



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:16 PM BST

PDB ID : 6JLP
Title : XFEL structure of cyanobacterial photosystem II (3F state, dataset2)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.50 Å(reported)

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

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

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

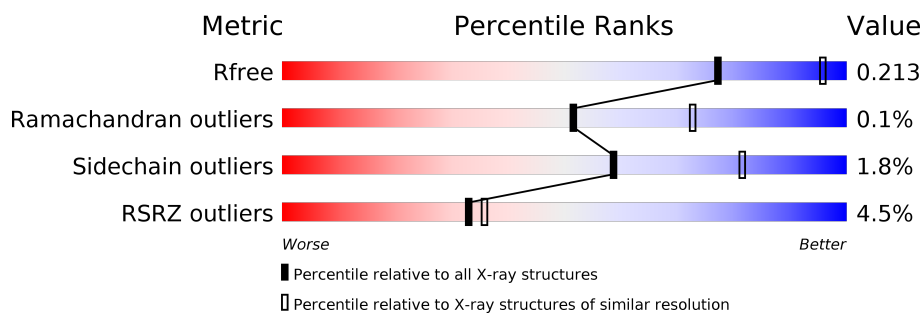
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div></div> <div>97%</div> <div>.</div> </div>
1	a	344	<div> <div>4%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>2%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>4%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>5%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div>%</div> <div>99%</div> <div></div> </div>

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Mol	Chain	Length	Quality of chain
4	d	342	% 99%
5	E	84	24% 96% .
5	e	84	10% 95% ..
6	F	44	11% 77% 23%
6	f	44	70% 27%
7	H	65	2% 97% .
7	h	65	3% 98% .
8	I	38	11% 95% 5%
8	i	38	8% 95% ..
9	J	39	26% 97% .
9	j	39	15% 100%
10	K	37	14% 97% .
10	k	37	95% 5%
11	L	37	97% .
11	l	37	100%
12	M	36	86% 8% 6%
12	m	36	89% 6% 6%
13	O	244	3% 98% .
13	o	244	% 97% .
14	T	32	3% 88% 6% 6%
14	t	32	88% 6% 6%
15	U	104	% 89% . 7%
15	u	104	90% . 7%
16	V	137	% 100%
16	v	137	% 98% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	406	X	-	-	-
23	CLA	D	407	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	a	412	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	b	620	X	-	-	-
23	CLA	b	621	X	-	-	-
23	CLA	b	622	X	-	-	-
23	CLA	b	623	X	-	-	-
23	CLA	b	624	X	-	-	-
23	CLA	b	625	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	c	515	X	-	-	-
23	CLA	c	516	X	-	-	-
23	CLA	c	517	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
23	CLA	d	405	X	-	-	-
26	GOL	V	202	-	-	-	X
27	LMT	C	521	-	-	-	X
27	LMT	F	101	-	-	-	X
27	LMT	a	419	-	-	-	X
27	LMT	b	630	-	-	-	X
34	DGD	d	408	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 55697 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	54	0
			3024	1969	499	538	18			
1	a	334	Total	C	N	O	S	0	56	0
			3020	1970	497	535	18			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		
21	a	1	Total	Fe	0	1
			1	1		

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

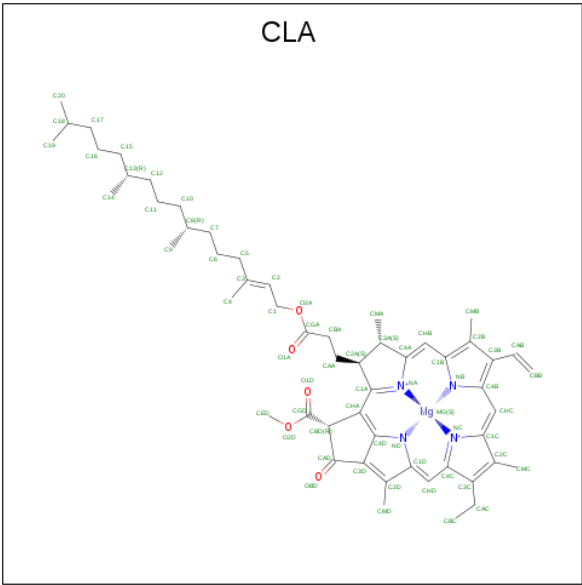
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

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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 CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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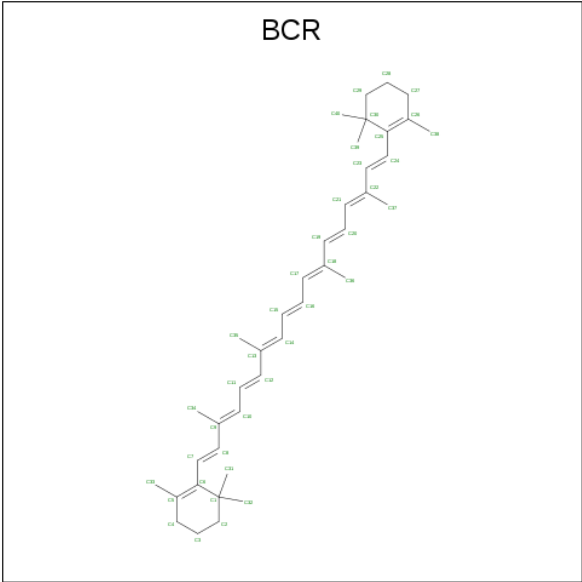
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N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

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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



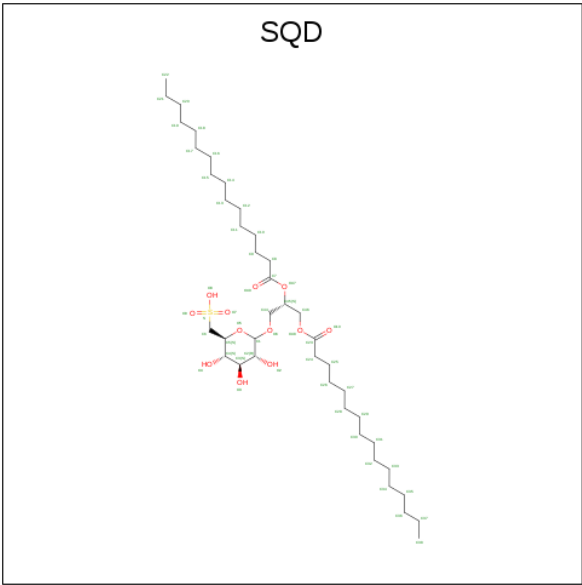
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

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

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



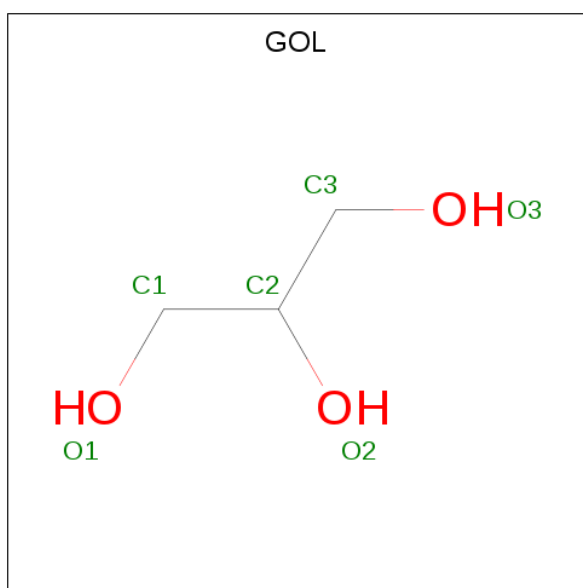
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O S 54 41 12 1	0	0
25	A	1	Total C O S 54 41 12 1	0	0
25	B	1	Total C O S 54 41 12 1	0	0

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

- Molecule 26 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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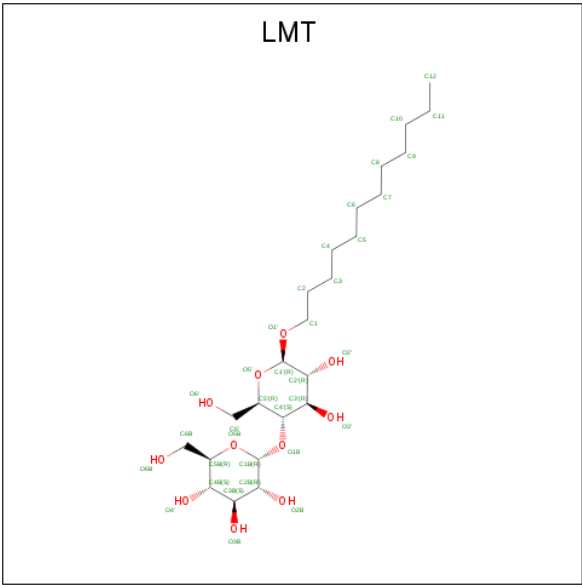
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	B	1	Total 6	C 3	O 3	0	0
26	B	1	Total 6	C 3	O 3	0	0
26	C	1	Total 6	C 3	O 3	0	0
26	C	1	Total 6	C 3	O 3	0	0
26	D	1	Total 6	C 3	O 3	0	0
26	F	1	Total 6	C 3	O 3	0	0
26	O	1	Total 6	C 3	O 3	0	0
26	T	1	Total 6	C 3	O 3	0	0
26	T	1	Total 6	C 3	O 3	0	0
26	V	1	Total 6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

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

- Molecule 27 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



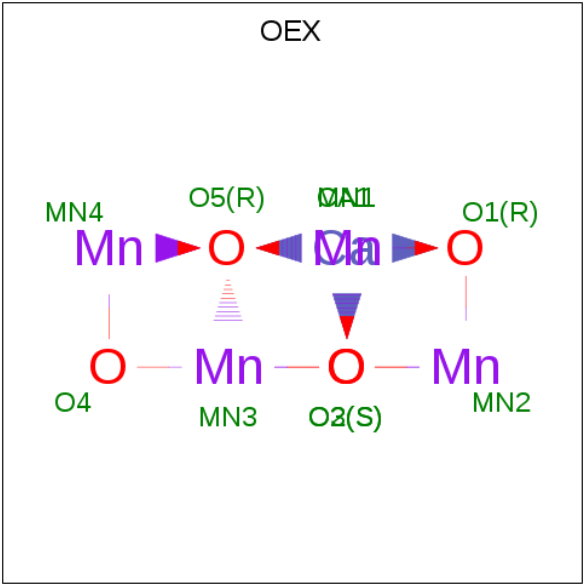
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			35	24	11		
27	C	1	Total	C	O	0	0
			35	24	11		
27	D	1	Total	C	O	0	0
			35	24	11		

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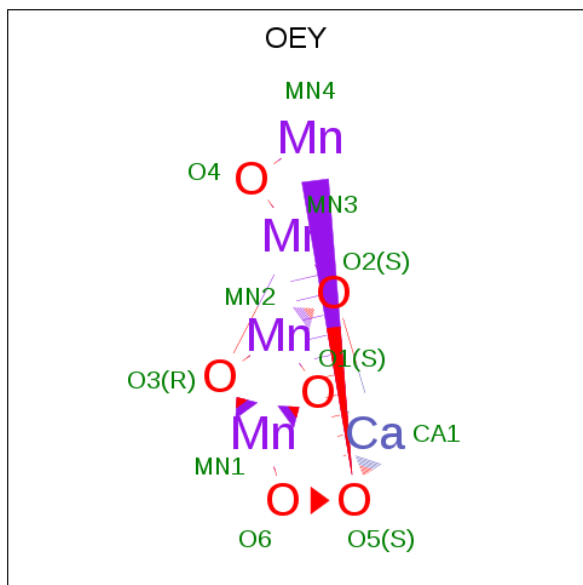
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	F	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	M	1	Total	C	O	0	0
			35	24	11		
27	T	1	Total	C	O	0	0
			25	19	6		
27	a	1	Total	C	O	0	0
			35	24	11		
27	a	1	Total	C	O	0	0
			35	24	11		
27	b	1	Total	C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

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



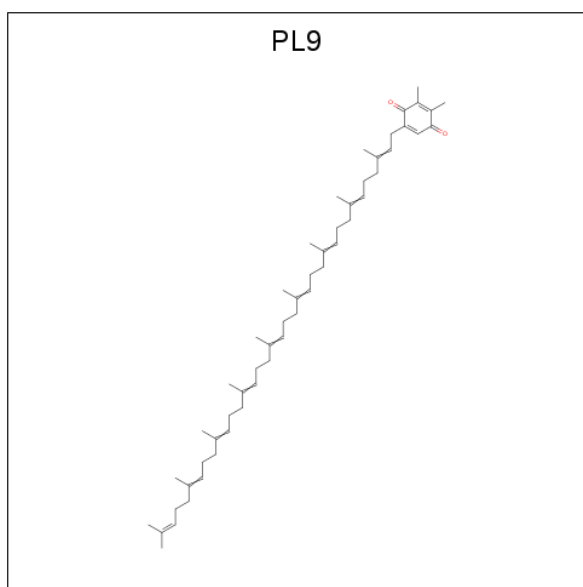
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
28	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 29 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

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



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

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

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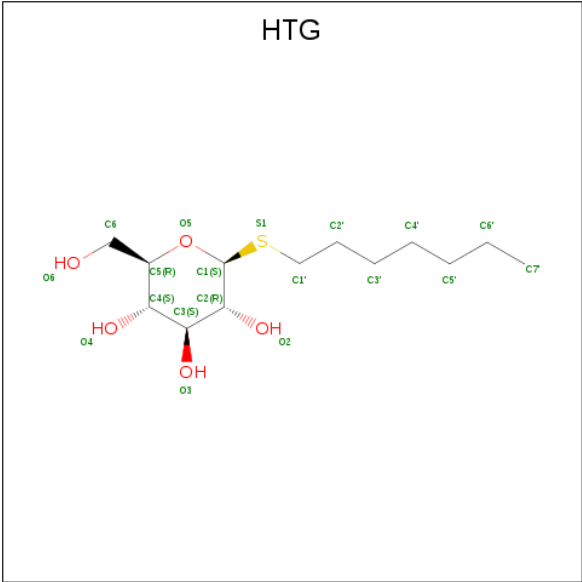
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 28 23 5	0	0
31	j	1	Total C 10 10	0	0
31	X	1	Total C O 18 16 2	0	0
31	d	3	Total C O 71 63 8	0	0
31	m	1	Total C 10 10	0	0
31	b	1	Total C O 33 28 5	0	0
31	M	1	Total C 10 10	0	0

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 33 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



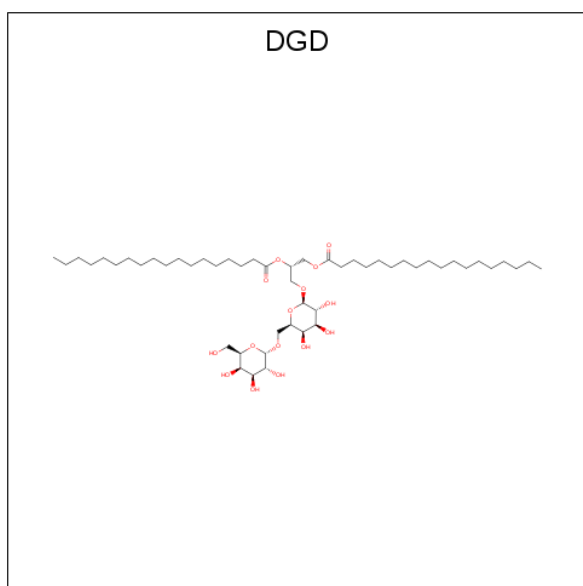
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	B	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	C	1	Total	C	O	S	0	0
			19	13	5	1		
33	D	1	Total	C	O	S	0	0
			16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

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

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



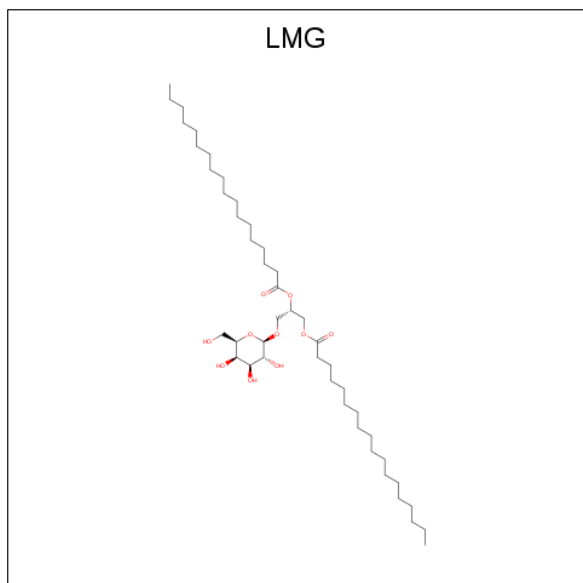
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	C	1	Total	C	O		0	0
			62	47	15			
34	D	1	Total	C	O		0	0
			52	42	10			
34	c	1	Total	C	O		0	0
			62	47	15			
34	c	1	Total	C	O		0	0
			62	47	15	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

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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



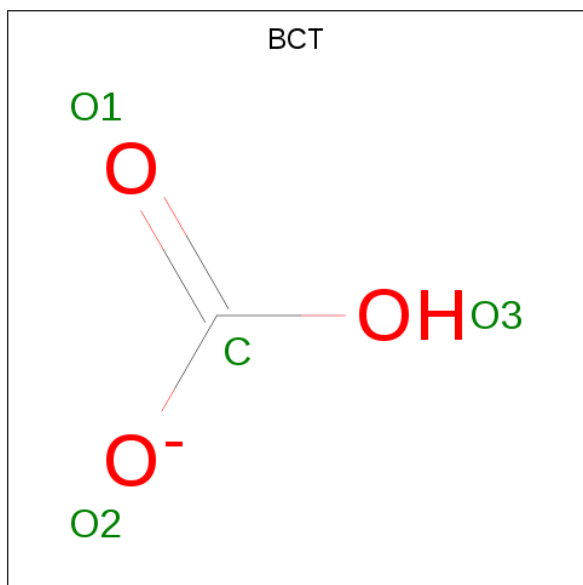
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		
35	C	1	Total	C	O	0	0
			51	41	10		
35	D	1	Total	C	O	0	0
			51	41	10		
35	M	1	Total	C	O	0	0
			51	41	10		
35	Z	1	Total	C	O	0	0
			37	27	10		
35	a	1	Total	C	O	0	0
			51	41	10		
35	b	1	Total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

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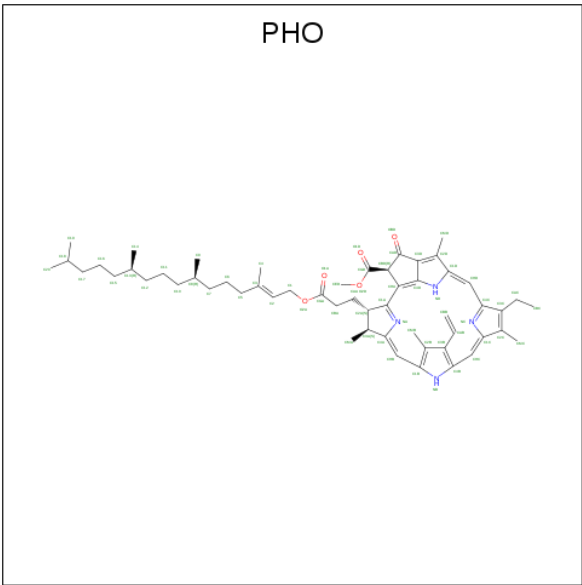
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	c	1	Total	C	O	0	0
			51	41	10		
35	d	1	Total	C	O	0	0
			51	41	10		
35	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 36 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



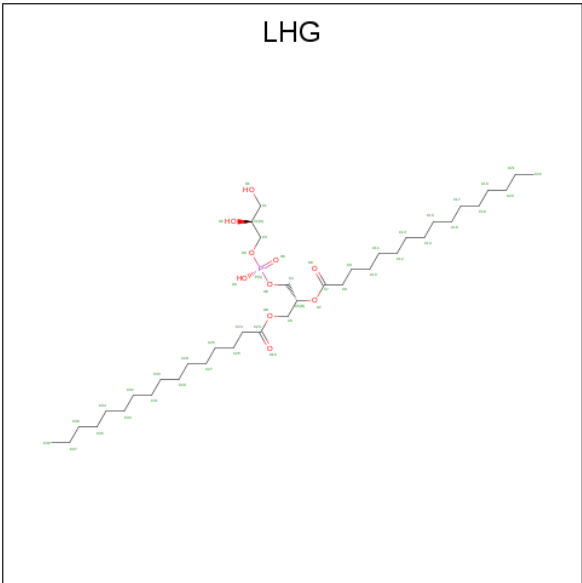
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	D	1	Total	C	O	0	1
			8	2	6		
36	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 37 is PHEOPHYTIN A (three-letter code: PHO) (formula: $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$).



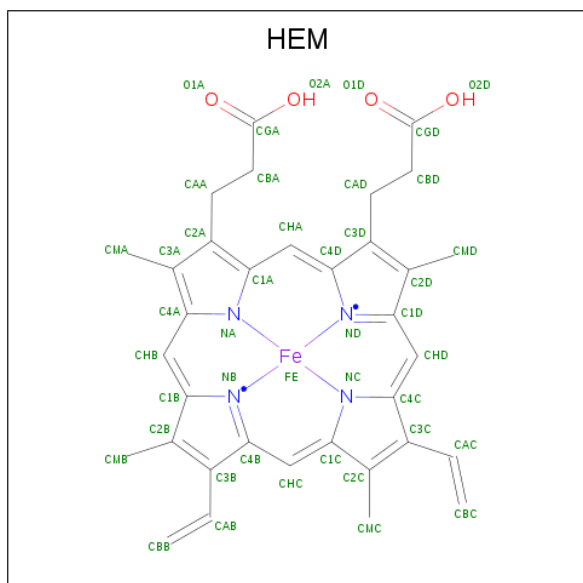
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	N	O	0	0
			64	55	4	5		
37	D	1	Total	C	N	O	0	1
			128	110	8	10		
37	a	1	Total	C	N	O	0	0
			64	55	4	5		
37	d	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

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

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

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	160	Total 172	O 172	0	14
41	B	286	Total 290	O 290	0	4
41	C	218	Total 222	O 222	0	5
41	D	146	Total 150	O 150	0	5
41	E	34	Total 35	O 35	0	1
41	F	11	Total 11	O 11	0	0
41	H	40	Total 40	O 40	0	0
41	I	6	Total 6	O 6	0	0
41	J	10	Total 10	O 10	0	0
41	K	9	Total 9	O 9	0	0
41	L	15	Total 16	O 16	0	1
41	M	23	Total 23	O 23	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	O	180	Total 182	O 182	0	2
41	T	16	Total 17	O 17	0	1
41	U	79	Total 79	O 79	0	0
41	V	122	Total 124	O 124	0	2
41	Y	4	Total 4	O 4	0	0
41	X	10	Total 10	O 10	0	0
41	Z	1	Total 1	O 1	0	0
41	a	146	Total 155	O 155	0	12
41	b	259	Total 262	O 262	0	3
41	c	204	Total 209	O 209	0	6
41	d	142	Total 145	O 145	0	3
41	e	18	Total 18	O 18	0	0
41	f	7	Total 7	O 7	0	0
41	h	44	Total 44	O 44	0	0
41	i	4	Total 4	O 4	0	0
41	j	7	Total 7	O 7	0	0
41	k	7	Total 7	O 7	0	0
41	l	8	Total 8	O 8	0	0
41	m	13	Total 13	O 13	0	0
41	o	154	Total 154	O 154	0	0
41	t	16	Total 16	O 16	0	0

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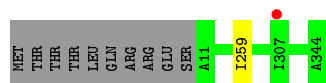
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	u	93	Total 93	O 93	0	0
41	v	79	Total 80	O 80	0	1
41	y	2	Total 2	O 2	0	0
41	x	6	Total 6	O 6	0	0

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

Chain A:  97%



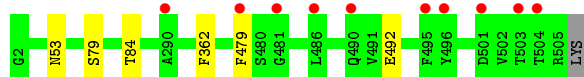
- Molecule 1: Photosystem II protein D1

Chain a:  96%



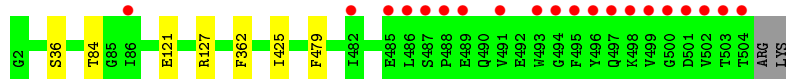
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  99%



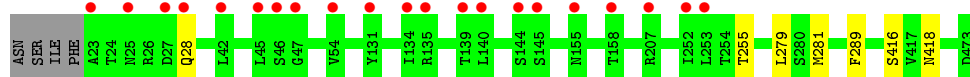
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  98%



- Molecule 3: Photosystem II CP43 reaction center protein

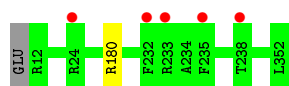
Chain C:  98%



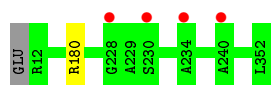
- Molecule 3: Photosystem II CP43 reaction center protein



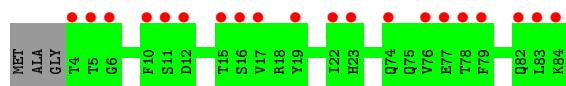
- Molecule 4: Photosystem II D2 protein



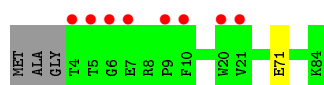
- Molecule 4: Photosystem II D2 protein



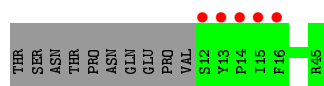
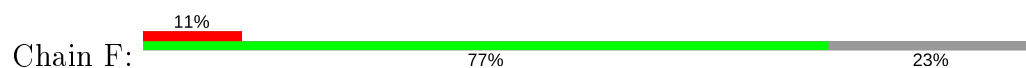
- Molecule 5: Cytochrome b559 subunit alpha



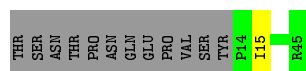
- Molecule 5: Cytochrome b559 subunit alpha



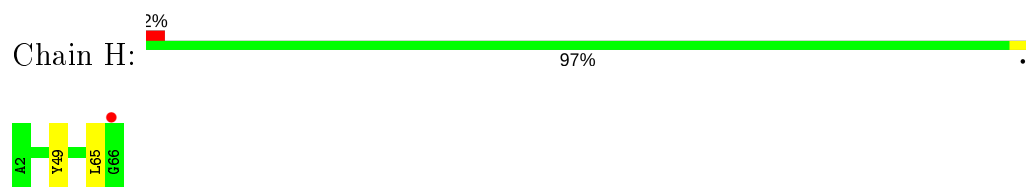
- Molecule 6: Cytochrome b559 subunit beta



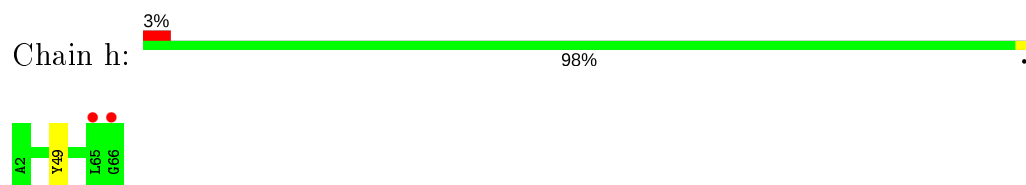
- Molecule 6: Cytochrome b559 subunit beta



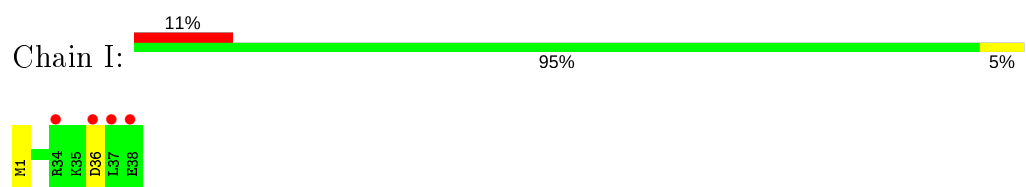
- Molecule 7: Photosystem II reaction center protein H



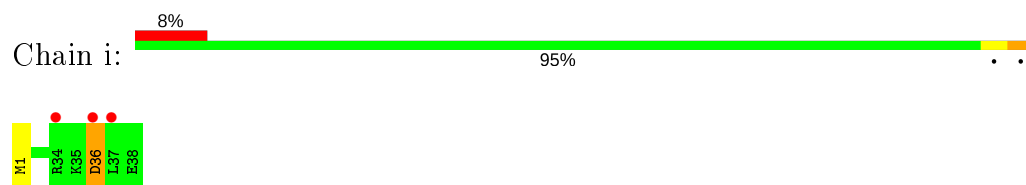
- Molecule 7: Photosystem II reaction center protein H



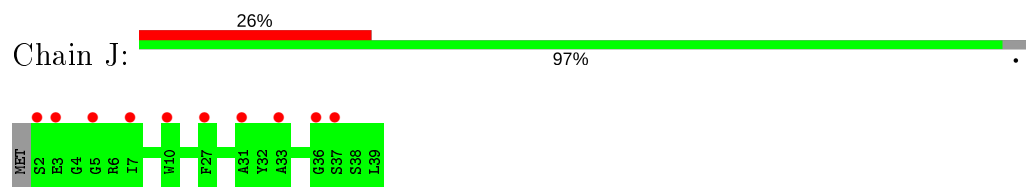
- Molecule 8: Photosystem II reaction center protein I



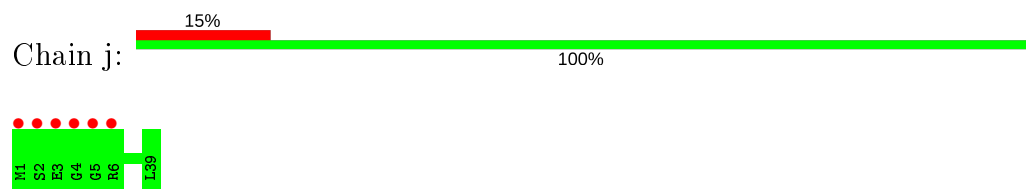
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

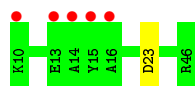


- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

Chain k: 95% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 97% .



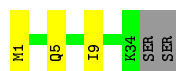
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%

There are no outlier residues recorded for this chain.

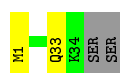
- Molecule 12: Photosystem II reaction center protein M

Chain M: 86% 8% 6%



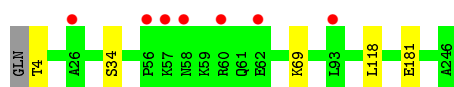
- Molecule 12: Photosystem II reaction center protein M

Chain m: 89% 6% 6%



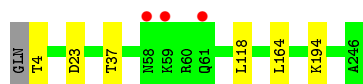
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 3% 98% .

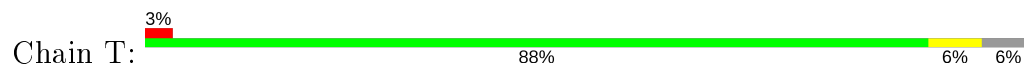


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

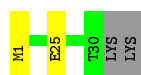
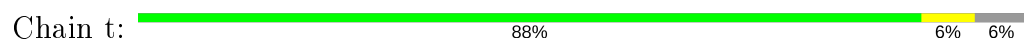
Chain o: % 97% .



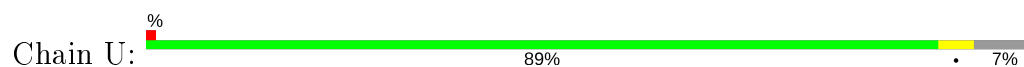
- Molecule 14: Photosystem II reaction center protein T



- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



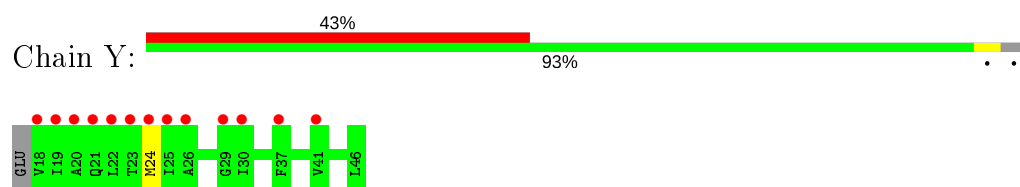
- Molecule 16: Cytochrome c-550



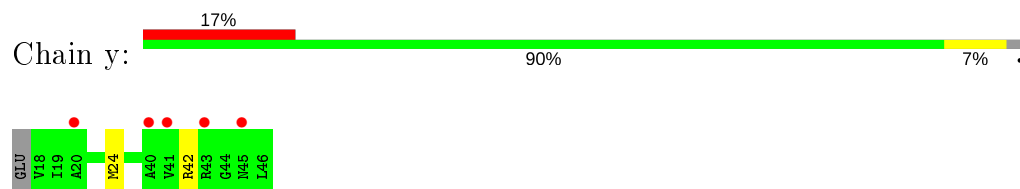
- Molecule 16: Cytochrome c-550



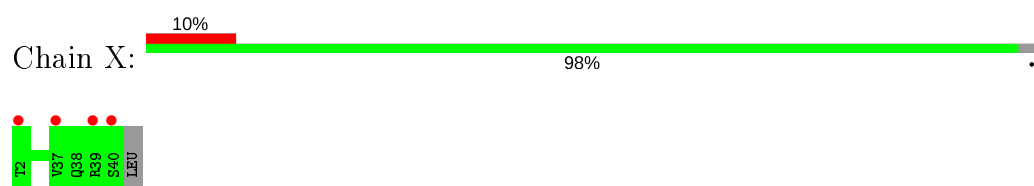
- Molecule 17: Photosystem II reaction center protein Ycf12



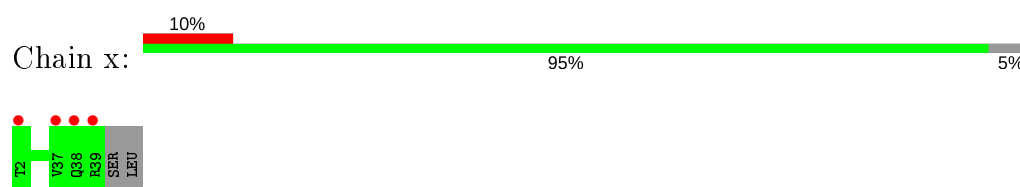
- Molecule 17: Photosystem II reaction center protein Ycf12



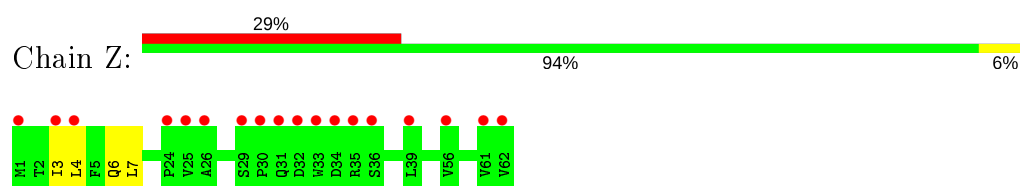
- Molecule 18: Photosystem II reaction center protein X



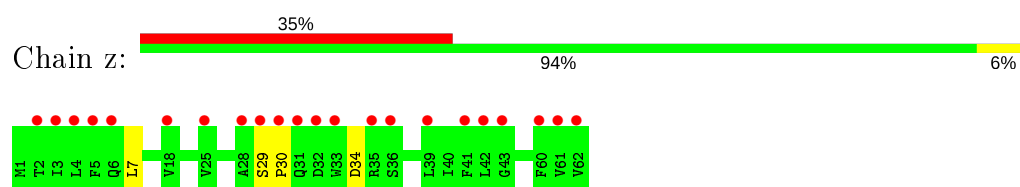
- Molecule 18: Photosystem II reaction center protein X



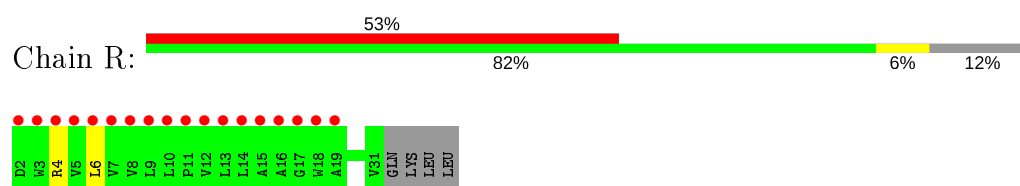
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 121.57 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.50) 99.2 (121.57-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.151 , 0.211 0.157 , 0.213	Depositor DCC
R_{free} test set	14865 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 79.9	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	0.96	EDS
Total number of atoms	55697	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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	0.43	0/3126	0.54	0/4257
1	a	0.44	0/3128	0.55	0/4260
2	B	0.42	0/4191	0.55	0/5709
2	b	0.43	0/4198	0.54	0/5720
3	C	0.39	0/3678	0.51	0/5007
3	c	0.39	0/3774	0.51	0/5135
4	D	0.46	0/2952	0.54	0/4021
4	d	0.45	0/2952	0.56	0/4021
5	E	0.33	0/693	0.49	0/944
5	e	0.35	0/695	0.50	0/948
6	F	0.40	0/284	0.52	0/387
6	f	0.41	0/265	0.53	0/360
7	H	0.36	0/535	0.53	0/728
7	h	0.35	0/524	0.53	0/713
8	I	0.38	0/311	0.51	0/419
8	i	0.39	0/311	0.50	0/419
9	J	0.35	0/278	0.40	0/376
9	j	0.36	0/286	0.45	0/386
10	K	0.34	0/303	0.49	0/416
10	k	0.37	0/303	0.52	0/416
11	L	0.44	0/319	0.49	0/433
11	l	0.45	0/319	0.46	0/433
12	M	0.49	0/270	0.68	0/368
12	m	0.45	0/262	0.57	0/357
13	O	0.39	0/1958	0.56	0/2654
13	o	0.38	0/1937	0.55	0/2625
14	T	0.51	0/266	0.54	0/362
14	t	0.52	0/266	0.53	0/362
15	U	0.38	0/785	0.54	0/1064
15	u	0.39	0/785	0.55	0/1064
16	V	0.37	0/1109	0.52	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.35	0/1098	0.51	0/1488
17	Y	0.35	0/216	0.47	0/289
17	y	0.32	0/216	0.45	0/289
18	X	0.34	0/290	0.47	0/392
18	x	0.34	0/284	0.48	0/384
19	Z	0.29	0/490	0.42	0/669
19	z	0.28	0/490	0.45	0/669
20	R	0.23	0/245	0.38	0/338
All	All	0.41	0/44392	0.53	0/60384

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/344 (112%)	378 (98%)	6 (2%)	1 (0%)	41	61
1	a	385/344 (112%)	377 (98%)	7 (2%)	1 (0%)	41	61
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	498 (97%)	14 (3%)	1 (0%)	47	68
3	C	461/455 (101%)	446 (97%)	13 (3%)	2 (0%)	34	54
3	c	473/455 (104%)	455 (96%)	16 (3%)	2 (0%)	34	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	355/342 (104%)	344 (97%)	11 (3%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	31 (97%)	1 (3%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	60 (94%)	4 (6%)	0	100	100
7	h	63/65 (97%)	57 (90%)	6 (10%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	7
9	J	36/39 (92%)	35 (97%)	1 (3%)	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%)	33 (94%)	2 (6%)	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%)	239 (96%)	10 (4%)	0	100	100
13	o	246/244 (101%)	236 (96%)	10 (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%)	92 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	Y	27/30 (90%)	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%)	57 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	16
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5431/5384 (101%)	5261 (97%)	161 (3%)	9 (0%)	51	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
2	b	127	ARG
3	c	416[A]	SER
3	c	416[B]	SER
19	z	30	PRO
8	i	36	ASP
1	a	259	ILE
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/279 (112%)	312 (100%)	0	100	100
1	a	312/279 (112%)	310 (99%)	2 (1%)	86	95
2	B	412/403 (102%)	406 (98%)	6 (2%)	65	85
2	b	413/403 (102%)	407 (98%)	6 (2%)	65	85
3	C	361/356 (101%)	355 (98%)	6 (2%)	60	82
3	c	371/356 (104%)	362 (98%)	9 (2%)	49	74
4	D	290/277 (105%)	289 (100%)	1 (0%)	92	97
4	d	290/277 (105%)	289 (100%)	1 (0%)	92	97
5	E	74/73 (101%)	74 (100%)	0	100	100
5	e	74/73 (101%)	73 (99%)	1 (1%)	67	86

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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	58
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	61
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	80
8	I	34/34 (100%)	33 (97%)	1 (3%)	42	69
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	69
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	27 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	64
10	k	30/30 (100%)	28 (93%)	2 (7%)	16	31
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	70
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	29 (94%)	2 (6%)	17	33
12	m	30/32 (94%)	29 (97%)	1 (3%)	38	64
13	O	214/207 (103%)	208 (97%)	6 (3%)	43	70
13	o	211/207 (102%)	205 (97%)	6 (3%)	43	70
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	27
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	27
15	U	84/89 (94%)	80 (95%)	4 (5%)	25	48
15	u	84/89 (94%)	81 (96%)	3 (4%)	35	61
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	115 (98%)	3 (2%)	47	73
17	Y	22/23 (96%)	21 (96%)	1 (4%)	27	51
17	y	22/23 (96%)	20 (91%)	2 (9%)	9	18
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%)	48 (92%)	4 (8%)	13	25
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	38
20	R	25/29 (86%)	23 (92%)	2 (8%)	12	23
All	All	4506/4403 (102%)	4423 (98%)	83 (2%)	59	81

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	79	SER
2	B	84	THR
2	B	362	PHE
2	B	479	PHE
2	B	492	GLU
3	C	28	GLN
3	C	255	THR
3	C	279	LEU
3	C	281	MET
3	C	289	PHE
3	C	418	ASN
4	D	180	ARG
7	H	49	TYR
7	H	65	LEU
8	I	36	ASP
10	K	23	ASP
11	L	13	ASN
12	M	5	GLN
12	M	9	ILE
13	O	4	THR
13	O	34	SER
13	O	69	LYS
13	O	118	LEU
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	8	GLU
15	U	59	GLU
15	U	70	ARG
15	U	73	GLN
17	Y	24	MET
19	Z	3	ILE
19	Z	4	LEU
19	Z	6	GLN
19	Z	7	LEU
20	R	4	ARG
20	R	6	LEU
1	a	12	ASN
1	a	257	ARG
2	b	36	SER
2	b	84	THR

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Mol	Chain	Res	Type
2	b	121	GLU
2	b	362	PHE
2	b	425	ILE
2	b	479	PHE
3	c	19	ASN
3	c	255	THR
3	c	289	PHE
3	c	391	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	180	ARG
5	e	71	GLU
6	f	15	ILE
7	h	49	TYR
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	37	THR
13	o	118	LEU
13	o	164	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	44	THR
15	u	61	VAL
15	u	86	GLU
16	v	2	GLU
16	v	6	GLU
16	v	90	GLU
17	y	24	MET
17	y	42	ARG
19	z	7	LEU
19	z	29	SER
19	z	34	ASP

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

Mol	Chain	Res	Type
1	A	315	ASN
2	B	53	ASN
2	B	331	ASN
2	B	490	GLN
2	B	497	GLN
3	C	201	ASN
3	C	418	ASN
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN
15	U	78	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
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
13	o	82	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	0.74	0	7,9,11	1.37	2 (28%)
12	FME	M	1	12	8,9,10	0.71	0	7,9,11	1.37	1 (14%)
8	FME	i	1	8	8,9,10	0.66	0	7,9,11	1.34	2 (28%)
12	FME	m	1	12	8,9,10	0.62	0	7,9,11	1.13	1 (14%)
14	FME	t	1	14	8,9,10	0.87	0	7,9,11	2.16	4 (57%)
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.61	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	-
12	FME	m	1	12	-	3/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.11	118.04	122.82
14	T	1	FME	CA-N-CN	-2.72	118.64	122.82
14	t	1	FME	O-C-CA	-2.62	117.90	124.78
12	M	1	FME	CA-N-CN	-2.47	119.02	122.82
14	T	1	FME	O-C-CA	-2.30	118.74	124.78
14	t	1	FME	C-CA-N	2.23	113.76	109.73
8	i	1	FME	CA-N-CN	-2.22	119.41	122.82
8	i	1	FME	O-C-CA	-2.16	119.12	124.78
8	I	1	FME	O-C-CA	-2.14	119.16	124.78
14	t	1	FME	O1-CN-N	-2.10	119.75	125.27
14	T	1	FME	C-CA-N	2.05	113.44	109.73
12	m	1	FME	O-C-CA	-2.04	119.44	124.78
8	I	1	FME	CA-N-CN	-2.02	119.72	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 18 are unknown and 24 are monoatomic - leaving 224 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PL9	A	416[A]	-	55,55,55	0.62	1 (1%)	68,69,69	1.76	21 (30%)
23	CLA	c	507	-	59,73,73	1.97	13 (22%)	67,113,113	2.16	20 (29%)
33	HTG	b	601	-	19,19,19	1.03	1 (5%)	23,24,24	1.20	2 (8%)
38	LHG	D	411	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	3 (5%)
26	GOL	B	628	-	5,5,5	0.38	0	5,5,5	0.33	0
24	BCR	b	628	-	41,41,41	1.06	1 (2%)	56,56,56	1.24	6 (10%)
26	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.21	0
30	PL9	d	407[A]	-	55,55,55	0.66	2 (3%)	68,69,69	1.55	13 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	GOL	B	633	-	5,5,5	0.41	0	5,5,5	0.45	0
35	LMG	D	417	40	51,51,55	0.93	2 (3%)	59,59,63	0.98	4 (6%)
23	CLA	c	509	-	59,73,73	1.98	13 (22%)	67,113,113	2.22	19 (28%)
23	CLA	B	612	-	59,73,73	2.04	13 (22%)	67,113,113	2.18	21 (31%)
35	LMG	c	522	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
26	GOL	C	525	-	5,5,5	0.44	0	5,5,5	0.61	0
24	BCR	B	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.52	12 (21%)
23	CLA	c	515	3	59,73,73	1.97	12 (20%)	67,113,113	2.08	22 (32%)
23	CLA	C	510	-	59,73,73	2.09	13 (22%)	67,113,113	2.18	24 (35%)
26	GOL	B	627	-	5,5,5	0.43	0	5,5,5	0.47	0
23	CLA	A	406	41	59,73,73	1.93	13 (22%)	67,113,113	2.12	24 (35%)
26	GOL	V	201	-	5,5,5	0.36	0	5,5,5	0.29	0
35	LMG	C	520	-	51,51,55	0.97	2 (3%)	59,59,63	1.08	4 (6%)
24	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	11 (19%)
24	BCR	T	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	15 (26%)
27	LMT	D	405	-	36,36,36	0.46	0	47,47,47	0.99	1 (2%)
34	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	1.02	5 (6%)
24	BCR	a	413	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	9 (16%)
23	CLA	C	508	41	59,73,73	1.97	13 (22%)	67,113,113	2.11	22 (32%)
23	CLA	C	502	-	59,73,73	2.01	13 (22%)	67,113,113	2.17	21 (31%)
24	BCR	c	527	-	41,41,41	1.04	1 (2%)	56,56,56	1.65	10 (17%)
27	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.83	0
33	HTG	c	525	-	19,19,19	1.01	2 (10%)	23,24,24	1.47	3 (13%)
23	CLA	b	621	-	59,73,73	2.04	12 (20%)	67,113,113	2.34	25 (37%)
34	DGD	h	102	-	63,63,67	0.89	3 (4%)	77,77,81	0.98	6 (7%)
35	LMG	M	101	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	4 (6%)
36	BCT	d	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
26	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.46	0
23	CLA	C	514	-	59,73,73	2.00	13 (22%)	67,113,113	2.10	22 (32%)
23	CLA	C	507	-	59,73,73	2.01	13 (22%)	67,113,113	2.16	23 (34%)
34	DGD	D	410	-	52,52,67	1.04	3 (5%)	60,60,81	1.18	5 (8%)
39	HEM	V	206	16	27,50,50	0.85	1 (3%)	17,82,82	1.60	3 (17%)
26	GOL	D	404	-	5,5,5	0.45	0	5,5,5	0.43	0
26	GOL	A	410	-	5,5,5	0.35	0	5,5,5	0.54	0
23	CLA	c	516	-	59,73,73	2.03	13 (22%)	67,113,113	2.29	21 (31%)
33	HTG	b	632	-	19,19,19	1.17	2 (10%)	23,24,24	2.03	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	615	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	20 (29%)
23	CLA	C	512	3	59,73,73	2.06	13 (22%)	67,113,113	2.11	20 (29%)
23	CLA	B	605	-	59,73,73	1.90	13 (22%)	67,113,113	2.22	21 (31%)
26	GOL	B	624	-	5,5,5	0.39	0	5,5,5	0.29	0
33	HTG	o	301	-	19,19,19	1.13	1 (5%)	23,24,24	1.37	1 (4%)
26	GOL	a	402	-	5,5,5	0.39	0	5,5,5	0.21	0
23	CLA	C	505	41	59,73,73	2.10	14 (23%)	67,113,113	2.21	23 (34%)
26	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.40	0
23	CLA	B	602	41	59,73,73	2.02	14 (23%)	67,113,113	2.18	20 (29%)
23	CLA	B	610	-	59,73,73	1.97	13 (22%)	67,113,113	2.15	21 (31%)
26	GOL	C	524	-	5,5,5	0.36	0	5,5,5	0.65	0
26	GOL	v	201	-	5,5,5	0.38	0	5,5,5	0.33	0
34	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.09	6 (7%)
23	CLA	a	410	41	59,73,73	2.00	12 (20%)	67,113,113	2.07	23 (34%)
23	CLA	c	512	-	59,73,73	2.07	13 (22%)	67,113,113	2.24	24 (35%)
26	GOL	O	301	-	5,5,5	0.37	0	5,5,5	0.36	0
23	CLA	b	611	-	59,73,73	2.04	13 (22%)	67,113,113	2.16	22 (32%)
26	GOL	A	411	-	5,5,5	0.41	0	5,5,5	0.25	0
23	CLA	B	609	-	59,73,73	2.02	15 (25%)	67,113,113	2.17	25 (37%)
39	HEM	e	101	5,6	27,50,50	0.81	1 (3%)	17,82,82	2.10	3 (17%)
26	GOL	c	501	-	5,5,5	0.44	0	5,5,5	0.43	0
24	BCR	d	406	-	41,41,41	1.08	1 (2%)	56,56,56	1.62	10 (17%)
33	HTG	V	207	-	19,19,19	1.04	2 (10%)	23,24,24	1.39	4 (17%)
23	CLA	C	503	-	59,73,73	2.04	13 (22%)	67,113,113	2.13	21 (31%)
25	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.18	4 (6%)
24	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.67	12 (21%)
25	SQD	f	102	-	42,43,54	1.20	3 (7%)	51,54,65	1.44	8 (15%)
34	DGD	C	516	-	63,63,67	0.86	2 (3%)	77,77,81	1.11	6 (7%)
37	PHO	D	402	-	67,69,69	2.13	16 (23%)	85,99,99	1.94	28 (32%)
24	BCR	B	618	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	8 (14%)
26	GOL	b	606	-	5,5,5	0.38	0	5,5,5	0.27	0
24	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	13 (23%)
25	SQD	A	409	-	53,54,54	0.99	3 (5%)	62,65,65	1.45	10 (16%)
27	LMT	M	104	-	36,36,36	0.55	0	47,47,47	0.99	3 (6%)
34	DGD	c	521	-	63,63,67	0.85	2 (3%)	77,77,81	1.06	3 (3%)
38	LHG	d	409	-	48,48,48	0.86	3 (6%)	51,54,54	1.00	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HTG	b	631	-	19,19,19	0.89	1 (5%)	23,24,24	1.38	3 (13%)
35	LMG	Z	101	-	37,37,55	0.97	3 (8%)	45,45,63	1.33	6 (13%)
34	DGD	c	520	-	63,63,67	0.89	2 (3%)	77,77,81	0.99	4 (5%)
23	CLA	A	405	41	59,73,73	2.03	13 (22%)	67,113,113	2.33	25 (37%)
33	HTG	B	623	-	19,19,19	1.06	2 (10%)	23,24,24	1.96	4 (17%)
28	OEX	a	417[A]	1,3,41	0,15,15	0.00	-	-		
23	CLA	c	510	-	59,73,73	1.97	12 (20%)	67,113,113	2.10	25 (37%)
27	LMT	M	105	-	36,36,36	0.48	0	47,47,47	0.88	1 (2%)
23	CLA	B	614	-	59,73,73	2.05	13 (22%)	67,113,113	2.16	23 (34%)
35	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.05	4 (6%)
24	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.70	11 (19%)
23	CLA	D	406	-	59,73,73	1.98	13 (22%)	67,113,113	2.24	21 (31%)
35	LMG	d	416	40	51,51,55	0.89	2 (3%)	59,59,63	1.10	5 (8%)
26	GOL	c	528	-	5,5,5	0.41	0	5,5,5	0.33	0
23	CLA	d	405	-	59,73,73	2.00	13 (22%)	67,113,113	2.18	23 (34%)
26	GOL	b	602	-	5,5,5	0.39	0	5,5,5	0.59	0
23	CLA	b	622	-	59,73,73	2.02	14 (23%)	67,113,113	2.15	23 (34%)
23	CLA	B	617	-	59,73,73	1.96	12 (20%)	67,113,113	2.23	21 (31%)
24	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.64	11 (19%)
23	CLA	c	513	-	59,73,73	2.08	13 (22%)	67,113,113	2.23	23 (34%)
24	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.56	13 (23%)
33	HTG	B	629	-	19,19,19	1.03	2 (10%)	23,24,24	1.42	1 (4%)
27	LMT	m	102	-	36,36,36	0.47	0	47,47,47	1.05	3 (6%)
27	LMT	a	404	-	36,36,36	0.57	1 (2%)	47,47,47	1.22	4 (8%)
38	LHG	d	411	-	48,48,48	0.93	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	604	-	59,73,73	2.04	13 (22%)	67,113,113	2.25	21 (31%)
35	LMG	c	523	-	51,51,55	0.95	2 (3%)	59,59,63	1.22	7 (11%)
38	LHG	D	413	-	48,48,48	0.95	2 (4%)	51,54,54	1.15	5 (9%)
24	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.53	10 (17%)
33	HTG	B	630	-	19,19,19	1.05	2 (10%)	23,24,24	1.36	1 (4%)
23	CLA	B	607	-	59,73,73	2.00	13 (22%)	67,113,113	2.21	21 (31%)
23	CLA	c	506	-	59,73,73	2.02	13 (22%)	67,113,113	2.10	21 (31%)
39	HEM	v	205	16	27,50,50	0.96	2 (7%)	17,82,82	1.58	2 (11%)
30	PL9	d	407[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.68	20 (29%)
38	LHG	d	410	-	48,48,48	0.89	2 (4%)	51,54,54	0.95	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	409	-	59,73,73	2.05	14 (23%)	67,113,113	2.21	21 (31%)
27	LMT	F	101	-	36,36,36	0.49	0	47,47,47	0.99	2 (4%)
26	GOL	V	203	-	5,5,5	0.35	0	5,5,5	0.43	0
23	CLA	b	618	-	59,73,73	1.99	12 (20%)	67,113,113	2.28	22 (32%)
35	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.18	4 (8%)
23	CLA	b	614	-	59,73,73	1.98	12 (20%)	67,113,113	2.29	21 (31%)
23	CLA	C	511	-	59,73,73	2.10	13 (22%)	67,113,113	2.17	23 (34%)
26	GOL	V	205	-	5,5,5	0.35	0	5,5,5	0.22	0
26	GOL	b	603	-	5,5,5	0.37	0	5,5,5	0.15	0
29	OEY	A	415[B]	1,3,41	0,16,16	0.00	-	-		
27	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.64	0
33	HTG	c	524	-	19,19,19	1.07	2 (10%)	23,24,24	1.65	2 (8%)
33	HTG	d	414	-	16,16,19	1.19	2 (12%)	20,21,24	1.84	2 (10%)
23	CLA	B	611	41	59,73,73	2.06	12 (20%)	67,113,113	2.15	25 (37%)
24	BCR	D	408	-	41,41,41	1.03	1 (2%)	56,56,56	1.77	12 (21%)
39	HEM	F	102	5,6	27,50,50	0.85	2 (7%)	17,82,82	2.31	3 (17%)
25	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.15	6 (9%)
23	CLA	b	625	-	59,73,73	1.99	14 (23%)	67,113,113	2.21	20 (29%)
37	PHO	D	403[B]	-	67,69,69	2.20	17 (25%)	85,99,99	1.85	22 (25%)
27	LMT	e	102	-	36,36,36	0.49	1 (2%)	47,47,47	0.80	0
26	GOL	b	604	-	5,5,5	0.34	0	5,5,5	0.26	0
37	PHO	D	403[A]	-	67,69,69	2.15	16 (23%)	85,99,99	1.94	20 (23%)
29	OEY	a	418[B]	1,3,41	0,16,16	0.00	-	-		
23	CLA	A	404	-	59,73,73	2.02	12 (20%)	67,113,113	2.28	23 (34%)
38	LHG	D	412	-	48,48,48	0.92	2 (4%)	51,54,54	0.82	2 (3%)
35	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	6 (10%)
34	DGD	d	408	-	63,63,67	0.95	2 (3%)	77,77,81	1.30	7 (9%)
23	CLA	b	623	-	59,73,73	1.96	12 (20%)	67,113,113	2.23	23 (34%)
23	CLA	A	407	-	59,73,73	2.01	13 (22%)	67,113,113	2.17	24 (35%)
30	PL9	D	409[A]	-	55,55,55	0.63	2 (3%)	68,69,69	1.66	20 (29%)
25	SQD	F	104	-	42,43,54	1.18	3 (7%)	51,54,65	1.62	10 (19%)
26	GOL	f	101	32	5,5,5	0.32	0	5,5,5	0.41	0
23	CLA	B	603	-	59,73,73	2.02	13 (22%)	67,113,113	2.25	24 (35%)
26	GOL	v	202	-	5,5,5	0.37	0	5,5,5	0.38	0
36	BCT	d	401[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	403	41	59,73,73	2.03	11 (18%)	67,113,113	2.24	24 (35%)
38	LHG	b	634	-	48,48,48	0.95	2 (4%)	51,54,54	1.04	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	506	-	59,73,73	1.99	14 (23%)	67,113,113	2.19	18 (26%)
23	CLA	b	624	-	59,73,73	2.01	13 (22%)	67,113,113	2.06	22 (32%)
23	CLA	b	610	41	59,73,73	2.08	13 (22%)	67,113,113	2.15	20 (29%)
23	CLA	d	404	-	59,73,73	1.97	14 (23%)	67,113,113	2.33	25 (37%)
23	CLA	b	620	-	59,73,73	1.97	12 (20%)	67,113,113	2.17	23 (34%)
23	CLA	C	509	-	59,73,73	2.09	13 (22%)	67,113,113	2.15	19 (28%)
24	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.30	7 (12%)
33	HTG	C	523	-	19,19,19	1.01	1 (5%)	23,24,24	1.76	4 (17%)
23	CLA	b	612	-	59,73,73	2.02	13 (22%)	67,113,113	2.36	23 (34%)
36	BCT	D	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
36	BCT	D	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
30	PL9	a	416[A]	-	55,55,55	0.61	2 (3%)	68,69,69	1.91	20 (29%)
30	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.83	21 (30%)
26	GOL	V	204	-	5,5,5	0.40	0	5,5,5	0.22	0
26	GOL	F	103	32	5,5,5	0.37	0	5,5,5	0.27	0
23	CLA	B	615	-	59,73,73	2.07	13 (22%)	67,113,113	2.24	24 (35%)
23	CLA	c	514	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	23 (34%)
37	PHO	d	402[A]	-	67,69,69	2.13	16 (23%)	85,99,99	2.01	22 (25%)
23	CLA	D	407	-	59,73,73	2.01	13 (22%)	67,113,113	2.08	22 (32%)
27	LMT	A	413	-	36,36,36	0.56	1 (2%)	47,47,47	1.30	7 (14%)
27	LMT	t	101	-	25,25,36	0.51	0	30,30,47	0.84	1 (3%)
23	CLA	B	608	41	59,73,73	1.96	14 (23%)	67,113,113	2.20	23 (34%)
30	PL9	A	416[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.77	22 (32%)
34	DGD	B	632	-	63,63,67	0.89	2 (3%)	77,77,81	1.10	6 (7%)
27	LMT	a	419	-	36,36,36	0.43	0	47,47,47	0.81	1 (2%)
35	LMG	b	629	-	51,51,55	0.91	2 (3%)	59,59,63	1.09	3 (5%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.09	4 (7%)
33	HTG	b	607	-	19,19,19	1.04	1 (5%)	23,24,24	1.78	4 (17%)
25	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.60	11 (17%)
27	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.06	3 (6%)
28	OEX	A	414[A]	1,3,41	0,15,15	0.00	-	-		
24	BCR	Y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.67	11 (19%)
26	GOL	B	626	-	5,5,5	0.38	0	5,5,5	0.47	0
23	CLA	b	616	41	59,73,73	2.01	13 (22%)	67,113,113	2.08	20 (29%)
23	CLA	b	617	-	59,73,73	2.02	13 (22%)	67,113,113	2.14	25 (37%)
23	CLA	C	513	-	59,73,73	2.06	13 (22%)	67,113,113	2.25	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PHO	d	402[B]	-	67,69,69	2.14	16 (23%)	85,99,99	1.94	21 (24%)
30	PL9	D	409[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.77	18 (26%)
24	BCR	K	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.45	8 (14%)
34	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.07	8 (10%)
23	CLA	c	511	41	59,73,73	2.01	12 (20%)	67,113,113	2.19	22 (32%)
26	GOL	B	625	-	5,5,5	0.42	0	5,5,5	0.46	0
26	GOL	c	502	-	5,5,5	0.43	0	5,5,5	0.42	0
23	CLA	B	606	-	59,73,73	2.01	13 (22%)	67,113,113	2.09	19 (28%)
26	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.29	0
23	CLA	c	505	-	59,73,73	1.97	14 (23%)	67,113,113	2.15	23 (34%)
27	LMT	T	104	-	25,25,36	0.55	1 (4%)	30,30,47	0.96	1 (3%)
23	CLA	B	616	-	59,73,73	2.03	13 (22%)	67,113,113	2.18	20 (29%)
23	CLA	c	517	-	59,73,73	2.03	13 (22%)	67,113,113	2.12	22 (32%)
33	HTG	B	622	-	19,19,19	0.87	1 (5%)	23,24,24	1.76	3 (13%)
23	CLA	a	412	-	59,73,73	2.00	12 (20%)	67,113,113	2.25	25 (37%)
26	GOL	t	103	-	5,5,5	0.49	0	5,5,5	0.22	0
38	LHG	E	101	-	41,41,48	1.02	2 (4%)	44,47,54	1.14	4 (9%)
24	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	9 (16%)
23	CLA	c	508	41	59,73,73	2.02	12 (20%)	67,113,113	2.26	24 (35%)
24	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.56	9 (16%)
25	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.37	8 (12%)
33	HTG	D	416	-	16,16,19	1.08	2 (12%)	20,21,24	1.44	1 (5%)
37	PHO	a	411	-	67,69,69	2.14	16 (23%)	85,99,99	1.89	21 (24%)
24	BCR	b	626	-	41,41,41	1.07	1 (2%)	56,56,56	1.55	7 (12%)
23	CLA	b	619	41	59,73,73	2.00	13 (22%)	67,113,113	2.13	23 (34%)
38	LHG	a	420	-	41,41,48	1.02	2 (4%)	44,47,54	0.99	2 (4%)
35	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.16	7 (11%)
33	HTG	C	522	-	19,19,19	1.00	2 (10%)	23,24,24	1.51	2 (8%)
23	CLA	B	613	-	59,73,73	1.99	14 (23%)	67,113,113	2.17	21 (31%)
33	HTG	b	608	-	19,19,19	1.08	2 (10%)	23,24,24	1.13	1 (4%)
24	BCR	A	408	-	41,41,41	1.07	1 (2%)	56,56,56	1.26	5 (8%)
26	GOL	b	605	-	5,5,5	0.39	0	5,5,5	0.26	0
26	GOL	v	203	-	5,5,5	0.38	0	5,5,5	0.24	0
25	SQD	a	414	-	53,54,54	0.97	3 (5%)	62,65,65	1.54	12 (19%)
23	CLA	C	504	-	59,73,73	2.04	13 (22%)	67,113,113	2.10	21 (31%)
23	CLA	b	613	-	59,73,73	2.03	13 (22%)	67,113,113	2.25	20 (29%)

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
30	PL9	A	416[A]	-	-	10/53/73/73	0/1/1/1
23	CLA	c	507	-	3/3/20/25	3/37/135/135	-
33	HTG	b	601	-	-	3/10/30/30	0/1/1/1
38	LHG	D	411	-	-	16/53/53/53	-
26	GOL	B	628	-	-	2/4/4/4	-
24	BCR	b	628	-	-	0/29/63/63	0/2/2/2
26	GOL	T	101	-	-	0/4/4/4	-
30	PL9	d	407[A]	-	-	8/53/73/73	0/1/1/1
26	GOL	B	633	-	-	0/4/4/4	-
35	LMG	D	417	40	-	9/46/66/70	0/1/1/1
23	CLA	c	509	-	2/2/20/25	8/37/135/135	-
23	CLA	B	612	-	3/3/20/25	5/37/135/135	-
35	LMG	c	522	-	-	17/46/66/70	0/1/1/1
26	GOL	C	525	-	-	2/4/4/4	-
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	c	515	3	3/3/20/25	5/37/135/135	-
23	CLA	C	510	-	3/3/20/25	10/37/135/135	-
39	HEM	F	102	5,6	-	0/6/54/54	-
26	GOL	B	627	-	-	4/4/4/4	-
23	CLA	A	406	41	2/2/20/25	4/37/135/135	-
26	GOL	V	201	-	-	2/4/4/4	-
35	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	BCR	K	103	-	-	4/29/63/63	0/2/2/2
24	BCR	T	103	-	-	1/29/63/63	0/2/2/2
27	LMT	D	405	-	-	11/21/61/61	0/2/2/2
34	DGD	C	518	-	-	9/51/91/95	0/2/2/2
24	BCR	a	413	-	-	1/29/63/63	0/2/2/2
23	CLA	C	508	41	3/3/20/25	5/37/135/135	-
23	CLA	C	502	-	3/3/20/25	10/37/135/135	-
24	BCR	c	527	-	-	0/29/63/63	0/2/2/2
27	LMT	M	102	-	-	7/21/61/61	0/2/2/2
33	HTG	c	525	-	-	0/10/30/30	0/1/1/1
23	CLA	b	621	-	3/3/20/25	4/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	h	102	-	-	8/51/91/95	0/2/2/2
35	LMG	M	101	-	-	7/46/66/70	0/1/1/1
26	GOL	a	401	-	-	2/4/4/4	-
23	CLA	C	514	-	3/3/20/25	9/37/135/135	-
23	CLA	C	507	-	3/3/20/25	9/37/135/135	-
34	DGD	D	410	-	-	18/47/67/95	0/1/1/2
39	HEM	V	206	16	-	0/6/54/54	-
26	GOL	D	404	-	-	2/4/4/4	-
26	GOL	A	410	-	-	1/4/4/4	-
23	CLA	c	516	-	3/3/20/25	7/37/135/135	-
33	HTG	b	632	-	-	4/10/30/30	0/1/1/1
23	CLA	b	615	-	3/3/20/25	8/37/135/135	-
23	CLA	C	512	3	3/3/20/25	3/37/135/135	-
23	CLA	B	605	-	3/3/20/25	4/37/135/135	-
26	GOL	B	624	-	-	0/4/4/4	-
33	HTG	V	207	-	-	4/10/30/30	0/1/1/1
33	HTG	o	301	-	-	3/10/30/30	0/1/1/1
26	GOL	a	402	-	-	2/4/4/4	-
26	GOL	V	202	-	-	4/4/4/4	-
23	CLA	B	602	41	3/3/20/25	14/37/135/135	-
23	CLA	B	610	-	2/2/20/25	8/37/135/135	-
26	GOL	C	524	-	-	1/4/4/4	-
26	GOL	v	201	-	-	2/4/4/4	-
34	DGD	c	519	-	-	13/51/91/95	0/2/2/2
23	CLA	a	410	41	2/2/20/25	7/37/135/135	-
23	CLA	c	512	-	3/3/20/25	4/37/135/135	-
26	GOL	O	301	-	-	0/4/4/4	-
23	CLA	b	611	-	2/2/20/25	3/37/135/135	-
26	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	609	-	2/2/20/25	1/37/135/135	-
39	HEM	e	101	5,6	-	0/6/54/54	-
26	GOL	c	501	-	-	2/4/4/4	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/20/25	9/37/135/135	-
23	CLA	C	503	-	2/2/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SQD	a	405	-	-	13/49/69/69	0/1/1/1
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	SQD	f	102	-	-	14/38/58/69	0/1/1/1
34	DGD	C	516	-	-	15/51/91/95	0/2/2/2
37	PHO	D	402	-	-	3/53/103/103	0/5/6/6
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	GOL	b	606	-	-	4/4/4/4	-
24	BCR	c	518	-	-	4/29/63/63	0/2/2/2
25	SQD	A	409	-	-	11/49/69/69	0/1/1/1
27	LMT	M	104	-	-	9/21/61/61	0/2/2/2
34	DGD	c	521	-	-	12/51/91/95	0/2/2/2
38	LHG	d	409	-	-	14/53/53/53	-
33	HTG	b	631	-	-	2/10/30/30	0/1/1/1
35	LMG	Z	101	-	-	15/31/51/70	0/1/1/1
34	DGD	c	520	-	-	17/51/91/95	0/2/2/2
23	CLA	A	405	41	3/3/20/25	7/37/135/135	-
33	HTG	B	623	-	-	3/10/30/30	0/1/1/1
23	CLA	c	510	-	3/3/20/25	17/37/135/135	-
27	LMT	M	105	-	-	7/21/61/61	0/2/2/2
23	CLA	B	614	-	3/3/20/25	9/37/135/135	-
35	LMG	C	519	-	-	10/46/66/70	0/1/1/1
24	BCR	k	102	-	-	6/29/63/63	0/2/2/2
23	CLA	D	406	-	1/1/20/25	1/37/135/135	-
35	LMG	d	416	40	-	10/46/66/70	0/1/1/1
26	GOL	c	528	-	-	0/4/4/4	-
23	CLA	d	405	-	3/3/20/25	7/37/135/135	-
26	GOL	b	602	-	-	0/4/4/4	-
23	CLA	b	622	-	3/3/20/25	5/37/135/135	-
23	CLA	B	617	-	3/3/20/25	7/37/135/135	-
24	BCR	C	515	-	-	6/29/63/63	0/2/2/2
23	CLA	c	513	-	3/3/20/25	16/37/135/135	-
24	BCR	t	102	-	-	3/29/63/63	0/2/2/2
33	HTG	B	629	-	-	1/10/30/30	0/1/1/1
27	LMT	m	102	-	-	7/21/61/61	0/2/2/2
27	LMT	a	404	-	-	5/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	d	411	-	-	18/53/53/53	-
23	CLA	B	604	-	3/3/20/25	7/37/135/135	-
35	LMG	c	523	-	-	5/46/66/70	0/1/1/1
38	LHG	D	413	-	-	20/53/53/53	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	HTG	B	630	-	-	1/10/30/30	0/1/1/1
23	CLA	B	607	-	2/2/20/25	6/37/135/135	-
23	CLA	c	506	-	3/3/20/25	3/37/135/135	-
39	HEM	v	205	16	-	0/6/54/54	-
30	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
38	LHG	d	410	-	-	11/53/53/53	-
23	CLA	a	409	-	3/3/20/25	5/37/135/135	-
27	LMT	F	101	-	-	4/21/61/61	0/2/2/2
26	GOL	V	203	-	-	1/4/4/4	-
23	CLA	b	618	-	3/3/20/25	5/37/135/135	-
35	LMG	z	101	-	-	16/34/54/70	0/1/1/1
23	CLA	b	614	-	3/3/20/25	7/37/135/135	-
23	CLA	C	511	-	3/3/20/25	10/37/135/135	-
26	GOL	V	205	-	-	4/4/4/4	-
26	GOL	b	603	-	-	0/4/4/4	-
23	CLA	b	620	-	3/3/20/25	8/37/135/135	-
27	LMT	b	630	-	-	3/17/37/61	0/1/1/2
33	HTG	c	524	-	-	3/10/30/30	0/1/1/1
33	HTG	d	414	-	-	0/7/27/30	0/1/1/1
23	CLA	B	611	41	3/3/20/25	4/37/135/135	-
24	BCR	D	408	-	-	8/29/63/63	0/2/2/2
23	CLA	A	404	-	3/3/20/25	4/37/135/135	-
25	SQD	A	412	-	-	14/49/69/69	0/1/1/1
23	CLA	b	625	-	3/3/20/25	8/37/135/135	-
37	PHO	D	403[B]	-	-	3/53/103/103	0/5/6/6
27	LMT	e	102	-	-	8/21/61/61	0/2/2/2
26	GOL	b	604	-	-	3/4/4/4	-
37	PHO	D	403[A]	-	-	2/53/103/103	0/5/6/6
38	LHG	D	412	-	-	11/53/53/53	-
35	LMG	a	415	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	DGD	d	408	-	-	24/51/91/95	0/2/2/2
23	CLA	b	623	-	3/3/20/25	20/37/135/135	-
23	CLA	A	407	-	3/3/20/25	8/37/135/135	-
30	PL9	D	409[A]	-	-	8/53/73/73	0/1/1/1
25	SQD	F	104	-	-	13/38/58/69	0/1/1/1
26	GOL	f	101	32	-	3/4/4/4	-
23	CLA	B	603	-	3/3/20/25	6/37/135/135	-
26	GOL	v	202	-	-	3/4/4/4	-
23	CLA	d	403	41	3/3/20/25	6/37/135/135	-
38	LHG	b	634	-	-	19/53/53/53	-
23	CLA	C	506	-	1/1/20/25	8/37/135/135	-
23	CLA	b	624	-	3/3/20/25	4/37/135/135	-
23	CLA	b	610	41	3/3/20/25	14/37/135/135	-
23	CLA	d	404	-	1/1/20/25	4/37/135/135	-
23	CLA	C	509	-	3/3/20/25	6/37/135/135	-
24	BCR	b	627	-	-	2/29/63/63	0/2/2/2
33	HTG	C	523	-	-	3/10/30/30	0/1/1/1
23	CLA	b	612	-	3/3/20/25	7/37/135/135	-
23	CLA	c	514	-	3/3/20/25	10/37/135/135	-
30	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
30	PL9	a	416[B]	-	-	13/53/73/73	0/1/1/1
26	GOL	V	204	-	-	2/4/4/4	-
26	GOL	F	103	32	-	0/4/4/4	-
23	CLA	B	615	-	3/3/20/25	18/37/135/135	-
23	CLA	B	608	41	3/3/20/25	4/37/135/135	-
37	PHO	d	402[A]	-	-	3/53/103/103	0/5/6/6
23	CLA	D	407	-	3/3/20/25	3/37/135/135	-
27	LMT	A	413	-	-	6/21/61/61	0/2/2/2
27	LMT	t	101	-	-	7/17/37/61	0/1/1/2
30	PL9	A	416[B]	-	-	11/53/73/73	0/1/1/1
34	DGD	B	632	-	-	11/51/91/95	0/2/2/2
27	LMT	a	419	-	-	4/21/61/61	0/2/2/2
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
38	LHG	L	101	-	-	13/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	HTG	b	607	-	-	1/10/30/30	0/1/1/1
25	SQD	L	102	-	-	23/49/69/69	0/1/1/1
27	LMT	C	521	-	-	10/21/61/61	0/2/2/2
23	CLA	C	505	41	3/3/20/25	8/37/135/135	-
24	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	GOL	B	626	-	-	2/4/4/4	-
23	CLA	b	616	41	2/2/20/25	1/37/135/135	-
23	CLA	b	617	-	2/2/20/25	3/37/135/135	-
23	CLA	C	513	-	3/3/20/25	12/37/135/135	-
37	PHO	d	402[B]	-	-	3/53/103/103	0/5/6/6
30	PL9	D	409[B]	-	-	8/53/73/73	0/1/1/1
24	BCR	K	101	-	-	3/29/63/63	0/2/2/2
34	DGD	C	517	-	-	16/51/91/95	0/2/2/2
23	CLA	c	511	41	3/3/20/25	6/37/135/135	-
26	GOL	B	625	-	-	2/4/4/4	-
26	GOL	c	502	-	-	2/4/4/4	-
23	CLA	B	606	-	3/3/20/25	3/37/135/135	-
26	GOL	T	102	-	-	2/4/4/4	-
23	CLA	c	505	-	3/3/20/25	5/37/135/135	-
27	LMT	T	104	-	-	7/17/37/61	0/1/1/2
23	CLA	B	616	-	3/3/20/25	9/37/135/135	-
23	CLA	c	517	-	3/3/20/25	5/37/135/135	-
33	HTG	B	622	-	-	5/10/30/30	0/1/1/1
23	CLA	a	412	-	3/3/20/25	10/37/135/135	-
26	GOL	t	103	-	-	0/4/4/4	-
38	LHG	E	101	-	-	19/46/46/53	-
24	BCR	h	101	-	-	1/29/63/63	0/2/2/2
23	CLA	c	508	41	3/3/20/25	5/37/135/135	-
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	SQD	B	621	-	-	23/49/69/69	0/1/1/1
33	HTG	D	416	-	-	0/7/27/30	0/1/1/1
37	PHO	a	411	-	-	6/53/103/103	0/5/6/6
24	BCR	b	626	-	-	2/29/63/63	0/2/2/2
23	CLA	b	619	41	3/3/20/25	6/37/135/135	-
38	LHG	a	420	-	-	17/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	C	501	-	-	17/46/66/70	0/1/1/1
33	HTG	C	522	-	-	0/10/30/30	0/1/1/1
33	HTG	b	608	-	-	0/10/30/30	0/1/1/1
24	BCR	A	408	-	-	4/29/63/63	0/2/2/2
26	GOL	b	605	-	-	2/4/4/4	-
26	GOL	v	203	-	-	2/4/4/4	-
25	SQD	a	414	-	-	11/49/69/69	0/1/1/1
23	CLA	C	504	-	3/3/20/25	2/37/135/135	-
23	CLA	b	613	-	3/3/20/25	3/37/135/135	-

All (1167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3B-C2B	6.63	1.49	1.40
23	C	510	CLA	C3B-C2B	6.56	1.49	1.40
23	A	405	CLA	C3B-C2B	6.54	1.49	1.40
23	B	605	CLA	C3B-C2B	6.52	1.49	1.40
23	c	513	CLA	C3B-C2B	6.43	1.49	1.40
23	C	512	CLA	C3B-C2B	6.42	1.49	1.40
23	b	621	CLA	C3B-C2B	6.40	1.49	1.40
23	c	512	CLA	C3B-C2B	6.39	1.49	1.40
23	b	622	CLA	C3B-C2B	6.34	1.49	1.40
23	D	406	CLA	C3B-C2B	6.33	1.49	1.40
23	C	509	CLA	C3B-C2B	6.31	1.49	1.40
23	B	615	CLA	C3B-C2B	6.30	1.49	1.40
23	c	508	CLA	C3B-C2B	6.29	1.49	1.40
23	C	503	CLA	C3B-C2B	6.27	1.49	1.40
23	A	404	CLA	C3B-C2B	6.24	1.49	1.40
23	C	513	CLA	C3B-C2B	6.23	1.49	1.40
23	b	610	CLA	C3D-C2D	6.23	1.50	1.39
23	b	624	CLA	C3D-C2D	6.22	1.50	1.39
23	d	403	CLA	C3B-C2B	6.20	1.49	1.40
23	C	513	CLA	C3D-C2D	6.20	1.50	1.39
23	c	515	CLA	C3B-C2B	6.19	1.49	1.40
23	b	619	CLA	C3B-C2B	6.18	1.48	1.40
23	C	505	CLA	C3D-C2D	6.13	1.50	1.39
23	B	612	CLA	C3D-C2D	6.10	1.50	1.39
23	B	616	CLA	C3D-C2D	6.09	1.50	1.39
23	c	514	CLA	C3B-C2B	6.09	1.48	1.40
23	C	511	CLA	C3B-C2B	6.08	1.48	1.40
37	d	402[B]	PHO	C3B-C2B	6.07	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C3B-C2B	6.07	1.48	1.40
23	C	503	CLA	C3D-C2D	6.06	1.50	1.39
23	B	614	CLA	C3B-C2B	6.05	1.48	1.40
23	c	505	CLA	C3B-C2B	6.03	1.48	1.40
23	B	611	CLA	C3B-C2B	6.02	1.48	1.40
23	b	617	CLA	C3D-C2D	6.02	1.50	1.39
23	B	617	CLA	C3B-C2B	6.02	1.48	1.40
23	d	405	CLA	C3D-C2D	6.01	1.50	1.39
23	d	403	CLA	C3D-C2D	6.00	1.50	1.39
23	B	606	CLA	C3B-C2B	5.99	1.48	1.40
23	b	620	CLA	C3B-C2B	5.98	1.48	1.40
23	b	618	CLA	C3D-C2D	5.96	1.50	1.39
23	C	504	CLA	C3D-C2D	5.96	1.50	1.39
37	D	403[A]	PHO	C3B-C2B	5.96	1.49	1.37
23	C	507	CLA	C3D-C2D	5.95	1.50	1.39
23	A	407	CLA	C3B-C2B	5.94	1.48	1.40
23	b	614	CLA	C3B-C2B	5.94	1.48	1.40
23	b	611	CLA	C3B-C2B	5.92	1.48	1.40
23	C	510	CLA	C3D-C2D	5.91	1.50	1.39
23	c	517	CLA	C3D-C2D	5.91	1.50	1.39
23	b	612	CLA	C3B-C2B	5.91	1.48	1.40
23	a	409	CLA	C3B-C2B	5.90	1.48	1.40
23	B	609	CLA	C3B-C2B	5.89	1.48	1.40
23	B	603	CLA	C3B-C2B	5.88	1.48	1.40
23	b	613	CLA	C3B-C2B	5.88	1.48	1.40
23	C	512	CLA	C3D-C2D	5.88	1.50	1.39
37	d	402[A]	PHO	C3C-C2C	5.85	1.49	1.36
37	d	402[B]	PHO	C3C-C2C	5.85	1.49	1.36
37	D	402	PHO	C3B-C2B	5.84	1.49	1.37
37	D	403[B]	PHO	C3B-C2B	5.84	1.49	1.37
23	B	608	CLA	C3B-C2B	5.83	1.48	1.40
23	b	616	CLA	C3D-C2D	5.83	1.49	1.39
23	b	621	CLA	C3D-C2D	5.83	1.49	1.39
23	c	506	CLA	C3D-C2D	5.82	1.49	1.39
37	D	403[A]	PHO	C3C-C2C	5.82	1.49	1.36
23	c	510	CLA	C3B-C2B	5.81	1.48	1.40
23	c	512	CLA	C3D-C2D	5.81	1.49	1.39
23	C	514	CLA	C3B-C2B	5.81	1.48	1.40
23	C	506	CLA	C3B-C2B	5.80	1.48	1.40
23	a	409	CLA	C3D-C2D	5.80	1.49	1.39
23	a	412	CLA	C3D-C2D	5.80	1.49	1.39
23	B	604	CLA	C3B-C2B	5.79	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C3D-C2D	5.79	1.49	1.39
23	A	406	CLA	C3D-C2D	5.78	1.49	1.39
23	C	511	CLA	C3D-C2D	5.78	1.49	1.39
23	d	404	CLA	C3B-C2B	5.78	1.48	1.40
23	A	404	CLA	C3D-C2D	5.77	1.49	1.39
23	B	614	CLA	C3D-C2D	5.77	1.49	1.39
23	A	405	CLA	C3D-C2D	5.75	1.49	1.39
23	c	516	CLA	C3D-C2D	5.74	1.49	1.39
23	B	615	CLA	C3D-C2D	5.74	1.49	1.39
37	a	411	PHO	C3C-C2C	5.74	1.48	1.36
23	A	407	CLA	C3D-C2D	5.73	1.49	1.39
23	a	412	CLA	C3B-C2B	5.73	1.48	1.40
23	b	625	CLA	C3B-C2B	5.72	1.48	1.40
23	b	623	CLA	C3B-C2B	5.71	1.48	1.40
23	B	612	CLA	C3B-C2B	5.70	1.48	1.40
23	b	610	CLA	C3B-C2B	5.70	1.48	1.40
23	C	514	CLA	C3D-C2D	5.69	1.49	1.39
37	d	402[A]	PHO	C3B-C2B	5.69	1.48	1.37
23	B	611	CLA	C3D-C2D	5.69	1.49	1.39
23	b	612	CLA	C3D-C2D	5.69	1.49	1.39
23	c	508	CLA	C3D-C2D	5.69	1.49	1.39
37	D	402	PHO	C3C-C2C	5.68	1.48	1.36
23	b	615	CLA	C3B-C2B	5.67	1.48	1.40
23	B	604	CLA	C3C-C2C	5.66	1.48	1.36
23	C	502	CLA	C3B-C2B	5.65	1.48	1.40
23	B	603	CLA	C3C-C2C	5.65	1.48	1.36
37	a	411	PHO	C3B-C2B	5.64	1.48	1.37
23	C	509	CLA	C3C-C2C	5.64	1.48	1.36
23	c	506	CLA	C3B-C2B	5.63	1.48	1.40
23	C	509	CLA	C3D-C2D	5.63	1.49	1.39
23	b	625	CLA	C3D-C2D	5.63	1.49	1.39
37	D	403[B]	PHO	C3C-C2C	5.62	1.48	1.36
23	B	611	CLA	C3C-C2C	5.61	1.48	1.36
23	B	609	CLA	C3D-C2D	5.61	1.49	1.39
23	C	507	CLA	C3B-C2B	5.61	1.48	1.40
23	d	404	CLA	C3D-C2D	5.60	1.49	1.39
23	b	613	CLA	OBD-CAD	5.58	1.30	1.22
23	a	410	CLA	C3B-C2B	5.58	1.48	1.40
23	C	504	CLA	C3B-C2B	5.58	1.48	1.40
23	B	615	CLA	C3C-C2C	5.57	1.48	1.36
23	b	615	CLA	C3C-C2C	5.57	1.48	1.36
23	b	610	CLA	C3C-C2C	5.57	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	407	CLA	C3B-C2B	5.57	1.48	1.40
23	b	620	CLA	C3D-C2D	5.57	1.49	1.39
23	B	602	CLA	C3B-C2B	5.56	1.48	1.40
23	a	412	CLA	C3C-C2C	5.55	1.48	1.36
23	b	613	CLA	C3D-C2D	5.55	1.49	1.39
23	D	407	CLA	C3D-C2D	5.54	1.49	1.39
23	c	509	CLA	C3B-C2B	5.54	1.48	1.40
23	A	405	CLA	C3C-C2C	5.54	1.48	1.36
23	B	616	CLA	O2D-CGD	5.54	1.46	1.33
23	B	613	CLA	C3D-C2D	5.53	1.49	1.39
23	b	622	CLA	C3C-C2C	5.53	1.48	1.36
23	c	514	CLA	C3D-C2D	5.52	1.49	1.39
23	D	406	CLA	C3D-C2D	5.52	1.49	1.39
23	C	511	CLA	C3C-C2C	5.52	1.48	1.36
23	C	508	CLA	C3B-C2B	5.51	1.48	1.40
23	B	607	CLA	C3B-C2B	5.50	1.48	1.40
23	c	511	CLA	CHC-C1C	5.50	1.49	1.35
23	C	513	CLA	C3C-C2C	5.50	1.48	1.36
23	B	607	CLA	C3C-C2C	5.50	1.48	1.36
23	B	602	CLA	C3D-C2D	5.50	1.49	1.39
23	c	511	CLA	C3D-C2D	5.49	1.49	1.39
23	c	507	CLA	C3B-C2B	5.49	1.48	1.40
23	c	515	CLA	C3D-C2D	5.49	1.49	1.39
23	b	622	CLA	C3D-C2D	5.48	1.49	1.39
23	c	517	CLA	C3B-C2B	5.48	1.48	1.40
23	C	502	CLA	CHC-C1C	5.47	1.49	1.35
23	c	505	CLA	C3D-C2D	5.47	1.49	1.39
23	C	504	CLA	C3C-C2C	5.47	1.48	1.36
23	c	507	CLA	C3C-C2C	5.46	1.48	1.36
23	b	622	CLA	O2D-CGD	5.46	1.46	1.33
23	C	508	CLA	C3D-C2D	5.46	1.49	1.39
23	b	614	CLA	C3D-C2D	5.45	1.49	1.39
23	c	516	CLA	C3B-C2B	5.45	1.47	1.40
23	b	614	CLA	C3C-C2C	5.44	1.48	1.36
23	B	604	CLA	CHC-C1C	5.44	1.48	1.35
23	C	508	CLA	CHC-C1C	5.43	1.48	1.35
23	c	513	CLA	C3D-C2D	5.42	1.49	1.39
23	B	616	CLA	C3B-C2B	5.41	1.47	1.40
23	C	510	CLA	C3C-C2C	5.40	1.48	1.36
23	D	406	CLA	C3C-C2C	5.40	1.48	1.36
23	C	502	CLA	C3D-C2D	5.40	1.49	1.39
23	a	412	CLA	O2D-CGD	5.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3D-C2D	5.39	1.49	1.39
23	b	617	CLA	C3C-C2C	5.39	1.48	1.36
23	b	624	CLA	C3B-C2B	5.39	1.47	1.40
23	b	623	CLA	C3D-C2D	5.39	1.49	1.39
23	c	514	CLA	C3C-C2C	5.38	1.48	1.36
23	b	618	CLA	C3B-C2B	5.37	1.47	1.40
23	c	509	CLA	CHC-C1C	5.36	1.48	1.35
23	B	617	CLA	C3C-C2C	5.36	1.48	1.36
23	C	504	CLA	CHC-C1C	5.35	1.48	1.35
23	b	612	CLA	C3C-C2C	5.35	1.48	1.36
23	B	606	CLA	C3D-C2D	5.34	1.49	1.39
23	b	624	CLA	OBD-CAD	5.34	1.29	1.22
23	a	410	CLA	C3D-C2D	5.34	1.49	1.39
24	k	101	BCR	C23-C22	-5.33	1.34	1.45
23	A	406	CLA	C3C-C2C	5.33	1.48	1.36
23	b	611	CLA	CHC-C1C	5.33	1.48	1.35
23	b	619	CLA	C3D-C2D	5.32	1.49	1.39
23	B	604	CLA	C3D-C2D	5.32	1.49	1.39
23	B	616	CLA	CHC-C1C	5.31	1.48	1.35
23	B	612	CLA	C3C-C2C	5.31	1.48	1.36
23	b	615	CLA	C3D-C2D	5.31	1.49	1.39
23	c	507	CLA	CHC-C1C	5.31	1.48	1.35
23	a	409	CLA	C3C-C2C	5.31	1.48	1.36
23	d	403	CLA	C3C-C2C	5.31	1.48	1.36
23	B	614	CLA	O2D-CGD	5.30	1.46	1.33
23	c	516	CLA	C3C-C2C	5.30	1.48	1.36
23	c	507	CLA	C3D-C2D	5.30	1.48	1.39
23	d	405	CLA	C3C-C2C	5.30	1.48	1.36
23	c	513	CLA	C3C-C2C	5.29	1.48	1.36
23	C	514	CLA	C3C-C2C	5.29	1.48	1.36
23	b	611	CLA	C3C-C2C	5.29	1.48	1.36
23	c	506	CLA	O2D-CGD	5.28	1.46	1.33
37	d	402[A]	PHO	CHC-C1C	5.28	1.48	1.38
23	c	516	CLA	CHC-C1C	5.28	1.48	1.35
23	b	616	CLA	C3C-C2C	5.27	1.47	1.36
37	D	403[B]	PHO	CHC-C1C	5.27	1.48	1.38
23	c	517	CLA	C3C-C2C	5.27	1.47	1.36
23	B	607	CLA	C3D-C2D	5.26	1.48	1.39
23	b	621	CLA	C3C-C2C	5.26	1.47	1.36
23	B	606	CLA	C3C-C2C	5.26	1.47	1.36
23	C	506	CLA	C3D-C2D	5.25	1.48	1.39
24	H	101	BCR	C23-C22	-5.25	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	411	PHO	CHC-C1C	5.25	1.48	1.38
37	D	402	PHO	CHB-C1B	5.25	1.48	1.38
23	b	617	CLA	CHC-C1C	5.25	1.48	1.35
23	c	510	CLA	O2D-CGD	5.24	1.46	1.33
23	C	508	CLA	C3C-C2C	5.24	1.47	1.36
23	c	508	CLA	O2D-CGD	5.24	1.46	1.33
23	c	506	CLA	C3C-C2C	5.24	1.47	1.36
23	c	512	CLA	O2D-CGD	5.24	1.46	1.33
23	C	503	CLA	C3C-C2C	5.24	1.47	1.36
23	c	512	CLA	C3C-C2C	5.23	1.47	1.36
23	a	410	CLA	CHC-C1C	5.23	1.48	1.35
23	b	624	CLA	C3C-C2C	5.23	1.47	1.36
23	b	623	CLA	C3C-C2C	5.23	1.47	1.36
23	b	610	CLA	CHC-C1C	5.23	1.48	1.35
23	D	407	CLA	CHC-C1C	5.22	1.48	1.35
23	c	511	CLA	C3C-C2C	5.22	1.47	1.36
23	c	511	CLA	C3B-C2B	5.22	1.47	1.40
23	B	617	CLA	C3D-C2D	5.22	1.48	1.39
23	c	508	CLA	CHC-C1C	5.22	1.48	1.35
23	C	503	CLA	CHC-C1C	5.21	1.48	1.35
23	b	619	CLA	C3C-C2C	5.21	1.47	1.36
23	a	410	CLA	OBD-CAD	5.20	1.29	1.22
24	K	103	BCR	C23-C22	-5.20	1.34	1.45
23	b	616	CLA	C3B-C2B	5.20	1.47	1.40
37	D	403[B]	PHO	CHB-C1B	5.19	1.48	1.38
23	C	511	CLA	O2D-CGD	5.19	1.45	1.33
23	b	625	CLA	CHC-C1C	5.19	1.48	1.35
23	B	603	CLA	CHC-C1C	5.18	1.48	1.35
23	D	407	CLA	C3C-C2C	5.18	1.47	1.36
23	b	618	CLA	CHC-C1C	5.18	1.48	1.35
23	B	602	CLA	C3C-C2C	5.18	1.47	1.36
23	b	617	CLA	C3B-C2B	5.18	1.47	1.40
23	c	505	CLA	C3C-C2C	5.18	1.47	1.36
23	B	613	CLA	CHC-C1C	5.18	1.48	1.35
23	b	612	CLA	CHC-C1C	5.18	1.48	1.35
37	D	403[A]	PHO	CHC-C1C	5.17	1.48	1.38
23	C	505	CLA	C3C-C2C	5.17	1.47	1.36
23	c	513	CLA	O2D-CGD	5.17	1.45	1.33
23	C	512	CLA	C3C-C2C	5.17	1.47	1.36
23	C	507	CLA	C3C-C2C	5.17	1.47	1.36
23	C	509	CLA	O2D-CGD	5.16	1.45	1.33
23	C	506	CLA	C3C-C2C	5.16	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	405	CLA	CHC-C1C	5.16	1.48	1.35
23	A	407	CLA	CHC-C1C	5.16	1.48	1.35
23	C	512	CLA	O2D-CGD	5.16	1.45	1.33
23	B	610	CLA	C3C-C2C	5.16	1.47	1.36
24	K	101	BCR	C23-C22	-5.15	1.34	1.45
23	c	513	CLA	CHC-C1C	5.15	1.48	1.35
23	B	602	CLA	O2D-CGD	5.15	1.45	1.33
23	b	620	CLA	O2D-CGD	5.15	1.45	1.33
23	c	515	CLA	CHC-C1C	5.15	1.48	1.35
23	b	616	CLA	O2D-CGD	5.15	1.45	1.33
23	D	407	CLA	O2D-CGD	5.14	1.45	1.33
23	b	618	CLA	O2D-CGD	5.14	1.45	1.33
23	B	603	CLA	C3D-C2D	5.14	1.48	1.39
37	D	403[A]	PHO	O2D-CGD	5.14	1.45	1.33
23	b	614	CLA	CHC-C1C	5.14	1.48	1.35
37	D	403[B]	PHO	O2D-CGD	5.14	1.45	1.33
23	B	608	CLA	C3D-C2D	5.14	1.48	1.39
23	c	510	CLA	C3C-C2C	5.13	1.47	1.36
23	d	405	CLA	C3B-C2B	5.13	1.47	1.40
23	B	614	CLA	C3C-C2C	5.13	1.47	1.36
23	b	611	CLA	OBD-CAD	5.13	1.29	1.22
23	B	612	CLA	O2D-CGD	5.13	1.45	1.33
23	B	607	CLA	CHC-C1C	5.13	1.48	1.35
23	C	514	CLA	CHC-C1C	5.13	1.48	1.35
23	C	505	CLA	O2D-CGD	5.12	1.45	1.33
23	B	611	CLA	CHC-C1C	5.12	1.48	1.35
23	C	512	CLA	CHC-C1C	5.11	1.48	1.35
23	B	606	CLA	O2D-CGD	5.11	1.45	1.33
23	c	515	CLA	C3C-C2C	5.11	1.47	1.36
23	B	609	CLA	C3C-C2C	5.11	1.47	1.36
23	C	511	CLA	OBD-CAD	5.11	1.29	1.22
24	a	413	BCR	C23-C22	-5.11	1.35	1.45
23	B	607	CLA	O2D-CGD	5.11	1.45	1.33
23	d	403	CLA	O2D-CGD	5.10	1.45	1.33
23	C	513	CLA	O2D-CGD	5.10	1.45	1.33
23	C	513	CLA	CHC-C1C	5.10	1.48	1.35
23	b	613	CLA	C3C-C2C	5.10	1.47	1.36
23	B	615	CLA	O2D-CGD	5.10	1.45	1.33
23	C	510	CLA	CHC-C1C	5.10	1.48	1.35
24	k	102	BCR	C23-C22	-5.10	1.35	1.45
37	D	403[B]	PHO	CHD-C1D	5.10	1.48	1.38
23	C	505	CLA	CHC-C1C	5.09	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	O2D-CGD	5.08	1.45	1.33
23	c	513	CLA	OBD-CAD	5.08	1.29	1.22
37	d	402[B]	PHO	CHB-C1B	5.08	1.48	1.38
37	d	402[B]	PHO	O2D-CGD	5.08	1.45	1.33
23	B	615	CLA	CHC-C1C	5.07	1.48	1.35
23	B	606	CLA	CHC-C1C	5.07	1.48	1.35
37	D	402	PHO	CHD-C1D	5.07	1.48	1.38
23	c	516	CLA	O2D-CGD	5.07	1.45	1.33
23	b	615	CLA	CHC-C1C	5.06	1.48	1.35
23	d	405	CLA	O2D-CGD	5.06	1.45	1.33
23	C	511	CLA	CHC-C1C	5.06	1.47	1.35
23	c	517	CLA	CHC-C1C	5.06	1.47	1.35
23	B	617	CLA	CHC-C1C	5.06	1.47	1.35
23	C	509	CLA	CHC-C1C	5.06	1.47	1.35
23	B	614	CLA	CHC-C1C	5.05	1.47	1.35
37	D	402	PHO	CHC-C1C	5.04	1.48	1.38
23	A	404	CLA	CHC-C1C	5.04	1.47	1.35
23	B	617	CLA	O2D-CGD	5.04	1.45	1.33
23	a	410	CLA	C3C-C2C	5.04	1.47	1.36
23	B	610	CLA	O2D-CGD	5.04	1.45	1.33
23	B	603	CLA	OBD-CAD	5.02	1.29	1.22
23	a	409	CLA	CHC-C1C	5.02	1.47	1.35
23	B	608	CLA	CHC-C1C	5.02	1.47	1.35
23	b	619	CLA	CHC-C1C	5.02	1.47	1.35
23	b	623	CLA	O2D-CGD	5.02	1.45	1.33
23	C	509	CLA	OBD-CAD	5.01	1.29	1.22
23	c	510	CLA	C3D-C2D	5.01	1.48	1.39
23	c	506	CLA	CHC-C1C	5.01	1.47	1.35
23	a	412	CLA	CHC-C1C	5.01	1.47	1.35
23	c	517	CLA	O2D-CGD	5.01	1.45	1.33
23	C	510	CLA	O2D-CGD	5.01	1.45	1.33
37	a	411	PHO	O2D-CGD	5.01	1.45	1.33
23	b	617	CLA	O2D-CGD	5.00	1.45	1.33
23	C	506	CLA	CHC-C1C	5.00	1.47	1.35
24	B	620	BCR	C23-C22	-5.00	1.35	1.45
23	b	616	CLA	CHC-C1C	5.00	1.47	1.35
24	Y	101	BCR	C23-C22	-5.00	1.35	1.45
23	b	618	CLA	C3C-C2C	4.99	1.47	1.36
37	d	402[B]	PHO	CHC-C1C	4.99	1.48	1.38
23	B	605	CLA	C3D-C2D	4.99	1.48	1.39
23	b	625	CLA	O2D-CGD	4.98	1.45	1.33
37	d	402[A]	PHO	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	621	CLA	CHC-C1C	4.98	1.47	1.35
23	B	612	CLA	OBD-CAD	4.98	1.29	1.22
23	a	409	CLA	OBD-CAD	4.98	1.29	1.22
23	c	509	CLA	C3C-C2C	4.97	1.47	1.36
23	A	406	CLA	O2D-CGD	4.97	1.45	1.33
23	A	407	CLA	C3C-C2C	4.97	1.47	1.36
23	b	623	CLA	CHC-C1C	4.96	1.47	1.35
24	c	527	BCR	C23-C22	-4.96	1.35	1.45
23	A	407	CLA	O2D-CGD	4.96	1.45	1.33
37	D	403[A]	PHO	CHB-C1B	4.96	1.48	1.38
23	B	605	CLA	CHC-C1C	4.96	1.47	1.35
37	a	411	PHO	CHB-C1B	4.96	1.48	1.38
23	C	507	CLA	CHC-C1C	4.95	1.47	1.35
23	b	625	CLA	C3C-C2C	4.95	1.47	1.36
23	B	609	CLA	CHC-C1C	4.95	1.47	1.35
37	a	411	PHO	CHD-C1D	4.95	1.48	1.38
23	B	610	CLA	CHC-C1C	4.95	1.47	1.35
24	b	628	BCR	C23-C22	-4.95	1.35	1.45
23	d	404	CLA	C3C-C2C	4.95	1.47	1.36
23	b	621	CLA	O2D-CGD	4.94	1.45	1.33
23	C	507	CLA	O2D-CGD	4.94	1.45	1.33
23	c	511	CLA	O2D-CGD	4.94	1.45	1.33
23	B	605	CLA	C3C-C2C	4.91	1.47	1.36
23	A	405	CLA	O2D-CGD	4.91	1.45	1.33
37	d	402[B]	PHO	CHD-C1D	4.91	1.48	1.38
23	c	510	CLA	CHC-C1C	4.91	1.47	1.35
23	b	612	CLA	O2D-CGD	4.91	1.45	1.33
23	B	616	CLA	C3C-C2C	4.90	1.47	1.36
23	c	512	CLA	CHC-C1C	4.90	1.47	1.35
23	B	608	CLA	O2D-CGD	4.89	1.45	1.33
23	C	502	CLA	C3C-C2C	4.89	1.47	1.36
23	B	610	CLA	C3B-C2B	4.89	1.47	1.40
23	B	604	CLA	O2D-CGD	4.89	1.45	1.33
23	B	609	CLA	O2D-CGD	4.89	1.45	1.33
24	A	408	BCR	C23-C22	-4.89	1.35	1.45
23	c	512	CLA	OBD-CAD	4.88	1.29	1.22
23	C	506	CLA	O2D-CGD	4.88	1.45	1.33
23	B	608	CLA	C3C-C2C	4.88	1.47	1.36
23	b	613	CLA	CHC-C1C	4.87	1.47	1.35
23	D	406	CLA	O2D-CGD	4.87	1.45	1.33
23	b	613	CLA	O2D-CGD	4.87	1.45	1.33
23	c	514	CLA	CHC-C1C	4.87	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C3B-C2B	4.87	1.47	1.40
24	T	103	BCR	C23-C22	-4.86	1.35	1.45
23	c	511	CLA	OBD-CAD	4.86	1.29	1.22
23	B	602	CLA	CHC-C1C	4.86	1.47	1.35
23	A	404	CLA	C3C-C2C	4.86	1.47	1.36
37	d	402[A]	PHO	CHB-C1B	4.86	1.48	1.38
23	b	621	CLA	OBD-CAD	4.85	1.29	1.22
23	c	517	CLA	OBD-CAD	4.85	1.29	1.22
23	c	505	CLA	CHC-C1C	4.85	1.47	1.35
23	d	404	CLA	CHC-C1C	4.84	1.47	1.35
23	B	613	CLA	C3C-C2C	4.84	1.47	1.36
23	b	620	CLA	CHC-C1C	4.83	1.47	1.35
24	C	515	BCR	C23-C22	-4.83	1.35	1.45
23	C	510	CLA	OBD-CAD	4.83	1.29	1.22
37	d	402[A]	PHO	CHD-C1D	4.82	1.48	1.38
23	B	611	CLA	OBD-CAD	4.82	1.29	1.22
23	A	406	CLA	CHC-C1C	4.82	1.47	1.35
24	b	626	BCR	C23-C22	-4.82	1.35	1.45
23	b	624	CLA	CHC-C1C	4.82	1.47	1.35
23	d	404	CLA	O2D-CGD	4.82	1.44	1.33
23	D	406	CLA	CHC-C1C	4.80	1.47	1.35
23	B	602	CLA	O2A-CGA	4.79	1.47	1.33
23	c	514	CLA	O2D-CGD	4.79	1.44	1.33
23	c	516	CLA	OBD-CAD	4.79	1.29	1.22
23	b	615	CLA	OBD-CAD	4.79	1.29	1.22
23	C	514	CLA	O2D-CGD	4.79	1.44	1.33
24	B	618	BCR	C23-C22	-4.79	1.35	1.45
23	c	507	CLA	O2D-CGD	4.79	1.44	1.33
23	c	508	CLA	C3C-C2C	4.78	1.46	1.36
37	D	402	PHO	O2D-CGD	4.78	1.44	1.33
23	d	403	CLA	CHC-C1C	4.78	1.47	1.35
23	C	504	CLA	O2D-CGD	4.77	1.44	1.33
23	B	603	CLA	O2D-CGD	4.77	1.44	1.33
24	d	406	BCR	C23-C22	-4.76	1.35	1.45
23	D	407	CLA	OBD-CAD	4.76	1.29	1.22
23	C	504	CLA	OBD-CAD	4.75	1.28	1.22
24	h	101	BCR	C23-C22	-4.75	1.35	1.45
23	A	407	CLA	OBD-CAD	4.75	1.28	1.22
23	b	611	CLA	O2D-CGD	4.74	1.44	1.33
23	b	622	CLA	CHC-C1C	4.74	1.47	1.35
23	C	505	CLA	OBD-CAD	4.74	1.28	1.22
23	b	620	CLA	C3C-C2C	4.74	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	O2D-CGD	4.73	1.44	1.33
23	b	614	CLA	O2D-CGD	4.72	1.44	1.33
23	B	616	CLA	OBD-CAD	4.72	1.28	1.22
23	b	617	CLA	OBD-CAD	4.71	1.28	1.22
23	B	614	CLA	OBD-CAD	4.70	1.28	1.22
24	t	102	BCR	C23-C22	-4.69	1.35	1.45
23	c	514	CLA	OBD-CAD	4.69	1.28	1.22
23	B	602	CLA	OBD-CAD	4.69	1.28	1.22
23	B	613	CLA	O2D-CGD	4.69	1.44	1.33
23	c	509	CLA	O2D-CGD	4.67	1.44	1.33
23	C	514	CLA	OBD-CAD	4.66	1.28	1.22
23	B	612	CLA	CHC-C1C	4.66	1.46	1.35
23	a	410	CLA	O2D-CGD	4.66	1.44	1.33
23	b	624	CLA	O2D-CGD	4.66	1.44	1.33
23	A	405	CLA	CHC-C1C	4.66	1.46	1.35
37	D	403[A]	PHO	CHD-C1D	4.65	1.47	1.38
23	C	502	CLA	OBD-CAD	4.65	1.28	1.22
24	c	518	BCR	C23-C22	-4.65	1.36	1.45
23	C	508	CLA	O2D-CGD	4.65	1.44	1.33
24	D	408	BCR	C23-C22	-4.65	1.36	1.45
23	c	510	CLA	OBD-CAD	4.65	1.28	1.22
23	c	509	CLA	OBD-CAD	4.64	1.28	1.22
23	b	620	CLA	OBD-CAD	4.64	1.28	1.22
23	A	404	CLA	O2D-CGD	4.64	1.44	1.33
23	C	513	CLA	OBD-CAD	4.64	1.28	1.22
23	c	509	CLA	C3D-C2D	4.64	1.47	1.39
23	C	502	CLA	O2D-CGD	4.63	1.44	1.33
23	B	615	CLA	OBD-CAD	4.63	1.28	1.22
23	C	503	CLA	O2D-CGD	4.63	1.44	1.33
23	C	506	CLA	OBD-CAD	4.62	1.28	1.22
23	A	406	CLA	OBD-CAD	4.62	1.28	1.22
23	b	615	CLA	O2D-CGD	4.62	1.44	1.33
23	c	515	CLA	O2D-CGD	4.61	1.44	1.33
23	d	405	CLA	OBD-CAD	4.60	1.28	1.22
24	b	627	BCR	C23-C22	-4.59	1.36	1.45
23	b	610	CLA	OBD-CAD	4.59	1.28	1.22
23	c	513	CLA	O2A-CGA	4.57	1.46	1.33
23	C	503	CLA	OBD-CAD	4.57	1.28	1.22
25	f	102	SQD	O47-C7	4.56	1.47	1.34
23	b	623	CLA	OBD-CAD	4.56	1.28	1.22
23	d	403	CLA	O2A-CGA	4.56	1.46	1.33
23	b	619	CLA	O2D-CGD	4.56	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	OBD-CAD	4.55	1.28	1.22
23	B	611	CLA	O2D-CGD	4.55	1.44	1.33
23	B	610	CLA	OBD-CAD	4.55	1.28	1.22
23	b	616	CLA	OBD-CAD	4.55	1.28	1.22
23	c	507	CLA	OBD-CAD	4.54	1.28	1.22
34	D	410	DGD	O1G-C1A	4.54	1.46	1.33
35	z	101	LMG	O8-C28	4.54	1.46	1.33
23	B	607	CLA	OBD-CAD	4.53	1.28	1.22
25	A	412	SQD	O48-C23	4.53	1.46	1.33
23	B	609	CLA	OBD-CAD	4.53	1.28	1.22
23	b	625	CLA	OBD-CAD	4.53	1.28	1.22
23	C	512	CLA	OBD-CAD	4.51	1.28	1.22
23	C	508	CLA	OBD-CAD	4.50	1.28	1.22
23	b	618	CLA	OBD-CAD	4.49	1.28	1.22
25	F	104	SQD	O47-C7	4.48	1.46	1.34
23	B	610	CLA	O2A-CGA	4.47	1.46	1.33
23	c	512	CLA	O2A-CGA	4.47	1.46	1.33
23	c	506	CLA	OBD-CAD	4.45	1.28	1.22
34	D	410	DGD	O2G-C1B	4.44	1.46	1.34
35	C	520	LMG	O7-C10	4.44	1.46	1.34
23	A	405	CLA	O2A-CGA	4.44	1.46	1.33
34	d	408	DGD	O2G-C1B	4.44	1.46	1.34
23	B	604	CLA	O2A-CGA	4.44	1.46	1.33
23	b	610	CLA	O2A-CGA	4.42	1.46	1.33
25	a	405	SQD	O48-C23	4.41	1.46	1.33
23	B	613	CLA	OBD-CAD	4.41	1.28	1.22
23	c	508	CLA	OBD-CAD	4.40	1.28	1.22
35	C	519	LMG	O8-C28	4.39	1.46	1.33
34	C	518	DGD	O1G-C1A	4.39	1.46	1.33
24	B	619	BCR	C23-C22	-4.38	1.36	1.45
23	C	502	CLA	O2A-CGA	4.38	1.46	1.33
23	A	404	CLA	OBD-CAD	4.38	1.28	1.22
23	b	619	CLA	OBD-CAD	4.38	1.28	1.22
33	o	301	HTG	C1'-S1	-4.37	1.75	1.81
23	B	615	CLA	O2A-CGA	4.37	1.46	1.33
23	B	609	CLA	O2A-CGA	4.37	1.46	1.33
23	C	509	CLA	O2A-CGA	4.36	1.46	1.33
23	B	606	CLA	OBD-CAD	4.36	1.28	1.22
38	D	413	LHG	O7-C7	4.36	1.46	1.34
34	d	408	DGD	O1G-C1A	4.35	1.46	1.33
23	d	405	CLA	O2A-CGA	4.35	1.46	1.33
23	c	511	CLA	O2A-CGA	4.34	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	621	SQD	O47-C7	4.34	1.46	1.34
37	d	402[B]	PHO	O2A-CGA	4.34	1.46	1.33
38	a	420	LHG	O8-C23	4.34	1.46	1.33
34	c	520	DGD	O1G-C1A	4.33	1.46	1.33
34	C	518	DGD	O2G-C1B	4.33	1.46	1.34
25	f	102	SQD	O48-C23	4.32	1.46	1.33
23	b	625	CLA	O2A-CGA	4.32	1.46	1.33
23	C	510	CLA	O2A-CGA	4.31	1.45	1.33
23	c	515	CLA	OBD-CAD	4.30	1.28	1.22
23	C	507	CLA	O2A-CGA	4.29	1.45	1.33
23	b	616	CLA	O2A-CGA	4.29	1.45	1.33
23	B	605	CLA	O2D-CGD	4.29	1.43	1.33
38	E	101	LHG	O8-C23	4.29	1.45	1.33
34	B	632	DGD	O1G-C1A	4.29	1.45	1.33
23	C	505	CLA	O2A-CGA	4.29	1.45	1.33
23	C	508	CLA	O2A-CGA	4.28	1.45	1.33
37	D	403[B]	PHO	O2A-CGA	4.27	1.45	1.33
35	c	523	LMG	O8-C28	4.26	1.45	1.33
38	d	411	LHG	O8-C23	4.26	1.45	1.33
38	L	101	LHG	O8-C23	4.26	1.45	1.33
23	B	607	CLA	O2A-CGA	4.25	1.45	1.33
35	M	101	LMG	O8-C28	4.25	1.45	1.33
25	a	405	SQD	O47-C7	4.25	1.46	1.34
23	b	624	CLA	O2A-CGA	4.25	1.45	1.33
23	B	606	CLA	O2A-CGA	4.24	1.45	1.33
23	c	517	CLA	O2A-CGA	4.24	1.45	1.33
23	b	612	CLA	OBD-CAD	4.24	1.28	1.22
23	C	507	CLA	OBD-CAD	4.23	1.28	1.22
23	A	405	CLA	OBD-CAD	4.23	1.28	1.22
35	C	501	LMG	O7-C10	4.23	1.46	1.34
37	d	402[A]	PHO	O2A-CGA	4.23	1.45	1.33
23	B	617	CLA	O2A-CGA	4.23	1.45	1.33
25	L	102	SQD	O47-C7	4.22	1.46	1.34
23	c	506	CLA	O2A-CGA	4.22	1.45	1.33
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33
23	a	409	CLA	O2D-CGD	4.21	1.43	1.33
23	D	406	CLA	O2A-CGA	4.21	1.45	1.33
23	a	410	CLA	O2A-CGA	4.21	1.45	1.33
23	C	512	CLA	O2A-CGA	4.20	1.45	1.33
23	C	511	CLA	O2A-CGA	4.20	1.45	1.33
35	a	415	LMG	O8-C28	4.20	1.45	1.33
23	A	404	CLA	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2A-CGA	4.19	1.45	1.33
23	B	617	CLA	OBD-CAD	4.19	1.28	1.22
34	C	517	DGD	O1G-C1A	4.19	1.45	1.33
23	c	505	CLA	OBD-CAD	4.18	1.28	1.22
38	b	634	LHG	O7-C7	4.18	1.46	1.34
38	d	410	LHG	O7-C7	4.18	1.46	1.34
23	B	605	CLA	OBD-CAD	4.18	1.28	1.22
34	h	102	DGD	O1G-C1A	4.16	1.45	1.33
23	c	516	CLA	O2A-CGA	4.16	1.45	1.33
23	B	616	CLA	O2A-CGA	4.16	1.45	1.33
37	D	402	PHO	O2A-CGA	4.15	1.45	1.33
38	D	412	LHG	O8-C23	4.15	1.45	1.33
23	d	403	CLA	OBD-CAD	4.15	1.28	1.22
23	C	514	CLA	O2A-CGA	4.15	1.45	1.33
23	b	621	CLA	O2A-CGA	4.15	1.45	1.33
35	C	520	LMG	O8-C28	4.14	1.45	1.33
35	C	501	LMG	O8-C28	4.14	1.45	1.33
23	c	508	CLA	O2A-CGA	4.14	1.45	1.33
38	b	634	LHG	O8-C23	4.14	1.45	1.33
25	a	414	SQD	O48-C23	4.14	1.45	1.33
35	c	523	LMG	O7-C10	4.14	1.46	1.34
23	c	515	CLA	O2A-CGA	4.13	1.45	1.33
38	E	101	LHG	O7-C7	4.13	1.46	1.34
23	b	617	CLA	O2A-CGA	4.13	1.45	1.33
35	Z	101	LMG	O7-C10	4.13	1.46	1.34
34	c	521	DGD	O1G-C1A	4.13	1.45	1.33
35	z	101	LMG	O7-C10	4.13	1.46	1.34
34	C	516	DGD	O2G-C1B	4.13	1.45	1.34
23	b	612	CLA	O2A-CGA	4.13	1.45	1.33
25	F	104	SQD	O48-C23	4.12	1.45	1.33
37	D	403[A]	PHO	O2A-CGA	4.11	1.45	1.33
23	b	611	CLA	O2A-CGA	4.11	1.45	1.33
35	c	522	LMG	O8-C28	4.11	1.45	1.33
23	B	603	CLA	O2A-CGA	4.11	1.45	1.33
23	d	404	CLA	O2A-CGA	4.08	1.45	1.33
25	A	412	SQD	O47-C7	4.08	1.45	1.34
23	a	412	CLA	O2A-CGA	4.07	1.45	1.33
23	B	614	CLA	O2A-CGA	4.07	1.45	1.33
34	c	519	DGD	O1G-C1A	4.07	1.45	1.33
35	D	417	LMG	O7-C10	4.07	1.45	1.34
23	C	506	CLA	O2A-CGA	4.06	1.45	1.33
23	b	620	CLA	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	622	CLA	OBD-CAD	4.05	1.28	1.22
33	b	632	HTG	C1'-S1	-4.05	1.76	1.81
23	b	623	CLA	O2A-CGA	4.05	1.45	1.33
23	D	407	CLA	O2A-CGA	4.04	1.45	1.33
35	d	416	LMG	O8-C28	4.04	1.45	1.33
23	A	407	CLA	O2A-CGA	4.04	1.45	1.33
23	a	412	CLA	OBD-CAD	4.03	1.27	1.22
23	b	615	CLA	O2A-CGA	4.03	1.45	1.33
38	a	420	LHG	O7-C7	4.03	1.45	1.34
25	L	102	SQD	O48-C23	4.03	1.45	1.33
23	C	503	CLA	O2A-CGA	4.02	1.45	1.33
38	D	413	LHG	O8-C23	4.02	1.45	1.33
25	A	409	SQD	O48-C23	4.01	1.45	1.33
34	C	516	DGD	O1G-C1A	4.01	1.45	1.33
23	c	510	CLA	O2A-CGA	4.00	1.45	1.33
23	B	612	CLA	O2A-CGA	4.00	1.45	1.33
35	b	629	LMG	O8-C28	4.00	1.45	1.33
35	C	519	LMG	O7-C10	4.00	1.45	1.34
35	D	417	LMG	O8-C28	3.99	1.45	1.33
35	M	101	LMG	O7-C10	3.99	1.45	1.34
23	c	514	CLA	O2A-CGA	3.99	1.45	1.33
23	B	608	CLA	O2A-CGA	3.99	1.45	1.33
38	D	411	LHG	O8-C23	3.98	1.45	1.33
34	h	102	DGD	O2G-C1B	3.98	1.45	1.34
25	B	621	SQD	O48-C23	3.97	1.44	1.33
23	c	505	CLA	O2A-CGA	3.96	1.44	1.33
38	d	411	LHG	O7-C7	3.96	1.45	1.34
35	d	416	LMG	O7-C10	3.96	1.45	1.34
25	A	409	SQD	O47-C7	3.95	1.45	1.34
34	c	521	DGD	O2G-C1B	3.95	1.45	1.34
34	B	632	DGD	O2G-C1B	3.95	1.45	1.34
23	B	613	CLA	O2A-CGA	3.94	1.44	1.33
23	b	618	CLA	O2A-CGA	3.94	1.44	1.33
35	a	415	LMG	O7-C10	3.94	1.45	1.34
37	a	411	PHO	OBD-CAD	3.93	1.29	1.22
34	c	520	DGD	O2G-C1B	3.93	1.45	1.34
23	D	406	CLA	OBD-CAD	3.93	1.27	1.22
23	C	504	CLA	O2A-CGA	3.93	1.44	1.33
23	b	613	CLA	O2A-CGA	3.92	1.44	1.33
35	b	629	LMG	O7-C10	3.90	1.45	1.34
34	C	517	DGD	O2G-C1B	3.90	1.45	1.34
33	b	607	HTG	C1'-S1	-3.90	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	403[B]	PHO	OBD-CAD	3.88	1.29	1.22
23	b	622	CLA	O2A-CGA	3.87	1.44	1.33
23	b	619	CLA	O2A-CGA	3.86	1.44	1.33
25	a	414	SQD	O47-C7	3.86	1.45	1.34
35	c	522	LMG	O7-C10	3.85	1.45	1.34
23	B	611	CLA	O2A-CGA	3.85	1.44	1.33
33	b	601	HTG	C1'-S1	-3.84	1.76	1.81
23	c	507	CLA	O2A-CGA	3.83	1.44	1.33
33	d	414	HTG	C1'-S1	-3.83	1.76	1.81
34	c	519	DGD	O2G-C1B	3.83	1.45	1.34
23	a	409	CLA	O2A-CGA	3.81	1.44	1.33
23	A	406	CLA	O2A-CGA	3.79	1.44	1.33
37	D	403[B]	PHO	CHC-C4B	3.79	1.49	1.40
37	d	402[A]	PHO	C3D-C2D	3.78	1.49	1.39
37	D	403[B]	PHO	C3D-C2D	3.78	1.49	1.39
23	b	614	CLA	O2A-CGA	3.77	1.44	1.33
23	d	404	CLA	OBD-CAD	3.77	1.27	1.22
23	B	608	CLA	OBD-CAD	3.75	1.27	1.22
38	d	409	LHG	O8-C23	3.74	1.44	1.33
37	a	411	PHO	CHC-C4B	3.73	1.49	1.40
33	B	629	HTG	C1'-S1	-3.73	1.76	1.81
37	a	411	PHO	O2A-CGA	3.72	1.44	1.33
33	B	630	HTG	C1'-S1	-3.66	1.76	1.81
38	L	101	LHG	O7-C7	3.65	1.44	1.34
33	V	207	HTG	C1'-S1	-3.64	1.76	1.81
37	D	403[A]	PHO	C3D-C2D	3.63	1.49	1.39
37	d	402[B]	PHO	OBD-CAD	3.63	1.28	1.22
23	B	605	CLA	O2A-CGA	3.62	1.43	1.33
37	D	403[A]	PHO	C4A-NA	-3.61	1.26	1.35
23	B	604	CLA	OBD-CAD	3.60	1.27	1.22
38	d	410	LHG	O8-C23	3.59	1.43	1.33
37	d	402[B]	PHO	CHC-C4B	3.59	1.48	1.40
33	b	608	HTG	C1'-S1	-3.59	1.76	1.81
33	B	623	HTG	C1'-S1	-3.57	1.76	1.81
37	D	402	PHO	C4A-NA	-3.57	1.26	1.35
38	D	412	LHG	O7-C7	3.57	1.44	1.34
37	D	402	PHO	C3D-C2D	3.56	1.48	1.39
37	a	411	PHO	C3D-C2D	3.55	1.48	1.39
37	d	402[A]	PHO	CHC-C4B	3.55	1.48	1.40
37	D	403[B]	PHO	C4A-NA	-3.55	1.26	1.35
37	D	403[B]	PHO	CHD-C4C	3.55	1.48	1.40
33	c	524	HTG	C1'-S1	-3.54	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	402	PHO	OBD-CAD	3.53	1.28	1.22
37	D	403[A]	PHO	CHC-C4B	3.53	1.48	1.40
33	c	525	HTG	C1'-S1	-3.52	1.76	1.81
37	d	402[B]	PHO	C3D-C2D	3.48	1.48	1.39
38	D	411	LHG	O7-C7	3.48	1.44	1.34
37	d	402[B]	PHO	C4A-NA	-3.48	1.26	1.35
23	a	409	CLA	C4C-C3C	3.47	1.51	1.45
33	C	523	HTG	C1'-S1	-3.46	1.77	1.81
33	C	522	HTG	C1'-S1	-3.42	1.77	1.81
37	D	402	PHO	CHD-C4C	3.39	1.48	1.40
38	d	409	LHG	O7-C7	3.36	1.43	1.34
37	a	411	PHO	C4A-NA	-3.34	1.27	1.35
37	a	411	PHO	CHB-C4A	3.32	1.48	1.40
37	D	403[A]	PHO	OBD-CAD	3.30	1.28	1.22
37	d	402[A]	PHO	C4A-NA	-3.29	1.27	1.35
33	b	631	HTG	C1'-S1	-3.27	1.77	1.81
37	D	402	PHO	CHB-C4A	3.26	1.48	1.40
37	d	402[A]	PHO	OBD-CAD	3.25	1.28	1.22
37	D	402	PHO	CHC-C4B	3.24	1.48	1.40
23	C	502	CLA	C1C-C2C	3.23	1.50	1.44
33	D	416	HTG	C1'-S1	-3.22	1.77	1.81
37	D	403[A]	PHO	CHD-C4C	3.21	1.47	1.40
33	B	622	HTG	C1'-S1	-3.20	1.77	1.81
23	D	407	CLA	C1D-C2D	3.14	1.49	1.42
37	D	403[A]	PHO	C3B-C4B	3.12	1.49	1.43
23	b	621	CLA	C1C-C2C	3.12	1.50	1.44
23	c	511	CLA	C1C-C2C	3.11	1.50	1.44
23	A	407	CLA	C1D-C2D	3.09	1.49	1.42
23	b	616	CLA	C1D-C2D	3.09	1.49	1.42
37	d	402[A]	PHO	CHD-C4C	3.09	1.47	1.40
23	A	404	CLA	C1D-C2D	3.09	1.49	1.42
37	D	403[B]	PHO	CHB-C4A	3.06	1.47	1.40
37	d	402[B]	PHO	CHD-C4C	3.05	1.47	1.40
37	d	402[A]	PHO	C3B-C4B	3.04	1.49	1.43
23	b	610	CLA	C1D-C2D	3.04	1.49	1.42
23	b	619	CLA	C1D-C2D	3.03	1.49	1.42
23	B	611	CLA	C1D-C2D	3.03	1.49	1.42
23	B	606	CLA	C1C-C2C	3.02	1.50	1.44
23	C	514	CLA	C1D-C2D	3.02	1.49	1.42
37	d	402[B]	PHO	CHB-C4A	3.00	1.47	1.40
37	D	403[B]	PHO	C3B-C4B	3.00	1.49	1.43
25	f	102	SQD	C6-S	-2.99	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	411	PHO	C3B-C4B	2.99	1.49	1.43
37	a	411	PHO	CHD-C4C	2.98	1.47	1.40
23	d	405	CLA	C1D-C2D	2.98	1.49	1.42
23	b	611	CLA	C1D-C2D	2.96	1.49	1.42
25	A	412	SQD	C6-S	-2.96	1.66	1.77
39	v	205	HEM	C3B-C2B	-2.95	1.36	1.40
23	c	509	CLA	C4C-C3C	2.95	1.50	1.45
23	C	511	CLA	C4C-C3C	2.94	1.50	1.45
23	a	409	CLA	C1D-C2D	2.93	1.49	1.42
23	b	615	CLA	C1D-C2D	2.93	1.49	1.42
23	C	507	CLA	C1D-C2D	2.93	1.49	1.42
23	C	509	CLA	C1D-C2D	2.93	1.49	1.42
23	b	624	CLA	C1D-C2D	2.92	1.49	1.42
23	B	608	CLA	C1D-C2D	2.92	1.49	1.42
23	B	610	CLA	C1D-C2D	2.92	1.49	1.42
23	B	606	CLA	C1D-C2D	2.89	1.49	1.42
23	d	404	CLA	C4C-C3C	2.89	1.50	1.45
37	d	402[A]	PHO	CHB-C4A	2.88	1.47	1.40
23	C	511	CLA	C1D-C2D	2.87	1.49	1.42
25	A	409	SQD	C6-S	-2.87	1.66	1.77
23	a	409	CLA	CHD-C4C	2.86	1.49	1.41
23	c	511	CLA	C1D-C2D	2.86	1.49	1.42
25	F	104	SQD	C6-S	-2.85	1.66	1.77
37	D	402	PHO	C3B-C4B	2.85	1.49	1.43
23	d	404	CLA	C1D-C2D	2.84	1.49	1.42
23	b	613	CLA	C1B-CHB	2.83	1.48	1.41
37	d	402[B]	PHO	C3B-C4B	2.83	1.49	1.43
23	B	613	CLA	C1B-CHB	2.83	1.48	1.41
33	c	524	HTG	C1-S1	-2.82	1.76	1.80
23	B	603	CLA	C1D-C2D	2.82	1.48	1.42
23	b	618	CLA	C1D-C2D	2.81	1.48	1.42
23	c	516	CLA	C1C-C2C	2.81	1.50	1.44
23	B	614	CLA	C1C-C2C	2.80	1.50	1.44
23	B	604	CLA	C1B-NB	-2.80	1.32	1.35
23	C	504	CLA	C1C-C2C	2.80	1.50	1.44
23	B	602	CLA	C1D-C2D	2.80	1.48	1.42
23	b	614	CLA	C1C-C2C	2.79	1.50	1.44
23	C	508	CLA	C1D-C2D	2.79	1.48	1.42
23	C	510	CLA	C1C-C2C	2.79	1.50	1.44
23	C	511	CLA	CHD-C4C	2.78	1.49	1.41
23	A	404	CLA	C4C-C3C	2.78	1.49	1.45
23	a	410	CLA	C1D-C2D	2.78	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4B-CHC	2.78	1.48	1.41
23	B	613	CLA	C1C-C2C	2.78	1.49	1.44
23	C	502	CLA	C1D-C2D	2.77	1.48	1.42
23	C	502	CLA	C4B-CHC	2.77	1.48	1.41
23	B	612	CLA	C1D-C2D	2.77	1.48	1.42
23	C	512	CLA	CHD-C4C	2.77	1.49	1.41
23	C	505	CLA	C1D-C2D	2.76	1.48	1.42
23	c	517	CLA	C1D-C2D	2.75	1.48	1.42
37	D	403[A]	PHO	CHB-C4A	2.75	1.46	1.40
23	c	514	CLA	C1D-C2D	2.75	1.48	1.42
23	b	621	CLA	C1B-CHB	2.74	1.48	1.41
23	C	504	CLA	C1D-C2D	2.74	1.48	1.42
23	c	510	CLA	C1D-C2D	2.73	1.48	1.42
23	b	620	CLA	C1D-C2D	2.73	1.48	1.42
23	c	508	CLA	C1D-C2D	2.73	1.48	1.42
25	a	405	SQD	C6-S	-2.73	1.67	1.77
23	B	613	CLA	C1D-C2D	2.73	1.48	1.42
23	B	614	CLA	C1D-C2D	2.73	1.48	1.42
23	c	517	CLA	C1C-C2C	2.73	1.49	1.44
23	B	611	CLA	CHD-C4C	2.73	1.48	1.41
23	B	603	CLA	C1C-C2C	2.73	1.49	1.44
23	C	506	CLA	C1D-C2D	2.73	1.48	1.42
23	c	514	CLA	CHD-C4C	2.73	1.48	1.41
23	c	511	CLA	C4B-CHC	2.72	1.48	1.41
23	C	510	CLA	C1D-C2D	2.72	1.48	1.42
23	b	617	CLA	C1D-C2D	2.72	1.48	1.42
23	c	512	CLA	C4C-C3C	2.72	1.49	1.45
23	c	507	CLA	C1D-C2D	2.71	1.48	1.42
23	C	506	CLA	C1B-CHB	2.71	1.48	1.41
23	B	606	CLA	C4B-CHC	2.71	1.48	1.41
23	B	604	CLA	C1C-C2C	2.71	1.49	1.44
23	b	625	CLA	C1D-C2D	2.71	1.48	1.42
23	b	610	CLA	CHD-C4C	2.71	1.48	1.41
23	c	509	CLA	C1D-C2D	2.70	1.48	1.42
23	B	607	CLA	C1D-C2D	2.70	1.48	1.42
23	c	510	CLA	C1B-CHB	2.70	1.48	1.41
23	b	624	CLA	C1B-CHB	2.70	1.48	1.41
23	C	504	CLA	CHD-C4C	2.70	1.48	1.41
23	d	403	CLA	CHD-C4C	2.69	1.48	1.41
23	A	406	CLA	C1D-C2D	2.69	1.48	1.42
23	B	614	CLA	C1B-CHB	2.69	1.48	1.41
23	b	613	CLA	C1C-C2C	2.68	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-C2C	2.68	1.49	1.44
23	c	513	CLA	C1B-CHB	2.68	1.48	1.41
23	C	504	CLA	C4B-CHC	2.67	1.48	1.41
23	c	505	CLA	C1B-CHB	2.67	1.48	1.41
23	B	615	CLA	C1D-C2D	2.67	1.48	1.42
25	B	621	SQD	C6-S	-2.67	1.67	1.77
23	A	404	CLA	CHD-C4C	2.67	1.48	1.41
23	B	612	CLA	CHD-C4C	2.67	1.48	1.41
23	d	403	CLA	C1D-C2D	2.66	1.48	1.42
23	b	617	CLA	C4B-CHC	2.66	1.48	1.41
23	c	515	CLA	C1D-C2D	2.66	1.48	1.42
23	B	608	CLA	C1B-NB	-2.66	1.32	1.35
23	c	514	CLA	C1B-CHB	2.66	1.48	1.41
23	b	615	CLA	C1C-C2C	2.65	1.49	1.44
23	B	611	CLA	C4B-CHC	2.65	1.48	1.41
35	Z	101	LMG	O8-C28	2.65	1.46	1.33
23	a	410	CLA	C1C-C2C	2.65	1.49	1.44
23	B	603	CLA	C4B-CHC	2.65	1.48	1.41
27	a	404	LMT	O1'-C1'	2.64	1.44	1.40
23	C	505	CLA	C1C-C2C	2.64	1.49	1.44
39	V	206	HEM	C3B-C2B	-2.64	1.36	1.40
23	A	405	CLA	C1D-C2D	2.63	1.48	1.42
23	c	506	CLA	C1B-CHB	2.63	1.48	1.41
23	b	622	CLA	C1D-C2D	2.63	1.48	1.42
23	c	513	CLA	C1D-C2D	2.63	1.48	1.42
23	b	614	CLA	C1D-C2D	2.62	1.48	1.42
33	D	416	HTG	C1-S1	-2.62	1.76	1.80
23	b	620	CLA	C1B-CHB	2.62	1.48	1.41
23	B	604	CLA	C1D-C2D	2.61	1.48	1.42
23	b	610	CLA	C1C-C2C	2.61	1.49	1.44
23	c	508	CLA	C1B-CHB	2.61	1.48	1.41
23	c	507	CLA	C1C-C2C	2.60	1.49	1.44
23	C	512	CLA	C4C-C3C	2.60	1.49	1.45
25	a	414	SQD	C6-S	-2.60	1.67	1.77
23	C	513	CLA	C1C-C2C	2.60	1.49	1.44
23	c	505	CLA	C1D-C2D	2.60	1.48	1.42
23	B	604	CLA	C4B-CHC	2.60	1.48	1.41
23	B	602	CLA	C1B-CHB	2.60	1.48	1.41
23	b	612	CLA	C1C-C2C	2.59	1.49	1.44
23	b	613	CLA	C4C-C3C	2.59	1.49	1.45
23	c	508	CLA	C1C-C2C	2.59	1.49	1.44
23	B	609	CLA	C1D-C2D	2.59	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	CHD-C4C	2.59	1.48	1.41
23	c	513	CLA	CHD-C4C	2.59	1.48	1.41
30	d	407[B]	PL9	C6-C5	2.59	1.48	1.35
23	b	622	CLA	C4C-C3C	2.59	1.49	1.45
23	c	507	CLA	C4B-CHC	2.59	1.48	1.41
23	c	513	CLA	C1C-C2C	2.59	1.49	1.44
23	b	619	CLA	C4C-C3C	2.58	1.49	1.45
23	b	623	CLA	C1B-CHB	2.58	1.48	1.41
23	B	609	CLA	CHD-C4C	2.58	1.48	1.41
30	a	416[B]	PL9	C6-C5	2.58	1.48	1.35
23	D	406	CLA	CHD-C4C	2.58	1.48	1.41
23	C	503	CLA	C1B-CHB	2.57	1.48	1.41
30	a	416[A]	PL9	C6-C5	2.57	1.48	1.35
23	C	511	CLA	C1B-CHB	2.57	1.48	1.41
30	D	409[A]	PL9	C6-C5	2.57	1.48	1.35
23	b	618	CLA	C1B-CHB	2.57	1.48	1.41
23	b	611	CLA	C1C-C2C	2.57	1.49	1.44
30	A	416[B]	PL9	C6-C5	2.57	1.48	1.35
23	C	514	CLA	CHD-C4C	2.56	1.48	1.41
23	B	610	CLA	CHD-C4C	2.56	1.48	1.41
23	D	407	CLA	CHD-C4C	2.56	1.48	1.41
23	b	618	CLA	C1C-C2C	2.56	1.49	1.44
25	L	102	SQD	C6-S	-2.55	1.68	1.77
23	c	516	CLA	CHD-C4C	2.55	1.48	1.41
23	c	509	CLA	C4B-CHC	2.55	1.48	1.41
23	b	622	CLA	C1B-CHB	2.55	1.48	1.41
23	B	615	CLA	C1B-CHB	2.55	1.48	1.41
23	B	610	CLA	C1B-CHB	2.55	1.48	1.41
23	c	512	CLA	C1B-CHB	2.55	1.48	1.41
30	A	416[A]	PL9	C6-C5	2.55	1.48	1.35
23	C	508	CLA	C1C-C2C	2.55	1.49	1.44
23	B	611	CLA	C4C-C3C	2.55	1.49	1.45
23	c	517	CLA	CHD-C4C	2.54	1.48	1.41
39	F	102	HEM	C3B-C2B	-2.54	1.36	1.40
23	b	610	CLA	C4B-CHC	2.54	1.48	1.41
23	A	404	CLA	C1C-C2C	2.54	1.49	1.44
23	B	607	CLA	C4C-C3C	2.54	1.49	1.45
23	b	623	CLA	C1D-C2D	2.54	1.48	1.42
23	B	605	CLA	C1C-C2C	2.54	1.49	1.44
23	C	505	CLA	C4C-C3C	2.54	1.49	1.45
23	C	509	CLA	C1B-CHB	2.53	1.48	1.41
23	B	616	CLA	C1D-C2D	2.53	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C4C-C3C	2.53	1.49	1.45
30	d	407[A]	PL9	C6-C5	2.53	1.48	1.35
23	B	614	CLA	CHD-C4C	2.53	1.48	1.41
23	C	503	CLA	C1D-C2D	2.53	1.48	1.42
23	c	516	CLA	C1D-C2D	2.52	1.48	1.42
23	c	509	CLA	C1C-C2C	2.52	1.49	1.44
23	C	512	CLA	C1B-CHB	2.52	1.48	1.41
23	C	506	CLA	C4C-C3C	2.52	1.49	1.45
23	C	505	CLA	CHD-C4C	2.52	1.48	1.41
23	C	513	CLA	CHD-C4C	2.52	1.48	1.41
23	c	506	CLA	C1D-C2D	2.51	1.48	1.42
23	A	407	CLA	C4B-CHC	2.51	1.48	1.41
23	C	503	CLA	C1C-C2C	2.51	1.49	1.44
23	b	612	CLA	C1D-C2D	2.51	1.48	1.42
23	b	611	CLA	CHD-C4C	2.51	1.48	1.41
23	C	509	CLA	C1C-C2C	2.51	1.49	1.44
23	C	512	CLA	C1D-C2D	2.51	1.48	1.42
23	b	614	CLA	C1B-CHB	2.51	1.48	1.41
23	b	625	CLA	C1B-CHB	2.50	1.47	1.41
23	A	405	CLA	C1C-C2C	2.50	1.49	1.44
23	c	508	CLA	C4B-CHC	2.50	1.47	1.41
23	b	615	CLA	C1B-CHB	2.50	1.47	1.41
30	D	409[B]	PL9	C6-C5	2.50	1.48	1.35
23	b	619	CLA	CHD-C4C	2.50	1.48	1.41
34	D	410	DGD	O3G-C1D	2.49	1.44	1.40
23	b	622	CLA	CHD-C4C	2.49	1.48	1.41
23	b	619	CLA	C4B-CHC	2.49	1.47	1.41
23	C	510	CLA	CHD-C4C	2.49	1.48	1.41
23	b	616	CLA	C1B-CHB	2.49	1.47	1.41
23	d	404	CLA	C1B-NB	-2.49	1.33	1.35
23	C	510	CLA	C1B-CHB	2.49	1.47	1.41
23	c	515	CLA	CHD-C4C	2.48	1.48	1.41
23	c	511	CLA	CHD-C4C	2.48	1.48	1.41
23	c	516	CLA	C4C-C3C	2.48	1.49	1.45
23	B	609	CLA	C1C-C2C	2.47	1.49	1.44
33	b	632	HTG	C1-S1	-2.47	1.76	1.80
23	b	621	CLA	C4B-CHC	2.47	1.47	1.41
23	c	509	CLA	CHD-C4C	2.47	1.48	1.41
23	c	517	CLA	C4B-CHC	2.47	1.47	1.41
23	C	507	CLA	C1B-CHB	2.46	1.47	1.41
23	B	602	CLA	CHD-C4C	2.46	1.48	1.41
23	A	406	CLA	C1C-C2C	2.46	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	CHD-C4C	2.46	1.48	1.41
23	c	509	CLA	C1B-CHB	2.46	1.47	1.41
23	B	613	CLA	C4B-CHC	2.46	1.47	1.41
23	B	612	CLA	C4C-C3C	2.46	1.49	1.45
23	d	404	CLA	CHD-C4C	2.46	1.48	1.41
23	C	513	CLA	C1D-C2D	2.46	1.48	1.42
23	C	502	CLA	CHD-C4C	2.46	1.48	1.41
23	B	614	CLA	C4B-CHC	2.46	1.47	1.41
23	c	506	CLA	C4B-CHC	2.46	1.47	1.41
23	a	412	CLA	CHD-C4C	2.46	1.48	1.41
23	b	613	CLA	C1D-C2D	2.45	1.48	1.42
23	a	412	CLA	C1D-C2D	2.45	1.48	1.42
23	C	507	CLA	C4C-C3C	2.45	1.49	1.45
33	d	414	HTG	C1-S1	-2.45	1.77	1.80
33	b	608	HTG	C1-S1	-2.45	1.77	1.80
23	B	603	CLA	C4C-C3C	2.45	1.49	1.45
23	B	610	CLA	C4C-C3C	2.44	1.49	1.45
23	b	617	CLA	C1C-C2C	2.44	1.49	1.44
23	C	509	CLA	CHD-C4C	2.44	1.48	1.41
23	C	508	CLA	C4B-CHC	2.44	1.47	1.41
23	C	503	CLA	CHD-C4C	2.44	1.48	1.41
23	c	508	CLA	CHD-C4C	2.44	1.48	1.41
23	c	505	CLA	C1C-C2C	2.43	1.49	1.44
23	b	617	CLA	CHD-C4C	2.43	1.48	1.41
23	B	609	CLA	C1C-NC	-2.43	1.34	1.37
23	B	606	CLA	CHD-C4C	2.43	1.48	1.41
23	D	407	CLA	C4C-C3C	2.43	1.49	1.45
23	b	611	CLA	C4B-CHC	2.43	1.47	1.41
23	A	406	CLA	CHD-C4C	2.43	1.48	1.41
23	c	506	CLA	CHD-C4C	2.43	1.48	1.41
23	C	514	CLA	C4B-CHC	2.43	1.47	1.41
23	B	608	CLA	CHD-C4C	2.43	1.48	1.41
23	d	405	CLA	C4B-CHC	2.42	1.47	1.41
23	B	607	CLA	CHD-C4C	2.42	1.48	1.41
23	C	502	CLA	C4C-C3C	2.42	1.49	1.45
33	C	522	HTG	C1-S1	-2.42	1.77	1.80
23	B	607	CLA	C1B-CHB	2.42	1.47	1.41
23	b	611	CLA	C4C-C3C	2.42	1.49	1.45
23	b	617	CLA	C1B-CHB	2.42	1.47	1.41
23	C	510	CLA	C4B-CHC	2.42	1.47	1.41
23	c	513	CLA	C4B-CHC	2.41	1.47	1.41
23	c	514	CLA	C4B-CHC	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	C1D-C2D	2.41	1.48	1.42
37	D	403[A]	PHO	C1A-NA	-2.41	1.32	1.37
23	D	406	CLA	C1D-C2D	2.41	1.48	1.42
23	c	505	CLA	C4C-C3C	2.41	1.49	1.45
23	C	508	CLA	CHD-C4C	2.41	1.48	1.41
23	C	504	CLA	C1B-CHB	2.41	1.47	1.41
23	C	511	CLA	C1C-C2C	2.41	1.49	1.44
23	B	615	CLA	CHD-C4C	2.41	1.48	1.41
27	A	413	LMT	O1'-C1'	2.41	1.44	1.40
23	B	605	CLA	C1B-CHB	2.40	1.47	1.41
23	c	517	CLA	C4C-C3C	2.40	1.49	1.45
23	B	615	CLA	C1C-C2C	2.40	1.49	1.44
23	C	511	CLA	C4B-CHC	2.40	1.47	1.41
23	D	406	CLA	C4C-C3C	2.40	1.49	1.45
23	c	510	CLA	CHD-C4C	2.40	1.48	1.41
23	B	608	CLA	C1B-CHB	2.40	1.47	1.41
23	B	602	CLA	C1C-C2C	2.39	1.49	1.44
23	B	608	CLA	C4B-CHC	2.39	1.47	1.41
23	d	405	CLA	CHD-C4C	2.39	1.48	1.41
23	B	609	CLA	C4C-C3C	2.39	1.49	1.45
33	V	207	HTG	C1-S1	-2.38	1.77	1.80
23	b	623	CLA	C1C-C2C	2.38	1.49	1.44
23	A	407	CLA	C1C-C2C	2.38	1.49	1.44
23	a	409	CLA	C1B-CHB	2.38	1.47	1.41
23	B	606	CLA	C4C-C3C	2.38	1.49	1.45
39	e	101	HEM	C3B-C2B	-2.38	1.37	1.40
23	A	407	CLA	CHD-C4C	2.38	1.47	1.41
23	d	404	CLA	C1C-C2C	2.38	1.49	1.44
23	C	513	CLA	C4B-CHC	2.38	1.47	1.41
23	B	614	CLA	C4C-C3C	2.38	1.49	1.45
23	B	608	CLA	C1C-C2C	2.37	1.49	1.44
23	b	612	CLA	C1B-CHB	2.37	1.47	1.41
23	b	623	CLA	CHD-C4C	2.37	1.47	1.41
23	c	516	CLA	C4B-CHC	2.36	1.47	1.41
23	D	407	CLA	C4B-CHC	2.36	1.47	1.41
23	B	602	CLA	C1C-NC	-2.36	1.34	1.37
23	B	611	CLA	C1B-CHB	2.36	1.47	1.41
23	b	622	CLA	C1C-C2C	2.35	1.49	1.44
23	C	512	CLA	C1C-C2C	2.35	1.49	1.44
23	b	615	CLA	CHD-C4C	2.35	1.47	1.41
23	B	607	CLA	C1C-C2C	2.35	1.49	1.44
23	C	504	CLA	C4C-C3C	2.35	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4C-C3C	2.35	1.49	1.45
23	b	624	CLA	C4B-CHC	2.35	1.47	1.41
23	B	606	CLA	C1B-CHB	2.35	1.47	1.41
23	C	502	CLA	C1B-CHB	2.35	1.47	1.41
23	C	513	CLA	C4C-C3C	2.35	1.49	1.45
23	B	607	CLA	C4B-CHC	2.34	1.47	1.41
23	C	505	CLA	C1B-CHB	2.34	1.47	1.41
23	C	513	CLA	C1B-CHB	2.34	1.47	1.41
23	b	612	CLA	C4C-C3C	2.34	1.49	1.45
23	D	407	CLA	C1C-C2C	2.33	1.49	1.44
23	b	610	CLA	C4C-C3C	2.33	1.49	1.45
23	b	611	CLA	C1B-CHB	2.33	1.47	1.41
23	C	509	CLA	C4C-C3C	2.33	1.49	1.45
23	B	613	CLA	CHD-C4C	2.33	1.47	1.41
23	B	605	CLA	CHD-C4C	2.33	1.47	1.41
23	c	514	CLA	C4C-C3C	2.33	1.49	1.45
23	C	506	CLA	CHD-C4C	2.33	1.47	1.41
23	c	505	CLA	CHD-C4C	2.33	1.47	1.41
23	B	617	CLA	C1B-CHB	2.32	1.47	1.41
23	a	409	CLA	C4B-CHC	2.32	1.47	1.41
23	C	514	CLA	C1B-CHB	2.32	1.47	1.41
23	c	512	CLA	C1D-C2D	2.32	1.47	1.42
23	C	514	CLA	C1C-C2C	2.32	1.49	1.44
23	b	616	CLA	C4B-CHC	2.32	1.47	1.41
23	c	511	CLA	C1B-CHB	2.32	1.47	1.41
23	c	507	CLA	CHD-C4C	2.32	1.47	1.41
23	a	410	CLA	CHD-C4C	2.32	1.47	1.41
23	B	617	CLA	C4B-CHC	2.32	1.47	1.41
23	B	608	CLA	C4C-C3C	2.31	1.49	1.45
23	b	623	CLA	C4B-CHC	2.31	1.47	1.41
23	c	512	CLA	C1C-C2C	2.31	1.49	1.44
23	C	503	CLA	C4B-CHC	2.31	1.47	1.41
23	b	625	CLA	C4B-CHC	2.31	1.47	1.41
23	c	512	CLA	CHD-C4C	2.31	1.47	1.41
23	B	612	CLA	C1B-CHB	2.31	1.47	1.41
23	c	510	CLA	C1B-NB	-2.30	1.33	1.35
23	c	516	CLA	C1B-CHB	2.30	1.47	1.41
23	b	619	CLA	C1B-CHB	2.30	1.47	1.41
23	b	618	CLA	C4B-CHC	2.29	1.47	1.41
37	D	403[A]	PHO	C4D-CHA	2.29	1.50	1.43
23	C	512	CLA	C4B-CHC	2.29	1.47	1.41
33	c	525	HTG	C1-S1	-2.29	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	515	CLA	C1C-C2C	2.29	1.49	1.44
23	c	515	CLA	C1B-CHB	2.29	1.47	1.41
23	b	613	CLA	C4B-CHC	2.28	1.47	1.41
23	B	603	CLA	C1B-CHB	2.28	1.47	1.41
23	A	405	CLA	CHD-C4C	2.28	1.47	1.41
23	c	513	CLA	C4C-C3C	2.28	1.49	1.45
23	B	602	CLA	C4B-CHC	2.27	1.47	1.41
23	b	617	CLA	C4C-C3C	2.27	1.49	1.45
23	b	618	CLA	CHD-C4C	2.27	1.47	1.41
37	d	402[B]	PHO	C1A-NA	-2.27	1.33	1.37
23	a	409	CLA	C1C-C2C	2.27	1.49	1.44
23	C	505	CLA	C4B-CHC	2.26	1.47	1.41
23	b	614	CLA	C4B-CHC	2.25	1.47	1.41
23	b	612	CLA	C4B-CHC	2.25	1.47	1.41
23	D	407	CLA	C1B-CHB	2.25	1.47	1.41
23	b	620	CLA	C4C-C3C	2.25	1.48	1.45
23	B	612	CLA	C1C-C2C	2.24	1.48	1.44
23	b	620	CLA	CHD-C4C	2.24	1.47	1.41
23	b	612	CLA	CHD-C4C	2.24	1.47	1.41
23	C	506	CLA	C4B-CHC	2.24	1.47	1.41
23	a	412	CLA	C1B-CHB	2.24	1.47	1.41
23	B	616	CLA	C1B-CHB	2.24	1.47	1.41
23	C	508	CLA	C4C-C3C	2.24	1.48	1.45
23	b	616	CLA	CHD-C4C	2.24	1.47	1.41
23	D	406	CLA	C1B-CHB	2.24	1.47	1.41
23	B	613	CLA	C4C-C3C	2.23	1.48	1.45
23	d	404	CLA	C1B-CHB	2.23	1.47	1.41
23	b	616	CLA	C4C-C3C	2.23	1.48	1.45
23	d	403	CLA	C1B-CHB	2.23	1.47	1.41
23	a	410	CLA	C1B-CHB	2.23	1.47	1.41
23	c	510	CLA	C4B-CHC	2.23	1.47	1.41
23	B	603	CLA	CHD-C4C	2.22	1.47	1.41
23	B	609	CLA	C4B-NB	-2.22	1.33	1.35
23	b	615	CLA	C4B-CHC	2.22	1.47	1.41
23	b	624	CLA	C4C-C3C	2.22	1.48	1.45
23	B	616	CLA	CHD-C4C	2.22	1.47	1.41
23	b	624	CLA	CHD-C4C	2.22	1.47	1.41
23	a	410	CLA	C4B-CHC	2.22	1.47	1.41
23	C	509	CLA	C4B-CHC	2.21	1.47	1.41
37	D	402	PHO	C4D-CHA	2.21	1.49	1.43
23	d	404	CLA	C4B-CHC	2.21	1.47	1.41
37	a	411	PHO	C4D-CHA	2.21	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CHD-C4C	2.21	1.47	1.41
23	C	506	CLA	C1C-C2C	2.21	1.48	1.44
23	B	604	CLA	C1B-CHB	2.21	1.47	1.41
23	C	514	CLA	C4C-C3C	2.20	1.48	1.45
23	B	609	CLA	C1B-CHB	2.20	1.47	1.41
37	d	402[A]	PHO	C4D-CHA	2.20	1.49	1.43
23	A	406	CLA	C4B-CHC	2.19	1.47	1.41
23	c	517	CLA	C1B-CHB	2.19	1.47	1.41
33	B	630	HTG	C1-S1	-2.19	1.77	1.80
23	B	616	CLA	C4C-C3C	2.19	1.48	1.45
23	a	412	CLA	C4B-CHC	2.19	1.47	1.41
23	b	622	CLA	C1C-NC	-2.19	1.34	1.37
23	C	508	CLA	C1B-CHB	2.19	1.47	1.41
23	B	615	CLA	C1B-NB	-2.19	1.33	1.35
33	B	623	HTG	C1-S1	-2.18	1.77	1.80
23	d	403	CLA	C1C-NC	-2.18	1.34	1.37
23	b	616	CLA	C1C-C2C	2.18	1.48	1.44
23	A	406	CLA	C1C-NC	-2.18	1.34	1.37
37	D	403[B]	PHO	C4D-CHA	2.18	1.49	1.43
37	a	411	PHO	C1A-NA	-2.17	1.33	1.37
23	b	625	CLA	CHD-C4C	2.17	1.47	1.41
23	C	507	CLA	C1C-C2C	2.17	1.48	1.44
23	B	615	CLA	C4B-CHC	2.17	1.47	1.41
23	B	612	CLA	C4B-CHC	2.16	1.47	1.41
23	c	505	CLA	C4B-CHC	2.16	1.47	1.41
37	d	402[A]	PHO	C1A-NA	-2.16	1.33	1.37
39	F	102	HEM	C4D-C3D	2.16	1.47	1.42
23	c	515	CLA	C4B-CHC	2.16	1.47	1.41
23	c	507	CLA	C4C-C3C	2.16	1.48	1.45
23	C	507	CLA	C4B-CHC	2.16	1.47	1.41
23	A	407	CLA	C4C-C3C	2.16	1.48	1.45
23	b	624	CLA	C1C-C2C	2.15	1.48	1.44
23	B	617	CLA	CHD-C4C	2.15	1.47	1.41
23	b	614	CLA	CHD-C4C	2.14	1.47	1.41
37	D	403[B]	PHO	C4C-C3C	2.13	1.49	1.45
23	B	602	CLA	C4C-C3C	2.12	1.48	1.45
23	a	412	CLA	C1C-C2C	2.12	1.48	1.44
23	A	405	CLA	C1B-CHB	2.12	1.46	1.41
23	D	406	CLA	C4B-CHC	2.12	1.46	1.41
23	b	610	CLA	C1B-CHB	2.12	1.46	1.41
23	d	405	CLA	C1C-C2C	2.12	1.48	1.44
23	d	405	CLA	C1B-CHB	2.11	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C1B-CHB	2.11	1.46	1.41
23	b	621	CLA	C1D-C2D	2.11	1.47	1.42
23	B	610	CLA	C4B-CHC	2.11	1.46	1.41
23	A	407	CLA	C1B-CHB	2.11	1.46	1.41
23	b	619	CLA	C1C-C2C	2.11	1.48	1.44
23	a	409	CLA	O2D-CED	-2.10	1.40	1.45
23	c	506	CLA	C1C-NC	-2.10	1.34	1.37
23	B	605	CLA	C4B-CHC	2.10	1.46	1.41
34	h	102	DGD	O5D-C1E	2.09	1.43	1.40
39	v	205	HEM	C4D-C3D	2.09	1.47	1.42
23	B	605	CLA	C1D-C2D	2.09	1.47	1.42
23	c	505	CLA	C1B-NB	-2.09	1.33	1.35
23	A	406	CLA	C4C-C3C	2.09	1.48	1.45
23	B	617	CLA	C1C-NC	-2.09	1.34	1.37
23	B	609	CLA	C4B-CHC	2.09	1.46	1.41
30	D	409[A]	PL9	C2-C3	2.09	1.40	1.34
23	b	620	CLA	C4B-CHC	2.08	1.46	1.41
23	c	512	CLA	C4B-CHC	2.08	1.46	1.41
37	d	402[B]	PHO	C4D-CHA	2.08	1.49	1.43
23	b	625	CLA	C1C-C2C	2.07	1.48	1.44
23	d	405	CLA	C4C-C3C	2.07	1.48	1.45
23	b	621	CLA	C1C-NC	-2.07	1.34	1.37
23	b	615	CLA	C4C-C3C	2.07	1.48	1.45
33	B	629	HTG	C1-S1	-2.07	1.77	1.80
23	B	613	CLA	C1B-NB	-2.06	1.33	1.35
23	b	625	CLA	C4C-C3C	2.06	1.48	1.45
23	b	625	CLA	C1C-NC	-2.06	1.34	1.37
27	T	104	LMT	O1'-C1'	2.05	1.43	1.40
23	B	610	CLA	C1C-C2C	2.05	1.48	1.44
23	c	506	CLA	C1C-C2C	2.05	1.48	1.44
37	D	403[B]	PHO	C1A-NA	-2.05	1.33	1.37
23	c	514	CLA	C1C-C2C	2.05	1.48	1.44
30	d	407[A]	PL9	C2-C3	2.04	1.40	1.34
38	d	409	LHG	O7-C5	-2.04	1.41	1.46
23	b	622	CLA	C4B-CHC	2.03	1.46	1.41
23	C	506	CLA	C1B-NB	-2.03	1.33	1.35
23	C	505	CLA	C1B-NB	-2.03	1.33	1.35
23	A	405	CLA	C4C-C3C	2.02	1.48	1.45
35	Z	101	LMG	O1-C1	2.02	1.43	1.40
23	A	404	CLA	C1B-CHB	2.01	1.46	1.41
30	a	416[A]	PL9	C2-C3	2.01	1.39	1.34
23	D	406	CLA	C1C-C2C	2.01	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	e	102	LMT	O1'-C1'	2.01	1.43	1.40
30	a	416[B]	PL9	C2-C3	2.01	1.39	1.34
23	A	405	CLA	C4B-CHC	2.01	1.46	1.41
37	D	402	PHO	C4C-C3C	2.00	1.48	1.45
23	B	605	CLA	C4C-C3C	2.00	1.48	1.45

All (2358) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	C4A-NA-C1A	-7.91	103.15	106.71
23	b	621	CLA	CHD-C4C-C3C	-7.54	113.75	124.84
23	c	509	CLA	C4A-NA-C1A	-7.19	103.47	106.71
23	b	611	CLA	C4A-NA-C1A	-6.96	103.58	106.71
23	b	612	CLA	C4A-NA-C1A	-6.95	103.58	106.71
37	d	402[B]	PHO	CMD-C2D-C1D	6.90	135.69	125.06
37	D	403[A]	PHO	CMD-C2D-C1D	6.74	135.44	125.06
23	c	511	CLA	CHD-C4C-C3C	-6.70	114.98	124.84
23	B	616	CLA	C4A-NA-C1A	-6.69	103.70	106.71
37	D	402	PHO	CMD-C2D-C1D	6.69	135.36	125.06
23	b	614	CLA	CHD-C4C-C3C	-6.66	115.05	124.84
33	d	414	HTG	C1'-S1-C1	6.65	112.53	100.09
37	a	411	PHO	CMD-C2D-C1D	6.59	135.21	125.06
37	d	402[A]	PHO	CMD-C2D-C1D	6.57	135.18	125.06
23	A	404	CLA	C4A-NA-C1A	-6.56	103.76	106.71
23	c	516	CLA	O2D-CGD-CBD	6.55	122.90	111.27
23	d	404	CLA	C2C-C1C-NC	6.48	116.04	109.97
23	c	507	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
39	F	102	HEM	CAD-CBD-CGD	6.43	123.47	112.67
37	D	403[B]	PHO	CMD-C2D-C1D	6.42	134.95	125.06
23	B	615	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
23	C	502	CLA	O2D-CGD-CBD	6.42	122.67	111.27
33	c	524	HTG	C1'-S1-C1	6.41	112.08	100.09
23	b	615	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
23	C	508	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
23	a	409	CLA	C4A-NA-C1A	-6.36	103.85	106.71
23	a	409	CLA	C2C-C1C-NC	6.34	115.91	109.97
23	b	623	CLA	O2D-CGD-CBD	6.34	122.53	111.27
23	b	625	CLA	CHD-C4C-C3C	-6.33	115.53	124.84
23	B	616	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
23	b	610	CLA	O2D-CGD-CBD	6.30	122.46	111.27
23	C	506	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	b	624	CLA	CHD-C4C-C3C	-6.29	115.60	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4A-NA-C1A	-6.27	103.89	106.71
23	c	512	CLA	C2C-C1C-NC	6.25	115.83	109.97
33	b	607	HTG	C1'-S1-C1	6.25	111.78	100.09
23	b	623	CLA	CHD-C4C-C3C	-6.24	115.66	124.84
33	B	622	HTG	C1'-S1-C1	6.19	111.66	100.09
23	c	516	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	C	504	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	B	602	CLA	O2D-CGD-CBD	6.17	122.23	111.27
23	b	618	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
33	C	522	HTG	C1'-S1-C1	6.16	111.60	100.09
23	c	515	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
23	B	602	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	c	508	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	B	617	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
23	D	406	CLA	C2C-C1C-NC	6.11	115.70	109.97
23	c	511	CLA	O2D-CGD-CBD	6.10	122.11	111.27
23	B	617	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	B	603	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
23	b	618	CLA	C4A-NA-C1A	-6.08	103.97	106.71
23	b	622	CLA	C2C-C1C-NC	6.06	115.65	109.97
23	B	614	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	C	513	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	B	604	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
23	c	507	CLA	C4A-NA-C1A	-5.99	104.01	106.71
23	B	606	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	C	513	CLA	O2D-CGD-CBD	5.99	121.91	111.27
23	b	613	CLA	C2C-C1C-NC	5.98	115.58	109.97
23	b	612	CLA	O2D-CGD-CBD	5.98	121.89	111.27
23	C	506	CLA	C2C-C1C-NC	5.97	115.57	109.97
23	D	406	CLA	C4A-NA-C1A	-5.97	104.02	106.71
23	a	410	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	A	405	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
23	b	613	CLA	O2D-CGD-CBD	5.94	121.82	111.27
23	c	514	CLA	C2C-C1C-NC	5.93	115.53	109.97
23	c	513	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
23	c	509	CLA	C2C-C1C-NC	5.93	115.53	109.97
23	C	503	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
23	B	604	CLA	O2D-CGD-CBD	5.92	121.78	111.27
23	B	617	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	C	502	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	B	610	CLA	C2C-C1C-NC	5.89	115.49	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C2C-C1C-NC	5.89	115.49	109.97
23	B	613	CLA	CHD-C4C-C3C	-5.89	116.19	124.84
24	D	408	BCR	C7-C8-C9	-5.89	117.34	126.23
23	A	405	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	607	CLA	C4A-NA-C1A	-5.86	104.07	106.71
23	B	604	CLA	C4A-NA-C1A	-5.85	104.08	106.71
23	C	509	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	B	609	CLA	C2C-C1C-NC	5.83	115.43	109.97
23	B	614	CLA	C2C-C1C-NC	5.82	115.43	109.97
33	B	623	HTG	C1'-S1-C1	5.82	110.98	100.09
25	L	102	SQD	O6-C1-C2	5.81	117.37	108.30
39	e	101	HEM	CAD-CBD-CGD	5.80	122.40	112.67
23	B	602	CLA	C2C-C1C-NC	5.77	115.38	109.97
23	b	625	CLA	C4A-NA-C1A	-5.77	104.11	106.71
23	b	622	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	b	619	CLA	C4A-NA-C1A	-5.77	104.11	106.71
23	C	504	CLA	C4A-NA-C1A	-5.77	104.11	106.71
23	B	612	CLA	C2C-C1C-NC	5.76	115.37	109.97
23	b	617	CLA	C4A-NA-C1A	-5.74	104.12	106.71
23	C	509	CLA	O2D-CGD-CBD	5.74	121.47	111.27
23	a	412	CLA	CHD-C4C-C3C	-5.73	116.42	124.84
23	A	404	CLA	C2C-C1C-NC	5.72	115.33	109.97
33	D	416	HTG	C1'-S1-C1	5.72	110.78	100.09
23	d	403	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	b	616	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
23	c	505	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	B	605	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	C	506	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	C	508	CLA	O2D-CGD-CBD	5.68	121.36	111.27
23	c	516	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	C	505	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	b	620	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	d	405	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
23	b	613	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
23	B	607	CLA	C2C-C1C-NC	5.66	115.27	109.97
23	d	405	CLA	C4A-NA-C1A	-5.65	104.17	106.71
23	B	607	CLA	O2D-CGD-CBD	5.65	121.31	111.27
23	c	510	CLA	C2C-C1C-NC	5.65	115.26	109.97
23	C	514	CLA	CHD-C4C-C3C	-5.64	116.54	124.84
23	B	612	CLA	C4A-NA-C1A	-5.63	104.17	106.71
23	B	613	CLA	O2D-CGD-CBD	5.63	121.27	111.27
23	A	406	CLA	CHD-C4C-C3C	-5.62	116.57	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	B	615	CLA	O2D-CGD-CBD	5.62	121.25	111.27
23	c	517	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	b	617	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	b	614	CLA	O2D-CGD-CBD	5.59	121.21	111.27
33	b	632	HTG	C1'-S1-C1	5.59	110.54	100.09
23	c	512	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	c	508	CLA	O2D-CGD-CBD	5.57	121.17	111.27
23	b	610	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	c	514	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
23	B	611	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
37	a	411	PHO	C3D-C2D-C1D	-5.56	97.77	105.87
23	C	507	CLA	C2C-C1C-NC	5.55	115.17	109.97
23	b	625	CLA	O2D-CGD-CBD	5.55	121.12	111.27
23	b	624	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	B	608	CLA	C2C-C1C-NC	5.53	115.16	109.97
23	b	614	CLA	C4A-NA-C1A	-5.53	104.22	106.71
23	B	605	CLA	O2D-CGD-CBD	5.53	121.09	111.27
23	C	510	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
37	d	402[B]	PHO	C3D-C2D-C1D	-5.52	97.83	105.87
23	C	512	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	b	610	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	A	407	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
33	b	632	HTG	O5-C1-C2	5.49	117.22	110.31
23	D	406	CLA	CHD-C4C-C3C	-5.49	116.77	124.84
25	f	102	SQD	O47-C7-C8	5.48	123.32	111.50
23	C	507	CLA	C4A-NA-C1A	-5.48	104.24	106.71
23	c	509	CLA	O2D-CGD-CBD	5.48	121.01	111.27
23	c	513	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	C	511	CLA	C2C-C1C-NC	5.47	115.09	109.97
23	c	512	CLA	O2D-CGD-CBD	5.46	120.98	111.27
23	b	616	CLA	C4A-NA-C1A	-5.45	104.25	106.71
23	b	619	CLA	C2C-C1C-NC	5.45	115.07	109.97
23	B	610	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
23	b	618	CLA	O2D-CGD-CBD	5.44	120.94	111.27
23	c	509	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
23	B	610	CLA	C4A-NA-C1A	-5.44	104.26	106.71
23	C	505	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	b	618	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	b	616	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	Y	101	BCR	C33-C5-C6	-5.41	118.46	124.53
23	c	505	CLA	C2C-C1C-NC	5.40	115.03	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	b	612	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	B	605	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	B	607	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
23	b	621	CLA	C3C-C4C-NC	5.36	116.58	110.57
33	B	630	HTG	C1'-S1-C1	5.36	110.11	100.09
23	c	506	CLA	C4A-NA-C1A	-5.35	104.30	106.71
23	b	619	CLA	CHD-C4C-C3C	-5.35	116.97	124.84
23	c	513	CLA	C2C-C1C-NC	5.35	114.98	109.97
23	C	505	CLA	C4A-NA-C1A	-5.34	104.31	106.71
37	d	402[A]	PHO	O2D-CGD-CBD	5.34	120.75	111.27
23	a	412	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	B	608	CLA	C4A-NA-C1A	-5.32	104.31	106.71
37	D	403[A]	PHO	C3D-C2D-C1D	-5.32	98.12	105.87
37	D	402	PHO	O2D-CGD-CBD	5.31	120.71	111.27
23	B	609	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
23	C	510	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	B	606	CLA	C4A-NA-C1A	-5.29	104.33	106.71
23	b	611	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	C	506	CLA	O2D-CGD-CBD	5.28	120.65	111.27
23	b	620	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
23	C	513	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	d	405	CLA	O2D-CGD-CBD	5.26	120.62	111.27
23	B	611	CLA	C4A-NA-C1A	-5.26	104.34	106.71
23	B	612	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
23	D	407	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.26	117.11	124.84
37	d	402[B]	PHO	C2D-C1D-ND	5.25	117.72	109.79
23	C	513	CLA	C4A-NA-C1A	-5.25	104.35	106.71
23	c	517	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	B	612	CLA	O2D-CGD-CBD	5.23	120.57	111.27
23	C	504	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	b	615	CLA	C2C-C1C-NC	5.21	114.85	109.97
23	c	516	CLA	C2C-C1C-NC	5.21	114.85	109.97
23	B	613	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	B	615	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	C	505	CLA	CHD-C4C-C3C	-5.17	117.23	124.84
23	C	511	CLA	O2D-CGD-CBD	5.16	120.44	111.27
23	b	620	CLA	O2D-CGD-CBD	5.16	120.44	111.27
33	B	623	HTG	O5-C1-C2	5.16	116.80	110.31
23	A	407	CLA	C2C-C1C-NC	5.16	114.80	109.97
23	a	412	CLA	O2D-CGD-CBD	5.16	120.43	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	F	104	SQD	O47-C7-C8	5.16	122.61	111.50
37	a	411	PHO	C2D-C1D-ND	5.16	117.57	109.79
37	D	403[A]	PHO	C2D-C1D-ND	5.15	117.56	109.79
23	C	502	CLA	C4A-NA-C1A	-5.14	104.39	106.71
23	B	603	CLA	O2D-CGD-CBD	5.14	120.40	111.27
23	A	405	CLA	O2D-CGD-CBD	5.14	120.40	111.27
23	A	407	CLA	C4A-NA-C1A	-5.14	104.40	106.71
23	C	507	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	b	621	CLA	O2D-CGD-CBD	5.13	120.38	111.27
23	C	512	CLA	C2C-C1C-NC	5.12	114.77	109.97
33	B	629	HTG	C1'-S1-C1	5.11	109.66	100.09
37	D	403[B]	PHO	C3D-C2D-C1D	-5.11	98.42	105.87
23	B	609	CLA	O2D-CGD-CBD	5.11	120.34	111.27
23	c	508	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	b	613	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	a	410	CLA	C4A-NA-C1A	-5.08	104.42	106.71
33	C	523	HTG	C1'-S1-C1	5.07	109.57	100.09
23	b	614	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.06	117.40	124.84
23	B	617	CLA	C2C-C1C-NC	5.05	114.70	109.97
37	d	402[A]	PHO	C3D-C2D-C1D	-5.05	98.51	105.87
23	B	603	CLA	C2C-C1C-NC	5.04	114.70	109.97
33	c	525	HTG	C1'-S1-C1	5.04	109.51	100.09
23	B	614	CLA	C4A-NA-C1A	-5.03	104.45	106.71
23	c	514	CLA	C4A-NA-C1A	-5.02	104.45	106.71
23	A	406	CLA	C2C-C1C-NC	5.02	114.67	109.97
23	b	623	CLA	C2C-C1C-NC	5.01	114.67	109.97
23	C	509	CLA	C2C-C1C-NC	5.01	114.67	109.97
23	c	505	CLA	C4A-NA-C1A	-5.01	104.45	106.71
23	C	511	CLA	C1-C2-C3	-5.00	117.40	126.04
23	b	615	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	A	405	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
37	D	402	PHO	C3D-C2D-C1D	-4.97	98.63	105.87
23	c	517	CLA	C2C-C1C-NC	4.97	114.63	109.97
23	D	407	CLA	O2D-CGD-CBD	4.96	120.08	111.27
37	D	403[A]	PHO	C1-C2-C3	-4.95	117.48	126.04
33	o	301	HTG	C1'-S1-C1	4.95	109.34	100.09
23	C	509	CLA	C4A-NA-C1A	-4.93	104.49	106.71
37	d	402[A]	PHO	C2D-C1D-ND	4.93	117.23	109.79
23	C	508	CLA	C2C-C1C-NC	4.91	114.58	109.97
23	c	506	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	B	605	CLA	C4A-NA-C1A	-4.91	104.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	O2D-CGD-CBD	4.90	119.98	111.27
23	B	615	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	C	514	CLA	C2C-C1C-NC	4.90	114.56	109.97
23	C	510	CLA	C1-C2-C3	-4.90	117.58	126.04
23	C	503	CLA	C2C-C1C-NC	4.89	114.55	109.97
37	D	402	PHO	C2D-C1D-ND	4.89	117.17	109.79
23	D	407	CLA	C2C-C1C-NC	4.89	114.55	109.97
33	C	523	HTG	C1-O5-C5	4.89	121.59	112.58
23	d	404	CLA	O2D-CGD-CBD	4.88	119.94	111.27
23	B	609	CLA	C4A-NA-C1A	-4.88	104.51	106.71
23	B	606	CLA	C2C-C1C-NC	4.87	114.54	109.97
23	A	407	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	c	505	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	c	508	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	c	512	CLA	C4A-NA-C1A	-4.85	104.52	106.71
23	C	511	CLA	C4A-NA-C1A	-4.85	104.53	106.71
25	B	621	SQD	O47-C7-C8	4.85	121.95	111.50
37	D	403[B]	PHO	C2D-C1D-ND	4.84	117.09	109.79
23	A	406	CLA	C4A-NA-C1A	-4.84	104.53	106.71
34	d	408	DGD	O6E-C5E-C4E	4.84	118.48	109.69
23	c	507	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	c	515	CLA	C4A-NA-C1A	-4.81	104.54	106.71
24	k	102	BCR	C33-C5-C6	-4.80	119.14	124.53
38	D	413	LHG	O7-C7-C8	4.79	121.83	111.50
37	d	402[A]	PHO	C1-C2-C3	-4.78	117.78	126.04
25	A	409	SQD	O47-C7-C8	4.78	121.80	111.50
23	C	504	CLA	O2D-CGD-CBD	4.77	119.74	111.27
24	C	515	BCR	C7-C8-C9	-4.76	119.04	126.23
23	C	506	CLA	C3C-C4C-NC	4.76	115.91	110.57
24	k	101	BCR	C20-C21-C22	-4.76	120.52	127.31
23	c	507	CLA	C1D-CHD-C4C	-4.75	116.29	122.56
23	C	512	CLA	C4A-NA-C1A	-4.75	104.57	106.71
24	k	102	BCR	C15-C14-C13	-4.74	120.55	127.31
34	d	408	DGD	O2G-C1B-C2B	4.74	121.71	111.50
35	c	523	LMG	O7-C10-C11	4.74	121.71	111.50
23	B	608	CLA	O2D-CGD-CBD	4.73	119.67	111.27
37	a	411	PHO	O2D-CGD-CBD	4.73	119.67	111.27
23	A	404	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
23	C	502	CLA	C2C-C1C-NC	4.71	114.39	109.97
23	d	403	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
23	b	610	CLA	C2C-C1C-NC	4.70	114.38	109.97
23	b	617	CLA	O2D-CGD-CBD	4.70	119.62	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	405	CLA	C2C-C1C-NC	4.69	114.37	109.97
23	C	510	CLA	O2D-CGD-CBD	4.69	119.60	111.27
23	b	620	CLA	C4A-NA-C1A	-4.68	104.60	106.71
23	b	617	CLA	C2C-C1C-NC	4.68	114.36	109.97
23	c	509	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	d	404	CLA	CHD-C4C-C3C	-4.66	117.98	124.84
23	C	514	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	B	604	CLA	C2C-C1C-NC	4.66	114.33	109.97
23	c	507	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	B	616	CLA	C2C-C1C-NC	4.65	114.33	109.97
23	c	514	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	B	611	CLA	C2C-C1C-NC	4.65	114.33	109.97
37	d	402[B]	PHO	O2D-CGD-CBD	4.64	119.52	111.27
23	B	611	CLA	O2D-CGD-CBD	4.64	119.50	111.27
23	B	613	CLA	C3C-C4C-NC	4.62	115.75	110.57
33	b	631	HTG	C1'-S1-C1	4.61	108.72	100.09
23	C	510	CLA	C4A-NA-C1A	-4.61	104.64	106.71
23	D	406	CLA	O2D-CGD-CBD	4.61	119.45	111.27
23	c	511	CLA	C4A-NA-C1A	-4.59	104.64	106.71
39	e	101	HEM	CBD-CAD-C3D	-4.55	104.10	112.48
23	C	507	CLA	O2D-CGD-CBD	4.55	119.35	111.27
34	c	519	DGD	O2G-C1B-C2B	4.54	121.29	111.50
23	b	611	CLA	C2C-C1C-NC	4.54	114.22	109.97
35	a	415	LMG	O7-C10-C11	4.53	121.26	111.50
23	A	406	CLA	O2D-CGD-CBD	4.52	119.30	111.27
30	A	416[B]	PL9	C7-C3-C4	4.52	120.55	116.88
23	C	514	CLA	O2D-CGD-CBD	4.51	119.29	111.27
23	C	508	CLA	C3C-C4C-NC	4.51	115.63	110.57
24	b	626	BCR	C15-C14-C13	-4.50	120.89	127.31
23	C	508	CLA	C4A-NA-C1A	-4.50	104.69	106.71
25	a	405	SQD	O8-S-C6	4.49	112.90	105.74
23	c	507	CLA	O2D-CGD-CBD	4.48	119.24	111.27
23	a	410	CLA	O2D-CGD-CBD	4.48	119.23	111.27
23	B	614	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	b	611	CLA	O2D-CGD-CBD	4.48	119.23	111.27
23	b	613	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	b	618	CLA	C3C-C4C-NC	4.47	115.59	110.57
24	c	527	BCR	C15-C14-C13	-4.47	120.93	127.31
23	A	404	CLA	CAC-C3C-C4C	4.47	130.61	124.81
23	c	517	CLA	O2D-CGD-CBD	4.47	119.21	111.27
23	b	622	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	b	615	CLA	O2D-CGD-CBD	4.46	119.19	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	402[B]	PHO	C1-C2-C3	-4.45	118.34	126.04
23	a	412	CLA	C1D-CHD-C4C	-4.45	116.68	122.56
37	D	403[A]	PHO	O2D-CGD-CBD	4.45	119.18	111.27
23	b	614	CLA	C3C-C4C-NC	4.45	115.56	110.57
23	B	606	CLA	O2D-CGD-CBD	4.44	119.17	111.27
23	C	512	CLA	C1D-CHD-C4C	-4.44	116.70	122.56
23	b	624	CLA	C3C-C4C-NC	4.43	115.54	110.57
25	a	414	SQD	O47-C7-C8	4.42	121.03	111.50
24	d	406	BCR	C33-C5-C6	-4.41	119.57	124.53
35	C	501	LMG	O7-C10-C11	4.41	121.00	111.50
23	B	616	CLA	C3C-C4C-NC	4.41	115.51	110.57
23	c	511	CLA	C3C-C4C-NC	4.41	115.51	110.57
23	C	504	CLA	C3C-C4C-NC	4.41	115.51	110.57
24	K	101	BCR	C7-C8-C9	-4.40	119.59	126.23
30	D	409[B]	PL9	C42-C43-C44	-4.40	117.07	127.66
35	C	520	LMG	O7-C10-C11	4.39	120.96	111.50
23	b	612	CLA	C1D-CHD-C4C	-4.39	116.77	122.56
23	a	409	CLA	CHD-C4C-C3C	-4.38	118.40	124.84
23	c	511	CLA	C2C-C1C-NC	4.38	114.07	109.97
23	C	503	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	D	407	CLA	C4A-NA-C1A	-4.37	104.74	106.71
23	a	410	CLA	C2C-C1C-NC	4.37	114.07	109.97
23	b	621	CLA	C2C-C1C-NC	4.36	114.06	109.97
23	b	625	CLA	C2C-C1C-NC	4.36	114.06	109.97
37	d	402[A]	PHO	C4C-C3C-C2C	-4.34	101.98	106.78
23	B	616	CLA	O2D-CGD-CBD	4.33	118.96	111.27
37	D	403[B]	PHO	C1-C2-C3	-4.32	118.57	126.04
23	B	603	CLA	C3C-C4C-NC	4.32	115.41	110.57
24	d	406	BCR	C7-C8-C9	-4.31	119.72	126.23
23	d	404	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
23	b	621	CLA	C1D-CHD-C4C	-4.31	116.87	122.56
23	B	602	CLA	C3C-C4C-NC	4.30	115.40	110.57
25	B	621	SQD	O6-C1-C2	4.30	115.01	108.30
23	b	616	CLA	C3C-C4C-NC	4.30	115.39	110.57
34	D	410	DGD	O2G-C1B-C2B	4.29	120.76	111.50
23	b	615	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	C	502	CLA	CMC-C2C-C1C	4.29	131.57	125.04
23	b	625	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	b	619	CLA	O2D-CGD-CBD	4.28	118.87	111.27
23	b	614	CLA	O2D-CGD-O1D	-4.28	115.47	123.84
25	a	414	SQD	O6-C1-C2	4.27	114.98	108.30
23	b	620	CLA	C3C-C4C-NC	4.27	115.36	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
24	H	101	BCR	C38-C26-C25	-4.27	119.73	124.53
23	A	405	CLA	CBC-CAC-C3C	-4.26	100.68	112.43
38	E	101	LHG	O7-C7-C8	4.25	120.67	111.50
27	a	404	LMT	C1'-O5'-C5'	4.25	122.03	113.69
23	b	624	CLA	C4A-NA-C1A	-4.25	104.80	106.71
23	B	605	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	b	622	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	C	503	CLA	O2D-CGD-CBD	4.24	118.81	111.27
23	C	502	CLA	O2D-CGD-O1D	-4.24	115.55	123.84
23	b	616	CLA	O2D-CGD-CBD	4.24	118.81	111.27
23	C	513	CLA	C3C-C4C-NC	4.24	115.32	110.57
23	b	622	CLA	C3B-C4B-NB	4.23	114.68	109.21
24	H	101	BCR	C24-C23-C22	-4.22	119.86	126.23
23	d	403	CLA	C4A-NA-C1A	-4.22	104.81	106.71
23	c	508	CLA	C3C-C4C-NC	4.21	115.30	110.57
23	c	512	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
24	T	103	BCR	C33-C5-C6	-4.21	119.80	124.53
25	L	102	SQD	O47-C7-C8	4.20	120.56	111.50
34	c	521	DGD	O2G-C1B-C2B	4.20	120.55	111.50
23	d	403	CLA	C3B-C4B-NB	4.20	114.64	109.21
38	d	411	LHG	O7-C7-C8	4.20	120.54	111.50
23	c	512	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	b	623	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	b	613	CLA	C1-C2-C3	-4.19	118.79	126.04
23	B	607	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	c	506	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	c	515	CLA	C2C-C1C-NC	4.18	113.89	109.97
25	a	414	SQD	O8-S-C6	4.18	112.40	105.74
23	B	617	CLA	C3C-C4C-NC	4.17	115.25	110.57
30	a	416[B]	PL9	C7-C8-C9	-4.16	119.86	126.79
23	C	503	CLA	C1D-CHD-C4C	-4.16	117.06	122.56
24	B	618	BCR	C33-C5-C6	-4.16	119.86	124.53
23	B	610	CLA	O2D-CGD-CBD	4.16	118.66	111.27
24	b	626	BCR	C33-C5-C6	-4.15	119.86	124.53
23	B	614	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
35	d	416	LMG	O7-C10-C11	4.15	120.44	111.50
23	C	503	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	b	621	CLA	C1-C2-C3	-4.14	118.88	126.04
23	B	617	CLA	C1D-CHD-C4C	-4.14	117.09	122.56
23	B	605	CLA	C3C-C4C-NC	4.14	115.21	110.57
25	A	409	SQD	O6-C1-C2	4.14	114.76	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	404	LMT	O5'-C5'-C4'	4.13	118.47	109.75
23	C	512	CLA	O2D-CGD-CBD	4.13	118.61	111.27
23	b	615	CLA	C1D-CHD-C4C	-4.13	117.11	122.56
23	b	620	CLA	CAC-C3C-C4C	4.13	130.16	124.81
23	d	403	CLA	O2D-CGD-CBD	4.12	118.58	111.27
23	c	506	CLA	O2D-CGD-CBD	4.11	118.57	111.27
23	c	505	CLA	C3C-C4C-NC	4.11	115.18	110.57
34	c	520	DGD	O2G-C1B-C2B	4.11	120.35	111.50
23	a	409	CLA	C1-C2-C3	-4.10	118.96	126.04
34	d	408	DGD	C3E-C4E-C5E	4.09	117.53	110.24
23	a	409	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	a	412	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	C	506	CLA	CAC-C3C-C4C	4.08	130.11	124.81
23	B	608	CLA	C1C-C2C-C3C	-4.08	102.66	106.96
27	D	405	LMT	O1B-C4'-C3'	4.08	118.14	107.28
23	C	502	CLA	C3C-C4C-NC	4.08	115.15	110.57
39	v	205	HEM	CBA-CAA-C2A	-4.08	104.97	112.49
37	D	403[B]	PHO	O2D-CGD-CBD	4.06	118.49	111.27
23	a	410	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	c	510	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	c	510	CLA	O2D-CGD-CBD	4.06	118.48	111.27
23	C	510	CLA	C3C-C4C-NC	4.05	115.12	110.57
23	B	602	CLA	C1D-CHD-C4C	-4.05	117.22	122.56
24	C	515	BCR	C33-C5-C6	-4.05	119.98	124.53
23	B	616	CLA	C1D-CHD-C4C	-4.04	117.22	122.56
24	Y	101	BCR	C16-C17-C18	-4.04	121.54	127.31
23	c	508	CLA	CMC-C2C-C1C	4.04	131.19	125.04
23	B	615	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	b	612	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	A	404	CLA	C1C-C2C-C3C	-4.02	102.72	106.96
38	b	634	LHG	O7-C7-C8	4.02	120.17	111.50
23	b	614	CLA	C1D-CHD-C4C	-4.02	117.26	122.56
23	B	612	CLA	C3C-C4C-NC	4.02	115.08	110.57
23	D	406	CLA	C1-C2-C3	-4.01	119.11	126.04
23	c	509	CLA	C1D-CHD-C4C	-4.01	117.27	122.56
23	B	615	CLA	C1D-CHD-C4C	-4.01	117.27	122.56
23	b	611	CLA	C3C-C4C-NC	4.01	115.06	110.57
23	b	618	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	604	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	B	609	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
25	F	104	SQD	O5-C5-C4	3.99	116.95	109.69
35	C	519	LMG	O7-C10-C11	3.99	120.11	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C3C-C4C-NC	3.99	115.05	110.57
39	F	102	HEM	CBA-CAA-C2A	-3.98	105.14	112.49
25	A	412	SQD	O47-C7-C8	3.98	120.08	111.50
34	D	410	DGD	C1D-C2D-C3D	3.98	118.28	110.00
23	C	504	CLA	C1D-CHD-C4C	-3.98	117.31	122.56
23	c	516	CLA	C1C-C2C-C3C	-3.98	102.78	106.96
23	B	607	CLA	C1-C2-C3	-3.98	119.17	126.04
23	B	607	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	C	512	CLA	CAC-C3C-C4C	3.95	129.94	124.81
25	B	621	SQD	O7-S-C6	3.95	111.64	106.94
23	C	503	CLA	C1-C2-C3	-3.95	119.21	126.04
23	b	612	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	b	625	CLA	C1D-CHD-C4C	-3.95	117.35	122.56
23	c	512	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	B	605	CLA	C3B-C4B-NB	3.94	114.30	109.21
23	c	513	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	b	613	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	B	609	CLA	C1D-CHD-C4C	-3.93	117.37	122.56
33	b	608	HTG	C1'-S1-C1	3.92	107.42	100.09
23	b	619	CLA	C3C-C4C-NC	3.92	114.97	110.57
33	V	207	HTG	C1'-S1-C1	3.91	107.41	100.09
23	C	505	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
30	d	407[B]	PL9	C42-C43-C44	-3.91	118.24	127.66
23	B	606	CLA	C3C-C4C-NC	3.91	114.96	110.57
23	A	406	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
23	c	514	CLA	C1C-C2C-C3C	-3.90	102.85	106.96
23	c	509	CLA	CAC-C3C-C4C	3.90	129.87	124.81
24	h	101	BCR	C38-C26-C25	-3.90	120.15	124.53
24	k	101	BCR	C15-C14-C13	-3.89	121.76	127.31
35	Z	101	LMG	O7-C10-C11	3.89	119.88	111.50
23	c	513	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	b	623	CLA	C4A-NA-C1A	-3.88	104.96	106.71
23	c	515	CLA	C1D-CHD-C4C	-3.88	117.44	122.56
23	c	510	CLA	C3B-C4B-NB	3.88	114.22	109.21
23	d	404	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	B	612	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	c	511	CLA	CMC-C2C-C1C	3.87	130.93	125.04
23	C	512	CLA	C3B-C4B-NB	3.86	114.21	109.21
23	B	613	CLA	C4A-NA-C1A	-3.86	104.97	106.71
23	d	403	CLA	CBC-CAC-C3C	-3.86	101.79	112.43
30	a	416[A]	PL9	C22-C23-C24	-3.86	118.37	127.66
23	c	508	CLA	C1D-CHD-C4C	-3.86	117.47	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C1D-CHD-C4C	-3.86	117.47	122.56
23	b	613	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	c	517	CLA	C1D-CHD-C4C	-3.85	117.48	122.56
23	b	614	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	c	510	CLA	C4A-NA-C1A	-3.85	104.98	106.71
23	b	616	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	C	507	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	A	404	CLA	CAA-C2A-C3A	-3.84	102.26	112.78
23	B	602	CLA	C3B-C4B-NB	3.84	114.17	109.21
39	F	102	HEM	CBD-CAD-C3D	-3.83	105.41	112.48
23	C	505	CLA	C3C-C4C-NC	3.83	114.87	110.57
23	c	514	CLA	C3B-C4B-NB	3.83	114.16	109.21
23	b	618	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	A	407	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	B	608	CLA	C1D-CHD-C4C	-3.82	117.51	122.56
23	C	509	CLA	C3B-C4B-NB	3.82	114.15	109.21
30	a	416[A]	PL9	C32-C33-C34	-3.82	118.47	127.66
25	L	102	SQD	C3-C4-C5	3.82	117.05	110.24
23	B	610	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	c	513	CLA	C1-O2A-CGA	3.81	126.45	116.44
23	c	516	CLA	C1D-CHD-C4C	-3.81	117.53	122.56
23	c	513	CLA	C1D-CHD-C4C	-3.81	117.53	122.56
37	D	403[A]	PHO	C4C-C3C-C2C	-3.81	102.56	106.78
23	C	505	CLA	C3B-C4B-NB	3.81	114.13	109.21
23	d	404	CLA	O2A-CGA-CBA	3.81	123.85	111.91
23	a	412	CLA	C4A-NA-C1A	-3.81	105.00	106.71
23	A	405	CLA	C3B-C4B-NB	3.80	114.13	109.21
34	C	516	DGD	O2G-C1B-C2B	3.80	119.70	111.50
23	b	612	CLA	CAA-C2A-C3A	-3.80	102.37	112.78
23	b	615	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
23	D	406	CLA	C3C-C4C-NC	3.80	114.83	110.57
24	b	626	BCR	C7-C8-C9	-3.80	120.50	126.23
23	B	615	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	B	620	BCR	C15-C14-C13	-3.80	121.89	127.31
34	C	517	DGD	O2G-C1B-C2B	3.80	119.68	111.50
37	d	402[B]	PHO	C4C-C3C-C2C	-3.80	102.58	106.78
23	B	602	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	A	405	CLA	C1D-CHD-C4C	-3.79	117.55	122.56
23	b	623	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
23	B	613	CLA	C1-C2-C3	-3.79	119.49	126.04
23	b	620	CLA	C1-C2-C3	-3.79	119.49	126.04
23	b	617	CLA	C3C-C4C-NC	3.79	114.82	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	622	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	c	508	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	B	609	CLA	C3C-C4C-NC	3.78	114.81	110.57
27	A	413	LMT	O5'-C5'-C4'	3.78	117.72	109.75
24	T	103	BCR	C11-C10-C9	-3.77	121.93	127.31
23	D	407	CLA	C4-C3-C5	3.77	121.61	115.27
23	c	515	CLA	O2D-CGD-CBD	3.76	117.96	111.27
23	c	516	CLA	C3C-C4C-NC	3.76	114.79	110.57
23	A	404	CLA	C1D-CHD-C4C	-3.76	117.60	122.56
23	c	517	CLA	C3C-C4C-NC	3.75	114.78	110.57
25	a	405	SQD	O47-C7-C8	3.75	119.59	111.50
23	A	404	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	B	604	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
23	d	405	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
23	b	623	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
23	B	610	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	B	604	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
23	c	514	CLA	C3C-C4C-NC	3.74	114.76	110.57
23	D	406	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	c	512	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
30	A	416[A]	PL9	C7-C3-C4	3.73	119.91	116.88
23	b	623	CLA	C1-C2-C3	-3.73	119.60	126.04
23	C	511	CLA	C4-C3-C5	3.72	121.53	115.27
27	C	521	LMT	C1'-O5'-C5'	3.72	120.99	113.69
23	C	513	CLA	C1D-CHD-C4C	-3.72	117.65	122.56
23	b	610	CLA	C1D-CHD-C4C	-3.72	117.65	122.56
23	B	605	CLA	C1-C2-C3	-3.71	119.62	126.04
23	C	510	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	b	621	CLA	C4-C3-C5	3.71	121.52	115.27
23	c	513	CLA	C1-C2-C3	-3.71	119.63	126.04
23	d	403	CLA	C1D-CHD-C4C	-3.71	117.67	122.56
35	M	101	LMG	O8-C28-C29	3.70	123.51	111.91
23	b	612	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
23	b	613	CLA	CAC-C3C-C4C	3.70	129.61	124.81
23	c	515	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	T	103	BCR	C15-C16-C17	-3.69	115.91	123.47
23	A	407	CLA	CAC-C3C-C4C	3.69	129.60	124.81
23	c	505	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
23	C	514	CLA	C1D-CHD-C4C	-3.69	117.69	122.56
23	D	407	CLA	C3C-C4C-NC	3.69	114.71	110.57
30	a	416[A]	PL9	C7-C3-C4	3.69	119.87	116.88
37	a	411	PHO	C4C-C3C-C2C	-3.69	102.70	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
23	A	406	CLA	C3C-C4C-NC	3.68	114.70	110.57
30	D	409[B]	PL9	C40-C39-C41	3.68	121.45	115.27
23	b	619	CLA	CAC-C3C-C4C	3.67	129.58	124.81
24	t	102	BCR	C33-C5-C6	-3.67	120.41	124.53
23	A	407	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
30	d	407[B]	PL9	C7-C8-C9	-3.67	120.68	126.79
24	c	518	BCR	C15-C14-C13	-3.67	122.08	127.31
23	c	514	CLA	C1-C2-C3	-3.67	119.70	126.04
23	B	612	CLA	C3B-C4B-NB	3.66	113.95	109.21
23	b	622	CLA	C1D-CHD-C4C	-3.66	117.72	122.56
23	a	412	CLA	C3B-C4B-NB	3.66	113.94	109.21
23	C	506	CLA	C1D-CHD-C4C	-3.66	117.73	122.56
23	c	510	CLA	C3C-C4C-NC	3.65	114.67	110.57
23	a	412	CLA	C3C-C4C-NC	3.65	114.67	110.57
23	b	610	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	b	612	CLA	C3B-C4B-NB	3.65	113.93	109.21
23	a	409	CLA	C3B-C4B-NB	3.65	113.92	109.21
23	B	606	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	C	514	CLA	C3C-C4C-NC	3.64	114.66	110.57
23	C	511	CLA	C3C-C4C-NC	3.64	114.65	110.57
39	v	205	HEM	CAD-CBD-CGD	3.64	118.77	112.67
23	b	621	CLA	C4C-C3C-C2C	-3.64	101.60	106.90
30	a	416[A]	PL9	C7-C8-C9	-3.63	120.74	126.79
23	C	508	CLA	C1D-CHD-C4C	-3.63	117.76	122.56
23	C	511	CLA	C3B-C4B-NB	3.63	113.91	109.21
23	c	505	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
25	A	412	SQD	O48-C23-C24	3.63	123.28	111.91
23	A	405	CLA	C4D-C3D-CAD	-3.62	106.45	108.47
23	c	511	CLA	C1-C2-C3	-3.61	119.79	126.04
30	a	416[A]	PL9	C15-C14-C16	3.61	121.35	115.27
23	b	625	CLA	C3B-C4B-NB	3.61	113.88	109.21
23	C	502	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	607	CLA	C1D-CHD-C4C	-3.61	117.79	122.56
37	a	411	PHO	CMB-C2B-C1B	3.61	130.62	125.06
23	B	603	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
23	C	513	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
23	B	603	CLA	C1D-CHD-C4C	-3.60	117.80	122.56
24	d	406	BCR	C38-C26-C25	-3.60	120.48	124.53
23	b	624	CLA	O2D-CGD-CBD	3.59	117.65	111.27
24	c	527	BCR	C16-C17-C18	-3.59	122.19	127.31
23	B	608	CLA	C3C-C4C-NC	3.59	114.60	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CAC-C3C-C4C	3.59	129.47	124.81
23	C	507	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	B	610	CLA	C3B-C4B-NB	3.58	113.84	109.21
23	C	514	CLA	C1-C2-C3	-3.58	119.85	126.04
23	a	410	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
23	B	611	CLA	C3C-C4C-NC	3.57	114.58	110.57
23	a	409	CLA	C3C-C4C-NC	3.57	114.58	110.57
23	B	604	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
23	b	625	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
23	b	623	CLA	C1D-CHD-C4C	-3.57	117.85	122.56
23	B	613	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	d	405	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	c	517	CLA	C1C-C2C-C3C	-3.57	103.21	106.96
23	a	409	CLA	CAA-C2A-C3A	-3.57	103.01	112.78
23	b	614	CLA	C4-C3-C5	3.56	121.27	115.27
23	B	614	CLA	C3B-C4B-NB	3.56	113.81	109.21
24	K	103	BCR	C7-C8-C9	-3.56	120.86	126.23
23	A	405	CLA	C4A-NA-C1A	-3.55	105.11	106.71
23	B	612	CLA	C1-C2-C3	-3.55	119.91	126.04
27	A	413	LMT	C1'-O5'-C5'	3.55	120.65	113.69
23	A	404	CLA	O2D-CGD-CBD	3.55	117.57	111.27
23	C	507	CLA	CAC-C3C-C4C	3.54	129.41	124.81
23	B	606	CLA	C1D-CHD-C4C	-3.54	117.88	122.56
23	C	504	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
24	D	408	BCR	C29-C30-C25	3.53	115.92	110.48
23	B	615	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	C	505	CLA	CMB-C2B-C3B	3.53	131.28	124.68
23	B	614	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	C	509	CLA	C1D-CHD-C4C	-3.53	117.90	122.56
23	C	511	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	c	505	CLA	CAC-C3C-C4C	3.53	129.38	124.81
23	C	506	CLA	C4C-C3C-C2C	-3.52	101.76	106.90
30	A	416[B]	PL9	C37-C38-C39	-3.52	119.18	127.66
23	c	511	CLA	C1D-CHD-C4C	-3.52	117.91	122.56
30	D	409[B]	PL9	C7-C8-C9	-3.52	120.93	126.79
23	b	621	CLA	CMC-C2C-C1C	3.52	130.39	125.04
23	c	513	CLA	C3B-C4B-NB	3.52	113.75	109.21
35	c	522	LMG	O7-C10-C11	3.51	119.08	111.50
23	b	613	CLA	CMC-C2C-C1C	3.51	130.39	125.04
23	c	511	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
33	b	601	HTG	C1'-S1-C1	3.51	106.66	100.09
23	c	506	CLA	C1D-CHD-C4C	-3.51	117.93	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	624	CLA	C3B-C4B-NB	3.51	113.74	109.21
35	z	101	LMG	O7-C10-C11	3.51	119.06	111.50
23	a	410	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
30	a	416[B]	PL9	C7-C3-C4	3.50	119.72	116.88
23	B	604	CLA	CMB-C2B-C3B	3.50	131.23	124.68
23	C	509	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
23	B	608	CLA	C4-C3-C5	3.50	121.15	115.27
23	C	512	CLA	C3C-C4C-NC	3.49	114.49	110.57
24	H	101	BCR	C7-C8-C9	-3.49	120.96	126.23
23	A	405	CLA	C3C-C4C-NC	3.48	114.48	110.57
23	B	611	CLA	C1D-CHD-C4C	-3.48	117.96	122.56
23	B	605	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
23	B	610	CLA	C1D-CHD-C4C	-3.47	117.97	122.56
23	b	620	CLA	C3B-C4B-NB	3.47	113.69	109.21
23	c	507	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
24	T	103	BCR	C21-C20-C19	-3.47	112.40	123.22
30	a	416[B]	PL9	C32-C33-C34	-3.46	119.32	127.66
23	b	621	CLA	CHD-C4C-NC	3.46	129.66	124.20
23	d	405	CLA	CBC-CAC-C3C	-3.46	102.89	112.43
23	C	505	CLA	C1D-CHD-C4C	-3.46	117.99	122.56
23	C	513	CLA	C3B-C4B-NB	3.46	113.68	109.21
23	C	514	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
24	D	408	BCR	C28-C27-C26	-3.46	107.91	114.08
23	b	615	CLA	C3B-C4B-NB	3.46	113.68	109.21
37	d	402[A]	PHO	O2D-CGD-O1D	-3.45	117.09	123.84
23	B	608	CLA	CMC-C2C-C1C	3.45	130.29	125.04
33	b	632	HTG	C1-O5-C5	3.45	118.94	112.58
23	b	620	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
34	h	102	DGD	O2G-C1B-C2B	3.45	118.93	111.50
23	c	505	CLA	C3B-C4B-NB	3.45	113.66	109.21
25	A	409	SQD	O8-S-C6	3.45	111.23	105.74
23	A	406	CLA	CBC-CAC-C3C	-3.44	102.94	112.43
37	D	402	PHO	C2A-C1A-NA	3.44	115.81	111.86
23	b	610	CLA	C3C-C4C-NC	3.44	114.43	110.57
35	c	522	LMG	O8-C28-C29	3.44	122.69	111.91
23	A	407	CLA	CMC-C2C-C1C	3.43	130.27	125.04
23	c	509	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
23	B	609	CLA	C3B-C4B-NB	3.43	113.65	109.21
34	B	632	DGD	O2G-C1B-C2B	3.43	118.89	111.50
34	c	519	DGD	C2G-O2G-C1B	-3.42	109.37	117.79
23	C	506	CLA	C3B-C4B-NB	3.42	113.63	109.21
23	d	404	CLA	C3B-C4B-NB	3.42	113.63	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	102	BCR	C16-C17-C18	-3.41	122.44	127.31
24	t	102	BCR	C3-C4-C5	-3.41	107.98	114.08
25	a	405	SQD	O48-C23-C24	3.41	122.62	111.91
30	A	416[A]	PL9	C32-C33-C34	-3.41	119.44	127.66
23	B	615	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
35	b	629	LMG	O8-C28-C29	3.41	122.60	111.91
39	V	206	HEM	CAD-CBD-CGD	3.41	118.39	112.67
23	B	604	CLA	O2A-CGA-CBA	3.40	122.59	111.91
24	k	101	BCR	C24-C23-C22	-3.40	121.10	126.23
38	a	420	LHG	O7-C7-C8	3.40	118.82	111.50
23	A	406	CLA	C4-C3-C5	3.40	120.99	115.27
23	c	507	CLA	C1-C2-C3	-3.40	120.17	126.04
24	K	103	BCR	C33-C5-C6	-3.39	120.72	124.53
23	b	617	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	A	404	CLA	CMB-C2B-C3B	3.39	131.03	124.68
30	A	416[B]	PL9	C20-C19-C21	3.39	120.98	115.27
23	B	608	CLA	CBC-CAC-C3C	-3.39	103.08	112.43
23	d	403	CLA	C3C-C4C-NC	3.39	114.37	110.57
23	a	409	CLA	CHC-C1C-C2C	-3.39	117.36	126.72
24	b	627	BCR	C15-C14-C13	-3.39	122.48	127.31
23	B	613	CLA	C4-C3-C5	3.38	120.96	115.27
38	D	411	LHG	O8-C23-C24	3.38	122.52	111.91
23	b	624	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	b	624	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
23	A	405	CLA	CAA-C2A-C3A	-3.37	103.54	112.78
24	B	619	BCR	C28-C27-C26	-3.37	108.05	114.08
23	A	404	CLA	C3C-C4C-NC	3.37	114.35	110.57
23	a	412	CLA	C1-C2-C3	-3.37	120.21	126.04
23	b	617	CLA	C1-C2-C3	-3.37	120.22	126.04
23	D	407	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
23	B	611	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
24	T	103	BCR	C12-C13-C14	-3.36	113.78	118.94
30	A	416[B]	PL9	C7-C3-C2	-3.36	118.88	123.30
34	B	632	DGD	C3G-O3G-C1D	-3.36	107.18	113.74
23	c	511	CLA	CHD-C4C-NC	3.36	129.49	124.20
30	D	409[B]	PL9	C27-C28-C29	-3.35	119.59	127.66
23	B	615	CLA	CHD-C4C-NC	3.35	129.48	124.20
23	d	403	CLA	C4D-C3D-CAD	-3.35	106.60	108.47
24	D	408	BCR	C38-C26-C25	-3.35	120.77	124.53
23	B	606	CLA	CMC-C2C-C1C	3.35	130.14	125.04
23	B	610	CLA	CHC-C1C-C2C	-3.35	117.47	126.72
24	c	518	BCR	C16-C17-C18	-3.34	122.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	103	BCR	C20-C21-C22	-3.34	122.54	127.31
34	d	408	DGD	O5D-C1E-C2E	3.34	113.52	108.30
23	a	409	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
23	b	625	CLA	CAC-C3C-C4C	3.34	129.14	124.81
23	D	407	CLA	CAC-C3C-C4C	3.34	129.14	124.81
25	f	102	SQD	C1-O5-C5	3.34	120.24	113.69
30	d	407[A]	PL9	C42-C43-C44	-3.34	119.62	127.66
23	c	515	CLA	CHD-C4C-NC	3.34	129.46	124.20
30	a	416[B]	PL9	C15-C14-C16	3.34	120.89	115.27
23	B	607	CLA	C4-C3-C5	3.34	120.88	115.27
23	C	506	CLA	C1C-C2C-C3C	-3.34	103.45	106.96
24	B	620	BCR	C28-C27-C26	-3.33	108.12	114.08
23	d	405	CLA	C3B-C4B-NB	3.33	113.52	109.21
23	A	405	CLA	CHD-C4C-NC	3.33	129.45	124.20
23	C	510	CLA	C3B-C4B-NB	3.33	113.52	109.21
23	B	604	CLA	CAA-C2A-C3A	-3.33	103.66	112.78
23	b	619	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	b	619	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
23	b	618	CLA	C1-C2-C3	-3.33	120.29	126.04
23	b	615	CLA	C4-C3-C5	3.33	120.87	115.27
23	C	510	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
23	c	515	CLA	C1-C2-C3	-3.32	120.30	126.04
23	B	608	CLA	C3B-C4B-NB	3.32	113.50	109.21
23	c	506	CLA	CAC-C3C-C4C	3.32	129.11	124.81
23	A	407	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	c	514	CLA	C4-C3-C5	3.31	120.84	115.27
23	B	608	CLA	CAA-C2A-C3A	-3.31	103.70	112.78
34	C	518	DGD	O2G-C1B-C2B	3.31	118.64	111.50
23	b	617	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
23	d	403	CLA	C1-C2-C3	-3.30	120.33	126.04
23	c	506	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
30	a	416[A]	PL9	C17-C18-C19	-3.30	119.71	127.66
23	B	613	CLA	CMC-C2C-C1C	3.30	130.07	125.04
24	D	408	BCR	C33-C5-C6	-3.30	120.82	124.53
23	c	510	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
25	a	414	SQD	C1-C2-C3	-3.30	103.13	110.00
23	d	405	CLA	C3C-C4C-NC	3.29	114.27	110.57
23	d	404	CLA	CAC-C3C-C4C	3.29	129.08	124.81
23	b	619	CLA	C1D-CHD-C4C	-3.29	118.21	122.56
23	B	617	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
23	b	618	CLA	C1D-CHD-C4C	-3.29	118.22	122.56
23	B	617	CLA	C3B-C4B-NB	3.29	113.46	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CHD-C4C-NC	3.29	129.38	124.20
23	B	603	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	b	621	CLA	C3B-C4B-NB	3.29	113.46	109.21
23	b	611	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	b	616	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	B	611	CLA	O2A-CGA-CBA	3.28	122.21	111.91
23	C	508	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	B	605	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	b	623	CLA	CMC-C2C-C1C	3.28	130.03	125.04
23	c	507	CLA	C4-C3-C5	3.27	120.78	115.27
30	a	416[B]	PL9	C22-C23-C24	-3.27	119.78	127.66
23	B	605	CLA	CMC-C2C-C1C	3.27	130.02	125.04
24	B	619	BCR	C37-C22-C21	-3.27	118.34	122.92
23	A	407	CLA	C4-C3-C5	3.27	120.77	115.27
24	D	408	BCR	C15-C14-C13	-3.27	122.64	127.31
23	C	507	CLA	CBC-CAC-C3C	-3.27	103.42	112.43
38	L	101	LHG	O7-C7-C8	3.27	118.54	111.50
23	b	622	CLA	CHC-C1C-C2C	-3.27	117.68	126.72
23	c	516	CLA	C1-C2-C3	-3.27	120.39	126.04
23	A	405	CLA	CMB-C2B-C3B	3.27	130.79	124.68
23	A	404	CLA	O2A-CGA-CBA	3.26	122.15	111.91
23	B	607	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	c	509	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	b	624	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	b	622	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	b	617	CLA	C1D-CHD-C4C	-3.25	118.27	122.56
24	a	413	BCR	C33-C5-C6	-3.25	120.88	124.53
23	C	505	CLA	CAC-C3C-C4C	3.25	129.03	124.81
23	b	618	CLA	CMC-C2C-C1C	3.25	129.99	125.04
24	C	515	BCR	C15-C14-C13	-3.25	122.67	127.31
23	B	605	CLA	O2A-CGA-O1A	-3.25	115.40	123.59
23	D	406	CLA	CHC-C1C-C2C	-3.25	117.74	126.72
23	C	502	CLA	CAC-C3C-C4C	3.25	129.02	124.81
23	C	503	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
37	D	403[A]	PHO	C4-C3-C5	3.24	120.72	115.27
30	D	409[B]	PL9	C10-C9-C11	3.24	120.71	115.27
23	d	403	CLA	CHC-C1C-C2C	-3.23	117.77	126.72
23	c	510	CLA	C1-C2-C3	-3.23	120.45	126.04
23	B	613	CLA	C3B-C4B-NB	3.23	113.39	109.21
23	A	407	CLA	C3B-C4B-NB	3.23	113.39	109.21
23	c	512	CLA	CHC-C1C-C2C	-3.23	117.79	126.72
23	c	505	CLA	C1D-CHD-C4C	-3.23	118.30	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	607	HTG	O5-C5-C4	3.23	115.55	109.69
30	A	416[A]	PL9	C20-C19-C21	3.22	120.69	115.27
23	C	507	CLA	CAA-C2A-C3A	-3.22	103.96	112.78
37	d	402[A]	PHO	C2B-C1B-NB	3.22	114.65	109.79
35	M	101	LMG	O7-C10-C11	3.22	118.44	111.50
23	C	512	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
23	a	412	CLA	C4-C3-C5	3.22	120.68	115.27
24	B	620	BCR	C38-C26-C25	-3.22	120.92	124.53
23	B	611	CLA	C1-C2-C3	-3.22	120.48	126.04
23	b	613	CLA	C1D-CHD-C4C	-3.21	118.32	122.56
23	B	617	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
23	C	507	CLA	C4-C3-C5	3.21	120.67	115.27
25	F	104	SQD	C1-O5-C5	3.21	119.98	113.69
37	d	402[A]	PHO	C4-C3-C5	3.21	120.66	115.27
23	C	511	CLA	CAC-C3C-C4C	3.20	128.97	124.81
23	b	623	CLA	C3B-C4B-NB	3.20	113.35	109.21
23	c	506	CLA	C1-C2-C3	-3.20	120.50	126.04
23	c	510	CLA	CHC-C1C-C2C	-3.20	117.86	126.72
23	b	614	CLA	C1-C2-C3	-3.20	120.51	126.04
24	K	101	BCR	C38-C26-C25	-3.20	120.94	124.53
23	C	503	CLA	C3B-C4B-NB	3.20	113.34	109.21
30	D	409[A]	PL9	C42-C43-C44	-3.20	119.96	127.66
30	a	416[A]	PL9	C37-C38-C39	-3.20	119.97	127.66
37	d	402[B]	PHO	C4-C3-C5	3.19	120.64	115.27
23	B	605	CLA	CAC-C3C-C4C	3.19	128.95	124.81
23	d	404	CLA	O2A-CGA-O1A	-3.19	115.53	123.59
30	a	416[B]	PL9	C27-C28-C29	-3.19	119.97	127.66
30	D	409[A]	PL9	C7-C8-C9	-3.19	121.48	126.79
23	C	508	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
38	D	411	LHG	O7-C7-C8	3.19	118.37	111.50
23	c	516	CLA	CBC-CAC-C3C	-3.19	103.65	112.43
23	B	612	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	d	405	CLA	CHD-C4C-NC	3.18	129.22	124.20
23	B	611	CLA	CAC-C3C-C4C	3.18	128.94	124.81
23	a	412	CLA	CBC-CAC-C3C	-3.18	103.66	112.43
30	a	416[A]	PL9	C20-C19-C21	3.18	120.62	115.27
23	C	507	CLA	C1-C2-C3	-3.18	120.54	126.04
37	D	403[B]	PHO	C4C-C3C-C2C	-3.18	103.26	106.78
23	B	616	CLA	CMC-C2C-C1C	3.18	129.88	125.04
23	b	621	CLA	C4A-NA-C1A	-3.18	105.28	106.71
23	C	502	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
25	F	104	SQD	C3-C4-C5	3.18	115.91	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
24	c	527	BCR	C11-C10-C9	-3.17	122.78	127.31
23	b	619	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	A	405	CLA	CHC-C1C-C2C	-3.17	117.95	126.72
30	a	416[A]	PL9	C27-C28-C29	-3.17	120.03	127.66
37	D	402	PHO	CHC-C1C-C2C	-3.17	117.76	125.73
23	C	507	CLA	C3B-C4B-NB	3.17	113.31	109.21
23	d	403	CLA	CHD-C4C-NC	3.17	129.19	124.20
30	a	416[A]	PL9	C10-C9-C11	3.17	120.60	115.27
23	b	625	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	C	507	CLA	CHC-C1C-C2C	-3.16	117.97	126.72
30	d	407[A]	PL9	C37-C38-C39	-3.16	120.05	127.66
25	A	409	SQD	C45-O47-C7	-3.16	110.01	117.79
23	C	503	CLA	C4D-C3D-CAD	-3.16	106.71	108.47
23	B	613	CLA	C2A-C1A-CHA	-3.16	118.34	123.86
23	c	517	CLA	CMC-C2C-C1C	3.16	129.85	125.04
24	A	408	BCR	C33-C5-C6	-3.16	120.98	124.53
23	B	605	CLA	O2A-CGA-CBA	3.15	121.81	111.91
23	a	412	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
30	a	416[B]	PL9	C10-C9-C11	3.15	120.57	115.27
30	A	416[A]	PL9	C37-C38-C39	-3.15	120.08	127.66
23	B	602	CLA	C4A-NA-C1A	-3.15	105.29	106.71
23	B	607	CLA	C3B-C4B-NB	3.15	113.28	109.21
30	D	409[A]	PL9	C10-C9-C11	3.14	120.56	115.27
30	D	409[A]	PL9	C37-C38-C39	-3.14	120.10	127.66
23	b	625	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	c	514	CLA	CHC-C1C-C2C	-3.14	118.04	126.72
23	B	613	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
35	C	501	LMG	O1-C1-C2	3.14	113.20	108.30
38	L	101	LHG	O8-C23-C24	3.14	121.76	111.91
23	A	404	CLA	CMC-C2C-C1C	3.14	129.82	125.04
35	C	519	LMG	O8-C28-C29	3.14	121.75	111.91
35	c	523	LMG	C3-C4-C5	3.13	115.83	110.24
34	C	518	DGD	O1G-C1A-C2A	3.13	121.74	111.91
23	b	615	CLA	CHD-C4C-NC	3.13	129.14	124.20
24	B	619	BCR	C15-C14-C13	-3.13	122.84	127.31
30	A	416[A]	PL9	C7-C8-C9	-3.13	121.58	126.79
23	d	405	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	B	616	CLA	CAC-C3C-C4C	3.13	128.87	124.81
30	a	416[B]	PL9	C42-C43-C44	-3.13	120.12	127.66
23	c	506	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
24	H	101	BCR	C16-C17-C18	-3.13	122.85	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C2A-C1A-CHA	-3.12	118.39	123.86
23	B	606	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
23	B	608	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	b	611	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	B	602	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
35	D	417	LMG	O7-C10-C11	3.12	118.22	111.50
23	c	517	CLA	CAC-C3C-C4C	3.12	128.86	124.81
30	D	409[B]	PL9	C22-C23-C24	-3.12	120.15	127.66
23	B	602	CLA	O2A-CGA-CBA	3.12	121.69	111.91
24	c	527	BCR	C28-C27-C26	-3.12	108.51	114.08
30	A	416[A]	PL9	C7-C3-C2	-3.12	119.20	123.30
24	Y	101	BCR	C15-C14-C13	-3.11	122.87	127.31
23	B	616	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
24	B	619	BCR	C29-C30-C25	3.11	115.27	110.48
23	C	505	CLA	CBC-CAC-C3C	-3.11	103.86	112.43
23	c	506	CLA	C4D-C3D-CAD	-3.11	106.74	108.47
23	B	605	CLA	CHC-C1C-C2C	-3.11	118.13	126.72
23	c	514	CLA	CBC-CAC-C3C	-3.11	103.87	112.43
23	b	612	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	B	611	CLA	CAA-C2A-C3A	-3.11	104.28	112.78
23	b	625	CLA	CHD-C4C-NC	3.10	129.09	124.20
37	D	403[B]	PHO	CAC-C3C-C4C	3.10	128.61	125.22
23	b	611	CLA	CAA-C2A-C3A	-3.10	104.30	112.78
23	B	616	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
23	b	620	CLA	O2D-CGD-O1D	-3.10	117.79	123.84
37	d	402[A]	PHO	C4D-CHA-C1A	-3.09	118.41	125.37
38	D	411	LHG	O8-C23-O10	-3.09	115.78	123.59
23	d	405	CLA	CHC-C1C-C2C	-3.09	118.17	126.72
23	B	615	CLA	O2A-CGA-CBA	3.09	121.61	111.91
37	D	402	PHO	C4C-C3C-C2C	-3.09	103.36	106.78
23	C	513	CLA	C1-C2-C3	-3.09	120.70	126.04
30	a	416[B]	PL9	C17-C18-C19	-3.09	120.23	127.66
33	c	525	HTG	C1-O5-C5	3.08	118.27	112.58
24	K	101	BCR	C15-C14-C13	-3.08	122.91	127.31
23	b	623	CLA	CHD-C4C-NC	3.08	129.06	124.20
23	c	515	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	B	612	CLA	CHC-C1C-C2C	-3.08	118.20	126.72
23	b	614	CLA	C3B-C4B-NB	3.08	113.19	109.21
23	b	622	CLA	C1-C2-C3	-3.07	120.73	126.04
30	d	407[B]	PL9	C27-C28-C29	-3.07	120.26	127.66
23	C	510	CLA	C1D-CHD-C4C	-3.07	118.51	122.56
23	B	614	CLA	CMC-C2C-C1C	3.07	129.71	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	O2D-CGD-CBD	3.07	116.72	111.27
30	d	407[A]	PL9	C27-C28-C29	-3.07	120.28	127.66
35	c	523	LMG	O6-C5-C4	3.07	115.26	109.69
30	a	416[A]	PL9	C42-C43-C44	-3.07	120.28	127.66
23	b	620	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
23	b	613	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	C	509	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	c	509	CLA	CHC-C1C-C2C	-3.06	118.24	126.72
23	C	510	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	c	515	CLA	C3B-C4B-NB	3.06	113.17	109.21
23	C	510	CLA	CMC-C2C-C1C	3.06	129.70	125.04
23	b	611	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	B	611	CLA	CHC-C1C-C2C	-3.06	118.26	126.72
23	d	405	CLA	CAC-C3C-C4C	3.06	128.78	124.81
38	d	410	LHG	O7-C7-C8	3.06	118.09	111.50
23	A	407	CLA	C1D-CHD-C4C	-3.06	118.52	122.56
23	b	618	CLA	O2A-CGA-CBA	3.06	121.50	111.91
23	c	516	CLA	C3B-C4B-NB	3.06	113.16	109.21
23	b	620	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	a	410	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
23	D	407	CLA	C3B-C4B-NB	3.05	113.16	109.21
23	C	507	CLA	C1D-CHD-C4C	-3.05	118.53	122.56
30	a	416[A]	PL9	C7-C3-C2	-3.05	119.28	123.30
23	C	504	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	B	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	b	615	CLA	C1-C2-C3	-3.05	120.77	126.04
23	B	615	CLA	C1-O2A-CGA	3.05	124.45	116.44
23	B	606	CLA	O2A-CGA-CBA	3.05	121.48	111.91
25	L	102	SQD	O7-S-C6	3.05	110.56	106.94
25	A	409	SQD	O48-C23-C24	3.05	121.47	111.91
23	B	606	CLA	CHD-C4C-NC	3.05	129.00	124.20
23	b	616	CLA	CHC-C1C-C2C	-3.05	118.30	126.72
24	k	102	BCR	C24-C23-C22	-3.04	121.64	126.23
23	C	511	CLA	C1D-CHD-C4C	-3.04	118.54	122.56
35	b	629	LMG	O7-C10-C11	3.04	118.05	111.50
23	B	615	CLA	C4-C3-C5	3.04	120.39	115.27
23	a	409	CLA	C4-C3-C5	3.04	120.39	115.27
30	A	416[B]	PL9	C32-C33-C34	-3.04	120.34	127.66
23	b	619	CLA	C1-C2-C3	-3.04	120.79	126.04
24	t	102	BCR	C11-C10-C9	-3.03	122.98	127.31
23	A	404	CLA	CHC-C1C-C2C	-3.03	118.33	126.72
30	a	416[B]	PL9	C20-C19-C21	3.03	120.37	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	102	BCR	C15-C16-C17	-3.03	117.26	123.47
23	C	503	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
23	B	607	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
23	B	611	CLA	CMB-C2B-C3B	3.03	130.34	124.68
23	b	621	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
23	d	404	CLA	CHC-C1C-C2C	-3.03	118.35	126.72
35	b	629	LMG	O8-C28-O10	-3.03	115.96	123.59
23	C	506	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
23	b	613	CLA	O2A-CGA-CBA	3.02	121.40	111.91
23	B	603	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
30	d	407[B]	PL9	C20-C19-C21	3.02	120.35	115.27
23	c	513	CLA	O2A-CGA-CBA	3.02	121.38	111.91
37	D	403[B]	PHO	C4D-CHA-C1A	-3.02	118.58	125.37
23	c	515	CLA	CAC-C3C-C4C	3.02	128.72	124.81
23	b	619	CLA	O2A-CGA-CBA	3.02	121.37	111.91
23	c	505	CLA	CHC-C1C-C2C	-3.01	118.38	126.72
23	b	610	CLA	C4-C3-C5	3.01	120.34	115.27
23	B	611	CLA	C3B-C4B-NB	3.01	113.10	109.21
23	a	409	CLA	O2A-CGA-CBA	3.01	121.36	111.91
23	c	513	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	B	604	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	b	610	CLA	C3B-C4B-NB	3.00	113.09	109.21
23	C	513	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	b	618	CLA	CBC-CAC-C3C	-3.00	104.16	112.43
37	D	402	PHO	C1C-C2C-C3C	-3.00	103.06	106.51
23	c	516	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
35	a	415	LMG	C8-O7-C10	-3.00	110.41	117.79
23	b	611	CLA	C1-C2-C3	-3.00	120.86	126.04
24	B	618	BCR	C34-C9-C10	-3.00	118.73	122.92
23	c	505	CLA	C4C-C3C-C2C	-2.99	102.53	106.90
23	B	616	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	b	611	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
23	C	504	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	b	610	CLA	CHD-C4C-NC	2.99	128.92	124.20
24	c	518	BCR	C38-C26-C25	-2.99	121.17	124.53
23	B	604	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	c	513	CLA	CMC-C2C-C1C	2.99	129.59	125.04
23	c	508	CLA	C4-C3-C5	2.99	120.30	115.27
30	A	416[B]	PL9	C22-C23-C24	-2.99	120.46	127.66
23	D	407	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	a	412	CLA	CHD-C4C-NC	2.99	128.91	124.20
34	D	410	DGD	O1G-C1A-C2A	2.99	121.28	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	O2A-CGA-CBA	2.99	121.28	111.91
23	c	510	CLA	CBC-CAC-C3C	-2.98	104.20	112.43
23	B	602	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
23	B	612	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	c	508	CLA	CAC-C3C-C4C	2.98	128.68	124.81
23	B	602	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
35	c	523	LMG	C8-O7-C10	-2.98	110.45	117.79
24	K	101	BCR	C16-C17-C18	-2.98	123.06	127.31
23	B	617	CLA	CHD-C4C-NC	2.98	128.90	124.20
27	T	104	LMT	C1'-O5'-C5'	2.98	119.53	113.69
23	C	509	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	d	404	CLA	C1-C2-C3	-2.98	120.89	126.04
23	c	515	CLA	C4-C3-C5	2.98	120.28	115.27
24	h	101	BCR	C10-C11-C12	-2.98	113.93	123.22
23	B	603	CLA	C3B-C4B-NB	2.98	113.06	109.21
30	a	416[B]	PL9	C7-C3-C2	-2.98	119.39	123.30
23	c	514	CLA	O2A-CGA-CBA	2.97	121.24	111.91
23	c	505	CLA	CBC-CAC-C3C	-2.97	104.23	112.43
23	C	513	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	C	508	CLA	CHD-C4C-NC	2.97	128.88	124.20
37	D	403[A]	PHO	C2B-C1B-NB	2.97	114.27	109.79
23	C	512	CLA	CHC-C1C-C2C	-2.97	118.52	126.72
23	B	614	CLA	O2A-CGA-CBA	2.97	121.21	111.91
23	c	510	CLA	O2A-CGA-O1A	-2.96	116.11	123.59
23	c	515	CLA	CBC-CAC-C3C	-2.96	104.26	112.43
23	a	409	CLA	O2A-CGA-O1A	-2.96	116.11	123.59
33	B	623	HTG	C1-C2-C3	2.96	116.44	110.59
23	b	614	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	D	406	CLA	C1D-CHD-C4C	-2.96	118.65	122.56
24	k	101	BCR	C16-C17-C18	-2.96	123.09	127.31
23	C	514	CLA	C3B-C4B-NB	2.96	113.03	109.21
30	A	416[A]	PL9	C22-C23-C24	-2.96	120.54	127.66
23	b	624	CLA	CHD-C4C-NC	2.96	128.86	124.20
23	c	508	CLA	CHD-C4C-NC	2.96	128.86	124.20
23	b	613	CLA	CHC-C1C-C2C	-2.95	118.55	126.72
23	C	509	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
23	a	410	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	c	508	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	b	616	CLA	C3B-C4B-NB	2.95	113.03	109.21
23	C	512	CLA	C1-C2-C3	-2.95	120.94	126.04
23	C	511	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
39	V	206	HEM	CBA-CAA-C2A	-2.95	107.05	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	516	CLA	C4-C3-C5	2.95	120.23	115.27
23	D	406	CLA	O2A-CGA-CBA	2.95	121.16	111.91
24	B	618	BCR	C7-C8-C9	-2.95	121.78	126.23
23	c	507	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	c	512	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
23	b	616	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
37	d	402[A]	PHO	CHC-C1C-C2C	-2.94	118.33	125.73
23	b	624	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
23	c	507	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
24	h	101	BCR	C7-C8-C9	-2.94	121.79	126.23
23	A	406	CLA	C3B-C4B-NB	2.94	113.01	109.21
23	D	407	CLA	C1D-CHD-C4C	-2.94	118.68	122.56
23	c	506	CLA	CHC-C1C-C2C	-2.94	118.59	126.72
23	b	618	CLA	C3B-C4B-NB	2.94	113.01	109.21
23	b	622	CLA	O2D-CGD-CBD	2.94	116.49	111.27
23	b	621	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
24	c	527	BCR	C33-C5-C6	-2.94	121.23	124.53
34	B	632	DGD	C2G-O2G-C1B	-2.93	110.57	117.79
38	E	101	LHG	O8-C23-C24	2.93	121.12	111.91
23	A	406	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
30	A	416[B]	PL9	C27-C28-C29	-2.93	120.60	127.66
23	B	617	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
25	L	102	SQD	O8-S-C6	2.93	110.41	105.74
23	C	513	CLA	CHC-C1C-C2C	-2.93	118.62	126.72
23	b	615	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	a	410	CLA	CHD-C4C-NC	2.93	128.82	124.20
23	B	614	CLA	C1-C2-C3	-2.93	120.98	126.04
30	d	407[A]	PL9	C40-C39-C41	2.92	120.19	115.27
24	B	619	BCR	C33-C5-C6	-2.92	121.25	124.53
24	d	406	BCR	C24-C23-C22	-2.92	121.82	126.23
23	B	604	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
23	a	410	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	C	512	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	C	505	CLA	CHC-C1C-C2C	-2.92	118.66	126.72
23	C	514	CLA	CHD-C4C-NC	2.92	128.80	124.20
37	D	402	PHO	C2B-C1B-NB	2.92	114.19	109.79
23	A	407	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
24	t	102	BCR	C21-C20-C19	-2.91	114.13	123.22
23	b	623	CLA	O2A-CGA-CBA	2.91	121.05	111.91
30	d	407[B]	PL9	C17-C18-C19	-2.91	120.65	127.66
23	D	406	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
30	A	416[A]	PL9	C27-C28-C29	-2.91	120.66	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	627	BCR	C29-C30-C25	2.91	114.96	110.48
30	D	409[B]	PL9	C12-C13-C14	-2.90	120.67	127.66
23	b	622	CLA	O2A-CGA-CBA	2.90	121.01	111.91
23	b	613	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	C	512	CLA	CHD-C4C-NC	2.90	128.77	124.20
23	B	614	CLA	C1D-CHD-C4C	-2.90	118.73	122.56
37	d	402[B]	PHO	CHC-C1C-C2C	-2.90	118.44	125.73
23	A	404	CLA	CAA-C2A-C1A	-2.90	102.48	111.97
30	A	416[A]	PL9	C42-C43-C44	-2.90	120.69	127.66
30	d	407[B]	PL9	C40-C39-C41	2.90	120.14	115.27
25	a	414	SQD	C45-O47-C7	-2.90	110.66	117.79
23	B	615	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
30	d	407[B]	PL9	C37-C38-C39	-2.90	120.69	127.66
23	B	616	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	b	620	CLA	O2A-CGA-CBA	2.89	120.99	111.91
23	B	602	CLA	CHD-C4C-NC	2.89	128.76	124.20
34	B	632	DGD	O1G-C1A-C2A	2.89	120.98	111.91
23	B	611	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	c	510	CLA	CHD-C4C-NC	2.89	128.75	124.20
24	c	527	BCR	C20-C21-C22	-2.89	123.19	127.31
23	b	617	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
25	F	104	SQD	O7-S-C6	2.89	110.37	106.94
23	C	511	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
25	F	104	SQD	O6-C1-C2	2.88	112.81	108.30
23	C	510	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
23	B	607	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
23	c	517	CLA	C4C-C3C-C2C	-2.88	102.69	106.90
23	C	513	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
30	D	409[B]	PL9	C36-C37-C38	-2.88	102.41	111.88
23	c	511	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
24	K	103	BCR	C24-C23-C22	-2.88	121.88	126.23
23	c	515	CLA	O2A-CGA-CBA	2.88	120.94	111.91
30	a	416[A]	PL9	C35-C34-C36	2.88	120.11	115.27
23	C	514	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	D	407	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	a	412	CLA	C4D-C3D-CAD	-2.88	106.87	108.47
23	B	613	CLA	CAC-C3C-C4C	2.88	128.54	124.81
23	B	609	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
23	B	615	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	B	604	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	c	515	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
23	A	406	CLA	CHD-C4C-NC	2.87	128.73	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	C3B-C4B-NB	2.87	112.92	109.21
33	C	523	HTG	O5-C5-C4	2.87	114.90	109.69
23	b	614	CLA	OBD-CAD-C3D	-2.87	123.22	127.98
23	a	410	CLA	C1D-CHD-C4C	-2.86	118.78	122.56
35	z	101	LMG	O8-C28-C29	2.86	120.89	111.91
23	C	513	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	c	512	CLA	C1-C2-C3	-2.86	121.09	126.04
30	a	416[A]	PL9	C25-C24-C26	2.86	120.08	115.27
23	b	624	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
23	b	617	CLA	C3B-C4B-NB	2.86	112.91	109.21
35	z	101	LMG	C8-O7-C10	-2.86	110.75	117.79
23	B	615	CLA	CMB-C2B-C3B	2.86	130.03	124.68
23	B	614	CLA	CHC-C1C-C2C	-2.86	118.81	126.72
24	C	515	BCR	C37-C22-C23	2.86	122.58	118.08
23	B	611	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
23	c	516	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	C	510	CLA	C1-O2A-CGA	2.86	123.94	116.44
23	a	410	CLA	O2A-CGA-O1A	-2.86	116.39	123.59
23	C	509	CLA	CHD-C4C-NC	2.85	128.70	124.20
23	c	508	CLA	CMB-C2B-C3B	2.85	130.02	124.68
25	a	414	SQD	O9-S-C6	2.85	110.33	106.94
23	b	623	CLA	CBC-CAC-C3C	-2.85	104.56	112.43
23	C	505	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	d	404	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	c	508	CLA	OBD-CAD-C3D	-2.85	123.25	127.98
23	C	502	CLA	CHD-C4C-NC	2.85	128.70	124.20
23	b	625	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
23	B	603	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	t	102	BCR	C15-C14-C13	2.85	131.38	127.31
30	a	416[B]	PL9	C35-C34-C36	2.85	120.07	115.27
23	b	615	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
23	C	504	CLA	CHD-C4C-NC	2.85	128.69	124.20
30	A	416[A]	PL9	C53-C6-C1	2.85	120.81	114.99
23	a	412	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	B	609	CLA	C4C-C3C-C2C	-2.85	102.75	106.90
23	B	603	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
24	c	518	BCR	C33-C5-C6	-2.84	121.33	124.53
33	B	622	HTG	C1-O5-C5	2.84	117.82	112.58
30	D	409[A]	PL9	C40-C39-C41	2.84	120.05	115.27
23	C	502	CLA	CBC-CAC-C3C	-2.84	104.60	112.43
23	b	621	CLA	O2A-CGA-CBA	2.84	120.82	111.91
23	b	612	CLA	CBC-CAC-C3C	-2.84	104.60	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	CMC-C2C-C1C	2.84	129.36	125.04
23	B	610	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
24	b	626	BCR	C16-C17-C18	-2.84	123.26	127.31
24	T	103	BCR	C35-C13-C12	2.84	122.55	118.08
23	b	611	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	C	503	CLA	O2A-CGA-CBA	2.84	120.81	111.91
37	D	403[A]	PHO	C2A-C1A-NA	2.84	115.12	111.86
24	b	628	BCR	C2-C1-C6	2.84	114.85	110.48
23	C	514	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
23	b	617	CLA	O2A-CGA-CBA	2.84	120.81	111.91
23	b	611	CLA	C1D-CHD-C4C	-2.83	118.82	122.56
23	c	511	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	B	603	CLA	OBD-CAD-C3D	-2.83	123.28	127.98
30	a	416[A]	PL9	C53-C6-C1	2.83	120.78	114.99
25	f	102	SQD	O5-C5-C4	2.83	114.84	109.69
23	C	514	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
23	a	410	CLA	O2A-CGA-CBA	2.83	120.79	111.91
23	B	608	CLA	C1-C2-C3	-2.83	121.15	126.04
24	c	518	BCR	C11-C10-C9	-2.83	123.27	127.31
24	b	627	BCR	C38-C26-C25	-2.83	121.35	124.53
23	b	620	CLA	C1D-CHD-C4C	-2.83	118.82	122.56
23	b	623	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
24	k	101	BCR	C11-C10-C9	-2.83	123.27	127.31
23	C	513	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
23	c	509	CLA	C3B-C4B-NB	2.83	112.87	109.21
25	L	102	SQD	C44-O6-C1	-2.83	108.22	113.74
37	d	402[B]	PHO	C4D-ND-C1D	-2.83	101.68	106.76
23	c	512	CLA	C4-C3-C5	2.83	120.02	115.27
23	b	619	CLA	CHC-C1C-C2C	-2.83	118.91	126.72
24	a	413	BCR	C20-C21-C22	-2.82	123.28	127.31
37	D	402	PHO	C4-C3-C5	2.82	120.02	115.27
23	b	614	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
23	C	503	CLA	CHD-C4C-NC	2.82	128.64	124.20
37	D	403[B]	PHO	C2A-C1A-NA	2.82	115.10	111.86
37	D	402	PHO	C4D-CHA-C1A	-2.82	119.03	125.37
23	B	608	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
23	d	403	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
23	C	514	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	b	615	CLA	CMB-C2B-C3B	2.82	129.94	124.68
23	c	513	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
23	b	612	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
37	D	403[A]	PHO	C4D-CHA-C1A	-2.81	119.04	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C3B-C4B-NB	2.81	112.84	109.21
23	A	406	CLA	C1-C2-C3	-2.81	121.19	126.04
23	B	614	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
23	b	616	CLA	C1D-CHD-C4C	-2.81	118.86	122.56
30	A	416[B]	PL9	C12-C13-C14	-2.81	120.90	127.66
23	D	406	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
23	A	406	CLA	CHC-C1C-C2C	-2.81	118.96	126.72
23	b	618	CLA	CHD-C4C-NC	2.81	128.62	124.20
25	a	414	SQD	C44-O6-C1	-2.80	108.26	113.74
23	B	606	CLA	C3B-C4B-NB	2.80	112.83	109.21
23	b	621	CLA	OBD-CAD-C3D	-2.80	123.33	127.98
23	A	406	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	c	516	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
23	C	513	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	A	406	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
37	d	402[A]	PHO	C2A-C1A-NA	2.80	115.07	111.86
23	C	504	CLA	C3B-C4B-NB	2.80	112.83	109.21
23	c	517	CLA	CHD-C4C-NC	2.80	128.61	124.20
24	c	518	BCR	C37-C22-C23	2.80	122.48	118.08
25	L	102	SQD	O48-C23-C24	2.79	120.68	111.91
23	a	412	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
35	Z	101	LMG	C9-O8-C28	2.79	124.12	117.10
23	B	614	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
23	c	508	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
30	D	409[A]	PL9	C22-C23-C24	-2.79	120.94	127.66
23	B	610	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
23	C	512	CLA	O2A-CGA-CBA	2.79	120.66	111.91
23	B	609	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	D	409[A]	PL9	C27-C28-C29	-2.79	120.95	127.66
23	A	407	CLA	C2A-C1A-CHA	-2.78	118.99	123.86
37	D	403[B]	PHO	C4-C3-C5	2.78	119.95	115.27
24	B	618	BCR	C16-C17-C18	-2.78	123.34	127.31
34	C	516	DGD	O1G-C1A-O1A	-2.78	116.57	123.59
23	c	511	CLA	C4-C3-C5	2.78	119.95	115.27
27	m	102	LMT	C1B-O5B-C5B	2.78	119.14	113.69
23	c	514	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	C	503	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	b	615	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	B	606	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
23	c	514	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	b	610	CLA	CMC-C2C-C1C	2.78	129.27	125.04
30	D	409[A]	PL9	C25-C24-C26	2.77	119.94	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	622	CLA	CED-O2D-CGD	2.77	122.21	115.94
30	D	409[B]	PL9	C53-C6-C1	2.77	120.66	114.99
23	c	517	CLA	O2A-CGA-CBA	2.77	120.61	111.91
23	B	610	CLA	CAC-C3C-C4C	2.77	128.41	124.81
35	Z	101	LMG	C1-O6-C5	2.77	119.13	113.69
24	k	102	BCR	C38-C26-C25	-2.77	121.42	124.53
23	b	623	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
23	b	618	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
23	c	506	CLA	CHD-C4C-NC	2.77	128.57	124.20
25	L	102	SQD	C1-C2-C3	-2.77	104.23	110.00
23	b	612	CLA	CMB-C2B-C3B	2.77	129.86	124.68
24	B	619	BCR	C2-C1-C6	2.77	114.74	110.48
23	b	617	CLA	CHD-C4C-NC	2.77	128.56	124.20
23	b	623	CLA	O2A-CGA-O1A	-2.76	116.61	123.59
24	B	618	BCR	C38-C26-C25	-2.76	121.42	124.53
30	A	416[B]	PL9	C53-C6-C1	2.76	120.64	114.99
37	D	403[A]	PHO	C4D-ND-C1D	-2.76	101.79	106.76
23	c	508	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
30	a	416[B]	PL9	C37-C38-C39	-2.76	121.01	127.66
23	B	604	CLA	C2A-C1A-CHA	-2.76	119.03	123.86
30	d	407[A]	PL9	C15-C14-C16	2.76	119.92	115.27
30	a	416[A]	PL9	C40-C39-C41	2.76	119.92	115.27
23	C	503	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	B	610	CLA	CMA-C3A-C4A	-2.76	104.35	111.77
30	a	416[B]	PL9	C25-C24-C26	2.76	119.91	115.27
27	M	104	LMT	O1B-C1B-C2B	2.76	115.25	108.10
30	a	416[B]	PL9	C40-C39-C41	2.76	119.91	115.27
23	C	506	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
30	d	407[A]	PL9	C53-C6-C1	2.75	120.62	114.99
23	d	403	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	A	407	CLA	CHC-C1C-C2C	-2.75	119.11	126.72
23	C	505	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	C	512	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
23	c	513	CLA	CMB-C2B-C3B	2.75	129.82	124.68
23	C	504	CLA	C4-C3-C5	2.75	119.89	115.27
23	a	409	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	C	512	CLA	CMC-C2C-C1C	2.74	129.22	125.04
37	d	402[A]	PHO	C3C-C4C-NC	2.74	114.53	110.28
23	c	517	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
24	B	620	BCR	C36-C18-C19	2.74	122.40	118.08
23	B	609	CLA	O2A-CGA-CBA	2.74	120.51	111.91
38	D	413	LHG	O8-C23-C24	2.74	120.51	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1D-CHD-C4C	-2.74	118.94	122.56
23	C	514	CLA	CAC-C3C-C4C	2.74	128.36	124.81
23	b	611	CLA	CMB-C2B-C3B	2.73	129.79	124.68
35	d	416	LMG	C4-C3-C2	-2.73	106.06	110.82
23	D	407	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
23	A	407	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
38	d	411	LHG	O8-C23-C24	2.73	120.47	111.91
30	A	416[A]	PL9	C15-C14-C16	2.73	119.86	115.27
23	b	617	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
37	d	402[B]	PHO	C2B-C1B-NB	2.72	113.90	109.79
25	f	102	SQD	O7-S-C6	2.72	110.17	106.94
23	C	507	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
23	B	614	CLA	OBD-CAD-C3D	-2.72	123.46	127.98
38	d	409	LHG	O7-C7-O9	-2.72	117.13	123.70
23	B	616	CLA	C3B-C4B-NB	2.72	112.73	109.21
37	d	402[A]	PHO	C4D-ND-C1D	-2.72	101.87	106.76
23	a	409	CLA	CAA-C2A-C1A	-2.72	103.06	111.97
25	F	104	SQD	O48-C23-C24	2.72	120.44	111.91
23	c	505	CLA	CMC-C2C-C1C	2.72	129.18	125.04
24	b	628	BCR	C24-C23-C22	-2.72	122.13	126.23
23	B	609	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	B	606	CLA	CAC-C3C-C4C	2.72	128.33	124.81
30	A	416[A]	PL9	C45-C44-C46	2.71	119.84	115.27
23	b	610	CLA	CHC-C1C-C2C	-2.71	119.21	126.72
23	C	508	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
23	b	614	CLA	CMC-C2C-C1C	2.71	129.17	125.04
24	K	101	BCR	C33-C5-C6	-2.71	121.48	124.53
23	B	617	CLA	OBD-CAD-C3D	-2.71	123.48	127.98
23	C	508	CLA	C1-C2-C3	-2.71	121.36	126.04
23	c	507	CLA	C3B-C4B-NB	2.71	112.71	109.21
23	c	513	CLA	C4-C3-C5	2.71	119.83	115.27
23	C	510	CLA	C4-C3-C5	2.71	119.82	115.27
38	b	634	LHG	O8-C23-C24	2.71	120.40	111.91
23	c	515	CLA	CMB-C2B-C3B	2.70	129.74	124.68
23	a	410	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
23	D	406	CLA	C4-C3-C5	2.70	119.82	115.27
23	b	612	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
37	d	402[A]	PHO	CHD-C1D-C2D	-2.70	118.93	125.73
23	a	409	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
23	b	623	CLA	CHC-C1C-C2C	-2.70	119.25	126.72
23	B	614	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	b	610	CLA	C2A-C1A-CHA	-2.70	119.14	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C10-C11-C12	-2.70	114.79	123.22
34	C	516	DGD	C3G-C2G-C1G	-2.70	105.41	111.79
30	a	416[A]	PL9	C30-C29-C31	2.70	119.81	115.27
23	d	405	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
23	c	515	CLA	CMC-C2C-C1C	2.70	129.15	125.04
30	A	416[A]	PL9	C25-C24-C26	2.70	119.81	115.27
24	K	103	BCR	C10-C11-C12	-2.70	114.81	123.22
24	C	515	BCR	C11-C10-C9	-2.69	123.46	127.31
34	D	410	DGD	O6D-C5D-C6D	2.69	112.11	106.67
23	a	410	CLA	C3B-C4B-NB	2.69	112.69	109.21
23	c	515	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
23	c	517	CLA	C1-C2-C3	-2.69	121.39	126.04
30	a	416[B]	PL9	C53-C6-C1	2.69	120.49	114.99
23	B	609	CLA	C1-C2-C3	-2.69	121.39	126.04
23	A	407	CLA	C1-C2-C3	-2.69	121.39	126.04
30	d	407[A]	PL9	C20-C19-C21	2.69	119.80	115.27
34	C	517	DGD	O1G-C1A-C2A	2.69	120.35	111.91
24	Y	101	BCR	C10-C11-C12	-2.69	114.83	123.22
23	a	412	CLA	CHB-C4A-NA	2.69	128.23	124.51
23	b	620	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
23	c	517	CLA	C3B-C4B-NB	2.69	112.69	109.21
23	c	508	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	C	502	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	c	505	CLA	OBD-CAD-C3D	-2.69	123.52	127.98
24	T	103	BCR	C16-C17-C18	-2.69	123.47	127.31
23	B	609	CLA	CBC-CAC-C3C	-2.69	105.03	112.43
34	c	521	DGD	O1G-C1A-C2A	2.69	120.33	111.91
23	D	406	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
35	a	415	LMG	C7-O1-C1	-2.68	108.50	113.74
23	b	618	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
23	b	618	CLA	C4-C3-C5	2.68	119.78	115.27
23	C	505	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
23	D	406	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
23	B	606	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
23	a	412	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	c	527	BCR	C35-C13-C14	-2.68	119.17	122.92
37	D	402	PHO	C16-C15-C13	-2.68	107.26	115.92
23	C	508	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
37	a	411	PHO	CHD-C1D-C2D	-2.68	119.00	125.73
37	d	402[B]	PHO	CHD-C1D-C2D	-2.68	119.00	125.73
30	d	407[A]	PL9	C10-C9-C11	2.67	119.77	115.27
23	B	611	CLA	O2A-CGA-O1A	-2.67	116.84	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	407[B]	PL9	C12-C13-C14	-2.67	121.22	127.66
37	D	403[B]	PHO	C1C-C2C-C3C	-2.67	103.44	106.51
23	c	516	CLA	CMC-C2C-C1C	2.67	129.11	125.04
23	b	625	CLA	C1-C2-C3	-2.67	121.42	126.04
23	C	504	CLA	O2A-CGA-CBA	2.67	120.28	111.91
30	A	416[B]	PL9	C15-C14-C16	2.67	119.76	115.27
23	b	618	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
37	d	402[B]	PHO	C2A-C1A-NA	2.67	114.92	111.86
23	b	619	CLA	CMB-C2B-C3B	2.67	129.67	124.68
30	A	416[B]	PL9	C42-C43-C44	-2.67	121.24	127.66
23	b	611	CLA	C4-C3-C5	2.66	119.75	115.27
23	C	509	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	b	611	CLA	CHC-C1C-C2C	-2.66	119.35	126.72
30	A	416[B]	PL9	C45-C44-C46	2.66	119.75	115.27
23	C	512	CLA	C4-C3-C5	2.66	119.75	115.27
23	B	617	CLA	O2A-CGA-CBA	2.66	120.26	111.91
23	C	502	CLA	C3B-C4B-NB	2.66	112.65	109.21
23	c	513	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
23	b	610	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
30	D	409[B]	PL9	C51-C49-C50	2.66	120.48	114.60
38	d	409	LHG	O8-C23-C24	2.66	120.25	111.91
33	C	523	HTG	O5-C1-C2	2.66	113.66	110.31
23	D	406	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	c	505	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
23	B	610	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	C	513	CLA	C4-C3-C5	2.66	119.74	115.27
23	b	612	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
24	b	628	BCR	C3-C4-C5	-2.65	109.34	114.08
23	C	510	CLA	CMB-C2B-C3B	2.65	129.64	124.68
23	b	625	CLA	OBD-CAD-C3D	-2.65	123.58	127.98
23	A	407	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	c	516	CLA	O2A-CGA-CBA	2.65	120.23	111.91
37	a	411	PHO	CBA-CAA-C2A	-2.65	106.04	113.86
23	c	505	CLA	CMB-C2B-C3B	2.65	129.64	124.68
37	a	411	PHO	C1C-C2C-C3C	-2.65	103.46	106.51
23	C	506	CLA	C1-O2A-CGA	2.65	123.40	116.44
23	c	512	CLA	CMB-C2B-C3B	2.65	129.63	124.68
23	C	510	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	c	518	BCR	C3-C4-C5	-2.65	109.35	114.08
23	c	505	CLA	CHD-C4C-NC	2.65	128.38	124.20
24	K	101	BCR	C11-C10-C9	-2.65	123.53	127.31
25	f	102	SQD	O47-C7-O49	-2.65	117.30	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
23	C	504	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
23	d	404	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	D	407	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
23	b	611	CLA	C1-O2A-CGA	2.64	123.38	116.44
37	D	403[A]	PHO	O2D-CGD-O1D	-2.64	118.68	123.84
23	B	617	CLA	C1-O2A-CGA	2.64	123.37	116.44
23	b	614	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
30	A	416[B]	PL9	C30-C29-C31	2.64	119.71	115.27
23	B	605	CLA	OBD-CAD-C3D	-2.64	123.60	127.98
23	c	516	CLA	CBA-CAA-C2A	-2.64	106.08	113.86
27	t	101	LMT	C1'-O5'-C5'	2.64	118.86	113.69
23	c	507	CLA	CAC-C3C-C4C	2.64	128.23	124.81
23	b	610	CLA	CAC-C3C-C4C	2.64	128.23	124.81
34	c	519	DGD	O2G-C1B-O1B	-2.63	117.33	123.70
23	b	615	CLA	C1-O2A-CGA	2.63	123.36	116.44
33	d	414	HTG	C1-O5-C5	2.63	117.44	112.58
23	d	403	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
23	b	620	CLA	CMC-C2C-C1C	2.63	129.05	125.04
24	D	408	BCR	C24-C23-C22	-2.63	122.26	126.23
23	B	610	CLA	C4D-C3D-CAD	-2.63	107.00	108.47
23	d	404	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	A	405	CLA	C1-C2-C3	-2.63	121.50	126.04
23	D	407	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
23	c	516	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
25	B	621	SQD	O48-C23-C24	2.62	120.13	111.91
38	D	412	LHG	O8-C23-C24	2.62	120.13	111.91
24	A	408	BCR	C8-C7-C6	-2.62	119.85	127.20
23	C	512	CLA	CMB-C2B-C3B	2.62	129.57	124.68
23	B	612	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
24	H	101	BCR	C16-C15-C14	-2.61	118.12	123.47
24	t	102	BCR	C1-C6-C7	2.61	123.17	115.78
23	B	609	CLA	CAC-C3C-C4C	2.61	128.20	124.81
37	D	402	PHO	C4D-ND-C1D	-2.61	102.06	106.76
37	a	411	PHO	CHC-C1C-C2C	-2.61	119.16	125.73
37	a	411	PHO	C2B-C1B-NB	2.61	113.73	109.79
27	M	104	LMT	O5'-C5'-C4'	2.61	115.26	109.75
23	B	614	CLA	C4-C3-C5	2.61	119.67	115.27
23	B	615	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
37	d	402[B]	PHO	C3C-C4C-NC	2.61	114.33	110.28
30	d	407[A]	PL9	C12-C13-C14	-2.61	121.38	127.66
23	B	613	CLA	O2A-CGA-CBA	2.61	120.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CMB-C2B-C3B	2.61	129.56	124.68
23	d	403	CLA	C4-C3-C5	2.61	119.66	115.27
23	B	616	CLA	C11-C10-C8	-2.61	107.49	115.92
23	D	406	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
37	D	403[A]	PHO	CHC-C1C-C2C	-2.61	119.17	125.73
23	B	603	CLA	C4-C3-C5	2.61	119.66	115.27
23	A	405	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
23	B	613	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
23	B	604	CLA	CMC-C2C-C1C	2.61	129.01	125.04
37	d	402[A]	PHO	CAC-C3C-C4C	2.61	128.06	125.22
37	a	411	PHO	C3C-C4C-NC	2.61	114.32	110.28
23	C	514	CLA	O2A-CGA-CBA	2.60	120.08	111.91
23	b	622	CLA	CHD-C4C-NC	2.60	128.31	124.20
30	A	416[A]	PL9	C30-C29-C31	2.60	119.65	115.27
23	b	624	CLA	C11-C10-C8	-2.60	107.52	115.92
24	B	620	BCR	C36-C18-C17	-2.60	119.28	122.92
23	D	407	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	B	603	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
38	d	409	LHG	O8-C23-O10	-2.60	117.03	123.59
23	C	503	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	c	513	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	c	507	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
30	D	409[B]	PL9	C37-C38-C39	-2.60	121.41	127.66
23	B	615	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	c	510	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	b	621	CLA	CMB-C2B-C3B	2.60	129.54	124.68
23	B	608	CLA	CHD-C4C-NC	2.60	128.29	124.20
23	b	616	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
23	C	505	CLA	C4-C3-C5	2.59	119.63	115.27
23	A	404	CLA	O2A-CGA-O1A	-2.59	117.05	123.59
23	d	404	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
30	A	416[A]	PL9	C12-C13-C14	-2.59	121.42	127.66
30	d	407[B]	PL9	C30-C29-C31	2.59	119.63	115.27
23	C	510	CLA	CHC-C1C-C2C	-2.59	119.56	126.72
35	C	501	LMG	C7-O1-C1	-2.59	108.68	113.74
24	C	515	BCR	C15-C16-C17	-2.59	118.17	123.47
23	B	607	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	d	405	CLA	C4D-C3D-CAD	-2.59	107.03	108.47
23	B	614	CLA	C7-C6-C5	-2.58	106.34	113.36
23	c	517	CLA	CAA-C2A-C3A	-2.58	105.71	112.78
37	D	402	PHO	C3A-C2A-C1A	-2.58	98.56	101.64
24	C	515	BCR	C21-C20-C19	-2.58	115.17	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	101	BCR	C34-C9-C8	2.58	122.14	118.08
25	F	104	SQD	C44-O6-C1	-2.58	108.70	113.74
23	c	515	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	K	101	BCR	C23-C24-C25	-2.58	119.97	127.20
37	D	403[B]	PHO	CHC-C1C-C2C	-2.57	119.26	125.73
23	C	508	CLA	OBD-CAD-C3D	-2.57	123.71	127.98
23	c	516	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	C	511	CLA	C4-C3-C2	-2.57	117.09	123.68
23	B	617	CLA	O1D-CGD-CBD	-2.57	119.23	124.48
30	D	409[A]	PL9	C53-C6-C1	2.57	120.24	114.99
23	a	412	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
37	d	402[B]	PHO	C1C-C2C-C3C	-2.57	103.56	106.51
37	D	403[B]	PHO	CMB-C2B-C1B	2.57	129.01	125.06
23	C	505	CLA	C4D-C3D-CAD	-2.56	107.04	108.47
33	V	207	HTG	C1-C2-C3	-2.56	105.53	110.59
24	a	413	BCR	C11-C10-C9	-2.56	123.65	127.31
23	c	508	CLA	CHC-C1C-C2C	-2.56	119.63	126.72
24	D	408	BCR	C10-C11-C12	-2.56	115.22	123.22
23	B	609	CLA	CMB-C2B-C3B	2.56	129.47	124.68
23	B	617	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
23	A	405	CLA	O2A-CGA-CBA	2.56	119.94	111.91
23	b	617	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
30	a	416[A]	PL9	C51-C49-C50	2.56	120.26	114.60
24	T	103	BCR	C34-C9-C10	-2.56	119.34	122.92
23	d	405	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
23	b	617	CLA	CMA-C3A-C4A	-2.56	104.89	111.77
23	d	404	CLA	C1D-CHD-C4C	-2.56	119.18	122.56
23	c	517	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	b	619	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
23	b	612	CLA	O2A-CGA-CBA	2.56	119.93	111.91
23	b	622	CLA	C4-C3-C5	2.55	119.57	115.27
25	A	412	SQD	O48-C23-O10	-2.55	117.15	123.59
23	B	610	CLA	CBC-CAC-C3C	-2.55	105.40	112.43
23	C	511	CLA	O2A-CGA-CBA	2.55	119.91	111.91
37	d	402[B]	PHO	O2A-CGA-CBA	2.55	119.90	111.91
23	a	409	CLA	CAC-C3C-C4C	2.55	128.11	124.81
30	A	416[B]	PL9	C25-C24-C26	2.55	119.55	115.27
23	a	409	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
23	b	616	CLA	CED-O2D-CGD	2.54	121.69	115.94
34	h	102	DGD	O1G-C1A-C2A	2.54	119.89	111.91
23	A	406	CLA	C1D-CHD-C4C	-2.54	119.20	122.56
23	b	616	CLA	CBC-CAC-C3C	-2.54	105.42	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
38	L	101	LHG	C5-O7-C7	-2.54	111.54	117.79
35	a	415	LMG	O8-C28-C29	2.54	119.88	111.91
33	V	207	HTG	O5-C5-C4	2.54	114.31	109.69
24	h	101	BCR	C20-C21-C22	-2.54	123.69	127.31
23	A	405	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
30	A	416[B]	PL9	C7-C8-C9	-2.54	122.57	126.79
23	b	624	CLA	CAC-C3C-C4C	2.54	128.10	124.81
23	b	621	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
30	A	416[A]	PL9	C17-C18-C19	-2.54	121.56	127.66
35	C	501	LMG	O8-C28-C29	2.54	119.86	111.91
30	D	409[A]	PL9	C20-C19-C21	2.53	119.53	115.27
23	b	611	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
24	a	413	BCR	C16-C17-C18	-2.53	123.69	127.31
37	D	402	PHO	C2C-C1C-NC	2.53	113.61	109.79
23	C	507	CLA	C4D-C3D-CAD	-2.53	107.06	108.47
24	h	101	BCR	C11-C10-C9	-2.53	123.70	127.31
23	B	616	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	c	510	CLA	C4-C3-C5	2.53	119.53	115.27
23	A	404	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
24	T	103	BCR	C1-C6-C7	2.53	122.94	115.78
24	c	518	BCR	C7-C8-C9	-2.53	122.41	126.23
23	D	407	CLA	CHD-C4C-NC	2.53	128.19	124.20
23	b	620	CLA	CBC-CAC-C3C	-2.53	105.46	112.43
23	B	605	CLA	C4-C3-C5	2.53	119.52	115.27
37	a	411	PHO	CBD-CHA-C1A	2.53	132.26	126.40
23	C	514	CLA	CMC-C2C-C1C	2.53	128.89	125.04
23	c	517	CLA	CHC-C1C-C2C	-2.53	119.73	126.72
23	C	509	CLA	C2A-C1A-CHA	-2.52	119.44	123.86
23	A	406	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	K	101	BCR	C20-C21-C22	-2.52	123.71	127.31
23	B	604	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
37	D	403[A]	PHO	C1C-C2C-C3C	-2.52	103.61	106.51
24	d	406	BCR	C37-C22-C23	2.52	122.04	118.08
23	C	507	CLA	CMB-C2B-C3B	2.52	129.39	124.68
23	B	612	CLA	CMC-C2C-C1C	2.52	128.87	125.04
23	C	510	CLA	CHD-C4C-NC	2.52	128.17	124.20
23	b	616	CLA	CHD-C4C-NC	2.51	128.17	124.20
37	D	403[A]	PHO	C3C-C4C-NC	2.51	114.18	110.28
23	B	605	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	a	413	BCR	C15-C14-C13	-2.51	123.72	127.31
23	a	412	CLA	CMA-C3A-C2A	-2.51	103.69	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	SQD	O47-C7-O49	-2.51	117.63	123.70
30	D	409[B]	PL9	C32-C33-C34	-2.51	121.61	127.66
23	B	615	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
35	c	522	LMG	O8-C28-O10	-2.51	117.25	123.59
37	D	403[B]	PHO	C4D-ND-C1D	-2.51	102.25	106.76
38	d	409	LHG	O7-C7-C8	2.51	116.91	111.50
30	A	416[B]	PL9	C17-C18-C19	-2.51	121.62	127.66
23	b	622	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
37	D	402	PHO	O2D-CGD-O1D	-2.51	118.94	123.84
23	b	625	CLA	C4-C3-C5	2.51	119.49	115.27
23	B	609	CLA	CHD-C4C-NC	2.50	128.15	124.20
35	C	520	LMG	O8-C28-C29	2.50	119.75	111.91
37	D	403[B]	PHO	C2B-C1B-NB	2.50	113.56	109.79
25	a	414	SQD	O48-C23-C24	2.50	119.75	111.91
23	c	517	CLA	C4-C3-C5	2.50	119.47	115.27
23	a	410	CLA	CHC-C1C-C2C	-2.49	119.82	126.72
33	B	622	HTG	C1-C2-C3	2.49	115.51	110.59
24	k	101	BCR	C36-C18-C19	2.49	122.00	118.08
23	A	406	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
23	C	514	CLA	C4-C3-C5	2.49	119.46	115.27
23	C	503	CLA	CMC-C2C-C1C	2.49	128.83	125.04
23	B	611	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	C	512	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	D	406	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	k	101	BCR	C10-C11-C12	-2.49	115.45	123.22
24	B	619	BCR	C31-C1-C6	-2.49	106.26	110.30
23	C	504	CLA	CMC-C2C-C1C	2.49	128.83	125.04
30	d	407[B]	PL9	C51-C49-C50	2.49	120.09	114.60
24	t	102	BCR	C29-C28-C27	-2.49	105.82	111.38
37	D	403[A]	PHO	CHD-C1D-C2D	-2.48	119.48	125.73
24	K	103	BCR	C31-C1-C6	-2.48	106.27	110.30
23	D	407	CLA	CMC-C2C-C1C	2.48	128.82	125.04
37	D	403[B]	PHO	CMC-C2C-C1C	2.48	128.88	125.06
27	A	413	LMT	C1B-O5B-C5B	2.48	118.56	113.69
23	C	507	CLA	CHD-C4C-NC	2.48	128.11	124.20
23	b	612	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
23	A	405	CLA	CMA-C3A-C2A	-2.48	103.83	113.83
24	c	518	BCR	C23-C24-C25	-2.48	120.24	127.20
23	C	514	CLA	CMB-C2B-C3B	2.48	129.31	124.68
37	a	411	PHO	CAC-C3C-C4C	2.48	127.92	125.22
23	B	606	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
23	B	603	CLA	CMA-C3A-C2A	-2.48	103.84	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	102	BCR	C21-C20-C19	-2.47	115.50	123.22
23	B	617	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
23	b	610	CLA	CMB-C2B-C3B	2.47	129.31	124.68
23	c	507	CLA	O2A-CGA-CBA	2.47	119.67	111.91
35	M	101	LMG	O8-C28-O10	-2.47	117.35	123.59
23	b	625	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
25	a	405	SQD	O48-C23-O10	-2.47	117.35	123.59
37	d	402[B]	PHO	C4D-CHA-C1A	-2.47	119.81	125.37
25	F	104	SQD	O47-C7-O49	-2.47	117.73	123.70
23	C	509	CLA	C4-C3-C5	2.47	119.42	115.27
23	b	618	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
30	d	407[B]	PL9	C15-C14-C16	2.47	119.42	115.27
23	c	506	CLA	O2A-CGA-CBA	2.47	119.65	111.91
23	d	403	CLA	C1-O2A-CGA	2.47	122.92	116.44
23	B	602	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
24	a	413	BCR	C8-C7-C6	-2.46	120.28	127.20
24	H	101	BCR	C11-C10-C9	-2.46	123.79	127.31
23	d	404	CLA	CMB-C2B-C3B	2.46	129.29	124.68
23	C	508	CLA	CMC-C2C-C1C	2.46	128.79	125.04
23	c	505	CLA	O2A-CGA-CBA	2.46	119.63	111.91
37	d	402[B]	PHO	C2C-C1C-NC	2.46	113.50	109.79
23	C	506	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	c	512	CLA	CHD-C4C-NC	2.46	128.08	124.20
23	B	617	CLA	CMB-C2B-C3B	2.46	129.28	124.68
30	D	409[B]	PL9	C17-C18-C19	-2.46	121.74	127.66
30	A	416[B]	PL9	C40-C39-C41	2.46	119.41	115.27
38	d	411	LHG	C5-O7-C7	-2.46	111.74	117.79
23	c	512	CLA	C4D-C3D-CAD	-2.46	107.10	108.47
27	C	521	LMT	O1B-C4'-C3'	2.46	113.81	107.28
23	c	505	CLA	C4D-C3D-CAD	-2.45	107.10	108.47
25	A	412	SQD	O8-S-C6	2.45	109.65	105.74
24	k	102	BCR	C10-C11-C12	-2.45	115.56	123.22
23	b	625	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
23	b	617	CLA	C11-C12-C13	-2.45	107.99	115.92
25	A	409	SQD	O48-C23-O10	-2.45	117.40	123.59
23	B	610	CLA	O2A-CGA-CBA	2.45	119.60	111.91
23	B	613	CLA	CHD-C4C-NC	2.45	128.07	124.20
35	c	523	LMG	O8-C28-C29	2.45	119.59	111.91
23	b	619	CLA	CHD-C4C-NC	2.45	128.06	124.20
37	D	403[B]	PHO	CBD-CHA-C1A	2.45	132.08	126.40
23	B	608	CLA	C1-O2A-CGA	2.45	122.86	116.44
24	B	620	BCR	C10-C11-C12	-2.45	115.58	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409[B]	PL9	C25-C24-C26	2.45	119.39	115.27
34	C	517	DGD	O3G-C1D-C2D	2.45	112.12	108.30
23	d	405	CLA	O2A-CGA-CBA	2.45	119.58	111.91
25	a	414	SQD	O47-C7-O49	-2.44	117.80	123.70
30	D	409[B]	PL9	C45-C44-C46	2.44	119.38	115.27
23	C	506	CLA	C4-C3-C5	2.44	119.38	115.27
23	B	616	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
23	B	609	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
30	a	416[B]	PL9	C30-C29-C31	2.44	119.37	115.27
34	B	632	DGD	O1G-C1A-O1A	-2.44	117.44	123.59
23	d	405	CLA	CMC-C2C-C1C	2.44	128.75	125.04
23	b	621	CLA	CMA-C3A-C4A	-2.44	105.22	111.77
24	t	102	BCR	C12-C13-C14	-2.44	115.20	118.94
30	d	407[B]	PL9	C10-C9-C11	2.44	119.37	115.27
23	A	406	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
23	B	612	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
24	t	102	BCR	C7-C6-C5	-2.43	115.57	121.46
24	c	518	BCR	C21-C20-C19	-2.43	115.64	123.22
24	T	103	BCR	C7-C6-C5	-2.43	115.58	121.46
23	c	508	CLA	CAA-C2A-C3A	-2.43	106.13	112.78
23	c	509	CLA	C1-C2-C3	-2.43	121.85	126.04
23	c	516	CLA	CMB-C2B-C3B	2.42	129.22	124.68
30	D	409[B]	PL9	C20-C19-C21	2.42	119.35	115.27
23	a	409	CLA	C7-C6-C5	-2.42	106.77	113.36
23	B	612	CLA	C4-C3-C5	2.42	119.35	115.27
23	A	407	CLA	OBD-CAD-C3D	-2.42	123.96	127.98
23	b	617	CLA	CMB-C2B-C3B	2.42	129.21	124.68
23	D	407	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
23	b	614	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
30	A	416[A]	PL9	C10-C9-C11	2.42	119.34	115.27
23	d	405	CLA	C4-C3-C5	2.42	119.34	115.27
37	a	411	PHO	C4D-CHA-C1A	-2.42	119.92	125.37
23	C	511	CLA	C6-C7-C8	-2.42	108.10	115.92
38	a	420	LHG	O8-C23-C24	2.42	119.50	111.91
23	c	514	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	B	605	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
30	D	409[B]	PL9	C15-C14-C16	2.41	119.33	115.27
23	C	502	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
38	D	413	LHG	O8-C23-O10	-2.41	117.50	123.59
23	B	608	CLA	C4C-C3C-C2C	-2.41	103.38	106.90
24	Y	101	BCR	C8-C7-C6	-2.41	120.44	127.20
23	b	622	CLA	OBD-CAD-C3D	-2.41	123.98	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409[A]	PL9	C12-C13-C14	-2.41	121.86	127.66
25	L	102	SQD	O47-C7-O49	-2.41	117.89	123.70
37	a	411	PHO	C4D-ND-C1D	-2.41	102.44	106.76
24	K	103	BCR	C2-C1-C6	2.41	114.19	110.48
23	c	512	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	c	513	CLA	CAC-C3C-C4C	2.41	127.93	124.81
23	B	614	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
23	C	508	CLA	C4-C3-C5	2.41	119.32	115.27
23	D	407	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
23	b	618	CLA	CAC-C3C-C4C	2.40	127.93	124.81
35	a	415	LMG	O6-C5-C4	2.40	114.06	109.69
23	C	511	CLA	CMB-C2B-C3B	2.40	129.17	124.68
23	C	513	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
23	b	614	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
23	b	619	CLA	C4-C3-C5	2.40	119.31	115.27
24	Y	101	BCR	C37-C22-C23	2.40	121.86	118.08
23	B	603	CLA	C1-C2-C3	-2.40	121.89	126.04
23	B	611	CLA	C11-C12-C13	-2.40	108.16	115.92
37	D	402	PHO	C1-C2-C3	-2.40	121.89	126.04
23	B	604	CLA	C4-C3-C5	2.40	119.30	115.27
23	B	613	CLA	C1D-CHD-C4C	-2.40	119.39	122.56
34	C	516	DGD	O1G-C1A-C2A	2.40	119.43	111.91
23	c	506	CLA	O2A-C1-C2	2.40	114.93	108.64
30	D	409[A]	PL9	C15-C14-C16	2.40	119.30	115.27
23	c	511	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
39	V	206	HEM	CBD-CAD-C3D	-2.40	108.06	112.48
23	b	612	CLA	CHD-C4C-NC	2.39	127.97	124.20
37	a	411	PHO	O1D-CGD-CBD	-2.39	119.59	124.48
27	F	101	LMT	O5'-C5'-C4'	2.39	114.79	109.75
23	B	608	CLA	CMB-C2B-C3B	2.39	129.15	124.68
35	Z	101	LMG	C8-O7-C10	-2.39	111.91	117.79
24	K	103	BCR	C29-C30-C25	2.39	114.16	110.48
23	B	616	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
23	c	509	CLA	O1D-CGD-CBD	-2.39	119.60	124.48
34	c	519	DGD	O1G-C1A-C2A	2.39	119.40	111.91
37	D	402	PHO	CBD-CHA-C1A	2.39	131.94	126.40
23	D	407	CLA	C1-C2-C3	-2.39	121.92	126.04
23	C	508	CLA	C3B-C4B-NB	2.39	112.29	109.21
23	C	507	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
25	A	409	SQD	C1-C2-C3	-2.38	105.04	110.00
34	h	102	DGD	O1G-C1A-O1A	-2.38	117.59	123.59
23	b	615	CLA	O2A-CGA-CBA	2.38	119.37	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	410	CLA	CMB-C2B-C3B	2.38	129.13	124.68
25	f	102	SQD	O48-C23-C24	2.38	119.37	111.91
23	C	508	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
25	A	409	SQD	C44-O6-C1	-2.38	109.10	113.74
23	C	511	CLA	CHD-C4C-NC	2.38	127.95	124.20
23	B	610	CLA	CMB-C2B-C1B	2.38	132.12	128.46
23	B	610	CLA	C1-O2A-CGA	2.37	122.67	116.44
23	C	511	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	c	512	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	a	410	CLA	C4-C3-C5	2.37	119.26	115.27
37	D	402	PHO	C4A-NA-C1A	-2.37	106.22	108.14
23	A	405	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
34	c	519	DGD	O3G-C3G-C2G	-2.37	105.18	110.90
23	b	620	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
30	d	407[B]	PL9	C45-C44-C46	2.37	119.26	115.27
23	B	614	CLA	CAC-C3C-C4C	2.37	127.88	124.81
30	D	409[A]	PL9	C17-C18-C19	-2.37	121.96	127.66
24	B	618	BCR	C21-C20-C19	-2.37	115.83	123.22
23	B	606	CLA	C4-C3-C5	2.37	119.25	115.27
30	a	416[B]	PL9	C51-C49-C50	2.37	119.83	114.60
30	A	416[A]	PL9	C40-C39-C41	2.37	119.25	115.27
23	c	513	CLA	OBD-CAD-C3D	-2.37	124.05	127.98
24	T	103	BCR	C37-C22-C23	2.36	121.80	118.08
30	D	409[A]	PL9	C45-C44-C46	2.36	119.25	115.27
23	b	617	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	b	624	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
23	B	608	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
23	a	412	CLA	O2A-CGA-CBA	2.36	119.31	111.91
23	b	621	CLA	C4D-C3D-CAD	-2.36	107.16	108.47
23	C	514	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
23	d	404	CLA	O2A-C1-C2	2.36	114.83	108.64
23	A	406	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	b	619	CLA	CMC-C2C-C1C	2.35	128.62	125.04
23	b	617	CLA	CBC-CAC-C3C	-2.35	105.94	112.43
37	d	402[A]	PHO	CBD-CHA-C1A	2.35	131.86	126.40
35	c	523	LMG	O7-C10-O9	-2.35	118.02	123.70
24	T	103	BCR	C37-C22-C21	-2.35	119.63	122.92
23	c	515	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
24	D	408	BCR	C38-C26-C27	2.35	118.13	113.62
34	d	408	DGD	O1G-C1A-C2A	2.35	119.28	111.91
23	b	619	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
24	b	626	BCR	C31-C1-C6	-2.35	106.49	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	D	403[B]	PHO	O2A-CGA-CBA	2.35	119.27	111.91
23	c	509	CLA	C4-C3-C5	2.35	119.22	115.27
23	d	403	CLA	C4C-C3C-C2C	-2.35	103.48	106.90
24	b	628	BCR	C8-C7-C6	-2.34	120.62	127.20
23	C	506	CLA	CMC-C2C-C1C	2.34	128.61	125.04
37	d	402[A]	PHO	C2C-C1C-NC	2.34	113.33	109.79
23	B	611	CLA	C6-C7-C8	-2.34	108.34	115.92
23	C	505	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	C	507	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	c	508	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	b	613	CLA	CHD-C4C-NC	2.34	127.89	124.20
30	D	409[A]	PL9	C35-C34-C36	2.34	119.20	115.27
23	b	623	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
23	C	511	CLA	CMC-C2C-C1C	2.33	128.59	125.04
37	D	403[A]	PHO	CAC-C3C-C4C	2.33	127.77	125.22
24	Y	101	BCR	C21-C20-C19	-2.33	115.94	123.22
23	B	616	CLA	C4-C3-C5	2.33	119.19	115.27
38	L	101	LHG	O8-C23-O10	-2.33	117.71	123.59
24	d	406	BCR	C16-C15-C14	-2.33	118.70	123.47
23	b	622	CLA	CAC-C3C-C4C	2.33	127.83	124.81
23	C	511	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
24	B	619	BCR	C37-C22-C23	2.33	121.75	118.08
23	b	612	CLA	CMA-C3A-C2A	-2.33	104.44	113.83
24	k	102	BCR	C34-C9-C8	2.33	121.74	118.08
24	Y	101	BCR	C15-C16-C17	-2.33	118.71	123.47
23	B	613	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	b	611	CLA	CHD-C4C-NC	2.33	127.87	124.20
23	b	610	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
23	C	509	CLA	O2A-CGA-CBA	2.32	119.20	111.91
27	A	413	LMT	C6'-C5'-C4'	-2.32	106.56	113.33
23	C	510	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	b	616	CLA	C4-C3-C5	2.32	119.18	115.27
24	T	103	BCR	C7-C8-C9	-2.32	122.73	126.23
23	c	506	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	c	506	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
38	d	410	LHG	O8-C23-O10	-2.32	117.74	123.59
23	b	618	CLA	C4D-C3D-CAD	-2.32	107.18	108.47
24	A	408	BCR	C29-C30-C25	2.32	114.05	110.48
23	B	603	CLA	CMC-C2C-C1C	2.32	128.57	125.04
34	C	516	DGD	C4E-C3E-C2E	-2.32	106.78	110.82
23	A	407	CLA	CHB-C4A-NA	2.32	127.71	124.51
23	B	605	CLA	CHD-C4C-NC	2.32	127.85	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	h	102	DGD	C3G-O3G-C1D	-2.32	109.22	113.74
23	c	511	CLA	O2A-CGA-CBA	2.31	119.17	111.91
23	d	404	CLA	C4-C3-C5	2.31	119.17	115.27
24	D	408	BCR	C21-C20-C19	-2.31	115.99	123.22
34	C	517	DGD	C1E-O6E-C5E	-2.31	109.15	113.69
24	B	618	BCR	C24-C23-C22	-2.31	122.74	126.23
23	c	514	CLA	CMB-C2B-C3B	2.31	129.00	124.68
23	b	615	CLA	CMC-C2C-C1C	2.31	128.56	125.04
30	D	409[A]	PL9	C32-C33-C34	-2.31	122.10	127.66
23	C	509	CLA	C1-C2-C3	-2.31	122.05	126.04
35	D	417	LMG	O8-C28-C29	2.31	119.15	111.91
24	h	101	BCR	C24-C23-C22	-2.31	122.75	126.23
23	a	410	CLA	CAC-C3C-C4C	2.31	127.81	124.81
24	b	627	BCR	C3-C4-C5	-2.31	109.96	114.08
27	C	521	LMT	O5'-C5'-C4'	2.31	114.62	109.75
23	b	617	CLA	CMC-C2C-C1C	2.31	128.55	125.04
37	D	402	PHO	CAC-C3C-C4C	2.31	127.74	125.22
24	k	102	BCR	C32-C1-C6	-2.31	106.56	110.30
37	a	411	PHO	C2C-C1C-NC	2.31	113.27	109.79
23	B	602	CLA	O1D-CGD-CBD	-2.31	119.77	124.48
23	c	517	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
24	d	406	BCR	C29-C28-C27	-2.30	106.23	111.38
30	a	416[A]	PL9	C45-C44-C46	2.30	119.15	115.27
37	D	403[B]	PHO	O2D-CGD-O1D	-2.30	119.33	123.84
24	d	406	BCR	C29-C30-C25	2.30	114.03	110.48
23	c	511	CLA	CHC-C1C-C2C	-2.30	120.35	126.72
23	B	617	CLA	CAC-C3C-C4C	2.30	127.80	124.81
30	a	416[B]	PL9	C45-C44-C46	2.30	119.14	115.27
30	d	407[A]	PL9	C45-C44-C46	2.30	119.14	115.27
23	B	609	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	B	604	CLA	C1-O2A-CGA	2.30	122.48	116.44
37	a	411	PHO	C4-C3-C5	2.30	119.14	115.27
23	a	412	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
23	C	507	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
25	a	414	SQD	O6-C44-C45	-2.30	105.36	110.90
24	C	515	BCR	C37-C22-C21	-2.30	119.71	122.92
23	b	616	CLA	O2A-CGA-CBA	2.29	119.11	111.91
23	c	509	CLA	O2D-CGD-O1D	-2.29	119.35	123.84
37	D	402	PHO	CHD-C1D-C2D	-2.29	119.96	125.73
23	C	502	CLA	OBD-CAD-C3D	-2.29	124.17	127.98
23	B	603	CLA	C11-C12-C13	-2.29	108.51	115.92
23	C	504	CLA	C4D-C3D-CAD	-2.29	107.19	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	b	613	CLA	OBD-CAD-C3D	-2.29	124.18	127.98
33	b	601	HTG	C1-O5-C5	2.29	116.80	112.58
23	c	512	CLA	O2A-CGA-CBA	2.29	119.09	111.91
23	B	607	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	B	612	CLA	CHD-C4C-NC	2.28	127.80	124.20
25	A	412	SQD	O9-S-C6	2.28	109.65	106.94
23	A	407	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
24	d	406	BCR	C28-C27-C26	-2.28	110.00	114.08
24	C	515	BCR	C24-C23-C22	-2.28	122.79	126.23
23	B	603	CLA	C11-C10-C8	-2.28	108.54	115.92
23	B	608	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	B	603	CLA	CAC-C3C-C4C	2.28	127.77	124.81
23	C	510	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
23	b	617	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	C	505	CLA	O2A-CGA-CBA	2.28	119.06	111.91
23	C	514	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
23	b	612	CLA	C7-C6-C5	-2.28	107.17	113.36
37	d	402[B]	PHO	O2D-CGD-O1D	-2.28	119.39	123.84
24	c	527	BCR	C8-C7-C6	-2.28	120.81	127.20
37	D	402	PHO	CBA-CAA-C2A	-2.28	107.14	113.86
23	c	512	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
23	D	406	CLA	OBD-CAD-C3D	-2.28	124.20	127.98
33	b	631	HTG	C1-O5-C5	2.28	116.78	112.58
23	b	619	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
23	c	507	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
35	d	416	LMG	O8-C28-O10	-2.27	117.85	123.59
34	C	518	DGD	O6D-C5D-C6D	2.27	111.25	106.67
23	c	511	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	B	616	CLA	C1-C2-C3	-2.27	122.11	126.04
23	b	624	CLA	O2A-CGA-CBA	2.27	119.03	111.91
23	B	607	CLA	CHD-C4C-NC	2.27	127.78	124.20
23	b	614	CLA	O2A-CGA-CBA	2.27	119.03	111.91
23	c	511	CLA	OBD-CAD-C3D	-2.27	124.21	127.98
23	C	513	CLA	CAC-C3C-C4C	2.27	127.75	124.81
37	D	403[B]	PHO	C2C-C1C-NC	2.27	113.21	109.79
24	c	527	BCR	C29-C30-C25	2.27	113.97	110.48
35	Z	101	LMG	O6-C5-C4	2.27	113.81	109.69
23	B	607	CLA	CMB-C2B-C3B	2.27	128.92	124.68
37	D	403[A]	PHO	O2A-CGA-CBA	2.26	119.01	111.91
23	c	514	CLA	CAC-C3C-C4C	2.26	127.75	124.81
23	c	514	CLA	C2A-C1A-CHA	-2.26	119.90	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	402[A]	PHO	C4A-NA-C1A	-2.26	106.31	108.14
23	B	609	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
38	d	410	LHG	O8-C23-C24	2.26	119.00	111.91
23	b	624	CLA	C4-C3-C5	2.26	119.07	115.27
23	c	507	CLA	CMB-C2B-C3B	2.26	128.90	124.68
30	D	409[A]	PL9	C51-C49-C50	2.26	119.59	114.60
23	c	515	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
25	B	621	SQD	O47-C7-O49	-2.26	118.25	123.70
23	b	612	CLA	C4-C3-C5	2.25	119.06	115.27
23	A	404	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	K	103	BCR	C15-C16-C17	-2.25	118.86	123.47
23	B	611	CLA	CMA-C3A-C4A	-2.25	105.73	111.77
23	b	621	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	c	505	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
30	A	416[A]	PL9	C8-C7-C3	2.25	118.34	111.98
23	B	615	CLA	CMC-C2C-C1C	2.25	128.46	125.04
23	A	405	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	b	623	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	A	404	CLA	C7-C6-C5	-2.25	107.25	113.36
23	C	502	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
23	c	510	CLA	CAC-C3C-C4C	2.25	127.72	124.81
23	C	513	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
24	b	628	BCR	C21-C20-C19	-2.25	116.21	123.22
23	C	513	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
35	C	519	LMG	C8-O7-C10	-2.25	112.26	117.79
23	A	405	CLA	C4-C3-C5	2.25	119.05	115.27
24	K	103	BCR	C28-C27-C26	-2.25	110.07	114.08
23	c	512	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
23	c	514	CLA	C4-C3-C2	-2.25	117.92	123.68
23	d	404	CLA	CMA-C3A-C2A	-2.25	104.77	113.83
23	C	502	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
24	b	627	BCR	C37-C22-C21	-2.24	119.78	122.92
23	D	407	CLA	O2A-CGA-CBA	2.24	118.95	111.91
30	A	416[B]	PL9	C35-C34-C36	2.24	119.05	115.27
23	d	404	CLA	C4D-C3D-CAD	-2.24	107.22	108.47
38	d	411	LHG	O7-C7-O9	-2.24	118.28	123.70
23	C	508	CLA	CMB-C2B-C3B	2.24	128.87	124.68
23	B	612	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
24	k	101	BCR	C33-C5-C6	-2.24	122.01	124.53
24	Y	101	BCR	C28-C27-C26	-2.24	110.08	114.08
23	C	508	CLA	O2A-CGA-CBA	2.24	118.93	111.91
23	c	507	CLA	O2D-CGD-O1D	-2.24	119.46	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	517	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
23	c	512	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
23	B	613	CLA	OBD-CAD-C3D	-2.24	124.27	127.98
23	a	410	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
27	m	102	LMT	O5'-C5'-C4'	2.23	114.46	109.75
23	C	504	CLA	CAC-C3C-C4C	2.23	127.71	124.81
23	b	613	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
30	A	416[B]	PL9	C10-C9-C11	2.23	119.02	115.27
30	A	416[B]	PL9	C51-C49-C50	2.23	119.52	114.60
34	c	520	DGD	O2G-C1B-O1B	-2.23	118.32	123.70
30	d	407[A]	PL9	C22-C23-C24	-2.23	122.30	127.66
37	D	403[A]	PHO	C2C-C1C-NC	2.23	113.15	109.79
23	B	611	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	A	404	CLA	CHD-C4C-NC	2.23	127.71	124.20
38	D	412	LHG	O8-C23-O10	-2.22	117.98	123.59
24	T	103	BCR	C2-C1-C6	2.22	113.90	110.48
23	C	504	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
25	A	412	SQD	O6-C44-C45	-2.22	105.54	110.90
23	C	513	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	B	607	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
35	a	415	LMG	O7-C10-O9	-2.22	118.34	123.70
34	c	520	DGD	C2G-O2G-C1B	-2.22	112.33	117.79
23	B	615	CLA	CED-O2D-CGD	2.22	120.95	115.94
23	b	621	CLA	C11-C10-C8	-2.22	108.75	115.92
23	b	611	CLA	C7-C6-C5	-2.22	107.33	113.36
23	c	512	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
23	b	617	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
23	c	510	CLA	OBD-CAD-C3D	-2.21	124.31	127.98
24	t	102	BCR	C2-C3-C4	-2.21	106.43	111.38
35	Z	101	LMG	C1-C2-C3	2.21	114.60	110.00
23	C	503	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	b	625	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
23	C	512	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
23	b	624	CLA	CMC-C2C-C1C	2.21	128.41	125.04
23	B	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	d	403	CLA	O2A-CGA-CBA	2.21	118.84	111.91
24	A	408	BCR	C15-C16-C17	-2.21	118.95	123.47
30	d	407[B]	PL9	C7-C3-C4	2.21	118.67	116.88
23	A	407	CLA	CMA-C3A-C4A	-2.21	105.84	111.77
23	C	502	CLA	C1-C2-C3	-2.21	122.22	126.04
23	b	619	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
27	M	105	LMT	C1B-O5B-C5B	2.21	118.02	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	402[B]	PHO	CMB-C2B-C1B	2.21	128.46	125.06
23	c	510	CLA	CMB-C2B-C3B	2.21	128.81	124.68
30	A	416[A]	PL9	C35-C34-C36	2.21	118.98	115.27
23	c	513	CLA	CBC-CAC-C3C	-2.20	106.35	112.43
23	c	507	CLA	CMC-C2C-C1C	2.20	128.40	125.04
23	B	612	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
23	d	403	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
33	V	207	HTG	O5-C1-C2	-2.20	107.54	110.31
37	D	402	PHO	CMB-C2B-C1B	2.20	128.46	125.06
23	c	509	CLA	C1-O2A-CGA	2.20	122.22	116.44
35	C	501	LMG	C8-O7-C10	-2.20	112.37	117.79
23	a	410	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
24	h	101	BCR	C29-C30-C25	2.20	113.87	110.48
23	c	510	CLA	CAA-C2A-C3A	-2.20	106.76	112.78
23	B	610	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
23	C	514	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
23	d	404	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
23	c	510	CLA	CGD-CBD-CAD	-2.20	103.62	110.73
24	k	101	BCR	C2-C1-C6	2.20	113.86	110.48
23	B	602	CLA	C4-C3-C5	2.20	118.97	115.27
23	d	405	CLA	CMB-C2B-C3B	2.20	128.79	124.68
35	C	520	LMG	C3-C4-C5	2.20	114.16	110.24
23	C	513	CLA	CMC-C2C-C1C	2.20	128.38	125.04
23	b	625	CLA	CMB-C2B-C3B	2.20	128.78	124.68
23	B	613	CLA	CBC-CAC-C3C	-2.19	106.38	112.43
34	C	518	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
23	c	510	CLA	CMC-C2C-C1C	2.19	128.38	125.04
37	d	402[A]	PHO	O2A-CGA-CBA	2.19	118.79	111.91
25	a	414	SQD	O48-C23-O10	-2.19	118.06	123.59
37	D	402	PHO	C1-O2A-CGA	2.19	122.19	116.44
34	h	102	DGD	C2G-O2G-C1B	-2.19	112.40	117.79
23	d	405	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
23	b	621	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
24	A	408	BCR	C20-C21-C22	-2.19	124.19	127.31
34	C	517	DGD	O1G-C1A-O1A	-2.19	118.07	123.59
23	B	607	CLA	O2A-CGA-CBA	2.19	118.77	111.91
23	b	621	CLA	CAC-C3C-C2C	2.19	131.27	127.53
24	b	628	BCR	C38-C26-C25	-2.19	122.07	124.53
24	Y	101	BCR	C23-C24-C25	-2.18	121.07	127.20
25	f	102	SQD	O8-S-C6	2.18	109.22	105.74
23	A	405	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
23	B	607	CLA	CMC-C2C-C1C	2.18	128.36	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	C1-O2A-CGA	2.18	122.17	116.44
27	m	102	LMT	C1-O1'-C1'	-2.18	110.22	113.84
30	d	407[A]	PL9	C25-C24-C26	2.18	118.94	115.27
24	b	626	BCR	C10-C11-C12	-2.18	116.42	123.22
23	a	412	CLA	CAC-C3C-C4C	2.18	127.64	124.81
24	H	101	BCR	C38-C26-C27	2.18	117.80	113.62
23	A	404	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
23	a	412	CLA	C1-O2A-CGA	2.17	122.15	116.44
23	B	605	CLA	CHA-C1A-NA	-2.17	121.42	126.40
35	d	416	LMG	O7-C10-O9	-2.17	118.46	123.70
23	b	624	CLA	C6-C7-C8	-2.17	108.90	115.92
23	b	623	CLA	CMB-C2B-C3B	2.17	128.74	124.68
27	A	413	LMT	C4B-C3B-C2B	-2.17	107.03	110.82
30	d	407[B]	PL9	C47-C48-C49	-2.17	120.33	127.75
23	C	502	CLA	C1-O2A-CGA	2.17	122.14	116.44
23	B	602	CLA	CAC-C3C-C4C	2.17	127.62	124.81
23	B	603	CLA	C1-O2A-CGA	2.17	122.13	116.44
25	F	104	SQD	C1-C2-C3	-2.17	105.48	110.00
23	c	509	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	C	506	CLA	CHD-C4C-NC	2.16	127.61	124.20
34	d	408	DGD	O2G-C1B-O1B	-2.16	118.47	123.70
33	B	623	HTG	C3-C4-C5	-2.16	106.38	110.24
37	d	402[B]	PHO	CBD-CHA-C1A	2.16	131.42	126.40
23	B	610	CLA	C1-C2-C3	-2.16	122.30	126.04
33	b	632	HTG	C1-C2-C3	2.16	114.86	110.59
24	D	408	BCR	C3-C4-C5	-2.16	110.22	114.08
33	b	632	HTG	C3-C4-C5	-2.16	106.38	110.24
30	A	416[B]	PL9	C47-C48-C49	-2.16	120.36	127.75
23	b	616	CLA	CAC-C3C-C4C	2.16	127.61	124.81
27	F	101	LMT	C1B-O5B-C5B	2.16	117.93	113.69
35	z	101	LMG	C7-O1-C1	-2.16	109.52	113.74
23	B	609	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	b	624	CLA	CMB-C2B-C1B	2.16	131.78	128.46
24	b	627	BCR	C8-C7-C6	-2.16	121.14	127.20
23	c	506	CLA	CMC-C2C-C1C	2.16	128.32	125.04
35	C	519	LMG	O8-C28-O10	-2.15	118.16	123.59
35	c	522	LMG	O6-C5-C4	2.15	113.61	109.69
24	B	619	BCR	C24-C23-C22	-2.15	122.98	126.23
23	c	508	CLA	C11-C10-C8	-2.15	108.96	115.92
23	b	622	CLA	C11-C10-C8	-2.15	108.96	115.92
23	d	405	CLA	CHC-C1C-NC	2.15	127.47	124.20
34	C	517	DGD	C3G-O3G-C1D	-2.15	109.54	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	B	614	CLA	CHB-C4A-NA	2.15	127.48	124.51
23	C	508	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
23	c	505	CLA	C4-C3-C5	2.15	118.89	115.27
27	a	419	LMT	C1B-O1B-C4'	-2.15	112.65	117.96
24	H	101	BCR	C21-C20-C19	-2.15	116.52	123.22
24	c	518	BCR	C35-C13-C14	-2.15	119.92	122.92
23	b	621	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
23	C	505	CLA	C1-O2A-CGA	2.15	122.07	116.44
23	c	510	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
24	c	527	BCR	C38-C26-C25	-2.14	122.12	124.53
23	B	608	CLA	CED-O2D-CGD	2.14	120.78	115.94
30	d	407[B]	PL9	C35-C34-C36	2.14	118.87	115.27
23	C	504	CLA	C1-C2-C3	-2.14	122.34	126.04
23	d	405	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	a	410	CLA	CMA-C3A-C2A	-2.14	105.20	113.83
23	C	503	CLA	CMB-C2B-C3B	2.14	128.68	124.68
23	b	618	CLA	C4-C3-C2	-2.14	118.20	123.68
23	b	616	CLA	CMA-C3A-C2A	-2.14	105.22	113.83
23	A	406	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	L	102	SQD	O48-C23-O10	-2.13	118.21	123.59
24	C	515	BCR	C16-C17-C18	-2.13	124.27	127.31
35	D	417	LMG	O8-C28-O10	-2.13	118.22	123.59
23	c	513	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
27	A	413	LMT	O5B-C5B-C4B	2.13	113.56	109.69
30	A	416[A]	PL9	C51-C49-C50	2.13	119.31	114.60
23	B	606	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
23	b	620	CLA	CHB-C4A-NA	2.13	127.45	124.51
23	B	615	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
38	D	413	LHG	C6-C5-C4	-2.13	106.75	111.79
23	C	502	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	b	622	CLA	CMB-C2B-C3B	2.13	128.66	124.68
30	a	416[B]	PL9	C10-C9-C8	-2.13	118.22	123.68
30	a	416[A]	PL9	C12-C13-C14	-2.13	122.54	127.66
37	D	402	PHO	O2A-CGA-CBA	2.12	118.57	111.91
38	E	101	LHG	O8-C23-O10	-2.12	118.23	123.59
23	b	620	CLA	CHD-C4C-NC	2.12	127.55	124.20
23	A	406	CLA	CMB-C2B-C1B	2.12	131.72	128.46
23	b	610	CLA	CHB-C4A-NA	2.12	127.44	124.51
35	d	416	LMG	O4-C4-C3	-2.12	105.45	110.35
37	a	411	PHO	CMC-C2C-C1C	2.12	128.33	125.06
34	c	521	DGD	O2G-C1B-O1B	-2.12	118.58	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	408	BCR	C37-C22-C21	-2.12	119.96	122.92
23	A	404	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
24	b	626	BCR	C24-C23-C22	-2.12	123.03	126.23
23	A	405	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
23	C	510	CLA	C11-C12-C13	-2.12	109.08	115.92
23	B	611	CLA	CHC-C1C-NC	2.12	127.42	124.20
23	c	508	CLA	C1-C2-C3	-2.12	122.38	126.04
23	B	603	CLA	O2A-CGA-CBA	2.12	118.55	111.91
37	D	402	PHO	CBC-CAC-C3C	-2.12	106.60	112.43
23	C	511	CLA	CED-O2D-CGD	2.12	120.72	115.94
23	c	506	CLA	CED-O2D-CGD	2.11	120.72	115.94
23	b	622	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
34	d	408	DGD	C1E-O6E-C5E	2.11	117.83	113.69
23	c	511	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	a	409	CLA	CHB-C4A-NA	2.11	127.43	124.51
30	a	416[B]	PL9	C12-C13-C14	-2.11	122.58	127.66
23	b	613	CLA	C6-C5-C3	-2.11	107.93	113.45
23	C	508	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	b	617	CLA	O2A-C1-C2	2.11	114.17	108.64
23	B	615	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
23	b	624	CLA	CHB-C4A-NA	2.11	127.42	124.51
34	c	519	DGD	O1G-C1A-O1A	-2.11	118.28	123.59
24	a	413	BCR	C36-C18-C19	2.11	121.39	118.08
37	D	403[A]	PHO	CBD-CHA-C1A	2.10	131.28	126.40
34	C	518	DGD	O3G-C3G-C2G	-2.10	105.82	110.90
23	C	505	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
23	B	612	CLA	O2A-CGA-CBA	2.10	118.50	111.91
24	t	102	BCR	C40-C30-C25	-2.10	106.89	110.30
23	B	611	CLA	C4-C3-C5	2.10	118.81	115.27
33	b	607	HTG	C6-C5-C4	-2.10	108.08	113.00
23	c	506	CLA	OBD-CAD-C3D	-2.10	124.49	127.98
24	K	103	BCR	C15-C14-C13	-2.10	124.31	127.31
23	c	505	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
23	c	508	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
33	C	522	HTG	C1-O5-C5	2.10	116.45	112.58
30	d	407[B]	PL9	C25-C24-C26	2.10	118.80	115.27
23	b	615	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
37	D	403[B]	PHO	CHD-C1D-C2D	-2.10	120.45	125.73
23	A	404	CLA	CHB-C4A-NA	2.10	127.41	124.51
23	C	504	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
24	B	618	BCR	C15-C14-C13	-2.10	124.32	127.31
23	B	609	CLA	C4-C3-C5	2.10	118.80	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	619	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
39	e	101	HEM	CMC-C2C-C3C	2.10	128.60	124.68
23	c	509	CLA	O2A-CGA-CBA	2.09	118.48	111.91
23	b	610	CLA	C1-O2A-CGA	2.09	121.94	116.44
23	C	505	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
34	c	520	DGD	O1G-C1A-C2A	2.09	118.48	111.91
24	a	413	BCR	C38-C26-C25	-2.09	122.18	124.53
23	C	508	CLA	CAC-C3C-C4C	2.09	127.52	124.81
24	a	413	BCR	C34-C9-C8	2.09	121.37	118.08
23	c	514	CLA	OBD-CAD-C3D	-2.09	124.51	127.98
30	d	407[B]	PL9	C36-C37-C38	-2.09	105.01	111.88
23	b	617	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	B	615	CLA	CAC-C3C-C4C	2.09	127.52	124.81
27	a	404	LMT	C6'-C5'-C4'	-2.09	107.25	113.33
23	c	517	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	d	404	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
23	c	510	CLA	CED-O2D-CGD	2.09	120.66	115.94
38	d	409	LHG	O4-P-O5	2.09	122.55	112.24
24	B	620	BCR	C8-C9-C10	-2.09	115.74	118.94
23	b	613	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
24	t	102	BCR	C28-C27-C26	-2.09	110.35	114.08
24	k	102	BCR	C8-C7-C6	-2.08	121.35	127.20
25	f	102	SQD	C4-C3-C2	-2.08	107.18	110.82
23	A	407	CLA	O2A-CGA-CBA	2.08	118.45	111.91
25	B	621	SQD	O8-S-C6	2.08	109.06	105.74
38	E	101	LHG	C5-O7-C7	-2.08	112.66	117.79
37	d	402[A]	PHO	C1C-C2C-C3C	-2.08	104.12	106.51
24	k	102	BCR	C40-C30-C25	-2.08	106.92	110.30
23	b	611	CLA	O2A-CGA-CBA	2.08	118.43	111.91
23	b	623	CLA	CAC-C3C-C4C	2.08	127.51	124.81
23	b	615	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	C	504	CLA	CAA-CBA-CGA	-2.08	107.18	113.25
27	a	404	LMT	O1'-C1'-C2'	2.08	111.55	108.30
35	D	417	LMG	O6-C5-C4	2.08	113.46	109.69
25	B	621	SQD	O48-C23-O10	-2.08	118.36	123.59
23	d	404	CLA	CHA-C1A-NA	-2.07	121.65	126.40
35	M	101	LMG	O1-C7-C8	-2.07	105.90	110.90
35	C	501	LMG	O7-C10-O9	-2.07	118.69	123.70
25	A	409	SQD	O9-S-C6	2.07	109.40	106.94
23	c	511	CLA	C3B-C4B-NB	2.07	111.89	109.21
23	b	614	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
34	C	516	DGD	O6D-C1D-O3G	-2.07	105.08	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	C6-C7-C8	-2.07	109.23	115.92
33	c	525	HTG	O5-C5-C4	2.07	113.45	109.69
23	A	407	CLA	CMA-C3A-C2A	-2.07	105.49	113.83
33	b	631	HTG	C1-C2-C3	2.07	114.67	110.59
30	D	409[B]	PL9	C47-C48-C49	-2.06	120.69	127.75
38	D	413	LHG	O7-C7-O9	-2.06	118.71	123.70
25	L	102	SQD	O6-C44-C45	2.06	115.88	110.90
23	b	622	CLA	CBC-CAC-C3C	-2.06	106.74	112.43
23	c	509	CLA	CHA-C1A-NA	-2.06	121.67	126.40
23	b	622	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
23	c	516	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
30	d	407[A]	PL9	C35-C34-C36	2.06	118.74	115.27
23	b	619	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
30	D	409[A]	PL9	C7-C3-C4	2.06	118.55	116.88
24	c	518	BCR	C34-C9-C8	2.06	121.32	118.08
23	b	620	CLA	OBD-CAD-C3D	-2.06	124.56	127.98
24	C	515	BCR	C20-C21-C22	-2.06	124.37	127.31
23	B	617	CLA	CED-O2D-CGD	2.06	120.59	115.94
23	c	512	CLA	CGD-CBD-CAD	-2.06	104.08	110.73
24	B	620	BCR	C16-C17-C18	-2.06	124.38	127.31
23	A	405	CLA	OBD-CAD-C3D	-2.05	124.57	127.98
24	b	627	BCR	C37-C22-C23	2.05	121.31	118.08
23	B	617	CLA	CHA-C1A-NA	-2.05	121.70	126.40
27	M	104	LMT	C1B-O5B-C5B	2.05	117.71	113.69
37	d	402[A]	PHO	C3A-C4A-CHB	-2.05	118.29	121.83
37	D	403[B]	PHO	C3C-C4C-NC	2.05	113.46	110.28
23	c	514	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
23	C	506	CLA	C1-C2-C3	-2.05	122.50	126.04
23	C	509	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	B	608	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	h	101	BCR	C37-C22-C21	-2.05	120.06	122.92
33	c	524	HTG	C1-O5-C5	2.05	116.35	112.58
24	d	406	BCR	C40-C30-C25	-2.04	106.98	110.30
23	c	510	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
23	B	611	CLA	CAA-CBA-CGA	-2.04	107.29	113.25
30	d	407[B]	PL9	C22-C23-C24	-2.04	122.75	127.66
23	d	403	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
34	h	102	DGD	C6D-C5D-C4D	2.04	116.35	112.09
35	c	523	LMG	O8-C28-O10	-2.04	118.45	123.59
35	C	520	LMG	C8-O7-C10	-2.04	112.77	117.79
23	d	403	CLA	C6-C7-C8	-2.04	109.33	115.92
25	B	621	SQD	C44-O6-C1	-2.04	109.76	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	410	DGD	O6D-C1D-C2D	2.04	114.66	110.35
23	A	406	CLA	CAA-CBA-CGA	2.04	119.20	113.25
30	D	409[A]	PL9	C30-C29-C31	2.03	118.69	115.27
23	B	614	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
23	b	620	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
23	C	503	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
34	C	517	DGD	O6E-C5E-C6E	2.03	111.48	106.44
24	B	619	BCR	C21-C20-C19	-2.03	116.89	123.22
23	D	406	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
23	B	612	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
24	H	101	BCR	C29-C30-C25	2.02	113.59	110.48
37	D	402	PHO	C3C-C4C-NC	2.02	113.41	110.28
23	c	515	CLA	C11-C10-C8	-2.02	109.39	115.92
23	B	607	CLA	OBD-CAD-C3D	-2.02	124.63	127.98
37	D	402	PHO	O1D-CGD-CBD	-2.02	120.35	124.48
23	c	512	CLA	OBD-CAD-C3D	-2.02	124.63	127.98
24	k	101	BCR	C23-C24-C25	-2.02	121.53	127.20
24	h	101	BCR	C16-C17-C18	-2.02	124.43	127.31
24	Y	101	BCR	C40-C30-C25	-2.02	107.03	110.30
23	C	511	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
34	B	632	DGD	O6E-C5E-C6E	2.02	111.45	106.44
23	b	620	CLA	C7-C6-C5	-2.02	107.88	113.36
23	C	510	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	a	412	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
23	b	616	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
23	c	507	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
30	d	407[B]	PL9	C53-C6-C1	2.01	119.11	114.99
24	k	101	BCR	C7-C8-C9	-2.01	123.19	126.23
37	d	402[B]	PHO	O2A-CGA-O1A	-2.01	118.51	123.59
23	B	604	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
30	A	416[B]	PL9	C8-C7-C3	2.01	117.67	111.98
24	B	620	BCR	C24-C23-C22	-2.01	123.19	126.23
24	c	518	BCR	C34-C9-C10	-2.01	120.10	122.92
35	C	501	LMG	O8-C28-O10	-2.01	118.52	123.59
23	b	611	CLA	CMC-C2C-C1C	2.01	128.10	125.04
25	a	414	SQD	C3-C4-C5	2.01	113.83	110.24
23	C	507	CLA	C1-O2A-CGA	2.01	121.72	116.44
23	A	406	CLA	O2A-CGA-CBA	2.01	118.22	111.91
24	T	103	BCR	C28-C27-C26	-2.01	110.49	114.08
23	C	510	CLA	CHB-C4A-NA	2.01	127.29	124.51
37	a	411	PHO	C1-O2A-CGA	2.01	121.71	116.44
27	A	413	LMT	C1B-O1B-C4'	-2.01	113.00	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	409[A]	PL9	C7-C3-C2	-2.01	120.66	123.30
23	c	511	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
23	b	624	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	B	616	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
33	b	607	HTG	C1-O5-C5	2.01	116.28	112.58
23	d	403	CLA	CHB-C4A-NA	2.01	127.29	124.51
24	B	619	BCR	C7-C8-C9	-2.01	123.20	126.23
24	B	619	BCR	C10-C11-C12	-2.00	116.96	123.22
23	c	511	CLA	CHB-C4A-NA	2.00	127.28	124.51
34	C	517	DGD	O2G-C1B-O1B	-2.00	118.86	123.70
23	C	507	CLA	O2A-CGA-CBA	2.00	118.19	111.91
35	c	522	LMG	C8-O7-C10	-2.00	112.86	117.79
23	B	609	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	b	623	CLA	C4-C3-C2	-2.00	118.55	123.68
23	C	509	CLA	CBC-CAC-C3C	-2.00	106.92	112.43

All (194) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	c	509	CLA	ND
23	c	509	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	c	515	CLA	NC
23	c	515	CLA	ND
23	c	515	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	A	406	CLA	NC
23	A	406	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	b	621	CLA	NC

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Mol	Chain	Res	Type	Atom
23	b	621	CLA	ND
23	b	621	CLA	NA
23	C	514	CLA	NC
23	C	514	CLA	ND
23	C	514	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	c	516	CLA	NC
23	c	516	CLA	ND
23	c	516	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	a	410	CLA	NC
23	a	410	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	B	609	CLA	NC
23	B	609	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA

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Mol	Chain	Res	Type	Atom
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	D	406	CLA	ND
23	d	405	CLA	NC
23	d	405	CLA	ND
23	d	405	CLA	NA
23	b	622	CLA	NC
23	b	622	CLA	ND
23	b	622	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	B	617	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	b	618	CLA	NC
23	b	618	CLA	ND
23	b	618	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	b	620	CLA	NC
23	b	620	CLA	ND
23	b	620	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	b	625	CLA	NC
23	b	625	CLA	ND
23	b	625	CLA	NA
23	b	623	CLA	NC
23	b	623	CLA	ND
23	b	623	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	ND
23	A	407	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	C	506	CLA	ND
23	b	624	CLA	NA
23	b	624	CLA	NC
23	b	624	CLA	ND
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	d	404	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	c	514	CLA	NC
23	c	514	CLA	ND
23	c	514	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	D	407	CLA	NC

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Mol	Chain	Res	Type	Atom
23	D	407	CLA	ND
23	D	407	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	617	CLA	NC
23	b	617	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	B	616	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	c	517	CLA	NC
23	c	517	CLA	ND
23	c	517	CLA	NA
23	a	412	CLA	NC
23	a	412	CLA	ND
23	a	412	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA

All (1396) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	D	411	LHG	C4-O6-P-O5
23	C	510	CLA	C2-C1-O2A-CGA
35	C	501	LMG	C11-C10-O7-C8
26	B	627	GOL	O1-C1-C2-C3
26	T	102	GOL	O1-C1-C2-C3
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
38	d	410	LHG	O2-C2-C3-O3
38	d	410	LHG	C3-O3-P-O4
34	D	410	DGD	C2B-C1B-O2G-C2G
34	D	410	DGD	C2D-C1D-O3G-C3G
34	D	410	DGD	O6D-C1D-O3G-C3G
26	D	404	GOL	C1-C2-C3-O3
33	b	632	HTG	C2'-C1'-S1-C1
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
33	V	207	HTG	O5-C1-S1-C1'
33	V	207	HTG	C2'-C1'-S1-C1
26	a	402	GOL	O1-C1-C2-C3
26	V	202	GOL	C1-C2-C3-O3
23	B	602	CLA	C11-C10-C8-C9
38	d	411	LHG	C4-O6-P-O4
23	c	512	CLA	CHA-CBD-CGD-O1D
23	c	512	CLA	CHA-CBD-CGD-O2D
35	C	520	LMG	C11-C10-O7-C8
24	d	406	BCR	C7-C8-C9-C10
24	d	406	BCR	C7-C8-C9-C34
24	d	406	BCR	C21-C22-C23-C24
24	d	406	BCR	C37-C22-C23-C24
24	d	406	BCR	C23-C24-C25-C30
25	a	405	SQD	O6-C44-C45-O47
25	a	405	SQD	O5-C5-C6-S
25	a	405	SQD	C5-C6-S-O7
25	a	405	SQD	C5-C6-S-O8
25	f	102	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
25	f	102	SQD	C8-C7-O47-C45
25	f	102	SQD	C5-C6-S-O7
25	f	102	SQD	C5-C6-S-O8
25	f	102	SQD	C5-C6-S-O9
24	B	618	BCR	C1-C6-C7-C8
27	t	101	LMT	C2'-C1'-O1'-C1
27	t	101	LMT	O5'-C1'-O1'-C1
26	b	606	GOL	O1-C1-C2-O2
26	b	606	GOL	O1-C1-C2-C3
27	M	104	LMT	O5'-C1'-O1'-C1
27	M	104	LMT	C2-C1-O1'-C1'
35	Z	101	LMG	O6-C1-O1-C7
35	Z	101	LMG	O9-C10-O7-C8
35	Z	101	LMG	C11-C10-O7-C8
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
33	B	623	HTG	O5-C1-S1-C1'
23	c	510	CLA	C1A-C2A-CAA-CBA
23	c	510	CLA	C3A-C2A-CAA-CBA
24	k	102	BCR	C1-C6-C7-C8
24	k	102	BCR	C5-C6-C7-C8
24	k	102	BCR	C21-C22-C23-C24
24	k	102	BCR	C37-C22-C23-C24
24	C	515	BCR	C7-C8-C9-C10
24	C	515	BCR	C7-C8-C9-C34
23	c	513	CLA	C2-C1-O2A-CGA
34	d	408	DGD	C2B-C1B-O2G-C2G
34	d	408	DGD	O1B-C1B-O2G-C2G
34	d	408	DGD	O6E-C1E-O5D-C6D
38	b	634	LHG	O1-C1-C2-C3
38	b	634	LHG	C4-O6-P-O3
38	b	634	LHG	C4-O6-P-O4
38	b	634	LHG	C4-O6-P-O5
38	D	413	LHG	C4-O6-P-O4
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
27	F	101	LMT	C2'-C1'-O1'-C1
27	F	101	LMT	O5'-C1'-O1'-C1
35	z	101	LMG	O9-C10-O7-C8
23	b	614	CLA	C4-C3-C5-C6
26	V	205	GOL	O1-C1-C2-C3
27	b	630	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
27	b	630	LMT	O5'-C1'-O1'-C1
30	a	416[A]	PL9	C12-C11-C9-C10
30	a	416[A]	PL9	C18-C19-C21-C22
30	a	416[A]	PL9	C20-C19-C21-C22
24	D	408	BCR	C7-C8-C9-C10
24	D	408	BCR	C7-C8-C9-C34
24	D	408	BCR	C21-C22-C23-C24
24	D	408	BCR	C37-C22-C23-C24
25	A	412	SQD	O6-C44-C45-O47
25	A	412	SQD	O5-C5-C6-S
27	e	102	LMT	C2'-C1'-O1'-C1
27	e	102	LMT	O5'-C1'-O1'-C1
26	b	604	GOL	O2-C2-C3-O3
38	D	412	LHG	C3-O3-P-O6
38	D	412	LHG	C4-O6-P-O4
23	b	623	CLA	CHA-CBD-CGD-O1D
23	b	623	CLA	CHA-CBD-CGD-O2D
23	b	623	CLA	CAD-CBD-CGD-O1D
23	b	623	CLA	CAD-CBD-CGD-O2D
23	b	623	CLA	C2-C3-C5-C6
23	b	623	CLA	C4-C3-C5-C6
25	F	104	SQD	O49-C7-O47-C45
25	F	104	SQD	C5-C6-S-O7
25	F	104	SQD	C5-C6-S-O8
25	F	104	SQD	C5-C6-S-O9
26	f	101	GOL	O1-C1-C2-C3
27	a	404	LMT	C2'-C1'-O1'-C1
27	a	404	LMT	O5'-C1'-O1'-C1
30	a	416[B]	PL9	C14-C16-C17-C18
30	a	416[B]	PL9	C25-C24-C26-C27
23	B	615	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O2D
27	A	413	LMT	C2'-C1'-O1'-C1
27	A	413	LMT	O5'-C1'-O1'-C1
26	A	411	GOL	C1-C2-C3-O3
26	B	626	GOL	O1-C1-C2-O2
26	B	626	GOL	O1-C1-C2-C3
38	L	101	LHG	C4-O6-P-O3
38	L	101	LHG	C4-O6-P-O4
38	L	101	LHG	C4-O6-P-O5
25	L	102	SQD	O5-C1-O6-C44
25	L	102	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
27	C	521	LMT	C2'-C1'-O1'-C1
27	C	521	LMT	O5'-C1'-O1'-C1
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	K	101	BCR	C37-C22-C23-C24
26	B	625	GOL	O1-C1-C2-O2
26	B	625	GOL	O1-C1-C2-C3
26	c	502	GOL	O1-C1-C2-C3
23	B	606	CLA	C2-C3-C5-C6
23	B	606	CLA	C4-C3-C5-C6
27	T	104	LMT	C2'-C1'-O1'-C1
27	T	104	LMT	O5'-C1'-O1'-C1
23	B	616	CLA	C11-C12-C13-C15
33	B	622	HTG	C2'-C1'-S1-C1
38	E	101	LHG	C4-O6-P-O5
23	c	508	CLA	C2-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
25	B	621	SQD	O5-C1-O6-C44
25	B	621	SQD	O49-C7-O47-C45
25	B	621	SQD	C5-C6-S-O7
25	B	621	SQD	C5-C6-S-O8
25	B	621	SQD	C5-C6-S-O9
26	v	202	GOL	O1-C1-C2-C3
27	a	419	LMT	C2'-C1'-O1'-C1
27	a	419	LMT	O5'-C1'-O1'-C1
38	a	420	LHG	O1-C1-C2-C3
38	a	420	LHG	O10-C23-O8-C6
38	a	420	LHG	C24-C23-O8-C6
26	b	605	GOL	O1-C1-C2-C3
26	v	203	GOL	O1-C1-C2-C3
23	c	505	CLA	CBD-CGD-O2D-CED
27	D	405	LMT	C3'-C4'-O1B-C1B
23	c	515	CLA	CBD-CGD-O2D-CED
38	E	101	LHG	O10-C23-O8-C6
27	C	521	LMT	O5B-C1B-O1B-C4'
35	C	501	LMG	O9-C10-O7-C8
34	D	410	DGD	O1B-C1B-O2G-C2G
35	C	520	LMG	O9-C10-O7-C8
23	c	510	CLA	C3-C5-C6-C7
23	B	617	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	b	623	CLA	C3-C5-C6-C7
23	A	407	CLA	C3-C5-C6-C7
23	B	615	CLA	C3-C5-C6-C7
23	D	407	CLA	C3-C5-C6-C7
38	E	101	LHG	C24-C23-O8-C6
35	z	101	LMG	C11-C10-O7-C8
25	F	104	SQD	C8-C7-O47-C45
25	L	102	SQD	C8-C7-O47-C45
25	B	621	SQD	C8-C7-O47-C45
23	C	510	CLA	CBD-CGD-O2D-CED
34	B	632	DGD	O6E-C5E-C6E-O5E
30	a	416[B]	PL9	C12-C11-C9-C10
23	B	615	CLA	C4-C3-C5-C6
27	M	104	LMT	O5'-C5'-C6'-O6'
35	c	522	LMG	C11-C10-O7-C8
27	C	521	LMT	C3'-C4'-O1B-C1B
35	C	520	LMG	O6-C5-C6-O5
23	c	513	CLA	CBD-CGD-O2D-CED
35	z	101	LMG	O6-C5-C6-O5
33	C	523	HTG	O5-C5-C6-O6
27	C	521	LMT	O5'-C5'-C6'-O6'
34	B	632	DGD	C4E-C5E-C6E-O5E
33	B	623	HTG	O5-C5-C6-O6
30	A	416[A]	PL9	C25-C24-C26-C27
30	a	416[A]	PL9	C15-C14-C16-C17
30	a	416[A]	PL9	C25-C24-C26-C27
30	a	416[B]	PL9	C15-C14-C16-C17
30	a	416[B]	PL9	C20-C19-C21-C22
30	A	416[B]	PL9	C25-C24-C26-C27
30	A	416[A]	PL9	C23-C24-C26-C27
23	b	614	CLA	C2-C3-C5-C6
30	a	416[A]	PL9	C13-C14-C16-C17
30	a	416[A]	PL9	C23-C24-C26-C27
30	a	416[B]	PL9	C13-C14-C16-C17
30	a	416[B]	PL9	C18-C19-C21-C22
30	a	416[B]	PL9	C23-C24-C26-C27
30	A	416[B]	PL9	C23-C24-C26-C27
27	M	102	LMT	O5B-C5B-C6B-O6B
23	C	510	CLA	O1A-CGA-O2A-C1
30	d	407[A]	PL9	C39-C41-C42-C43
30	D	409[B]	PL9	C39-C41-C42-C43
23	C	510	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
34	d	408	DGD	O6D-C5D-C6D-O5D
23	c	515	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	O1D-CGD-O2D-CED
38	E	101	LHG	C1-C2-C3-O3
38	d	411	LHG	C24-C23-O8-C6
38	D	413	LHG	C24-C23-O8-C6
35	Z	101	LMG	C10-C11-C12-C13
33	B	623	HTG	C4-C5-C6-O6
35	a	415	LMG	C17-C18-C19-C20
25	B	621	SQD	C7-C8-C9-C10
35	Z	101	LMG	C2-C1-O1-C7
34	d	408	DGD	C2E-C1E-O5D-C6D
23	b	612	CLA	C4-C3-C5-C6
23	b	612	CLA	C2-C3-C5-C6
23	B	615	CLA	C2-C3-C5-C6
23	C	502	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	B	617	CLA	C6-C7-C8-C9
23	b	623	CLA	C11-C10-C8-C9
23	B	607	CLA	C2A-CAA-CBA-CGA
24	C	515	BCR	C11-C12-C13-C35
35	c	522	LMG	O9-C10-O7-C8
27	M	102	LMT	C4B-C5B-C6B-O6B
27	M	104	LMT	C4'-C5'-C6'-O6'
35	C	520	LMG	C28-C29-C30-C31
38	d	411	LHG	O10-C23-O8-C6
38	D	413	LHG	O10-C23-O8-C6
27	m	102	LMT	O5'-C5'-C6'-O6'
23	b	624	CLA	C10-C11-C12-C13
23	B	615	CLA	C8-C10-C11-C12
23	B	615	CLA	C10-C11-C12-C13
35	Z	101	LMG	O6-C5-C6-O5
35	C	520	LMG	C10-C11-C12-C13
34	d	408	DGD	C4E-C5E-C6E-O5E
23	a	409	CLA	C2C-C3C-CAC-CBC
23	C	502	CLA	C15-C16-C17-C18
23	b	615	CLA	C13-C15-C16-C17
23	A	407	CLA	C13-C15-C16-C17
23	b	612	CLA	C5-C6-C7-C8
23	c	514	CLA	C8-C10-C11-C12
27	a	404	LMT	C3-C4-C5-C6
26	f	101	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
38	D	411	LHG	C23-C24-C25-C26
25	A	412	SQD	C23-C24-C25-C26
23	b	623	CLA	C5-C6-C7-C8
27	D	405	LMT	O1'-C1-C2-C3
35	b	629	LMG	C30-C31-C32-C33
23	C	514	CLA	CBD-CGD-O2D-CED
23	c	510	CLA	CBD-CGD-O2D-CED
38	D	412	LHG	C32-C33-C34-C35
23	B	602	CLA	C10-C11-C12-C13
23	b	615	CLA	C12-C13-C15-C16
23	b	623	CLA	C12-C13-C15-C16
23	B	614	CLA	CBD-CGD-O2D-CED
27	D	405	LMT	O5'-C1'-O1'-C1
23	B	612	CLA	C15-C16-C17-C18
23	C	507	CLA	C13-C15-C16-C17
23	A	407	CLA	C8-C10-C11-C12
30	d	407[B]	PL9	C39-C41-C42-C43
30	a	416[A]	PL9	C9-C11-C12-C13
30	a	416[B]	PL9	C9-C11-C12-C13
34	c	519	DGD	O6D-C5D-C6D-O5D
23	C	509	CLA	C10-C11-C12-C13
23	C	505	CLA	C15-C16-C17-C18
23	c	517	CLA	C10-C11-C12-C13
23	c	516	CLA	CBA-CGA-O2A-C1
23	C	513	CLA	CBA-CGA-O2A-C1
23	B	617	CLA	C10-C11-C12-C13
27	T	104	LMT	O1'-C1-C2-C3
35	z	101	LMG	C4-C5-C6-O5
23	c	513	CLA	O1A-CGA-O2A-C1
23	A	404	CLA	C13-C15-C16-C17
23	A	407	CLA	C10-C11-C12-C13
23	B	616	CLA	C8-C10-C11-C12
23	a	412	CLA	C15-C16-C17-C18
38	d	410	LHG	C3-O3-P-O6
38	E	101	LHG	C3-O3-P-O6
38	a	420	LHG	C3-O3-P-O6
38	a	420	LHG	C4-O6-P-O3
27	M	105	LMT	O5'-C5'-C6'-O6'
23	a	412	CLA	C3-C5-C6-C7
27	C	521	LMT	C5'-C4'-O1B-C1B
23	c	513	CLA	CBA-CGA-O2A-C1
38	a	420	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C5-C6-C7-C8
23	c	508	CLA	C15-C16-C17-C18
34	d	408	DGD	C4D-C5D-C6D-O5D
23	B	615	CLA	C5-C6-C7-C8
23	b	615	CLA	C2A-CAA-CBA-CGA
23	b	620	CLA	C16-C17-C18-C19
23	B	605	CLA	C3-C5-C6-C7
34	C	516	DGD	O6D-C5D-C6D-O5D
38	D	411	LHG	C34-C35-C36-C37
38	a	420	LHG	C24-C25-C26-C27
33	b	632	HTG	C1'-C2'-C3'-C4'
35	C	501	LMG	C14-C15-C16-C17
35	C	501	LMG	C32-C33-C34-C35
34	D	410	DGD	C2A-C3A-C4A-C5A
35	Z	101	LMG	C19-C20-C21-C22
34	d	408	DGD	C8B-C9B-CAB-CBB
33	B	622	HTG	C2'-C3'-C4'-C5'
23	C	510	CLA	O1D-CGD-O2D-CED
34	c	519	DGD	C4D-C5D-C6D-O5D
34	D	410	DGD	C3B-C4B-C5B-C6B
27	t	101	LMT	C3-C4-C5-C6
35	C	519	LMG	C11-C12-C13-C14
35	C	519	LMG	C12-C13-C14-C15
27	e	102	LMT	C4-C5-C6-C7
34	B	632	DGD	C7A-C8A-C9A-CAA
35	M	101	LMG	C29-C30-C31-C32
34	C	517	DGD	C9A-CAA-CBA-CCA
34	C	517	DGD	CBB-CCB-CDB-CEB
25	a	414	SQD	C11-C12-C13-C14
25	A	409	SQD	C14-C15-C16-C17
38	E	101	LHG	O2-C2-C3-O3
34	c	520	DGD	C9A-CAA-CBA-CCA
35	M	101	LMG	C33-C34-C35-C36
23	c	513	CLA	C3-C5-C6-C7
27	D	405	LMT	C2'-C1'-O1'-C1
27	M	102	LMT	C2'-C1'-O1'-C1
34	c	520	DGD	C2E-C1E-O5D-C6D
34	c	519	DGD	C2E-C1E-O5D-C6D
27	M	104	LMT	C2'-C1'-O1'-C1
34	C	517	DGD	C2E-C1E-O5D-C6D
33	b	631	HTG	C2'-C3'-C4'-C5'
25	A	409	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	L	102	SQD	C12-C13-C14-C15
34	C	517	DGD	C4B-C5B-C6B-C7B
23	b	617	CLA	C13-C15-C16-C17
23	C	503	CLA	C16-C17-C18-C19
23	a	412	CLA	C16-C17-C18-C19
23	B	610	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
34	c	521	DGD	C5B-C6B-C7B-C8B
35	a	415	LMG	C12-C13-C14-C15
30	d	407[A]	PL9	C13-C14-C16-C17
23	C	507	CLA	C6-C7-C8-C9
23	a	410	CLA	C14-C13-C15-C16
23	c	513	CLA	C11-C10-C8-C9
23	B	604	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	b	619	CLA	C11-C12-C13-C14
34	c	521	DGD	CBA-CCA-CDA-CEA
34	d	408	DGD	CAA-CBA-CCA-CDA
38	D	413	LHG	C29-C30-C31-C32
25	F	104	SQD	C34-C35-C36-C37
25	L	102	SQD	C29-C30-C31-C32
34	C	517	DGD	C8B-C9B-CAB-CBB
23	C	508	CLA	C2A-CAA-CBA-CGA
23	c	516	CLA	O1A-CGA-O2A-C1
24	b	626	BCR	C36-C18-C19-C20
35	c	522	LMG	C34-C35-C36-C37
38	D	411	LHG	O1-C1-C2-C3
26	B	627	GOL	C1-C2-C3-O3
26	V	201	GOL	O1-C1-C2-C3
38	d	409	LHG	O1-C1-C2-C3
26	v	201	GOL	O1-C1-C2-C3
38	d	411	LHG	O1-C1-C2-C3
26	c	501	GOL	O1-C1-C2-C3
26	b	606	GOL	C1-C2-C3-O3
38	D	413	LHG	O1-C1-C2-C3
26	V	205	GOL	C1-C2-C3-O3
26	b	604	GOL	O1-C1-C2-C3
26	b	604	GOL	C1-C2-C3-O3
33	C	523	HTG	S1-C1'-C2'-C3'
23	b	624	CLA	C5-C6-C7-C8
25	a	405	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
35	a	415	LMG	C10-C11-C12-C13
34	D	410	DGD	C8B-C9B-CAB-CBB
34	d	408	DGD	C5A-C6A-C7A-C8A
38	b	634	LHG	C10-C11-C12-C13
34	C	518	DGD	CAA-CBA-CCA-CDA
25	L	102	SQD	C32-C33-C34-C35
27	T	104	LMT	C11-C10-C9-C8
23	C	503	CLA	C16-C17-C18-C20
27	M	102	LMT	O5'-C1'-O1'-C1
34	C	517	DGD	O6E-C1E-O5D-C6D
23	b	610	CLA	C8-C10-C11-C12
35	D	417	LMG	C19-C20-C21-C22
34	C	516	DGD	C4B-C5B-C6B-C7B
25	A	409	SQD	C9-C10-C11-C12
34	d	408	DGD	C2A-C3A-C4A-C5A
35	z	101	LMG	C12-C13-C14-C15
34	C	516	DGD	C4D-C5D-C6D-O5D
23	C	506	CLA	CBD-CGD-O2D-CED
34	c	519	DGD	C8A-C9A-CAA-CBA
35	d	416	LMG	C38-C39-C40-C41
25	A	412	SQD	C11-C12-C13-C14
35	a	415	LMG	C33-C34-C35-C36
23	b	613	CLA	C13-C15-C16-C17
38	d	409	LHG	C25-C26-C27-C28
38	d	411	LHG	C31-C32-C33-C34
34	c	519	DGD	C7B-C8B-C9B-CAB
35	d	416	LMG	C14-C15-C16-C17
34	d	408	DGD	C2A-C1A-O1G-C1G
23	C	511	CLA	CBA-CGA-O2A-C1
34	D	410	DGD	C6A-C7A-C8A-C9A
25	f	102	SQD	C24-C25-C26-C27
38	d	411	LHG	C29-C30-C31-C32
38	b	634	LHG	C32-C33-C34-C35
25	a	414	SQD	C33-C34-C35-C36
23	C	513	CLA	O1A-CGA-O2A-C1
23	b	624	CLA	C16-C17-C18-C19
35	C	520	LMG	C14-C15-C16-C17
27	t	101	LMT	C7-C8-C9-C10
35	d	416	LMG	C15-C16-C17-C18
35	d	416	LMG	C16-C17-C18-C19
38	L	101	LHG	C12-C13-C14-C15
27	T	104	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
35	a	415	LMG	C7-C8-C9-O8
34	c	521	DGD	CBB-CCB-CDB-CEB
38	L	101	LHG	C13-C14-C15-C16
27	T	104	LMT	C4-C5-C6-C7
23	B	602	CLA	C3-C5-C6-C7
23	C	513	CLA	C3-C5-C6-C7
30	D	409[B]	PL9	C15-C14-C16-C17
30	d	407[A]	PL9	C43-C44-C46-C47
23	B	610	CLA	C2-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
27	t	101	LMT	C11-C10-C9-C8
26	B	627	GOL	O1-C1-C2-O2
26	B	627	GOL	O2-C2-C3-O3
26	T	102	GOL	O1-C1-C2-O2
26	D	404	GOL	O2-C2-C3-O3
26	a	402	GOL	O1-C1-C2-O2
26	v	201	GOL	O1-C1-C2-O2
38	d	411	LHG	O1-C1-C2-O2
26	V	205	GOL	O2-C2-C3-O3
26	A	411	GOL	O2-C2-C3-O3
26	b	605	GOL	O1-C1-C2-O2
26	v	203	GOL	O1-C1-C2-O2
38	L	101	LHG	C14-C15-C16-C17
23	a	412	CLA	C16-C17-C18-C20
23	C	510	CLA	C3-C5-C6-C7
27	C	521	LMT	O5B-C5B-C6B-O6B
38	d	410	LHG	C1-C2-C3-O3
35	M	101	LMG	C35-C36-C37-C38
25	a	414	SQD	C9-C10-C11-C12
27	T	104	LMT	C1-C2-C3-C4
23	B	617	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C2-C1-O2A-CGA
25	B	621	SQD	C34-C35-C36-C37
23	b	623	CLA	C13-C15-C16-C17
23	C	511	CLA	O1A-CGA-O2A-C1
34	c	520	DGD	C4A-C5A-C6A-C7A
23	b	620	CLA	C16-C17-C18-C20
34	D	410	DGD	C1B-C2B-C3B-C4B
24	d	406	BCR	C23-C24-C25-C26
24	B	618	BCR	C5-C6-C7-C8
24	C	515	BCR	C1-C6-C7-C8
24	C	515	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	c	521	DGD	C6B-C7B-C8B-C9B
25	a	414	SQD	C30-C31-C32-C33
23	c	512	CLA	C15-C16-C17-C18
25	A	412	SQD	C18-C19-C20-C21
38	D	411	LHG	C27-C28-C29-C30
23	B	614	CLA	C13-C15-C16-C17
33	c	524	HTG	C2'-C3'-C4'-C5'
30	d	407[A]	PL9	C45-C44-C46-C47
37	D	402	PHO	C4-C3-C5-C6
30	D	409[A]	PL9	C15-C14-C16-C17
23	C	507	CLA	C6-C7-C8-C10
37	D	402	PHO	C2-C3-C5-C6
23	c	513	CLA	C12-C13-C15-C16
23	B	604	CLA	C6-C7-C8-C10
30	d	407[B]	PL9	C13-C14-C16-C17
23	C	511	CLA	C2-C3-C5-C6
23	C	511	CLA	C6-C7-C8-C10
23	b	623	CLA	C11-C12-C13-C15
30	D	409[A]	PL9	C28-C29-C31-C32
23	b	612	CLA	C6-C7-C8-C10
23	C	513	CLA	C11-C10-C8-C7
30	D	409[B]	PL9	C13-C14-C16-C17
34	d	408	DGD	O1A-C1A-O1G-C1G
24	T	103	BCR	C13-C14-C15-C16
35	a	415	LMG	O9-C10-O7-C8
35	c	523	LMG	C10-C11-C12-C13
23	c	515	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
25	L	102	SQD	C35-C36-C37-C38
25	a	414	SQD	C27-C28-C29-C30
35	C	520	LMG	C37-C38-C39-C40
35	b	629	LMG	C38-C39-C40-C41
25	a	405	SQD	C31-C32-C33-C34
23	a	409	CLA	C4C-C3C-CAC-CBC
33	b	631	HTG	C3'-C4'-C5'-C6'
34	c	521	DGD	C7B-C8B-C9B-CAB
35	z	101	LMG	C15-C16-C17-C18
27	a	419	LMT	C6-C7-C8-C9
23	C	502	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C16-C17-C18-C20
34	c	520	DGD	O6E-C1E-O5D-C6D
34	c	519	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
34	d	408	DGD	O6D-C1D-O3G-C3G
23	b	623	CLA	C10-C11-C12-C13
38	D	411	LHG	C24-C25-C26-C27
27	M	104	LMT	C11-C10-C9-C8
25	A	409	SQD	C8-C7-O47-C45
35	a	415	LMG	C11-C10-O7-C8
38	D	413	LHG	C28-C29-C30-C31
25	a	414	SQD	C29-C30-C31-C32
23	B	613	CLA	CBD-CGD-O2D-CED
34	c	521	DGD	C7A-C8A-C9A-CAA
25	f	102	SQD	C31-C32-C33-C34
34	d	408	DGD	C2D-C1D-O3G-C3G
35	a	415	LMG	C31-C32-C33-C34
34	h	102	DGD	CAA-CBA-CCA-CDA
30	d	407[A]	PL9	C15-C14-C16-C17
23	C	511	CLA	C4-C3-C5-C6
30	D	409[A]	PL9	C45-C44-C46-C47
27	e	102	LMT	C4'-C5'-C6'-O6'
27	b	630	LMT	C3'-C4'-O1B-C1B
30	a	416[A]	PL9	C12-C11-C9-C8
30	A	416[A]	PL9	C4-C3-C7-C8
30	a	416[A]	PL9	C4-C3-C7-C8
30	A	416[B]	PL9	C4-C3-C7-C8
34	d	408	DGD	C9B-CAB-CBB-CCB
23	B	612	CLA	C14-C13-C15-C16
23	c	513	CLA	C14-C13-C15-C16
23	b	623	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C11-C12-C13-C14
25	A	412	SQD	C24-C25-C26-C27
25	F	104	SQD	C31-C32-C33-C34
35	a	415	LMG	C29-C30-C31-C32
38	a	420	LHG	C14-C15-C16-C17
27	D	405	LMT	O5B-C5B-C6B-O6B
24	A	408	BCR	C36-C18-C19-C20
33	b	601	HTG	C2'-C3'-C4'-C5'
25	B	621	SQD	C32-C33-C34-C35
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
35	C	501	LMG	C36-C37-C38-C39
23	c	510	CLA	C15-C16-C17-C18
38	D	412	LHG	C4-O6-P-O3
35	C	520	LMG	C13-C14-C15-C16
38	b	634	LHG	C27-C28-C29-C30
25	A	412	SQD	C30-C31-C32-C33
34	C	517	DGD	C8A-C9A-CAA-CBA
25	L	102	SQD	C10-C11-C12-C13
23	b	610	CLA	C10-C11-C12-C13
23	a	412	CLA	C10-C11-C12-C13
27	M	104	LMT	C2B-C1B-O1B-C4'
38	b	634	LHG	O6-C4-C5-C6
38	L	101	LHG	O6-C4-C5-C6
35	c	522	LMG	C16-C17-C18-C19
25	A	409	SQD	C15-C16-C17-C18
38	E	101	LHG	C23-C24-C25-C26
34	C	516	DGD	O6E-C5E-C6E-O5E
23	a	410	CLA	C10-C11-C12-C13
23	b	624	CLA	C16-C17-C18-C20
35	a	415	LMG	C35-C36-C37-C38
34	c	520	DGD	C8B-C9B-CAB-CBB
33	b	632	HTG	S1-C1'-C2'-C3'
33	b	632	HTG	O5-C5-C6-O6
35	D	417	LMG	C13-C14-C15-C16
34	h	102	DGD	C5B-C6B-C7B-C8B
38	b	634	LHG	C28-C29-C30-C31
25	F	104	SQD	C32-C33-C34-C35
38	d	411	LHG	C33-C34-C35-C36
23	c	515	CLA	O1A-CGA-O2A-C1
25	B	621	SQD	C11-C10-C9-C8
23	B	611	CLA	C2A-CAA-CBA-CGA
35	c	522	LMG	C7-C8-C9-O8
34	D	410	DGD	O1G-C1G-C2G-C3G
34	c	519	DGD	C2A-C3A-C4A-C5A
25	a	405	SQD	O6-C44-C45-C46
35	b	629	LMG	C40-C41-C42-C43
25	B	621	SQD	C44-C45-C46-O48
25	a	414	SQD	O6-C44-C45-C46
34	c	519	DGD	O6E-C5E-C6E-O5E
27	M	104	LMT	O5B-C5B-C6B-O6B
23	B	602	CLA	C15-C16-C17-C18
34	c	520	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
34	c	520	DGD	C5D-C6D-O5D-C1E
27	D	405	LMT	C2-C3-C4-C5
34	B	632	DGD	CDA-CEA-CFA-CGA
38	D	411	LHG	C33-C34-C35-C36
38	b	634	LHG	C9-C10-C11-C12
23	C	504	CLA	C8-C10-C11-C12
25	B	621	SQD	C33-C34-C35-C36
35	D	417	LMG	O6-C5-C6-O5
35	d	416	LMG	O6-C5-C6-O5
38	D	411	LHG	O1-C1-C2-O2
26	V	202	GOL	O2-C2-C3-O3
26	V	205	GOL	O1-C1-C2-O2
26	c	502	GOL	O1-C1-C2-O2
26	v	202	GOL	O1-C1-C2-O2
34	c	520	DGD	C3B-C4B-C5B-C6B
27	m	102	LMT	C9-C10-C11-C12
23	D	407	CLA	C8-C10-C11-C12
25	L	102	SQD	C28-C29-C30-C31
23	c	513	CLA	O1D-CGD-O2D-CED
23	b	623	CLA	C15-C16-C17-C18
27	A	413	LMT	O5B-C5B-C6B-O6B
35	C	501	LMG	C30-C31-C32-C33
34	C	516	DGD	C1A-C2A-C3A-C4A
23	B	611	CLA	C16-C17-C18-C19
38	d	410	LHG	C24-C23-O8-C6
23	C	512	CLA	CBA-CGA-O2A-C1
25	L	102	SQD	C24-C23-O48-C46
25	A	412	SQD	C15-C16-C17-C18
34	C	518	DGD	C6B-C7B-C8B-C9B
25	B	621	SQD	C46-C45-O47-C7
25	A	409	SQD	O49-C7-O47-C45
23	c	517	CLA	C2-C1-O2A-CGA
34	D	410	DGD	C7A-C8A-C9A-CAA
23	C	514	CLA	C3-C5-C6-C7
23	C	503	CLA	C3-C5-C6-C7
25	B	621	SQD	C9-C10-C11-C12
23	c	510	CLA	O1D-CGD-O2D-CED
23	B	611	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C19
35	c	522	LMG	C10-C11-C12-C13
35	C	519	LMG	C28-C29-C30-C31
35	d	416	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	f	102	SQD	C26-C27-C28-C29
34	c	519	DGD	C9A-CAA-CBA-CCA
25	a	405	SQD	C23-C24-C25-C26
25	A	412	SQD	C7-C8-C9-C10
33	b	601	HTG	S1-C1'-C2'-C3'
38	b	634	LHG	C11-C12-C13-C14
35	Z	101	LMG	O1-C7-C8-O7
33	b	601	HTG	C3'-C4'-C5'-C6'
23	b	625	CLA	C10-C11-C12-C13
23	C	512	CLA	O1A-CGA-O2A-C1
25	a	405	SQD	C28-C29-C30-C31
23	B	616	CLA	C4-C3-C5-C6
23	B	612	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	a	410	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
23	c	513	CLA	C6-C7-C8-C10
23	A	407	CLA	C6-C7-C8-C10
30	D	409[A]	PL9	C13-C14-C16-C17
23	C	506	CLA	C11-C12-C13-C15
23	b	610	CLA	C6-C7-C8-C10
23	B	615	CLA	C12-C13-C15-C16
35	C	501	LMG	C33-C34-C35-C36
34	c	519	DGD	C8B-C9B-CAB-CBB
23	b	615	CLA	C14-C13-C15-C16
23	c	513	CLA	C6-C7-C8-C9
23	A	407	CLA	C6-C7-C8-C9
23	b	610	CLA	C6-C7-C8-C9
23	b	610	CLA	C11-C10-C8-C9
23	b	612	CLA	C6-C7-C8-C9
23	c	514	CLA	C11-C12-C13-C14
35	c	522	LMG	C38-C39-C40-C41
35	d	416	LMG	C19-C20-C21-C22
34	B	632	DGD	C5B-C6B-C7B-C8B
23	c	510	CLA	O1A-CGA-O2A-C1
33	b	607	HTG	C4'-C5'-C6'-C7'
24	K	101	BCR	C21-C22-C23-C24
35	C	519	LMG	C35-C36-C37-C38
23	B	614	CLA	O1D-CGD-O2D-CED
34	h	102	DGD	CDA-CEA-CFA-CGA
23	c	514	CLA	CBA-CGA-O2A-C1
33	o	301	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
38	d	410	LHG	O10-C23-O8-C6
23	d	405	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	C13-C15-C16-C17
35	a	415	LMG	C14-C15-C16-C17
23	B	616	CLA	C2-C3-C5-C6
34	C	517	DGD	C1A-C2A-C3A-C4A
27	e	102	LMT	C9-C10-C11-C12
25	B	621	SQD	C17-C18-C19-C20
23	C	514	CLA	O1D-CGD-O2D-CED
27	M	105	LMT	C5-C6-C7-C8
34	c	521	DGD	C2A-C1A-O1G-C1G
38	D	413	LHG	C10-C11-C12-C13
25	L	102	SQD	O10-C23-O48-C46
23	B	610	CLA	C3A-C2A-CAA-CBA
23	b	618	CLA	C3A-C2A-CAA-CBA
34	d	408	DGD	C2B-C3B-C4B-C5B
24	h	101	BCR	C9-C10-C11-C12
38	d	411	LHG	C35-C36-C37-C38
34	C	517	DGD	C4A-C5A-C6A-C7A
23	C	509	CLA	C3-C5-C6-C7
23	b	621	CLA	C8-C10-C11-C12
38	D	411	LHG	C15-C16-C17-C18
35	b	629	LMG	C37-C38-C39-C40
35	c	522	LMG	O1-C7-C8-C9
38	d	411	LHG	C4-C5-C6-O8
35	Z	101	LMG	O1-C7-C8-C9
38	D	413	LHG	C4-C5-C6-O8
25	A	412	SQD	O6-C44-C45-C46
25	L	102	SQD	C44-C45-C46-O48
38	E	101	LHG	C4-C5-C6-O8
35	M	101	LMG	C15-C16-C17-C18
23	C	514	CLA	C5-C6-C7-C8
23	B	613	CLA	C8-C10-C11-C12
30	d	407[B]	PL9	C45-C44-C46-C47
23	b	619	CLA	C16-C17-C18-C20
38	a	420	LHG	C25-C26-C27-C28
38	E	101	LHG	C16-C17-C18-C19
38	D	411	LHG	C3-O3-P-O6
35	C	501	LMG	C10-C11-C12-C13
26	b	606	GOL	O2-C2-C3-O3
38	b	634	LHG	O1-C1-C2-O2
26	V	204	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	f	102	SQD	C25-C26-C27-C28
34	C	516	DGD	C1B-C2B-C3B-C4B
34	B	632	DGD	O2G-C1B-C2B-C3B
23	c	514	CLA	O1A-CGA-O2A-C1
35	b	629	LMG	C36-C37-C38-C39
34	c	520	DGD	C2A-C3A-C4A-C5A
34	c	520	DGD	C9B-CAB-CBB-CCB
33	o	301	HTG	C3'-C4'-C5'-C6'
35	c	522	LMG	O1-C7-C8-O7
35	c	522	LMG	O7-C8-C9-O8
38	d	411	LHG	O7-C5-C6-O8
25	f	102	SQD	O6-C44-C45-O47
38	D	413	LHG	O7-C5-C6-O8
25	a	414	SQD	O6-C44-C45-O47
34	C	516	DGD	C3A-C4A-C5A-C6A
35	z	101	LMG	C13-C14-C15-C16
30	D	409[A]	PL9	C9-C11-C12-C13
30	D	409[A]	PL9	C39-C41-C42-C43
23	c	515	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	625	CLA	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9
27	M	102	LMT	C11-C10-C9-C8
34	h	102	DGD	C9B-CAB-CBB-CCB
38	d	411	LHG	C2-C3-O3-P
27	m	102	LMT	C1-C2-C3-C4
38	d	409	LHG	C11-C10-C9-C8
38	d	409	LHG	C15-C16-C17-C18
38	d	411	LHG	C11-C10-C9-C8
35	C	519	LMG	C29-C30-C31-C32
27	a	404	LMT	C2-C3-C4-C5
24	d	406	BCR	C1-C6-C7-C8
24	d	406	BCR	C5-C6-C7-C8
24	c	518	BCR	C1-C6-C7-C8
24	c	518	BCR	C5-C6-C7-C8
24	k	102	BCR	C23-C24-C25-C26
24	k	102	BCR	C23-C24-C25-C30
24	D	408	BCR	C23-C24-C25-C26
24	A	408	BCR	C1-C6-C7-C8
24	A	408	BCR	C5-C6-C7-C8
25	F	104	SQD	C30-C31-C32-C33
24	K	103	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	c	522	LMG	C21-C22-C23-C24
23	a	412	CLA	CBA-CGA-O2A-C1
24	K	103	BCR	C17-C18-C19-C20
34	C	516	DGD	C5B-C6B-C7B-C8B
23	c	516	CLA	C15-C16-C17-C18
34	c	519	DGD	CAB-CBB-CCB-CDB
34	B	632	DGD	C5A-C6A-C7A-C8A
38	L	101	LHG	C35-C36-C37-C38
23	A	406	CLA	C13-C15-C16-C17
34	c	520	DGD	C6A-C7A-C8A-C9A
23	a	410	CLA	C12-C13-C15-C16
30	d	407[B]	PL9	C43-C44-C46-C47
23	b	625	CLA	C11-C12-C13-C15
23	c	514	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
27	e	102	LMT	C1-C2-C3-C4
23	A	405	CLA	C2C-C3C-CAC-CBC
23	C	510	CLA	C13-C15-C16-C17
24	t	102	BCR	C13-C14-C15-C16
23	b	619	CLA	C16-C17-C18-C19
25	L	102	SQD	C27-C28-C29-C30
38	d	411	LHG	C7-C8-C9-C10
23	C	510	CLA	C10-C11-C12-C13
23	B	617	CLA	C13-C15-C16-C17
23	B	602	CLA	C2A-CAA-CBA-CGA
34	C	518	DGD	C2A-C3A-C4A-C5A
34	d	408	DGD	C3A-C4A-C5A-C6A
33	c	524	HTG	C2'-C1'-S1-C1
33	B	622	HTG	C4-C5-C6-O6
23	B	610	CLA	CBA-CGA-O2A-C1
23	b	610	CLA	CBA-CGA-O2A-C1
35	D	417	LMG	C12-C13-C14-C15
35	M	101	LMG	C16-C17-C18-C19
27	M	104	LMT	O5B-C1B-O1B-C4'
23	B	614	CLA	C15-C16-C17-C18
33	B	629	HTG	C2'-C3'-C4'-C5'
37	a	411	PHO	C2B-C3B-CAB-CBB
37	a	411	PHO	CAD-CBD-CGD-O2D
23	B	613	CLA	CAD-CBD-CGD-O2D
23	b	622	CLA	CAD-CBD-CGD-O2D
25	L	102	SQD	C46-C45-O47-C7
23	C	513	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	b	619	CLA	CAD-CBD-CGD-O2D
23	b	613	CLA	CAD-CBD-CGD-O2D
34	d	408	DGD	C4A-C5A-C6A-C7A
38	b	634	LHG	C31-C32-C33-C34
23	d	403	CLA	C2C-C3C-CAC-CBC
23	C	514	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	CBA-CGA-O2A-C1
25	B	621	SQD	C24-C23-O48-C46
27	M	105	LMT	O5'-C1'-O1'-C1
34	d	408	DGD	O1G-C1G-C2G-C3G
35	z	101	LMG	O1-C7-C8-C9
35	z	101	LMG	C7-C8-C9-O8
25	F	104	SQD	C44-C45-C46-O48
34	c	521	DGD	O1A-C1A-O1G-C1G
38	b	634	LHG	O6-C4-C5-O7
23	c	513	CLA	C15-C16-C17-C18
27	a	404	LMT	C6-C7-C8-C9
25	a	414	SQD	C15-C16-C17-C18
35	z	101	LMG	C16-C17-C18-C19
23	B	602	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CHA-CBD-CGD-O1D
23	B	610	CLA	O1A-CGA-O2A-C1
23	a	412	CLA	O1A-CGA-O2A-C1
35	C	501	LMG	C2-C1-O1-C7
35	C	501	LMG	O1-C7-C8-O7
34	D	410	DGD	O1G-C1G-C2G-O2G
35	z	101	LMG	O1-C7-C8-O7
25	L	102	SQD	O47-C45-C46-O48
23	A	407	CLA	C15-C16-C17-C18
23	B	615	CLA	O1A-CGA-O2A-C1
35	D	417	LMG	C34-C35-C36-C37
35	C	520	LMG	C29-C30-C31-C32
35	M	101	LMG	C36-C37-C38-C39
34	C	517	DGD	C3A-C4A-C5A-C6A
38	d	409	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
26	C	524	GOL	O1-C1-C2-O2
26	c	501	GOL	O1-C1-C2-O2
38	D	413	LHG	O1-C1-C2-O2
38	a	420	LHG	O1-C1-C2-O2
35	c	523	LMG	C37-C38-C39-C40
30	A	416[A]	PL9	C15-C14-C16-C17
30	d	407[A]	PL9	C28-C29-C31-C32
30	d	407[B]	PL9	C28-C29-C31-C32
23	B	605	CLA	C6-C7-C8-C9
23	C	506	CLA	O1D-CGD-O2D-CED
38	E	101	LHG	C26-C27-C28-C29
23	b	610	CLA	O1A-CGA-O2A-C1
27	t	101	LMT	C2-C3-C4-C5
34	C	518	DGD	C8A-C9A-CAA-CBA
23	C	514	CLA	O1A-CGA-O2A-C1
24	c	518	BCR	C7-C8-C9-C34
26	v	202	GOL	C1-C2-C3-O3
24	A	408	BCR	C17-C18-C19-C20
38	d	409	LHG	C26-C27-C28-C29
27	D	405	LMT	C5-C6-C7-C8
38	E	101	LHG	C4-O6-P-O3
38	E	101	LHG	C24-C25-C26-C27
35	Z	101	LMG	C4-C5-C6-O5
35	a	415	LMG	C18-C19-C20-C21
35	a	415	LMG	C30-C31-C32-C33
23	c	517	CLA	C3-C5-C6-C7
38	D	412	LHG	C3-O3-P-O4
38	D	412	LHG	C4-O6-P-O5
38	E	101	LHG	C3-O3-P-O5
38	a	420	LHG	C3-O3-P-O5
38	a	420	LHG	C4-O6-P-O5
35	C	501	LMG	O6-C1-O1-C7
34	C	516	DGD	O6E-C1E-O5D-C6D
25	A	412	SQD	C24-C23-O48-C46
35	M	101	LMG	C40-C41-C42-C43
25	B	621	SQD	O10-C23-O48-C46
23	C	502	CLA	C2A-CAA-CBA-CGA
34	D	410	DGD	C2B-C3B-C4B-C5B
23	B	602	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
25	a	405	SQD	C5-C6-S-O9
25	A	409	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
34	h	102	DGD	O2G-C1B-C2B-C3B
38	d	411	LHG	C25-C26-C27-C28
23	c	513	CLA	C10-C11-C12-C13
35	a	415	LMG	O6-C5-C6-O5
38	d	409	LHG	C33-C34-C35-C36
23	C	502	CLA	C11-C12-C13-C15
33	V	207	HTG	C2-C1-S1-C1'
23	b	625	CLA	C12-C13-C15-C16
38	L	101	LHG	O6-C4-C5-O7
23	c	511	CLA	C11-C10-C8-C7
38	D	413	LHG	C30-C31-C32-C33
35	d	416	LMG	C35-C36-C37-C38
38	a	420	LHG	C8-C7-O7-C5
27	m	102	LMT	C2-C3-C4-C5
27	A	413	LMT	O1'-C1-C2-C3
23	A	405	CLA	C15-C16-C17-C18
23	B	604	CLA	C13-C15-C16-C17
35	C	520	LMG	C4-C5-C6-O5
35	C	501	LMG	O1-C7-C8-C9
34	C	516	DGD	C1G-C2G-C3G-O3G
34	C	518	DGD	C9A-CAA-CBA-CCA
38	a	420	LHG	O9-C7-O7-C5
34	C	516	DGD	O2G-C2G-C3G-O3G
35	a	415	LMG	O7-C8-C9-O8
25	F	104	SQD	O47-C45-C46-O48
25	L	102	SQD	O6-C44-C45-O47
38	E	101	LHG	O7-C5-C6-O8
34	C	516	DGD	C3B-C4B-C5B-C6B
38	D	412	LHG	C26-C27-C28-C29
23	C	502	CLA	O1D-CGD-O2D-CED
35	b	629	LMG	C10-C11-C12-C13
35	C	520	LMG	C8-C7-O1-C1
34	C	517	DGD	C2G-C3G-O3G-C1D
38	D	413	LHG	C2-C3-O3-P
23	B	602	CLA	C8-C10-C11-C12
30	D	409[B]	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
27	M	105	LMT	C11-C10-C9-C8
23	b	610	CLA	CAA-CBA-CGA-O2A
25	F	104	SQD	C26-C27-C28-C29
23	a	410	CLA	C11-C10-C8-C9
23	b	622	CLA	C6-C7-C8-C9
23	b	625	CLA	C14-C13-C15-C16
23	B	603	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	b	621	CLA	CBD-CGD-O2D-CED
33	V	207	HTG	C4'-C5'-C6'-C7'
30	a	416[A]	PL9	C14-C16-C17-C18
25	A	412	SQD	O10-C23-O48-C46
23	B	602	CLA	CAA-CBA-CGA-O2A
23	B	613	CLA	O1D-CGD-O2D-CED
35	C	501	LMG	C39-C40-C41-C42
34	c	520	DGD	C4B-C5B-C6B-C7B
34	C	518	DGD	CBA-CCA-CDA-CEA
34	c	520	DGD	C7A-C8A-C9A-CAA
25	B	621	SQD	C12-C13-C14-C15
35	c	522	LMG	C36-C37-C38-C39
23	b	620	CLA	C8-C10-C11-C12
27	C	521	LMT	C3-C4-C5-C6
34	B	632	DGD	C7B-C8B-C9B-CAB
38	L	101	LHG	C17-C18-C19-C20
23	c	505	CLA	C2A-CAA-CBA-CGA
23	c	516	CLA	C2-C1-O2A-CGA
34	C	518	DGD	C2A-C1A-O1G-C1G
34	C	518	DGD	O1A-C1A-O1G-C1G
34	B	632	DGD	C6B-C7B-C8B-C9B
23	b	623	CLA	CBD-CGD-O2D-CED
27	e	102	LMT	C5-C6-C7-C8
24	D	408	BCR	C23-C24-C25-C30
30	A	416[B]	PL9	C43-C44-C46-C47
35	d	416	LMG	C29-C30-C31-C32
34	C	517	DGD	CAB-CBB-CCB-CDB
35	b	629	LMG	C34-C35-C36-C37
34	h	102	DGD	CCA-CDA-CEA-CFA
38	D	413	LHG	C12-C13-C14-C15
34	C	516	DGD	C2E-C1E-O5D-C6D
33	B	622	HTG	C4'-C5'-C6'-C7'
25	B	621	SQD	O47-C45-C46-O48
38	L	101	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
23	d	405	CLA	O1D-CGD-O2D-CED
25	L	102	SQD	O6-C44-C45-C46
30	a	416[A]	PL9	C45-C44-C46-C47
30	A	416[B]	PL9	C15-C14-C16-C17
34	c	521	DGD	C3A-C4A-C5A-C6A
33	B	622	HTG	C1'-C2'-C3'-C4'
23	c	507	CLA	C5-C6-C7-C8
23	B	605	CLA	C6-C7-C8-C10
23	D	406	CLA	C12-C13-C15-C16
23	A	407	CLA	C12-C13-C15-C16
23	b	610	CLA	C11-C10-C8-C7
23	C	505	CLA	C12-C13-C15-C16
23	C	502	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	a	410	CLA	C11-C12-C13-C14
24	H	101	BCR	C9-C10-C11-C12
35	C	519	LMG	C31-C32-C33-C34
23	B	617	CLA	C8-C10-C11-C12
26	A	410	GOL	C1-C2-C3-O3
33	C	523	HTG	C4-C5-C6-O6
23	c	517	CLA	C4-C3-C5-C6
26	V	201	GOL	O1-C1-C2-O2
34	C	517	DGD	C6B-C7B-C8B-C9B
25	L	102	SQD	C33-C34-C35-C36
23	b	621	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C5-C6-C7-C8
33	c	524	HTG	C3'-C4'-C5'-C6'
34	D	410	DGD	C7B-C8B-C9B-CAB
35	a	415	LMG	C34-C35-C36-C37
23	A	404	CLA	C16-C17-C18-C19
35	b	629	LMG	C39-C40-C41-C42
30	d	407[B]	PL9	C15-C14-C16-C17
25	A	409	SQD	C10-C11-C12-C13
35	a	415	LMG	C36-C37-C38-C39
30	A	416[A]	PL9	C13-C14-C16-C17
37	a	411	PHO	C2-C3-C5-C6
23	B	614	CLA	C2-C1-O2A-CGA
23	b	622	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
27	M	105	LMT	C2'-C1'-O1'-C1
34	D	410	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C2A-CAA-CBA-CGA
35	c	523	LMG	O7-C8-C9-O8
38	D	413	LHG	C9-C10-C11-C12
38	d	409	LHG	C7-C8-C9-C10
23	C	514	CLA	C3A-C2A-CAA-CBA
23	B	608	CLA	C3A-C2A-CAA-CBA
23	a	409	CLA	C13-C15-C16-C17
27	M	102	LMT	O5'-C5'-C6'-O6'
25	A	412	SQD	C26-C27-C28-C29
30	d	407[A]	PL9	C30-C29-C31-C32
37	a	411	PHO	C4-C3-C5-C6
30	a	416[A]	PL9	C43-C44-C46-C47
23	B	602	CLA	C14-C13-C15-C16
23	B	610	CLA	C6-C7-C8-C9
23	B	604	CLA	C14-C13-C15-C16
23	b	620	CLA	C11-C12-C13-C14
23	D	407	CLA	C6-C7-C8-C9
23	C	505	CLA	C11-C12-C13-C14
27	M	102	LMT	C6-C7-C8-C9
38	D	411	LHG	C28-C29-C30-C31
38	d	409	LHG	C1-C2-C3-O3
38	D	412	LHG	C9-C10-C11-C12
38	b	634	LHG	C30-C31-C32-C33
35	a	415	LMG	C19-C20-C21-C22
23	b	614	CLA	C8-C10-C11-C12
24	b	626	BCR	C17-C18-C19-C20
23	b	625	CLA	C4-C3-C5-C6
30	A	416[B]	PL9	C45-C44-C46-C47
23	c	505	CLA	C1A-C2A-CAA-CBA
38	d	409	LHG	C32-C33-C34-C35
25	A	409	SQD	C12-C13-C14-C15
38	D	412	LHG	C33-C34-C35-C36
23	C	507	CLA	C16-C17-C18-C20
23	A	406	CLA	C11-C10-C8-C7
23	C	502	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C7
23	d	404	CLA	C11-C12-C13-C15
38	d	411	LHG	C4-O6-P-O3
38	D	413	LHG	C4-O6-P-O3
35	c	522	LMG	C33-C34-C35-C36
35	C	501	LMG	C13-C14-C15-C16
34	C	516	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
23	b	623	CLA	C2A-CAA-CBA-CGA
23	b	619	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C10-C11-C12-C13
25	f	102	SQD	C33-C34-C35-C36
27	A	413	LMT	C6-C7-C8-C9
34	c	520	DGD	C3A-C4A-C5A-C6A
30	D	409[B]	PL9	C45-C44-C46-C47
30	A	416[B]	PL9	C13-C14-C16-C17
27	D	405	LMT	C2B-C1B-O1B-C4'
34	c	519	DGD	C4B-C5B-C6B-C7B
27	M	105	LMT	C9-C10-C11-C12
35	D	417	LMG	C30-C31-C32-C33
25	F	104	SQD	O6-C44-C45-O47
27	M	105	LMT	C4'-C5'-C6'-O6'
23	C	509	CLA	C13-C15-C16-C17
27	t	101	LMT	C4-C5-C6-C7
30	A	416[A]	PL9	C19-C21-C22-C23
30	a	416[A]	PL9	C39-C41-C42-C43
30	A	416[B]	PL9	C19-C21-C22-C23
23	d	405	CLA	C4-C3-C5-C6
23	C	507	CLA	C2-C1-O2A-CGA
23	b	623	CLA	C2-C1-O2A-CGA
30	A	416[A]	PL9	C43-C44-C46-C47
23	b	625	CLA	C2-C3-C5-C6
30	D	409[B]	PL9	C43-C44-C46-C47
23	c	517	CLA	C2-C3-C5-C6
23	b	623	CLA	C14-C13-C15-C16
27	D	405	LMT	C6-C7-C8-C9
23	c	509	CLA	O1A-CGA-O2A-C1
35	c	522	LMG	C32-C33-C34-C35
34	C	518	DGD	C3B-C4B-C5B-C6B
35	D	417	LMG	C21-C22-C23-C24
34	c	520	DGD	C2B-C3B-C4B-C5B
23	A	404	CLA	C15-C16-C17-C18
23	B	604	CLA	C16-C17-C18-C20
24	K	103	BCR	C1-C6-C7-C8
24	a	413	BCR	C1-C6-C7-C8
24	H	101	BCR	C23-C24-C25-C30
24	D	408	BCR	C1-C6-C7-C8
24	D	408	BCR	C5-C6-C7-C8
24	b	627	BCR	C23-C24-C25-C26
24	b	627	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	K	101	BCR	C23-C24-C25-C30
25	f	102	SQD	O6-C44-C45-C46
26	V	202	GOL	O1-C1-C2-C3
26	V	203	GOL	O1-C1-C2-C3
25	L	102	SQD	C11-C12-C13-C14
23	b	610	CLA	C4-C3-C5-C6
23	a	412	CLA	C4-C3-C5-C6
24	c	518	BCR	C7-C8-C9-C10
24	C	515	BCR	C11-C12-C13-C14
23	A	406	CLA	C16-C17-C18-C20
27	F	101	LMT	O1'-C1-C2-C3
23	A	405	CLA	O1A-CGA-O2A-C1
25	a	405	SQD	C45-C44-O6-C1
35	z	101	LMG	C8-C7-O1-C1
34	C	517	DGD	C5D-C6D-O5D-C1E
27	D	405	LMT	O5B-C1B-O1B-C4'
23	d	403	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
38	D	413	LHG	C13-C14-C15-C16
23	d	403	CLA	C15-C16-C17-C18
27	a	419	LMT	C7-C8-C9-C10
25	B	621	SQD	C19-C20-C21-C22
23	b	616	CLA	C3-C5-C6-C7
35	D	417	LMG	C14-C15-C16-C17
30	A	416[A]	PL9	C30-C29-C31-C32
23	C	508	CLA	C4-C3-C5-C6
23	C	514	CLA	C4-C3-C5-C6
35	b	629	LMG	C29-C30-C31-C32
23	B	612	CLA	C2-C3-C5-C6
23	B	602	CLA	C11-C10-C8-C7
23	d	405	CLA	C11-C10-C8-C7
30	a	416[B]	PL9	C43-C44-C46-C47
30	D	409[B]	PL9	C28-C29-C31-C32
23	a	412	CLA	C2-C3-C5-C6
23	b	613	CLA	C11-C12-C13-C15
38	a	420	LHG	C13-C14-C15-C16
26	a	401	GOL	O2-C2-C3-O3
26	V	202	GOL	O1-C1-C2-O2
35	d	416	LMG	C36-C37-C38-C39
38	D	412	LHG	C31-C32-C33-C34
38	E	101	LHG	C11-C12-C13-C14
35	Z	101	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
35	z	101	LMG	O7-C8-C9-O8
35	C	519	LMG	O10-C28-O8-C9
34	c	521	DGD	CAB-CBB-CCB-CDB
35	z	101	LMG	C18-C19-C20-C21
23	B	607	CLA	C13-C15-C16-C17
38	b	634	LHG	O7-C7-C8-C9
38	a	420	LHG	O8-C23-C24-C25
35	C	501	LMG	C21-C22-C23-C24
34	c	520	DGD	O2G-C1B-C2B-C3B
23	C	507	CLA	C4-C3-C5-C6
30	D	409[A]	PL9	C35-C34-C36-C37
30	a	416[B]	PL9	C45-C44-C46-C47
30	A	416[B]	PL9	C30-C29-C31-C32
27	m	102	LMT	C4'-C5'-C6'-O6'
30	a	416[B]	PL9	C12-C11-C9-C8
38	d	409	LHG	O8-C23-C24-C25
23	C	513	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	C11-C10-C8-C9
23	b	618	CLA	C6-C7-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
38	d	409	LHG	C13-C14-C15-C16
34	d	408	DGD	C7B-C8B-C9B-CAB
23	C	506	CLA	O1A-CGA-O2A-C1
35	Z	101	LMG	O7-C10-C11-C12
23	C	511	CLA	CAA-CBA-CGA-O2A
23	c	507	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	c	516	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
37	D	402	PHO	CAD-CBD-CGD-O2D
23	B	617	CLA	CAD-CBD-CGD-O2D
23	C	511	CLA	CAD-CBD-CGD-O2D
23	B	611	CLA	CAD-CBD-CGD-O2D
23	b	625	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
27	C	521	LMT	C4'-C5'-C6'-O6'
23	C	511	CLA	C2-C1-O2A-CGA
38	D	411	LHG	C25-C26-C27-C28
30	A	416[A]	PL9	C20-C19-C21-C22
30	A	416[A]	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C4-C3-C5-C6
27	m	102	LMT	C11-C10-C9-C8
38	b	634	LHG	C17-C18-C19-C20
30	D	409[B]	PL9	C33-C34-C36-C37
38	L	101	LHG	O7-C7-C8-C9
38	E	101	LHG	O8-C23-C24-C25
25	L	102	SQD	C7-C8-C9-C10
35	Z	101	LMG	C7-C8-C9-O8
34	D	410	DGD	O1G-C1A-C2A-C3A
34	c	521	DGD	O1G-C1A-C2A-C3A
38	E	101	LHG	C15-C16-C17-C18
37	a	411	PHO	O2A-C1-C2-C3
23	B	614	CLA	O2A-C1-C2-C3
23	d	405	CLA	O2A-C1-C2-C3
23	b	622	CLA	O2A-C1-C2-C3
23	b	620	CLA	O1A-CGA-O2A-C1
37	a	411	PHO	C4B-C3B-CAB-CBB
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	607	CLA	C10-C11-C12-C13
27	F	101	LMT	C1-C2-C3-C4
34	h	102	DGD	C6A-C7A-C8A-C9A
23	b	611	CLA	O1A-CGA-O2A-C1
23	c	509	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	b	611	CLA	CHA-CBD-CGD-O1D
23	b	611	CLA	CHA-CBD-CGD-O2D
37	D	403[B]	PHO	CHA-CBD-CGD-O1D
37	D	403[B]	PHO	CHA-CBD-CGD-O2D
23	B	613	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	c	513	CLA	CHA-CBD-CGD-O1D
23	c	513	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O2D
37	D	403[A]	PHO	CHA-CBD-CGD-O1D
37	D	403[A]	PHO	CHA-CBD-CGD-O2D
23	B	603	CLA	CHA-CBD-CGD-O1D
23	B	603	CLA	CHA-CBD-CGD-O2D
23	d	403	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CHA-CBD-CGD-O1D
23	B	615	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
37	d	402[A]	PHO	CHA-CBD-CGD-O1D
37	d	402[A]	PHO	CHA-CBD-CGD-O2D
23	B	608	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	CHA-CBD-CGD-O1D
37	d	402[B]	PHO	CHA-CBD-CGD-O1D
37	d	402[B]	PHO	CHA-CBD-CGD-O2D
23	c	511	CLA	CHA-CBD-CGD-O2D
30	A	416[B]	PL9	C20-C19-C21-C22
23	b	619	CLA	C15-C16-C17-C18
25	L	102	SQD	C24-C25-C26-C27
35	c	522	LMG	O7-C10-C11-C12
38	D	411	LHG	C13-C14-C15-C16
25	A	409	SQD	O6-C44-C45-O47
34	d	408	DGD	CAB-CBB-CCB-CDB
37	d	402[B]	PHO	C8-C10-C11-C12
23	B	616	CLA	C5-C6-C7-C8
25	B	621	SQD	C35-C36-C37-C38
34	d	408	DGD	O2G-C1B-C2B-C3B
27	A	413	LMT	C11-C10-C9-C8
26	B	628	GOL	O2-C2-C3-O3
26	C	525	GOL	O1-C1-C2-O2
23	d	405	CLA	C15-C16-C17-C18
23	d	403	CLA	C4C-C3C-CAC-CBC
38	E	101	LHG	C11-C10-C9-C8
23	A	405	CLA	CBA-CGA-O2A-C1
23	b	620	CLA	CBA-CGA-O2A-C1
34	B	632	DGD	O1B-C1B-C2B-C3B
23	B	614	CLA	CAA-CBA-CGA-O2A
23	b	617	CLA	C4-C3-C5-C6
25	A	409	SQD	C18-C19-C20-C21
35	c	523	LMG	C31-C32-C33-C34
30	a	416[B]	PL9	C4-C3-C7-C8
38	d	410	LHG	C14-C15-C16-C17
27	e	102	LMT	C2B-C1B-O1B-C4'
35	z	101	LMG	O6-C1-O1-C7
23	c	514	CLA	CAA-CBA-CGA-O2A
35	c	522	LMG	C19-C20-C21-C22
23	c	509	CLA	C11-C12-C13-C14
23	A	406	CLA	C11-C10-C8-C9
23	B	607	CLA	C11-C12-C13-C14
23	B	615	CLA	C6-C7-C8-C9
35	c	523	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
38	b	634	LHG	C23-C24-C25-C26
25	f	102	SQD	O47-C7-C8-C9
38	d	410	LHG	C28-C29-C30-C31
38	D	412	LHG	C13-C14-C15-C16
34	D	410	DGD	O1A-C1A-C2A-C3A
38	d	410	LHG	C34-C35-C36-C37
23	A	405	CLA	C4C-C3C-CAC-CBC
38	D	411	LHG	C11-C12-C13-C14
34	B	632	DGD	CCA-CDA-CEA-CFA
25	L	102	SQD	C11-C10-C9-C8
38	a	420	LHG	O10-C23-C24-C25
25	a	414	SQD	C35-C36-C37-C38
26	B	628	GOL	C1-C2-C3-O3
26	C	525	GOL	O1-C1-C2-C3
26	a	401	GOL	C1-C2-C3-O3
26	V	204	GOL	C1-C2-C3-O3
25	a	405	SQD	O48-C23-C24-C25
34	c	521	DGD	O1A-C1A-C2A-C3A
37	d	402[A]	PHO	C2C-C3C-CAC-CBC
23	C	512	CLA	C1A-C2A-CAA-CBA
23	b	618	CLA	C1A-C2A-CAA-CBA
23	d	404	CLA	C1A-C2A-CAA-CBA
23	a	409	CLA	C16-C17-C18-C19
23	c	510	CLA	C2-C1-O2A-CGA
23	a	409	CLA	C2-C1-O2A-CGA
23	b	617	CLA	C2-C1-O2A-CGA
23	c	509	CLA	CBA-CGA-O2A-C1
23	B	613	CLA	CBA-CGA-O2A-C1
35	C	519	LMG	C29-C28-O8-C9
38	d	409	LHG	O10-C23-C24-C25
35	Z	101	LMG	O9-C10-C11-C12
38	b	634	LHG	O9-C7-C8-C9
23	C	511	CLA	CAA-CBA-CGA-O1A
35	Z	101	LMG	C13-C14-C15-C16
34	D	410	DGD	C1G-C2G-C3G-O3G
23	b	621	CLA	C3-C5-C6-C7
35	D	417	LMG	O7-C10-C11-C12
23	b	623	CLA	C8-C10-C11-C12
38	D	411	LHG	C4-O6-P-O3
23	c	510	CLA	C13-C15-C16-C17
33	o	301	HTG	C2'-C3'-C4'-C5'
23	C	513	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
38	E	101	LHG	O10-C23-C24-C25
35	C	519	LMG	C16-C17-C18-C19
23	B	603	CLA	C8-C10-C11-C12
38	D	411	LHG	C3-O3-P-O5
38	d	411	LHG	C4-O6-P-O5
38	D	413	LHG	C4-O6-P-O5
23	b	614	CLA	C16-C17-C18-C19
35	c	522	LMG	O9-C10-C11-C12
33	B	630	HTG	S1-C1'-C2'-C3'
25	L	102	SQD	C31-C32-C33-C34
24	K	103	BCR	C5-C6-C7-C8
24	t	102	BCR	C1-C6-C7-C8
24	t	102	BCR	C5-C6-C7-C8
34	C	517	DGD	C6A-C7A-C8A-C9A
25	B	621	SQD	C15-C16-C17-C18
23	B	616	CLA	C10-C11-C12-C13
34	C	517	DGD	C1B-C2B-C3B-C4B
38	d	410	LHG	C11-C10-C9-C8
25	B	621	SQD	O48-C23-C24-C25
23	c	511	CLA	C2A-CAA-CBA-CGA
38	L	101	LHG	O9-C7-C8-C9
23	b	615	CLA	C10-C11-C12-C13
23	C	510	CLA	C8-C10-C11-C12
23	C	513	CLA	C10-C11-C12-C13
23	c	509	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	B	610	CLA	CAD-CBD-CGD-O1D
23	B	604	CLA	CAD-CBD-CGD-O1D
23	b	618	CLA	CAD-CBD-CGD-O1D
23	d	403	CLA	CAD-CBD-CGD-O1D
23	b	612	CLA	CAD-CBD-CGD-O1D
23	B	608	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
23	B	613	CLA	O1A-CGA-O2A-C1
23	b	618	CLA	O1A-CGA-O2A-C1
34	c	520	DGD	O1B-C1B-C2B-C3B
35	C	501	LMG	C31-C32-C33-C34
23	b	615	CLA	C11-C10-C8-C9
23	d	405	CLA	C11-C10-C8-C9
23	b	620	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	d	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	509	CLA	C6-C7-C8-C9
23	b	612	CLA	C11-C10-C8-C9
26	f	101	GOL	O2-C2-C3-O3
38	d	409	LHG	C24-C25-C26-C27
38	D	413	LHG	C25-C26-C27-C28
25	A	412	SQD	C16-C17-C18-C19
23	C	505	CLA	C13-C15-C16-C17
35	C	520	LMG	C38-C39-C40-C41
23	C	506	CLA	CAA-CBA-CGA-O2A
30	d	407[B]	PL9	C11-C12-C13-C14
30	A	416[B]	PL9	C26-C27-C28-C29
25	a	414	SQD	C26-C27-C28-C29
25	f	102	SQD	O49-C7-C8-C9
23	B	614	CLA	CAA-CBA-CGA-O1A
23	B	612	CLA	C4-C3-C5-C6
30	D	409[A]	PL9	C30-C29-C31-C32
23	c	507	CLA	C6-C7-C8-C10
30	d	407[A]	PL9	C18-C19-C21-C22
23	c	509	CLA	C11-C12-C13-C15
23	a	410	CLA	C11-C12-C13-C15
23	b	620	CLA	C12-C13-C15-C16
23	B	603	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
23	c	516	CLA	CAA-CBA-CGA-O1A
34	d	408	DGD	O1B-C1B-C2B-C3B
38	d	410	LHG	C16-C17-C18-C19
34	c	519	DGD	CCA-CDA-CEA-CFA
23	c	509	CLA	CAA-CBA-CGA-O2A
23	c	516	CLA	CAA-CBA-CGA-O2A
23	b	622	CLA	CAA-CBA-CGA-O2A
35	z	101	LMG	O7-C10-C11-C12
23	d	404	CLA	CAA-CBA-CGA-O2A
34	h	102	DGD	C7A-C8A-C9A-CAA
34	C	516	DGD	C4A-C5A-C6A-C7A
23	B	613	CLA	C3-C5-C6-C7
23	c	511	CLA	C5-C6-C7-C8
27	D	405	LMT	C4-C5-C6-C7
23	B	613	CLA	CAA-CBA-CGA-O2A
27	m	102	LMT	O5'-C1'-O1'-C1
23	a	412	CLA	C8-C10-C11-C12
23	C	506	CLA	CAA-CBA-CGA-O1A
23	c	514	CLA	CAA-CBA-CGA-O1A

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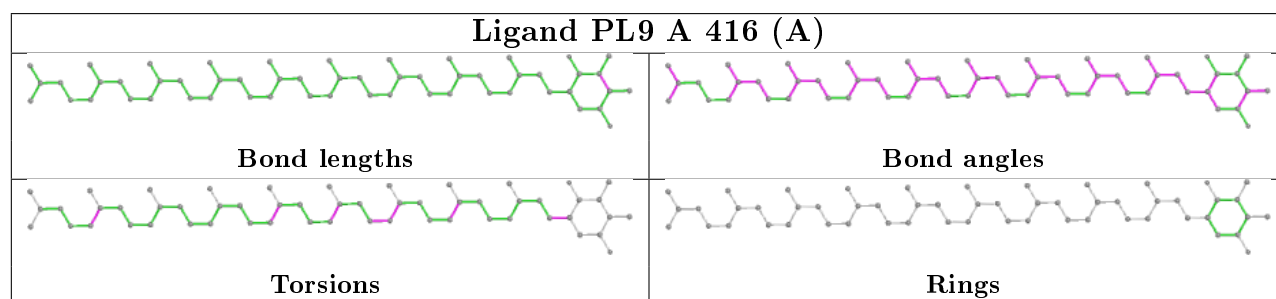
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Mol	Chain	Res	Type	Atoms
38	D	413	LHG	C17-C18-C19-C20
27	C	521	LMT	C2-C3-C4-C5
35	b	629	LMG	C4-C5-C6-O5
38	d	411	LHG	O8-C23-C24-C25
38	D	413	LHG	O8-C23-C24-C25
35	a	415	LMG	O8-C28-C29-C30
25	a	405	SQD	O10-C23-C24-C25
23	A	404	CLA	C2A-CAA-CBA-CGA
23	B	609	CLA	C16-C17-C18-C19
23	C	508	CLA	C5-C6-C7-C8
37	D	403[B]	PHO	NC-C1C-CHC-C4B
23	c	509	CLA	CAA-CBA-CGA-O1A
23	B	608	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
35	C	501	LMG	O8-C28-C29-C30
35	C	519	LMG	O7-C10-C11-C12
23	B	615	CLA	CAA-CBA-CGA-O2A

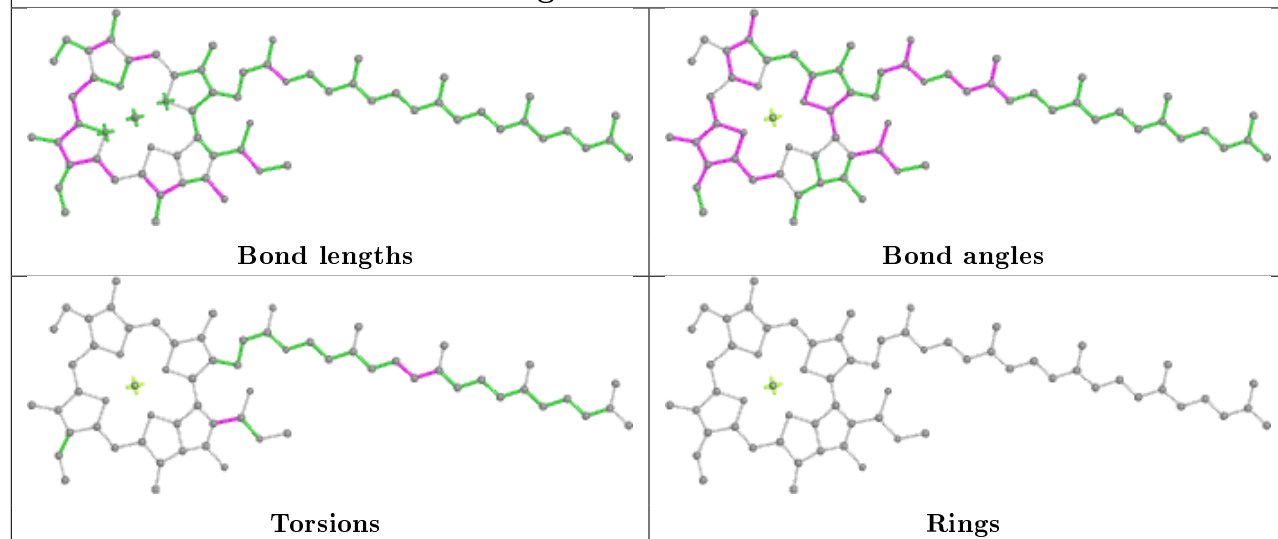
There are no ring outliers.

No monomer is involved in short contacts.

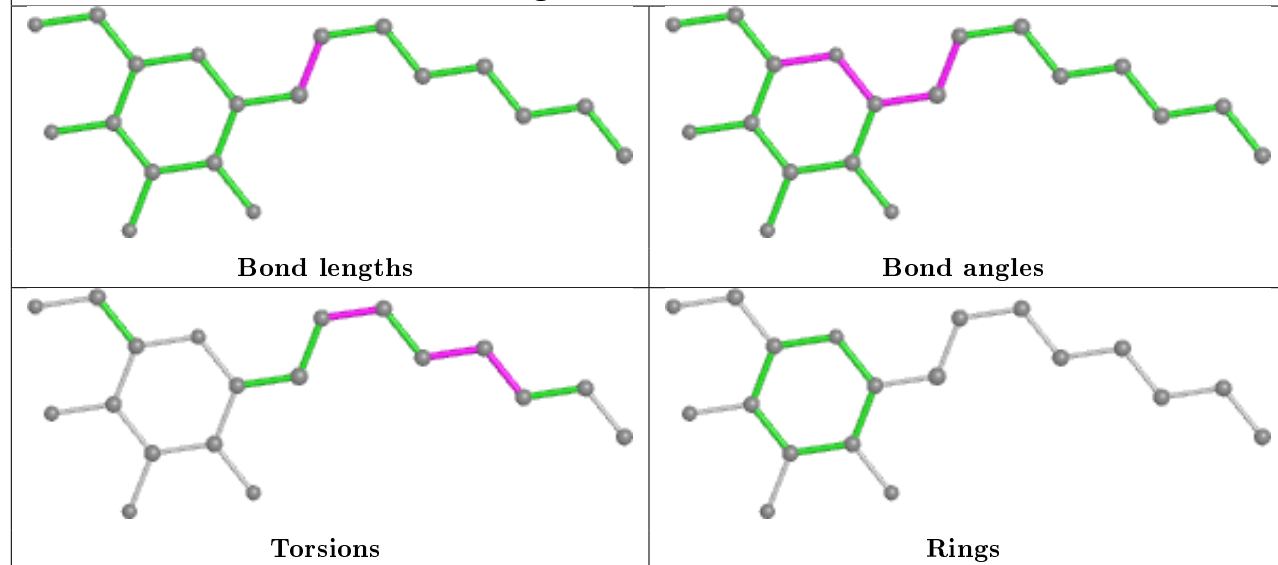
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

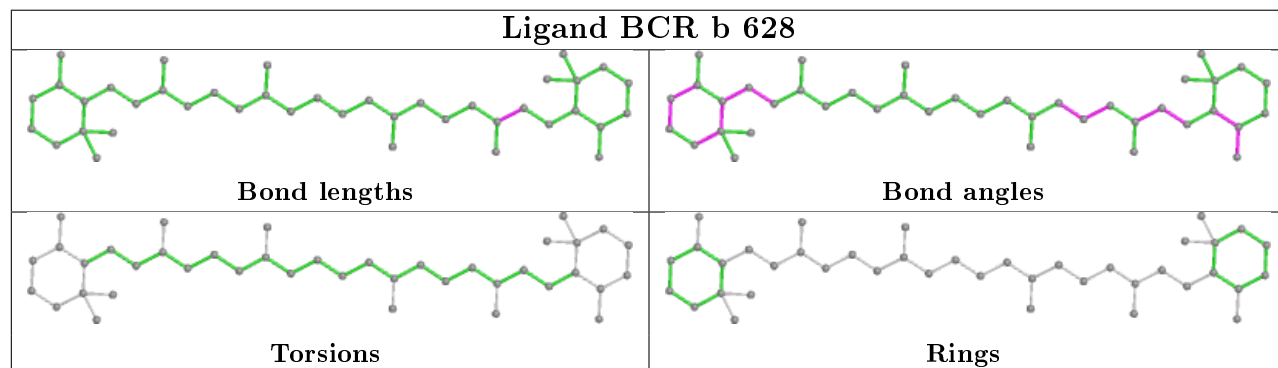
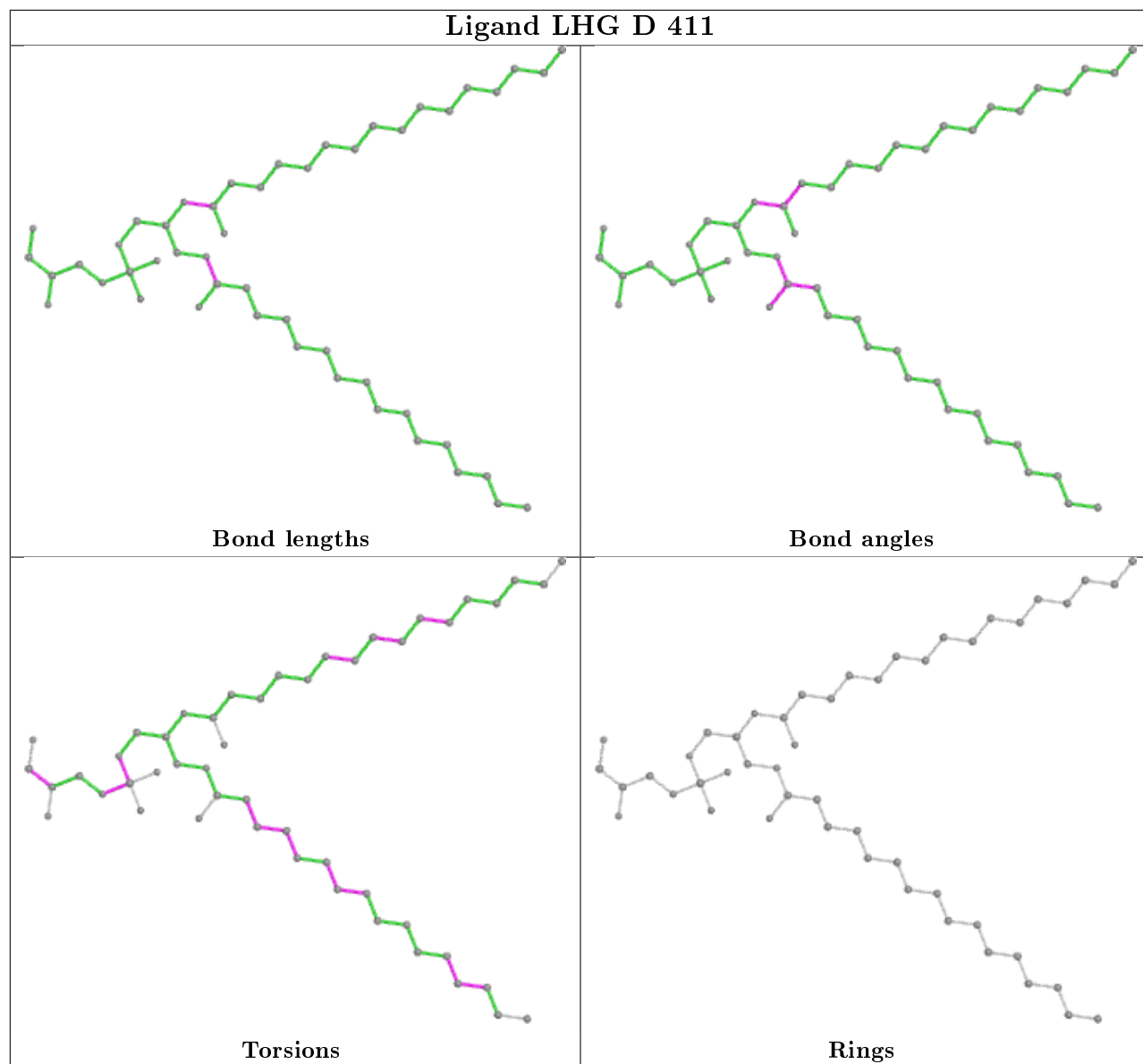


Ligand CLA c 507

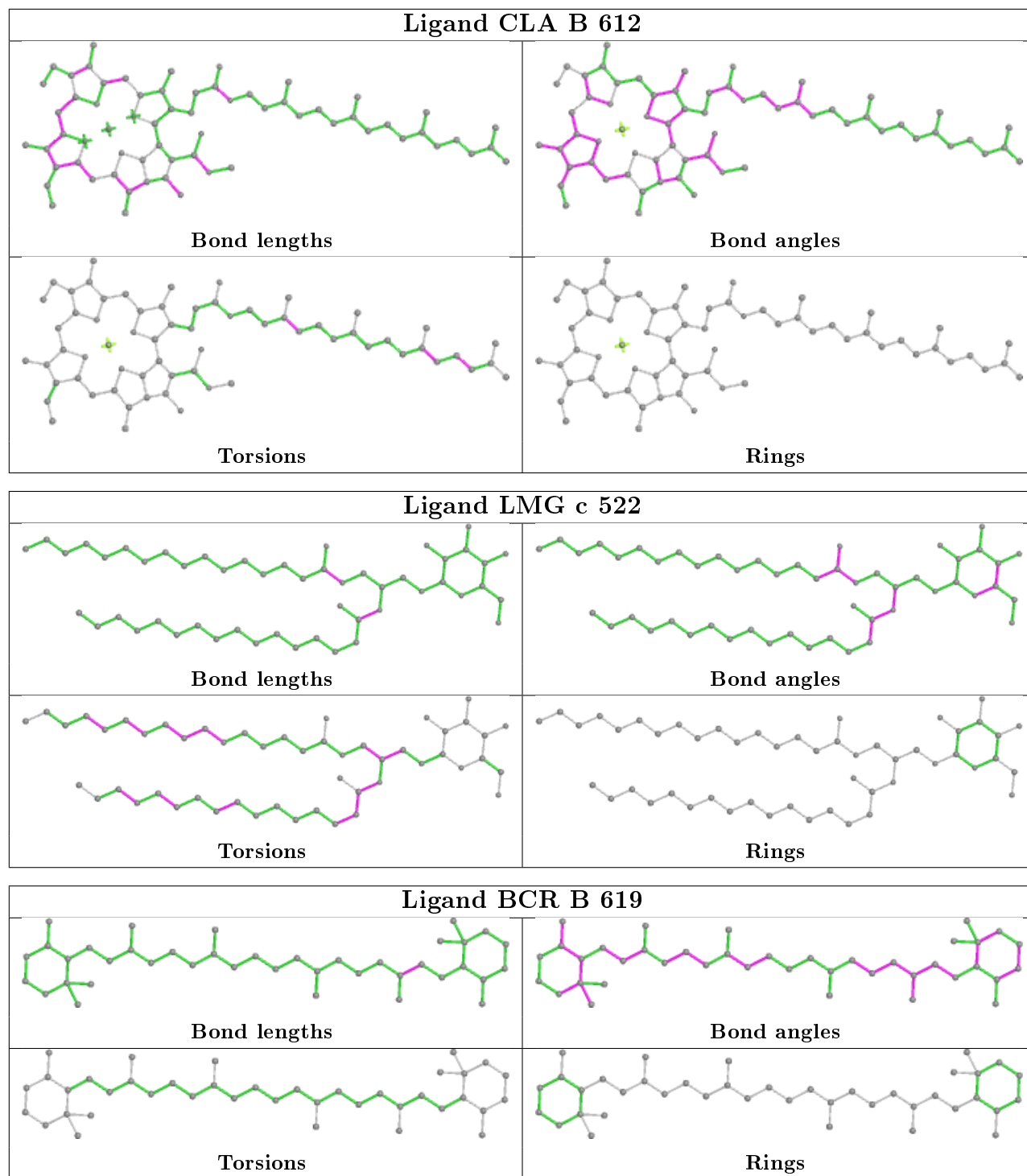


Ligand HTG b 601

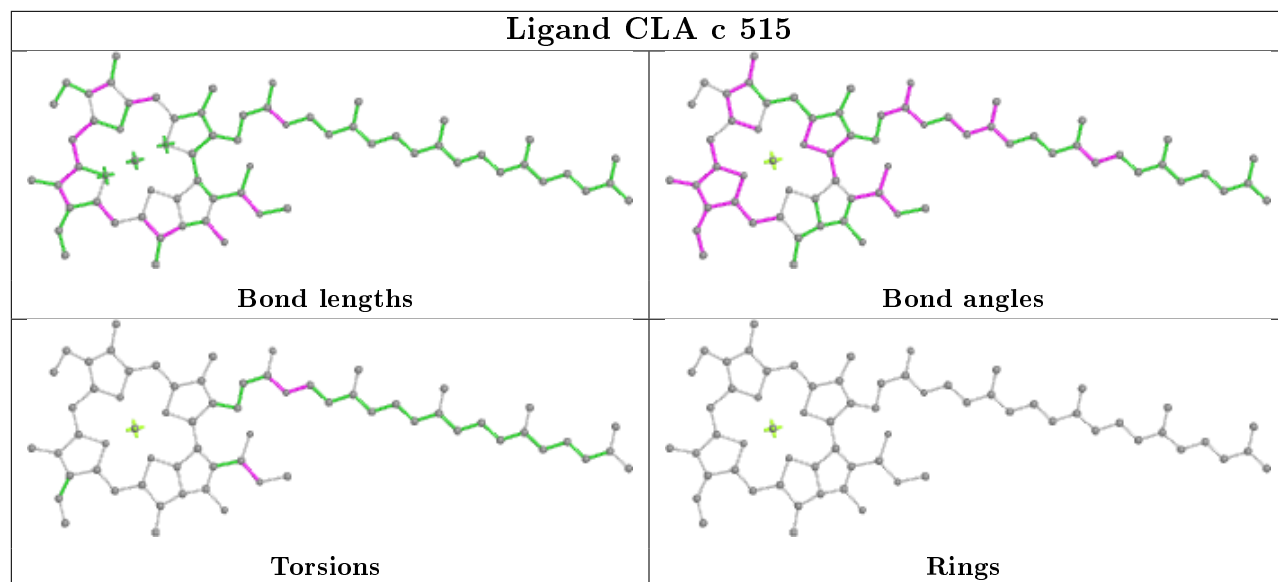




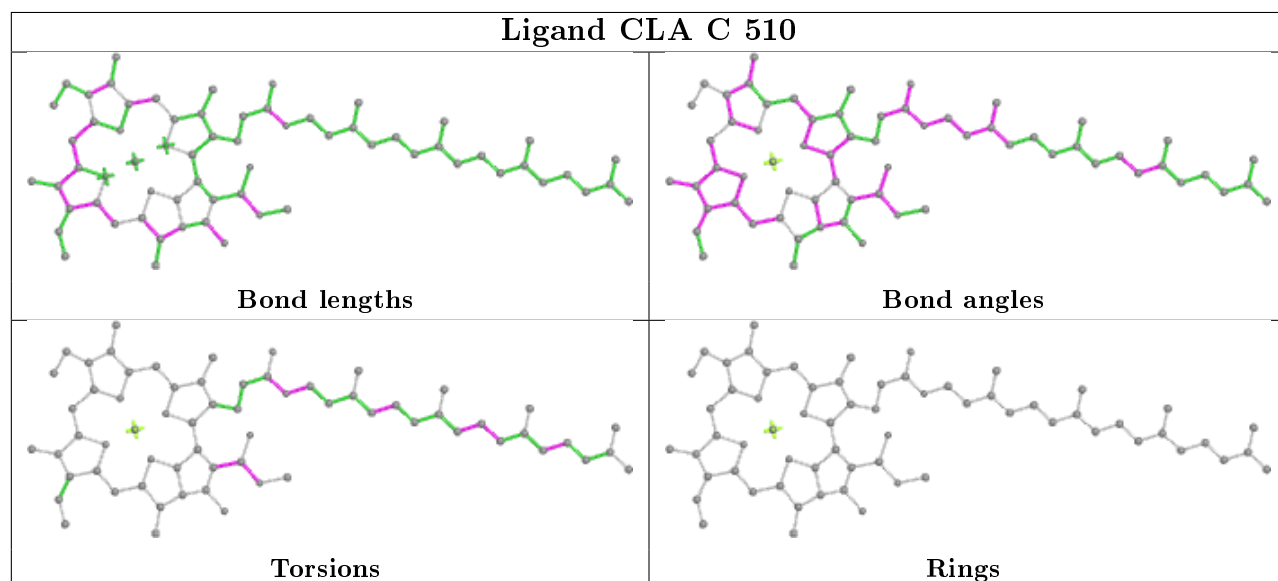
Ligand PL9 d 407 (A)	
<p>Bond lengths</p>	<p>Bond angles</p>
<p>Torsions</p>	<p>Rings</p>
Ligand LMG D 417	
<p>Bond lengths</p>	<p>Bond angles</p>
<p>Torsions</p>	<p>Rings</p>
Ligand CLA c 509	
<p>Bond lengths</p>	<p>Bond angles</p>
<p>Torsions</p>	<p>Rings</p>



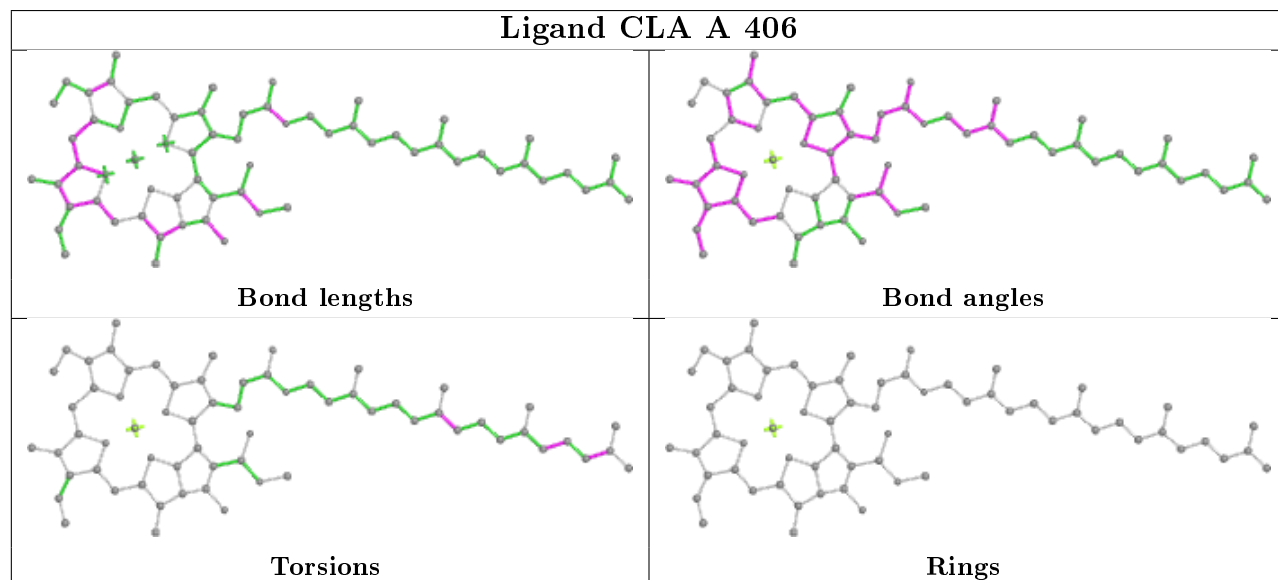
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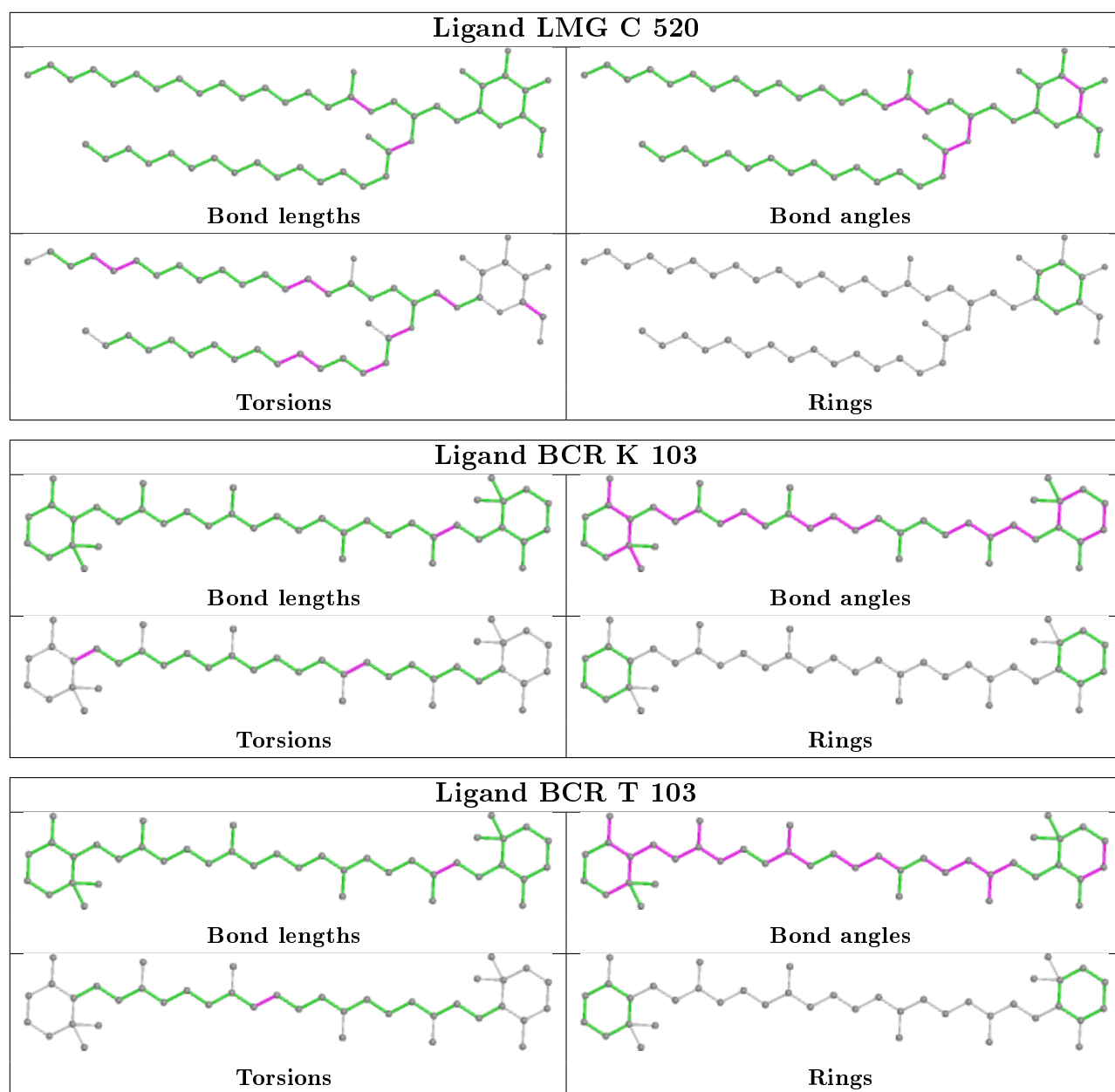


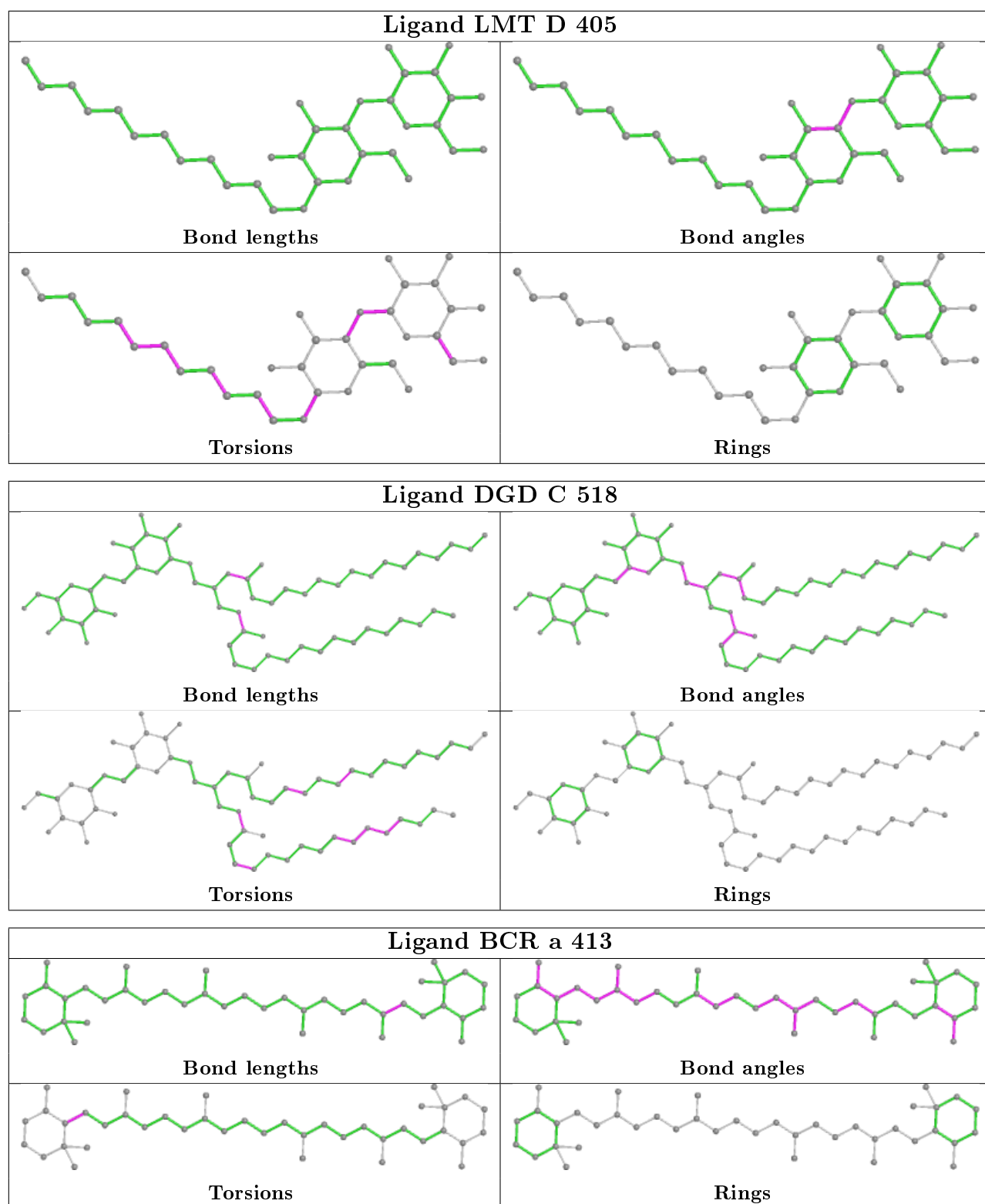
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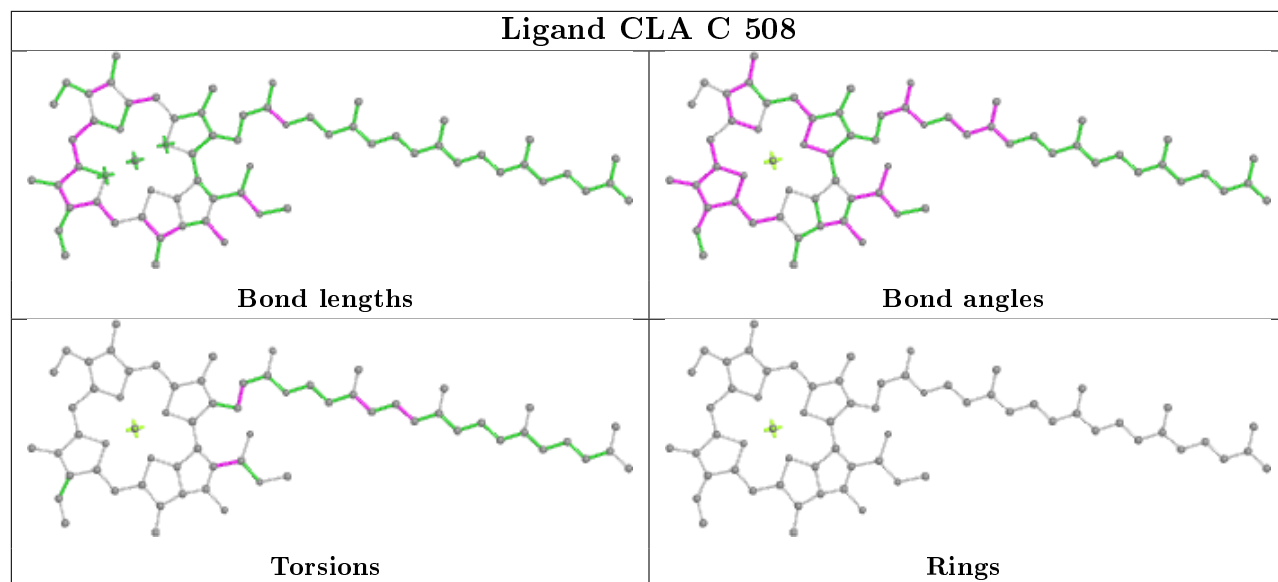
Ligand CLA A 406



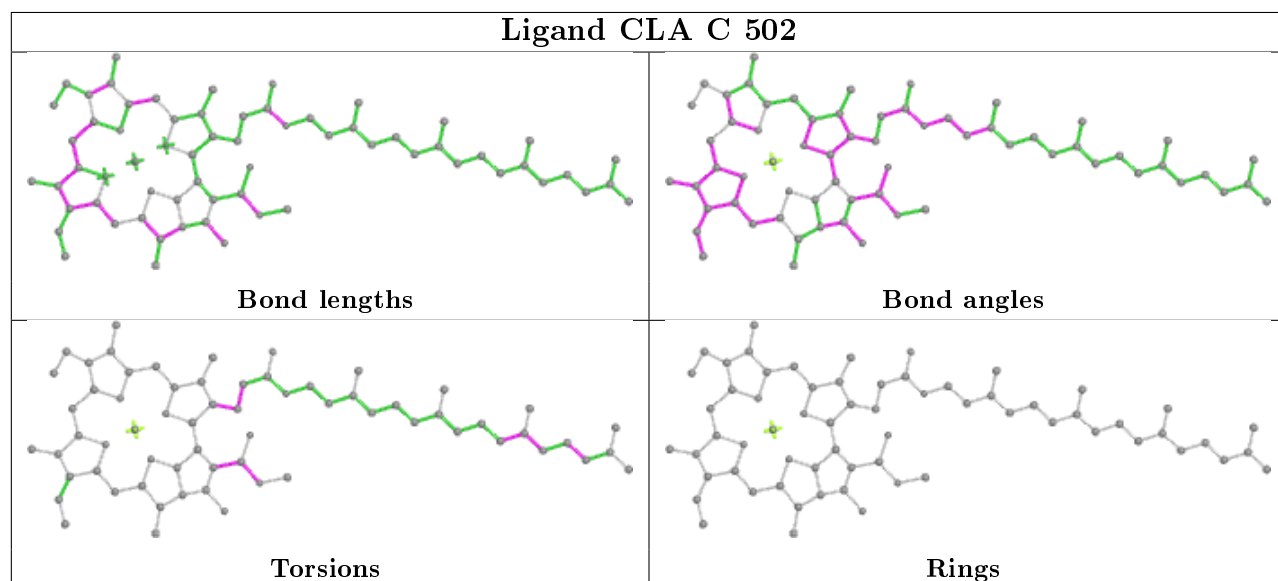




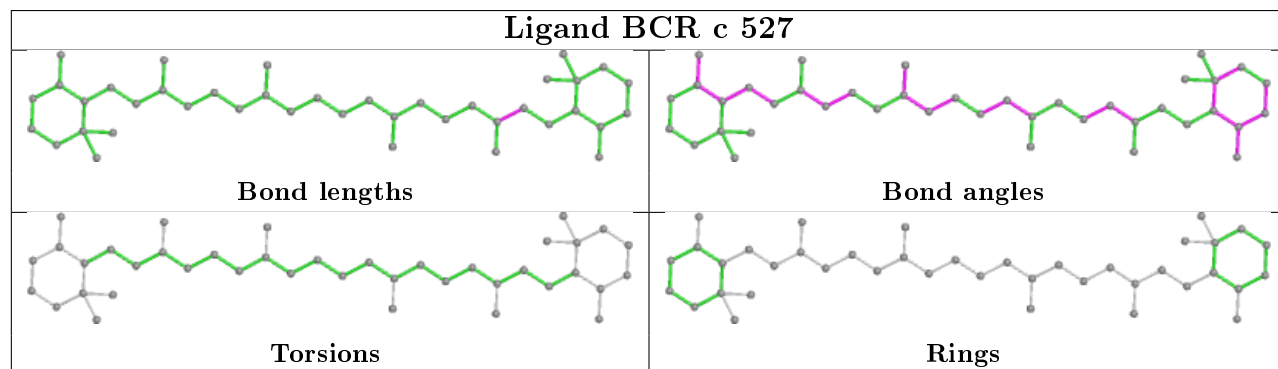
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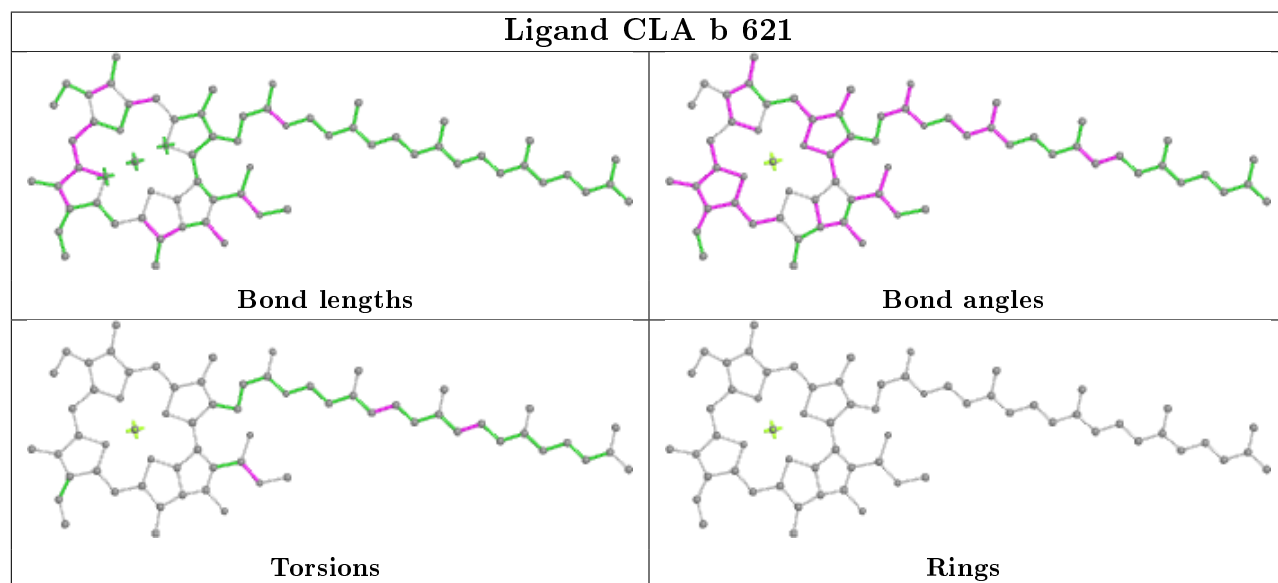
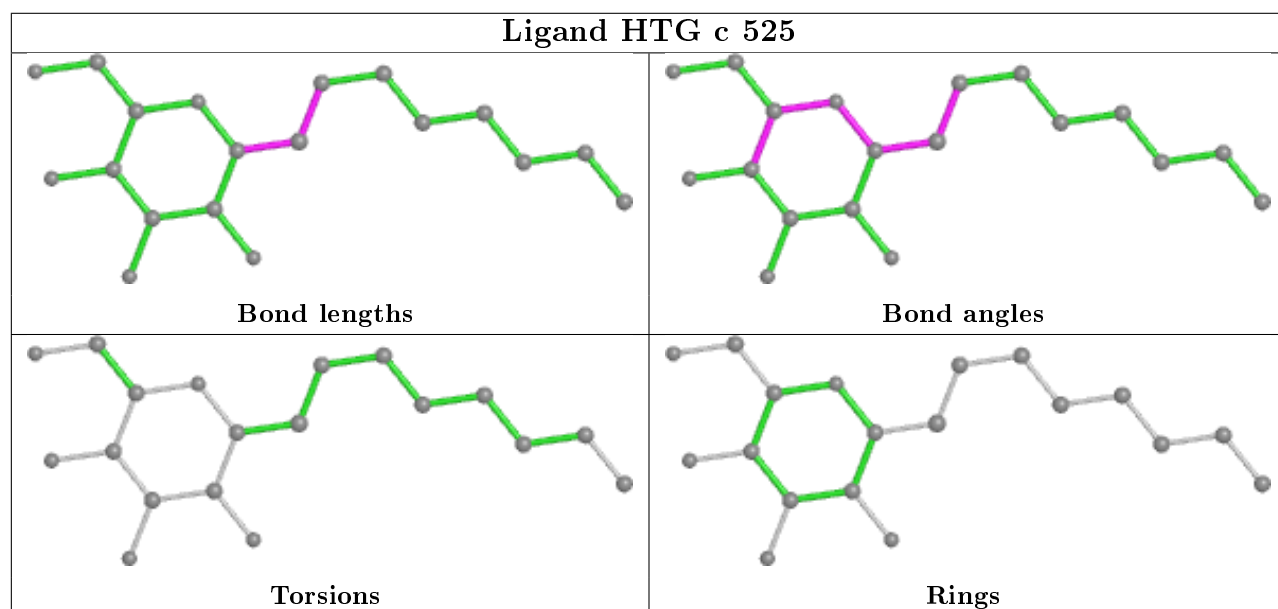
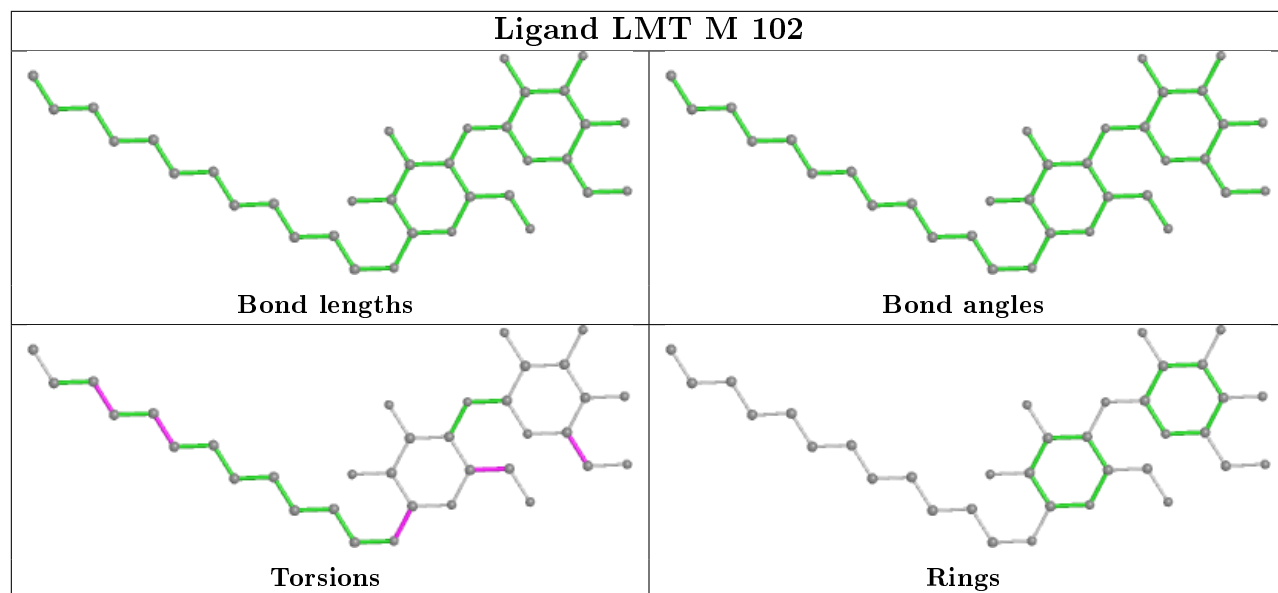


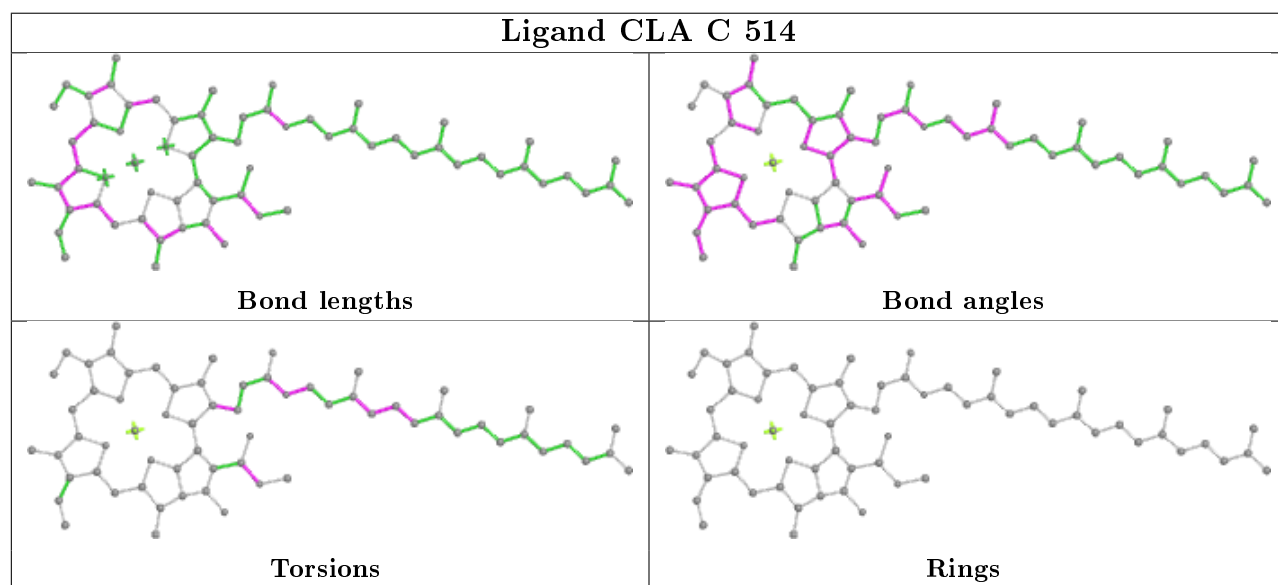
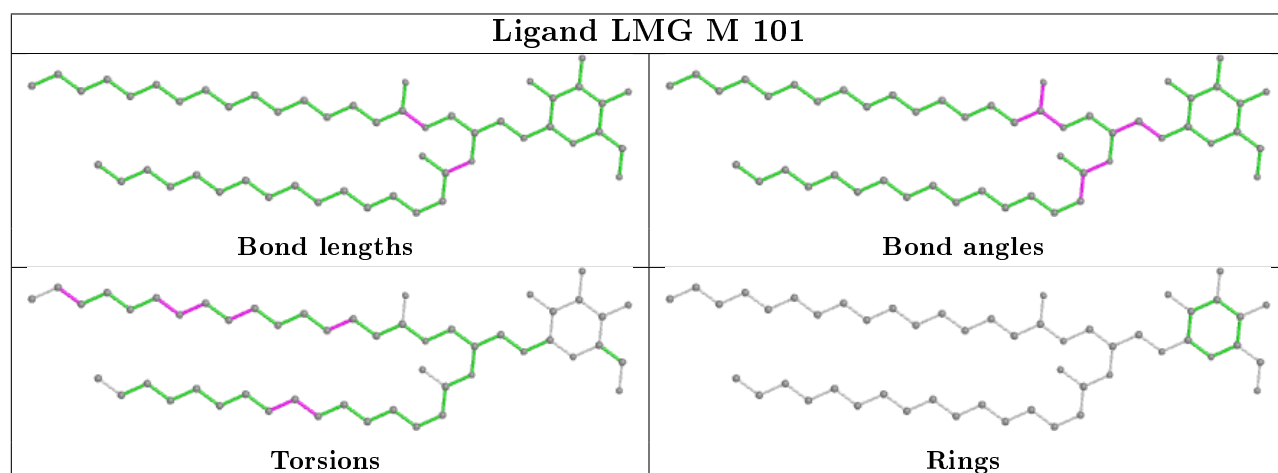
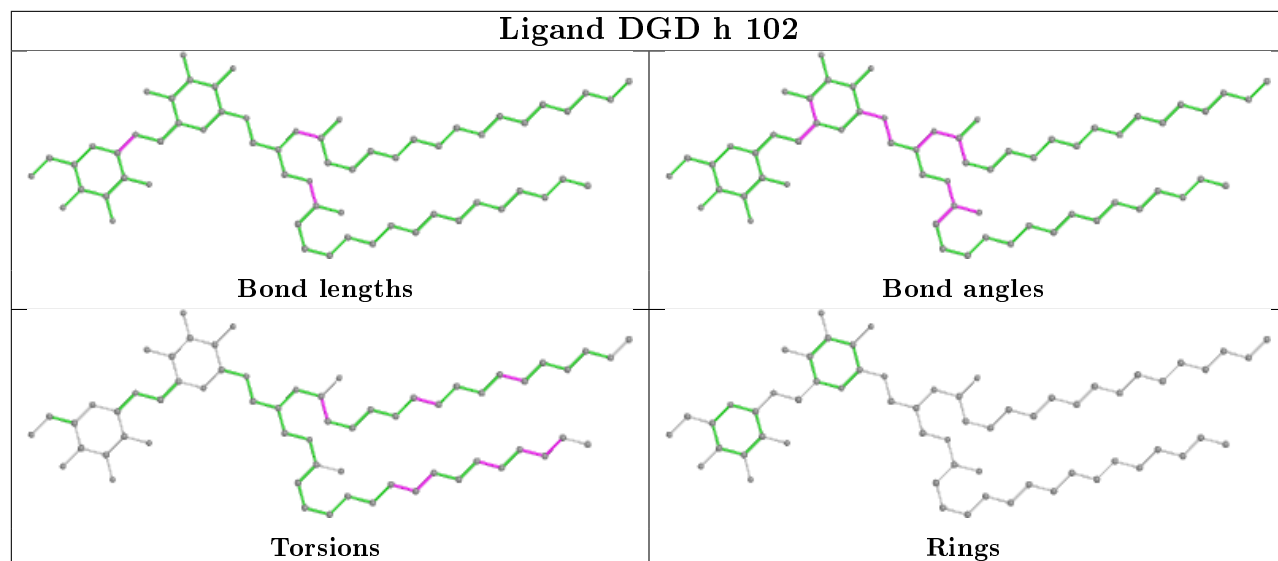
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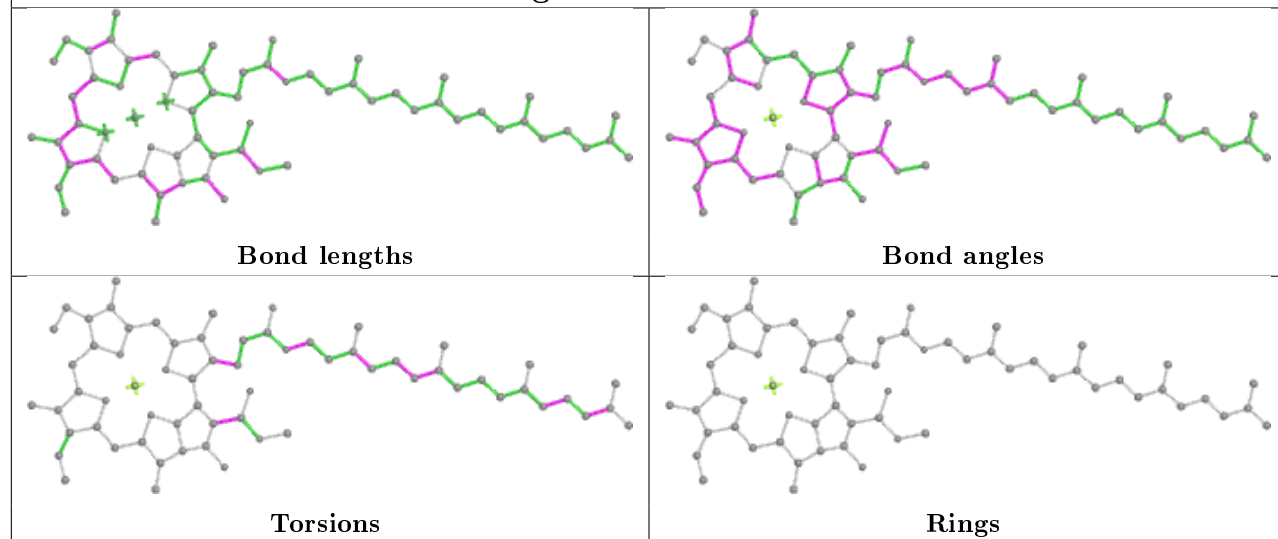
Ligand BCR c 527



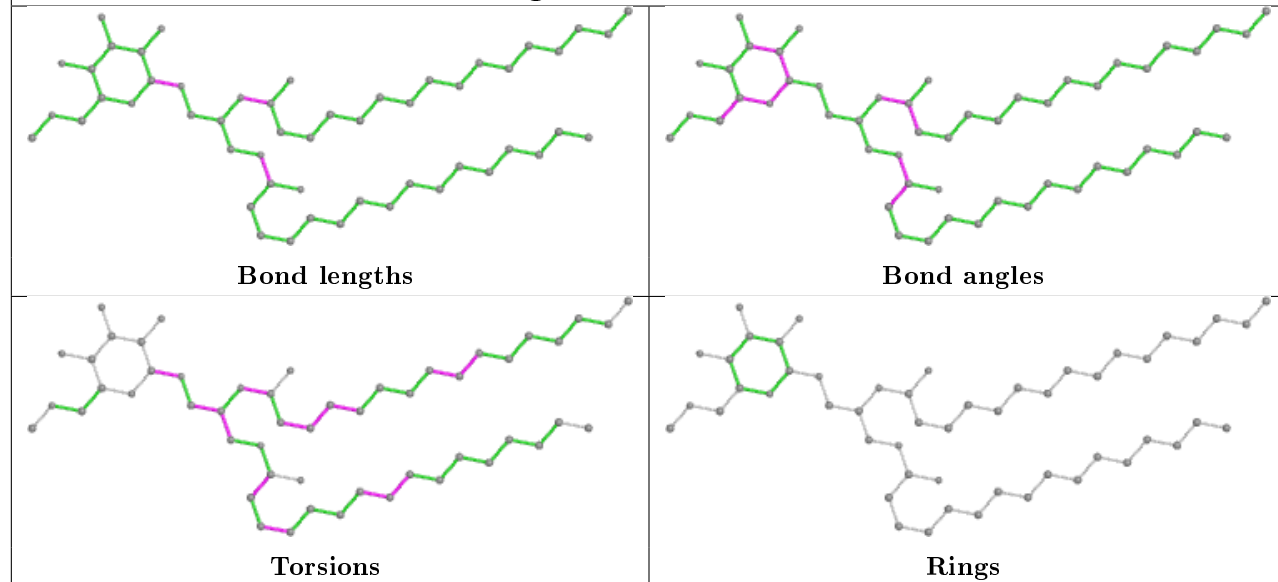




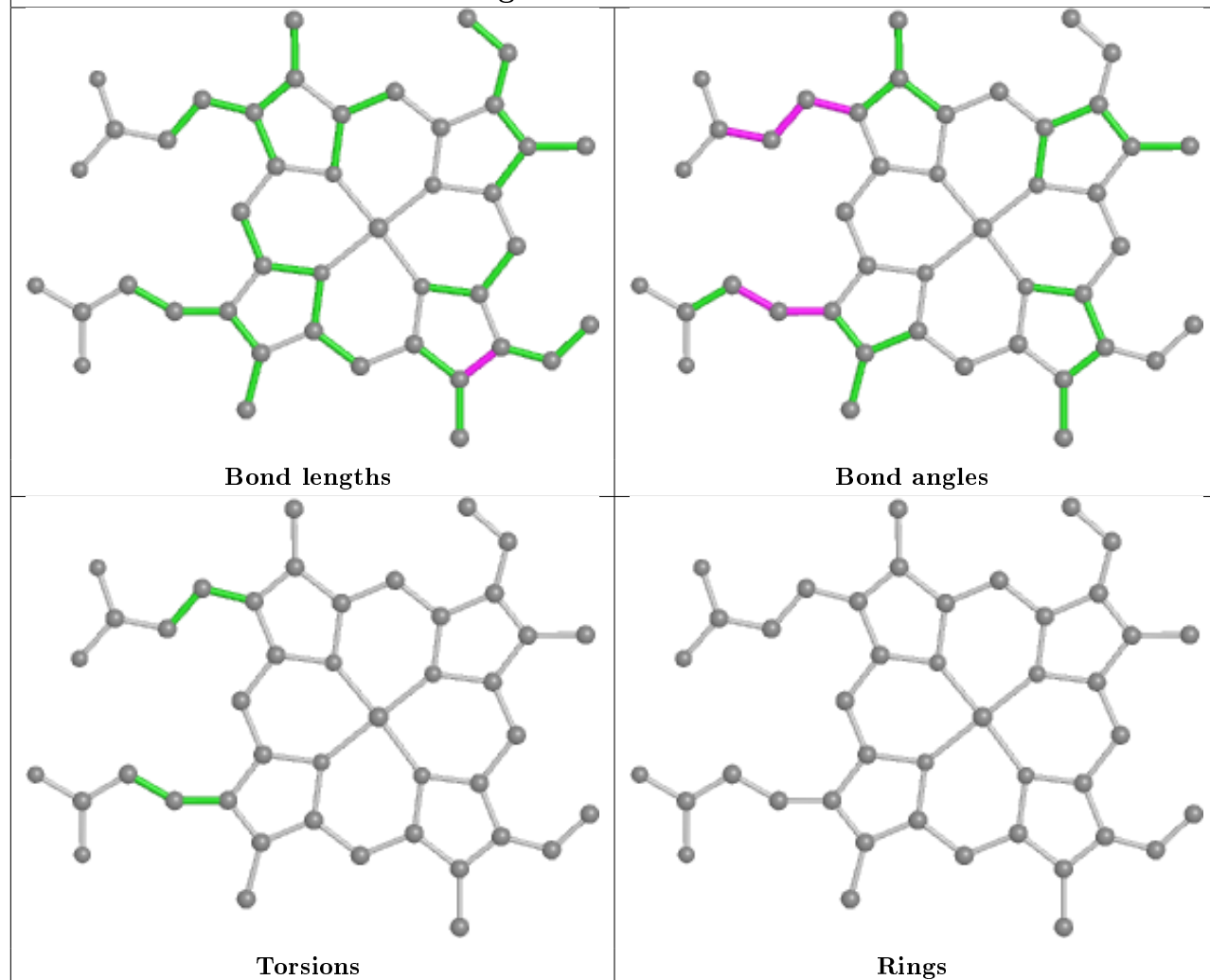
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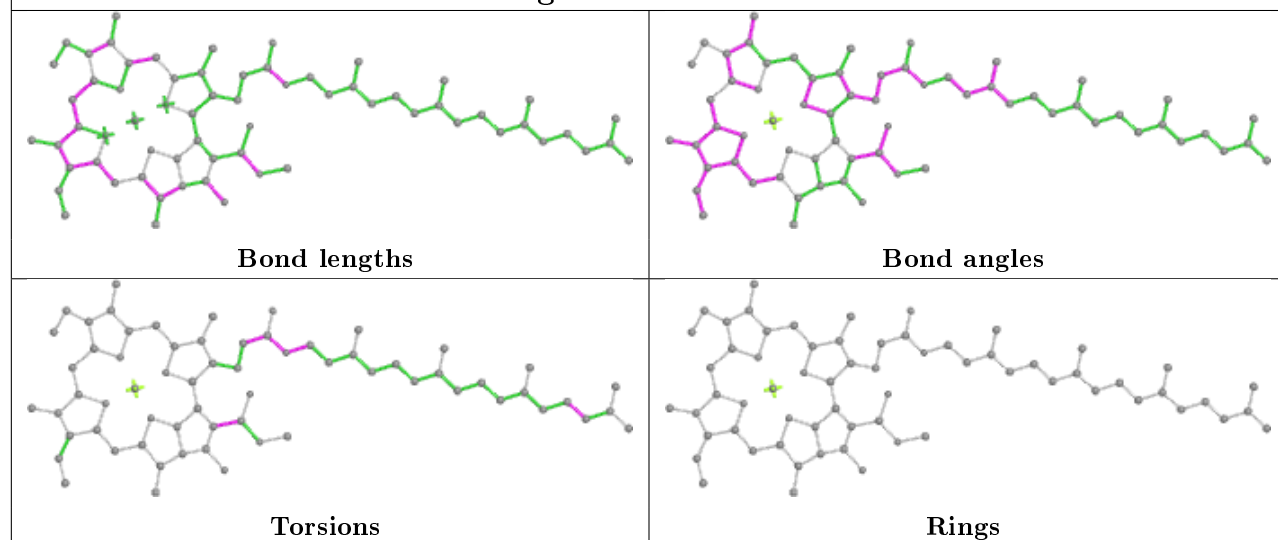
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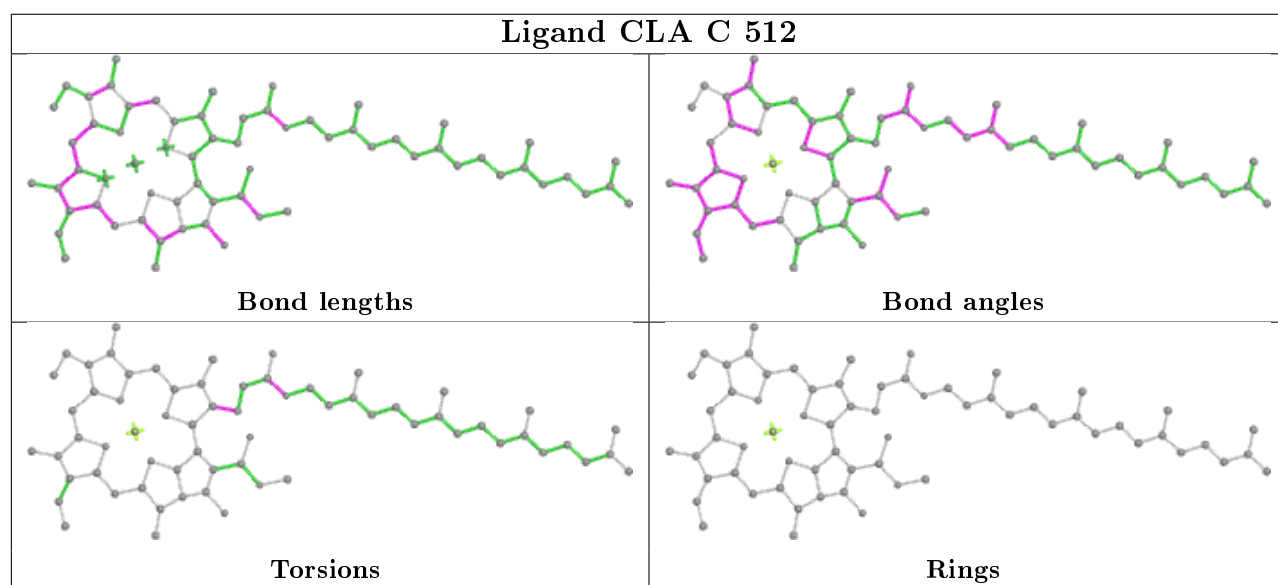
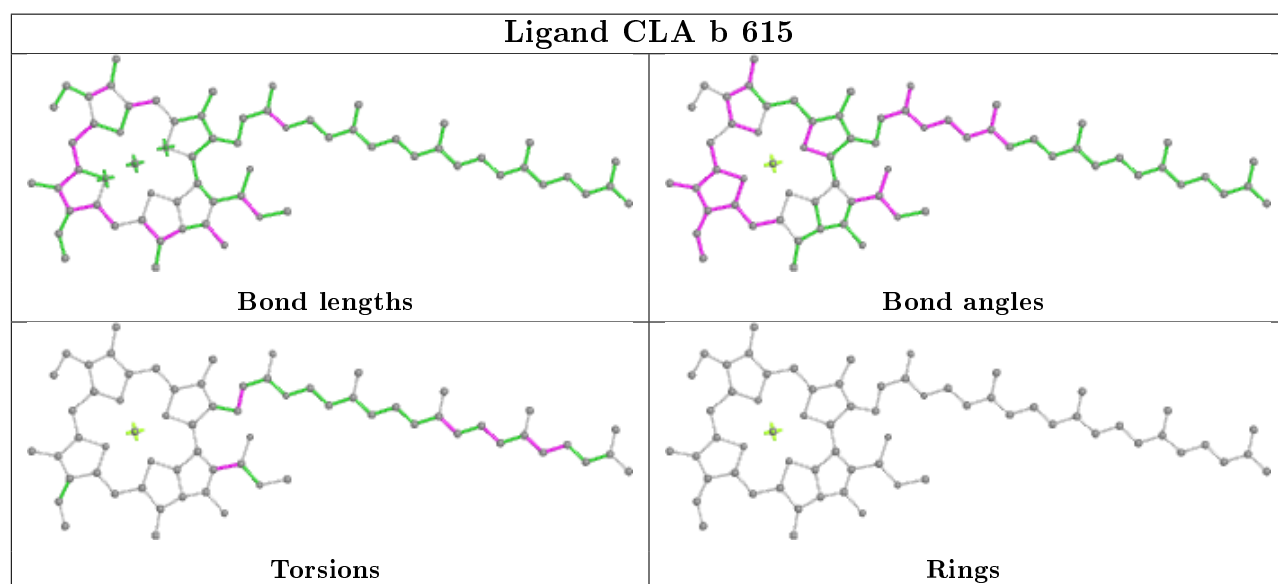
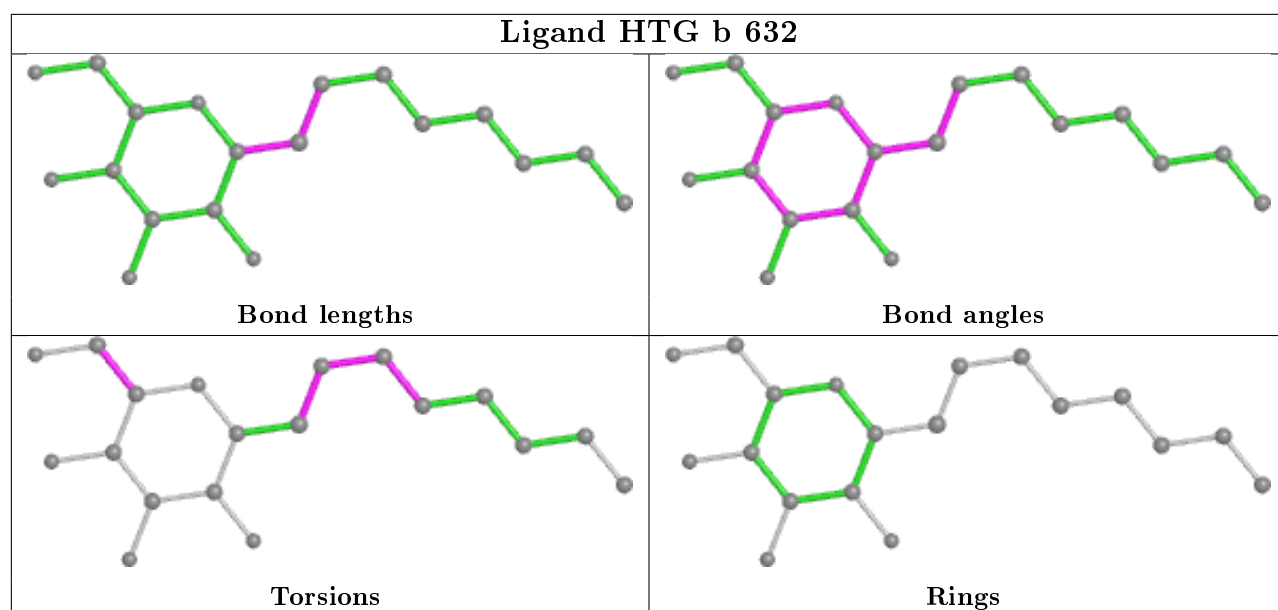


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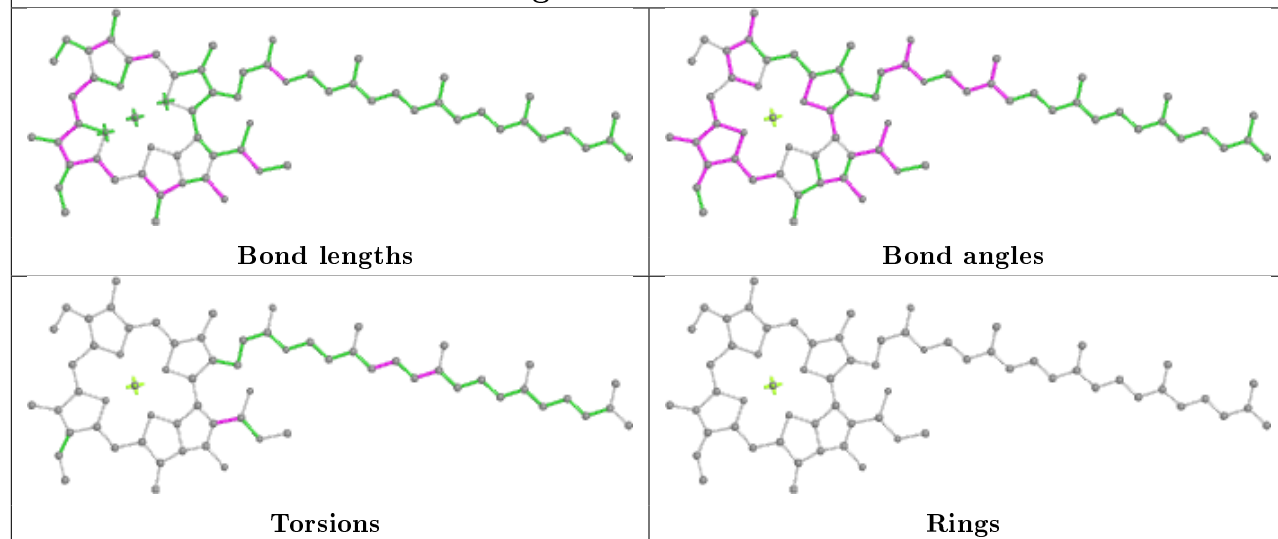


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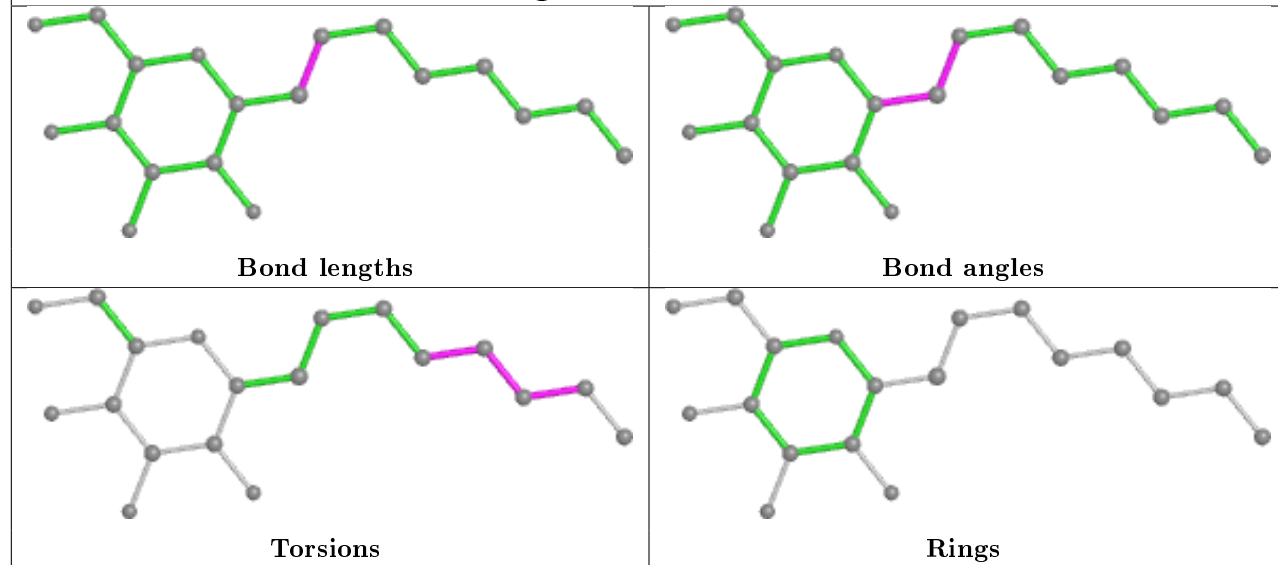




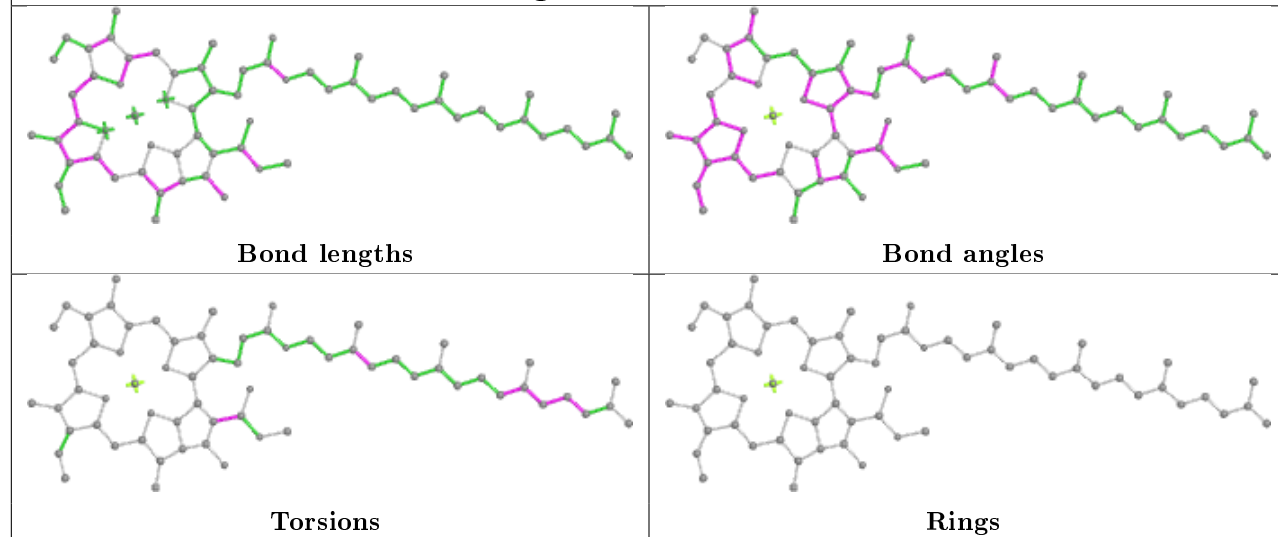
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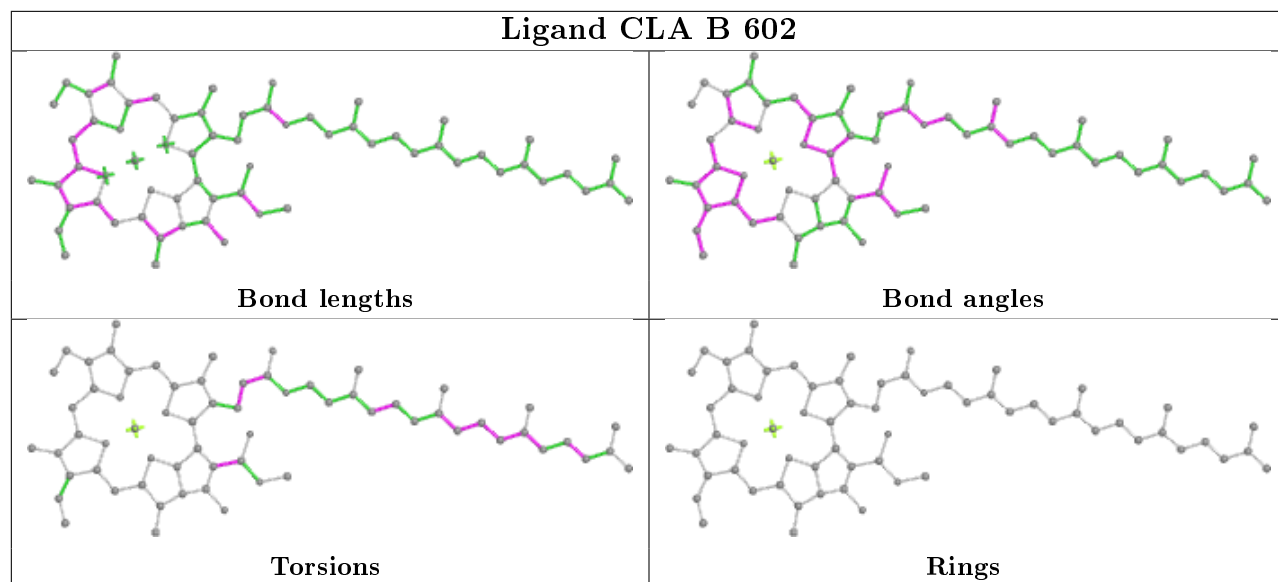
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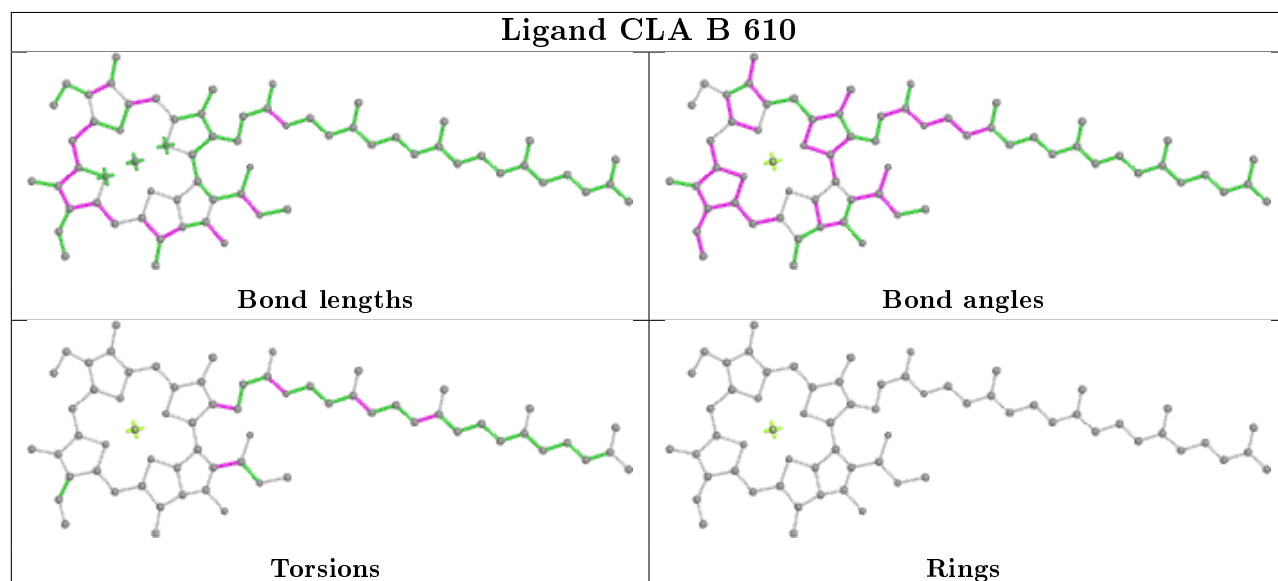
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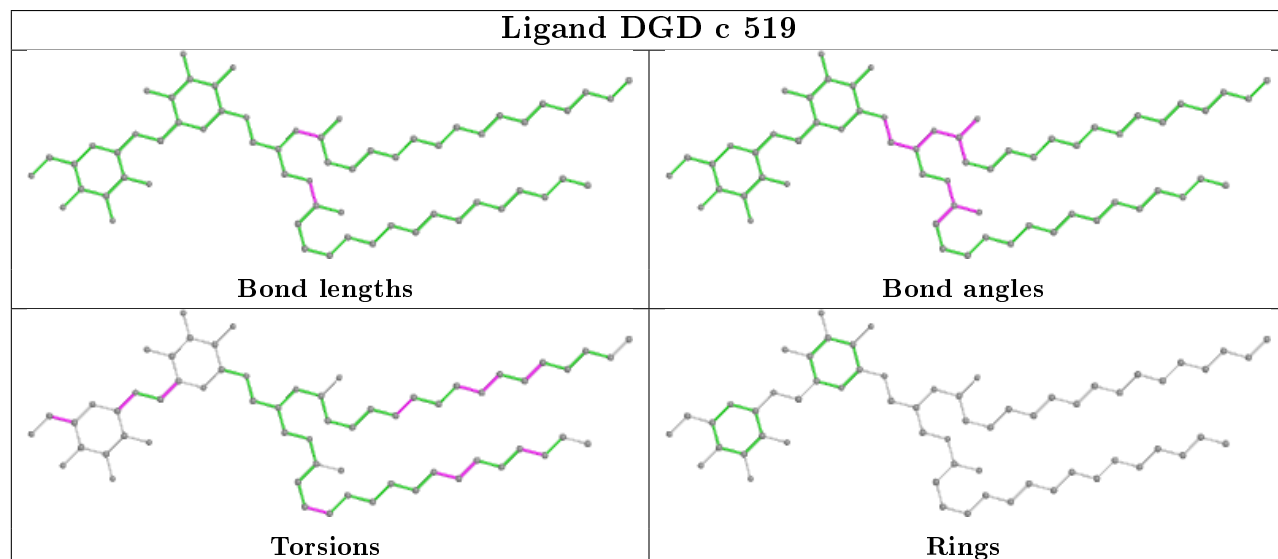
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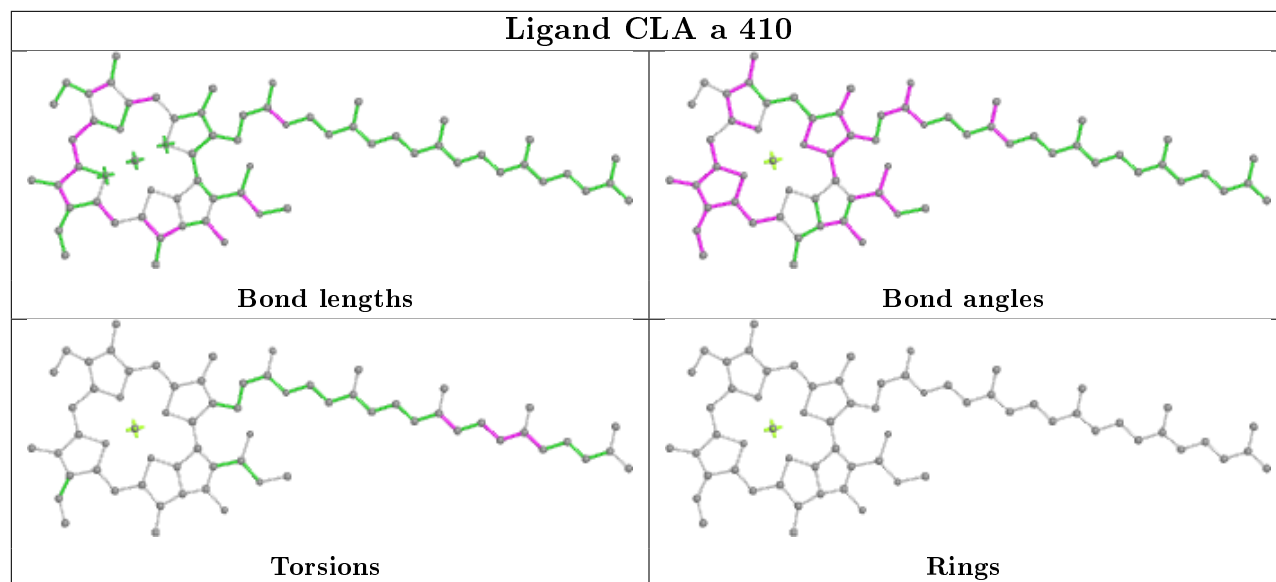
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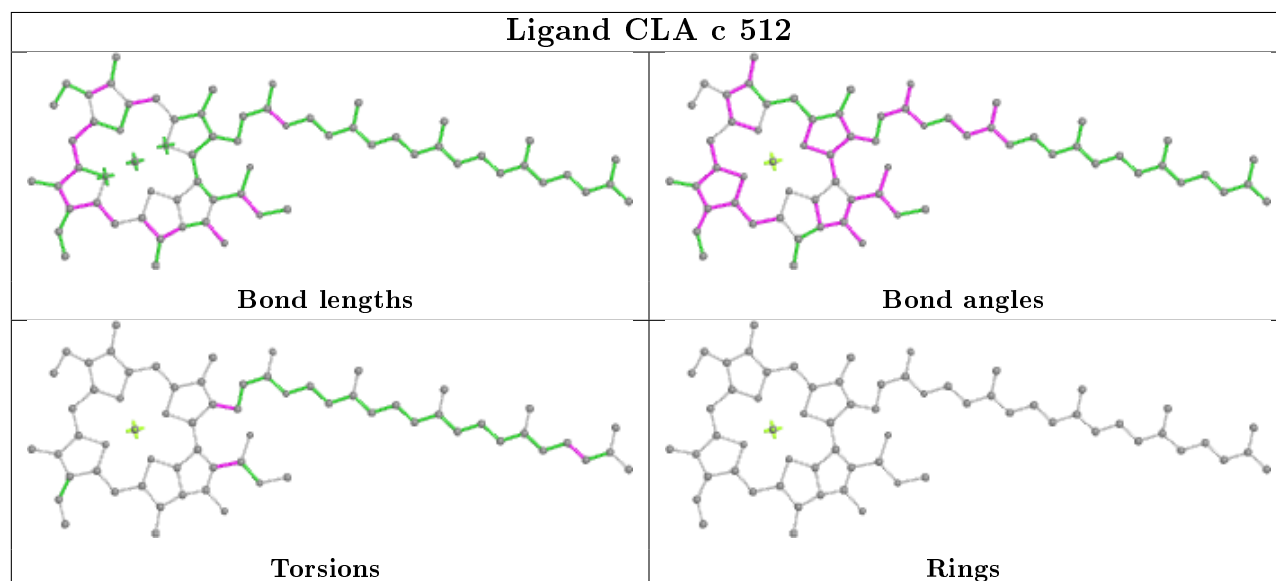
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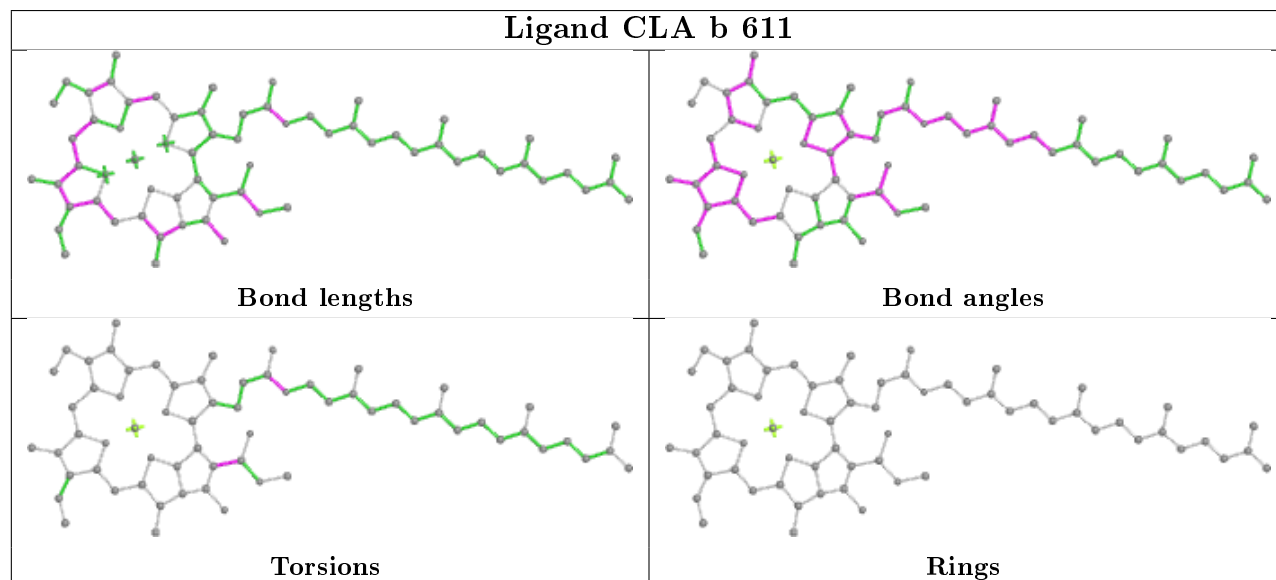
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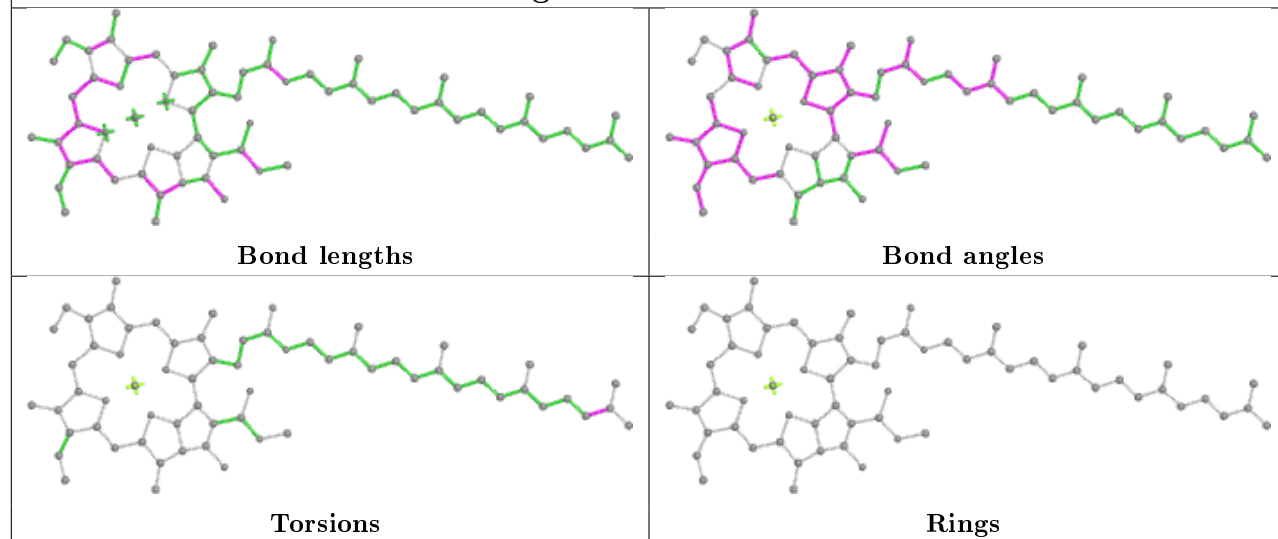
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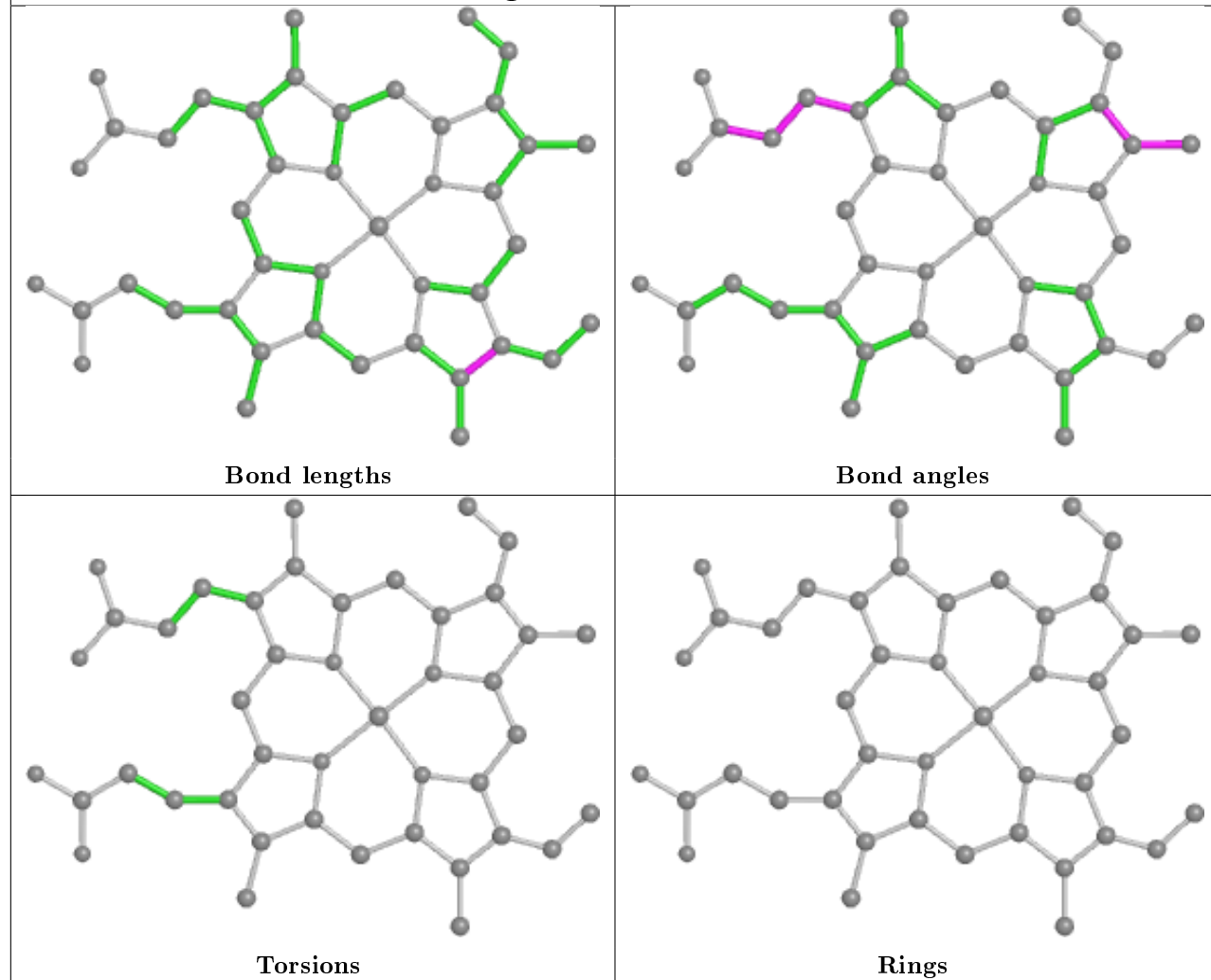
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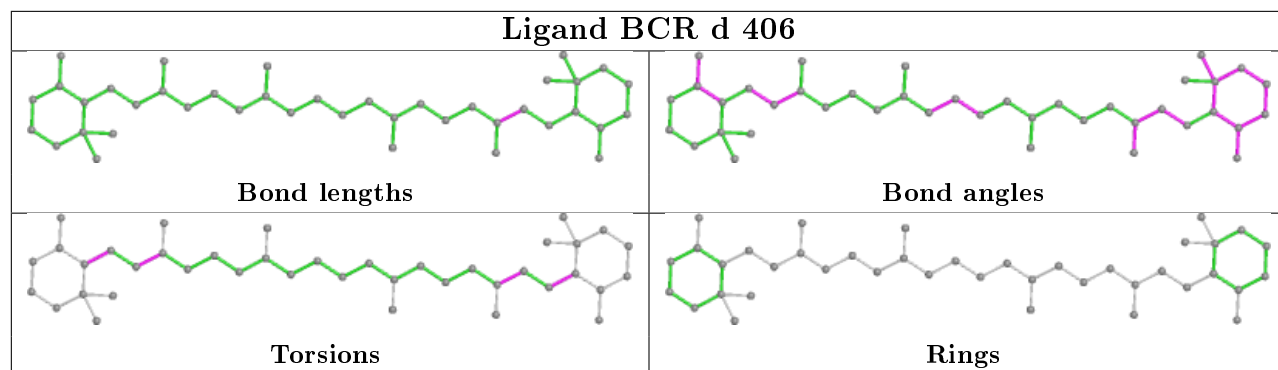
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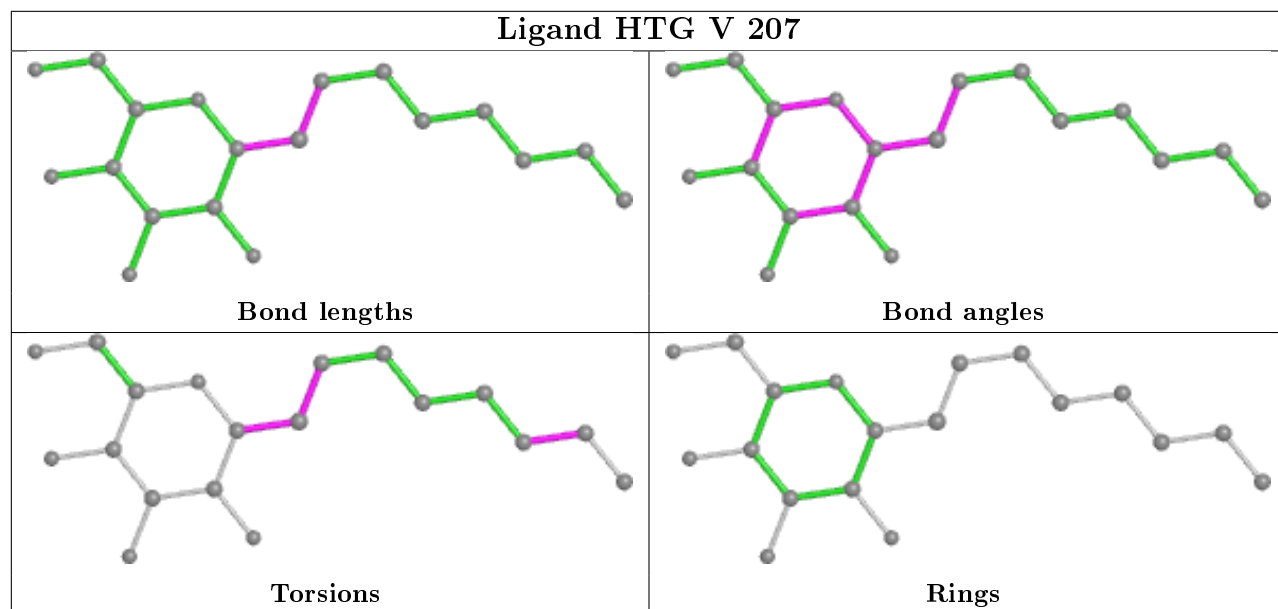
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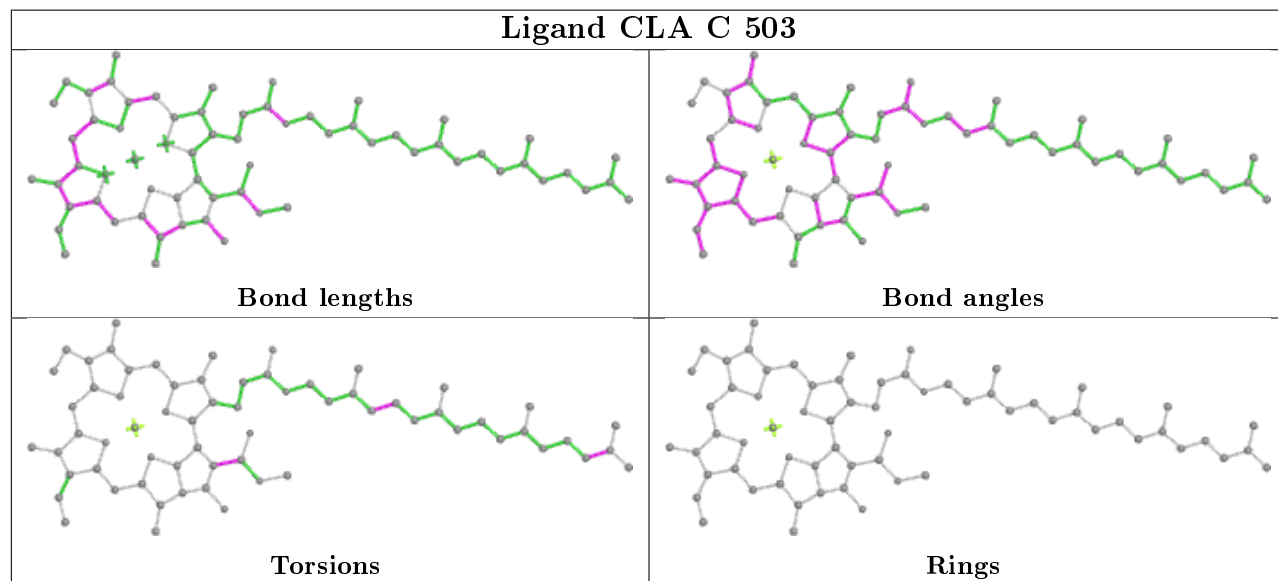
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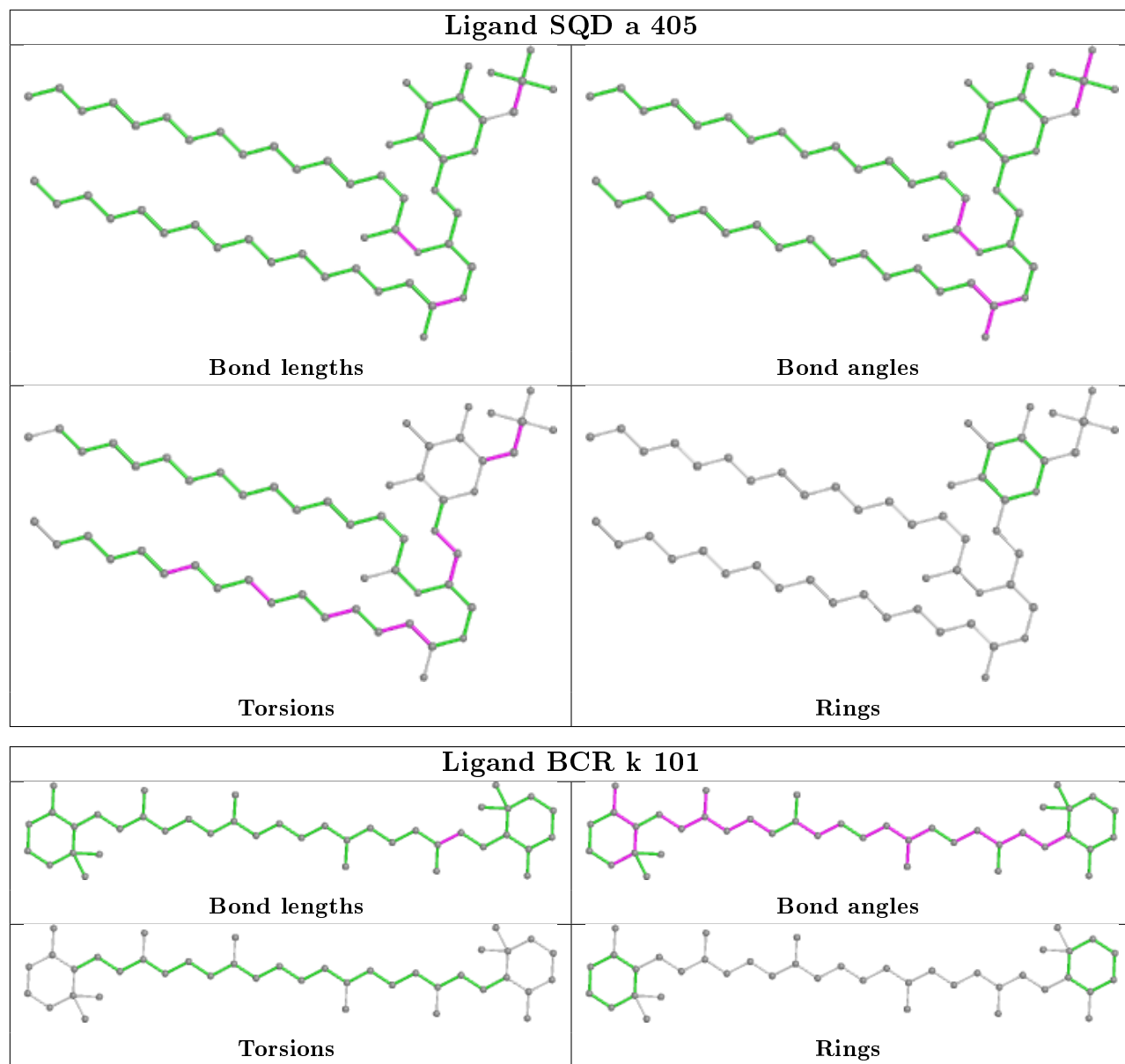


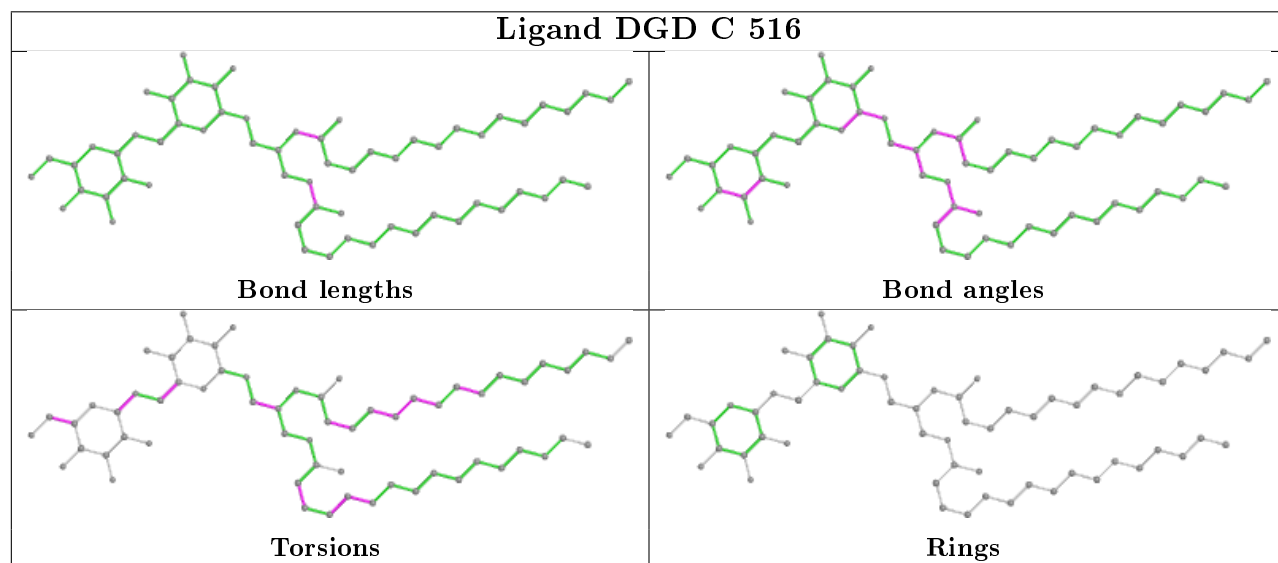
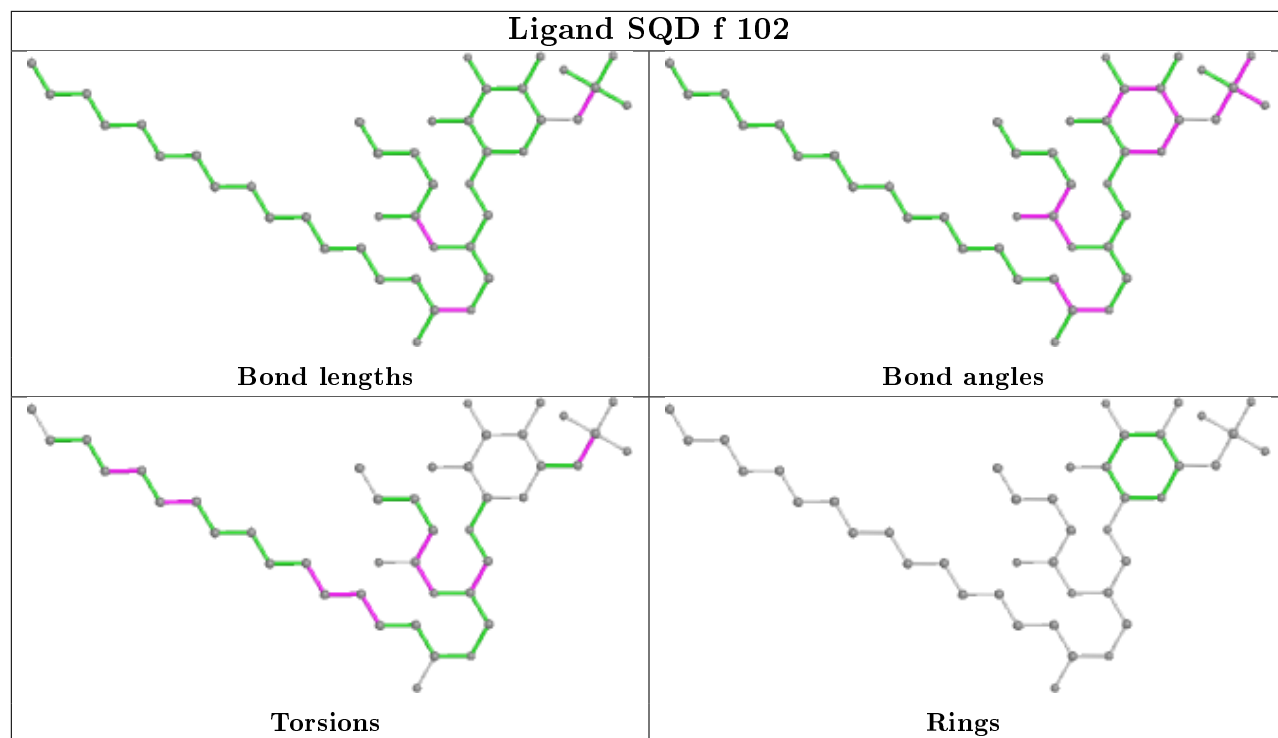
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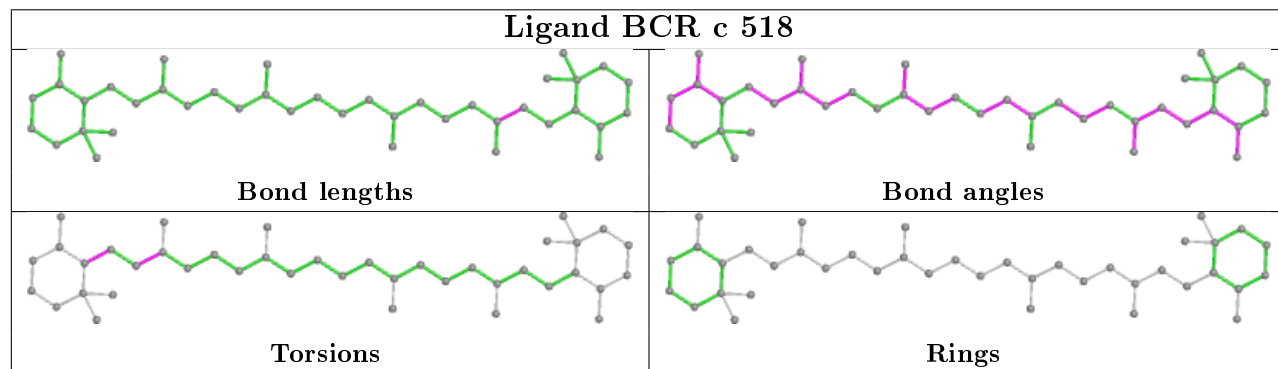
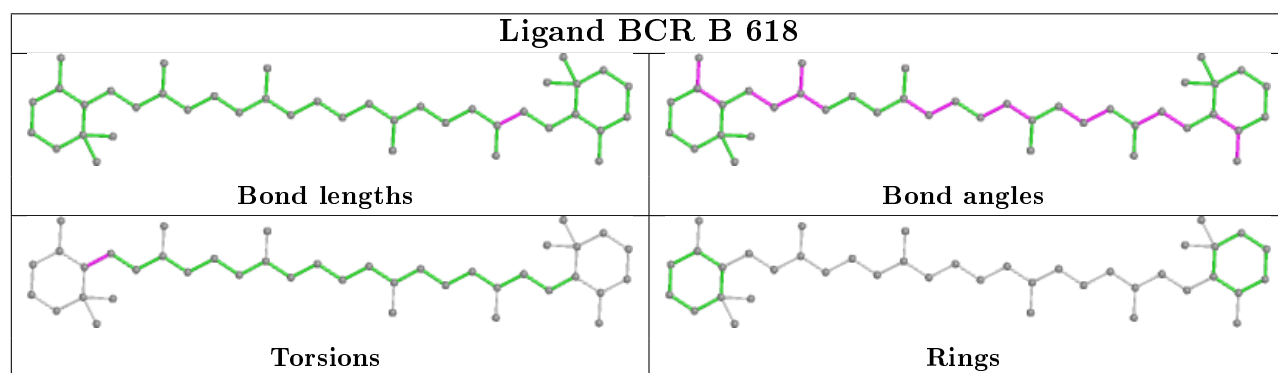
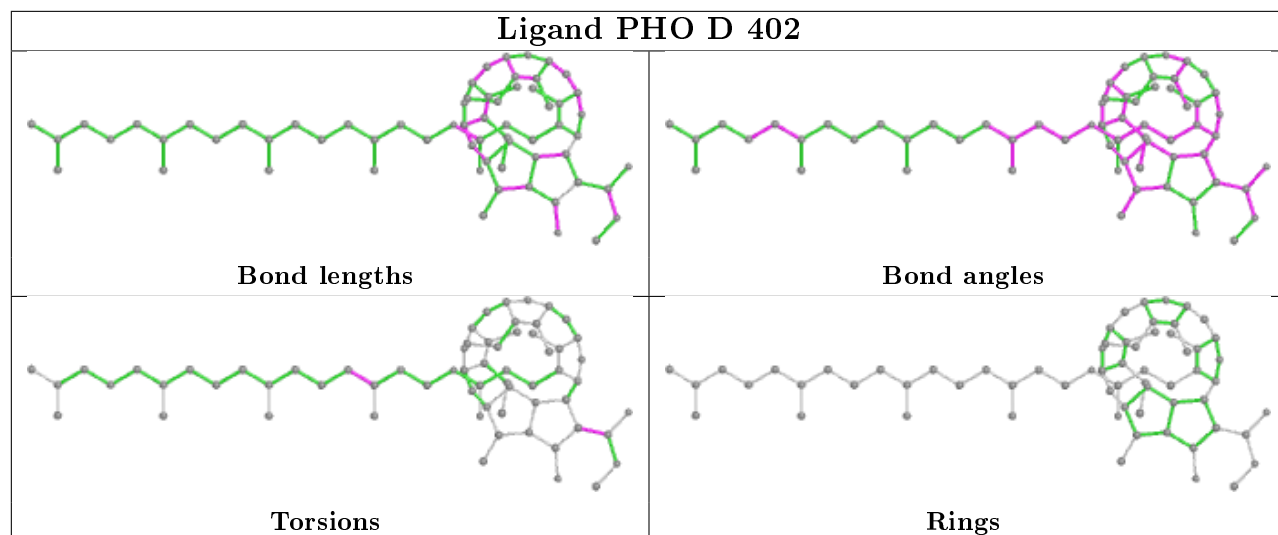


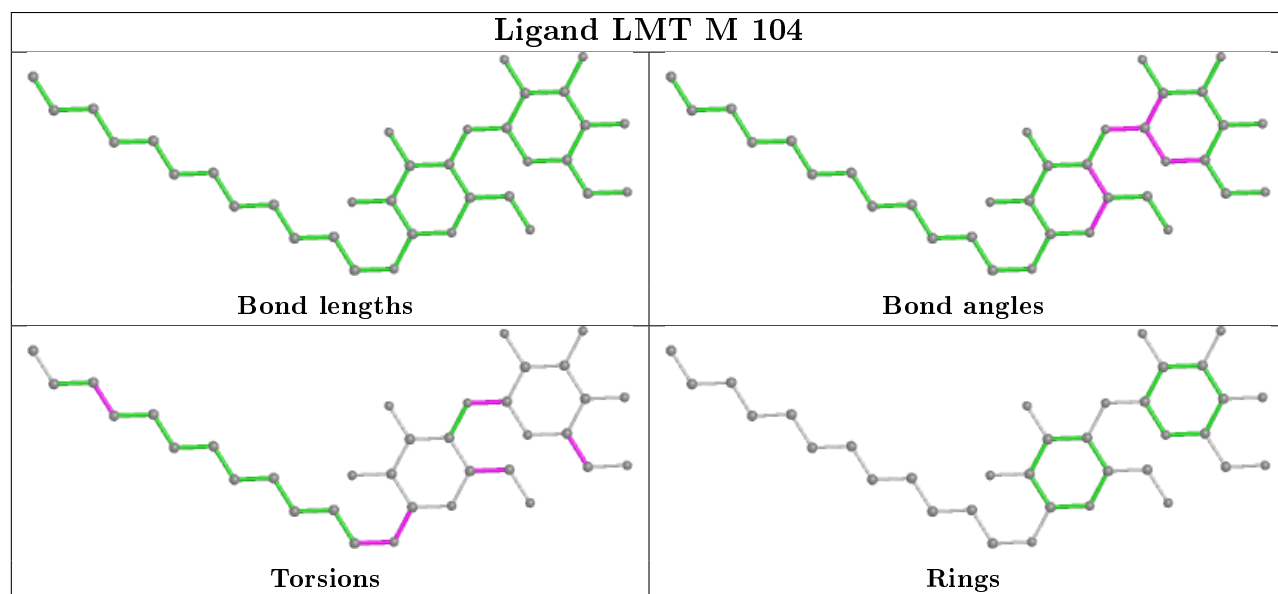
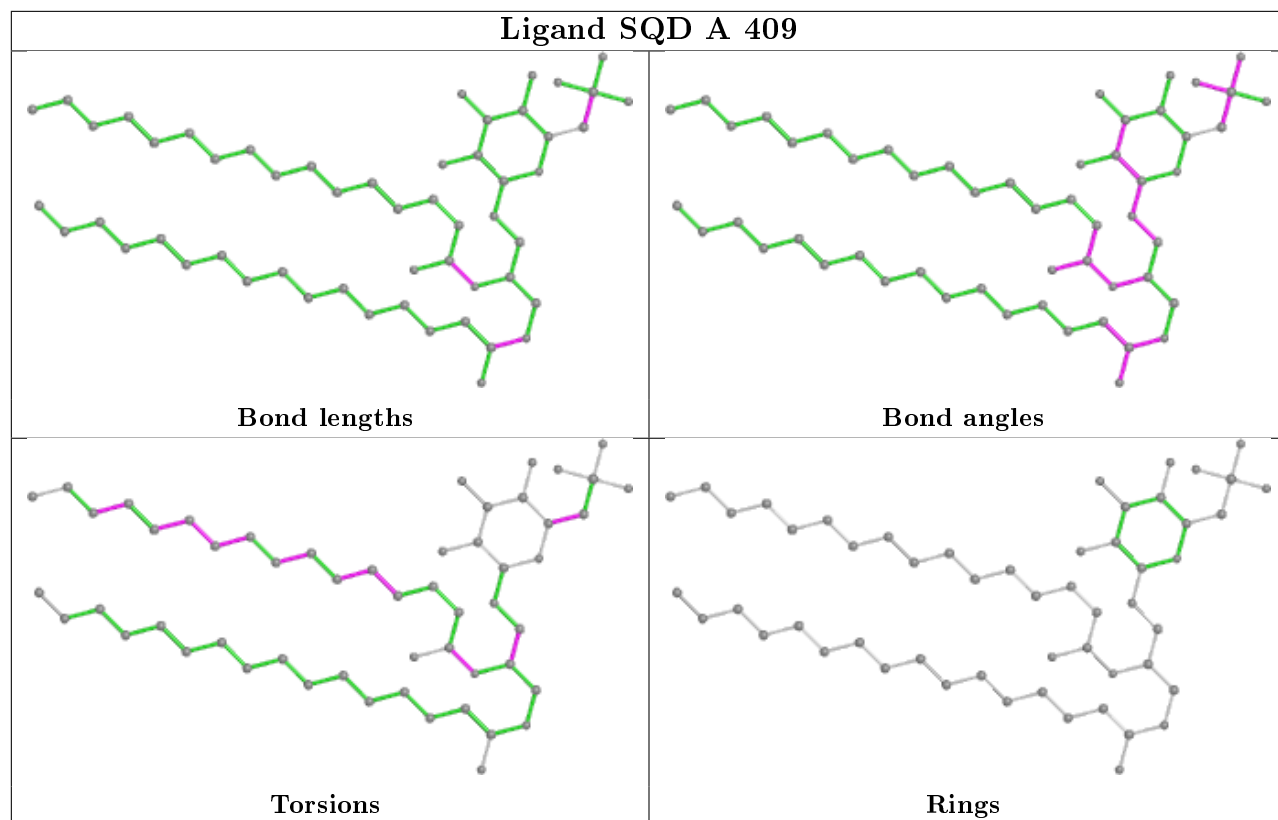
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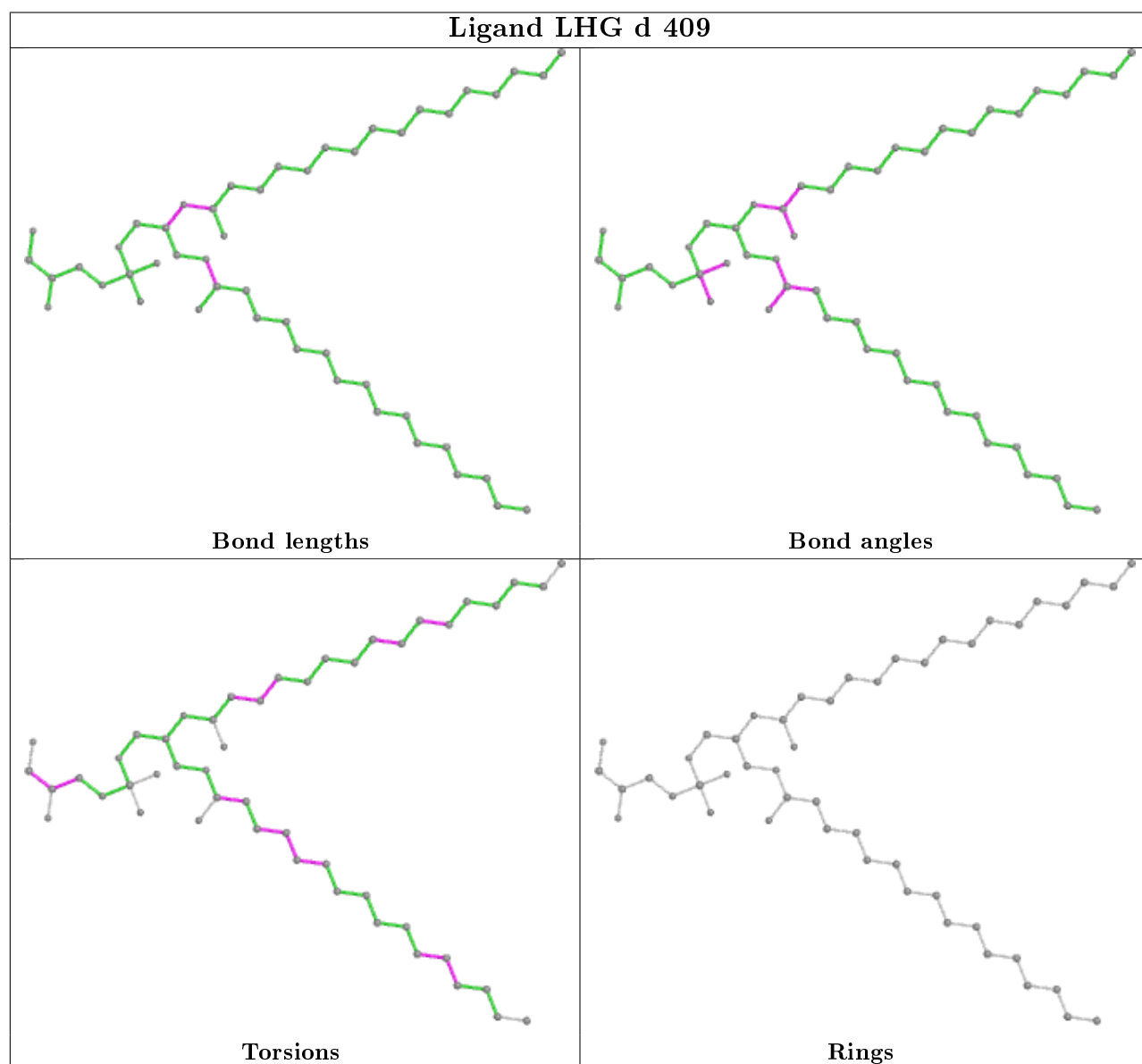
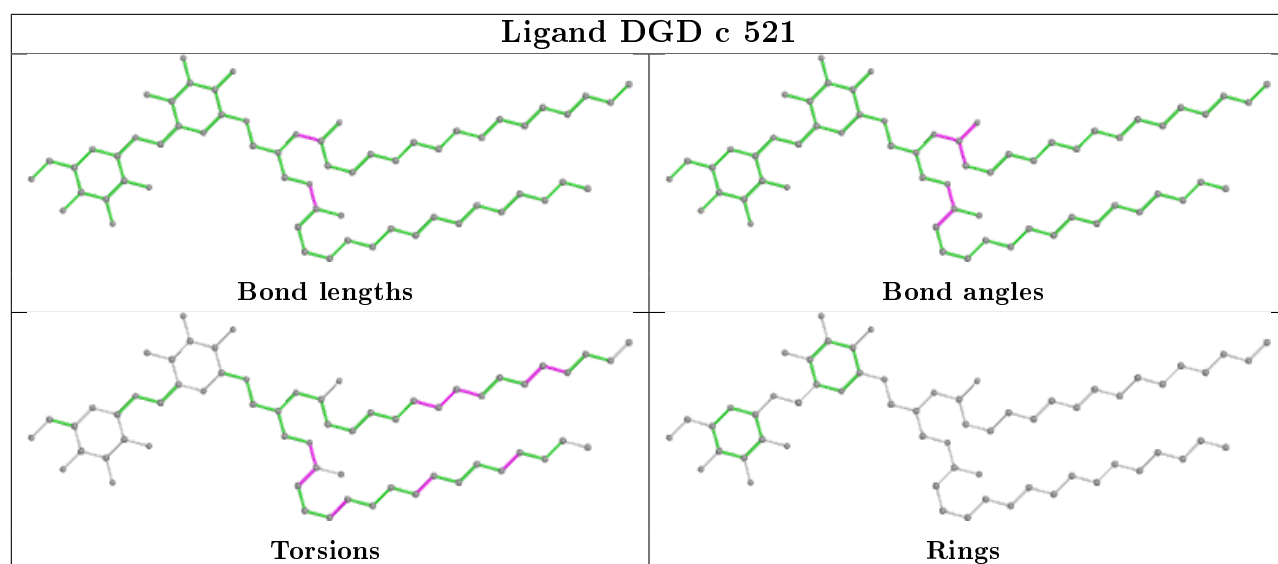


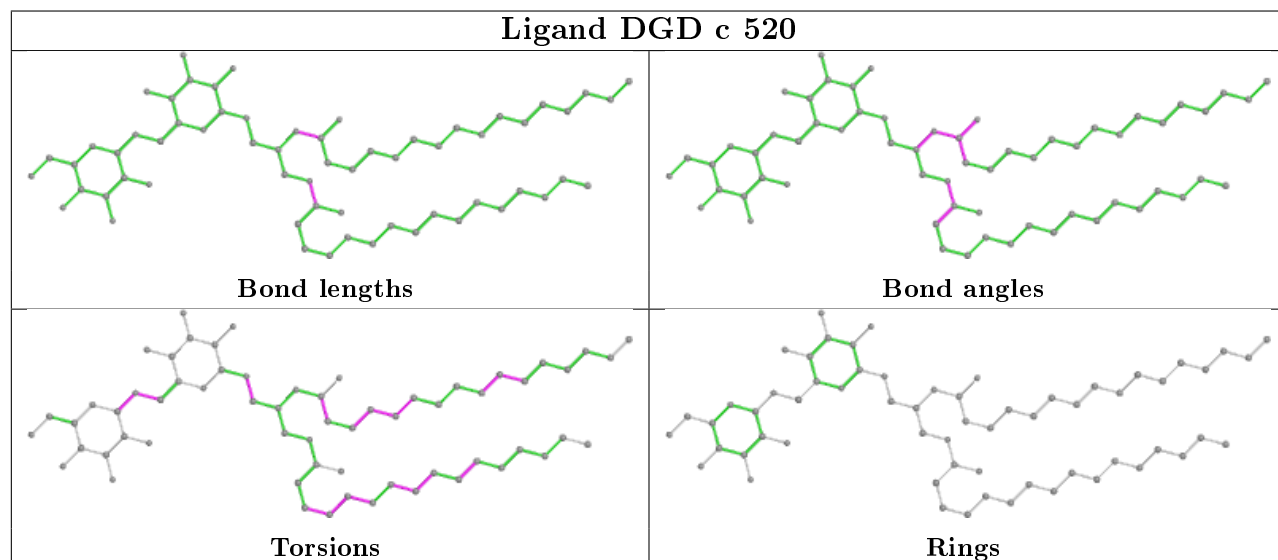
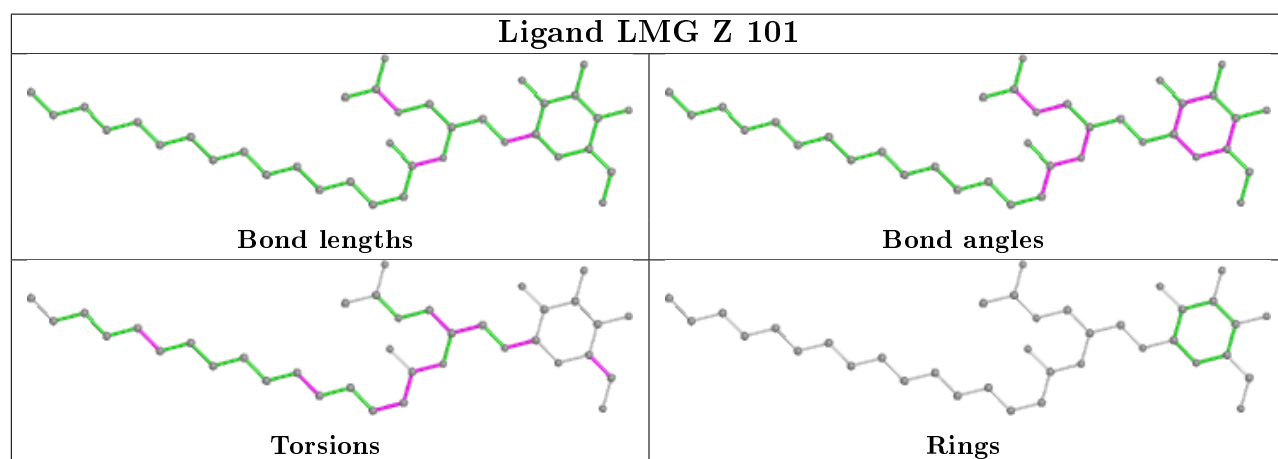
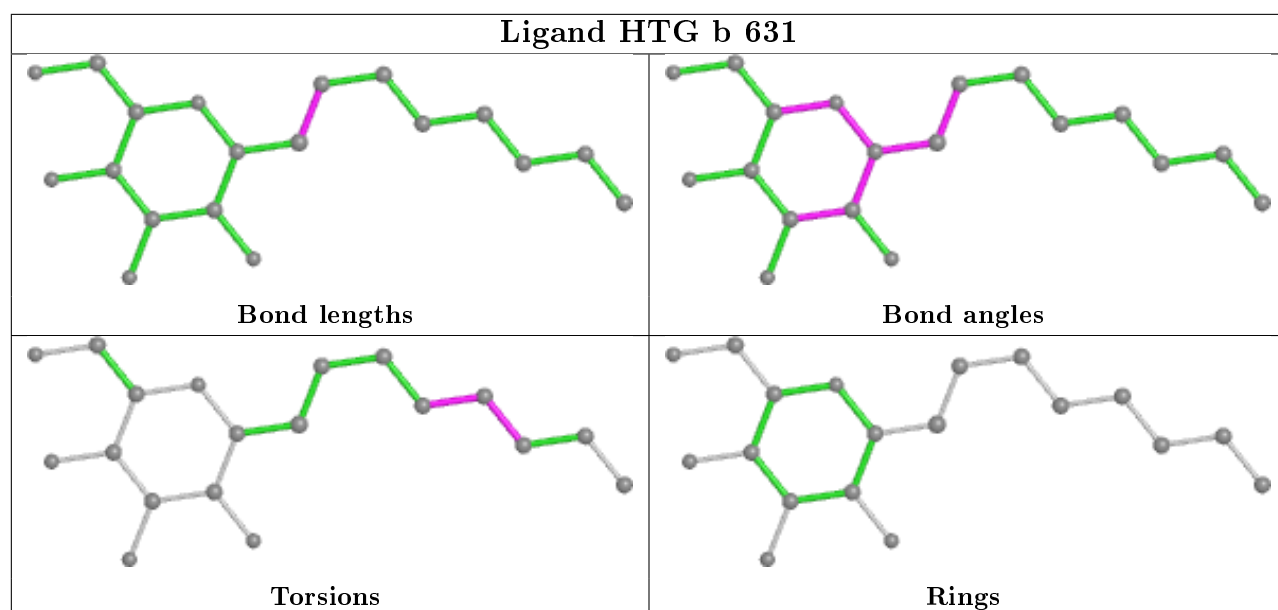




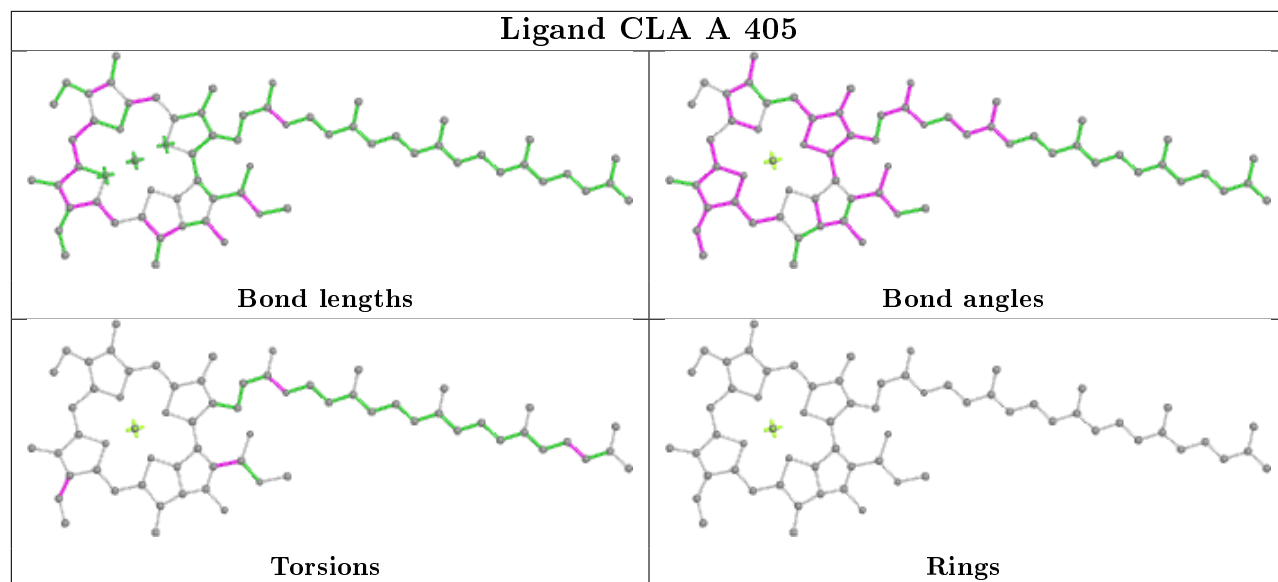




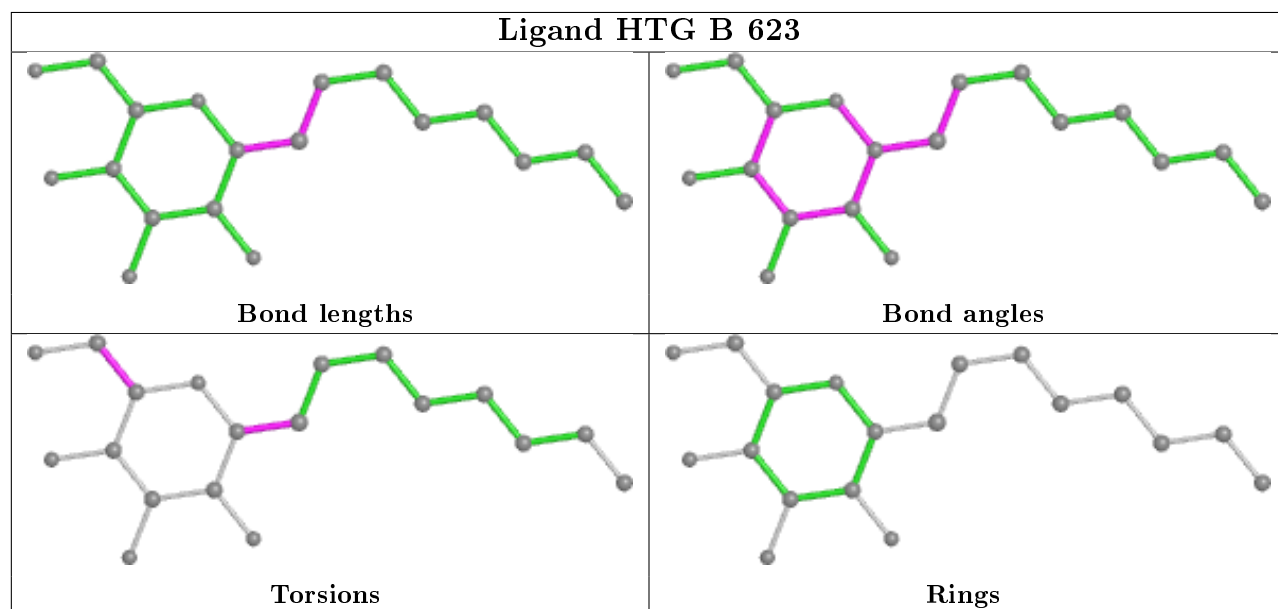




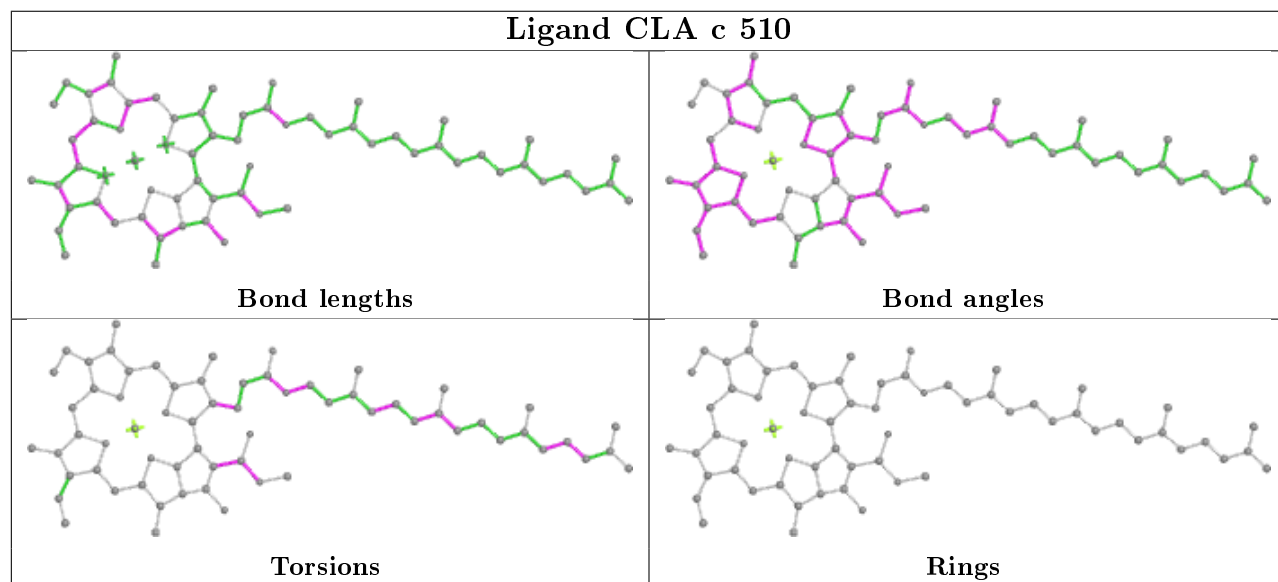
Ligand CLA A 405

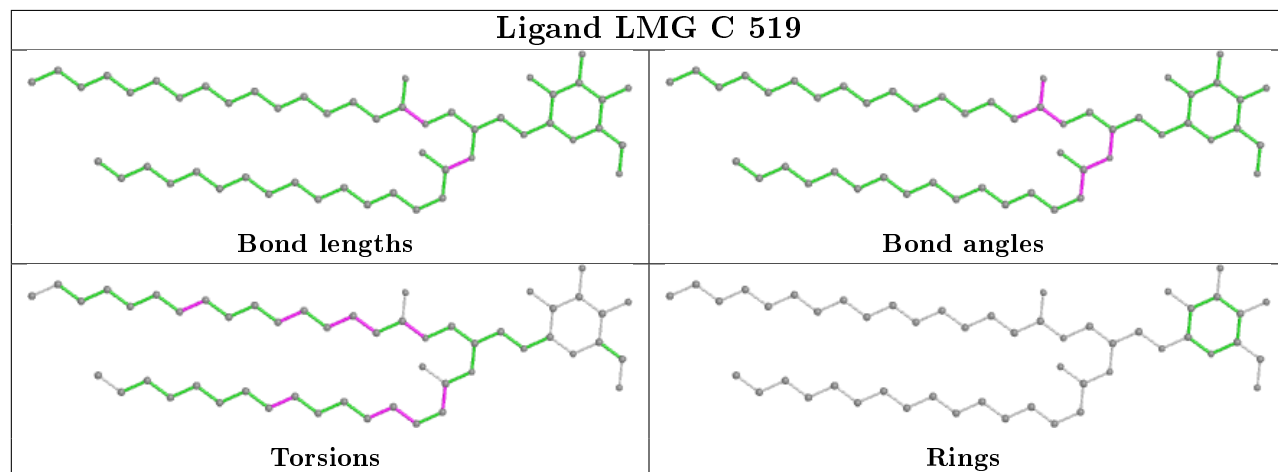
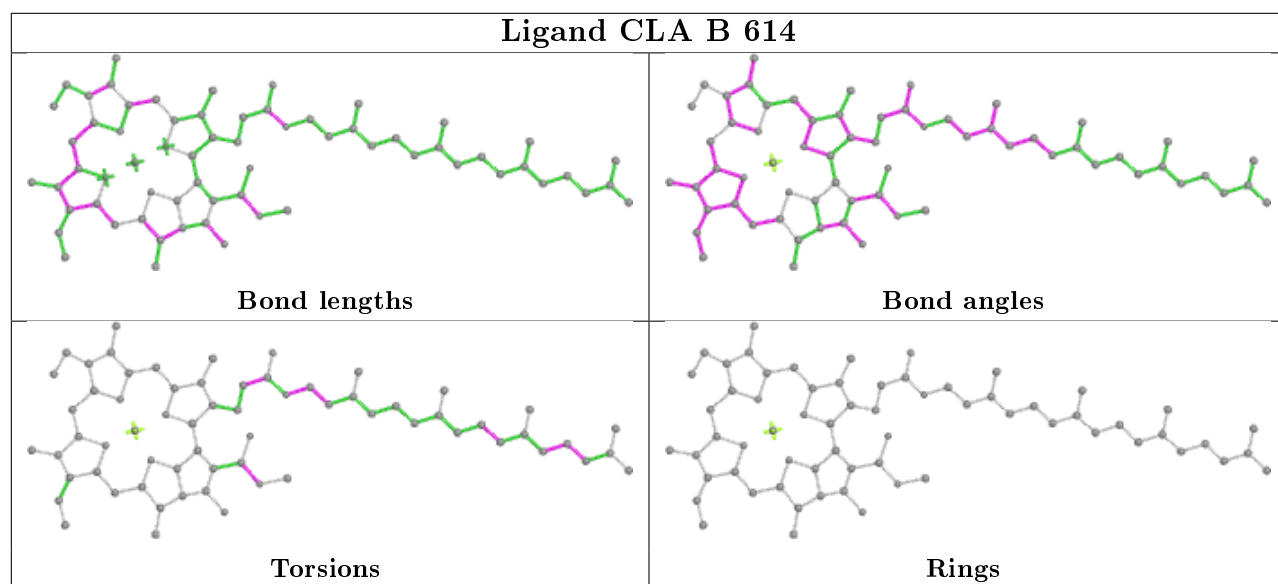
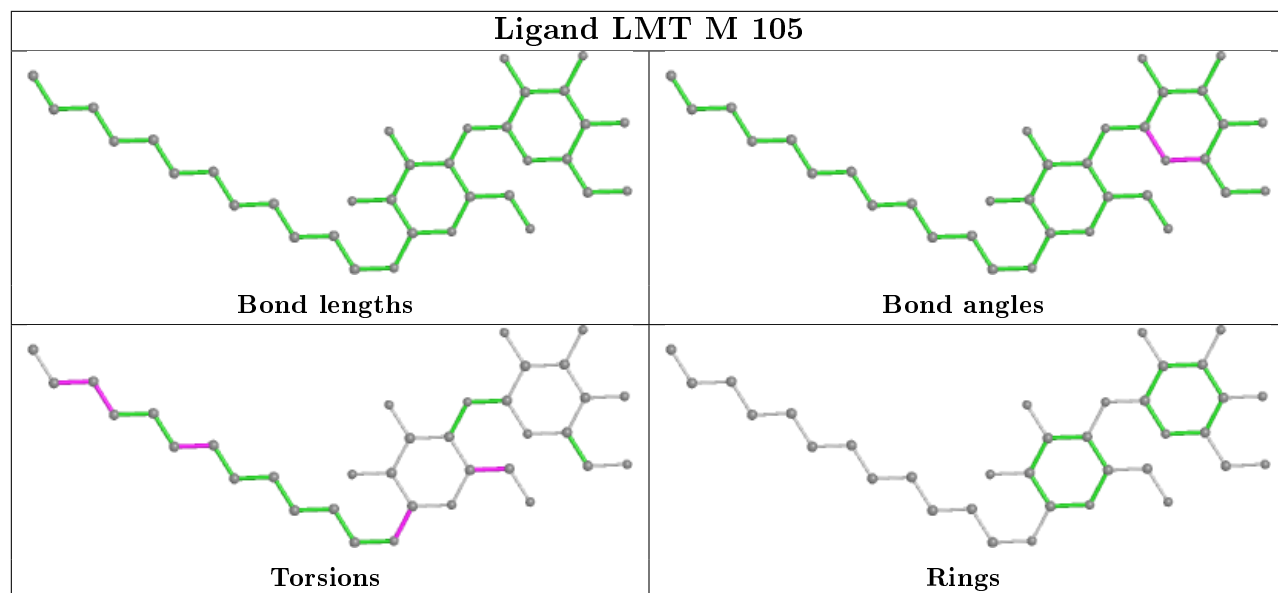


Ligand HTG B 623

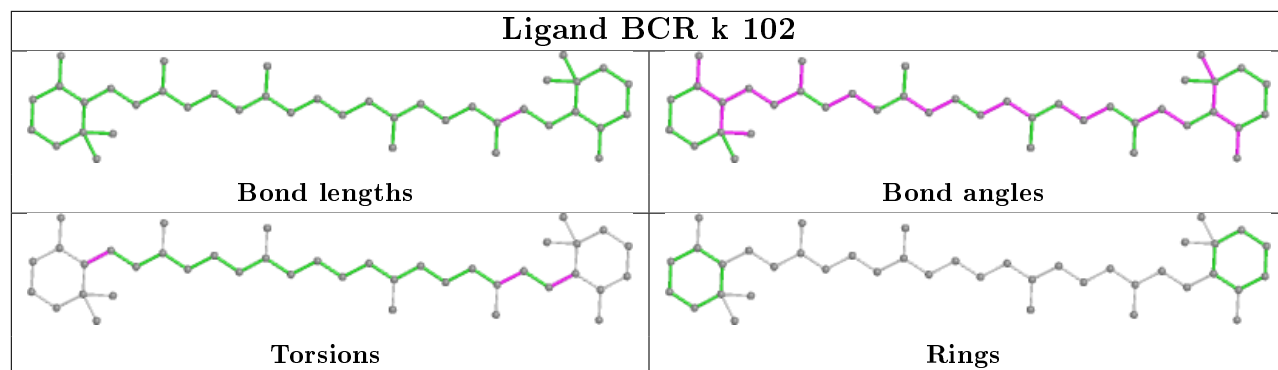


Ligand CLA c 510

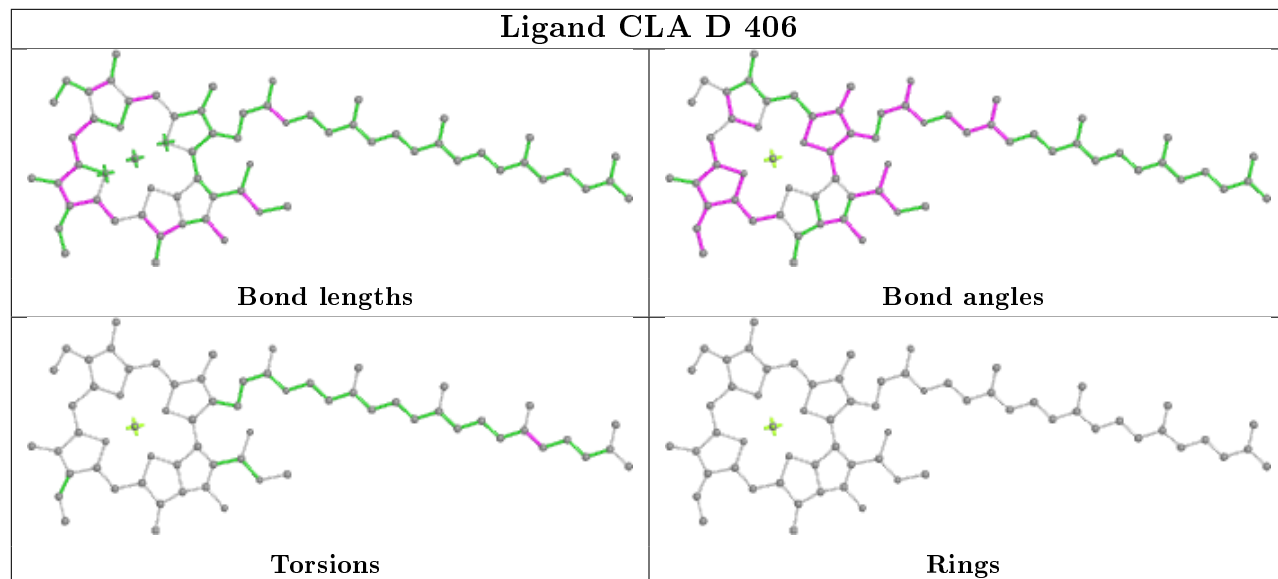




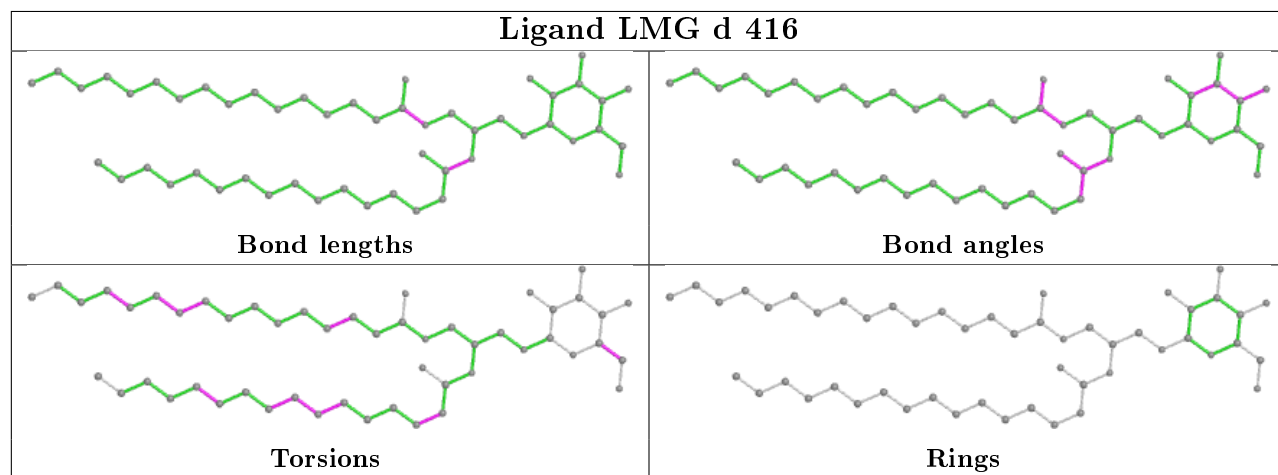
Ligand BCR k 102



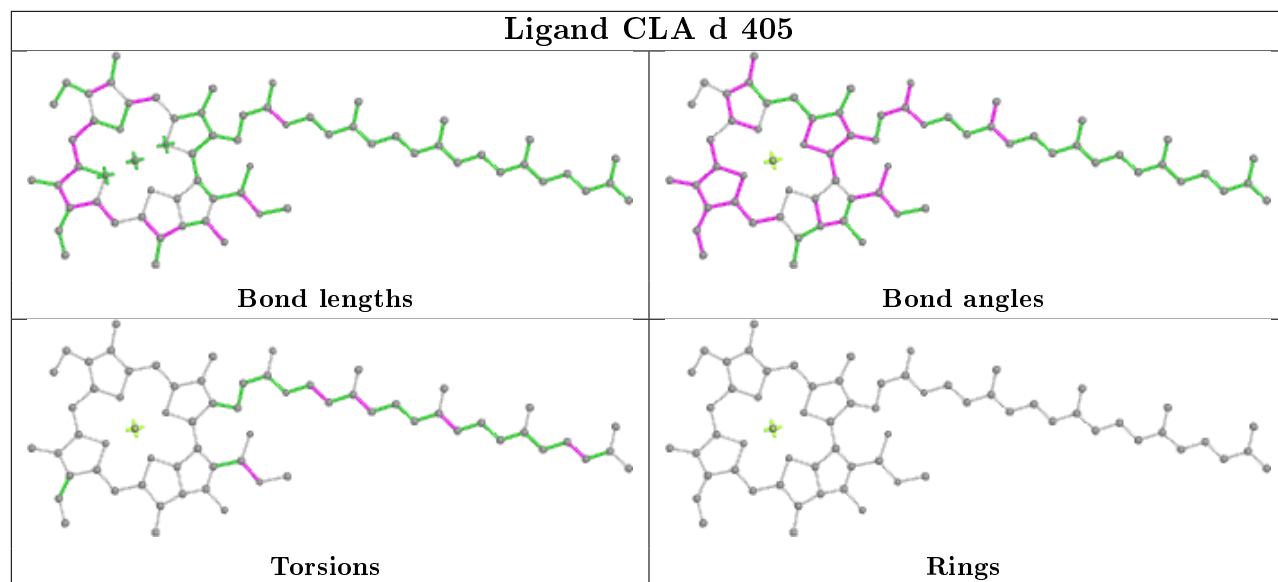
Ligand CLA D 406



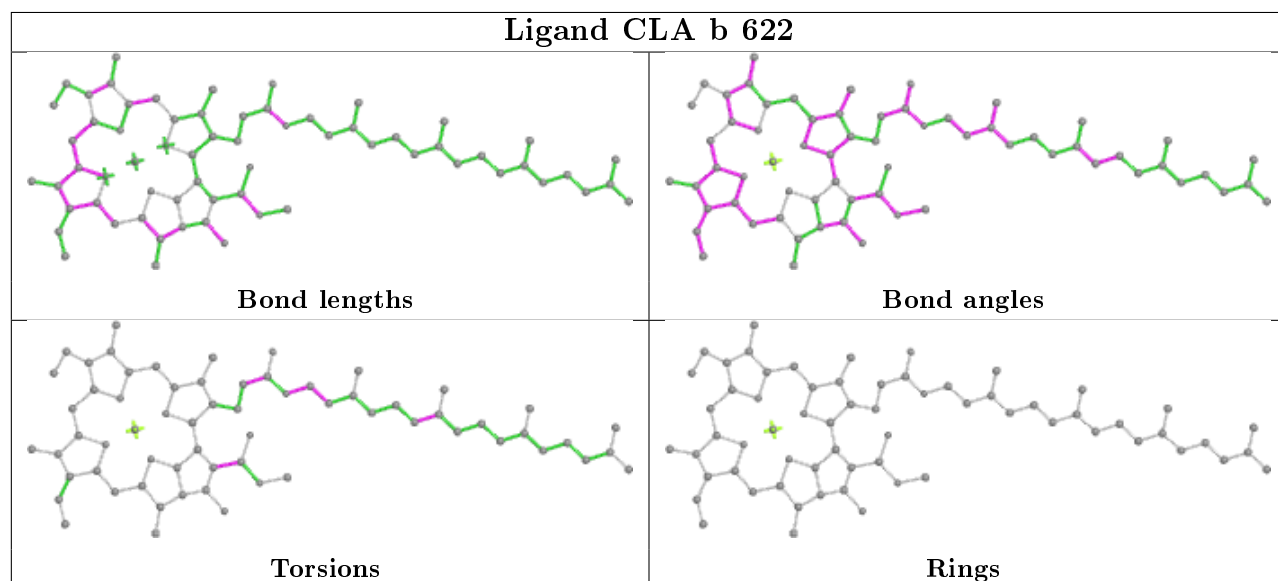
Ligand LMG d 416



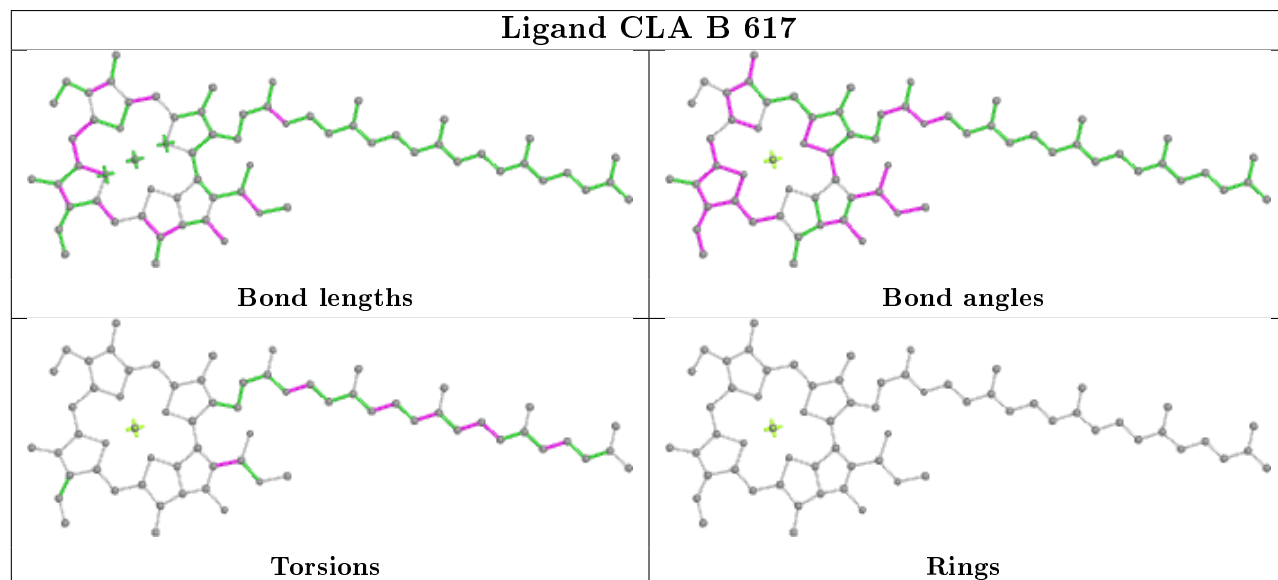
Ligand CLA d 405

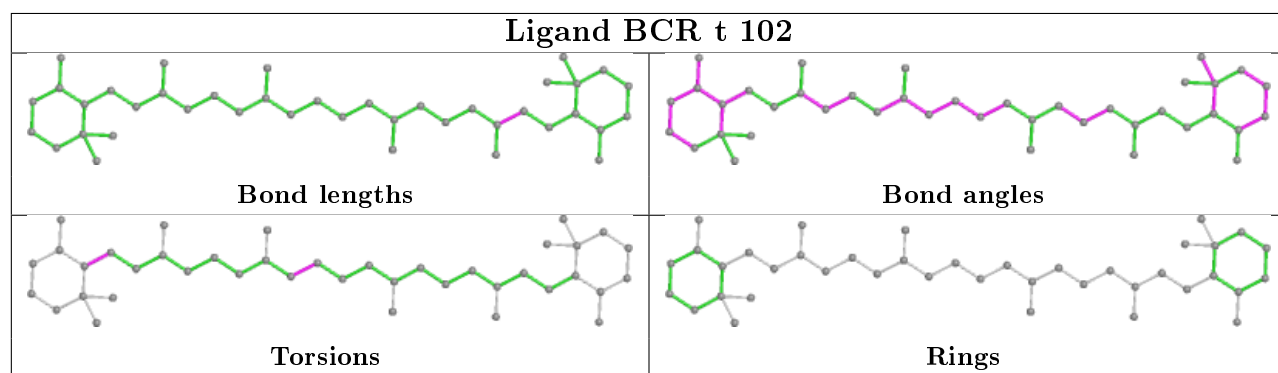
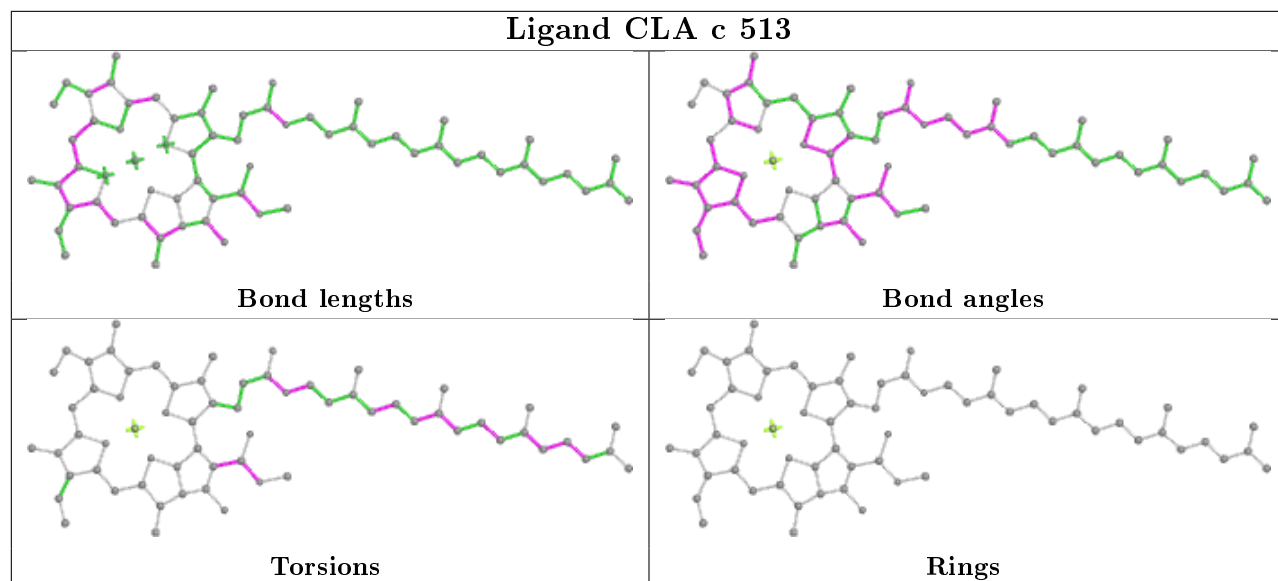
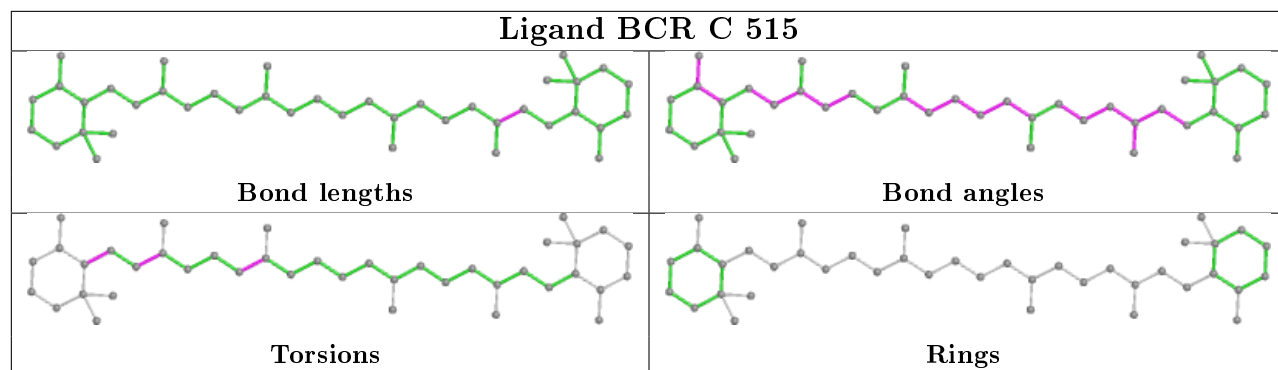


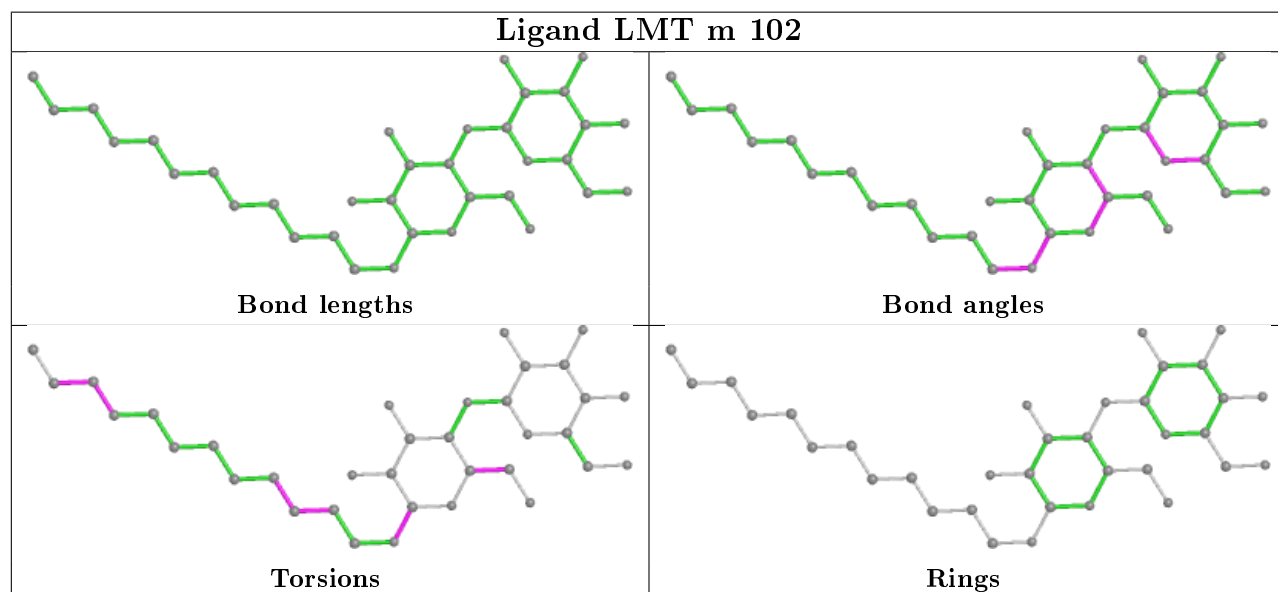
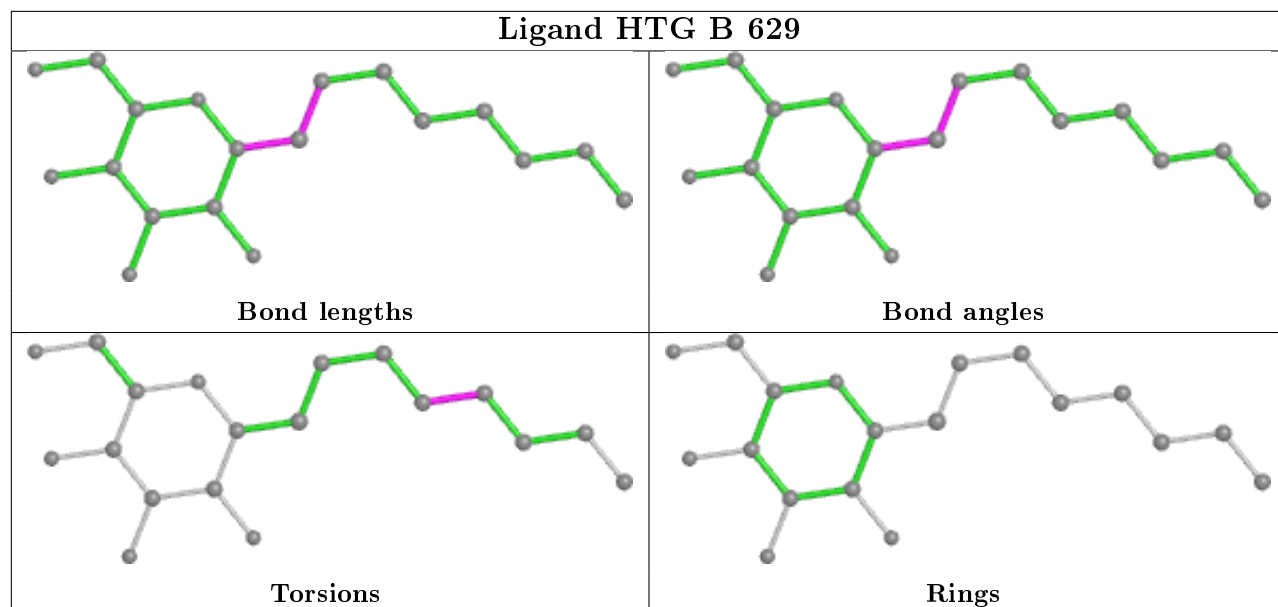
Ligand CLA b 622

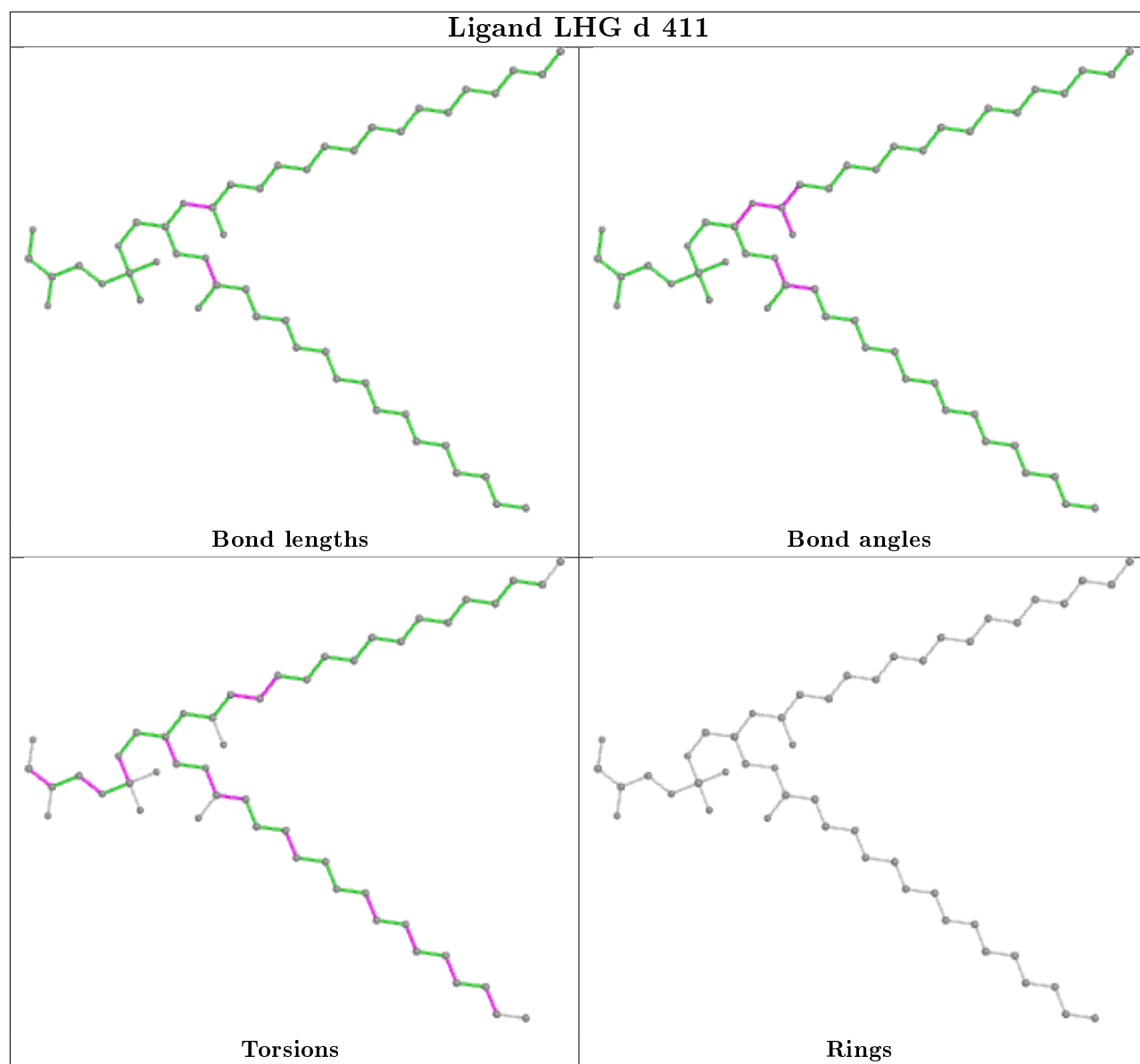
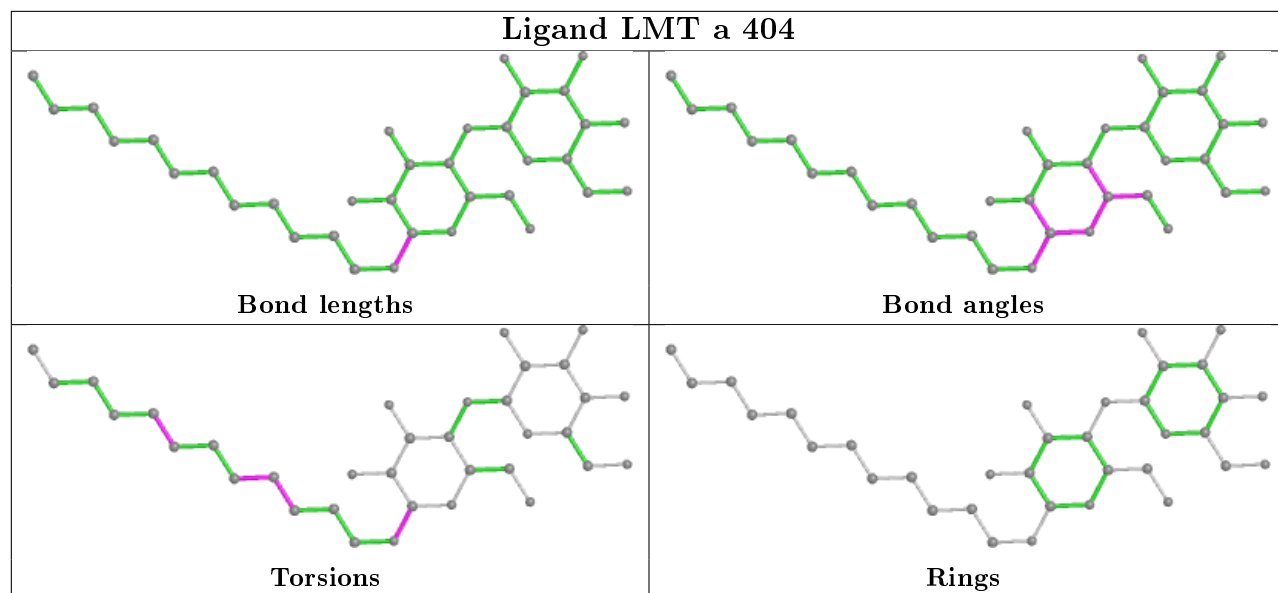


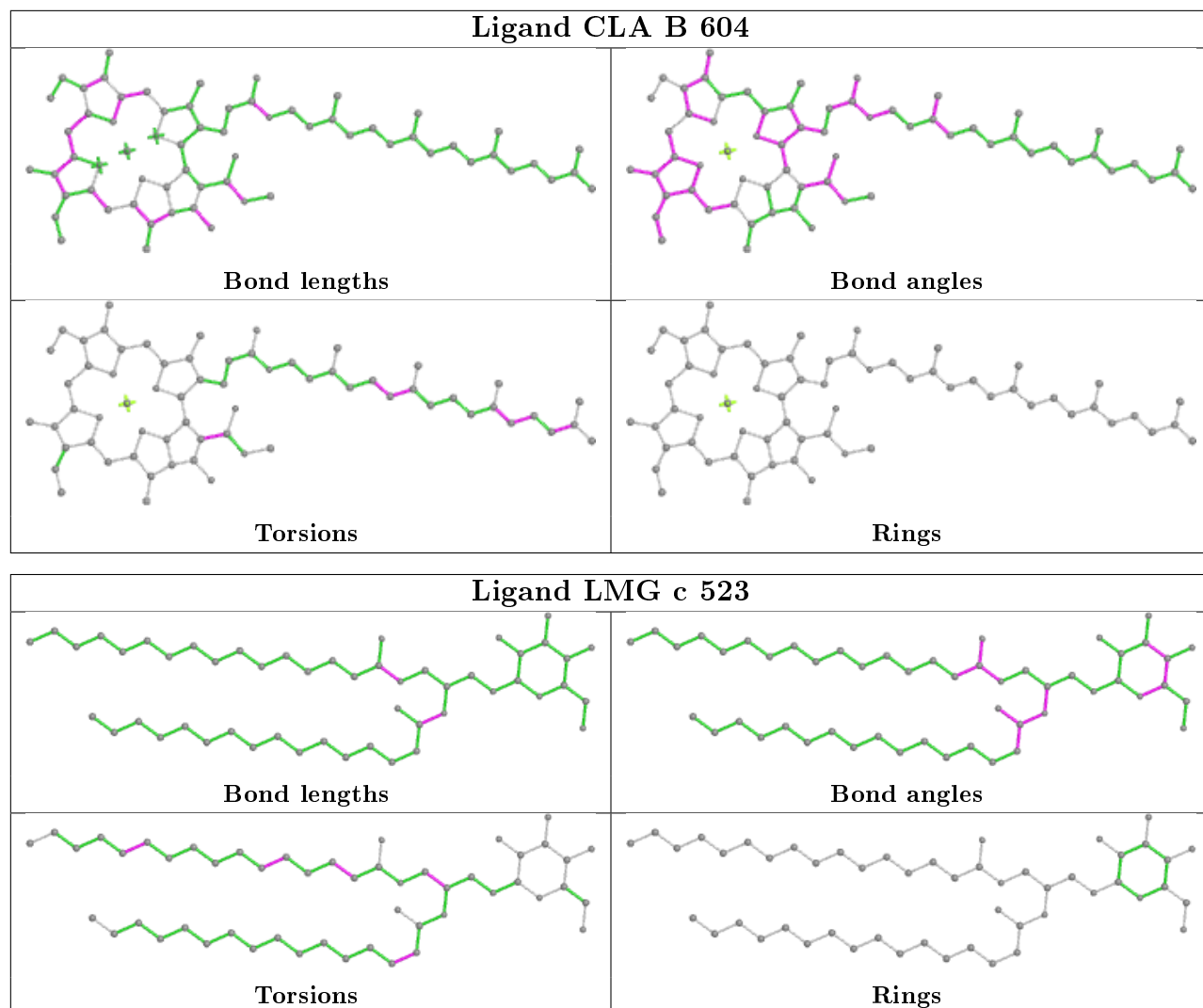
Ligand CLA B 617

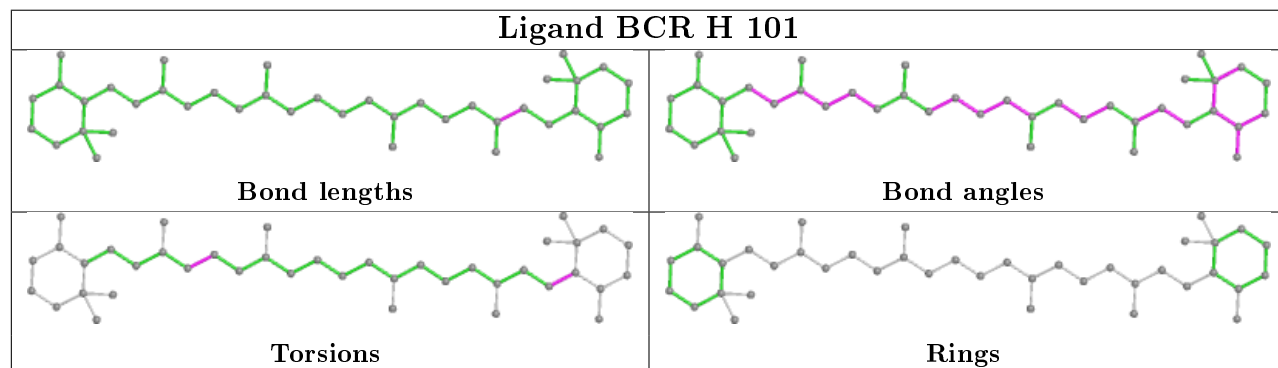
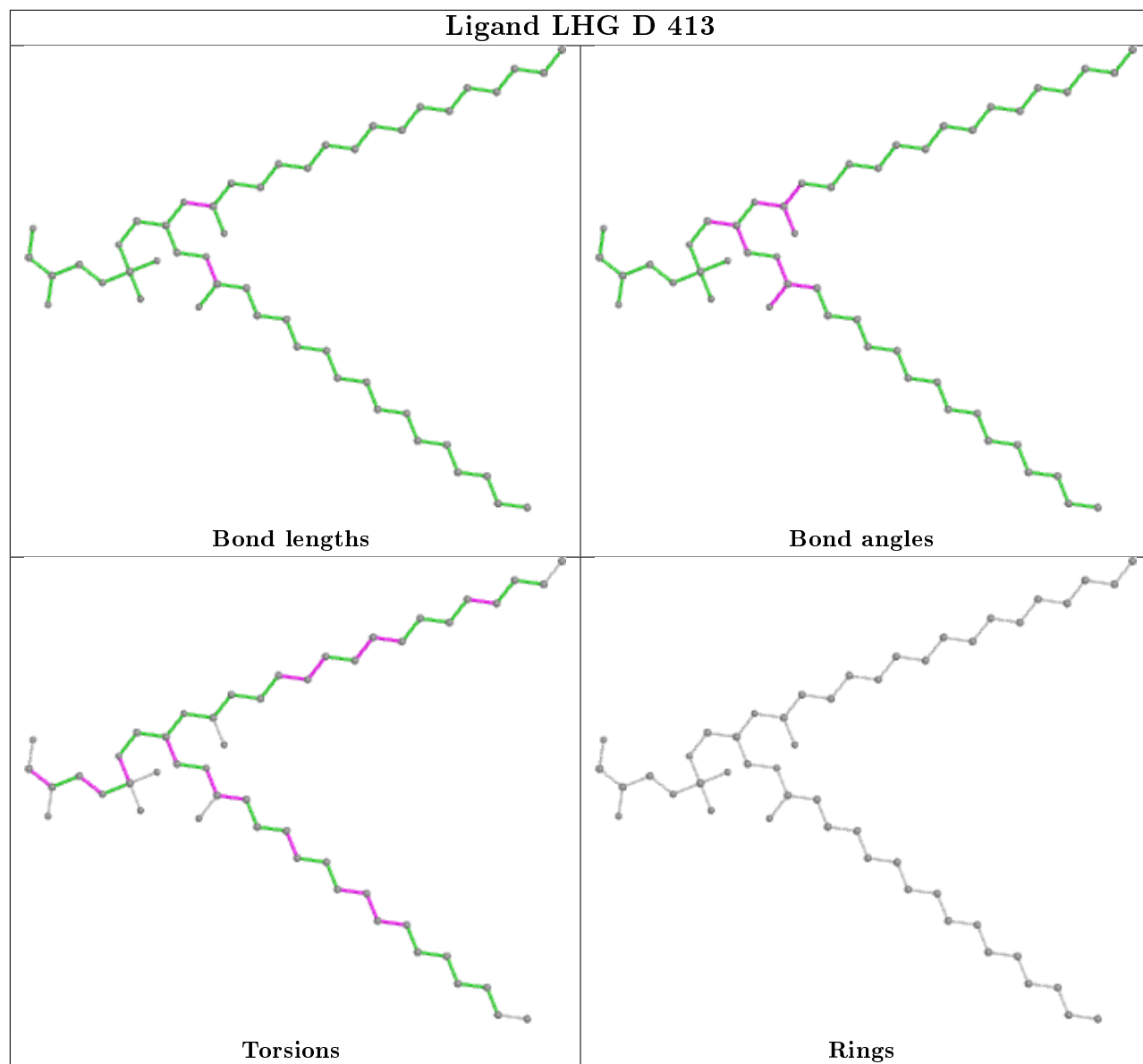


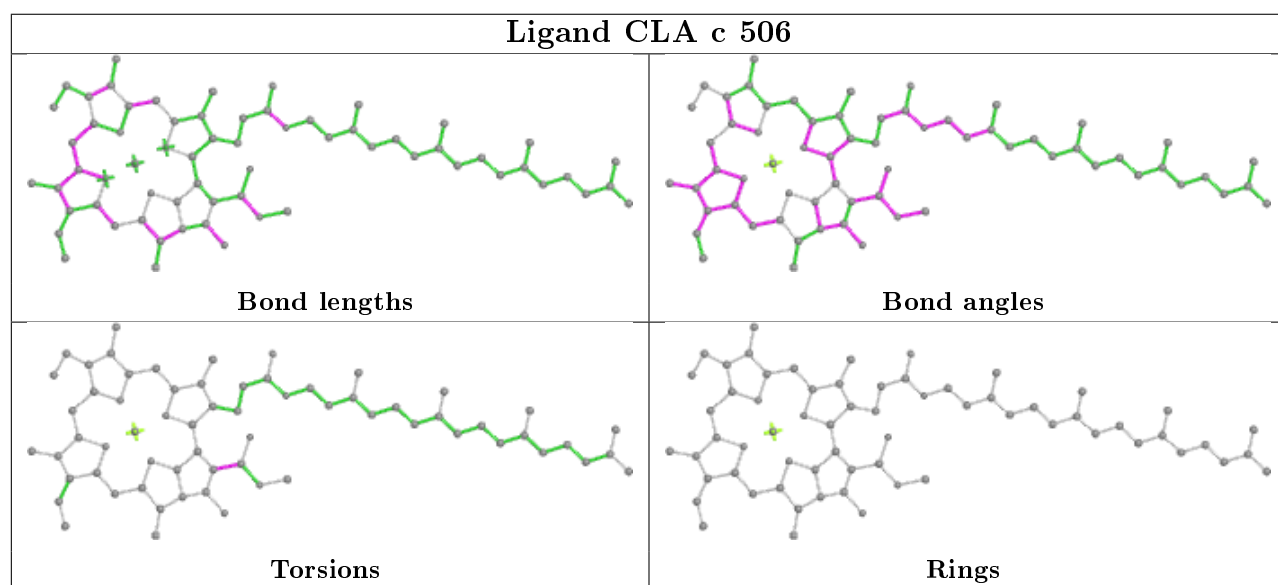
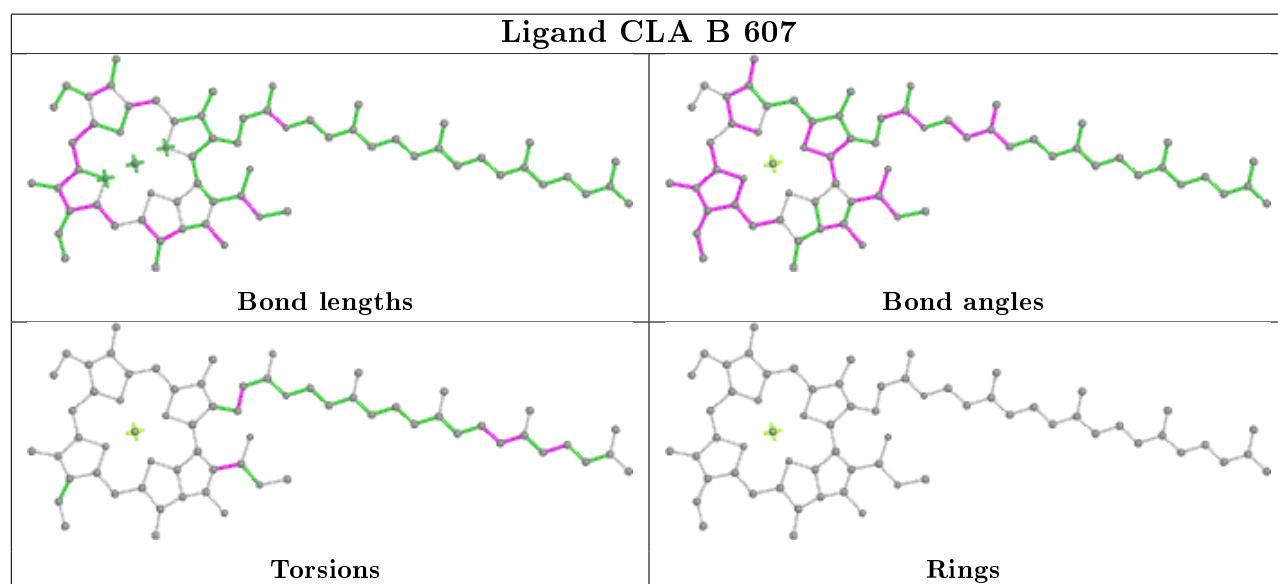
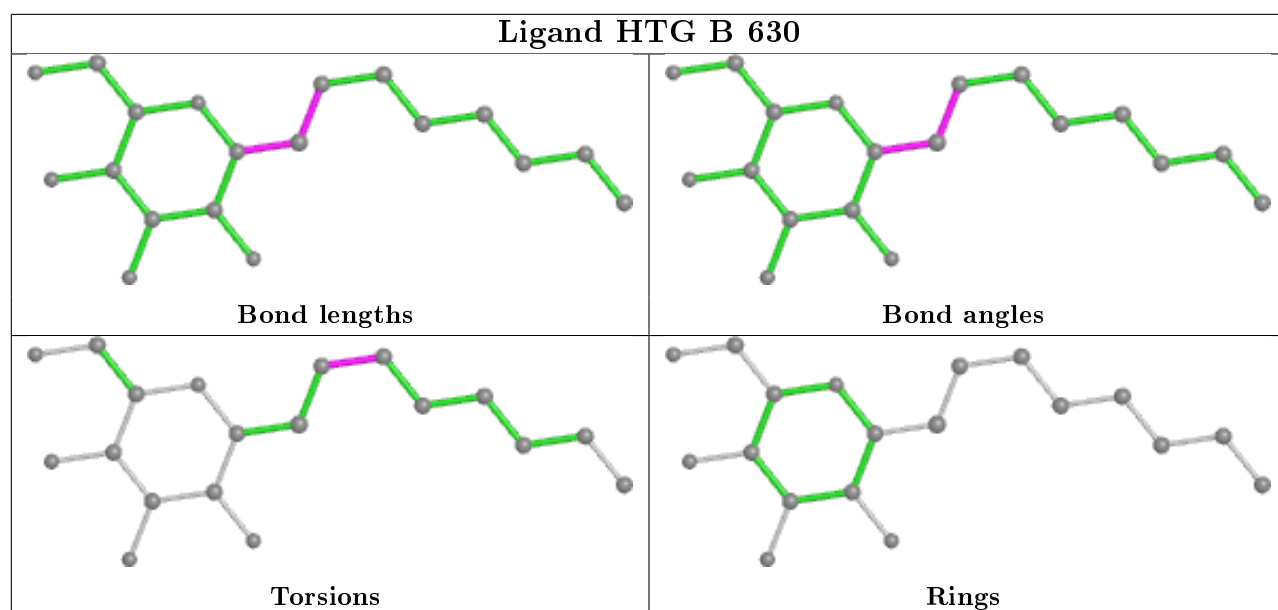


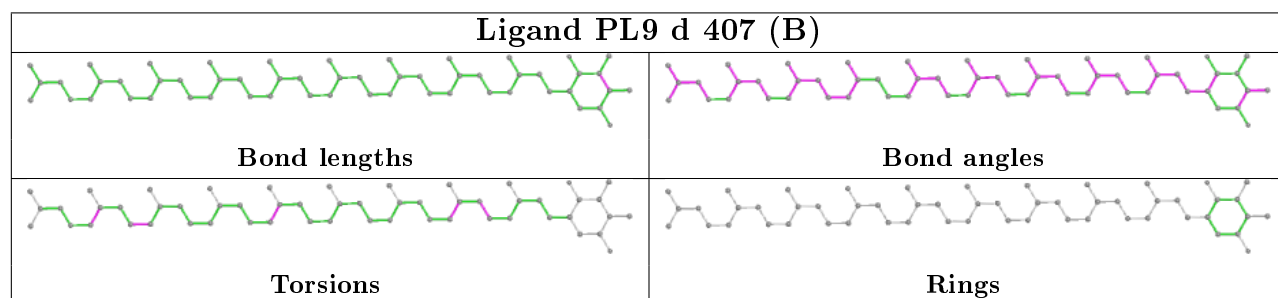
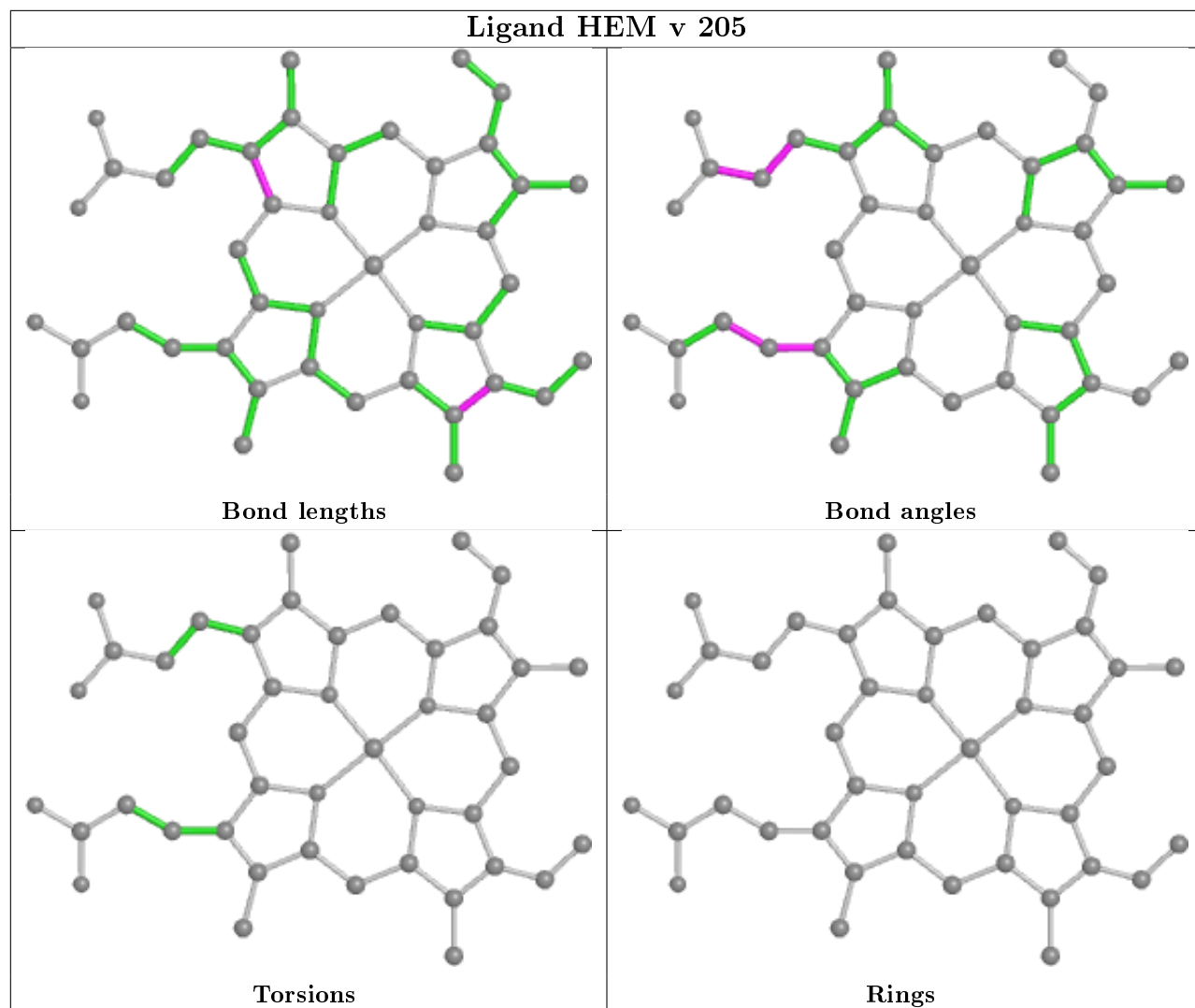


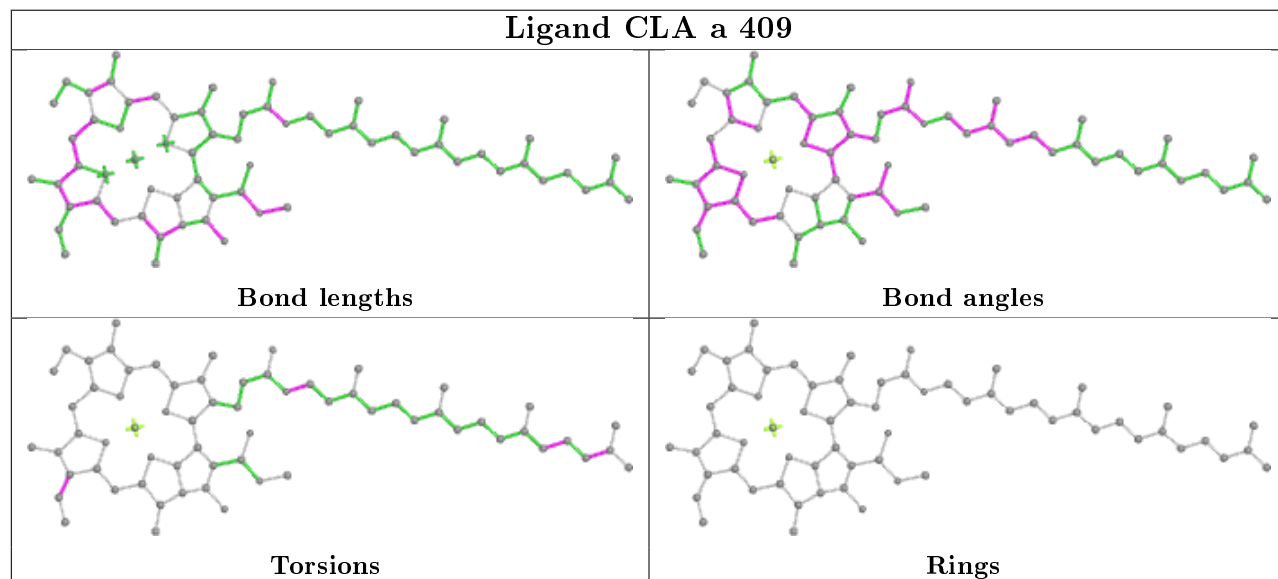
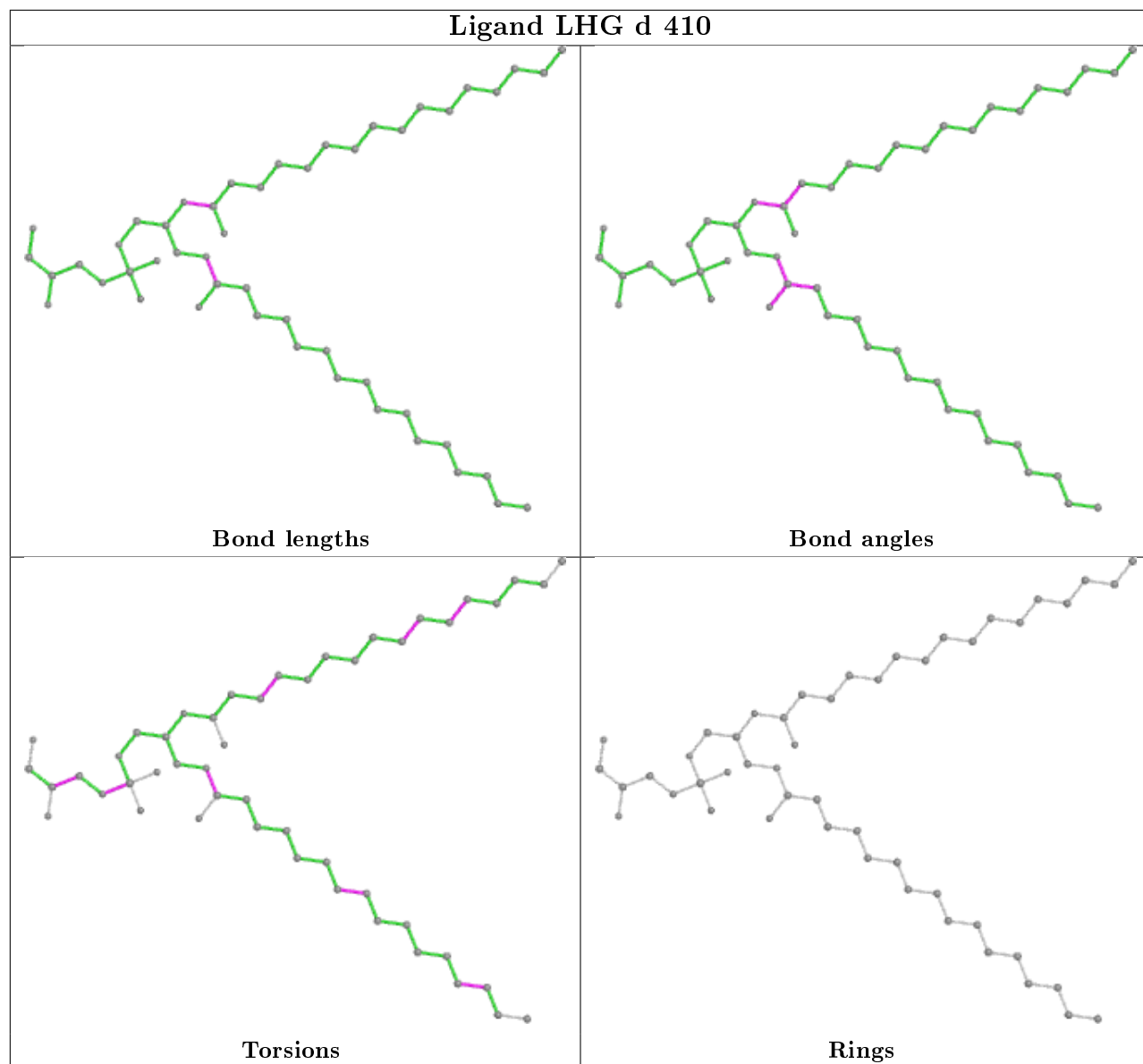


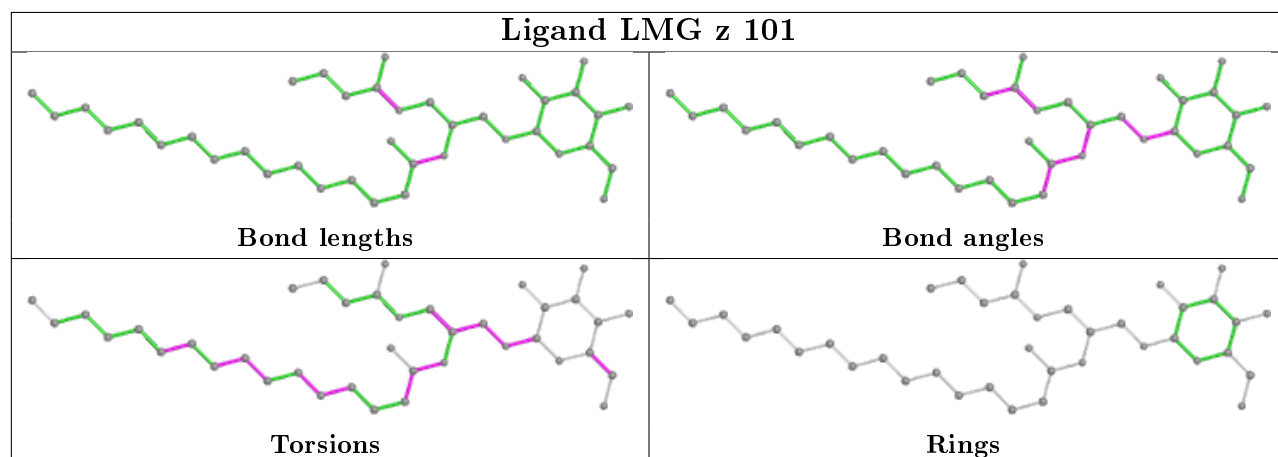
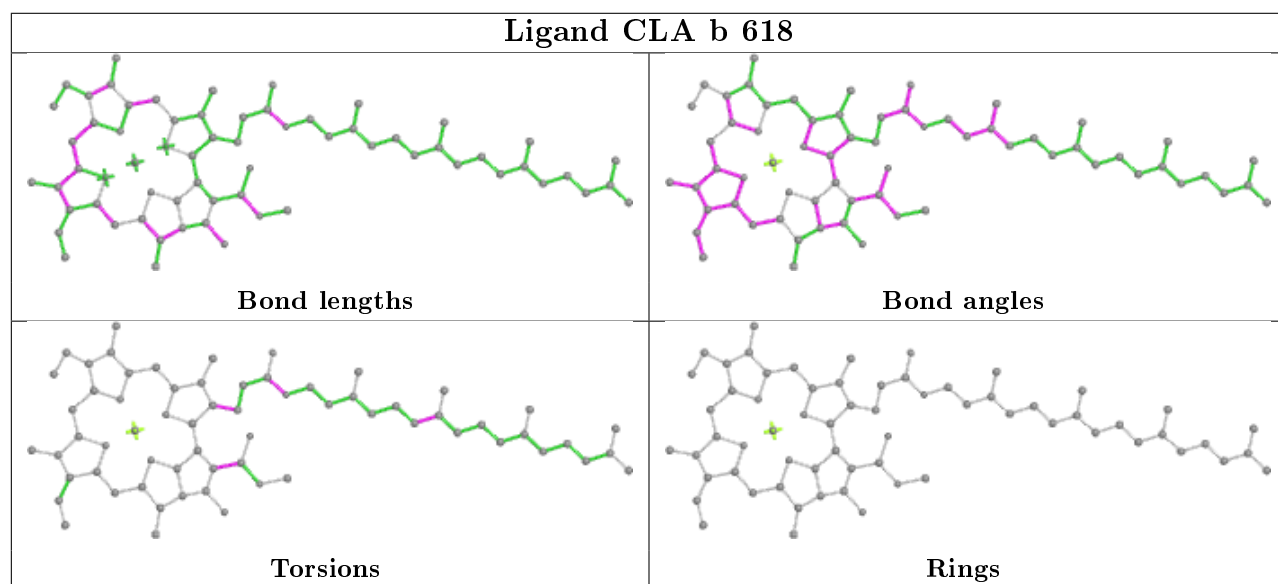
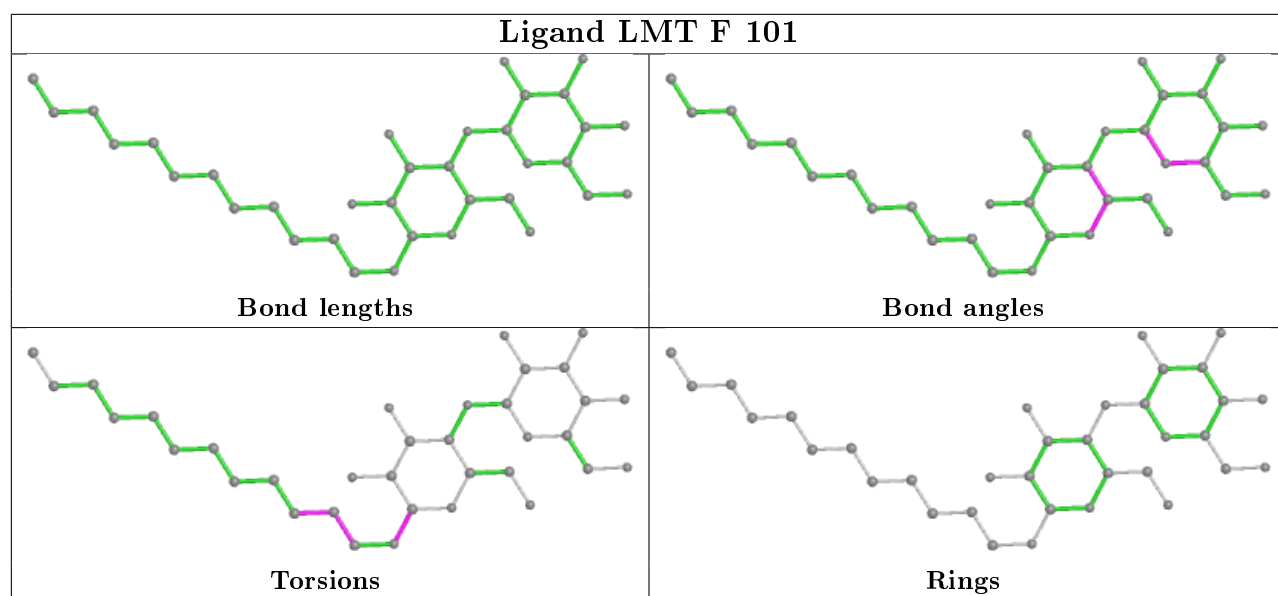




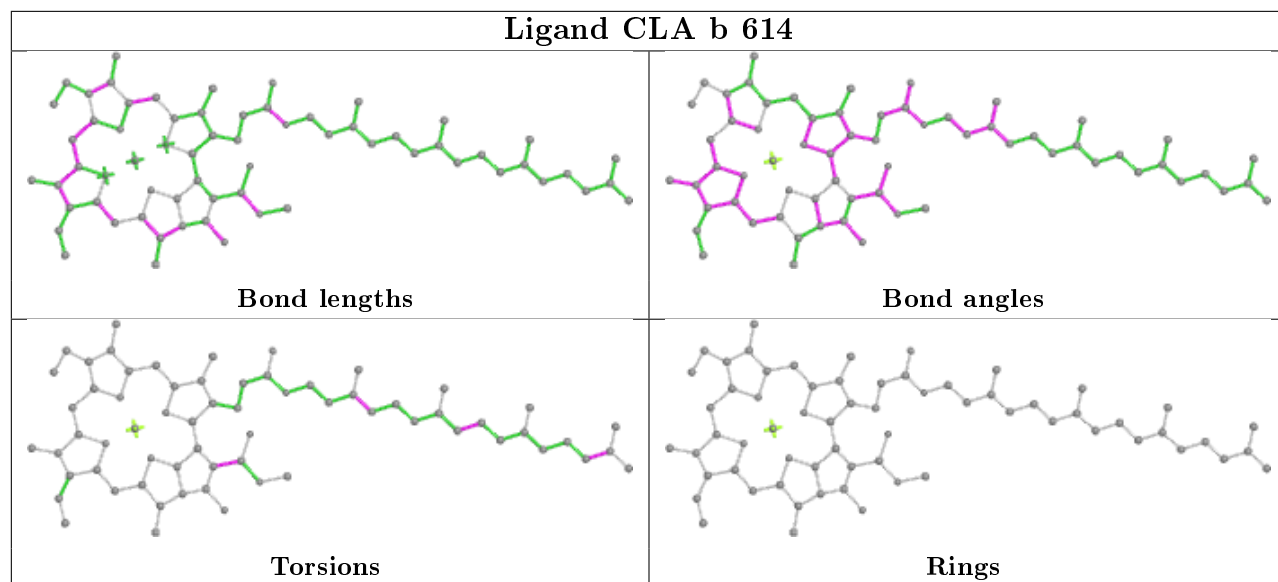




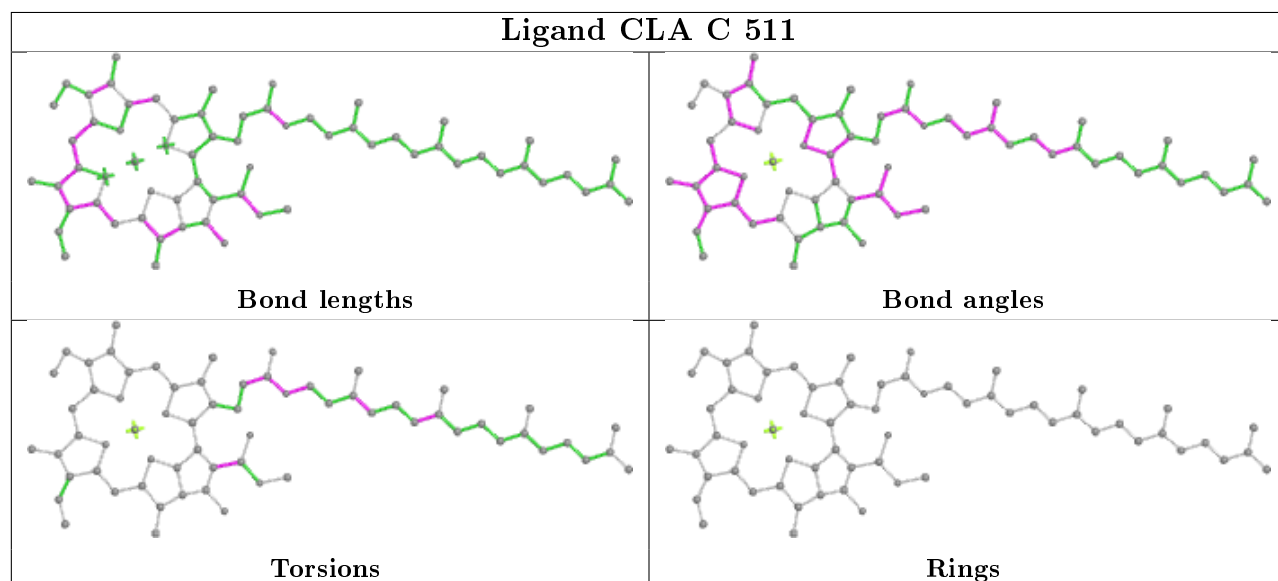




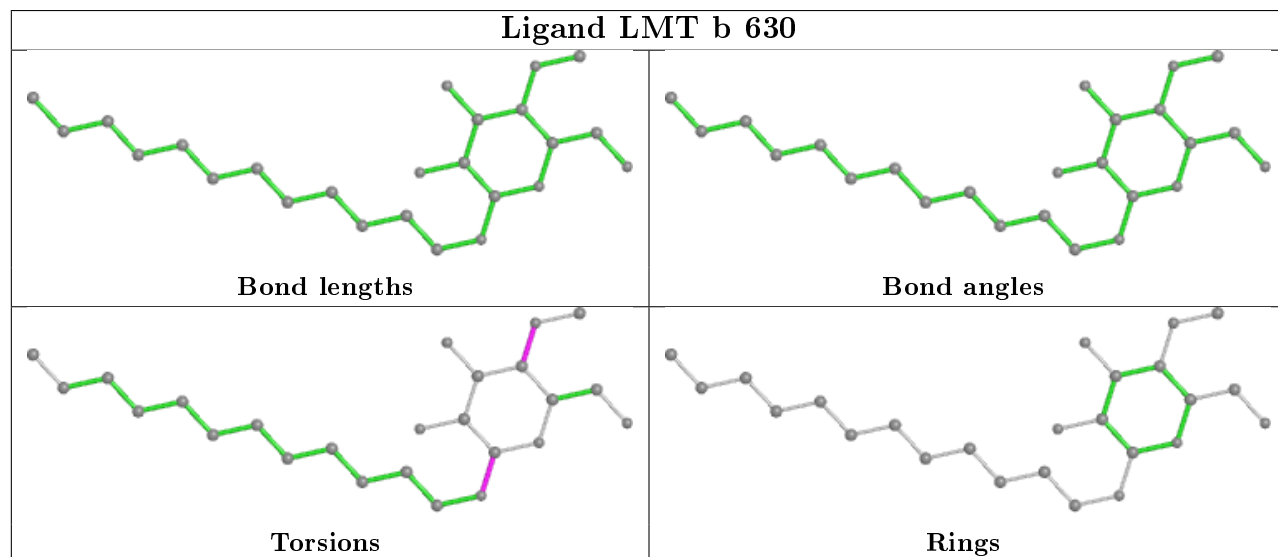
Ligand CLA b 614

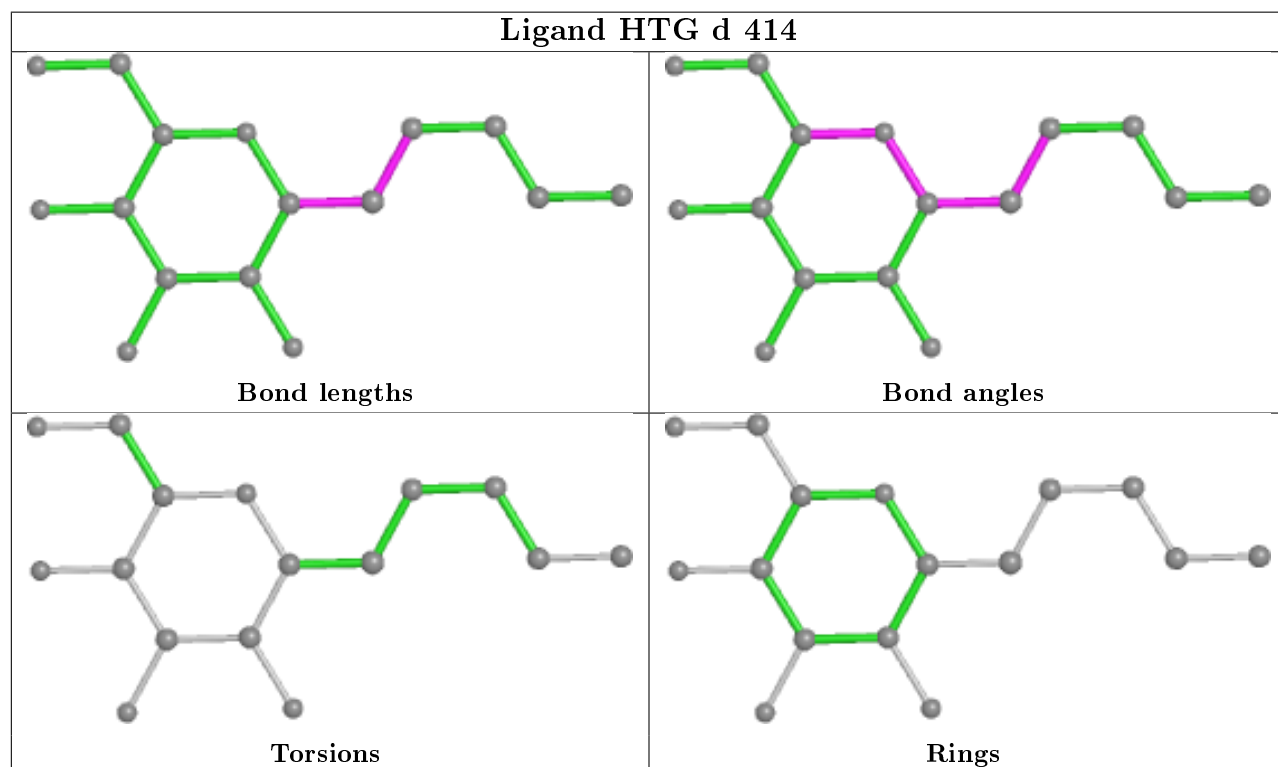
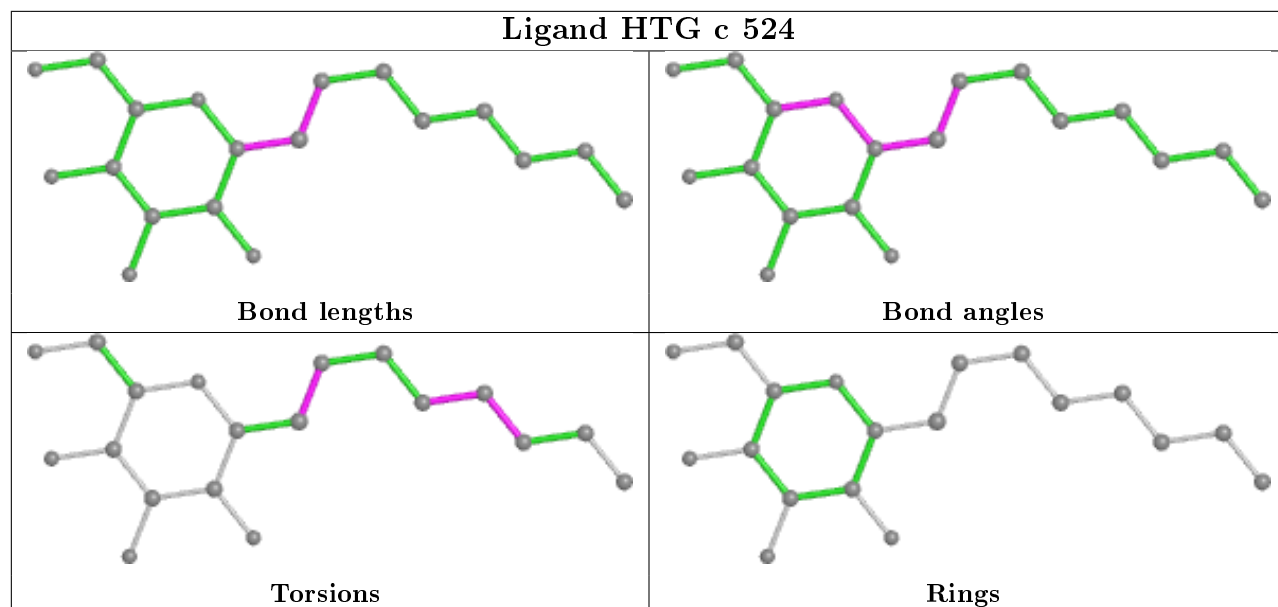


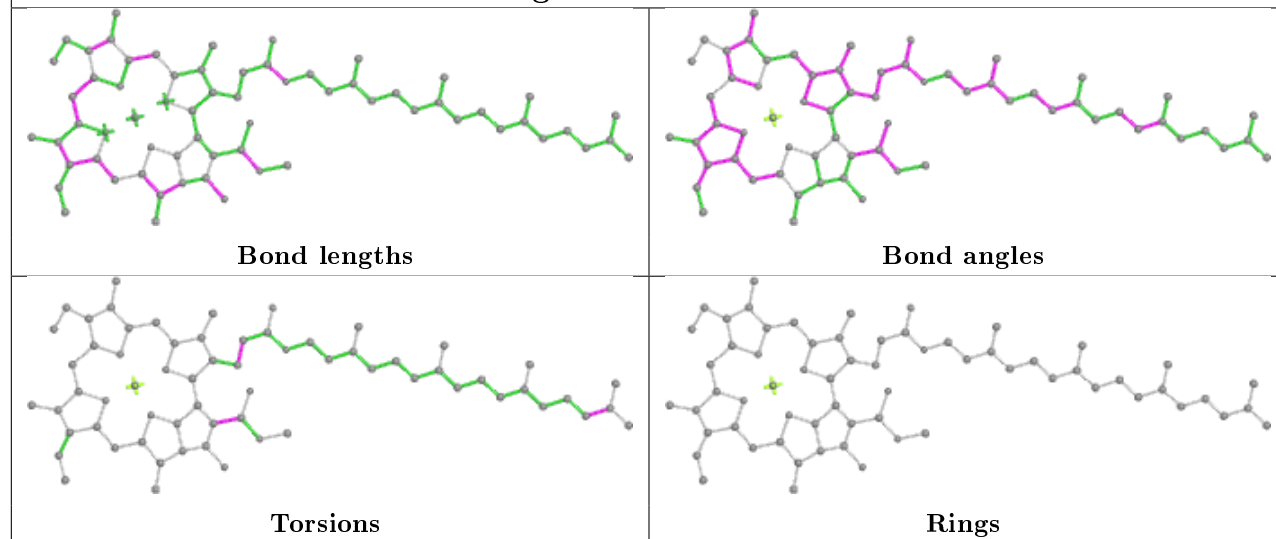
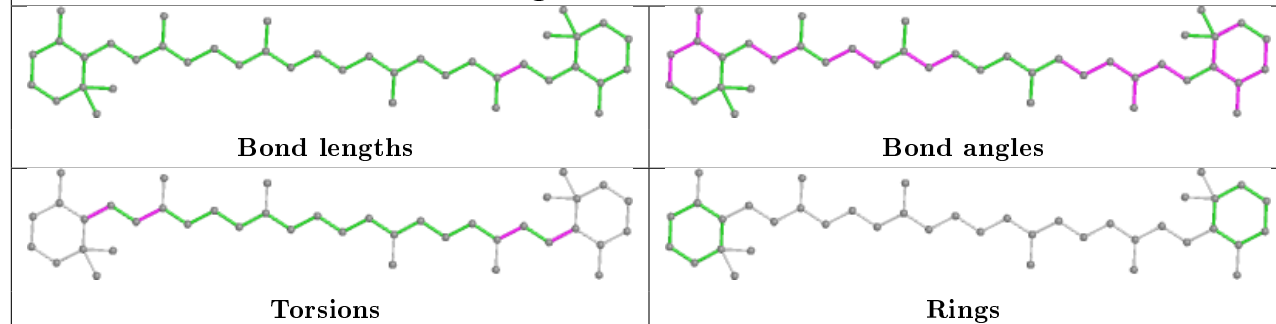
Ligand CLA C 511

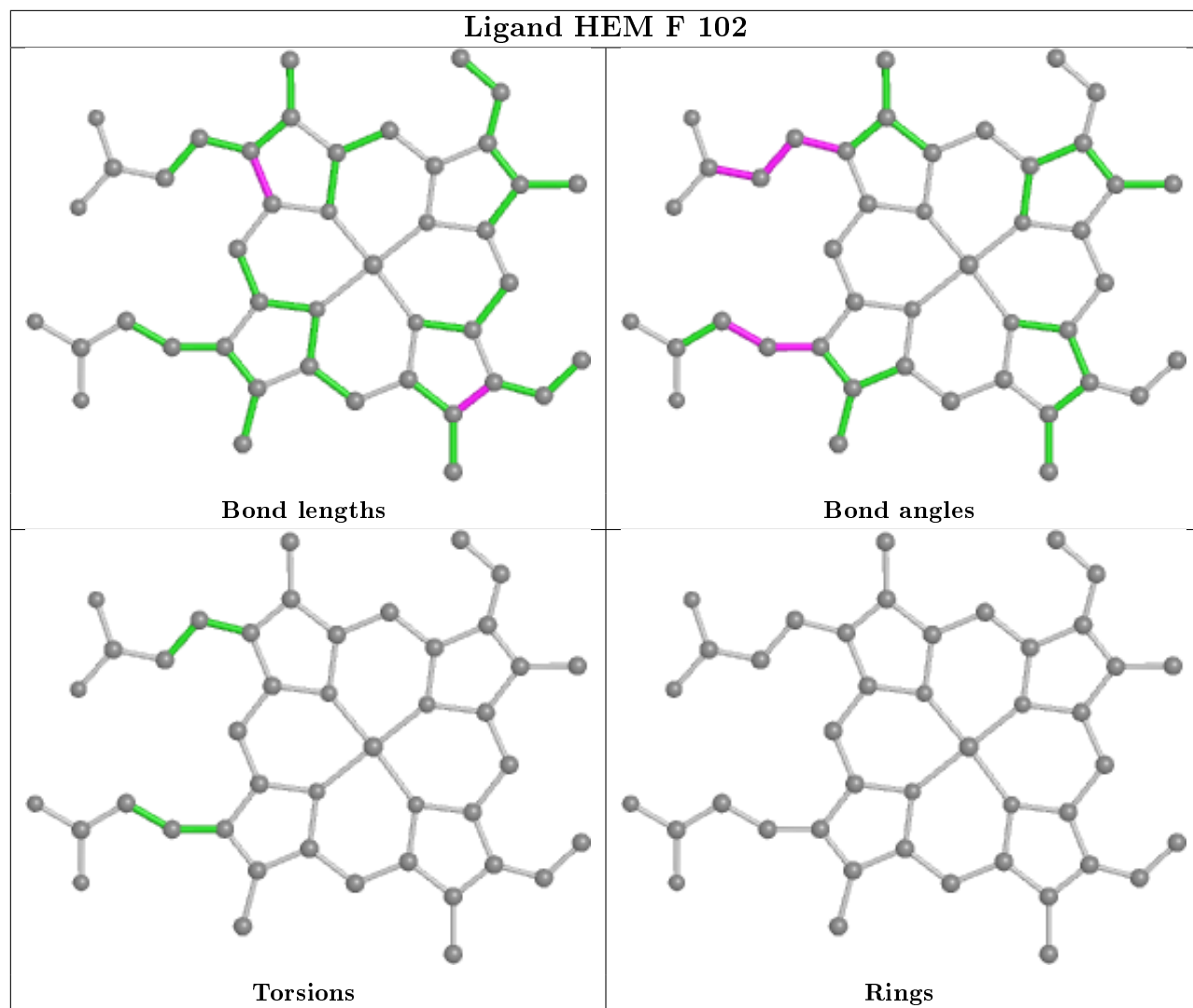


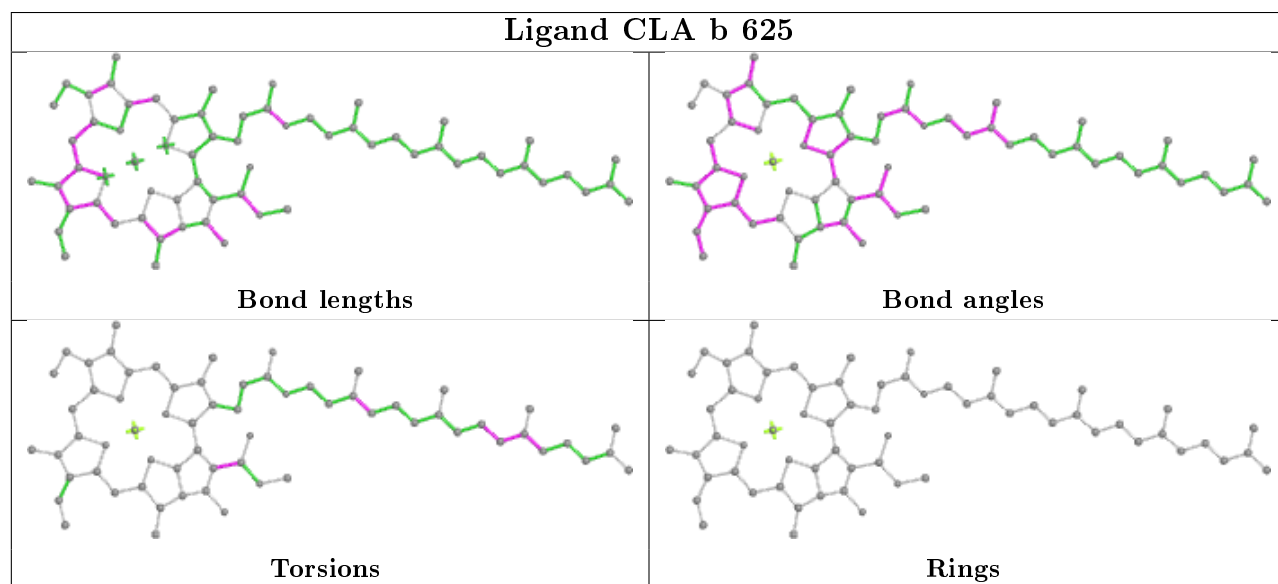
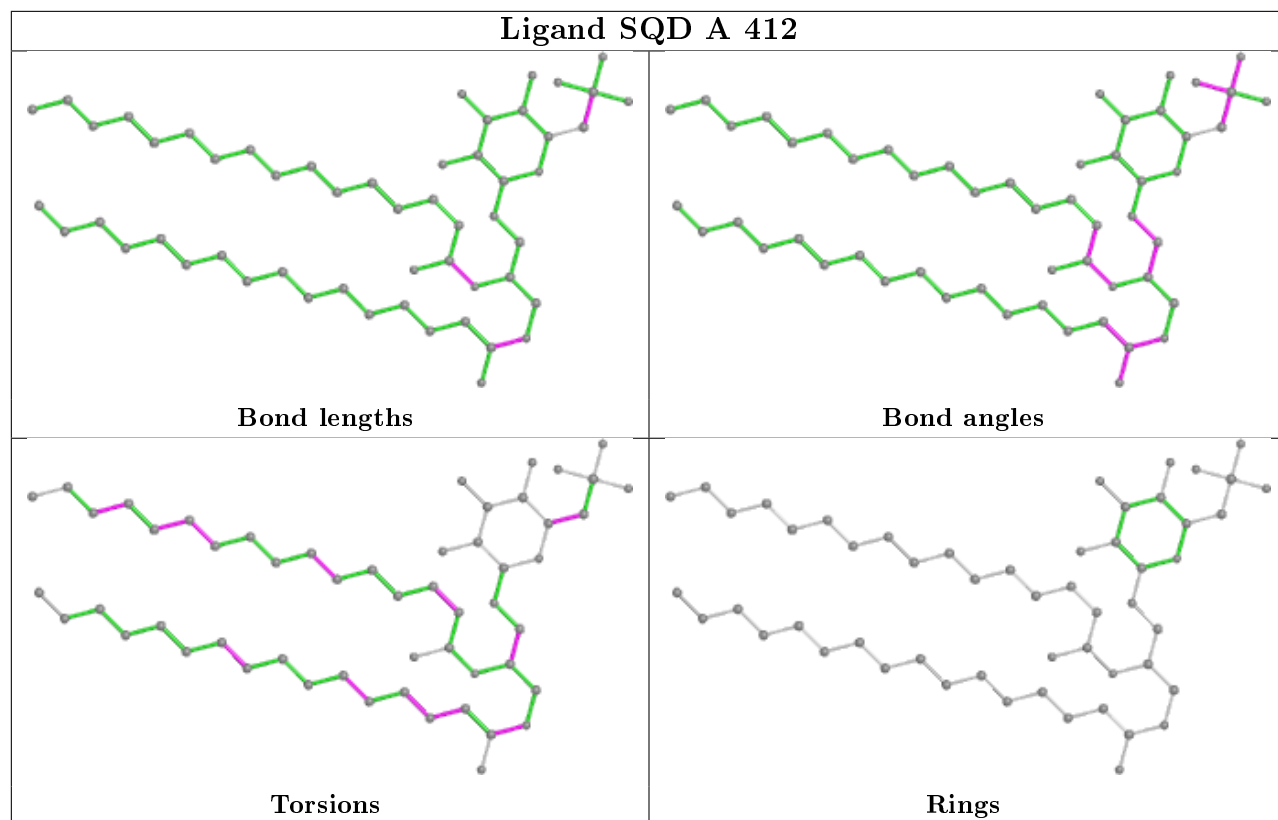
Ligand LMT b 630

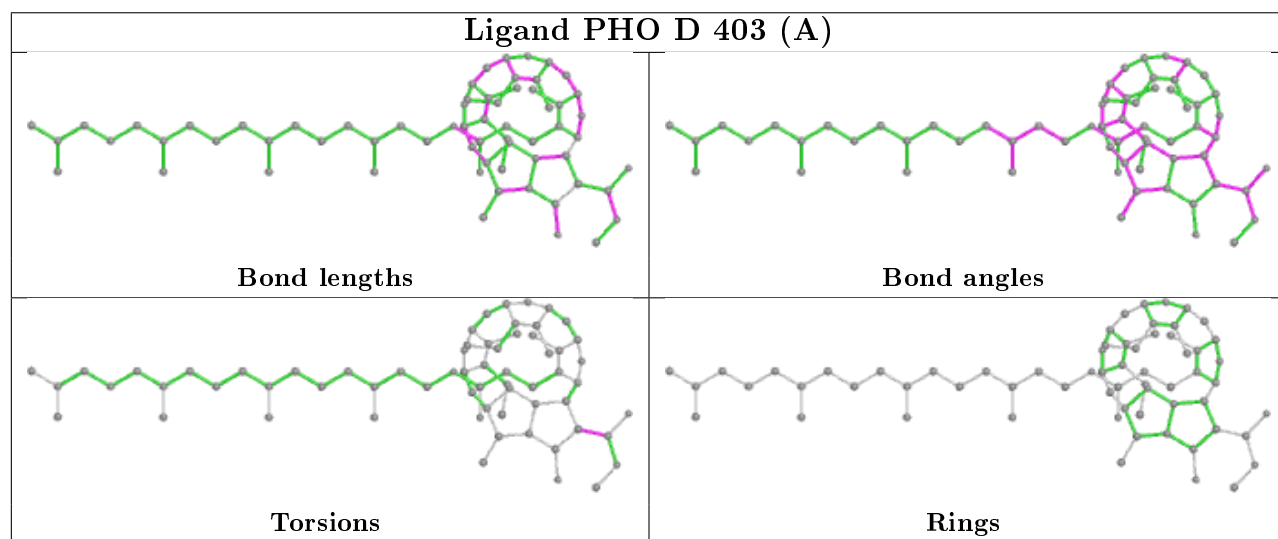
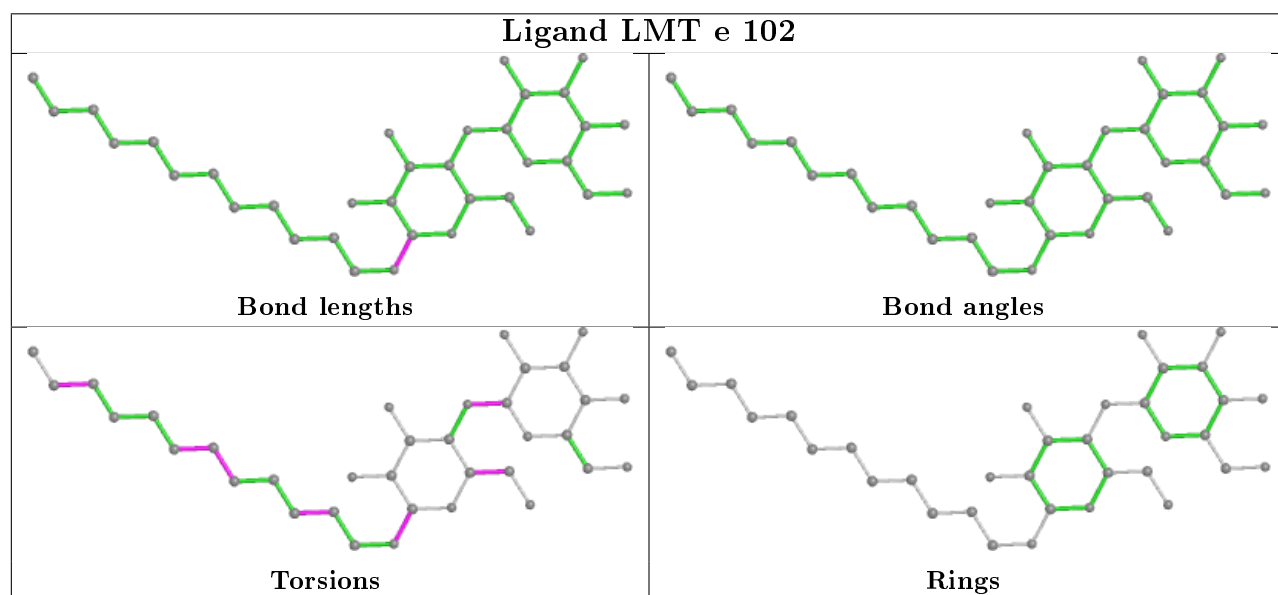
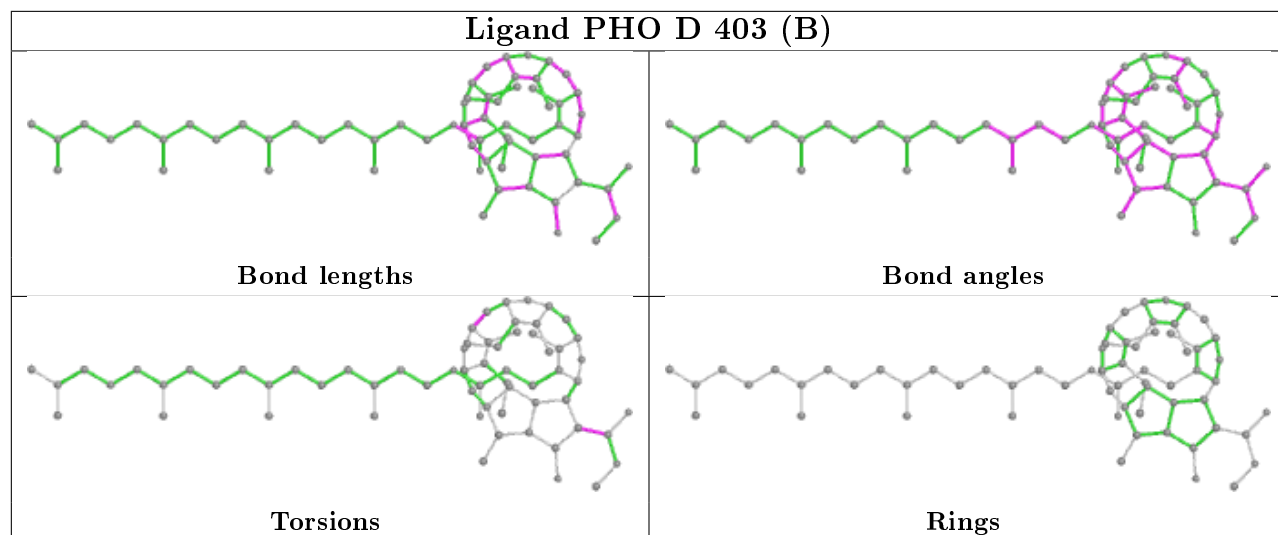




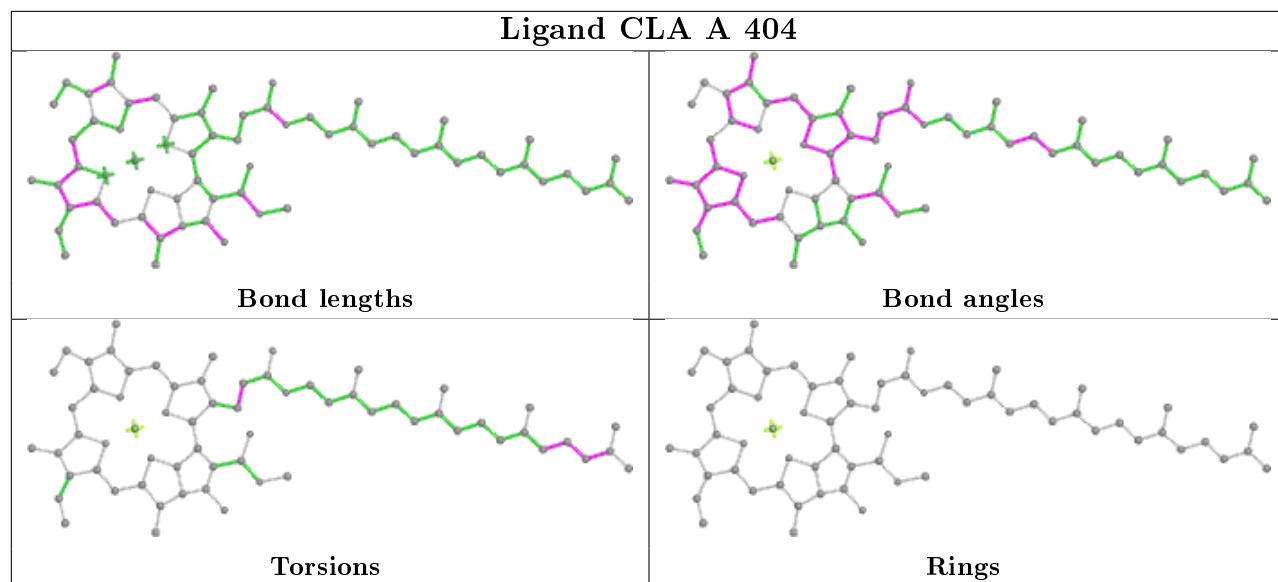
Ligand CLA B 611**Ligand BCR D 408**



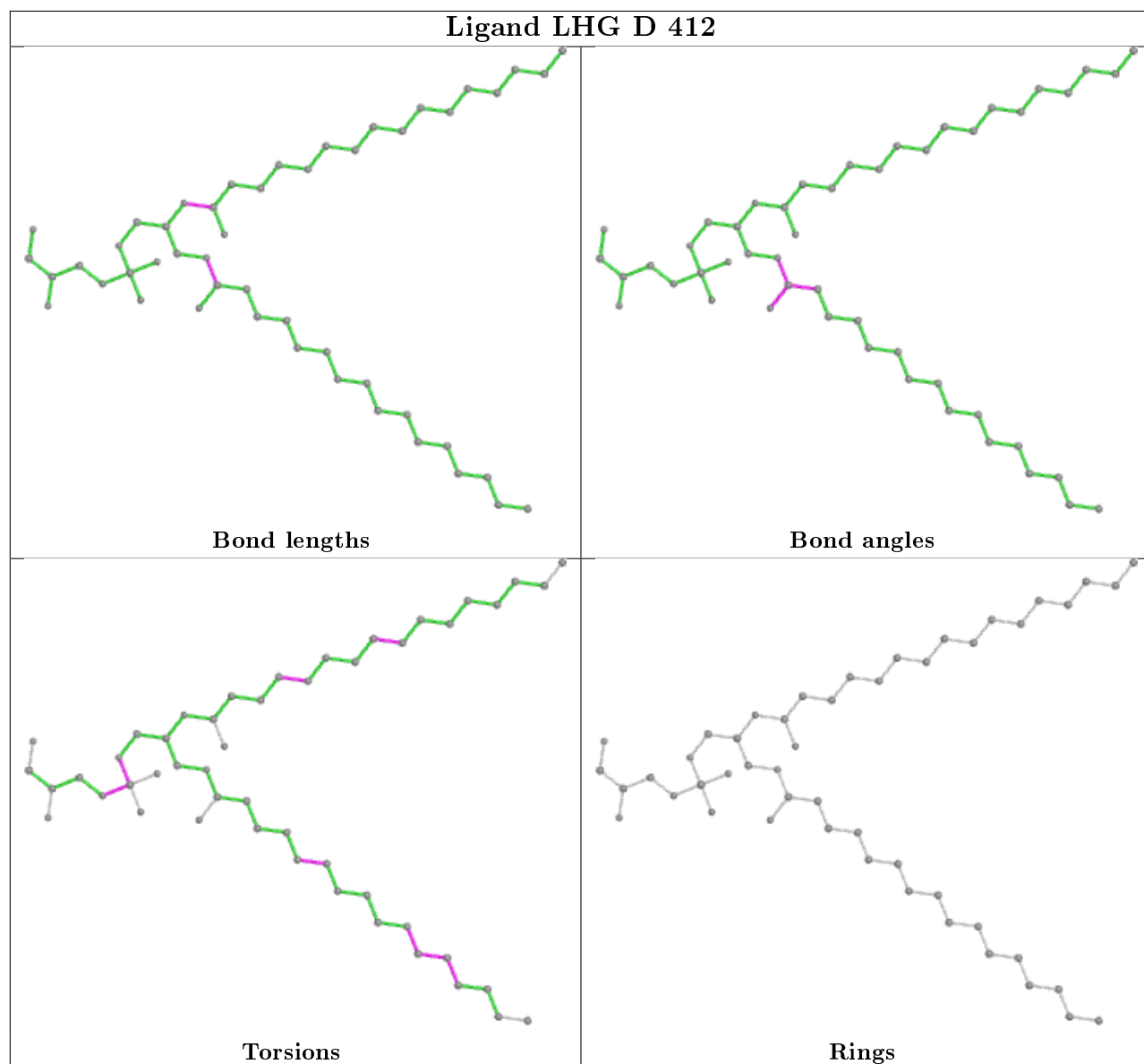


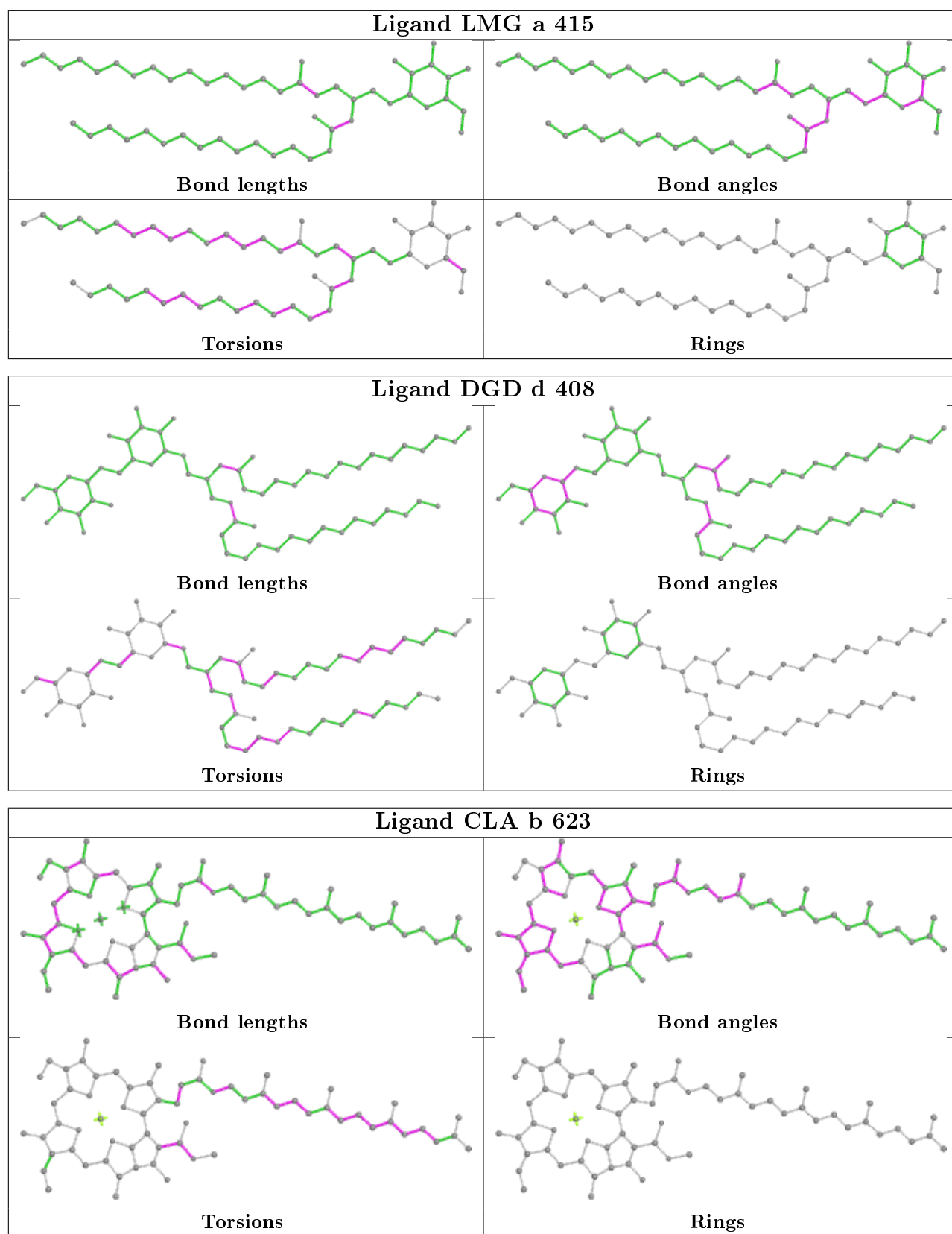


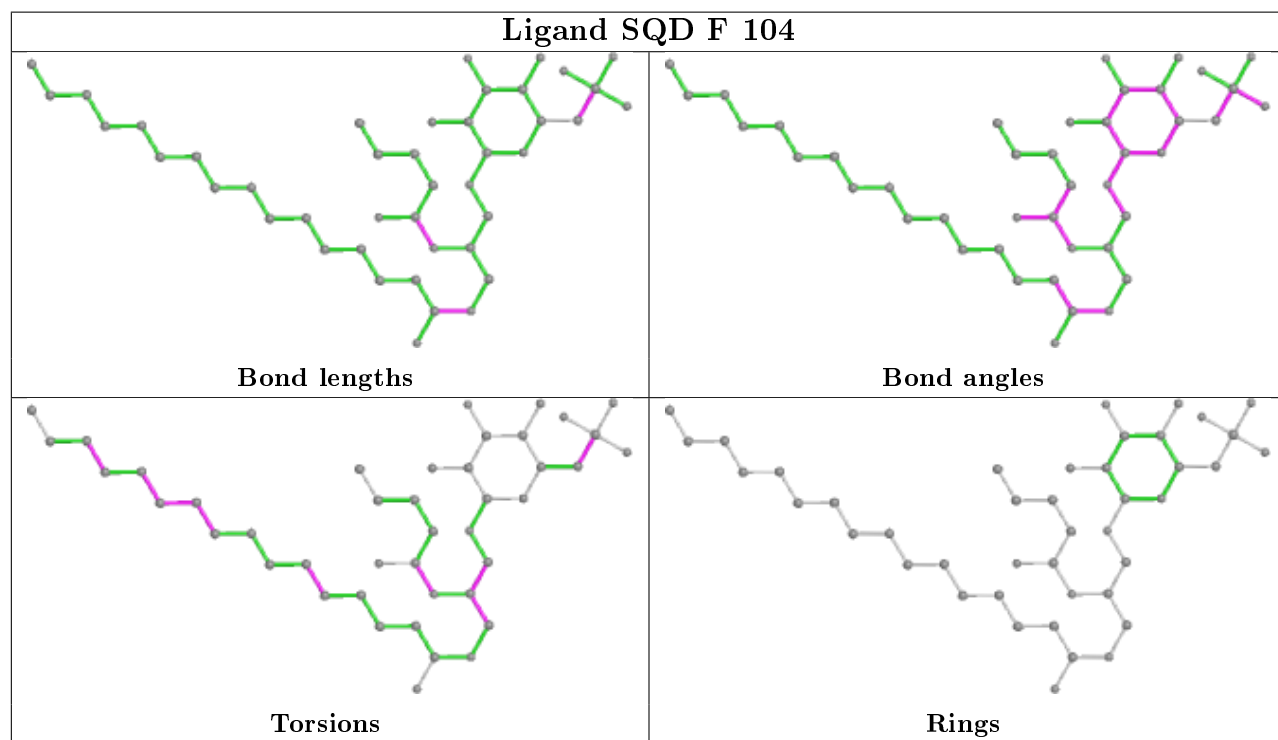
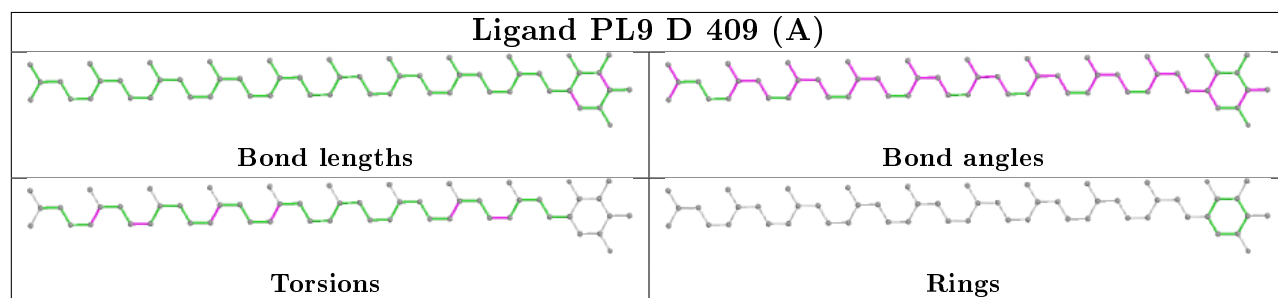
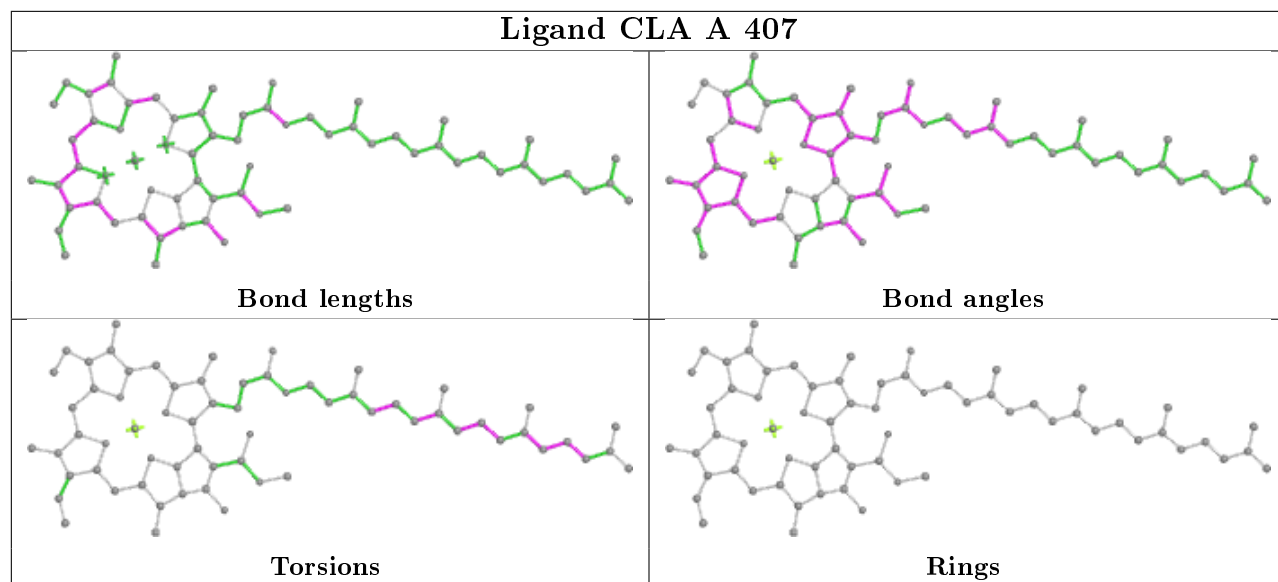
Ligand CLA A 404

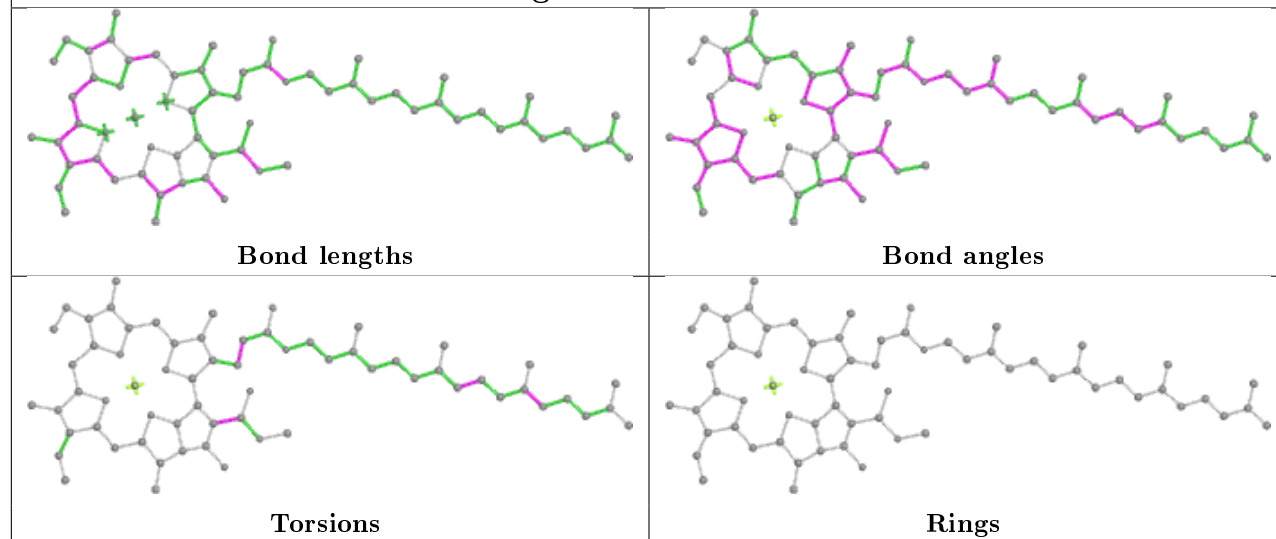
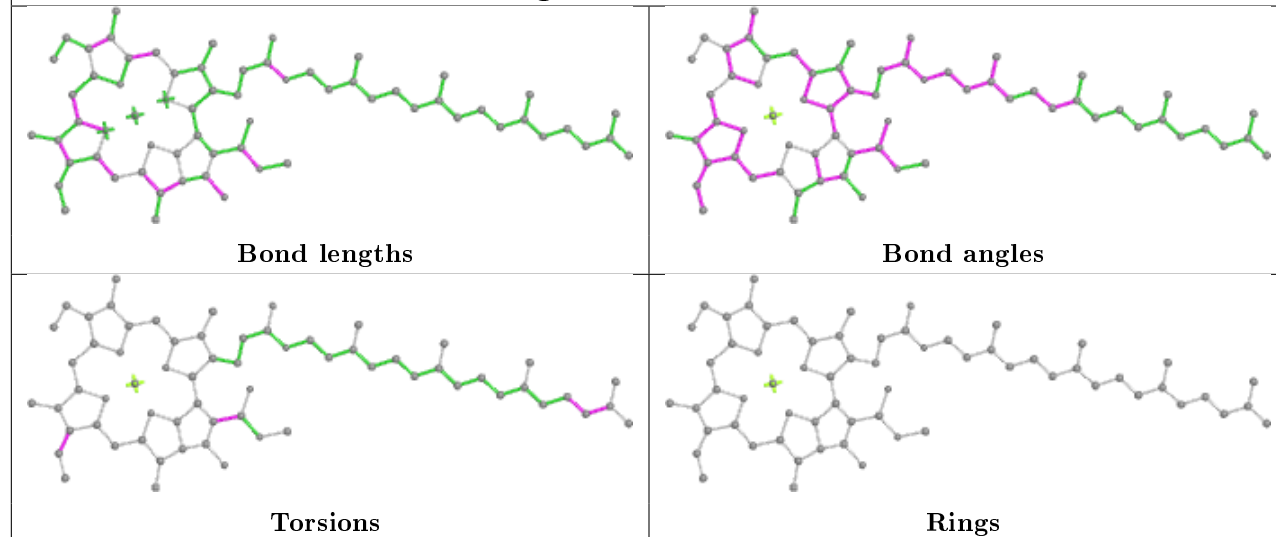


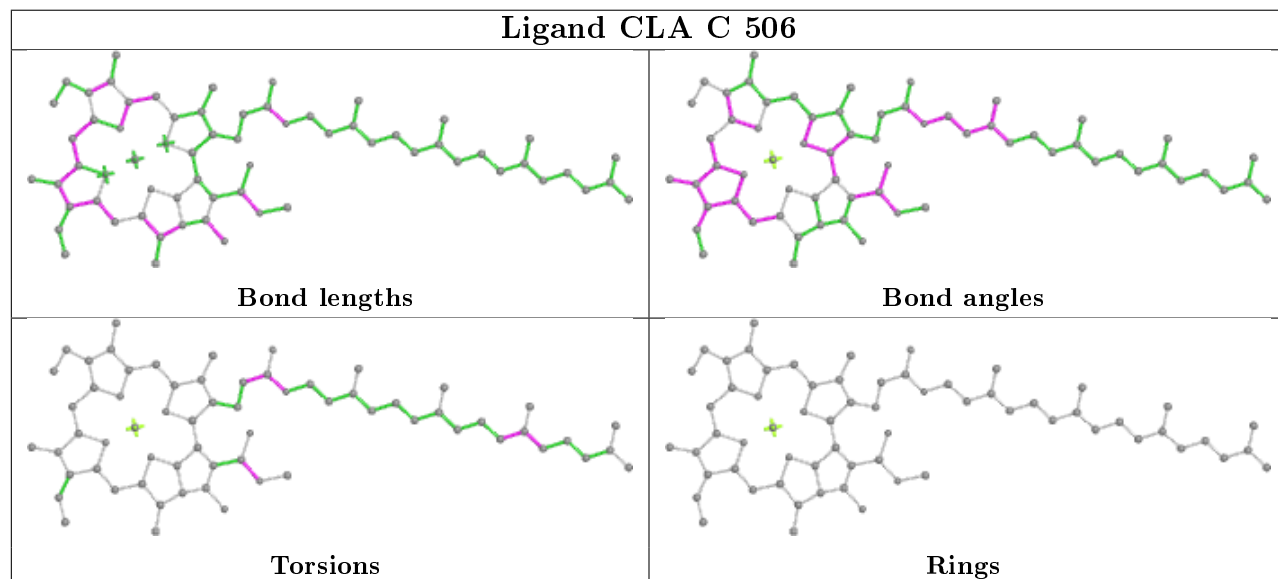
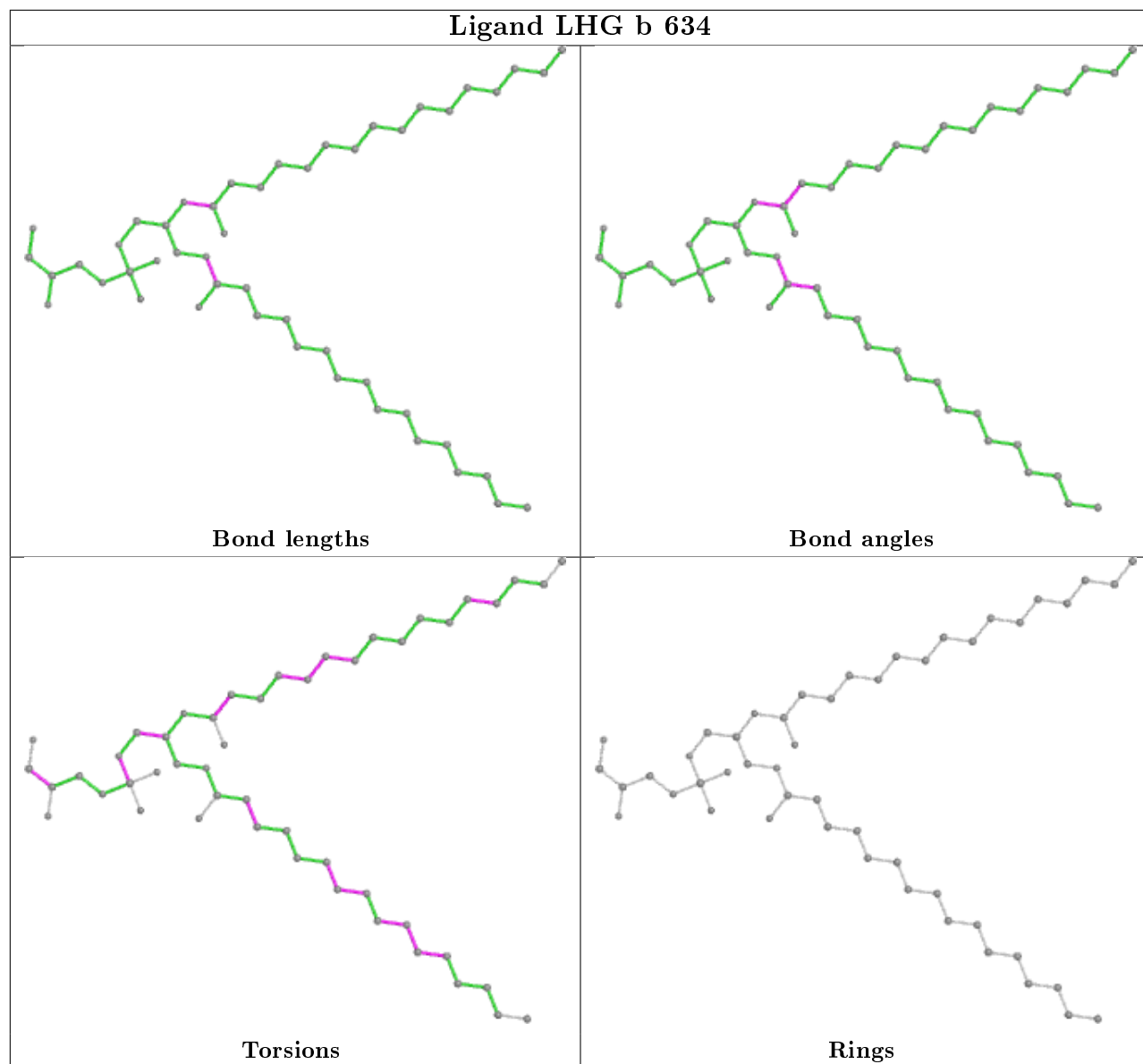
Ligand LHG D 412



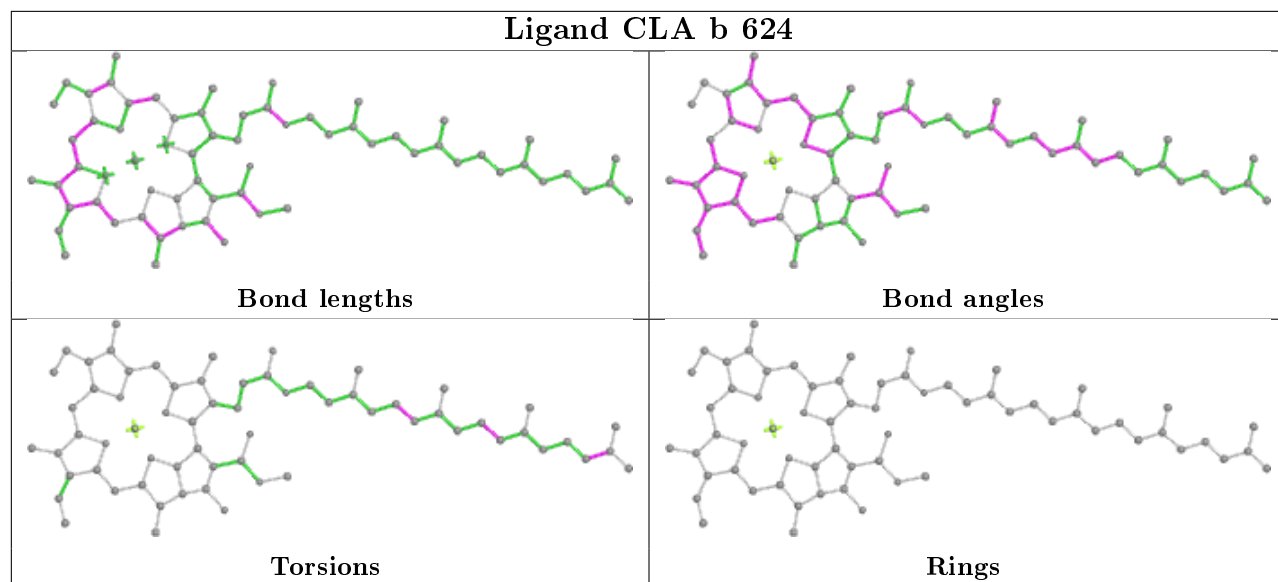




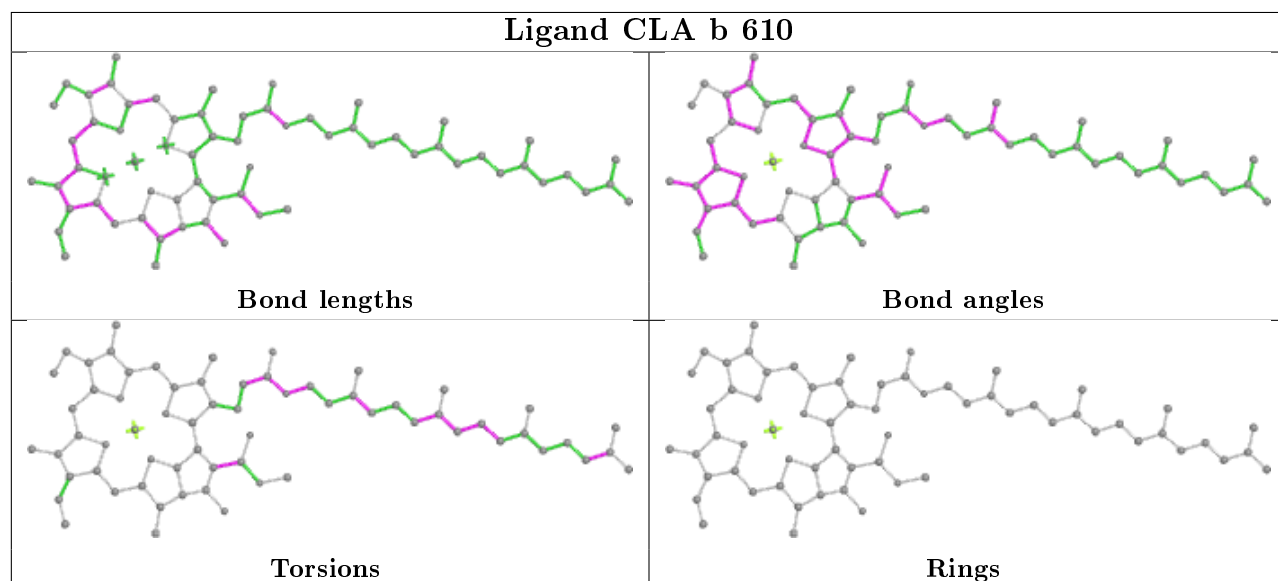
Ligand CLA B 603**Ligand CLA d 403**



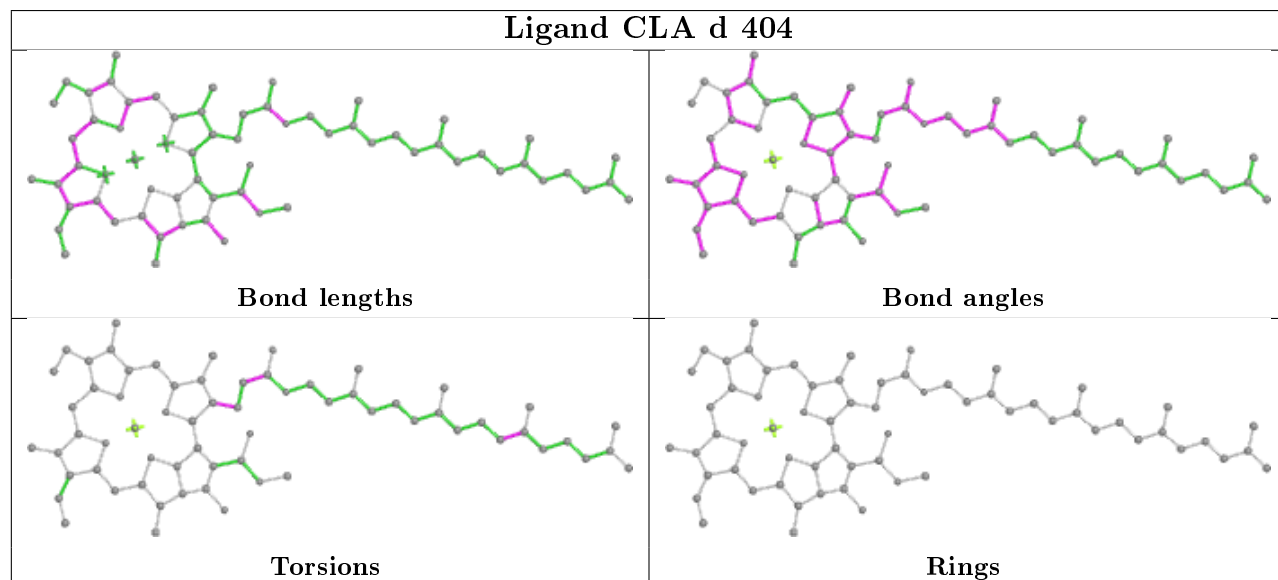
Ligand CLA b 624



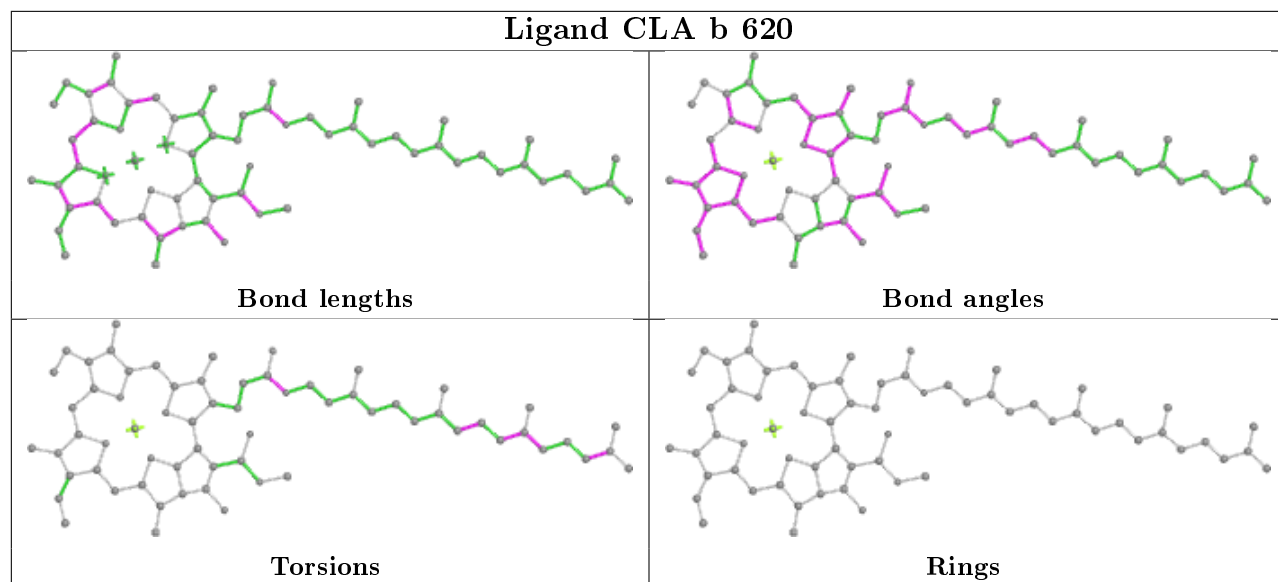
Ligand CLA b 610



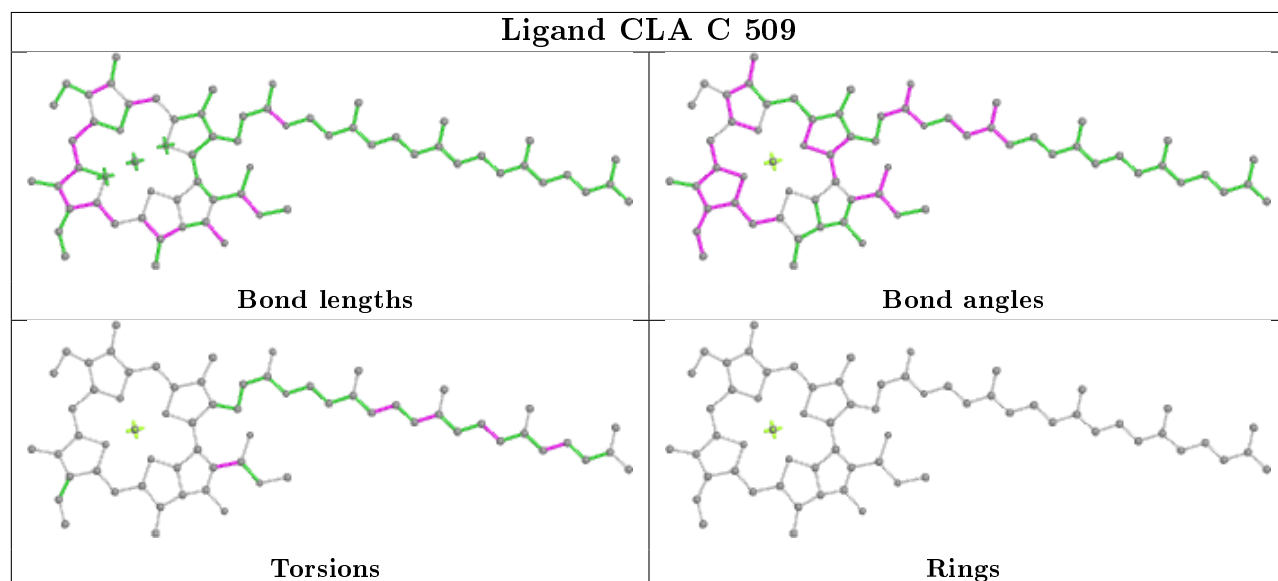
Ligand CLA d 404



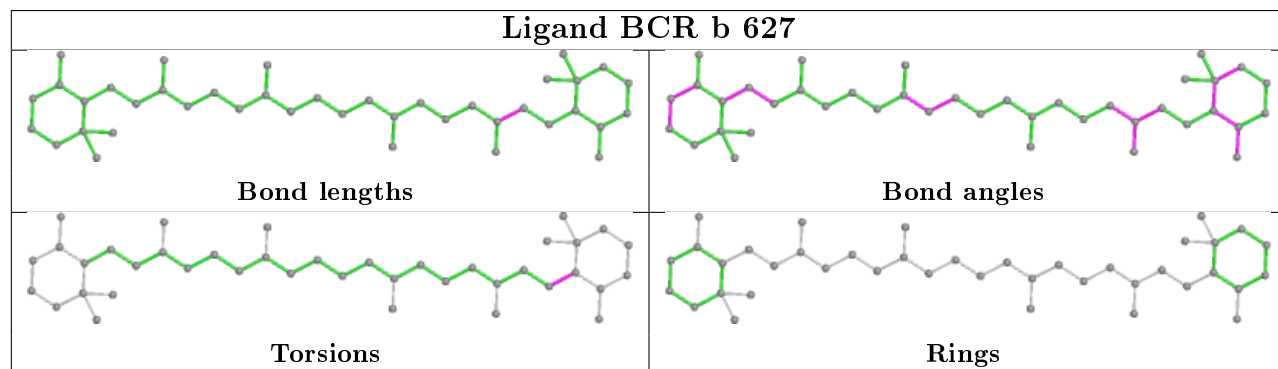
Ligand CLA b 620

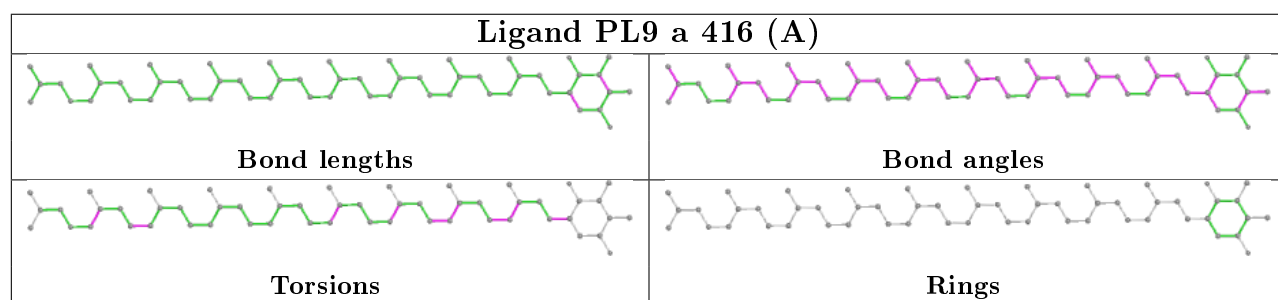
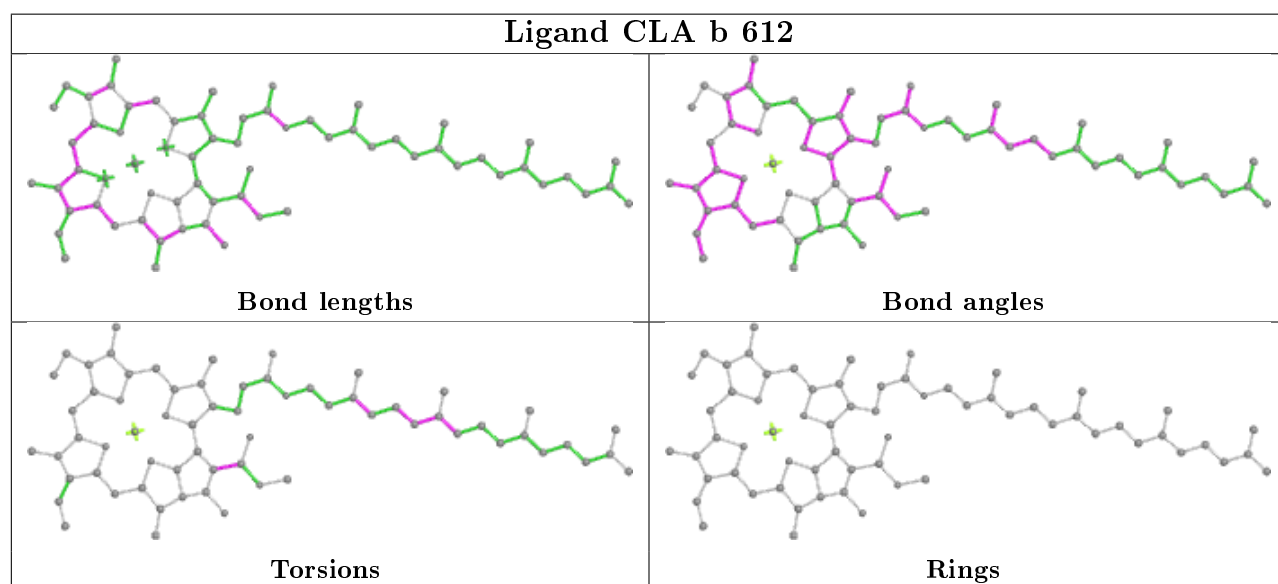
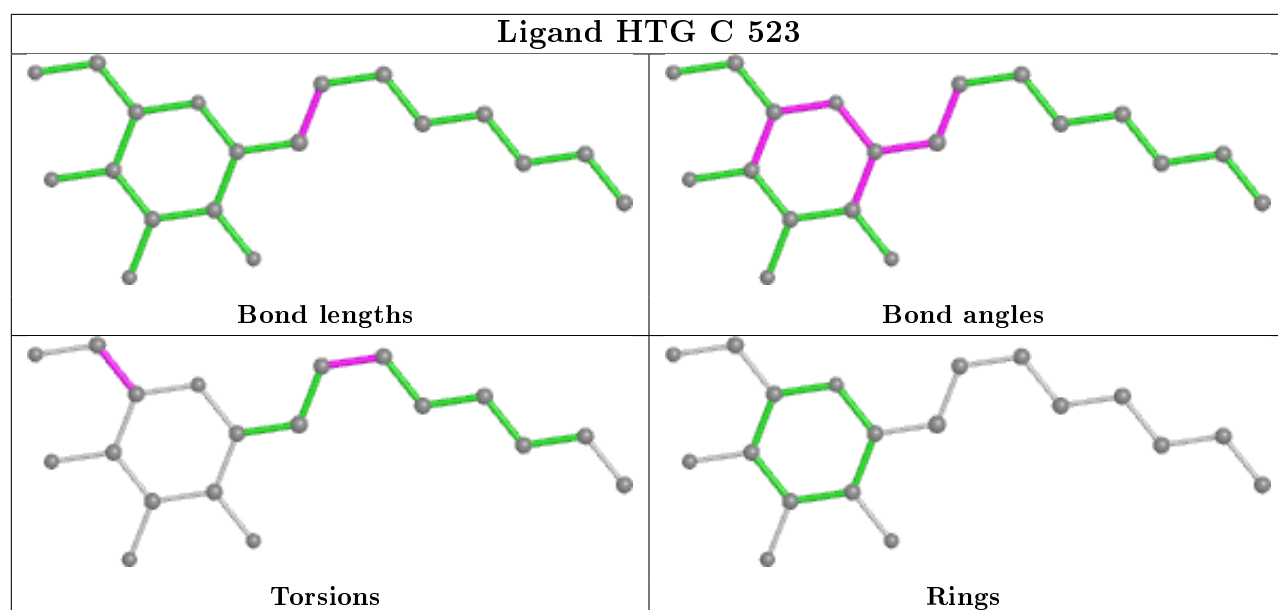


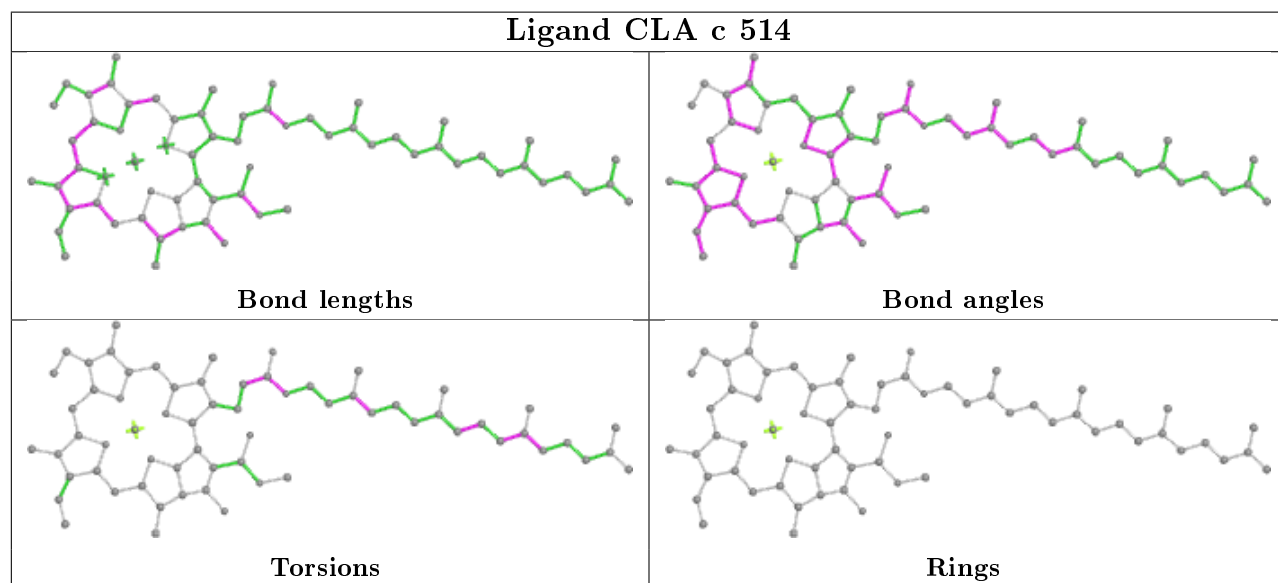
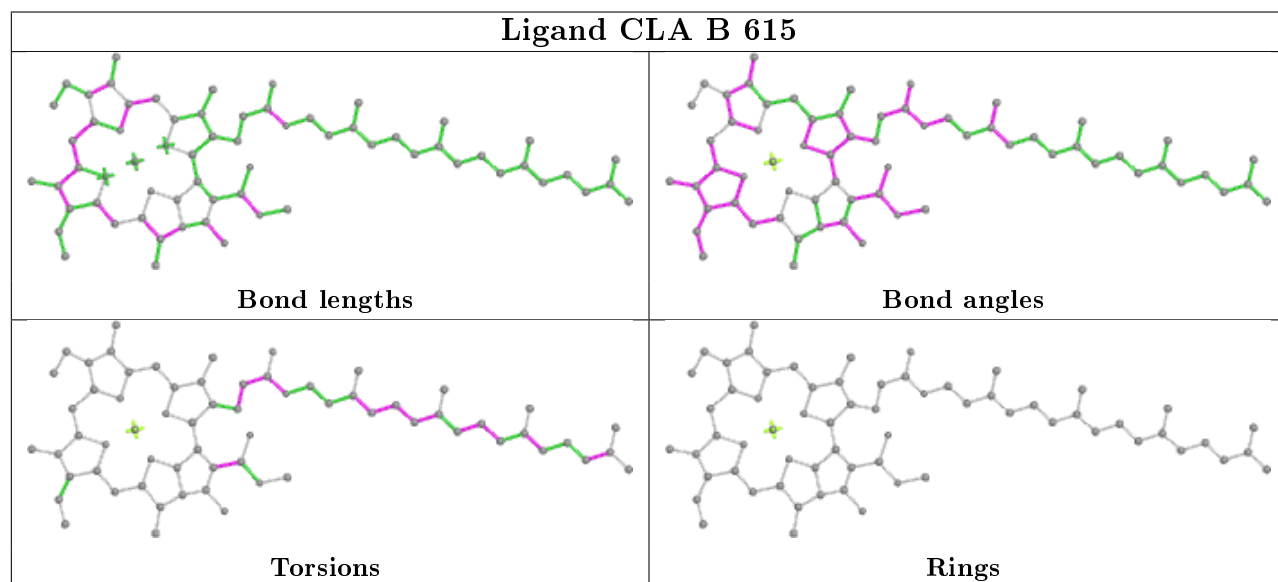
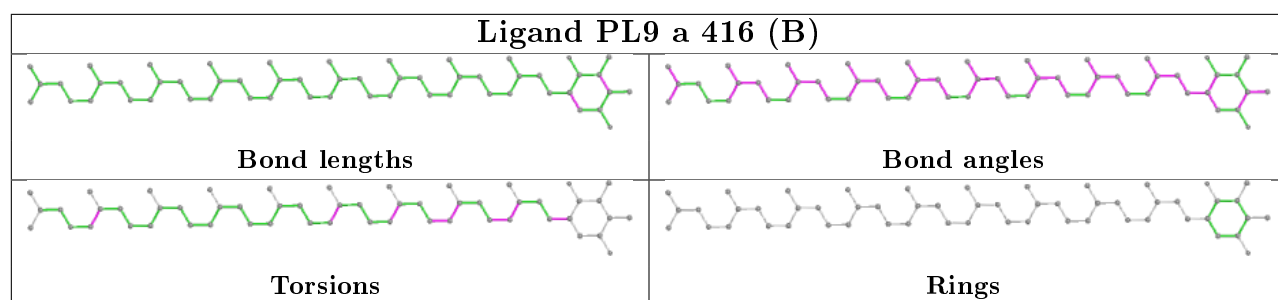
Ligand CLA C 509

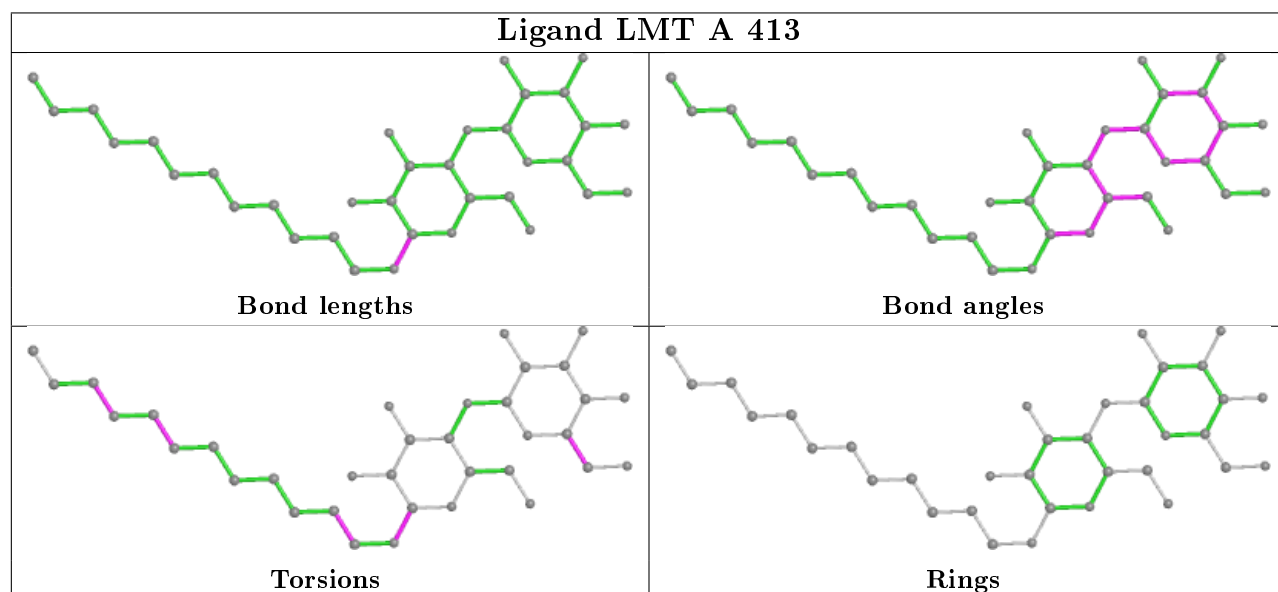
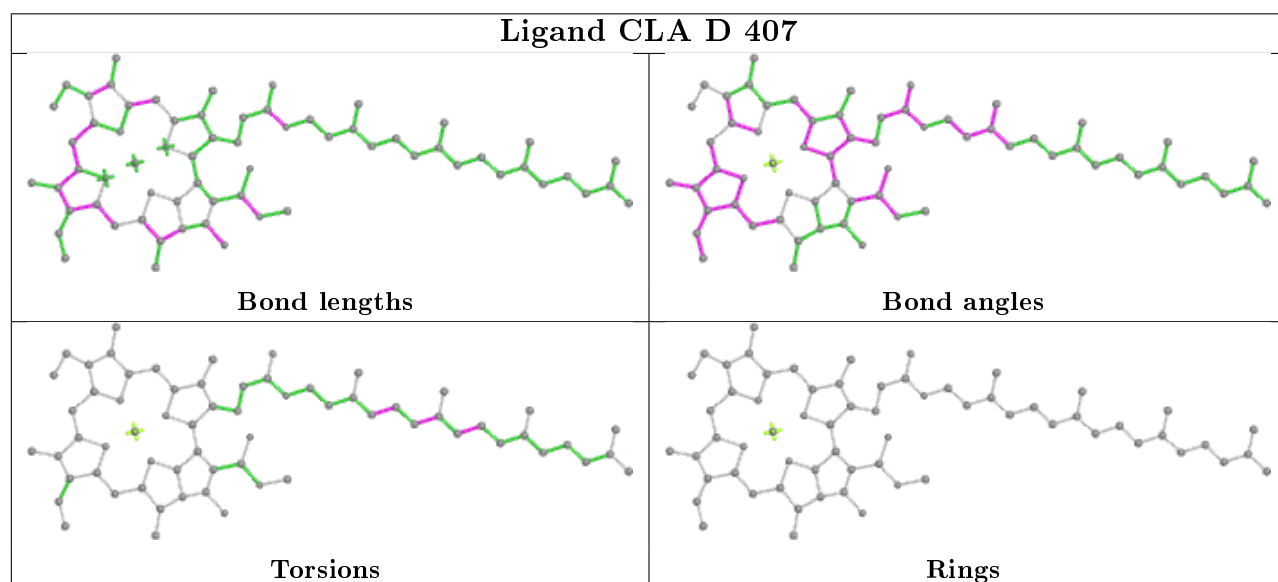
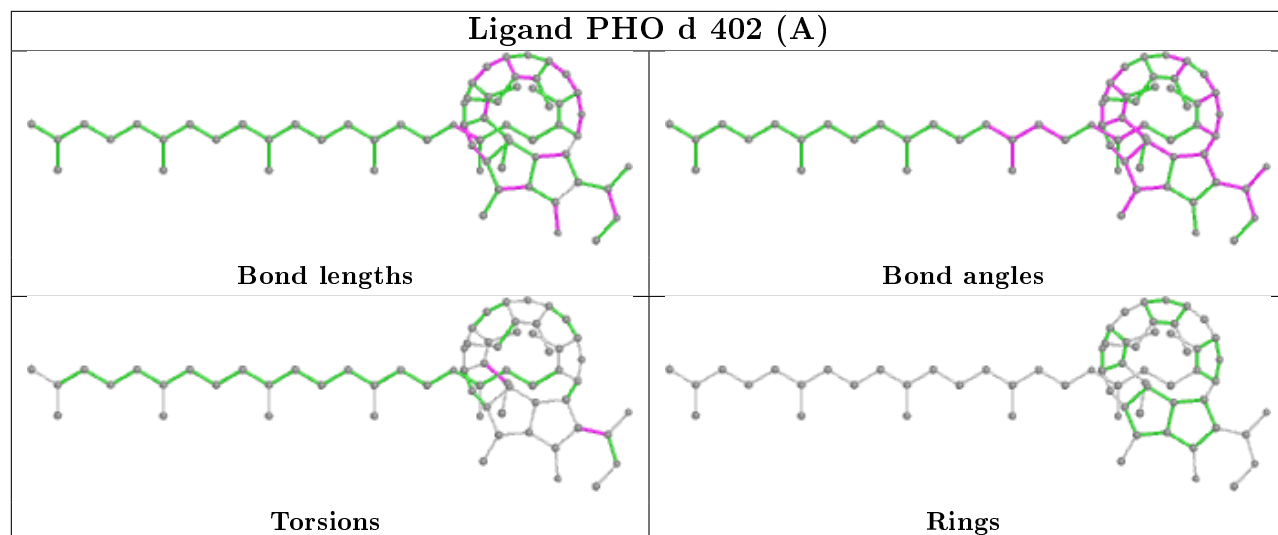


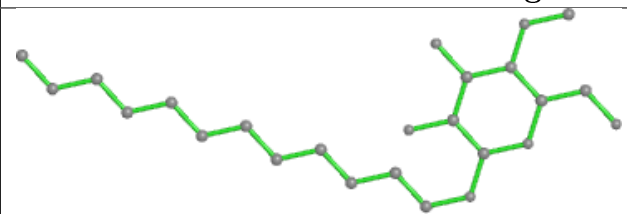
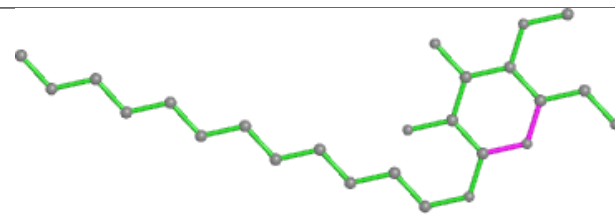
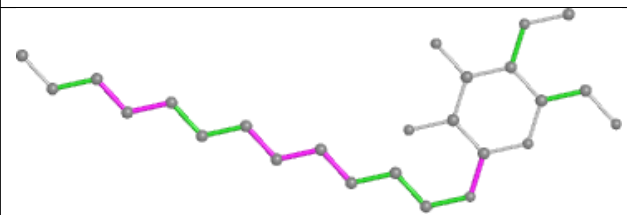
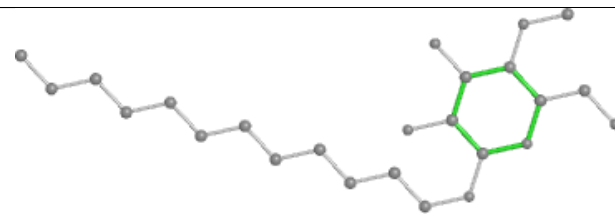
Ligand BCR b 627

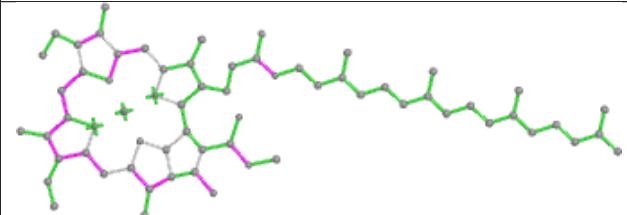
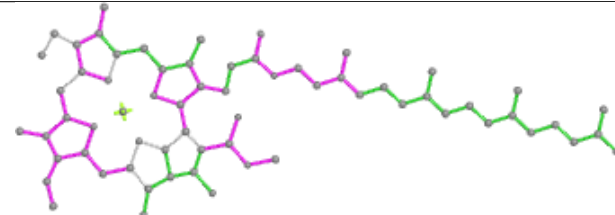
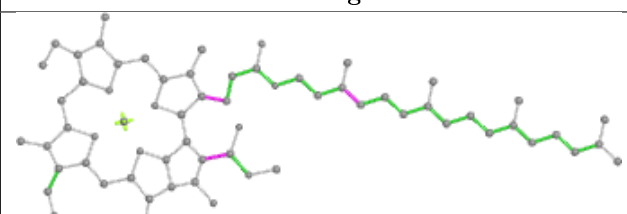
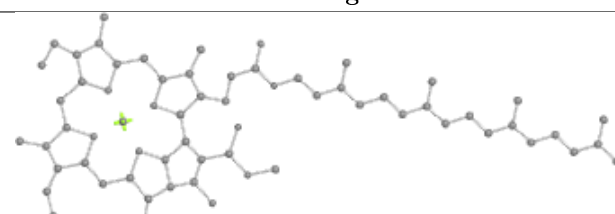


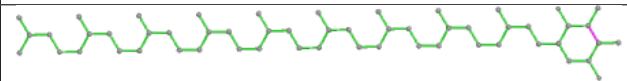
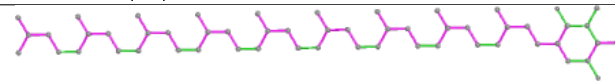
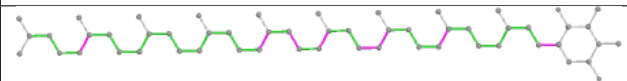
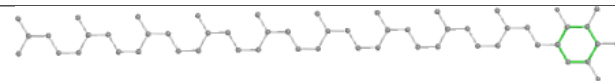


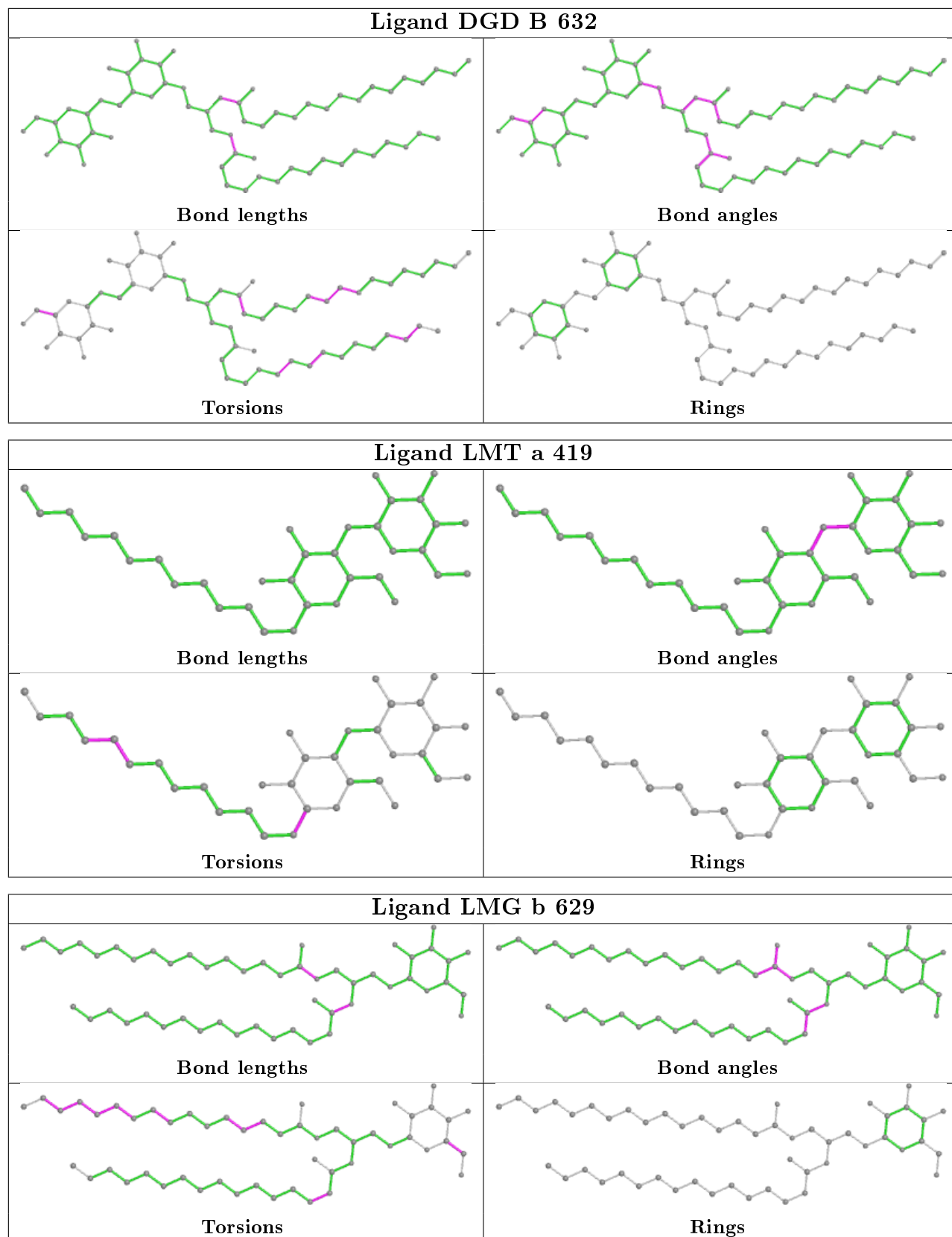


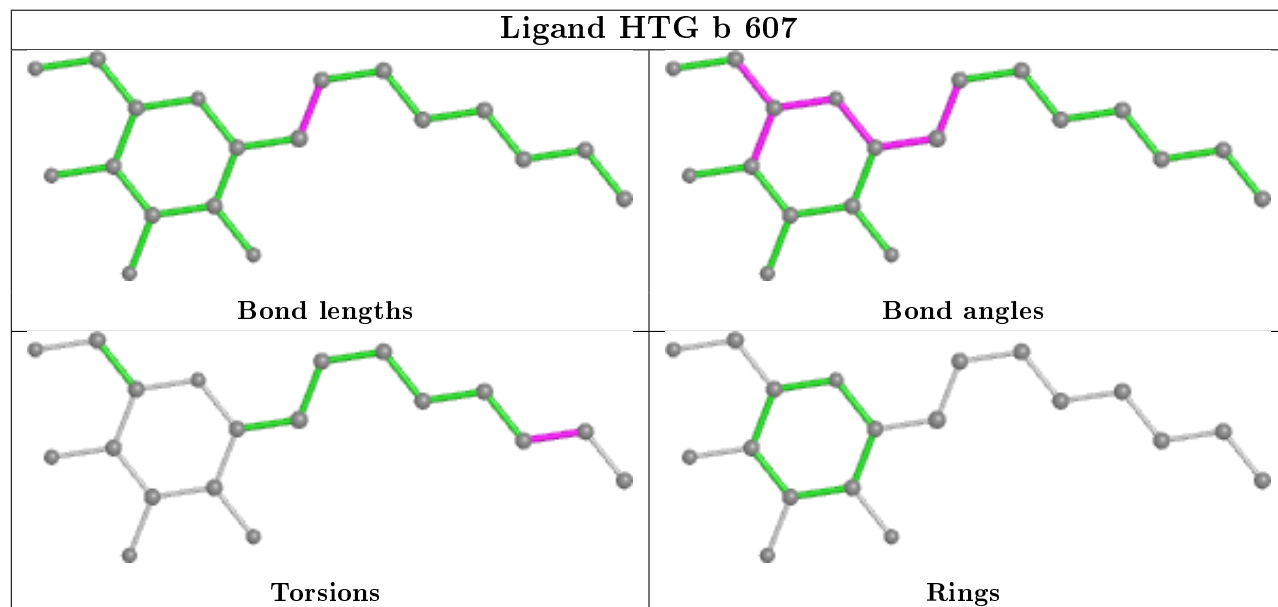
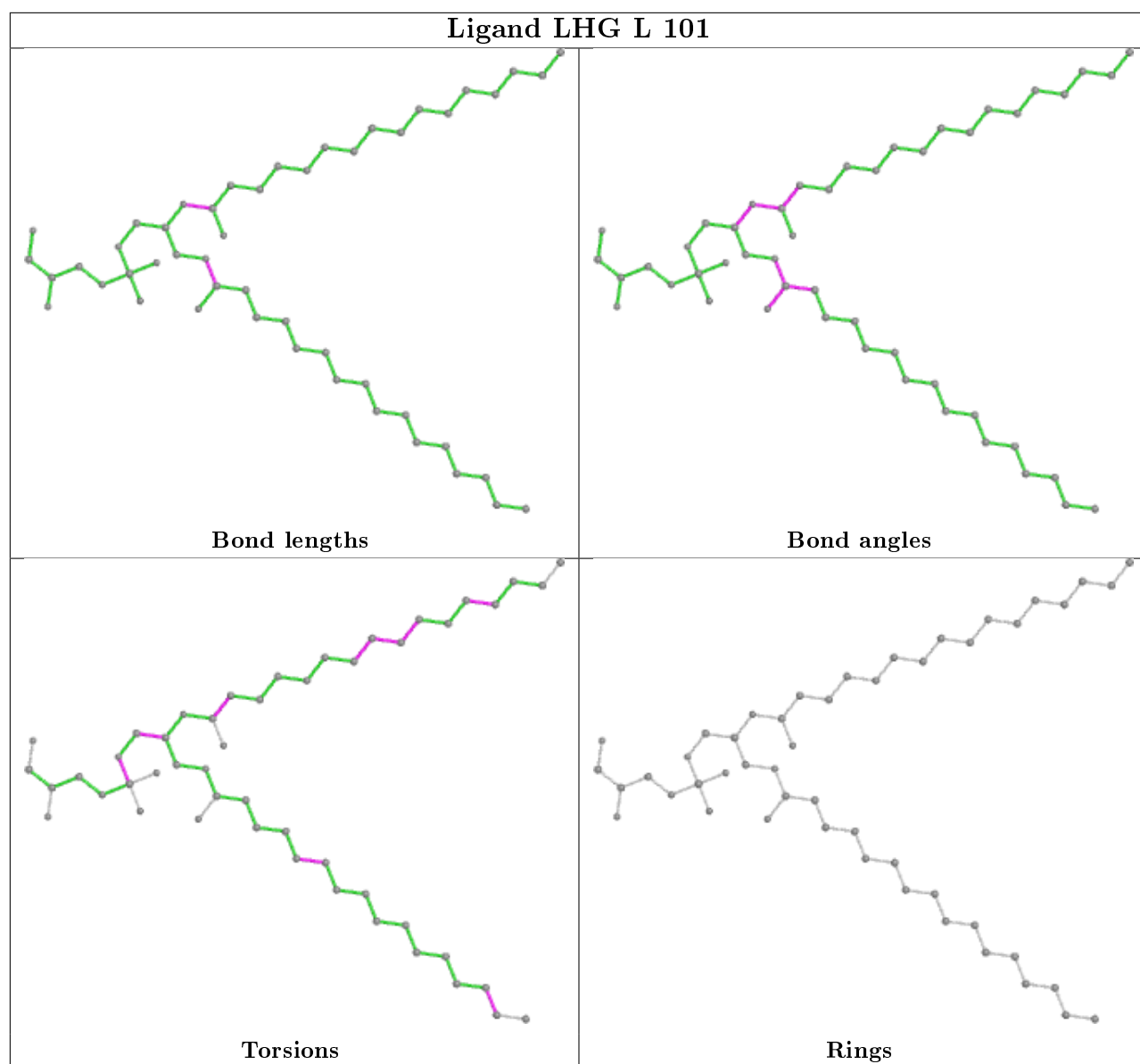


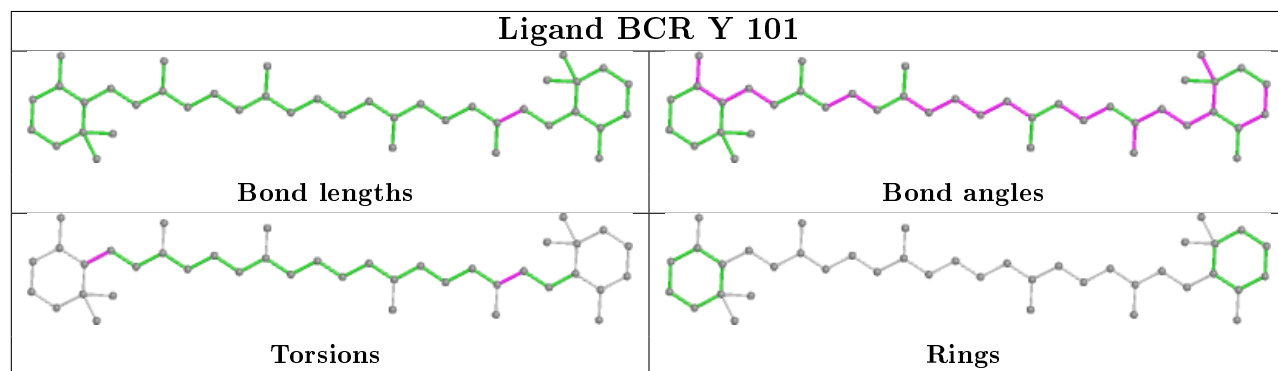
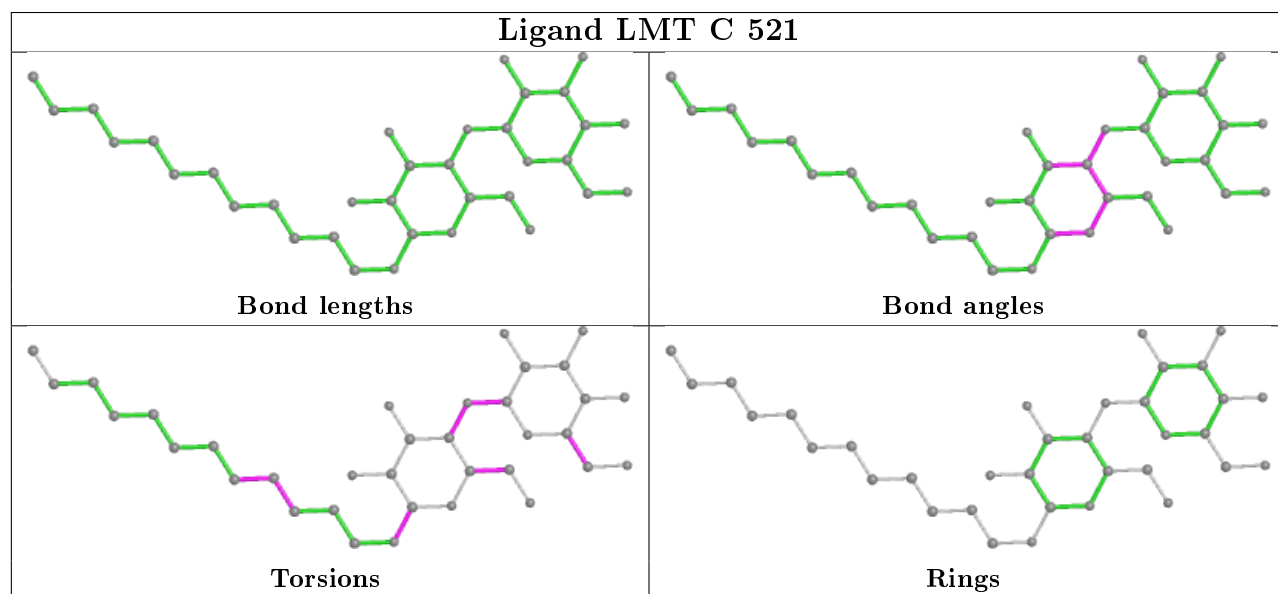
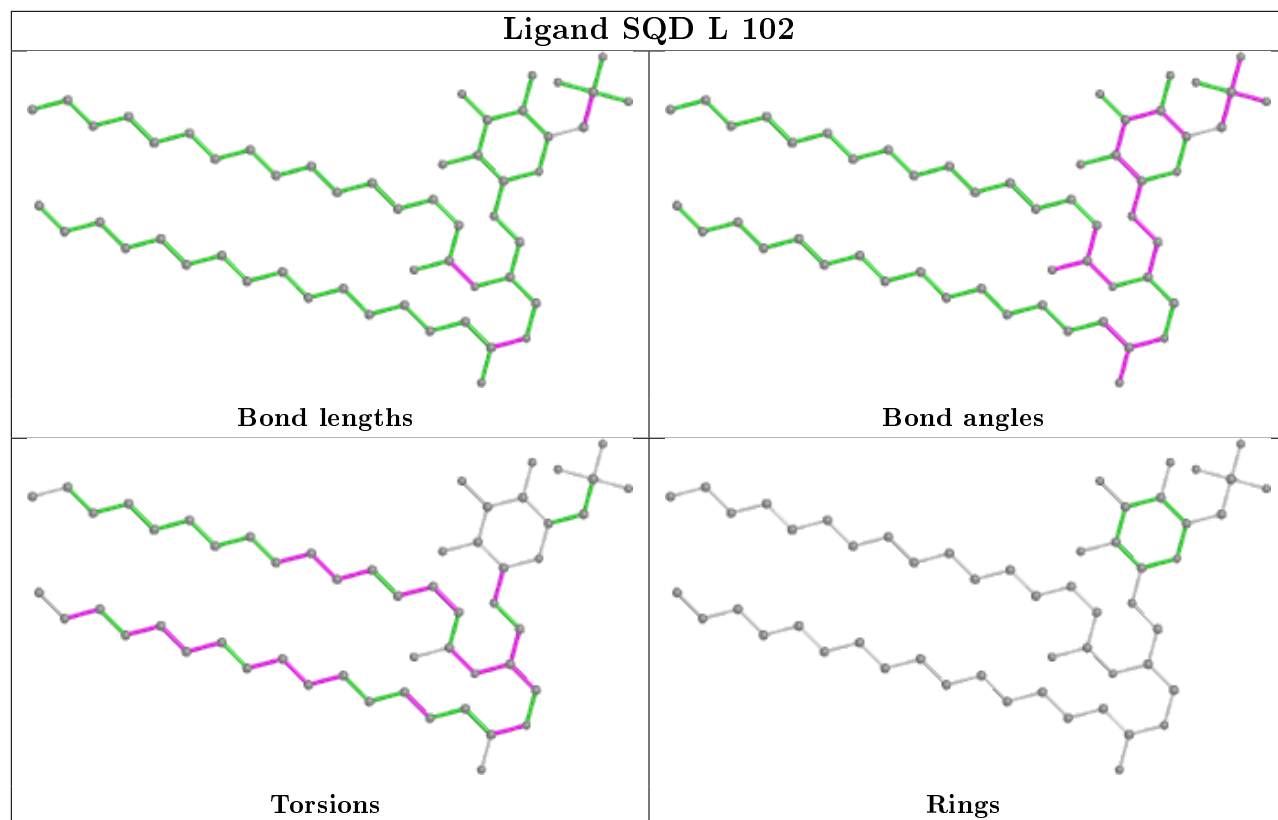
Ligand LMT t 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

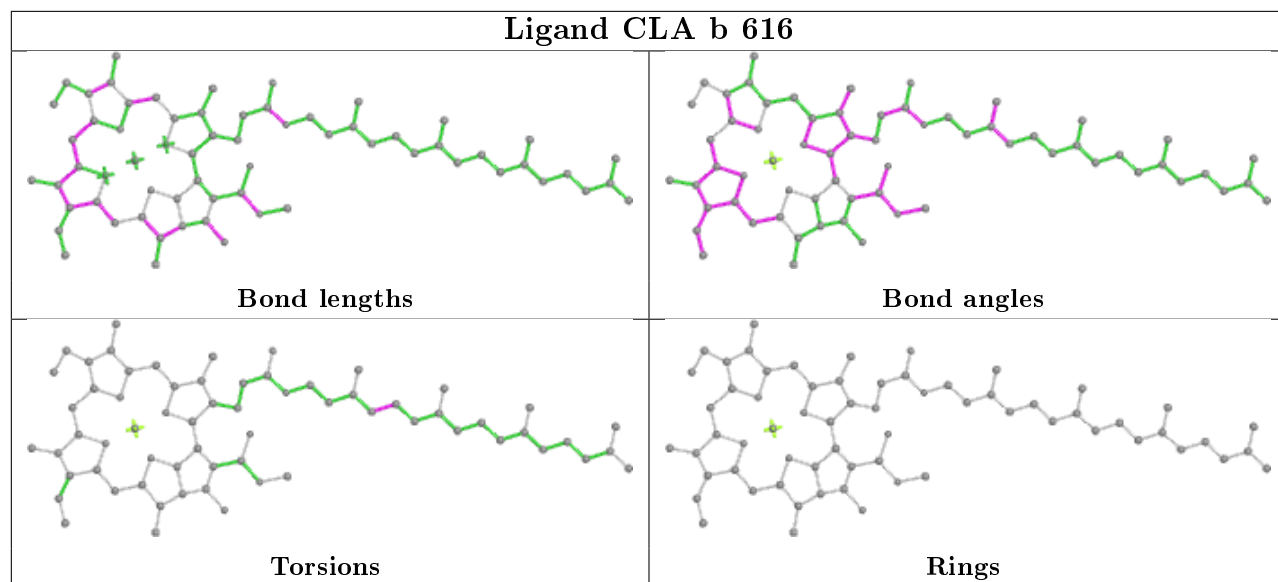
Ligand PL9 A 416 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings



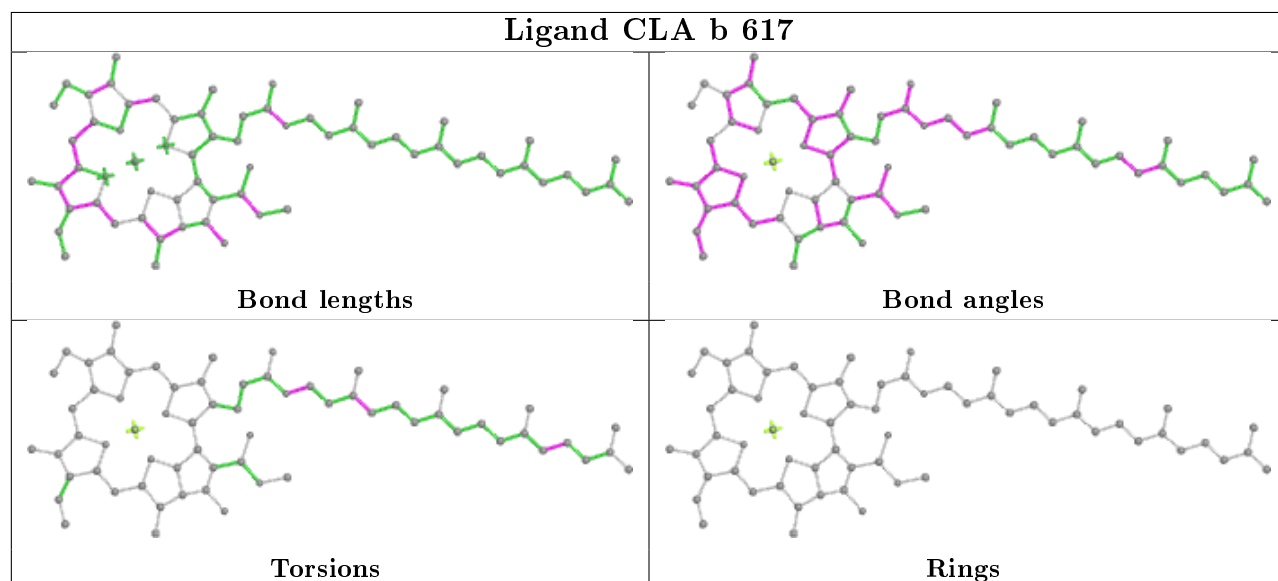




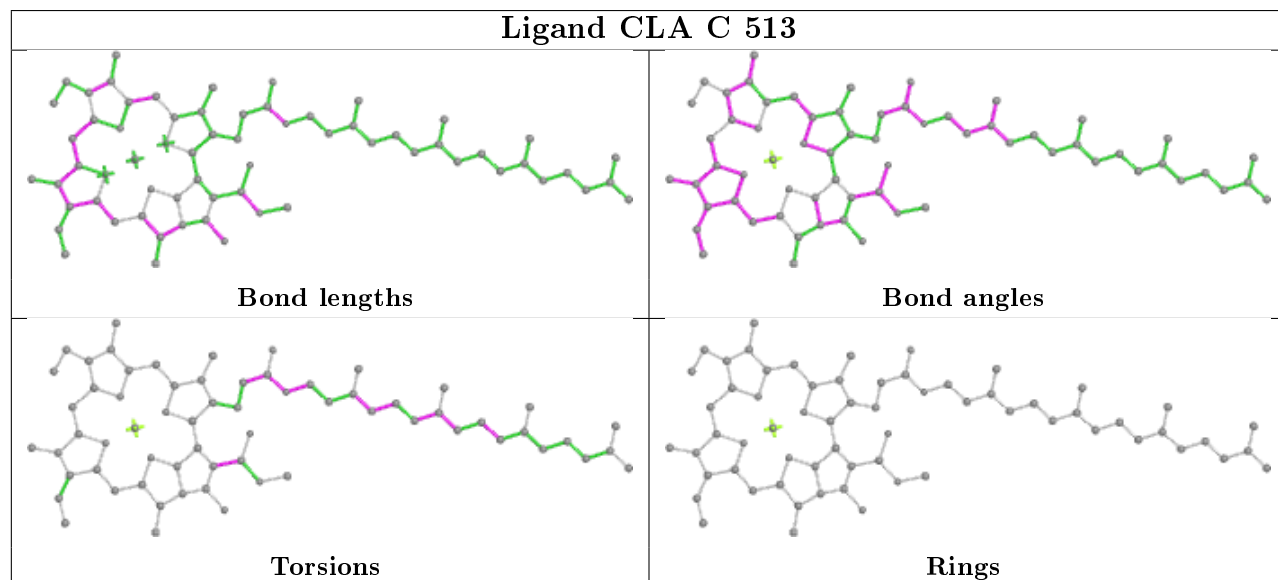
Ligand CLA b 616

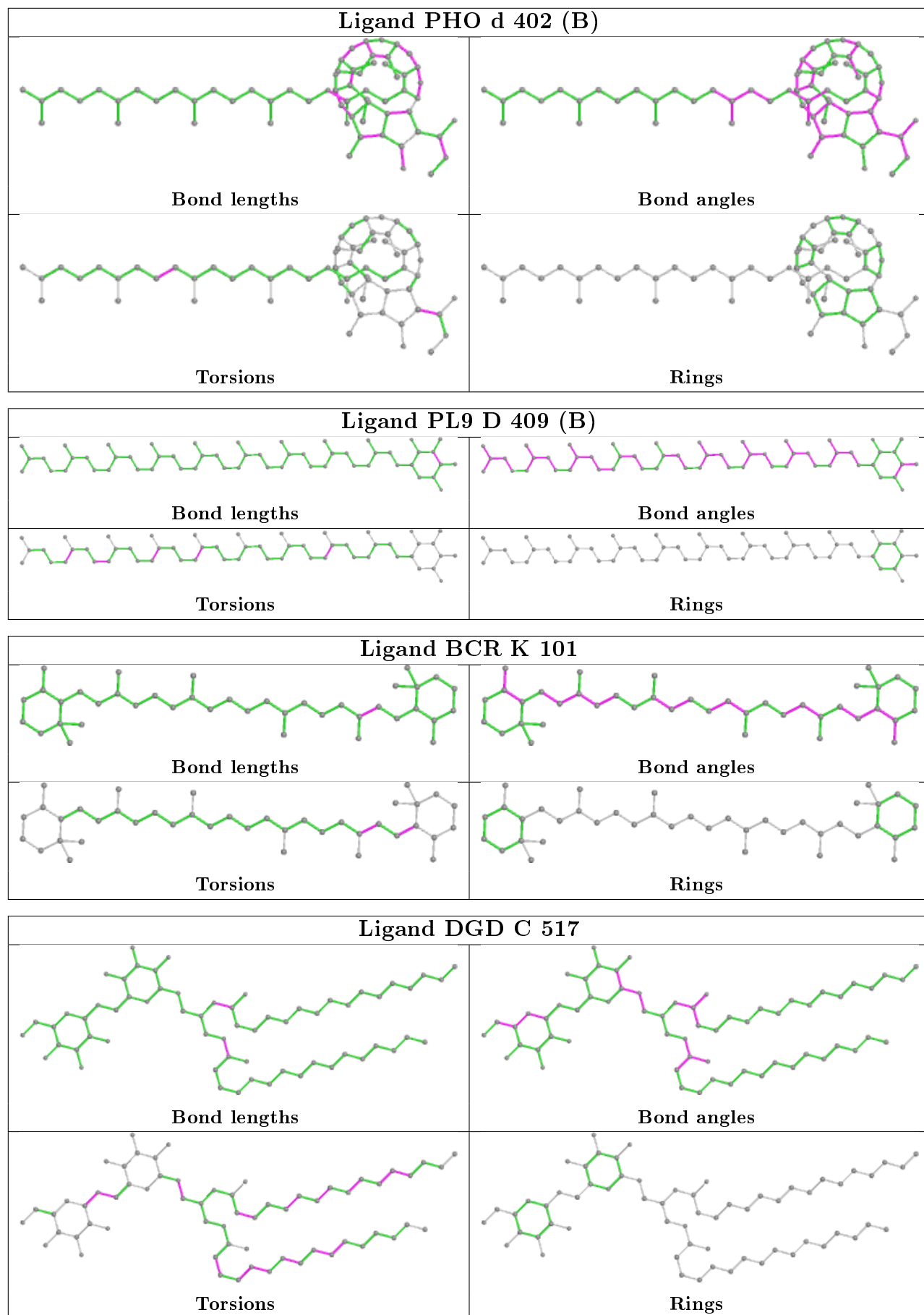


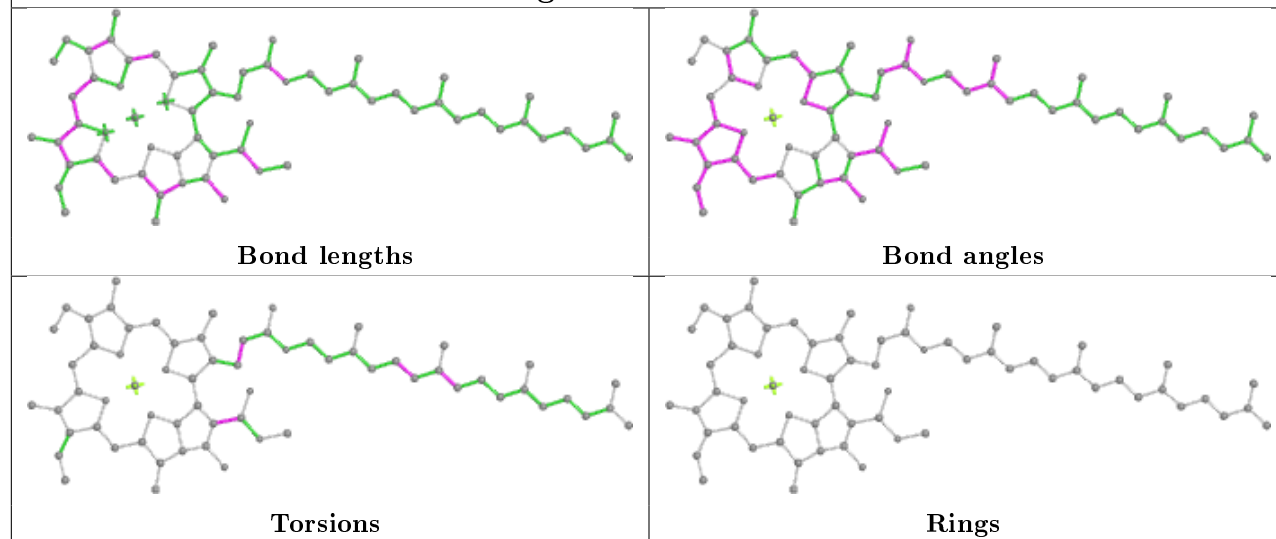
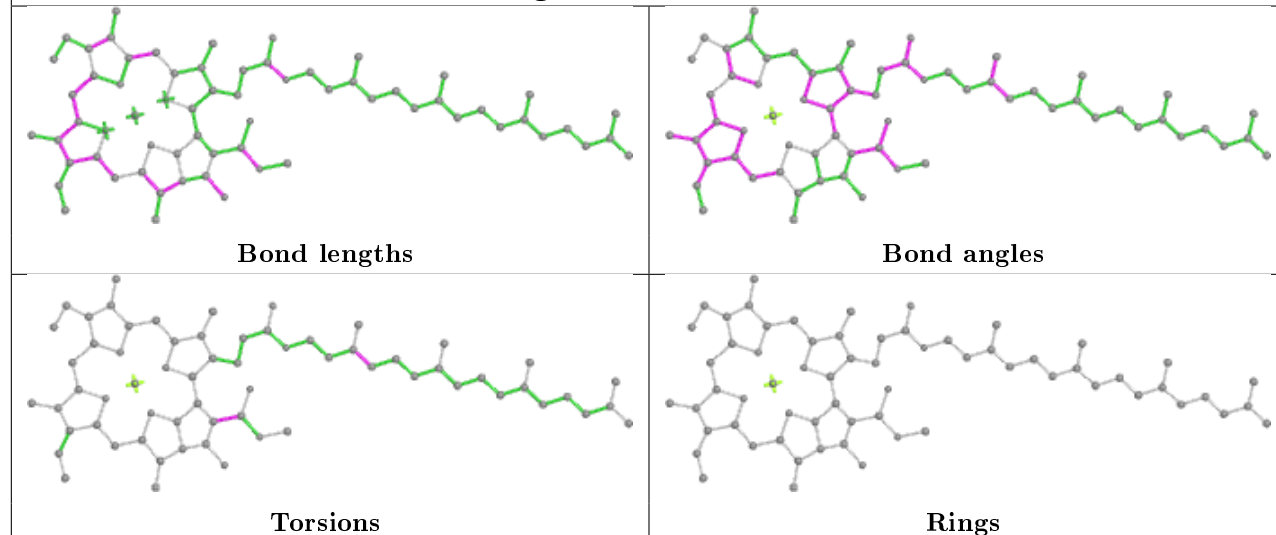
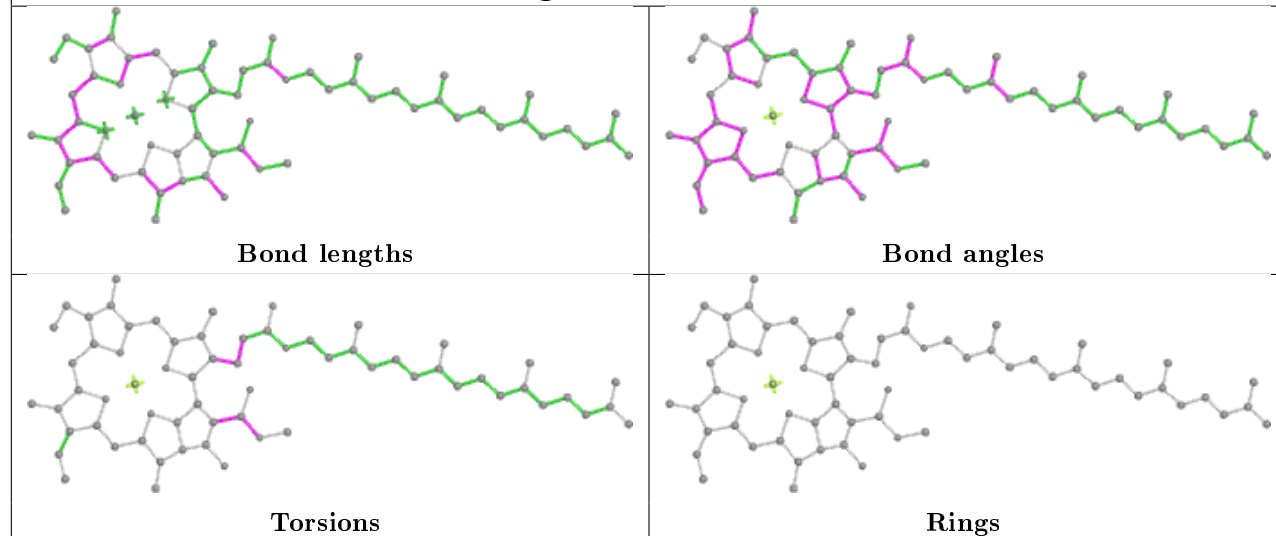
Ligand CLA b 617

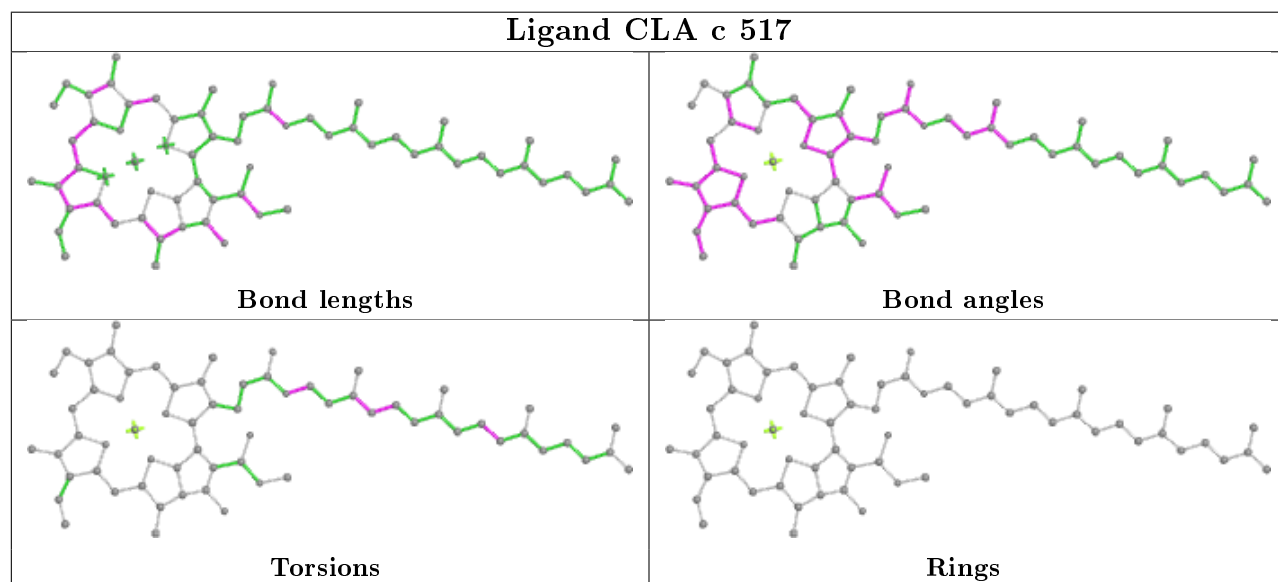
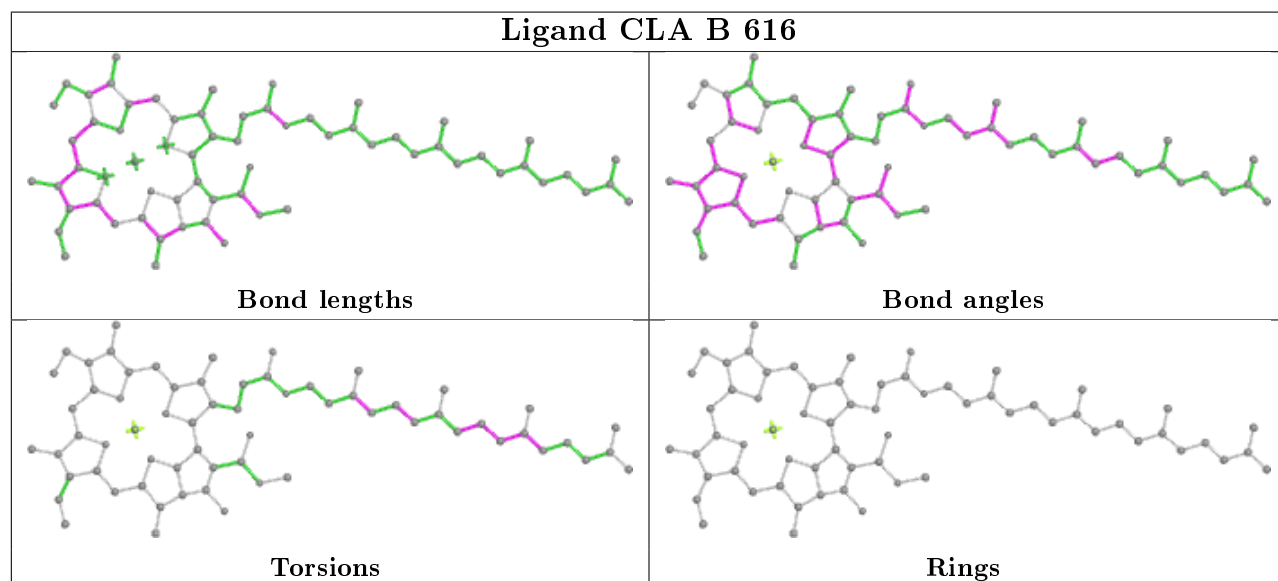
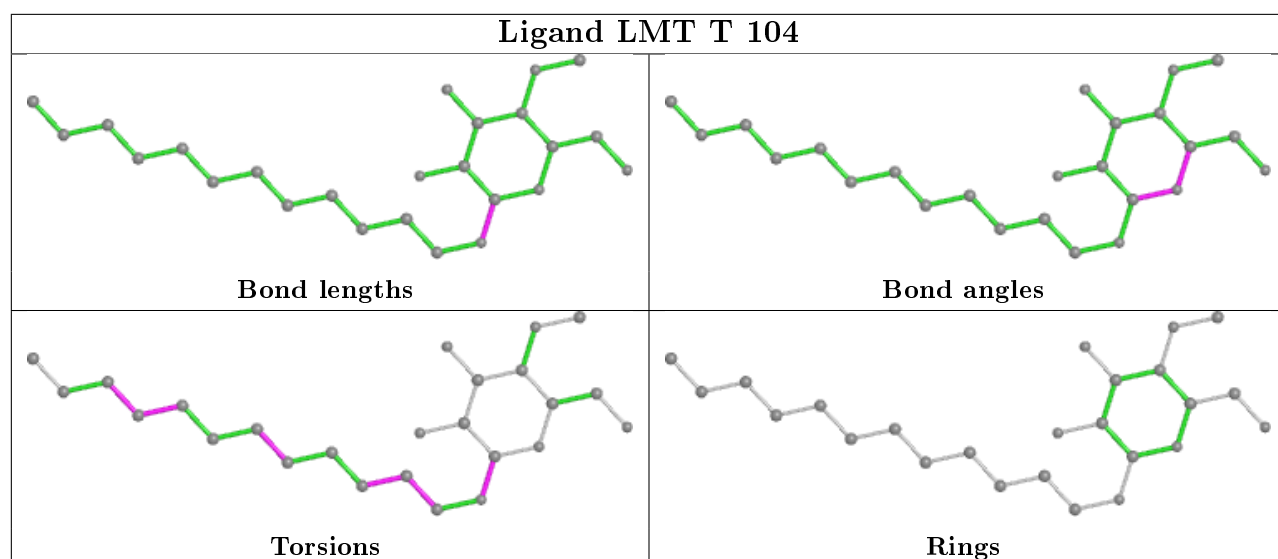


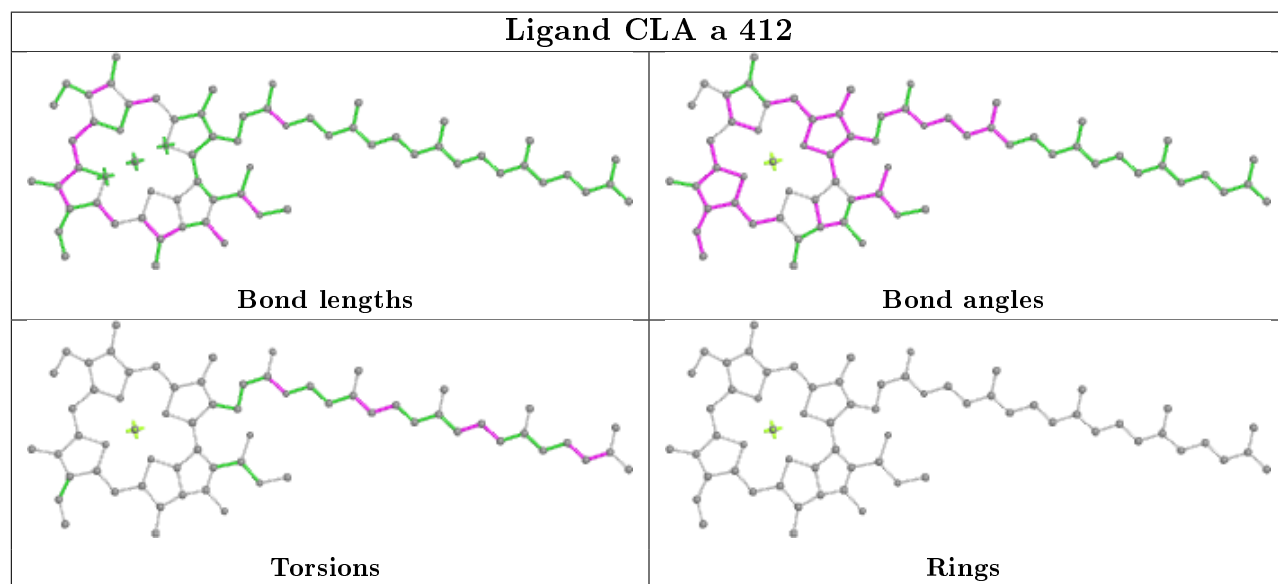
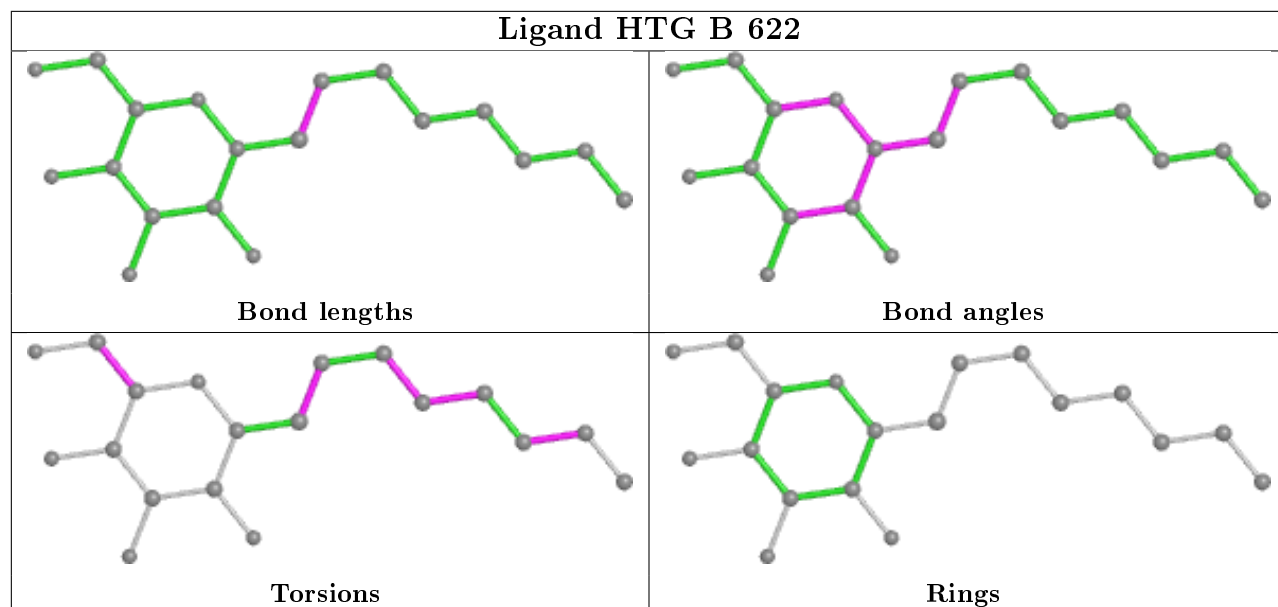
Ligand CLA C 513

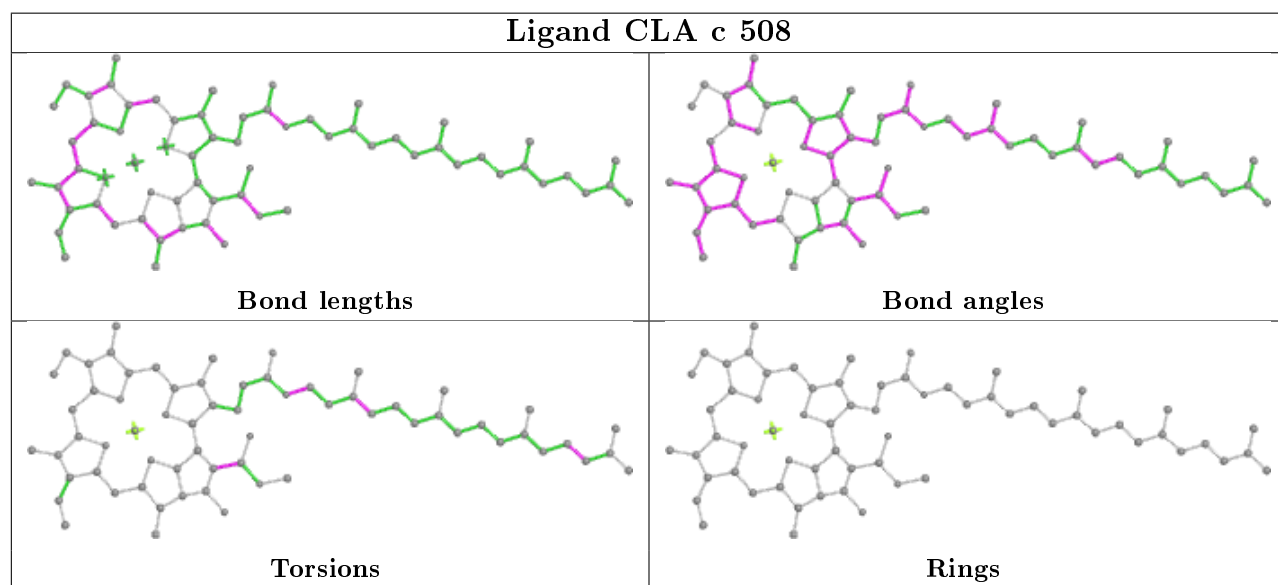
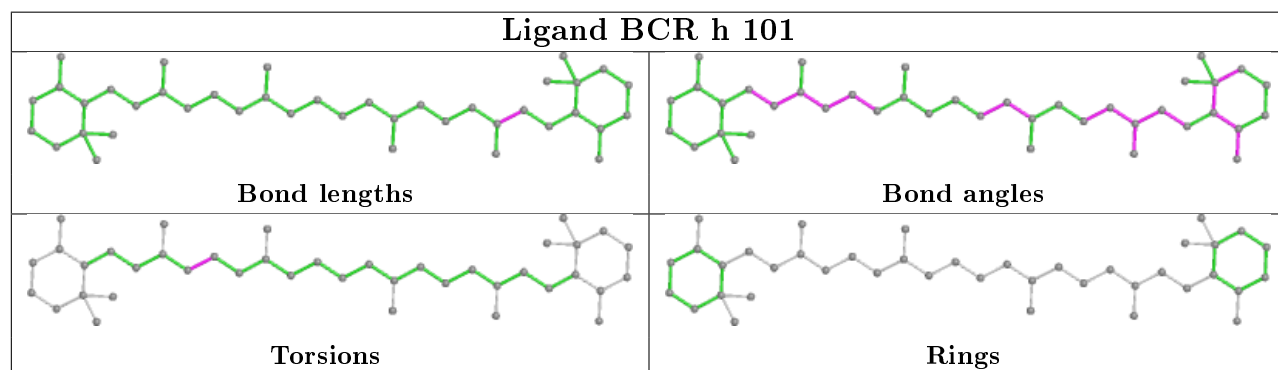
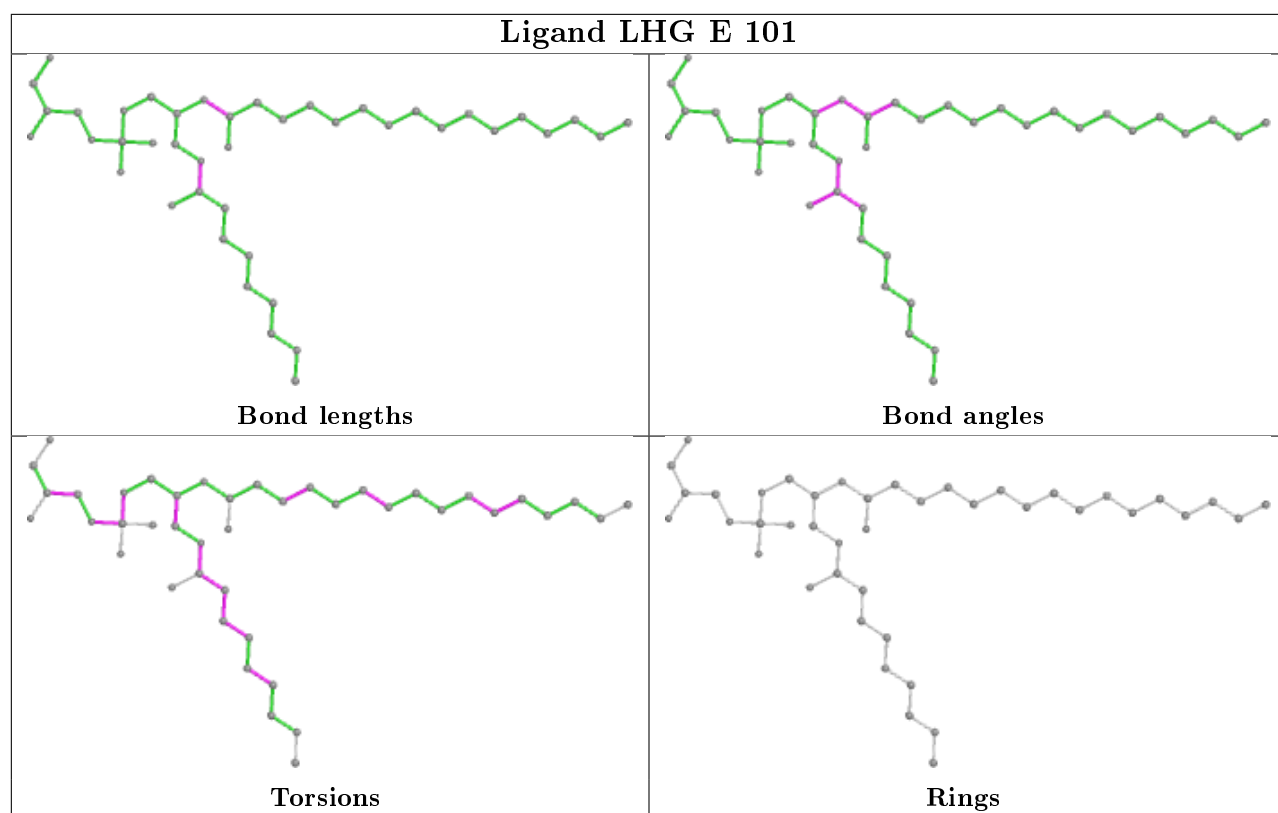


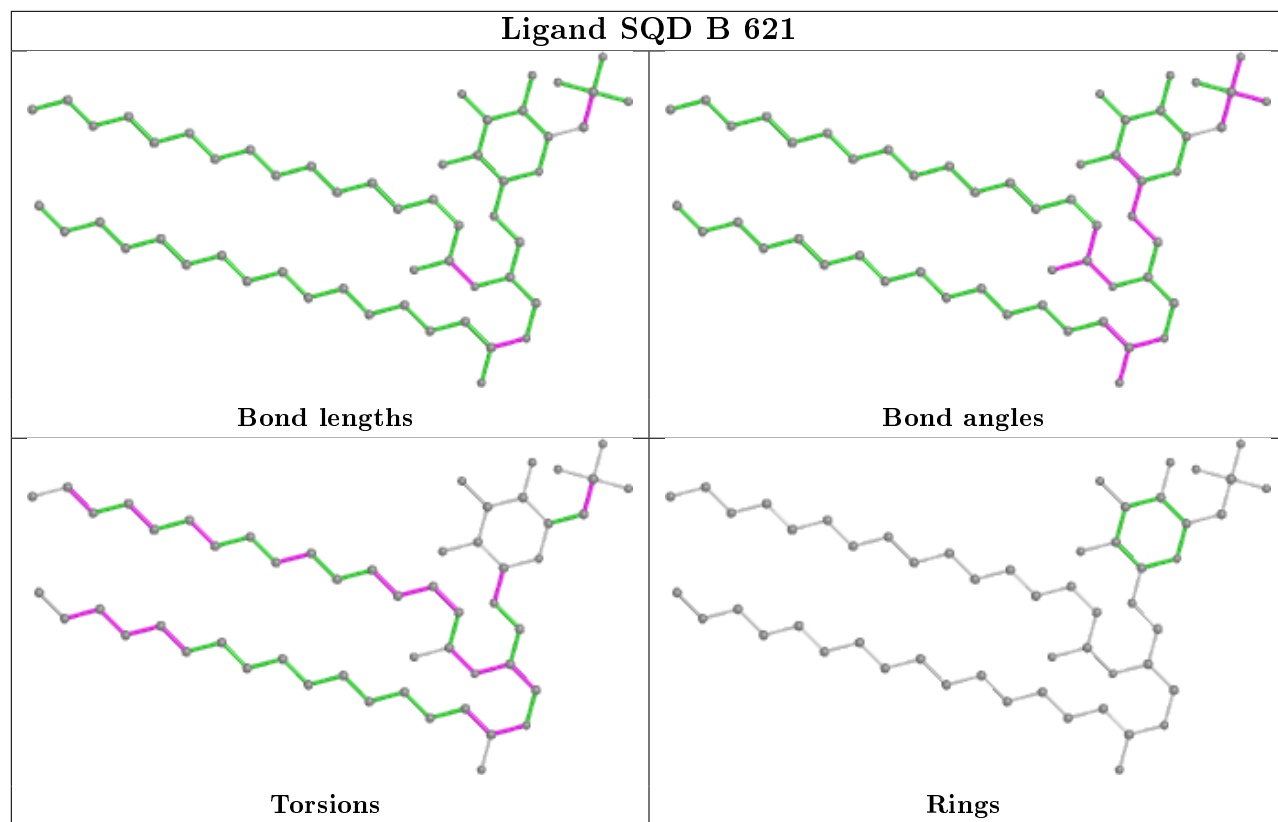
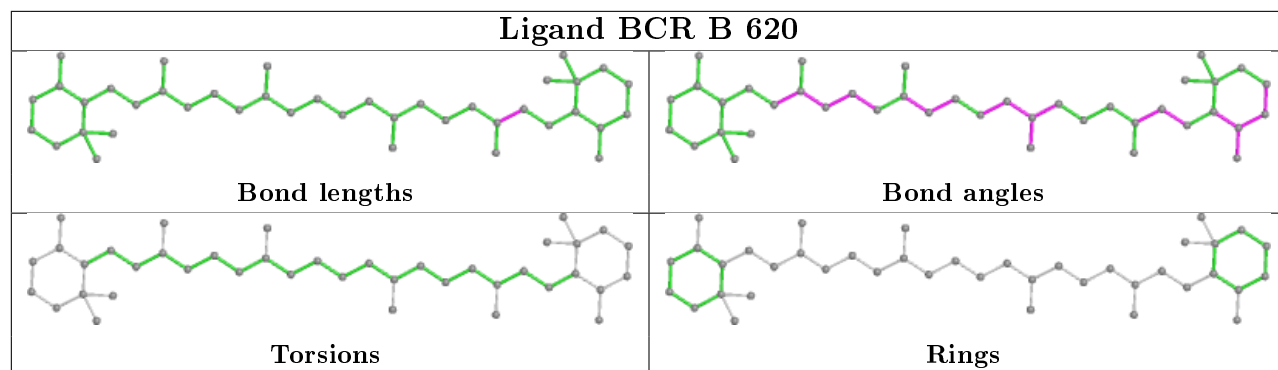


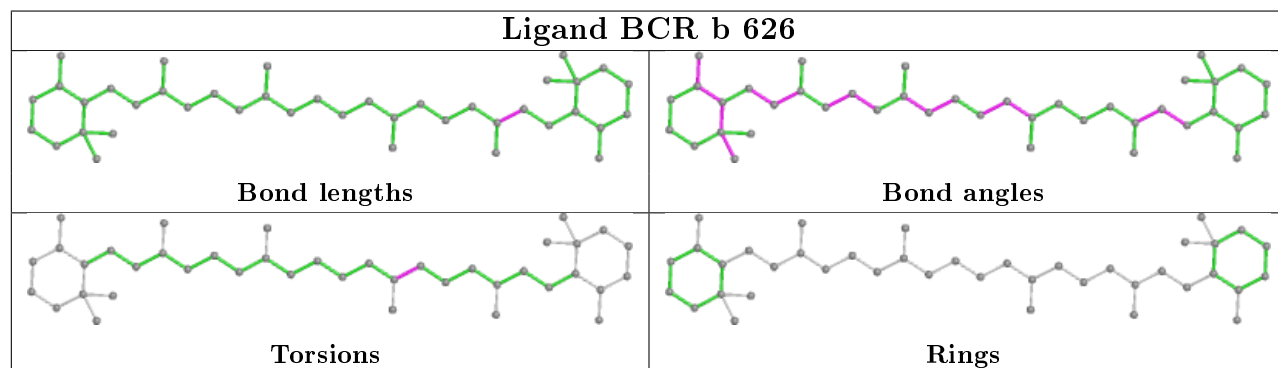
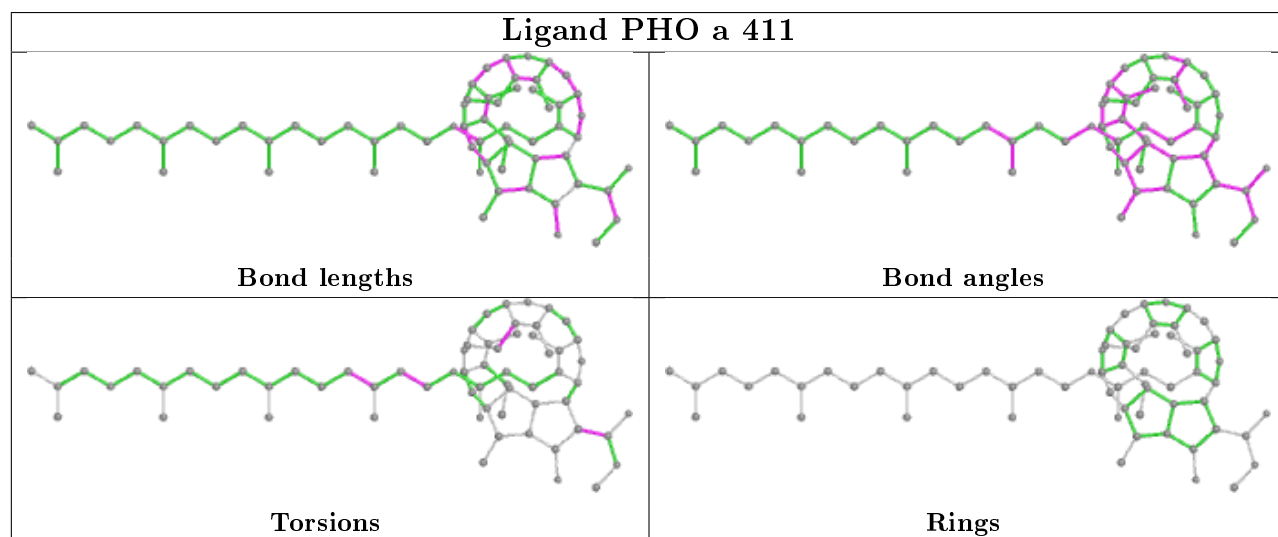
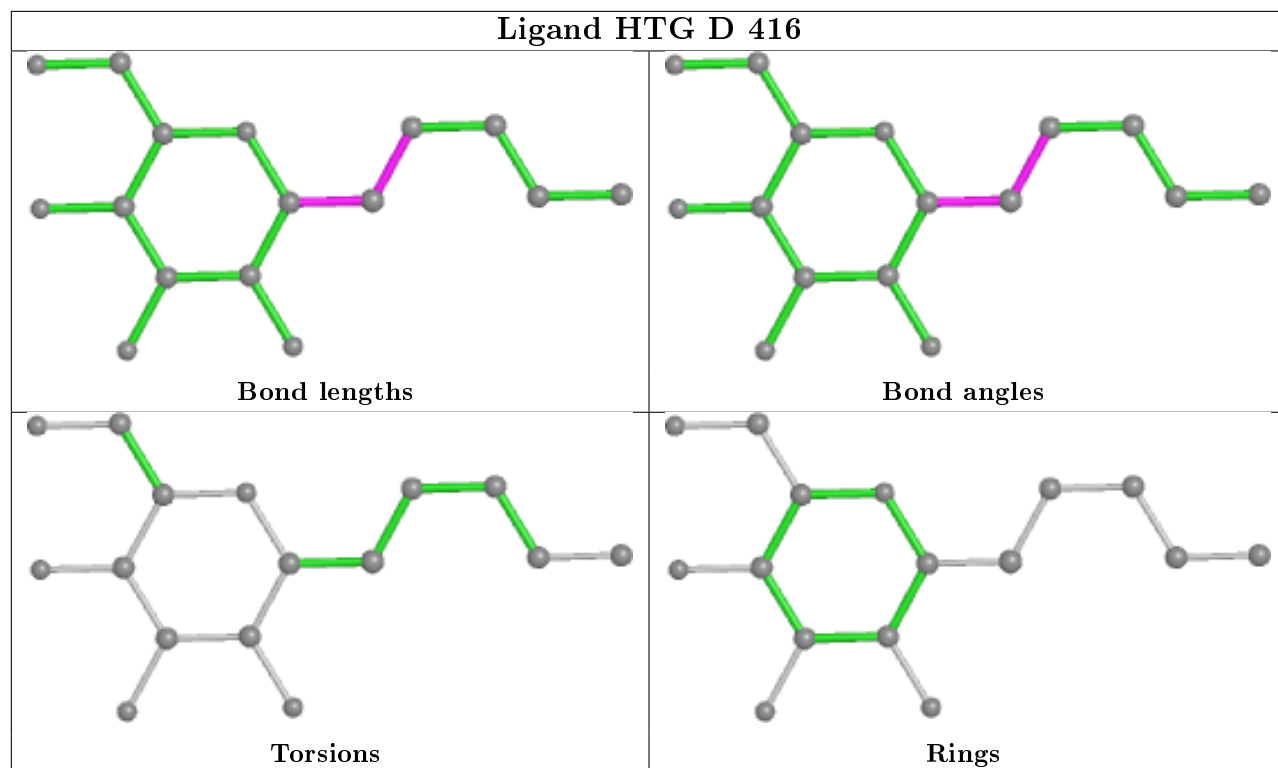
Ligand CLA c 511**Ligand CLA B 606****Ligand CLA c 505**



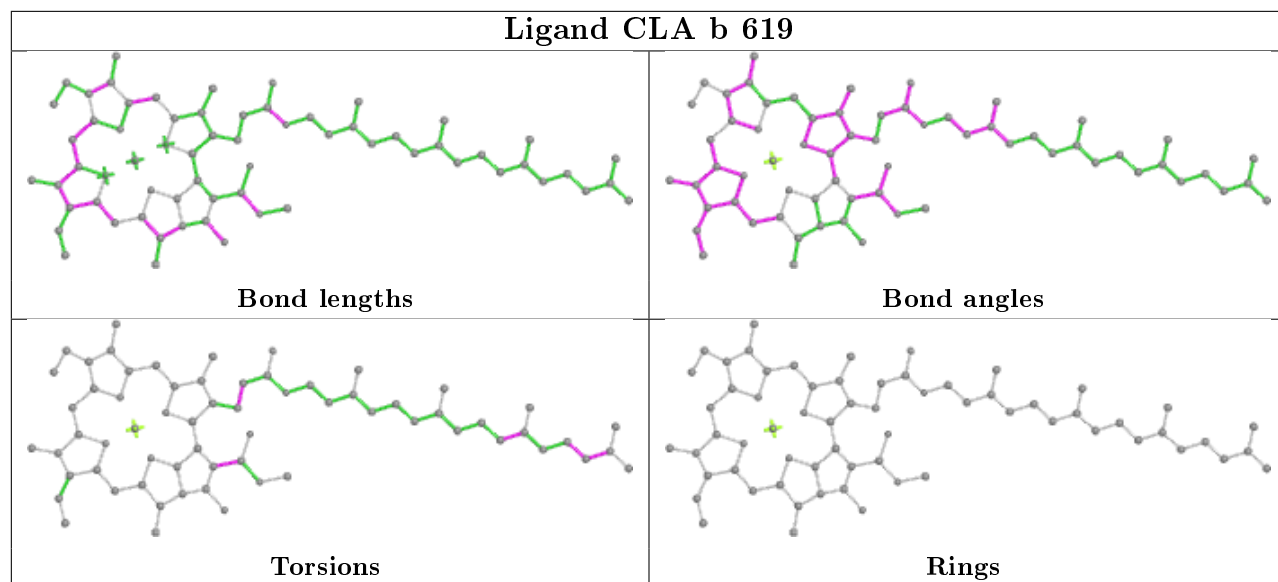




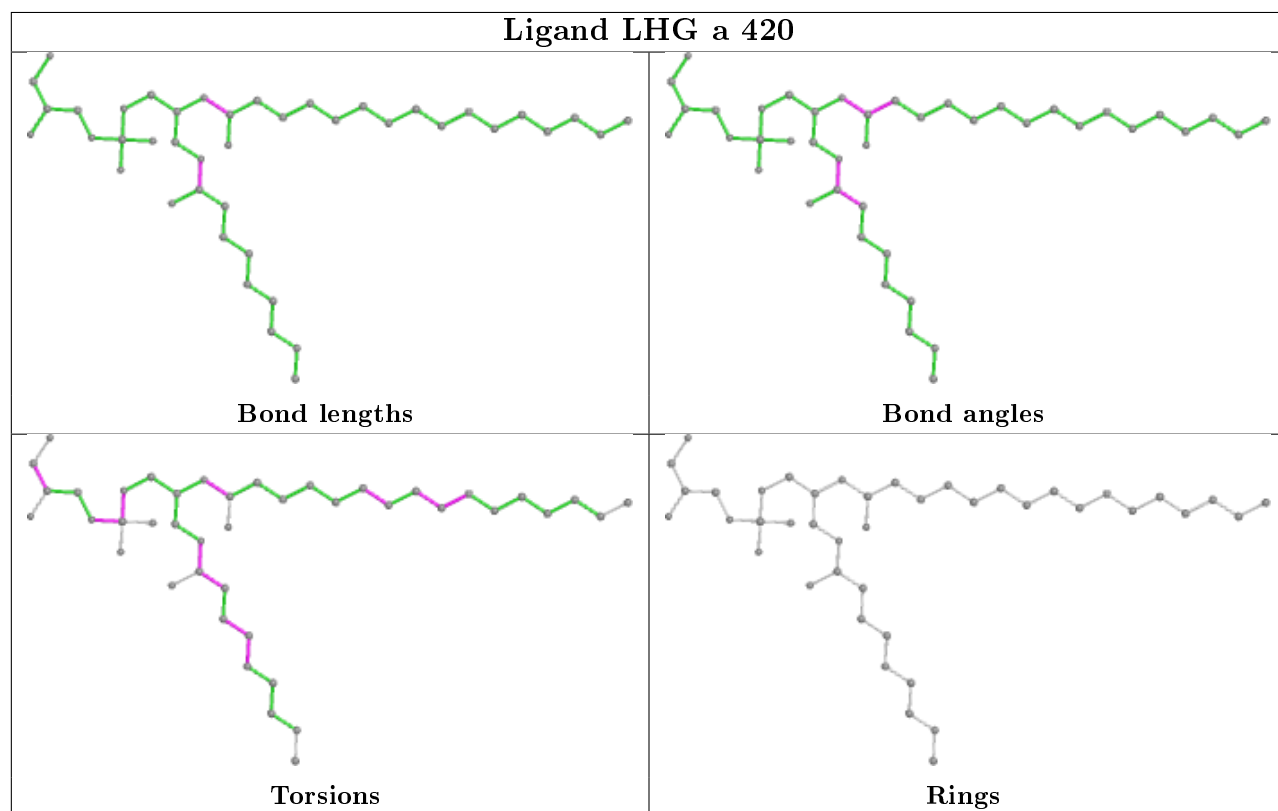


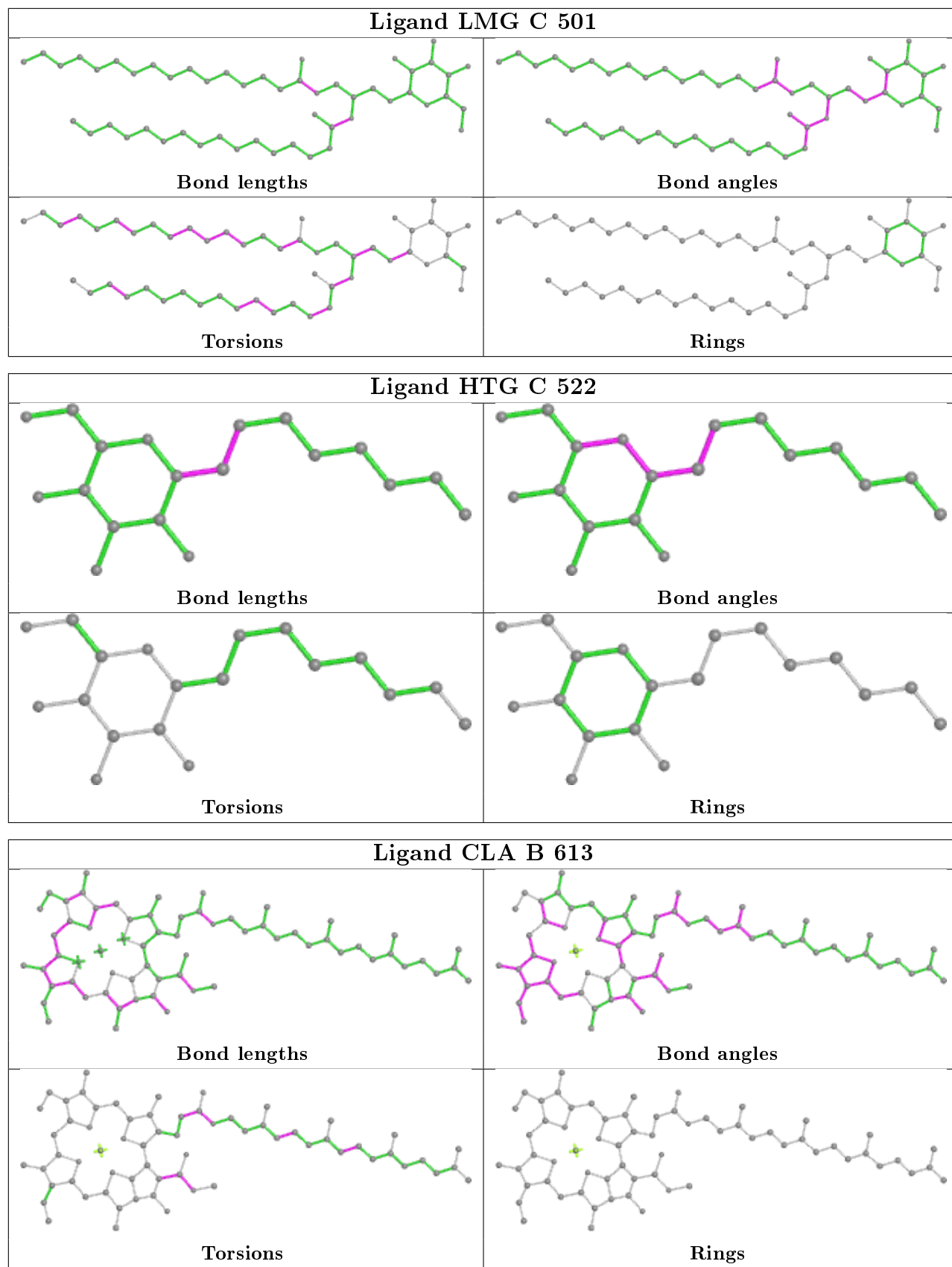


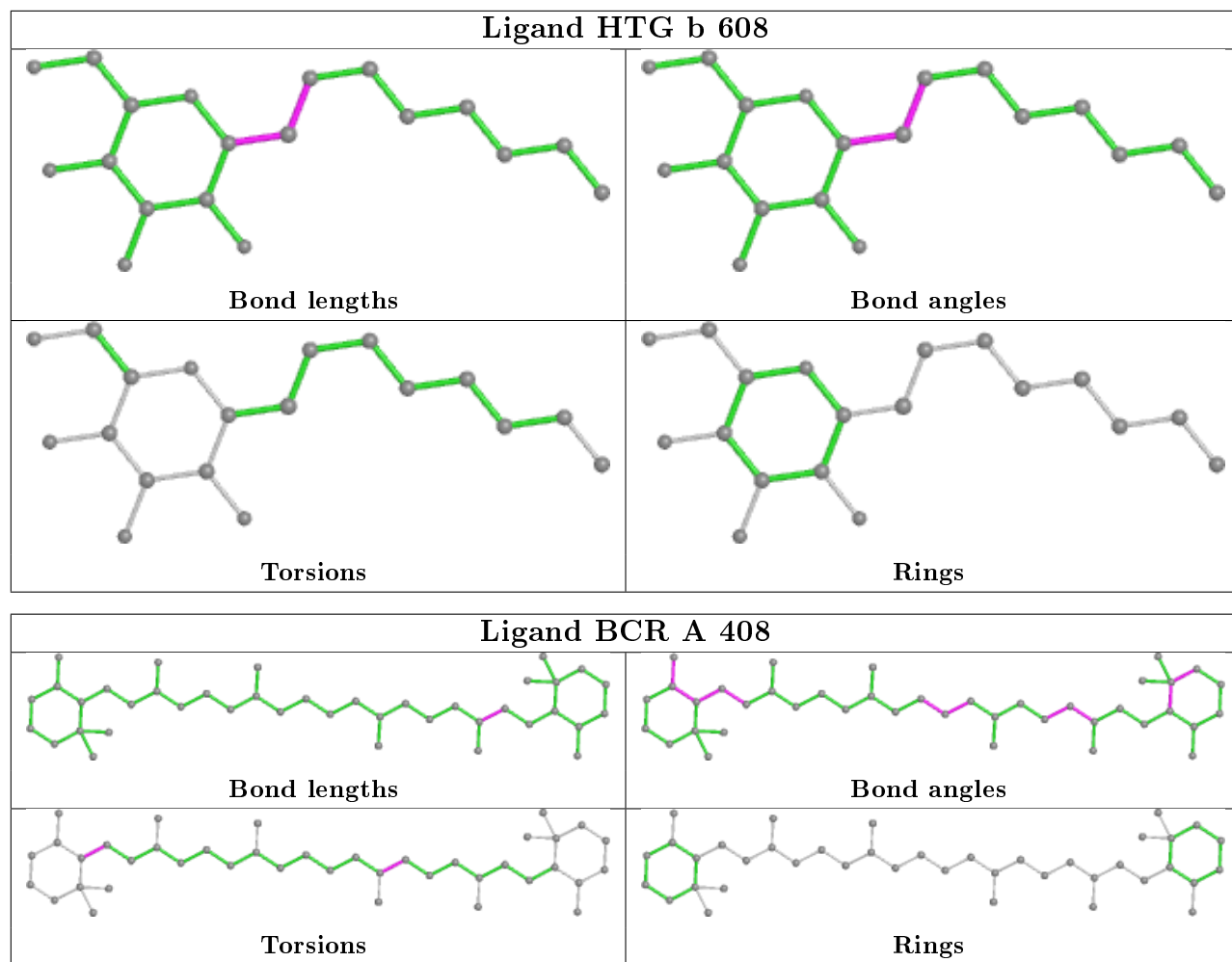
Ligand CLA b 619

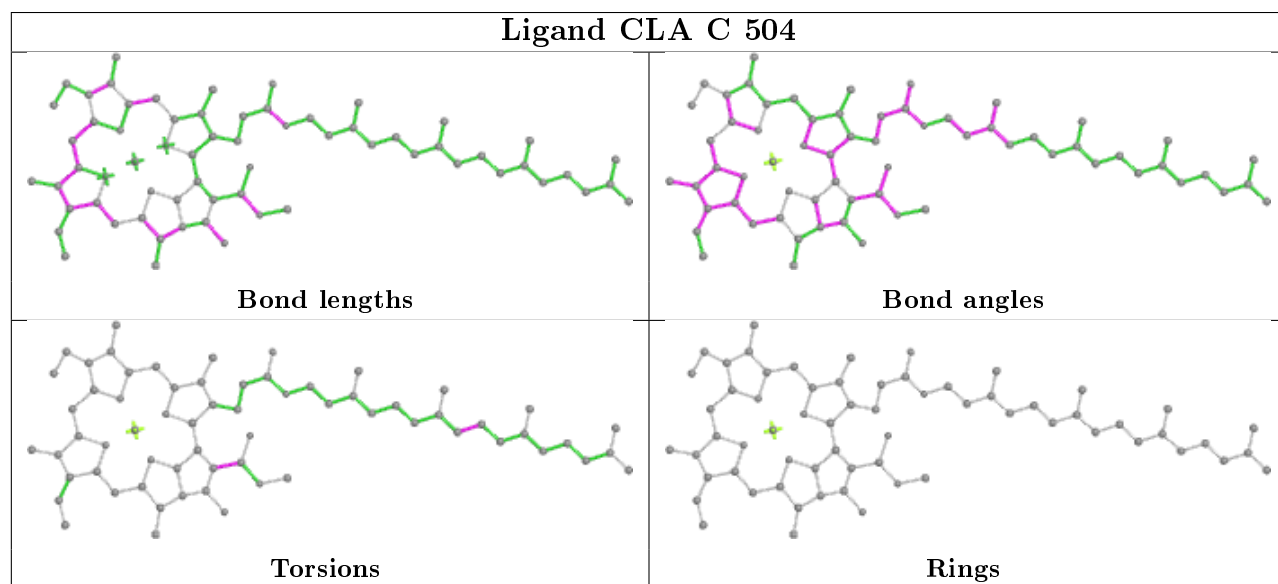
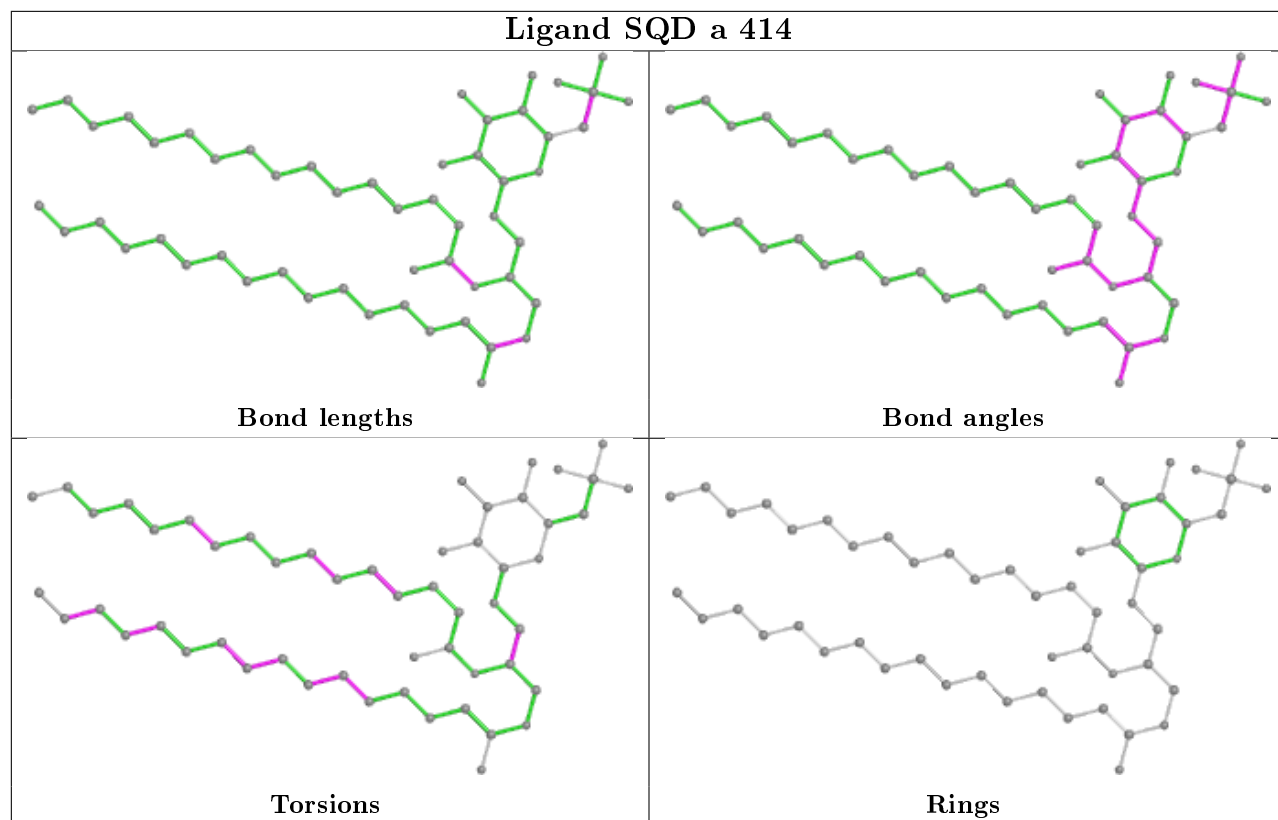


Ligand LHG a 420

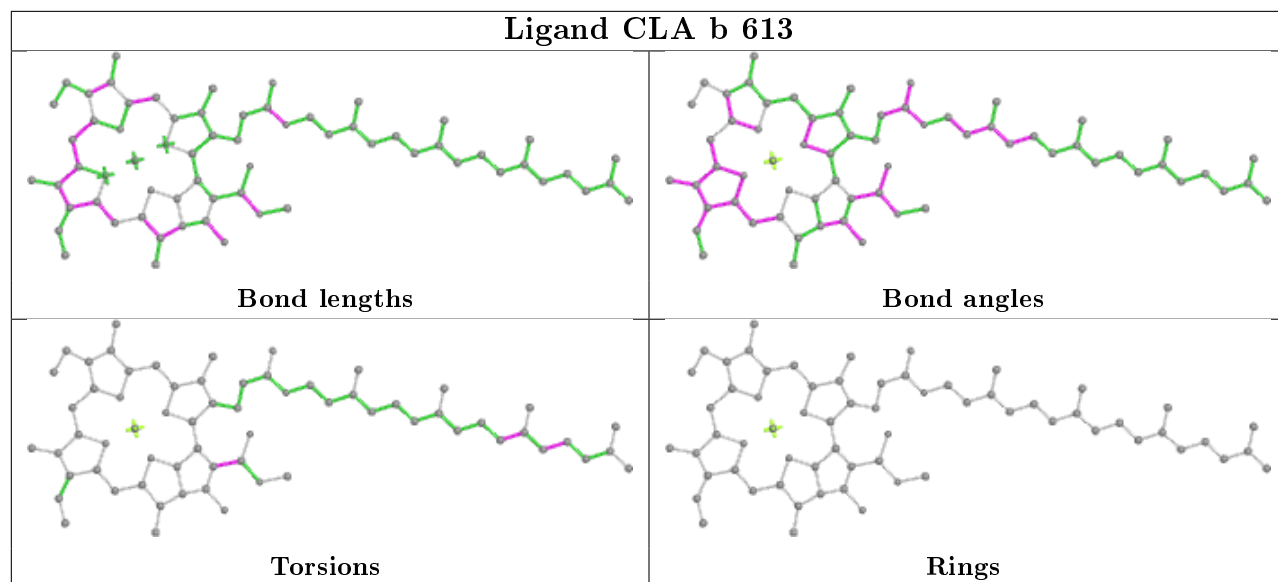




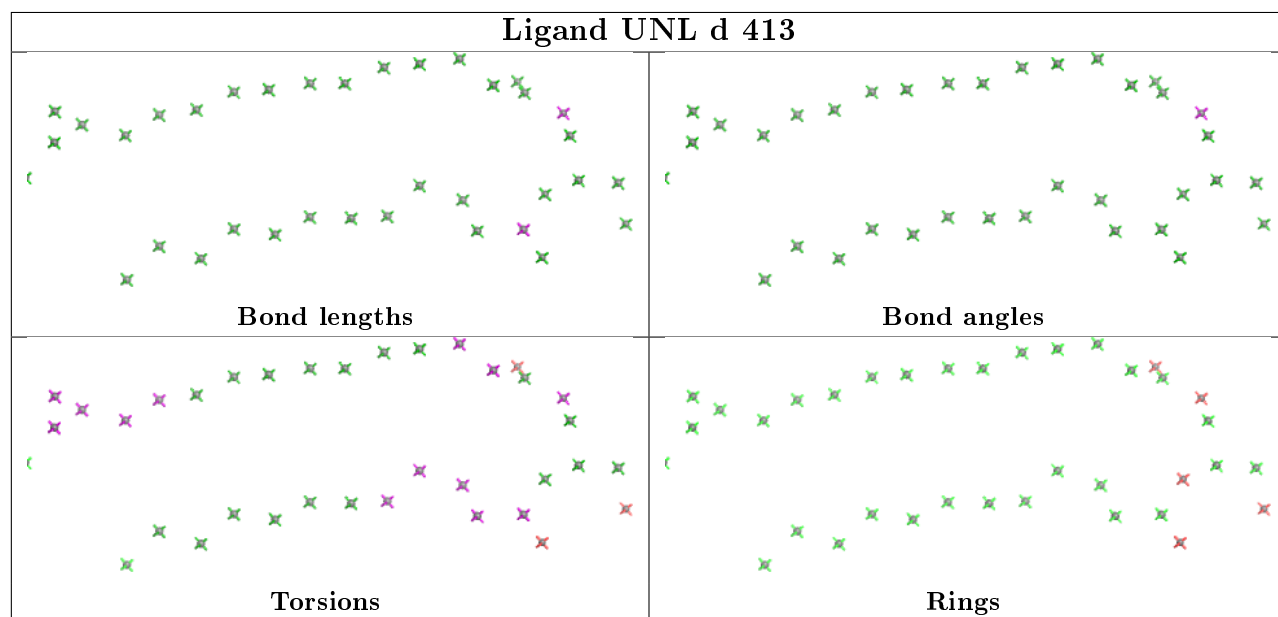


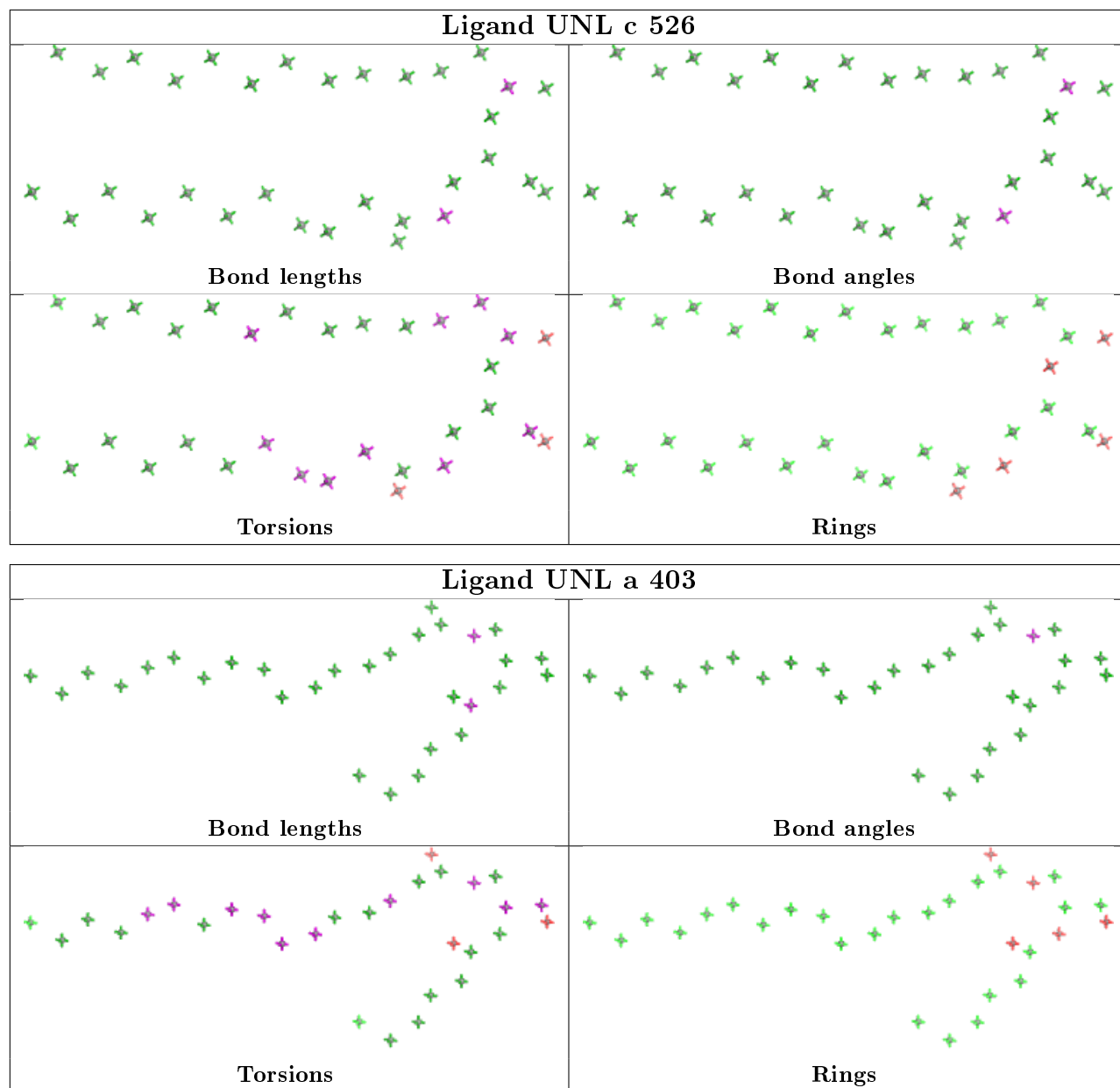


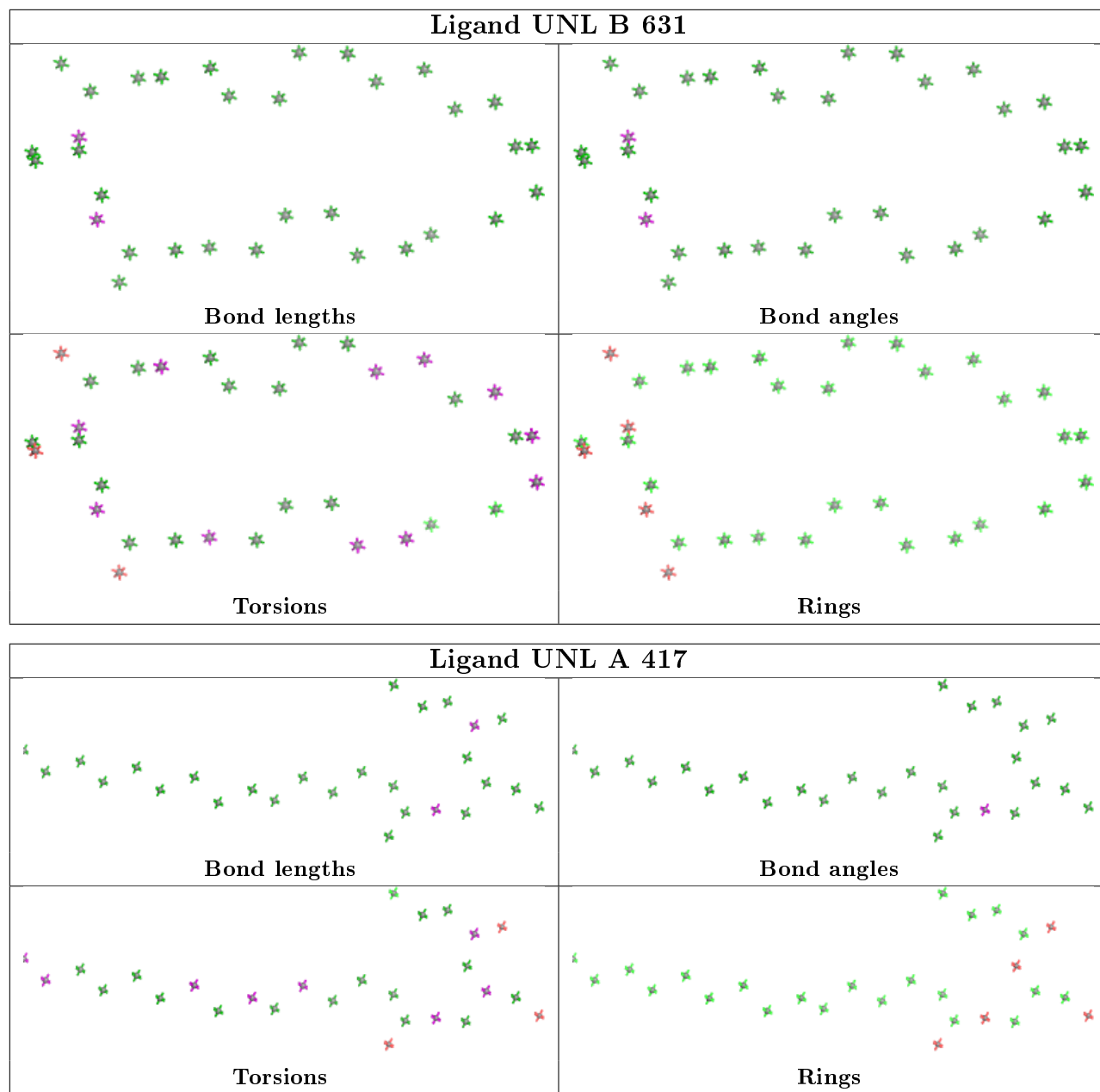
Ligand CLA b 613

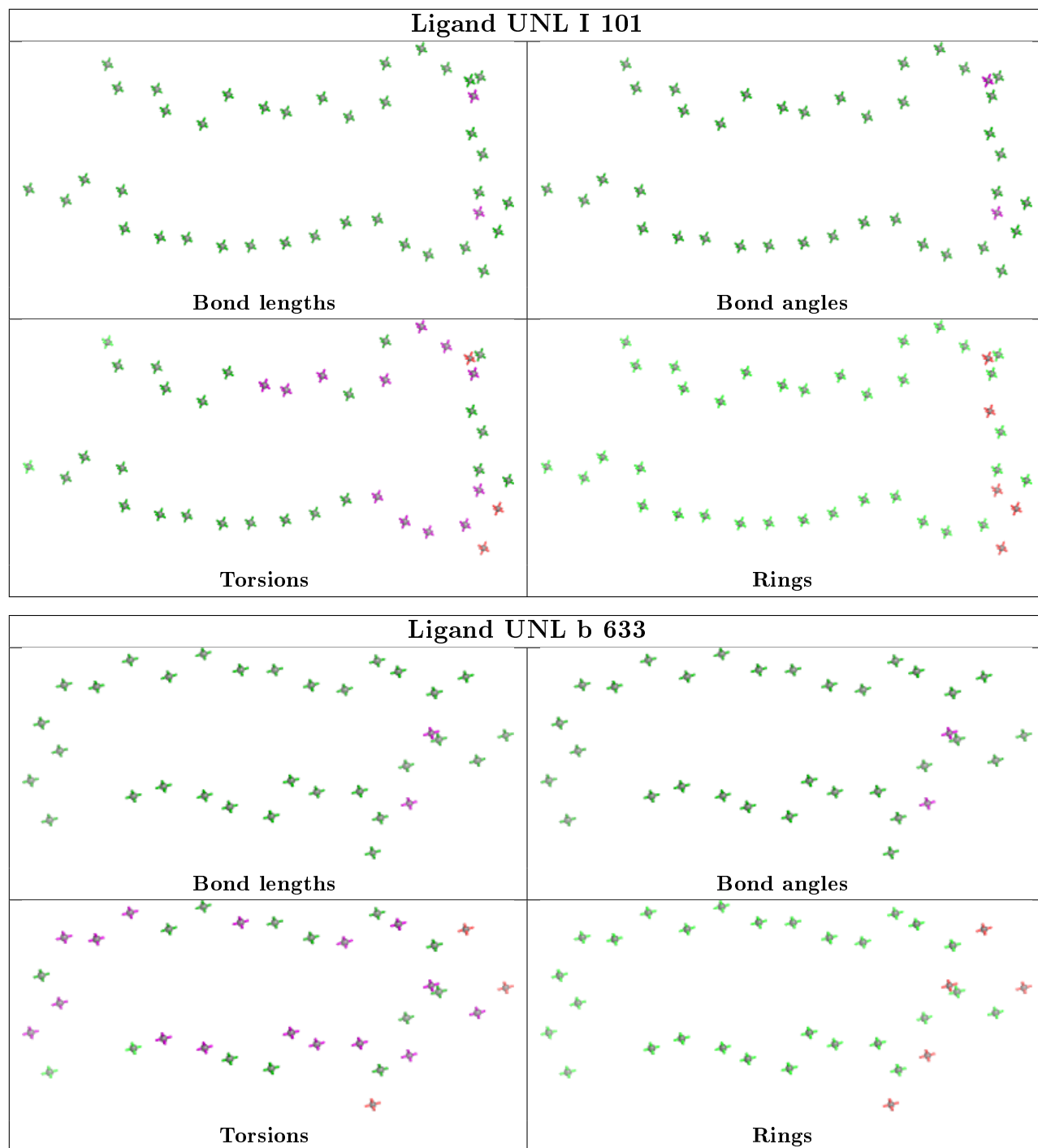


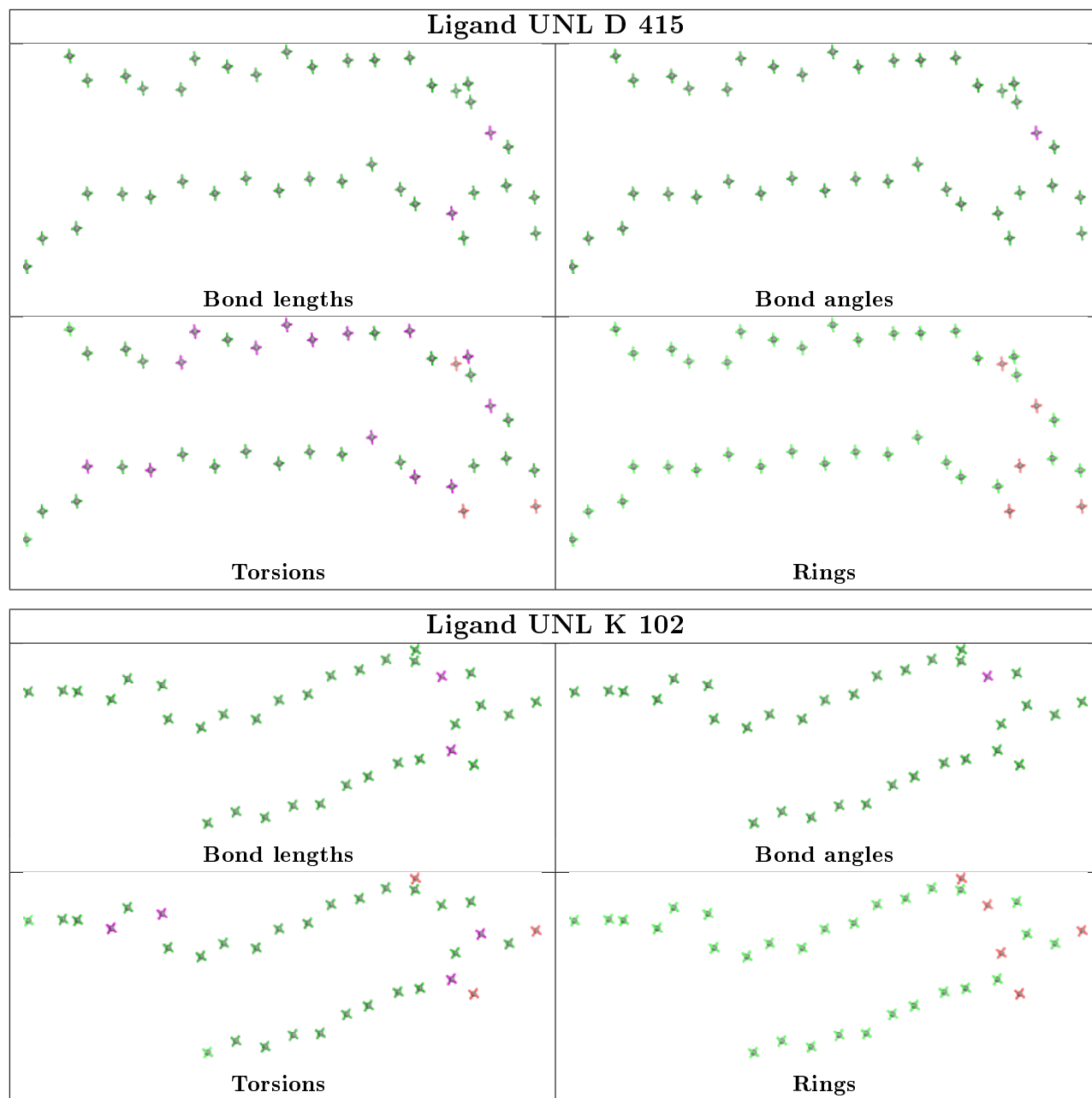
Ligand UNL d 413

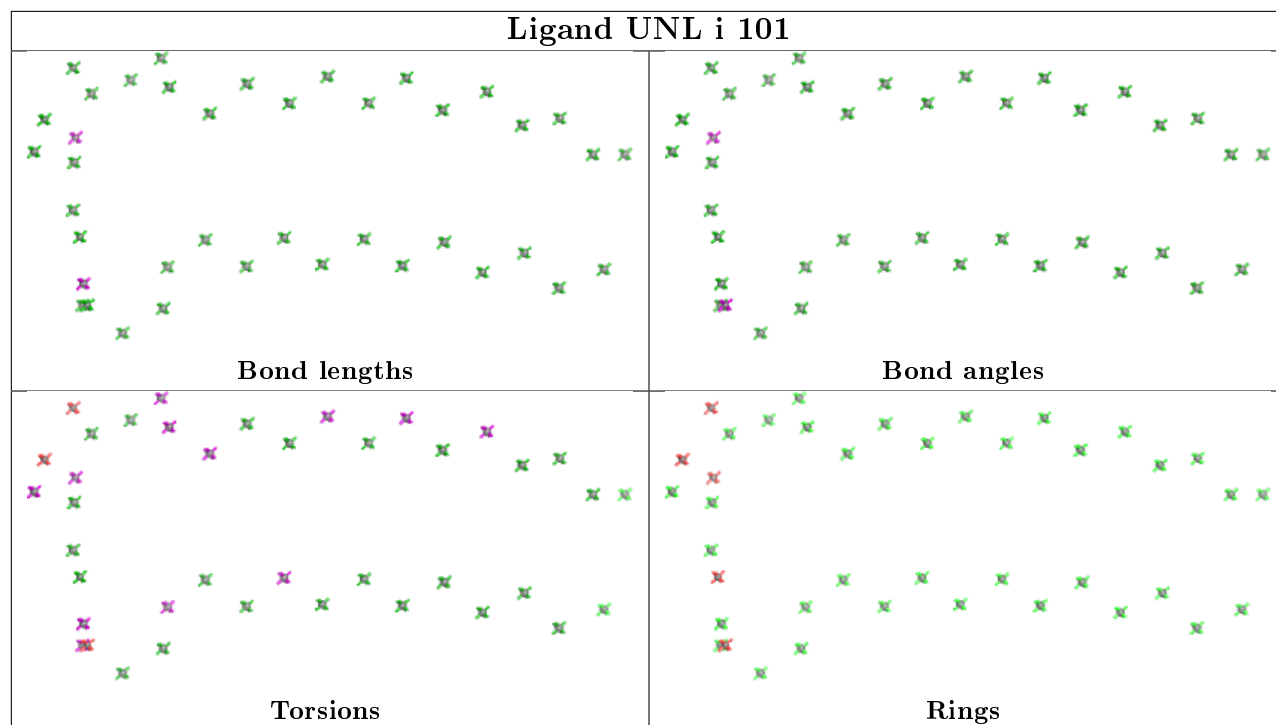












5.7 Other polymers [i](#)

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%)	0.19	1 (0%) 94 94	36, 47, 80, 129	0
1	a	334/344 (97%)	0.31	13 (3%) 39 42	36, 49, 88, 147	0
2	B	504/505 (99%)	0.21	10 (1%) 65 68	38, 52, 93, 149	0
2	b	503/505 (99%)	0.30	20 (3%) 38 41	37, 53, 104, 202	0
3	C	451/455 (99%)	0.34	21 (4%) 31 33	42, 62, 91, 136	0
3	c	455/455 (100%)	0.16	4 (0%) 84 86	46, 66, 87, 123	0
4	D	341/342 (99%)	0.13	5 (1%) 73 75	34, 49, 82, 143	0
4	d	341/342 (99%)	0.21	4 (1%) 79 80	36, 51, 77, 115	0
5	E	81/84 (96%)	1.26	20 (24%) 0 0	56, 85, 117, 162	0
5	e	81/84 (96%)	0.70	8 (9%) 7 7	58, 79, 131, 187	0
6	F	34/44 (77%)	0.62	5 (14%) 2 2	58, 72, 120, 130	0
6	f	32/44 (72%)	0.11	0 100 100	58, 68, 128, 159	0
7	H	65/65 (100%)	0.18	1 (1%) 73 75	52, 65, 85, 166	0
7	h	65/65 (100%)	0.11	2 (3%) 49 52	52, 65, 85, 169	0
8	I	37/38 (97%)	0.46	4 (10%) 5 5	50, 64, 136, 194	0
8	i	37/38 (97%)	0.36	3 (8%) 12 12	48, 61, 131, 164	0
9	J	38/39 (97%)	1.17	10 (26%) 0 0	63, 79, 167, 195	0
9	j	39/39 (100%)	0.66	6 (15%) 2 1	58, 71, 149, 191	0
10	K	37/37 (100%)	0.72	5 (13%) 3 2	65, 79, 98, 119	0
10	k	37/37 (100%)	0.37	0 100 100	61, 75, 97, 119	0
11	L	37/37 (100%)	0.09	0 100 100	36, 42, 101, 127	0
11	l	37/37 (100%)	0.17	0 100 100	35, 43, 104, 138	0
12	M	33/36 (91%)	0.18	0 100 100	33, 43, 76, 131	0
12	m	33/36 (91%)	0.36	0 100 100	37, 44, 89, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.29	7 (2%) 51 55	36, 58, 101, 145	0
13	o	243/244 (99%)	0.18	3 (1%) 79 80	38, 61, 115, 178	0
14	T	29/32 (90%)	0.34	1 (3%) 45 48	36, 42, 77, 145	0
14	t	29/32 (90%)	0.25	0 100 100	36, 44, 75, 144	0
15	U	97/104 (93%)	0.11	1 (1%) 82 84	45, 57, 90, 133	0
15	u	97/104 (93%)	0.07	0 100 100	46, 61, 79, 123	0
16	V	137/137 (100%)	0.23	1 (0%) 87 89	44, 59, 83, 114	0
16	v	137/137 (100%)	0.11	1 (0%) 87 89	48, 70, 103, 132	0
17	Y	29/30 (96%)	3.70	13 (44%) 0 0	80, 102, 195, 215	0
17	y	29/30 (96%)	1.01	5 (17%) 1 1	80, 94, 148, 163	0
18	X	39/40 (97%)	0.48	4 (10%) 6 6	63, 72, 125, 163	0
18	x	38/40 (95%)	0.53	4 (10%) 6 6	64, 74, 130, 159	0
19	Z	62/62 (100%)	1.45	18 (29%) 0 0	82, 99, 136, 151	0
19	z	62/62 (100%)	1.27	22 (35%) 0 0	80, 100, 152, 195	0
20	R	18/34 (52%)	5.46	18 (100%) 0 0	111, 147, 171, 187	0
All	All	5275/5384 (97%)	0.34	240 (4%) 33 36	33, 58, 110, 215	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	18.4
17	Y	19	ILE	15.8
17	Y	20	ALA	12.3
2	b	494	GLY	10.6
17	Y	21	GLN	10.1
20	R	6	LEU	9.8
20	R	18	TRP	9.2
5	e	5	THR	8.5
20	R	8	VAL	8.1
20	R	5	VAL	7.8
2	b	495	PHE	7.8
17	Y	25	ILE	7.5
20	R	15	ALA	7.3
17	Y	22	LEU	7.1
20	R	16	ALA	7.0
2	b	496	TYR	6.9
19	z	3	ILE	6.4

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Mol	Chain	Res	Type	RSRZ
19	Z	62	VAL	6.0
9	j	1	MET	6.0
18	x	2	THR	5.9
19	Z	31	GLN	5.9
2	b	504	THR	5.8
7	h	65	LEU	5.8
5	E	84	LYS	5.7
20	R	17	GLY	5.7
5	E	83	LEU	5.7
19	Z	61	VAL	5.7
17	Y	26	ALA	5.5
5	e	4	THR	5.5
9	j	2	SER	5.4
19	Z	36	SER	5.4
2	b	493	TRP	5.3
18	x	37	VAL	5.3
20	R	12	VAL	5.2
17	Y	23	THR	5.1
20	R	13	LEU	5.1
5	E	79	PHE	5.0
2	b	487	SER	5.0
5	E	19	TYR	4.9
8	I	36	ASP	4.8
20	R	11	PRO	4.8
13	O	56	PRO	4.8
18	x	38	GLN	4.7
5	E	5	THR	4.7
5	E	82	GLN	4.7
19	Z	33	TRP	4.6
8	I	34	ARG	4.6
1	a	264[A]	SER	4.6
8	i	37	LEU	4.6
2	b	501	ASP	4.6
19	z	33	TRP	4.5
17	y	20	ALA	4.4
9	j	4	GLY	4.4
20	R	9	LEU	4.3
8	i	36	ASP	4.3
2	b	486	LEU	4.3
20	R	2	ASP	4.3
2	B	496	TYR	4.2
2	b	489	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
10	K	14	ALA	4.2
19	z	32	ASP	4.1
2	b	502	VAL	4.1
7	h	66	GLY	4.1
20	R	14	LEU	4.1
19	Z	30	PRO	4.1
19	Z	25	VAL	4.1
2	B	479	PHE	4.0
2	b	497	GLN	4.0
7	H	66	GLY	4.0
13	o	59	LYS	4.0
2	b	488	PRO	4.0
9	J	2	SER	3.9
3	C	145[A]	SER	3.9
2	b	491	VAL	3.9
6	F	16	PHE	3.9
17	y	41	VAL	3.9
17	Y	24	MET	3.8
17	Y	30	ILE	3.8
2	b	503	THR	3.8
3	c	140	LEU	3.7
20	R	3	TRP	3.7
13	O	62	GLU	3.6
19	Z	32	ASP	3.6
3	C	25	ASN	3.6
13	o	58	ASN	3.6
19	z	41	PHE	3.6
5	E	11	SER	3.6
13	o	61	GLN	3.6
19	z	5	PHE	3.6
20	R	4	ARG	3.5
5	E	4	THR	3.5
3	C	131	TYR	3.5
3	c	143	TYR	3.5
6	F	15	ILE	3.5
5	e	10	PHE	3.5
4	D	238[A]	THR	3.4
5	E	17	VAL	3.4
19	z	30	PRO	3.4
8	I	38	GLU	3.3
2	B	495	PHE	3.3
2	B	503	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	b	499	VAL	3.3
18	X	2	THR	3.3
14	T	30	THR	3.3
19	z	36	SER	3.2
3	C	253	LEU	3.1
20	R	7	VAL	3.1
19	Z	35	ARG	3.1
19	z	35	ARG	3.1
17	y	40	ALA	3.1
9	J	5	GLY	3.1
3	C	139	THR	3.1
6	F	12	SER	3.1
9	j	5	GLY	3.1
1	a	11	ALA	3.0
4	D	235[A]	PHE	3.0
2	B	504	THR	3.0
19	Z	4	LEU	3.0
10	K	15	TYR	3.0
8	I	37	LEU	3.0
2	b	500	GLY	3.0
4	D	24	ARG	2.9
2	B	290	ALA	2.9
3	C	252	ILE	2.9
1	a	265[A]	PHE	2.9
19	z	62	VAL	2.9
2	b	485	GLU	2.9
5	E	23	HIS	2.9
3	C	155	ASN	2.8
1	a	262	TYR	2.8
5	E	15	THR	2.8
20	R	19	ALA	2.8
9	j	3	GLU	2.8
1	a	256	GLY	2.8
5	E	78	THR	2.8
19	Z	39	LEU	2.8
5	E	6	GLY	2.8
3	C	28	GLN	2.8
19	z	39	LEU	2.8
3	c	21	ILE	2.8
9	J	27	PHE	2.8
19	z	18	VAL	2.7
5	e	6	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
19	Z	3	ILE	2.7
19	Z	24	PRO	2.7
9	J	36	GLY	2.7
8	i	34	ARG	2.7
5	E	76	VAL	2.7
4	d	230	SER	2.7
6	F	14	PRO	2.7
19	z	61	VAL	2.7
18	X	39	ARG	2.7
1	a	229	GLU	2.7
4	D	232	PHE	2.7
19	z	28	ALA	2.6
5	e	7	GLU	2.6
19	z	31	GLN	2.6
3	C	45	LEU	2.6
16	v	17	LYS	2.6
19	Z	1	MET	2.6
19	z	42	LEU	2.6
5	E	10	PHE	2.6
9	J	3	GLU	2.6
9	J	31	ALA	2.6
9	J	33	ALA	2.6
19	Z	29	SER	2.6
3	C	140	LEU	2.5
15	U	73	GLN	2.5
13	O	60	ARG	2.5
4	d	240[A]	ALA	2.5
13	O	26	ALA	2.5
20	R	10	LEU	2.5
4	d	234[A]	ALA	2.5
9	J	7	ILE	2.5
18	x	39	ARG	2.5
5	e	9	PRO	2.5
1	a	246[A]	TYR	2.5
2	b	482	ILE	2.5
5	E	16	SER	2.4
19	z	4	LEU	2.4
1	a	261	GLN	2.4
19	z	43	GLY	2.4
9	J	37	SER	2.4
6	F	13	TYR	2.4
3	C	23	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	54	VAL	2.3
5	E	74	GLN	2.3
19	z	25	VAL	2.3
13	O	58	ASN	2.3
2	B	486	LEU	2.3
19	Z	56	VAL	2.3
1	A	307	ILE	2.3
3	C	135	ARG	2.3
3	C	207	ARG	2.3
5	E	22	ILE	2.3
19	Z	26	ALA	2.3
19	Z	34	ASP	2.3
1	a	263	ALA	2.3
17	Y	37	PHE	2.3
19	z	29	SER	2.2
3	C	134	ILE	2.2
3	C	47	GLY	2.2
17	Y	29	GLY	2.2
3	C	158	THR	2.2
19	z	60	PHE	2.2
17	y	43	ARG	2.2
16	V	71	GLY	2.2
2	b	498	LYS	2.2
5	e	21	VAL	2.2
19	z	2	THR	2.2
2	B	481	GLY	2.2
18	X	37	VAL	2.2
1	a	248[A]	ILE	2.2
3	C	42	LEU	2.2
18	X	40	SER	2.2
1	a	252[A]	HIS	2.2
2	b	86[A]	ILE	2.2
4	D	233[A]	ARG	2.2
17	Y	41	VAL	2.2
10	K	16	ALA	2.2
13	O	93	LEU	2.2
19	z	6	GLN	2.1
1	a	15	GLU	2.1
9	j	6	ARG	2.1
1	a	19	ASN	2.1
10	K	10	LYS	2.1
2	B	490	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
4	d	228	GLY	2.1
13	O	57	LYS	2.1
5	e	20	TRP	2.1
5	E	12	ASP	2.1
3	C	144	SER	2.1
5	E	77	GLU	2.1
9	J	10	TRP	2.1
3	C	27	ASP	2.0
10	K	13	GLU	2.0
3	C	46	SER	2.0
17	y	45	ASN	2.0
3	c	175	LEU	2.0
2	B	501	ASP	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	0.94	0.16	38,48,56,93	0
14	FME	t	1	10/11	0.95	0.15	28,39,49,95	0
8	FME	i	1	10/11	0.95	0.15	41,58,64,68	0
12	FME	m	1	10/11	0.96	0.19	35,51,97,107	0
8	FME	I	1	10/11	0.97	0.14	39,51,61,66	0
12	FME	M	1	10/11	0.97	0.20	31,47,94,99	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
27	LMT	F	101	35/35	0.28	0.58	133,171,182,184	0
34	DGD	d	408	62/66	0.33	0.49	87,130,176,182	0
27	LMT	b	630	25/35	0.50	0.41	85,107,156,159	0
31	UNL	J	101	10/-	0.51	0.31	70,104,114,115	0
27	LMT	a	419	35/35	0.52	0.42	98,142,160,162	0
27	LMT	C	521	35/35	0.55	0.41	103,145,170,173	0
31	UNL	j	101	10/-	0.56	0.31	59,89,101,103	0
38	LHG	a	420	42/49	0.56	0.34	92,136,181,183	0
31	UNL	c	526	32/-	0.58	0.29	82,100,140,147	0
31	UNL	K	102	34/-	0.58	0.27	94,127,136,139	0
34	DGD	D	410	52/66	0.60	0.39	74,109,157,168	0
38	LHG	E	101	42/49	0.62	0.30	89,127,142,147	0
27	LMT	a	404	35/35	0.63	0.29	55,101,126,145	0
32	CA	b	609	1/1	0.63	0.12	131,131,131,131	0
27	LMT	m	102	35/35	0.64	0.29	51,111,129,130	0
31	UNL	a	403	30/-	0.65	0.31	67,93,124,131	0
27	LMT	D	405	35/35	0.65	0.31	84,132,152,153	0
33	HTG	D	416	16/19	0.65	0.29	70,134,155,156	0
31	UNL	b	633	33/-	0.66	0.29	55,88,143,145	0
27	LMT	e	102	35/35	0.66	0.32	86,136,156,157	0
25	SQD	f	102	43/54	0.67	0.31	106,125,157,166	0
22	CL	U	201	1/1	0.67	0.10	120,120,120,120	0
33	HTG	B	630	19/19	0.68	0.25	58,118,140,169	0
35	LMG	C	519	51/55	0.68	0.26	59,102,122,125	0
33	HTG	d	414	16/19	0.69	0.24	75,116,122,125	0
31	UNL	A	417	28/-	0.70	0.27	63,89,113,115	0
27	LMT	M	105	35/35	0.70	0.30	50,99,119,121	0
35	LMG	Z	101	37/55	0.70	0.32	67,138,150,151	0
27	LMT	A	413	35/35	0.71	0.26	57,91,114,119	0
33	HTG	b	608	19/19	0.71	0.22	58,116,151,164	0
26	GOL	v	201	6/6	0.72	0.30	78,98,103,104	0
33	HTG	B	623	19/19	0.74	0.24	85,137,145,176	0
34	DGD	C	517	62/66	0.74	0.26	55,74,100,114	0
27	LMT	M	104	35/35	0.74	0.28	44,109,152,157	0
26	GOL	V	202	6/6	0.74	0.57	88,95,99,99	0
35	LMG	z	101	39/55	0.75	0.31	74,125,149,162	0
33	HTG	b	631	19/19	0.76	0.30	66,80,98,102	0
31	UNL	B	631	33/-	0.76	0.32	61,83,134,137	0
33	HTG	b	632	19/19	0.77	0.27	80,134,152,155	0
30	PL9	a	416[A]	55/55	0.77	0.28	91,109,122,123	55
30	PL9	a	416[B]	55/55	0.77	0.28	92,108,122,124	55
35	LMG	C	520	51/55	0.77	0.35	63,125,134,137	0
31	UNL	m	101	10/-	0.77	0.34	46,60,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	HTG	C	523	19/19	0.78	0.30	78,110,127,130	0
27	LMT	T	104	25/35	0.79	0.30	44,81,135,142	0
30	PL9	A	416[A]	55/55	0.79	0.29	86,107,117,119	55
26	GOL	O	301	6/6	0.79	0.17	81,84,87,87	0
32	CA	f	103	1/1	0.79	0.13	127,127,127,127	0
32	CA	B	601	1/1	0.79	0.07	131,131,131,131	0
30	PL9	A	416[B]	55/55	0.79	0.29	86,107,117,119	55
25	SQD	a	405	54/54	0.80	0.24	50,82,127,132	0
26	GOL	V	205	6/6	0.80	0.20	87,100,106,115	0
31	UNL	d	413	36/-	0.81	0.25	64,85,131,137	0
25	SQD	L	102	54/54	0.81	0.23	42,76,124,140	0
31	UNL	M	103	10/-	0.81	0.30	52,63,78,80	0
33	HTG	c	525	19/19	0.81	0.31	86,116,133,149	0
25	SQD	A	412	54/54	0.82	0.23	56,77,134,138	0
35	LMG	c	522	51/55	0.82	0.23	64,95,120,122	0
23	CLA	c	517	65/65	0.82	0.23	80,95,105,107	0
31	UNL	I	101	40/-	0.82	0.28	58,93,150,153	0
25	SQD	B	621	54/54	0.82	0.24	53,79,156,160	0
27	LMT	t	101	25/35	0.82	0.31	45,80,143,149	0
25	SQD	F	104	43/54	0.82	0.29	91,122,143,145	0
27	LMT	M	102	35/35	0.82	0.24	42,101,123,131	0
34	DGD	C	518	62/66	0.83	0.20	51,64,88,105	0
31	UNL	D	415	40/-	0.83	0.22	62,86,130,137	0
35	LMG	c	523	51/55	0.83	0.26	65,117,129,133	0
26	GOL	v	202	6/6	0.83	0.29	103,105,109,122	0
23	CLA	C	514	65/65	0.83	0.29	71,91,120,124	0
22	CL	v	204	1/1	0.83	0.12	120,120,120,120	0
31	UNL	i	101	40/-	0.83	0.24	50,87,139,142	0
26	GOL	a	402	6/6	0.83	0.27	103,108,108,109	0
35	LMG	M	101	51/55	0.84	0.23	39,59,75,91	0
35	LMG	b	629	51/55	0.85	0.24	40,54,76,84	0
35	LMG	C	501	51/55	0.85	0.22	62,84,103,107	0
33	HTG	b	607	19/19	0.85	0.17	53,83,94,95	0
34	DGD	h	102	62/66	0.85	0.22	36,58,75,82	0
23	CLA	C	505	65/65	0.85	0.24	47,67,101,108	0
33	HTG	c	524	19/19	0.86	0.18	99,106,117,119	0
25	SQD	A	409	54/54	0.86	0.24	55,98,108,111	0
33	HTG	B	629	19/19	0.86	0.17	48,88,113,116	0
33	HTG	C	522	19/19	0.86	0.24	84,94,135,137	0
35	LMG	a	415	51/55	0.86	0.20	59,85,101,114	0
34	DGD	B	632	62/66	0.86	0.21	43,59,89,105	0
25	SQD	a	414	54/54	0.86	0.19	56,83,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	HTG	B	622	19/19	0.87	0.22	63,75,85,91	0
26	GOL	C	524	6/6	0.87	0.38	88,89,103,104	0
33	HTG	b	601	19/19	0.87	0.20	49,65,76,77	0
31	UNL	X	101	18/-	0.87	0.22	69,87,109,111	0
34	DGD	c	520	62/66	0.87	0.20	49,66,111,127	0
33	HTG	V	207	19/19	0.88	0.36	80,105,126,240	0
31	UNL	d	415	18/-	0.88	0.22	67,80,109,116	0
39	HEM	F	102	43/43	0.88	0.24	59,85,111,234	0
38	LHG	D	413	49/49	0.89	0.26	51,78,118,126	0
35	LMG	D	417	51/55	0.89	0.21	50,76,125,133	0
23	CLA	c	511	65/65	0.89	0.19	52,65,77,82	0
26	GOL	T	101	6/6	0.89	0.30	58,81,84,93	0
26	GOL	T	102	6/6	0.89	0.49	107,116,118,122	0
34	DGD	c	521	62/66	0.90	0.19	51,61,98,109	0
23	CLA	b	611	65/65	0.90	0.20	43,52,62,70	0
23	CLA	B	602	65/65	0.90	0.20	53,75,112,132	0
23	CLA	c	510	65/65	0.90	0.18	57,75,99,102	0
38	LHG	D	411	49/49	0.90	0.24	40,52,64,80	0
23	CLA	b	616	65/65	0.90	0.20	29,42,50,53	0
33	HTG	o	301	19/19	0.90	0.19	51,74,87,91	0
35	LMG	d	416	51/55	0.90	0.20	53,66,107,118	0
23	CLA	c	512	65/65	0.90	0.17	47,57,115,122	0
23	CLA	C	507	65/65	0.90	0.17	59,78,118,125	0
26	GOL	A	411	6/6	0.90	0.20	84,86,91,92	0
23	CLA	C	512	65/65	0.90	0.20	54,76,92,97	0
26	GOL	f	101	6/6	0.90	0.23	85,90,93,96	0
23	CLA	C	502	65/65	0.91	0.17	51,62,88,93	0
34	DGD	C	516	62/66	0.91	0.18	40,56,87,95	0
23	CLA	B	607	65/65	0.91	0.18	37,52,91,95	0
23	CLA	c	507	65/65	0.91	0.18	53,64,74,93	0
26	GOL	A	410	6/6	0.91	0.20	49,56,61,66	0
23	CLA	c	508	65/65	0.91	0.17	50,64,81,86	0
23	CLA	b	618	65/65	0.91	0.20	47,55,66,73	0
23	CLA	C	513	65/65	0.91	0.17	71,87,94,97	0
32	CA	C	526	1/1	0.91	0.12	83,83,83,83	0
24	BCR	K	101	40/40	0.91	0.21	64,83,92,94	0
26	GOL	b	606	6/6	0.91	0.24	75,87,92,94	0
23	CLA	B	614	65/65	0.91	0.18	32,43,62,72	0
26	GOL	c	502	6/6	0.91	0.42	81,89,105,110	0
23	CLA	c	509	65/65	0.91	0.17	45,56,73,77	0
38	LHG	d	411	49/49	0.91	0.22	47,63,114,118	0
26	GOL	b	605	6/6	0.91	0.22	69,87,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	610	65/65	0.91	0.20	53,84,129,138	0
26	GOL	B	627	6/6	0.92	0.33	58,78,80,82	0
26	GOL	t	103	6/6	0.92	0.36	72,88,96,97	0
26	GOL	B	633	6/6	0.92	0.16	56,60,61,63	0
31	UNL	d	412	17/-	0.92	0.23	62,71,93,94	0
23	CLA	C	511	65/65	0.92	0.17	54,71,85,96	0
34	DGD	c	519	62/66	0.92	0.18	42,62,92,96	0
23	CLA	D	407	65/65	0.92	0.17	48,62,108,118	0
23	CLA	c	516	65/65	0.92	0.16	64,78,87,94	0
24	BCR	c	527	40/40	0.92	0.17	72,89,97,102	0
23	CLA	b	615	65/65	0.92	0.17	39,51,93,95	0
38	LHG	b	634	49/49	0.92	0.22	35,50,62,72	0
23	CLA	b	625	65/65	0.92	0.18	46,59,103,110	0
23	CLA	C	509	65/65	0.92	0.17	49,67,135,141	0
23	CLA	c	515	65/65	0.92	0.21	54,71,88,93	0
23	CLA	c	514	65/65	0.92	0.16	51,64,72,82	0
23	CLA	C	504	65/65	0.92	0.21	54,67,80,86	0
23	CLA	C	508	65/65	0.93	0.18	53,72,85,89	0
38	LHG	d	409	49/49	0.93	0.22	40,56,63,69	0
26	GOL	B	626	6/6	0.93	0.25	83,86,88,89	0
24	BCR	k	102	40/40	0.93	0.16	57,73,91,92	0
38	LHG	d	410	49/49	0.93	0.24	34,46,66,84	0
26	GOL	c	528	6/6	0.93	0.19	77,90,101,113	0
24	BCR	h	101	40/40	0.93	0.18	48,66,72,78	0
23	CLA	d	405	65/65	0.93	0.19	47,61,114,122	0
23	CLA	b	623	65/65	0.93	0.18	34,45,91,105	0
24	BCR	Y	101	40/40	0.93	0.19	61,79,92,106	0
26	GOL	V	204	6/6	0.93	0.31	70,71,74,75	0
23	CLA	c	513	65/65	0.93	0.17	55,68,82,88	0
26	GOL	F	103	6/6	0.93	0.30	98,110,118,121	0
23	CLA	B	615	65/65	0.93	0.20	32,45,99,102	0
23	CLA	B	610	65/65	0.93	0.17	42,55,66,79	0
24	BCR	H	101	40/40	0.93	0.18	47,60,78,78	0
23	CLA	d	403	65/65	0.93	0.18	34,41,48,51	0
23	CLA	C	510	65/65	0.93	0.18	54,74,91,95	0
23	CLA	b	624	65/65	0.93	0.17	42,53,71,76	0
23	CLA	B	608	65/65	0.93	0.18	29,43,55,67	0
23	CLA	A	404	65/65	0.94	0.18	33,39,50,61	0
23	CLA	a	409	65/65	0.94	0.19	36,42,50,72	0
30	PL9	d	407[A]	55/55	0.94	0.22	33,45,54,57	55
24	BCR	b	627	40/40	0.94	0.19	32,48,64,70	0
23	CLA	B	616	65/65	0.94	0.17	41,52,67,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	UNL	D	414	17/-	0.94	0.20	48,71,87,90	0
23	CLA	b	612	65/65	0.94	0.17	42,54,63,67	0
23	CLA	a	412	65/65	0.94	0.21	41,55,120,125	0
38	LHG	L	101	49/49	0.94	0.22	37,50,58,62	0
36	BCT	D	401[B]	4/4	0.94	0.21	75,76,81,89	4
24	BCR	k	101	40/40	0.94	0.19	59,76,86,87	0
23	CLA	D	406	65/65	0.94	0.17	32,40,65,75	0
23	CLA	B	612	65/65	0.94	0.19	34,45,53,61	0
24	BCR	K	103	40/40	0.94	0.16	62,74,82,87	0
24	BCR	d	406	40/40	0.94	0.19	52,61,83,87	0
23	CLA	b	620	65/65	0.94	0.19	34,48,58,63	0
23	CLA	b	617	65/65	0.94	0.17	44,55,66,69	0
23	CLA	B	603	65/65	0.94	0.17	43,53,60,68	0
37	PHO	d	402[B]	64/64	0.94	0.20	39,50,55,57	64
24	BCR	C	515	40/40	0.94	0.18	51,63,78,78	0
30	PL9	d	407[B]	55/55	0.94	0.22	35,45,53,58	55
37	PHO	d	402[A]	64/64	0.94	0.20	37,50,55,59	64
26	GOL	v	203	6/6	0.94	0.21	65,68,73,74	0
36	BCT	D	401[A]	4/4	0.94	0.21	76,77,81,89	4
24	BCR	D	408	40/40	0.94	0.18	49,68,101,109	0
23	CLA	A	406	65/65	0.95	0.17	35,46,104,109	0
23	CLA	A	407	65/65	0.95	0.16	42,56,118,126	0
30	PL9	D	409[A]	55/55	0.95	0.22	30,43,51,65	55
23	CLA	b	622	65/65	0.95	0.19	34,46,55,70	0
23	CLA	B	617	65/65	0.95	0.21	45,61,139,140	0
23	CLA	B	604	65/65	0.95	0.18	38,52,60,64	0
37	PHO	D	403[B]	64/64	0.95	0.18	39,48,54,59	64
26	GOL	V	203	6/6	0.95	0.17	51,70,86,89	0
23	CLA	B	609	65/65	0.95	0.18	40,51,63,66	0
32	CA	F	105	1/1	0.95	0.06	119,119,119,119	0
23	CLA	C	506	65/65	0.95	0.16	46,59,74,81	0
30	PL9	D	409[B]	55/55	0.95	0.22	30,43,51,61	55
23	CLA	B	605	65/65	0.95	0.17	33,43,69,75	0
23	CLA	b	619	65/65	0.95	0.18	42,54,69,72	0
23	CLA	A	405	65/65	0.95	0.17	32,39,46,51	0
23	CLA	b	614	65/65	0.95	0.17	36,45,58,64	0
23	CLA	d	404	65/65	0.95	0.17	35,43,59,65	0
23	CLA	B	606	65/65	0.95	0.16	34,44,55,62	0
37	PHO	D	403[A]	64/64	0.95	0.18	41,48,54,59	64
38	LHG	D	412	49/49	0.95	0.22	35,46,75,85	0
23	CLA	c	505	65/65	0.95	0.16	52,67,76,79	0
23	CLA	B	613	65/65	0.95	0.17	35,45,55,58	0

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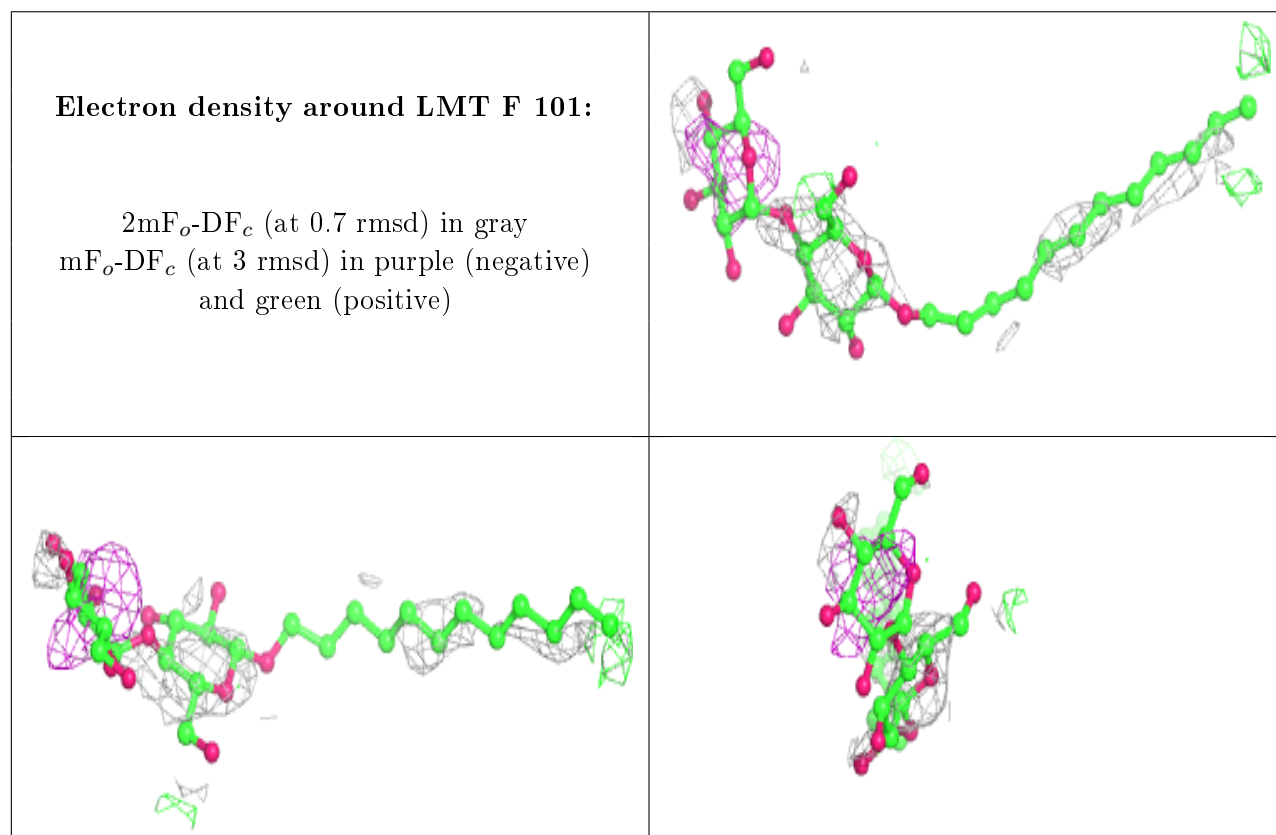
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	b	621	65/65	0.95	0.17	36,46,58,63	0
23	CLA	b	613	65/65	0.95	0.17	34,45,72,79	0
26	GOL	V	201	6/6	0.96	0.29	63,81,87,88	0
26	GOL	b	602	6/6	0.96	0.28	63,68,78,79	0
39	HEM	e	101	43/43	0.96	0.20	73,94,130,141	0
24	BCR	T	103	40/40	0.96	0.17	29,49,65,68	0
26	GOL	B	624	6/6	0.96	0.21	64,74,77,86	0
23	CLA	B	611	65/65	0.96	0.19	43,55,62,65	0
23	CLA	c	506	65/65	0.96	0.17	51,62,84,87	0
39	HEM	v	205	43/43	0.96	0.17	53,63,78,80	0
23	CLA	C	503	65/65	0.96	0.16	48,66,75,83	0
26	GOL	D	404	6/6	0.96	0.39	51,61,73,76	0
24	BCR	b	626	40/40	0.96	0.18	33,45,53,54	0
26	GOL	B	625	6/6	0.96	0.31	49,66,85,101	0
24	BCR	t	102	40/40	0.96	0.20	37,52,68,71	0
23	CLA	a	410	65/65	0.96	0.19	37,49,104,112	0
26	GOL	b	604	6/6	0.96	0.22	65,84,86,92	0
32	CA	O	302	1/1	0.96	0.05	90,90,90,90	0
26	GOL	B	628	6/6	0.96	0.39	55,87,89,91	0
24	BCR	A	408	40/40	0.96	0.18	33,46,55,56	0
26	GOL	a	401	6/6	0.96	0.26	53,59,71,80	0
37	PHO	D	402	64/64	0.96	0.17	31,41,49,51	0
24	BCR	a	413	40/40	0.96	0.19	34,47,57,60	0
24	BCR	B	619	40/40	0.96	0.19	36,47,58,66	0
24	BCR	c	518	40/40	0.96	0.19	50,65,74,77	0
26	GOL	b	603	6/6	0.97	0.21	60,70,74,75	0
24	BCR	B	618	40/40	0.97	0.21	31,44,56,59	0
37	PHO	a	411	64/64	0.97	0.20	33,43,54,58	0
24	BCR	b	628	40/40	0.97	0.19	42,55,65,67	0
32	CA	o	302	1/1	0.97	0.06	96,96,96,96	0
40	MG	J	102	1/1	0.97	0.13	62,62,62,62	0
24	BCR	B	620	40/40	0.97	0.20	43,50,60,77	0
39	HEM	V	206	43/43	0.97	0.14	47,53,63,69	0
36	BCT	d	401[B]	4/4	0.98	0.27	71,74,75,77	4
26	GOL	c	501	6/6	0.98	0.24	55,59,61,62	0
26	GOL	C	525	6/6	0.98	0.22	53,59,63,63	0
36	BCT	d	401[A]	4/4	0.98	0.27	72,74,75,77	4
32	CA	c	504	1/1	0.98	0.06	84,84,84,84	0
22	CL	A	403[B]	1/1	0.99	0.16	44,44,44,44	1
40	MG	j	102	1/1	0.99	0.14	72,72,72,72	0
22	CL	a	408[A]	1/1	0.99	0.18	46,46,46,46	1
32	CA	c	503	1/1	0.99	0.10	79,79,79,79	0

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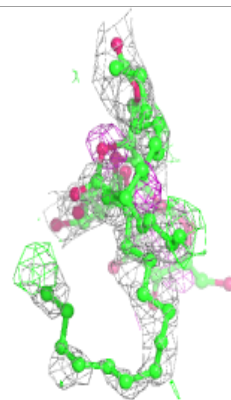
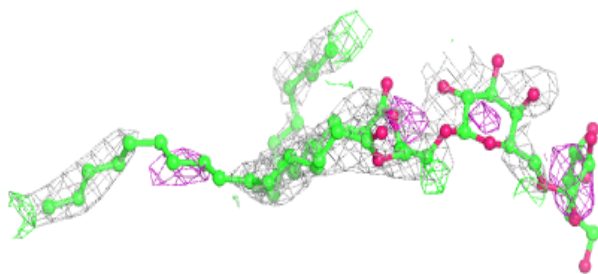
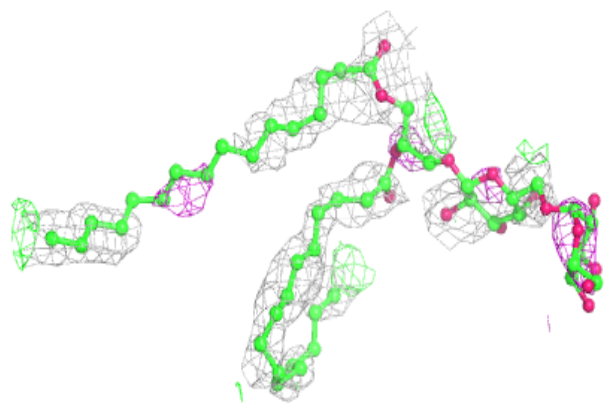
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	OEY	a	418[B]	11/11	0.99	0.14	40,46,55,59	11
21	FE2	a	406[B]	1/1	0.99	0.09	60,60,60,60	0
21	FE2	A	401[A]	1/1	0.99	0.08	72,72,72,72	1
22	CL	a	408[B]	1/1	0.99	0.18	46,46,46,46	1
28	OEX	a	417[A]	10/10	0.99	0.13	40,47,52,54	10
22	CL	a	407[A]	1/1	0.99	0.14	43,43,43,43	1
21	FE2	A	401[B]	1/1	0.99	0.08	73,73,73,73	1
28	OEX	A	414[A]	10/10	0.99	0.15	49,56,74,80	10
22	CL	A	403[A]	1/1	0.99	0.16	44,44,44,44	1
22	CL	a	407[B]	1/1	0.99	0.14	46,46,46,46	1
29	OEY	A	415[B]	11/11	0.99	0.14	49,56,78,79	11
22	CL	A	402[A]	1/1	1.00	0.17	40,40,40,40	1
22	CL	A	402[B]	1/1	1.00	0.17	40,40,40,40	1

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

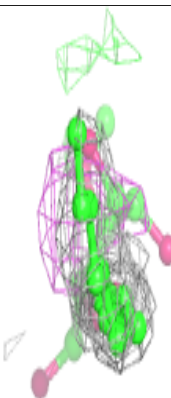
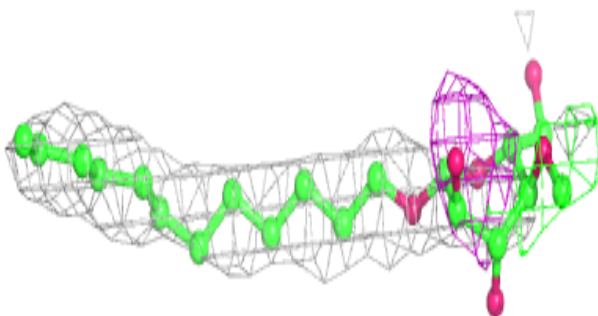
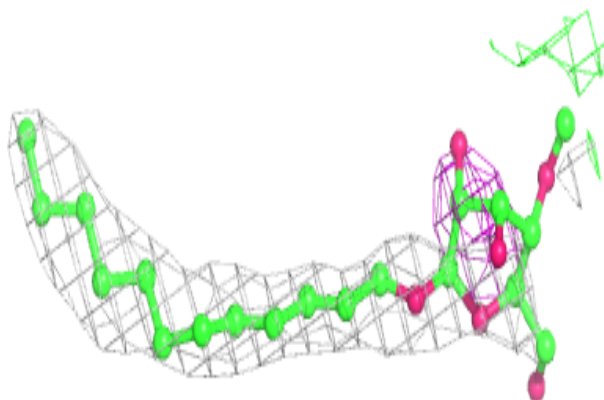


Electron density around DGD d 408:

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

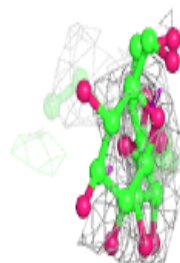
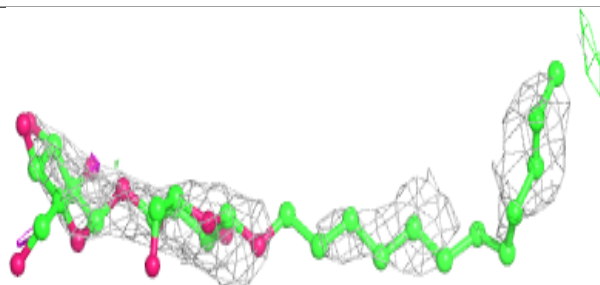
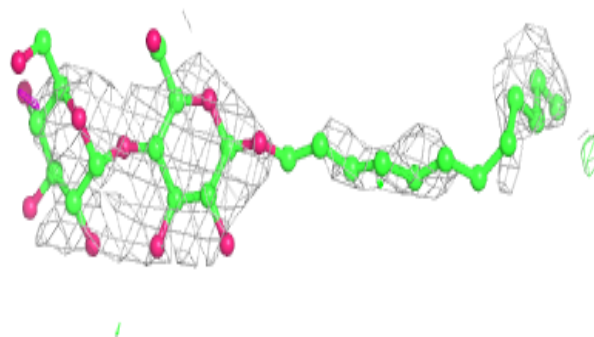
**Electron density around LMT b 630:**

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

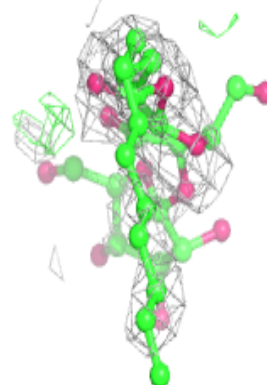
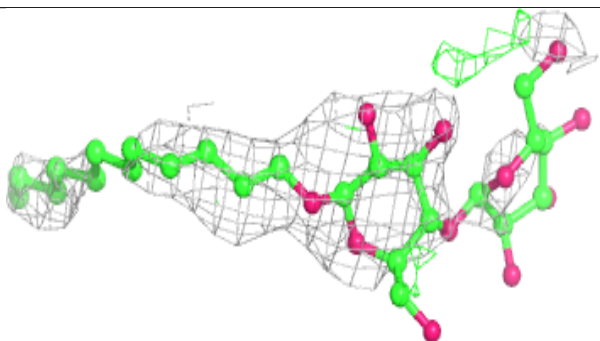
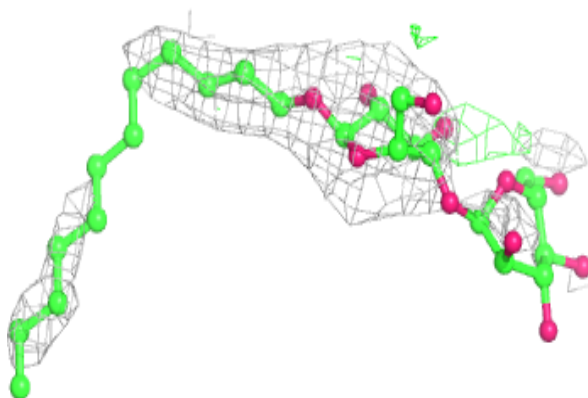


Electron density around LMT a 419:

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

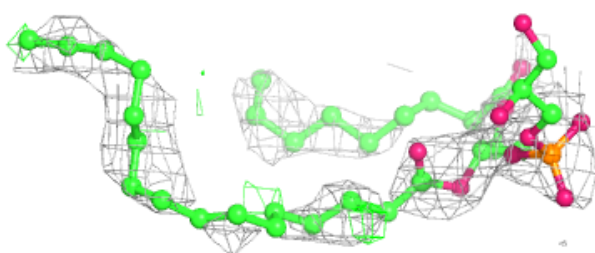
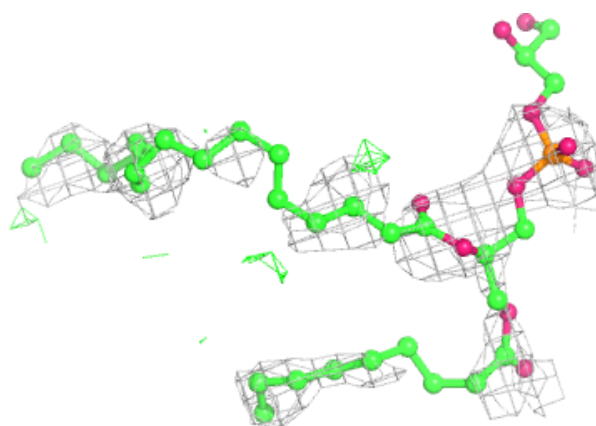
**Electron density around LMT C 521:**

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

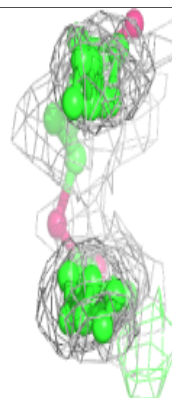
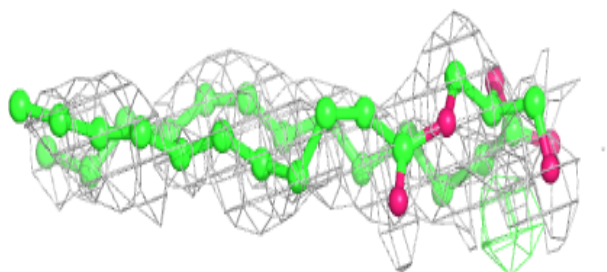
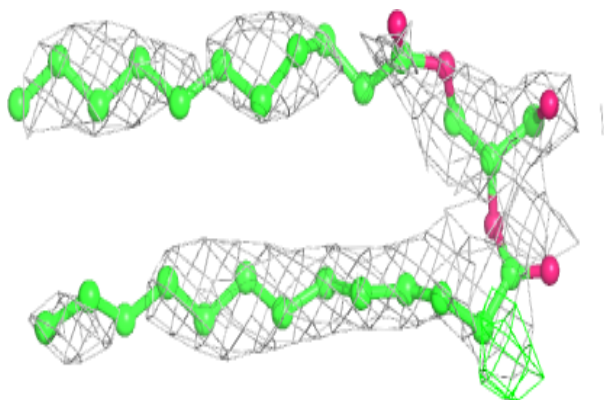


Electron density around LHG a 420:

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

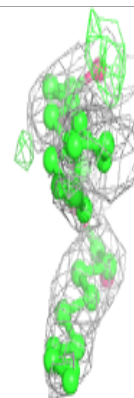
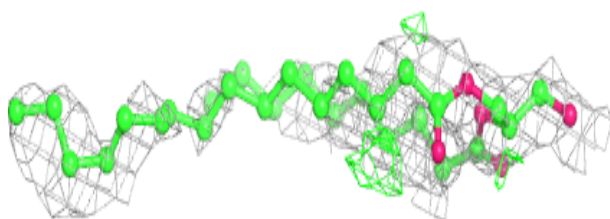
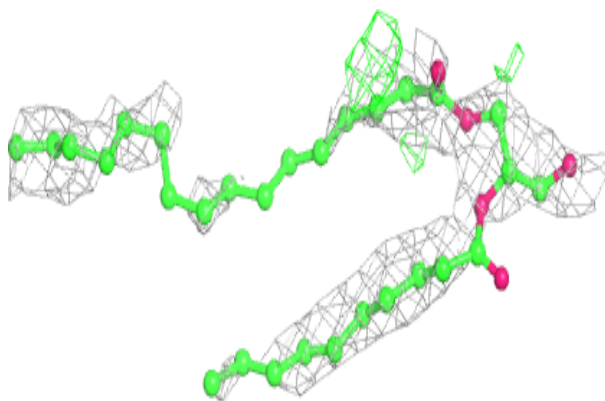
**Electron density around UNL c 526:**

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

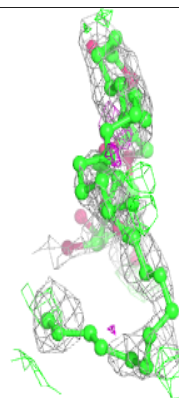
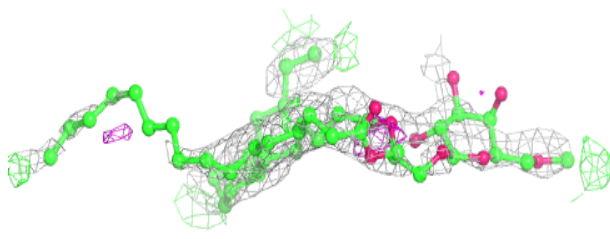
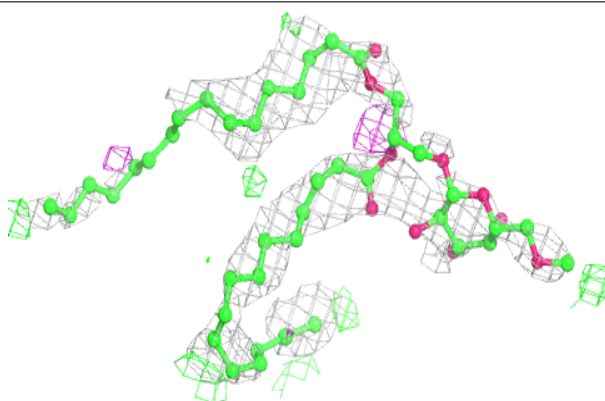


Electron density around UNL K 102:

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

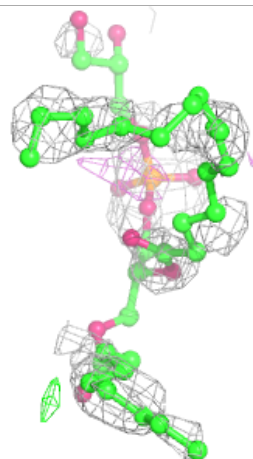
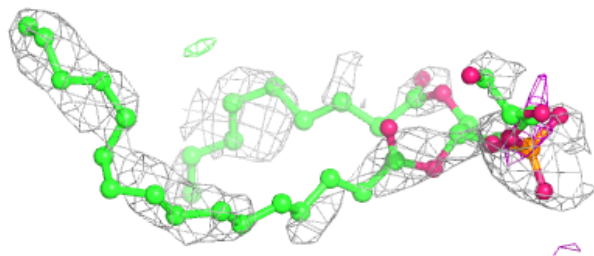
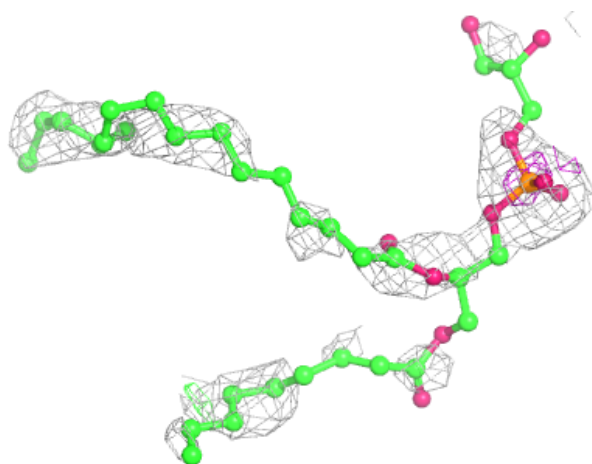
**Electron density around DGD D 410:**

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



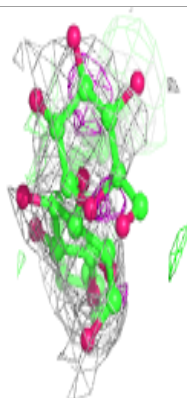
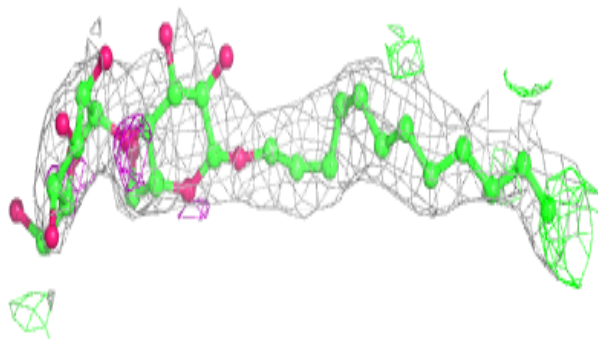
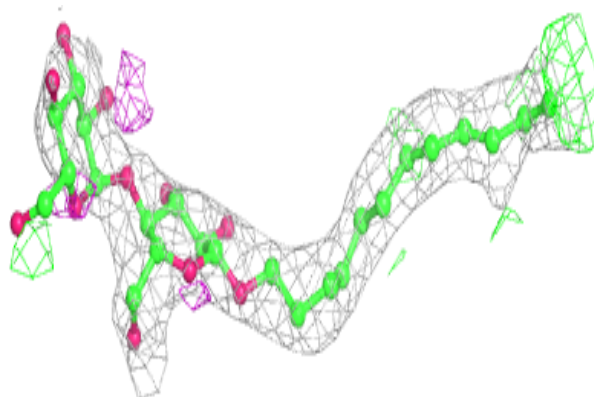
Electron density around LHG E 101:

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

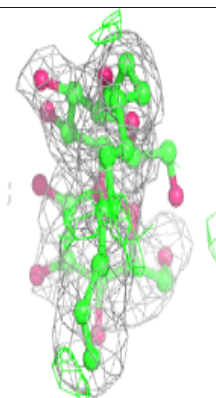
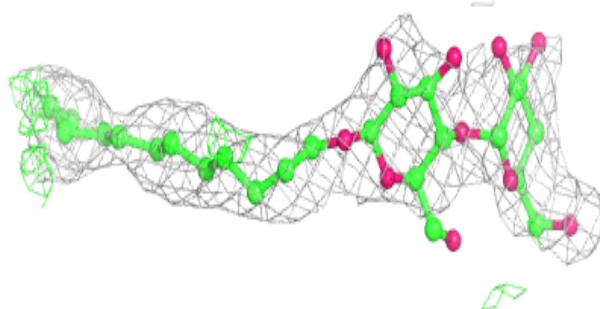
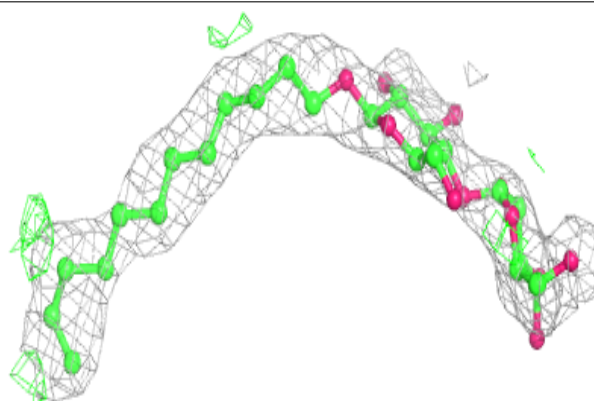


Electron density around LMT a 404:

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

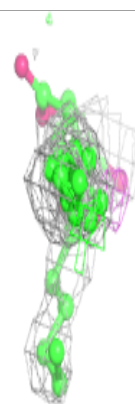
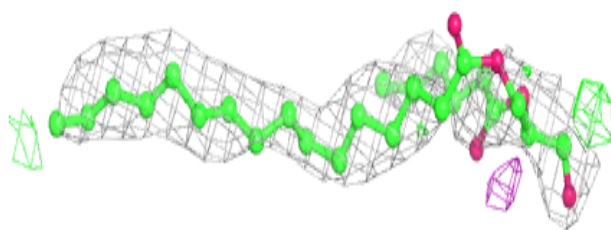
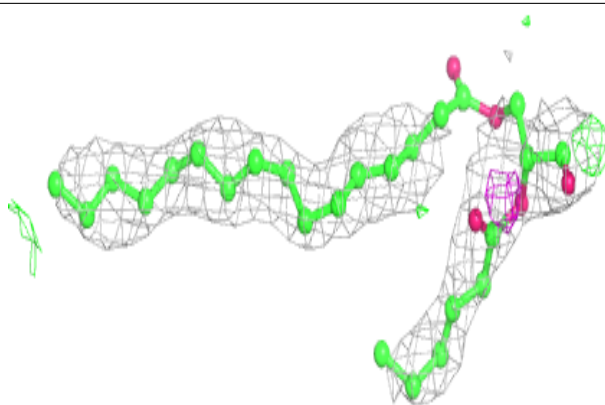
**Electron density around LMT m 102:**

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

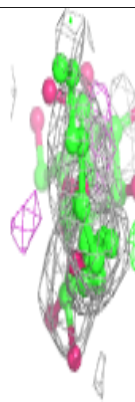
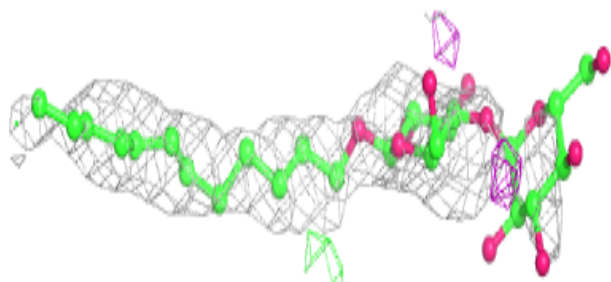
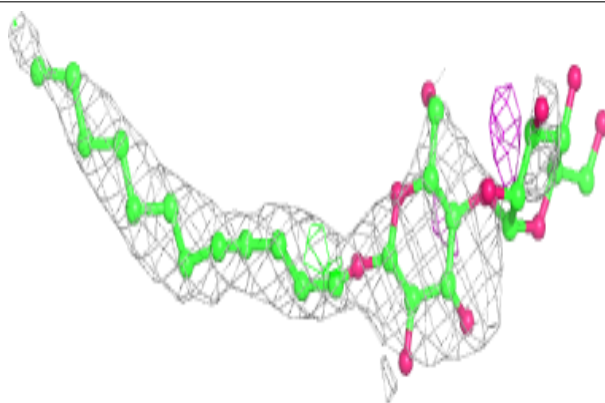


Electron density around UNL a 403:

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

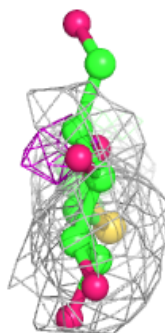
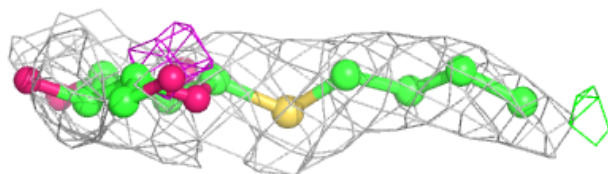
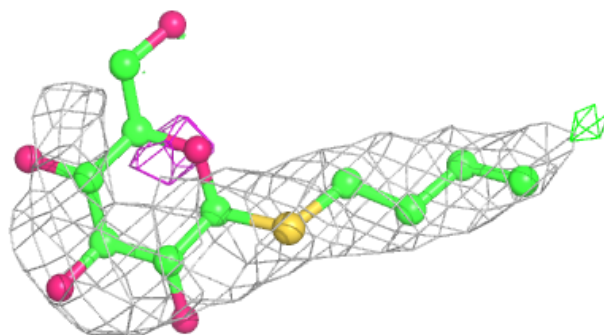
**Electron density around LMT D 405:**

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

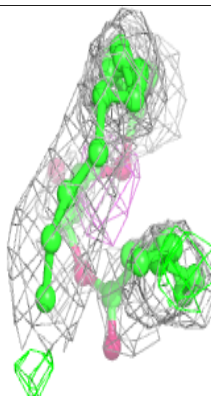
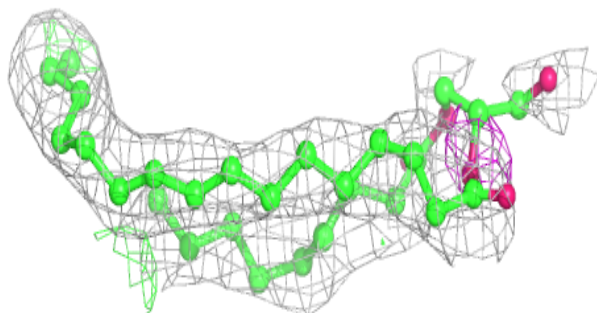
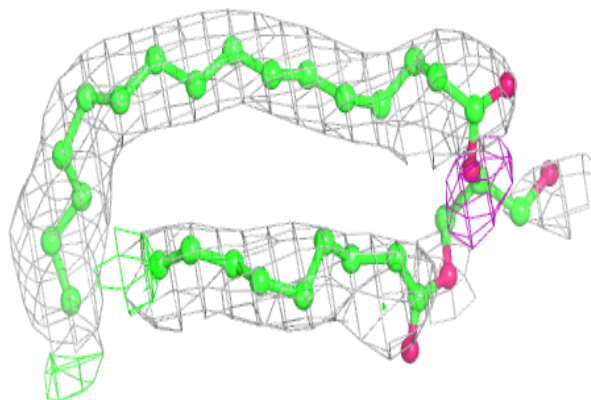


Electron density around HTG D 416:

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

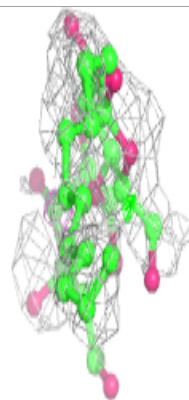
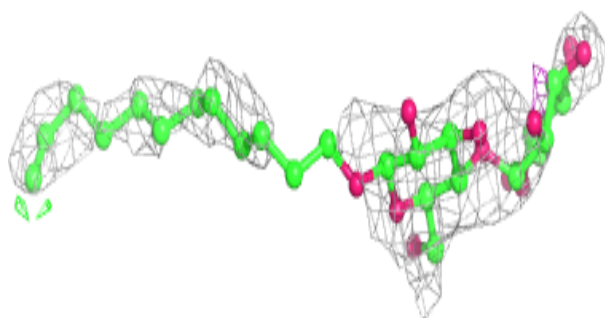
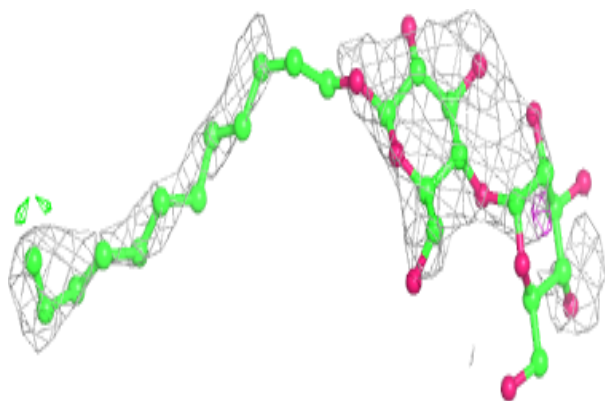
**Electron density around UNL b 633:**

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

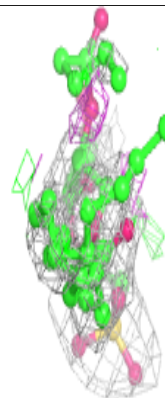
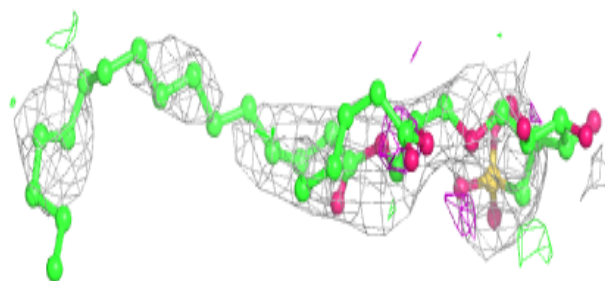
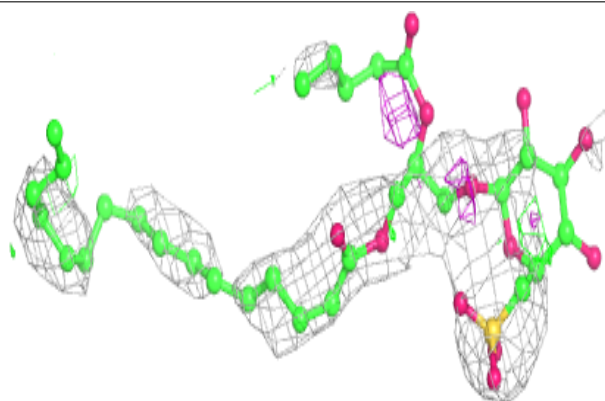


Electron density around LMT e 102:

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

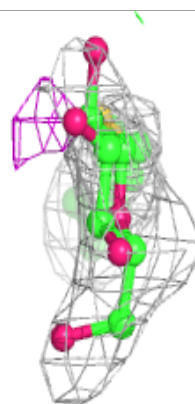
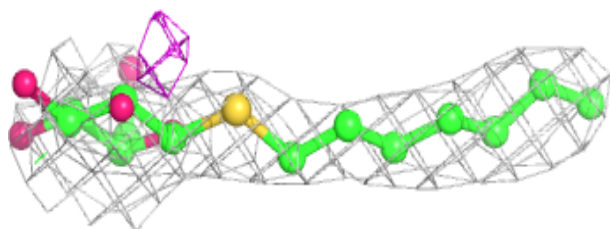
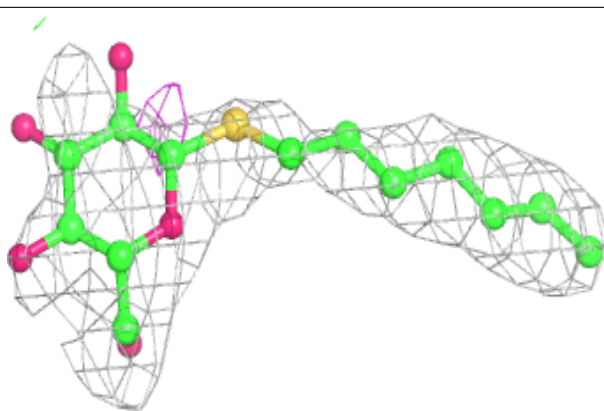
**Electron density around SQD f 102:**

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

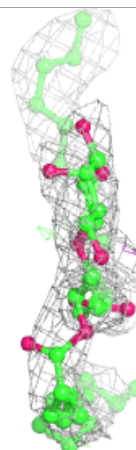
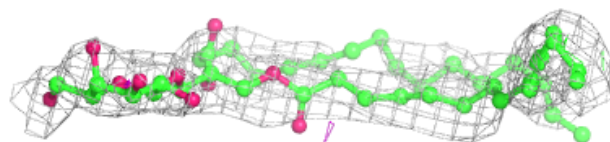
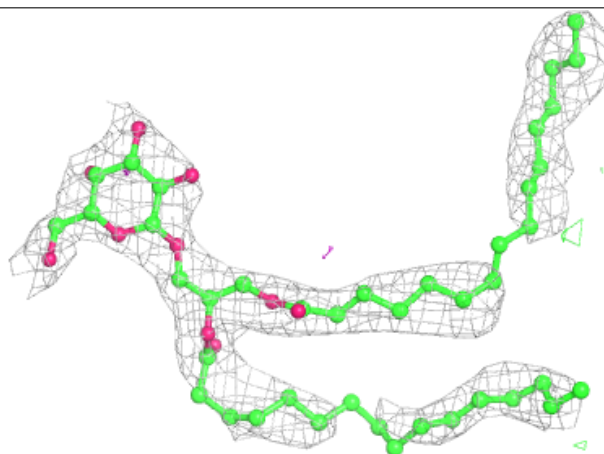


Electron density around HTG B 630:

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

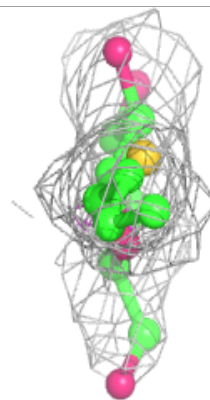
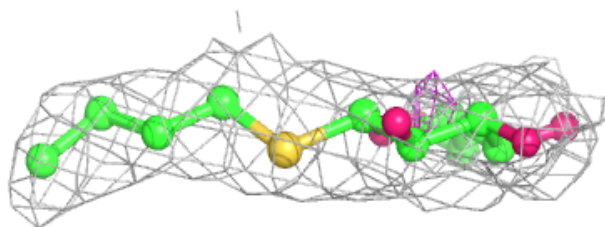
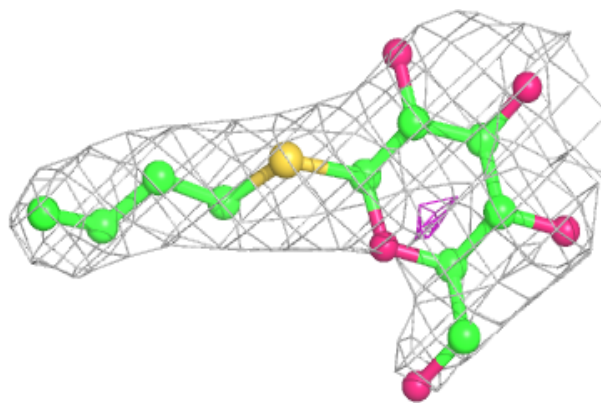
**Electron density around LMG C 519:**

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

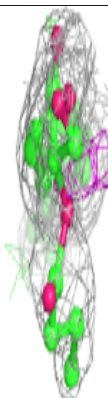
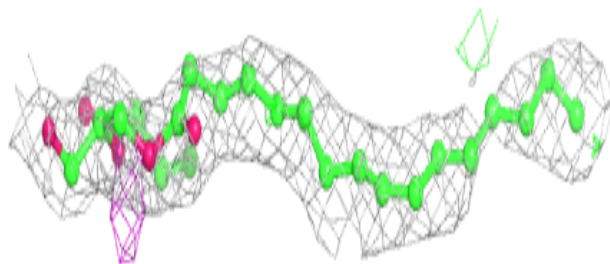
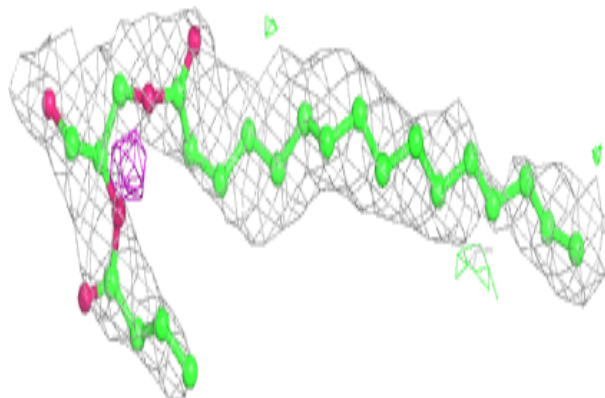


Electron density around HTG d 414:

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

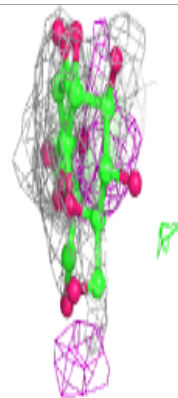
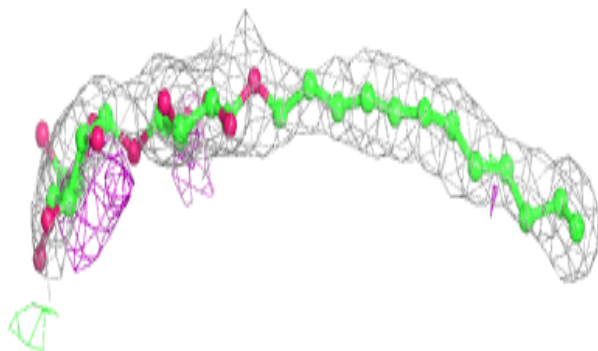
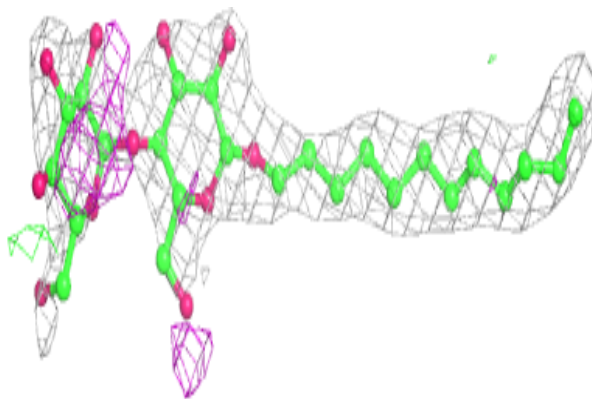
**Electron density around UNL A 417:**

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

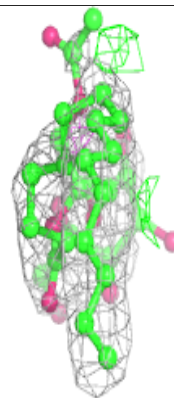
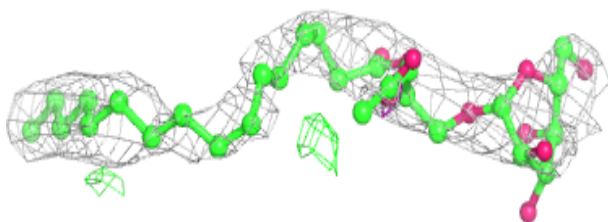
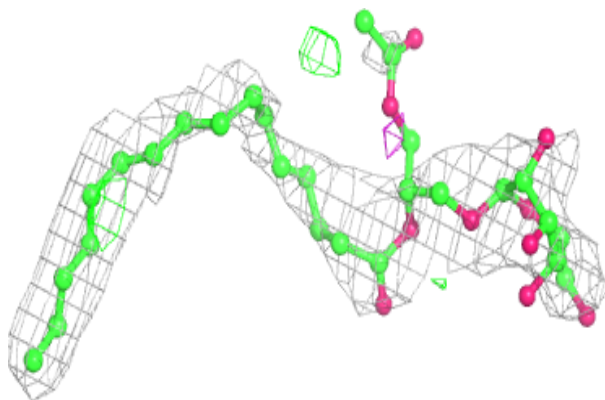


Electron density around LMT M 105:

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

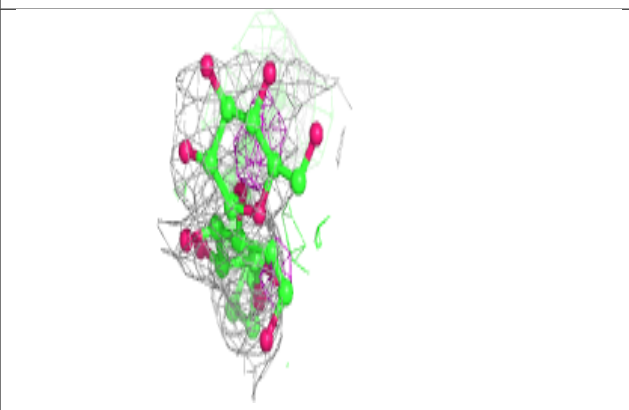
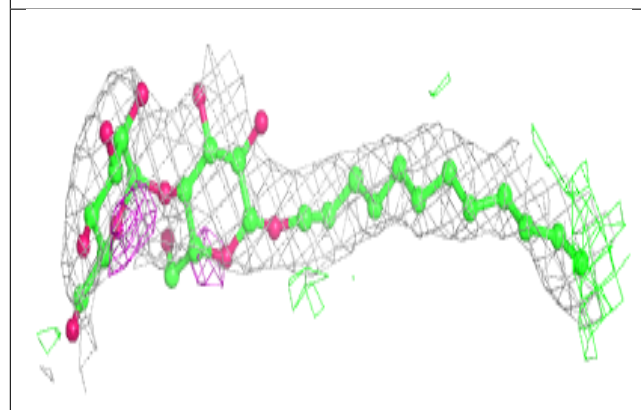
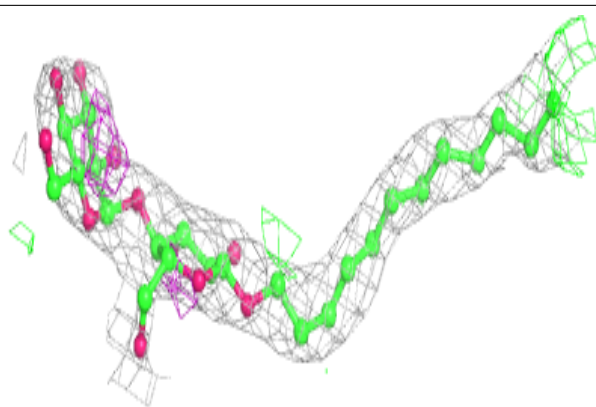
**Electron density around LMG Z 101:**

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

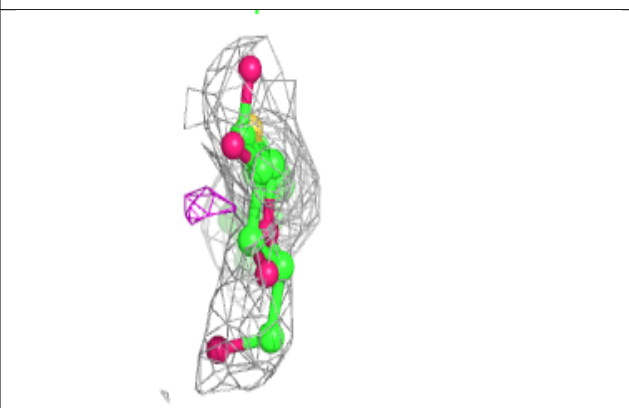
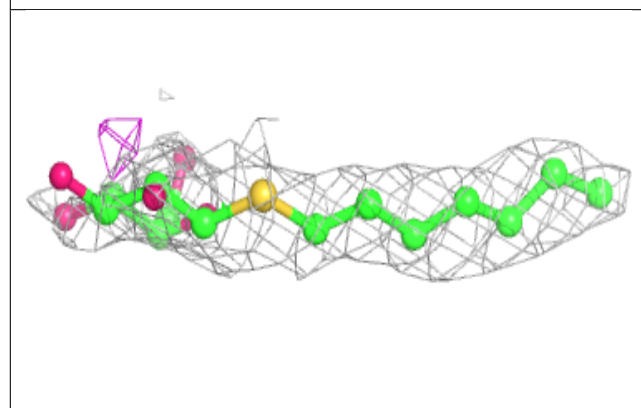
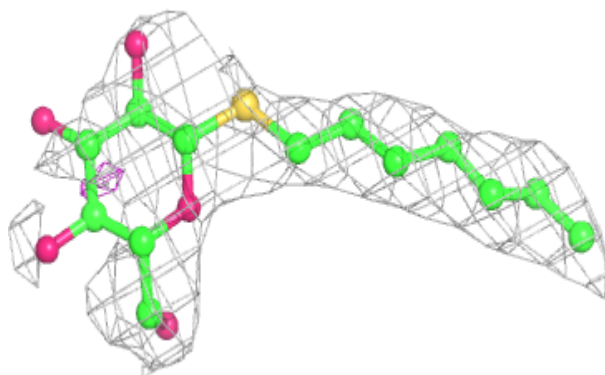


Electron density around LMT A 413:

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

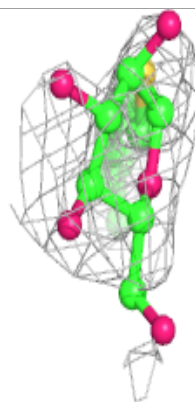
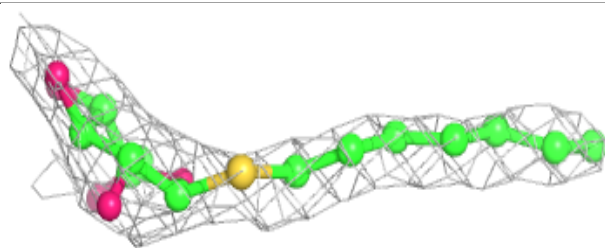
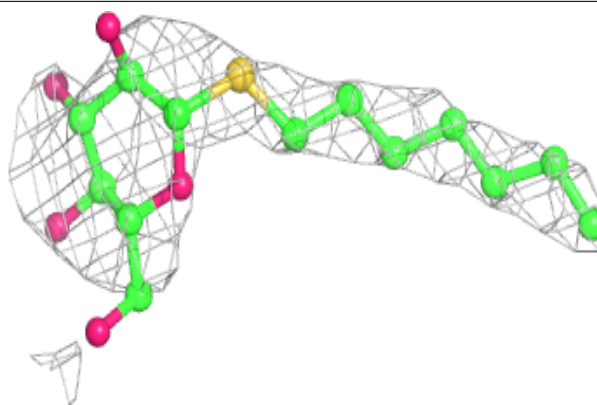
**Electron density around HTG b 608:**

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

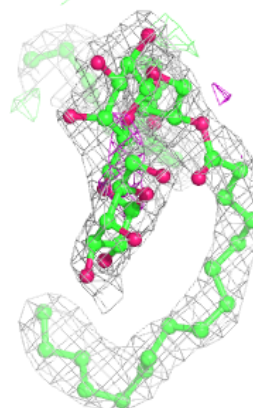
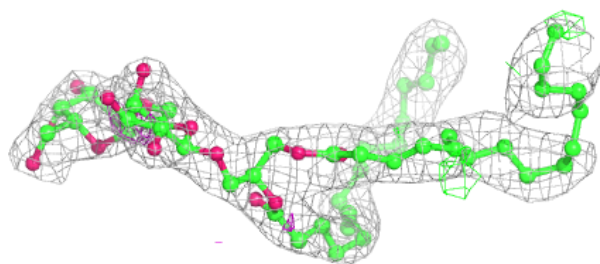
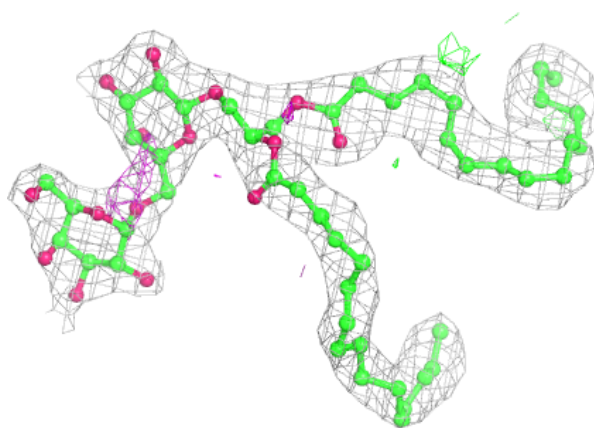


Electron density around HTG B 623:

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

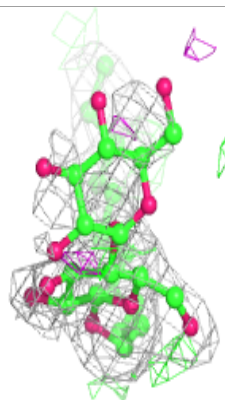
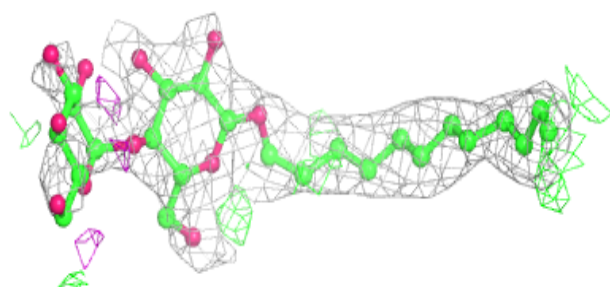
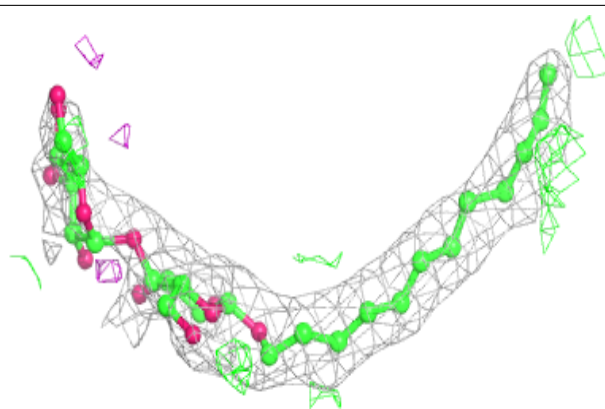
**Electron density around DGD C 517:**

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

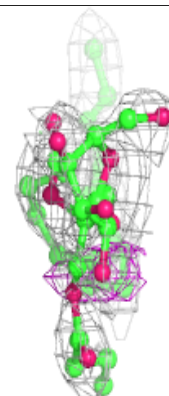
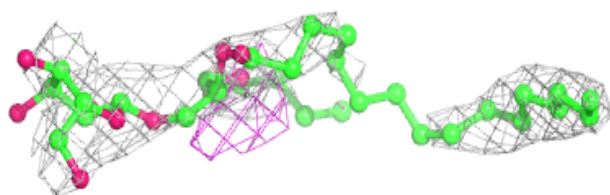
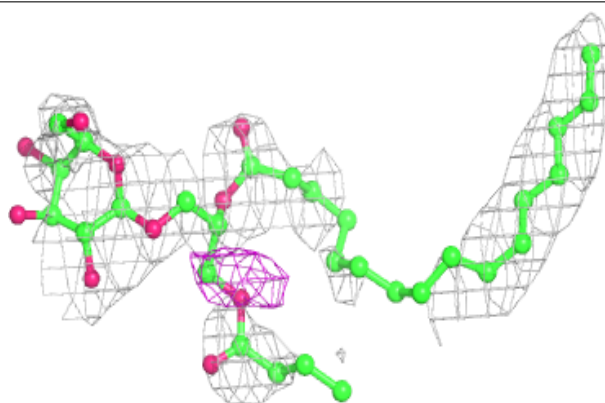


Electron density around LMT M 104:

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

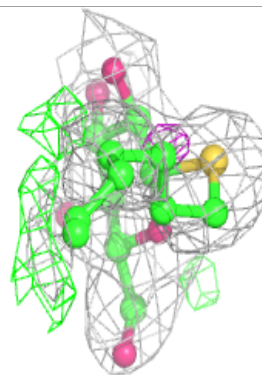
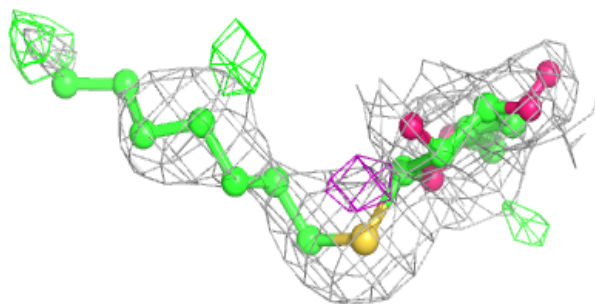
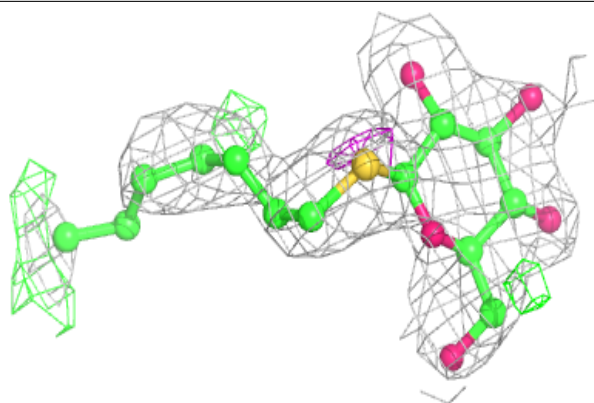
**Electron density around LMG z 101:**

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

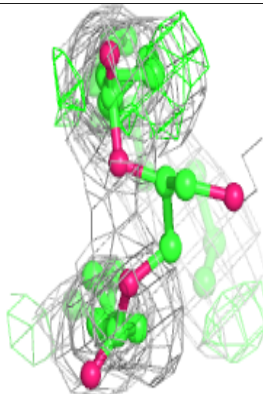
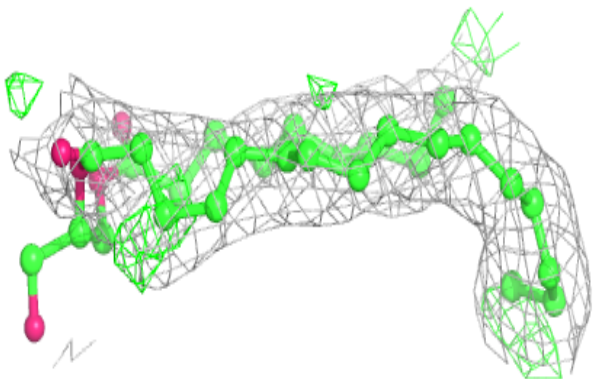
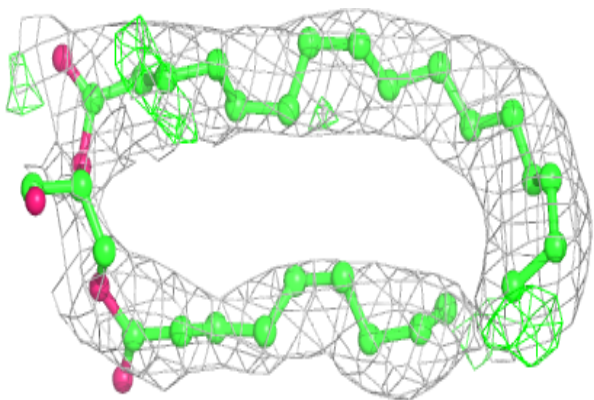


Electron density around HTG b 631:

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

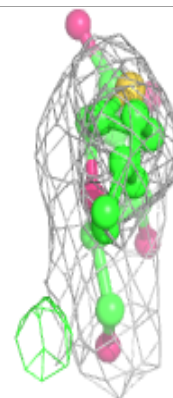
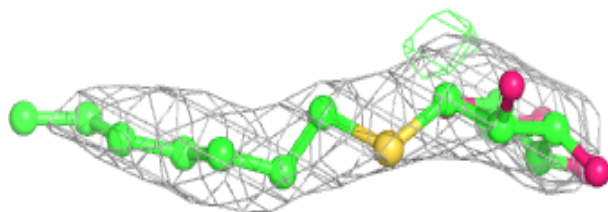
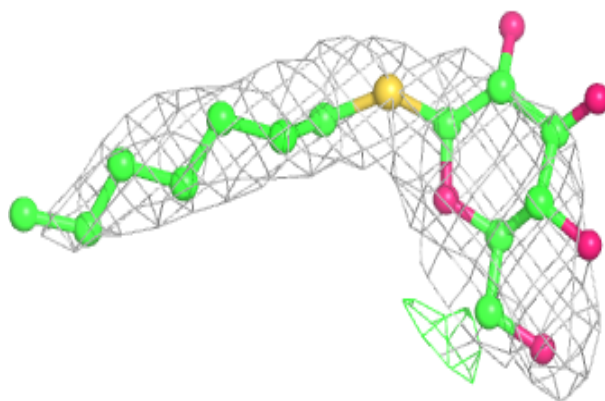
**Electron density around UNL B 631:**

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

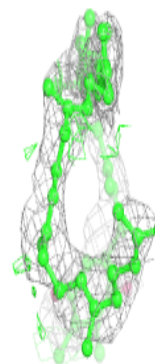
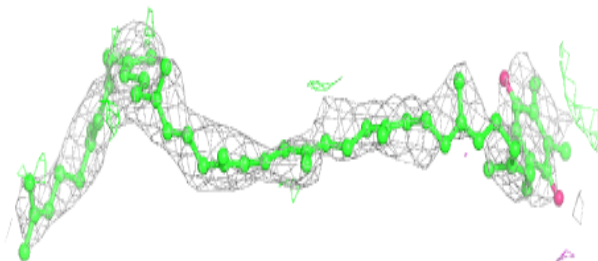
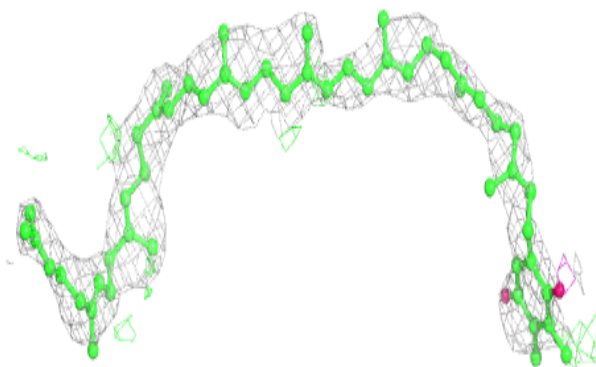


Electron density around HTG b 632:

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

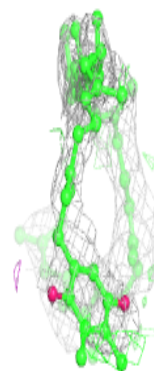
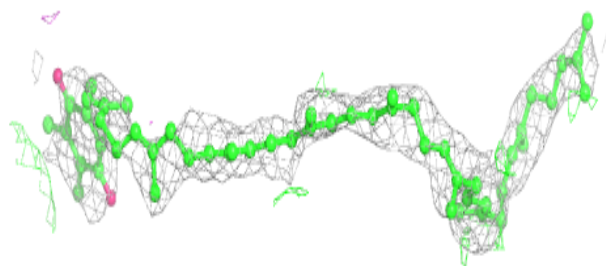
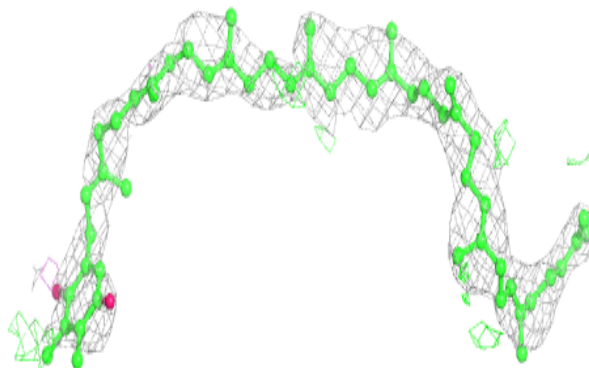
**Electron density around PL9 a 416 (A):**

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

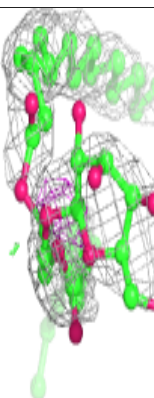
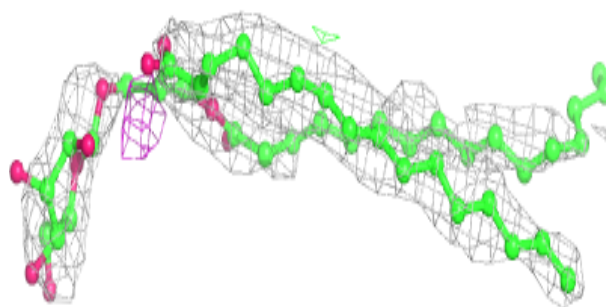
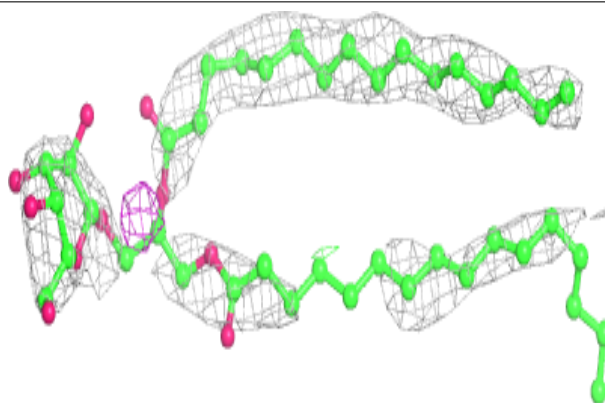


Electron density around PL9 a 416 (B):

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

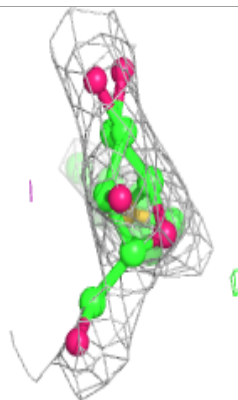
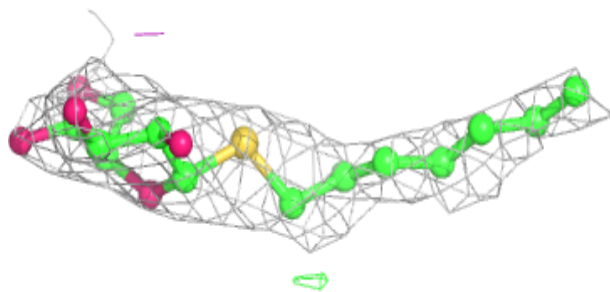
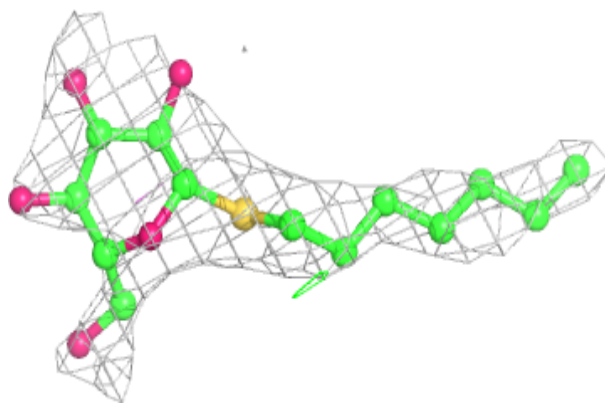
**Electron density around LMG C 520:**

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

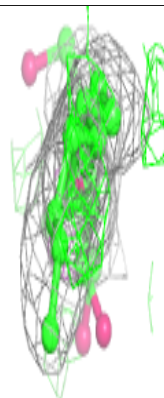
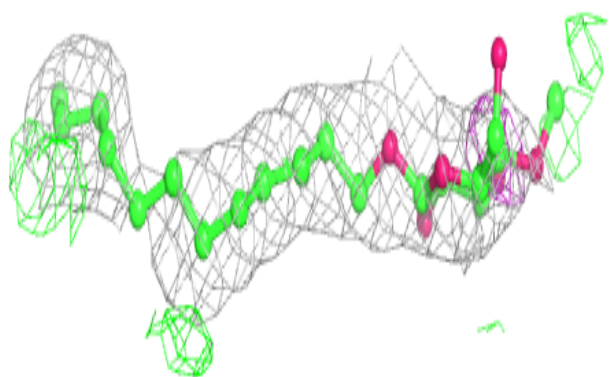
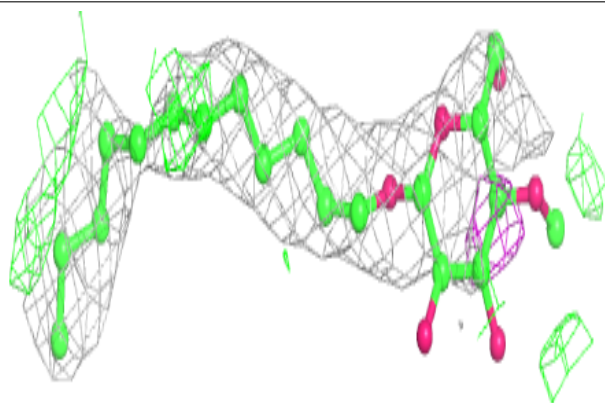


Electron density around HTG C 523:

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

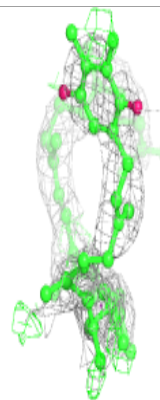
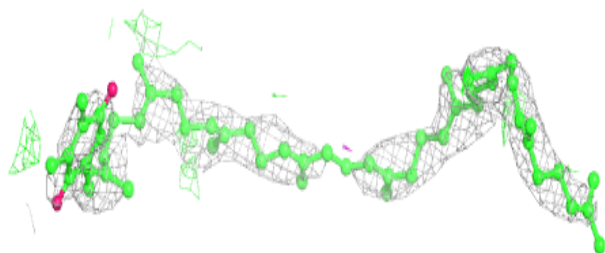
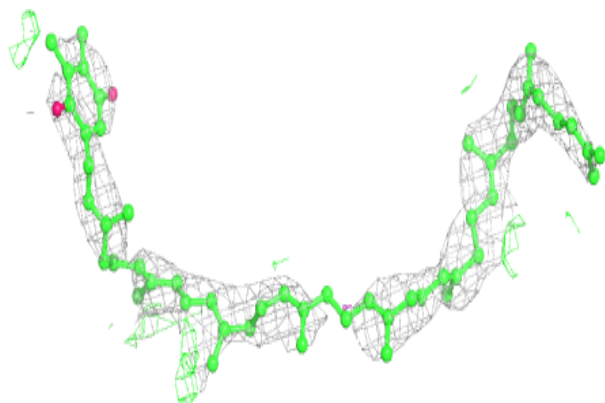
**Electron density around LMT T 104:**

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

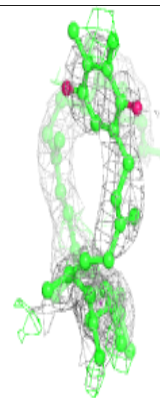
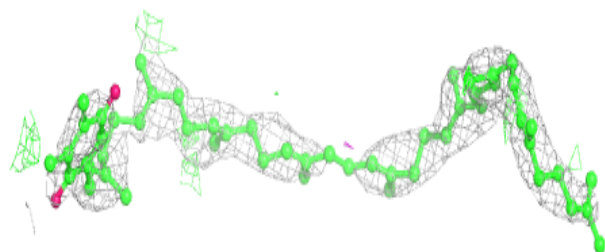
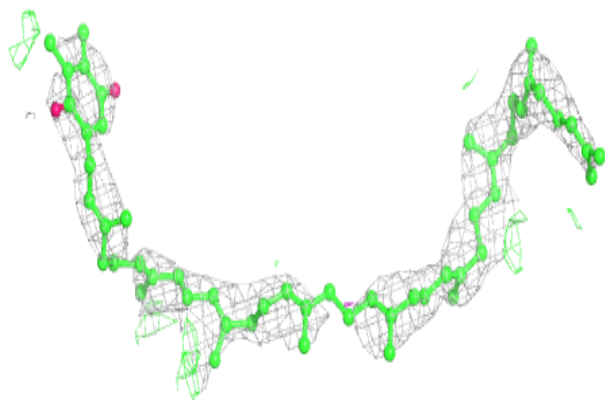


Electron density around PL9 A 416 (A):

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

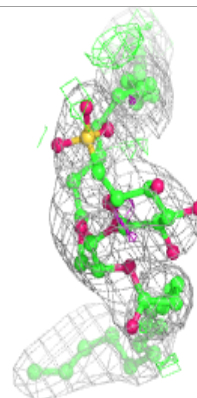
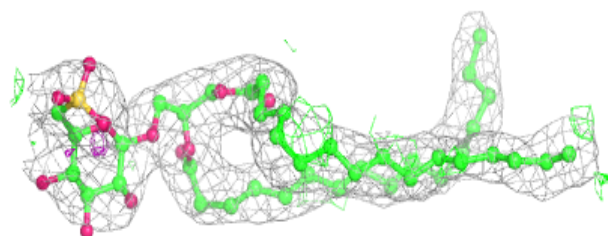
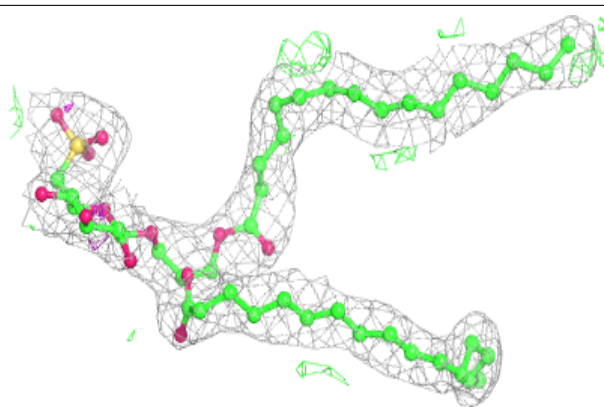
**Electron density around PL9 A 416 (B):**

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

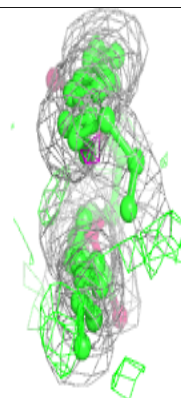
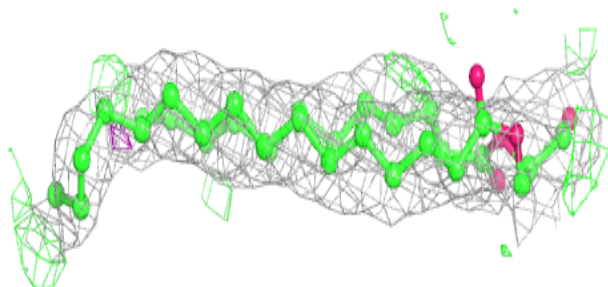
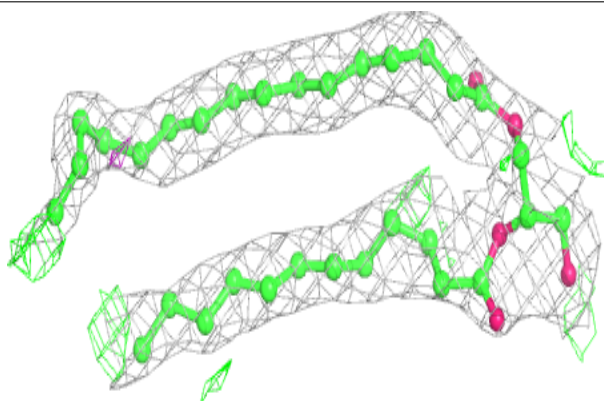


Electron density around SQD a 405:

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

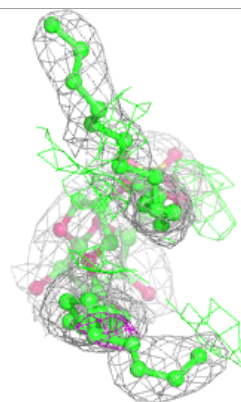
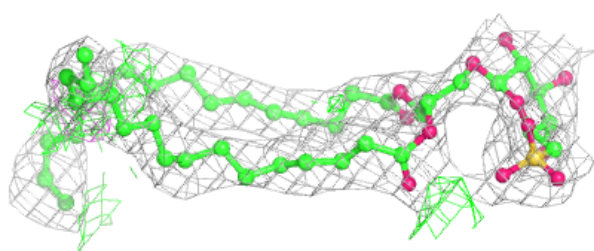
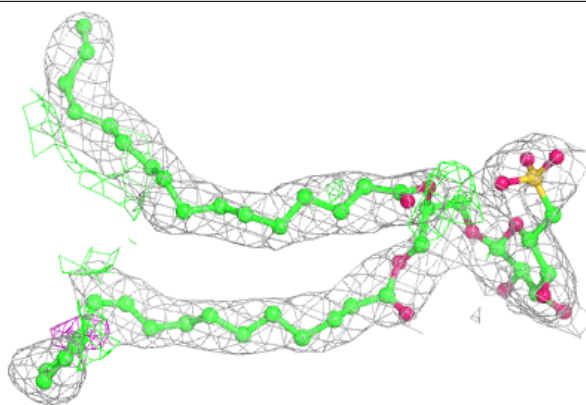
**Electron density around UNL d 413:**

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

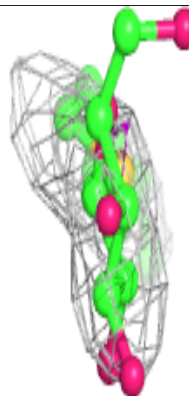
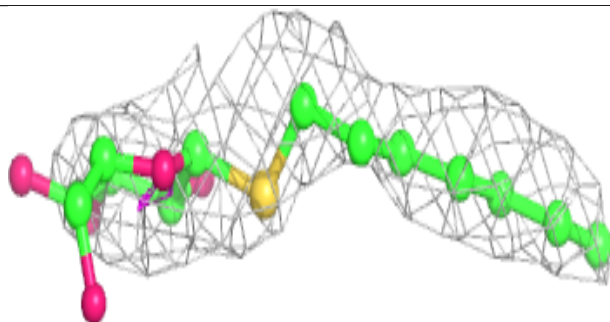
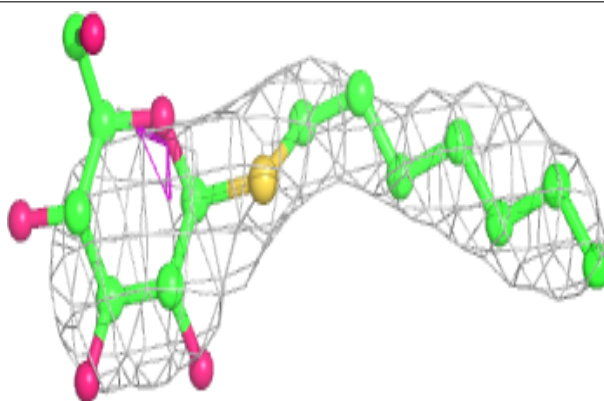


Electron density around SQD L 102:

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

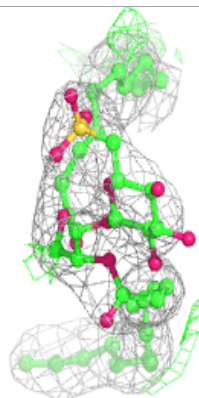
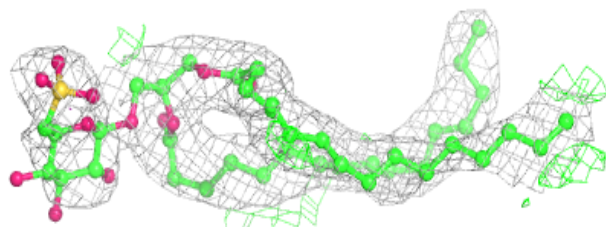
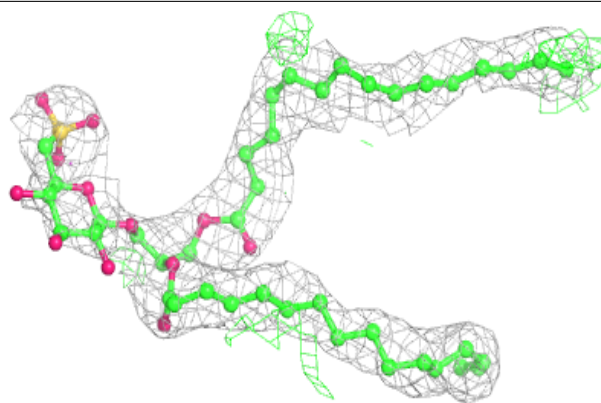
**Electron density around HTG c 525:**

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



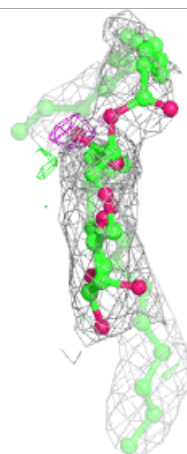
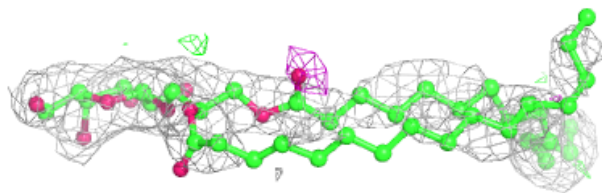
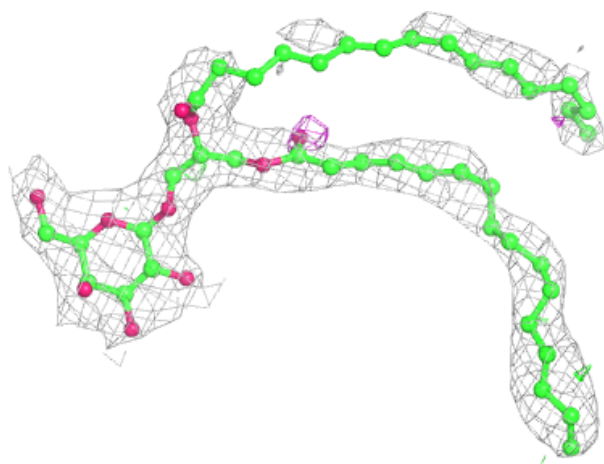
Electron density around SQD A 412:

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



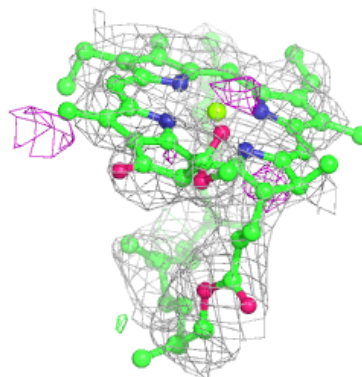
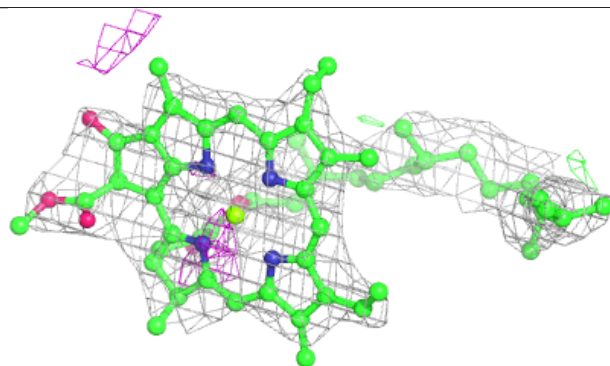
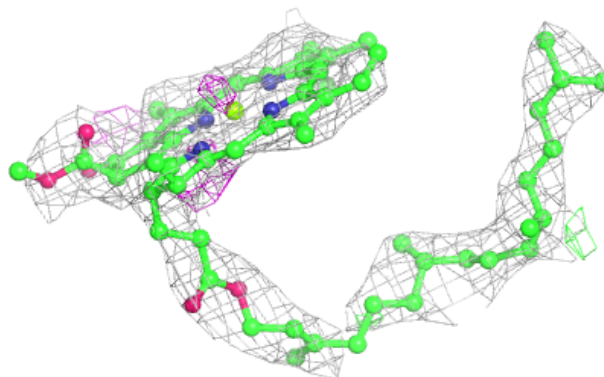
Electron density around LMG c 522:

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

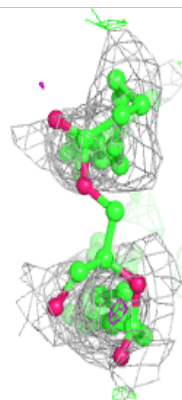
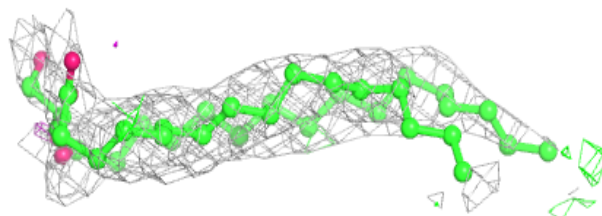
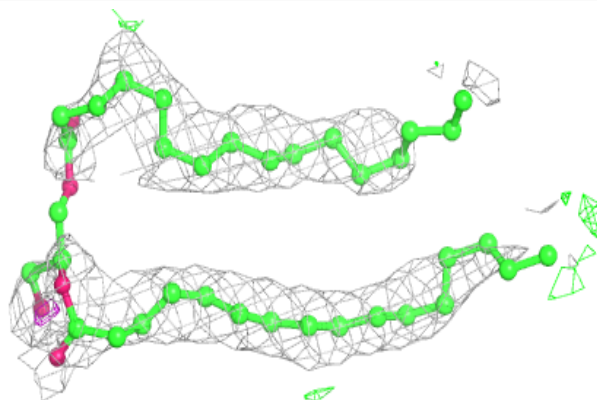


Electron density around CLA c 517:

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

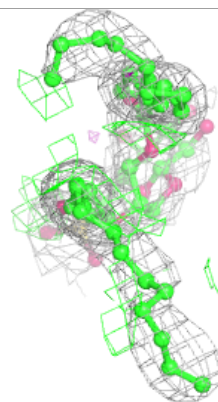
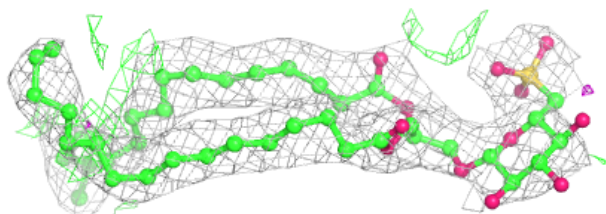
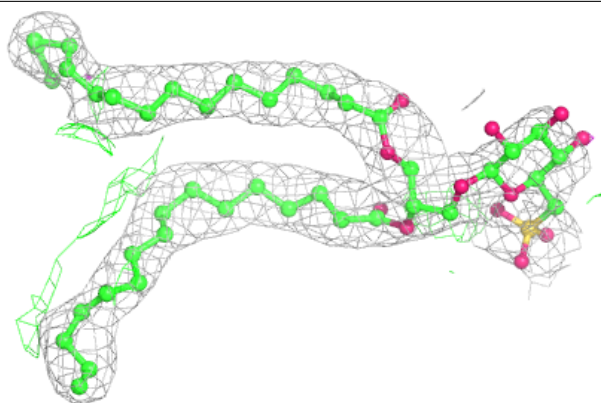
**Electron density around UNL I 101:**

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

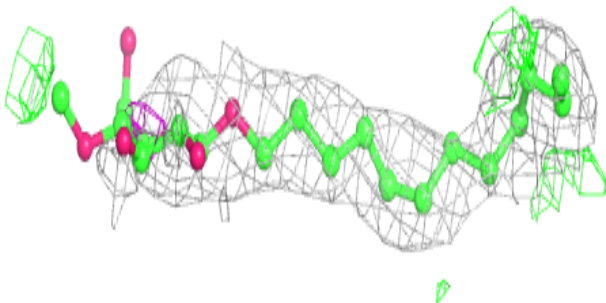
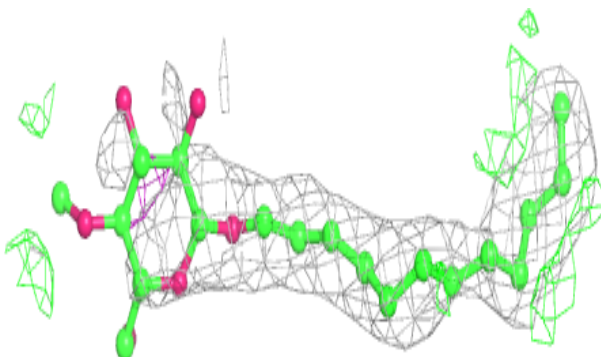


Electron density around SQD B 621:

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

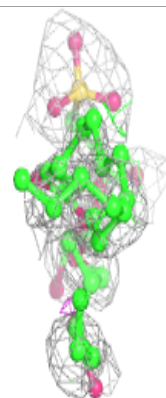
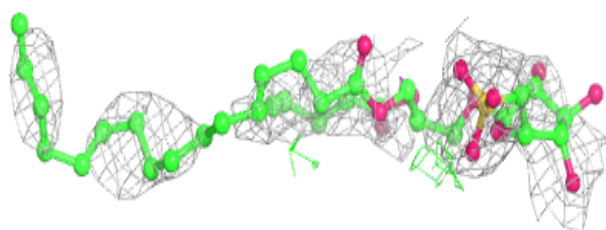
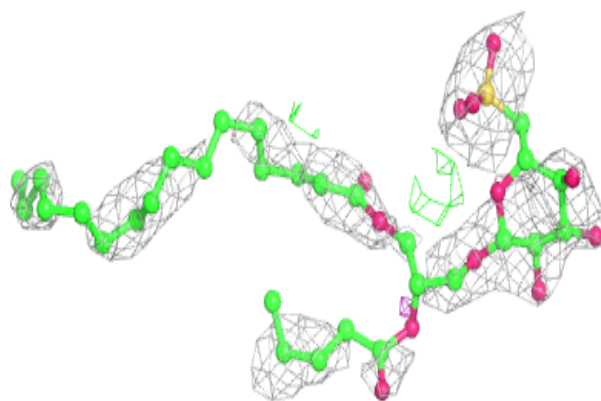
**Electron density around LMT t 101:**

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

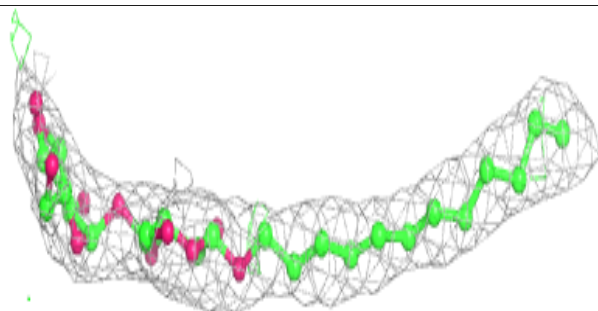
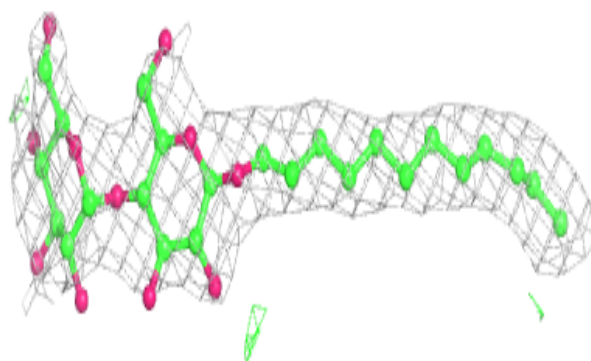


Electron density around SQD F 104:

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

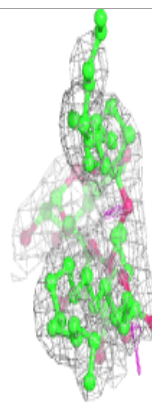
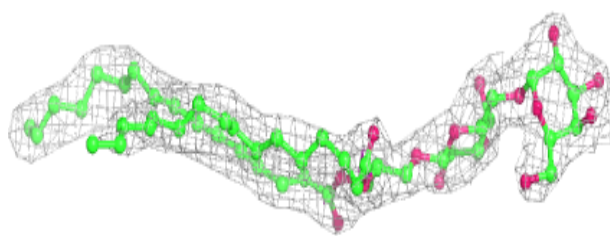
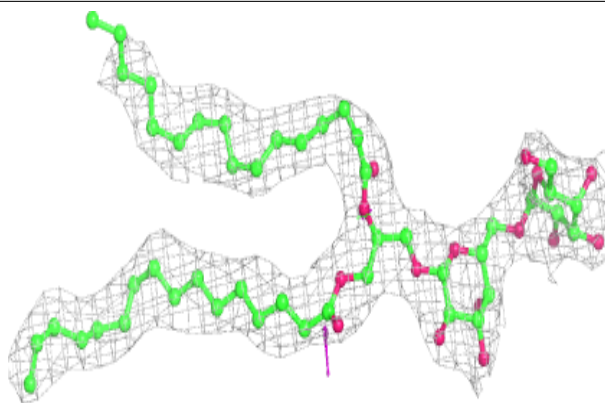
**Electron density around LMT M 102:**

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

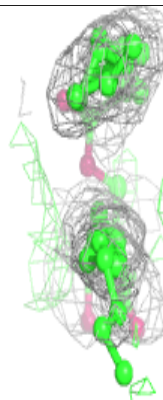
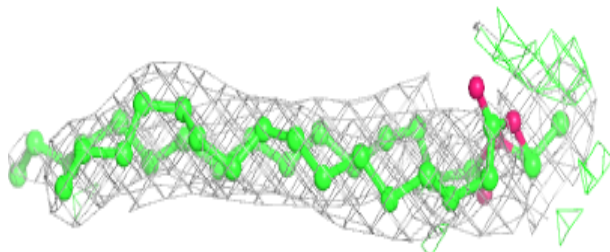
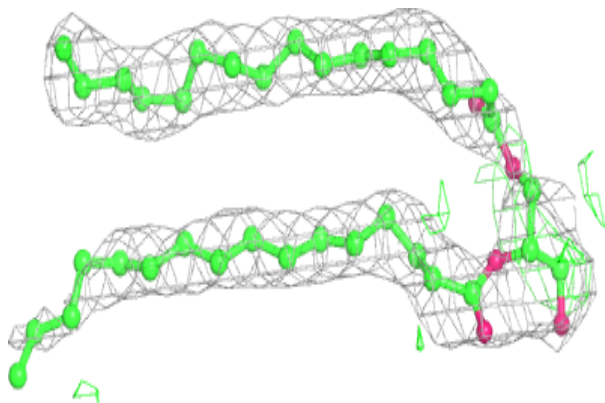


Electron density around DGD C 518:

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

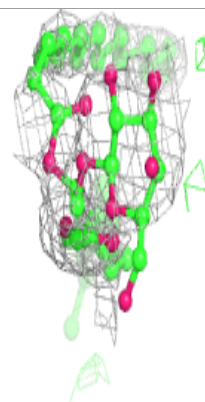
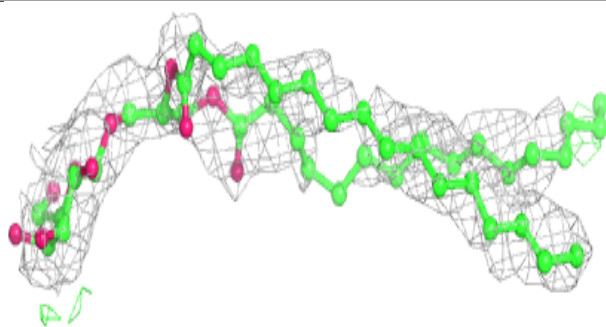
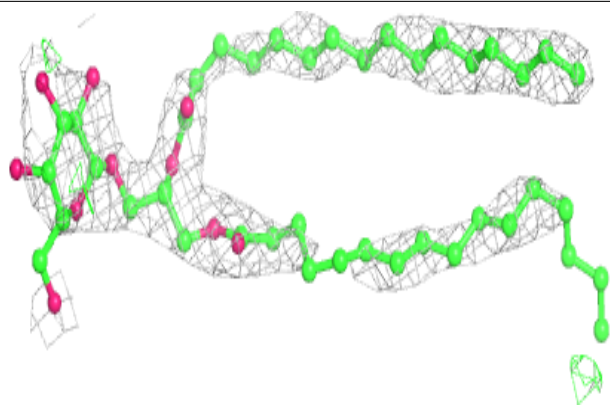
**Electron density around UNL D 415:**

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

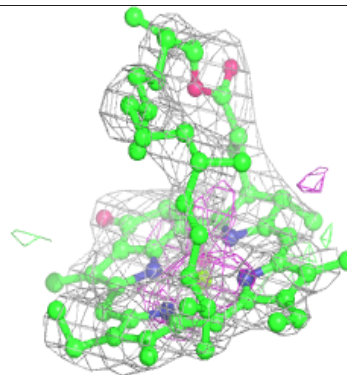
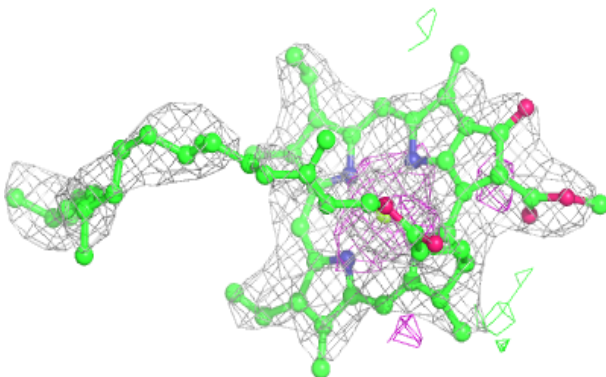
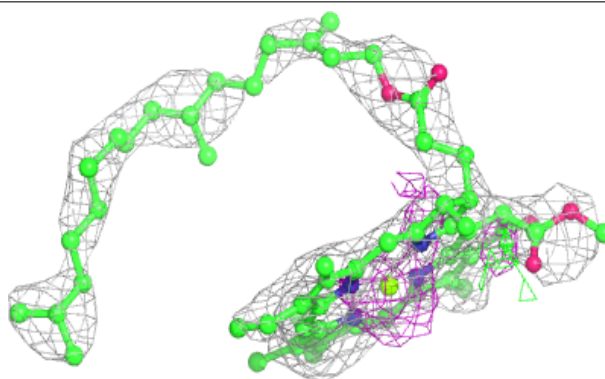


Electron density around LMG c 523:

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

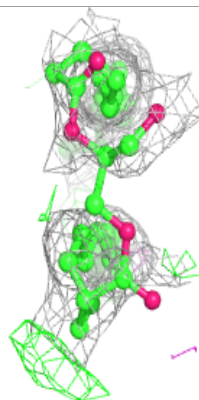
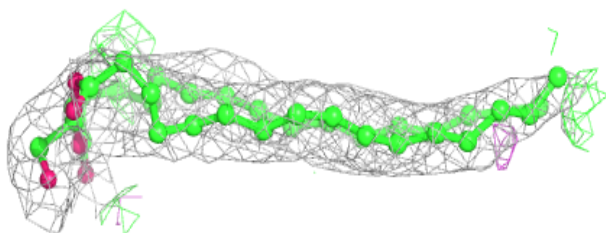
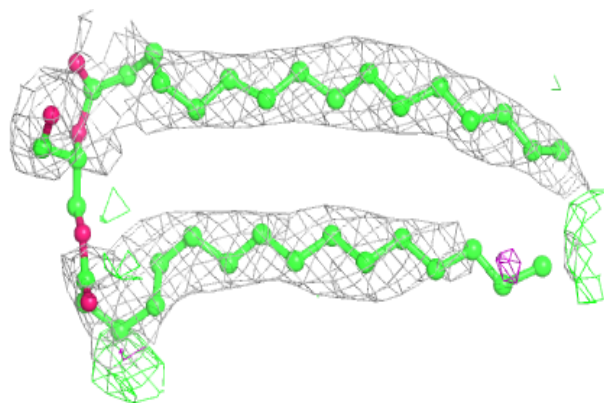
**Electron density around CLA C 514:**

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

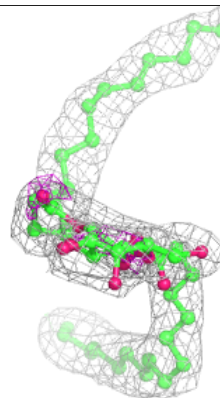
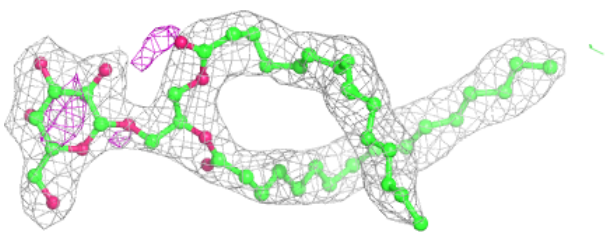
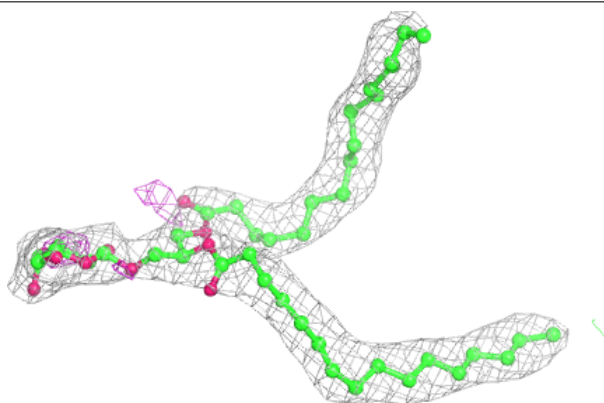


Electron density around UNL i 101:

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

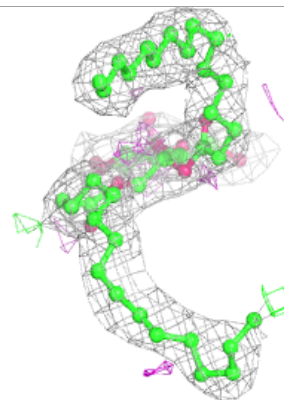
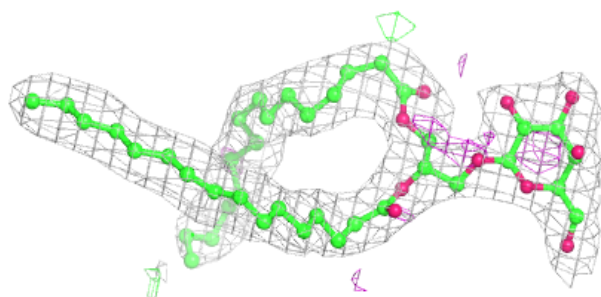
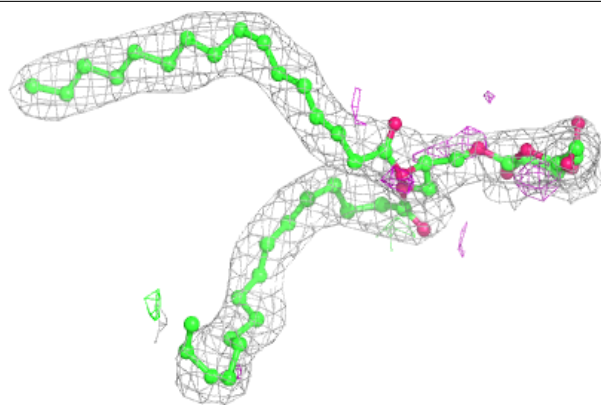
**Electron density around LMG M 101:**

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

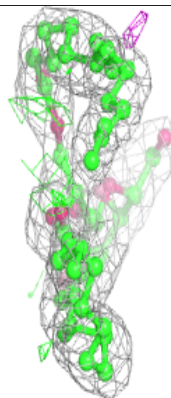
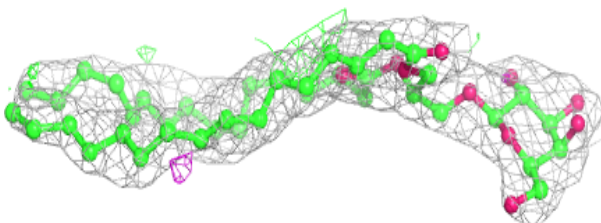
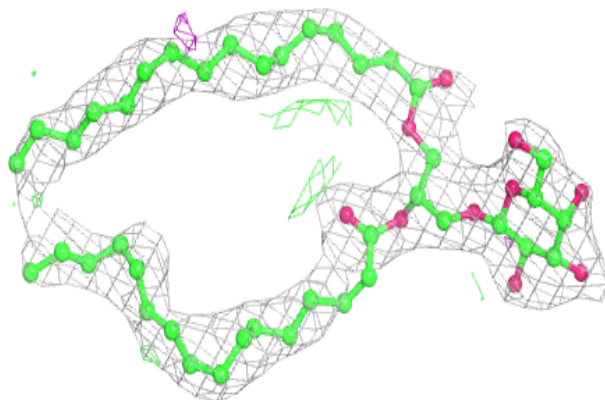


Electron density around LMG b 629:

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

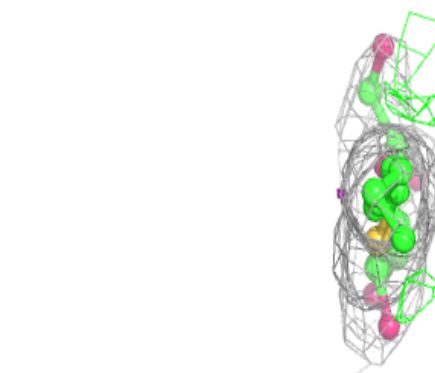
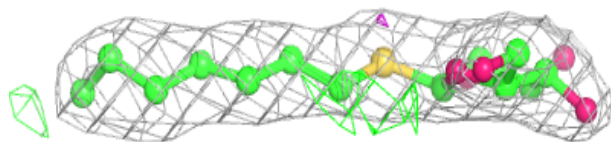
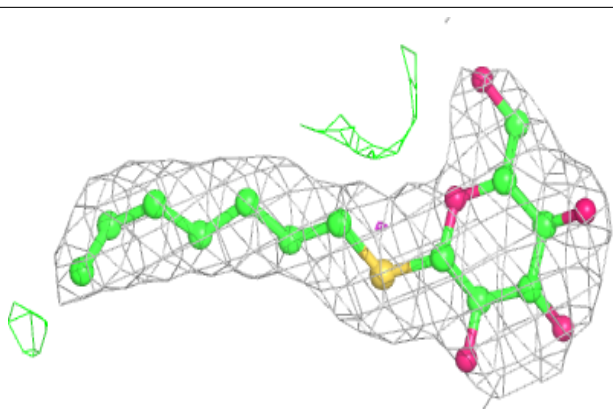
**Electron density around LMG C 501:**

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

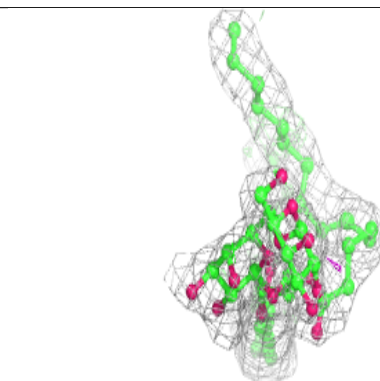
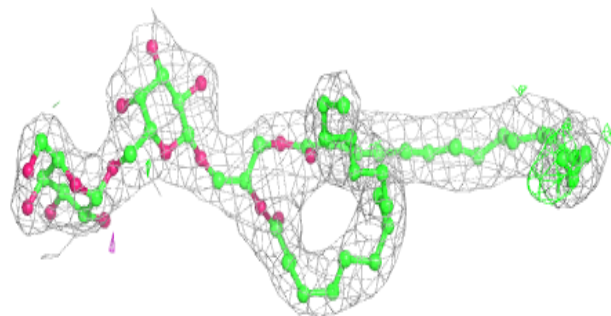
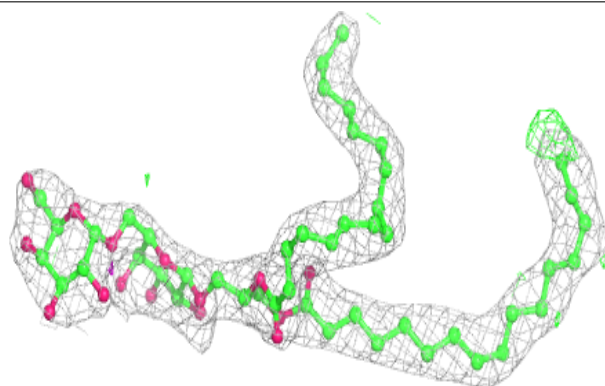


Electron density around HTG b 607:

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

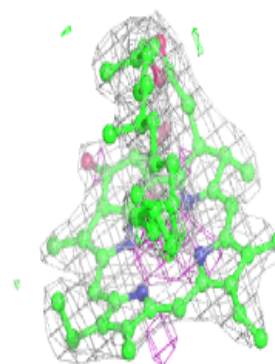
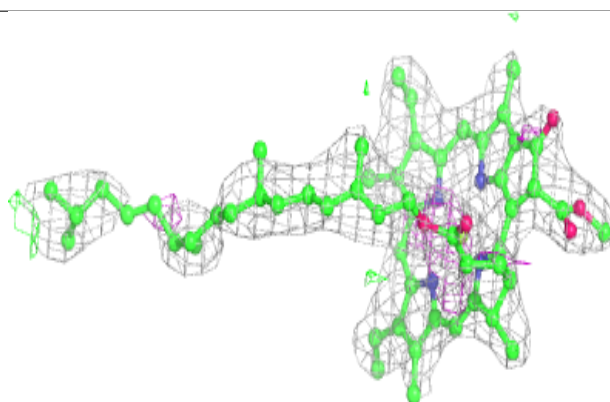
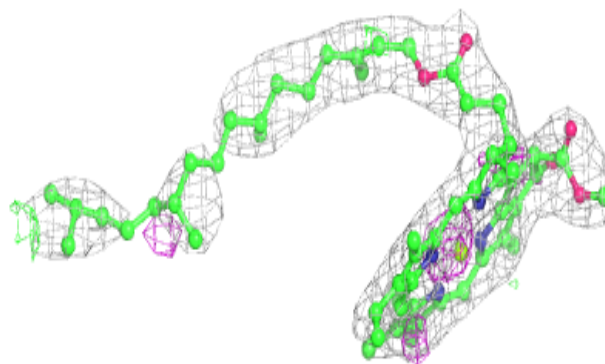
**Electron density around DGD h 102:**

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

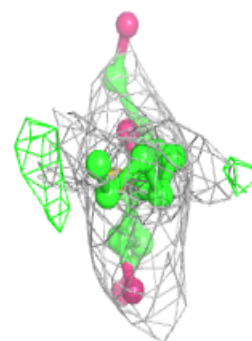
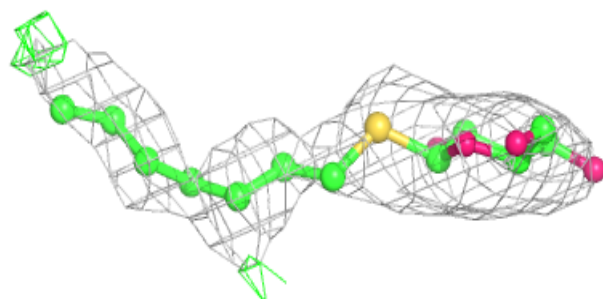
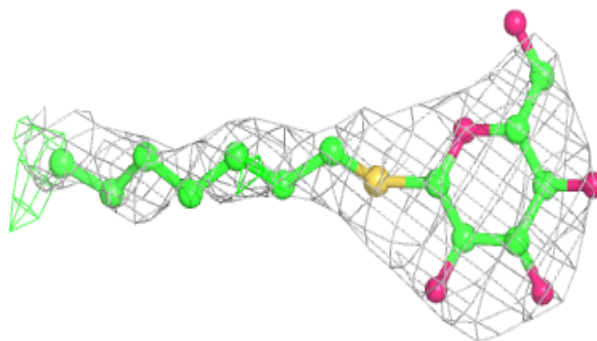


Electron density around CLA C 505:

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

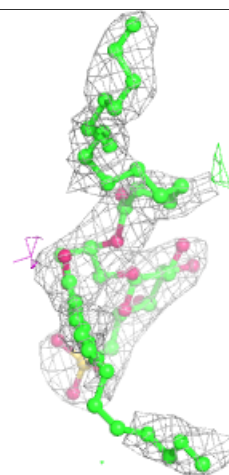
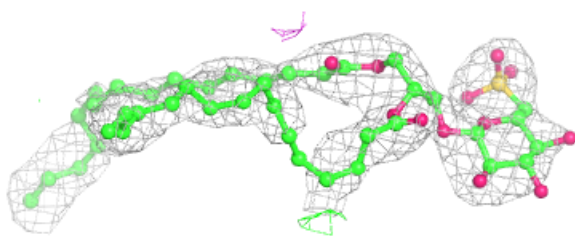
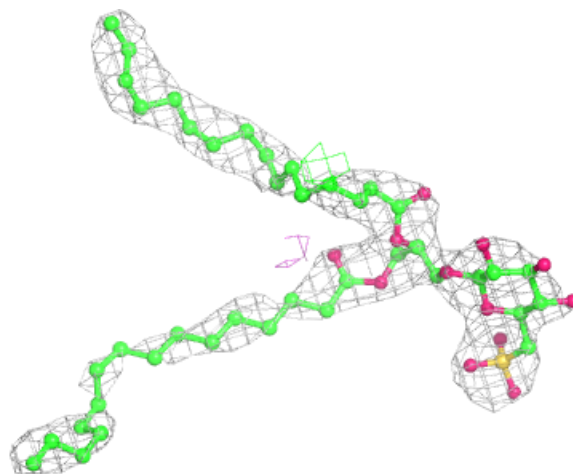
**Electron density around HTG c 524:**

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



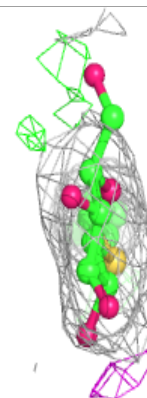
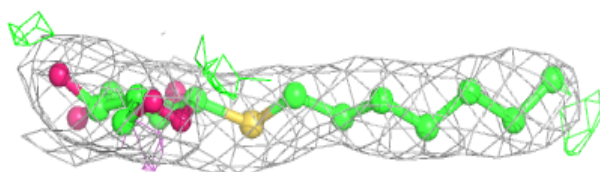
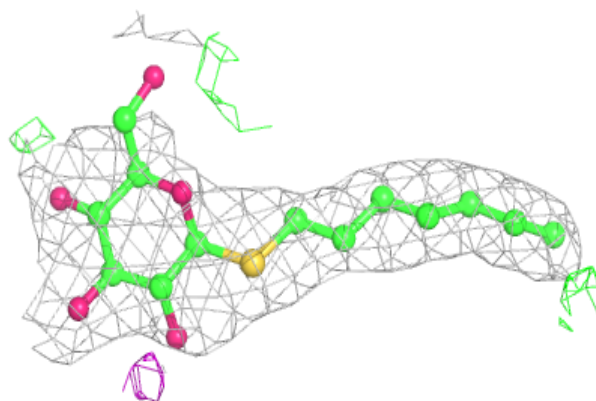
Electron density around SQD A 409:

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

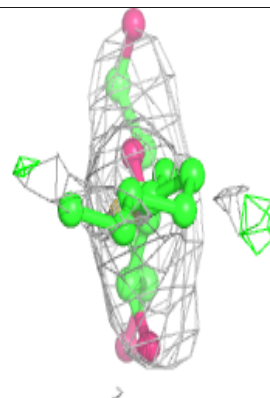
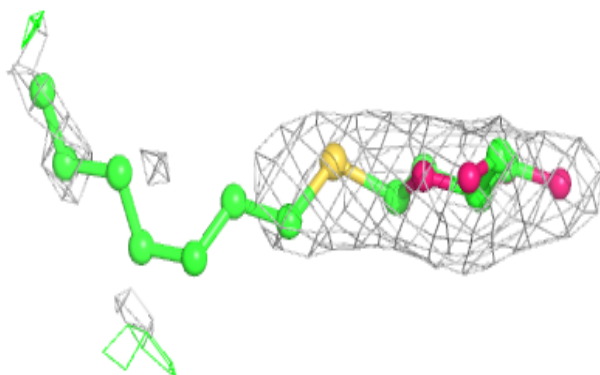
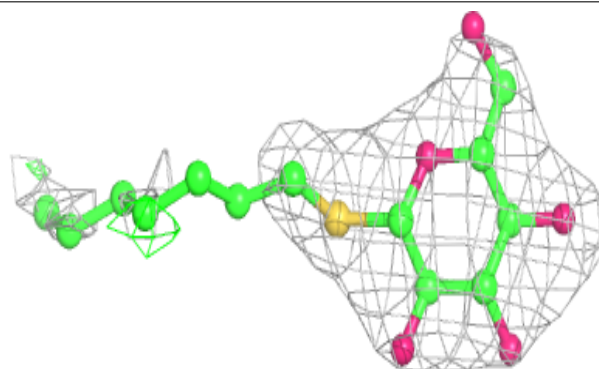


Electron density around HTG B 629:

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

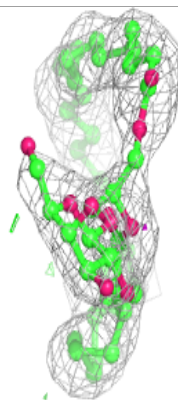
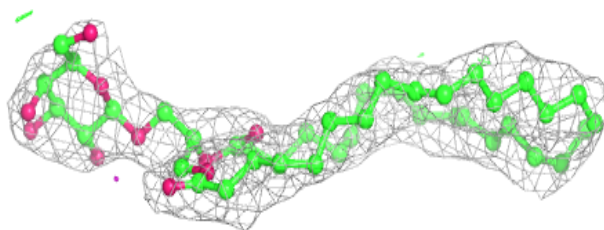
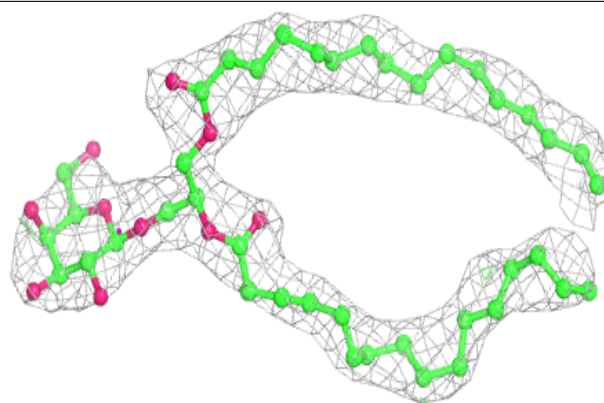
**Electron density around HTG C 522:**

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

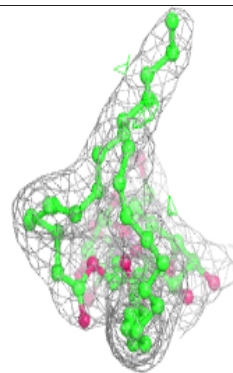
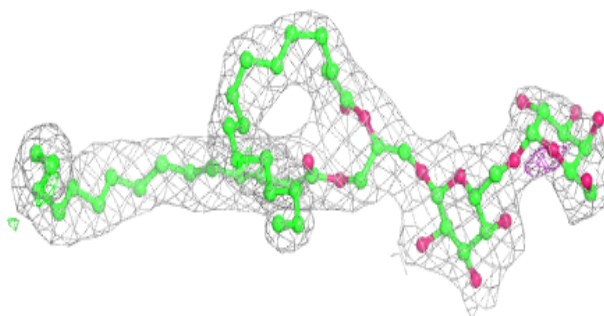
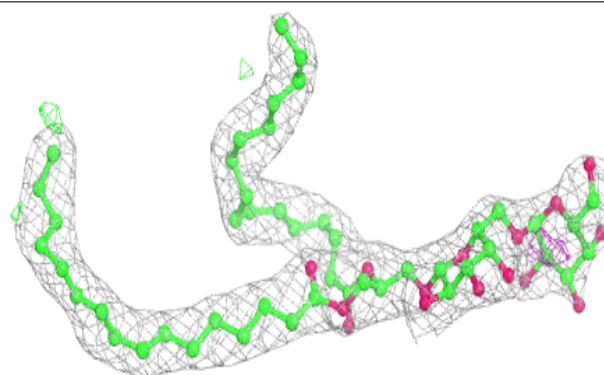


Electron density around LMG a 415:

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

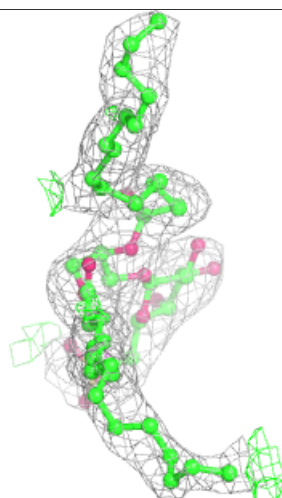
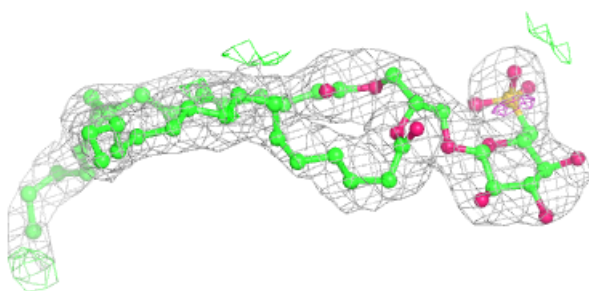
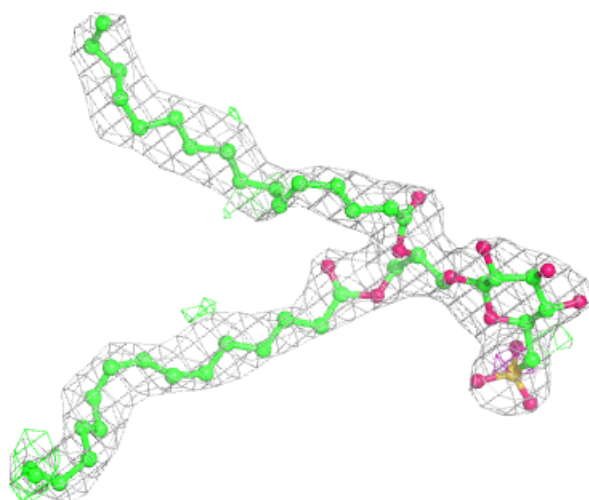
**Electron density around DGD B 632:**

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



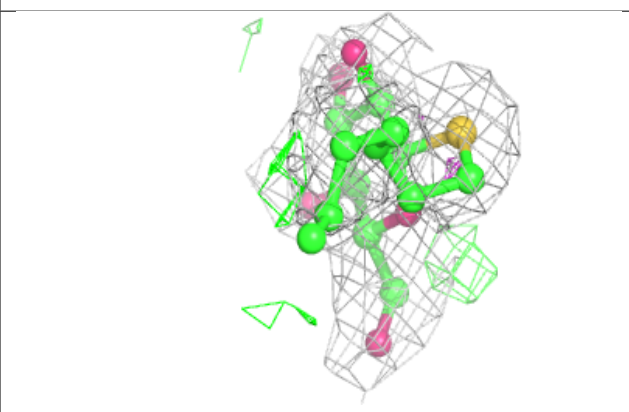
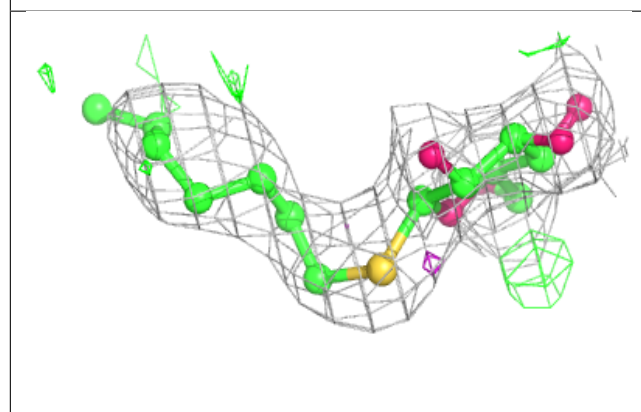
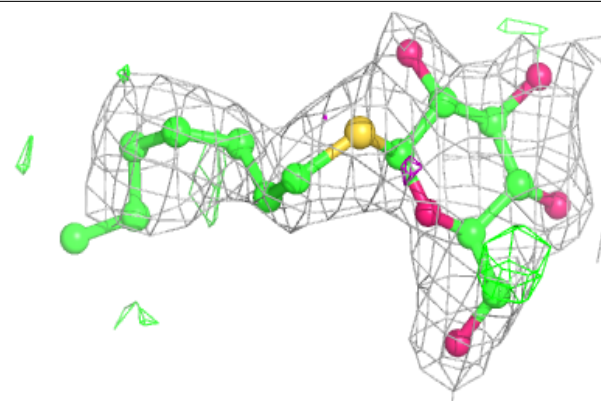
Electron density around SQD a 414:

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

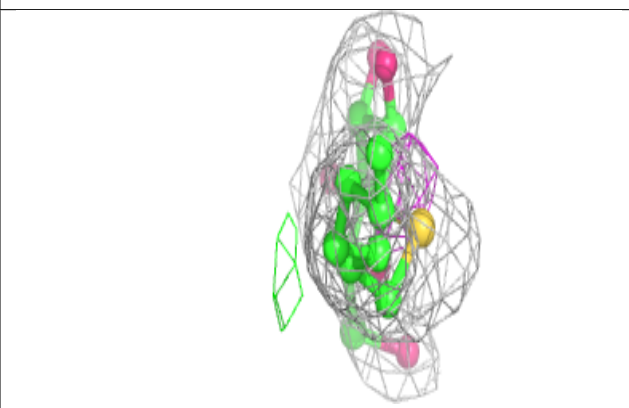
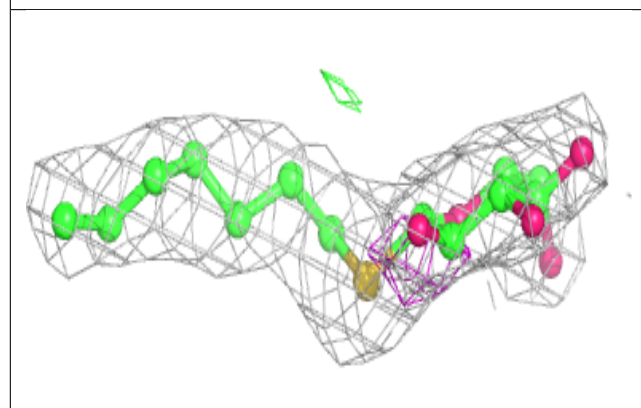
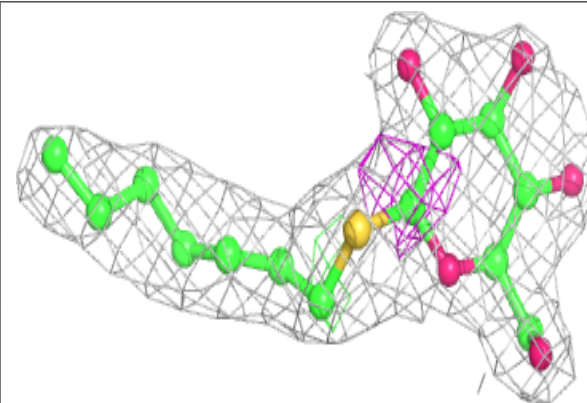


Electron density around HTG B 622:

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

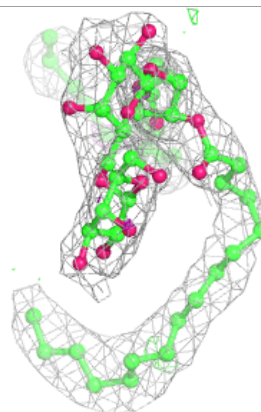
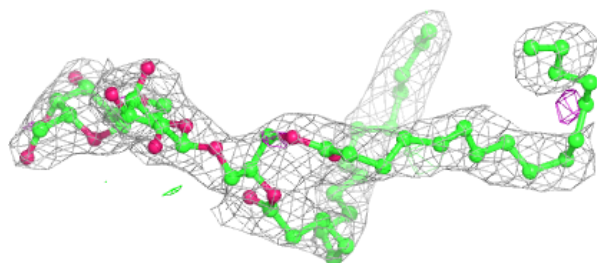
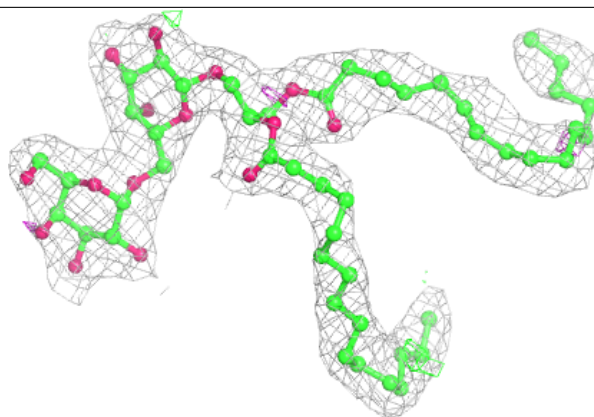
**Electron density around HTG b 601:**

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

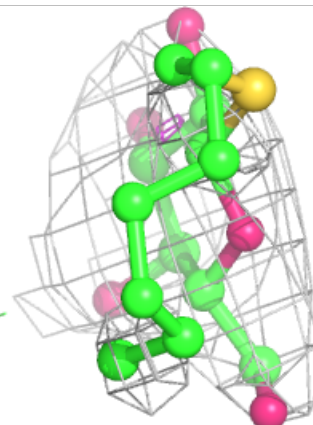
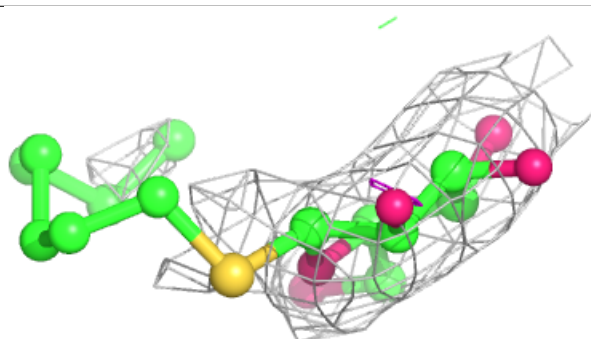
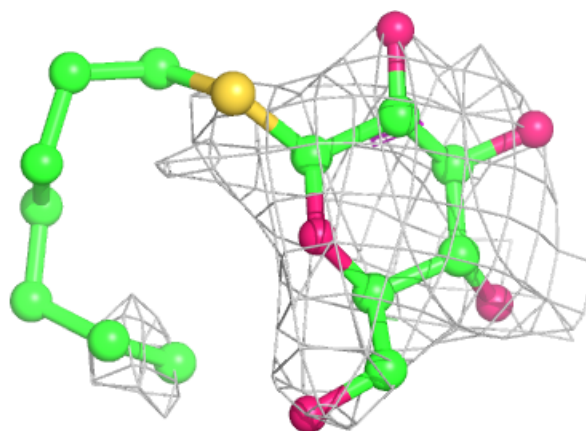


Electron density around DGD c 520:

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

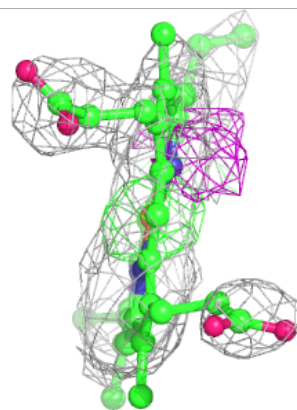
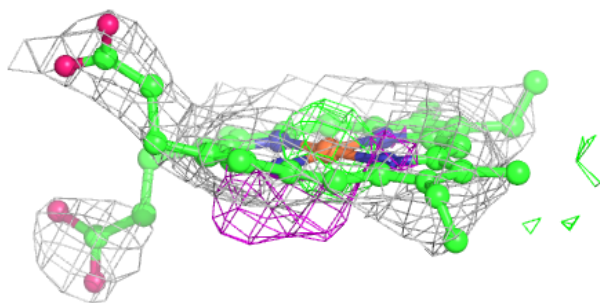
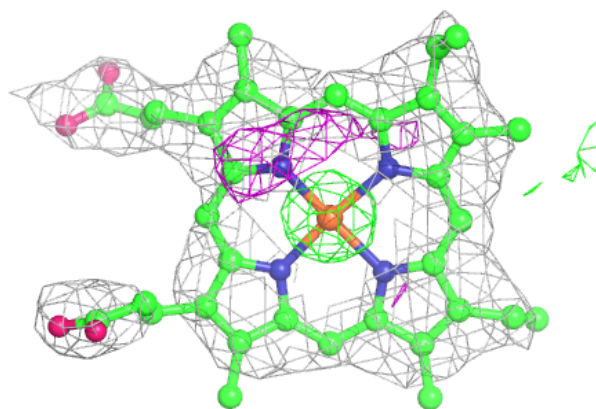
**Electron density around HTG V 207:**

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



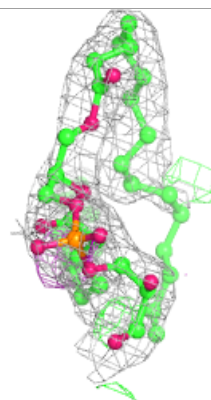
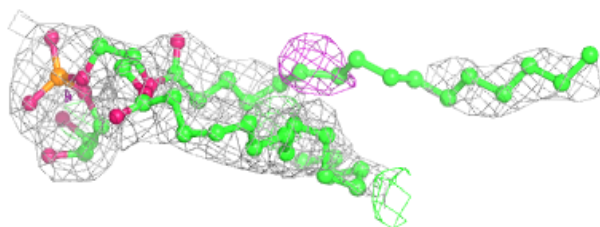
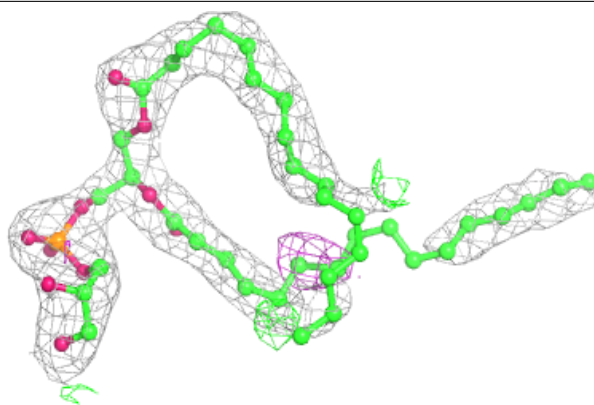
Electron density around HEM F 102:

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

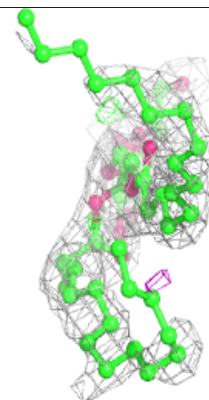
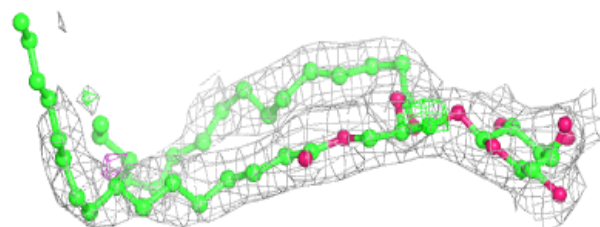
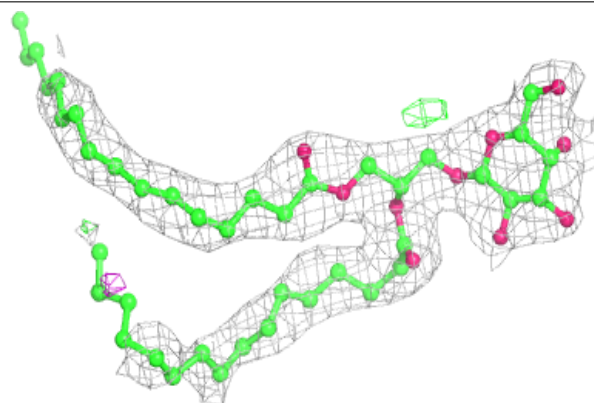


Electron density around LHG D 413:

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

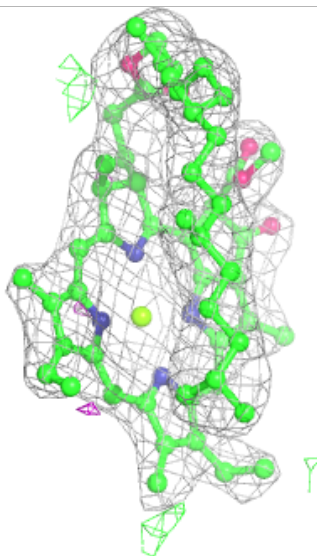
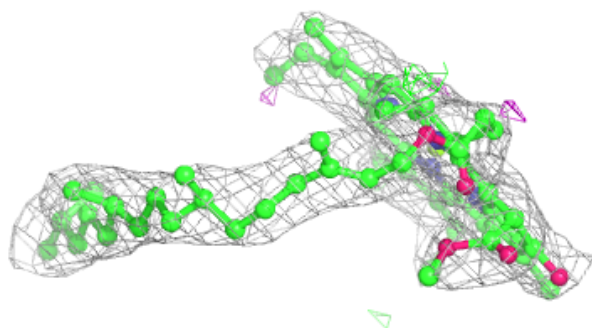
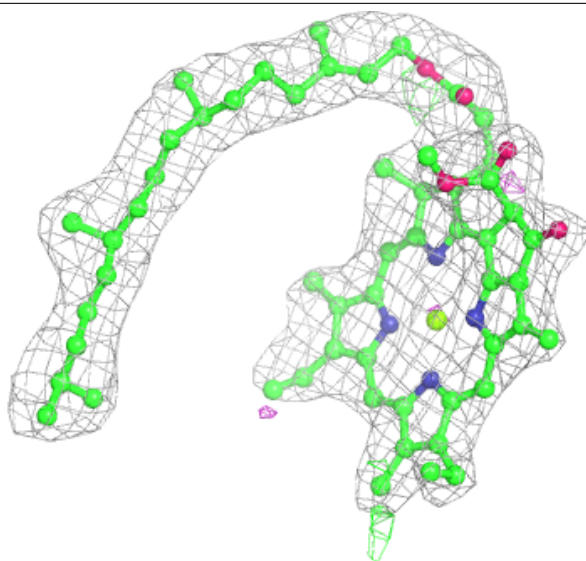
**Electron density around LMG D 417:**

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



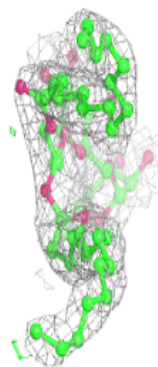
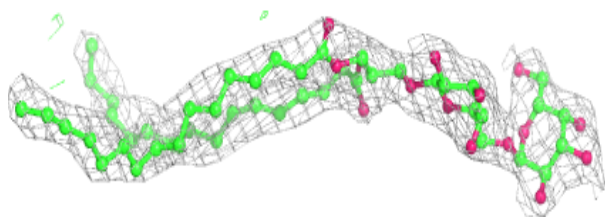
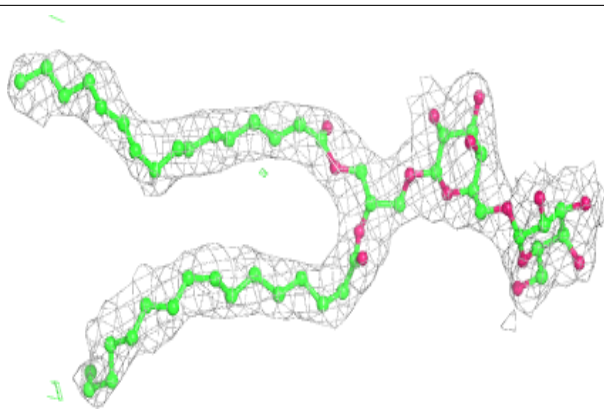
Electron density around CLA c 511:

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

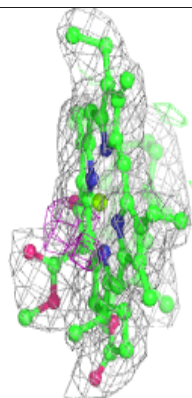
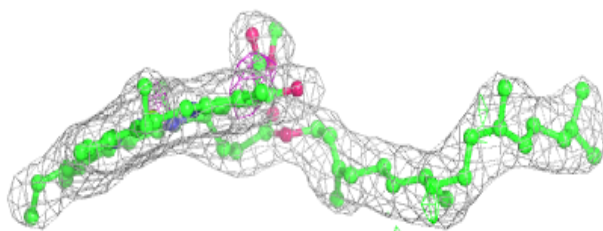
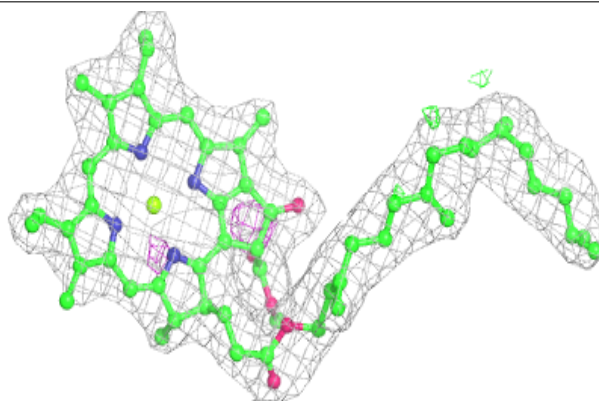


Electron density around DGD c 521:

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

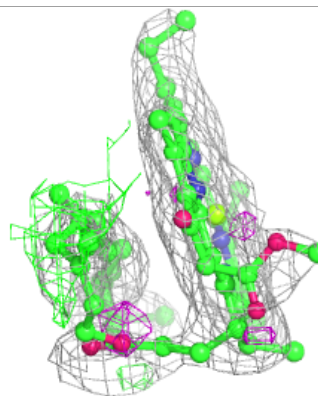
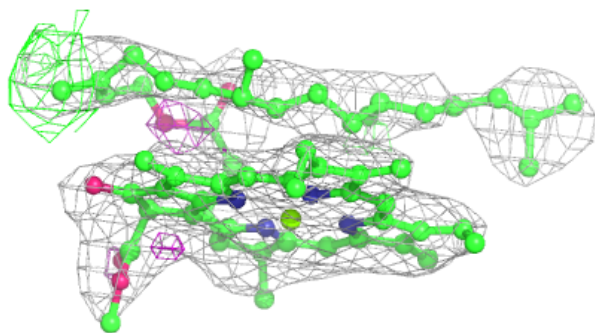
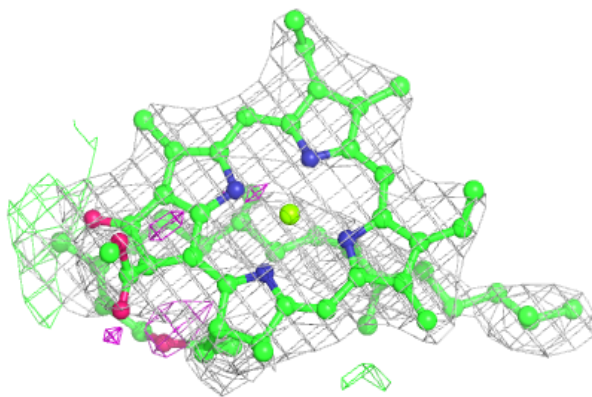
**Electron density around CLA b 611:**

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

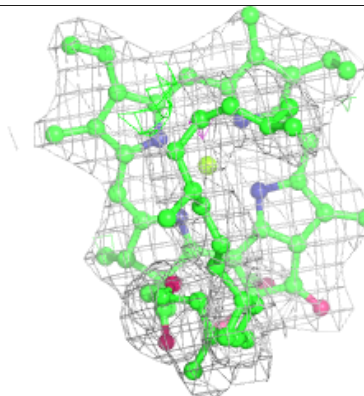
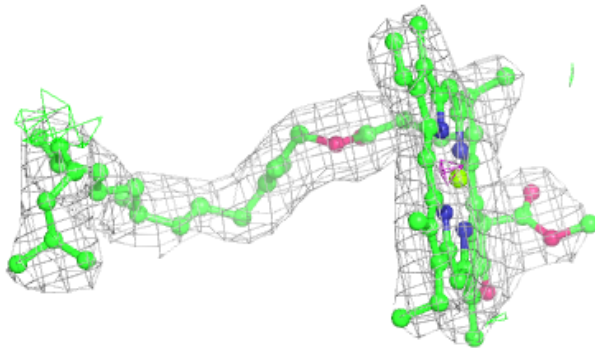
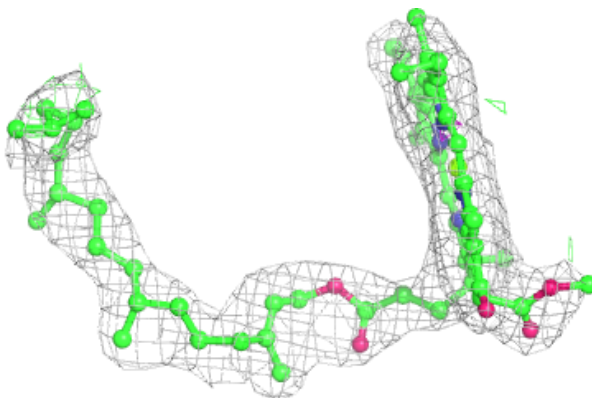


Electron density around CLA B 602:

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

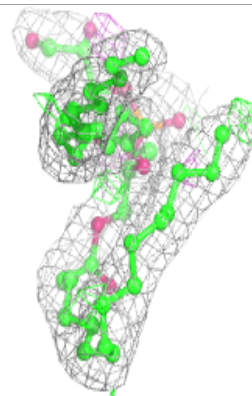
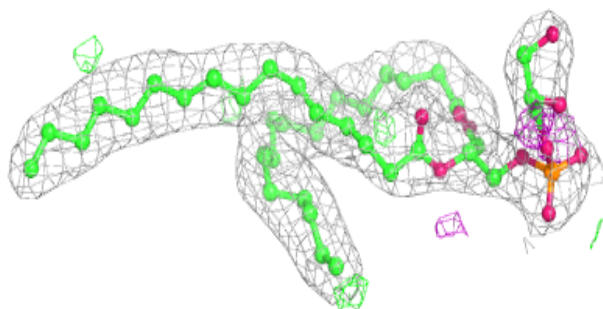
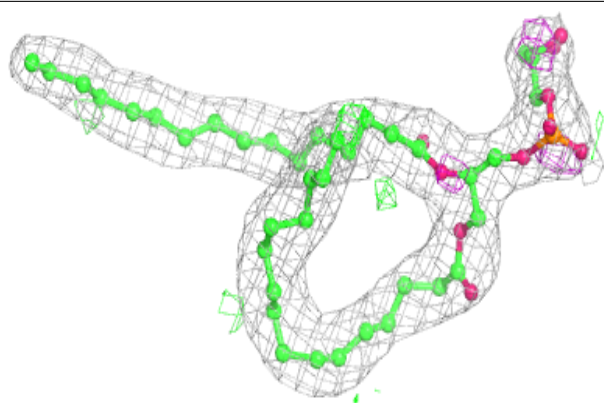
**Electron density around CLA c 510:**

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

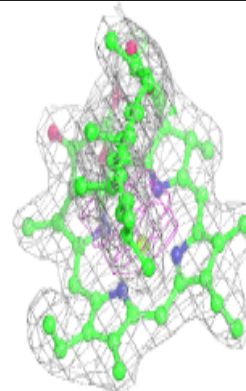
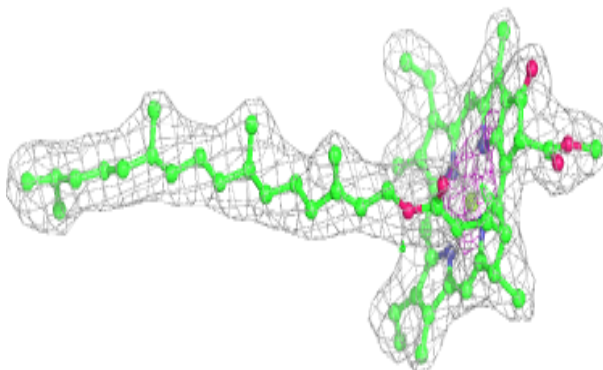
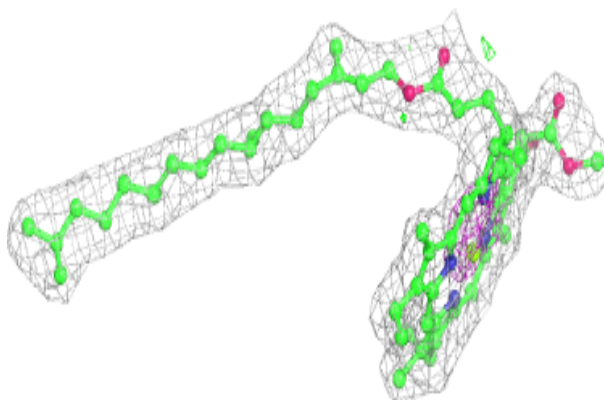


Electron density around LHG D 411:

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

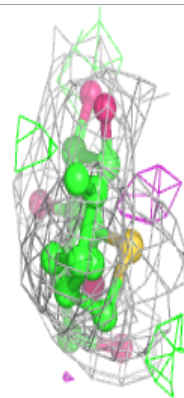
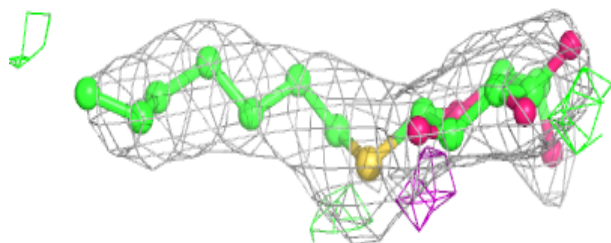
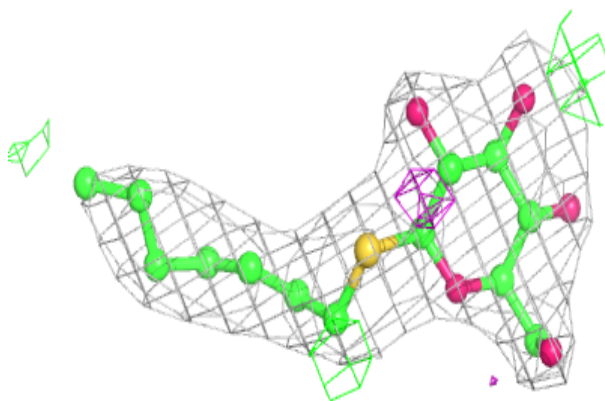
**Electron density around CLA b 616:**

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

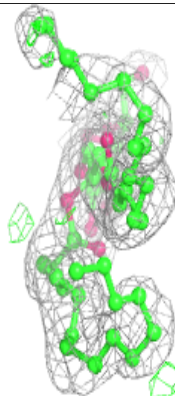
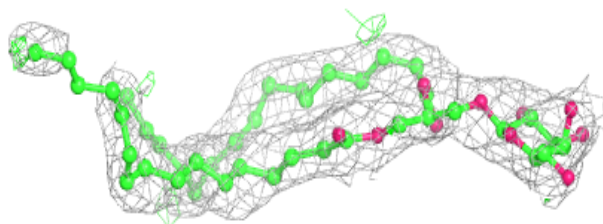
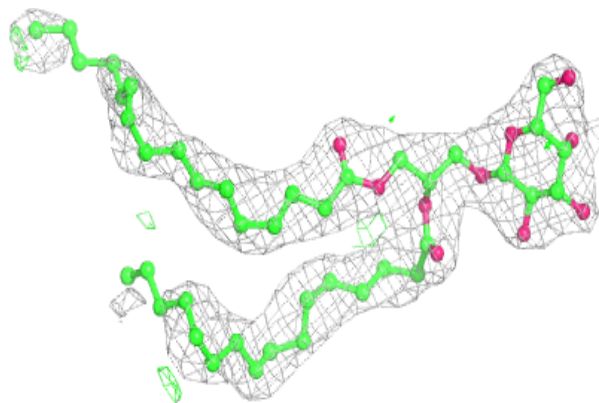


Electron density around HTG o 301:

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

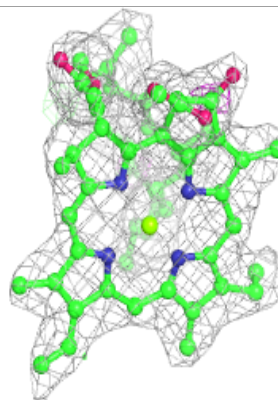
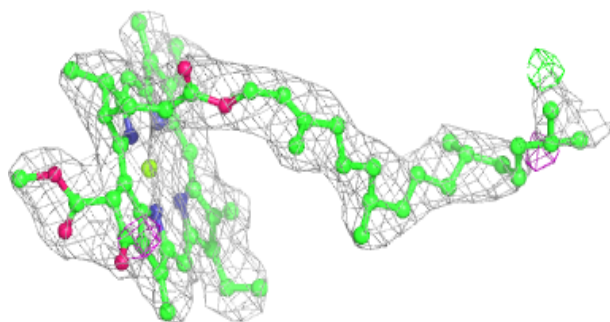
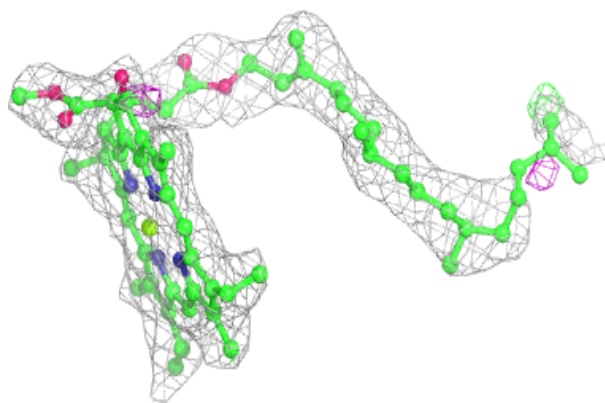
**Electron density around LMG d 416:**

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

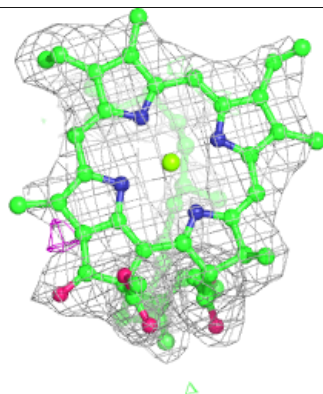
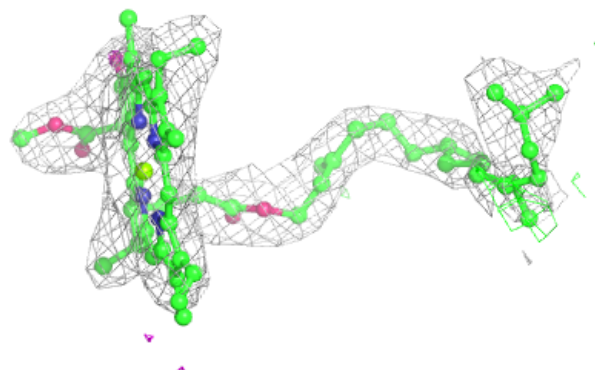
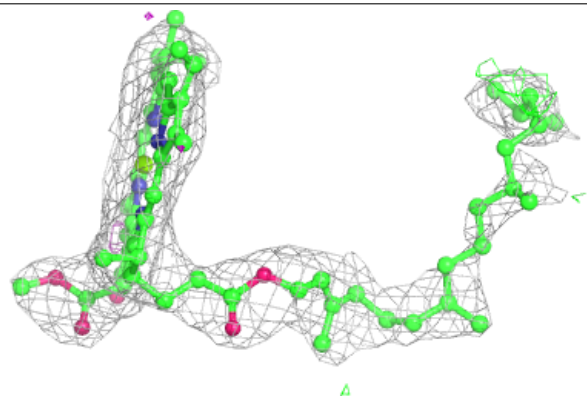


Electron density around CLA c 512:

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

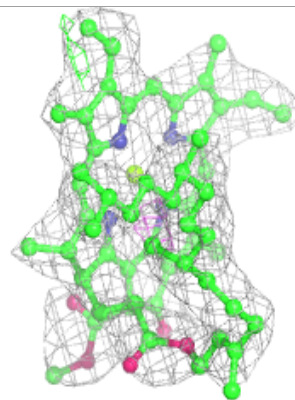
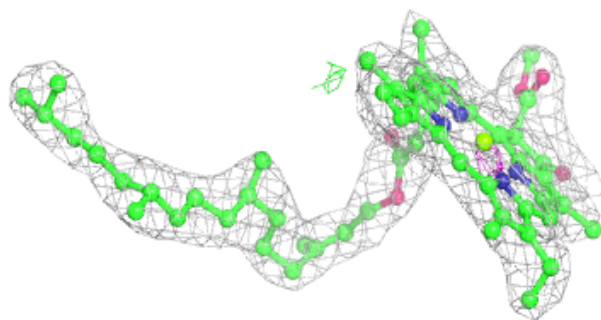
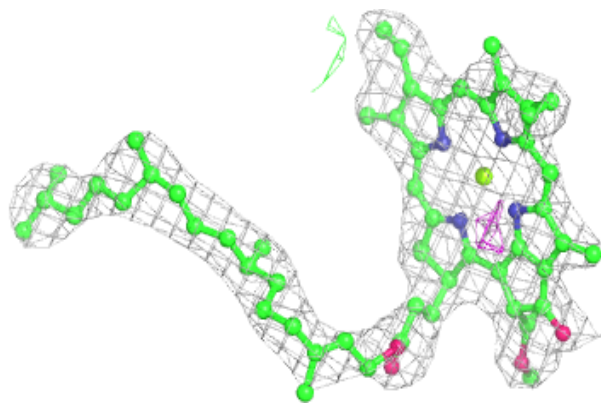
**Electron density around CLA C 507:**

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

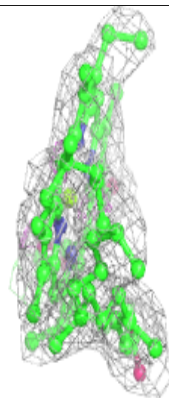
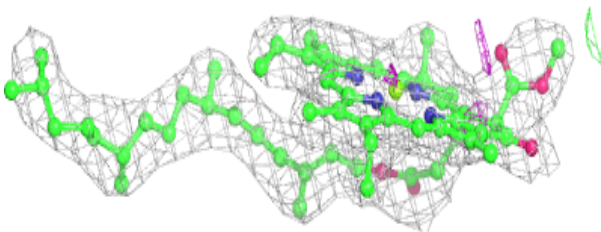
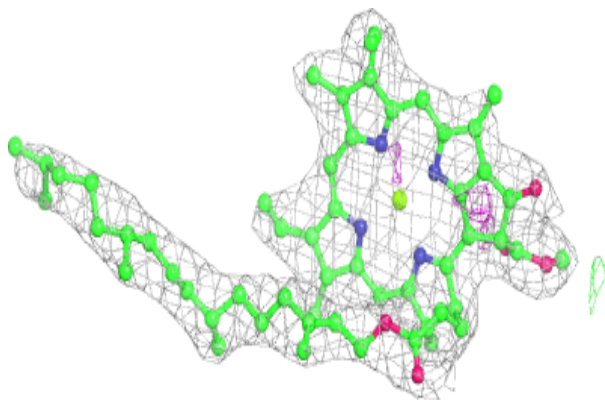


Electron density around CLA C 512:

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

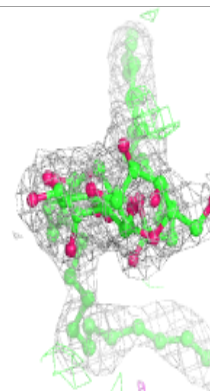
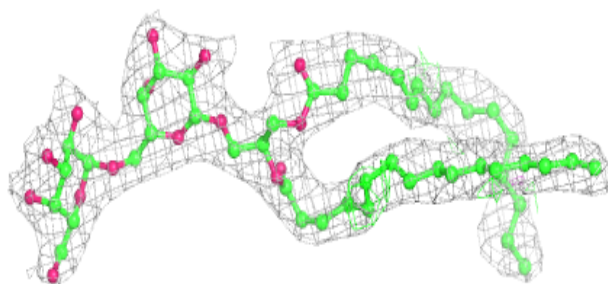
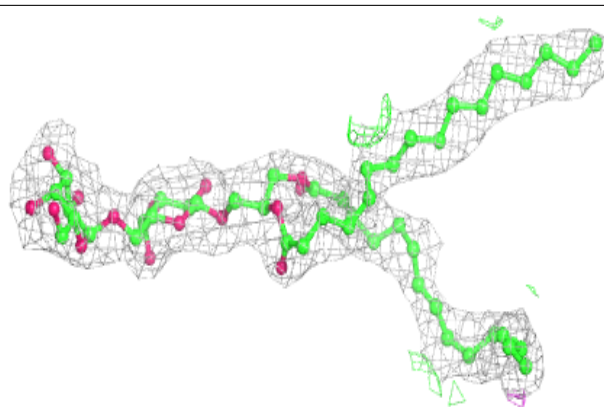
**Electron density around CLA C 502:**

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

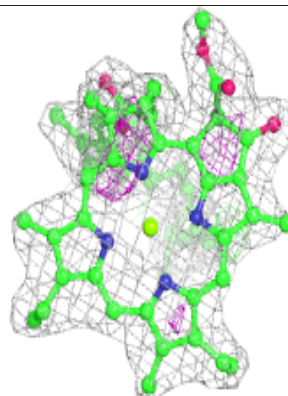
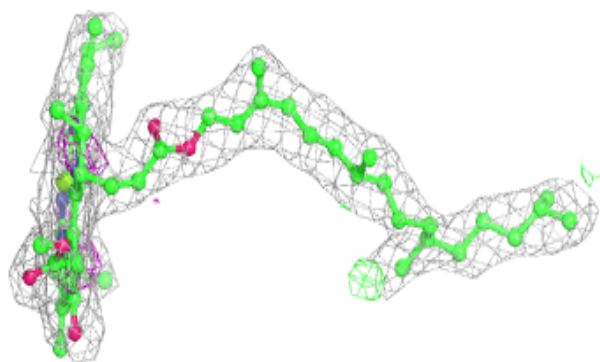
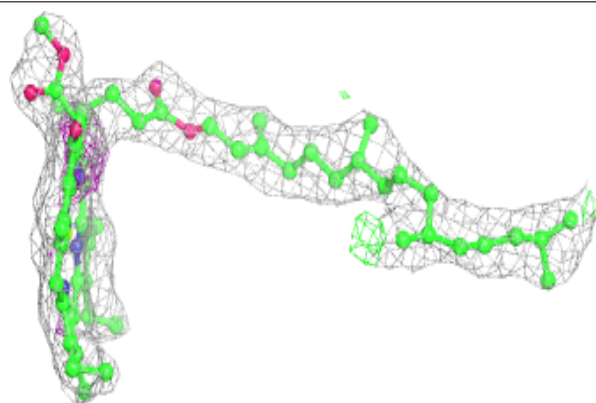


Electron density around DGD C 516:

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

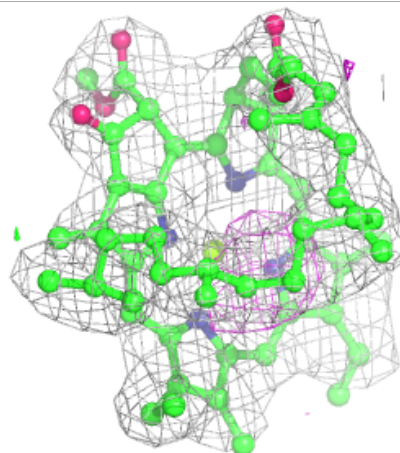
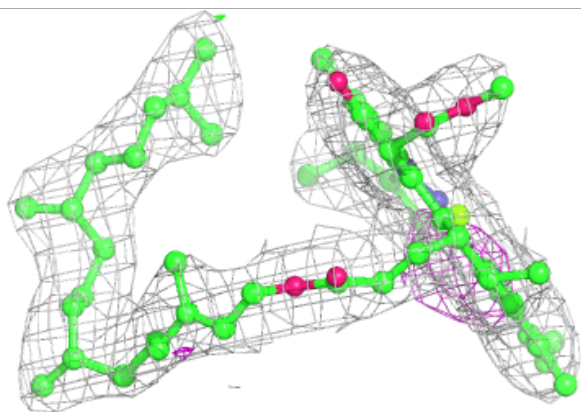
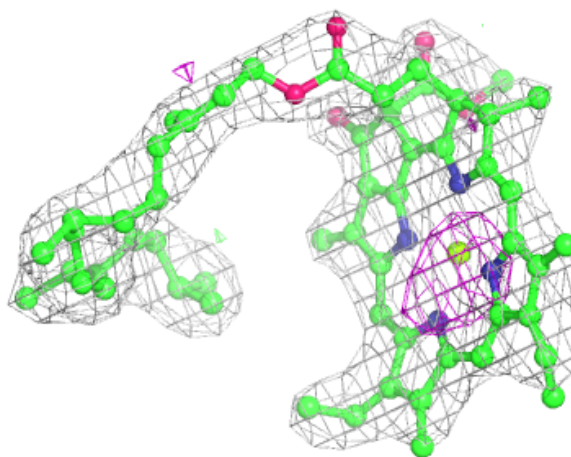
**Electron density around CLA B 607:**

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



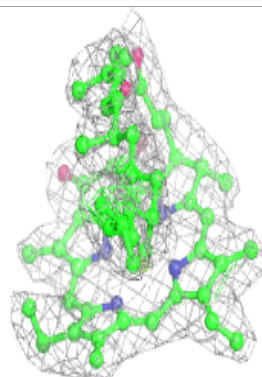
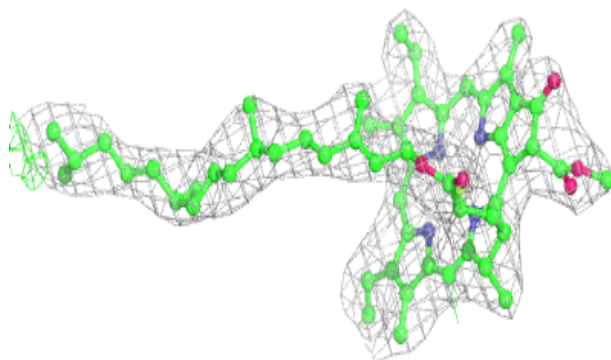
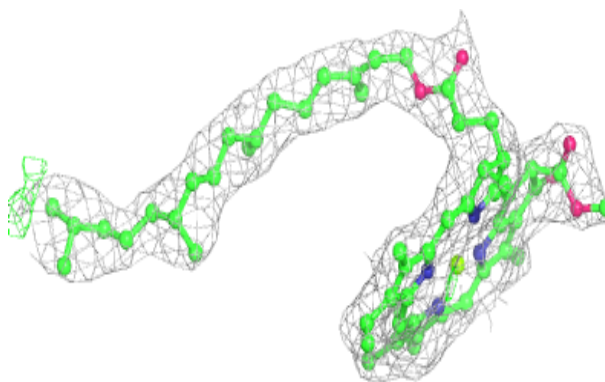
Electron density around CLA c 507:

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

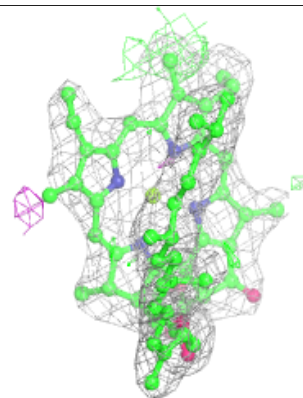
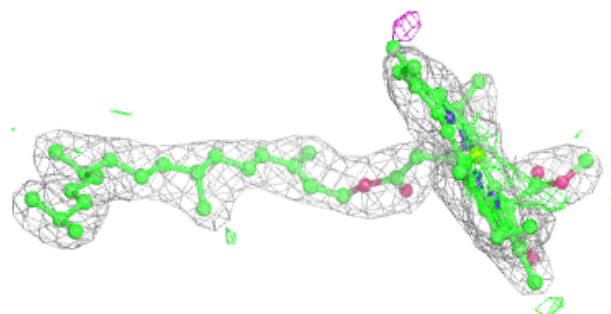
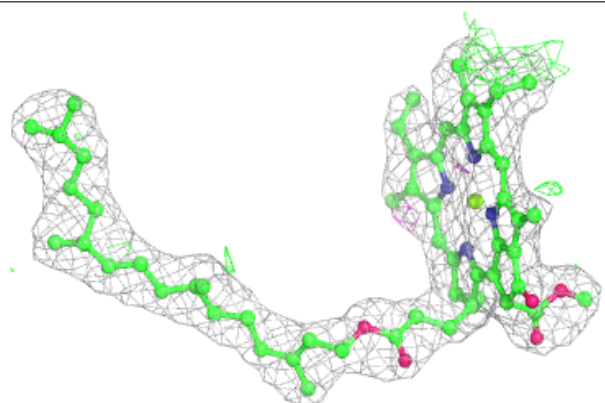


Electron density around CLA c 508:

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

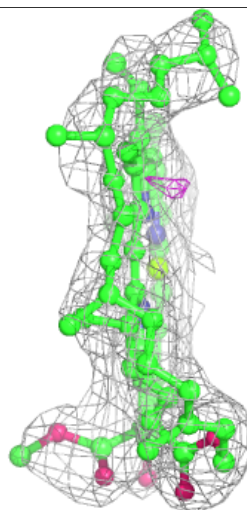
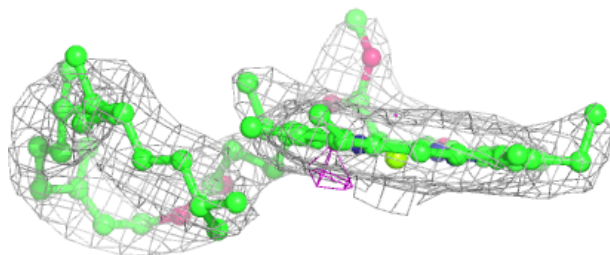
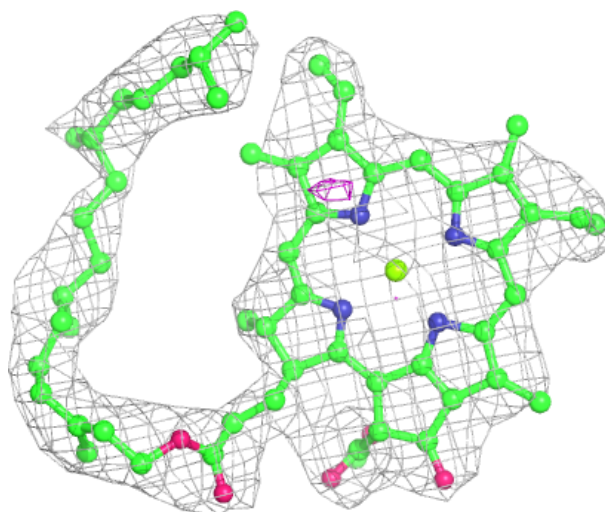
**Electron density around CLA b 618:**

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



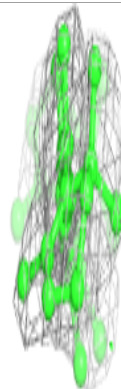
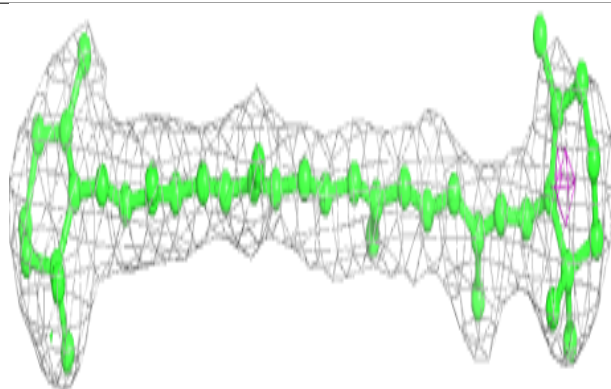
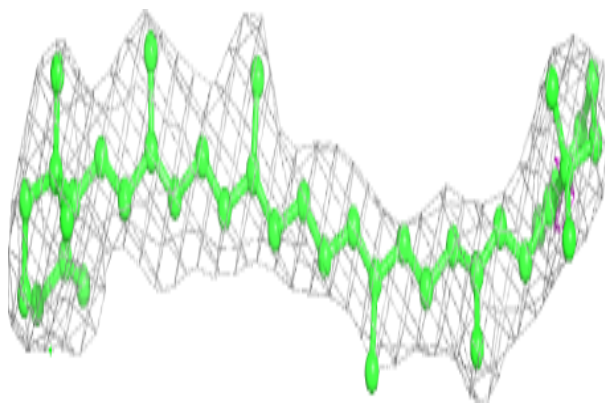
Electron density around CLA C 513:

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



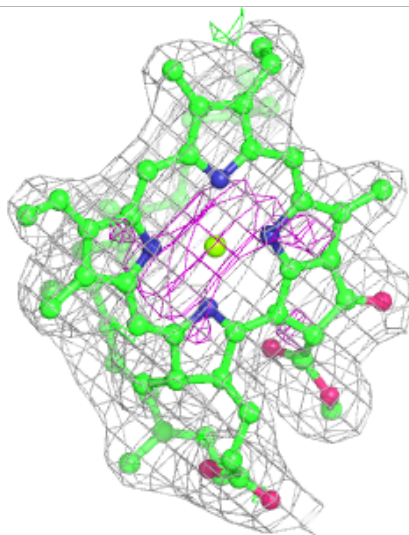
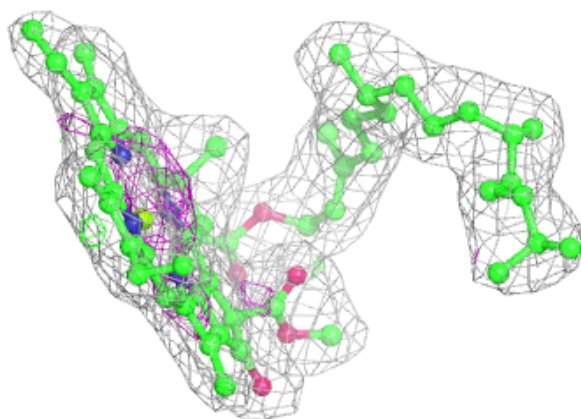
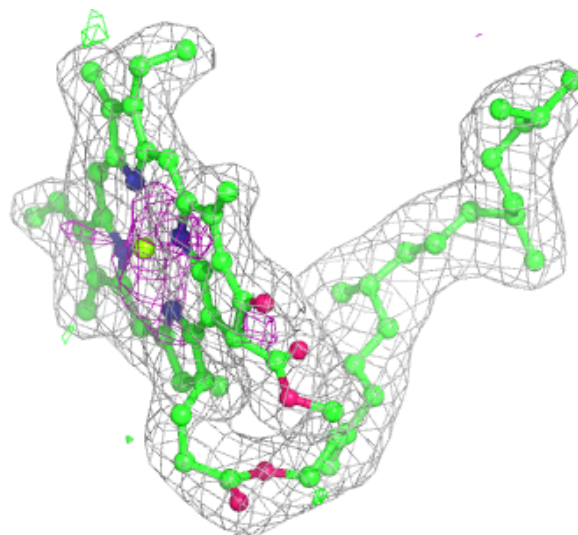
Electron density around BCR K 101:

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



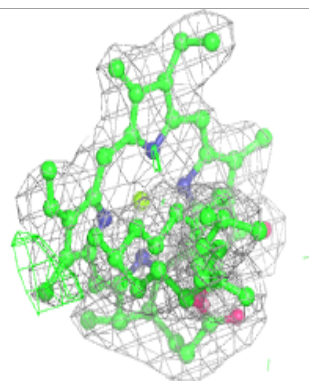
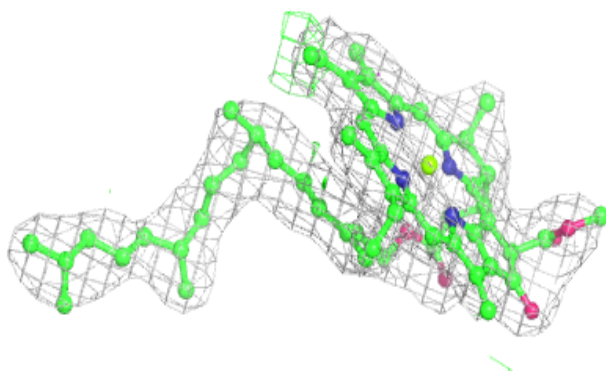
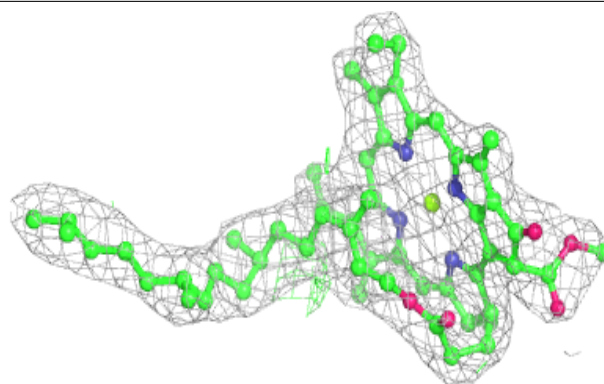
Electron density around CLA B 614:

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

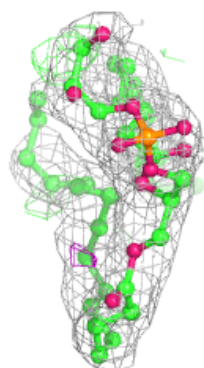
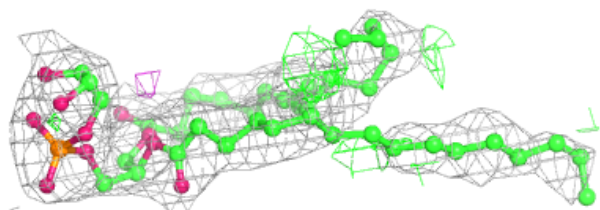
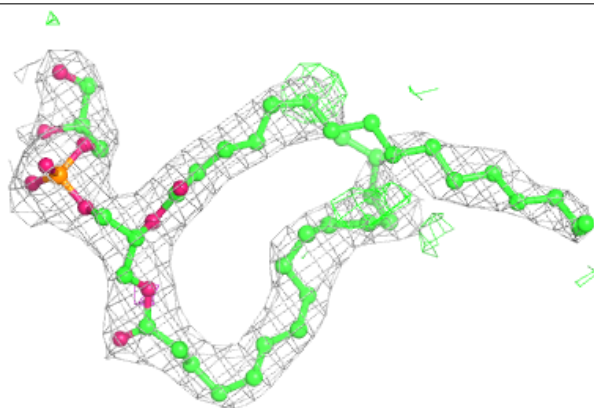


Electron density around CLA c 509:

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

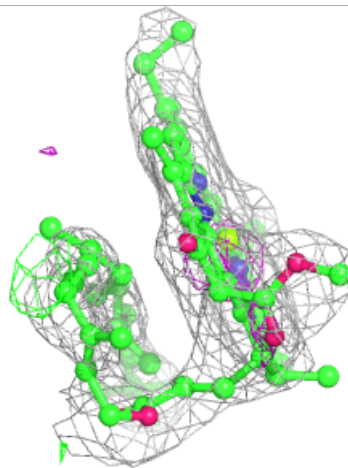
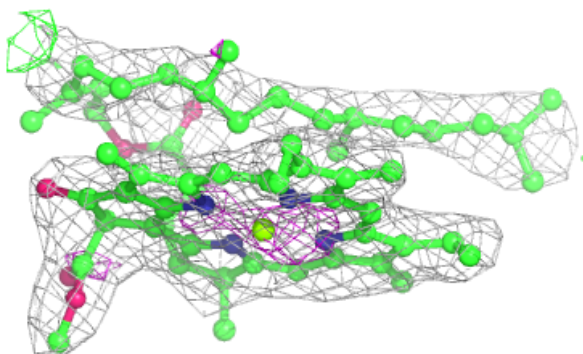
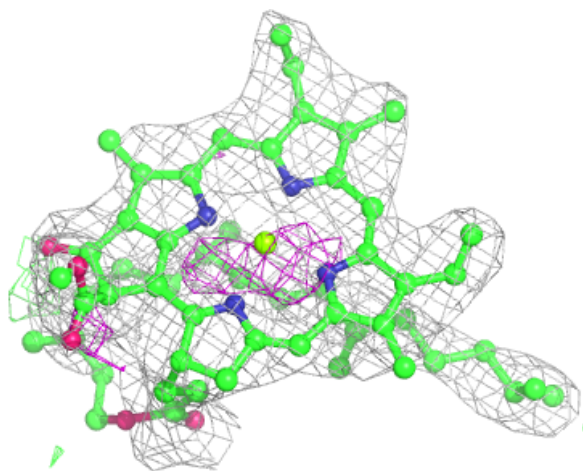
**Electron density around LHG d 411:**

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



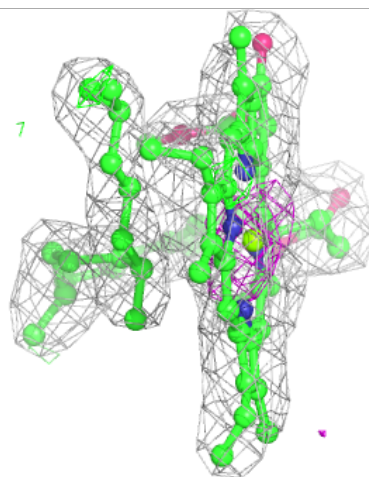
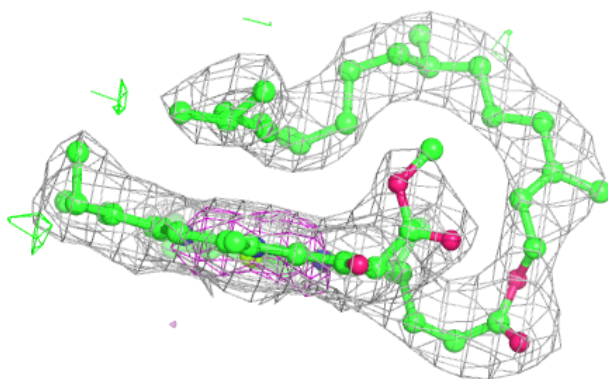
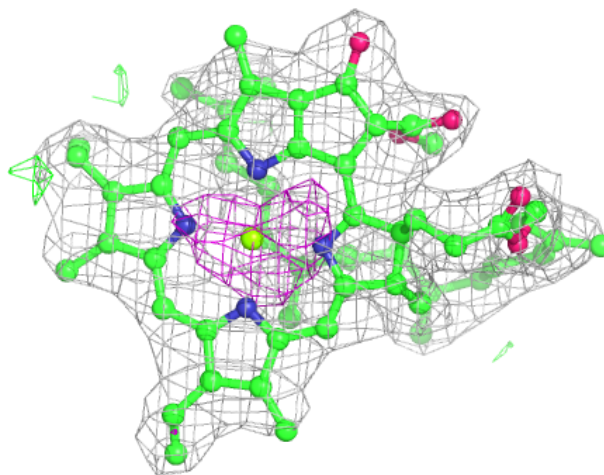
Electron density around CLA b 610:

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



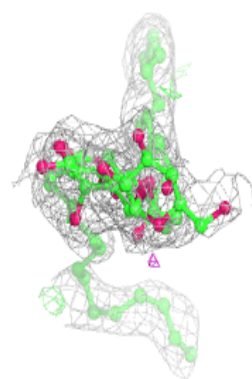
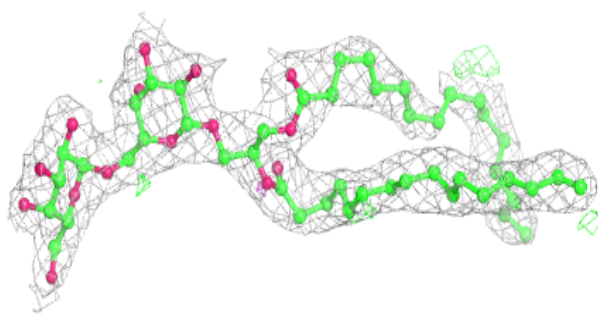
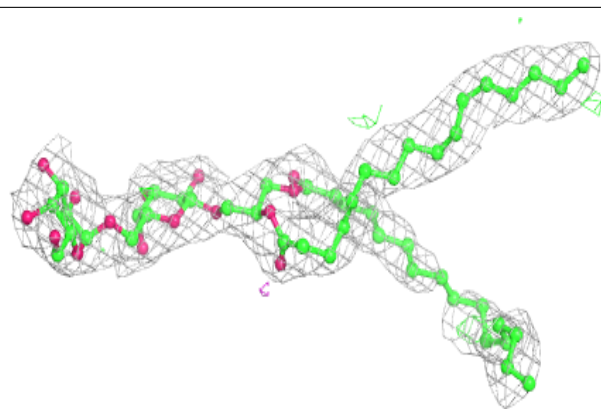
Electron density around CLA C 511:

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

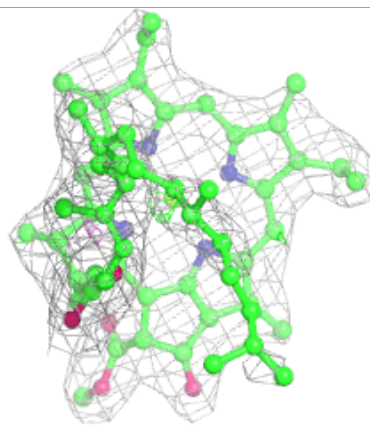
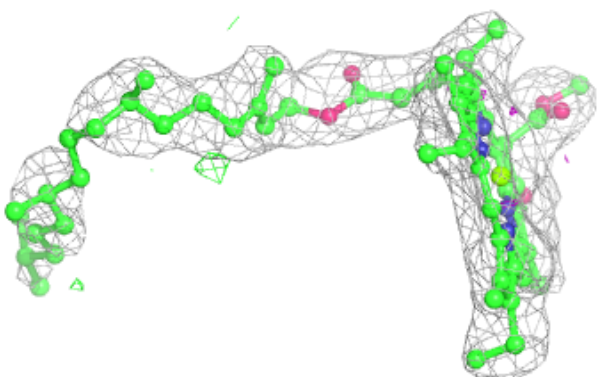
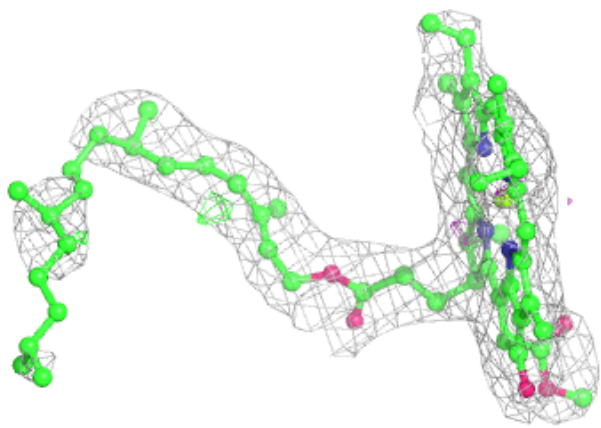


Electron density around DGD c 519:

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

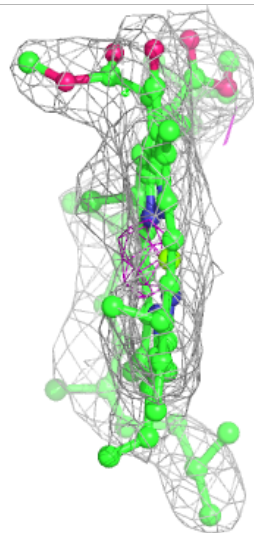
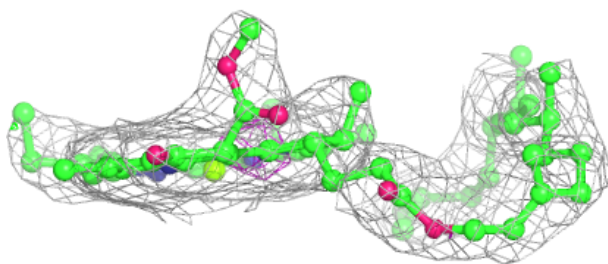
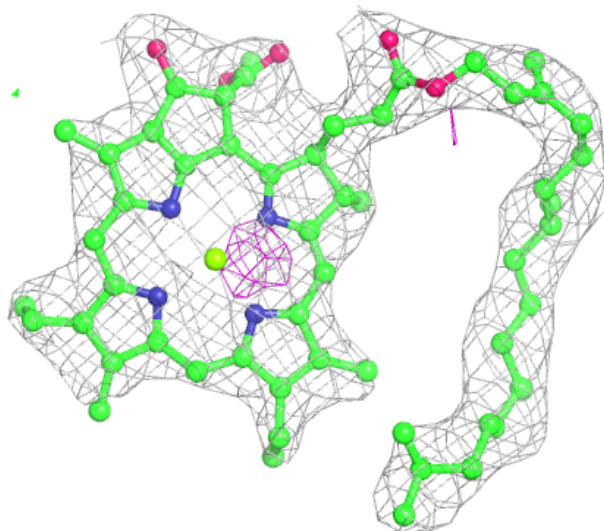
**Electron density around CLA D 407:**

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



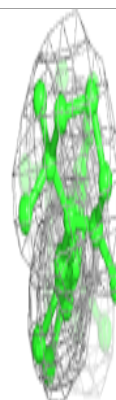
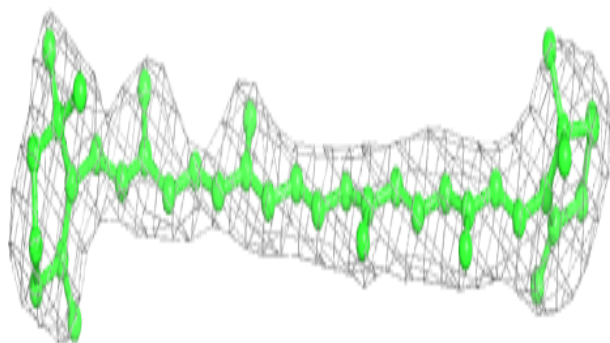
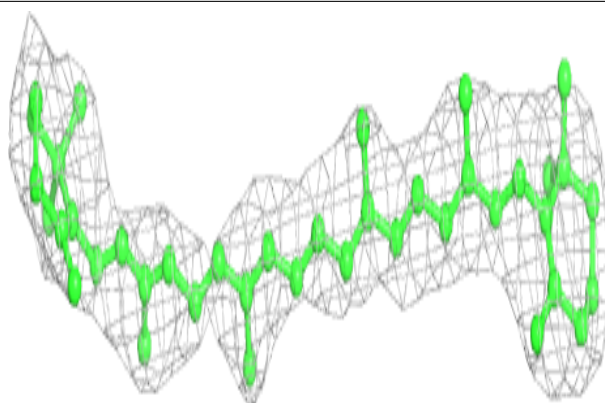
Electron density around CLA c 516:

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

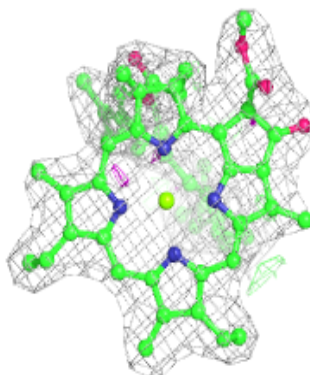
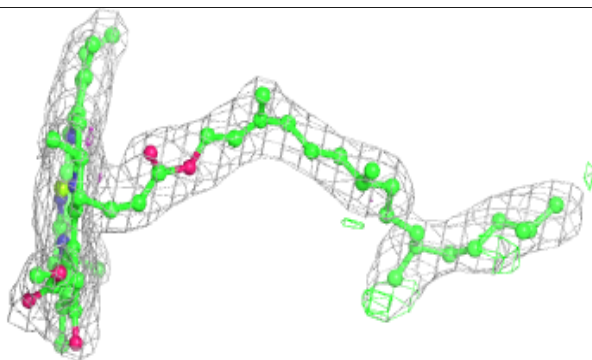
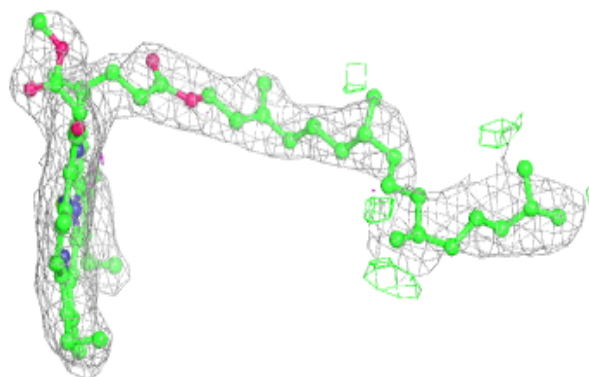


Electron density around BCR c 527:

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

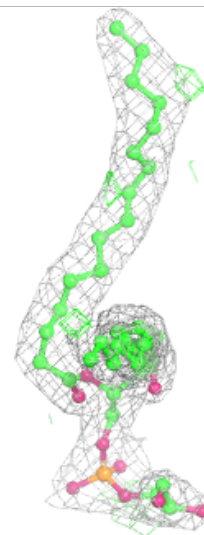
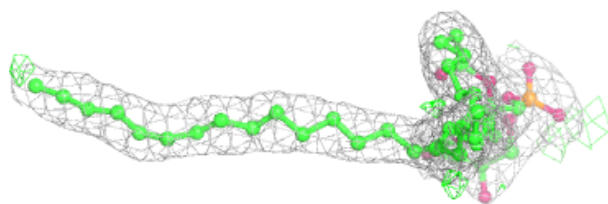
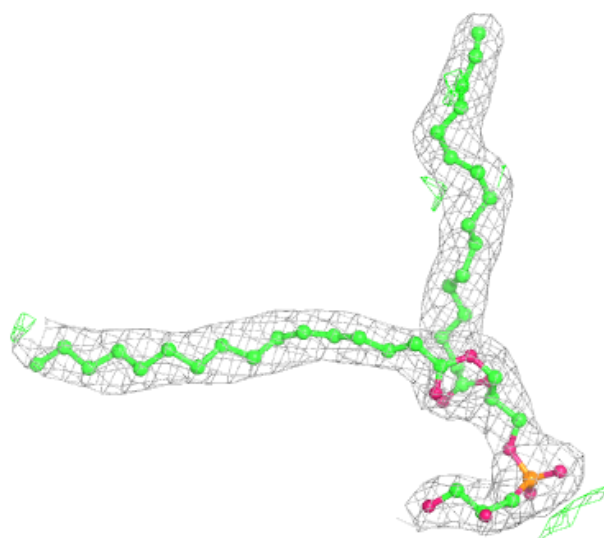
**Electron density around CLA b 615:**

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



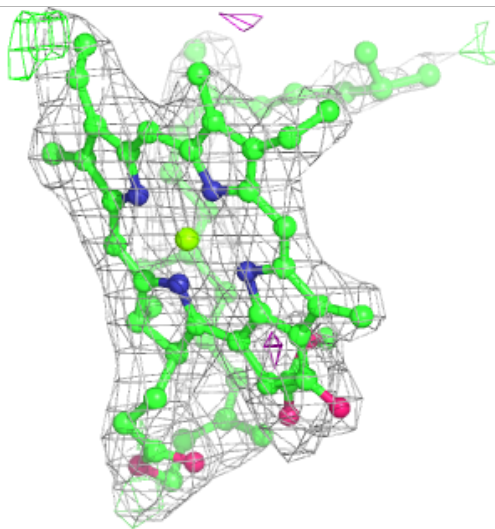
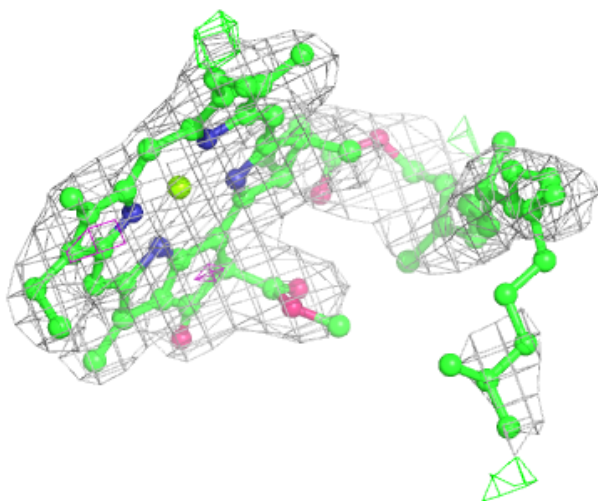
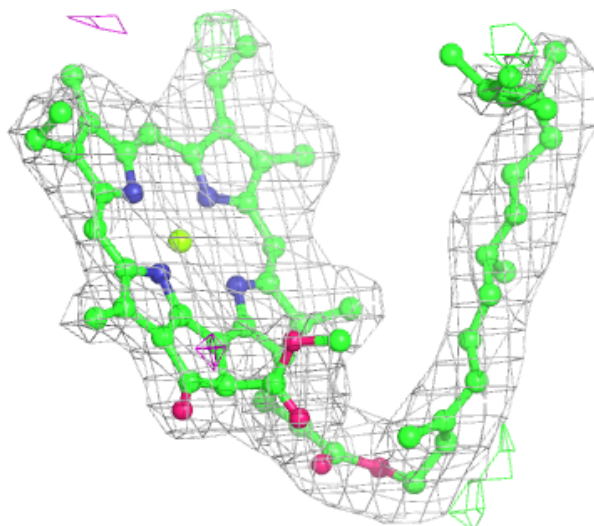
Electron density around LHG b 634:

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



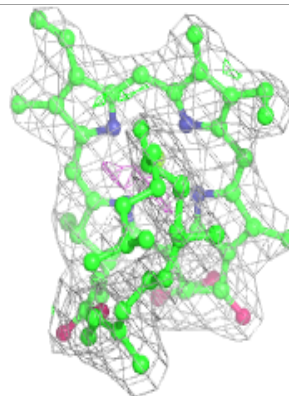
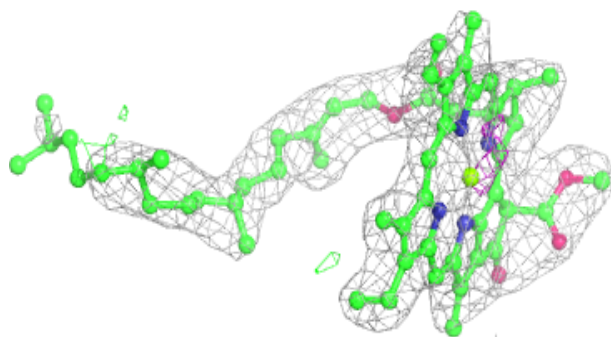
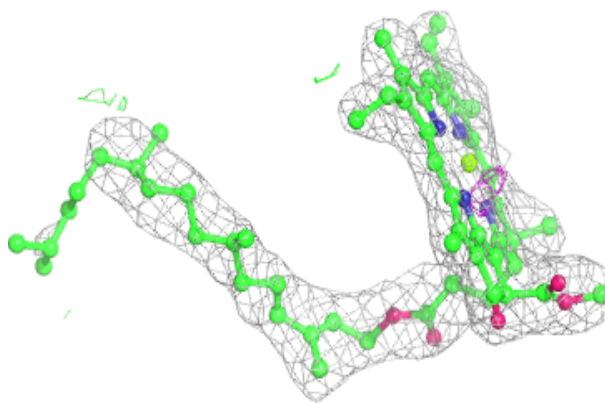
Electron density around CLA b 625:

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

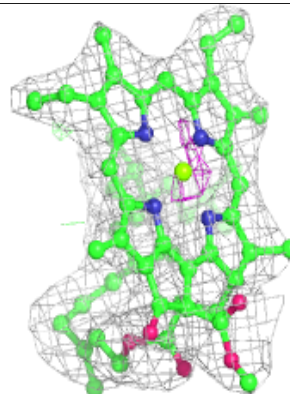
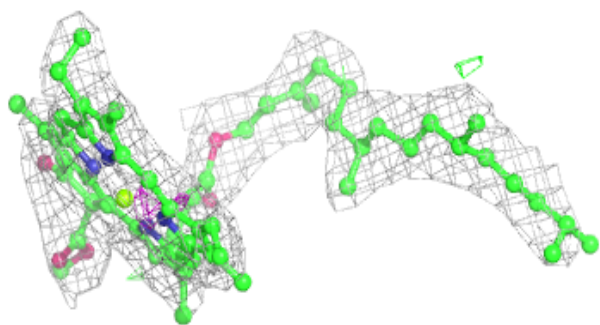
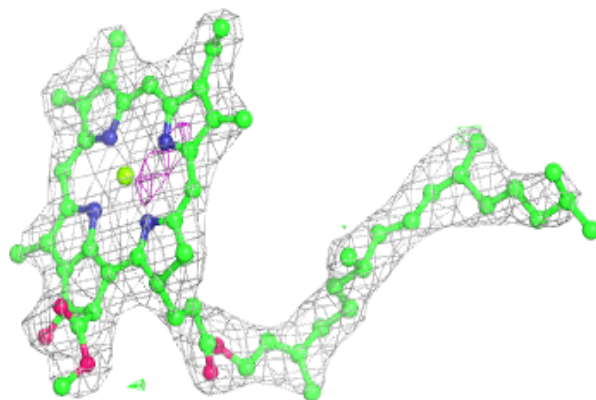


Electron density around CLA C 509:

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

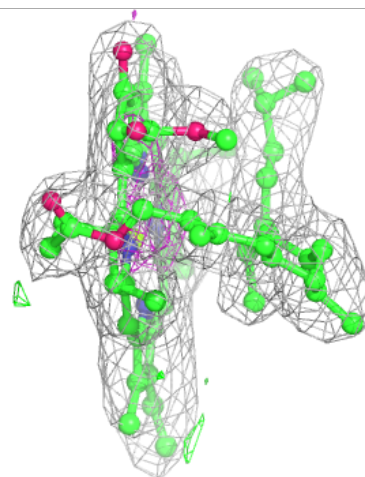
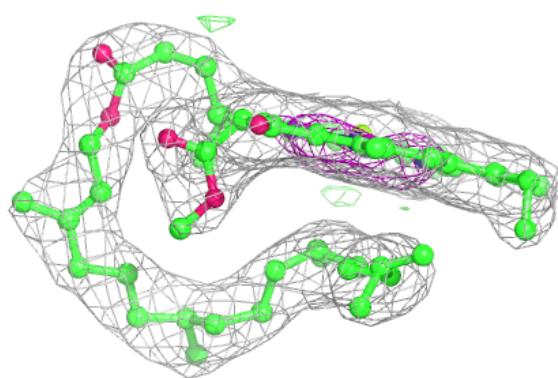
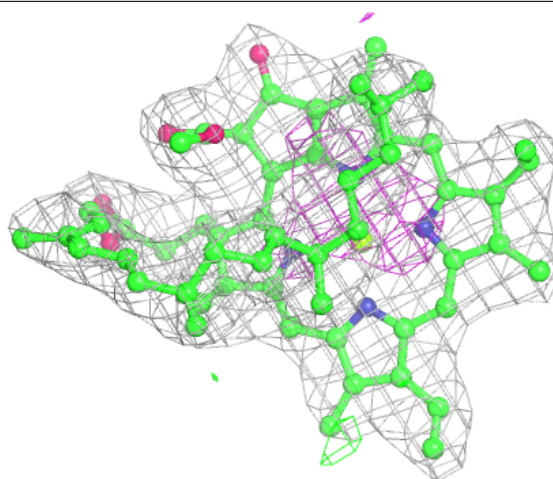
**Electron density around CLA c 515:**

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



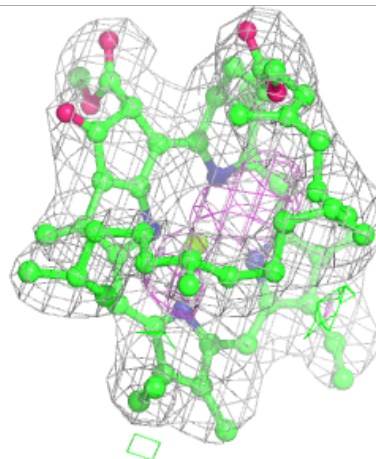
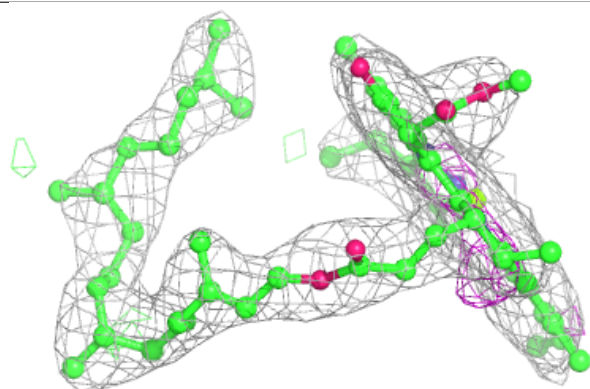
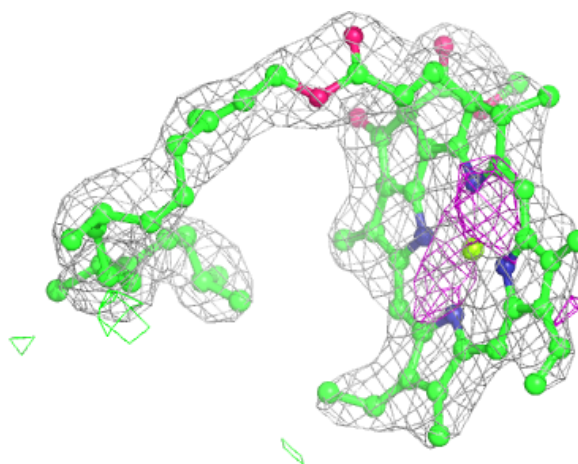
Electron density around CLA c 514:

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



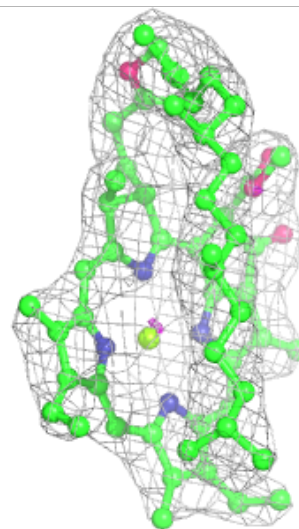
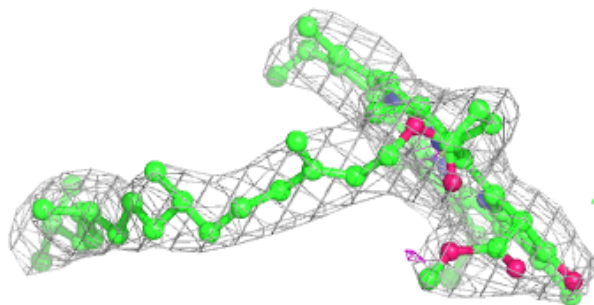
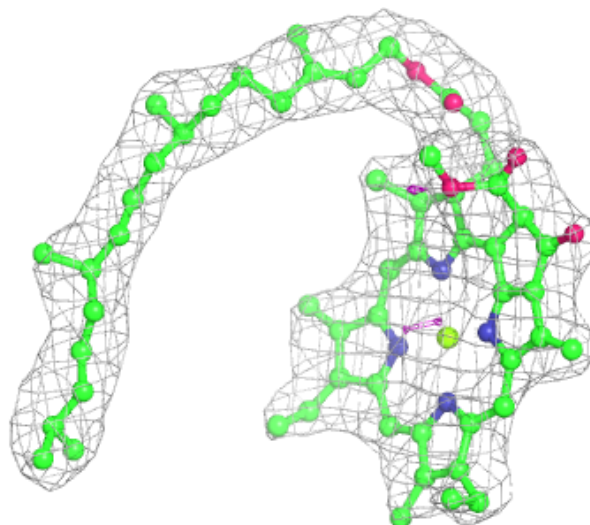
Electron density around CLA C 504:

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



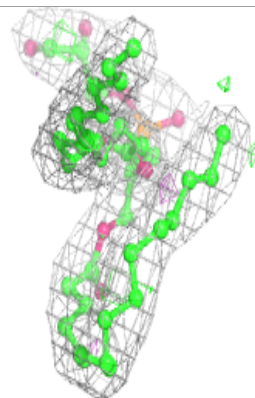
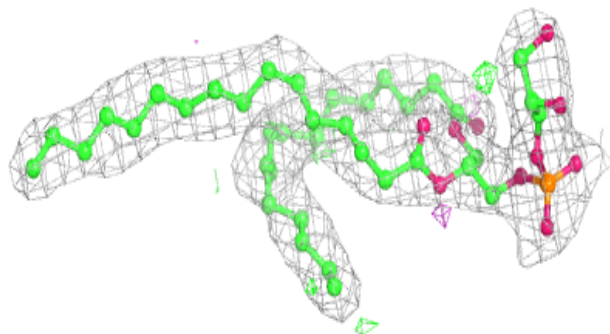
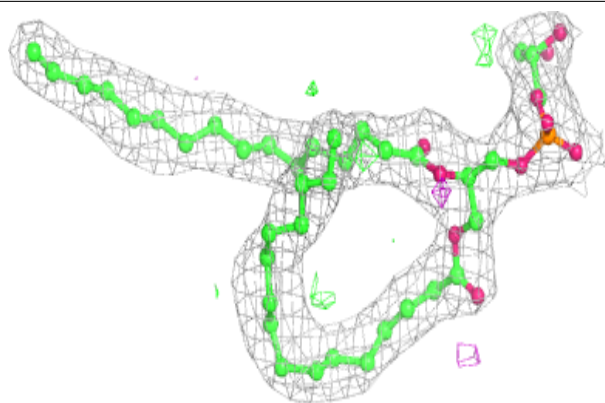
Electron density around CLA C 508:

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

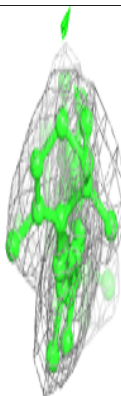
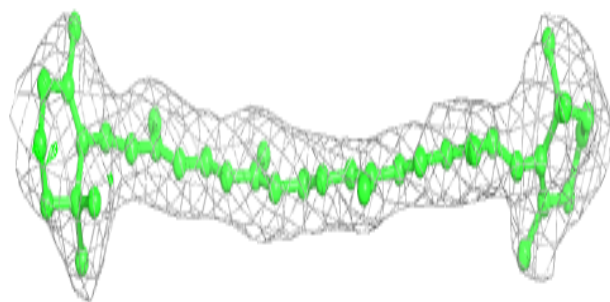
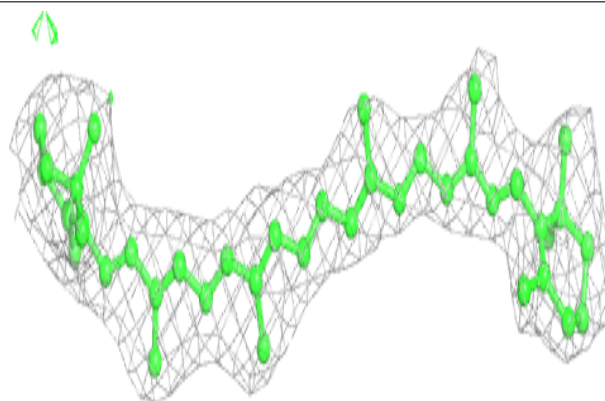


Electron density around LHG d 409:

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

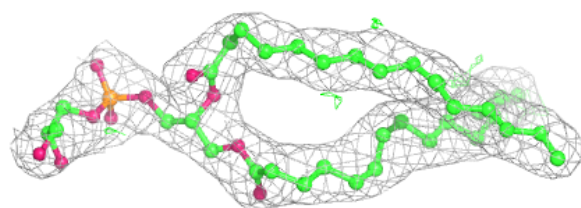
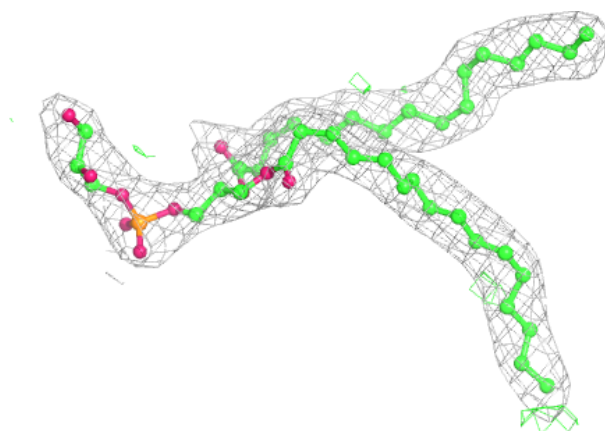
**Electron density around BCR k 102:**

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

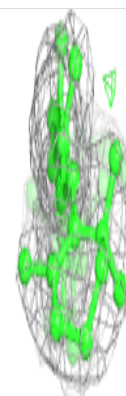
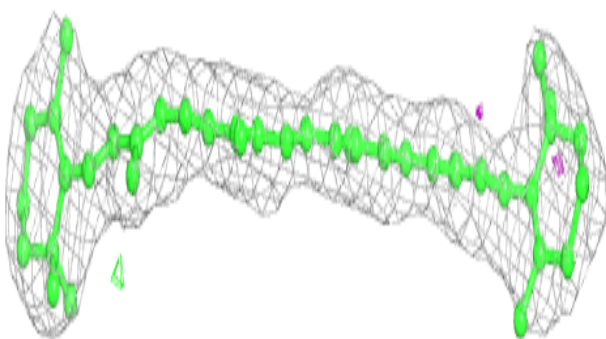
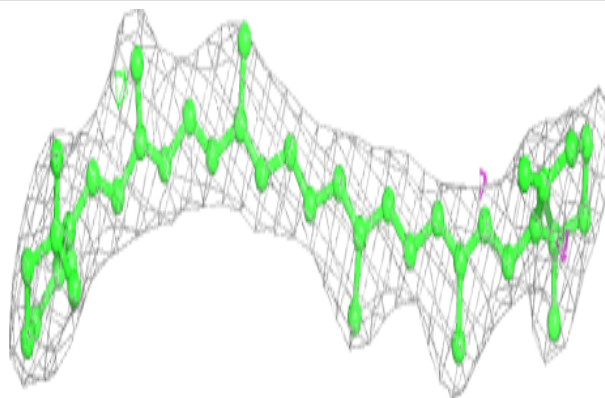


Electron density around LHG d 410:

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

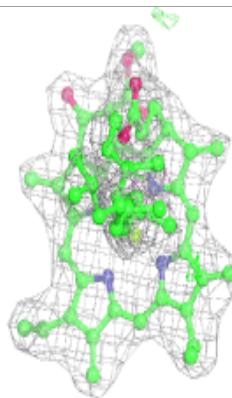
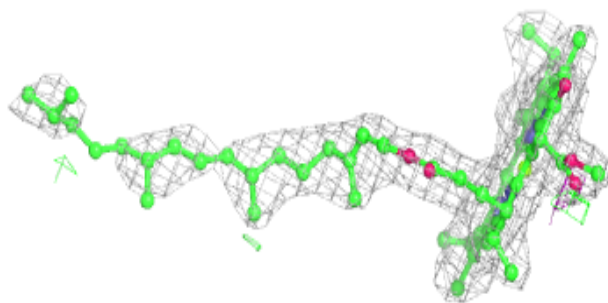
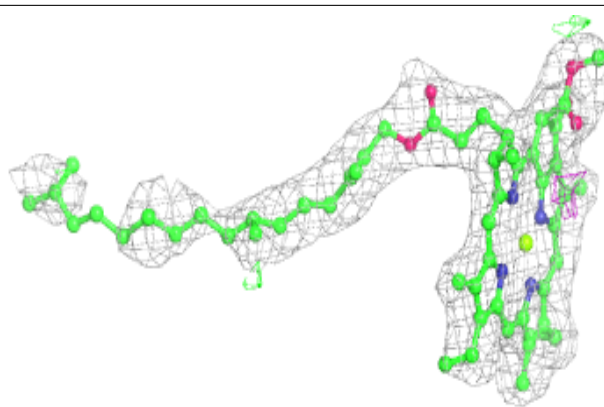
**Electron density around BCR h 101:**

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

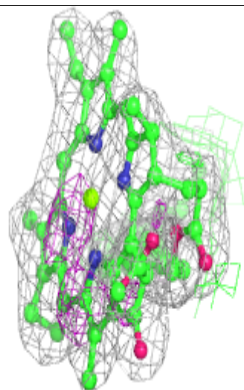
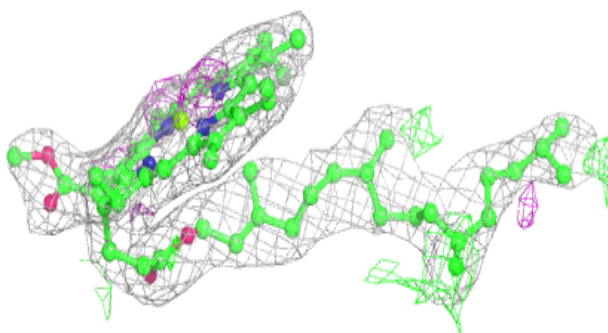
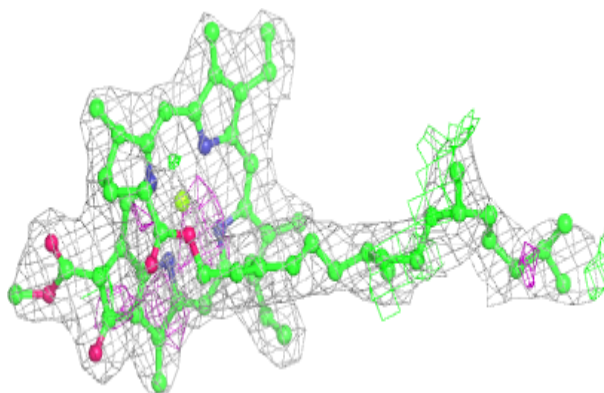


Electron density around CLA d 405:

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

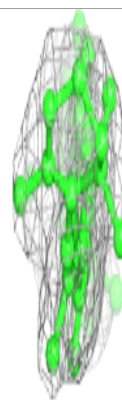
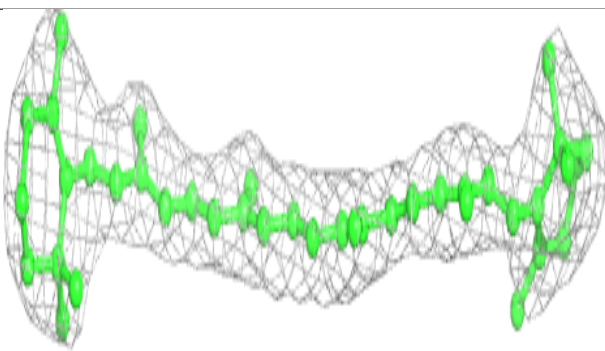
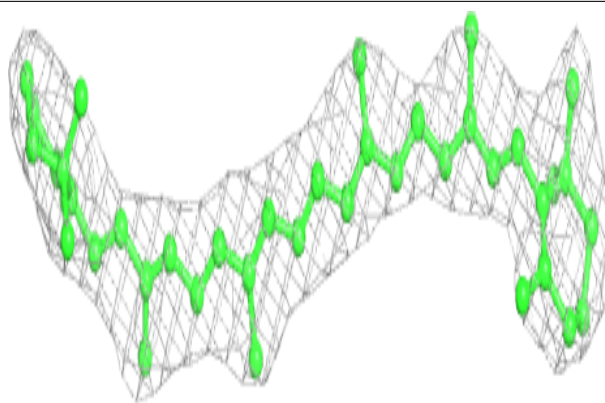
**Electron density around CLA b 623:**

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

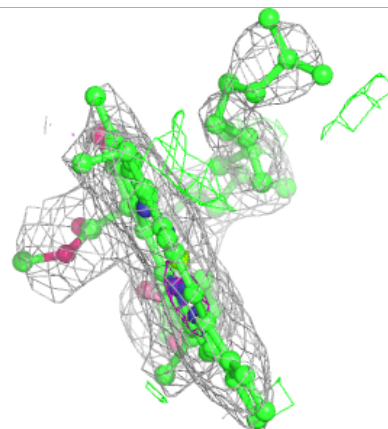
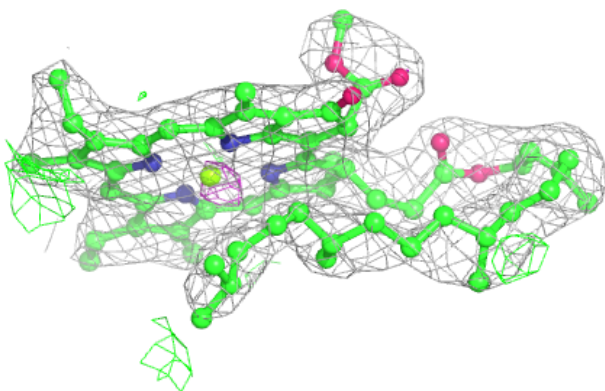
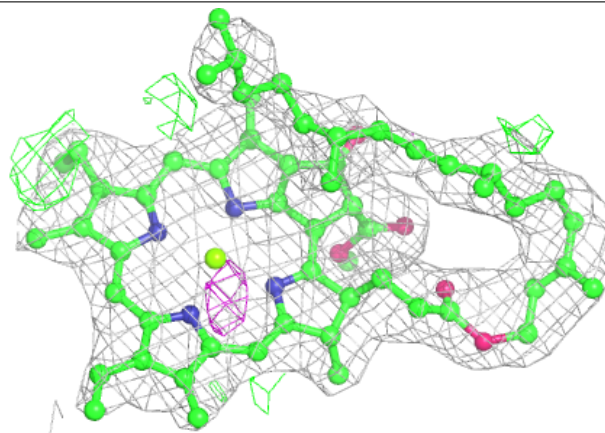


Electron density around BCR Y 101:

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

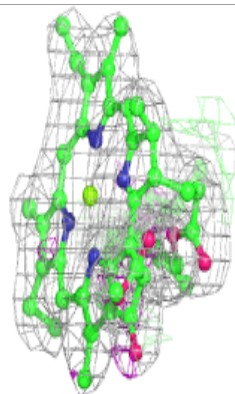
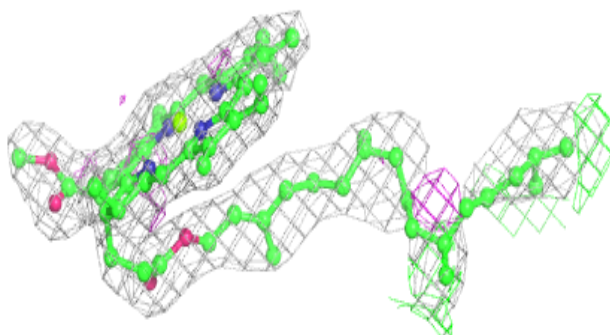
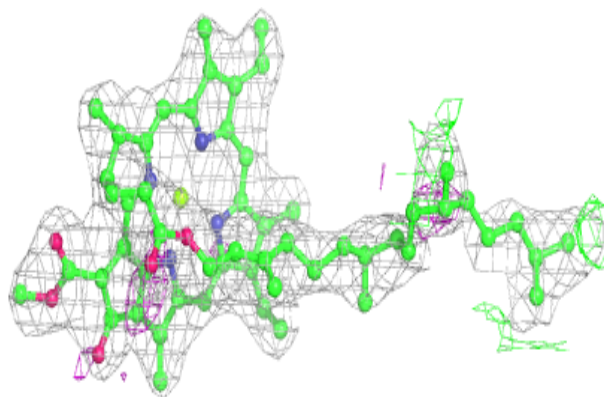
**Electron density around CLA c 513:**

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

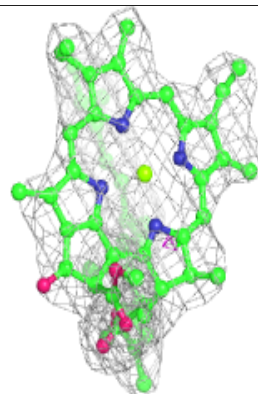
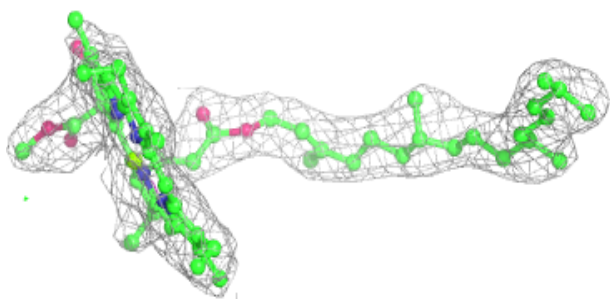
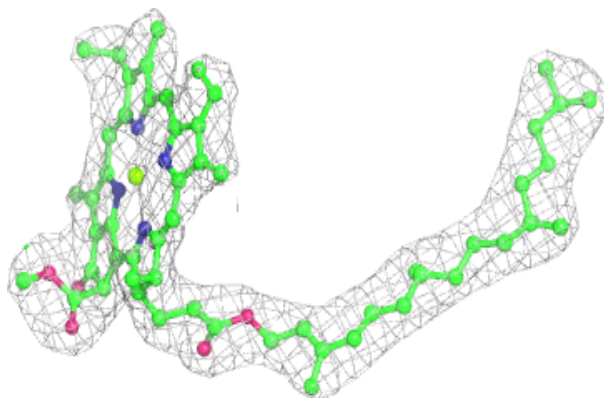


Electron density around CLA B 615:

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

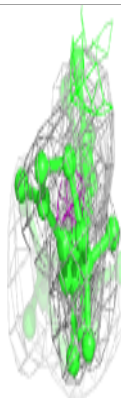
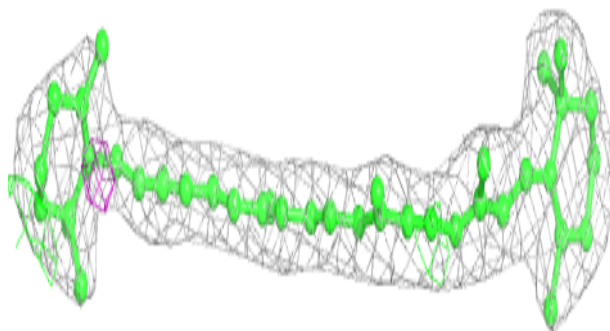
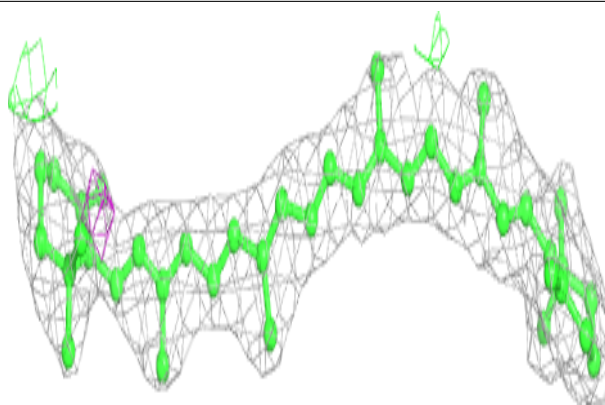
**Electron density around CLA B 610:**

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

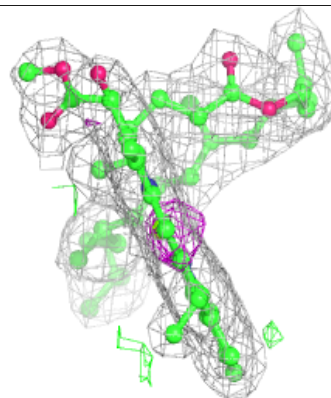
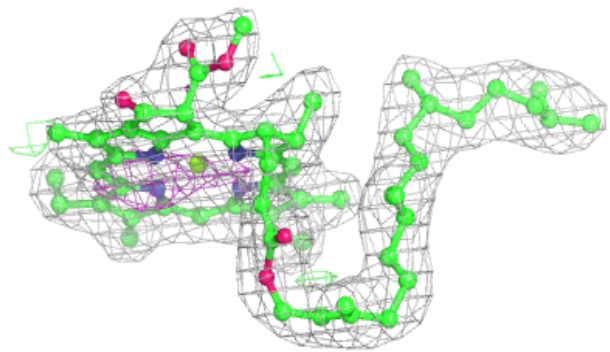
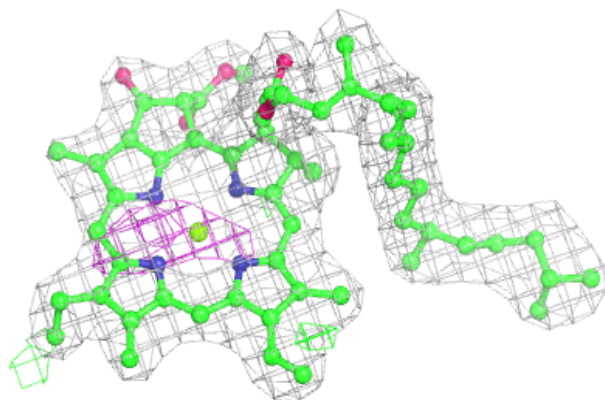


Electron density around BCR H 101:

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

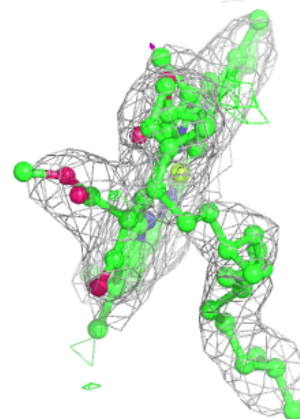
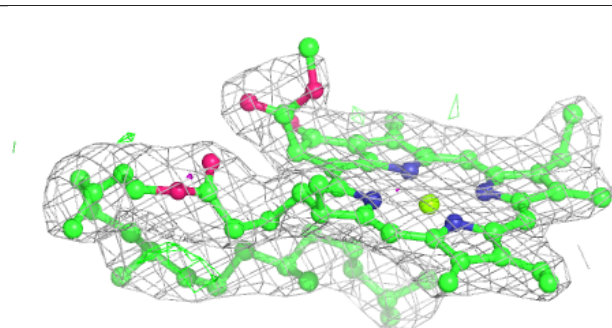
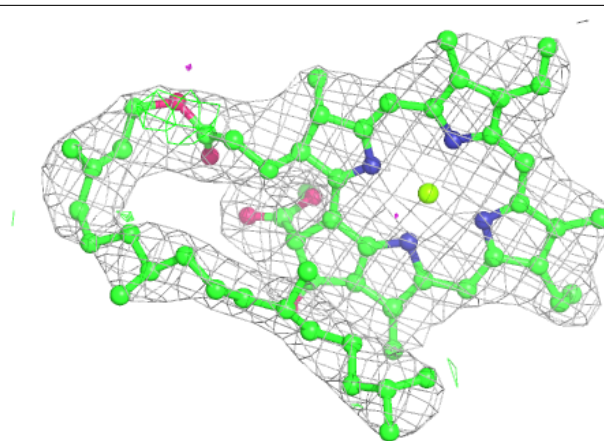
**Electron density around CLA d 403:**

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



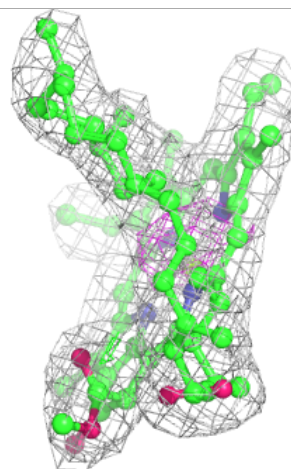
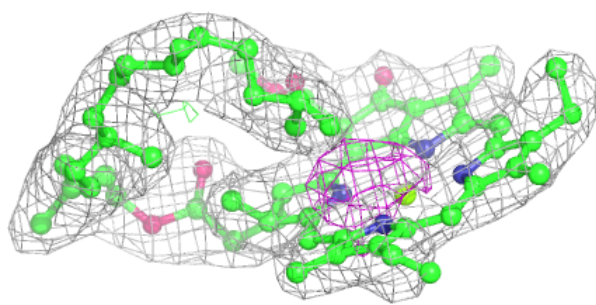
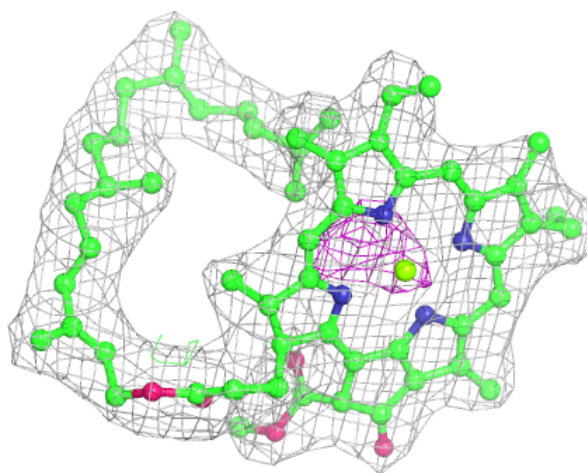
Electron density around CLA C 510:

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



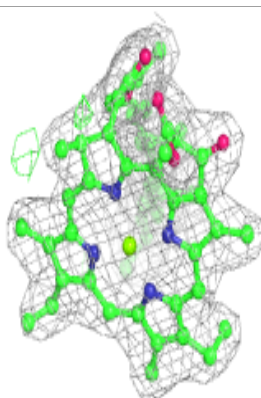
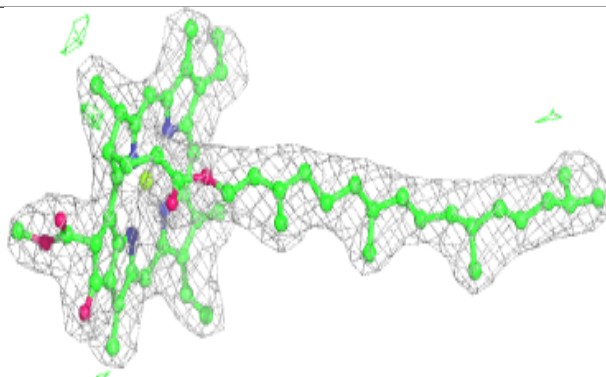
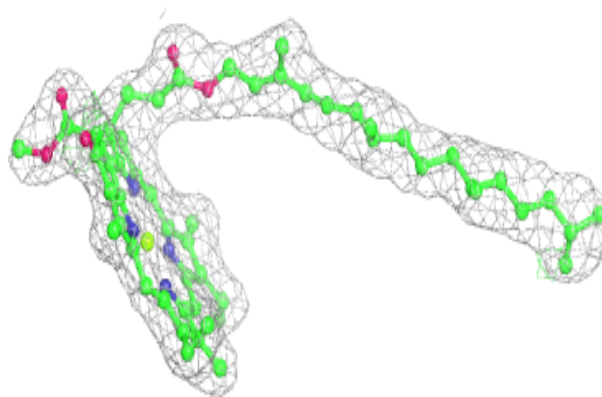
Electron density around CLA b 624:

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

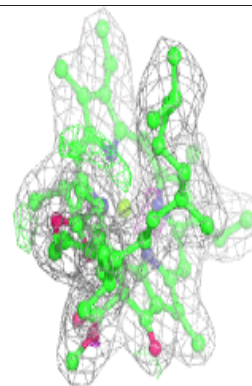
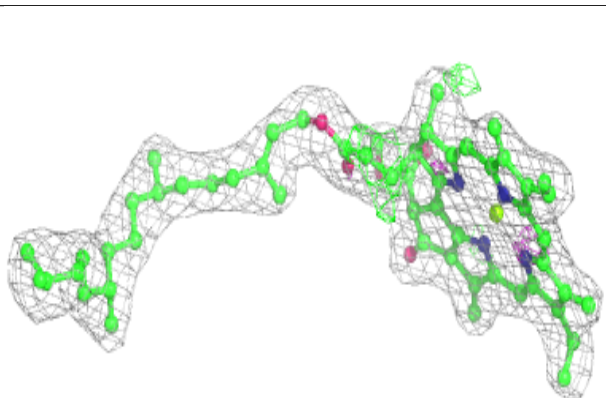
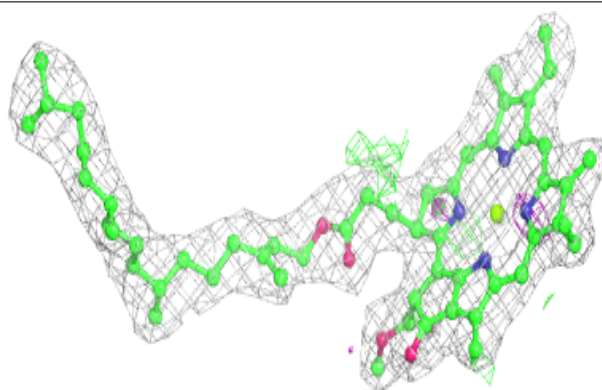


Electron density around CLA B 608:

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

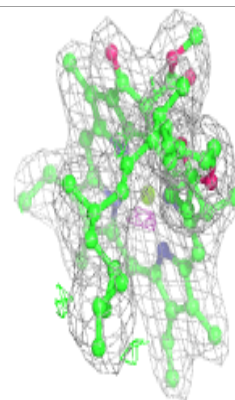
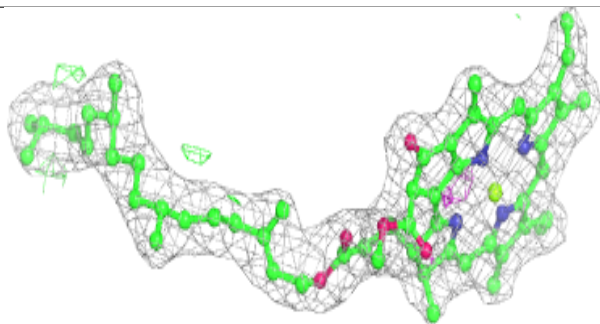
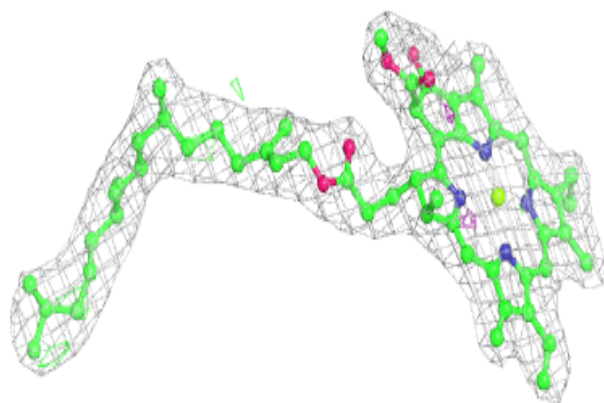
**Electron density around CLA A 404:**

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

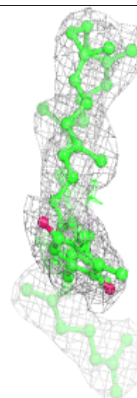
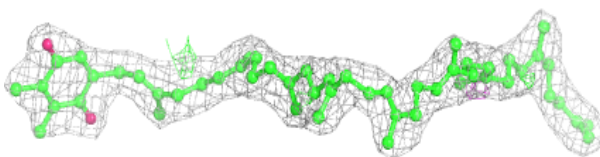
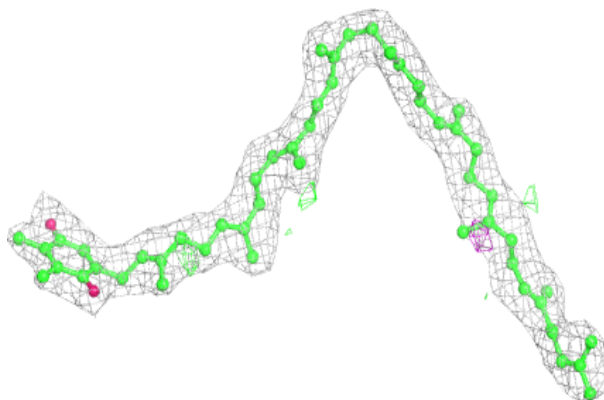


Electron density around CLA a 409:

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

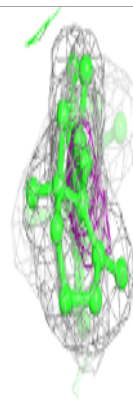
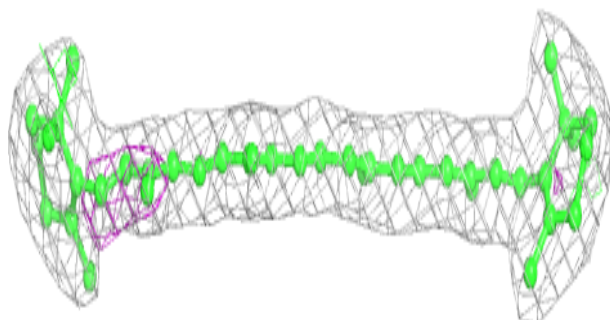
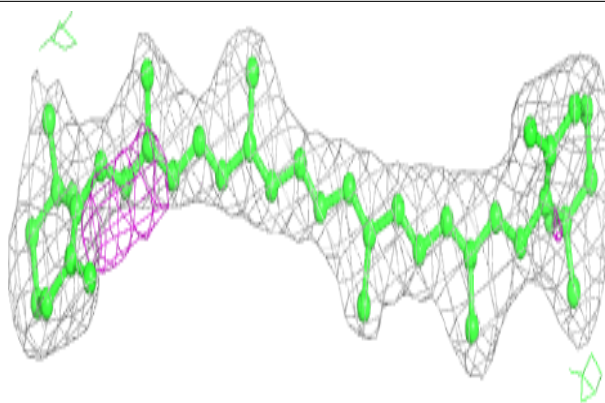
**Electron density around PL9 d 407 (A):**

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



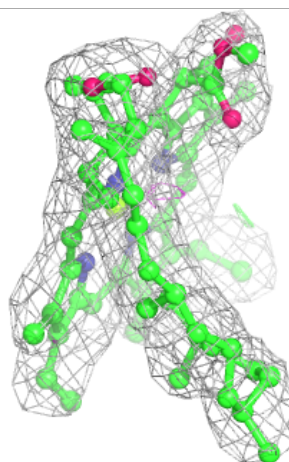
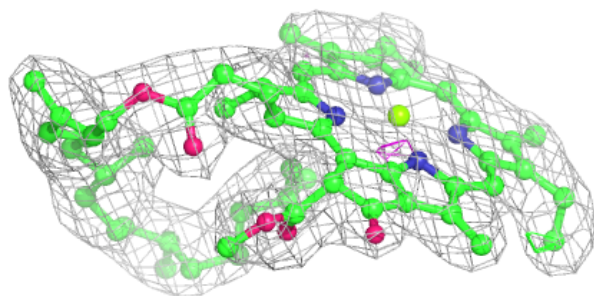
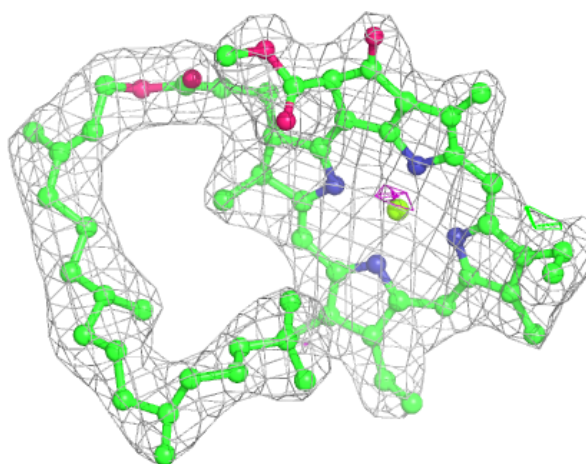
Electron density around BCR b 627:

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



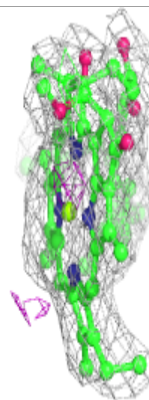
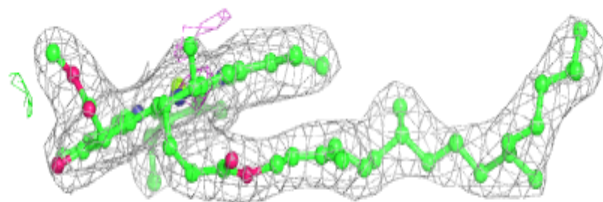
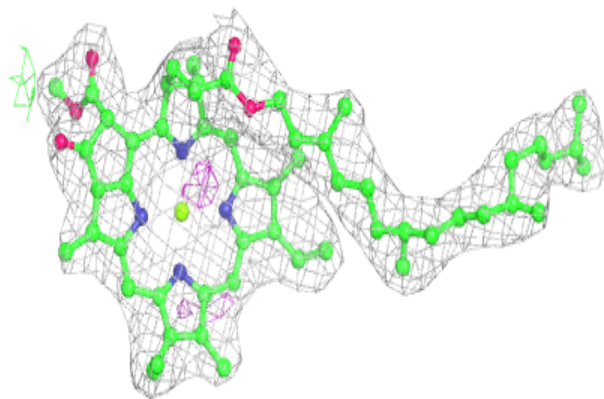
Electron density around CLA B 616:

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

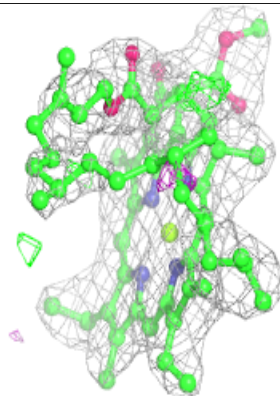
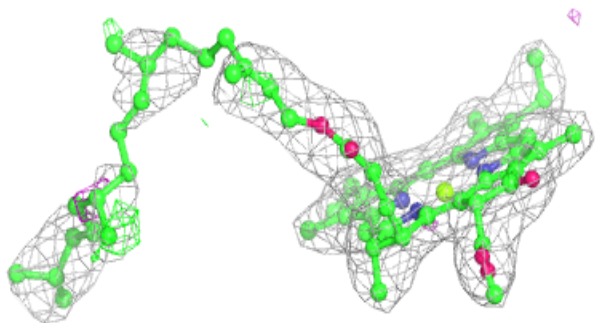
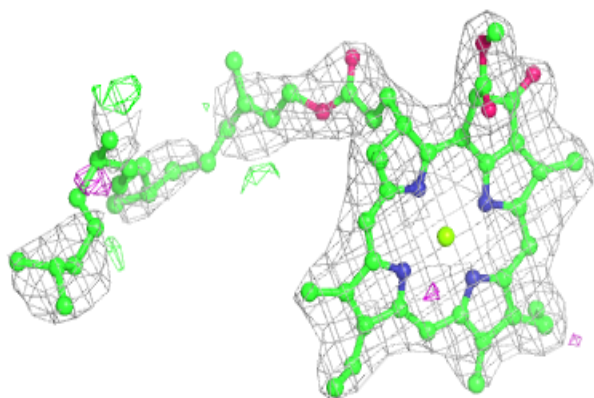


Electron density around CLA b 612:

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

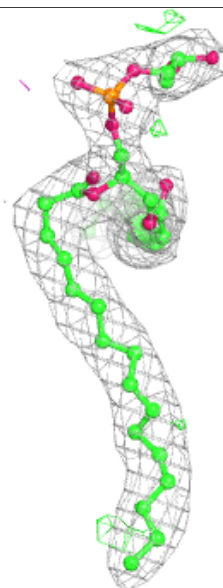
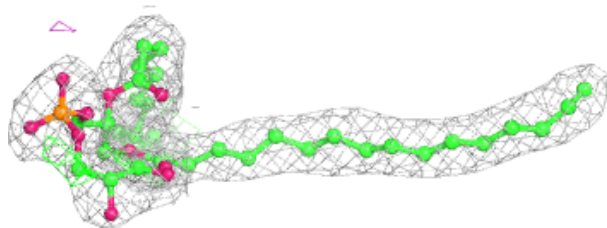
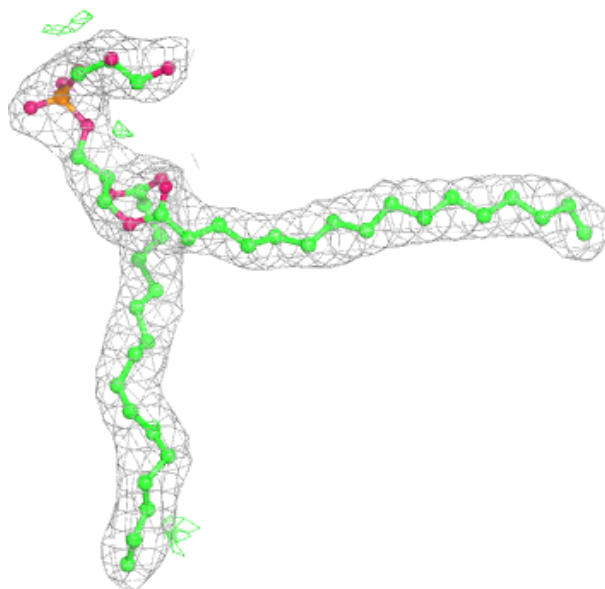
**Electron density around CLA a 412:**

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



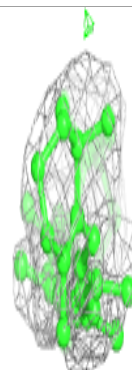
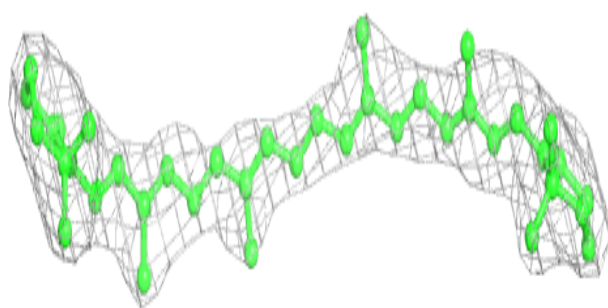
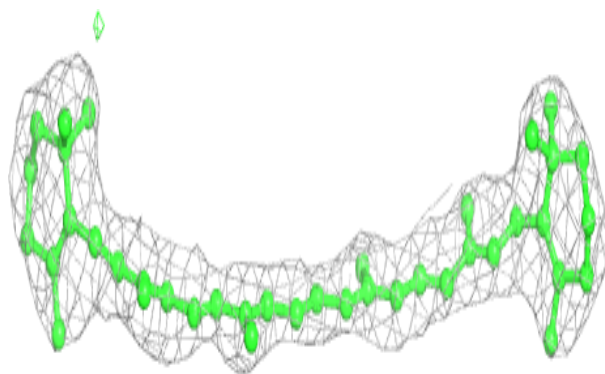
Electron density around LHG L 101:

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

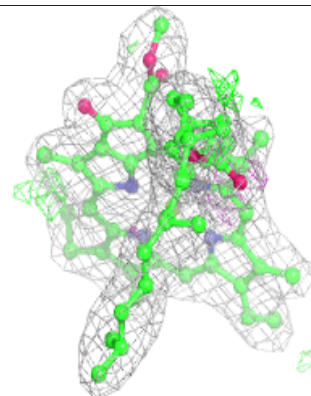
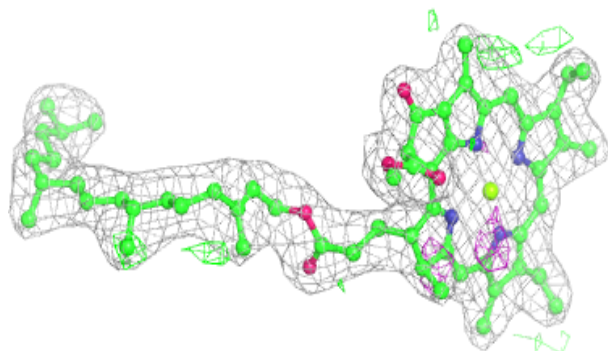
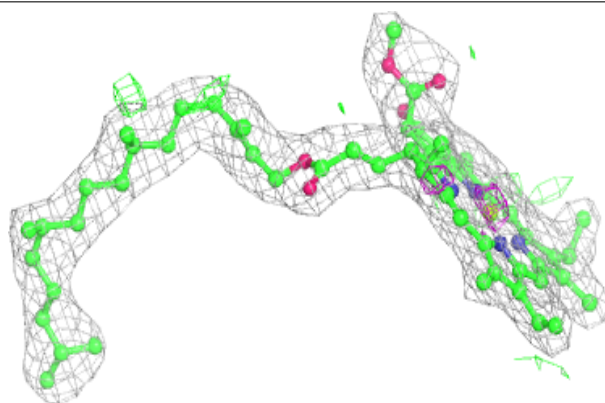


Electron density around BCR k 101:

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

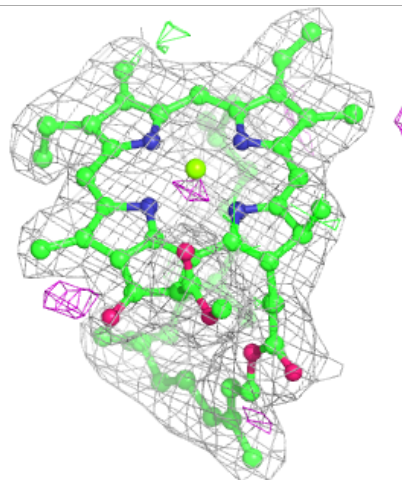
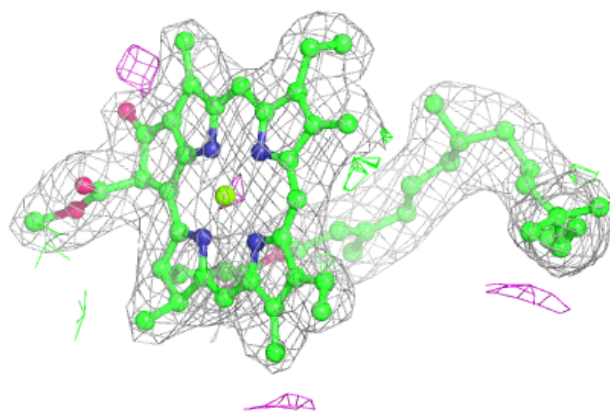
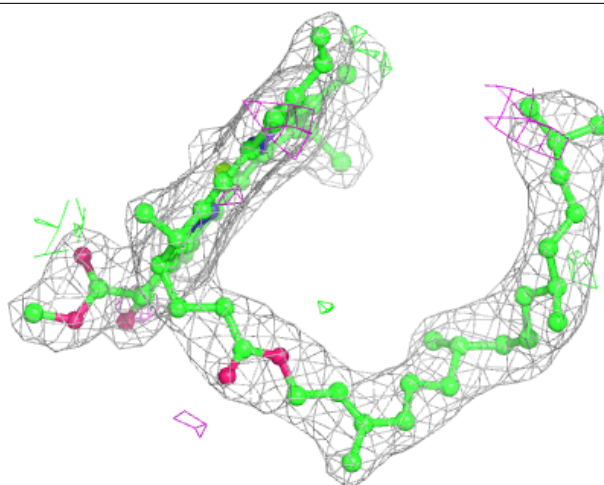
**Electron density around CLA D 406:**

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



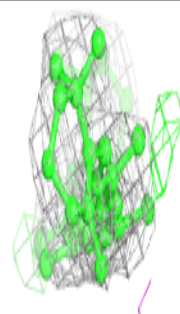
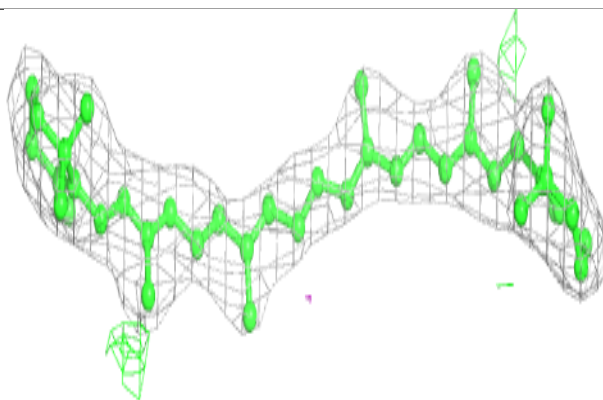
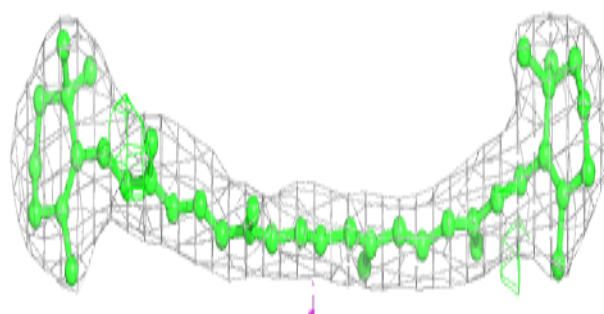
Electron density around CLA B 612:

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

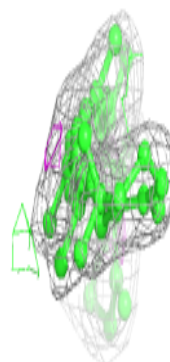
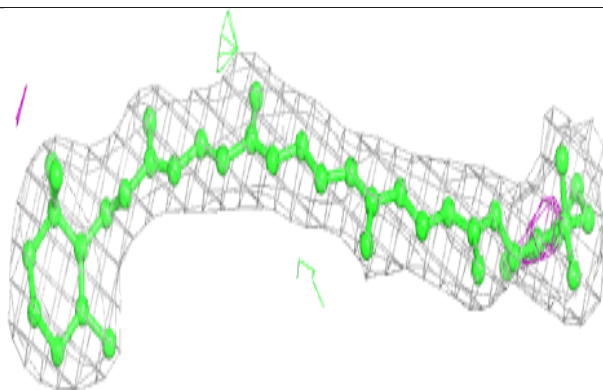
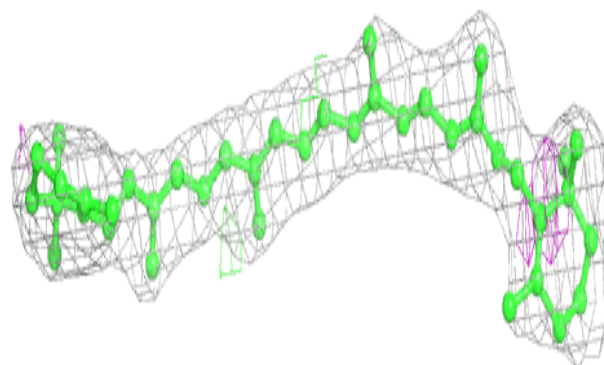


Electron density around BCR K 103:

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

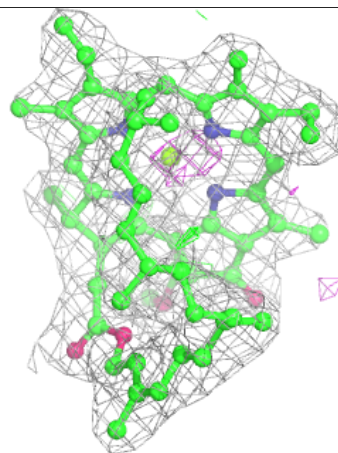
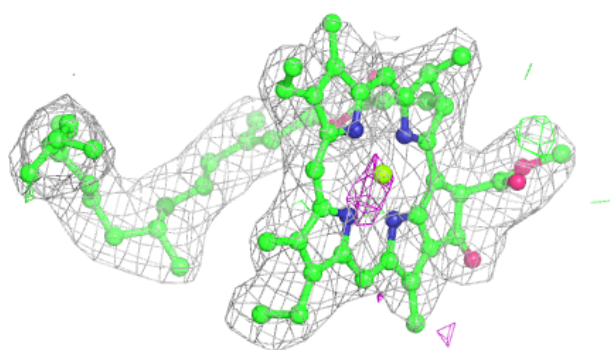
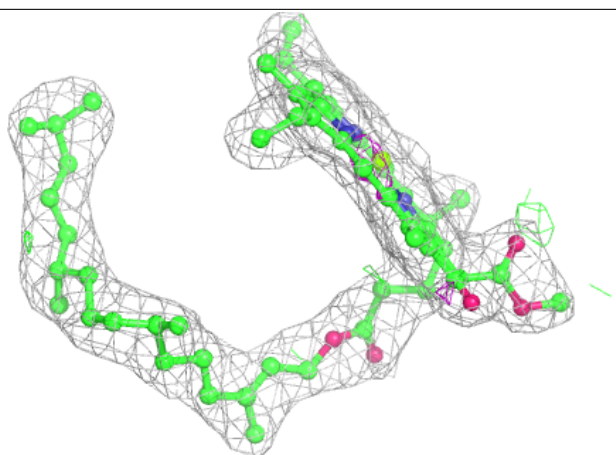
**Electron density around BCR d 406:**

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

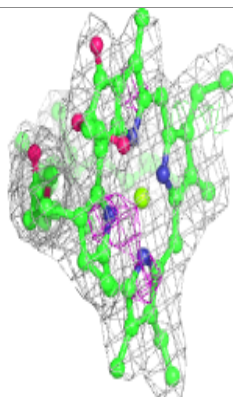
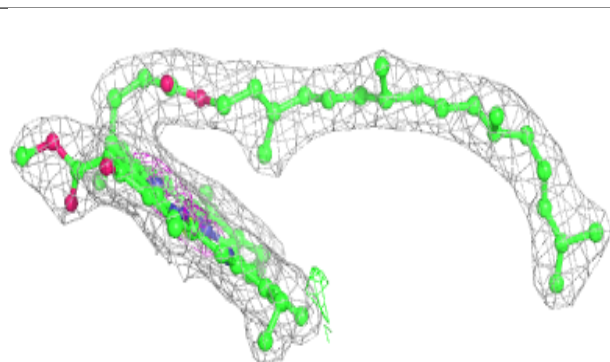
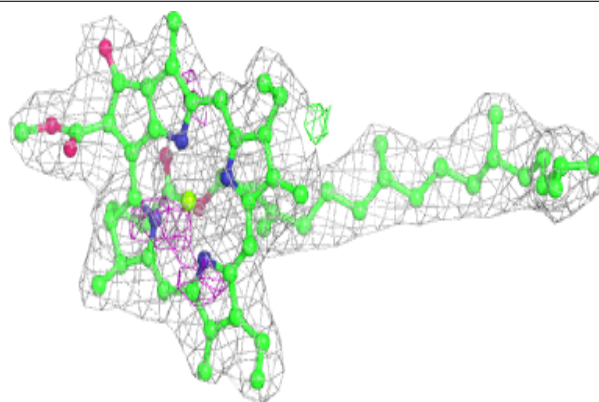


Electron density around CLA b 620:

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

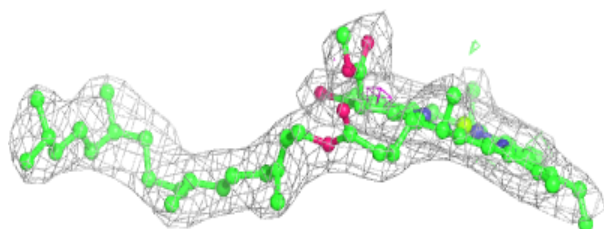
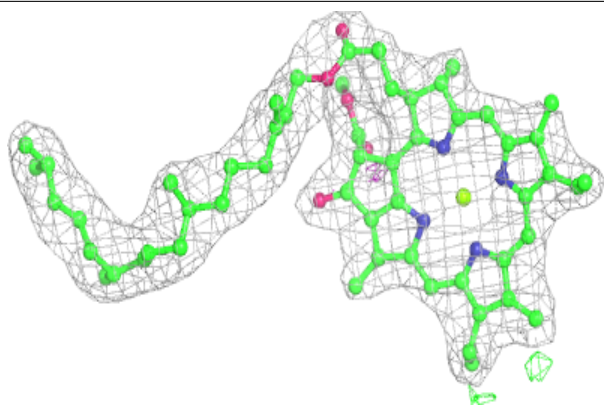
**Electron density around CLA b 617:**

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



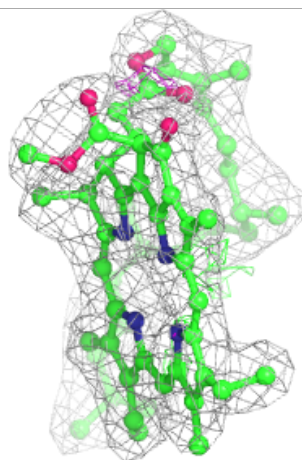
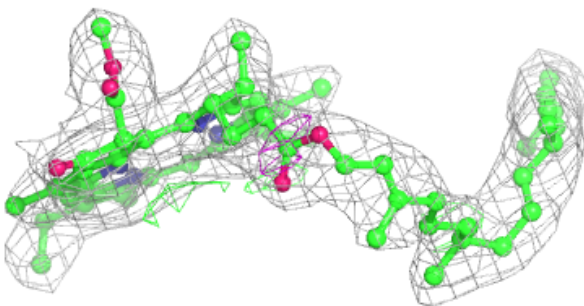
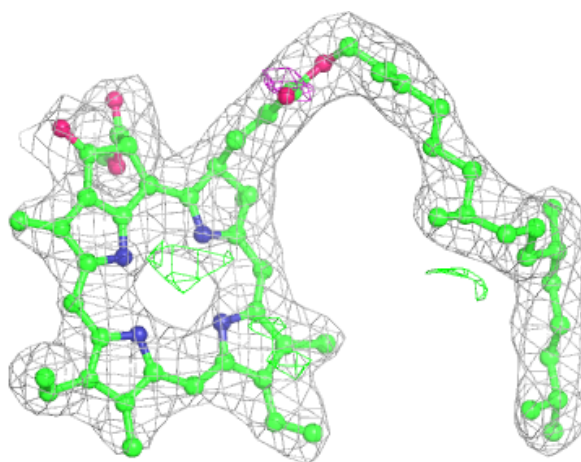
Electron density around CLA B 603:

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



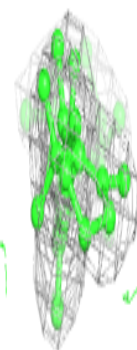
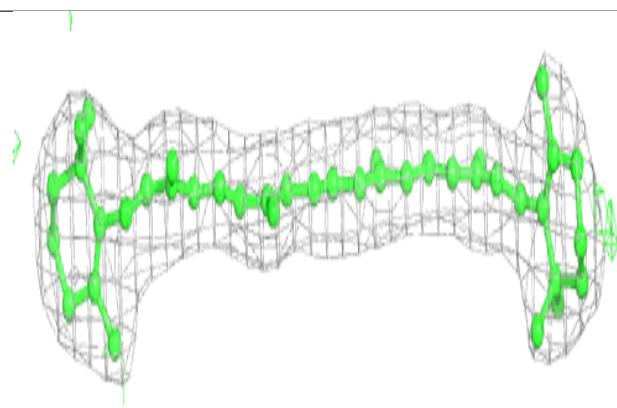
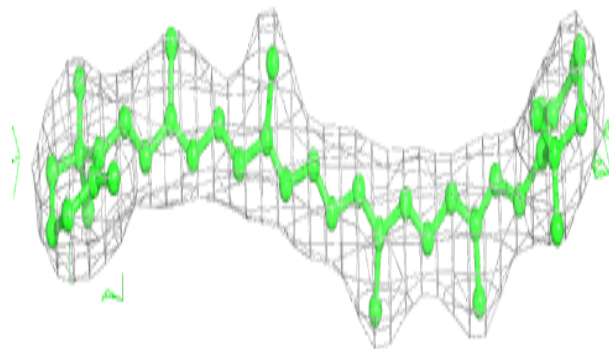
Electron density around PHO d 402 (B):

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

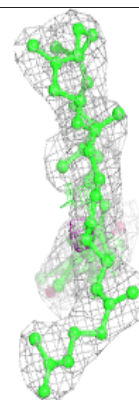
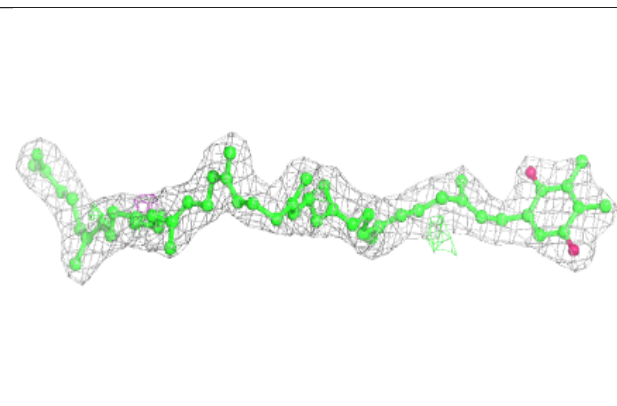
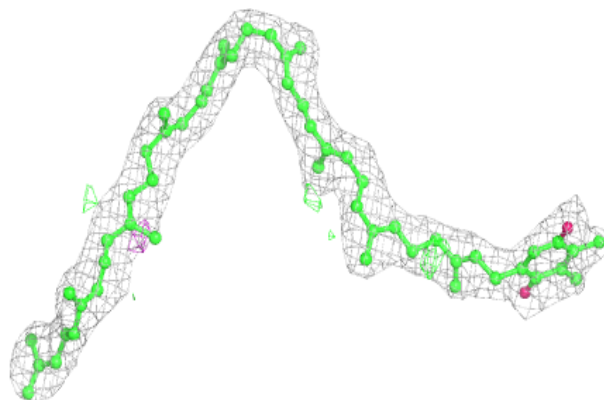


Electron density around BCR C 515:

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

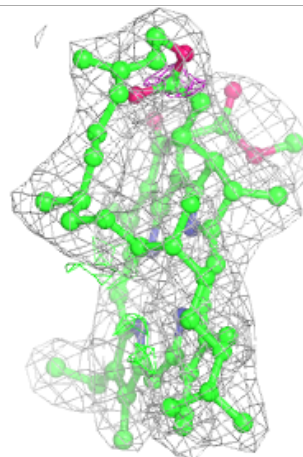
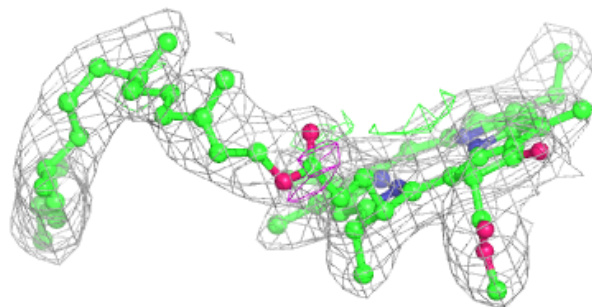
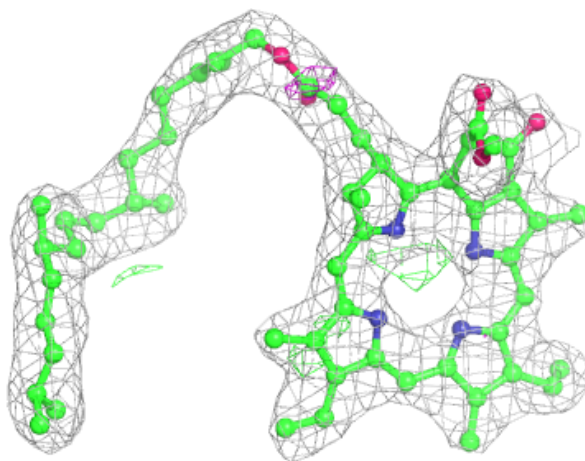
**Electron density around PL9 d 407 (B):**

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



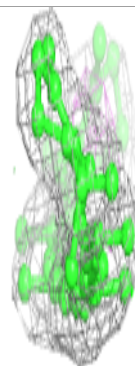
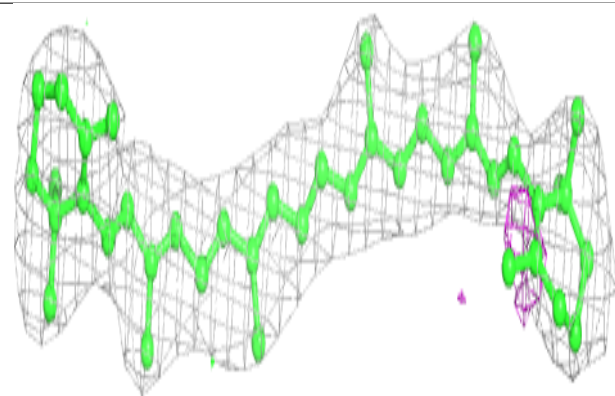
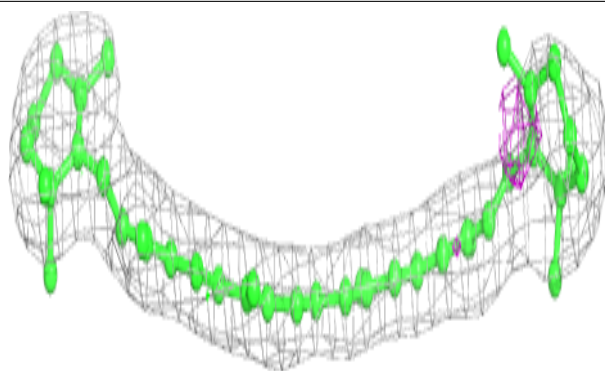
Electron density around PHO d 402 (A):

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

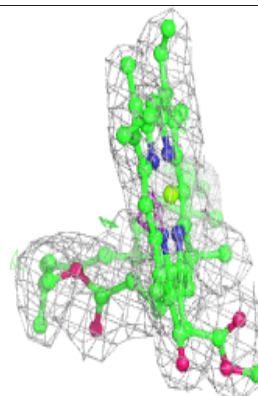
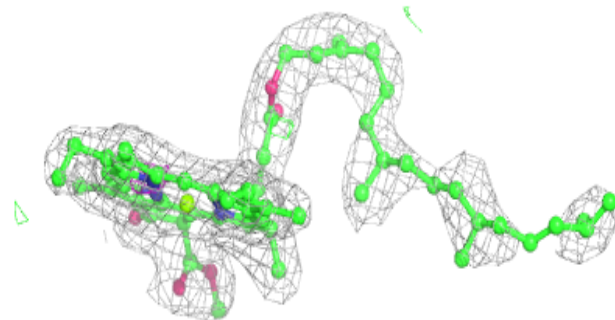
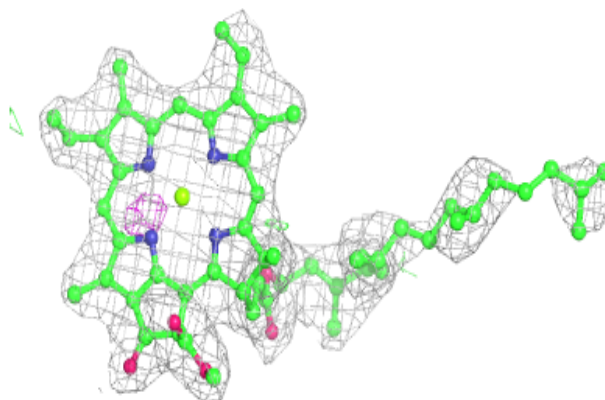


Electron density around BCR D 408:

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

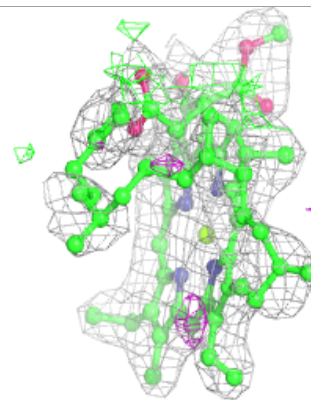
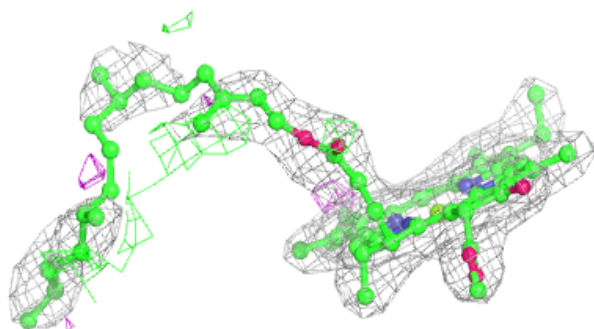
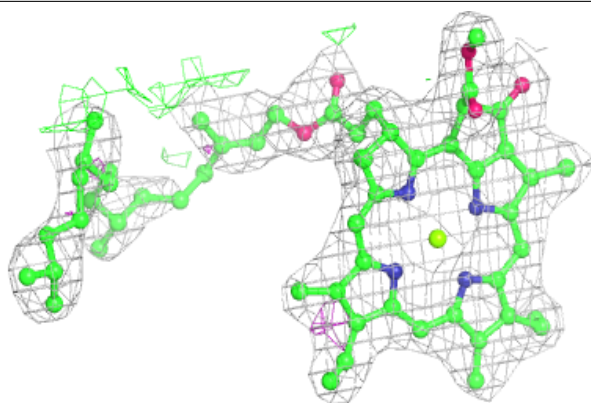
**Electron density around CLA A 406:**

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

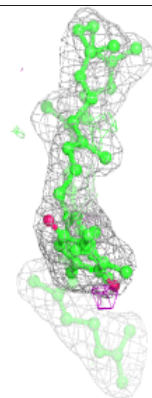
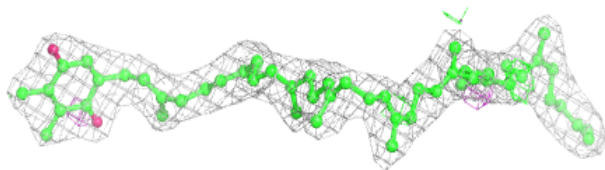
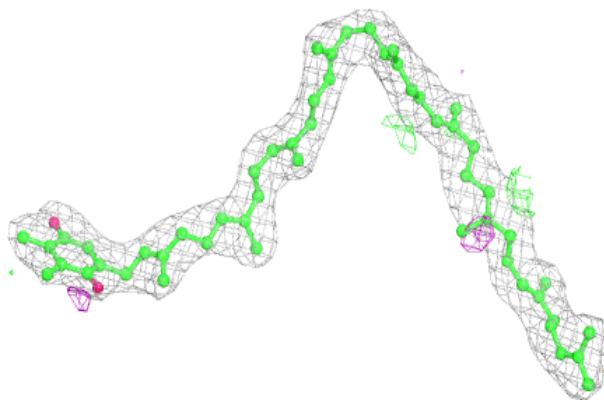


Electron density around CLA A 407:

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

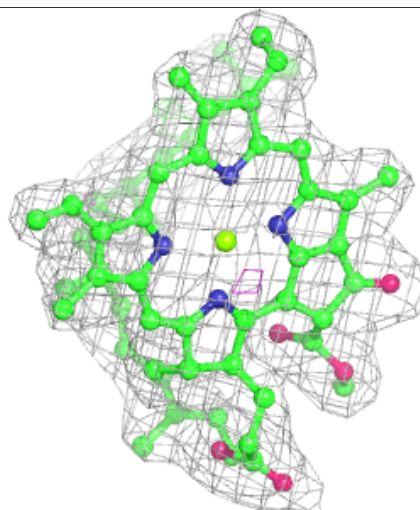
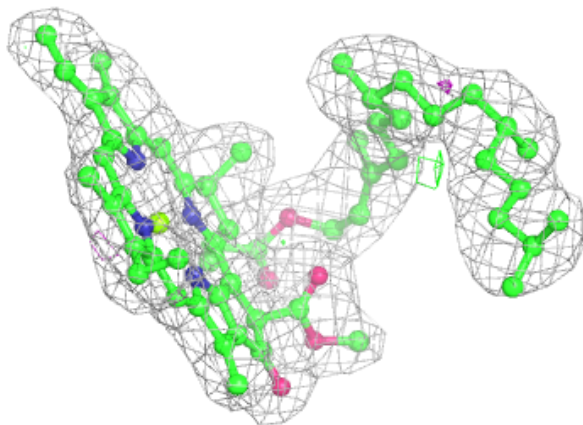
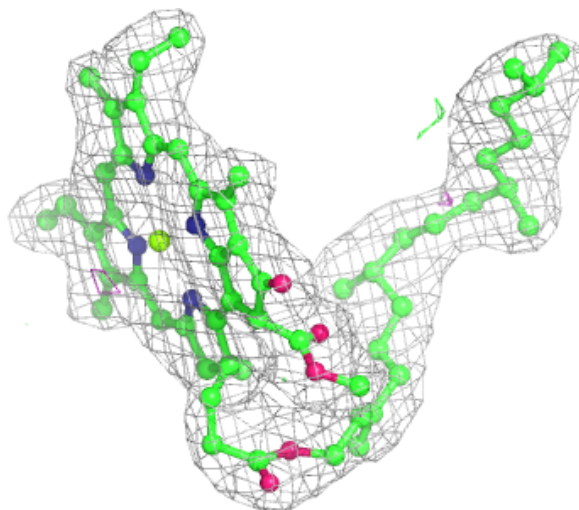
**Electron density around PL9 D 409 (A):**

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



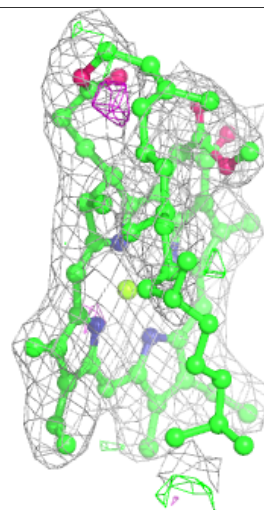
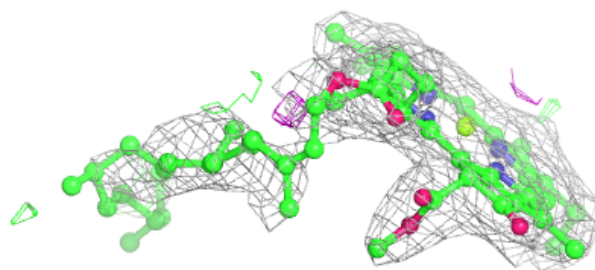
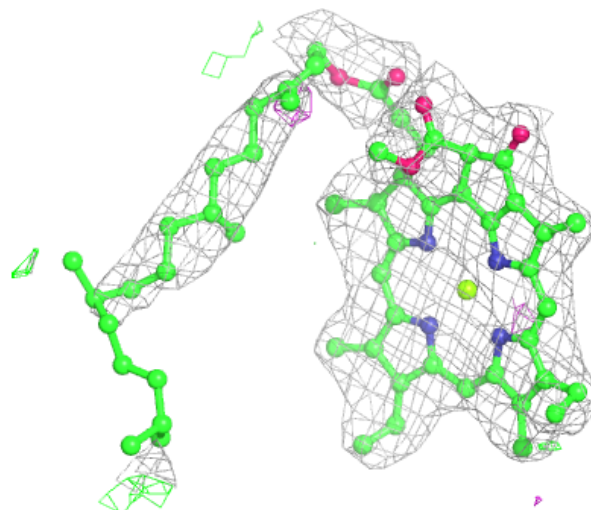
Electron density around CLA b 622:

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



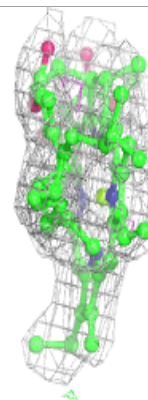
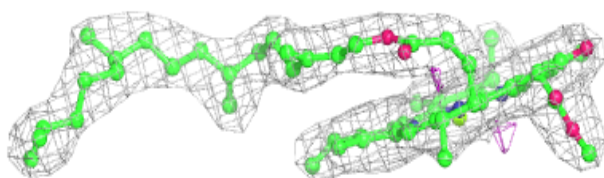
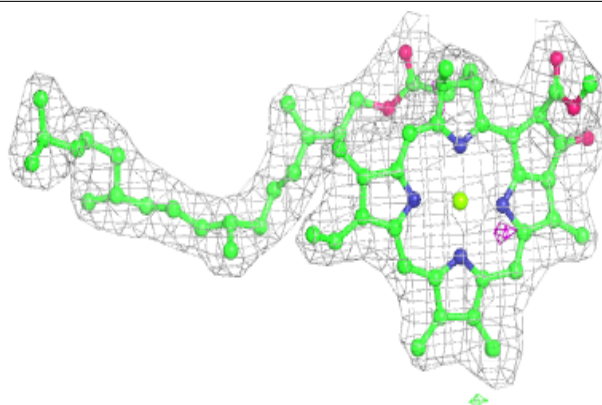
Electron density around CLA B 617:

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

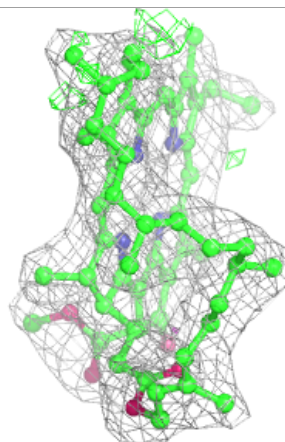
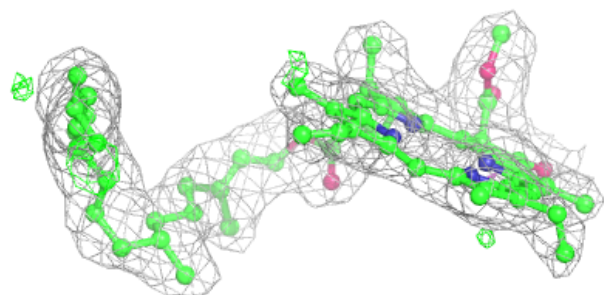
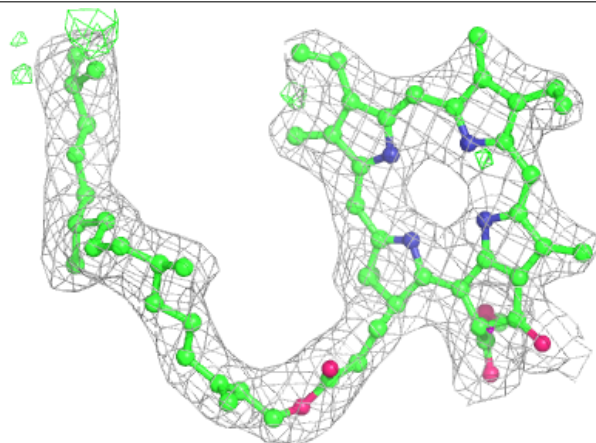


Electron density around CLA B 604:

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

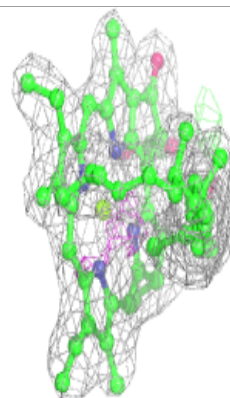
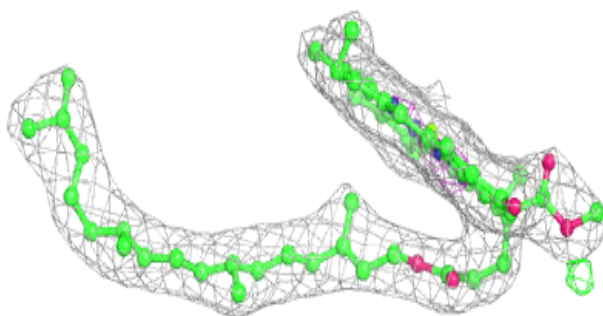
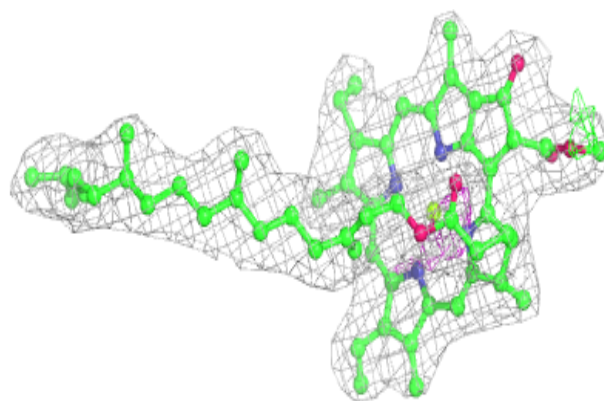
**Electron density around PHO D 403 (B):**

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

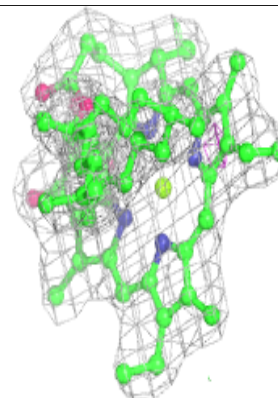
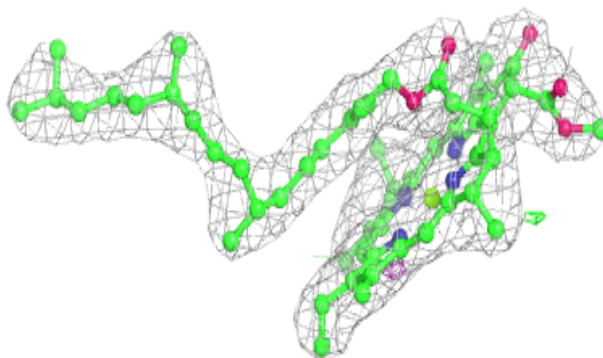
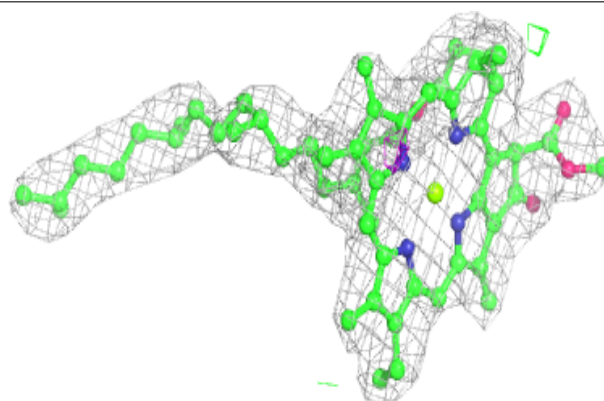


Electron density around CLA B 609:

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

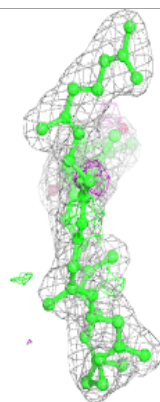
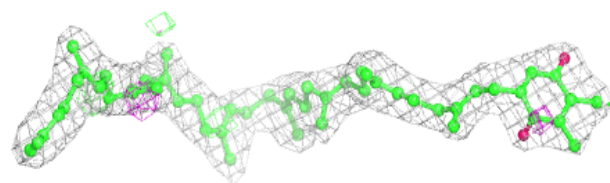
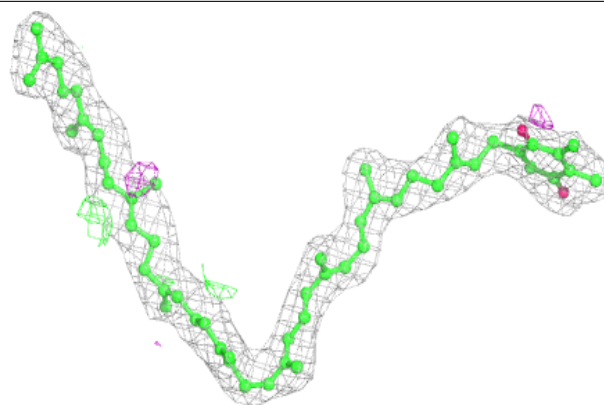
**Electron density around CLA C 506:**

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

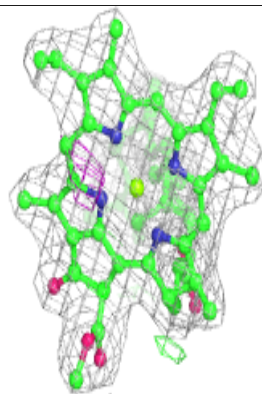
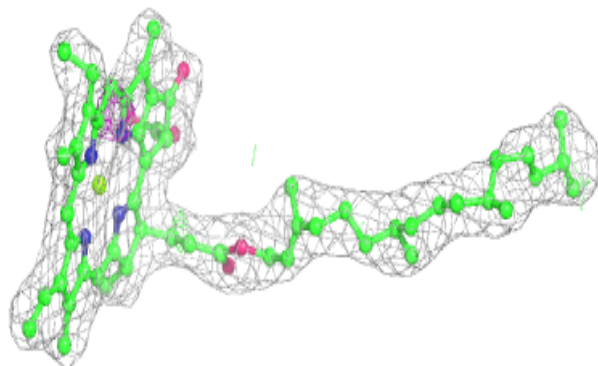
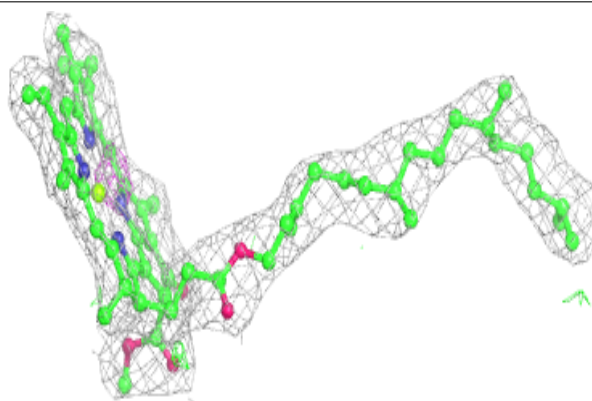


Electron density around PL9 D 409 (B):

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

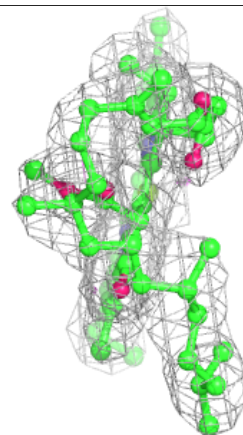
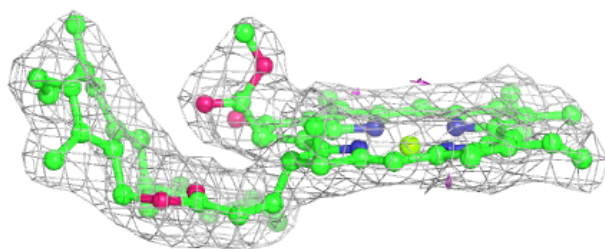
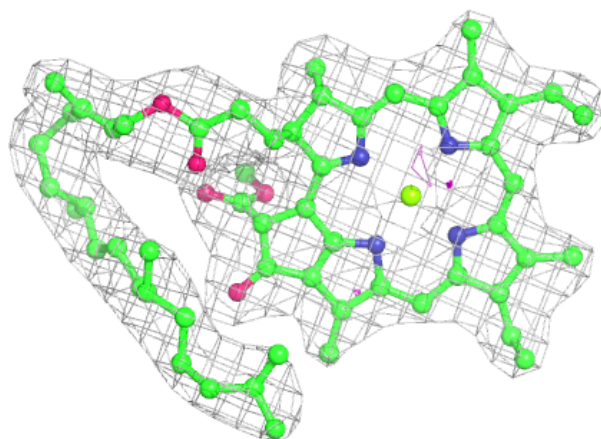
**Electron density around CLA B 605:**

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

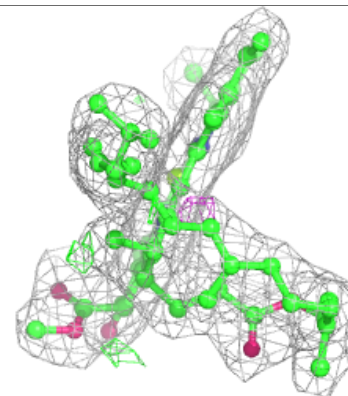
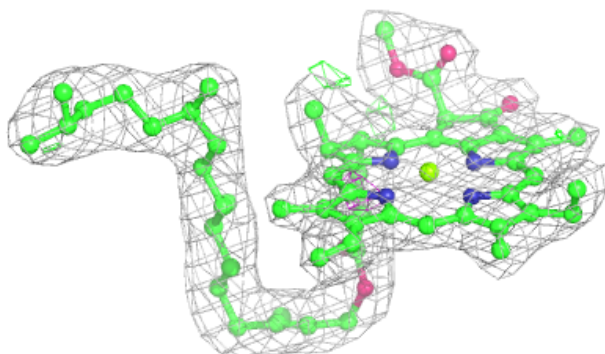
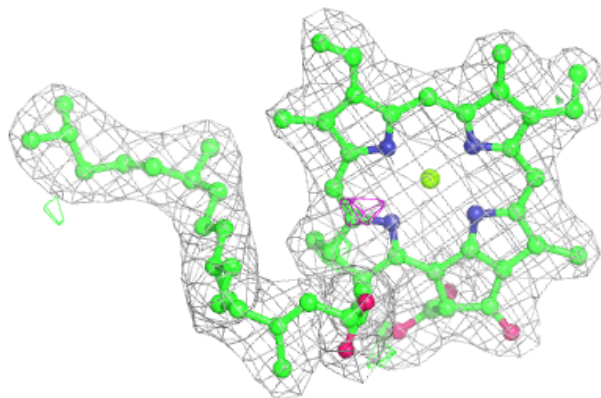


Electron density around CLA b 619:

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

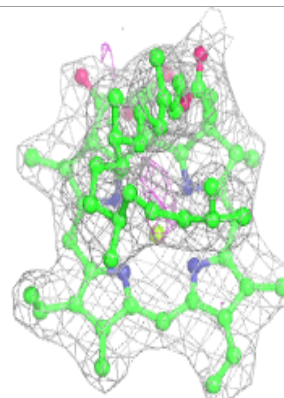
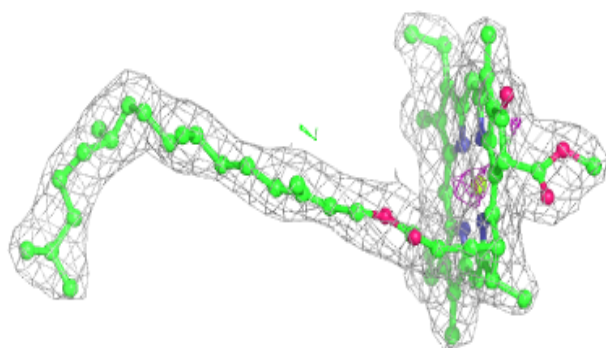
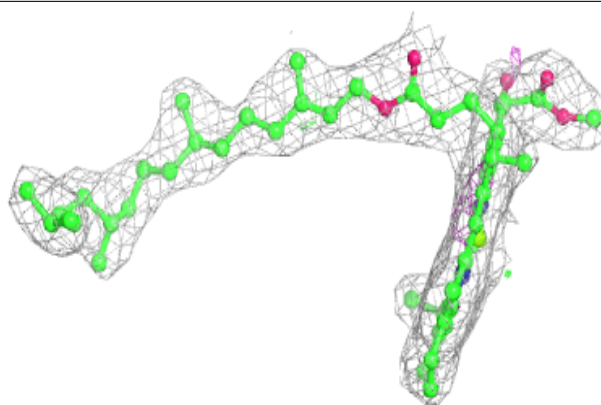
**Electron density around CLA A 405:**

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

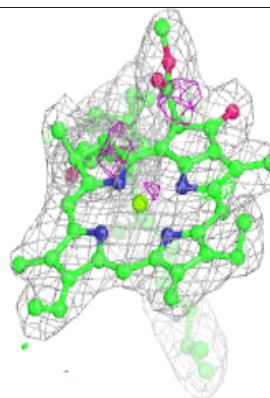
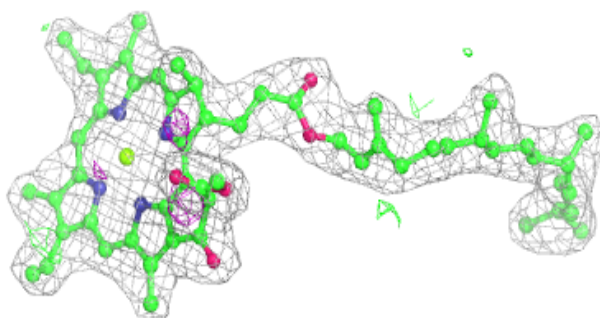
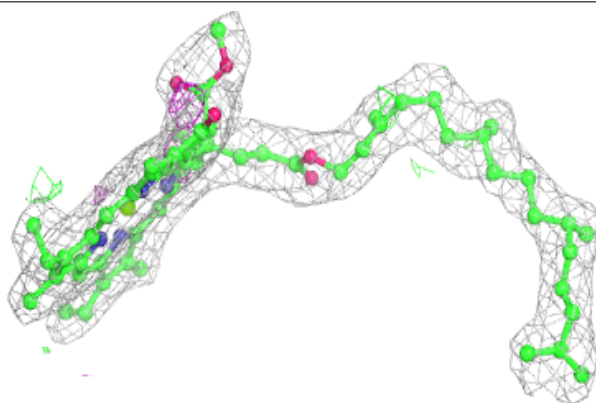


Electron density around CLA b 614:

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

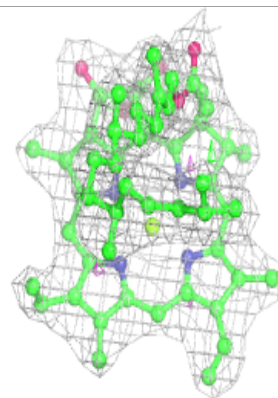
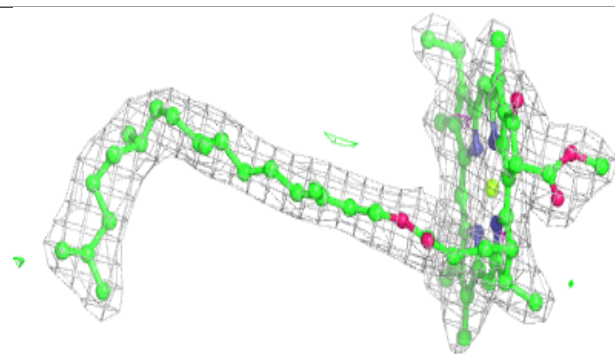
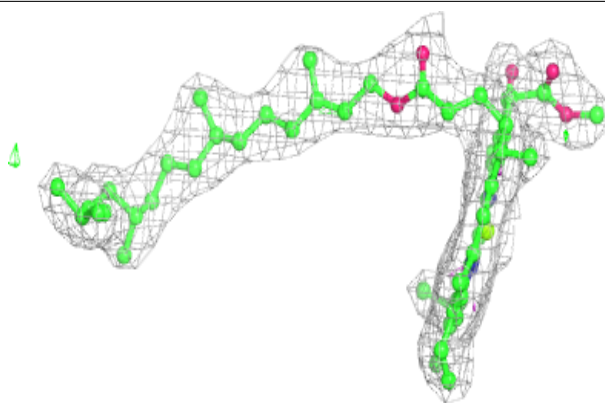
**Electron density around CLA d 404:**

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

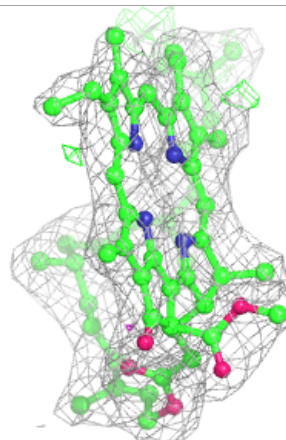
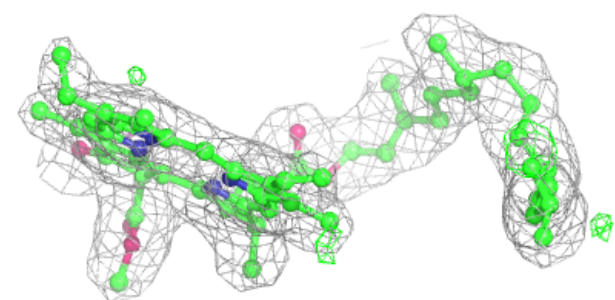
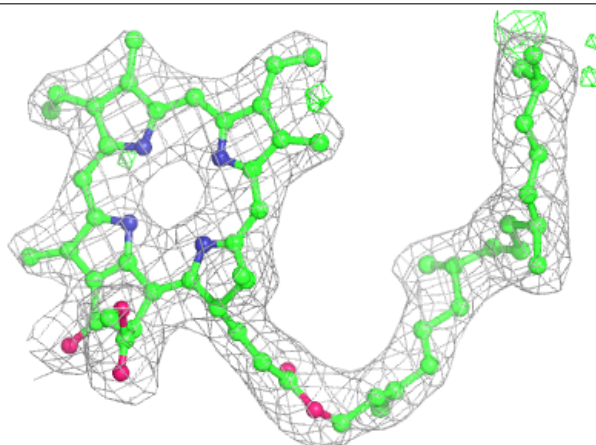


Electron density around CLA B 606:

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

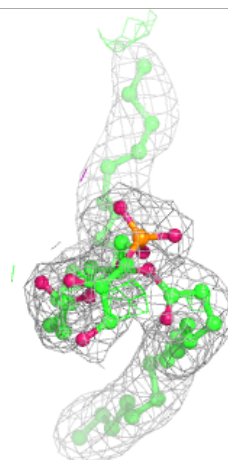
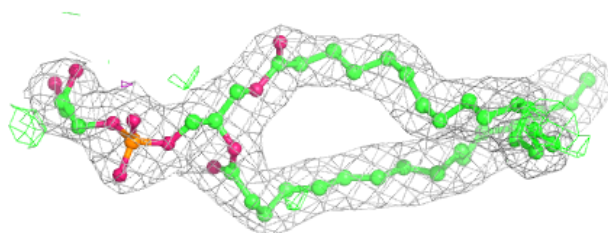
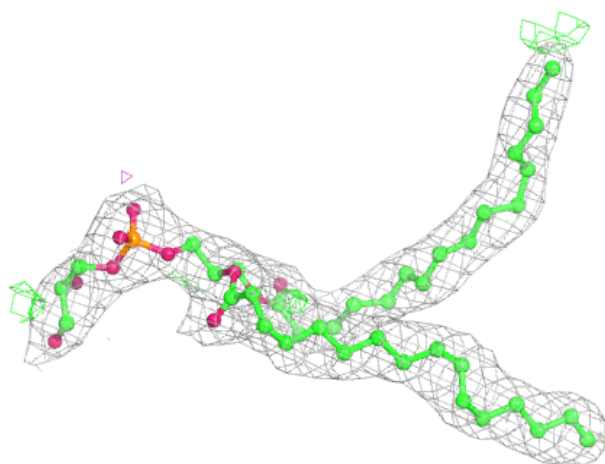
**Electron density around PHO D 403 (A):**

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



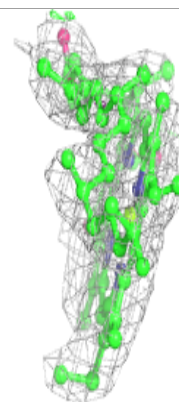
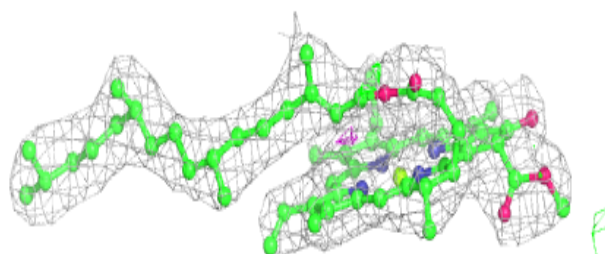
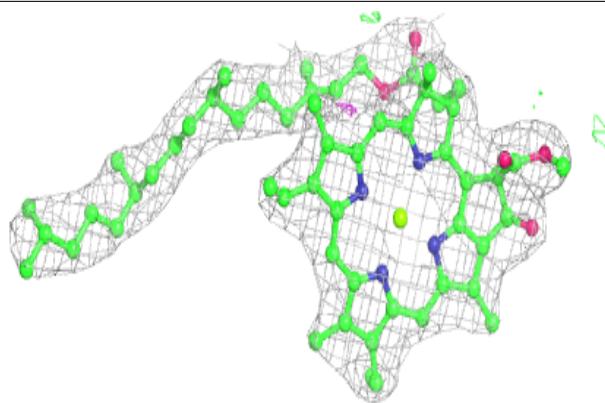
Electron density around LHG D 412:

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

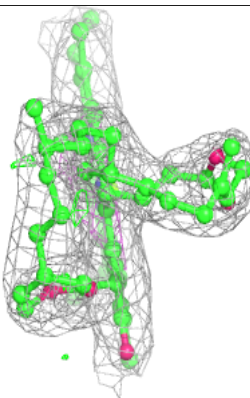
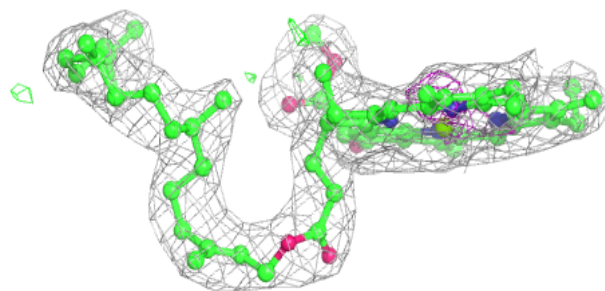
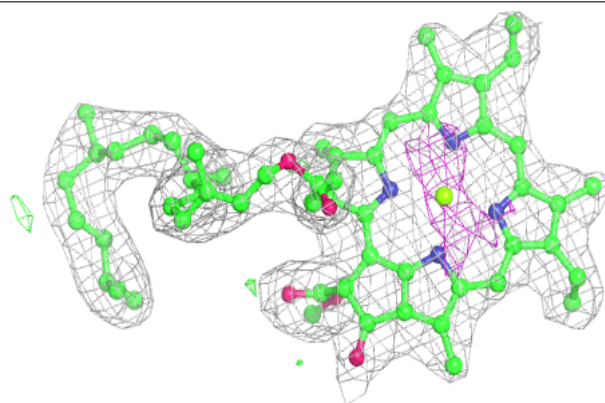


Electron density around CLA c 505:

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

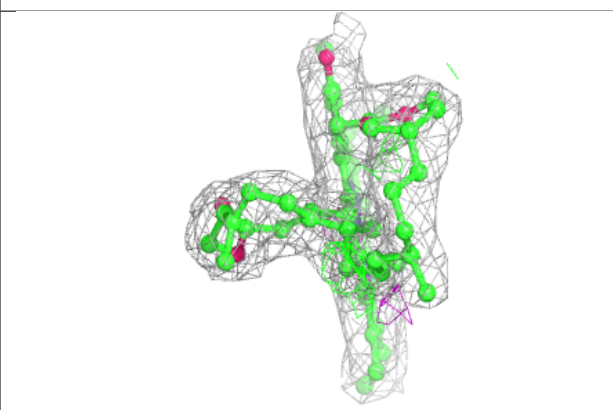
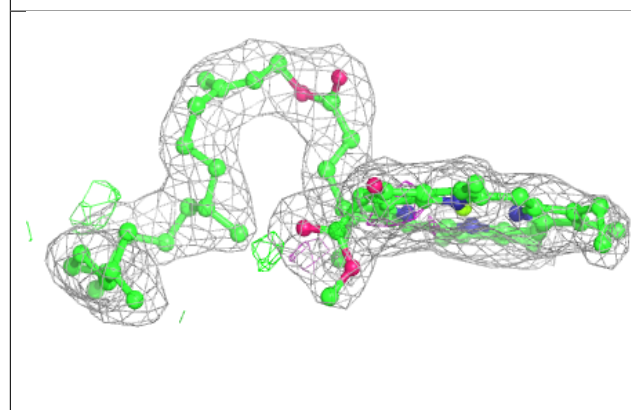
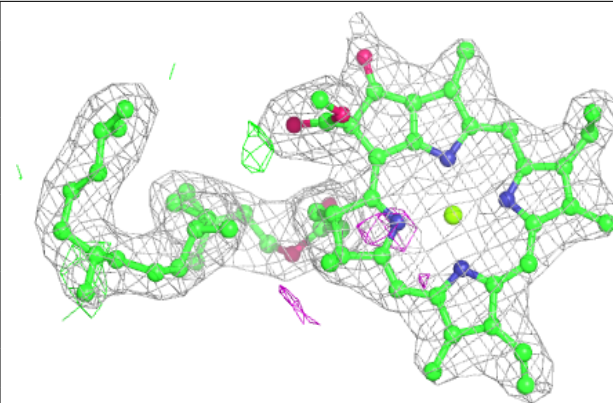
**Electron density around CLA B 613:**

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

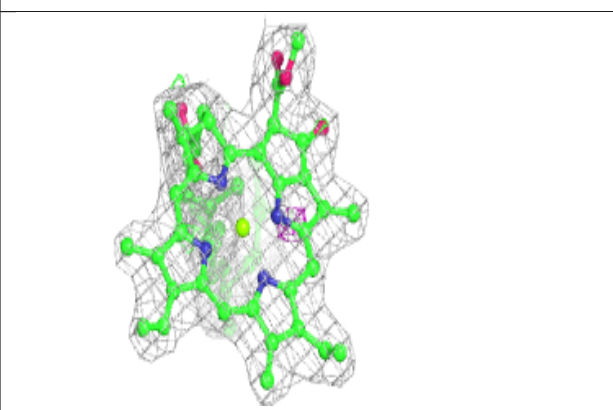
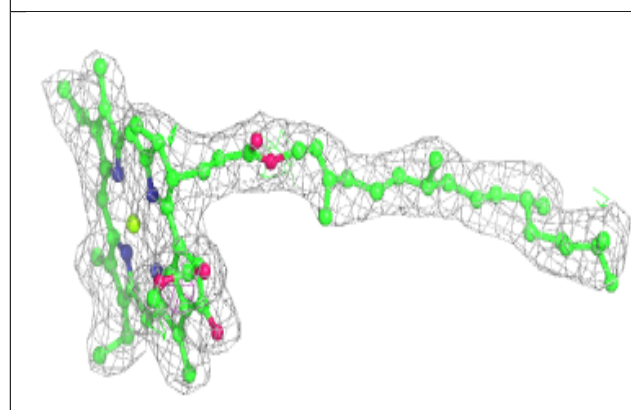
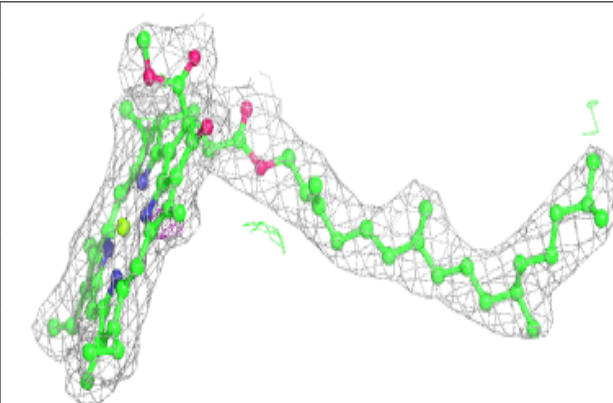


Electron density around CLA b 621:

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

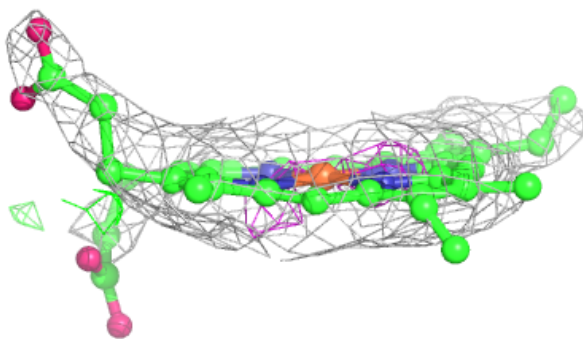
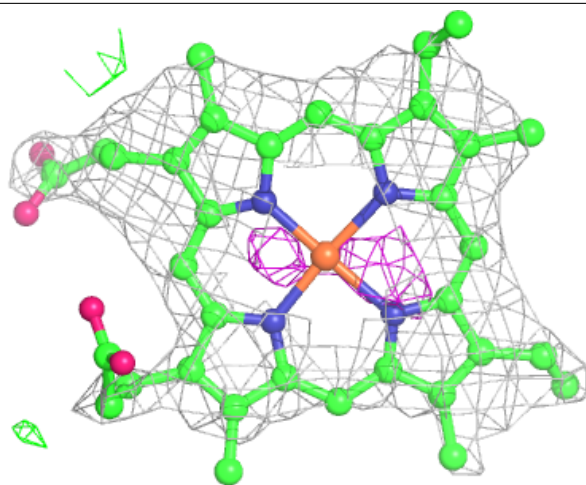
**Electron density around CLA b 613:**

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



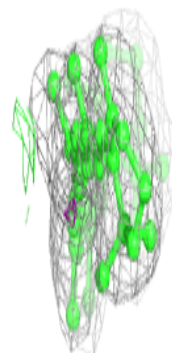
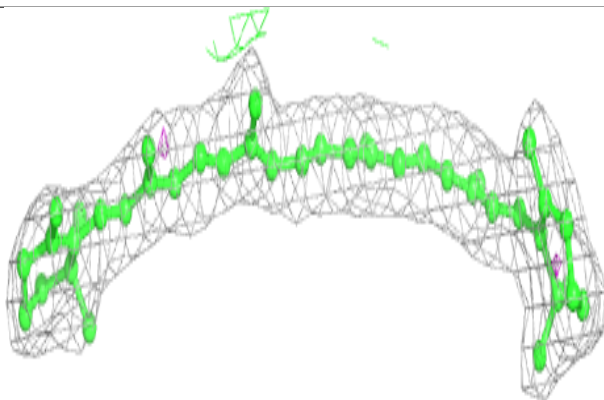
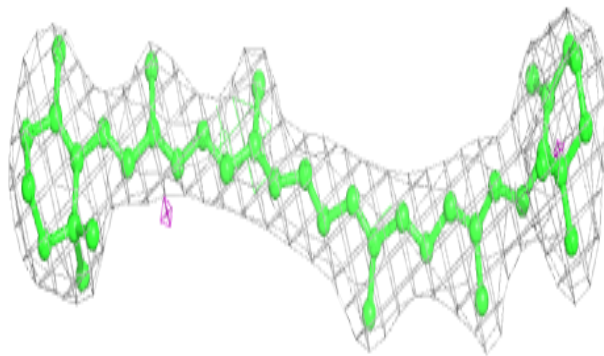
Electron density around HEM e 101:

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

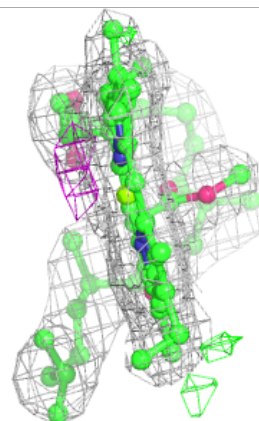
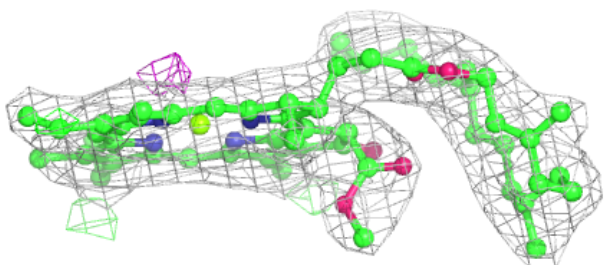
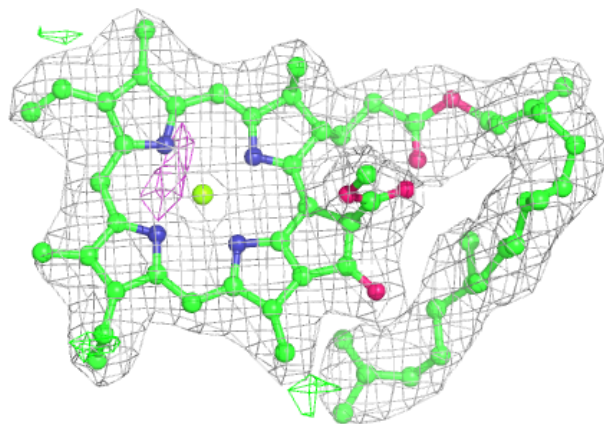


Electron density around BCR T 103:

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

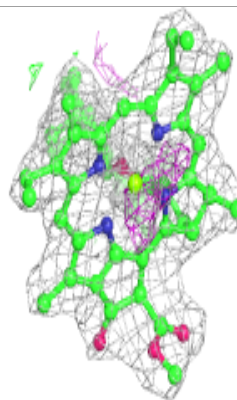
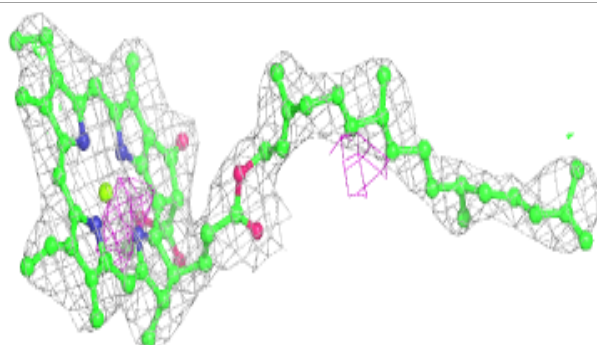
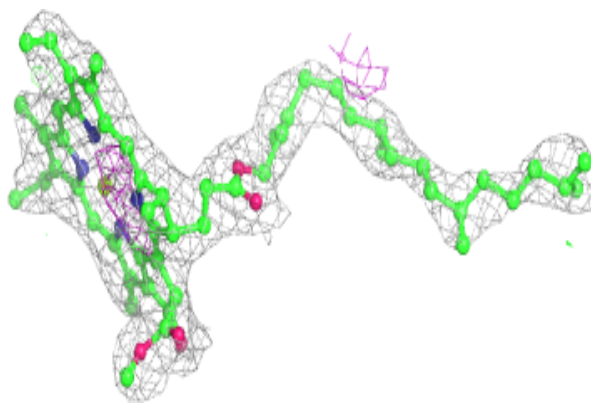
**Electron density around CLA B 611:**

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



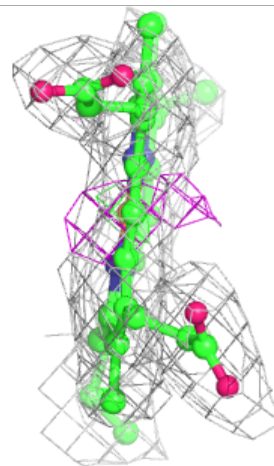
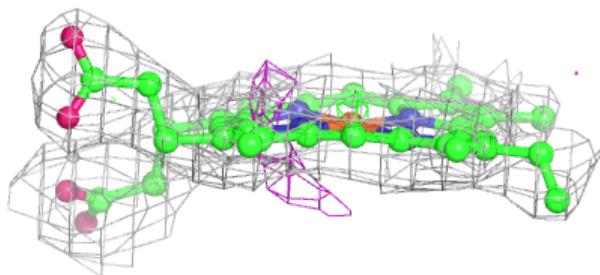
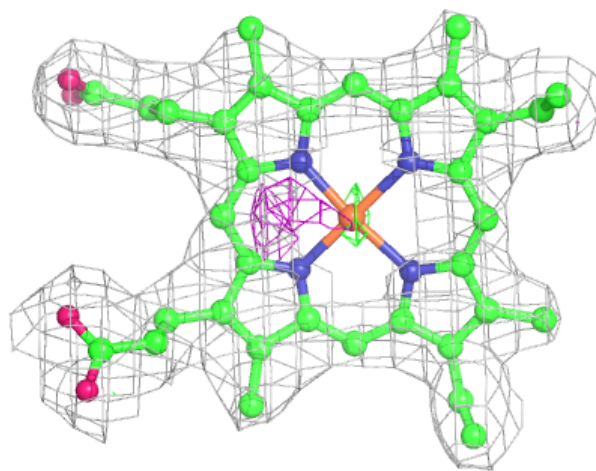
Electron density around CLA c 506:

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



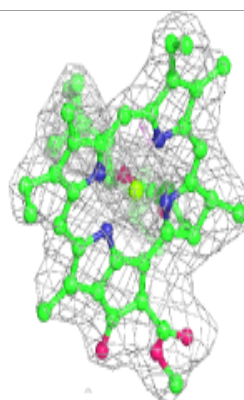
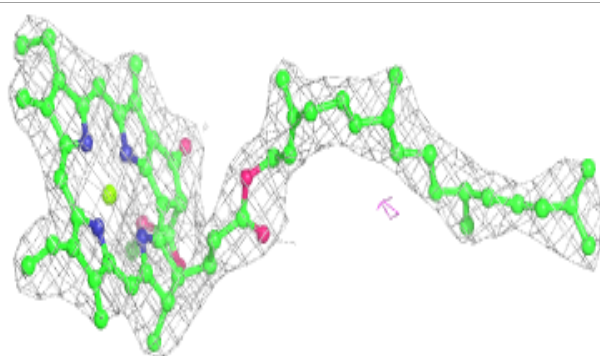
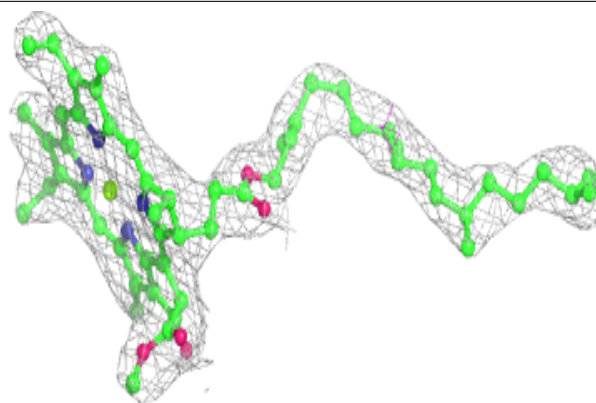
Electron density around HEM v 205:

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

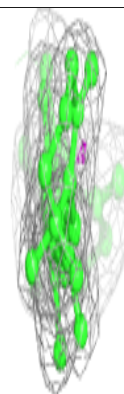
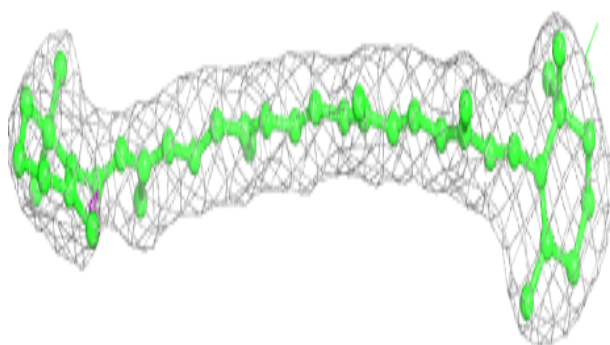
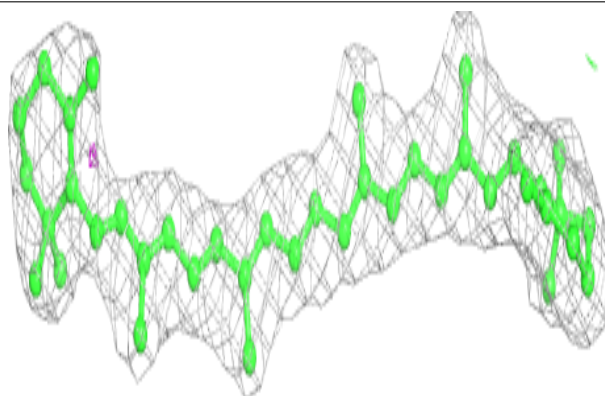


Electron density around CLA C 503:

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

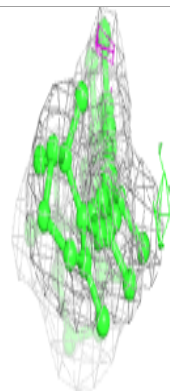
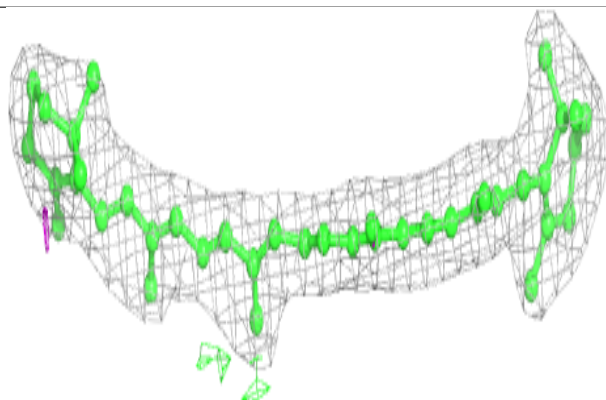
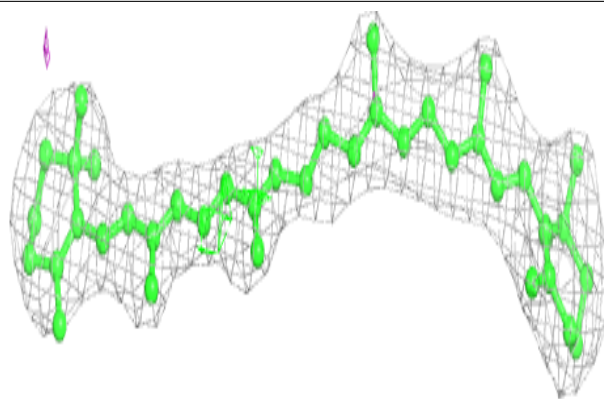
**Electron density around BCR b 626:**

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

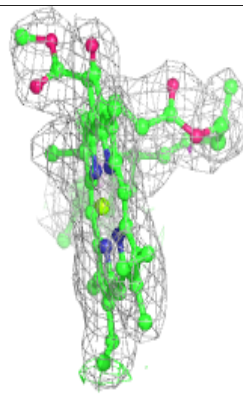
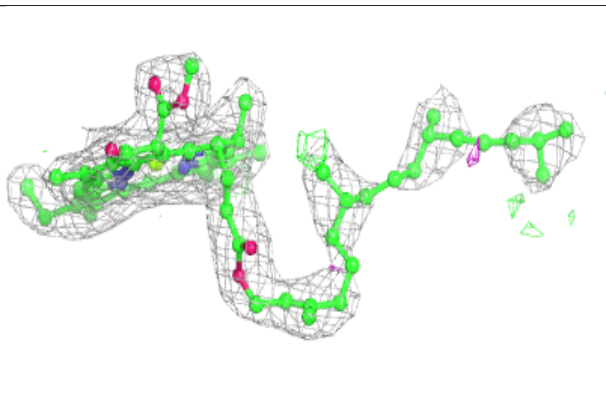
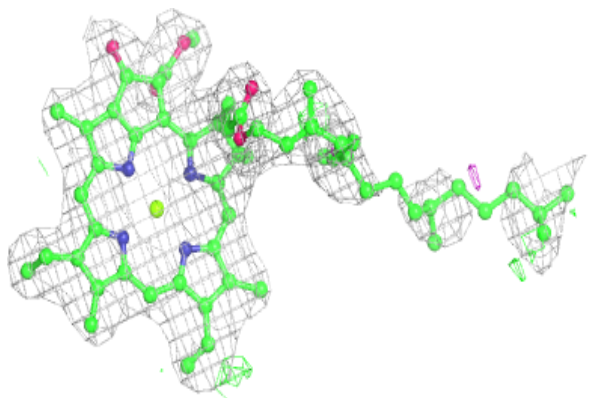


Electron density around BCR t 102:

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

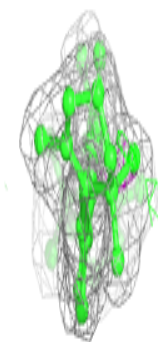
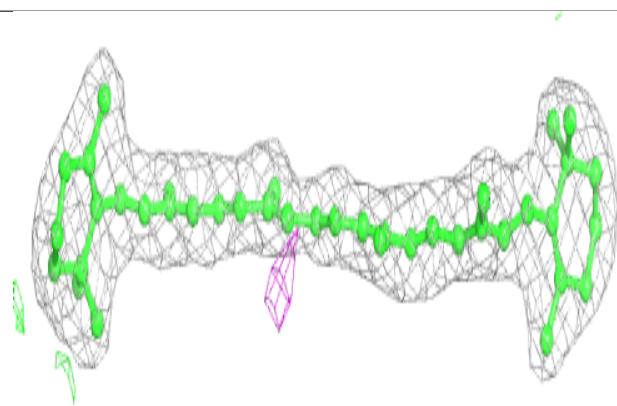
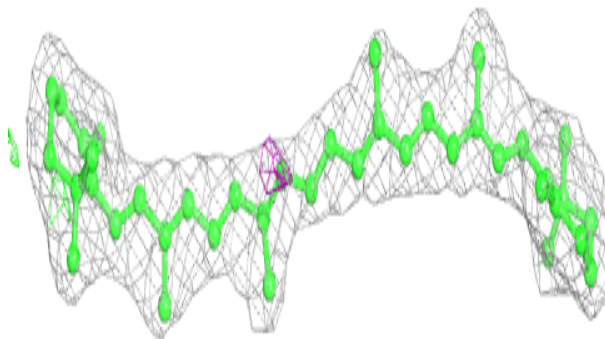
**Electron density around CLA a 410:**

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

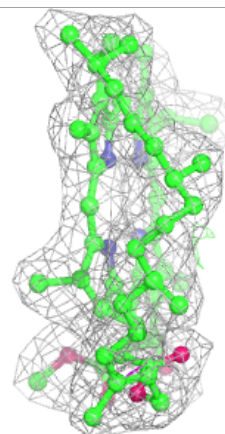
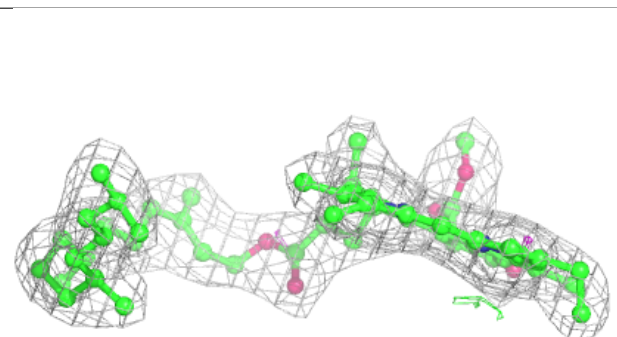
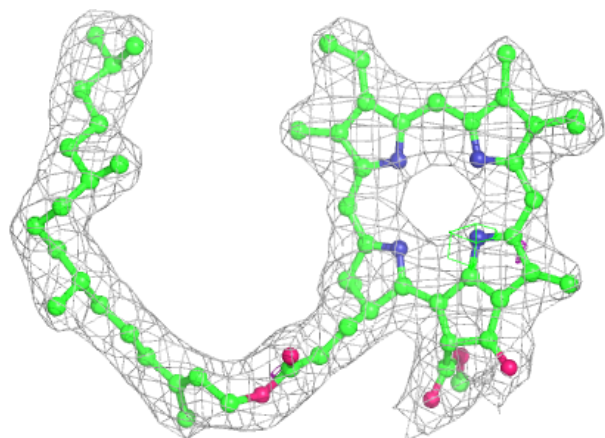


Electron density around BCR A 408:

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

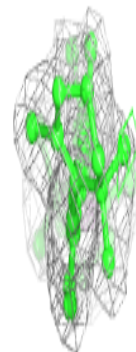
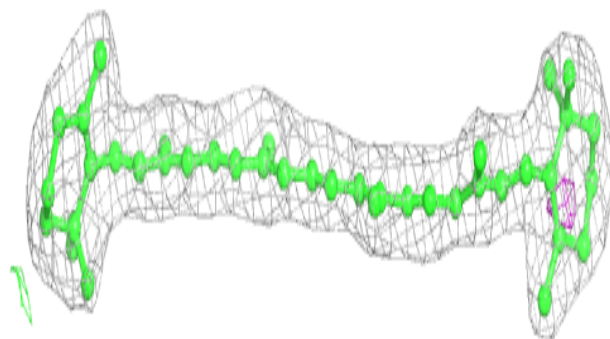
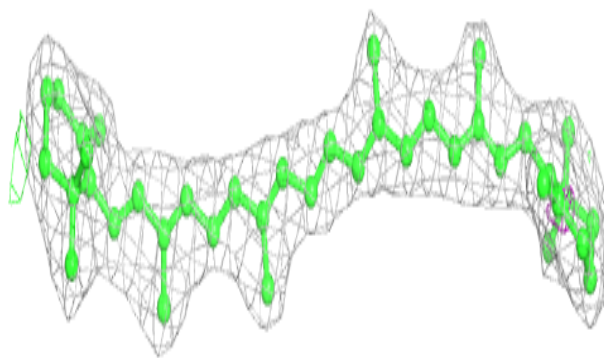
**Electron density around PHO D 402:**

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

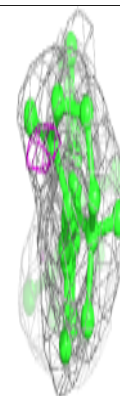
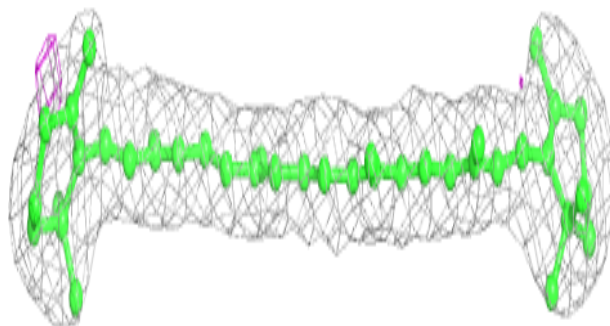
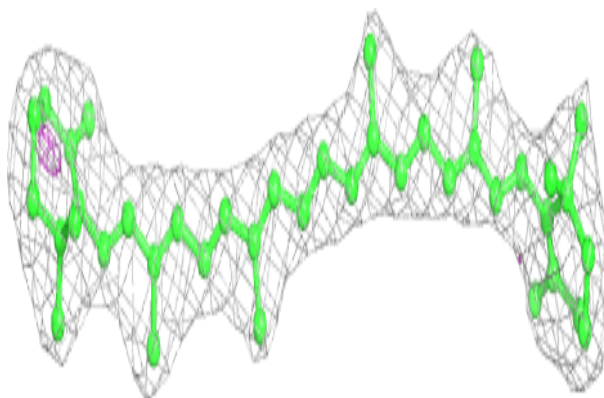


Electron density around BCR a 413:

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

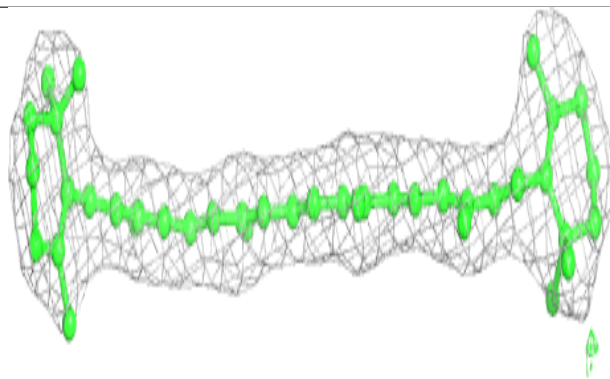
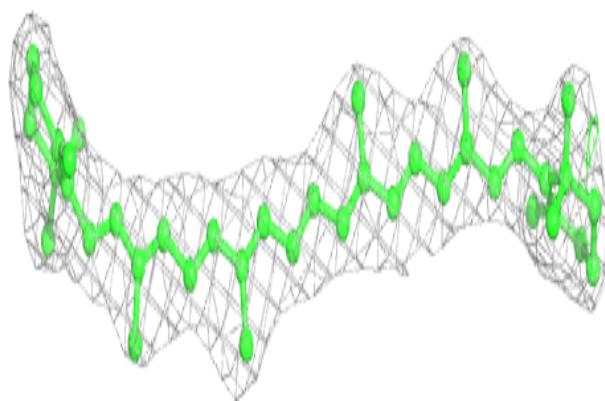
**Electron density around BCR B 619:**

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

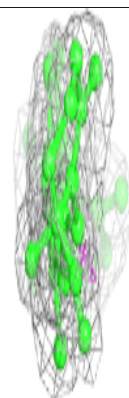
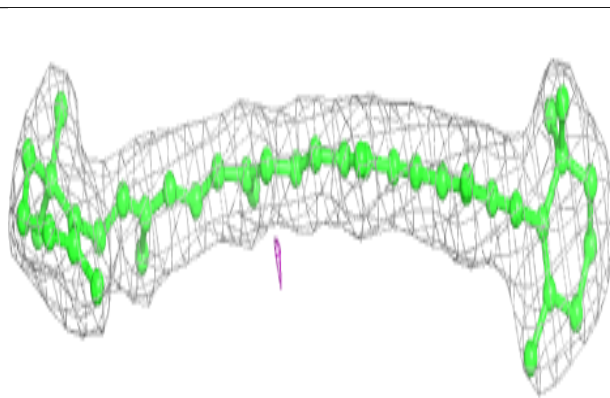
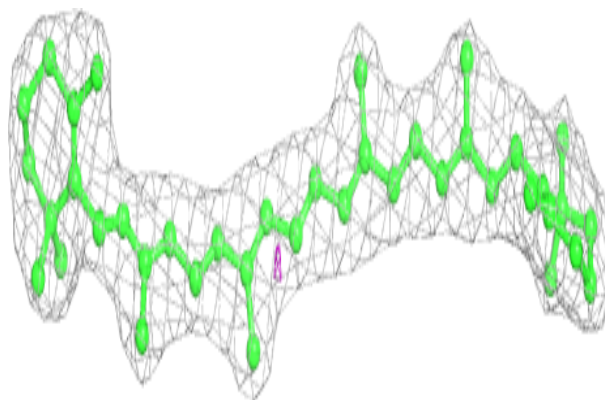


Electron density around BCR c 518:

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

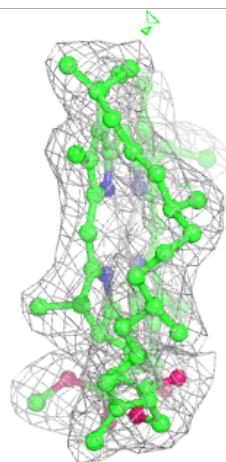
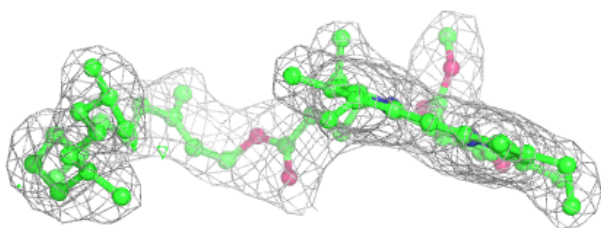
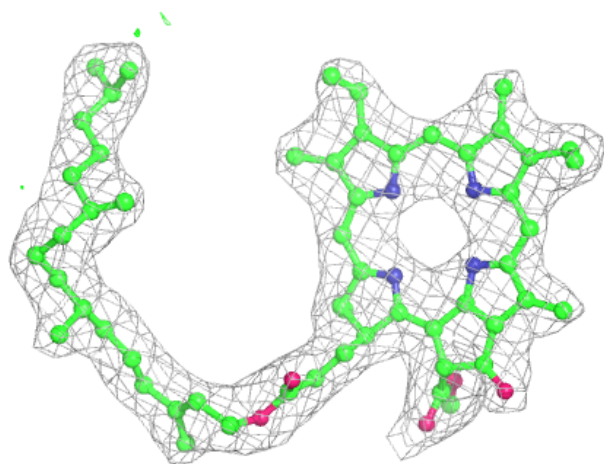
**Electron density around BCR B 618:**

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



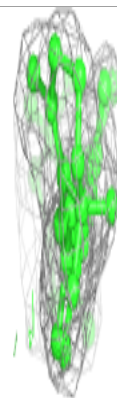
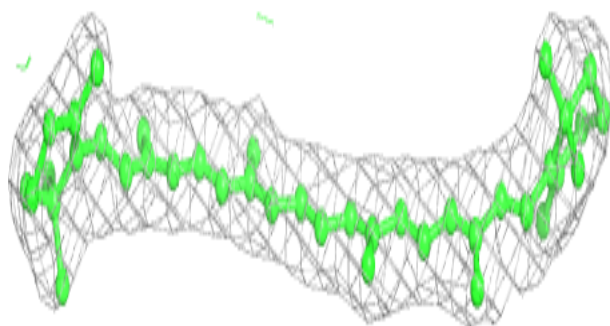
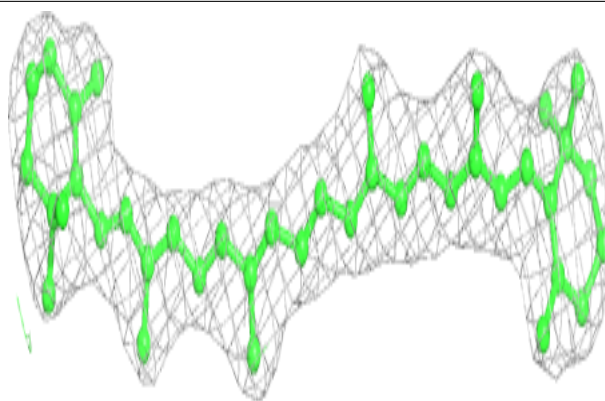
Electron density around PHO a 411:

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

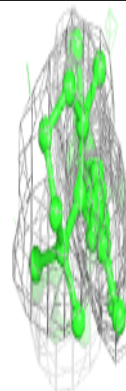
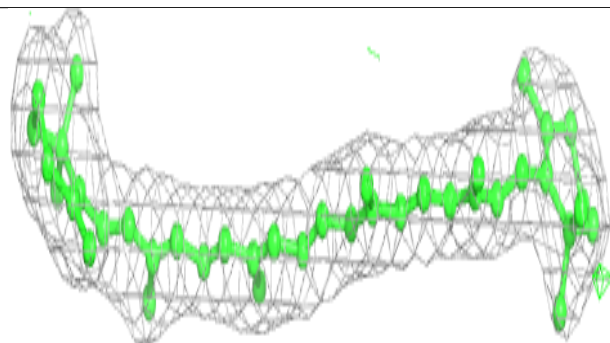
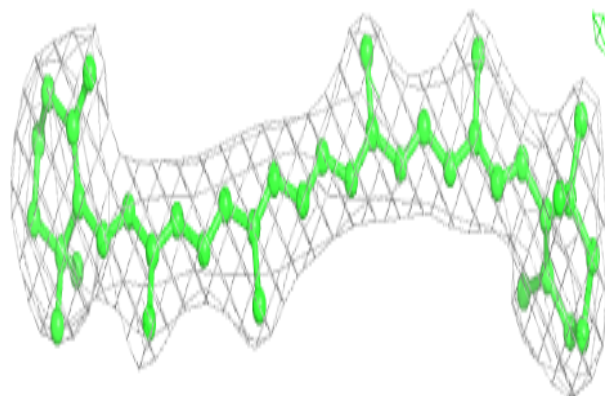


Electron density around BCR b 628:

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

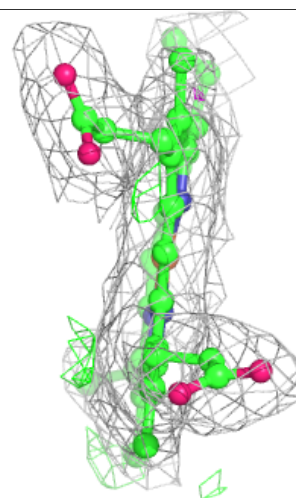
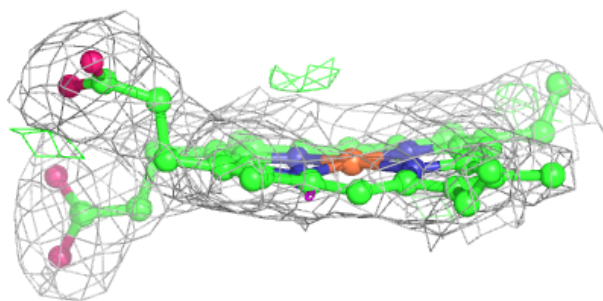
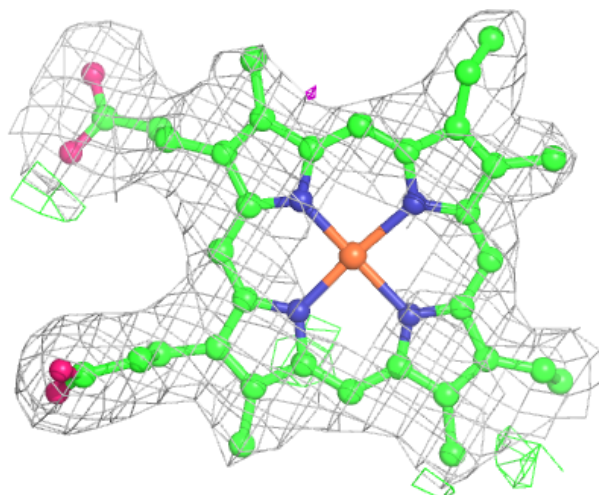
**Electron density around BCR B 620:**

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



Electron density around HEM V 206:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.