.21
24	c	514	CLA	C3B-C4B-NB	3.61	113.87	109.21
24	B	604	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
32	D	407[B]	PL9	C10-C9-C11	3.60	121.33	115.27
24	c	515	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	c	505	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	c	514	CLA	C1D-CHD-C4C	-3.59	117.81	122.56
34	D	415	LMG	O7-C10-C11	3.59	119.24	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	CAC-C3C-C4C	3.59	129.47	124.81
24	c	512	CLA	C1D-CHD-C4C	-3.58	117.83	122.56
32	a	416[B]	PL9	C32-C33-C34	-3.58	119.04	127.66
24	C	504	CLA	C3C-C4C-NC	3.58	114.58	110.57
24	c	509	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
24	c	506	CLA	C1-C2-C3	-3.57	119.86	126.04
24	c	516	CLA	C3C-C4C-NC	3.57	114.58	110.57
24	b	610	CLA	O2D-CGD-O1D	-3.57	116.86	123.84
24	a	409	CLA	CAA-C2A-C3A	-3.57	103.01	112.78
26	H	101	BCR	C24-C23-C22	-3.56	120.85	126.23
24	B	616	CLA	CMC-C2C-C1C	3.56	130.47	125.04
24	D	404	CLA	C3B-C4B-NB	3.56	113.82	109.21
24	B	614	CLA	C3B-C4B-NB	3.56	113.81	109.21
24	c	515	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
26	d	406	BCR	C38-C26-C25	-3.56	120.53	124.53
24	b	624	CLA	O2D-CGD-CBD	3.55	117.58	111.27
24	a	409	CLA	C3C-C4C-NC	3.55	114.56	110.57
24	d	405	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
26	T	103	BCR	C12-C13-C14	-3.55	113.50	118.94
24	C	507	CLA	C1D-CHD-C4C	-3.55	117.88	122.56
24	b	617	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
26	d	406	BCR	C24-C23-C22	-3.55	120.88	126.23
32	a	416[B]	PL9	C7-C8-C9	-3.54	120.89	126.79
32	D	407[A]	PL9	C40-C39-C41	3.54	121.22	115.27
24	c	506	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
24	b	623	CLA	C1D-CHD-C4C	-3.54	117.89	122.56
34	d	415	LMG	O7-C10-C11	3.54	119.13	111.50
32	D	407[A]	PL9	C42-C43-C44	-3.54	119.15	127.66
24	B	602	CLA	C3B-C4B-NB	3.53	113.78	109.21
24	b	614	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	C	505	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
24	c	505	CLA	CAC-C3C-C4C	3.53	129.39	124.81
26	c	526	BCR	C33-C5-C6	-3.53	120.57	124.53
24	d	404	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
27	A	411	SQD	C45-O47-C7	-3.52	109.12	117.79
24	b	615	CLA	C3B-C4B-NB	3.52	113.76	109.21
32	a	416[B]	PL9	C15-C14-C16	3.52	121.19	115.27
24	B	611	CLA	C1D-CHD-C4C	-3.52	117.92	122.56
24	c	512	CLA	C3B-C4B-NB	3.52	113.75	109.21
24	c	517	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
24	B	611	CLA	C3C-C4C-NC	3.51	114.51	110.57
24	C	513	CLA	C1-C2-C3	-3.51	119.97	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
24	c	507	CLA	C1-C2-C3	-3.51	119.97	126.04
24	C	504	CLA	C3B-C4B-NB	3.51	113.74	109.21
24	B	603	CLA	C1D-CHD-C4C	-3.51	117.93	122.56
24	B	609	CLA	C3C-C4C-NC	3.50	114.50	110.57
24	B	613	CLA	C4-C3-C5	3.50	121.16	115.27
24	D	405	CLA	O2D-CGD-O1D	-3.50	117.00	123.84
24	B	602	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
32	a	416[A]	PL9	C7-C8-C9	-3.50	120.97	126.79
24	A	406	CLA	CAA-C2A-C3A	-3.49	103.21	112.78
26	H	101	BCR	C16-C17-C18	-3.49	122.32	127.31
24	b	625	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
24	C	513	CLA	C3C-C4C-NC	3.49	114.49	110.57
24	b	610	CLA	C3C-C4C-NC	3.49	114.49	110.57
24	b	614	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
26	b	627	BCR	C29-C30-C25	3.49	115.85	110.48
24	a	410	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
24	b	621	CLA	C4C-C3C-C2C	-3.49	101.82	106.90
24	c	512	CLA	C1-C2-C3	-3.48	120.02	126.04
24	A	406	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
24	a	412	CLA	C3C-C4C-NC	3.48	114.47	110.57
25	d	402[A]	PHO	C4-C3-C5	3.48	121.12	115.27
24	B	611	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
24	c	516	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
27	a	405	SQD	O48-C23-C24	3.48	122.83	111.91
37	C	517	DGD	O2G-C1B-C2B	3.48	119.00	111.50
26	h	101	BCR	C38-C26-C25	-3.48	120.62	124.53
39	E	103	HEM	CBA-CAA-C2A	-3.48	106.07	112.49
24	b	613	CLA	C3B-C4B-NB	3.47	113.70	109.21
24	B	614	CLA	C1-C2-C3	-3.47	120.04	126.04
27	f	102	SQD	C1-O5-C5	3.47	120.50	113.69
24	b	621	CLA	C3B-C4B-NB	3.47	113.69	109.21
24	c	511	CLA	CMC-C2C-C1C	3.47	130.32	125.04
24	D	404	CLA	CBC-CAC-C3C	-3.47	102.87	112.43
24	C	511	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
24	b	622	CLA	C1-C2-C3	-3.46	120.06	126.04
25	D	401[B]	PHO	O2D-CGD-CBD	3.46	117.42	111.27
24	c	511	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	B	609	CLA	CHC-C1C-C2C	-3.46	117.15	126.72
34	z	101	LMG	O7-C10-C11	3.46	118.95	111.50
38	L	101	LHG	O7-C7-C8	3.46	118.95	111.50
32	A	417[A]	PL9	C7-C3-C4	3.46	119.69	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
24	b	612	CLA	C3B-C4B-NB	3.45	113.68	109.21
24	A	406	CLA	C3C-C4C-NC	3.45	114.44	110.57
24	b	621	CLA	O2A-CGA-CBA	3.45	122.74	111.91
24	a	412	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
24	B	614	CLA	CAC-C3C-C4C	3.45	129.28	124.81
24	d	404	CLA	O2A-CGA-CBA	3.44	122.70	111.91
26	B	620	BCR	C28-C27-C26	-3.44	107.94	114.08
24	b	616	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
24	D	405	CLA	C4-C3-C5	3.43	121.04	115.27
24	B	608	CLA	CAA-C2A-C3A	-3.43	103.40	112.78
24	b	624	CLA	C3B-C4B-NB	3.42	113.63	109.21
24	b	622	CLA	O2D-CGD-CBD	3.41	117.33	111.27
24	b	616	CLA	CBC-CAC-C3C	-3.41	103.03	112.43
32	A	417[A]	PL9	C37-C38-C39	-3.41	119.45	127.66
32	a	416[B]	PL9	C22-C23-C24	-3.40	119.47	127.66
24	b	620	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	c	507	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
24	b	623	CLA	C3B-C4B-NB	3.40	113.61	109.21
24	C	502	CLA	CAC-C3C-C4C	3.40	129.22	124.81
26	b	626	BCR	C16-C17-C18	-3.40	122.46	127.31
34	k	101	LMG	O7-C10-C11	3.40	118.82	111.50
24	B	615	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
24	c	510	CLA	CBC-CAC-C3C	-3.39	103.08	112.43
27	F	101	SQD	C3-C4-C5	3.39	116.29	110.24
32	A	417[A]	PL9	C20-C19-C21	3.39	120.97	115.27
24	B	615	CLA	C3B-C4B-NB	3.39	113.59	109.21
24	b	625	CLA	C3B-C4B-NB	3.38	113.59	109.21
24	C	508	CLA	C1D-CHD-C4C	-3.38	118.09	122.56
24	b	621	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
26	a	413	BCR	C20-C21-C22	-3.38	122.49	127.31
24	C	509	CLA	CAC-C3C-C4C	3.38	129.19	124.81
24	b	625	CLA	CAC-C3C-C4C	3.38	129.19	124.81
24	c	512	CLA	C4-C3-C5	3.38	120.95	115.27
24	b	620	CLA	CHC-C1C-C2C	-3.37	117.39	126.72
24	C	506	CLA	C4-C3-C5	3.37	120.94	115.27
24	A	409	CLA	C4-C3-C5	3.37	120.94	115.27
24	B	608	CLA	C1D-CHD-C4C	-3.37	118.11	122.56
26	Y	101	BCR	C10-C11-C12	-3.36	112.73	123.22
26	Y	101	BCR	C24-C23-C22	-3.36	121.16	126.23
24	B	610	CLA	CHC-C1C-C2C	-3.36	117.44	126.72
24	B	611	CLA	O2A-CGA-CBA	3.36	122.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	625	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
32	D	407[A]	PL9	C7-C8-C9	-3.35	121.22	126.79
24	D	405	CLA	CAC-C3C-C4C	3.35	129.15	124.81
24	b	614	CLA	O2A-CGA-O1A	-3.35	115.15	123.59
24	c	516	CLA	O2D-CGD-O1D	-3.34	117.30	123.84
24	B	609	CLA	C1D-CHD-C4C	-3.34	118.14	122.56
24	B	607	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
24	b	613	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
26	B	619	BCR	C28-C27-C26	-3.34	108.12	114.08
24	c	505	CLA	C3B-C4B-NB	3.34	113.52	109.21
29	C	521	LMT	C1'-O5'-C5'	3.33	120.23	113.69
24	B	610	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
24	c	515	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	B	612	CLA	C3B-C4B-NB	3.33	113.51	109.21
24	b	619	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
25	A	408	PHO	C4C-C3C-C2C	-3.33	103.10	106.78
32	A	417[B]	PL9	C20-C19-C21	3.33	120.87	115.27
24	C	510	CLA	CAC-C3C-C4C	3.33	129.12	124.81
29	C	521	LMT	O1B-C4'-C3'	3.33	116.13	107.28
24	b	613	CLA	CAC-C3C-C4C	3.32	129.12	124.81
37	h	102	DGD	O2G-C1B-C2B	3.32	118.66	111.50
24	C	512	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	b	624	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	c	506	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
36	b	608	HTG	C1'-S1-C1	3.32	106.30	100.09
32	a	416[B]	PL9	C27-C28-C29	-3.32	119.68	127.66
24	b	621	CLA	C4-C3-C5	3.31	120.84	115.27
25	d	402[B]	PHO	CHC-C1C-C2C	-3.31	117.40	125.73
24	b	611	CLA	CAA-C2A-C3A	-3.31	103.71	112.78
26	D	406	BCR	C28-C27-C26	-3.31	108.17	114.08
24	a	412	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
24	B	604	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
27	a	414	SQD	C1-C2-C3	-3.31	103.11	110.00
24	B	608	CLA	C3B-C4B-NB	3.31	113.48	109.21
24	b	612	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
24	c	516	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
24	B	605	CLA	CAC-C3C-C4C	3.30	129.09	124.81
24	a	412	CLA	C1-C2-C3	-3.30	120.33	126.04
24	d	403	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
24	B	611	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
24	D	404	CLA	O2A-CGA-CBA	3.30	122.25	111.91
24	A	406	CLA	CHC-C1C-C2C	-3.29	117.62	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	102	BCR	C15-C16-C17	-3.29	116.73	123.47
24	c	511	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
24	b	614	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
37	H	102	DGD	O2G-C1B-C2B	3.29	118.59	111.50
24	d	403	CLA	C3C-C4C-NC	3.29	114.26	110.57
24	C	501	CLA	CBC-CAC-C3C	-3.29	103.37	112.43
24	A	405	CLA	O2A-CGA-CBA	3.29	122.22	111.91
24	B	617	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
32	A	417[B]	PL9	C22-C23-C24	-3.29	119.75	127.66
24	c	515	CLA	C3B-C4B-NB	3.28	113.45	109.21
24	B	608	CLA	CAC-C3C-C4C	3.28	129.07	124.81
24	c	515	CLA	C1-C2-C3	-3.28	120.37	126.04
24	c	516	CLA	CBC-CAC-C3C	-3.28	103.39	112.43
32	A	417[A]	PL9	C32-C33-C34	-3.28	119.77	127.66
25	A	408	PHO	CHC-C1C-C2C	-3.28	117.49	125.73
24	c	506	CLA	CAC-C3C-C4C	3.27	129.06	124.81
24	B	614	CLA	CMB-C2B-C3B	3.27	130.80	124.68
24	b	622	CLA	C1D-CHD-C4C	-3.27	118.24	122.56
24	d	404	CLA	C1-C2-C3	-3.27	120.39	126.04
32	a	416[A]	PL9	C17-C18-C19	-3.27	119.79	127.66
24	C	508	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
24	C	502	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
24	B	611	CLA	CHD-C4C-NC	3.27	129.35	124.20
26	K	101	BCR	C24-C23-C22	-3.26	121.30	126.23
24	B	606	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
25	D	401[A]	PHO	C4-C3-C5	3.26	120.76	115.27
26	B	619	BCR	C33-C5-C6	-3.26	120.87	124.53
24	B	604	CLA	CMB-C2B-C3B	3.26	130.77	124.68
24	b	610	CLA	CHD-C4C-NC	3.26	129.34	124.20
32	D	407[A]	PL9	C10-C9-C11	3.26	120.75	115.27
24	B	604	CLA	O2A-CGA-O1A	-3.25	115.38	123.59
24	B	615	CLA	C1C-C2C-C3C	-3.25	103.53	106.96
24	C	502	CLA	C3B-C4B-NB	3.25	113.42	109.21
24	D	405	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
26	t	102	BCR	C20-C21-C22	-3.25	122.67	127.31
24	c	509	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
25	d	402[B]	PHO	C4-C3-C5	3.24	120.73	115.27
24	A	405	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
32	a	416[B]	PL9	C17-C18-C19	-3.24	119.85	127.66
32	A	417[B]	PL9	C7-C8-C9	-3.24	121.39	126.79
24	b	619	CLA	C3B-C4B-NB	3.24	113.40	109.21
26	d	406	BCR	C29-C30-C25	3.24	115.47	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
24	c	510	CLA	C1D-CHD-C4C	-3.24	118.28	122.56
24	C	503	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
26	c	518	BCR	C38-C26-C25	-3.24	120.89	124.53
24	B	612	CLA	CMC-C2C-C1C	3.23	129.97	125.04
24	D	404	CLA	CHC-C1C-C2C	-3.23	117.77	126.72
32	a	416[A]	PL9	C20-C19-C21	3.23	120.71	115.27
24	b	618	CLA	C1D-CHD-C4C	-3.23	118.29	122.56
32	A	417[B]	PL9	C32-C33-C34	-3.23	119.88	127.66
24	B	616	CLA	O2D-CGD-CBD	3.23	117.01	111.27
24	d	405	CLA	C3B-C4B-NB	3.23	113.38	109.21
27	F	101	SQD	C1-C2-C3	-3.23	103.27	110.00
24	A	407	CLA	C3B-C4B-NB	3.22	113.37	109.21
24	b	624	CLA	C4-C3-C5	3.22	120.68	115.27
24	c	511	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
24	c	506	CLA	C4D-C3D-CAD	-3.22	106.68	108.47
38	b	634	LHG	O7-C7-C8	3.21	118.43	111.50
24	B	612	CLA	CMA-C3A-C4A	-3.21	103.14	111.77
39	V	205	HEM	CBA-CAA-C2A	-3.21	106.56	112.49
32	D	407[B]	PL9	C40-C39-C41	3.21	120.68	115.27
24	c	510	CLA	C3C-C4C-NC	3.21	114.17	110.57
24	B	612	CLA	CAC-C3C-C4C	3.21	128.98	124.81
32	A	417[B]	PL9	C7-C3-C2	-3.21	119.08	123.30
24	C	509	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
32	a	416[A]	PL9	C42-C43-C44	-3.21	119.94	127.66
24	c	510	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
26	A	410	BCR	C33-C5-C6	-3.21	120.93	124.53
39	v	206	HEM	CBA-CAA-C2A	-3.20	106.59	112.49
24	b	624	CLA	C4D-C3D-CAD	-3.20	106.69	108.47
24	c	508	CLA	CMC-C2C-C1C	3.20	129.91	125.04
24	c	512	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	C	512	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
24	B	613	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
25	D	401[A]	PHO	CHC-C1C-C2C	-3.19	117.69	125.73
24	c	506	CLA	C3B-C4B-NB	3.19	113.34	109.21
24	c	513	CLA	C1-C2-C3	-3.19	120.52	126.04
24	b	618	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
32	a	416[A]	PL9	C10-C9-C11	3.19	120.64	115.27
36	c	524	HTG	C1-O5-C5	3.19	118.47	112.58
25	a	411	PHO	O1D-CGD-CBD	-3.19	117.95	124.48
24	B	604	CLA	O2A-CGA-CBA	3.19	121.90	111.91
32	d	407[B]	PL9	C40-C39-C41	3.19	120.63	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C4-C3-C5	3.18	120.62	115.27
25	d	402[A]	PHO	C4D-CHA-C1A	-3.18	118.21	125.37
24	c	515	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	B	616	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
24	C	503	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
24	a	412	CLA	CHC-C1C-C2C	-3.18	117.93	126.72
24	b	614	CLA	C2A-C1A-CHA	-3.18	118.31	123.86
26	D	406	BCR	C33-C5-C6	-3.17	120.97	124.53
24	C	509	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	b	617	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	a	410	CLA	OBD-CAD-C3D	-3.17	122.72	127.98
26	T	103	BCR	C15-C16-C17	-3.17	116.98	123.47
24	C	502	CLA	C4D-C3D-CAD	-3.17	106.70	108.47
24	a	410	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
38	D	411	LHG	O8-C23-C24	3.17	121.85	111.91
24	B	617	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	A	409	CLA	C1D-CHD-C4C	-3.17	118.38	122.56
24	c	506	CLA	CHC-C1C-C2C	-3.17	117.97	126.72
24	B	605	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
24	b	611	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
24	C	506	CLA	C3B-C4B-NB	3.16	113.30	109.21
24	b	611	CLA	C1D-CHD-C4C	-3.16	118.39	122.56
24	B	614	CLA	C4-C3-C5	3.16	120.58	115.27
26	B	618	BCR	C7-C8-C9	-3.16	121.47	126.23
24	C	505	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
26	B	620	BCR	C36-C18-C19	3.15	123.05	118.08
24	b	618	CLA	C3B-C4B-NB	3.15	113.28	109.21
24	d	405	CLA	CHD-C4C-NC	3.15	129.17	124.20
24	B	606	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	c	517	CLA	CMC-C2C-C1C	3.15	129.84	125.04
26	Y	101	BCR	C40-C30-C25	-3.15	105.19	110.30
26	T	103	BCR	C21-C20-C19	-3.15	113.39	123.22
27	L	102	SQD	O8-S-C6	3.15	110.76	105.74
26	C	514	BCR	C15-C14-C13	-3.15	122.82	127.31
24	c	513	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
24	B	616	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
24	A	405	CLA	CHC-C1C-C2C	-3.14	118.02	126.72
24	B	607	CLA	CMC-C2C-C1C	3.14	129.83	125.04
24	C	504	CLA	CMB-C2B-C3B	3.14	130.56	124.68
24	A	405	CLA	C1C-C2C-C3C	-3.14	103.65	106.96
24	B	608	CLA	CMC-C2C-C1C	3.14	129.82	125.04
24	B	616	CLA	CAC-C3C-C4C	3.14	128.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CHD-C4C-NC	3.14	129.15	124.20
34	b	629	LMG	O7-C10-C11	3.14	118.26	111.50
24	c	513	CLA	CMB-C2B-C3B	3.14	130.55	124.68
32	D	407[B]	PL9	C36-C37-C38	-3.14	101.58	111.88
24	c	510	CLA	C1-C2-C3	-3.13	120.62	126.04
24	a	412	CLA	CBC-CAC-C3C	-3.13	103.79	112.43
26	t	102	BCR	C7-C8-C9	-3.13	121.50	126.23
24	B	613	CLA	C1D-CHD-C4C	-3.13	118.42	122.56
24	B	609	CLA	CAC-C3C-C4C	3.13	128.87	124.81
24	c	506	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
26	a	413	BCR	C15-C14-C13	-3.13	122.84	127.31
24	c	509	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
24	b	610	CLA	C3B-C4B-NB	3.13	113.25	109.21
24	C	506	CLA	CAA-C2A-C3A	-3.12	104.22	112.78
26	Y	101	BCR	C16-C17-C18	-3.12	122.85	127.31
24	c	513	CLA	CAC-C3C-C4C	3.12	128.86	124.81
32	D	407[B]	PL9	C27-C28-C29	-3.12	120.14	127.66
24	B	605	CLA	CHC-C1C-C2C	-3.12	118.09	126.72
24	c	509	CLA	C1-C2-C3	-3.12	120.65	126.04
24	C	504	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	b	624	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
24	C	504	CLA	CBC-CAC-C3C	-3.12	103.84	112.43
24	C	513	CLA	CAC-C3C-C4C	3.12	128.85	124.81
24	b	611	CLA	C3B-C4B-NB	3.11	113.24	109.21
24	A	409	CLA	C3B-C4B-NB	3.11	113.24	109.21
32	A	417[A]	PL9	C53-C6-C1	3.11	121.36	114.99
24	b	619	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
24	A	405	CLA	O2D-CGD-CBD	3.11	116.80	111.27
38	E	101	LHG	O8-C23-C24	3.11	121.67	111.91
24	B	612	CLA	C1-C2-C3	-3.11	120.67	126.04
26	K	101	BCR	C33-C5-C6	-3.11	121.04	124.53
24	B	606	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	b	616	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	b	621	CLA	O2A-CGA-O1A	-3.11	115.75	123.59
24	C	502	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
38	d	409	LHG	O7-C7-C8	3.11	118.19	111.50
24	b	611	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
24	B	607	CLA	C4-C3-C5	3.11	120.50	115.27
32	D	407[B]	PL9	C22-C23-C24	-3.10	120.19	127.66
32	d	407[A]	PL9	C40-C39-C41	3.10	120.49	115.27
34	C	519	LMG	O8-C28-C29	3.10	121.64	111.91
24	C	508	CLA	CHC-C1C-C2C	-3.10	118.14	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	C3B-C4B-NB	3.10	113.22	109.21
24	b	613	CLA	C1-C2-C3	-3.10	120.68	126.04
24	b	624	CLA	CHD-C4C-NC	3.10	129.08	124.20
24	B	606	CLA	C2A-C1A-CHA	-3.10	118.45	123.86
24	D	404	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
24	A	409	CLA	CAA-C2A-C3A	-3.10	104.30	112.78
24	d	403	CLA	C2A-C1A-CHA	-3.10	118.45	123.86
24	C	506	CLA	CHC-C1C-C2C	-3.09	118.16	126.72
24	B	605	CLA	C1D-CHD-C4C	-3.09	118.47	122.56
24	d	404	CLA	C3B-C4B-NB	3.09	113.21	109.21
24	C	506	CLA	C1D-CHD-C4C	-3.09	118.48	122.56
26	b	628	BCR	C15-C14-C13	-3.09	122.90	127.31
24	D	405	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	B	616	CLA	CHD-C4C-NC	3.09	129.08	124.20
24	B	602	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	C	505	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
24	c	505	CLA	CBC-CAC-C3C	-3.09	103.93	112.43
24	b	615	CLA	CMB-C2B-C3B	3.08	130.45	124.68
24	c	517	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
24	b	621	CLA	CHD-C4C-NC	3.08	129.06	124.20
24	c	515	CLA	C4-C3-C5	3.08	120.46	115.27
24	B	603	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
24	a	409	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
24	c	505	CLA	C1D-CHD-C4C	-3.08	118.50	122.56
24	c	508	CLA	C4-C3-C5	3.08	120.45	115.27
29	m	103	LMT	C1B-O5B-C5B	3.08	119.73	113.69
24	B	614	CLA	CMC-C2C-C1C	3.07	129.72	125.04
32	D	407[A]	PL9	C36-C37-C38	-3.07	101.80	111.88
24	a	409	CLA	CAA-C2A-C1A	-3.07	101.92	111.97
24	B	604	CLA	C3B-C4B-NB	3.06	113.17	109.21
25	d	402[B]	PHO	C4D-ND-C1D	-3.06	101.25	106.76
24	c	517	CLA	CAC-C3C-C4C	3.06	128.79	124.81
24	B	606	CLA	CAC-C3C-C4C	3.06	128.78	124.81
24	b	613	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	c	507	CLA	C3B-C4B-NB	3.06	113.17	109.21
24	d	405	CLA	CMC-C2C-C1C	3.06	129.70	125.04
24	b	614	CLA	CHD-C4C-NC	3.06	129.03	124.20
24	b	615	CLA	C4-C3-C5	3.06	120.42	115.27
24	A	407	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	B	611	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
24	b	612	CLA	CAC-C3C-C4C	3.06	128.78	124.81
34	k	101	LMG	O8-C28-C29	3.06	121.50	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	B	615	CLA	O2A-CGA-CBA	3.06	121.50	111.91
36	B	624	HTG	C1-O5-C5	3.05	118.21	112.58
37	e	101	DGD	O5D-C1E-C2E	3.05	113.07	108.30
24	c	514	CLA	CHC-C1C-C2C	-3.05	118.27	126.72
24	c	510	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
24	B	605	CLA	O2A-CGA-CBA	3.05	121.49	111.91
24	B	602	CLA	O2A-CGA-CBA	3.05	121.48	111.91
27	F	101	SQD	C44-O6-C1	-3.05	107.78	113.74
24	C	503	CLA	C4-C3-C5	3.05	120.40	115.27
24	C	502	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	c	516	CLA	C1-C2-C3	-3.05	120.77	126.04
34	c	522	LMG	C3-C4-C5	3.05	115.68	110.24
32	a	416[A]	PL9	C27-C28-C29	-3.05	120.32	127.66
24	B	602	CLA	CHD-C4C-NC	3.05	129.01	124.20
24	c	515	CLA	CHD-C4C-NC	3.05	129.00	124.20
32	A	417[A]	PL9	C45-C44-C46	3.05	120.40	115.27
32	A	417[A]	PL9	C22-C23-C24	-3.05	120.32	127.66
24	c	516	CLA	C4-C3-C5	3.05	120.39	115.27
26	C	514	BCR	C33-C5-C6	-3.04	121.11	124.53
24	C	504	CLA	CMC-C2C-C1C	3.04	129.67	125.04
25	d	402[A]	PHO	C2B-C1B-NB	3.04	114.38	109.79
37	D	408	DGD	O1G-C1A-C2A	3.04	121.45	111.91
26	d	406	BCR	C16-C15-C14	-3.04	117.25	123.47
24	a	409	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	B	603	CLA	CHD-C4C-NC	3.04	128.99	124.20
24	a	409	CLA	C4-C3-C5	3.04	120.38	115.27
24	b	614	CLA	C4-C3-C5	3.04	120.38	115.27
32	D	407[A]	PL9	C15-C14-C16	3.04	120.38	115.27
24	B	611	CLA	C4C-C3C-C2C	-3.03	102.47	106.90
24	c	515	CLA	O2A-CGA-CBA	3.03	121.43	111.91
24	b	625	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
24	b	613	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
32	a	416[B]	PL9	C20-C19-C21	3.03	120.37	115.27
24	C	512	CLA	C1-C2-C3	-3.03	120.80	126.04
24	b	610	CLA	C4-C3-C5	3.03	120.37	115.27
24	c	509	CLA	C3B-C4B-NB	3.03	113.12	109.21
25	d	402[A]	PHO	CHD-C1D-C2D	-3.03	118.12	125.73
24	C	503	CLA	CMC-C2C-C1C	3.03	129.65	125.04
24	a	409	CLA	O2D-CGD-CBD	3.02	116.64	111.27
26	H	101	BCR	C31-C1-C6	-3.02	105.39	110.30
24	A	407	CLA	CBC-CAC-C3C	-3.02	104.09	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	SQD	C1-O5-C5	-3.02	107.75	113.69
24	C	512	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
32	a	416[B]	PL9	C10-C9-C11	3.02	120.36	115.27
32	a	416[B]	PL9	C42-C43-C44	-3.02	120.39	127.66
38	d	408	LHG	O8-C23-O10	-3.02	115.97	123.59
24	d	405	CLA	CAC-C3C-C4C	3.02	128.73	124.81
24	b	619	CLA	CHC-C1C-C2C	-3.02	118.37	126.72
24	b	612	CLA	CBC-CAC-C3C	-3.02	104.11	112.43
24	c	508	CLA	C3B-C4B-NB	3.02	113.11	109.21
32	a	416[B]	PL9	C7-C3-C2	-3.02	119.33	123.30
25	D	401[B]	PHO	CHC-C1C-C2C	-3.02	118.14	125.73
38	a	420	LHG	O7-C7-C8	3.01	118.00	111.50
24	B	613	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
24	a	410	CLA	C3B-C4B-NB	3.01	113.11	109.21
24	C	507	CLA	CMC-C2C-C1C	3.01	129.63	125.04
29	M	104	LMT	O5'-C5'-C4'	3.01	116.10	109.75
37	C	518	DGD	O2G-C1B-C2B	3.01	117.99	111.50
24	C	512	CLA	C3B-C4B-NB	3.01	113.10	109.21
24	b	612	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
26	T	103	BCR	C35-C13-C12	3.01	122.82	118.08
24	C	501	CLA	CHD-C4C-NC	3.01	128.94	124.20
37	H	102	DGD	O1G-C1A-C2A	3.01	121.34	111.91
24	b	621	CLA	C1-C2-C3	-3.01	120.84	126.04
37	C	518	DGD	O1G-C1A-C2A	3.01	121.34	111.91
24	d	405	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
24	a	409	CLA	O2A-CGA-O1A	-3.00	116.02	123.59
24	C	510	CLA	C1D-CHD-C4C	-3.00	118.60	122.56
24	b	623	CLA	CHC-C1C-C2C	-3.00	118.42	126.72
26	k	102	BCR	C24-C23-C22	-3.00	121.70	126.23
24	b	614	CLA	C3B-C4B-NB	3.00	113.09	109.21
32	A	417[B]	PL9	C27-C28-C29	-3.00	120.44	127.66
24	B	615	CLA	CHD-C4C-NC	3.00	128.93	124.20
24	C	510	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
24	C	511	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
32	a	416[A]	PL9	C35-C34-C36	2.99	120.31	115.27
34	Z	101	LMG	C1-O6-C5	2.99	119.56	113.69
24	b	622	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
32	d	407[A]	PL9	C10-C9-C11	2.99	120.30	115.27
24	a	412	CLA	CMA-C3A-C4A	-2.99	103.74	111.77
24	b	624	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	D	404	CLA	C1D-CHD-C4C	-2.99	118.61	122.56
27	A	413	SQD	O8-S-C6	2.99	110.50	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C3B-C4B-NB	2.99	113.07	109.21
25	d	402[A]	PHO	CAC-C3C-C4C	2.99	128.48	125.22
24	C	505	CLA	C3B-C4B-NB	2.98	113.07	109.21
26	Y	101	BCR	C38-C26-C25	-2.98	121.18	124.53
24	B	612	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	A	406	CLA	O2A-CGA-O1A	-2.98	116.07	123.59
24	b	623	CLA	CBC-CAC-C3C	-2.98	104.22	112.43
24	c	513	CLA	CMC-C2C-C1C	2.98	129.57	125.04
24	A	407	CLA	C4-C3-C5	2.98	120.28	115.27
24	C	504	CLA	CAC-C3C-C4C	2.98	128.67	124.81
24	c	505	CLA	CMC-C2C-C1C	2.98	129.57	125.04
25	d	402[B]	PHO	C4D-CHA-C1A	-2.98	118.67	125.37
36	C	523	HTG	O5-C5-C4	2.98	115.10	109.69
26	D	406	BCR	C29-C30-C25	2.98	115.06	110.48
24	B	604	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
25	A	408	PHO	C1C-C2C-C3C	-2.97	103.09	106.51
24	B	606	CLA	CHD-C4C-NC	2.97	128.89	124.20
24	A	409	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
38	D	409	LHG	O7-C7-C8	2.97	117.90	111.50
34	b	629	LMG	O8-C28-C29	2.97	121.22	111.91
24	c	505	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
26	C	515	BCR	C24-C23-C22	-2.96	121.75	126.23
24	B	617	CLA	CHC-C1C-C2C	-2.96	118.52	126.72
24	B	606	CLA	CMC-C2C-C1C	2.96	129.55	125.04
38	d	408	LHG	O7-C7-C8	2.96	117.89	111.50
24	C	508	CLA	CMB-C2B-C3B	2.96	130.22	124.68
24	C	513	CLA	C3B-C4B-NB	2.96	113.04	109.21
24	a	409	CLA	O2A-CGA-CBA	2.96	121.20	111.91
32	A	417[A]	PL9	C7-C8-C9	-2.96	121.87	126.79
24	c	509	CLA	CAC-C3C-C4C	2.96	128.65	124.81
24	A	409	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
24	B	614	CLA	CHC-C1C-C2C	-2.96	118.55	126.72
32	a	416[A]	PL9	C53-C6-C1	2.95	121.03	114.99
24	b	623	CLA	CMC-C2C-C1C	2.95	129.53	125.04
24	b	625	CLA	C1-C2-C3	-2.95	120.94	126.04
34	c	522	LMG	O6-C5-C4	2.95	115.06	109.69
24	B	608	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
38	L	101	LHG	C5-O7-C7	-2.95	110.52	117.79
24	D	405	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
27	L	102	SQD	O48-C23-C24	2.95	121.17	111.91
24	a	412	CLA	CHD-C4C-NC	2.95	128.85	124.20
24	b	619	CLA	C1D-CHD-C4C	-2.95	118.67	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	411	SQD	O48-C23-C24	2.95	121.15	111.91
25	d	402[A]	PHO	C3C-C4C-NC	2.95	114.85	110.28
26	c	518	BCR	C33-C5-C6	-2.94	121.22	124.53
25	D	401[A]	PHO	C2B-C1B-NB	2.94	114.23	109.79
24	b	615	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
24	C	510	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
24	b	625	CLA	CHD-C4C-NC	2.94	128.83	124.20
26	h	101	BCR	C16-C17-C18	-2.94	123.12	127.31
24	B	612	CLA	C1D-CHD-C4C	-2.94	118.68	122.56
25	D	401[B]	PHO	C4D-CHA-C1A	-2.94	118.76	125.37
24	C	508	CLA	CAC-C3C-C4C	2.94	128.62	124.81
24	d	403	CLA	C1-C2-C3	-2.93	120.97	126.04
24	B	610	CLA	CAC-C3C-C4C	2.93	128.62	124.81
32	A	417[A]	PL9	C8-C7-C3	2.93	120.27	111.98
24	c	509	CLA	CHC-C1C-C2C	-2.93	118.61	126.72
24	C	508	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
34	M	101	LMG	O8-C28-C29	2.93	121.11	111.91
24	b	622	CLA	OBD-CAD-C3D	-2.93	123.11	127.98
24	C	507	CLA	CHD-C4C-NC	2.93	128.82	124.20
24	a	412	CLA	C4-C3-C5	2.93	120.20	115.27
24	b	620	CLA	C1D-CHD-C4C	-2.93	118.70	122.56
24	c	512	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
32	d	407[A]	PL9	C37-C38-C39	-2.92	120.62	127.66
24	a	410	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	B	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
32	a	416[B]	PL9	C37-C38-C39	-2.92	120.63	127.66
32	D	407[B]	PL9	C53-C6-C1	2.92	120.96	114.99
24	a	412	CLA	CHB-C4A-NA	2.92	128.55	124.51
24	C	506	CLA	CMC-C2C-C1C	2.92	129.48	125.04
24	C	501	CLA	CAC-C3C-C4C	2.92	128.60	124.81
24	C	511	CLA	CMB-C2B-C3B	2.92	130.14	124.68
24	c	508	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	b	612	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
24	B	606	CLA	O2A-CGA-O1A	-2.91	116.24	123.59
26	h	101	BCR	C7-C8-C9	-2.91	121.83	126.23
24	c	507	CLA	C4-C3-C5	2.91	120.17	115.27
24	d	403	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	A	408	PHO	C4D-CHA-C1A	-2.91	118.82	125.37
24	b	615	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	C	502	CLA	CHD-C4C-NC	2.91	128.79	124.20
24	b	623	CLA	O2A-CGA-CBA	2.91	121.04	111.91
24	B	613	CLA	C3B-C4B-NB	2.91	112.97	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
27	a	414	SQD	C45-O47-C7	-2.91	110.63	117.79
24	c	511	CLA	C4-C3-C5	2.91	120.16	115.27
24	c	505	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
24	c	515	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
26	B	620	BCR	C38-C26-C25	-2.90	121.27	124.53
24	b	617	CLA	CMC-C2C-C1C	2.90	129.46	125.04
32	a	416[A]	PL9	C40-C39-C41	2.90	120.15	115.27
24	d	404	CLA	CMC-C2C-C1C	2.90	129.45	125.04
24	C	513	CLA	CHC-C1C-C2C	-2.90	118.70	126.72
24	c	516	CLA	CHD-C4C-NC	2.90	128.77	124.20
24	c	508	CLA	CAC-C3C-C4C	2.89	128.57	124.81
24	c	516	CLA	CMB-C2B-C3B	2.89	130.09	124.68
24	d	405	CLA	CBC-CAC-C3C	-2.89	104.46	112.43
24	B	617	CLA	CHD-C4C-NC	2.89	128.76	124.20
24	b	625	CLA	O2A-CGA-CBA	2.89	120.98	111.91
24	B	607	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
24	b	616	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	d	404	CLA	C4-C3-C5	2.89	120.13	115.27
24	c	512	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
24	a	410	CLA	C4-C3-C5	2.88	120.12	115.27
26	D	406	BCR	C15-C14-C13	-2.88	123.19	127.31
32	a	416[A]	PL9	C37-C38-C39	-2.88	120.72	127.66
26	d	406	BCR	C15-C14-C13	-2.88	123.20	127.31
32	d	407[B]	PL9	C10-C9-C11	2.88	120.12	115.27
24	B	613	CLA	CHD-C4C-NC	2.88	128.74	124.20
25	D	401[B]	PHO	C4-C3-C5	2.88	120.12	115.27
24	b	623	CLA	CAC-C3C-C4C	2.88	128.55	124.81
32	A	417[B]	PL9	C53-C6-C1	2.88	120.88	114.99
24	B	614	CLA	C1D-CHD-C4C	-2.88	118.76	122.56
32	a	416[B]	PL9	C35-C34-C36	2.88	120.11	115.27
24	b	622	CLA	O2A-CGA-CBA	2.88	120.94	111.91
26	c	518	BCR	C11-C10-C9	-2.88	123.20	127.31
27	a	414	SQD	O9-S-C6	2.88	110.36	106.94
24	B	607	CLA	CMB-C2B-C3B	2.88	130.06	124.68
27	f	102	SQD	O5-C5-C4	2.88	114.92	109.69
24	b	618	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
37	c	519	DGD	C2G-O2G-C1B	-2.88	110.71	117.79
26	c	518	BCR	C3-C4-C5	-2.88	108.94	114.08
24	b	610	CLA	CMB-C2B-C3B	2.87	130.06	124.68
24	b	611	CLA	C1-C2-C3	-2.87	121.07	126.04
24	B	602	CLA	O2D-CGD-O1D	-2.87	118.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
25	d	402[A]	PHO	C2A-C1A-NA	2.87	115.16	111.86
25	a	411	PHO	CMB-C2B-C1B	2.87	129.49	125.06
24	b	620	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
38	D	409	LHG	O8-C23-C24	2.87	120.91	111.91
24	D	405	CLA	CAA-C2A-C3A	-2.87	104.93	112.78
24	A	409	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	d	404	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
37	C	516	DGD	C3G-C2G-C1G	-2.87	105.01	111.79
24	b	611	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	b	613	CLA	C4D-C3D-CAD	-2.86	106.87	108.47
36	B	624	HTG	C1-C2-C3	2.86	116.24	110.59
24	C	512	CLA	CHD-C4C-NC	2.86	128.72	124.20
24	b	618	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
32	D	407[A]	PL9	C53-C6-C1	2.86	120.84	114.99
32	A	417[A]	PL9	C12-C13-C14	-2.86	120.77	127.66
24	C	508	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	D	404	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
24	D	405	CLA	CBC-CAC-C3C	-2.86	104.56	112.43
25	d	402[B]	PHO	C2A-C1A-NA	2.85	115.14	111.86
24	b	611	CLA	C4-C3-C5	2.85	120.07	115.27
26	k	102	BCR	C3-C4-C5	-2.85	108.98	114.08
24	C	509	CLA	CMC-C2C-C1C	2.85	129.38	125.04
24	b	612	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	C	509	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
32	d	407[B]	PL9	C12-C13-C14	-2.85	120.79	127.66
24	b	612	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	b	614	CLA	OBD-CAD-C3D	-2.85	123.25	127.98
24	d	403	CLA	CHD-C4C-NC	2.85	128.69	124.20
39	V	205	HEM	CAD-CBD-CGD	2.85	117.45	112.67
24	d	404	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
34	C	519	LMG	C8-O7-C10	-2.85	110.78	117.79
24	c	513	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
26	y	101	BCR	C10-C11-C12	-2.85	114.34	123.22
37	h	102	DGD	O1G-C1A-C2A	2.85	120.84	111.91
24	B	610	CLA	C1-O2A-CGA	2.84	123.91	116.44
24	B	603	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
24	C	511	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
24	C	503	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
24	b	617	CLA	O2A-CGA-CBA	2.84	120.83	111.91
24	B	604	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	b	617	CLA	CHD-C4C-NC	2.84	128.68	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	402[B]	PHO	C2B-C1B-NB	2.84	114.08	109.79
27	A	411	SQD	O9-S-C6	2.84	110.31	106.94
24	b	616	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	c	517	CLA	C2A-C1A-CHA	-2.84	118.90	123.86
24	c	511	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	c	508	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
25	d	402[B]	PHO	CAC-C3C-C4C	2.84	128.32	125.22
24	b	620	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
24	c	515	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
24	B	602	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
24	b	613	CLA	O2A-CGA-CBA	2.84	120.81	111.91
26	C	514	BCR	C38-C26-C25	-2.84	121.34	124.53
27	F	101	SQD	O48-C23-C24	2.84	120.81	111.91
26	B	619	BCR	C37-C22-C21	-2.83	118.95	122.92
32	A	417[A]	PL9	C27-C28-C29	-2.83	120.84	127.66
24	b	616	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
24	B	616	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
24	b	617	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
24	c	505	CLA	OBD-CAD-C3D	-2.83	123.29	127.98
24	D	404	CLA	CHD-C4C-NC	2.83	128.66	124.20
24	B	605	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	c	518	BCR	C21-C20-C19	-2.83	114.40	123.22
24	B	608	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
24	C	509	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
24	b	615	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
26	b	627	BCR	C38-C26-C25	-2.82	121.36	124.53
37	H	102	DGD	O1G-C1A-O1A	-2.82	116.47	123.59
24	b	619	CLA	CMB-C2B-C3B	2.82	129.96	124.68
25	A	408	PHO	CAC-C3C-C4C	2.82	128.30	125.22
24	c	508	CLA	CMB-C2B-C3B	2.82	129.95	124.68
24	B	603	CLA	C4-C3-C5	2.82	120.01	115.27
25	A	408	PHO	C2B-C1B-NB	2.82	114.04	109.79
24	c	506	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	B	615	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
24	b	612	CLA	CMC-C2C-C1C	2.81	129.32	125.04
24	C	504	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
24	b	612	CLA	CHD-C4C-NC	2.81	128.63	124.20
26	k	102	BCR	C15-C14-C13	-2.81	123.30	127.31
24	b	617	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
26	K	101	BCR	C3-C4-C5	-2.81	109.06	114.08
24	B	607	CLA	CHD-C4C-NC	2.81	128.63	124.20
25	d	402[A]	PHO	C4D-ND-C1D	-2.81	101.71	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	CBC-CAC-C3C	-2.81	104.69	112.43
26	b	628	BCR	C3-C4-C5	-2.81	109.07	114.08
24	b	618	CLA	C1-C2-C3	-2.81	121.19	126.04
24	B	615	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
38	d	408	LHG	O8-C23-C24	2.81	120.71	111.91
24	C	507	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
24	B	614	CLA	O2D-CGD-CBD	2.80	116.25	111.27
24	b	610	CLA	CHC-C1C-C2C	-2.80	118.97	126.72
25	a	411	PHO	CHC-C1C-C2C	-2.80	118.69	125.73
24	B	613	CLA	C1-C2-C3	-2.80	121.20	126.04
32	a	416[A]	PL9	C25-C24-C26	2.80	119.97	115.27
24	a	409	CLA	CMB-C2B-C3B	2.79	129.91	124.68
34	z	101	LMG	O8-C28-C29	2.79	120.68	111.91
24	b	621	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	B	612	CLA	CHC-C1C-C2C	-2.79	118.99	126.72
24	C	505	CLA	CHC-C1C-C2C	-2.79	119.00	126.72
24	b	611	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
24	C	510	CLA	C4-C3-C5	2.79	119.97	115.27
37	c	521	DGD	O1G-C1A-C2A	2.79	120.66	111.91
24	c	510	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	b	618	CLA	C4-C3-C5	2.79	119.96	115.27
24	b	619	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
24	B	613	CLA	C2A-C1A-CHA	-2.79	118.99	123.86
24	B	616	CLA	C3B-C4B-NB	2.79	112.81	109.21
24	C	501	CLA	C3B-C4B-NB	2.79	112.81	109.21
24	B	605	CLA	CMC-C2C-C1C	2.78	129.28	125.04
24	B	614	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	B	609	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
24	B	610	CLA	CMB-C2B-C1B	2.78	132.74	128.46
24	b	618	CLA	CHD-C4C-NC	2.78	128.58	124.20
24	c	510	CLA	CHD-C4C-NC	2.78	128.58	124.20
24	b	614	CLA	O2A-CGA-CBA	2.78	120.63	111.91
34	z	101	LMG	C8-O7-C10	-2.78	110.95	117.79
25	d	402[A]	PHO	CHC-C1C-C2C	-2.78	118.74	125.73
24	c	516	CLA	O2A-CGA-CBA	2.78	120.62	111.91
34	a	415	LMG	C7-O1-C1	-2.78	108.31	113.74
26	Y	101	BCR	C15-C16-C17	-2.78	117.79	123.47
26	K	101	BCR	C10-C11-C12	-2.77	114.56	123.22
24	A	405	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
26	t	102	BCR	C21-C20-C19	-2.77	114.56	123.22
25	A	408	PHO	C2A-C1A-NA	2.77	115.04	111.86
24	d	403	CLA	CMA-C3A-C2A	-2.77	102.66	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	511	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	C	506	CLA	C1-C2-C3	-2.77	121.25	126.04
24	b	619	CLA	O2A-CGA-CBA	2.77	120.60	111.91
24	D	404	CLA	CAA-C2A-C3A	-2.77	105.20	112.78
24	d	405	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
24	a	410	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
24	B	605	CLA	OBD-CAD-C3D	-2.77	123.39	127.98
24	C	511	CLA	CMC-C2C-C1C	2.77	129.25	125.04
32	a	416[B]	PL9	C53-C6-C1	2.77	120.64	114.99
24	c	513	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
24	A	407	CLA	C1D-CHD-C4C	-2.77	118.91	122.56
25	a	411	PHO	CBA-CAA-C2A	-2.76	105.70	113.86
26	b	628	BCR	C38-C26-C25	-2.76	121.42	124.53
24	b	617	CLA	C3B-C4B-NB	2.76	112.78	109.21
26	c	526	BCR	C20-C21-C22	-2.76	123.37	127.31
24	A	407	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
24	C	503	CLA	CHD-C4C-NC	2.76	128.55	124.20
24	d	405	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
24	B	610	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
26	c	526	BCR	C28-C27-C26	-2.76	109.16	114.08
24	B	604	CLA	C4-C3-C5	2.76	119.91	115.27
34	M	101	LMG	O7-C10-C11	2.75	117.44	111.50
24	c	514	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	b	615	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
24	c	516	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	b	616	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	c	517	CLA	CHD-C4C-NC	2.75	128.54	124.20
26	B	618	BCR	C16-C17-C18	-2.75	123.39	127.31
34	b	629	LMG	O8-C28-O10	-2.75	116.65	123.59
24	d	404	CLA	C4D-C3D-CAD	-2.75	106.94	108.47
24	B	614	CLA	O2A-CGA-CBA	2.75	120.53	111.91
24	B	607	CLA	C3B-C4B-NB	2.75	112.76	109.21
26	K	101	BCR	C20-C21-C22	-2.75	123.39	127.31
24	c	517	CLA	C3B-C4B-NB	2.75	112.76	109.21
24	c	514	CLA	CHD-C4C-NC	2.75	128.53	124.20
24	d	404	CLA	CAC-C3C-C4C	2.74	128.37	124.81
24	C	505	CLA	C4-C3-C5	2.74	119.88	115.27
38	d	409	LHG	O8-C23-O10	-2.74	116.67	123.59
38	d	408	LHG	O7-C7-O9	-2.74	117.08	123.70
26	t	102	BCR	C37-C22-C23	2.74	122.39	118.08
24	b	615	CLA	CMC-C2C-C1C	2.74	129.21	125.04
26	b	628	BCR	C8-C7-C6	-2.74	119.51	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
32	d	407[B]	PL9	C27-C28-C29	-2.74	121.07	127.66
32	d	407[A]	PL9	C27-C28-C29	-2.73	121.08	127.66
24	a	410	CLA	O2A-CGA-CBA	2.73	120.48	111.91
34	Z	101	LMG	C8-O7-C10	-2.73	111.07	117.79
32	A	417[B]	PL9	C45-C44-C46	2.73	119.86	115.27
24	d	404	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
32	D	407[B]	PL9	C25-C24-C26	2.73	119.86	115.27
24	c	507	CLA	CAC-C3C-C4C	2.73	128.35	124.81
24	C	509	CLA	C1-O2A-CGA	2.73	123.60	116.44
32	D	407[B]	PL9	C37-C38-C39	-2.73	121.09	127.66
24	c	515	CLA	CMC-C2C-C1C	2.73	129.19	125.04
32	d	407[A]	PL9	C20-C19-C21	2.72	119.85	115.27
32	A	417[B]	PL9	C15-C14-C16	2.72	119.85	115.27
26	t	102	BCR	C1-C6-C7	2.72	123.48	115.78
32	a	416[B]	PL9	C25-C24-C26	2.72	119.85	115.27
26	a	413	BCR	C37-C22-C21	-2.72	119.11	122.92
24	B	616	CLA	C1-C2-C3	-2.72	121.34	126.04
24	c	511	CLA	C1-C2-C3	-2.72	121.34	126.04
32	D	407[A]	PL9	C7-C3-C4	2.72	119.09	116.88
25	D	401[B]	PHO	CAC-C3C-C4C	2.72	128.19	125.22
24	c	510	CLA	CMB-C2B-C3B	2.72	129.76	124.68
24	d	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.90
26	b	626	BCR	C29-C30-C25	2.72	114.66	110.48
24	c	507	CLA	CHD-C4C-NC	2.72	128.48	124.20
38	L	101	LHG	O8-C23-C24	2.72	120.43	111.91
24	b	620	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
24	C	508	CLA	O2A-CGA-CBA	2.71	120.42	111.91
32	A	417[B]	PL9	C42-C43-C44	-2.71	121.13	127.66
24	c	508	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	C	502	CLA	O2A-CGA-CBA	2.71	120.41	111.91
24	b	623	CLA	CHD-C4C-NC	2.71	128.47	124.20
25	a	411	PHO	CED-O2D-CGD	2.71	122.06	115.94
24	b	612	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	B	615	CLA	C4-C3-C5	2.70	119.82	115.27
25	D	401[A]	PHO	O2D-CGD-O1D	-2.70	118.55	123.84
24	D	405	CLA	C1-C2-C3	-2.70	121.37	126.04
24	a	410	CLA	CMC-C2C-C1C	2.70	129.15	125.04
24	b	622	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
29	M	104	LMT	O1B-C1B-C2B	2.70	115.10	108.10
27	a	414	SQD	C44-O6-C1	-2.70	108.47	113.74
24	C	506	CLA	C4D-C3D-CAD	-2.70	106.97	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	SQD	O48-C23-C24	2.70	120.38	111.91
24	B	606	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	B	607	CLA	OBD-CAD-C3D	-2.70	123.50	127.98
24	B	603	CLA	C1-C2-C3	-2.70	121.38	126.04
25	d	402[B]	PHO	CHD-C1D-C2D	-2.70	118.95	125.73
29	m	103	LMT	O5'-C5'-C4'	2.69	115.43	109.75
24	C	502	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
26	B	619	BCR	C29-C30-C25	2.69	114.63	110.48
24	B	607	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	C	512	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
24	B	617	CLA	O2A-CGA-CBA	2.69	120.34	111.91
24	B	617	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	C	509	CLA	C4-C3-C5	2.69	119.79	115.27
24	C	507	CLA	C1-C2-C3	-2.69	121.40	126.04
24	c	505	CLA	O2A-CGA-CBA	2.69	120.33	111.91
25	D	401[A]	PHO	C3C-C4C-NC	2.68	114.44	110.28
24	B	604	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
24	c	514	CLA	O2A-CGA-CBA	2.68	120.33	111.91
24	c	508	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
24	B	606	CLA	O2A-CGA-CBA	2.68	120.33	111.91
24	A	407	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
25	A	408	PHO	O2D-CGD-O1D	-2.68	118.60	123.84
24	C	503	CLA	CAC-C3C-C4C	2.68	128.29	124.81
24	B	613	CLA	CMB-C2B-C3B	2.68	129.69	124.68
24	B	607	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
25	A	408	PHO	C4D-ND-C1D	-2.68	101.95	106.76
24	C	513	CLA	C4C-C3C-C2C	-2.68	103.00	106.90
24	b	620	CLA	O2A-CGA-CBA	2.67	120.30	111.91
24	A	405	CLA	O2A-CGA-O1A	-2.67	116.84	123.59
24	b	617	CLA	CMB-C2B-C3B	2.67	129.68	124.68
24	c	517	CLA	O2A-CGA-CBA	2.67	120.30	111.91
32	d	407[B]	PL9	C37-C38-C39	-2.67	121.22	127.66
24	c	513	CLA	CHD-C4C-NC	2.67	128.41	124.20
32	D	407[A]	PL9	C25-C24-C26	2.67	119.77	115.27
24	b	623	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
25	d	402[A]	PHO	C4A-NA-C1A	-2.67	105.98	108.14
38	d	410	LHG	O8-C23-C24	2.67	120.29	111.91
32	A	417[A]	PL9	C25-C24-C26	2.67	119.76	115.27
25	d	402[B]	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
27	a	414	SQD	O47-C7-O49	-2.67	117.26	123.70
25	A	408	PHO	C2C-C1C-NC	2.67	113.81	109.79
24	c	516	CLA	C3B-C4B-NB	2.66	112.66	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	417[A]	PL9	C30-C29-C31	2.66	119.75	115.27
24	b	618	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
26	a	413	BCR	C38-C26-C25	-2.66	121.54	124.53
26	b	627	BCR	C37-C22-C21	-2.66	119.19	122.92
26	h	101	BCR	C24-C23-C22	-2.66	122.21	126.23
24	C	508	CLA	C1-C2-C3	-2.66	121.44	126.04
24	c	517	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
24	C	508	CLA	C4D-C3D-CAD	-2.66	106.99	108.47
27	A	413	SQD	O48-C23-O10	-2.66	116.88	123.59
24	C	510	CLA	O2A-CGA-CBA	2.66	120.26	111.91
26	h	101	BCR	C10-C11-C12	-2.66	114.92	123.22
24	a	412	CLA	CMA-C3A-C2A	-2.66	103.11	113.83
24	b	623	CLA	CMB-C2B-C3B	2.66	129.65	124.68
32	D	407[B]	PL9	C51-C49-C50	2.66	120.47	114.60
25	D	401[B]	PHO	C2A-C1A-NA	2.66	114.91	111.86
24	a	409	CLA	CAC-C3C-C4C	2.66	128.26	124.81
24	c	507	CLA	CHC-C1C-C2C	-2.66	119.37	126.72
25	a	411	PHO	C4-C3-C5	2.66	119.74	115.27
24	B	614	CLA	CED-O2D-CGD	2.65	121.94	115.94
25	D	401[A]	PHO	C2A-C1A-NA	2.65	114.91	111.86
26	a	413	BCR	C33-C5-C6	-2.65	121.55	124.53
24	B	607	CLA	CAA-C2A-C3A	-2.65	105.52	112.78
25	D	401[A]	PHO	CAC-C3C-C4C	2.65	128.11	125.22
25	D	401[B]	PHO	C4D-ND-C1D	-2.65	102.00	106.76
24	c	511	CLA	C3B-C4B-NB	2.65	112.63	109.21
24	A	407	CLA	C1-C2-C3	-2.65	121.46	126.04
24	d	404	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
32	A	417[B]	PL9	C12-C13-C14	-2.65	121.29	127.66
24	C	511	CLA	CHD-C4C-NC	2.65	128.37	124.20
24	B	611	CLA	C4-C3-C5	2.64	119.72	115.27
24	B	610	CLA	C4D-C3D-CAD	-2.64	107.00	108.47
24	b	611	CLA	CMB-C2B-C3B	2.64	129.62	124.68
24	C	510	CLA	C6-C7-C8	-2.64	107.38	115.92
24	c	509	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
26	c	518	BCR	C7-C8-C9	-2.64	122.24	126.23
24	A	407	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
24	C	504	CLA	CHD-C4C-NC	2.64	128.37	124.20
26	c	518	BCR	C37-C22-C23	2.64	122.24	118.08
24	C	507	CLA	O2A-CGA-CBA	2.64	120.19	111.91
24	B	615	CLA	CAC-C3C-C4C	2.64	128.24	124.81
24	C	506	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
24	a	410	CLA	C2A-C1A-CHA	-2.64	119.25	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CMB-C2B-C3B	2.64	129.61	124.68
24	C	513	CLA	CMC-C2C-C1C	2.64	129.05	125.04
24	B	608	CLA	C1-O2A-CGA	2.64	123.36	116.44
26	t	102	BCR	C11-C10-C9	-2.64	123.55	127.31
26	k	102	BCR	C36-C18-C19	2.63	122.23	118.08
24	B	607	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	B	603	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
26	t	102	BCR	C33-C5-C4	2.63	118.67	113.62
24	D	404	CLA	C4-C3-C5	2.63	119.69	115.27
25	A	408	PHO	CMB-C2B-C1B	2.63	129.11	125.06
24	B	609	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
24	c	513	CLA	O2A-CGA-CBA	2.62	120.14	111.91
24	c	505	CLA	CHD-C4C-NC	2.62	128.34	124.20
24	b	621	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
24	b	623	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
24	b	621	CLA	CHC-C1C-C2C	-2.62	119.46	126.72
32	d	407[A]	PL9	C53-C6-C1	2.62	120.35	114.99
36	C	523	HTG	O5-C1-C2	2.62	113.61	110.31
24	C	512	CLA	O2A-CGA-CBA	2.62	120.14	111.91
24	d	405	CLA	C4-C3-C5	2.62	119.68	115.27
24	c	511	CLA	CAC-C3C-C4C	2.62	128.21	124.81
27	f	102	SQD	O47-C7-O49	-2.62	117.37	123.70
26	c	526	BCR	C16-C17-C18	-2.62	123.57	127.31
24	C	510	CLA	CMB-C2B-C3B	2.62	129.57	124.68
24	c	516	CLA	CMC-C2C-C1C	2.62	129.02	125.04
24	C	506	CLA	OBD-CAD-C3D	-2.62	123.64	127.98
24	C	513	CLA	CMB-C2B-C3B	2.62	129.57	124.68
24	a	412	CLA	CAA-C2A-C3A	-2.62	105.62	112.78
24	C	503	CLA	C3B-C4B-NB	2.61	112.59	109.21
24	C	509	CLA	CHD-C4C-NC	2.61	128.32	124.20
26	y	101	BCR	C40-C30-C25	-2.61	106.06	110.30
24	b	610	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
24	b	624	CLA	CAC-C3C-C4C	2.61	128.20	124.81
24	b	622	CLA	C4-C3-C5	2.61	119.67	115.27
24	c	506	CLA	O2A-C1-C2	2.61	115.50	108.64
32	d	407[B]	PL9	C20-C19-C21	2.61	119.66	115.27
24	B	606	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
24	c	505	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
26	d	406	BCR	C33-C5-C6	-2.61	121.60	124.53
27	f	102	SQD	O7-S-C6	2.61	110.04	106.94
24	c	509	CLA	C4-C3-C5	2.61	119.66	115.27
34	Z	101	LMG	O6-C5-C4	2.61	114.43	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
32	D	407[A]	PL9	C22-C23-C24	-2.61	121.39	127.66
24	C	512	CLA	CMC-C2C-C1C	2.60	129.01	125.04
24	b	619	CLA	C4-C3-C5	2.60	119.65	115.27
24	C	501	CLA	C4C-C3C-C2C	-2.60	103.10	106.90
26	C	515	BCR	C15-C16-C17	-2.60	118.14	123.47
24	d	403	CLA	C1-O2A-CGA	2.60	123.27	116.44
24	b	615	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
24	C	509	CLA	O2A-CGA-CBA	2.60	120.06	111.91
24	B	608	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
32	D	407[A]	PL9	C37-C38-C39	-2.60	121.41	127.66
25	d	402[B]	PHO	C2C-C1C-NC	2.60	113.71	109.79
24	b	617	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
27	A	411	SQD	O48-C23-O10	-2.60	117.04	123.59
24	C	511	CLA	O2A-CGA-CBA	2.60	120.05	111.91
24	C	512	CLA	C4-C3-C5	2.59	119.64	115.27
36	b	602	HTG	C1-O5-C5	2.59	117.36	112.58
24	c	514	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
24	B	610	CLA	CHD-C4C-NC	2.59	128.29	124.20
32	D	407[B]	PL9	C12-C13-C14	-2.59	121.42	127.66
24	c	506	CLA	O2A-CGA-CBA	2.59	120.05	111.91
26	y	101	BCR	C16-C17-C18	-2.59	123.61	127.31
24	C	508	CLA	CHD-C4C-NC	2.59	128.28	124.20
24	B	612	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
24	B	610	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
24	c	506	CLA	CHD-C4C-NC	2.59	128.28	124.20
24	b	611	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
24	c	516	CLA	CHC-C1C-C2C	-2.59	119.57	126.72
24	c	515	CLA	CMB-C2B-C3B	2.59	129.52	124.68
26	K	101	BCR	C2-C1-C6	2.58	114.46	110.48
32	a	416[A]	PL9	C30-C29-C31	2.58	119.61	115.27
32	d	407[B]	PL9	C25-C24-C26	2.58	119.61	115.27
37	C	517	DGD	O1G-C1A-C2A	2.58	120.00	111.91
32	A	417[A]	PL9	C15-C14-C16	2.58	119.61	115.27
24	C	506	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
24	c	516	CLA	CBA-CAA-C2A	-2.58	106.25	113.86
24	B	613	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
24	b	619	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
32	a	416[B]	PL9	C40-C39-C41	2.58	119.60	115.27
24	a	410	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
24	C	505	CLA	C1-O2A-CGA	2.57	123.20	116.44
24	A	406	CLA	C4C-C3C-C2C	-2.57	103.15	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
32	A	417[B]	PL9	C25-C24-C26	2.57	119.59	115.27
24	a	412	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
25	d	402[B]	PHO	C3C-C4C-NC	2.57	114.26	110.28
32	D	407[B]	PL9	C7-C3-C4	2.57	118.96	116.88
38	b	634	LHG	O8-C23-C24	2.57	119.96	111.91
25	D	401[B]	PHO	C2B-C1B-NB	2.57	113.66	109.79
24	b	618	CLA	O2A-CGA-CBA	2.56	119.96	111.91
24	A	409	CLA	CMC-C2C-C1C	2.56	128.94	125.04
24	c	508	CLA	O2A-CGA-CBA	2.56	119.95	111.91
24	A	409	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	B	610	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
24	B	610	CLA	C1-C2-C3	-2.56	121.61	126.04
24	C	513	CLA	CHD-C4C-NC	2.56	128.24	124.20
24	C	513	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
24	b	614	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
24	c	513	CLA	OBD-CAD-C3D	-2.56	123.73	127.98
26	B	620	BCR	C36-C18-C17	-2.56	119.34	122.92
25	D	401[B]	PHO	CMB-C2B-C1B	2.56	129.00	125.06
24	b	616	CLA	CAC-C3C-C4C	2.56	128.13	124.81
26	T	103	BCR	C15-C14-C13	2.56	130.96	127.31
32	D	407[B]	PL9	C7-C3-C2	-2.55	119.94	123.30
26	T	103	BCR	C2-C1-C6	2.55	114.41	110.48
24	C	512	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
24	a	412	CLA	O2A-CGA-CBA	2.55	119.91	111.91
24	b	611	CLA	C1-O2A-CGA	2.55	123.14	116.44
24	b	614	CLA	C4D-C3D-CAD	-2.55	107.05	108.47
32	a	416[A]	PL9	C51-C49-C50	2.55	120.23	114.60
24	B	608	CLA	C4-C3-C5	2.55	119.56	115.27
24	b	623	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
26	K	101	BCR	C29-C30-C25	2.55	114.40	110.48
26	H	101	BCR	C16-C15-C14	-2.55	118.26	123.47
24	B	605	CLA	C4-C3-C5	2.55	119.55	115.27
24	B	607	CLA	O2A-CGA-CBA	2.54	119.89	111.91
37	C	516	DGD	O1G-C1A-O1A	-2.54	117.18	123.59
27	f	102	SQD	O48-C23-C24	2.54	119.88	111.91
32	D	407[A]	PL9	C27-C28-C29	-2.54	121.54	127.66
26	B	620	BCR	C24-C23-C22	-2.54	122.40	126.23
24	c	508	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
26	k	102	BCR	C11-C10-C9	-2.54	123.69	127.31
24	A	409	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	C	513	CLA	C2A-C1A-CHA	-2.54	119.42	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	520	DGD	C2G-O2G-C1B	-2.54	111.54	117.79
25	d	402[B]	PHO	CBD-CHA-C1A	2.54	132.29	126.40
24	B	603	CLA	CMB-C2B-C3B	2.54	129.42	124.68
32	a	416[B]	PL9	C45-C44-C46	2.54	119.54	115.27
24	b	624	CLA	C11-C10-C8	-2.54	107.72	115.92
26	T	103	BCR	C1-C6-C7	2.53	122.95	115.78
24	C	512	CLA	CAC-C3C-C4C	2.53	128.09	124.81
24	a	409	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
34	Z	101	LMG	C1-C2-C3	2.53	115.26	110.00
25	D	401[A]	PHO	C1C-C2C-C3C	-2.53	103.61	106.51
27	L	102	SQD	C44-O6-C1	-2.53	108.80	113.74
26	y	101	BCR	C21-C20-C19	-2.53	115.33	123.22
25	a	411	PHO	C3C-C4C-NC	2.53	114.20	110.28
26	C	514	BCR	C20-C21-C22	-2.53	123.70	127.31
24	B	615	CLA	OBD-CAD-C3D	-2.53	123.79	127.98
24	c	508	CLA	O2A-CGA-O1A	-2.53	117.22	123.59
24	B	611	CLA	C1-C2-C3	-2.52	121.68	126.04
24	B	603	CLA	CMA-C3A-C2A	-2.52	103.65	113.83
27	A	411	SQD	O47-C7-O49	-2.52	117.60	123.70
36	V	206	HTG	O5-C1-C2	-2.52	107.14	110.31
24	c	512	CLA	CHD-C4C-NC	2.52	128.18	124.20
24	c	514	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
24	c	510	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
24	b	617	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
38	a	420	LHG	O8-C23-C24	2.52	119.82	111.91
34	a	415	LMG	O8-C28-C29	2.52	119.82	111.91
24	C	508	CLA	C4-C3-C5	2.52	119.51	115.27
24	b	611	CLA	CAC-C3C-C4C	2.52	128.07	124.81
24	B	602	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
24	D	404	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
24	B	604	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
24	b	610	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
24	B	612	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
24	b	611	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
24	c	510	CLA	C4-C3-C5	2.51	119.50	115.27
24	d	404	CLA	C1D-CHD-C4C	-2.51	119.25	122.56
24	c	511	CLA	O1D-CGD-CBD	-2.51	119.35	124.48
26	b	626	BCR	C37-C22-C21	-2.51	119.41	122.92
34	Z	101	LMG	C9-O8-C28	2.51	123.41	117.10
26	c	526	BCR	C29-C30-C25	2.51	114.34	110.48
24	B	612	CLA	CMB-C2B-C3B	2.51	129.37	124.68
24	D	405	CLA	O2A-CGA-CBA	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	417[B]	PL9	C8-C7-C3	2.51	119.06	111.98
24	b	618	CLA	CMC-C2C-C1C	2.51	128.85	125.04
24	B	614	CLA	OBD-CAD-C3D	-2.50	123.82	127.98
24	c	512	CLA	CAA-C2A-C3A	-2.50	105.92	112.78
32	A	417[B]	PL9	C17-C18-C19	-2.50	121.63	127.66
36	b	607	HTG	C1-O5-C5	2.50	117.20	112.58
24	A	405	CLA	CMA-C3A-C4A	-2.50	105.05	111.77
24	B	611	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
24	B	613	CLA	O2A-CGA-CBA	2.50	119.76	111.91
24	C	511	CLA	C4-C3-C5	2.50	119.48	115.27
24	B	616	CLA	C4-C3-C5	2.50	119.47	115.27
24	b	625	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
25	a	411	PHO	CBD-CHA-C1A	2.49	132.19	126.40
24	D	404	CLA	CMC-C2C-C1C	2.49	128.83	125.04
32	A	417[A]	PL9	C42-C43-C44	-2.49	121.66	127.66
38	d	408	LHG	C5-O7-C7	-2.49	111.66	117.79
24	c	517	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
24	b	616	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	h	101	BCR	C11-C10-C9	-2.49	123.76	127.31
25	D	401[A]	PHO	C2C-C1C-NC	2.49	113.55	109.79
24	B	614	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	C	504	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
24	B	617	CLA	OBD-CAD-C3D	-2.48	123.86	127.98
26	C	514	BCR	C23-C24-C25	-2.48	120.23	127.20
32	d	407[B]	PL9	C17-C18-C19	-2.48	121.68	127.66
24	d	403	CLA	OBD-CAD-C3D	-2.48	123.87	127.98
24	d	405	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
24	b	623	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
25	A	408	PHO	C4-C3-C5	2.47	119.43	115.27
25	a	411	PHO	C4D-CHA-C1A	-2.47	119.81	125.37
26	C	514	BCR	C16-C17-C18	-2.47	123.78	127.31
39	v	206	HEM	CAD-CBD-CGD	2.47	116.81	112.67
24	C	513	CLA	O2A-CGA-CBA	2.47	119.65	111.91
27	F	101	SQD	O47-C7-O49	-2.47	117.74	123.70
24	C	506	CLA	CHD-C4C-NC	2.47	128.09	124.20
24	C	506	CLA	CMB-C2B-C3B	2.47	129.29	124.68
24	C	508	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
24	b	615	CLA	O2A-CGA-CBA	2.47	119.65	111.91
38	d	409	LHG	C6-C5-C4	-2.47	105.96	111.79
37	C	517	DGD	O6E-C5E-C6E	2.47	112.56	106.44
26	k	102	BCR	C10-C11-C12	-2.46	115.53	123.22
37	H	102	DGD	C3G-O3G-C1D	-2.46	108.92	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410	BCR	C2-C1-C6	2.46	114.28	110.48
24	b	613	CLA	C6-C5-C3	-2.46	107.00	113.45
26	b	628	BCR	C21-C20-C19	-2.46	115.53	123.22
32	D	407[A]	PL9	C42-C41-C39	-2.46	104.88	112.98
32	A	417[B]	PL9	C10-C9-C11	2.46	119.41	115.27
24	A	406	CLA	C1-C2-C3	-2.46	121.79	126.04
29	M	104	LMT	C1B-O5B-C5B	2.46	118.52	113.69
26	y	101	BCR	C37-C22-C23	2.46	121.95	118.08
24	c	510	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	c	509	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
24	C	503	CLA	O2A-CGA-CBA	2.46	119.62	111.91
34	k	101	LMG	C8-O7-C10	-2.46	111.74	117.79
27	A	411	SQD	C1-C2-C3	-2.46	104.88	110.00
32	A	417[A]	PL9	C10-C9-C11	2.46	119.40	115.27
24	c	505	CLA	C4D-C3D-CAD	-2.46	107.10	108.47
32	a	416[A]	PL9	C7-C3-C2	-2.46	120.07	123.30
26	B	620	BCR	C10-C11-C12	-2.46	115.55	123.22
24	b	613	CLA	CHD-C4C-NC	2.46	128.07	124.20
27	f	102	SQD	O8-S-C6	2.46	109.65	105.74
36	V	206	HTG	C1-C2-C3	-2.45	105.74	110.59
24	c	513	CLA	C1-O2A-CGA	2.45	122.88	116.44
24	B	612	CLA	C4D-C3D-CAD	-2.45	107.10	108.47
24	a	412	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
37	C	517	DGD	C1E-O6E-C5E	-2.45	108.87	113.69
34	c	522	LMG	O8-C28-C29	2.45	119.60	111.91
24	c	511	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
25	d	402[B]	PHO	C1C-C2C-C3C	-2.45	103.70	106.51
24	b	612	CLA	C4-C3-C5	2.45	119.39	115.27
24	B	610	CLA	C4-C3-C5	2.45	119.39	115.27
25	A	408	PHO	C1-C2-C3	-2.45	121.81	126.04
34	C	520	LMG	C3-C4-C5	2.45	114.60	110.24
24	C	513	CLA	C4-C3-C5	2.45	119.39	115.27
26	K	101	BCR	C31-C1-C6	-2.44	106.33	110.30
24	C	501	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
25	D	401[A]	PHO	C4D-ND-C1D	-2.44	102.37	106.76
34	A	419	LMG	C8-O7-C10	-2.44	111.77	117.79
32	D	407[A]	PL9	C51-C49-C50	2.44	120.00	114.60
24	B	608	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
24	B	609	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	a	410	CLA	CAC-C3C-C4C	2.44	127.97	124.81
26	y	101	BCR	C32-C1-C6	-2.44	106.34	110.30
24	C	501	CLA	C1-C2-C3	-2.44	121.83	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
24	c	515	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
24	B	616	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
36	b	608	HTG	O5-C1-C2	2.44	113.38	110.31
24	c	509	CLA	CHD-C4C-NC	2.44	128.04	124.20
24	c	514	CLA	CAC-C3C-C4C	2.43	127.97	124.81
24	A	407	CLA	CAA-C2A-C3A	-2.43	106.11	112.78
24	c	508	CLA	OBD-CAD-C3D	-2.43	123.94	127.98
24	C	505	CLA	CMC-C2C-C1C	2.43	128.74	125.04
26	B	619	BCR	C30-C25-C26	-2.43	119.19	122.61
24	b	615	CLA	C1-O2A-CGA	2.43	122.82	116.44
26	c	526	BCR	C11-C10-C9	-2.43	123.84	127.31
24	B	615	CLA	C1-O2A-CGA	2.43	122.82	116.44
32	A	417[B]	PL9	C30-C29-C31	2.43	119.36	115.27
24	c	512	CLA	O2A-CGA-CBA	2.43	119.53	111.91
26	B	618	BCR	C21-C20-C19	-2.43	115.64	123.22
25	A	408	PHO	CBA-CAA-C2A	-2.43	106.70	113.86
32	D	407[A]	PL9	C12-C13-C14	-2.43	121.81	127.66
24	C	507	CLA	CAC-C3C-C4C	2.43	127.96	124.81
24	b	616	CLA	CGD-CBD-CAD	-2.43	102.88	110.73
24	B	609	CLA	CMB-C2B-C3B	2.42	129.21	124.68
24	D	404	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
24	b	617	CLA	C11-C12-C13	-2.42	108.09	115.92
24	B	613	CLA	CAC-C3C-C4C	2.42	127.95	124.81
26	b	628	BCR	C2-C1-C6	2.42	114.21	110.48
24	B	611	CLA	CAA-CBA-CGA	-2.42	106.18	113.25
24	b	614	CLA	CMC-C2C-C1C	2.42	128.72	125.04
24	c	505	CLA	CMB-C2B-C3B	2.42	129.20	124.68
32	D	407[B]	PL9	C45-C44-C46	2.42	119.33	115.27
26	d	406	BCR	C38-C26-C27	2.42	118.26	113.62
38	D	411	LHG	O8-C23-O10	-2.42	117.50	123.59
32	d	407[B]	PL9	C22-C23-C24	-2.41	121.85	127.66
24	d	405	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
24	B	615	CLA	CMB-C2B-C3B	2.41	129.19	124.68
24	c	514	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
24	D	405	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
24	a	410	CLA	C1-C2-C3	-2.41	121.88	126.04
37	D	408	DGD	O6D-C5D-C6D	2.41	111.53	106.67
25	a	411	PHO	C2B-C1B-NB	2.41	113.42	109.79
34	z	101	LMG	C7-O1-C1	-2.41	109.04	113.74
25	a	411	PHO	C4D-ND-C1D	-2.41	102.44	106.76
26	T	103	BCR	C7-C6-C5	-2.41	115.64	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	h	102	DGD	O1G-C1A-O1A	-2.40	117.52	123.59
32	a	416[B]	PL9	C30-C29-C31	2.40	119.31	115.27
24	b	619	CLA	CAA-CBA-CGA	-2.40	106.23	113.25
24	b	612	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
25	D	401[B]	PHO	CBD-CHA-C1A	2.40	131.97	126.40
24	b	617	CLA	CAC-C3C-C4C	2.40	127.92	124.81
24	a	410	CLA	CMA-C3A-C2A	-2.40	104.16	113.83
24	B	609	CLA	O2A-CGA-CBA	2.40	119.43	111.91
26	B	620	BCR	C16-C17-C18	-2.39	123.89	127.31
25	d	402[A]	PHO	CMB-C2B-C1B	2.39	128.75	125.06
26	t	102	BCR	C7-C6-C5	-2.39	115.66	121.46
24	C	504	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
26	D	406	BCR	C10-C11-C12	-2.39	115.75	123.22
32	d	407[B]	PL9	C7-C3-C4	2.39	118.82	116.88
24	C	509	CLA	C11-C12-C13	-2.39	108.20	115.92
24	c	516	CLA	C11-C12-C13	-2.39	108.20	115.92
29	M	102	LMT	O5'-C1'-O1'	-2.39	104.32	109.97
24	d	405	CLA	O2A-CGA-CBA	2.39	119.40	111.91
24	d	403	CLA	C4C-C3C-C2C	-2.39	103.42	106.90
27	B	621	SQD	O48-C23-C24	2.39	119.40	111.91
24	c	512	CLA	CMB-C2B-C3B	2.39	129.14	124.68
24	C	503	CLA	CHC-C1C-C2C	-2.38	120.12	126.72
25	a	411	PHO	C2C-C1C-NC	2.38	113.39	109.79
25	a	411	PHO	C1C-C2C-C3C	-2.38	103.77	106.51
24	c	516	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
24	B	608	CLA	OBD-CAD-C3D	-2.38	124.02	127.98
34	d	415	LMG	O8-C28-C29	2.38	119.39	111.91
26	D	406	BCR	C21-C20-C19	-2.38	115.78	123.22
25	a	411	PHO	CHD-C1D-C2D	-2.38	119.74	125.73
24	B	610	CLA	CMA-C3A-C4A	-2.38	105.37	111.77
24	D	404	CLA	C4D-C3D-CAD	-2.38	107.14	108.47
36	b	632	HTG	C1-O5-C5	2.38	116.97	112.58
27	L	102	SQD	O47-C7-O49	-2.38	117.95	123.70
24	b	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
24	b	625	CLA	C1C-C2C-C3C	-2.38	104.46	106.96
27	F	101	SQD	O7-S-C6	2.38	109.76	106.94
37	e	101	DGD	O1G-C1A-C2A	2.37	119.36	111.91
26	T	103	BCR	C16-C17-C18	-2.37	123.92	127.31
25	D	401[B]	PHO	O2A-CGA-CBA	2.37	119.36	111.91
34	M	101	LMG	O1-C7-C8	-2.37	105.17	110.90
27	a	405	SQD	O48-C23-O10	-2.37	117.60	123.59
24	B	609	CLA	CHD-C4C-NC	2.37	127.94	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	401[B]	PHO	C1C-C2C-C3C	-2.37	103.78	106.51
26	b	627	BCR	C20-C21-C22	-2.37	123.93	127.31
26	C	515	BCR	C21-C20-C19	-2.37	115.82	123.22
24	b	612	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
24	d	405	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
24	A	405	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
26	b	626	BCR	C37-C22-C23	2.37	121.81	118.08
26	B	619	BCR	C24-C23-C22	-2.37	122.66	126.23
27	A	411	SQD	C44-O6-C1	-2.36	109.12	113.74
26	K	101	BCR	C15-C16-C17	-2.36	118.63	123.47
24	B	611	CLA	C11-C12-C13	-2.36	108.28	115.92
24	C	510	CLA	CHD-C4C-NC	2.36	127.92	124.20
24	C	501	CLA	C4-C3-C5	2.36	119.24	115.27
24	c	515	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
24	c	514	CLA	C4-C3-C2	-2.36	117.63	123.68
32	d	407[B]	PL9	C36-C37-C38	-2.36	104.13	111.88
24	c	507	CLA	O2A-CGA-CBA	2.36	119.31	111.91
24	c	514	CLA	C6-C7-C8	-2.36	108.30	115.92
34	C	520	LMG	O8-C28-C29	2.36	119.30	111.91
38	d	409	LHG	O8-C23-C24	2.35	119.30	111.91
24	C	501	CLA	O2A-CGA-CBA	2.35	119.30	111.91
39	V	205	HEM	CBD-CAD-C3D	-2.35	108.14	112.48
24	A	409	CLA	O2A-CGA-O1A	-2.35	117.65	123.59
24	b	613	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
24	c	513	CLA	C4-C3-C5	2.35	119.23	115.27
32	D	407[A]	PL9	C40-C39-C38	-2.35	117.64	123.68
27	L	102	SQD	C1-C2-C3	-2.35	105.10	110.00
24	b	618	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
25	d	402[B]	PHO	O2A-CGA-CBA	2.35	119.28	111.91
24	a	409	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	b	619	CLA	CHD-C4C-NC	2.35	127.90	124.20
24	d	403	CLA	C4D-C3D-CAD	-2.35	107.16	108.47
24	C	502	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
32	d	407[A]	PL9	C12-C13-C14	-2.35	122.01	127.66
24	c	517	CLA	C1-C2-C3	-2.35	121.99	126.04
32	A	417[B]	PL9	C40-C39-C41	2.35	119.22	115.27
24	B	611	CLA	O2A-CGA-O1A	-2.34	117.67	123.59
24	B	608	CLA	CHD-C4C-NC	2.34	127.90	124.20
26	b	626	BCR	C36-C18-C17	-2.34	119.64	122.92
32	D	407[A]	PL9	C32-C33-C34	-2.34	122.02	127.66
24	B	615	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
24	B	604	CLA	CMC-C2C-C1C	2.34	128.60	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	O2A-CGA-CBA	2.34	119.25	111.91
24	b	614	CLA	CMA-C3A-C2A	-2.34	104.40	113.83
24	c	507	CLA	OBD-CAD-C3D	-2.34	124.10	127.98
24	B	611	CLA	CMB-C2B-C3B	2.33	129.05	124.68
24	C	511	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
24	B	617	CLA	CAC-C3C-C4C	2.33	127.83	124.81
27	B	621	SQD	O47-C7-O49	-2.33	118.07	123.70
27	F	101	SQD	C1-O5-C5	2.33	118.26	113.69
24	B	615	CLA	CMC-C2C-C1C	2.33	128.59	125.04
24	c	507	CLA	CMC-C2C-C1C	2.33	128.59	125.04
24	c	508	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
36	B	632	HTG	C1-O5-C5	2.33	116.87	112.58
24	C	505	CLA	CHD-C4C-NC	2.33	127.87	124.20
39	f	101	HEM	CMA-C3A-C4A	-2.33	124.89	128.46
24	B	617	CLA	C1-O2A-CGA	2.33	122.55	116.44
24	b	625	CLA	CMB-C2B-C3B	2.33	129.03	124.68
24	C	508	CLA	CBC-CAC-C3C	-2.33	106.02	112.43
24	C	501	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
37	e	101	DGD	C1E-O6E-C5E	2.32	118.25	113.69
26	c	526	BCR	C38-C26-C25	-2.32	121.92	124.53
24	b	610	CLA	CMC-C2C-C1C	2.32	128.58	125.04
26	B	620	BCR	C29-C30-C25	2.32	114.05	110.48
24	B	614	CLA	CHD-C4C-NC	2.32	127.86	124.20
24	C	510	CLA	CMC-C2C-C1C	2.32	128.57	125.04
24	d	403	CLA	C4-C3-C5	2.32	119.17	115.27
26	t	102	BCR	C2-C1-C6	2.32	114.05	110.48
24	b	612	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
32	d	407[A]	PL9	C25-C24-C26	2.32	119.17	115.27
24	c	514	CLA	CMB-C2B-C3B	2.32	129.01	124.68
34	c	522	LMG	C8-O7-C10	-2.31	112.10	117.79
24	B	616	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
24	B	608	CLA	C1-C2-C3	-2.31	122.04	126.04
24	C	505	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
24	b	611	CLA	CMC-C2C-C1C	2.31	128.56	125.04
24	b	614	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
38	D	409	LHG	O8-C23-O10	-2.31	117.76	123.59
24	b	613	CLA	CMB-C2B-C3B	2.31	129.00	124.68
24	A	409	CLA	O2A-CGA-CBA	2.31	119.16	111.91
24	B	612	CLA	C4-C3-C5	2.31	119.16	115.27
32	d	407[A]	PL9	C15-C14-C16	2.31	119.16	115.27
37	C	516	DGD	C4E-C3E-C2E	-2.31	106.79	110.82
24	B	606	CLA	C4-C3-C5	2.31	119.15	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	417[A]	PL9	C17-C18-C19	-2.31	122.10	127.66
24	C	509	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
32	a	416[B]	PL9	C51-C49-C50	2.31	119.69	114.60
27	L	102	SQD	O7-S-C6	2.30	109.68	106.94
24	d	404	CLA	CHD-C4C-NC	2.30	127.83	124.20
24	C	513	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
24	c	513	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
25	d	402[A]	PHO	C2C-C1C-NC	2.30	113.26	109.79
26	t	102	BCR	C12-C13-C14	-2.30	115.41	118.94
26	c	518	BCR	C34-C9-C10	-2.30	119.70	122.92
24	C	512	CLA	OBD-CAD-C3D	-2.30	124.17	127.98
34	A	419	LMG	O8-C28-C29	2.30	119.12	111.91
24	b	618	CLA	CAC-C3C-C4C	2.30	127.79	124.81
26	b	628	BCR	C16-C15-C14	-2.30	118.77	123.47
24	B	612	CLA	CHD-C4C-NC	2.30	127.82	124.20
24	C	507	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
24	a	409	CLA	CMC-C2C-C1C	2.30	128.53	125.04
25	a	411	PHO	O2A-CGA-CBA	2.29	119.11	111.91
34	d	415	LMG	C6-C5-C4	-2.29	107.63	113.00
24	b	618	CLA	C1-O2A-CGA	2.29	122.46	116.44
24	B	617	CLA	CED-O2D-CGD	2.29	121.12	115.94
26	T	103	BCR	C37-C22-C23	2.29	121.69	118.08
24	B	613	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
24	B	602	CLA	C1-O2A-CGA	2.29	122.46	116.44
32	d	407[B]	PL9	C45-C44-C46	2.29	119.12	115.27
37	c	519	DGD	O2G-C1B-O1B	-2.29	118.17	123.70
24	b	611	CLA	O2A-CGA-CBA	2.29	119.09	111.91
25	d	402[B]	PHO	C3A-C4A-CHB	-2.29	117.87	121.83
26	D	406	BCR	C16-C17-C18	-2.29	124.04	127.31
24	c	512	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
24	c	511	CLA	O2A-CGA-CBA	2.29	119.09	111.91
32	d	407[B]	PL9	C30-C29-C31	2.29	119.12	115.27
24	C	508	CLA	CHB-C4A-NA	2.29	127.67	124.51
24	C	504	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
24	c	510	CLA	C4C-C3C-C2C	-2.28	103.57	106.90
25	d	402[A]	PHO	CBD-CHA-C1A	2.28	131.70	126.40
26	Y	101	BCR	C21-C20-C19	-2.28	116.09	123.22
24	A	407	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	A	406	CLA	O2A-CGA-CBA	2.28	119.07	111.91
24	D	405	CLA	CHD-C4C-NC	2.28	127.80	124.20
24	A	406	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
24	c	515	CLA	C2A-C1A-CHA	-2.28	119.87	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
24	B	614	CLA	C7-C6-C5	-2.28	107.17	113.36
24	c	508	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
25	A	408	PHO	CBD-CHA-C1A	2.28	131.68	126.40
24	b	622	CLA	CED-O2D-CGD	2.28	121.08	115.94
32	D	407[B]	PL9	C17-C18-C19	-2.27	122.18	127.66
24	C	502	CLA	C4-C3-C5	2.27	119.09	115.27
36	b	602	HTG	C1'-S1-C1	2.27	104.34	100.09
36	b	607	HTG	O5-C5-C4	2.27	113.82	109.69
39	V	205	HEM	C1D-C2D-C3D	-2.27	105.42	107.00
32	A	417[B]	PL9	C35-C34-C36	2.27	119.09	115.27
32	A	417[A]	PL9	C7-C3-C2	-2.27	120.32	123.30
37	C	517	DGD	C3G-O3G-C1D	-2.27	109.31	113.74
24	C	507	CLA	C4-C3-C5	2.27	119.09	115.27
37	c	519	DGD	O3G-C3G-C2G	-2.27	105.43	110.90
26	H	101	BCR	C10-C11-C12	-2.27	116.15	123.22
24	A	406	CLA	OBD-CAD-C3D	-2.26	124.22	127.98
34	a	415	LMG	O7-C10-O9	-2.26	118.23	123.70
24	a	409	CLA	C1-C2-C3	-2.26	122.13	126.04
24	c	513	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
24	A	406	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
25	D	401[B]	PHO	CED-O2D-CGD	2.26	121.05	115.94
26	d	406	BCR	C21-C20-C19	-2.26	116.17	123.22
34	d	415	LMG	C1-O6-C5	2.26	118.12	113.69
29	E	102	LMT	O5'-C5'-C4'	2.26	114.51	109.75
24	C	507	CLA	C3B-C4B-NB	2.26	112.13	109.21
37	C	518	DGD	O3G-C3G-C2G	-2.26	105.45	110.90
24	c	509	CLA	CMC-C2C-C1C	2.26	128.47	125.04
24	B	612	CLA	C1-O2A-CGA	2.26	122.36	116.44
24	b	617	CLA	C11-C10-C8	-2.26	108.63	115.92
32	D	407[B]	PL9	C15-C14-C16	2.25	119.06	115.27
24	C	510	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
24	A	407	CLA	CMC-C2C-C1C	2.25	128.47	125.04
34	d	415	LMG	O6-C5-C4	2.25	113.78	109.69
24	C	502	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
26	B	620	BCR	C37-C22-C23	2.25	121.62	118.08
24	B	603	CLA	CMC-C2C-C1C	2.25	128.46	125.04
24	B	608	CLA	CMB-C2B-C3B	2.25	128.88	124.68
24	B	617	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
24	C	507	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
37	c	520	DGD	O1G-C1A-C2A	2.24	118.95	111.91
24	B	603	CLA	C11-C12-C13	-2.24	108.67	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	CLA	CAC-C3C-C4C	2.24	127.72	124.81
24	c	505	CLA	C4-C3-C5	2.24	119.04	115.27
26	D	406	BCR	C38-C26-C27	2.24	117.92	113.62
25	D	401[A]	PHO	C4D-CHA-C1A	-2.24	120.33	125.37
24	C	502	CLA	CED-O2D-CGD	2.24	121.00	115.94
24	b	612	CLA	CMA-C3A-C2A	-2.24	104.79	113.83
32	D	407[B]	PL9	C32-C33-C34	-2.24	122.27	127.66
24	C	510	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
34	b	629	LMG	O6-C5-C6	2.24	112.00	106.44
24	b	613	CLA	CHA-C1A-NA	-2.24	121.27	126.40
24	d	403	CLA	O2A-CGA-CBA	2.24	118.93	111.91
24	C	504	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
37	C	517	DGD	O1G-C1A-O1A	-2.24	117.95	123.59
24	C	513	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
24	B	608	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	b	619	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
27	A	413	SQD	O9-S-C6	2.23	109.59	106.94
24	c	507	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
24	c	510	CLA	OBD-CAD-C3D	-2.23	124.28	127.98
24	b	619	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
24	C	512	CLA	CHB-C4A-NA	2.22	127.59	124.51
25	D	401[B]	PHO	C3C-C4C-NC	2.22	113.73	110.28
24	b	625	CLA	CHC-C1C-NC	2.22	127.58	124.20
27	A	413	SQD	O6-C44-C45	-2.22	105.54	110.90
26	t	102	BCR	C35-C13-C12	2.22	121.58	118.08
24	B	611	CLA	CMA-C3A-C2A	-2.22	104.87	113.83
24	b	621	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
26	C	515	BCR	C11-C10-C9	-2.22	124.14	127.31
29	M	104	LMT	O5B-C5B-C4B	2.22	113.72	109.69
38	E	101	LHG	O8-C23-O10	-2.22	118.00	123.59
24	b	620	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
24	b	620	CLA	O2A-CGA-O1A	-2.21	118.00	123.59
24	B	604	CLA	C1-O2A-CGA	2.21	122.25	116.44
24	a	409	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	c	517	CLA	C4-C3-C5	2.21	118.99	115.27
24	B	602	CLA	CAC-C3C-C4C	2.21	127.68	124.81
34	D	415	LMG	O8-C28-O10	-2.21	118.02	123.59
24	C	506	CLA	O2A-CGA-CBA	2.21	118.84	111.91
24	c	507	CLA	C1-O2A-CGA	2.21	122.24	116.44
37	c	520	DGD	C3B-C2B-C1B	-2.21	105.59	113.62
24	B	609	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
24	b	625	CLA	OBD-CAD-C3D	-2.21	124.32	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	D	407[B]	PL9	C30-C29-C31	2.21	118.98	115.27
24	b	610	CLA	CBC-CAC-C3C	-2.21	106.35	112.43
25	A	408	PHO	C16-C15-C13	-2.21	108.79	115.92
24	B	603	CLA	O2A-CGA-CBA	2.20	118.82	111.91
24	A	406	CLA	C6-C7-C8	-2.20	108.80	115.92
24	B	605	CLA	CHA-C1A-NA	-2.20	121.36	126.40
24	B	615	CLA	CED-O2D-CGD	2.20	120.92	115.94
24	B	611	CLA	C6-C7-C8	-2.20	108.81	115.92
24	C	509	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
26	d	406	BCR	C10-C11-C12	-2.20	116.35	123.22
34	C	519	LMG	O8-C28-O10	-2.20	118.05	123.59
24	B	603	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
26	C	514	BCR	C11-C10-C9	-2.20	124.18	127.31
24	B	617	CLA	C4-C3-C5	2.20	118.96	115.27
32	d	407[B]	PL9	C15-C14-C16	2.19	118.96	115.27
26	a	413	BCR	C36-C18-C19	2.19	121.53	118.08
24	B	604	CLA	OBD-CAD-C3D	-2.19	124.34	127.98
24	b	620	CLA	CHD-C4C-NC	2.19	127.66	124.20
37	c	519	DGD	O1G-C1A-C2A	2.19	118.79	111.91
24	B	607	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
37	e	101	DGD	O2G-C1B-O1B	-2.19	118.41	123.70
26	b	626	BCR	C36-C18-C19	2.19	121.53	118.08
24	b	625	CLA	C4-C3-C5	2.19	118.95	115.27
24	c	507	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	b	619	CLA	OBD-CAD-C3D	-2.19	124.35	127.98
24	A	405	CLA	CHB-C4A-NA	2.19	127.54	124.51
24	A	407	CLA	CMA-C3A-C4A	-2.19	105.90	111.77
26	T	103	BCR	C34-C9-C10	-2.19	119.86	122.92
27	a	414	SQD	O48-C23-O10	-2.19	118.08	123.59
25	D	401[B]	PHO	C2C-C1C-NC	2.18	113.09	109.79
32	D	407[B]	PL9	C20-C19-C21	2.18	118.94	115.27
29	m	103	LMT	C1'-O5'-C5'	2.18	117.97	113.69
24	b	623	CLA	C4-C3-C5	2.18	118.94	115.27
24	b	615	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
36	b	608	HTG	C1-O5-C5	2.18	116.60	112.58
24	A	409	CLA	C1-C2-C3	-2.18	122.27	126.04
24	B	603	CLA	C1-O2A-CGA	2.18	122.16	116.44
24	b	620	CLA	CHB-C4A-NA	2.18	127.53	124.51
38	E	101	LHG	C5-O7-C7	-2.18	112.42	117.79
24	b	621	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
26	y	101	BCR	C29-C30-C25	2.18	113.83	110.48
24	D	404	CLA	OBD-CAD-C3D	-2.18	124.37	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
36	B	631	HTG	C6-C5-C4	-2.18	107.91	113.00
38	d	410	LHG	O8-C23-O10	-2.17	118.10	123.59
24	A	407	CLA	CHB-C4A-NA	2.17	127.52	124.51
24	b	610	CLA	C4D-C3D-CAD	-2.17	107.26	108.47
24	C	510	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
37	C	517	DGD	O3G-C1D-C2D	2.17	111.69	108.30
24	C	512	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
26	c	526	BCR	C35-C13-C14	-2.17	119.88	122.92
26	B	620	BCR	C8-C7-C6	-2.17	121.10	127.20
24	C	507	CLA	CMB-C2B-C3B	2.17	128.74	124.68
26	a	413	BCR	C37-C22-C23	2.17	121.50	118.08
24	D	405	CLA	OBD-CAD-C3D	-2.17	124.38	127.98
26	A	410	BCR	C38-C26-C25	-2.17	122.09	124.53
32	A	417[B]	PL9	C51-C49-C50	2.17	119.39	114.60
24	B	617	CLA	CMB-C2B-C3B	2.17	128.73	124.68
26	B	618	BCR	C15-C14-C13	-2.17	124.22	127.31
24	c	516	CLA	CAC-C3C-C4C	2.16	127.62	124.81
26	d	406	BCR	C34-C9-C10	-2.16	119.89	122.92
24	B	614	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
25	A	408	PHO	CHD-C1D-C2D	-2.16	120.30	125.73
26	B	620	BCR	C37-C22-C21	-2.16	119.90	122.92
24	c	517	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
37	c	519	DGD	O1G-C1A-O1A	-2.16	118.14	123.59
27	L	102	SQD	C1-O5-C5	-2.16	109.45	113.69
24	b	616	CLA	O2A-CGA-CBA	2.16	118.68	111.91
24	C	511	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
24	C	512	CLA	CMB-C2B-C3B	2.16	128.71	124.68
24	B	616	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
24	C	508	CLA	CHC-C1C-NC	2.15	127.47	124.20
24	B	604	CLA	CAC-C3C-C4C	2.15	127.60	124.81
32	D	407[A]	PL9	C20-C19-C21	2.15	118.89	115.27
24	a	409	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
26	B	618	BCR	C38-C26-C25	-2.15	122.11	124.53
24	c	510	CLA	CED-O2D-CGD	2.15	120.80	115.94
24	A	409	CLA	CHD-C4C-NC	2.15	127.59	124.20
24	A	405	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	B	610	CLA	O2A-CGA-CBA	2.15	118.64	111.91
24	b	624	CLA	O2A-CGA-CBA	2.14	118.64	111.91
27	F	101	SQD	O48-C23-O10	-2.14	118.19	123.59
24	c	517	CLA	CBC-CAC-C3C	-2.14	106.53	112.43
36	V	206	HTG	C3-C4-C5	2.14	114.06	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	517	DGD	O6D-C5D-C6D	2.14	110.99	106.67
24	c	517	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
24	B	602	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
32	a	416[A]	PL9	C45-C44-C46	2.14	118.87	115.27
24	A	406	CLA	CMA-C3A-C2A	-2.14	105.21	113.83
32	D	407[A]	PL9	C35-C34-C36	2.14	118.86	115.27
24	B	607	CLA	CAC-C3C-C4C	2.13	127.58	124.81
24	c	512	CLA	CAC-C3C-C4C	2.13	127.58	124.81
24	C	510	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
32	a	416[A]	PL9	C8-C7-C3	2.13	118.00	111.98
32	d	407[A]	PL9	C40-C39-C38	-2.13	118.22	123.68
24	c	512	CLA	CMC-C2C-C1C	2.13	128.28	125.04
24	A	409	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
26	Y	101	BCR	C35-C13-C12	2.13	121.43	118.08
26	d	406	BCR	C40-C30-C25	-2.13	106.85	110.30
24	C	509	CLA	C4D-C3D-CAD	-2.13	107.28	108.47
25	D	401[B]	PHO	C3A-C2A-C1A	-2.12	99.11	101.64
37	H	102	DGD	C3E-C4E-C5E	-2.12	106.45	110.24
26	k	102	BCR	C7-C8-C9	-2.12	123.03	126.23
27	A	411	SQD	C1-O5-C5	-2.12	109.53	113.69
24	B	602	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	B	611	CLA	CAC-C3C-C4C	2.12	127.56	124.81
34	k	101	LMG	O8-C28-O10	-2.12	118.25	123.59
24	C	501	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	c	513	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
24	c	508	CLA	C5-C3-C2	-2.12	116.84	121.12
26	k	102	BCR	C34-C9-C8	2.11	121.41	118.08
37	c	521	DGD	O1G-C1A-O1A	-2.11	118.25	123.59
32	d	407[A]	PL9	C36-C37-C38	-2.11	104.94	111.88
24	b	625	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
27	L	102	SQD	C4-C3-C2	2.11	114.51	110.82
26	b	628	BCR	C11-C10-C9	-2.11	124.30	127.31
24	B	612	CLA	O2A-CGA-CBA	2.11	118.53	111.91
24	B	603	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
25	D	401[A]	PHO	O2A-CGA-CBA	2.11	118.53	111.91
29	C	521	LMT	O5'-C5'-C4'	2.11	114.20	109.75
24	a	412	CLA	C4A-NA-C1A	-2.11	105.76	106.71
24	c	509	CLA	O2A-CGA-CBA	2.11	118.53	111.91
29	A	414	LMT	C4B-C3B-C2B	-2.11	107.14	110.82
24	B	616	CLA	O2A-CGA-CBA	2.11	118.52	111.91
38	D	410	LHG	O7-C7-C8	2.11	116.04	111.50
26	b	628	BCR	C10-C11-C12	-2.10	116.65	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	415	LMG	O8-C28-C29	2.10	118.51	111.91
32	D	407[A]	PL9	C47-C48-C49	-2.10	120.56	127.75
25	d	402[A]	PHO	C1C-C2C-C3C	-2.10	104.09	106.51
24	A	409	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
24	a	412	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
26	K	101	BCR	C15-C14-C13	-2.10	124.31	127.31
26	B	619	BCR	C2-C1-C6	2.10	113.72	110.48
26	b	627	BCR	C35-C13-C14	-2.10	119.98	122.92
29	A	414	LMT	C6'-C5'-C4'	-2.10	107.21	113.33
24	c	510	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
32	A	417[A]	PL9	C47-C46-C44	-2.10	106.06	112.98
24	B	614	CLA	CHB-C4A-NA	2.10	127.42	124.51
24	B	605	CLA	CHD-C4C-NC	2.10	127.51	124.20
24	b	611	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
32	A	417[B]	PL9	C47-C48-C49	-2.10	120.58	127.75
24	C	503	CLA	C1-C2-C3	-2.10	122.42	126.04
24	C	510	CLA	C4-C3-C2	-2.10	118.30	123.68
34	k	101	LMG	O6-C5-C6	2.10	111.65	106.44
26	a	413	BCR	C40-C30-C25	-2.10	106.90	110.30
37	D	408	DGD	O6D-C1D-C2D	2.10	114.79	110.35
32	D	407[B]	PL9	C47-C48-C49	-2.10	120.59	127.75
24	c	515	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
24	b	610	CLA	CAA-CBA-CGA	-2.10	107.13	113.25
24	C	508	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	a	411	PHO	C16-C15-C13	-2.09	109.15	115.92
36	d	413	HTG	C1-O5-C5	2.09	116.44	112.58
38	L	101	LHG	O8-C23-O10	-2.09	118.31	123.59
26	d	406	BCR	C7-C8-C9	-2.09	123.07	126.23
24	b	625	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
24	c	507	CLA	CBC-CAC-C3C	-2.09	106.66	112.43
38	L	101	LHG	O4-P-O5	2.09	122.58	112.24
29	T	104	LMT	C6'-C5'-C4'	-2.09	107.24	113.33
32	A	417[A]	PL9	C51-C49-C50	2.09	119.22	114.60
34	d	415	LMG	C4-C3-C2	-2.09	107.17	110.82
26	b	626	BCR	C20-C21-C22	-2.09	124.33	127.31
24	c	511	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
24	d	405	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	d	402[A]	PHO	C3A-C4A-CHB	-2.09	118.22	121.83
24	b	610	CLA	C1-O2A-CGA	2.09	121.92	116.44
24	B	609	CLA	CHB-C4A-NA	2.09	127.40	124.51
32	D	407[B]	PL9	C10-C9-C8	-2.09	118.33	123.68
29	a	404	LMT	C1B-O1B-C4'	-2.08	112.81	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C3C-C4C-NC	2.08	113.51	110.28
24	b	615	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	b	622	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
24	B	607	CLA	C1-C2-C3	-2.08	122.44	126.04
24	d	404	CLA	CAA-C2A-C3A	-2.08	107.08	112.78
24	B	611	CLA	CBC-CAC-C3C	-2.08	106.69	112.43
26	k	102	BCR	C2-C1-C6	2.08	113.69	110.48
29	t	101	LMT	C1'-O5'-C5'	2.08	117.77	113.69
24	B	615	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	b	624	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
24	b	624	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
34	C	519	LMG	O7-C10-O9	-2.08	118.68	123.70
24	A	406	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
24	A	405	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
24	c	506	CLA	CMB-C2B-C3B	2.08	128.56	124.68
24	B	611	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
26	c	518	BCR	C34-C9-C8	2.07	121.35	118.08
26	t	102	BCR	C29-C28-C27	-2.07	106.74	111.38
36	c	523	HTG	C1-O5-C5	2.07	116.40	112.58
24	C	504	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
24	b	616	CLA	CMA-C3A-C2A	-2.07	105.48	113.83
24	c	512	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
24	d	403	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	d	404	CLA	CMB-C2B-C3B	2.07	128.55	124.68
24	D	405	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	c	511	CLA	OBD-CAD-C3D	-2.07	124.55	127.98
24	b	617	CLA	C4-C3-C5	2.07	118.75	115.27
24	C	511	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
26	C	515	BCR	C28-C27-C26	-2.06	110.39	114.08
26	B	618	BCR	C24-C23-C22	-2.06	123.11	126.23
32	d	407[A]	PL9	C35-C34-C36	2.06	118.74	115.27
24	b	619	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
24	a	409	CLA	CHB-C4A-NA	2.06	127.36	124.51
37	C	516	DGD	O1G-C1A-C2A	2.06	118.38	111.91
24	b	620	CLA	CMC-C2C-C1C	2.06	128.18	125.04
24	C	502	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
32	A	417[A]	PL9	C40-C39-C41	2.06	118.74	115.27
32	d	407[A]	PL9	C22-C23-C24	-2.06	122.70	127.66
24	B	606	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
37	C	518	DGD	O1G-C1A-O1A	-2.06	118.40	123.59
24	B	609	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
26	T	103	BCR	C33-C5-C4	2.06	117.56	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	406	BCR	C37-C22-C23	2.06	121.31	118.08
24	b	616	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
36	b	607	HTG	C6-C5-C4	-2.05	108.19	113.00
24	A	406	CLA	CAA-CBA-CGA	2.05	119.26	113.25
25	d	402[B]	PHO	C4-C3-C2	-2.05	118.41	123.68
26	K	101	BCR	C36-C18-C19	2.05	121.31	118.08
26	y	101	BCR	C8-C7-C6	-2.05	121.44	127.20
24	B	610	CLA	CED-O2D-CGD	2.05	120.58	115.94
24	b	610	CLA	C11-C12-C13	-2.05	109.29	115.92
26	D	406	BCR	C1-C6-C7	2.05	121.58	115.78
27	L	102	SQD	O48-C23-O10	-2.05	118.42	123.59
26	B	618	BCR	C16-C15-C14	-2.05	119.28	123.47
24	C	509	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
24	b	614	CLA	CAC-C3C-C2C	2.05	131.03	127.53
24	B	611	CLA	CHC-C1C-NC	2.05	127.31	124.20
24	C	502	CLA	CMB-C2B-C3B	2.05	128.51	124.68
24	D	404	CLA	CMB-C2B-C3B	2.05	128.51	124.68
24	B	612	CLA	CHB-C4A-NA	2.05	127.34	124.51
37	c	520	DGD	O5D-C1E-C2E	2.05	111.50	108.30
24	b	618	CLA	CED-O2D-CGD	2.04	120.56	115.94
24	c	508	CLA	CHB-C4A-NA	2.04	127.34	124.51
24	b	620	CLA	C7-C6-C5	-2.04	107.81	113.36
24	D	405	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
32	d	407[A]	PL9	O1-C4-C3	-2.04	118.47	120.72
29	a	419	LMT	C1B-O1B-C4'	-2.04	112.92	117.96
24	b	625	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	m	103	LMT	O5B-C5B-C4B	2.04	113.40	109.69
34	Z	101	LMG	O6-C1-C2	2.04	114.67	110.35
24	C	508	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
26	K	101	BCR	C16-C17-C18	-2.04	124.40	127.31
24	B	609	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
24	c	506	CLA	OBD-CAD-C3D	-2.04	124.60	127.98
26	b	626	BCR	C10-C11-C12	-2.04	116.86	123.22
24	c	506	CLA	C3D-CAD-CBD	2.04	110.28	107.61
32	d	407[B]	PL9	C32-C33-C34	-2.04	122.76	127.66
24	A	405	CLA	CED-O2D-CGD	2.03	120.54	115.94
29	e	102	LMT	O5'-C5'-C4'	2.03	114.04	109.75
34	c	522	LMG	O7-C10-O9	-2.03	118.79	123.70
24	b	615	CLA	CAC-C3C-C4C	2.03	127.45	124.81
24	A	407	CLA	CAA-C2A-C1A	-2.03	105.31	111.97
26	h	101	BCR	C36-C18-C17	-2.03	120.08	122.92
26	C	515	BCR	C37-C22-C23	2.03	121.28	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	f	101	HEM	CMC-C2C-C3C	2.03	128.48	124.68
34	b	629	LMG	C9-C8-C7	-2.03	106.98	111.79
26	D	406	BCR	C3-C4-C5	-2.03	110.45	114.08
24	C	510	CLA	CHB-C4A-NA	2.03	127.32	124.51
34	c	522	LMG	O8-C28-O10	-2.03	118.47	123.59
25	D	401[A]	PHO	C3A-C4A-NA	2.03	116.51	113.05
24	D	405	CLA	CMC-C2C-C1C	2.03	128.13	125.04
24	B	609	CLA	C1-C2-C3	-2.03	122.54	126.04
26	a	413	BCR	C8-C7-C6	-2.03	121.51	127.20
24	b	625	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
24	b	611	CLA	CHB-C4A-NA	2.02	127.31	124.51
26	C	515	BCR	C15-C14-C13	-2.02	124.42	127.31
24	b	615	CLA	CHA-C1A-NA	-2.02	121.77	126.40
24	b	619	CLA	CHA-C1A-NA	-2.02	121.77	126.40
26	k	102	BCR	C37-C22-C21	-2.02	120.09	122.92
24	c	505	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
26	B	619	BCR	C31-C1-C6	-2.02	107.03	110.30
24	b	621	CLA	CMB-C2B-C3B	2.02	128.45	124.68
26	B	619	BCR	C37-C22-C23	2.02	121.25	118.08
38	d	409	LHG	O7-C7-O9	-2.02	118.83	123.70
37	C	517	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
26	Y	101	BCR	C37-C22-C23	2.02	121.25	118.08
37	C	516	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
25	D	401[A]	PHO	CHD-C1D-C2D	-2.01	120.66	125.73
24	c	511	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	C	511	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	C	508	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
25	D	401[B]	PHO	CHC-C1C-NC	2.01	128.77	124.58
29	M	104	LMT	C1'-O5'-C5'	2.01	117.64	113.69
26	b	627	BCR	C33-C5-C6	-2.01	122.27	124.53
24	b	617	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
24	C	506	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
24	C	505	CLA	C1-C2-C3	-2.01	122.57	126.04
24	B	602	CLA	CMC-C2C-C1C	2.01	128.10	125.04
24	c	512	CLA	OBD-CAD-C3D	-2.01	124.64	127.98
24	c	509	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
34	d	415	LMG	O8-C28-O10	-2.01	118.53	123.59
24	C	503	CLA	C1-O2A-CGA	2.01	121.71	116.44
38	D	410	LHG	O8-C23-C24	2.01	118.20	111.91
26	h	101	BCR	C16-C15-C14	-2.01	119.37	123.47
26	C	515	BCR	C3-C4-C5	-2.00	110.50	114.08
32	A	417[A]	PL9	C16-C17-C18	-2.00	105.30	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
24	B	617	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
24	b	618	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
26	d	406	BCR	C29-C28-C27	-2.00	106.90	111.38
24	c	514	CLA	OBD-CAD-C3D	-2.00	124.66	127.98
24	b	622	CLA	CHC-C1C-NC	2.00	127.24	124.20
24	A	407	CLA	O2A-CGA-CBA	2.00	118.19	111.91
24	b	615	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
37	c	520	DGD	O2G-C1B-O1B	-2.00	118.87	123.70
24	b	610	CLA	CHB-C4A-NA	2.00	127.28	124.51

All (191) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	c	517	CLA	NC
24	c	517	CLA	NA
24	d	404	CLA	ND
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	b	622	CLA	NC
24	b	622	CLA	ND
24	b	622	CLA	NA
24	D	404	CLA	ND
24	d	403	CLA	ND
24	d	403	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	615	CLA	NA
24	B	609	CLA	NC

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Mol	Chain	Res	Type	Atom
24	B	609	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	D	405	CLA	NC
24	D	405	CLA	ND
24	D	405	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	a	409	CLA	NC
24	a	409	CLA	ND
24	a	409	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	603	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	c	505	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	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	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	b	614	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	614	CLA	ND
24	b	614	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	618	CLA	NA
24	c	514	CLA	NC
24	c	514	CLA	ND
24	c	514	CLA	NA
24	a	412	CLA	NC
24	a	412	CLA	ND
24	a	412	CLA	NA
24	c	506	CLA	ND
24	c	506	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	c	509	CLA	ND
24	c	509	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	b	623	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	623	CLA	ND
24	b	623	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	NA
24	c	516	CLA	NC
24	c	516	CLA	ND
24	c	516	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	b	625	CLA	NA
24	b	625	CLA	NC
24	b	625	CLA	ND
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	c	515	CLA	NC
24	c	515	CLA	ND
24	c	515	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	ND
24	b	620	CLA	NA
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	d	405	CLA	NC
24	d	405	CLA	ND
24	d	405	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	A	407	CLA	NC
24	A	407	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	501	CLA	NC
24	C	501	CLA	ND
24	C	501	CLA	NA
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	b	619	CLA	NA
24	a	410	CLA	NC
24	a	410	CLA	NA
24	A	409	CLA	NC
24	A	409	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	b	624	CLA	NA
24	b	624	CLA	NC
24	b	624	CLA	ND
24	C	505	CLA	ND
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	ND
24	c	508	CLA	NA
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA

All (1405) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	z	101	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	z	101	LMG	O9-C10-O7-C8
28	D	402	GOL	C1-C2-C3-O3
26	C	515	BCR	C7-C8-C9-C10
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C37-C22-C23-C24
28	v	202	GOL	O1-C1-C2-C3
36	c	523	HTG	C2'-C1'-S1-C1
24	b	615	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O2D
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
34	C	520	LMG	C11-C10-O7-C8
28	b	606	GOL	O1-C1-C2-O2
28	b	606	GOL	O1-C1-C2-C3
38	D	409	LHG	C4-O6-P-O5
28	T	102	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-C3
26	d	406	BCR	C21-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
32	a	416[B]	PL9	C9-C11-C12-C13
36	b	632	HTG	C2'-C1'-S1-C1
28	B	627	GOL	O1-C1-C2-O2
24	C	509	CLA	C2-C1-O2A-CGA
37	D	408	DGD	C2B-C1B-O2G-C2G
37	D	408	DGD	O1B-C1B-O2G-C2G
37	D	408	DGD	C2D-C1D-O3G-C3G
37	D	408	DGD	O6D-C1D-O3G-C3G
29	a	419	LMT	C2'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
28	a	421	GOL	O1-C1-C2-C3
26	t	102	BCR	C7-C8-C9-C10
26	t	102	BCR	C7-C8-C9-C34
29	b	630	LMT	C2'-C1'-O1'-C1
29	b	630	LMT	O5'-C1'-O1'-C1
24	b	614	CLA	C4-C3-C5-C6
28	B	626	GOL	O1-C1-C2-O2
28	B	626	GOL	O1-C1-C2-C3
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
38	a	420	LHG	C3-O3-P-O5
38	a	420	LHG	C3-O3-P-O6
38	a	420	LHG	C4-O6-P-O5
38	a	420	LHG	C24-C23-O8-C6
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C5-C6-S-O7
28	B	629	GOL	O1-C1-C2-C3
29	t	101	LMT	C2'-C1'-O1'-C1
29	t	101	LMT	O5'-C1'-O1'-C1
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
29	e	102	LMT	C2'-C1'-O1'-C1
29	e	102	LMT	O5'-C1'-O1'-C1
29	A	414	LMT	C2'-C1'-O1'-C1
29	A	414	LMT	O5'-C1'-O1'-C1
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	Y	101	BCR	C21-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
38	d	408	LHG	C4-O6-P-O5
28	a	401	GOL	C1-C2-C3-O3
38	E	101	LHG	C4-O6-P-O3
38	E	101	LHG	C4-O6-P-O5
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C7-C8-C9-C34
26	D	406	BCR	C21-C22-C23-C24
26	D	406	BCR	C37-C22-C23-C24
26	D	406	BCR	C23-C24-C25-C30
34	A	419	LMG	C11-C10-O7-C8
28	V	201	GOL	C1-C2-C3-O3
38	d	409	LHG	C3-O3-P-O4
36	V	206	HTG	C2-C1-S1-C1'
36	V	206	HTG	O5-C1-S1-C1'
36	V	206	HTG	C2'-C1'-S1-C1
38	D	410	LHG	C4-O6-P-O4
28	a	402	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	M	104	LMT	O5'-C1'-O1'-C1
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
29	T	104	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
37	e	101	DGD	C2B-C1B-O2G-C2G
37	e	101	DGD	O1B-C1B-O2G-C2G
37	e	101	DGD	C2D-C1D-O3G-C3G
37	e	101	DGD	O6E-C1E-O5D-C6D
27	A	413	SQD	O6-C44-C45-O47
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
38	L	101	LHG	C4-O6-P-O4
28	b	604	GOL	C1-C2-C3-O3
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
29	E	102	LMT	C2'-C1'-O1'-C1
29	E	102	LMT	O5'-C1'-O1'-C1
28	c	502	GOL	O1-C1-C2-C3
29	C	521	LMT	C2'-C1'-O1'-C1
29	C	521	LMT	O5'-C1'-O1'-C1
36	B	623	HTG	C2'-C1'-S1-C1
36	B	624	HTG	O5-C1-S1-C1'
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
28	b	605	GOL	O1-C1-C2-C3
24	c	508	CLA	C2-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
38	b	634	LHG	O1-C1-C2-C3
38	b	634	LHG	C4-O6-P-O4
29	C	521	LMT	C3'-C4'-O1B-C1B
38	a	420	LHG	O10-C23-O8-C6
38	E	101	LHG	O10-C23-O8-C6
29	D	403	LMT	C3'-C4'-O1B-C1B
38	E	101	LHG	C24-C23-O8-C6
24	c	515	CLA	CBD-CGD-O2D-CED
34	C	520	LMG	O9-C10-O7-C8
34	A	419	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	c	510	CLA	C3-C5-C6-C7
24	a	412	CLA	C3-C5-C6-C7
24	b	623	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	A	409	CLA	C3-C5-C6-C7
34	z	101	LMG	O6-C5-C6-O5
34	z	101	LMG	C11-C10-O7-C8
27	L	102	SQD	C8-C7-O47-C45
27	F	101	SQD	C8-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
32	a	416[A]	PL9	C12-C11-C9-C10
32	a	416[A]	PL9	C20-C19-C21-C22
32	a	416[B]	PL9	C12-C11-C9-C10
24	B	615	CLA	C4-C3-C5-C6
24	b	623	CLA	C4-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
24	C	509	CLA	CBD-CGD-O2D-CED
24	B	607	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C3-C5-C6-C7
24	d	405	CLA	CBD-CGD-O2D-CED
36	c	523	HTG	S1-C1'-C2'-C3'
29	M	104	LMT	O5'-C5'-C6'-O6'
36	B	624	HTG	O5-C5-C6-O6
24	b	613	CLA	CBD-CGD-O2D-CED
24	C	501	CLA	CBD-CGD-O2D-CED
24	c	507	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	C3-C5-C6-C7
24	a	410	CLA	CBD-CGD-O2D-CED
36	C	523	HTG	O5-C5-C6-O6
34	C	520	LMG	O6-C5-C6-O5
29	m	103	LMT	O5'-C5'-C6'-O6'
34	z	101	LMG	C4-C5-C6-O5
37	e	101	DGD	C4E-C5E-C6E-O5E
29	M	102	LMT	O5B-C5B-C6B-O6B
34	a	415	LMG	C17-C18-C19-C20
24	B	606	CLA	C4-C3-C5-C6
32	A	417[A]	PL9	C25-C24-C26-C27
32	a	416[A]	PL9	C15-C14-C16-C17
32	a	416[A]	PL9	C25-C24-C26-C27
32	a	416[B]	PL9	C15-C14-C16-C17
32	a	416[B]	PL9	C20-C19-C21-C22
32	a	416[B]	PL9	C25-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
32	A	417[B]	PL9	C25-C24-C26-C27
29	M	104	LMT	C4'-C5'-C6'-O6'
24	B	606	CLA	C2-C3-C5-C6
32	A	417[A]	PL9	C23-C24-C26-C27
32	a	416[A]	PL9	C13-C14-C16-C17
32	a	416[A]	PL9	C23-C24-C26-C27
32	a	416[B]	PL9	C13-C14-C16-C17
32	a	416[B]	PL9	C18-C19-C21-C22
32	a	416[B]	PL9	C23-C24-C26-C27
32	A	417[B]	PL9	C23-C24-C26-C27
24	C	509	CLA	O1A-CGA-O2A-C1
29	e	102	LMT	C4'-C5'-C6'-O6'
37	e	101	DGD	O6D-C1D-O3G-C3G
32	d	407[B]	PL9	C39-C41-C42-C43
32	d	407[A]	PL9	C39-C41-C42-C43
32	D	407[A]	PL9	C39-C41-C42-C43
32	D	407[B]	PL9	C39-C41-C42-C43
38	D	411	LHG	C24-C23-O8-C6
24	C	509	CLA	CBA-CGA-O2A-C1
27	A	413	SQD	C18-C19-C20-C21
38	D	411	LHG	O10-C23-O8-C6
24	a	412	CLA	O1A-CGA-O2A-C1
24	a	412	CLA	CBA-CGA-O2A-C1
24	b	623	CLA	CBD-CGD-O2D-CED
29	m	102	LMT	O5'-C5'-C6'-O6'
34	d	415	LMG	C19-C20-C21-C22
24	B	615	CLA	C8-C10-C11-C12
24	C	508	CLA	C10-C11-C12-C13
38	E	101	LHG	O2-C2-C3-O3
37	c	521	DGD	C1A-C2A-C3A-C4A
37	e	101	DGD	C2E-C1E-O5D-C6D
34	Z	101	LMG	C2-C1-O1-C7
32	a	416[A]	PL9	C12-C11-C9-C8
24	c	510	CLA	C6-C7-C8-C9
24	B	602	CLA	C11-C10-C8-C9
24	b	620	CLA	C11-C12-C13-C14
24	B	617	CLA	C6-C7-C8-C9
24	c	513	CLA	C11-C10-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	b	615	CLA	C2A-CAA-CBA-CGA
26	t	102	BCR	C11-C12-C13-C35
26	b	628	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
24	C	506	CLA	C5-C6-C7-C8
29	C	521	LMT	O5B-C5B-C6B-O6B
37	H	102	DGD	O6E-C5E-C6E-O5E
24	B	616	CLA	C8-C10-C11-C12
24	B	615	CLA	C10-C11-C12-C13
24	b	624	CLA	C10-C11-C12-C13
38	d	410	LHG	C25-C26-C27-C28
34	Z	101	LMG	C10-C11-C12-C13
24	c	505	CLA	CBD-CGD-O2D-CED
29	M	102	LMT	O5'-C5'-C6'-O6'
24	b	615	CLA	C10-C11-C12-C13
24	b	615	CLA	C13-C15-C16-C17
24	B	615	CLA	C5-C6-C7-C8
24	c	513	CLA	C13-C15-C16-C17
24	A	409	CLA	C13-C15-C16-C17
28	B	629	GOL	O2-C2-C3-O3
28	a	402	GOL	O1-C1-C2-O2
37	C	517	DGD	C1B-C2B-C3B-C4B
34	k	101	LMG	C10-C11-C12-C13
27	A	413	SQD	C23-C24-C25-C26
27	B	621	SQD	C7-C8-C9-C10
34	c	522	LMG	C10-C11-C12-C13
37	C	517	DGD	CBB-CCB-CDB-CEB
24	c	512	CLA	C15-C16-C17-C18
24	A	409	CLA	C10-C11-C12-C13
38	d	410	LHG	C24-C23-O8-C6
37	C	516	DGD	O6D-C5D-C6D-O5D
38	D	409	LHG	C23-C24-C25-C26
34	a	415	LMG	C10-C11-C12-C13
37	C	516	DGD	C2A-C3A-C4A-C5A
29	T	104	LMT	O1'-C1-C2-C3
29	m	102	LMT	C4'-C5'-C6'-O6'
24	d	405	CLA	C4-C3-C5-C6
36	B	624	HTG	C4-C5-C6-O6
24	b	615	CLA	C11-C10-C8-C7
24	b	615	CLA	C12-C13-C15-C16
24	B	616	CLA	C11-C12-C13-C15
24	a	410	CLA	C6-C7-C8-C10
38	b	634	LHG	C7-C8-C9-C10
24	c	517	CLA	C10-C11-C12-C13
24	b	623	CLA	C5-C6-C7-C8
24	b	623	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	M	102	LMT	C4B-C5B-C6B-O6B
37	H	102	DGD	C4E-C5E-C6E-O5E
38	D	410	LHG	C32-C33-C34-C35
29	e	102	LMT	O5'-C5'-C6'-O6'
24	a	410	CLA	C10-C11-C12-C13
32	a	416[A]	PL9	C9-C11-C12-C13
38	E	101	LHG	C23-C24-C25-C26
36	b	632	HTG	S1-C1'-C2'-C3'
24	c	515	CLA	O1D-CGD-O2D-CED
24	B	605	CLA	C3-C5-C6-C7
24	B	602	CLA	C10-C11-C12-C13
38	d	410	LHG	O10-C23-O8-C6
34	C	520	LMG	C4-C5-C6-O5
24	C	509	CLA	C13-C15-C16-C17
24	b	620	CLA	C8-C10-C11-C12
24	b	610	CLA	C8-C10-C11-C12
24	B	617	CLA	C10-C11-C12-C13
38	E	101	LHG	C3-O3-P-O6
38	d	409	LHG	C3-O3-P-O6
38	L	101	LHG	C4-O6-P-O3
38	b	634	LHG	C4-O6-P-O3
27	L	102	SQD	C24-C23-O48-C46
27	B	621	SQD	C24-C23-O48-C46
38	a	420	LHG	C11-C12-C13-C14
24	a	412	CLA	C15-C16-C17-C18
38	E	101	LHG	C7-C8-C9-C10
38	E	101	LHG	C1-C2-C3-O3
32	a	416[A]	PL9	C30-C29-C31-C32
24	b	622	CLA	C16-C17-C18-C19
37	C	518	DGD	C6B-C7B-C8B-C9B
27	F	101	SQD	C26-C27-C28-C29
37	C	516	DGD	C4B-C5B-C6B-C7B
37	e	101	DGD	C2A-C3A-C4A-C5A
34	k	101	LMG	C11-C10-O7-C8
24	C	506	CLA	C13-C15-C16-C17
36	b	632	HTG	C1'-C2'-C3'-C4'
34	M	101	LMG	C29-C30-C31-C32
37	c	519	DGD	C8B-C9B-CAB-CBB
37	C	517	DGD	C9A-CAA-CBA-CCA
34	C	519	LMG	C11-C12-C13-C14
37	D	408	DGD	C7A-C8A-C9A-CAA
27	A	411	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
38	d	410	LHG	C29-C30-C31-C32
37	e	101	DGD	C5A-C6A-C7A-C8A
24	b	610	CLA	C16-C17-C18-C20
37	C	516	DGD	C4D-C5D-C6D-O5D
37	C	518	DGD	CAA-CBA-CCA-CDA
37	c	520	DGD	C9A-CAA-CBA-CCA
29	M	104	LMT	C2-C3-C4-C5
34	k	101	LMG	O9-C10-O7-C8
34	C	519	LMG	C12-C13-C14-C15
34	k	101	LMG	C32-C33-C34-C35
34	A	419	LMG	C30-C31-C32-C33
27	a	414	SQD	C11-C12-C13-C14
37	e	101	DGD	O6D-C5D-C6D-O5D
37	C	518	DGD	O6E-C5E-C6E-O5E
37	e	101	DGD	O6E-C5E-C6E-O5E
27	a	405	SQD	C23-C24-C25-C26
37	C	517	DGD	C2E-C1E-O5D-C6D
37	c	520	DGD	C2E-C1E-O5D-C6D
29	M	104	LMT	C2'-C1'-O1'-C1
38	D	409	LHG	C11-C12-C13-C14
27	L	102	SQD	C29-C30-C31-C32
29	t	101	LMT	C3-C4-C5-C6
37	e	101	DGD	C8B-C9B-CAB-CBB
36	B	623	HTG	C2'-C3'-C4'-C5'
27	B	621	SQD	O10-C23-O48-C46
24	a	412	CLA	C16-C17-C18-C19
24	C	509	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	O1D-CGD-O2D-CED
32	d	407[B]	PL9	C15-C14-C16-C17
32	d	407[B]	PL9	C45-C44-C46-C47
32	d	407[A]	PL9	C45-C44-C46-C47
32	D	407[B]	PL9	C45-C44-C46-C47
37	c	519	DGD	CAB-CBB-CCB-CDB
38	b	634	LHG	C33-C34-C35-C36
32	a	416[A]	PL9	C18-C19-C21-C22
24	b	615	CLA	C14-C13-C15-C16
24	b	623	CLA	C11-C10-C8-C9
24	b	625	CLA	C11-C12-C13-C14
24	c	513	CLA	C14-C13-C15-C16
24	C	510	CLA	C6-C7-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	d	405	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	L	102	SQD	C32-C33-C34-C35
27	F	101	SQD	C34-C35-C36-C37
34	d	415	LMG	C16-C17-C18-C19
37	c	521	DGD	C7A-C8A-C9A-CAA
38	b	634	LHG	C11-C10-C9-C8
29	T	104	LMT	C11-C10-C9-C8
38	b	634	LHG	C27-C28-C29-C30
28	o	301	GOL	O1-C1-C2-C3
38	D	409	LHG	O1-C1-C2-C3
28	B	627	GOL	O1-C1-C2-C3
28	O	301	GOL	C1-C2-C3-O3
28	B	628	GOL	O1-C1-C2-C3
28	B	629	GOL	C1-C2-C3-O3
28	V	202	GOL	O1-C1-C2-C3
28	v	204	GOL	O1-C1-C2-C3
28	V	204	GOL	C1-C2-C3-O3
28	v	203	GOL	O1-C1-C2-C3
24	C	501	CLA	C15-C16-C17-C18
27	L	102	SQD	C14-C15-C16-C17
38	E	101	LHG	C24-C25-C26-C27
37	c	521	DGD	C6A-C7A-C8A-C9A
37	H	102	DGD	C7A-C8A-C9A-CAA
34	z	101	LMG	C12-C13-C14-C15
34	C	520	LMG	C14-C15-C16-C17
37	D	408	DGD	C2A-C3A-C4A-C5A
29	m	103	LMT	C2-C3-C4-C5
29	e	102	LMT	C4-C5-C6-C7
27	a	414	SQD	C15-C16-C17-C18
24	b	610	CLA	C16-C17-C18-C19
24	b	620	CLA	C16-C17-C18-C19
36	B	623	HTG	C4-C5-C6-O6
37	C	517	DGD	O6E-C1E-O5D-C6D
37	c	520	DGD	O6E-C1E-O5D-C6D
37	h	102	DGD	CAA-CBA-CCA-CDA
34	d	415	LMG	C38-C39-C40-C41
34	Z	101	LMG	C19-C20-C21-C22
38	D	409	LHG	C24-C25-C26-C27
38	a	420	LHG	C24-C25-C26-C27
34	d	415	LMG	C14-C15-C16-C17
27	a	414	SQD	C9-C10-C11-C12
29	T	104	LMT	C4-C5-C6-C7
38	L	101	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	C	516	DGD	C1B-C2B-C3B-C4B
27	L	102	SQD	O10-C23-O48-C46
29	t	101	LMT	C11-C10-C9-C8
36	b	631	HTG	C3'-C4'-C5'-C6'
34	a	415	LMG	C14-C15-C16-C17
29	M	104	LMT	C2-C1-O1'-C1'
37	c	519	DGD	C5A-C6A-C7A-C8A
36	b	607	HTG	C2'-C3'-C4'-C5'
24	a	409	CLA	CBD-CGD-O2D-CED
24	B	605	CLA	CBD-CGD-O2D-CED
34	z	101	LMG	C13-C14-C15-C16
37	c	519	DGD	C7B-C8B-C9B-CAB
32	D	407[A]	PL9	C15-C14-C16-C17
32	d	407[B]	PL9	C13-C14-C16-C17
32	D	407[B]	PL9	C43-C44-C46-C47
34	d	415	LMG	C35-C36-C37-C38
28	D	402	GOL	O2-C2-C3-O3
28	v	202	GOL	O1-C1-C2-O2
28	a	421	GOL	O1-C1-C2-O2
28	B	629	GOL	O1-C1-C2-O2
28	a	401	GOL	O2-C2-C3-O3
28	V	201	GOL	O2-C2-C3-O3
28	v	204	GOL	O1-C1-C2-O2
28	V	204	GOL	O2-C2-C3-O3
28	b	605	GOL	O1-C1-C2-O2
34	C	520	LMG	C28-C29-C30-C31
37	c	519	DGD	O6D-C5D-C6D-O5D
29	A	414	LMT	C6-C7-C8-C9
38	L	101	LHG	C12-C13-C14-C15
34	b	629	LMG	C38-C39-C40-C41
37	e	101	DGD	C2A-C1A-O1G-C1G
37	D	408	DGD	C6A-C7A-C8A-C9A
36	b	602	HTG	C3'-C4'-C5'-C6'
27	L	102	SQD	C28-C29-C30-C31
38	d	408	LHG	C25-C26-C27-C28
34	A	419	LMG	C14-C15-C16-C17
27	B	621	SQD	C11-C10-C9-C8
24	b	610	CLA	C2-C1-O2A-CGA
24	B	617	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
36	c	523	HTG	C1'-C2'-C3'-C4'
37	c	519	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
37	D	408	DGD	C8B-C9B-CAB-CBB
34	b	629	LMG	C37-C38-C39-C40
37	C	517	DGD	CAB-CBB-CCB-CDB
27	A	411	SQD	C13-C14-C15-C16
29	a	404	LMT	C7-C8-C9-C10
34	b	629	LMG	C30-C31-C32-C33
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	406	BCR	C23-C24-C25-C26
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
27	A	411	SQD	C15-C16-C17-C18
29	a	404	LMT	C2-C3-C4-C5
27	f	102	SQD	C24-C25-C26-C27
37	e	101	DGD	C7B-C8B-C9B-CAB
38	L	101	LHG	C13-C14-C15-C16
24	c	516	CLA	CBA-CGA-O2A-C1
24	b	615	CLA	C15-C16-C17-C18
24	b	613	CLA	C13-C15-C16-C17
24	b	610	CLA	C10-C11-C12-C13
24	A	407	CLA	C13-C15-C16-C17
24	c	513	CLA	C15-C16-C17-C18
34	d	415	LMG	C15-C16-C17-C18
36	b	631	HTG	C2'-C3'-C4'-C5'
37	c	521	DGD	CBB-CCB-CDB-CEB
24	B	610	CLA	C4-C3-C5-C6
32	d	407[B]	PL9	C43-C44-C46-C47
24	b	612	CLA	C6-C7-C8-C10
24	B	604	CLA	C6-C7-C8-C10
24	B	602	CLA	C11-C10-C8-C7
24	b	625	CLA	C11-C12-C13-C15
32	d	407[A]	PL9	C43-C44-C46-C47
24	c	513	CLA	C12-C13-C15-C16
32	D	407[A]	PL9	C13-C14-C16-C17
32	D	407[B]	PL9	C28-C29-C31-C32
24	B	610	CLA	C2-C3-C5-C6
24	C	506	CLA	C6-C7-C8-C10
37	e	101	DGD	O1A-C1A-O1G-C1G
37	C	517	DGD	C4B-C5B-C6B-C7B
24	a	412	CLA	C10-C11-C12-C13
24	B	616	CLA	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	501	CLA	O1D-CGD-O2D-CED
38	d	409	LHG	C24-C23-O8-C6
24	A	409	CLA	CBA-CGA-O2A-C1
37	C	516	DGD	C6A-C7A-C8A-C9A
34	C	519	LMG	C31-C32-C33-C34
27	a	414	SQD	C29-C30-C31-C32
37	C	516	DGD	C3B-C4B-C5B-C6B
37	C	517	DGD	C1A-C2A-C3A-C4A
24	a	410	CLA	O1D-CGD-O2D-CED
34	k	101	LMG	C36-C37-C38-C39
34	D	415	LMG	C19-C20-C21-C22
29	T	104	LMT	C1-C2-C3-C4
29	A	414	LMT	O1'-C1-C2-C3
29	C	521	LMT	O5B-C1B-O1B-C4'
24	c	515	CLA	CBA-CGA-O2A-C1
24	b	623	CLA	C10-C11-C12-C13
27	L	102	SQD	C35-C36-C37-C38
34	A	419	LMG	C39-C40-C41-C42
34	A	419	LMG	C10-C11-C12-C13
27	A	413	SQD	C24-C25-C26-C27
24	B	602	CLA	C8-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
24	b	612	CLA	CBD-CGD-O2D-CED
34	A	419	LMG	C13-C14-C15-C16
37	H	102	DGD	C7B-C8B-C9B-CAB
37	C	516	DGD	C2E-C1E-O5D-C6D
24	B	614	CLA	C13-C15-C16-C17
27	L	102	SQD	C10-C11-C12-C13
24	A	406	CLA	C2C-C3C-CAC-CBC
27	L	102	SQD	C13-C14-C15-C16
29	C	521	LMT	O5'-C5'-C6'-O6'
25	a	411	PHO	C4-C3-C5-C6
32	D	407[A]	PL9	C45-C44-C46-C47
29	b	630	LMT	C3'-C4'-O1B-C1B
25	a	411	PHO	C2-C3-C5-C6
24	d	405	CLA	C2-C3-C5-C6
32	A	417[A]	PL9	C4-C3-C7-C8
32	a	416[A]	PL9	C4-C3-C7-C8
32	a	416[B]	PL9	C4-C3-C7-C8
32	A	417[B]	PL9	C4-C3-C7-C8
24	b	615	CLA	C11-C10-C8-C9
24	b	612	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C6-C7-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C9
24	b	623	CLA	C11-C12-C13-C14
24	C	501	CLA	C14-C13-C15-C16
24	a	410	CLA	C6-C7-C8-C9
24	B	611	CLA	C2A-CAA-CBA-CGA
24	b	612	CLA	C5-C6-C7-C8
38	D	409	LHG	C34-C35-C36-C37
24	c	516	CLA	O1A-CGA-O2A-C1
38	d	409	LHG	O10-C23-O8-C6
24	A	409	CLA	O1A-CGA-O2A-C1
24	b	622	CLA	C16-C17-C18-C20
24	B	616	CLA	C16-C17-C18-C20
24	a	412	CLA	C16-C17-C18-C20
24	B	611	CLA	C16-C17-C18-C20
24	b	624	CLA	C16-C17-C18-C20
37	c	520	DGD	C3B-C4B-C5B-C6B
29	M	102	LMT	C1-C2-C3-C4
38	d	408	LHG	C4-O6-P-O3
38	D	410	LHG	C4-O6-P-O3
37	h	102	DGD	C6A-C7A-C8A-C9A
27	F	101	SQD	C30-C31-C32-C33
24	C	511	CLA	CBA-CGA-O2A-C1
27	a	405	SQD	C25-C26-C27-C28
37	D	408	DGD	C1B-C2B-C3B-C4B
37	c	519	DGD	O6E-C5E-C6E-O5E
38	d	408	LHG	C32-C33-C34-C35
24	b	613	CLA	O1D-CGD-O2D-CED
24	c	513	CLA	C3-C5-C6-C7
36	C	523	HTG	S1-C1'-C2'-C3'
29	m	103	LMT	C1-C2-C3-C4
36	b	602	HTG	C2'-C3'-C4'-C5'
24	C	509	CLA	C5-C6-C7-C8
34	C	520	LMG	C39-C40-C41-C42
37	c	520	DGD	C2A-C3A-C4A-C5A
27	a	414	SQD	C30-C31-C32-C33
24	c	515	CLA	O1A-CGA-O2A-C1
34	A	419	LMG	C36-C37-C38-C39
24	b	624	CLA	C16-C17-C18-C19
24	C	509	CLA	C3-C5-C6-C7
29	m	102	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
37	D	408	DGD	O1G-C1G-C2G-C3G
38	a	420	LHG	C4-C5-C6-O8
27	F	101	SQD	C44-C45-C46-O48
37	c	521	DGD	CBA-CCA-CDA-CEA
37	c	521	DGD	C7B-C8B-C9B-CAB
27	a	414	SQD	O6-C44-C45-C46
37	e	101	DGD	O1G-C1G-C2G-C3G
27	B	621	SQD	C44-C45-C46-O48
34	Z	101	LMG	C7-C8-C9-O8
27	a	405	SQD	O6-C44-C45-C46
24	c	507	CLA	C8-C10-C11-C12
37	c	520	DGD	C2G-C3G-O3G-C1D
37	c	520	DGD	C5D-C6D-O5D-C1E
34	b	629	LMG	C40-C41-C42-C43
34	A	419	LMG	O6-C5-C6-O5
24	b	612	CLA	C10-C11-C12-C13
36	b	607	HTG	C4'-C5'-C6'-C7'
37	e	101	DGD	C4D-C5D-C6D-O5D
34	C	520	LMG	C10-C11-C12-C13
24	C	511	CLA	O1A-CGA-O2A-C1
29	D	403	LMT	O1'-C1-C2-C3
34	A	419	LMG	C12-C13-C14-C15
24	C	503	CLA	C8-C10-C11-C12
37	D	408	DGD	C3B-C4B-C5B-C6B
37	C	516	DGD	O6E-C5E-C6E-O5E
28	V	202	GOL	O1-C1-C2-O2
28	b	604	GOL	O2-C2-C3-O3
28	c	502	GOL	O1-C1-C2-O2
34	a	415	LMG	C12-C13-C14-C15
36	c	524	HTG	C4-C5-C6-O6
24	A	409	CLA	C8-C10-C11-C12
27	a	414	SQD	C19-C20-C21-C22
29	m	103	LMT	C4'-C5'-C6'-O6'
24	a	409	CLA	C2C-C3C-CAC-CBC
25	d	402[B]	PHO	C2C-C3C-CAC-CBC
36	b	632	HTG	O5-C5-C6-O6
29	D	403	LMT	O5B-C5B-C6B-O6B
29	A	414	LMT	O5B-C5B-C6B-O6B
24	c	514	CLA	C4-C3-C5-C6
24	b	625	CLA	C4-C3-C5-C6
24	C	510	CLA	C4-C3-C5-C6
37	c	520	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
27	F	101	SQD	C7-C8-C9-C10
24	c	513	CLA	C16-C17-C18-C19
34	Z	101	LMG	O6-C5-C6-O5
24	c	510	CLA	C15-C16-C17-C18
24	b	617	CLA	C13-C15-C16-C17
29	e	102	LMT	C9-C10-C11-C12
34	d	415	LMG	O6-C5-C6-O5
29	M	104	LMT	O5B-C5B-C6B-O6B
34	D	415	LMG	O6-C5-C6-O5
24	D	405	CLA	C3-C5-C6-C7
38	L	101	LHG	C35-C36-C37-C38
37	C	517	DGD	C4A-C5A-C6A-C7A
27	A	411	SQD	C12-C13-C14-C15
27	F	101	SQD	C31-C32-C33-C34
24	A	409	CLA	C15-C16-C17-C18
38	D	411	LHG	O7-C5-C6-O8
38	E	101	LHG	O7-C5-C6-O8
27	f	102	SQD	O6-C44-C45-O47
34	a	415	LMG	O7-C8-C9-O8
34	Z	101	LMG	O1-C7-C8-O7
38	D	411	LHG	C29-C30-C31-C32
37	c	521	DGD	C6B-C7B-C8B-C9B
24	A	405	CLA	C13-C15-C16-C17
24	b	623	CLA	C15-C16-C17-C18
37	h	102	DGD	CDA-CEA-CFA-CGA
32	D	407[B]	PL9	C15-C14-C16-C17
24	D	404	CLA	C12-C13-C15-C16
24	B	615	CLA	C12-C13-C15-C16
24	c	514	CLA	C2-C3-C5-C6
24	b	623	CLA	C11-C12-C13-C15
24	C	512	CLA	C11-C10-C8-C7
24	C	501	CLA	C12-C13-C15-C16
24	A	409	CLA	C6-C7-C8-C10
24	C	510	CLA	C2-C3-C5-C6
37	h	102	DGD	O2G-C1B-C2B-C3B
24	b	612	CLA	C11-C10-C8-C9
24	c	514	CLA	C6-C7-C8-C9
24	B	605	CLA	C6-C7-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	A	409	CLA	C6-C7-C8-C9
24	B	602	CLA	C2A-CAA-CBA-CGA
37	h	102	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
37	c	520	DGD	C4A-C5A-C6A-C7A
37	c	519	DGD	C4D-C5D-C6D-O5D
26	b	626	BCR	C36-C18-C19-C20
26	K	101	BCR	C36-C18-C19-C20
24	c	510	CLA	C16-C17-C18-C19
29	t	101	LMT	C2-C3-C4-C5
29	M	102	LMT	C4'-C5'-C6'-O6'
24	B	615	CLA	CBA-CGA-O2A-C1
24	b	614	CLA	C8-C10-C11-C12
29	m	102	LMT	C11-C10-C9-C8
24	c	516	CLA	C15-C16-C17-C18
32	a	416[A]	PL9	C39-C41-C42-C43
34	k	101	LMG	C21-C22-C23-C24
27	A	413	SQD	C30-C31-C32-C33
27	B	621	SQD	C17-C18-C19-C20
34	a	415	LMG	C33-C34-C35-C36
34	b	629	LMG	C33-C34-C35-C36
24	C	507	CLA	C15-C16-C17-C18
24	C	501	CLA	C13-C15-C16-C17
24	B	616	CLA	C4-C3-C5-C6
25	A	408	PHO	C4-C3-C5-C6
24	B	616	CLA	C2-C3-C5-C6
25	A	408	PHO	C2-C3-C5-C6
24	b	625	CLA	C2-C3-C5-C6
34	A	419	LMG	C29-C30-C31-C32
24	c	505	CLA	O1D-CGD-O2D-CED
38	d	410	LHG	C33-C34-C35-C36
29	E	102	LMT	C2-C3-C4-C5
24	b	623	CLA	C16-C17-C18-C19
37	C	518	DGD	C2A-C1A-O1G-C1G
37	c	521	DGD	C2A-C1A-O1G-C1G
36	B	631	HTG	C4'-C5'-C6'-C7'
36	B	623	HTG	O5-C5-C6-O6
24	C	513	CLA	C3A-C2A-CAA-CBA
24	a	412	CLA	C3A-C2A-CAA-CBA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	610	CLA	C3A-C2A-CAA-CBA
34	M	101	LMG	C31-C32-C33-C34
29	b	630	LMT	C6-C7-C8-C9
27	f	102	SQD	C31-C32-C33-C34
36	B	624	HTG	C3'-C4'-C5'-C6'
37	c	521	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
38	L	101	LHG	C26-C27-C28-C29
34	a	415	LMG	C35-C36-C37-C38
34	C	519	LMG	C29-C28-O8-C9
24	b	610	CLA	CBA-CGA-O2A-C1
24	C	512	CLA	CBA-CGA-O2A-C1
37	c	519	DGD	C3A-C4A-C5A-C6A
34	k	101	LMG	C39-C40-C41-C42
24	C	504	CLA	C13-C15-C16-C17
38	D	411	LHG	C4-C5-C6-O8
34	k	101	LMG	C7-C8-C9-O8
27	L	102	SQD	C44-C45-C46-O48
38	E	101	LHG	C4-C5-C6-O8
34	a	415	LMG	C7-C8-C9-O8
27	a	405	SQD	C29-C30-C31-C32
37	e	101	DGD	C2B-C3B-C4B-C5B
24	B	615	CLA	O1A-CGA-O2A-C1
32	a	416[A]	PL9	C45-C44-C46-C47
32	a	416[A]	PL9	C28-C29-C31-C32
37	c	520	DGD	C6A-C7A-C8A-C9A
24	c	514	CLA	C8-C10-C11-C12
38	D	411	LHG	C12-C13-C14-C15
38	D	409	LHG	O1-C1-C2-O2
28	B	628	GOL	O1-C1-C2-O2
38	b	634	LHG	O1-C1-C2-O2
37	C	518	DGD	C9A-CAA-CBA-CCA
24	b	625	CLA	C16-C17-C18-C19
24	c	513	CLA	C16-C17-C18-C20
24	B	614	CLA	C10-C11-C12-C13
29	m	102	LMT	C5-C6-C7-C8
27	a	405	SQD	C28-C29-C30-C31
34	z	101	LMG	C15-C16-C17-C18
37	D	408	DGD	O2G-C2G-C3G-O3G
27	L	102	SQD	O47-C45-C46-O48
27	F	101	SQD	O47-C45-C46-O48
27	a	414	SQD	O6-C44-C45-O47
27	B	621	SQD	O47-C45-C46-O48
37	c	521	DGD	C5B-C6B-C7B-C8B
27	B	621	SQD	C19-C20-C21-C22
29	M	102	LMT	O5'-C1'-O1'-C1
37	C	516	DGD	O6E-C1E-O5D-C6D
24	A	405	CLA	C15-C16-C17-C18
24	B	607	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	D	407[B]	PL9	C9-C11-C12-C13
29	M	104	LMT	C2B-C1B-O1B-C4'
37	c	519	DGD	CCA-CDA-CEA-CFA
38	d	410	LHG	C35-C36-C37-C38
24	C	510	CLA	C2-C1-O2A-CGA
24	b	623	CLA	O1D-CGD-O2D-CED
34	b	629	LMG	C17-C18-C19-C20
24	B	616	CLA	C14-C13-C15-C16
24	b	618	CLA	C6-C7-C8-C9
24	c	513	CLA	C6-C7-C8-C9
24	a	410	CLA	C11-C10-C8-C9
27	f	102	SQD	C25-C26-C27-C28
32	A	417[A]	PL9	C2-C3-C7-C8
24	D	405	CLA	C8-C10-C11-C12
24	b	623	CLA	C16-C17-C18-C20
26	H	101	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
26	c	518	BCR	C1-C6-C7-C8
26	c	518	BCR	C5-C6-C7-C8
34	k	101	LMG	C20-C21-C22-C23
27	A	411	SQD	C18-C19-C20-C21
29	a	404	LMT	C3-C4-C5-C6
34	C	520	LMG	C29-C30-C31-C32
38	E	101	LHG	C25-C26-C27-C28
27	A	413	SQD	C11-C12-C13-C14
34	a	415	LMG	C29-C30-C31-C32
36	B	623	HTG	C4'-C5'-C6'-C7'
26	C	515	BCR	C21-C22-C23-C24
26	K	101	BCR	C17-C18-C19-C20
24	c	513	CLA	C10-C11-C12-C13
27	A	413	SQD	C7-C8-C9-C10
38	E	101	LHG	C8-C7-O7-C5
37	C	517	DGD	C8A-C9A-CAA-CBA
38	d	408	LHG	C33-C34-C35-C36
38	E	101	LHG	C19-C20-C21-C22
24	b	620	CLA	C16-C17-C18-C20
38	d	410	LHG	C11-C10-C9-C8
34	b	629	LMG	C39-C40-C41-C42
34	A	419	LMG	C11-C12-C13-C14
27	L	102	SQD	C33-C34-C35-C36
24	d	404	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
32	a	416[A]	PL9	C43-C44-C46-C47
24	b	612	CLA	C11-C10-C8-C7
24	c	510	CLA	C6-C7-C8-C10
24	c	514	CLA	C6-C7-C8-C10
24	b	610	CLA	C6-C7-C8-C10
24	B	617	CLA	C6-C7-C8-C10
24	B	605	CLA	C6-C7-C8-C10
24	c	513	CLA	C6-C7-C8-C10
24	C	501	CLA	C11-C12-C13-C15
24	a	410	CLA	C11-C10-C8-C7
24	C	505	CLA	C11-C12-C13-C15
34	b	629	LMG	C35-C36-C37-C38
26	h	101	BCR	C9-C10-C11-C12
37	C	517	DGD	C3B-C4B-C5B-C6B
38	D	411	LHG	C28-C29-C30-C31
24	b	615	CLA	C8-C10-C11-C12
24	C	509	CLA	C10-C11-C12-C13
24	d	405	CLA	C15-C16-C17-C18
27	A	411	SQD	C8-C7-O47-C45
38	L	101	LHG	C17-C18-C19-C20
24	A	406	CLA	C3-C5-C6-C7
27	f	102	SQD	C26-C27-C28-C29
24	C	510	CLA	CBA-CGA-O2A-C1
34	M	101	LMG	C16-C17-C18-C19
37	H	102	DGD	C5A-C6A-C7A-C8A
24	b	622	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
27	L	102	SQD	C46-C45-O47-C7
24	b	625	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
34	A	419	LMG	C32-C33-C34-C35
37	C	518	DGD	CDA-CEA-CFA-CGA
24	b	610	CLA	O1A-CGA-O2A-C1
32	A	417[A]	PL9	C15-C14-C16-C17
37	C	517	DGD	C8B-C9B-CAB-CBB
29	D	403	LMT	O5'-C1'-O1'-C1
34	A	419	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
32	D	407[B]	PL9	C13-C14-C16-C17
32	D	407[A]	PL9	C9-C11-C12-C13
34	z	101	LMG	O1-C7-C8-C9
27	A	413	SQD	O6-C44-C45-C46
34	a	415	LMG	C31-C32-C33-C34
37	h	102	DGD	CCA-CDA-CEA-CFA
29	a	419	LMT	C6-C7-C8-C9
38	d	408	LHG	C29-C30-C31-C32
27	a	414	SQD	C33-C34-C35-C36
24	a	409	CLA	O1D-CGD-O2D-CED
38	E	101	LHG	O9-C7-O7-C5
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
24	B	608	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O1D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	c	516	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
34	C	519	LMG	O10-C28-O8-C9
34	D	415	LMG	C13-C14-C15-C16
29	D	403	LMT	C2'-C1'-O1'-C1
34	A	419	LMG	O1-C7-C8-O7
34	Z	101	LMG	O7-C8-C9-O8
37	C	518	DGD	O1A-C1A-O1G-C1G
24	C	512	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	O1A-CGA-O2A-C1
38	D	410	LHG	C13-C14-C15-C16
27	a	405	SQD	C31-C32-C33-C34
24	c	510	CLA	C16-C17-C18-C20
28	V	204	GOL	O1-C1-C2-O2
28	C	524	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
24	b	625	CLA	C10-C11-C12-C13
38	D	409	LHG	C25-C26-C27-C28
27	A	411	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	c	521	DGD	O1A-C1A-O1G-C1G
32	A	417[A]	PL9	C13-C14-C16-C17
34	C	520	LMG	C13-C14-C15-C16
27	A	411	SQD	O49-C7-O47-C45
24	D	405	CLA	C11-C10-C8-C9
24	b	610	CLA	C6-C7-C8-C9
24	A	407	CLA	C11-C10-C8-C9
24	B	610	CLA	C6-C7-C8-C9
24	c	514	CLA	O1A-CGA-O2A-C1
29	M	102	LMT	C11-C10-C9-C8
27	B	621	SQD	C14-C15-C16-C17
27	F	101	SQD	C5-C6-S-O8
27	a	414	SQD	C5-C6-S-O8
24	B	602	CLA	C16-C17-C18-C20
29	e	102	LMT	C2B-C1B-O1B-C4'
37	e	101	DGD	C3A-C4A-C5A-C6A
26	H	101	BCR	C7-C8-C9-C34
26	c	518	BCR	C7-C8-C9-C34
27	a	414	SQD	C34-C35-C36-C37
28	v	201	GOL	O1-C1-C2-C3
28	V	204	GOL	O1-C1-C2-C3
29	m	103	LMT	O1'-C1-C2-C3
26	H	101	BCR	C7-C8-C9-C10
36	V	206	HTG	C4-C5-C6-O6
37	D	408	DGD	C4B-C5B-C6B-C7B
27	a	414	SQD	C17-C18-C19-C20
27	a	405	SQD	C24-C25-C26-C27
24	c	510	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	c	515	CLA	C1A-C2A-CAA-CBA
24	C	501	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	b	619	CLA	C16-C17-C18-C20
24	B	604	CLA	C5-C6-C7-C8
24	a	409	CLA	C4C-C3C-CAC-CBC
26	T	103	BCR	C13-C14-C15-C16
26	t	102	BCR	C13-C14-C15-C16
38	D	409	LHG	C4-O6-P-O3
34	Z	101	LMG	C13-C14-C15-C16
37	D	408	DGD	C2B-C3B-C4B-C5B
38	D	411	LHG	C2-C3-O3-P
38	d	410	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
32	D	407[A]	PL9	C43-C44-C46-C47
38	d	408	LHG	C4-O6-P-O4
38	E	101	LHG	C3-O3-P-O5
38	D	410	LHG	C4-O6-P-O5
38	L	101	LHG	C4-O6-P-O5
38	b	634	LHG	C4-O6-P-O5
24	b	619	CLA	C16-C17-C18-C19
38	L	101	LHG	C23-C24-C25-C26
38	L	101	LHG	O6-C4-C5-C6
38	b	634	LHG	O6-C4-C5-C6
32	a	416[A]	PL9	C14-C16-C17-C18
34	D	415	LMG	C34-C35-C36-C37
24	B	614	CLA	C15-C16-C17-C18
38	D	411	LHG	C10-C11-C12-C13
24	B	606	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
27	F	101	SQD	C5-C6-S-O9
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	602	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
27	B	621	SQD	C5-C6-S-O7
24	B	610	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
24	B	602	CLA	CAA-CBA-CGA-O2A
38	d	410	LHG	C24-C25-C26-C27
27	a	414	SQD	C35-C36-C37-C38
37	e	101	DGD	CAB-CBB-CCB-CDB
38	D	409	LHG	C33-C34-C35-C36
24	c	514	CLA	CBA-CGA-O2A-C1
37	C	517	DGD	CCA-CDA-CEA-CFA
24	B	616	CLA	C12-C13-C15-C16
24	c	510	CLA	C11-C10-C8-C7
38	a	420	LHG	C23-C24-C25-C26
24	b	625	CLA	C12-C13-C15-C16
24	A	407	CLA	C11-C10-C8-C7
24	C	505	CLA	C12-C13-C15-C16
24	C	506	CLA	C12-C13-C15-C16
37	h	102	DGD	C9B-CAB-CBB-CCB
24	C	509	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	m	103	LMT	C3-C4-C5-C6
34	M	101	LMG	C33-C34-C35-C36
34	D	415	LMG	C30-C31-C32-C33
34	D	415	LMG	C20-C21-C22-C23
37	D	408	DGD	C1G-C2G-C3G-O3G
27	L	102	SQD	C31-C32-C33-C34
34	A	419	LMG	O1-C7-C8-C9
37	e	101	DGD	CAA-CBA-CCA-CDA
34	Z	101	LMG	O1-C7-C8-C9
24	B	613	CLA	CBD-CGD-O2D-CED
34	k	101	LMG	O1-C7-C8-O7
34	k	101	LMG	O7-C8-C9-O8
38	a	420	LHG	O7-C5-C6-O8
37	e	101	DGD	O1G-C1G-C2G-O2G
27	a	405	SQD	C27-C28-C29-C30
37	C	517	DGD	C5D-C6D-O5D-C1E
24	c	508	CLA	C15-C16-C17-C18
27	a	414	SQD	C27-C28-C29-C30
24	b	614	CLA	O1A-CGA-O2A-C1
32	A	417[B]	PL9	C15-C14-C16-C17
38	d	408	LHG	C11-C10-C9-C8
29	T	104	LMT	C7-C8-C9-C10
24	B	616	CLA	C11-C12-C13-C14
24	B	615	CLA	C6-C7-C8-C9
24	c	510	CLA	C11-C10-C8-C9
24	a	410	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	A	405	CLA	CBD-CGD-O2D-CED
38	d	408	LHG	C26-C27-C28-C29
37	c	520	DGD	C2B-C3B-C4B-C5B
36	c	524	HTG	O5-C5-C6-O6
34	a	415	LMG	C21-C22-C23-C24
27	B	621	SQD	C31-C32-C33-C34
37	c	520	DGD	C5B-C6B-C7B-C8B
38	d	409	LHG	O2-C2-C3-O3
34	D	415	LMG	C16-C17-C18-C19
38	d	410	LHG	C30-C31-C32-C33
24	b	610	CLA	CAA-CBA-CGA-O2A
34	d	415	LMG	C29-C30-C31-C32
34	a	415	LMG	C30-C31-C32-C33
24	C	503	CLA	C5-C6-C7-C8
34	M	101	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C46-C45-O47-C7
24	B	603	CLA	C2A-CAA-CBA-CGA
37	e	101	DGD	C4A-C5A-C6A-C7A
34	c	522	LMG	O9-C10-O7-C8
24	d	404	CLA	C2-C1-O2A-CGA
24	c	516	CLA	C2-C1-O2A-CGA
24	b	622	CLA	O1D-CGD-O2D-CED
24	C	508	CLA	C3-C5-C6-C7
27	A	413	SQD	C15-C16-C17-C18
27	f	102	SQD	C30-C31-C32-C33
27	A	413	SQD	C24-C23-O48-C46
27	A	413	SQD	O10-C23-O48-C46
24	B	613	CLA	C8-C10-C11-C12
32	D	407[B]	PL9	C30-C29-C31-C32
37	C	517	DGD	C5A-C6A-C7A-C8A
24	b	611	CLA	C16-C17-C18-C19
34	c	522	LMG	C11-C10-O7-C8
37	c	519	DGD	O6E-C1E-O5D-C6D
29	m	102	LMT	O5'-C1'-O1'-C1
29	m	103	LMT	O5'-C1'-O1'-C1
29	M	102	LMT	C2'-C1'-O1'-C1
32	a	416[B]	PL9	C14-C16-C17-C18
32	A	417[B]	PL9	C19-C21-C22-C23
34	A	419	LMG	C2-C1-O1-C7
24	d	403	CLA	C2C-C3C-CAC-CBC
34	z	101	LMG	O1-C7-C8-O7
34	c	522	LMG	O7-C8-C9-O8
38	a	420	LHG	C4-O6-P-O3
38	D	410	LHG	C3-O3-P-O6
36	B	622	HTG	C4'-C5'-C6'-C7'
29	e	102	LMT	C5-C6-C7-C8
27	B	621	SQD	C15-C16-C17-C18
37	H	102	DGD	C6B-C7B-C8B-C9B
34	k	101	LMG	O1-C7-C8-C9
27	f	102	SQD	O6-C44-C45-C46
32	d	407[B]	PL9	C18-C19-C21-C22
24	b	610	CLA	C11-C10-C8-C7
32	A	417[B]	PL9	C43-C44-C46-C47
24	C	510	CLA	C6-C7-C8-C10
34	C	519	LMG	C29-C30-C31-C32
29	D	403	LMT	C5-C6-C7-C8
24	d	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	625	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
29	m	102	LMT	C1-C2-C3-C4
38	a	420	LHG	C14-C15-C16-C17
24	b	614	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C9-C10-C11-C12
27	A	413	SQD	C26-C27-C28-C29
24	B	602	CLA	C16-C17-C18-C19
37	C	517	DGD	C3A-C4A-C5A-C6A
24	C	510	CLA	C8-C10-C11-C12
37	C	518	DGD	C8A-C9A-CAA-CBA
37	c	520	DGD	C3A-C4A-C5A-C6A
32	a	416[B]	PL9	C12-C11-C9-C8
34	C	519	LMG	C16-C17-C18-C19
37	C	518	DGD	C3B-C4B-C5B-C6B
24	c	510	CLA	C13-C15-C16-C17
24	c	507	CLA	C5-C6-C7-C8
25	a	411	PHO	C2C-C3C-CAC-CBC
24	c	505	CLA	C2A-CAA-CBA-CGA
27	A	413	SQD	O5-C1-O6-C44
32	A	417[A]	PL9	C19-C21-C22-C23
37	e	101	DGD	CCA-CDA-CEA-CFA
34	b	629	LMG	C16-C17-C18-C19
24	b	625	CLA	C16-C17-C18-C20
32	d	407[A]	PL9	C30-C29-C31-C32
32	d	407[A]	PL9	C28-C29-C31-C32
37	C	516	DGD	C7B-C8B-C9B-CAB
27	F	101	SQD	C32-C33-C34-C35
34	z	101	LMG	C16-C17-C18-C19
24	A	406	CLA	C4C-C3C-CAC-CBC
24	b	622	CLA	C2-C1-O2A-CGA
24	B	606	CLA	C10-C11-C12-C13
34	C	520	LMG	C15-C16-C17-C18
27	a	414	SQD	C16-C17-C18-C19
37	c	519	DGD	C2E-C1E-O5D-C6D
34	d	415	LMG	C36-C37-C38-C39
27	L	102	SQD	O6-C44-C45-O47
24	c	511	CLA	C2A-CAA-CBA-CGA
38	d	410	LHG	O7-C5-C6-O8
34	M	101	LMG	C20-C21-C22-C23
34	C	520	LMG	C37-C38-C39-C40
24	C	502	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
37	D	408	DGD	C4A-C5A-C6A-C7A
32	A	417[A]	PL9	C45-C44-C46-C47
37	H	102	DGD	O2G-C1B-C2B-C3B
24	B	602	CLA	C14-C13-C15-C16
24	C	504	CLA	C11-C12-C13-C14
24	b	619	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16
38	D	409	LHG	C27-C28-C29-C30
38	d	410	LHG	C9-C10-C11-C12
36	b	607	HTG	C3'-C4'-C5'-C6'
29	D	403	LMT	C2-C3-C4-C5
36	d	413	HTG	C1'-C2'-C3'-C4'
36	B	623	HTG	C1'-C2'-C3'-C4'
38	D	409	LHG	C28-C29-C30-C31
34	D	415	LMG	C14-C15-C16-C17
29	C	521	LMT	C5'-C4'-O1B-C1B
29	T	104	LMT	C4'-C5'-C6'-O6'
29	e	102	LMT	O5B-C1B-O1B-C4'
29	M	104	LMT	O5B-C1B-O1B-C4'
34	M	101	LMG	C7-C8-O7-C10
32	A	417[B]	PL9	C45-C44-C46-C47
37	c	519	DGD	C2A-C3A-C4A-C5A
24	D	405	CLA	C11-C10-C8-C7
24	C	504	CLA	C12-C13-C15-C16
27	A	411	SQD	C16-C17-C18-C19
29	m	102	LMT	O1'-C1-C2-C3
29	D	403	LMT	C4-C5-C6-C7
34	c	522	LMG	C31-C32-C33-C34
27	A	413	SQD	C25-C26-C27-C28
27	B	621	SQD	C35-C36-C37-C38
24	b	623	CLA	C2A-CAA-CBA-CGA
24	b	619	CLA	C2A-CAA-CBA-CGA
24	B	612	CLA	C10-C11-C12-C13
24	C	508	CLA	C5-C6-C7-C8
38	b	634	LHG	O6-C4-C5-O7
29	C	521	LMT	C4B-C5B-C6B-O6B
38	E	101	LHG	C15-C16-C17-C18
38	d	408	LHG	C34-C35-C36-C37
29	M	102	LMT	C7-C8-C9-C10
37	C	517	DGD	C7B-C8B-C9B-CAB
24	c	506	CLA	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	c	517	CLA	C4-C3-C5-C6
24	a	412	CLA	C4-C3-C5-C6
32	D	407[B]	PL9	C35-C34-C36-C37
24	a	409	CLA	C13-C15-C16-C17
27	A	413	SQD	C2-C1-O6-C44
27	F	101	SQD	O6-C44-C45-O47
27	A	411	SQD	C7-C8-C9-C10
36	C	522	HTG	C1'-C2'-C3'-C4'
24	C	507	CLA	C2A-CAA-CBA-CGA
34	a	415	LMG	C19-C20-C21-C22
38	E	101	LHG	C10-C11-C12-C13
27	B	621	SQD	C32-C33-C34-C35
29	T	104	LMT	O5'-C5'-C6'-O6'
24	c	511	CLA	C5-C6-C7-C8
29	a	404	LMT	C6-C7-C8-C9
24	c	517	CLA	C2-C1-O2A-CGA
24	B	614	CLA	C2-C1-O2A-CGA
24	b	623	CLA	C2-C1-O2A-CGA
24	c	515	CLA	C2-C1-O2A-CGA
32	A	417[A]	PL9	C43-C44-C46-C47
37	C	516	DGD	O2G-C1B-C2B-C3B
24	B	606	CLA	O1A-CGA-O2A-C1
29	a	404	LMT	C9-C10-C11-C12
38	d	410	LHG	C31-C32-C33-C34
26	c	526	BCR	C1-C6-C7-C8
26	b	627	BCR	C23-C24-C25-C30
26	H	101	BCR	C23-C24-C25-C30
26	C	514	BCR	C1-C6-C7-C8
26	b	626	BCR	C1-C6-C7-C8
26	Y	101	BCR	C23-C24-C25-C26
26	Y	101	BCR	C23-C24-C25-C30
34	M	101	LMG	C36-C37-C38-C39
34	a	415	LMG	O8-C28-C29-C30
29	e	102	LMT	C1-C2-C3-C4
38	a	420	LHG	O1-C1-C2-C3
28	C	525	GOL	O1-C1-C2-C3
38	E	101	LHG	C16-C17-C18-C19
24	C	513	CLA	C4-C3-C5-C6
32	a	416[B]	PL9	C45-C44-C46-C47
24	b	610	CLA	C4-C3-C5-C6
26	c	518	BCR	C7-C8-C9-C10
24	A	407	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	C	516	DGD	C5B-C6B-C7B-C8B
24	c	517	CLA	C2-C3-C5-C6
24	a	412	CLA	C2-C3-C5-C6
32	A	417[B]	PL9	C13-C14-C16-C17
37	c	519	DGD	C5D-C6D-O5D-C1E
34	C	520	LMG	C8-C7-O1-C1
37	H	102	DGD	C8A-C9A-CAA-CBA
24	A	405	CLA	C16-C17-C18-C19
29	M	102	LMT	C5-C6-C7-C8
24	b	622	CLA	CBD-CGD-O2D-CED
29	t	101	LMT	C4-C5-C6-C7
24	B	608	CLA	C2A-CAA-CBA-CGA
37	C	518	DGD	CBA-CCA-CDA-CEA
24	C	513	CLA	C3-C5-C6-C7
34	a	415	LMG	C22-C23-C24-C25
24	C	508	CLA	C13-C15-C16-C17
32	A	417[A]	PL9	C20-C19-C21-C22
32	A	417[A]	PL9	C40-C39-C41-C42
32	A	417[B]	PL9	C30-C29-C31-C32
32	A	417[A]	PL9	C9-C11-C12-C13
24	B	614	CLA	C12-C13-C15-C16
27	a	405	SQD	C24-C23-O48-C46
28	D	402	GOL	O1-C1-C2-O2
28	O	301	GOL	O2-C2-C3-O3
28	C	525	GOL	O1-C1-C2-O2
36	C	523	HTG	C4-C5-C6-O6
38	b	634	LHG	C23-C24-C25-C26
38	d	409	LHG	C35-C36-C37-C38
29	m	102	LMT	C2'-C1'-O1'-C1
29	m	103	LMT	C2'-C1'-O1'-C1
37	D	408	DGD	O1G-C1G-C2G-O2G
38	d	409	LHG	O7-C5-C6-O8
37	h	102	DGD	O1B-C1B-C2B-C3B
37	c	520	DGD	O2G-C1B-C2B-C3B
24	C	512	CLA	CAA-CBA-CGA-O2A
37	h	102	DGD	C9A-CAA-CBA-CCA
36	b	602	HTG	C1'-C2'-C3'-C4'
32	d	407[B]	PL9	C35-C34-C36-C37
32	A	417[A]	PL9	C30-C29-C31-C32
32	a	416[B]	PL9	C43-C44-C46-C47
37	c	520	DGD	C8A-C9A-CAA-CBA
24	C	509	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	C	510	CLA	CAA-CBA-CGA-O2A
24	D	404	CLA	C14-C13-C15-C16
24	b	625	CLA	C6-C7-C8-C9
34	c	522	LMG	C37-C38-C39-C40
24	b	624	CLA	C13-C15-C16-C17
37	D	408	DGD	C9B-CAB-CBB-CCB
34	c	522	LMG	C34-C35-C36-C37
24	b	618	CLA	C3A-C2A-CAA-CBA
24	A	407	CLA	C3A-C2A-CAA-CBA
27	a	405	SQD	O10-C23-O48-C46
24	b	612	CLA	CAD-CBD-CGD-O2D
24	B	604	CLA	CAD-CBD-CGD-O2D
24	b	621	CLA	CAD-CBD-CGD-O2D
25	A	408	PHO	CAD-CBD-CGD-O2D
25	a	411	PHO	CAD-CBD-CGD-O2D
24	C	503	CLA	CAD-CBD-CGD-O2D
24	b	623	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CAD-CBD-CGD-O2D
24	C	505	CLA	CAD-CBD-CGD-O2D
29	A	414	LMT	C11-C10-C9-C8
34	d	415	LMG	C17-C18-C19-C20
24	d	403	CLA	C13-C15-C16-C17
25	d	402[B]	PHO	C8-C10-C11-C12
24	C	513	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA
38	a	420	LHG	O8-C23-C24-C25
27	f	102	SQD	O47-C7-C8-C9
32	D	407[A]	PL9	C35-C34-C36-C37
26	t	102	BCR	C11-C12-C13-C14
26	k	102	BCR	C17-C18-C19-C20
26	b	626	BCR	C17-C18-C19-C20
34	a	415	LMG	O6-C5-C6-O5
38	a	420	LHG	C13-C14-C15-C16
37	C	516	DGD	C1G-C2G-C3G-O3G
27	A	411	SQD	C11-C10-C9-C8
24	C	501	CLA	C16-C17-C18-C20
24	B	614	CLA	O2A-C1-C2-C3
24	b	622	CLA	O2A-C1-C2-C3
25	a	411	PHO	O2A-C1-C2-C3
24	b	613	CLA	O2A-C1-C2-C3
24	d	405	CLA	O2A-C1-C2-C3
24	C	513	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
38	D	411	LHG	C17-C18-C19-C20
34	a	415	LMG	C18-C19-C20-C21
24	b	611	CLA	C16-C17-C18-C20
24	B	606	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
25	D	401[A]	PHO	CHA-CBD-CGD-O1D
25	D	401[A]	PHO	CHA-CBD-CGD-O2D
25	D	401[B]	PHO	CHA-CBD-CGD-O1D
25	D	401[B]	PHO	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
25	d	402[A]	PHO	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
24	B	608	CLA	CHA-CBD-CGD-O2D
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	513	CLA	CHA-CBD-CGD-O1D
24	c	513	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O2D
25	d	402[B]	PHO	CHA-CBD-CGD-O1D
38	E	101	LHG	O8-C23-C24-C25
37	c	521	DGD	O1G-C1A-C2A-C3A
37	e	101	DGD	O2G-C1B-C2B-C3B
24	C	513	CLA	CBA-CGA-O2A-C1
29	D	403	LMT	O5B-C1B-O1B-C4'
37	C	517	DGD	C6B-C7B-C8B-C9B
37	c	520	DGD	C4B-C5B-C6B-C7B
38	d	409	LHG	C11-C10-C9-C8
38	L	101	LHG	O7-C7-C8-C9
27	L	102	SQD	C27-C28-C29-C30
24	B	602	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C3-C5-C6-C7
24	B	613	CLA	O1D-CGD-O2D-CED
37	C	517	DGD	O2G-C1B-C2B-C3B
38	a	420	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	CAA-CBA-CGA-O2A
37	D	408	DGD	CBA-CCA-CDA-CEA
24	b	620	CLA	C11-C12-C13-C15
24	c	513	CLA	C11-C10-C8-C7
24	a	410	CLA	C12-C13-C15-C16
29	E	102	LMT	C1-C2-C3-C4
24	C	506	CLA	C16-C17-C18-C20
24	b	622	CLA	CAA-CBA-CGA-O2A
24	c	516	CLA	CAA-CBA-CGA-O2A
34	A	419	LMG	O8-C28-C29-C30
34	Z	101	LMG	O7-C10-C11-C12
24	a	410	CLA	C11-C12-C13-C14
37	D	408	DGD	O1G-C1A-C2A-C3A
27	B	621	SQD	C5-C6-S-O8
27	f	102	SQD	C35-C36-C37-C38
24	B	615	CLA	C2A-CAA-CBA-CGA
32	a	416[B]	PL9	C26-C27-C28-C29
37	c	520	DGD	O1B-C1B-C2B-C3B
34	k	101	LMG	C35-C36-C37-C38
29	a	419	LMT	C7-C8-C9-C10
24	c	510	CLA	C4-C3-C5-C6
24	B	607	CLA	C4-C3-C5-C6
28	A	412	GOL	C1-C2-C3-O3
28	D	402	GOL	O1-C1-C2-C3
28	F	103	GOL	O1-C1-C2-C3
28	O	301	GOL	O1-C1-C2-C3
32	d	407[B]	PL9	C28-C29-C31-C32
32	A	417[A]	PL9	C28-C29-C31-C32
34	b	629	LMG	O8-C28-C29-C30
26	b	628	BCR	C11-C12-C13-C14
24	c	517	CLA	C1A-C2A-CAA-CBA
24	B	610	CLA	C1A-C2A-CAA-CBA
24	a	409	CLA	C16-C17-C18-C19
24	b	614	CLA	C16-C17-C18-C19
27	f	102	SQD	O49-C7-C8-C9
24	c	508	CLA	C2-C1-O2A-CGA
24	B	606	CLA	CBA-CGA-O2A-C1
27	A	413	SQD	C13-C14-C15-C16
27	L	102	SQD	O6-C44-C45-C46
37	H	102	DGD	CCA-CDA-CEA-CFA
38	D	409	LHG	C17-C18-C19-C20
24	d	403	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
37	D	408	DGD	O1A-C1A-C2A-C3A
24	C	512	CLA	CAA-CBA-CGA-O1A
34	Z	101	LMG	O9-C10-C11-C12
37	h	102	DGD	C7B-C8B-C9B-CAB
38	d	409	LHG	C26-C27-C28-C29
38	b	634	LHG	C31-C32-C33-C34
24	c	516	CLA	CAA-CBA-CGA-O1A
24	C	510	CLA	CAA-CBA-CGA-O1A
24	b	620	CLA	O1A-CGA-O2A-C1
38	D	409	LHG	C4-O6-P-O4
32	a	416[A]	PL9	C3-C7-C8-C9
38	D	411	LHG	C4-O6-P-O5
38	d	409	LHG	C4-O6-P-O5
24	b	612	CLA	O1D-CGD-O2D-CED
24	d	403	CLA	C4C-C3C-CAC-CBC
38	a	420	LHG	O10-C23-C24-C25
37	c	521	DGD	O1A-C1A-C2A-C3A
36	B	622	HTG	S1-C1'-C2'-C3'
26	H	101	BCR	C23-C24-C25-C26
26	t	102	BCR	C1-C6-C7-C8
26	t	102	BCR	C5-C6-C7-C8
29	C	521	LMT	C3-C4-C5-C6
24	b	622	CLA	C13-C15-C16-C17
38	L	101	LHG	O9-C7-C8-C9
24	d	403	CLA	C15-C16-C17-C18
29	D	403	LMT	C2B-C1B-O1B-C4'
24	C	513	CLA	C8-C10-C11-C12
34	M	101	LMG	C15-C16-C17-C18
37	c	520	DGD	C1A-C2A-C3A-C4A
26	H	101	BCR	C9-C10-C11-C12
32	a	416[B]	PL9	C21-C22-C23-C24
32	A	417[B]	PL9	C26-C27-C28-C29
24	d	403	CLA	CAD-CBD-CGD-O1D
24	b	618	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	O5-C5-C6-S
24	c	509	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	C3-C5-C6-C7
24	c	516	CLA	CAD-CBD-CGD-O1D
27	A	413	SQD	O5-C5-C6-S
24	C	506	CLA	CAD-CBD-CGD-O1D
34	M	101	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
38	d	410	LHG	C7-C8-C9-C10
37	C	517	DGD	O1B-C1B-C2B-C3B
37	e	101	DGD	O1B-C1B-C2B-C3B
24	d	403	CLA	C11-C10-C8-C9
24	C	504	CLA	C14-C13-C15-C16
24	c	508	CLA	C14-C13-C15-C16
28	o	301	GOL	O1-C1-C2-O2
25	d	402[B]	PHO	C4C-C3C-CAC-CBC
24	b	624	CLA	C5-C6-C7-C8
24	b	622	CLA	O1A-CGA-O2A-C1
34	C	519	LMG	O7-C10-C11-C12
38	b	634	LHG	O7-C7-C8-C9
38	d	410	LHG	C14-C15-C16-C17
34	k	101	LMG	O7-C10-C11-C12
38	d	410	LHG	O8-C23-C24-C25
24	C	505	CLA	CAA-CBA-CGA-O2A
37	c	519	DGD	CBA-CCA-CDA-CEA
37	C	518	DGD	C2B-C3B-C4B-C5B
34	A	419	LMG	C16-C17-C18-C19
29	M	104	LMT	O1'-C1-C2-C3
24	d	403	CLA	C11-C10-C8-C7
24	B	604	CLA	C11-C10-C8-C7
24	C	509	CLA	C11-C12-C13-C15
24	c	514	CLA	C12-C13-C15-C16
38	d	408	LHG	C7-C8-C9-C10
24	C	504	CLA	C11-C12-C13-C15
24	A	409	CLA	C12-C13-C15-C16
24	c	508	CLA	C12-C13-C15-C16
38	E	101	LHG	O10-C23-C24-C25
37	C	518	DGD	C8B-C9B-CAB-CBB
38	E	101	LHG	O7-C7-C8-C9
24	C	501	CLA	CAA-CBA-CGA-O2A
26	T	103	BCR	C11-C12-C13-C14
38	b	634	LHG	O9-C7-C8-C9
32	a	416[A]	PL9	C2-C3-C7-C8
29	t	101	LMT	C7-C8-C9-C10
37	c	521	DGD	C8A-C9A-CAA-CBA
24	c	506	CLA	C16-C17-C18-C20
29	m	102	LMT	C2-C1-O1'-C1'
24	c	509	CLA	CAA-CBA-CGA-O2A
38	d	408	LHG	O8-C23-C24-C25
34	M	101	LMG	O6-C1-O1-C7

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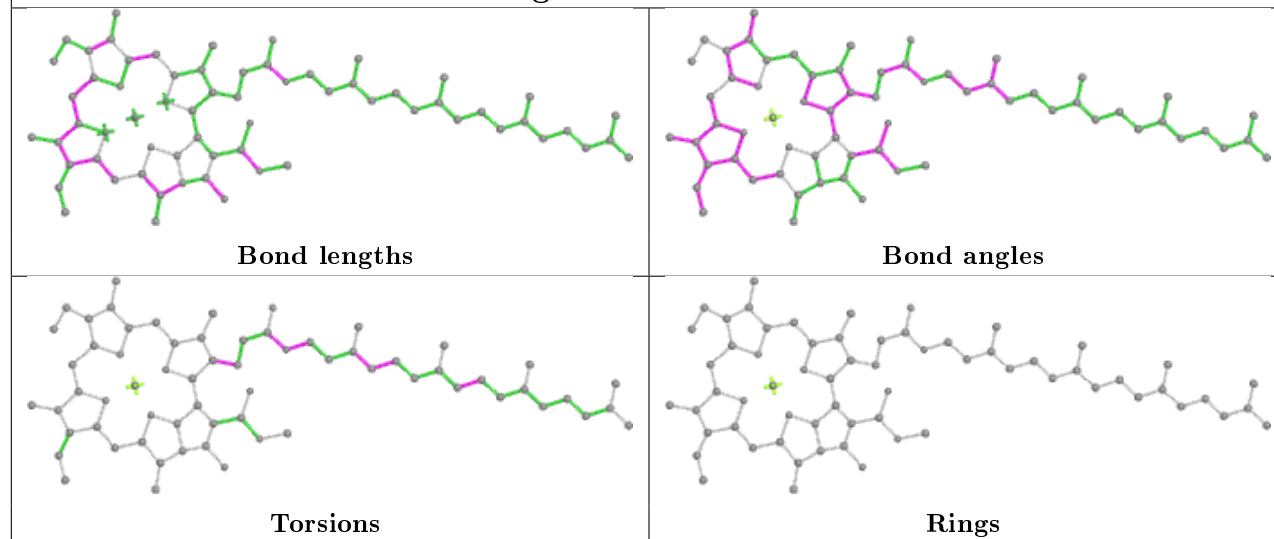
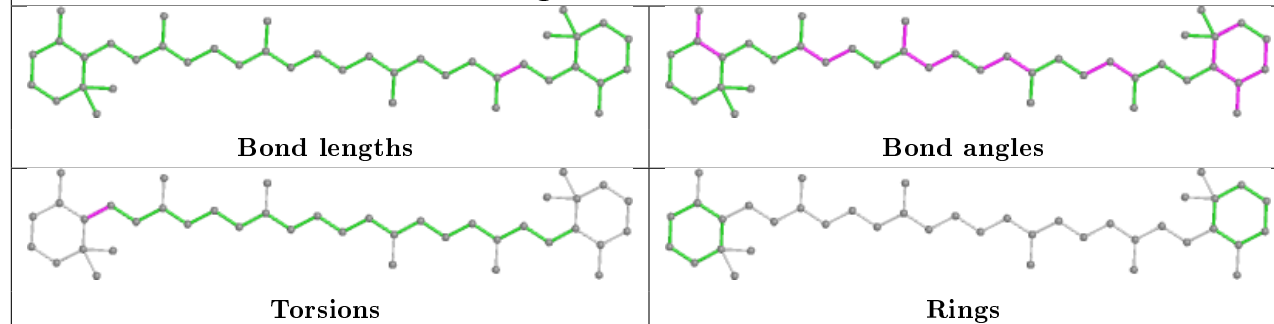
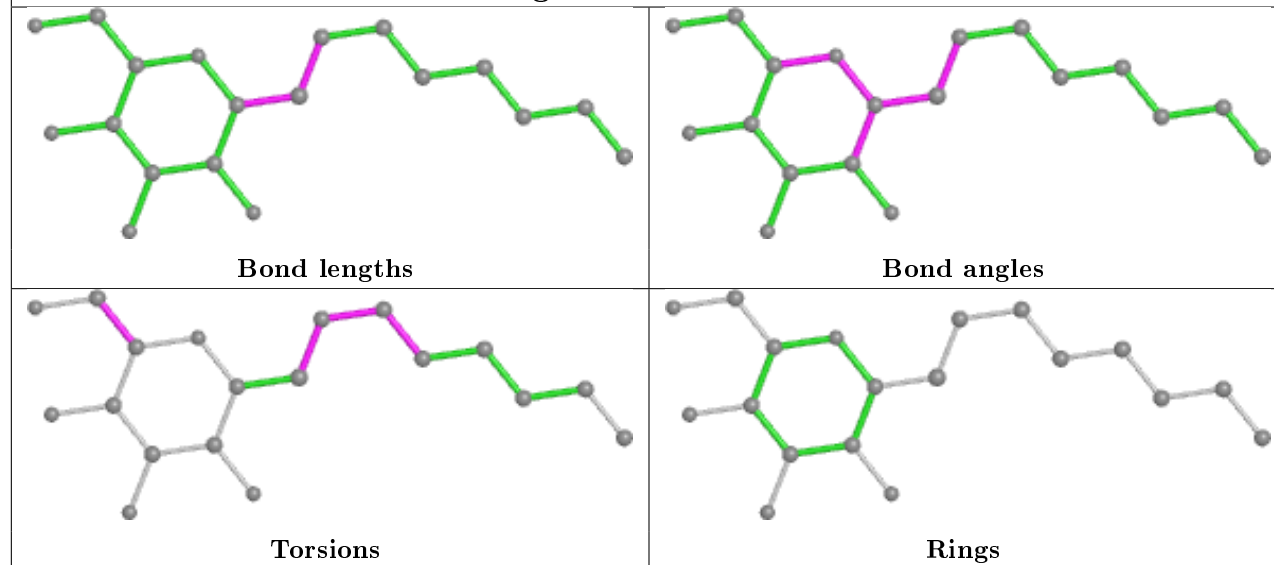
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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	CAA-CBA-CGA-O1A
24	b	622	CLA	CAA-CBA-CGA-O1A
24	c	509	CLA	CAA-CBA-CGA-O1A
34	b	629	LMG	O10-C28-C29-C30
24	b	620	CLA	CBA-CGA-O2A-C1
24	b	623	CLA	C8-C10-C11-C12
24	b	619	CLA	C5-C6-C7-C8
24	b	619	CLA	C15-C16-C17-C18
34	z	101	LMG	O8-C28-C29-C30
38	D	411	LHG	O8-C23-C24-C25
38	a	420	LHG	C15-C16-C17-C18
37	H	102	DGD	C5B-C6B-C7B-C8B
24	c	507	CLA	C15-C16-C17-C18
24	B	602	CLA	CBD-CGD-O2D-CED
38	d	408	LHG	O10-C23-C24-C25
24	b	612	CLA	C4-C3-C5-C6
34	M	101	LMG	O8-C28-C29-C30
24	B	615	CLA	CAA-CBA-CGA-O2A

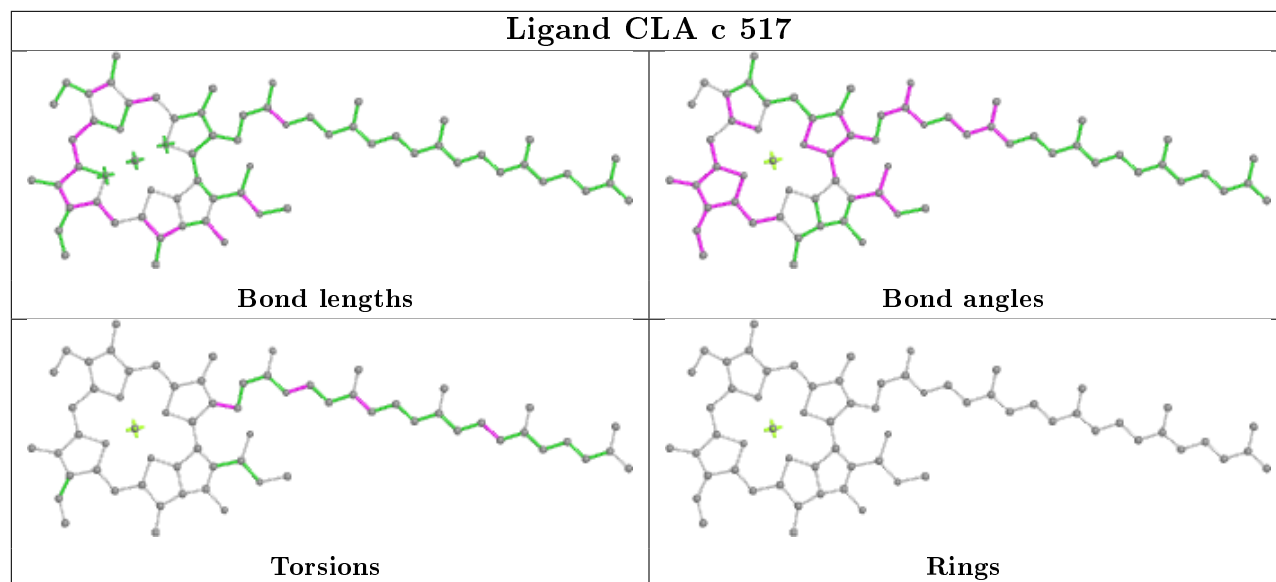
There are no ring outliers.

No monomer is involved in short contacts.

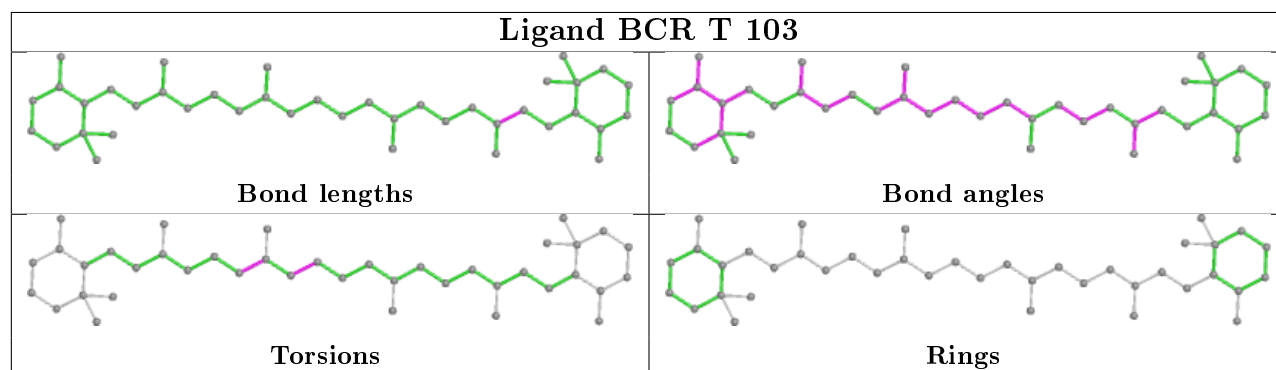
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA C 513**Ligand BCR c 526****Ligand HTG b 632**

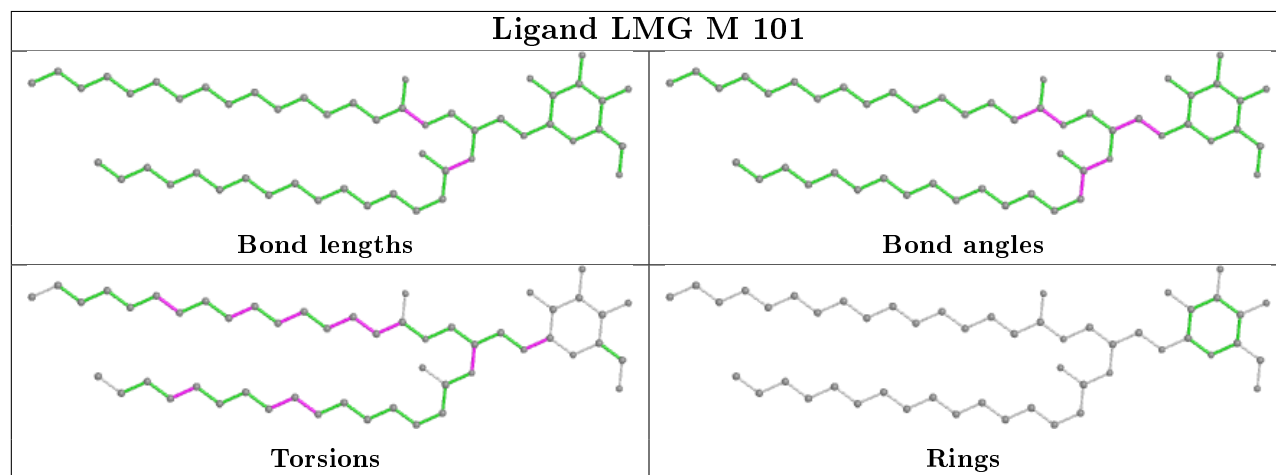
Ligand CLA c 517



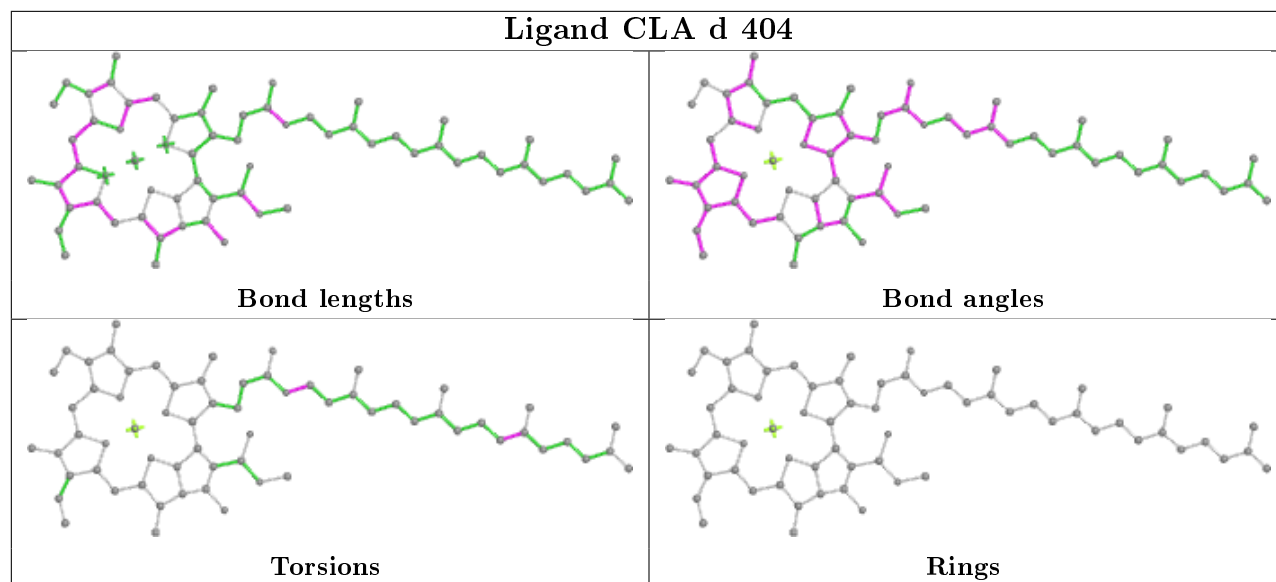
Ligand BCR T 103



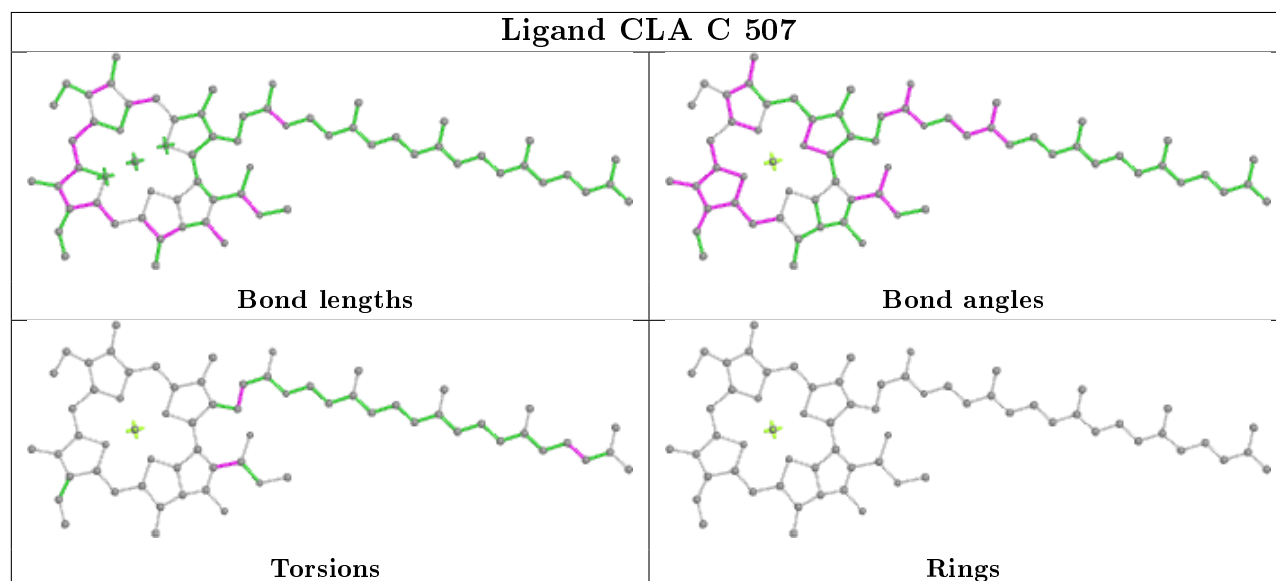
Ligand LMG M 101



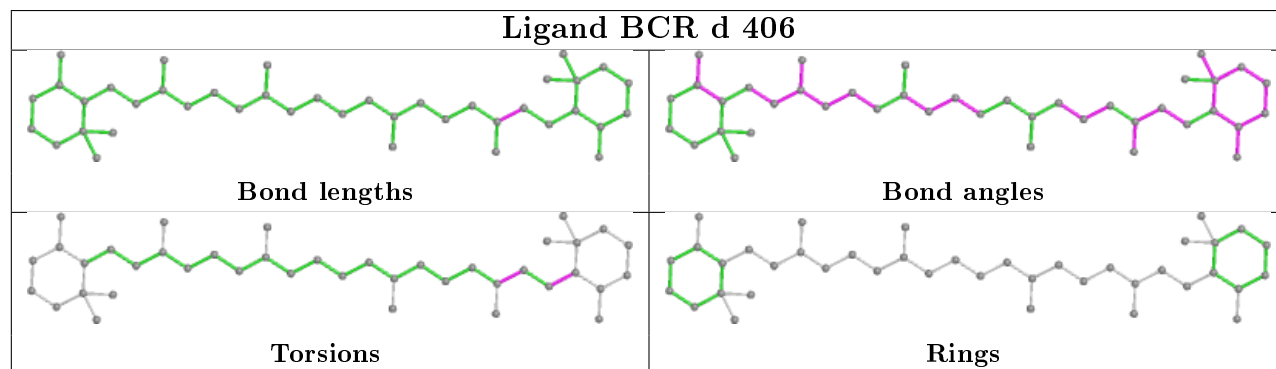
Ligand CLA d 404



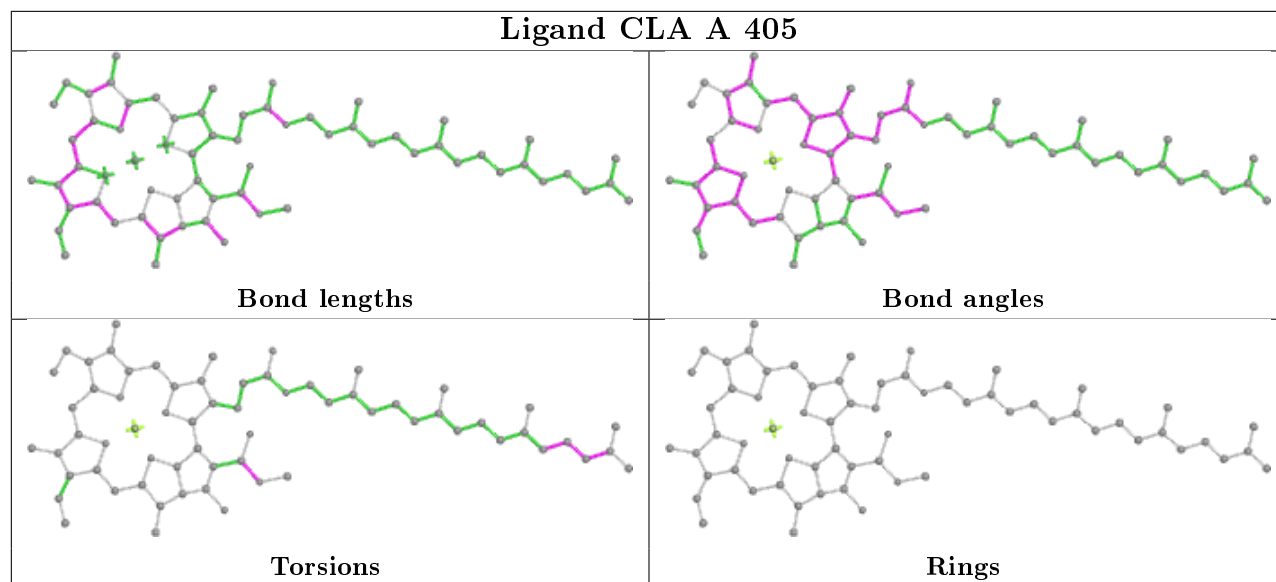
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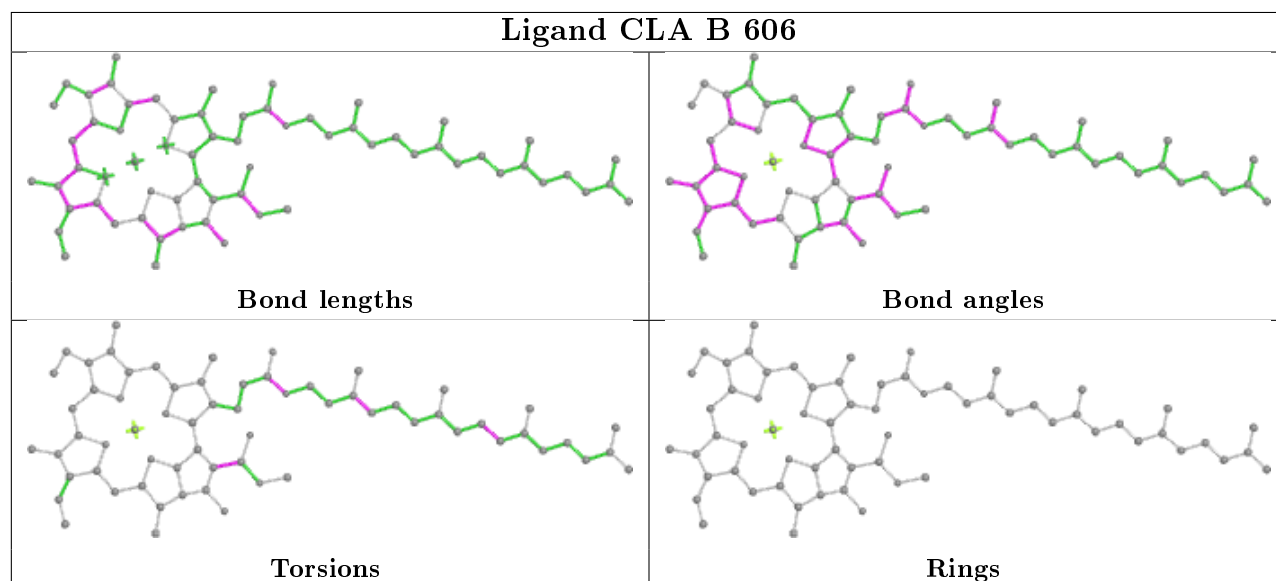
Ligand BCR d 406



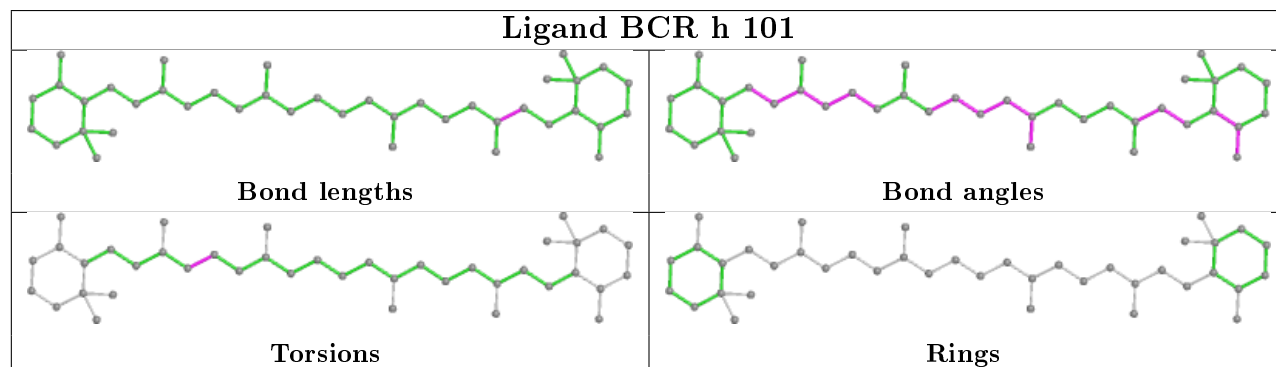
Ligand CLA A 405

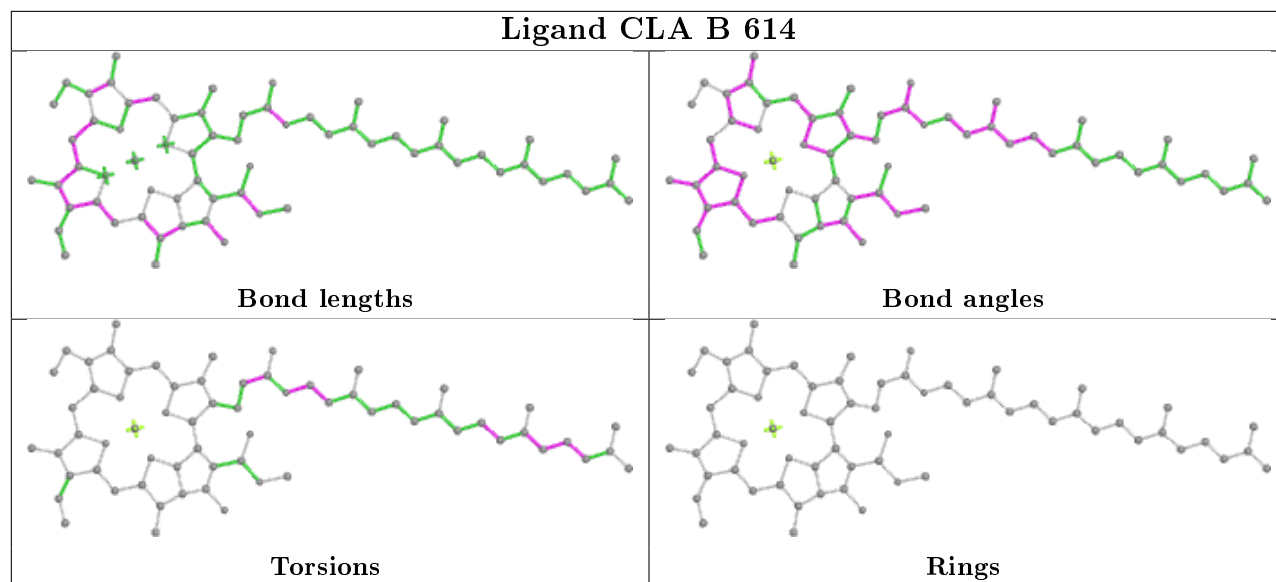
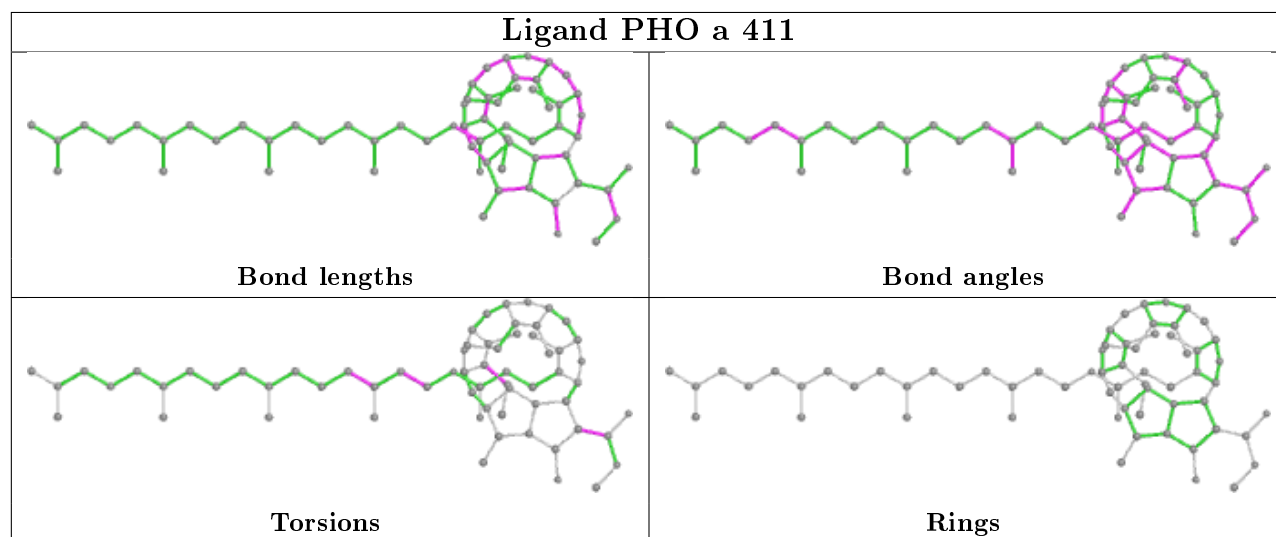


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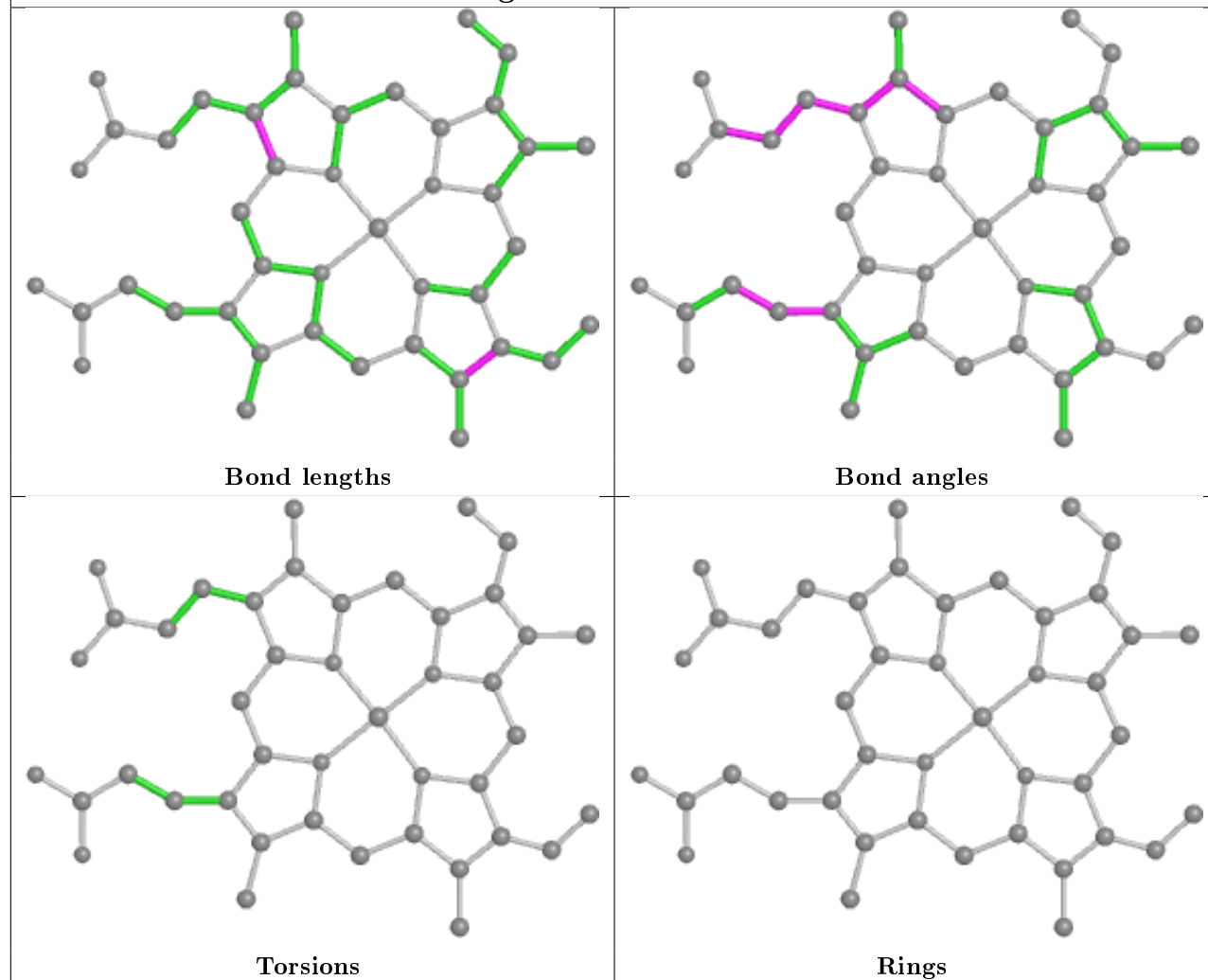


Ligand BCR h 101

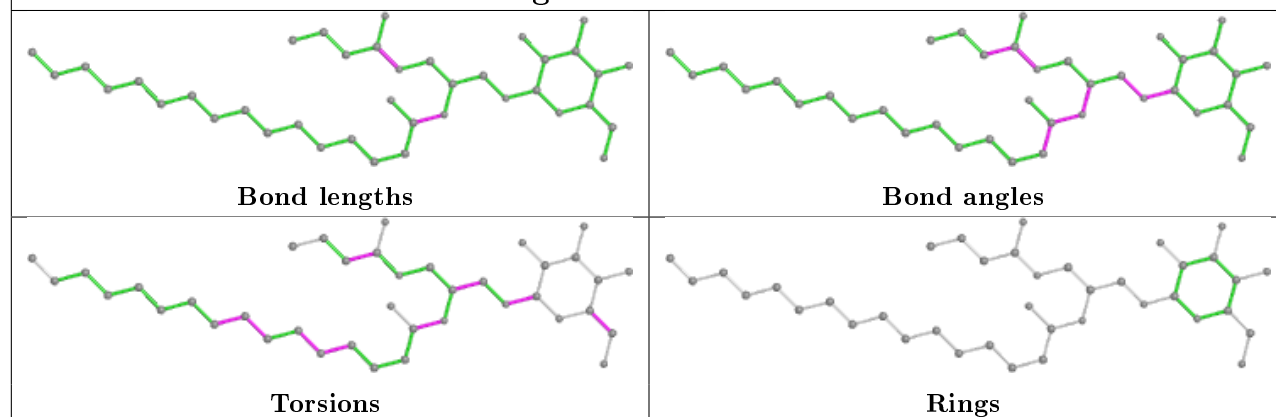


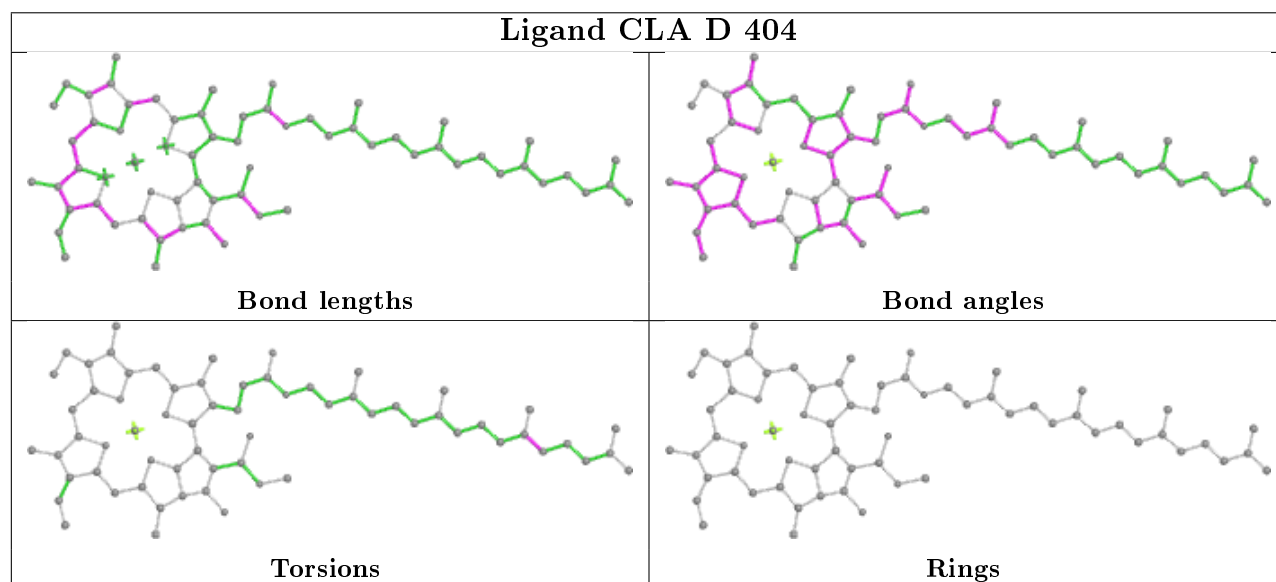
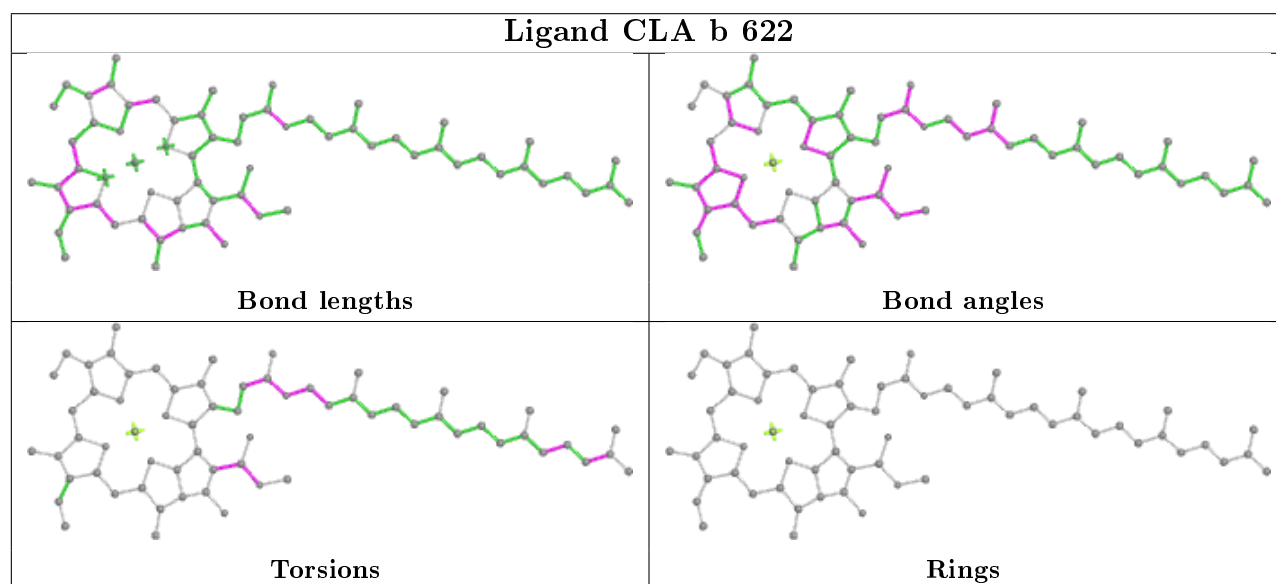
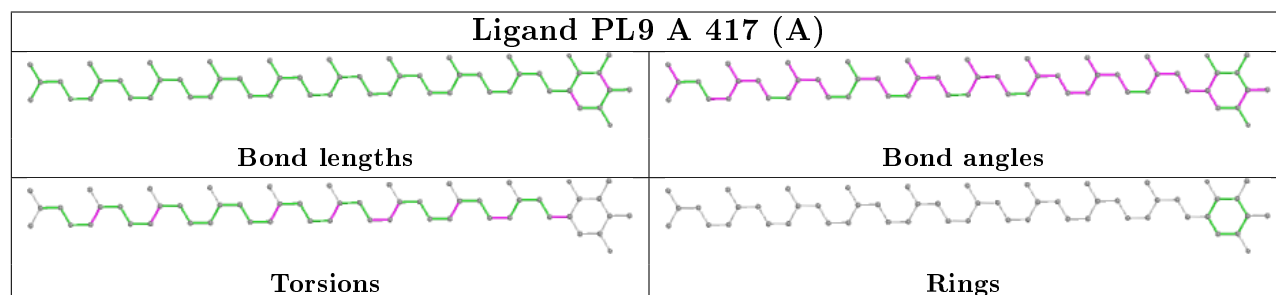
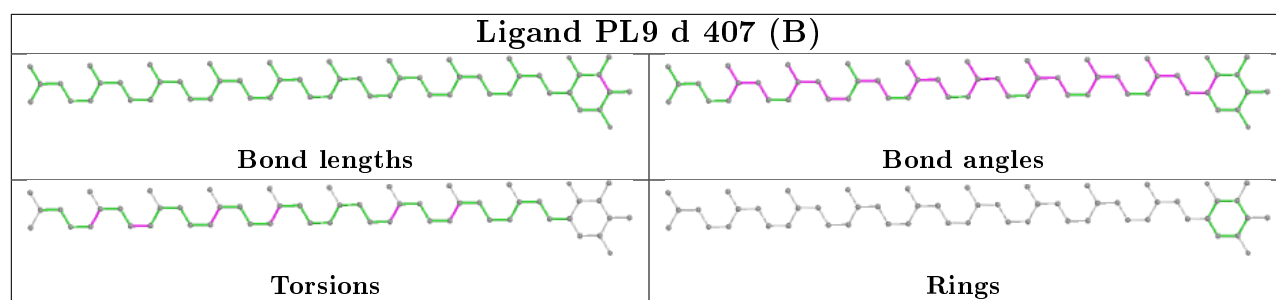
Ligand CLA B 614**Ligand PHO a 411**

Ligand HEM V 205

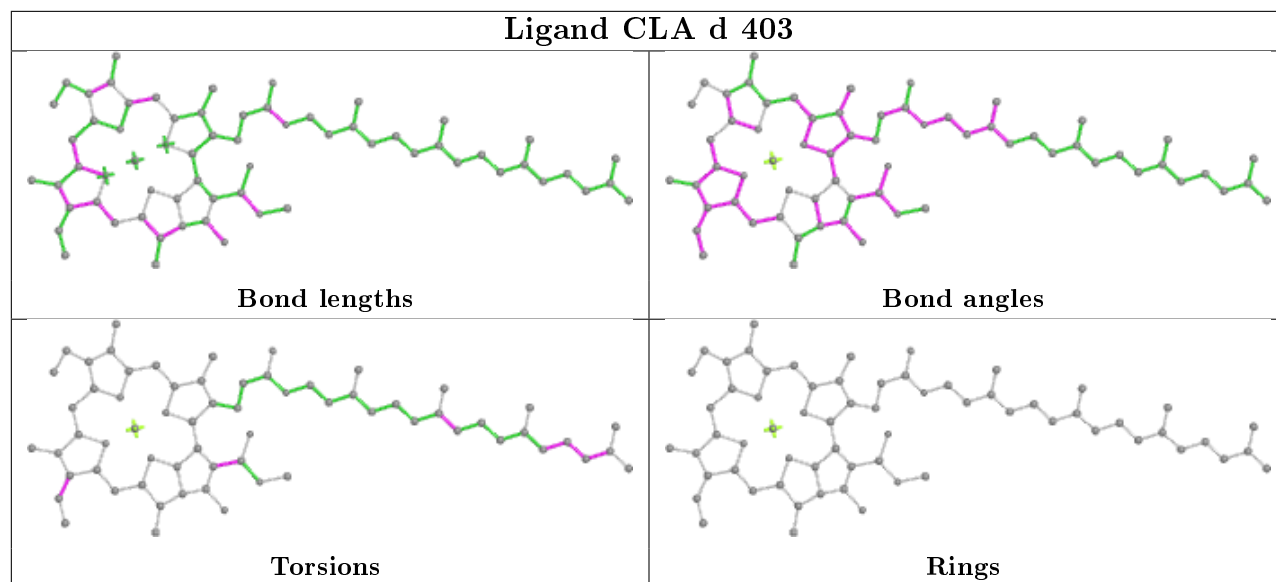


Ligand LMG z 101

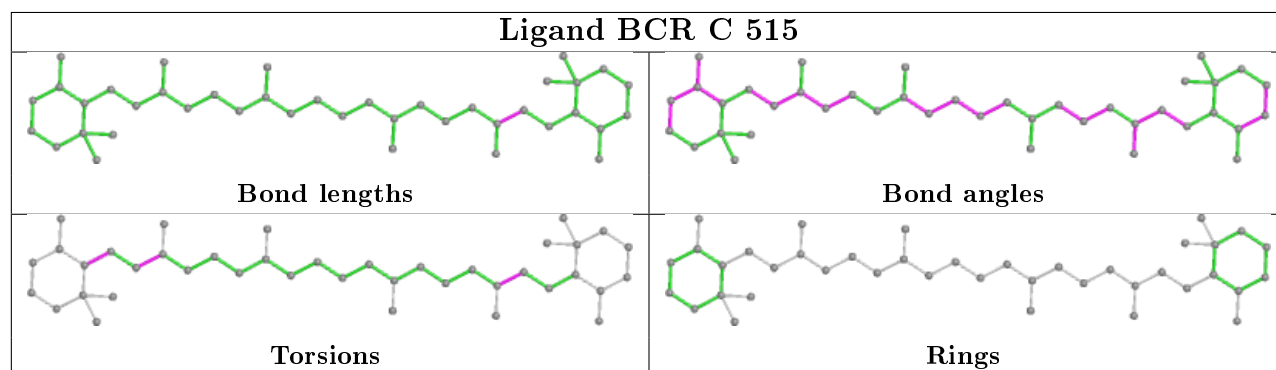




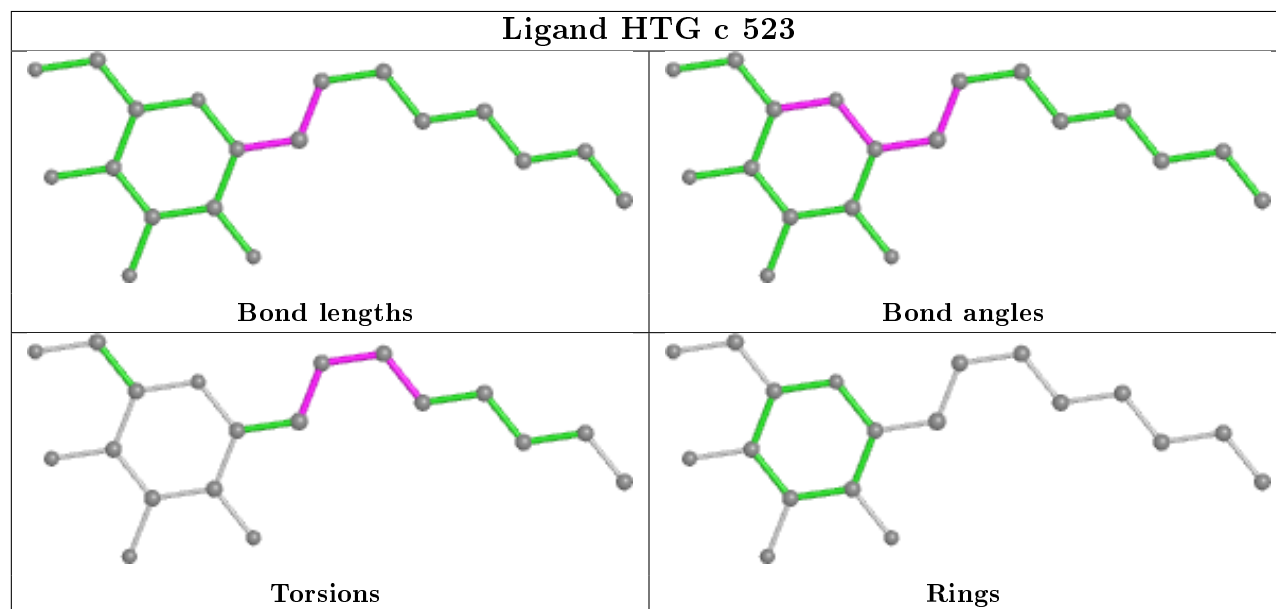
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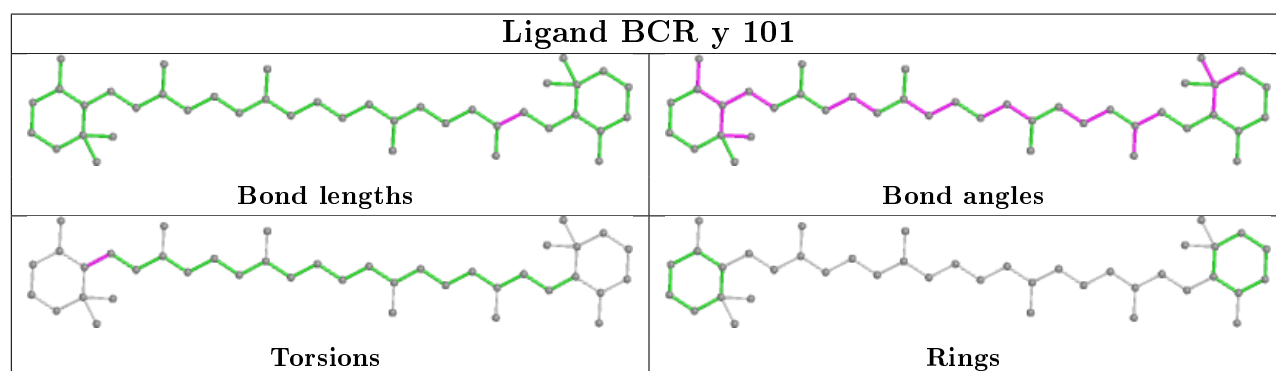
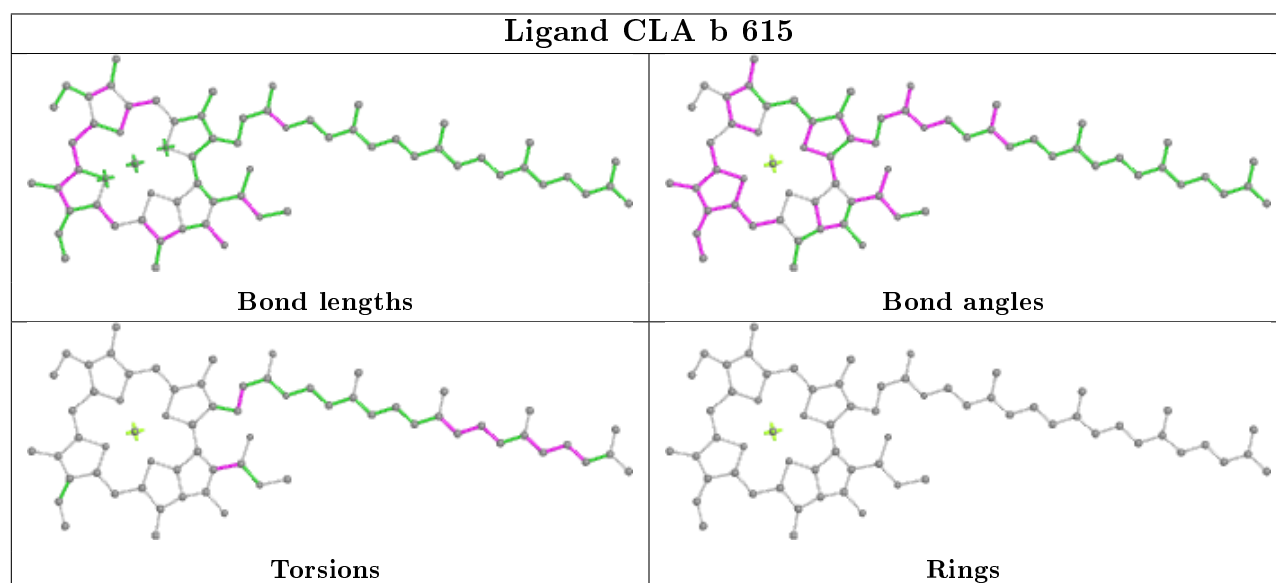
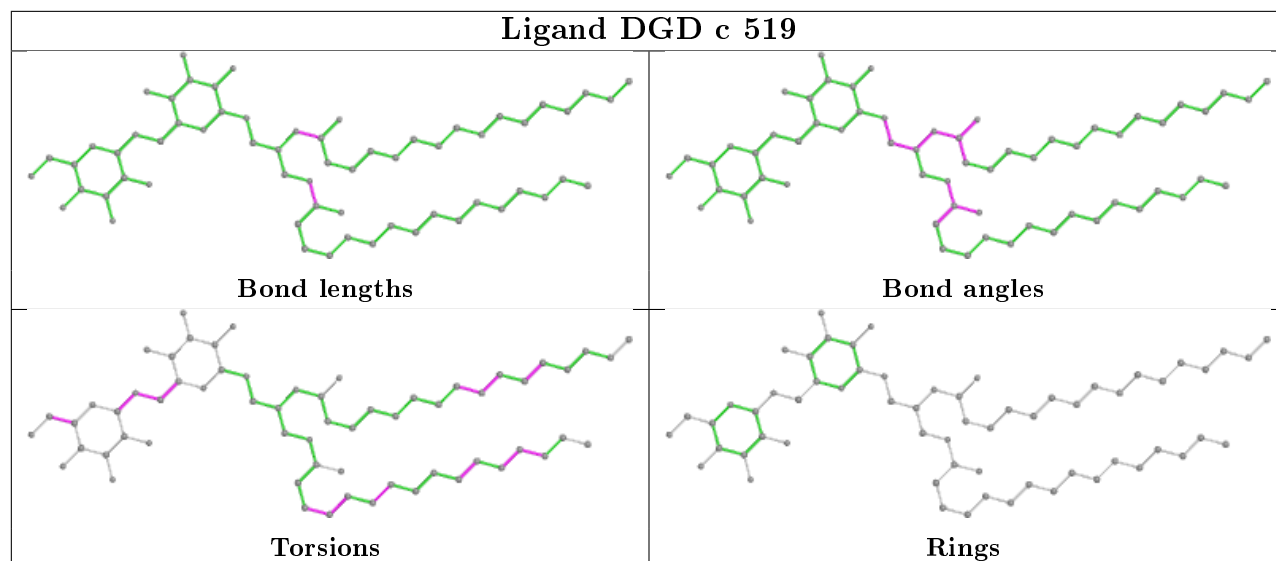


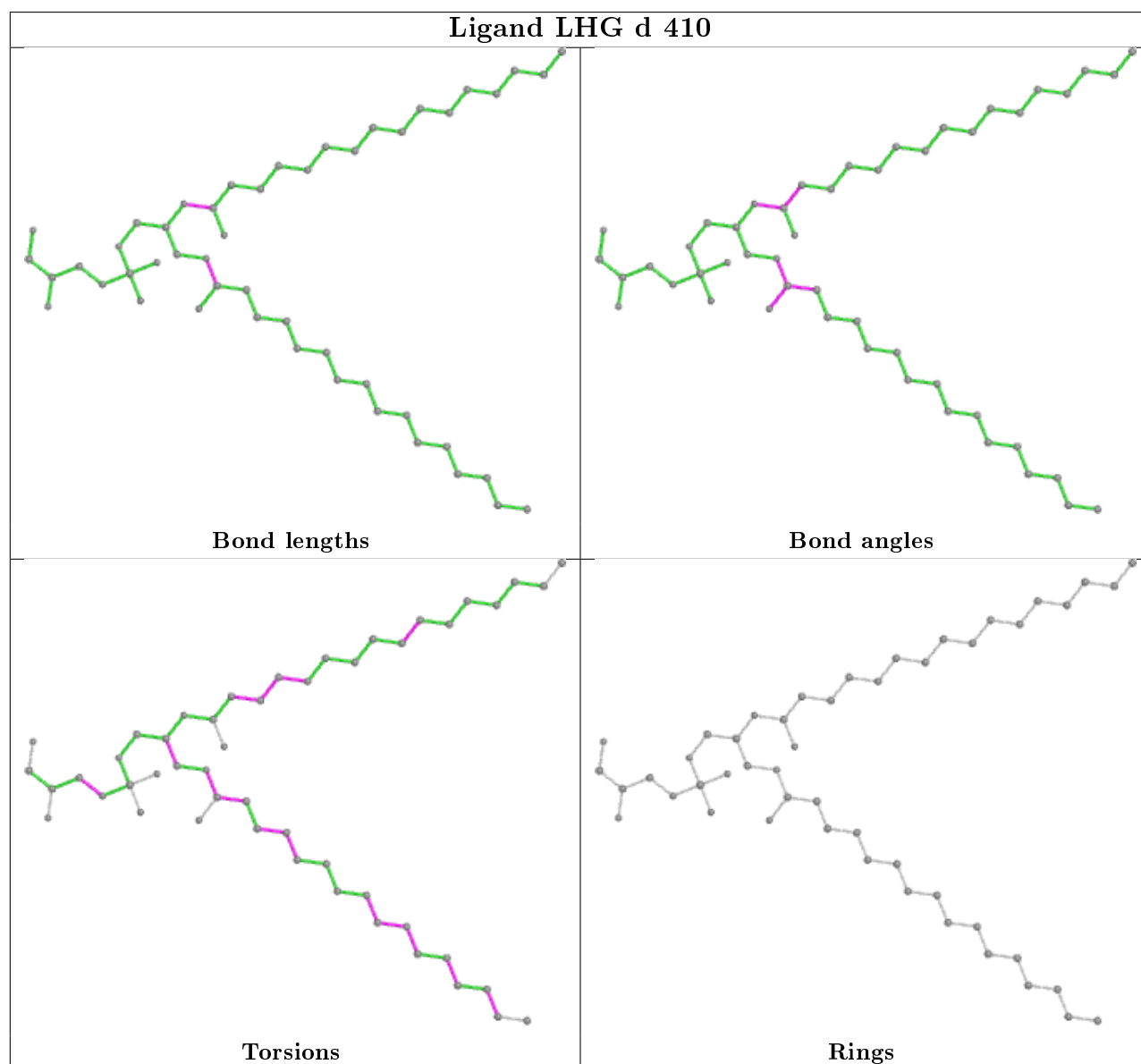
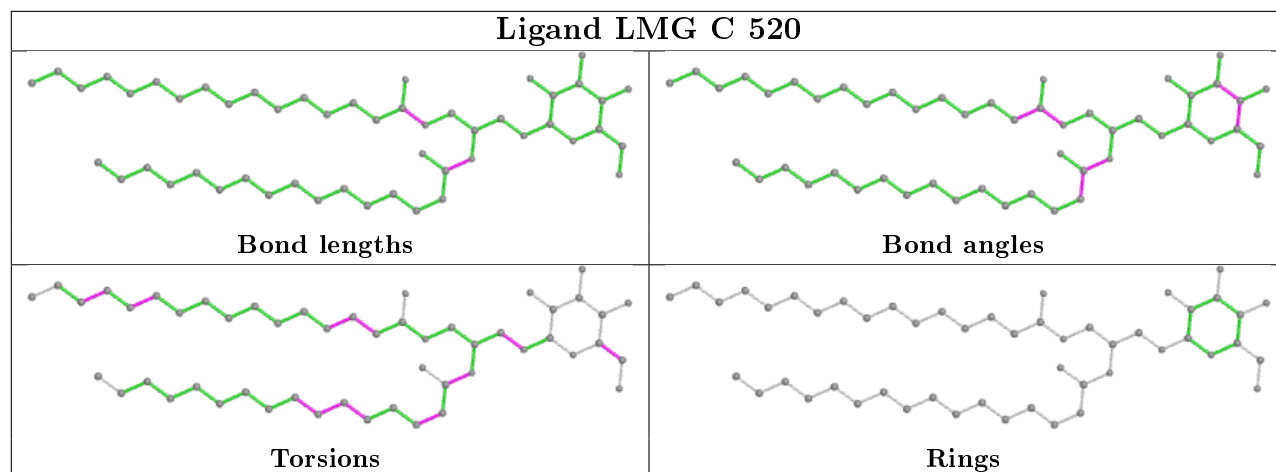
Ligand BCR C 515



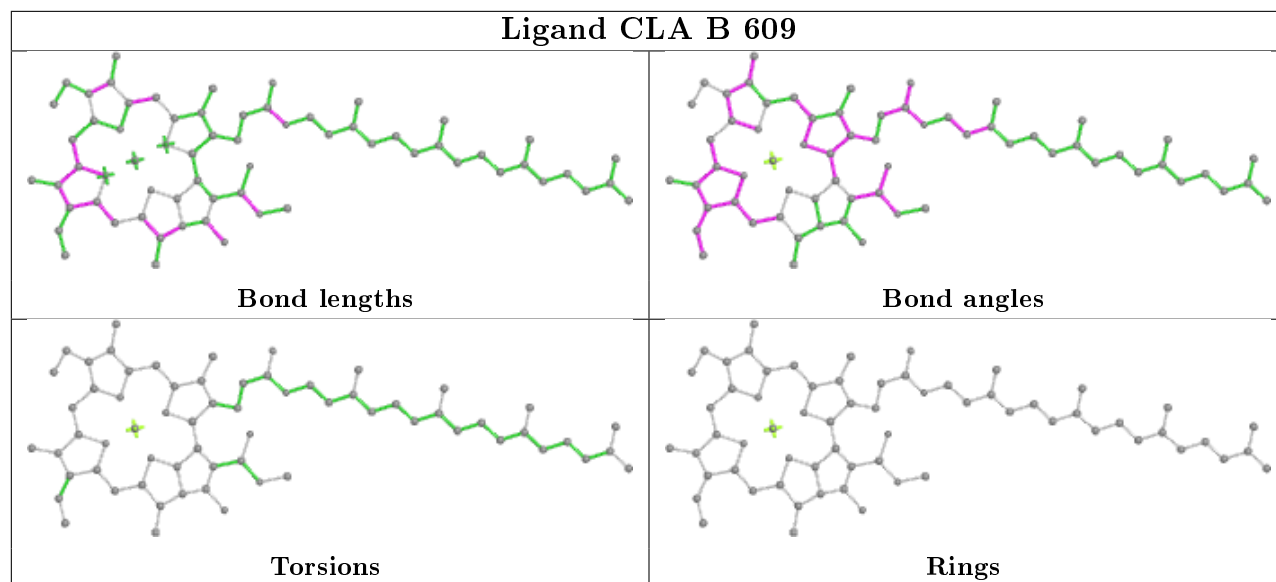
Ligand HTG c 523



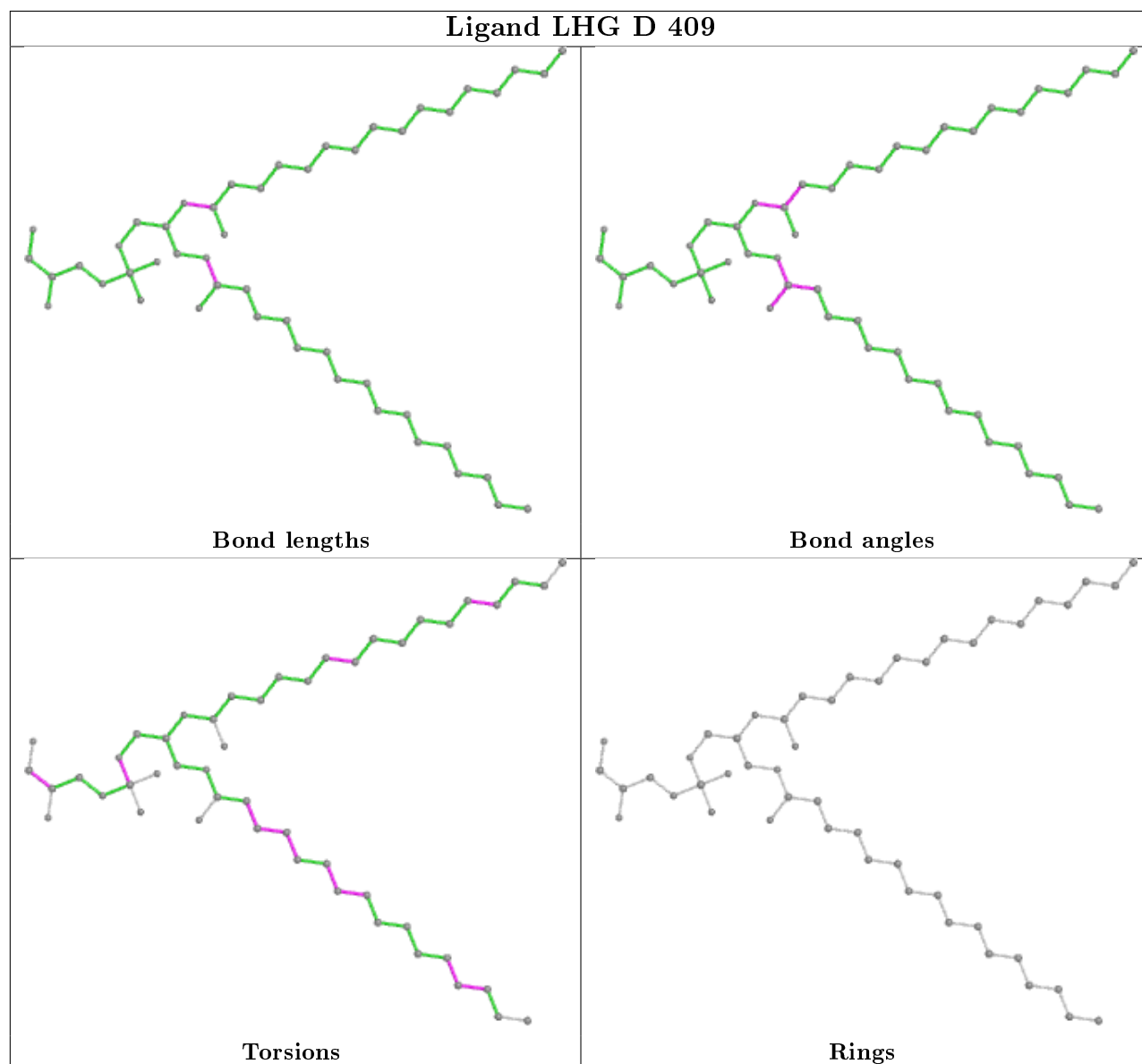


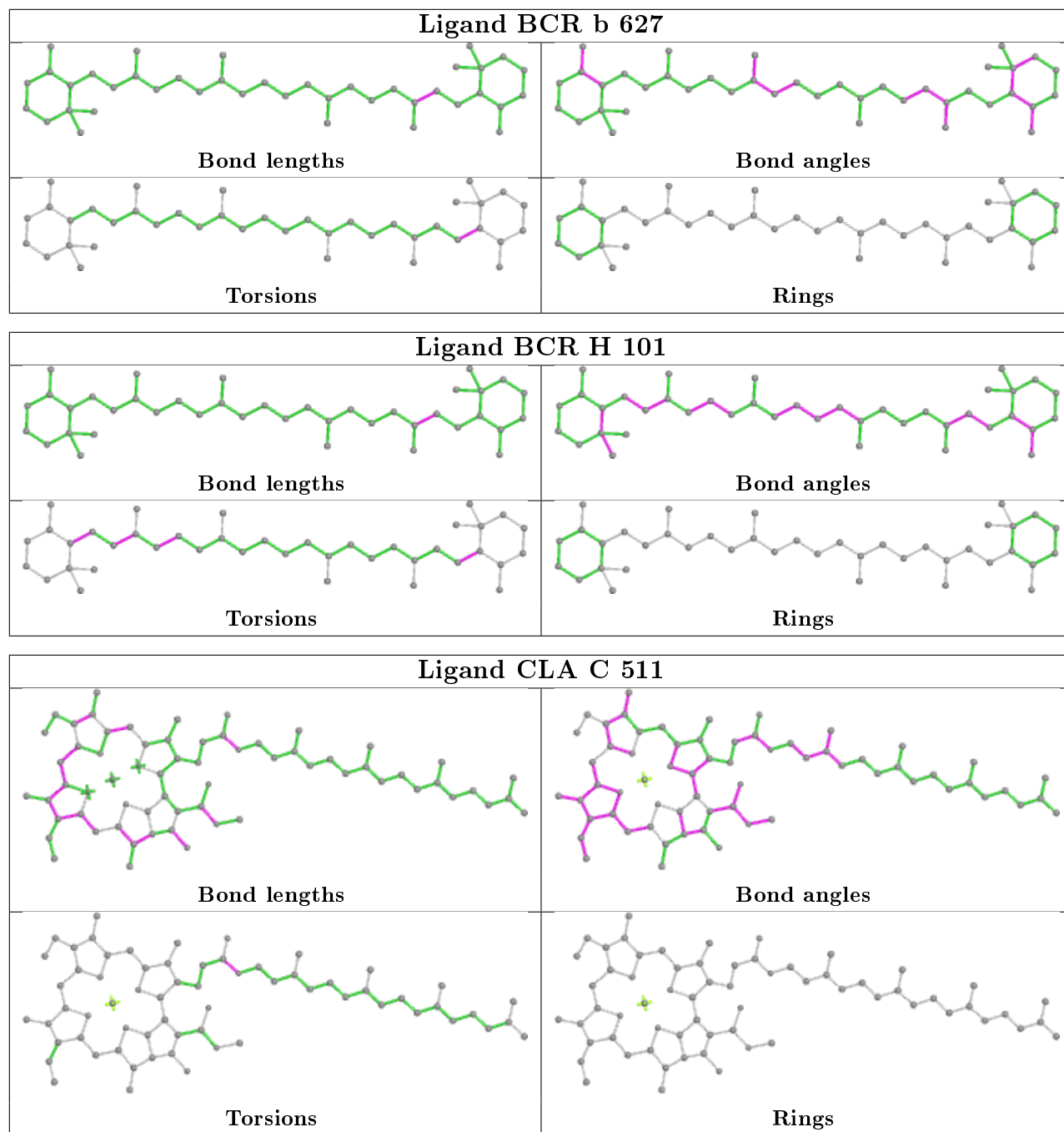


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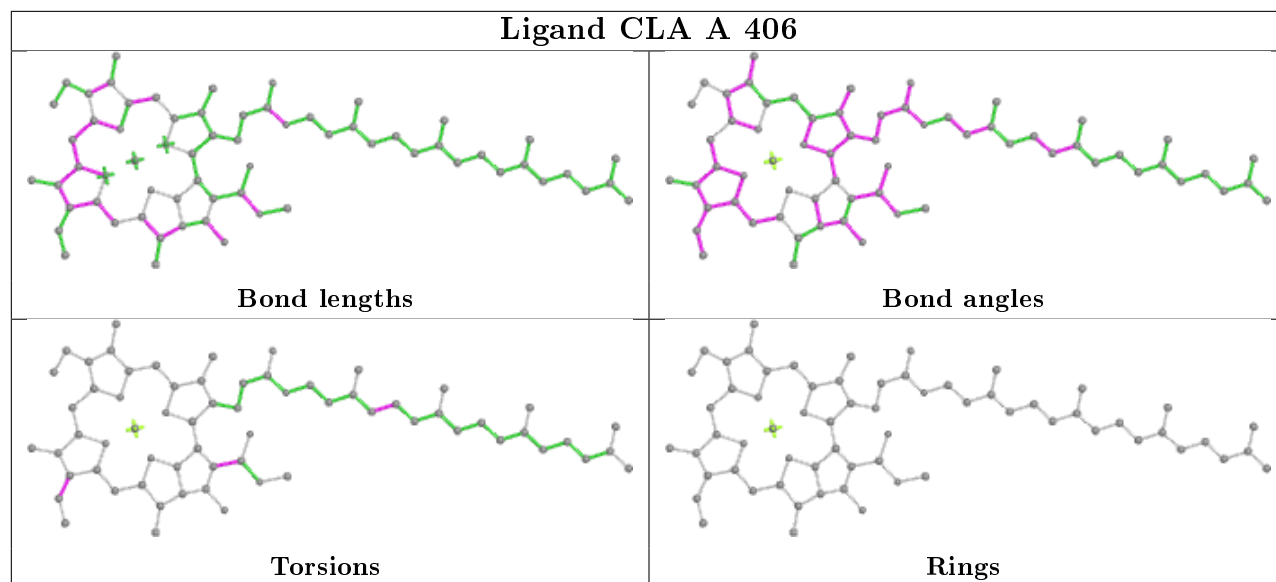


Ligand LHG D 409

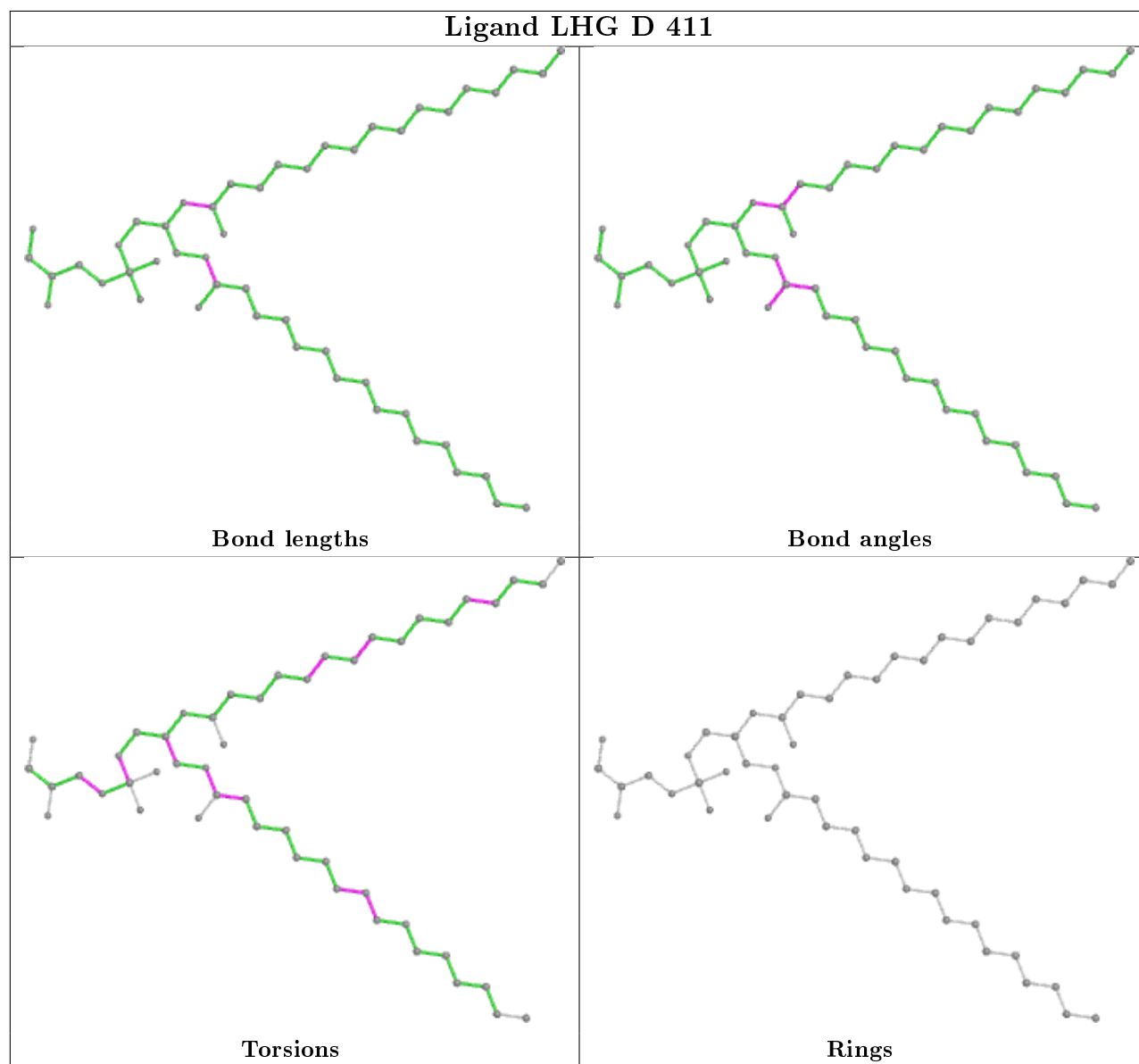


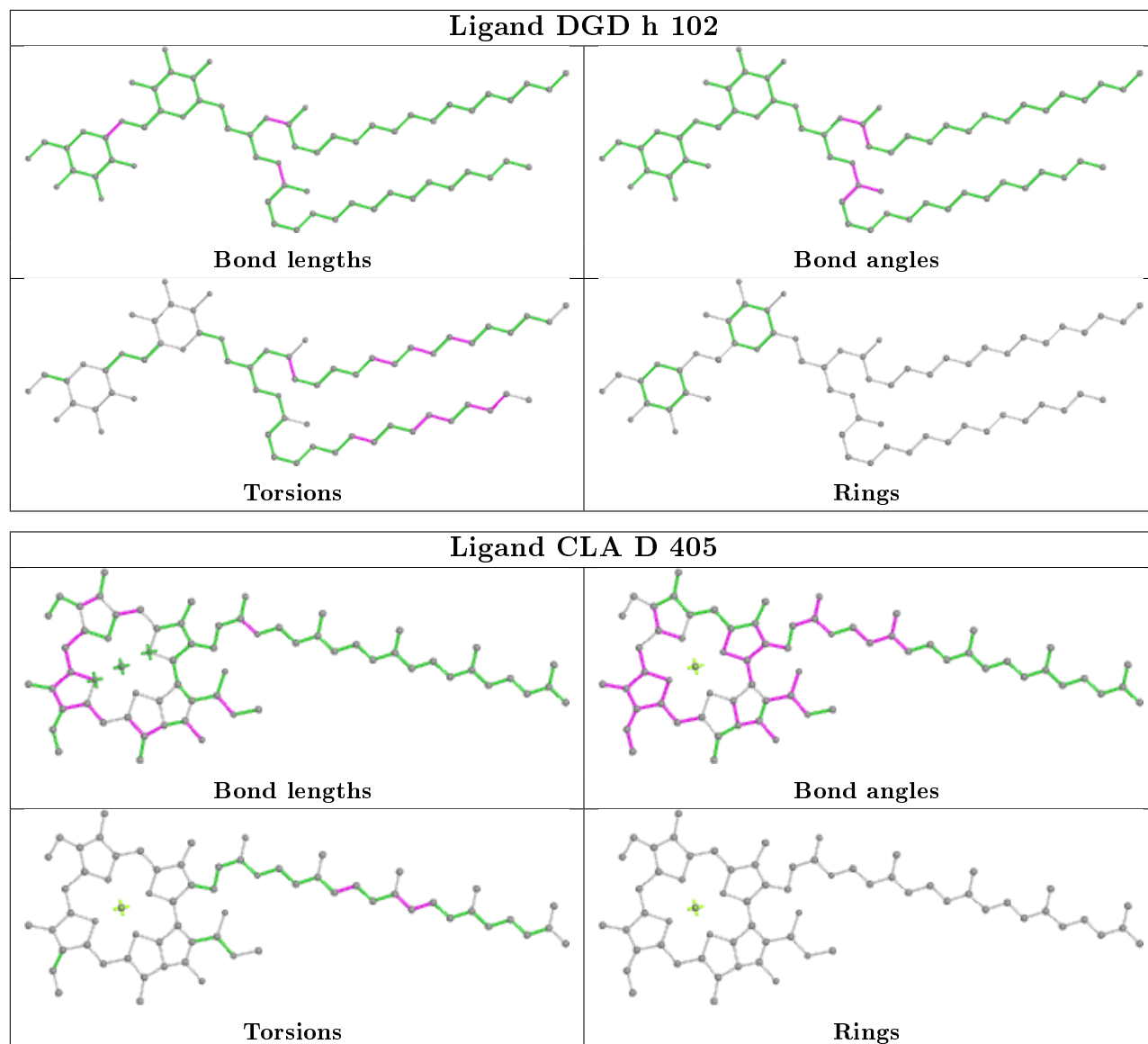


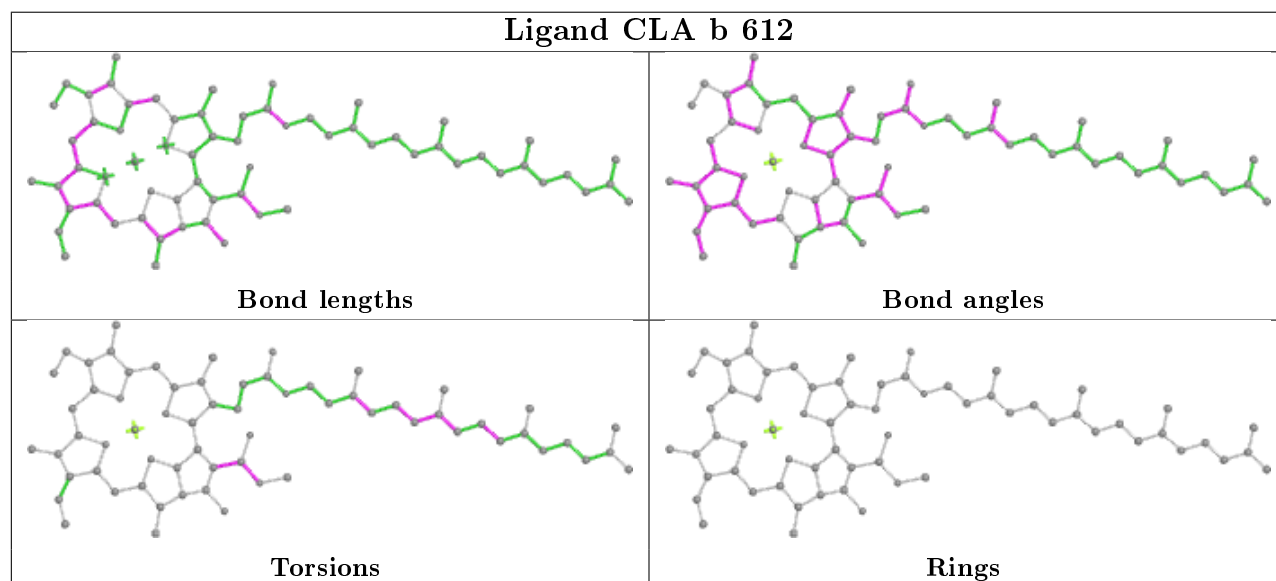
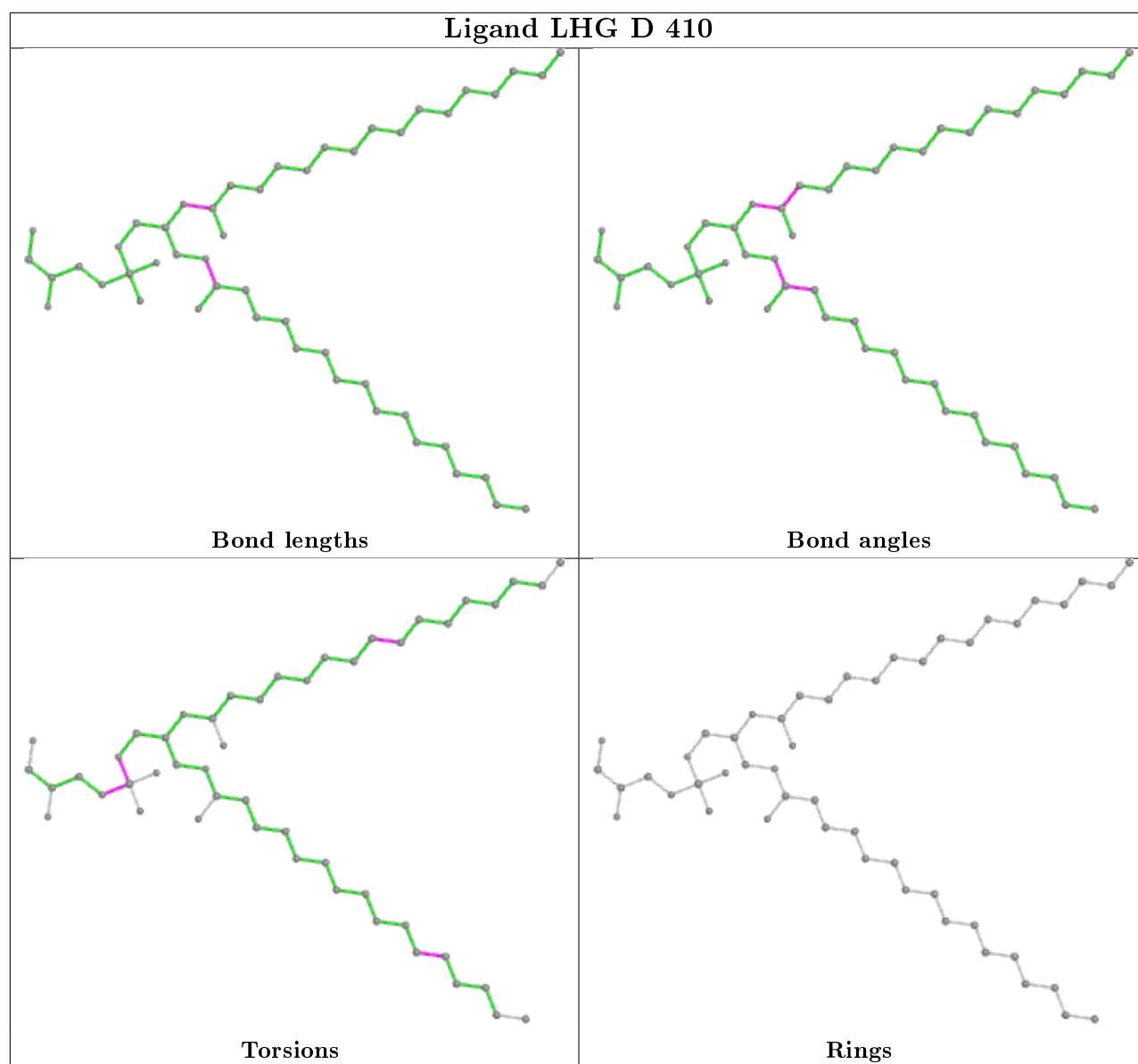
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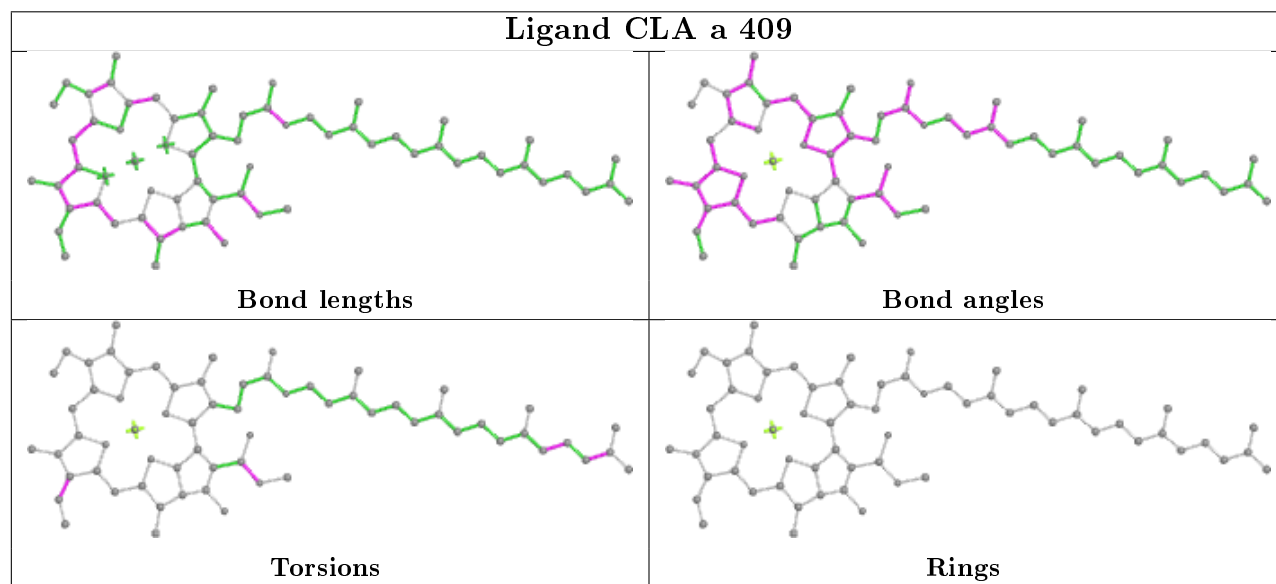
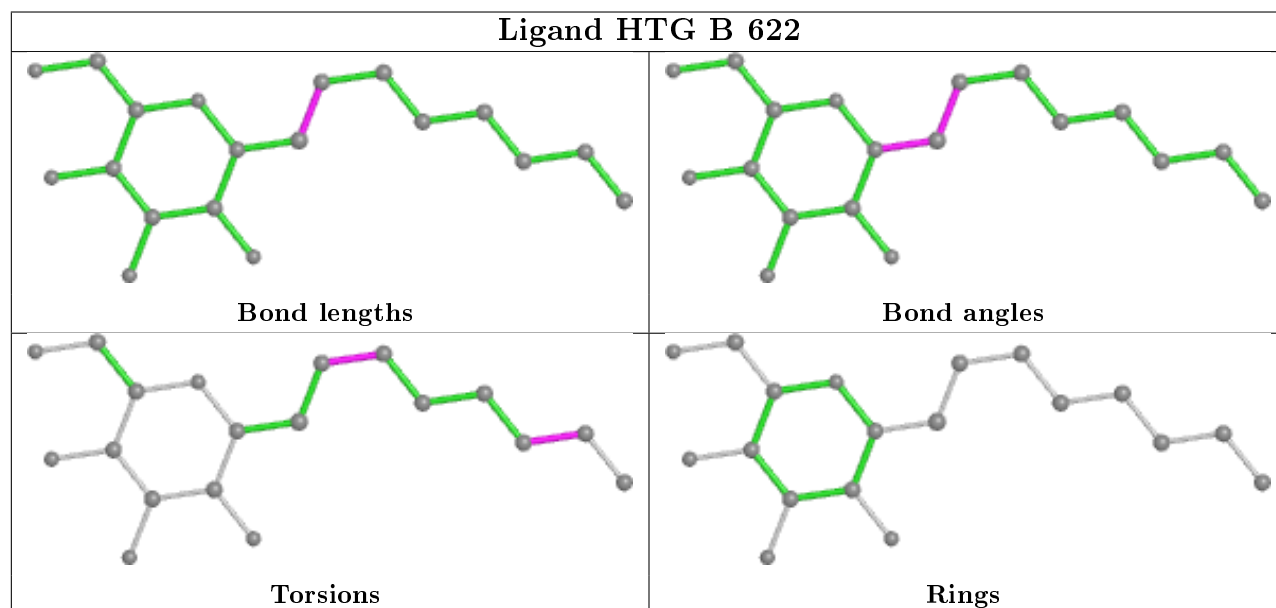
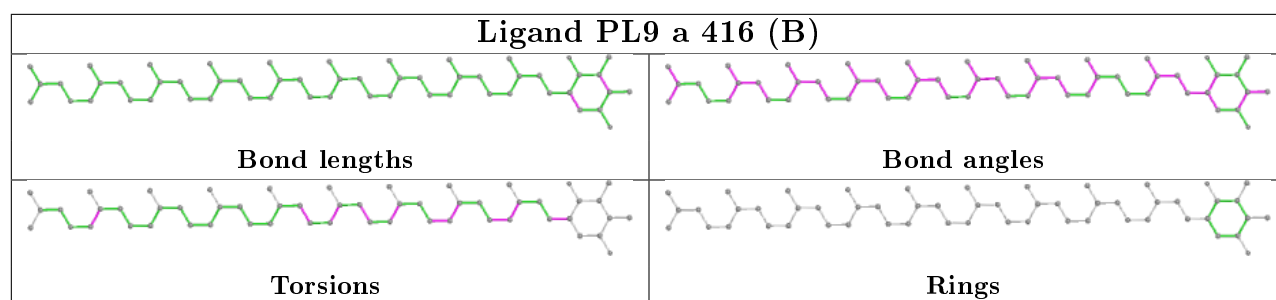


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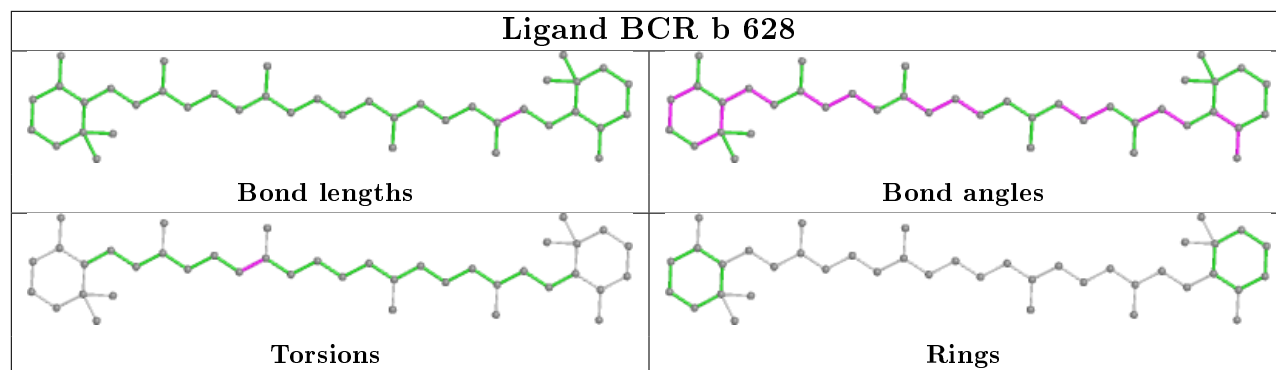




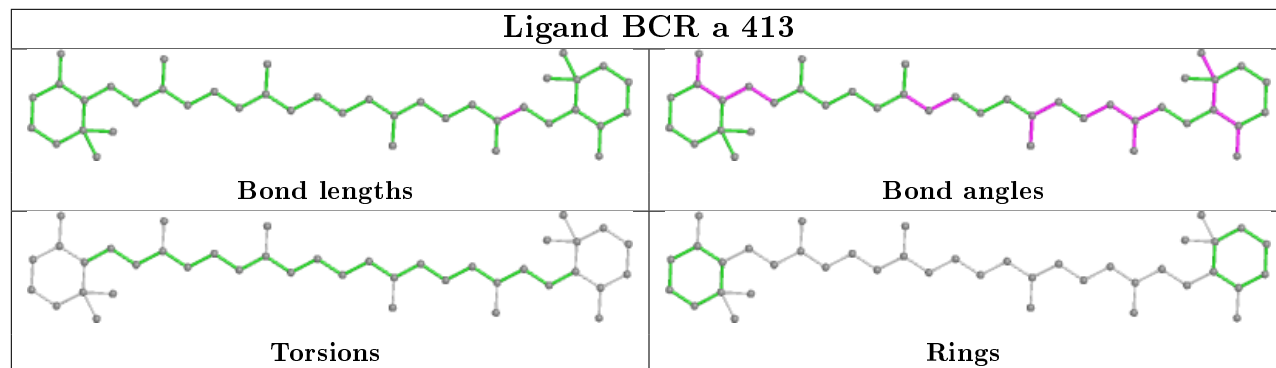




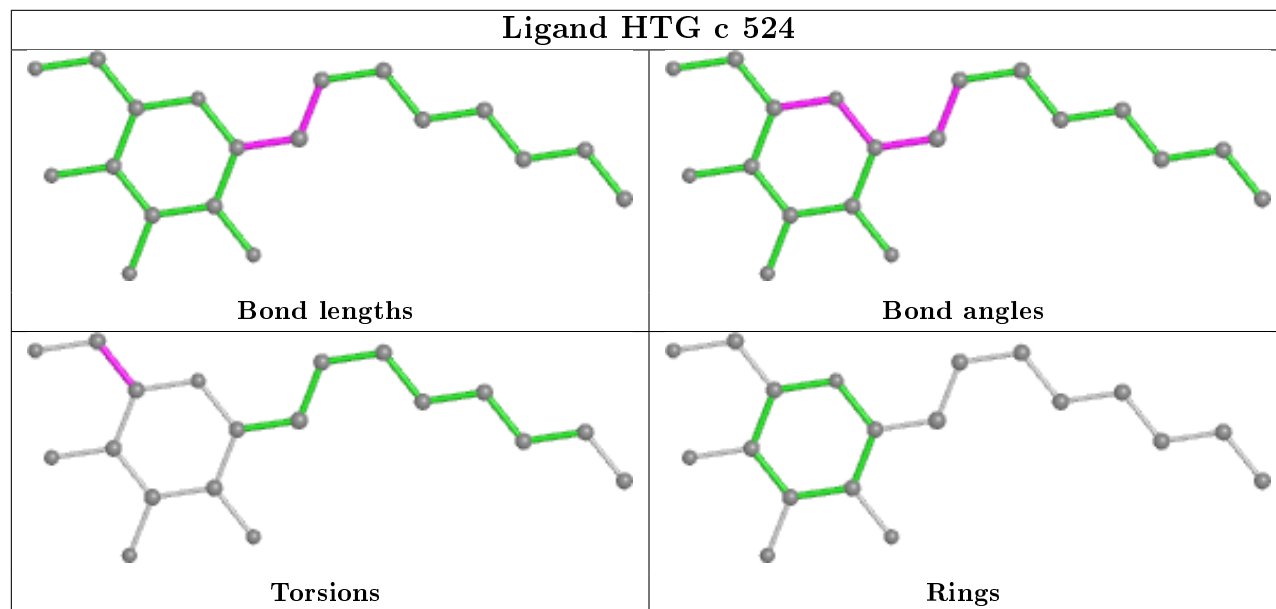
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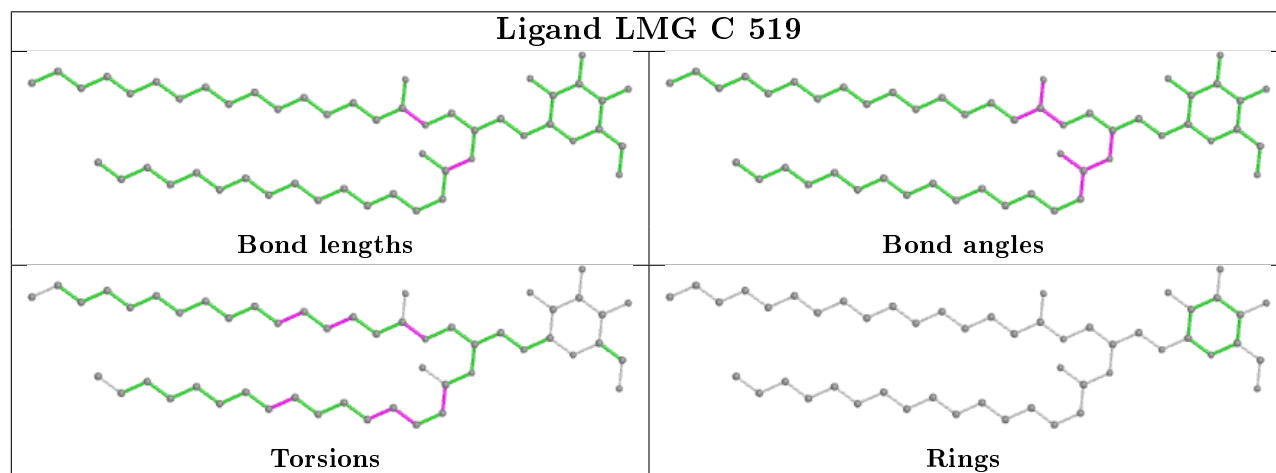
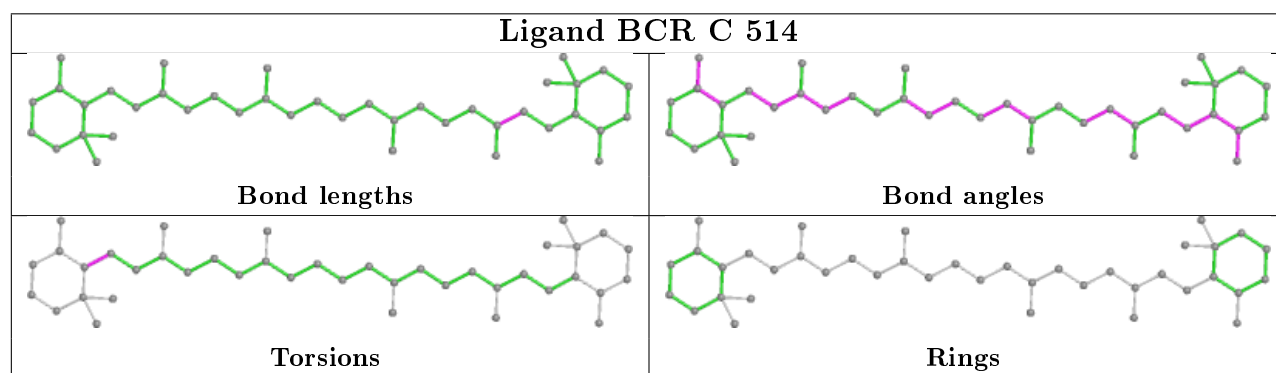
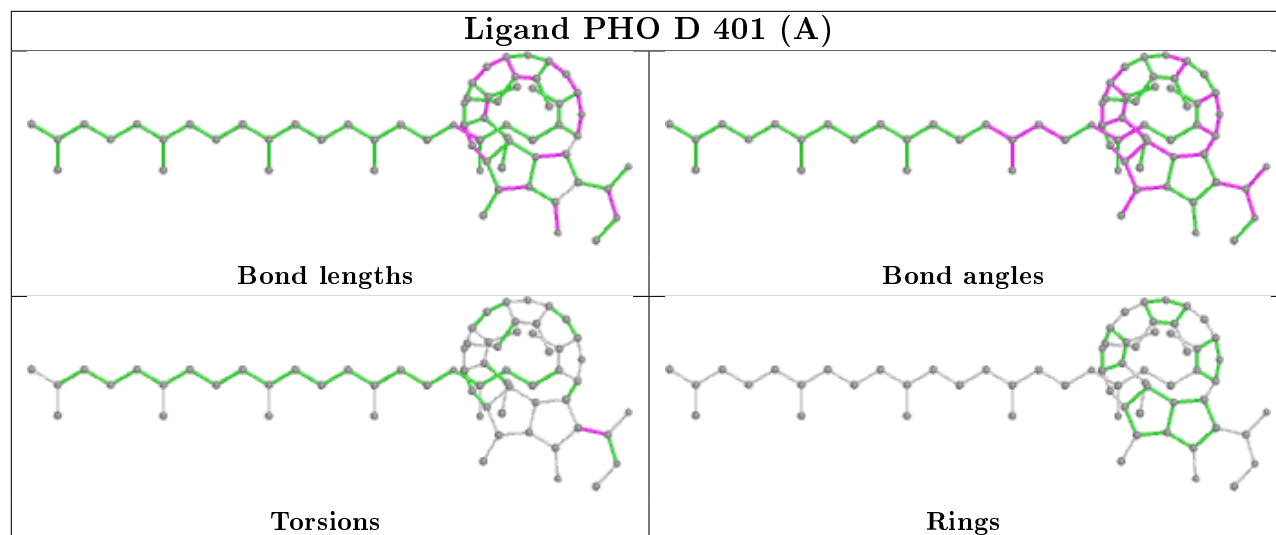


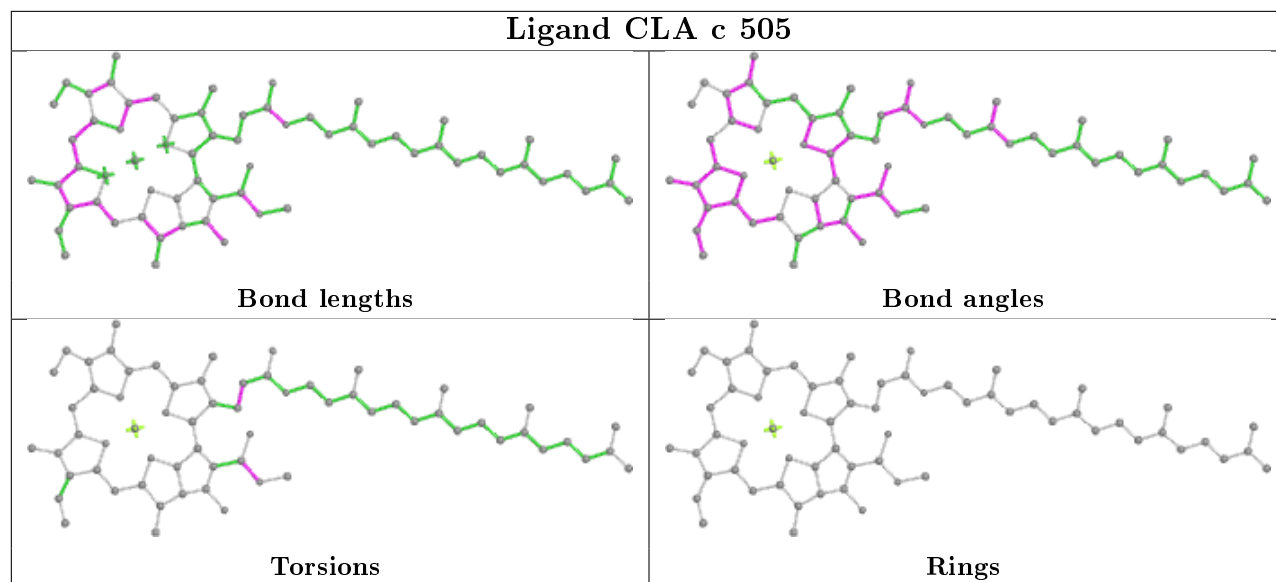
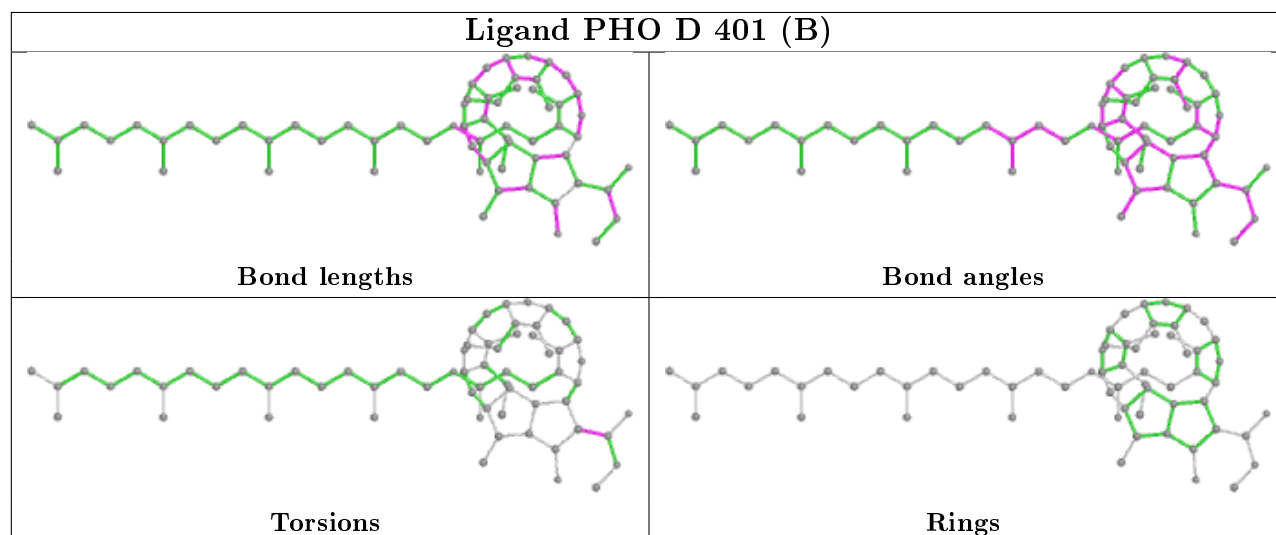
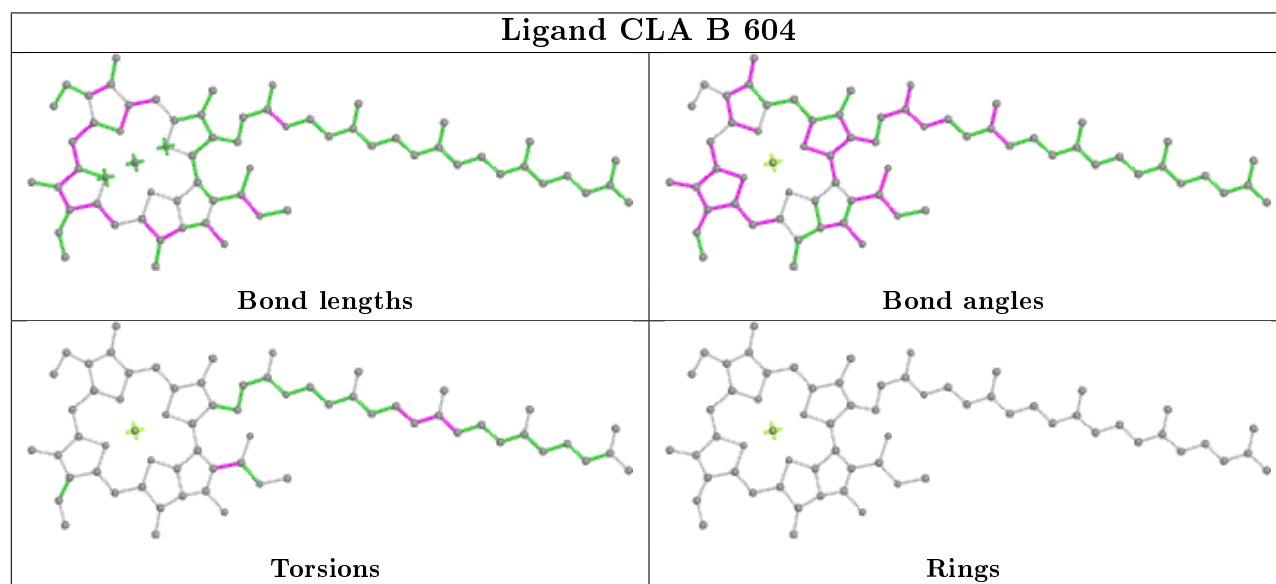
Ligand BCR a 413

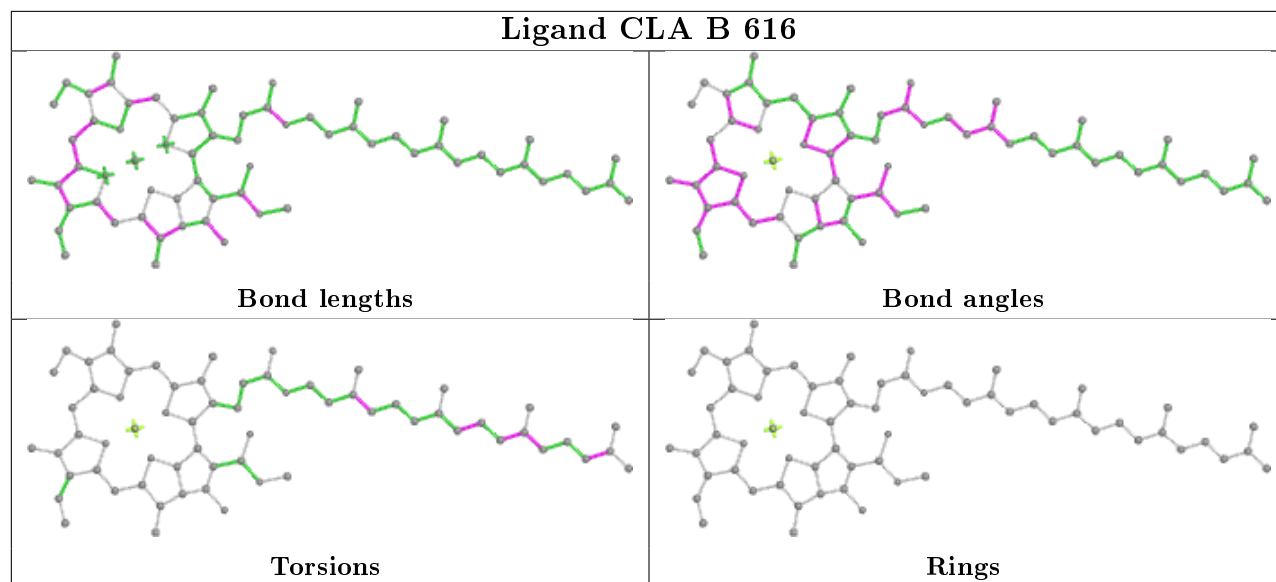
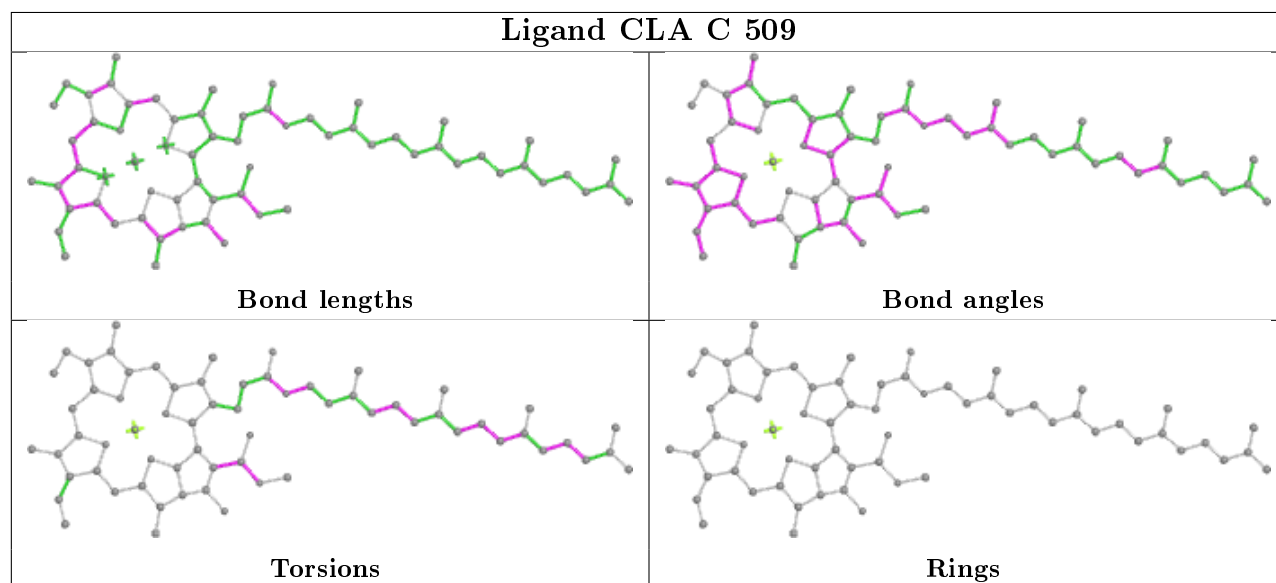


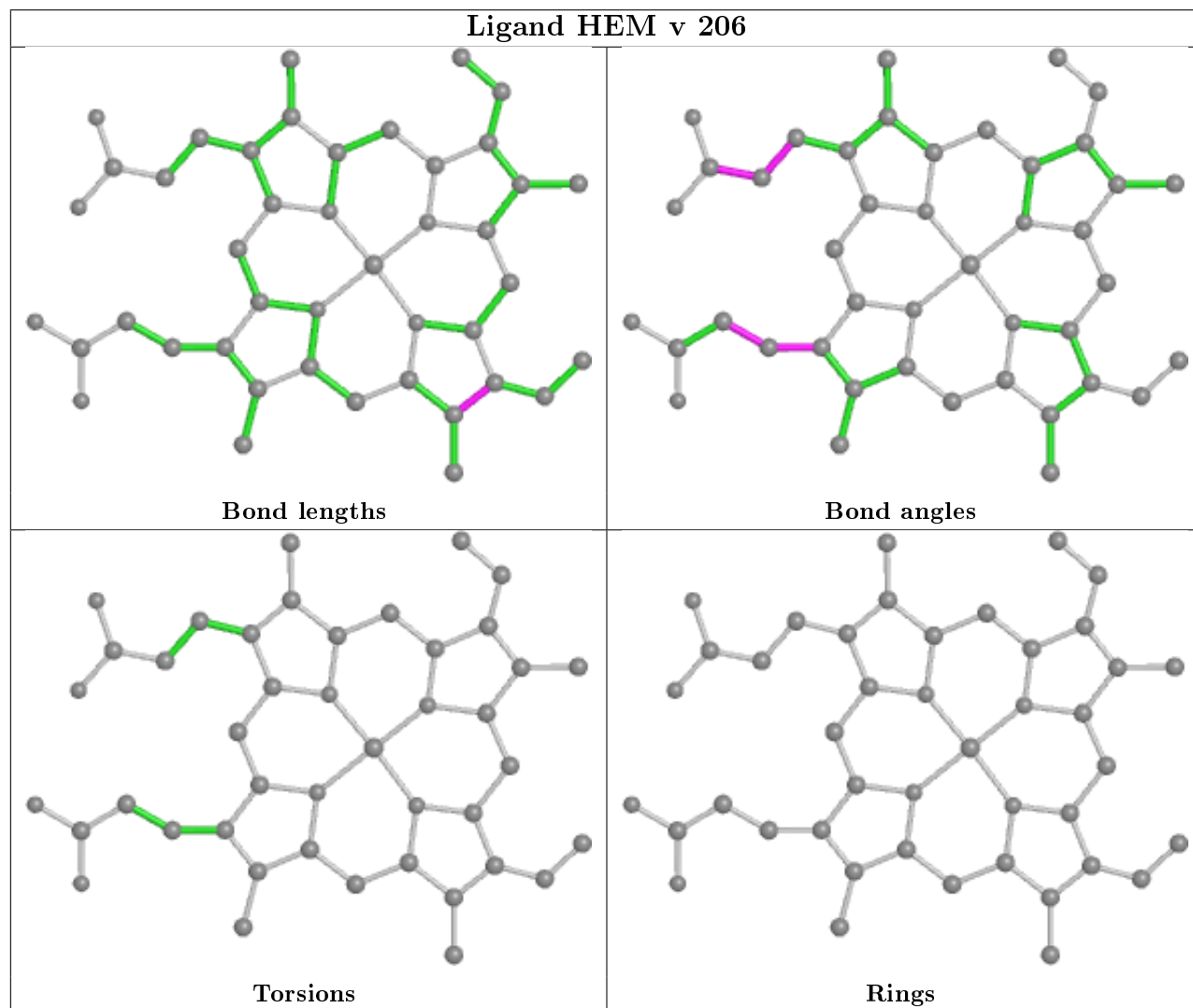
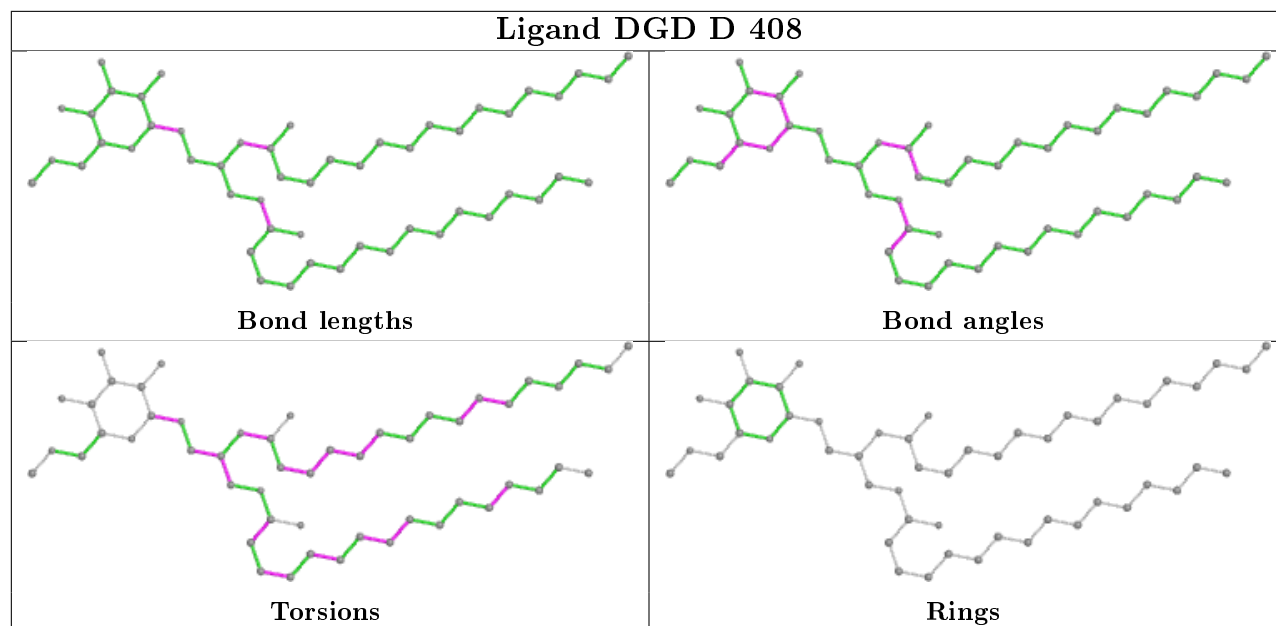
Ligand HTG c 524



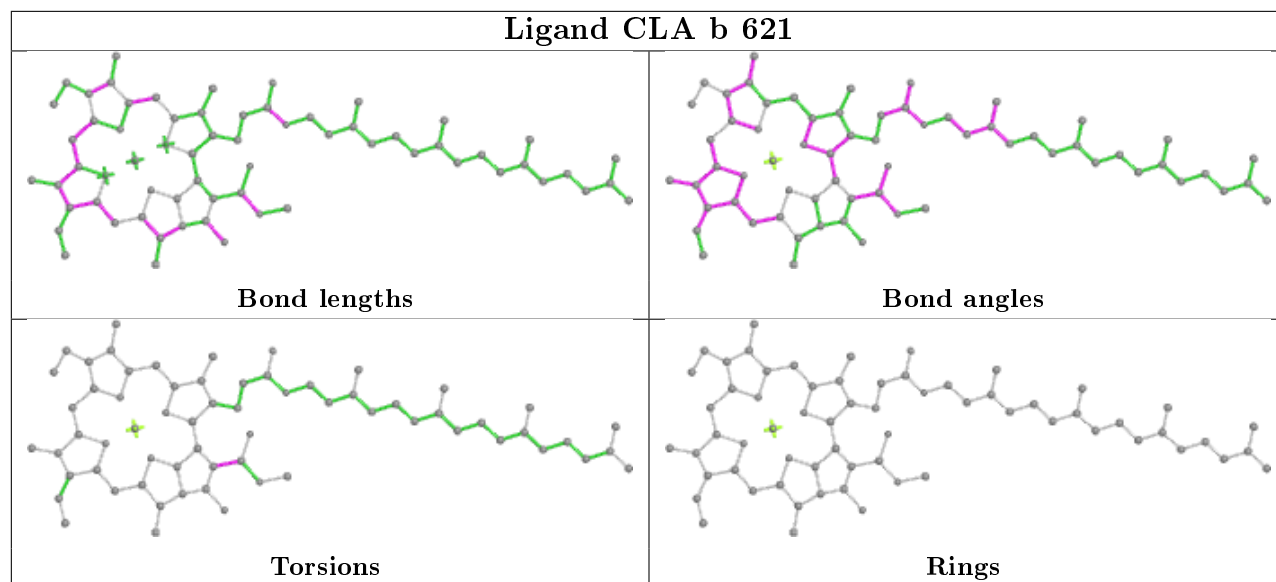


Ligand CLA c 505**Ligand PHO D 401 (B)****Ligand CLA B 604**

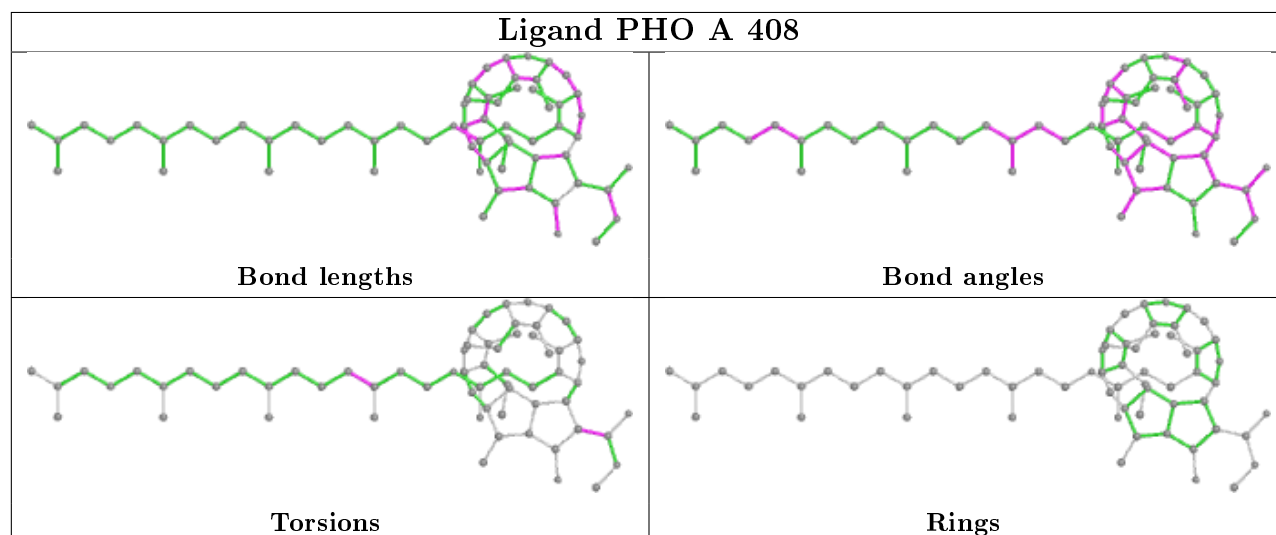
Ligand CLA B 616**Ligand CLA C 509**



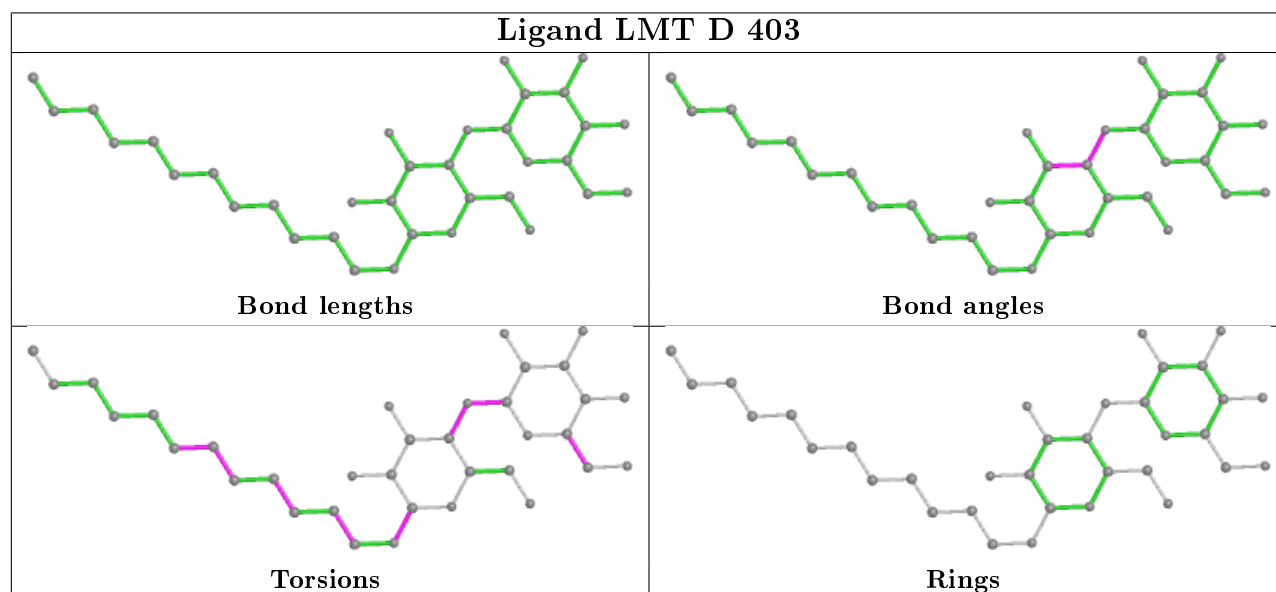
Ligand CLA b 621

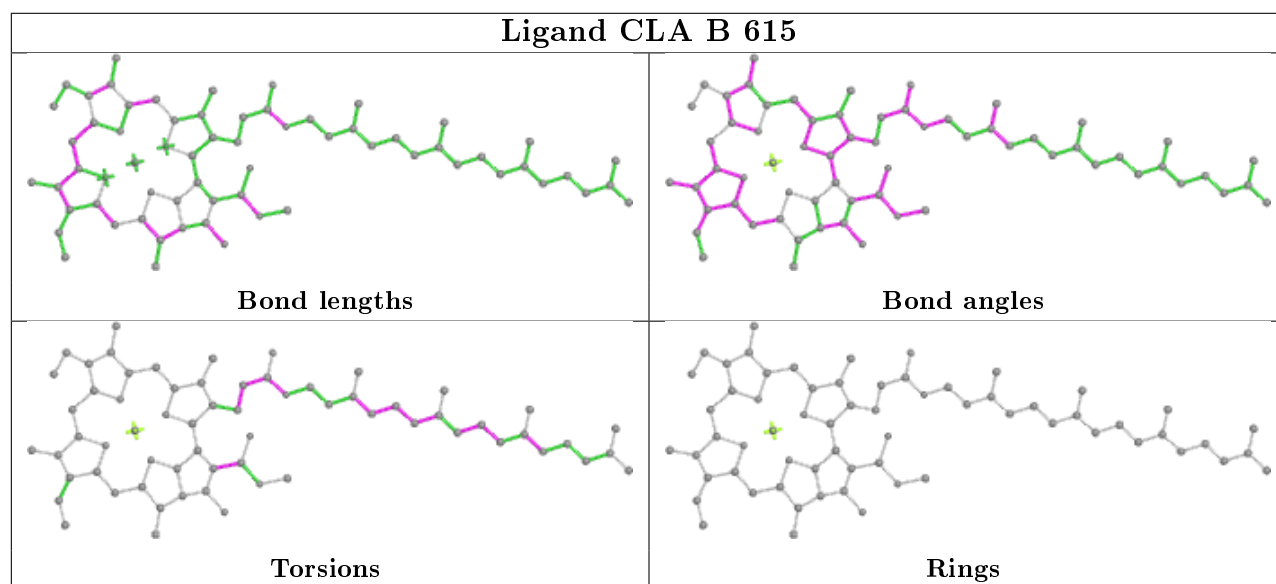
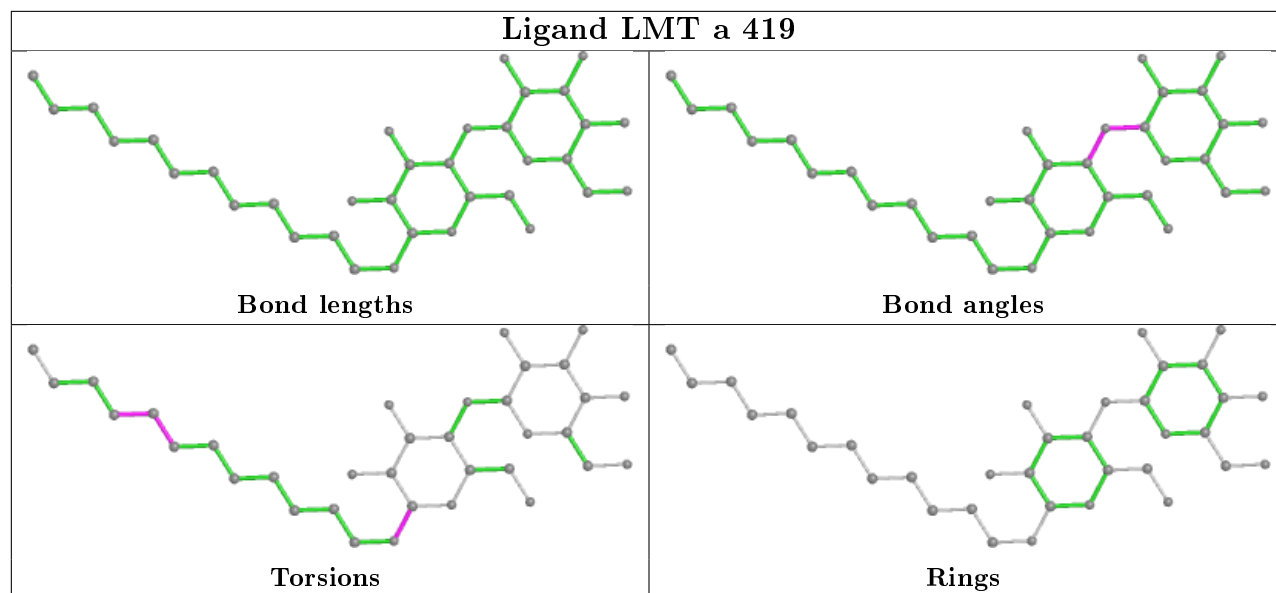


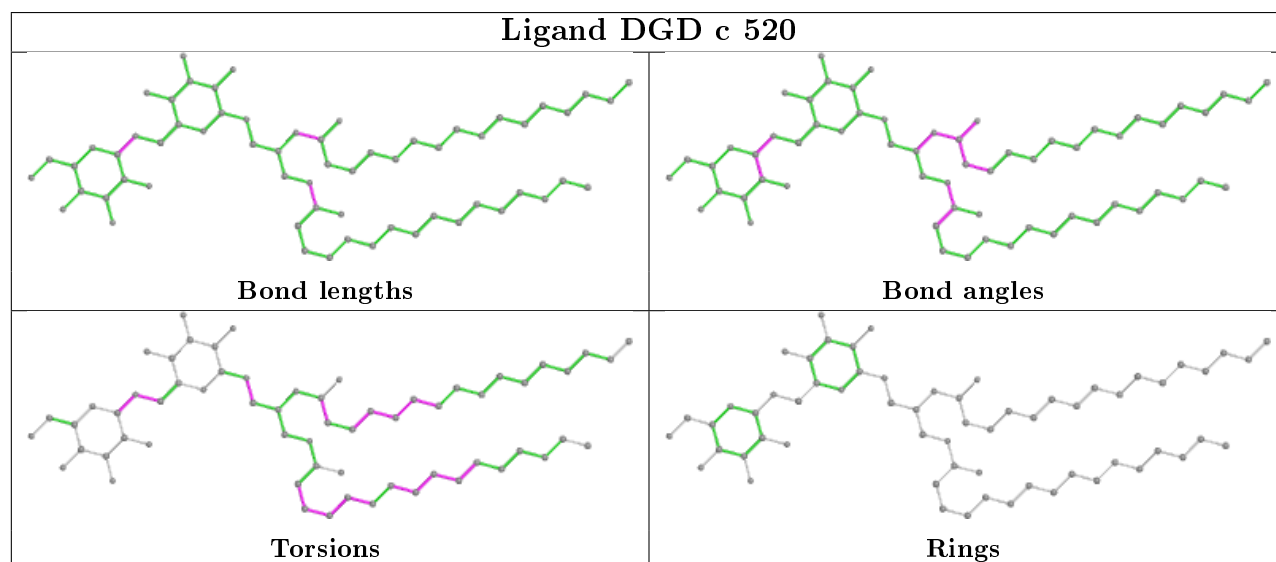
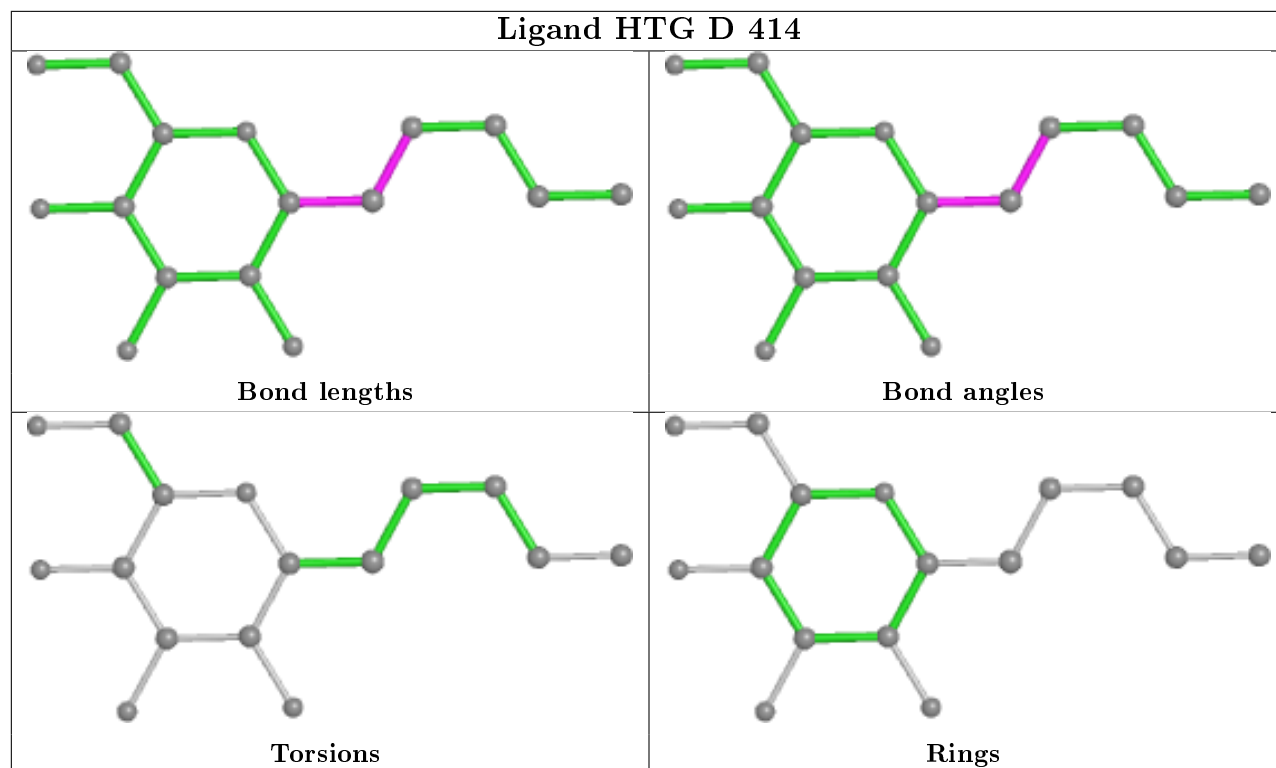
Ligand PHO A 408

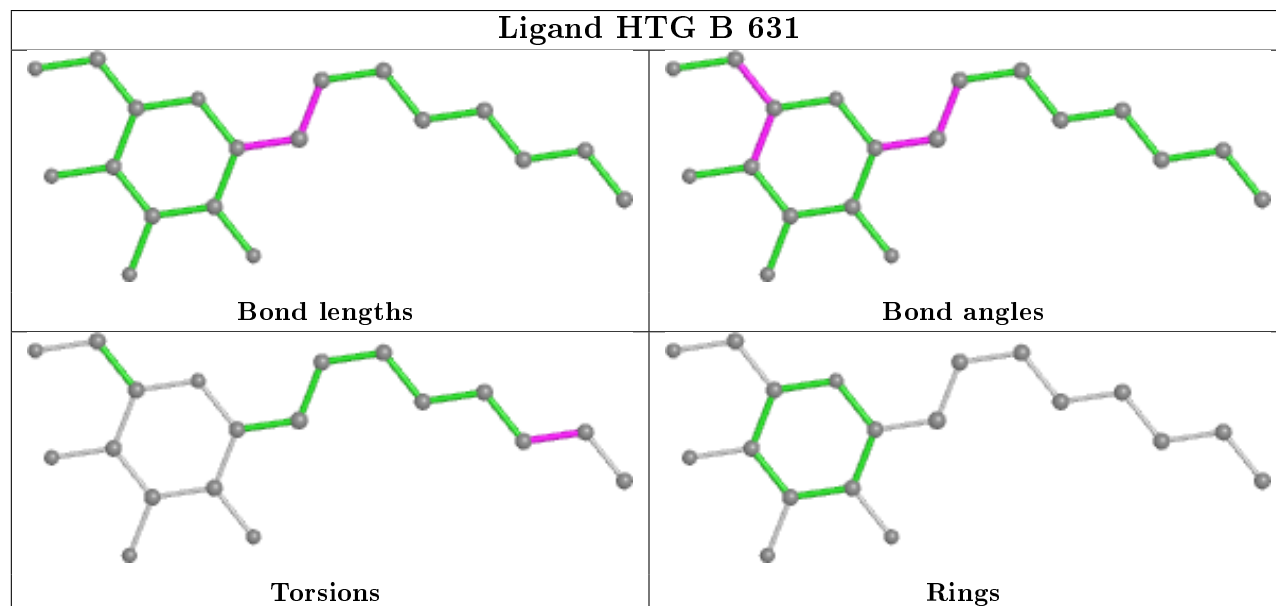
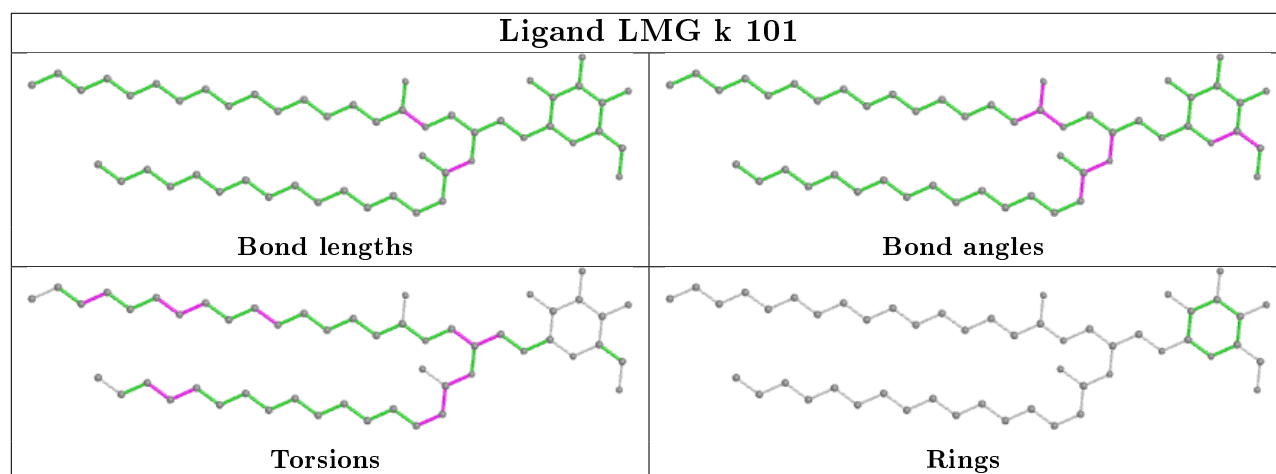
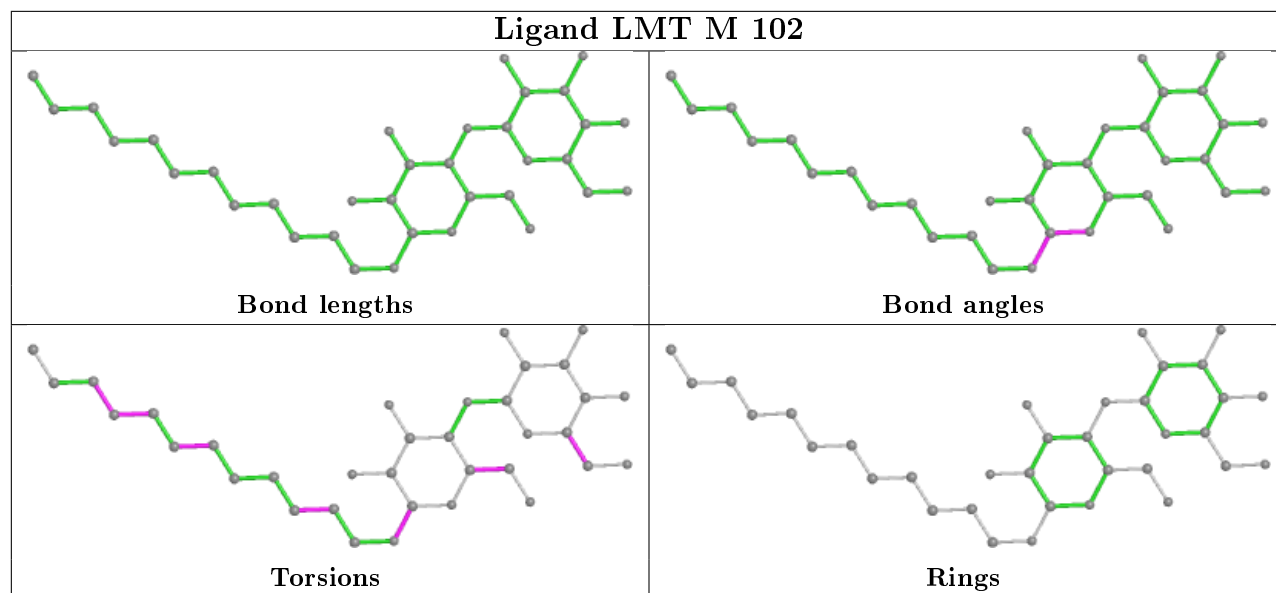


Ligand LMT D 403

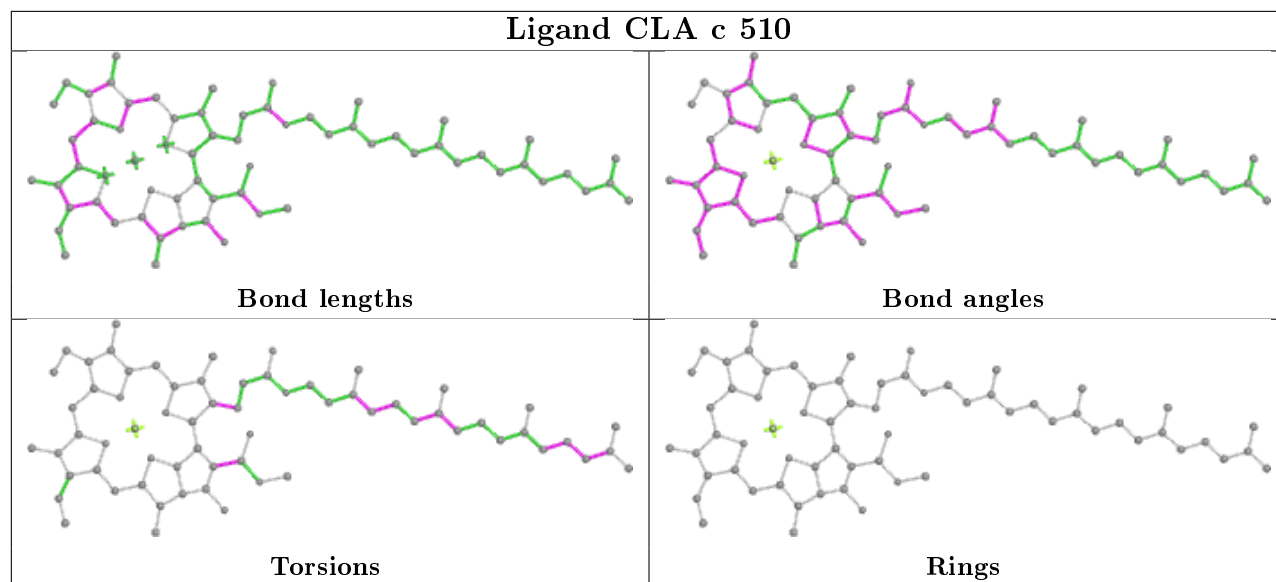




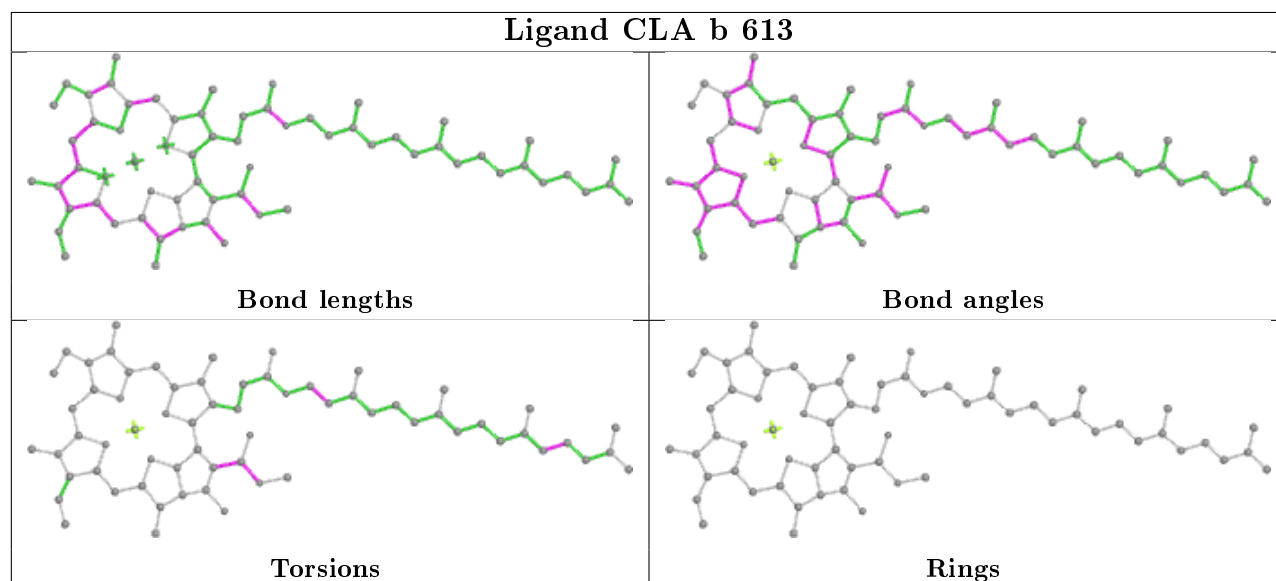




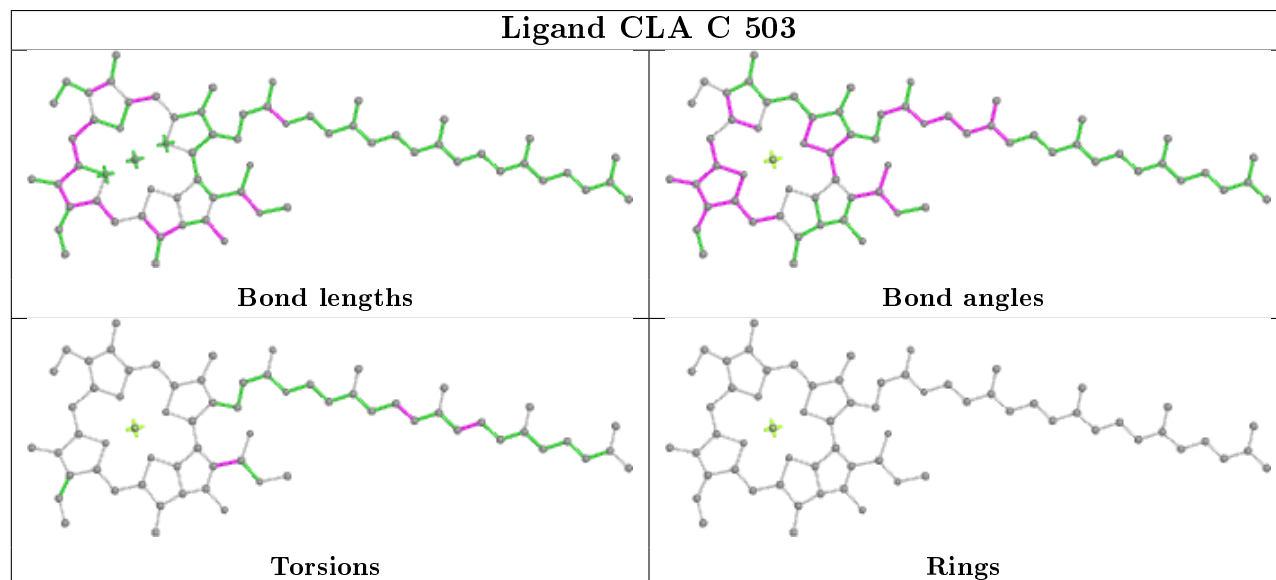
Ligand CLA c 510

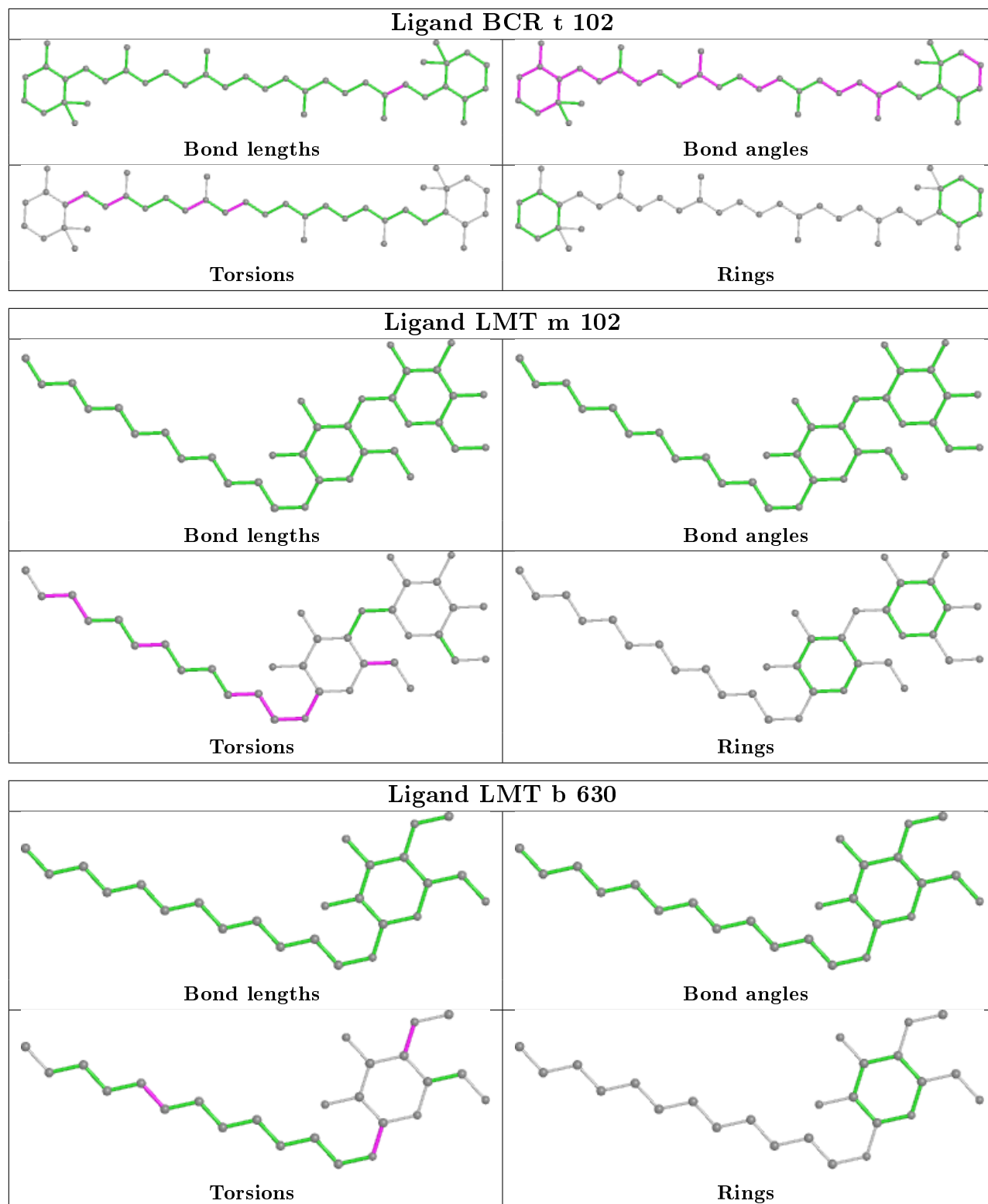


Ligand CLA b 613

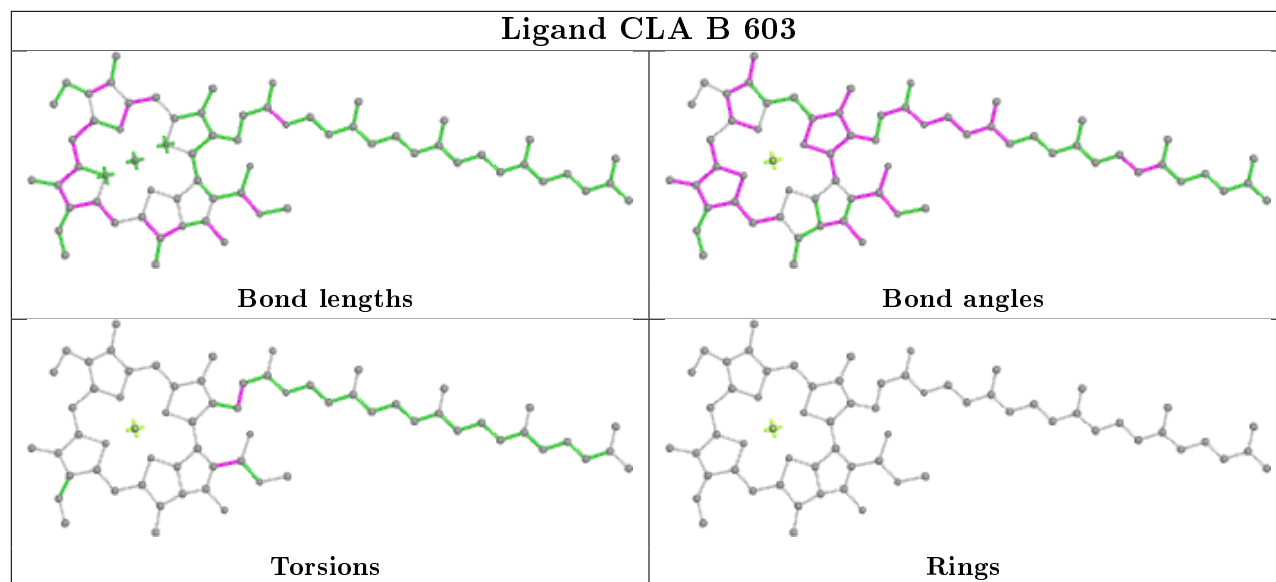


Ligand CLA C 503

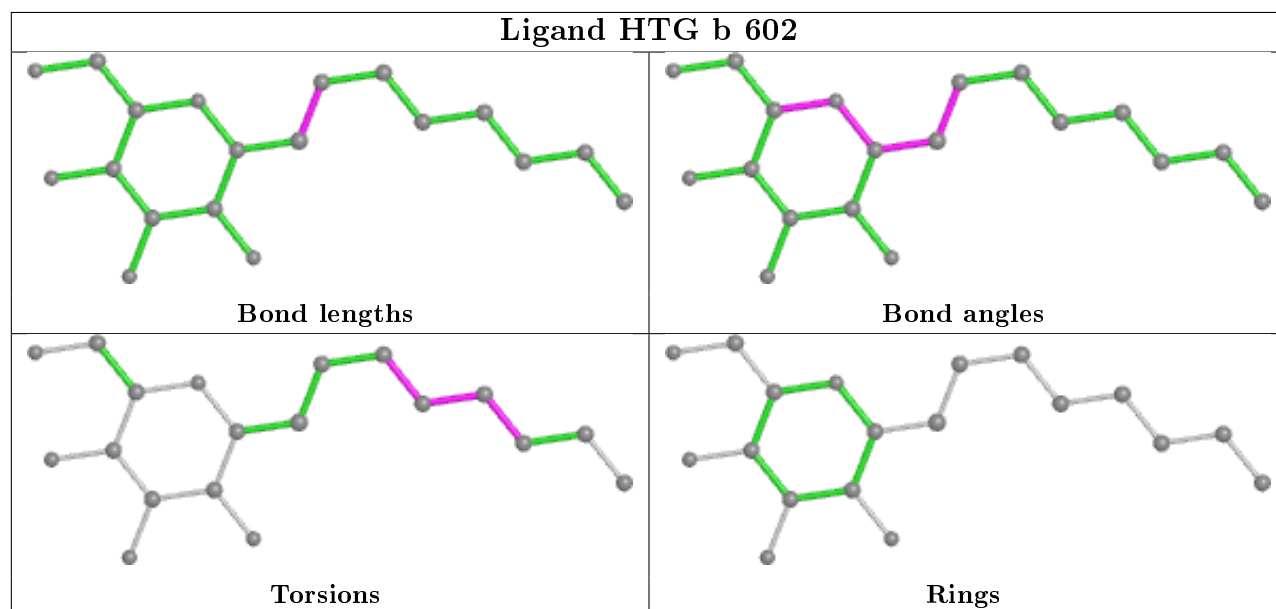




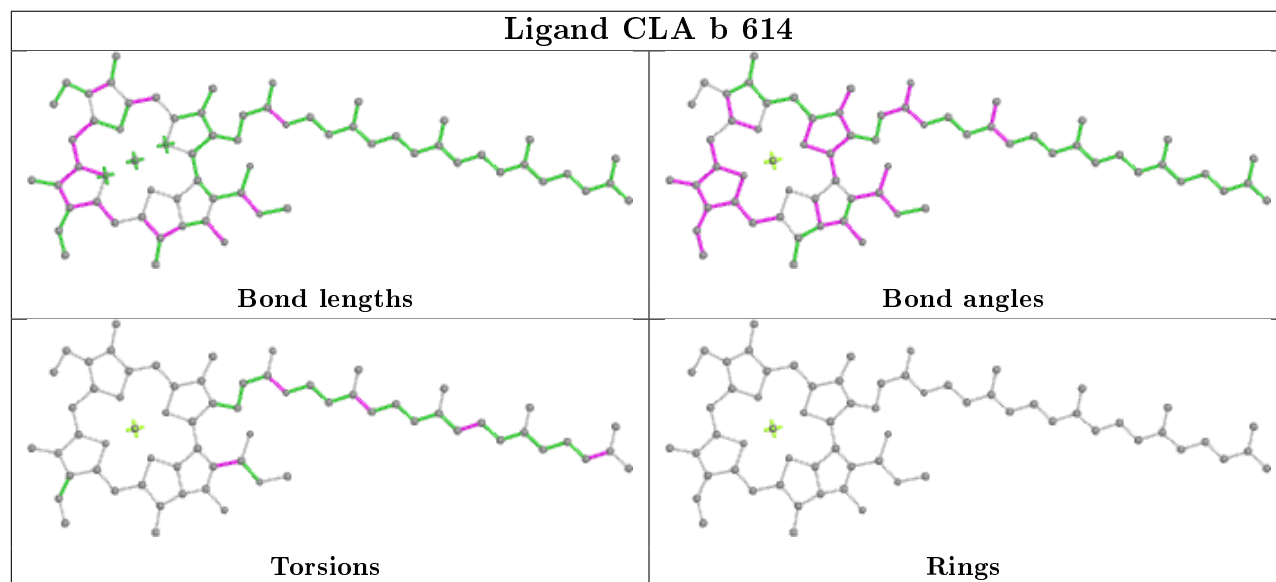
Ligand CLA B 603



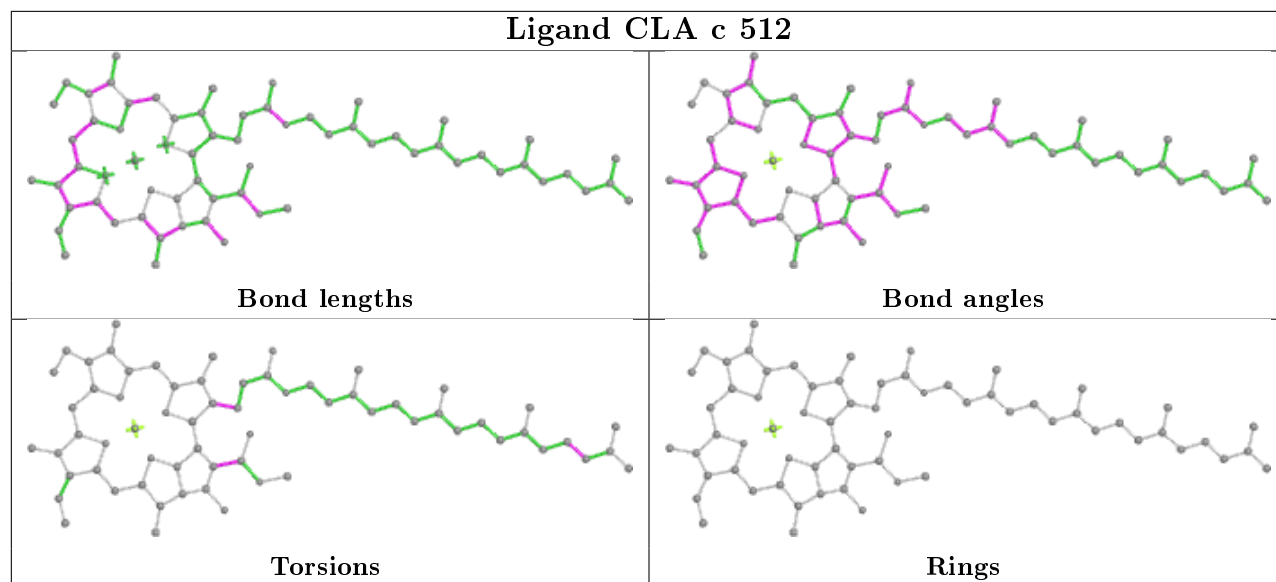
Ligand HTG b 602



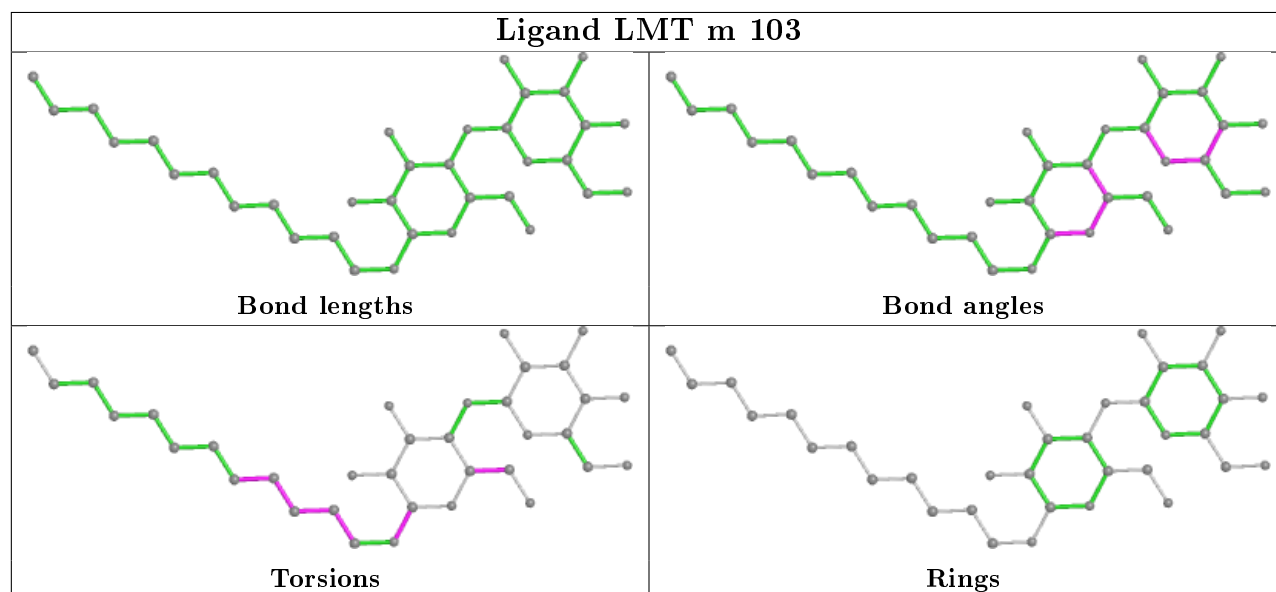
Ligand CLA b 614



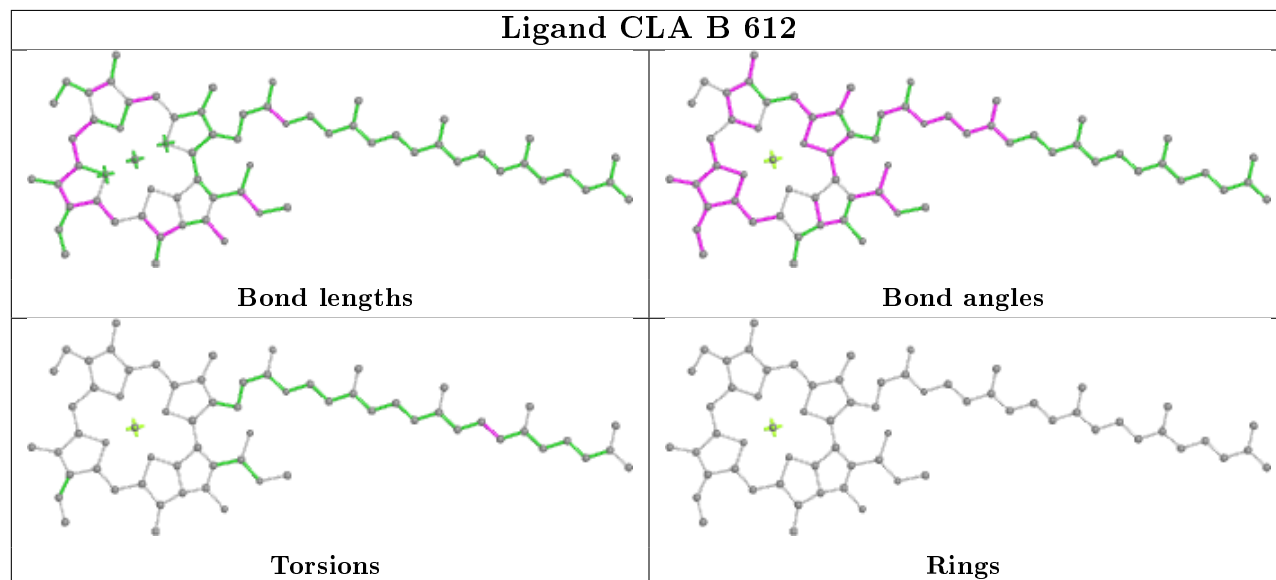
Ligand CLA c 512

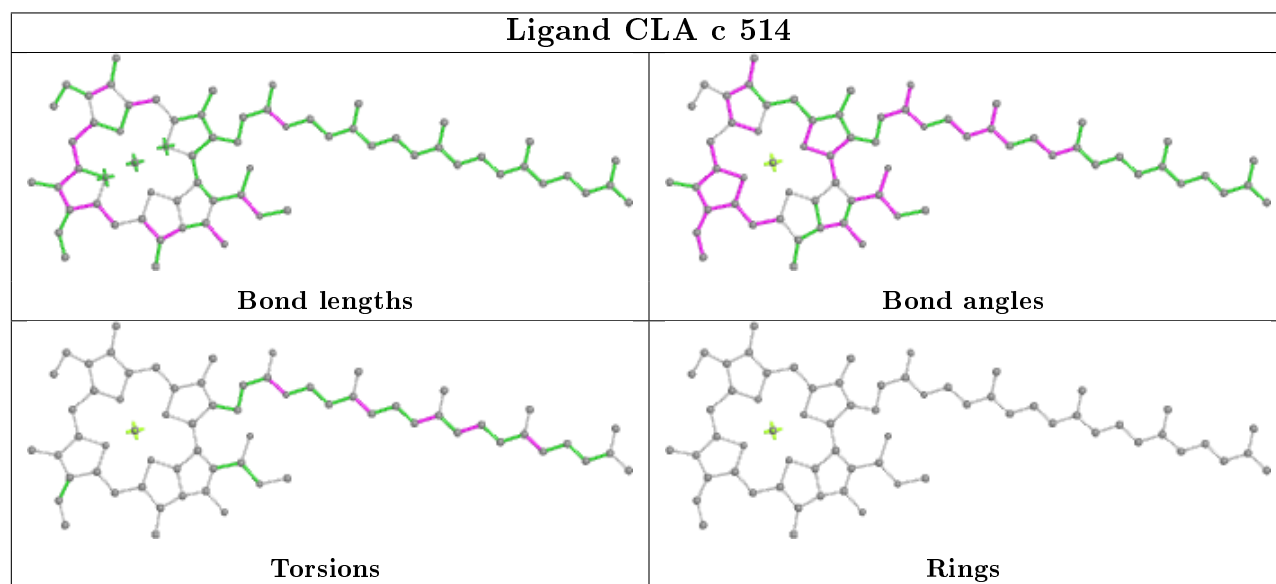
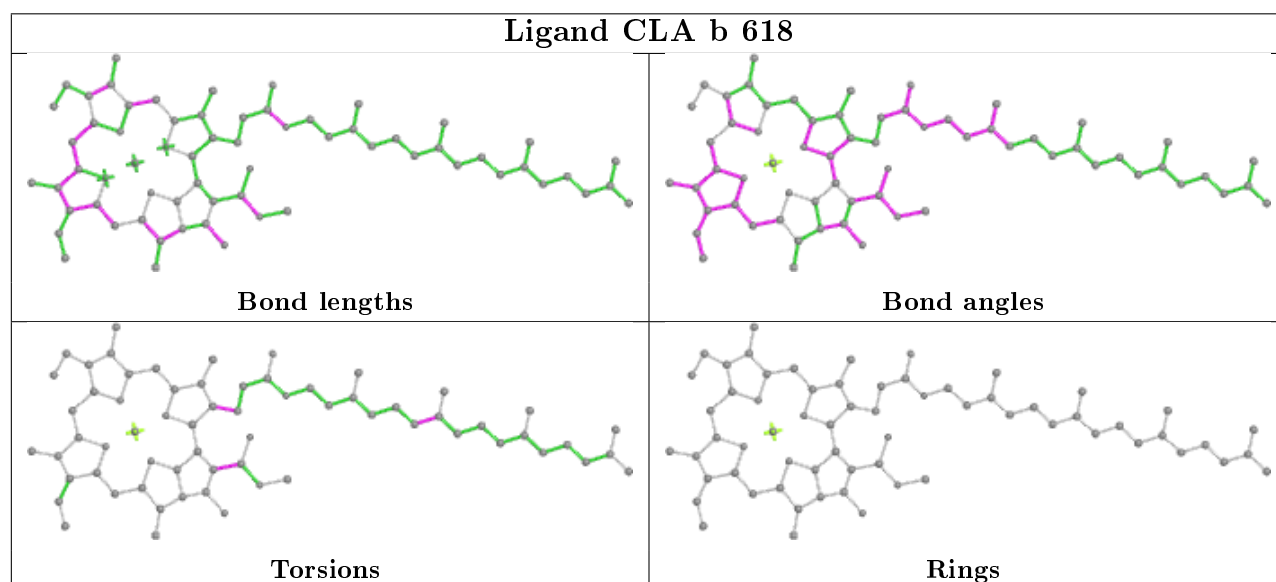
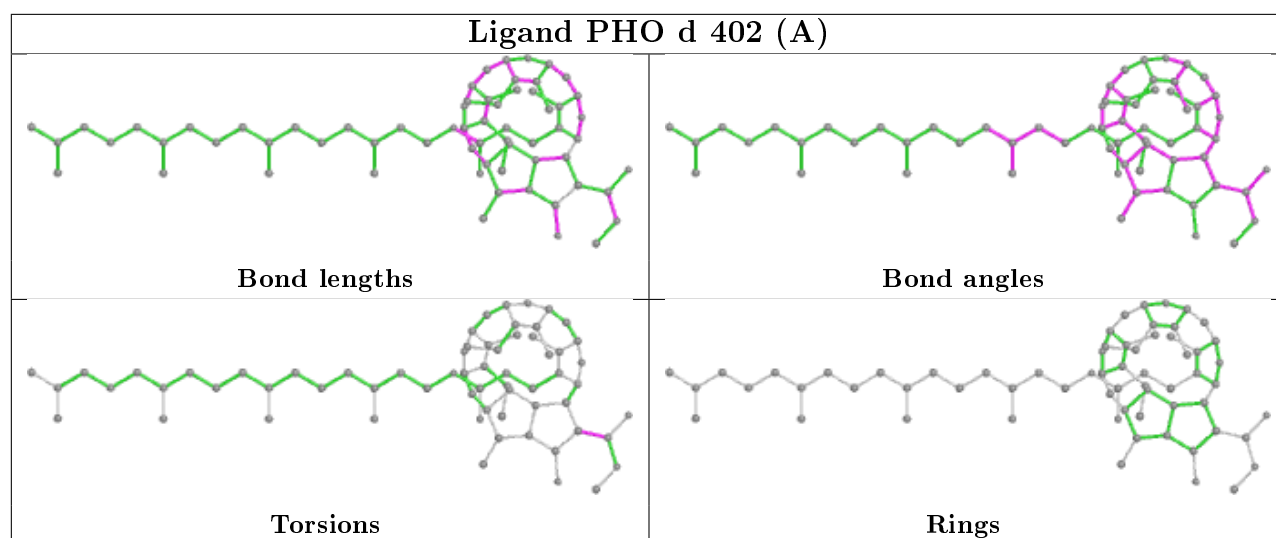


Ligand LMT m 103

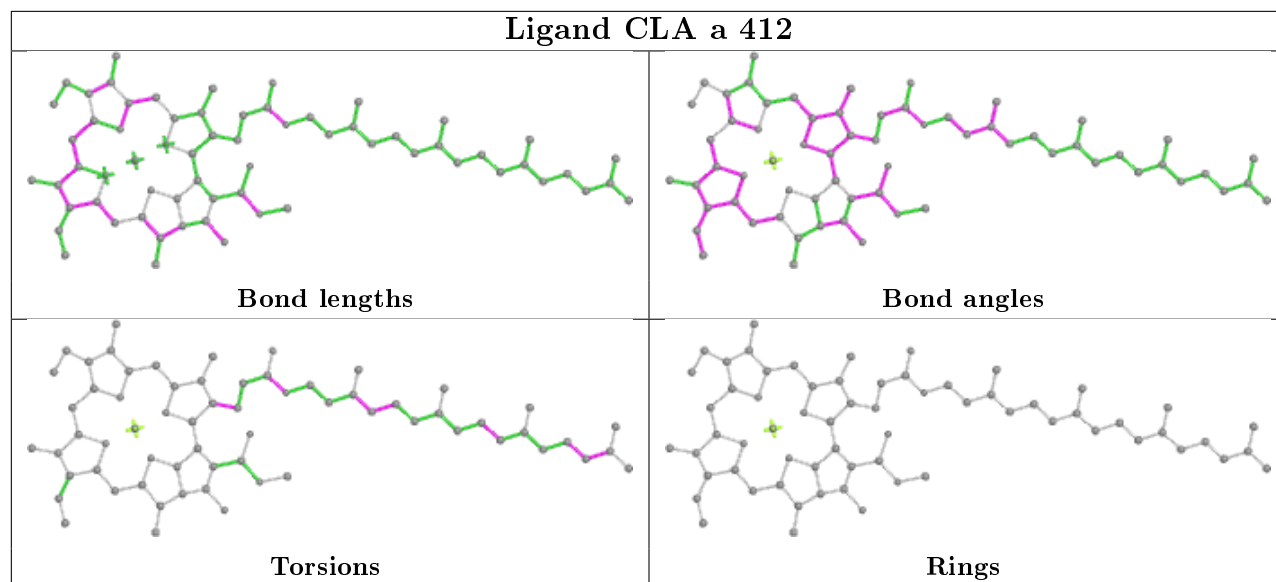


Ligand CLA B 612

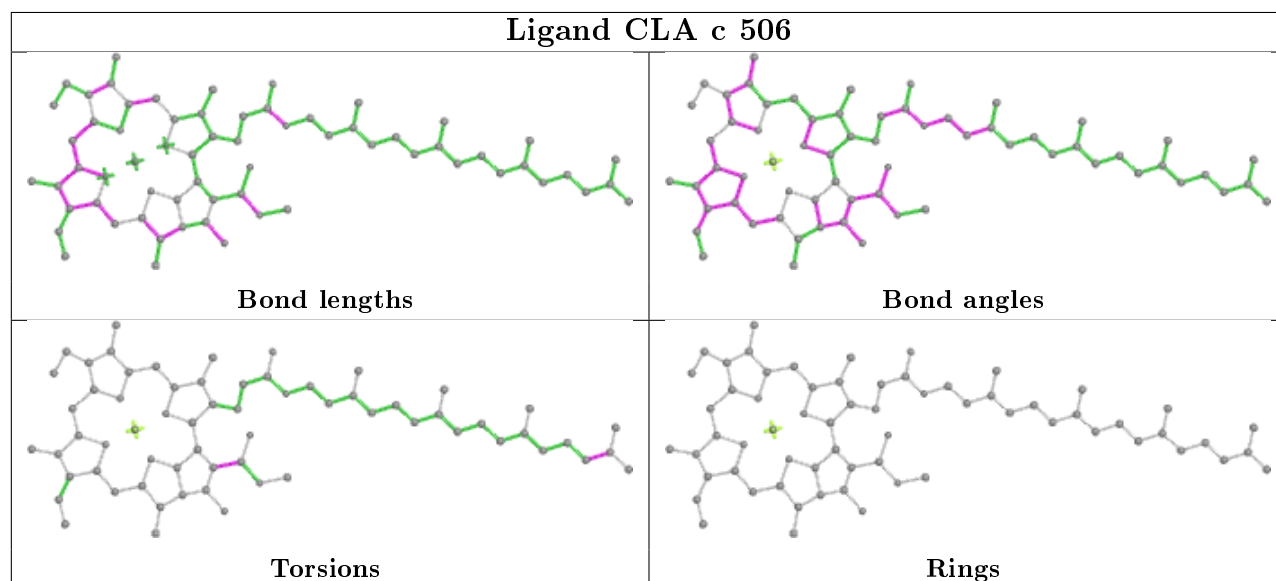




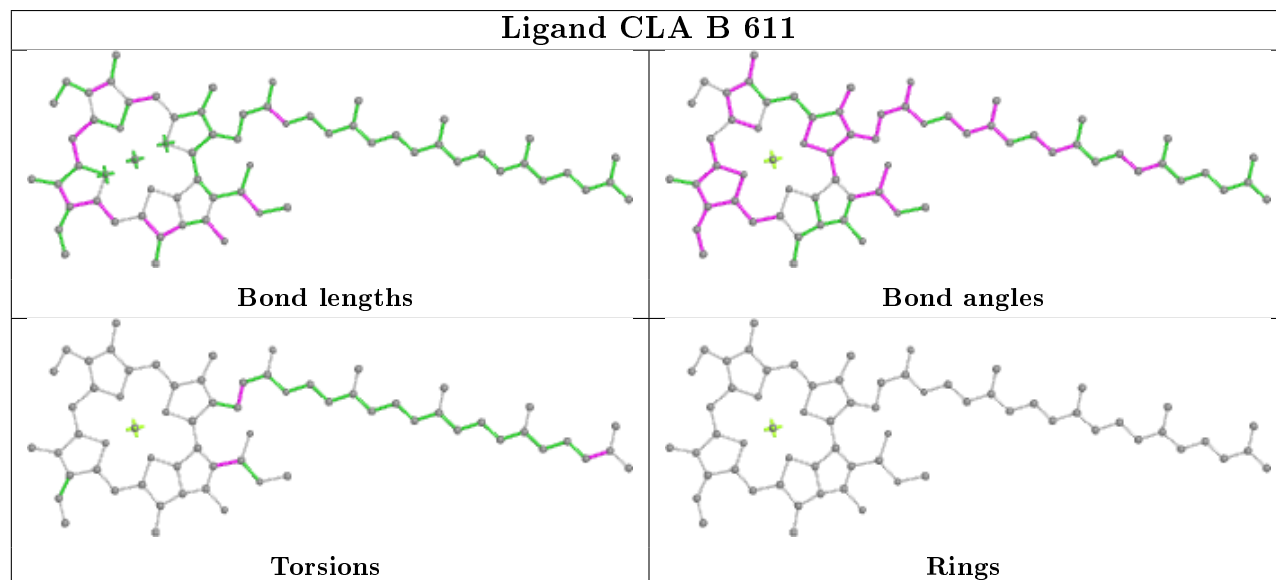
Ligand CLA a 412

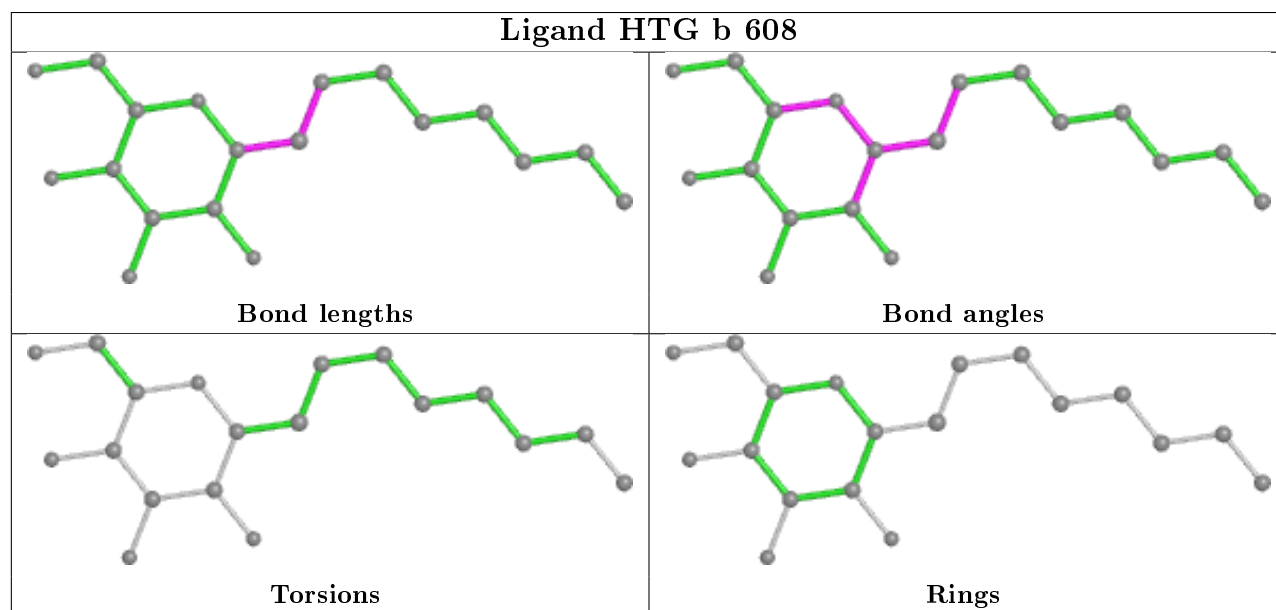
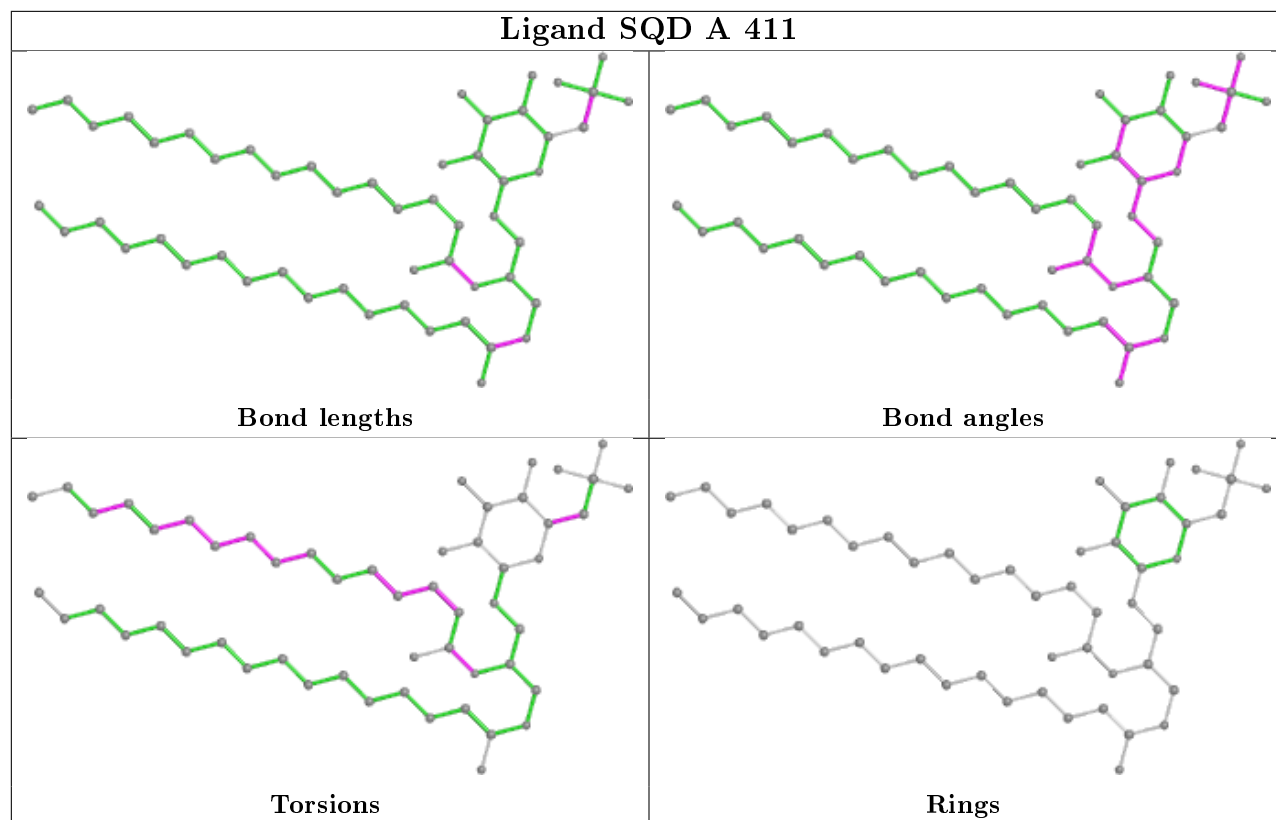


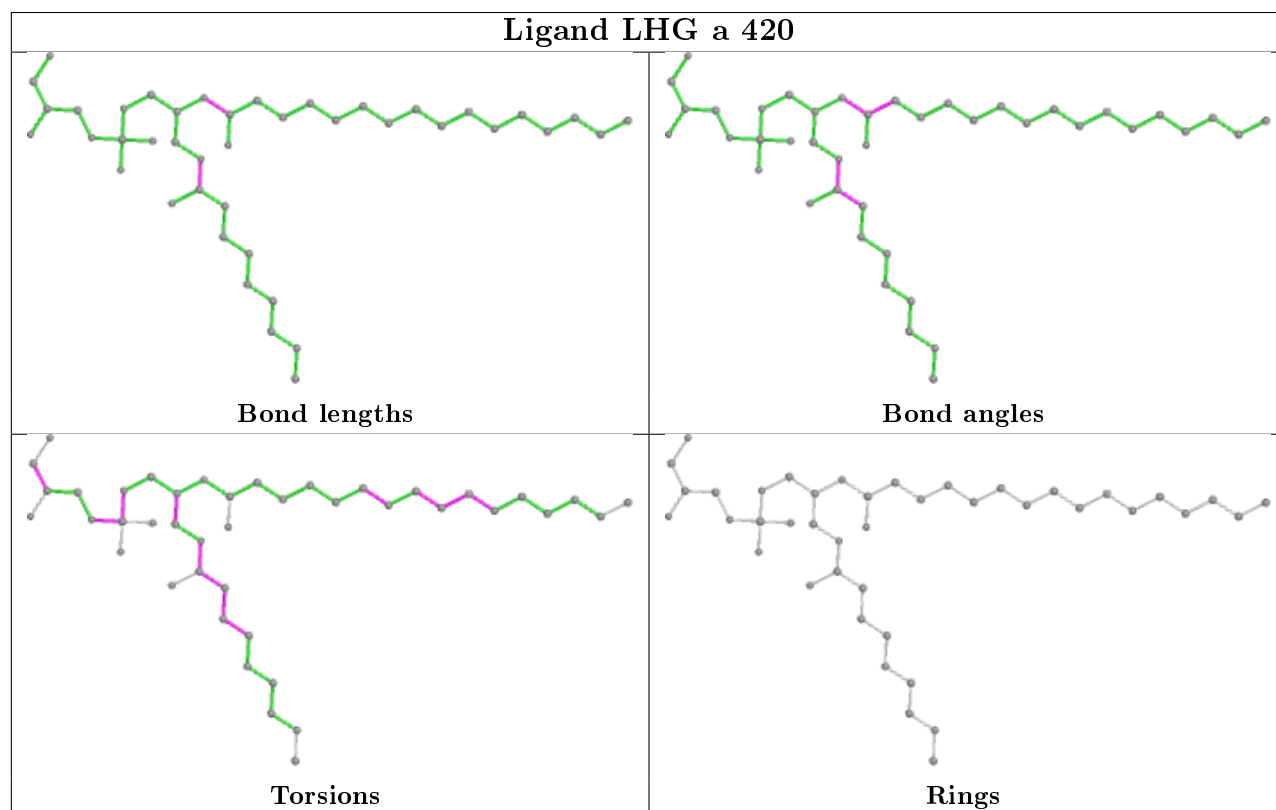
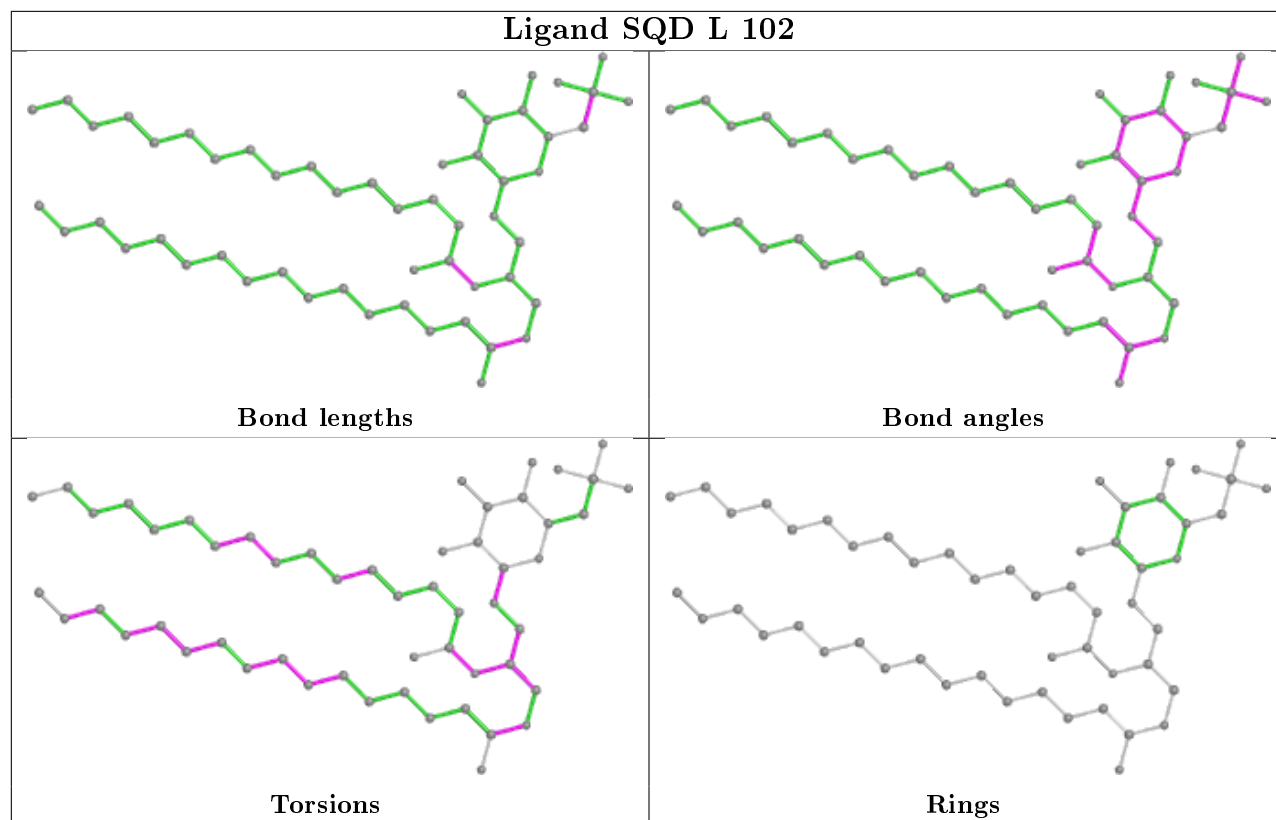
Ligand CLA c 506



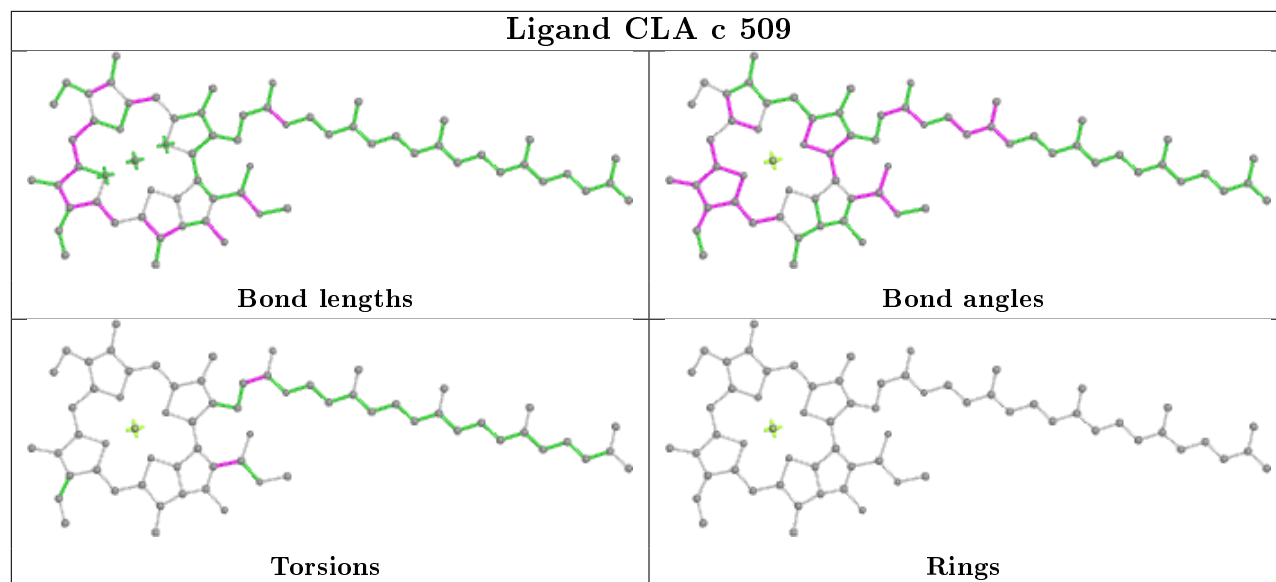
Ligand CLA B 611



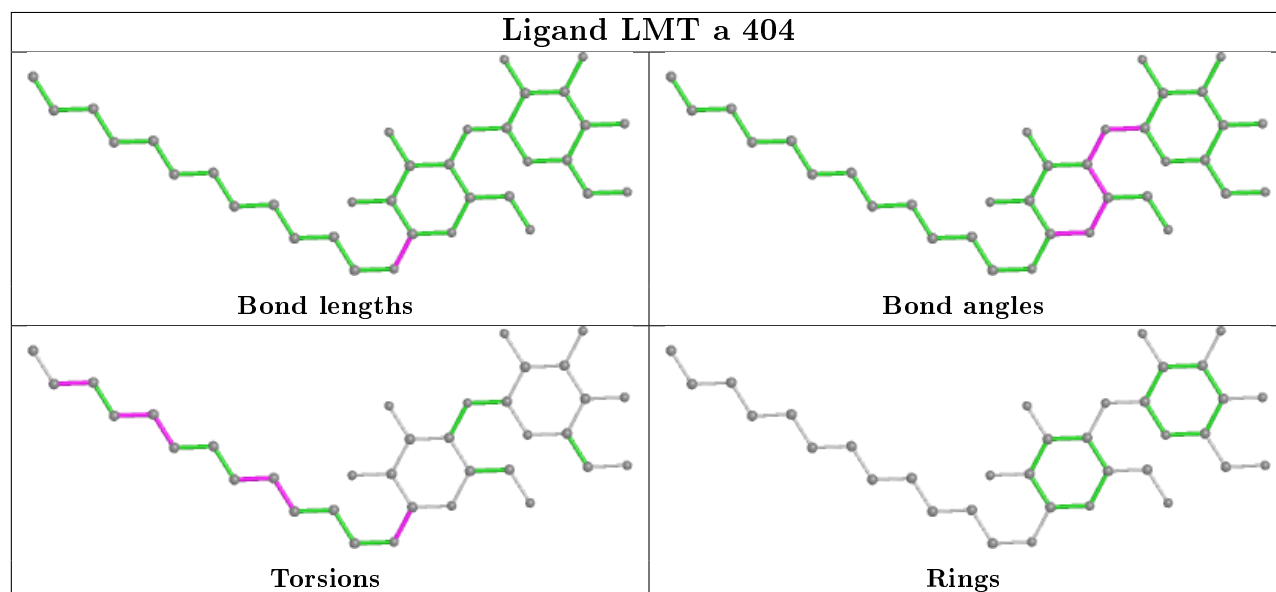




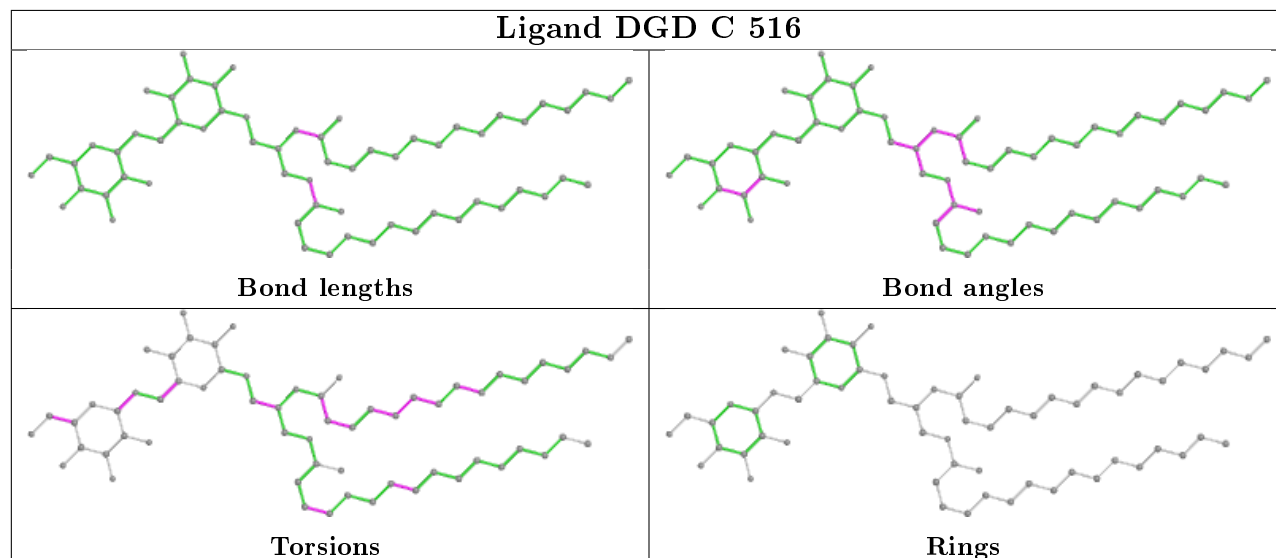
Ligand CLA c 509

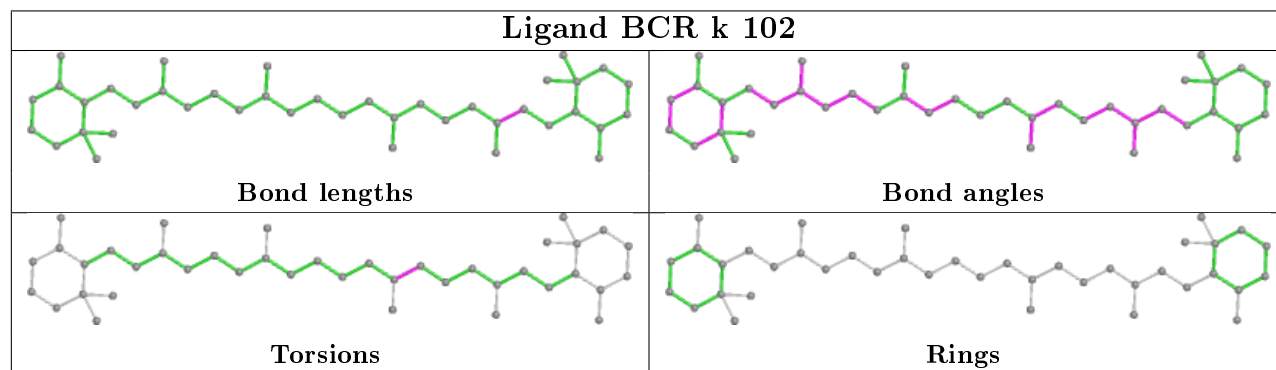
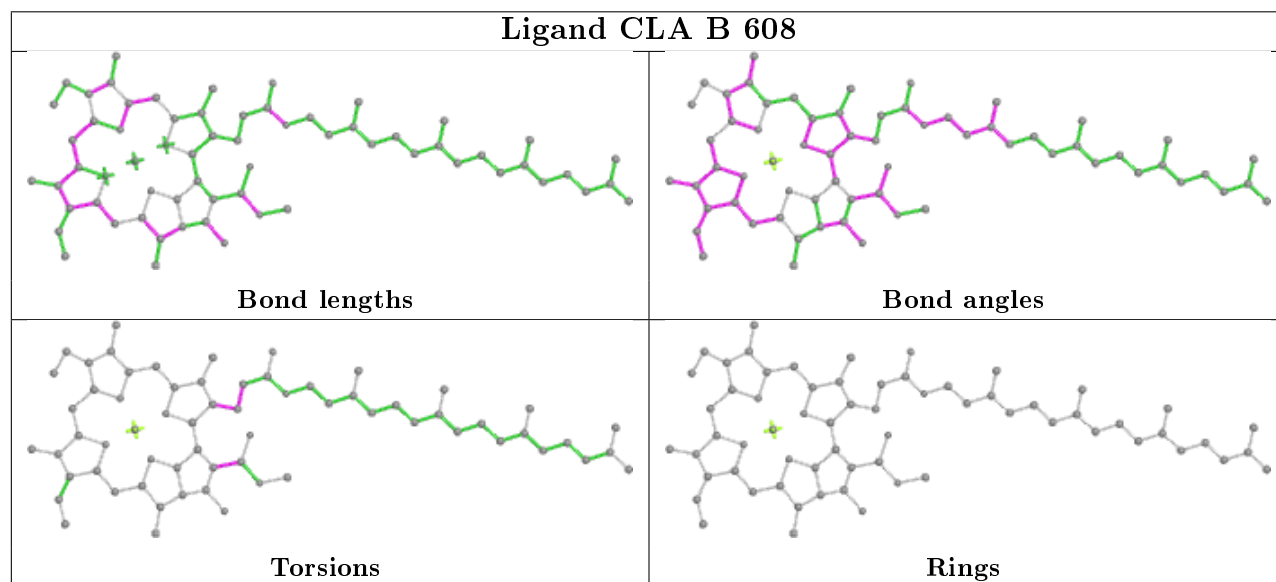
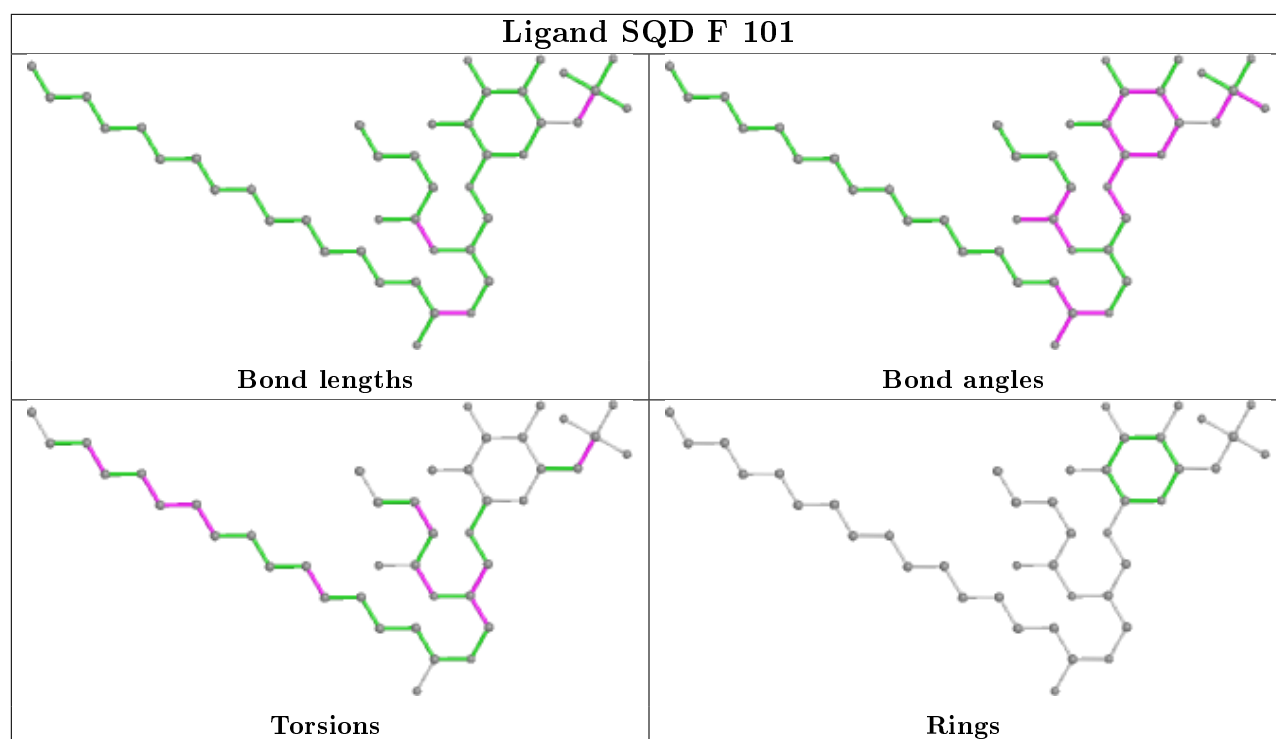


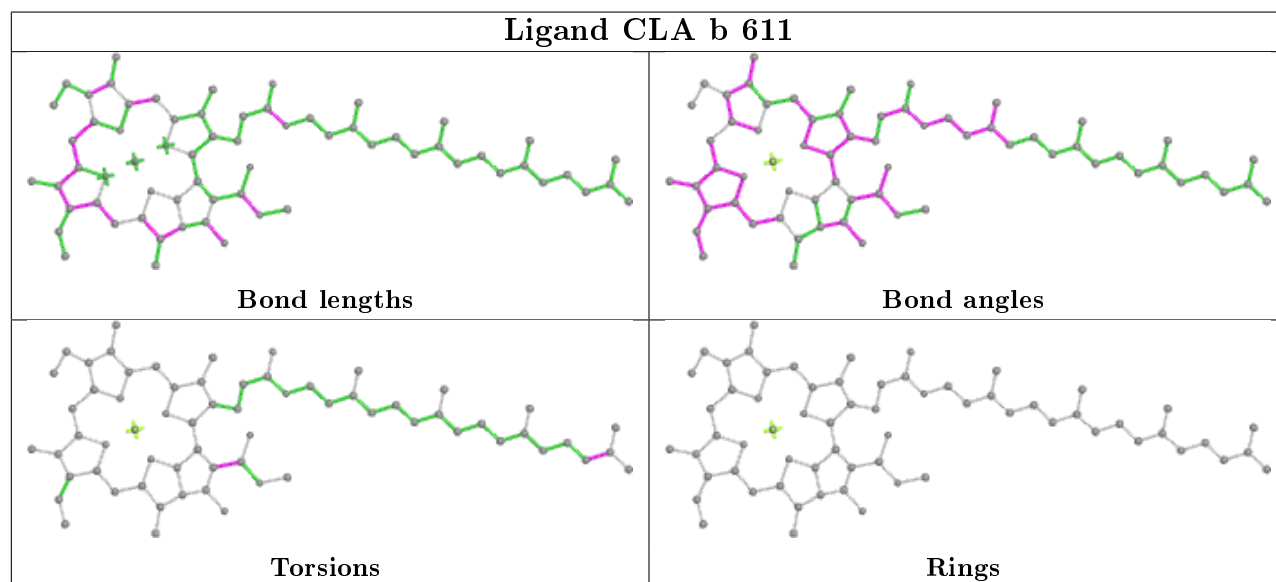
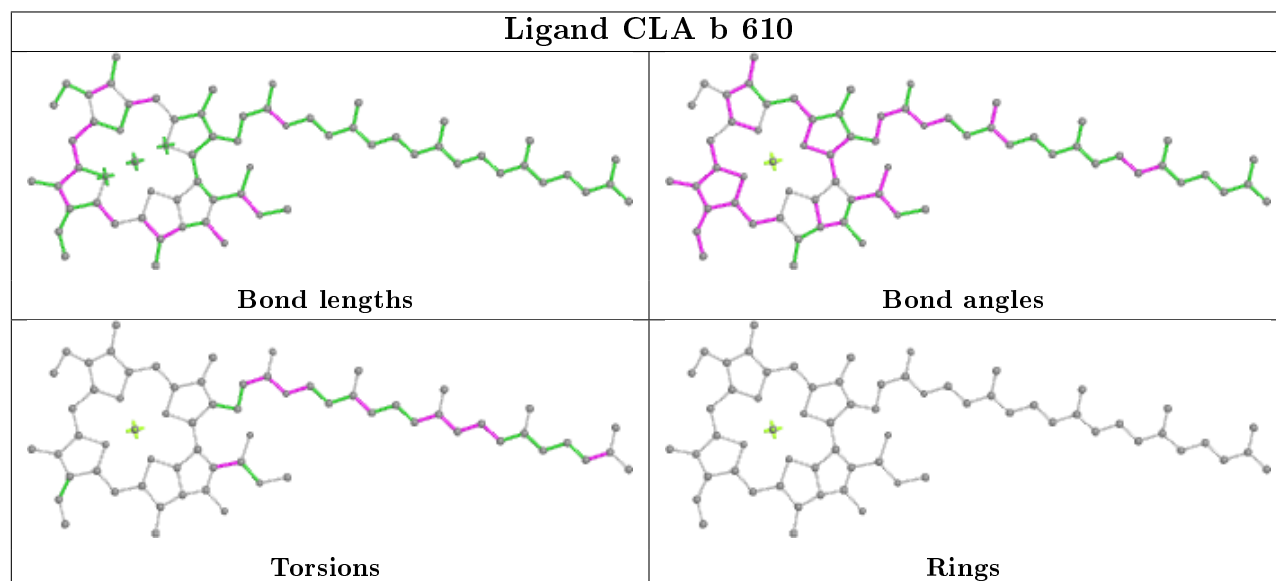
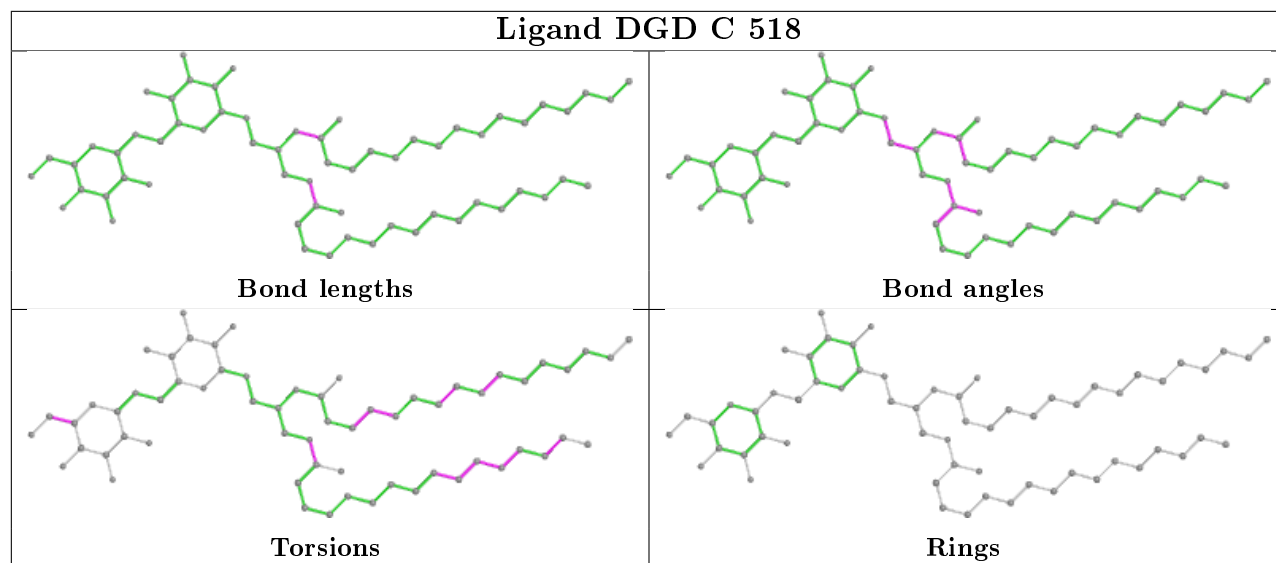
Ligand LMT a 404

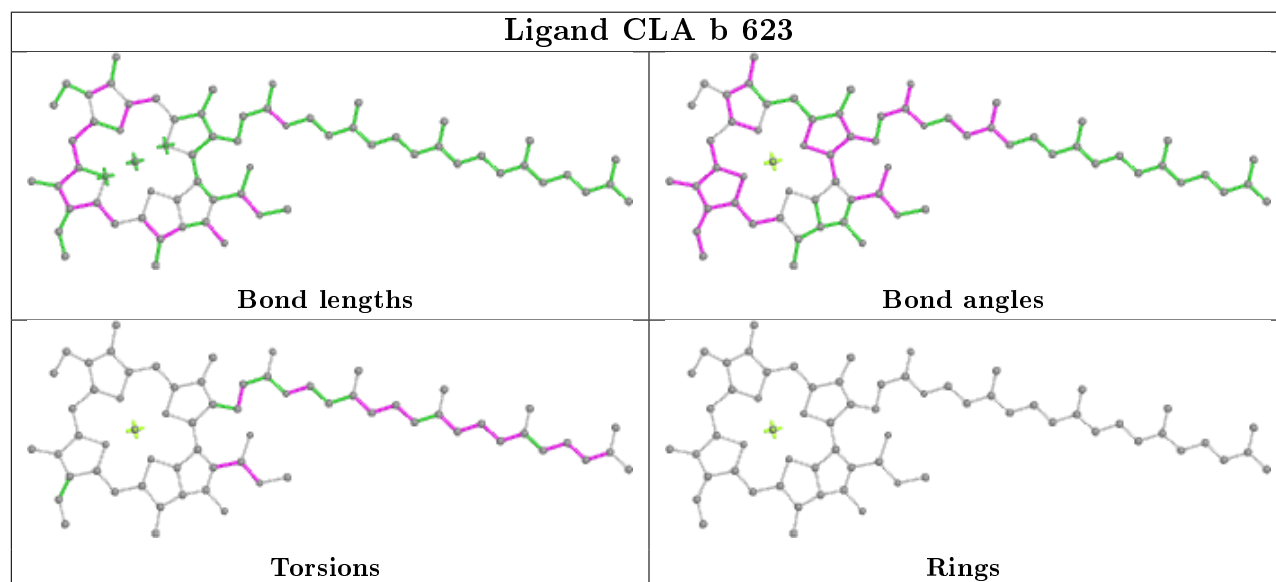
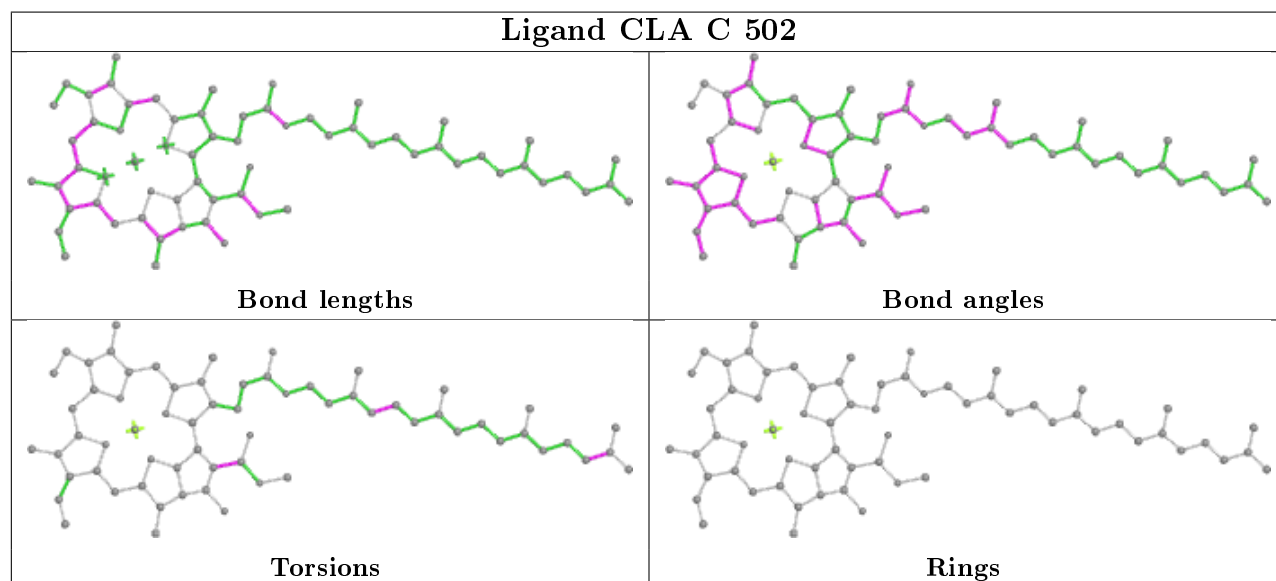
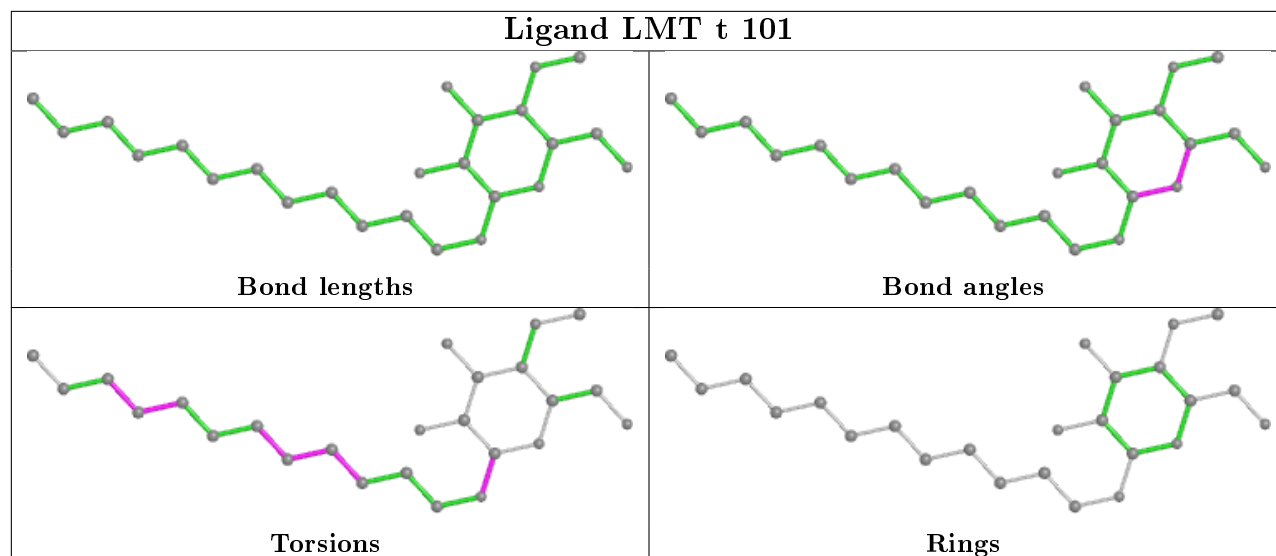


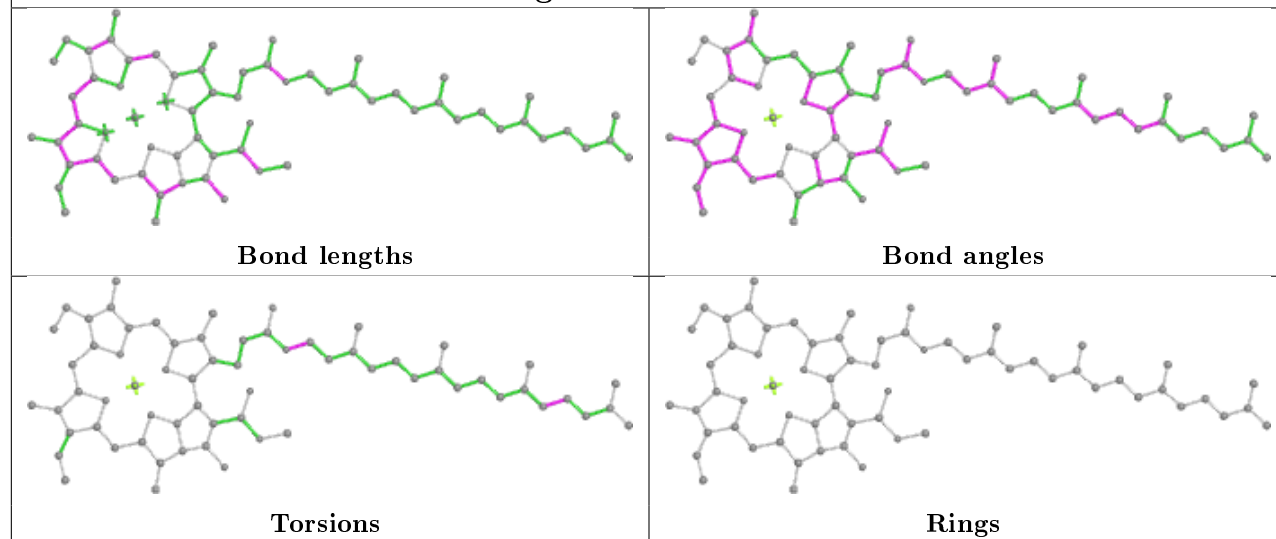
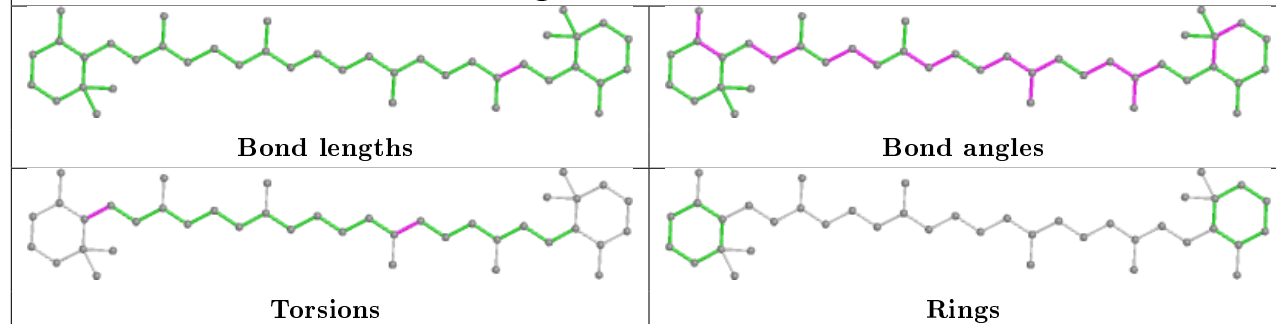
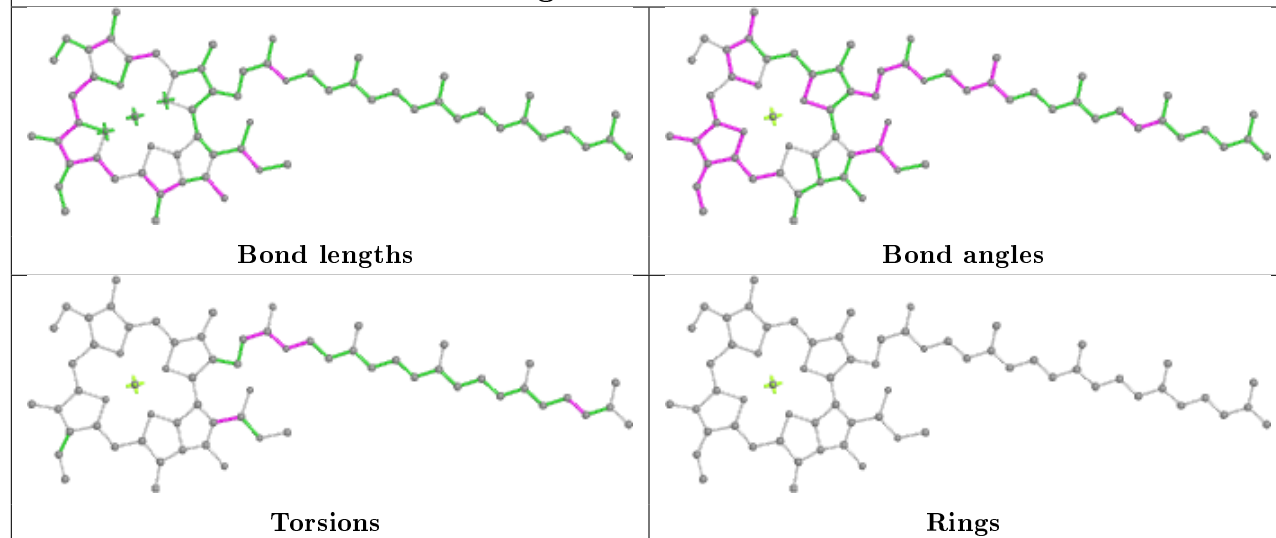
Ligand DGD C 516

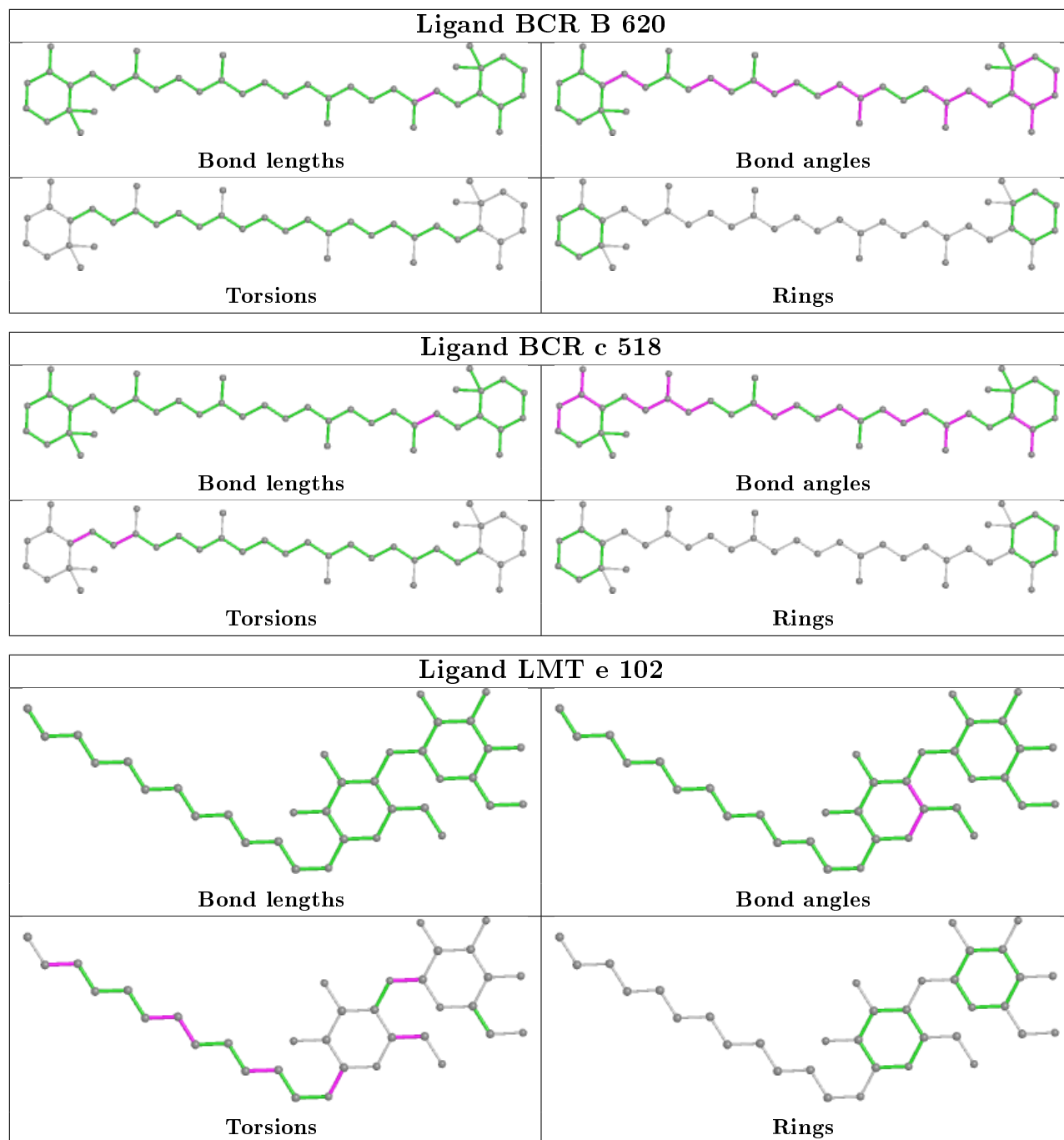




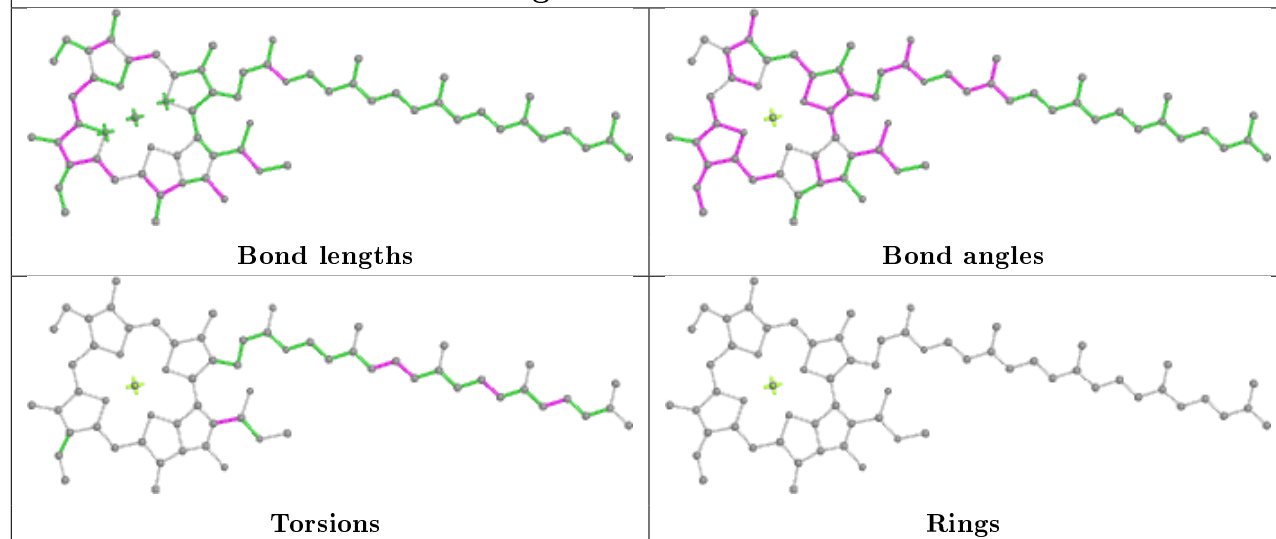




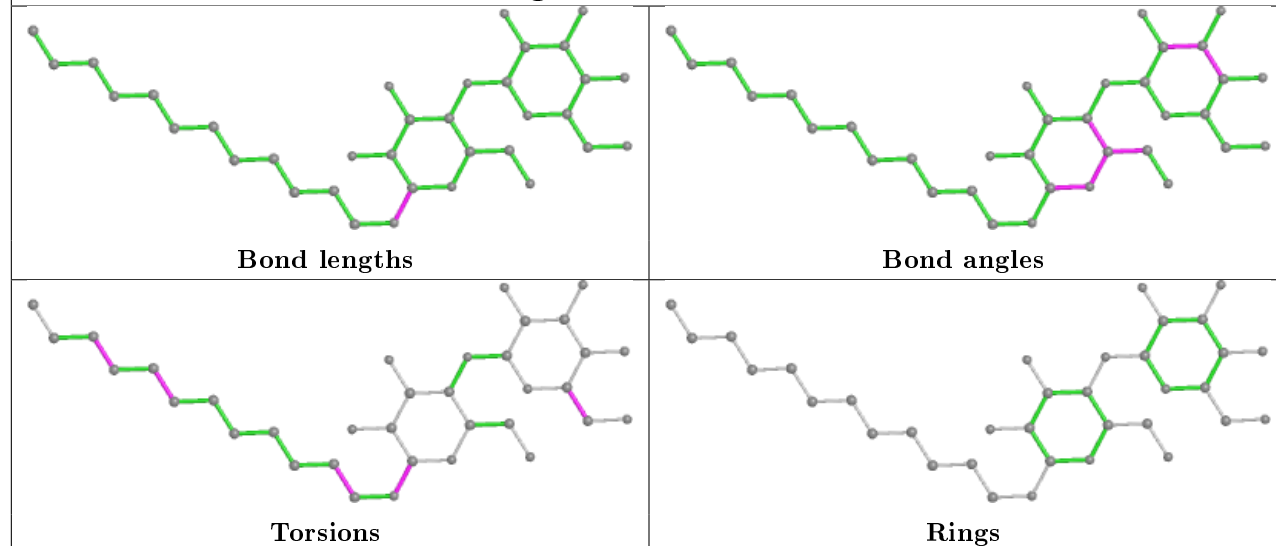
Ligand CLA b 617**Ligand BCR b 626****Ligand CLA c 516**



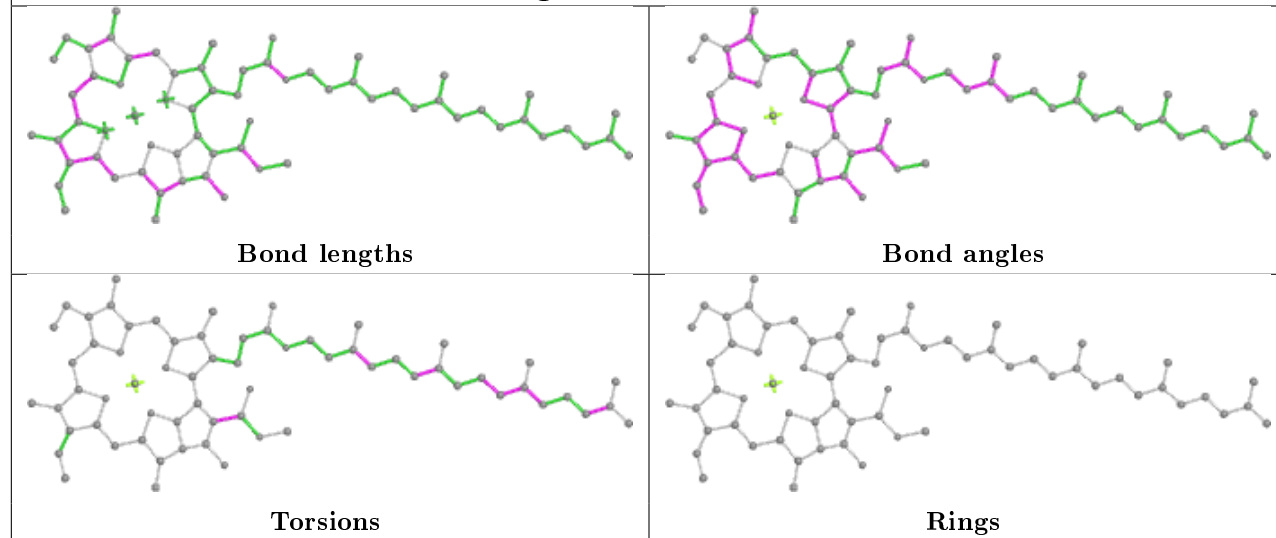
Ligand CLA C 508

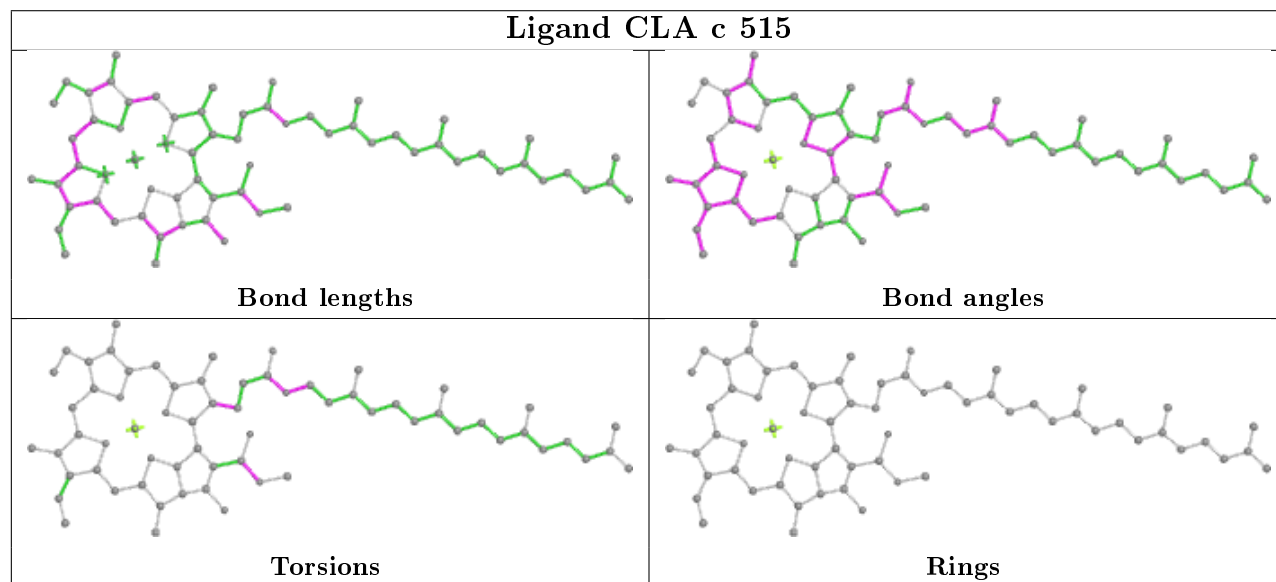
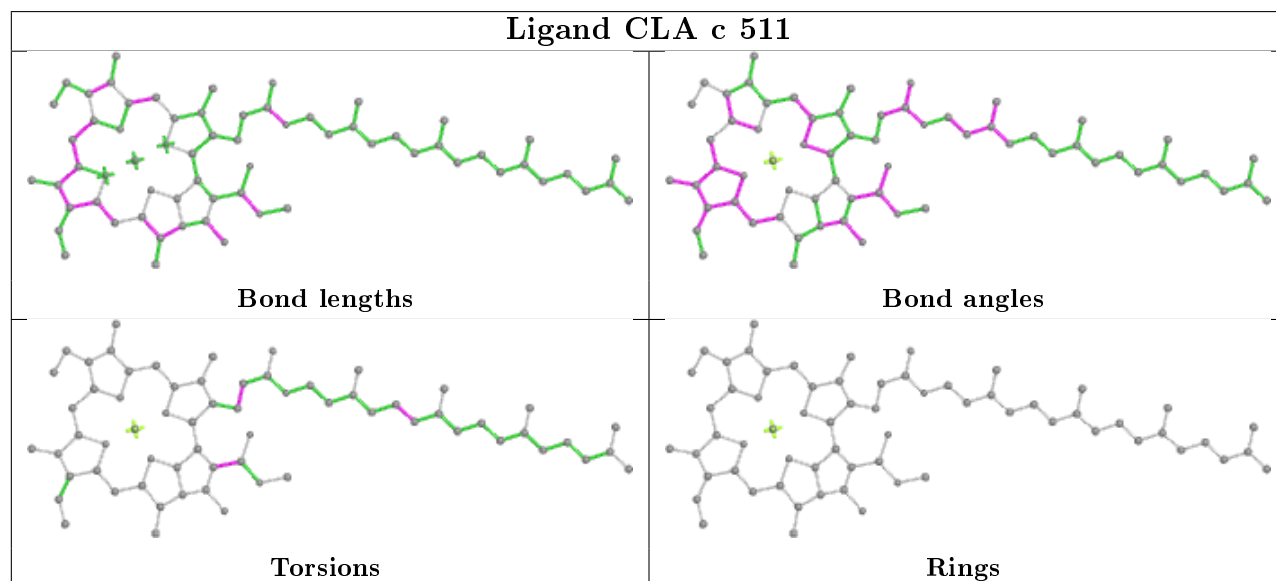
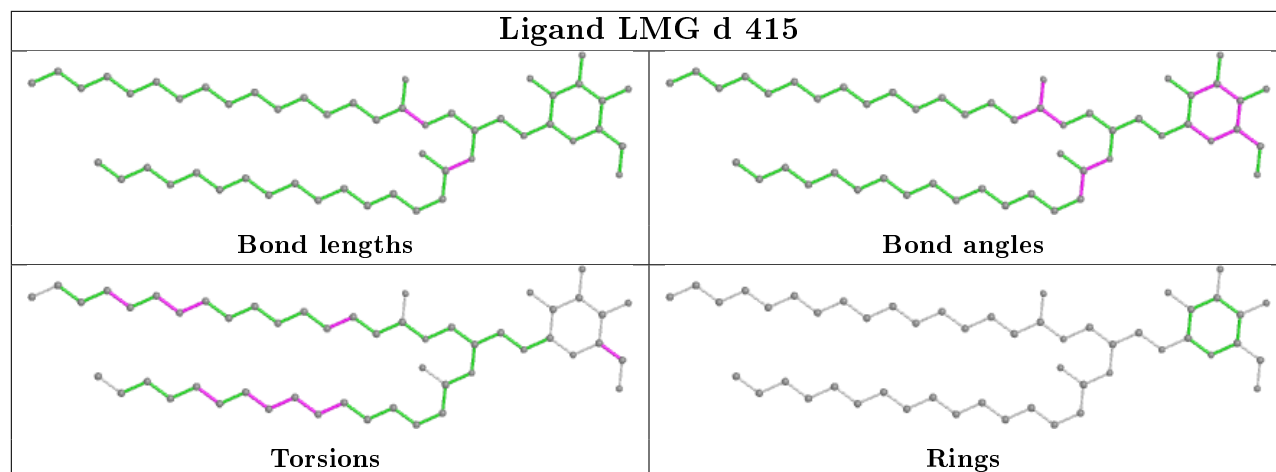


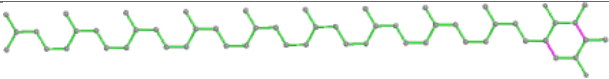
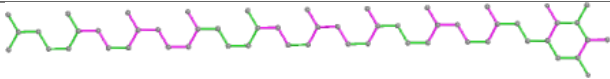
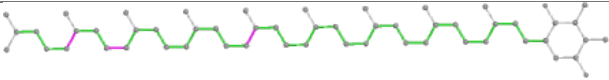
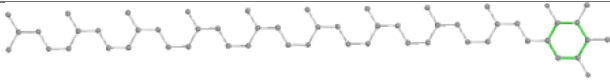
Ligand LMT A 414

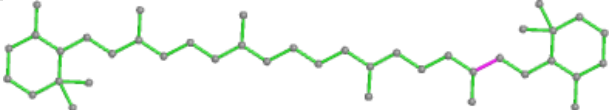
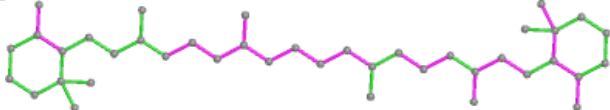
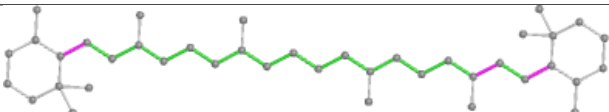
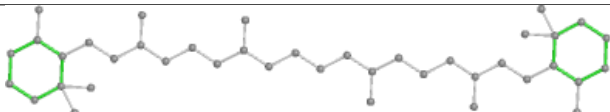


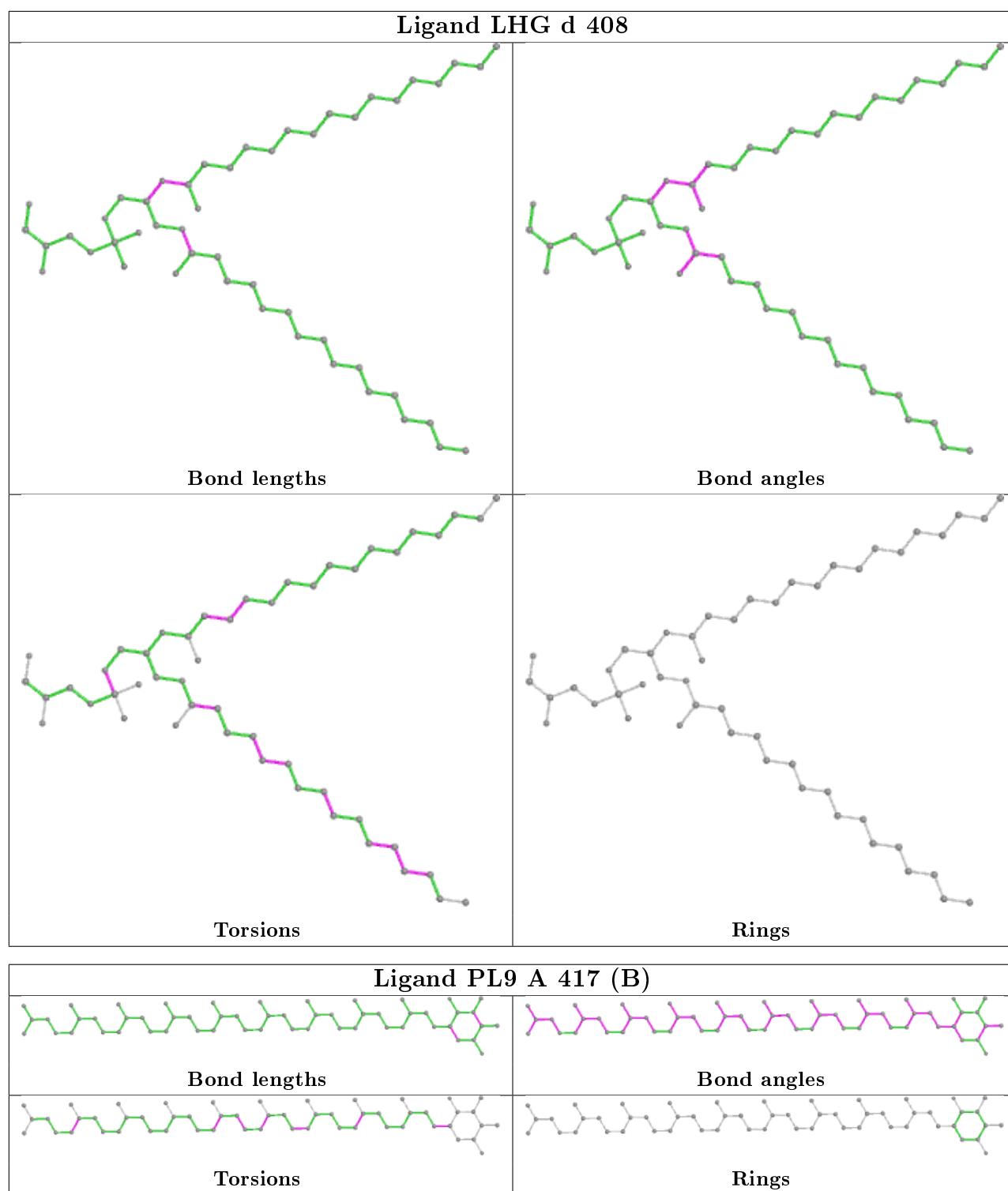
Ligand CLA b 625

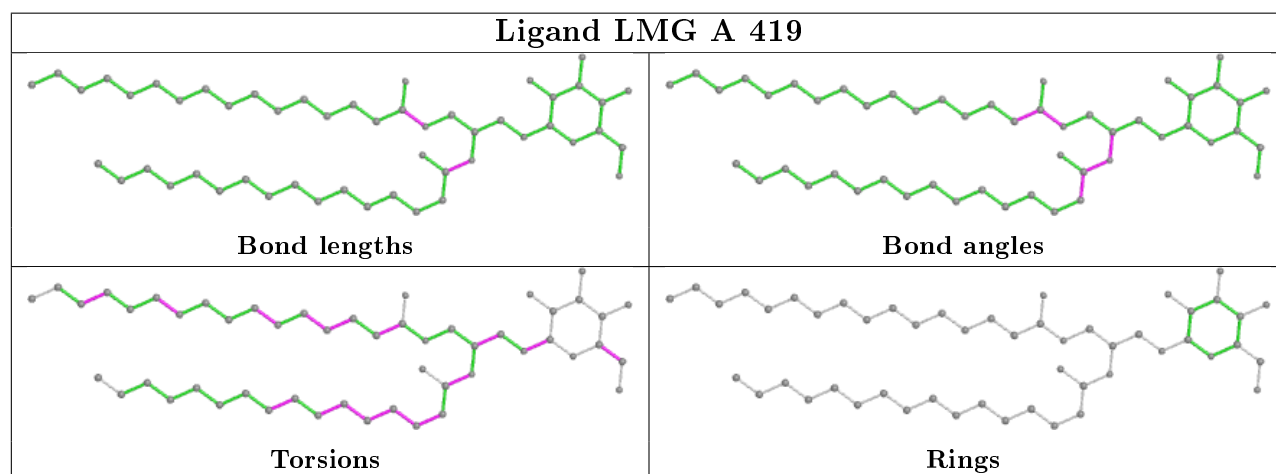
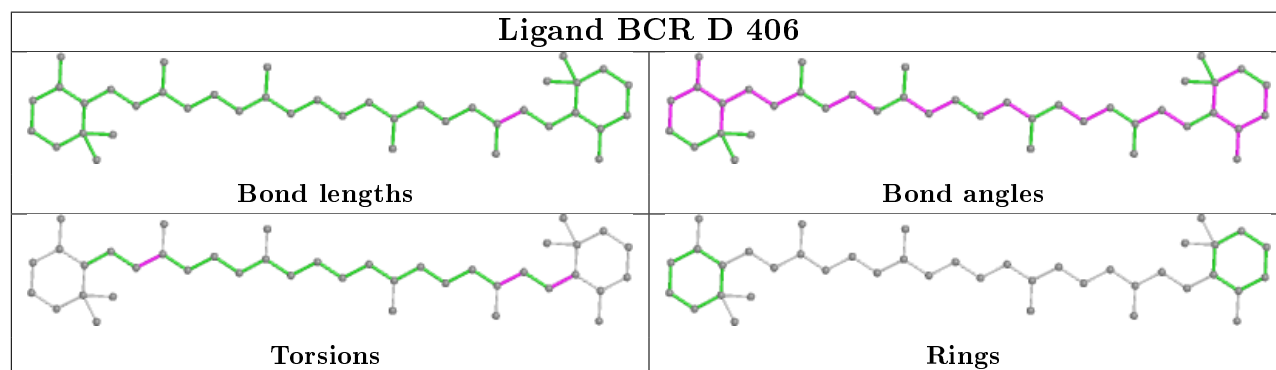
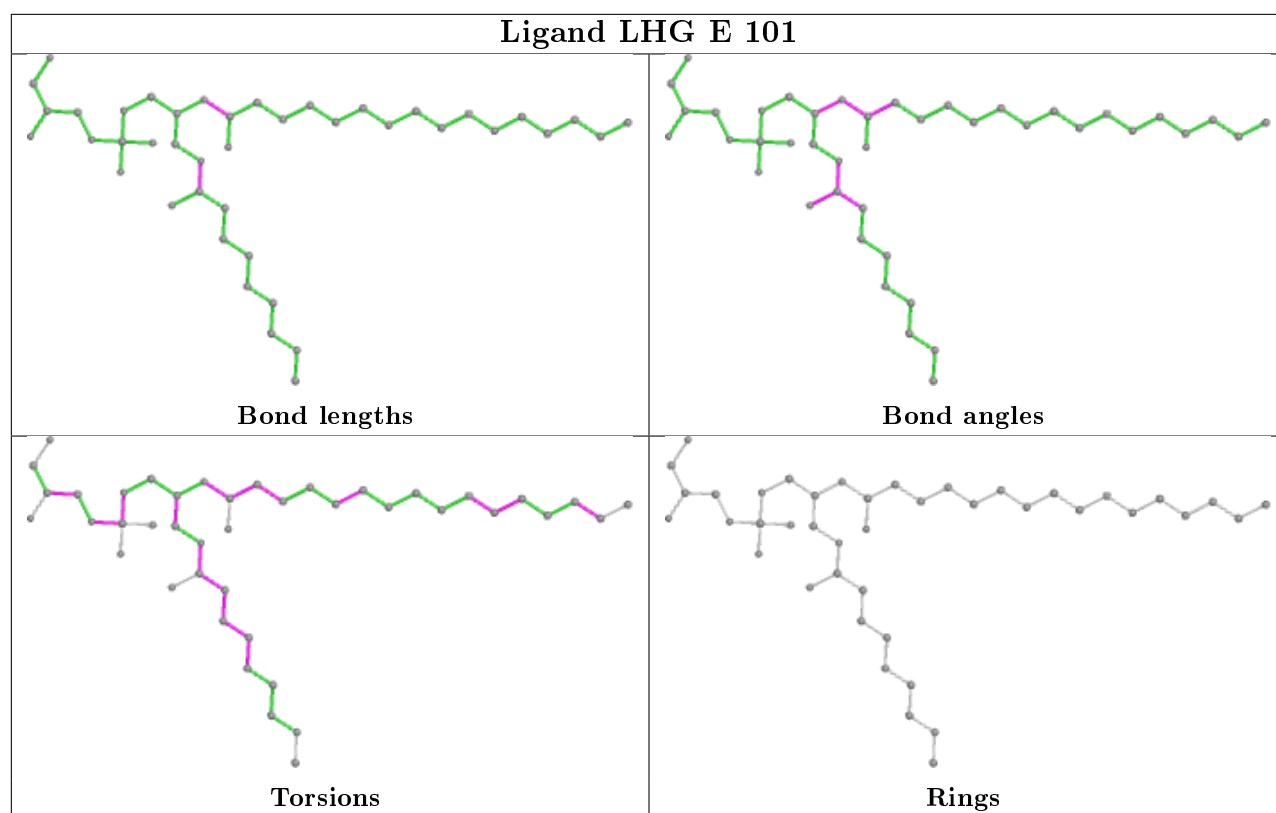




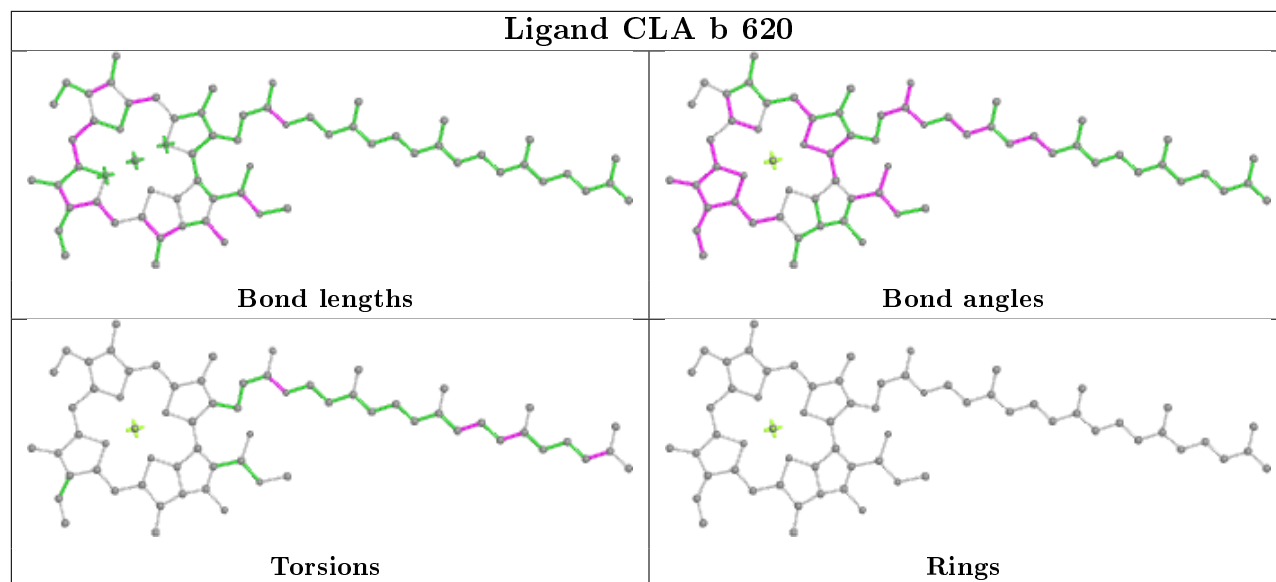
Ligand PL9 d 407 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR Y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

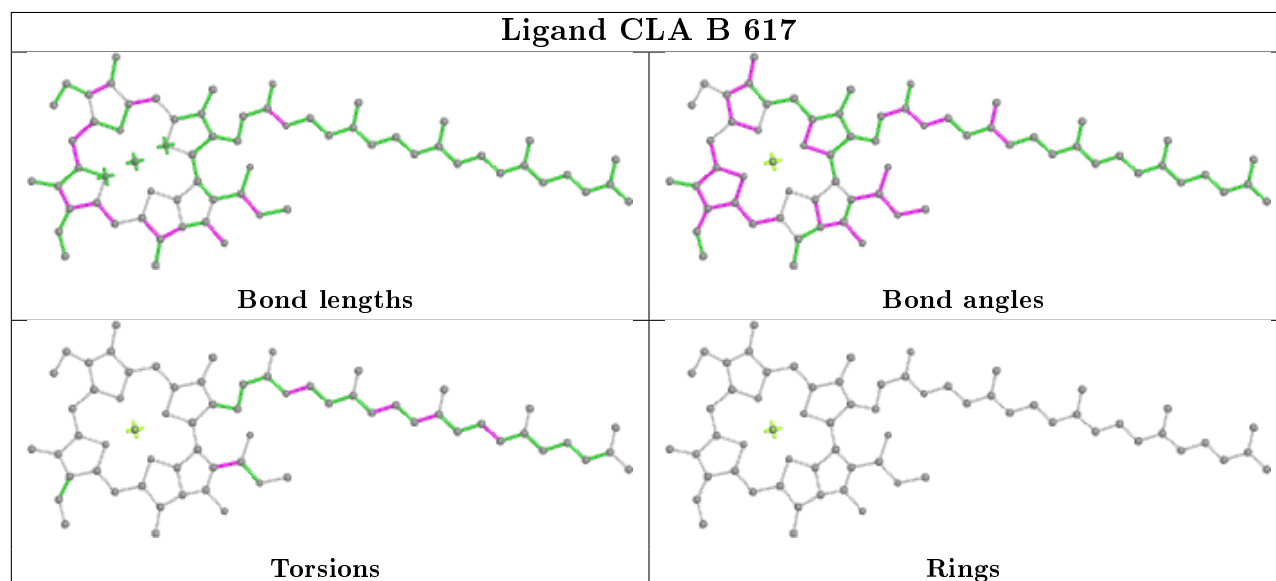




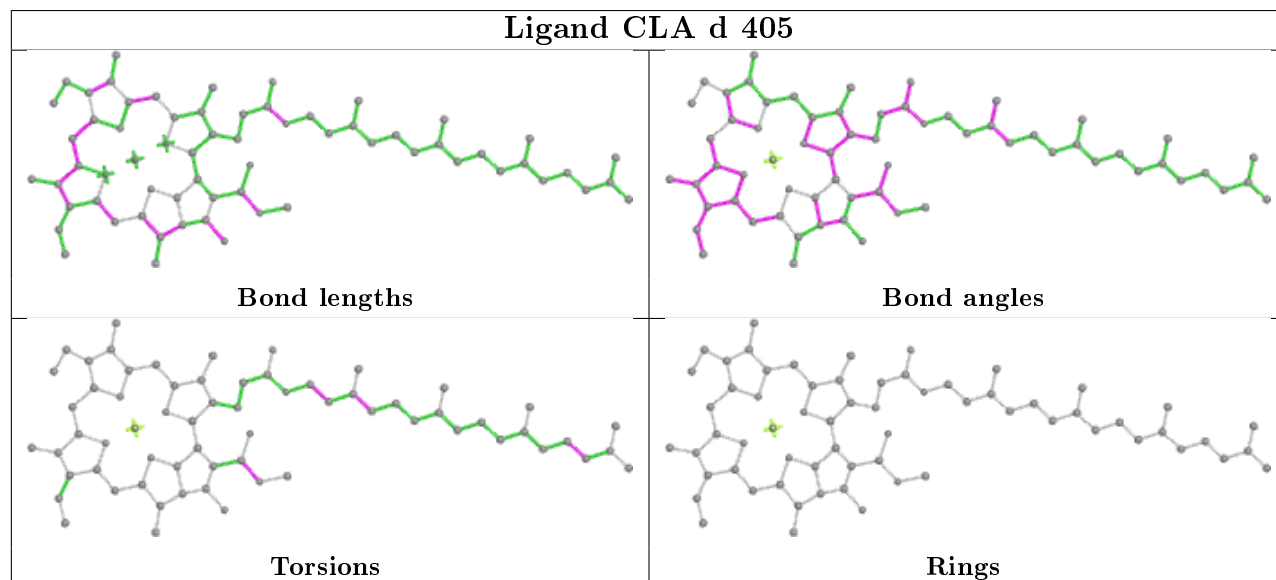
Ligand CLA b 620



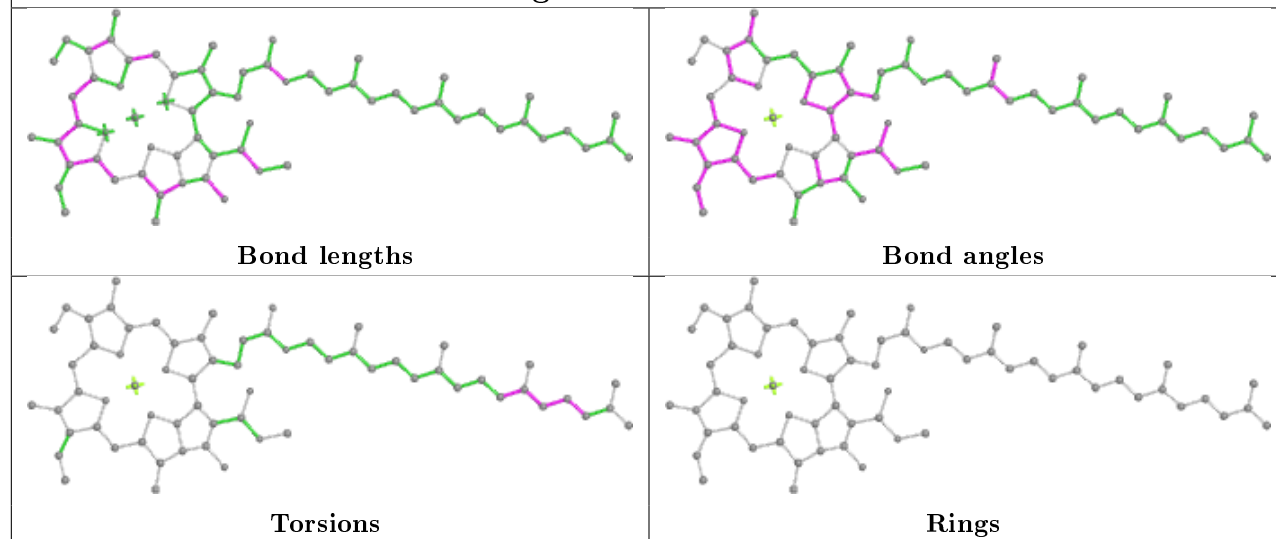
Ligand CLA B 617



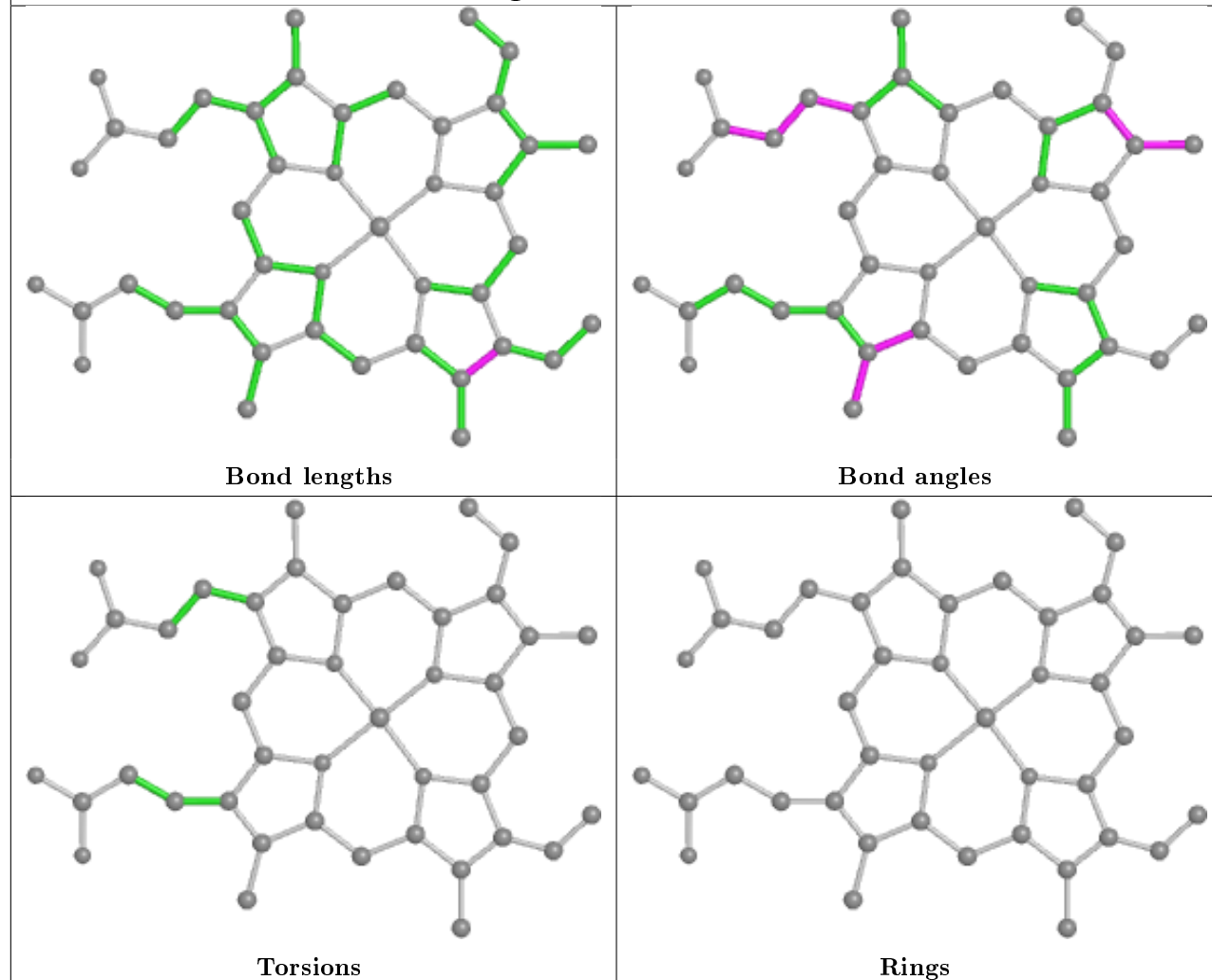
Ligand CLA d 405

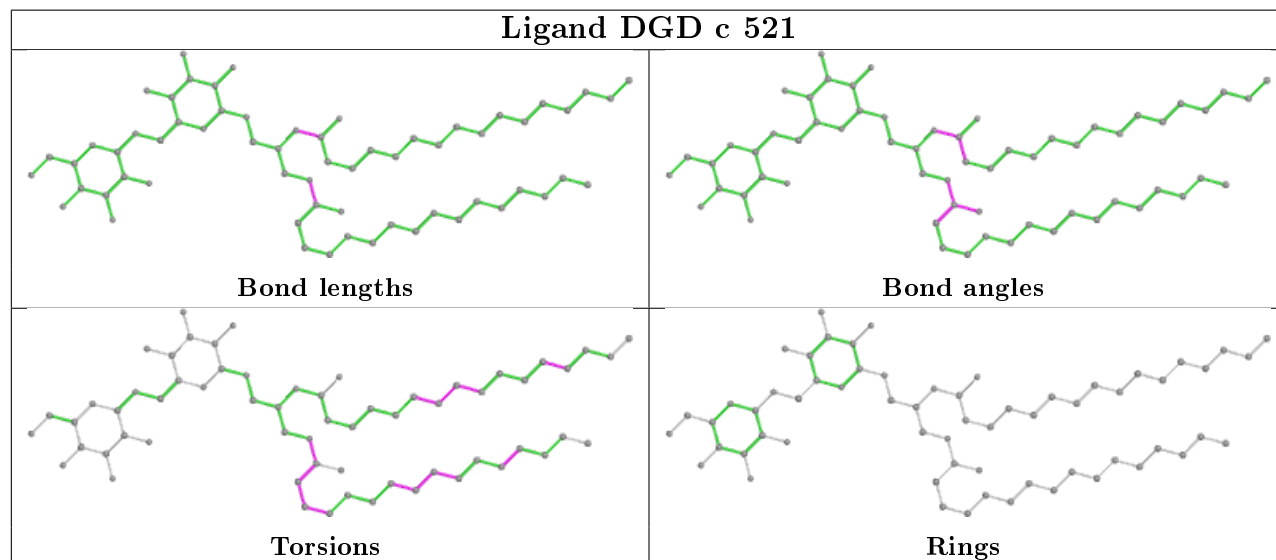
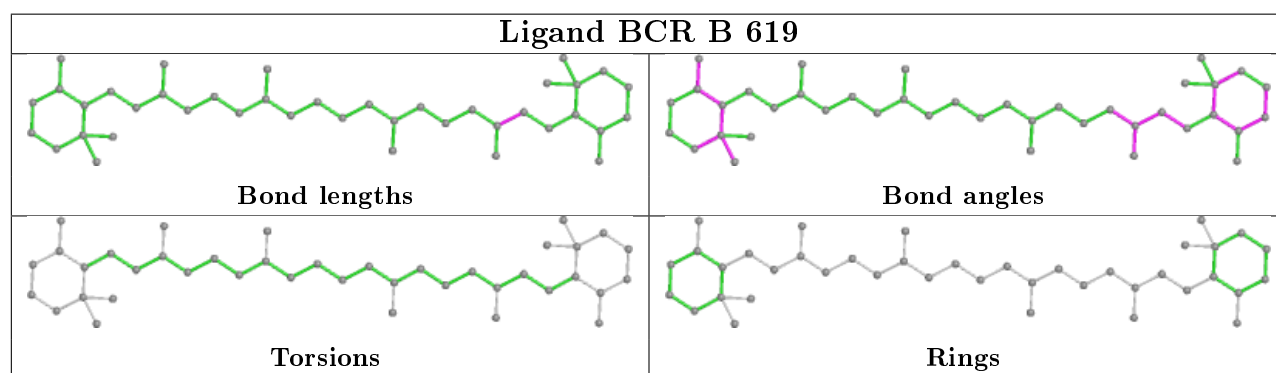
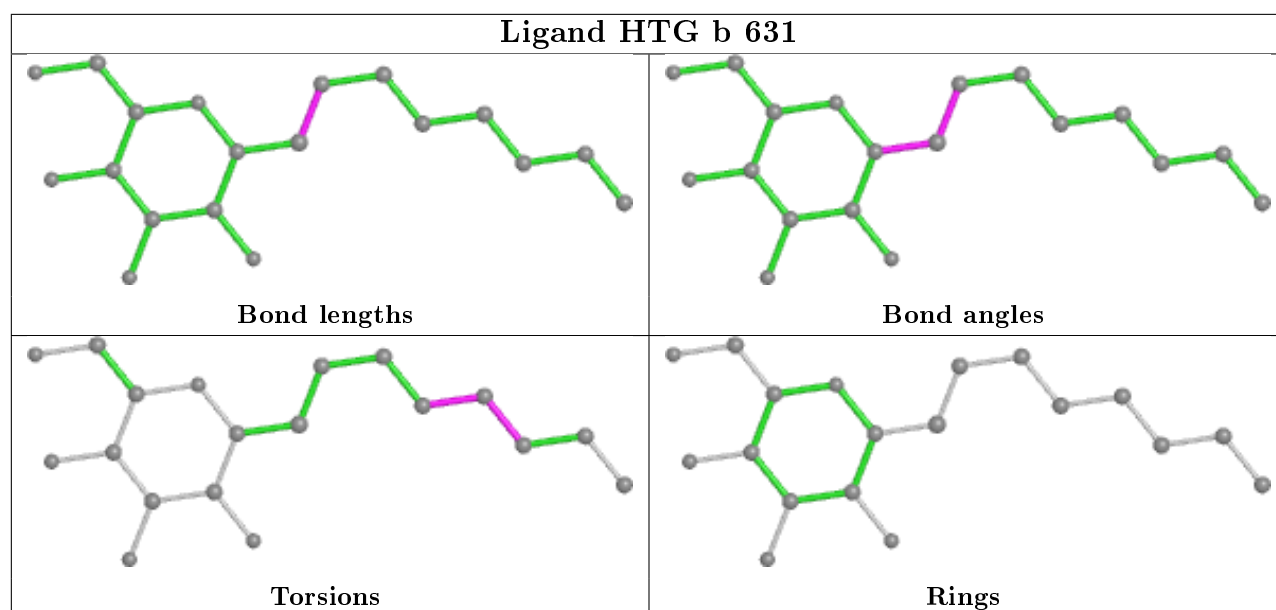


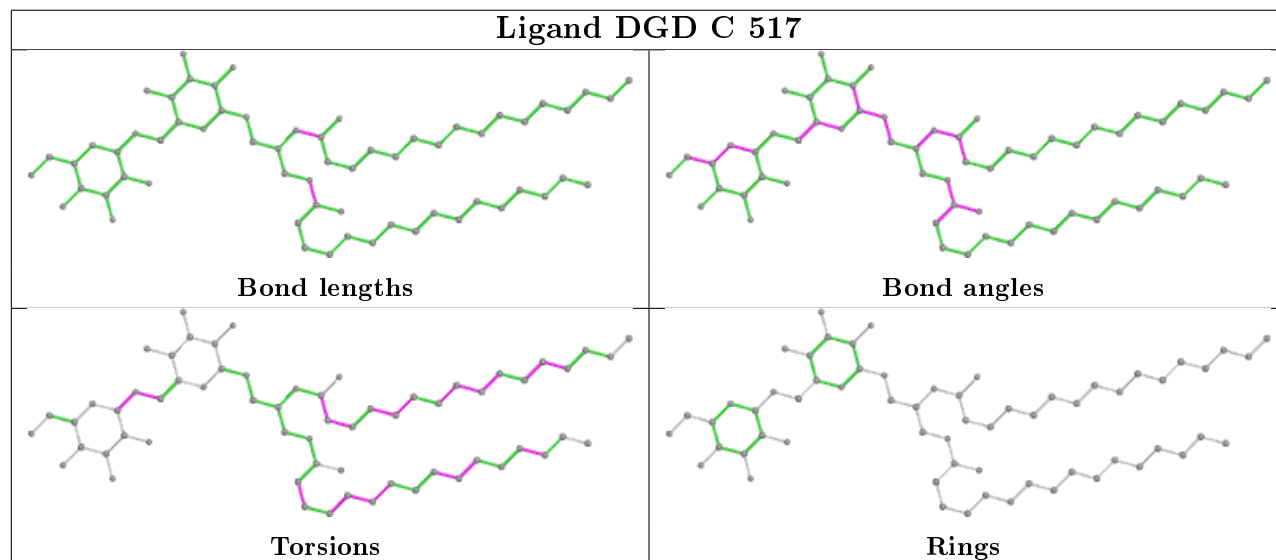
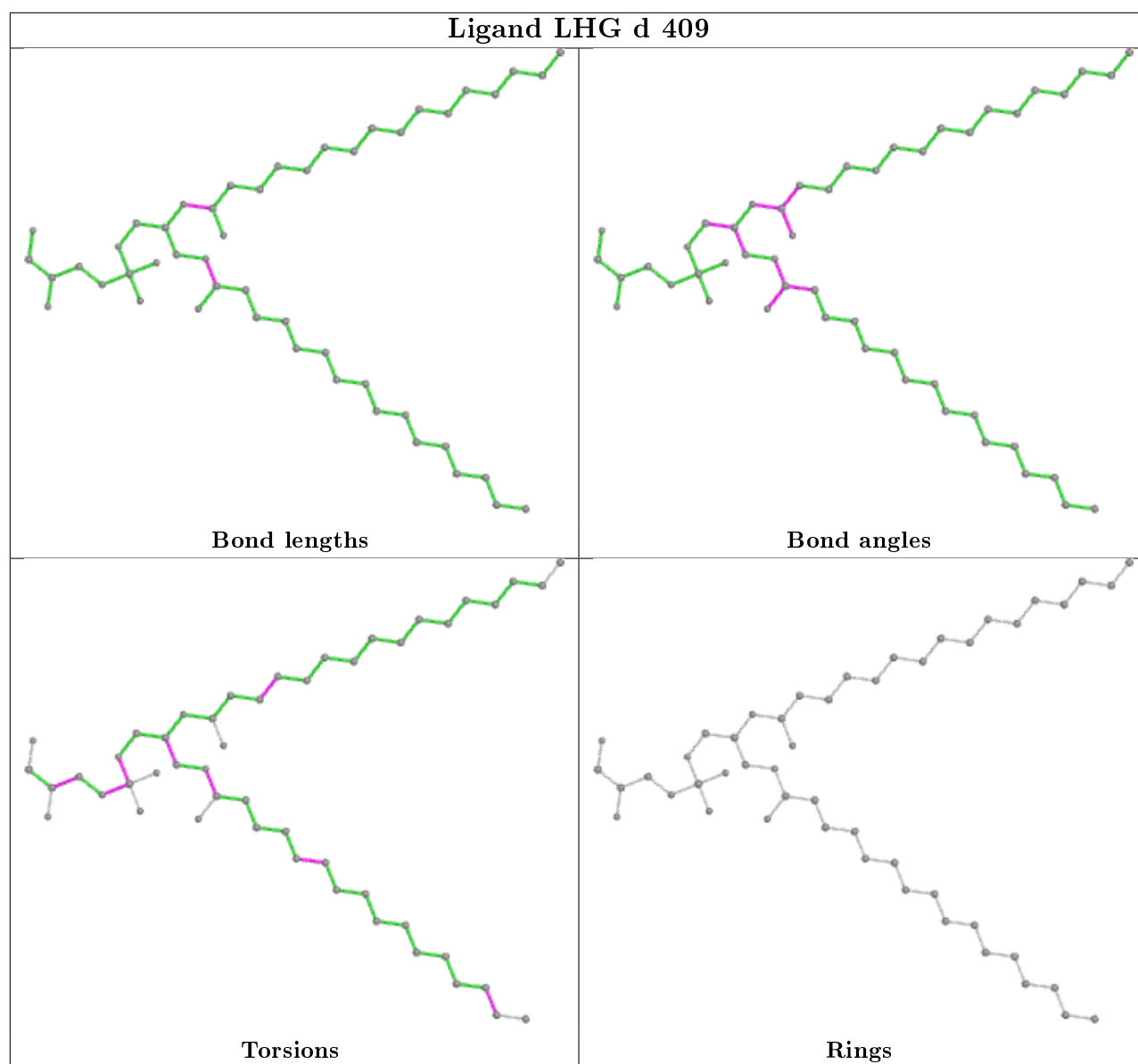
Ligand CLA C 504



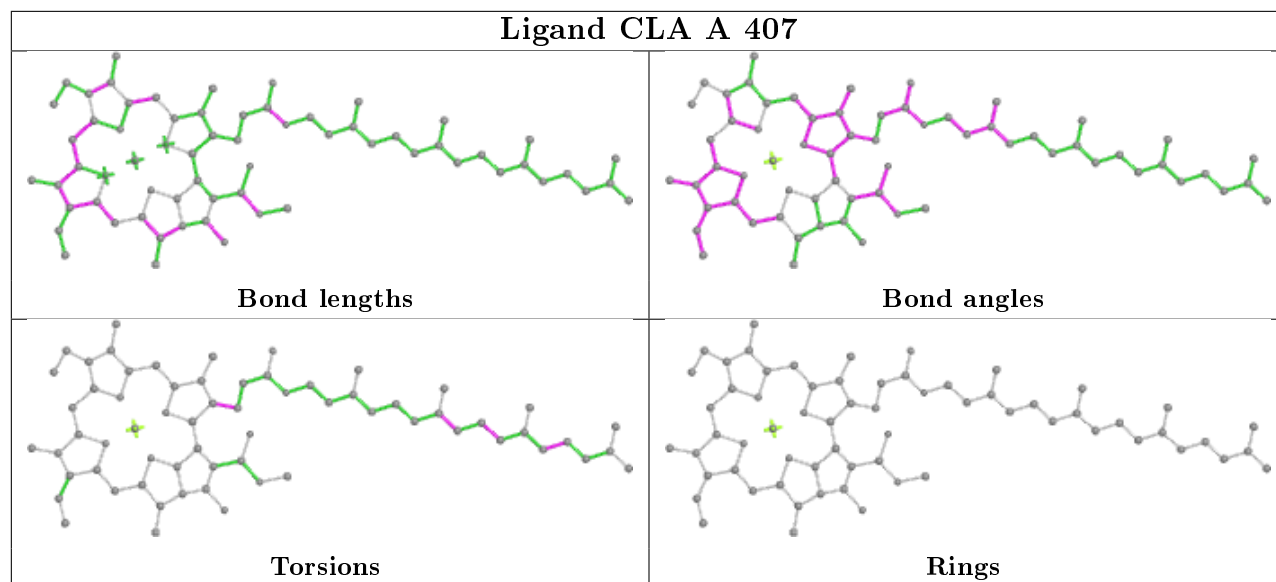
Ligand HEM f 101



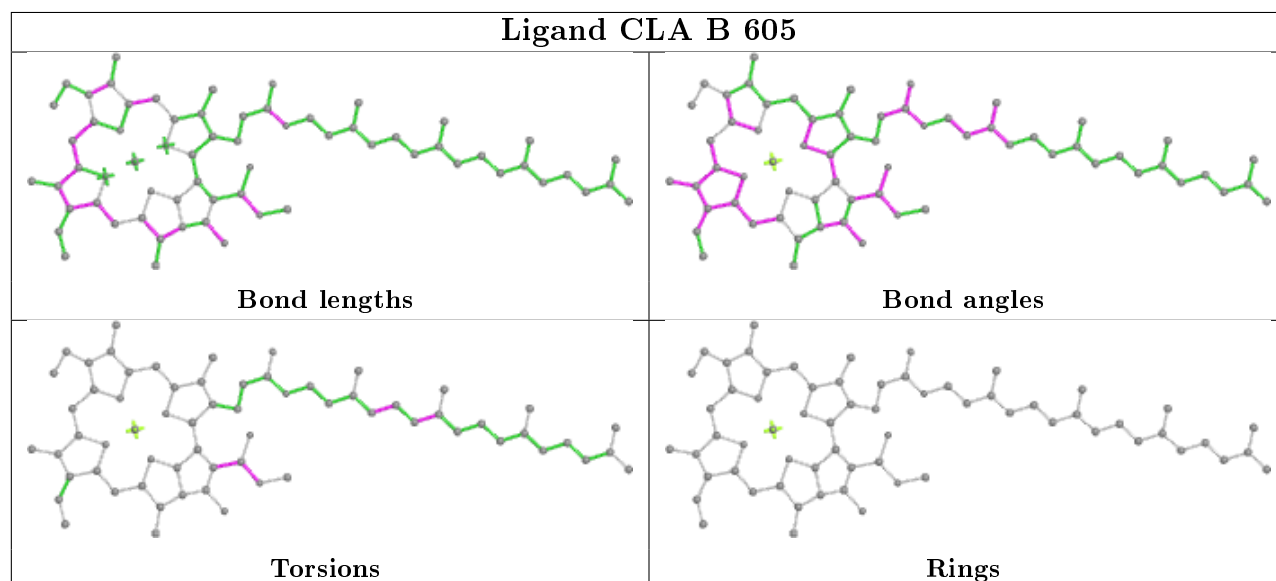




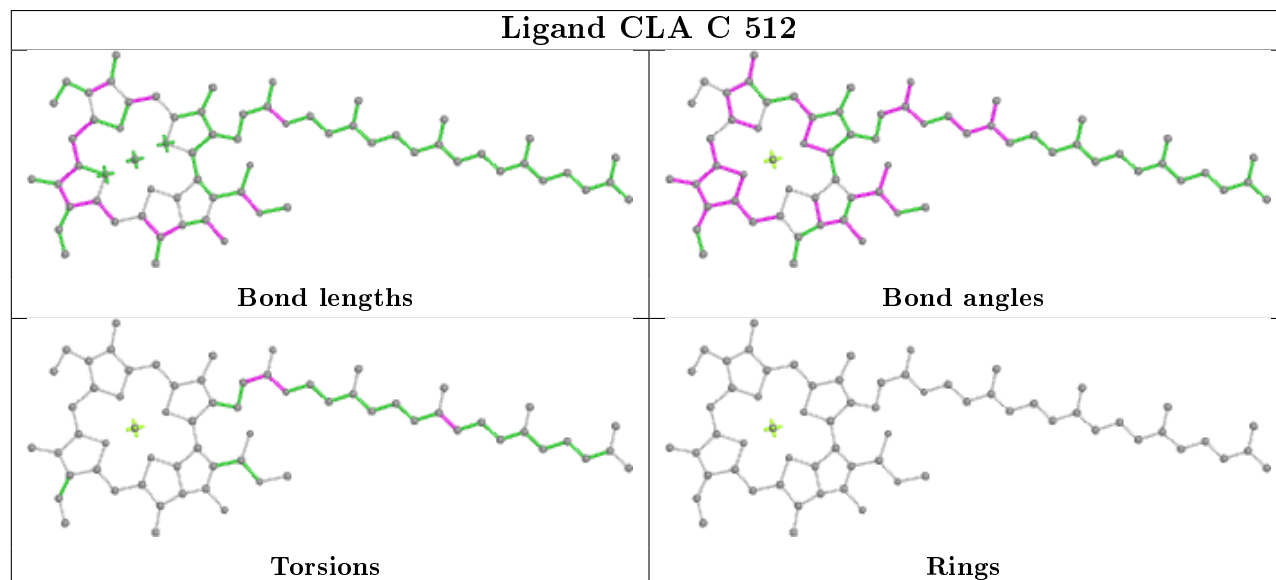
Ligand CLA A 407



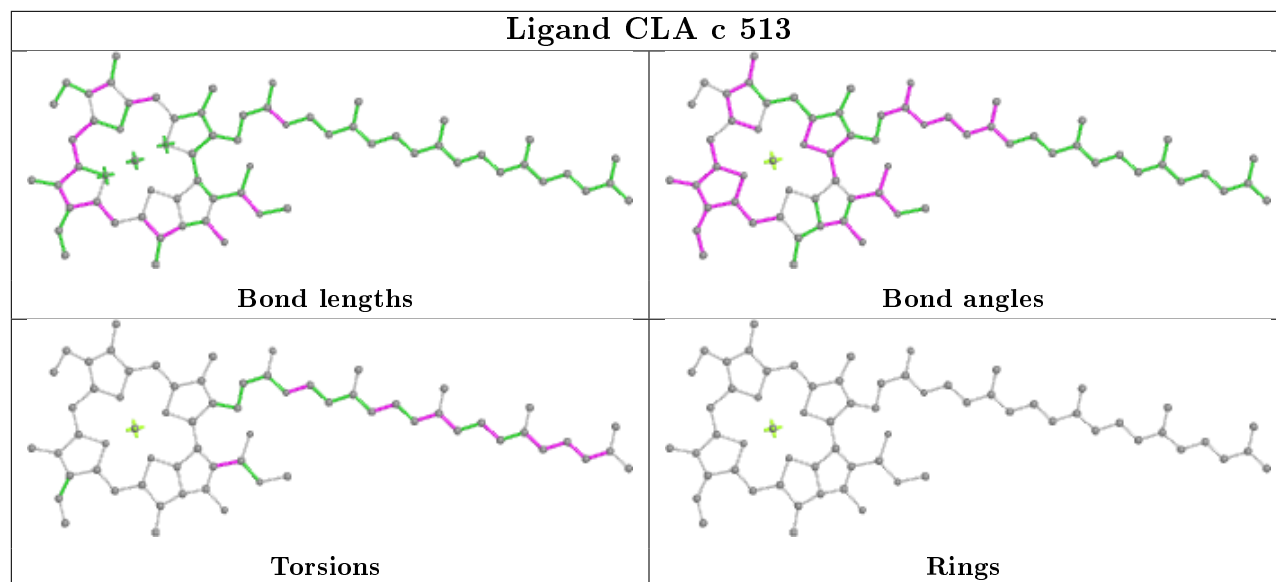
Ligand CLA B 605



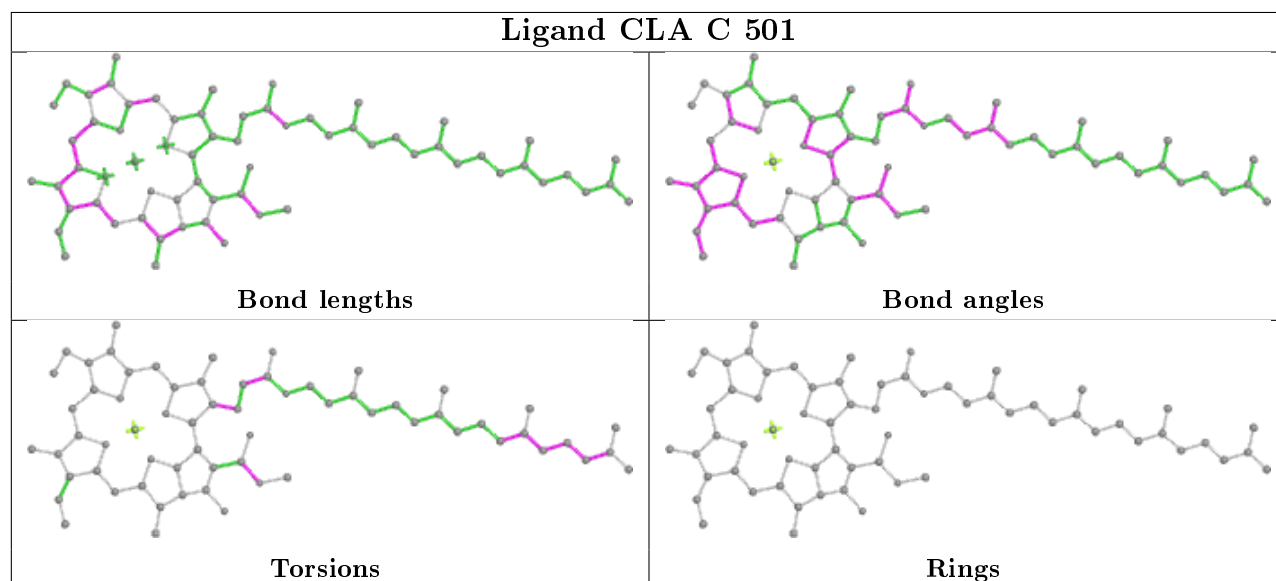
Ligand CLA C 512



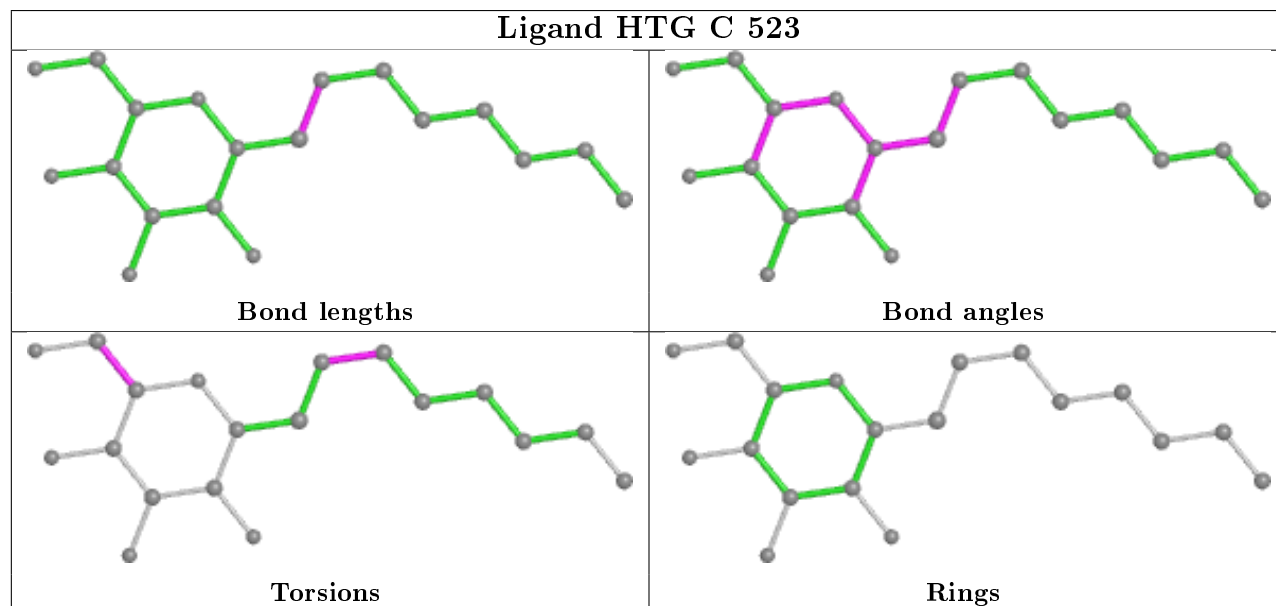
Ligand CLA c 513



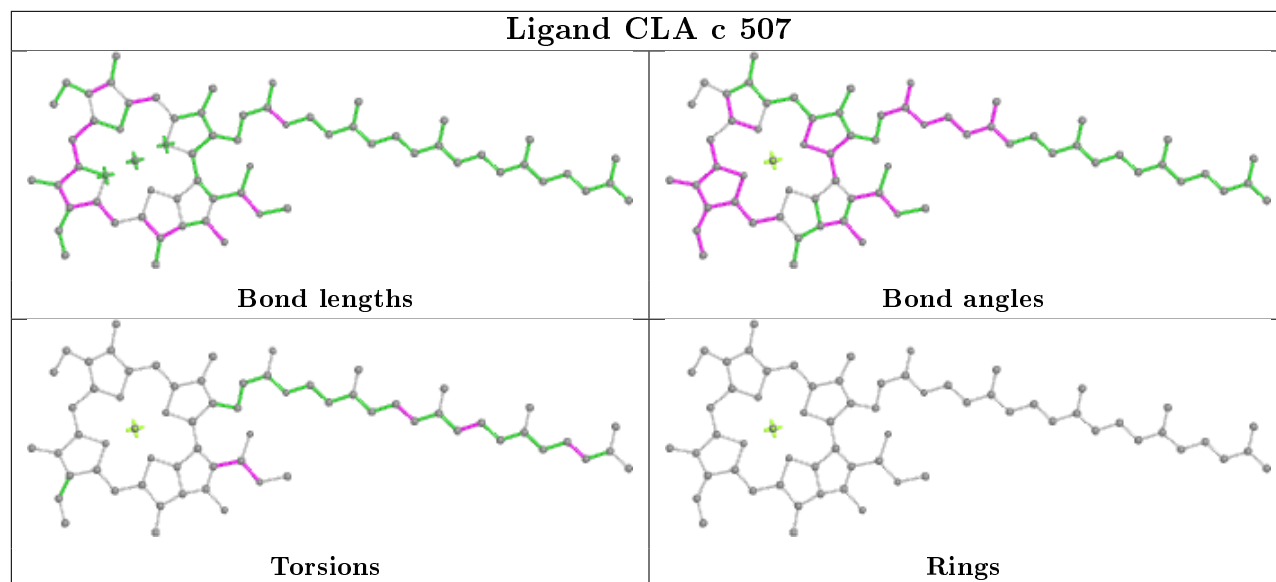
Ligand CLA C 501



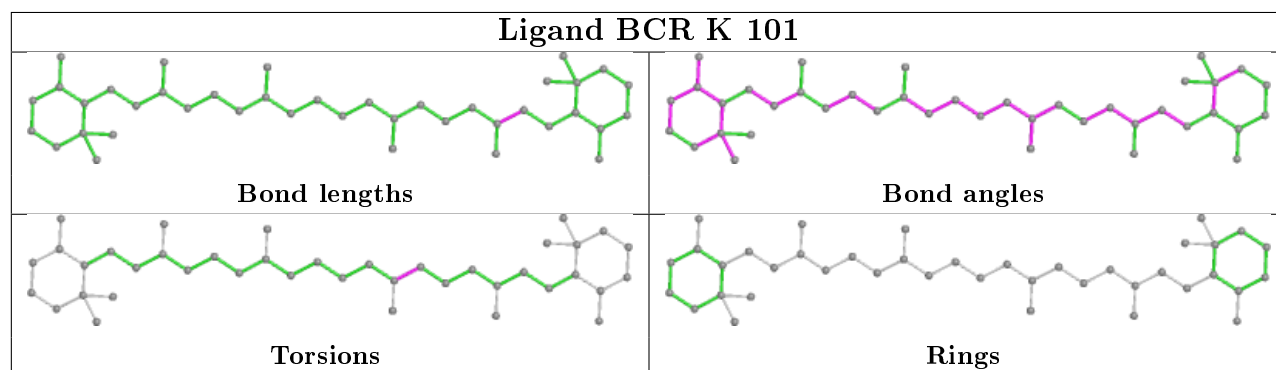
Ligand HTG C 523



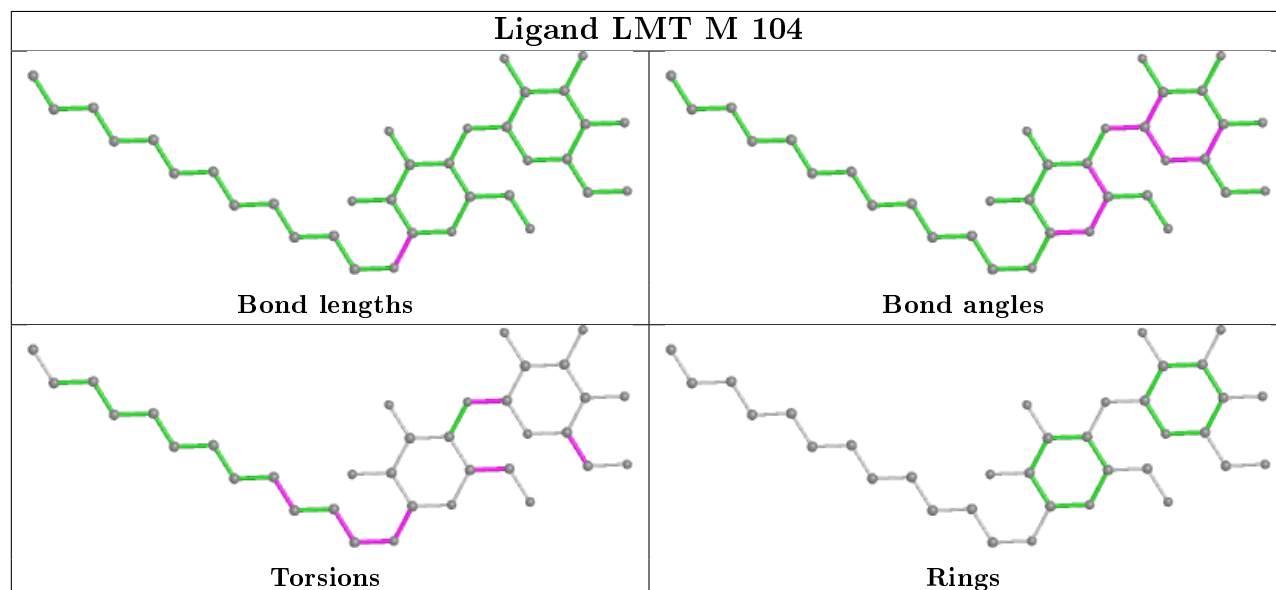
Ligand CLA c 507

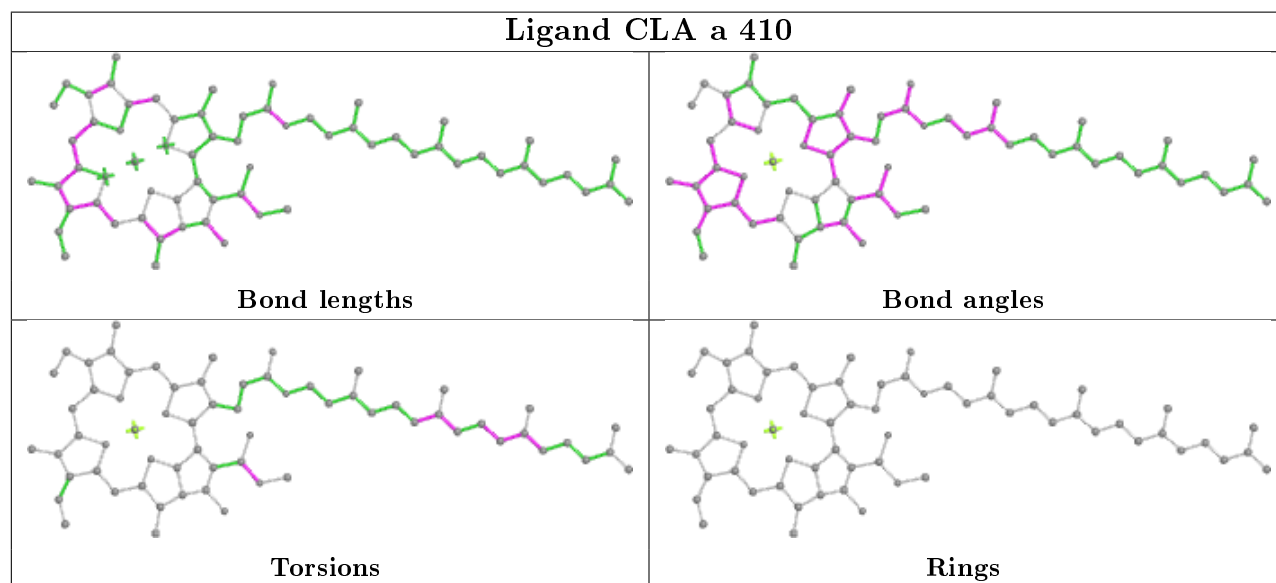
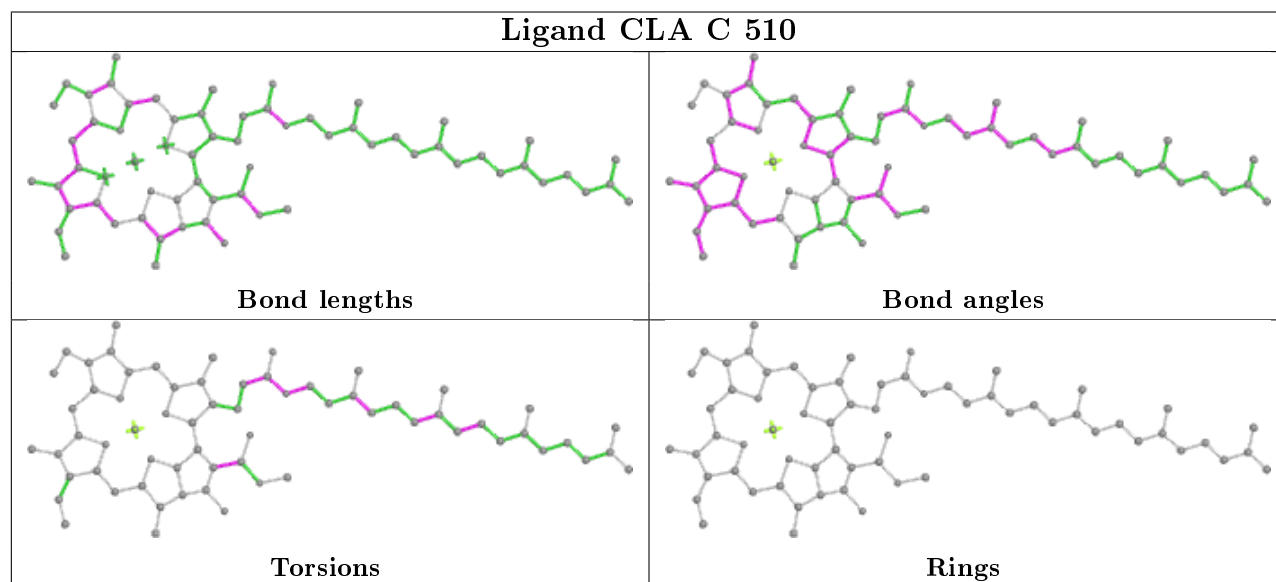
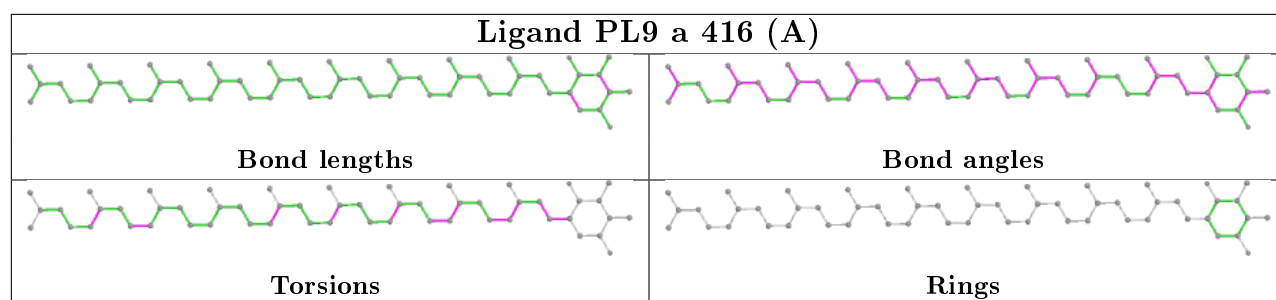


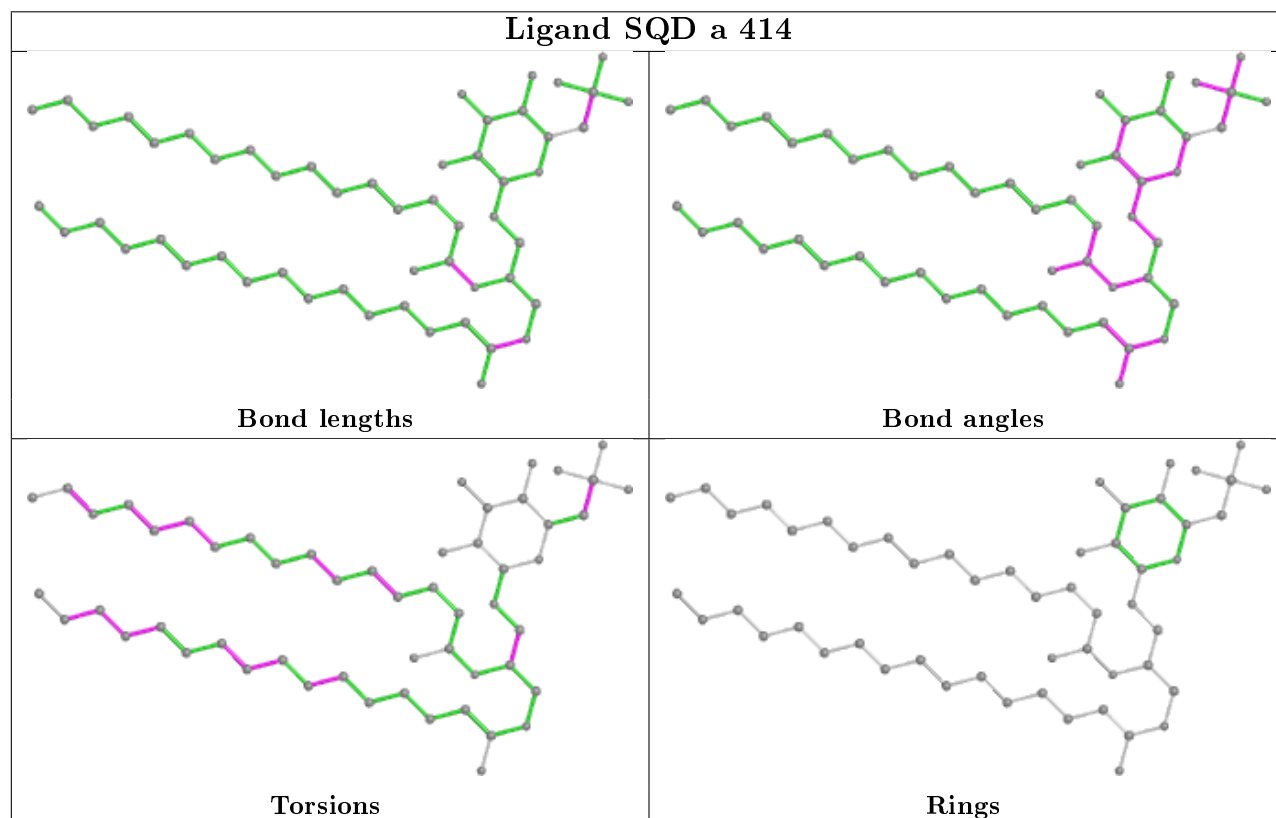
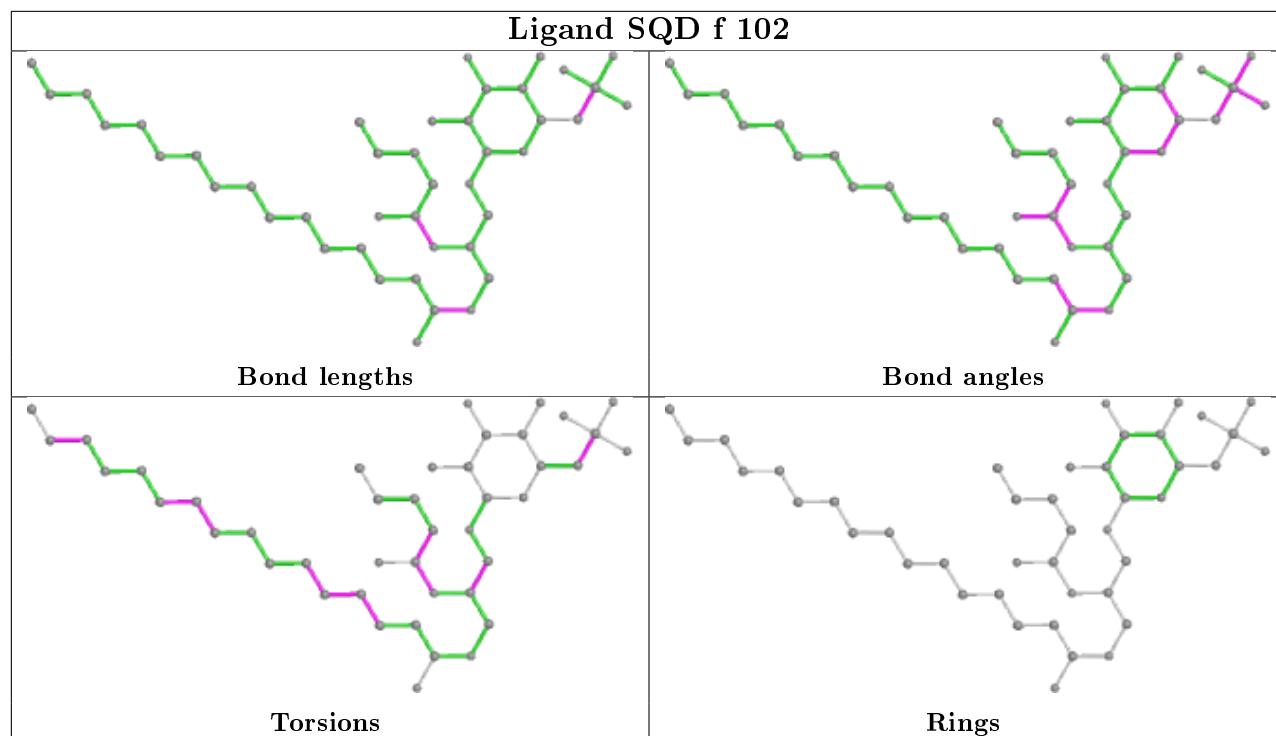
Ligand BCR K 101

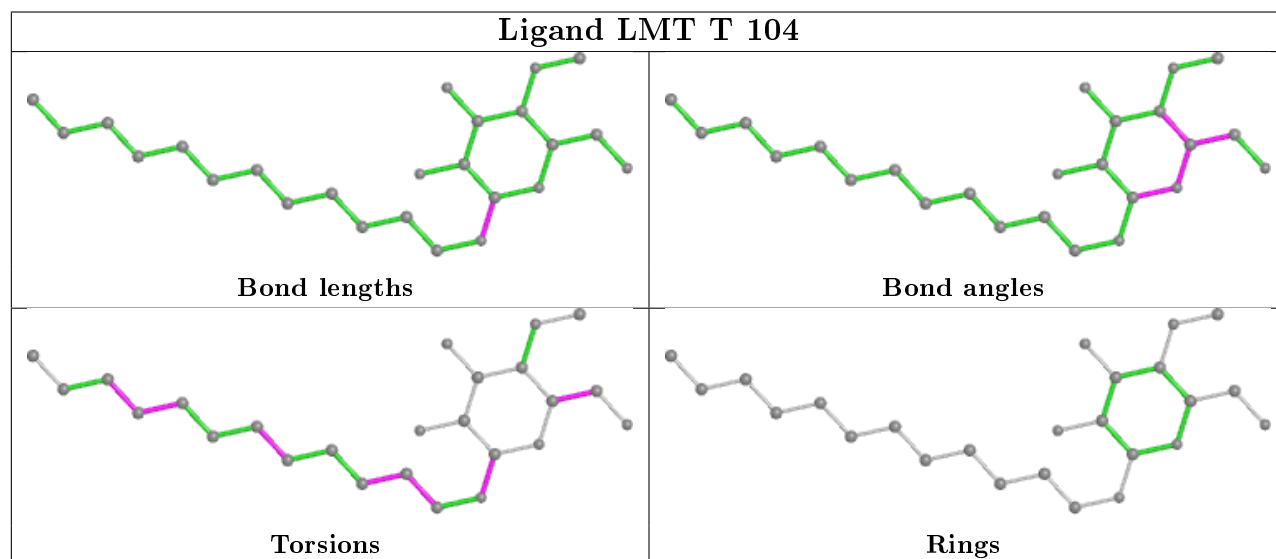
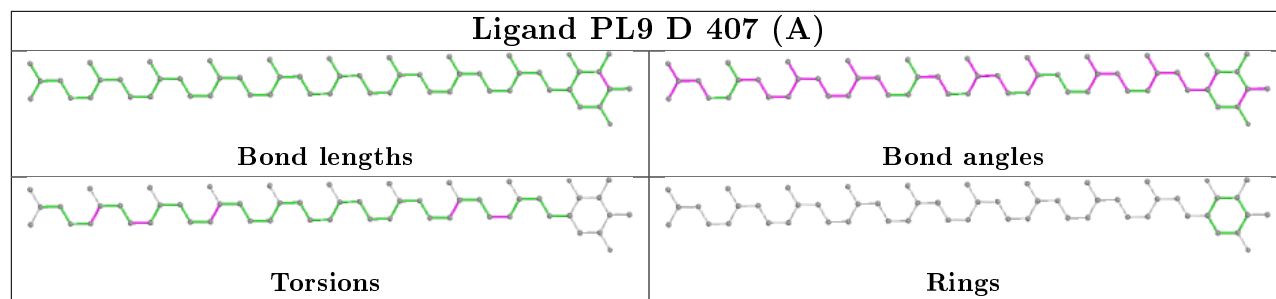


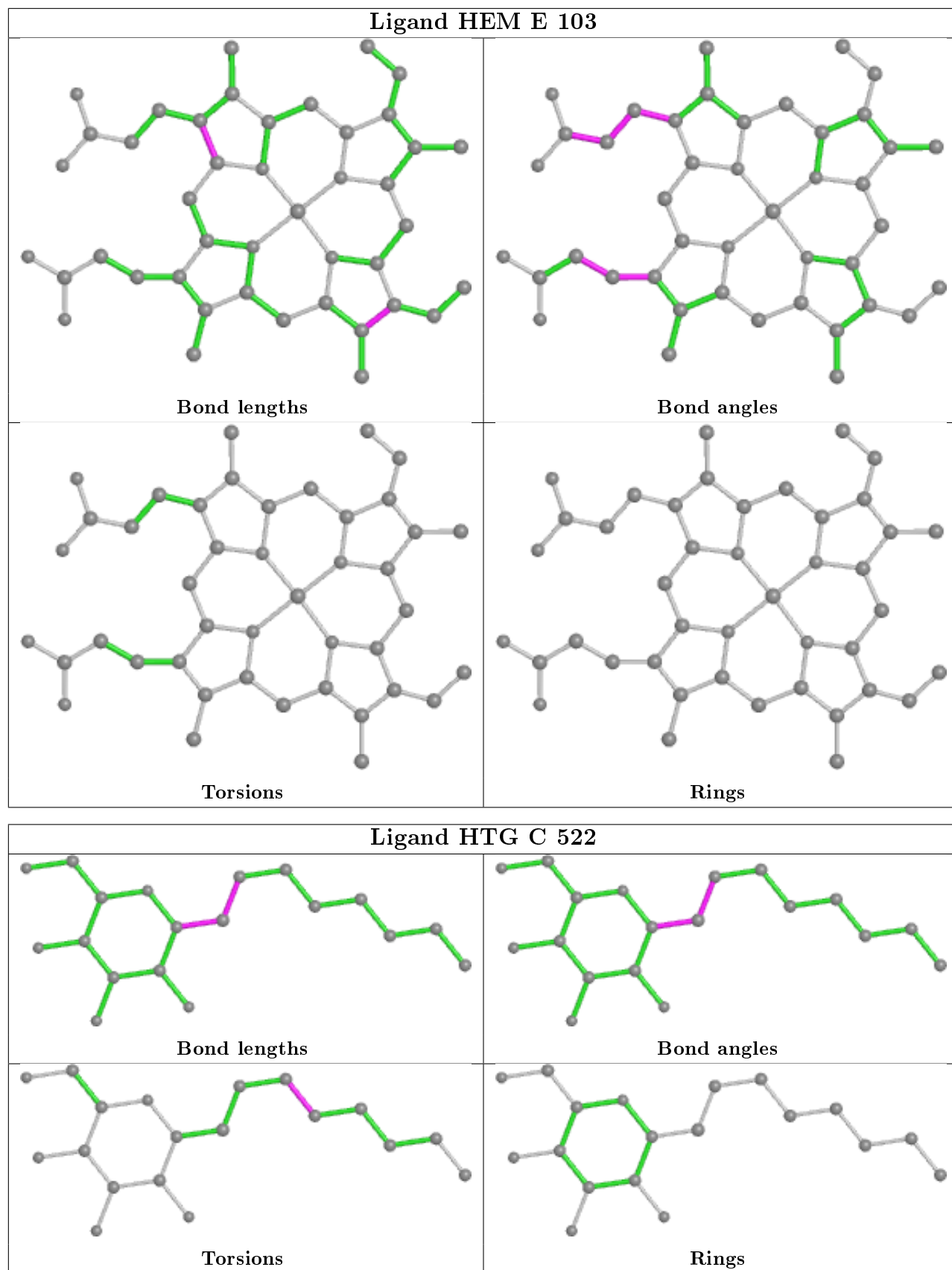
Ligand LMT M 104

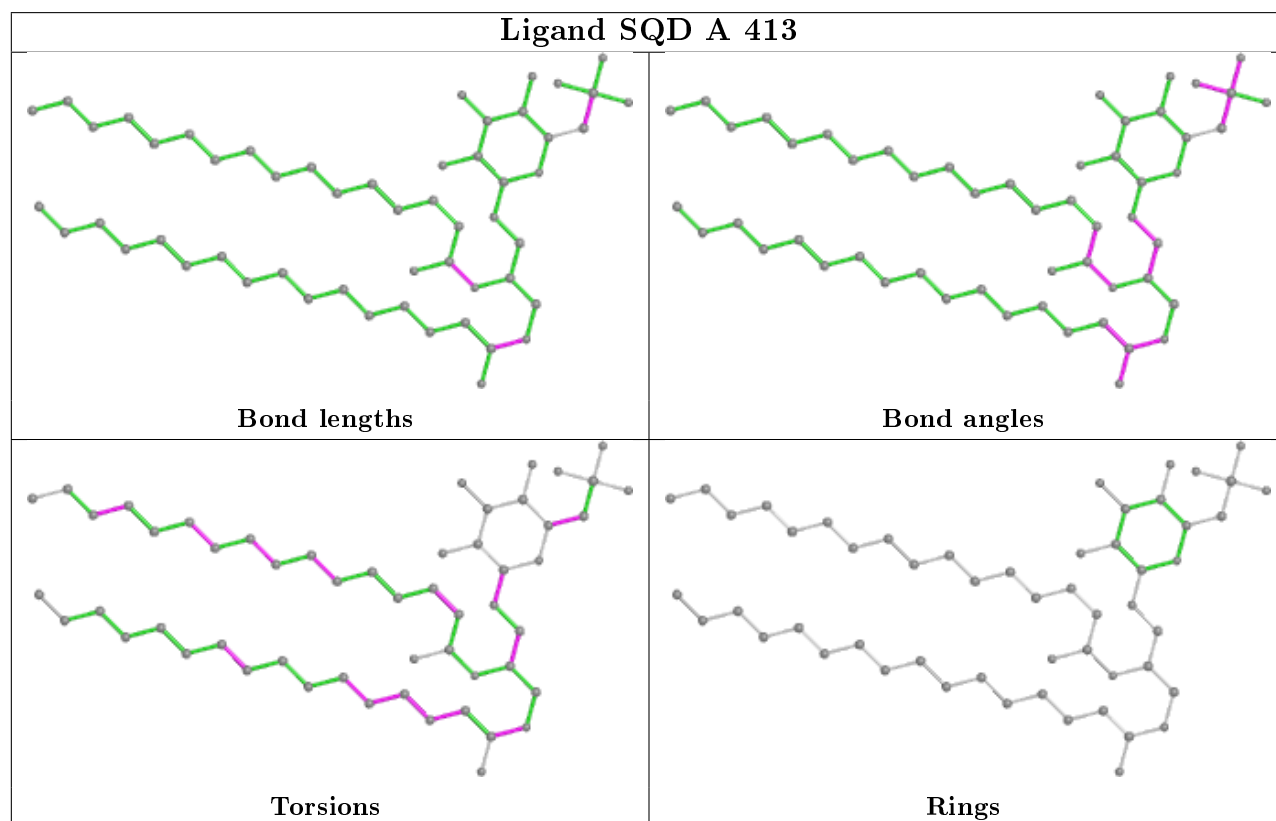
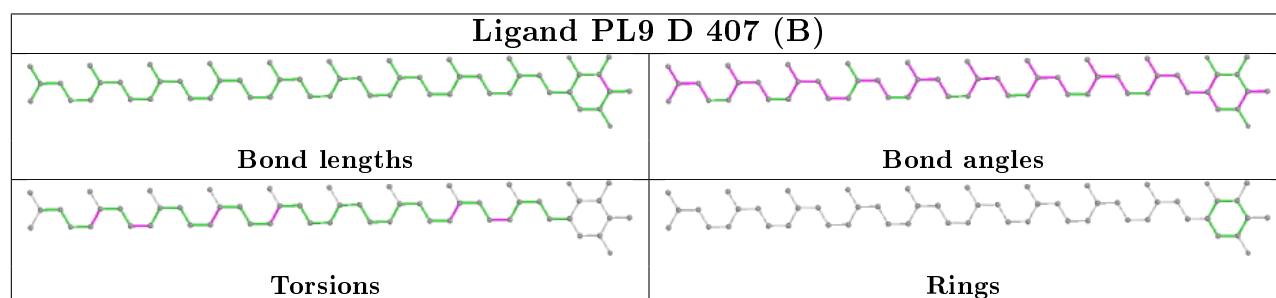
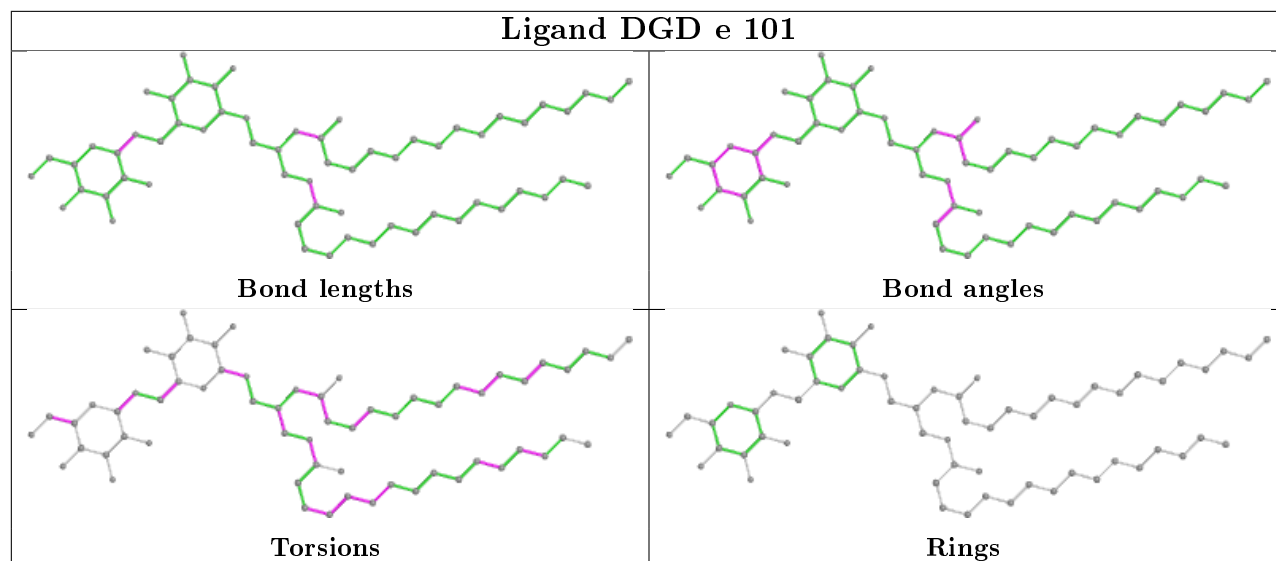


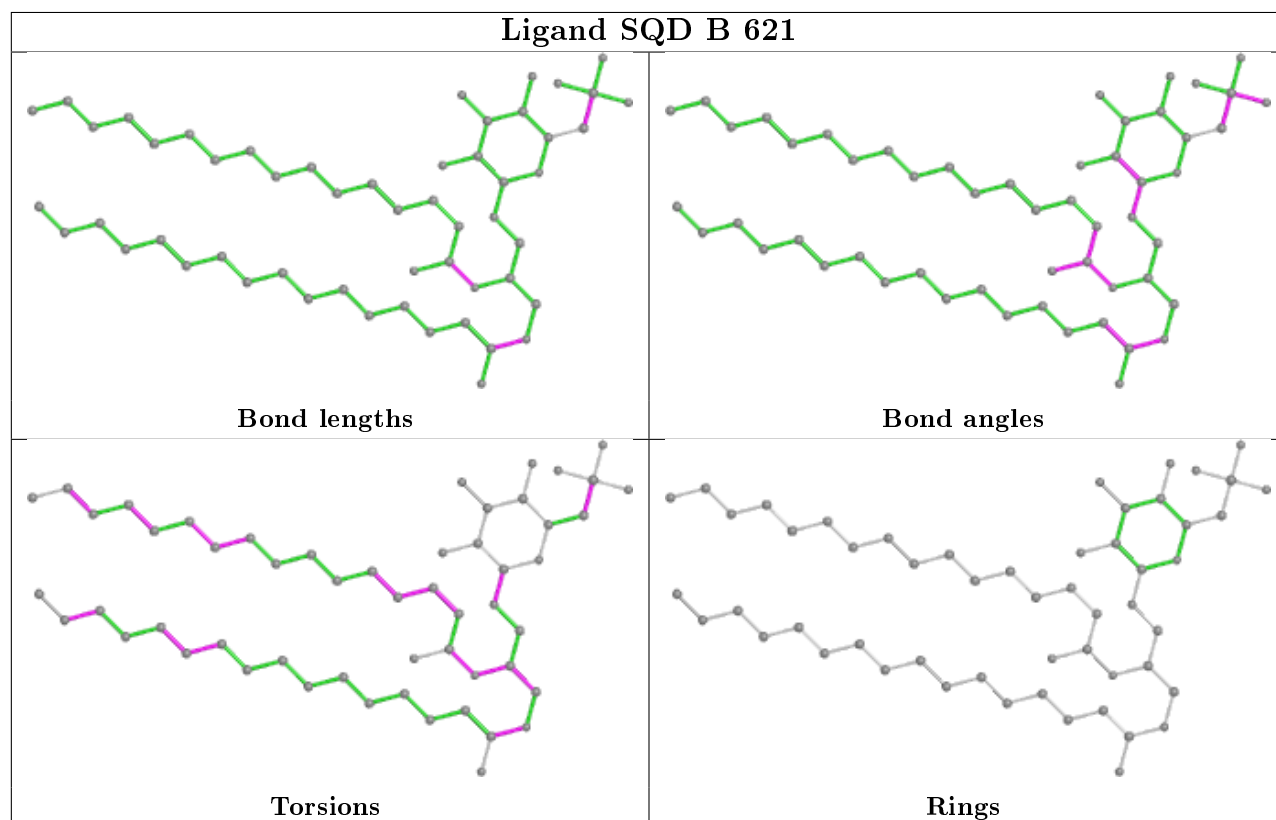
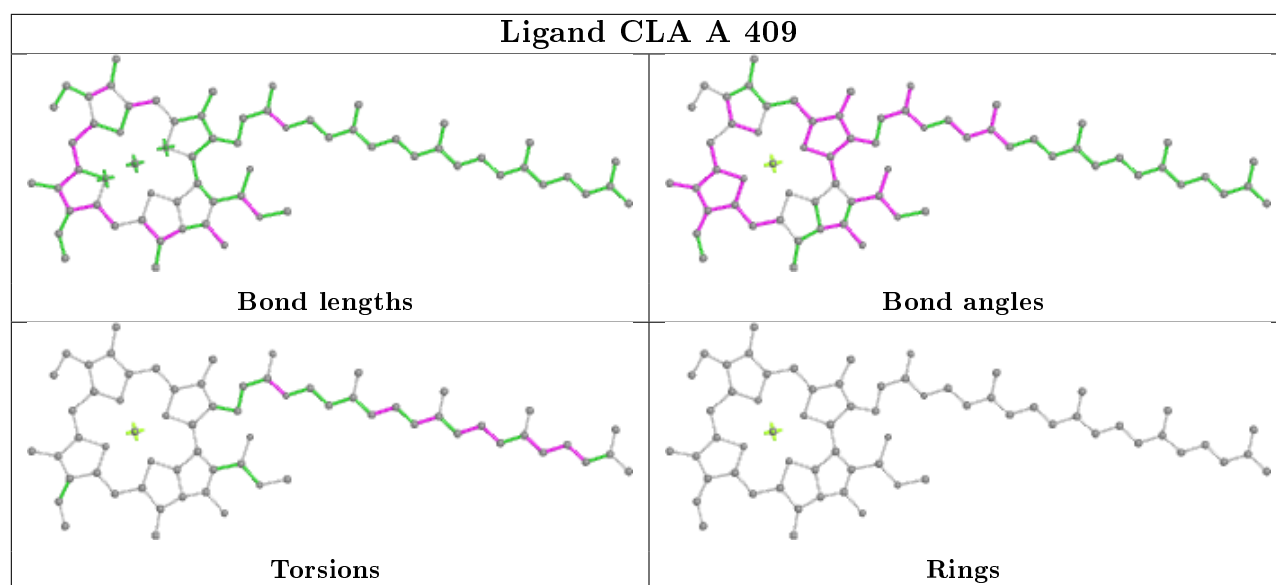




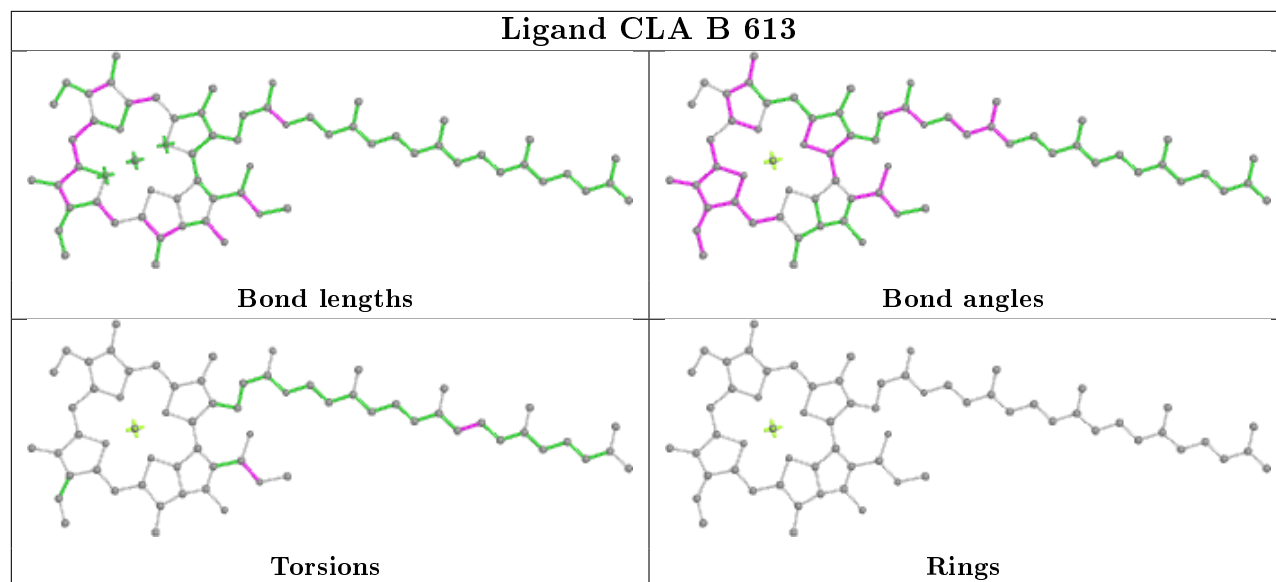




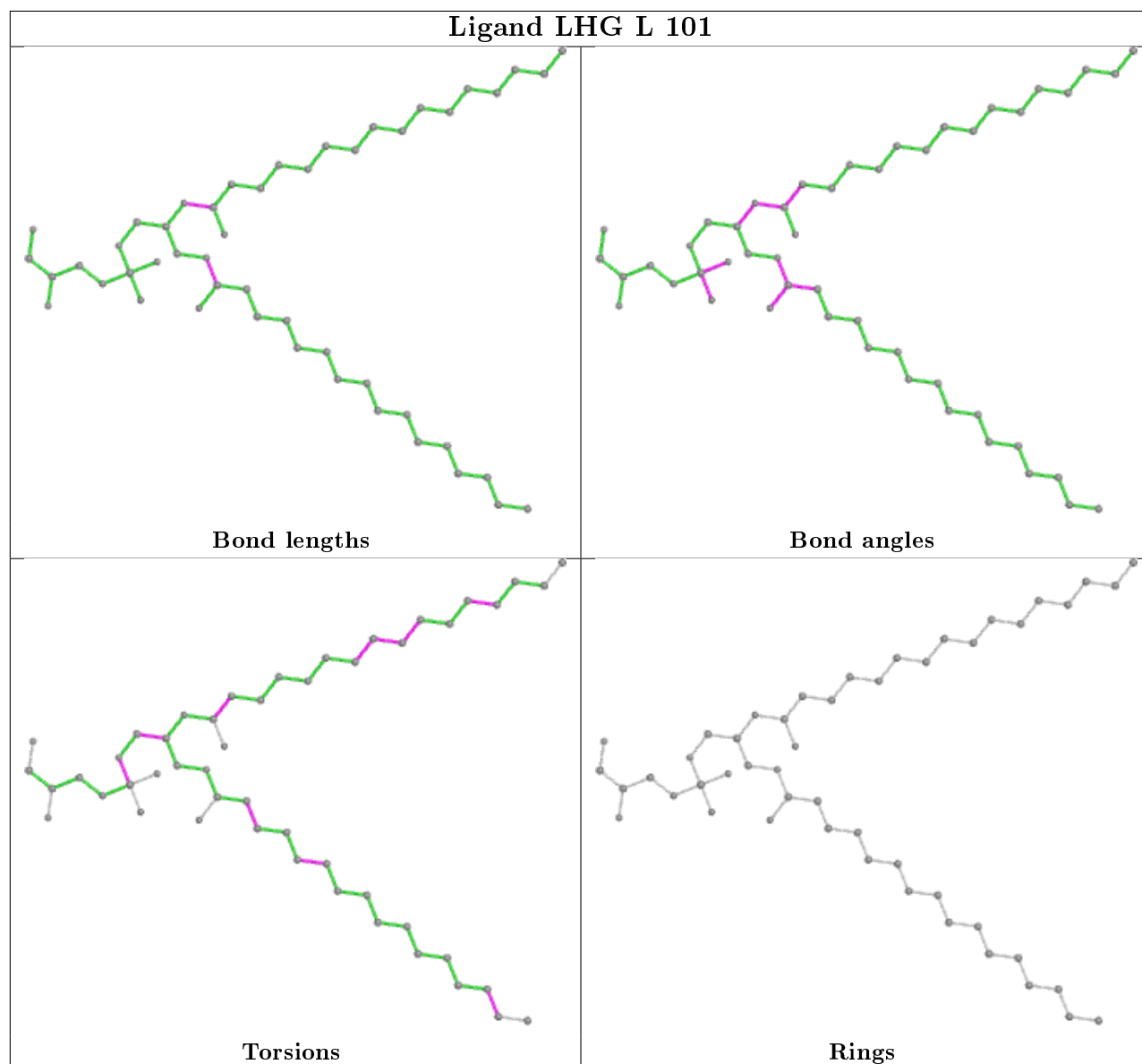


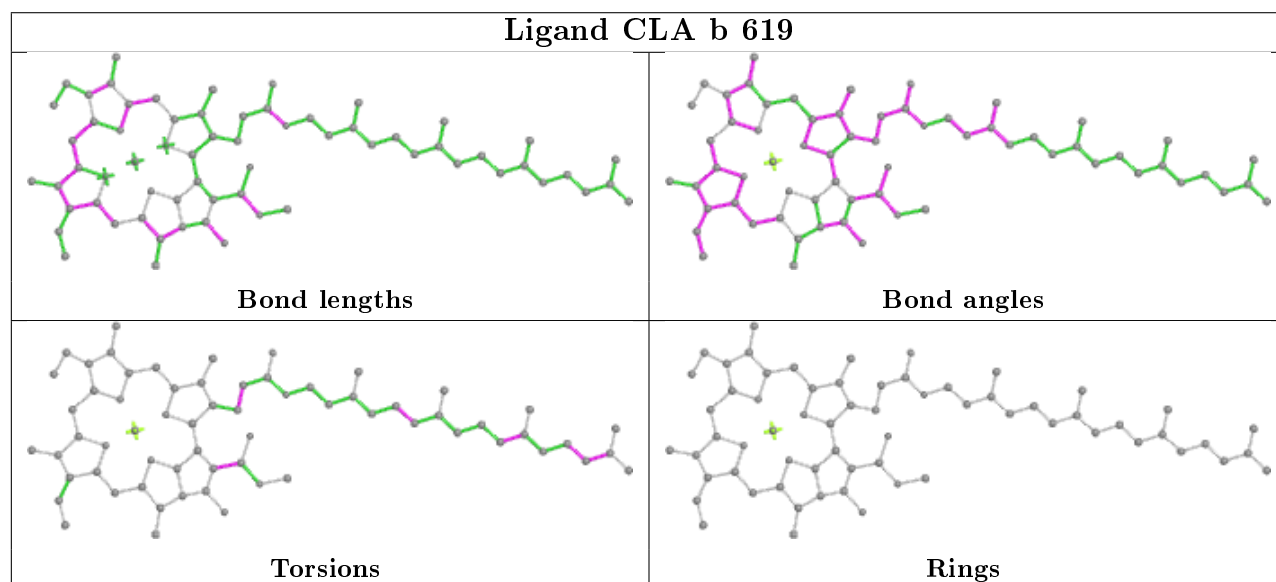
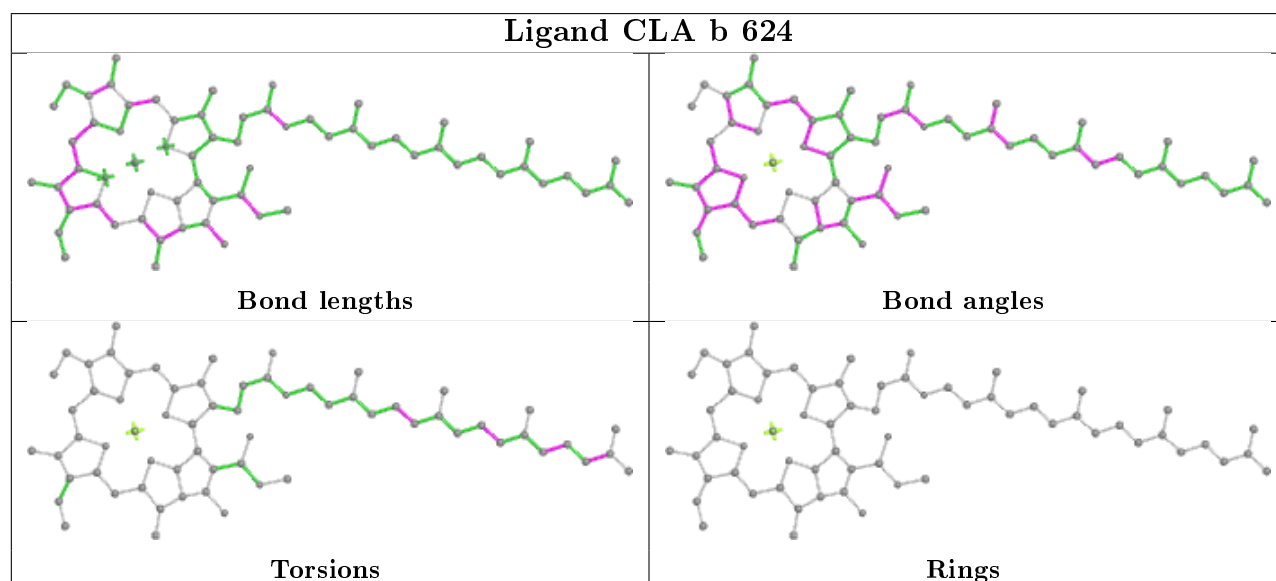
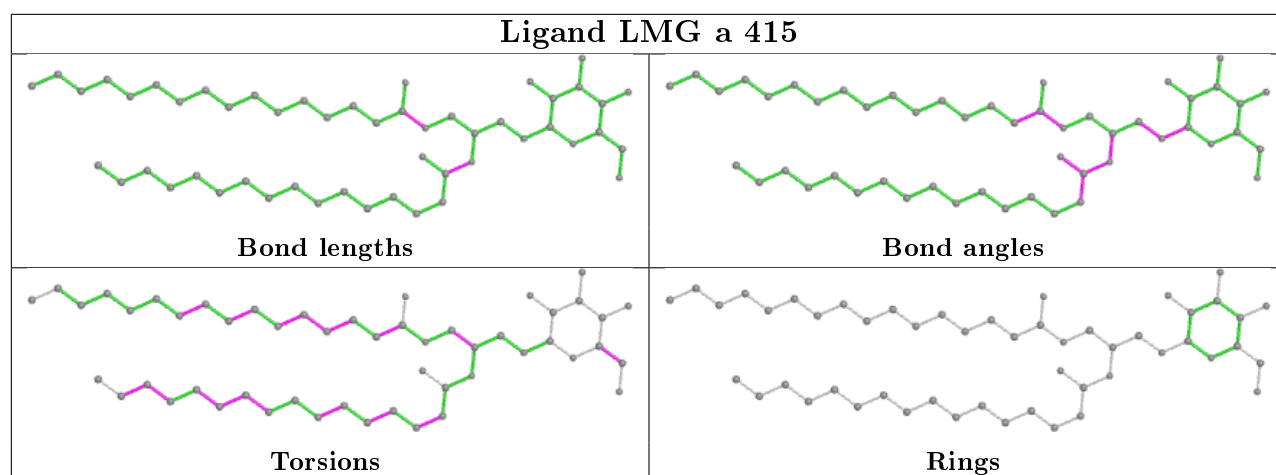


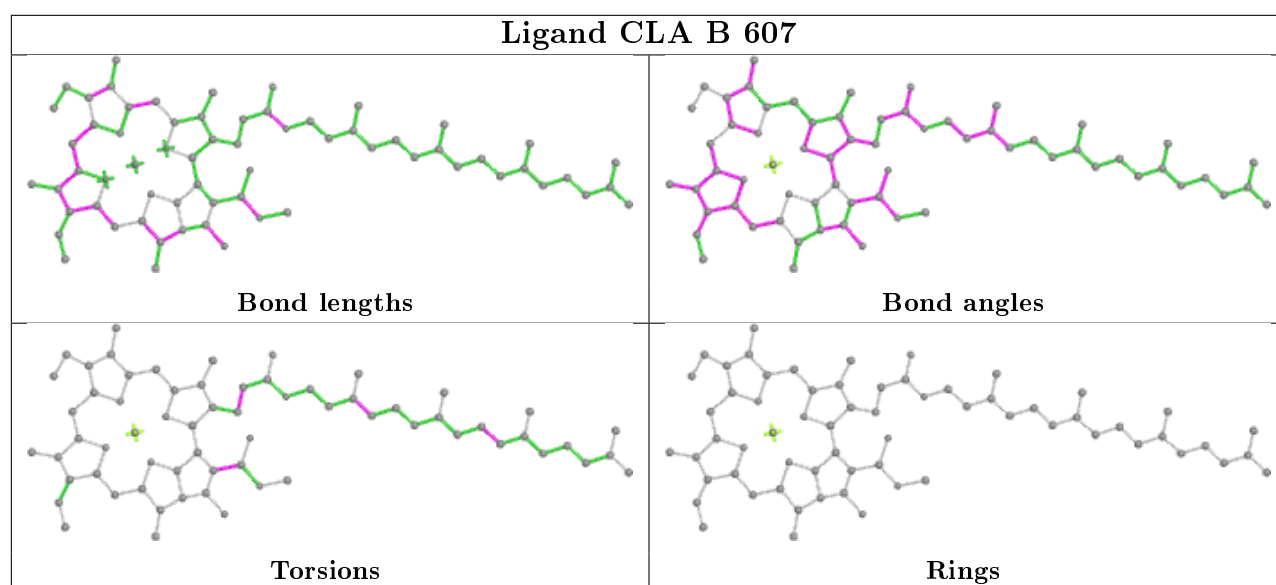
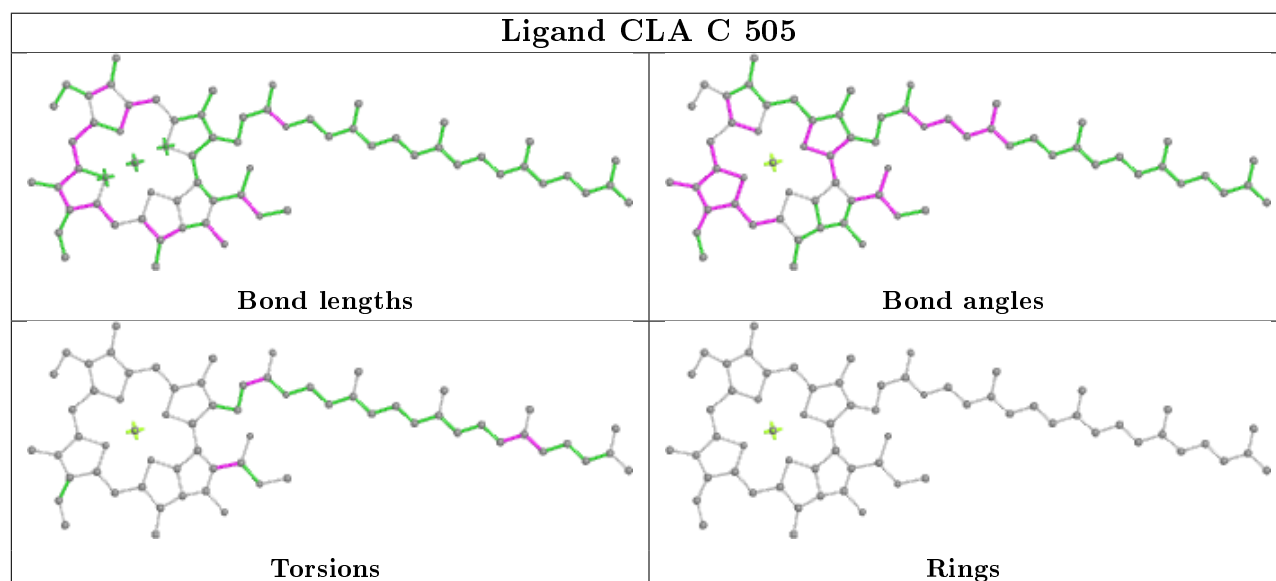
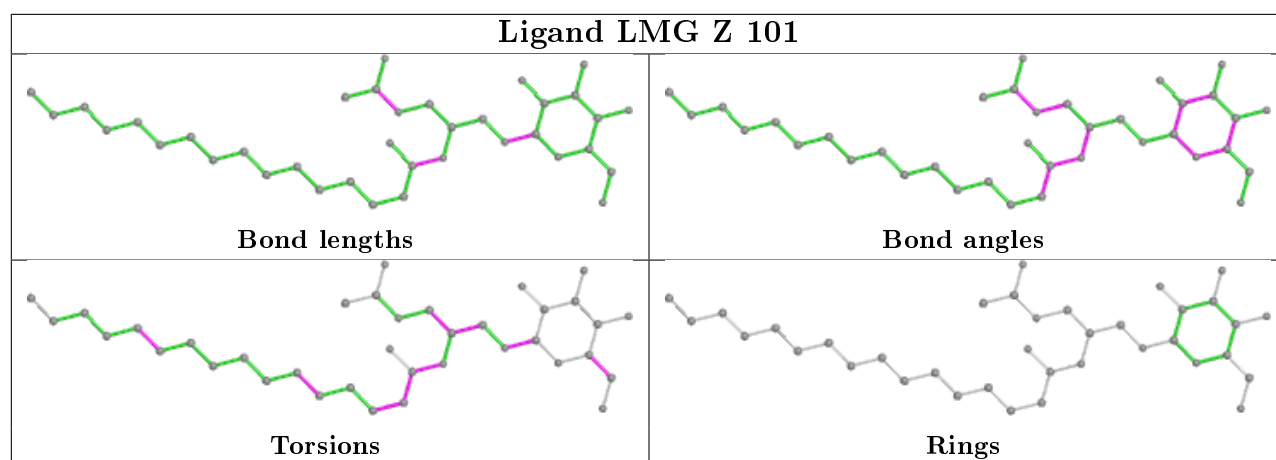
Ligand CLA B 613



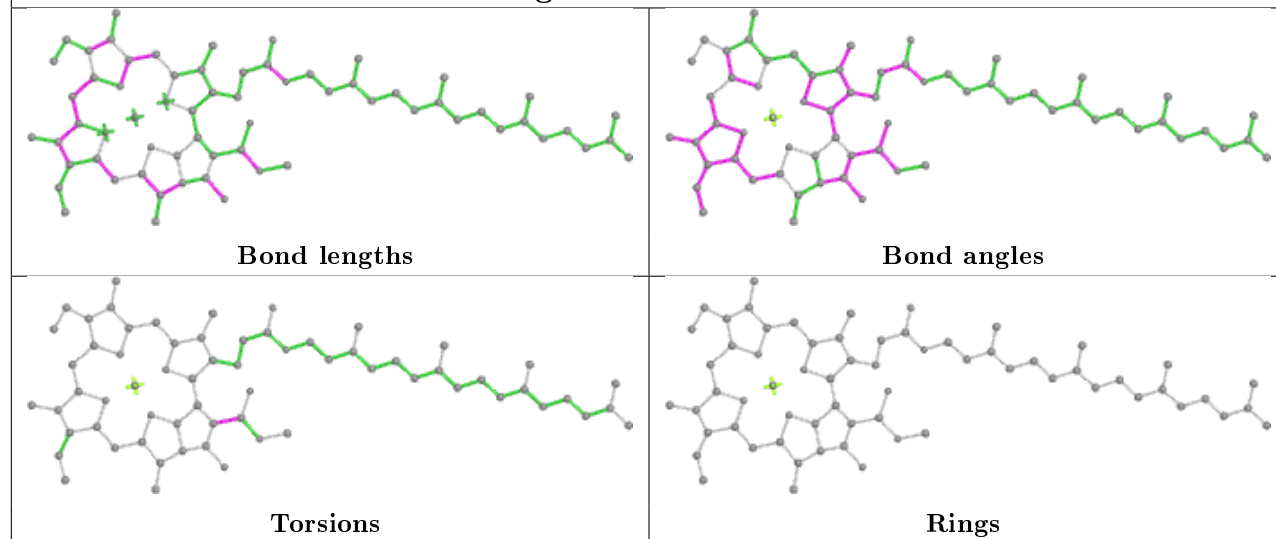
Ligand LHG L 101



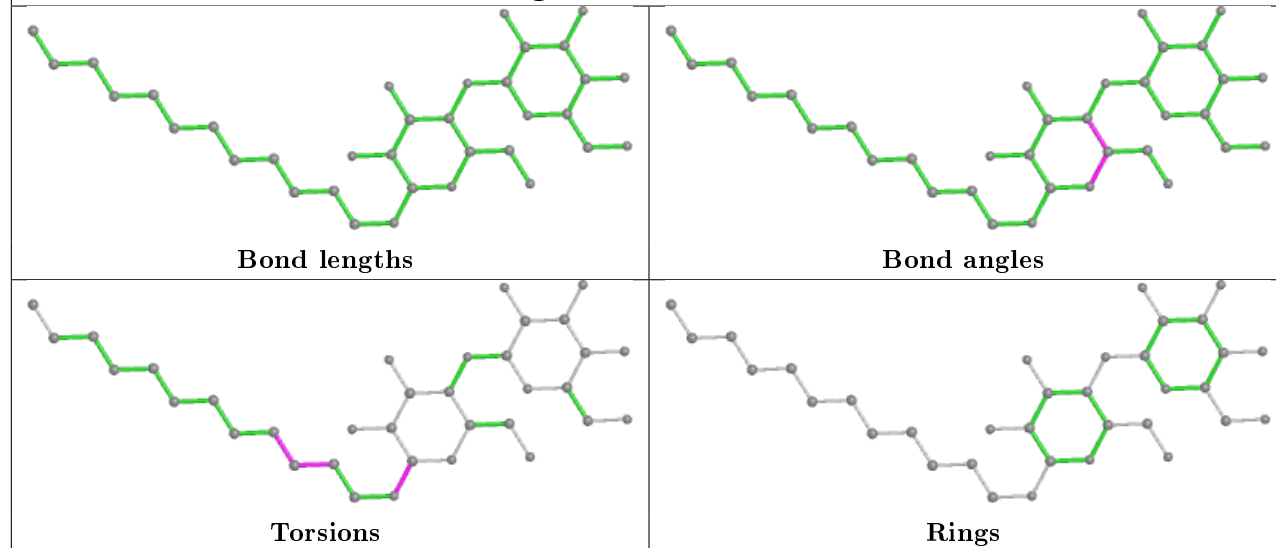




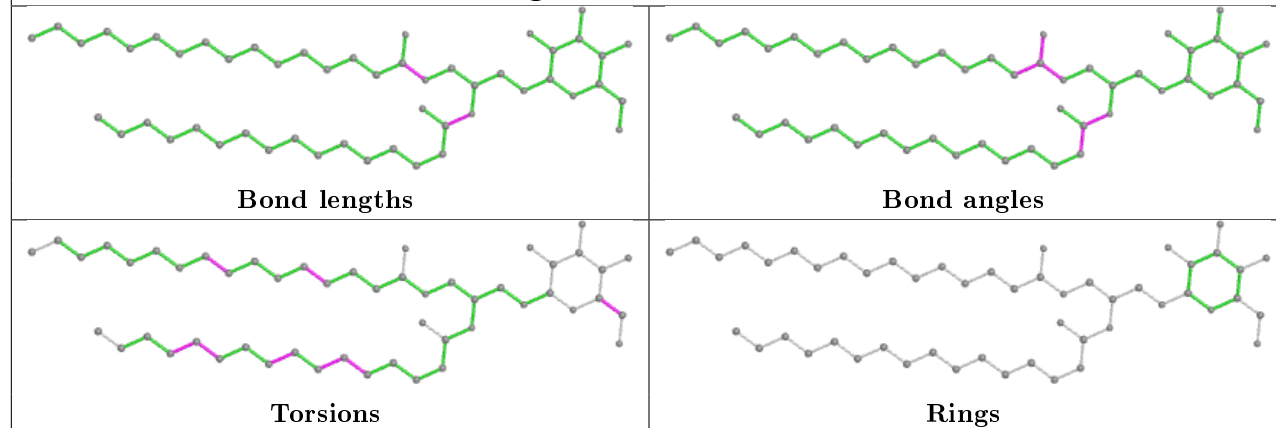
Ligand CLA b 616

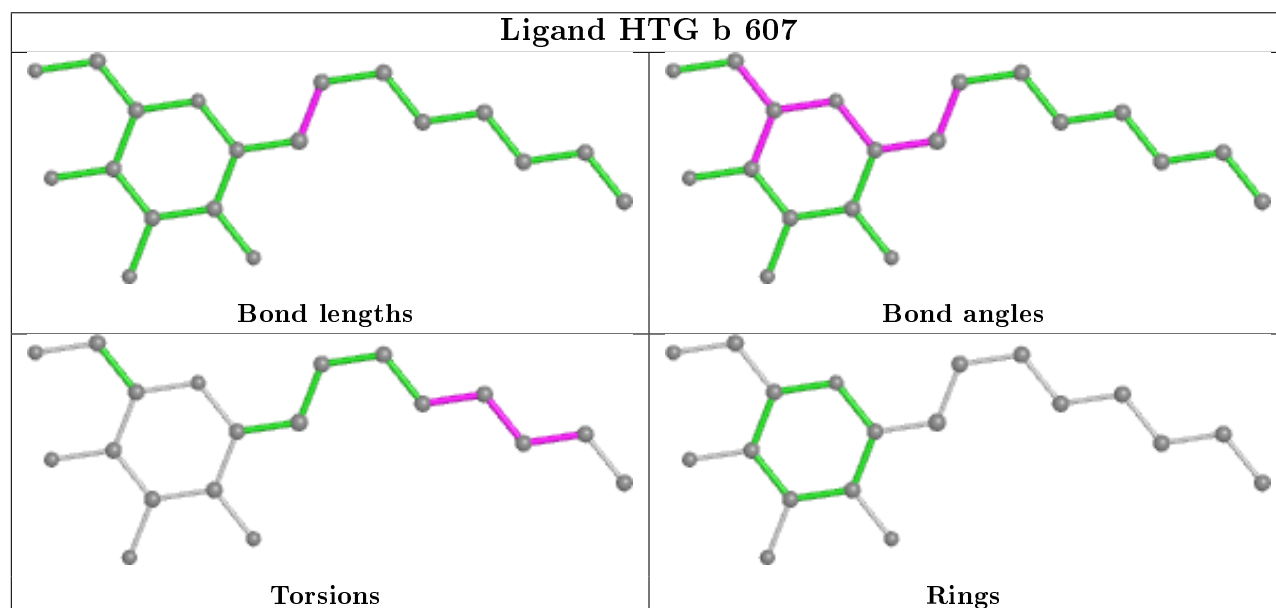
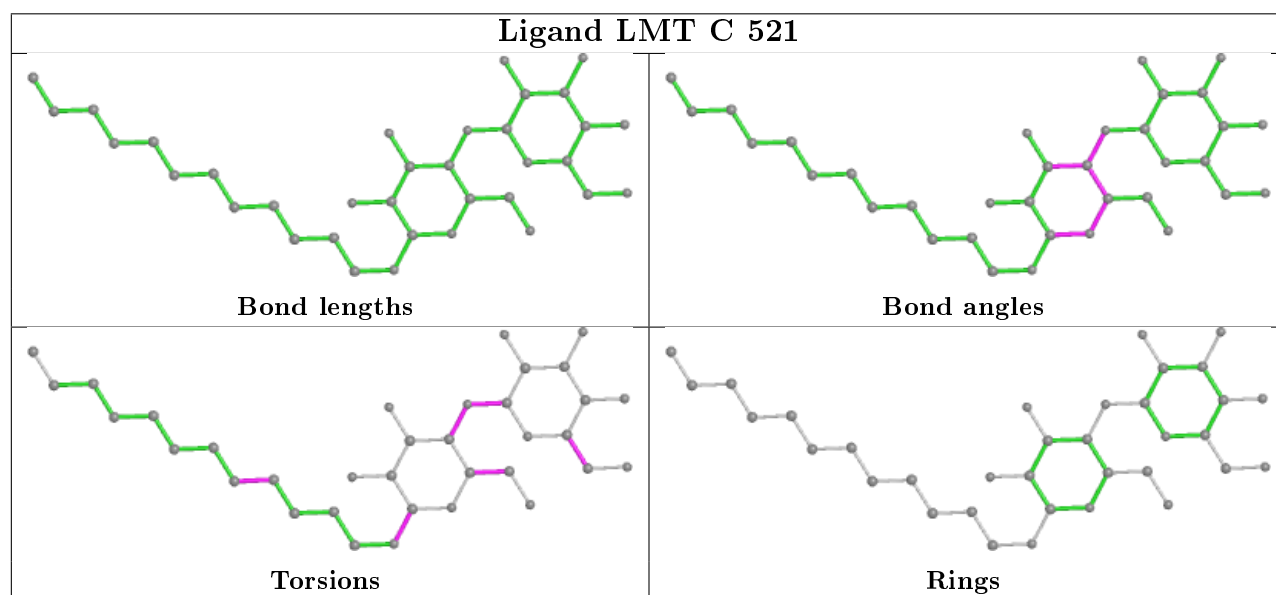
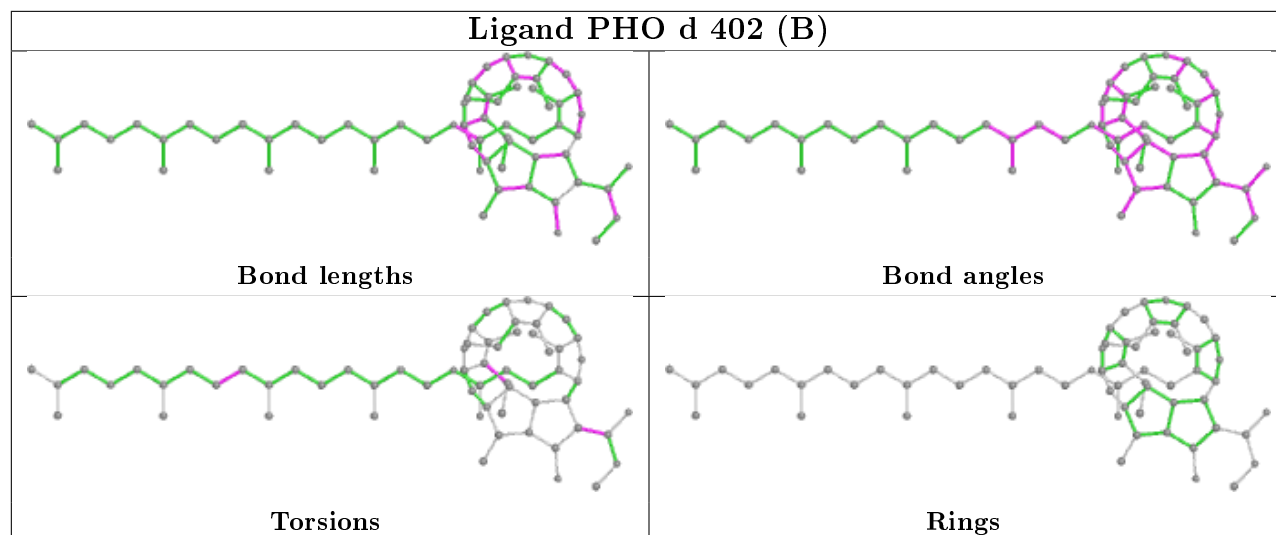


Ligand LMT E 102

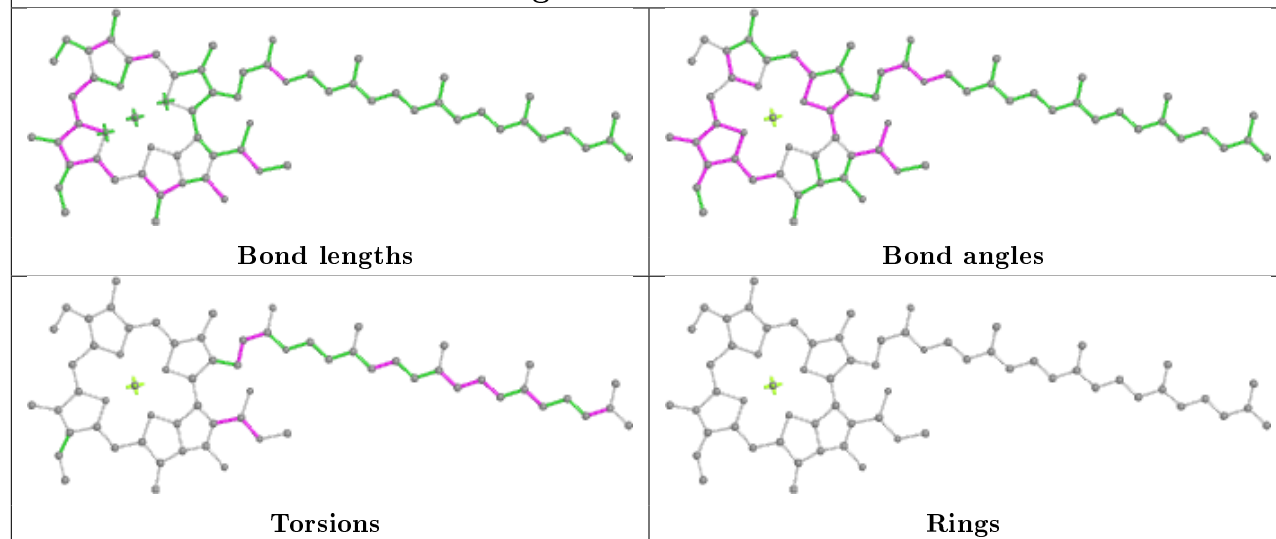


Ligand LMG D 415

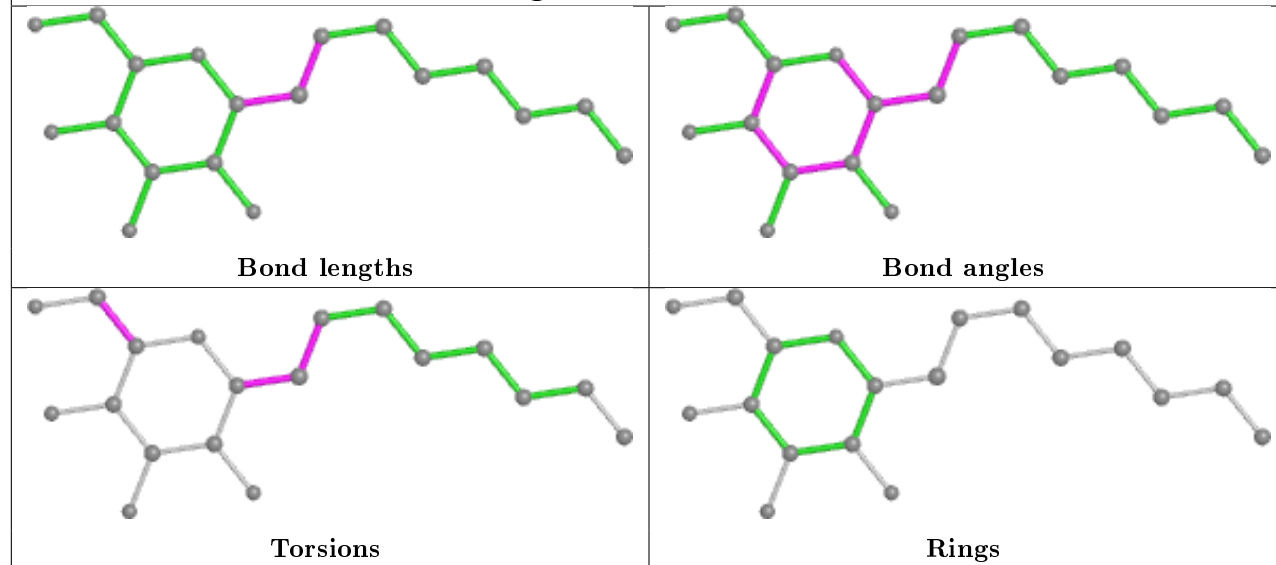




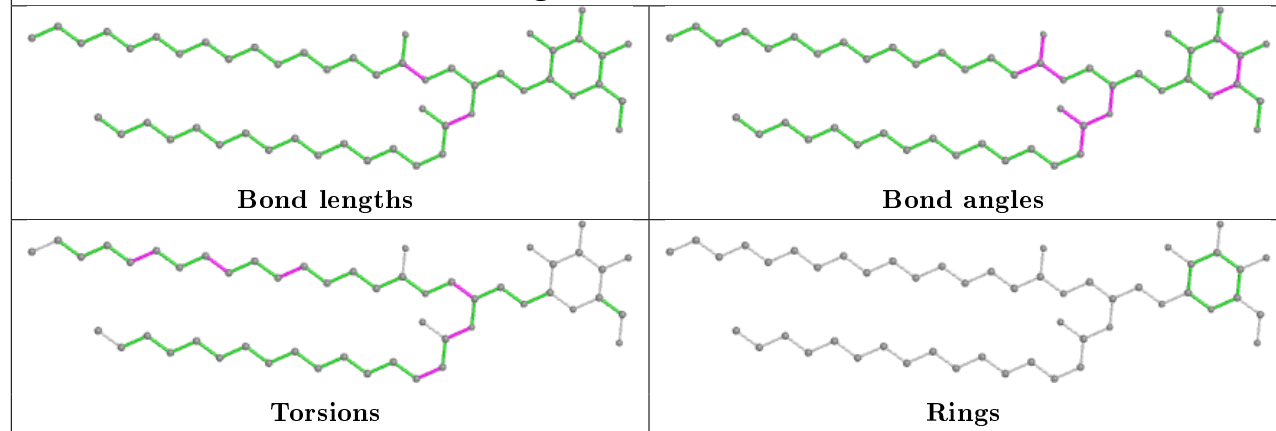
Ligand CLA B 602

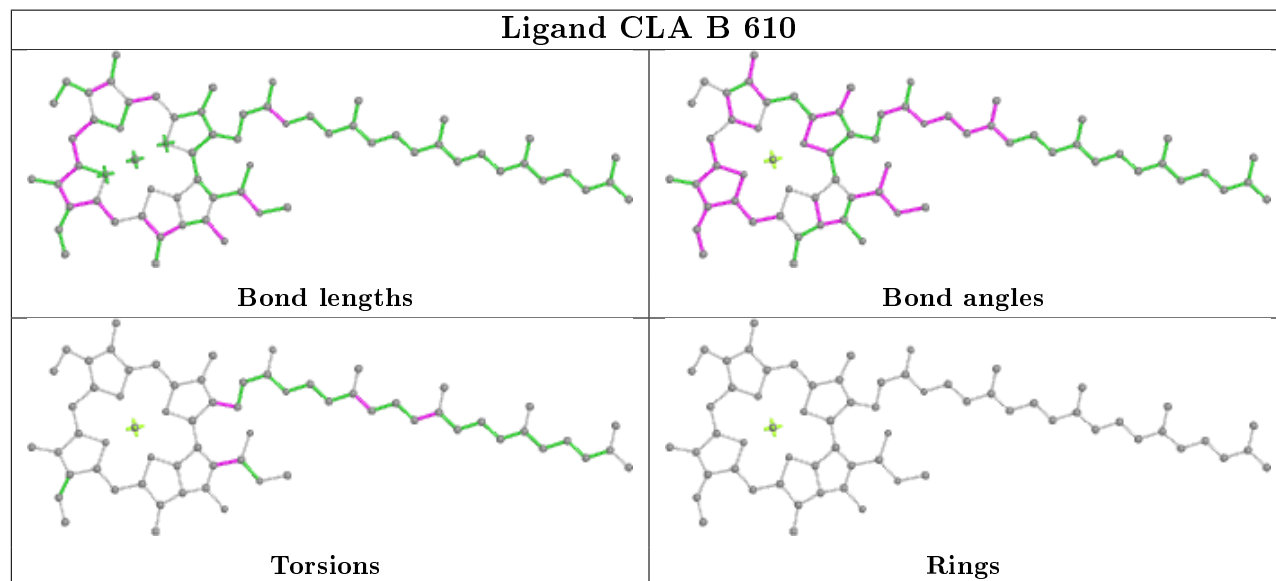
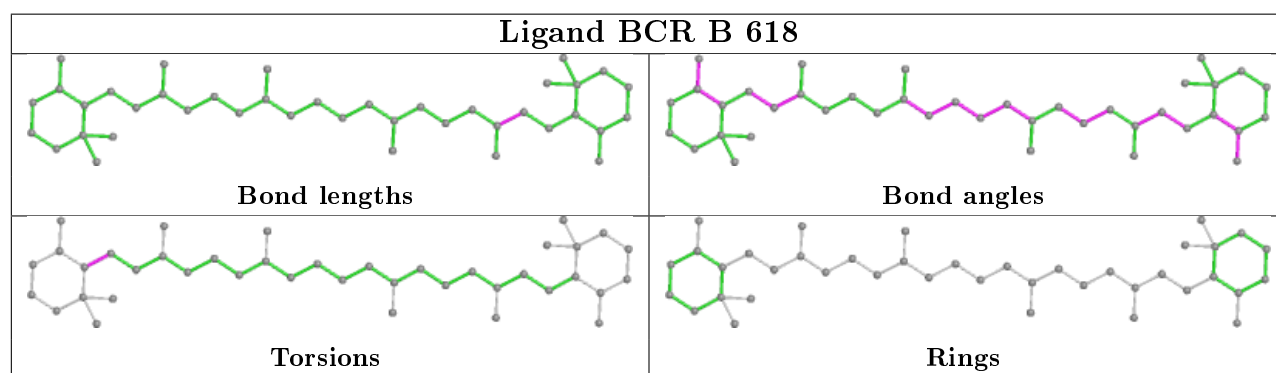
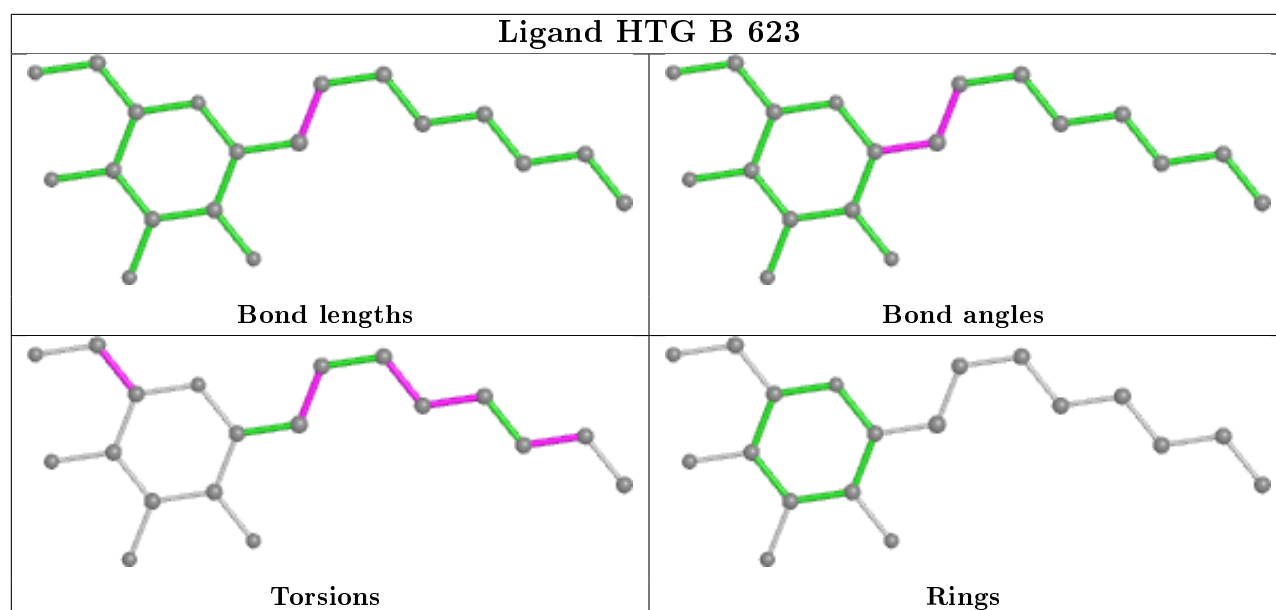


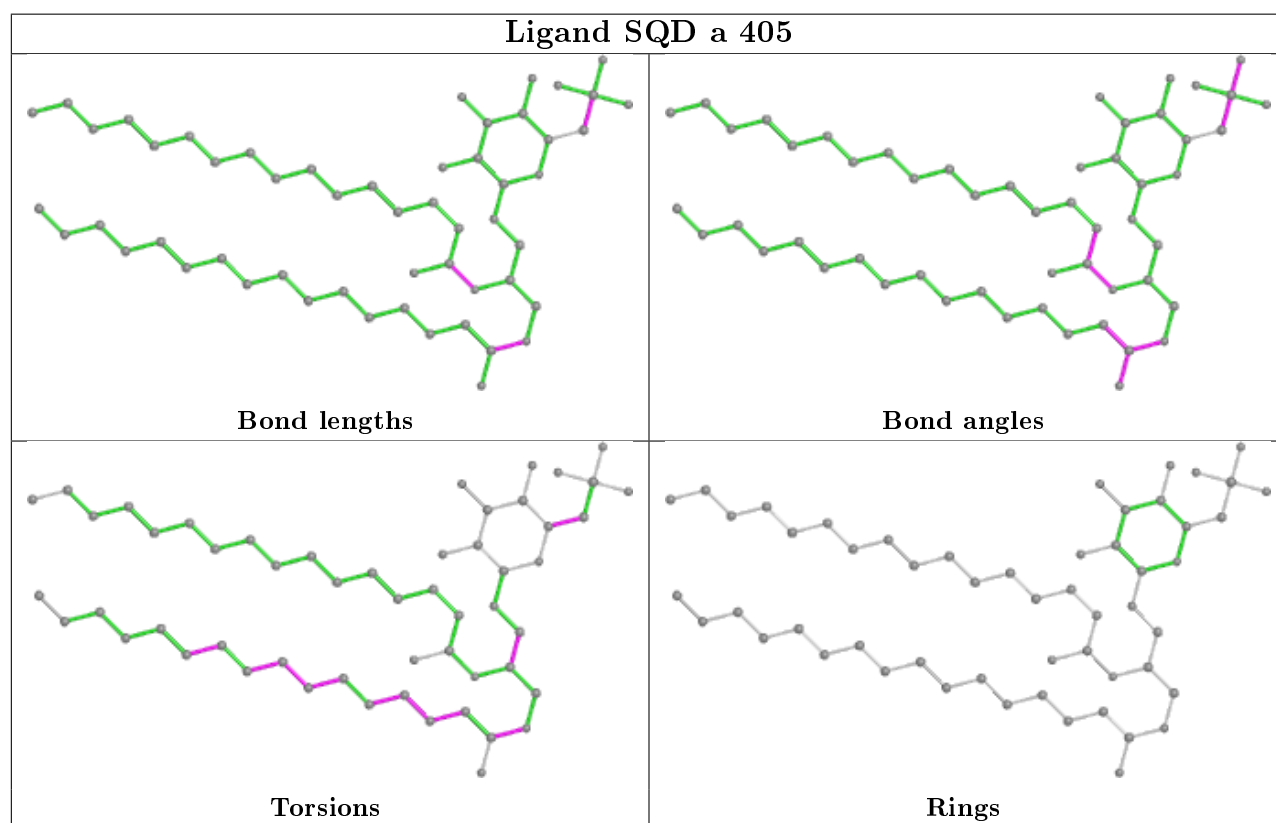
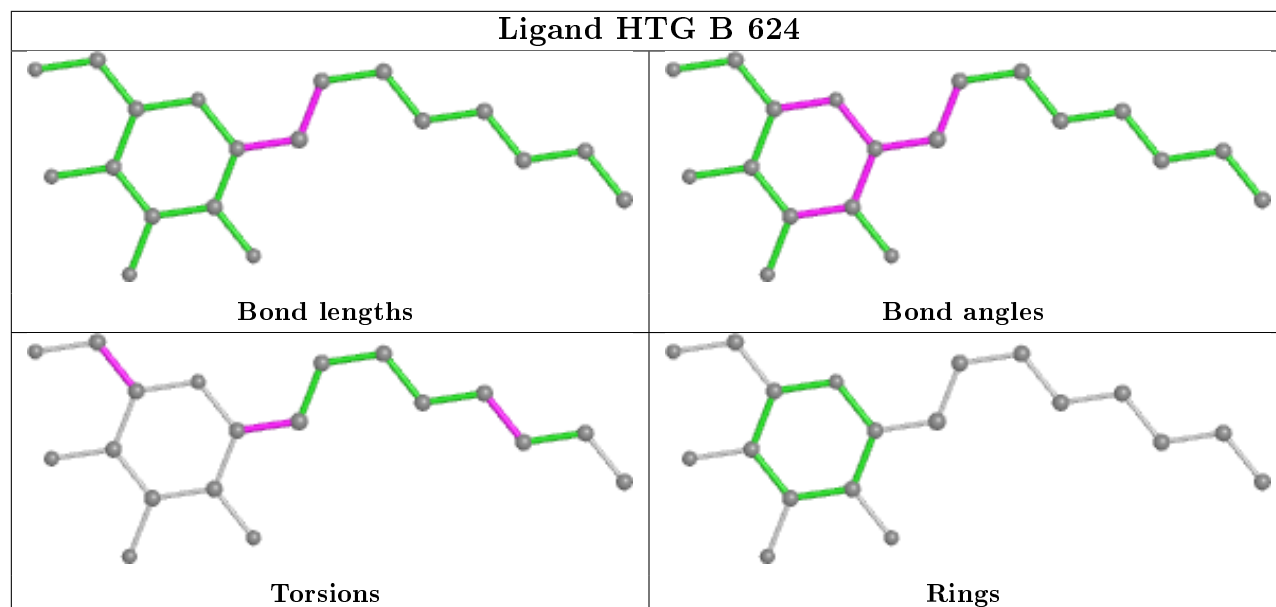
Ligand HTG V 206

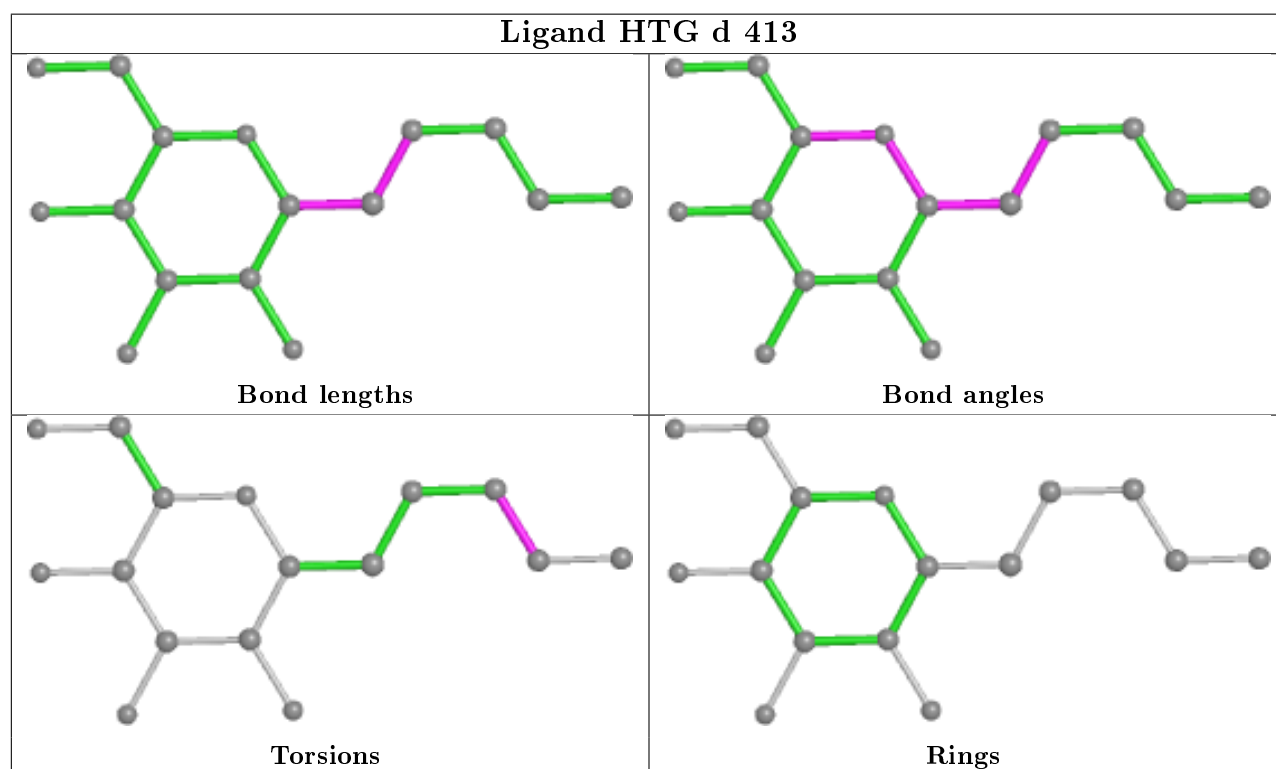
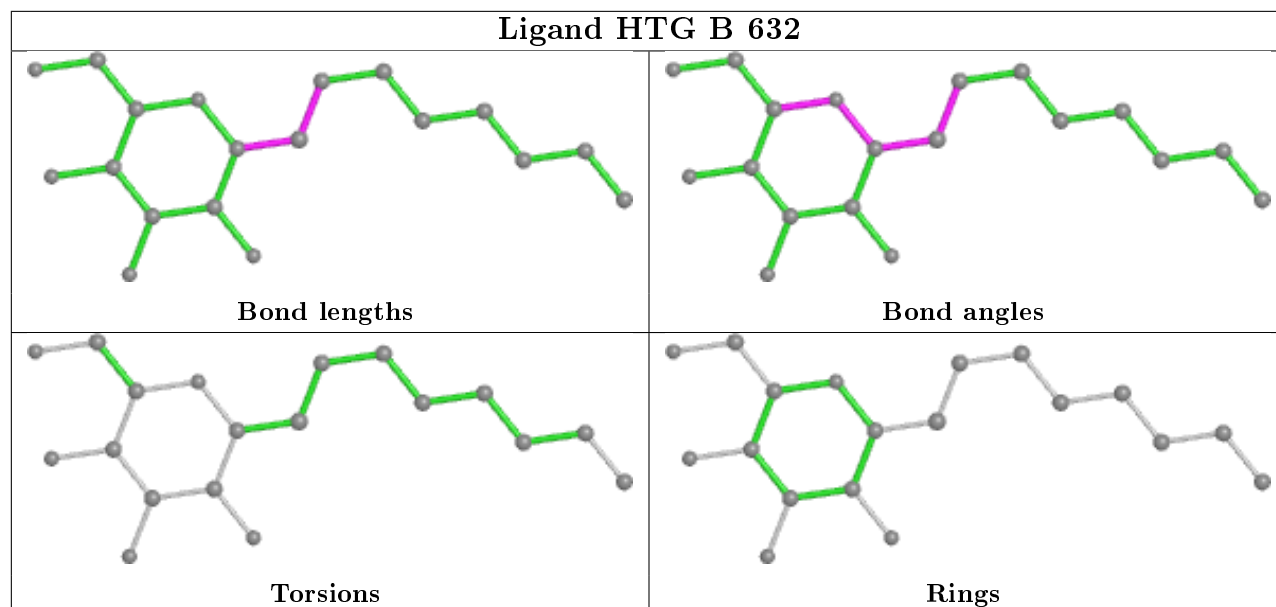


Ligand LMG c 522

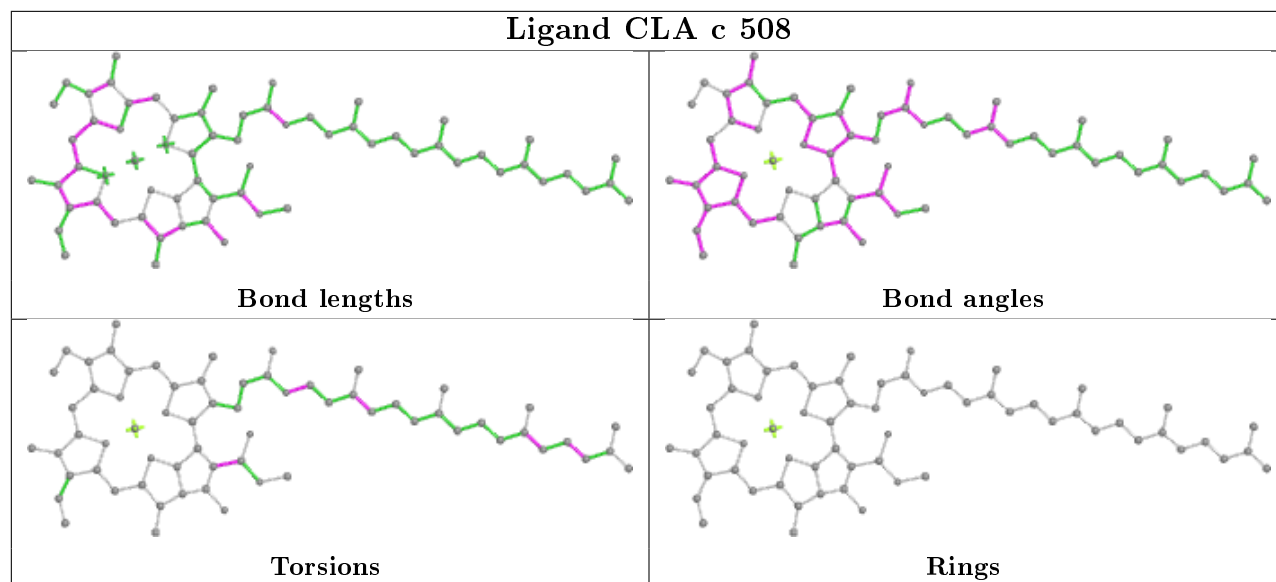




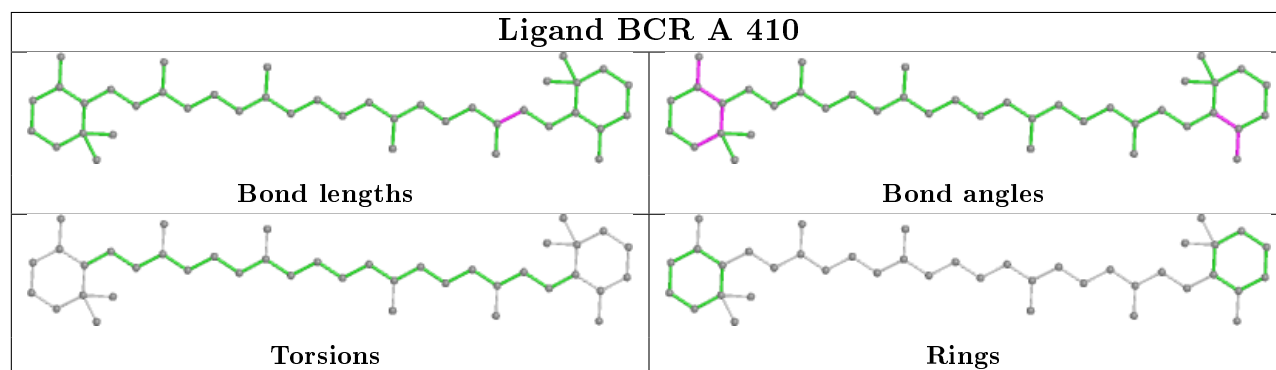




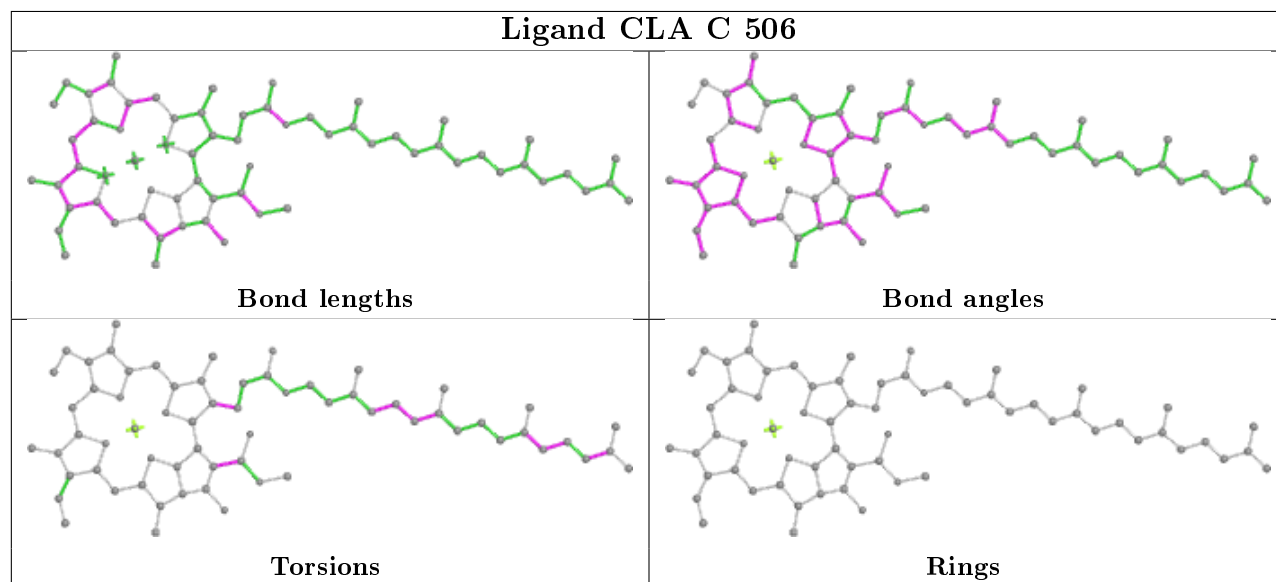
Ligand CLA c 508



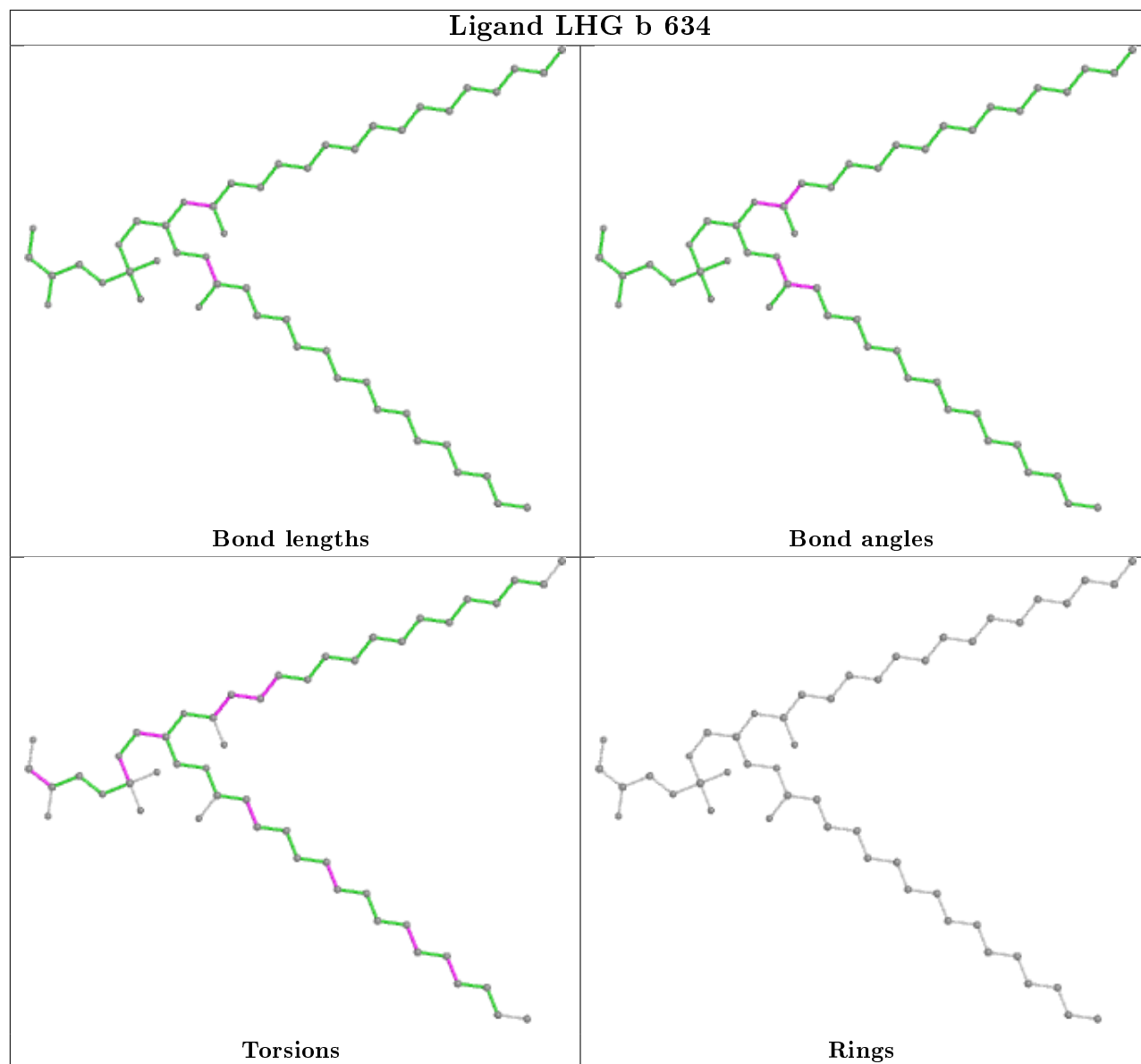
Ligand BCR A 410



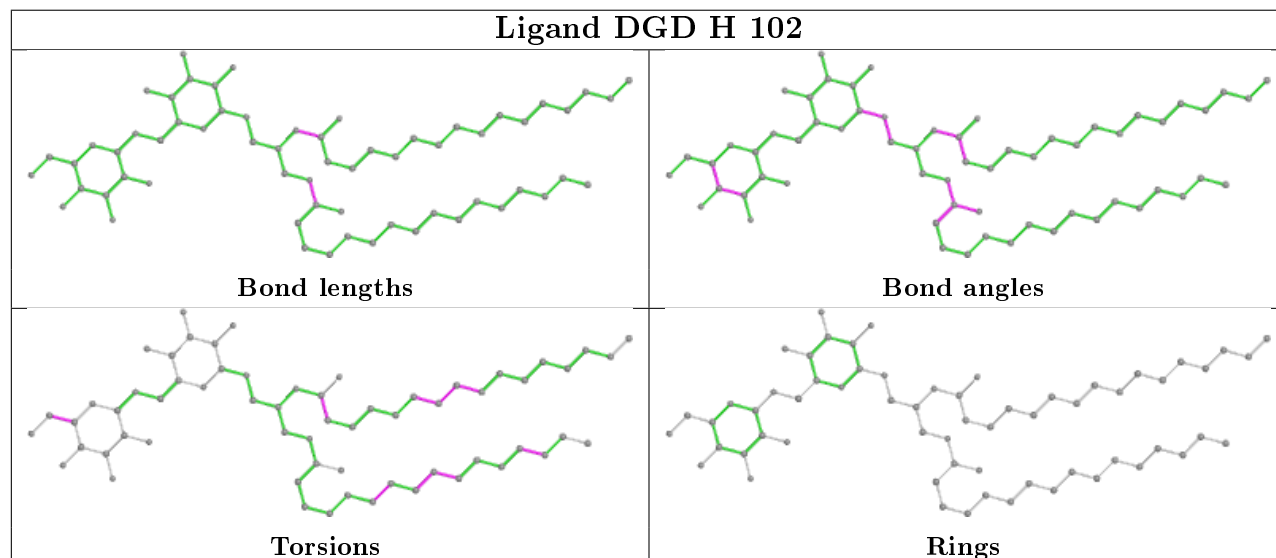
Ligand CLA C 506

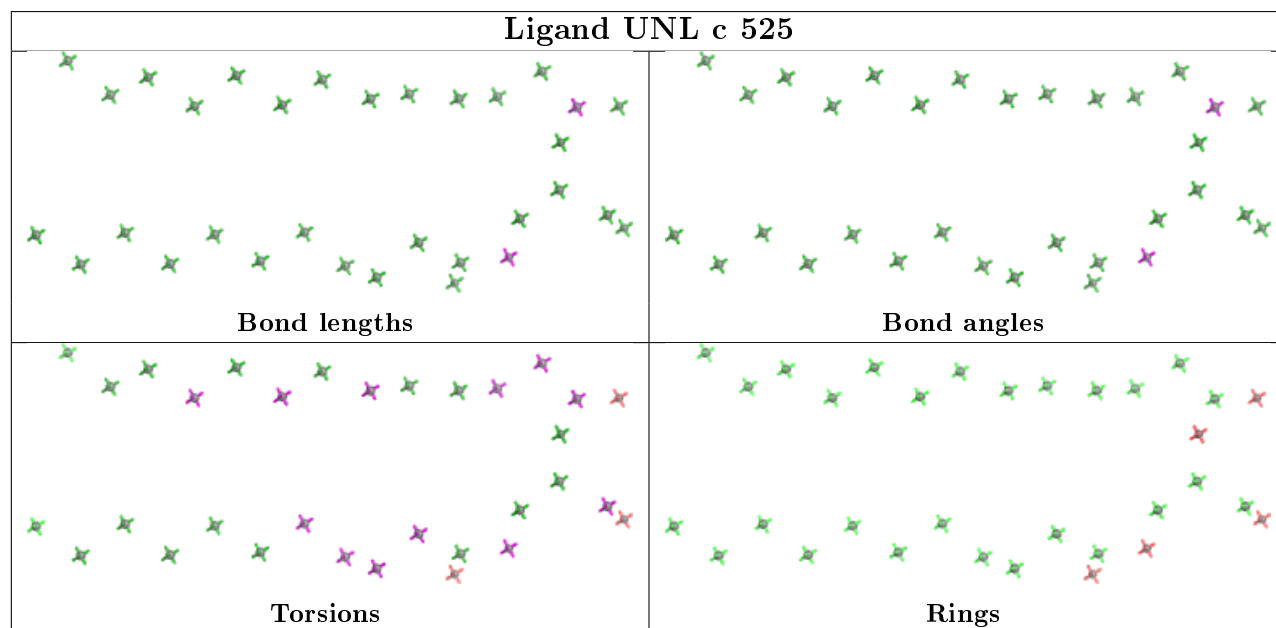
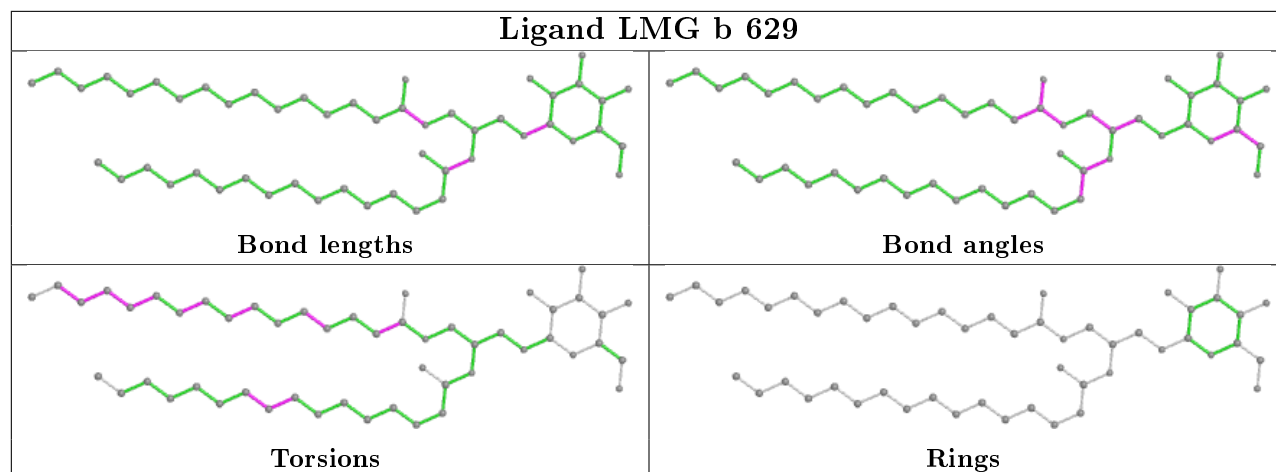


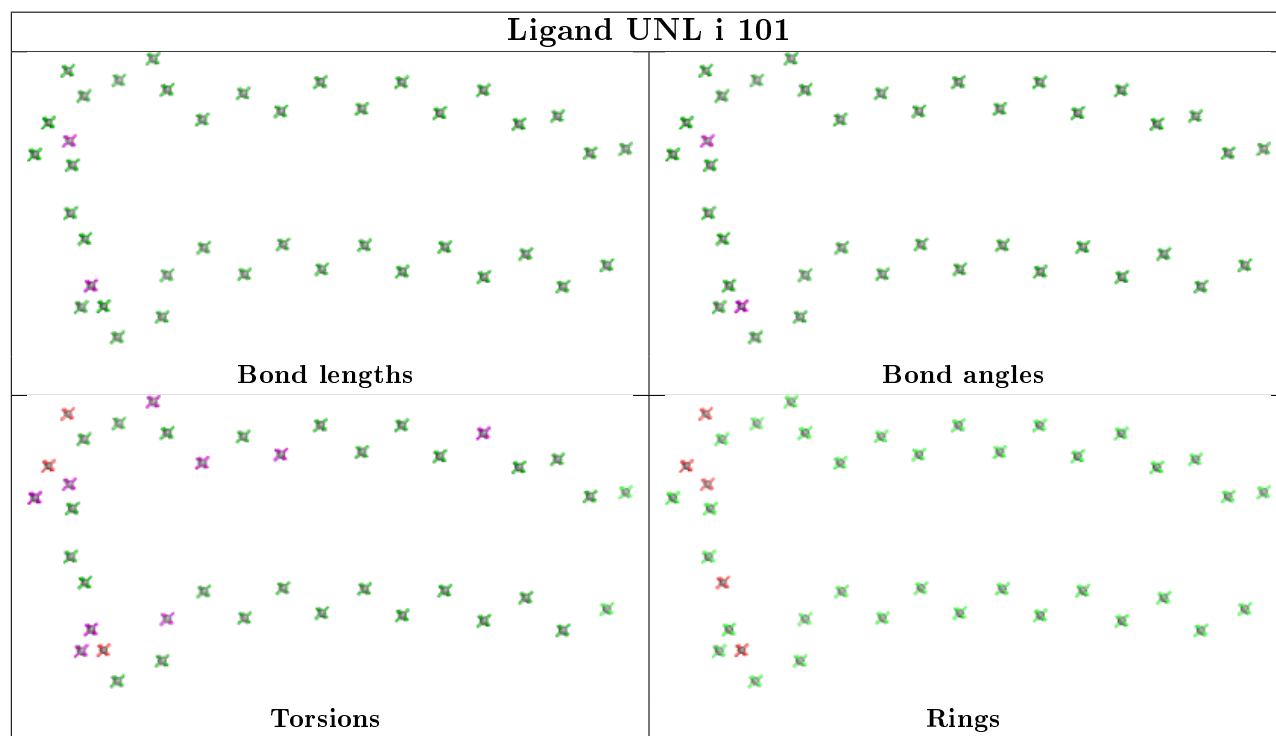
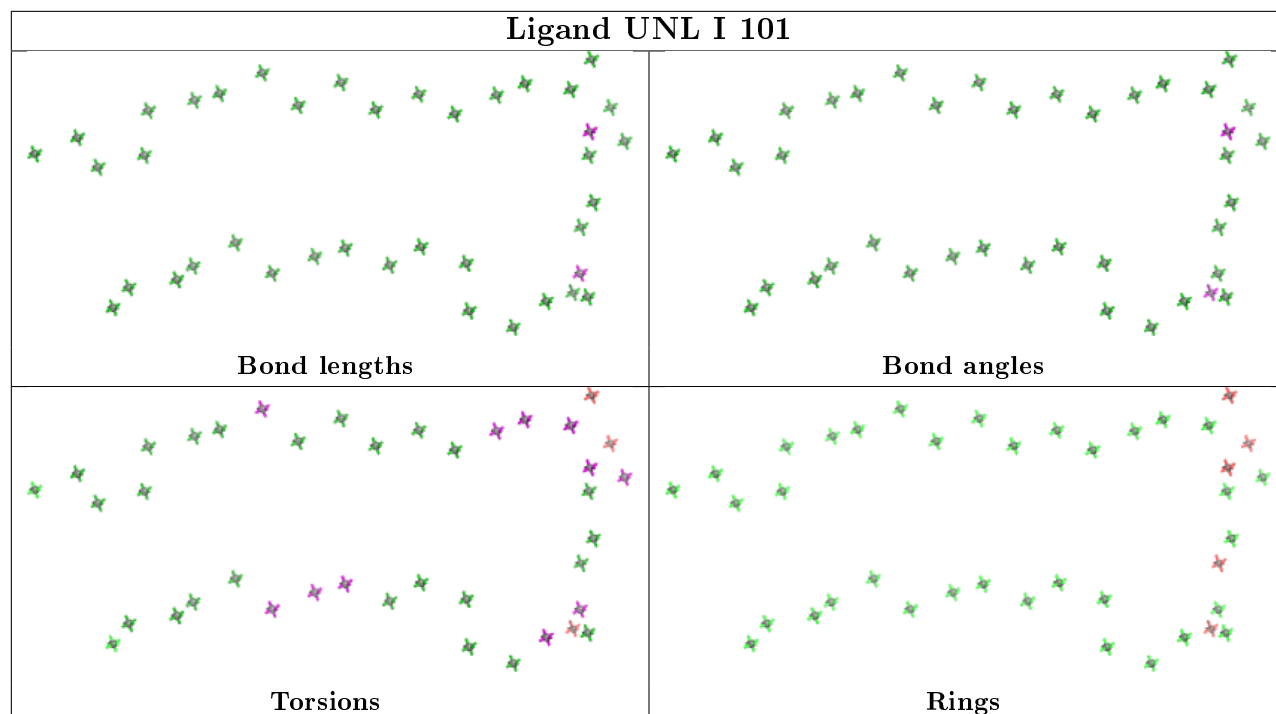
Ligand LHG b 634

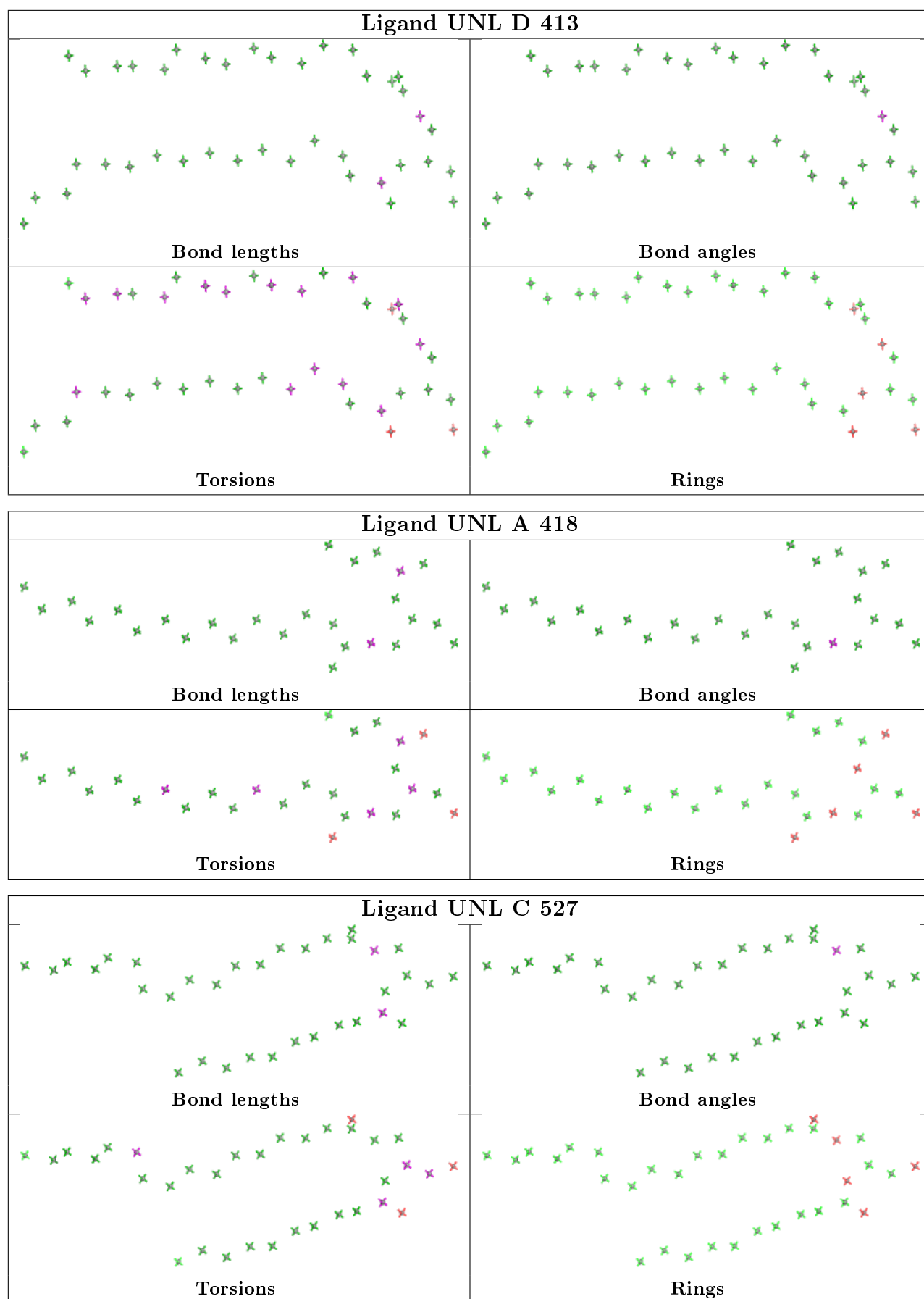


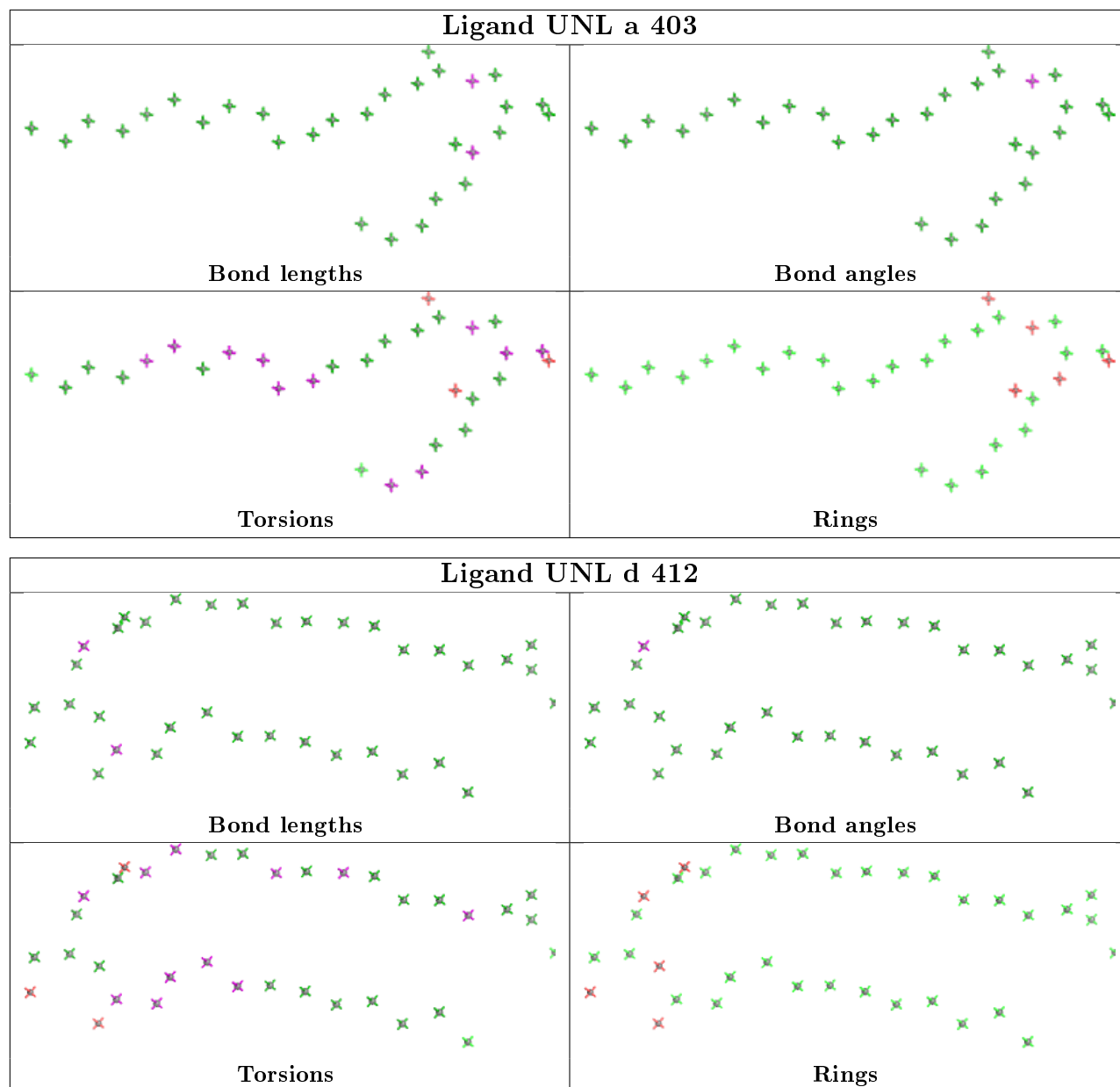
Ligand DGD H 102

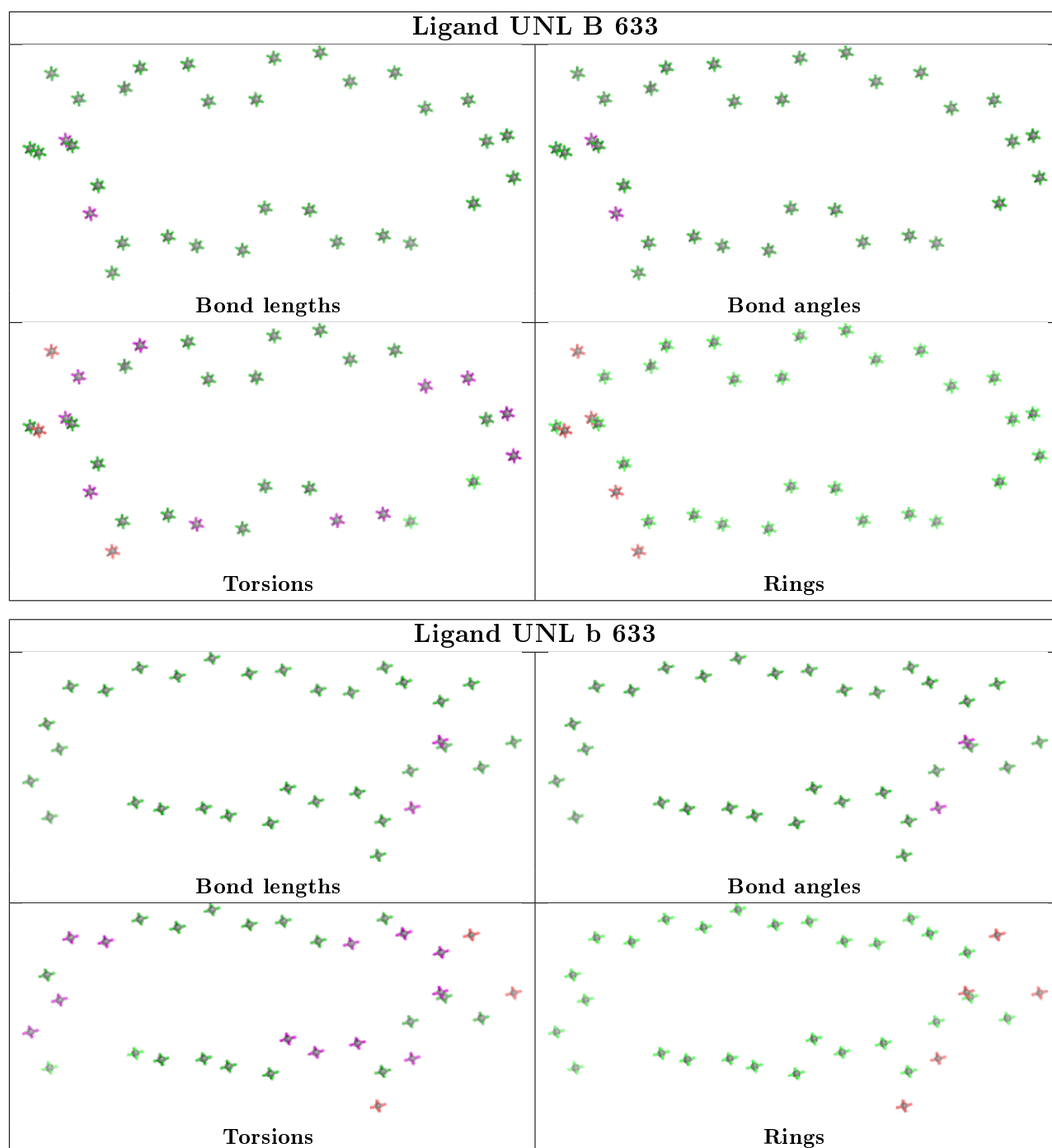












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	334/344 (97%)	0.25	9 (2%) 54 52	37, 49, 79, 117	0
1	a	334/344 (97%)	0.27	12 (3%) 42 42	37, 50, 87, 160	0
2	B	504/505 (99%)	0.20	24 (4%) 30 29	39, 54, 93, 141	0
2	b	503/505 (99%)	0.37	41 (8%) 11 10	41, 54, 99, 194	0
3	C	451/455 (99%)	0.22	33 (7%) 15 13	42, 63, 87, 140	0
3	c	455/455 (100%)	0.23	36 (7%) 12 11	46, 66, 87, 139	0
4	D	341/342 (99%)	0.24	15 (4%) 34 33	38, 51, 79, 139	0
4	d	341/342 (99%)	0.11	10 (2%) 51 50	39, 52, 79, 122	0
5	E	81/84 (96%)	2.26	37 (45%) 0 0	58, 79, 113, 169	0
5	e	81/84 (96%)	0.38	10 (12%) 4 3	58, 80, 131, 187	0
6	F	34/44 (77%)	1.07	8 (23%) 0 0	59, 70, 111, 118	0
6	f	32/44 (72%)	-0.01	1 (3%) 49 47	57, 69, 132, 154	0
7	H	65/65 (100%)	-0.06	5 (7%) 13 12	52, 65, 86, 160	0
7	h	65/65 (100%)	0.53	8 (12%) 4 3	54, 67, 85, 172	0
8	I	37/38 (97%)	0.13	4 (10%) 5 5	53, 67, 127, 178	0
8	i	37/38 (97%)	0.16	5 (13%) 3 2	49, 64, 131, 156	0
9	J	38/39 (97%)	1.17	8 (21%) 1 0	58, 76, 160, 184	0
9	j	39/39 (100%)	0.28	3 (7%) 13 12	59, 71, 147, 178	0
10	K	37/37 (100%)	0.41	4 (10%) 5 5	65, 77, 94, 113	0
10	k	37/37 (100%)	0.17	2 (5%) 25 24	65, 76, 98, 113	0
11	L	37/37 (100%)	1.17	12 (32%) 0 0	39, 44, 98, 137	0
11	l	37/37 (100%)	1.28	14 (37%) 0 0	40, 46, 98, 140	0
12	M	33/36 (91%)	1.85	16 (48%) 0 0	39, 46, 80, 122	0
12	m	33/36 (91%)	1.74	16 (48%) 0 0	39, 48, 87, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.13	9 (3%) 41 41	41, 59, 100, 159	0
13	o	243/244 (99%)	0.33	26 (10%) 6 5	43, 63, 115, 176	0
14	T	29/32 (90%)	1.09	7 (24%) 0 0	39, 45, 78, 136	0
14	t	29/32 (90%)	1.18	8 (27%) 0 0	39, 45, 71, 137	0
15	U	97/104 (93%)	-0.28	0 100 100	46, 59, 89, 121	0
15	u	97/104 (93%)	-0.37	0 100 100	47, 61, 81, 129	0
16	V	137/137 (100%)	-0.23	0 100 100	46, 59, 83, 119	0
16	v	137/137 (100%)	-0.05	3 (2%) 62 60	48, 69, 98, 139	0
17	Y	29/30 (96%)	4.06	17 (58%) 0 0	81, 91, 187, 209	0
17	y	29/30 (96%)	0.64	5 (17%) 1 1	82, 96, 146, 162	0
18	X	39/40 (97%)	1.34	15 (38%) 0 0	62, 73, 120, 151	0
18	x	38/40 (95%)	0.81	7 (18%) 1 1	63, 72, 133, 157	0
19	Z	62/62 (100%)	2.37	31 (50%) 0 0	78, 93, 132, 152	0
19	z	62/62 (100%)	2.22	28 (45%) 0 0	83, 97, 151, 188	0
20	R	18/34 (52%)	7.41	18 (100%) 0 0	96, 143, 171, 174	0
All	All	5275/5384 (97%)	0.39	507 (9%) 8 7	37, 59, 107, 209	0

All (507) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	23.2
17	Y	19	ILE	12.6
20	R	8	VAL	12.3
20	R	18	TRP	11.5
17	Y	20	ALA	10.8
20	R	15	ALA	10.6
20	R	6	LEU	10.3
20	R	5	VAL	9.1
18	x	37	VAL	8.3
2	b	496	TYR	8.2
5	E	84	LYS	8.0
2	b	495	PHE	7.8
9	J	5	GLY	7.8
19	Z	31	GLN	7.7
17	Y	21	GLN	7.6
2	b	494	GLY	7.6
2	b	503	THR	7.4

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Mol	Chain	Res	Type	RSRZ
2	b	504	THR	7.3
19	z	5	PHE	7.2
20	R	9	LEU	7.2
17	Y	22	LEU	7.2
5	E	19	TYR	7.1
20	R	12	VAL	7.1
20	R	13	LEU	7.0
19	z	3	ILE	6.9
18	x	2	THR	6.9
19	Z	33	TRP	6.8
20	R	3	TRP	6.7
5	E	17	VAL	6.7
2	B	496	TYR	6.6
19	Z	61	VAL	6.6
20	R	7	VAL	6.5
17	Y	26	ALA	6.5
17	y	20	ALA	6.3
2	b	487	SER	6.3
20	R	11	PRO	6.2
6	F	16	PHE	6.2
20	R	16	ALA	6.1
2	b	499	VAL	6.1
2	b	489	GLU	6.0
5	E	5	THR	6.0
8	i	37	LEU	5.9
20	R	17	GLY	5.9
3	c	143	TYR	5.8
5	E	6	GLY	5.8
3	c	140	LEU	5.8
2	b	502	VAL	5.8
17	Y	25	ILE	5.8
6	F	15	ILE	5.7
20	R	14	LEU	5.7
2	B	495	PHE	5.7
19	z	33	TRP	5.7
5	e	4	THR	5.7
5	E	83	LEU	5.7
3	C	253	LEU	5.6
20	R	10	LEU	5.5
2	b	497	GLN	5.5
20	R	2	ASP	5.5
19	Z	32	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
19	z	61	VAL	5.4
7	h	65	LEU	5.4
19	Z	62	VAL	5.4
16	v	17	LYS	5.3
5	E	4	THR	5.3
8	I	34	ARG	5.3
17	Y	23	THR	5.2
2	b	501	ASP	5.2
5	E	11	SER	5.2
2	B	290	ALA	5.2
19	z	62	VAL	5.1
20	R	4	ARG	5.0
19	Z	36	SER	5.0
18	X	2	THR	5.0
12	M	16[A]	LEU	5.0
18	x	38	GLN	5.0
20	R	19	ALA	4.9
7	H	64	ALA	4.9
5	E	22	ILE	4.9
3	C	145[A]	SER	4.9
2	b	486	LEU	4.9
13	O	62	GLU	4.8
5	E	20	TRP	4.8
19	z	41	PHE	4.8
2	B	494	GLY	4.8
5	e	5	THR	4.8
19	z	32	ASP	4.8
19	Z	1	MET	4.8
19	Z	25	VAL	4.8
18	X	37	VAL	4.7
7	h	66	GLY	4.7
2	B	504	THR	4.7
5	E	15	THR	4.7
19	Z	35	ARG	4.7
19	z	42	LEU	4.7
6	F	13	TYR	4.7
5	E	79	PHE	4.7
5	E	82	GLN	4.6
5	E	16	SER	4.6
5	E	10	PHE	4.5
19	Z	3	ILE	4.5
2	b	85	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
19	z	60	PHE	4.5
9	J	7	ILE	4.4
12	m	9	ILE	4.4
4	D	17	ILE	4.4
19	Z	30	PRO	4.4
2	b	493	TRP	4.4
3	C	23	ALA	4.3
3	C	131	TYR	4.3
2	b	126	PRO	4.3
5	E	78	THR	4.3
13	o	25	THR	4.3
13	o	26	ALA	4.3
9	J	3	GLU	4.3
6	F	14	PRO	4.2
13	O	56	PRO	4.2
19	z	7	LEU	4.2
5	E	21	VAL	4.1
13	O	25	THR	4.1
8	i	36	ASP	4.1
3	C	252	ILE	4.1
5	E	23	HIS	4.0
1	a	11	ALA	4.0
3	C	28	GLN	4.0
2	b	127	ARG	4.0
1	A	13	LEU	4.0
12	m	13	LEU	4.0
9	J	6	ARG	4.0
19	Z	4	LEU	4.0
18	x	39	ARG	3.9
2	b	294	SER	3.9
19	z	56	VAL	3.9
19	Z	29	SER	3.9
17	Y	41	VAL	3.9
5	E	9	PRO	3.9
3	C	143	TYR	3.9
9	j	1	MET	3.9
18	X	4	THR	3.9
3	C	155	ASN	3.9
2	B	501	ASP	3.8
4	D	238[A]	THR	3.8
4	D	12	ARG	3.8
2	b	485	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
9	j	3	GLU	3.8
18	X	40	SER	3.8
19	Z	26	ALA	3.8
14	t	4	ILE	3.8
3	c	207	ARG	3.7
3	c	200	THR	3.7
9	J	2	SER	3.7
12	M	14	PHE	3.7
1	a	15	GLU	3.7
4	d	17	ILE	3.7
2	B	502	VAL	3.7
2	b	491	VAL	3.7
3	c	158	THR	3.7
1	A	77	ILE	3.6
12	m	16	LEU	3.6
7	h	22	ALA	3.6
3	c	155	ASN	3.6
17	Y	40	ALA	3.6
18	X	32	SER	3.6
18	X	3	ILE	3.6
1	A	12	ASN	3.6
3	c	260	ALA	3.6
13	O	26	ALA	3.6
17	Y	37	PHE	3.5
2	b	297	THR	3.5
12	M	15	VAL	3.5
3	c	144	SER	3.5
19	z	35	ARG	3.5
3	C	134	ILE	3.5
3	C	139	THR	3.5
12	M	12	ALA	3.5
2	b	301	ALA	3.5
19	Z	56	VAL	3.4
5	E	25	ILE	3.4
2	B	497	GLN	3.4
19	Z	39	LEU	3.4
2	b	293	ALA	3.4
13	o	28	GLY	3.4
19	z	30	PRO	3.4
11	l	31	PHE	3.4
18	X	35	ASP	3.4
3	C	181	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
3	c	257	PHE	3.4
3	c	159	THR	3.4
5	e	6	GLY	3.4
9	J	4	GLY	3.3
5	E	74	GLN	3.3
12	M	20	VAL	3.3
2	b	296	ALA	3.3
14	t	12	CYS	3.3
13	o	132	ASN	3.3
3	c	175	LEU	3.3
19	Z	34	ASP	3.3
3	C	254	THR	3.3
5	E	18	ARG	3.3
10	K	14	ALA	3.3
18	X	39	ARG	3.3
3	C	47	GLY	3.3
18	x	33	GLN	3.3
19	z	36	SER	3.3
19	Z	38	GLN	3.3
3	c	253	LEU	3.3
12	m	12	ALA	3.3
12	m	15	VAL	3.3
2	b	488	PRO	3.2
11	l	26	VAL	3.2
12	m	20	VAL	3.2
7	H	65	LEU	3.2
17	Y	39	LEU	3.2
19	z	43	GLY	3.2
13	O	27	ARG	3.2
12	M	9	ILE	3.2
18	X	6	SER	3.2
2	B	503	THR	3.2
12	M	13	LEU	3.2
2	b	129	GLY	3.2
2	b	490	GLN	3.2
7	h	23	PRO	3.2
19	Z	27	TYR	3.1
3	C	207	ARG	3.1
11	L	26	VAL	3.1
13	o	204	VAL	3.1
11	l	24[A]	ILE	3.1
17	Y	30	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
3	c	259	TRP	3.1
13	o	21	THR	3.1
3	C	257	PHE	3.1
12	m	14	PHE	3.1
3	C	27	ASP	3.1
3	C	250	TRP	3.1
3	C	140	LEU	3.1
13	o	202	ALA	3.1
19	z	2	THR	3.1
19	Z	41	PHE	3.1
19	z	1	MET	3.1
2	b	500	GLY	3.1
2	B	296	ALA	3.1
11	l	28	ALA	3.1
2	b	498	LYS	3.1
3	c	251	HIS	3.1
11	l	21	LEU	3.1
12	M	8	LEU	3.1
19	z	59	PHE	3.0
18	X	38	GLN	3.0
3	c	256	PRO	3.0
3	c	254	THR	3.0
2	b	484	PRO	3.0
5	E	75	GLN	3.0
19	z	38	GLN	3.0
13	o	23	ASP	3.0
1	a	264[A]	SER	3.0
12	M	19	SER	3.0
5	e	74	GLN	3.0
13	o	209	GLY	3.0
3	c	147	PHE	3.0
6	F	12	SER	3.0
5	E	42	LEU	3.0
19	Z	54	VAL	2.9
1	A	176	ILE	2.9
5	E	72	ALA	2.9
11	L	29	LEU	2.9
11	L	30	LEU	2.9
11	l	23	LEU	2.9
12	m	10	ALA	2.9
19	z	4	LEU	2.9
8	I	36	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
3	c	145	SER	2.9
6	F	20	TRP	2.9
12	M	24	ILE	2.9
3	C	45	LEU	2.9
6	F	17	THR	2.9
12	m	17	VAL	2.9
18	x	3	ILE	2.9
1	a	225	ARG	2.9
19	z	6	GLN	2.9
12	M	18	PRO	2.9
13	o	141	ASP	2.8
1	a	256	GLY	2.8
3	C	54	VAL	2.8
18	X	33	GLN	2.8
2	B	293	ALA	2.8
8	I	37	LEU	2.8
12	M	11	THR	2.8
5	E	12	ASP	2.8
4	D	24	ARG	2.8
13	o	35	SER	2.8
2	B	489	GLU	2.8
14	T	8	PHE	2.8
13	o	140	THR	2.8
19	z	40	ILE	2.8
5	E	24	SER	2.8
4	d	20	ASP	2.8
6	F	34	LEU	2.7
3	C	157	MET	2.7
1	a	53	ILE	2.7
2	b	161	LEU	2.7
3	c	204	LEU	2.7
19	Z	24	PRO	2.7
12	M	17	VAL	2.7
2	B	479	PHE	2.7
11	l	22	LEU	2.7
4	d	21	TRP	2.7
1	a	263	ALA	2.7
1	a	248[A]	ILE	2.7
13	o	24	ASP	2.7
14	T	4	ILE	2.7
3	c	141	GLU	2.7
4	d	238[A]	THR	2.7

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Mol	Chain	Res	Type	RSRZ
14	t	8	PHE	2.7
19	z	39	LEU	2.7
2	B	285	ASN	2.7
3	c	162	GLY	2.7
11	L	24[A]	ILE	2.7
2	b	295	GLY	2.7
19	Z	22	GLY	2.7
5	E	76	VAL	2.6
3	c	255	THR	2.6
2	b	298	LEU	2.6
12	m	8	LEU	2.6
2	b	285[A]	ASN	2.6
12	M	10	ALA	2.6
1	a	229	GLU	2.6
5	E	7	GLU	2.6
19	Z	42	LEU	2.6
2	b	139	PHE	2.6
6	f	14	PRO	2.6
13	o	59	LYS	2.6
3	c	206	PRO	2.6
5	E	14	ILE	2.6
10	k	12	PRO	2.6
11	L	35	PHE	2.6
8	i	38	GLU	2.6
2	B	295	GLY	2.6
2	b	290	ALA	2.6
11	L	23	LEU	2.6
5	e	71	GLU	2.6
19	Z	2	THR	2.6
3	c	50	LEU	2.6
12	M	5	GLN	2.6
8	i	34	ARG	2.6
13	o	139	SER	2.6
2	B	297	THR	2.5
12	m	11	THR	2.5
16	v	19	ILE	2.5
3	C	25	ASN	2.5
13	o	213	GLY	2.5
5	E	77	GLU	2.5
13	O	60	ARG	2.5
3	c	201	ASN	2.5
18	X	36	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	493	TRP	2.5
11	L	27	LEU	2.5
10	k	17	ILE	2.5
17	Y	44	GLY	2.5
14	t	17	PHE	2.5
4	d	16	ASP	2.5
11	l	27	LEU	2.5
11	L	31	PHE	2.5
2	B	490	GLN	2.5
18	X	31	ILE	2.5
2	B	483	ASP	2.5
3	C	48	LYS	2.4
11	l	25	LEU	2.4
1	A	49	VAL	2.4
7	H	48	ILE	2.4
4	d	195	PRO	2.4
19	Z	43	GLY	2.4
11	L	22	LEU	2.4
7	H	54	ILE	2.4
12	m	24	ILE	2.4
2	B	505	ARG	2.4
14	T	5	THR	2.4
5	e	77	GLU	2.4
11	l	30	LEU	2.4
14	T	7	VAL	2.4
19	z	53	VAL	2.4
19	Z	60	PHE	2.4
9	J	10	TRP	2.4
11	l	32	SER	2.4
14	t	13	ILE	2.4
14	T	10	PHE	2.4
5	E	26	THR	2.4
12	m	19	SER	2.4
2	B	499	VAL	2.4
13	o	58	ASN	2.4
4	D	235[A]	PHE	2.4
17	Y	43	ARG	2.4
13	o	137	THR	2.4
3	C	144	SER	2.4
11	L	19	LEU	2.4
4	D	27	PHE	2.3
19	Z	8	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
18	x	35	ASP	2.3
3	c	146	PHE	2.3
3	C	158	THR	2.3
5	e	61	ARG	2.3
3	c	153	ASP	2.3
13	O	36	GLN	2.3
13	o	36	GLN	2.3
11	L	28	ALA	2.3
3	C	26	ARG	2.3
4	D	103	ARG	2.3
5	E	71	GLU	2.3
8	I	38	GLU	2.3
2	b	223	GLN	2.3
9	J	8	PRO	2.3
14	T	14	ILE	2.3
1	a	19	ASN	2.3
19	Z	17	PHE	2.3
2	b	165	GLY	2.3
9	j	2	SER	2.3
10	K	15	TYR	2.3
2	B	324	LEU	2.3
2	b	218	LEU	2.3
5	E	46	VAL	2.3
7	h	64	ALA	2.3
17	Y	24	MET	2.3
3	C	46	SER	2.3
12	m	7	GLY	2.3
3	c	134	ILE	2.3
12	m	5	GLN	2.2
5	E	13	ILE	2.2
2	b	292	LEU	2.2
17	y	22	LEU	2.2
14	t	7	VAL	2.2
17	y	18	VAL	2.2
2	b	302	TRP	2.2
11	l	29	LEU	2.2
4	D	195	PRO	2.2
13	o	200	ASN	2.2
8	i	33	LYS	2.2
13	o	208	THR	2.2
12	m	18	PRO	2.2
3	C	135	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	15	GLU	2.2
7	h	26	GLY	2.2
19	z	25	VAL	2.2
2	B	492	GLU	2.2
3	c	203	THR	2.2
3	C	147	PHE	2.2
14	t	10	PHE	2.2
17	Y	45	ASN	2.2
3	c	161	LEU	2.2
13	o	61	GLN	2.2
10	K	41	ALA	2.2
3	c	149	TYR	2.1
5	e	72	ALA	2.1
4	d	24	ARG	2.1
4	D	232	PHE	2.1
3	c	142	GLU	2.1
7	h	57	GLY	2.1
4	D	313	THR	2.1
1	A	78	ILE	2.1
1	a	77	ILE	2.1
17	y	25	ILE	2.1
2	B	291	SER	2.1
4	D	300	SER	2.1
1	a	262	TYR	2.1
13	o	133	VAL	2.1
5	E	61	ARG	2.1
13	O	58	ASN	2.1
3	c	131	TYR	2.1
4	D	239[A]	GLN	2.1
1	A	71	LEU	2.1
4	D	273	PHE	2.1
17	y	21	GLN	2.1
3	C	133	ALA	2.1
19	z	54	VAL	2.1
13	o	5	LEU	2.1
16	v	12	LEU	2.1
3	C	270	ALA	2.1
5	e	68	ASP	2.1
19	Z	21	ILE	2.1
11	l	35	PHE	2.1
12	M	6	LEU	2.1
4	D	98	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
7	H	66	GLY	2.1
13	o	91	GLY	2.1
3	c	250	TRP	2.1
4	d	204	VAL	2.0
3	c	160	ILE	2.0
11	l	34	TYR	2.0
13	o	38	TYR	2.0
4	d	205	LEU	2.0
5	e	79	PHE	2.0
14	T	17	PHE	2.0
19	z	12	LEU	2.0
18	X	8	LYS	2.0
1	A	183	MET	2.0
5	E	68	ASP	2.0
3	C	132	HIS	2.0
3	C	251	HIS	2.0
4	D	193	LEU	2.0
11	L	21	LEU	2.0
19	Z	52	LEU	2.0
4	d	14	TRP	2.0
10	K	39	TRP	2.0
2	b	128	THR	2.0
7	h	63	LYS	2.0
13	O	57	LYS	2.0
19	z	31	GLN	2.0
3	c	249	ILE	2.0
14	t	14	ILE	2.0
18	X	34	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, 95th 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 ²)	Q<0.9
14	FME	T	1	10/11	0.91	0.30	40,51,58,129	0
8	FME	i	1	10/11	0.93	0.17	45,62,71,72	0
14	FME	t	1	10/11	0.93	0.29	33,45,52,103	0
12	FME	m	1	10/11	0.95	0.27	37,59,100,111	0
8	FME	I	1	10/11	0.95	0.13	36,59,66,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	FME	M	1	10/11	0.97	0.24	38,56,95,98	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, 95th 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(\AA^2)	Q<0.9
37	DGD	e	101	62/66	0.28	0.48	89,127,190,192	0
33	UNL	C	527	34/-	0.38	0.33	92,125,135,139	0
29	LMT	E	102	35/35	0.44	0.46	116,153,169,172	0
33	UNL	a	403	30/-	0.46	0.35	77,96,125,131	0
29	LMT	b	630	25/35	0.53	0.39	80,112,160,160	0
33	UNL	A	418	28/-	0.53	0.28	65,94,113,117	0
37	DGD	D	408	52/66	0.53	0.46	75,107,156,165	0
29	LMT	m	102	35/35	0.54	0.38	56,93,121,125	0
38	LHG	E	101	42/49	0.56	0.34	73,119,141,142	0
33	UNL	j	101	10/-	0.56	0.42	76,91,98,99	0
33	UNL	B	633	33/-	0.57	0.30	62,87,128,133	0
38	LHG	a	420	42/49	0.58	0.33	75,138,182,183	0
33	UNL	c	525	32/-	0.58	0.40	85,102,136,143	0
29	LMT	C	521	35/35	0.58	0.39	96,134,162,166	0
36	HTG	D	414	16/19	0.59	0.28	81,137,154,157	0
36	HTG	d	413	16/19	0.59	0.32	72,110,117,122	0
27	SQD	f	102	43/54	0.60	0.31	109,123,162,167	0
29	LMT	a	419	35/35	0.61	0.49	104,129,159,162	0
29	LMT	e	102	35/35	0.62	0.31	86,143,166,167	0
29	LMT	M	102	35/35	0.62	0.31	46,102,124,132	0
29	LMT	m	103	35/35	0.62	0.45	46,103,128,129	0
33	UNL	J	101	10/-	0.64	0.27	61,84,93,93	0
22	CL	v	205	1/1	0.66	0.22	128,128,128,128	0
34	LMG	Z	101	37/55	0.66	0.39	72,131,146,147	0
29	LMT	D	403	35/35	0.67	0.31	75,127,151,153	0
36	HTG	B	632	19/19	0.67	0.25	55,118,140,210	0
29	LMT	A	414	35/35	0.67	0.34	59,96,114,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	LMT	M	104	35/35	0.68	0.58	56,102,155,159	0
32	PL9	A	417[B]	55/55	0.68	0.31	84,104,120,121	55
32	PL9	A	417[A]	55/55	0.68	0.31	85,104,120,121	55
29	LMT	a	404	35/35	0.69	0.38	42,99,122,150	0
36	HTG	B	624	19/19	0.69	0.35	78,133,147,176	0
34	LMG	C	519	51/55	0.70	0.23	62,99,117,120	0
27	SQD	L	102	54/54	0.70	0.34	54,82,126,138	0
34	LMG	z	101	39/55	0.71	0.41	77,125,148,160	0
36	HTG	C	523	19/19	0.71	0.42	78,117,141,143	0
36	HTG	c	524	19/19	0.71	0.44	90,122,133,164	0
32	PL9	a	416[A]	55/55	0.72	0.31	87,114,123,124	55
32	PL9	a	416[B]	55/55	0.72	0.31	87,114,123,124	55
33	UNL	i	101	40/-	0.72	0.24	54,88,139,142	0
33	UNL	b	633	33/-	0.72	0.24	58,97,147,148	0
27	SQD	B	621	54/54	0.73	0.46	56,82,141,145	0
36	HTG	b	608	19/19	0.73	0.21	55,112,147,160	0
33	UNL	m	101	10/-	0.74	0.75	64,66,90,92	0
27	SQD	A	413	54/54	0.74	0.27	56,81,130,137	0
33	UNL	d	412	36/-	0.75	0.21	69,89,135,139	0
27	SQD	a	405	54/54	0.76	0.30	40,83,122,127	0
36	HTG	b	607	19/19	0.76	0.22	52,88,101,103	0
37	DGD	h	102	62/66	0.76	0.20	44,60,79,85	0
29	LMT	t	101	25/35	0.77	0.55	52,86,147,149	0
22	CL	U	201	1/1	0.77	0.31	117,117,117,117	0
29	LMT	T	104	25/35	0.77	0.44	43,83,140,150	0
33	UNL	I	101	40/-	0.77	0.25	60,95,150,153	0
28	GOL	A	412	6/6	0.77	0.23	76,86,88,92	0
28	GOL	v	202	6/6	0.78	0.29	83,96,98,100	0
37	DGD	C	517	62/66	0.78	0.21	55,71,102,113	0
33	UNL	D	413	40/-	0.78	0.18	63,88,132,140	0
34	LMG	a	415	51/55	0.79	0.21	61,90,100,101	0
33	UNL	M	103	10/-	0.79	0.52	48,53,74,76	0
34	LMG	k	101	51/55	0.79	0.24	62,94,123,126	0
36	HTG	B	631	19/19	0.79	0.20	52,105,123,128	0
36	HTG	b	632	19/19	0.79	0.41	77,138,158,165	0
33	UNL	d	414	18/-	0.80	0.25	76,84,116,118	0
34	LMG	c	522	51/55	0.80	0.34	59,111,124,132	0
34	LMG	C	520	51/55	0.80	0.30	67,122,137,143	0
34	LMG	A	419	51/55	0.80	0.23	57,90,109,115	0
28	GOL	V	201	6/6	0.80	0.47	81,91,96,100	0
28	GOL	T	101	6/6	0.80	0.34	70,88,93,93	0
35	CA	F	102	1/1	0.81	0.05	119,119,119,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CA	f	103	1/1	0.81	0.07	124,124,124,124	0
36	HTG	B	623	19/19	0.81	0.20	60,79,91,92	0
28	GOL	b	606	6/6	0.81	0.22	70,91,98,100	0
36	HTG	b	631	19/19	0.81	0.25	67,83,98,102	0
27	SQD	F	101	43/54	0.81	0.37	80,119,134,139	0
28	GOL	O	301	6/6	0.81	0.15	74,89,90,93	0
37	DGD	H	102	62/66	0.81	0.20	41,58,95,103	0
37	DGD	c	520	62/66	0.82	0.23	47,65,115,133	0
28	GOL	t	103	6/6	0.82	0.29	60,88,99,102	0
27	SQD	A	411	54/54	0.82	0.23	52,94,103,105	0
28	GOL	V	204	6/6	0.83	0.15	90,103,105,112	0
24	CLA	C	513	65/65	0.83	0.39	61,87,117,123	0
24	CLA	C	504	65/65	0.83	0.19	45,67,93,102	0
34	LMG	M	101	51/55	0.83	0.41	41,61,83,89	0
34	LMG	b	629	51/55	0.83	0.35	40,57,76,83	0
37	DGD	C	518	62/66	0.84	0.19	45,63,82,96	0
28	GOL	B	629	6/6	0.84	0.23	55,69,74,78	0
24	CLA	b	611	65/65	0.84	0.18	41,57,65,73	0
28	GOL	v	203	6/6	0.84	0.28	96,105,112,124	0
33	UNL	X	101	18/-	0.84	0.22	70,77,101,105	0
27	SQD	a	414	54/54	0.84	0.25	54,87,114,116	0
36	HTG	c	523	19/19	0.84	0.27	91,114,126,129	0
38	LHG	D	409	49/49	0.85	0.39	39,56,65,72	0
28	GOL	T	102	6/6	0.85	0.29	104,114,118,118	0
36	HTG	b	602	19/19	0.85	0.19	46,64,75,77	0
26	BCR	H	101	40/40	0.85	0.19	45,64,78,85	0
24	CLA	c	517	65/65	0.86	0.33	76,94,106,111	0
37	DGD	c	521	62/66	0.86	0.23	51,62,87,100	0
34	LMG	d	415	51/55	0.86	0.27	53,70,112,122	0
24	CLA	C	506	65/65	0.86	0.18	52,75,116,119	0
28	GOL	b	601	6/6	0.86	0.20	55,59,64,68	0
28	GOL	a	402	6/6	0.86	0.20	93,97,103,103	0
24	CLA	b	616	65/65	0.87	0.26	31,42,54,62	0
24	CLA	c	507	65/65	0.87	0.20	50,62,75,87	0
24	CLA	c	510	65/65	0.87	0.18	52,74,96,102	0
38	LHG	d	408	49/49	0.87	0.31	44,60,70,72	0
35	CA	b	609	1/1	0.87	0.40	134,134,134,134	0
24	CLA	b	618	65/65	0.87	0.18	45,57,67,77	0
36	HTG	V	206	19/19	0.87	0.22	62,103,129,237	0
26	BCR	C	514	40/40	0.88	0.21	58,81,93,94	0
28	GOL	D	402	6/6	0.88	0.29	55,64,73,77	0
24	CLA	b	615	65/65	0.88	0.18	41,54,100,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMG	D	415	51/55	0.88	0.19	51,73,119,129	0
24	CLA	B	607	65/65	0.88	0.17	40,54,94,98	0
28	GOL	o	301	6/6	0.88	0.23	84,90,97,98	0
38	LHG	b	634	49/49	0.88	0.32	39,54,68,82	0
38	LHG	D	411	49/49	0.88	0.23	51,71,118,127	0
24	CLA	c	512	65/65	0.88	0.16	44,59,125,141	0
37	DGD	c	519	62/66	0.89	0.16	41,62,97,101	0
24	CLA	B	602	65/65	0.89	0.23	57,74,114,132	0
24	CLA	b	610	65/65	0.89	0.34	57,79,127,133	0
28	GOL	C	524	6/6	0.89	0.23	86,89,104,108	0
24	CLA	B	603	65/65	0.89	0.15	40,53,62,66	0
24	CLA	C	511	65/65	0.89	0.20	56,74,89,101	0
24	CLA	c	508	65/65	0.89	0.18	49,62,85,99	0
24	CLA	B	614	65/65	0.89	0.30	31,45,67,82	0
24	CLA	b	624	65/65	0.89	0.14	42,56,74,78	0
24	CLA	c	509	65/65	0.89	0.14	43,56,75,78	0
38	LHG	d	410	49/49	0.89	0.24	42,65,113,119	0
28	GOL	c	502	6/6	0.90	0.27	85,111,119,127	0
38	LHG	d	409	49/49	0.90	0.34	35,51,69,90	0
36	HTG	C	522	19/19	0.90	0.22	91,102,119,121	0
24	CLA	C	510	65/65	0.90	0.14	55,71,84,92	0
28	GOL	F	103	6/6	0.90	0.23	88,95,100,104	0
32	PL9	D	407[B]	55/55	0.90	0.38	34,45,53,67	55
24	CLA	b	620	65/65	0.90	0.18	35,49,59,65	0
28	GOL	a	421	6/6	0.90	0.26	88,100,106,106	0
26	BCR	d	406	40/40	0.90	0.23	48,61,83,91	0
24	CLA	C	501	65/65	0.90	0.15	50,62,87,97	0
24	CLA	B	615	65/65	0.90	0.30	34,46,97,100	0
24	CLA	c	511	65/65	0.90	0.16	53,68,79,83	0
24	CLA	c	515	65/65	0.90	0.17	51,73,89,101	0
24	CLA	C	503	65/65	0.90	0.19	50,62,77,82	0
36	HTG	B	622	19/19	0.90	0.23	53,65,88,92	0
26	BCR	c	526	40/40	0.90	0.21	72,87,94,96	0
32	PL9	D	407[A]	55/55	0.90	0.38	34,45,52,64	55
28	GOL	v	201	6/6	0.91	0.16	74,84,87,96	0
26	BCR	b	627	40/40	0.91	0.29	37,52,68,78	0
32	PL9	d	407[A]	55/55	0.91	0.34	31,46,53,59	55
32	PL9	d	407[B]	55/55	0.91	0.34	31,45,55,63	55
24	CLA	C	508	65/65	0.91	0.14	46,66,133,146	0
24	CLA	B	612	65/65	0.91	0.25	35,46,54,63	0
38	LHG	L	101	49/49	0.91	0.38	39,52,64,67	0
26	BCR	D	406	40/40	0.91	0.15	52,65,99,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	b	625	65/65	0.91	0.15	40,61,106,112	0
28	GOL	V	203	6/6	0.91	0.18	68,76,82,85	0
24	CLA	b	623	65/65	0.91	0.22	31,47,93,106	0
24	CLA	b	617	65/65	0.92	0.12	43,57,64,73	0
26	BCR	y	101	40/40	0.92	0.15	58,70,81,83	0
26	BCR	b	626	40/40	0.92	0.29	36,49,59,64	0
35	CA	B	601	1/1	0.92	0.36	135,135,135,135	0
24	CLA	B	610	65/65	0.92	0.15	38,58,67,75	0
24	CLA	B	608	65/65	0.92	0.32	32,45,58,70	0
37	DGD	C	516	62/66	0.92	0.20	40,58,89,91	0
33	UNL	d	411	17/-	0.92	0.17	57,77,101,101	0
24	CLA	C	507	65/65	0.92	0.17	51,71,84,91	0
28	GOL	B	626	6/6	0.92	0.24	56,67,87,100	0
24	CLA	c	514	65/65	0.92	0.14	47,64,74,80	0
24	CLA	b	622	65/65	0.92	0.22	36,49,62,68	0
28	GOL	b	603	6/6	0.92	0.30	60,73,78,87	0
33	UNL	D	412	17/-	0.92	0.15	46,71,89,96	0
38	LHG	D	410	49/49	0.92	0.33	34,49,75,92	0
24	CLA	C	512	65/65	0.92	0.20	62,81,95,102	0
24	CLA	c	516	65/65	0.93	0.24	63,79,91,99	0
24	CLA	B	616	65/65	0.93	0.16	40,56,68,77	0
24	CLA	C	509	65/65	0.93	0.16	49,72,86,92	0
24	CLA	d	403	65/65	0.93	0.26	35,44,53,57	0
26	BCR	K	101	40/40	0.93	0.14	58,71,80,87	0
24	CLA	D	405	65/65	0.93	0.17	47,62,111,116	0
28	GOL	b	605	6/6	0.93	0.20	66,82,107,110	0
24	CLA	B	613	65/65	0.93	0.16	32,47,57,60	0
24	CLA	b	619	65/65	0.93	0.14	41,58,66,77	0
24	CLA	d	405	65/65	0.93	0.14	49,64,115,122	0
28	GOL	V	202	6/6	0.93	0.19	54,65,76,78	0
26	BCR	Y	101	40/40	0.93	0.15	62,72,92,98	0
24	CLA	c	513	65/65	0.93	0.17	53,68,85,94	0
40	MG	j	102	1/1	0.94	0.13	70,70,70,70	0
24	CLA	A	405	65/65	0.94	0.25	32,41,52,62	0
24	CLA	B	617	65/65	0.94	0.21	45,62,136,139	0
35	CA	c	504	1/1	0.94	0.06	84,84,84,84	0
23	BCT	A	404[B]	4/4	0.94	0.17	71,72,78,90	4
24	CLA	a	409	65/65	0.94	0.26	34,44,56,71	0
24	CLA	c	505	65/65	0.94	0.14	50,67,75,77	0
25	PHO	D	401[B]	64/64	0.94	0.18	40,50,59,64	64
25	PHO	d	402[B]	64/64	0.94	0.20	40,50,56,60	64
25	PHO	d	402[A]	64/64	0.94	0.20	39,50,56,59	64

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	B	604	65/65	0.94	0.16	43,55,63,68	0
26	BCR	k	102	40/40	0.94	0.17	54,75,85,87	0
26	BCR	h	101	40/40	0.94	0.17	46,66,76,77	0
28	GOL	v	204	6/6	0.94	0.15	59,64,71,78	0
23	BCT	A	404[A]	4/4	0.94	0.17	72,74,78,88	4
26	BCR	B	619	40/40	0.94	0.36	37,51,64,71	0
24	CLA	b	612	65/65	0.94	0.13	45,55,63,71	0
24	CLA	c	506	65/65	0.94	0.15	47,61,79,88	0
24	CLA	C	502	65/65	0.94	0.14	45,66,73,81	0
26	BCR	T	103	40/40	0.94	0.27	32,51,66,72	0
24	CLA	b	621	65/65	0.94	0.13	35,50,59,63	0
24	CLA	B	605	65/65	0.94	0.18	31,45,75,79	0
28	GOL	b	604	6/6	0.94	0.33	62,73,80,84	0
28	GOL	a	401	6/6	0.94	0.26	55,63,75,82	0
25	PHO	A	408	64/64	0.94	0.25	28,44,52,61	0
25	PHO	D	401[A]	64/64	0.94	0.18	41,51,60,63	64
24	CLA	C	505	65/65	0.94	0.13	48,60,75,91	0
26	BCR	c	518	40/40	0.94	0.14	49,63,73,78	0
24	CLA	b	614	65/65	0.95	0.14	36,46,60,70	0
24	CLA	B	611	65/65	0.95	0.18	42,56,67,71	0
24	CLA	A	406	65/65	0.95	0.29	31,42,51,53	0
26	BCR	B	618	40/40	0.95	0.41	36,49,59,62	0
26	BCR	B	620	40/40	0.95	0.20	39,53,64,79	0
28	GOL	B	628	6/6	0.95	0.17	56,69,75,78	0
24	CLA	b	613	65/65	0.95	0.14	32,48,75,84	0
26	BCR	C	515	40/40	0.95	0.16	47,63,75,80	0
26	BCR	t	102	40/40	0.95	0.38	36,53,75,77	0
24	CLA	A	409	65/65	0.95	0.16	40,58,123,132	0
28	GOL	B	627	6/6	0.95	0.22	71,86,88,88	0
24	CLA	B	609	65/65	0.95	0.15	42,53,62,66	0
26	BCR	b	628	40/40	0.95	0.15	41,59,69,72	0
26	BCR	A	410	40/40	0.95	0.20	37,48,57,65	0
24	CLA	B	606	65/65	0.95	0.16	36,47,58,61	0
24	CLA	a	412	65/65	0.95	0.18	40,59,116,123	0
24	CLA	a	410	65/65	0.95	0.24	38,51,113,120	0
28	GOL	B	634	6/6	0.95	0.19	56,58,65,66	0
28	GOL	B	630	6/6	0.96	0.25	59,95,102,108	0
35	CA	O	302	1/1	0.96	0.13	100,100,100,100	0
39	HEM	E	103	43/43	0.96	0.28	63,82,103,115	0
23	BCT	d	401[B]	4/4	0.96	0.20	85,85,88,93	4
24	CLA	d	404	65/65	0.96	0.22	32,45,58,73	0
24	CLA	A	407	65/65	0.96	0.16	33,47,101,110	0

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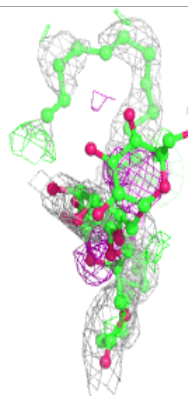
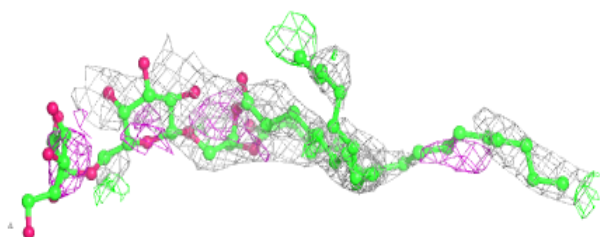
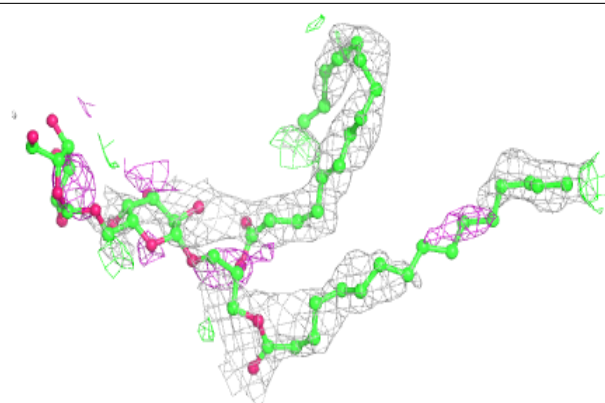
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	BCT	d	401[A]	4/4	0.96	0.20	86,88,90,94	4
25	PHO	a	411	64/64	0.96	0.28	38,45,54,63	0
26	BCR	a	413	40/40	0.96	0.20	34,47,58,61	0
35	CA	o	302	1/1	0.97	0.07	97,97,97,97	0
28	GOL	B	625	6/6	0.97	0.12	55,65,74,83	0
28	GOL	C	525	6/6	0.97	0.22	52,54,59,60	0
28	GOL	c	501	6/6	0.97	0.17	47,52,56,58	0
22	CL	A	403[B]	1/1	0.97	0.12	45,45,45,45	1
22	CL	A	403[A]	1/1	0.97	0.12	47,47,47,47	1
24	CLA	D	404	65/65	0.97	0.21	30,42,61,69	0
39	HEM	V	205	43/43	0.97	0.14	44,53,65,67	0
39	HEM	f	101	43/43	0.97	0.13	66,90,130,144	0
40	MG	J	102	1/1	0.97	0.09	71,71,71,71	0
30	OEX	a	417[A]	10/10	0.98	0.13	47,51,57,61	10
39	HEM	v	206	43/43	0.98	0.11	51,65,74,75	0
31	OEY	a	418[B]	10/11	0.98	0.13	47,51,57,60	10
22	CL	a	408[A]	1/1	0.98	0.14	49,49,49,49	1
22	CL	a	408[B]	1/1	0.98	0.14	49,49,49,49	1
35	CA	C	526	1/1	0.98	0.24	87,87,87,87	0
35	CA	c	503	1/1	0.99	0.21	77,77,77,77	0
22	CL	A	402[A]	1/1	0.99	0.25	41,41,41,41	1
22	CL	a	407[B]	1/1	0.99	0.16	45,45,45,45	1
30	OEX	A	415[A]	10/10	0.99	0.12	47,57,59,70	10
22	CL	a	407[A]	1/1	0.99	0.16	43,43,43,43	1
21	FE2	a	406[B]	1/1	0.99	0.11	62,62,62,62	1
31	OEY	A	416[B]	10/11	0.99	0.12	43,52,60,68	10
21	FE2	a	406[A]	1/1	0.99	0.11	62,62,62,62	1
21	FE2	A	401[B]	1/1	0.99	0.10	65,65,65,65	1
22	CL	A	402[B]	1/1	0.99	0.25	41,41,41,41	1
21	FE2	A	401[A]	1/1	0.99	0.10	66,66,66,66	1

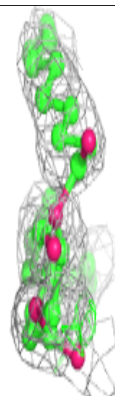
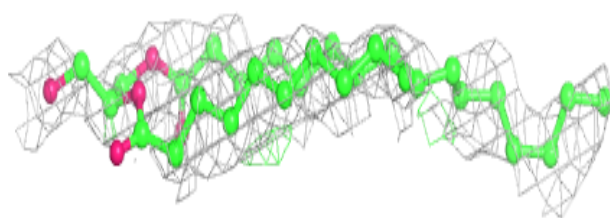
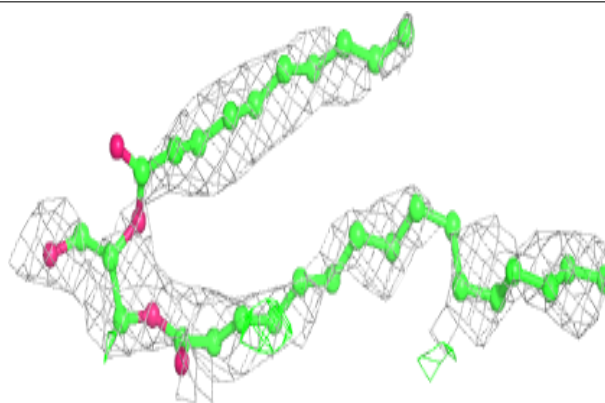
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD e 101:

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

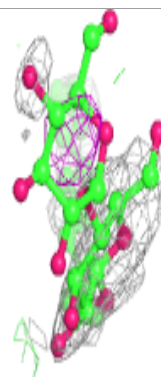
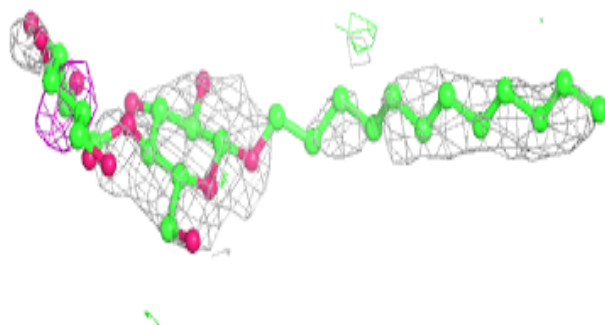
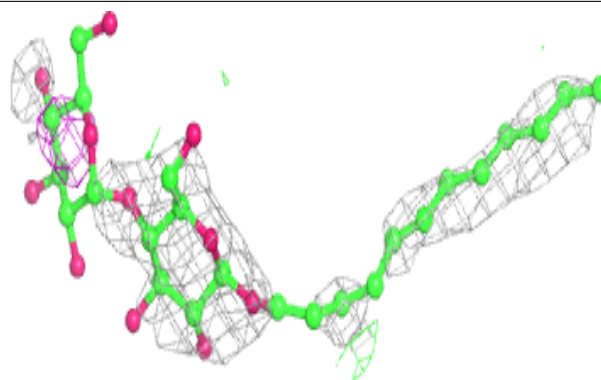
**Electron density around UNL C 527:**

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

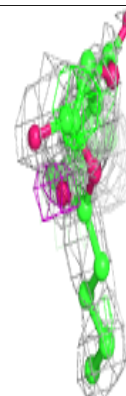
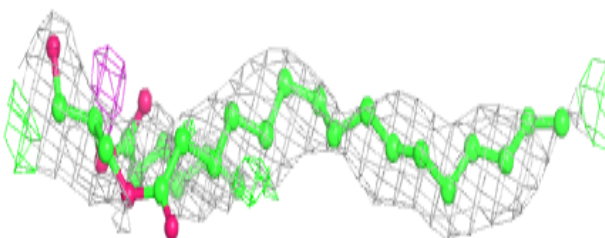
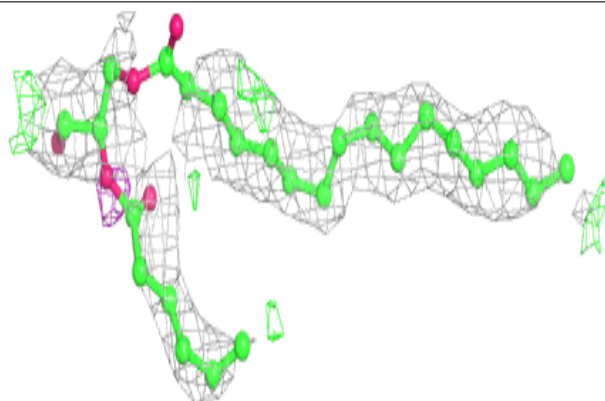


Electron density around LMT E 102:

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

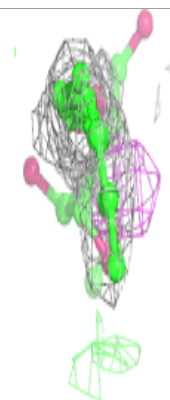
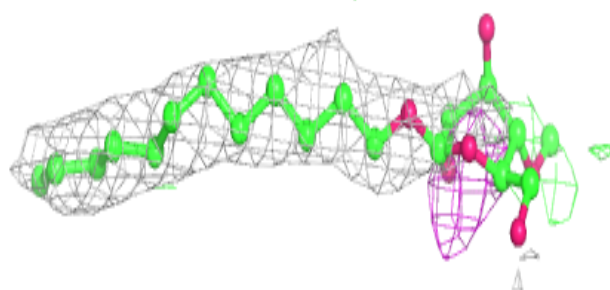
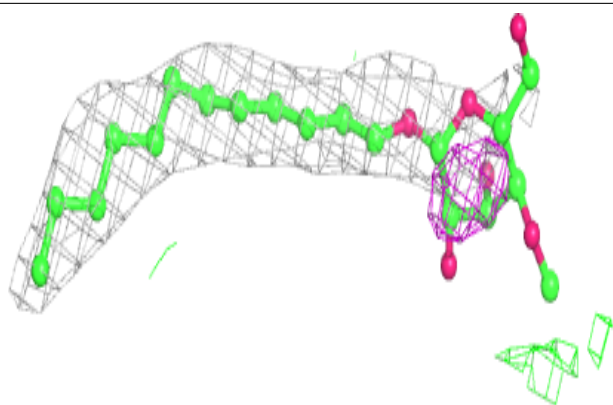
**Electron density around UNL a 403:**

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

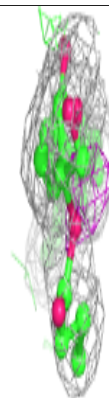
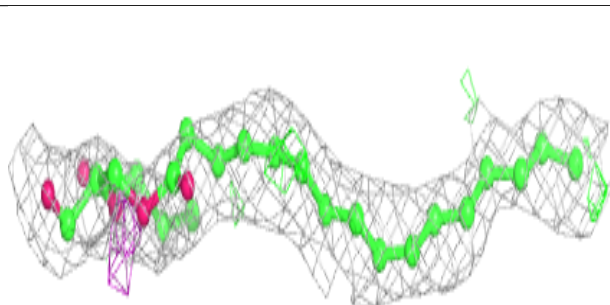
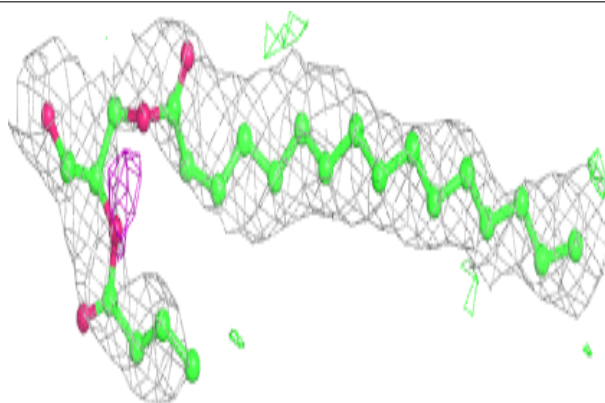


Electron density around LMT b 630:

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

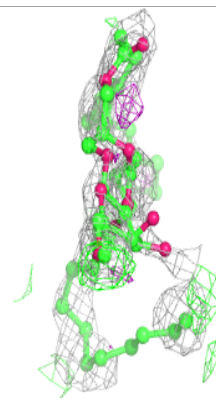
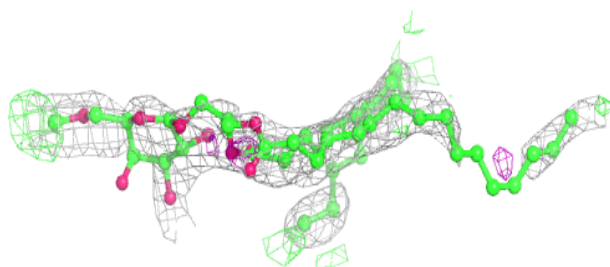
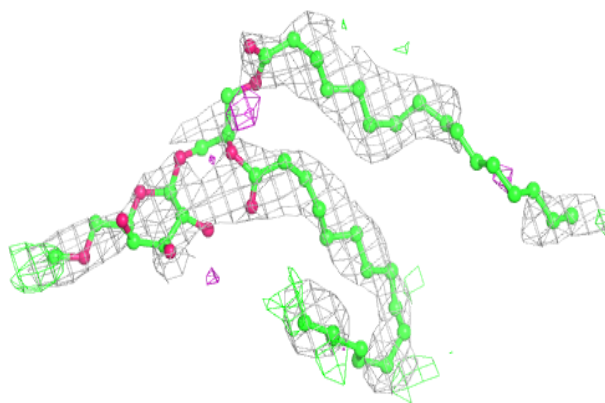
**Electron density around UNL A 418:**

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

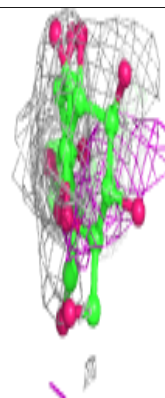
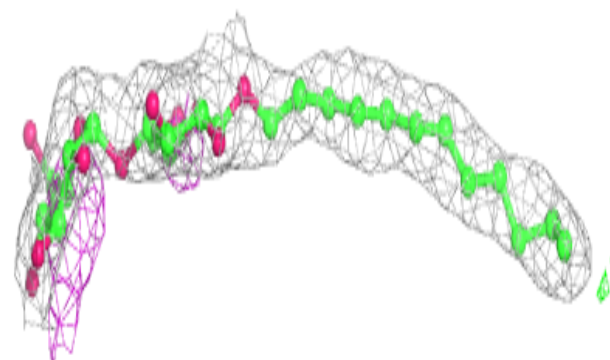
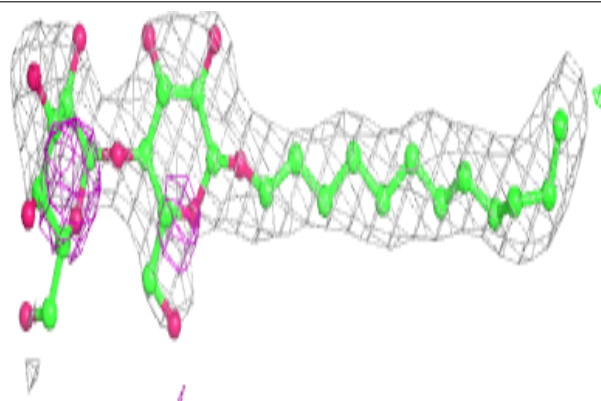


Electron density around DGD D 408:

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

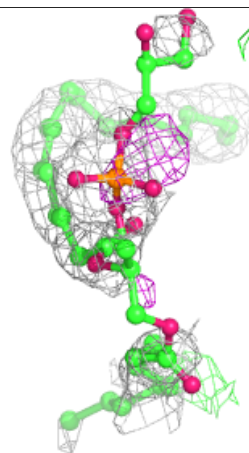
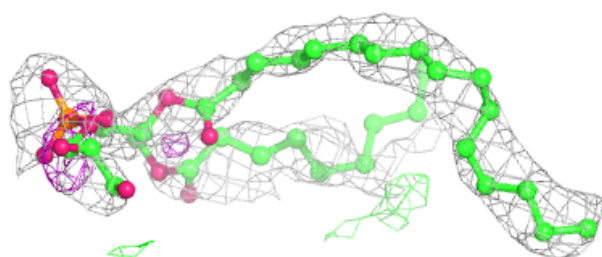
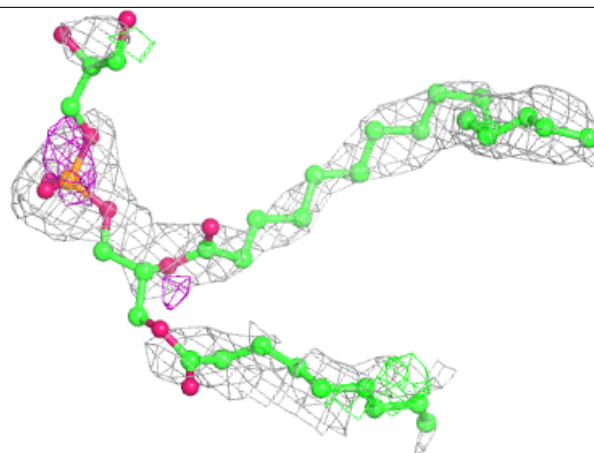
**Electron density around LMT m 102:**

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

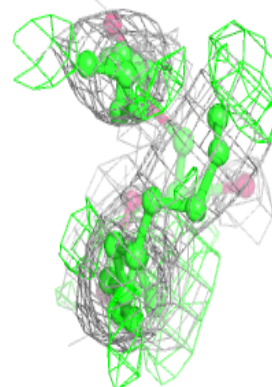
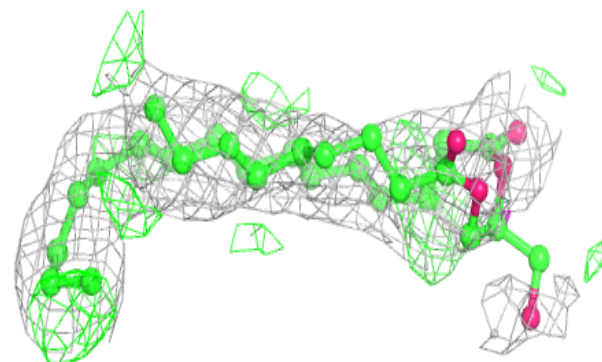
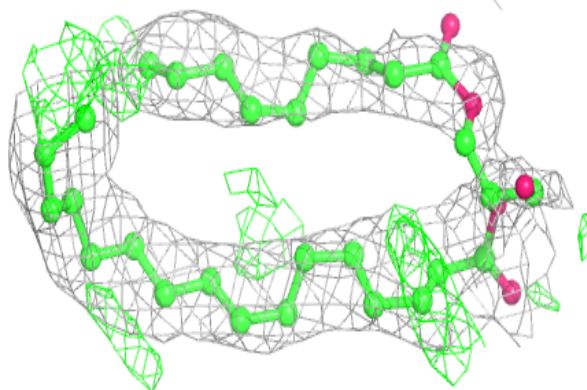


Electron density around LHG E 101:

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

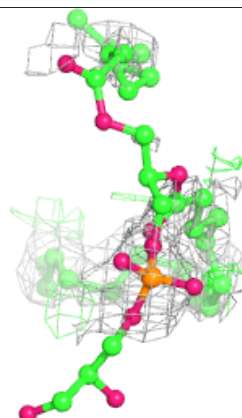
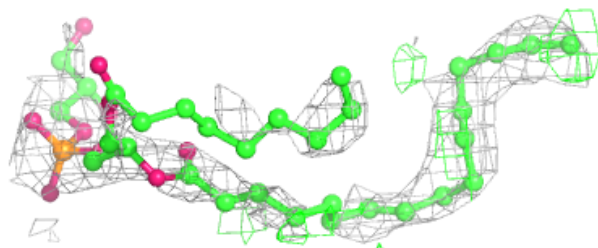
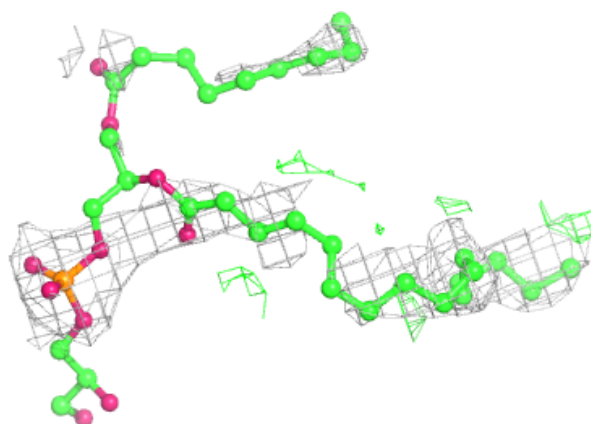
**Electron density around UNL B 633:**

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

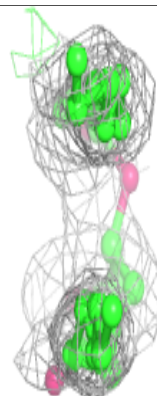
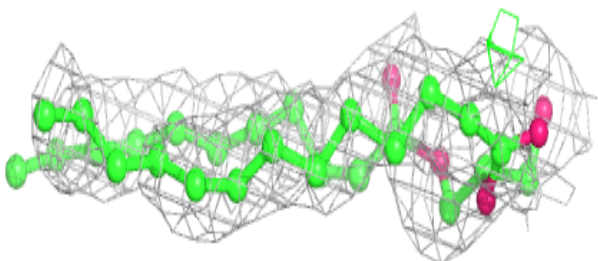
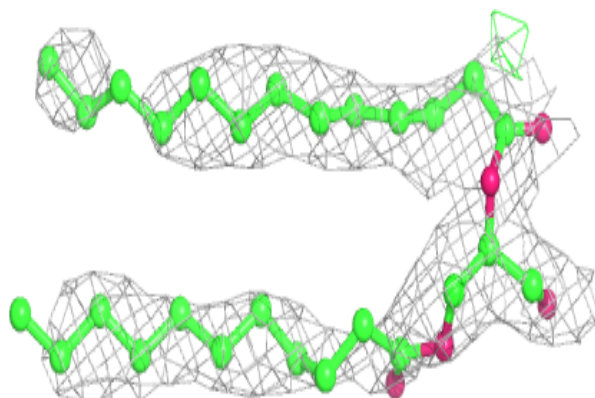


Electron density around LHG a 420:

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

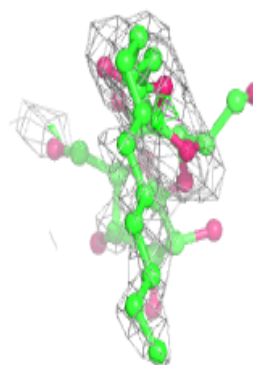
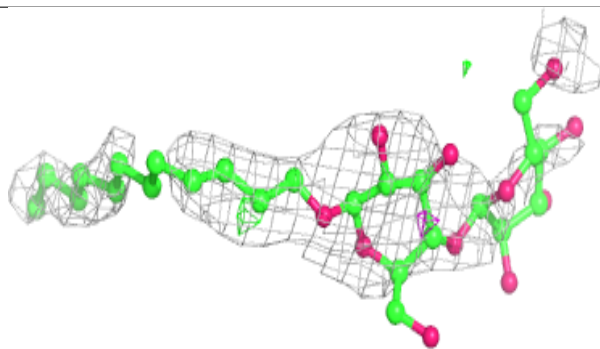
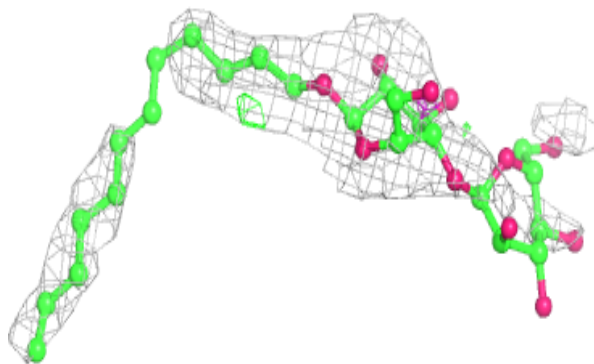
**Electron density around UNL c 525:**

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

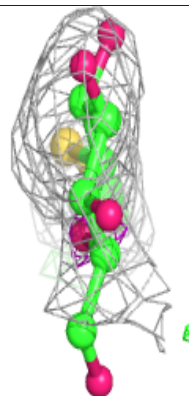
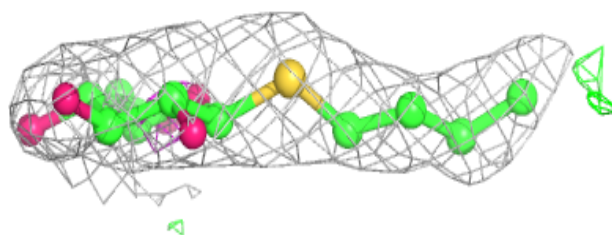
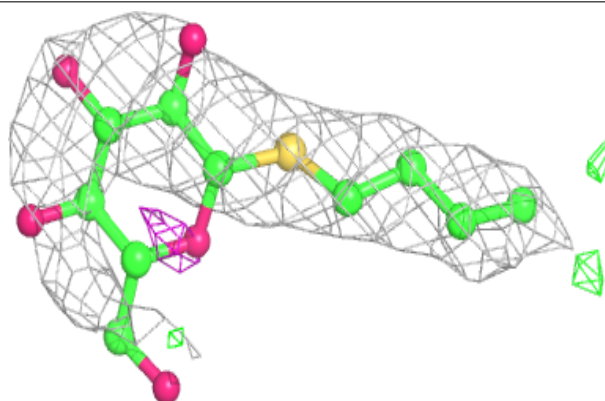


Electron density around LMT C 521:

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

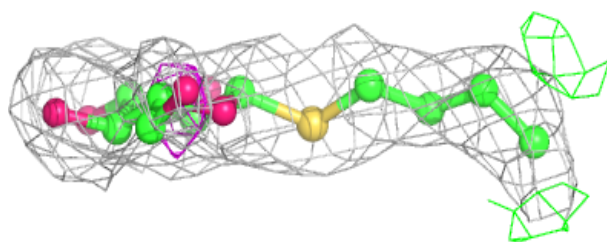
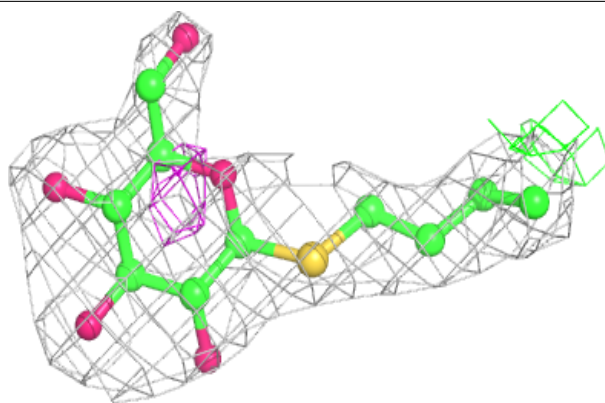
**Electron density around HTG D 414:**

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

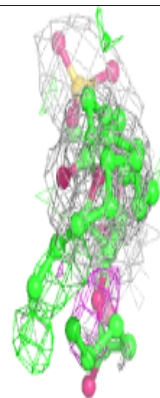
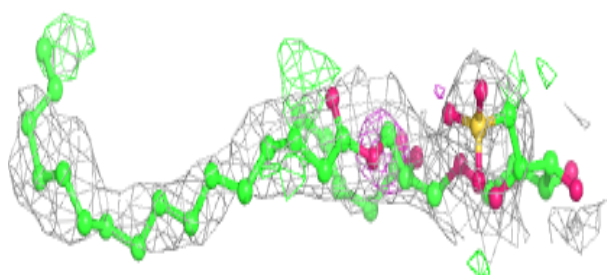
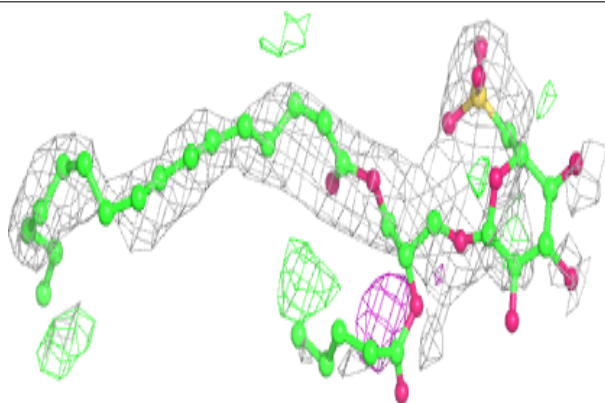


Electron density around HTG d 413:

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

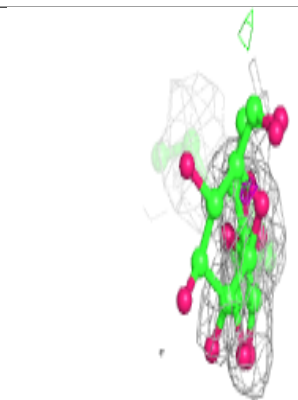
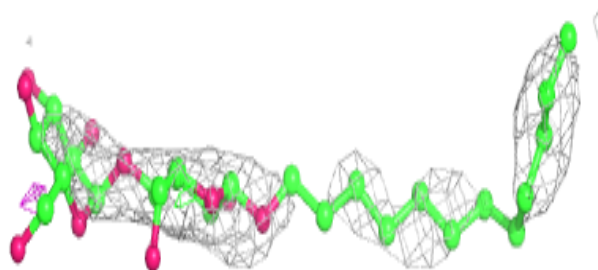
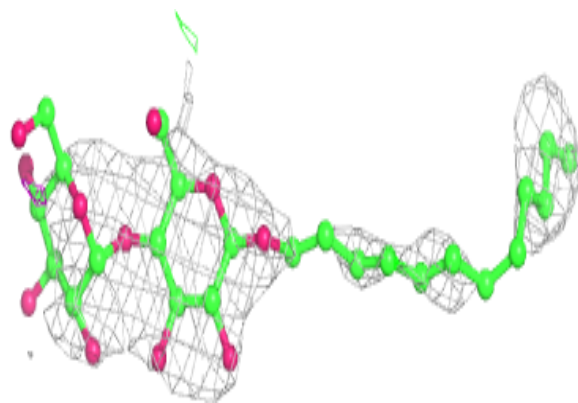
**Electron density around SQD f 102:**

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

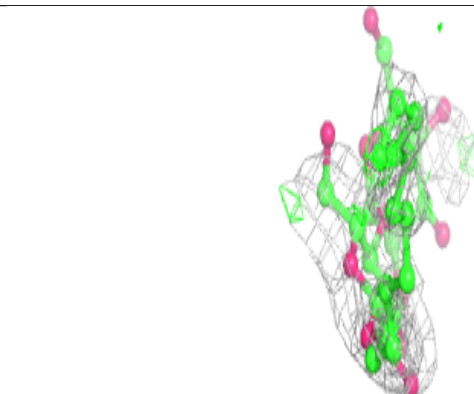
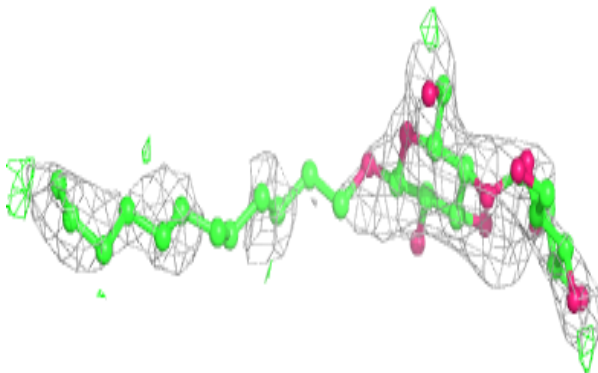
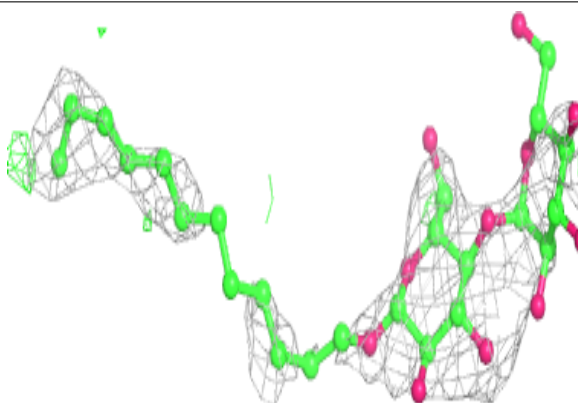


Electron density around LMT a 419:

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

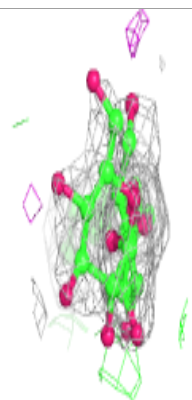
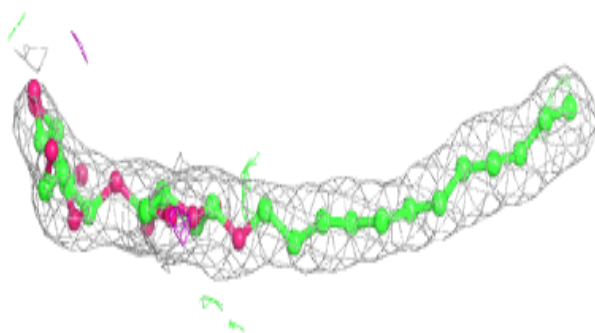
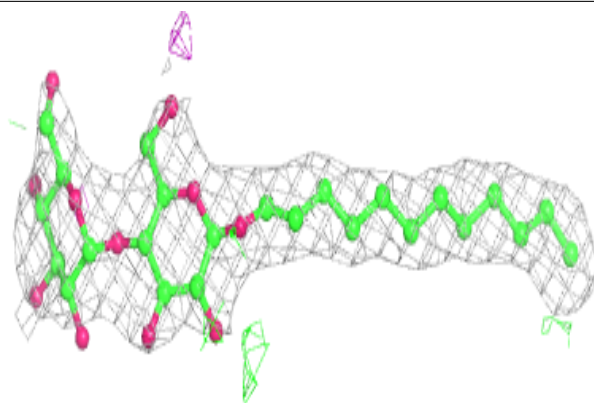
**Electron density around LMT e 102:**

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

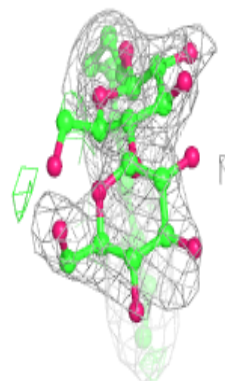
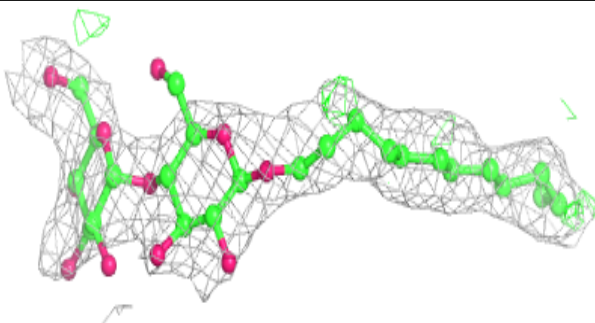
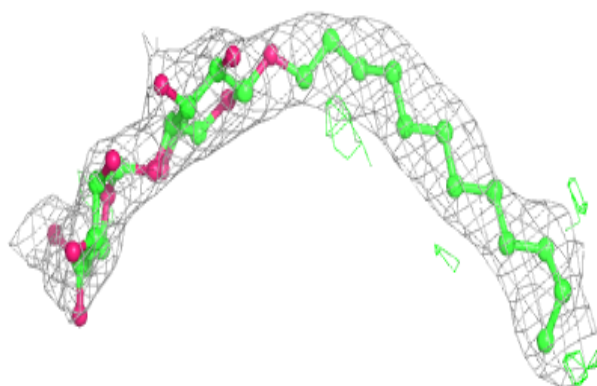


Electron density around LMT M 102:

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

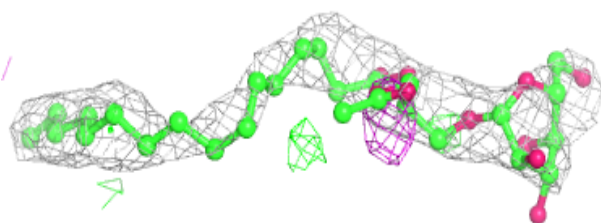
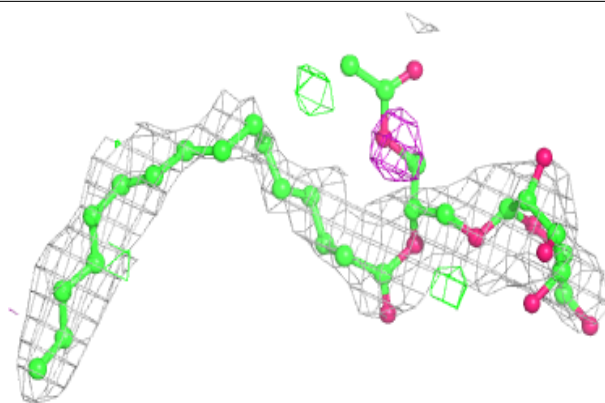
**Electron density around LMT m 103:**

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

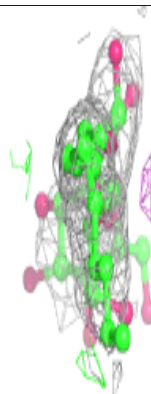
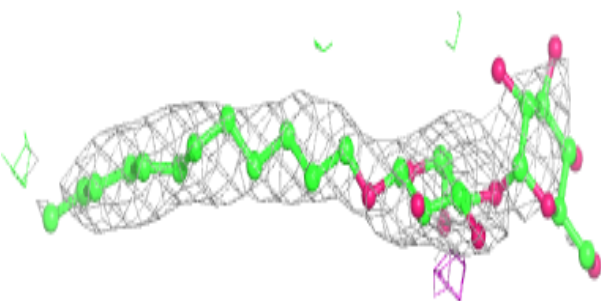
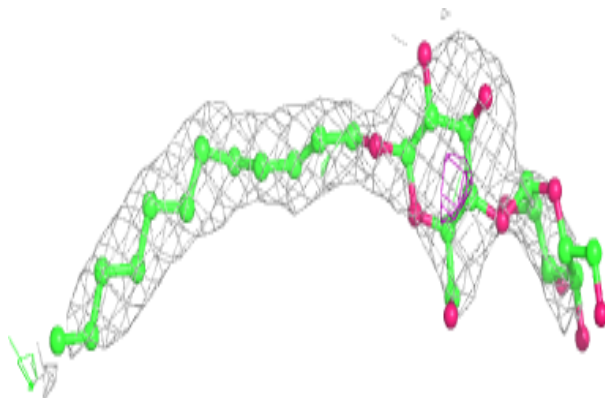


Electron density around LMG Z 101:

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

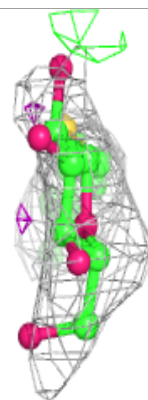
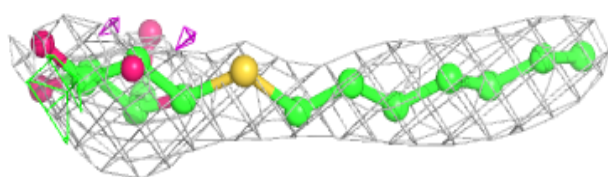
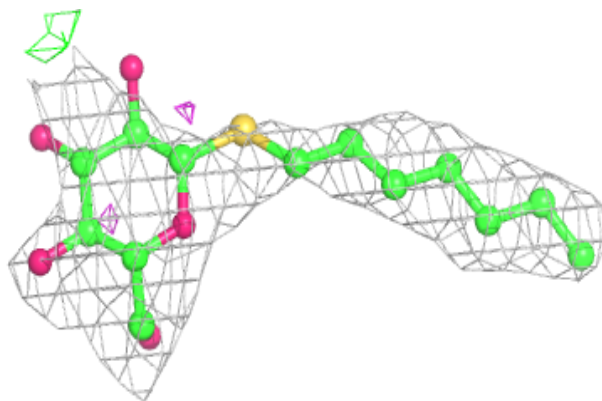
**Electron density around LMT D 403:**

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

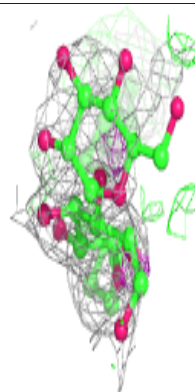
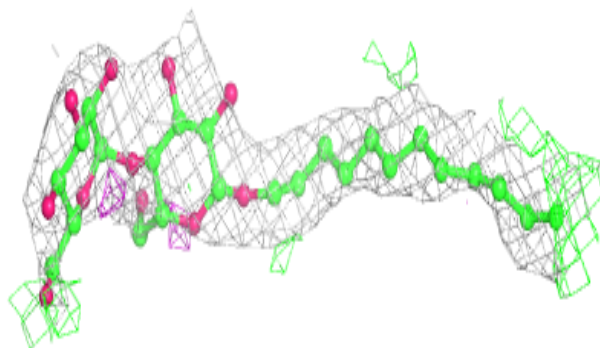
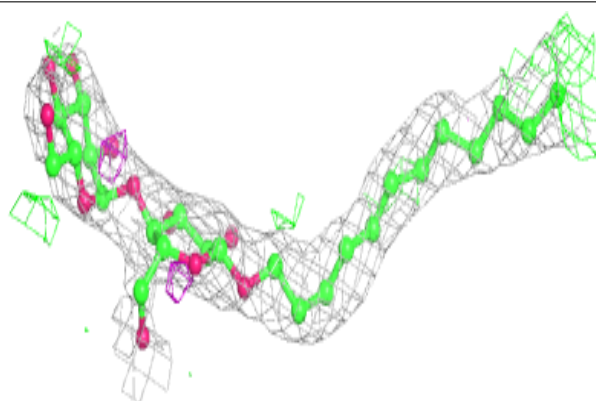


Electron density around HTG B 632:

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

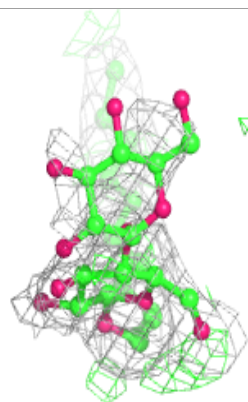
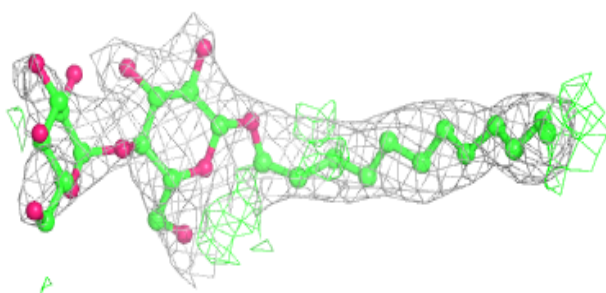
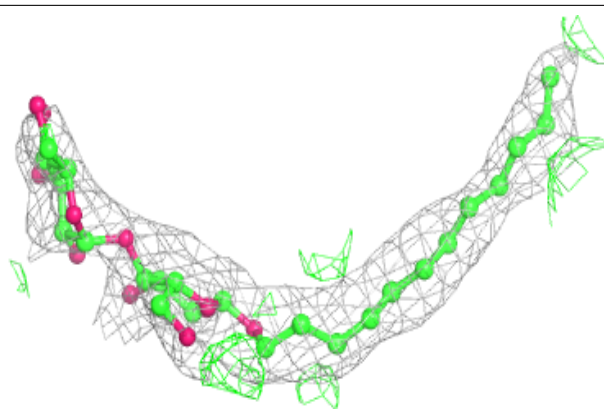
**Electron density around LMT A 414:**

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

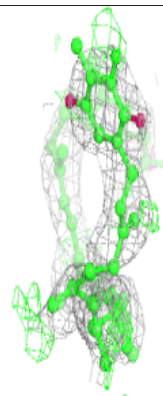
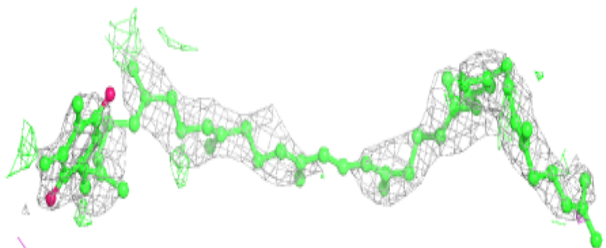
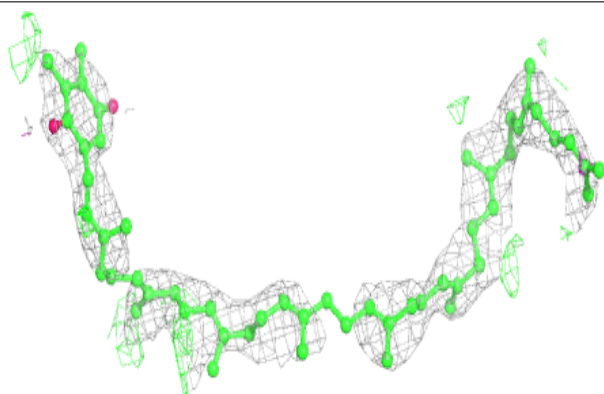


Electron density around LMT M 104:

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

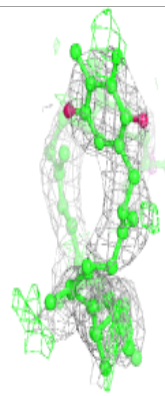
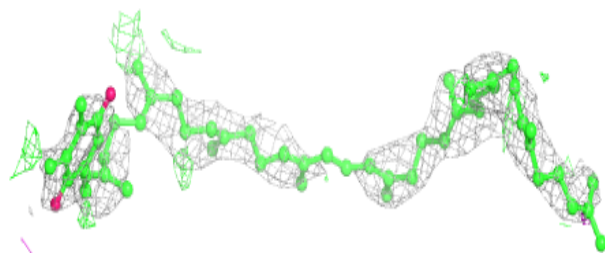
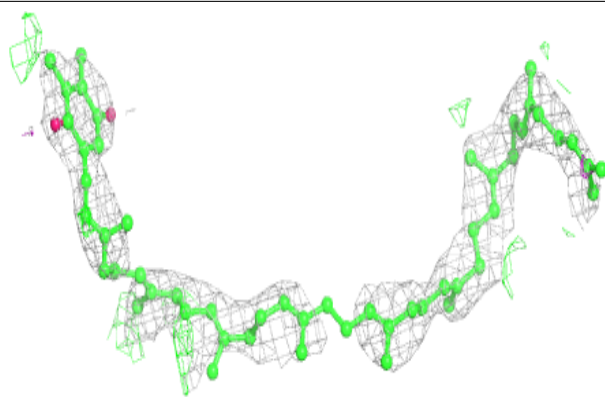
**Electron density around PL9 A 417 (B):**

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

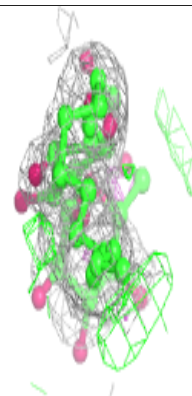
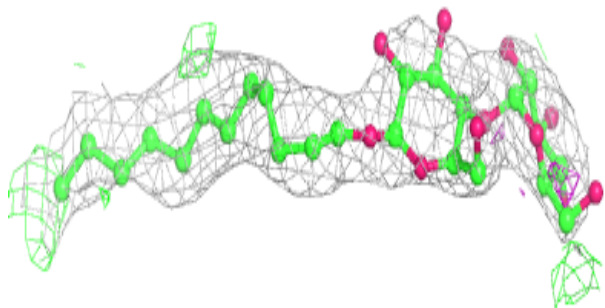
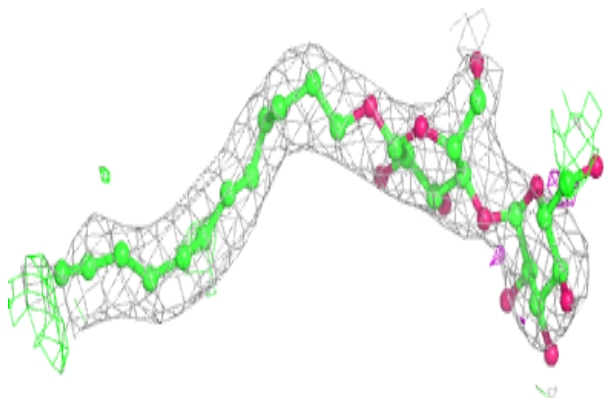


Electron density around PL9 A 417 (A):

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

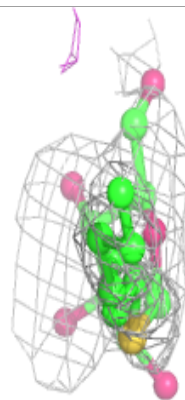
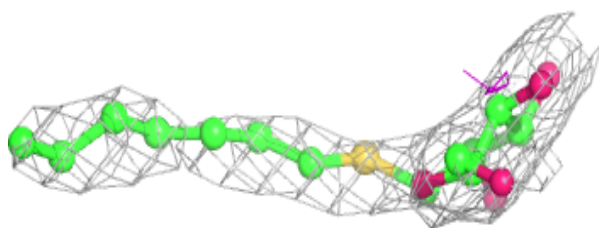
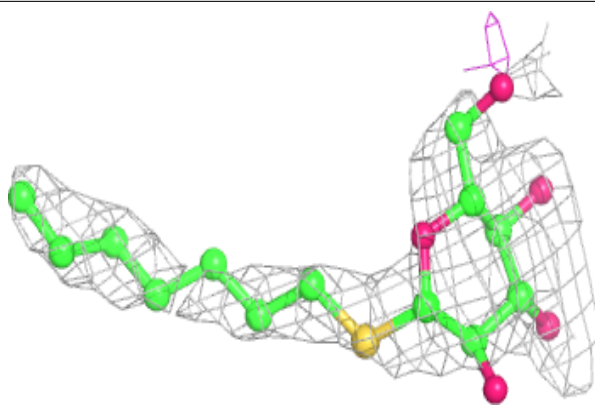
**Electron density around LMT a 404:**

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



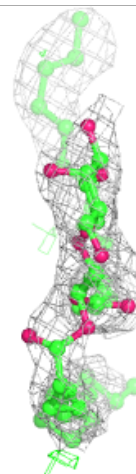
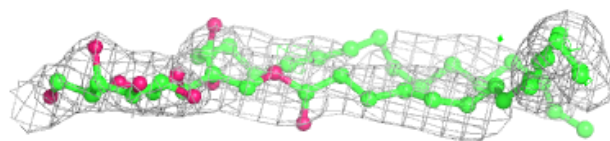
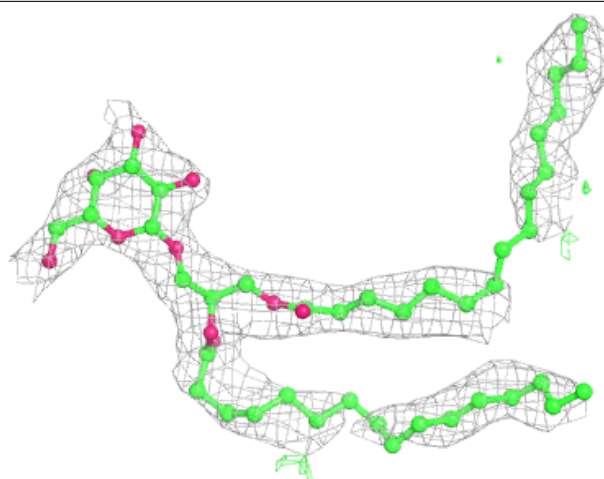
Electron density around HTG B 624:

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



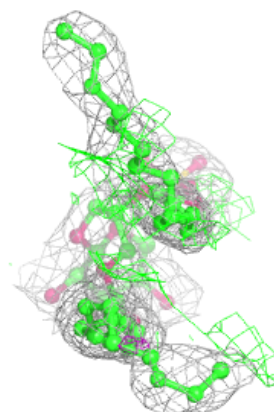
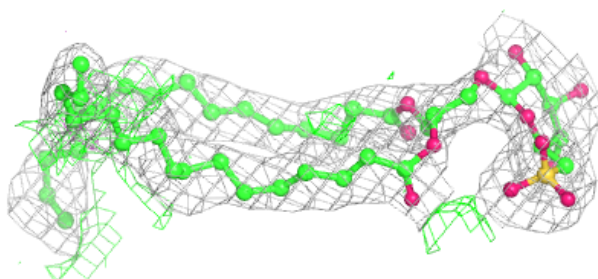
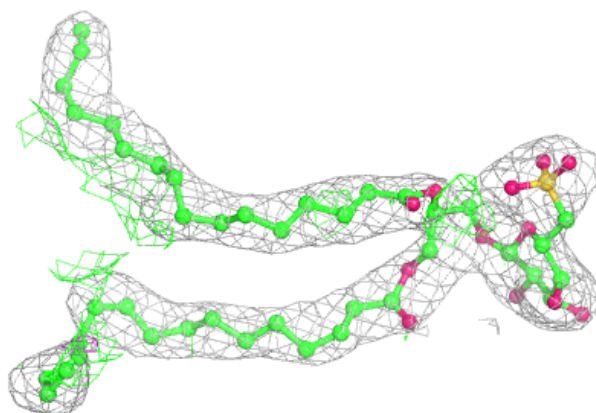
Electron density around LMG C 519:

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

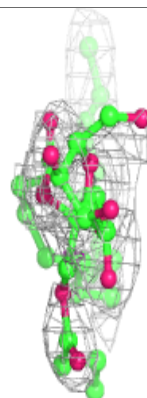
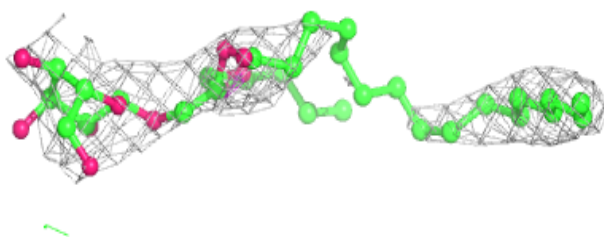
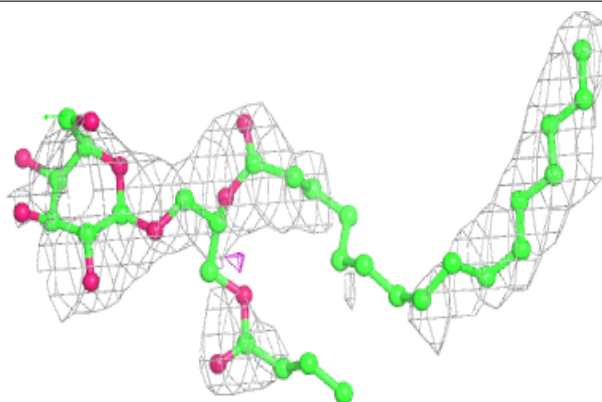


Electron density around SQD L 102:

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

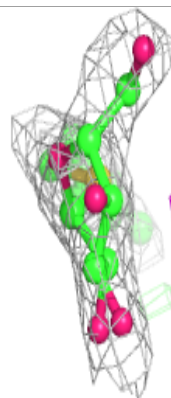
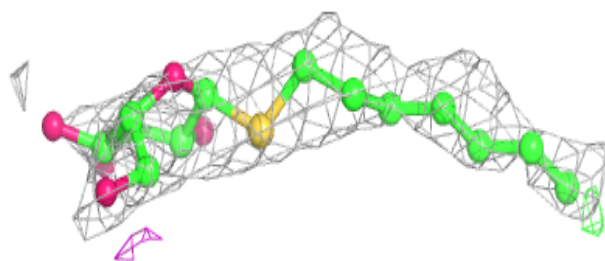
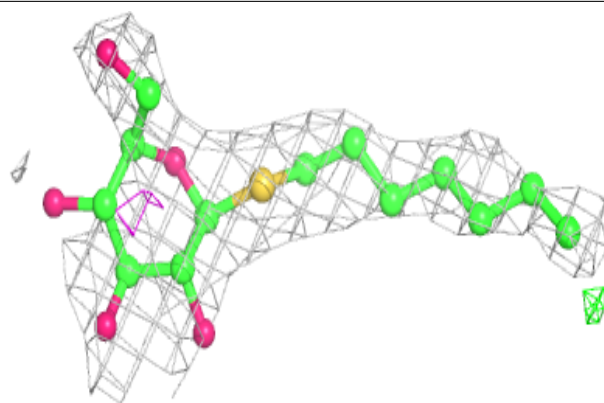
**Electron density around LMG z 101:**

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

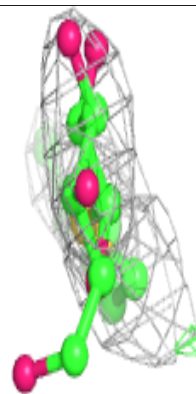
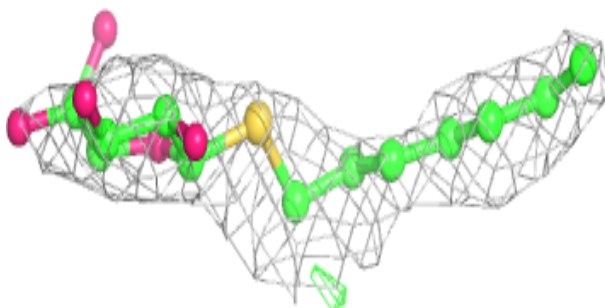
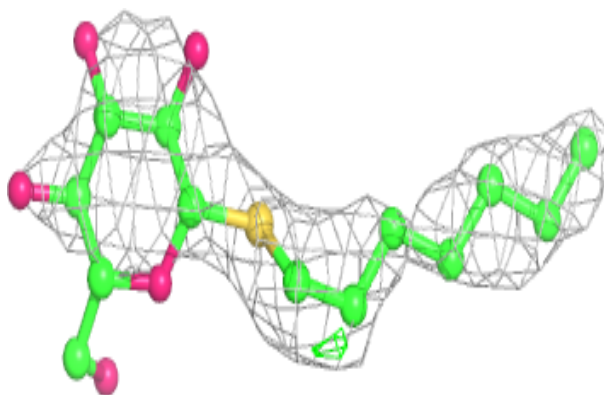


Electron density around HTG C 523:

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

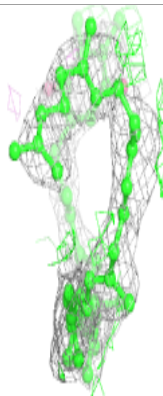
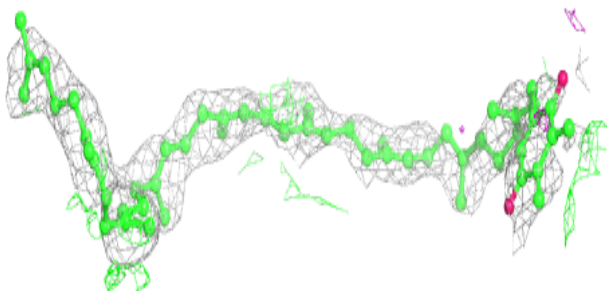
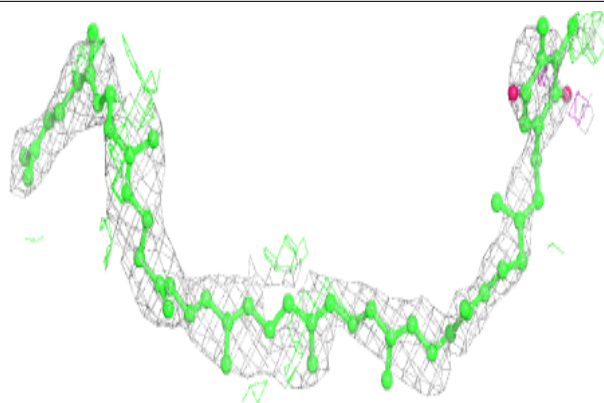
**Electron density around HTG c 524:**

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

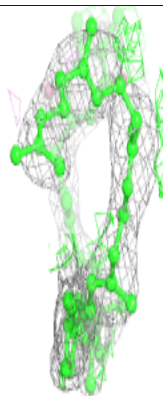
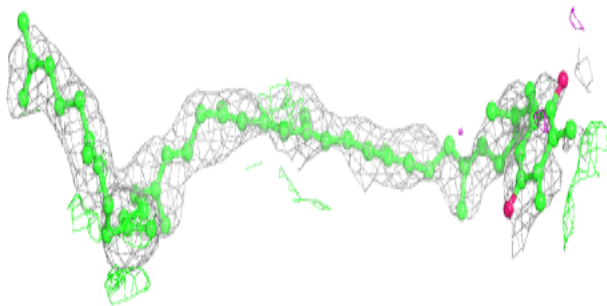
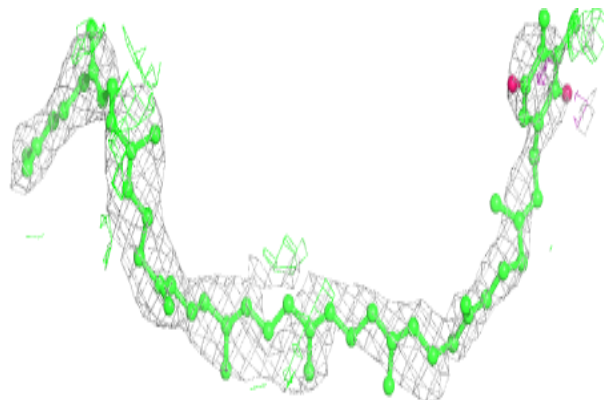


Electron density around PL9 a 416 (A):

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

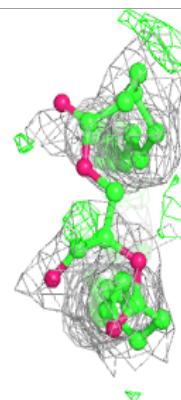
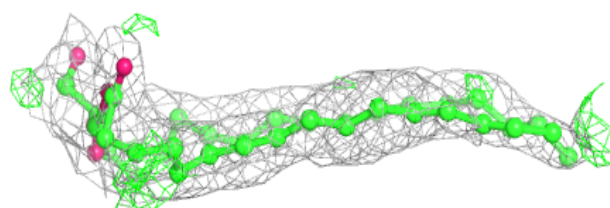
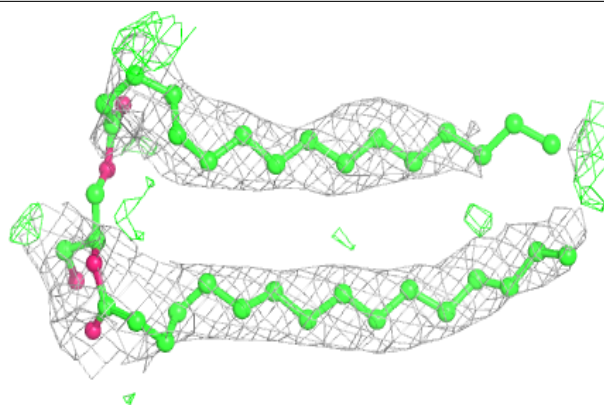
**Electron density around PL9 a 416 (B):**

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

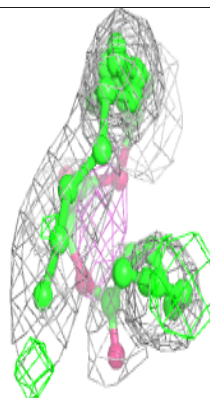
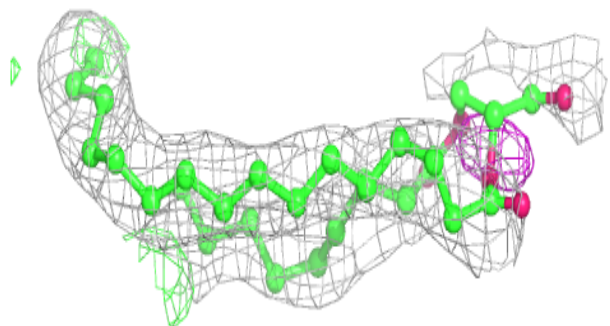
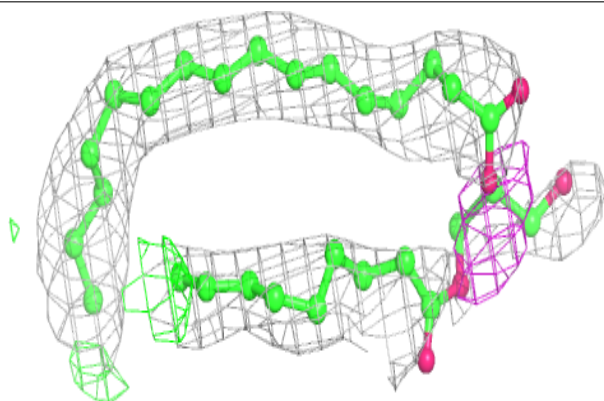


Electron density around UNL i 101:

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

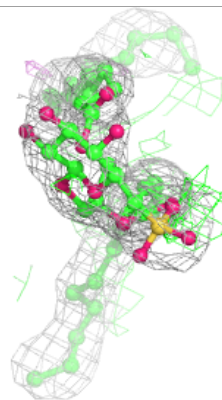
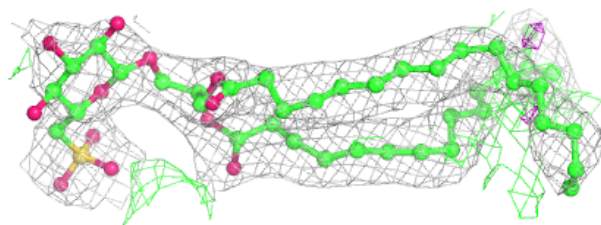
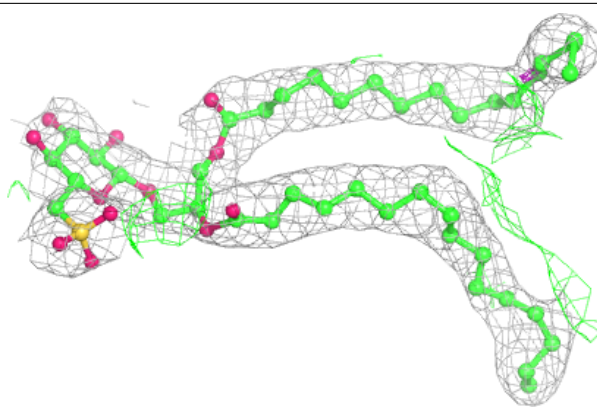
**Electron density around UNL b 633:**

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

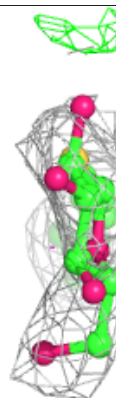
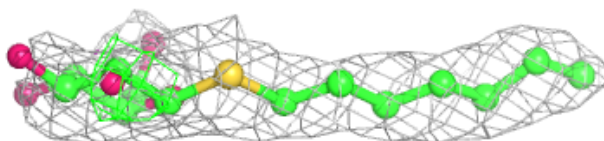
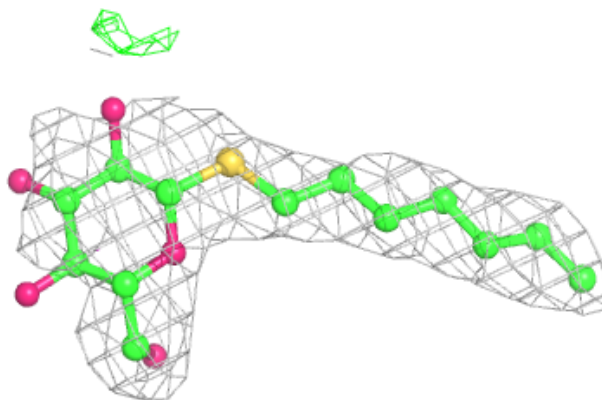


Electron density around SQD B 621:

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

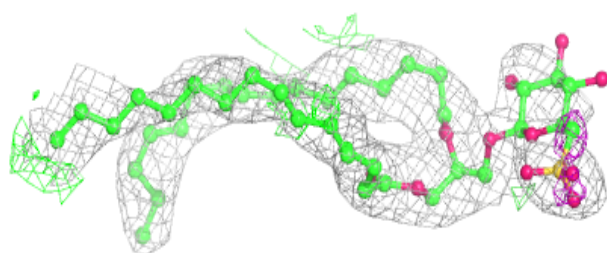
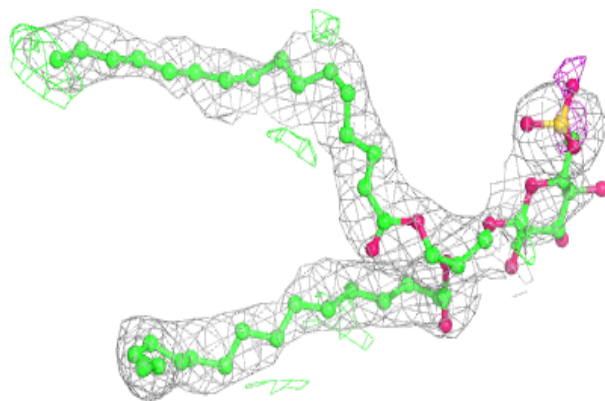
**Electron density around HTG b 608:**

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

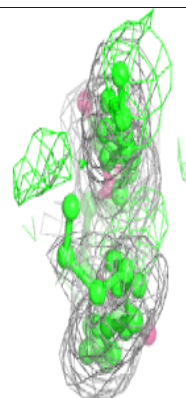
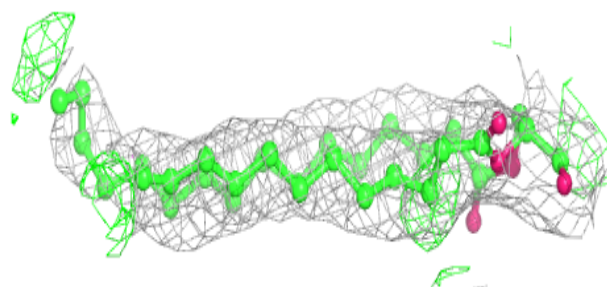
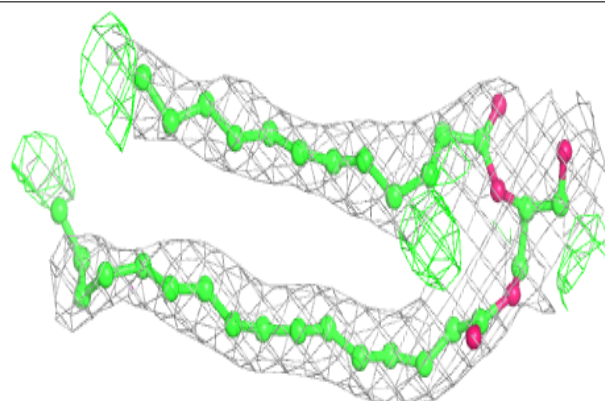


Electron density around SQD A 413:

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

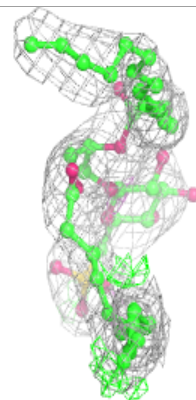
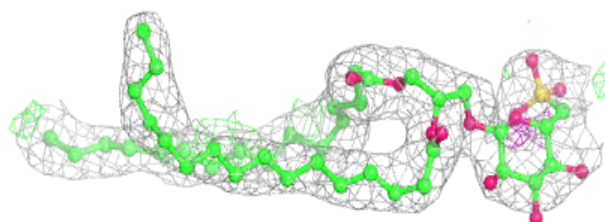
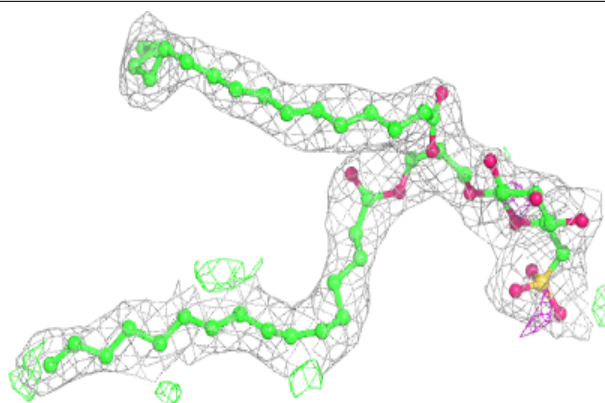
**Electron density around UNL d 412:**

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

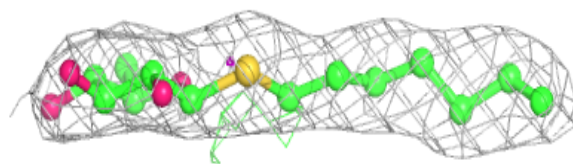
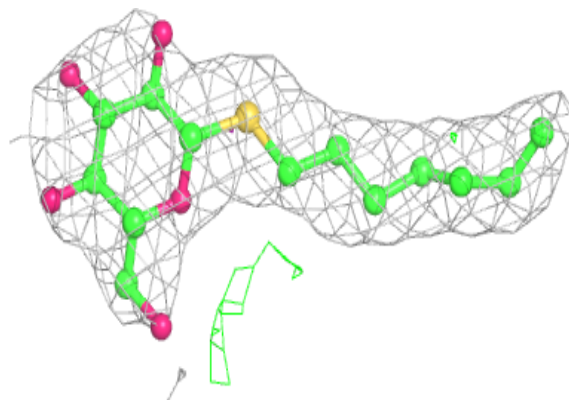


Electron density around SQD a 405:

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

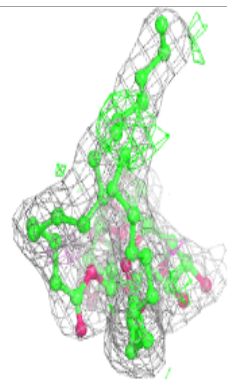
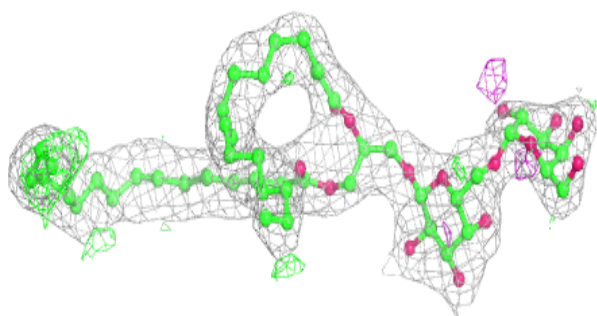
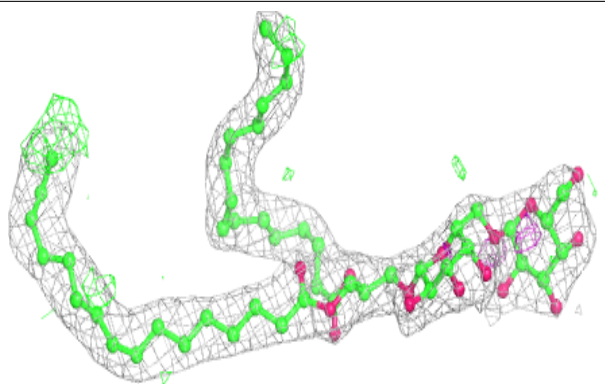
**Electron density around HTG b 607:**

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

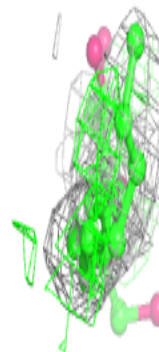
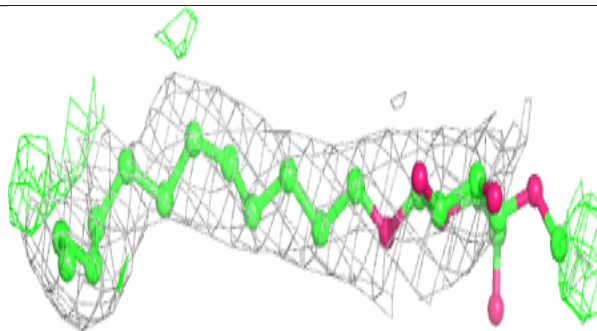
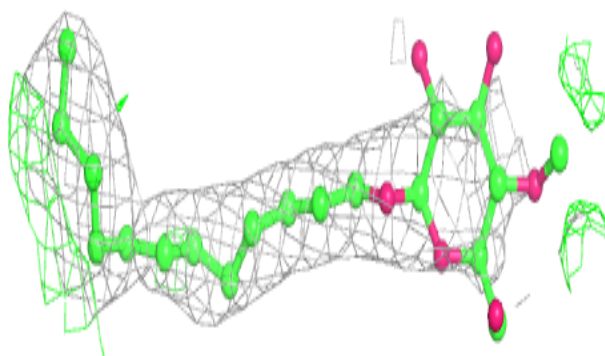


Electron density around DGD h 102:

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

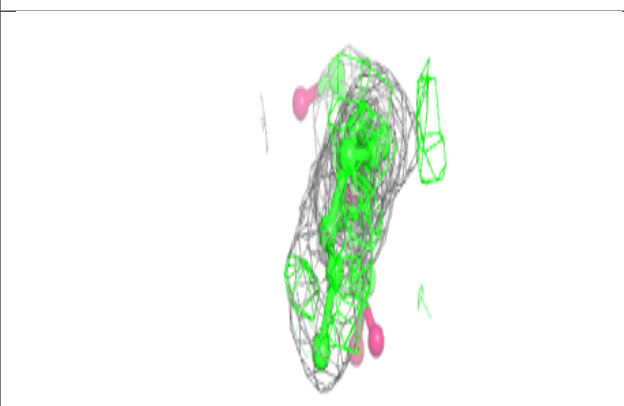
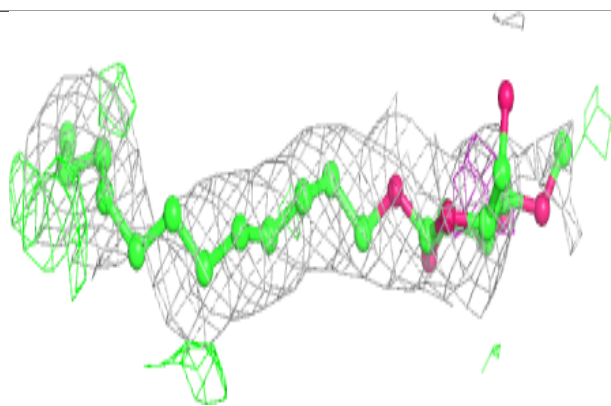
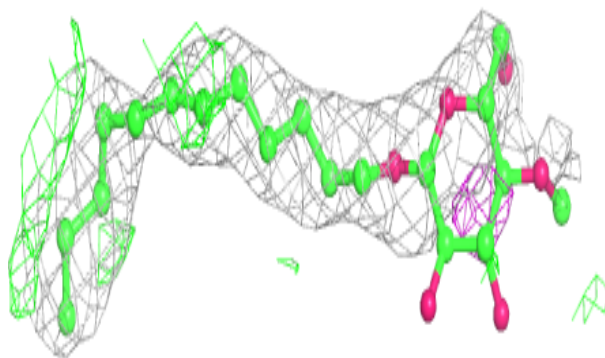
**Electron density around LMT t 101:**

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

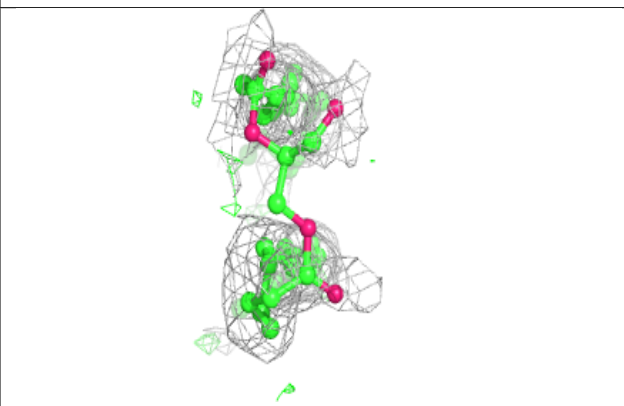
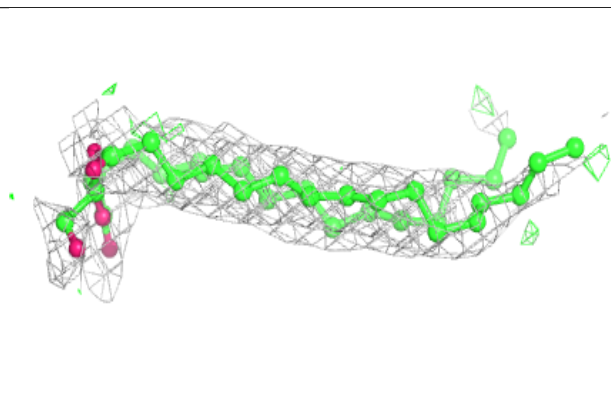
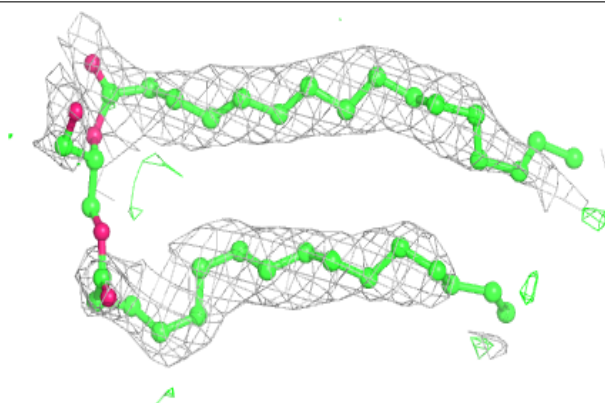


Electron density around LMT T 104:

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

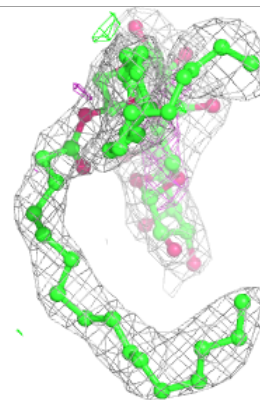
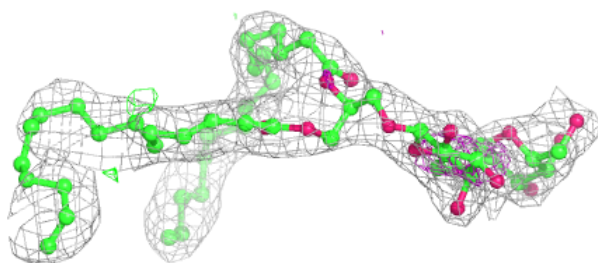
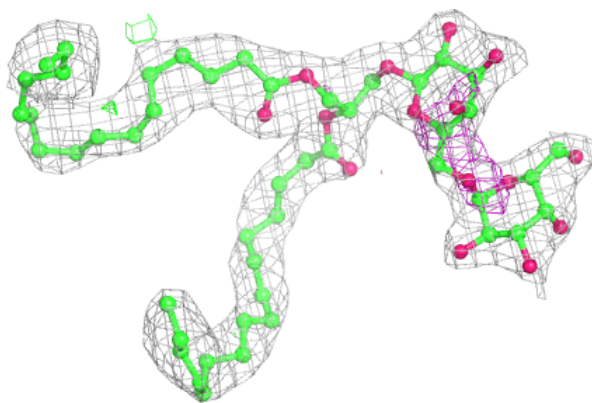
**Electron density around UNL I 101:**

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

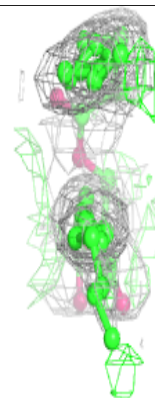
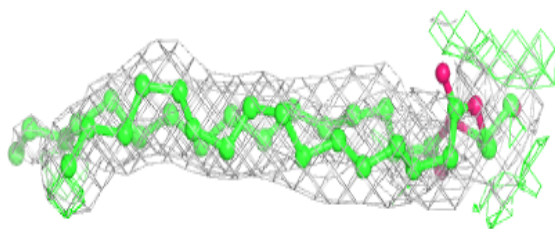
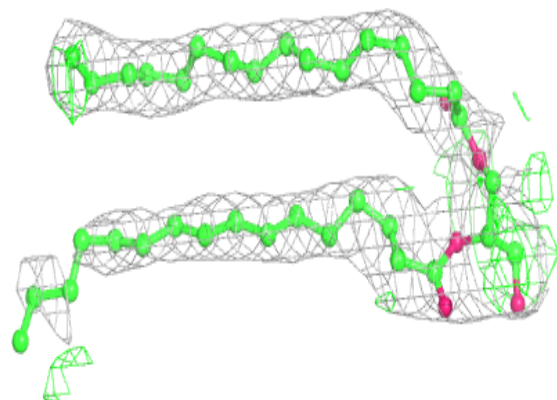


Electron density around DGD C 517:

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

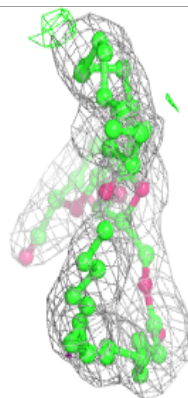
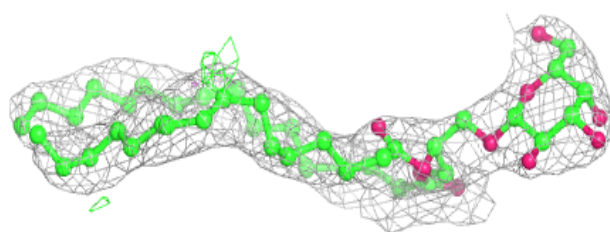
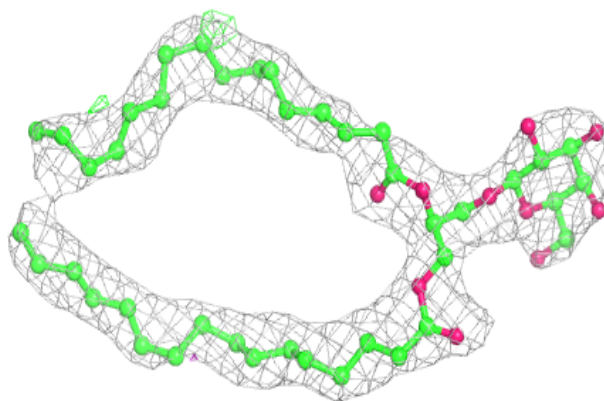
**Electron density around UNL D 413:**

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

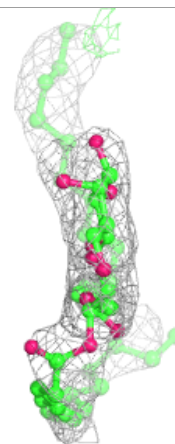
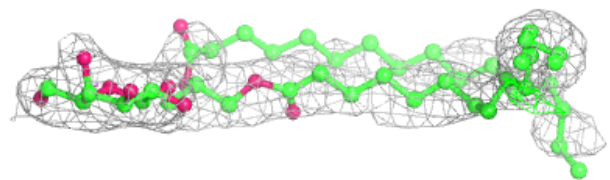
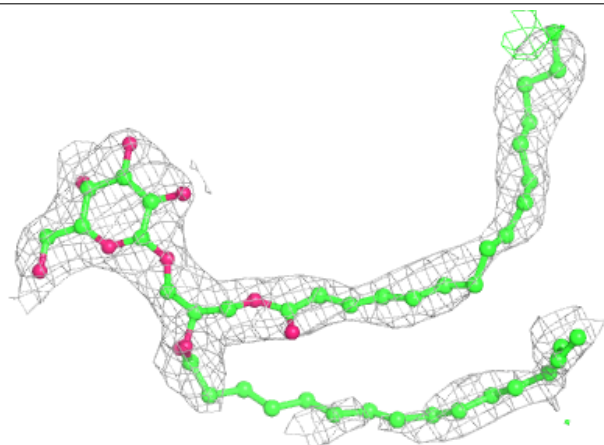


Electron density around LMG a 415:

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

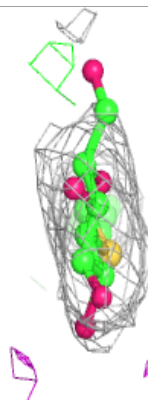
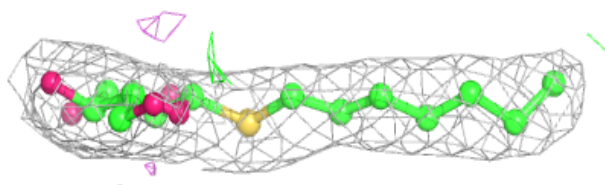
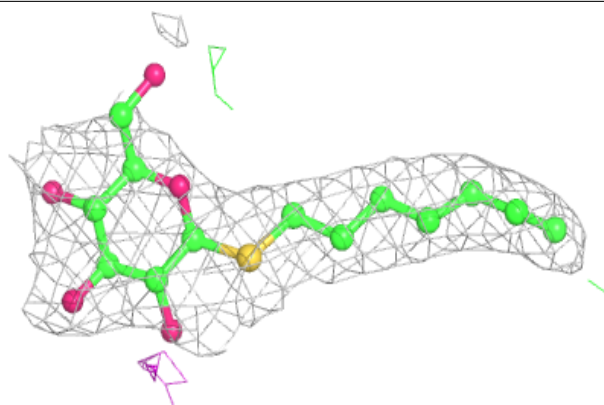
**Electron density around LMG k 101:**

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

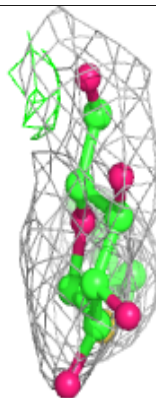
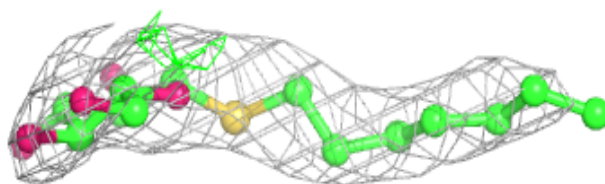
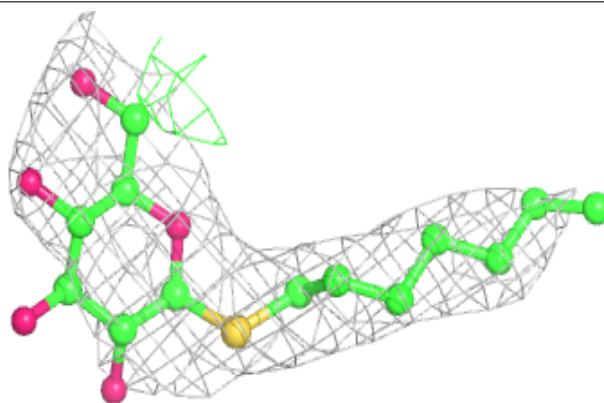


Electron density around HTG B 631:

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

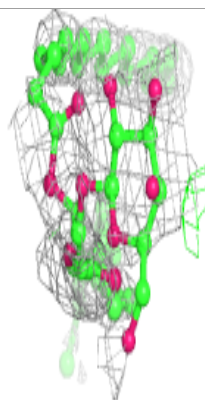
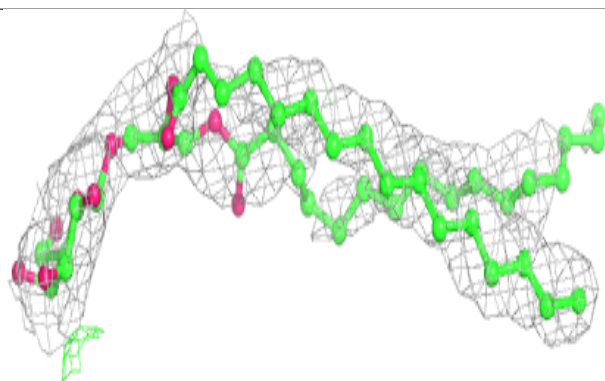
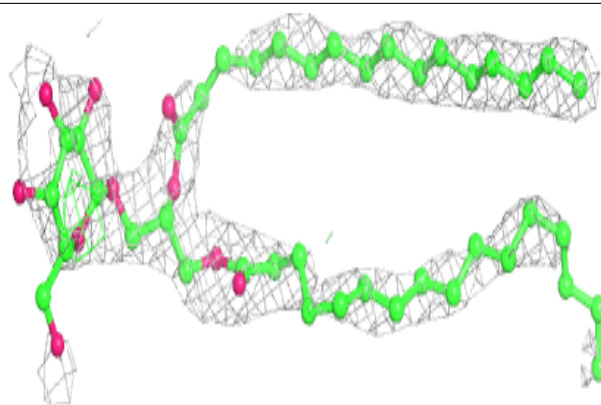
**Electron density around HTG b 632:**

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

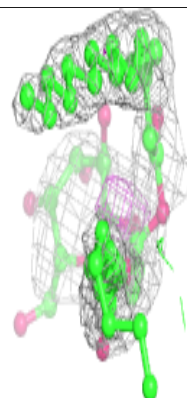
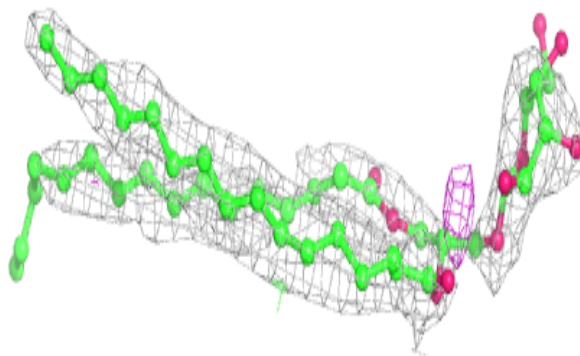
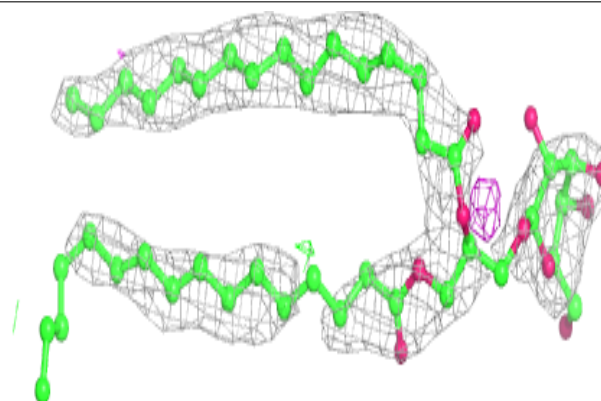


Electron density around LMG c 522:

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

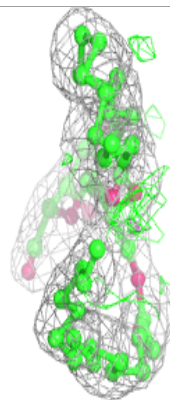
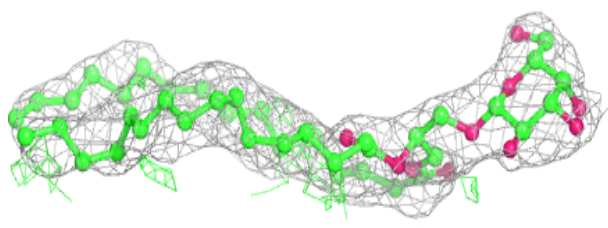
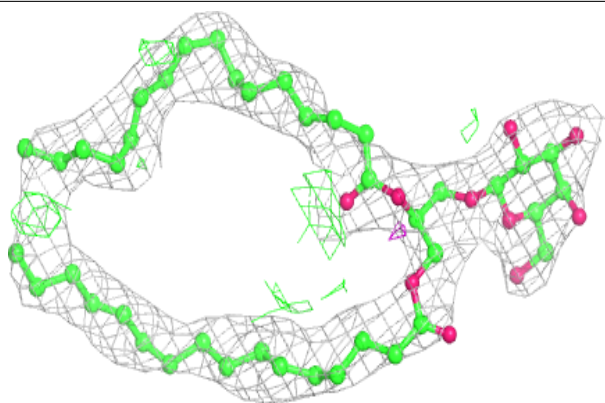
**Electron density around LMG C 520:**

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

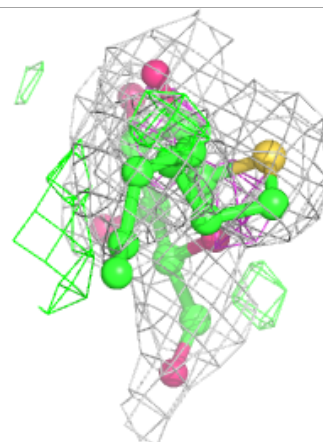
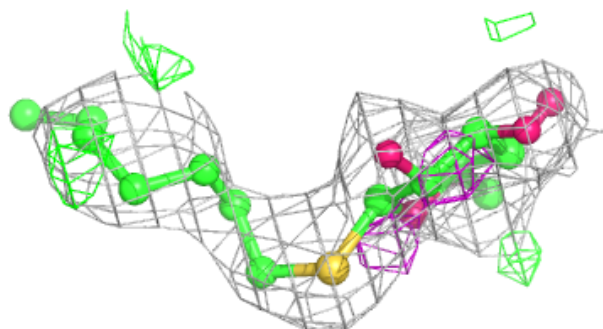
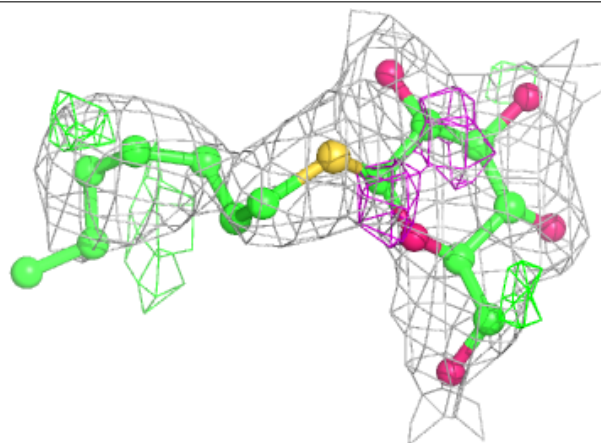


Electron density around LMG A 419:

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

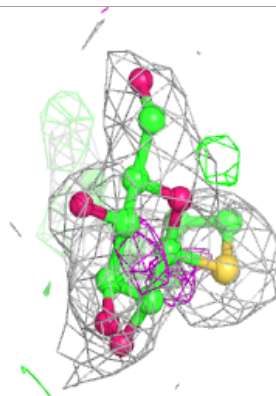
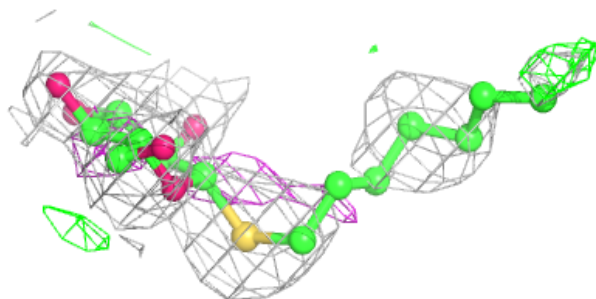
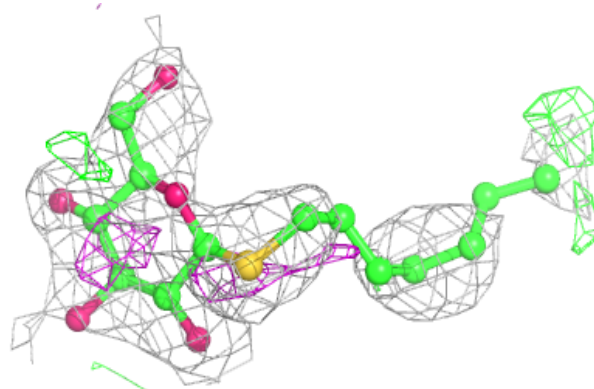
**Electron density around HTG B 623:**

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

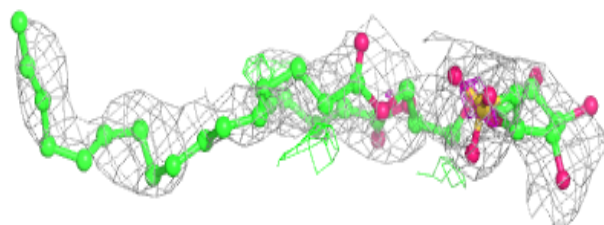
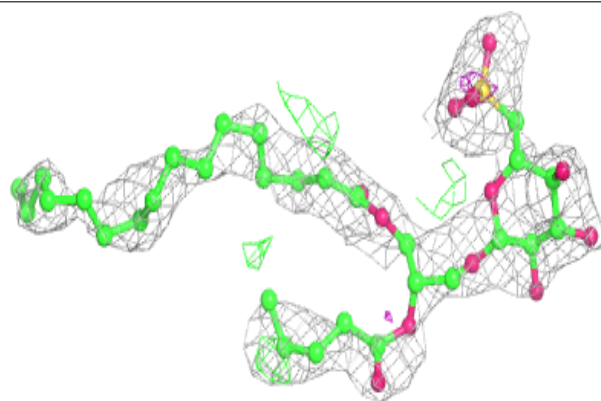


Electron density around HTG b 631:

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

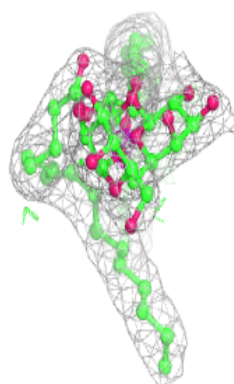
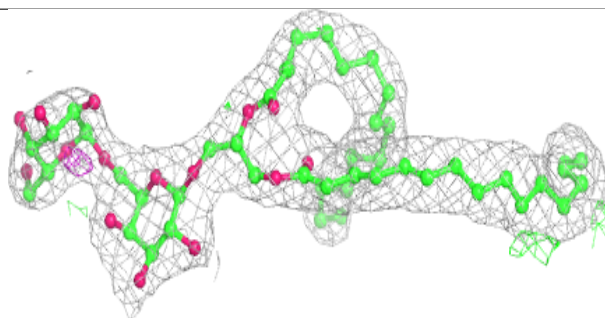
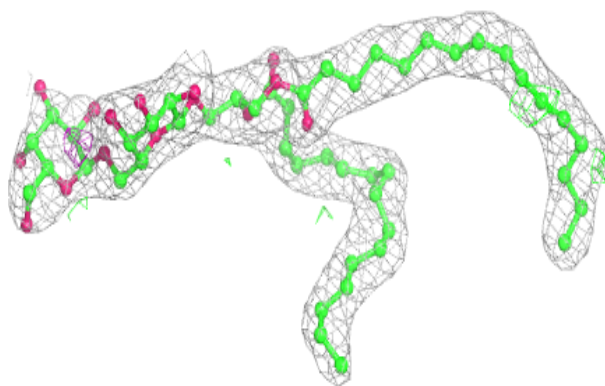
**Electron density around SQD F 101:**

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

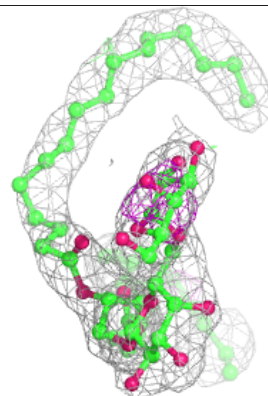
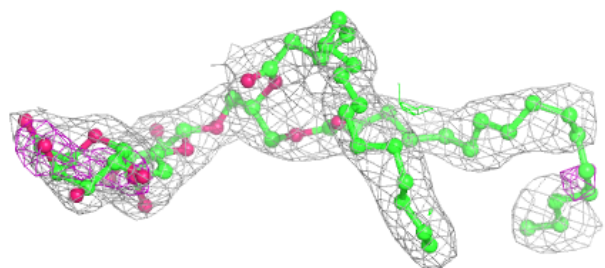
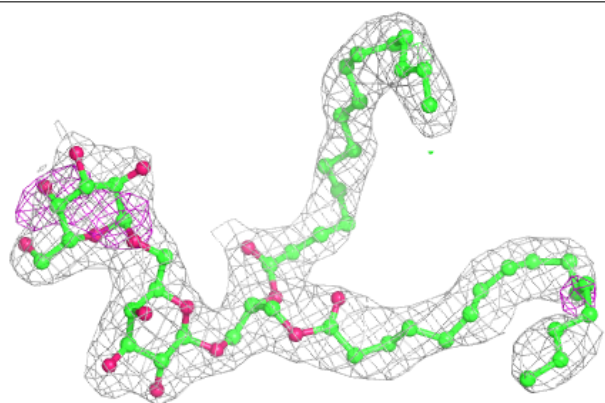


Electron density around DGD H 102:

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

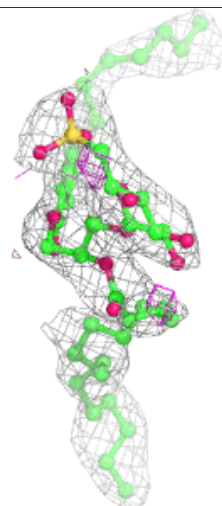
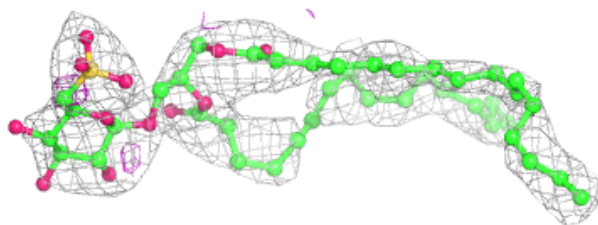
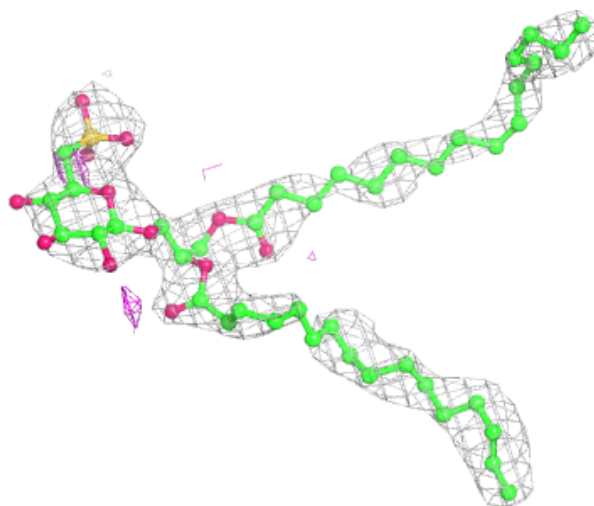
**Electron density around DGD c 520:**

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



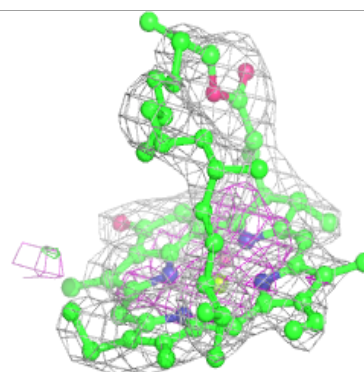
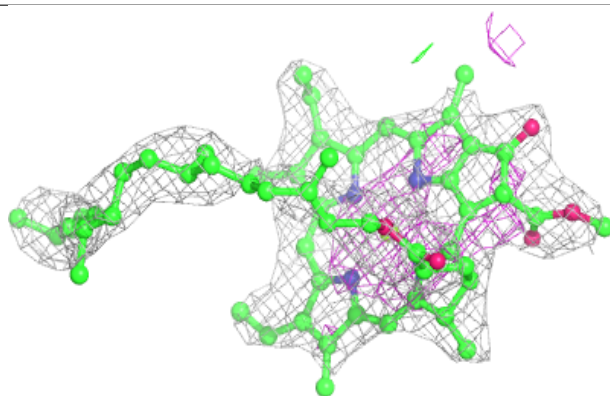
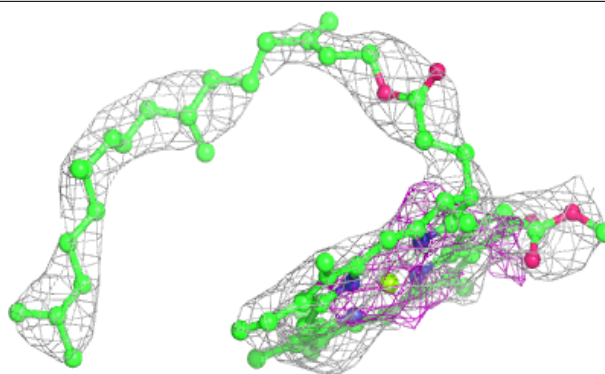
Electron density around SQD A 411:

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

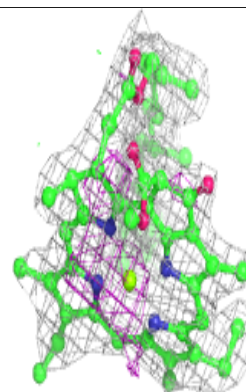
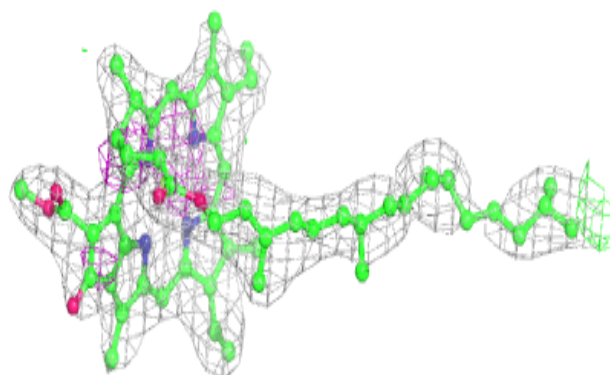
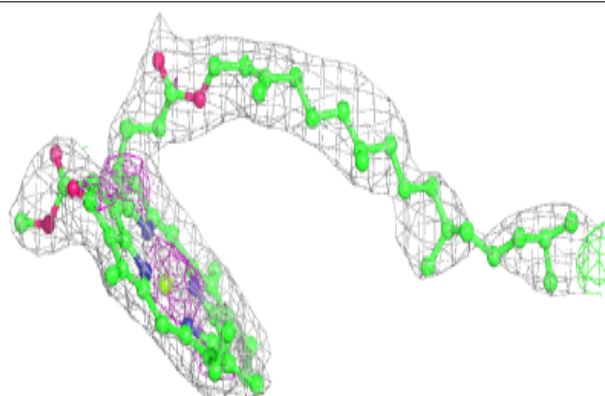


Electron density around CLA C 513:

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

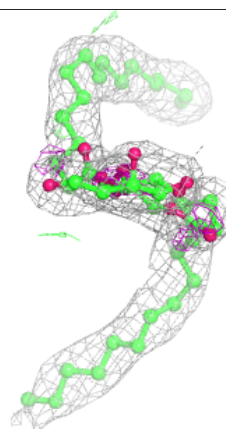
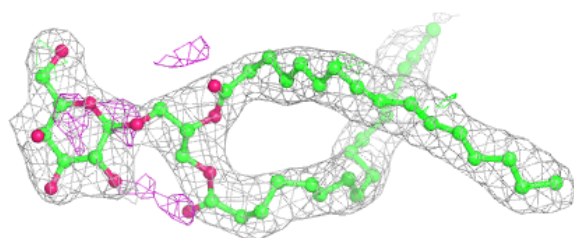
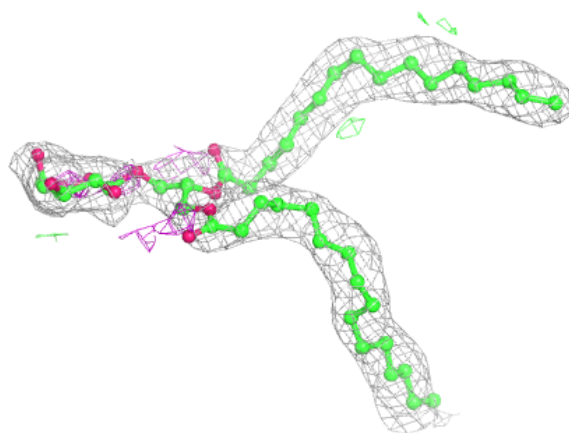
**Electron density around CLA C 504:**

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

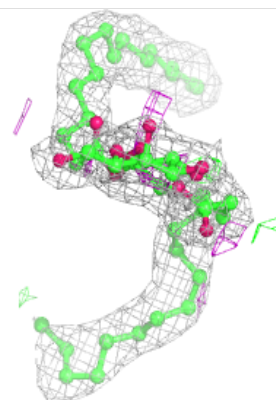
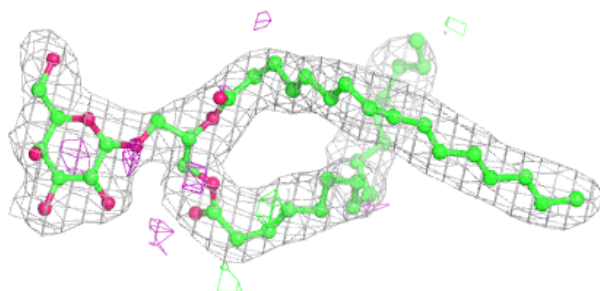
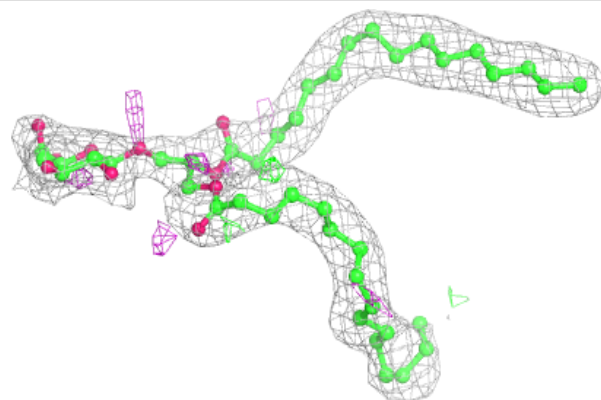


Electron density around LMG M 101:

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

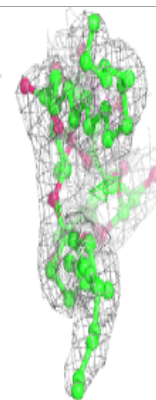
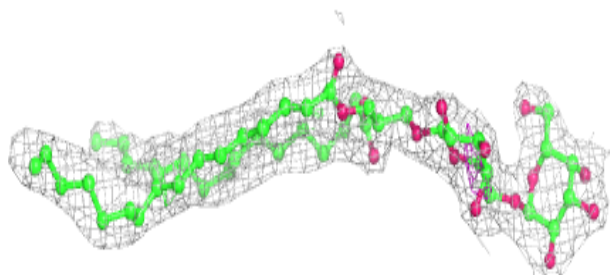
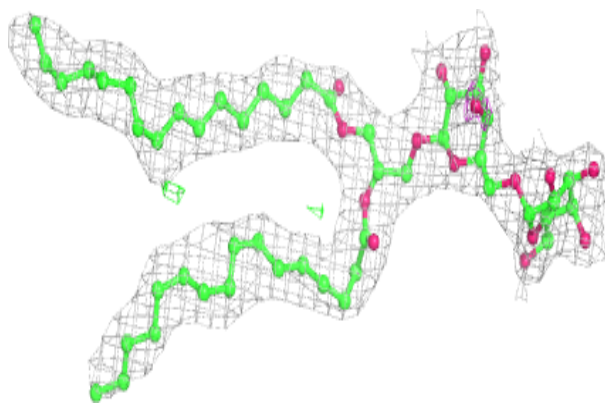
**Electron density around LMG b 629:**

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

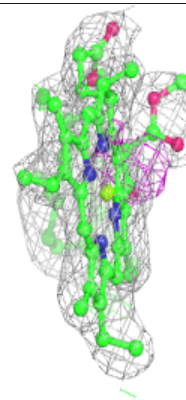
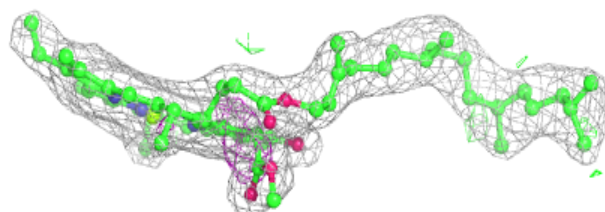
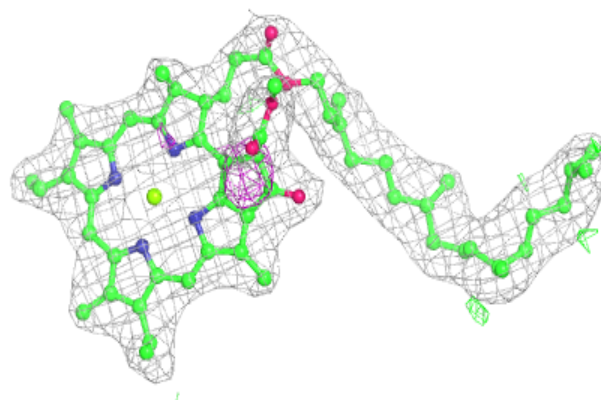


Electron density around DGD C 518:

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

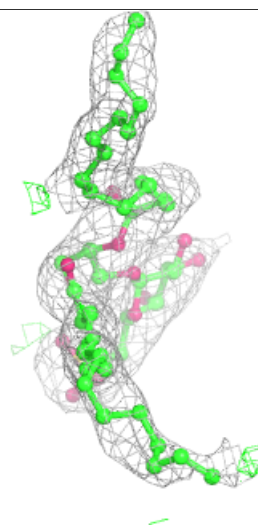
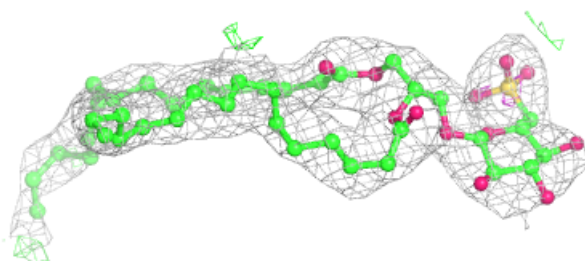
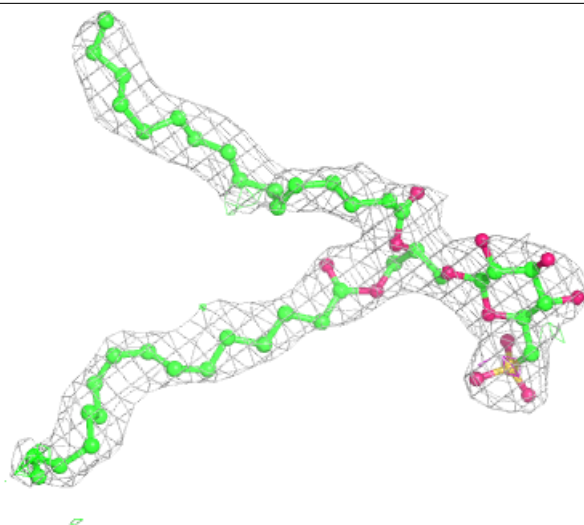
**Electron density around CLA b 611:**

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



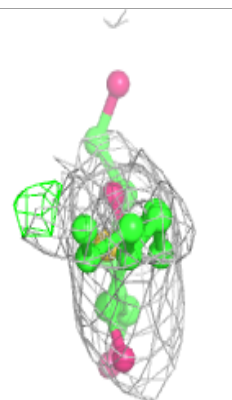
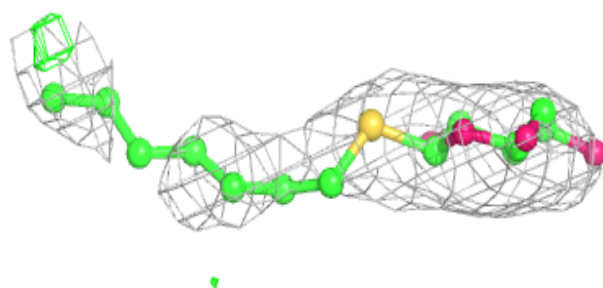
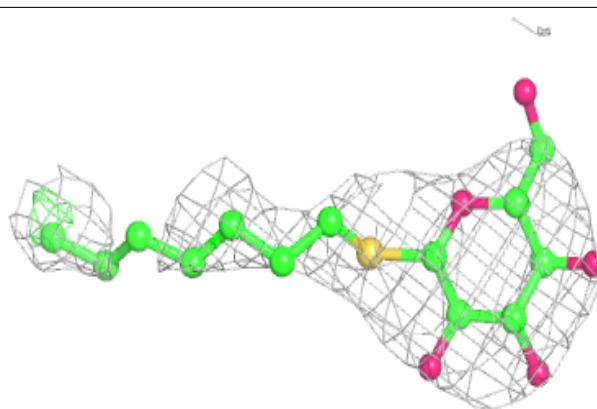
Electron density around SQD a 414:

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

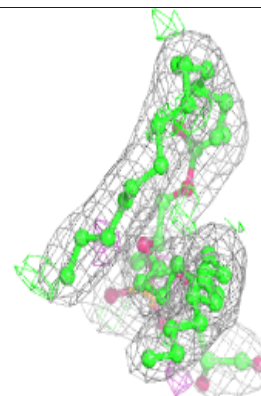
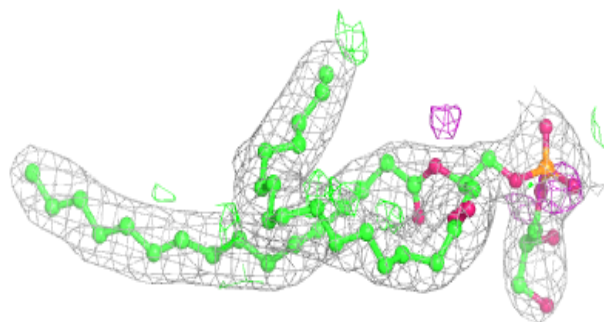
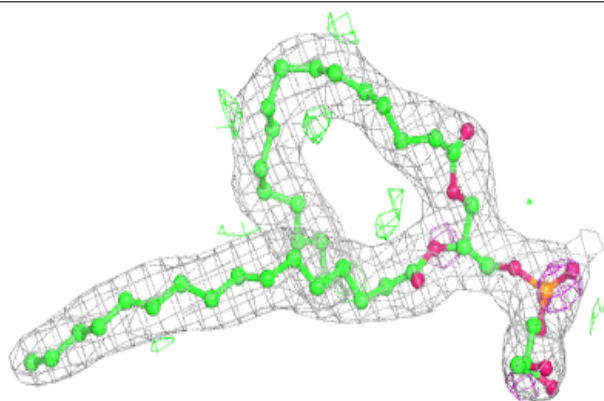


Electron density around HTG c 523:

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

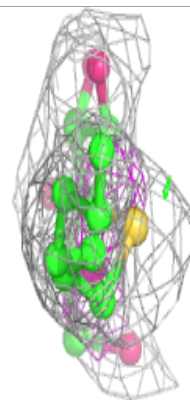
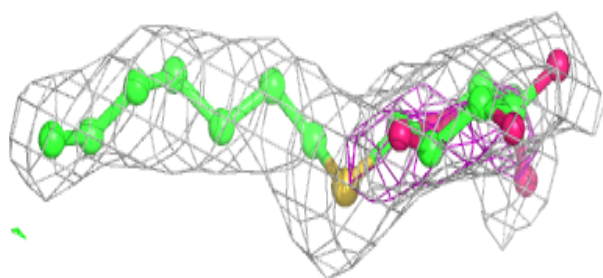
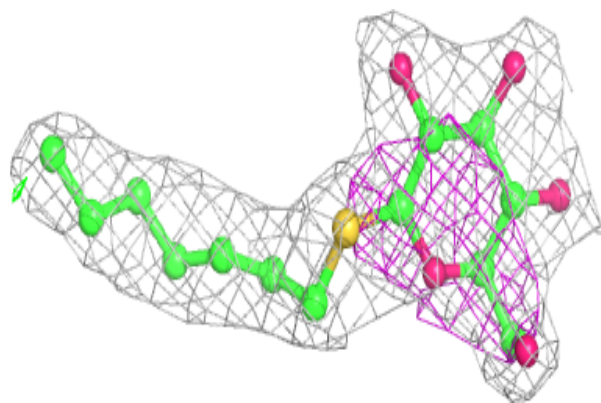
**Electron density around LHG D 409:**

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

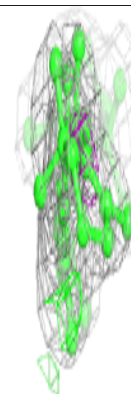
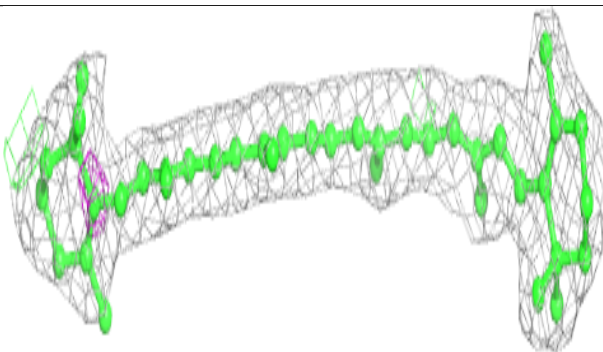
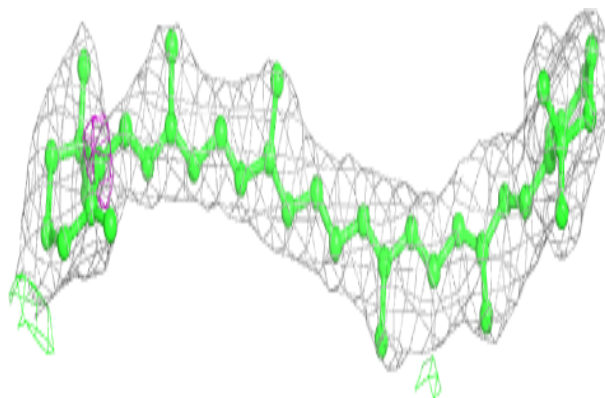


Electron density around HTG b 602:

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

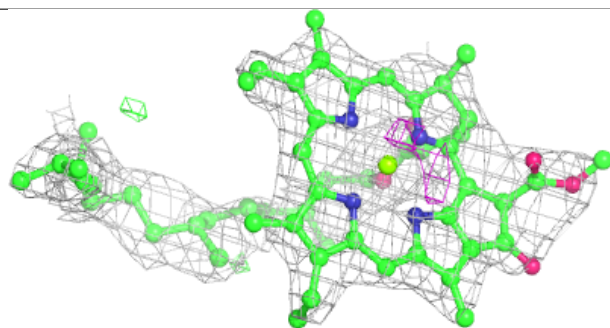
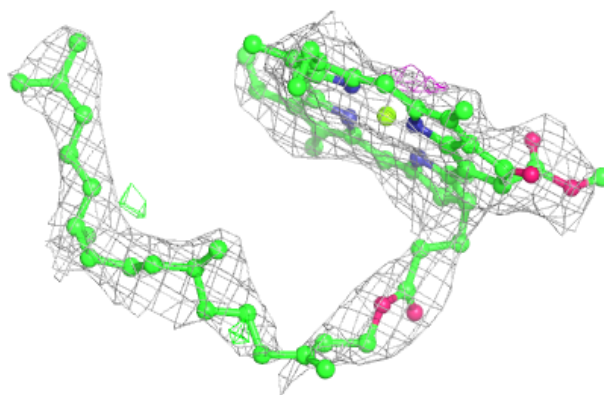
**Electron density around BCR H 101:**

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

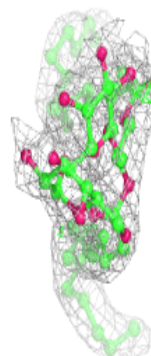
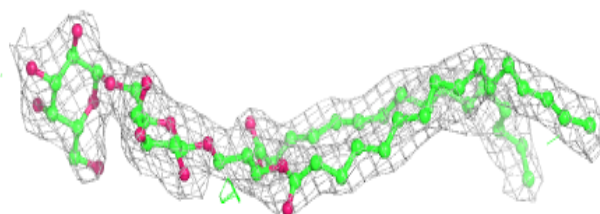
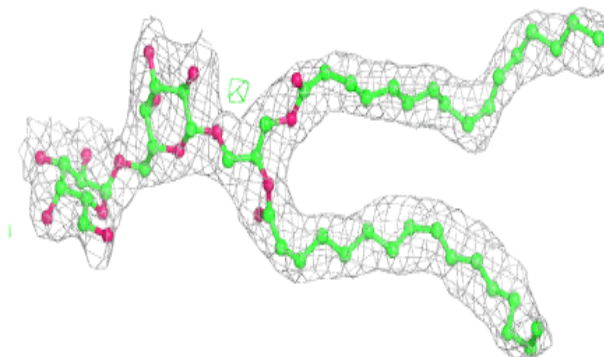


Electron density around CLA c 517:

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

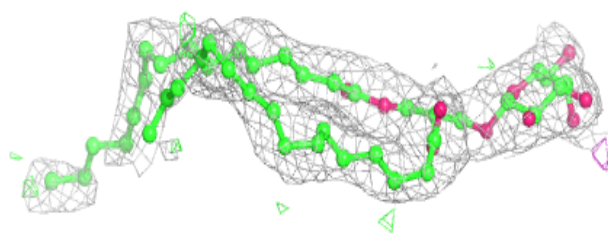
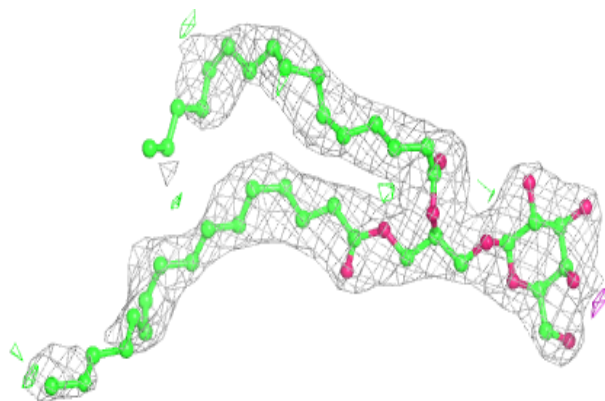
**Electron density around DGD c 521:**

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

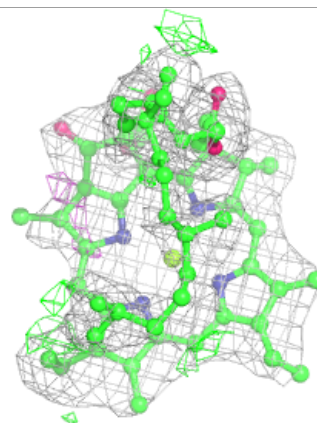
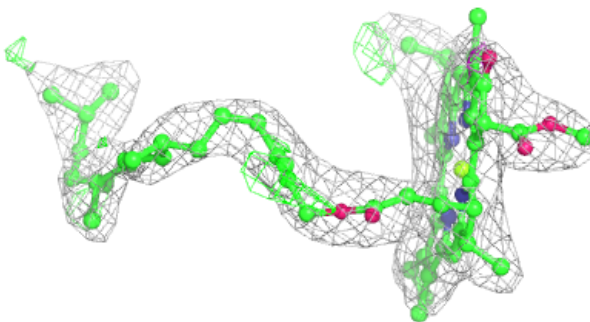
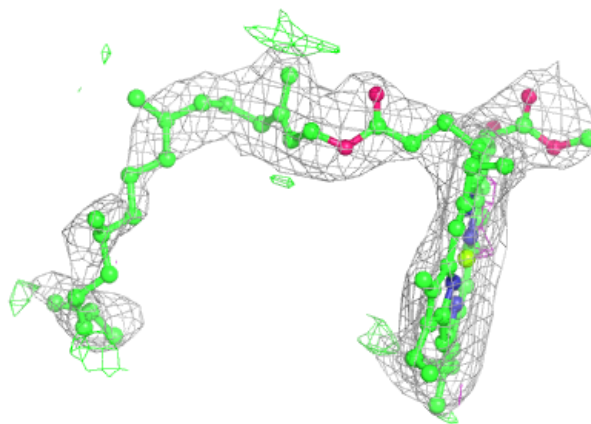


Electron density around LMG d 415:

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

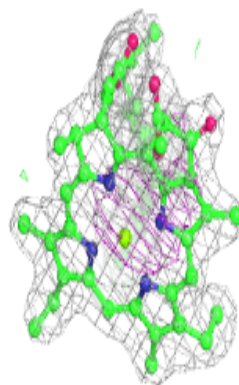
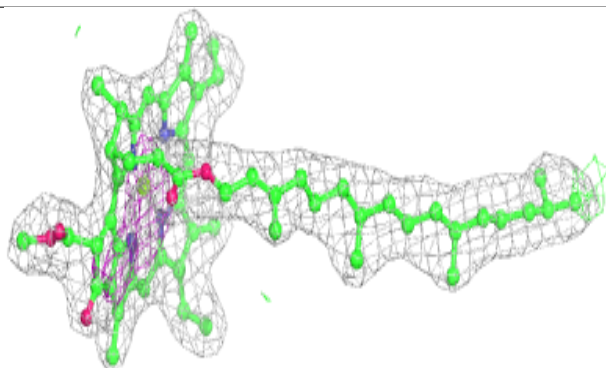
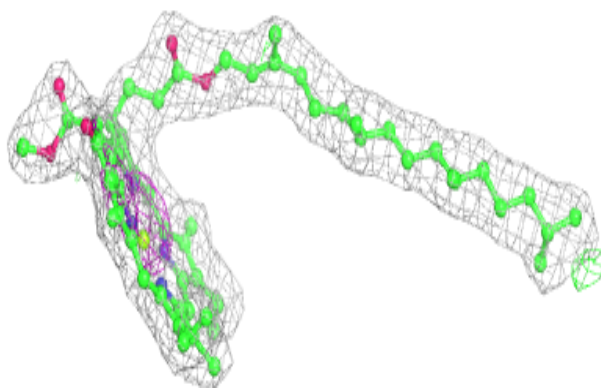
**Electron density around CLA C 506:**

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



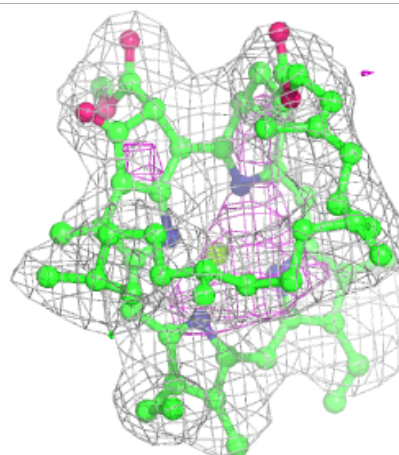
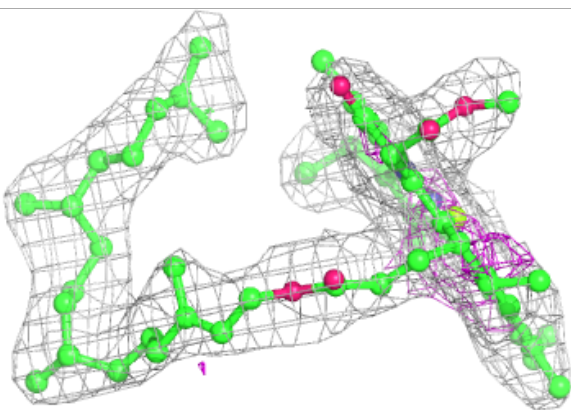
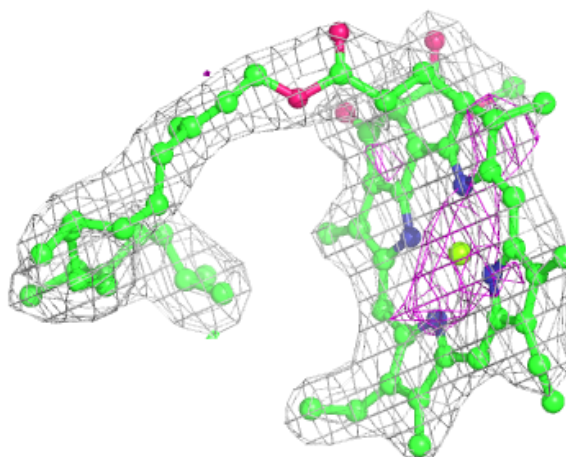
Electron density around CLA b 616:

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



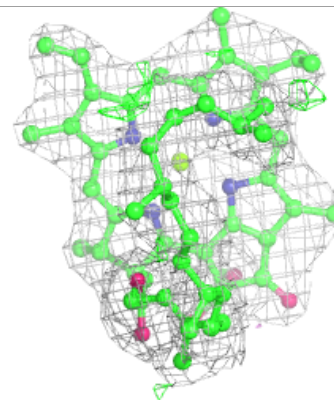
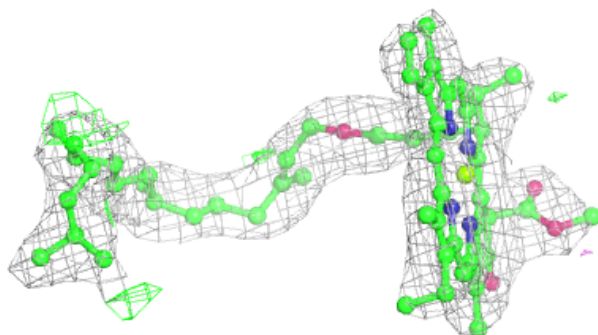
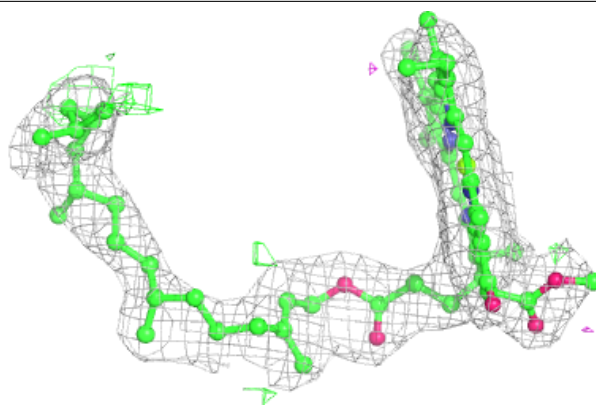
Electron density around CLA c 507:

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

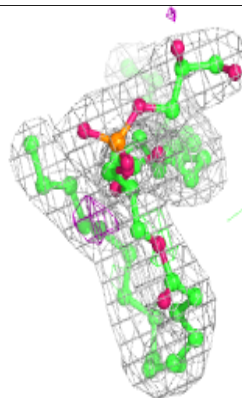
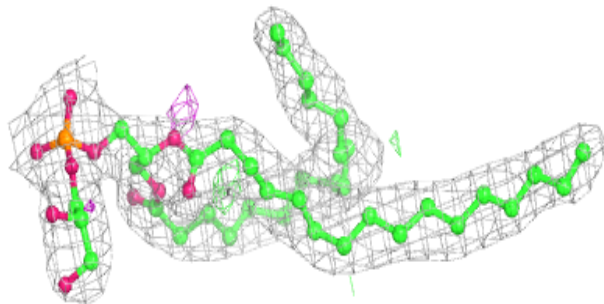
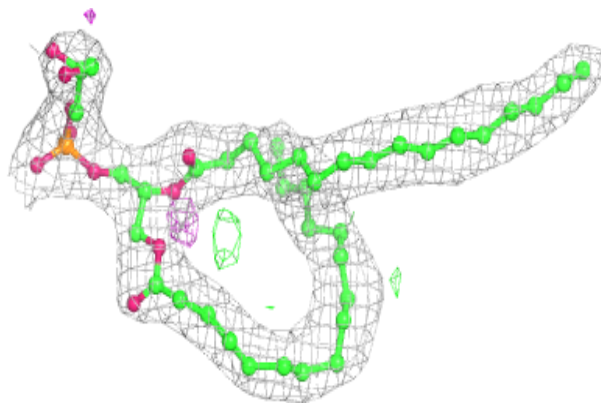


Electron density around CLA c 510:

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

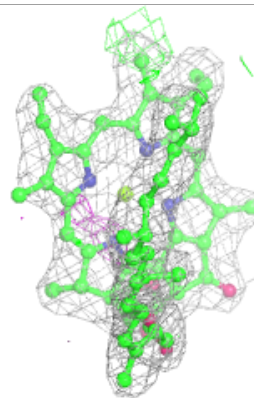
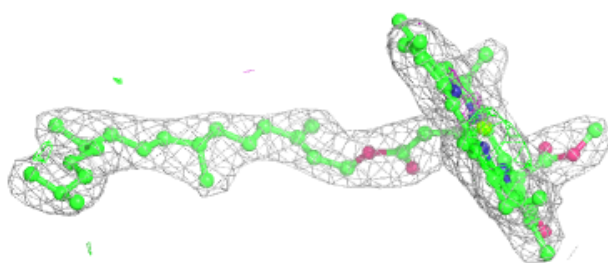
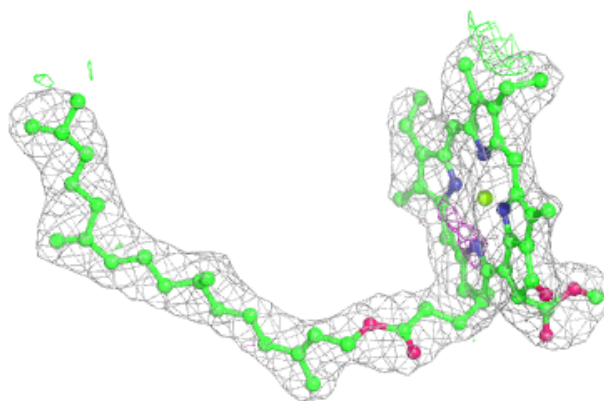
**Electron density around LHG d 408:**

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

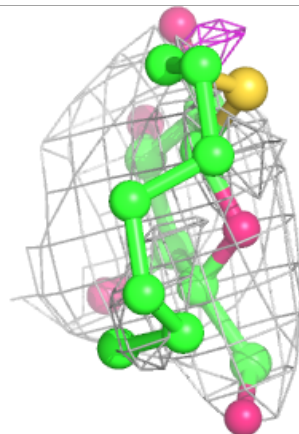
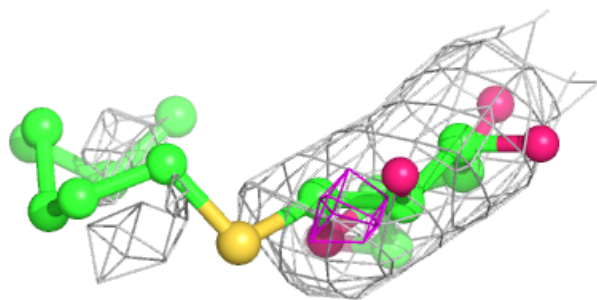
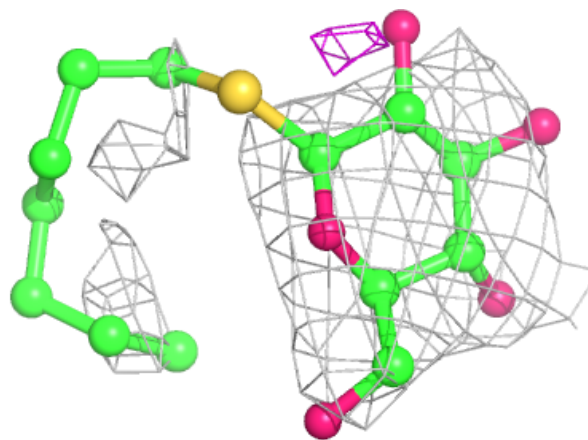


Electron density around CLA b 618:

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

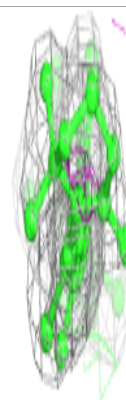
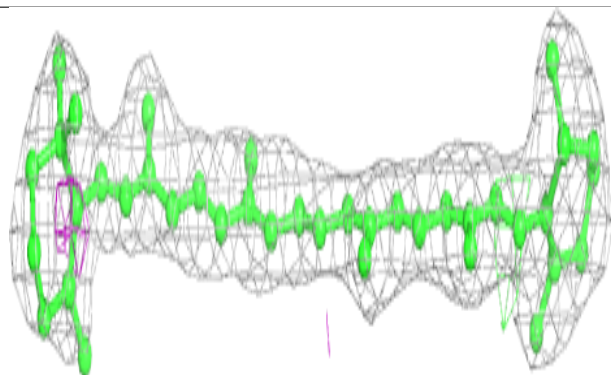
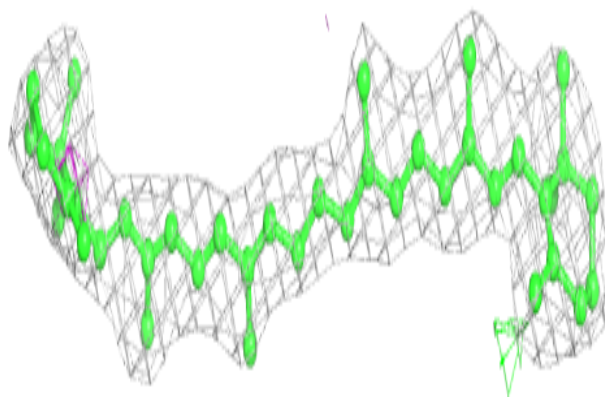
**Electron density around HTG V 206:**

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

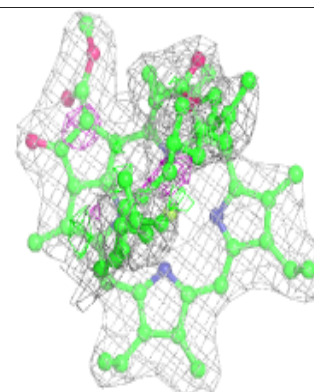
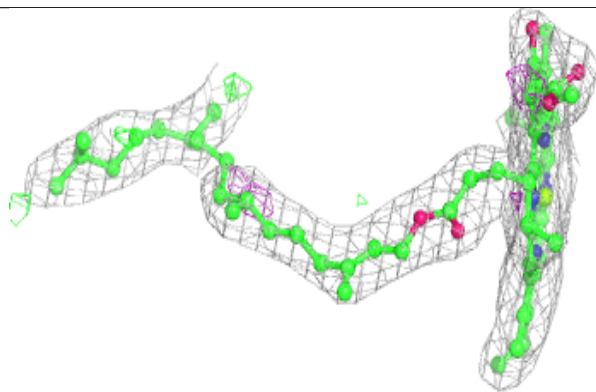
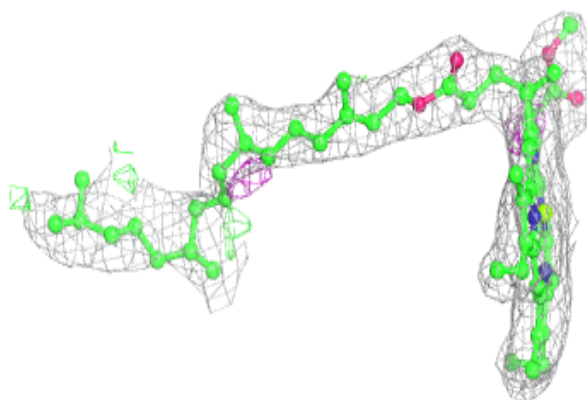


Electron density around BCR C 514:

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

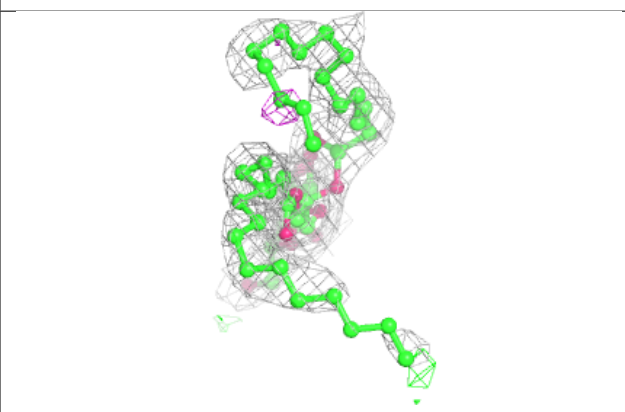
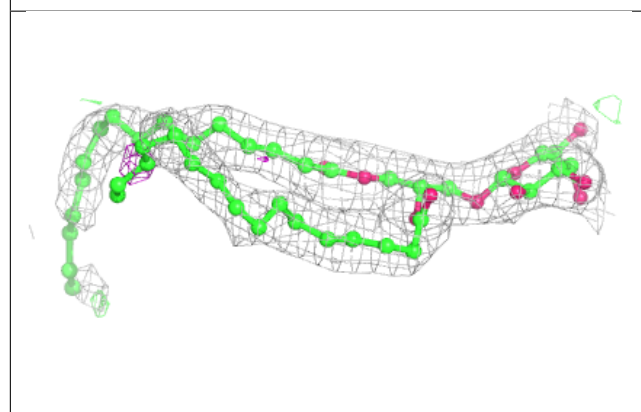
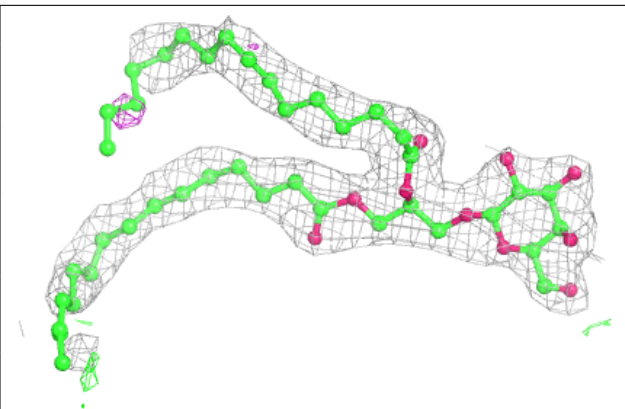
**Electron density around CLA b 615:**

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

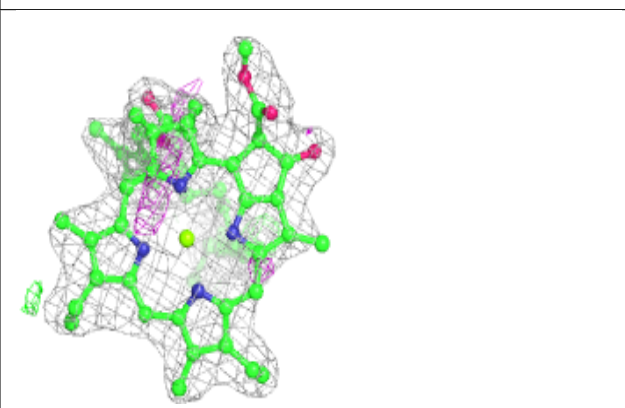
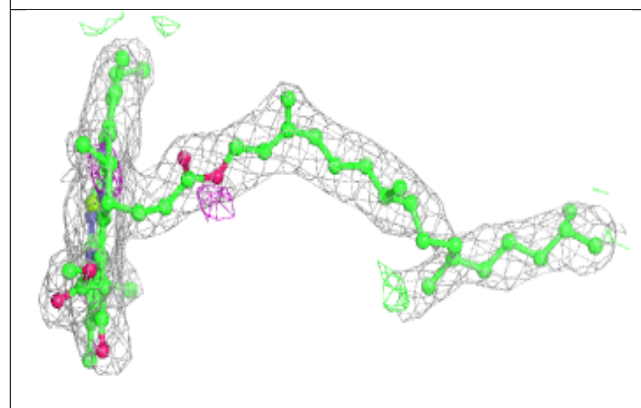
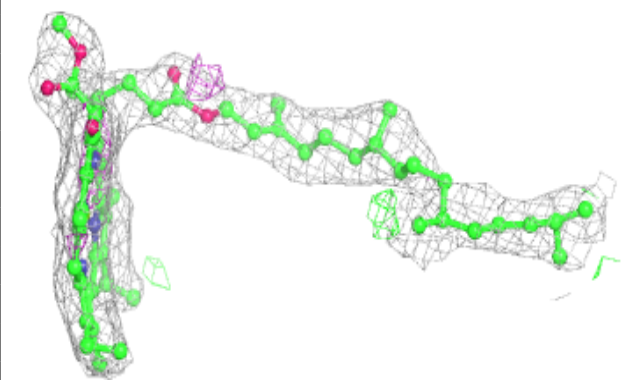


Electron density around LMG D 415:

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

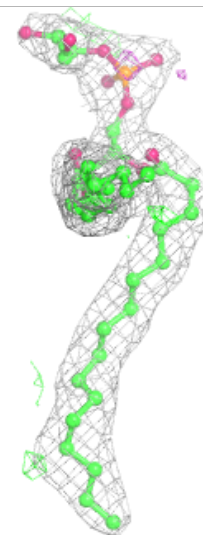
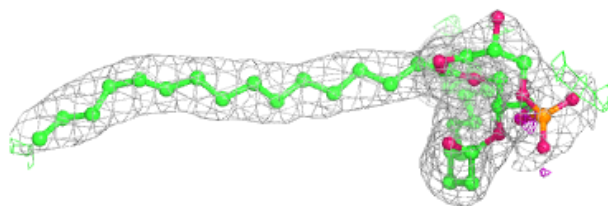
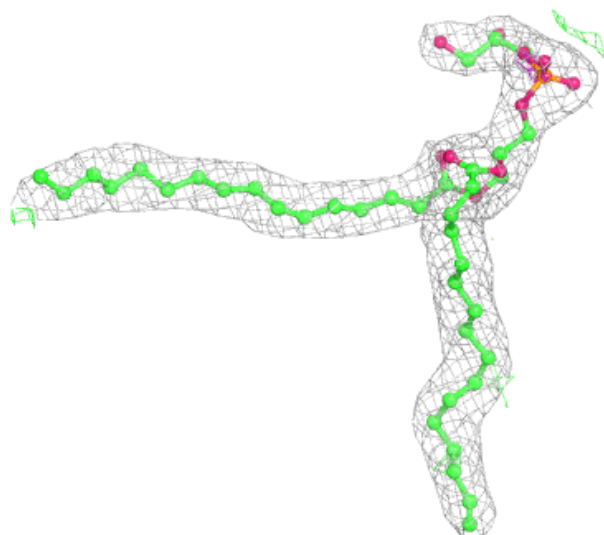
**Electron density around CLA B 607:**

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



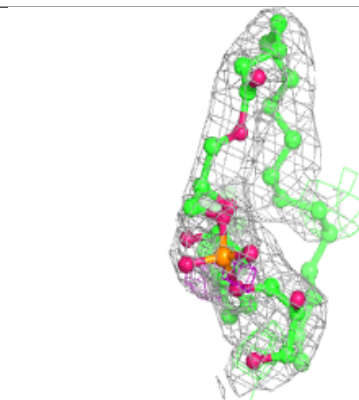
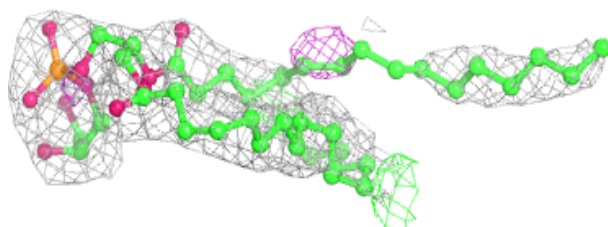
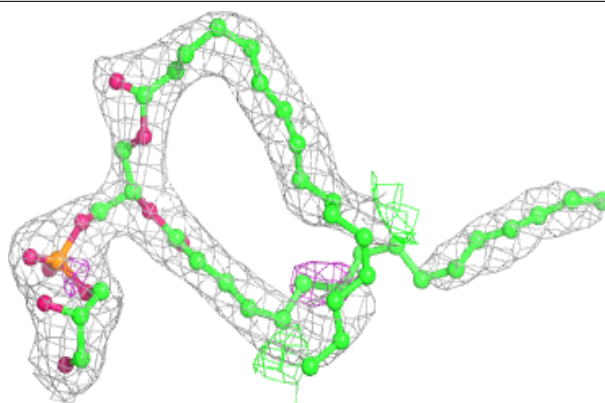
Electron density around LHG b 634:

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

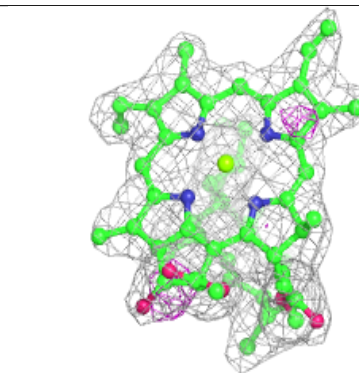
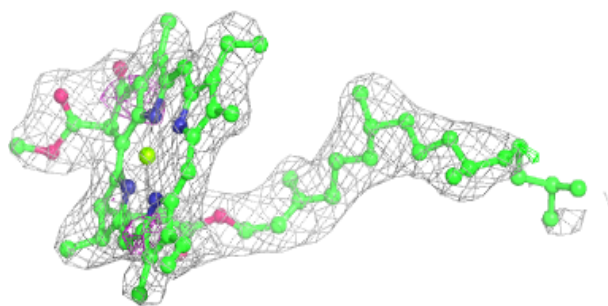
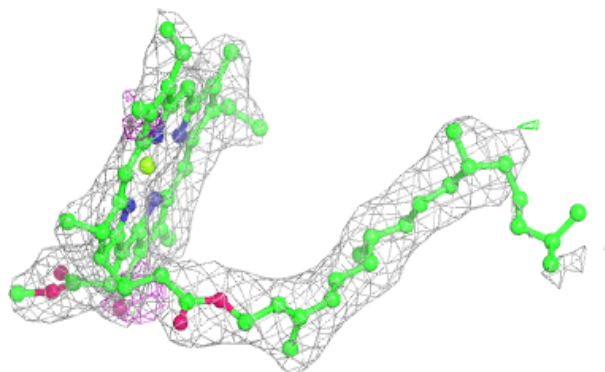


Electron density around LHG D 411:

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

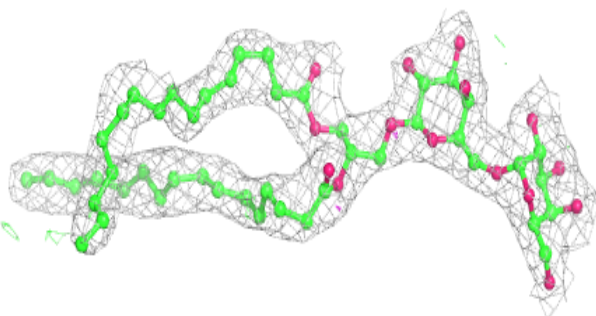
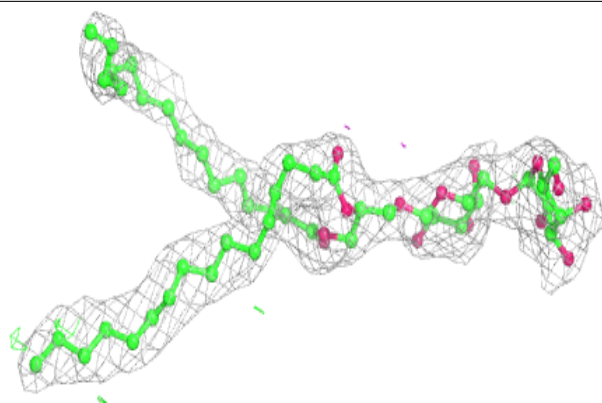
**Electron density around CLA c 512:**

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

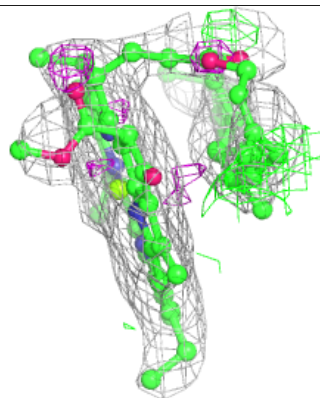
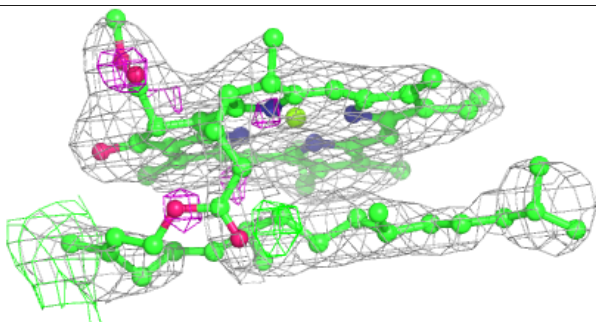
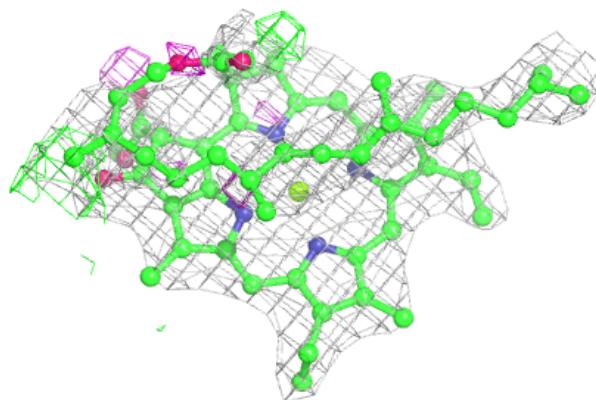


Electron density around DGD c 519:

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

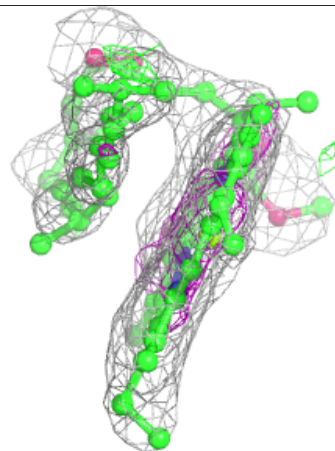
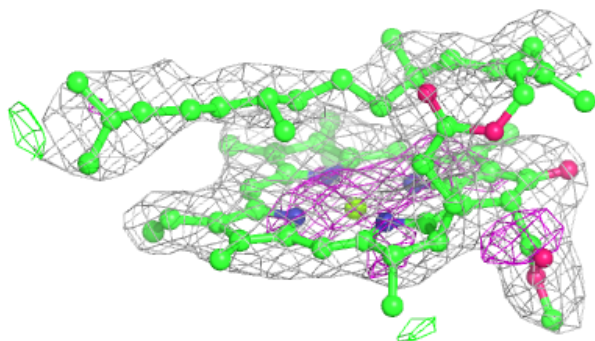
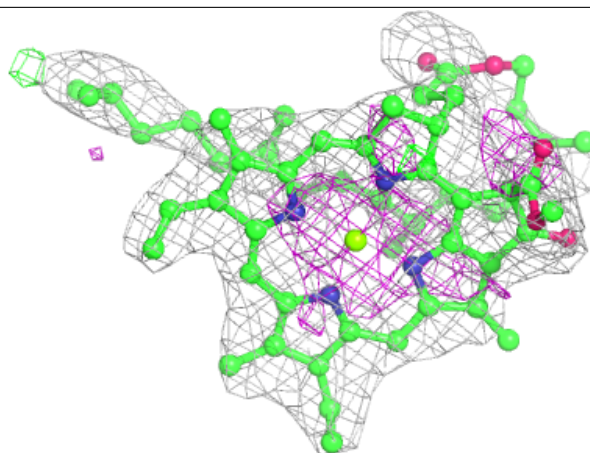
**Electron density around CLA B 602:**

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

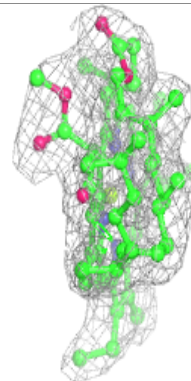
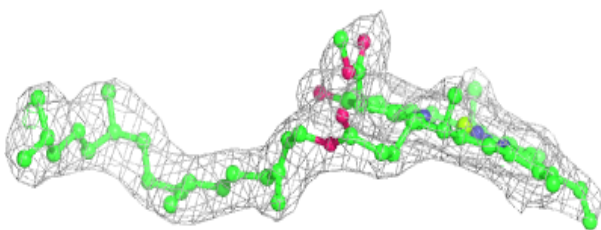
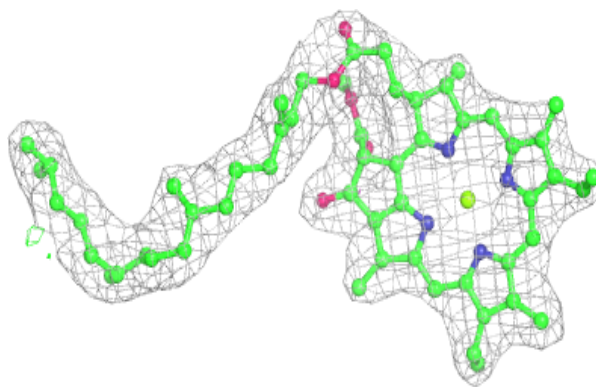


Electron density around CLA b 610:

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

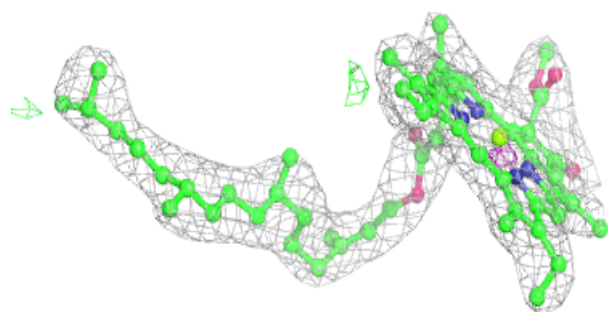
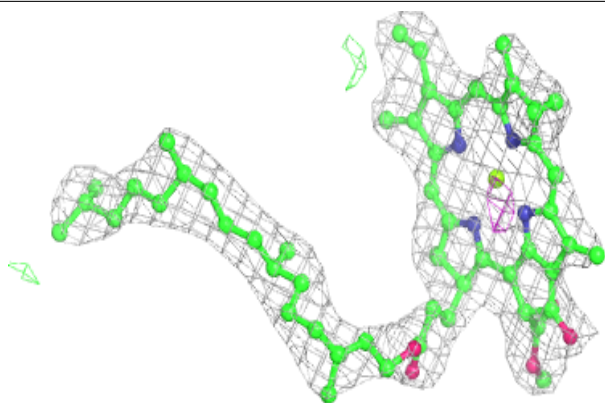
**Electron density around CLA B 603:**

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

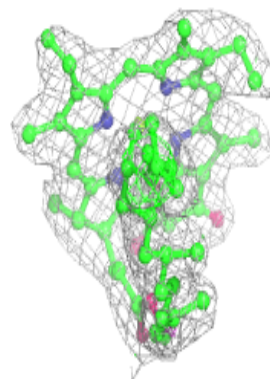
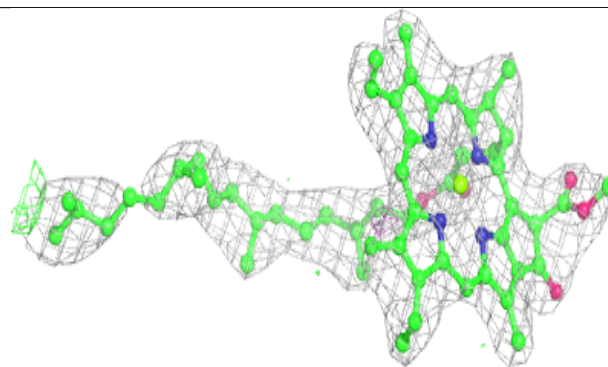
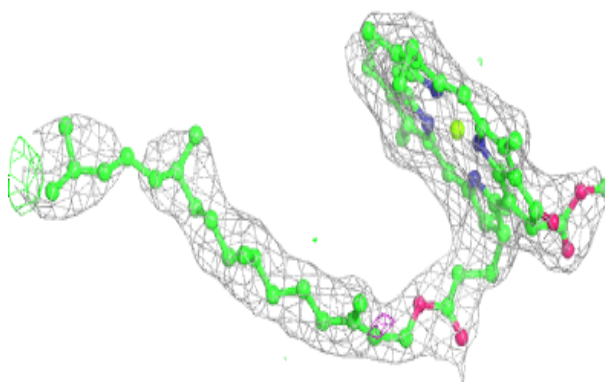


Electron density around CLA C 511:

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

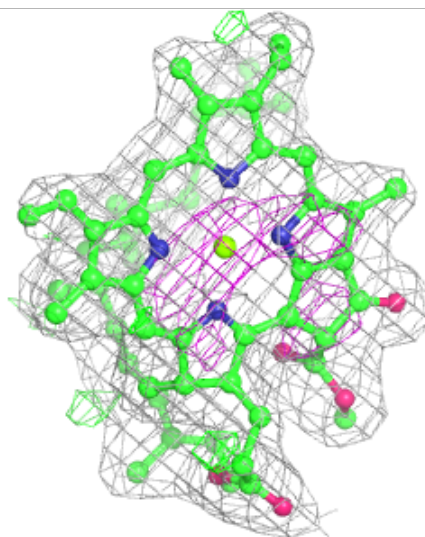
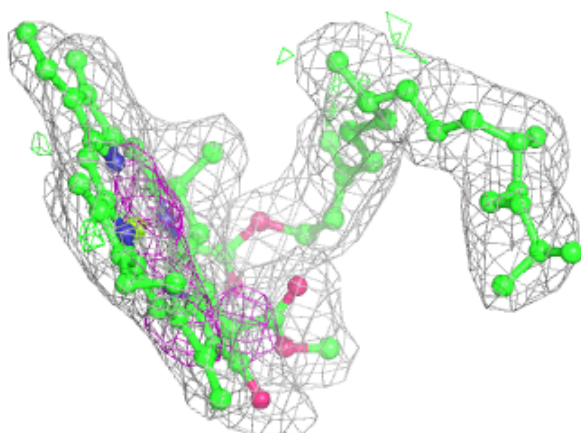
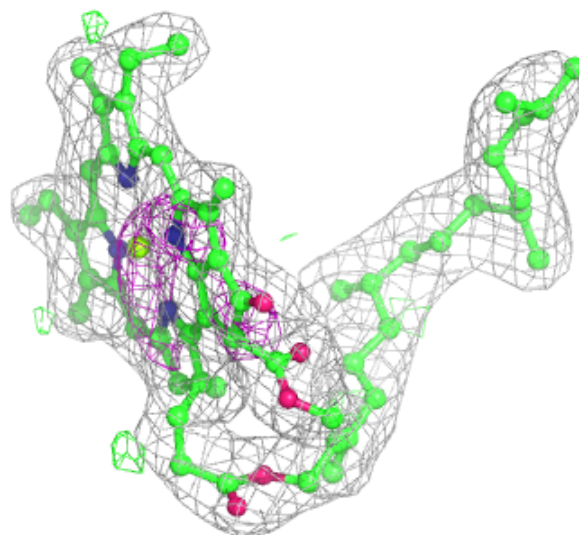
**Electron density around CLA c 508:**

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



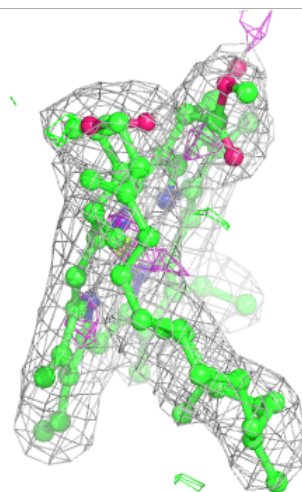
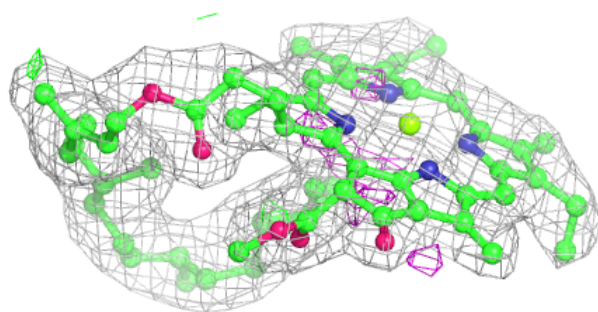
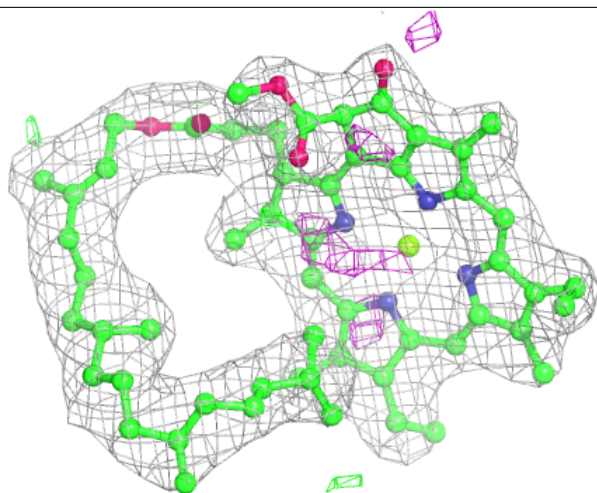
Electron density around CLA B 614:

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



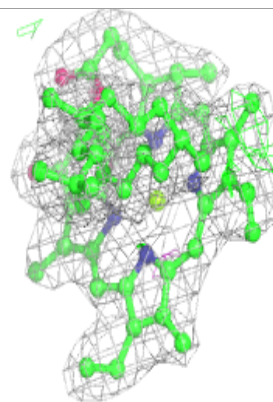
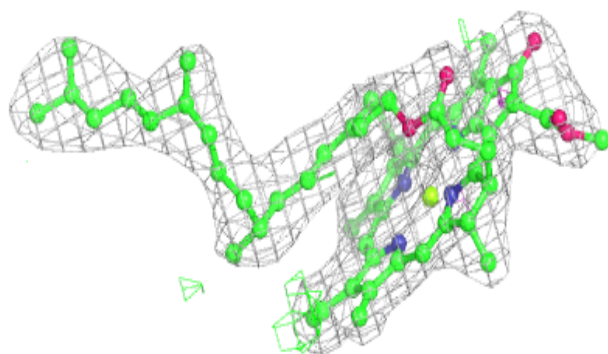
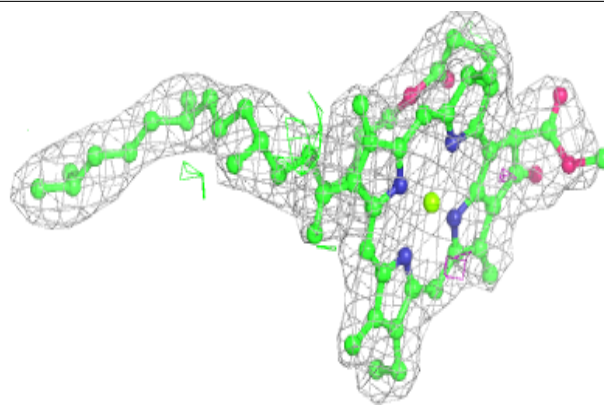
Electron density around CLA b 624:

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

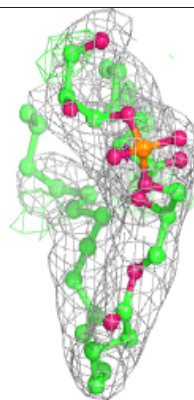
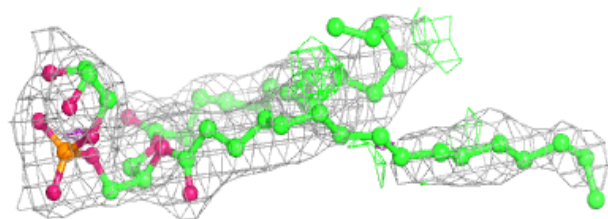
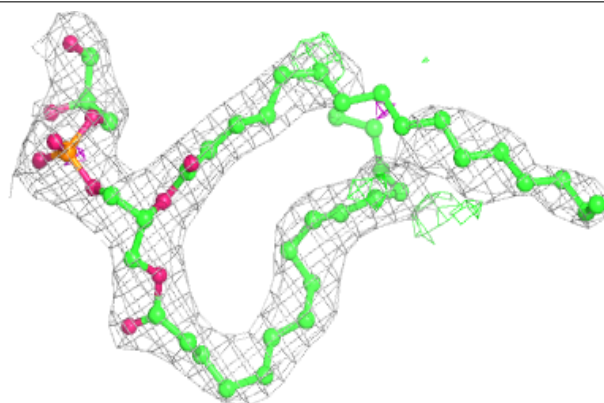


Electron density around CLA c 509:

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

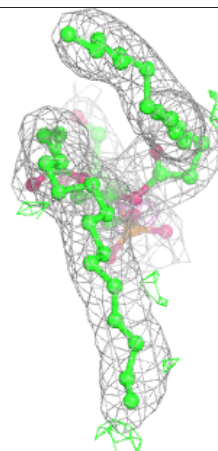
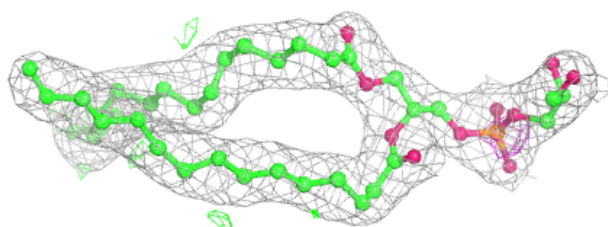
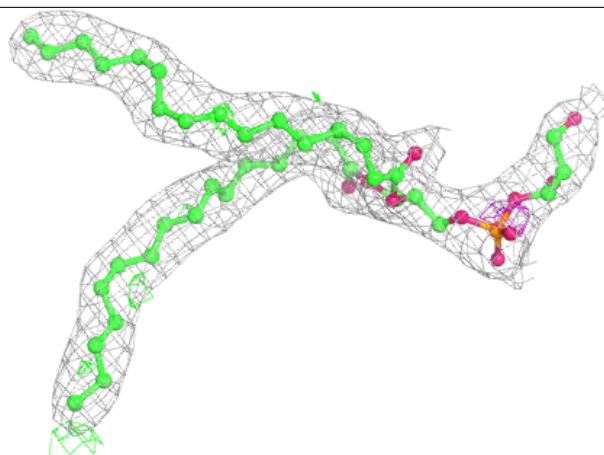
**Electron density around LHG d 410:**

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

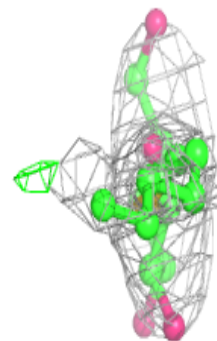
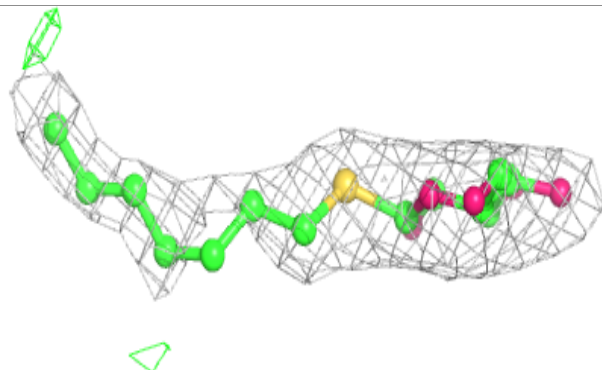
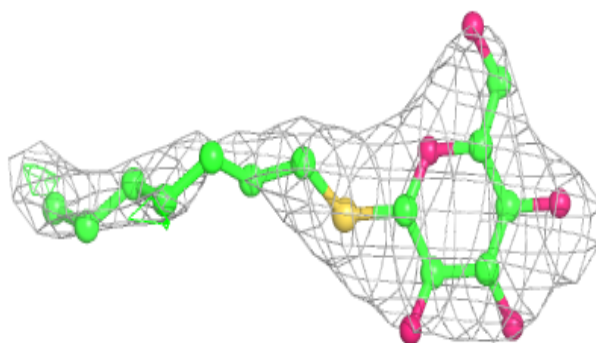


Electron density around LHG d 409:

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

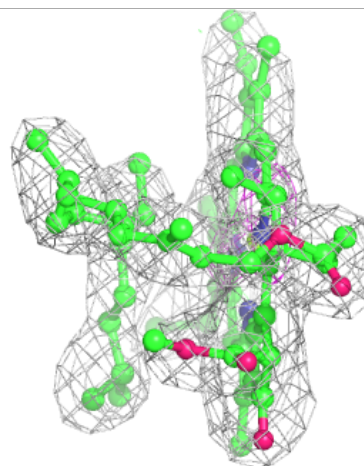
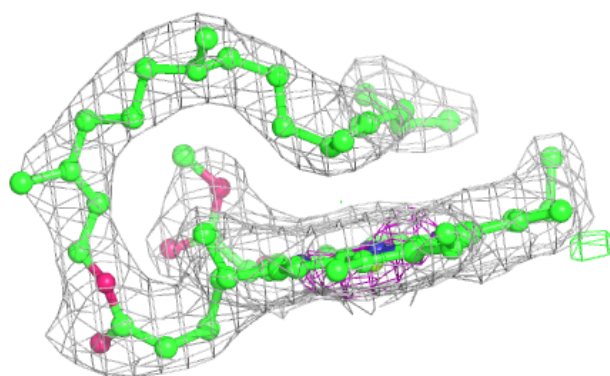
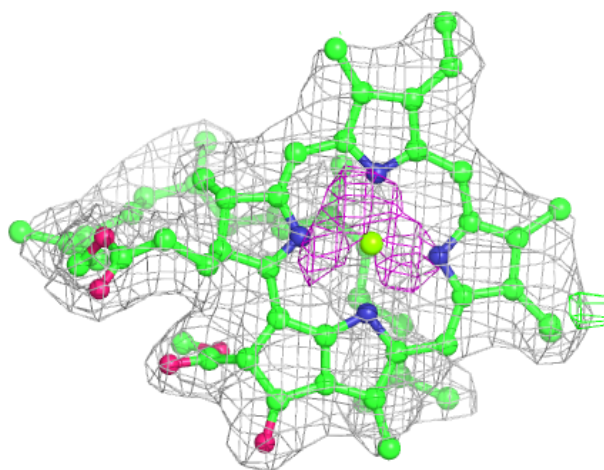
**Electron density around HTG C 522:**

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



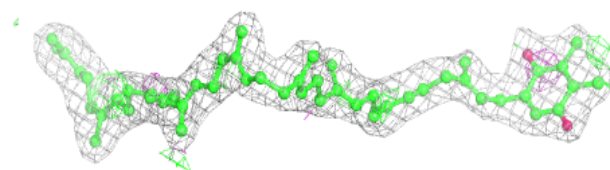
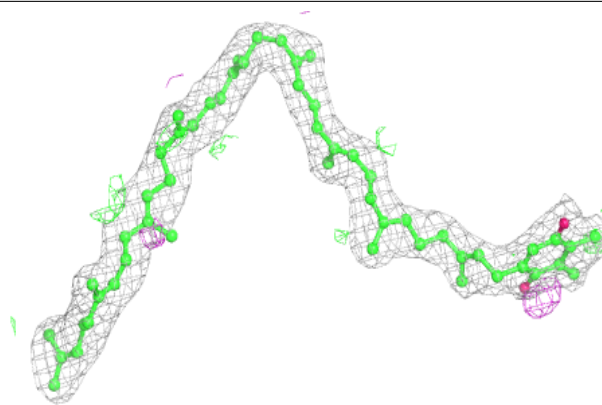
Electron density around CLA C 510:

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



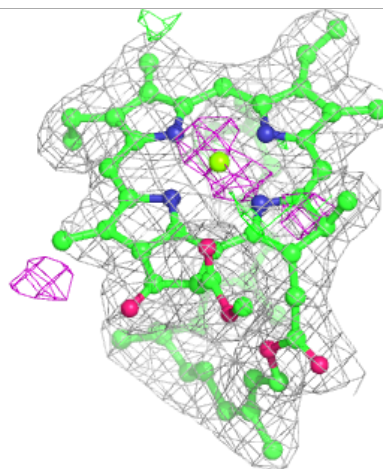
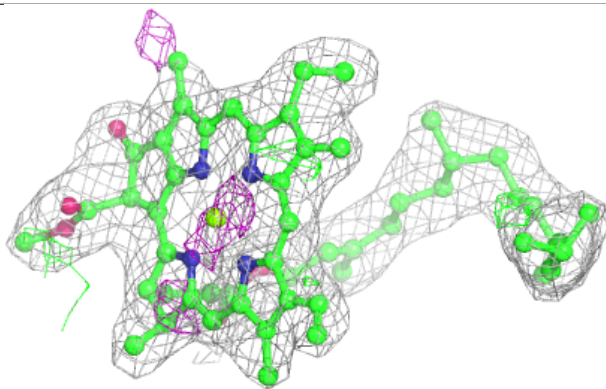
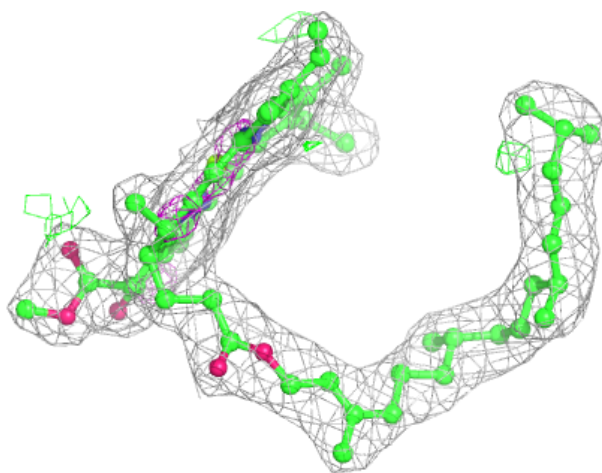
Electron density around PL9 D 407 (B):

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



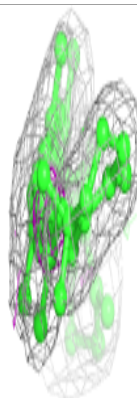
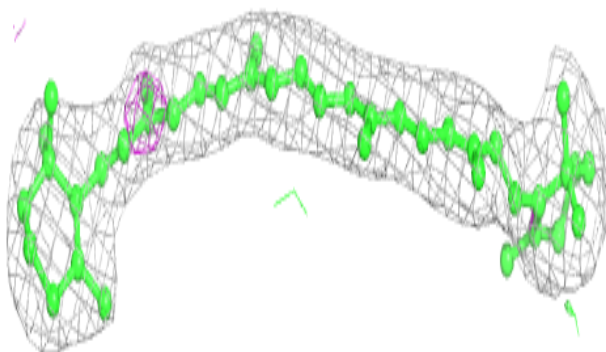
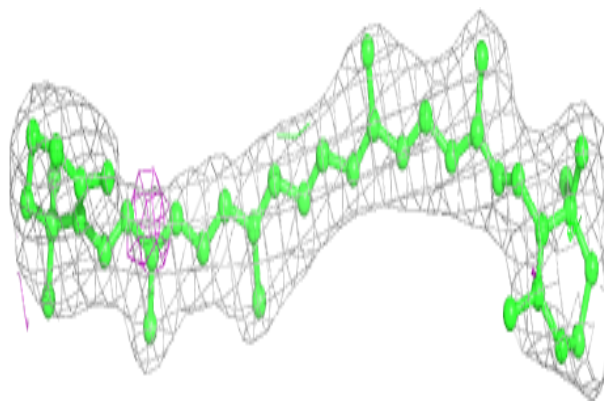
Electron density around CLA b 620:

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

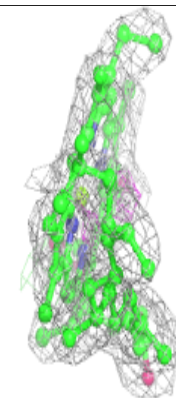
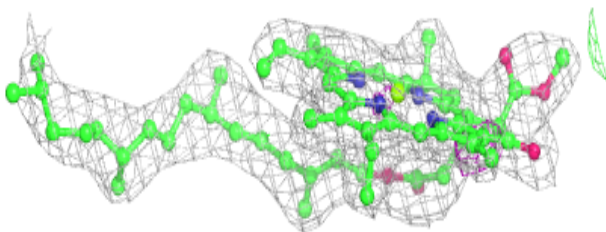
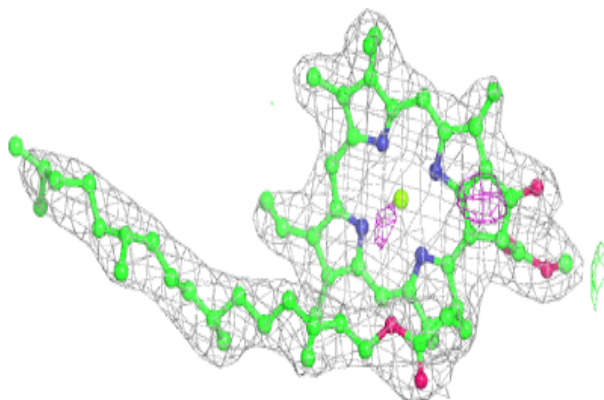


Electron density around BCR d 406:

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

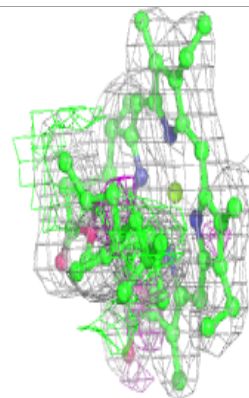
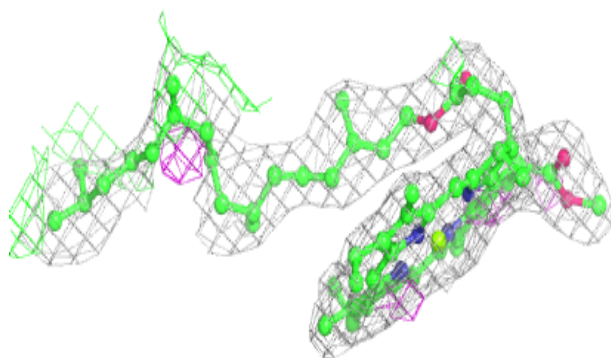
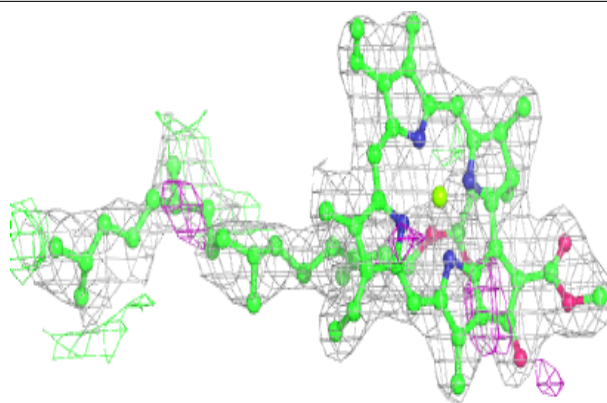
**Electron density around CLA C 501:**

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



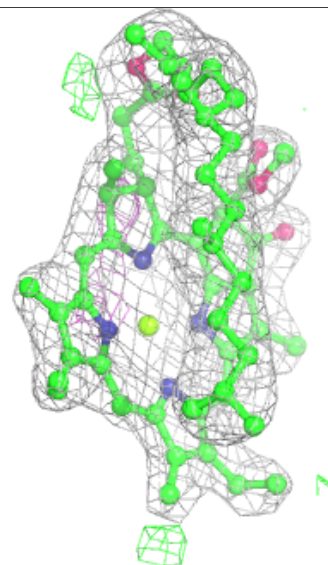
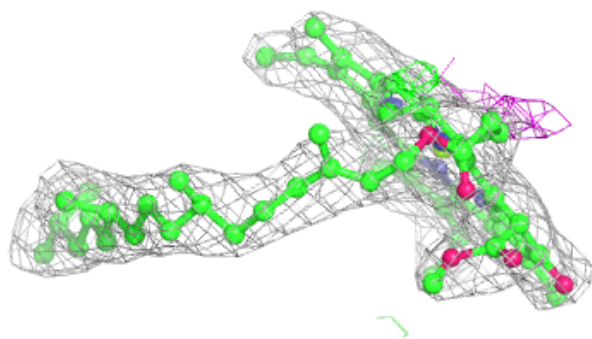
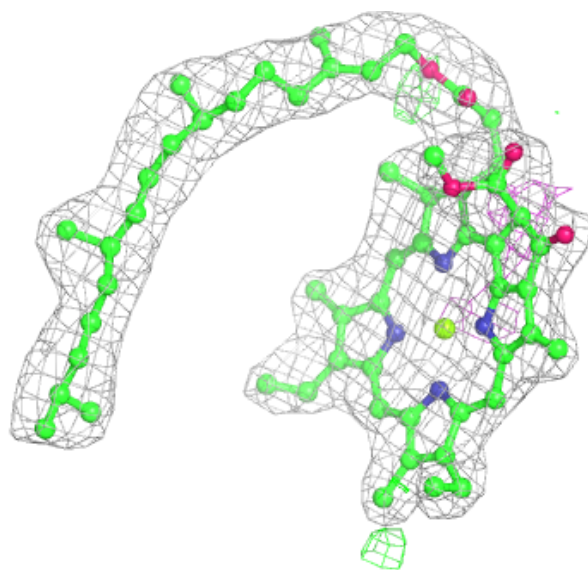
Electron density around CLA B 615:

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



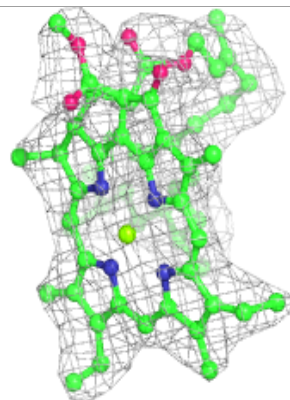
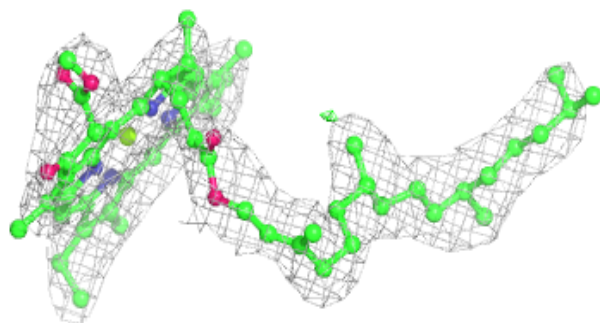
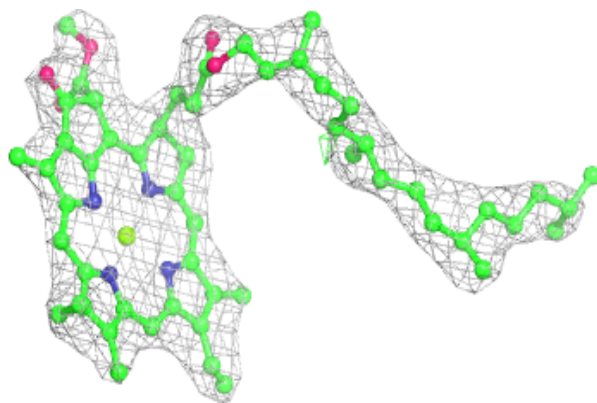
Electron density around CLA c 511:

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



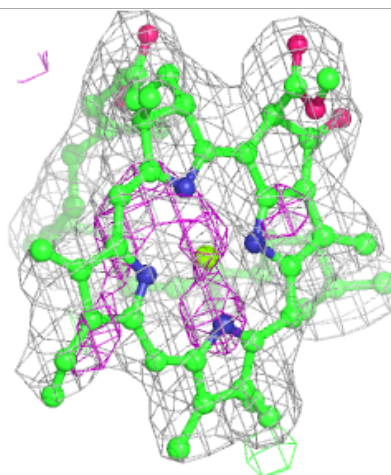
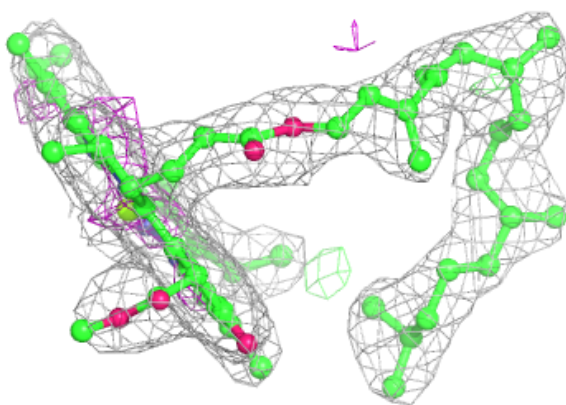
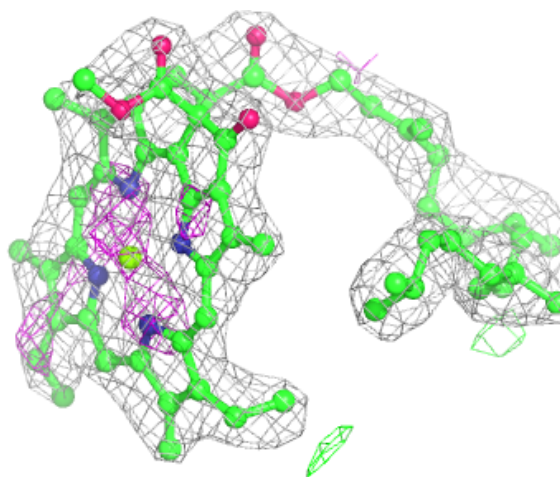
Electron density around CLA c 515:

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



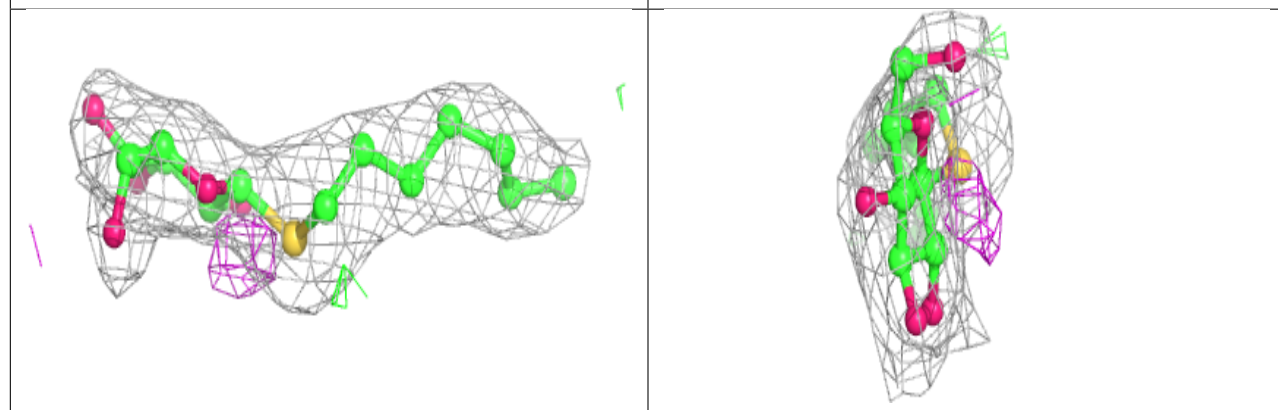
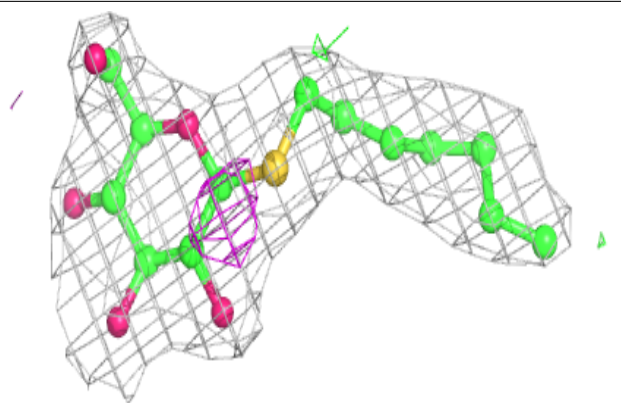
Electron density around CLA C 503:

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

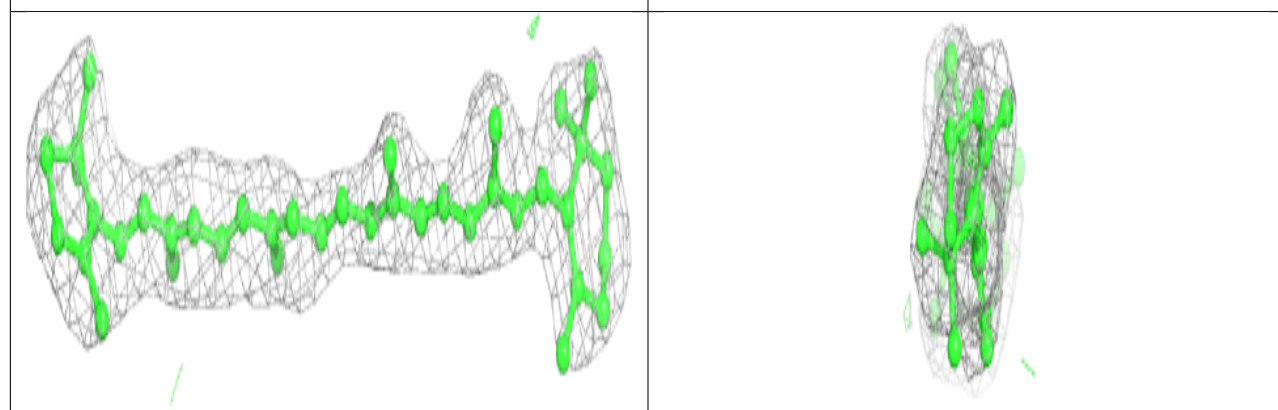
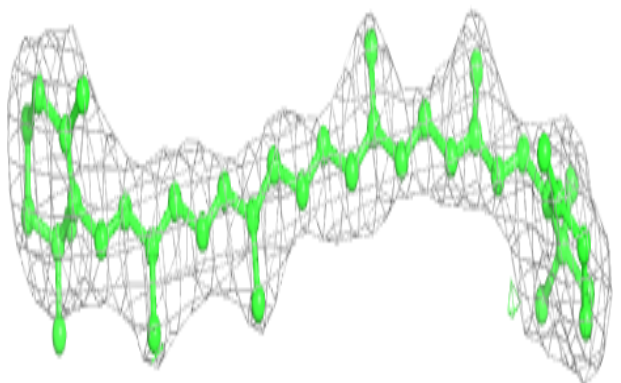


Electron density around HTG B 622:

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

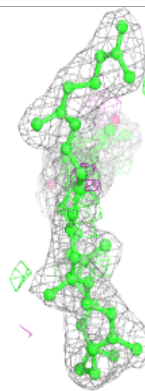
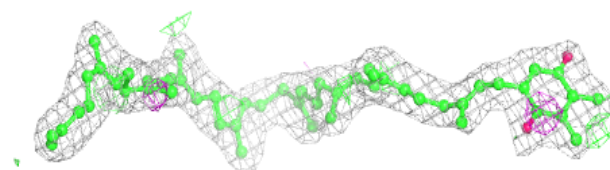
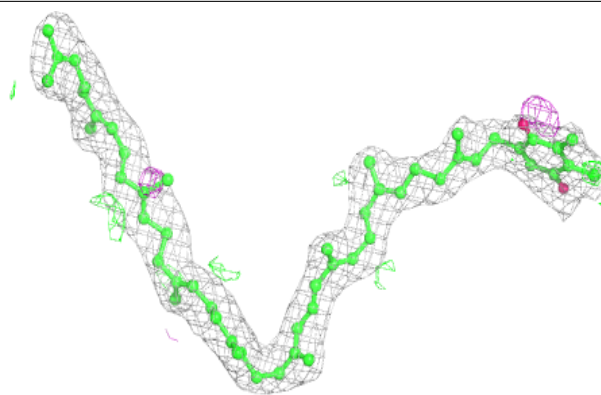
**Electron density around BCR c 526:**

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

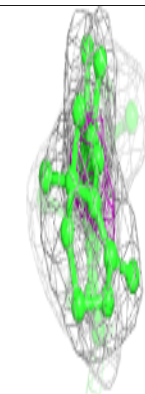
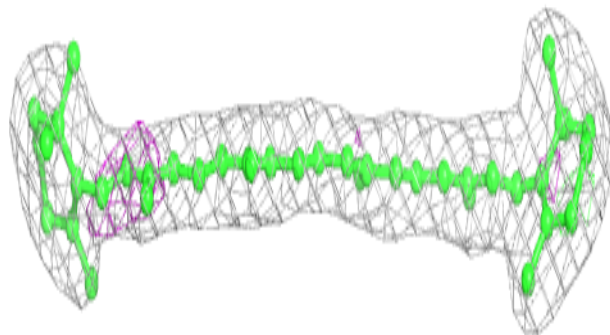
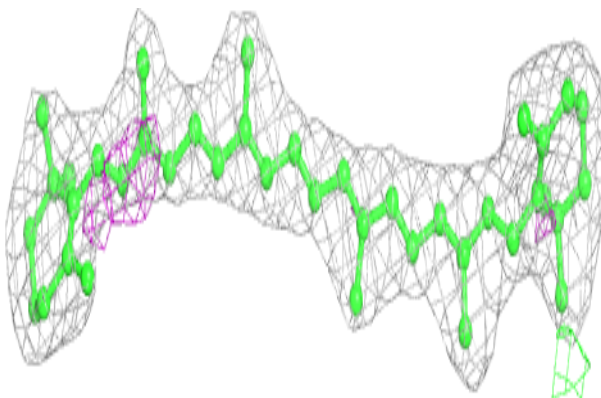


Electron density around PL9 D 407 (A):

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

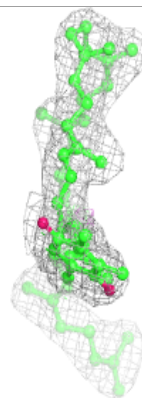
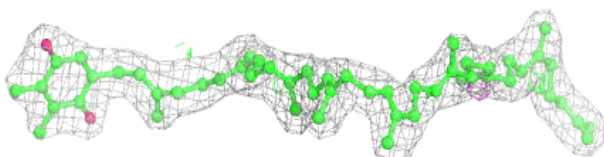
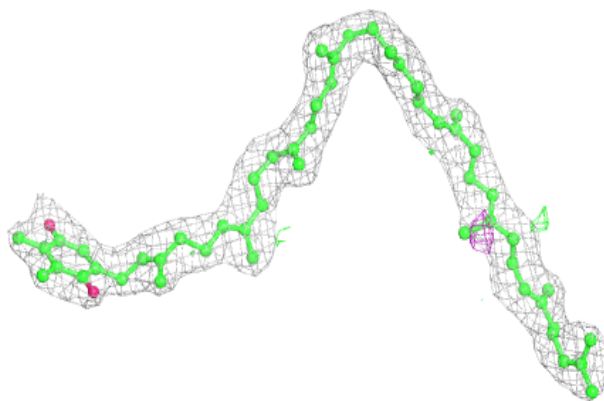
**Electron density around BCR b 627:**

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

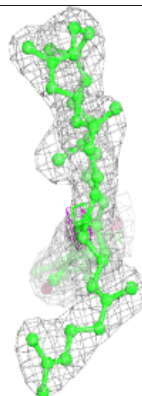
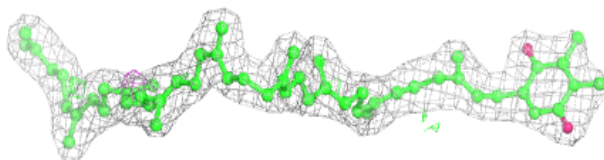
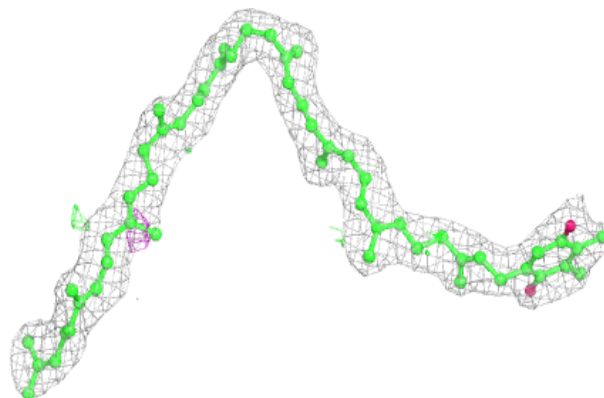


Electron density around PL9 d 407 (A):

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

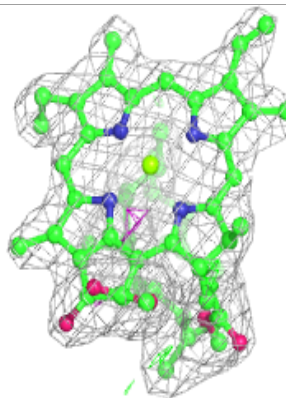
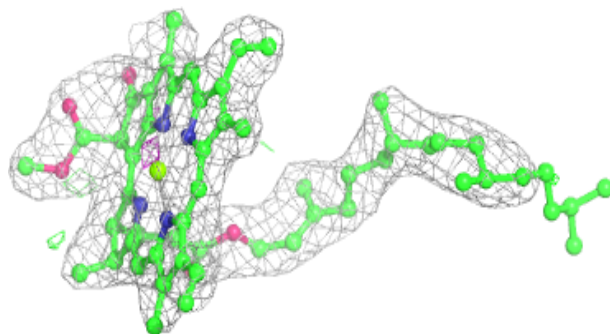
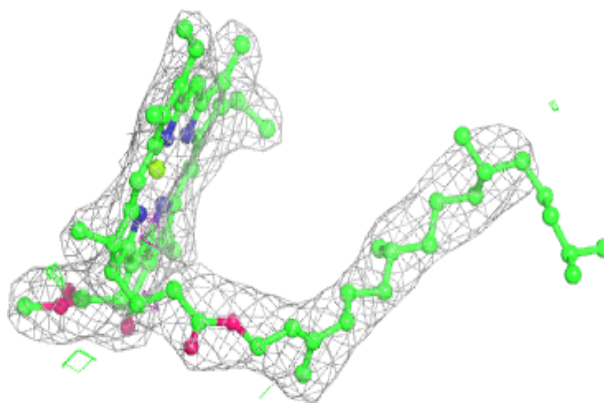
**Electron density around PL9 d 407 (B):**

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



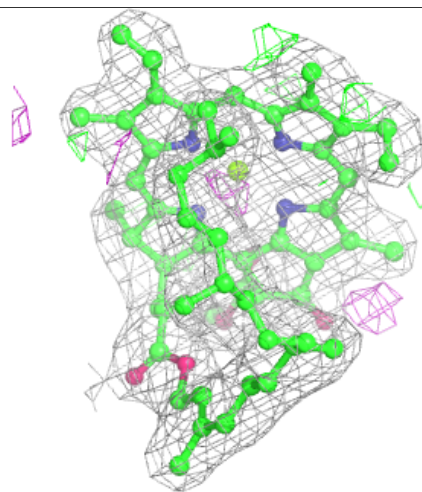
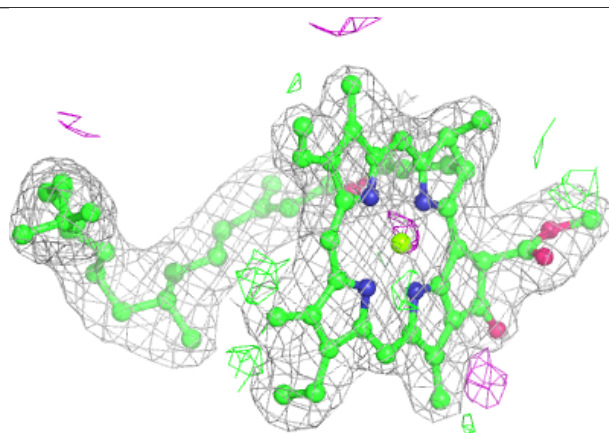
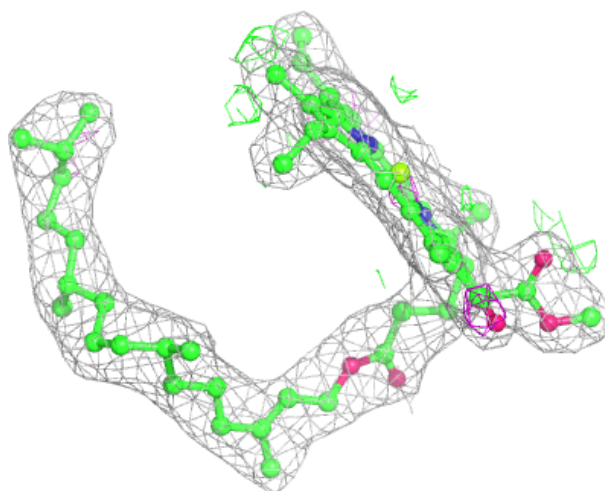
Electron density around CLA C 508:

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



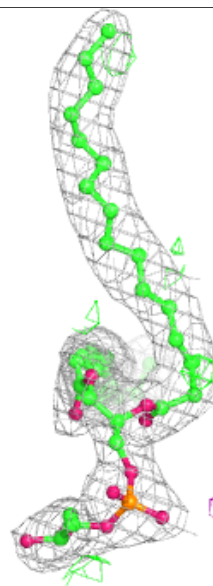
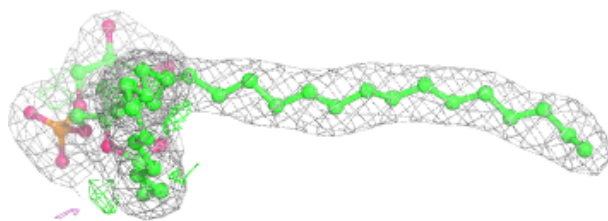
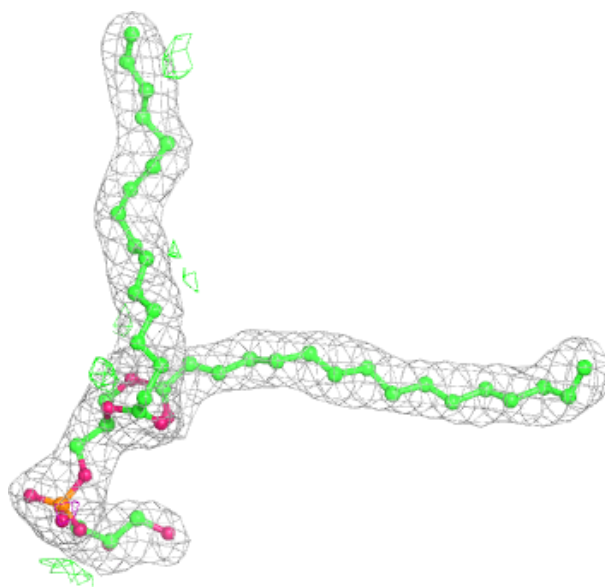
Electron density around CLA B 612:

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



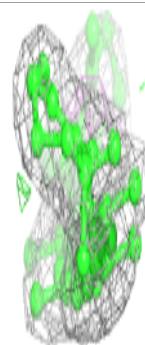
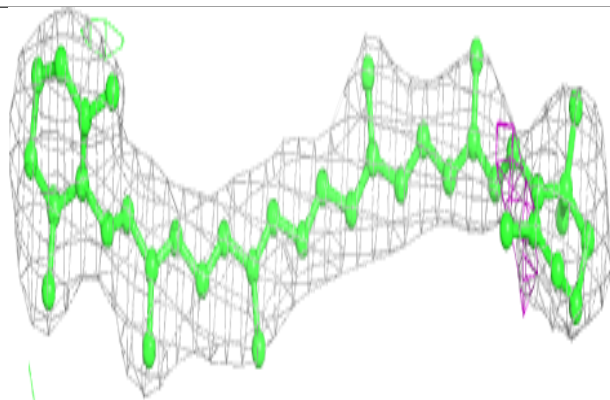
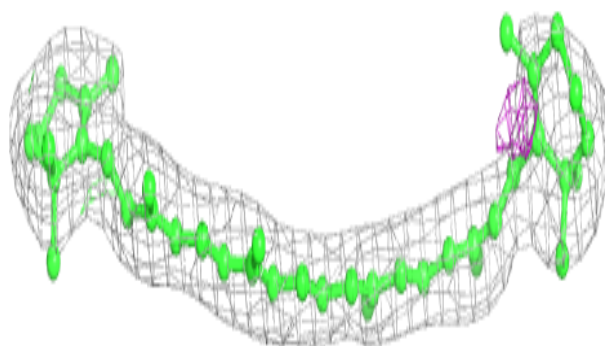
Electron density around LHG L 101:

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



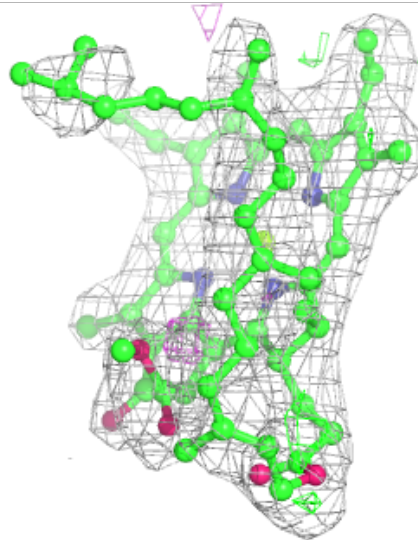
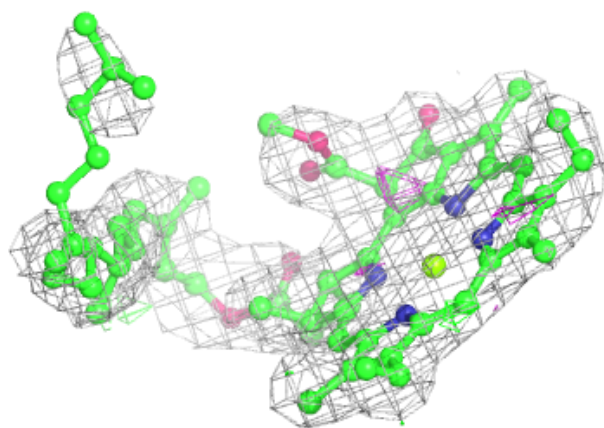
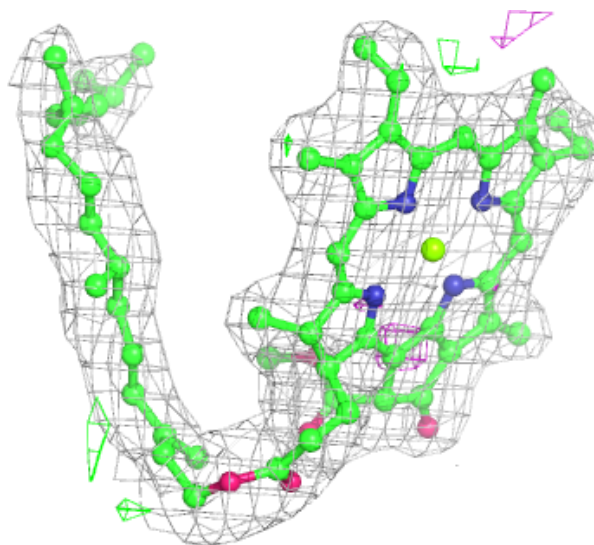
Electron density around BCR D 406:

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



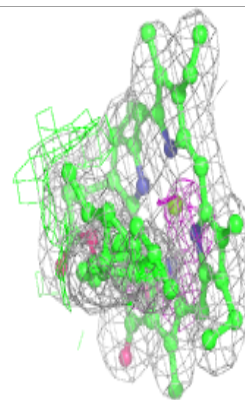
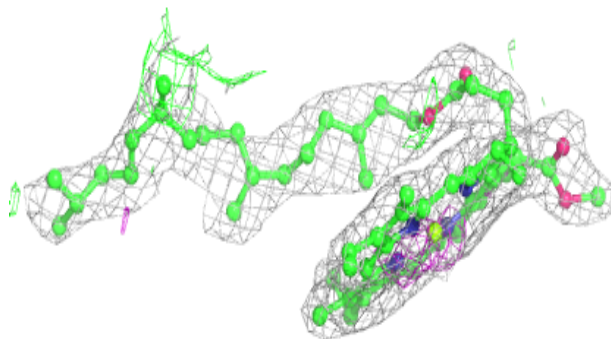
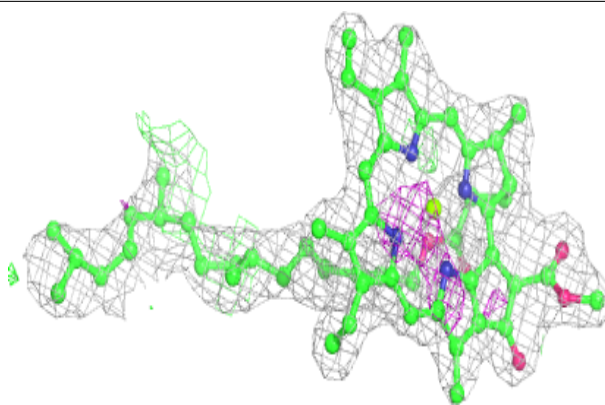
Electron density around CLA b 625:

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

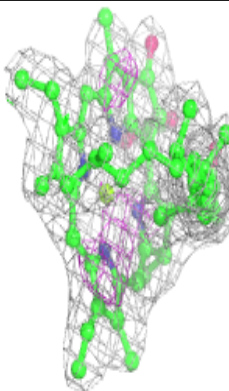
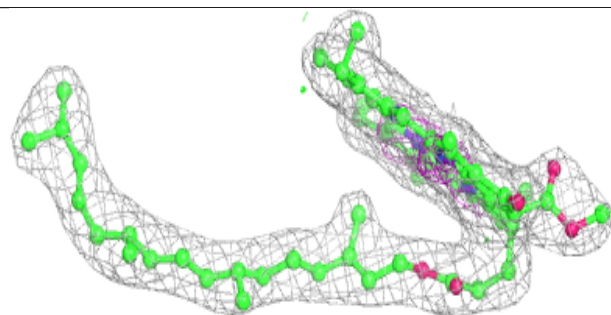
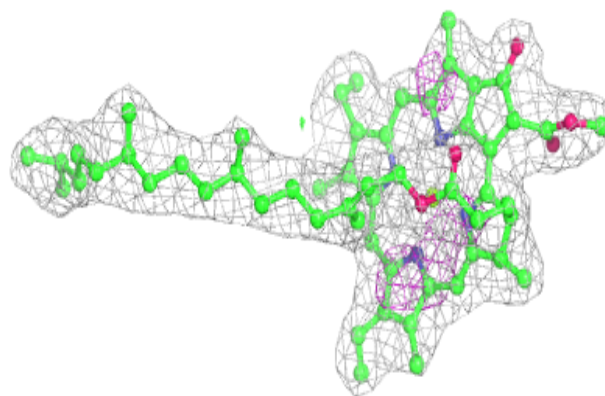


Electron density around CLA b 623:

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

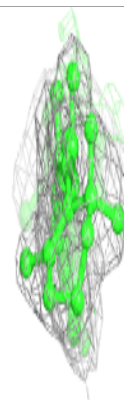
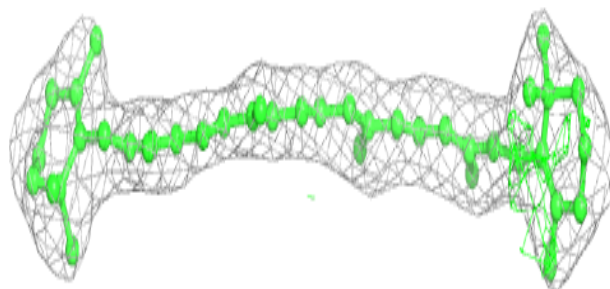
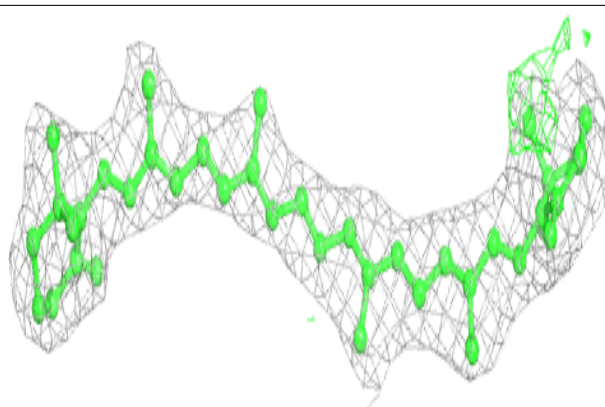
**Electron density around CLA b 617:**

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

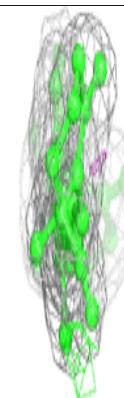
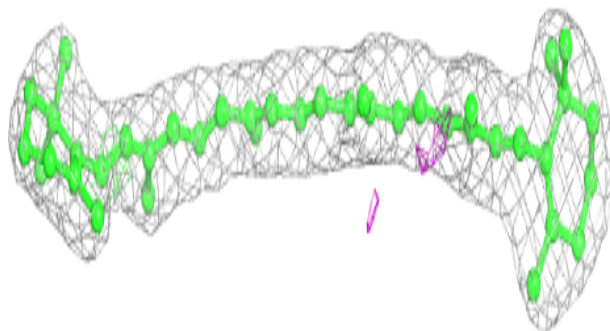
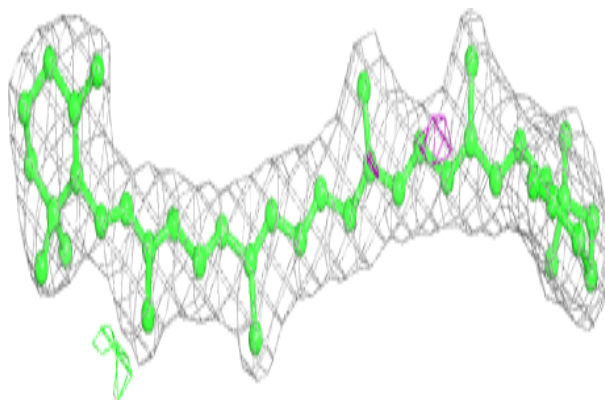


Electron density around BCR y 101:

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

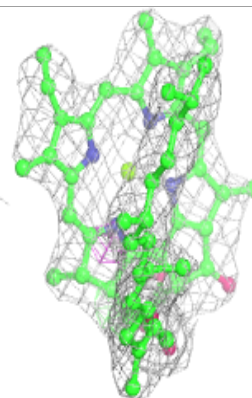
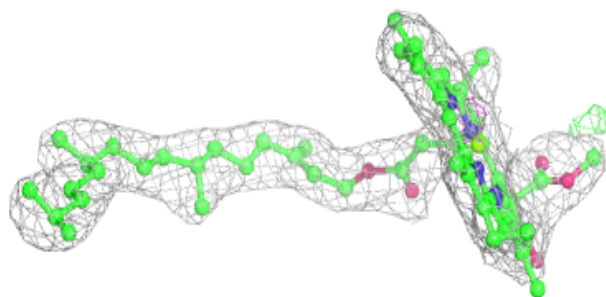
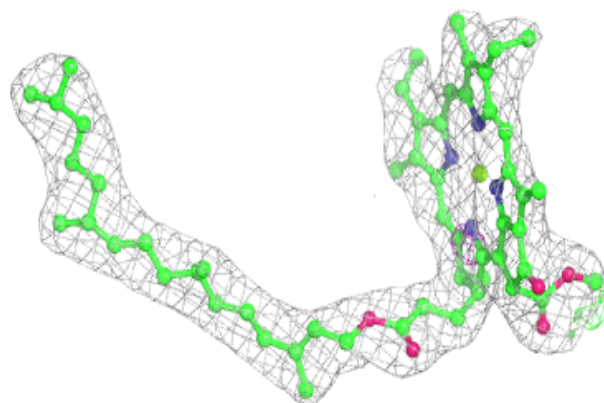
**Electron density around BCR b 626:**

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

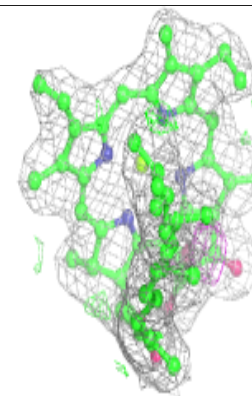
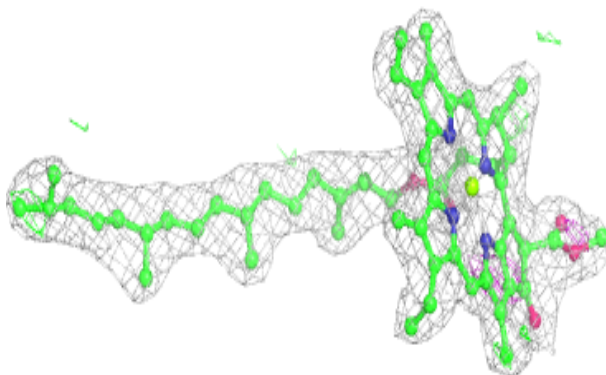
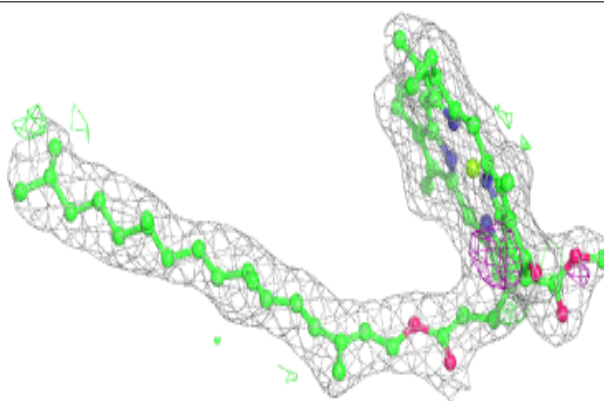


Electron density around CLA B 610:

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

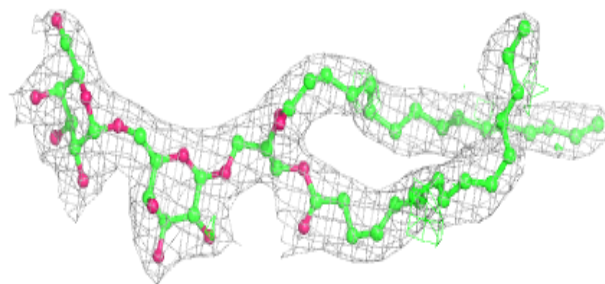
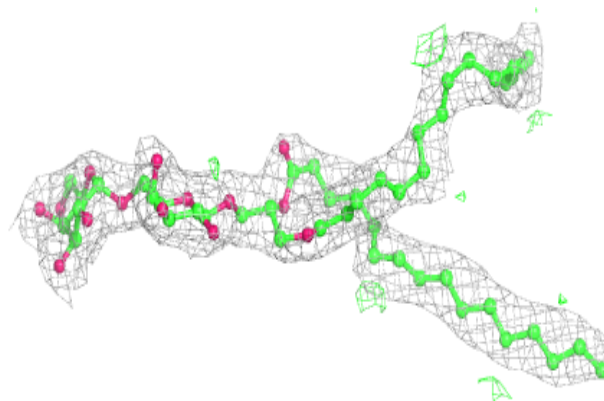
**Electron density around CLA B 608:**

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



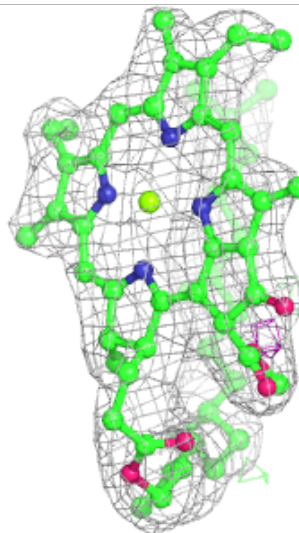
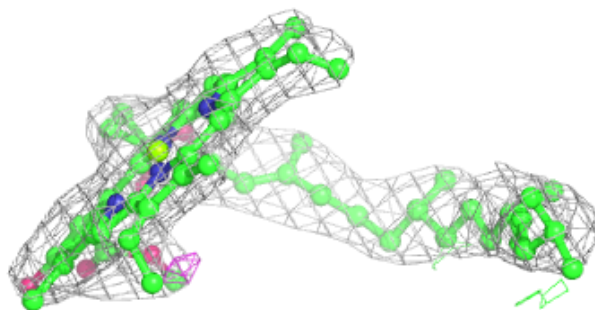
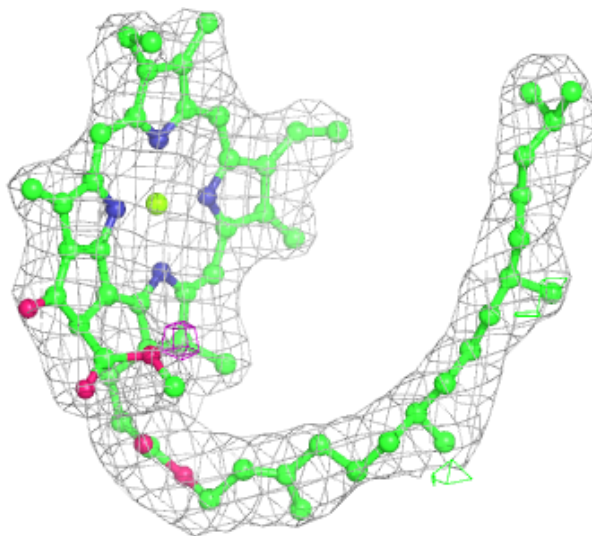
Electron density around DGD C 516:

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



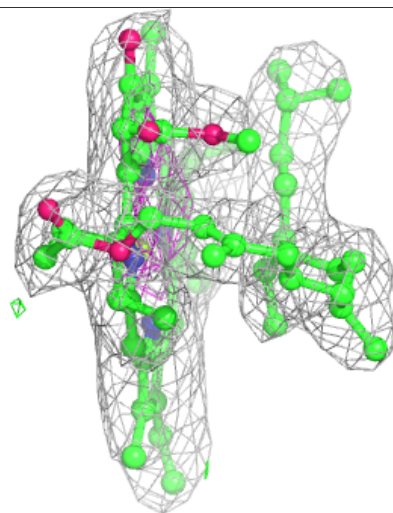
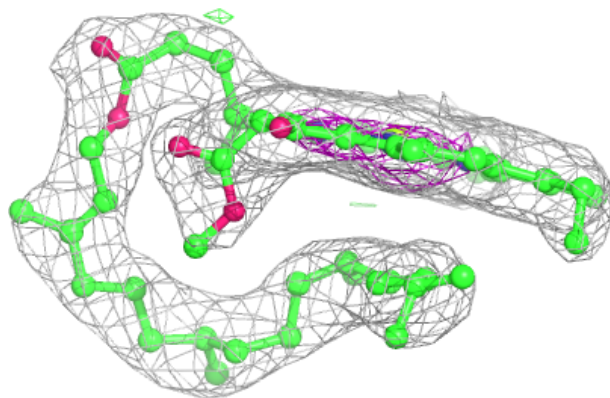
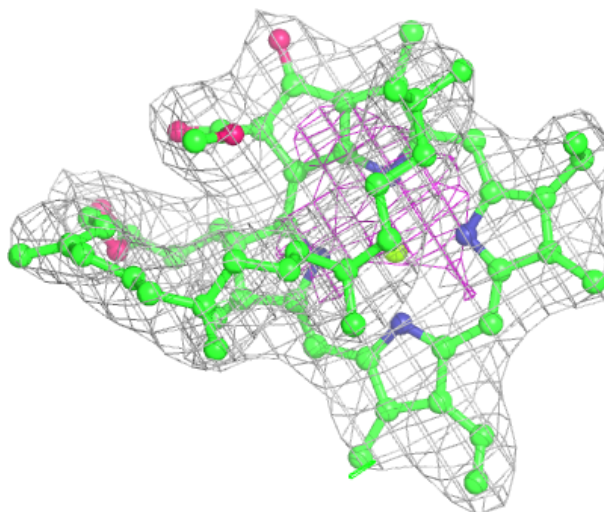
Electron density around CLA C 507:

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



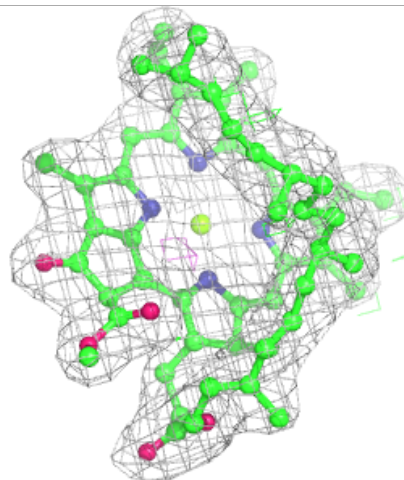
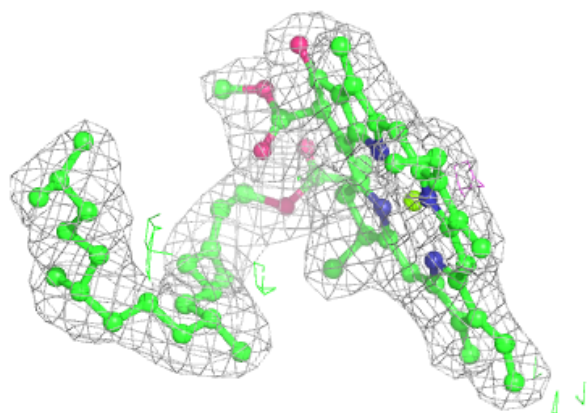
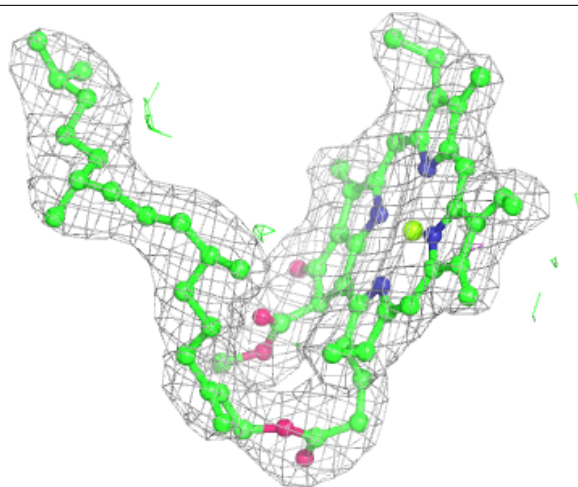
Electron density around CLA c 514:

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



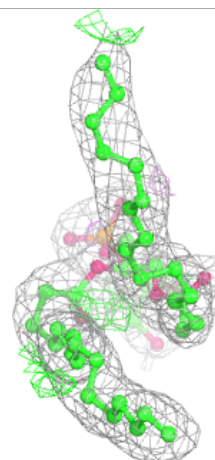
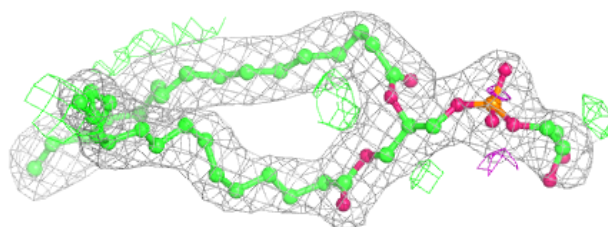
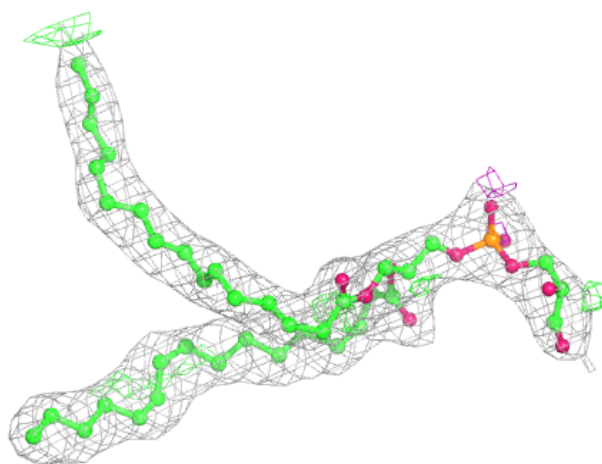
Electron density around CLA b 622:

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



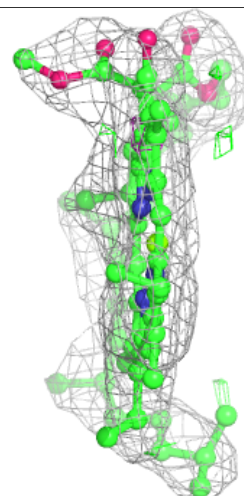
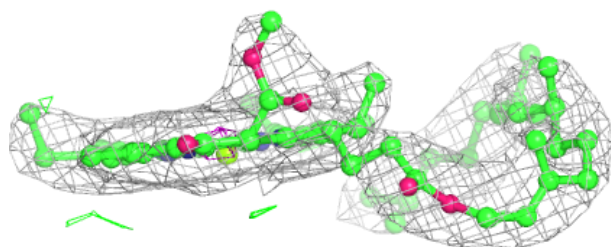
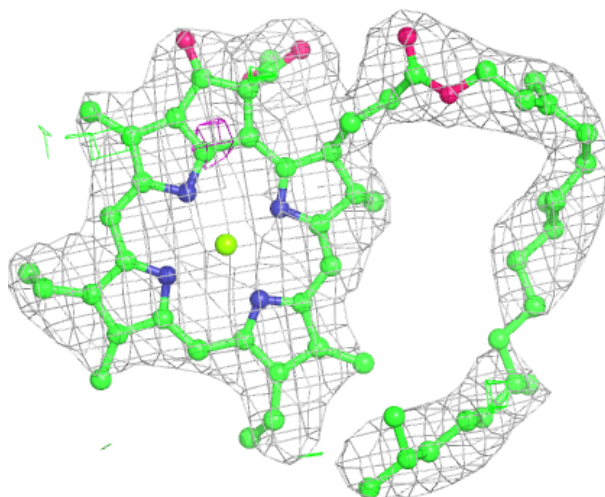
Electron density around LHG D 410:

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



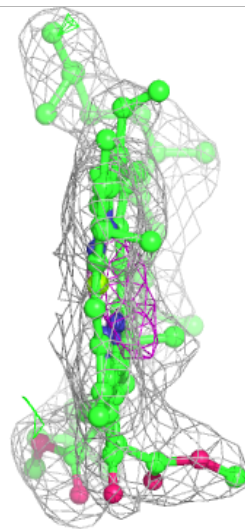
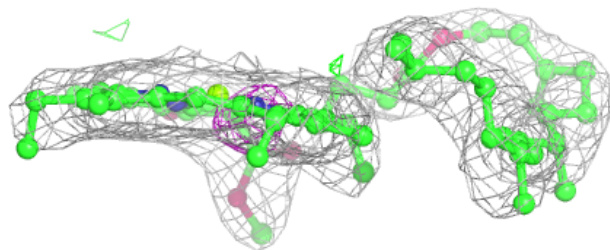
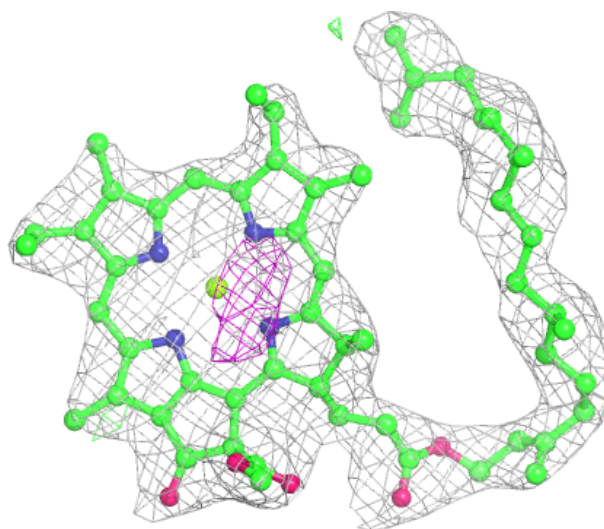
Electron density around CLA C 512:

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



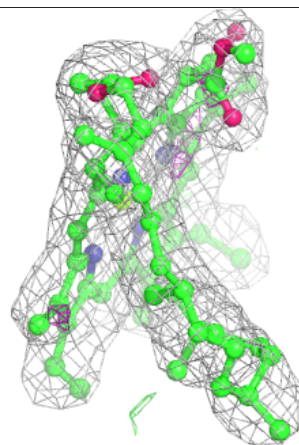
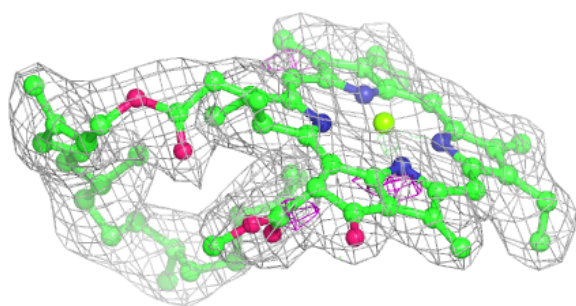
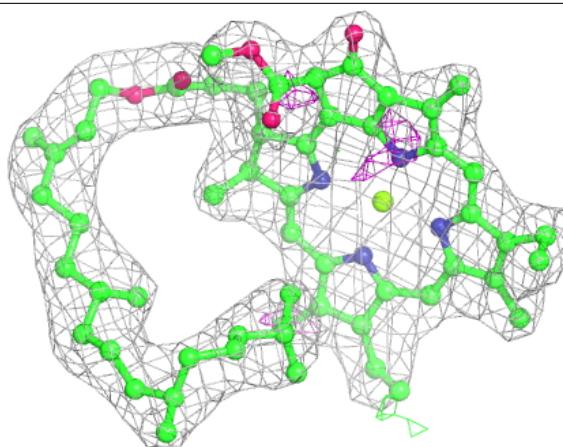
Electron density around CLA c 516:

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



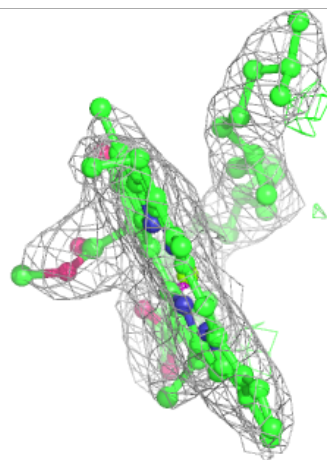
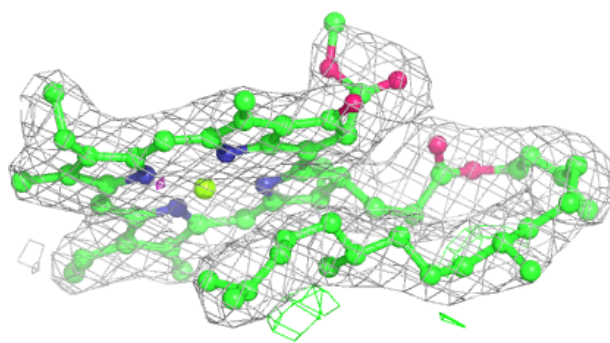
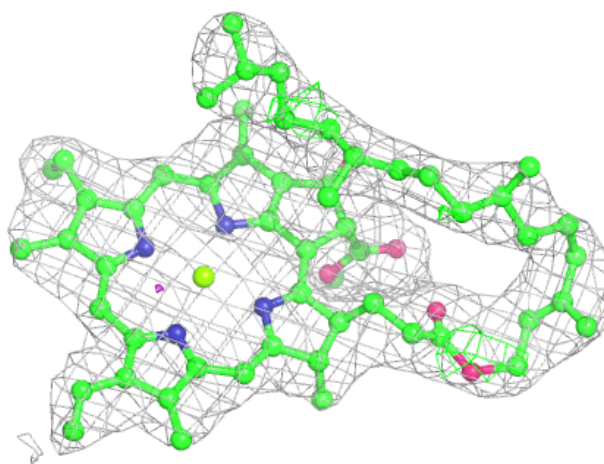
Electron density around CLA B 616:

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



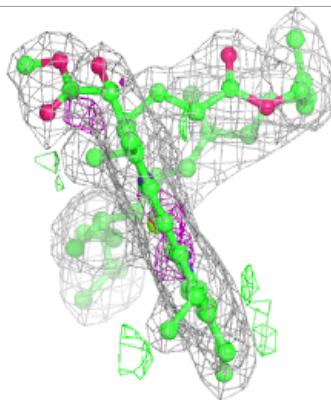
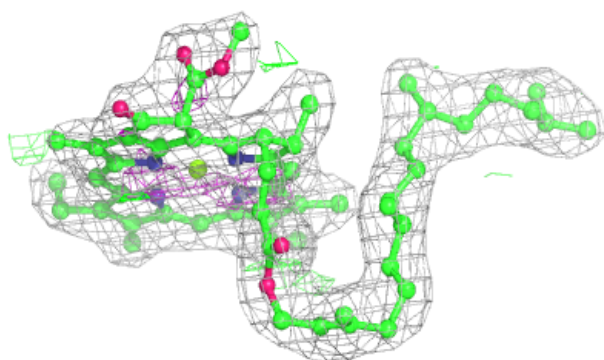
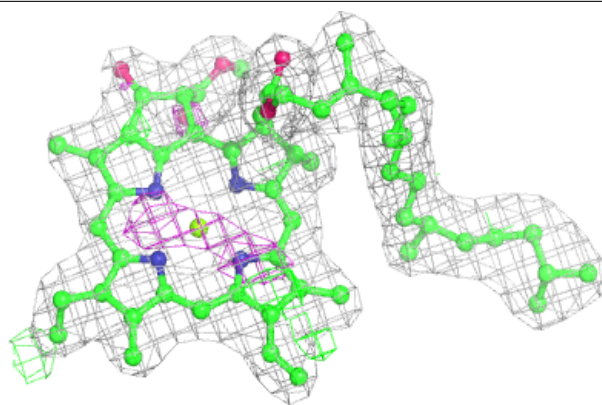
Electron density around CLA C 509:

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

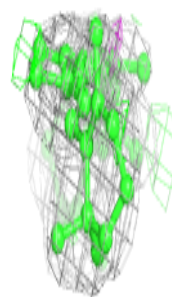
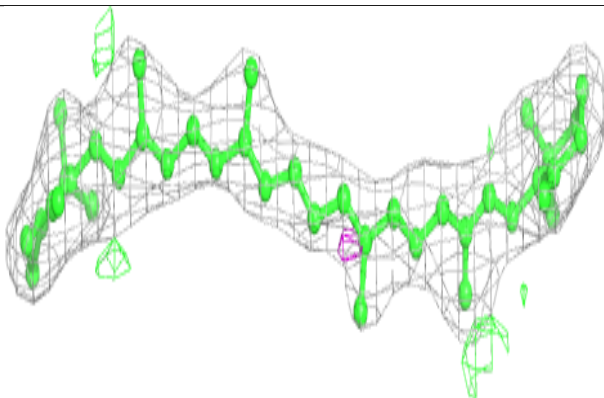
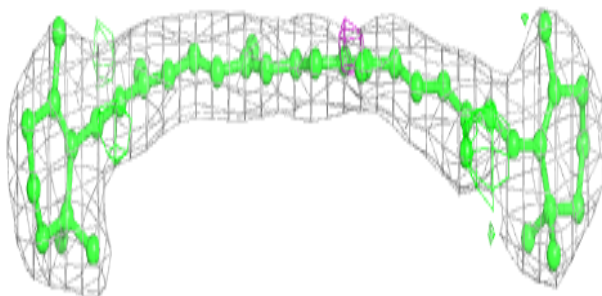


Electron density around CLA d 403:

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

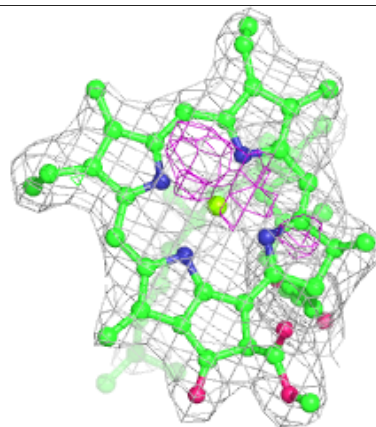
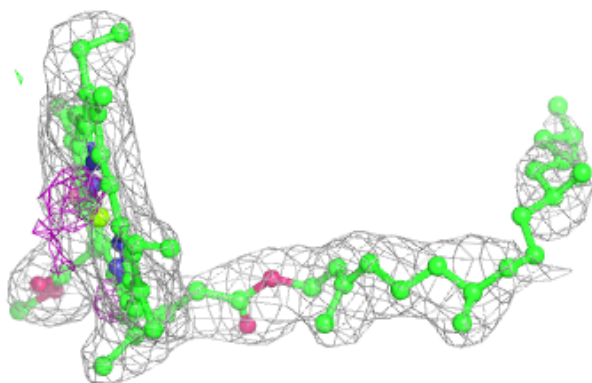
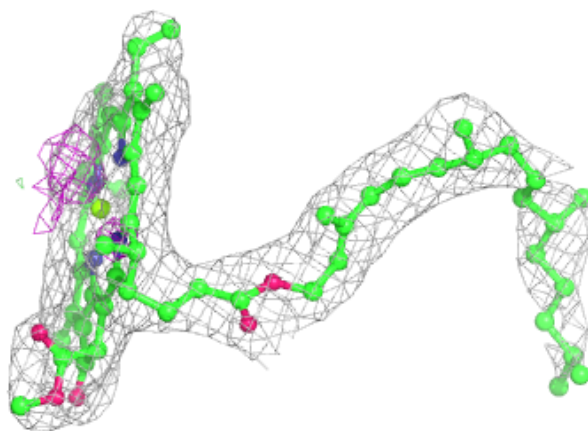
**Electron density around BCR K 101:**

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

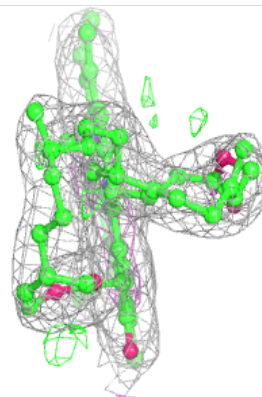
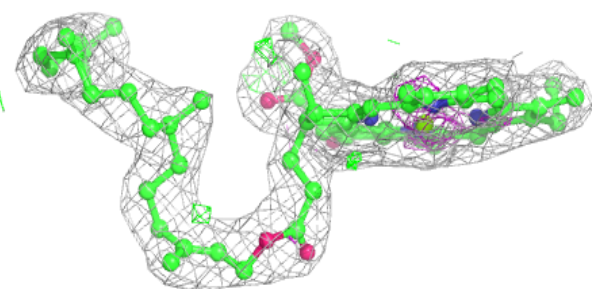
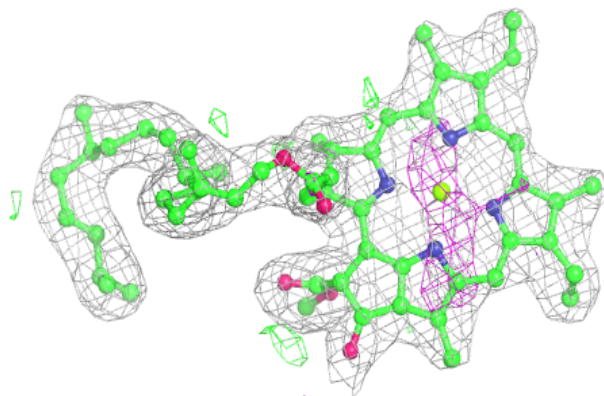


Electron density around CLA D 405:

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

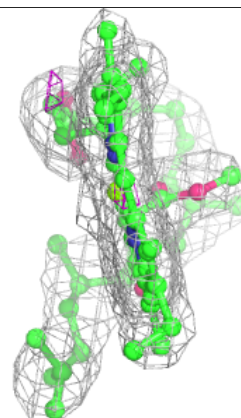
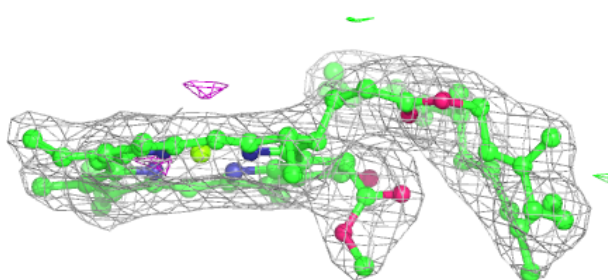
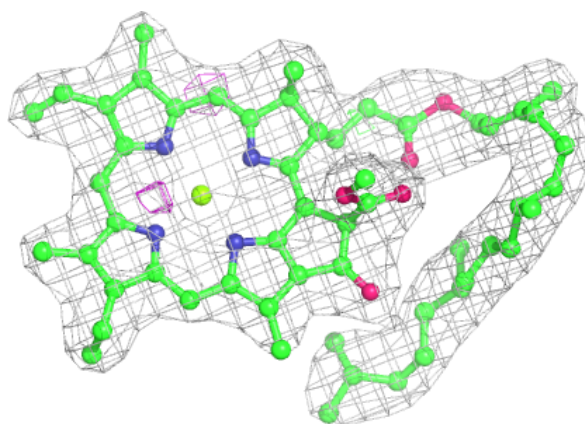
**Electron density around CLA B 613:**

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

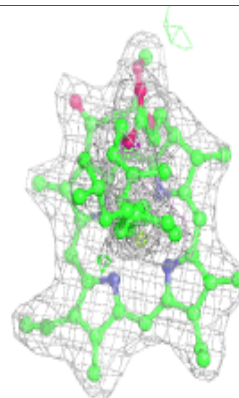
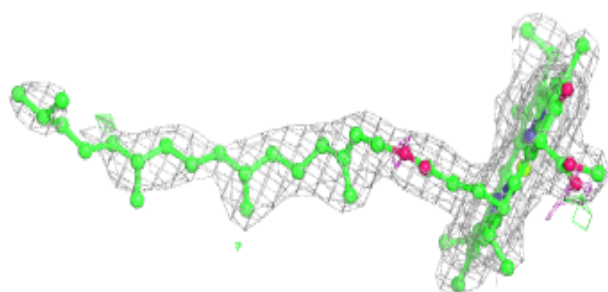
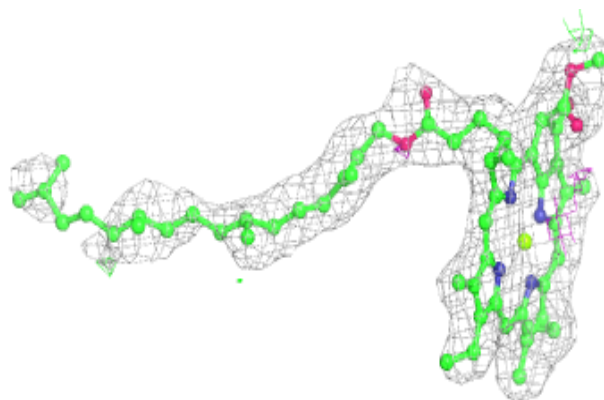


Electron density around CLA b 619:

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

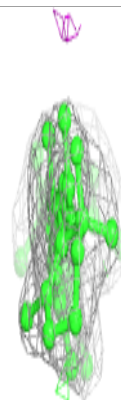
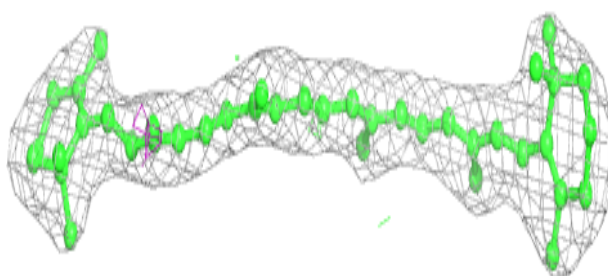
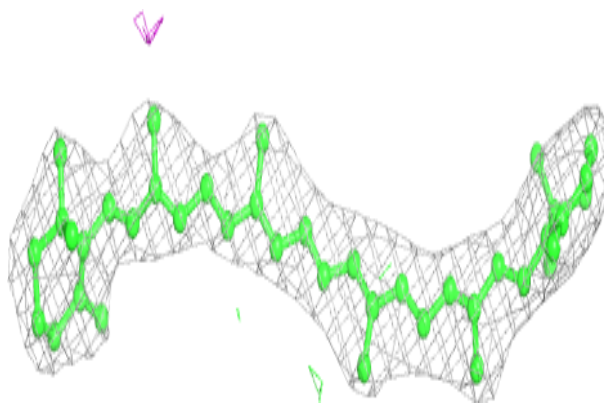
**Electron density around CLA d 405:**

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

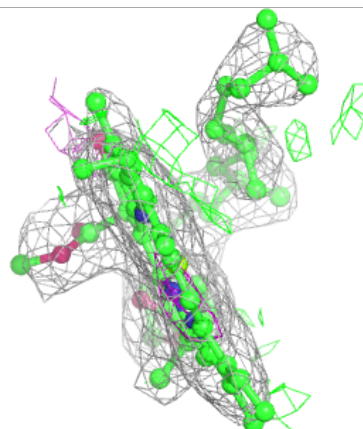
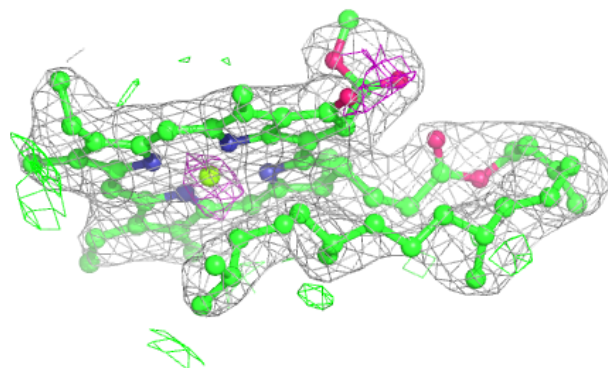
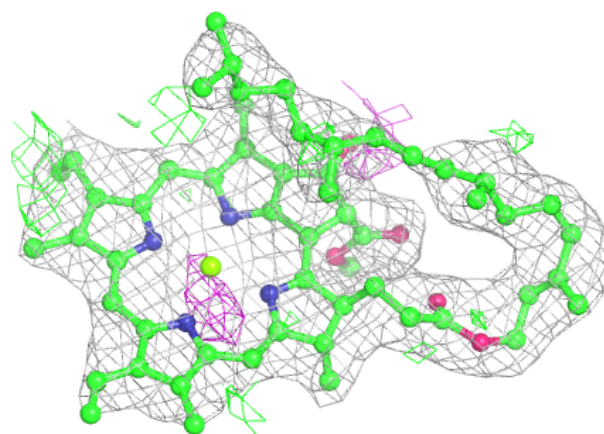


Electron density around BCR Y 101:

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

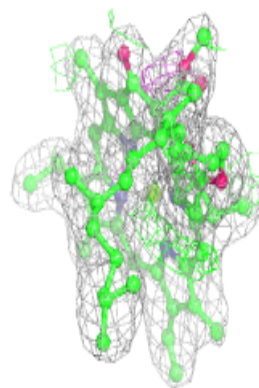
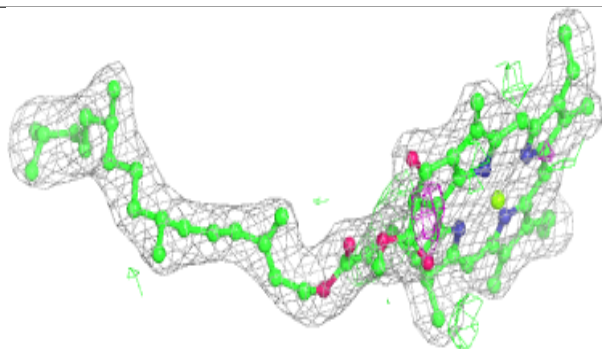
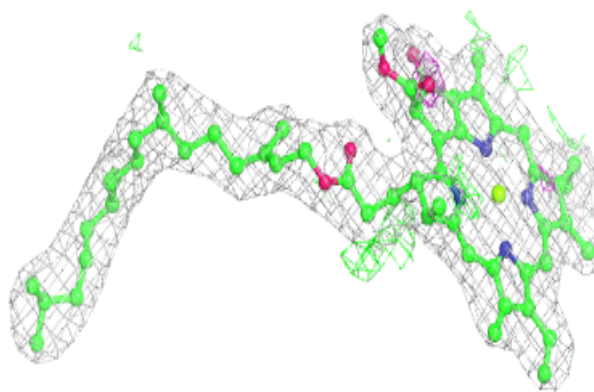
**Electron density around CLA c 513:**

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



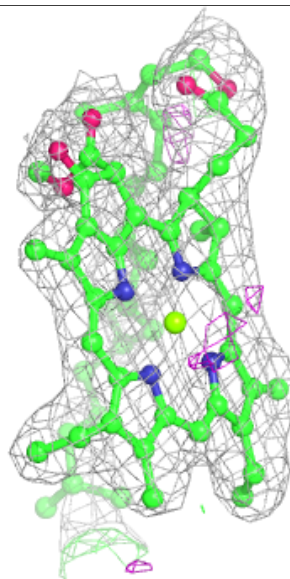
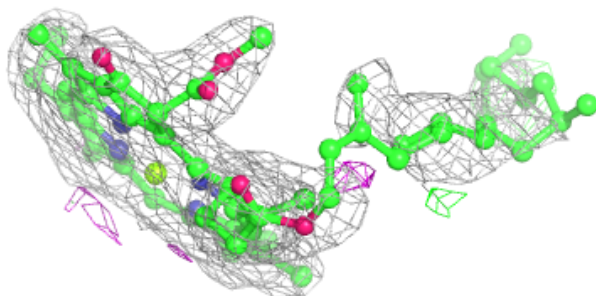
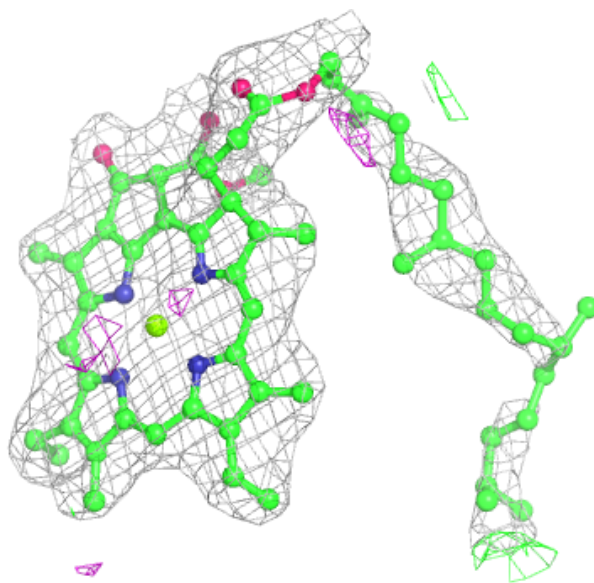
Electron density around CLA A 405:

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



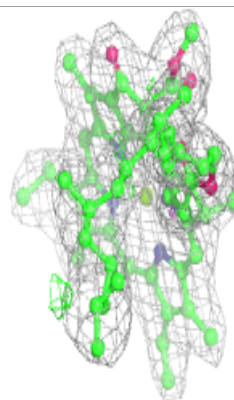
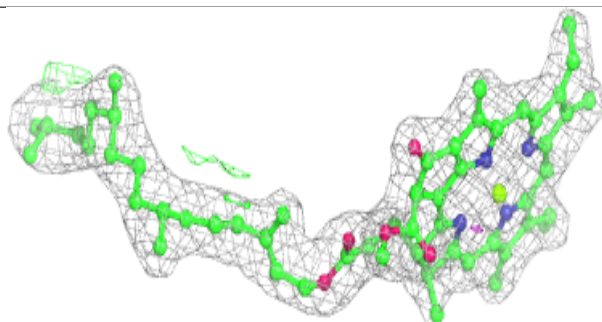
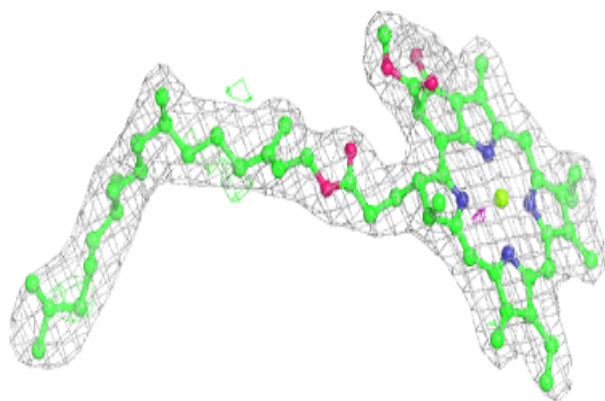
Electron density around CLA B 617:

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

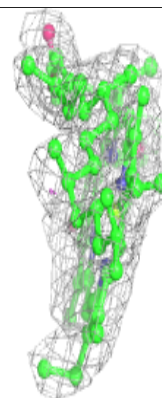
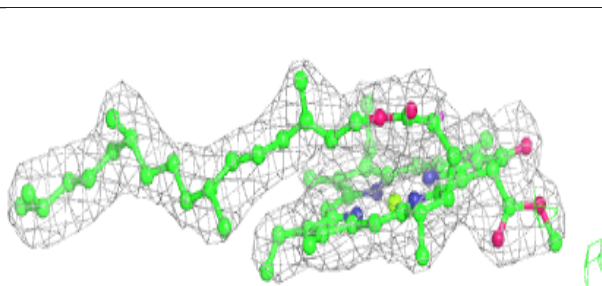
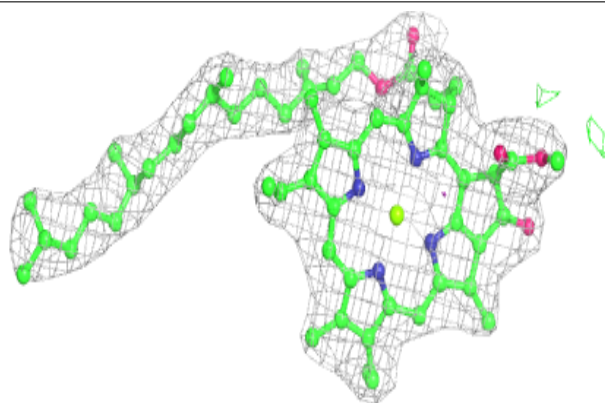


Electron density around CLA a 409:

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

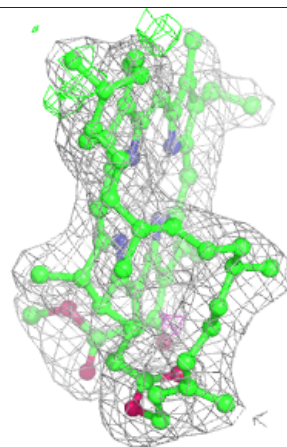
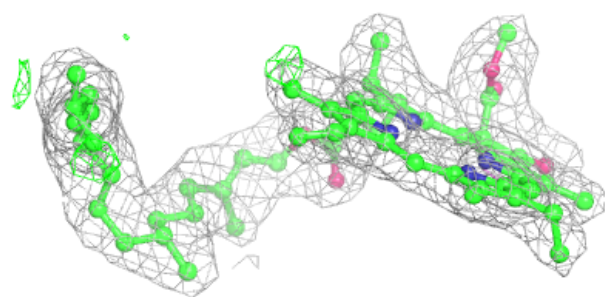
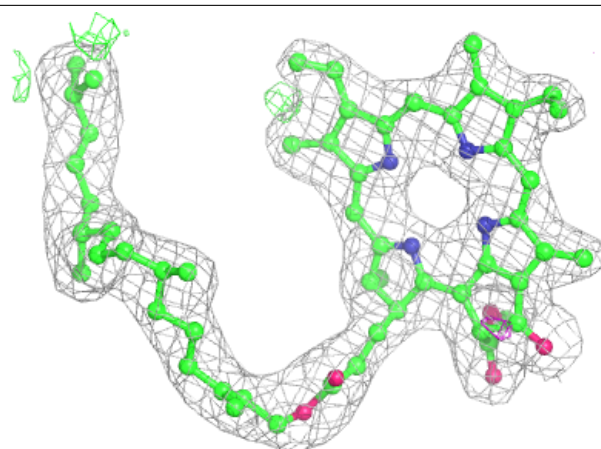
**Electron density around CLA c 505:**

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



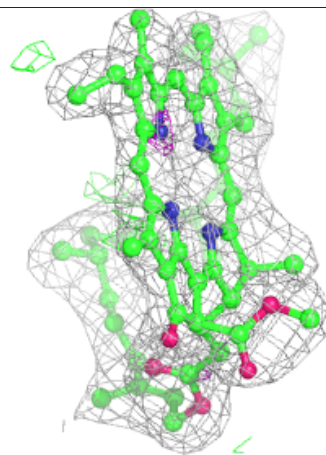
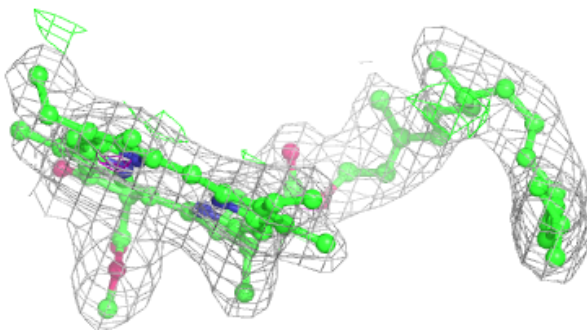
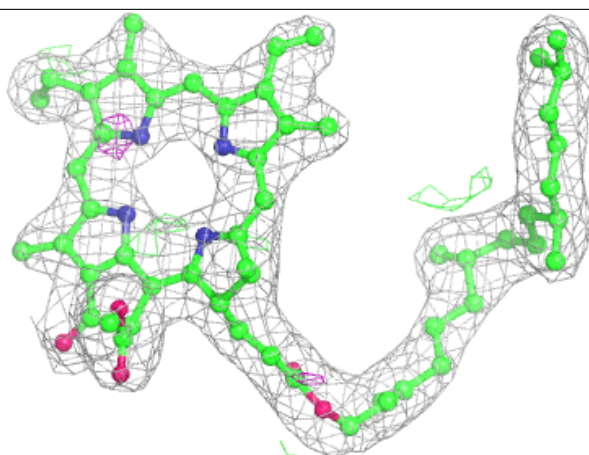
Electron density around PHO D 401 (B):

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



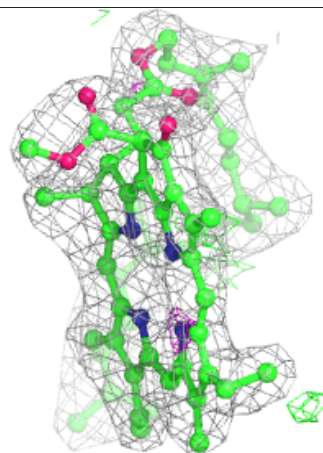
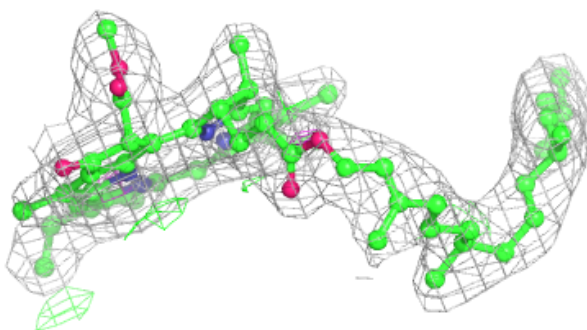
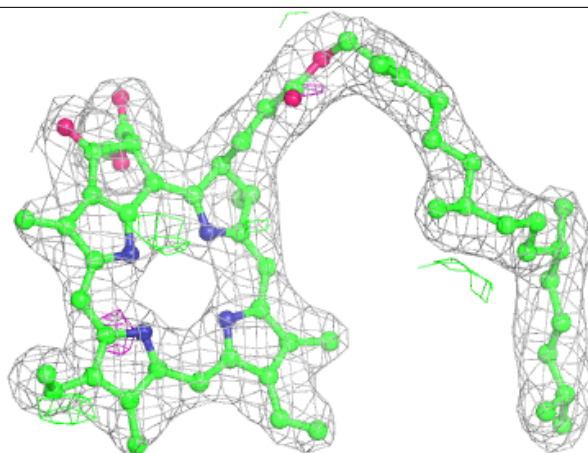
Electron density around PHO d 402 (B):

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

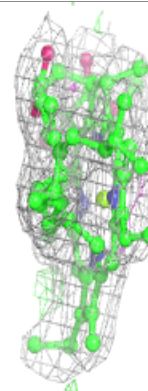
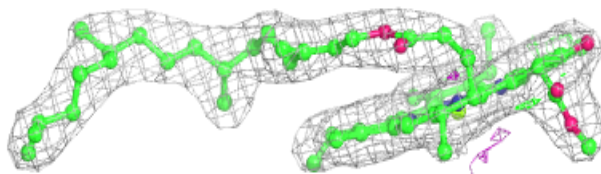
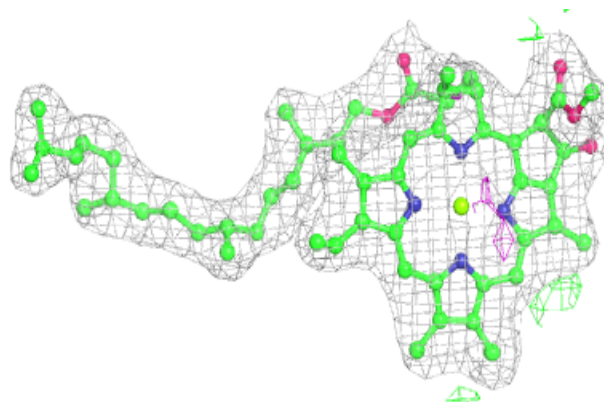


Electron density around PHO d 402 (A):

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

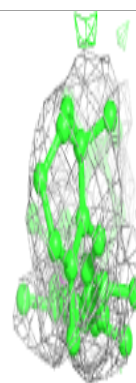
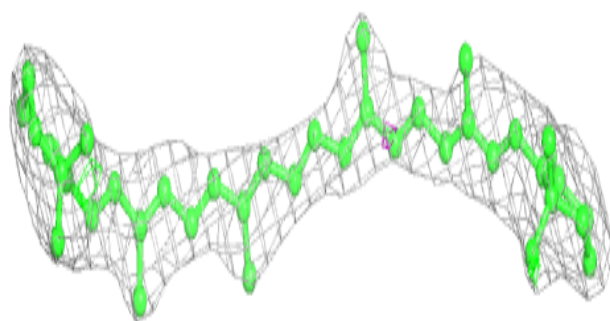
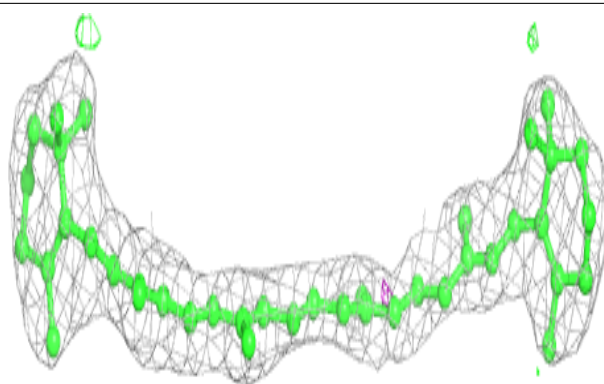
**Electron density around CLA B 604:**

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

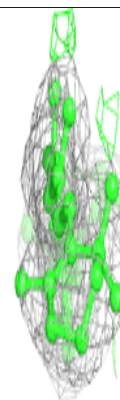
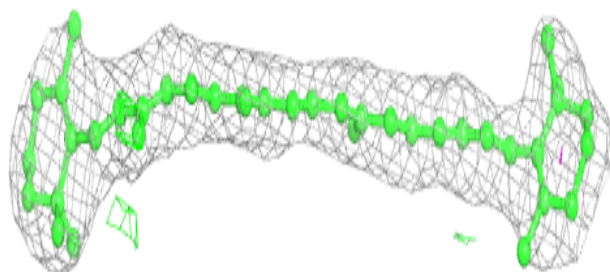
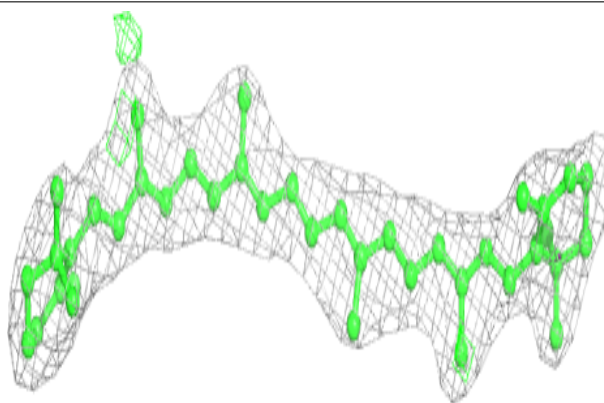


Electron density around BCR k 102:

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

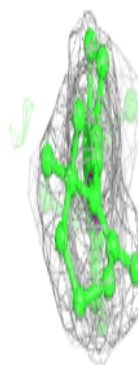
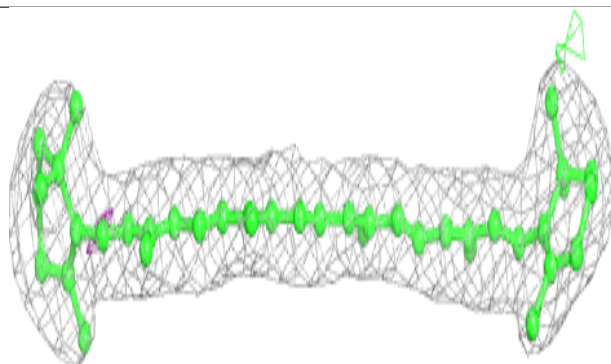
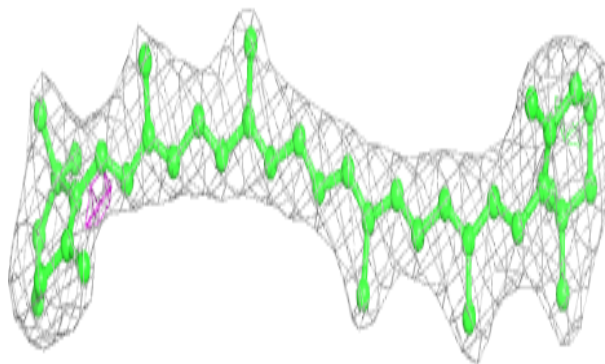
**Electron density around BCR h 101:**

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

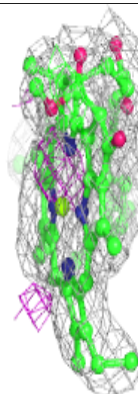
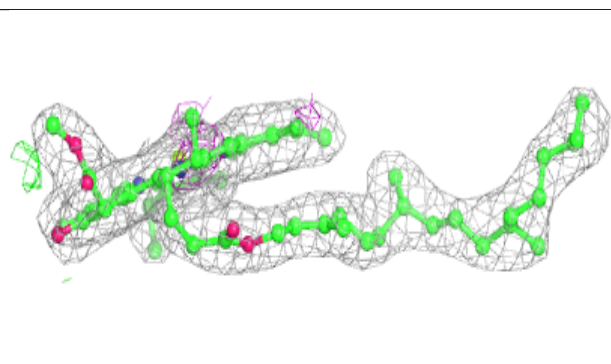
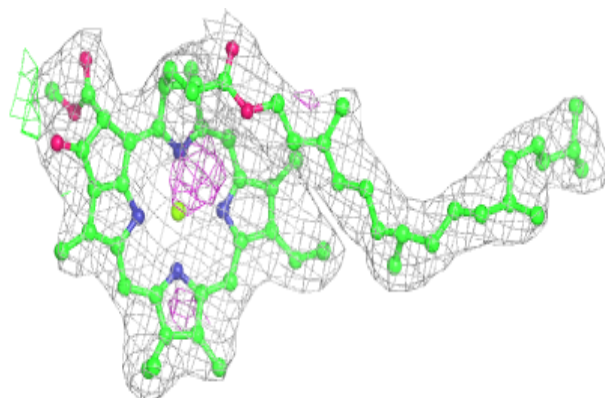


Electron density around BCR B 619:

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

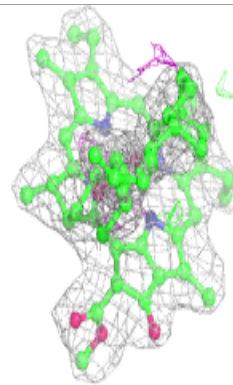
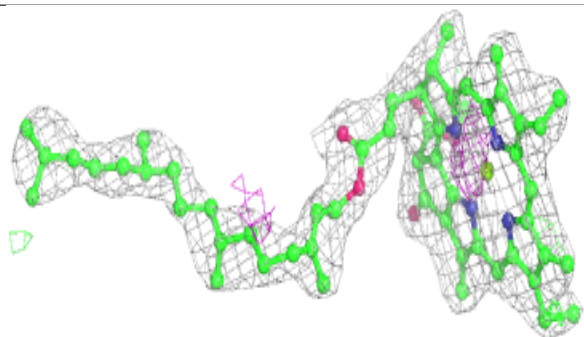
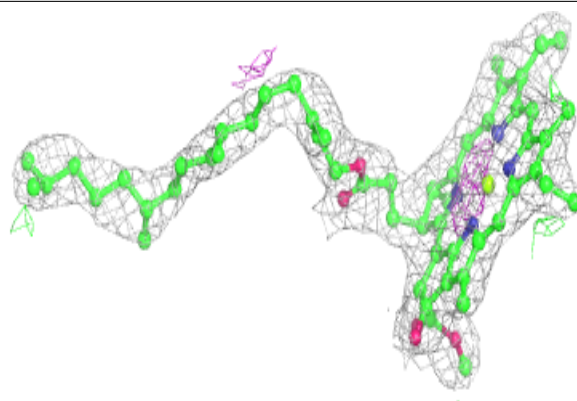
**Electron density around CLA b 612:**

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

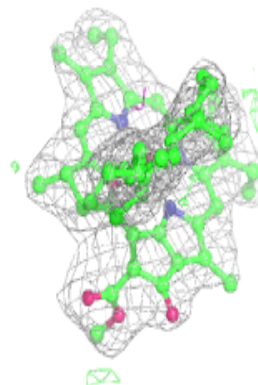
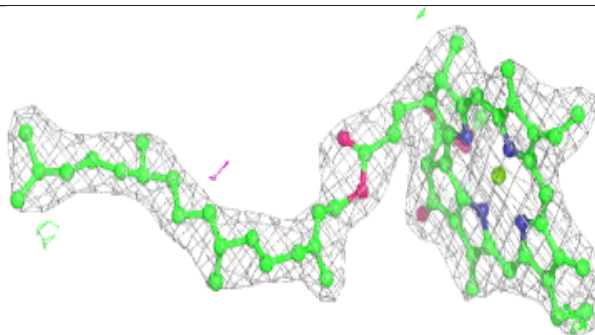
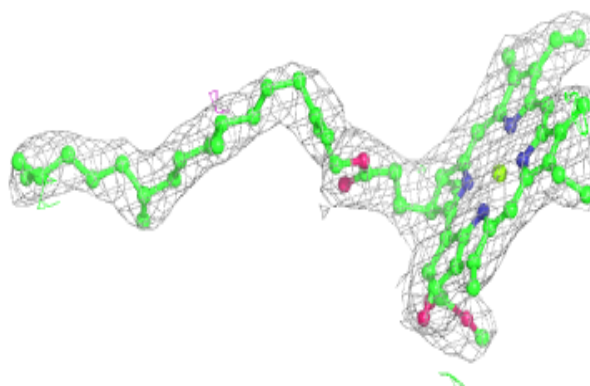


Electron density around CLA c 506:

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

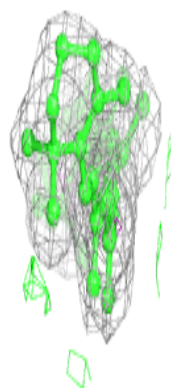
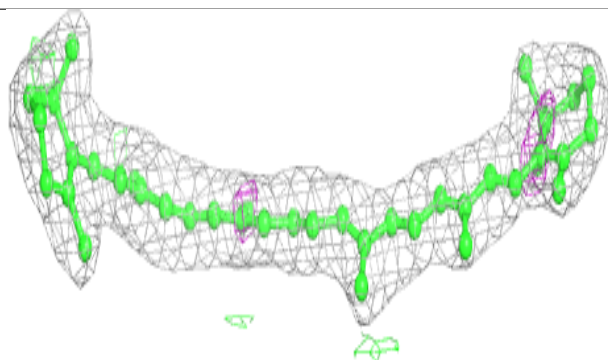
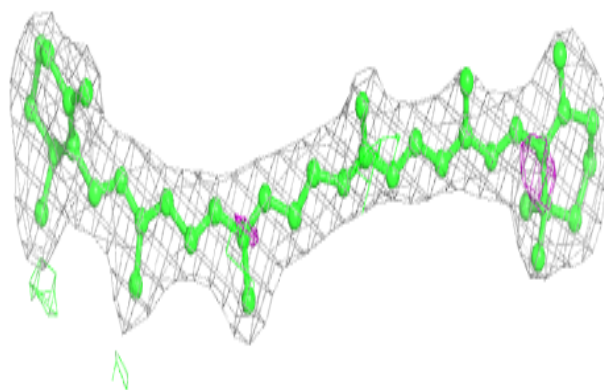
**Electron density around CLA C 502:**

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

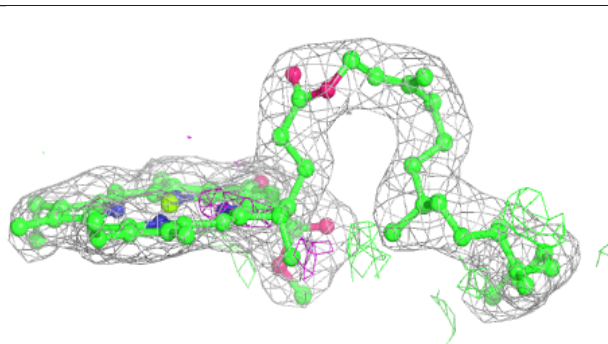
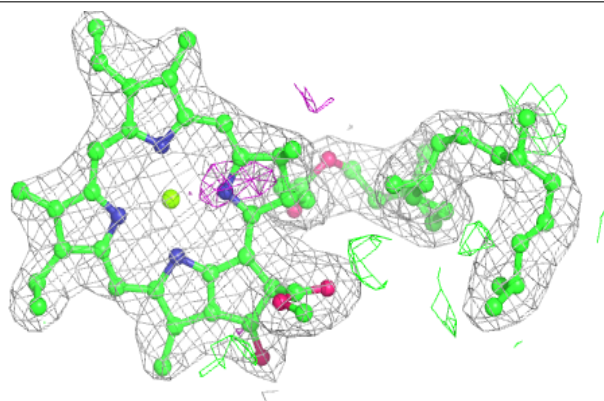


Electron density around BCR T 103:

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

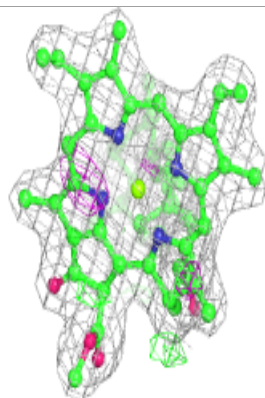
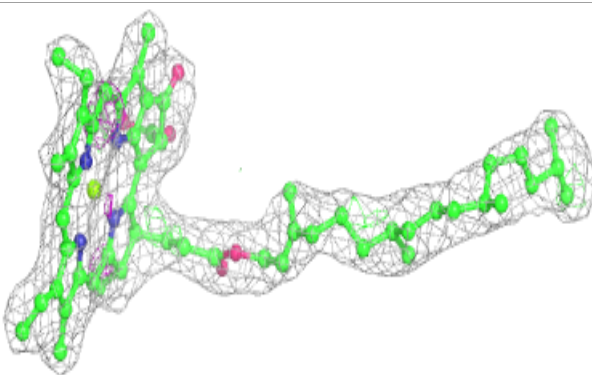
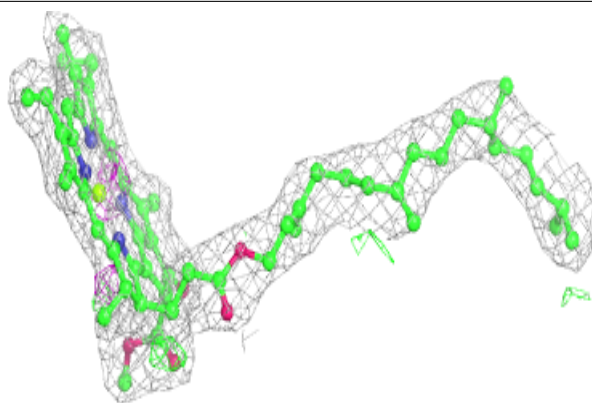
**Electron density around CLA b 621:**

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

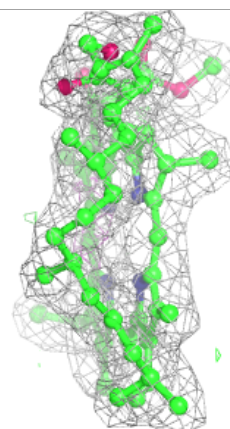
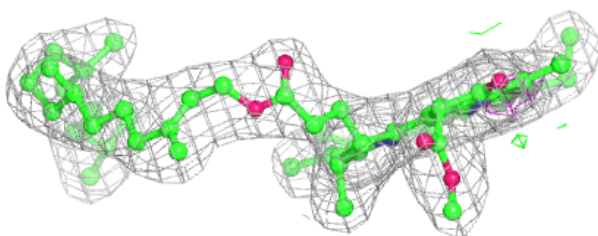
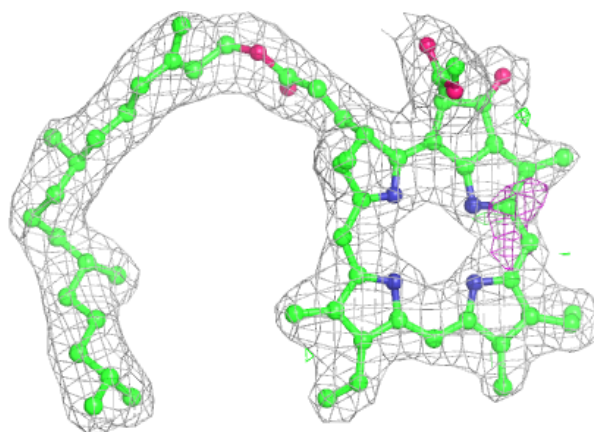


Electron density around CLA B 605:

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

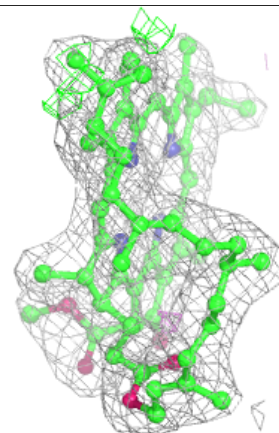
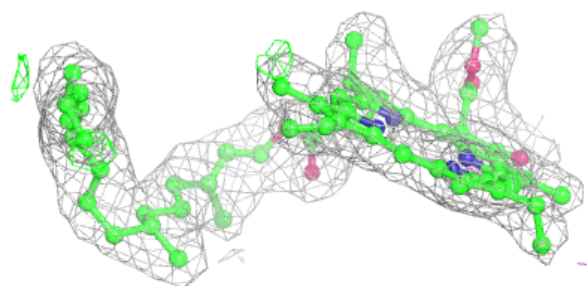
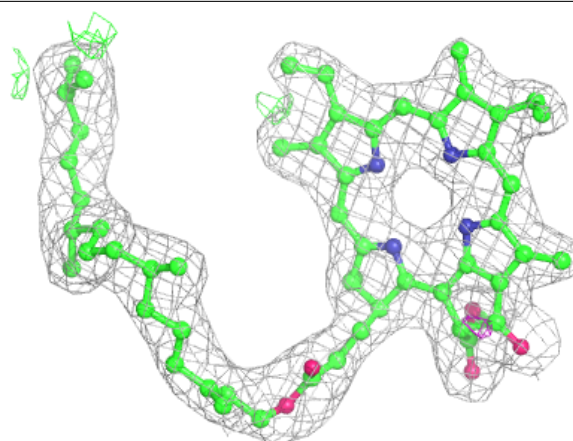
**Electron density around PHO A 408:**

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

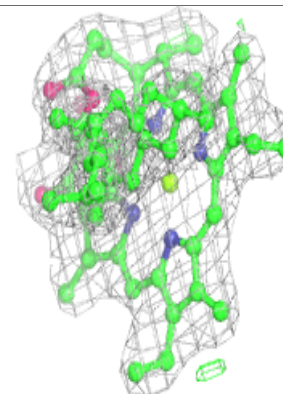
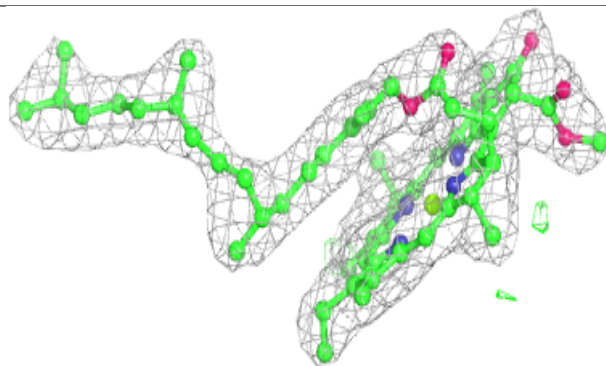
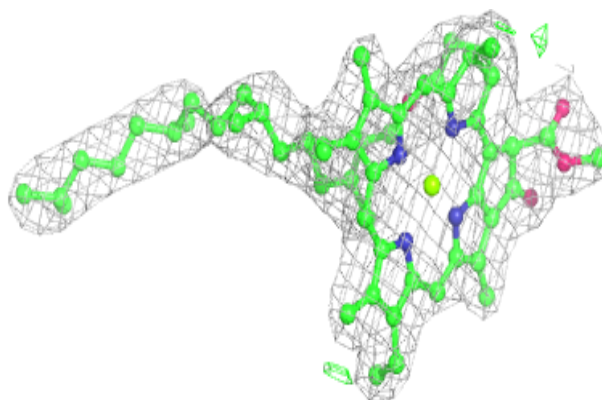


Electron density around PHO D 401 (A):

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

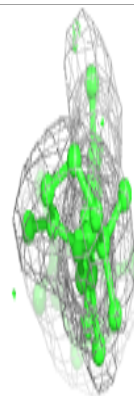
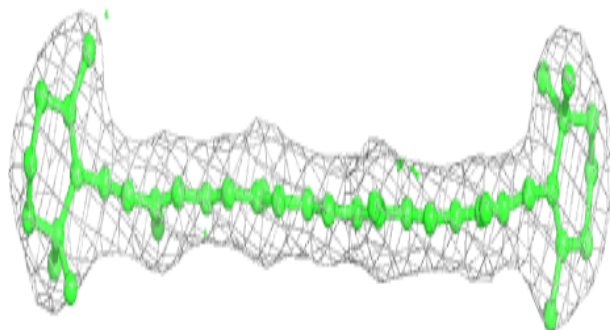
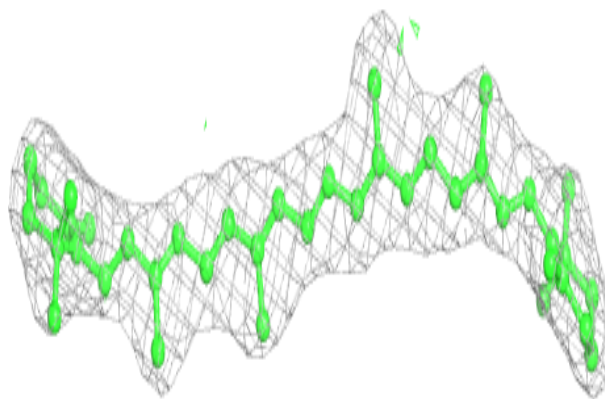
**Electron density around CLA C 505:**

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

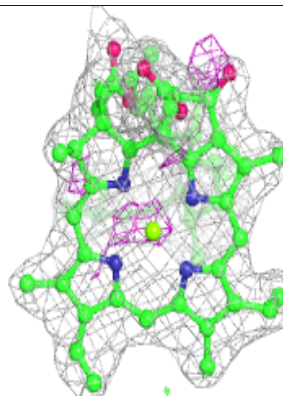
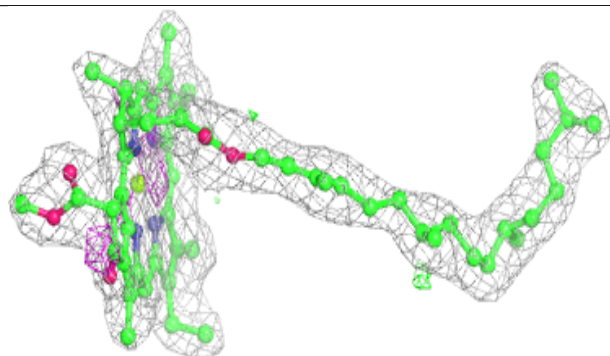
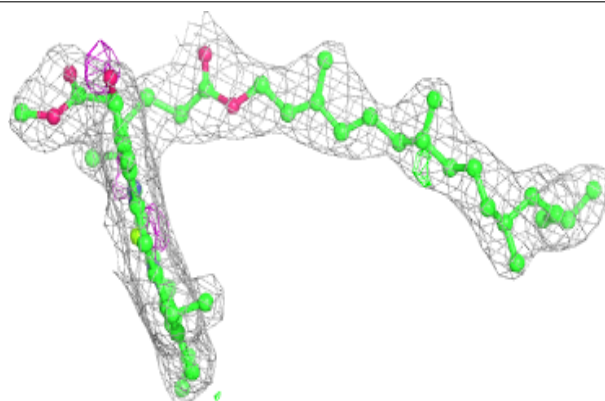


Electron density around BCR c 518:

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

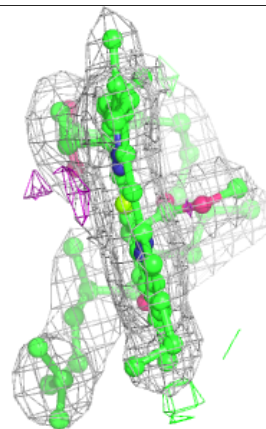
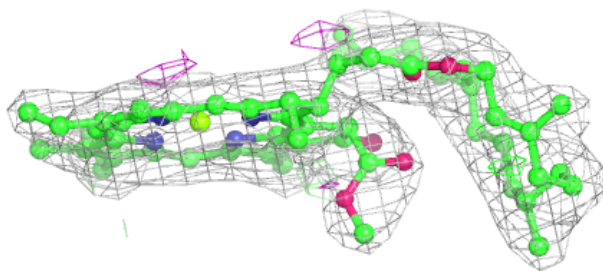
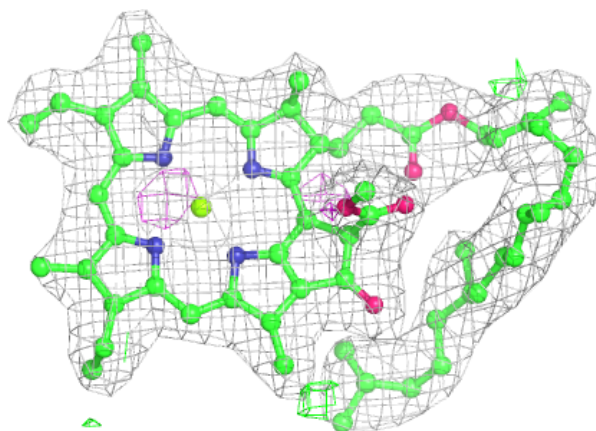
**Electron density around CLA b 614:**

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

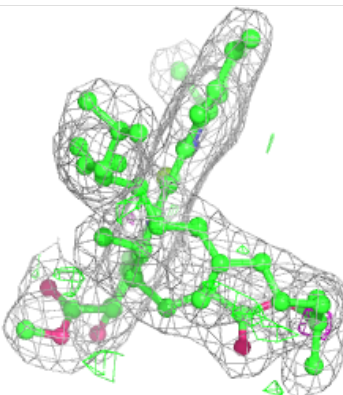
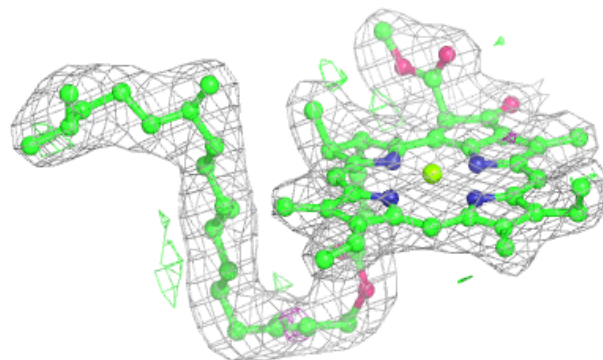
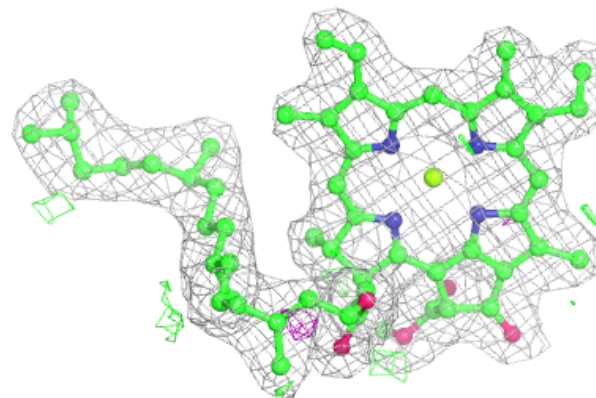


Electron density around CLA B 611:

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

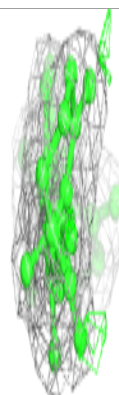
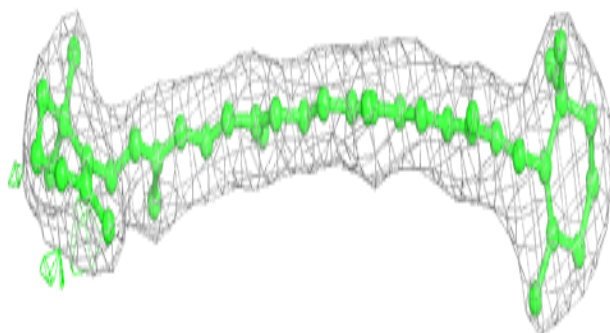
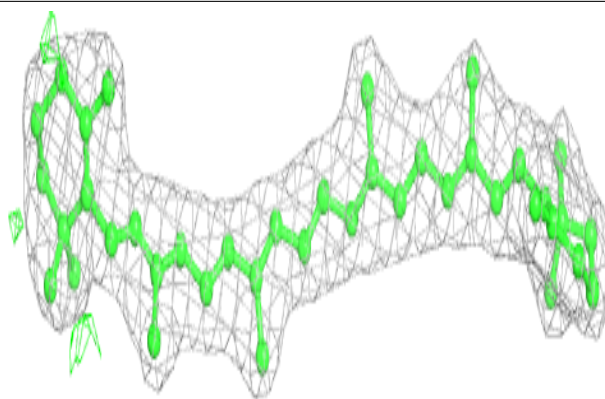
**Electron density around CLA A 406:**

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

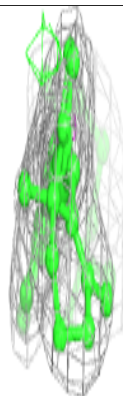
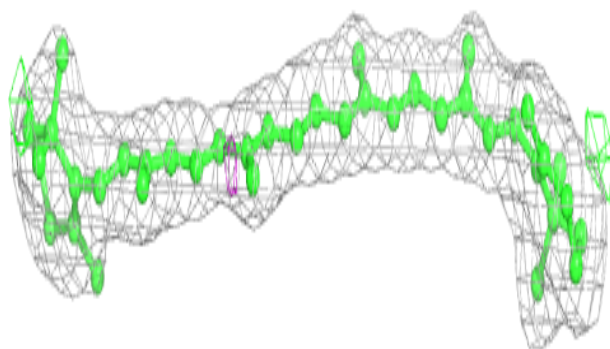
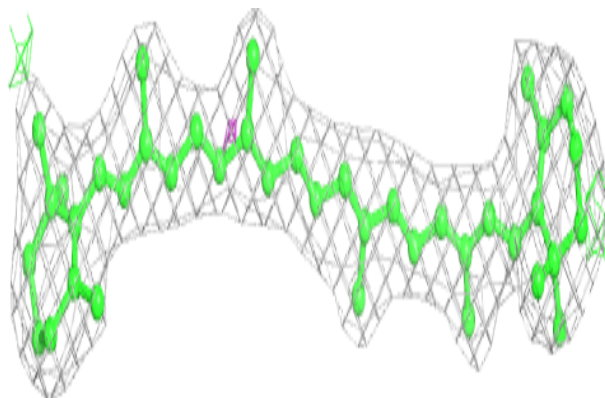


Electron density around BCR B 618:

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

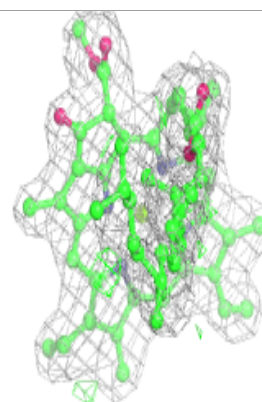
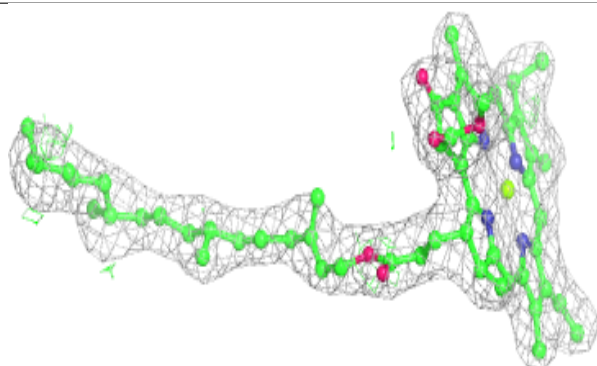
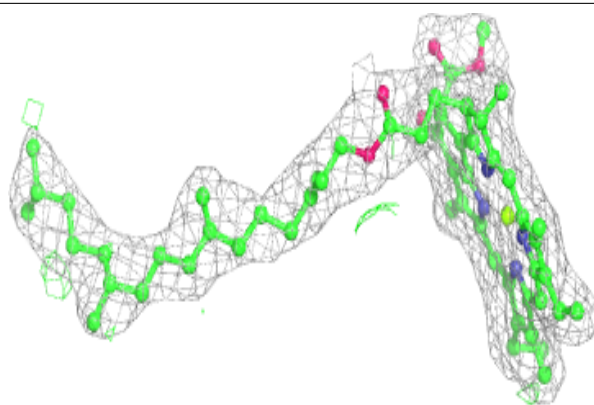
**Electron density around BCR B 620:**

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

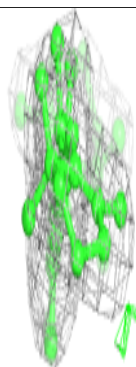
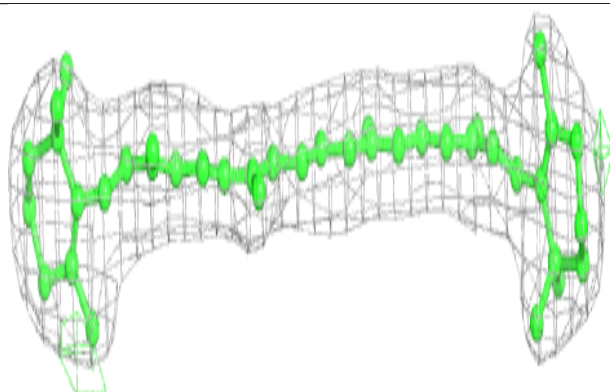
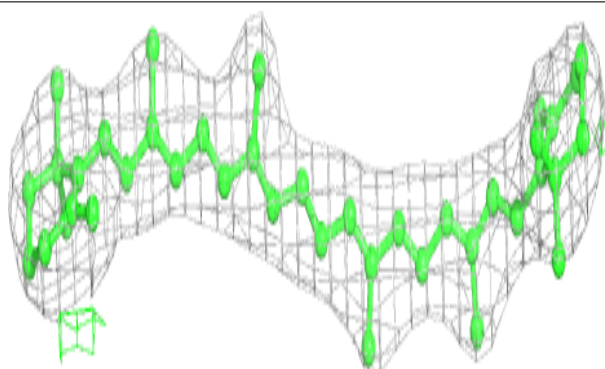


Electron density around CLA b 613:

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

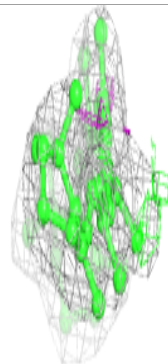
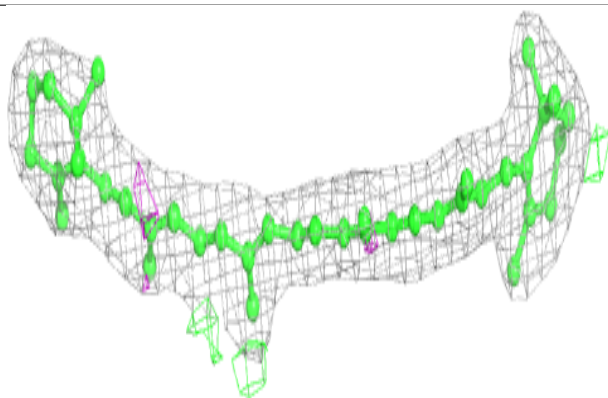
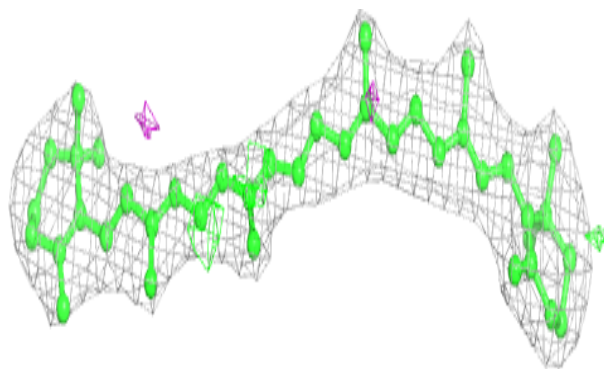
**Electron density around BCR C 515:**

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

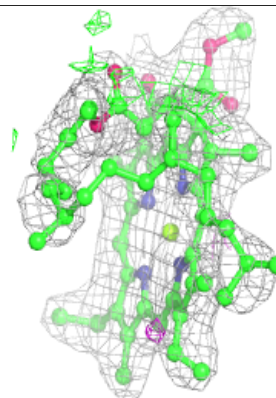
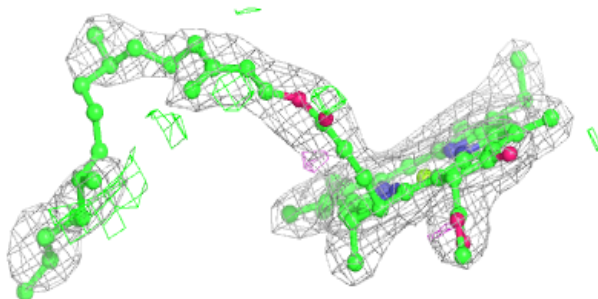
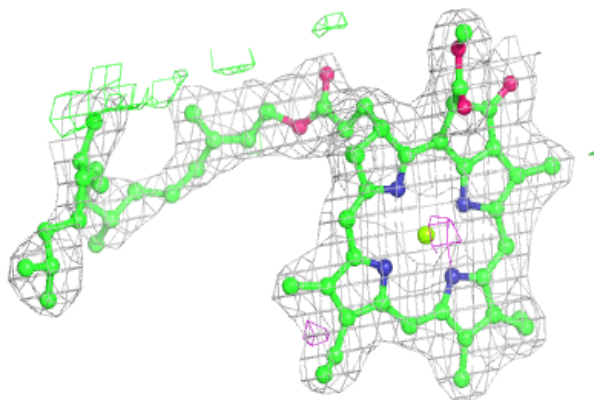


Electron density around BCR t 102:

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

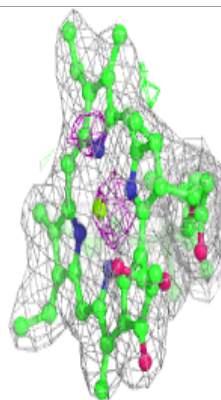
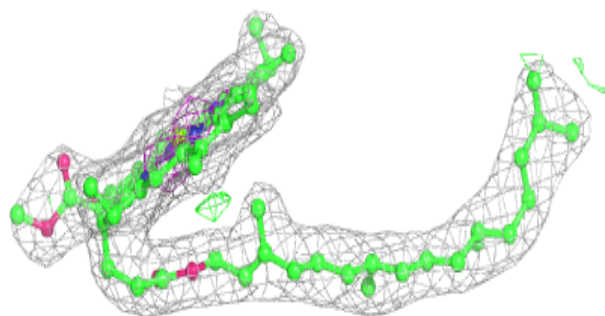
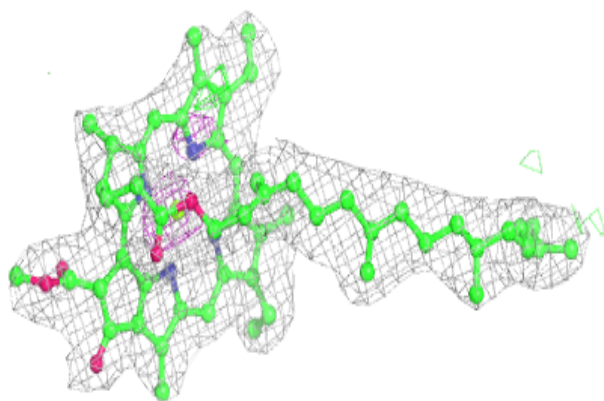
**Electron density around CLA A 409:**

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

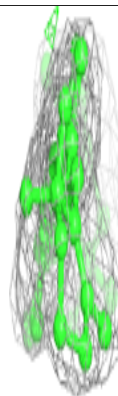
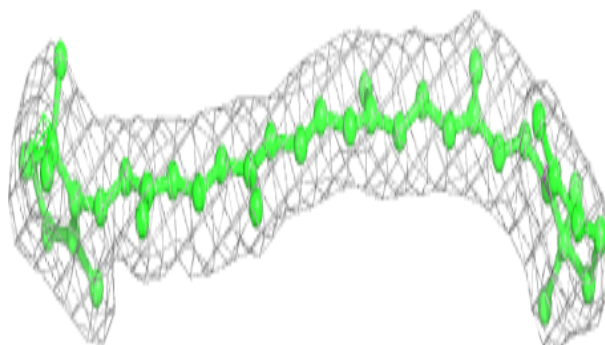
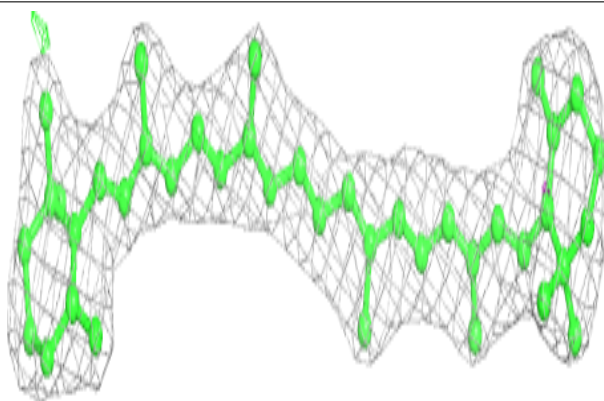


Electron density around CLA B 609:

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

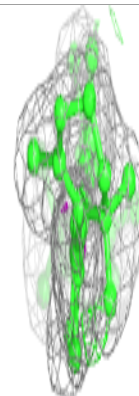
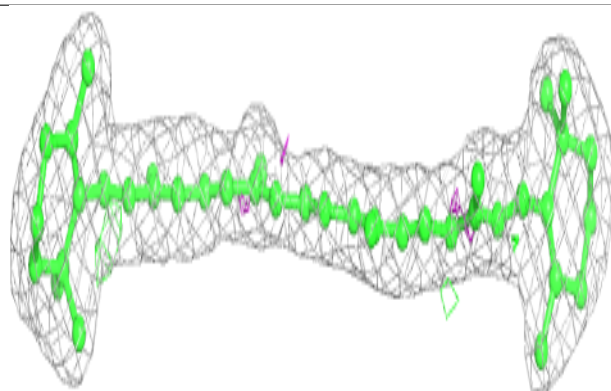
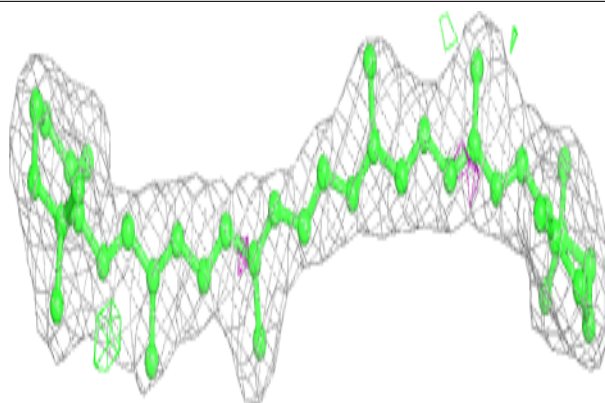
**Electron density around BCR b 628:**

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

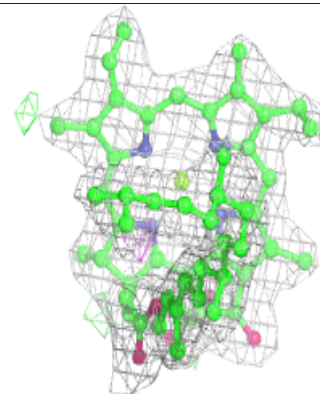
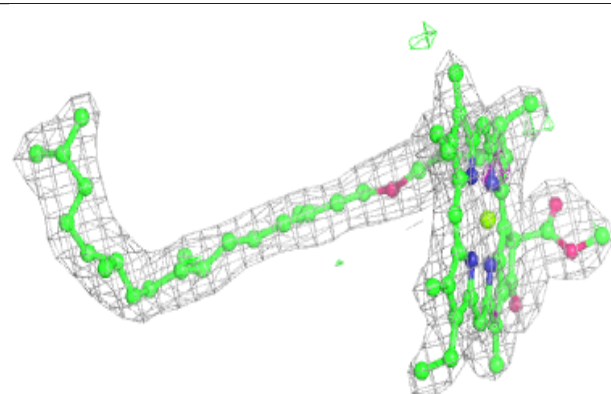
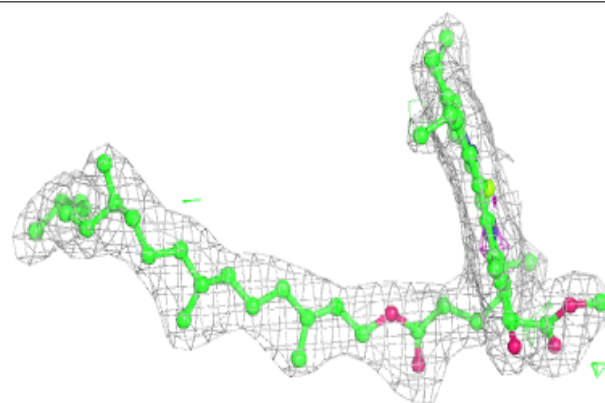


Electron density around BCR A 410:

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

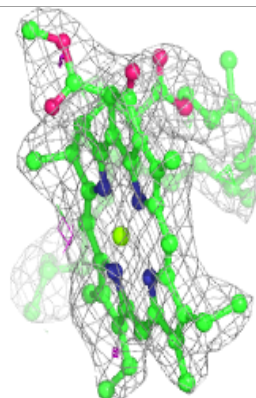
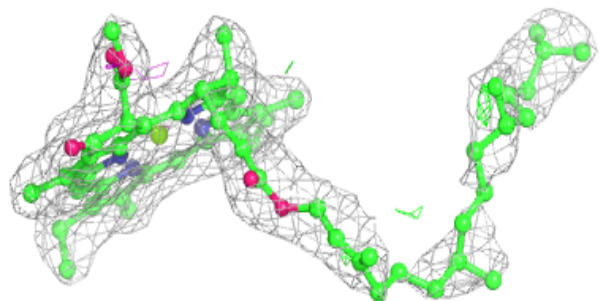
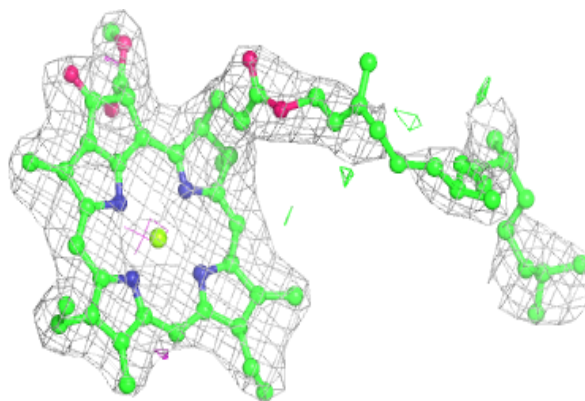
**Electron density around CLA B 606:**

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

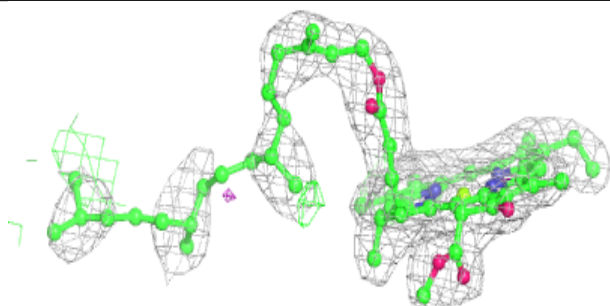
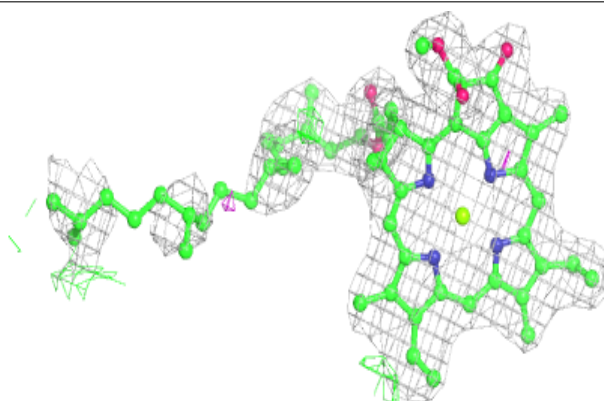


Electron density around CLA a 412:

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

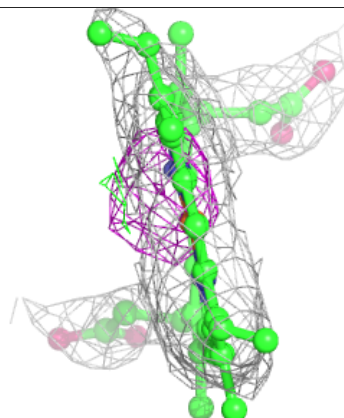
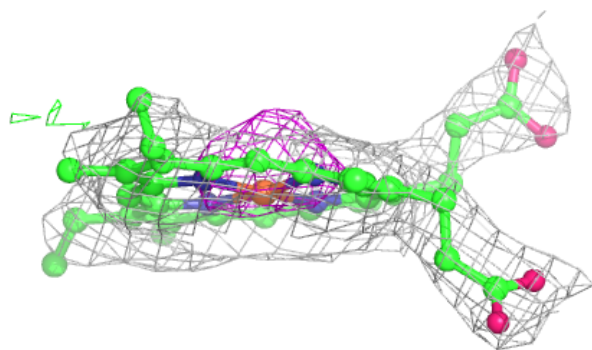
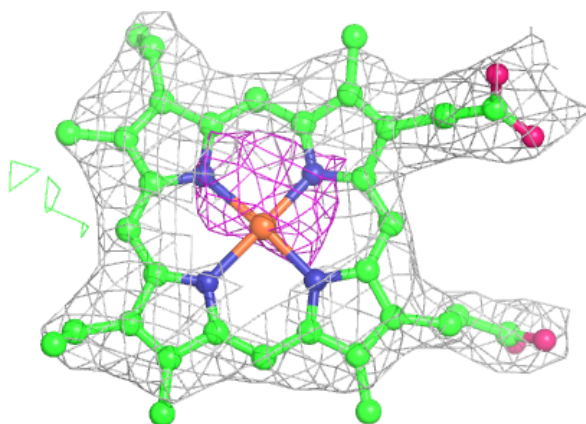
**Electron density around CLA a 410:**

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

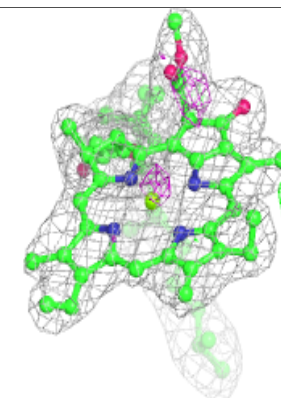
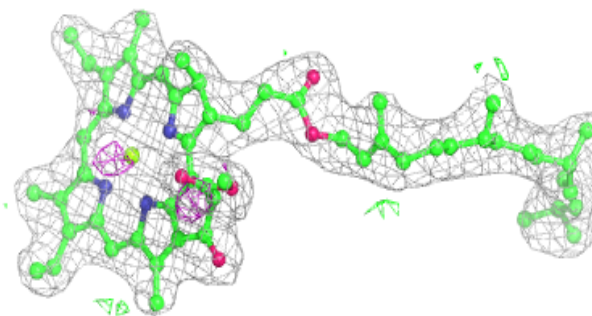
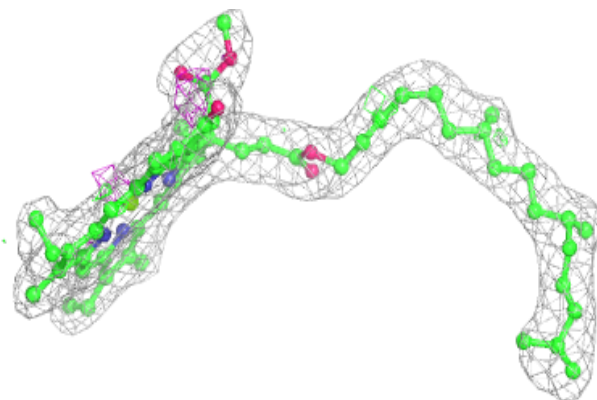


Electron density around HEM E 103:

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

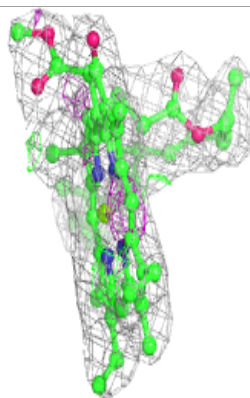
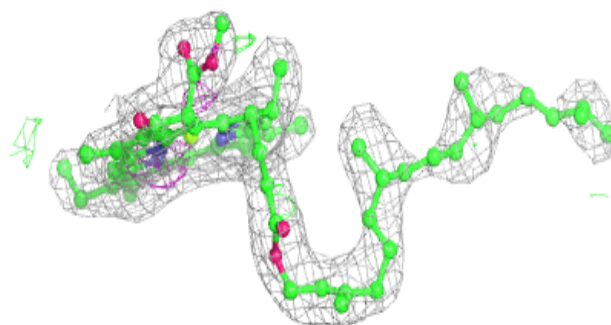
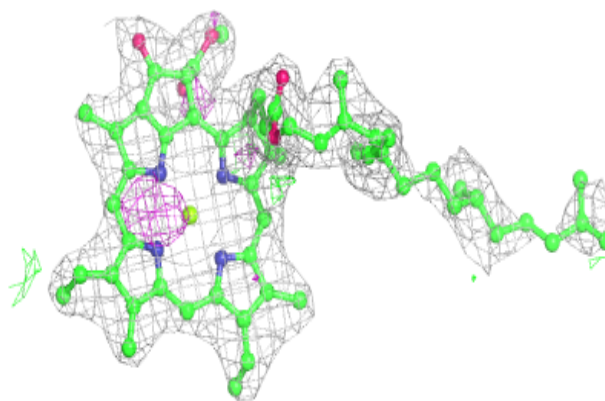
**Electron density around CLA d 404:**

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

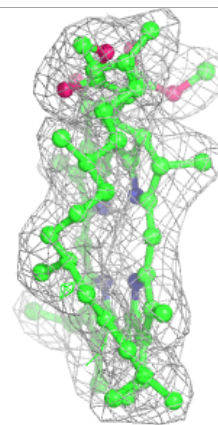
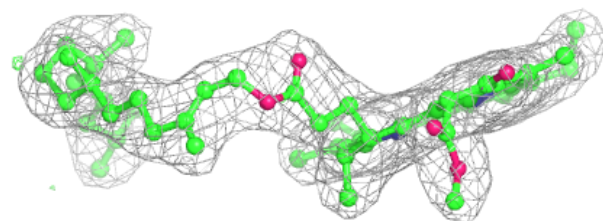
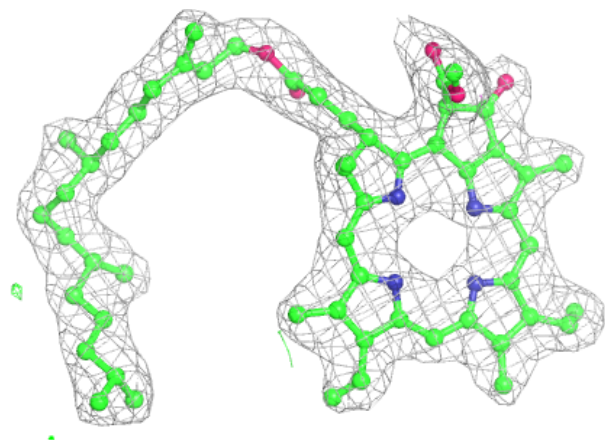


Electron density around CLA A 407:

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

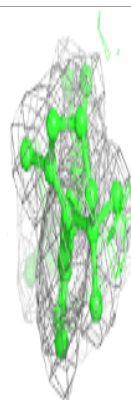
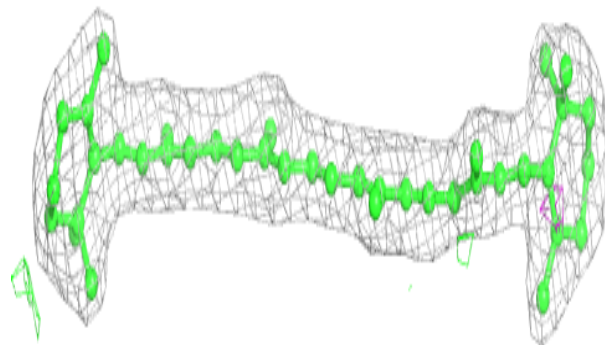
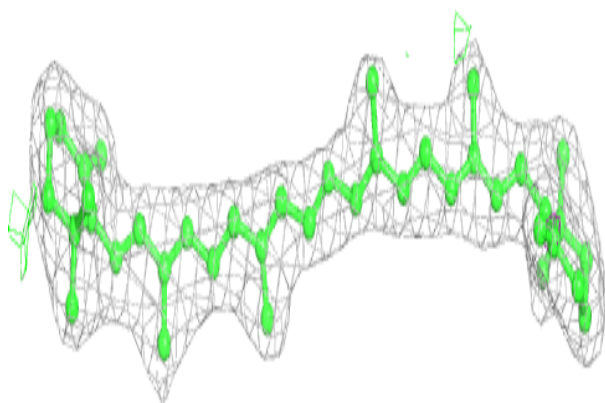
**Electron density around PHO a 411:**

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

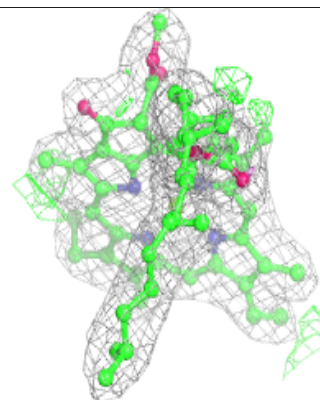
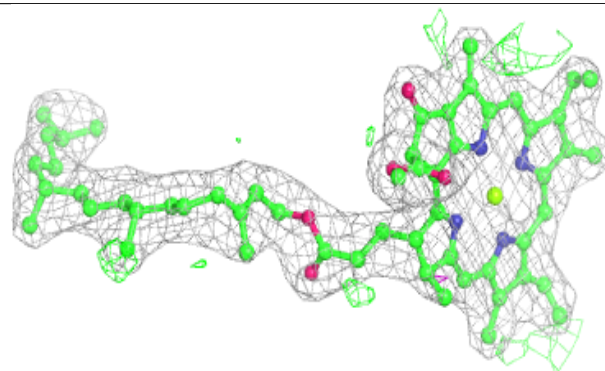
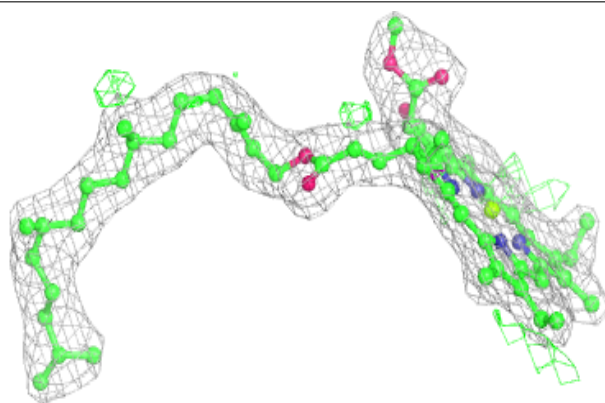


Electron density around BCR a 413:

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

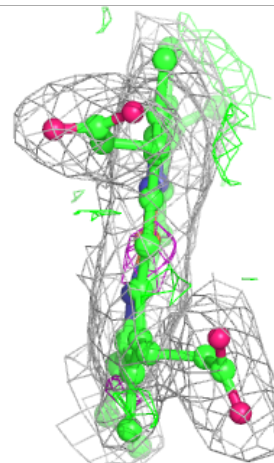
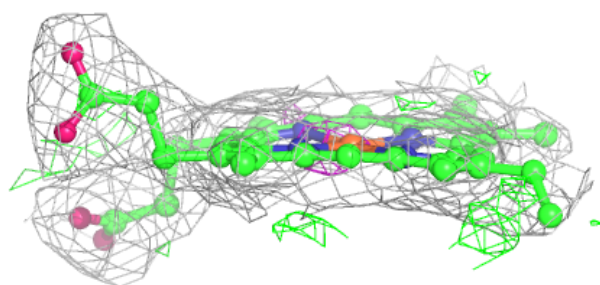
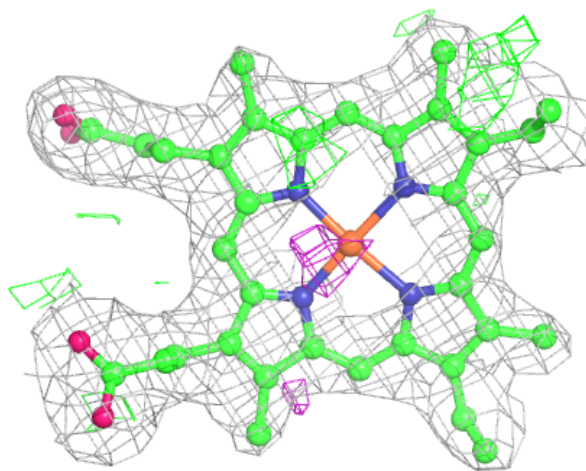
**Electron density around CLA D 404:**

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



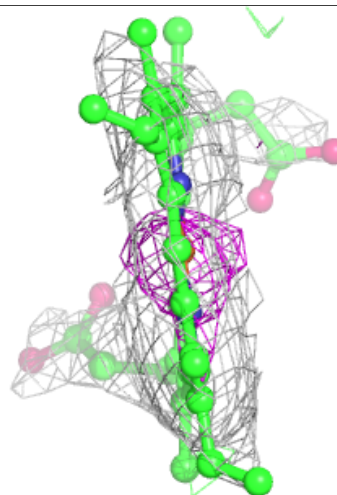
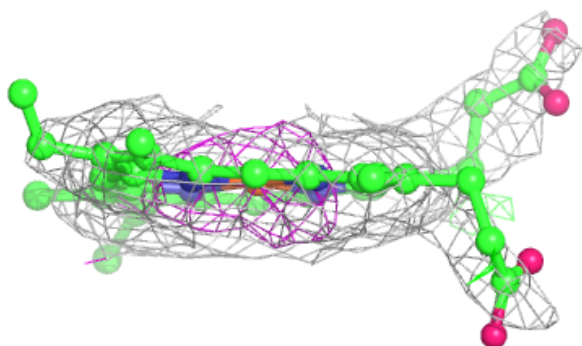
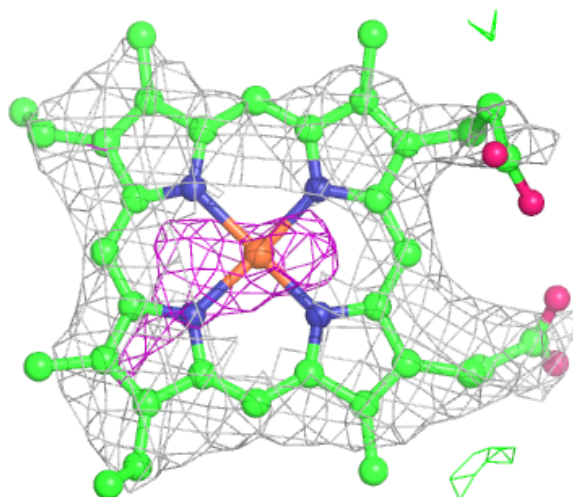
Electron density around HEM V 205:

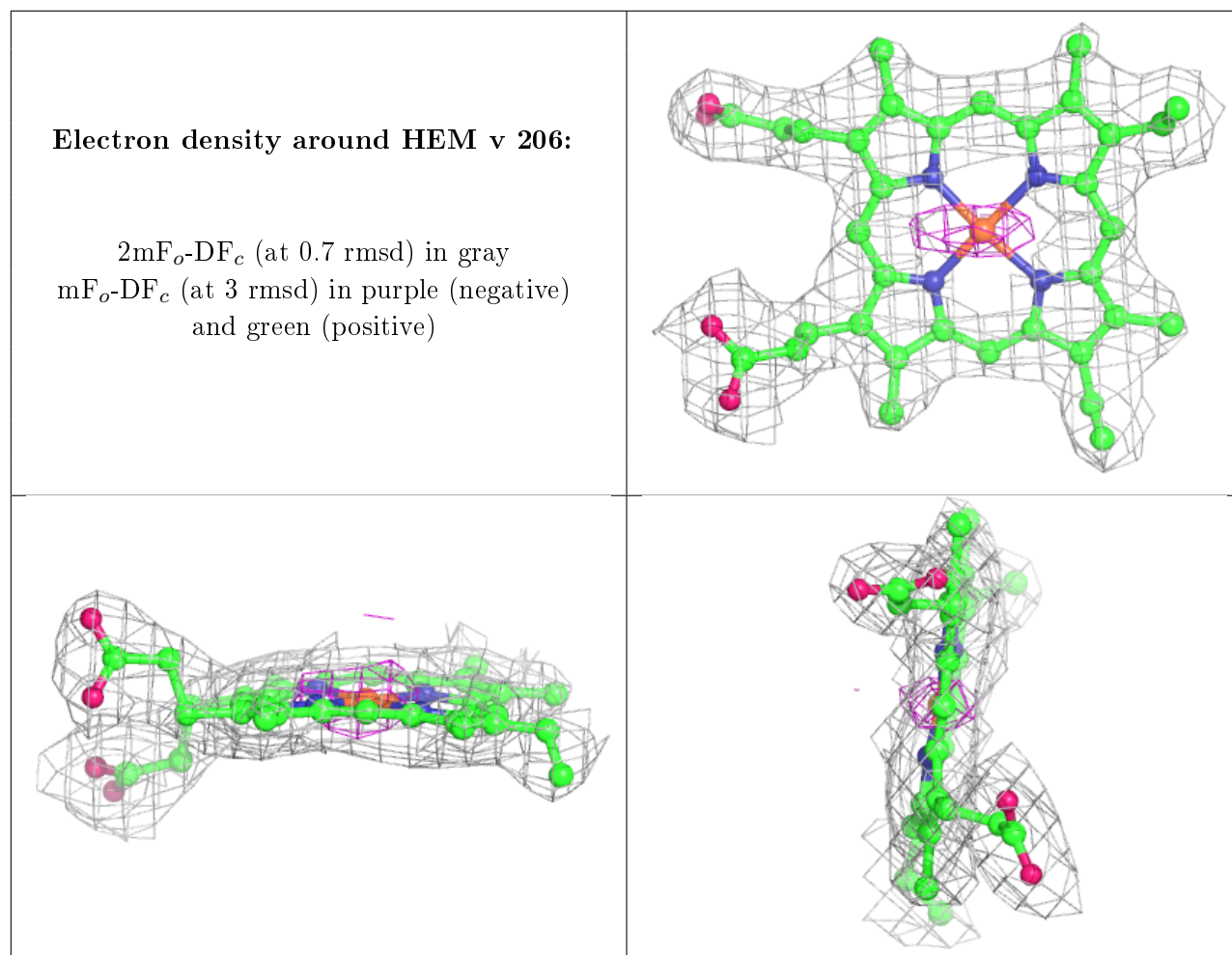
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.