



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2021 – 10:31 PM JST

PDB ID : 7CJJ
Title : Photosystem II structure in the S2 state
Authors : Li, H.; Shen, J.-R.; Suga, M.
Deposited on : 2020-07-11
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
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)	:	2.18

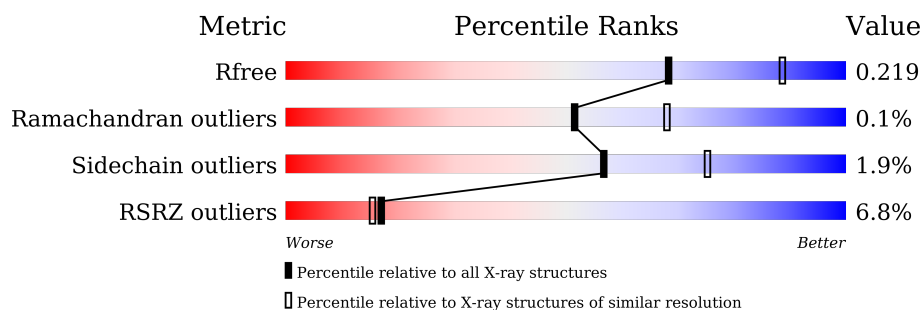
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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>2%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
2	B	505	<div> <div>5%</div> <div>99%</div> <div>.</div> </div>
2	b	505	<div> <div>9%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>4%</div> <div>98%</div> <div>..</div> </div>
3	c	455	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
4	D	342	<div> <div>2%</div> <div>99%</div> <div>.</div> </div>

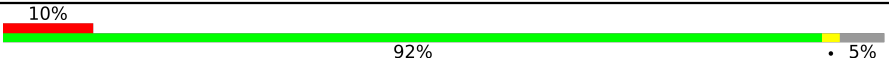
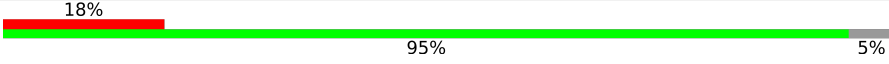
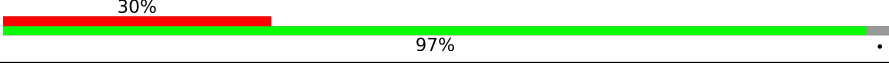
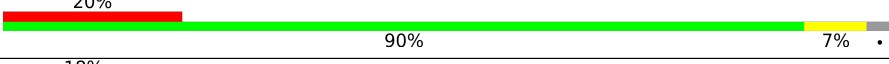
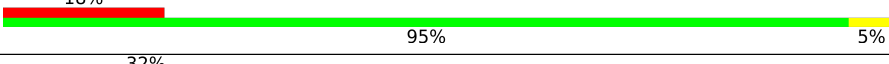
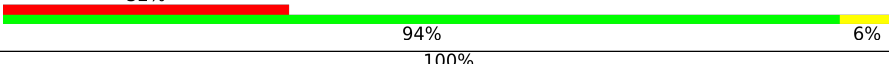

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16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

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Mol	Chain	Length	Quality of chain
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
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	403	X	-	-	-
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	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	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	403	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	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	c	503	X	-	-	-
23	CLA	c	504	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	515	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
26	SQD	f	101	-	-	-	X
30	UNL	A	414	-	-	-	X
32	HTG	b	622	-	-	-	X
33	LMT	C	526	-	-	-	X
33	LMT	F	101	-	-	-	X
33	LMT	a	418	-	-	-	X
33	LMT	e	101	-	-	-	X
34	LMG	C	522	-	-	-	X
34	LMG	c	522	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53612 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	18	0
			2773	1805	459	494	15			
1	a	334	Total	C	N	O	S	0	19	0
			2781	1811	460	495	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4050	2650	677	710	13			
2	b	504	Total	C	N	O	S	0	4	0
			3998	2622	665	698	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	5	0
			3522	2300	589	620	13			
3	c	455	Total	C	N	O	S	0	3	0
			3543	2316	592	622	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	4	0
			2764	1828	454	470	12			
4	d	341	Total	C	N	O	S	0	4	0
			2755	1823	453	467	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			668	435	108	125			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

- 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	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			517	345	85	85	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	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
			277	185	43	48	1			

- 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	36	Total	C	N	O	0	1	0
			304	203	48	53			
11	l	36	Total	C	N	O	0	1	0
			304	203	48	53			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	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	3	0
			1886	1177	318	386	5			
13	o	243	Total	C	N	O	S	0	2	0
			1879	1173	317	384	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	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	0	0
			765	486	128	151				
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	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

- 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	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

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

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

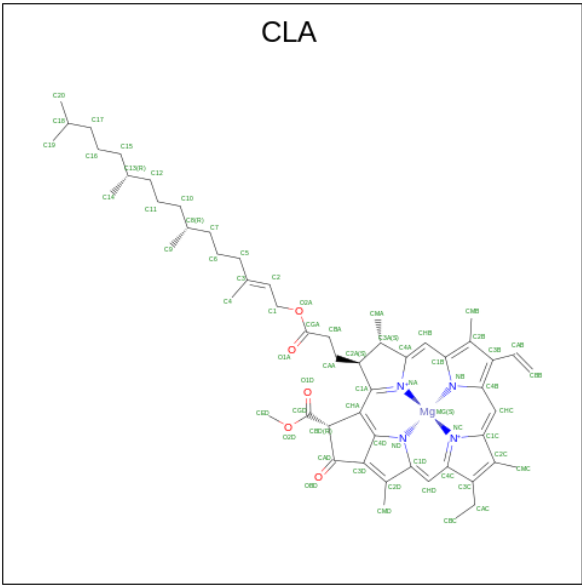
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	1	Total	Cl	0	0
			1	1		
22	C	1	Total	Cl	0	0
			1	1		

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

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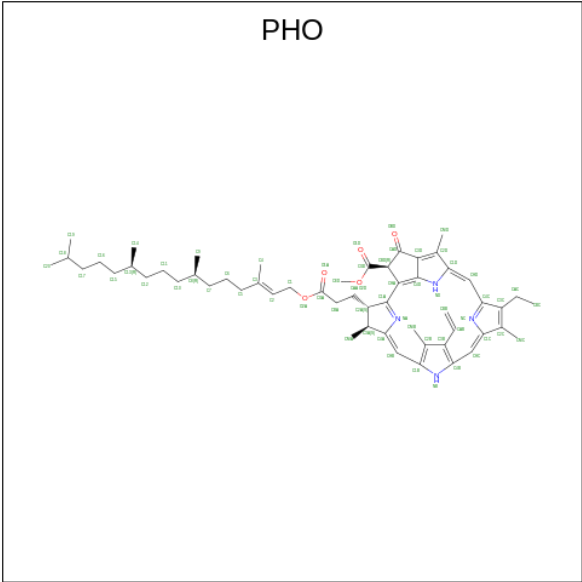
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N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

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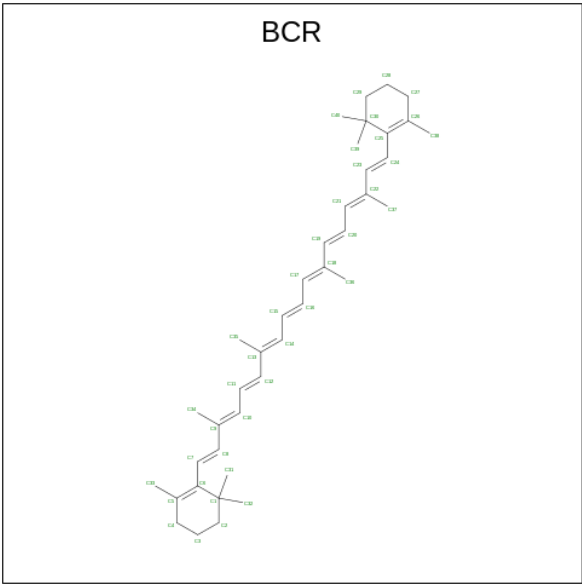
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



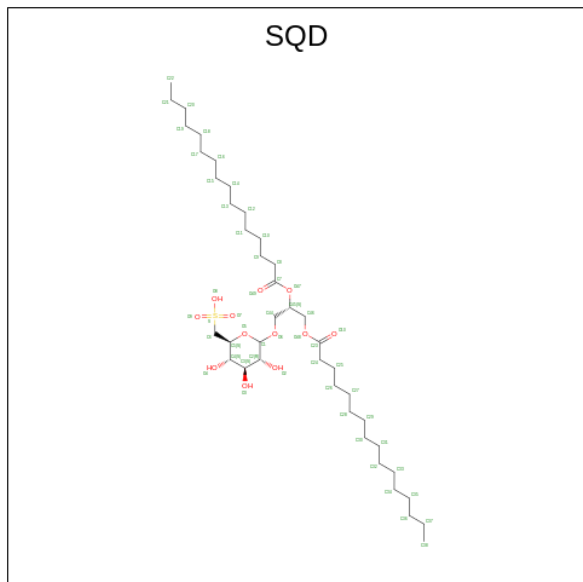
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



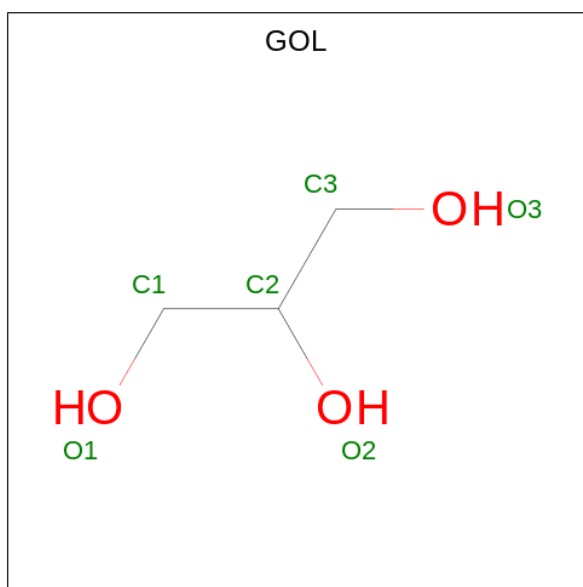
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



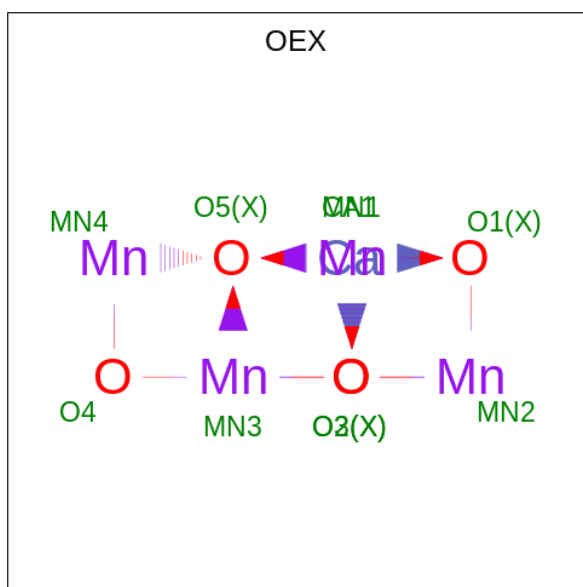
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0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

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



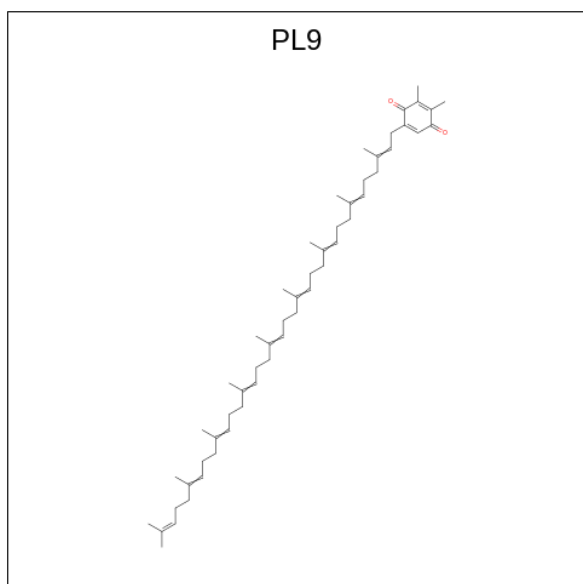
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	c	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	0
			6	3	3		

- 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 20	Ca 2	Mn 8	O 10	0	1
28	a	1	Total 20	Ca 2	Mn 8	O 10	0	1

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



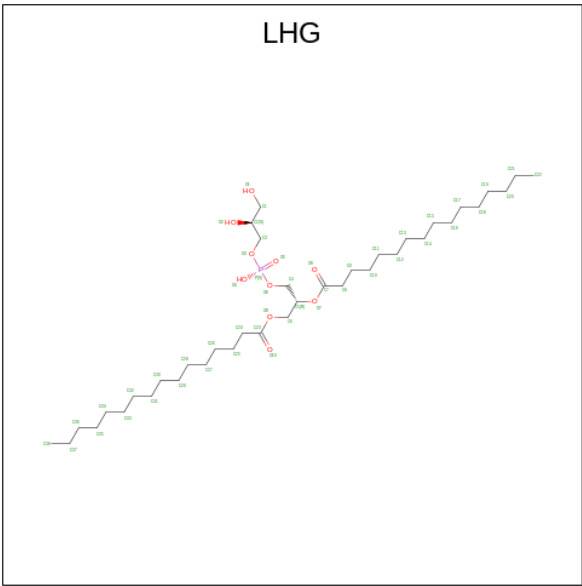
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	1
			110	106	4		
29	D	1	Total	C	O	0	0
			55	53	2		
29	a	1	Total	C	O	0	1
			110	106	4		
29	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

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

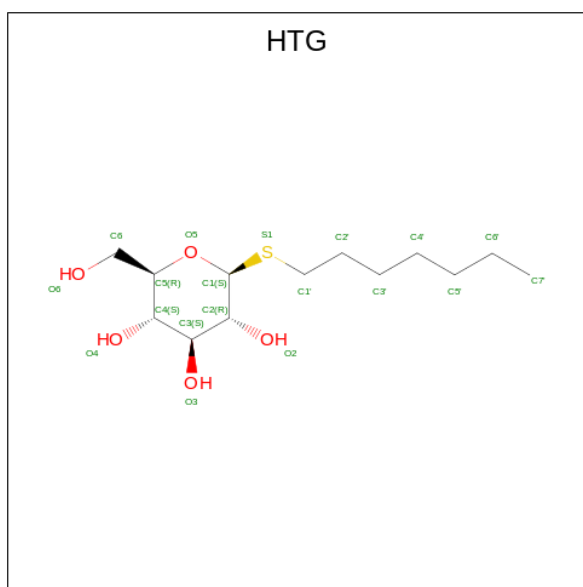
- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: C₃₈H₇₅O₁₀P).



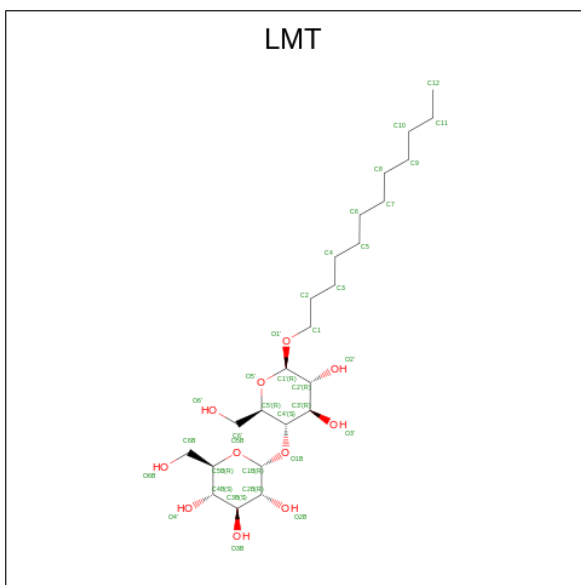
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	L	1	Total	C	O	P	0	0
			49	38	10	1		
31	a	1	Total	C	O	P	0	0
			42	31	10	1		
31	b	1	Total	C	O	P	0	0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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



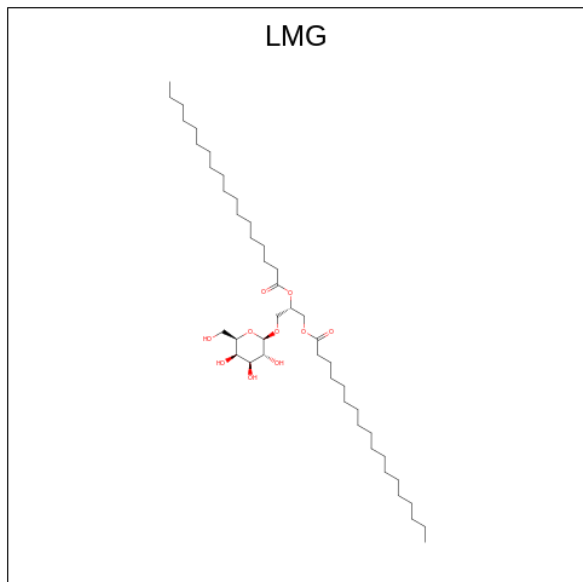
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			16	10	5	1		
32	V	1	Total	C	O		0	0
			11	6	5			
32	b	1	Total	C	O	S	0	0
			19	13	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		
32	c	1	Total	C	O	S	0	0
			19	13	5	1		
32	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



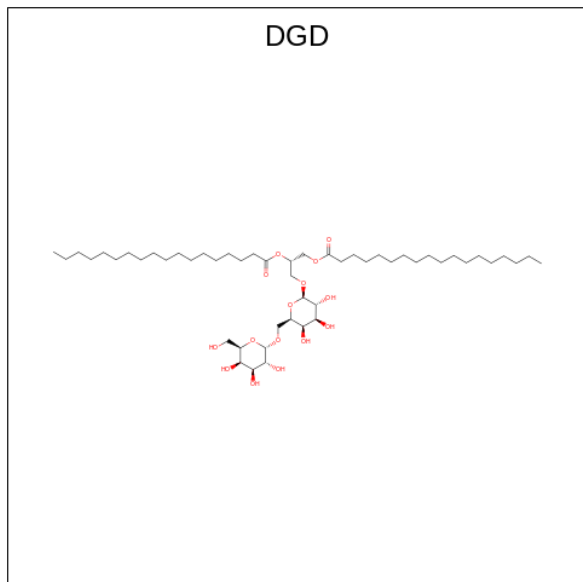
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total 35	C 24	O 11	0	0
33	B	1	Total 25	C 19	O 6	0	0
33	B	1	Total 26	C 19	O 7	0	0
33	C	1	Total 35	C 24	O 11	0	0
33	D	1	Total 35	C 24	O 11	0	0
33	F	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	M	1	Total 35	C 24	O 11	0	0
33	a	1	Total 35	C 24	O 11	0	0
33	a	1	Total 35	C 24	O 11	0	0
33	b	1	Total 25	C 19	O 6	0	0
33	b	1	Total 25	C 19	O 6	0	0
33	e	1	Total 35	C 24	O 11	0	0
33	m	1	Total 35	C 24	O 11	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 36 is CALCIUM ION (three-letter code: CA) (formula: Ca).

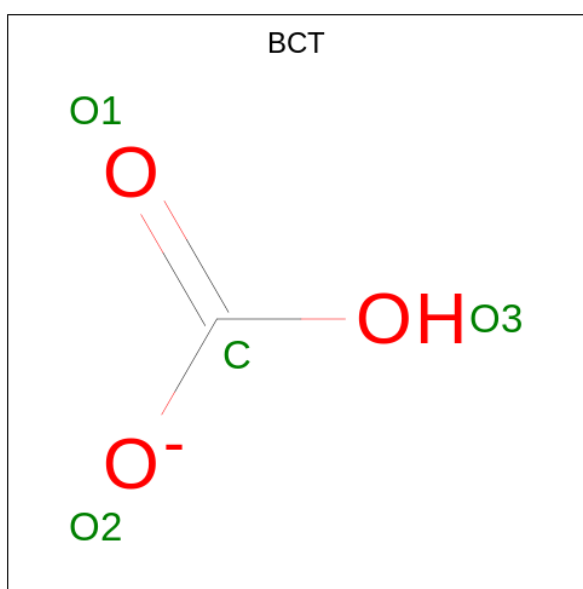
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	C	1	Total	Ca	0	0
			1	1		
36	F	1	Total	Ca	0	0
			1	1		

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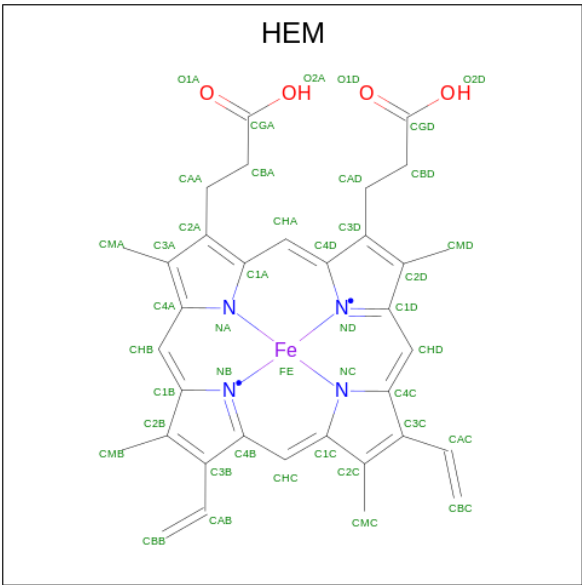
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Ca	0	0
			1	1		
36	a	1	Total	Ca	0	0
			1	1		
36	c	2	Total	Ca	0	0
			2	2		
36	o	1	Total	Ca	0	0
			1	1		

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).

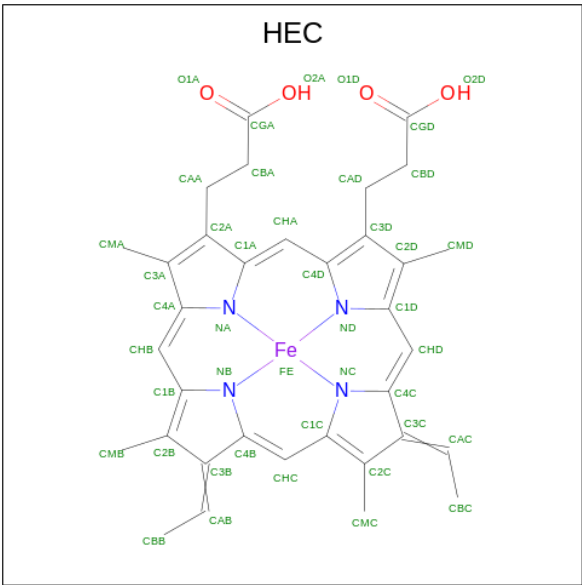


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	147	Total	O	0	11
			157	157		
41	B	218	Total	O	0	0
			218	218		
41	C	188	Total	O	0	4
			191	191		
41	D	124	Total	O	0	2
			126	126		
41	E	24	Total	O	0	0
			24	24		
41	F	8	Total	O	0	0
			8	8		
41	H	28	Total	O	0	0
			28	28		
41	I	4	Total	O	0	0
			4	4		
41	J	6	Total	O	0	0
			6	6		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	8	Total O 8 8	0	0
41	M	18	Total O 18 18	0	0
41	O	118	Total O 118 118	0	0
41	T	14	Total O 14 14	0	0
41	U	56	Total O 56 56	0	0
41	V	95	Total O 95 95	0	0
41	X	10	Total O 10 10	0	0
41	Y	1	Total O 1 1	0	0
41	R	1	Total O 1 1	0	0
41	a	139	Total O 150 150	0	12
41	b	220	Total O 220 220	0	0
41	c	169	Total O 172 172	0	4
41	d	129	Total O 129 129	0	0
41	e	15	Total O 15 15	0	0
41	f	5	Total O 5 5	0	0
41	h	22	Total O 22 22	0	0
41	i	1	Total O 1 1	0	0
41	j	4	Total O 4 4	0	0
41	k	5	Total O 5 5	0	0
41	l	8	Total O 8 8	0	0
41	m	10	Total O 10 10	0	0

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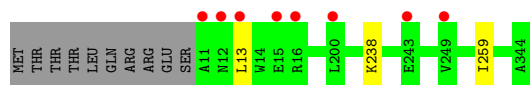
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	o	99	Total 99	O 99	0	0
41	t	10	Total 10	O 10	0	0
41	u	68	Total 68	O 68	0	0
41	v	57	Total 57	O 57	0	0
41	x	10	Total 10	O 10	0	0
41	y	4	Total 4	O 4	0	0

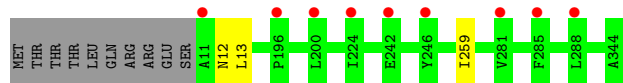
3 Residue-property plots [i](#)

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

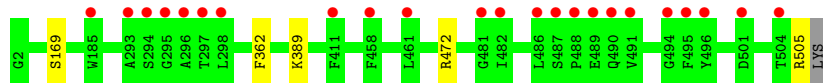
- Molecule 1: Photosystem II protein D1



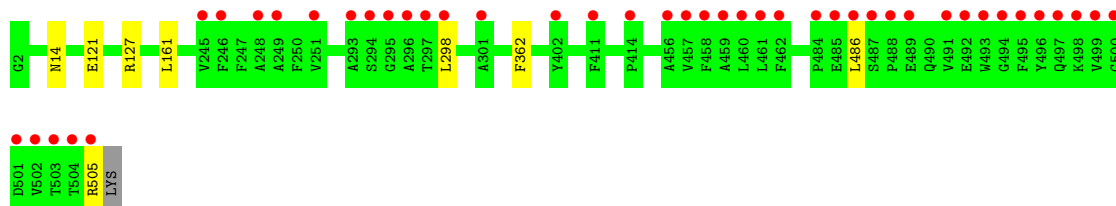
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

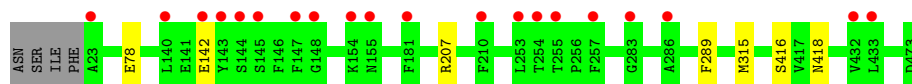


- Molecule 2: Photosystem II CP47 reaction center protein

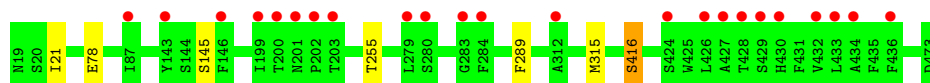


- Molecule 3: Photosystem II CP43 reaction center protein

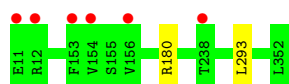




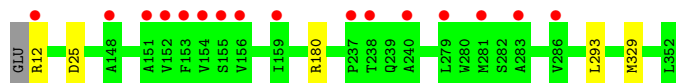
- Molecule 3: Photosystem II CP43 reaction center protein



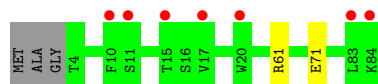
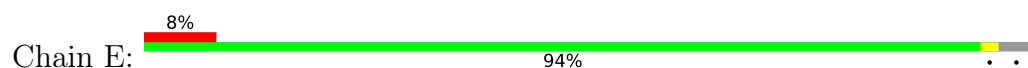
- Molecule 4: Photosystem II D2 protein



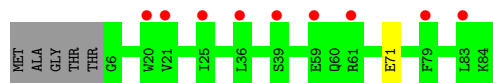
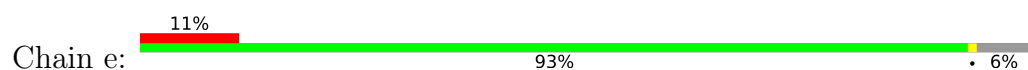
- Molecule 4: Photosystem II D2 protein



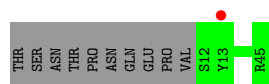
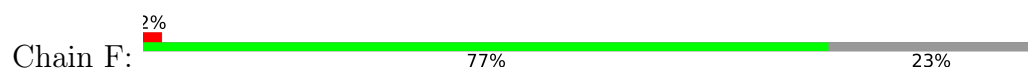
- Molecule 5: Cytochrome b559 subunit alpha



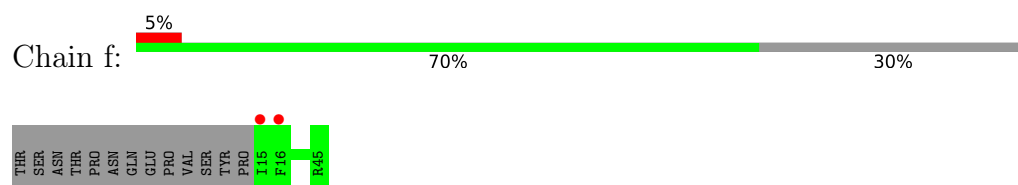
- Molecule 5: Cytochrome b559 subunit alpha



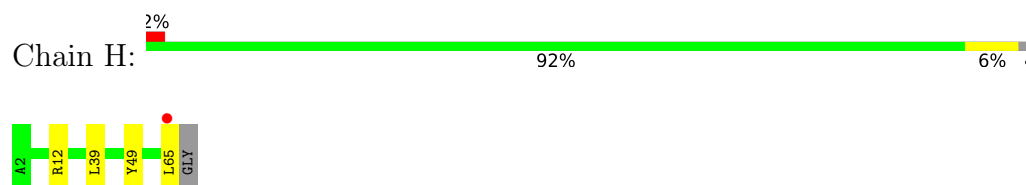
- Molecule 6: Cytochrome b559 subunit beta



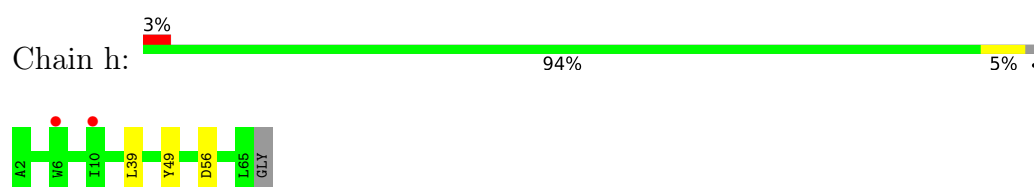
- Molecule 6: Cytochrome b559 subunit beta



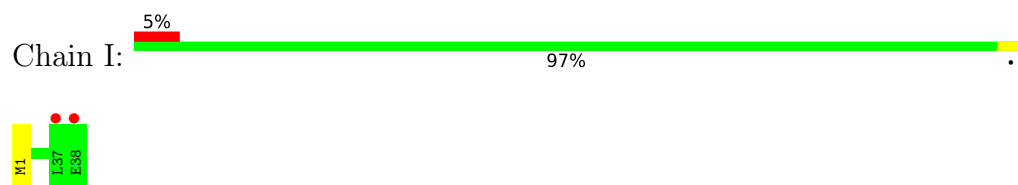
- Molecule 7: Photosystem II reaction center protein H



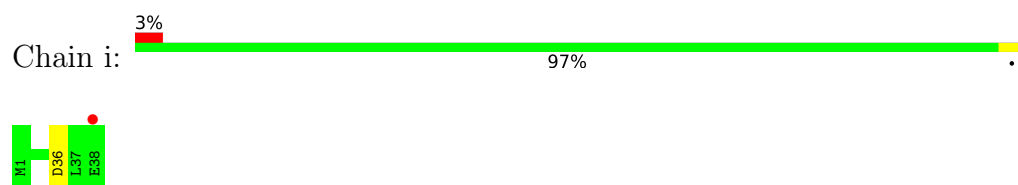
- Molecule 7: Photosystem II reaction center protein H



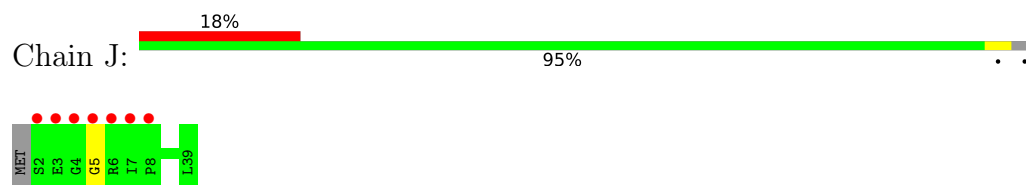
- Molecule 8: Photosystem II reaction center protein I



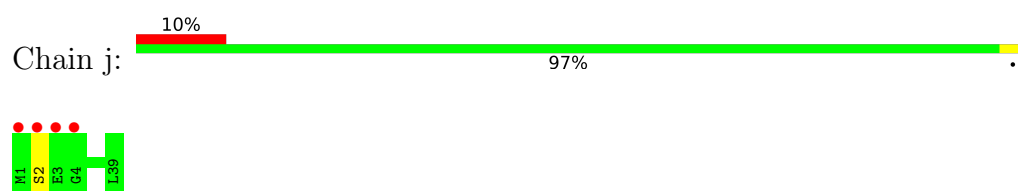
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

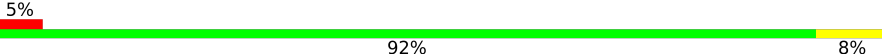


- Molecule 10: Photosystem II reaction center protein K

Chain K:  92% 8%



- Molecule 10: Photosystem II reaction center protein K

Chain k:  5% 92% 8%



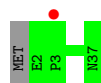
- Molecule 11: Photosystem II reaction center protein L

Chain L:  97% .



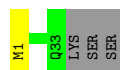
- Molecule 11: Photosystem II reaction center protein L

Chain l:  3% 97% .




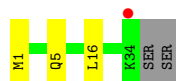
- Molecule 12: Photosystem II reaction center protein M

Chain M:  89% . 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  3% 86% 8% 6%

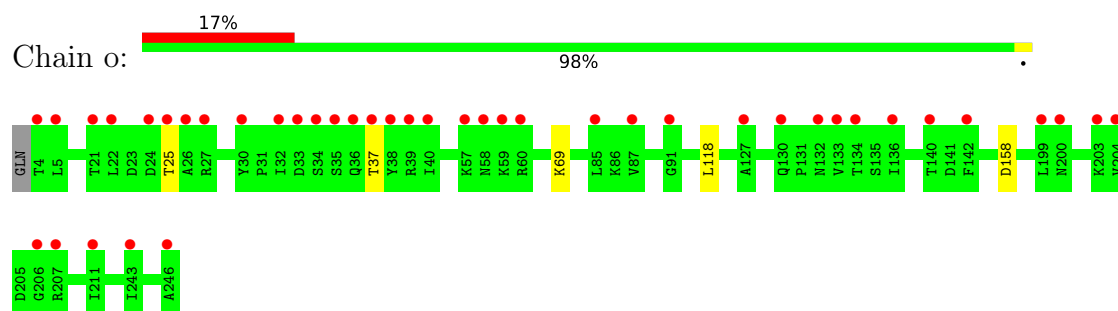


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

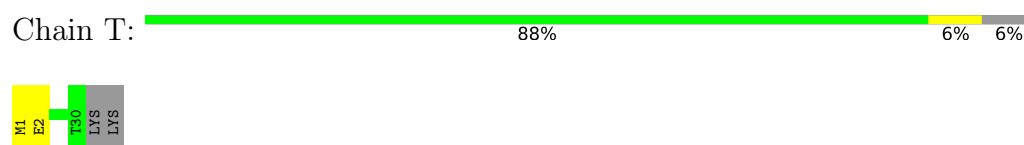
Chain O:  9% 98% .



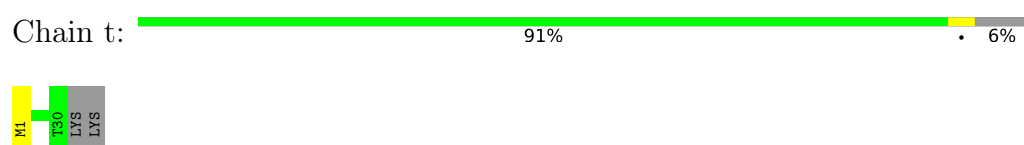
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



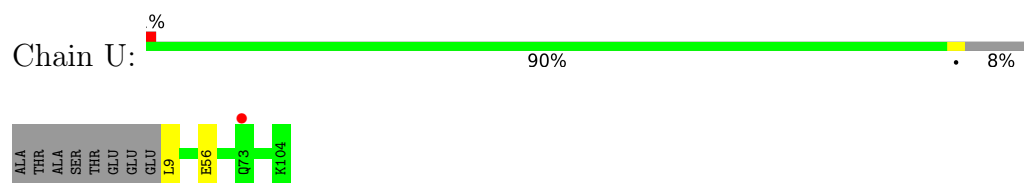
- Molecule 14: Photosystem II reaction center protein T



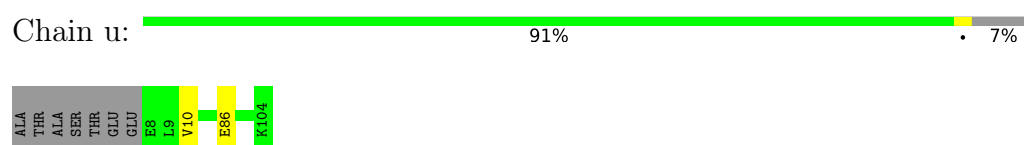
- Molecule 14: Photosystem II reaction center protein T



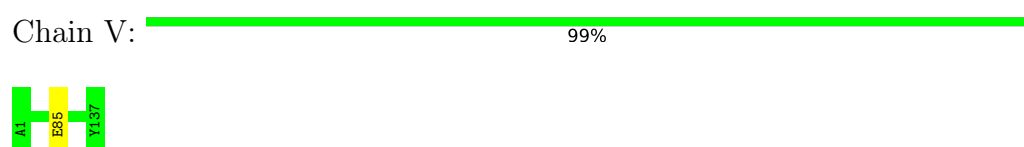
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

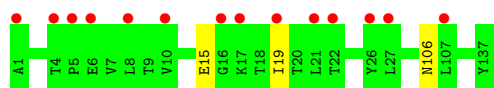


- Molecule 16: Cytochrome c-550

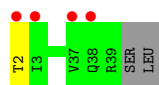
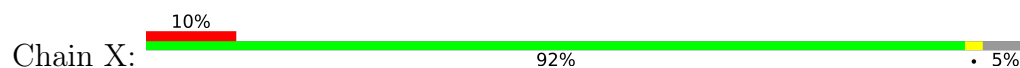


- Molecule 16: Cytochrome c-550

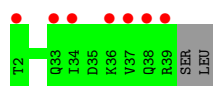




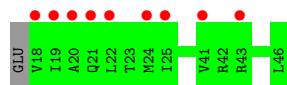
- Molecule 17: Photosystem II reaction center protein X



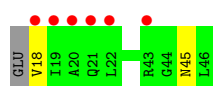
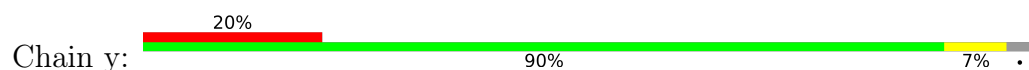
- Molecule 17: Photosystem II reaction center protein X



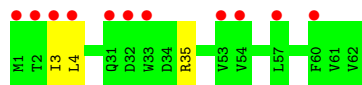
- Molecule 18: Photosystem II reaction center protein Ycf12



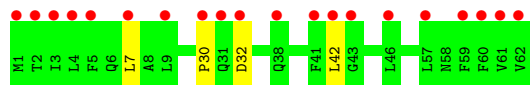
- Molecule 18: Photosystem II reaction center protein Ycf12



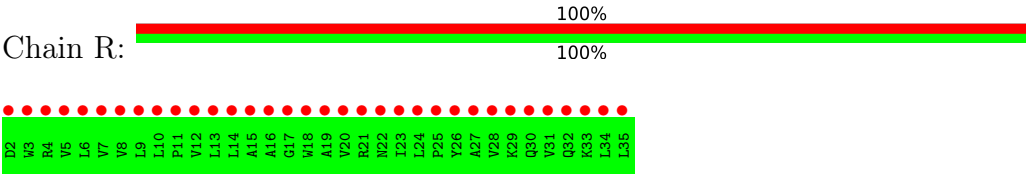
- Molecule 19: Photosystem II reaction center protein Z



- 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	125.75Å 231.63Å 288.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.90 – 2.40 52.70 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.90-2.40) 82.1 (52.70-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.168 , 0.218 0.169 , 0.219	Depositor DCC
R_{free} test set	16450 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53612	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% 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: PL9, CL, CLA, SQD, MG, FME, BCR, HTG, LMG, UNL, LMT, GOL, DGD, FE2, LHG, CA, HEM, BCT, OEX, HEC, PHO

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	0/2861	0.56	0/3897
1	a	0.40	0/2869	0.54	0/3908
2	B	0.41	0/4190	0.55	0/5708
2	b	0.40	0/4138	0.53	0/5640
3	C	0.39	0/3635	0.51	0/4948
3	c	0.36	0/3657	0.49	0/4978
4	D	0.43	0/2861	0.55	0/3897
4	d	0.41	0/2852	0.54	0/3885
5	E	0.34	0/687	0.50	0/936
5	e	0.36	0/667	0.47	0/908
6	F	0.38	0/284	0.48	0/387
6	f	0.32	0/257	0.47	0/349
7	H	0.35	0/530	0.56	0/723
7	h	0.34	0/519	0.55	0/708
8	I	0.35	0/311	0.50	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.33	0/278	0.51	0/376
9	j	0.32	0/283	0.52	0/383
10	K	0.35	0/303	0.51	0/416
10	k	0.35	0/303	0.50	0/416
11	L	0.44	0/311	0.51	0/423
11	l	0.42	0/311	0.51	0/423
12	M	0.45	0/261	0.54	0/357
12	m	0.39	0/262	0.51	0/357
13	O	0.40	0/1917	0.58	0/2599
13	o	0.37	0/1910	0.59	1/2589 (0.0%)
14	T	0.46	0/257	0.50	0/349
14	t	0.45	0/257	0.44	0/349
15	U	0.38	0/776	0.55	0/1052
15	u	0.36	0/785	0.58	0/1064
16	V	0.37	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.34	0/1085	0.52	0/1473
17	X	0.31	0/284	0.48	0/384
17	x	0.30	0/284	0.45	0/384
18	Y	0.29	0/216	0.45	0/289
18	y	0.30	0/216	0.44	0/289
19	Z	0.31	0/490	0.40	0/669
19	z	0.31	0/490	0.41	0/669
20	R	0.28	0/279	0.46	0/383
All	All	0.39	0/43272	0.53	1/58876 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.20	122.98	118.30

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	349/344 (102%)	345 (99%)	3 (1%)	1 (0%)	41	55
1	a	350/344 (102%)	345 (99%)	4 (1%)	1 (0%)	41	55
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	496 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	454/455 (100%)	447 (98%)	5 (1%)	2 (0%)	34	48
3	c	456/455 (100%)	445 (98%)	10 (2%)	1 (0%)	47	62
4	D	344/342 (101%)	334 (97%)	10 (3%)	0	100	100
4	d	343/342 (100%)	331 (96%)	12 (4%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
7	h	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	32 (89%)	3 (8%)	1 (3%)	5	4
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	244/244 (100%)	236 (97%)	7 (3%)	1 (0%)	34	48
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
19	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	9	11
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	5286/5384 (98%)	5165 (98%)	113 (2%)	8 (0%)	51	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416	SER
13	O	61	GLN
19	z	30	PRO
9	J	5	GLY
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	286/279 (102%)	284 (99%)	2 (1%)	84	92
1	a	287/279 (103%)	285 (99%)	2 (1%)	84	92
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	85
2	b	406/403 (101%)	398 (98%)	8 (2%)	55	74
3	C	357/356 (100%)	351 (98%)	6 (2%)	60	78
3	c	359/356 (101%)	352 (98%)	7 (2%)	57	75
4	D	281/277 (101%)	279 (99%)	2 (1%)	84	92
4	d	280/277 (101%)	275 (98%)	5 (2%)	59	76
5	E	73/73 (100%)	71 (97%)	2 (3%)	44	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	70/73 (96%)	69 (99%)	1 (1%)	67	82
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	50 (91%)	5 (9%)	9	14
7	h	54/54 (100%)	51 (94%)	3 (6%)	21	34
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	62
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	33	51
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	11
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	11
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	28 (93%)	2 (7%)	16	26
13	O	209/207 (101%)	205 (98%)	4 (2%)	57	75
13	o	208/207 (100%)	204 (98%)	4 (2%)	57	75
14	T	26/28 (93%)	25 (96%)	1 (4%)	33	51
14	t	26/28 (93%)	26 (100%)	0	100	100
15	U	83/89 (93%)	81 (98%)	2 (2%)	49	68
15	u	84/89 (94%)	82 (98%)	2 (2%)	49	68
16	V	117/117 (100%)	116 (99%)	1 (1%)	78	90
16	v	117/117 (100%)	114 (97%)	3 (3%)	46	66
17	X	31/33 (94%)	30 (97%)	1 (3%)	39	59
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	20 (91%)	2 (9%)	9	14
19	Z	52/52 (100%)	49 (94%)	3 (6%)	20	32
19	z	52/52 (100%)	49 (94%)	3 (6%)	20	32
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4392/4403 (100%)	4308 (98%)	84 (2%)	57	75

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	238	LYS
2	B	169	SER
2	B	362	PHE
2	B	389	LYS
2	B	472	ARG
2	B	505	ARG
3	C	78	GLU
3	C	142	GLU
3	C	207	ARG
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	180	ARG
4	D	293	LEU
5	E	61	ARG
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	39	LEU
7	H	49	TYR
7	H	65	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
13	O	4	THR
13	O	60	ARG
13	O	118	LEU
13	O	181	GLU
14	T	2	GLU
15	U	9	LEU
15	U	56	GLU
16	V	85	GLU
17	X	2	THR
19	Z	3	ILE
19	Z	4	LEU
19	Z	35	ARG
1	a	12	ASN
1	a	13	LEU
2	b	14	ASN
2	b	121	GLU
2	b	127	ARG

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Mol	Chain	Res	Type
2	b	161	LEU
2	b	298	LEU
2	b	362	PHE
2	b	486	LEU
2	b	505	ARG
3	c	21	ILE
3	c	78	GLU
3	c	145	SER
3	c	255	THR
3	c	289	PHE
3	c	315	MET
3	c	416	SER
4	d	12	ARG
4	d	25	ASP
4	d	180	ARG
4	d	293	LEU
4	d	329	MET
5	e	71	GLU
7	h	39	LEU
7	h	49	TYR
7	h	56	ASP
8	i	36	ASP
9	j	2	SER
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
12	m	16	LEU
13	o	25	THR
13	o	37	THR
13	o	69	LYS
13	o	118	LEU
15	u	10	VAL
15	u	86	GLU
16	v	15	GLU
16	v	19	ILE
16	v	106	ASN
18	y	18	VAL
18	y	45	ASN
19	z	7	LEU
19	z	32	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
13	O	80	GLN
13	o	88	ASN
13	o	196	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.61	0	7,9,11	1.18	1 (14%)
8	FME	I	1	8	8,9,10	0.63	0	7,9,11	1.14	1 (14%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.21	1 (14%)
14	FME	t	1	14	8,9,10	0.61	0	7,9,11	1.50	2 (28%)
8	FME	i	1	8	8,9,10	0.59	0	7,9,11	0.93	0
12	FME	M	1	12	8,9,10	0.59	0	7,9,11	1.55	2 (28%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	1	FME	O-C-CA	-2.72	117.65	124.78
12	M	1	FME	CA-N-CN	-2.68	118.70	122.82
14	t	1	FME	O-C-CA	-2.56	118.08	124.78
14	t	1	FME	CA-N-CN	-2.42	119.10	122.82
12	M	1	FME	O-C-CA	-2.21	118.99	124.78
8	I	1	FME	O-C-CA	-2.10	119.28	124.78
12	m	1	FME	O-C-CA	-2.09	119.31	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
12	M	1	FME	CB-CA-N-CN
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 224 ligands modelled in this entry, 17 are monoatomic and 18 are unknown - leaving 189 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	$\# Z > 2$
23	CLA	B	601	41	59,73,73	2.08	14 (23%)	67,113,113	2.10	21 (31%)
31	LHG	D	408	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
24	PHO	a	406	-	67,69,69	2.13	16 (23%)	85,99,99	1.91	23 (27%)
29	PL9	A	413[B]	-	55,55,55	0.63	2 (3%)	68,69,69	2.02	23 (33%)
23	CLA	a	407	-	59,73,73	1.96	14 (23%)	67,113,113	2.29	24 (35%)
25	BCR	b	619	-	41,41,41	1.17	2 (4%)	56,56,56	1.65	13 (23%)
23	CLA	B	607	41	59,73,73	1.98	13 (22%)	67,113,113	2.20	21 (31%)
26	SQD	B	620	-	53,54,54	1.01	3 (5%)	62,65,65	1.51	9 (14%)
34	LMG	Z	101	-	37,37,55	1.01	3 (8%)	45,45,63	1.49	6 (13%)
35	DGD	c	518	-	63,63,67	0.90	2 (3%)	77,77,81	1.09	5 (6%)
25	BCR	C	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.59	11 (19%)
27	GOL	A	410	-	5,5,5	1.09	0	5,5,5	0.90	0
25	BCR	k	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.59	13 (23%)
23	CLA	C	514	-	59,73,73	2.07	13 (22%)	67,113,113	2.24	22 (32%)
34	LMG	d	411	39	51,51,55	0.91	2 (3%)	59,59,63	0.92	1 (1%)
23	CLA	b	606	-	59,73,73	1.92	12 (20%)	67,113,113	2.28	23 (34%)
25	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.66	11 (19%)
26	SQD	A	411	-	53,54,54	1.05	3 (5%)	62,65,65	1.28	8 (12%)
33	LMT	b	620	-	25,25,36	0.51	0	30,30,47	0.61	0
32	HTG	b	621	-	19,19,19	1.01	2 (10%)	23,24,24	1.35	4 (17%)
23	CLA	b	603	-	59,73,73	2.08	13 (22%)	67,113,113	2.27	21 (31%)
27	GOL	v	201	-	5,5,5	1.19	0	5,5,5	0.85	0
24	PHO	A	406	-	67,69,69	2.13	16 (23%)	85,99,99	1.90	23 (27%)
33	LMT	B	630	-	26,26,36	0.51	0	31,31,47	1.00	1 (3%)
34	LMG	D	412	39	51,51,55	0.87	3 (5%)	59,59,63	1.08	5 (8%)
23	CLA	C	509	41	59,73,73	2.01	13 (22%)	67,113,113	2.17	20 (29%)
25	BCR	d	404	-	41,41,41	1.19	2 (4%)	56,56,56	1.81	14 (25%)
27	GOL	a	410	-	5,5,5	0.89	0	5,5,5	1.04	0
32	HTG	c	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.33	1 (4%)
34	LMG	C	502	-	51,51,55	0.93	2 (3%)	59,59,63	1.02	2 (3%)
23	CLA	C	512	-	59,73,73	1.99	14 (23%)	67,113,113	2.21	21 (31%)
23	CLA	b	608	-	59,73,73	2.02	13 (22%)	67,113,113	2.21	26 (38%)
23	CLA	B	611	-	59,73,73	2.02	14 (23%)	67,113,113	2.31	23 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	613	-	59,73,73	2.02	12 (20%)	67,113,113	2.26	24 (35%)
31	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.05	2 (4%)
23	CLA	c	503	-	59,73,73	1.98	14 (23%)	67,113,113	2.16	24 (35%)
27	GOL	C	524	-	5,5,5	1.10	0	5,5,5	1.09	0
23	CLA	b	610	41	59,73,73	1.95	14 (23%)	67,113,113	2.33	25 (37%)
31	LHG	d	406	-	48,48,48	0.90	2 (4%)	51,54,54	1.12	5 (9%)
23	CLA	c	512	-	59,73,73	1.95	13 (22%)	67,113,113	2.22	24 (35%)
33	LMT	M	103	-	36,36,36	0.52	0	47,47,47	1.07	3 (6%)
33	LMT	M	102	-	36,36,36	0.43	0	47,47,47	0.93	2 (4%)
26	SQD	a	411	-	53,54,54	1.04	3 (5%)	62,65,65	1.25	7 (11%)
23	CLA	C	511	-	59,73,73	2.08	14 (23%)	67,113,113	2.20	21 (31%)
23	CLA	C	505	-	59,73,73	2.00	13 (22%)	67,113,113	2.20	20 (29%)
25	BCR	B	618	-	41,41,41	0.92	1 (2%)	56,56,56	1.59	12 (21%)
27	GOL	b	623	-	5,5,5	0.95	0	5,5,5	1.10	0
27	GOL	B	628	-	5,5,5	1.05	0	5,5,5	0.91	0
23	CLA	B	602	-	59,73,73	2.01	13 (22%)	67,113,113	2.34	24 (35%)
25	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	8 (14%)
25	BCR	A	408	-	41,41,41	1.10	1 (2%)	56,56,56	1.38	6 (10%)
28	OEX	A	412[A]	3,1,41	0,15,15	0.00	-	-	-	-
33	LMT	D	402	-	36,36,36	0.55	1 (2%)	47,47,47	0.77	0
23	CLA	c	513	3	59,73,73	1.97	13 (22%)	67,113,113	2.21	25 (37%)
23	CLA	a	405	41	59,73,73	1.96	12 (20%)	67,113,113	2.18	23 (34%)
37	BCT	D	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
25	BCR	h	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	9 (16%)
23	CLA	b	612	-	59,73,73	2.04	13 (22%)	67,113,113	2.35	23 (34%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	4 (6%)
33	LMT	a	412	-	36,36,36	0.64	1 (2%)	47,47,47	1.29	5 (10%)
27	GOL	b	627	-	5,5,5	0.98	0	5,5,5	1.02	0
27	GOL	c	527	-	5,5,5	0.81	0	5,5,5	1.07	0
34	LMG	M	101	-	51,51,55	1.03	2 (3%)	59,59,63	1.07	3 (5%)
29	PL9	a	414[B]	-	55,55,55	0.67	2 (3%)	68,69,69	1.94	19 (27%)
23	CLA	B	608	-	59,73,73	1.98	13 (22%)	67,113,113	2.21	25 (37%)
37	BCT	d	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	C	508	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	24 (35%)
23	CLA	C	504	-	59,73,73	2.03	12 (20%)	67,113,113	2.10	20 (29%)
26	SQD	a	409	-	53,54,54	1.00	3 (5%)	62,65,65	1.68	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	OEX	a	413[A]	3,1,41	0,15,15	0.00	-	-		
25	BCR	b	617	-	41,41,41	1.11	1 (2%)	56,56,56	1.48	8 (14%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.47	11 (19%)
23	CLA	A	407	-	59,73,73	2.00	13 (22%)	67,113,113	2.20	24 (35%)
23	CLA	c	509	41	59,73,73	2.02	13 (22%)	67,113,113	2.17	20 (29%)
23	CLA	A	404	41	59,73,73	1.95	14 (23%)	67,113,113	2.20	25 (37%)
23	CLA	c	511	-	59,73,73	2.12	14 (23%)	67,113,113	2.26	23 (34%)
23	CLA	D	404	-	59,73,73	2.01	12 (20%)	67,113,113	2.18	23 (34%)
32	HTG	D	411	-	16,16,19	1.05	2 (12%)	20,21,24	1.41	1 (5%)
34	LMG	c	522	-	51,51,55	0.97	2 (3%)	59,59,63	1.20	6 (10%)
35	DGD	h	103	-	63,63,67	0.91	3 (4%)	77,77,81	1.06	4 (5%)
33	LMT	e	101	-	36,36,36	0.52	1 (2%)	47,47,47	0.92	3 (6%)
27	GOL	B	623	-	5,5,5	0.87	0	5,5,5	1.04	0
23	CLA	b	601	41	59,73,73	2.07	13 (22%)	67,113,113	2.23	22 (32%)
23	CLA	c	506	41	59,73,73	2.13	14 (23%)	67,113,113	2.20	24 (35%)
23	CLA	b	611	-	59,73,73	1.94	13 (22%)	67,113,113	2.21	20 (29%)
34	LMG	c	521	-	51,51,55	0.92	2 (3%)	59,59,63	1.06	5 (8%)
24	PHO	A	415	-	67,69,69	2.10	17 (25%)	85,99,99	2.04	20 (23%)
23	CLA	b	605	-	59,73,73	1.98	14 (23%)	67,113,113	2.25	22 (32%)
23	CLA	b	604	-	59,73,73	1.97	13 (22%)	67,113,113	2.21	21 (31%)
33	LMT	m	103	-	36,36,36	0.46	0	47,47,47	1.06	3 (6%)
38	HEM	E	102	5,6	27,50,50	0.85	1 (3%)	17,82,82	2.14	4 (23%)
23	CLA	A	405	41	59,73,73	1.99	11 (18%)	67,113,113	2.10	18 (26%)
34	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.20	7 (11%)
35	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.13	5 (6%)
33	LMT	F	101	-	36,36,36	0.55	1 (2%)	47,47,47	1.18	5 (10%)
23	CLA	c	510	-	59,73,73	2.11	14 (23%)	67,113,113	2.39	22 (32%)
26	SQD	L	102	-	53,54,54	1.03	3 (5%)	62,65,65	1.64	9 (14%)
40	HEC	v	202	16	26,50,50	2.24	3 (11%)	18,82,82	2.03	5 (27%)
26	SQD	A	409	-	53,54,54	0.96	3 (5%)	62,65,65	2.05	11 (17%)
23	CLA	B	605	-	59,73,73	2.00	12 (20%)	67,113,113	2.29	21 (31%)
23	CLA	C	510	-	59,73,73	2.09	14 (23%)	67,113,113	2.32	21 (31%)
23	CLA	c	514	-	59,73,73	2.01	13 (22%)	67,113,113	2.23	24 (35%)
23	CLA	c	504	-	59,73,73	2.01	13 (22%)	67,113,113	2.09	21 (31%)
33	LMT	B	629	-	25,25,36	0.42	0	30,30,47	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMT	B	627	-	36,36,36	0.43	0	47,47,47	1.14	4 (8%)
24	PHO	a	416	-	67,69,69	2.14	19 (28%)	85,99,99	2.10	23 (27%)
29	PL9	D	406	-	55,55,55	0.68	2 (3%)	68,69,69	1.67	20 (29%)
32	HTG	b	624	-	19,19,19	1.03	2 (10%)	23,24,24	1.40	4 (17%)
31	LHG	L	101	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	5 (9%)
23	CLA	C	503	-	59,73,73	1.95	13 (22%)	67,113,113	2.25	23 (34%)
25	BCR	c	517	-	41,41,41	1.07	1 (2%)	56,56,56	1.60	12 (21%)
27	GOL	c	502	-	5,5,5	1.05	0	5,5,5	0.91	0
25	BCR	D	405	-	41,41,41	1.01	1 (2%)	56,56,56	1.78	17 (30%)
23	CLA	B	610	41	59,73,73	2.03	13 (22%)	67,113,113	2.24	23 (34%)
29	PL9	A	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
33	LMT	b	626	-	25,25,36	0.56	1 (4%)	30,30,47	1.12	3 (10%)
35	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	1.01	4 (5%)
23	CLA	B	614	-	59,73,73	1.94	13 (22%)	67,113,113	2.33	25 (37%)
23	CLA	B	616	-	59,73,73	1.96	13 (22%)	67,113,113	2.21	20 (29%)
23	CLA	b	602	-	59,73,73	2.05	13 (22%)	67,113,113	2.35	25 (37%)
28	OEX	A	412[B]	3,1,41	0,15,15	0.00	-	-		
32	HTG	h	101	-	16,16,19	1.16	2 (12%)	20,21,24	2.03	7 (35%)
25	BCR	a	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.48	9 (16%)
23	CLA	c	515	-	59,73,73	2.03	13 (22%)	67,113,113	2.16	23 (34%)
26	SQD	D	413	-	42,43,54	1.15	3 (7%)	51,54,65	1.87	11 (21%)
33	LMT	C	526	-	36,36,36	0.52	1 (2%)	47,47,47	1.12	3 (6%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.74	16 (28%)
37	BCT	D	401[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
34	LMG	C	522	-	51,51,55	1.04	3 (5%)	59,59,63	1.38	7 (11%)
34	LMG	C	521	-	51,51,55	0.98	2 (3%)	59,59,63	1.02	3 (5%)
35	DGD	c	520	-	63,63,67	0.87	2 (3%)	77,77,81	1.05	7 (9%)
23	CLA	b	607	41	59,73,73	1.96	15 (25%)	67,113,113	2.20	20 (29%)
40	HEC	V	201	16	26,50,50	2.17	4 (15%)	18,82,82	2.28	7 (38%)
23	CLA	B	606	-	59,73,73	1.96	13 (22%)	67,113,113	2.30	23 (34%)
23	CLA	C	513	3	59,73,73	2.06	14 (23%)	67,113,113	2.11	22 (32%)
23	CLA	b	609	-	59,73,73	2.02	13 (22%)	67,113,113	2.20	23 (34%)
23	CLA	c	507	-	59,73,73	2.03	13 (22%)	67,113,113	2.19	18 (26%)
28	OEX	a	413[B]	3,1,41	0,15,15	0.00	-	-		
32	HTG	b	622	-	19,19,19	1.02	1 (5%)	23,24,24	1.62	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	HTG	B	624	-	19,19,19	1.12	2 (10%)	23,24,24	1.41	3 (13%)
23	CLA	c	508	-	59,73,73	2.02	14 (23%)	67,113,113	2.21	23 (34%)
23	CLA	b	615	-	59,73,73	1.97	12 (20%)	67,113,113	2.09	21 (31%)
33	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.97	2 (4%)
27	GOL	O	302	-	5,5,5	0.89	0	5,5,5	0.98	0
23	CLA	C	507	-	59,73,73	1.93	13 (22%)	67,113,113	2.16	21 (31%)
23	CLA	B	603	-	59,73,73	2.05	14 (23%)	67,113,113	2.28	22 (32%)
23	CLA	A	403	-	59,73,73	1.99	13 (22%)	67,113,113	2.23	27 (40%)
26	SQD	f	101	-	42,43,54	1.16	3 (7%)	51,54,65	1.28	6 (11%)
23	CLA	B	609	-	59,73,73	1.93	13 (22%)	67,113,113	2.10	18 (26%)
23	CLA	a	404	41	59,73,73	2.01	13 (22%)	67,113,113	2.26	26 (38%)
23	CLA	C	506	41	59,73,73	2.02	13 (22%)	67,113,113	2.24	28 (41%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.09	3 (6%)
23	CLA	b	614	-	59,73,73	1.98	14 (23%)	67,113,113	2.33	23 (34%)
23	CLA	b	616	-	59,73,73	1.94	13 (22%)	67,113,113	2.49	25 (37%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	8 (14%)
23	CLA	B	604	-	59,73,73	2.00	14 (23%)	67,113,113	2.34	21 (31%)
32	HTG	B	622	-	19,19,19	0.85	1 (5%)	23,24,24	1.39	1 (4%)
23	CLA	D	403	-	59,73,73	1.97	13 (22%)	67,113,113	2.26	22 (32%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	10 (17%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	1.16	4 (5%)
25	BCR	B	631	-	41,41,41	1.06	1 (2%)	56,56,56	1.44	11 (19%)
23	CLA	d	403	-	59,73,73	2.04	13 (22%)	67,113,113	2.21	22 (32%)
25	BCR	B	617	-	41,41,41	1.07	1 (2%)	56,56,56	1.15	5 (8%)
23	CLA	B	613	-	59,73,73	2.00	14 (23%)	67,113,113	2.17	21 (31%)
23	CLA	d	402	-	59,73,73	1.93	12 (20%)	67,113,113	2.29	27 (40%)
27	GOL	B	626	-	5,5,5	0.87	0	5,5,5	1.13	0
23	CLA	B	612	-	59,73,73	1.98	12 (20%)	67,113,113	2.41	22 (32%)
31	LHG	d	408	-	48,48,48	0.90	2 (4%)	51,54,54	1.10	5 (9%)
25	BCR	H	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	10 (17%)
31	LHG	D	407	-	48,48,48	0.89	3 (6%)	51,54,54	0.98	3 (5%)
29	PL9	a	414[A]	-	55,55,55	0.64	1 (1%)	68,69,69	2.01	21 (30%)
23	CLA	C	515	-	59,73,73	1.98	13 (22%)	67,113,113	2.19	21 (31%)
23	CLA	a	403	-	59,73,73	2.01	13 (22%)	67,113,113	2.36	27 (40%)
37	BCT	d	401[A]	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	505	-	59,73,73	1.91	13 (22%)	67,113,113	2.19	22 (32%)
31	LHG	d	407	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
31	LHG	b	628	-	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
32	HTG	B	621	-	19,19,19	0.98	1 (5%)	23,24,24	1.60	4 (17%)
23	CLA	B	615	-	59,73,73	1.97	12 (20%)	67,113,113	2.31	23 (34%)
29	PL9	d	405	-	55,55,55	0.70	2 (3%)	68,69,69	1.63	18 (26%)
38	HEM	e	102	5,6	27,50,50	0.92	1 (3%)	17,82,82	2.08	3 (17%)
35	DGD	H	102	-	63,63,67	0.84	3 (4%)	77,77,81	1.07	7 (9%)
35	DGD	C	520	-	63,63,67	0.84	2 (3%)	77,77,81	1.02	4 (5%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.34	8 (14%)
32	HTG	V	202	-	11,11,19	0.19	0	15,15,24	1.21	1 (6%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.85	15 (26%)
32	HTG	C	523	-	19,19,19	0.92	1 (5%)	23,24,24	1.47	2 (8%)
31	LHG	A	416	-	48,48,48	0.88	2 (4%)	51,54,54	1.22	5 (9%)
31	LHG	a	419	-	41,41,48	1.05	2 (4%)	44,47,54	0.96	2 (4%)

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
23	CLA	B	601	41	3/3/20/25	11/37/135/135	-
31	LHG	D	408	-	-	11/53/53/53	-
24	PHO	a	406	-	-	8/53/103/103	0/5/6/6
29	PL9	A	413[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	a	407	-	3/3/20/25	11/37/135/135	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	B	607	41	3/3/20/25	3/37/135/135	-
26	SQD	B	620	-	-	19/49/69/69	0/1/1/1
34	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
35	DGD	c	518	-	-	18/51/91/95	0/2/2/2
25	BCR	C	517	-	-	3/29/63/63	0/2/2/2
27	GOL	A	410	-	-	3/4/4/4	-
25	BCR	k	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	514	-	3/3/20/25	16/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	d	411	39	-	9/46/66/70	0/1/1/1
23	CLA	b	606	-	3/3/20/25	11/37/135/135	-
25	BCR	k	102	-	-	5/29/63/63	0/2/2/2
26	SQD	A	411	-	-	14/49/69/69	0/1/1/1
33	LMT	b	620	-	-	6/17/37/61	0/1/1/2
32	HTG	b	621	-	-	5/10/30/30	0/1/1/1
23	CLA	b	603	-	2/2/20/25	5/37/135/135	-
27	GOL	v	201	-	-	2/4/4/4	-
24	PHO	A	406	-	-	2/53/103/103	0/5/6/6
33	LMT	B	630	-	-	8/17/38/61	0/1/1/2
34	LMG	D	412	39	-	9/46/66/70	0/1/1/1
23	CLA	C	509	41	3/3/20/25	5/37/135/135	-
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
27	GOL	a	410	-	-	4/4/4/4	-
32	HTG	c	523	-	-	4/10/30/30	0/1/1/1
34	LMG	C	502	-	-	24/46/66/70	0/1/1/1
23	CLA	C	512	-	3/3/20/25	10/37/135/135	-
23	CLA	b	608	-	3/3/20/25	5/37/135/135	-
23	CLA	B	611	-	3/3/20/25	2/37/135/135	-
23	CLA	b	613	-	3/3/20/25	2/37/135/135	-
31	LHG	E	101	-	-	17/46/46/53	-
23	CLA	c	503	-	3/3/20/25	6/37/135/135	-
27	GOL	C	524	-	-	0/4/4/4	-
23	CLA	b	610	41	3/3/20/25	8/37/135/135	-
31	LHG	d	406	-	-	20/53/53/53	-
23	CLA	c	512	-	3/3/20/25	9/37/135/135	-
33	LMT	M	103	-	-	9/21/61/61	0/2/2/2
33	LMT	M	102	-	-	7/21/61/61	0/2/2/2
26	SQD	a	411	-	-	17/49/69/69	0/1/1/1
23	CLA	C	511	-	3/3/20/25	3/37/135/135	-
23	CLA	C	505	-	3/3/20/25	5/37/135/135	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	GOL	b	623	-	-	2/4/4/4	-
27	GOL	B	628	-	-	0/4/4/4	-
23	CLA	B	602	-	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
33	LMT	D	402	-	-	10/21/61/61	0/2/2/2
23	CLA	c	513	3	3/3/20/25	6/37/135/135	-
23	CLA	a	405	41	2/2/20/25	8/37/135/135	-
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
23	CLA	b	612	-	3/3/20/25	6/37/135/135	-
34	LMG	m	101	-	-	11/46/66/70	0/1/1/1
33	LMT	a	412	-	-	7/21/61/61	0/2/2/2
27	GOL	b	627	-	-	0/4/4/4	-
27	GOL	c	527	-	-	0/4/4/4	-
34	LMG	M	101	-	-	18/46/66/70	0/1/1/1
29	PL9	a	414[B]	-	-	16/53/73/73	0/1/1/1
23	CLA	B	608	-	2/2/20/25	2/37/135/135	-
23	CLA	C	508	-	3/3/20/25	12/37/135/135	-
23	CLA	C	504	-	2/2/20/25	8/37/135/135	-
26	SQD	a	409	-	-	12/49/69/69	0/1/1/1
25	BCR	b	617	-	-	4/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	A	407	-	3/3/20/25	8/37/135/135	-
23	CLA	c	509	41	3/3/20/25	8/37/135/135	-
23	CLA	A	404	41	3/3/20/25	6/37/135/135	-
23	CLA	c	511	-	3/3/20/25	12/37/135/135	-
23	CLA	D	404	-	3/3/20/25	9/37/135/135	-
32	HTG	D	411	-	-	2/7/27/30	0/1/1/1
34	LMG	c	522	-	-	9/46/66/70	0/1/1/1
35	DGD	h	103	-	-	11/51/91/95	0/2/2/2
33	LMT	e	101	-	-	9/21/61/61	0/2/2/2
27	GOL	B	623	-	-	2/4/4/4	-
23	CLA	b	601	41	3/3/20/25	15/37/135/135	-
23	CLA	c	506	41	3/3/20/25	4/37/135/135	-
23	CLA	b	611	-	3/3/20/25	3/37/135/135	-
34	LMG	c	521	-	-	6/46/66/70	0/1/1/1
24	PHO	A	415	-	-	3/53/103/103	0/5/6/6
23	CLA	b	605	-	3/3/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	604	-	3/3/20/25	13/37/135/135	-
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
38	HEM	E	102	5,6	-	0/6/54/54	-
23	CLA	A	405	41	2/2/20/25	5/37/135/135	-
34	LMG	a	417	-	-	12/46/66/70	0/1/1/1
35	DGD	C	518	-	-	16/51/91/95	0/2/2/2
33	LMT	F	101	-	-	5/21/61/61	0/2/2/2
23	CLA	c	510	-	3/3/20/25	10/37/135/135	-
26	SQD	L	102	-	-	19/49/69/69	0/1/1/1
40	HEC	v	202	16	-	0/6/54/54	-
26	SQD	A	409	-	-	15/49/69/69	0/1/1/1
23	CLA	B	605	-	2/2/20/25	8/37/135/135	-
23	CLA	C	510	-	3/3/20/25	7/37/135/135	-
23	CLA	c	514	-	3/3/20/25	9/37/135/135	-
23	CLA	c	504	-	3/3/20/25	3/37/135/135	-
33	LMT	B	629	-	-	4/17/37/61	0/1/1/2
33	LMT	B	627	-	-	9/21/61/61	0/2/2/2
24	PHO	a	416	-	-	5/53/103/103	0/5/6/6
29	PL9	D	406	-	-	7/53/73/73	0/1/1/1
32	HTG	b	624	-	-	2/10/30/30	0/1/1/1
31	LHG	L	101	-	-	16/53/53/53	-
23	CLA	C	503	-	3/3/20/25	5/37/135/135	-
25	BCR	c	517	-	-	2/29/63/63	0/2/2/2
27	GOL	c	502	-	-	0/4/4/4	-
25	BCR	D	405	-	-	8/29/63/63	0/2/2/2
23	CLA	B	610	41	3/3/20/25	8/37/135/135	-
29	PL9	A	413[A]	-	-	17/53/73/73	0/1/1/1
33	LMT	b	626	-	-	9/17/37/61	0/1/1/2
35	DGD	c	519	-	-	17/51/91/95	0/2/2/2
23	CLA	B	614	-	3/3/20/25	11/37/135/135	-
23	CLA	B	616	-	3/3/20/25	7/37/135/135	-
23	CLA	b	602	-	2/2/20/25	3/37/135/135	-
32	HTG	h	101	-	-	3/7/27/30	0/1/1/1
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
23	CLA	c	515	-	3/3/20/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	D	413	-	-	12/38/58/69	0/1/1/1
33	LMT	C	526	-	-	8/21/61/61	0/2/2/2
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
34	LMG	C	522	-	-	11/46/66/70	0/1/1/1
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
35	DGD	c	520	-	-	10/51/91/95	0/2/2/2
23	CLA	b	607	41	3/3/20/25	1/37/135/135	-
40	HEC	V	201	16	-	0/6/54/54	-
23	CLA	B	606	-	3/3/20/25	12/37/135/135	-
23	CLA	C	513	3	3/3/20/25	5/37/135/135	-
23	CLA	b	609	-	3/3/20/25	8/37/135/135	-
23	CLA	c	507	-	1/1/20/25	5/37/135/135	-
32	HTG	b	622	-	-	2/10/30/30	0/1/1/1
32	HTG	B	624	-	-	5/10/30/30	0/1/1/1
23	CLA	c	508	-	3/3/20/25	10/37/135/135	-
23	CLA	b	615	-	3/3/20/25	11/37/135/135	-
33	LMT	a	418	-	-	4/21/61/61	0/2/2/2
27	GOL	O	302	-	-	4/4/4/4	-
23	CLA	C	507	-	1/1/20/25	6/37/135/135	-
23	CLA	B	603	-	2/2/20/25	6/37/135/135	-
23	CLA	A	403	-	3/3/20/25	3/37/135/135	-
26	SQD	f	101	-	-	14/38/58/69	0/1/1/1
23	CLA	B	609	-	2/2/20/25	6/37/135/135	-
23	CLA	a	404	41	3/3/20/25	11/37/135/135	-
23	CLA	C	506	41	3/3/20/25	6/37/135/135	-
34	LMG	z	101	-	-	7/34/54/70	0/1/1/1
23	CLA	b	614	-	3/3/20/25	13/37/135/135	-
23	CLA	b	616	-	3/3/20/25	10/37/135/135	-
25	BCR	c	516	-	-	2/29/63/63	0/2/2/2
23	CLA	B	604	-	3/3/20/25	8/37/135/135	-
23	CLA	D	403	-	1/1/20/25	4/37/135/135	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
35	DGD	C	519	-	-	17/51/91/95	0/2/2/2
25	BCR	B	631	-	-	4/29/63/63	0/2/2/2
23	CLA	d	403	-	3/3/20/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
23	CLA	B	613	-	3/3/20/25	9/37/135/135	-
23	CLA	d	402	-	1/1/20/25	3/37/135/135	-
27	GOL	B	626	-	-	3/4/4/4	-
23	CLA	B	612	-	3/3/20/25	7/37/135/135	-
31	LHG	d	408	-	-	9/53/53/53	-
25	BCR	H	101	-	-	1/29/63/63	0/2/2/2
31	LHG	D	407	-	-	15/53/53/53	-
29	PL9	a	414[A]	-	-	18/53/73/73	0/1/1/1
23	CLA	C	515	-	3/3/20/25	7/37/135/135	-
23	CLA	a	403	-	3/3/20/25	6/37/135/135	-
23	CLA	c	505	-	3/3/20/25	3/37/135/135	-
31	LHG	d	407	-	-	23/53/53/53	-
31	LHG	b	628	-	-	13/53/53/53	-
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
23	CLA	B	615	-	3/3/20/25	8/37/135/135	-
29	PL9	d	405	-	-	7/53/73/73	0/1/1/1
38	HEM	e	102	5,6	-	0/6/54/54	-
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
35	DGD	C	520	-	-	7/51/91/95	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
32	HTG	V	202	-	-	1/2/19/30	0/1/1/1
25	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
32	HTG	C	523	-	-	2/10/30/30	0/1/1/1
31	LHG	A	416	-	-	16/53/53/53	-
31	LHG	a	419	-	-	19/46/46/53	-

All (1146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C3B-C2B	7.24	1.50	1.40
23	c	506	CLA	C3B-C2B	7.17	1.50	1.40
23	a	403	CLA	C3B-C2B	6.92	1.50	1.40
23	A	403	CLA	C3B-C2B	6.89	1.49	1.40
23	c	511	CLA	C3B-C2B	6.89	1.49	1.40
23	a	404	CLA	C3D-C2D	6.88	1.51	1.39
23	b	612	CLA	C3B-C2B	6.83	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C3B-C2B	6.78	1.49	1.40
23	B	615	CLA	C3D-C2D	6.77	1.51	1.39
23	C	511	CLA	C3B-C2B	6.61	1.49	1.40
23	B	613	CLA	C3B-C2B	6.56	1.49	1.40
23	B	612	CLA	C3B-C2B	6.48	1.49	1.40
23	b	603	CLA	C3B-C2B	6.46	1.49	1.40
23	b	613	CLA	C3B-C2B	6.43	1.49	1.40
23	B	603	CLA	C3B-C2B	6.41	1.49	1.40
23	C	509	CLA	C3B-C2B	6.37	1.49	1.40
23	b	609	CLA	C3B-C2B	6.33	1.49	1.40
23	C	513	CLA	C3B-C2B	6.32	1.49	1.40
23	B	608	CLA	C3B-C2B	6.31	1.49	1.40
23	c	513	CLA	C3B-C2B	6.31	1.49	1.40
23	C	514	CLA	C3B-C2B	6.30	1.49	1.40
23	B	604	CLA	C3B-C2B	6.27	1.49	1.40
23	b	601	CLA	C3D-C2D	6.25	1.50	1.39
23	b	614	CLA	C3B-C2B	6.23	1.49	1.40
40	v	202	HEC	C3B-C2B	-6.21	1.34	1.40
23	d	403	CLA	C3D-C2D	6.15	1.50	1.39
23	C	506	CLA	C3B-C2B	6.13	1.48	1.40
23	c	506	CLA	C3D-C2D	6.13	1.50	1.39
23	b	613	CLA	C3D-C2D	6.11	1.50	1.39
23	C	504	CLA	C3B-C2B	6.08	1.48	1.40
23	b	604	CLA	C3B-C2B	6.08	1.48	1.40
23	b	602	CLA	C3B-C2B	6.06	1.48	1.40
23	c	508	CLA	C3B-C2B	6.05	1.48	1.40
24	a	406	PHO	C3B-C2B	6.05	1.49	1.37
23	c	504	CLA	C3B-C2B	6.04	1.48	1.40
23	a	405	CLA	C3D-C2D	6.03	1.50	1.39
23	c	512	CLA	C3B-C2B	6.03	1.48	1.40
23	B	606	CLA	C3B-C2B	6.02	1.48	1.40
23	B	607	CLA	C3B-C2B	5.99	1.48	1.40
24	A	406	PHO	C3C-C2C	5.97	1.49	1.36
23	b	611	CLA	C3B-C2B	5.97	1.48	1.40
23	C	512	CLA	C3D-C2D	5.95	1.50	1.39
23	b	601	CLA	C3B-C2B	5.95	1.48	1.40
23	d	402	CLA	C3B-C2B	5.93	1.48	1.40
23	C	510	CLA	C3C-C2C	5.93	1.49	1.36
23	C	514	CLA	C3D-C2D	5.93	1.50	1.39
23	A	407	CLA	C3B-C2B	5.89	1.48	1.40
23	C	504	CLA	C3D-C2D	5.89	1.50	1.39
23	c	510	CLA	C3D-C2D	5.89	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	201	HEC	C3B-C2B	-5.88	1.34	1.40
23	B	601	CLA	C3B-C2B	5.88	1.48	1.40
23	D	404	CLA	C3D-C2D	5.87	1.49	1.39
23	C	515	CLA	C3B-C2B	5.87	1.48	1.40
24	A	415	PHO	C3B-C2B	5.85	1.49	1.37
24	A	406	PHO	C3B-C2B	5.84	1.49	1.37
24	A	415	PHO	C3C-C2C	5.84	1.49	1.36
23	B	611	CLA	C3B-C2B	5.84	1.48	1.40
23	C	506	CLA	C3D-C2D	5.83	1.49	1.39
23	D	403	CLA	C3B-C2B	5.83	1.48	1.40
23	c	507	CLA	C3D-C2D	5.82	1.49	1.39
23	b	606	CLA	C3B-C2B	5.82	1.48	1.40
23	B	610	CLA	C3D-C2D	5.81	1.49	1.39
23	C	512	CLA	C3B-C2B	5.81	1.48	1.40
23	A	405	CLA	C3D-C2D	5.80	1.49	1.39
23	c	509	CLA	C3D-C2D	5.80	1.49	1.39
23	a	407	CLA	C3B-C2B	5.80	1.48	1.40
23	c	504	CLA	C3D-C2D	5.79	1.49	1.39
23	c	503	CLA	C3D-C2D	5.79	1.49	1.39
23	c	503	CLA	C3B-C2B	5.79	1.48	1.40
23	c	515	CLA	C3B-C2B	5.77	1.48	1.40
23	b	614	CLA	C3D-C2D	5.77	1.49	1.39
24	a	406	PHO	C3C-C2C	5.77	1.49	1.36
23	B	610	CLA	C3C-C2C	5.76	1.49	1.36
23	c	507	CLA	C3C-C2C	5.76	1.49	1.36
23	B	602	CLA	C3D-C2D	5.76	1.49	1.39
23	b	608	CLA	C3B-C2B	5.75	1.48	1.40
24	a	416	PHO	C3B-C2B	5.75	1.48	1.37
23	C	511	CLA	C3D-C2D	5.73	1.49	1.39
23	C	513	CLA	C3D-C2D	5.70	1.49	1.39
23	C	515	CLA	C3D-C2D	5.69	1.49	1.39
25	d	404	BCR	C23-C22	-5.68	1.33	1.45
23	b	616	CLA	C3B-C2B	5.68	1.48	1.40
23	a	405	CLA	C3B-C2B	5.67	1.48	1.40
23	B	602	CLA	CHC-C1C	5.66	1.49	1.35
23	B	605	CLA	CHC-C1C	5.65	1.49	1.35
23	b	610	CLA	C3D-C2D	5.65	1.49	1.39
23	b	601	CLA	C3C-C2C	5.65	1.48	1.36
23	B	611	CLA	C3D-C2D	5.64	1.49	1.39
23	b	615	CLA	C3D-C2D	5.64	1.49	1.39
23	B	610	CLA	C3B-C2B	5.63	1.48	1.40
23	c	508	CLA	C3D-C2D	5.63	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C3D-C2D	5.62	1.49	1.39
23	C	505	CLA	C3D-C2D	5.62	1.49	1.39
23	a	403	CLA	C3D-C2D	5.62	1.49	1.39
23	c	514	CLA	C3D-C2D	5.61	1.49	1.39
23	c	515	CLA	C3D-C2D	5.59	1.49	1.39
23	C	510	CLA	C3D-C2D	5.59	1.49	1.39
23	b	609	CLA	C3D-C2D	5.59	1.49	1.39
23	B	611	CLA	C3C-C2C	5.59	1.48	1.36
23	c	510	CLA	C3C-C2C	5.58	1.48	1.36
23	C	507	CLA	C3D-C2D	5.58	1.49	1.39
23	B	603	CLA	C3D-C2D	5.57	1.49	1.39
23	b	602	CLA	C3D-C2D	5.57	1.49	1.39
23	c	511	CLA	C3D-C2D	5.57	1.49	1.39
23	A	407	CLA	C3D-C2D	5.56	1.49	1.39
23	C	513	CLA	O2D-CGD	5.55	1.46	1.33
23	B	601	CLA	C3D-C2D	5.55	1.49	1.39
23	B	604	CLA	C3D-C2D	5.54	1.49	1.39
24	a	416	PHO	C3C-C2C	5.54	1.48	1.36
23	B	613	CLA	C3D-C2D	5.53	1.49	1.39
23	C	505	CLA	C3B-C2B	5.53	1.48	1.40
23	B	616	CLA	C3D-C2D	5.53	1.49	1.39
23	C	508	CLA	C3D-C2D	5.53	1.49	1.39
23	B	609	CLA	C3D-C2D	5.52	1.49	1.39
23	C	514	CLA	C3C-C2C	5.49	1.48	1.36
23	d	403	CLA	CHC-C1C	5.49	1.49	1.35
23	d	403	CLA	C3B-C2B	5.49	1.48	1.40
23	b	605	CLA	C3B-C2B	5.49	1.48	1.40
23	a	407	CLA	C3C-C2C	5.48	1.48	1.36
40	v	202	HEC	C3D-C2D	5.48	1.53	1.37
23	b	605	CLA	C3C-C2C	5.47	1.48	1.36
23	B	612	CLA	C3D-C2D	5.47	1.49	1.39
23	B	605	CLA	C3D-C2D	5.47	1.49	1.39
23	b	615	CLA	C3C-C2C	5.47	1.48	1.36
23	b	611	CLA	C3D-C2D	5.47	1.49	1.39
23	D	403	CLA	C3C-C2C	5.46	1.48	1.36
23	B	616	CLA	C3B-C2B	5.46	1.47	1.40
40	V	201	HEC	C3C-C2C	-5.46	1.35	1.40
23	B	601	CLA	C3C-C2C	5.45	1.48	1.36
23	C	509	CLA	C3C-C2C	5.45	1.48	1.36
23	B	608	CLA	C3D-C2D	5.45	1.49	1.39
23	c	513	CLA	C3D-C2D	5.44	1.49	1.39
23	A	407	CLA	C3C-C2C	5.43	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C3C-C2C	5.43	1.48	1.36
23	b	607	CLA	C3C-C2C	5.42	1.48	1.36
23	A	403	CLA	C3D-C2D	5.42	1.49	1.39
23	b	612	CLA	C3C-C2C	5.42	1.48	1.36
23	C	515	CLA	C3C-C2C	5.42	1.48	1.36
23	C	508	CLA	C3B-C2B	5.41	1.47	1.40
23	b	610	CLA	C3B-C2B	5.41	1.47	1.40
23	c	509	CLA	CHC-C1C	5.41	1.48	1.35
23	a	404	CLA	C3C-C2C	5.41	1.48	1.36
23	B	614	CLA	C3D-C2D	5.41	1.49	1.39
23	A	405	CLA	C3C-C2C	5.41	1.48	1.36
23	b	607	CLA	C3D-C2D	5.40	1.49	1.39
23	b	603	CLA	C3C-C2C	5.39	1.48	1.36
23	A	404	CLA	C3C-C2C	5.39	1.48	1.36
23	b	612	CLA	C3D-C2D	5.39	1.49	1.39
23	C	505	CLA	C3C-C2C	5.38	1.48	1.36
23	C	509	CLA	C3D-C2D	5.38	1.49	1.39
23	b	609	CLA	CHC-C1C	5.37	1.48	1.35
23	c	509	CLA	OBD-CAD	5.37	1.29	1.22
23	C	511	CLA	C3C-C2C	5.37	1.48	1.36
23	c	515	CLA	C3C-C2C	5.37	1.48	1.36
23	d	403	CLA	C3C-C2C	5.36	1.48	1.36
23	B	607	CLA	CHC-C1C	5.36	1.48	1.35
23	c	514	CLA	CHC-C1C	5.35	1.48	1.35
23	c	504	CLA	C3C-C2C	5.35	1.48	1.36
23	B	606	CLA	C3D-C2D	5.35	1.49	1.39
23	B	614	CLA	C3C-C2C	5.35	1.48	1.36
23	D	404	CLA	C3C-C2C	5.34	1.48	1.36
23	d	402	CLA	C3D-C2D	5.34	1.49	1.39
25	b	619	BCR	C23-C22	-5.32	1.34	1.45
23	c	511	CLA	O2D-CGD	5.32	1.46	1.33
23	c	512	CLA	C3D-C2D	5.31	1.49	1.39
24	A	415	PHO	CHC-C1C	5.30	1.48	1.38
25	k	101	BCR	C23-C22	-5.29	1.34	1.45
23	c	506	CLA	C3C-C2C	5.29	1.48	1.36
23	c	515	CLA	CHC-C1C	5.29	1.48	1.35
23	B	605	CLA	O2D-CGD	5.29	1.46	1.33
23	c	505	CLA	C3D-C2D	5.29	1.48	1.39
23	C	504	CLA	CHC-C1C	5.28	1.48	1.35
23	C	503	CLA	C3B-C2B	5.28	1.47	1.40
23	c	511	CLA	C3C-C2C	5.27	1.47	1.36
23	b	603	CLA	O2D-CGD	5.27	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C3D-C2D	5.26	1.48	1.39
23	c	514	CLA	C3C-C2C	5.26	1.47	1.36
23	A	404	CLA	C3D-C2D	5.25	1.48	1.39
24	A	406	PHO	CHB-C1B	5.25	1.48	1.38
23	b	603	CLA	C3D-C2D	5.24	1.48	1.39
24	a	406	PHO	CHB-C1B	5.24	1.48	1.38
23	c	508	CLA	C3C-C2C	5.24	1.47	1.36
23	b	613	CLA	C3C-C2C	5.24	1.47	1.36
23	b	608	CLA	CHC-C1C	5.23	1.48	1.35
23	B	601	CLA	CHC-C1C	5.23	1.48	1.35
23	A	405	CLA	CHC-C1C	5.23	1.48	1.35
23	b	605	CLA	OBD-CAD	5.23	1.29	1.22
23	c	507	CLA	CHC-C1C	5.23	1.48	1.35
23	C	514	CLA	CHC-C1C	5.22	1.48	1.35
24	a	416	PHO	CHB-C1B	5.22	1.48	1.38
23	c	514	CLA	O2D-CGD	5.22	1.45	1.33
23	A	404	CLA	C3B-C2B	5.22	1.47	1.40
23	b	615	CLA	C3B-C2B	5.21	1.47	1.40
23	C	503	CLA	C3D-C2D	5.21	1.48	1.39
24	a	416	PHO	CHC-C1C	5.20	1.48	1.38
23	b	610	CLA	C3C-C2C	5.20	1.47	1.36
23	D	404	CLA	CHC-C1C	5.19	1.48	1.35
23	c	505	CLA	C3C-C2C	5.19	1.47	1.36
23	A	407	CLA	O2D-CGD	5.19	1.45	1.33
23	c	507	CLA	C3B-C2B	5.19	1.47	1.40
23	c	510	CLA	O2D-CGD	5.18	1.45	1.33
23	b	606	CLA	C3C-C2C	5.18	1.47	1.36
23	a	404	CLA	C3B-C2B	5.18	1.47	1.40
24	A	406	PHO	CHC-C1C	5.18	1.48	1.38
23	B	605	CLA	C3C-C2C	5.18	1.47	1.36
23	b	614	CLA	O2D-CGD	5.17	1.45	1.33
23	B	613	CLA	CHC-C1C	5.17	1.48	1.35
23	b	603	CLA	OBD-CAD	5.17	1.29	1.22
23	b	602	CLA	CHC-C1C	5.17	1.48	1.35
23	C	512	CLA	CHC-C1C	5.16	1.48	1.35
23	B	603	CLA	C3C-C2C	5.16	1.47	1.36
23	A	404	CLA	CHC-C1C	5.16	1.48	1.35
23	b	605	CLA	C3D-C2D	5.16	1.48	1.39
23	B	609	CLA	O2D-CGD	5.16	1.45	1.33
23	c	512	CLA	C3C-C2C	5.16	1.47	1.36
23	C	507	CLA	C3C-C2C	5.15	1.47	1.36
23	b	602	CLA	C3C-C2C	5.15	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	515	CLA	CHC-C1C	5.15	1.48	1.35
23	c	504	CLA	O2D-CGD	5.15	1.45	1.33
23	b	615	CLA	OBD-CAD	5.15	1.29	1.22
23	B	611	CLA	O2D-CGD	5.14	1.45	1.33
23	b	616	CLA	CHC-C1C	5.14	1.48	1.35
23	B	614	CLA	C3B-C2B	5.14	1.47	1.40
23	B	601	CLA	O2D-CGD	5.14	1.45	1.33
25	A	408	BCR	C23-C22	-5.14	1.34	1.45
23	B	615	CLA	C3C-C2C	5.14	1.47	1.36
23	B	616	CLA	C3C-C2C	5.14	1.47	1.36
23	a	407	CLA	CHC-C1C	5.14	1.48	1.35
23	B	610	CLA	CHC-C1C	5.13	1.48	1.35
23	C	507	CLA	CHC-C1C	5.13	1.48	1.35
23	b	609	CLA	C3C-C2C	5.13	1.47	1.36
23	B	602	CLA	C3C-C2C	5.12	1.47	1.36
23	B	605	CLA	C3B-C2B	5.12	1.47	1.40
23	c	503	CLA	C3C-C2C	5.12	1.47	1.36
23	C	506	CLA	O2D-CGD	5.12	1.45	1.33
23	B	602	CLA	C3B-C2B	5.12	1.47	1.40
23	B	604	CLA	C3C-C2C	5.12	1.47	1.36
23	B	606	CLA	C3C-C2C	5.11	1.47	1.36
23	C	504	CLA	C3C-C2C	5.11	1.47	1.36
23	B	610	CLA	OBD-CAD	5.11	1.29	1.22
23	b	604	CLA	C3C-C2C	5.11	1.47	1.36
23	a	403	CLA	C3C-C2C	5.10	1.47	1.36
23	a	403	CLA	CHC-C1C	5.10	1.48	1.35
23	c	508	CLA	CHC-C1C	5.10	1.48	1.35
23	b	616	CLA	O2D-CGD	5.09	1.45	1.33
23	C	513	CLA	CHC-C1C	5.09	1.48	1.35
23	b	611	CLA	O2D-CGD	5.09	1.45	1.33
23	c	510	CLA	CHC-C1C	5.08	1.48	1.35
23	B	616	CLA	CHC-C1C	5.08	1.48	1.35
23	B	604	CLA	CHC-C1C	5.08	1.48	1.35
23	b	601	CLA	CHC-C1C	5.07	1.48	1.35
25	B	631	BCR	C23-C22	-5.07	1.35	1.45
24	a	406	PHO	CHD-C1D	5.07	1.48	1.38
23	c	514	CLA	C3B-C2B	5.06	1.47	1.40
25	b	617	BCR	C23-C22	-5.06	1.35	1.45
23	b	602	CLA	O2D-CGD	5.06	1.45	1.33
23	b	608	CLA	C3C-C2C	5.06	1.47	1.36
23	b	608	CLA	C3D-C2D	5.06	1.48	1.39
23	b	606	CLA	CHC-C1C	5.06	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CHC-C1C	5.05	1.47	1.35
23	B	612	CLA	CHC-C1C	5.05	1.47	1.35
23	B	608	CLA	C3C-C2C	5.04	1.47	1.36
25	K	101	BCR	C23-C22	-5.04	1.35	1.45
23	b	610	CLA	CHC-C1C	5.03	1.47	1.35
23	b	611	CLA	C3C-C2C	5.03	1.47	1.36
23	B	609	CLA	CHC-C1C	5.03	1.47	1.35
23	c	515	CLA	O2D-CGD	5.03	1.45	1.33
23	C	510	CLA	CHC-C1C	5.03	1.47	1.35
24	A	406	PHO	CHD-C1D	5.03	1.48	1.38
23	c	509	CLA	O2D-CGD	5.02	1.45	1.33
24	a	416	PHO	O2D-CGD	5.02	1.45	1.33
23	C	503	CLA	OBD-CAD	5.02	1.29	1.22
23	C	508	CLA	CHC-C1C	5.02	1.47	1.35
23	C	512	CLA	C3C-C2C	5.02	1.47	1.36
24	A	415	PHO	CHB-C1B	5.02	1.48	1.38
23	C	506	CLA	CHC-C1C	5.02	1.47	1.35
23	B	606	CLA	CHC-C1C	5.02	1.47	1.35
23	b	603	CLA	CHC-C1C	5.01	1.47	1.35
23	c	513	CLA	C3C-C2C	5.01	1.47	1.36
23	C	504	CLA	O2D-CGD	5.01	1.45	1.33
23	b	607	CLA	C3B-C2B	5.01	1.47	1.40
23	b	616	CLA	C3C-C2C	5.01	1.47	1.36
23	c	508	CLA	O2D-CGD	5.01	1.45	1.33
23	A	407	CLA	CHC-C1C	5.01	1.47	1.35
23	A	405	CLA	O2D-CGD	5.01	1.45	1.33
23	B	615	CLA	O2D-CGD	5.01	1.45	1.33
23	D	404	CLA	C3B-C2B	5.01	1.47	1.40
23	b	605	CLA	CHC-C1C	5.01	1.47	1.35
25	k	102	BCR	C23-C22	-5.01	1.35	1.45
23	b	606	CLA	C3D-C2D	5.00	1.48	1.39
23	b	607	CLA	CHC-C1C	5.00	1.47	1.35
23	B	607	CLA	C3D-C2D	4.99	1.48	1.39
23	c	513	CLA	CHC-C1C	4.99	1.47	1.35
23	D	404	CLA	O2D-CGD	4.98	1.45	1.33
23	C	508	CLA	O2D-CGD	4.98	1.45	1.33
23	B	603	CLA	CHC-C1C	4.98	1.47	1.35
23	a	405	CLA	CHC-C1C	4.97	1.47	1.35
23	B	613	CLA	O2D-CGD	4.97	1.45	1.33
23	C	505	CLA	CHC-C1C	4.96	1.47	1.35
23	B	611	CLA	OBD-CAD	4.96	1.29	1.22
23	c	511	CLA	CHC-C1C	4.96	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	202	HEC	C3C-C2C	-4.95	1.35	1.40
23	B	614	CLA	CHC-C1C	4.95	1.47	1.35
23	c	506	CLA	O2D-CGD	4.95	1.45	1.33
23	B	602	CLA	O2D-CGD	4.94	1.45	1.33
23	c	509	CLA	C3B-C2B	4.94	1.47	1.40
23	b	613	CLA	O2D-CGD	4.93	1.45	1.33
23	b	608	CLA	O2D-CGD	4.92	1.45	1.33
23	b	615	CLA	CHC-C1C	4.92	1.47	1.35
23	b	614	CLA	C3C-C2C	4.91	1.47	1.36
23	C	505	CLA	O2D-CGD	4.91	1.45	1.33
25	c	517	BCR	C23-C22	-4.91	1.35	1.45
25	C	516	BCR	C23-C22	-4.91	1.35	1.45
23	C	509	CLA	CHC-C1C	4.90	1.47	1.35
23	D	404	CLA	OBD-CAD	4.90	1.29	1.22
23	b	608	CLA	OBD-CAD	4.90	1.29	1.22
24	A	415	PHO	O2D-CGD	4.90	1.45	1.33
23	B	616	CLA	O2D-CGD	4.90	1.45	1.33
23	c	507	CLA	O2D-CGD	4.90	1.45	1.33
23	A	403	CLA	C3C-C2C	4.89	1.47	1.36
23	A	405	CLA	C3B-C2B	4.89	1.47	1.40
23	C	507	CLA	O2D-CGD	4.89	1.45	1.33
23	C	511	CLA	OBD-CAD	4.89	1.29	1.22
23	b	614	CLA	CHC-C1C	4.89	1.47	1.35
23	d	402	CLA	C3C-C2C	4.88	1.47	1.36
40	V	201	HEC	C3D-C2D	4.88	1.52	1.37
23	C	506	CLA	C3C-C2C	4.88	1.47	1.36
23	C	508	CLA	C3C-C2C	4.87	1.47	1.36
23	c	509	CLA	C3C-C2C	4.87	1.47	1.36
23	b	604	CLA	O2D-CGD	4.87	1.45	1.33
23	a	404	CLA	CHC-C1C	4.87	1.47	1.35
23	b	606	CLA	OBD-CAD	4.87	1.29	1.22
23	B	615	CLA	CHC-C1C	4.87	1.47	1.35
25	b	618	BCR	C23-C22	-4.86	1.35	1.45
23	c	503	CLA	CHC-C1C	4.86	1.47	1.35
23	B	609	CLA	C3C-C2C	4.86	1.47	1.36
25	c	516	BCR	C23-C22	-4.85	1.35	1.45
23	c	504	CLA	CHC-C1C	4.85	1.47	1.35
23	D	403	CLA	CHC-C1C	4.84	1.47	1.35
23	b	609	CLA	O2D-CGD	4.83	1.45	1.33
23	a	407	CLA	C3D-C2D	4.83	1.48	1.39
23	b	607	CLA	O2D-CGD	4.83	1.45	1.33
23	c	506	CLA	CHC-C1C	4.83	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	O2D-CGD	4.83	1.45	1.33
23	b	604	CLA	CHC-C1C	4.83	1.47	1.35
23	C	507	CLA	C3B-C2B	4.82	1.47	1.40
23	B	609	CLA	C3B-C2B	4.82	1.47	1.40
23	c	514	CLA	OBD-CAD	4.82	1.29	1.22
23	C	504	CLA	OBD-CAD	4.81	1.29	1.22
23	c	505	CLA	C3B-C2B	4.81	1.47	1.40
24	a	406	PHO	CHC-C1C	4.81	1.48	1.38
23	C	514	CLA	OBD-CAD	4.81	1.29	1.22
23	B	606	CLA	O2D-CGD	4.80	1.44	1.33
23	a	405	CLA	C3C-C2C	4.80	1.46	1.36
25	T	101	BCR	C23-C22	-4.80	1.35	1.45
23	a	404	CLA	O2D-CGD	4.80	1.44	1.33
23	c	511	CLA	OBD-CAD	4.79	1.29	1.22
23	B	615	CLA	C3B-C2B	4.79	1.47	1.40
23	C	511	CLA	CHC-C1C	4.79	1.47	1.35
23	C	514	CLA	O2D-CGD	4.78	1.44	1.33
23	C	509	CLA	O2D-CGD	4.78	1.44	1.33
23	c	510	CLA	OBD-CAD	4.78	1.29	1.22
23	c	512	CLA	OBD-CAD	4.78	1.29	1.22
23	b	601	CLA	O2D-CGD	4.77	1.44	1.33
25	H	101	BCR	C23-C22	-4.77	1.35	1.45
25	h	102	BCR	C23-C22	-4.76	1.35	1.45
23	A	405	CLA	OBD-CAD	4.76	1.29	1.22
23	B	601	CLA	O2A-CGA	4.76	1.47	1.33
34	M	101	LMG	O8-C28	4.74	1.47	1.33
23	c	512	CLA	CHC-C1C	4.74	1.47	1.35
23	b	605	CLA	O2D-CGD	4.73	1.44	1.33
23	a	407	CLA	O2D-CGD	4.72	1.44	1.33
23	b	613	CLA	CHC-C1C	4.72	1.47	1.35
23	C	511	CLA	O2D-CGD	4.72	1.44	1.33
23	B	611	CLA	CHC-C1C	4.72	1.47	1.35
23	B	601	CLA	OBD-CAD	4.71	1.28	1.22
23	C	503	CLA	CHC-C1C	4.70	1.47	1.35
23	b	611	CLA	CHC-C1C	4.70	1.47	1.35
23	B	614	CLA	O2D-CGD	4.70	1.44	1.33
23	b	601	CLA	O2A-CGA	4.70	1.47	1.33
23	c	503	CLA	O2D-CGD	4.69	1.44	1.33
23	b	612	CLA	CHC-C1C	4.69	1.47	1.35
23	D	403	CLA	C3D-C2D	4.69	1.47	1.39
23	C	515	CLA	O2D-CGD	4.69	1.44	1.33
23	d	402	CLA	OBD-CAD	4.68	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	CHC-C1C	4.68	1.47	1.35
23	c	506	CLA	OBD-CAD	4.67	1.28	1.22
23	B	603	CLA	O2D-CGD	4.67	1.44	1.33
25	a	408	BCR	C23-C22	-4.66	1.35	1.45
23	B	615	CLA	OBD-CAD	4.66	1.28	1.22
23	B	608	CLA	CHC-C1C	4.65	1.46	1.35
25	B	619	BCR	C23-C22	-4.65	1.36	1.45
23	C	513	CLA	C3C-C2C	4.64	1.46	1.36
23	B	612	CLA	C3C-C2C	4.64	1.46	1.36
23	B	613	CLA	C3C-C2C	4.64	1.46	1.36
25	B	617	BCR	C23-C22	-4.64	1.36	1.45
23	B	612	CLA	O2D-CGD	4.62	1.44	1.33
23	B	607	CLA	C3C-C2C	4.62	1.46	1.36
23	d	403	CLA	O2D-CGD	4.61	1.44	1.33
23	b	612	CLA	O2D-CGD	4.61	1.44	1.33
23	c	508	CLA	OBD-CAD	4.61	1.28	1.22
23	b	604	CLA	OBD-CAD	4.60	1.28	1.22
23	A	404	CLA	O2D-CGD	4.57	1.44	1.33
23	A	403	CLA	CHC-C1C	4.57	1.46	1.35
25	C	517	BCR	C23-C22	-4.57	1.36	1.45
26	A	411	SQD	O48-C23	4.57	1.46	1.33
24	a	406	PHO	O2D-CGD	4.56	1.44	1.33
23	c	507	CLA	OBD-CAD	4.55	1.28	1.22
24	A	406	PHO	O2D-CGD	4.55	1.44	1.33
23	C	503	CLA	O2D-CGD	4.55	1.44	1.33
23	B	604	CLA	OBD-CAD	4.54	1.28	1.22
23	A	404	CLA	OBD-CAD	4.54	1.28	1.22
23	c	513	CLA	O2D-CGD	4.53	1.44	1.33
34	M	101	LMG	O7-C10	4.52	1.47	1.34
23	c	512	CLA	O2D-CGD	4.50	1.44	1.33
23	C	512	CLA	O2D-CGD	4.50	1.44	1.33
23	A	403	CLA	O2D-CGD	4.49	1.44	1.33
23	B	609	CLA	O2A-CGA	4.49	1.46	1.33
23	C	510	CLA	O2D-CGD	4.49	1.44	1.33
23	b	610	CLA	O2D-CGD	4.49	1.44	1.33
23	C	510	CLA	OBD-CAD	4.49	1.28	1.22
23	B	607	CLA	O2D-CGD	4.48	1.44	1.33
23	c	505	CLA	O2D-CGD	4.48	1.44	1.33
23	a	403	CLA	OBD-CAD	4.47	1.28	1.22
23	a	405	CLA	OBD-CAD	4.47	1.28	1.22
25	D	405	BCR	C23-C22	-4.47	1.36	1.45
23	b	601	CLA	OBD-CAD	4.47	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	522	LMG	O7-C10	4.46	1.46	1.34
34	C	521	LMG	O8-C28	4.46	1.46	1.33
23	C	505	CLA	OBD-CAD	4.45	1.28	1.22
23	C	509	CLA	OBD-CAD	4.45	1.28	1.22
23	c	514	CLA	O2A-CGA	4.45	1.46	1.33
34	C	522	LMG	O8-C28	4.44	1.46	1.33
23	B	604	CLA	O2D-CGD	4.44	1.44	1.33
23	a	407	CLA	O2A-CGA	4.44	1.46	1.33
31	E	101	LHG	O8-C23	4.43	1.46	1.33
23	a	403	CLA	O2D-CGD	4.42	1.44	1.33
23	b	602	CLA	OBD-CAD	4.42	1.28	1.22
23	c	513	CLA	O2A-CGA	4.42	1.46	1.33
23	D	403	CLA	O2D-CGD	4.42	1.44	1.33
23	d	402	CLA	O2D-CGD	4.41	1.43	1.33
23	b	610	CLA	OBD-CAD	4.40	1.28	1.22
26	D	413	SQD	O47-C7	4.39	1.46	1.34
23	d	403	CLA	OBD-CAD	4.39	1.28	1.22
31	a	419	LHG	O8-C23	4.38	1.46	1.33
23	B	603	CLA	OBD-CAD	4.38	1.28	1.22
23	c	510	CLA	O2A-CGA	4.37	1.46	1.33
34	z	101	LMG	O8-C28	4.37	1.46	1.33
23	C	506	CLA	O2A-CGA	4.37	1.46	1.33
31	a	419	LHG	O7-C7	4.36	1.46	1.34
23	a	405	CLA	O2D-CGD	4.36	1.43	1.33
26	L	102	SQD	O48-C23	4.36	1.46	1.33
23	C	513	CLA	O2A-CGA	4.35	1.46	1.33
23	B	608	CLA	OBD-CAD	4.35	1.28	1.22
34	c	522	LMG	O8-C28	4.35	1.46	1.33
23	B	616	CLA	OBD-CAD	4.33	1.28	1.22
23	C	508	CLA	OBD-CAD	4.33	1.28	1.22
23	D	403	CLA	OBD-CAD	4.32	1.28	1.22
26	B	620	SQD	O47-C7	4.32	1.46	1.34
26	f	101	SQD	O47-C7	4.32	1.46	1.34
35	c	520	DGD	O1G-C1A	4.31	1.45	1.33
35	c	518	DGD	O1G-C1A	4.31	1.45	1.33
23	c	515	CLA	O2A-CGA	4.31	1.45	1.33
23	c	511	CLA	O2A-CGA	4.31	1.45	1.33
23	C	508	CLA	O2A-CGA	4.30	1.45	1.33
23	b	602	CLA	O2A-CGA	4.30	1.45	1.33
23	C	514	CLA	O2A-CGA	4.29	1.45	1.33
24	A	415	PHO	CHD-C1D	4.29	1.47	1.38
23	b	613	CLA	OBD-CAD	4.29	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	O2A-CGA	4.29	1.45	1.33
26	a	411	SQD	O48-C23	4.28	1.45	1.33
23	c	507	CLA	O2A-CGA	4.28	1.45	1.33
34	c	522	LMG	O7-C10	4.28	1.46	1.34
23	C	513	CLA	OBD-CAD	4.27	1.28	1.22
23	B	608	CLA	O2A-CGA	4.27	1.45	1.33
25	Y	101	BCR	C23-C22	-4.26	1.36	1.45
23	d	402	CLA	O2A-CGA	4.26	1.45	1.33
23	B	607	CLA	OBD-CAD	4.26	1.28	1.22
23	B	602	CLA	OBD-CAD	4.26	1.28	1.22
23	D	403	CLA	O2A-CGA	4.26	1.45	1.33
23	c	504	CLA	OBD-CAD	4.26	1.28	1.22
23	a	404	CLA	OBD-CAD	4.25	1.28	1.22
35	C	520	DGD	O1G-C1A	4.25	1.45	1.33
24	a	416	PHO	CHD-C1D	4.25	1.46	1.38
23	a	404	CLA	O2A-CGA	4.24	1.45	1.33
34	Z	101	LMG	O7-C10	4.24	1.46	1.34
34	d	411	LMG	O8-C28	4.23	1.45	1.33
23	b	611	CLA	O2A-CGA	4.22	1.45	1.33
23	b	612	CLA	O2A-CGA	4.22	1.45	1.33
23	B	612	CLA	OBD-CAD	4.22	1.28	1.22
23	C	504	CLA	O2A-CGA	4.21	1.45	1.33
26	a	411	SQD	O47-C7	4.21	1.46	1.34
34	C	521	LMG	O7-C10	4.21	1.46	1.34
35	h	103	DGD	O1G-C1A	4.20	1.45	1.33
34	m	101	LMG	O8-C28	4.20	1.45	1.33
31	b	628	LHG	O8-C23	4.20	1.45	1.33
23	C	515	CLA	O2A-CGA	4.20	1.45	1.33
23	A	407	CLA	O2A-CGA	4.19	1.45	1.33
26	a	409	SQD	O48-C23	4.19	1.45	1.33
23	B	607	CLA	O2A-CGA	4.19	1.45	1.33
23	d	403	CLA	O2A-CGA	4.19	1.45	1.33
23	b	609	CLA	OBD-CAD	4.18	1.28	1.22
26	L	102	SQD	O47-C7	4.18	1.46	1.34
23	b	616	CLA	OBD-CAD	4.17	1.28	1.22
24	a	406	PHO	C3D-C2D	4.16	1.50	1.39
26	a	409	SQD	O47-C7	4.16	1.46	1.34
34	c	521	LMG	O8-C28	4.15	1.45	1.33
26	A	411	SQD	O47-C7	4.14	1.46	1.34
23	C	509	CLA	O2A-CGA	4.13	1.45	1.33
34	c	521	LMG	O7-C10	4.13	1.46	1.34
23	c	515	CLA	OBD-CAD	4.13	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	502	LMG	O8-C28	4.13	1.45	1.33
23	b	612	CLA	OBD-CAD	4.13	1.28	1.22
23	C	510	CLA	O2A-CGA	4.12	1.45	1.33
23	C	506	CLA	OBD-CAD	4.12	1.28	1.22
23	B	605	CLA	OBD-CAD	4.12	1.28	1.22
23	B	606	CLA	O2A-CGA	4.12	1.45	1.33
24	A	406	PHO	O2A-CGA	4.12	1.45	1.33
35	c	518	DGD	O2G-C1B	4.11	1.45	1.34
34	C	502	LMG	O7-C10	4.11	1.45	1.34
23	b	614	CLA	O2A-CGA	4.10	1.45	1.33
26	B	620	SQD	O48-C23	4.10	1.45	1.33
23	B	608	CLA	O2D-CGD	4.09	1.43	1.33
35	c	519	DGD	O1G-C1A	4.09	1.45	1.33
23	C	505	CLA	O2A-CGA	4.09	1.45	1.33
34	a	417	LMG	O8-C28	4.09	1.45	1.33
23	c	509	CLA	O2A-CGA	4.09	1.45	1.33
23	b	614	CLA	OBD-CAD	4.08	1.28	1.22
31	D	408	LHG	O7-C7	4.08	1.45	1.34
26	D	413	SQD	O48-C23	4.08	1.45	1.33
31	b	628	LHG	O7-C7	4.07	1.45	1.34
31	L	101	LHG	O8-C23	4.07	1.45	1.33
23	B	603	CLA	O2A-CGA	4.07	1.45	1.33
34	z	101	LMG	O7-C10	4.06	1.45	1.34
23	B	610	CLA	O2D-CGD	4.06	1.43	1.33
35	C	519	DGD	O1G-C1A	4.05	1.45	1.33
31	E	101	LHG	O7-C7	4.05	1.45	1.34
35	C	518	DGD	O1G-C1A	4.04	1.45	1.33
23	B	609	CLA	OBD-CAD	4.04	1.27	1.22
23	b	609	CLA	O2A-CGA	4.03	1.45	1.33
23	c	504	CLA	O2A-CGA	4.03	1.45	1.33
26	f	101	SQD	O48-C23	4.02	1.45	1.33
31	d	408	LHG	O8-C23	4.02	1.45	1.33
23	B	613	CLA	O2A-CGA	4.01	1.45	1.33
23	C	507	CLA	OBD-CAD	4.01	1.27	1.22
23	b	606	CLA	O2D-CGD	4.01	1.43	1.33
23	c	513	CLA	OBD-CAD	4.00	1.27	1.22
23	c	508	CLA	O2A-CGA	4.00	1.45	1.33
23	c	506	CLA	O2A-CGA	4.00	1.45	1.33
23	C	512	CLA	OBD-CAD	3.99	1.27	1.22
23	C	511	CLA	O2A-CGA	3.99	1.45	1.33
25	B	618	BCR	C23-C22	-3.98	1.37	1.45
34	a	417	LMG	O7-C10	3.98	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	O2A-CGA	3.98	1.45	1.33
35	C	518	DGD	O2G-C1B	3.98	1.45	1.34
23	c	505	CLA	O2A-CGA	3.97	1.45	1.33
23	c	503	CLA	OBD-CAD	3.97	1.27	1.22
31	d	408	LHG	O7-C7	3.96	1.45	1.34
23	b	615	CLA	O2A-CGA	3.95	1.44	1.33
23	B	615	CLA	O2A-CGA	3.94	1.44	1.33
34	m	101	LMG	O7-C10	3.93	1.45	1.34
24	a	406	PHO	OBD-CAD	3.93	1.29	1.22
31	A	416	LHG	O7-C7	3.93	1.45	1.34
23	a	405	CLA	O2A-CGA	3.93	1.44	1.33
35	h	103	DGD	O2G-C1B	3.92	1.45	1.34
23	A	404	CLA	O2A-CGA	3.92	1.44	1.33
26	A	409	SQD	O48-C23	3.91	1.44	1.33
23	B	616	CLA	O2A-CGA	3.91	1.44	1.33
35	C	519	DGD	O2G-C1B	3.91	1.45	1.34
23	b	616	CLA	O2A-CGA	3.90	1.44	1.33
23	A	403	CLA	OBD-CAD	3.90	1.27	1.22
23	C	503	CLA	O2A-CGA	3.90	1.44	1.33
34	d	411	LMG	O7-C10	3.90	1.45	1.34
23	D	404	CLA	O2A-CGA	3.89	1.44	1.33
23	B	614	CLA	O2A-CGA	3.89	1.44	1.33
35	c	519	DGD	O2G-C1B	3.88	1.45	1.34
23	B	614	CLA	OBD-CAD	3.87	1.27	1.22
23	A	407	CLA	OBD-CAD	3.87	1.27	1.22
31	D	407	LHG	O8-C23	3.86	1.44	1.33
23	b	604	CLA	O2A-CGA	3.86	1.44	1.33
23	b	603	CLA	O2A-CGA	3.85	1.44	1.33
23	B	606	CLA	OBD-CAD	3.85	1.27	1.22
23	C	512	CLA	O2A-CGA	3.85	1.44	1.33
23	b	613	CLA	O2A-CGA	3.84	1.44	1.33
23	c	503	CLA	O2A-CGA	3.83	1.44	1.33
23	C	507	CLA	O2A-CGA	3.83	1.44	1.33
23	B	612	CLA	O2A-CGA	3.82	1.44	1.33
31	d	406	LHG	O7-C7	3.82	1.45	1.34
31	d	406	LHG	O8-C23	3.81	1.44	1.33
32	h	101	HTG	C1'-S1	-3.81	1.76	1.81
31	D	408	LHG	O8-C23	3.80	1.44	1.33
35	C	520	DGD	O2G-C1B	3.80	1.45	1.34
24	a	416	PHO	C3D-C2D	3.79	1.49	1.39
34	D	412	LMG	O8-C28	3.79	1.44	1.33
23	c	505	CLA	OBD-CAD	3.78	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	407	LHG	O8-C23	3.78	1.44	1.33
23	B	604	CLA	O2A-CGA	3.78	1.44	1.33
23	b	611	CLA	OBD-CAD	3.77	1.27	1.22
24	a	416	PHO	CHC-C4B	3.76	1.49	1.40
35	H	102	DGD	O1G-C1A	3.76	1.44	1.33
23	b	607	CLA	OBD-CAD	3.75	1.27	1.22
26	A	409	SQD	O47-C7	3.74	1.44	1.34
24	a	406	PHO	O2A-CGA	3.74	1.44	1.33
24	A	415	PHO	C3D-C2D	3.74	1.49	1.39
23	a	403	CLA	O2A-CGA	3.73	1.44	1.33
35	c	520	DGD	O2G-C1B	3.73	1.44	1.34
24	a	416	PHO	O2A-CGA	3.73	1.44	1.33
32	b	622	HTG	C1'-S1	-3.72	1.76	1.81
23	b	606	CLA	O2A-CGA	3.71	1.44	1.33
23	C	515	CLA	OBD-CAD	3.71	1.27	1.22
31	d	407	LHG	O7-C7	3.70	1.44	1.34
24	A	415	PHO	O2A-CGA	3.70	1.44	1.33
23	B	613	CLA	OBD-CAD	3.70	1.27	1.22
23	A	403	CLA	O2A-CGA	3.67	1.44	1.33
24	A	406	PHO	OBD-CAD	3.66	1.28	1.22
23	B	610	CLA	O2A-CGA	3.66	1.44	1.33
24	a	416	PHO	OBD-CAD	3.63	1.28	1.22
23	b	607	CLA	O2A-CGA	3.62	1.43	1.33
34	D	412	LMG	O7-C10	3.60	1.44	1.34
23	B	602	CLA	O2A-CGA	3.59	1.43	1.33
32	B	621	HTG	C1'-S1	-3.58	1.76	1.81
23	B	611	CLA	O2A-CGA	3.57	1.43	1.33
24	A	415	PHO	OBD-CAD	3.57	1.28	1.22
35	H	102	DGD	O2G-C1B	3.57	1.44	1.34
31	A	416	LHG	O8-C23	3.57	1.43	1.33
23	B	612	CLA	C1C-C2C	3.54	1.51	1.44
23	c	512	CLA	O2A-CGA	3.53	1.43	1.33
32	B	624	HTG	C1'-S1	-3.52	1.76	1.81
31	D	407	LHG	O7-C7	3.50	1.44	1.34
23	B	602	CLA	C1C-C2C	3.49	1.51	1.44
23	A	405	CLA	O2A-CGA	3.48	1.43	1.33
31	L	101	LHG	O7-C7	3.46	1.44	1.34
23	b	605	CLA	O2A-CGA	3.46	1.43	1.33
24	a	416	PHO	CHB-C4A	3.44	1.48	1.40
32	b	624	HTG	C1'-S1	-3.44	1.77	1.81
24	a	406	PHO	CHC-C4B	3.43	1.48	1.40
23	B	614	CLA	C4B-NB	-3.42	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	415	PHO	C4A-NA	-3.39	1.27	1.35
32	b	621	HTG	C1'-S1	-3.39	1.77	1.81
24	A	406	PHO	C3D-C2D	3.37	1.48	1.39
24	A	406	PHO	C4A-NA	-3.33	1.27	1.35
32	c	523	HTG	C1'-S1	-3.33	1.77	1.81
23	c	511	CLA	C4C-C3C	3.31	1.50	1.45
23	b	610	CLA	O2A-CGA	3.29	1.42	1.33
23	C	508	CLA	C1D-C2D	3.25	1.49	1.42
23	B	605	CLA	C4B-CHC	3.23	1.50	1.41
24	a	406	PHO	CHB-C4A	3.23	1.48	1.40
24	A	415	PHO	CHC-C4B	3.20	1.47	1.40
24	a	416	PHO	C4A-NA	-3.20	1.27	1.35
23	a	407	CLA	OBD-CAD	3.20	1.26	1.22
23	c	506	CLA	C1D-C2D	3.17	1.49	1.42
24	A	406	PHO	CHB-C4A	3.17	1.47	1.40
32	D	411	HTG	C1'-S1	-3.17	1.77	1.81
23	b	605	CLA	C1D-C2D	3.15	1.49	1.42
23	c	509	CLA	C1D-C2D	3.15	1.49	1.42
24	A	406	PHO	CHD-C4C	3.13	1.47	1.40
23	D	403	CLA	C1B-CHB	3.12	1.49	1.41
32	C	523	HTG	C1'-S1	-3.11	1.77	1.81
24	a	406	PHO	CHD-C4C	3.10	1.47	1.40
23	D	404	CLA	C1D-C2D	3.09	1.49	1.42
23	B	603	CLA	C1B-NB	-3.07	1.32	1.35
23	c	513	CLA	C1B-CHB	3.07	1.49	1.41
23	a	405	CLA	C1C-C2C	3.07	1.50	1.44
23	B	609	CLA	C1D-C2D	3.07	1.49	1.42
23	B	606	CLA	C1D-C2D	3.05	1.49	1.42
24	A	406	PHO	CHC-C4B	3.05	1.47	1.40
23	B	602	CLA	C4B-CHC	3.05	1.49	1.41
23	d	403	CLA	C1D-C2D	3.04	1.49	1.42
23	B	611	CLA	C1C-C2C	3.02	1.50	1.44
23	c	506	CLA	C4C-C3C	3.02	1.50	1.45
23	B	603	CLA	C1C-C2C	3.01	1.50	1.44
23	a	407	CLA	C1C-C2C	3.01	1.50	1.44
23	A	404	CLA	C1D-C2D	3.00	1.49	1.42
23	c	515	CLA	C1D-C2D	3.00	1.49	1.42
24	a	416	PHO	C3B-C4B	3.00	1.49	1.43
24	a	416	PHO	CHD-C4C	2.99	1.47	1.40
26	f	101	SQD	C6-S	-2.98	1.66	1.77
23	C	513	CLA	C1D-C2D	2.98	1.49	1.42
23	b	608	CLA	C1D-C2D	2.98	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C1D-C2D	2.97	1.49	1.42
32	B	624	HTG	C1-S1	-2.97	1.76	1.80
23	B	612	CLA	C1B-CHB	2.97	1.49	1.41
23	c	505	CLA	C1C-C2C	2.96	1.50	1.44
23	A	405	CLA	CHD-C4C	2.96	1.49	1.41
23	c	507	CLA	C1C-C2C	2.95	1.50	1.44
23	B	601	CLA	C1D-C2D	2.95	1.49	1.42
23	b	602	CLA	C1D-C2D	2.93	1.49	1.42
23	b	612	CLA	C1B-NB	-2.93	1.32	1.35
23	b	606	CLA	C1D-C2D	2.93	1.49	1.42
23	B	607	CLA	C1C-C2C	2.92	1.50	1.44
23	c	509	CLA	C1C-C2C	2.92	1.50	1.44
23	b	609	CLA	C1D-C2D	2.90	1.49	1.42
23	C	506	CLA	C1C-C2C	2.90	1.50	1.44
23	b	610	CLA	C1C-C2C	2.89	1.50	1.44
38	e	102	HEM	C3B-C2B	-2.89	1.36	1.40
26	a	409	SQD	C6-S	-2.89	1.66	1.77
32	B	622	HTG	C1'-S1	-2.89	1.77	1.81
23	C	511	CLA	C1D-C2D	2.89	1.49	1.42
23	C	515	CLA	C1C-C2C	2.87	1.50	1.44
23	b	603	CLA	C1C-C2C	2.87	1.50	1.44
23	c	503	CLA	C1B-CHB	2.87	1.49	1.41
23	C	511	CLA	C1C-C2C	2.87	1.50	1.44
23	B	605	CLA	C1D-C2D	2.87	1.49	1.42
23	B	613	CLA	C1D-C2D	2.86	1.49	1.42
24	A	415	PHO	CHB-C4A	2.86	1.47	1.40
23	c	505	CLA	C4C-C3C	2.86	1.50	1.45
23	b	612	CLA	C1D-C2D	2.85	1.49	1.42
23	B	616	CLA	C4B-CHC	2.84	1.48	1.41
23	b	607	CLA	C1B-CHB	2.84	1.48	1.41
23	b	607	CLA	C1B-NB	-2.84	1.32	1.35
23	c	515	CLA	C1C-C2C	2.83	1.50	1.44
23	B	610	CLA	C4C-C3C	2.83	1.49	1.45
23	C	503	CLA	C1C-C2C	2.83	1.50	1.44
23	B	601	CLA	C4B-CHC	2.82	1.48	1.41
23	D	404	CLA	C1B-CHB	2.82	1.48	1.41
23	b	610	CLA	C1B-CHB	2.82	1.48	1.41
23	A	404	CLA	C4B-CHC	2.82	1.48	1.41
26	A	409	SQD	C6-S	-2.81	1.67	1.77
23	C	512	CLA	C1C-C2C	2.81	1.50	1.44
24	a	406	PHO	C4A-NA	-2.81	1.28	1.35
23	c	509	CLA	CHD-C4C	2.81	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C1D-C2D	2.81	1.48	1.42
23	c	515	CLA	CHD-C4C	2.80	1.49	1.41
23	b	616	CLA	C4B-CHC	2.80	1.48	1.41
23	B	610	CLA	C1D-C2D	2.79	1.48	1.42
23	a	403	CLA	C1D-C2D	2.79	1.48	1.42
23	b	615	CLA	C4C-C3C	2.79	1.49	1.45
23	A	407	CLA	C1C-C2C	2.77	1.49	1.44
23	d	403	CLA	CHD-C4C	2.77	1.49	1.41
24	A	415	PHO	CHD-C4C	2.77	1.46	1.40
23	b	609	CLA	C1C-C2C	2.77	1.49	1.44
23	A	403	CLA	C1D-C2D	2.77	1.48	1.42
23	c	509	CLA	C4B-CHC	2.76	1.48	1.41
23	B	602	CLA	C1D-C2D	2.76	1.48	1.42
33	a	412	LMT	O1'-C1'	2.76	1.44	1.40
23	B	607	CLA	C1B-CHB	2.76	1.48	1.41
23	c	507	CLA	C4B-CHC	2.75	1.48	1.41
23	b	602	CLA	C1C-C2C	2.75	1.49	1.44
23	c	514	CLA	C4B-CHC	2.75	1.48	1.41
23	a	404	CLA	C1C-C2C	2.75	1.49	1.44
23	b	610	CLA	C4B-CHC	2.75	1.48	1.41
23	b	611	CLA	C1D-C2D	2.75	1.48	1.42
23	A	407	CLA	C1D-C2D	2.75	1.48	1.42
23	A	405	CLA	C1D-C2D	2.74	1.48	1.42
23	B	615	CLA	C1C-C2C	2.74	1.49	1.44
23	D	404	CLA	C1C-C2C	2.74	1.49	1.44
23	b	602	CLA	C4C-C3C	2.74	1.49	1.45
23	c	511	CLA	C1D-C2D	2.74	1.48	1.42
23	C	508	CLA	CHD-C4C	2.74	1.49	1.41
23	b	601	CLA	C1D-C2D	2.73	1.48	1.42
23	B	614	CLA	C4B-CHC	2.73	1.48	1.41
23	b	602	CLA	CHD-C4C	2.73	1.48	1.41
23	C	503	CLA	C4B-CHC	2.72	1.48	1.41
23	A	403	CLA	C1C-C2C	2.72	1.49	1.44
23	b	616	CLA	C1C-C2C	2.72	1.49	1.44
23	B	607	CLA	C4B-CHC	2.71	1.48	1.41
23	A	405	CLA	C4C-C3C	2.71	1.49	1.45
23	C	505	CLA	C1D-C2D	2.70	1.48	1.42
23	D	403	CLA	CHD-C4C	2.70	1.48	1.41
26	D	413	SQD	C6-S	-2.70	1.67	1.77
23	c	506	CLA	C1B-CHB	2.70	1.48	1.41
26	B	620	SQD	C6-S	-2.69	1.67	1.77
29	A	413[B]	PL9	C6-C5	2.69	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	C4B-CHC	2.69	1.48	1.41
23	b	601	CLA	CHD-C4C	2.68	1.48	1.41
23	B	604	CLA	C1B-CHB	2.68	1.48	1.41
23	D	403	CLA	C4C-C3C	2.68	1.49	1.45
23	c	503	CLA	C1C-C2C	2.68	1.49	1.44
23	C	508	CLA	C4C-C3C	2.68	1.49	1.45
23	b	603	CLA	C4C-C3C	2.68	1.49	1.45
26	A	411	SQD	C6-S	-2.67	1.67	1.77
23	B	603	CLA	C1B-CHB	2.67	1.48	1.41
23	C	513	CLA	C1B-CHB	2.67	1.48	1.41
23	C	504	CLA	C1B-CHB	2.67	1.48	1.41
29	A	413[A]	PL9	C6-C5	2.66	1.49	1.35
23	c	508	CLA	CHD-C4C	2.66	1.48	1.41
23	c	504	CLA	C1D-C2D	2.66	1.48	1.42
23	b	607	CLA	C1D-C2D	2.66	1.48	1.42
23	b	605	CLA	C4B-CHC	2.66	1.48	1.41
26	a	411	SQD	C6-S	-2.65	1.67	1.77
23	C	507	CLA	C4C-C3C	2.65	1.49	1.45
23	c	515	CLA	C4C-C3C	2.65	1.49	1.45
23	c	514	CLA	C1D-C2D	2.65	1.48	1.42
23	d	403	CLA	C4B-CHC	2.65	1.48	1.41
23	B	616	CLA	C1C-C2C	2.65	1.49	1.44
23	C	510	CLA	C1B-CHB	2.64	1.48	1.41
23	B	614	CLA	C1B-CHB	2.64	1.48	1.41
26	L	102	SQD	C6-S	-2.64	1.67	1.77
29	a	414[A]	PL9	C6-C5	2.64	1.49	1.35
23	b	608	CLA	CHD-C4C	2.64	1.48	1.41
23	b	603	CLA	C1D-C2D	2.64	1.48	1.42
23	B	613	CLA	C1B-CHB	2.64	1.48	1.41
23	c	511	CLA	CHD-C4C	2.63	1.48	1.41
24	A	406	PHO	C3B-C4B	2.63	1.48	1.43
29	a	414[B]	PL9	C6-C5	2.63	1.49	1.35
23	C	513	CLA	C1C-C2C	2.63	1.49	1.44
23	B	613	CLA	C1C-C2C	2.63	1.49	1.44
23	B	606	CLA	C1B-CHB	2.62	1.48	1.41
23	C	514	CLA	C1C-C2C	2.62	1.49	1.44
23	b	606	CLA	C1C-C2C	2.62	1.49	1.44
23	B	610	CLA	C4B-CHC	2.62	1.48	1.41
23	C	507	CLA	C1C-C2C	2.62	1.49	1.44
23	D	403	CLA	C1C-C2C	2.62	1.49	1.44
23	a	405	CLA	C1D-C2D	2.62	1.48	1.42
23	D	403	CLA	C1D-C2D	2.62	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	C1C-C2C	2.62	1.49	1.44
23	C	512	CLA	C1B-CHB	2.61	1.48	1.41
23	C	509	CLA	C1C-C2C	2.61	1.49	1.44
23	b	604	CLA	C4B-CHC	2.61	1.48	1.41
23	B	607	CLA	C4C-C3C	2.61	1.49	1.45
23	C	514	CLA	C1D-C2D	2.61	1.48	1.42
32	b	624	HTG	C1-S1	-2.61	1.76	1.80
23	C	511	CLA	CHD-C4C	2.60	1.48	1.41
23	c	512	CLA	C1B-CHB	2.60	1.48	1.41
23	b	613	CLA	C1B-CHB	2.60	1.48	1.41
23	A	407	CLA	CHD-C4C	2.59	1.48	1.41
23	C	509	CLA	C1D-C2D	2.59	1.48	1.42
23	B	604	CLA	CHD-C4C	2.59	1.48	1.41
23	B	604	CLA	C1C-C2C	2.59	1.49	1.44
23	C	513	CLA	CHD-C4C	2.59	1.48	1.41
23	C	511	CLA	C4C-C3C	2.59	1.49	1.45
23	c	503	CLA	C1D-C2D	2.59	1.48	1.42
23	a	407	CLA	C4B-CHC	2.58	1.48	1.41
23	C	515	CLA	C1D-C2D	2.58	1.48	1.42
23	c	503	CLA	CHD-C4C	2.58	1.48	1.41
23	c	505	CLA	C1B-CHB	2.58	1.48	1.41
23	c	506	CLA	C1C-C2C	2.58	1.49	1.44
24	A	415	PHO	C1A-NA	-2.58	1.32	1.37
23	c	514	CLA	C1C-C2C	2.58	1.49	1.44
23	b	605	CLA	C1B-NB	-2.58	1.32	1.35
23	b	608	CLA	C1B-CHB	2.58	1.48	1.41
23	a	404	CLA	C4B-CHC	2.58	1.48	1.41
23	C	504	CLA	C1C-C2C	2.58	1.49	1.44
23	a	407	CLA	C1D-C2D	2.58	1.48	1.42
24	A	415	PHO	C3B-C4B	2.57	1.48	1.43
23	C	515	CLA	C1B-CHB	2.56	1.48	1.41
23	C	505	CLA	C1C-C2C	2.56	1.49	1.44
23	C	504	CLA	C4B-CHC	2.56	1.48	1.41
23	b	612	CLA	C1B-CHB	2.56	1.48	1.41
23	B	611	CLA	C1B-CHB	2.55	1.48	1.41
23	B	601	CLA	C1C-C2C	2.55	1.49	1.44
23	C	512	CLA	C4B-CHC	2.55	1.48	1.41
23	c	507	CLA	C4C-C3C	2.55	1.49	1.45
24	a	406	PHO	C4C-C3C	2.55	1.49	1.45
23	b	613	CLA	C1C-C2C	2.55	1.49	1.44
23	B	616	CLA	C1D-C2D	2.54	1.48	1.42
23	B	608	CLA	C1C-C2C	2.54	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C1C-C2C	2.54	1.49	1.44
23	c	508	CLA	C1D-C2D	2.54	1.48	1.42
23	a	403	CLA	CHD-C4C	2.54	1.48	1.41
23	C	507	CLA	C1D-C2D	2.54	1.48	1.42
34	Z	101	LMG	O8-C28	2.54	1.45	1.33
23	B	614	CLA	C1D-C2D	2.53	1.48	1.42
23	c	513	CLA	C1D-C2D	2.53	1.48	1.42
25	b	619	BCR	C30-C25	-2.53	1.50	1.53
23	c	504	CLA	C1B-CHB	2.53	1.48	1.41
23	a	403	CLA	C1C-C2C	2.53	1.49	1.44
23	B	614	CLA	C1C-C2C	2.53	1.49	1.44
23	C	512	CLA	C1D-C2D	2.52	1.48	1.42
23	B	609	CLA	C1C-C2C	2.52	1.49	1.44
23	A	405	CLA	C4B-CHC	2.52	1.48	1.41
23	b	608	CLA	C1C-C2C	2.52	1.49	1.44
23	c	506	CLA	CHD-C4C	2.52	1.48	1.41
23	a	404	CLA	C1D-C2D	2.51	1.48	1.42
23	C	511	CLA	C1B-CHB	2.51	1.48	1.41
23	C	506	CLA	C1B-CHB	2.51	1.48	1.41
23	c	505	CLA	C4B-CHC	2.51	1.48	1.41
23	C	507	CLA	CHD-C4C	2.51	1.48	1.41
23	C	505	CLA	CHD-C4C	2.50	1.48	1.41
23	c	512	CLA	C1D-C2D	2.50	1.48	1.42
23	b	604	CLA	C1D-C2D	2.50	1.48	1.42
23	b	611	CLA	C1B-CHB	2.50	1.47	1.41
23	b	602	CLA	C4B-CHC	2.50	1.47	1.41
23	b	609	CLA	C4B-CHC	2.50	1.47	1.41
23	B	615	CLA	C1D-C2D	2.49	1.48	1.42
23	B	603	CLA	C1D-C2D	2.48	1.48	1.42
23	a	407	CLA	C1B-CHB	2.48	1.47	1.41
23	C	507	CLA	C1B-CHB	2.48	1.47	1.41
38	E	102	HEM	C3B-C2B	-2.48	1.36	1.40
23	C	508	CLA	C1C-C2C	2.48	1.49	1.44
23	C	507	CLA	C4B-CHC	2.48	1.47	1.41
23	C	512	CLA	CHD-C4C	2.48	1.48	1.41
23	c	505	CLA	CHD-C4C	2.48	1.48	1.41
23	C	505	CLA	C1B-CHB	2.47	1.47	1.41
23	b	603	CLA	C1B-CHB	2.47	1.47	1.41
23	B	601	CLA	CHD-C4C	2.47	1.48	1.41
23	c	512	CLA	CHD-C4C	2.47	1.48	1.41
23	c	511	CLA	C1C-C2C	2.47	1.49	1.44
23	C	503	CLA	CHD-C4C	2.47	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	CHD-C4C	2.47	1.48	1.41
23	B	610	CLA	CHD-C4C	2.46	1.48	1.41
23	b	612	CLA	C4B-CHC	2.46	1.47	1.41
23	C	509	CLA	C4C-C3C	2.46	1.49	1.45
23	B	604	CLA	C4B-CHC	2.46	1.47	1.41
23	c	514	CLA	C4C-C3C	2.46	1.49	1.45
23	c	508	CLA	C4B-CHC	2.46	1.47	1.41
23	C	515	CLA	C4B-CHC	2.46	1.47	1.41
23	b	611	CLA	CHD-C4C	2.46	1.48	1.41
23	B	607	CLA	C1D-C2D	2.45	1.48	1.42
23	a	407	CLA	C1B-NB	-2.45	1.33	1.35
23	C	505	CLA	C4C-C3C	2.45	1.49	1.45
23	D	404	CLA	C4B-CHC	2.45	1.47	1.41
23	B	602	CLA	CHD-C4C	2.45	1.48	1.41
23	B	609	CLA	C1B-CHB	2.45	1.47	1.41
23	B	615	CLA	C4B-CHC	2.45	1.47	1.41
23	c	503	CLA	C4C-C3C	2.45	1.49	1.45
23	b	604	CLA	C1B-CHB	2.44	1.47	1.41
23	B	616	CLA	C1B-CHB	2.44	1.47	1.41
23	c	505	CLA	C1D-C2D	2.44	1.48	1.42
23	C	511	CLA	C4B-CHC	2.44	1.47	1.41
23	d	402	CLA	C4C-C3C	2.44	1.49	1.45
23	c	507	CLA	C1D-C2D	2.43	1.48	1.42
23	C	513	CLA	C4C-C3C	2.43	1.49	1.45
23	B	602	CLA	C1B-CHB	2.43	1.47	1.41
23	C	512	CLA	C4C-C3C	2.43	1.49	1.45
34	C	522	LMG	O1-C1	2.43	1.44	1.40
23	b	614	CLA	C1B-CHB	2.43	1.47	1.41
23	B	605	CLA	C1C-C2C	2.43	1.49	1.44
23	c	508	CLA	C1C-C2C	2.43	1.49	1.44
23	A	403	CLA	C1B-CHB	2.42	1.47	1.41
23	b	616	CLA	C1B-CHB	2.42	1.47	1.41
23	b	613	CLA	C1D-C2D	2.42	1.48	1.42
23	a	404	CLA	CHD-C4C	2.42	1.48	1.41
23	C	503	CLA	C1B-CHB	2.41	1.47	1.41
23	B	609	CLA	CHD-C4C	2.41	1.48	1.41
23	b	608	CLA	C4B-CHC	2.41	1.47	1.41
23	b	606	CLA	CHD-C4C	2.41	1.48	1.41
23	c	512	CLA	C1C-C2C	2.41	1.49	1.44
23	C	515	CLA	CHD-C4C	2.41	1.48	1.41
23	c	503	CLA	C4B-CHC	2.41	1.47	1.41
29	d	405	PL9	C6-C5	2.40	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	CHD-C4C	2.40	1.48	1.41
23	C	514	CLA	C4B-CHC	2.40	1.47	1.41
23	b	614	CLA	C4B-CHC	2.40	1.47	1.41
23	b	615	CLA	CHD-C4C	2.40	1.48	1.41
23	B	611	CLA	C1D-C2D	2.39	1.48	1.42
23	b	613	CLA	C4C-C3C	2.39	1.49	1.45
23	c	514	CLA	C1B-CHB	2.39	1.47	1.41
23	b	607	CLA	C1C-C2C	2.39	1.49	1.44
33	D	402	LMT	O1'-C1'	2.38	1.44	1.40
23	B	613	CLA	C1B-NB	-2.38	1.33	1.35
23	B	613	CLA	C4C-C3C	2.38	1.49	1.45
23	b	603	CLA	CHD-C4C	2.38	1.47	1.41
23	B	615	CLA	C1B-CHB	2.38	1.47	1.41
23	C	506	CLA	C1D-C2D	2.38	1.47	1.42
23	c	504	CLA	CHD-C4C	2.38	1.47	1.41
23	B	607	CLA	CHD-C4C	2.37	1.47	1.41
23	B	608	CLA	C1D-C2D	2.37	1.47	1.42
23	c	514	CLA	CHD-C4C	2.36	1.47	1.41
23	b	609	CLA	C1B-CHB	2.36	1.47	1.41
23	c	510	CLA	CHD-C4C	2.36	1.47	1.41
23	b	610	CLA	C1B-NB	-2.36	1.33	1.35
23	c	507	CLA	CHD-C4C	2.36	1.47	1.41
23	a	405	CLA	C4B-CHC	2.36	1.47	1.41
32	D	411	HTG	C1-S1	-2.35	1.77	1.80
23	b	605	CLA	C1B-CHB	2.35	1.47	1.41
23	C	510	CLA	C1D-C2D	2.35	1.47	1.42
23	b	605	CLA	CHD-C4C	2.34	1.47	1.41
23	b	614	CLA	C1D-C2D	2.34	1.47	1.42
23	B	610	CLA	C1B-CHB	2.34	1.47	1.41
23	C	506	CLA	CHD-C4C	2.34	1.47	1.41
23	A	407	CLA	C4C-C3C	2.34	1.49	1.45
23	b	607	CLA	C4C-C3C	2.34	1.49	1.45
23	B	601	CLA	C1B-NB	-2.34	1.33	1.35
23	C	505	CLA	C4B-CHC	2.34	1.47	1.41
23	c	511	CLA	C1B-CHB	2.34	1.47	1.41
23	b	614	CLA	C1C-C2C	2.34	1.49	1.44
24	A	406	PHO	C4C-C3C	2.33	1.49	1.45
35	h	103	DGD	O5D-C1E	2.33	1.44	1.40
23	c	510	CLA	C1C-C2C	2.32	1.49	1.44
23	C	514	CLA	C4C-C3C	2.32	1.49	1.45
23	b	612	CLA	C4C-C3C	2.32	1.49	1.45
23	B	612	CLA	C1D-C2D	2.32	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	C4B-CHC	2.32	1.47	1.41
23	c	512	CLA	C4B-CHC	2.32	1.47	1.41
23	b	604	CLA	C1C-C2C	2.32	1.49	1.44
23	B	606	CLA	C1C-C2C	2.32	1.49	1.44
23	b	601	CLA	C4B-CHC	2.32	1.47	1.41
23	A	403	CLA	C4C-C3C	2.31	1.49	1.45
23	B	608	CLA	C4C-C3C	2.31	1.49	1.45
23	b	610	CLA	C4C-C3C	2.31	1.49	1.45
23	c	510	CLA	C1B-CHB	2.31	1.47	1.41
23	B	609	CLA	C4B-CHC	2.31	1.47	1.41
23	c	504	CLA	C4B-CHC	2.31	1.47	1.41
23	c	507	CLA	C1B-CHB	2.31	1.47	1.41
23	b	608	CLA	C4C-C3C	2.31	1.49	1.45
23	c	508	CLA	C1B-CHB	2.31	1.47	1.41
23	a	407	CLA	C4C-C3C	2.31	1.49	1.45
31	D	407	LHG	O7-C5	-2.31	1.40	1.46
23	A	404	CLA	CHD-C4C	2.31	1.47	1.41
23	b	609	CLA	CHD-C4C	2.30	1.47	1.41
23	d	403	CLA	C1C-C2C	2.30	1.49	1.44
23	c	513	CLA	C4B-CHC	2.30	1.47	1.41
31	L	101	LHG	O7-C5	-2.30	1.40	1.46
23	b	601	CLA	C1C-C2C	2.30	1.49	1.44
23	C	513	CLA	C1C-NC	-2.30	1.34	1.37
25	d	404	BCR	C30-C25	-2.29	1.50	1.53
23	b	601	CLA	C1B-CHB	2.29	1.47	1.41
29	D	406	PL9	C6-C5	2.29	1.47	1.35
23	c	504	CLA	C1C-C2C	2.29	1.49	1.44
23	B	612	CLA	C4B-CHC	2.29	1.47	1.41
24	A	415	PHO	C4D-CHA	2.28	1.49	1.43
23	B	612	CLA	C4C-C3C	2.28	1.49	1.45
23	B	616	CLA	CHD-C4C	2.28	1.47	1.41
23	b	611	CLA	C4B-CHC	2.28	1.47	1.41
23	b	609	CLA	C1C-NC	-2.28	1.34	1.37
33	C	526	LMT	O1'-C1'	2.28	1.44	1.40
35	H	102	DGD	O5D-C1E	2.28	1.44	1.40
23	b	604	CLA	CHD-C4C	2.27	1.47	1.41
23	C	509	CLA	C1B-CHB	2.27	1.47	1.41
23	a	405	CLA	C1B-CHB	2.27	1.47	1.41
23	B	614	CLA	CHD-C4C	2.27	1.47	1.41
23	c	512	CLA	C4C-C3C	2.27	1.48	1.45
23	B	608	CLA	C4B-CHC	2.27	1.47	1.41
23	c	510	CLA	C1C-NC	-2.26	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C4C-C3C	2.26	1.48	1.45
23	C	512	CLA	C1B-NB	-2.26	1.33	1.35
29	D	406	PL9	C2-C3	2.25	1.40	1.34
23	C	508	CLA	C1B-CHB	2.25	1.47	1.41
24	a	406	PHO	C3B-C4B	2.25	1.47	1.43
23	c	506	CLA	C4B-CHC	2.25	1.47	1.41
23	c	515	CLA	C1B-CHB	2.25	1.47	1.41
23	C	513	CLA	C4B-CHC	2.24	1.47	1.41
32	c	523	HTG	C1-S1	-2.24	1.77	1.80
23	b	605	CLA	C1C-C2C	2.24	1.48	1.44
23	B	606	CLA	CHD-C4C	2.24	1.47	1.41
23	b	611	CLA	C1C-C2C	2.24	1.48	1.44
23	b	610	CLA	C1D-C2D	2.24	1.47	1.42
23	c	508	CLA	C1B-NB	-2.24	1.33	1.35
23	B	608	CLA	C1B-CHB	2.24	1.47	1.41
23	c	506	CLA	C1C-NC	-2.24	1.34	1.37
23	C	503	CLA	C4C-C3C	2.24	1.48	1.45
23	c	503	CLA	C1C-NC	-2.23	1.34	1.37
23	C	510	CLA	C4C-C3C	2.23	1.48	1.45
23	B	602	CLA	C4C-C3C	2.22	1.48	1.45
23	B	610	CLA	C1C-C2C	2.22	1.48	1.44
23	b	614	CLA	C1B-NB	-2.22	1.33	1.35
23	B	616	CLA	C1B-NB	-2.22	1.33	1.35
23	b	613	CLA	CHD-C4C	2.22	1.47	1.41
23	c	510	CLA	C4C-C3C	2.22	1.48	1.45
23	c	510	CLA	C4B-CHC	2.22	1.47	1.41
29	A	413[A]	PL9	C2-C3	2.21	1.40	1.34
23	C	504	CLA	C1D-C2D	2.21	1.47	1.42
23	C	509	CLA	CHD-C4C	2.21	1.47	1.41
23	c	509	CLA	C1B-CHB	2.21	1.47	1.41
23	c	504	CLA	C4C-C3C	2.21	1.48	1.45
23	C	510	CLA	C4B-CHC	2.21	1.47	1.41
34	Z	101	LMG	O1-C1	2.21	1.44	1.40
23	b	607	CLA	C4B-CHC	2.20	1.47	1.41
23	B	605	CLA	CHD-C4C	2.20	1.47	1.41
23	b	607	CLA	CHD-C4C	2.20	1.47	1.41
23	A	403	CLA	C4B-CHC	2.20	1.47	1.41
23	B	608	CLA	CHD-C4C	2.20	1.47	1.41
23	B	606	CLA	C4B-CHC	2.20	1.47	1.41
23	C	515	CLA	C4C-C3C	2.20	1.48	1.45
23	b	601	CLA	C1C-NC	-2.20	1.34	1.37
23	A	407	CLA	C1B-CHB	2.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416	PHO	C4D-CHA	2.19	1.49	1.43
23	d	402	CLA	C1B-CHB	2.19	1.47	1.41
23	a	405	CLA	CHD-C4C	2.19	1.47	1.41
23	a	403	CLA	C4B-CHC	2.19	1.47	1.41
23	d	402	CLA	C4B-CHC	2.18	1.47	1.41
24	A	406	PHO	C1C-C2C	2.18	1.50	1.45
23	B	603	CLA	C4B-CHC	2.18	1.47	1.41
23	b	603	CLA	C4B-CHC	2.18	1.47	1.41
23	a	404	CLA	C4C-C3C	2.18	1.48	1.45
23	C	514	CLA	C1B-CHB	2.18	1.47	1.41
23	A	404	CLA	C1B-CHB	2.18	1.47	1.41
24	a	416	PHO	C1B-C2B	2.18	1.50	1.45
23	d	403	CLA	C1B-CHB	2.18	1.47	1.41
23	b	606	CLA	C4B-CHC	2.18	1.47	1.41
29	d	405	PL9	C2-C3	2.18	1.40	1.34
23	c	511	CLA	C4B-CHC	2.17	1.47	1.41
23	B	603	CLA	C4C-C3C	2.17	1.48	1.45
23	B	604	CLA	C1D-C2D	2.17	1.47	1.42
23	C	504	CLA	CHD-C4C	2.17	1.47	1.41
23	b	602	CLA	C1B-CHB	2.17	1.47	1.41
23	c	515	CLA	C4B-CHC	2.17	1.47	1.41
33	F	101	LMT	O1'-C1'	2.17	1.43	1.40
23	C	506	CLA	C4B-CHC	2.16	1.47	1.41
23	C	510	CLA	CHD-C4C	2.16	1.47	1.41
23	B	603	CLA	CHD-C4C	2.16	1.47	1.41
23	b	612	CLA	C4B-NB	-2.16	1.33	1.35
23	B	604	CLA	MG-NA	2.16	2.11	2.06
29	A	413[B]	PL9	C2-C3	2.16	1.40	1.34
23	b	615	CLA	C1B-CHB	2.16	1.47	1.41
23	b	616	CLA	CHD-C4C	2.15	1.47	1.41
23	c	510	CLA	C1D-C2D	2.15	1.47	1.42
23	b	616	CLA	C1D-C2D	2.15	1.47	1.42
23	B	604	CLA	C4C-C3C	2.14	1.48	1.45
23	D	404	CLA	CHD-C4C	2.14	1.47	1.41
23	B	606	CLA	MG-NA	2.14	2.11	2.06
23	a	404	CLA	C1B-CHB	2.13	1.46	1.41
23	b	606	CLA	C1B-CHB	2.13	1.46	1.41
23	C	508	CLA	C4B-CHC	2.13	1.46	1.41
23	C	510	CLA	C1C-NC	-2.13	1.34	1.37
23	B	611	CLA	CHD-C4C	2.13	1.47	1.41
33	e	101	LMT	O1'-C1'	2.13	1.43	1.40
23	a	407	CLA	CHD-C4C	2.13	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C1C-NC	-2.12	1.34	1.37
23	b	614	CLA	C4C-C3C	2.12	1.48	1.45
23	B	613	CLA	C4B-CHC	2.11	1.46	1.41
23	c	511	CLA	C1B-NB	-2.11	1.33	1.35
23	B	611	CLA	C4C-C3C	2.11	1.48	1.45
23	a	403	CLA	C4C-C3C	2.10	1.48	1.45
24	a	416	PHO	C1B-NB	-2.10	1.34	1.38
23	b	616	CLA	C1B-NB	-2.10	1.33	1.35
33	b	626	LMT	O1'-C1'	2.10	1.43	1.40
23	C	510	CLA	C1C-C2C	2.10	1.48	1.44
23	c	513	CLA	C1C-C2C	2.10	1.48	1.44
23	B	605	CLA	C1B-NB	-2.10	1.33	1.35
32	h	101	HTG	C1-S1	-2.09	1.77	1.80
23	c	513	CLA	C4C-C3C	2.09	1.48	1.45
23	b	614	CLA	CHD-C4C	2.09	1.47	1.41
24	a	416	PHO	C1A-NA	-2.09	1.33	1.37
23	d	402	CLA	C1B-NB	-2.08	1.33	1.35
23	a	403	CLA	C1B-CHB	2.08	1.46	1.41
23	A	403	CLA	CHD-C4C	2.08	1.47	1.41
23	A	404	CLA	C1B-NB	-2.08	1.33	1.35
23	A	404	CLA	C4C-C3C	2.08	1.48	1.45
40	V	201	HEC	C3C-C4C	2.08	1.46	1.43
23	b	604	CLA	C1A-CHA	2.07	1.51	1.43
23	B	611	CLA	C1B-NB	-2.07	1.33	1.35
29	a	414[B]	PL9	C2-C3	2.07	1.40	1.34
23	B	611	CLA	C4B-CHC	2.05	1.46	1.41
34	D	412	LMG	O7-C8	-2.05	1.41	1.46
23	c	508	CLA	C4C-C3C	2.05	1.48	1.45
24	a	406	PHO	C4D-CHA	2.04	1.49	1.43
23	b	615	CLA	C4B-CHC	2.04	1.46	1.41
24	A	415	PHO	C1B-NB	-2.04	1.34	1.38
23	b	605	CLA	C4C-C3C	2.04	1.48	1.45
23	c	509	CLA	C4C-C3C	2.04	1.48	1.45
23	d	403	CLA	C4C-C3C	2.04	1.48	1.45
23	D	403	CLA	C4B-CHC	2.03	1.46	1.41
23	B	613	CLA	CHD-C4C	2.03	1.46	1.41
23	b	611	CLA	C4C-C3C	2.03	1.48	1.45
35	C	519	DGD	O3G-C1D	2.03	1.43	1.40
33	a	418	LMT	O1'-C1'	2.03	1.43	1.40
23	B	601	CLA	C1B-CHB	2.03	1.46	1.41
23	B	601	CLA	C4C-C3C	2.03	1.48	1.45
23	b	610	CLA	CHD-C4C	2.02	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHD-C4C	2.02	1.46	1.41
24	a	416	PHO	C4C-C3C	2.02	1.48	1.45
23	C	506	CLA	C4C-C3C	2.02	1.48	1.45
23	b	607	CLA	C1A-CHA	2.01	1.51	1.43
32	b	621	HTG	O5-C1	2.00	1.45	1.42

All (2318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	C4A-NA-C1A	-8.14	103.05	106.71
23	b	616	CLA	C4A-NA-C1A	-7.71	103.24	106.71
23	B	615	CLA	CHD-C4C-C3C	-7.46	113.88	124.84
23	B	602	CLA	C4A-NA-C1A	-7.41	103.38	106.71
24	A	415	PHO	CMD-C2D-C1D	7.41	136.47	125.06
23	d	403	CLA	C4A-NA-C1A	-7.39	103.38	106.71
23	b	616	CLA	CHD-C4C-C3C	-7.35	114.03	124.84
26	A	409	SQD	O6-C1-C2	7.26	119.64	108.30
23	B	614	CLA	CHD-C4C-C3C	-7.18	114.28	124.84
23	b	602	CLA	C4A-NA-C1A	-7.17	103.48	106.71
24	A	406	PHO	CMD-C2D-C1D	7.14	136.07	125.06
23	B	612	CLA	CHD-C4C-C3C	-7.12	114.37	124.84
23	B	605	CLA	C4A-NA-C1A	-7.03	103.54	106.71
23	C	505	CLA	C4A-NA-C1A	-6.93	103.59	106.71
23	B	606	CLA	O2D-CGD-CBD	6.87	123.48	111.27
23	c	507	CLA	C4A-NA-C1A	-6.72	103.69	106.71
23	B	616	CLA	CHD-C4C-C3C	-6.71	114.97	124.84
29	a	414[B]	PL9	C7-C3-C4	6.65	122.28	116.88
23	B	603	CLA	CHD-C4C-C3C	-6.65	115.07	124.84
23	C	504	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	a	405	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	B	616	CLA	C4A-NA-C1A	-6.60	103.74	106.71
23	b	610	CLA	CHD-C4C-C3C	-6.60	115.13	124.84
23	b	605	CLA	CHD-C4C-C3C	-6.59	115.15	124.84
23	B	602	CLA	CHD-C4C-C3C	-6.59	115.15	124.84
23	B	605	CLA	CHD-C4C-C3C	-6.57	115.18	124.84
23	b	616	CLA	O2D-CGD-CBD	6.52	122.86	111.27
23	b	604	CLA	O2D-CGD-CBD	6.51	122.84	111.27
23	A	407	CLA	C4A-NA-C1A	-6.46	103.80	106.71
23	b	613	CLA	C2C-C1C-NC	6.44	116.01	109.97
23	B	611	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
23	C	515	CLA	CHD-C4C-C3C	-6.43	115.38	124.84
38	e	102	HEM	CAD-CBD-CGD	6.43	123.46	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	O2D-CGD-CBD	6.43	122.69	111.27
23	b	601	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
23	c	510	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
23	d	402	CLA	C2C-C1C-NC	6.40	115.97	109.97
23	b	608	CLA	C4A-NA-C1A	-6.40	103.83	106.71
23	C	510	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
23	c	515	CLA	C4A-NA-C1A	-6.39	103.83	106.71
23	b	609	CLA	CHD-C4C-C3C	-6.36	115.48	124.84
23	B	616	CLA	O2D-CGD-CBD	6.34	122.53	111.27
32	b	622	HTG	C1'-S1-C1	6.32	111.91	100.09
23	a	407	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	B	606	CLA	C4A-NA-C1A	-6.25	103.89	106.71
23	B	604	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	c	514	CLA	C4A-NA-C1A	-6.23	103.90	106.71
23	C	505	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
23	c	510	CLA	C2C-C1C-NC	6.22	115.80	109.97
23	b	614	CLA	O2D-CGD-CBD	6.20	122.28	111.27
23	c	513	CLA	CHD-C4C-C3C	-6.19	115.73	124.84
23	B	604	CLA	O2D-CGD-CBD	6.18	122.26	111.27
23	b	606	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	b	609	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	D	404	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
24	a	416	PHO	CMD-C2D-C1D	6.16	134.55	125.06
23	B	610	CLA	O2D-CGD-CBD	6.15	122.20	111.27
23	B	607	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	C	506	CLA	C2C-C1C-NC	6.15	115.73	109.97
23	C	509	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	C	510	CLA	C2C-C1C-NC	6.14	115.73	109.97
32	C	523	HTG	C1'-S1-C1	6.14	111.58	100.09
23	b	601	CLA	O2D-CGD-CBD	6.14	122.17	111.27
23	A	404	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	B	612	CLA	O2D-CGD-CBD	6.13	122.15	111.27
23	b	606	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	B	608	CLA	CHD-C4C-C3C	-6.12	115.84	124.84
23	C	503	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	b	614	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
38	E	102	HEM	CAD-CBD-CGD	6.10	122.90	112.67
23	a	404	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
23	b	602	CLA	O2D-CGD-CBD	6.06	122.04	111.27
23	D	403	CLA	C2C-C1C-NC	6.05	115.64	109.97
23	c	509	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	b	611	CLA	C4A-NA-C1A	-6.04	103.99	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
23	b	611	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	C	514	CLA	C4A-NA-C1A	-6.02	104.00	106.71
23	b	603	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
24	A	415	PHO	C3D-C2D-C1D	-6.00	97.13	105.87
23	B	601	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
26	A	409	SQD	C1-C2-C3	-5.98	97.54	110.00
25	Y	101	BCR	C33-C5-C6	-5.97	117.82	124.53
23	C	511	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
24	a	406	PHO	CMD-C2D-C1D	5.97	134.25	125.06
23	A	405	CLA	C4A-NA-C1A	-5.96	104.03	106.71
23	c	504	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
23	b	615	CLA	C2C-C1C-NC	5.96	115.56	109.97
23	c	509	CLA	O2D-CGD-CBD	5.96	121.86	111.27
23	c	507	CLA	O2D-CGD-CBD	5.95	121.85	111.27
23	b	604	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	C	503	CLA	C4A-NA-C1A	-5.94	104.03	106.71
23	B	609	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	c	511	CLA	C2C-C1C-NC	5.94	115.53	109.97
23	b	613	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	C	507	CLA	C4A-NA-C1A	-5.93	104.04	106.71
23	A	403	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	C	514	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	B	601	CLA	O2D-CGD-CBD	5.90	121.76	111.27
23	C	509	CLA	O2D-CGD-CBD	5.89	121.74	111.27
26	D	413	SQD	O6-C1-C2	5.89	117.50	108.30
23	a	403	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	606	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	c	512	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	C	512	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	c	508	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	c	505	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	C	514	CLA	O2D-CGD-CBD	5.83	121.63	111.27
23	B	609	CLA	C4A-NA-C1A	-5.82	104.09	106.71
23	C	508	CLA	C4A-NA-C1A	-5.82	104.09	106.71
23	b	611	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	c	506	CLA	C2C-C1C-NC	5.80	115.40	109.97
23	b	612	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
26	L	102	SQD	O6-C1-C2	5.79	117.33	108.30
23	C	506	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
23	B	603	CLA	O2D-CGD-CBD	5.76	121.51	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	C2D-C1D-ND	5.76	118.48	109.79
23	c	507	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
23	c	503	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
23	c	504	CLA	C2C-C1C-NC	5.75	115.36	109.97
32	D	411	HTG	C1'-S1-C1	5.75	110.85	100.09
23	b	606	CLA	O2D-CGD-CBD	5.74	121.46	111.27
23	c	514	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
24	a	416	PHO	C3D-C2D-C1D	-5.73	97.53	105.87
23	c	514	CLA	O2D-CGD-CBD	5.73	121.44	111.27
23	b	612	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	c	510	CLA	O2D-CGD-CBD	5.72	121.44	111.27
23	b	614	CLA	C2C-C1C-NC	5.71	115.32	109.97
23	C	503	CLA	O2D-CGD-CBD	5.70	121.40	111.27
23	b	603	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	a	404	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	C	510	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	B	611	CLA	C2C-C1C-NC	5.68	115.30	109.97
24	a	416	PHO	C2D-C1D-ND	5.67	118.35	109.79
23	c	506	CLA	O2D-CGD-CBD	5.66	121.33	111.27
23	B	607	CLA	C2C-C1C-NC	5.66	115.28	109.97
23	b	604	CLA	C2C-C1C-NC	5.66	115.28	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
23	a	405	CLA	C4A-NA-C1A	-5.65	104.17	106.71
23	B	613	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	b	601	CLA	C4A-NA-C1A	-5.63	104.17	106.71
26	A	409	SQD	C1-O5-C5	-5.63	102.64	113.69
29	a	414[A]	PL9	C7-C3-C4	5.63	121.45	116.88
23	C	511	CLA	C2C-C1C-NC	5.63	115.24	109.97
23	c	512	CLA	C2C-C1C-NC	5.62	115.24	109.97
23	B	612	CLA	C3C-C4C-NC	5.61	116.86	110.57
23	c	503	CLA	C2C-C1C-NC	5.61	115.22	109.97
24	a	406	PHO	O2D-CGD-CBD	5.60	121.23	111.27
32	h	101	HTG	C1'-S1-C1	5.60	110.57	100.09
23	a	403	CLA	C4A-NA-C1A	-5.60	104.19	106.71
23	d	402	CLA	CHD-C4C-C3C	-5.59	116.61	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	C	513	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
23	B	604	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	b	605	CLA	C4A-NA-C1A	-5.57	104.20	106.71
23	b	612	CLA	O2D-CGD-CBD	5.57	121.17	111.27
23	c	508	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	b	612	CLA	C4A-NA-C1A	-5.55	104.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	416	PHO	O2D-CGD-CBD	5.55	121.13	111.27
23	C	513	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	b	610	CLA	O2D-CGD-CBD	5.52	121.08	111.27
23	c	505	CLA	C2C-C1C-NC	5.51	115.14	109.97
23	B	608	CLA	C2C-C1C-NC	5.51	115.14	109.97
23	b	610	CLA	C2C-C1C-NC	5.51	115.13	109.97
26	a	409	SQD	O6-C1-C2	5.50	116.89	108.30
23	c	509	CLA	C4A-NA-C1A	-5.48	104.24	106.71
23	b	607	CLA	C2C-C1C-NC	5.47	115.09	109.97
23	A	407	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	C	512	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	B	613	CLA	C1-C2-C3	-5.42	116.67	126.04
23	C	507	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	a	403	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
23	A	405	CLA	O2D-CGD-CBD	5.41	120.89	111.27
23	d	402	CLA	C4A-NA-C1A	-5.41	104.27	106.71
23	d	403	CLA	CHD-C4C-C3C	-5.40	116.90	124.84
23	c	508	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	C	505	CLA	C2C-C1C-NC	5.39	115.02	109.97
23	C	512	CLA	O2D-CGD-CBD	5.38	120.83	111.27
23	C	511	CLA	O2D-CGD-CBD	5.38	120.82	111.27
23	B	611	CLA	O2D-CGD-CBD	5.38	120.82	111.27
23	D	404	CLA	O2D-CGD-CBD	5.38	120.82	111.27
23	D	404	CLA	C4A-NA-C1A	-5.37	104.29	106.71
26	B	620	SQD	O47-C7-C8	5.36	123.04	111.50
23	C	509	CLA	C2C-C1C-NC	5.36	114.99	109.97
23	C	507	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	B	604	CLA	C4A-NA-C1A	-5.35	104.30	106.71
32	c	523	HTG	C1'-S1-C1	5.35	110.09	100.09
23	c	515	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
23	B	603	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	B	610	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	c	511	CLA	C4A-NA-C1A	-5.31	104.32	106.71
29	A	413[A]	PL9	C7-C3-C4	5.31	121.19	116.88
23	C	508	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	B	605	CLA	O2D-CGD-CBD	5.27	120.64	111.27
25	k	102	BCR	C33-C5-C6	-5.26	118.62	124.53
23	d	403	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	B	609	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	b	615	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	b	602	CLA	C2C-C1C-NC	5.19	114.83	109.97
23	A	407	CLA	C2C-C1C-NC	5.18	114.82	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	O2D-CGD-CBD	5.16	120.45	111.27
25	D	405	BCR	C7-C8-C9	-5.15	118.46	126.23
23	A	403	CLA	CHD-C4C-C3C	-5.14	117.29	124.84
23	C	514	CLA	C2C-C1C-NC	5.13	114.78	109.97
23	B	603	CLA	C3C-C4C-NC	5.13	116.32	110.57
23	B	610	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	A	405	CLA	CHD-C4C-C3C	-5.12	117.31	124.84
26	A	409	SQD	O47-C7-C8	5.12	122.53	111.50
23	b	603	CLA	O2D-CGD-CBD	5.12	120.36	111.27
23	c	507	CLA	C2C-C1C-NC	5.12	114.76	109.97
23	a	407	CLA	O2D-CGD-CBD	5.11	120.35	111.27
23	b	607	CLA	C4A-NA-C1A	-5.11	104.41	106.71
23	a	407	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	B	615	CLA	C4A-NA-C1A	-5.10	104.41	106.71
24	a	416	PHO	C1-C2-C3	-5.10	117.23	126.04
32	B	622	HTG	C1'-S1-C1	5.09	109.61	100.09
23	C	512	CLA	C4A-NA-C1A	-5.08	104.42	106.71
23	c	513	CLA	C2C-C1C-NC	5.08	114.73	109.97
23	b	608	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
23	B	606	CLA	C2C-C1C-NC	5.06	114.72	109.97
23	b	615	CLA	CHD-C4C-C3C	-5.06	117.39	124.84
23	B	607	CLA	C4A-NA-C1A	-5.06	104.43	106.71
40	V	201	HEC	CBD-CAD-C3D	-5.06	103.15	112.49
23	c	505	CLA	C4A-NA-C1A	-5.06	104.43	106.71
23	C	510	CLA	C3C-C4C-NC	5.05	116.24	110.57
24	a	406	PHO	C3D-C2D-C1D	-5.05	98.51	105.87
23	A	405	CLA	C2C-C1C-NC	5.05	114.70	109.97
23	c	513	CLA	O2D-CGD-CBD	5.05	120.24	111.27
26	f	101	SQD	O47-C7-C8	5.05	122.38	111.50
23	b	607	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	c	515	CLA	C2C-C1C-NC	5.02	114.67	109.97
23	B	615	CLA	C3C-C4C-NC	5.01	116.19	110.57
23	c	505	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	B	610	CLA	CHD-C4C-C3C	-5.00	117.49	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.00	117.50	124.84
23	c	511	CLA	O2D-CGD-CBD	4.96	120.09	111.27
23	C	503	CLA	C2C-C1C-NC	4.96	114.62	109.97
23	D	403	CLA	CHD-C4C-C3C	-4.95	117.56	124.84
23	C	515	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	C	508	CLA	CHD-C4C-C3C	-4.94	117.58	124.84
23	c	511	CLA	CHD-C4C-C3C	-4.93	117.59	124.84
23	A	404	CLA	O2D-CGD-CBD	4.91	120.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	413	SQD	C44-O6-C1	-4.91	104.14	113.74
26	L	102	SQD	O47-C7-C8	4.91	122.08	111.50
23	b	611	CLA	O2D-CGD-CBD	4.90	119.98	111.27
23	b	603	CLA	C4A-NA-C1A	-4.90	104.50	106.71
23	a	407	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	B	615	CLA	C2C-C1C-NC	4.89	114.55	109.97
23	B	604	CLA	C3C-C4C-NC	4.89	116.05	110.57
23	B	613	CLA	C3C-C4C-NC	4.88	116.04	110.57
23	A	404	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	A	403	CLA	CAA-C2A-C3A	-4.85	99.49	112.78
23	B	603	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	b	613	CLA	C1-C2-C3	-4.85	117.65	126.04
23	a	403	CLA	C1D-CHD-C4C	-4.85	116.16	122.56
23	b	605	CLA	O2D-CGD-CBD	4.84	119.87	111.27
23	b	610	CLA	C3C-C4C-NC	4.84	116.00	110.57
23	C	515	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	b	613	CLA	C3C-C4C-NC	4.83	115.99	110.57
23	C	504	CLA	O2D-CGD-CBD	4.83	119.84	111.27
23	C	506	CLA	C3C-C4C-NC	4.83	115.98	110.57
23	b	605	CLA	C2C-C1C-NC	4.82	114.48	109.97
23	c	514	CLA	C2C-C1C-NC	4.79	114.46	109.97
23	C	504	CLA	C3C-C4C-NC	4.78	115.93	110.57
23	C	508	CLA	O2D-CGD-CBD	4.78	119.75	111.27
25	b	617	BCR	C7-C8-C9	-4.77	119.03	126.23
23	B	601	CLA	C4A-NA-C1A	-4.75	104.57	106.71
26	D	413	SQD	O47-C7-C8	4.75	121.73	111.50
23	b	601	CLA	C2C-C1C-NC	4.75	114.42	109.97
23	b	614	CLA	C4A-NA-C1A	-4.74	104.58	106.71
24	A	406	PHO	C3D-C2D-C1D	-4.74	98.97	105.87
23	B	616	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	c	505	CLA	C3C-C4C-NC	4.73	115.87	110.57
23	b	616	CLA	C1D-CHD-C4C	-4.72	116.33	122.56
24	a	406	PHO	C2D-C1D-ND	4.72	116.91	109.79
23	C	509	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	C	504	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	B	612	CLA	O2D-CGD-O1D	-4.70	114.65	123.84
23	c	512	CLA	O2D-CGD-CBD	4.70	119.62	111.27
23	B	608	CLA	O2D-CGD-CBD	4.69	119.60	111.27
23	C	506	CLA	O2D-CGD-CBD	4.69	119.59	111.27
23	B	604	CLA	C1D-CHD-C4C	-4.68	116.38	122.56
32	B	621	HTG	O5-C1-C2	4.68	116.20	110.31
23	b	603	CLA	C1D-CHD-C4C	-4.68	116.38	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	PHO	C2D-C1D-ND	4.68	116.85	109.79
29	a	414[A]	PL9	C15-C14-C16	4.68	123.14	115.27
23	a	404	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	c	503	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	a	405	CLA	C2C-C1C-NC	4.66	114.33	109.97
23	c	510	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	B	602	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	B	611	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
23	C	515	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	b	608	CLA	O2D-CGD-CBD	4.64	119.52	111.27
23	a	407	CLA	C3C-C4C-NC	4.64	115.78	110.57
23	b	605	CLA	C4-C3-C5	4.64	123.08	115.27
23	c	507	CLA	C3C-C4C-NC	4.63	115.76	110.57
23	B	607	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	b	608	CLA	C2C-C1C-NC	4.61	114.29	109.97
23	B	607	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	503	CLA	O2D-CGD-CBD	4.60	119.44	111.27
23	B	614	CLA	C2C-C1C-NC	4.59	114.28	109.97
23	B	612	CLA	C2C-C1C-NC	4.59	114.27	109.97
23	b	606	CLA	C2C-C1C-NC	4.58	114.26	109.97
23	C	515	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	D	404	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	b	616	CLA	C3C-C4C-NC	4.58	115.70	110.57
23	d	402	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
29	a	414[A]	PL9	C37-C38-C39	-4.57	116.66	127.66
23	a	404	CLA	C4A-NA-C1A	-4.57	104.65	106.71
23	b	609	CLA	C3C-C4C-NC	4.57	115.69	110.57
23	c	509	CLA	CMC-C2C-C1C	4.56	131.99	125.04
23	C	511	CLA	C3C-C4C-NC	4.56	115.68	110.57
23	D	403	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
23	C	506	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	c	504	CLA	O2D-CGD-CBD	4.53	119.33	111.27
23	C	511	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	a	404	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
23	B	609	CLA	C3C-C4C-NC	4.53	115.65	110.57
24	A	415	PHO	C1-C2-C3	-4.52	118.22	126.04
26	a	409	SQD	O47-C7-C8	4.52	121.24	111.50
25	b	619	BCR	C38-C26-C25	-4.52	119.46	124.53
23	C	503	CLA	C1D-CHD-C4C	-4.52	116.60	122.56
24	A	415	PHO	C4C-C3C-C2C	-4.51	101.79	106.78
23	b	614	CLA	C3C-C4C-NC	4.50	115.61	110.57
23	a	403	CLA	C1C-C2C-C3C	-4.49	102.23	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	CMC-C2C-C1C	4.48	131.86	125.04
23	c	505	CLA	C1D-CHD-C4C	-4.48	116.64	122.56
23	B	605	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	B	614	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	B	602	CLA	CMC-C2C-C1C	4.46	131.83	125.04
23	a	405	CLA	C3C-C4C-NC	4.45	115.56	110.57
23	b	612	CLA	C3C-C4C-NC	4.45	115.56	110.57
23	c	509	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	c	511	CLA	CAC-C3C-C4C	4.44	130.58	124.81
23	B	611	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	c	508	CLA	O2D-CGD-CBD	4.43	119.15	111.27
23	b	603	CLA	C3C-C4C-NC	4.43	115.54	110.57
25	B	618	BCR	C15-C14-C13	-4.42	121.00	127.31
23	B	602	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	D	403	CLA	C1-C2-C3	-4.42	118.40	126.04
25	c	517	BCR	C7-C8-C9	-4.41	119.58	126.23
23	C	506	CLA	C1C-C2C-C3C	-4.41	102.33	106.96
23	b	613	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
23	b	609	CLA	O2D-CGD-CBD	4.39	119.08	111.27
26	B	620	SQD	O6-C1-C2	4.39	115.16	108.30
29	A	413[A]	PL9	C15-C14-C16	4.39	122.66	115.27
34	C	522	LMG	O6-C5-C4	4.39	117.67	109.69
23	b	610	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	C	504	CLA	C2C-C1C-NC	4.38	114.08	109.97
23	C	513	CLA	O2D-CGD-CBD	4.38	119.06	111.27
23	C	507	CLA	C3C-C4C-NC	4.38	115.48	110.57
23	b	604	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
23	d	402	CLA	C3C-C4C-NC	4.37	115.47	110.57
23	D	404	CLA	C2C-C1C-NC	4.37	114.06	109.97
25	d	404	BCR	C7-C8-C9	-4.36	119.65	126.23
23	b	607	CLA	C3C-C4C-NC	4.35	115.44	110.57
23	b	616	CLA	OBD-CAD-C3D	-4.34	120.78	127.98
23	c	504	CLA	C1C-C2C-C3C	-4.34	102.40	106.96
23	B	611	CLA	C1-C2-C3	-4.33	118.55	126.04
23	B	611	CLA	C4A-NA-C1A	-4.33	104.76	106.71
23	b	604	CLA	C3C-C4C-NC	4.32	115.42	110.57
23	C	510	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
24	A	406	PHO	O2D-CGD-CBD	4.32	118.94	111.27
25	d	404	BCR	C15-C14-C13	-4.31	121.16	127.31
23	b	606	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
23	c	511	CLA	C1-C2-C3	-4.31	118.59	126.04
23	b	609	CLA	C2C-C1C-NC	4.30	114.00	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C2C-C1C-NC	4.29	113.99	109.97
34	M	101	LMG	O7-C10-C11	4.28	120.73	111.50
23	b	611	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	B	606	CLA	C3C-C4C-NC	4.28	115.37	110.57
34	Z	101	LMG	O7-C10-C11	4.26	120.69	111.50
23	c	503	CLA	C3C-C4C-NC	4.26	115.35	110.57
29	a	414[B]	PL9	C7-C3-C2	-4.26	117.70	123.30
33	C	526	LMT	C1'-O5'-C5'	4.26	122.05	113.69
23	a	407	CLA	OBD-CAD-C3D	-4.26	120.91	127.98
23	C	508	CLA	CAC-C3C-C4C	4.25	130.33	124.81
29	A	413[B]	PL9	C15-C14-C16	4.25	122.42	115.27
25	T	101	BCR	C15-C16-C17	-4.25	114.77	123.47
34	C	522	LMG	O7-C10-C11	4.23	120.62	111.50
31	A	416	LHG	O7-C7-C8	4.23	120.61	111.50
23	A	404	CLA	CBC-CAC-C3C	-4.22	100.80	112.43
23	B	610	CLA	CAC-C3C-C4C	4.22	130.28	124.81
23	B	614	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
23	B	613	CLA	C3B-C4B-NB	4.21	114.66	109.21
23	b	613	CLA	C3B-C4B-NB	4.20	114.65	109.21
26	A	409	SQD	O9-S-C6	4.20	111.93	106.94
33	F	101	LMT	C1B-O5B-C5B	4.20	121.93	113.69
23	C	514	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	C	505	CLA	C1D-CHD-C4C	-4.19	117.03	122.56
23	B	612	CLA	C4A-NA-C1A	-4.19	104.82	106.71
29	a	414[B]	PL9	C37-C38-C39	-4.19	117.58	127.66
38	e	102	HEM	CBD-CAD-C3D	-4.18	104.77	112.48
23	B	601	CLA	C2C-C1C-NC	4.18	113.89	109.97
23	b	606	CLA	C1D-CHD-C4C	-4.18	117.04	122.56
23	C	510	CLA	C1D-CHD-C4C	-4.18	117.04	122.56
23	b	605	CLA	C3C-C4C-NC	4.18	115.25	110.57
23	B	615	CLA	C1D-CHD-C4C	-4.17	117.05	122.56
23	A	403	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	c	510	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	b	610	CLA	C1D-CHD-C4C	-4.17	117.06	122.56
23	c	510	CLA	C1D-CHD-C4C	-4.16	117.07	122.56
23	B	609	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	B	614	CLA	C1D-CHD-C4C	-4.16	117.07	122.56
34	a	417	LMG	O7-C10-C11	4.15	120.45	111.50
29	D	406	PL9	C42-C43-C44	-4.15	117.67	127.66
33	a	412	LMT	C1B-O5B-C5B	4.15	121.83	113.69
23	c	510	CLA	C1-C2-C3	-4.15	118.87	126.04
23	A	407	CLA	C1C-C2C-C3C	-4.14	102.60	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413[B]	PL9	C37-C38-C39	-4.13	117.71	127.66
31	D	408	LHG	O7-C7-C8	4.13	120.40	111.50
25	b	617	BCR	C33-C5-C6	-4.13	119.89	124.53
23	c	505	CLA	CAC-C3C-C4C	4.13	130.16	124.81
23	c	506	CLA	C4A-NA-C1A	-4.12	104.85	106.71
23	A	404	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
23	C	512	CLA	C1-C2-C3	-4.12	118.92	126.04
23	c	514	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	C	512	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
23	B	608	CLA	C3C-C4C-NC	4.12	115.19	110.57
29	A	413[B]	PL9	C7-C3-C4	4.12	120.22	116.88
40	v	202	HEC	CBD-CAD-C3D	-4.11	104.90	112.49
23	c	512	CLA	C4A-NA-C1A	-4.09	104.87	106.71
23	C	505	CLA	C3C-C4C-NC	4.09	115.16	110.57
23	c	513	CLA	C3C-C4C-NC	4.09	115.16	110.57
23	C	513	CLA	C4A-NA-C1A	-4.08	104.87	106.71
23	A	403	CLA	O2A-CGA-CBA	4.07	124.69	111.91
29	a	414[A]	PL9	C7-C3-C2	-4.07	117.95	123.30
23	b	610	CLA	C1-C2-C3	-4.06	119.01	126.04
23	b	601	CLA	C1D-CHD-C4C	-4.06	117.19	122.56
23	d	402	CLA	O2D-CGD-CBD	4.06	118.49	111.27
25	B	631	BCR	C33-C5-C6	-4.06	119.97	124.53
23	c	504	CLA	C4A-NA-C1A	-4.05	104.88	106.71
25	d	404	BCR	C38-C26-C25	-4.05	119.98	124.53
23	b	614	CLA	O2D-CGD-O1D	-4.05	115.93	123.84
25	K	101	BCR	C7-C8-C9	-4.04	120.12	126.23
23	a	403	CLA	CAA-C2A-C3A	-4.04	101.71	112.78
23	d	403	CLA	C2C-C1C-NC	4.03	113.74	109.97
23	C	503	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	C	505	CLA	O2D-CGD-CBD	4.02	118.41	111.27
31	E	101	LHG	O7-C7-C8	4.02	120.16	111.50
32	h	101	HTG	O5-C5-C4	4.02	116.99	109.69
23	C	513	CLA	C3B-C4B-NB	4.02	114.40	109.21
23	c	513	CLA	O2D-CGD-O1D	-4.02	115.99	123.84
23	c	513	CLA	C1-C2-C3	-4.01	119.10	126.04
23	B	616	CLA	C2C-C1C-NC	4.00	113.72	109.97
34	C	502	LMG	O7-C10-C11	4.00	120.12	111.50
23	A	407	CLA	C1-C2-C3	-4.00	119.13	126.04
23	c	503	CLA	C1C-C2C-C3C	-4.00	102.76	106.96
23	c	508	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	b	601	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	c	512	CLA	C1C-C2C-C3C	-3.98	102.77	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413[B]	PL9	C10-C9-C11	3.98	121.96	115.27
23	b	603	CLA	C3B-C4B-NB	3.98	114.35	109.21
23	b	612	CLA	C1-C2-C3	-3.97	119.17	126.04
23	B	606	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
23	C	513	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	c	515	CLA	O2D-CGD-CBD	3.97	118.32	111.27
23	A	403	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	B	608	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	a	416	PHO	C4C-C3C-C2C	-3.97	102.39	106.78
23	B	607	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
34	c	522	LMG	O7-C10-C11	3.96	120.04	111.50
29	A	413[A]	PL9	C37-C38-C39	-3.96	118.13	127.66
38	E	102	HEM	CBA-CAA-C2A	-3.96	105.19	112.49
23	b	611	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
23	C	512	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	c	504	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	610	CLA	O2A-CGA-CBA	3.94	124.28	111.91
26	a	409	SQD	C44-O6-C1	-3.94	106.04	113.74
23	c	506	CLA	C3B-C4B-NB	3.94	114.30	109.21
29	A	413[A]	PL9	C27-C28-C29	-3.94	118.18	127.66
25	Y	101	BCR	C37-C22-C23	3.93	124.28	118.08
24	a	416	PHO	C4-C3-C5	3.93	121.88	115.27
23	B	602	CLA	C2C-C1C-NC	3.93	113.65	109.97
40	V	201	HEC	CMB-C2B-C1B	-3.93	122.43	128.46
25	C	517	BCR	C7-C8-C9	-3.93	120.30	126.23
23	c	506	CLA	C3C-C4C-NC	3.92	114.97	110.57
34	Z	101	LMG	C1-C2-C3	3.92	118.16	110.00
23	b	614	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
23	C	510	CLA	C3B-C4B-NB	3.92	114.28	109.21
23	b	613	CLA	O2A-CGA-O1A	-3.92	113.71	123.59
25	k	102	BCR	C15-C14-C13	-3.91	121.73	127.31
23	a	404	CLA	C1D-CHD-C4C	-3.91	117.40	122.56
23	b	612	CLA	C3B-C4B-NB	3.90	114.25	109.21
31	d	406	LHG	O7-C7-C8	3.90	119.91	111.50
23	B	615	CLA	C4D-C3D-CAD	-3.90	106.30	108.47
23	c	513	CLA	C4A-NA-C1A	-3.90	104.95	106.71
23	c	515	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	B	610	CLA	O2A-CGA-CBA	3.89	124.11	111.91
23	c	512	CLA	C1D-CHD-C4C	-3.89	117.43	122.56
23	B	612	CLA	CAC-C3C-C4C	3.88	129.85	124.81
25	T	101	BCR	C11-C10-C9	-3.88	121.77	127.31
23	C	515	CLA	C1-C2-C3	-3.88	119.34	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	O2D-CGD-CBD	3.87	118.15	111.27
23	B	613	CLA	C4A-NA-C1A	-3.86	104.97	106.71
31	d	408	LHG	O7-C7-C8	3.86	119.82	111.50
23	c	510	CLA	C4A-NA-C1A	-3.86	104.97	106.71
23	c	512	CLA	C3B-C4B-NB	3.86	114.20	109.21
23	A	407	CLA	O2D-CGD-CBD	3.86	118.13	111.27
23	b	602	CLA	CAC-C3C-C4C	3.85	129.81	124.81
23	B	602	CLA	CAA-C2A-C3A	-3.85	102.24	112.78
23	b	616	CLA	CHD-C4C-NC	3.85	130.27	124.20
23	C	511	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	c	511	CLA	C3B-C4B-NB	3.85	114.19	109.21
23	a	405	CLA	O2D-CGD-CBD	3.85	118.10	111.27
25	K	101	BCR	C24-C23-C22	-3.85	120.42	126.23
35	C	519	DGD	O2G-C1B-C2B	3.83	119.77	111.50
23	b	612	CLA	O2D-CGD-O1D	-3.83	116.34	123.84
23	C	510	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	b	606	CLA	C3C-C4C-NC	3.83	114.87	110.57
23	b	612	CLA	CMB-C2B-C3B	3.83	131.84	124.68
25	D	405	BCR	C38-C26-C25	-3.83	120.23	124.53
23	c	512	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	B	610	CLA	O2D-CGD-O1D	-3.82	116.37	123.84
23	b	608	CLA	C1-C2-C3	-3.82	119.43	126.04
26	A	411	SQD	C3-C4-C5	3.82	117.05	110.24
23	c	511	CLA	C3C-C4C-NC	3.82	114.85	110.57
23	c	503	CLA	O2D-CGD-O1D	-3.82	116.38	123.84
25	d	404	BCR	C28-C27-C26	-3.81	107.27	114.08
23	D	403	CLA	C3C-C4C-NC	3.81	114.85	110.57
25	h	102	BCR	C7-C8-C9	-3.81	120.47	126.23
32	B	624	HTG	C1'-S1-C1	3.81	107.21	100.09
23	b	616	CLA	O2D-CGD-O1D	-3.80	116.40	123.84
23	b	614	CLA	C1D-CHD-C4C	-3.80	117.54	122.56
23	c	511	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
25	A	408	BCR	C24-C23-C22	-3.80	120.49	126.23
23	d	402	CLA	C3B-C4B-NB	3.80	114.12	109.21
26	a	411	SQD	O7-S-C6	3.80	111.45	106.94
26	A	409	SQD	C44-O6-C1	-3.80	106.32	113.74
23	b	616	CLA	C2C-C1C-NC	3.80	113.53	109.97
23	B	601	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	C	504	CLA	C1-C2-C3	-3.79	119.48	126.04
23	a	403	CLA	O2D-CGD-CBD	3.79	118.00	111.27
23	B	602	CLA	C1D-CHD-C4C	-3.79	117.56	122.56
23	b	603	CLA	C1C-C2C-C3C	-3.79	102.97	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C1-C2-C3	-3.78	119.50	126.04
23	A	407	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	B	605	CLA	C4-C3-C5	3.78	121.62	115.27
34	C	522	LMG	C3-C4-C5	3.77	116.97	110.24
23	c	508	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	C	514	CLA	C1D-CHD-C4C	-3.77	117.58	122.56
23	a	404	CLA	C3C-C4C-NC	3.76	114.79	110.57
23	B	614	CLA	CHD-C4C-NC	3.76	130.13	124.20
29	A	413[B]	PL9	C32-C33-C34	-3.76	118.61	127.66
23	b	615	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	c	506	CLA	CAC-C3C-C4C	3.76	129.69	124.81
23	c	508	CLA	C1D-CHD-C4C	-3.76	117.60	122.56
35	c	519	DGD	O2G-C1B-C2B	3.75	119.59	111.50
23	D	403	CLA	O2D-CGD-CBD	3.75	117.94	111.27
23	b	610	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
35	C	518	DGD	O1G-C1A-C2A	3.75	123.68	111.91
25	a	408	BCR	C24-C23-C22	-3.75	120.56	126.23
23	b	614	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	B	608	CLA	C1D-CHD-C4C	-3.75	117.61	122.56
23	b	608	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	B	604	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
23	b	602	CLA	C1-C2-C3	-3.75	119.56	126.04
23	C	515	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
25	H	101	BCR	C38-C26-C25	-3.74	120.33	124.53
23	b	605	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
23	C	506	CLA	C1D-CHD-C4C	-3.74	117.62	122.56
23	a	407	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	509	CLA	C4A-NA-C1A	-3.73	105.03	106.71
40	v	202	HEC	CBA-CAA-C2A	-3.73	105.61	112.48
23	a	405	CLA	CMC-C2C-C1C	3.73	130.72	125.04
26	a	411	SQD	O47-C7-C8	3.73	119.54	111.50
23	b	612	CLA	CAC-C3C-C4C	3.73	129.65	124.81
23	b	607	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
23	a	403	CLA	C3C-C4C-NC	3.73	114.75	110.57
23	A	403	CLA	O2A-CGA-O1A	-3.72	114.20	123.59
23	c	510	CLA	O2D-CGD-O1D	-3.72	116.57	123.84
33	M	103	LMT	C1'-O5'-C5'	3.72	120.98	113.69
23	b	613	CLA	O2A-CGA-CBA	3.71	123.56	111.91
34	z	101	LMG	O7-C10-C11	3.71	119.50	111.50
25	C	516	BCR	C7-C8-C9	-3.71	120.63	126.23
23	b	606	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
23	B	612	CLA	C1-C2-C3	-3.71	119.62	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	OBD-CAD-C3D	-3.71	121.82	127.98
34	c	522	LMG	O6-C5-C4	3.71	116.43	109.69
26	a	409	SQD	C1-C2-C3	-3.71	102.27	110.00
29	d	405	PL9	C40-C39-C41	3.71	121.51	115.27
26	D	413	SQD	C1-O5-C5	-3.71	106.41	113.69
23	b	615	CLA	O2D-CGD-CBD	3.71	117.85	111.27
26	a	409	SQD	O8-S-C6	3.70	111.64	105.74
31	L	101	LHG	O7-C7-C8	3.70	119.48	111.50
23	c	509	CLA	C3C-C4C-NC	3.70	114.72	110.57
40	v	202	HEC	CMC-C2C-C1C	-3.70	122.78	128.46
29	a	414[A]	PL9	C27-C28-C29	-3.69	118.76	127.66
23	B	610	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	C	510	CLA	C4C-C3C-C2C	-3.69	101.52	106.90
23	B	611	CLA	C3B-C4B-NB	3.69	113.98	109.21
23	B	603	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	a	403	CLA	C3B-C4B-NB	3.69	113.98	109.21
23	c	509	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
25	Y	101	BCR	C16-C17-C18	-3.68	122.06	127.31
23	B	608	CLA	C4A-NA-C1A	-3.68	105.05	106.71
25	C	516	BCR	C16-C17-C18	-3.68	122.06	127.31
23	c	514	CLA	C1D-CHD-C4C	-3.68	117.71	122.56
23	C	513	CLA	C1D-CHD-C4C	-3.68	117.71	122.56
23	c	510	CLA	C3B-C4B-NB	3.67	113.95	109.21
23	b	612	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
23	B	615	CLA	CED-O2D-CGD	3.67	124.23	115.94
23	a	403	CLA	CAC-C3C-C4C	3.66	129.56	124.81
23	B	610	CLA	CAA-C2A-C3A	-3.66	102.75	112.78
23	b	602	CLA	C3C-C4C-NC	3.66	114.68	110.57
23	A	404	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	b	604	CLA	C3B-C4B-NB	3.66	113.94	109.21
23	c	512	CLA	CBC-CAC-C3C	-3.66	102.35	112.43
23	B	606	CLA	C3B-C4B-NB	3.65	113.93	109.21
23	B	603	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
34	c	521	LMG	O7-C10-C11	3.65	119.36	111.50
23	d	402	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
23	B	612	CLA	C1D-CHD-C4C	-3.64	117.75	122.56
23	B	607	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
23	b	606	CLA	C1-C2-C3	-3.64	119.75	126.04
23	B	613	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
32	b	621	HTG	C1-O5-C5	3.64	119.29	112.58
23	C	505	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
25	b	619	BCR	C11-C10-C9	-3.64	122.12	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	CHD-C4C-NC	3.64	129.93	124.20
34	m	101	LMG	O7-C10-C11	3.64	119.33	111.50
23	A	403	CLA	CAC-C3C-C4C	3.63	129.53	124.81
23	b	612	CLA	C1D-CHD-C4C	-3.63	117.76	122.56
35	C	518	DGD	O2G-C1B-C2B	3.63	119.33	111.50
23	B	608	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
23	A	405	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	c	506	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	C	508	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	b	613	CLA	O2D-CGD-CBD	3.63	117.71	111.27
23	D	404	CLA	CAC-C3C-C4C	3.62	129.51	124.81
23	C	514	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	C	513	CLA	CAC-C3C-C4C	3.61	129.50	124.81
23	B	608	CLA	C3B-C4B-NB	3.61	113.88	109.21
23	b	607	CLA	C3B-C4B-NB	3.61	113.87	109.21
26	a	409	SQD	C1-O5-C5	-3.61	106.61	113.69
23	C	503	CLA	C1C-C2C-C3C	-3.61	103.17	106.96
23	B	605	CLA	C1D-CHD-C4C	-3.61	117.80	122.56
38	E	102	HEM	CBD-CAD-C3D	-3.60	105.84	112.48
23	B	606	CLA	C1D-CHD-C4C	-3.60	117.80	122.56
23	a	405	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	C	505	CLA	C1-C2-C3	-3.60	119.82	126.04
23	A	403	CLA	CMB-C2B-C3B	3.60	131.41	124.68
29	d	405	PL9	C42-C43-C44	-3.60	119.00	127.66
23	B	613	CLA	CAC-C3C-C4C	3.60	129.47	124.81
23	C	513	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	A	404	CLA	C3C-C4C-NC	3.59	114.60	110.57
25	C	516	BCR	C15-C14-C13	-3.59	122.18	127.31
23	c	513	CLA	C3B-C4B-NB	3.59	113.85	109.21
23	B	615	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	b	615	CLA	C3B-C4B-NB	3.59	113.85	109.21
35	c	518	DGD	O2G-C1B-C2B	3.59	119.23	111.50
23	C	511	CLA	C1D-CHD-C4C	-3.59	117.83	122.56
23	c	515	CLA	C1D-CHD-C4C	-3.59	117.83	122.56
23	B	614	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	c	514	CLA	CAC-C3C-C4C	3.58	129.46	124.81
25	c	516	BCR	C11-C10-C9	-3.58	122.20	127.31
35	C	520	DGD	O2G-C1B-C2B	3.58	119.21	111.50
34	C	521	LMG	O7-C10-C11	3.58	119.21	111.50
23	B	604	CLA	C1C-C2C-C3C	-3.58	103.20	106.96
23	b	605	CLA	C1D-CHD-C4C	-3.57	117.84	122.56
23	c	513	CLA	C1D-CHD-C4C	-3.57	117.85	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	PHO	CHC-C1C-C2C	-3.57	116.75	125.73
25	d	404	BCR	C33-C5-C6	-3.57	120.52	124.53
23	B	612	CLA	C4C-C3C-C2C	-3.56	101.71	106.90
23	c	506	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
23	c	507	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	c	508	CLA	C1-C2-C3	-3.56	119.89	126.04
23	c	510	CLA	C4D-C3D-CAD	-3.55	106.49	108.47
23	C	506	CLA	C3B-C4B-NB	3.55	113.81	109.21
25	C	517	BCR	C3-C4-C5	-3.55	107.73	114.08
33	b	626	LMT	C1'-O5'-C5'	3.55	120.66	113.69
23	b	615	CLA	C3C-C4C-NC	3.55	114.56	110.57
23	b	610	CLA	O2A-CGA-O1A	-3.55	114.63	123.59
29	A	413[A]	PL9	C20-C19-C21	3.55	121.24	115.27
23	b	603	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
23	C	509	CLA	C1D-CHD-C4C	-3.55	117.88	122.56
23	b	607	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
23	b	608	CLA	C3B-C4B-NB	3.54	113.79	109.21
26	A	411	SQD	O47-C7-C8	3.54	119.14	111.50
29	A	413[A]	PL9	C25-C24-C26	3.54	121.23	115.27
23	b	602	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
24	A	415	PHO	C4-C3-C5	3.54	121.23	115.27
23	B	604	CLA	O2A-CGA-O1A	-3.54	114.66	123.59
23	B	614	CLA	C4A-NA-C1A	-3.54	105.12	106.71
23	b	611	CLA	C3B-C4B-NB	3.54	113.78	109.21
25	b	619	BCR	C39-C30-C25	-3.54	104.56	110.30
25	b	619	BCR	C15-C14-C13	-3.54	122.26	127.31
31	A	416	LHG	O8-C23-O10	-3.53	114.67	123.59
23	B	603	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	c	508	CLA	C3B-C4B-NB	3.52	113.77	109.21
23	b	614	CLA	C1-C2-C3	-3.52	119.95	126.04
23	C	507	CLA	CAC-C3C-C4C	3.52	129.38	124.81
23	B	604	CLA	C1-C2-C3	-3.52	119.95	126.04
23	B	602	CLA	CAC-C3C-C4C	3.52	129.38	124.81
23	b	606	CLA	C4-C3-C5	3.52	121.19	115.27
24	a	416	PHO	O2D-CGD-O1D	-3.52	116.96	123.84
23	C	512	CLA	C1D-CHD-C4C	-3.52	117.92	122.56
23	B	609	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
23	b	609	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
26	B	620	SQD	C3-C4-C5	3.51	116.50	110.24
23	b	602	CLA	O2D-CGD-O1D	-3.51	116.98	123.84
32	b	624	HTG	C1'-S1-C1	3.50	106.65	100.09
23	B	606	CLA	C1C-C2C-C3C	-3.50	103.27	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
23	b	608	CLA	CBC-CAC-C3C	-3.50	102.78	112.43
33	M	103	LMT	O5'-C5'-C4'	3.50	117.13	109.75
23	a	407	CLA	C3B-C4B-NB	3.50	113.73	109.21
23	C	509	CLA	C4C-C3C-C2C	-3.49	101.80	106.90
23	C	510	CLA	C4A-NA-C1A	-3.49	105.14	106.71
23	b	604	CLA	C4A-NA-C1A	-3.49	105.14	106.71
26	L	102	SQD	C1-C2-C3	-3.49	102.72	110.00
23	d	402	CLA	C4-C3-C5	3.49	121.14	115.27
29	A	413[B]	PL9	C7-C8-C9	-3.49	120.98	126.79
23	B	613	CLA	CMC-C2C-C1C	3.48	130.34	125.04
26	a	411	SQD	O48-C23-C24	3.48	122.82	111.91
23	a	404	CLA	O2D-CGD-O1D	-3.48	117.04	123.84
23	C	508	CLA	C1-C2-C3	-3.48	120.03	126.04
23	B	610	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	c	515	CLA	C3B-C4B-NB	3.48	113.70	109.21
29	A	413[B]	PL9	C27-C28-C29	-3.47	119.29	127.66
24	A	406	PHO	C4D-CHA-C1A	-3.47	117.55	125.37
23	D	404	CLA	C3B-C4B-NB	3.47	113.70	109.21
23	b	612	CLA	C4-C3-C5	3.47	121.10	115.27
29	a	414[B]	PL9	C25-C24-C26	3.47	121.10	115.27
23	A	404	CLA	CAA-C2A-C3A	-3.47	103.29	112.78
23	a	407	CLA	O2D-CGD-O1D	-3.46	117.06	123.84
23	C	508	CLA	C3C-C4C-NC	3.46	114.45	110.57
23	D	404	CLA	C1D-CHD-C4C	-3.46	118.00	122.56
34	D	412	LMG	O7-C10-C11	3.46	118.95	111.50
23	C	514	CLA	C3B-C4B-NB	3.45	113.67	109.21
23	c	507	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	B	616	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
23	A	403	CLA	C4A-NA-C1A	-3.45	105.16	106.71
23	c	515	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
32	V	202	HTG	C1-O5-C5	3.45	116.86	112.19
23	c	505	CLA	C4C-C3C-C2C	-3.45	101.88	106.90
23	b	605	CLA	O2A-CGA-O1A	-3.44	114.91	123.59
23	b	601	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
25	k	101	BCR	C24-C23-C22	-3.44	121.04	126.23
23	c	504	CLA	CMC-C2C-C1C	3.44	130.27	125.04
25	Y	101	BCR	C15-C14-C13	-3.43	122.41	127.31
23	A	405	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
23	A	404	CLA	C1D-CHD-C4C	-3.43	118.03	122.56
23	A	405	CLA	O2A-CGA-O1A	-3.43	114.94	123.59
23	C	508	CLA	O2D-CGD-O1D	-3.43	117.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	CHC-C1C-C2C	-3.42	117.26	126.72
23	b	605	CLA	CHD-C4C-NC	3.42	129.59	124.20
23	b	609	CLA	C1-C2-C3	-3.42	120.13	126.04
25	b	619	BCR	C34-C9-C10	-3.41	118.14	122.92
23	B	615	CLA	CMC-C2C-C1C	3.41	130.23	125.04
23	d	402	CLA	C1-C2-C3	-3.41	120.15	126.04
23	A	405	CLA	C3C-C4C-NC	3.41	114.39	110.57
23	b	607	CLA	C1D-CHD-C4C	-3.41	118.06	122.56
23	C	511	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
23	A	403	CLA	C3B-C4B-NB	3.40	113.60	109.21
23	C	504	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
23	A	404	CLA	CHD-C4C-NC	3.40	129.56	124.20
23	b	601	CLA	CHD-C4C-NC	3.40	129.56	124.20
23	C	511	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
23	b	601	CLA	C3B-C4B-NB	3.40	113.60	109.21
31	b	628	LHG	O7-C7-C8	3.40	118.82	111.50
25	c	517	BCR	C33-C5-C6	-3.39	120.72	124.53
23	b	616	CLA	CMC-C2C-C1C	3.39	130.21	125.04
23	B	616	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
23	C	509	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	c	505	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
23	b	606	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	c	514	CLA	C1-C2-C3	-3.38	120.20	126.04
23	D	404	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
24	A	415	PHO	O2D-CGD-O1D	-3.38	117.24	123.84
23	B	603	CLA	C4C-C3C-C2C	-3.38	101.98	106.90
25	D	405	BCR	C24-C23-C22	-3.37	121.15	126.23
26	D	413	SQD	O8-S-C6	3.37	111.10	105.74
29	A	413[A]	PL9	C7-C3-C2	-3.37	118.87	123.30
29	a	414[B]	PL9	C32-C33-C34	-3.37	119.56	127.66
25	C	517	BCR	C33-C5-C6	-3.36	120.75	124.53
25	D	405	BCR	C28-C27-C26	-3.36	108.08	114.08
23	c	505	CLA	C3B-C4B-NB	3.36	113.56	109.21
25	b	618	BCR	C15-C14-C13	-3.36	122.52	127.31
23	c	503	CLA	O2A-CGA-O1A	-3.36	115.11	123.59
23	a	403	CLA	C4-C3-C5	3.36	120.92	115.27
23	B	601	CLA	C1D-CHD-C4C	-3.35	118.13	122.56
23	c	515	CLA	CAC-C3C-C4C	3.35	129.16	124.81
23	a	407	CLA	C1D-CHD-C4C	-3.35	118.14	122.56
23	b	615	CLA	C1D-CHD-C4C	-3.35	118.14	122.56
34	C	521	LMG	O8-C28-C29	3.35	122.41	111.91
23	B	611	CLA	OBD-CAD-C3D	-3.34	122.43	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C29-C30-C25	3.34	115.63	110.48
23	C	508	CLA	C3B-C4B-NB	3.34	113.53	109.21
29	A	413[B]	PL9	C42-C43-C44	-3.34	119.61	127.66
25	a	408	BCR	C11-C10-C9	-3.34	122.54	127.31
23	A	407	CLA	C3B-C4B-NB	3.34	113.52	109.21
23	b	604	CLA	C1-C2-C3	-3.34	120.27	126.04
23	b	616	CLA	CBC-CAC-C3C	-3.33	103.24	112.43
23	C	511	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
29	a	414[A]	PL9	C37-C36-C34	-3.33	102.02	112.98
23	b	602	CLA	C3B-C4B-NB	3.33	113.51	109.21
24	a	406	PHO	C4C-C3C-C2C	-3.33	103.10	106.78
23	c	507	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	d	402	CLA	C1D-CHD-C4C	-3.33	118.17	122.56
23	B	613	CLA	O2D-CGD-CBD	3.32	117.17	111.27
23	B	607	CLA	C4-C3-C5	3.32	120.86	115.27
25	d	404	BCR	C40-C30-C25	-3.32	104.91	110.30
23	b	609	CLA	CMB-C2B-C3B	3.32	130.89	124.68
23	b	602	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
23	b	603	CLA	O2A-CGA-O1A	-3.31	115.23	123.59
23	C	515	CLA	C1C-C2C-C3C	-3.31	103.47	106.96
23	b	601	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	b	608	CLA	CMC-C2C-C1C	3.31	130.08	125.04
23	b	608	CLA	C3C-C4C-NC	3.31	114.29	110.57
25	H	101	BCR	C7-C8-C9	-3.31	121.23	126.23
25	b	619	BCR	C24-C23-C22	-3.31	121.23	126.23
23	B	611	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
35	C	519	DGD	O1G-C1A-C2A	3.31	122.30	111.91
23	C	515	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
23	C	506	CLA	C1-C2-C3	-3.31	120.32	126.04
23	D	403	CLA	C3B-C4B-NB	3.31	113.49	109.21
23	a	404	CLA	C4D-C3D-CAD	-3.31	106.63	108.47
23	C	509	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
25	H	101	BCR	C24-C23-C22	-3.30	121.25	126.23
23	a	405	CLA	C1D-CHD-C4C	-3.30	118.21	122.56
23	b	610	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
23	b	608	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
25	K	101	BCR	C38-C26-C25	-3.29	120.83	124.53
23	C	504	CLA	C1D-CHD-C4C	-3.29	118.22	122.56
34	C	522	LMG	O8-C28-C29	3.29	122.23	111.91
23	B	607	CLA	CAA-C2A-C3A	-3.29	103.77	112.78
34	Z	101	LMG	O6-C1-C2	3.29	117.31	110.35
23	C	503	CLA	O2D-CGD-O1D	-3.29	117.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C3B-C4B-NB	3.28	113.45	109.21
23	b	605	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
25	T	101	BCR	C33-C5-C6	-3.28	120.84	124.53
24	A	406	PHO	C4C-C3C-C2C	-3.28	103.15	106.78
25	h	102	BCR	C16-C17-C18	-3.28	122.63	127.31
23	a	403	CLA	O2A-CGA-CBA	3.28	122.19	111.91
23	b	612	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
29	a	414[B]	PL9	C20-C19-C21	3.28	120.78	115.27
24	A	406	PHO	CAC-C3C-C4C	3.27	128.79	125.22
23	B	605	CLA	O2A-CGA-O1A	-3.27	115.33	123.59
23	B	605	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	b	601	CLA	C4-C3-C5	3.27	120.77	115.27
29	A	413[A]	PL9	C53-C6-C1	3.27	121.67	114.99
23	b	616	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
23	c	510	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
23	D	404	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
26	a	411	SQD	C3-C4-C5	3.26	116.06	110.24
23	c	512	CLA	C4-C3-C5	3.26	120.76	115.27
29	a	414[A]	PL9	C7-C8-C9	-3.26	121.36	126.79
23	a	403	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	B	614	CLA	OBD-CAD-C3D	-3.26	122.57	127.98
25	H	101	BCR	C11-C10-C9	-3.26	122.66	127.31
29	A	413[B]	PL9	C20-C19-C21	3.26	120.75	115.27
29	a	414[B]	PL9	C27-C28-C29	-3.25	119.82	127.66
35	C	518	DGD	O1G-C1A-O1A	-3.25	115.38	123.59
23	B	611	CLA	CMC-C2C-C1C	3.25	129.99	125.04
23	B	605	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	c	509	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	C	503	CLA	C1-C2-C3	-3.25	120.42	126.04
23	C	512	CLA	C3B-C4B-NB	3.25	113.41	109.21
23	a	405	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	B	608	CLA	CMC-C2C-C1C	3.25	129.99	125.04
26	D	413	SQD	C1-C2-C3	-3.25	103.23	110.00
23	b	605	CLA	C2A-C1A-CHA	-3.25	118.18	123.86
23	B	602	CLA	CHD-C4C-NC	3.25	129.32	124.20
40	V	201	HEC	C1D-C2D-C3D	-3.24	104.74	107.00
29	A	413[A]	PL9	C10-C9-C11	3.24	120.72	115.27
31	a	419	LHG	O7-C7-C8	3.23	118.47	111.50
23	A	404	CLA	OBD-CAD-C3D	-3.23	122.61	127.98
23	a	404	CLA	CHD-C4C-NC	3.23	129.30	124.20
23	C	505	CLA	C4-C3-C5	3.23	120.71	115.27
24	a	416	PHO	C4D-CHA-C1A	-3.23	118.10	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CHD-C4C-NC	3.23	129.29	124.20
23	c	513	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
23	A	407	CLA	CAA-C2A-C3A	-3.22	103.95	112.78
25	b	618	BCR	C24-C23-C22	-3.22	121.36	126.23
23	a	407	CLA	CMC-C2C-C1C	3.22	129.95	125.04
23	B	613	CLA	C4-C3-C5	3.22	120.69	115.27
23	B	604	CLA	C3B-C4B-NB	3.22	113.38	109.21
23	b	607	CLA	CAA-C2A-C3A	-3.22	103.96	112.78
23	a	403	CLA	CHC-C1C-C2C	-3.22	117.82	126.72
23	a	403	CLA	CMB-C2B-C3B	3.21	130.69	124.68
23	b	614	CLA	O2A-CGA-CBA	3.21	121.99	111.91
23	b	609	CLA	C4D-C3D-CAD	-3.21	106.68	108.47
23	c	514	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
23	D	403	CLA	O2A-CGA-CBA	3.21	121.98	111.91
31	b	628	LHG	O8-C23-C24	3.21	121.98	111.91
26	A	409	SQD	O48-C23-C24	3.21	121.97	111.91
29	a	414[A]	PL9	C25-C24-C26	3.21	120.66	115.27
23	b	615	CLA	CAC-C3C-C4C	3.20	128.97	124.81
26	L	102	SQD	O8-S-C6	3.20	110.84	105.74
23	b	608	CLA	CAC-C3C-C4C	3.20	128.96	124.81
23	C	514	CLA	CMB-C2B-C3B	3.20	130.66	124.68
23	d	403	CLA	C1D-CHD-C4C	-3.20	118.34	122.56
23	D	404	CLA	CAA-C2A-C3A	-3.20	104.03	112.78
23	C	503	CLA	C4-C3-C5	3.20	120.65	115.27
23	c	515	CLA	C1-C2-C3	-3.20	120.52	126.04
25	B	631	BCR	C3-C4-C5	-3.20	108.37	114.08
23	B	603	CLA	CAA-C2A-C3A	-3.19	104.03	112.78
23	C	510	CLA	CHC-C1C-C2C	-3.19	117.89	126.72
23	B	605	CLA	CHD-C4C-NC	3.19	129.23	124.20
23	c	506	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	b	612	CLA	O2A-CGA-CBA	3.18	121.90	111.91
23	d	403	CLA	C3C-C4C-NC	3.18	114.14	110.57
23	b	614	CLA	C4D-C3D-CAD	-3.18	106.70	108.47
23	b	604	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
23	B	609	CLA	C3B-C4B-NB	3.18	113.32	109.21
23	c	503	CLA	C3B-C4B-NB	3.18	113.32	109.21
23	A	405	CLA	CAA-C2A-C3A	-3.18	104.08	112.78
25	B	618	BCR	C37-C22-C21	-3.17	118.48	122.92
23	B	608	CLA	CMB-C2B-C3B	3.17	130.61	124.68
33	C	526	LMT	O1B-C4'-C3'	3.17	115.71	107.28
23	C	503	CLA	CMC-C2C-C1C	3.17	129.87	125.04
25	C	516	BCR	C33-C5-C6	-3.17	120.97	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	406	PL9	C30-C29-C31	3.17	120.60	115.27
23	B	604	CLA	C4-C3-C5	3.16	120.59	115.27
25	k	101	BCR	C3-C4-C5	-3.16	108.43	114.08
23	c	503	CLA	C1D-CHD-C4C	-3.16	118.38	122.56
25	B	619	BCR	C7-C8-C9	-3.16	121.46	126.23
23	C	506	CLA	OBD-CAD-C3D	-3.16	122.73	127.98
23	b	608	CLA	CMB-C2B-C3B	3.16	130.59	124.68
34	m	101	LMG	O8-C28-C29	3.16	121.82	111.91
23	B	616	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	C	510	CLA	C4-C3-C5	3.16	120.58	115.27
23	b	613	CLA	CHC-C1C-C2C	-3.15	118.00	126.72
23	c	513	CLA	CAC-C3C-C4C	3.15	128.90	124.81
25	K	101	BCR	C15-C14-C13	-3.15	122.81	127.31
29	d	405	PL9	C37-C38-C39	-3.15	120.07	127.66
23	A	404	CLA	C4-C3-C5	3.15	120.56	115.27
23	B	606	CLA	CHC-C1C-C2C	-3.15	118.02	126.72
25	k	101	BCR	C11-C10-C9	-3.15	122.82	127.31
23	b	614	CLA	CMC-C2C-C1C	3.15	129.83	125.04
23	C	507	CLA	C1D-CHD-C4C	-3.15	118.41	122.56
23	B	608	CLA	CBC-CAC-C3C	-3.14	103.76	112.43
23	B	615	CLA	C4-C3-C5	3.14	120.56	115.27
23	C	505	CLA	CHD-C4C-NC	3.14	129.16	124.20
31	d	406	LHG	O8-C23-O10	-3.14	115.66	123.59
23	B	604	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
29	D	406	PL9	C22-C23-C24	-3.14	120.10	127.66
23	B	616	CLA	CHD-C4C-NC	3.14	129.15	124.20
25	T	101	BCR	C39-C30-C25	-3.14	105.21	110.30
24	a	416	PHO	CHD-C1D-C2D	-3.14	117.84	125.73
23	d	403	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
23	b	607	CLA	CHC-C1C-C2C	-3.14	118.05	126.72
23	B	601	CLA	CHD-C4C-NC	3.13	129.14	124.20
23	c	509	CLA	O2A-CGA-CBA	3.13	121.74	111.91
23	B	601	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	d	403	CLA	C1-C2-C3	-3.13	120.63	126.04
23	C	514	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	B	608	CLA	CMA-C3A-C4A	-3.13	103.36	111.77
23	b	607	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	d	403	CLA	CAA-C2A-C3A	-3.13	104.22	112.78
23	b	610	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	b	606	CLA	CMC-C2C-C1C	3.12	129.80	125.04
23	C	515	CLA	C3B-C4B-NB	3.12	113.25	109.21
25	b	617	BCR	C16-C17-C18	-3.12	122.85	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C2A-C1A-CHA	-3.12	118.40	123.86
23	b	611	CLA	C1D-CHD-C4C	-3.12	118.44	122.56
23	B	610	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	B	602	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	c	505	CLA	CMC-C2C-C1C	3.12	129.79	125.04
23	b	604	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	c	512	CLA	C1-C2-C3	-3.12	120.65	126.04
23	b	611	CLA	CMC-C2C-C1C	3.12	129.78	125.04
23	B	610	CLA	CHC-C1C-C2C	-3.11	118.11	126.72
26	A	411	SQD	O48-C23-C24	3.11	121.68	111.91
23	C	515	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
23	B	607	CLA	C1D-CHD-C4C	-3.11	118.45	122.56
23	B	615	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
26	L	102	SQD	O7-S-C6	3.11	110.64	106.94
23	c	509	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
23	c	513	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	c	504	CLA	C1-C2-C3	-3.11	120.67	126.04
23	b	605	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
25	T	101	BCR	C15-C14-C13	3.11	131.75	127.31
23	B	614	CLA	O2A-CGA-O1A	-3.11	115.75	123.59
23	B	614	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	C	510	CLA	CMB-C2B-C3B	3.10	130.49	124.68
23	c	511	CLA	O2A-CGA-CBA	3.10	121.65	111.91
24	A	415	PHO	CHC-C1C-C2C	-3.10	117.92	125.73
24	a	406	PHO	C1C-C2C-C3C	-3.10	102.95	106.51
23	B	609	CLA	O2A-CGA-CBA	3.10	121.64	111.91
23	C	512	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	B	612	CLA	C4-C3-C5	3.10	120.48	115.27
35	h	103	DGD	O2G-C1B-C2B	3.10	118.17	111.50
23	a	404	CLA	CBC-CAC-C3C	-3.10	103.90	112.43
29	A	413[B]	PL9	C7-C3-C2	-3.09	119.23	123.30
25	k	102	BCR	C24-C23-C22	-3.09	121.56	126.23
23	C	507	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	B	611	CLA	CHD-C4C-NC	3.09	129.07	124.20
23	B	614	CLA	C4-C3-C5	3.09	120.47	115.27
25	k	101	BCR	C15-C14-C13	-3.09	122.90	127.31
23	a	403	CLA	CMC-C2C-C1C	3.09	129.74	125.04
23	b	610	CLA	C4-C3-C5	3.08	120.46	115.27
23	B	601	CLA	O2A-CGA-CBA	3.08	121.58	111.91
23	D	403	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
23	C	503	CLA	CHD-C4C-NC	3.08	129.06	124.20
29	A	413[B]	PL9	C25-C24-C26	3.08	120.45	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	PHO	C2C-C1C-NC	3.08	114.43	109.79
23	C	505	CLA	C3B-C4B-NB	3.08	113.19	109.21
23	C	504	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	c	513	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
33	B	629	LMT	C1-O1'-C1'	-3.07	108.75	113.84
23	b	601	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
23	B	612	CLA	CMB-C2B-C3B	3.07	130.42	124.68
33	a	412	LMT	O5'-C5'-C4'	3.07	116.23	109.75
23	A	403	CLA	C1D-CHD-C4C	-3.07	118.51	122.56
25	k	101	BCR	C29-C30-C25	3.07	115.20	110.48
23	a	405	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
35	h	103	DGD	O1G-C1A-C2A	3.07	121.53	111.91
23	c	515	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	b	604	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
23	B	601	CLA	C1C-C2C-C3C	-3.06	103.73	106.96
23	d	403	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
23	c	505	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
23	b	611	CLA	O2A-CGA-CBA	3.06	121.51	111.91
23	B	612	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
23	C	503	CLA	C3B-C4B-NB	3.06	113.16	109.21
23	B	609	CLA	CMB-C2B-C1B	3.06	133.16	128.46
23	b	609	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	H	101	BCR	C31-C1-C6	-3.05	105.35	110.30
23	a	407	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	c	509	CLA	C4-C3-C5	3.05	120.40	115.27
26	f	101	SQD	O7-S-C6	3.05	110.56	106.94
23	B	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
29	a	414[A]	PL9	C42-C43-C44	-3.05	120.32	127.66
23	a	403	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
23	B	603	CLA	C1D-CHD-C4C	-3.05	118.54	122.56
23	C	507	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
31	d	407	LHG	C6-C5-C4	-3.05	104.58	111.79
29	A	413[A]	PL9	C42-C43-C44	-3.04	120.33	127.66
23	b	604	CLA	CMC-C2C-C1C	3.04	129.68	125.04
23	c	511	CLA	CHC-C1C-C2C	-3.04	118.30	126.72
24	a	406	PHO	CMB-C2B-C1B	3.04	129.75	125.06
23	c	512	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
23	B	615	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	b	613	CLA	C4-C3-C5	3.03	120.37	115.27
23	b	603	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	c	503	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
24	a	406	PHO	CAC-C3C-C4C	3.03	128.53	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
26	L	102	SQD	C1-O5-C5	-3.03	107.75	113.69
23	B	608	CLA	CHD-C4C-NC	3.03	128.97	124.20
23	D	404	CLA	O2A-CGA-CBA	3.02	121.40	111.91
23	C	504	CLA	CHD-C4C-NC	3.02	128.97	124.20
23	B	612	CLA	C3B-C4B-NB	3.02	113.12	109.21
23	c	511	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	a	407	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
24	a	416	PHO	CAC-C3C-C4C	3.02	128.51	125.22
23	d	403	CLA	CHD-C4C-NC	3.02	128.96	124.20
24	a	406	PHO	O2A-CGA-CBA	3.02	121.38	111.91
23	B	609	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
23	C	508	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
23	B	607	CLA	CBC-CAC-C3C	-3.02	104.12	112.43
23	c	508	CLA	CHD-C4C-NC	3.02	128.96	124.20
23	c	506	CLA	CHC-C1C-C2C	-3.02	118.38	126.72
23	C	512	CLA	CMC-C2C-C1C	3.02	129.63	125.04
23	b	613	CLA	C4C-C3C-C2C	-3.01	102.50	106.90
23	b	612	CLA	CHC-C1C-C2C	-3.01	118.39	126.72
25	Y	101	BCR	C38-C26-C25	-3.01	121.14	124.53
29	D	406	PL9	C53-C6-C1	3.01	121.15	114.99
23	c	508	CLA	O2A-CGA-O1A	-3.01	115.99	123.59
23	C	504	CLA	C1C-C2C-C3C	-3.01	103.79	106.96
25	k	102	BCR	C38-C26-C25	-3.01	121.15	124.53
23	c	510	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
23	d	403	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
23	B	614	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	c	512	CLA	CHC-C1C-C2C	-3.01	118.40	126.72
23	C	511	CLA	CAC-C3C-C4C	3.01	128.71	124.81
29	a	414[A]	PL9	C32-C33-C34	-3.00	120.42	127.66
35	c	520	DGD	O2G-C1B-C2B	3.00	117.98	111.50
23	A	403	CLA	O2D-CGD-CBD	3.00	116.60	111.27
23	A	405	CLA	C4D-C3D-CAD	-3.00	106.80	108.47
25	B	618	BCR	C28-C27-C26	-3.00	108.72	114.08
25	B	619	BCR	C24-C23-C22	-3.00	121.70	126.23
23	c	504	CLA	C3B-C4B-NB	3.00	113.09	109.21
23	c	504	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	c	511	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
26	A	409	SQD	O48-C23-O10	-3.00	116.03	123.59
23	c	514	CLA	C4-C3-C5	2.99	120.31	115.27
23	B	601	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
23	c	514	CLA	C4C-C3C-C2C	-2.99	102.53	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2A-CGA-O1A	-2.99	116.04	123.59
23	B	609	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	a	416	PHO	C4D-ND-C1D	-2.99	101.38	106.76
29	A	413[B]	PL9	C17-C18-C19	-2.99	120.46	127.66
29	a	414[A]	PL9	C22-C23-C24	-2.99	120.46	127.66
26	B	620	SQD	O7-S-C6	2.99	110.49	106.94
23	b	603	CLA	O2A-CGA-CBA	2.99	121.28	111.91
29	a	414[B]	PL9	C15-C14-C16	2.99	120.30	115.27
23	C	515	CLA	CHD-C4C-NC	2.99	128.91	124.20
23	c	512	CLA	CHD-C4C-NC	2.99	128.91	124.20
25	B	619	BCR	C29-C30-C25	2.98	115.07	110.48
32	B	621	HTG	C1-C2-C3	2.98	116.48	110.59
23	b	602	CLA	CMC-C2C-C1C	2.98	129.58	125.04
23	B	610	CLA	C3B-C4B-NB	2.98	113.06	109.21
23	D	403	CLA	CHC-C1C-C2C	-2.98	118.48	126.72
23	B	606	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	A	407	CLA	CMA-C3A-C2A	-2.98	101.81	113.83
23	A	407	CLA	CBC-CAC-C3C	-2.98	104.22	112.43
25	D	405	BCR	C37-C22-C23	2.98	122.77	118.08
32	b	621	HTG	C1'-S1-C1	2.98	105.66	100.09
23	B	611	CLA	CBC-CAC-C3C	-2.98	104.22	112.43
32	h	101	HTG	C1-O5-C5	2.98	118.07	112.58
23	B	616	CLA	O2A-CGA-CBA	2.98	121.25	111.91
25	C	517	BCR	C38-C26-C25	-2.98	121.19	124.53
29	A	413[B]	PL9	C22-C23-C24	-2.98	120.50	127.66
23	C	511	CLA	CMB-C2B-C3B	2.97	130.24	124.68
23	b	613	CLA	CAC-C3C-C4C	2.97	128.67	124.81
23	B	606	CLA	C4-C3-C5	2.97	120.27	115.27
23	B	611	CLA	C1D-CHD-C4C	-2.97	118.64	122.56
23	c	508	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
23	C	514	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	b	616	CLA	O2A-CGA-CBA	2.96	121.21	111.91
23	B	614	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
25	c	516	BCR	C20-C21-C22	-2.96	123.08	127.31
23	a	407	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
23	c	511	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	b	610	CLA	CHD-C4C-NC	2.96	128.87	124.20
23	A	407	CLA	CMC-C2C-C1C	2.96	129.54	125.04
26	L	102	SQD	C3-C4-C5	2.96	115.52	110.24
23	c	503	CLA	CHC-C1C-C2C	-2.96	118.54	126.72
29	a	414[B]	PL9	C53-C6-C1	2.96	121.04	114.99
23	B	605	CLA	C2A-C1A-CHA	-2.95	118.70	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	O2A-CGA-O1A	-2.95	116.15	123.59
23	b	613	CLA	C1D-CHD-C4C	-2.95	118.67	122.56
35	C	519	DGD	O1G-C1A-O1A	-2.95	116.15	123.59
25	c	517	BCR	C15-C16-C17	-2.95	117.43	123.47
23	a	405	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	b	611	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
23	c	513	CLA	CBC-CAC-C3C	-2.95	104.31	112.43
29	D	406	PL9	C25-C24-C26	2.94	120.22	115.27
23	B	601	CLA	CAC-C3C-C4C	2.94	128.63	124.81
23	A	403	CLA	C2A-C1A-CHA	-2.94	118.71	123.86
23	C	505	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
34	c	522	LMG	O8-C28-C29	2.94	121.14	111.91
29	a	414[B]	PL9	C37-C36-C34	-2.94	103.31	112.98
25	c	516	BCR	C38-C26-C25	-2.94	121.23	124.53
23	c	511	CLA	C1-O2A-CGA	2.94	124.15	116.44
25	k	101	BCR	C34-C9-C8	2.94	122.70	118.08
23	A	407	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
23	B	602	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
23	b	609	CLA	CHD-C4C-NC	2.93	128.83	124.20
26	A	409	SQD	C45-O47-C7	-2.93	110.57	117.79
23	a	404	CLA	C3B-C4B-NB	2.93	113.00	109.21
25	B	618	BCR	C29-C30-C25	2.93	115.00	110.48
23	c	511	CLA	CMB-C2B-C3B	2.93	130.16	124.68
23	A	405	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
35	H	102	DGD	C3G-O3G-C1D	-2.93	108.02	113.74
23	c	514	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	C	508	CLA	CMC-C2C-C1C	2.93	129.50	125.04
31	D	408	LHG	O8-C23-C24	2.93	121.10	111.91
34	D	412	LMG	O8-C28-O10	-2.92	116.21	123.59
40	V	201	HEC	CMB-C2B-C3B	2.92	129.26	125.82
23	c	510	CLA	CHD-C4C-NC	2.92	128.81	124.20
23	a	405	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
29	A	413[B]	PL9	C53-C6-C1	2.92	120.96	114.99
24	A	415	PHO	C3C-C4C-NC	2.92	114.81	110.28
23	c	504	CLA	CBC-CAC-C3C	-2.92	104.39	112.43
25	D	405	BCR	C37-C22-C21	-2.92	118.84	122.92
26	a	409	SQD	O9-S-C6	2.92	110.40	106.94
32	B	624	HTG	O5-C5-C4	2.92	114.99	109.69
29	A	413[A]	PL9	C17-C18-C19	-2.91	120.64	127.66
23	c	504	CLA	C4D-C3D-CAD	-2.91	106.84	108.47
23	c	508	CLA	C4D-C3D-CAD	-2.91	106.85	108.47
23	C	513	CLA	C4C-C3C-C2C	-2.91	102.65	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	CLA	O2A-CGA-CBA	2.91	121.04	111.91
25	c	517	BCR	C15-C14-C13	-2.91	123.16	127.31
23	C	514	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
23	C	509	CLA	C3B-C4B-NB	2.91	112.97	109.21
31	E	101	LHG	O8-C23-C24	2.91	121.03	111.91
23	a	407	CLA	C4-C3-C5	2.91	120.16	115.27
23	A	405	CLA	O2A-CGA-CBA	2.90	121.02	111.91
23	b	607	CLA	C1-O2A-CGA	2.90	124.06	116.44
29	a	414[B]	PL9	C45-C44-C46	2.90	120.15	115.27
23	C	513	CLA	CMC-C2C-C1C	2.90	129.46	125.04
40	V	201	HEC	CAD-CBD-CGD	-2.90	107.80	112.67
23	C	505	CLA	CMC-C2C-C1C	2.90	129.46	125.04
23	C	513	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
23	c	511	CLA	C1D-CHD-C4C	-2.90	118.73	122.56
23	C	512	CLA	CHD-C4C-NC	2.90	128.77	124.20
25	T	101	BCR	C12-C13-C14	-2.90	114.50	118.94
23	C	515	CLA	CMC-C2C-C1C	2.90	129.45	125.04
23	b	609	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
23	b	603	CLA	CHC-C1C-C2C	-2.90	118.71	126.72
23	d	403	CLA	O2A-CGA-CBA	2.90	120.99	111.91
32	B	624	HTG	C3-C4-C5	2.89	115.40	110.24
23	a	405	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
26	L	102	SQD	C44-O6-C1	-2.89	108.08	113.74
25	D	405	BCR	C29-C30-C25	2.89	114.93	110.48
23	B	603	CLA	C4-C3-C5	2.89	120.13	115.27
24	A	406	PHO	C2A-C1A-NA	2.89	115.18	111.86
23	C	505	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
23	b	611	CLA	C1-C2-C3	-2.89	121.05	126.04
23	B	614	CLA	O2A-CGA-CBA	2.88	120.96	111.91
23	B	606	CLA	CAC-C3C-C4C	2.88	128.55	124.81
23	d	402	CLA	O2A-CGA-CBA	2.88	120.96	111.91
23	c	513	CLA	CHC-C1C-C2C	-2.88	118.74	126.72
25	c	516	BCR	C15-C14-C13	-2.88	123.20	127.31
23	b	615	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	B	612	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	B	614	CLA	CMC-C2C-C1C	2.88	129.42	125.04
23	d	403	CLA	CMC-C2C-C1C	2.88	129.42	125.04
23	c	508	CLA	CMB-C2B-C3B	2.88	130.06	124.68
23	c	512	CLA	O2A-CGA-CBA	2.87	120.93	111.91
25	a	408	BCR	C33-C5-C6	-2.87	121.30	124.53
23	d	402	CLA	CHC-C1C-C2C	-2.87	118.78	126.72
23	B	607	CLA	C3B-C4B-NB	2.87	112.92	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	PHO	C1C-C2C-C3C	-2.87	103.21	106.51
23	B	616	CLA	C3B-C4B-NB	2.87	112.92	109.21
31	A	416	LHG	O8-C23-C24	2.87	120.91	111.91
23	C	513	CLA	C4-C3-C5	2.87	120.09	115.27
23	B	613	CLA	O2A-CGA-CBA	2.87	120.90	111.91
23	B	601	CLA	C3B-C4B-NB	2.86	112.91	109.21
25	d	404	BCR	C24-C23-C22	-2.86	121.91	126.23
23	C	512	CLA	CMB-C2B-C3B	2.86	130.03	124.68
23	C	511	CLA	O2A-CGA-O1A	-2.86	116.37	123.59
29	A	413[A]	PL9	C22-C23-C24	-2.86	120.77	127.66
23	A	407	CLA	C4-C3-C5	2.86	120.08	115.27
40	V	201	HEC	CMC-C2C-C1C	-2.86	124.07	128.46
23	B	608	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	c	509	CLA	CAC-C3C-C4C	2.86	128.52	124.81
31	d	408	LHG	O8-C23-C24	2.86	120.87	111.91
23	b	614	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
29	D	406	PL9	C45-C44-C46	2.86	120.07	115.27
29	d	405	PL9	C31-C32-C33	-2.85	102.50	111.88
24	A	406	PHO	CBD-CHA-C1A	2.85	133.02	126.40
23	b	614	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
29	D	406	PL9	C51-C49-C50	2.85	120.90	114.60
24	A	415	PHO	C4D-ND-C1D	-2.85	101.64	106.76
23	D	404	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
23	b	602	CLA	C1D-CHD-C4C	-2.85	118.80	122.56
23	B	602	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
29	D	406	PL9	C10-C9-C11	2.84	120.06	115.27
23	C	507	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	B	608	CLA	C4C-C3C-C2C	-2.84	102.75	106.90
23	b	602	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
25	H	101	BCR	C16-C17-C18	-2.84	123.26	127.31
23	a	403	CLA	CMA-C3A-C4A	-2.84	104.14	111.77
23	a	404	CLA	CMA-C3A-C2A	-2.84	102.38	113.83
23	b	614	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
23	b	614	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
34	z	101	LMG	O8-C28-C29	2.83	120.80	111.91
34	c	521	LMG	O8-C28-C29	2.83	120.80	111.91
25	b	617	BCR	C29-C30-C25	2.83	114.84	110.48
23	A	403	CLA	CMC-C2C-C1C	2.83	129.35	125.04
23	a	404	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
23	b	616	CLA	C1-C2-C3	-2.83	121.16	126.04
23	b	610	CLA	CBC-CAC-C3C	-2.83	104.64	112.43
23	B	612	CLA	O2A-CGA-CBA	2.82	120.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	SQD	O5-C5-C4	2.82	114.82	109.69
29	a	414[A]	PL9	C10-C9-C11	2.82	120.02	115.27
34	c	521	LMG	O1-C7-C8	-2.82	104.09	110.90
24	a	406	PHO	CBD-CHA-C1A	2.82	132.95	126.40
25	h	102	BCR	C24-C23-C22	-2.82	121.97	126.23
25	B	618	BCR	C16-C17-C18	-2.82	123.28	127.31
23	C	503	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	b	611	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	c	514	CLA	O2A-CGA-CBA	2.82	120.75	111.91
23	b	609	CLA	C1D-CHD-C4C	-2.82	118.84	122.56
23	B	610	CLA	CAA-CBA-CGA	-2.82	105.02	113.25
23	C	509	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
23	c	513	CLA	CMC-C2C-C1C	2.82	129.33	125.04
29	a	414[A]	PL9	C20-C19-C21	2.82	120.01	115.27
29	a	414[B]	PL9	C42-C43-C44	-2.82	120.88	127.66
23	c	505	CLA	OBD-CAD-C3D	-2.82	123.31	127.98
23	c	508	CLA	CMC-C2C-C1C	2.82	129.33	125.04
26	a	409	SQD	O48-C23-C24	2.81	120.74	111.91
23	B	610	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
23	C	506	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	B	614	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	a	404	CLA	CMC-C2C-C1C	2.81	129.32	125.04
35	C	520	DGD	O1G-C1A-C2A	2.81	120.73	111.91
23	B	614	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	B	604	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	C	507	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	C	512	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
23	C	514	CLA	C1-C2-C3	-2.81	121.19	126.04
23	B	604	CLA	C6-C7-C8	-2.81	106.84	115.92
23	a	405	CLA	C3B-C4B-NB	2.81	112.84	109.21
23	B	611	CLA	CHC-C1C-C2C	-2.81	118.95	126.72
23	b	602	CLA	C4C-C3C-C2C	-2.81	102.81	106.90
23	B	616	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
23	b	605	CLA	CED-O2D-CGD	2.81	122.28	115.94
23	B	613	CLA	C4D-C3D-CAD	-2.80	106.91	108.47
23	B	603	CLA	O2A-CGA-O1A	-2.80	116.51	123.59
23	A	405	CLA	CHC-C1C-C2C	-2.80	118.96	126.72
23	C	503	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	b	611	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
23	C	508	CLA	C1D-CHD-C4C	-2.80	118.86	122.56
29	A	413[A]	PL9	C32-C33-C34	-2.80	120.92	127.66
25	B	619	BCR	C2-C3-C4	-2.80	105.13	111.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C4A-NA-C1A	-2.80	105.45	106.71
23	B	614	CLA	C1-C2-C3	-2.80	121.21	126.04
25	D	405	BCR	C33-C5-C6	-2.79	121.39	124.53
35	c	520	DGD	O1G-C1A-C2A	2.79	120.67	111.91
34	Z	101	LMG	C4-C3-C2	2.79	115.70	110.82
23	b	603	CLA	C4-C3-C5	2.79	119.96	115.27
23	b	602	CLA	C11-C12-C13	-2.79	106.90	115.92
23	a	407	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
23	a	404	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
23	B	613	CLA	CMB-C2B-C3B	2.79	129.90	124.68
23	b	607	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
23	B	603	CLA	CHD-C4C-NC	2.79	128.60	124.20
24	a	406	PHO	C4D-CHA-C1A	-2.79	119.10	125.37
23	B	607	CLA	C4C-C3C-C2C	-2.79	102.84	106.90
25	k	101	BCR	C16-C17-C18	-2.78	123.34	127.31
23	c	507	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	c	503	CLA	CAC-C3C-C4C	2.78	128.42	124.81
31	d	406	LHG	O8-C23-C24	2.78	120.64	111.91
23	B	605	CLA	O2A-CGA-CBA	2.78	120.63	111.91
23	C	510	CLA	OBD-CAD-C3D	-2.78	123.36	127.98
23	B	605	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
25	d	404	BCR	C16-C17-C18	-2.78	123.34	127.31
23	b	603	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	b	607	CLA	CHD-C4C-NC	2.78	128.58	124.20
32	b	624	HTG	O5-C5-C4	2.78	114.74	109.69
23	a	407	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	c	508	CLA	CHC-C1C-C2C	-2.78	119.04	126.72
23	b	612	CLA	CMC-C2C-C1C	2.78	129.27	125.04
23	C	514	CLA	O2A-CGA-CBA	2.77	120.61	111.91
23	A	405	CLA	C3B-C4B-NB	2.77	112.80	109.21
23	d	403	CLA	C3B-C4B-NB	2.77	112.80	109.21
23	c	509	CLA	C1-C2-C3	-2.77	121.25	126.04
34	c	522	LMG	C3-C4-C5	2.77	115.18	110.24
23	b	610	CLA	C3B-C4B-NB	2.77	112.79	109.21
23	C	514	CLA	CHD-C4C-NC	2.77	128.57	124.20
29	d	405	PL9	C36-C34-C33	-2.77	115.52	121.12
23	d	403	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
23	c	513	CLA	C4-C3-C5	2.77	119.92	115.27
23	c	513	CLA	O2A-CGA-CBA	2.77	120.59	111.91
23	b	616	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
23	a	404	CLA	CHC-C1C-C2C	-2.76	119.07	126.72
23	a	407	CLA	C1-C2-C3	-2.76	121.26	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	B	616	CLA	CMC-C2C-C1C	2.76	129.25	125.04
23	c	507	CLA	C1D-CHD-C4C	-2.76	118.91	122.56
29	d	405	PL9	C10-C9-C11	2.76	119.91	115.27
23	C	512	CLA	O2A-CGA-CBA	2.76	120.56	111.91
29	A	413[B]	PL9	C45-C44-C46	2.76	119.91	115.27
23	B	605	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
29	D	406	PL9	C37-C38-C39	-2.75	121.03	127.66
23	c	512	CLA	CMC-C2C-C1C	2.75	129.23	125.04
23	C	506	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	c	515	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
34	a	417	LMG	C7-O1-C1	-2.75	108.37	113.74
23	c	510	CLA	CMB-C2B-C3B	2.75	129.82	124.68
31	d	407	LHG	O8-C23-C24	2.75	120.53	111.91
23	c	509	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
23	C	509	CLA	OBD-CAD-C3D	-2.75	123.42	127.98
23	C	506	CLA	C4D-C3D-CAD	-2.75	106.94	108.47
24	a	416	PHO	C3C-C4C-NC	2.75	114.54	110.28
23	B	601	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	b	616	CLA	C3B-C4B-NB	2.74	112.76	109.21
23	a	404	CLA	CMB-C2B-C1B	2.74	132.68	128.46
23	d	402	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
23	D	404	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	B	612	CLA	C4D-C3D-CAD	-2.74	106.94	108.47
23	A	403	CLA	CAA-C2A-C1A	-2.74	103.01	111.97
23	b	605	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
23	c	504	CLA	C2A-C1A-CHA	-2.74	119.08	123.86
23	d	403	CLA	CMB-C2B-C3B	2.73	129.79	124.68
23	b	614	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	C	508	CLA	CBC-CAC-C3C	-2.73	104.89	112.43
23	B	606	CLA	CMB-C2B-C3B	2.73	129.79	124.68
23	C	513	CLA	CMB-C2B-C3B	2.73	129.79	124.68
34	D	412	LMG	O8-C28-C29	2.73	120.48	111.91
23	A	404	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
23	c	509	CLA	C1D-CHD-C4C	-2.73	118.95	122.56
23	b	606	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
24	A	406	PHO	C1-C2-C3	-2.73	121.32	126.04
23	B	609	CLA	C1D-CHD-C4C	-2.73	118.96	122.56
25	k	101	BCR	C36-C18-C19	2.73	122.38	118.08
23	A	405	CLA	CMA-C3A-C2A	-2.73	102.82	113.83
29	d	405	PL9	C53-C6-C1	2.73	120.57	114.99
23	B	602	CLA	C2A-C1A-CHA	-2.73	119.09	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
24	A	406	PHO	C4D-ND-C1D	-2.72	101.86	106.76
25	a	408	BCR	C39-C30-C25	-2.72	105.88	110.30
23	B	611	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
23	b	610	CLA	CMC-C2C-C1C	2.72	129.19	125.04
24	A	415	PHO	C2B-C1B-NB	2.72	113.90	109.79
23	B	607	CLA	CMC-C2C-C1C	2.72	129.18	125.04
23	b	611	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	A	413[B]	PL9	C16-C14-C13	-2.72	115.62	121.12
29	A	413[A]	PL9	C40-C39-C41	2.72	119.84	115.27
23	b	604	CLA	CHD-C4C-NC	2.72	128.49	124.20
29	a	414[B]	PL9	C17-C18-C19	-2.72	121.12	127.66
23	C	503	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
23	c	503	CLA	CMC-C2C-C1C	2.71	129.17	125.04
23	B	605	CLA	CAC-C3C-C4C	2.71	128.33	124.81
24	a	416	PHO	CBD-CHA-C1A	2.71	132.69	126.40
25	Y	101	BCR	C34-C9-C8	2.71	122.35	118.08
23	c	515	CLA	CMB-C2B-C3B	2.71	129.75	124.68
25	C	517	BCR	C15-C16-C17	-2.71	117.92	123.47
25	b	618	BCR	C3-C4-C5	-2.71	109.24	114.08
23	a	404	CLA	C1-C2-C3	-2.71	121.36	126.04
23	B	602	CLA	O2A-CGA-O1A	-2.71	116.76	123.59
29	d	405	PL9	C22-C23-C24	-2.71	121.14	127.66
23	B	607	CLA	CHD-C4C-NC	2.71	128.47	124.20
29	A	413[A]	PL9	C30-C29-C31	2.71	119.82	115.27
23	b	610	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
31	A	416	LHG	C5-O7-C7	-2.70	111.13	117.79
23	c	514	CLA	CHC-C1C-C2C	-2.70	119.24	126.72
33	a	412	LMT	O5B-C5B-C4B	2.70	114.60	109.69
23	C	506	CLA	CMC-C2C-C1C	2.70	129.15	125.04
25	k	102	BCR	C10-C11-C12	-2.70	114.79	123.22
23	C	512	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
29	a	414[A]	PL9	C53-C6-C1	2.69	120.50	114.99
23	B	604	CLA	C11-C12-C13	-2.69	107.22	115.92
23	C	506	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
23	b	606	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
23	B	615	CLA	C11-C10-C8	-2.69	107.23	115.92
23	a	407	CLA	CMA-C3A-C2A	-2.69	102.98	113.83
23	C	512	CLA	CHC-C1C-C2C	-2.69	119.28	126.72
23	b	603	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	D	403	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
23	a	407	CLA	C2A-C1A-CHA	-2.69	119.16	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	SQD	O48-C23-C24	2.69	120.34	111.91
23	C	507	CLA	CMB-C2B-C1B	2.69	132.59	128.46
23	B	613	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
23	c	510	CLA	C4-C3-C5	2.68	119.79	115.27
23	b	601	CLA	CHC-C1C-C2C	-2.68	119.30	126.72
23	b	605	CLA	C3B-C4B-NB	2.68	112.68	109.21
23	c	503	CLA	C4-C3-C5	2.68	119.78	115.27
23	c	504	CLA	CHC-C1C-C2C	-2.68	119.31	126.72
25	C	516	BCR	C38-C26-C25	-2.68	121.52	124.53
33	B	627	LMT	C1-O1'-C1'	-2.68	109.40	113.84
31	d	406	LHG	C5-O7-C7	-2.68	111.19	117.79
23	B	615	CLA	CMB-C2B-C1B	2.68	132.58	128.46
26	D	413	SQD	O48-C23-C24	2.68	120.31	111.91
26	a	411	SQD	O48-C23-O10	-2.68	116.84	123.59
23	B	603	CLA	O2A-CGA-CBA	2.68	120.30	111.91
35	c	520	DGD	C2G-O2G-C1B	-2.67	111.21	117.79
23	a	405	CLA	CAC-C3C-C4C	2.67	128.28	124.81
23	B	610	CLA	C1D-CHD-C4C	-2.67	119.03	122.56
23	D	404	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
23	B	606	CLA	CHD-C4C-NC	2.67	128.41	124.20
23	b	613	CLA	C4D-C3D-CAD	-2.67	106.98	108.47
23	C	511	CLA	CHC-C1C-C2C	-2.67	119.34	126.72
23	B	609	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	a	405	CLA	C1-C2-C3	-2.67	121.43	126.04
23	c	506	CLA	CHD-C4C-NC	2.67	128.41	124.20
25	C	516	BCR	C23-C24-C25	-2.67	119.71	127.20
26	L	102	SQD	O48-C23-C24	2.66	120.27	111.91
25	A	408	BCR	C31-C1-C6	-2.66	105.98	110.30
26	D	413	SQD	O7-S-C6	2.66	110.10	106.94
29	A	413[A]	PL9	C45-C44-C46	2.66	119.75	115.27
23	b	606	CLA	C1-O2A-CGA	2.66	123.43	116.44
23	B	606	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
23	A	407	CLA	C1D-CHD-C4C	-2.66	119.05	122.56
23	B	607	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	b	612	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	c	514	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	C	505	CLA	O2A-CGA-CBA	2.66	120.25	111.91
23	a	403	CLA	CHB-C4A-NA	2.66	128.19	124.51
29	A	413[B]	PL9	C35-C34-C36	2.66	119.74	115.27
29	A	413[B]	PL9	C30-C29-C31	2.65	119.73	115.27
26	A	411	SQD	O5-C5-C4	2.65	114.51	109.69
23	b	608	CLA	CHC-C1C-C2C	-2.65	119.38	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	405	BCR	C3-C4-C5	-2.65	109.34	114.08
23	A	407	CLA	C4D-C3D-CAD	-2.65	106.99	108.47
23	A	407	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	b	601	CLA	O2A-CGA-CBA	2.65	120.23	111.91
23	B	603	CLA	CMC-C2C-C1C	2.65	129.08	125.04
29	A	413[B]	PL9	C40-C39-C41	2.65	119.73	115.27
25	k	102	BCR	C29-C28-C27	-2.65	105.46	111.38
23	d	402	CLA	CMC-C2C-C1C	2.65	129.07	125.04
23	c	507	CLA	C3B-C4B-NB	2.65	112.63	109.21
23	B	605	CLA	CMC-C2C-C1C	2.65	129.07	125.04
23	C	508	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	b	612	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
29	D	406	PL9	C40-C39-C41	2.65	119.72	115.27
23	A	403	CLA	CHC-C1C-C2C	-2.65	119.40	126.72
23	a	403	CLA	CHD-C4C-NC	2.64	128.37	124.20
23	b	613	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	c	506	CLA	CED-O2D-CGD	2.64	121.92	115.94
23	B	603	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
23	C	515	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	C	503	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
24	a	416	PHO	C2B-C1B-NB	2.64	113.77	109.79
25	b	618	BCR	C8-C7-C6	-2.64	119.80	127.20
23	b	608	CLA	C11-C10-C8	-2.64	107.40	115.92
23	b	604	CLA	C11-C12-C13	-2.64	107.40	115.92
24	a	416	PHO	CHC-C1C-C2C	-2.63	119.10	125.73
23	C	514	CLA	C4-C3-C5	2.63	119.70	115.27
23	c	508	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	B	604	CLA	CMB-C2B-C3B	2.63	129.60	124.68
23	c	504	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
31	L	101	LHG	O8-C23-C24	2.63	120.17	111.91
25	b	619	BCR	C7-C8-C9	-2.63	122.26	126.23
23	c	506	CLA	C1-O2A-CGA	2.63	123.35	116.44
23	c	504	CLA	C1D-CHD-C4C	-2.63	119.08	122.56
23	c	515	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
24	a	406	PHO	C1-C2-C3	-2.63	121.49	126.04
23	C	513	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	b	608	CLA	CHD-C4C-NC	2.63	128.34	124.20
23	B	611	CLA	CED-O2D-CGD	2.63	121.88	115.94
23	C	509	CLA	CHD-C4C-NC	2.63	128.34	124.20
23	c	510	CLA	O2A-CGA-CBA	2.63	120.15	111.91
24	a	416	PHO	CMB-C2B-C1B	2.63	129.11	125.06
23	C	508	CLA	O2A-CGA-CBA	2.63	120.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	521	LMG	O8-C28-O10	-2.63	116.97	123.59
23	C	508	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
29	a	414[A]	PL9	C17-C18-C19	-2.62	121.34	127.66
24	a	406	PHO	O2A-CGA-O1A	-2.62	116.97	123.59
25	B	617	BCR	C33-C5-C6	-2.62	121.58	124.53
23	c	514	CLA	C3B-C4B-NB	2.62	112.60	109.21
23	a	403	CLA	C1-C2-C3	-2.62	121.51	126.04
23	b	614	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	c	505	CLA	C4-C3-C5	2.62	119.68	115.27
23	c	503	CLA	CBC-CAC-C3C	-2.62	105.21	112.43
23	d	403	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	c	515	CLA	CMC-C2C-C1C	2.62	129.03	125.04
34	a	417	LMG	C30-C29-C28	-2.62	104.10	113.62
23	c	510	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	C	511	CLA	CMC-C2C-C1C	2.62	129.02	125.04
25	Y	101	BCR	C40-C30-C25	-2.62	106.06	110.30
25	D	405	BCR	C21-C20-C19	-2.62	115.06	123.22
23	d	403	CLA	C4D-C3D-CAD	-2.61	107.01	108.47
23	B	604	CLA	O2A-CGA-CBA	2.61	120.11	111.91
23	C	505	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
23	C	510	CLA	CHD-C4C-NC	2.61	128.32	124.20
24	a	406	PHO	C2B-C1B-NB	2.61	113.73	109.79
23	d	403	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
23	B	607	CLA	C1-O2A-CGA	2.61	123.29	116.44
23	D	403	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
24	A	406	PHO	O2D-CGD-O1D	-2.61	118.74	123.84
23	b	602	CLA	CHC-C1C-C2C	-2.61	119.51	126.72
25	K	101	BCR	C3-C4-C5	-2.61	109.42	114.08
23	C	515	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
23	b	608	CLA	C1D-CHD-C4C	-2.60	119.12	122.56
23	b	608	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
23	b	602	CLA	CMB-C2B-C3B	2.60	129.55	124.68
31	d	408	LHG	O8-C23-O10	-2.60	117.03	123.59
23	b	608	CLA	C4-C3-C5	2.60	119.65	115.27
23	C	504	CLA	C3B-C4B-NB	2.60	112.57	109.21
23	A	404	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	C	506	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
25	B	618	BCR	C2-C1-C6	2.60	114.48	110.48
29	d	405	PL9	C35-C34-C36	2.60	119.64	115.27
25	T	101	BCR	C16-C17-C18	-2.60	123.60	127.31
23	C	508	CLA	C4-C3-C5	2.60	119.64	115.27
29	A	413[A]	PL9	C7-C8-C9	-2.60	122.47	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	411	SQD	O8-S-C6	2.60	109.88	105.74
23	c	508	CLA	C4-C3-C5	2.60	119.64	115.27
23	A	405	CLA	CHD-C4C-NC	2.60	128.29	124.20
25	b	618	BCR	C15-C16-C17	-2.59	118.16	123.47
23	b	603	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
23	c	512	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
35	c	519	DGD	C2G-O2G-C1B	-2.59	111.41	117.79
23	b	614	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
29	d	405	PL9	C20-C19-C21	2.59	119.63	115.27
29	a	414[A]	PL9	C45-C44-C46	2.59	119.62	115.27
23	b	604	CLA	O2A-CGA-O1A	-2.59	117.07	123.59
25	A	408	BCR	C38-C26-C25	-2.58	121.63	124.53
23	B	604	CLA	CHD-C4C-NC	2.58	128.28	124.20
25	k	102	BCR	C21-C20-C19	-2.58	115.16	123.22
24	a	416	PHO	C2A-C1A-NA	2.58	114.83	111.86
23	d	402	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
23	b	602	CLA	C4-C3-C5	2.58	119.61	115.27
23	C	510	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
25	c	516	BCR	C33-C5-C6	-2.58	121.63	124.53
23	b	614	CLA	C4-C3-C5	2.58	119.61	115.27
23	c	503	CLA	CHD-C4C-NC	2.58	128.27	124.20
40	v	202	HEC	CMB-C2B-C1B	-2.58	124.50	128.46
23	B	611	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
23	C	512	CLA	C4-C3-C5	2.58	119.60	115.27
25	T	101	BCR	C29-C28-C27	-2.57	105.62	111.38
23	c	503	CLA	OBD-CAD-C3D	-2.57	123.71	127.98
23	C	506	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
23	A	407	CLA	O2A-CGA-CBA	2.57	119.97	111.91
23	C	511	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	C	505	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
25	b	618	BCR	C38-C26-C25	-2.57	121.64	124.53
23	b	601	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
23	B	612	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
23	C	509	CLA	O2A-CGA-CBA	2.57	119.97	111.91
23	B	603	CLA	CMB-C2B-C3B	2.57	129.48	124.68
25	B	618	BCR	C37-C22-C23	2.57	122.12	118.08
23	D	403	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
35	H	102	DGD	O1G-C1A-O1A	-2.57	117.11	123.59
23	C	509	CLA	CMB-C2B-C3B	2.57	129.48	124.68
24	A	406	PHO	C2B-C1B-NB	2.57	113.66	109.79
25	b	618	BCR	C39-C30-C25	-2.57	106.14	110.30
23	b	611	CLA	CAC-C3C-C4C	2.56	128.14	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C4-C3-C5	2.56	119.58	115.27
23	B	609	CLA	CHD-C4C-NC	2.56	128.24	124.20
25	C	517	BCR	C11-C10-C9	-2.56	123.65	127.31
25	B	631	BCR	C2-C1-C6	2.56	114.42	110.48
23	c	503	CLA	C7-C6-C5	-2.56	106.41	113.36
25	d	404	BCR	C21-C20-C19	-2.56	115.23	123.22
23	c	508	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
23	B	608	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
23	b	609	CLA	C3B-C4B-NB	2.56	112.52	109.21
23	B	606	CLA	O2A-CGA-CBA	2.56	119.93	111.91
25	d	404	BCR	C10-C11-C12	-2.56	115.24	123.22
23	c	508	CLA	O2A-CGA-CBA	2.56	119.93	111.91
23	d	402	CLA	CMB-C2B-C3B	2.56	129.46	124.68
23	a	405	CLA	CBC-CAC-C3C	-2.56	105.39	112.43
23	C	515	CLA	C4D-C3D-CAD	-2.56	107.05	108.47
34	d	411	LMG	O7-C10-C11	2.55	117.01	111.50
23	C	513	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	c	506	CLA	CMC-C2C-C1C	2.55	128.93	125.04
23	A	403	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
23	B	611	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	A	404	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
23	C	509	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
23	b	601	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
23	c	511	CLA	OBD-CAD-C3D	-2.55	123.75	127.98
26	A	409	SQD	O47-C7-O49	-2.55	117.55	123.70
23	B	608	CLA	O2A-CGA-CBA	2.54	119.89	111.91
23	c	506	CLA	C4-C3-C5	2.54	119.55	115.27
23	D	404	CLA	C1-O2A-CGA	2.54	123.12	116.44
23	b	601	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
33	F	101	LMT	O5B-C1B-C2B	2.54	115.73	110.35
35	H	102	DGD	O1G-C1A-C2A	2.54	119.88	111.91
31	d	406	LHG	O7-C7-O9	-2.54	117.56	123.70
23	B	613	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
23	c	512	CLA	C11-C10-C8	-2.54	107.71	115.92
23	B	605	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
25	B	631	BCR	C21-C20-C19	-2.54	115.29	123.22
23	A	407	CLA	C4C-C3C-C2C	-2.54	103.20	106.90
23	B	601	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
24	A	406	PHO	CHC-C1C-C2C	-2.53	119.36	125.73
23	b	608	CLA	C4C-C3C-C2C	-2.53	103.20	106.90
23	C	506	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
23	b	606	CLA	OBD-CAD-C3D	-2.53	123.78	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
23	A	403	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	C	511	CLA	O2A-CGA-CBA	2.53	119.84	111.91
23	B	612	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
23	c	506	CLA	CAA-C2A-C3A	-2.53	105.86	112.78
23	d	403	CLA	C4-C3-C5	2.53	119.52	115.27
23	c	505	CLA	O2A-CGA-O1A	-2.53	117.22	123.59
23	C	504	CLA	O2A-CGA-CBA	2.52	119.83	111.91
23	b	603	CLA	CAC-C3C-C4C	2.52	128.08	124.81
23	b	610	CLA	CHC-C1C-C2C	-2.52	119.74	126.72
23	b	608	CLA	O2A-CGA-CBA	2.52	119.83	111.91
23	b	615	CLA	O2A-CGA-CBA	2.52	119.82	111.91
26	B	620	SQD	O48-C23-C24	2.52	119.82	111.91
23	b	615	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
23	D	403	CLA	CMC-C2C-C1C	2.52	128.88	125.04
23	a	404	CLA	C1-O2A-CGA	2.52	123.06	116.44
23	c	506	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
23	B	610	CLA	C1-C2-C3	-2.52	121.68	126.04
23	B	601	CLA	CHC-C1C-C2C	-2.52	119.75	126.72
24	a	406	PHO	O2D-CGD-O1D	-2.52	118.91	123.84
23	D	403	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
25	H	101	BCR	C10-C11-C12	-2.52	115.36	123.22
25	B	631	BCR	C7-C8-C9	-2.52	122.43	126.23
23	B	615	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
23	c	515	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
31	D	407	LHG	O8-C23-C24	2.52	119.80	111.91
23	C	515	CLA	C4-C3-C5	2.52	119.50	115.27
23	C	509	CLA	C1-C2-C3	-2.51	121.69	126.04
23	B	616	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
24	A	415	PHO	CAC-C3C-C4C	2.51	127.96	125.22
23	C	506	CLA	C4-C3-C5	2.51	119.50	115.27
23	b	609	CLA	O2A-CGA-CBA	2.51	119.78	111.91
23	C	504	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
23	c	513	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
23	D	404	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	C	503	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	c	505	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
23	B	605	CLA	C3B-C4B-NB	2.51	112.45	109.21
29	D	406	PL9	O2-C1-C6	-2.51	116.25	120.59
23	b	604	CLA	O2A-CGA-CBA	2.50	119.77	111.91
23	c	512	CLA	CAC-C3C-C4C	2.50	128.06	124.81
23	C	513	CLA	CED-O2D-CGD	2.50	121.59	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
23	b	601	CLA	CMB-C2B-C3B	2.50	129.35	124.68
23	b	604	CLA	O1D-CGD-CBD	-2.50	119.38	124.48
25	h	102	BCR	C36-C18-C17	-2.50	119.43	122.92
23	c	505	CLA	O2A-CGA-CBA	2.49	119.73	111.91
25	T	101	BCR	C7-C8-C9	-2.49	122.47	126.23
23	A	404	CLA	C3B-C4B-NB	2.49	112.43	109.21
25	B	617	BCR	C7-C8-C9	-2.49	122.47	126.23
25	a	408	BCR	C38-C26-C25	-2.49	121.73	124.53
34	a	417	LMG	O6-C5-C4	2.49	114.21	109.69
31	d	407	LHG	O8-C23-O10	-2.49	117.31	123.59
23	B	607	CLA	OBD-CAD-C3D	-2.49	123.85	127.98
25	B	619	BCR	C3-C4-C5	-2.49	109.64	114.08
25	B	631	BCR	C11-C10-C9	-2.49	123.76	127.31
25	A	408	BCR	C15-C14-C13	-2.48	123.77	127.31
24	A	406	PHO	CMC-C2C-C1C	2.48	128.89	125.06
23	d	402	CLA	C4D-C3D-CAD	-2.48	107.09	108.47
29	d	405	PL9	C51-C49-C50	2.48	120.08	114.60
23	c	514	CLA	O1D-CGD-CBD	-2.48	119.41	124.48
31	a	419	LHG	O8-C23-C24	2.48	119.69	111.91
33	C	526	LMT	O5'-C5'-C4'	2.48	114.98	109.75
23	b	612	CLA	CHD-C4C-NC	2.48	128.11	124.20
23	C	512	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
25	D	405	BCR	C10-C11-C12	-2.48	115.48	123.22
23	A	404	CLA	C4A-NA-C1A	-2.48	105.59	106.71
23	B	611	CLA	C4-C3-C5	2.48	119.44	115.27
23	b	615	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
23	b	616	CLA	OBD-CAD-CBD	2.48	129.43	125.89
35	H	102	DGD	O2G-C1B-C2B	2.47	116.83	111.50
29	d	405	PL9	C36-C37-C38	-2.47	103.76	111.88
23	b	606	CLA	CMB-C2B-C3B	2.47	129.30	124.68
23	b	606	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
40	v	202	HEC	C1D-C2D-C3D	-2.47	105.28	107.00
23	D	403	CLA	CMB-C2B-C3B	2.47	129.29	124.68
23	B	603	CLA	CMA-C3A-C2A	-2.47	103.87	113.83
24	a	406	PHO	C3C-C4C-NC	2.47	114.10	110.28
23	c	514	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
35	H	102	DGD	O4D-C4D-C5D	-2.47	103.18	109.30
23	d	402	CLA	CAC-C3C-C4C	2.46	128.01	124.81
23	B	601	CLA	CAA-C2A-C3A	-2.46	106.03	112.78
23	a	403	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
23	c	504	CLA	O2A-CGA-CBA	2.46	119.64	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	517	BCR	C36-C18-C19	2.46	121.96	118.08
25	b	619	BCR	C8-C9-C10	2.46	122.72	118.94
29	D	406	PL9	C15-C14-C16	2.46	119.41	115.27
23	B	602	CLA	CED-O2D-CGD	2.46	121.50	115.94
23	b	606	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
23	b	607	CLA	C4-C3-C5	2.46	119.41	115.27
29	a	414[B]	PL9	C30-C29-C31	2.46	119.41	115.27
23	b	613	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	T	101	BCR	C21-C20-C19	-2.46	115.55	123.22
23	B	603	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	A	404	CLA	C2A-C1A-CHA	-2.46	119.57	123.86
23	C	508	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
23	b	611	CLA	OBD-CAD-C3D	-2.45	123.91	127.98
23	d	403	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
33	F	101	LMT	C4B-C3B-C2B	-2.45	106.55	110.82
23	b	612	CLA	OBD-CAD-C3D	-2.45	123.91	127.98
25	T	101	BCR	C10-C11-C12	-2.45	115.57	123.22
24	A	406	PHO	CHD-C1D-C2D	-2.45	119.57	125.73
25	B	619	BCR	C10-C11-C12	-2.45	115.58	123.22
23	C	515	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
29	a	414[B]	PL9	C12-C13-C14	-2.45	121.77	127.66
25	C	516	BCR	C11-C10-C9	-2.45	123.82	127.31
34	Z	101	LMG	C1-O6-C5	2.45	118.49	113.69
25	c	517	BCR	C21-C20-C19	-2.44	115.59	123.22
29	D	406	PL9	C17-C18-C19	-2.44	121.78	127.66
23	b	603	CLA	CMC-C2C-C1C	2.44	128.76	125.04
23	c	508	CLA	CBC-CAC-C3C	-2.44	105.69	112.43
24	A	415	PHO	CMB-C2B-C1B	2.44	128.82	125.06
23	b	615	CLA	CHD-C4C-NC	2.44	128.05	124.20
23	b	609	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
23	c	515	CLA	CHD-C4C-NC	2.44	128.04	124.20
25	D	405	BCR	C16-C17-C18	-2.44	123.83	127.31
25	h	102	BCR	C10-C11-C12	-2.44	115.61	123.22
35	c	519	DGD	O1G-C1A-C2A	2.44	119.56	111.91
23	B	602	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
29	D	406	PL9	C36-C37-C38	-2.44	103.87	111.88
23	C	513	CLA	CBC-CAC-C3C	-2.43	105.72	112.43
29	D	406	PL9	C20-C19-C21	2.43	119.36	115.27
23	C	515	CLA	CAC-C3C-C4C	2.43	127.96	124.81
25	c	516	BCR	C8-C7-C6	-2.43	120.38	127.20
23	B	612	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
23	C	503	CLA	O2A-CGA-CBA	2.43	119.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	PHO	C3C-C4C-NC	2.43	114.05	110.28
25	K	101	BCR	C10-C11-C12	-2.43	115.64	123.22
23	C	509	CLA	C11-C12-C13	-2.43	108.07	115.92
23	A	407	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	C	505	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	a	405	CLA	C4-C3-C5	2.43	119.36	115.27
23	c	512	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
35	c	518	DGD	O6D-C1D-O3G	-2.43	104.23	109.97
25	C	516	BCR	C20-C21-C22	-2.43	123.85	127.31
23	c	506	CLA	CMB-C2B-C3B	2.43	129.22	124.68
25	h	102	BCR	C38-C26-C25	-2.42	121.81	124.53
23	b	607	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
26	B	620	SQD	O9-S-C6	2.42	109.82	106.94
31	d	407	LHG	O7-C7-C8	2.42	116.72	111.50
23	B	607	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
23	C	513	CLA	C1-C2-C3	-2.42	121.85	126.04
25	B	619	BCR	C21-C20-C19	-2.42	115.66	123.22
23	d	402	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
23	c	509	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
29	A	413[A]	PL9	C16-C14-C13	-2.42	116.22	121.12
23	B	606	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
23	c	507	CLA	C4-C3-C5	2.42	119.33	115.27
29	A	413[B]	PL9	C21-C22-C23	-2.41	103.95	111.88
23	B	610	CLA	CMA-C3A-C4A	-2.41	105.29	111.77
23	a	405	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
23	C	507	CLA	CHD-C4C-NC	2.41	128.00	124.20
23	b	613	CLA	CMB-C2B-C3B	2.41	129.19	124.68
25	T	101	BCR	C16-C15-C14	2.41	128.41	123.47
25	h	102	BCR	C34-C9-C8	2.41	121.87	118.08
25	a	408	BCR	C29-C30-C25	2.41	114.19	110.48
25	B	617	BCR	C16-C17-C18	-2.41	123.88	127.31
24	a	406	PHO	C3A-C4A-CHB	-2.41	117.67	121.83
23	a	407	CLA	CHC-C1C-C2C	-2.41	120.07	126.72
23	a	407	CLA	CAC-C3C-C4C	2.40	127.93	124.81
24	a	416	PHO	CMC-C2C-C1C	2.40	128.76	125.06
34	Z	101	LMG	C9-C8-C7	-2.40	106.11	111.79
23	C	510	CLA	C1-C2-C3	-2.40	121.89	126.04
23	b	604	CLA	C4C-C3C-C2C	-2.40	103.40	106.90
23	a	405	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
35	h	103	DGD	O1G-C1A-O1A	-2.40	117.54	123.59
23	c	514	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	d	404	BCR	C29-C30-C25	2.40	114.17	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	415	PHO	C2C-C1C-NC	2.39	113.40	109.79
23	c	514	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	B	631	BCR	C1-C6-C7	2.39	122.54	115.78
23	a	404	CLA	C4C-C3C-C2C	-2.39	103.41	106.90
25	K	101	BCR	C36-C18-C19	2.39	121.84	118.08
23	C	515	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
23	C	508	CLA	CHD-C4C-NC	2.39	127.97	124.20
31	A	416	LHG	O7-C7-O9	-2.39	117.93	123.70
23	b	616	CLA	CMB-C2B-C3B	2.39	129.14	124.68
25	c	517	BCR	C37-C22-C23	2.39	121.84	118.08
23	C	504	CLA	CBC-CAC-C3C	-2.39	105.85	112.43
32	h	101	HTG	C6-C5-C4	-2.39	107.42	113.00
25	B	619	BCR	C38-C26-C25	-2.38	121.85	124.53
23	A	407	CLA	CMB-C2B-C3B	2.38	129.14	124.68
23	c	509	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
25	C	517	BCR	C29-C30-C25	2.38	114.14	110.48
25	C	516	BCR	C37-C22-C23	2.38	121.82	118.08
23	c	507	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	B	606	CLA	OBD-CAD-C3D	-2.38	124.04	127.98
33	b	626	LMT	O1'-C1'-C2'	2.38	112.01	108.30
34	z	101	LMG	C8-O7-C10	-2.37	111.94	117.79
31	D	407	LHG	O8-C23-O10	-2.37	117.60	123.59
25	Y	101	BCR	C37-C22-C21	-2.37	119.60	122.92
26	A	411	SQD	O7-S-C6	2.37	109.76	106.94
23	C	508	CLA	CGD-CBD-CAD	-2.37	103.05	110.73
23	C	506	CLA	O2A-CGA-CBA	2.37	119.34	111.91
23	b	609	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	b	602	CLA	C1-O2A-CGA	2.37	122.66	116.44
23	B	605	CLA	C7-C6-C5	-2.37	106.93	113.36
23	A	403	CLA	CHB-C4A-NA	2.37	127.79	124.51
31	D	407	LHG	O7-C7-C8	2.37	116.60	111.50
23	c	505	CLA	CMB-C2B-C1B	2.37	132.10	128.46
23	B	616	CLA	CHC-C1C-C2C	-2.37	120.18	126.72
23	a	404	CLA	CAA-CBA-CGA	2.37	120.17	113.25
35	c	518	DGD	C2G-O2G-C1B	-2.36	111.97	117.79
23	c	507	CLA	CAC-C3C-C4C	2.36	127.88	124.81
31	D	408	LHG	O8-C23-O10	-2.36	117.62	123.59
25	b	619	BCR	C21-C20-C19	-2.36	115.84	123.22
24	A	415	PHO	C6-C5-C3	-2.36	107.26	113.45
23	c	511	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
24	A	415	PHO	CHD-C1D-C2D	-2.36	119.79	125.73
23	b	603	CLA	CMA-C3A-C2A	-2.36	104.30	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	414[A]	PL9	C30-C29-C31	2.36	119.24	115.27
33	m	103	LMT	C1-O1'-C1'	-2.36	109.93	113.84
23	B	610	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
23	c	511	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
23	c	509	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
23	C	512	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	d	405	PL9	C27-C28-C29	-2.35	121.99	127.66
23	b	616	CLA	C4-C3-C5	2.35	119.23	115.27
23	c	509	CLA	C3B-C4B-NB	2.35	112.25	109.21
23	d	402	CLA	CHD-C4C-NC	2.35	127.91	124.20
34	D	412	LMG	C7-O1-C1	-2.35	109.15	113.74
25	b	619	BCR	C35-C13-C14	-2.35	119.64	122.92
23	C	509	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	C	510	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	B	609	CLA	C4-C3-C5	2.34	119.22	115.27
33	m	103	LMT	O5B-C5B-C6B	2.34	112.26	106.44
32	B	621	HTG	O2-C2-C3	-2.34	104.93	110.35
23	b	613	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	B	615	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	c	511	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
25	k	102	BCR	C16-C17-C18	-2.34	123.97	127.31
23	C	506	CLA	CED-O2D-CGD	2.34	121.23	115.94
23	C	514	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	C	504	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
23	b	609	CLA	CAC-C3C-C4C	2.34	127.85	124.81
25	B	631	BCR	C36-C18-C19	2.34	121.76	118.08
23	b	615	CLA	C4-C3-C5	2.34	119.20	115.27
23	C	511	CLA	C11-C12-C13	-2.34	108.37	115.92
23	c	506	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
23	C	507	CLA	C1-C2-C3	-2.33	122.01	126.04
29	D	406	PL9	C25-C24-C23	-2.33	117.70	123.68
23	c	505	CLA	CHD-C4C-NC	2.33	127.87	124.20
23	C	504	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
26	a	409	SQD	O6-C44-C45	-2.33	105.29	110.90
25	K	101	BCR	C33-C5-C6	-2.33	121.92	124.53
23	C	510	CLA	O2A-CGA-O1A	-2.32	117.72	123.59
23	C	514	CLA	CAC-C3C-C4C	2.32	127.83	124.81
23	B	609	CLA	OBD-CAD-C3D	-2.32	124.12	127.98
23	b	608	CLA	CMA-C3A-C4A	-2.32	105.53	111.77
31	d	408	LHG	C5-O7-C7	-2.32	112.08	117.79
25	d	404	BCR	C16-C15-C14	-2.32	118.72	123.47
23	c	507	CLA	CHD-C4C-NC	2.32	127.86	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	CMC-C2C-C1C	2.32	128.57	125.04
34	c	521	LMG	O8-C28-O10	-2.32	117.74	123.59
34	c	522	LMG	O8-C28-O10	-2.32	117.75	123.59
23	b	601	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
23	c	510	CLA	CAC-C3C-C2C	2.31	131.49	127.53
26	f	101	SQD	O8-S-C6	2.31	109.43	105.74
25	b	619	BCR	C16-C17-C18	-2.31	124.01	127.31
23	c	506	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
23	B	616	CLA	CAC-C3C-C4C	2.31	127.81	124.81
23	A	403	CLA	CMA-C3A-C2A	-2.31	104.51	113.83
23	c	515	CLA	C4-C3-C5	2.31	119.16	115.27
23	C	514	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
25	c	517	BCR	C36-C18-C19	2.31	121.72	118.08
29	A	413[A]	PL9	C47-C48-C49	-2.31	119.86	127.75
24	A	406	PHO	O2A-CGA-CBA	2.31	119.15	111.91
25	Y	101	BCR	C28-C27-C26	-2.31	109.96	114.08
23	b	601	CLA	C1-O2A-CGA	2.31	122.50	116.44
25	D	405	BCR	C11-C10-C9	-2.31	124.02	127.31
23	c	503	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
23	a	403	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
23	a	405	CLA	CHC-C1C-C2C	-2.30	120.35	126.72
23	b	603	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
33	B	627	LMT	O1B-C4'-C3'	2.30	113.40	107.28
23	b	602	CLA	CHD-C4C-NC	2.30	127.83	124.20
25	k	102	BCR	C7-C8-C9	-2.30	122.76	126.23
23	b	601	CLA	CAC-C3C-C2C	2.30	131.46	127.53
23	C	505	CLA	OBD-CAD-C3D	-2.30	124.17	127.98
24	a	416	PHO	CBA-CAA-C2A	-2.30	107.08	113.86
24	A	406	PHO	C2C-C1C-NC	2.30	113.26	109.79
32	b	624	HTG	C4-C3-C2	-2.30	106.81	110.82
23	C	510	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
23	C	514	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
40	V	201	HEC	CAA-CBA-CGA	-2.30	108.82	112.67
25	k	101	BCR	C7-C8-C9	-2.29	122.77	126.23
23	a	403	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
26	B	620	SQD	C1-C2-C3	-2.29	105.22	110.00
35	C	519	DGD	C1E-O6E-C5E	-2.29	109.19	113.69
24	a	406	PHO	O1D-CGD-CBD	-2.29	119.80	124.48
32	B	621	HTG	C1-O5-C5	2.29	116.80	112.58
23	c	504	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	b	615	CLA	C11-C12-C13	-2.29	108.52	115.92
23	b	614	CLA	CMB-C2B-C3B	2.29	128.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
25	B	617	BCR	C29-C30-C25	2.29	114.00	110.48
29	d	405	PL9	C47-C48-C49	-2.29	119.94	127.75
23	c	508	CLA	CAC-C3C-C4C	2.28	127.77	124.81
23	B	616	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
23	b	602	CLA	CMA-C3A-C2A	-2.28	104.61	113.83
23	C	504	CLA	CMC-C2C-C1C	2.28	128.52	125.04
31	L	101	LHG	O4-P-O5	2.28	123.52	112.24
23	A	403	CLA	CBC-CAC-C3C	-2.28	106.14	112.43
33	b	626	LMT	O5'-C5'-C4'	2.28	114.56	109.75
25	c	516	BCR	C35-C13-C14	-2.28	119.73	122.92
23	B	616	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
34	a	417	LMG	C8-O7-C10	-2.28	112.18	117.79
23	c	513	CLA	C11-C12-C13	-2.28	108.55	115.92
29	d	405	PL9	C15-C14-C16	2.28	119.11	115.27
23	C	514	CLA	CMC-C2C-C1C	2.28	128.51	125.04
23	B	610	CLA	CHD-C4C-NC	2.28	127.79	124.20
23	b	605	CLA	C5-C3-C2	-2.28	116.51	121.12
23	A	404	CLA	CMB-C2B-C1B	2.27	131.96	128.46
23	c	504	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
33	m	103	LMT	O6'-C6'-C5'	-2.27	103.50	111.29
35	C	518	DGD	C2G-O2G-C1B	-2.27	112.20	117.79
23	c	505	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
23	B	606	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
23	D	404	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	C	507	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
23	B	602	CLA	O2A-CGA-CBA	2.27	119.03	111.91
23	c	505	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
23	A	404	CLA	C1-C2-C3	-2.27	122.12	126.04
23	b	616	CLA	CHC-C1C-C2C	-2.26	120.46	126.72
23	C	507	CLA	O2A-CGA-CBA	2.26	119.01	111.91
24	A	406	PHO	C4-C3-C5	2.26	119.08	115.27
33	a	418	LMT	O5B-C5B-C4B	2.26	113.80	109.69
32	b	624	HTG	C6-C5-C4	-2.26	107.71	113.00
23	b	604	CLA	CAC-C3C-C4C	2.26	127.74	124.81
29	A	413[B]	PL9	C51-C49-C50	2.26	119.60	114.60
23	c	513	CLA	C1-O2A-CGA	2.26	122.37	116.44
35	H	102	DGD	C3E-C4E-C5E	-2.26	106.21	110.24
23	c	504	CLA	C4-C3-C5	2.26	119.07	115.27
33	M	103	LMT	O1B-C1B-C2B	2.26	113.95	108.10
26	a	409	SQD	C45-O47-C7	-2.26	112.23	117.79
24	a	416	PHO	C1C-C2C-C3C	-2.26	103.92	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C4D-C3D-CAD	-2.26	107.21	108.47
31	b	628	LHG	O8-C23-O10	-2.26	117.90	123.59
23	B	601	CLA	CMB-C2B-C3B	2.26	128.90	124.68
23	B	608	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	b	605	CLA	CMC-C2C-C1C	2.25	128.47	125.04
23	C	515	CLA	CMB-C2B-C3B	2.25	128.89	124.68
23	c	512	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
29	a	414[A]	PL9	C47-C48-C49	-2.25	120.06	127.75
31	L	101	LHG	O8-C23-O10	-2.25	117.92	123.59
23	C	511	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
23	B	608	CLA	C11-C12-C13	-2.25	108.66	115.92
26	f	101	SQD	O47-C7-O49	-2.25	118.28	123.70
25	B	618	BCR	C15-C16-C17	-2.25	118.88	123.47
23	D	403	CLA	C4-C3-C5	2.24	119.04	115.27
23	c	509	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
23	D	404	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
23	B	613	CLA	C1D-CHD-C4C	-2.24	119.60	122.56
23	b	609	CLA	C16-C15-C13	-2.24	108.68	115.92
25	a	408	BCR	C10-C11-C12	-2.24	116.23	123.22
23	B	614	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
34	M	101	LMG	C9-C8-C7	-2.24	106.50	111.79
23	B	610	CLA	CMC-C2C-C1C	2.24	128.45	125.04
25	a	408	BCR	C15-C16-C17	-2.24	118.89	123.47
32	h	101	HTG	C1-C2-C3	-2.24	106.17	110.59
23	B	607	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	C	506	CLA	C3D-CAD-CBD	2.24	110.55	107.61
23	B	615	CLA	CAC-C3C-C4C	2.23	127.71	124.81
29	D	406	PL9	C42-C41-C39	-2.23	105.63	112.98
25	B	618	BCR	C7-C8-C9	-2.23	122.86	126.23
25	a	408	BCR	C8-C7-C6	-2.23	120.94	127.20
23	C	504	CLA	CED-O2D-CGD	2.23	120.98	115.94
25	T	101	BCR	C34-C9-C8	2.23	121.59	118.08
34	m	101	LMG	O8-C28-O10	-2.23	117.97	123.59
29	a	414[B]	PL9	C51-C49-C50	2.23	119.52	114.60
23	b	615	CLA	CMB-C2B-C1B	2.23	131.89	128.46
23	c	503	CLA	CMB-C2B-C3B	2.23	128.84	124.68
25	B	617	BCR	C38-C26-C25	-2.23	122.03	124.53
26	a	411	SQD	O5-C5-C4	2.23	113.74	109.69
35	C	518	DGD	O6E-C5E-C4E	2.22	113.73	109.69
24	a	406	PHO	CHD-C1D-C2D	-2.22	120.14	125.73
26	D	413	SQD	O48-C23-O10	-2.22	117.98	123.59
34	c	522	LMG	C1-O6-C5	2.22	118.05	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	T	101	BCR	C1-C6-C7	2.22	122.06	115.78
33	e	101	LMT	O1'-C1'-C2'	2.22	111.77	108.30
23	b	608	CLA	OBD-CAD-C3D	-2.22	124.30	127.98
25	H	101	BCR	C29-C30-C25	2.22	113.89	110.48
23	c	504	CLA	CAC-C3C-C4C	2.22	127.69	124.81
23	B	615	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
23	b	605	CLA	C6-C7-C8	-2.22	108.75	115.92
29	A	413[A]	PL9	C51-C49-C50	2.22	119.50	114.60
35	H	102	DGD	O6E-C5E-C6E	2.22	111.94	106.44
23	B	613	CLA	CHD-C4C-NC	2.21	127.69	124.20
26	A	409	SQD	O9-S-O7	-2.21	106.29	113.95
23	B	614	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
35	c	520	DGD	O2G-C1B-O1B	-2.21	118.36	123.70
23	b	611	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
35	c	518	DGD	O1G-C1A-C2A	2.21	118.84	111.91
23	c	515	CLA	CED-O2D-CGD	2.21	120.93	115.94
29	d	405	PL9	C25-C24-C26	2.21	118.98	115.27
33	B	629	LMT	C3'-C4'-C5'	-2.20	105.88	110.93
23	c	513	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
23	b	610	CLA	OBD-CAD-C3D	-2.20	124.33	127.98
25	Y	101	BCR	C15-C16-C17	-2.20	118.97	123.47
23	B	608	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
23	A	404	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
25	Y	101	BCR	C10-C11-C12	-2.20	116.36	123.22
23	A	403	CLA	CHD-C4C-NC	2.20	127.67	124.20
26	A	411	SQD	O48-C23-O10	-2.20	118.05	123.59
26	A	411	SQD	O6-C1-C2	2.20	111.73	108.30
29	A	413[A]	PL9	C35-C34-C36	2.19	118.96	115.27
25	A	408	BCR	C34-C9-C8	2.19	121.53	118.08
23	c	506	CLA	O2A-CGA-CBA	2.19	118.80	111.91
23	B	602	CLA	C4-C3-C5	2.19	118.96	115.27
25	c	516	BCR	C34-C9-C10	-2.19	119.85	122.92
25	Y	101	BCR	C33-C5-C4	2.19	117.82	113.62
24	A	415	PHO	C4D-CHA-C1A	-2.19	120.44	125.37
29	a	414[A]	PL9	C47-C46-C44	-2.19	105.78	112.98
23	C	512	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
23	A	403	CLA	OBD-CAD-C3D	-2.19	124.35	127.98
23	c	513	CLA	CMB-C2B-C3B	2.19	128.77	124.68
23	B	604	CLA	C11-C10-C8	-2.19	108.85	115.92
23	C	506	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	C	510	CLA	CAC-C3C-C2C	2.18	131.26	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	404	BCR	C23-C24-C25	-2.18	121.07	127.20
23	b	613	CLA	CED-O2D-CGD	2.18	120.87	115.94
23	c	505	CLA	C11-C12-C13	-2.18	108.87	115.92
25	C	517	BCR	C39-C30-C25	-2.18	106.77	110.30
32	b	621	HTG	O2-C2-C3	-2.18	105.32	110.35
23	B	602	CLA	C1-C2-C3	-2.18	122.28	126.04
23	c	506	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
34	a	417	LMG	C3-C4-C5	2.17	114.12	110.24
23	B	605	CLA	CAA-C2A-C3A	-2.17	106.83	112.78
26	D	413	SQD	O47-C7-O49	-2.17	118.45	123.70
25	c	517	BCR	C28-C27-C26	-2.17	110.20	114.08
34	C	502	LMG	O8-C28-C29	2.17	118.73	111.91
25	c	517	BCR	C37-C22-C21	-2.17	119.88	122.92
23	a	404	CLA	OBD-CAD-C3D	-2.17	124.37	127.98
25	C	516	BCR	C3-C4-C5	-2.17	110.20	114.08
23	a	403	CLA	CBC-CAC-C3C	-2.17	106.44	112.43
23	c	515	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	a	405	CLA	O2A-CGA-CBA	2.17	118.72	111.91
23	D	403	CLA	CAC-C3C-C4C	2.17	127.63	124.81
23	d	402	CLA	C4-C3-C2	-2.17	118.11	123.68
23	B	614	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	b	602	CLA	O2A-CGA-CBA	2.17	118.71	111.91
23	a	404	CLA	C4-C3-C5	2.17	118.92	115.27
29	a	414[B]	PL9	C40-C39-C41	2.17	118.92	115.27
25	k	101	BCR	C10-C11-C12	-2.17	116.45	123.22
26	f	101	SQD	O48-C23-O10	-2.17	118.12	123.59
35	c	520	DGD	O3G-C3G-C2G	-2.17	105.67	110.90
38	e	102	HEM	C3C-C4C-NC	-2.17	106.85	110.94
31	D	408	LHG	C6-C5-C4	-2.17	106.67	111.79
24	a	416	PHO	C2C-C1C-NC	2.17	113.06	109.79
38	E	102	HEM	C3C-C4C-NC	-2.16	106.86	110.94
34	C	522	LMG	O8-C28-O10	-2.16	118.14	123.59
25	b	617	BCR	C24-C23-C22	-2.16	122.97	126.23
23	B	615	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
23	B	608	CLA	OBD-CAD-C3D	-2.16	124.39	127.98
23	B	616	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
32	h	101	HTG	C3-C4-C5	2.16	114.09	110.24
23	C	509	CLA	C6-C7-C8	-2.16	108.94	115.92
34	C	522	LMG	C9-C8-C7	-2.16	106.69	111.79
26	B	620	SQD	O47-C7-O49	-2.16	118.49	123.70
23	C	503	CLA	OBD-CAD-C3D	-2.16	124.40	127.98
23	b	615	CLA	C4D-C3D-CAD	-2.16	107.27	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CHB-C4A-NA	2.16	127.49	124.51
23	C	507	CLA	CHA-C1A-NA	-2.15	121.46	126.40
23	c	508	CLA	C2A-C1A-CHA	-2.15	120.09	123.86
23	b	615	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
35	c	519	DGD	O1G-C1A-O1A	-2.15	118.16	123.59
23	c	514	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	L	101	LHG	O7-C7-O9	-2.15	118.50	123.70
25	b	618	BCR	C2-C1-C6	2.15	113.79	110.48
23	C	503	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
29	A	413[B]	PL9	C37-C36-C34	-2.15	105.90	112.98
23	C	507	CLA	C4-C3-C5	2.15	118.89	115.27
23	B	607	CLA	O2A-CGA-CBA	2.15	118.66	111.91
23	b	605	CLA	O2A-CGA-CBA	2.15	118.65	111.91
33	B	627	LMT	C3B-C4B-C5B	2.15	114.07	110.24
33	B	630	LMT	C3'-C4'-C5'	-2.15	106.00	110.93
23	b	610	CLA	CAA-CBA-CGA	-2.15	106.98	113.25
23	B	610	CLA	CMA-C3A-C2A	-2.15	105.17	113.83
23	a	403	CLA	CAA-C2A-C1A	-2.15	104.94	111.97
29	d	405	PL9	C7-C8-C9	-2.15	123.22	126.79
23	D	403	CLA	CHD-C4C-NC	2.15	127.58	124.20
33	M	102	LMT	O5B-C5B-C6B	2.15	111.77	106.44
23	b	613	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
23	b	611	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
23	C	513	CLA	C1-O2A-CGA	2.14	122.07	116.44
34	a	417	LMG	O7-C10-O9	-2.14	118.52	123.70
23	B	603	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
24	a	406	PHO	CBA-CAA-C2A	-2.14	107.54	113.86
29	D	406	PL9	C27-C28-C29	-2.14	122.51	127.66
35	h	103	DGD	O3G-C1D-C2D	2.14	111.64	108.30
23	c	503	CLA	C4D-C3D-CAD	-2.14	107.28	108.47
25	B	618	BCR	C10-C11-C12	-2.14	116.55	123.22
23	c	507	CLA	C1-C2-C3	-2.14	122.35	126.04
23	D	404	CLA	C4-C3-C5	2.13	118.86	115.27
23	b	609	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
25	H	101	BCR	C16-C15-C14	-2.13	119.10	123.47
23	b	607	CLA	CAC-C3C-C4C	2.13	127.58	124.81
23	b	610	CLA	CAC-C3C-C4C	2.13	127.58	124.81
25	c	517	BCR	C16-C17-C18	-2.13	124.27	127.31
34	M	101	LMG	C9-O8-C28	2.13	125.02	117.12
33	F	101	LMT	O5'-C5'-C4'	2.13	114.25	109.75
29	D	406	PL9	C32-C33-C34	-2.13	122.53	127.66
29	a	414[A]	PL9	C40-C39-C41	2.13	118.85	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	408	LHG	O7-C7-O9	-2.13	118.56	123.70
25	Y	101	BCR	C16-C15-C14	-2.13	119.11	123.47
25	b	617	BCR	C39-C30-C25	-2.13	106.85	110.30
23	c	511	CLA	CHD-C4C-NC	2.13	127.56	124.20
25	k	101	BCR	C20-C21-C22	-2.13	124.28	127.31
23	c	507	CLA	CMC-C2C-C1C	2.12	128.27	125.04
23	B	613	CLA	CED-O2D-CGD	2.12	120.73	115.94
25	k	102	BCR	C40-C30-C25	-2.12	106.86	110.30
23	a	407	CLA	CMB-C2B-C3B	2.12	128.64	124.68
23	C	506	CLA	CMB-C2B-C3B	2.12	128.64	124.68
23	B	601	CLA	C1-O2A-CGA	2.12	122.00	116.44
23	b	606	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
33	B	627	LMT	O1B-C4'-C5'	-2.12	103.64	109.45
25	D	405	BCR	C30-C25-C24	2.12	121.77	115.78
23	B	611	CLA	C1-O2A-CGA	2.12	122.00	116.44
23	c	512	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	C	506	CLA	C1-O2A-CGA	2.12	122.00	116.44
34	c	521	LMG	C8-O7-C10	-2.12	112.58	117.79
23	C	503	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
23	A	404	CLA	CMA-C3A-C4A	-2.12	106.09	111.77
23	B	616	CLA	C4-C3-C5	2.12	118.83	115.27
29	a	414[B]	PL9	C47-C48-C49	-2.12	120.52	127.75
23	c	512	CLA	CMB-C2B-C3B	2.12	128.64	124.68
25	k	101	BCR	C34-C9-C10	-2.11	119.96	122.92
23	d	402	CLA	C6-C5-C3	2.11	118.99	113.45
25	B	631	BCR	C35-C13-C12	2.11	121.40	118.08
23	B	609	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
23	b	602	CLA	C6-C7-C8	-2.11	109.10	115.92
23	A	407	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
23	b	604	CLA	C6-C7-C8	-2.11	109.11	115.92
25	T	101	BCR	C7-C6-C5	-2.11	116.36	121.46
23	B	615	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
23	b	616	CLA	CHA-C1A-NA	-2.11	121.57	126.40
23	B	608	CLA	C1-C2-C3	-2.11	122.40	126.04
23	c	513	CLA	CAA-CBA-CGA	-2.11	107.10	113.25
32	b	622	HTG	O5-C1-C2	2.10	112.96	110.31
25	Y	101	BCR	C11-C10-C9	-2.10	124.31	127.31
23	a	407	CLA	C3D-CAD-CBD	2.10	110.38	107.61
23	c	503	CLA	C1-C2-C3	-2.10	122.40	126.04
23	B	606	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
35	c	518	DGD	O3G-C3G-C2G	-2.10	105.82	110.90
26	a	411	SQD	C1-O5-C5	2.10	117.81	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	403	CLA	C1-C2-C3	-2.10	122.41	126.04
23	b	608	CLA	C11-C12-C13	-2.10	109.13	115.92
23	A	404	CLA	CAA-CBA-CGA	2.10	119.38	113.25
23	b	609	CLA	CBC-CAC-C3C	-2.10	106.65	112.43
23	c	514	CLA	CBA-CAA-C2A	-2.10	107.67	113.86
24	a	406	PHO	C4D-ND-C1D	-2.10	102.99	106.76
25	T	101	BCR	C34-C9-C10	-2.09	119.99	122.92
24	A	406	PHO	CBA-CAA-C2A	-2.09	107.69	113.86
24	A	406	PHO	C3A-C2A-C1A	-2.09	99.15	101.64
35	c	520	DGD	O3G-C1D-C2D	-2.09	105.04	108.30
33	a	412	LMT	O1B-C1B-C2B	2.09	113.51	108.10
23	b	609	CLA	OBD-CAD-C3D	-2.09	124.52	127.98
25	A	408	BCR	C33-C5-C6	-2.09	122.19	124.53
23	b	607	CLA	CAA-CBA-CGA	2.08	119.34	113.25
25	D	405	BCR	C40-C30-C25	-2.08	106.92	110.30
23	b	602	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
23	b	604	CLA	C4-C3-C5	2.08	118.78	115.27
25	C	517	BCR	C21-C20-C19	-2.08	116.73	123.22
23	B	604	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
23	B	614	CLA	C3D-CAD-CBD	2.08	110.34	107.61
23	B	608	CLA	CAC-C3C-C4C	2.08	127.51	124.81
23	B	602	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
33	e	101	LMT	C1B-C2B-C3B	2.08	114.32	110.00
23	b	616	CLA	C4D-C3D-CAD	-2.08	107.31	108.47
23	c	514	CLA	CMB-C2B-C3B	2.08	128.56	124.68
25	k	101	BCR	C16-C15-C14	-2.08	119.22	123.47
23	b	607	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
23	B	611	CLA	CHB-C4A-NA	2.07	127.38	124.51
23	b	605	CLA	CMB-C2B-C3B	2.07	128.56	124.68
32	h	101	HTG	O5-C1-C2	-2.07	107.70	110.31
33	a	418	LMT	C1B-O1B-C4'	-2.07	112.83	117.96
23	b	601	CLA	C5-C3-C2	-2.07	116.92	121.12
23	B	612	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
29	A	413[B]	PL9	C47-C48-C49	-2.07	120.67	127.75
29	a	414[A]	PL9	C16-C14-C13	-2.07	116.92	121.12
26	a	409	SQD	O48-C23-O10	-2.07	118.36	123.59
23	C	505	CLA	CHA-C1A-NA	-2.07	121.65	126.40
23	C	503	CLA	C7-C6-C5	-2.07	107.73	113.36
23	D	404	CLA	C2A-C1A-CHA	-2.07	120.24	123.86
23	B	603	CLA	OBD-CAD-C3D	-2.07	124.55	127.98
23	C	513	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	B	609	CLA	CAC-C3C-C4C	2.07	127.49	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
23	b	610	CLA	CMB-C2B-C1B	2.07	131.64	128.46
23	B	608	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
25	b	618	BCR	C37-C22-C21	-2.07	120.03	122.92
23	B	601	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
23	a	404	CLA	CHB-C4A-NA	2.06	127.36	124.51
23	B	601	CLA	CMA-C3A-C2A	-2.06	105.51	113.83
25	B	618	BCR	C30-C25-C26	-2.06	119.71	122.61
23	B	613	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
23	b	614	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
23	C	508	CLA	CMB-C2B-C3B	2.06	128.53	124.68
33	e	101	LMT	C4B-C3B-C2B	2.06	114.42	110.82
23	A	404	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
25	b	617	BCR	C36-C18-C19	2.06	121.32	118.08
23	d	402	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
23	C	506	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	h	102	BCR	C37-C22-C21	-2.06	120.04	122.92
23	b	613	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
23	D	404	CLA	CMB-C2B-C1B	2.05	131.62	128.46
24	a	416	PHO	C3A-C4A-CHB	-2.05	118.28	121.83
23	C	504	CLA	CMB-C2B-C1B	2.05	131.62	128.46
35	C	520	DGD	O2G-C1B-O1B	-2.05	118.75	123.70
33	a	412	LMT	C2'-C3'-C4'	2.05	114.36	109.68
25	D	405	BCR	C15-C14-C13	-2.05	124.39	127.31
25	h	102	BCR	C20-C21-C22	-2.05	124.39	127.31
23	b	616	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	b	612	CLA	C11-C10-C8	-2.05	109.30	115.92
23	b	616	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
23	c	512	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	b	610	CLA	C4-C3-C2	-2.05	118.43	123.68
25	b	618	BCR	C11-C10-C9	-2.04	124.39	127.31
23	b	610	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
23	c	515	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
25	B	631	BCR	C7-C6-C5	-2.04	116.51	121.46
35	C	520	DGD	O1G-C1A-O1A	-2.04	118.43	123.59
23	b	605	CLA	CAC-C3C-C4C	2.04	127.46	124.81
25	c	517	BCR	C24-C23-C22	-2.04	123.15	126.23
23	B	602	CLA	C11-C12-C13	-2.04	109.32	115.92
34	D	412	LMG	O7-C10-O9	-2.04	118.77	123.70
25	B	618	BCR	C31-C1-C6	-2.04	106.99	110.30
29	D	406	PL9	C7-C3-C4	2.04	118.53	116.88
34	m	101	LMG	C7-O1-C1	-2.04	109.76	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	C1D-CHD-C4C	-2.04	119.87	122.56
23	b	608	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	b	606	CLA	CAC-C3C-C4C	2.04	127.45	124.81
23	c	506	CLA	C1-C2-C3	-2.04	122.52	126.04
23	c	514	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
23	C	506	CLA	CHB-C4A-NA	2.03	127.33	124.51
34	C	522	LMG	O6-C1-C2	-2.03	106.04	110.35
23	a	405	CLA	C1-O2A-CGA	2.03	121.78	116.44
23	a	403	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
24	A	415	PHO	C2A-C1A-NA	2.03	114.19	111.86
25	k	102	BCR	C28-C27-C26	-2.03	110.45	114.08
23	A	403	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
23	C	508	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	B	602	CLA	CMA-C3A-C4A	-2.03	106.32	111.77
23	C	507	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
23	A	403	CLA	CAA-CBA-CGA	-2.03	107.33	113.25
25	C	517	BCR	C36-C18-C17	-2.03	120.08	122.92
32	b	621	HTG	O2-C2-C1	2.03	113.99	110.27
23	c	510	CLA	CHB-C4A-NA	2.03	127.31	124.51
23	A	405	CLA	CMA-C3A-C4A	-2.02	106.33	111.77
23	c	510	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
33	F	101	LMT	O5B-C5B-C4B	2.02	113.37	109.69
23	C	514	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
25	b	619	BCR	C33-C5-C6	-2.02	122.26	124.53
25	D	405	BCR	C38-C26-C27	2.02	117.50	113.62
23	C	506	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
23	d	402	CLA	OBD-CAD-C3D	-2.02	124.62	127.98
23	c	513	CLA	C11-C10-C8	-2.02	109.39	115.92
25	b	619	BCR	C29-C30-C25	2.02	113.59	110.48
23	B	606	CLA	CMC-C2C-C1C	2.02	128.11	125.04
24	A	415	PHO	O2A-CGA-O1A	-2.02	118.50	123.59
25	d	404	BCR	C35-C13-C14	-2.02	120.10	122.92
23	B	606	CLA	CHC-C1C-NC	2.02	127.26	124.20
25	B	631	BCR	C29-C30-C25	2.02	113.58	110.48
35	c	520	DGD	O1G-C1A-O1A	-2.01	118.51	123.59
26	D	413	SQD	C3-C4-C5	2.01	113.83	110.24
29	A	413[A]	PL9	C37-C36-C34	-2.01	106.35	112.98
23	B	615	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
23	A	407	CLA	C3D-CAD-CBD	2.01	110.25	107.61
23	C	511	CLA	C16-C15-C13	-2.01	109.42	115.92
23	b	612	CLA	C11-C12-C13	-2.01	109.42	115.92
23	B	611	CLA	C4D-C3D-CAD	-2.01	107.35	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C4D-C3D-CAD	-2.01	107.35	108.47
25	b	617	BCR	C20-C21-C22	-2.01	124.44	127.31
23	c	515	CLA	C1-O2A-CGA	2.01	121.71	116.44
23	d	402	CLA	C2A-C1A-CHA	-2.01	120.35	123.86
25	H	101	BCR	C7-C6-C5	2.01	126.33	121.46
25	Y	101	BCR	C21-C20-C19	-2.01	116.95	123.22
25	c	517	BCR	C29-C30-C25	2.01	113.57	110.48
32	C	523	HTG	O5-C5-C6	2.01	111.43	106.44
29	d	405	PL9	C30-C29-C31	2.01	118.65	115.27
23	C	513	CLA	C11-C10-C8	-2.01	109.44	115.92
23	b	613	CLA	C16-C15-C13	-2.01	109.44	115.92
23	a	404	CLA	O2A-CGA-CBA	2.00	118.20	111.91
29	a	414[B]	PL9	C35-C34-C36	2.00	118.64	115.27
33	M	102	LMT	O1B-C1B-C2B	2.00	113.29	108.10
23	B	602	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
23	D	404	CLA	C1-C2-C3	-2.00	122.58	126.04
23	c	511	CLA	C2A-C1A-CHA	-2.00	120.36	123.86

All (193) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	403	CLA	NA
23	A	403	CLA	NC
23	A	403	CLA	ND
23	A	404	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	405	CLA	NA
23	A	405	CLA	NC
23	A	407	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	ND
23	B	601	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	602	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	604	CLA	NA
23	B	604	CLA	NC

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Mol	Chain	Res	Type	Atom
23	B	604	CLA	ND
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	606	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	607	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	608	CLA	NA
23	B	608	CLA	NC
23	B	609	CLA	NC
23	B	609	CLA	ND
23	B	610	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	611	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	612	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	613	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	614	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	615	CLA	NA
23	B	615	CLA	ND
23	B	615	CLA	NC
23	B	616	CLA	NA
23	B	616	CLA	ND
23	B	616	CLA	NC
23	C	503	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	504	CLA	NA
23	C	504	CLA	NC
23	C	505	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	506	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	509	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	510	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	511	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	512	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	513	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	514	CLA	NA
23	C	514	CLA	NC
23	C	514	CLA	ND
23	C	515	CLA	NA
23	C	515	CLA	NC
23	C	515	CLA	ND
23	D	403	CLA	ND
23	D	404	CLA	NA
23	D	404	CLA	NC
23	D	404	CLA	ND
23	a	403	CLA	NA
23	a	403	CLA	NC
23	a	403	CLA	ND
23	a	404	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	405	CLA	NA
23	a	405	CLA	NC
23	a	407	CLA	NA
23	a	407	CLA	NC

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Mol	Chain	Res	Type	Atom
23	a	407	CLA	ND
23	b	601	CLA	NA
23	b	601	CLA	NC
23	b	601	CLA	ND
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	603	CLA	NC
23	b	603	CLA	ND
23	b	604	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	605	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	606	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	607	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	608	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	609	CLA	NA
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	610	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	611	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	612	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	613	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	614	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	615	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	615	CLA	ND
23	b	615	CLA	NC
23	b	616	CLA	NA
23	b	616	CLA	ND
23	b	616	CLA	NC
23	c	503	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	504	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	505	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	506	CLA	NA
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	509	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	510	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	511	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	512	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	513	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	514	CLA	NA
23	c	514	CLA	NC
23	c	514	CLA	ND
23	c	515	CLA	NA
23	c	515	CLA	NC
23	c	515	CLA	ND

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Mol	Chain	Res	Type	Atom
23	d	402	CLA	ND
23	d	403	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND

All (1338) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	407	CLA	C2-C3-C5-C6
23	A	407	CLA	C4-C3-C5-C6
23	B	605	CLA	C6-C7-C8-C9
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	609	CLA	C1A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	C14-C13-C15-C16
23	C	506	CLA	C2-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	C	509	CLA	C2-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	C	510	CLA	CHA-CBD-CGD-O1D
23	D	404	CLA	C2-C3-C5-C6
23	D	404	CLA	C4-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	C6-C7-C8-C9
23	c	509	CLA	C2-C3-C5-C6
23	c	509	CLA	C4-C3-C5-C6
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	515	CLA	C2-C3-C5-C6
23	c	515	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	d	403	CLA	C2-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
25	D	405	BCR	C7-C8-C9-C34
25	D	405	BCR	C21-C22-C23-C24
25	D	405	BCR	C37-C22-C23-C24
25	D	405	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	Y	101	BCR	C21-C22-C23-C24
25	Y	101	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
25	b	619	BCR	C7-C8-C9-C34
25	d	404	BCR	C23-C24-C25-C30
25	k	101	BCR	C7-C8-C9-C34
25	k	102	BCR	C1-C6-C7-C8
25	k	102	BCR	C5-C6-C7-C8
26	A	411	SQD	O6-C44-C45-O47
26	B	620	SQD	C8-C7-O47-C45
26	D	413	SQD	O49-C7-O47-C45
26	D	413	SQD	C8-C7-O47-C45
26	L	102	SQD	O49-C7-O47-C45
26	L	102	SQD	C8-C7-O47-C45
26	a	411	SQD	C5-C6-S-O7
26	a	411	SQD	C5-C6-S-O8
26	a	411	SQD	C5-C6-S-O9
26	f	101	SQD	C2-C1-O6-C44
26	f	101	SQD	O5-C1-O6-C44
26	f	101	SQD	C8-C7-O47-C45
27	B	623	GOL	C1-C2-C3-O3
27	a	410	GOL	O1-C1-C2-C3
27	b	623	GOL	C1-C2-C3-O3
27	v	201	GOL	O1-C1-C2-C3
29	A	413[A]	PL9	C19-C21-C22-C23
29	A	413[A]	PL9	C23-C24-C26-C27
29	A	413[A]	PL9	C25-C24-C26-C27
29	A	413[B]	PL9	C15-C14-C16-C17
29	A	413[B]	PL9	C24-C26-C27-C28
29	A	413[B]	PL9	C35-C34-C36-C37
29	a	414[A]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C15-C14-C16-C17
29	a	414[A]	PL9	C19-C21-C22-C23
29	a	414[B]	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	a	414[B]	PL9	C25-C24-C26-C27
31	D	407	LHG	C3-O3-P-O4
31	D	407	LHG	C4-O6-P-O4
31	E	101	LHG	C3-O3-P-O4
31	E	101	LHG	C3-O3-P-O5
31	E	101	LHG	C3-O3-P-O6
31	L	101	LHG	C3-O3-P-O4
31	L	101	LHG	C4-O6-P-O4
31	L	101	LHG	C4-O6-P-O5
31	a	419	LHG	C3-O3-P-O4
31	a	419	LHG	C3-O3-P-O5
31	a	419	LHG	C3-O3-P-O6
31	a	419	LHG	O10-C23-O8-C6
31	a	419	LHG	C24-C23-O8-C6
31	b	628	LHG	C4-O6-P-O3
31	b	628	LHG	C4-O6-P-O4
31	b	628	LHG	C4-O6-P-O5
31	d	406	LHG	C3-O3-P-O4
31	d	406	LHG	C3-O3-P-O5
31	d	406	LHG	C3-O3-P-O6
31	d	407	LHG	O2-C2-C3-O3
31	d	407	LHG	C3-O3-P-O4
31	d	407	LHG	C4-O6-P-O4
32	B	621	HTG	C2'-C1'-S1-C1
32	b	621	HTG	C2'-C1'-S1-C1
33	B	630	LMT	O5'-C1'-O1'-C1
33	B	630	LMT	C2-C1-O1'-C1'
33	C	526	LMT	C2'-C1'-O1'-C1
33	C	526	LMT	O5'-C1'-O1'-C1
33	D	402	LMT	C2'-C1'-O1'-C1
33	D	402	LMT	O5'-C1'-O1'-C1
33	F	101	LMT	C2'-C1'-O1'-C1
33	F	101	LMT	O5'-C1'-O1'-C1
33	M	103	LMT	C2'-C1'-O1'-C1
33	M	103	LMT	O5'-C1'-O1'-C1
33	a	412	LMT	C2'-C1'-O1'-C1
33	a	412	LMT	O5'-C1'-O1'-C1
33	a	418	LMT	C2'-C1'-O1'-C1
33	a	418	LMT	O5'-C1'-O1'-C1
33	b	620	LMT	O5'-C1'-O1'-C1
33	b	626	LMT	C2'-C1'-O1'-C1
33	b	626	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
33	b	626	LMT	C2-C1-O1'-C1'
33	e	101	LMT	C2'-C1'-O1'-C1
34	C	522	LMG	C11-C10-O7-C8
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	a	417	LMG	O9-C10-O7-C8
34	a	417	LMG	C11-C10-O7-C8
34	c	522	LMG	C11-C10-O7-C8
34	z	101	LMG	O6-C1-O1-C7
34	z	101	LMG	C11-C10-O7-C8
33	C	526	LMT	C3'-C4'-O1B-C1B
31	E	101	LHG	O10-C23-O8-C6
31	E	101	LHG	C24-C23-O8-C6
23	C	505	CLA	CBD-CGD-O2D-CED
23	b	615	CLA	C13-C15-C16-C17
26	B	620	SQD	O49-C7-O47-C45
26	f	101	SQD	O49-C7-O47-C45
34	c	522	LMG	O9-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	a	407	CLA	C3-C5-C6-C7
23	c	508	CLA	C3-C5-C6-C7
23	c	514	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
23	b	604	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	C4-C3-C5-C6
29	A	413[A]	PL9	C13-C14-C16-C17
29	A	413[B]	PL9	C13-C14-C16-C17
23	C	503	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
26	f	101	SQD	C24-C23-O48-C46
34	C	502	LMG	O6-C5-C6-O5
23	c	503	CLA	CBD-CGD-O2D-CED
34	C	522	LMG	O9-C10-O7-C8
23	b	601	CLA	CBD-CGD-O2D-CED
31	D	407	LHG	O2-C2-C3-O3
23	A	407	CLA	C3-C5-C6-C7
23	B	604	CLA	C3-C5-C6-C7
23	C	508	CLA	C3-C5-C6-C7
23	C	514	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
23	D	404	CLA	C3-C5-C6-C7
33	M	103	LMT	O5'-C5'-C6'-O6'
32	c	523	HTG	O5-C5-C6-O6
33	F	101	LMT	O5'-C5'-C6'-O6'
32	B	624	HTG	O5-C5-C6-O6
32	c	523	HTG	C4-C5-C6-O6
23	B	605	CLA	C3-C5-C6-C7
34	a	417	LMG	O6-C5-C6-O5
26	f	101	SQD	O10-C23-O48-C46
33	B	627	LMT	O5B-C5B-C6B-O6B
33	e	101	LMT	O5'-C5'-C6'-O6'
34	c	522	LMG	O6-C5-C6-O5
23	B	605	CLA	C4-C3-C5-C6
23	B	616	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	A	413[A]	PL9	C15-C14-C16-C17
29	A	413[B]	PL9	C30-C29-C31-C32
29	a	414[A]	PL9	C25-C24-C26-C27
23	B	605	CLA	C2-C3-C5-C6
23	B	616	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	A	413[B]	PL9	C28-C29-C31-C32
29	a	414[A]	PL9	C23-C24-C26-C27
29	a	414[B]	PL9	C23-C24-C26-C27
34	C	502	LMG	C4-C5-C6-O5
26	B	620	SQD	O5-C1-O6-C44
33	e	101	LMT	O5'-C1'-O1'-C1
34	c	522	LMG	O6-C1-O1-C7
29	A	413[B]	PL9	C14-C16-C17-C18
29	A	413[B]	PL9	C19-C21-C22-C23
29	D	406	PL9	C39-C41-C42-C43
29	a	414[A]	PL9	C24-C26-C27-C28
29	a	414[A]	PL9	C29-C31-C32-C33
29	a	414[B]	PL9	C39-C41-C42-C43
29	d	405	PL9	C39-C41-C42-C43
31	b	628	LHG	C7-C8-C9-C10
33	C	526	LMT	O5B-C5B-C6B-O6B
33	B	627	LMT	C3'-C4'-O1B-C1B
23	C	505	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	c	514	CLA	C15-C16-C17-C18
33	B	630	LMT	C2'-C1'-O1'-C1
33	b	620	LMT	C2'-C1'-O1'-C1
29	A	413[A]	PL9	C12-C11-C9-C10
23	b	604	CLA	C2-C3-C5-C6
23	B	602	CLA	C6-C7-C8-C9
23	B	610	CLA	C11-C12-C13-C14
23	C	514	CLA	C6-C7-C8-C9
23	C	515	CLA	C14-C13-C15-C16
23	b	610	CLA	C11-C12-C13-C14
23	b	615	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	C	515	CLA	CBD-CGD-O2D-CED
33	b	626	LMT	C11-C10-C9-C8
23	b	610	CLA	C2A-CAA-CBA-CGA
25	B	631	BCR	C11-C12-C13-C35
25	b	619	BCR	C37-C22-C23-C24
25	d	404	BCR	C7-C8-C9-C34
34	C	522	LMG	O6-C5-C6-O5
35	C	519	DGD	C5A-C6A-C7A-C8A
33	M	103	LMT	C4'-C5'-C6'-O6'
26	f	101	SQD	C23-C24-C25-C26
23	c	511	CLA	O1A-CGA-O2A-C1
23	c	508	CLA	C15-C16-C17-C18
23	c	510	CLA	C10-C11-C12-C13
26	A	409	SQD	C11-C10-C9-C8
23	B	602	CLA	C15-C16-C17-C18
23	b	616	CLA	C13-C15-C16-C17
31	d	406	LHG	C23-C24-C25-C26
34	Z	101	LMG	C10-C11-C12-C13
35	c	519	DGD	C1B-C2B-C3B-C4B
26	A	409	SQD	C18-C19-C20-C21
23	A	404	CLA	C15-C16-C17-C18
23	A	407	CLA	C5-C6-C7-C8
23	B	606	CLA	C15-C16-C17-C18
23	B	614	CLA	C10-C11-C12-C13
23	C	508	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
33	B	627	LMT	C4B-C5B-C6B-O6B
31	E	101	LHG	C26-C27-C28-C29
27	A	410	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	v	201	GOL	O1-C1-C2-O2
26	D	413	SQD	C7-C8-C9-C10
23	a	405	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	C15-C16-C17-C18
23	C	514	CLA	C15-C16-C17-C18
33	C	526	LMT	O1'-C1-C2-C3
23	c	511	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C8-C10-C11-C12
23	C	511	CLA	C13-C15-C16-C17
23	C	510	CLA	CBD-CGD-O2D-CED
34	a	417	LMG	C4-C5-C6-O5
23	C	510	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
23	c	507	CLA	C11-C12-C13-C15
25	T	101	BCR	C13-C14-C15-C16
23	B	610	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C10-C11-C12-C13
23	D	403	CLA	C15-C16-C17-C18
23	c	509	CLA	C8-C10-C11-C12
35	C	519	DGD	CBB-CCB-CDB-CEB
33	e	101	LMT	C4'-C5'-C6'-O6'
33	B	627	LMT	C5'-C4'-O1B-C1B
33	M	102	LMT	O5'-C1'-O1'-C1
35	C	519	DGD	O6E-C1E-O5D-C6D
23	B	614	CLA	C8-C10-C11-C12
23	C	514	CLA	C13-C15-C16-C17
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
29	A	413[A]	PL9	C24-C26-C27-C28
29	a	414[B]	PL9	C14-C16-C17-C18
29	a	414[B]	PL9	C24-C26-C27-C28
29	d	405	PL9	C34-C36-C37-C38
32	b	624	HTG	S1-C1'-C2'-C3'
23	C	510	CLA	C5-C6-C7-C8
23	a	404	CLA	CBD-CGD-O2D-CED
34	c	522	LMG	C4-C5-C6-O5
23	B	613	CLA	C15-C16-C17-C18
23	B	614	CLA	C5-C6-C7-C8
23	b	603	CLA	C13-C15-C16-C17
23	b	616	CLA	C10-C11-C12-C13
23	A	405	CLA	C15-C16-C17-C18
23	C	504	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C8-C10-C11-C12
23	c	512	CLA	C10-C11-C12-C13
31	D	407	LHG	C3-O3-P-O6
31	L	101	LHG	C4-O6-P-O3
31	d	407	LHG	C3-O3-P-O6
31	A	416	LHG	C23-C24-C25-C26
23	B	601	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	C4E-C5E-C6E-O5E
31	a	419	LHG	C23-C24-C25-C26
31	d	407	LHG	C1-C2-C3-O3
23	B	603	CLA	C8-C10-C11-C12
23	c	509	CLA	C15-C16-C17-C18
33	m	103	LMT	O5'-C5'-C6'-O6'
23	b	604	CLA	C3-C5-C6-C7
23	d	403	CLA	CBA-CGA-O2A-C1
31	D	408	LHG	C24-C23-O8-C6
31	D	408	LHG	C33-C34-C35-C36
34	M	101	LMG	C36-C37-C38-C39
26	B	620	SQD	C10-C11-C12-C13
31	L	101	LHG	C25-C26-C27-C28
31	b	628	LHG	C25-C26-C27-C28
33	b	620	LMT	C5-C6-C7-C8
34	C	522	LMG	C36-C37-C38-C39
34	D	412	LMG	C19-C20-C21-C22
35	C	518	DGD	C4B-C5B-C6B-C7B
23	a	407	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
31	d	408	LHG	C24-C23-O8-C6
26	A	409	SQD	C9-C10-C11-C12
31	D	408	LHG	C28-C29-C30-C31
34	C	502	LMG	C34-C35-C36-C37
34	d	411	LMG	C21-C22-C23-C24
35	H	102	DGD	C7B-C8B-C9B-CAB
26	B	620	SQD	C46-C45-O47-C7
23	b	605	CLA	C13-C15-C16-C17
31	b	628	LHG	C14-C15-C16-C17
31	d	408	LHG	C29-C30-C31-C32
35	c	519	DGD	C7A-C8A-C9A-CAA
35	c	519	DGD	C9A-CAA-CBA-CCA
26	A	411	SQD	C27-C28-C29-C30
34	C	502	LMG	C18-C19-C20-C21
34	C	521	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
33	B	627	LMT	C4'-C5'-C6'-O6'
23	C	503	CLA	O1D-CGD-O2D-CED
23	c	503	CLA	O1D-CGD-O2D-CED
31	d	406	LHG	O2-C2-C3-O3
33	M	102	LMT	C2'-C1'-O1'-C1
34	C	502	LMG	C2-C1-O1-C7
34	M	101	LMG	C2-C1-O1-C7
35	C	519	DGD	C2E-C1E-O5D-C6D
26	a	409	SQD	C30-C31-C32-C33
23	b	608	CLA	C15-C16-C17-C18
23	c	511	CLA	C15-C16-C17-C18
31	D	408	LHG	O10-C23-O8-C6
23	B	615	CLA	C16-C17-C18-C19
23	b	609	CLA	C16-C17-C18-C20
23	b	604	CLA	O1D-CGD-O2D-CED
23	C	507	CLA	C4-C3-C5-C6
23	C	512	CLA	C4-C3-C5-C6
23	c	512	CLA	C4-C3-C5-C6
29	d	405	PL9	C15-C14-C16-C17
26	a	411	SQD	C16-C17-C18-C19
31	D	408	LHG	C32-C33-C34-C35
31	L	101	LHG	C17-C18-C19-C20
34	C	521	LMG	C21-C22-C23-C24
34	m	101	LMG	C14-C15-C16-C17
23	C	507	CLA	C2-C3-C5-C6
23	B	610	CLA	C14-C13-C15-C16
23	D	404	CLA	C11-C10-C8-C9
23	a	405	CLA	C11-C12-C13-C14
26	A	411	SQD	C26-C27-C28-C29
32	B	624	HTG	C2'-C3'-C4'-C5'
34	C	502	LMG	C14-C15-C16-C17
35	C	518	DGD	C3A-C4A-C5A-C6A
35	C	519	DGD	C8A-C9A-CAA-CBA
23	A	407	CLA	C15-C16-C17-C18
23	B	602	CLA	C13-C15-C16-C17
23	D	403	CLA	C13-C15-C16-C17
23	d	403	CLA	O1A-CGA-O2A-C1
26	A	411	SQD	C17-C18-C19-C20
27	A	410	GOL	O1-C1-C2-C3
27	A	410	GOL	C1-C2-C3-O3
27	B	626	GOL	C1-C2-C3-O3
27	O	302	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
27	O	302	GOL	C1-C2-C3-O3
27	a	410	GOL	C1-C2-C3-O3
31	A	416	LHG	O1-C1-C2-C3
31	D	408	LHG	O1-C1-C2-C3
31	d	406	LHG	O1-C1-C2-C3
32	b	621	HTG	S1-C1'-C2'-C3'
25	D	405	BCR	C7-C8-C9-C10
34	M	101	LMG	O9-C10-O7-C8
23	b	606	CLA	C15-C16-C17-C18
31	d	407	LHG	C33-C34-C35-C36
33	B	629	LMT	C11-C10-C9-C8
34	C	502	LMG	C12-C13-C14-C15
35	h	103	DGD	CCB-CDB-CEB-CFB
31	D	407	LHG	C12-C13-C14-C15
31	D	408	LHG	C12-C13-C14-C15
31	E	101	LHG	C10-C11-C12-C13
34	C	521	LMG	C30-C31-C32-C33
34	C	522	LMG	C17-C18-C19-C20
32	h	101	HTG	O5-C5-C6-O6
34	Z	101	LMG	O6-C5-C6-O5
23	a	407	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
34	C	502	LMG	O6-C1-O1-C7
23	b	608	CLA	C13-C15-C16-C17
29	A	413[A]	PL9	C14-C16-C17-C18
26	A	409	SQD	C15-C16-C17-C18
31	d	408	LHG	C28-C29-C30-C31
33	D	402	LMT	C5-C6-C7-C8
34	M	101	LMG	C29-C30-C31-C32
33	a	412	LMT	C1-C2-C3-C4
34	C	522	LMG	C18-C19-C20-C21
34	D	412	LMG	C35-C36-C37-C38
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	O1A-CGA-O2A-C1
26	L	102	SQD	C13-C14-C15-C16
34	C	502	LMG	C17-C18-C19-C20
35	h	103	DGD	CAB-CBB-CCB-CDB
35	c	518	DGD	O6D-C5D-C6D-O5D
31	A	416	LHG	C26-C27-C28-C29
23	C	508	CLA	C3A-C2A-CAA-CBA
23	B	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	a	411	SQD	C25-C26-C27-C28
31	D	408	LHG	C29-C30-C31-C32
31	d	406	LHG	C34-C35-C36-C37
35	H	102	DGD	C9A-CAA-CBA-CCA
35	c	518	DGD	C8B-C9B-CAB-CBB
31	b	628	LHG	C16-C17-C18-C19
31	d	407	LHG	C32-C33-C34-C35
34	c	522	LMG	C30-C31-C32-C33
33	e	101	LMT	C5-C6-C7-C8
35	c	519	DGD	C7B-C8B-C9B-CAB
26	B	620	SQD	C7-C8-C9-C10
33	M	103	LMT	O1'-C1-C2-C3
33	m	103	LMT	O1'-C1-C2-C3
34	C	521	LMG	C17-C18-C19-C20
29	D	406	PL9	C30-C29-C31-C32
23	C	512	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
23	c	512	CLA	C2-C3-C5-C6
29	D	406	PL9	C28-C29-C31-C32
29	d	405	PL9	C13-C14-C16-C17
26	A	409	SQD	C8-C7-O47-C45
34	M	101	LMG	C11-C10-O7-C8
27	O	302	GOL	O1-C1-C2-O2
27	O	302	GOL	O2-C2-C3-O3
27	b	623	GOL	O2-C2-C3-O3
34	D	412	LMG	C30-C31-C32-C33
34	c	521	LMG	C36-C37-C38-C39
34	d	411	LMG	C38-C39-C40-C41
23	B	615	CLA	C16-C17-C18-C20
35	h	103	DGD	C5B-C6B-C7B-C8B
35	c	518	DGD	C4D-C5D-C6D-O5D
26	L	102	SQD	C27-C28-C29-C30
33	D	402	LMT	C7-C8-C9-C10
23	C	512	CLA	C8-C10-C11-C12
33	B	627	LMT	O5'-C5'-C6'-O6'
33	b	626	LMT	C5-C6-C7-C8
26	A	409	SQD	O49-C7-O47-C45
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
32	B	624	HTG	C4-C5-C6-O6
33	D	402	LMT	C4'-C5'-C6'-O6'
26	A	411	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	E	101	LHG	C24-C25-C26-C27
23	A	403	CLA	C13-C15-C16-C17
31	d	408	LHG	O10-C23-O8-C6
31	E	101	LHG	C23-C24-C25-C26
25	D	405	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C26
34	C	502	LMG	C37-C38-C39-C40
23	b	601	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	CBA-CGA-O2A-C1
23	c	514	CLA	CBA-CGA-O2A-C1
26	L	102	SQD	C24-C23-O48-C46
34	C	502	LMG	C11-C10-O7-C8
31	a	419	LHG	C13-C14-C15-C16
34	C	502	LMG	C16-C17-C18-C19
34	d	411	LMG	C28-C29-C30-C31
33	F	101	LMT	C4'-C5'-C6'-O6'
35	H	102	DGD	C5B-C6B-C7B-C8B
23	b	605	CLA	C8-C10-C11-C12
23	c	510	CLA	C8-C10-C11-C12
31	E	101	LHG	C11-C10-C9-C8
31	a	419	LHG	C18-C19-C20-C21
24	a	406	PHO	C4-C3-C5-C6
23	D	404	CLA	C11-C10-C8-C7
23	a	407	CLA	C6-C7-C8-C10
24	a	406	PHO	C2-C3-C5-C6
23	c	513	CLA	O1A-CGA-O2A-C1
23	C	506	CLA	C8-C10-C11-C12
35	c	518	DGD	C2A-C1A-O1G-C1G
34	m	101	LMG	C39-C40-C41-C42
33	M	103	LMT	C2B-C1B-O1B-C4'
33	D	402	LMT	C3-C4-C5-C6
34	C	521	LMG	C13-C14-C15-C16
34	C	521	LMG	C29-C30-C31-C32
23	A	407	CLA	C13-C15-C16-C17
26	D	413	SQD	C30-C31-C32-C33
31	A	416	LHG	C18-C19-C20-C21
32	b	621	HTG	C2'-C3'-C4'-C5'
33	b	626	LMT	C3-C4-C5-C6
34	Z	101	LMG	C16-C17-C18-C19
34	a	417	LMG	C36-C37-C38-C39
33	B	629	LMT	O1'-C1-C2-C3
23	B	601	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C16-C17-C18-C19
32	C	523	HTG	C4-C5-C6-O6
33	m	103	LMT	O5'-C1'-O1'-C1
34	M	101	LMG	O6-C1-O1-C7
29	A	413[A]	PL9	C9-C11-C12-C13
29	a	414[A]	PL9	C39-C41-C42-C43
26	D	413	SQD	C28-C29-C30-C31
34	C	522	LMG	C33-C34-C35-C36
31	d	407	LHG	C34-C35-C36-C37
34	a	417	LMG	C30-C31-C32-C33
34	C	502	LMG	O9-C10-O7-C8
34	a	417	LMG	C32-C33-C34-C35
35	c	519	DGD	C6A-C7A-C8A-C9A
26	D	413	SQD	C2-C1-O6-C44
26	A	409	SQD	O6-C44-C45-O47
26	a	411	SQD	O6-C44-C45-O47
26	f	101	SQD	O47-C45-C46-O48
31	L	101	LHG	C24-C25-C26-C27
23	a	404	CLA	C16-C17-C18-C20
23	b	609	CLA	C16-C17-C18-C19
23	c	507	CLA	C4-C3-C5-C6
29	A	413[B]	PL9	C33-C34-C36-C37
29	D	406	PL9	C13-C14-C16-C17
29	A	413[A]	PL9	C4-C3-C7-C8
29	A	413[B]	PL9	C4-C3-C7-C8
29	a	414[A]	PL9	C4-C3-C7-C8
29	a	414[B]	PL9	C4-C3-C7-C8
23	a	405	CLA	C14-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C9
23	c	507	CLA	C11-C12-C13-C14
23	c	515	CLA	C6-C7-C8-C9
23	a	403	CLA	C2A-CAA-CBA-CGA
26	a	409	SQD	C9-C10-C11-C12
34	a	417	LMG	C14-C15-C16-C17
32	b	622	HTG	O5-C5-C6-O6
34	D	412	LMG	C38-C39-C40-C41
34	M	101	LMG	C32-C33-C34-C35
25	k	101	BCR	C7-C8-C9-C10
23	C	503	CLA	C1A-C2A-CAA-CBA
23	b	615	CLA	C16-C17-C18-C19
26	A	409	SQD	C12-C13-C14-C15
34	c	522	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	C	504	CLA	C15-C16-C17-C18
31	D	407	LHG	C4-O6-P-O3
31	d	407	LHG	C4-O6-P-O3
35	C	519	DGD	C8B-C9B-CAB-CBB
35	c	518	DGD	C3A-C4A-C5A-C6A
23	c	511	CLA	C10-C11-C12-C13
31	d	406	LHG	C33-C34-C35-C36
34	d	411	LMG	C10-C11-C12-C13
35	C	520	DGD	C9A-CAA-CBA-CCA
23	b	610	CLA	C16-C17-C18-C20
23	b	601	CLA	C3-C5-C6-C7
32	c	523	HTG	S1-C1'-C2'-C3'
34	M	101	LMG	C28-C29-C30-C31
33	B	627	LMT	C6-C7-C8-C9
35	c	518	DGD	O6E-C5E-C6E-O5E
23	B	604	CLA	C4-C3-C5-C6
23	b	601	CLA	C4-C3-C5-C6
29	D	406	PL9	C15-C14-C16-C17
29	a	414[B]	PL9	C30-C29-C31-C32
35	C	518	DGD	C6B-C7B-C8B-C9B
35	c	519	DGD	CCA-CDA-CEA-CFA
23	c	514	CLA	O1A-CGA-O2A-C1
26	L	102	SQD	O10-C23-O48-C46
31	A	416	LHG	C32-C33-C34-C35
34	D	412	LMG	O6-C5-C6-O5
33	e	101	LMT	C2B-C1B-O1B-C4'
26	B	620	SQD	C44-C45-C46-O48
26	a	409	SQD	O6-C44-C45-C46
32	B	621	HTG	C3'-C4'-C5'-C6'
34	C	522	LMG	C7-C8-C9-O8
35	C	520	DGD	C6B-C7B-C8B-C9B
34	d	411	LMG	O6-C5-C6-O5
23	D	404	CLA	C10-C11-C12-C13
34	c	521	LMG	C40-C41-C42-C43
35	C	518	DGD	O6D-C5D-C6D-O5D
35	c	519	DGD	C2G-C3G-O3G-C1D
35	c	519	DGD	C5D-C6D-O5D-C1E
32	B	624	HTG	C4'-C5'-C6'-C7'
32	b	624	HTG	C4'-C5'-C6'-C7'
31	d	407	LHG	C13-C14-C15-C16
34	c	521	LMG	C32-C33-C34-C35
35	c	518	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	CBA-CCA-CDA-CEA
23	b	616	CLA	C15-C16-C17-C18
35	C	519	DGD	CDA-CEA-CFA-CGA
27	B	623	GOL	O2-C2-C3-O3
27	B	626	GOL	O2-C2-C3-O3
27	a	410	GOL	O1-C1-C2-O2
31	d	406	LHG	O1-C1-C2-O2
34	m	101	LMG	C11-C10-O7-C8
29	a	414[A]	PL9	C30-C29-C31-C32
31	E	101	LHG	C7-C8-C9-C10
23	C	513	CLA	CBA-CGA-O2A-C1
26	a	411	SQD	C26-C27-C28-C29
31	d	407	LHG	C30-C31-C32-C33
31	d	408	LHG	C11-C10-C9-C8
33	b	620	LMT	C3-C4-C5-C6
34	C	502	LMG	C35-C36-C37-C38
35	C	518	DGD	O6E-C5E-C6E-O5E
23	A	407	CLA	C8-C10-C11-C12
23	C	514	CLA	C2-C1-O2A-CGA
35	c	518	DGD	C1A-C2A-C3A-C4A
23	b	614	CLA	C3-C5-C6-C7
32	B	621	HTG	C2'-C3'-C4'-C5'
33	D	402	LMT	C4-C5-C6-C7
31	d	408	LHG	C9-C10-C11-C12
33	C	526	LMT	C4-C5-C6-C7
23	C	514	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
23	a	404	CLA	C16-C17-C18-C19
34	D	412	LMG	C12-C13-C14-C15
35	H	102	DGD	CCA-CDA-CEA-CFA
33	b	620	LMT	C3'-C4'-O1B-C1B
33	m	103	LMT	C2'-C1'-O1'-C1
26	a	409	SQD	O6-C44-C45-O47
31	E	101	LHG	O7-C5-C6-O8
23	a	405	CLA	O1D-CGD-O2D-CED
23	a	405	CLA	C10-C11-C12-C13
23	C	513	CLA	O1A-CGA-O2A-C1
34	z	101	LMG	C4-C5-C6-O5
26	A	411	SQD	C30-C31-C32-C33
26	L	102	SQD	C14-C15-C16-C17
34	M	101	LMG	C17-C18-C19-C20
34	m	101	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C6-C7-C8-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	a	403	CLA	C12-C13-C15-C16
23	a	405	CLA	C11-C12-C13-C15
23	b	601	CLA	C2-C3-C5-C6
23	b	610	CLA	C12-C13-C15-C16
23	b	614	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	512	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
29	a	414[B]	PL9	C28-C29-C31-C32
23	B	602	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	512	CLA	C14-C13-C15-C16
23	C	515	CLA	C6-C7-C8-C9
23	C	515	CLA	C11-C10-C8-C9
23	a	403	CLA	C14-C13-C15-C16
23	b	610	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	d	402	CLA	C11-C12-C13-C14
34	C	521	LMG	C31-C32-C33-C34
23	C	512	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C8-C10-C11-C12
23	c	511	CLA	C16-C17-C18-C20
25	b	619	BCR	C21-C22-C23-C24
31	D	407	LHG	C1-C2-C3-O3
23	B	606	CLA	C8-C10-C11-C12
26	a	411	SQD	C19-C20-C21-C22
23	C	514	CLA	C10-C11-C12-C13
23	b	602	CLA	C10-C11-C12-C13
23	b	604	CLA	C13-C15-C16-C17
35	C	519	DGD	CAB-CBB-CCB-CDB
31	b	628	LHG	C10-C11-C12-C13
31	b	628	LHG	C34-C35-C36-C37
23	B	610	CLA	C15-C16-C17-C18
31	a	419	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	413[B]	PL9	C39-C41-C42-C43
29	a	414[A]	PL9	C9-C11-C12-C13
33	B	630	LMT	C4-C5-C6-C7
33	B	630	LMT	C3-C4-C5-C6
23	c	513	CLA	C8-C10-C11-C12
35	c	520	DGD	O6E-C5E-C6E-O5E
23	c	506	CLA	C4-C3-C5-C6
29	a	414[A]	PL9	C28-C29-C31-C32
34	a	417	LMG	C20-C21-C22-C23
34	m	101	LMG	C38-C39-C40-C41
23	b	615	CLA	C5-C6-C7-C8
35	C	518	DGD	C3B-C4B-C5B-C6B
23	A	405	CLA	C16-C17-C18-C20
33	b	626	LMT	C1-C2-C3-C4
26	A	409	SQD	C14-C15-C16-C17
34	M	101	LMG	C29-C28-O8-C9
35	C	519	DGD	C2A-C3A-C4A-C5A
23	b	609	CLA	C3A-C2A-CAA-CBA
35	C	518	DGD	C5A-C6A-C7A-C8A
33	e	101	LMT	C2-C1-O1'-C1'
26	a	409	SQD	C26-C27-C28-C29
23	B	611	CLA	C8-C10-C11-C12
23	a	404	CLA	C13-C15-C16-C17
26	A	409	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
31	E	101	LHG	C4-C5-C6-O8
31	a	419	LHG	C4-C5-C6-O8
32	V	202	HTG	O5-C5-C6-O6
34	Z	101	LMG	C7-C8-C9-O8
34	M	101	LMG	C34-C35-C36-C37
34	a	417	LMG	C40-C41-C42-C43
26	A	411	SQD	C7-C8-C9-C10
35	c	520	DGD	CDB-CEB-CFB-CGB
35	H	102	DGD	O6E-C5E-C6E-O5E
23	C	505	CLA	C10-C11-C12-C13
26	a	411	SQD	C31-C32-C33-C34
34	C	522	LMG	C32-C33-C34-C35
33	M	103	LMT	O5B-C1B-O1B-C4'
23	b	603	CLA	C16-C17-C18-C20
23	a	404	CLA	O1D-CGD-O2D-CED
35	h	103	DGD	CDB-CEB-CFB-CGB
26	B	620	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	a	419	LHG	C4-O6-P-O3
23	C	512	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
31	A	416	LHG	O1-C1-C2-O2
23	C	508	CLA	C13-C15-C16-C17
33	C	526	LMT	C3-C4-C5-C6
34	c	521	LMG	C30-C31-C32-C33
35	c	518	DGD	C2B-C3B-C4B-C5B
23	C	515	CLA	O1D-CGD-O2D-CED
31	a	419	LHG	O6-C4-C5-O7
35	H	102	DGD	CBB-CCB-CDB-CEB
23	C	514	CLA	O1A-CGA-O2A-C1
23	B	609	CLA	C13-C15-C16-C17
34	C	521	LMG	C12-C13-C14-C15
26	a	409	SQD	C33-C34-C35-C36
34	C	502	LMG	C32-C33-C34-C35
31	a	419	LHG	O7-C5-C6-O8
34	C	522	LMG	O7-C8-C9-O8
26	a	411	SQD	C24-C23-O48-C46
23	c	510	CLA	C5-C6-C7-C8
23	c	514	CLA	C10-C11-C12-C13
33	e	101	LMT	O5B-C1B-O1B-C4'
35	C	519	DGD	C6A-C7A-C8A-C9A
26	a	411	SQD	O5-C1-O6-C44
35	c	518	DGD	O6E-C1E-O5D-C6D
35	c	520	DGD	CBA-CCA-CDA-CEA
34	m	101	LMG	O9-C10-O7-C8
23	b	608	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C5-C6-C7-C8
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	C14-C13-C15-C16
23	D	404	CLA	C14-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C9
23	c	504	CLA	C14-C13-C15-C16
29	a	414[B]	PL9	C2-C3-C7-C8
23	b	611	CLA	C8-C10-C11-C12
23	B	608	CLA	C16-C17-C18-C20
23	a	403	CLA	C16-C17-C18-C19
25	C	517	BCR	C1-C6-C7-C8
25	C	517	BCR	C5-C6-C7-C8
25	D	405	BCR	C1-C6-C7-C8
25	D	405	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	Y	101	BCR	C23-C24-C25-C30
25	b	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	k	102	BCR	C23-C24-C25-C26
26	L	102	SQD	C15-C16-C17-C18
35	h	103	DGD	O2G-C1B-C2B-C3B
25	B	631	BCR	C11-C12-C13-C14
25	d	404	BCR	C7-C8-C9-C10
25	d	404	BCR	C21-C22-C23-C24
35	C	518	DGD	C4D-C5D-C6D-O5D
23	a	404	CLA	C15-C16-C17-C18
33	b	626	LMT	C4-C5-C6-C7
23	a	403	CLA	C16-C17-C18-C20
33	M	102	LMT	C4B-C5B-C6B-O6B
24	a	416	PHO	C2C-C3C-CAC-CBC
31	b	628	LHG	O6-C4-C5-C6
31	d	406	LHG	C29-C30-C31-C32
23	A	405	CLA	C12-C13-C15-C16
23	B	605	CLA	C6-C7-C8-C10
23	B	609	CLA	C2-C3-C5-C6
23	B	616	CLA	C12-C13-C15-C16
23	C	515	CLA	C11-C10-C8-C7
23	D	404	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	609	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
23	b	615	CLA	C12-C13-C15-C16
23	c	508	CLA	C6-C7-C8-C10
23	c	508	CLA	C11-C10-C8-C7
23	d	402	CLA	C11-C12-C13-C15
31	d	406	LHG	C16-C17-C18-C19
26	a	411	SQD	C30-C31-C32-C33
35	C	519	DGD	C9B-CAB-CBB-CCB
35	c	518	DGD	C2A-C3A-C4A-C5A
26	B	620	SQD	C29-C30-C31-C32
31	d	407	LHG	C29-C30-C31-C32
23	a	407	CLA	CBA-CGA-O2A-C1
31	d	406	LHG	C24-C23-O8-C6
31	d	407	LHG	C24-C23-O8-C6
26	D	413	SQD	C34-C35-C36-C37
31	D	407	LHG	C18-C19-C20-C21
34	a	417	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C13-C15-C16-C17
23	B	604	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
23	c	514	CLA	CAD-CBD-CGD-O2D
23	d	403	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
24	A	415	PHO	CAD-CBD-CGD-O2D
24	a	406	PHO	C2B-C3B-CAB-CBB
24	a	406	PHO	CAD-CBD-CGD-O2D
26	L	102	SQD	C46-C45-O47-C7
23	b	607	CLA	C3-C5-C6-C7
23	B	610	CLA	C13-C15-C16-C17
26	A	411	SQD	C24-C23-O48-C46
35	c	520	DGD	C2A-C1A-O1G-C1G
26	f	101	SQD	C33-C34-C35-C36
31	A	416	LHG	C11-C10-C9-C8
33	C	526	LMT	C4B-C5B-C6B-O6B
26	L	102	SQD	O5-C1-O6-C44
29	A	413[A]	PL9	C44-C46-C47-C48
23	c	512	CLA	O1A-CGA-O2A-C1
34	M	101	LMG	O10-C28-O8-C9
31	b	628	LHG	O6-C4-C5-O7
33	F	101	LMT	C6-C7-C8-C9
33	m	103	LMT	C4'-C5'-C6'-O6'
26	a	411	SQD	O10-C23-O48-C46
23	c	511	CLA	C16-C17-C18-C19
32	b	621	HTG	C4'-C5'-C6'-C7'
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	a	407	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	O1D-CGD-O2D-CED
35	c	518	DGD	C2E-C1E-O5D-C6D
29	A	413[B]	PL9	C2-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
26	a	411	SQD	C18-C19-C20-C21
26	B	620	SQD	O47-C45-C46-O48
26	L	102	SQD	O47-C45-C46-O48
35	c	518	DGD	CAA-CBA-CCA-CDA
31	d	407	LHG	O10-C23-O8-C6
26	a	411	SQD	C24-C25-C26-C27
31	a	419	LHG	C16-C17-C18-C19
31	d	407	LHG	C9-C10-C11-C12
23	A	405	CLA	C16-C17-C18-C19
23	b	603	CLA	C16-C17-C18-C19
27	a	410	GOL	O2-C2-C3-O3
31	D	407	LHG	C11-C12-C13-C14
35	H	102	DGD	CAA-CBA-CCA-CDA
23	a	403	CLA	C15-C16-C17-C18
23	B	609	CLA	C4-C3-C5-C6
31	d	407	LHG	C25-C26-C27-C28
31	L	101	LHG	C27-C28-C29-C30
26	A	411	SQD	O49-C7-O47-C45
23	B	612	CLA	C10-C11-C12-C13
23	d	403	CLA	C14-C13-C15-C16
33	a	412	LMT	C4-C5-C6-C7
23	C	510	CLA	O1D-CGD-O2D-CED
31	L	101	LHG	C23-C24-C25-C26
33	D	402	LMT	C6-C7-C8-C9
35	H	102	DGD	O2G-C1B-C2B-C3B
35	C	518	DGD	CCB-CDB-CEB-CFB
31	d	406	LHG	O10-C23-O8-C6
25	b	617	BCR	C36-C18-C19-C20
34	C	521	LMG	C15-C16-C17-C18
23	B	601	CLA	C3-C5-C6-C7
33	b	620	LMT	C6-C7-C8-C9
35	h	103	DGD	CAA-CBA-CCA-CDA
23	D	404	CLA	C1A-C2A-CAA-CBA
23	a	405	CLA	C1A-C2A-CAA-CBA
32	C	523	HTG	O5-C5-C6-O6
23	A	407	CLA	C16-C17-C18-C19
34	c	522	LMG	C29-C28-O8-C9
26	a	411	SQD	C27-C28-C29-C30
31	A	416	LHG	C29-C30-C31-C32
29	a	414[B]	PL9	C35-C34-C36-C37
31	D	408	LHG	C2-C3-O3-P
31	d	408	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
29	A	413[A]	PL9	C3-C7-C8-C9
31	D	407	LHG	C4-O6-P-O5
31	d	406	LHG	C4-O6-P-O5
31	d	407	LHG	C4-O6-P-O5
33	B	627	LMT	C4-C5-C6-C7
24	a	406	PHO	C2C-C3C-CAC-CBC
26	B	620	SQD	C33-C34-C35-C36
31	a	419	LHG	C25-C26-C27-C28
34	M	101	LMG	C20-C21-C22-C23
23	B	606	CLA	C16-C17-C18-C20
34	C	502	LMG	C38-C39-C40-C41
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
35	C	520	DGD	C9B-CAB-CBB-CCB
26	A	411	SQD	O10-C23-O48-C46
35	c	520	DGD	O1A-C1A-O1G-C1G
23	C	507	CLA	C10-C11-C12-C13
23	c	512	CLA	CBA-CGA-O2A-C1
31	A	416	LHG	C9-C10-C11-C12
31	E	101	LHG	C17-C18-C19-C20
23	C	514	CLA	C16-C17-C18-C20
23	B	610	CLA	C11-C12-C13-C15
23	C	515	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	b	615	CLA	C6-C7-C8-C10
23	c	503	CLA	C11-C12-C13-C15
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
26	L	102	SQD	C28-C29-C30-C31
31	A	416	LHG	C19-C20-C21-C22
26	L	102	SQD	C12-C13-C14-C15
23	b	606	CLA	C8-C10-C11-C12
26	A	411	SQD	O6-C44-C45-C46
26	L	102	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
26	f	101	SQD	C44-C45-C46-O48
31	d	407	LHG	C28-C29-C30-C31
34	C	502	LMG	O1-C7-C8-C9
35	C	518	DGD	C2B-C3B-C4B-C5B
35	h	103	DGD	CBA-CCA-CDA-CEA
34	Z	101	LMG	O7-C8-C9-O8
35	C	519	DGD	C9A-CAA-CBA-CCA
23	B	602	CLA	O2A-C1-C2-C3
33	M	102	LMT	C9-C10-C11-C12
35	C	519	DGD	C2G-C3G-O3G-C1D
23	a	407	CLA	C5-C6-C7-C8
23	b	610	CLA	C13-C15-C16-C17
32	b	622	HTG	C3'-C4'-C5'-C6'
29	a	414[A]	PL9	C12-C11-C9-C10
34	C	502	LMG	C13-C14-C15-C16
33	D	402	LMT	O5'-C5'-C6'-O6'
23	c	506	CLA	C2-C3-C5-C6
29	a	414[B]	PL9	C43-C44-C46-C47
33	a	418	LMT	C2-C3-C4-C5
23	A	405	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	b	609	CLA	C14-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C14
34	c	522	LMG	O10-C28-O8-C9
34	C	522	LMG	C12-C13-C14-C15
23	B	608	CLA	C16-C17-C18-C19
29	A	413[B]	PL9	C9-C11-C12-C13
29	a	414[B]	PL9	C34-C36-C37-C38
26	A	409	SQD	C33-C34-C35-C36
35	H	102	DGD	C6B-C7B-C8B-C9B
23	C	505	CLA	C15-C16-C17-C18
35	c	518	DGD	CDA-CEA-CFA-CGA
25	b	617	BCR	C17-C18-C19-C20
25	k	102	BCR	C21-C22-C23-C24
34	M	101	LMG	C33-C34-C35-C36
26	B	620	SQD	C34-C35-C36-C37
35	c	518	DGD	C6B-C7B-C8B-C9B
23	b	601	CLA	CAA-CBA-CGA-O2A
29	A	413[A]	PL9	C12-C11-C9-C8
23	B	601	CLA	CAA-CBA-CGA-O2A
23	C	503	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	c	515	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
26	B	620	SQD	C11-C10-C9-C8
23	C	514	CLA	C16-C17-C18-C19
26	B	620	SQD	C19-C20-C21-C22
24	a	416	PHO	CBD-CGD-O2D-CED
35	C	518	DGD	C5B-C6B-C7B-C8B
26	B	620	SQD	C24-C23-O48-C46
31	A	416	LHG	C34-C35-C36-C37
23	B	613	CLA	C13-C15-C16-C17
23	B	603	CLA	C4-C3-C5-C6
31	d	407	LHG	C11-C10-C9-C8
34	C	502	LMG	C21-C22-C23-C24
25	Y	101	BCR	C23-C24-C25-C26
25	k	102	BCR	C23-C24-C25-C30
34	M	101	LMG	C15-C16-C17-C18
31	d	408	LHG	C10-C11-C12-C13
26	D	413	SQD	O5-C1-O6-C44
34	C	502	LMG	O1-C7-C8-O7
31	E	101	LHG	C4-O6-P-O3
33	M	102	LMT	C7-C8-C9-C10
33	a	418	LMT	C4-C5-C6-C7
26	B	620	SQD	C30-C31-C32-C33
26	L	102	SQD	C19-C20-C21-C22
31	D	407	LHG	C16-C17-C18-C19
35	H	102	DGD	CDB-CEB-CFB-CGB
23	B	612	CLA	CBA-CGA-O2A-C1
31	d	407	LHG	C4-C5-C6-O8
23	B	615	CLA	C11-C12-C13-C15
23	d	403	CLA	C12-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	c	508	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C12-C13-C14
31	d	407	LHG	C31-C32-C33-C34
23	c	509	CLA	C2A-CAA-CBA-CGA
23	B	606	CLA	C16-C17-C18-C19
31	L	101	LHG	C12-C13-C14-C15
33	B	630	LMT	O1'-C1-C2-C3
34	z	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C5-C6-C7-C8
31	D	407	LHG	C28-C29-C30-C31
32	D	411	HTG	C4-C5-C6-O6
23	C	514	CLA	CBD-CGD-O2D-CED
26	f	101	SQD	C29-C30-C31-C32
31	D	408	LHG	C30-C31-C32-C33
26	D	413	SQD	C24-C23-O48-C46
31	D	408	LHG	C9-C10-C11-C12
31	d	406	LHG	C27-C28-C29-C30
29	A	413[A]	PL9	C2-C3-C7-C8
23	B	612	CLA	O1A-CGA-O2A-C1
26	B	620	SQD	O10-C23-O48-C46
34	C	521	LMG	C36-C37-C38-C39
35	c	520	DGD	C4A-C5A-C6A-C7A
23	a	407	CLA	C15-C16-C17-C18
23	B	614	CLA	C2A-CAA-CBA-CGA
35	c	519	DGD	O6E-C1E-O5D-C6D
34	Z	101	LMG	C14-C15-C16-C17
29	a	414[B]	PL9	C29-C31-C32-C33
29	d	405	PL9	C9-C11-C12-C13
23	B	613	CLA	C10-C11-C12-C13
23	b	612	CLA	C8-C10-C11-C12
31	A	416	LHG	C10-C11-C12-C13
35	C	519	DGD	CCA-CDA-CEA-CFA
35	C	519	DGD	C6B-C7B-C8B-C9B
26	A	409	SQD	C13-C14-C15-C16
23	c	515	CLA	O1A-CGA-O2A-C1
26	D	413	SQD	O10-C23-O48-C46
33	B	630	LMT	C5-C6-C7-C8
23	c	508	CLA	C2-C1-O2A-CGA
23	b	604	CLA	C2C-C3C-CAC-CBC
35	c	519	DGD	CDA-CEA-CFA-CGA
26	a	409	SQD	C34-C35-C36-C37
35	c	519	DGD	C2E-C1E-O5D-C6D
26	L	102	SQD	C18-C19-C20-C21
26	B	620	SQD	C14-C15-C16-C17
32	B	624	HTG	C3'-C4'-C5'-C6'
35	C	520	DGD	C5B-C6B-C7B-C8B
29	a	414[B]	PL9	C45-C44-C46-C47
23	B	613	CLA	C11-C12-C13-C14
23	a	407	CLA	C11-C10-C8-C9
23	b	601	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	c	510	CLA	C6-C7-C8-C9
23	c	513	CLA	C11-C10-C8-C9
24	A	415	PHO	C6-C7-C8-C9
35	c	519	DGD	CBA-CCA-CDA-CEA
23	B	603	CLA	C13-C15-C16-C17
23	B	604	CLA	C13-C15-C16-C17
26	f	101	SQD	C28-C29-C30-C31
34	C	521	LMG	C34-C35-C36-C37
23	A	404	CLA	C2C-C3C-CAC-CBC
35	c	519	DGD	C6B-C7B-C8B-C9B
31	L	101	LHG	C35-C36-C37-C38
33	a	412	LMT	C9-C10-C11-C12
33	B	629	LMT	C3-C4-C5-C6
23	c	515	CLA	CBA-CGA-O2A-C1
33	B	627	LMT	O5'-C1'-O1'-C1
33	a	412	LMT	C6-C7-C8-C9
24	a	416	PHO	O1D-CGD-O2D-CED
35	C	520	DGD	C4B-C5B-C6B-C7B
34	M	101	LMG	C7-C8-O7-C10
23	C	508	CLA	C1A-C2A-CAA-CBA
34	a	417	LMG	O8-C28-C29-C30
23	B	613	CLA	C11-C10-C8-C7
23	C	514	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
23	a	405	CLA	C12-C13-C15-C16
23	b	604	CLA	C12-C13-C15-C16
23	b	608	CLA	C11-C12-C13-C15
23	b	616	CLA	C12-C13-C15-C16
23	c	515	CLA	C12-C13-C15-C16
23	c	504	CLA	C3-C5-C6-C7
25	H	101	BCR	C9-C10-C11-C12
31	L	101	LHG	C3-O3-P-O6
26	a	409	SQD	C27-C28-C29-C30
33	e	101	LMT	C4-C5-C6-C7
34	C	502	LMG	O8-C28-C29-C30
23	b	615	CLA	C15-C16-C17-C18
31	d	406	LHG	C26-C27-C28-C29
35	c	519	DGD	C2A-C3A-C4A-C5A
26	A	411	SQD	C8-C7-O47-C45
23	C	504	CLA	C3-C5-C6-C7
33	m	103	LMT	C3-C4-C5-C6
34	d	411	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
29	D	406	PL9	C35-C34-C36-C37
26	D	413	SQD	C26-C27-C28-C29
35	c	520	DGD	C2B-C3B-C4B-C5B
29	a	414[A]	PL9	C43-C44-C46-C47
33	B	629	LMT	C4-C5-C6-C7
35	C	518	DGD	CBB-CCB-CDB-CEB
35	h	103	DGD	C8B-C9B-CAB-CBB
35	C	518	DGD	C7A-C8A-C9A-CAA
23	b	616	CLA	C4-C3-C5-C6
29	a	414[A]	PL9	C45-C44-C46-C47
23	c	513	CLA	C2-C1-O2A-CGA
35	c	520	DGD	O6D-C5D-C6D-O5D
23	B	606	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
33	b	626	LMT	C7-C8-C9-C10
29	a	414[A]	PL9	C2-C3-C7-C8
34	c	521	LMG	C31-C32-C33-C34
35	C	519	DGD	C5B-C6B-C7B-C8B
23	B	605	CLA	C13-C15-C16-C17
24	a	416	PHO	C8-C10-C11-C12
26	a	409	SQD	C25-C26-C27-C28
23	A	403	CLA	C2A-CAA-CBA-CGA
25	c	516	BCR	C1-C6-C7-C8
25	c	516	BCR	C23-C24-C25-C30
25	c	517	BCR	C1-C6-C7-C8
31	L	101	LHG	C9-C10-C11-C12
35	C	520	DGD	C7A-C8A-C9A-CAA
26	A	411	SQD	C16-C17-C18-C19
35	C	520	DGD	C8A-C9A-CAA-CBA
23	B	615	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
25	k	101	BCR	C17-C18-C19-C20
23	C	510	CLA	C13-C15-C16-C17
31	a	419	LHG	C17-C18-C19-C20
35	c	519	DGD	C5B-C6B-C7B-C8B
23	B	604	CLA	C4C-C3C-CAC-CBC
31	d	407	LHG	C23-C24-C25-C26
34	D	412	LMG	C18-C19-C20-C21
29	A	413[B]	PL9	C40-C39-C41-C42
29	a	414[A]	PL9	C14-C16-C17-C18
35	h	103	DGD	C9A-CAA-CBA-CCA
23	B	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C11-C10-C8-C7
23	B	613	CLA	C12-C13-C15-C16
23	C	508	CLA	C2-C3-C5-C6
23	C	513	CLA	C6-C7-C8-C10
23	a	404	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
29	A	413[A]	PL9	C43-C44-C46-C47
34	C	521	LMG	C32-C33-C34-C35
23	C	512	CLA	C10-C11-C12-C13
32	B	621	HTG	C1'-C2'-C3'-C4'
23	B	613	CLA	CAA-CBA-CGA-O2A
34	m	101	LMG	C2-C1-O1-C7
31	d	407	LHG	O7-C5-C6-O8
31	b	628	LHG	O7-C7-C8-C9
26	A	411	SQD	C31-C32-C33-C34
26	a	409	SQD	C35-C36-C37-C38
23	c	515	CLA	C10-C11-C12-C13
23	B	606	CLA	C4-C3-C5-C6
29	D	406	PL9	C45-C44-C46-C47
29	d	405	PL9	C45-C44-C46-C47
23	B	605	CLA	C14-C13-C15-C16
23	C	508	CLA	C6-C7-C8-C9
23	C	511	CLA	C6-C7-C8-C9
23	b	606	CLA	C6-C7-C8-C9
23	b	611	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
23	c	515	CLA	C14-C13-C15-C16
31	D	407	LHG	C26-C27-C28-C29
31	d	406	LHG	C11-C10-C9-C8
23	B	612	CLA	C3A-C2A-CAA-CBA
23	b	612	CLA	C3A-C2A-CAA-CBA
23	B	612	CLA	CAA-CBA-CGA-O2A
23	C	514	CLA	CAA-CBA-CGA-O2A
34	D	412	LMG	O7-C10-C11-C12
23	B	603	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAA-CBA-CGA-O2A
26	f	101	SQD	O48-C23-C24-C25
34	C	502	LMG	O7-C10-C11-C12
23	c	508	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	a	409	SQD	C31-C32-C33-C34
23	c	510	CLA	C13-C15-C16-C17
23	b	616	CLA	C2-C3-C5-C6
29	a	414[A]	PL9	C12-C11-C9-C8
23	c	512	CLA	CAA-CBA-CGA-O2A
34	Z	101	LMG	O7-C10-C11-C12
31	L	101	LHG	C15-C16-C17-C18
34	z	101	LMG	O6-C5-C6-O5
32	c	523	HTG	C1'-C2'-C3'-C4'
23	D	403	CLA	C2C-C3C-CAC-CBC
31	D	407	LHG	C15-C16-C17-C18
35	C	518	DGD	CDB-CEB-CFB-CGB
23	C	511	CLA	O2A-C1-C2-C3
24	A	406	PHO	O2A-C1-C2-C3
24	a	406	PHO	O2A-C1-C2-C3
32	h	101	HTG	C4-C5-C6-O6
35	c	520	DGD	CAB-CBB-CCB-CDB
24	a	406	PHO	C4B-C3B-CAB-CBB
23	b	602	CLA	C2A-CAA-CBA-CGA
23	B	602	CLA	C3-C5-C6-C7
35	c	519	DGD	CBB-CCB-CDB-CEB
34	m	101	LMG	C33-C34-C35-C36
23	A	404	CLA	CHA-CBD-CGD-O1D
23	A	404	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	B	616	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	a	404	CLA	CHA-CBD-CGD-O1D
23	a	404	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	508	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-O2D
24	a	416	PHO	CHA-CBD-CGD-O2D
29	A	413[A]	PL9	C45-C44-C46-C47
23	B	606	CLA	C2-C3-C5-C6
34	d	411	LMG	C19-C20-C21-C22
32	D	411	HTG	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
23	a	404	CLA	C2C-C3C-CAC-CBC
31	d	408	LHG	C31-C32-C33-C34
31	L	101	LHG	O7-C7-C8-C9
23	C	512	CLA	CAA-CBA-CGA-O2A
23	c	514	CLA	CAA-CBA-CGA-O2A
31	A	416	LHG	O8-C23-C24-C25
23	A	403	CLA	C16-C17-C18-C19
27	B	626	GOL	O1-C1-C2-O2
34	m	101	LMG	C13-C14-C15-C16
31	d	406	LHG	O8-C23-C24-C25
35	H	102	DGD	C5A-C6A-C7A-C8A
23	C	514	CLA	C6-C7-C8-C10
34	m	101	LMG	O6-C1-O1-C7
26	L	102	SQD	O48-C23-C24-C25
35	c	518	DGD	O2G-C1B-C2B-C3B
32	b	621	HTG	C3'-C4'-C5'-C6'
23	C	514	CLA	C14-C13-C15-C16
23	a	407	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	616	CLA	C14-C13-C15-C16
23	B	604	CLA	C2C-C3C-CAC-CBC
31	a	419	LHG	C28-C29-C30-C31
23	B	602	CLA	C2A-CAA-CBA-CGA
25	k	101	BCR	C36-C18-C19-C20
31	b	628	LHG	O9-C7-C8-C9
23	B	603	CLA	C2-C3-C5-C6
26	a	409	SQD	C13-C14-C15-C16
23	c	512	CLA	CAA-CBA-CGA-O1A
25	C	517	BCR	C7-C8-C9-C10
35	h	103	DGD	C2A-C3A-C4A-C5A
23	b	609	CLA	C1A-C2A-CAA-CBA
33	D	402	LMT	C4B-C5B-C6B-O6B
24	A	415	PHO	NC-C1C-CHC-C4B
34	M	101	LMG	O1-C7-C8-C9
23	B	602	CLA	C16-C17-C18-C20
23	B	612	CLA	CAA-CBA-CGA-O1A
23	C	514	CLA	CAA-CBA-CGA-O1A
31	A	416	LHG	O10-C23-C24-C25
31	L	101	LHG	O9-C7-C8-C9
23	b	604	CLA	C4C-C3C-CAC-CBC
26	A	409	SQD	O47-C7-C8-C9
35	C	519	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	CAA-CBA-CGA-O1A
23	c	514	CLA	CAA-CBA-CGA-O1A
26	f	101	SQD	O10-C23-C24-C25
34	D	412	LMG	O9-C10-C11-C12
35	c	518	DGD	O1B-C1B-C2B-C3B
29	A	413[B]	PL9	C43-C44-C46-C47
31	E	101	LHG	C4-O6-P-O5
29	d	405	PL9	C11-C12-C13-C14
31	d	406	LHG	O10-C23-C24-C25
25	B	631	BCR	C1-C6-C7-C8
25	B	631	BCR	C5-C6-C7-C8
25	c	517	BCR	C5-C6-C7-C8
23	C	508	CLA	C5-C6-C7-C8
35	c	519	DGD	C1A-C2A-C3A-C4A
23	b	612	CLA	CAA-CBA-CGA-O1A
34	C	502	LMG	O9-C10-C11-C12
35	c	518	DGD	C7A-C8A-C9A-CAA
23	b	612	CLA	C10-C11-C12-C13
35	h	103	DGD	O1B-C1B-C2B-C3B
34	C	502	LMG	C15-C16-C17-C18
34	C	521	LMG	O7-C10-C11-C12
23	b	602	CLA	C8-C10-C11-C12
23	c	505	CLA	C15-C16-C17-C18
33	a	412	LMT	C2-C3-C4-C5
34	Z	101	LMG	O9-C10-C11-C12
26	B	620	SQD	C11-C12-C13-C14
29	a	414[B]	PL9	C11-C12-C13-C14
31	A	416	LHG	C24-C23-O8-C6
23	A	404	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	C	508	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
31	a	419	LHG	O8-C23-C24-C25
34	c	521	LMG	O7-C10-C11-C12
23	B	601	CLA	C6-C7-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	a	404	CLA	C6-C7-C8-C9
23	b	604	CLA	C14-C13-C15-C16
31	d	406	LHG	C31-C32-C33-C34
33	B	630	LMT	C6-C7-C8-C9
24	a	406	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	A	416	LHG	O10-C23-O8-C6
23	b	613	CLA	CAA-CBA-CGA-O2A
33	M	103	LMT	C9-C10-C11-C12
23	b	604	CLA	C10-C11-C12-C13
35	c	520	DGD	C3B-C4B-C5B-C6B
34	m	101	LMG	C17-C18-C19-C20
35	H	102	DGD	C8A-C9A-CAA-CBA
23	C	509	CLA	C5-C6-C7-C8
29	A	413[A]	PL9	C46-C47-C48-C49
26	D	413	SQD	C31-C32-C33-C34
35	C	518	DGD	CAB-CBB-CCB-CDB
23	B	603	CLA	C6-C7-C8-C10
23	C	503	CLA	C11-C12-C13-C15
23	C	508	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
32	B	621	HTG	C2-C1-S1-C1'
32	h	101	HTG	C2-C1-S1-C1'
31	a	419	LHG	O10-C23-C24-C25
35	H	102	DGD	O1B-C1B-C2B-C3B
34	d	411	LMG	O7-C10-C11-C12
31	D	407	LHG	C33-C34-C35-C36
33	M	103	LMT	C2-C1-O1'-C1'
34	M	101	LMG	C14-C15-C16-C17
23	C	513	CLA	C8-C10-C11-C12
23	b	609	CLA	C15-C16-C17-C18
23	c	503	CLA	C8-C10-C11-C12
23	c	511	CLA	C8-C10-C11-C12
23	c	513	CLA	C15-C16-C17-C18
26	A	409	SQD	O49-C7-C8-C9
26	L	102	SQD	O10-C23-C24-C25
23	A	404	CLA	C4C-C3C-CAC-CBC
26	A	409	SQD	C27-C28-C29-C30
23	B	612	CLA	C8-C10-C11-C12
33	M	102	LMT	O5B-C5B-C6B-O6B
34	z	101	LMG	O7-C10-C11-C12
34	d	411	LMG	O9-C10-C11-C12
23	C	505	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
33	M	102	LMT	C2-C3-C4-C5
35	C	518	DGD	C8A-C9A-CAA-CBA
23	C	512	CLA	CAA-CBA-CGA-O1A

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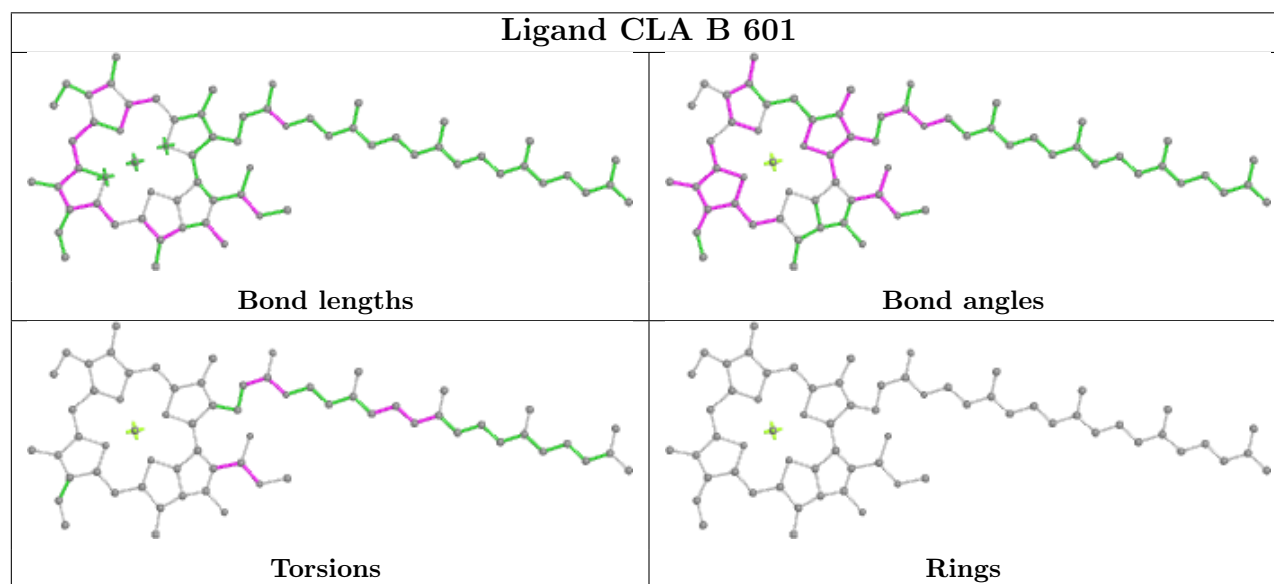
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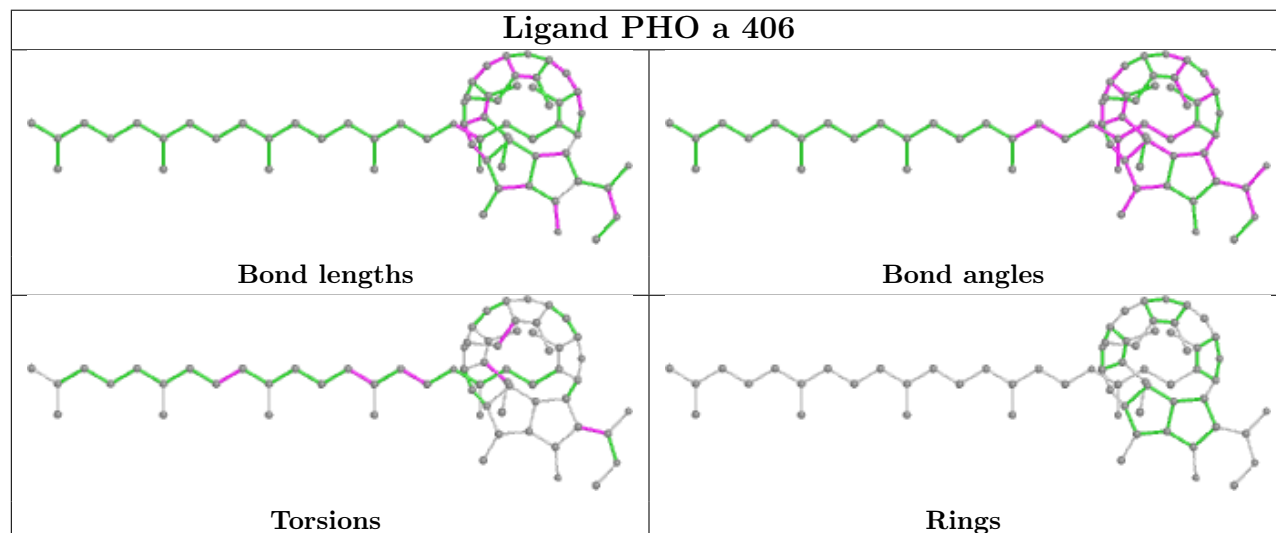
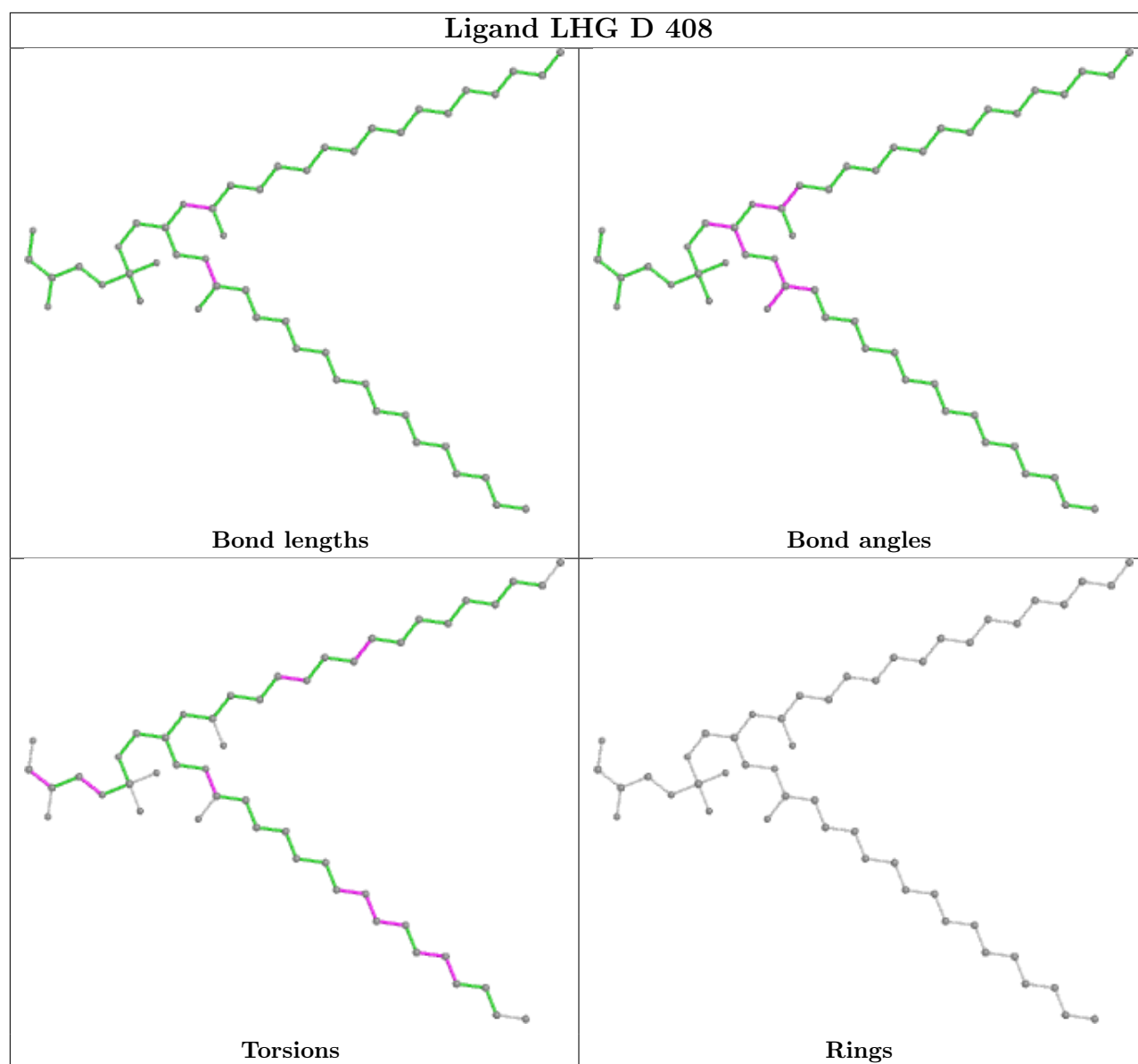
Mol	Chain	Res	Type	Atoms
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31	E	101	LHG	C25-C26-C27-C28

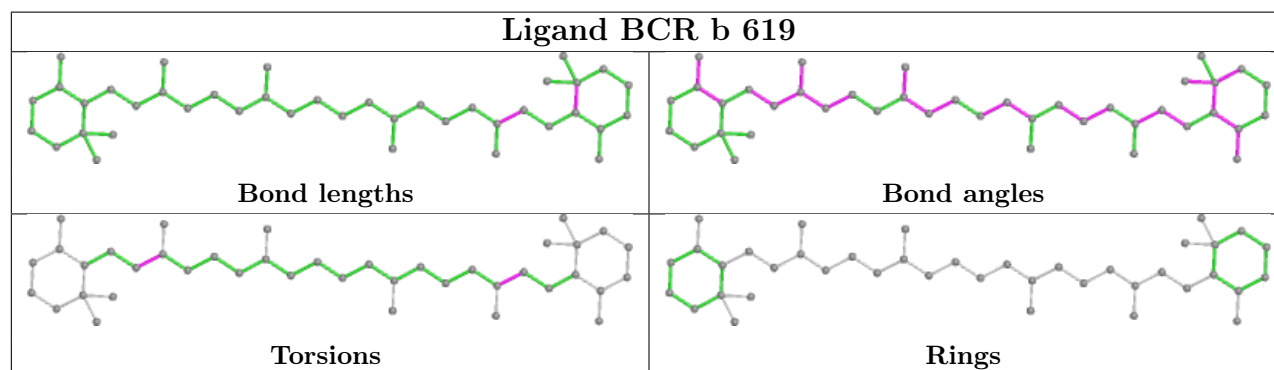
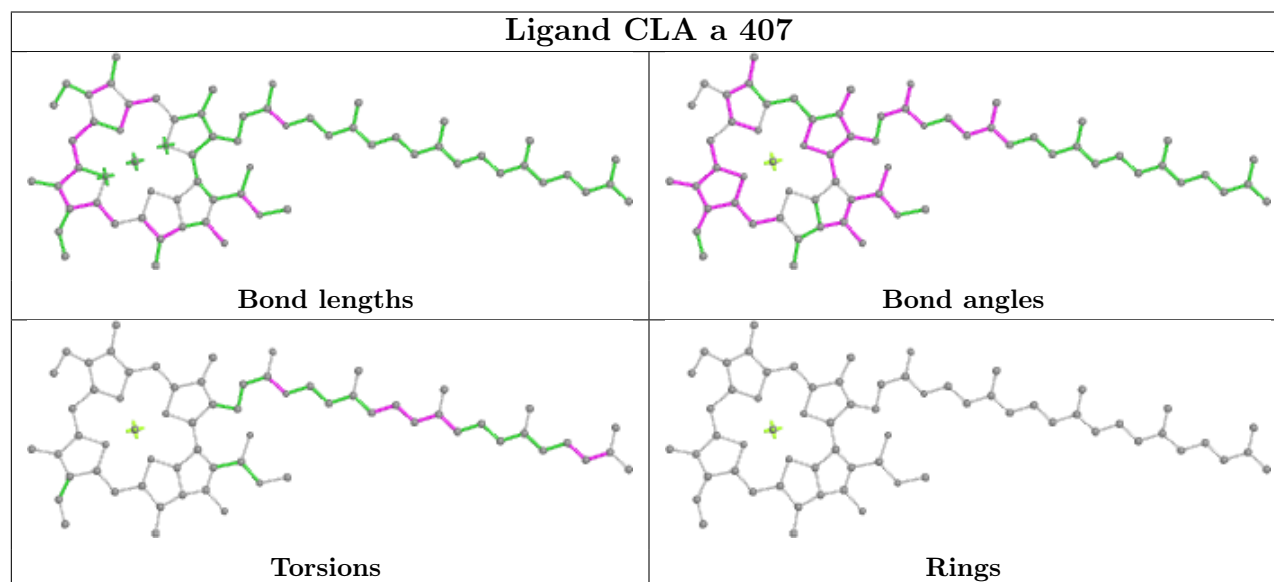
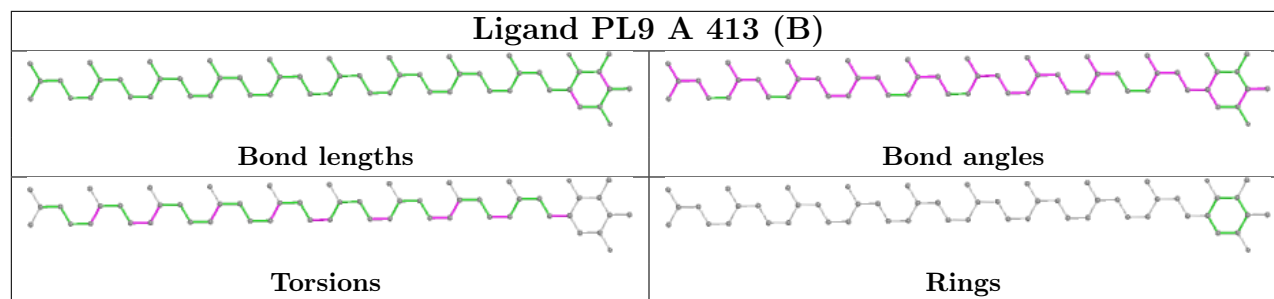
There are no ring outliers.

No monomer is involved in short contacts.

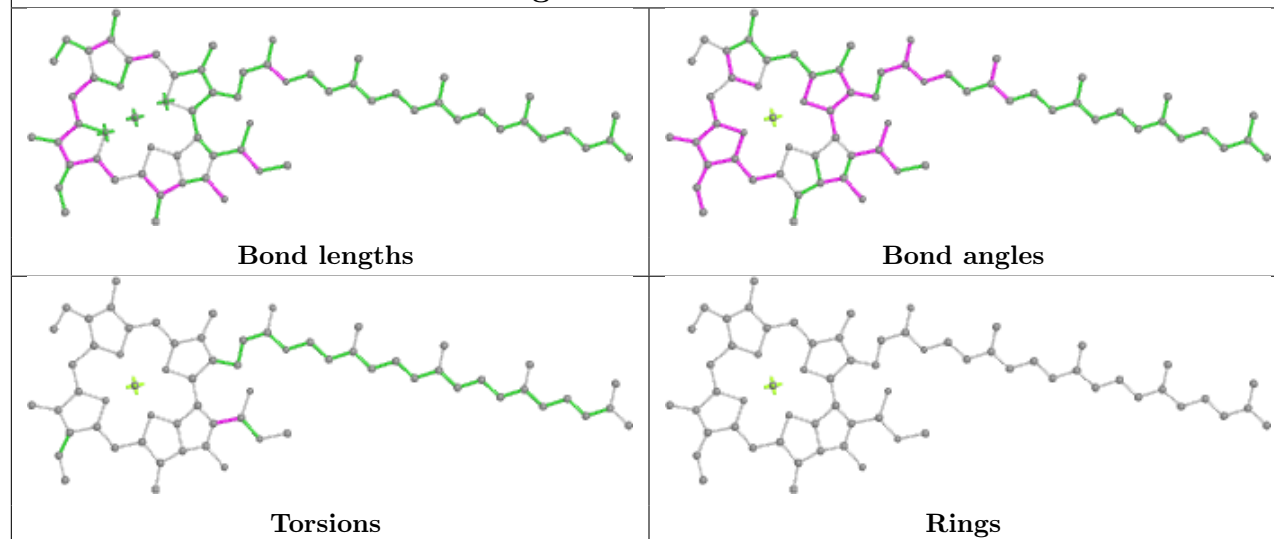
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



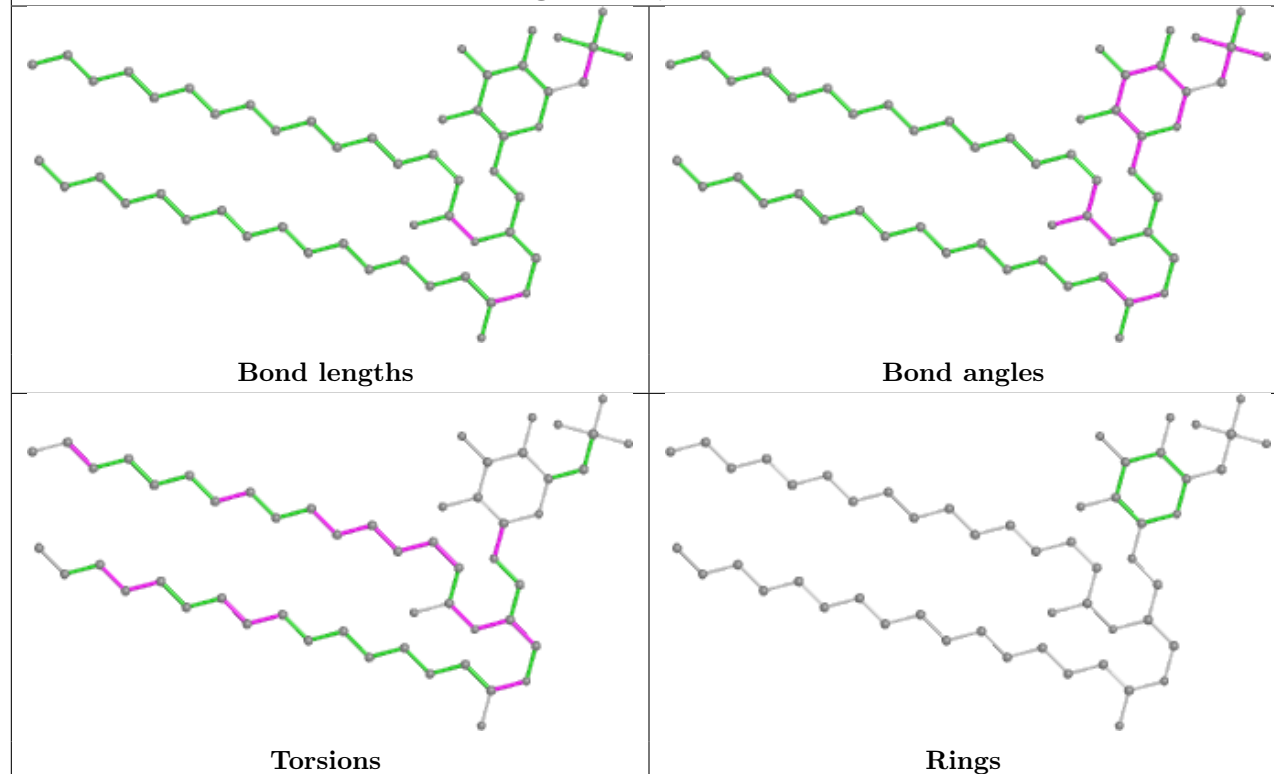


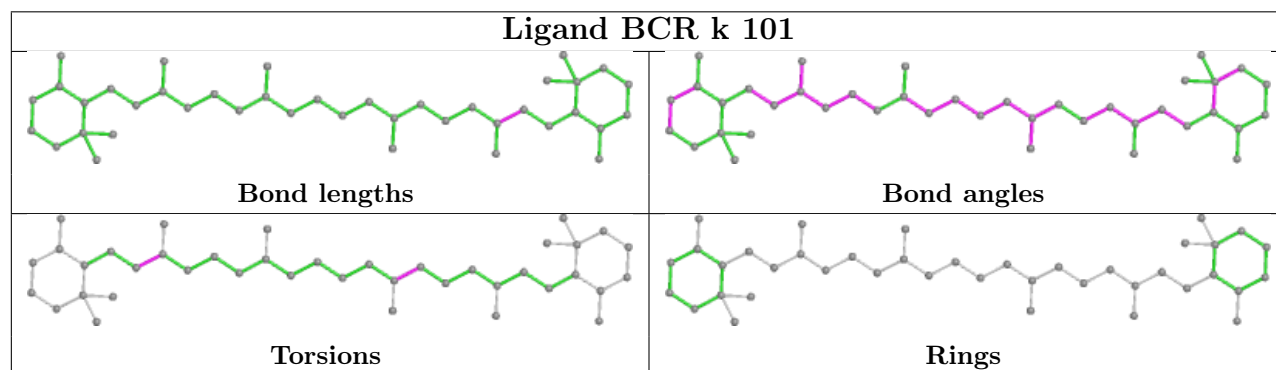
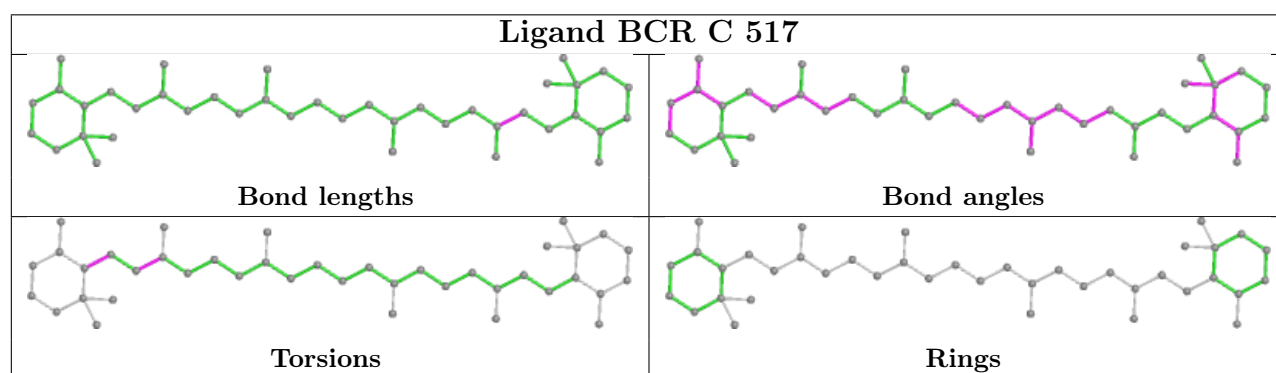
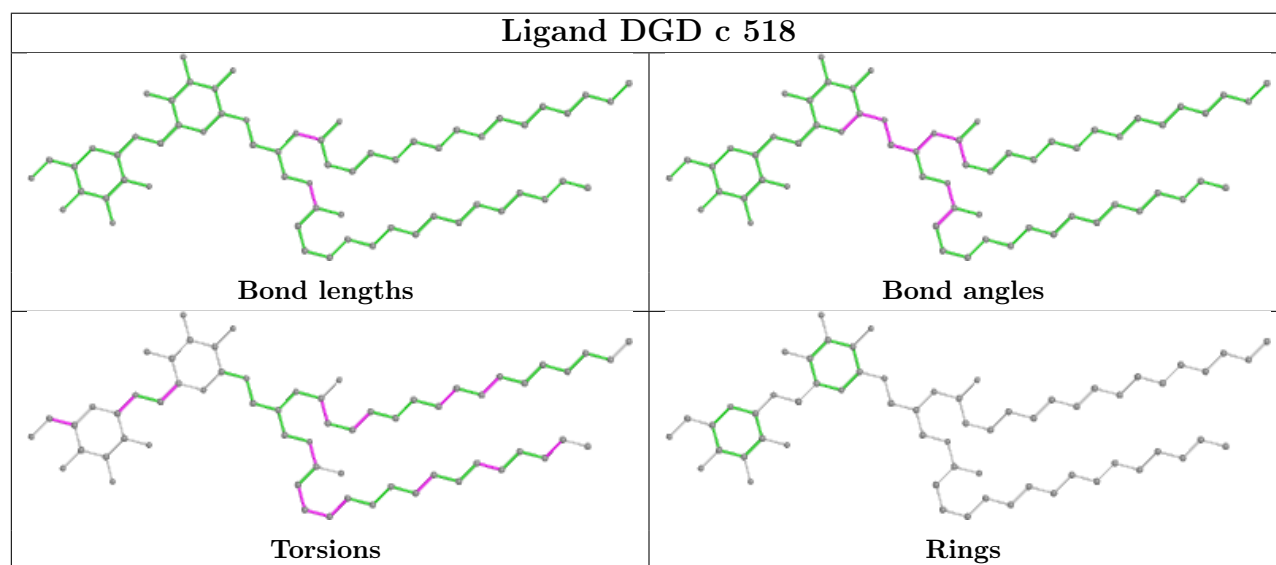
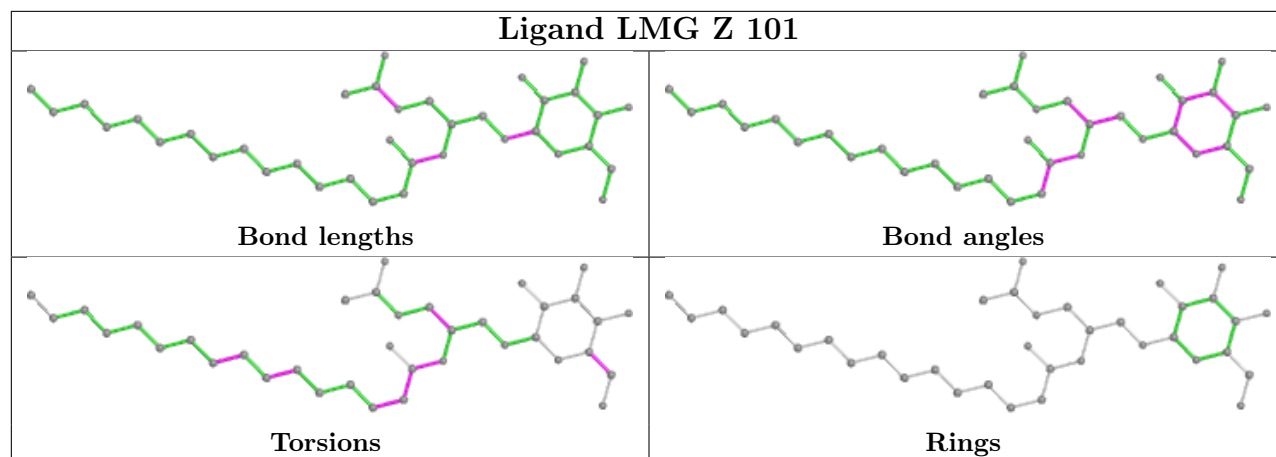


Ligand CLA B 607

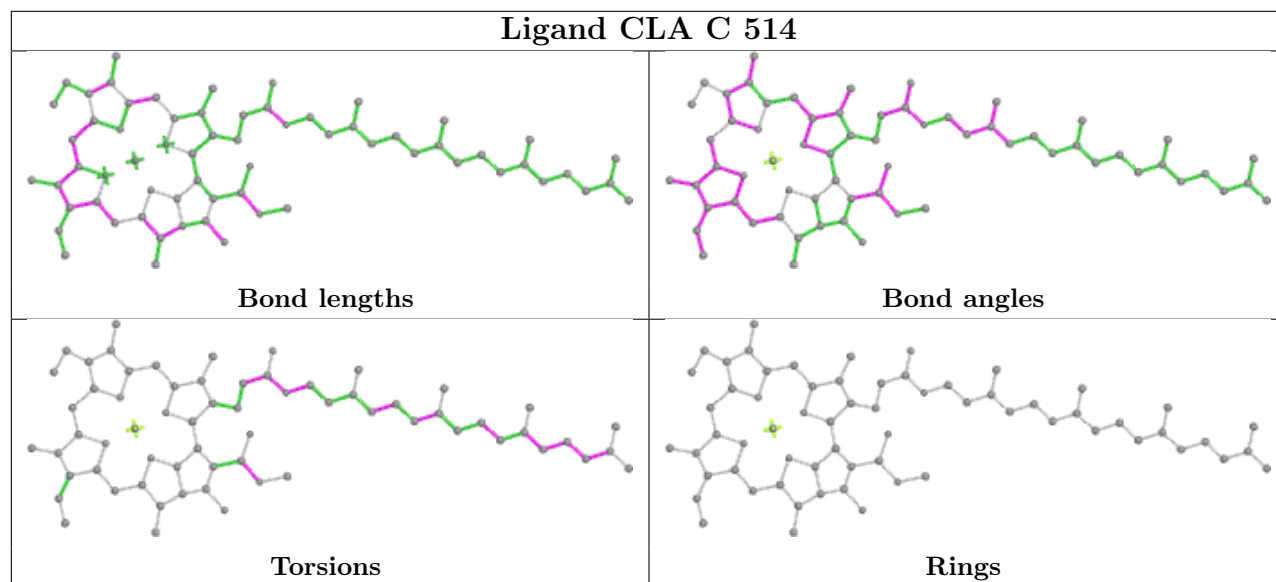


Ligand SQD B 620

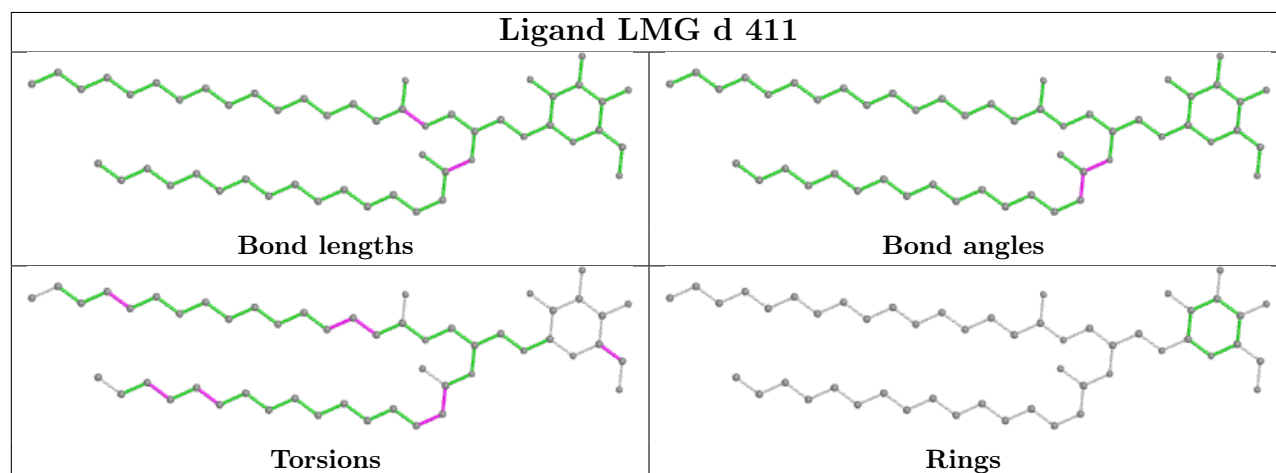




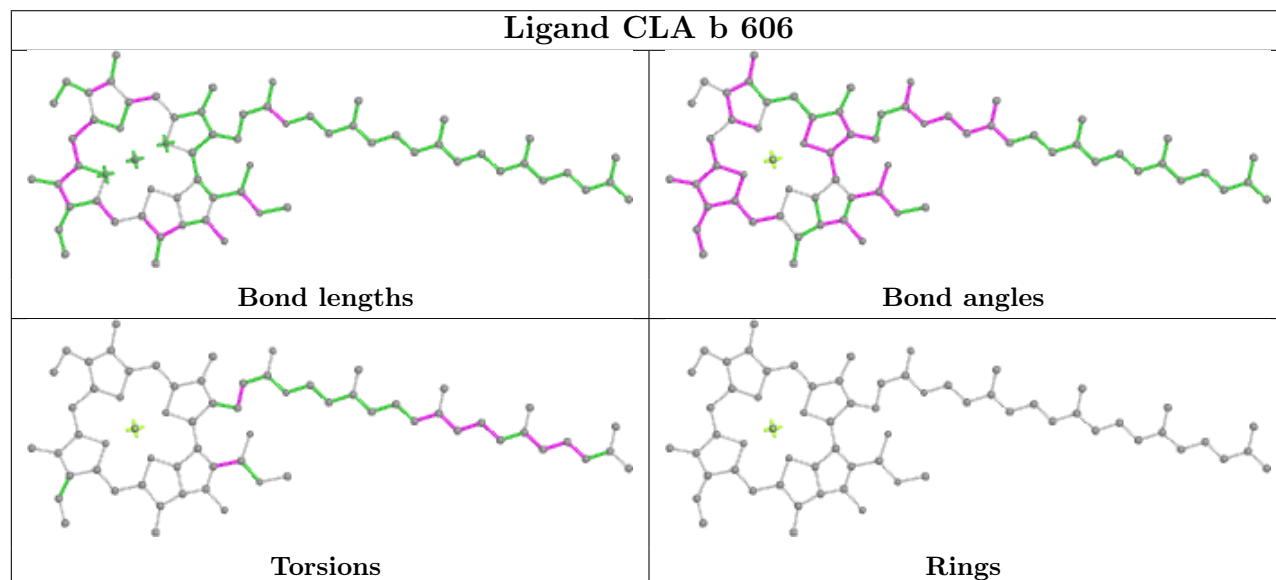
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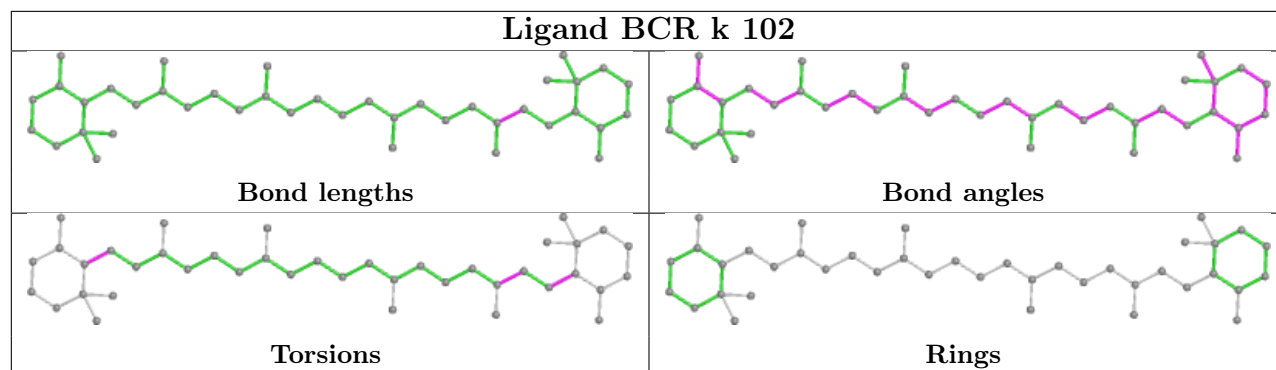
Ligand LMG d 411



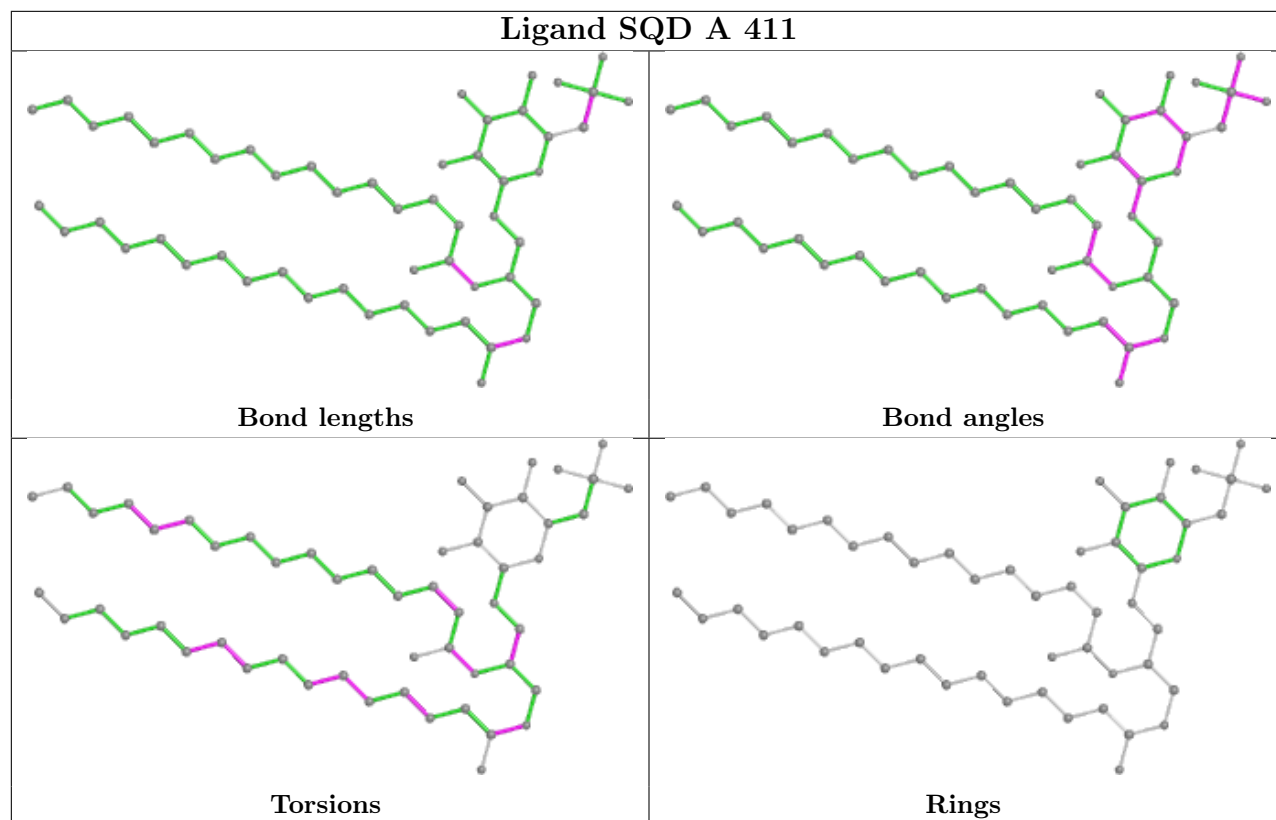
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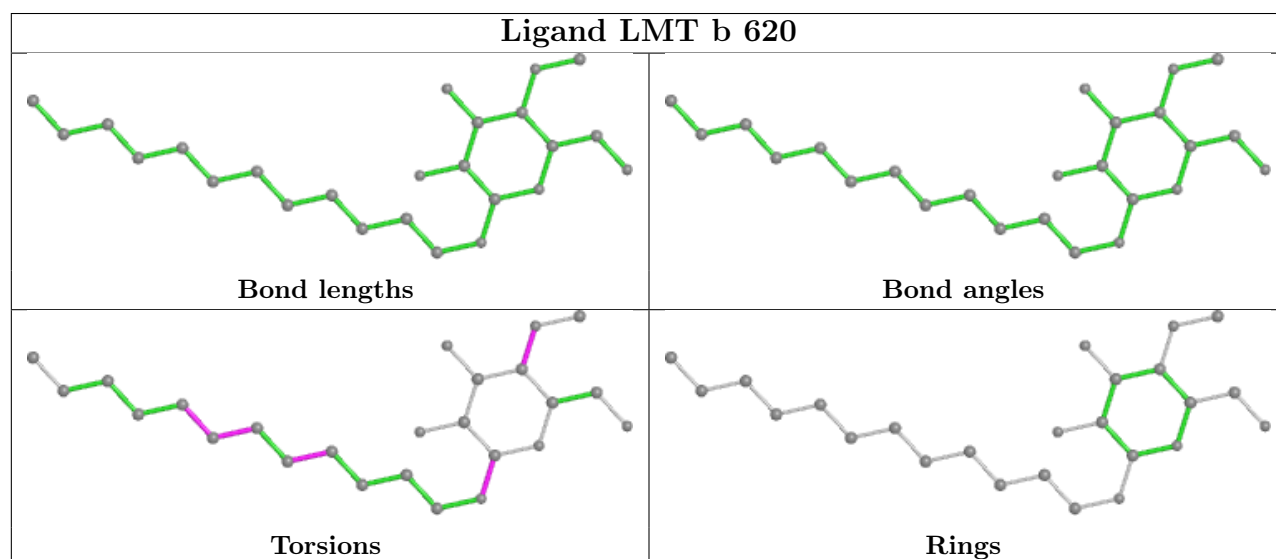
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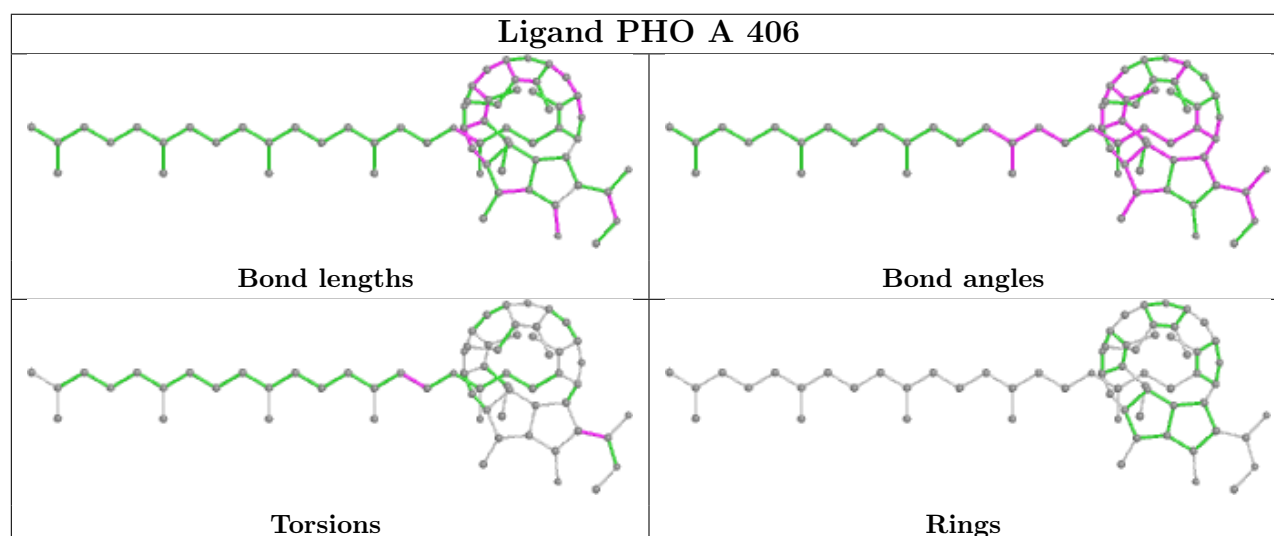
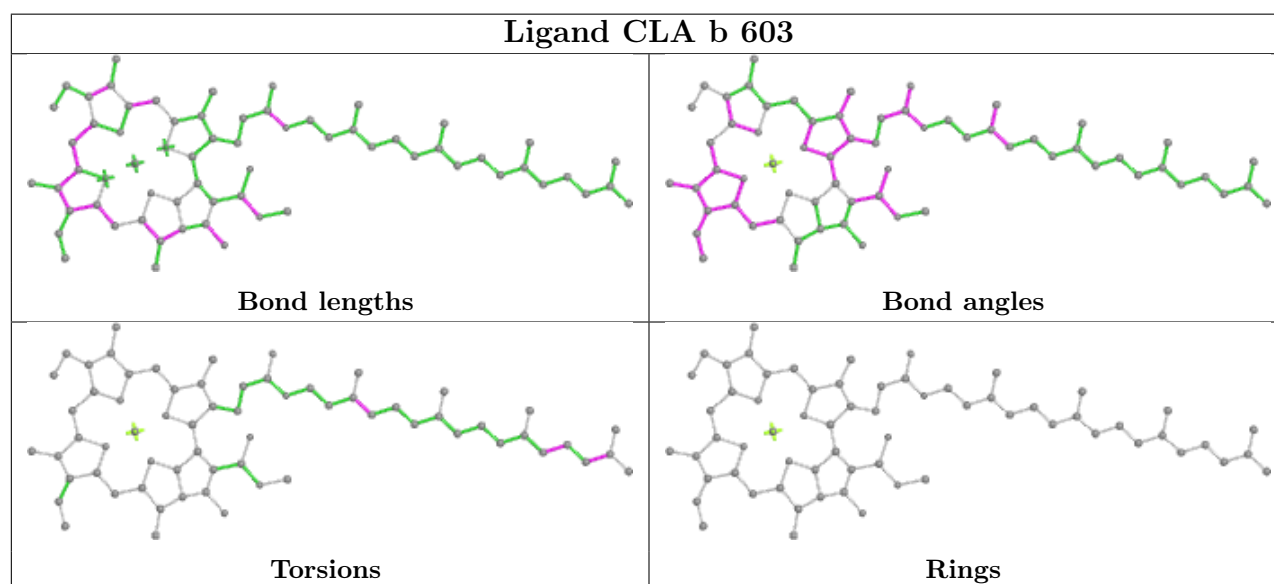
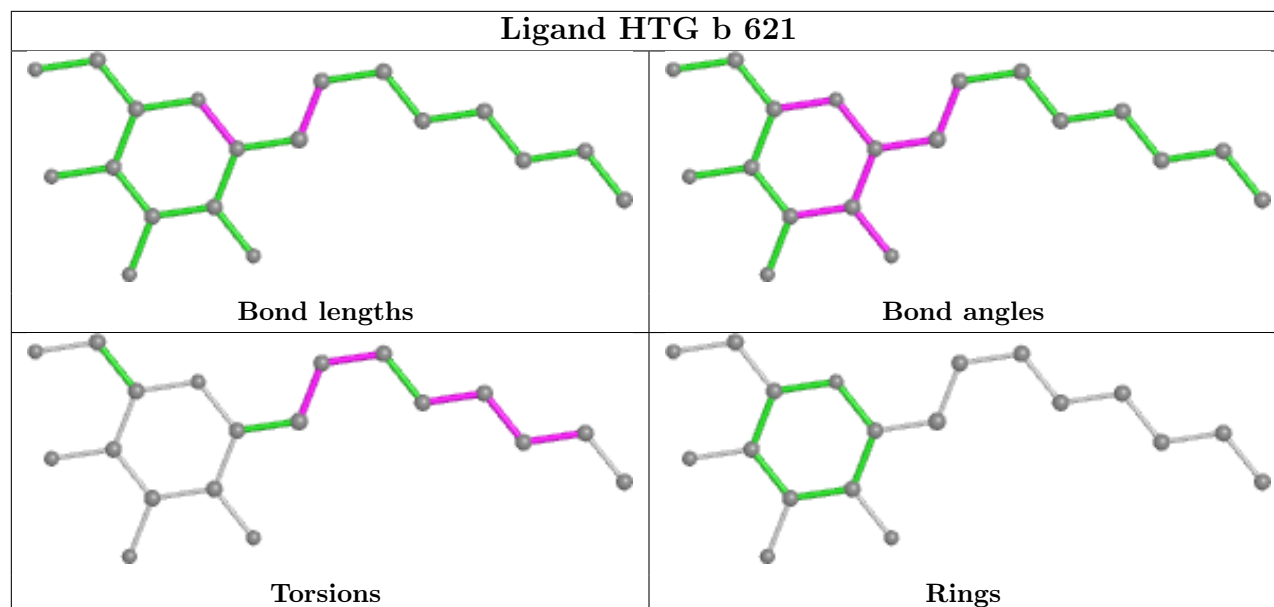


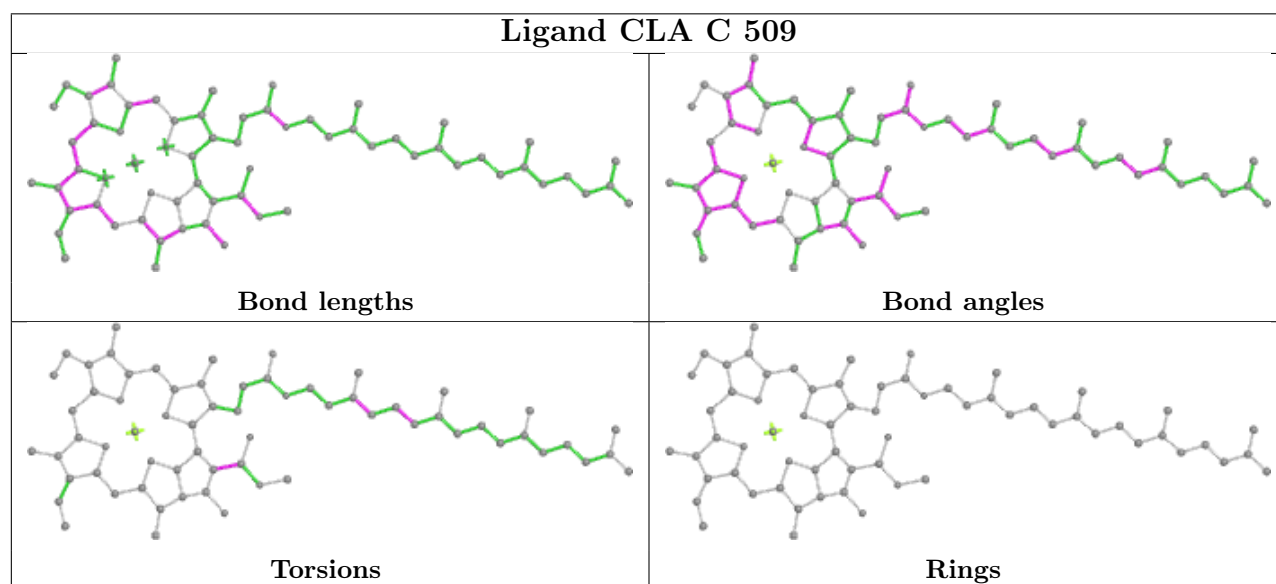
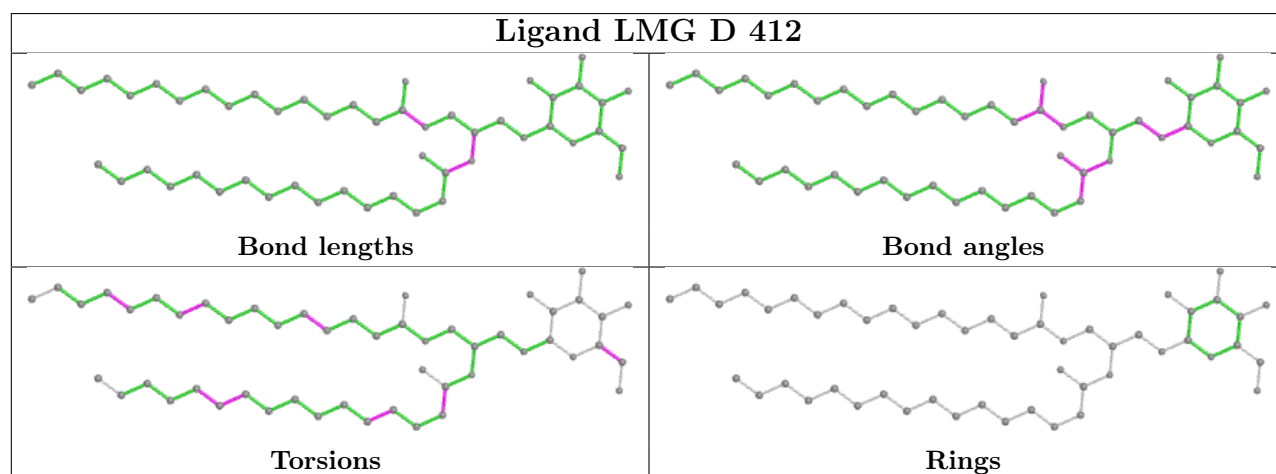
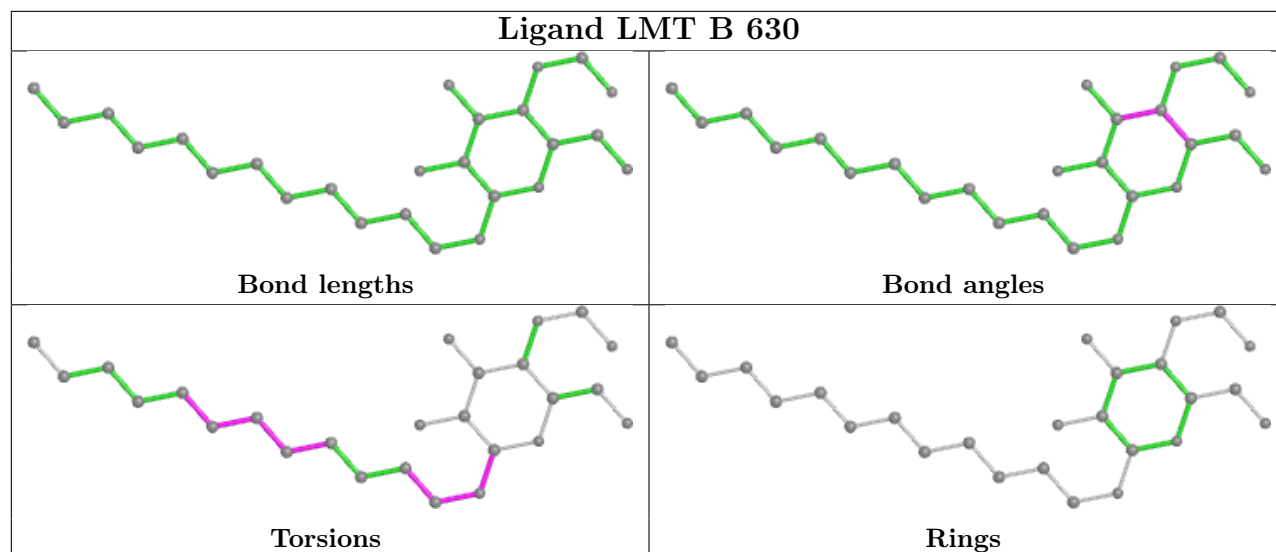
Ligand SQD A 411



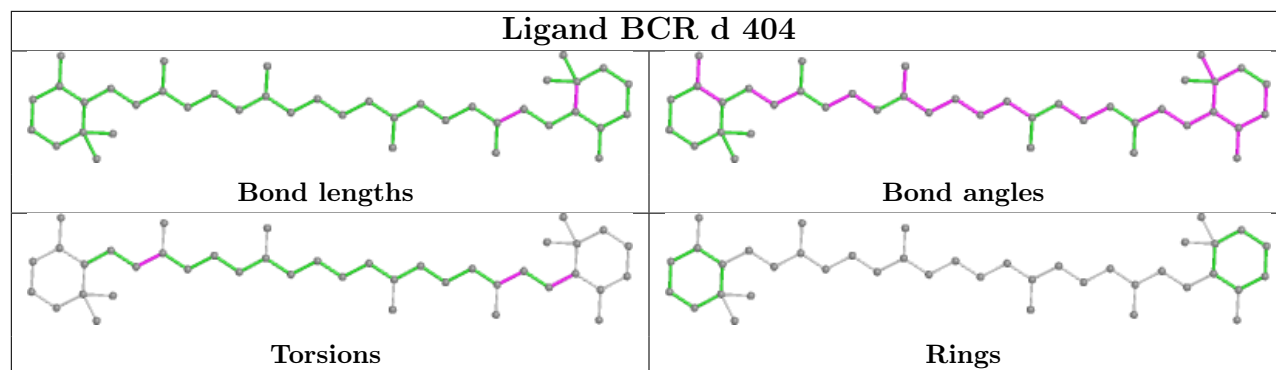
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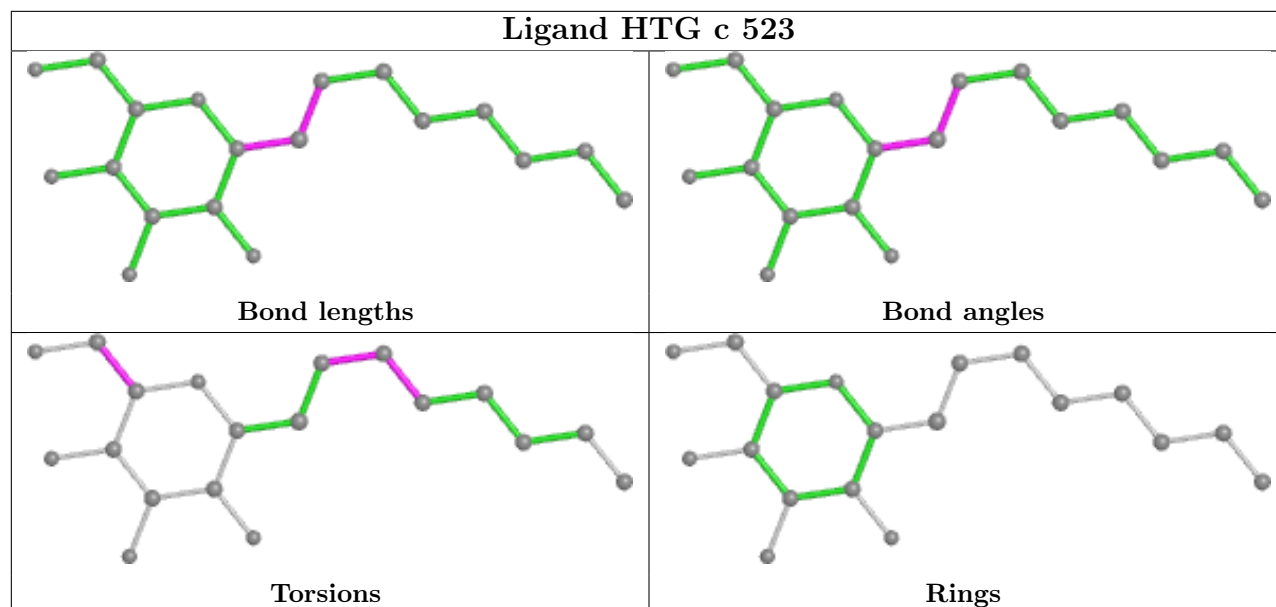




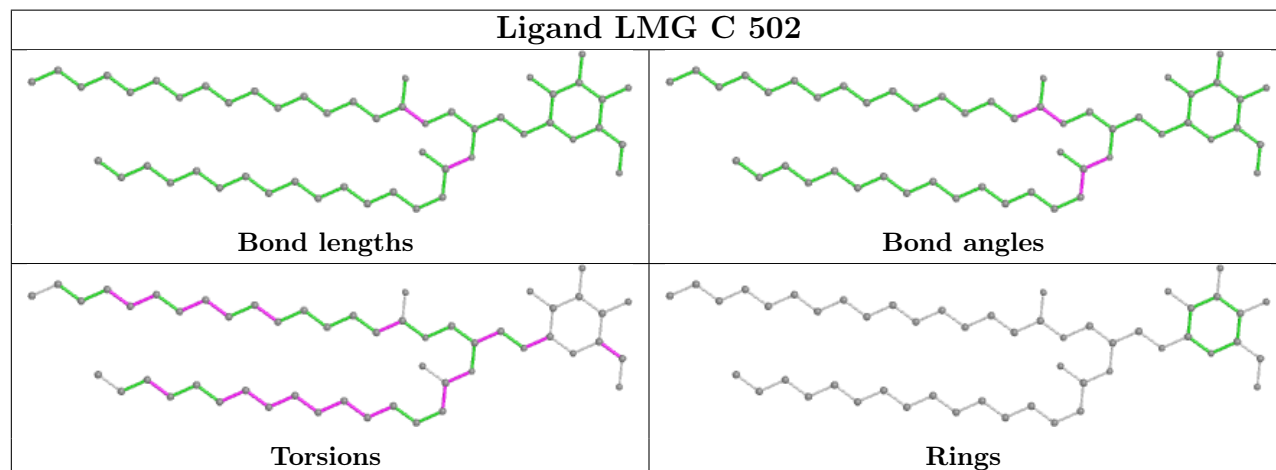
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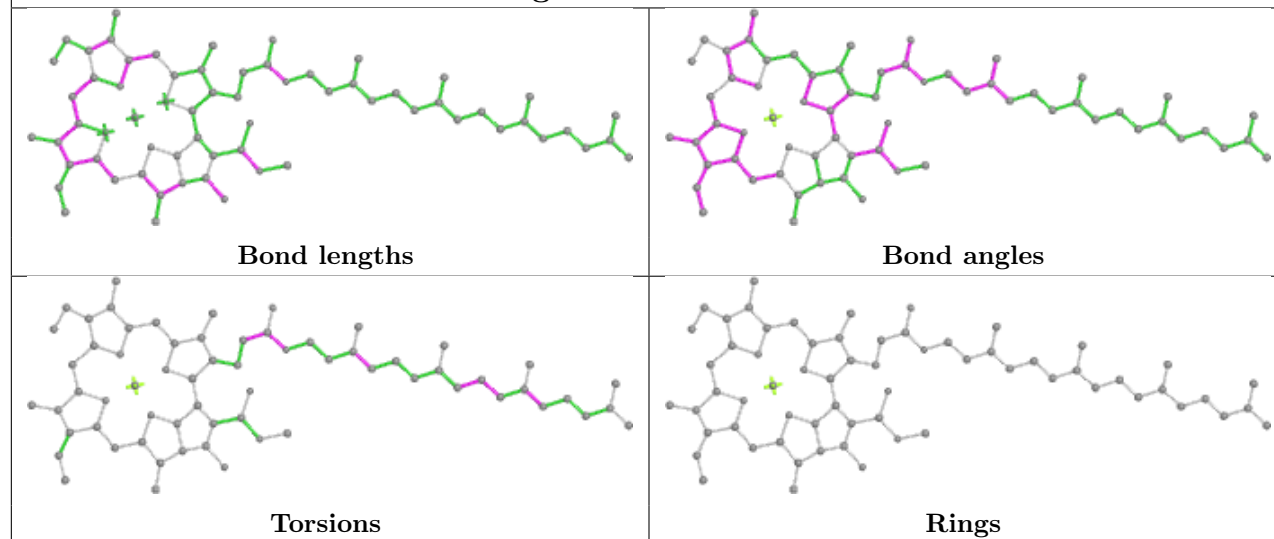
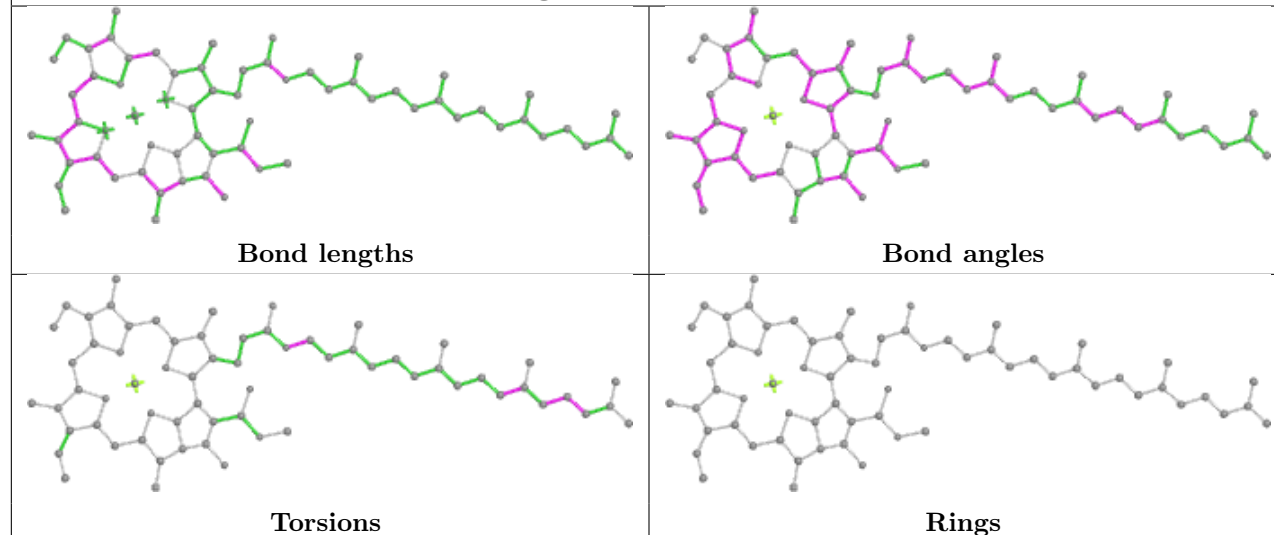
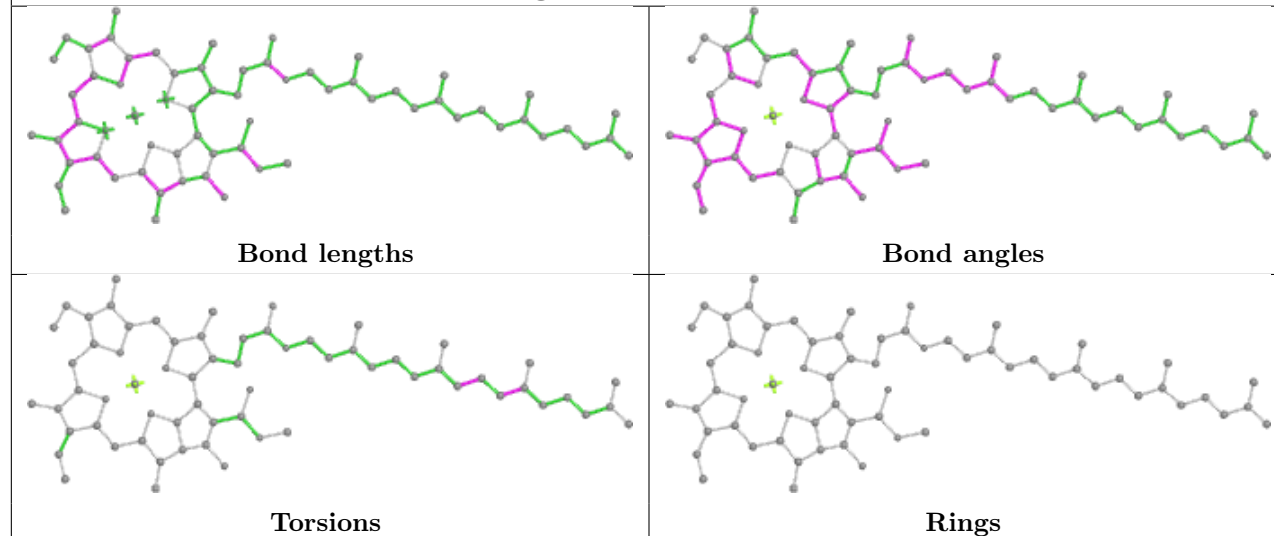


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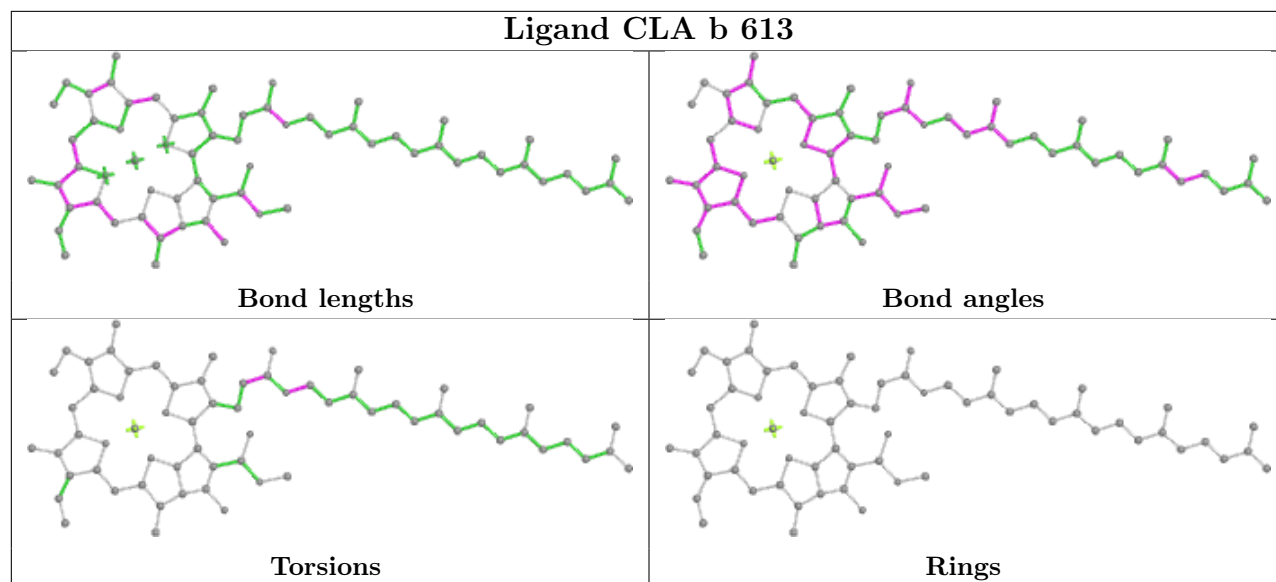


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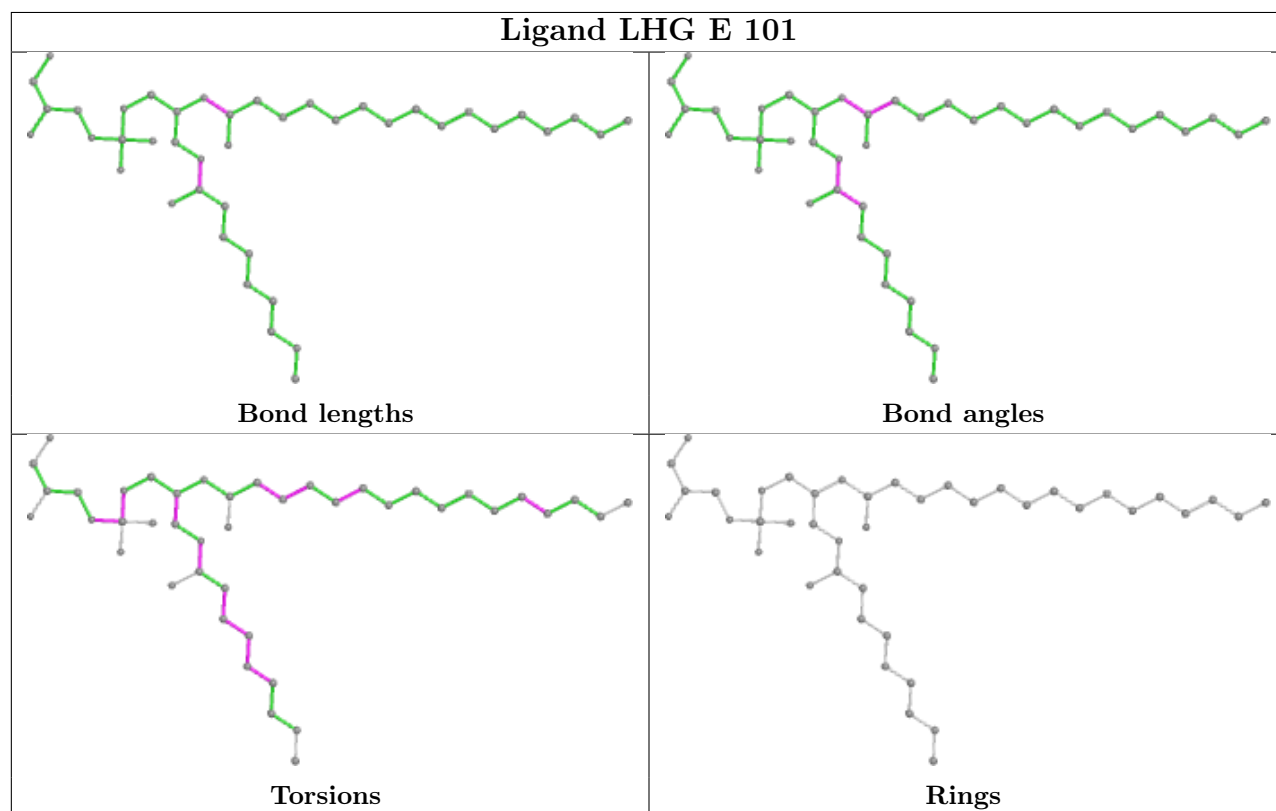


Ligand CLA C 512**Ligand CLA b 608****Ligand CLA B 611**

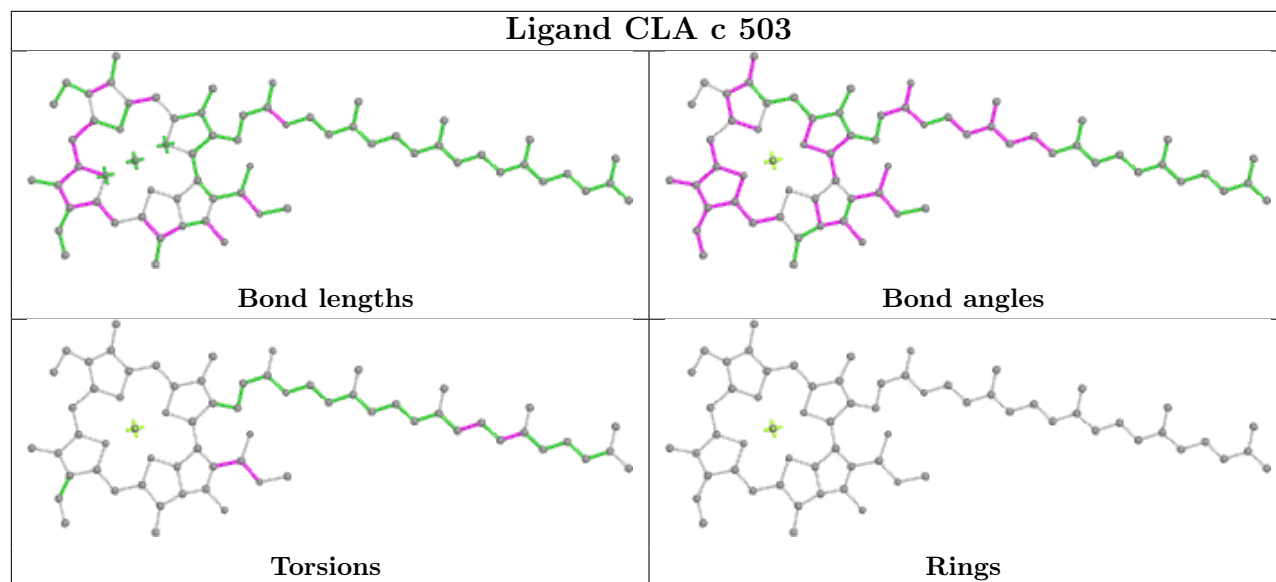
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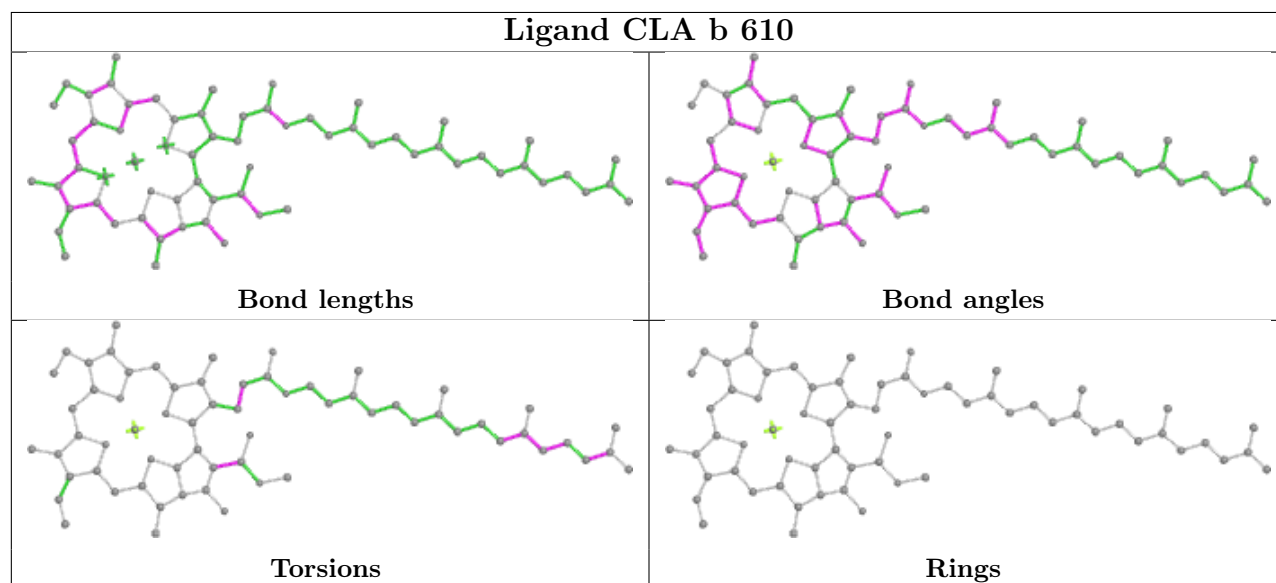
Ligand LHG E 101



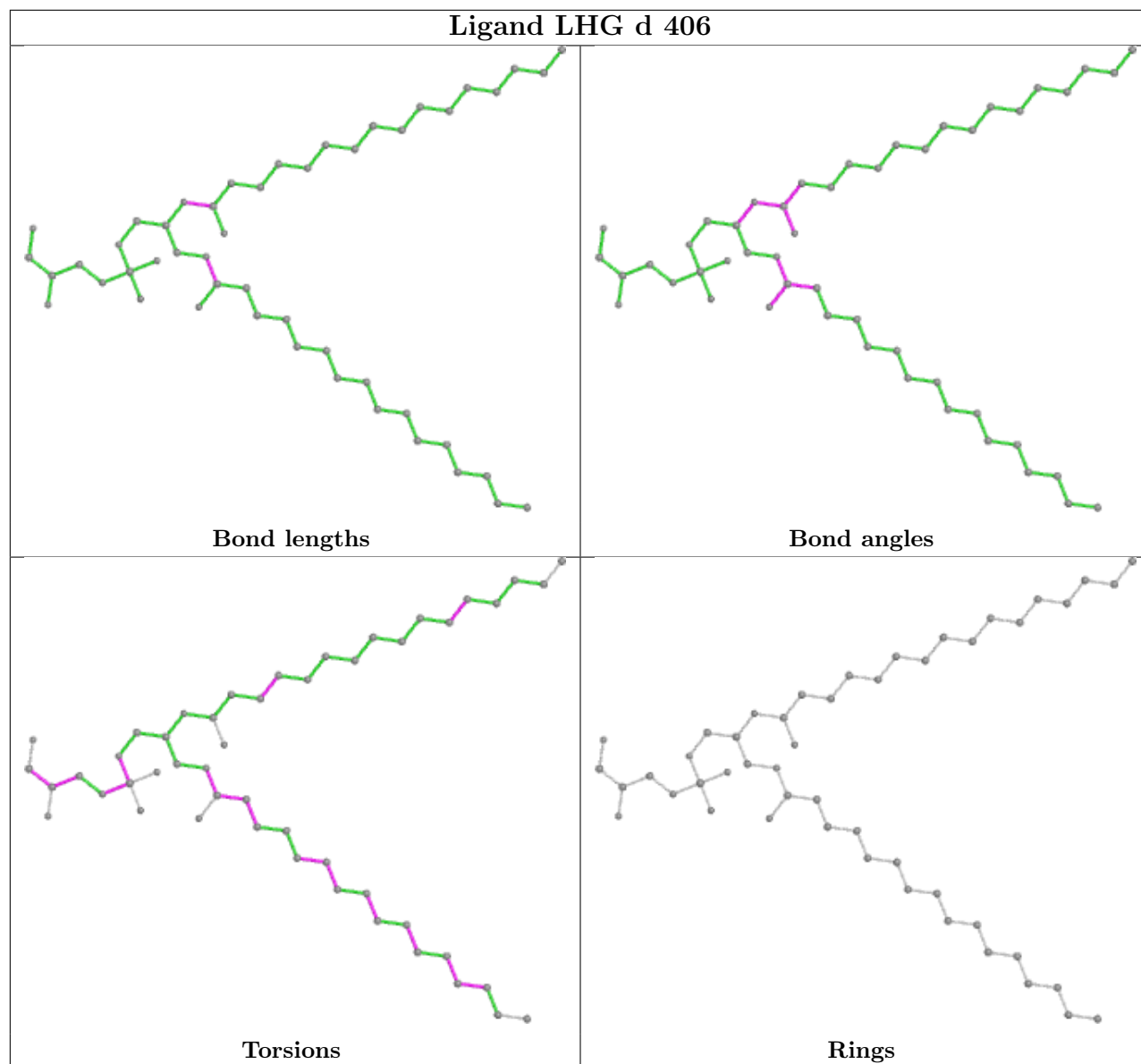
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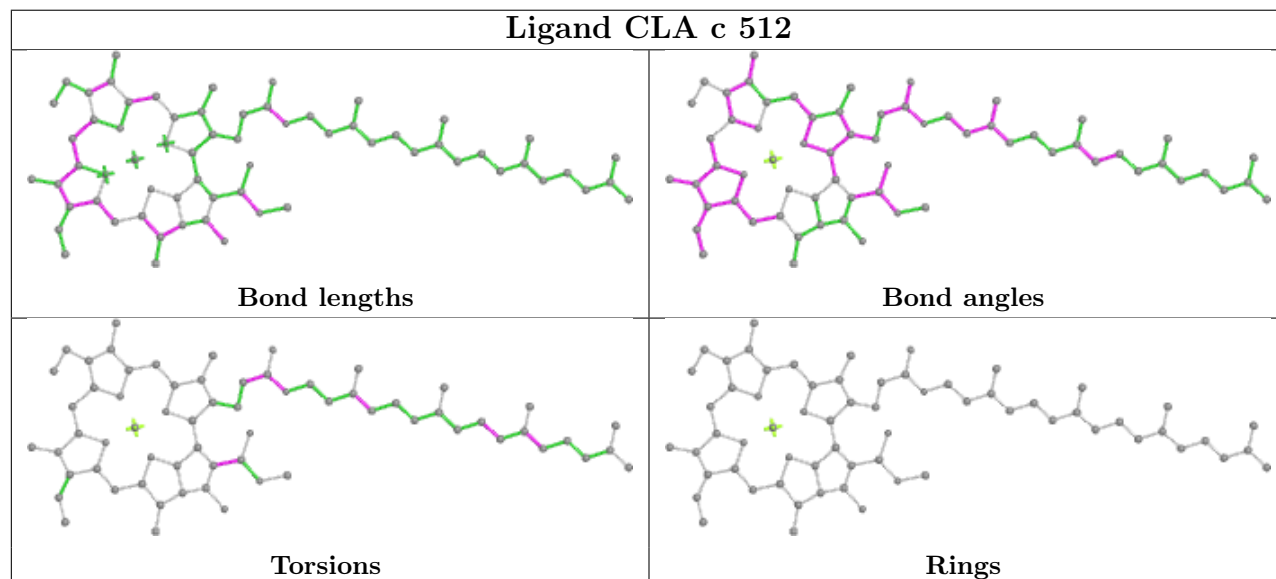
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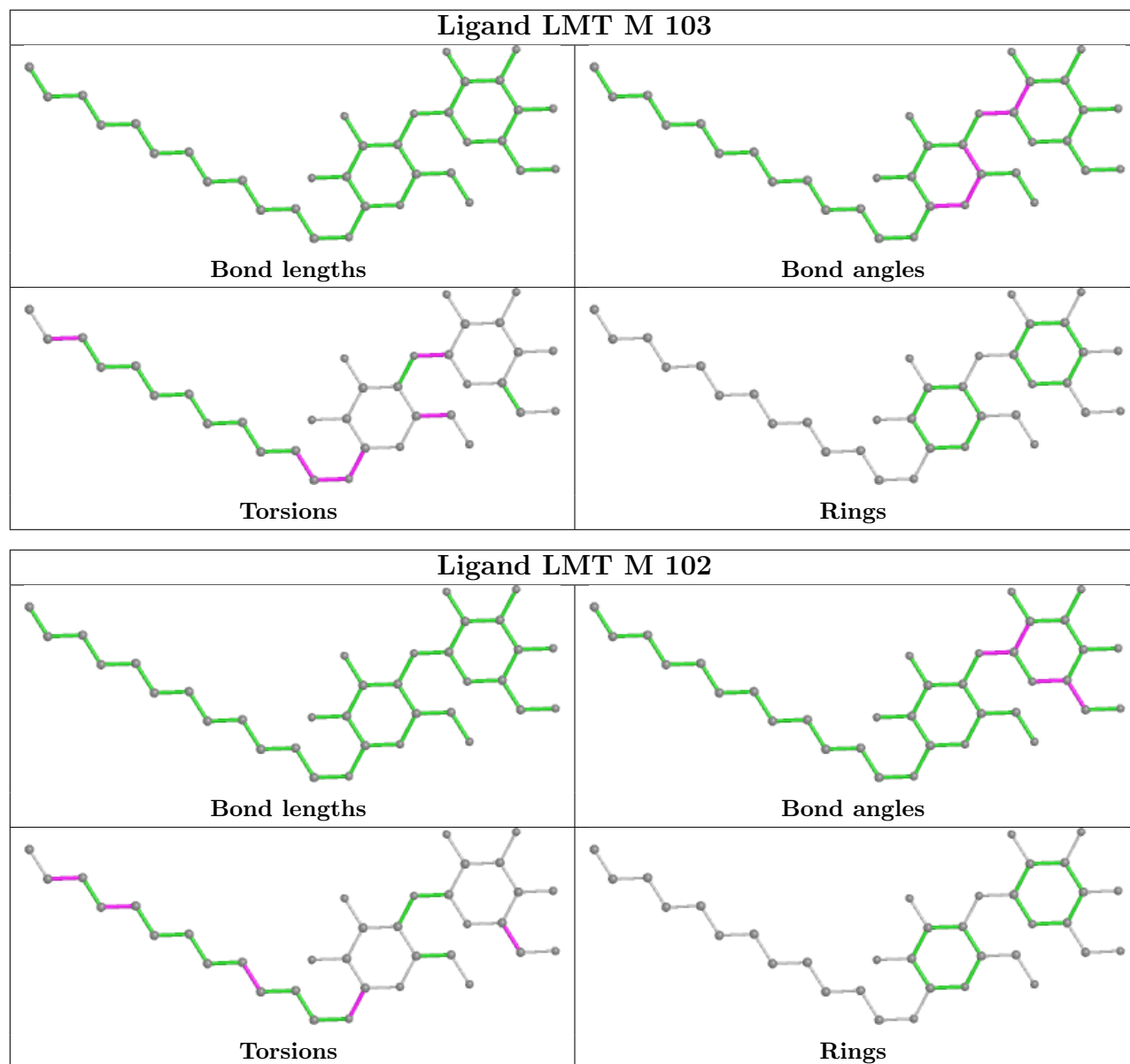


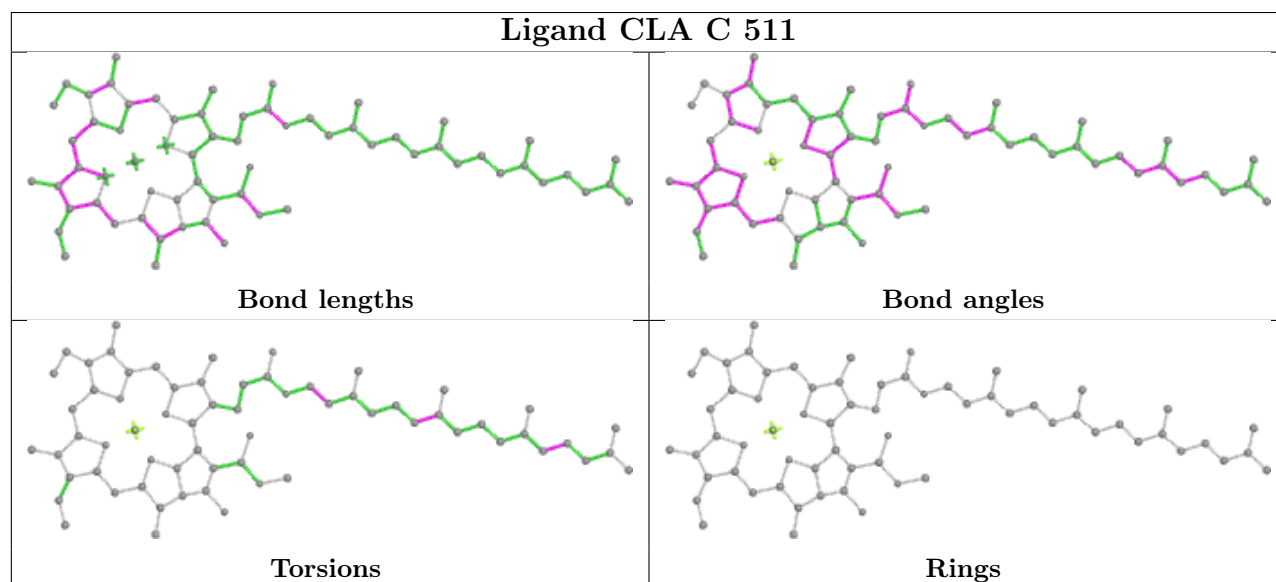
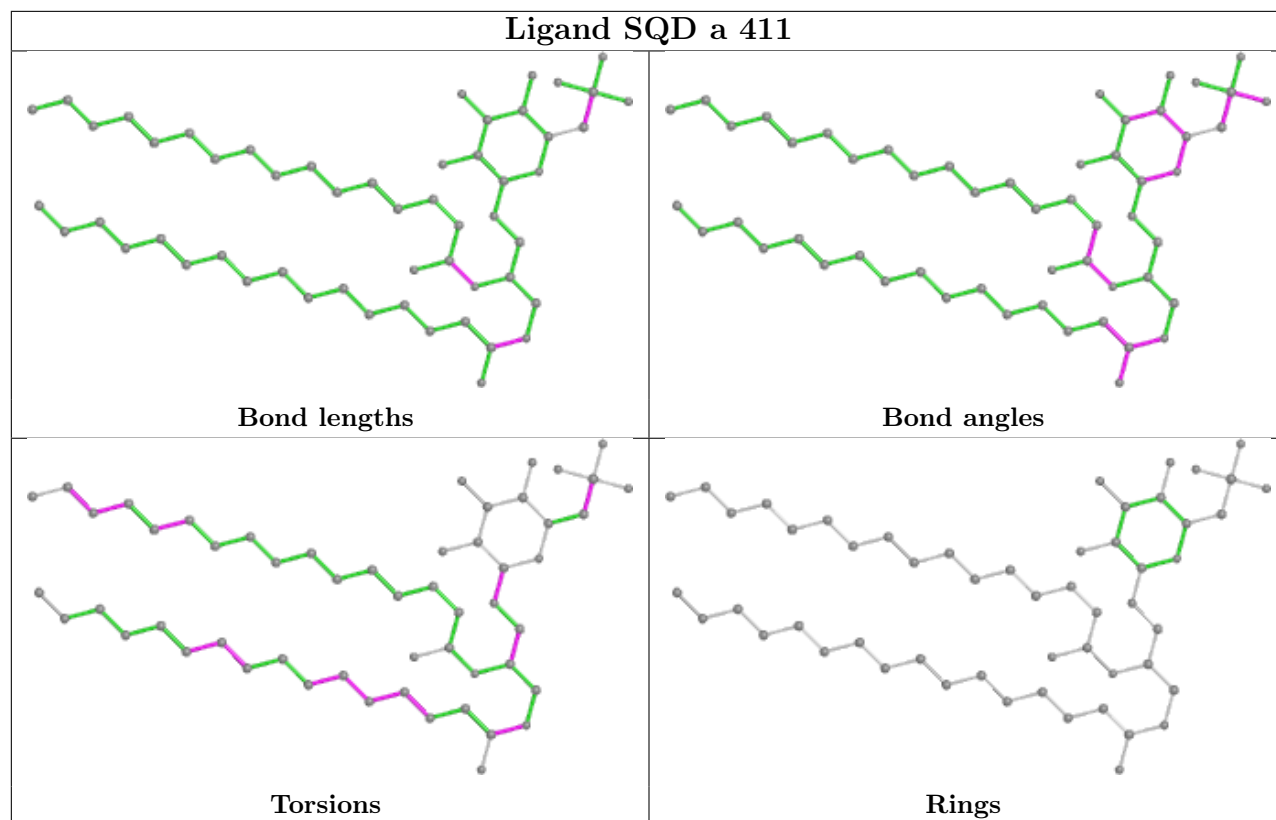
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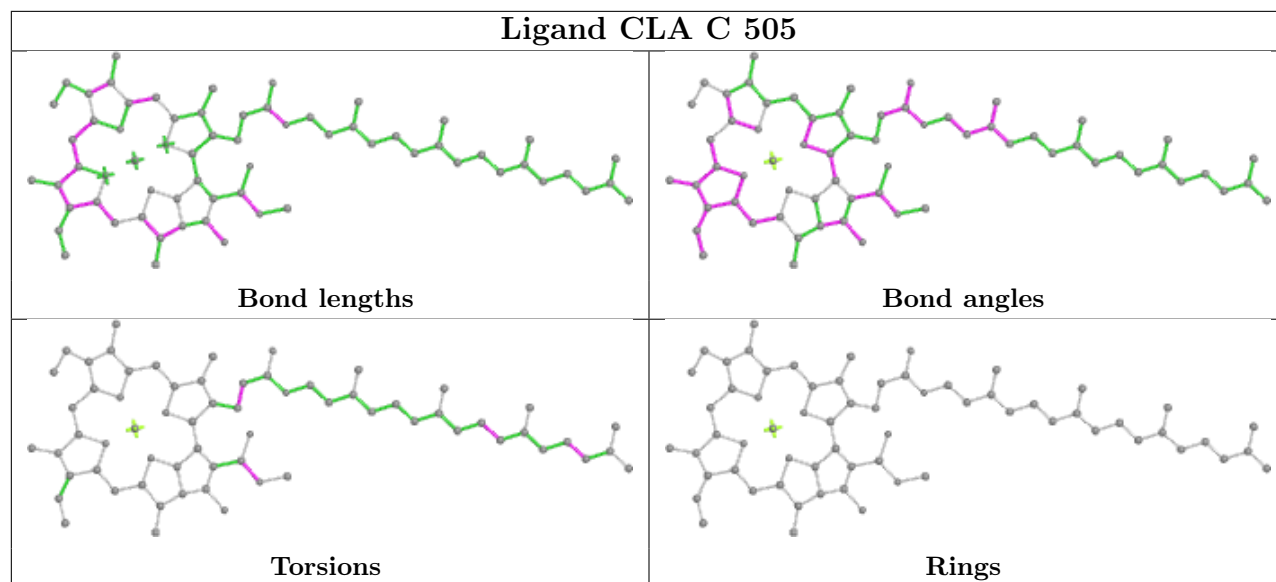
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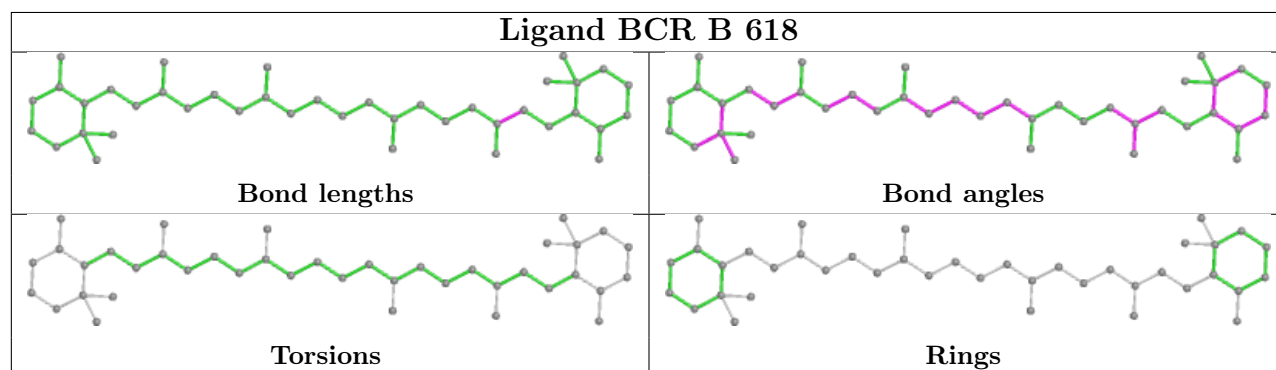




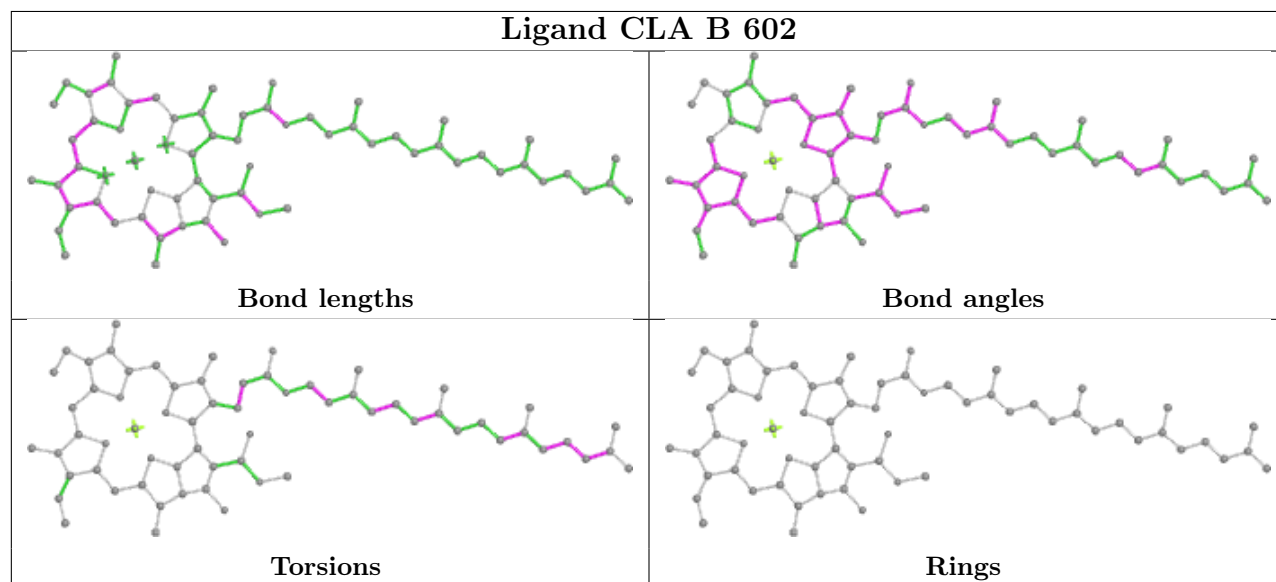
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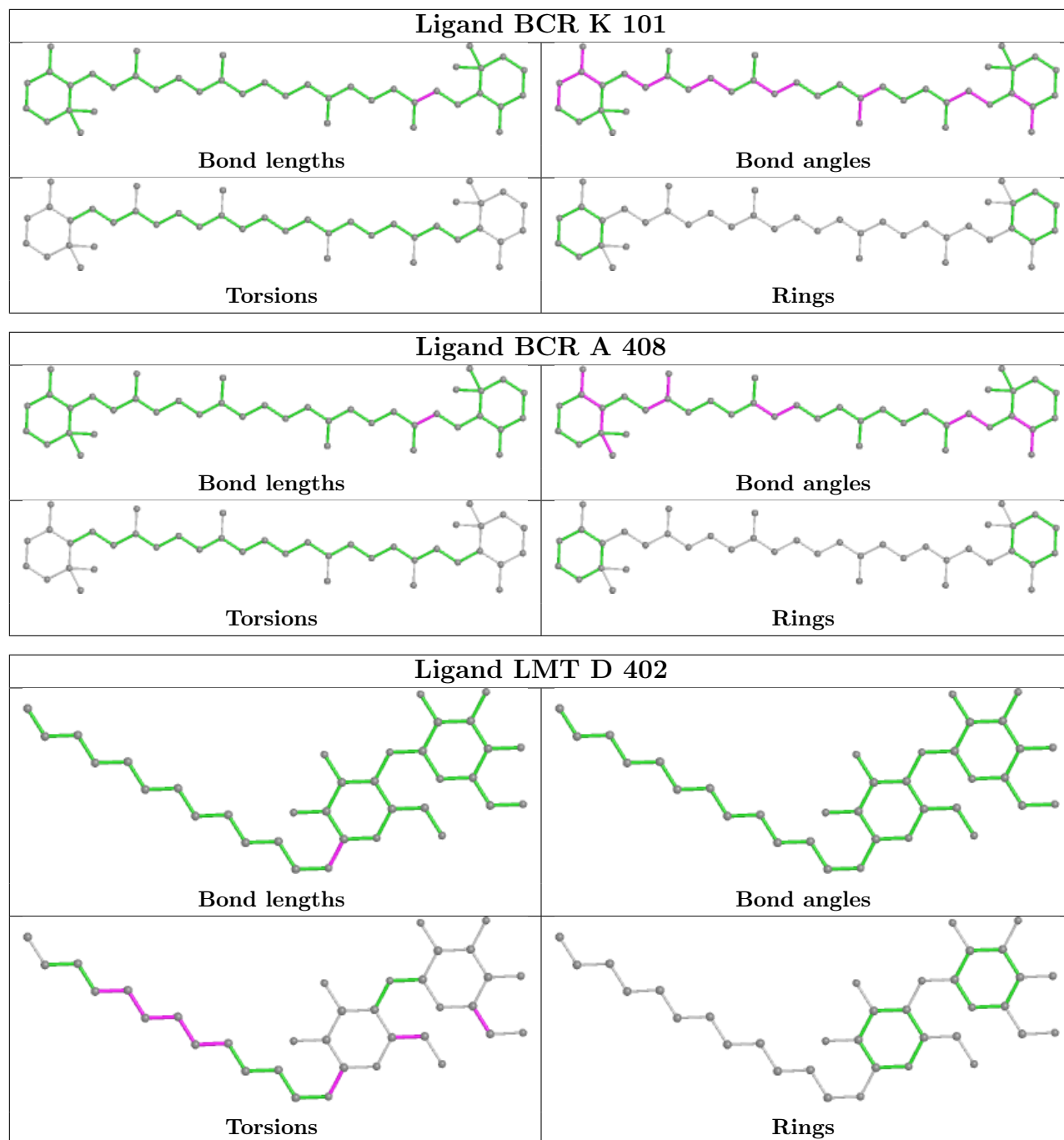


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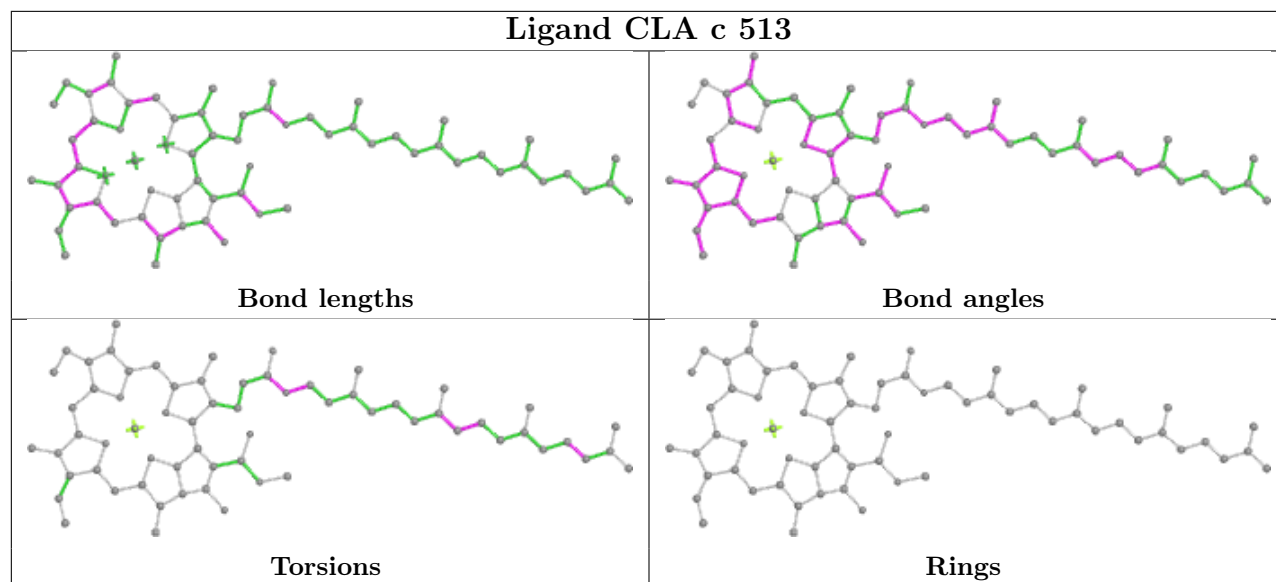


Ligand CLA B 602

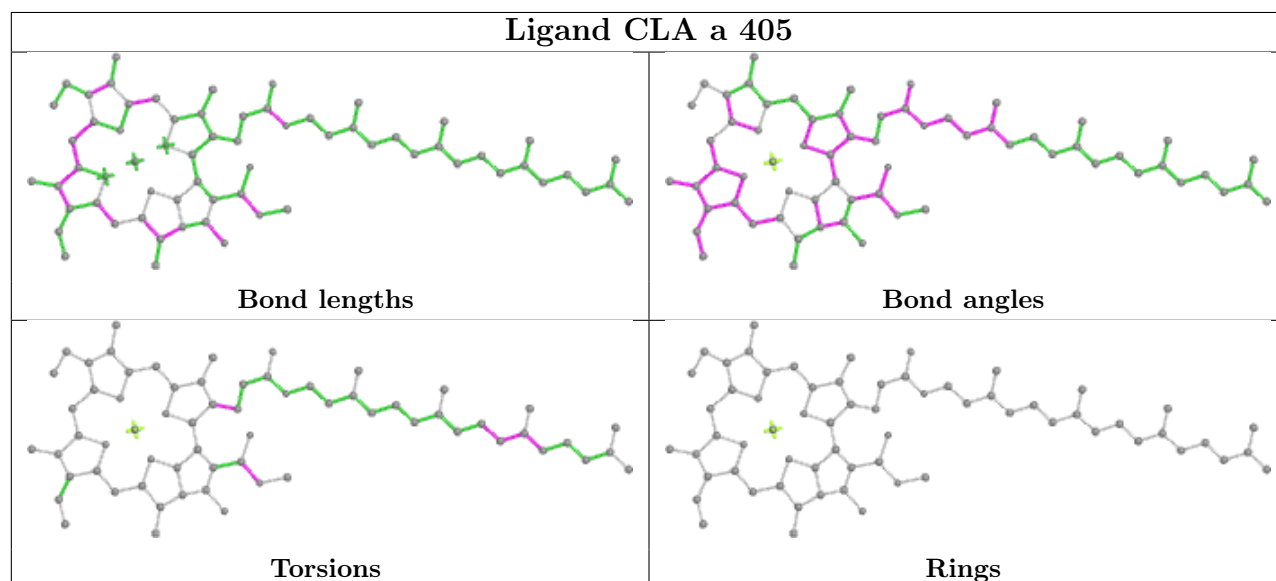




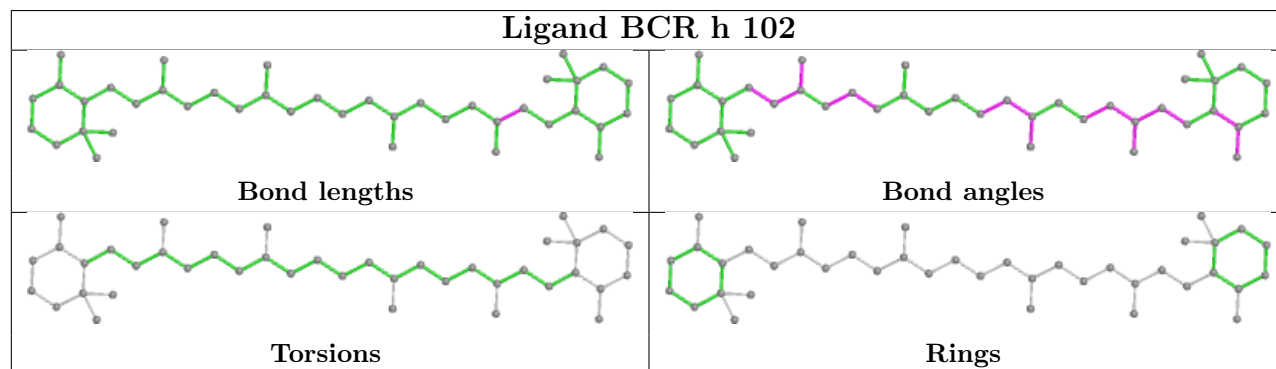
Ligand CLA c 513



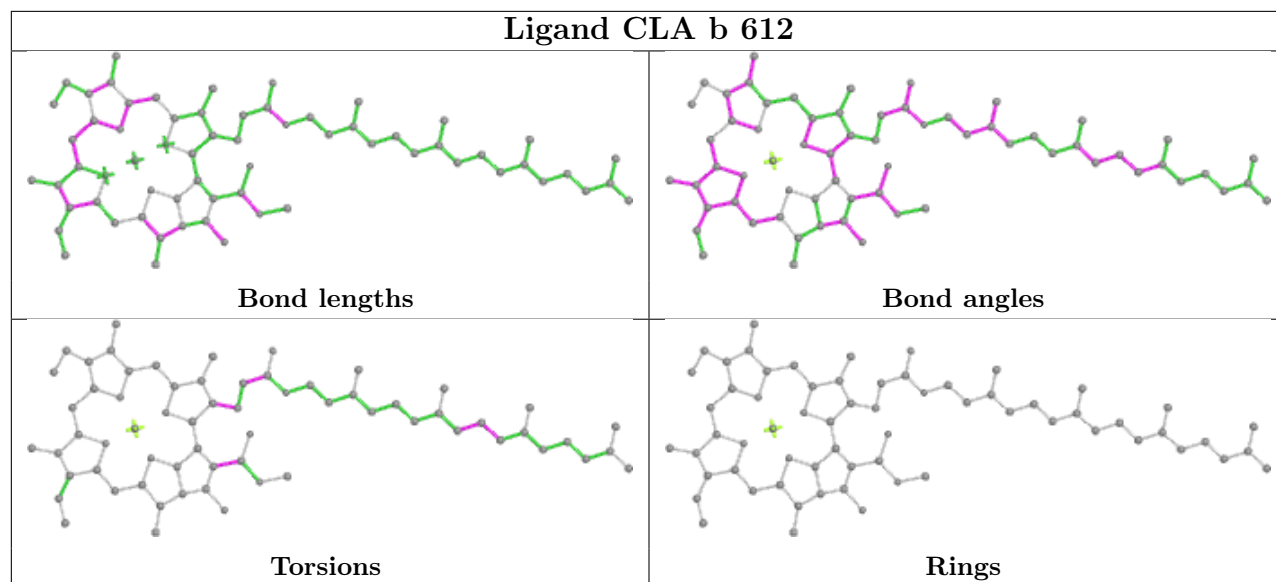
Ligand CLA a 405



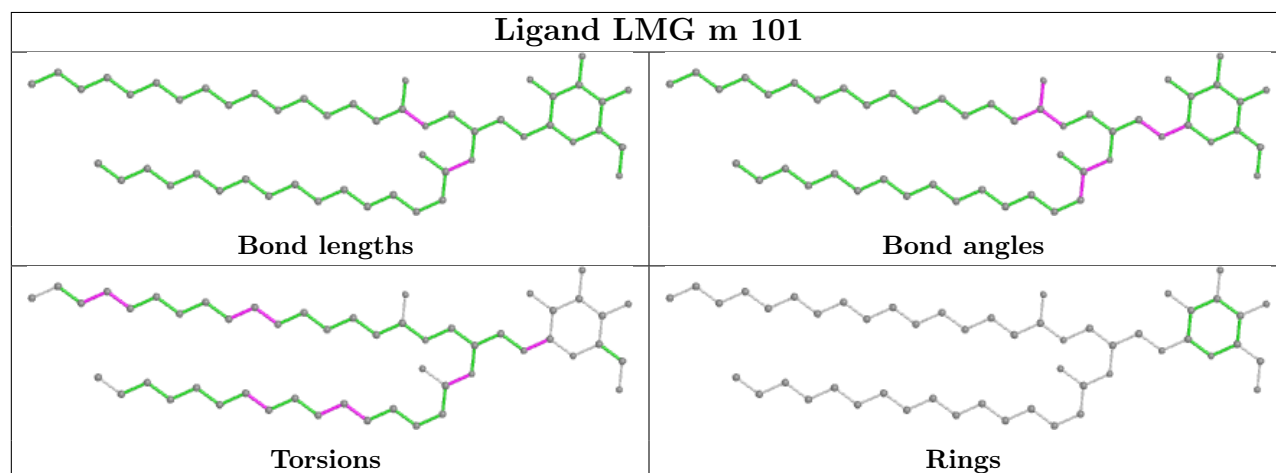
Ligand BCR h 102



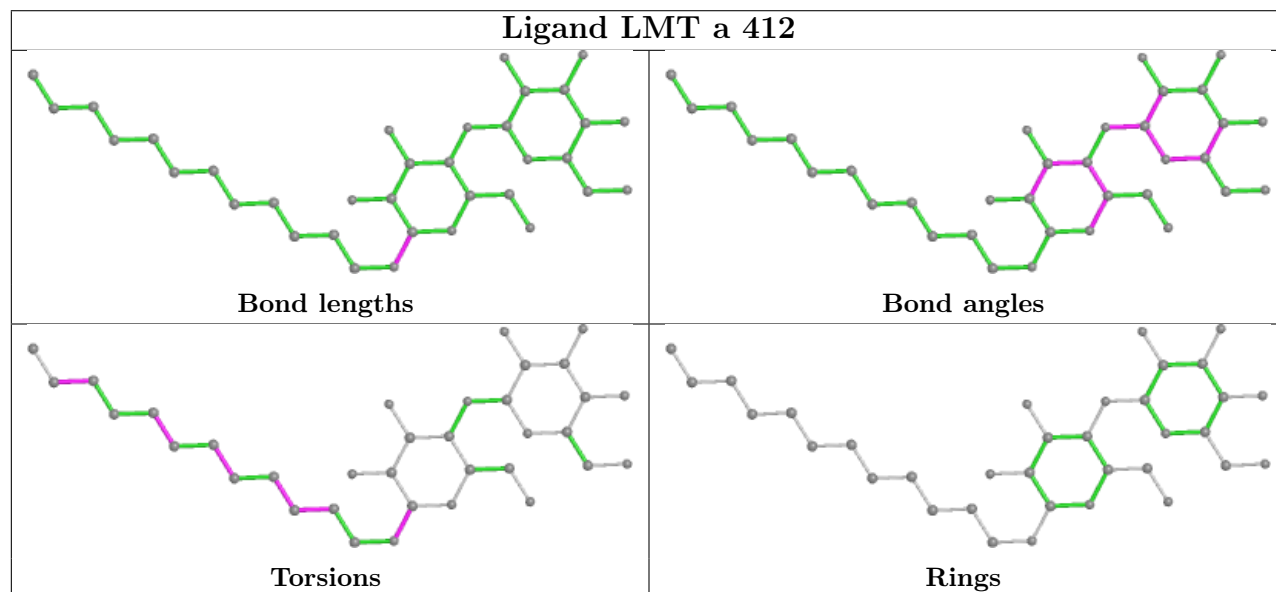
Ligand CLA b 612

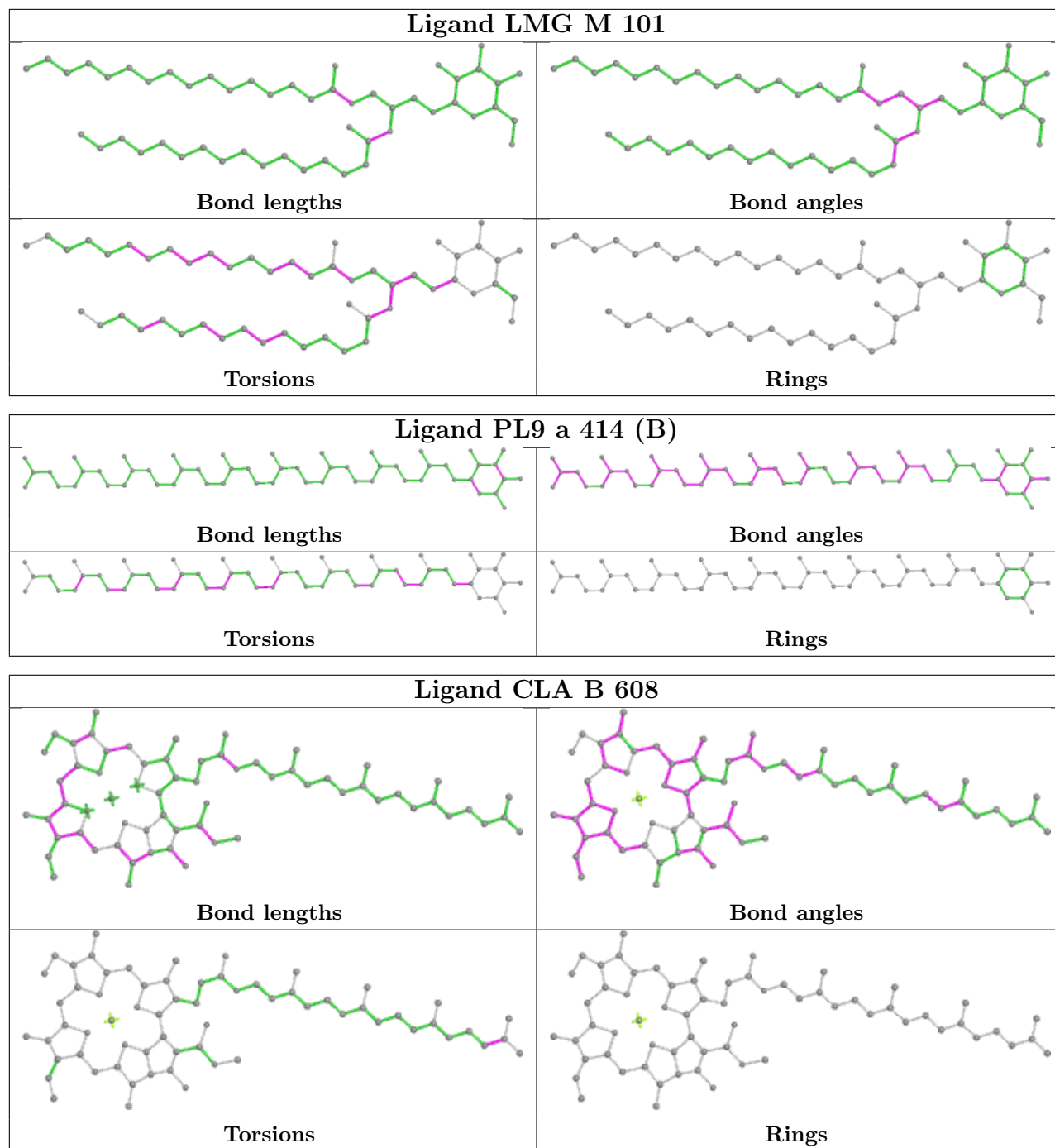


Ligand LMG m 101

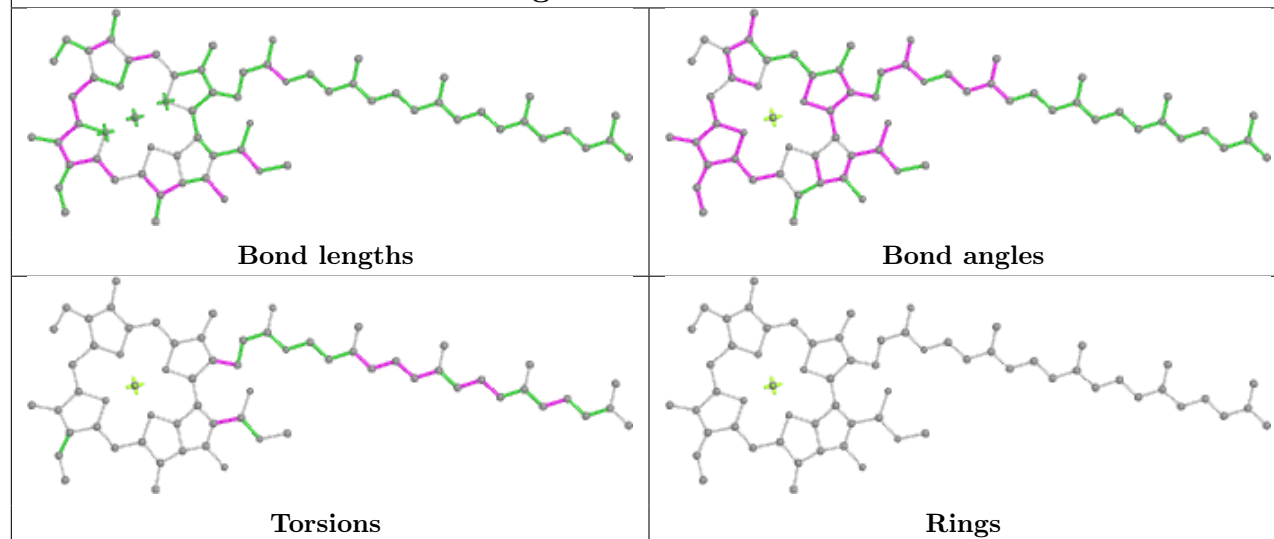


Ligand LMT a 412

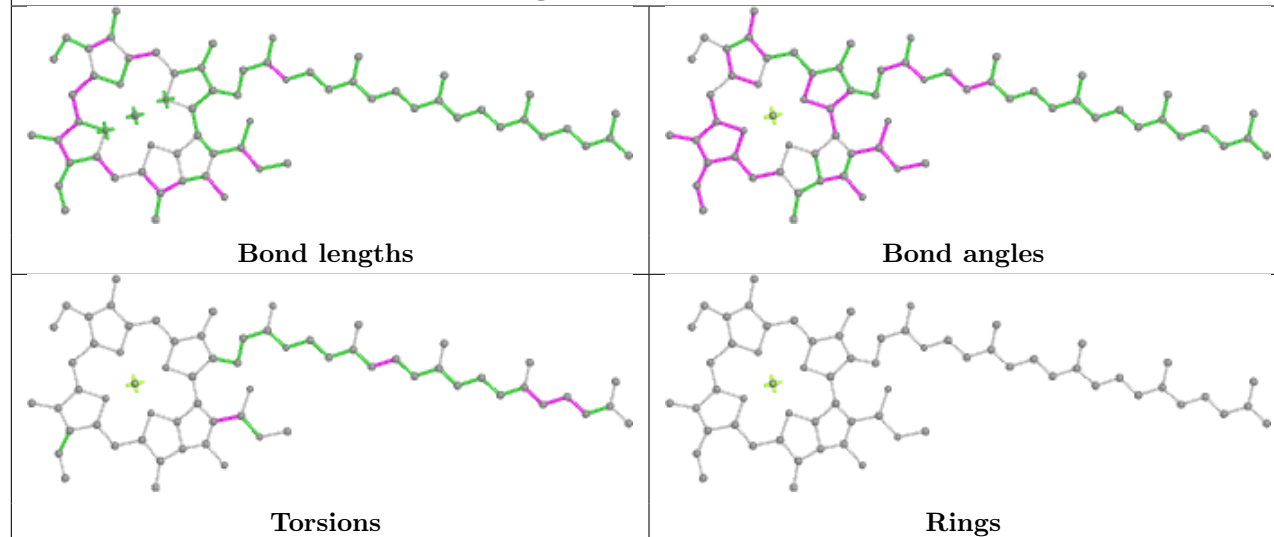


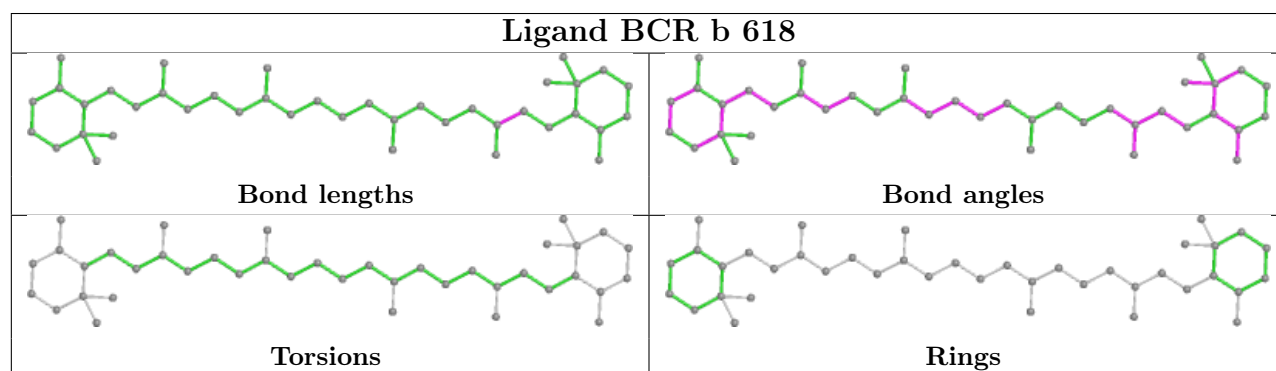
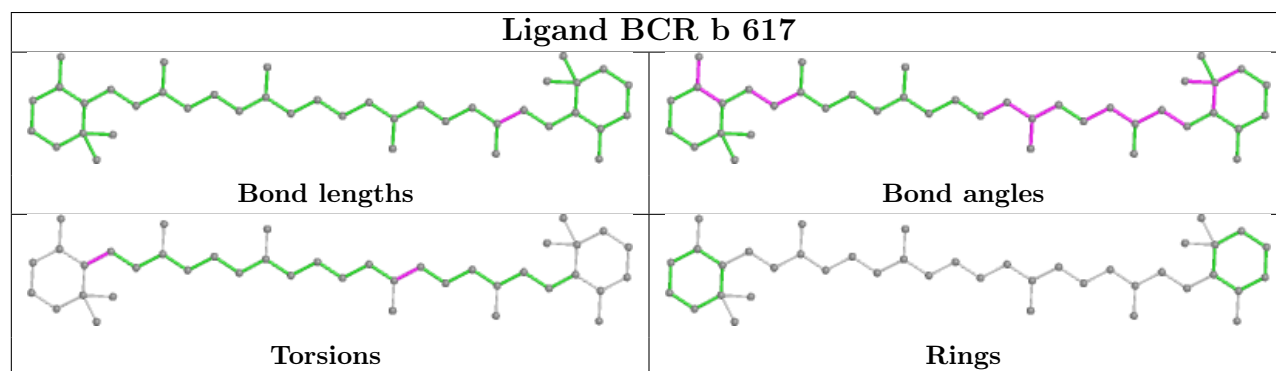
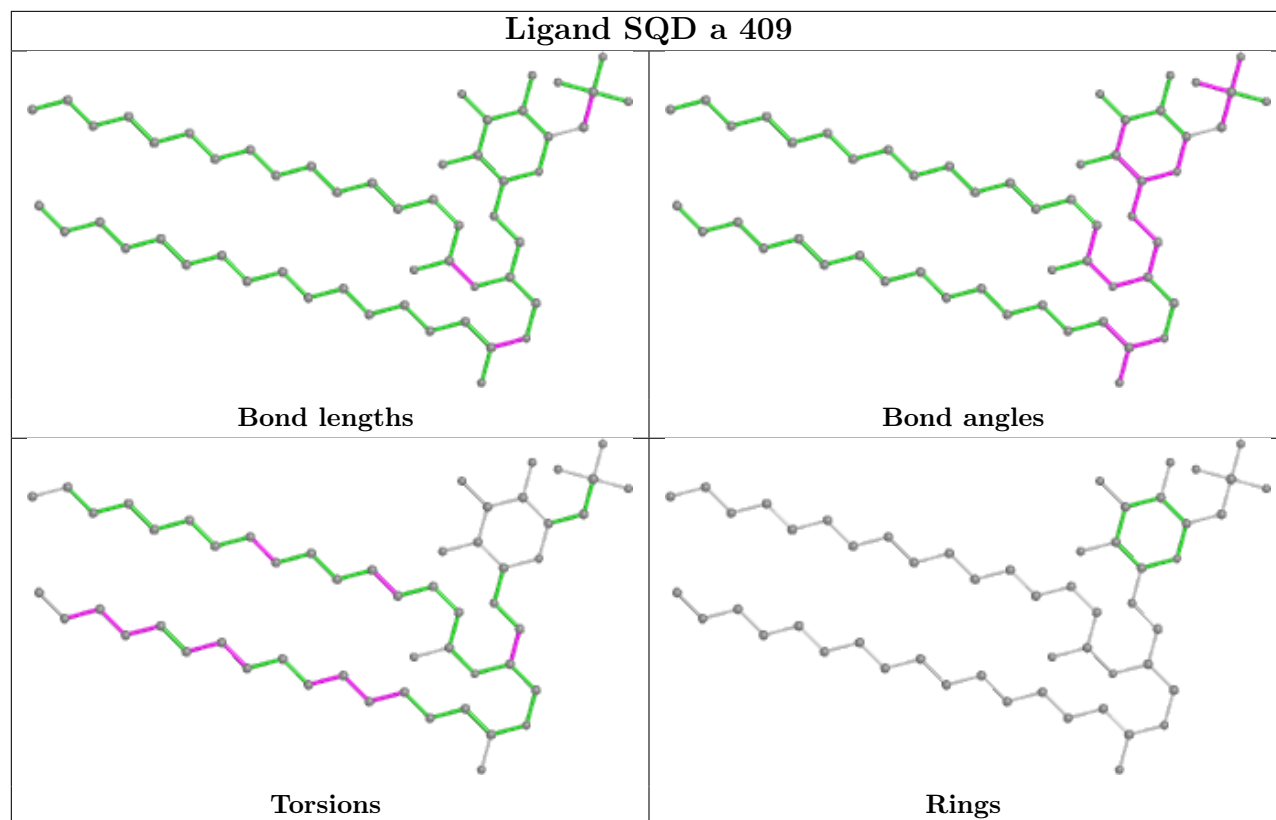


Ligand CLA C 508

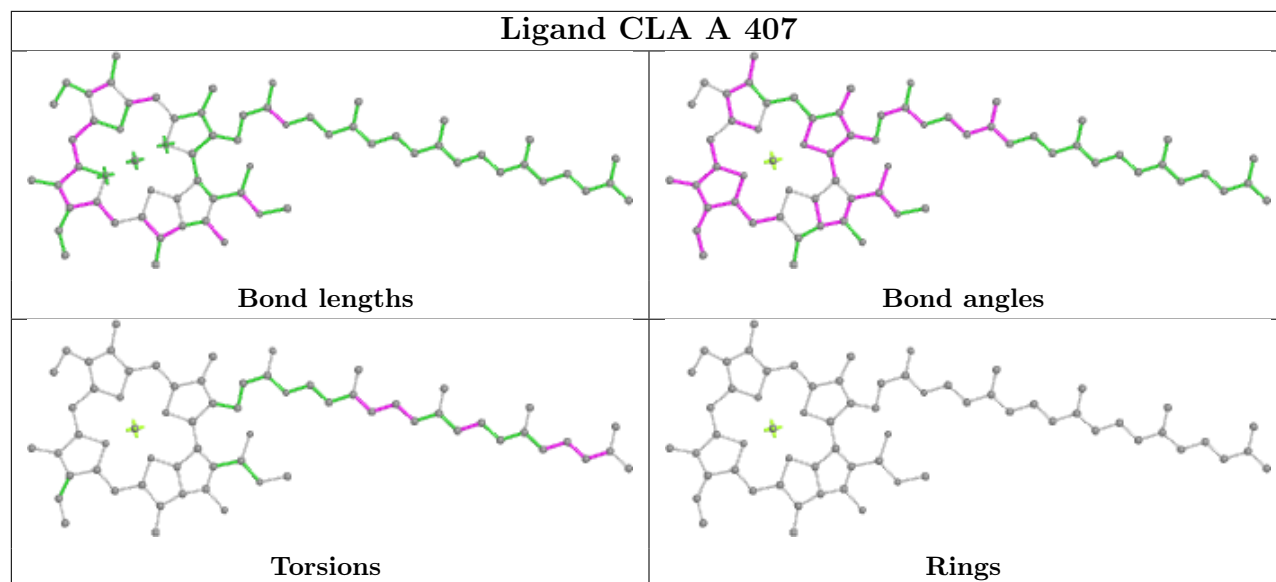


Ligand CLA C 504

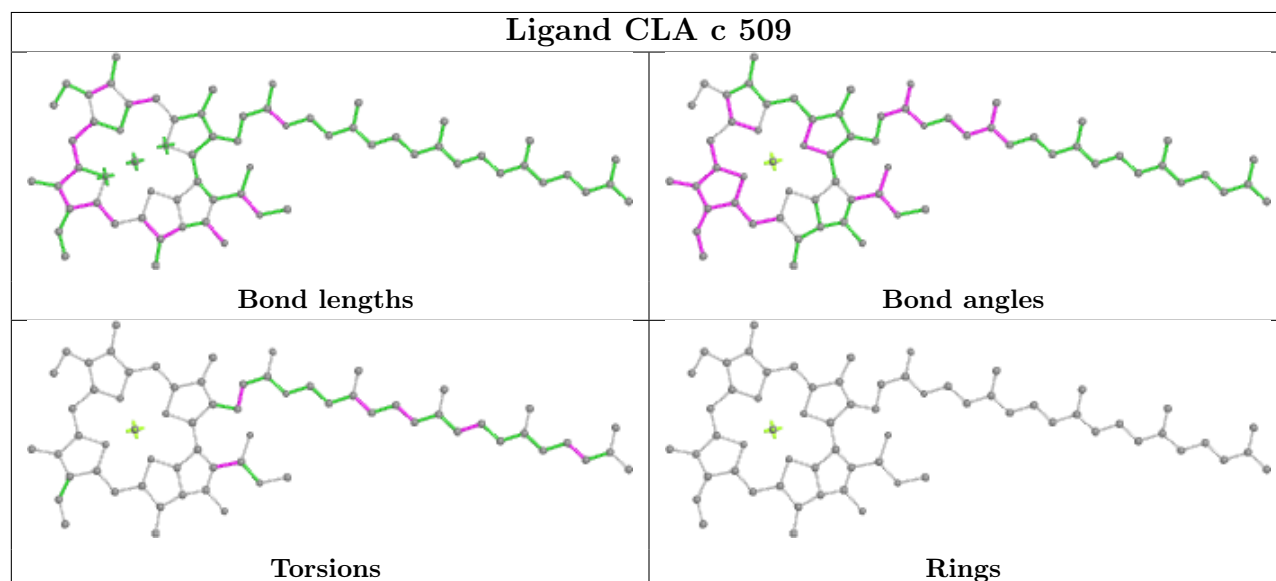




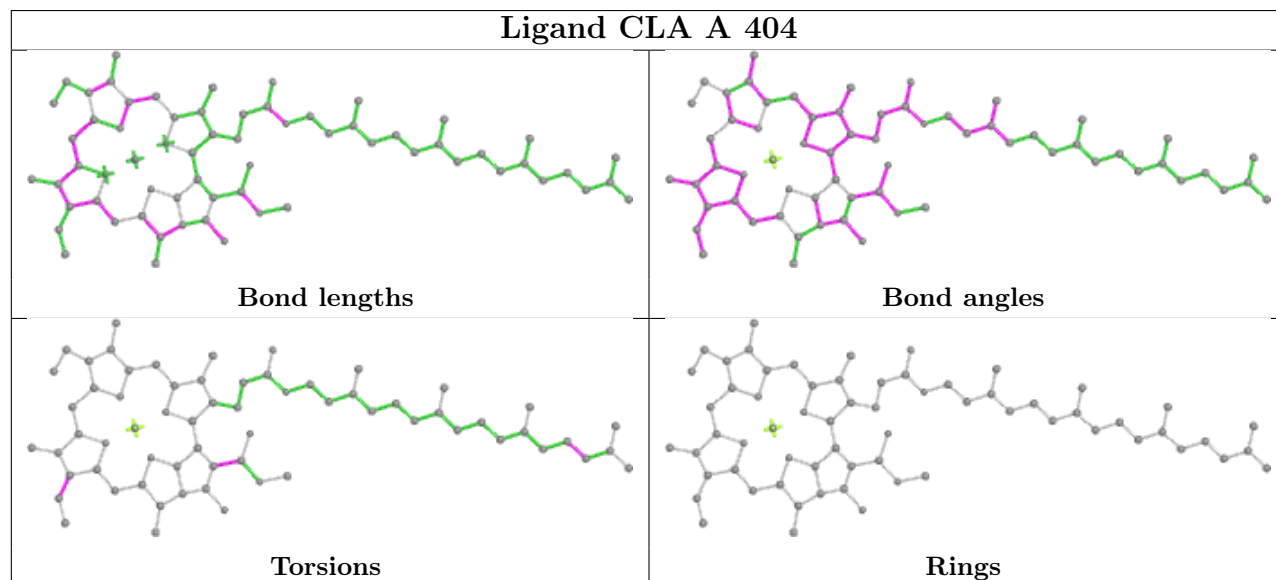
Ligand CLA A 407



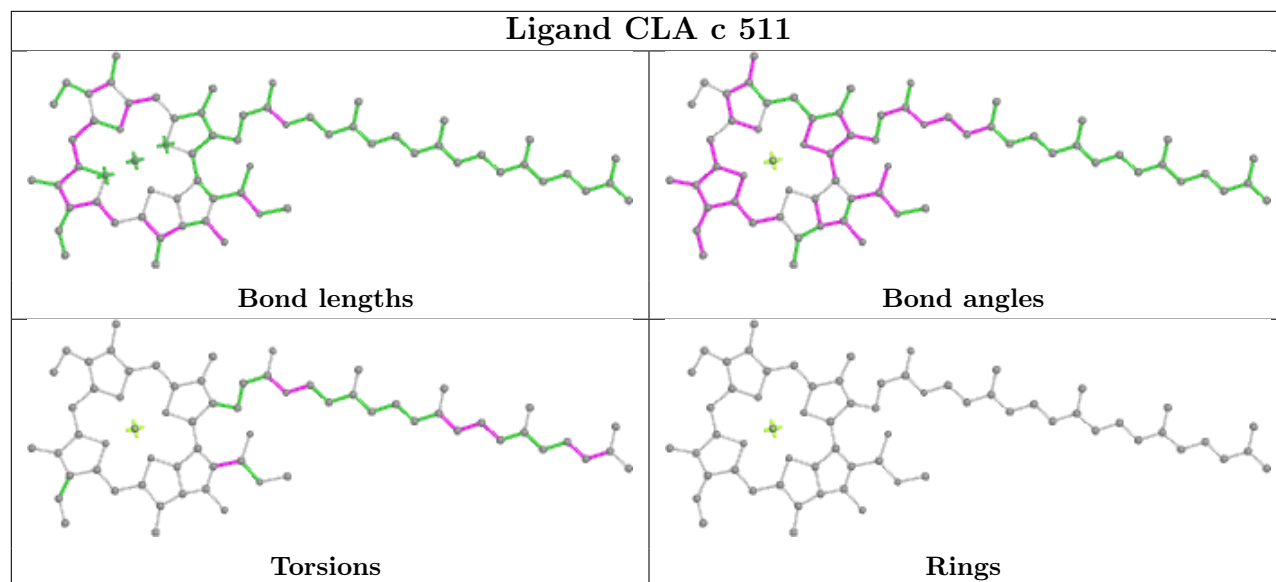
Ligand CLA c 509



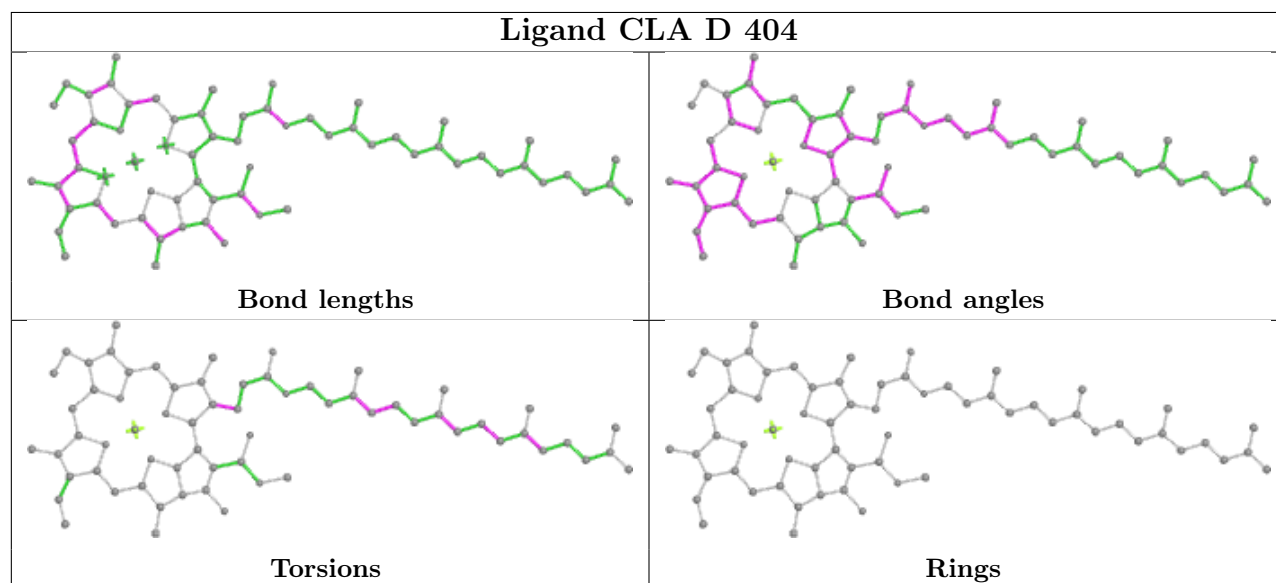
Ligand CLA A 404

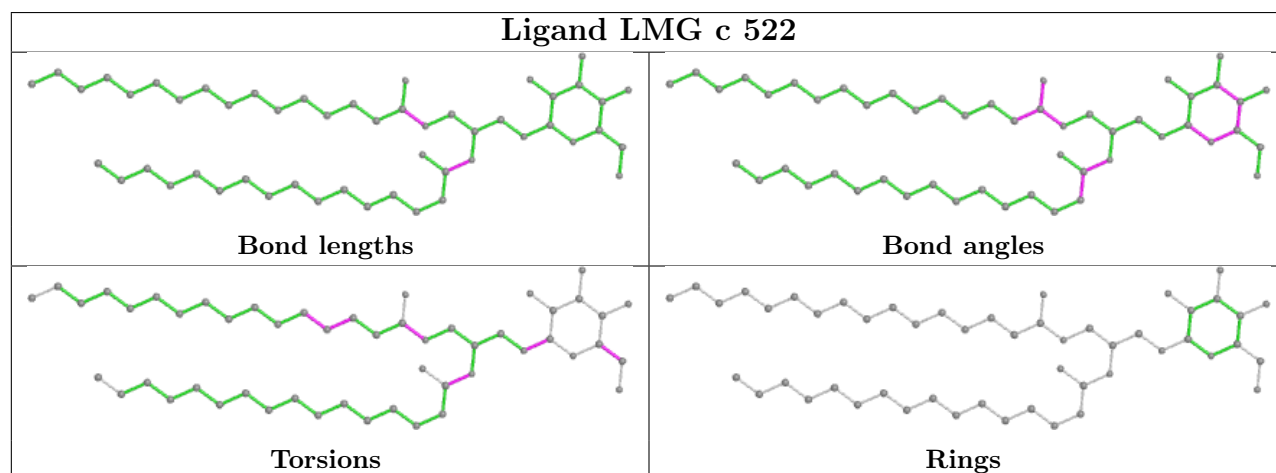
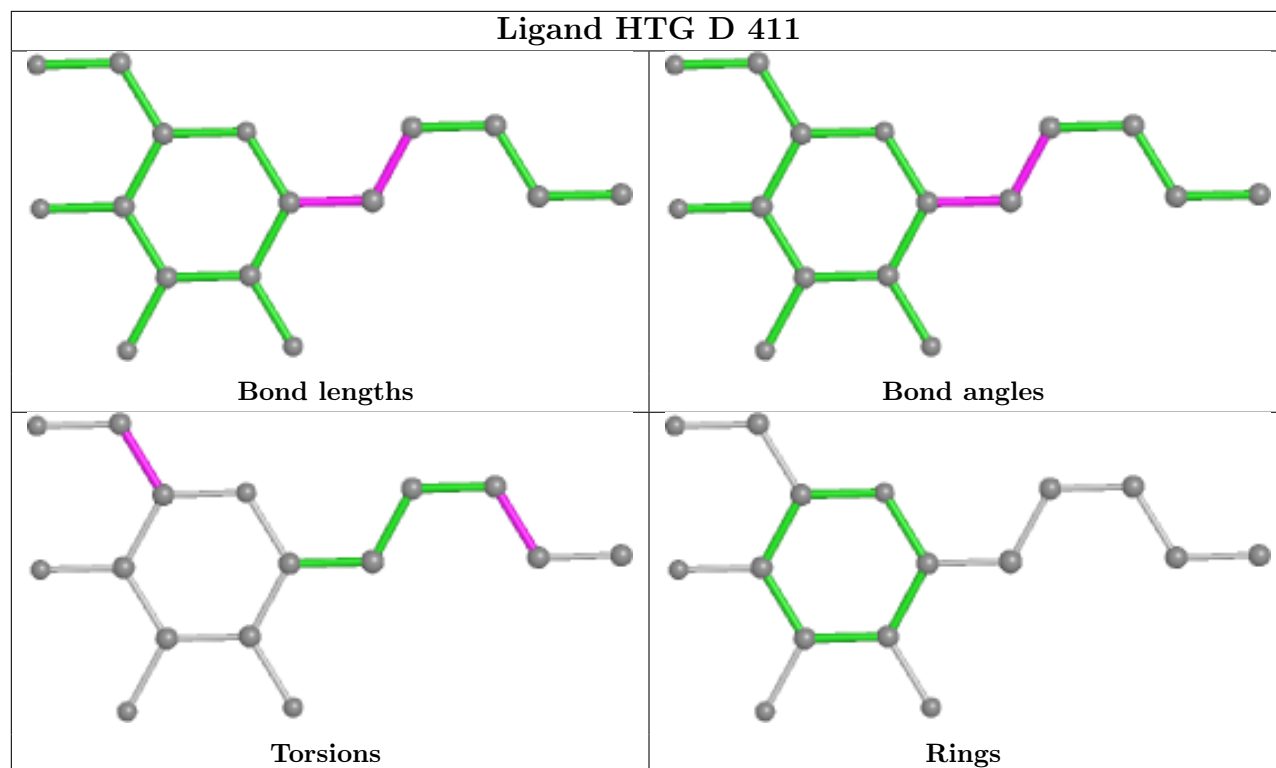


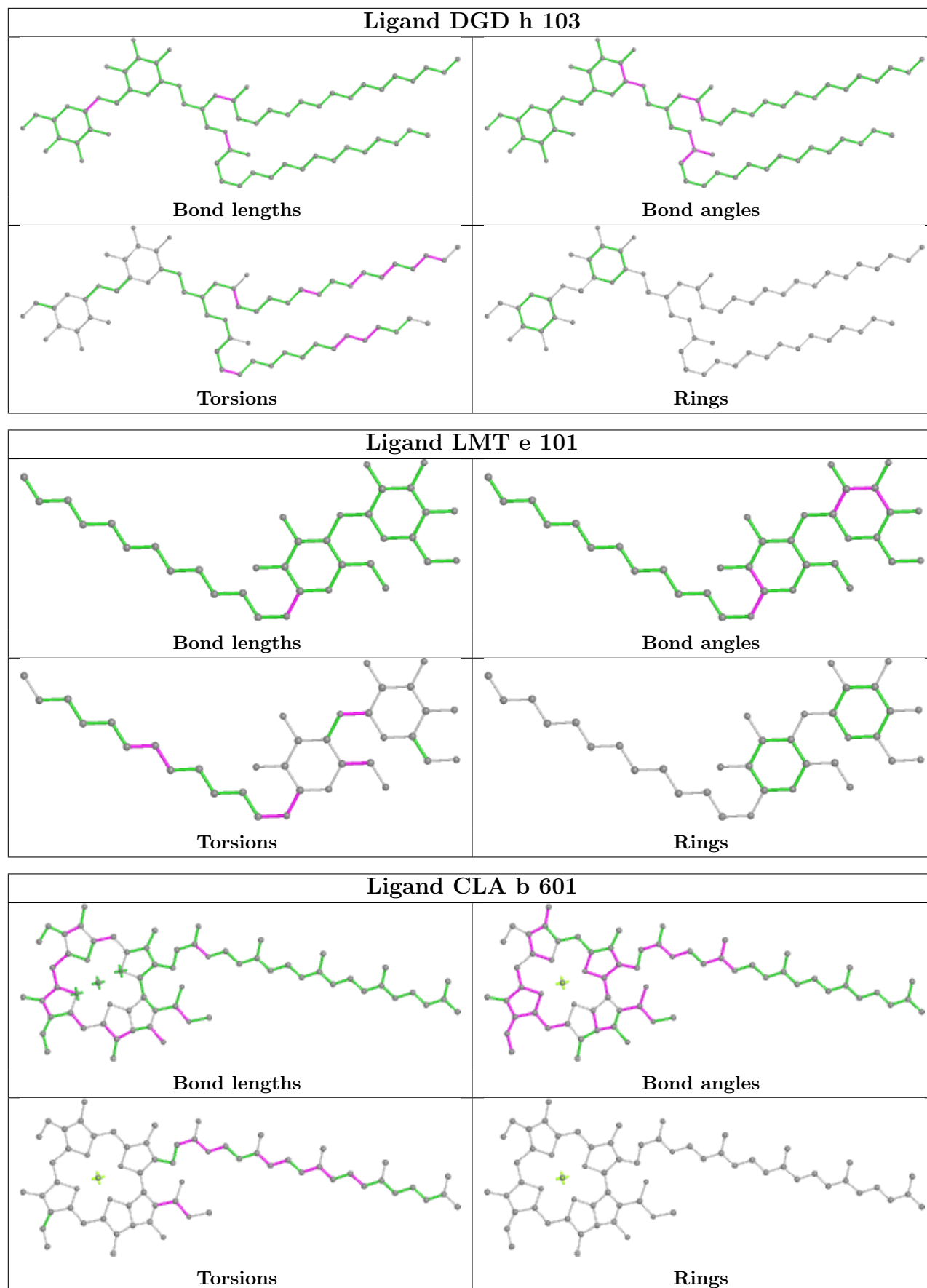
Ligand CLA c 511



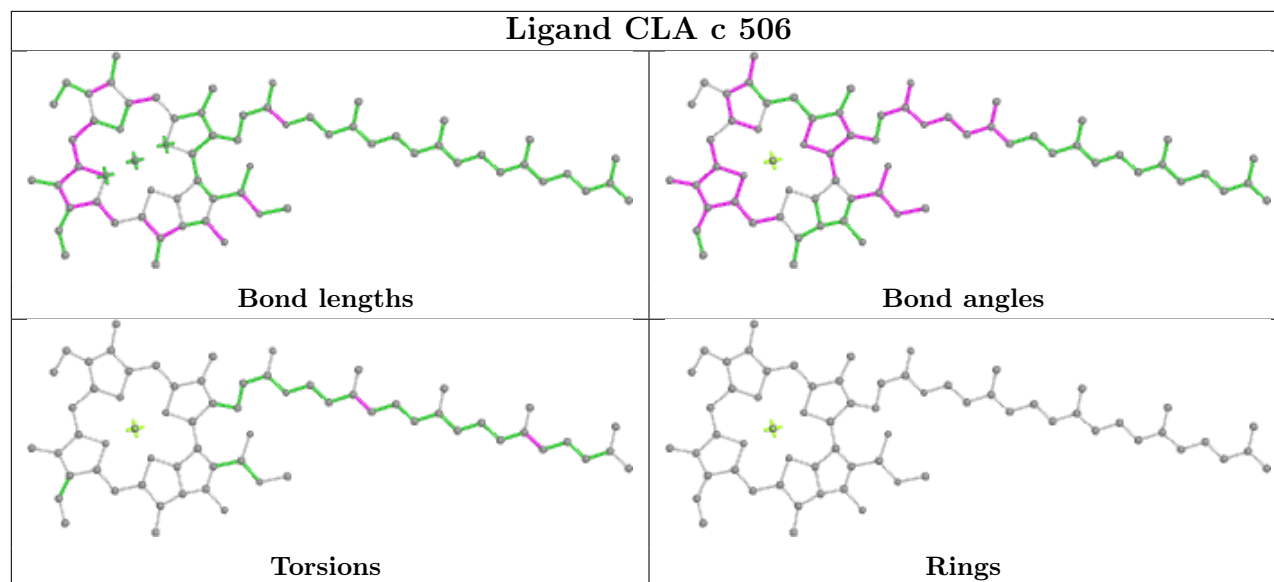
Ligand CLA D 404



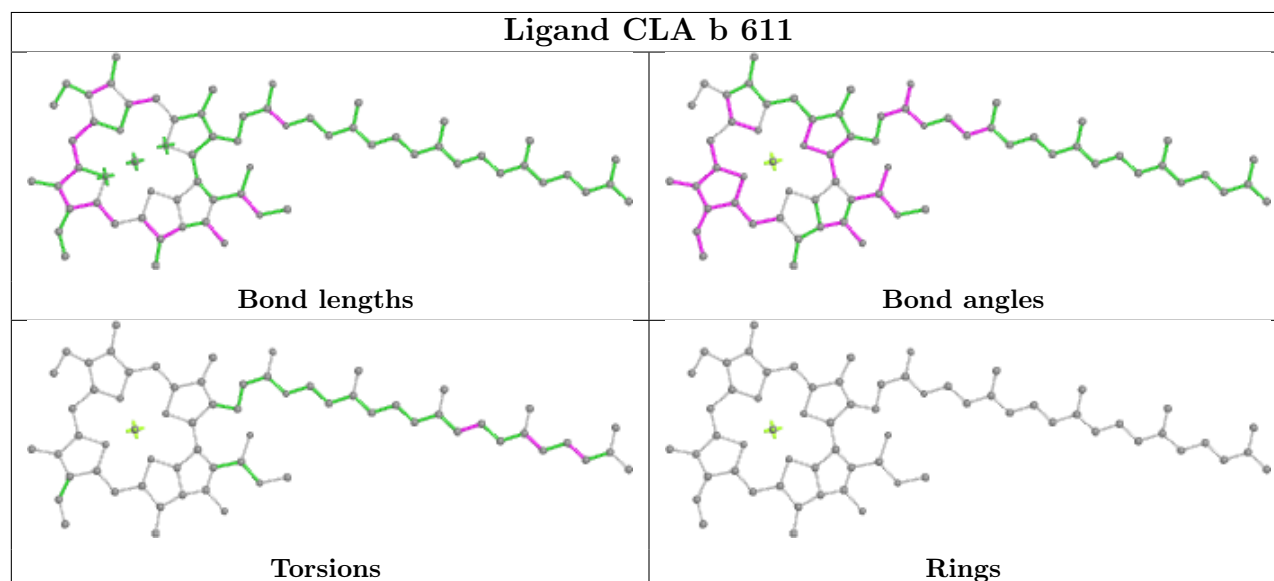




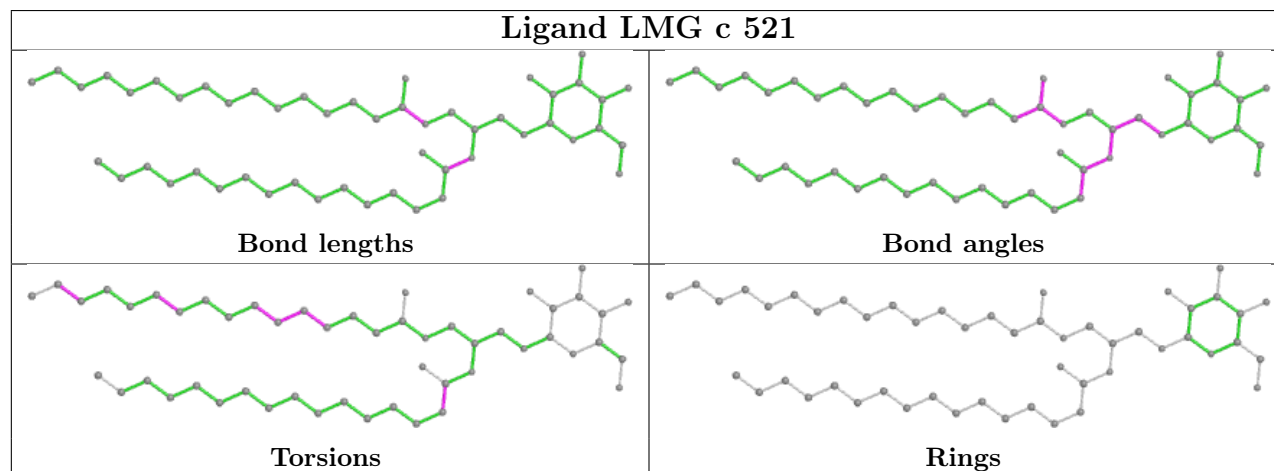
Ligand CLA c 506

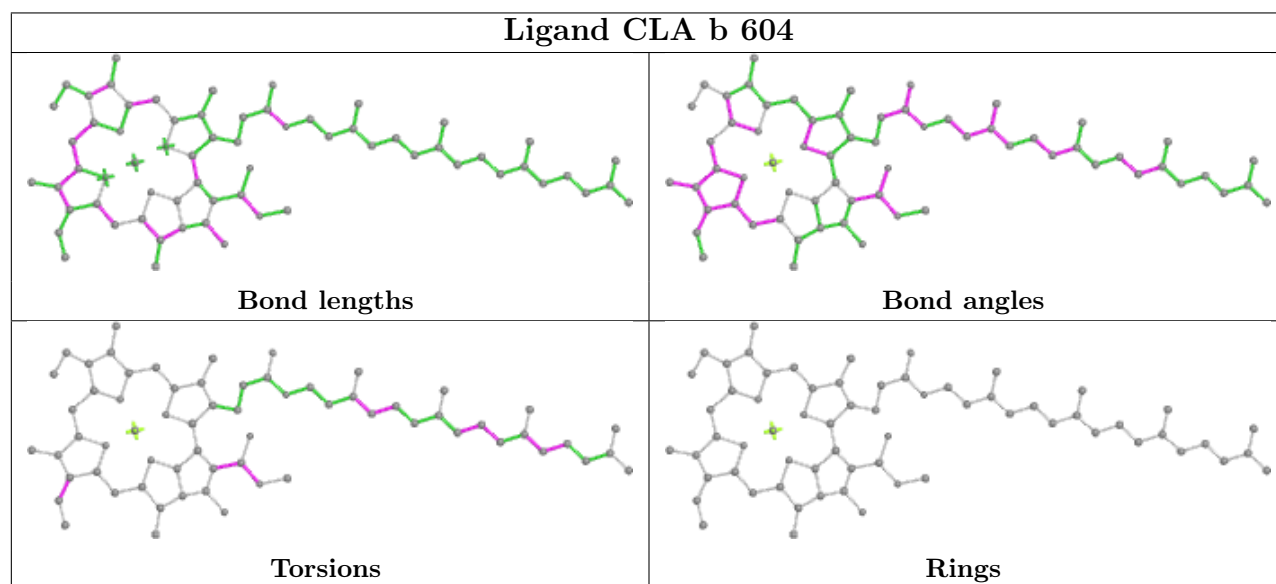
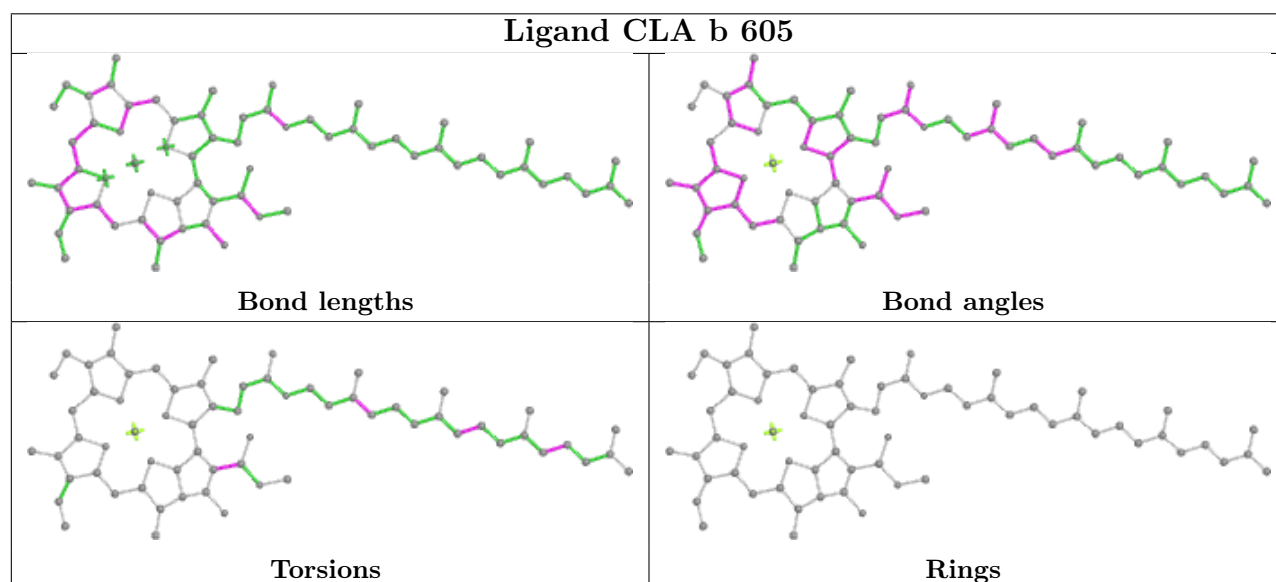
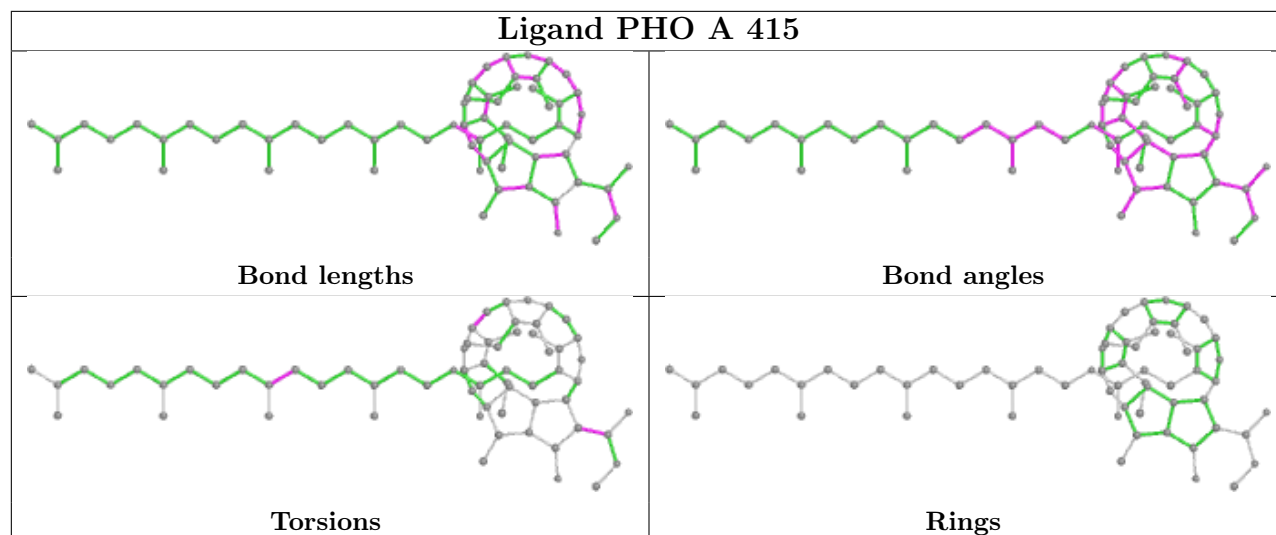


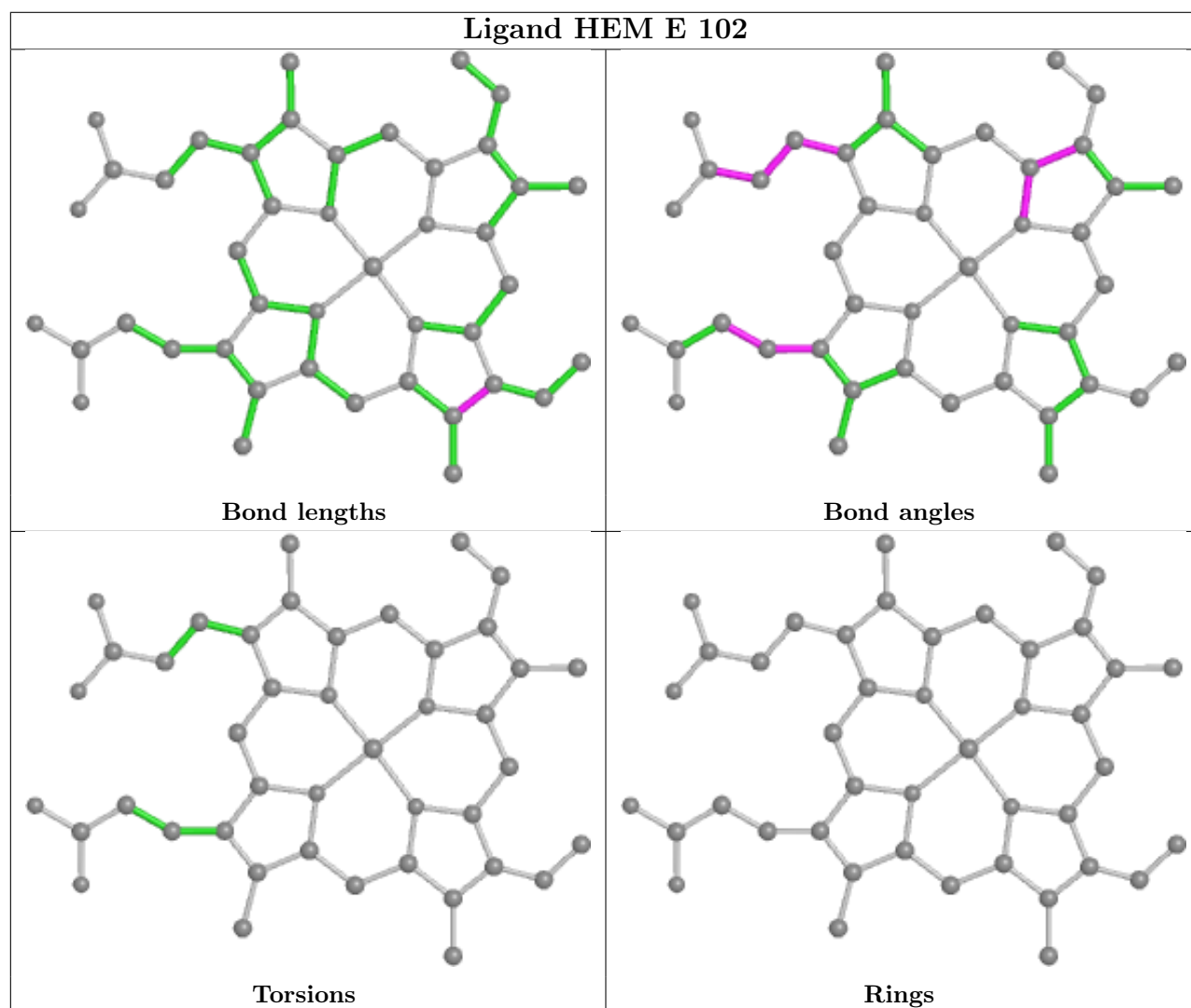
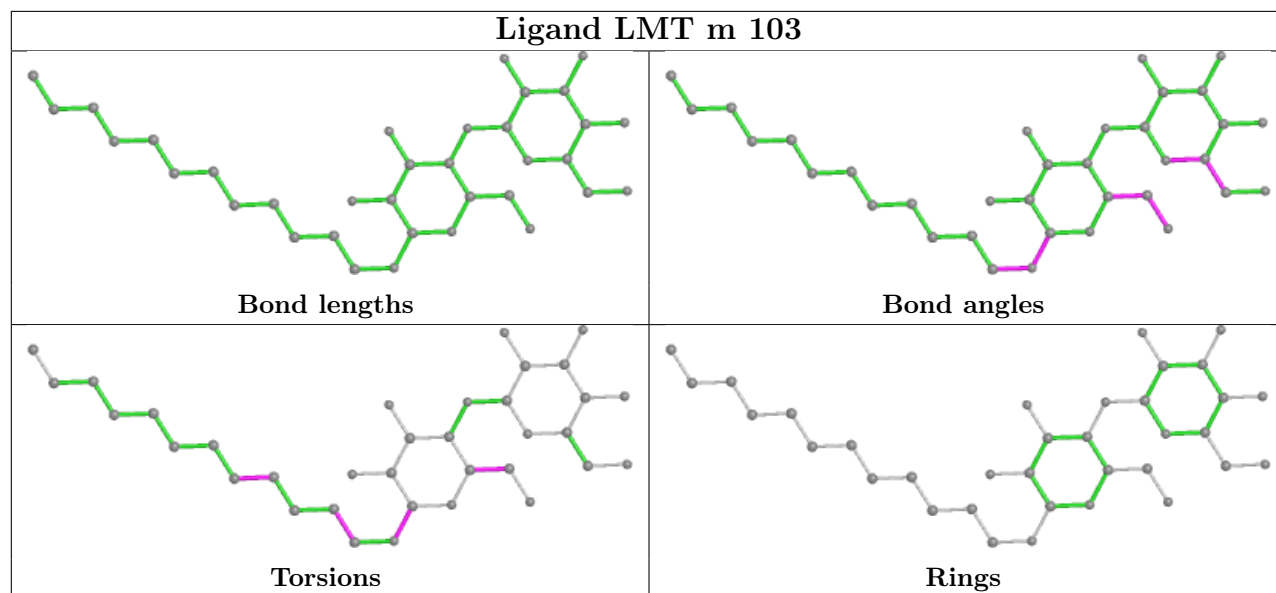
Ligand CLA b 611

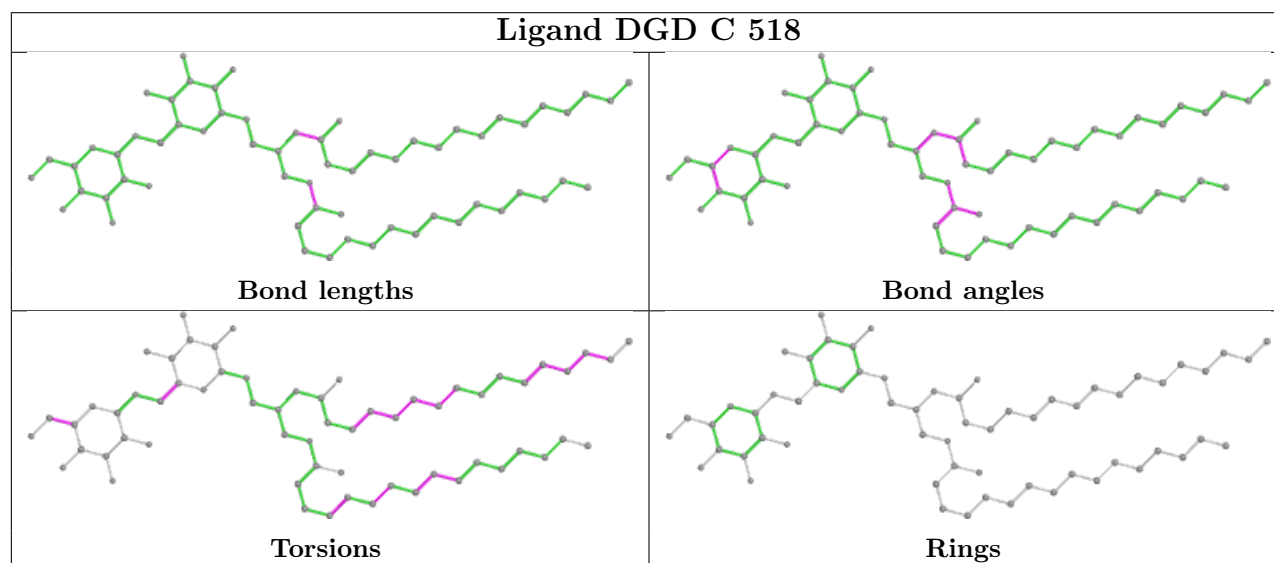
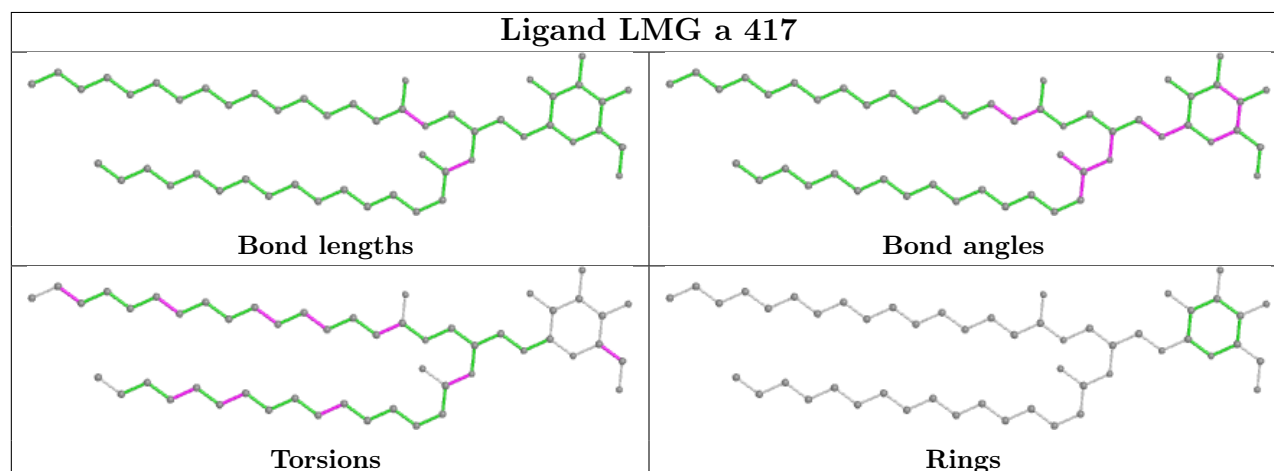
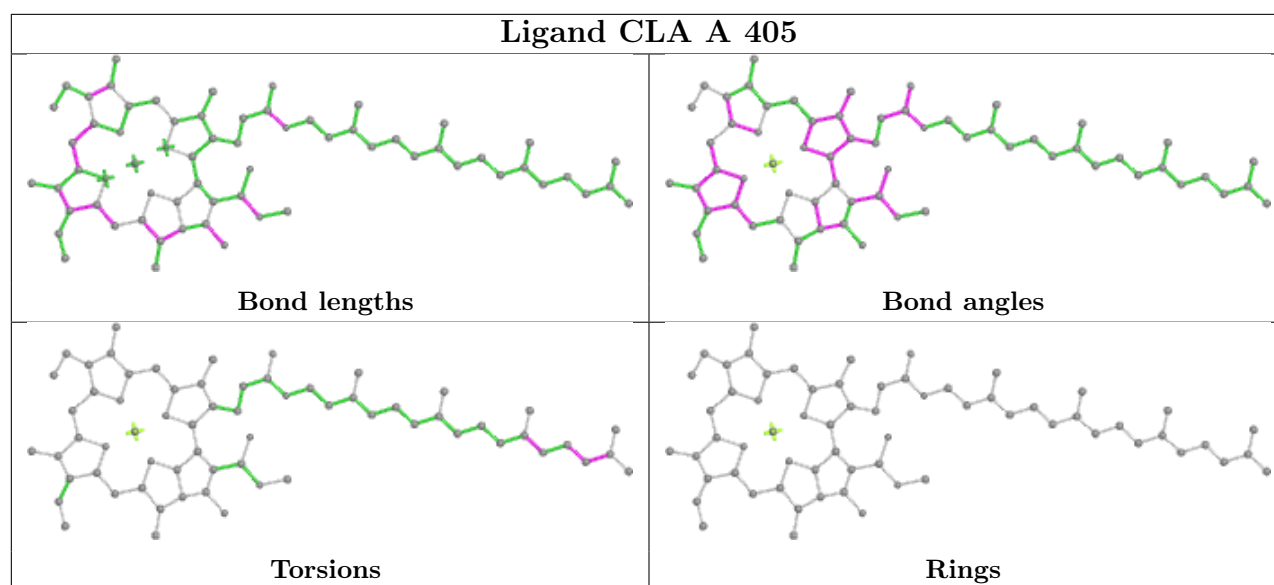


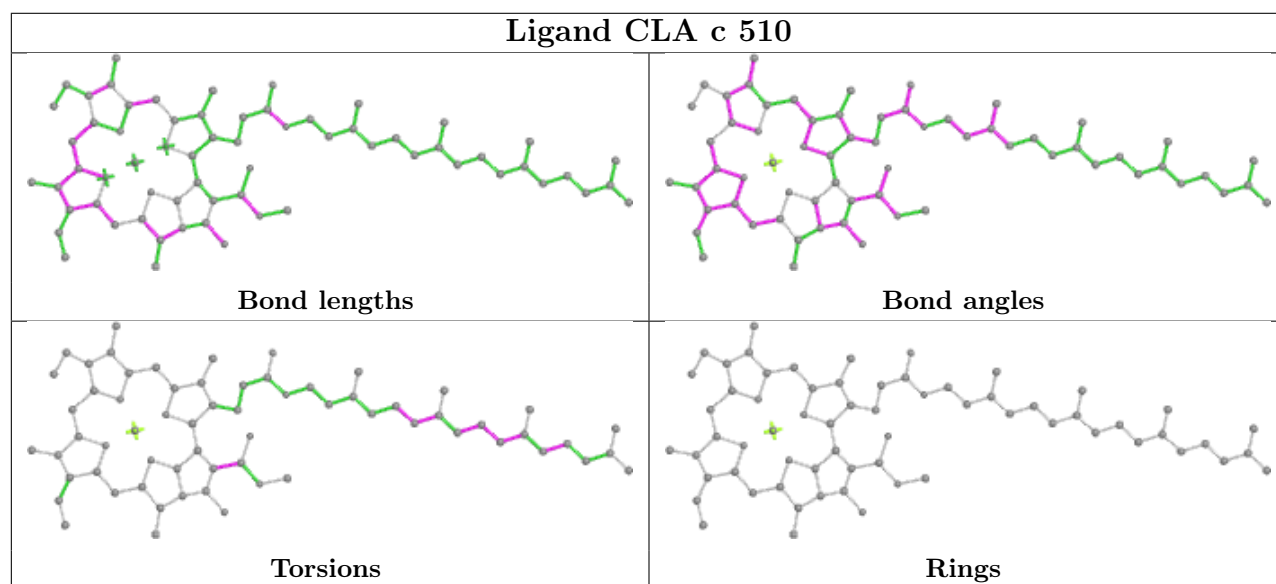
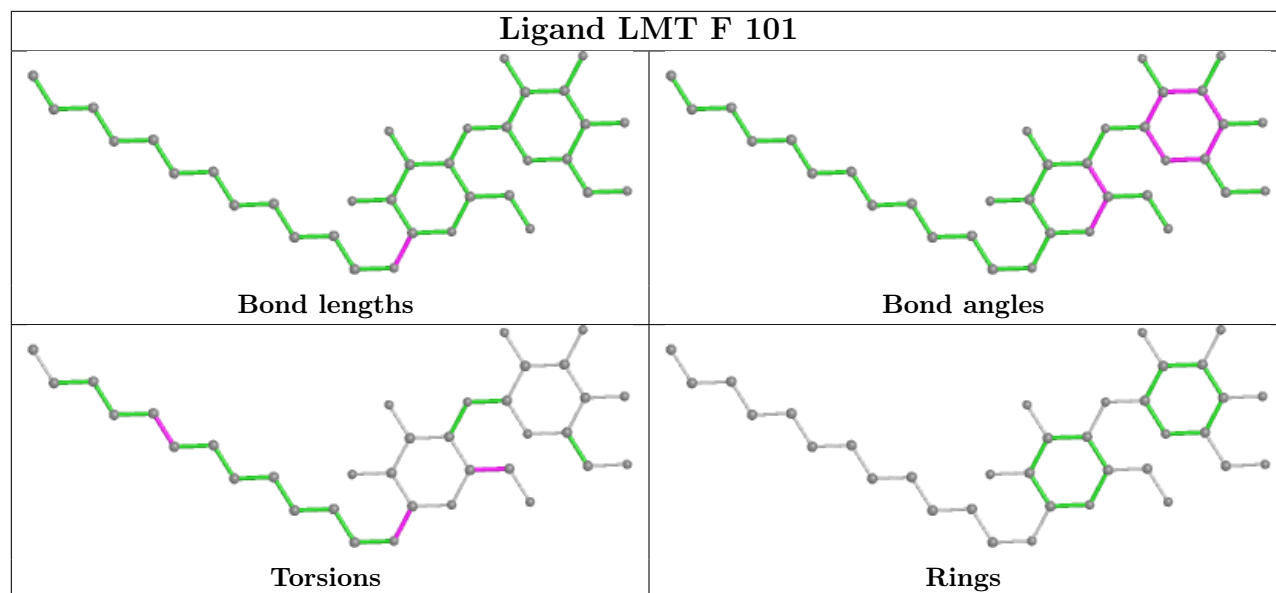
Ligand LMG c 521

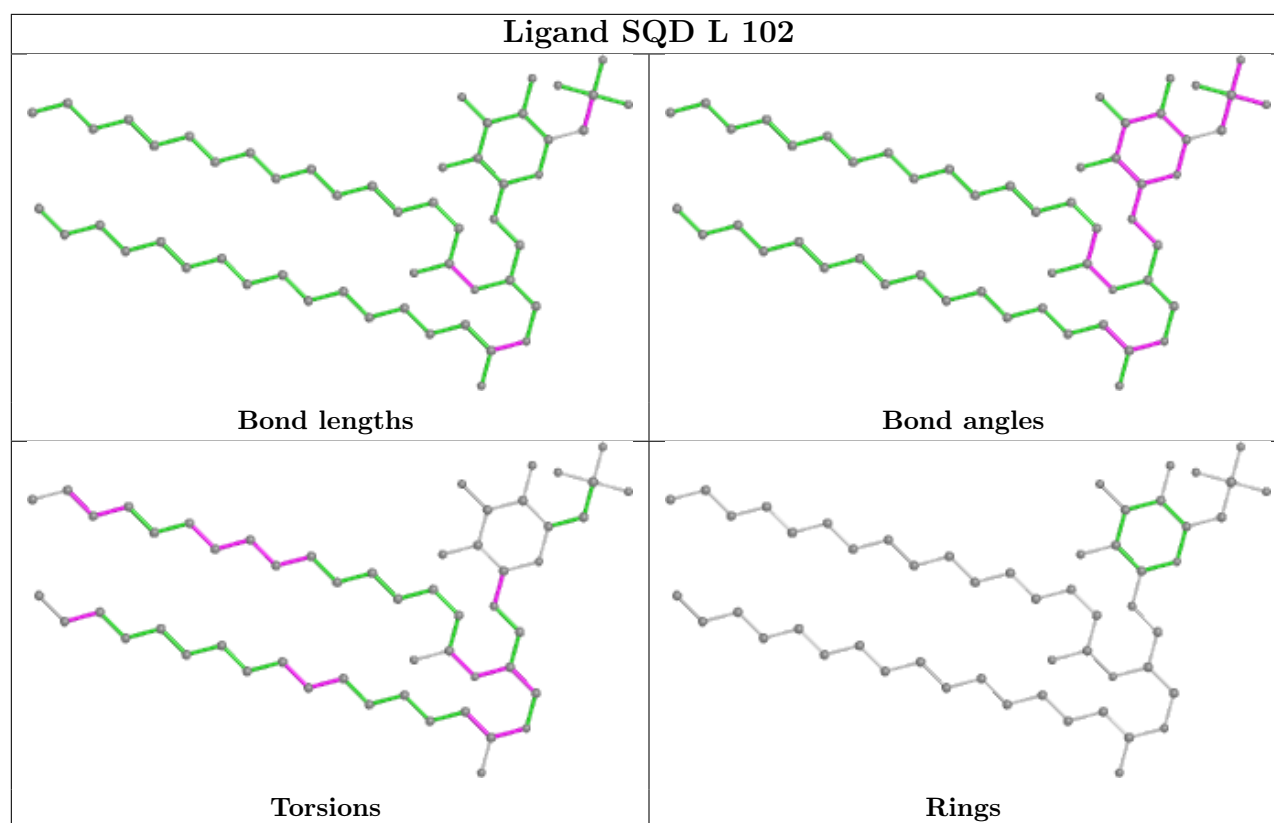




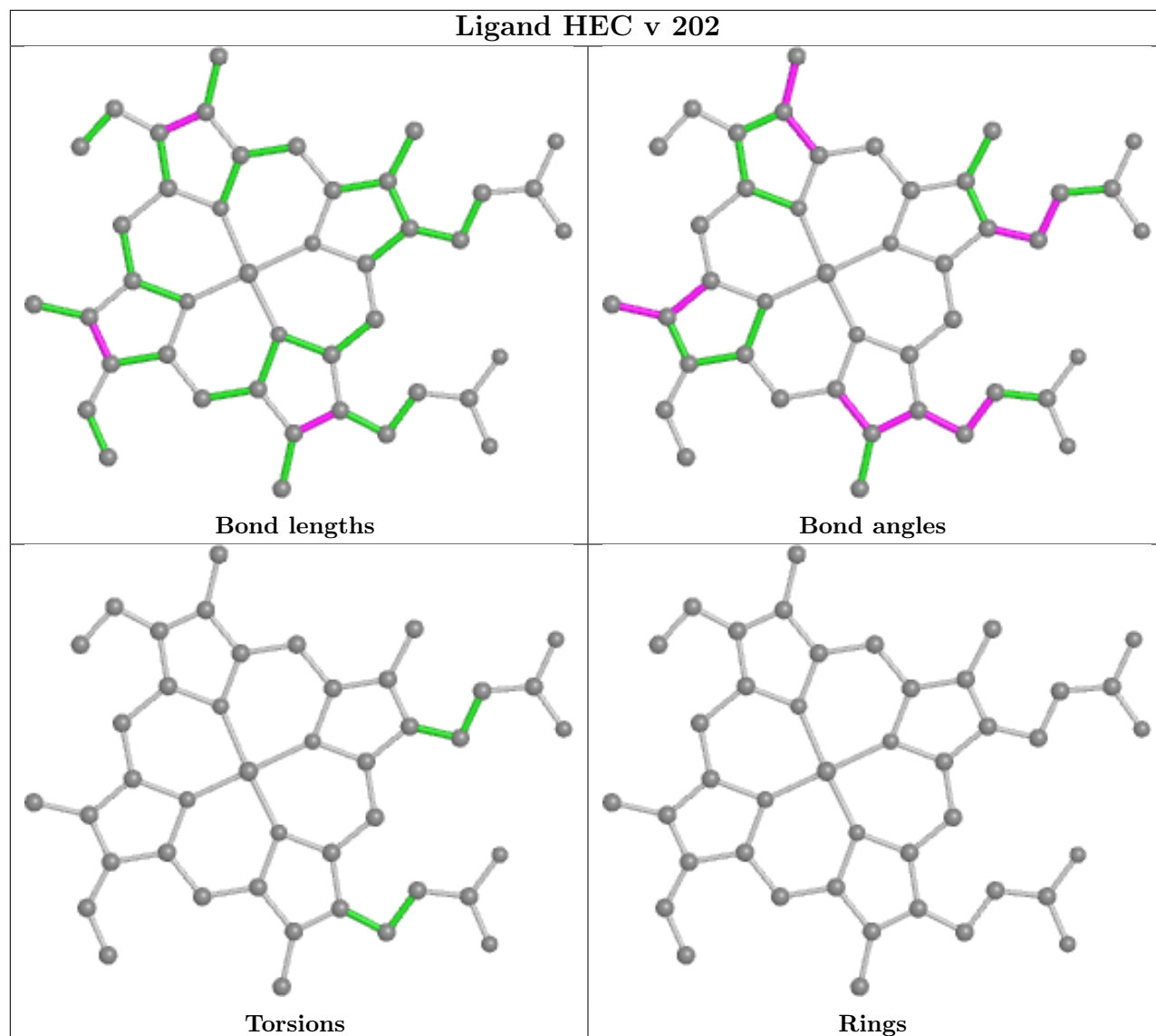


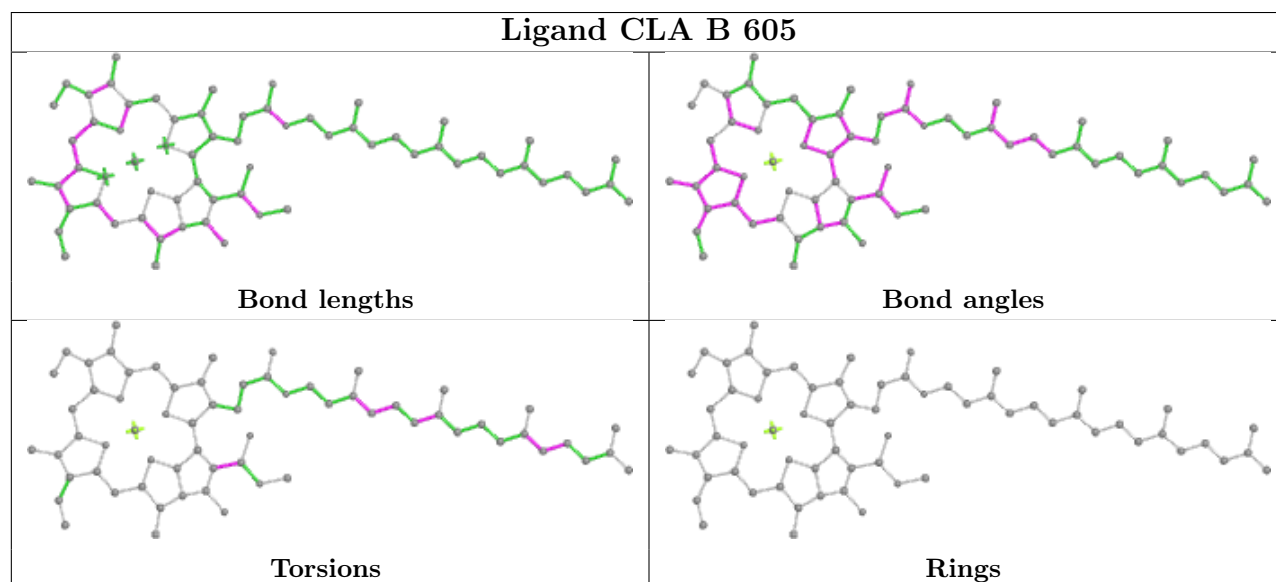
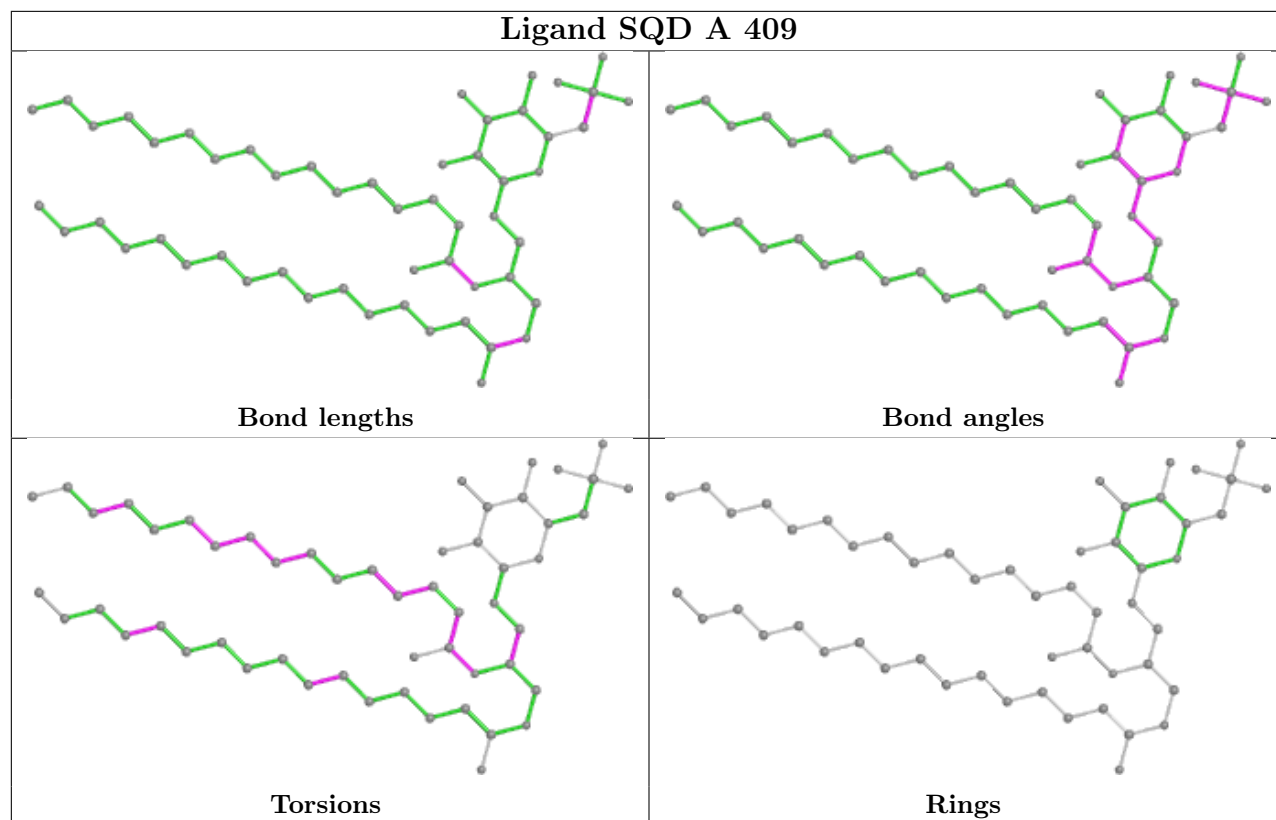




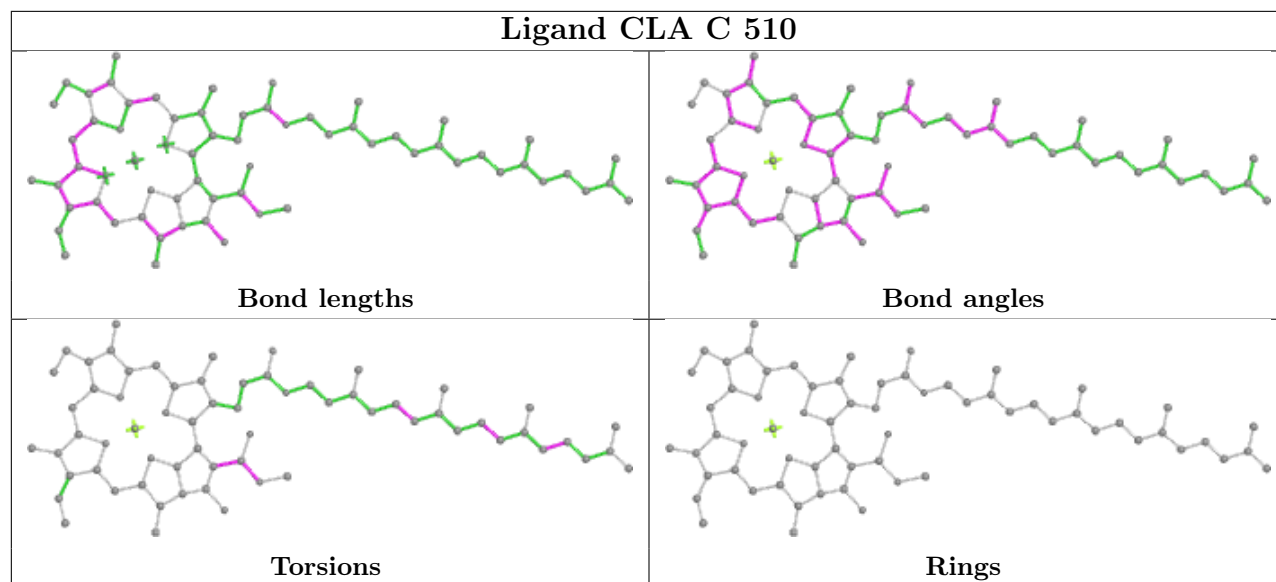


Ligand HEC v 202

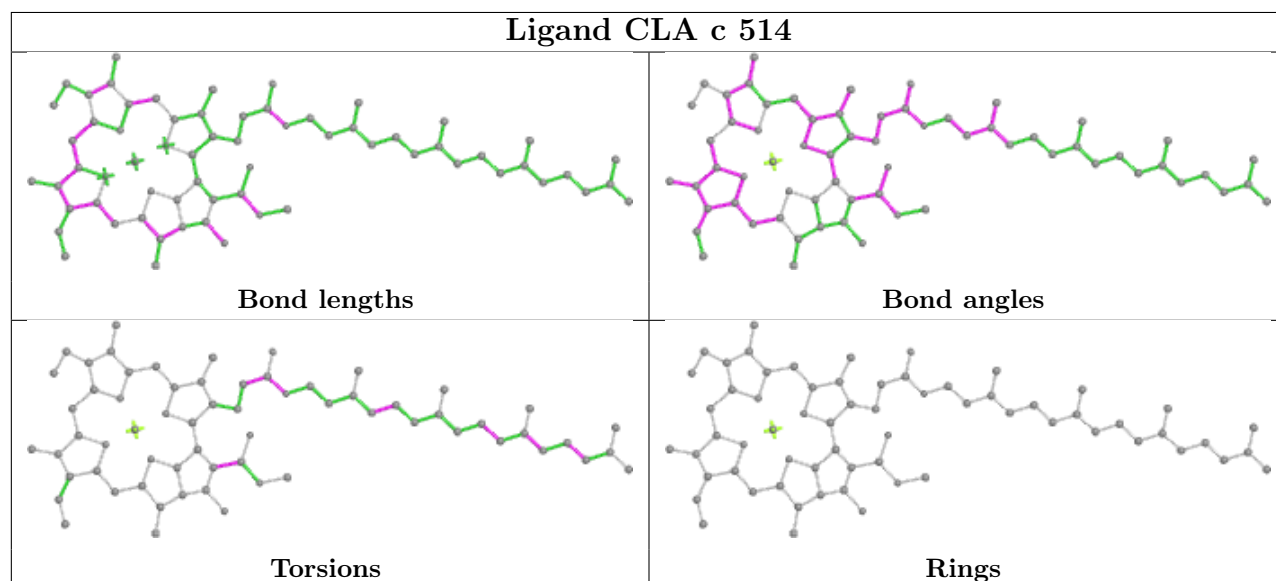




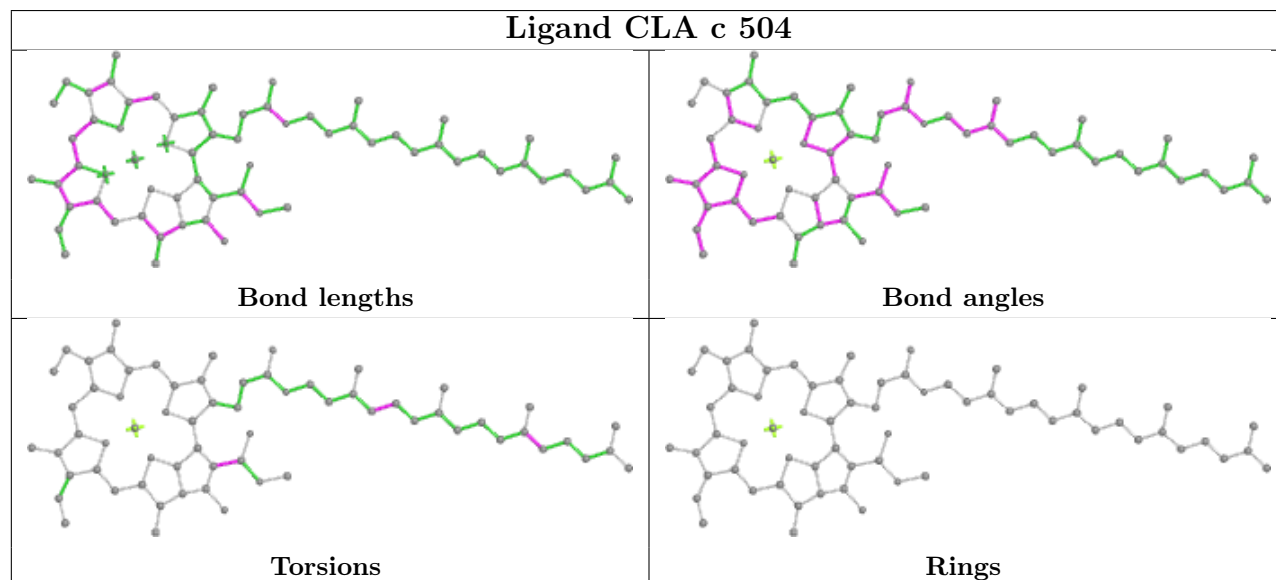
Ligand CLA C 510

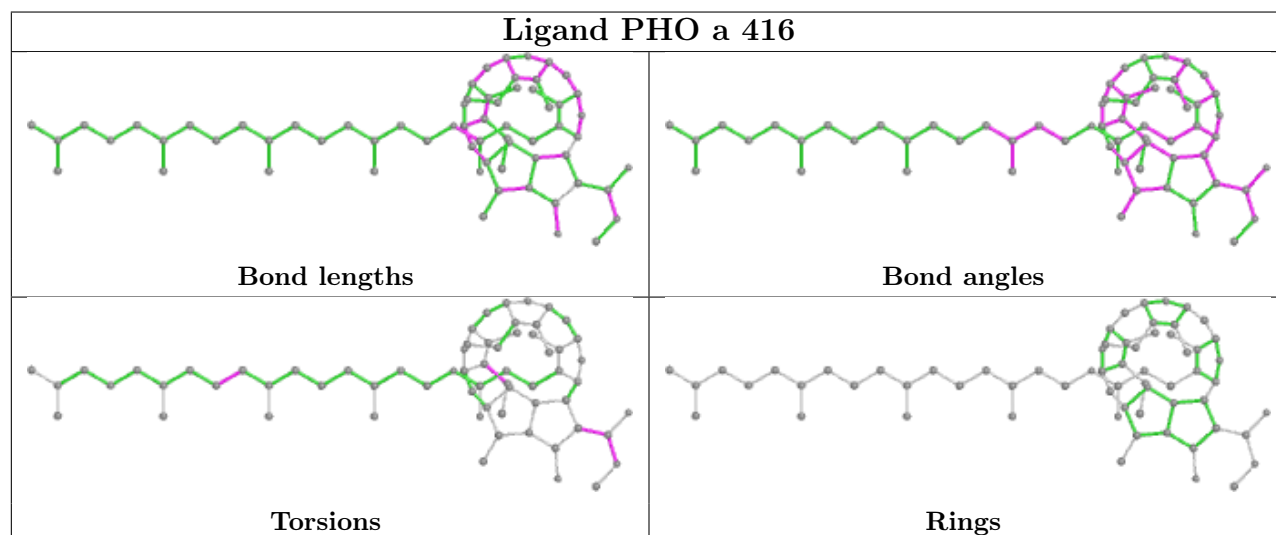
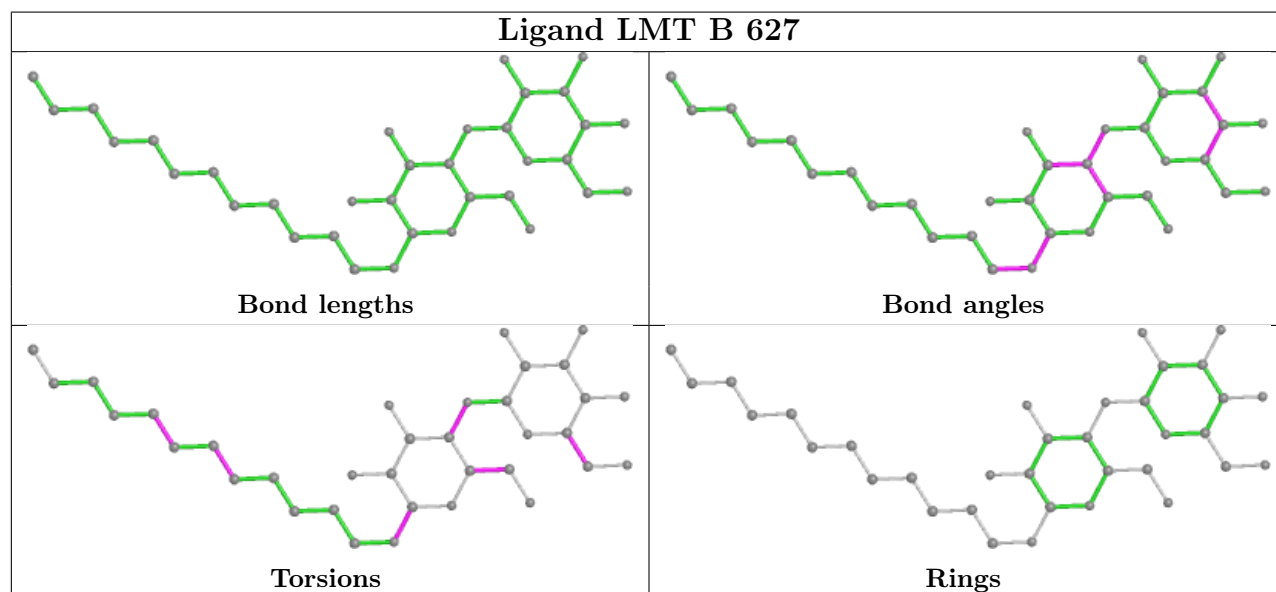
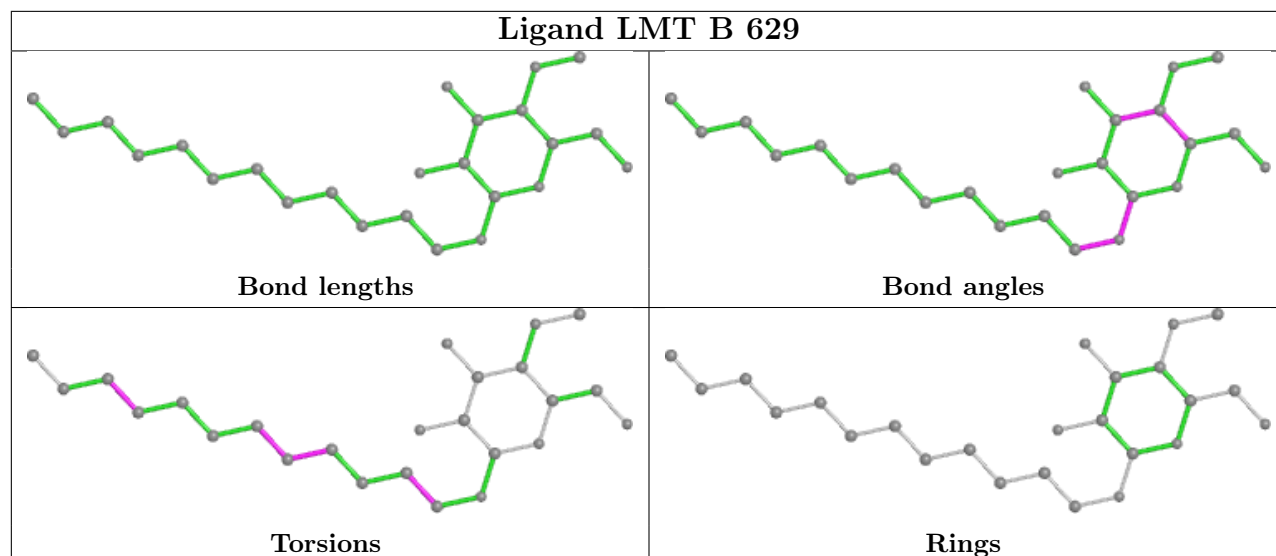


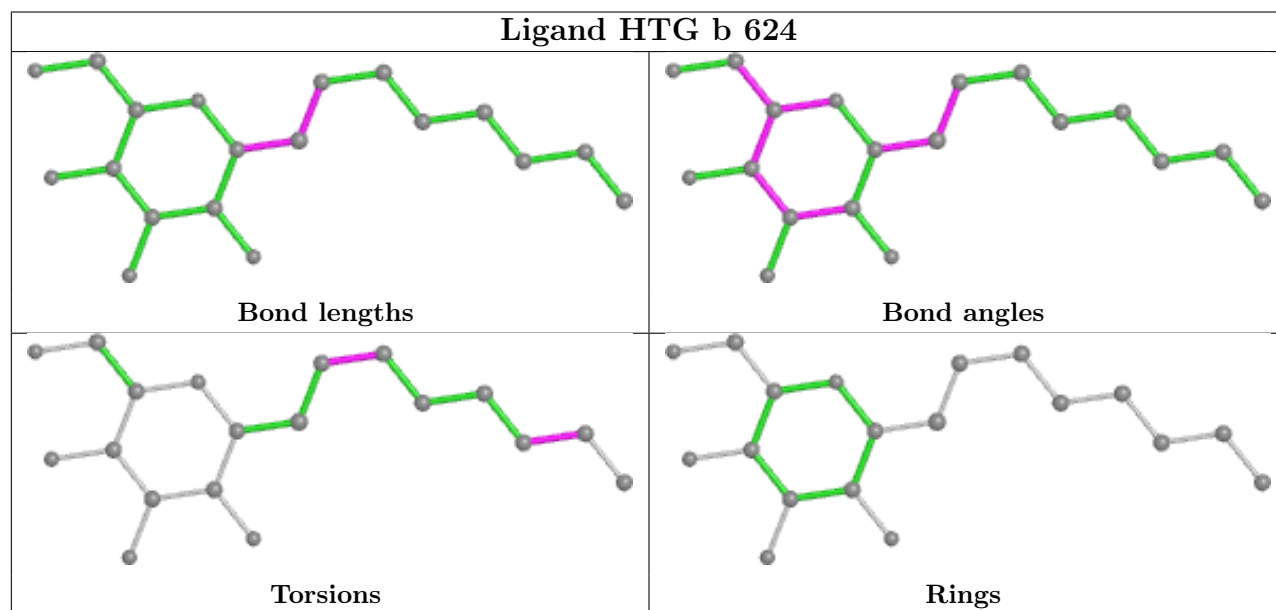
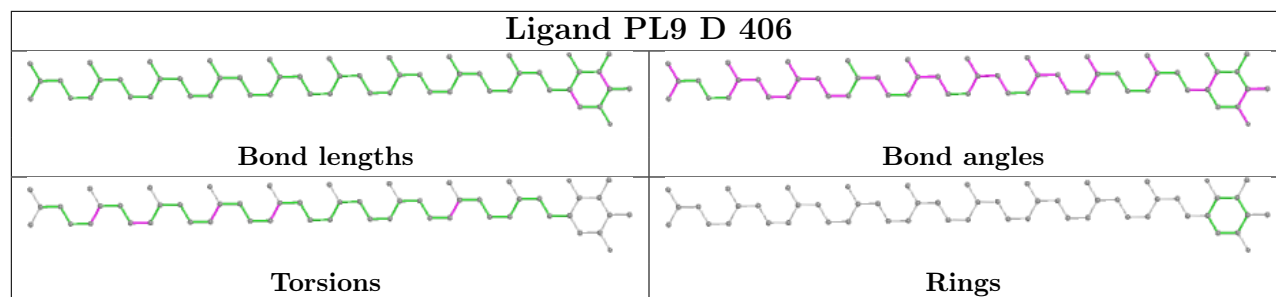
Ligand CLA c 514



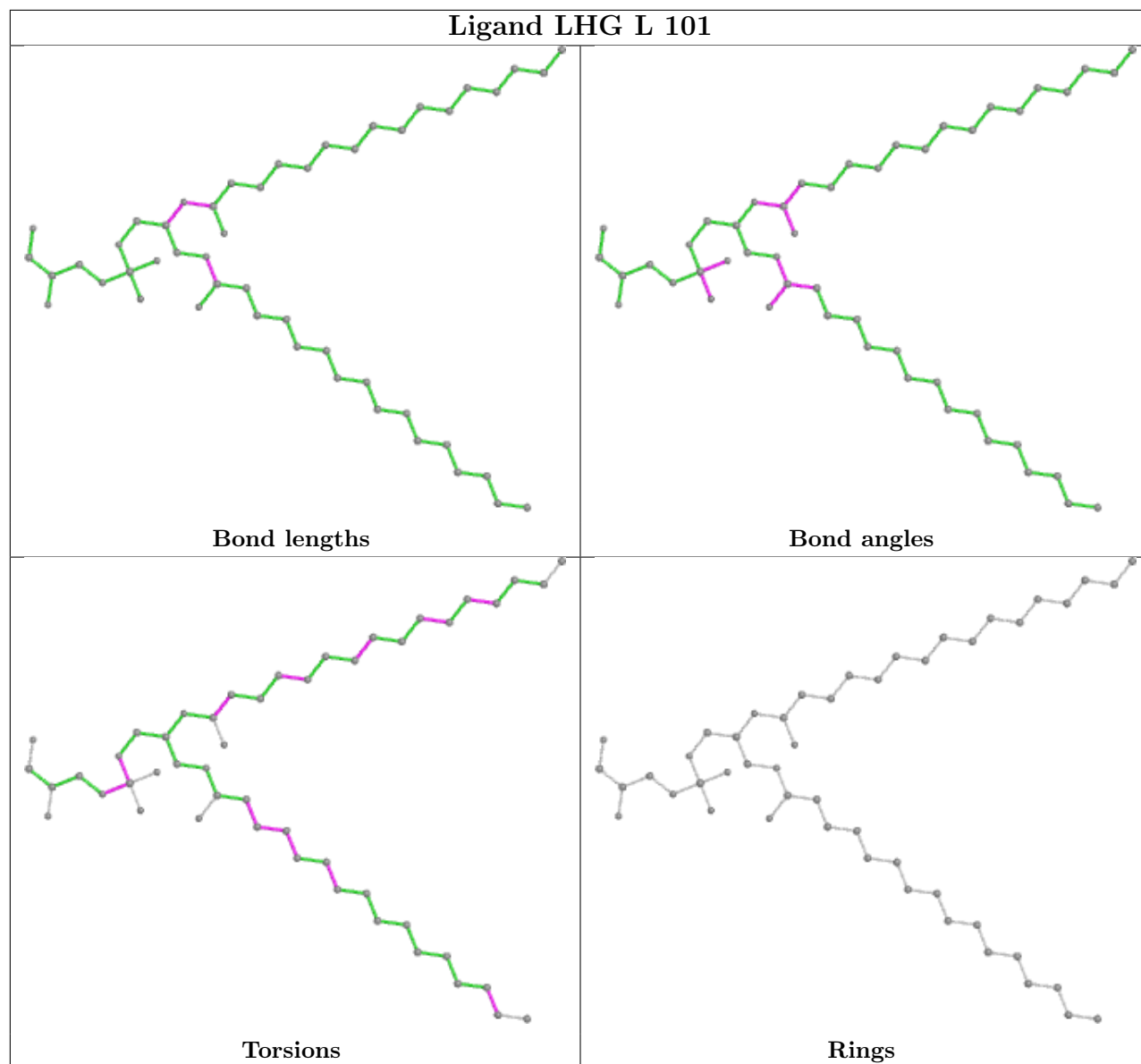
Ligand CLA c 504



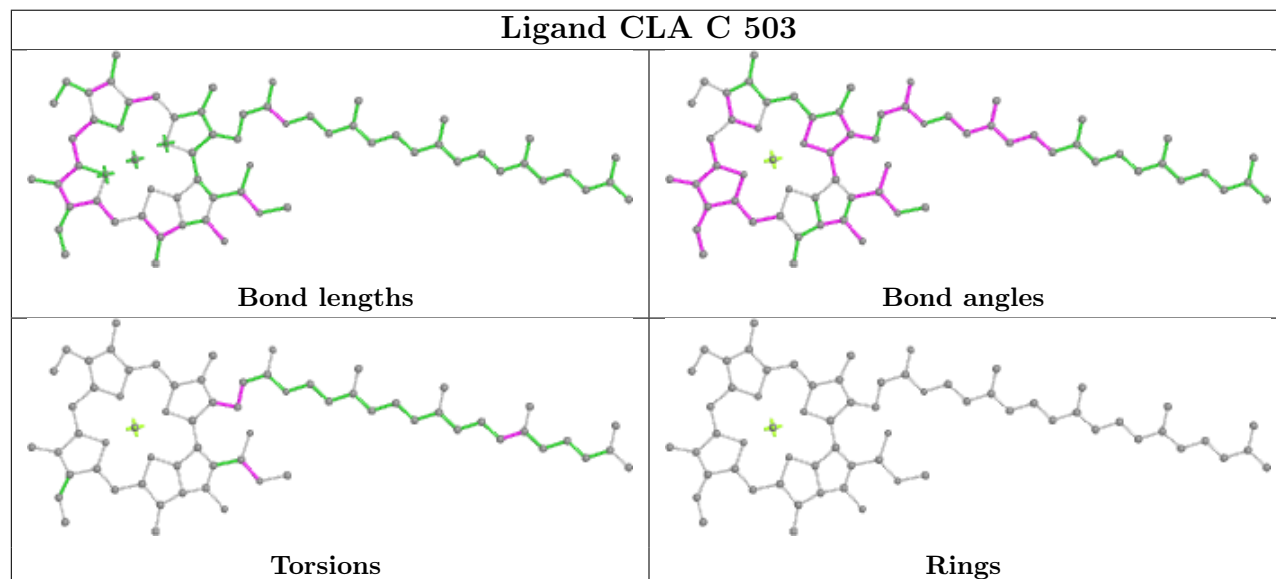


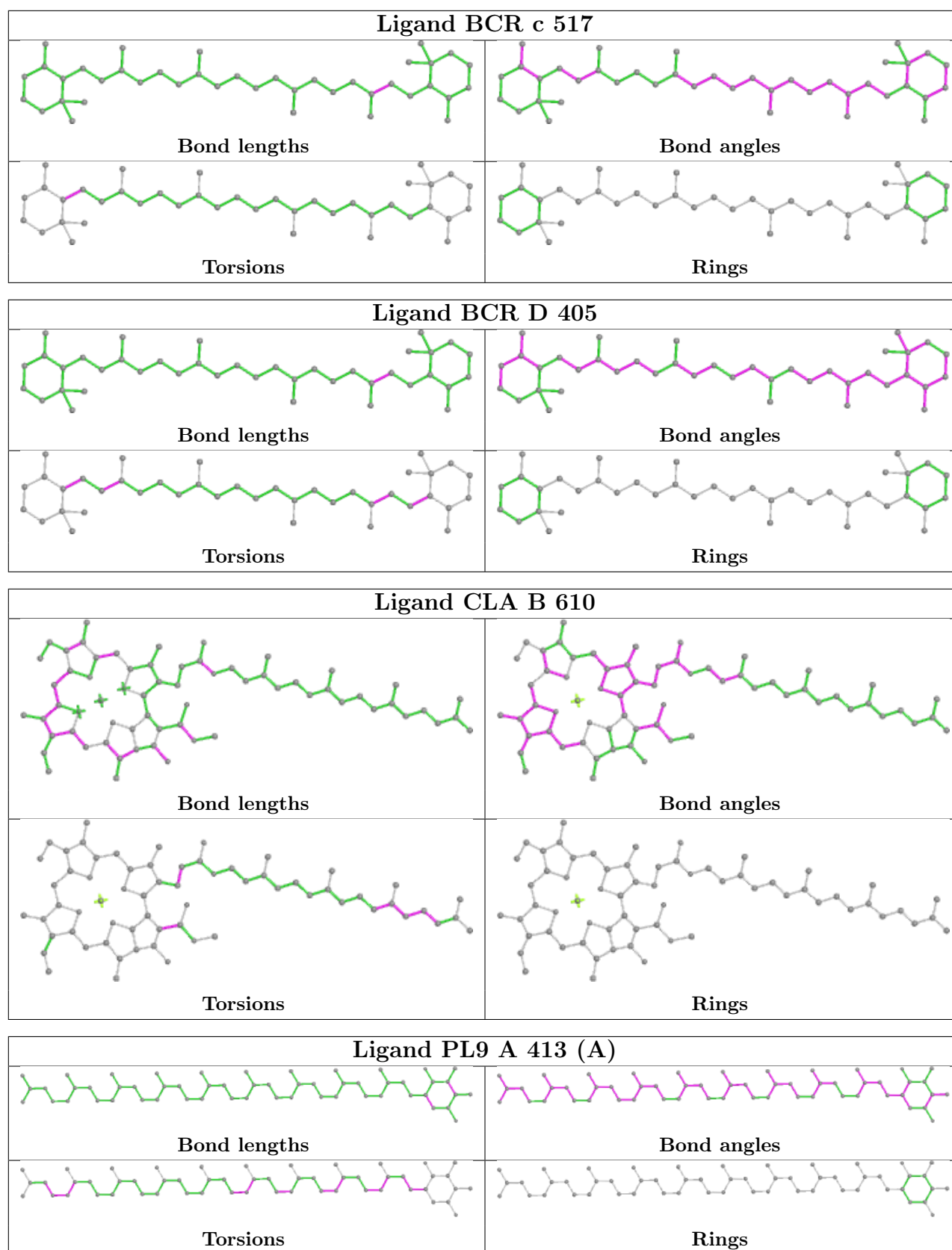


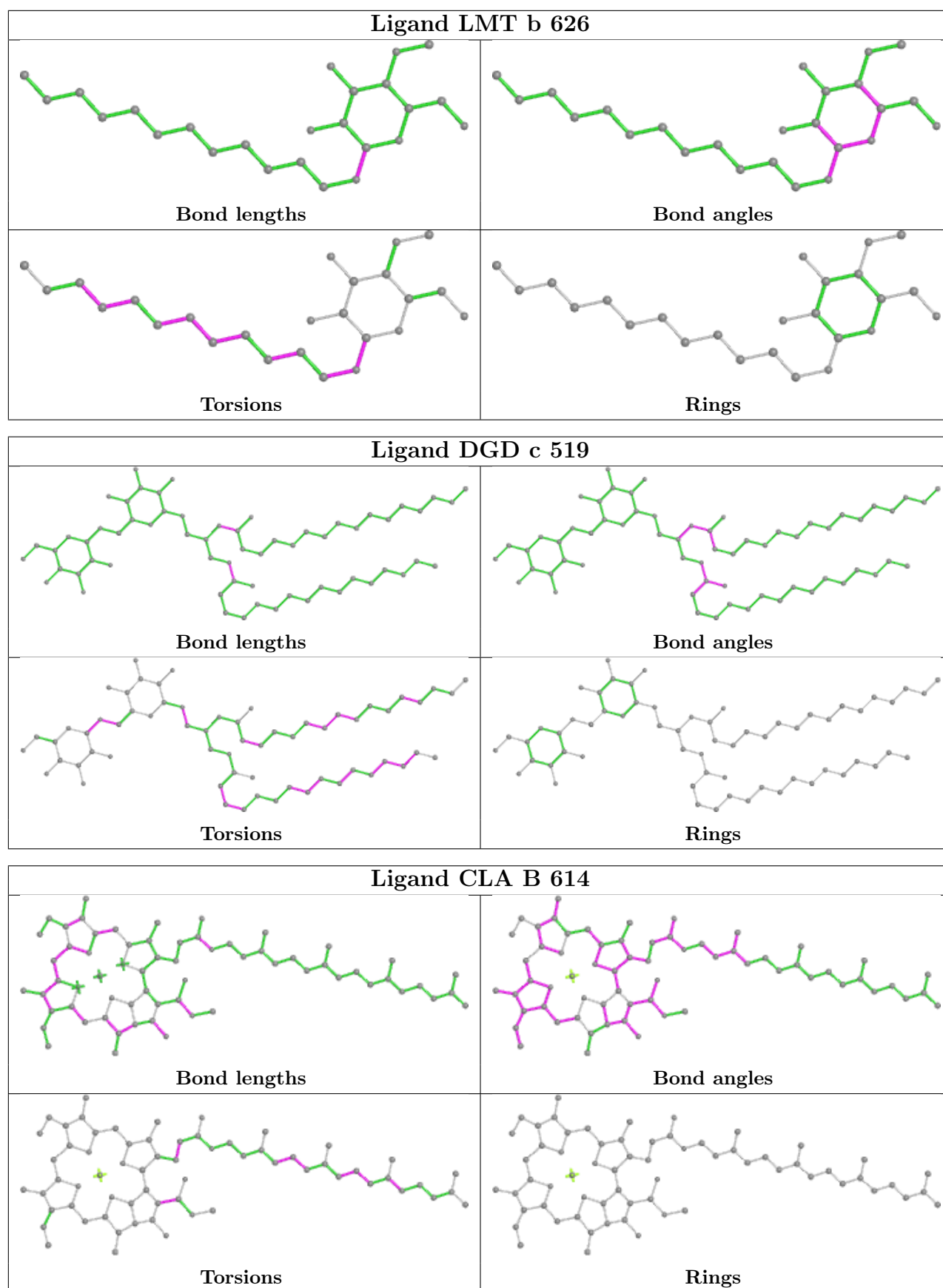
Ligand LHG L 101

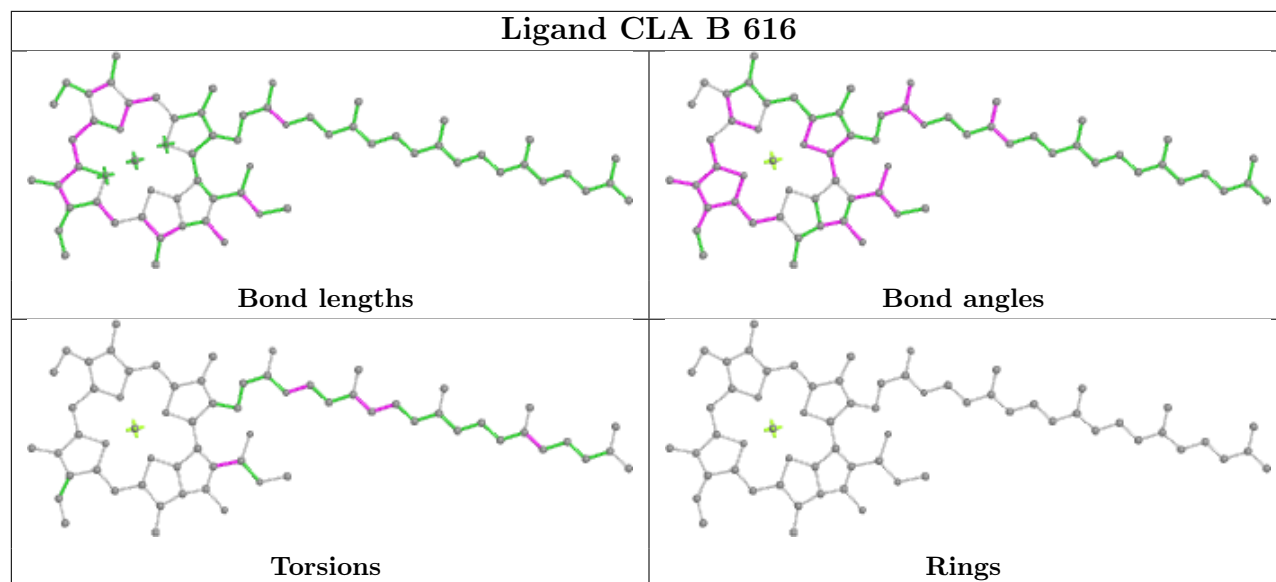
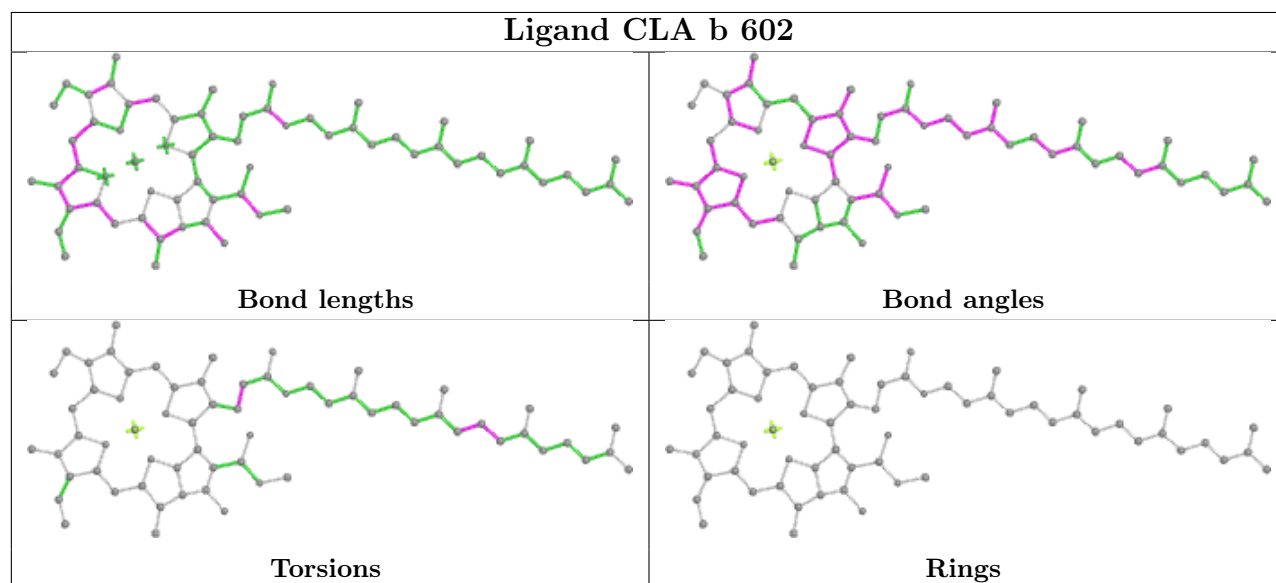


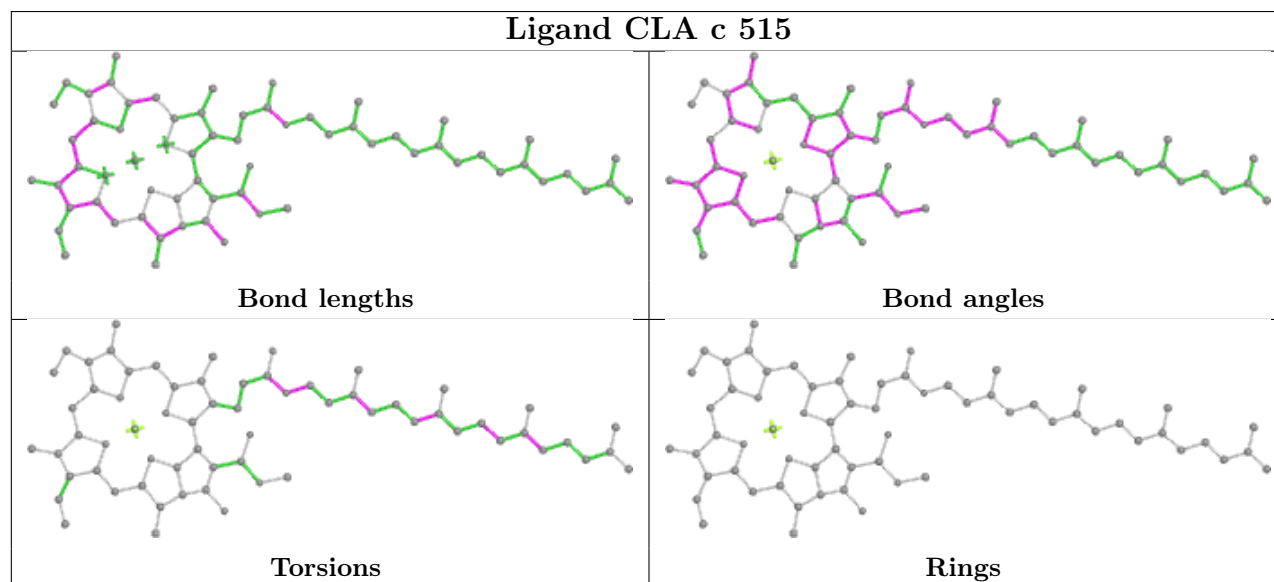
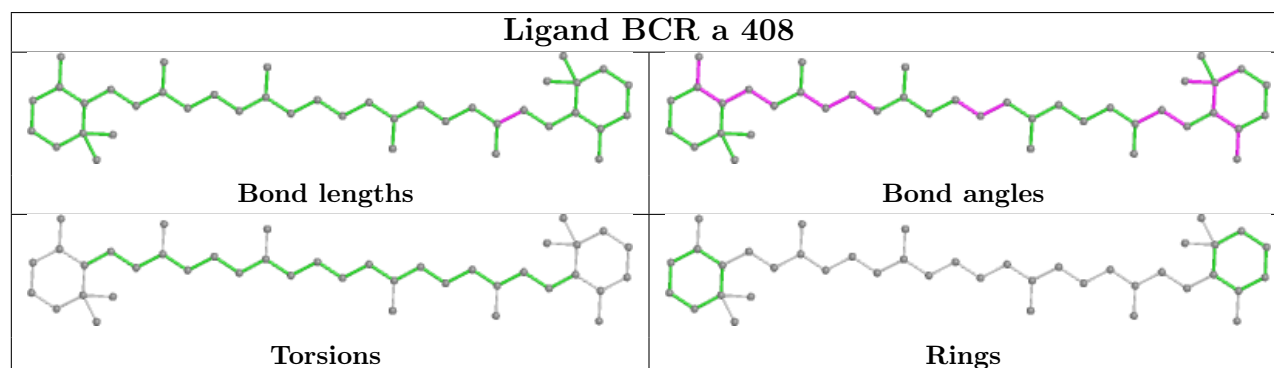
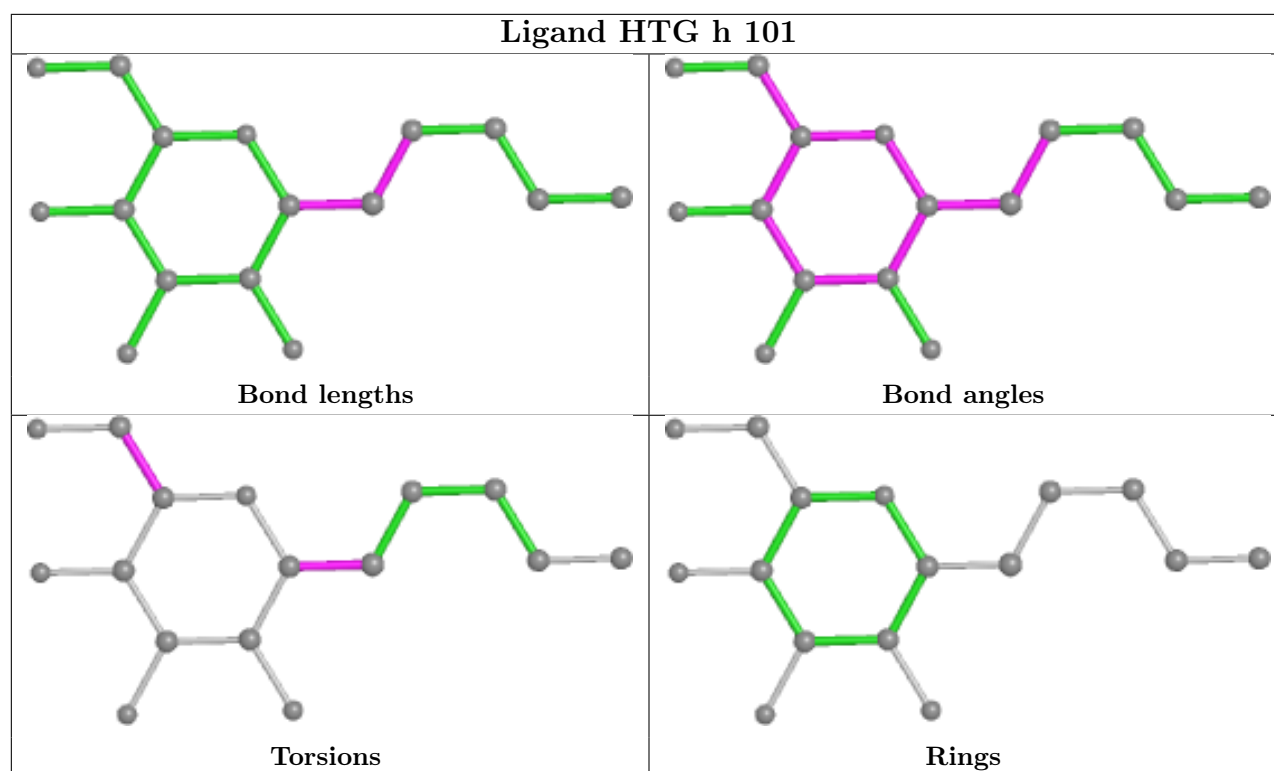
Ligand CLA C 503

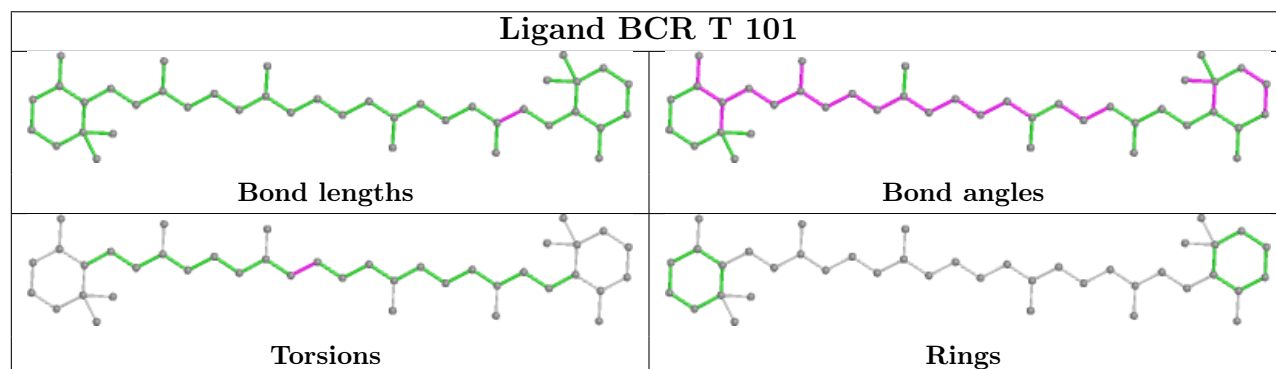
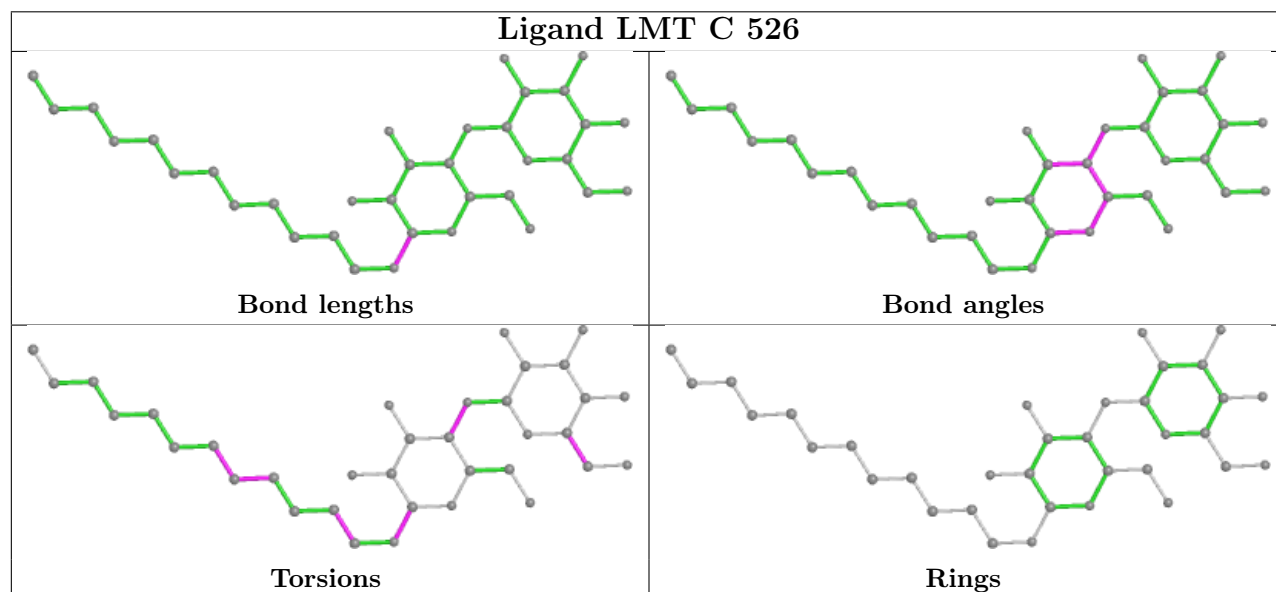
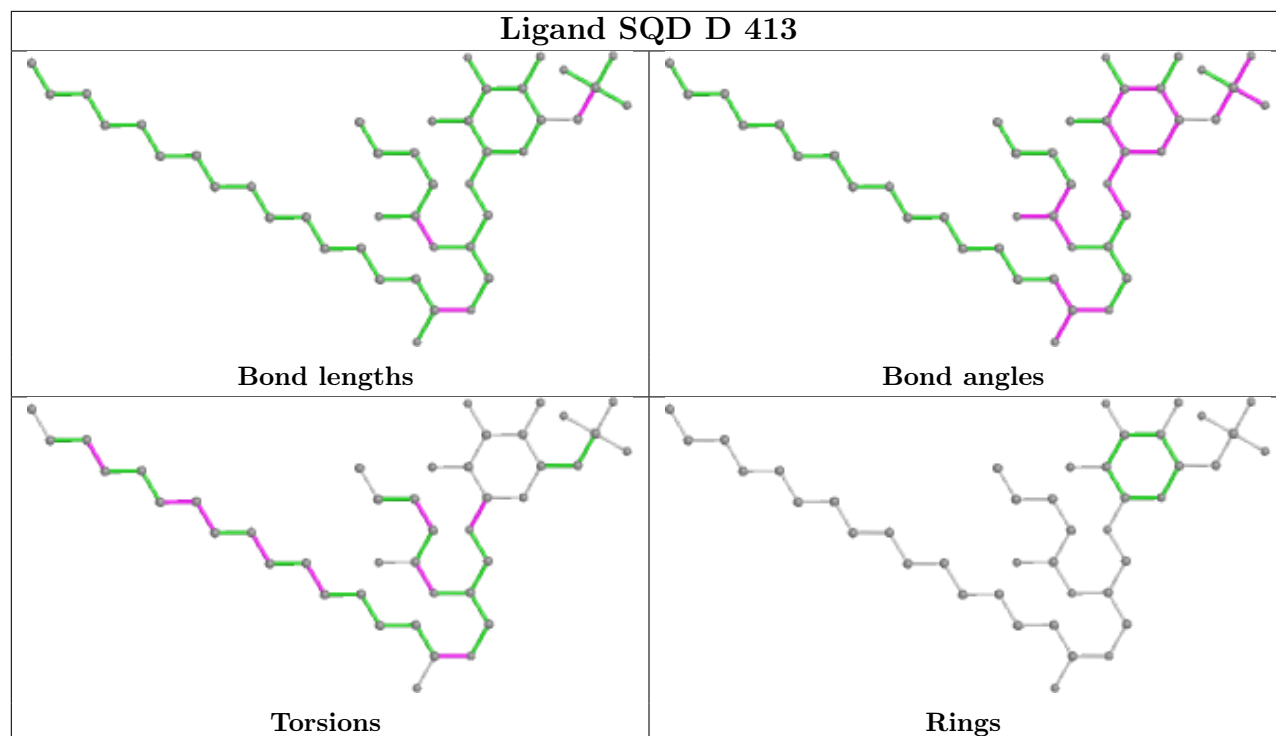


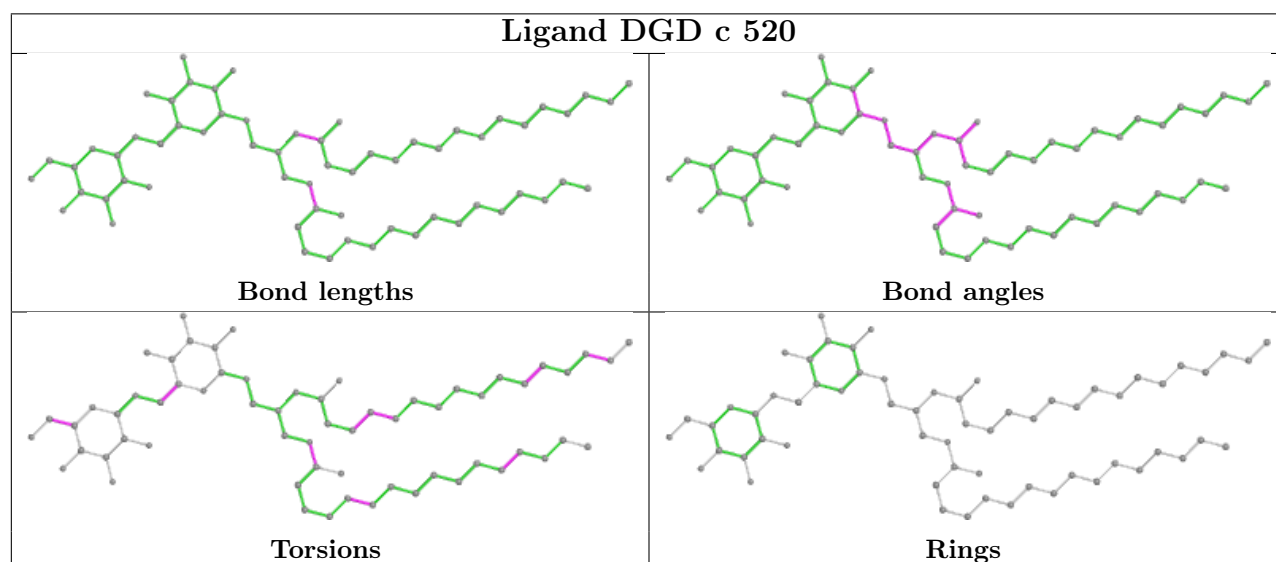
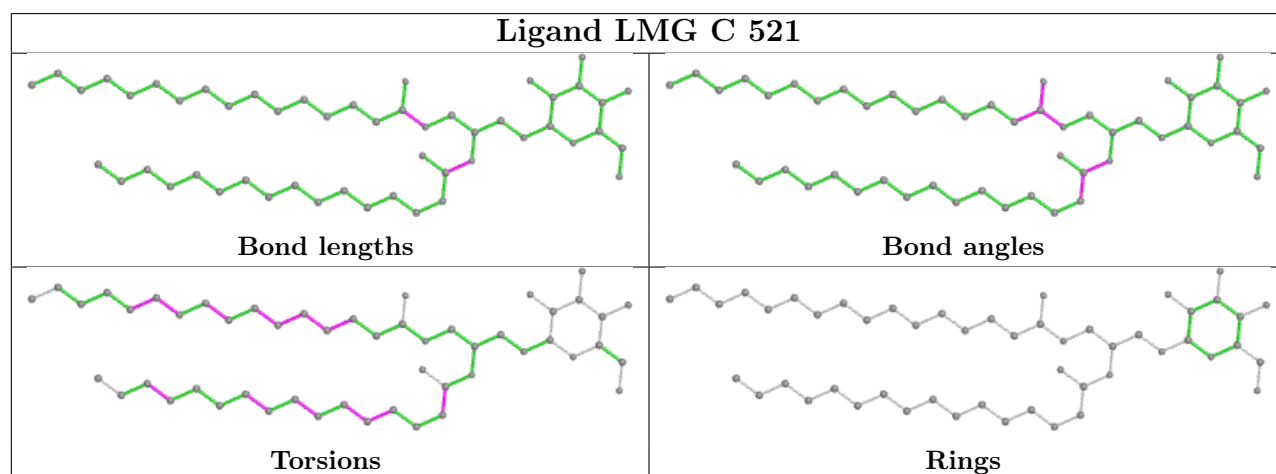
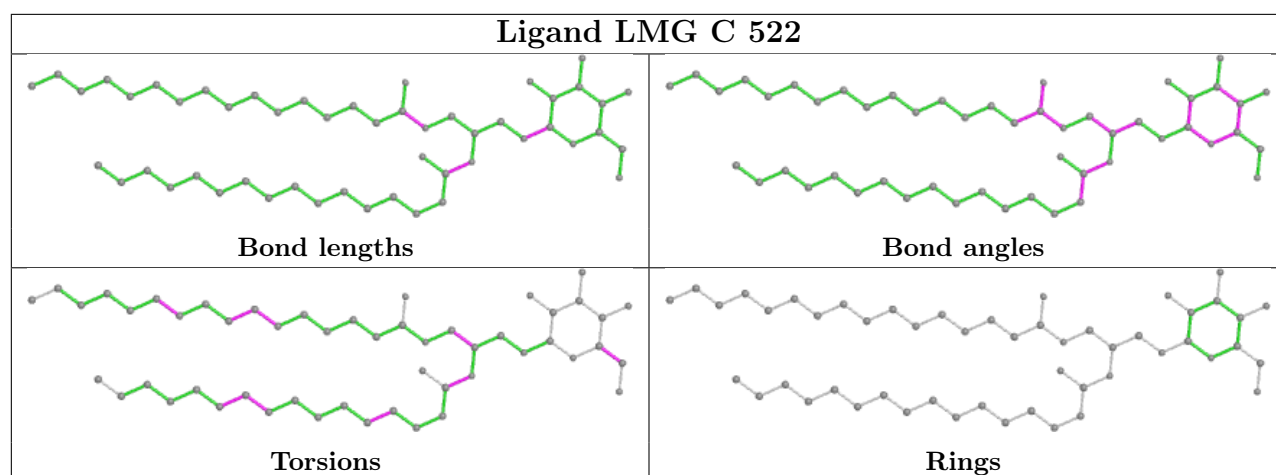




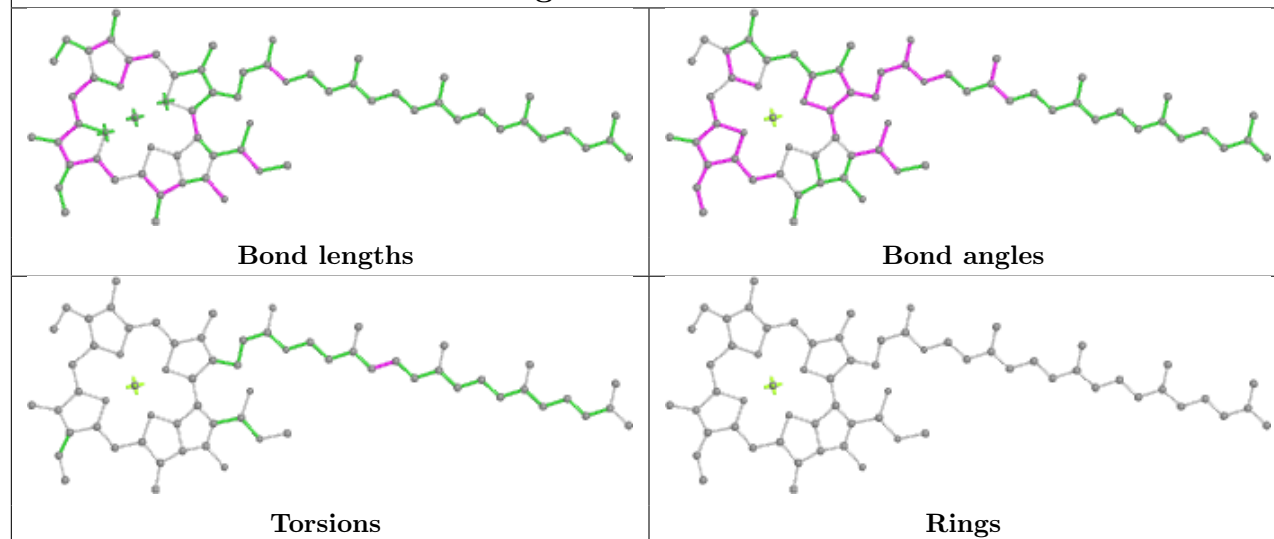
Ligand CLA B 616**Ligand CLA b 602**



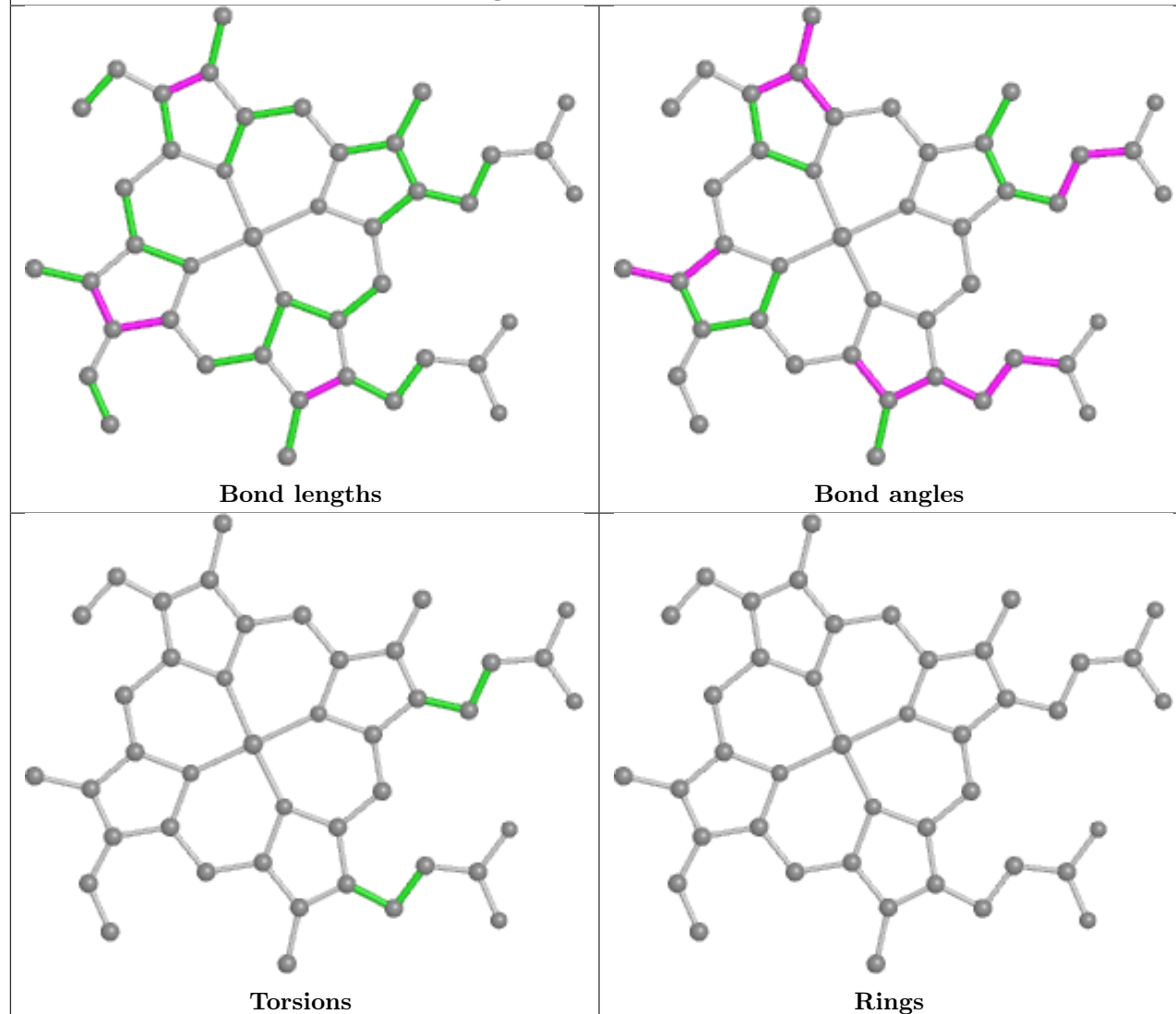




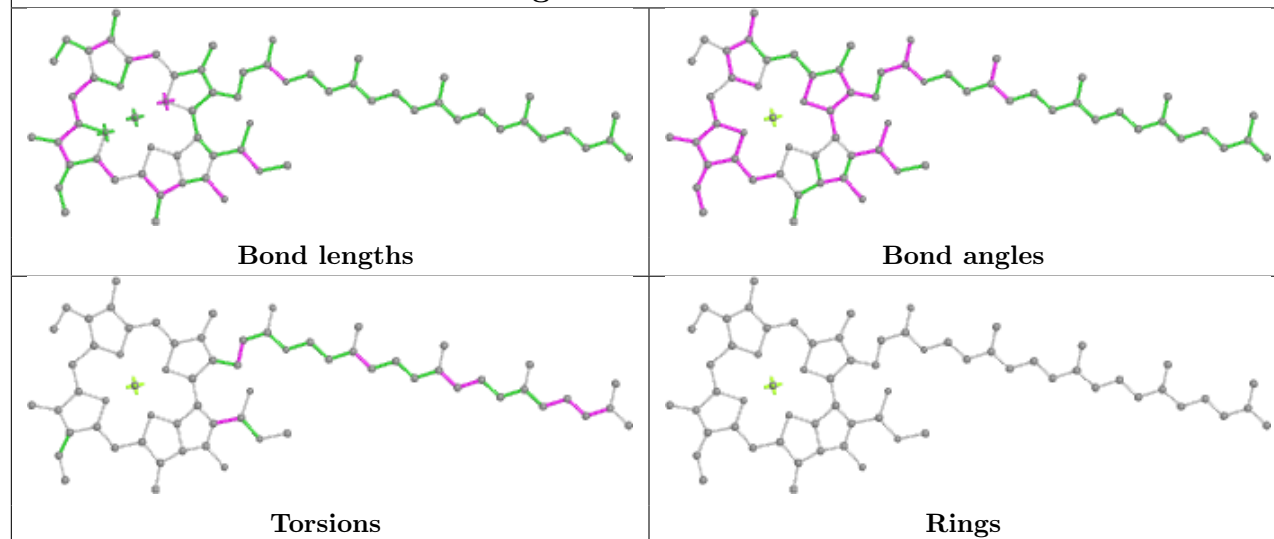
Ligand CLA b 607



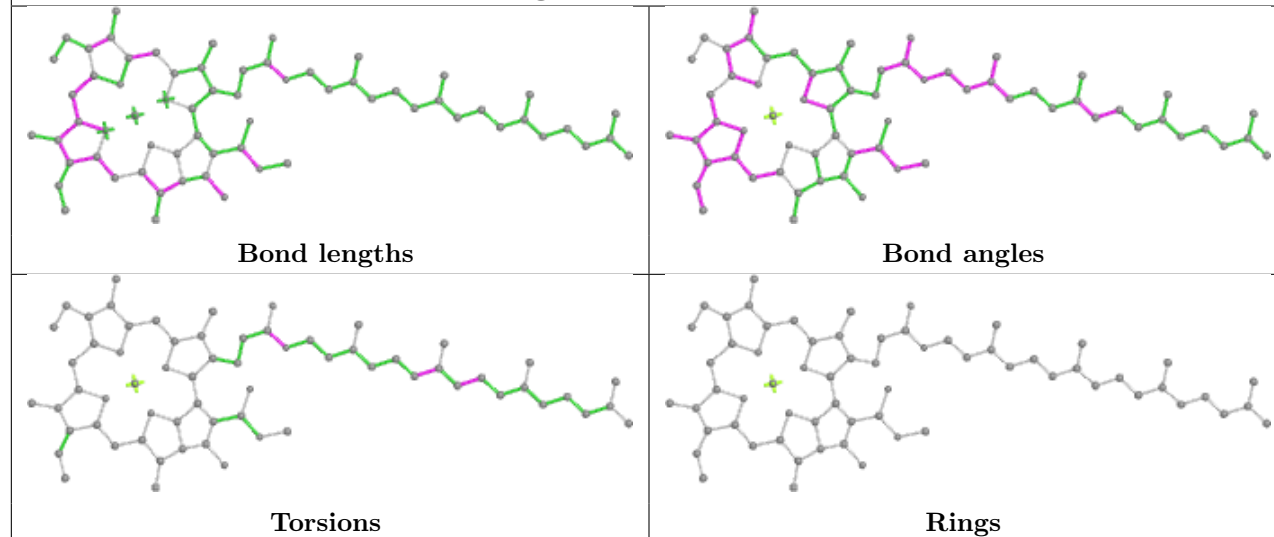
Ligand HEC V 201



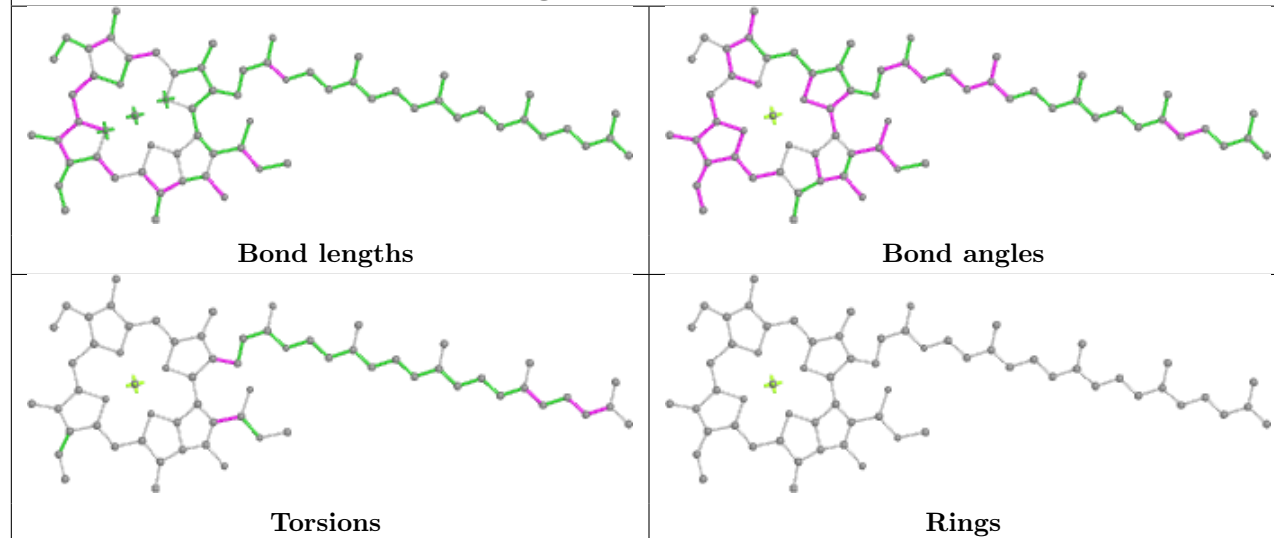
Ligand CLA B 606



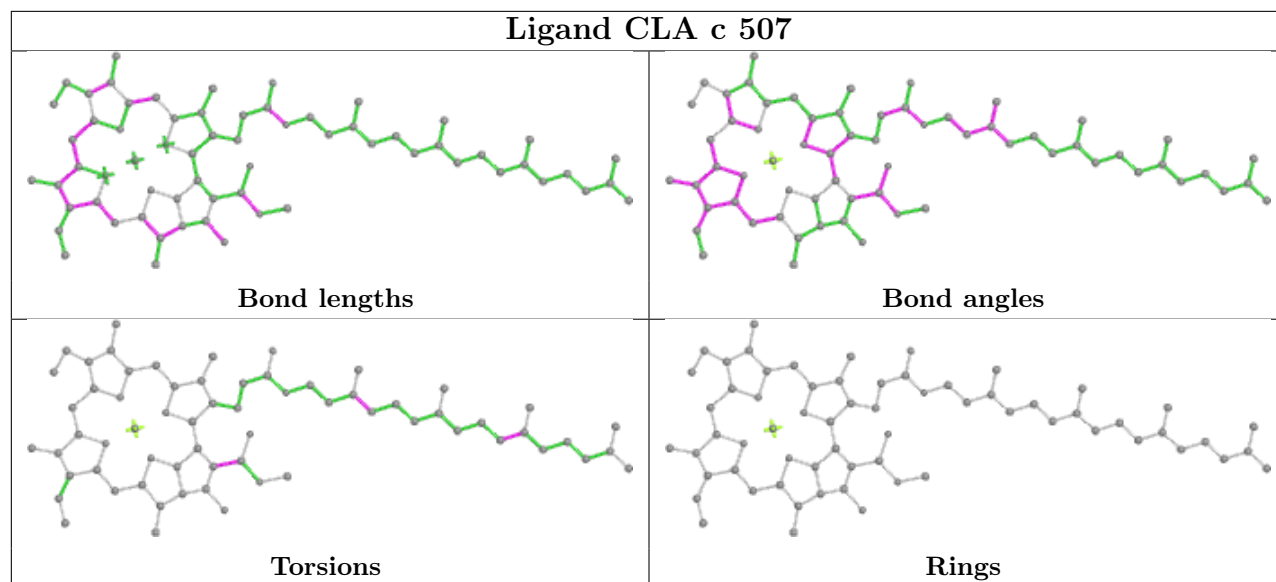
Ligand CLA C 513



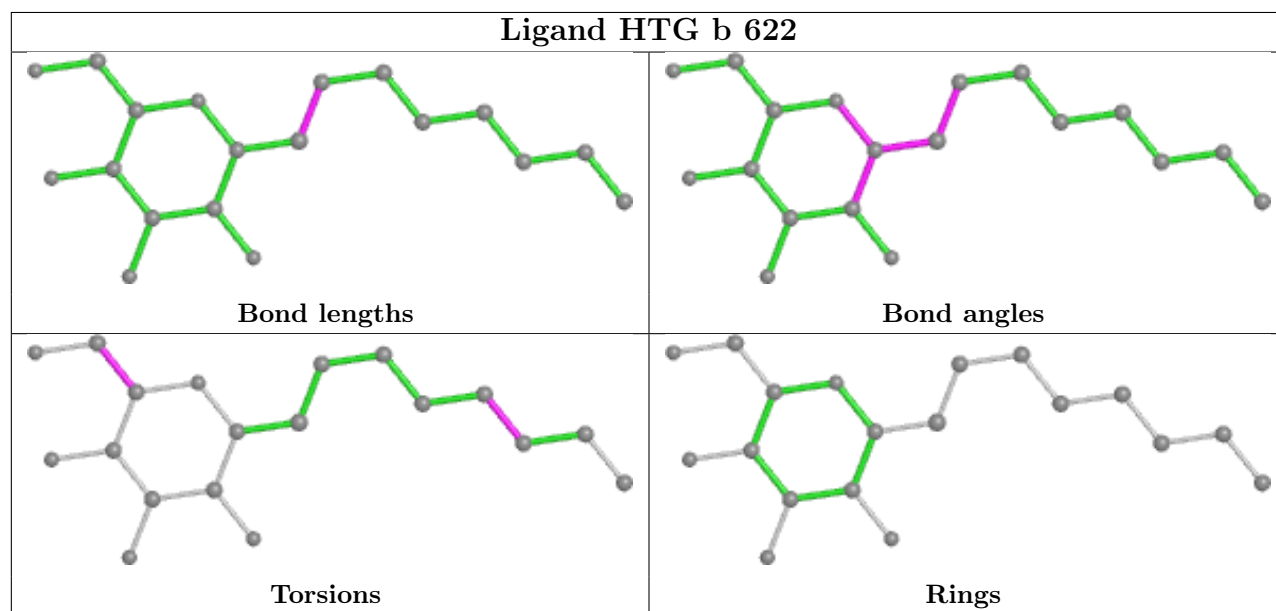
Ligand CLA b 609

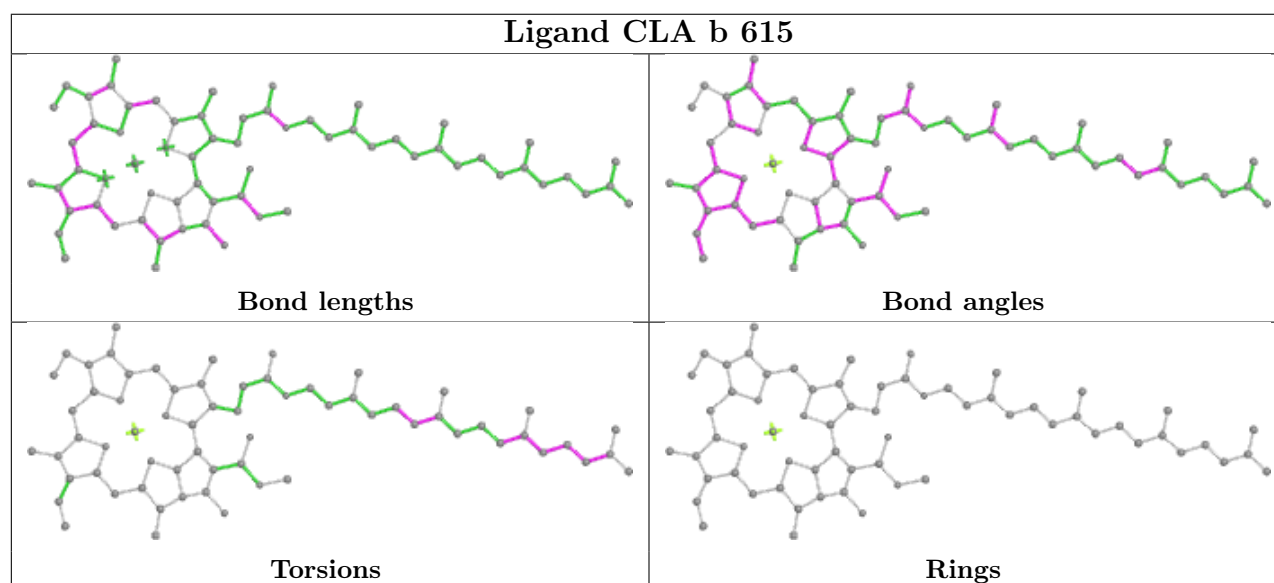
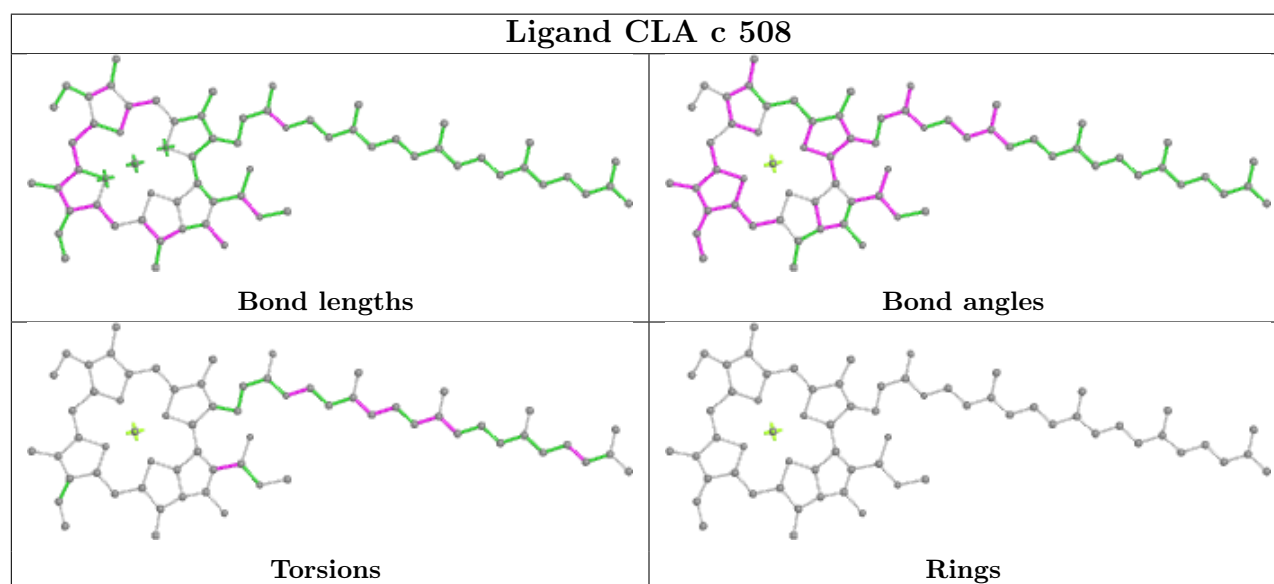
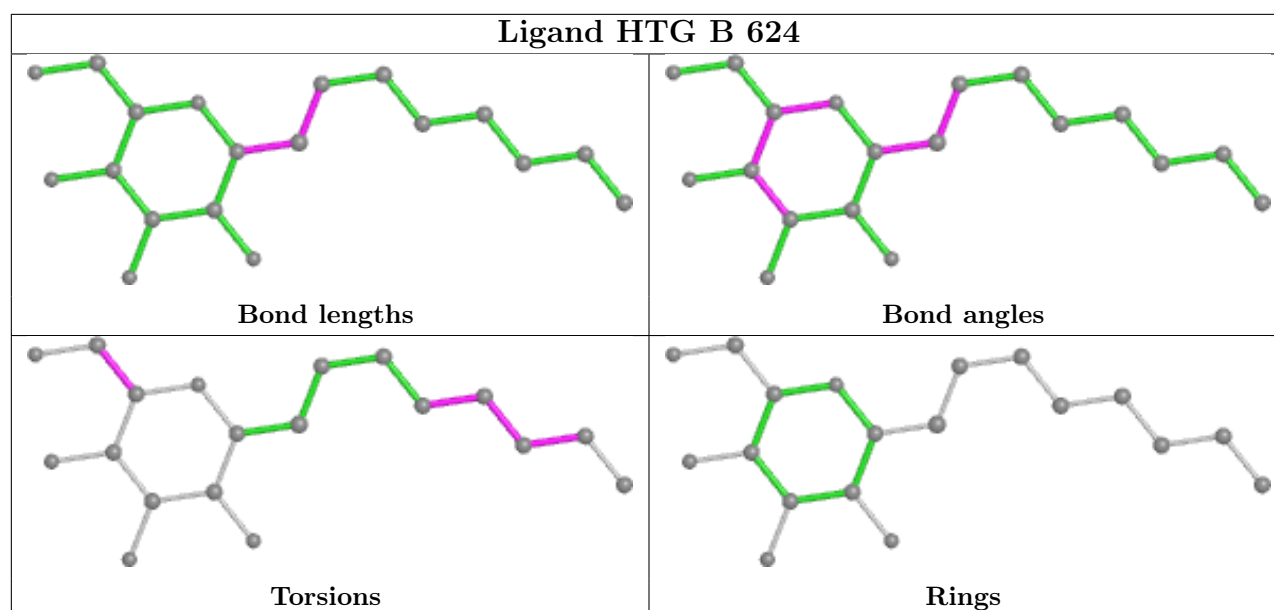


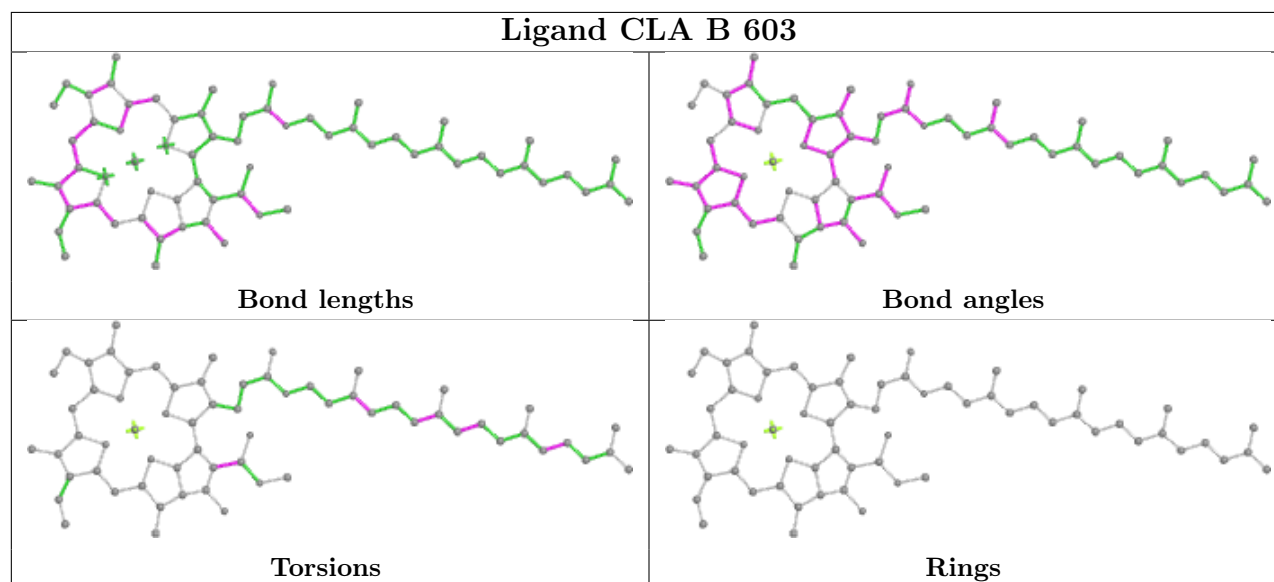
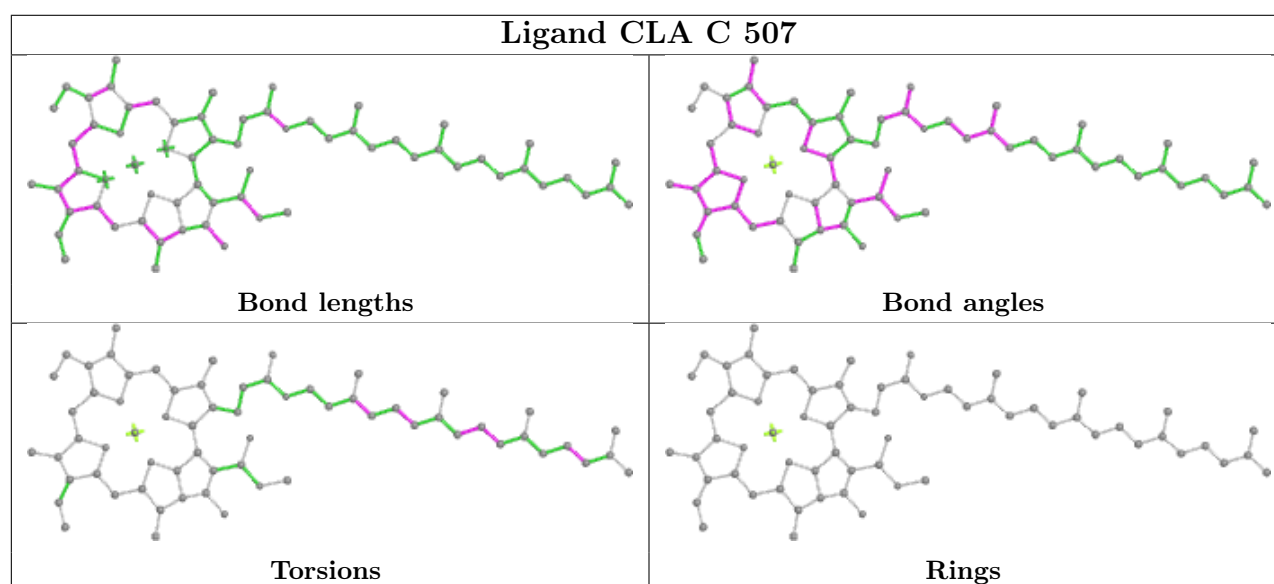
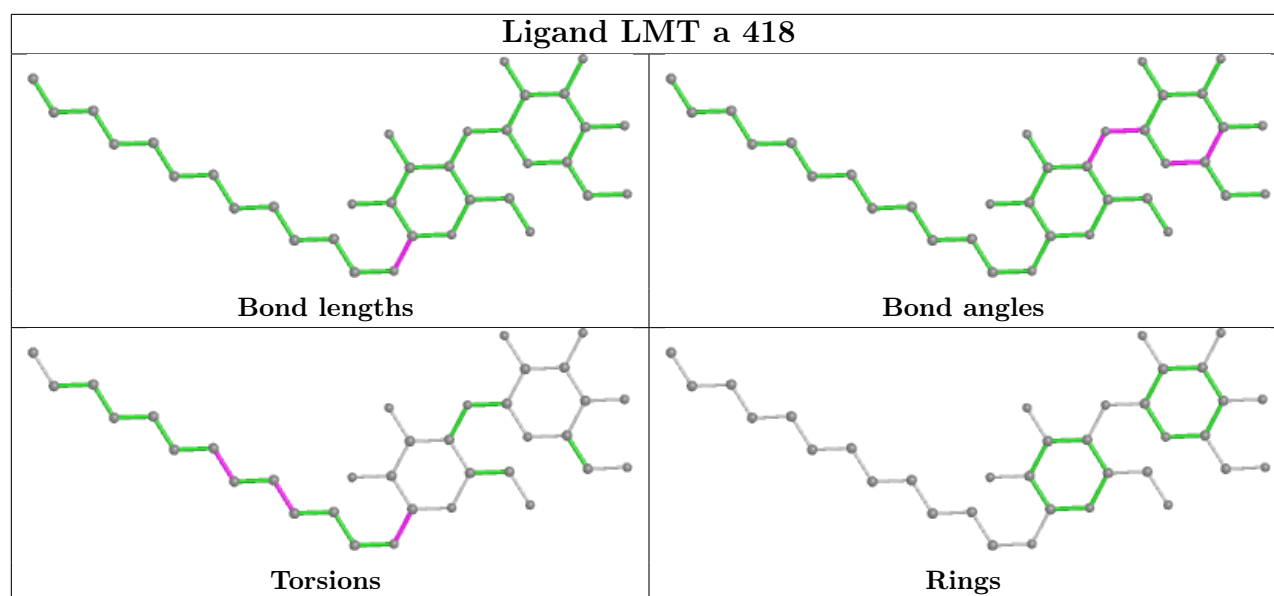
Ligand CLA c 507

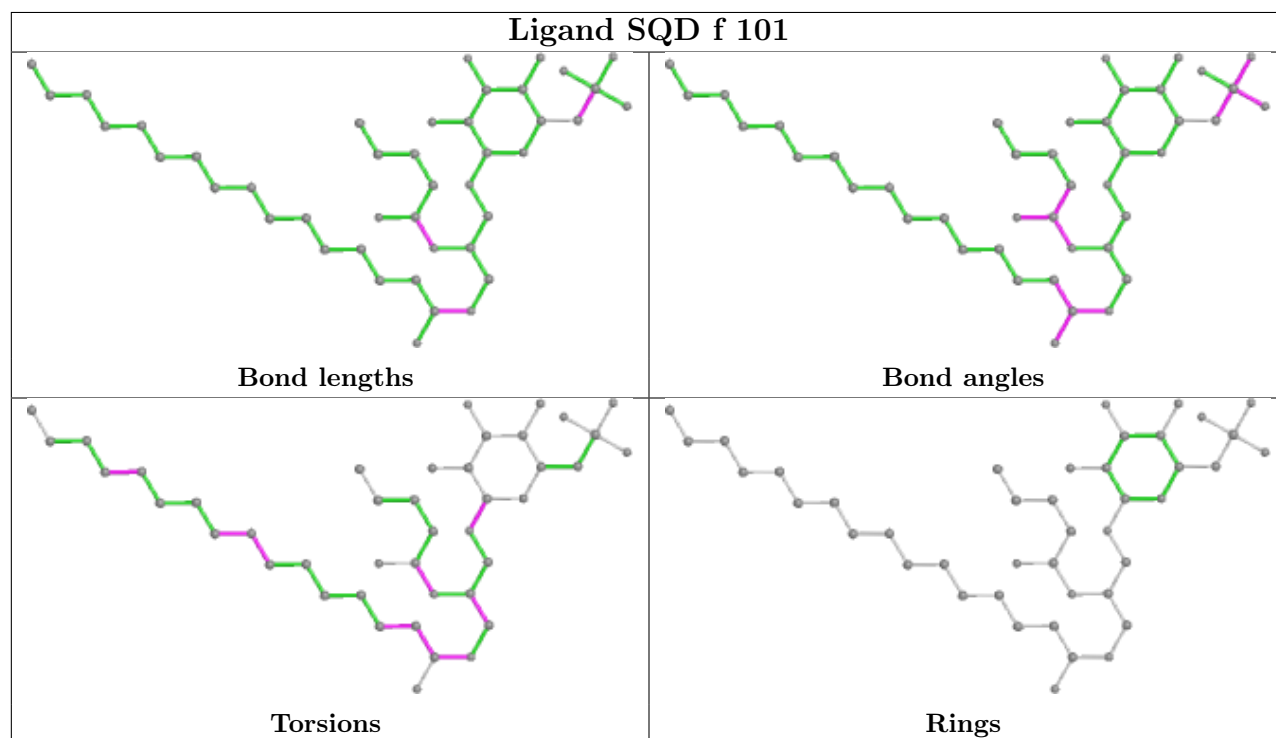
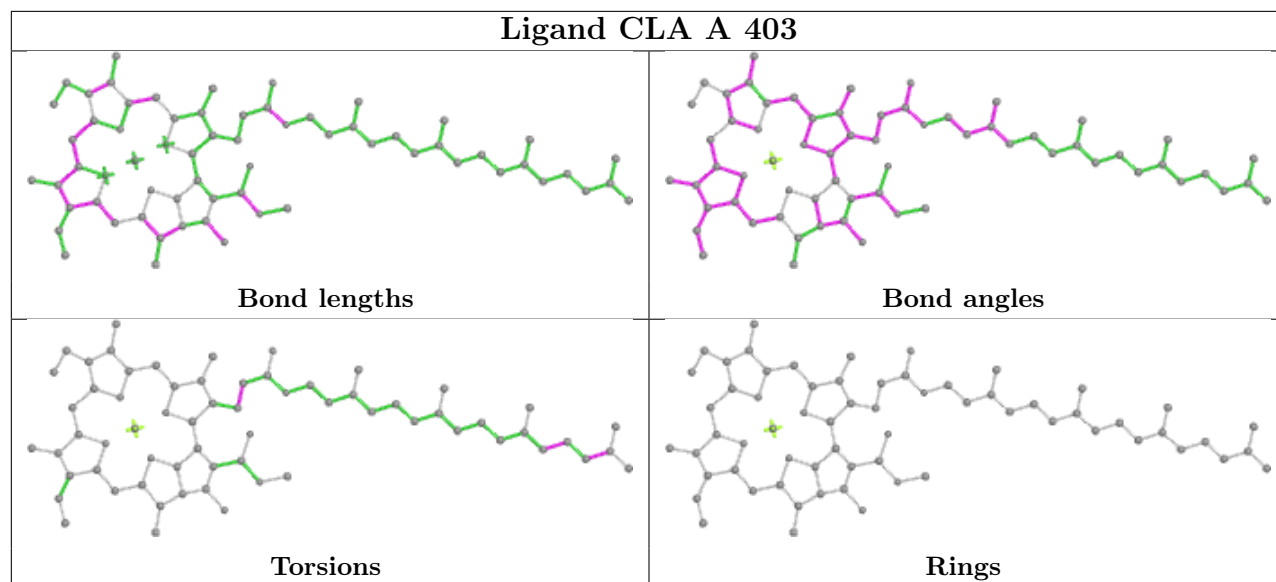


Ligand HTG b 622

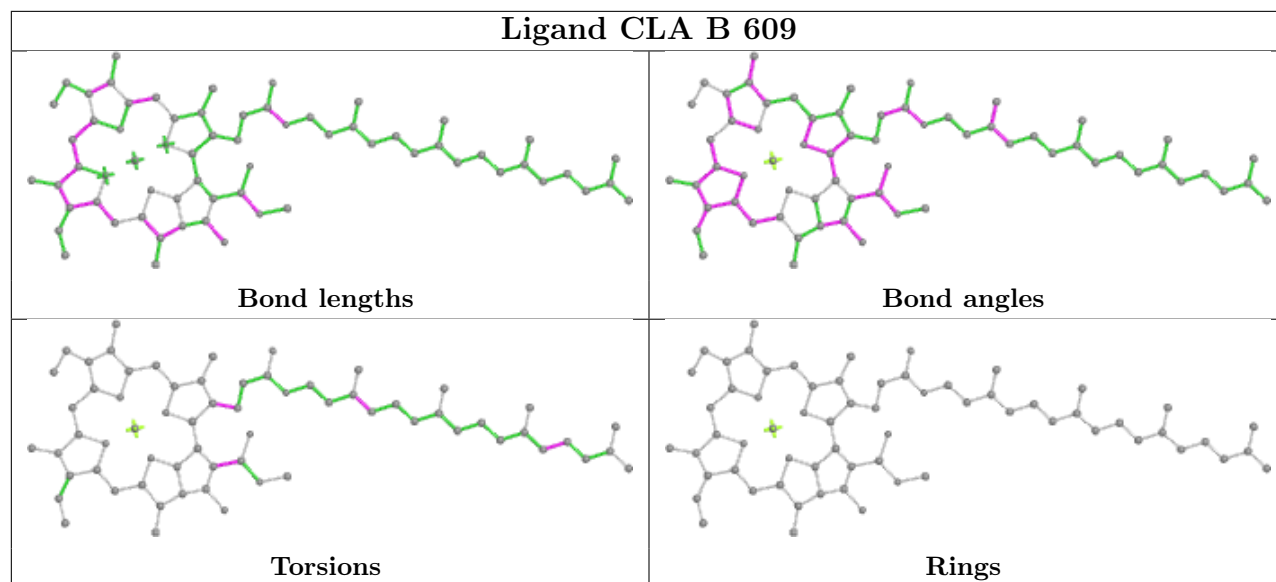




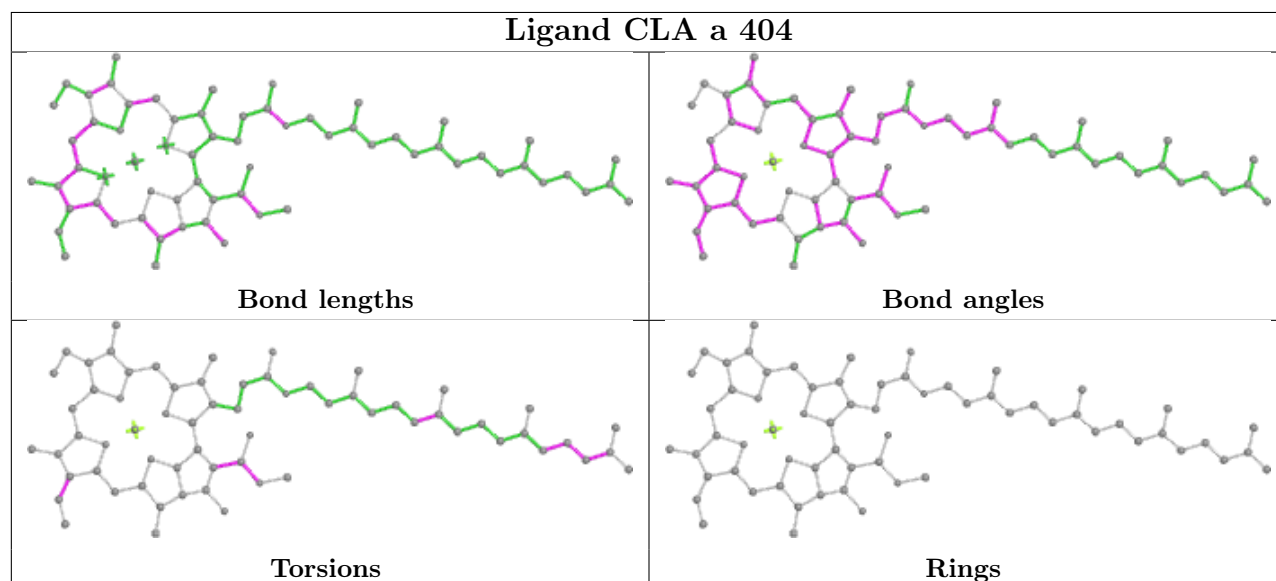




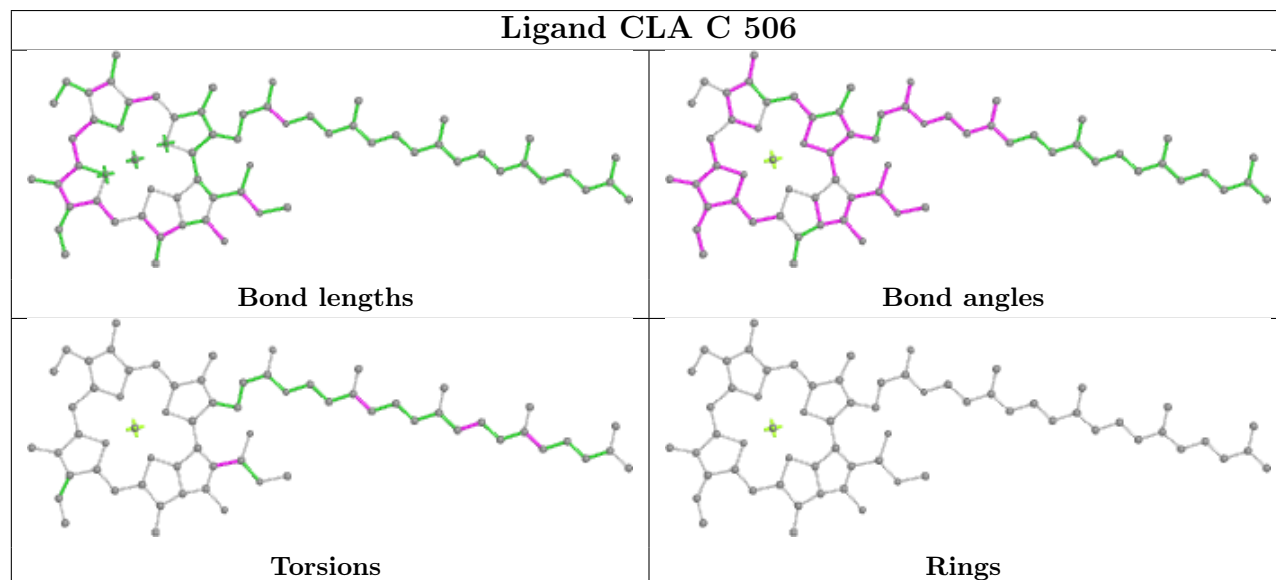
Ligand CLA B 609

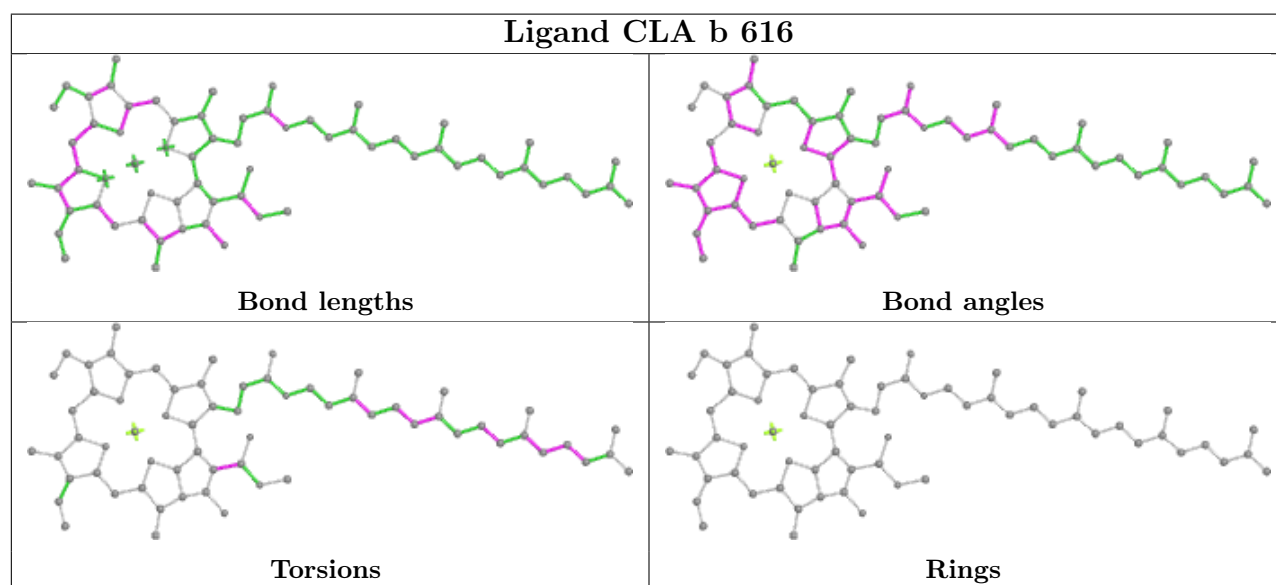
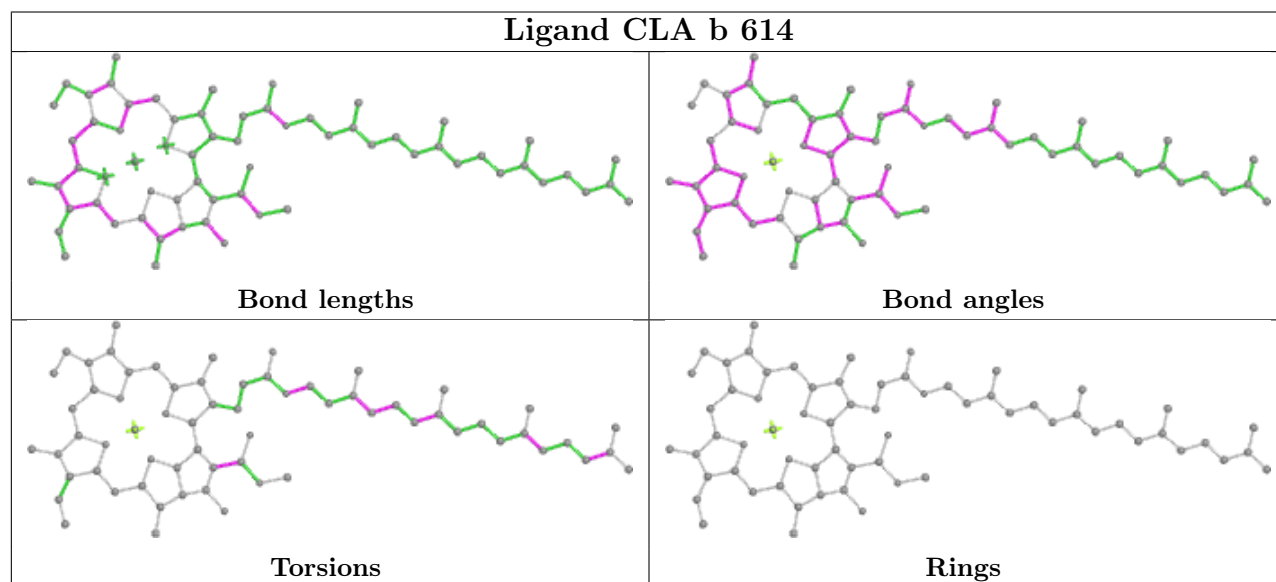
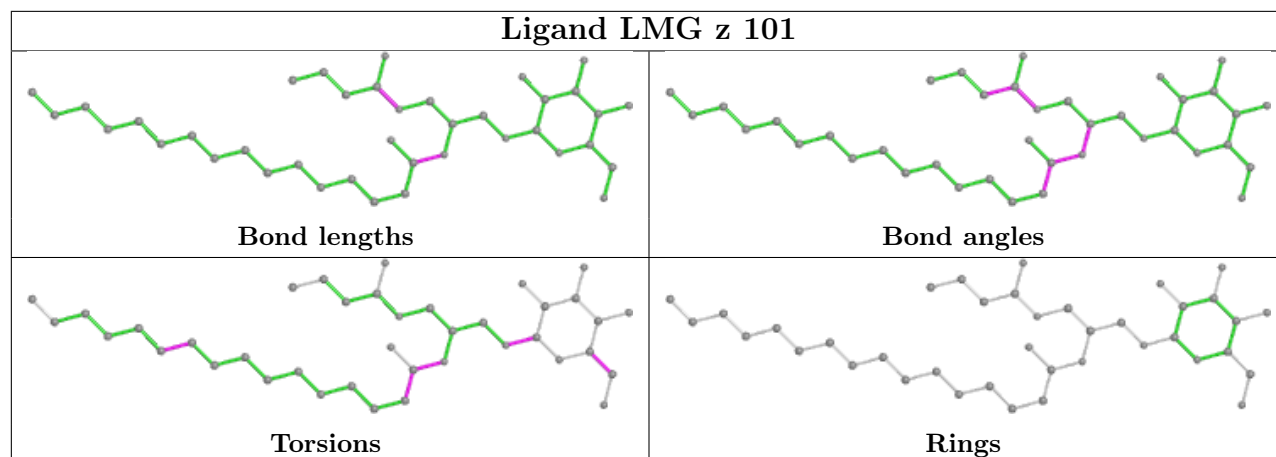


Ligand CLA a 404

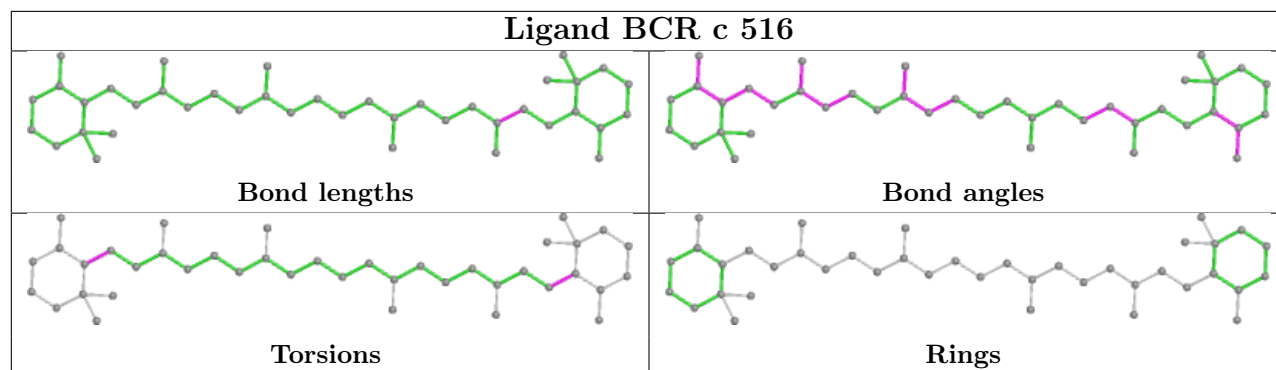


Ligand CLA C 506

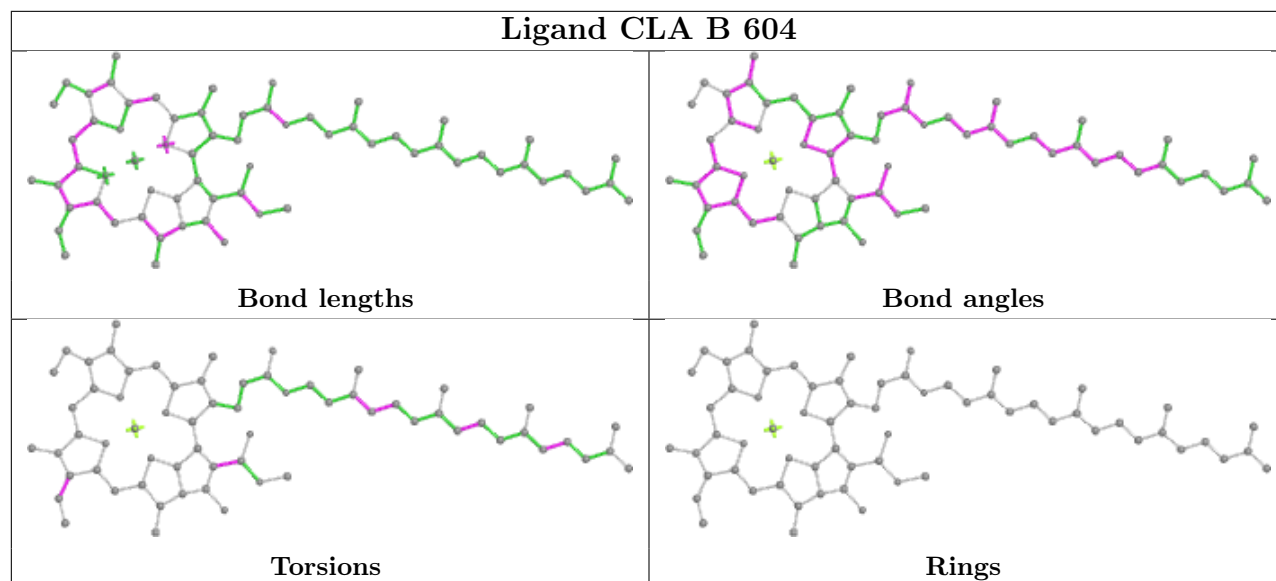




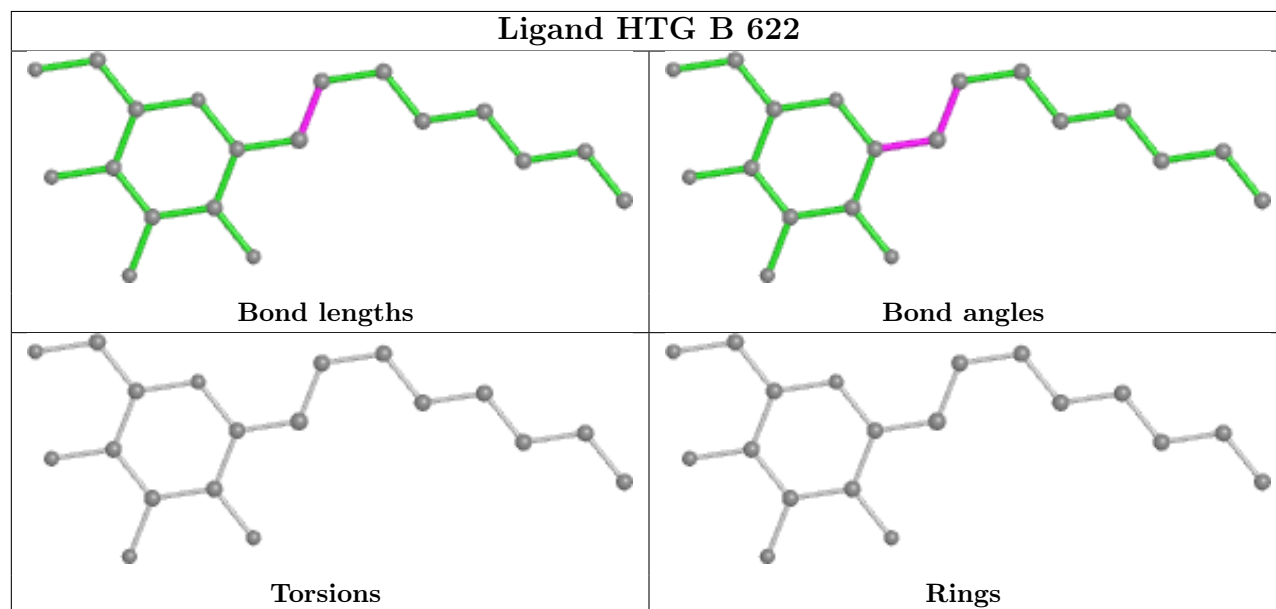
Ligand BCR c 516

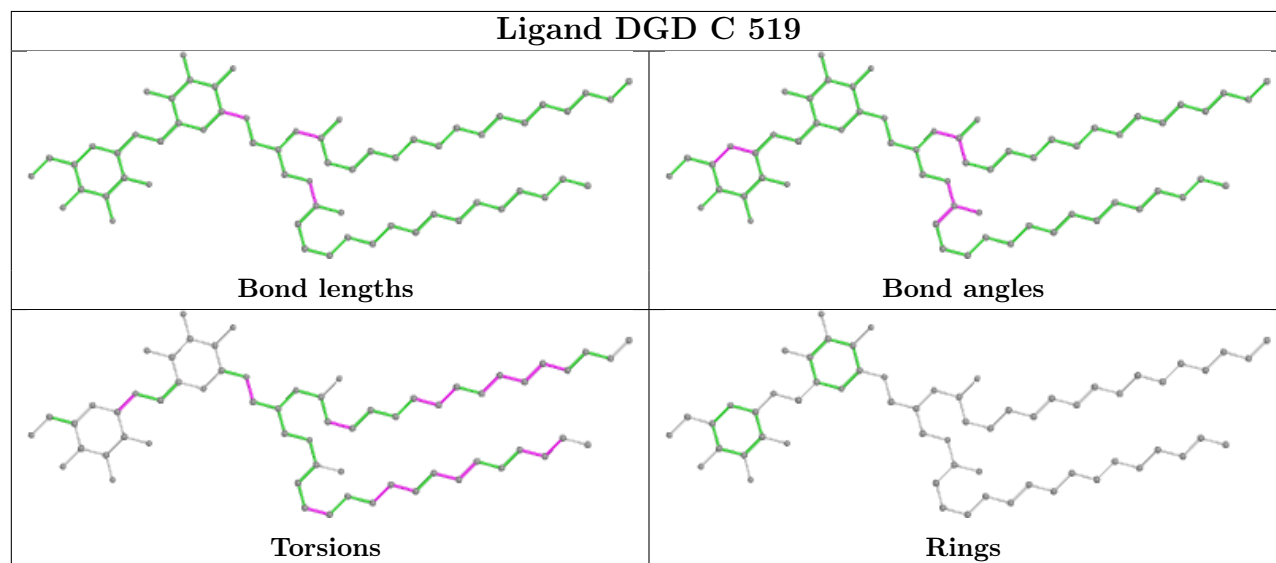
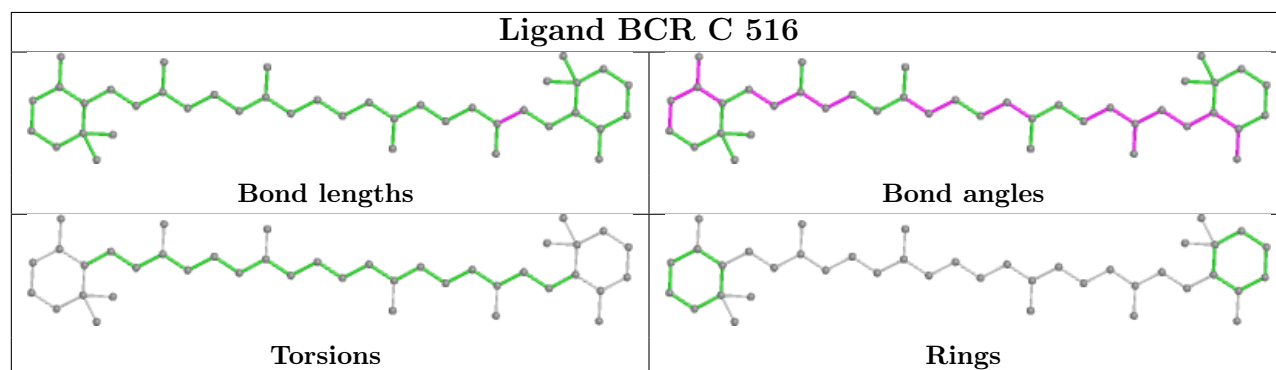
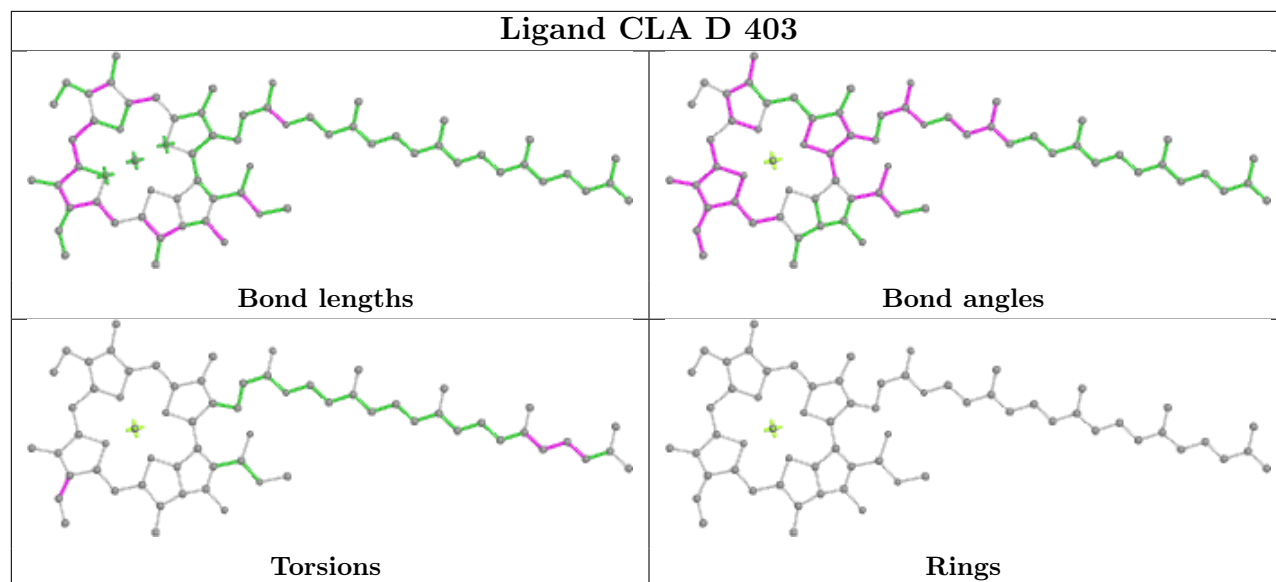


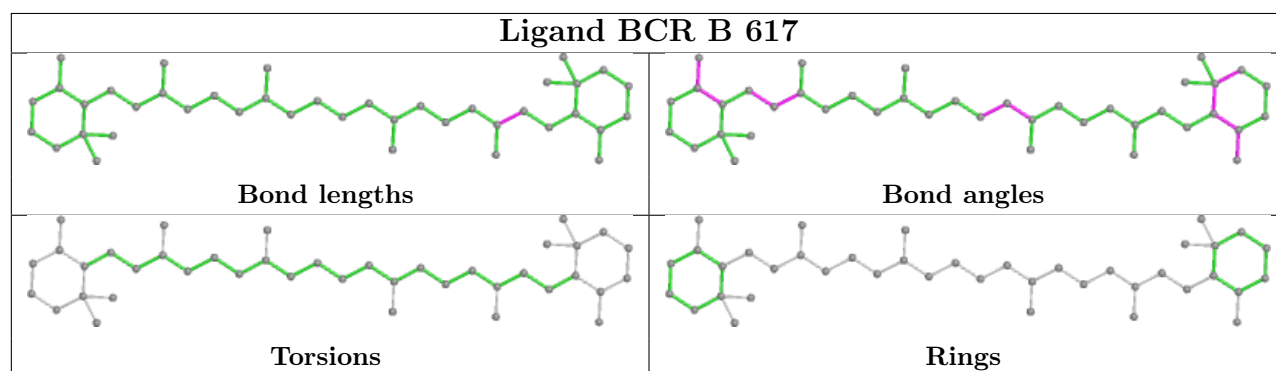
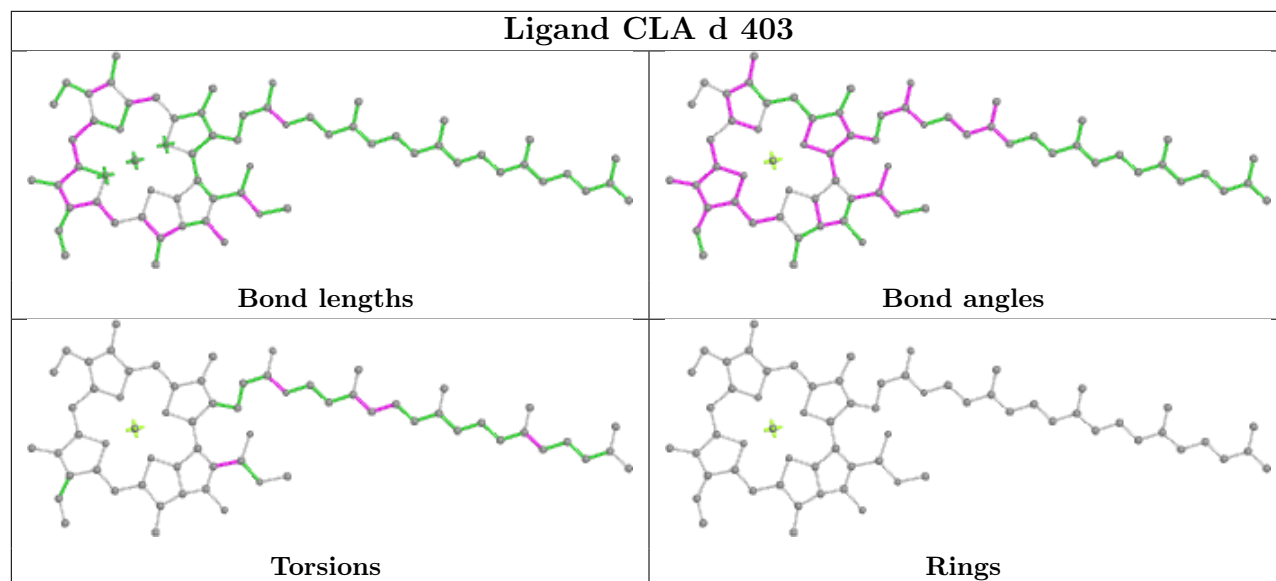
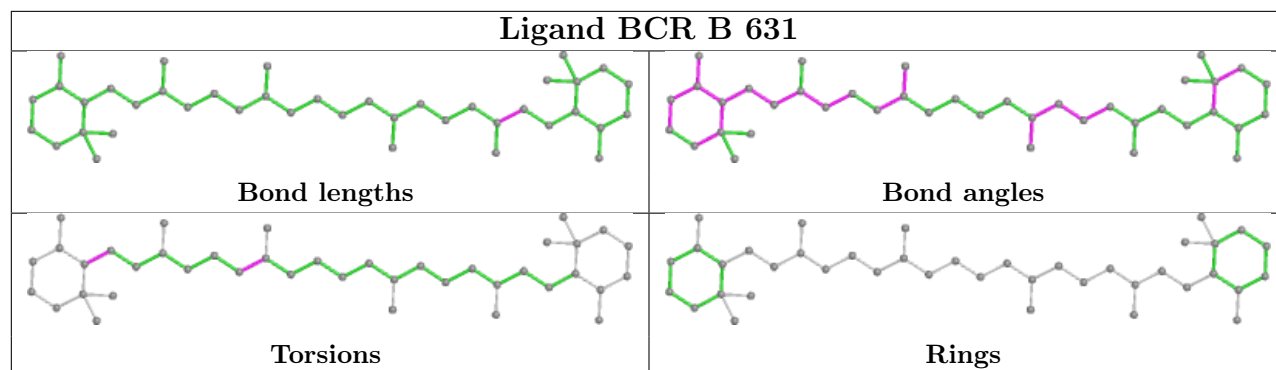
Ligand CLA B 604



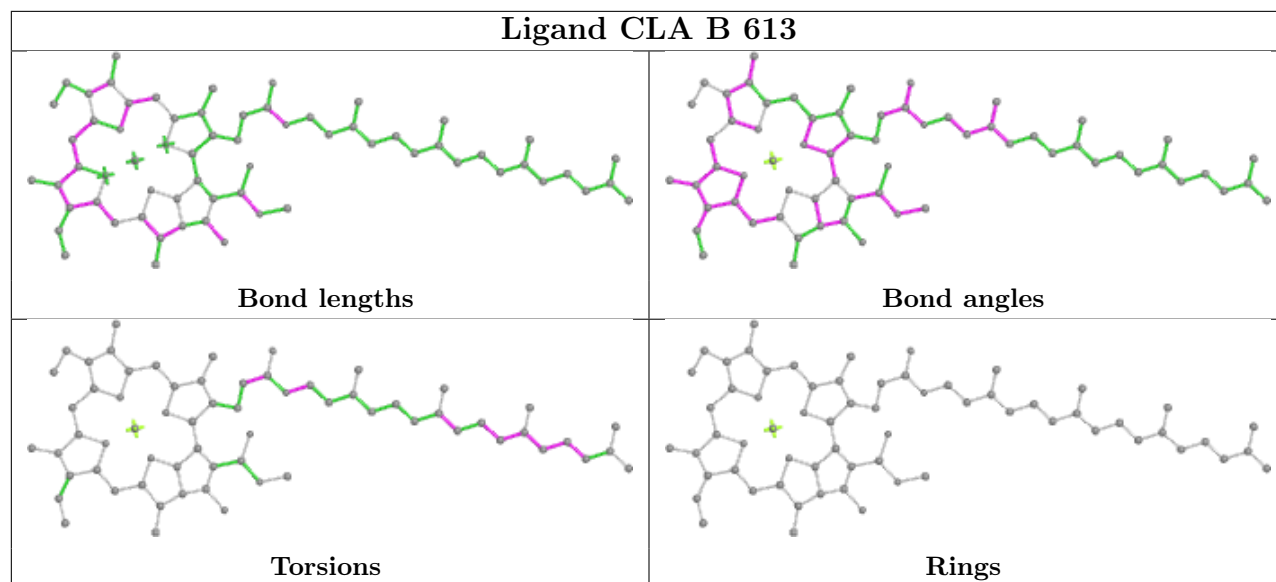
Ligand HTG B 622



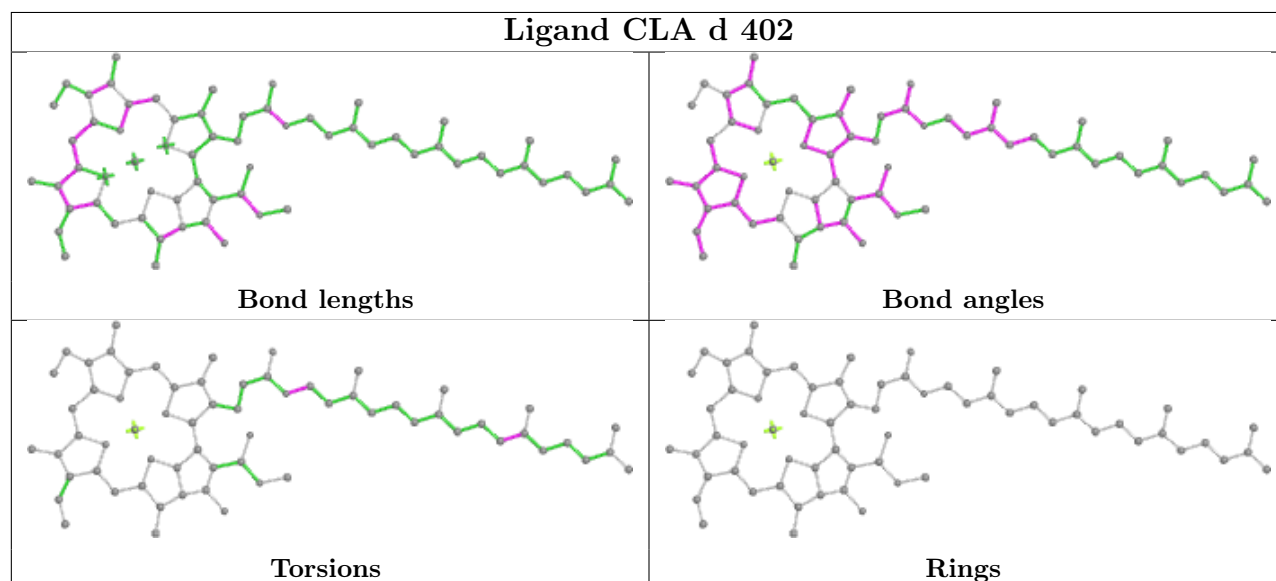




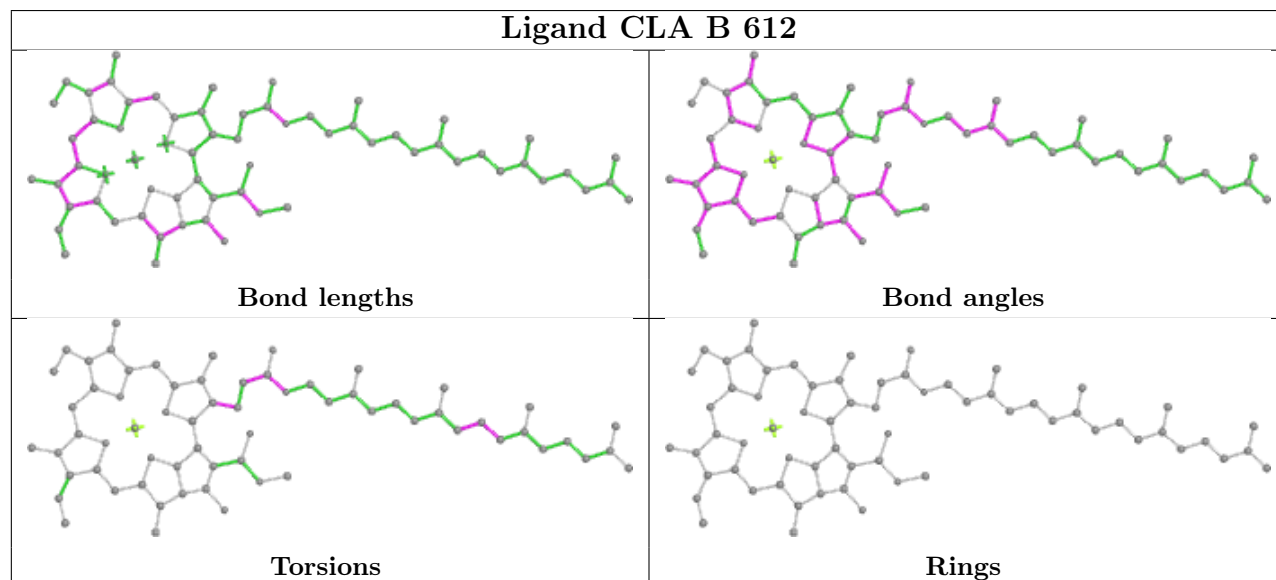
Ligand CLA B 613



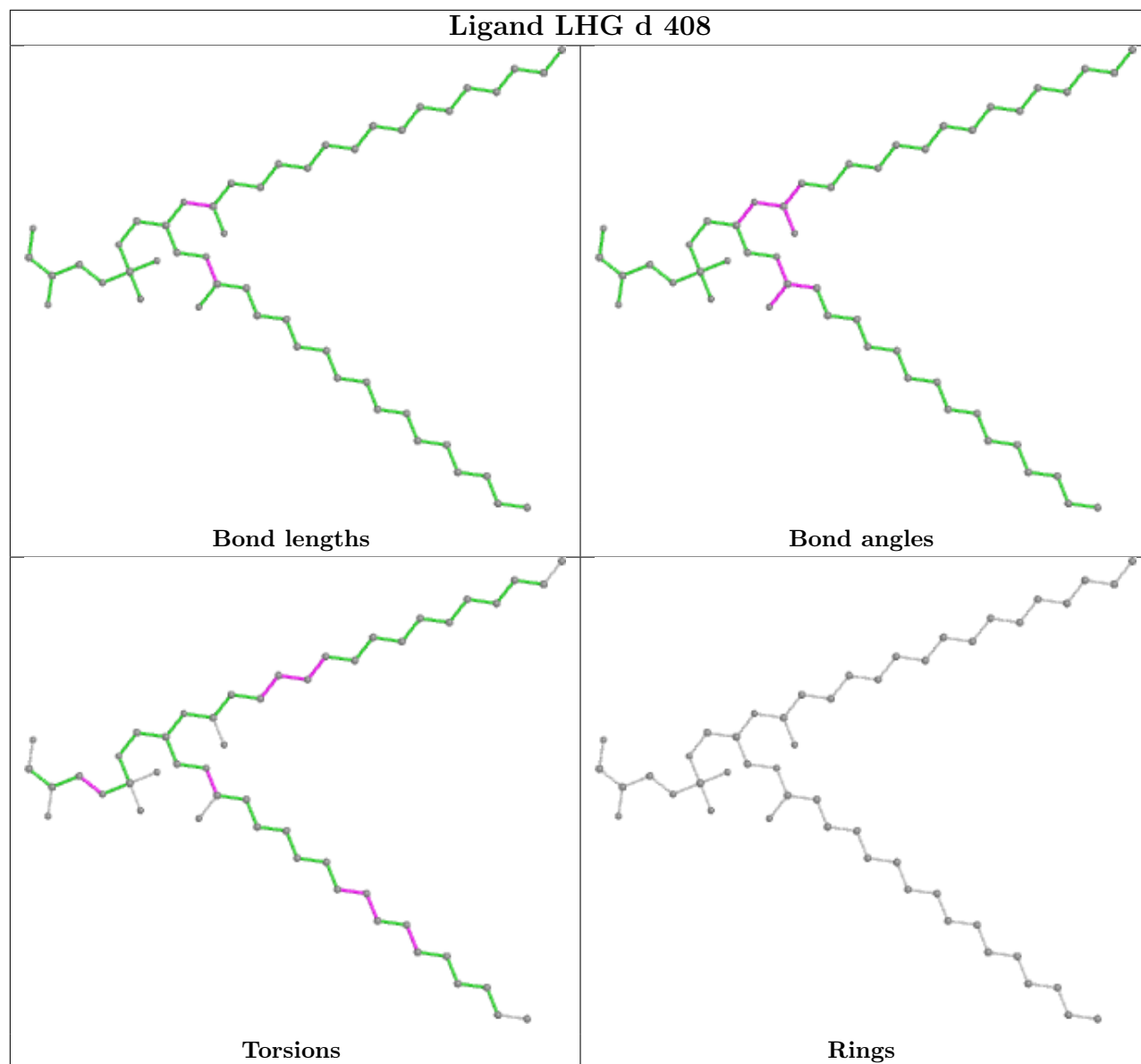
Ligand CLA d 402



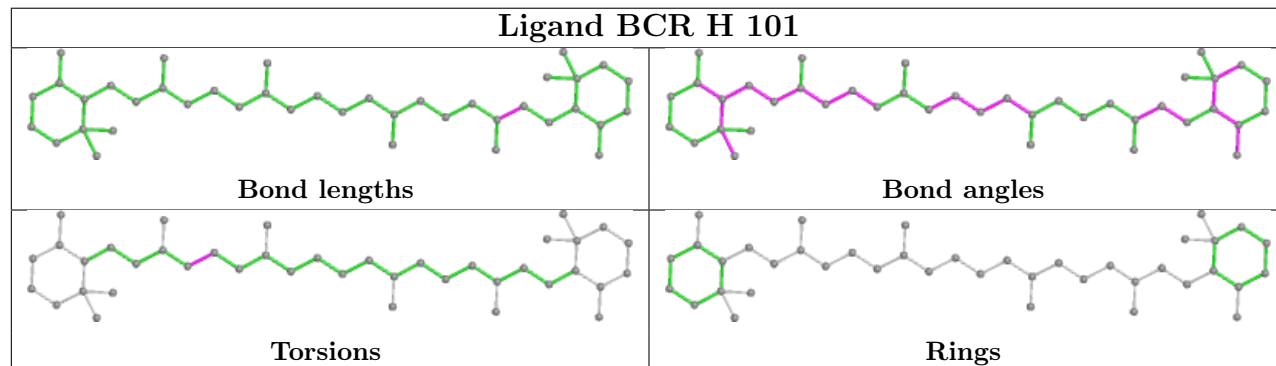
Ligand CLA B 612

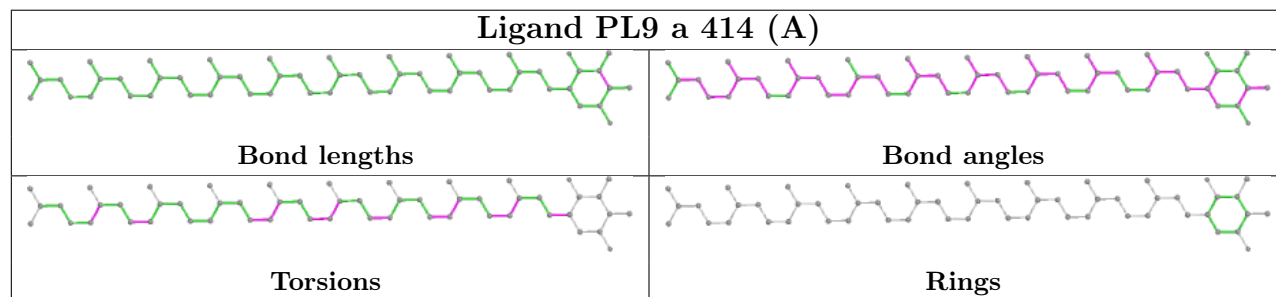
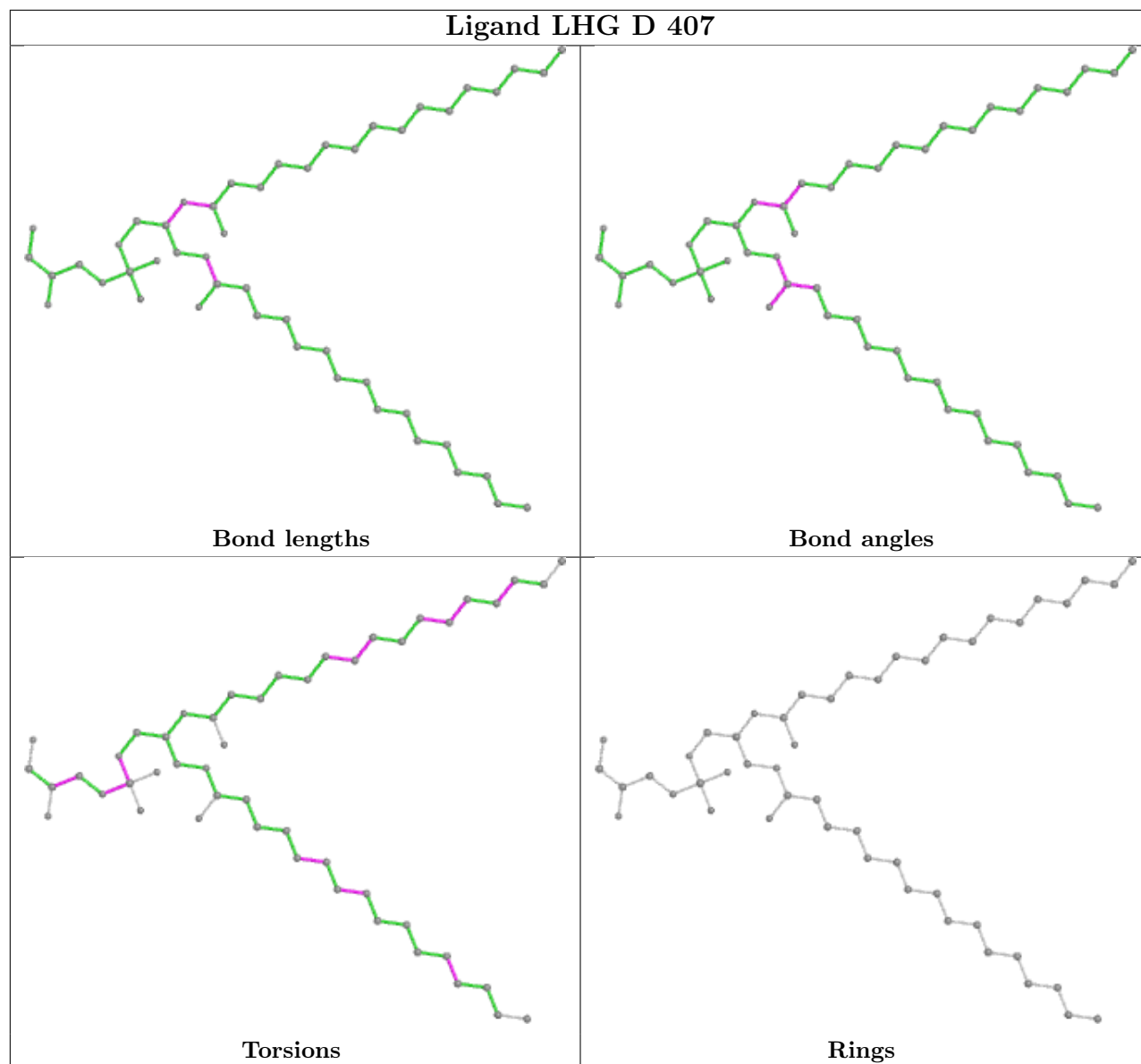


Ligand LHG d 408

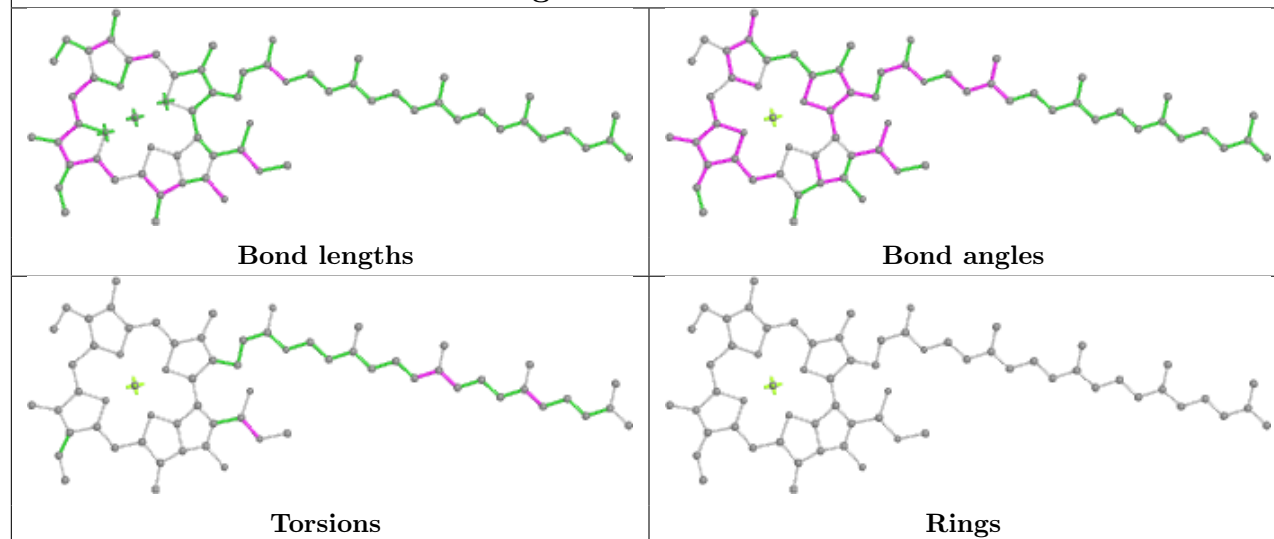


Ligand BCR H 101

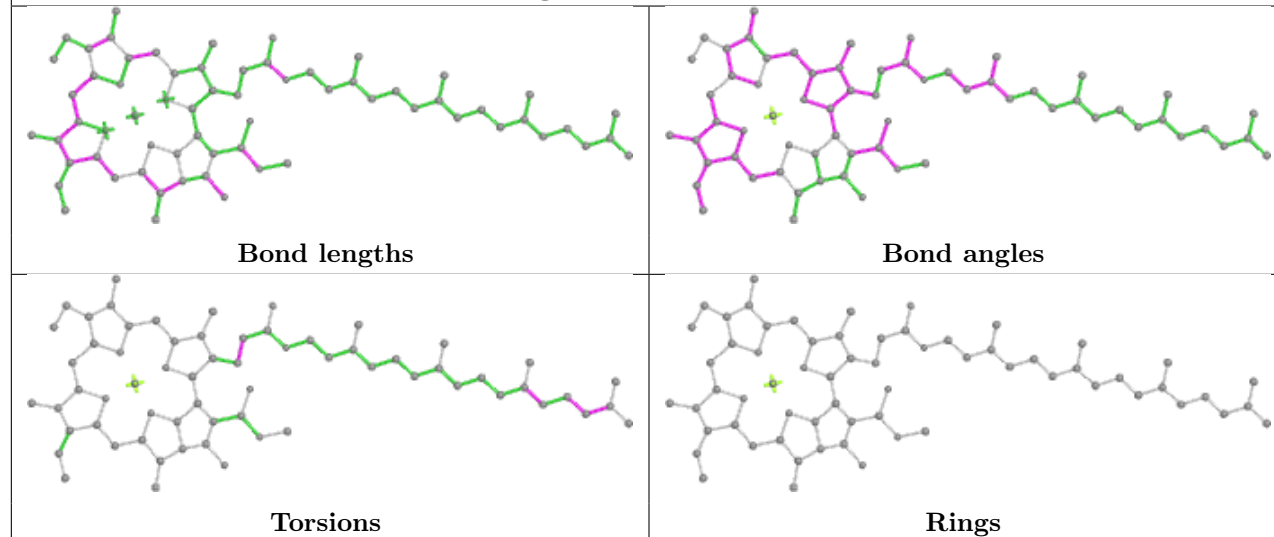




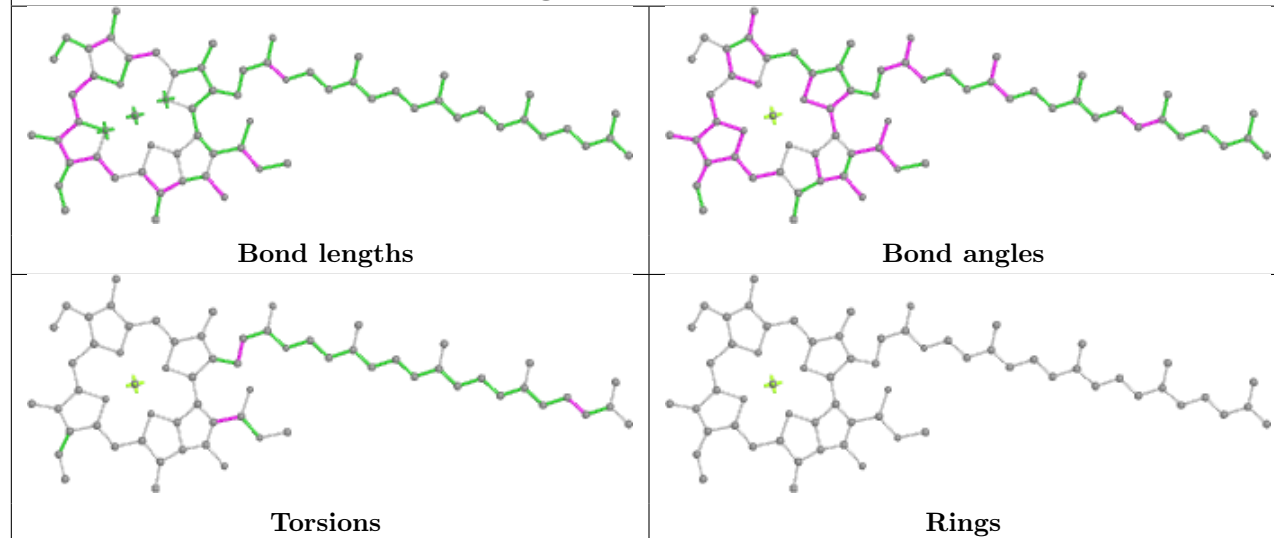
Ligand CLA C 515

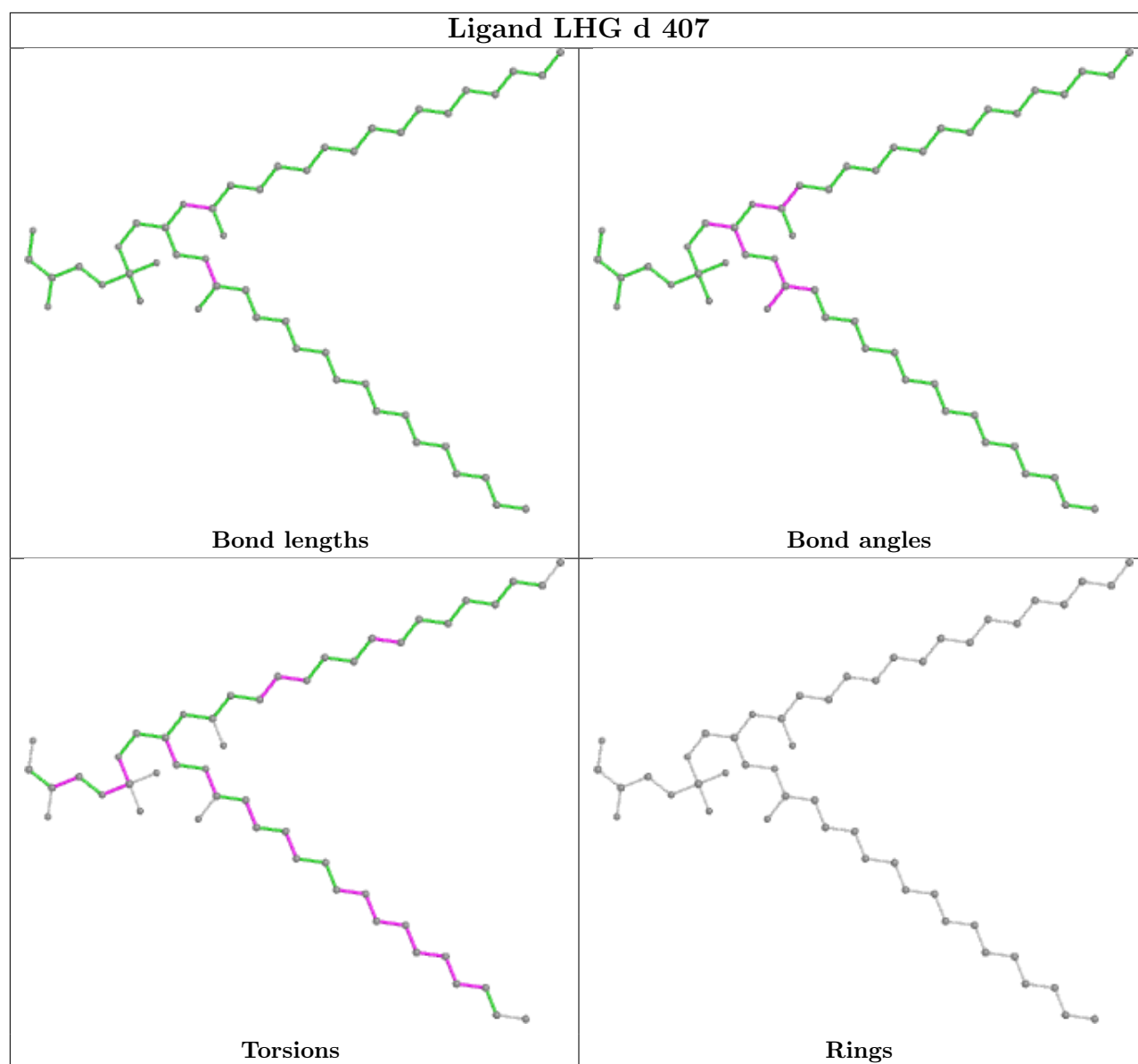


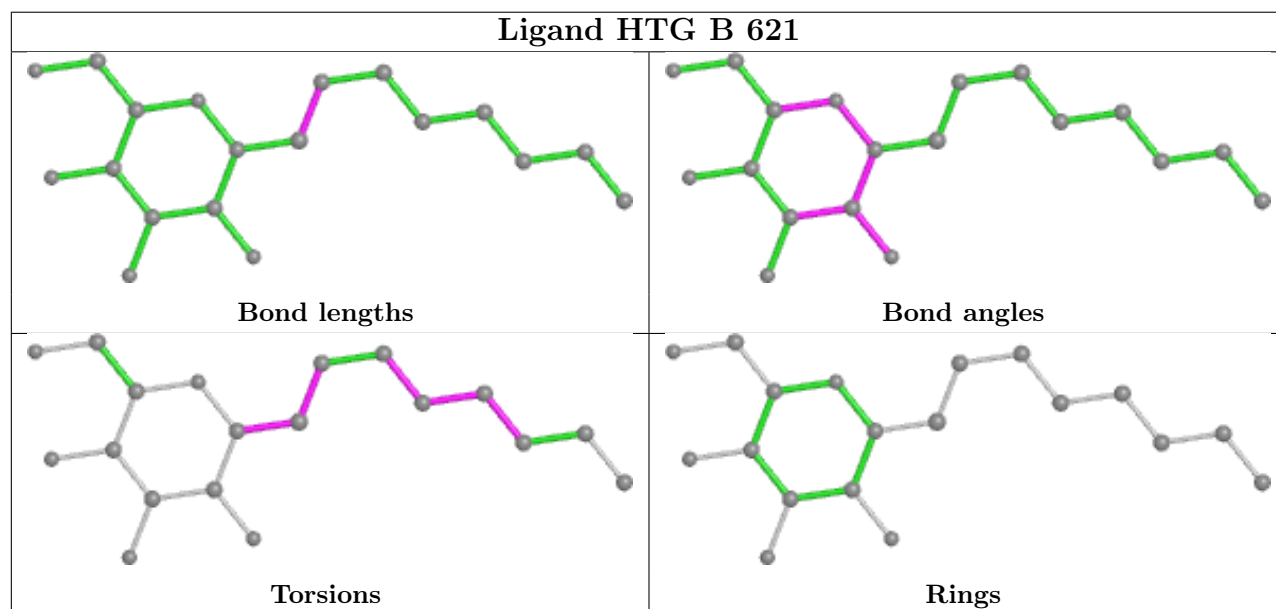
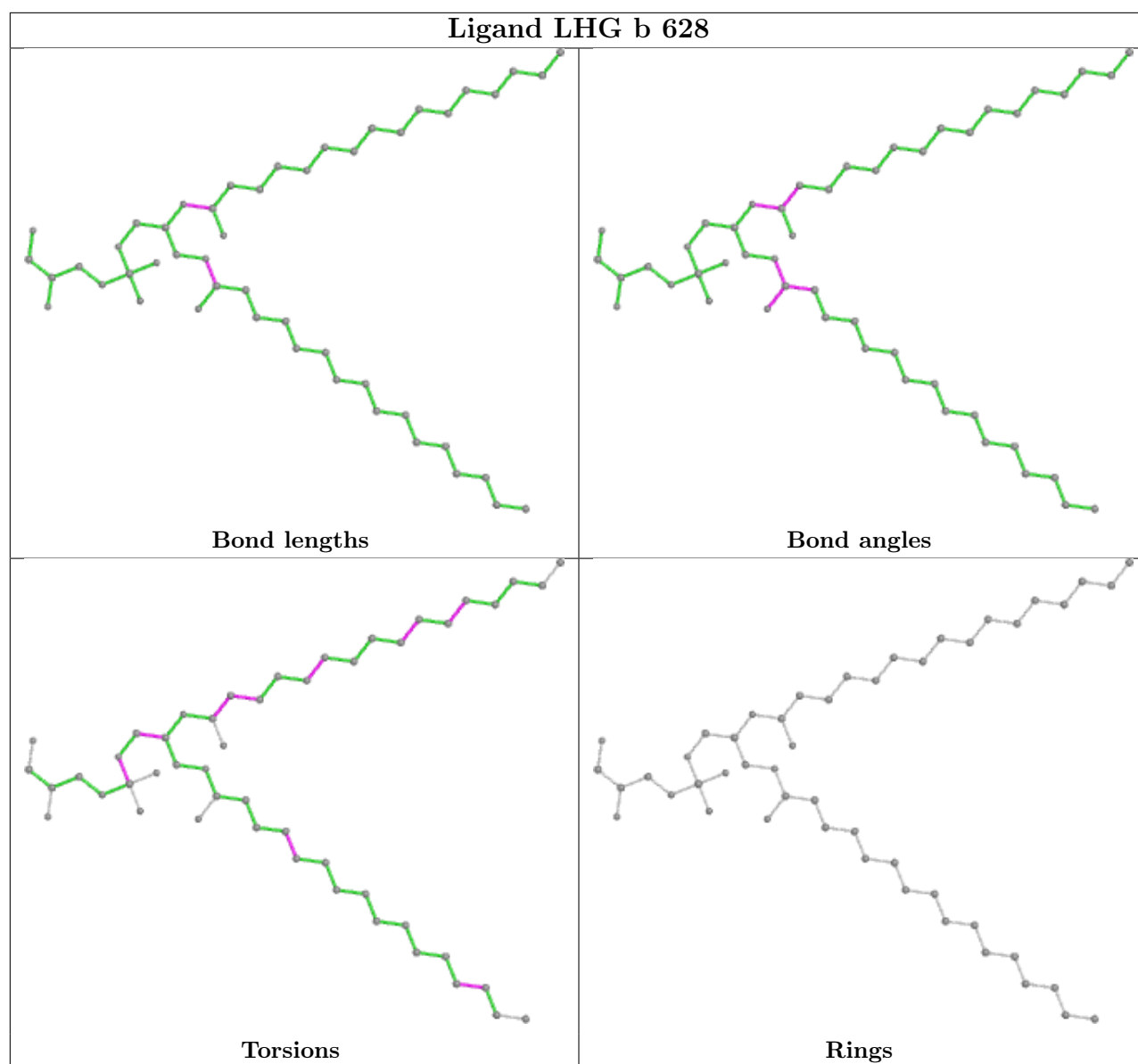
Ligand CLA a 403

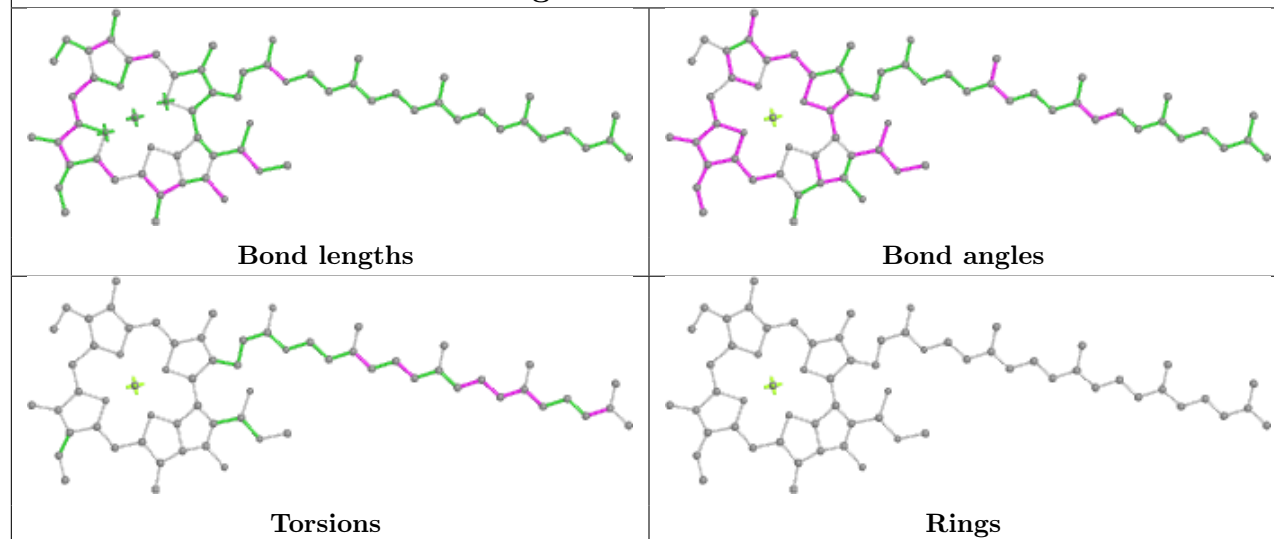
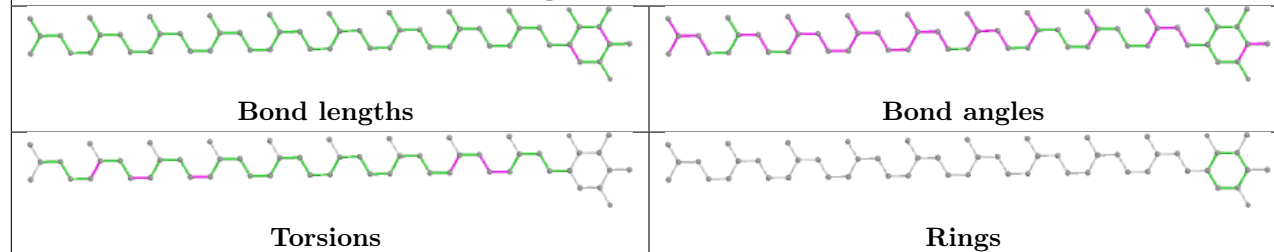


Ligand CLA c 505

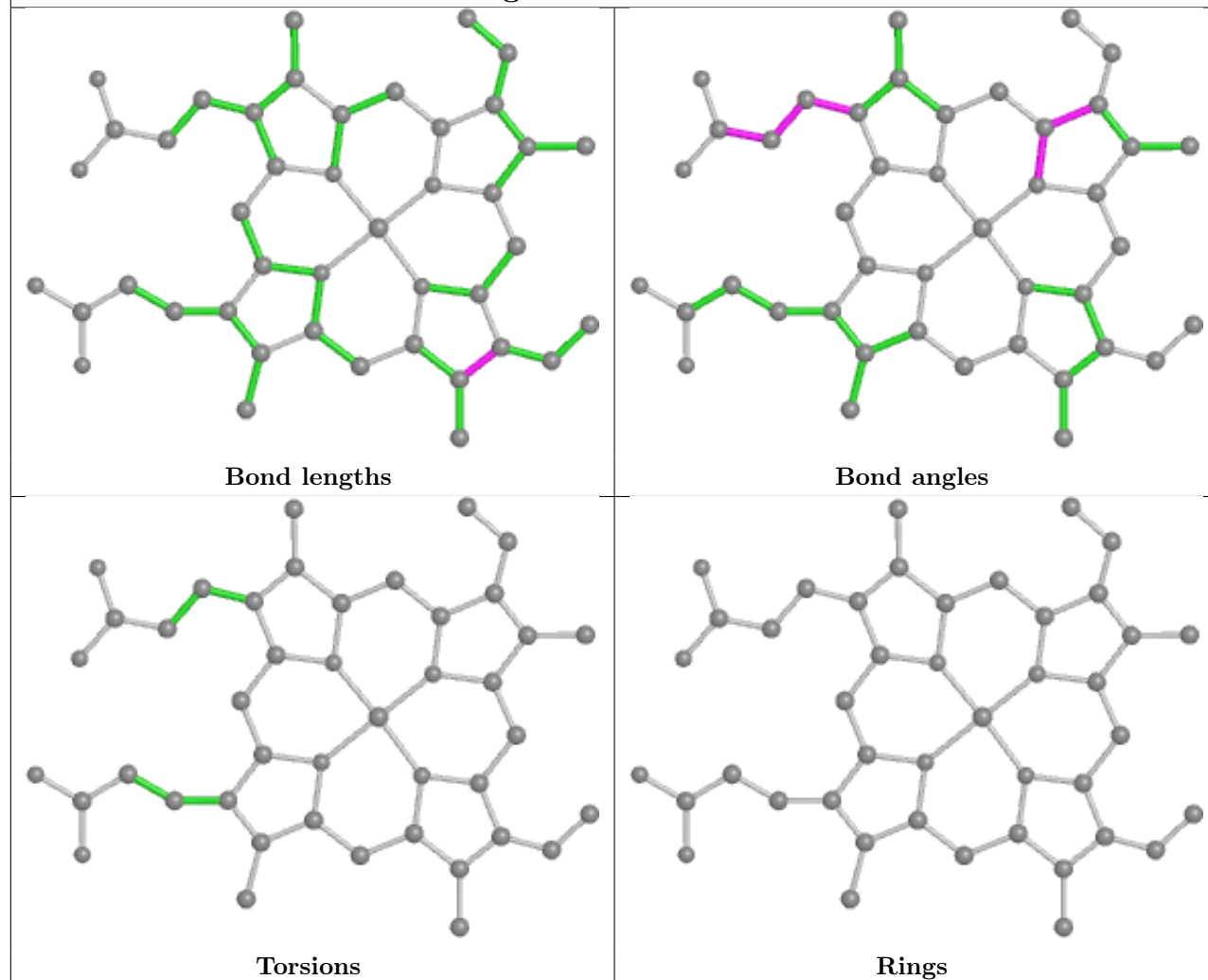




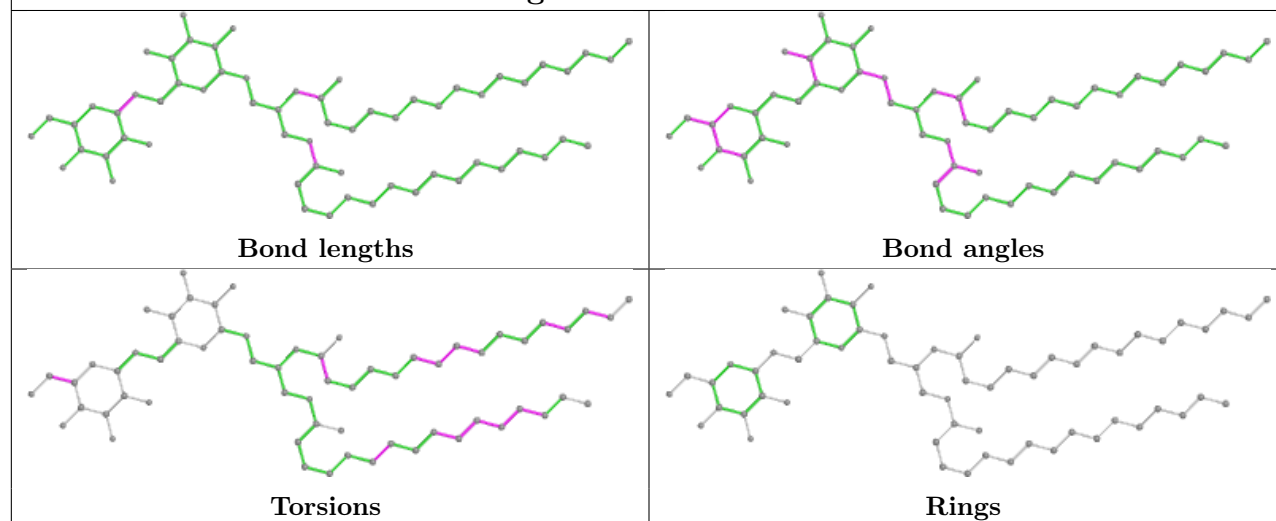


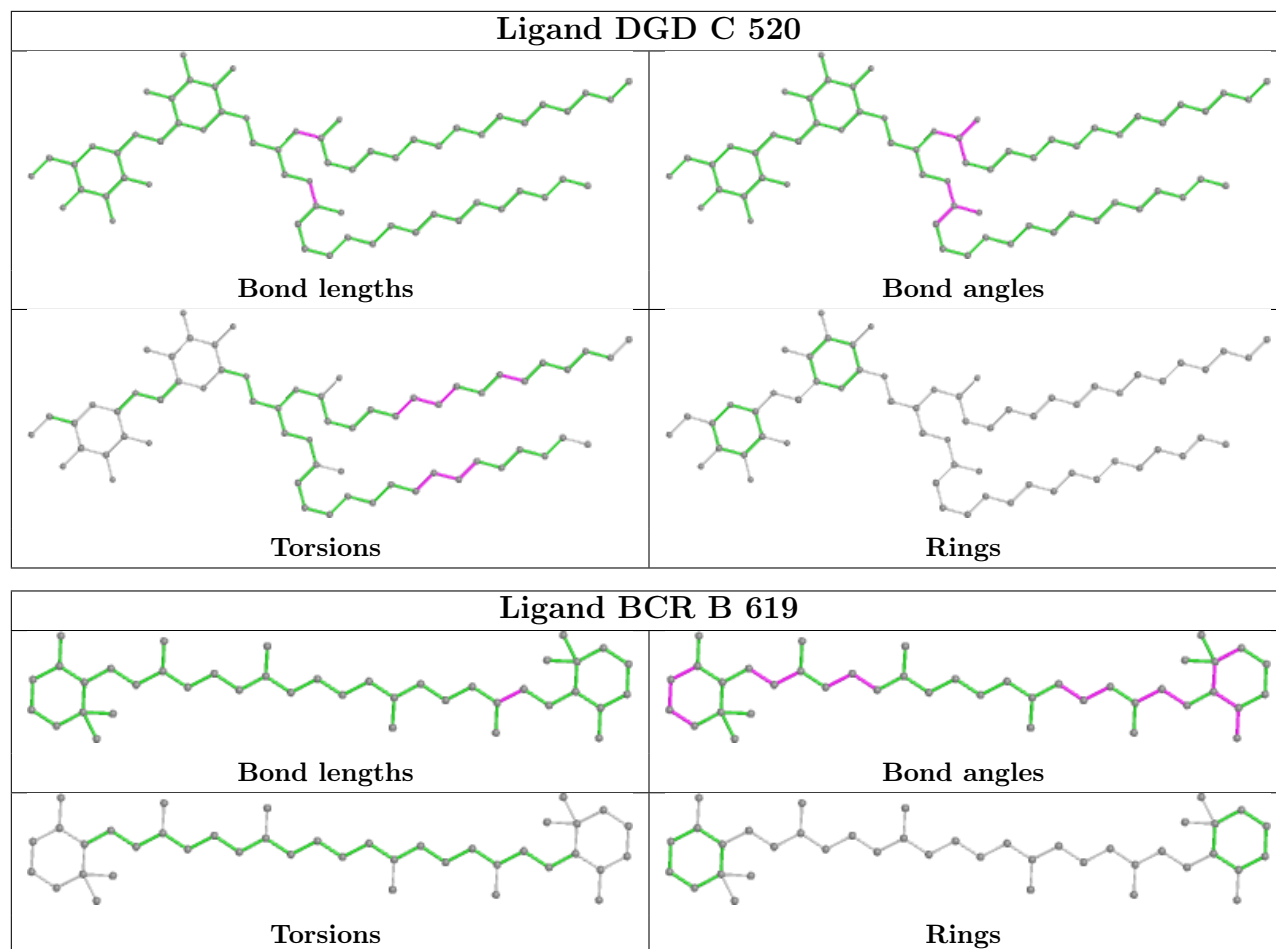
Ligand CLA B 615**Ligand PL9 d 405**

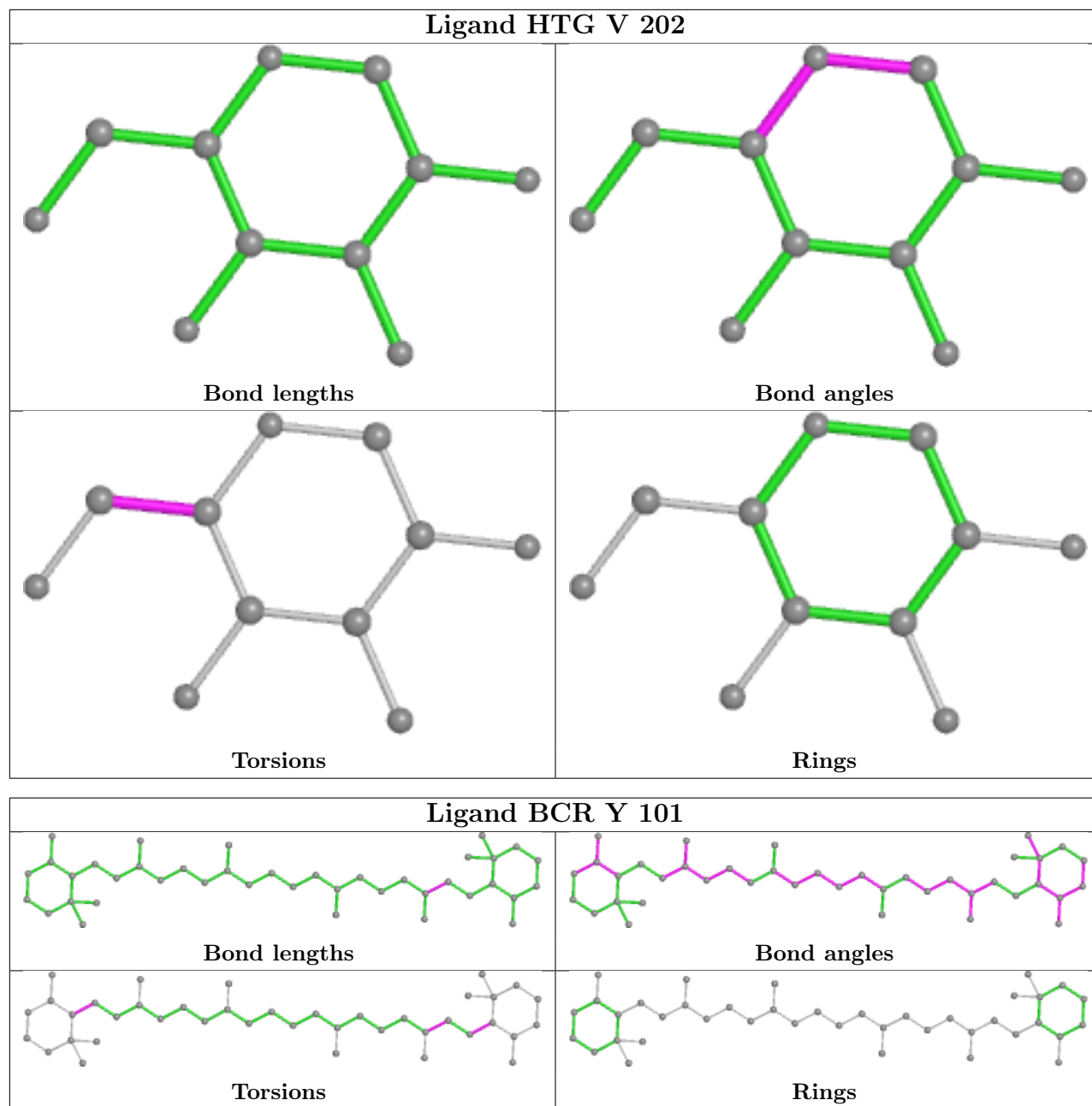
Ligand HEM e 102

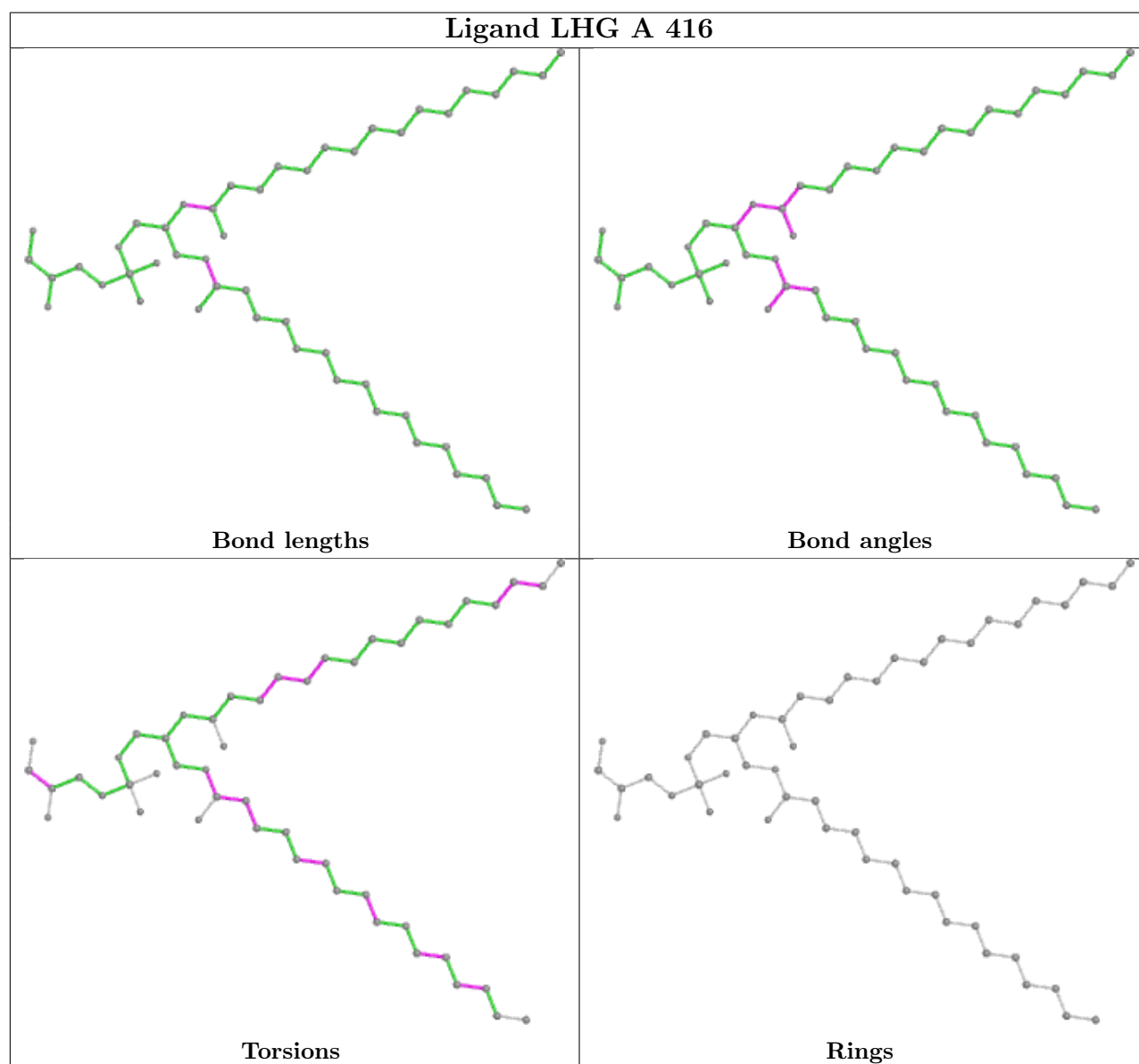
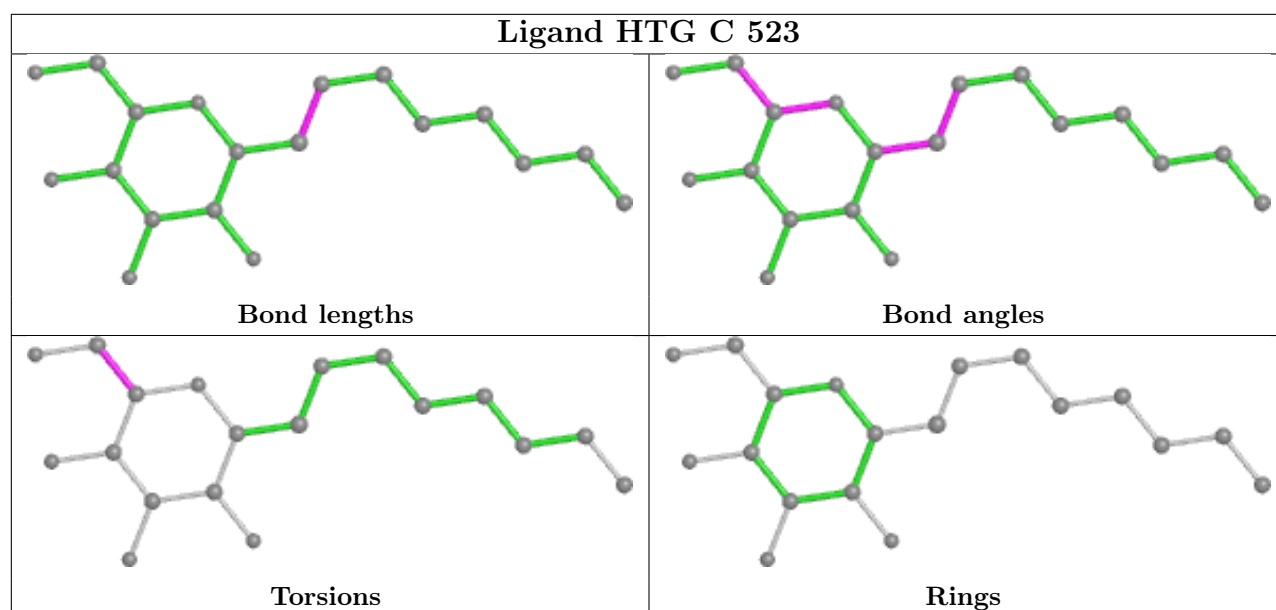


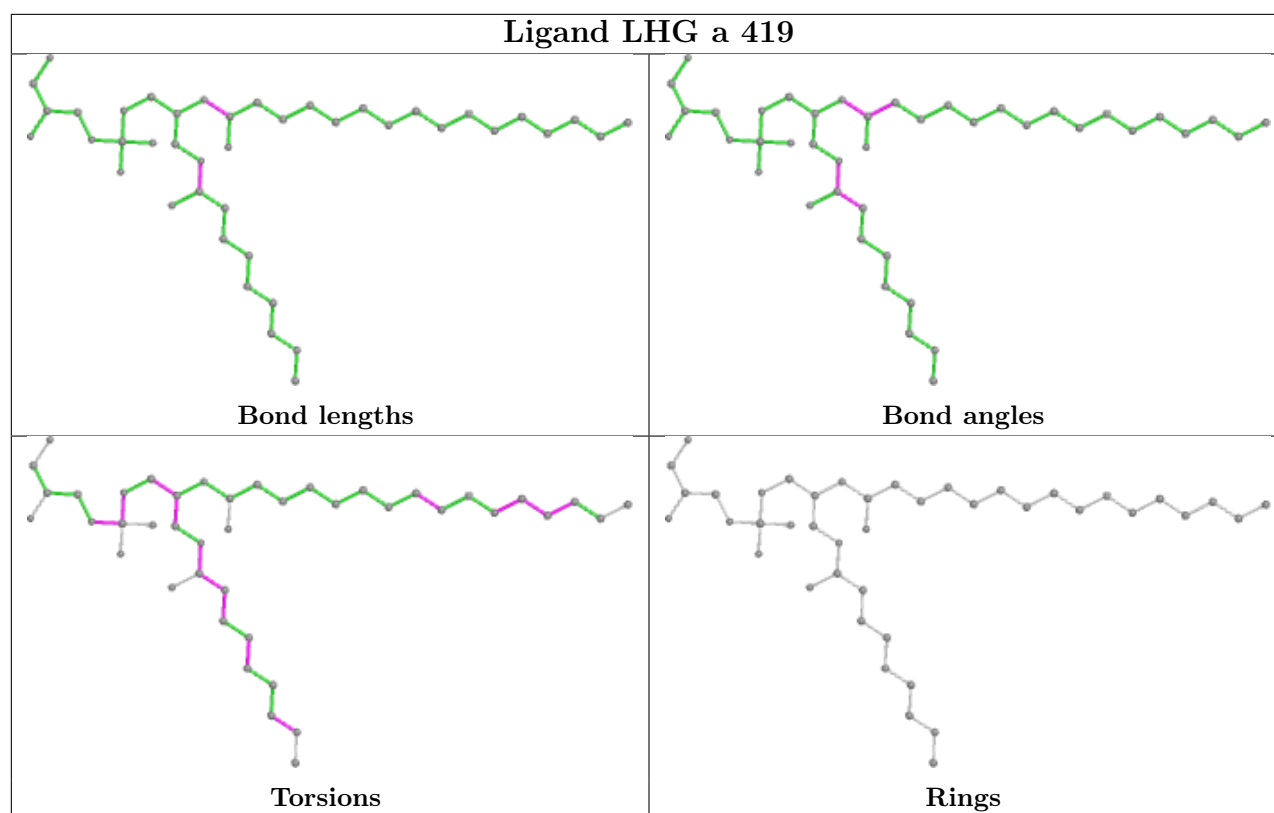
Ligand DGD H 102











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.11	8 (2%) 59 57	34, 44, 69, 128	0
1	a	334/344 (97%)	-0.02	9 (2%) 54 52	37, 48, 78, 110	0
2	B	504/505 (99%)	-0.32	23 (4%) 32 31	37, 49, 81, 127	0
2	b	504/505 (99%)	-0.11	43 (8%) 10 10	39, 53, 92, 158	0
3	C	451/455 (99%)	-0.24	20 (4%) 34 33	40, 56, 82, 156	0
3	c	455/455 (100%)	-0.05	23 (5%) 28 26	44, 64, 86, 133	0
4	D	342/342 (100%)	-0.22	6 (1%) 68 66	35, 45, 68, 139	0
4	d	341/342 (99%)	-0.18	16 (4%) 31 30	38, 50, 73, 129	0
5	E	81/84 (96%)	0.24	7 (8%) 10 9	51, 70, 96, 139	0
5	e	79/84 (94%)	0.30	9 (11%) 5 4	59, 74, 116, 157	0
6	F	34/44 (77%)	-0.35	1 (2%) 51 50	50, 62, 85, 108	0
6	f	31/44 (70%)	-0.19	2 (6%) 18 17	58, 67, 92, 144	0
7	H	64/65 (98%)	-0.54	1 (1%) 72 70	43, 59, 81, 133	0
7	h	64/65 (98%)	0.05	2 (3%) 49 47	52, 65, 91, 105	0
8	I	37/38 (97%)	-0.28	2 (5%) 25 24	49, 60, 124, 148	0
8	i	37/38 (97%)	-0.44	1 (2%) 54 52	52, 60, 114, 145	0
9	J	38/39 (97%)	0.31	7 (18%) 1 1	50, 70, 131, 177	0
9	j	39/39 (100%)	0.08	4 (10%) 6 6	58, 73, 125, 165	0
10	K	37/37 (100%)	-0.62	0 100 100	58, 67, 89, 113	0
10	k	37/37 (100%)	-0.10	2 (5%) 25 24	66, 73, 95, 113	0
11	L	36/37 (97%)	-0.32	0 100 100	35, 41, 93, 140	0
11	l	36/37 (97%)	-0.15	1 (2%) 53 51	37, 42, 105, 134	0
12	M	32/36 (88%)	-0.34	0 100 100	38, 44, 73, 146	0
12	m	33/36 (91%)	-0.35	1 (3%) 50 49	38, 44, 82, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.03	22 (9%) 9 8	35, 60, 113, 178	0
13	o	243/244 (99%)	0.42	42 (17%) 1 1	40, 61, 119, 171	0
14	T	29/32 (90%)	-0.53	0 100 100	38, 43, 83, 104	0
14	t	29/32 (90%)	-0.42	0 100 100	38, 46, 74, 139	0
15	U	96/104 (92%)	-0.38	1 (1%) 82 80	44, 56, 88, 92	0
15	u	97/104 (93%)	-0.59	0 100 100	48, 61, 80, 129	0
16	V	137/137 (100%)	-0.51	0 100 100	43, 55, 80, 112	0
16	v	137/137 (100%)	0.10	14 (10%) 6 6	50, 69, 103, 131	0
17	X	38/40 (95%)	-0.09	4 (10%) 6 5	54, 69, 91, 110	0
17	x	38/40 (95%)	0.57	7 (18%) 1 1	60, 74, 124, 157	0
18	Y	29/30 (96%)	1.57	9 (31%) 0 0	67, 89, 136, 169	0
18	y	29/30 (96%)	0.45	6 (20%) 1 0	75, 87, 113, 116	0
19	Z	62/62 (100%)	0.76	11 (17%) 1 1	69, 83, 138, 186	0
19	z	62/62 (100%)	1.43	20 (32%) 0 0	76, 95, 137, 185	0
20	R	34/34 (100%)	4.62	34 (100%) 0 0	91, 106, 138, 142	0
All	All	5283/5384 (98%)	-0.06	358 (6%) 17 15	34, 56, 99, 186	0

All (358) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	Y	19	ILE	9.3
17	x	38	GLN	8.9
20	R	6	LEU	8.0
1	A	11	ALA	6.6
20	R	5	VAL	6.2
20	R	15	ALA	6.2
20	R	18	TRP	6.0
3	C	143	TYR	5.9
13	o	4	THR	5.8
2	b	499	VAL	5.8
20	R	14	LEU	5.8
20	R	19	ALA	5.7
20	R	3	TRP	5.6
20	R	35	LEU	5.5
5	E	84	LYS	5.3
20	R	4	ARG	5.2
20	R	20	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
20	R	8	VAL	5.2
13	O	27	ARG	5.2
17	x	37	VAL	5.1
1	A	13	LEU	5.1
3	c	143	TYR	5.0
20	R	12	VAL	5.0
20	R	31	VAL	5.0
20	R	7	VAL	4.9
13	o	27	ARG	4.9
9	J	4	GLY	4.9
18	y	19	ILE	4.9
20	R	16	ALA	4.8
2	b	495	PHE	4.8
20	R	33	LYS	4.8
13	o	22	LEU	4.7
20	R	34	LEU	4.6
13	o	133	VAL	4.6
20	R	17	GLY	4.6
19	z	5	PHE	4.5
20	R	2	ASP	4.5
9	j	2	SER	4.5
13	o	5	LEU	4.5
5	e	59	GLU	4.4
20	R	10	LEU	4.4
4	d	12	ARG	4.4
20	R	32	GLN	4.4
19	z	42	LEU	4.4
2	b	504	THR	4.4
2	b	486	LEU	4.3
18	Y	18	VAL	4.3
20	R	13	LEU	4.3
2	b	500	GLY	4.3
20	R	9	LEU	4.3
1	a	11	ALA	4.3
3	C	155	ASN	4.2
13	O	60	ARG	4.2
4	D	238	THR	4.2
20	R	21	ARG	4.2
19	Z	3	ILE	4.2
9	j	3	GLU	4.1
12	m	34	LYS	4.1
20	R	26	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	b	484	PRO	4.0
20	R	24	LEU	4.0
9	J	7	ILE	3.9
13	O	5	LEU	3.9
19	Z	31	GLN	3.9
19	z	60	PHE	3.8
2	b	503	THR	3.8
9	J	3	GLU	3.8
18	Y	41	VAL	3.8
2	B	494	GLY	3.8
13	o	25	THR	3.8
2	b	497	GLN	3.8
9	J	6	ARG	3.7
17	x	39	ARG	3.7
10	k	18	PHE	3.7
2	b	496	TYR	3.7
5	E	83	LEU	3.7
13	O	4	THR	3.7
13	O	28	GLY	3.7
13	o	26	ALA	3.7
2	B	293	ALA	3.7
2	b	296	ALA	3.7
16	v	21	LEU	3.7
18	y	18	VAL	3.7
18	Y	43	ARG	3.7
2	b	488	PRO	3.7
9	J	2	SER	3.6
18	Y	20	ALA	3.6
13	o	206	GLY	3.6
2	B	504	THR	3.6
6	f	15	ILE	3.6
13	O	133	VAL	3.6
2	b	485	GLU	3.6
3	c	426	LEU	3.5
19	z	46	LEU	3.5
17	x	33	GLN	3.5
3	c	428	THR	3.5
13	o	134	THR	3.5
2	b	294	SER	3.5
13	o	32	ILE	3.5
2	b	293	ALA	3.5
18	y	20	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
20	R	27	ALA	3.5
13	o	58	ASN	3.5
3	C	145[A]	SER	3.5
1	A	12	ASN	3.5
2	B	490	GLN	3.4
5	E	17	VAL	3.4
3	c	433	LEU	3.4
3	c	429	SER	3.4
13	o	35	SER	3.4
19	z	31	GLN	3.4
5	E	11	SER	3.4
19	Z	32	ASP	3.4
2	b	498	LYS	3.3
2	b	493	TRP	3.3
3	c	430	HIS	3.3
13	o	203	LYS	3.3
2	B	297	THR	3.3
13	o	204	VAL	3.3
2	b	494	GLY	3.3
13	o	24	ASP	3.2
20	R	29	LYS	3.2
13	O	139	SER	3.2
2	b	461	LEU	3.2
13	O	204	VAL	3.2
7	h	6	TRP	3.2
20	R	23	ILE	3.2
20	R	11	PRO	3.2
13	o	36	GLN	3.2
17	x	2	THR	3.2
3	c	203	THR	3.2
19	z	2	THR	3.2
19	Z	60	PHE	3.2
18	Y	21	GLN	3.2
4	d	152	VAL	3.2
3	C	253	LEU	3.2
16	v	26	TYR	3.2
8	I	38	GLU	3.1
16	v	17	LYS	3.1
20	R	25	PRO	3.1
13	o	38	TYR	3.1
1	A	15	GLU	3.0
2	b	489	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
19	Z	53	VAL	3.0
2	B	489	GLU	3.0
13	o	33	ASP	3.0
17	X	37	VAL	3.0
10	k	17	ILE	3.0
19	z	41	PHE	3.0
2	B	496	TYR	3.0
13	o	34	SER	3.0
2	b	457	VAL	3.0
2	b	487	SER	3.0
19	z	7	LEU	3.0
1	a	285	PHE	2.9
5	e	39	SER	2.9
13	O	25	THR	2.9
13	o	60	ARG	2.9
20	R	22	ASN	2.9
6	F	13	TYR	2.9
13	O	132	ASN	2.9
17	X	2	THR	2.9
17	X	38	GLN	2.9
2	B	495	PHE	2.9
2	b	298	LEU	2.9
17	x	36	LYS	2.9
1	a	224	ILE	2.8
2	b	248	ALA	2.8
19	z	61	VAL	2.8
4	d	151	ALA	2.8
13	O	21	THR	2.8
2	B	185	TRP	2.8
13	o	136	ILE	2.8
4	d	283	ALA	2.8
13	o	246	ALA	2.8
20	R	30	GLN	2.8
19	z	1	MET	2.8
9	J	5	GLY	2.8
13	o	87	VAL	2.8
4	D	12	ARG	2.8
3	c	200	THR	2.8
2	b	460	LEU	2.8
1	a	246[A]	TYR	2.8
18	y	21	GLN	2.8
13	o	243	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
19	Z	1	MET	2.8
2	B	295	GLY	2.7
2	b	249	ALA	2.7
1	A	249	VAL	2.7
2	b	402	TYR	2.7
2	b	505	ARG	2.7
5	E	15	THR	2.7
13	o	142	PHE	2.7
18	Y	25	ILE	2.7
3	C	23	ALA	2.7
13	o	37	THR	2.7
17	x	34	ILE	2.7
19	z	3	ILE	2.7
19	Z	4	LEU	2.7
19	z	32	ASP	2.7
13	O	138	THR	2.7
16	v	1	ALA	2.7
3	C	181	PHE	2.7
3	c	312	ALA	2.7
3	C	257	PHE	2.7
13	o	40	ILE	2.7
13	o	30	TYR	2.7
2	b	491	VAL	2.6
13	O	87	VAL	2.6
2	b	459	ALA	2.6
13	O	22	LEU	2.6
6	f	16	PHE	2.6
13	O	130	GLN	2.6
9	j	1	MET	2.6
2	B	296	ALA	2.6
13	O	26	ALA	2.6
20	R	28	VAL	2.6
5	e	83	LEU	2.6
19	z	9	LEU	2.6
3	c	199	ILE	2.6
19	z	62	VAL	2.6
3	c	283	GLY	2.6
4	D	154	VAL	2.6
13	o	21	THR	2.6
13	o	140	THR	2.6
2	B	298	LEU	2.6
9	j	4	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
4	d	238	THR	2.6
19	z	59	PHE	2.5
13	o	127	ALA	2.5
18	y	43	ARG	2.5
3	c	427	ALA	2.5
2	b	502	VAL	2.5
2	b	458	PHE	2.5
5	e	79	PHE	2.5
13	o	59	LYS	2.5
3	c	284	PHE	2.5
4	D	153	PHE	2.5
3	C	154	LYS	2.5
2	b	245	VAL	2.5
7	H	65	LEU	2.5
13	o	130	GLN	2.5
13	o	39	ARG	2.5
2	b	246	PHE	2.5
3	c	436	PHE	2.5
2	b	456	ALA	2.5
16	v	5	PRO	2.5
4	D	11	GLU	2.5
4	d	279	LEU	2.4
3	c	201	ASN	2.4
2	B	486	LEU	2.4
2	B	461	LEU	2.4
13	o	199	LEU	2.4
3	C	148	GLY	2.4
3	c	202	PRO	2.4
4	d	240	ALA	2.4
19	Z	2	THR	2.4
13	O	23	ASP	2.4
3	C	147	PHE	2.4
3	c	424	SER	2.4
4	d	155	SER	2.4
9	J	8	PRO	2.3
19	z	4	LEU	2.3
19	z	57	LEU	2.3
1	a	281	VAL	2.3
4	d	159	ILE	2.3
3	c	146	PHE	2.3
2	B	491	VAL	2.3
3	C	142	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	156	VAL	2.3
2	b	411	PHE	2.3
3	C	144	SER	2.3
8	i	38	GLU	2.3
16	v	16	GLY	2.3
5	e	25	ILE	2.3
16	v	8	LEU	2.3
4	d	154	VAL	2.3
13	o	200	ASN	2.3
2	B	294	SER	2.3
13	o	211	ILE	2.3
2	b	297	THR	2.3
1	A	200	LEU	2.3
1	a	242	GLU	2.3
8	I	37	LEU	2.3
2	B	488	PRO	2.2
13	O	56	PRO	2.2
16	v	10	VAL	2.2
15	U	73	GLN	2.2
2	b	501	ASP	2.2
19	Z	33	TRP	2.2
3	C	140	LEU	2.2
3	C	433	LEU	2.2
7	h	10	ILE	2.2
11	l	3	PRO	2.2
1	A	243	GLU	2.2
2	b	492	GLU	2.2
2	B	487	SER	2.2
13	O	62	GLU	2.2
2	B	481	GLY	2.2
2	b	462	PHE	2.2
13	o	132	ASN	2.2
5	E	20	TRP	2.2
4	d	156	VAL	2.2
3	c	87	ILE	2.2
2	B	411	PHE	2.2
2	B	501	ASP	2.2
18	Y	22	LEU	2.2
13	O	61	GLN	2.2
16	v	19	ILE	2.2
1	A	16	ARG	2.2
3	C	283	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
16	v	6	GLU	2.2
3	C	286	ALA	2.1
2	b	295	GLY	2.1
19	z	43	GLY	2.1
1	a	196	PRO	2.1
3	c	279	LEU	2.1
5	e	36	LEU	2.1
4	d	281	MET	2.1
13	O	24	ASP	2.1
13	o	207	ARG	2.1
3	C	255	THR	2.1
13	O	134	THR	2.1
19	z	30	PRO	2.1
2	B	458	PHE	2.1
1	a	200	LEU	2.1
1	a	288	LEU	2.1
13	o	57	LYS	2.1
16	v	107	LEU	2.1
13	o	91	GLY	2.1
4	d	237	PRO	2.1
2	B	482	ILE	2.1
5	e	20	TRP	2.1
2	b	301	ALA	2.1
3	C	210	PHE	2.1
4	d	153	PHE	2.1
16	v	27	LEU	2.1
18	y	22	LEU	2.1
19	z	38	GLN	2.1
3	C	254	THR	2.0
3	c	432	VAL	2.0
16	v	4	THR	2.0
16	v	22	THR	2.0
3	c	280	SER	2.0
3	c	434	ALA	2.0
5	e	21	VAL	2.0
13	o	85	LEU	2.0
17	X	3	ILE	2.0
2	b	414	PRO	2.0
4	d	148	ALA	2.0
2	b	251	VAL	2.0
3	C	432	VAL	2.0
4	d	286	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
19	Z	54	VAL	2.0
5	e	61	ARG	2.0
19	Z	57	LEU	2.0
5	E	10	PHE	2.0
18	Y	24	MET	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
12	FME	M	1	10/11	0.96	0.13	31,59,83,93	0
8	FME	I	1	10/11	0.97	0.14	46,67,72,75	0
14	FME	T	1	10/11	0.97	0.09	39,48,63,64	0
8	FME	i	1	10/11	0.97	0.11	52,62,75,81	0
12	FME	m	1	10/11	0.98	0.08	38,52,79,90	0
14	FME	t	1	10/11	0.98	0.08	35,44,61,70	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(Å ²)	Q<0.9
34	LMG	C	522	51/55	0.47	0.44	76,125,159,161	0
33	LMT	C	526	35/35	0.53	0.55	93,147,159,160	0
33	LMT	a	412	35/35	0.54	0.39	63,131,144,146	0
33	LMT	F	101	35/35	0.54	0.41	105,152,164,167	0
32	HTG	D	411	16/19	0.60	0.33	82,116,129,129	0
33	LMT	M	103	35/35	0.60	0.32	75,140,160,163	0
30	UNL	A	414	28/-	0.61	0.46	88,103,120,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMG	c	522	51/55	0.62	0.41	80,125,151,152	0
33	LMT	D	402	35/35	0.63	0.35	75,130,140,142	0
32	HTG	b	622	19/19	0.63	0.57	86,138,148,150	0
30	UNL	C	527	34/-	0.63	0.36	83,110,123,129	0
33	LMT	m	103	35/35	0.64	0.38	59,97,109,113	0
30	UNL	I	101	40/-	0.65	0.28	74,108,148,149	0
30	UNL	j	101	10/-	0.65	0.34	81,90,102,103	0
30	UNL	b	625	33/-	0.66	0.36	65,94,146,147	0
33	LMT	e	101	35/35	0.68	0.62	121,173,177,179	0
30	UNL	a	415	30/-	0.69	0.31	100,110,133,140	0
31	LHG	E	101	42/49	0.70	0.26	74,114,131,133	0
33	LMT	M	102	35/35	0.71	0.27	54,105,130,138	0
30	UNL	i	101	40/-	0.73	0.31	72,97,151,154	0
33	LMT	b	620	25/35	0.73	0.24	90,129,147,148	0
27	GOL	B	626	6/6	0.73	0.27	82,99,100,103	0
34	LMG	Z	101	37/55	0.74	0.32	73,129,162,169	0
33	LMT	B	627	35/35	0.74	0.28	68,112,127,131	0
29	PL9	A	413[A]	55/55	0.75	0.32	89,97,103,104	55
30	UNL	d	410	36/-	0.75	0.26	72,92,117,120	0
30	UNL	J	101	10/-	0.75	0.29	69,84,88,90	0
29	PL9	A	413[B]	55/55	0.75	0.32	88,97,104,104	55
31	LHG	a	419	42/49	0.76	0.34	86,136,170,174	0
33	LMT	a	418	35/35	0.76	0.51	113,144,152,153	0
30	UNL	B	625	33/-	0.76	0.24	56,105,148,152	0
30	UNL	c	526	32/-	0.76	0.37	91,111,125,129	0
27	GOL	c	527	6/6	0.77	0.37	105,109,114,116	0
26	SQD	f	101	43/54	0.77	0.45	111,129,159,160	0
33	LMT	B	629	25/35	0.78	0.22	56,79,132,133	0
30	UNL	m	102	10/-	0.79	0.23	59,67,88,90	0
32	HTG	B	622	19/19	0.79	0.35	79,89,99,100	0
33	LMT	b	626	25/35	0.79	0.22	46,70,129,135	0
27	GOL	O	302	6/6	0.79	0.27	78,84,85,85	0
29	PL9	a	414[A]	55/55	0.80	0.29	93,104,111,112	55
33	LMT	B	630	26/35	0.80	0.24	78,117,140,143	0
32	HTG	h	101	16/19	0.80	0.30	99,134,140,142	0
29	PL9	a	414[B]	55/55	0.80	0.29	92,104,111,112	55
34	LMG	a	417	51/55	0.81	0.22	59,90,115,128	0
32	HTG	b	621	19/19	0.81	0.20	61,78,111,112	0
27	GOL	B	628	6/6	0.82	0.41	90,102,105,109	0
32	HTG	c	523	19/19	0.82	0.30	119,131,139,141	0
26	SQD	L	102	54/54	0.82	0.21	55,91,118,119	0
36	CA	F	102	1/1	0.82	0.07	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	LMG	z	101	39/55	0.83	0.29	81,136,147,148	0
30	UNL	l	101	10/-	0.83	0.24	63,74,83,85	0
32	HTG	V	202	11/19	0.84	0.39	109,114,122,124	0
32	HTG	B	621	19/19	0.84	0.23	72,87,118,120	0
34	LMG	c	521	51/55	0.84	0.30	66,93,123,128	0
30	UNL	D	410	40/-	0.85	0.23	52,87,126,132	0
25	BCR	h	102	40/40	0.85	0.18	50,66,74,75	0
36	CA	c	525	1/1	0.85	0.05	81,81,81,81	0
34	LMG	C	521	51/55	0.86	0.22	59,84,115,118	0
26	SQD	A	411	54/54	0.87	0.17	60,84,125,128	0
32	HTG	C	523	19/19	0.87	0.33	108,122,132,133	0
27	GOL	b	623	6/6	0.87	0.18	87,92,94,102	0
26	SQD	B	620	54/54	0.87	0.17	60,89,121,127	0
35	DGD	h	103	62/66	0.87	0.25	46,62,73,78	0
34	LMG	M	101	51/55	0.87	0.19	48,69,87,101	0
23	CLA	C	515	65/65	0.87	0.22	59,76,108,109	0
30	UNL	d	412	18/-	0.88	0.20	72,81,121,124	0
26	SQD	a	411	54/54	0.88	0.16	63,89,126,130	0
25	BCR	H	101	40/40	0.88	0.18	47,59,77,80	0
30	UNL	D	409	17/-	0.88	0.30	60,78,113,114	0
30	UNL	X	101	18/-	0.88	0.15	57,74,95,98	0
31	LHG	A	416	49/49	0.88	0.24	41,61,78,84	0
27	GOL	v	201	6/6	0.89	0.21	59,82,83,86	0
36	CA	O	301	1/1	0.89	0.18	118,118,118,118	0
34	LMG	m	101	51/55	0.89	0.22	53,69,98,101	0
35	DGD	C	519	62/66	0.90	0.18	45,64,116,121	0
35	DGD	c	519	62/66	0.90	0.20	51,73,114,122	0
23	CLA	C	514	65/65	0.90	0.18	55,69,119,122	0
25	BCR	k	102	40/40	0.90	0.17	58,72,89,92	0
34	LMG	C	502	51/55	0.90	0.20	58,89,113,120	0
30	UNL	d	409	17/-	0.90	0.22	68,84,106,108	0
26	SQD	D	413	43/54	0.91	0.22	70,105,125,136	0
23	CLA	c	514	65/65	0.91	0.17	62,80,117,125	0
23	CLA	B	602	65/65	0.91	0.16	40,51,74,84	0
35	DGD	C	520	62/66	0.91	0.19	43,57,92,104	0
35	DGD	H	102	62/66	0.91	0.22	41,57,76,80	0
36	CA	o	301	1/1	0.91	0.10	104,104,104,104	0
29	PL9	d	405	55/55	0.92	0.19	36,47,56,65	0
27	GOL	b	627	6/6	0.92	0.29	91,93,95,97	0
23	CLA	C	508	65/65	0.92	0.14	51,69,117,126	0
27	GOL	A	410	6/6	0.92	0.17	65,67,74,83	0
23	CLA	b	609	65/65	0.92	0.14	49,57,76,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	c	504	65/65	0.92	0.26	49,58,73,89	0
25	BCR	k	101	40/40	0.92	0.16	60,73,84,87	0
23	CLA	c	505	65/65	0.92	0.19	52,65,75,81	0
26	SQD	A	409	54/54	0.93	0.17	57,74,105,111	0
23	CLA	c	515	65/65	0.93	0.26	68,85,111,112	0
23	CLA	C	506	65/65	0.93	0.17	43,53,92,102	0
34	LMG	D	412	51/55	0.93	0.18	46,69,108,116	0
31	LHG	b	628	49/49	0.93	0.18	42,54,68,80	0
25	BCR	d	404	40/40	0.93	0.13	52,64,87,93	0
27	GOL	a	410	6/6	0.93	0.20	60,70,83,86	0
23	CLA	B	609	65/65	0.93	0.13	45,54,72,80	0
23	CLA	D	404	65/65	0.93	0.17	43,55,120,122	0
23	CLA	b	601	65/65	0.93	0.22	58,80,119,128	0
23	CLA	d	403	65/65	0.94	0.15	49,60,108,119	0
26	SQD	a	409	54/54	0.94	0.20	62,81,108,113	0
29	PL9	D	406	55/55	0.94	0.18	32,44,58,67	0
32	HTG	b	624	19/19	0.94	0.13	64,77,95,104	0
25	BCR	C	516	40/40	0.94	0.13	64,80,88,91	0
23	CLA	b	616	65/65	0.94	0.17	41,58,112,116	0
25	BCR	b	618	40/40	0.94	0.22	39,53,69,75	0
27	GOL	B	623	6/6	0.94	0.21	79,89,96,98	0
23	CLA	C	509	65/65	0.94	0.12	48,57,78,86	0
34	LMG	d	411	51/55	0.94	0.14	53,67,107,116	0
23	CLA	b	602	65/65	0.94	0.18	48,56,68,81	0
23	CLA	c	506	65/65	0.94	0.26	51,59,100,110	0
31	LHG	L	101	49/49	0.94	0.16	41,52,63,88	0
23	CLA	c	509	65/65	0.94	0.14	55,65,78,87	0
23	CLA	c	510	65/65	0.94	0.25	48,59,116,123	0
31	LHG	d	407	49/49	0.94	0.15	39,51,69,80	0
35	DGD	c	520	62/66	0.94	0.16	49,60,97,101	0
31	LHG	d	408	49/49	0.94	0.21	56,66,109,120	0
23	CLA	c	513	65/65	0.94	0.14	56,66,80,83	0
27	GOL	c	502	6/6	0.94	0.25	67,70,80,85	0
23	CLA	B	601	65/65	0.94	0.26	54,73,118,127	0
23	CLA	b	612	65/65	0.94	0.18	38,47,59,75	0
23	CLA	B	603	65/65	0.95	0.14	38,49,65,68	0
23	CLA	c	507	65/65	0.95	0.14	44,57,80,84	0
23	CLA	a	407	65/65	0.95	0.16	40,51,124,127	0
23	CLA	B	611	65/65	0.95	0.17	35,41,60,68	0
23	CLA	B	616	65/65	0.95	0.17	45,56,134,137	0
23	CLA	b	604	65/65	0.95	0.24	35,46,105,111	0
23	CLA	C	510	65/65	0.95	0.19	44,55,118,130	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	0.95	0.16	44,52,66,73	0
23	CLA	C	512	65/65	0.95	0.21	47,57,77,83	0
25	BCR	C	517	40/40	0.95	0.13	50,61,74,79	0
31	LHG	D	407	49/49	0.95	0.15	41,50,67,84	0
31	LHG	D	408	49/49	0.95	0.19	43,60,115,123	0
35	DGD	C	518	62/66	0.95	0.23	41,57,98,102	0
23	CLA	b	614	65/65	0.95	0.14	36,45,103,107	0
25	BCR	K	101	40/40	0.95	0.14	57,69,78,81	0
25	BCR	Y	101	40/40	0.95	0.12	53,67,77,84	0
25	BCR	b	617	40/40	0.95	0.15	39,49,57,59	0
31	LHG	d	406	49/49	0.95	0.25	50,62,82,94	0
23	CLA	C	513	65/65	0.95	0.13	51,65,83,84	0
25	BCR	c	516	40/40	0.95	0.16	68,85,89,95	0
23	CLA	C	503	65/65	0.95	0.14	47,56,66,81	0
36	CA	a	420	1/1	0.95	0.27	108,108,108,108	0
36	CA	c	524	1/1	0.95	0.07	75,75,75,75	0
23	CLA	C	505	65/65	0.95	0.13	48,58,73,76	0
32	HTG	B	624	19/19	0.95	0.11	63,79,90,90	0
23	CLA	b	611	65/65	0.96	0.22	38,47,70,82	0
24	PHO	A	415	64/64	0.96	0.24	36,46,53,54	0
25	BCR	A	408	40/40	0.96	0.12	35,46,55,56	0
25	BCR	B	618	40/40	0.96	0.17	39,53,64,68	0
25	BCR	B	619	40/40	0.96	0.10	43,55,74,76	0
25	BCR	B	631	40/40	0.96	0.15	36,57,68,70	0
23	CLA	B	614	65/65	0.96	0.14	34,44,96,103	0
23	CLA	a	405	65/65	0.96	0.21	40,50,112,117	0
25	BCR	D	405	40/40	0.96	0.15	48,57,94,99	0
23	CLA	b	615	65/65	0.96	0.11	41,52,73,79	0
23	CLA	B	607	65/65	0.96	0.16	32,42,62,72	0
25	BCR	T	101	40/40	0.96	0.14	35,51,63,63	0
23	CLA	c	503	65/65	0.96	0.13	56,63,75,79	0
25	BCR	a	408	40/40	0.96	0.11	38,48,56,59	0
23	CLA	A	407	65/65	0.96	0.12	39,47,109,116	0
23	CLA	C	504	65/65	0.96	0.18	44,57,77,85	0
35	DGD	c	518	62/66	0.96	0.20	46,59,90,92	0
23	CLA	b	603	65/65	0.96	0.16	41,53,74,81	0
25	BCR	c	517	40/40	0.96	0.12	54,67,73,75	0
23	CLA	B	610	65/65	0.96	0.15	42,50,63,75	0
23	CLA	c	508	65/65	0.96	0.13	56,69,122,127	0
23	CLA	b	605	65/65	0.96	0.16	36,47,67,70	0
23	CLA	b	606	65/65	0.96	0.13	40,52,114,120	0
23	CLA	b	607	65/65	0.96	0.18	33,43,72,80	0

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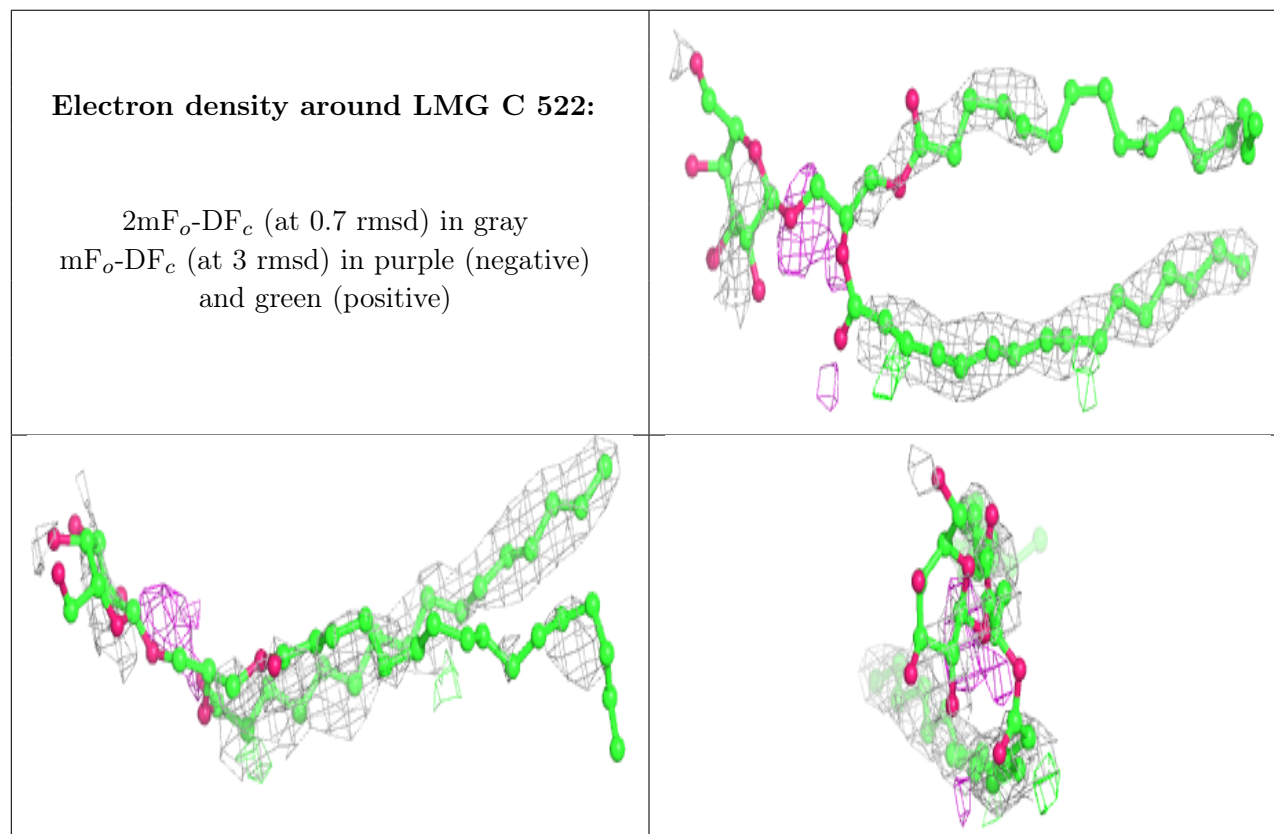
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	B	604	65/65	0.96	0.19	34,41,98,103	0
23	CLA	C	507	65/65	0.96	0.15	43,52,86,87	0
37	BCT	d	401[A]	4/4	0.96	0.12	55,59,59,60	4
37	BCT	d	401[B]	4/4	0.96	0.12	53,58,60,67	4
39	MG	J	102	1/1	0.96	0.14	56,56,56,56	0
24	PHO	A	406	64/64	0.97	0.15	33,41,49,58	0
23	CLA	C	511	65/65	0.97	0.13	49,58,76,83	0
24	PHO	a	416	64/64	0.97	0.18	40,48,55,63	0
25	BCR	b	619	40/40	0.97	0.11	46,55,77,86	0
23	CLA	B	613	65/65	0.97	0.23	36,43,86,93	0
25	BCR	B	617	40/40	0.97	0.14	38,47,58,61	0
27	GOL	C	524	6/6	0.97	0.16	49,58,63,63	0
23	CLA	B	608	65/65	0.97	0.18	39,49,66,67	0
23	CLA	B	615	65/65	0.97	0.12	40,47,75,84	0
23	CLA	b	613	65/65	0.97	0.26	34,45,80,86	0
23	CLA	B	605	65/65	0.97	0.12	37,43,59,71	0
23	CLA	c	511	65/65	0.97	0.19	54,63,79,88	0
23	CLA	c	512	65/65	0.97	0.29	52,61,74,79	0
23	CLA	B	606	65/65	0.97	0.12	39,50,95,104	0
23	CLA	a	403	65/65	0.97	0.19	37,43,66,74	0
23	CLA	A	405	65/65	0.97	0.21	34,46,107,111	0
38	HEM	e	102	43/43	0.97	0.19	63,77,113,121	0
23	CLA	b	608	65/65	0.97	0.21	45,53,68,73	0
39	MG	j	102	1/1	0.97	0.08	61,61,61,61	0
40	HEC	v	202	43/43	0.97	0.12	53,60,67,72	0
23	CLA	a	404	65/65	0.98	0.15	35,43,52,58	0
23	CLA	A	403	65/65	0.98	0.21	34,38,63,71	0
37	BCT	D	401[A]	4/4	0.98	0.09	57,57,60,62	4
37	BCT	D	401[B]	4/4	0.98	0.09	59,59,61,64	4
23	CLA	d	402	65/65	0.98	0.22	37,44,70,78	0
36	CA	C	525	1/1	0.98	0.21	68,68,68,68	0
38	HEM	E	102	43/43	0.98	0.13	58,65,82,93	0
23	CLA	D	403	65/65	0.98	0.24	33,40,57,69	0
23	CLA	B	612	65/65	0.98	0.15	36,44,58,67	0
23	CLA	A	404	65/65	0.98	0.18	32,40,51,56	0
40	HEC	V	201	43/43	0.98	0.09	44,51,55,56	0
24	PHO	a	406	64/64	0.98	0.14	35,44,51,58	0
21	FE2	a	401[A]	1/1	0.99	0.02	56,56,56,56	1
21	FE2	a	401[B]	1/1	0.99	0.02	63,63,63,63	1
22	CL	C	501	1/1	0.99	0.12	43,43,43,43	0
22	CL	c	501	1/1	0.99	0.11	46,46,46,46	0
28	OEX	A	412[A]	10/10	0.99	0.10	42,45,49,49	10

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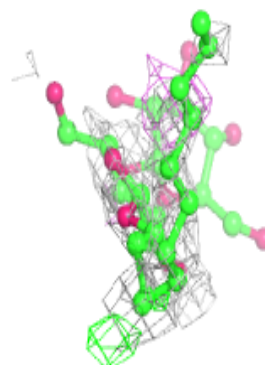
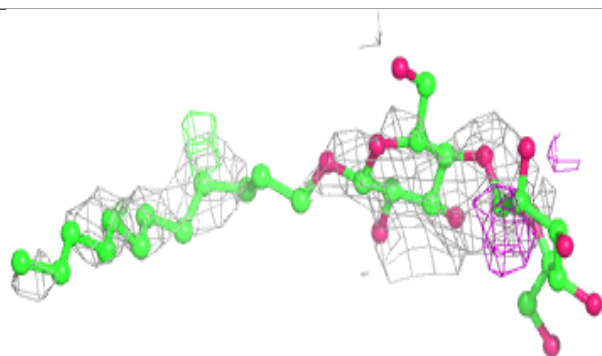
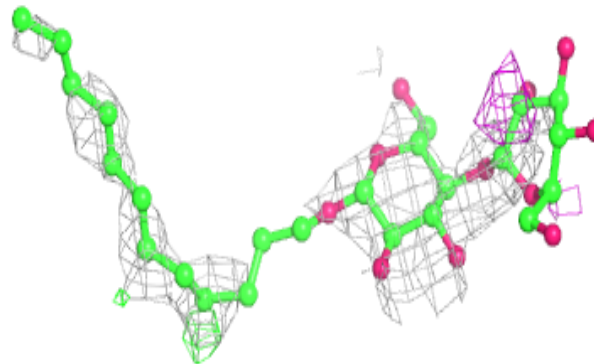
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	OEX	A	412[B]	10/10	0.99	0.10	39,46,51,51	10
22	CL	a	402	1/1	1.00	0.08	46,46,46,46	0
21	FE2	A	401[B]	1/1	1.00	0.03	57,57,57,57	1
22	CL	A	402	1/1	1.00	0.09	39,39,39,39	0
21	FE2	A	401[A]	1/1	1.00	0.03	54,54,54,54	1
28	OEX	a	413[A]	10/10	1.00	0.10	46,48,52,56	10
28	OEX	a	413[B]	10/10	1.00	0.10	44,50,54,54	10

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

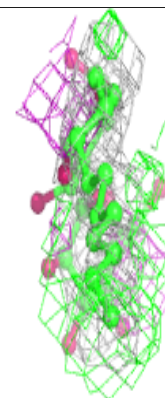
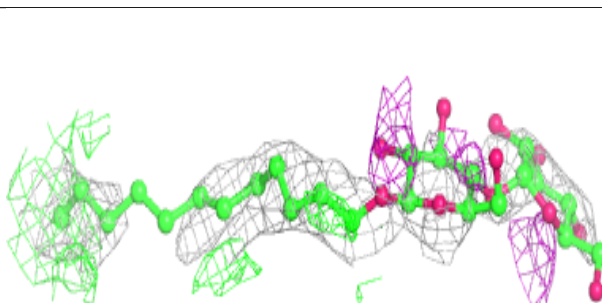
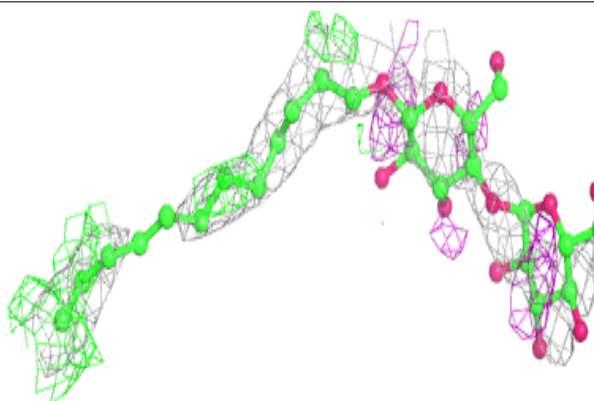


Electron density around LMT C 526:

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

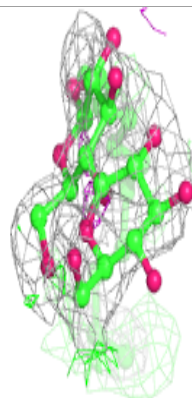
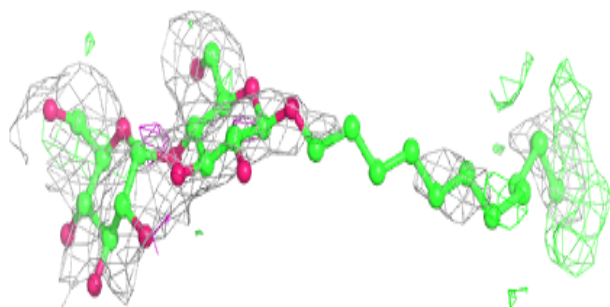
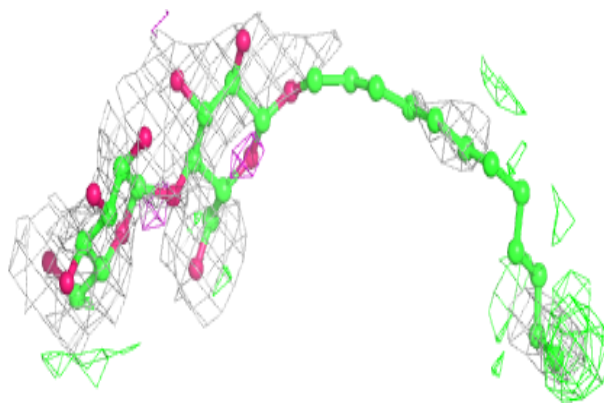
**Electron density around LMT a 412:**

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

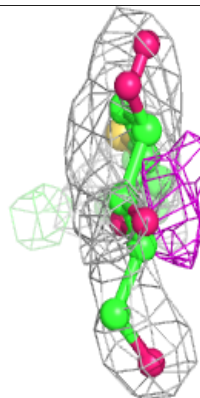
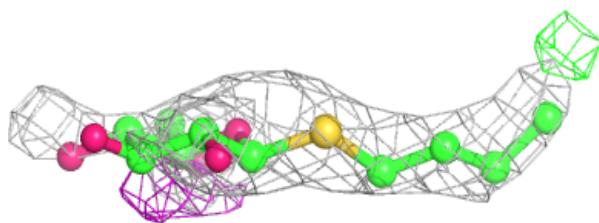
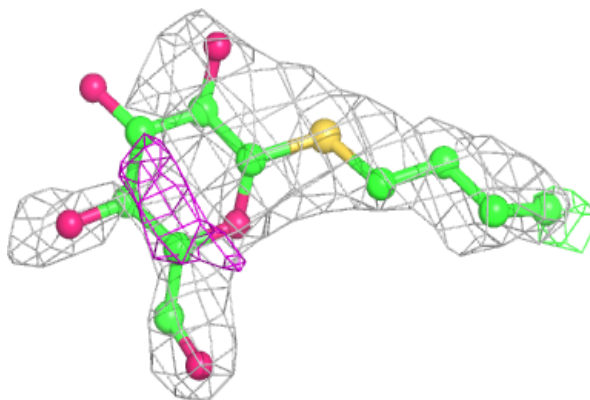


Electron density around LMT F 101:

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

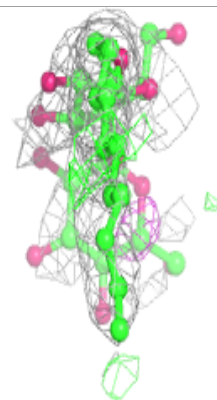
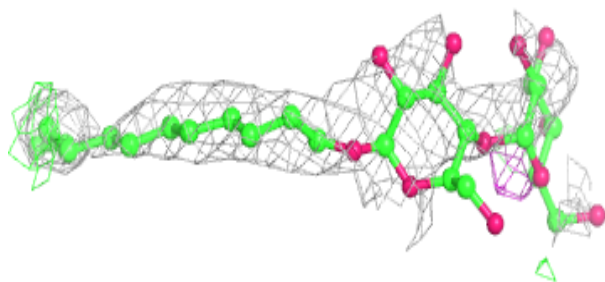
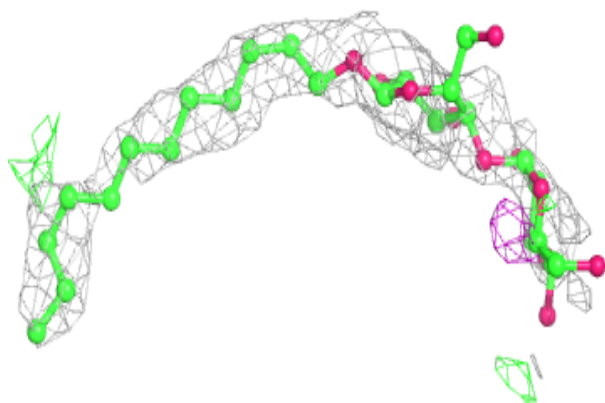
**Electron density around HTG D 411:**

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

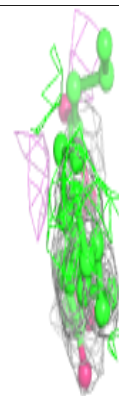
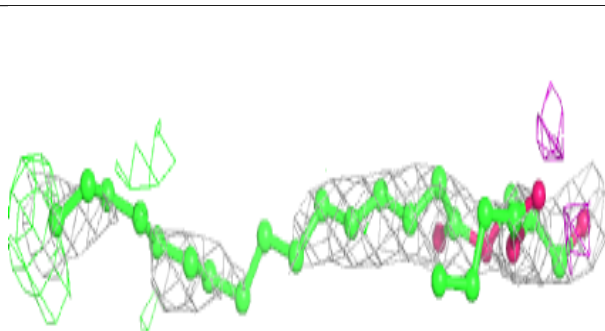
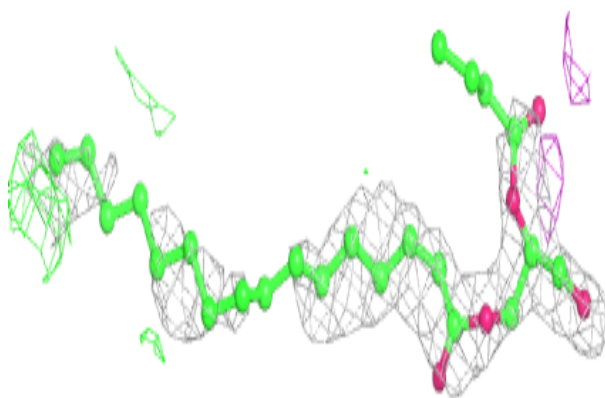


Electron density around LMT M 103:

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

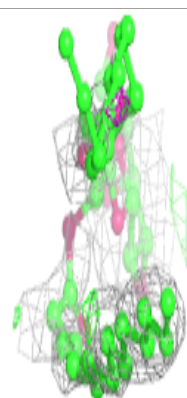
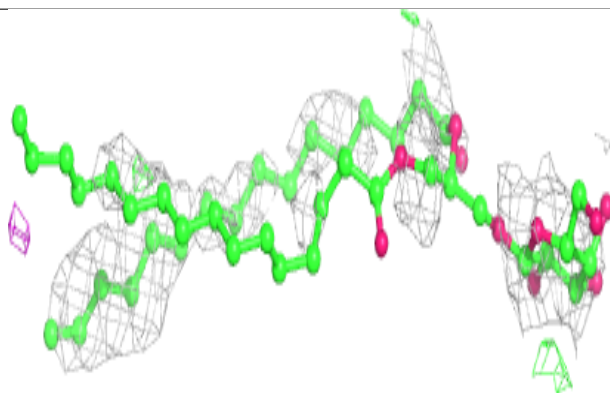
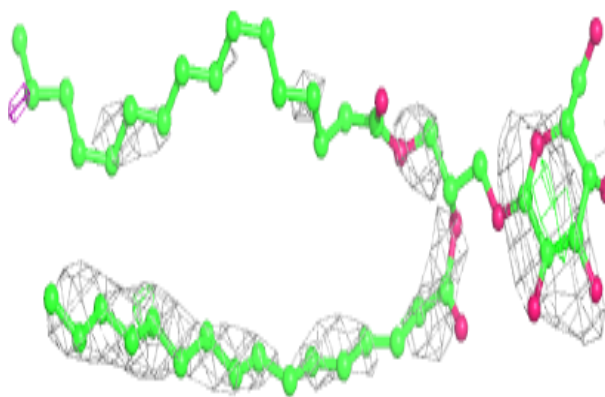
**Electron density around UNL A 414:**

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

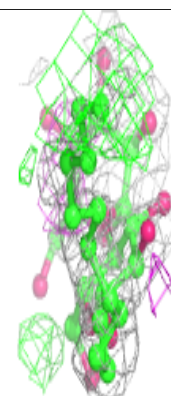
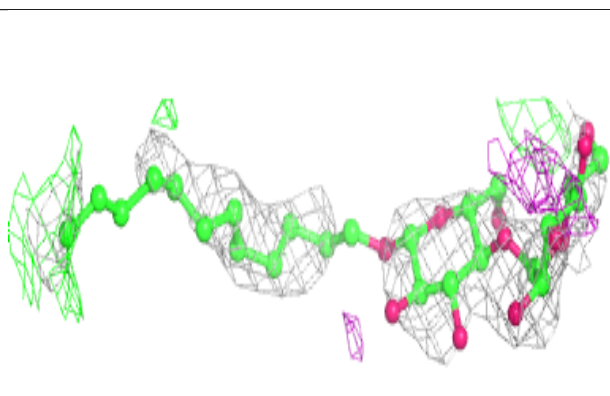
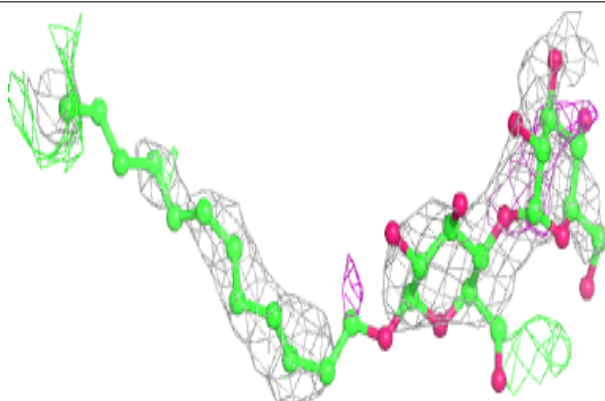


Electron density around LMG c 522:

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

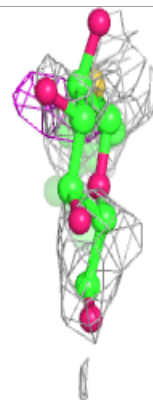
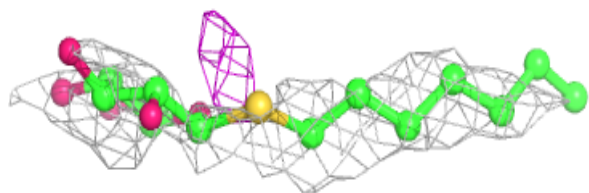
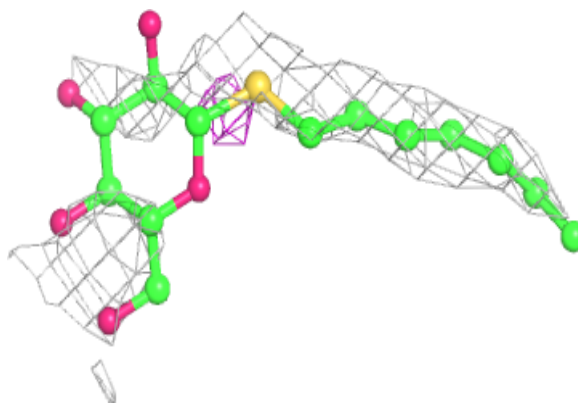
**Electron density around LMT D 402:**

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

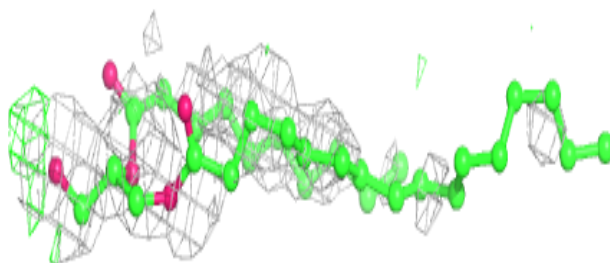
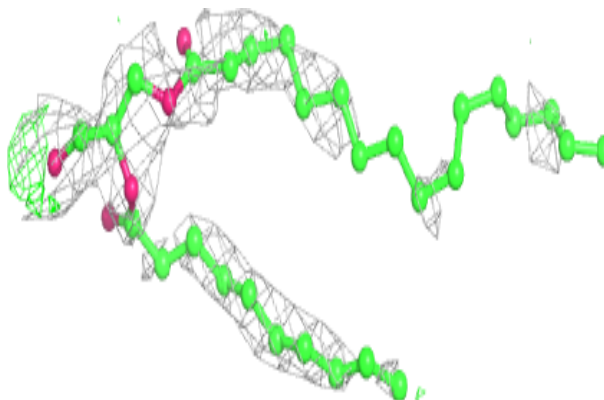


Electron density around HTG b 622:

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

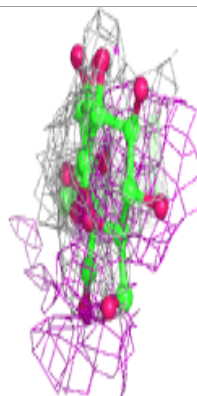
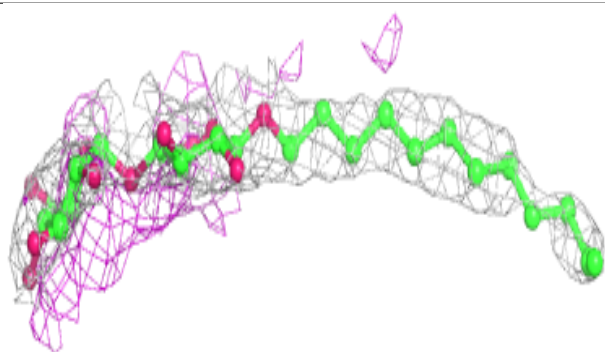
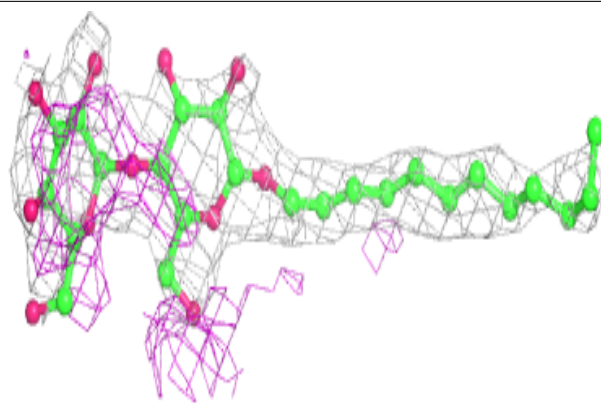
**Electron density around UNL C 527:**

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

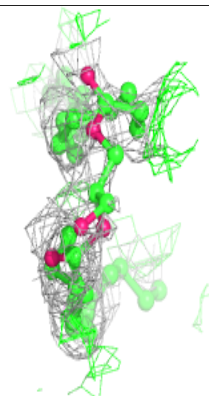
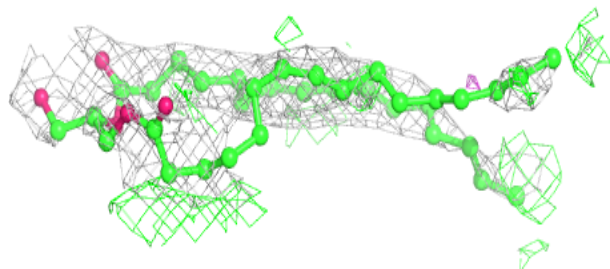
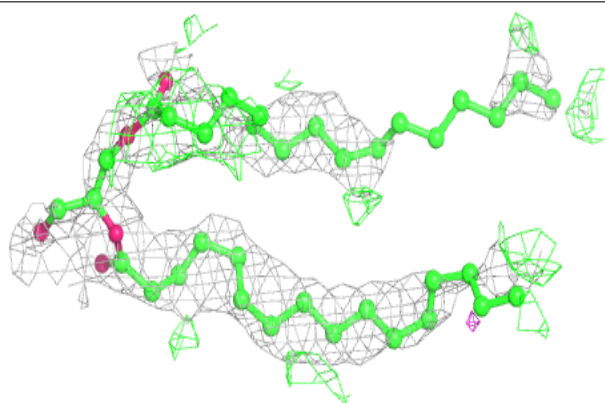


Electron density around LMT m 103:

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

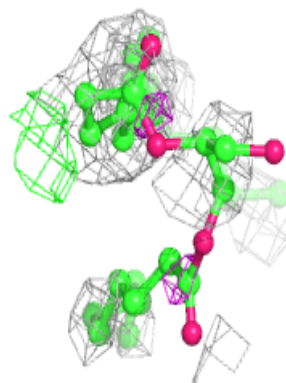
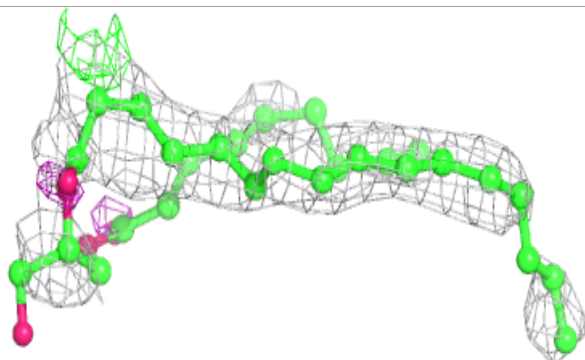
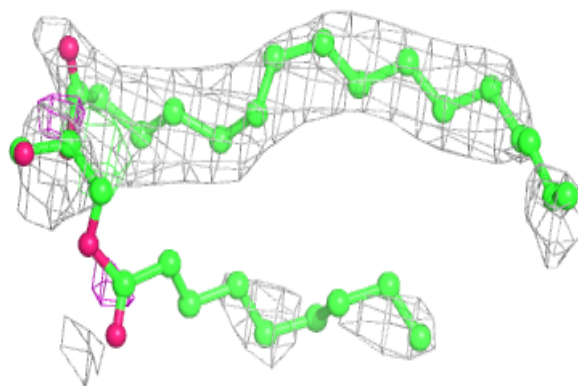
**Electron density around UNL I 101:**

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

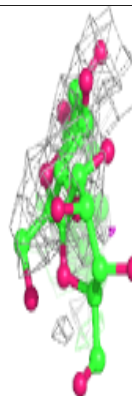
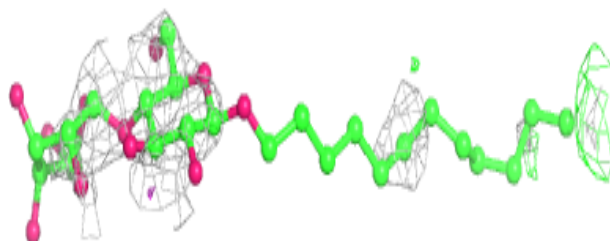
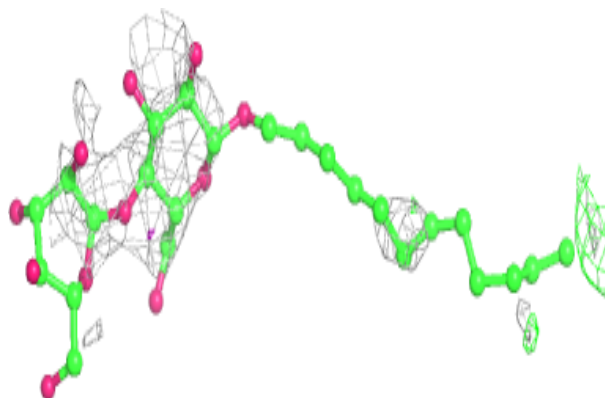


Electron density around UNL b 625:

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

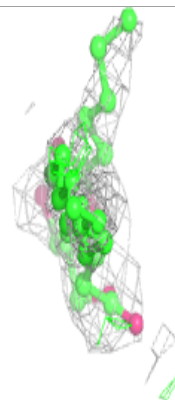
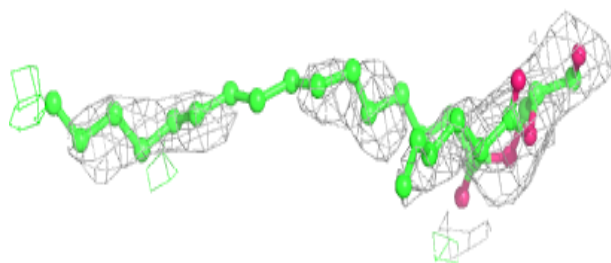
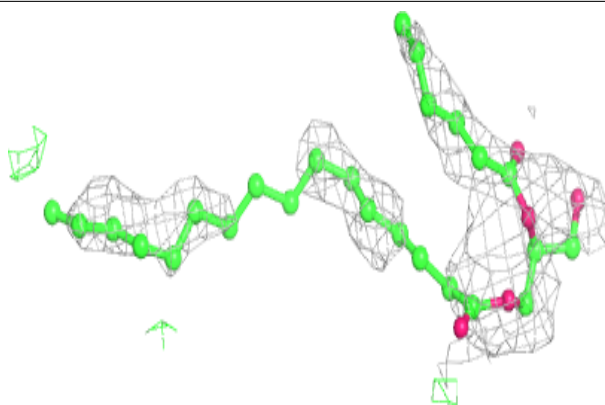
**Electron density around LMT e 101:**

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



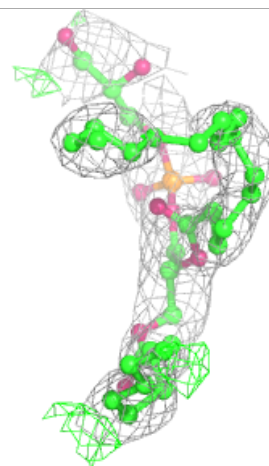
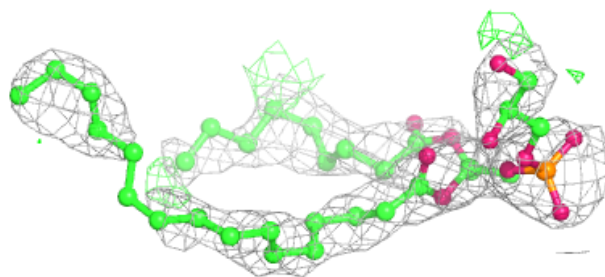
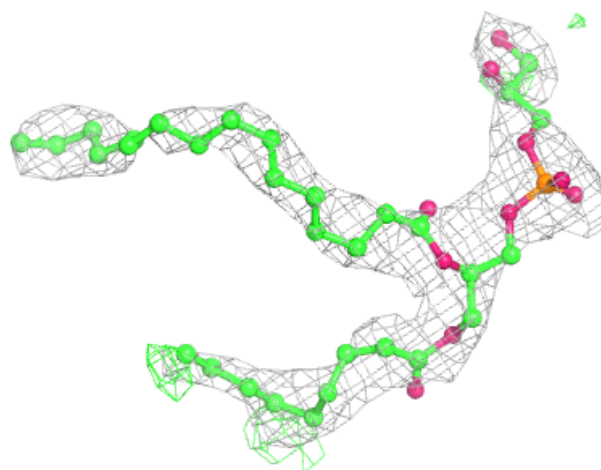
Electron density around UNL a 415:

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



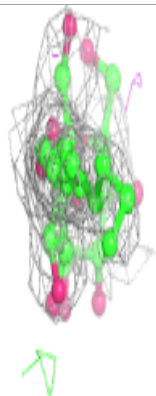
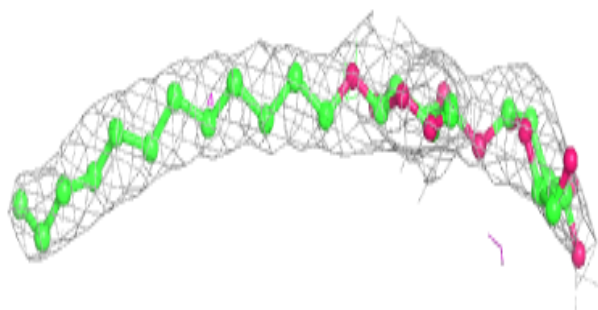
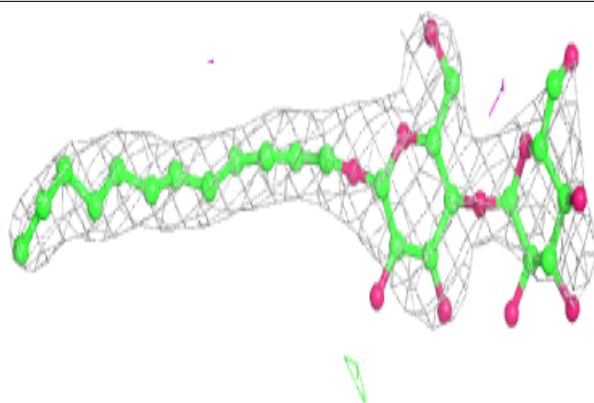
Electron density around LHG E 101:

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

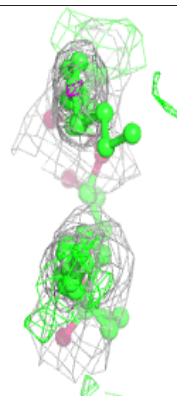
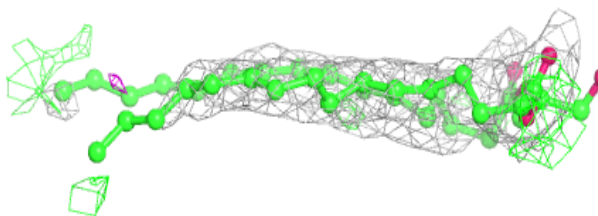
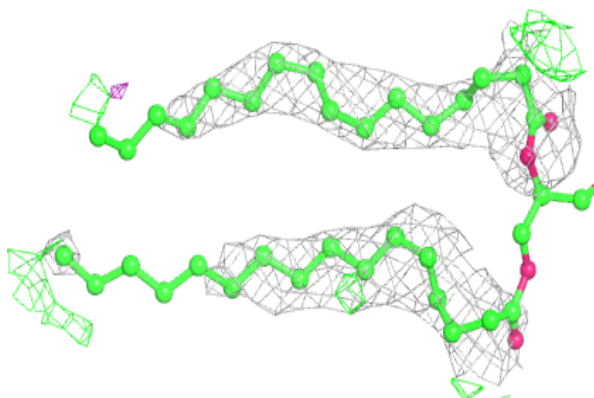


Electron density around LMT M 102:

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

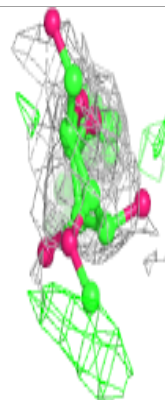
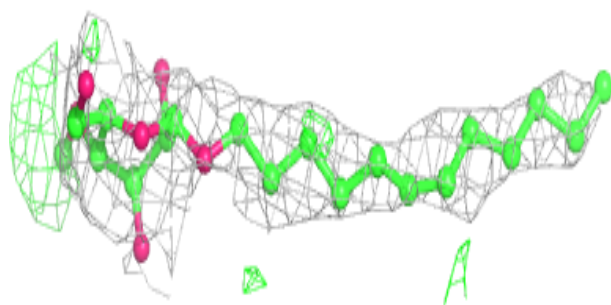
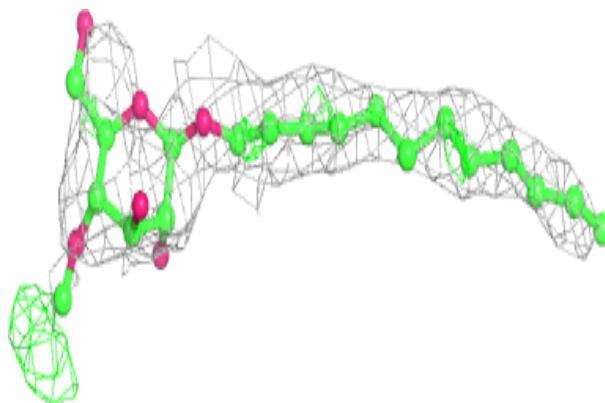
**Electron density around UNL i 101:**

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

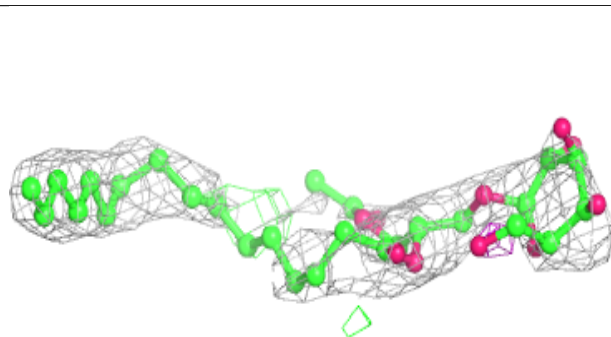
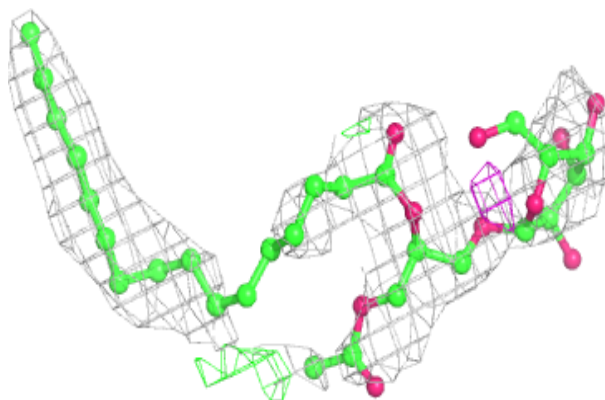


Electron density around LMT b 620:

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

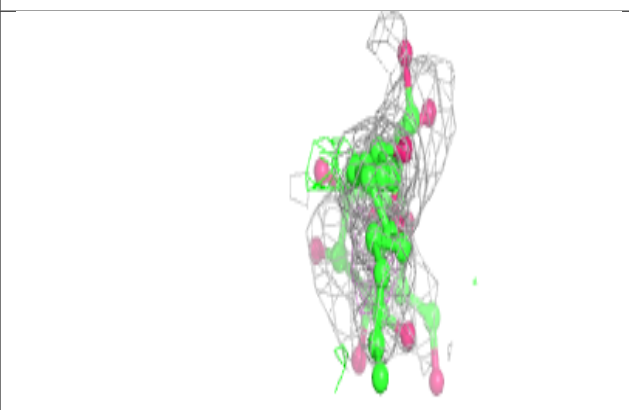
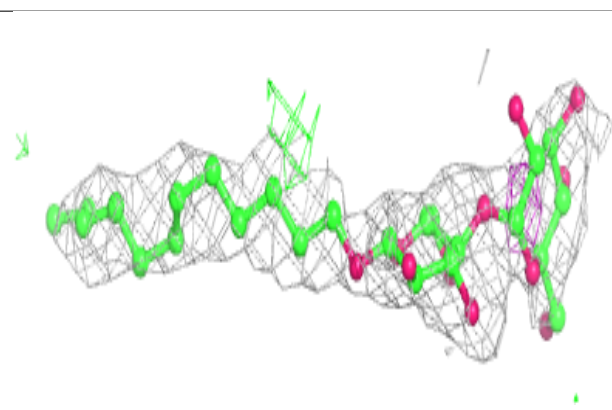
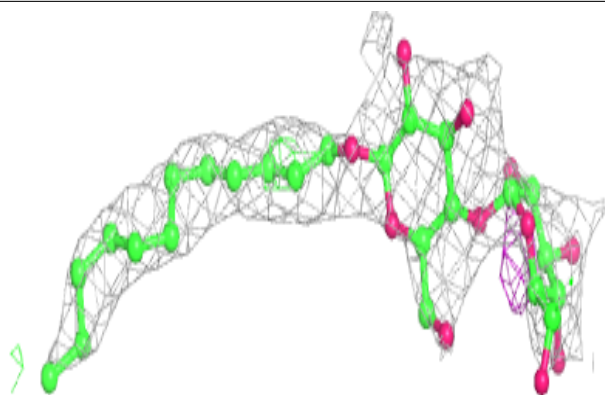
**Electron density around LMG Z 101:**

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

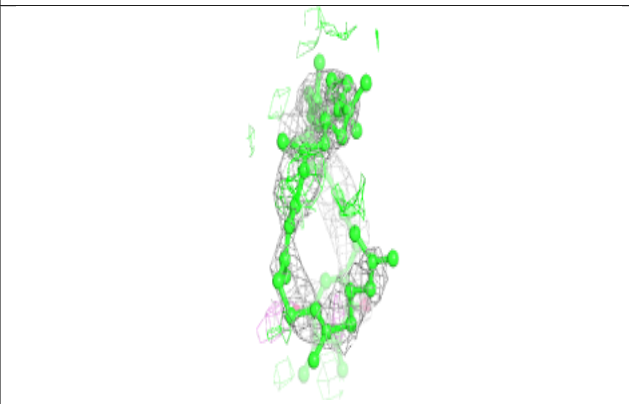
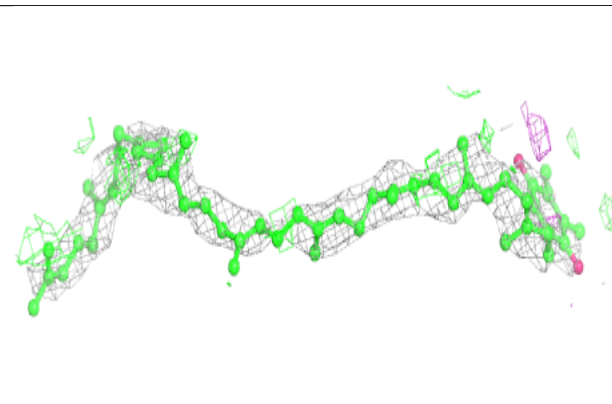
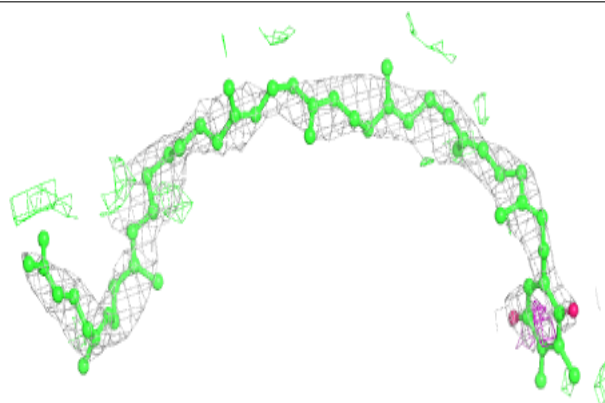


Electron density around LMT B 627:

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

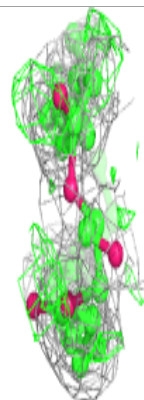
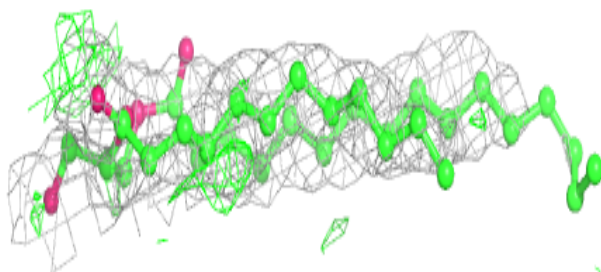
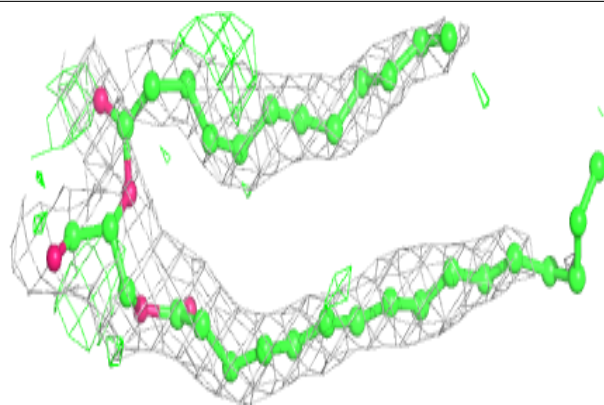
**Electron density around PL9 A 413 (A):**

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

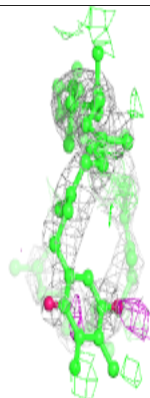
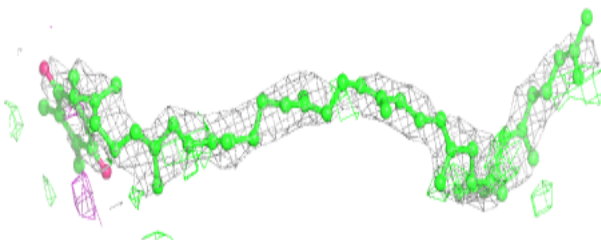
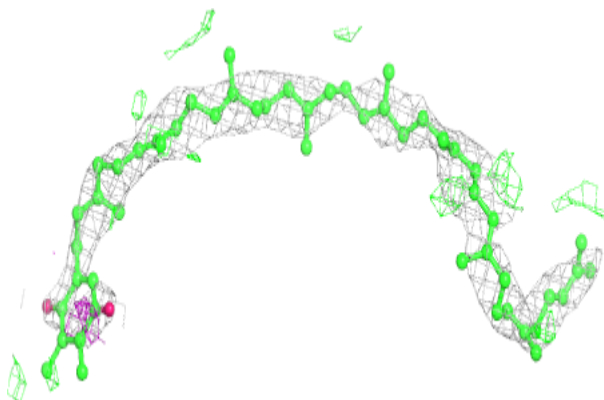


Electron density around UNL d 410:

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

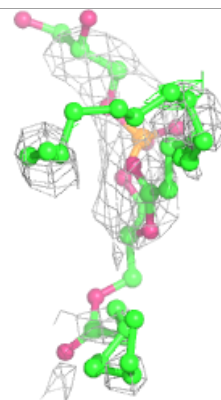
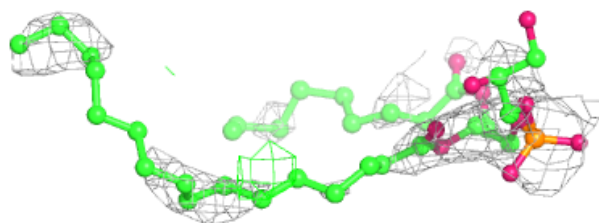
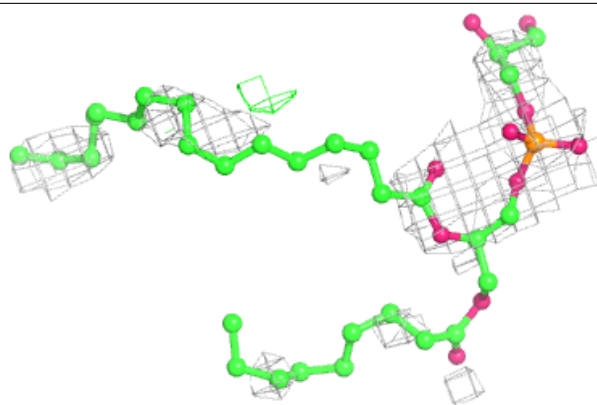
**Electron density around PL9 A 413 (B):**

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

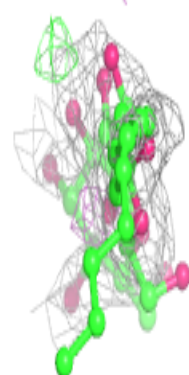
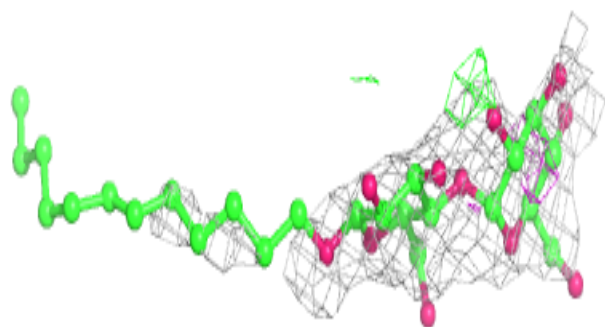
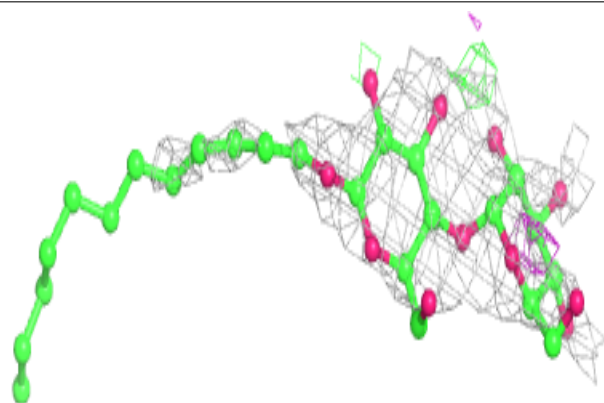


Electron density around LHG a 419:

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

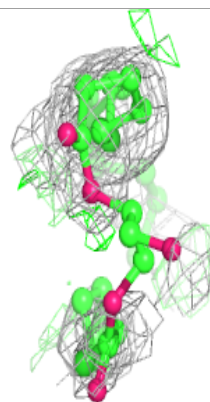
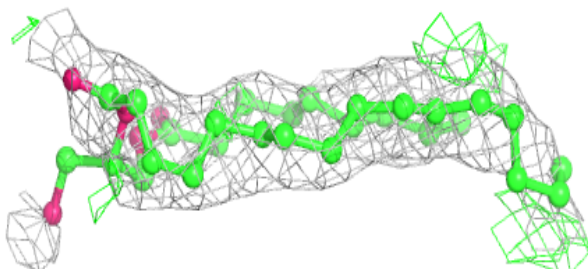
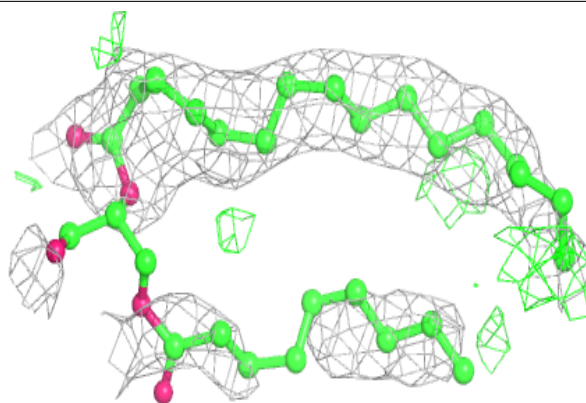
**Electron density around LMT a 418:**

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

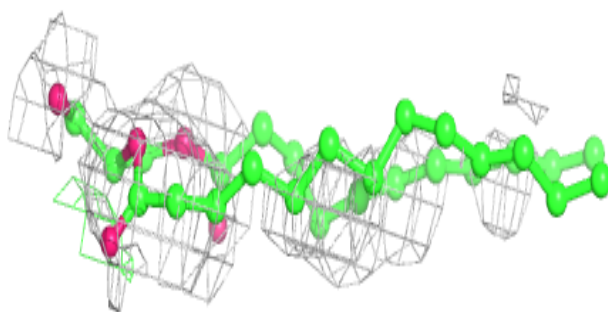
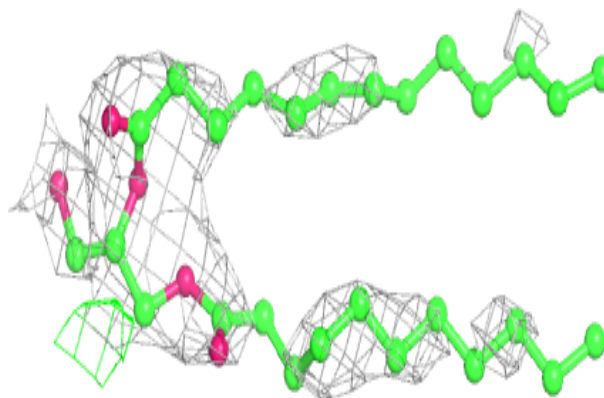


Electron density around UNL B 625:

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

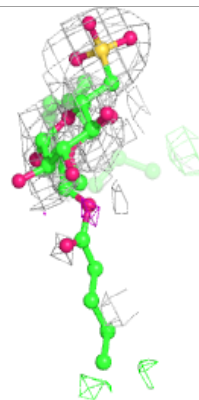
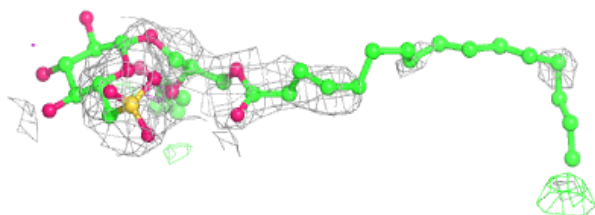
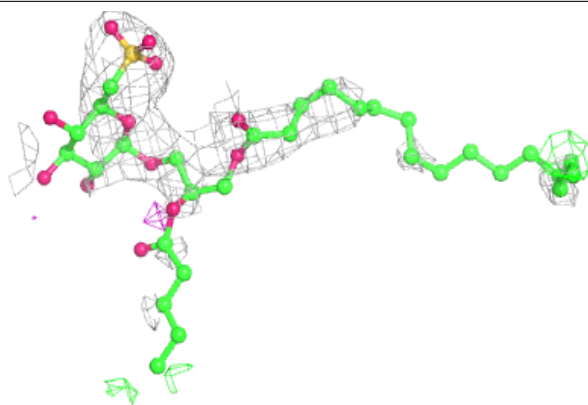
**Electron density around UNL c 526:**

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

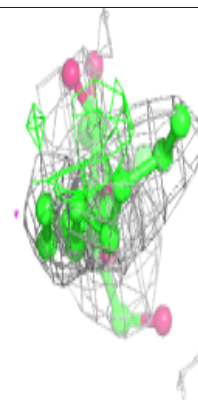
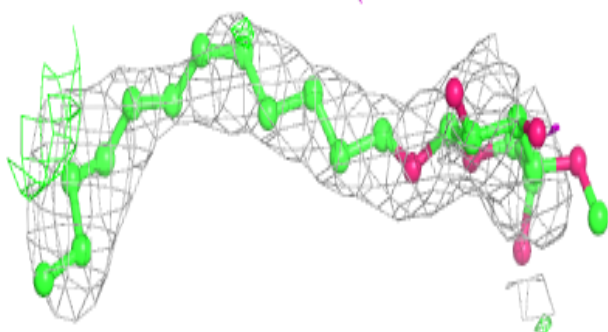
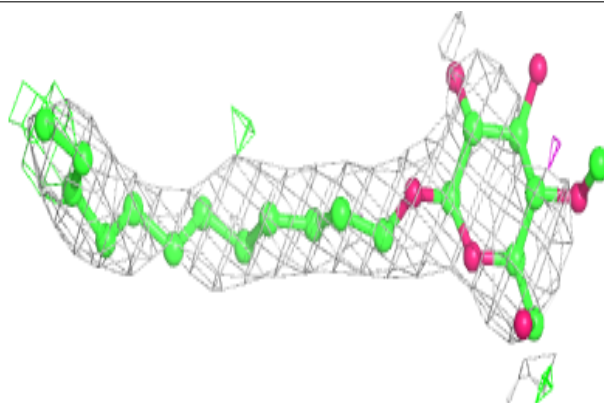


Electron density around SQD f 101:

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

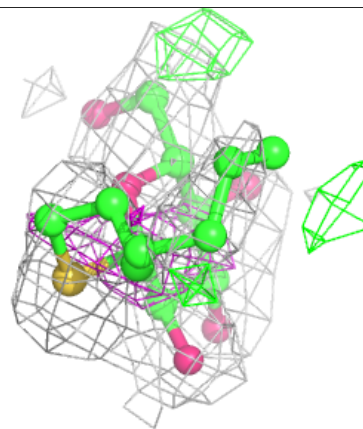
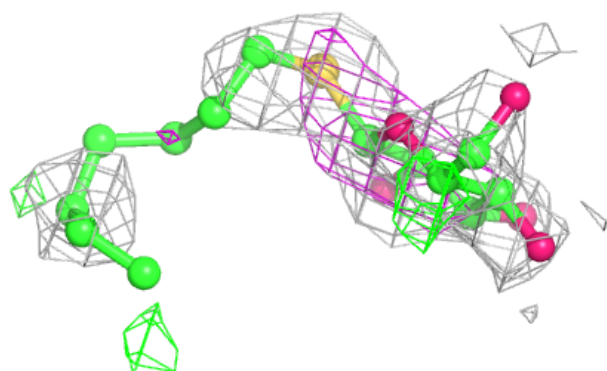
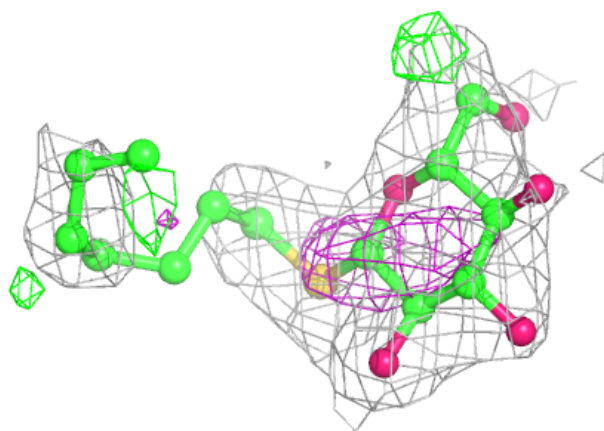
**Electron density around LMT B 629:**

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

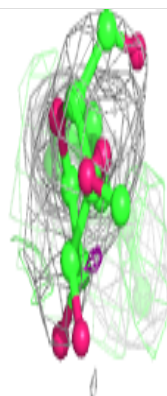
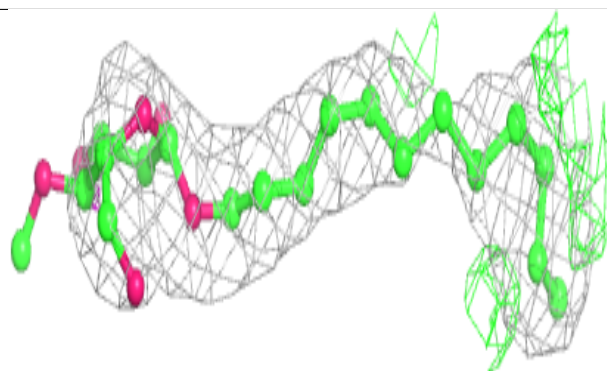
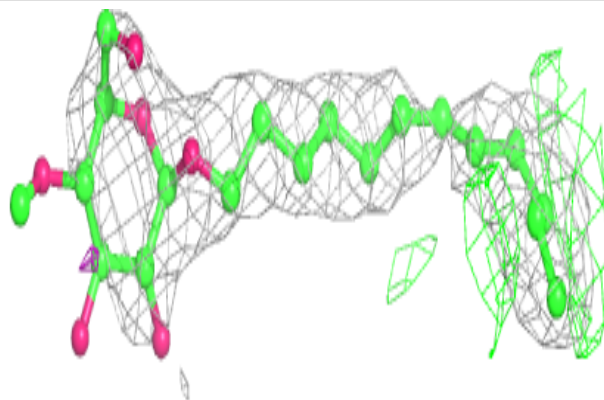


Electron density around HTG B 622:

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

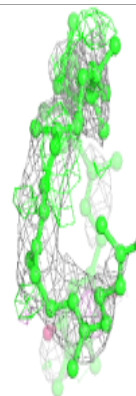
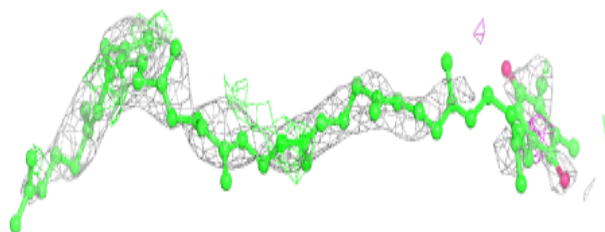
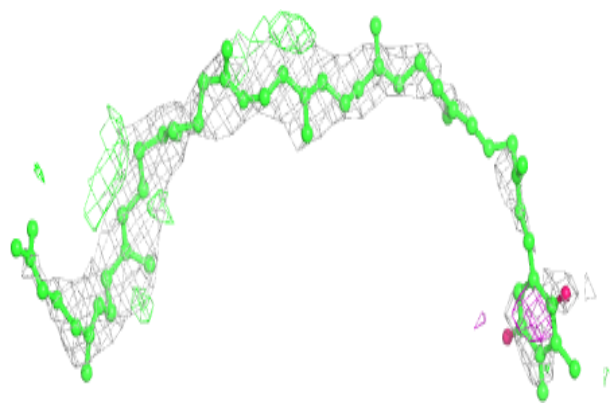
**Electron density around LMT b 626:**

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

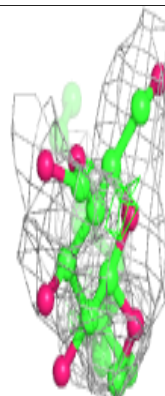
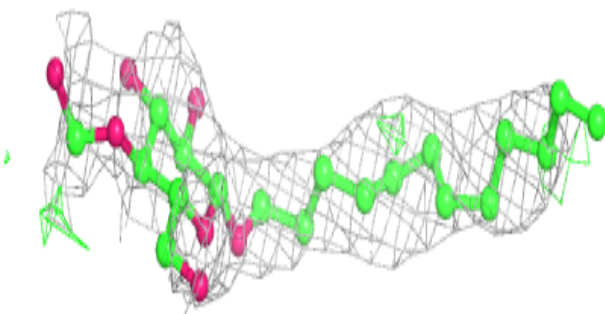
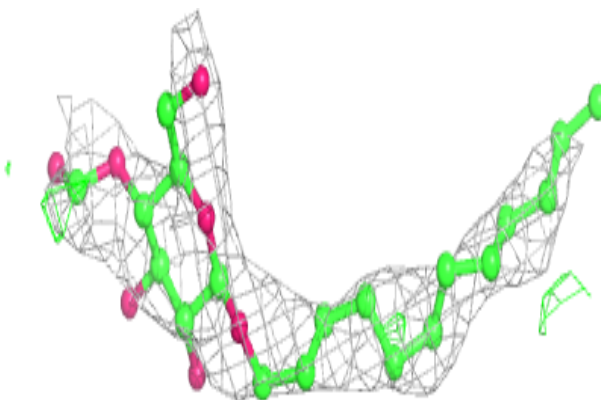


Electron density around PL9 a 414 (A):

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

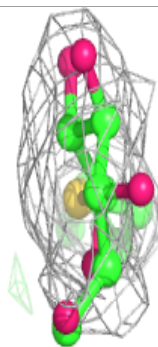
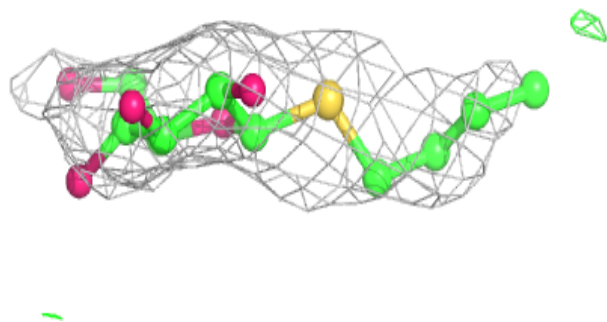
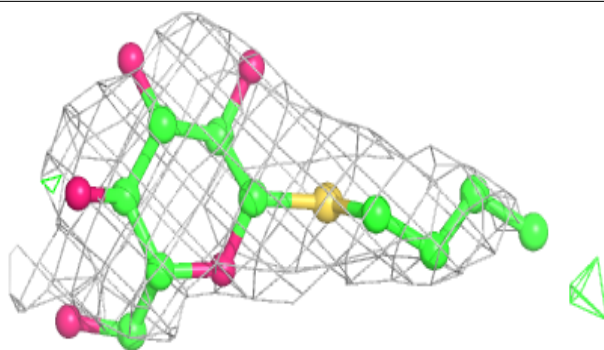
**Electron density around LMT B 630:**

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

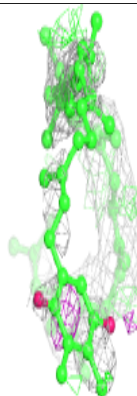
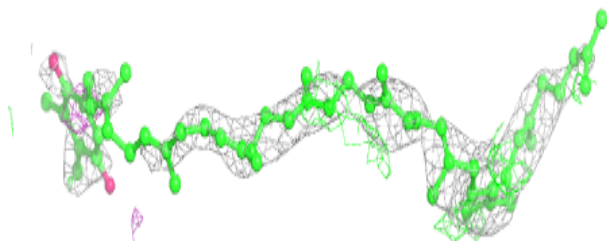
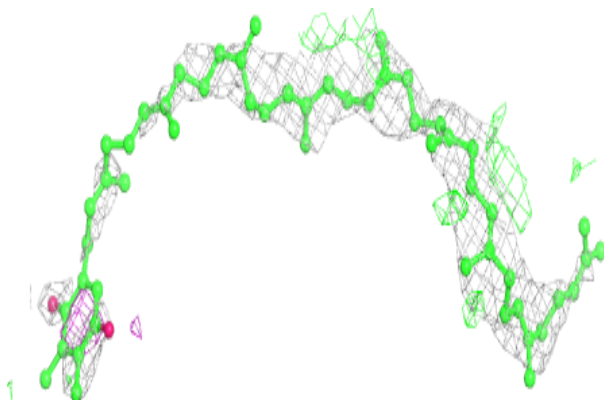


Electron density around HTG h 101:

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

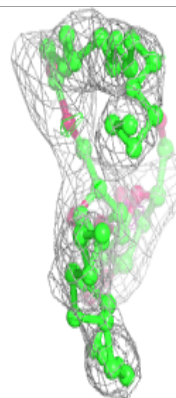
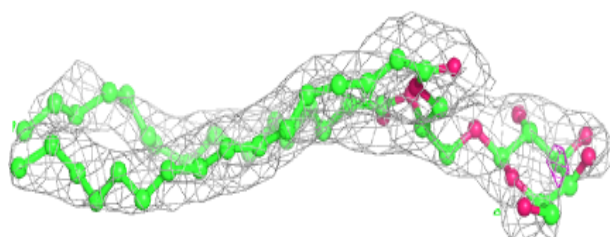
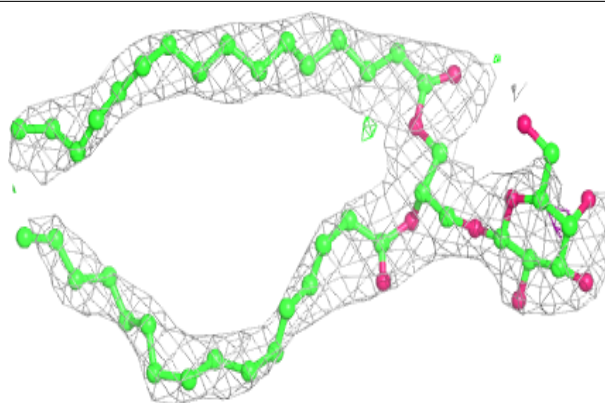
**Electron density around PL9 a 414 (B):**

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

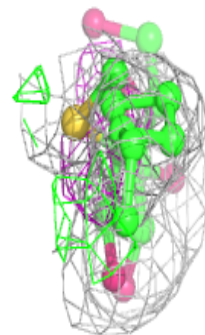
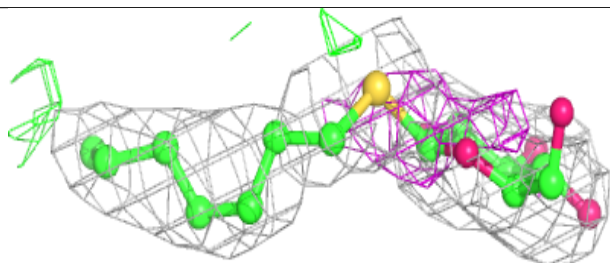
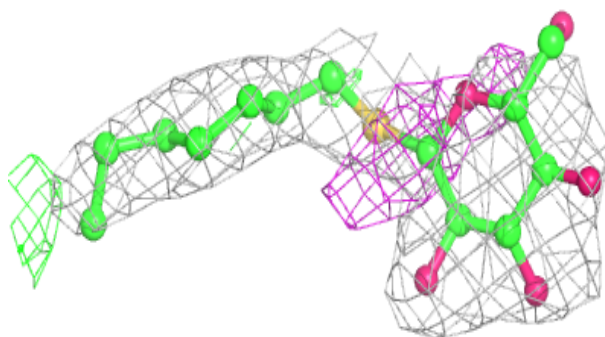


Electron density around LMG a 417:

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

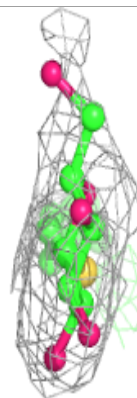
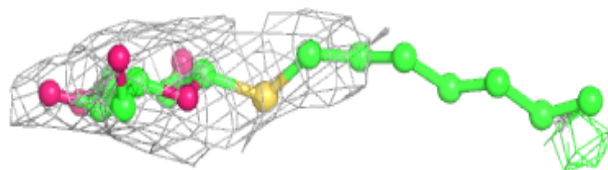
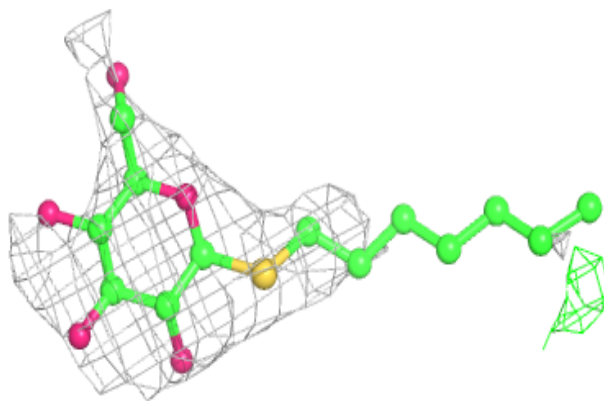
**Electron density around HTG b 621:**

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

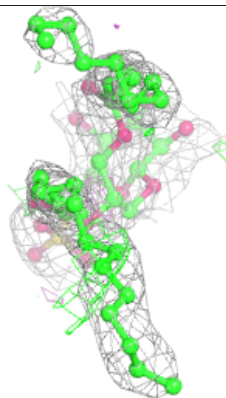
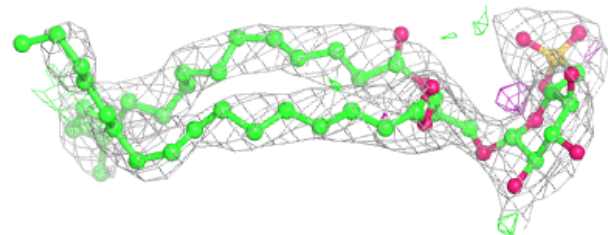
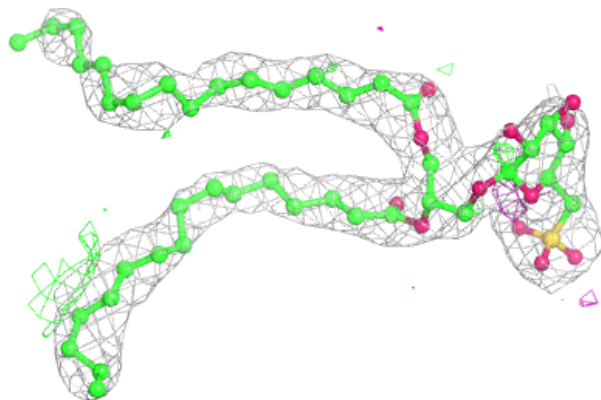


Electron density around HTG c 523:

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

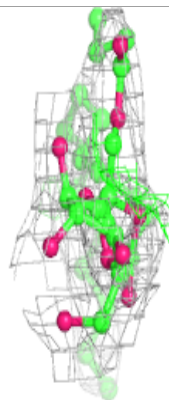
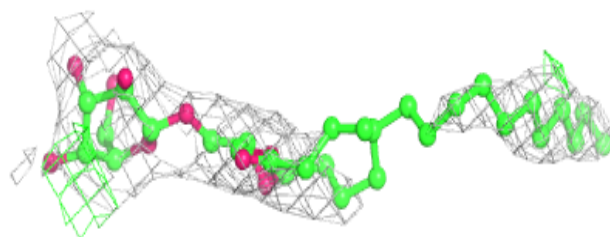
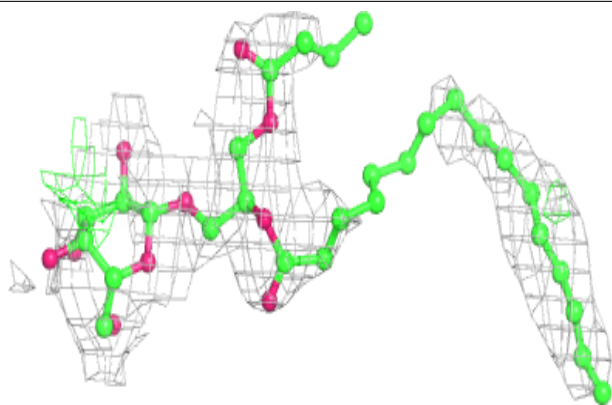
**Electron density around SQD L 102:**

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



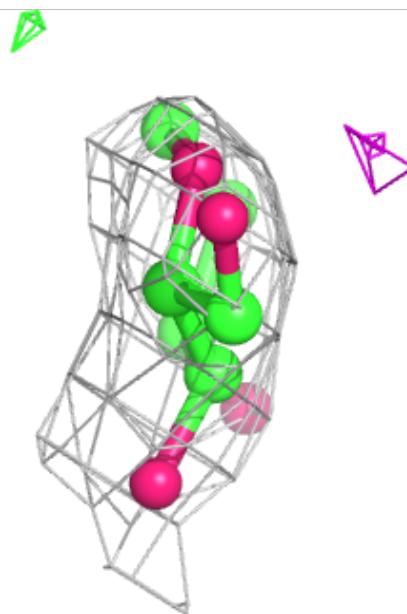
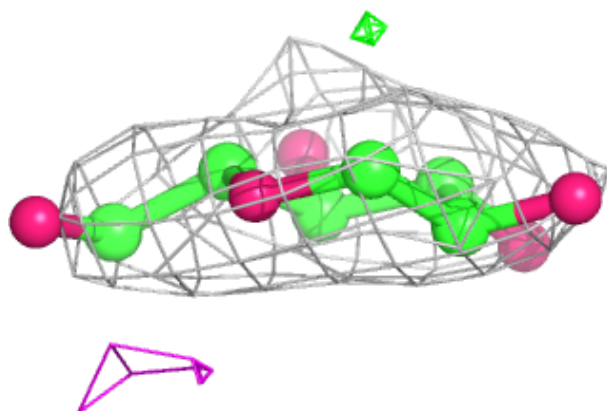
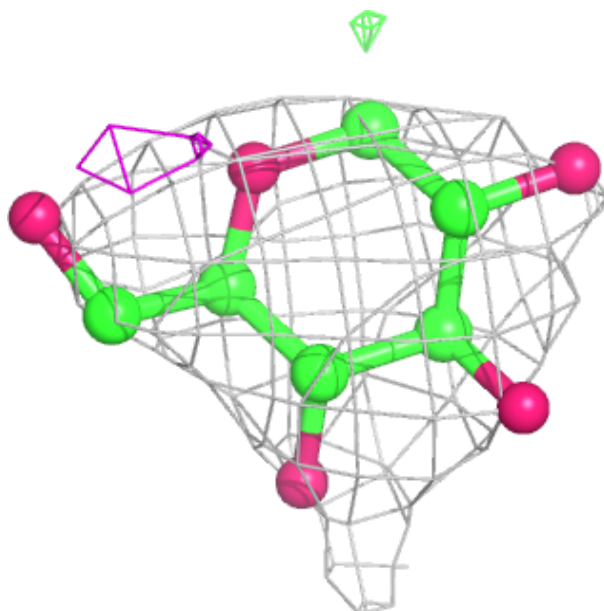
Electron density around LMG z 101:

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



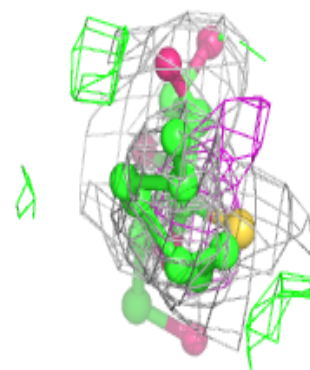
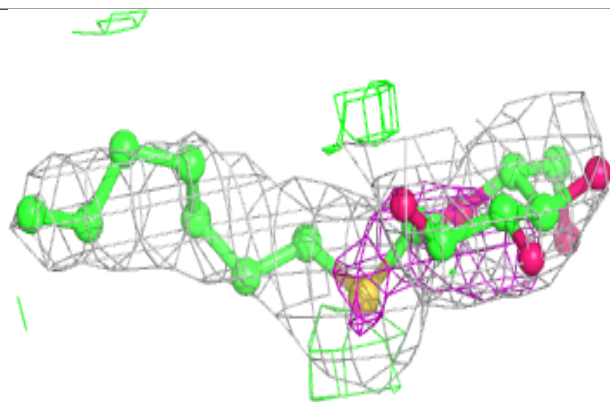
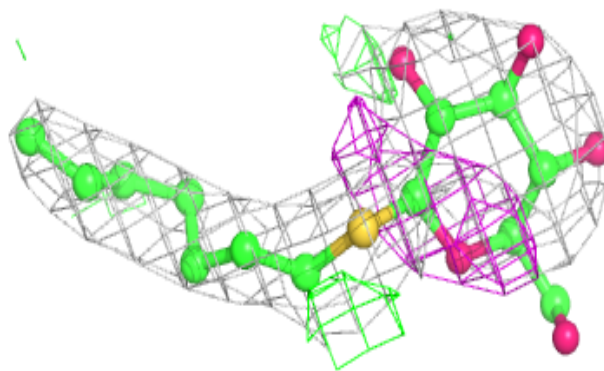
Electron density around HTG V 202:

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



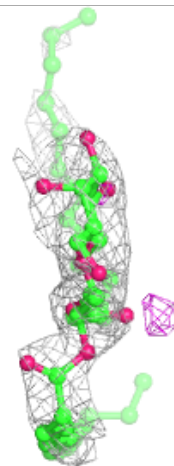
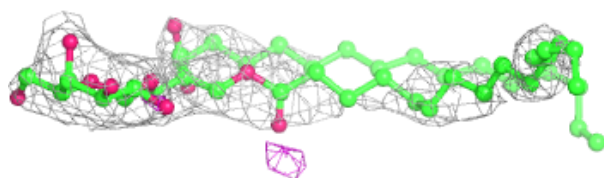
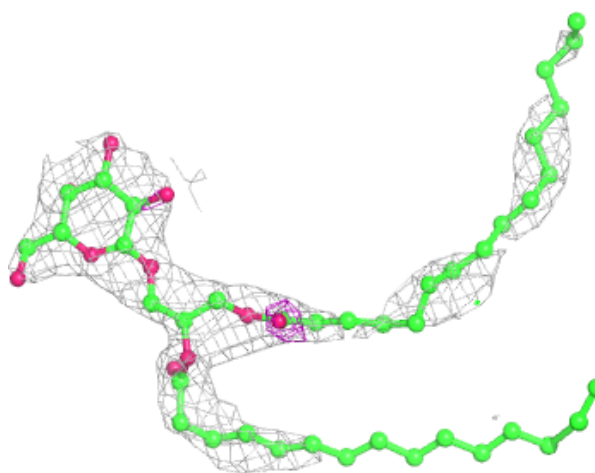
Electron density around HTG B 621:

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



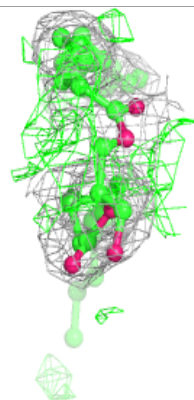
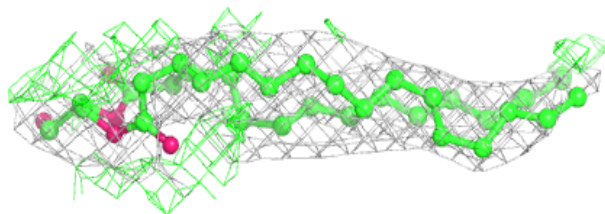
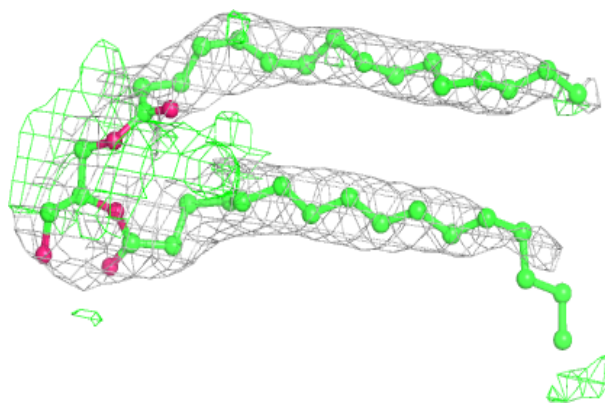
Electron density around LMG c 521:

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

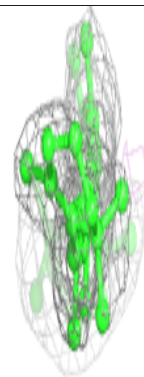
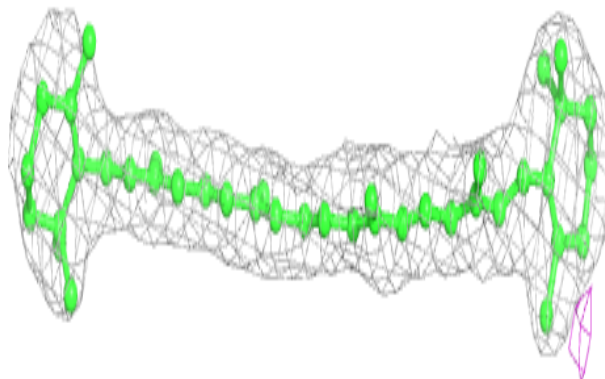
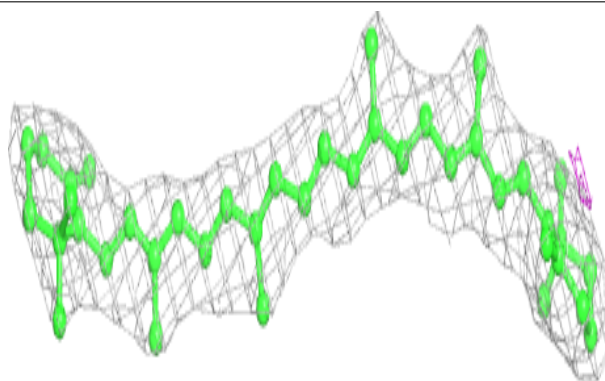


Electron density around UNL D 410:

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

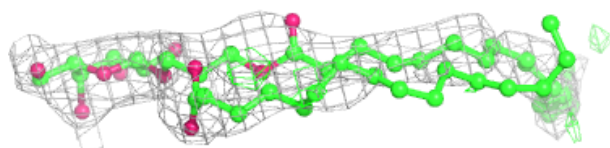
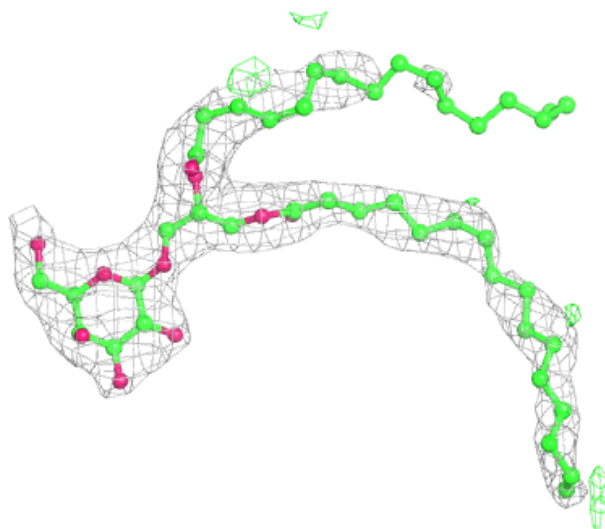
**Electron density around BCR h 102:**

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



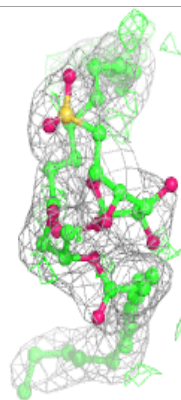
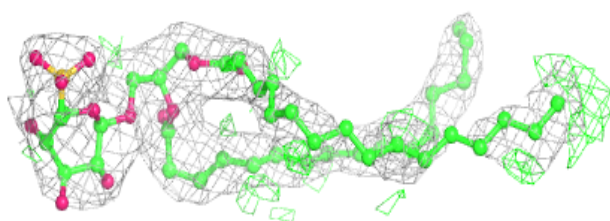
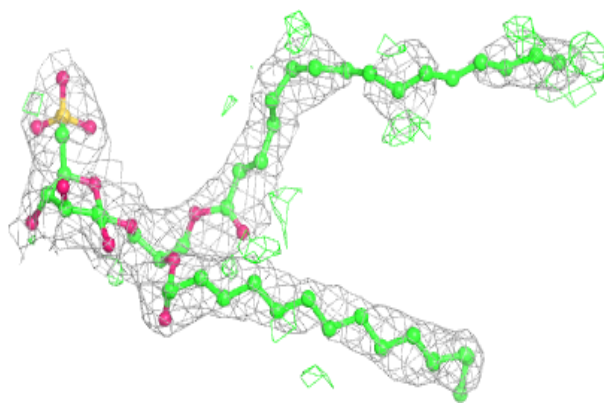
Electron density around LMG C 521:

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

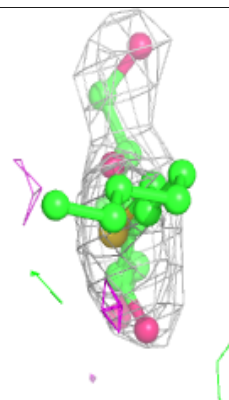
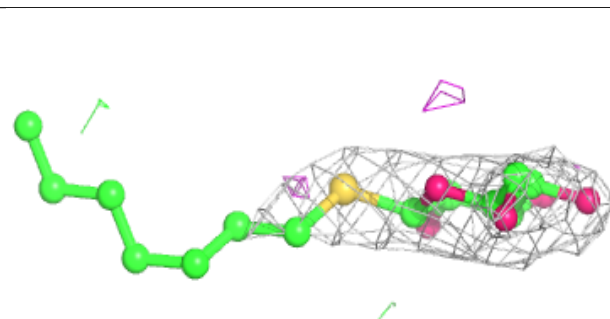
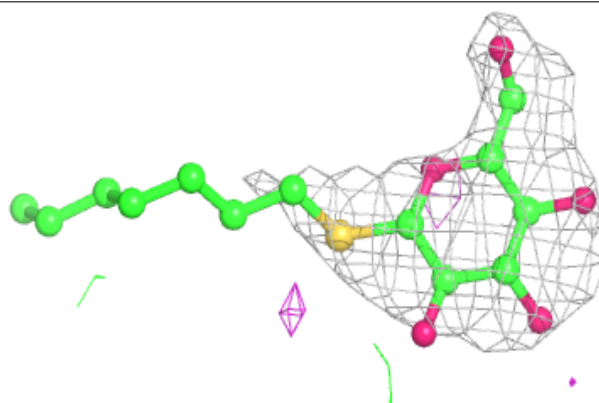


Electron density around SQD A 411:

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

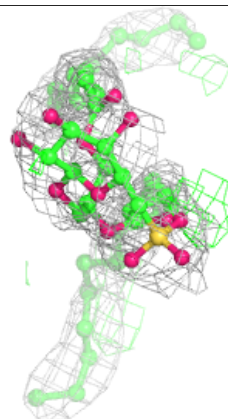
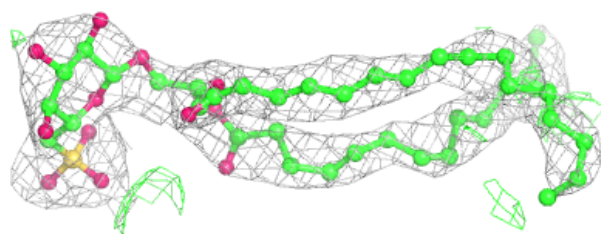
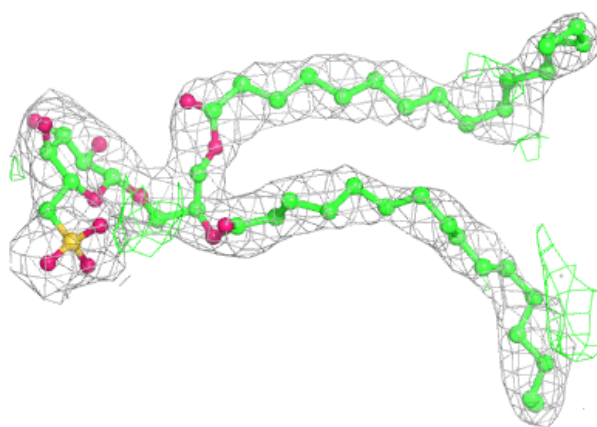
**Electron density around HTG C 523:**

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

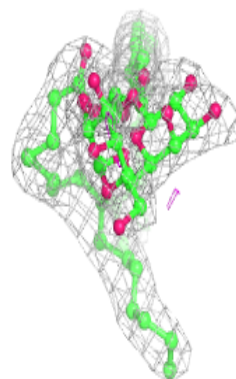
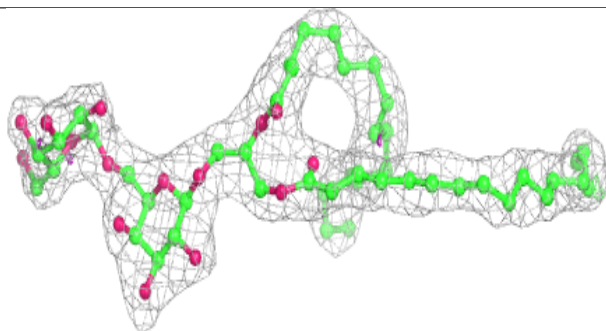
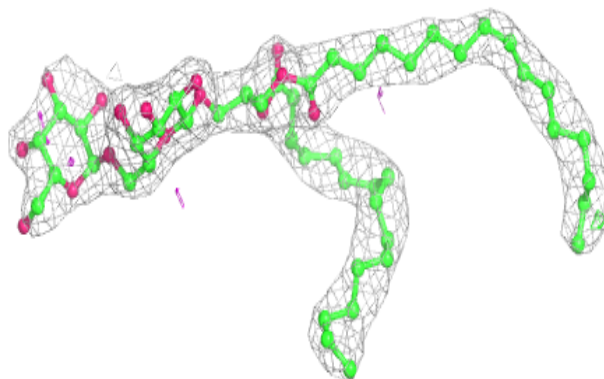


Electron density around SQD B 620:

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

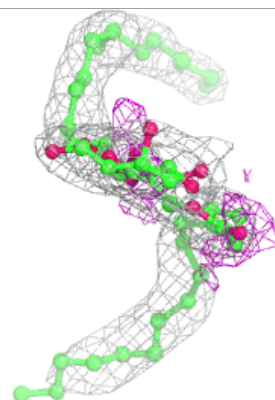
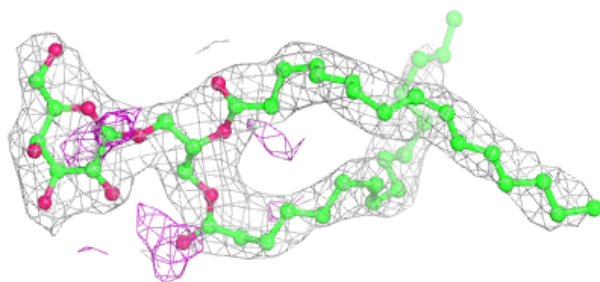
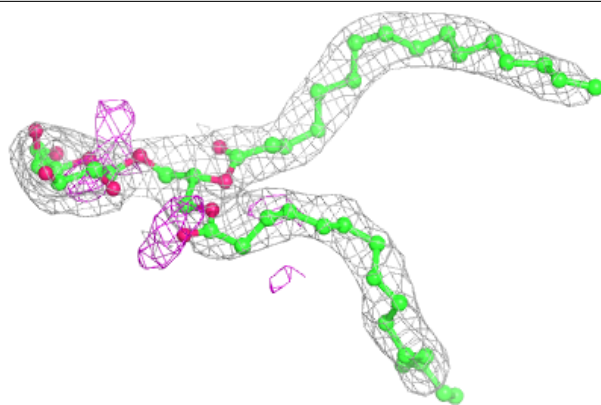
**Electron density around DGD h 103:**

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

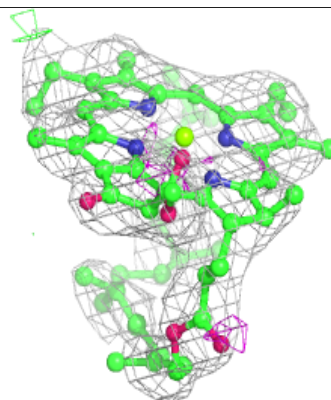
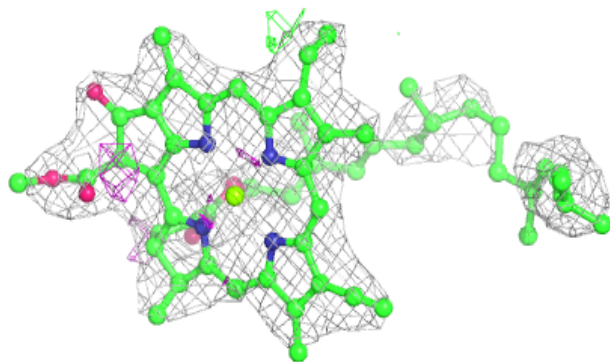
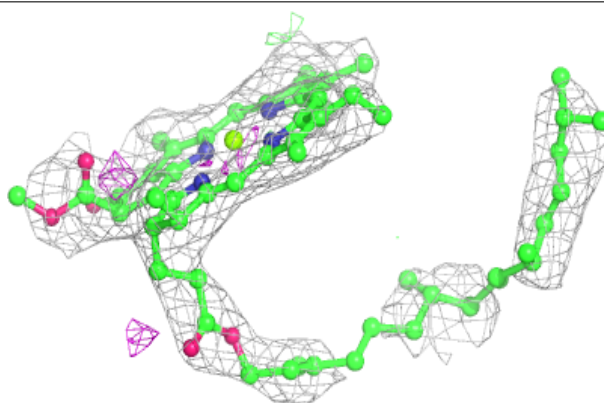


Electron density around LMG M 101:

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

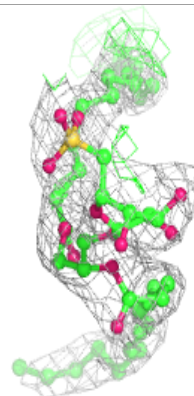
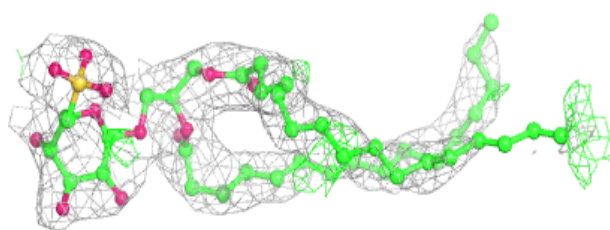
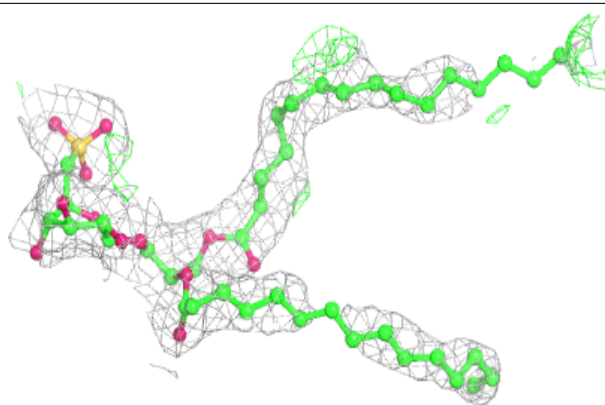
**Electron density around CLA C 515:**

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

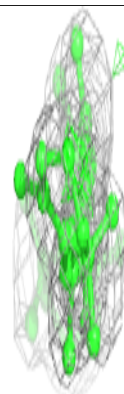
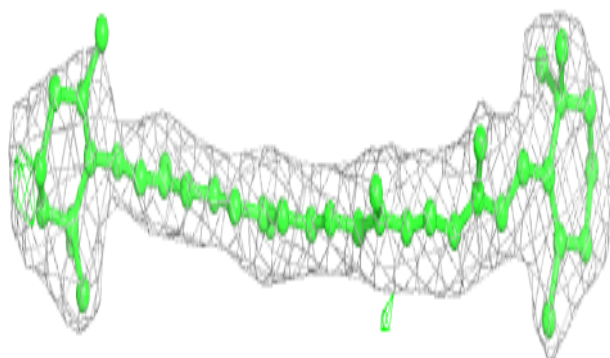
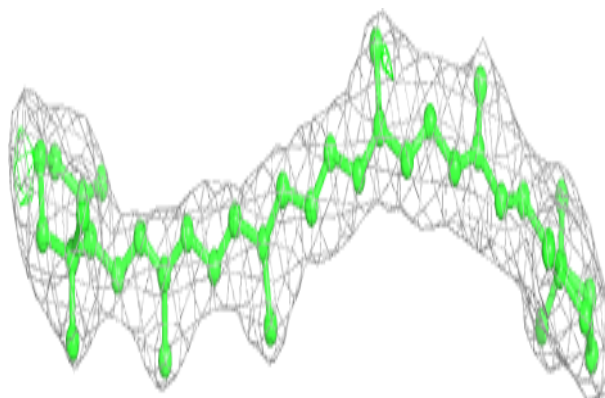


Electron density around SQD a 411:

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

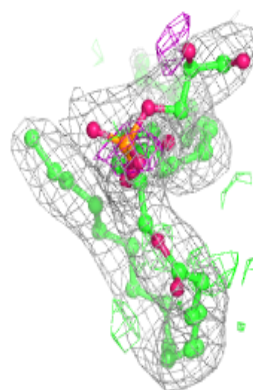
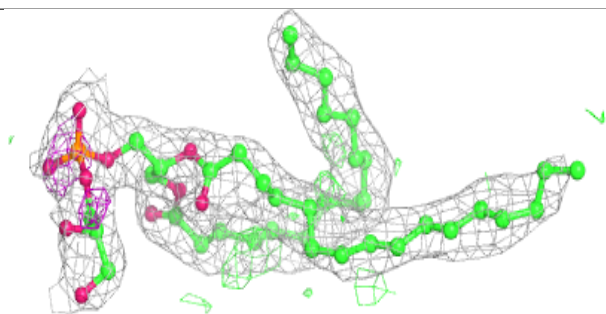
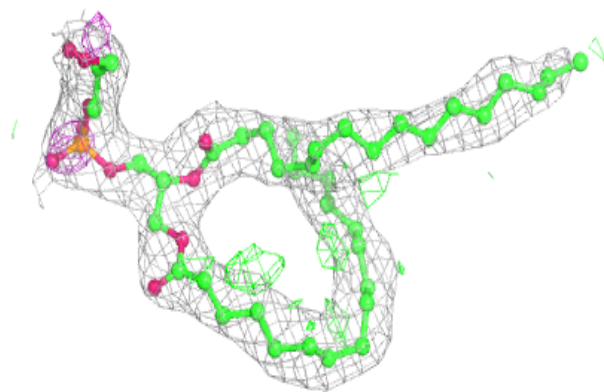
**Electron density around BCR H 101:**

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

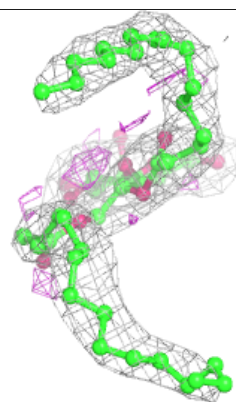
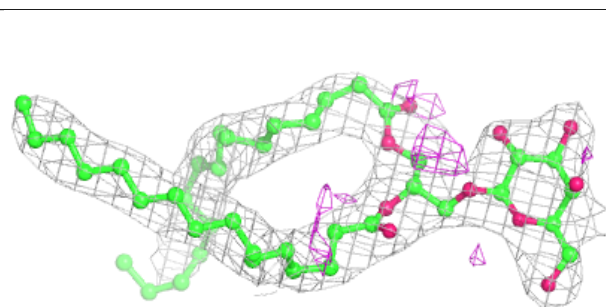
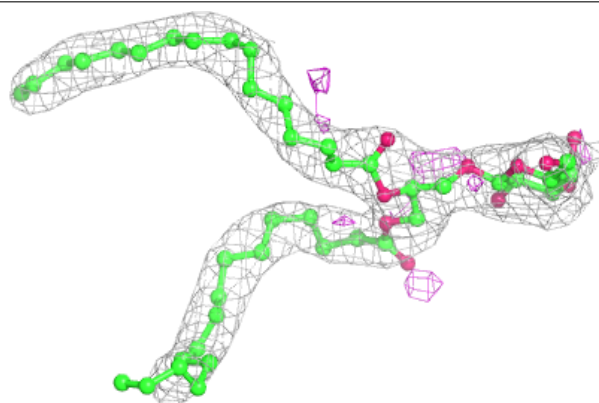


Electron density around LHG A 416:

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

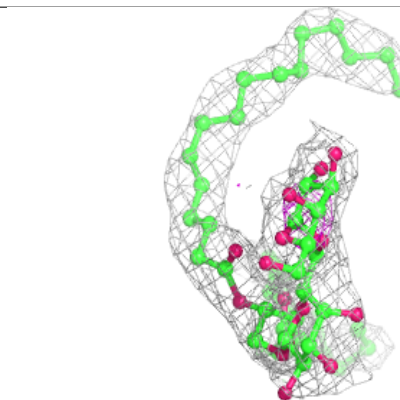
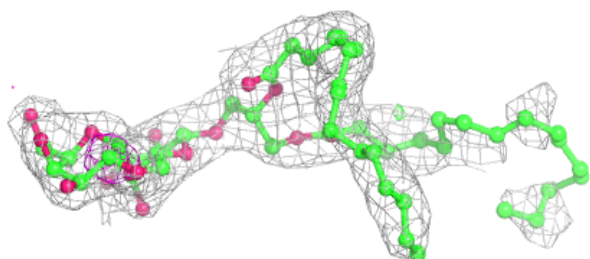
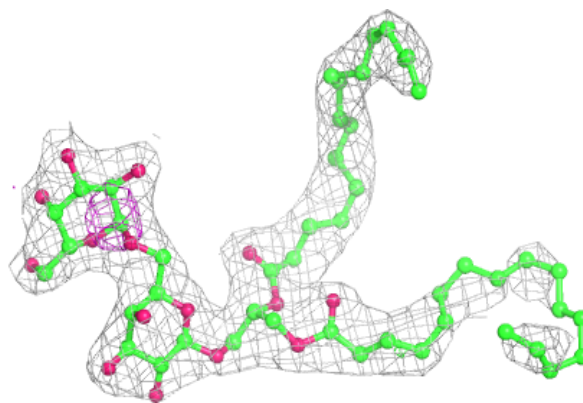
**Electron density around LMG m 101:**

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

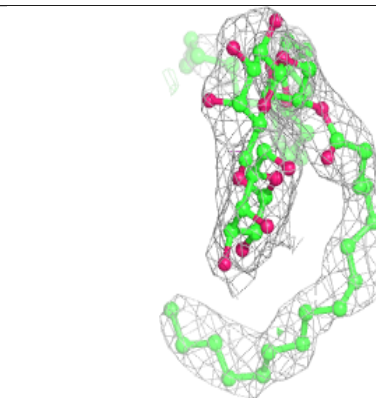
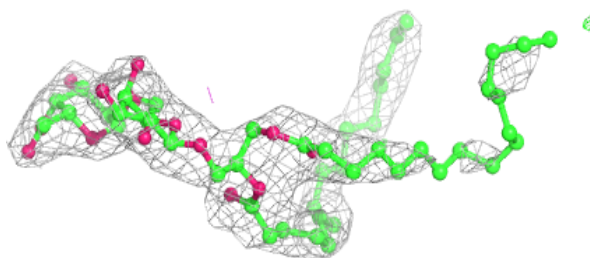
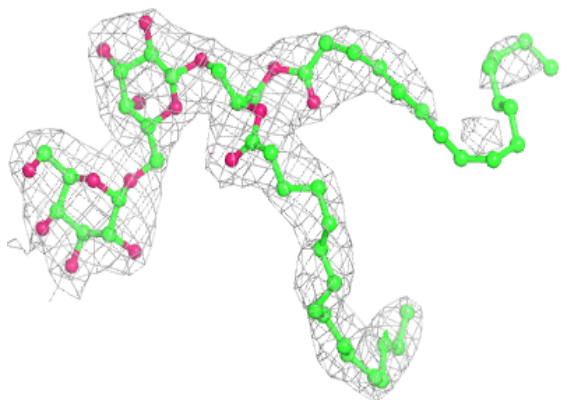


Electron density around DGD C 519:

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

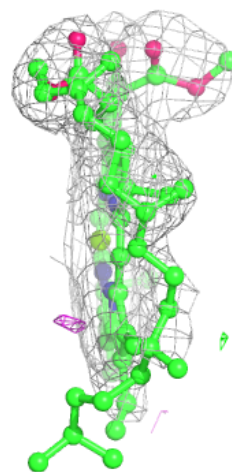
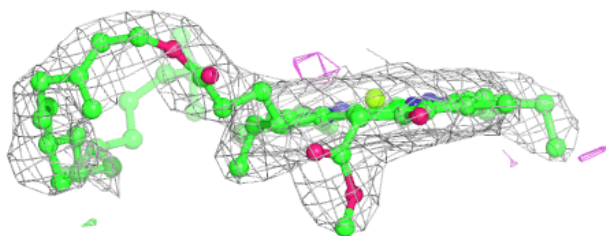
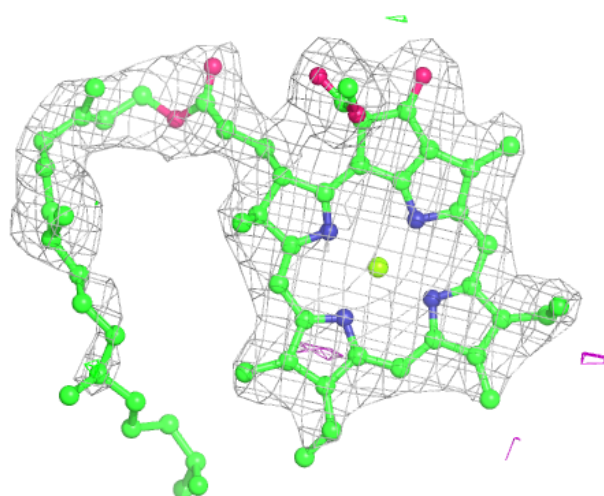
**Electron density around DGD c 519:**

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



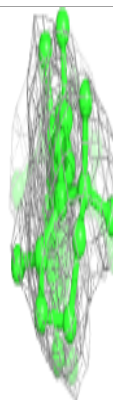
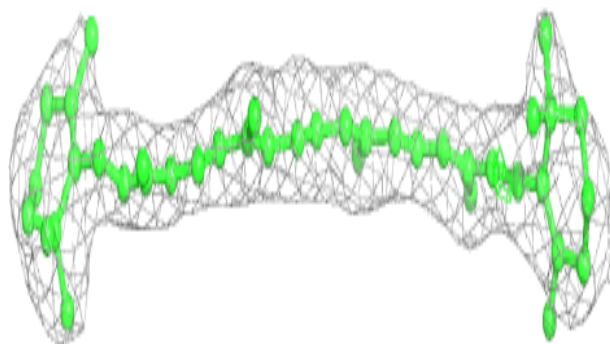
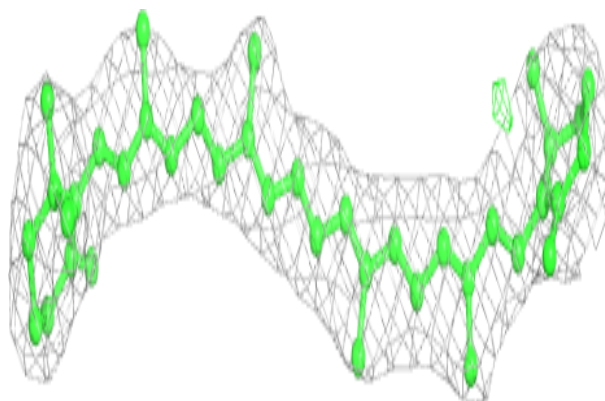
Electron density around CLA C 514:

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

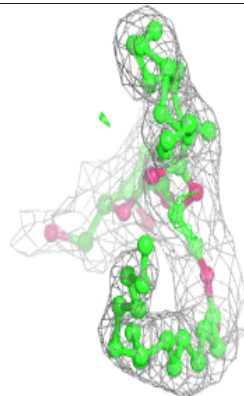
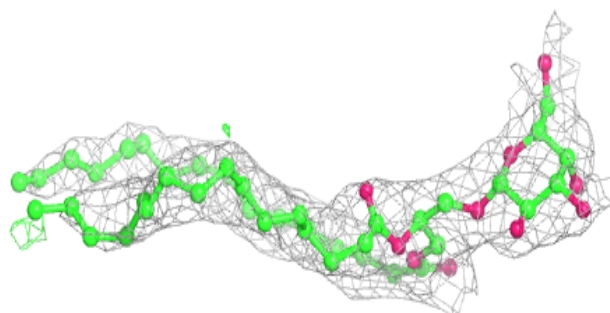
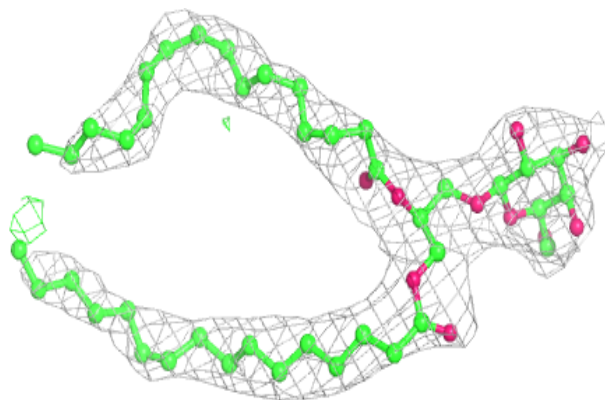


Electron density around BCR k 102:

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

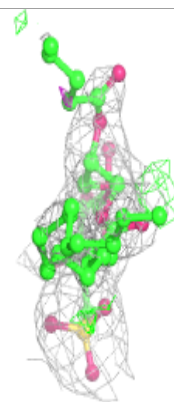
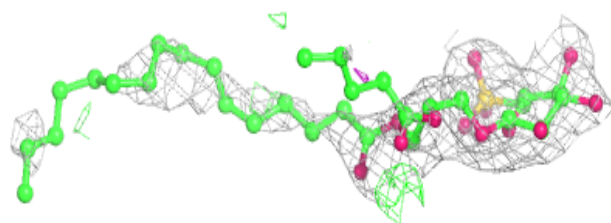
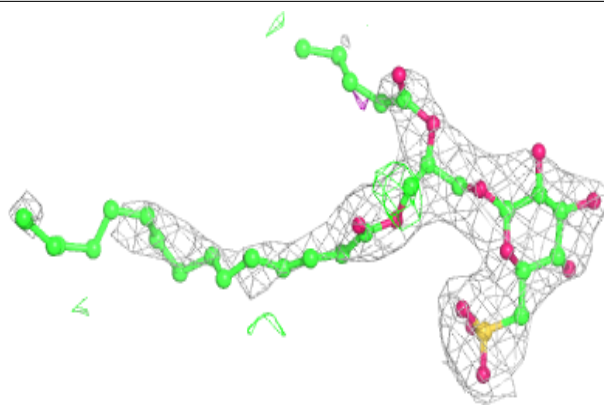
**Electron density around LMG C 502:**

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



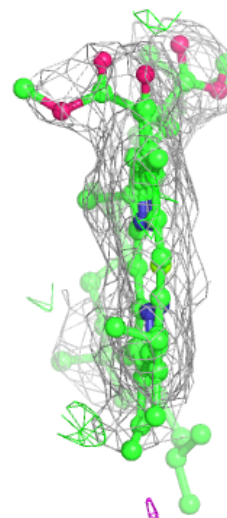
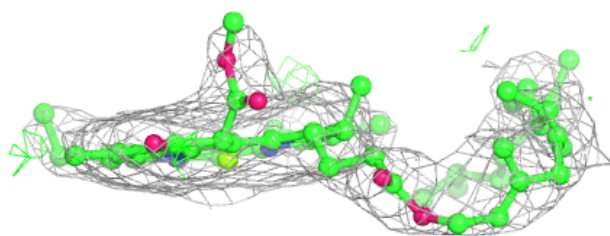
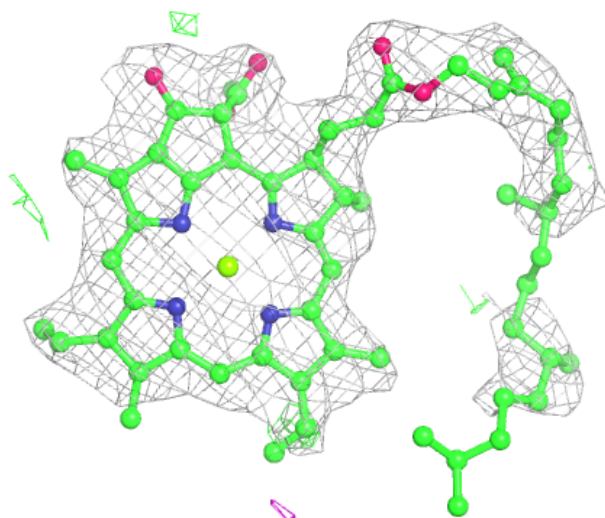
Electron density around SQD D 413:

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



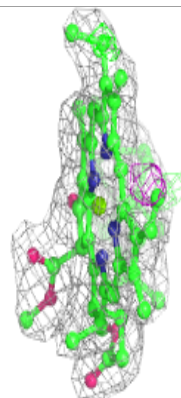
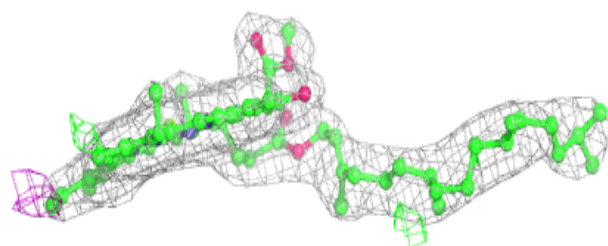
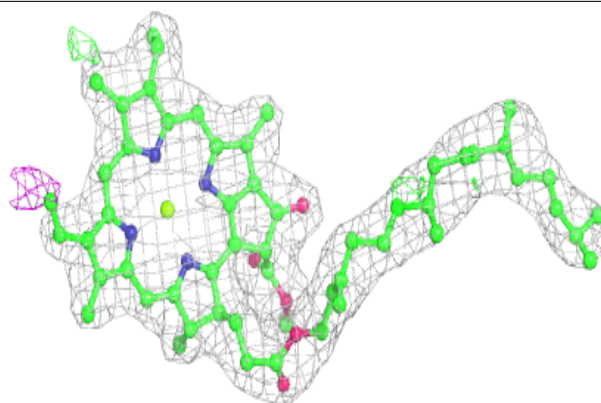
Electron density around CLA c 514:

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

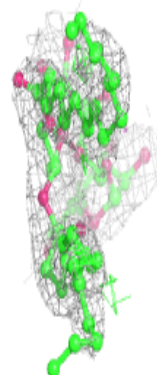
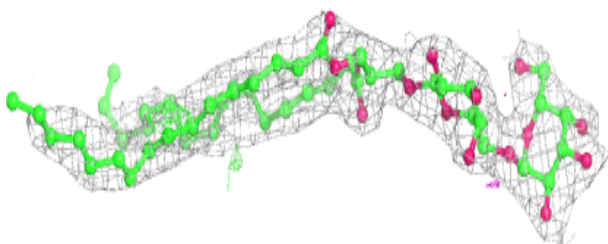
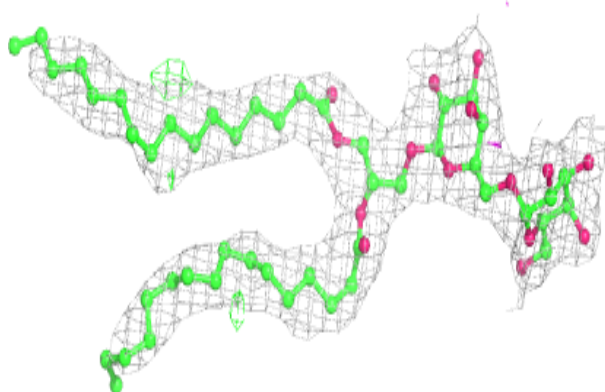


Electron density around CLA B 602:

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

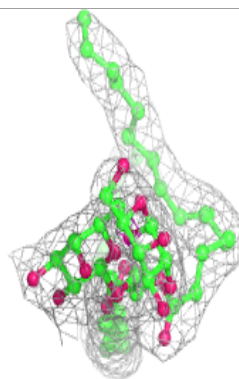
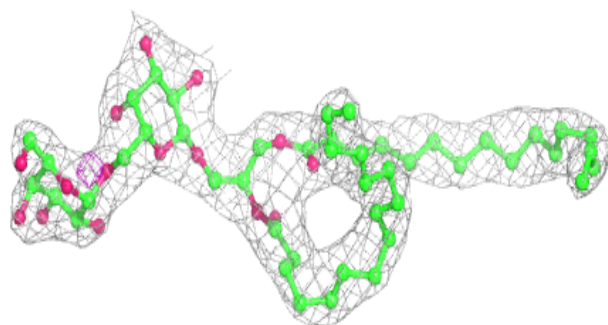
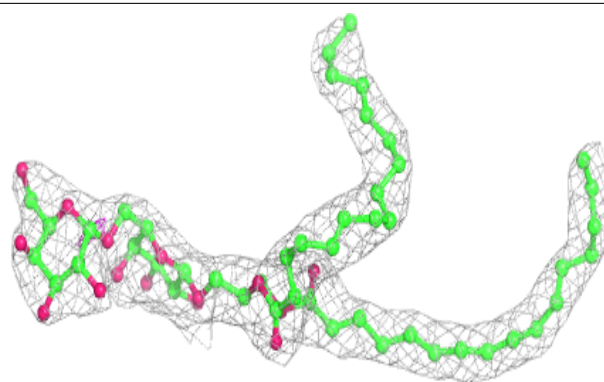
**Electron density around DGD C 520:**

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

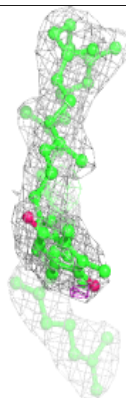
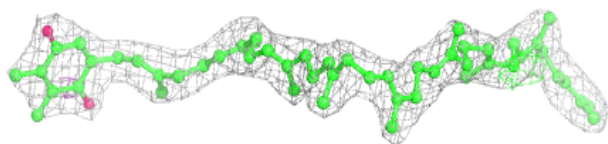
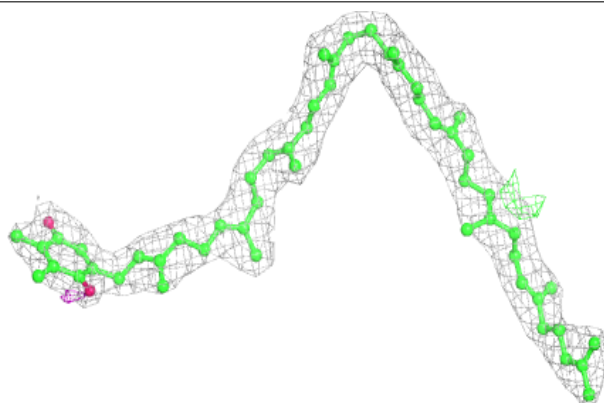


Electron density around DGD H 102:

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

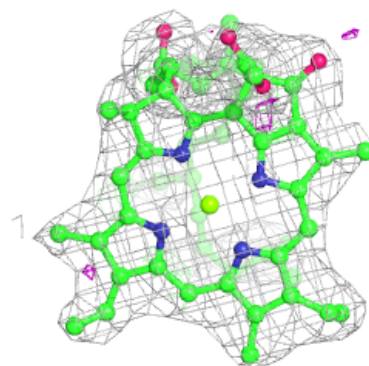
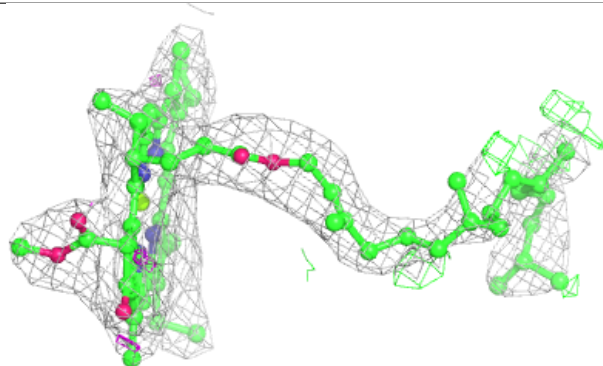
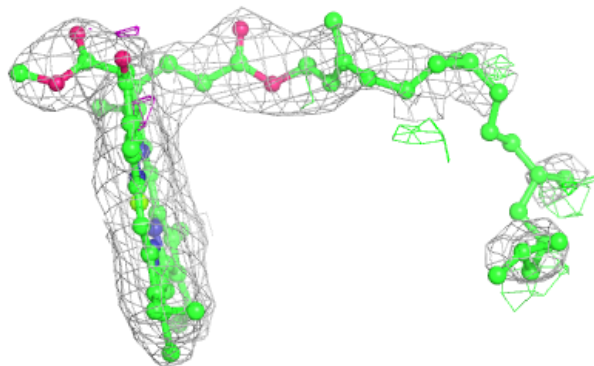
**Electron density around PL9 d 405:**

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

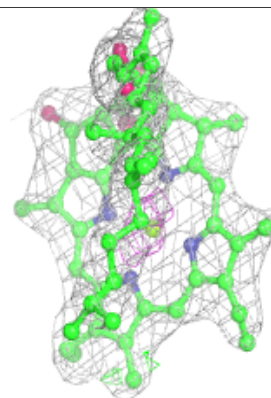
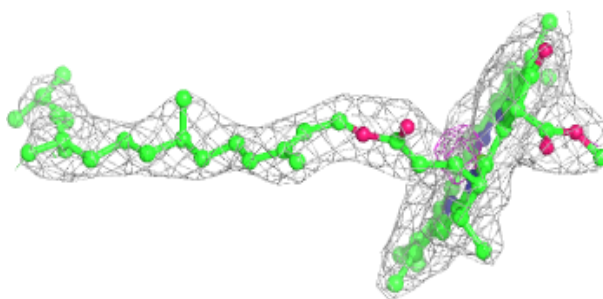
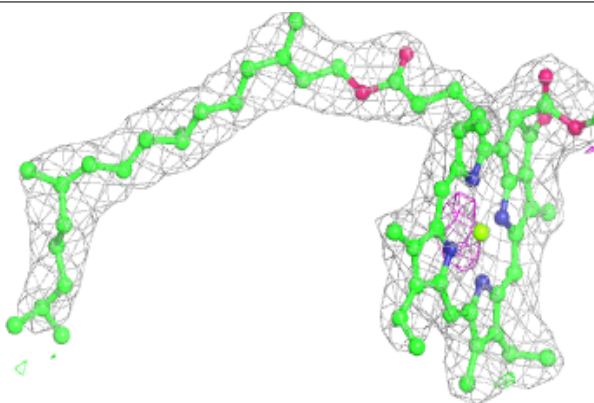


Electron density around CLA C 508:

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

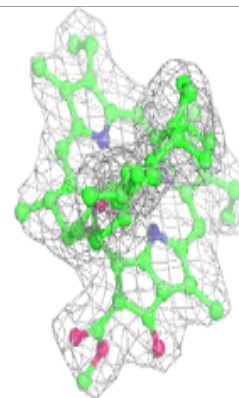
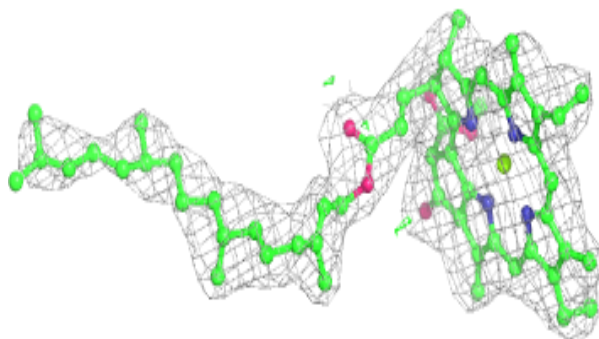
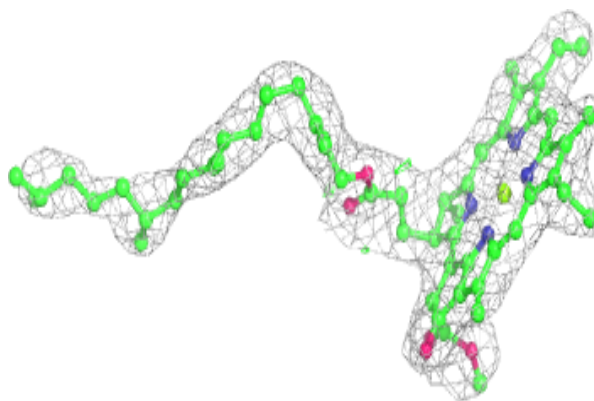
**Electron density around CLA b 609:**

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

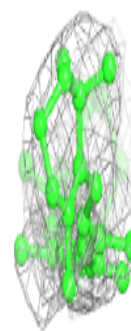
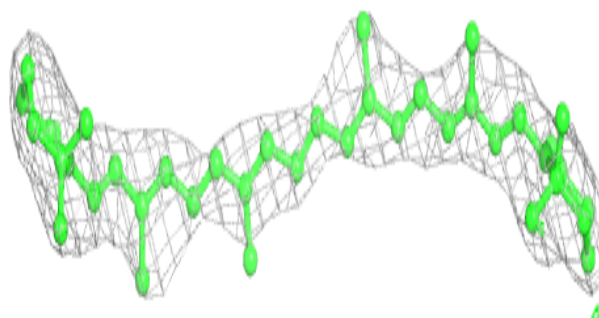
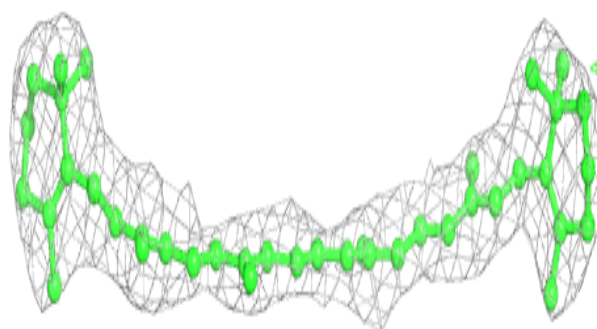


Electron density around CLA c 504:

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

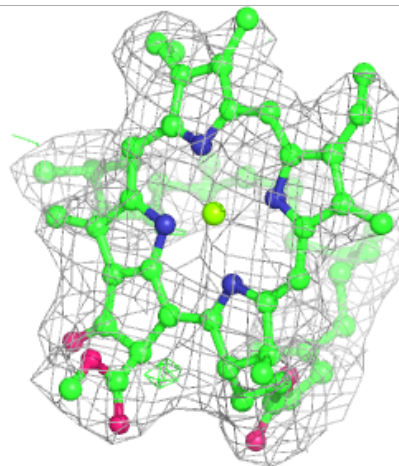
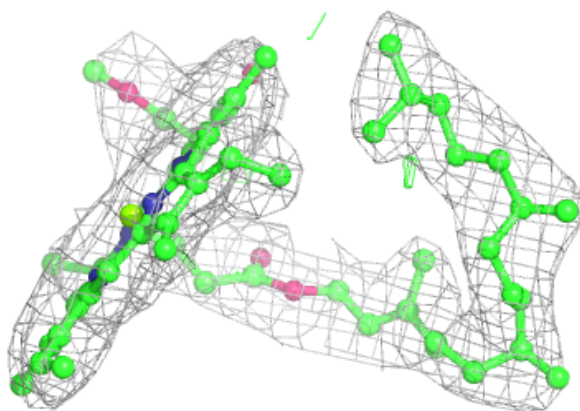
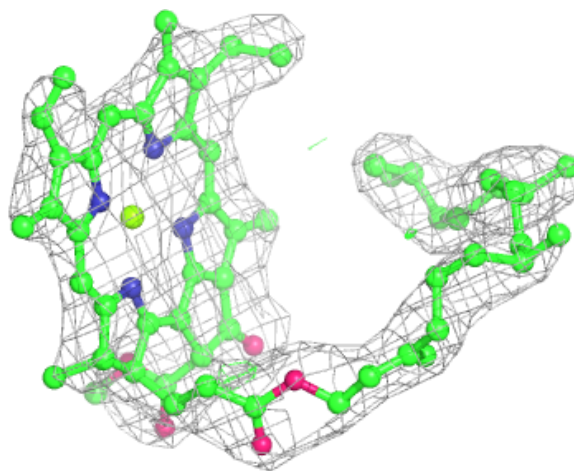
**Electron density around BCR k 101:**

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



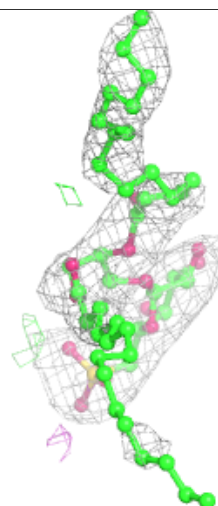
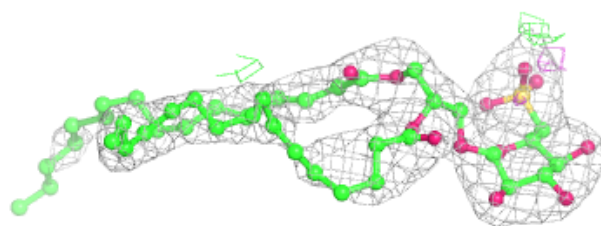
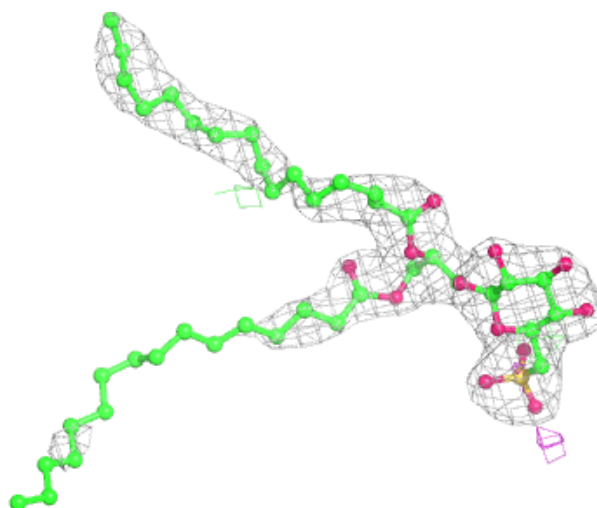
Electron density around CLA c 505:

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



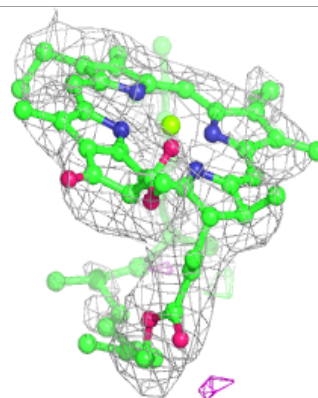
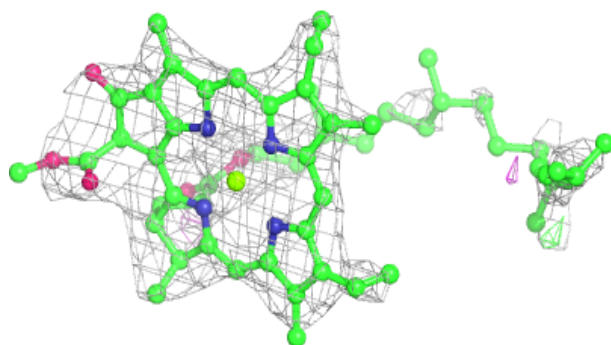
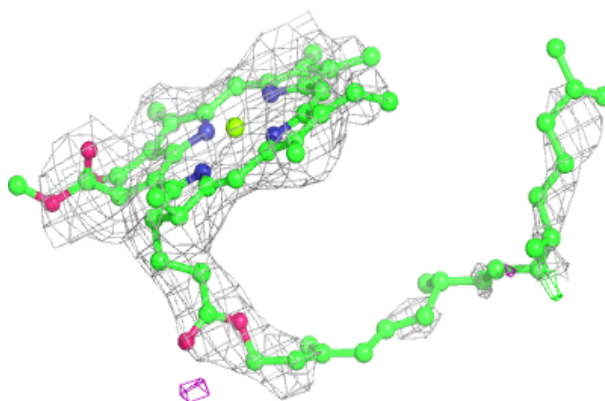
Electron density around SQD A 409:

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

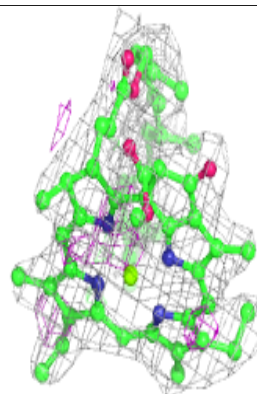
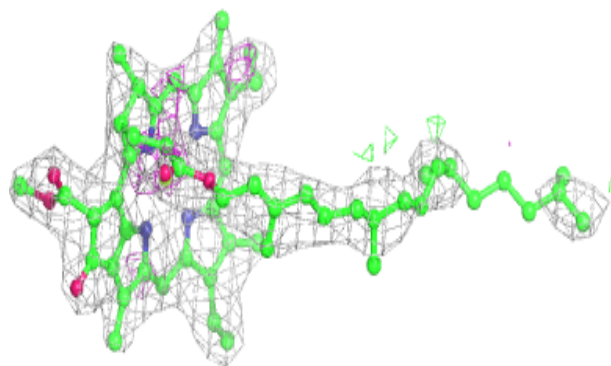
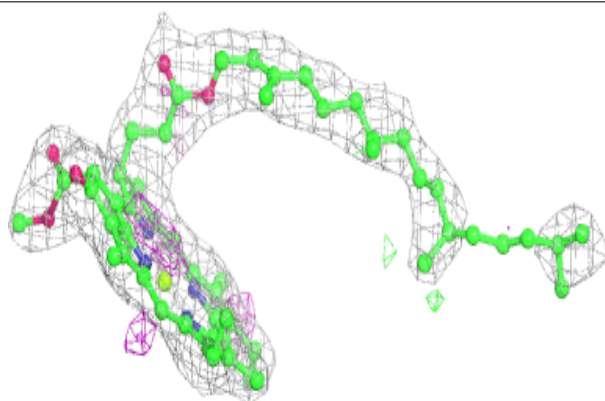


Electron density around CLA c 515:

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

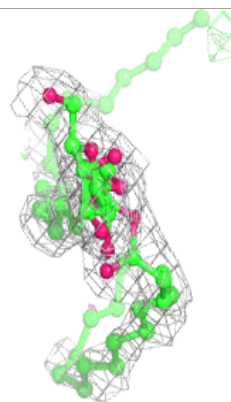
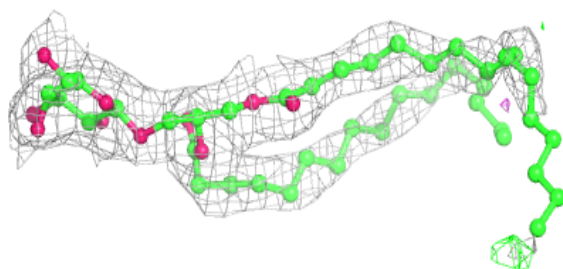
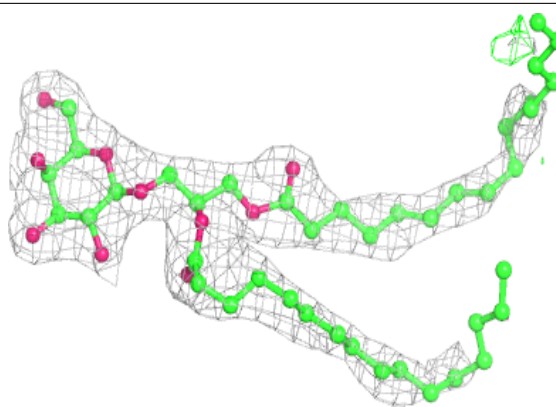
**Electron density around CLA C 506:**

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



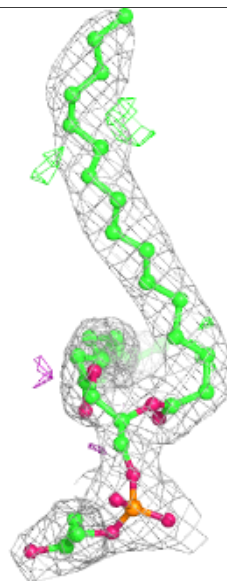
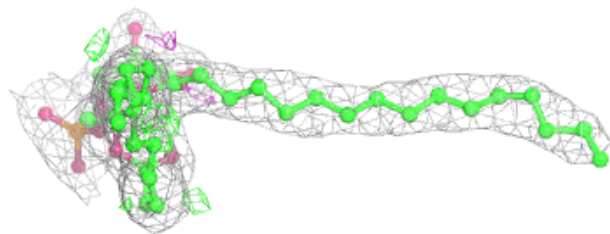
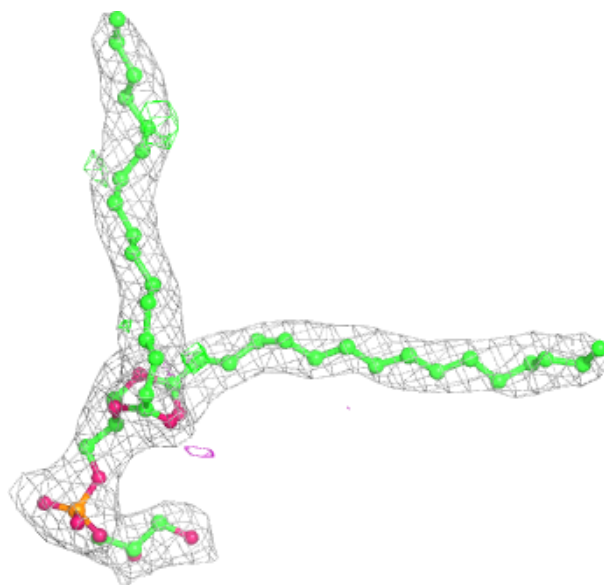
Electron density around LMG D 412:

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



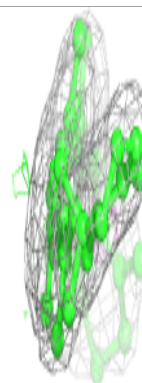
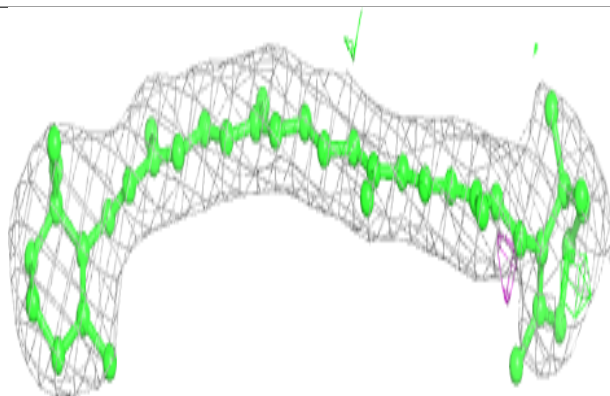
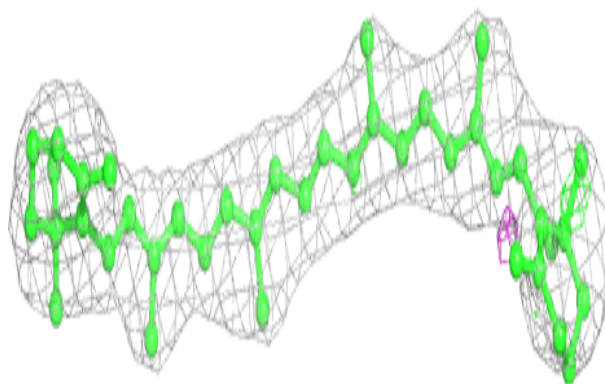
Electron density around LHG b 628:

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

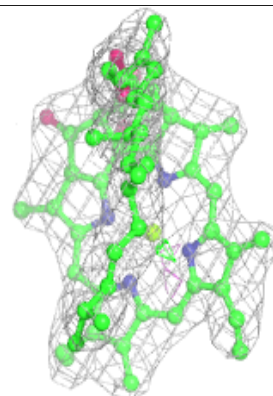
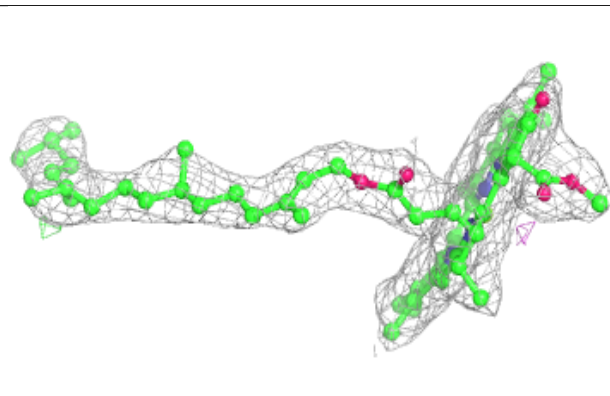
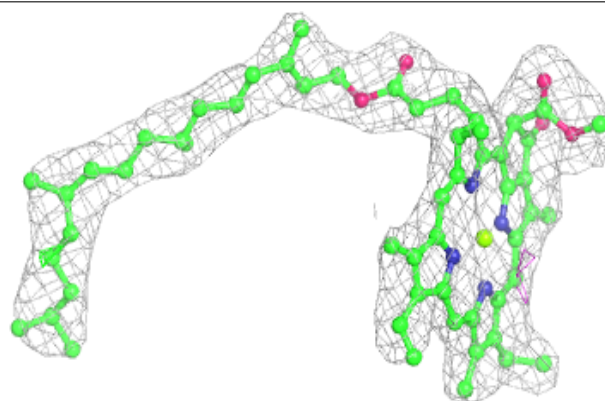


Electron density around BCR d 404:

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

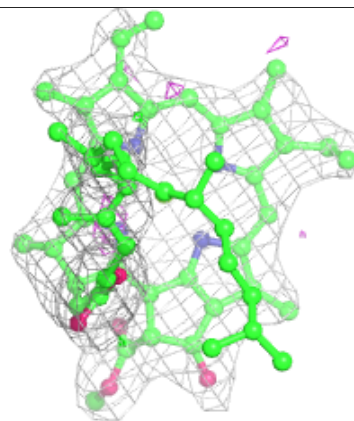
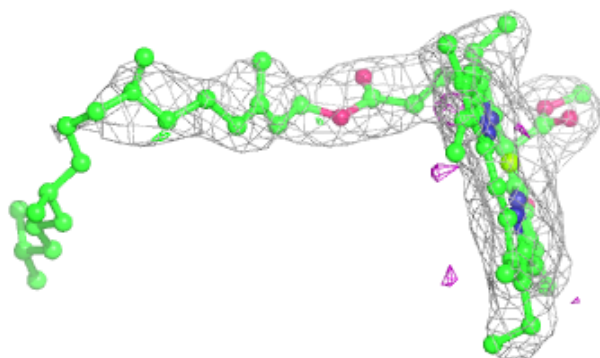
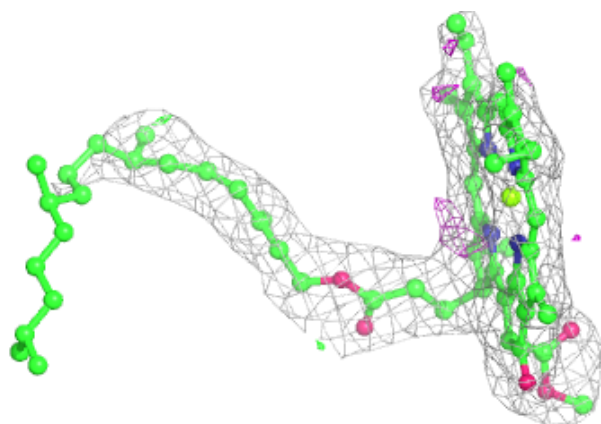
**Electron density around CLA B 609:**

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



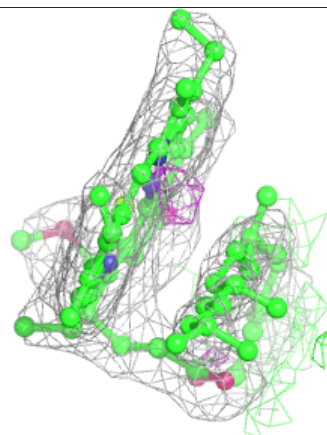
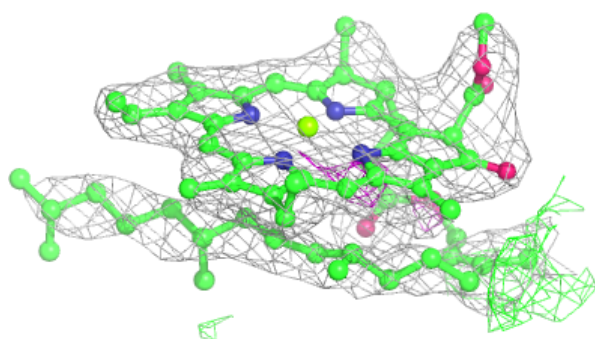
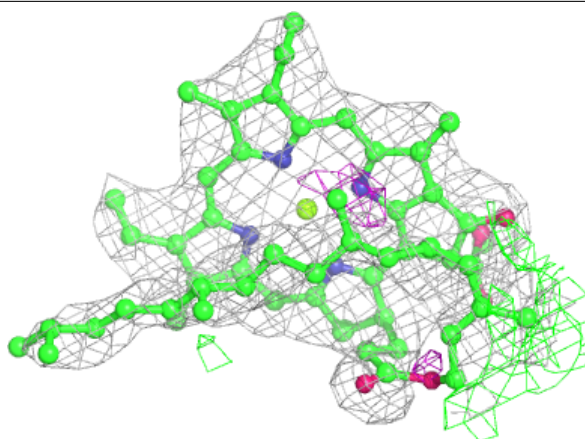
Electron density around CLA D 404:

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

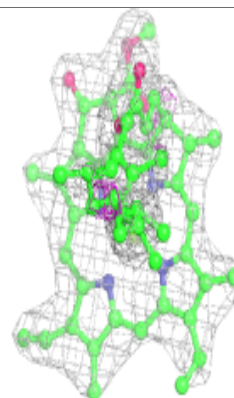
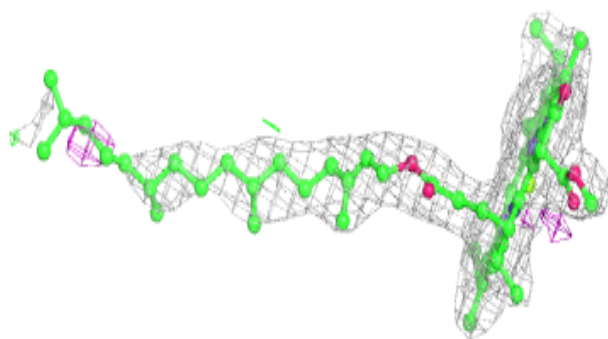
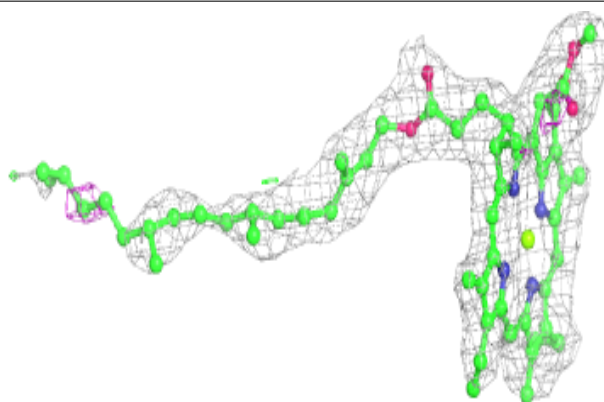


Electron density around CLA b 601:

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

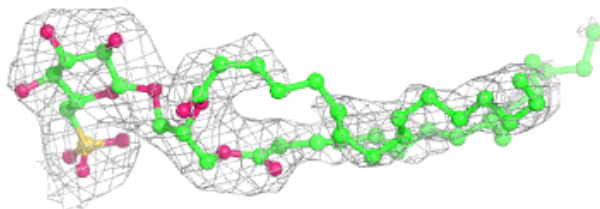
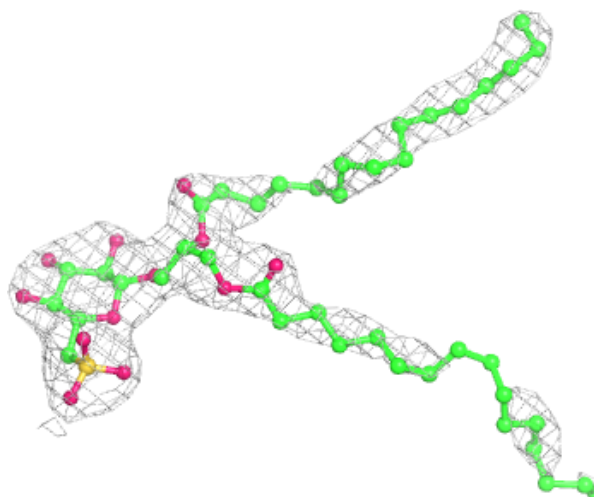
**Electron density around CLA d 403:**

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



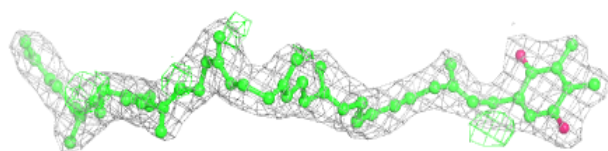
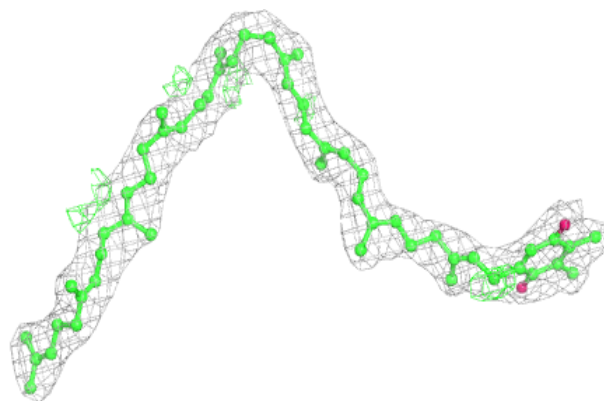
Electron density around SQD a 409:

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

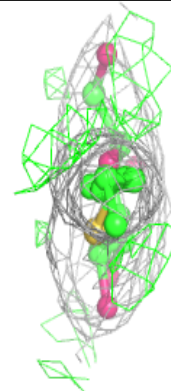
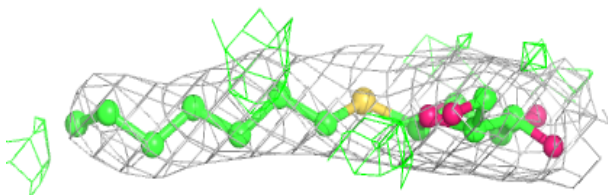
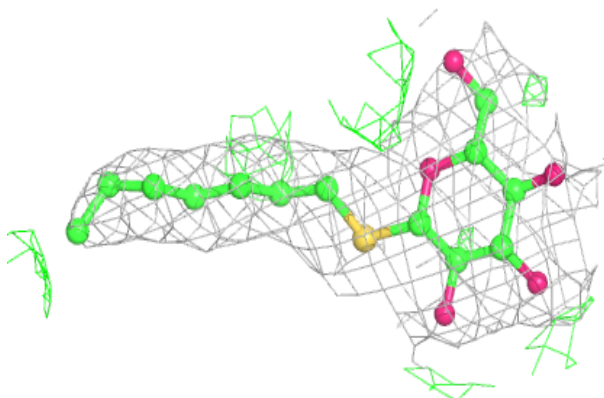


Electron density around PL9 D 406:

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

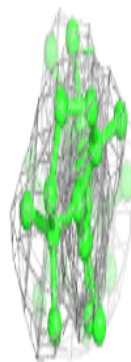
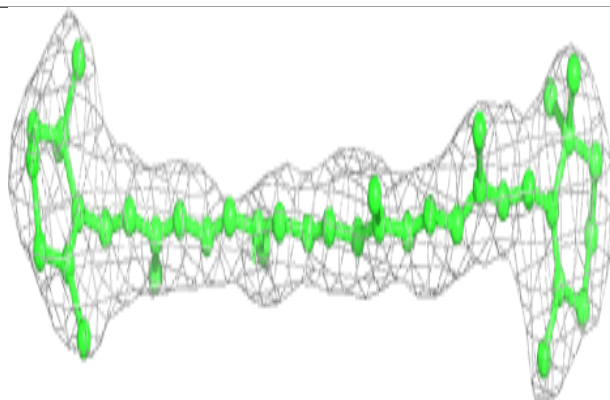
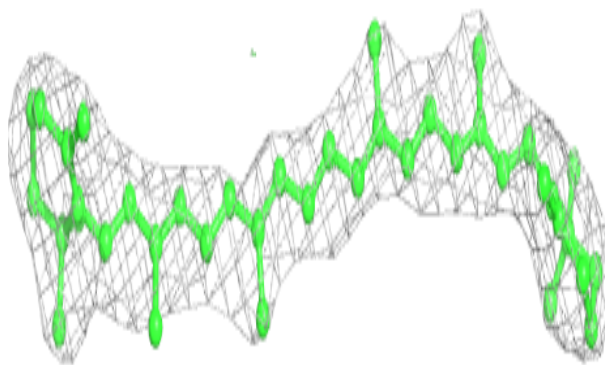
**Electron density around HTG b 624:**

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



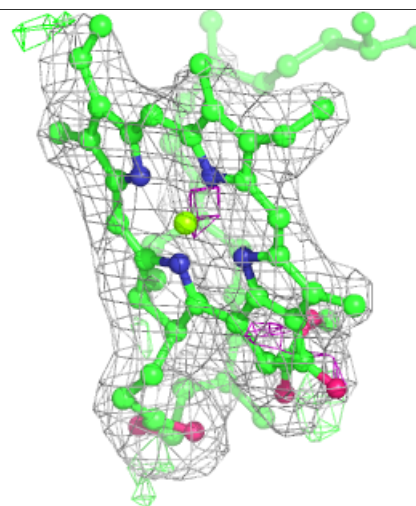
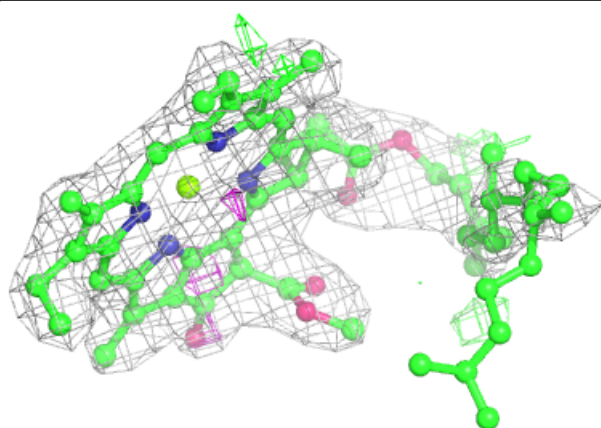
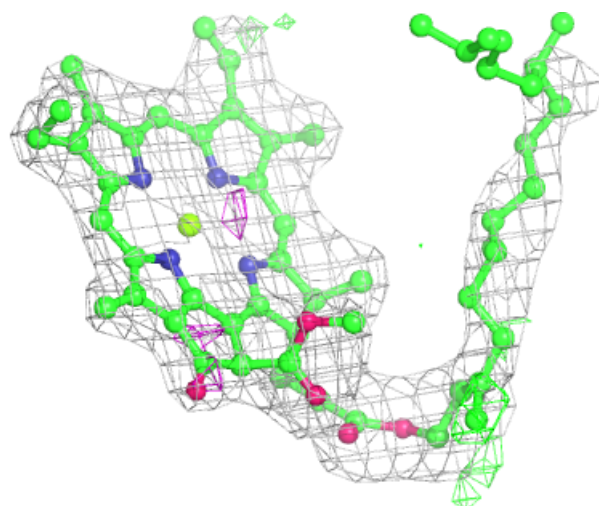
Electron density around BCR C 516:

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



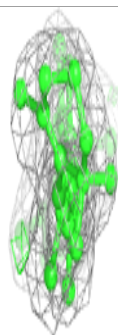
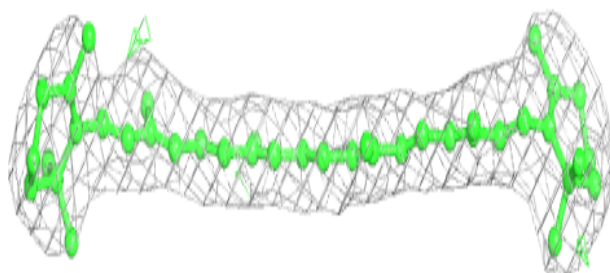
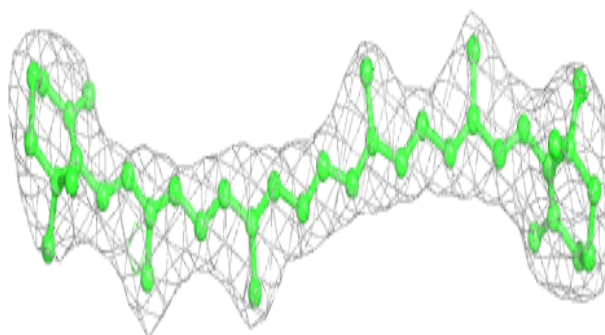
Electron density around CLA b 616:

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



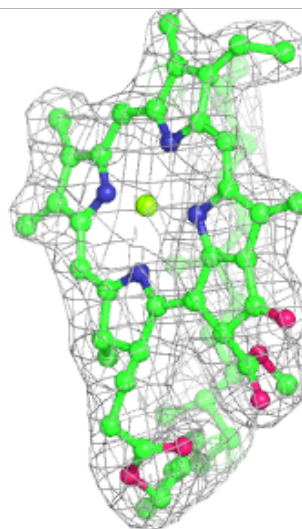
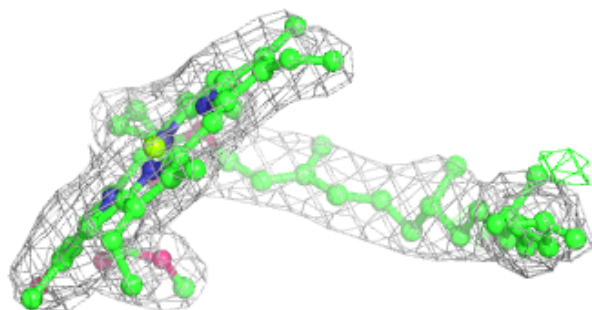
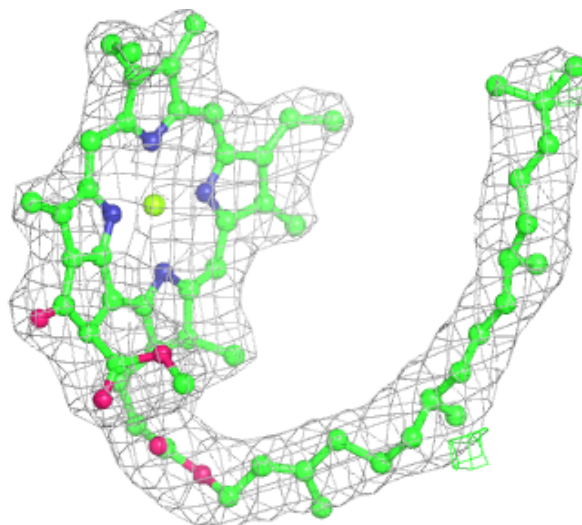
Electron density around BCR b 618:

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



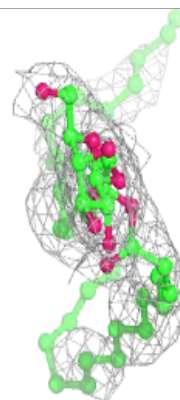
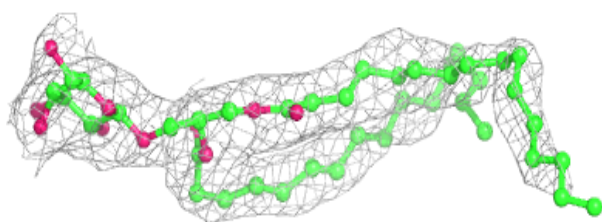
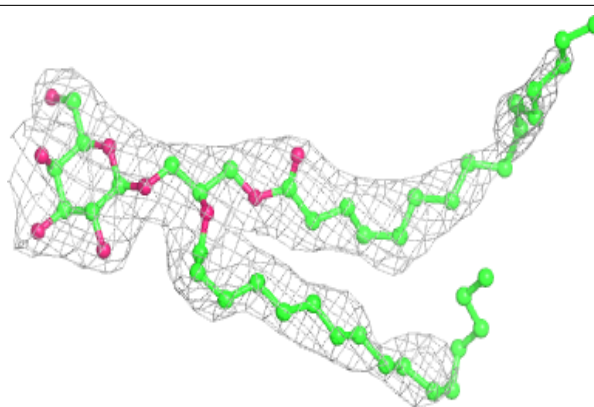
Electron density around CLA C 509:

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

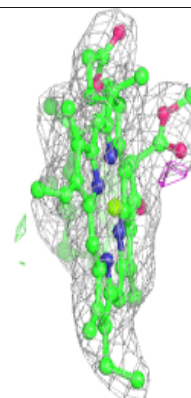
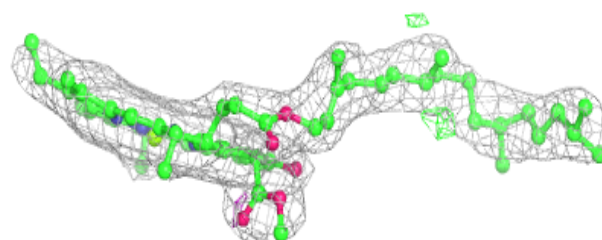
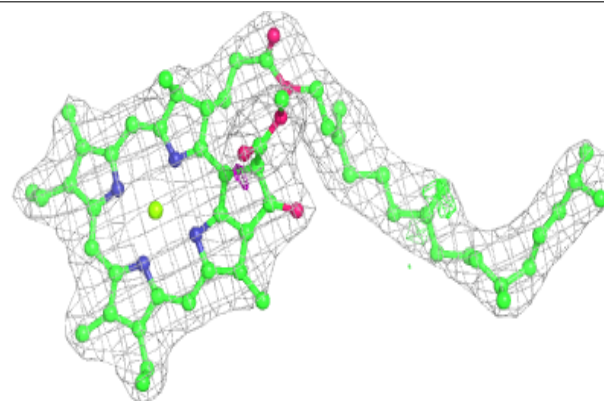


Electron density around LMG d 411:

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

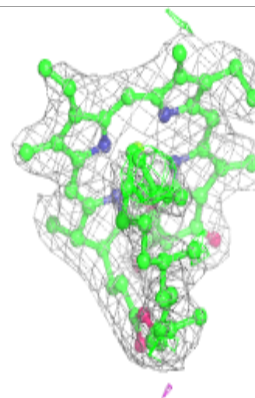
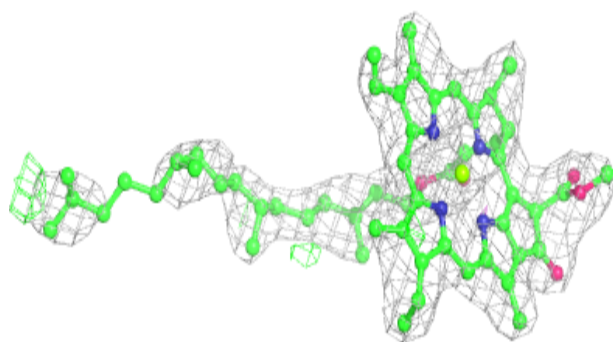
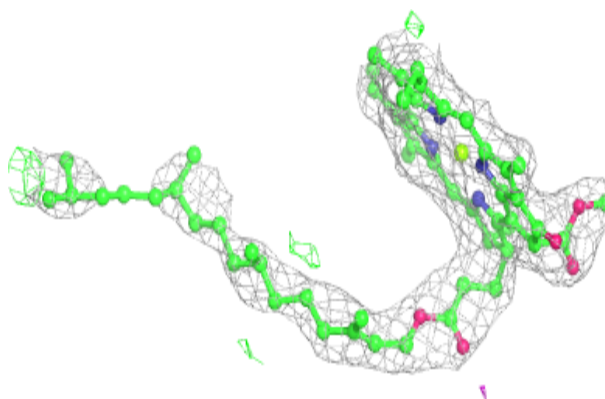
**Electron density around CLA b 602:**

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



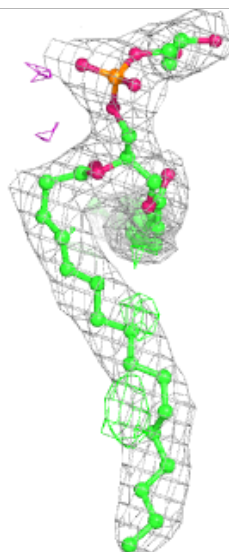
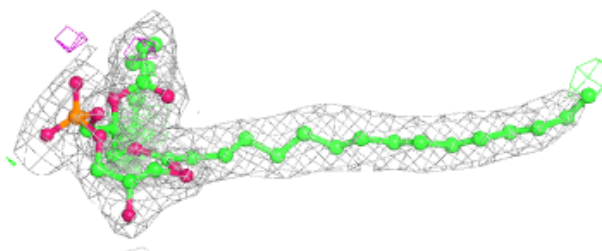
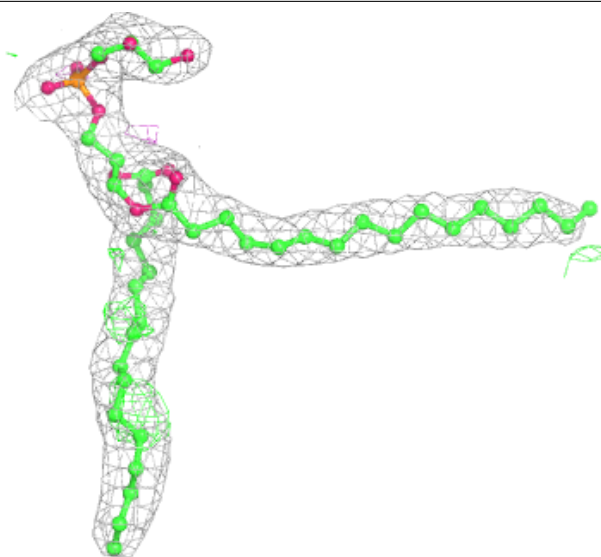
Electron density around CLA c 506:

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



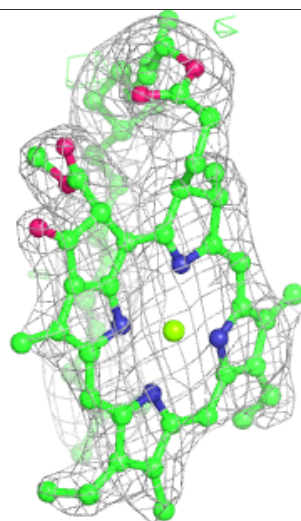
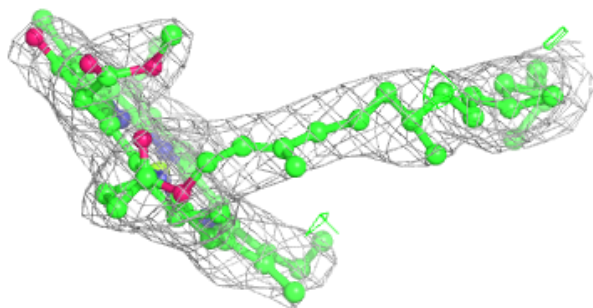
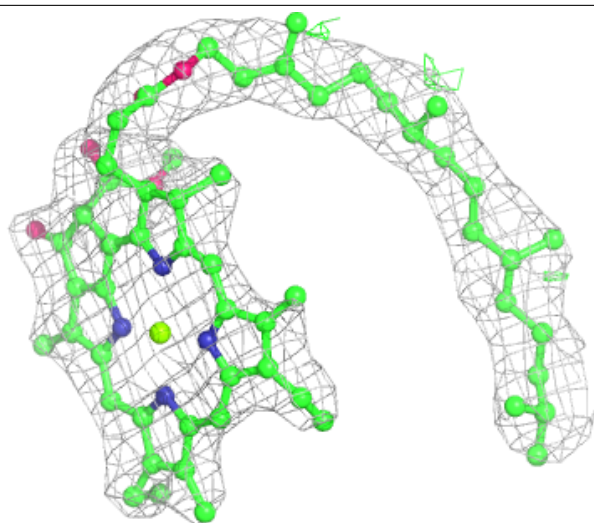
Electron density around LHG L 101:

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



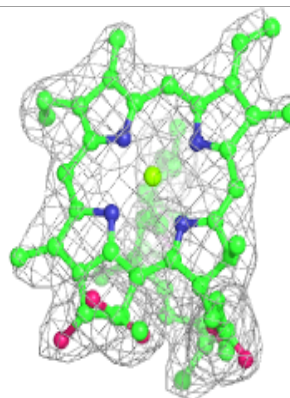
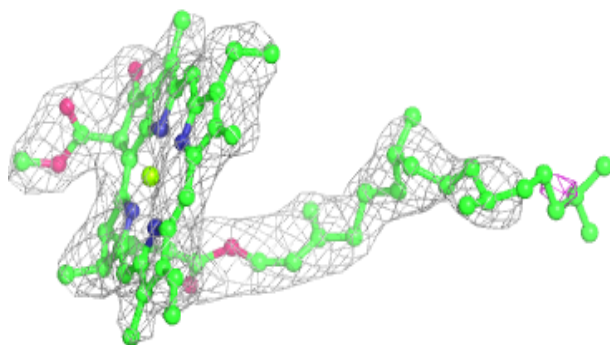
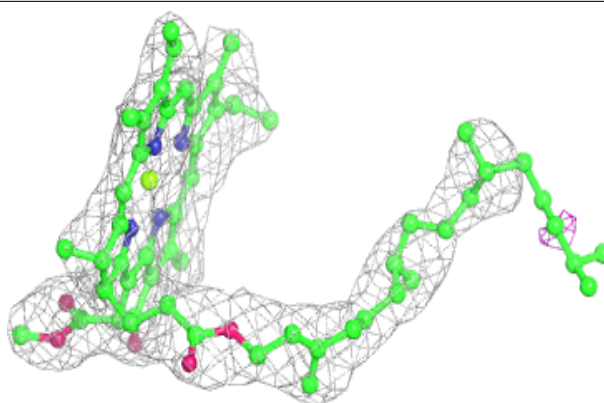
Electron density around CLA c 509:

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

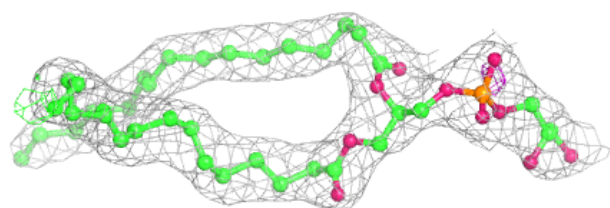
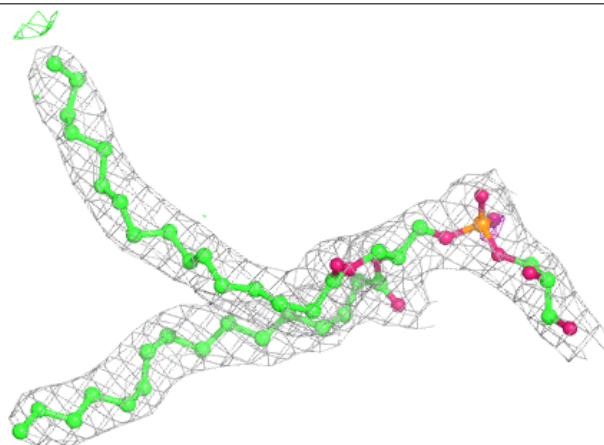


Electron density around CLA c 510:

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

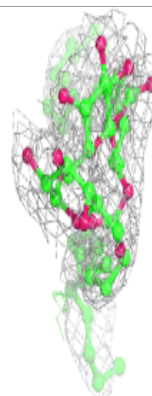
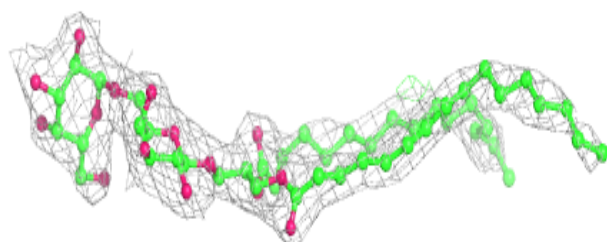
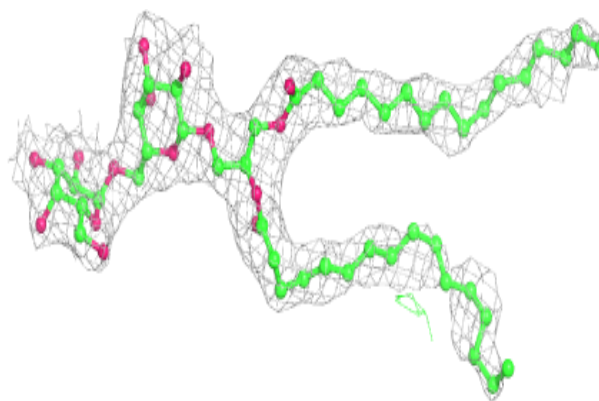
**Electron density around LHG d 407:**

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

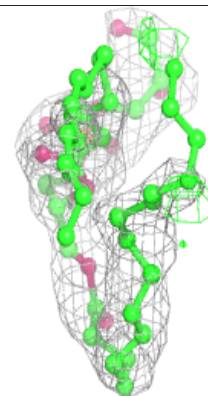
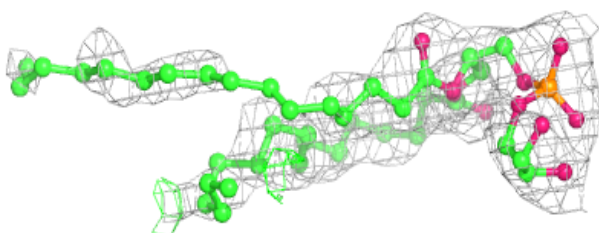
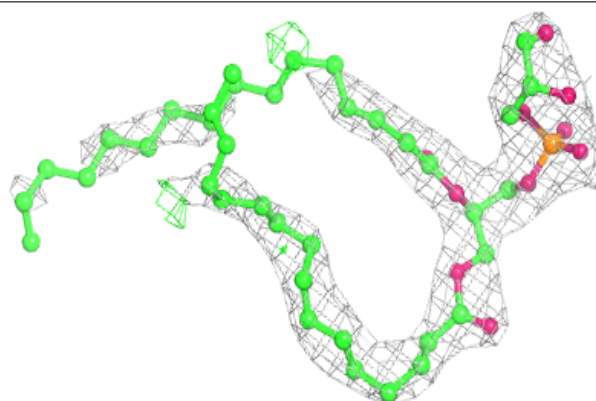


Electron density around DGD c 520:

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

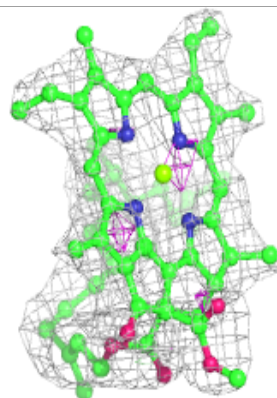
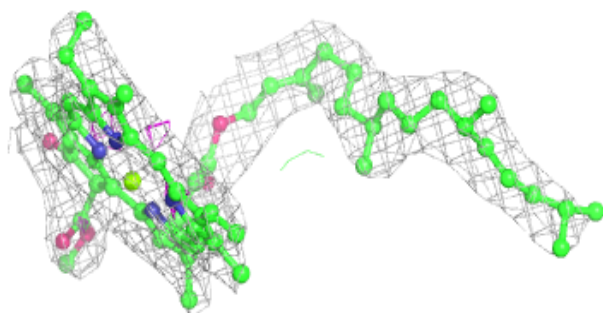
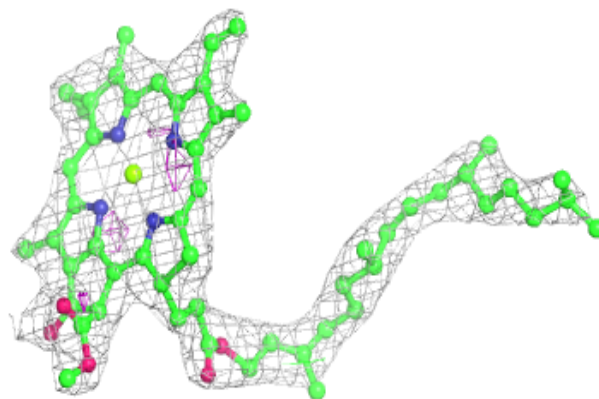
**Electron density around LHG d 408:**

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

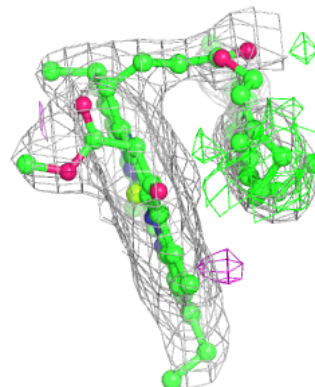
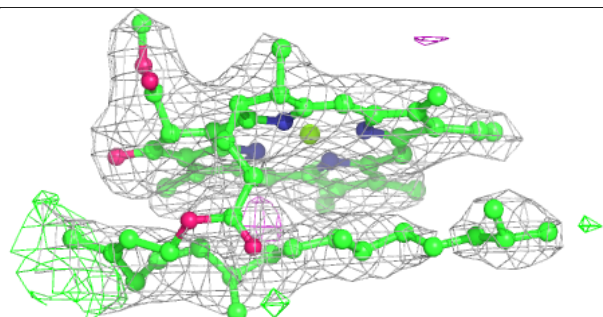
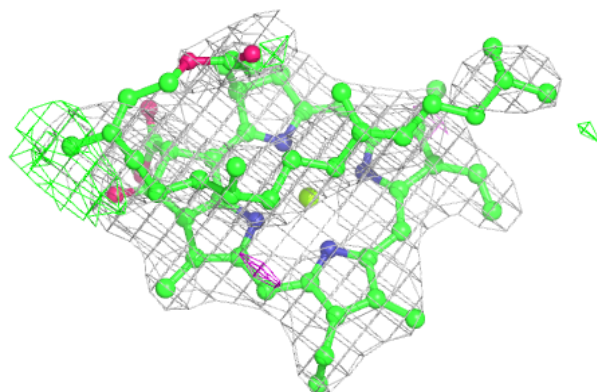


Electron density around CLA c 513:

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

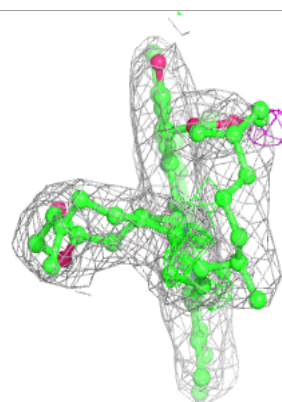
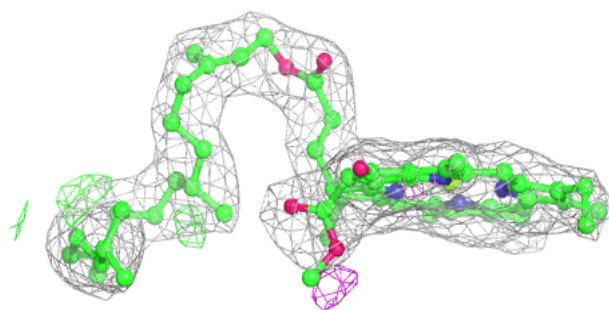
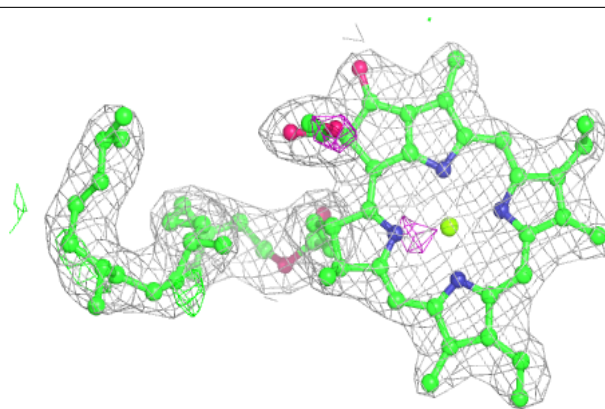
**Electron density around CLA B 601:**

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

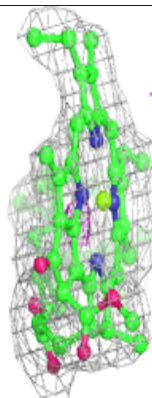
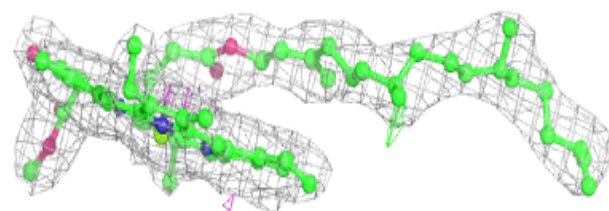
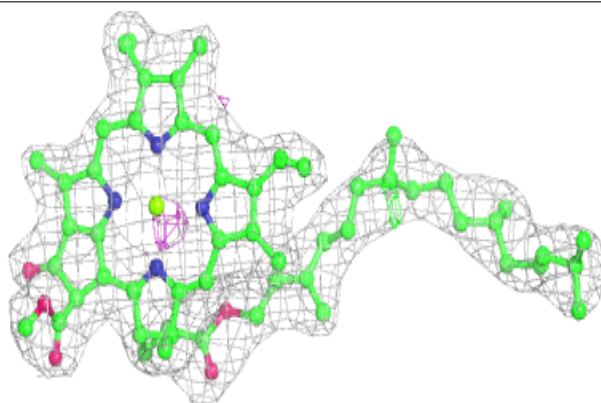


Electron density around CLA b 612:

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

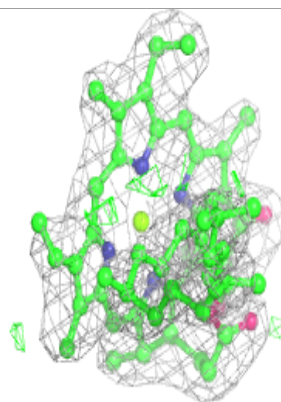
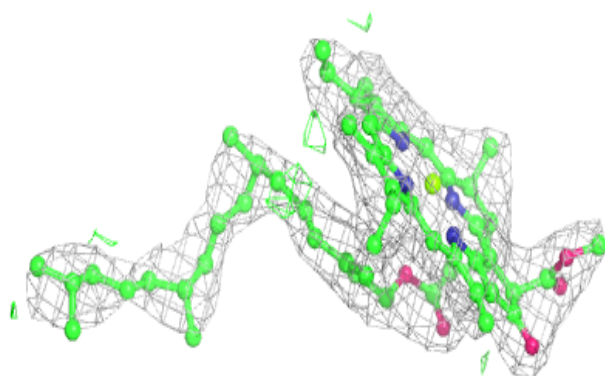
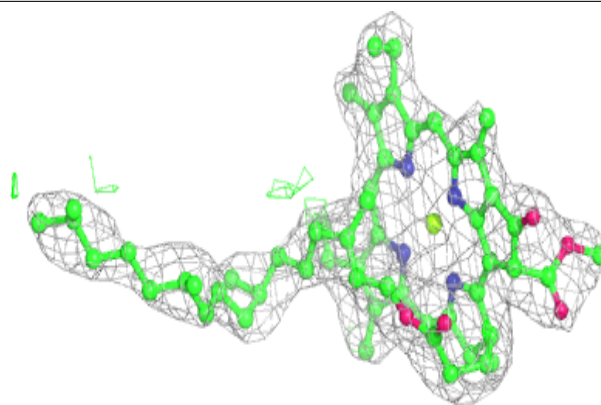
**Electron density around CLA B 603:**

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

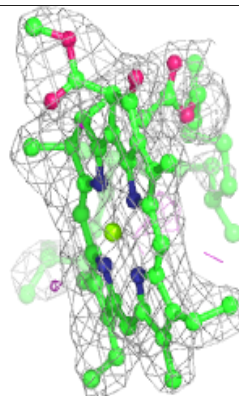
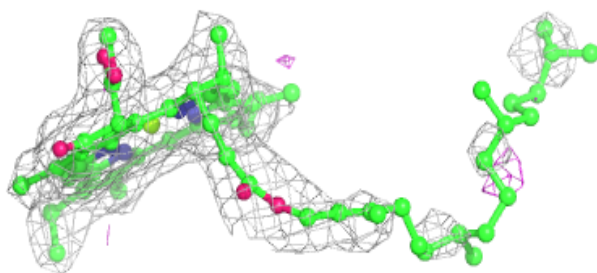
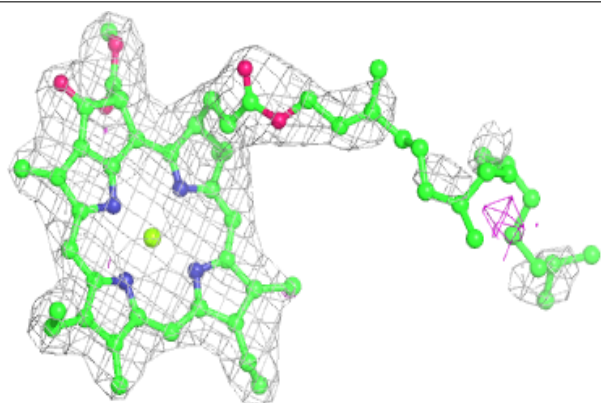


Electron density around CLA c 507:

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

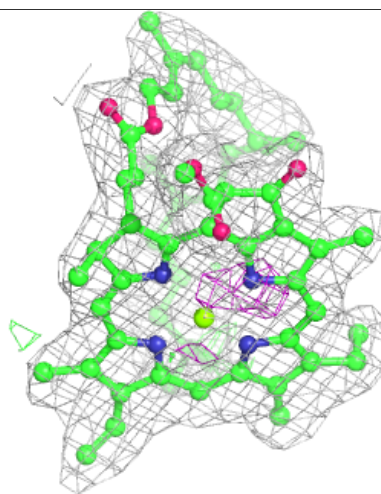
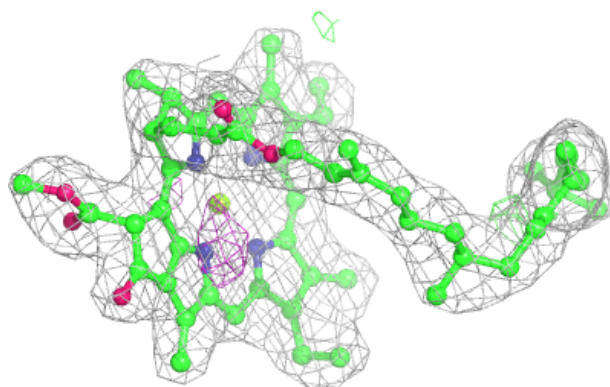
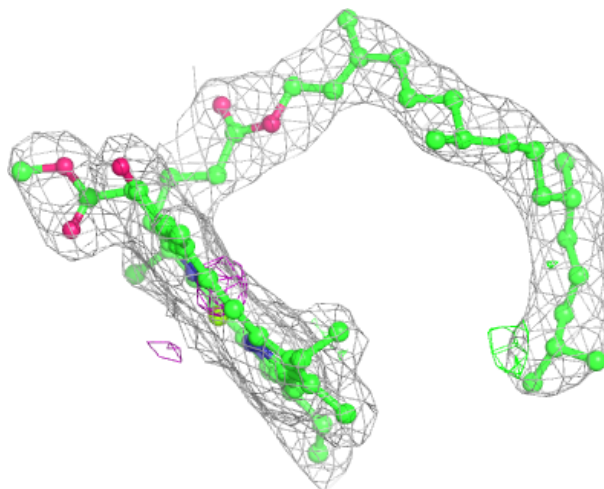
**Electron density around CLA a 407:**

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



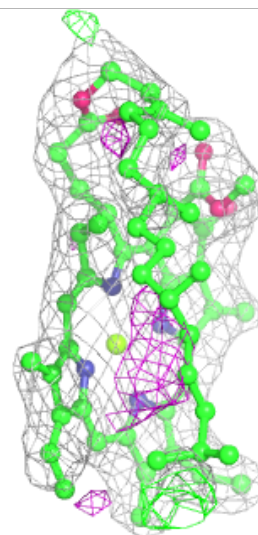
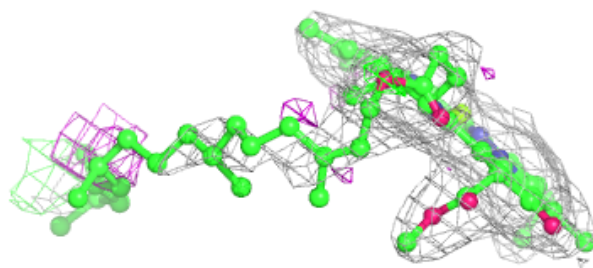
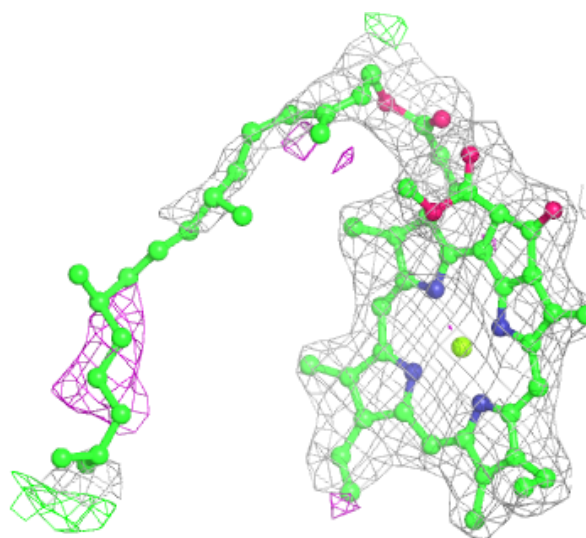
Electron density around CLA B 611:

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



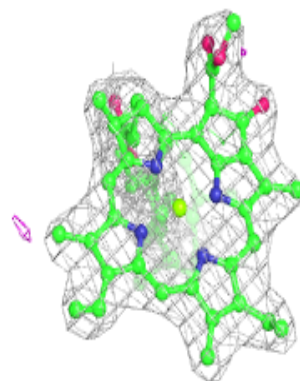
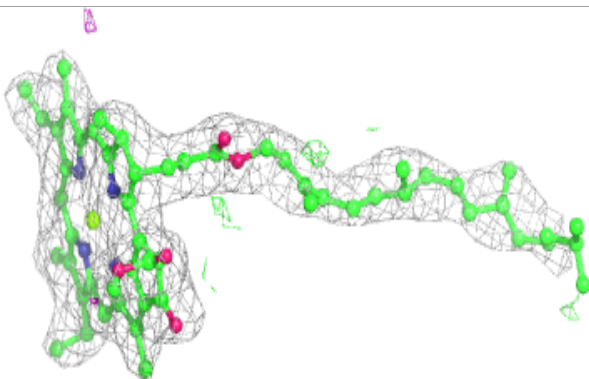
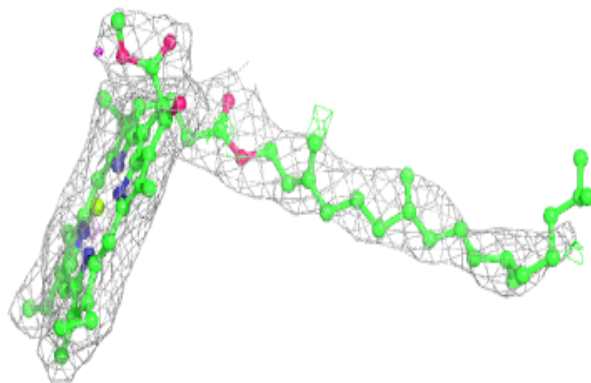
Electron density around CLA B 616:

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

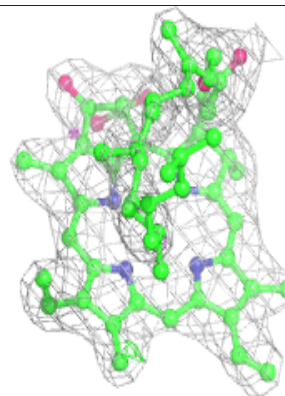
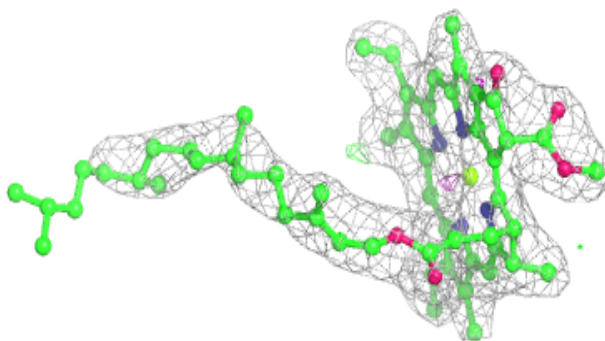
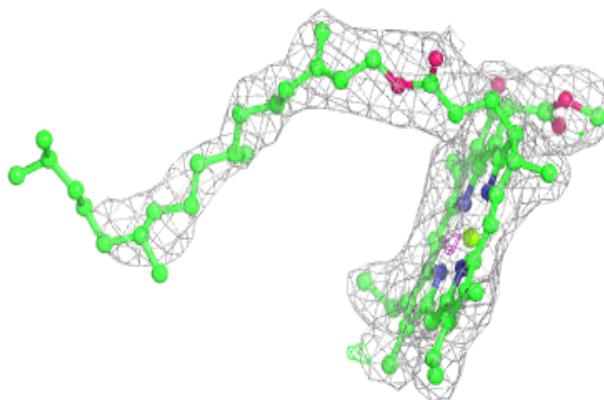


Electron density around CLA b 604:

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

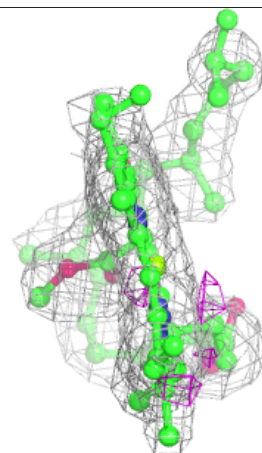
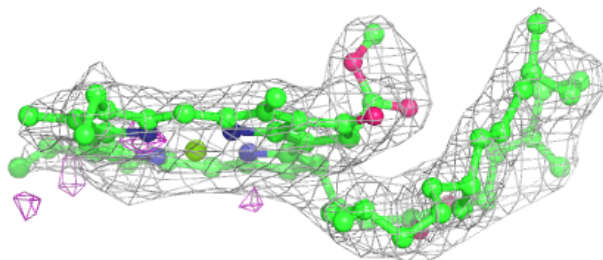
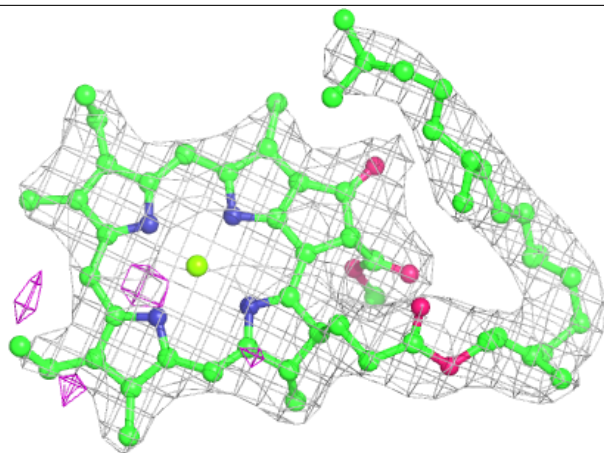
**Electron density around CLA C 510:**

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



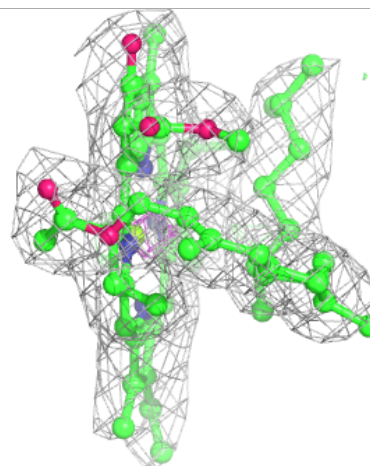
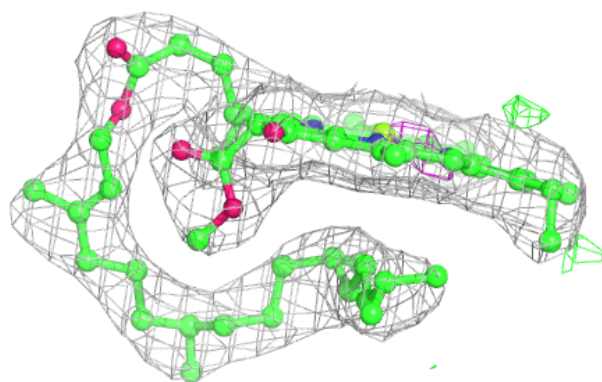
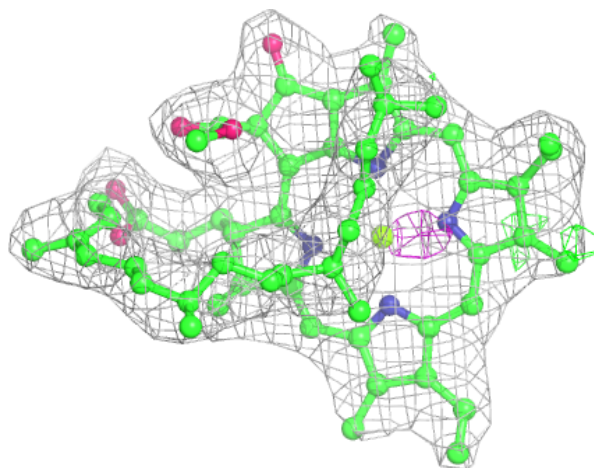
Electron density around CLA b 610:

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



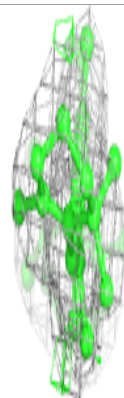
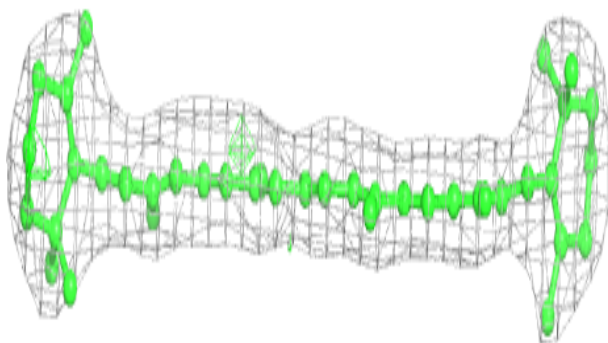
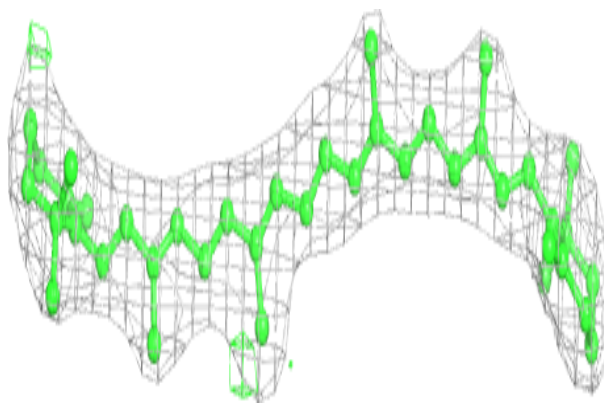
Electron density around CLA C 512:

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

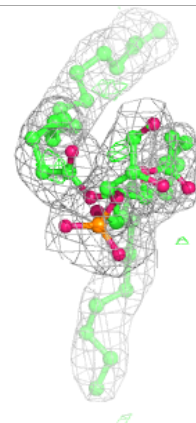
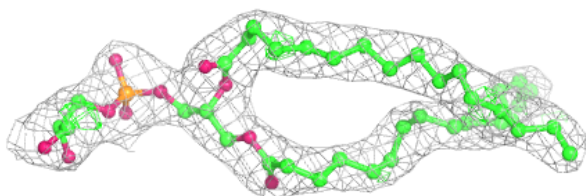
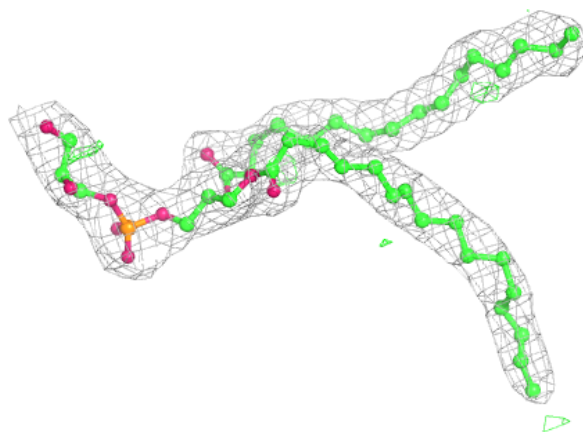


Electron density around BCR C 517:

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

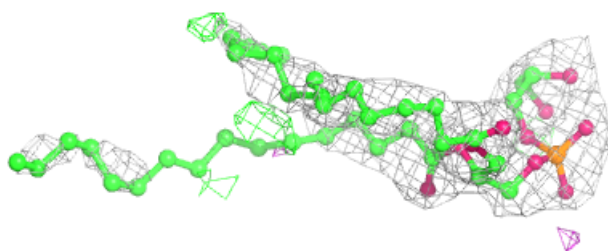
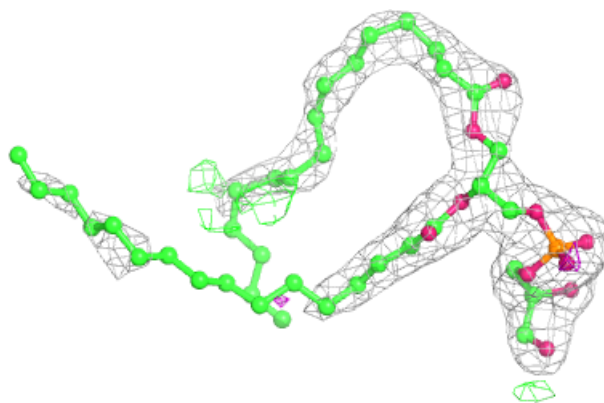
**Electron density around LHG D 407:**

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

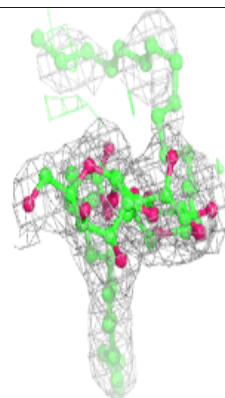
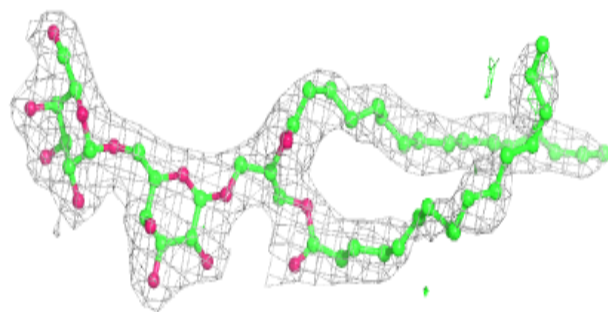
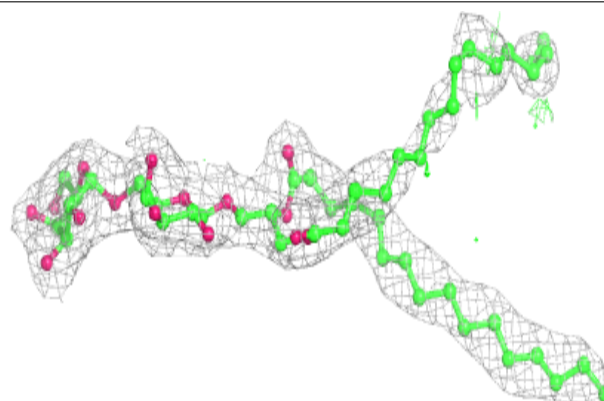


Electron density around LHG D 408:

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

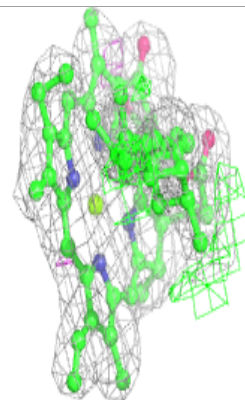
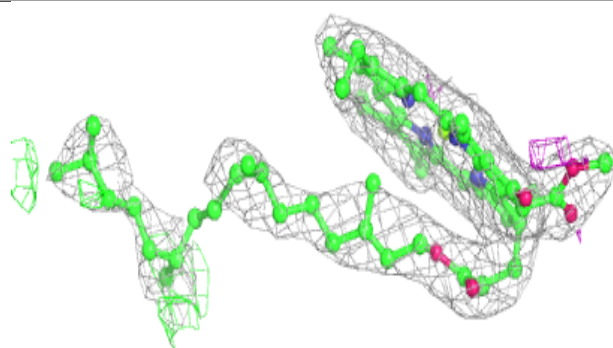
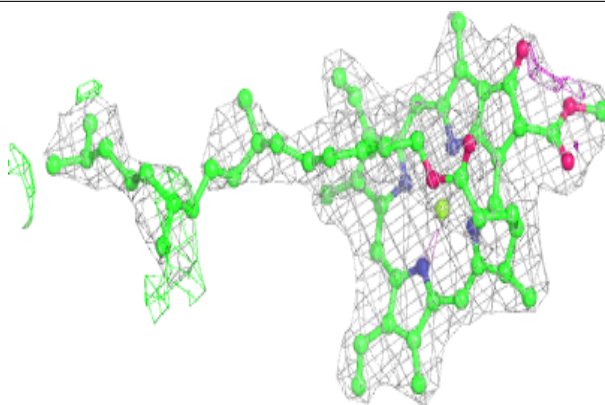
**Electron density around DGD C 518:**

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

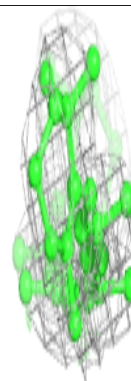
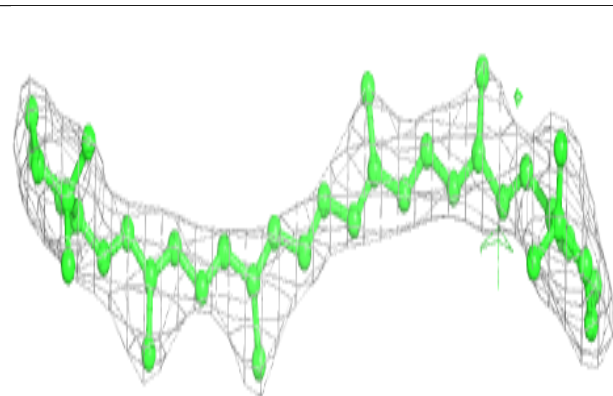
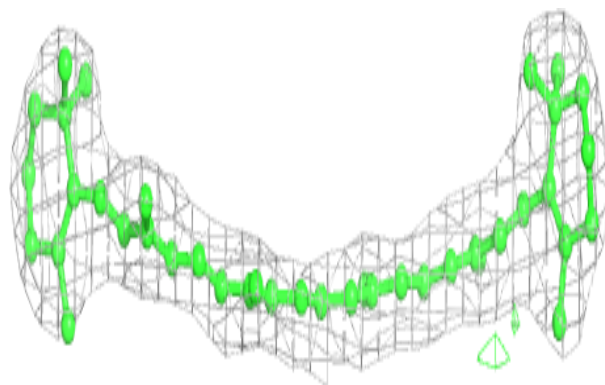


Electron density around CLA b 614:

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

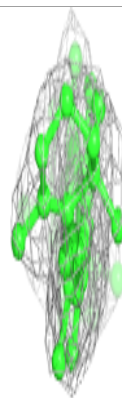
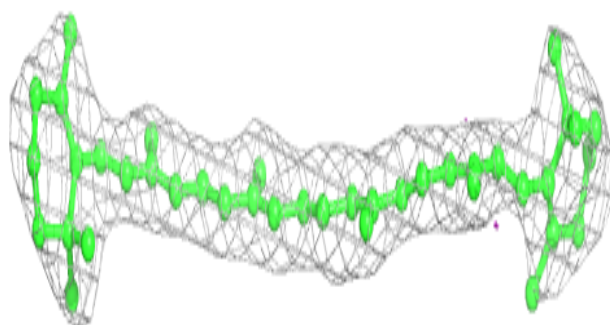
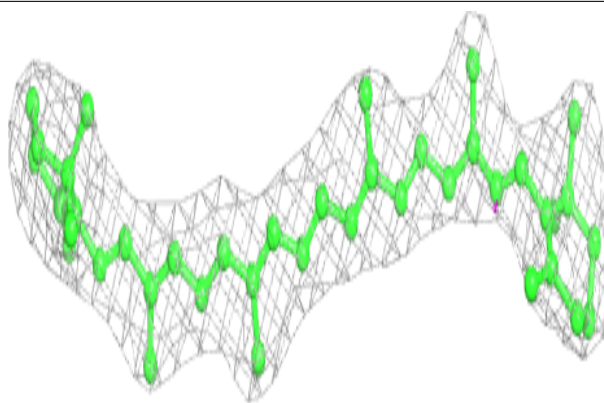
**Electron density around BCR K 101:**

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

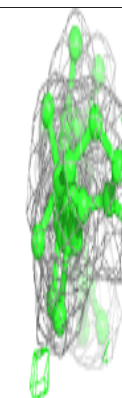
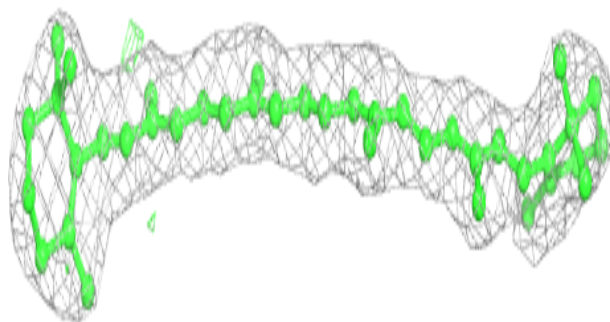
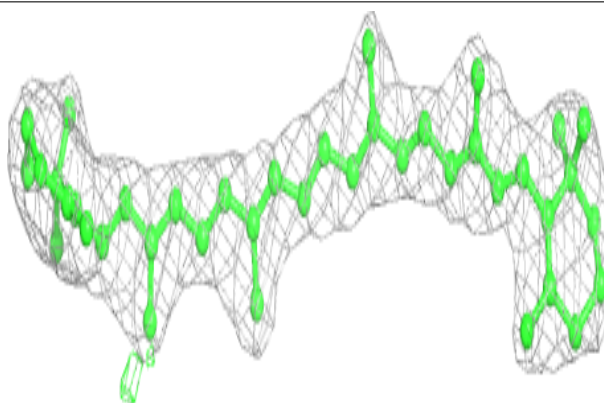


Electron density around BCR Y 101:

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

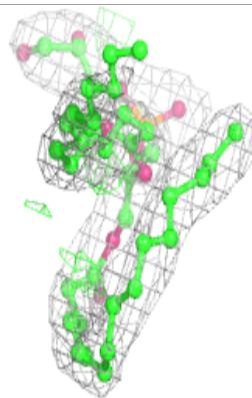
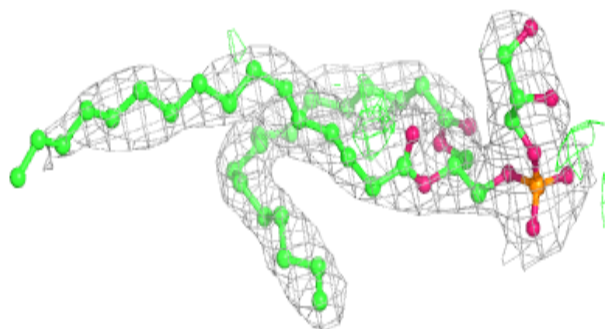
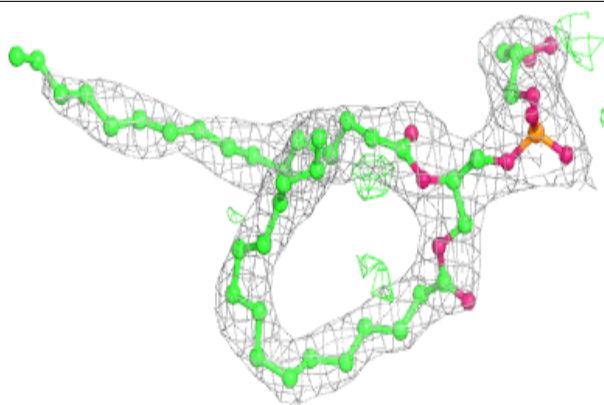
**Electron density around BCR b 617:**

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

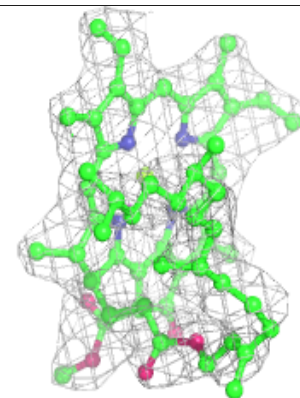
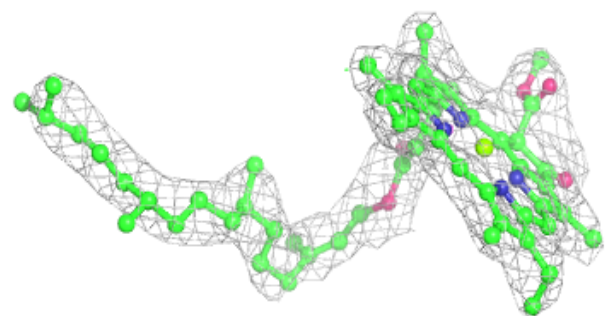
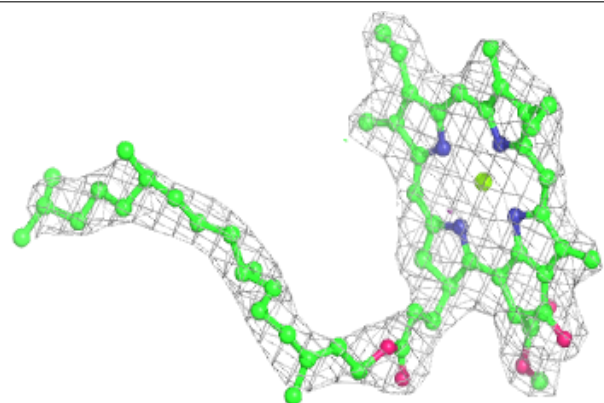


Electron density around LHG d 406:

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

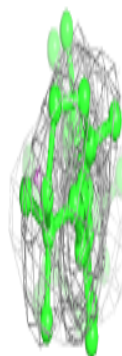
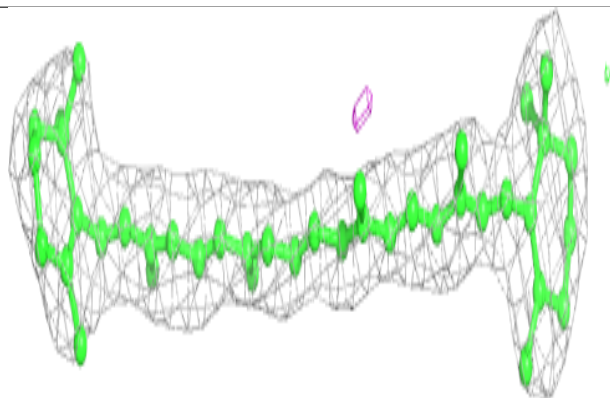
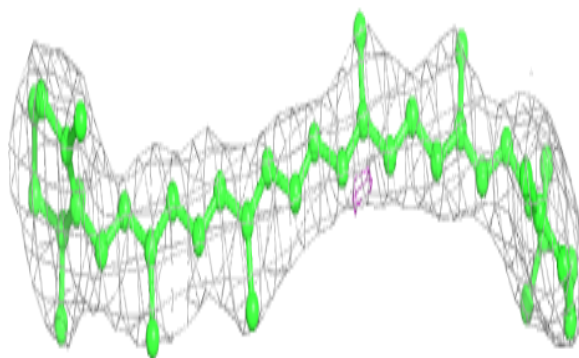
**Electron density around CLA C 513:**

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

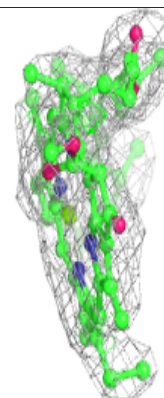
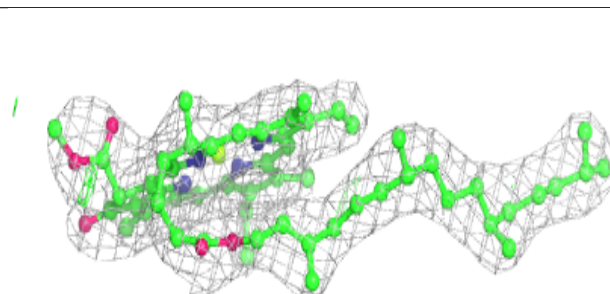
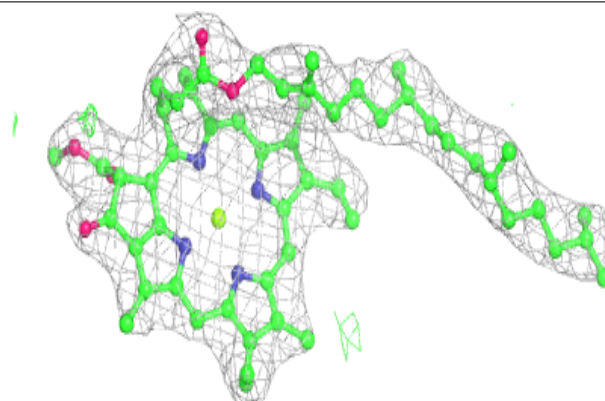


Electron density around BCR c 516:

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

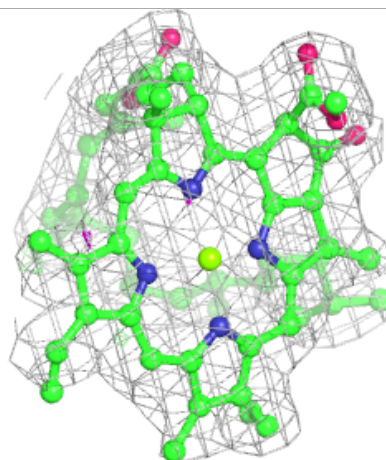
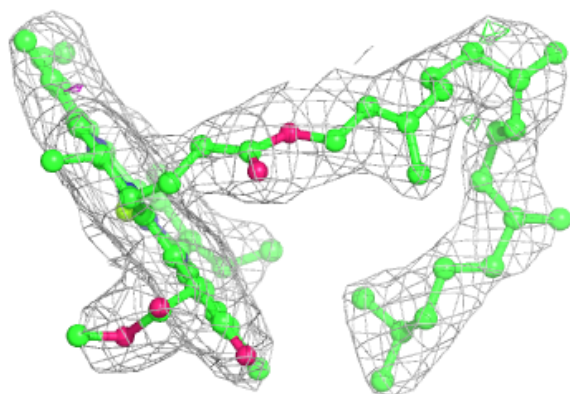
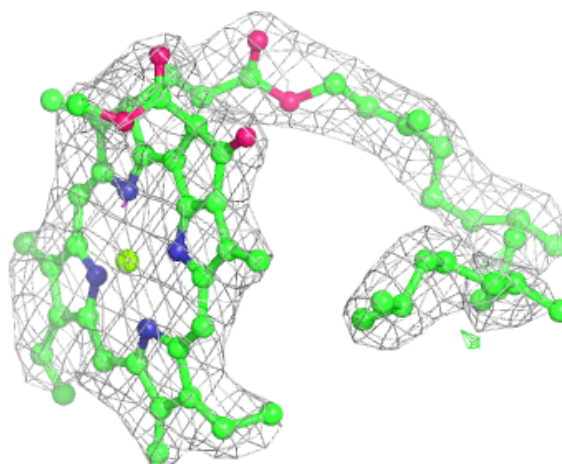
**Electron density around CLA C 503:**

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



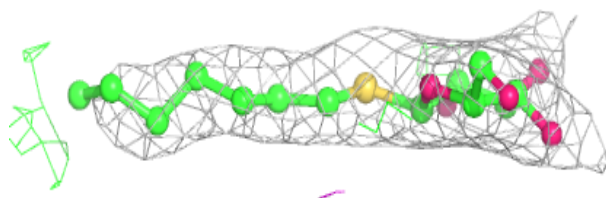
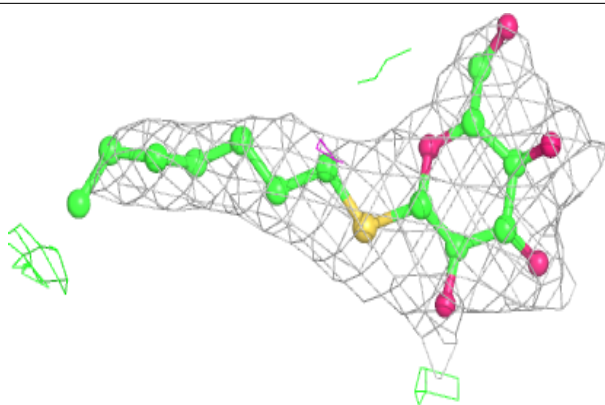
Electron density around CLA C 505:

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



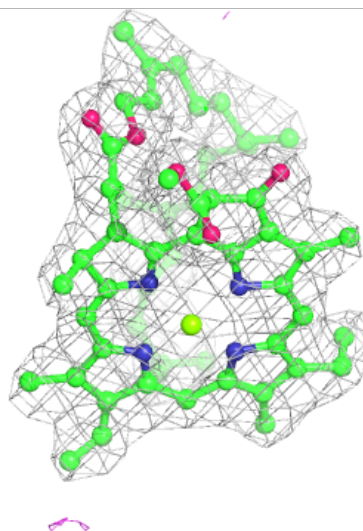
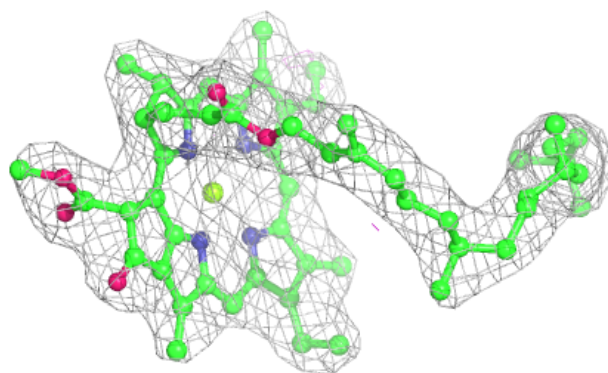
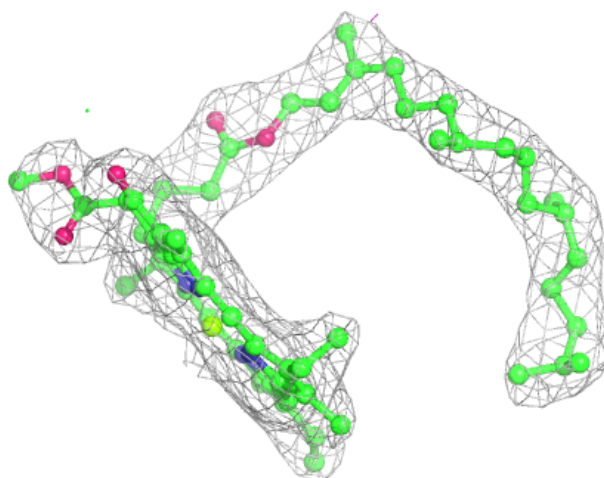
Electron density around HTG B 624:

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



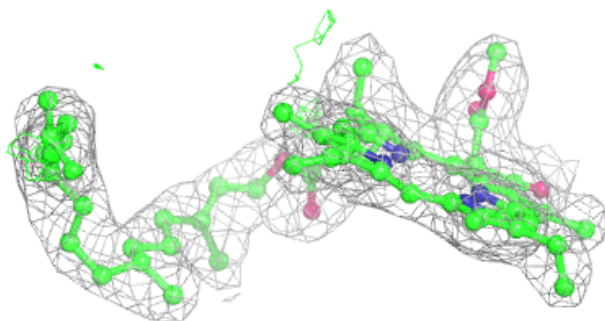
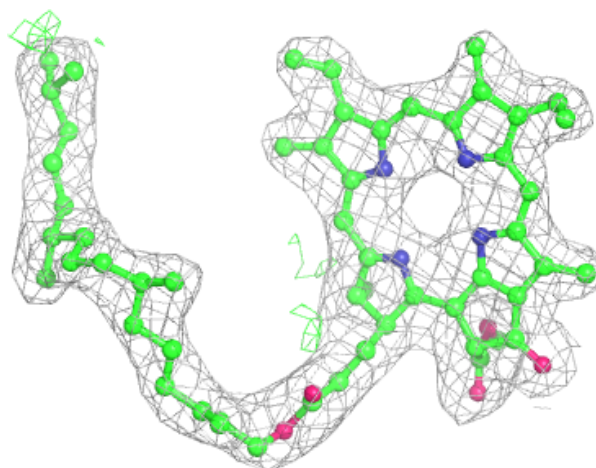
Electron density around CLA b 611:

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



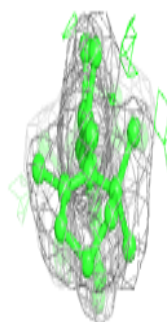
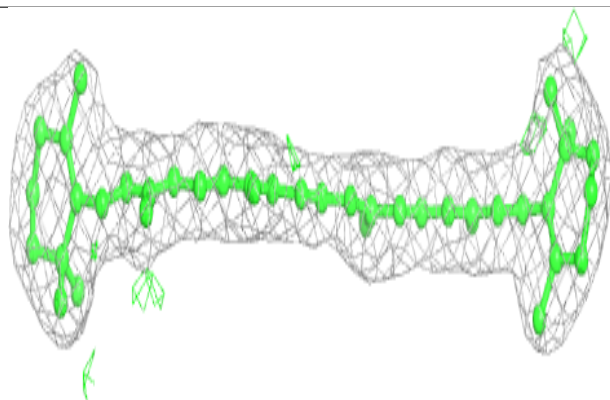
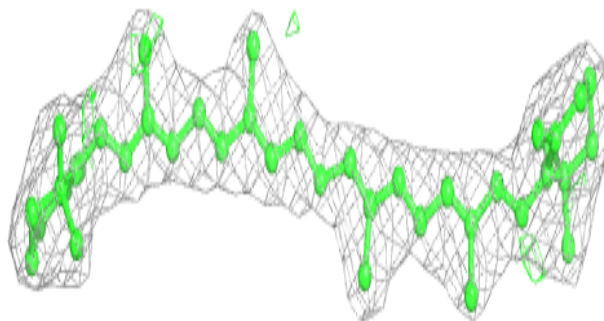
Electron density around PHO A 415:

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

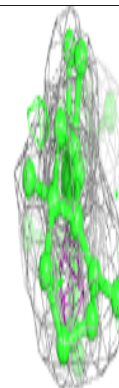
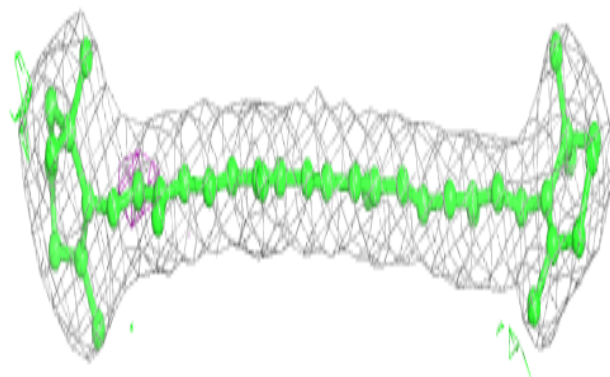
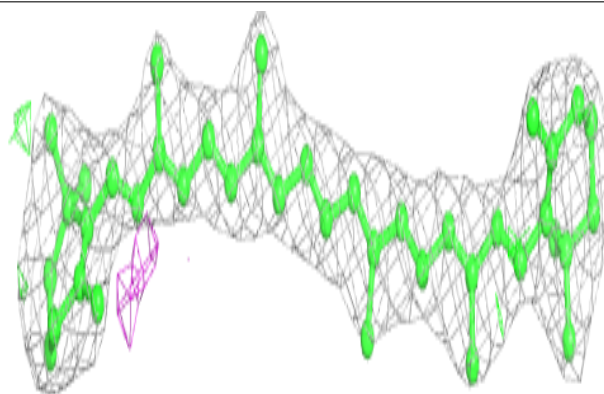


Electron density around BCR A 408:

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

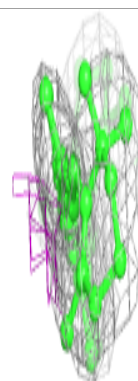
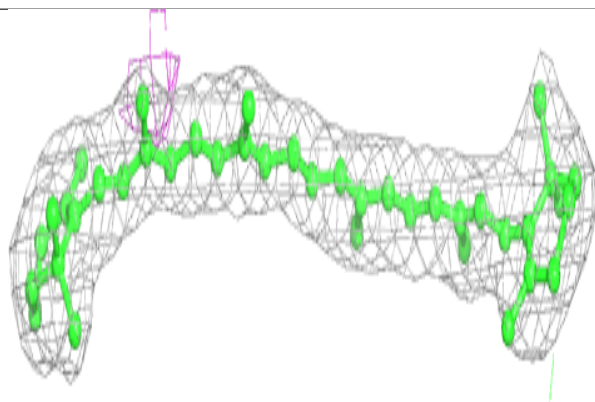
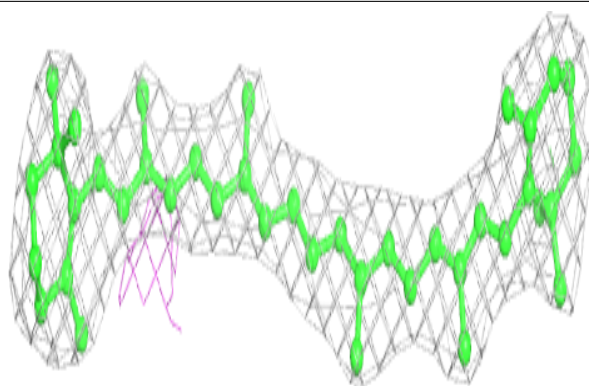
**Electron density around BCR B 618:**

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

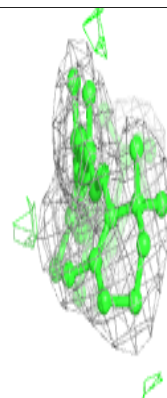
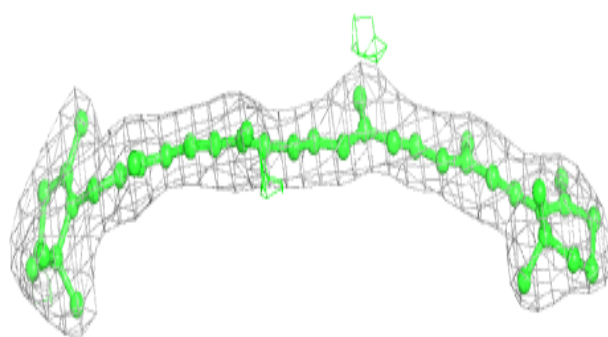
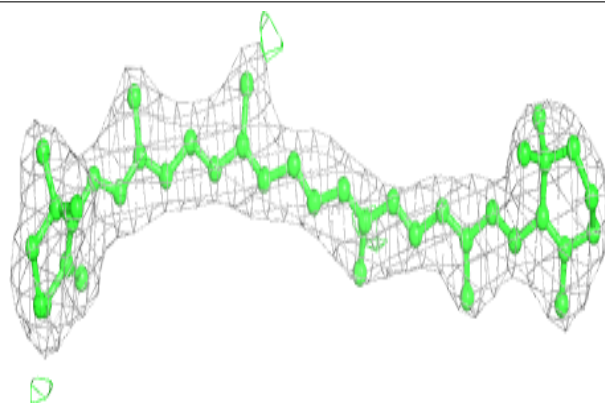


Electron density around BCR B 619:

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

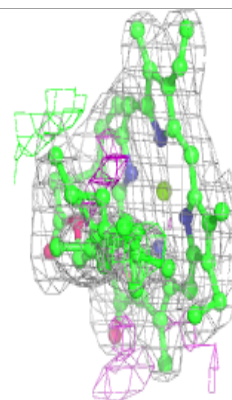
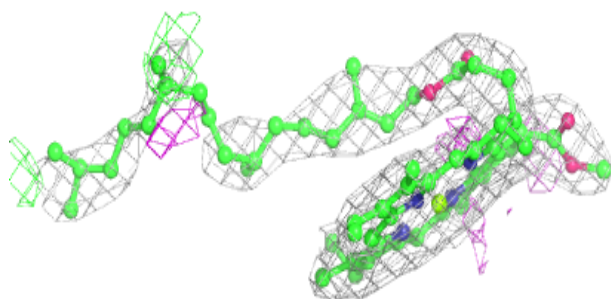
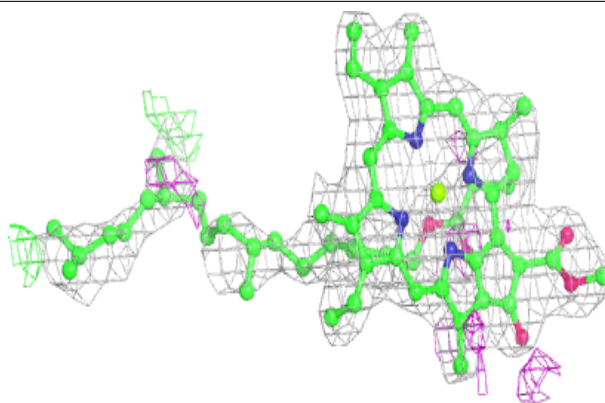
**Electron density around BCR B 631:**

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

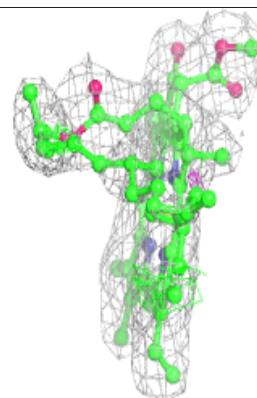
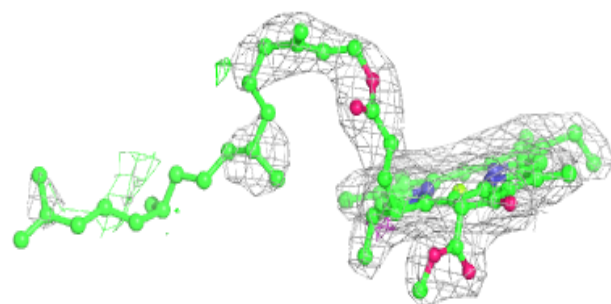
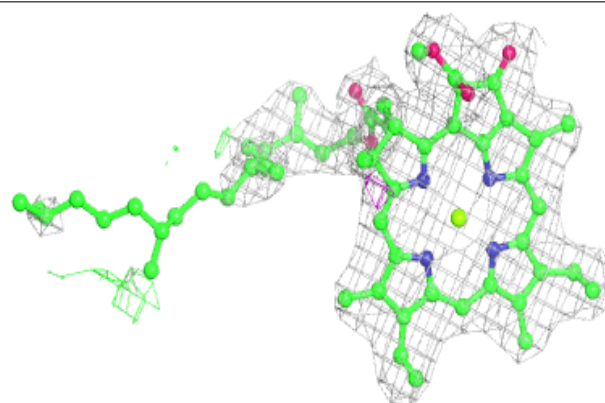


Electron density around CLA B 614:

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

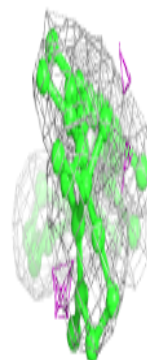
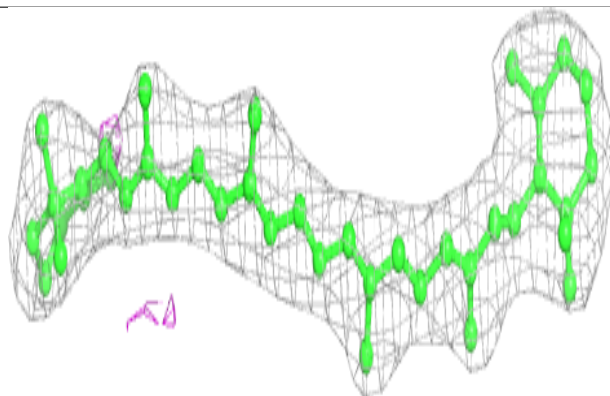
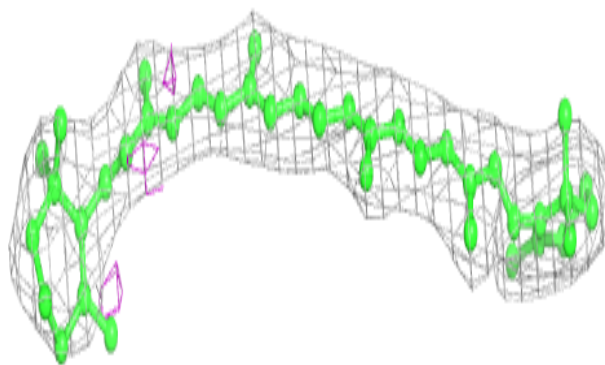
**Electron density around CLA a 405:**

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



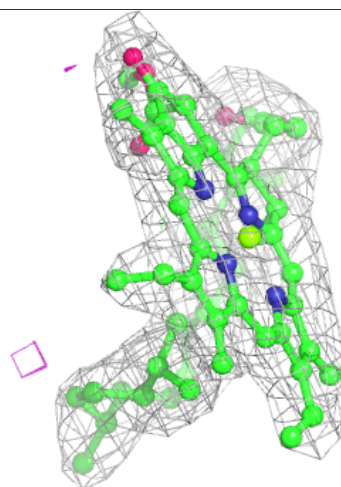
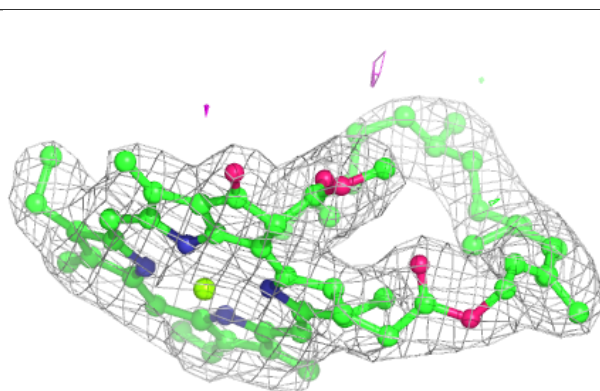
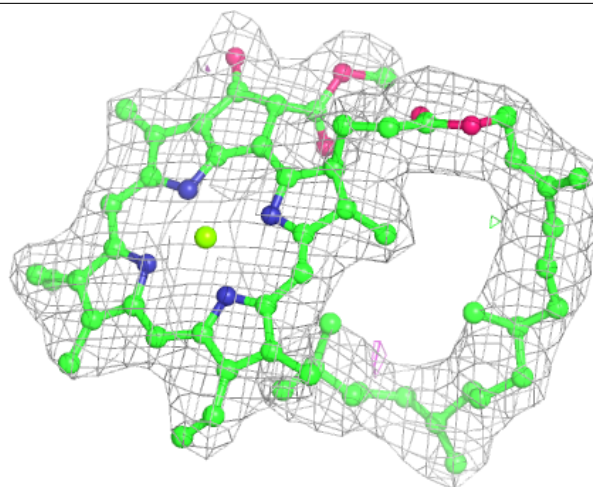
Electron density around BCR D 405:

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



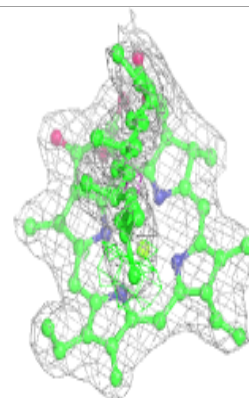
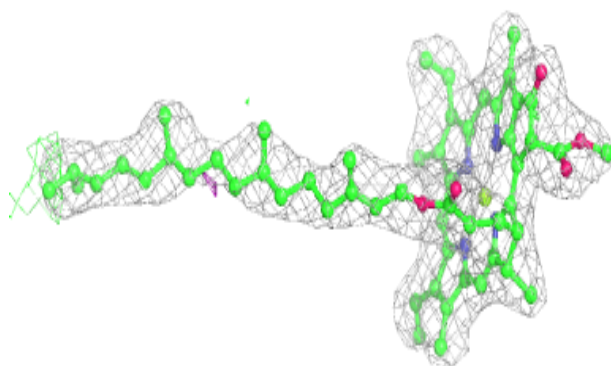
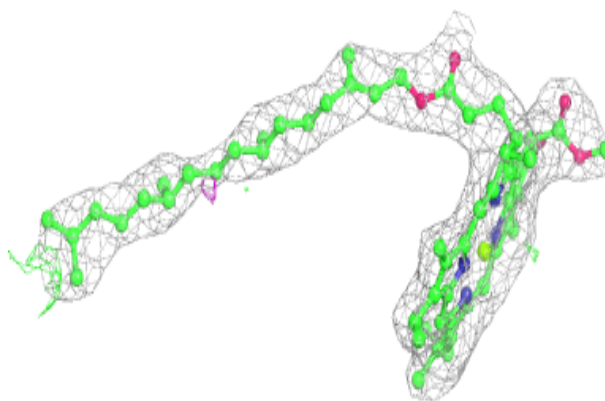
Electron density around CLA b 615:

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

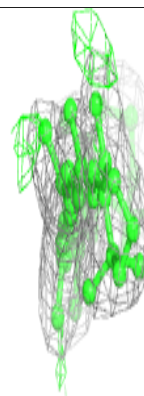
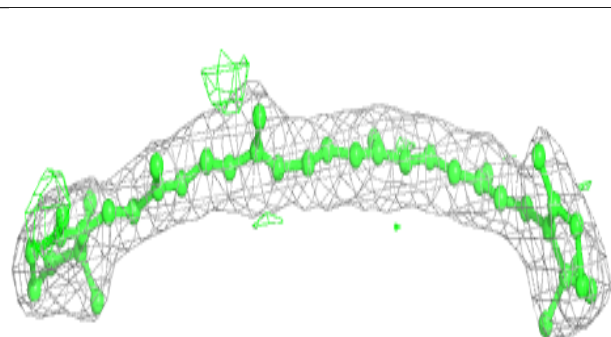
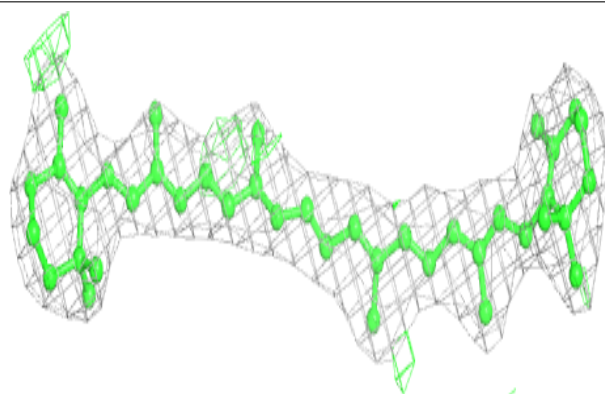


Electron density around CLA B 607:

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

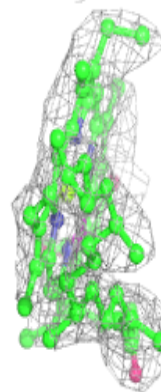
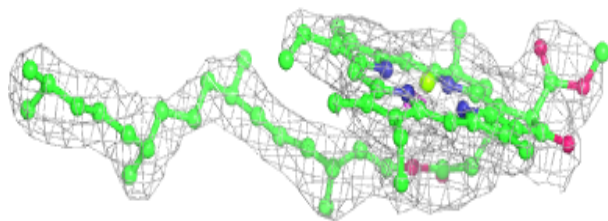
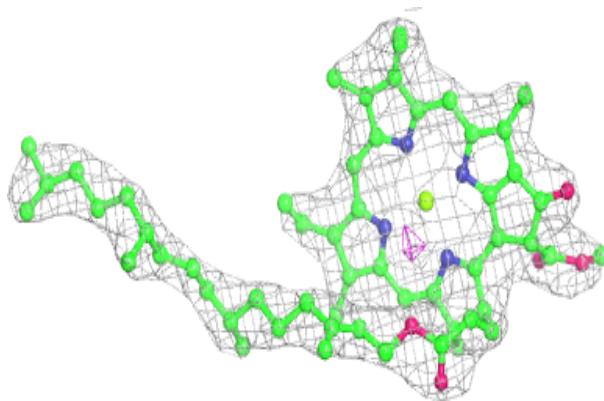
**Electron density around BCR T 101:**

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

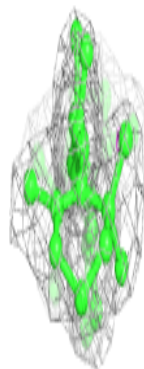
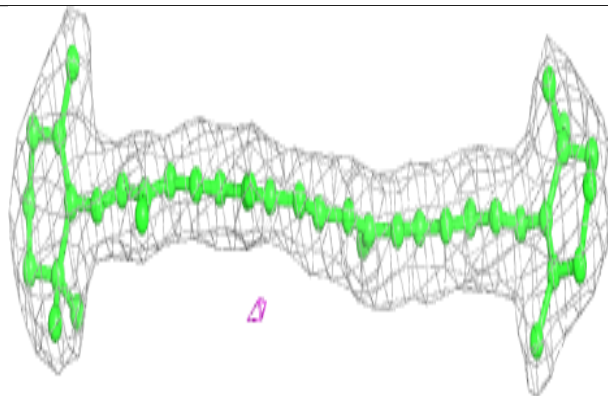
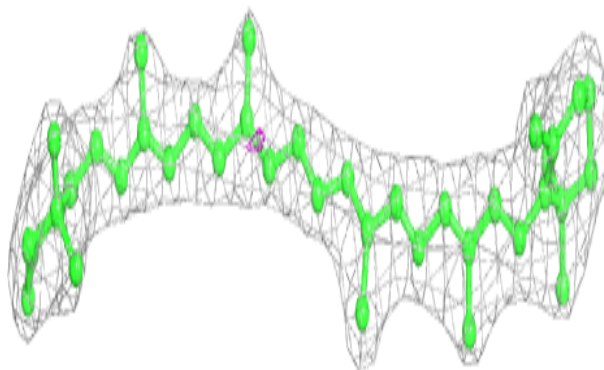


Electron density around CLA c 503:

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

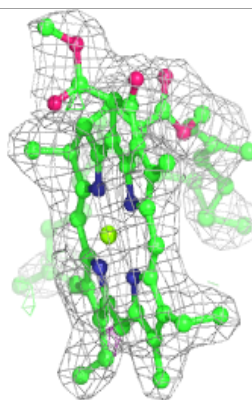
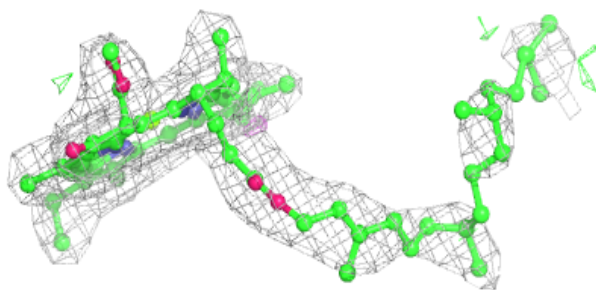
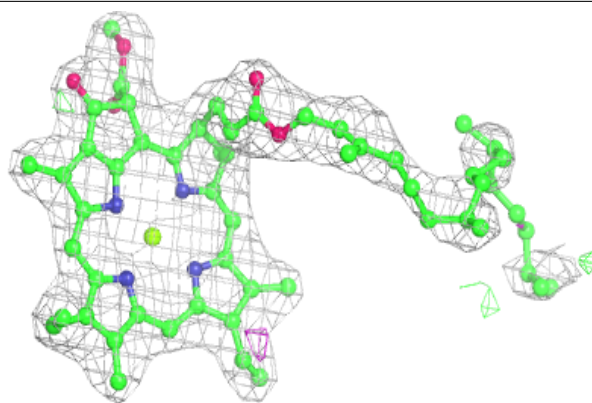
**Electron density around BCR a 408:**

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

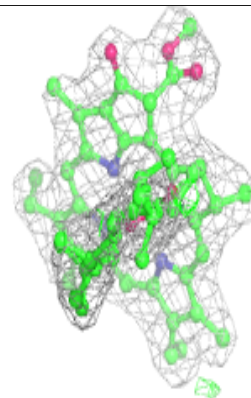
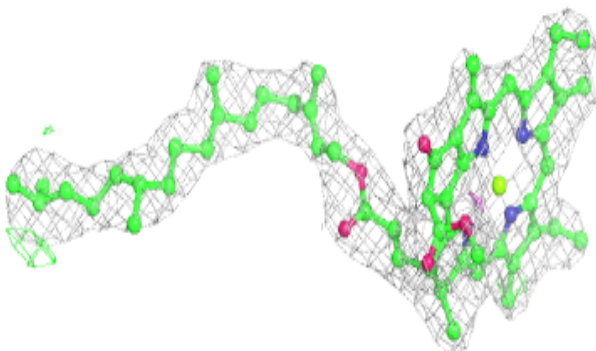
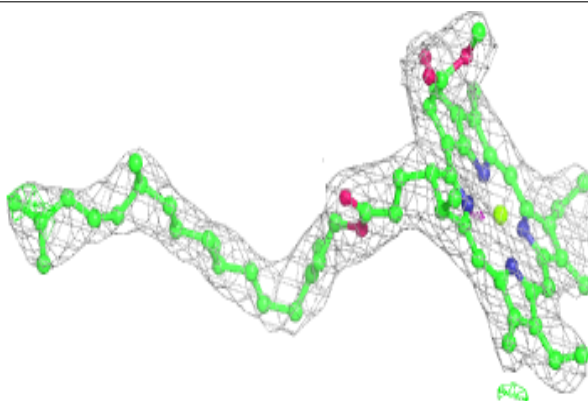


Electron density around CLA A 407:

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

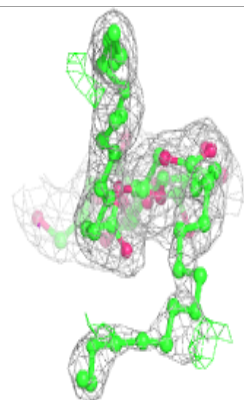
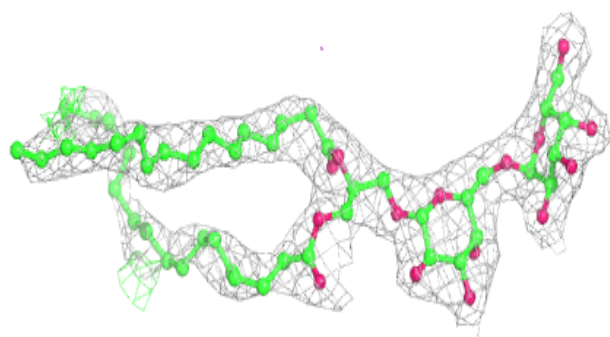
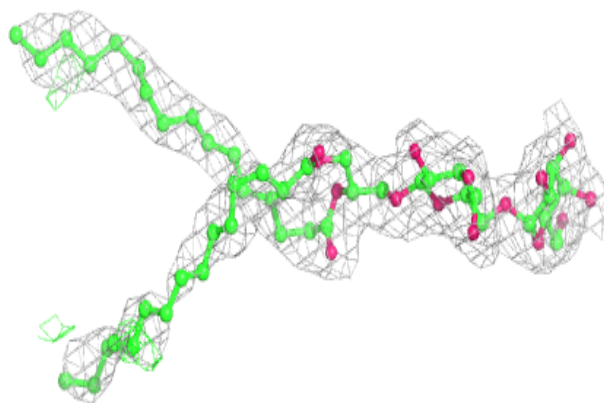
**Electron density around CLA C 504:**

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

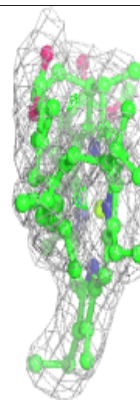
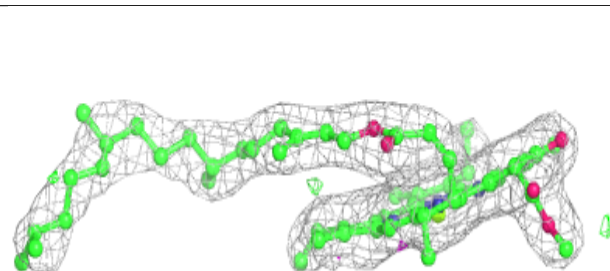
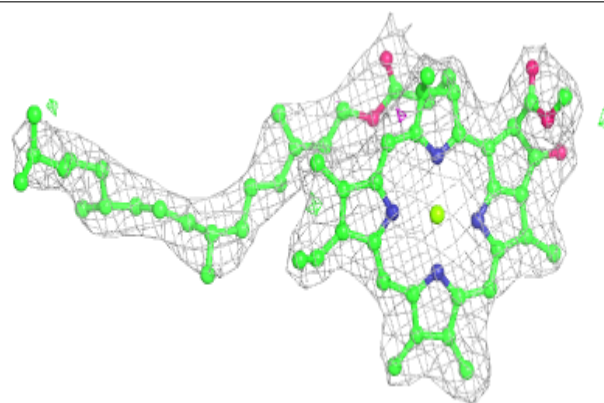


Electron density around DGD c 518:

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

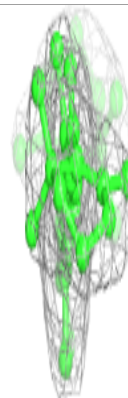
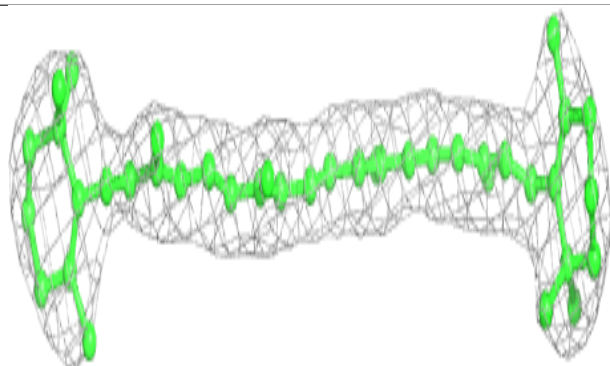
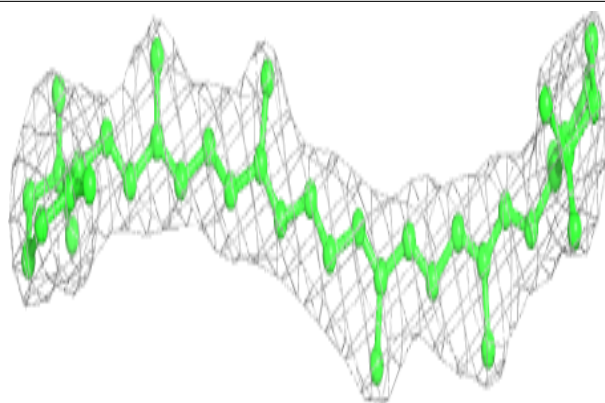
**Electron density around CLA b 603:**

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

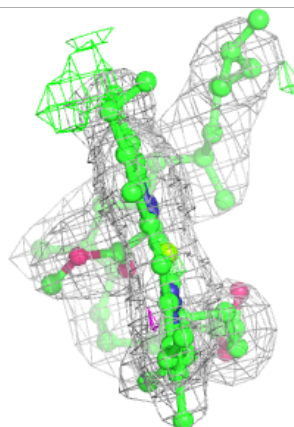
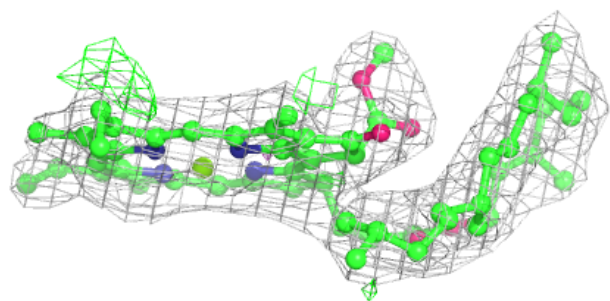
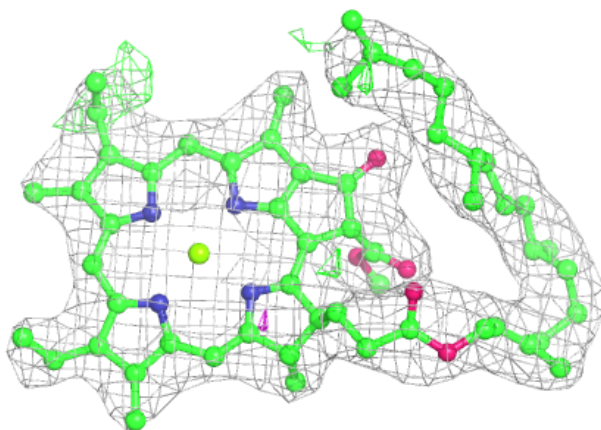


Electron density around BCR c 517:

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

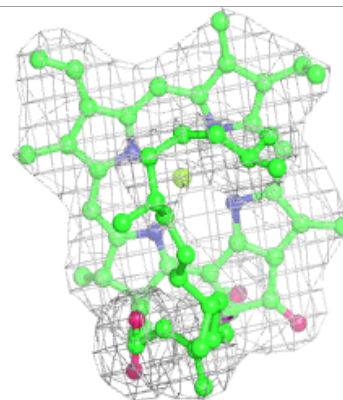
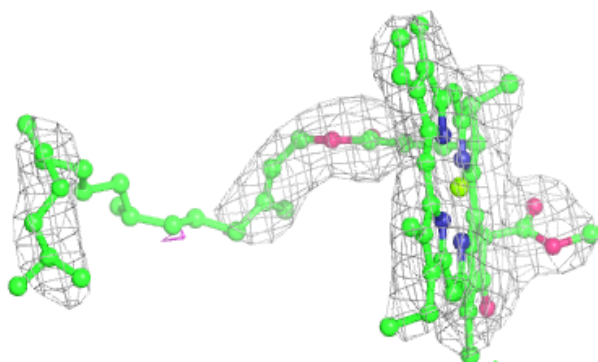
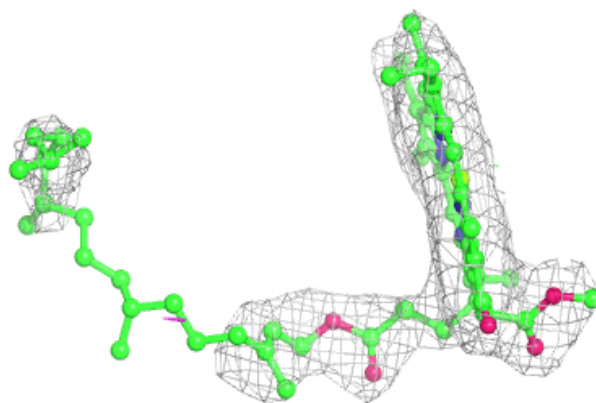
**Electron density around CLA B 610:**

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

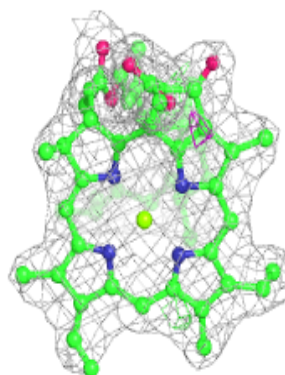
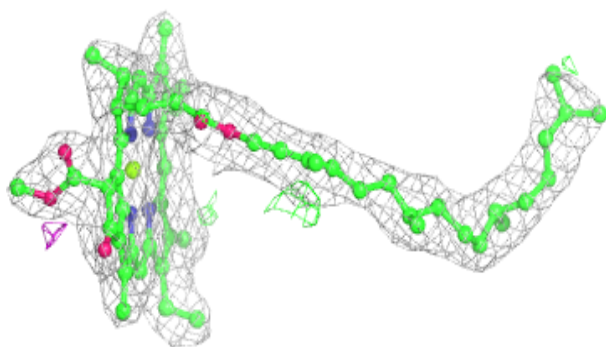
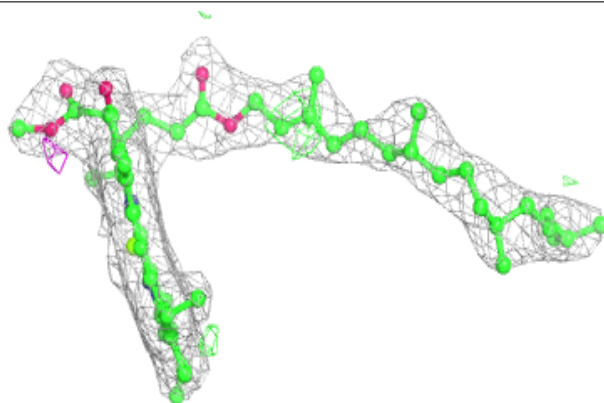


Electron density around CLA c 508:

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

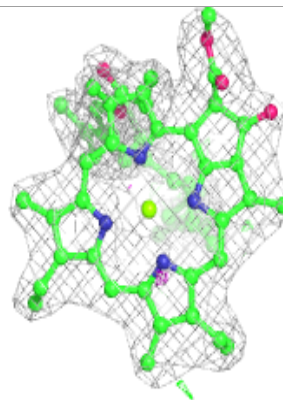
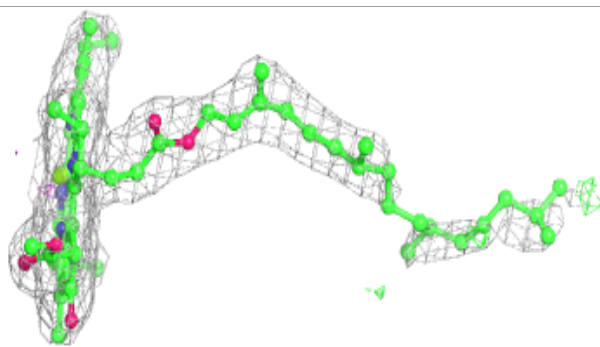
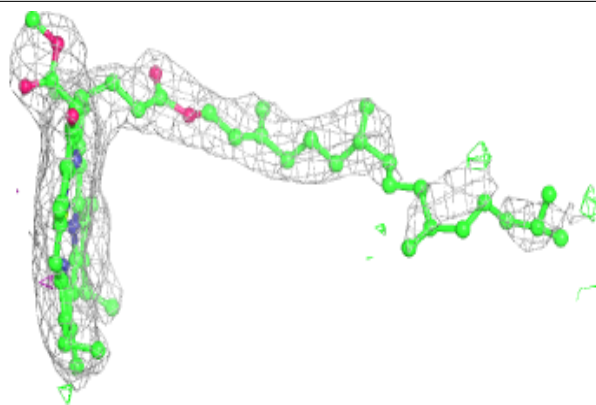
**Electron density around CLA b 605:**

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

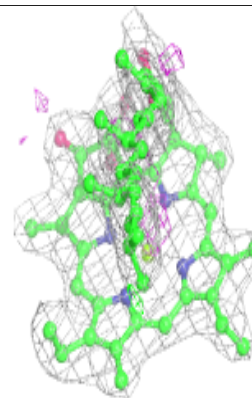
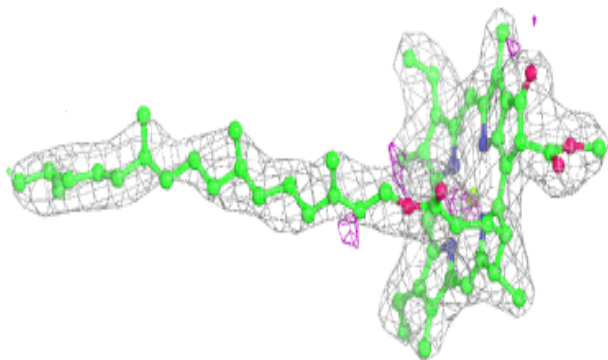
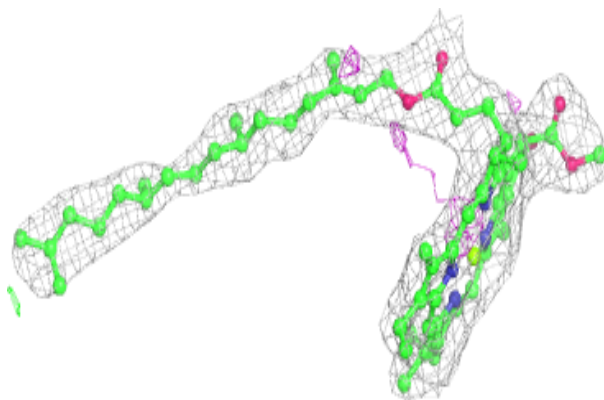


Electron density around CLA b 606:

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

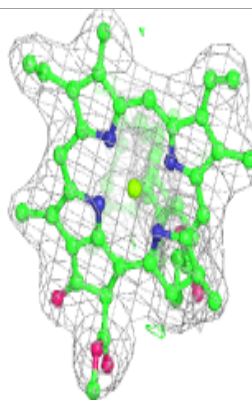
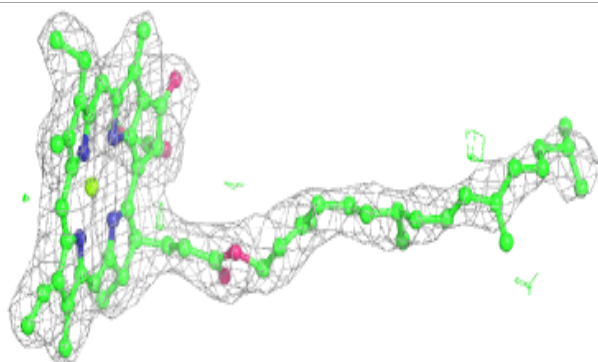
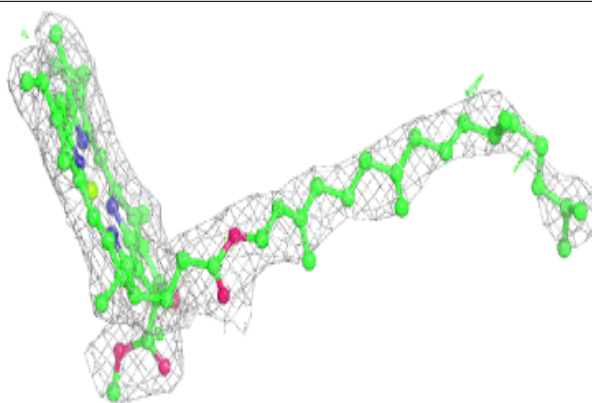
**Electron density around CLA b 607:**

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

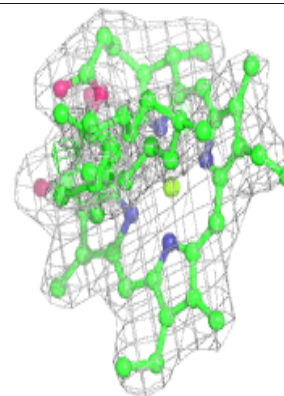
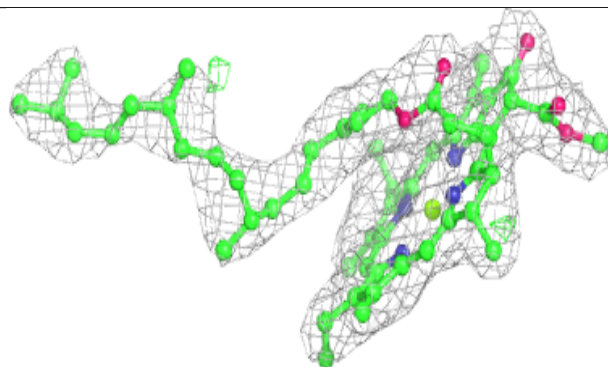
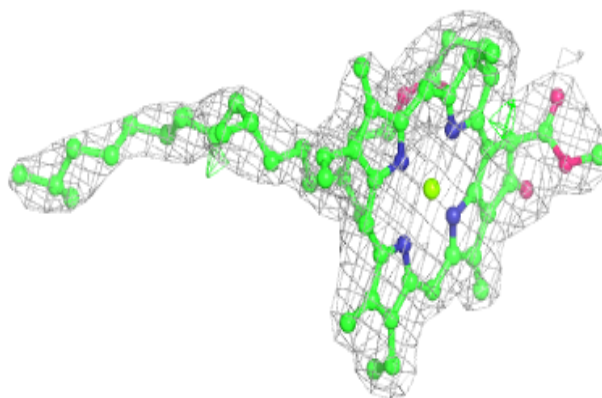


Electron density around CLA B 604:

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

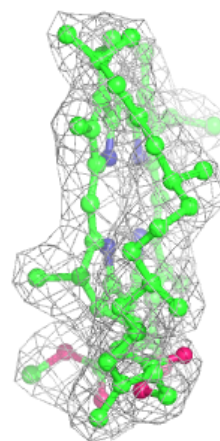
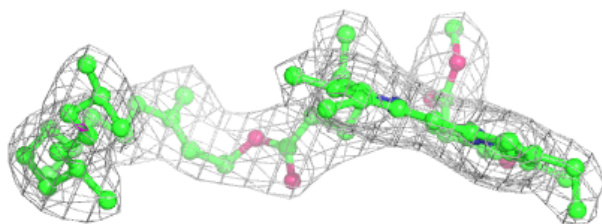
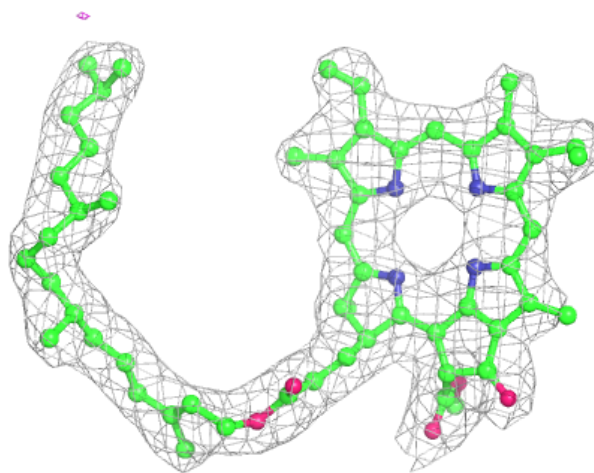
**Electron density around CLA C 507:**

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



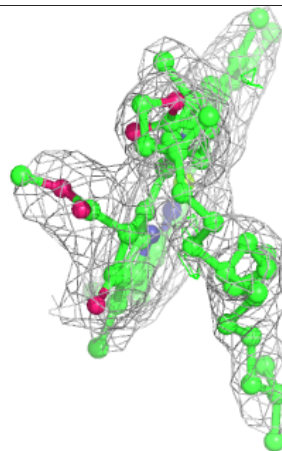
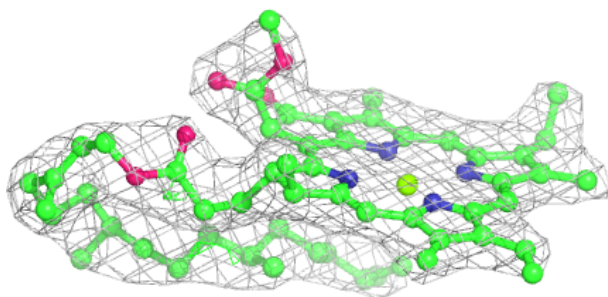
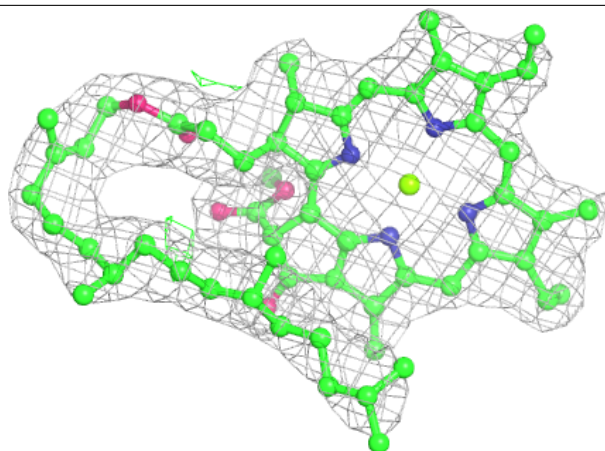
Electron density around PHO A 406:

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



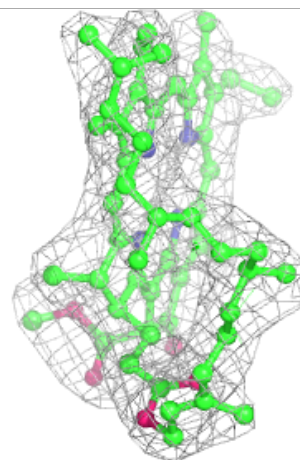
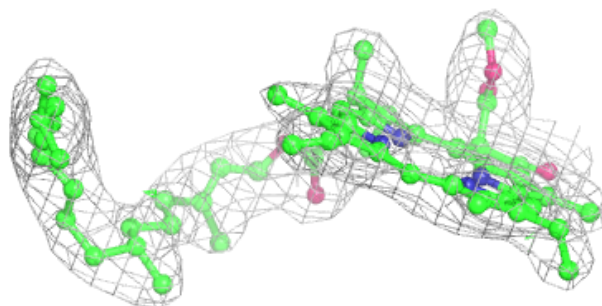
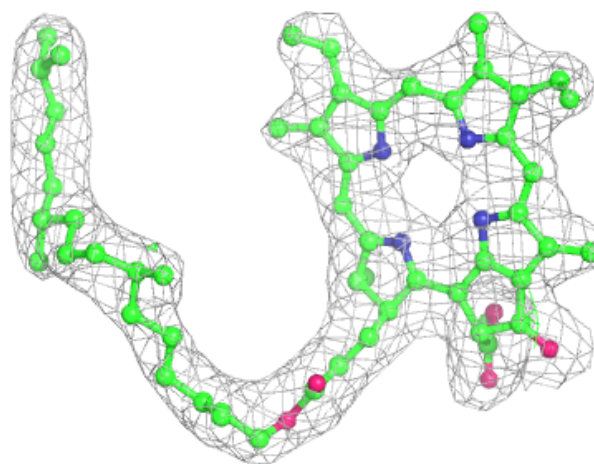
Electron density around CLA C 511:

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



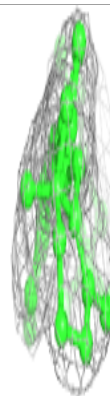
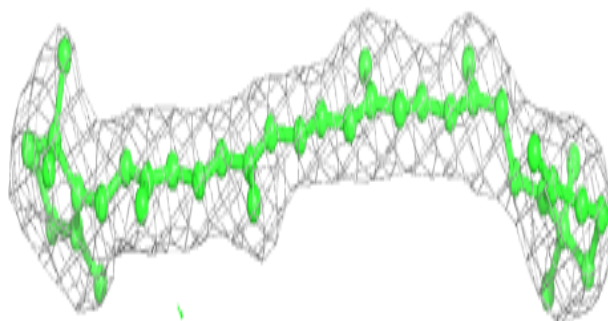
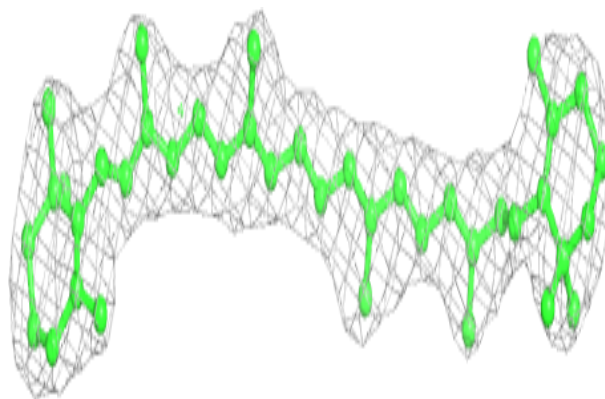
Electron density around PHO a 416:

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



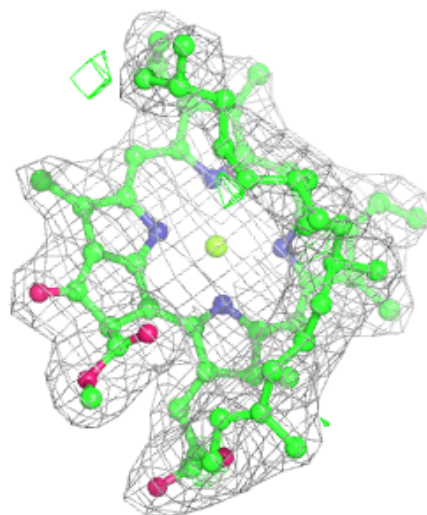
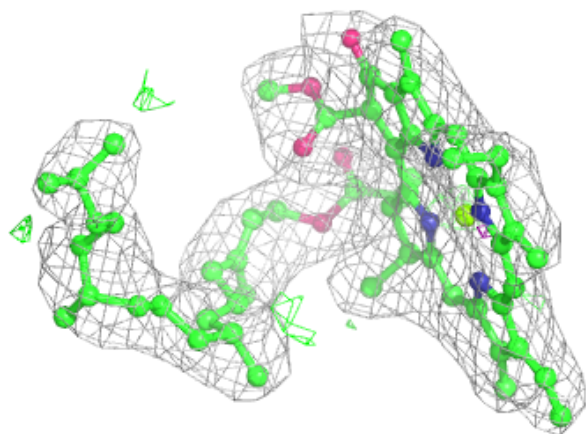
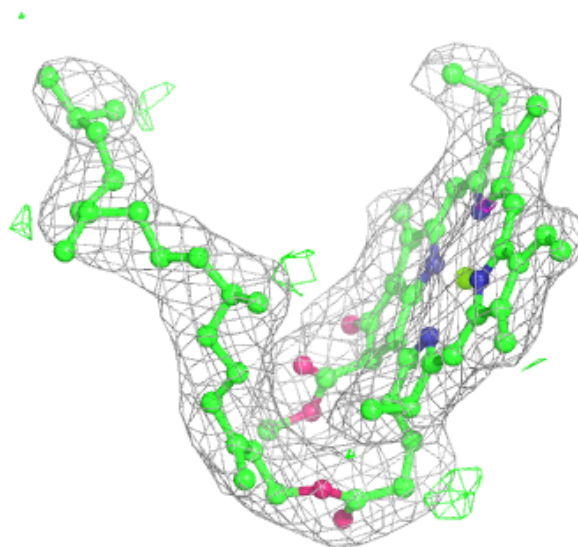
Electron density around BCR b 619:

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



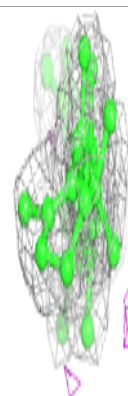
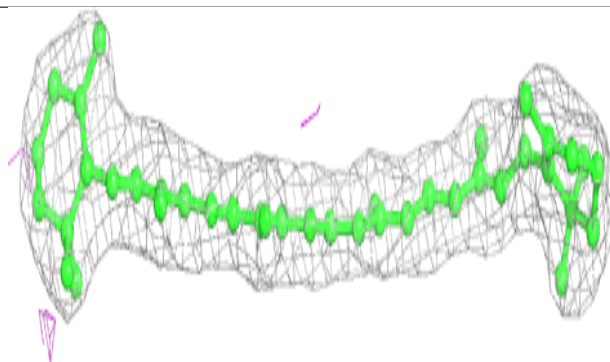
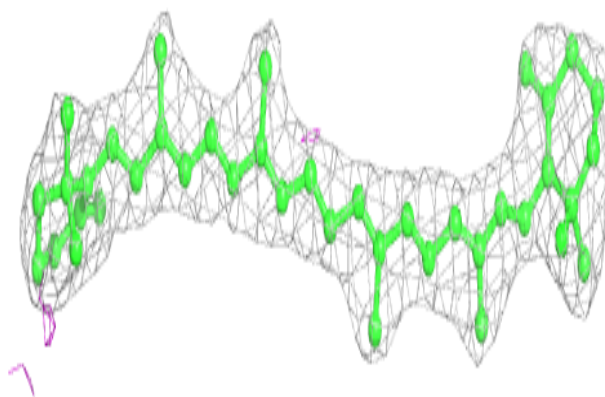
Electron density around CLA B 613:

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

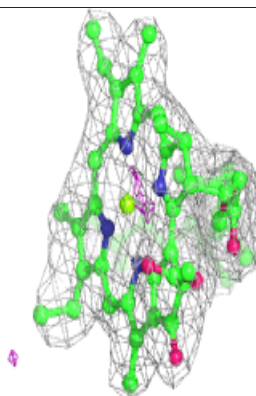
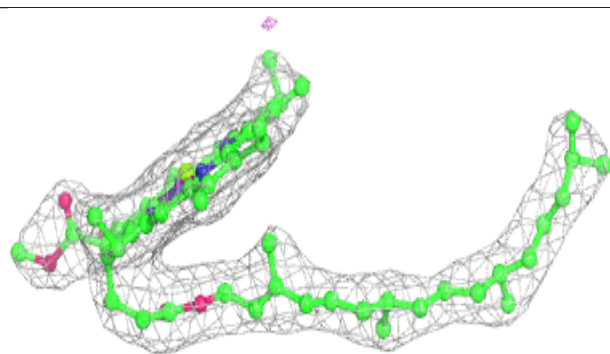
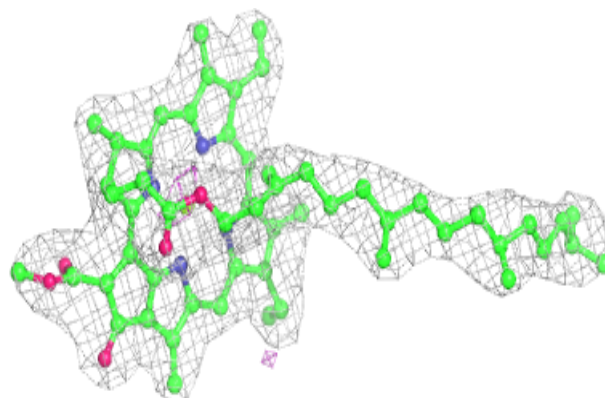


Electron density around BCR B 617:

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

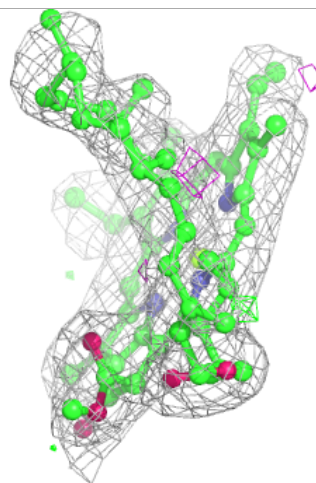
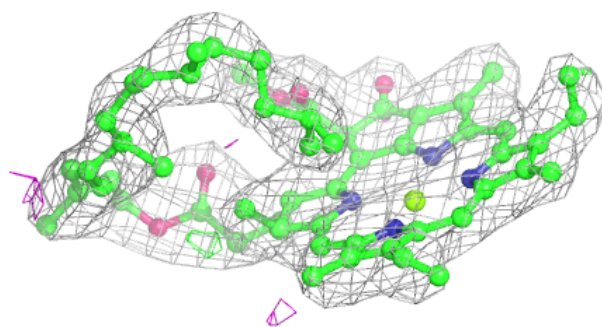
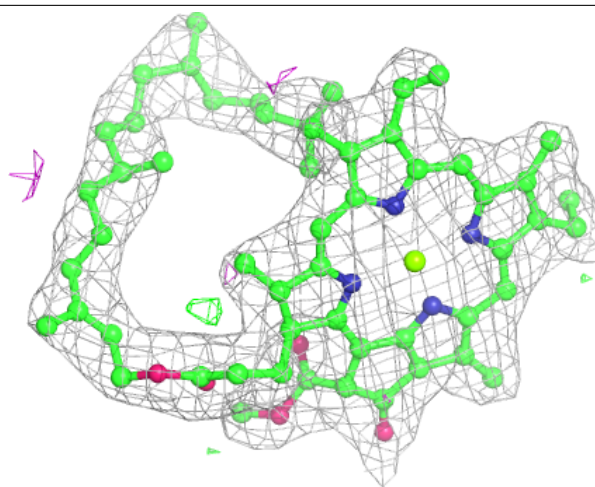
**Electron density around CLA B 608:**

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



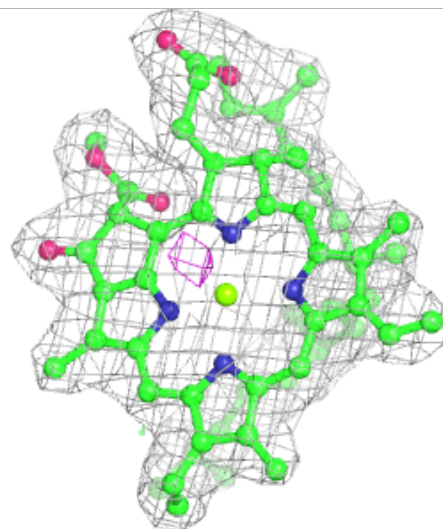
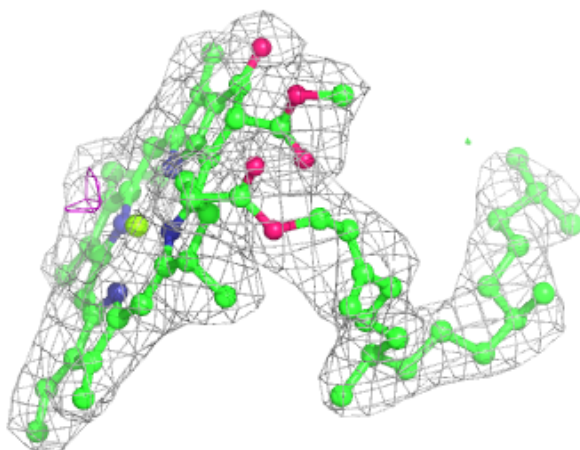
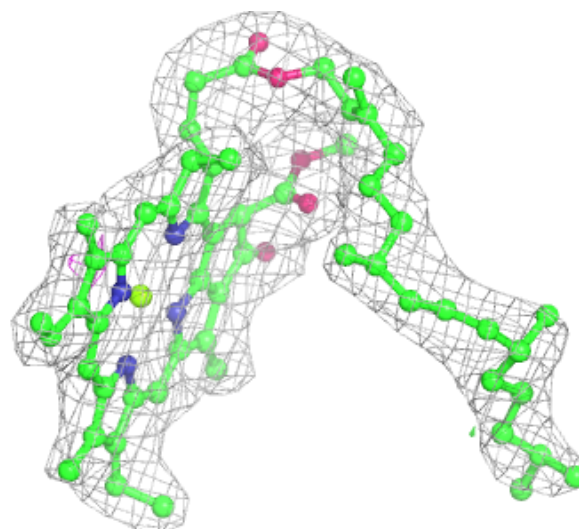
Electron density around CLA B 615:

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



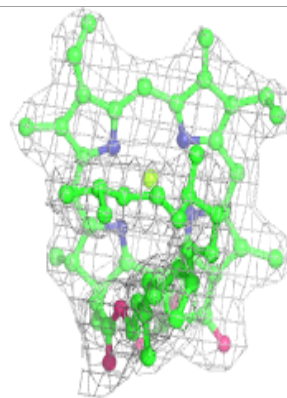
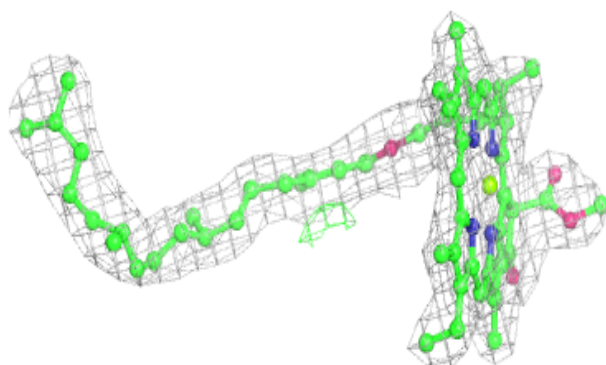
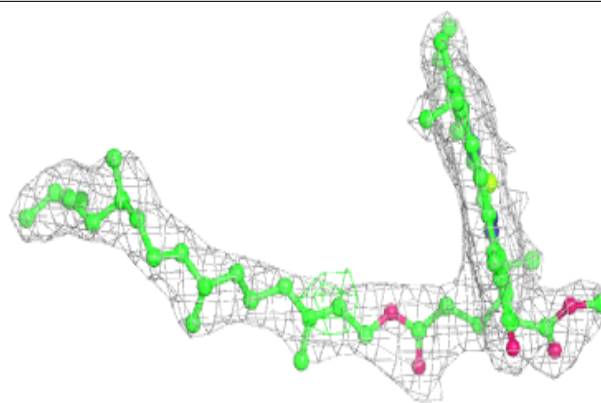
Electron density around CLA b 613:

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

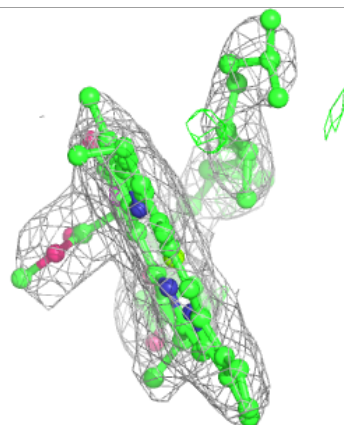
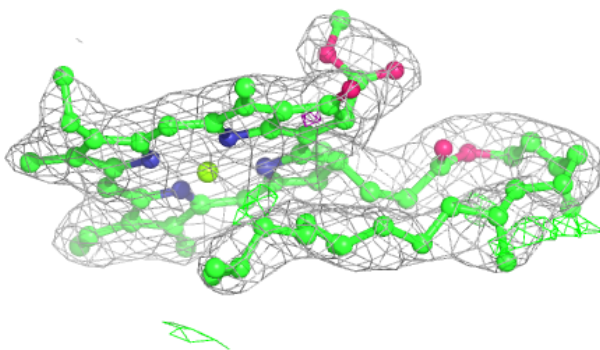
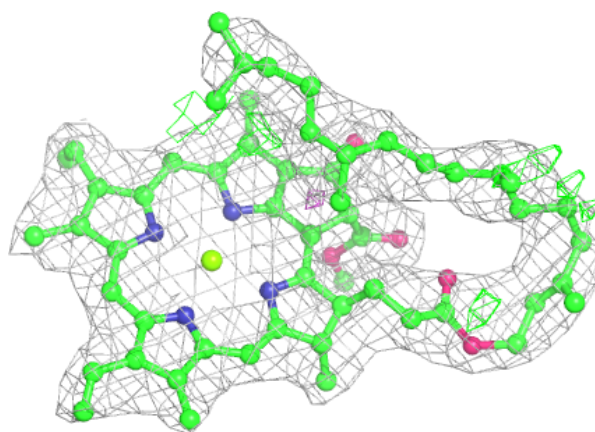


Electron density around CLA B 605:

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

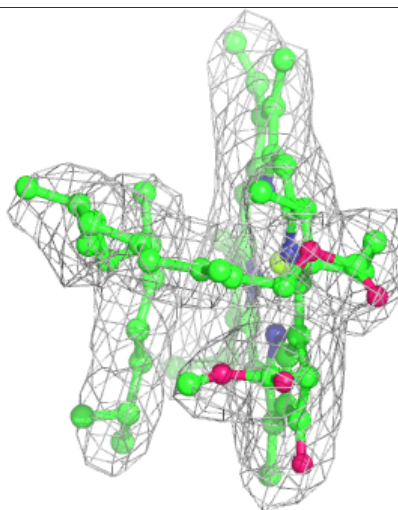
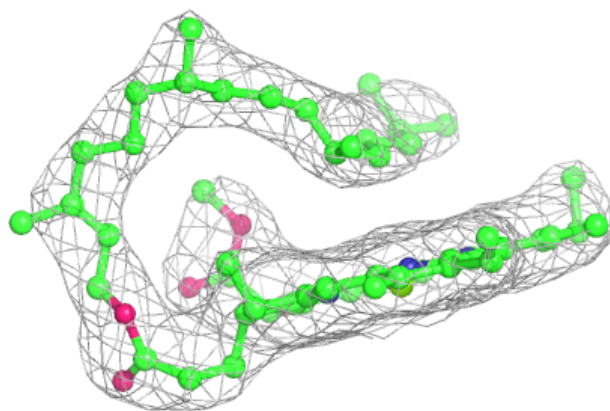
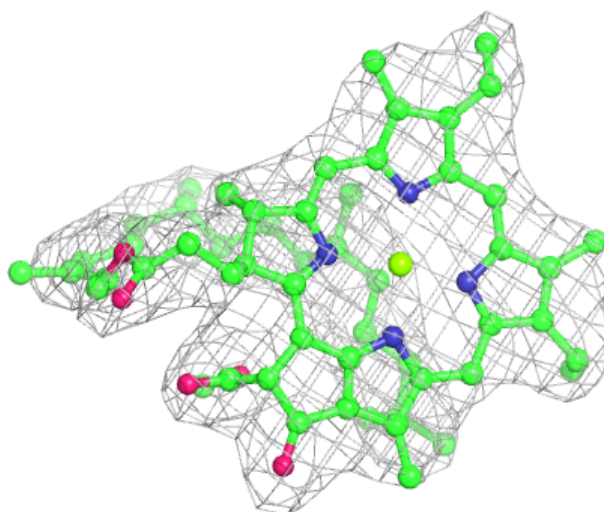
**Electron density around CLA c 511:**

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



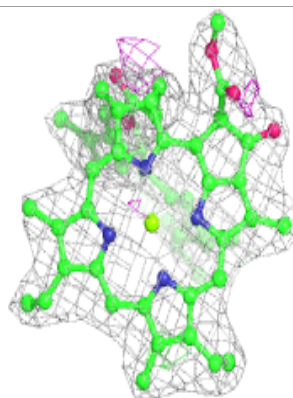
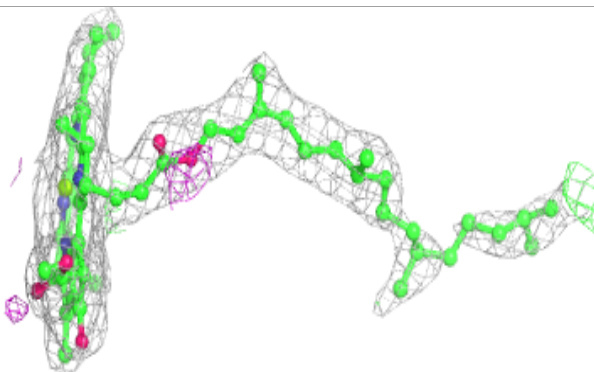
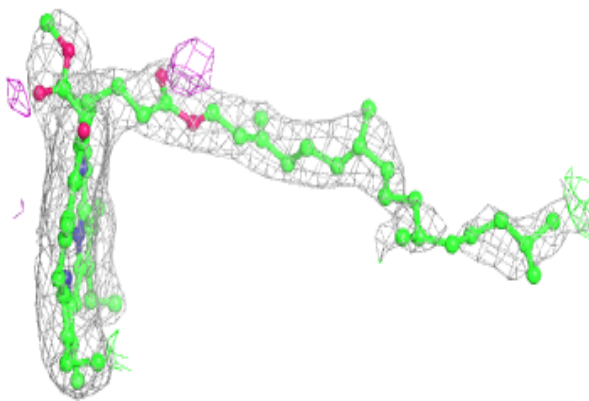
Electron density around CLA c 512:

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

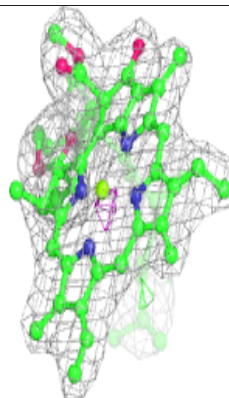
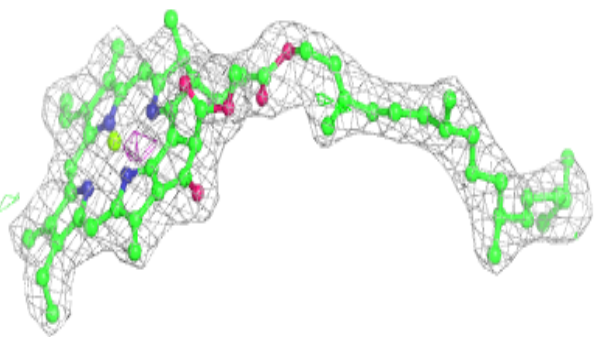
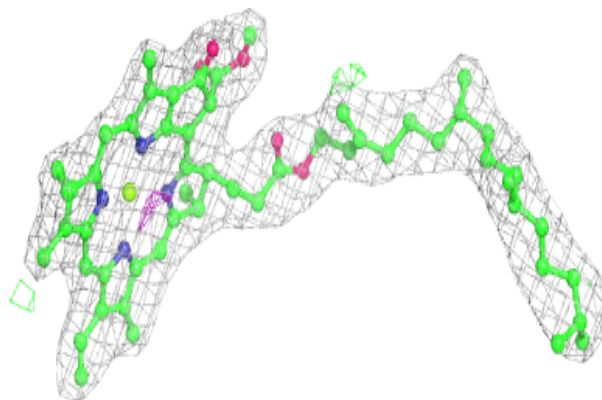


Electron density around CLA B 606:

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

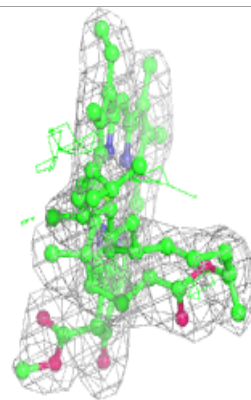
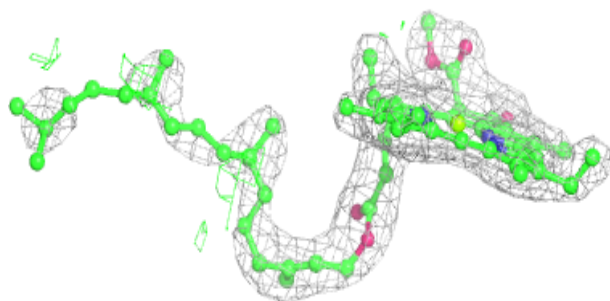
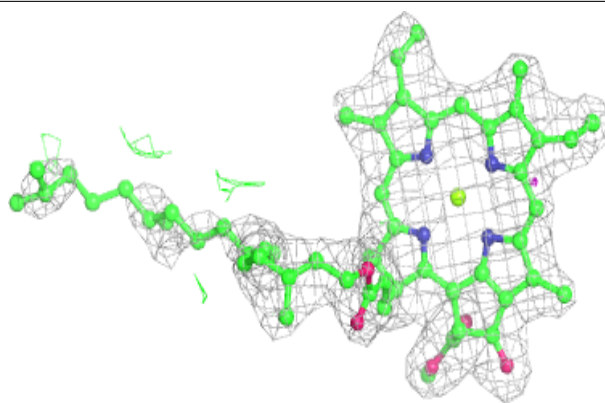
**Electron density around CLA a 403:**

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



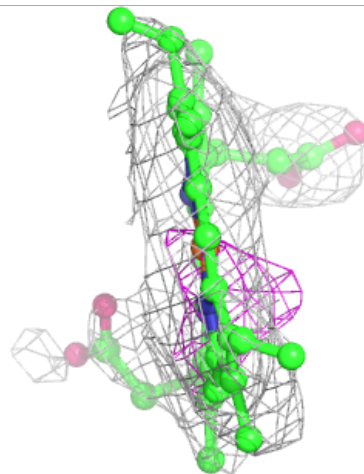
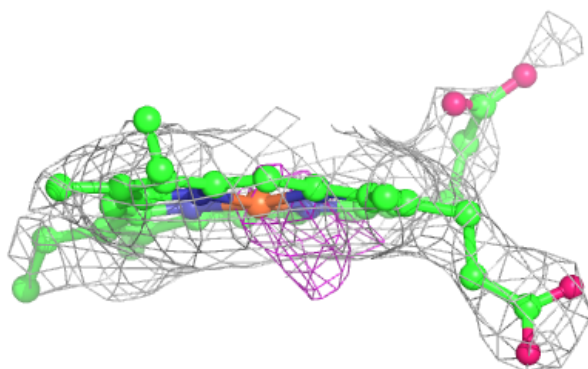
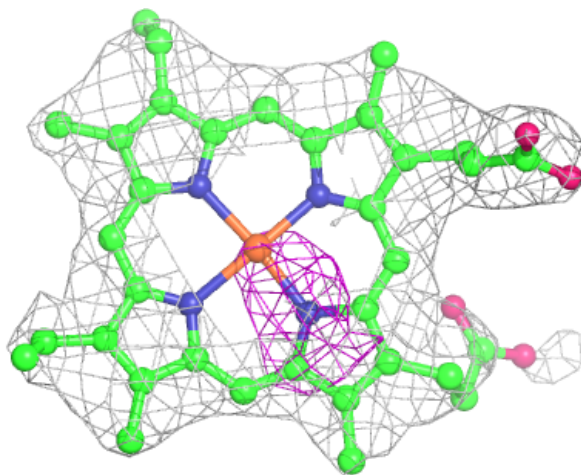
Electron density around CLA A 405:

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



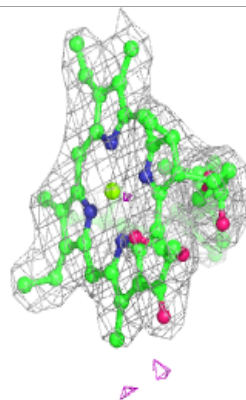
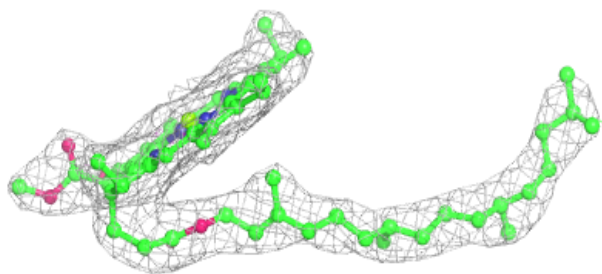
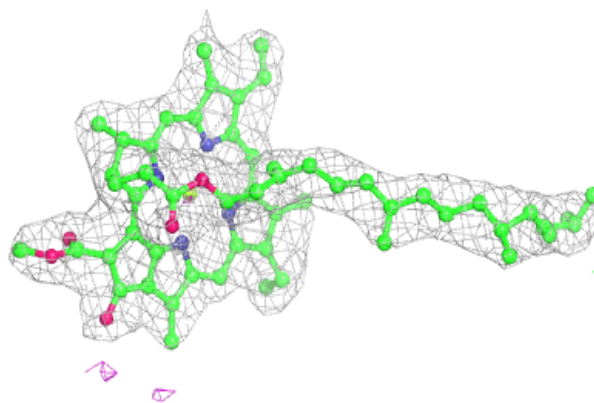
Electron density around HEM e 102:

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



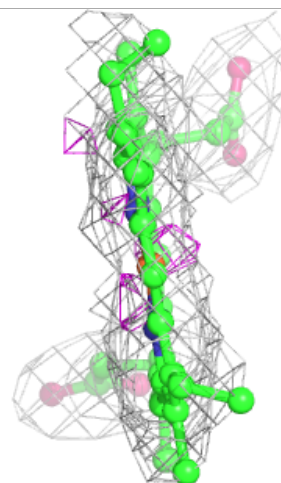
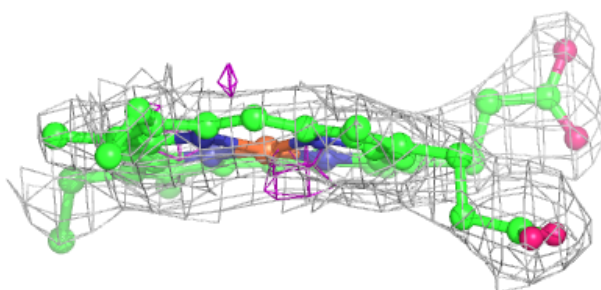
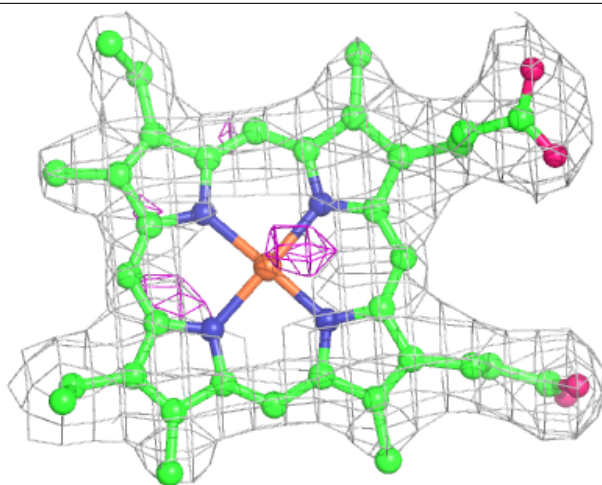
Electron density around CLA b 608:

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



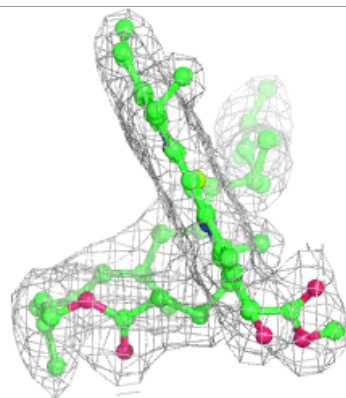
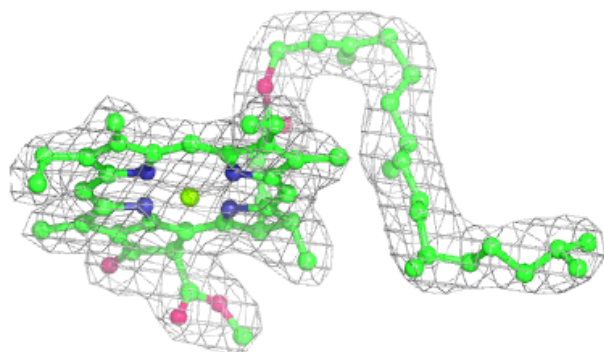
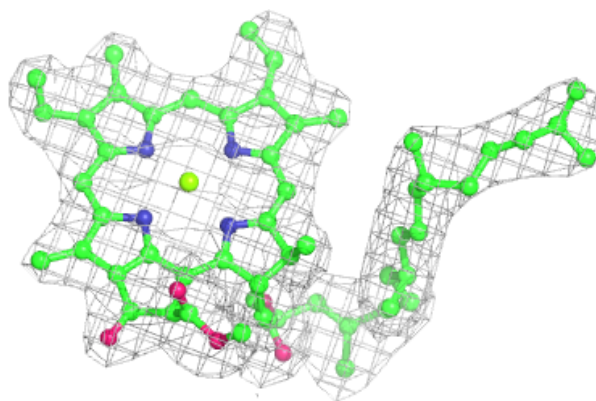
Electron density around HEC v 202:

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

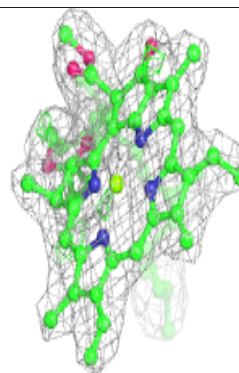
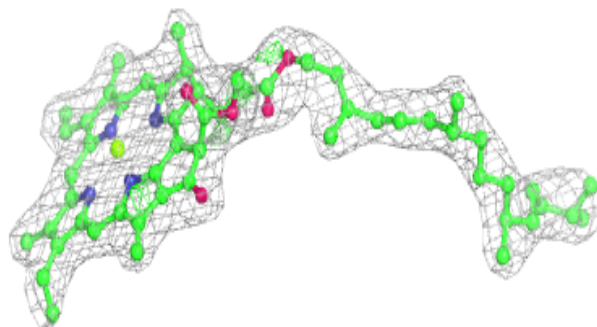
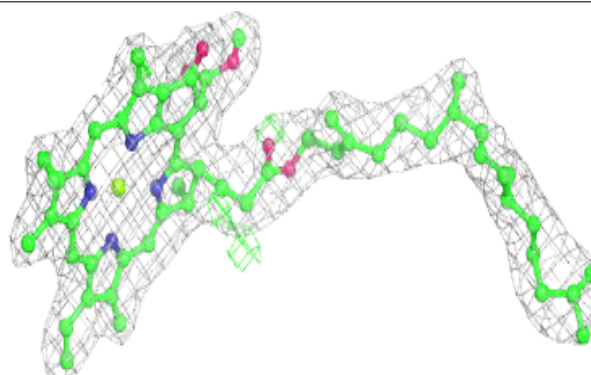


Electron density around CLA a 404:

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

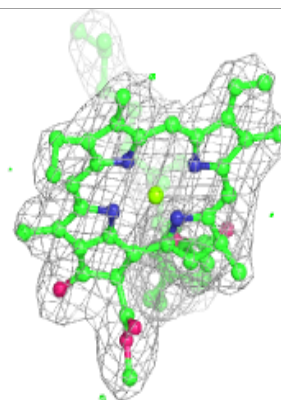
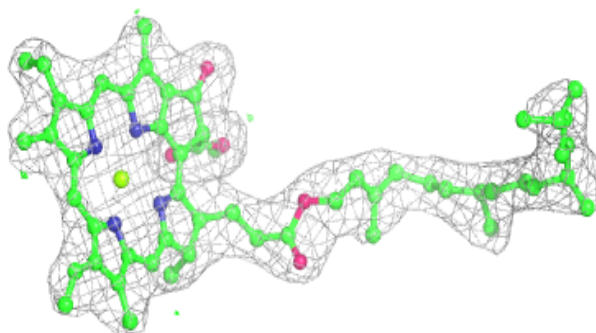
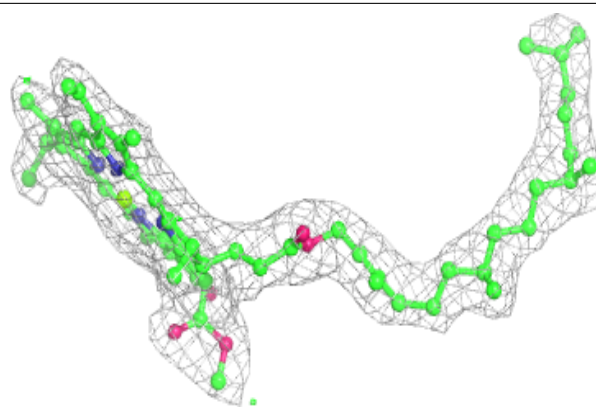
**Electron density around CLA A 403:**

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



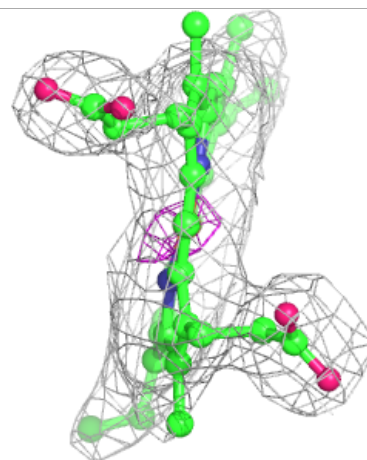
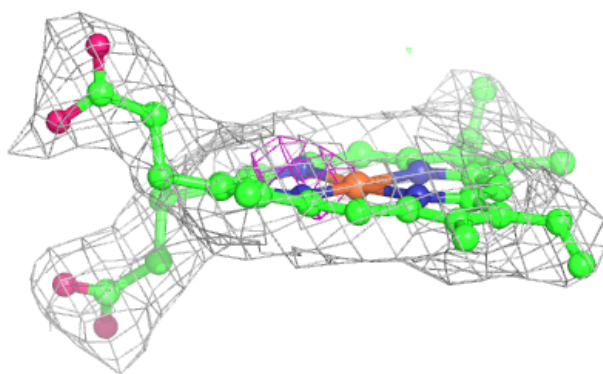
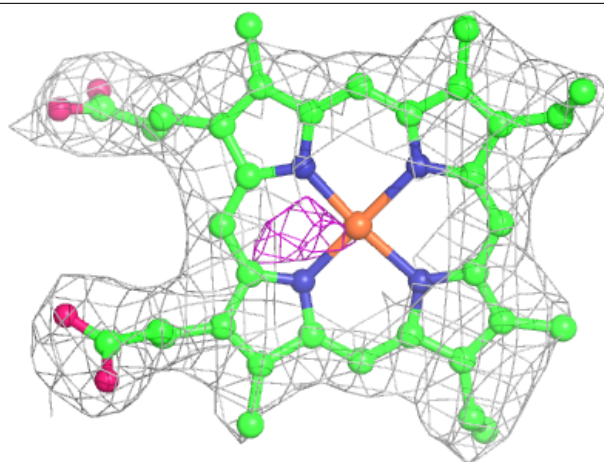
Electron density around CLA d 402:

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



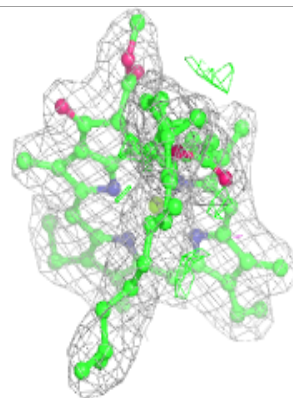
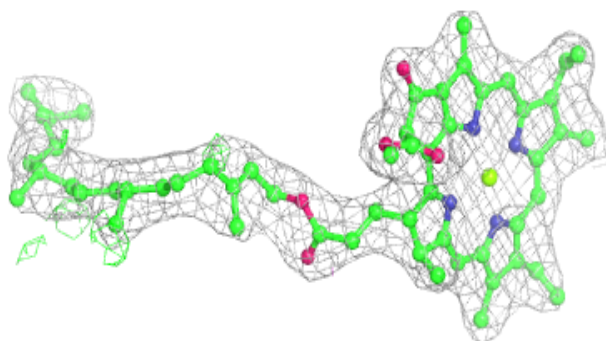
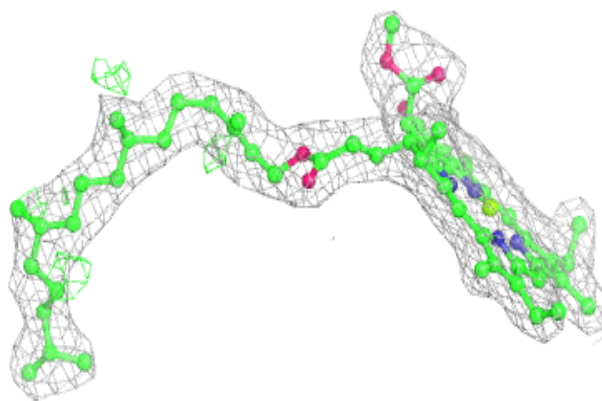
Electron density around HEM E 102:

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

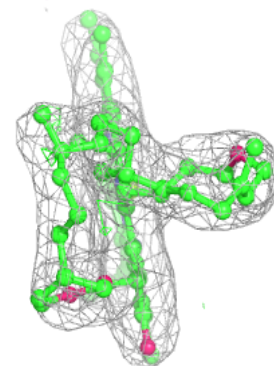
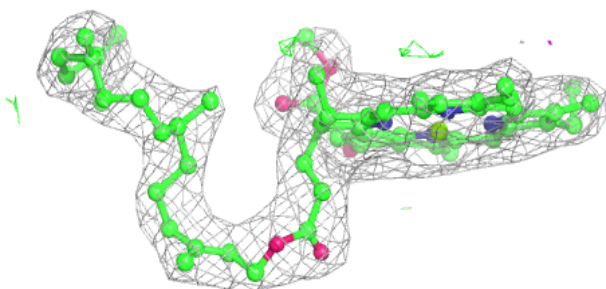
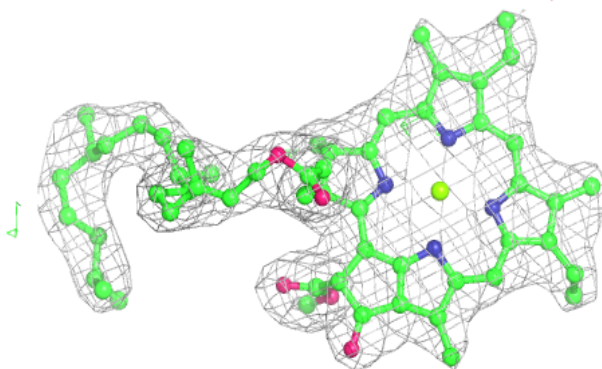


Electron density around CLA D 403:

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

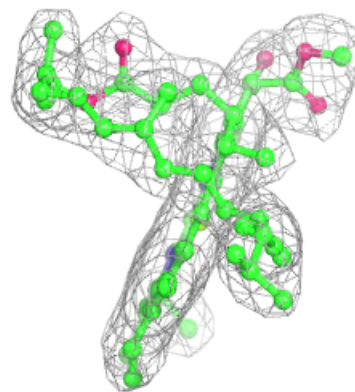
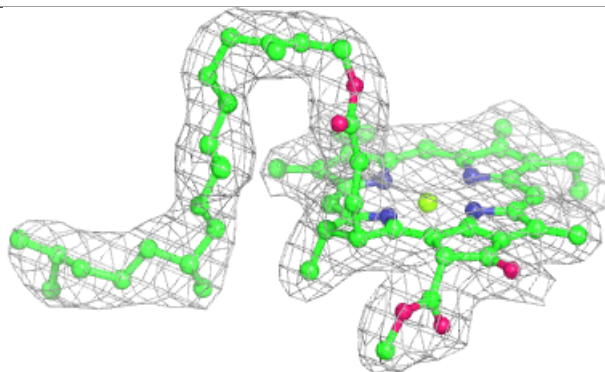
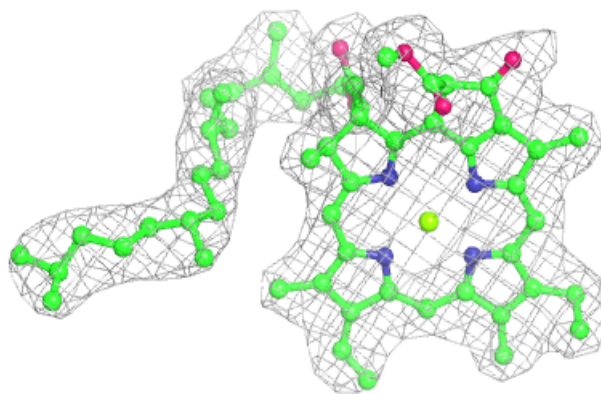
**Electron density around CLA B 612:**

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



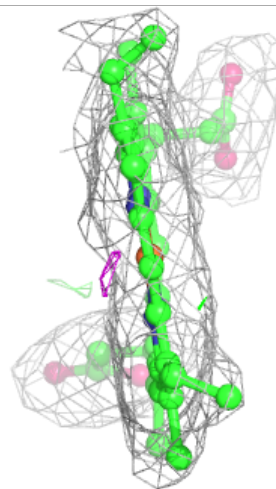
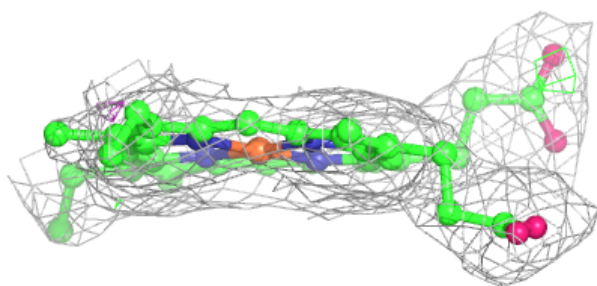
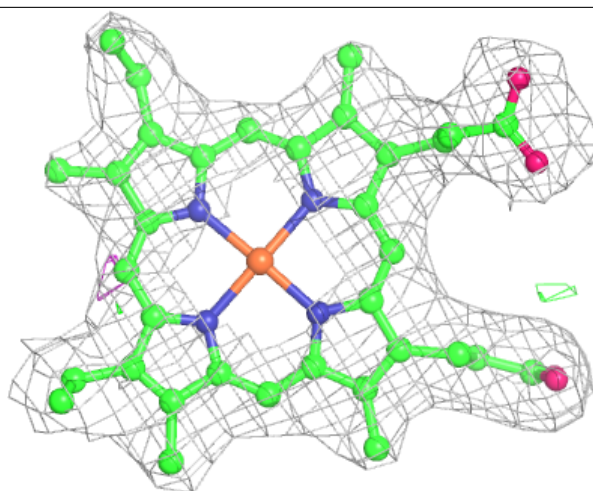
Electron density around CLA A 404:

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



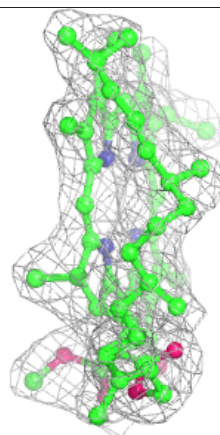
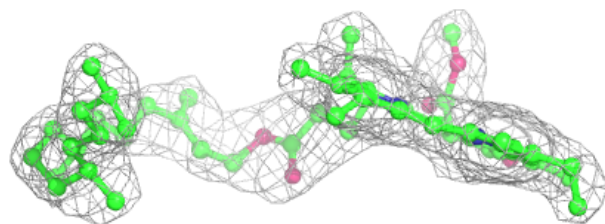
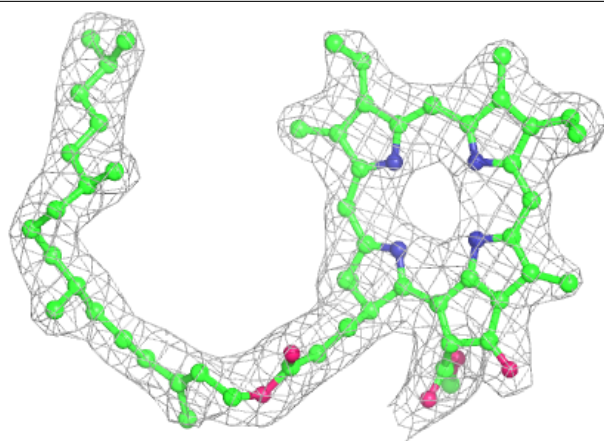
Electron density around HEC V 201:

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



Electron density around PHO a 406:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.