



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2020 – 10:52 AM BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

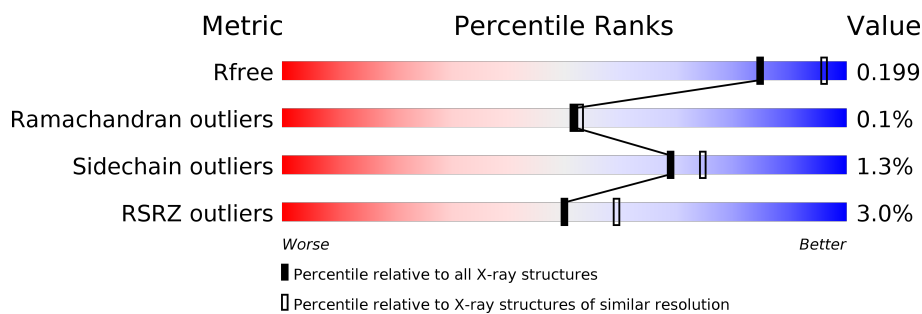
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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

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

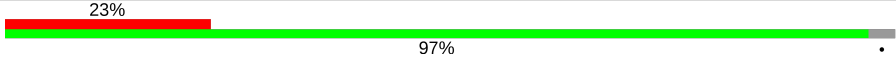
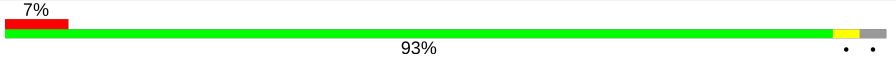
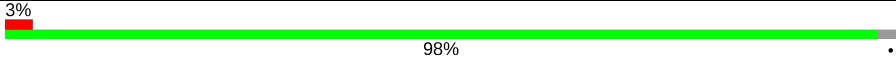
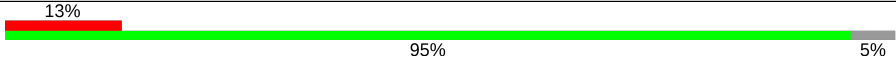
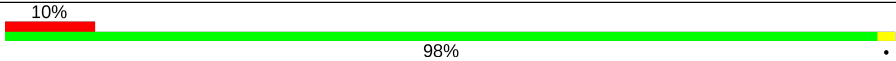
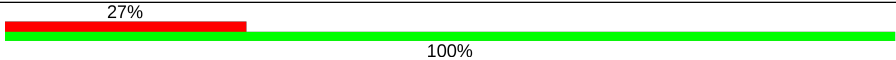

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Mol	Chain	Length	Quality of chain
4	d	342	99%
5	E	84	10%
5	e	84	11%
6	F	44	5%
6	f	44	5%
7	H	65	5%
7	h	65	3%
8	I	38	5%
8	i	38	5%
9	J	39	8%
9	j	39	13%
10	K	37	
10	k	37	
11	L	37	
11	l	37	5%
12	M	36	6%
12	m	36	
13	O	244	2%
13	o	244	2%
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	407	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	410	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	c	517	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-

2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	6	0
			3544	2323	589	619	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	12			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

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

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

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

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

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

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

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

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

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

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

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

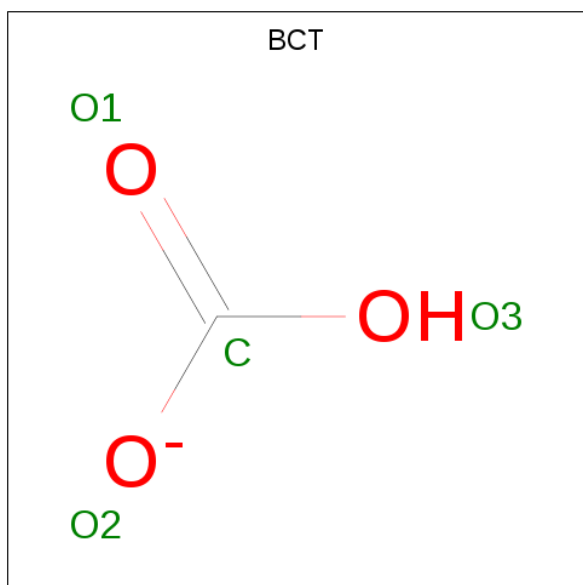
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

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

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



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

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



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

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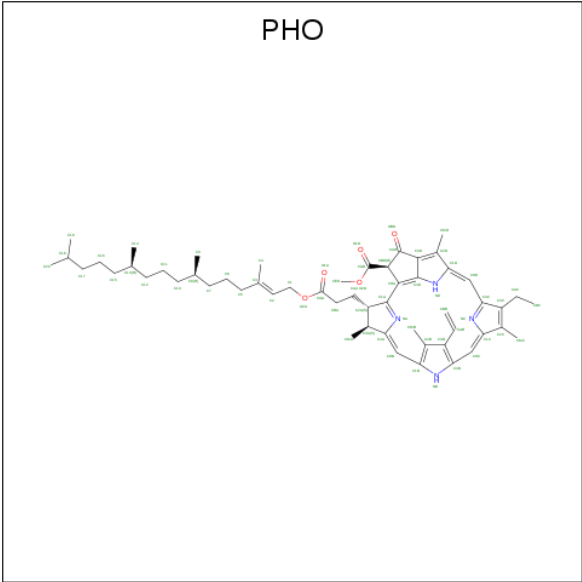
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24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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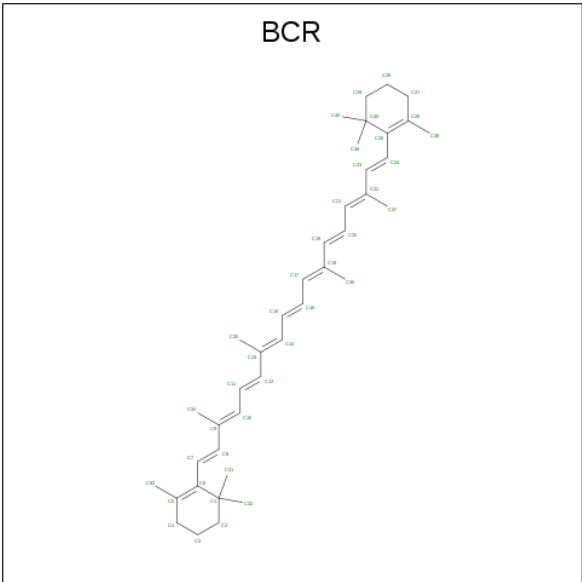
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



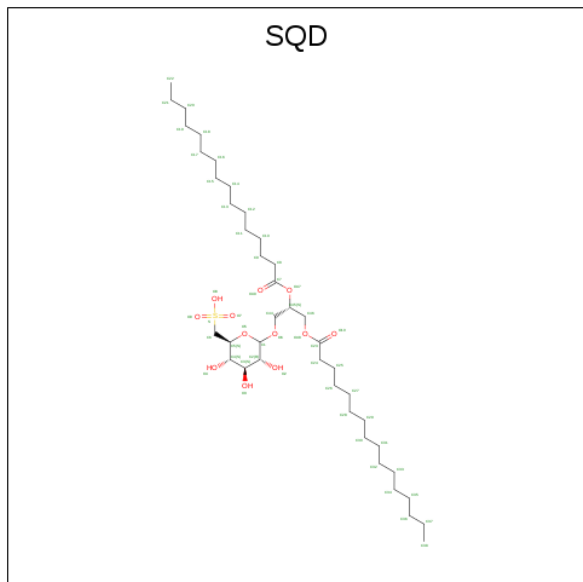
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



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

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



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

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



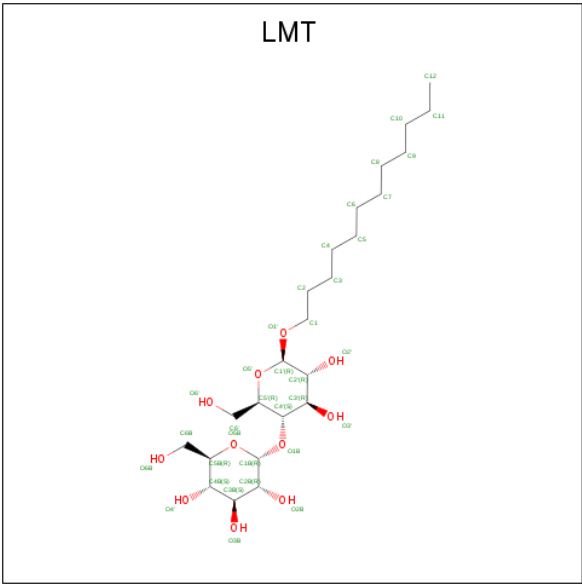
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

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

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



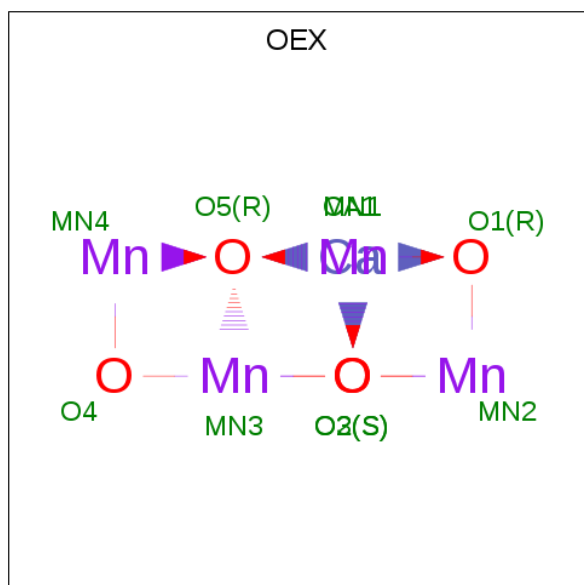
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C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

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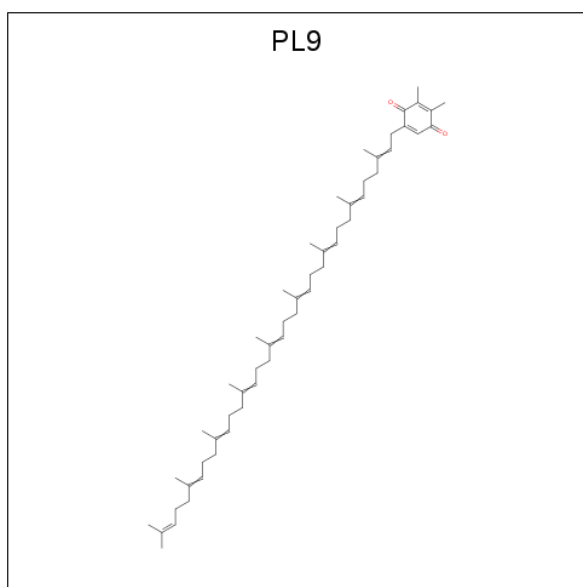
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	f	1	Total	C	O	0	0
			35	24	11		
29	m	1	Total	C	O	0	0
			35	24	11		

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



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

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



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

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

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

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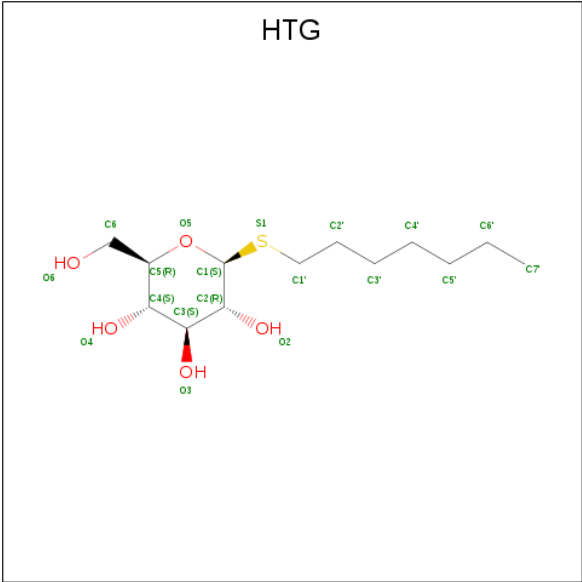
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	j	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0
32	d	3	Total C O 71 63 8	0	0
32	m	1	Total C 10 10	0	0
32	b	1	Total C O 33 28 5	0	0
32	M	1	Total C 10 10	0	0

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



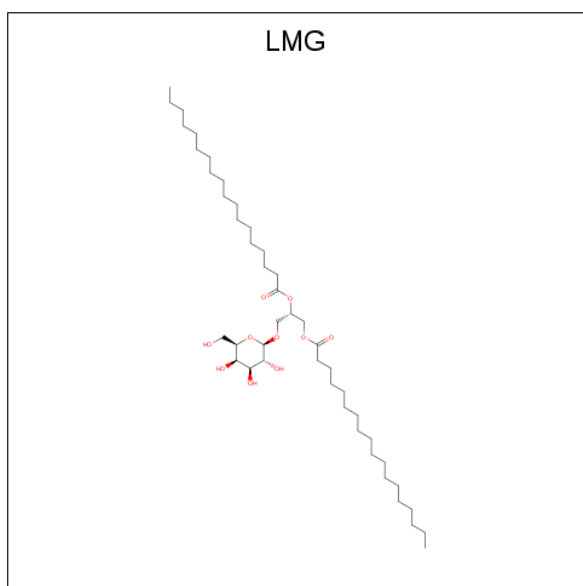
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19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

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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



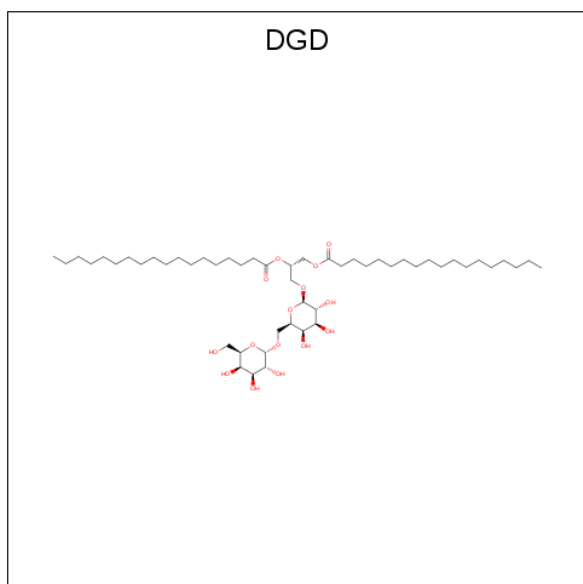
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			51	41	10			
35	C	1	Total	C	O		0	0
			51	41	10			
35	C	1	Total	C	O		0	0
			51	41	10			
35	J	1	Total	C	O		0	0
			51	41	10			
35	M	1	Total	C	O		0	0
			51	41	10			
35	Z	1	Total	C	O		0	0
			37	27	10			
35	a	1	Total	C	O		0	0
			51	41	10	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

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

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



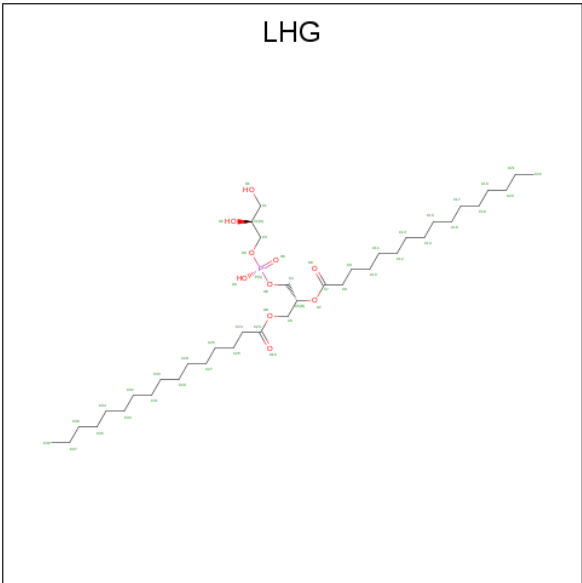
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			52	42	10		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



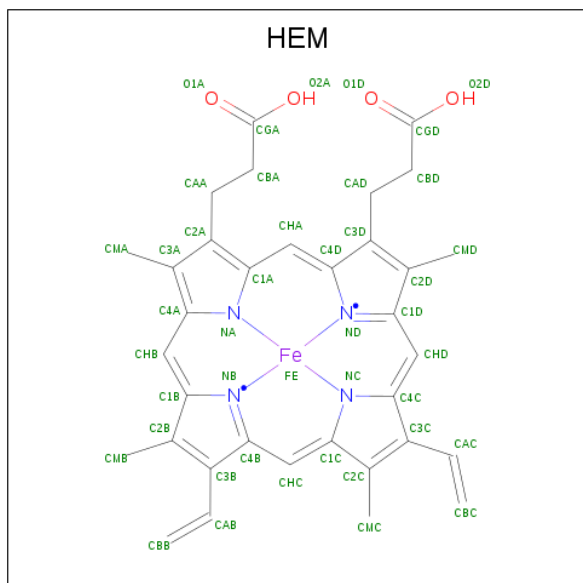
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	D	1	Total	C	O	P	0	0
			49	38	10	1		
37	E	1	Total	C	O	P	0	0
			42	31	10	1		
37	L	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0
			49	38	10	1		
37	d	1	Total	C	O	P	0	0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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	e	1	Total	C	O	P	0	0
			42	31	10	1		
37	l	1	Total	C	O	P	0	0
			49	38	10	1		

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



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

- 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	A	163	Total O 166 166	0	3
40	B	291	Total O 295 295	0	4
40	C	230	Total O 232 232	0	2
40	D	139	Total O 143 143	0	4
40	E	34	Total O 34 34	0	0
40	F	8	Total O 8 8	0	0
40	H	43	Total O 44 44	0	1
40	I	4	Total O 4 4	0	0
40	J	11	Total O 11 11	0	0
40	K	7	Total O 7 7	0	0
40	L	16	Total O 17 17	0	1
40	M	24	Total O 24 24	0	0
40	O	177	Total O 179 179	0	2
40	T	16	Total O 17 17	0	1
40	U	85	Total O 85 85	0	0
40	V	115	Total O 117 117	0	2
40	Y	4	Total O 4 4	0	0
40	X	8	Total O 8 8	0	0
40	Z	1	Total O 1 1	0	0
40	a	158	Total O 159 159	0	1
40	b	258	Total O 261 261	0	3
40	c	201	Total O 204 204	0	3

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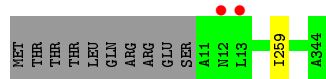
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	d	128	Total 131	O 131	0	3
40	e	20	Total 20	O 20	0	0
40	f	8	Total 8	O 8	0	0
40	h	42	Total 42	O 42	0	0
40	i	6	Total 6	O 6	0	0
40	j	6	Total 6	O 6	0	0
40	k	7	Total 7	O 7	0	0
40	l	8	Total 8	O 8	0	0
40	m	14	Total 14	O 14	0	0
40	o	163	Total 163	O 163	0	0
40	t	9	Total 9	O 9	0	0
40	u	91	Total 91	O 91	0	0
40	v	82	Total 83	O 83	0	1
40	y	2	Total 2	O 2	0	0
40	x	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

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

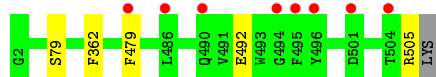
- Molecule 1: Photosystem II protein D1



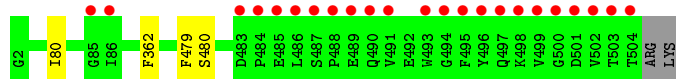
- Molecule 1: Photosystem II protein D1



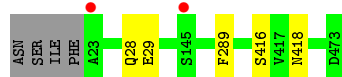
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



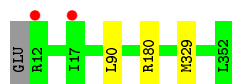
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



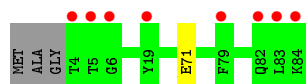
- Molecule 4: Photosystem II D2 protein



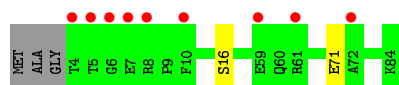
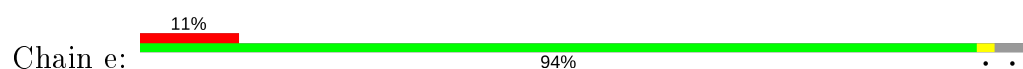
- Molecule 4: Photosystem II D2 protein



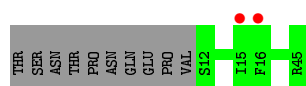
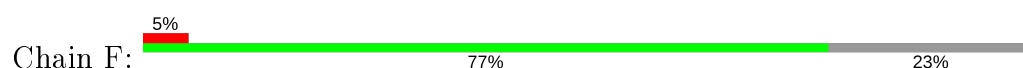
- Molecule 5: Cytochrome b559 subunit alpha



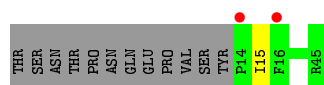
- Molecule 5: Cytochrome b559 subunit alpha



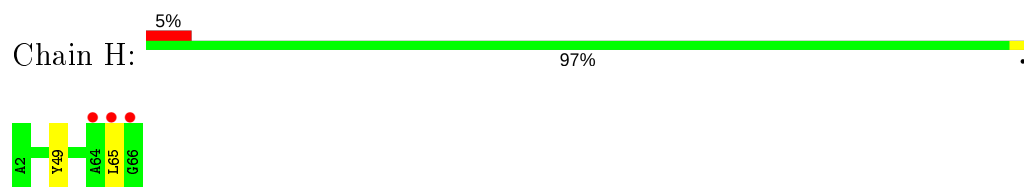
- Molecule 6: Cytochrome b559 subunit beta



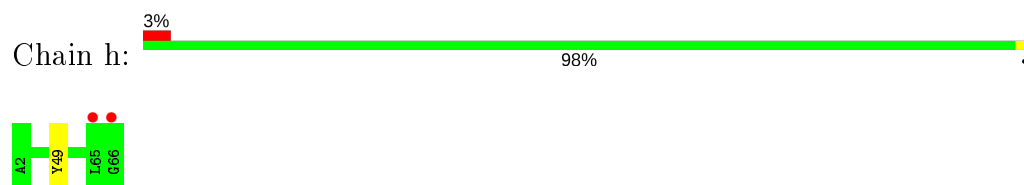
- Molecule 6: Cytochrome b559 subunit beta



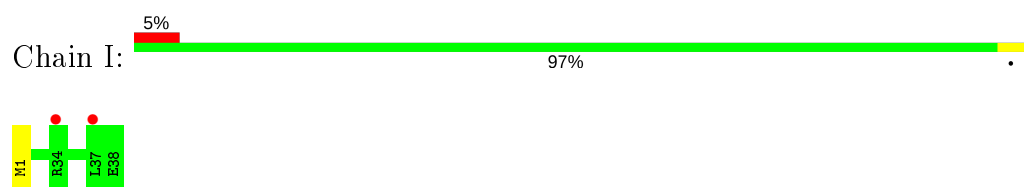
- Molecule 7: Photosystem II reaction center protein H



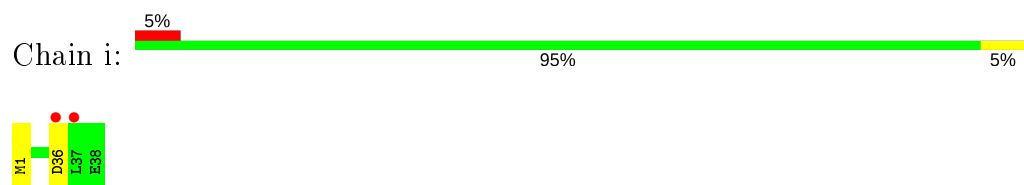
- Molecule 7: Photosystem II reaction center protein H



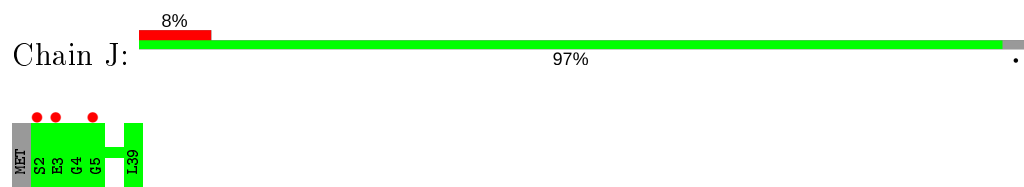
- Molecule 8: Photosystem II reaction center protein I



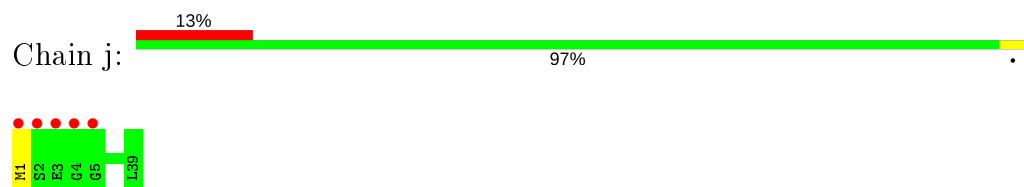
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

Chain k: 97%



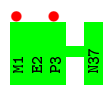
- Molecule 11: Photosystem II reaction center protein L

Chain L: 97%



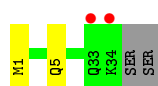
- Molecule 11: Photosystem II reaction center protein L

Chain l: 100%



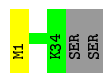
- Molecule 12: Photosystem II reaction center protein M

Chain M: 89%



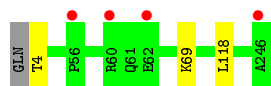
- Molecule 12: Photosystem II reaction center protein M

Chain m: 92%



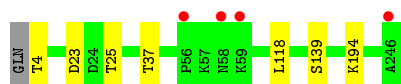
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 98%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 97%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 88% 6% 6%



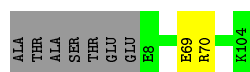
- Molecule 14: Photosystem II reaction center protein T

Chain t: 88% 6% 6%



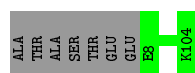
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 91% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 93% 7%



- Molecule 16: Cytochrome c-550

Chain V: 100%

There are no outlier residues recorded for this chain.

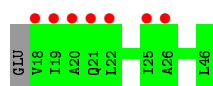
- Molecule 16: Cytochrome c-550

Chain v: 99%

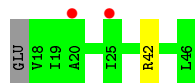


- Molecule 17: Photosystem II reaction center protein Ycf12

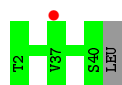
Chain Y: 23% 97%



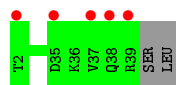
- Molecule 17: Photosystem II reaction center protein Ycf12



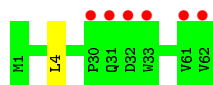
- Molecule 18: Photosystem II reaction center protein X



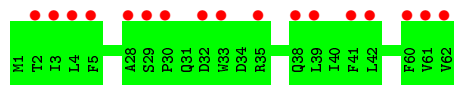
- Molecule 18: Photosystem II reaction center protein X



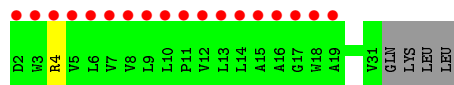
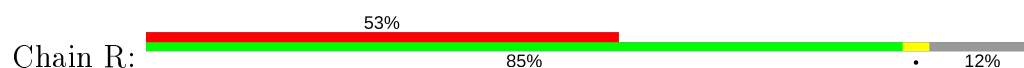
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 178.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.9 (178.86-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.152 , 0.198 0.154 , 0.199	Depositor DCC
R_{free} test set	26827 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.684	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 79.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54101	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.47	0/2728	0.57	0/3719
1	a	0.47	0/2748	0.56	0/3746
2	B	0.45	0/4191	0.53	0/5709
2	b	0.43	0/4198	0.53	0/5720
3	C	0.39	0/3626	0.50	0/4936
3	c	0.39	0/3676	0.51	0/5004
4	D	0.50	0/2818	0.56	0/3840
4	d	0.47	0/2818	0.54	0/3840
5	E	0.34	0/693	0.50	0/944
5	e	0.36	0/695	0.50	0/948
6	F	0.41	0/284	0.52	0/387
6	f	0.42	0/265	0.52	0/360
7	H	0.39	0/535	0.56	0/728
7	h	0.34	0/524	0.52	0/713
8	I	0.35	0/311	0.49	0/419
8	i	0.36	0/311	0.46	0/419
9	J	0.34	0/278	0.42	0/376
9	j	0.34	0/286	0.46	0/386
10	K	0.34	0/303	0.52	0/416
10	k	0.38	0/303	0.50	0/416
11	L	0.44	0/319	0.48	0/433
11	l	0.46	0/319	0.44	0/433
12	M	0.49	0/270	0.58	0/368
12	m	0.45	0/262	0.54	0/357
13	O	0.38	0/1958	0.56	0/2654
13	o	0.38	0/1937	0.55	0/2625
14	T	0.48	0/266	0.54	0/362
14	t	0.51	0/266	0.51	0/362
15	U	0.38	0/785	0.53	0/1064
15	u	0.41	0/785	0.54	0/1064
16	V	0.38	0/1096	0.51	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.36	0/1085	0.52	0/1473
17	Y	0.37	0/216	0.51	0/289
17	y	0.31	0/216	0.46	0/289
18	X	0.31	0/290	0.47	0/392
18	x	0.32	0/284	0.47	0/384
19	Z	0.31	0/490	0.44	0/669
19	z	0.31	0/490	0.48	0/669
20	R	0.23	0/245	0.37	0/338
All	All	0.42	0/43170	0.53	0/58738

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	327 (98%)	7 (2%)	1 (0%)	41	37
1	a	338/344 (98%)	332 (98%)	5 (2%)	1 (0%)	41	37
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	502 (98%)	11 (2%)	0	100	100
3	C	453/455 (100%)	444 (98%)	7 (2%)	2 (0%)	34	29
3	c	459/455 (101%)	449 (98%)	8 (2%)	2 (0%)	34	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	60 (94%)	4 (6%)	0	100	100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	36 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5282/5384 (98%)	5166 (98%)	110 (2%)	6 (0%)	51	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	a	259	ILE
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	272/279 (98%)	272 (100%)	0	100	100
1	a	275/279 (99%)	274 (100%)	1 (0%)	91	93
2	B	412/403 (102%)	407 (99%)	5 (1%)	71	76
2	b	413/403 (102%)	409 (99%)	4 (1%)	76	81
3	C	356/356 (100%)	352 (99%)	4 (1%)	73	78
3	c	362/356 (102%)	354 (98%)	8 (2%)	52	55
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	78
4	d	277/277 (100%)	274 (99%)	3 (1%)	73	78
5	E	74/73 (101%)	73 (99%)	1 (1%)	67	72
5	e	74/73 (101%)	72 (97%)	2 (3%)	44	46
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	31
7	H	55/54 (102%)	53 (96%)	2 (4%)	35	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	61
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	42	42
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	34	32
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	37
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	37
11	L	36/35 (103%)	35 (97%)	1 (3%)	43	44
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	31/32 (97%)	30 (97%)	1 (3%)	39	38
12	m	30/32 (94%)	30 (100%)	0	100	100
13	O	214/207 (103%)	211 (99%)	3 (1%)	67	72
13	o	211/207 (102%)	204 (97%)	7 (3%)	38	37
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	9
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	9
15	U	84/89 (94%)	83 (99%)	1 (1%)	71	76
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	118 (100%)	0	100	100
16	v	117/117 (100%)	115 (98%)	2 (2%)	60	65
17	Y	22/23 (96%)	22 (100%)	0	100	100
17	y	22/23 (96%)	21 (96%)	1 (4%)	27	24
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	57	61
19	z	52/52 (100%)	52 (100%)	0	100	100
20	R	25/29 (86%)	24 (96%)	1 (4%)	31	29
All	All	4387/4403 (100%)	4326 (99%)	61 (1%)	69	72

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	79	SER
2	B	362	PHE

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Mol	Chain	Res	Type
2	B	479	PHE
2	B	492	GLU
2	B	505	ARG
3	C	28	GLN
3	C	29	GLU
3	C	289	PHE
3	C	418	ASN
4	D	90	LEU
4	D	180	ARG
4	D	329	MET
5	E	71	GLU
7	H	49	TYR
7	H	65	LEU
10	K	17	ILE
11	L	13	ASN
12	M	5	GLN
13	O	4	THR
13	O	69	LYS
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	70	ARG
19	Z	4	LEU
20	R	4	ARG
1	a	12	ASN
2	b	80	ILE
2	b	362	PHE
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	289	PHE
3	c	391	ARG
3	c	416[A]	SER
3	c	416[B]	SER
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	180	ARG
4	d	329	MET
5	e	16	SER
5	e	71	GLU

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Mol	Chain	Res	Type
6	f	15	ILE
7	h	49	TYR
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
13	o	4	THR
13	o	23	ASP
13	o	25	THR
13	o	37	THR
13	o	118	LEU
13	o	139	SER
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
16	v	2	GLU
16	v	110	LYS
17	y	42	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
2	B	53	ASN
2	B	331	ASN
2	B	490	GLN
4	D	61	HIS
4	D	83	ASN
4	D	332	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN
19	Z	58	ASN
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
13	o	124	ASN
13	o	147	ASN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	FME	M	1	12	8,9,10	0.63	0	7,9,11	1.36	2 (28%)
12	FME	m	1	12	8,9,10	0.68	0	7,9,11	1.53	2 (28%)
14	FME	T	1	14	8,9,10	0.71	0	7,9,11	1.36	1 (14%)
8	FME	I	1	8	8,9,10	0.66	0	7,9,11	1.17	1 (14%)
14	FME	t	1	14	8,9,10	0.85	0	7,9,11	2.25	4 (57%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.37	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	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.38	117.62	122.82
14	t	1	FME	C-CA-N	2.62	114.47	109.73
12	m	1	FME	CA-N-CN	-2.46	119.03	122.82
8	i	1	FME	CA-N-CN	-2.45	119.05	122.82
14	t	1	FME	O1-CN-N	-2.43	118.87	125.27
14	T	1	FME	O-C-CA	-2.30	118.76	124.78
14	t	1	FME	O-C-CA	-2.28	118.80	124.78
8	I	1	FME	O-C-CA	-2.19	119.04	124.78
12	m	1	FME	O1-CN-N	-2.16	119.58	125.27
8	i	1	FME	O-C-CA	-2.08	119.33	124.78
12	M	1	FME	O-C-CA	-2.07	119.35	124.78
12	M	1	FME	CA-N-CN	-2.03	119.69	122.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	O1-CN-N-CA
8	I	1	FME	O1-CN-N-CA
12	m	1	FME	CA-CB-CG-SD
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 251 ligands modelled in this entry, 18 are unknown and 19 are monoatomic - leaving 214 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	B	620	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	10 (17%)
24	CLA	B	607	-	59,73,73	1.96	13 (22%)	67,113,113	2.26	23 (34%)
28	GOL	B	626	-	5,5,5	0.43	0	5,5,5	0.30	0
25	PHO	a	411	-	67,69,69	2.15	17 (25%)	85,99,99	1.86	23 (27%)
27	SQD	A	415	-	53,54,54	1.05	3 (5%)	62,65,65	1.15	4 (6%)
28	GOL	b	602	-	5,5,5	0.41	0	5,5,5	0.44	0
23	BCT	A	404	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	B	609	-	59,73,73	2.00	13 (22%)	67,113,113	2.15	24 (35%)
24	CLA	B	604	-	59,73,73	2.06	14 (23%)	67,113,113	2.28	22 (32%)
34	HTG	B	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.09	1 (4%)
24	CLA	a	412	-	59,73,73	1.98	13 (22%)	67,113,113	2.19	24 (35%)
28	GOL	V	201	-	5,5,5	0.37	0	5,5,5	0.32	0
28	GOL	a	401	-	5,5,5	0.42	0	5,5,5	0.46	0
26	BCR	D	404	-	41,41,41	1.05	1 (2%)	56,56,56	1.73	14 (25%)
38	HEM	E	102	5,6	27,50,50	0.83	1 (3%)	17,82,82	2.28	3 (17%)
24	CLA	b	623	-	59,73,73	1.98	12 (20%)	67,113,113	2.30	26 (38%)
26	BCR	Y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	9 (16%)
26	BCR	C	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	13 (23%)
35	LMG	Z	101	-	37,37,55	0.96	2 (5%)	45,45,63	1.38	6 (13%)
24	CLA	b	612	-	59,73,73	2.00	13 (22%)	67,113,113	2.38	25 (37%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.21	0
25	PHO	d	401	-	67,69,69	2.12	17 (25%)	85,99,99	2.09	23 (27%)
24	CLA	D	402	-	59,73,73	1.95	13 (22%)	67,113,113	2.29	25 (37%)
26	BCR	b	628	-	41,41,41	1.07	1 (2%)	56,56,56	1.25	7 (12%)
24	CLA	c	515	3	59,73,73	2.00	13 (22%)	67,113,113	2.08	23 (34%)
31	PL9	a	416	-	55,55,55	0.64	2 (3%)	68,69,69	1.91	18 (26%)
24	CLA	b	615	-	59,73,73	1.94	13 (22%)	67,113,113	2.37	22 (32%)
37	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
29	LMT	m	102	-	36,36,36	0.49	0	47,47,47	0.98	2 (4%)
24	CLA	B	602	40	59,73,73	2.02	13 (22%)	67,113,113	2.14	20 (29%)
28	GOL	t	102	-	5,5,5	0.45	0	5,5,5	0.12	0
37	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.11	5 (9%)
24	CLA	B	616	-	59,73,73	1.94	12 (20%)	67,113,113	2.12	21 (31%)
24	CLA	C	504	-	59,73,73	2.01	13 (22%)	67,113,113	2.03	18 (26%)
35	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	0.98	3 (5%)
35	LMG	c	522	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.57	7 (12%)
27	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.47	8 (15%)
25	PHO	D	401	-	67,69,69	2.12	17 (25%)	85,99,99	1.91	22 (25%)
24	CLA	B	615	-	59,73,73	2.01	13 (22%)	67,113,113	2.25	21 (31%)
24	CLA	B	610	-	59,73,73	1.98	13 (22%)	67,113,113	2.17	23 (34%)
34	HTG	B	624	-	19,19,19	0.78	1 (5%)	23,24,24	1.56	3 (13%)
37	LHG	D	408	-	48,48,48	0.89	2 (4%)	51,54,54	0.89	4 (7%)
34	HTG	b	632	-	19,19,19	1.14	2 (10%)	23,24,24	1.75	3 (13%)
36	DGD	C	519	-	63,63,67	0.87	2 (3%)	77,77,81	0.88	2 (2%)
24	CLA	c	505	-	59,73,73	2.00	13 (22%)	67,113,113	2.15	21 (31%)
28	GOL	b	605	-	5,5,5	0.37	0	5,5,5	0.30	0
37	LHG	d	409	-	48,48,48	0.93	2 (4%)	51,54,54	1.05	2 (3%)
24	CLA	C	509	-	59,73,73	2.05	13 (22%)	67,113,113	2.21	22 (32%)
24	CLA	C	508	40	59,73,73	1.99	13 (22%)	67,113,113	2.08	20 (29%)
24	CLA	b	622	-	59,73,73	2.03	12 (20%)	67,113,113	2.15	22 (32%)
24	CLA	C	514	-	59,73,73	1.99	13 (22%)	67,113,113	2.07	23 (34%)
34	HTG	d	412	-	16,16,19	1.22	2 (12%)	20,21,24	1.80	3 (15%)
36	DGD	D	406	-	52,52,67	1.02	3 (5%)	60,60,81	1.21	5 (8%)
28	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.32	0
24	CLA	A	406	40	59,73,73	2.01	13 (22%)	67,113,113	2.33	25 (37%)
24	CLA	c	511	40	59,73,73	2.00	13 (22%)	67,113,113	2.24	20 (29%)
38	HEM	V	205	16	27,50,50	0.84	2 (7%)	17,82,82	1.40	1 (5%)
37	LHG	d	408	-	48,48,48	0.88	2 (4%)	51,54,54	1.00	4 (7%)
36	DGD	h	102	-	63,63,67	0.91	3 (4%)	77,77,81	0.92	4 (5%)
24	CLA	C	512	3	59,73,73	2.04	12 (20%)	67,113,113	2.14	23 (34%)
24	CLA	c	509	-	59,73,73	1.96	13 (22%)	67,113,113	2.23	17 (25%)
28	GOL	B	627	-	5,5,5	0.30	0	5,5,5	0.45	0
28	GOL	v	203	-	5,5,5	0.41	0	5,5,5	0.27	0
28	GOL	f	101	33	5,5,5	0.32	0	5,5,5	0.49	0
24	CLA	C	510	-	59,73,73	2.09	13 (22%)	67,113,113	2.21	21 (31%)
29	LMT	a	404	-	36,36,36	0.48	1 (2%)	47,47,47	1.10	2 (4%)
24	CLA	b	618	-	59,73,73	1.95	12 (20%)	67,113,113	2.13	22 (32%)
24	CLA	d	402	40	59,73,73	2.03	13 (22%)	67,113,113	2.24	23 (34%)
35	LMG	C	521	-	51,51,55	0.95	2 (3%)	59,59,63	1.18	5 (8%)
24	CLA	C	506	-	59,73,73	1.93	13 (22%)	67,113,113	2.16	18 (26%)
29	LMT	F	102	-	36,36,36	0.46	0	47,47,47	1.01	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	516	-	59,73,73	2.02	12 (20%)	67,113,113	2.27	23 (34%)
34	HTG	b	607	-	19,19,19	1.08	2 (10%)	23,24,24	1.32	1 (4%)
29	LMT	C	522	-	36,36,36	0.50	0	47,47,47	1.22	3 (6%)
24	CLA	b	616	40	59,73,73	1.97	14 (23%)	67,113,113	2.15	22 (32%)
24	CLA	c	513	-	59,73,73	2.06	13 (22%)	67,113,113	2.21	21 (31%)
34	HTG	b	608	-	19,19,19	1.07	2 (10%)	23,24,24	1.27	3 (13%)
29	LMT	b	630	-	25,25,36	0.52	0	30,30,47	0.64	0
28	GOL	V	203	-	5,5,5	0.40	0	5,5,5	0.28	0
28	GOL	A	412	-	5,5,5	0.32	0	5,5,5	0.36	0
24	CLA	C	503	-	59,73,73	2.02	13 (22%)	67,113,113	2.17	22 (32%)
28	GOL	F	101	33	5,5,5	0.37	0	5,5,5	0.22	0
24	CLA	b	624	-	59,73,73	1.99	13 (22%)	67,113,113	2.11	19 (28%)
24	CLA	B	613	-	59,73,73	2.04	13 (22%)	67,113,113	2.23	22 (32%)
27	SQD	A	411	-	53,54,54	0.96	3 (5%)	62,65,65	1.52	11 (17%)
28	GOL	T	101	-	5,5,5	0.43	0	5,5,5	0.17	0
27	SQD	L	102	-	53,54,54	1.02	3 (5%)	62,65,65	1.58	10 (16%)
26	BCR	B	619	-	41,41,41	1.10	1 (2%)	56,56,56	1.38	6 (10%)
27	SQD	a	414	-	53,54,54	0.97	3 (5%)	62,65,65	1.59	13 (20%)
24	CLA	C	505	40	59,73,73	2.05	13 (22%)	67,113,113	2.19	22 (32%)
26	BCR	c	518	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	8 (14%)
37	LHG	D	409	-	48,48,48	0.96	2 (4%)	51,54,54	1.04	3 (5%)
34	HTG	b	631	-	19,19,19	0.79	1 (5%)	23,24,24	1.26	2 (8%)
24	CLA	B	612	-	59,73,73	1.99	13 (22%)	67,113,113	2.27	20 (29%)
24	CLA	C	507	-	59,73,73	1.99	13 (22%)	67,113,113	2.17	22 (32%)
24	CLA	b	621	-	59,73,73	2.02	15 (25%)	67,113,113	2.29	24 (35%)
23	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
28	GOL	v	202	-	5,5,5	0.34	0	5,5,5	0.28	0
24	CLA	C	502	-	59,73,73	1.95	12 (20%)	67,113,113	2.19	23 (34%)
34	HTG	B	633	-	19,19,19	1.03	2 (10%)	23,24,24	1.41	1 (4%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.57	0
36	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.12	7 (9%)
29	LMT	a	419	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
28	GOL	c	502	-	5,5,5	0.40	0	5,5,5	0.48	0
36	DGD	c	521	-	63,63,67	0.89	2 (3%)	77,77,81	1.01	4 (5%)
34	HTG	c	524	-	19,19,19	1.04	2 (10%)	23,24,24	1.49	1 (4%)
30	OEX	A	417	1,3,40	0,15,15	0.00	-	-	-	-
24	CLA	c	507	-	59,73,73	1.98	13 (22%)	67,113,113	2.08	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	K	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.43	11 (19%)
24	CLA	B	606	-	59,73,73	1.99	12 (20%)	67,113,113	2.17	22 (32%)
24	CLA	A	407	40	59,73,73	1.99	13 (22%)	67,113,113	2.14	22 (32%)
35	LMG	M	101	-	51,51,55	0.94	2 (3%)	59,59,63	1.02	3 (5%)
29	LMT	M	105	-	36,36,36	0.47	0	47,47,47	0.85	0
36	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.12	7 (9%)
26	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.57	9 (16%)
24	CLA	C	513	-	59,73,73	2.01	13 (22%)	67,113,113	2.22	22 (32%)
24	CLA	a	409	-	59,73,73	2.01	13 (22%)	67,113,113	2.21	25 (37%)
34	HTG	C	523	-	19,19,19	0.99	2 (10%)	23,24,24	1.58	2 (8%)
24	CLA	c	514	-	59,73,73	2.02	13 (22%)	67,113,113	2.21	24 (35%)
24	CLA	b	625	-	59,73,73	2.01	13 (22%)	67,113,113	2.28	22 (32%)
24	CLA	B	617	-	59,73,73	2.00	13 (22%)	67,113,113	2.23	21 (31%)
29	LMT	f	103	-	36,36,36	0.48	0	47,47,47	0.94	2 (4%)
28	GOL	B	628	-	5,5,5	0.36	0	5,5,5	0.52	0
36	DGD	H	102	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	6 (7%)
38	HEM	e	103	5,6	27,50,50	0.80	1 (3%)	17,82,82	1.72	3 (17%)
34	HTG	c	525	-	19,19,19	1.03	2 (10%)	23,24,24	1.49	3 (13%)
26	BCR	d	405	-	41,41,41	1.06	1 (2%)	56,56,56	1.65	13 (23%)
28	GOL	a	402	-	5,5,5	0.38	0	5,5,5	0.27	0
28	GOL	C	525	-	5,5,5	0.38	0	5,5,5	0.73	0
25	PHO	A	408	-	67,69,69	2.12	17 (25%)	85,99,99	1.91	19 (22%)
28	GOL	B	629	-	5,5,5	0.37	0	5,5,5	0.28	0
29	LMT	M	102	-	36,36,36	0.40	0	47,47,47	0.90	1 (2%)
24	CLA	D	403	-	59,73,73	2.01	14 (23%)	67,113,113	2.16	21 (31%)
24	CLA	b	614	-	59,73,73	1.99	13 (22%)	67,113,113	2.26	20 (29%)
28	GOL	b	603	-	5,5,5	0.33	0	5,5,5	0.20	0
27	SQD	B	621	-	53,54,54	1.01	3 (5%)	62,65,65	1.53	9 (14%)
26	BCR	b	626	-	41,41,41	1.02	1 (2%)	56,56,56	1.45	8 (14%)
24	CLA	b	611	-	59,73,73	2.02	13 (22%)	67,113,113	2.27	22 (32%)
34	HTG	B	632	-	19,19,19	1.02	2 (10%)	23,24,24	1.39	3 (13%)
28	GOL	o	301	-	5,5,5	0.38	0	5,5,5	0.26	0
29	LMT	T	104	-	25,25,36	0.52	0	30,30,47	0.92	1 (3%)
26	BCR	T	103	-	41,41,41	1.08	1 (2%)	56,56,56	1.62	13 (23%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.36	0
26	BCR	b	627	-	41,41,41	1.00	1 (2%)	56,56,56	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	d	403	-	59,73,73	2.01	13 (22%)	67,113,113	2.19	21 (31%)
26	BCR	a	413	-	41,41,41	1.07	1 (2%)	56,56,56	1.14	4 (7%)
37	LHG	E	101	-	41,41,48	1.03	2 (4%)	44,47,54	1.10	3 (6%)
26	BCR	A	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.23	7 (12%)
24	CLA	A	405	-	59,73,73	2.02	14 (23%)	67,113,113	2.25	24 (35%)
35	LMG	a	415	-	51,51,55	0.90	2 (3%)	59,59,63	1.17	5 (8%)
24	CLA	a	410	40	59,73,73	1.97	14 (23%)	67,113,113	2.15	24 (35%)
31	PL9	d	406	-	55,55,55	0.71	2 (3%)	68,69,69	1.54	16 (23%)
24	CLA	C	511	-	59,73,73	2.03	13 (22%)	67,113,113	2.18	25 (37%)
36	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.98	4 (5%)
24	CLA	B	611	40	59,73,73	2.02	13 (22%)	67,113,113	2.20	26 (38%)
28	GOL	T	102	-	5,5,5	0.40	0	5,5,5	0.30	0
37	LHG	d	407	-	48,48,48	0.88	3 (6%)	51,54,54	1.04	5 (9%)
35	LMG	j	101	39	51,51,55	0.92	2 (3%)	59,59,63	1.04	3 (5%)
24	CLA	d	404	-	59,73,73	2.02	14 (23%)	67,113,113	2.14	24 (35%)
28	GOL	C	526	-	5,5,5	0.34	0	5,5,5	0.52	0
27	SQD	F	103	-	42,43,54	1.15	3 (7%)	51,54,65	1.59	11 (21%)
24	CLA	b	617	-	59,73,73	2.03	13 (22%)	67,113,113	2.17	23 (34%)
26	BCR	H	101	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	9 (16%)
26	BCR	c	527	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	8 (14%)
29	LMT	B	622	-	36,36,36	0.43	0	47,47,47	1.06	2 (4%)
29	LMT	B	635	-	25,25,36	0.55	1 (4%)	30,30,47	0.80	1 (3%)
34	HTG	b	601	-	19,19,19	0.96	1 (5%)	23,24,24	1.04	1 (4%)
24	CLA	c	508	40	59,73,73	2.02	14 (23%)	67,113,113	2.22	24 (35%)
29	LMT	A	416	-	36,36,36	0.56	1 (2%)	47,47,47	1.28	3 (6%)
34	HTG	C	524	-	19,19,19	1.01	2 (10%)	23,24,24	1.78	4 (17%)
28	GOL	B	631	-	5,5,5	0.37	0	5,5,5	0.38	0
27	SQD	a	405	-	53,54,54	1.06	3 (5%)	62,65,65	1.24	6 (9%)
24	CLA	c	512	-	59,73,73	2.05	13 (22%)	67,113,113	2.22	23 (34%)
24	CLA	b	613	-	59,73,73	1.98	13 (22%)	67,113,113	2.32	25 (37%)
24	CLA	b	619	40	59,73,73	2.03	14 (23%)	67,113,113	2.18	23 (34%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.04	4 (8%)
31	PL9	A	418	-	55,55,55	0.66	2 (3%)	68,69,69	1.77	20 (29%)
28	GOL	O	301	-	5,5,5	0.35	0	5,5,5	0.40	0
35	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.10	4 (6%)
28	GOL	V	204	-	5,5,5	0.35	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.83	4 (17%)
35	LMG	J	101	39	51,51,55	0.86	2 (3%)	59,59,63	0.99	4 (6%)
34	HTG	D	412	-	16,16,19	1.10	2 (12%)	20,21,24	1.49	1 (5%)
35	LMG	b	629	-	51,51,55	0.90	2 (3%)	59,59,63	1.01	3 (5%)
24	CLA	B	603	-	59,73,73	2.05	14 (23%)	67,113,113	2.24	21 (31%)
28	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.24	0
24	CLA	c	510	-	59,73,73	2.00	14 (23%)	67,113,113	2.17	25 (37%)
28	GOL	A	414	-	5,5,5	0.39	0	5,5,5	0.17	0
26	BCR	t	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	16 (28%)
24	CLA	b	610	40	59,73,73	2.02	13 (22%)	67,113,113	2.18	18 (26%)
24	CLA	c	506	-	59,73,73	1.99	14 (23%)	67,113,113	2.20	23 (34%)
37	LHG	e	102	-	41,41,48	1.03	2 (4%)	44,47,54	0.93	2 (4%)
24	CLA	B	605	-	59,73,73	1.92	14 (23%)	67,113,113	2.26	21 (31%)
24	CLA	c	517	-	59,73,73	2.01	13 (22%)	67,113,113	2.14	23 (34%)
35	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.11	3 (6%)
37	LHG	l	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.98	3 (5%)
28	GOL	c	501	-	5,5,5	0.37	0	5,5,5	0.29	0
36	DGD	C	518	-	63,63,67	0.89	2 (3%)	77,77,81	1.02	5 (6%)
36	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.21	7 (9%)
30	OEX	a	417	1,3,40	0,15,15	0.00	-	-	-	-
24	CLA	B	608	40	59,73,73	1.98	14 (23%)	67,113,113	2.14	23 (34%)
26	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	11 (19%)
26	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	11 (19%)
24	CLA	b	620	-	59,73,73	1.99	12 (20%)	67,113,113	2.13	21 (31%)
24	CLA	B	614	-	59,73,73	2.01	13 (22%)	67,113,113	2.13	22 (32%)
26	BCR	B	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	7 (12%)
38	HEM	v	205	16	27,50,50	0.84	1 (3%)	17,82,82	1.30	1 (5%)
28	GOL	A	413	-	5,5,5	0.46	0	5,5,5	0.46	0
28	GOL	b	606	-	5,5,5	0.37	0	5,5,5	0.28	0
35	LMG	c	523	-	51,51,55	0.96	2 (3%)	59,59,63	1.22	7 (11%)
24	CLA	A	409	-	59,73,73	2.03	13 (22%)	67,113,113	2.15	24 (35%)
34	HTG	V	206	-	19,19,19	1.04	2 (10%)	23,24,24	1.30	3 (13%)
31	PL9	D	405	-	55,55,55	0.65	1 (1%)	68,69,69	1.71	18 (26%)

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
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	B	607	-	2/2/20/25	5/37/135/135	-
28	GOL	B	626	-	-	2/4/4/4	-
25	PHO	a	411	-	-	6/53/103/103	0/5/6/6
27	SQD	A	415	-	-	14/49/69/69	0/1/1/1
28	GOL	b	602	-	-	4/4/4/4	-
35	LMG	C	520	-	-	11/46/66/70	0/1/1/1
24	CLA	B	609	-	2/2/20/25	1/37/135/135	-
24	CLA	B	604	-	3/3/20/25	6/37/135/135	-
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	a	412	-	3/3/20/25	9/37/135/135	-
28	GOL	V	204	-	-	0/4/4/4	-
28	GOL	V	201	-	-	2/4/4/4	-
28	GOL	a	401	-	-	2/4/4/4	-
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
38	HEM	E	102	5,6	-	0/6/54/54	-
24	CLA	b	623	-	3/3/20/25	20/37/135/135	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	BCR	C	516	-	-	4/29/63/63	0/2/2/2
35	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
24	CLA	b	612	-	2/2/20/25	5/37/135/135	-
28	GOL	v	201	-	-	2/4/4/4	-
25	PHO	d	401	-	-	1/53/103/103	0/5/6/6
24	CLA	D	402	-	1/1/20/25	0/37/135/135	-
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
24	CLA	c	515	3	3/3/20/25	5/37/135/135	-
31	PL9	a	416	-	-	15/53/73/73	0/1/1/1
24	CLA	b	615	-	2/2/20/25	11/37/135/135	-
37	LHG	L	101	-	-	15/53/53/53	-
29	LMT	m	102	-	-	5/21/61/61	0/2/2/2
25	PHO	D	401	-	-	5/53/103/103	0/5/6/6
28	GOL	t	102	-	-	0/4/4/4	-
37	LHG	D	407	-	-	13/53/53/53	-
24	CLA	B	616	-	3/3/20/25	9/37/135/135	-
24	CLA	C	504	-	3/3/20/25	1/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1
35	LMG	c	522	-	-	13/46/66/70	0/1/1/1
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
24	CLA	B	602	40	3/3/20/25	12/37/135/135	-
24	CLA	b	620	-	2/2/20/25	3/37/135/135	-
24	CLA	B	615	-	3/3/20/25	14/37/135/135	-
24	CLA	B	610	-	3/3/20/25	5/37/135/135	-
34	HTG	B	624	-	-	5/10/30/30	0/1/1/1
37	LHG	D	408	-	-	11/53/53/53	-
34	HTG	b	632	-	-	5/10/30/30	0/1/1/1
36	DGD	C	519	-	-	8/51/91/95	0/2/2/2
24	CLA	c	505	-	3/3/20/25	3/37/135/135	-
28	GOL	b	605	-	-	2/4/4/4	-
37	LHG	d	409	-	-	13/53/53/53	-
24	CLA	C	509	-	3/3/20/25	5/37/135/135	-
24	CLA	C	508	40	3/3/20/25	5/37/135/135	-
24	CLA	b	622	-	3/3/20/25	4/37/135/135	-
24	CLA	C	514	-	3/3/20/25	6/37/135/135	-
34	HTG	d	412	-	-	0/7/27/30	0/1/1/1
36	DGD	D	406	-	-	21/47/67/95	0/1/1/2
28	GOL	V	202	-	-	2/4/4/4	-
24	CLA	A	406	40	2/2/20/25	4/37/135/135	-
24	CLA	c	511	40	3/3/20/25	5/37/135/135	-
38	HEM	V	205	16	-	0/6/54/54	-
37	LHG	d	408	-	-	9/53/53/53	-
36	DGD	h	102	-	-	10/51/91/95	0/2/2/2
24	CLA	C	512	3	3/3/20/25	3/37/135/135	-
24	CLA	c	509	-	2/2/20/25	4/37/135/135	-
28	GOL	B	627	-	-	2/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
28	GOL	f	101	33	-	3/4/4/4	-
24	CLA	C	510	-	3/3/20/25	11/37/135/135	-
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
24	CLA	b	618	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	C	521	-	-	9/46/66/70	0/1/1/1
24	CLA	C	506	-	1/1/20/25	4/37/135/135	-
29	LMT	F	102	-	-	3/21/61/61	0/2/2/2
24	CLA	c	516	-	3/3/20/25	9/37/135/135	-
34	HTG	b	607	-	-	2/10/30/30	0/1/1/1
29	LMT	C	522	-	-	10/21/61/61	0/2/2/2
24	CLA	b	616	40	3/3/20/25	2/37/135/135	-
24	CLA	c	513	-	3/3/20/25	11/37/135/135	-
34	HTG	b	608	-	-	1/10/30/30	0/1/1/1
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
28	GOL	V	203	-	-	1/4/4/4	-
28	GOL	A	412	-	-	0/4/4/4	-
24	CLA	C	503	-	2/2/20/25	3/37/135/135	-
28	GOL	F	101	33	-	2/4/4/4	-
24	CLA	b	624	-	3/3/20/25	4/37/135/135	-
24	CLA	B	613	-	3/3/20/25	1/37/135/135	-
27	SQD	A	411	-	-	11/49/69/69	0/1/1/1
28	GOL	T	101	-	-	0/4/4/4	-
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	a	414	-	-	15/49/69/69	0/1/1/1
24	CLA	C	505	40	3/3/20/25	6/37/135/135	-
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
37	LHG	D	409	-	-	14/53/53/53	-
34	HTG	b	631	-	-	3/10/30/30	0/1/1/1
24	CLA	B	612	-	2/2/20/25	4/37/135/135	-
24	CLA	C	507	-	3/3/20/25	9/37/135/135	-
24	CLA	b	621	-	3/3/20/25	2/37/135/135	-
28	GOL	v	202	-	-	3/4/4/4	-
24	CLA	C	502	-	3/3/20/25	5/37/135/135	-
34	HTG	B	633	-	-	0/10/30/30	0/1/1/1
28	GOL	B	636	-	-	0/4/4/4	-
36	DGD	c	519	-	-	15/51/91/95	0/2/2/2
29	LMT	a	419	-	-	5/21/61/61	0/2/2/2
28	GOL	c	502	-	-	0/4/4/4	-
36	DGD	c	521	-	-	16/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	c	524	-	-	3/10/30/30	0/1/1/1
24	CLA	c	507	-	3/3/20/25	2/37/135/135	-
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	606	-	3/3/20/25	6/37/135/135	-
24	CLA	A	407	40	2/2/20/25	3/37/135/135	-
35	LMG	M	101	-	-	7/46/66/70	0/1/1/1
29	LMT	M	105	-	-	7/21/61/61	0/2/2/2
36	DGD	C	517	-	-	16/51/91/95	0/2/2/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
24	CLA	C	513	-	3/3/20/25	10/37/135/135	-
24	CLA	a	409	-	3/3/20/25	6/37/135/135	-
34	HTG	C	523	-	-	0/10/30/30	0/1/1/1
24	CLA	c	514	-	3/3/20/25	9/37/135/135	-
24	CLA	b	625	-	3/3/20/25	8/37/135/135	-
24	CLA	B	617	-	3/3/20/25	6/37/135/135	-
38	HEM	e	103	5,6	-	2/6/54/54	-
29	LMT	f	103	-	-	10/21/61/61	0/2/2/2
28	GOL	B	628	-	-	2/4/4/4	-
36	DGD	H	102	-	-	13/51/91/95	0/2/2/2
24	CLA	c	512	-	3/3/20/25	4/37/135/135	-
34	HTG	c	525	-	-	0/10/30/30	0/1/1/1
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
28	GOL	a	402	-	-	2/4/4/4	-
28	GOL	C	525	-	-	2/4/4/4	-
25	PHO	A	408	-	-	2/53/103/103	0/5/6/6
28	GOL	B	629	-	-	3/4/4/4	-
29	LMT	M	102	-	-	5/21/61/61	0/2/2/2
24	CLA	D	403	-	3/3/20/25	5/37/135/135	-
24	CLA	b	614	-	2/2/20/25	3/37/135/135	-
28	GOL	b	603	-	-	0/4/4/4	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
24	CLA	b	611	-	2/2/20/25	5/37/135/135	-
34	HTG	B	632	-	-	3/10/30/30	0/1/1/1
28	GOL	o	301	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
26	BCR	T	103	-	-	2/29/63/63	0/2/2/2
28	GOL	B	630	-	-	4/4/4/4	-
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
24	CLA	d	403	-	1/1/20/25	2/37/135/135	-
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
37	LHG	E	101	-	-	22/46/46/53	-
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
24	CLA	A	405	-	3/3/20/25	4/37/135/135	-
35	LMG	a	415	-	-	18/46/66/70	0/1/1/1
24	CLA	a	410	40	2/2/20/25	10/37/135/135	-
31	PL9	d	406	-	-	3/53/73/73	0/1/1/1
24	CLA	C	511	-	3/3/20/25	8/37/135/135	-
36	DGD	c	520	-	-	16/51/91/95	0/2/2/2
24	CLA	B	611	40	3/3/20/25	6/37/135/135	-
28	GOL	T	102	-	-	2/4/4/4	-
37	LHG	d	407	-	-	12/53/53/53	-
35	LMG	j	101	39	-	12/46/66/70	0/1/1/1
24	CLA	d	404	-	3/3/20/25	3/37/135/135	-
28	GOL	C	526	-	-	0/4/4/4	-
24	CLA	b	617	-	2/2/20/25	3/37/135/135	-
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
29	LMT	B	622	-	-	10/21/61/61	0/2/2/2
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
34	HTG	b	601	-	-	3/10/30/30	0/1/1/1
24	CLA	c	508	40	3/3/20/25	8/37/135/135	-
29	LMT	A	416	-	-	5/21/61/61	0/2/2/2
34	HTG	C	524	-	-	3/10/30/30	0/1/1/1
28	GOL	B	631	-	-	0/4/4/4	-
27	SQD	a	405	-	-	16/49/69/69	0/1/1/1
24	CLA	b	613	-	3/3/20/25	3/37/135/135	-
24	CLA	b	619	40	3/3/20/25	6/37/135/135	-
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2
31	PL9	A	418	-	-	13/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	O	301	-	-	2/4/4/4	-
35	LMG	C	501	-	-	18/46/66/70	0/1/1/1
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
34	HTG	B	625	-	-	5/10/30/30	0/1/1/1
35	LMG	J	101	39	-	9/46/66/70	0/1/1/1
34	HTG	D	412	-	-	1/7/27/30	0/1/1/1
35	LMG	b	629	-	-	10/46/66/70	0/1/1/1
24	CLA	B	603	-	3/3/20/25	5/37/135/135	-
28	GOL	b	604	-	-	2/4/4/4	-
24	CLA	c	510	-	3/3/20/25	14/37/135/135	-
28	GOL	A	414	-	-	2/4/4/4	-
26	BCR	t	101	-	-	3/29/63/63	0/2/2/2
24	CLA	b	610	40	3/3/20/25	16/37/135/135	-
24	CLA	c	506	-	2/2/20/25	5/37/135/135	-
37	LHG	e	102	-	-	20/46/46/53	-
24	CLA	B	605	-	3/3/20/25	6/37/135/135	-
24	CLA	c	517	-	3/3/20/25	5/37/135/135	-
35	LMG	z	101	-	-	13/34/54/70	0/1/1/1
37	LHG	l	101	-	-	14/53/53/53	-
28	GOL	c	501	-	-	0/4/4/4	-
36	DGD	C	518	-	-	18/51/91/95	0/2/2/2
36	DGD	e	101	-	-	26/51/91/95	0/2/2/2
24	CLA	B	608	40	3/3/20/25	2/37/135/135	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
24	CLA	d	402	40	3/3/20/25	7/37/135/135	-
24	CLA	B	614	-	3/3/20/25	7/37/135/135	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
38	HEM	v	205	16	-	0/6/54/54	-
28	GOL	A	413	-	-	2/4/4/4	-
28	GOL	b	606	-	-	3/4/4/4	-
35	LMG	c	523	-	-	3/46/66/70	0/1/1/1
24	CLA	A	409	-	2/2/20/25	8/37/135/135	-
34	HTG	V	206	-	-	4/10/30/30	0/1/1/1
31	PL9	D	405	-	-	8/53/73/73	0/1/1/1

All (1143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3B-C2B	6.54	1.49	1.40
24	C	505	CLA	C3B-C2B	6.48	1.49	1.40
24	B	605	CLA	C3B-C2B	6.45	1.49	1.40
24	c	513	CLA	C3B-C2B	6.44	1.49	1.40
24	B	613	CLA	C3B-C2B	6.38	1.49	1.40
24	C	509	CLA	C3B-C2B	6.34	1.49	1.40
24	d	402	CLA	C3B-C2B	6.31	1.49	1.40
24	b	613	CLA	C3B-C2B	6.30	1.49	1.40
24	a	409	CLA	C3B-C2B	6.28	1.49	1.40
24	b	620	CLA	C3B-C2B	6.26	1.49	1.40
24	b	621	CLA	C3B-C2B	6.25	1.49	1.40
24	B	617	CLA	C3B-C2B	6.24	1.49	1.40
24	C	512	CLA	C3B-C2B	6.23	1.49	1.40
24	b	622	CLA	C3B-C2B	6.23	1.49	1.40
24	D	402	CLA	C3B-C2B	6.23	1.49	1.40
24	c	510	CLA	C3B-C2B	6.21	1.49	1.40
24	c	506	CLA	C3D-C2D	6.21	1.50	1.39
24	c	505	CLA	C3B-C2B	6.18	1.48	1.40
24	c	512	CLA	C3B-C2B	6.17	1.48	1.40
24	b	625	CLA	C3B-C2B	6.13	1.48	1.40
24	d	404	CLA	C3B-C2B	6.11	1.48	1.40
24	b	625	CLA	C3D-C2D	6.09	1.50	1.39
24	c	511	CLA	C3B-C2B	6.09	1.48	1.40
24	A	406	CLA	C3B-C2B	6.09	1.48	1.40
24	c	515	CLA	C3B-C2B	6.07	1.48	1.40
25	d	401	PHO	C3C-C2C	6.07	1.49	1.36
24	B	603	CLA	C3B-C2B	6.07	1.48	1.40
24	C	503	CLA	C3D-C2D	6.06	1.50	1.39
24	B	610	CLA	C3D-C2D	6.02	1.50	1.39
24	B	614	CLA	C3B-C2B	6.02	1.48	1.40
24	c	514	CLA	C3B-C2B	6.01	1.48	1.40
24	C	511	CLA	C3B-C2B	6.01	1.48	1.40
24	B	611	CLA	C3D-C2D	6.00	1.50	1.39
24	A	406	CLA	C3D-C2D	6.00	1.50	1.39
24	B	609	CLA	C3D-C2D	6.00	1.50	1.39
24	b	619	CLA	C3B-C2B	5.97	1.48	1.40
24	c	508	CLA	C3B-C2B	5.97	1.48	1.40
24	b	612	CLA	C3B-C2B	5.96	1.48	1.40
24	B	604	CLA	C3D-C2D	5.96	1.50	1.39
24	C	503	CLA	C3B-C2B	5.96	1.48	1.40
24	b	623	CLA	C3B-C2B	5.95	1.48	1.40
24	c	515	CLA	C3D-C2D	5.94	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	507	CLA	C3D-C2D	5.94	1.50	1.39
24	B	612	CLA	C3D-C2D	5.93	1.50	1.39
24	B	615	CLA	C3B-C2B	5.93	1.48	1.40
24	A	405	CLA	C3B-C2B	5.92	1.48	1.40
24	b	610	CLA	C3B-C2B	5.91	1.48	1.40
24	C	512	CLA	C3D-C2D	5.91	1.50	1.39
24	C	513	CLA	C3D-C2D	5.90	1.50	1.39
24	b	617	CLA	C3B-C2B	5.89	1.48	1.40
25	A	408	PHO	C3B-C2B	5.88	1.49	1.37
24	A	409	CLA	C3D-C2D	5.87	1.50	1.39
24	c	512	CLA	C3D-C2D	5.87	1.50	1.39
24	d	403	CLA	C3B-C2B	5.87	1.48	1.40
24	B	609	CLA	C3B-C2B	5.87	1.48	1.40
24	C	505	CLA	C3D-C2D	5.87	1.49	1.39
24	b	610	CLA	C3D-C2D	5.86	1.49	1.39
24	B	612	CLA	C3B-C2B	5.85	1.48	1.40
24	C	504	CLA	C3D-C2D	5.84	1.49	1.39
24	A	409	CLA	C3B-C2B	5.84	1.48	1.40
24	b	623	CLA	C3D-C2D	5.84	1.49	1.39
24	C	508	CLA	C3B-C2B	5.80	1.48	1.40
24	C	506	CLA	C3B-C2B	5.80	1.48	1.40
24	b	615	CLA	C3B-C2B	5.80	1.48	1.40
24	D	403	CLA	C3B-C2B	5.79	1.48	1.40
24	B	606	CLA	C3D-C2D	5.78	1.49	1.39
24	C	510	CLA	C3D-C2D	5.78	1.49	1.39
25	a	411	PHO	C3C-C2C	5.77	1.49	1.36
24	B	607	CLA	C3B-C2B	5.76	1.48	1.40
24	d	402	CLA	C3D-C2D	5.76	1.49	1.39
24	b	624	CLA	C3D-C2D	5.75	1.49	1.39
24	D	403	CLA	C3D-C2D	5.73	1.49	1.39
24	c	509	CLA	C3B-C2B	5.73	1.48	1.40
24	c	516	CLA	C3B-C2B	5.73	1.48	1.40
24	b	622	CLA	C3D-C2D	5.72	1.49	1.39
25	D	401	PHO	C3B-C2B	5.71	1.48	1.37
24	C	513	CLA	C3B-C2B	5.71	1.48	1.40
24	A	405	CLA	C3D-C2D	5.70	1.49	1.39
24	B	614	CLA	C3D-C2D	5.70	1.49	1.39
24	B	602	CLA	C3B-C2B	5.69	1.48	1.40
25	D	401	PHO	C3C-C2C	5.69	1.48	1.36
25	a	411	PHO	C3B-C2B	5.69	1.48	1.37
24	c	506	CLA	C3B-C2B	5.68	1.48	1.40
24	b	621	CLA	C3D-C2D	5.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	516	CLA	C3D-C2D	5.67	1.49	1.39
24	B	608	CLA	C3B-C2B	5.67	1.48	1.40
24	C	504	CLA	C3C-C2C	5.66	1.48	1.36
24	B	603	CLA	C3C-C2C	5.65	1.48	1.36
24	c	511	CLA	C3D-C2D	5.65	1.49	1.39
24	b	618	CLA	C3D-C2D	5.65	1.49	1.39
24	c	505	CLA	C3D-C2D	5.64	1.49	1.39
24	C	511	CLA	C3D-C2D	5.64	1.49	1.39
24	b	611	CLA	C3D-C2D	5.63	1.49	1.39
24	c	514	CLA	C3D-C2D	5.61	1.49	1.39
24	C	509	CLA	C3C-C2C	5.61	1.48	1.36
24	C	508	CLA	C3D-C2D	5.60	1.49	1.39
24	b	613	CLA	C3D-C2D	5.59	1.49	1.39
24	b	617	CLA	C3D-C2D	5.58	1.49	1.39
24	C	514	CLA	C3D-C2D	5.57	1.49	1.39
24	c	510	CLA	C3D-C2D	5.57	1.49	1.39
24	b	611	CLA	C3B-C2B	5.57	1.48	1.40
24	c	513	CLA	C3D-C2D	5.56	1.49	1.39
24	B	604	CLA	C3C-C2C	5.56	1.48	1.36
24	B	602	CLA	C3D-C2D	5.56	1.49	1.39
24	A	407	CLA	C3D-C2D	5.56	1.49	1.39
24	b	624	CLA	C3B-C2B	5.55	1.48	1.40
24	D	402	CLA	C3D-C2D	5.55	1.49	1.39
24	B	617	CLA	C3D-C2D	5.54	1.49	1.39
24	b	610	CLA	C3C-C2C	5.54	1.48	1.36
24	a	410	CLA	C3B-C2B	5.54	1.48	1.40
24	c	508	CLA	C3D-C2D	5.53	1.49	1.39
24	a	412	CLA	C3D-C2D	5.52	1.49	1.39
24	B	615	CLA	C3D-C2D	5.51	1.49	1.39
24	c	517	CLA	C3B-C2B	5.50	1.48	1.40
24	b	620	CLA	C3D-C2D	5.49	1.49	1.39
25	d	401	PHO	C3B-C2B	5.49	1.48	1.37
25	A	408	PHO	C3C-C2C	5.49	1.48	1.36
24	C	502	CLA	C3D-C2D	5.49	1.49	1.39
24	B	613	CLA	C3D-C2D	5.48	1.49	1.39
24	d	403	CLA	C3D-C2D	5.48	1.49	1.39
24	A	407	CLA	C3C-C2C	5.48	1.48	1.36
24	C	503	CLA	CHC-C1C	5.48	1.49	1.35
24	C	507	CLA	C3B-C2B	5.47	1.48	1.40
24	B	604	CLA	C3B-C2B	5.47	1.48	1.40
24	c	517	CLA	C3C-C2C	5.46	1.48	1.36
24	d	404	CLA	C3D-C2D	5.46	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C3D-C2D	5.46	1.49	1.39
24	B	611	CLA	C3C-C2C	5.46	1.48	1.36
24	c	517	CLA	C3D-C2D	5.45	1.49	1.39
24	b	619	CLA	C3C-C2C	5.45	1.48	1.36
24	b	617	CLA	C3C-C2C	5.44	1.48	1.36
24	C	514	CLA	C3B-C2B	5.44	1.47	1.40
25	d	401	PHO	CHC-C1C	5.44	1.49	1.38
24	B	611	CLA	C3B-C2B	5.43	1.47	1.40
24	b	614	CLA	C3C-C2C	5.43	1.48	1.36
24	D	402	CLA	C3C-C2C	5.42	1.48	1.36
24	A	407	CLA	C3B-C2B	5.42	1.47	1.40
24	B	610	CLA	CHC-C1C	5.41	1.48	1.35
24	b	622	CLA	C3C-C2C	5.41	1.48	1.36
24	b	614	CLA	C3B-C2B	5.40	1.47	1.40
24	b	612	CLA	C3D-C2D	5.40	1.49	1.39
26	k	101	BCR	C23-C22	-5.39	1.34	1.45
24	c	512	CLA	C3C-C2C	5.39	1.48	1.36
24	C	509	CLA	C3D-C2D	5.38	1.49	1.39
24	c	516	CLA	CHC-C1C	5.38	1.48	1.35
24	a	409	CLA	C3C-C2C	5.37	1.48	1.36
24	C	510	CLA	C3C-C2C	5.37	1.48	1.36
24	A	405	CLA	CHC-C1C	5.37	1.48	1.35
24	C	514	CLA	C3C-C2C	5.37	1.48	1.36
24	c	509	CLA	C3D-C2D	5.37	1.49	1.39
24	c	514	CLA	C3C-C2C	5.36	1.48	1.36
24	C	504	CLA	CHC-C1C	5.36	1.48	1.35
24	D	403	CLA	C3C-C2C	5.35	1.48	1.36
24	b	619	CLA	C3D-C2D	5.35	1.49	1.39
24	A	406	CLA	C3C-C2C	5.34	1.48	1.36
24	C	513	CLA	C3C-C2C	5.33	1.48	1.36
24	b	613	CLA	C3C-C2C	5.33	1.48	1.36
24	B	603	CLA	C3D-C2D	5.33	1.49	1.39
24	C	511	CLA	C3C-C2C	5.32	1.48	1.36
26	b	628	BCR	C23-C22	-5.32	1.34	1.45
24	a	412	CLA	C3C-C2C	5.31	1.48	1.36
24	B	606	CLA	O2D-CGD	5.31	1.46	1.33
24	b	616	CLA	C3B-C2B	5.31	1.47	1.40
24	b	611	CLA	C3C-C2C	5.30	1.48	1.36
24	c	507	CLA	CHC-C1C	5.30	1.48	1.35
24	b	616	CLA	C3D-C2D	5.29	1.48	1.39
24	b	616	CLA	C3C-C2C	5.29	1.48	1.36
24	C	502	CLA	CHC-C1C	5.28	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C3C-C2C	5.28	1.48	1.36
25	D	401	PHO	CHD-C1D	5.28	1.48	1.38
24	C	508	CLA	CHC-C1C	5.27	1.48	1.35
24	b	621	CLA	O2D-CGD	5.27	1.46	1.33
24	a	412	CLA	C3B-C2B	5.27	1.47	1.40
24	c	510	CLA	C3C-C2C	5.26	1.47	1.36
24	C	503	CLA	C3C-C2C	5.26	1.47	1.36
24	c	508	CLA	C3C-C2C	5.26	1.47	1.36
24	B	602	CLA	C3C-C2C	5.26	1.47	1.36
24	b	622	CLA	O2D-CGD	5.25	1.46	1.33
24	a	410	CLA	C3D-C2D	5.25	1.48	1.39
25	d	401	PHO	CHB-C1B	5.25	1.48	1.38
24	C	504	CLA	C3B-C2B	5.24	1.47	1.40
24	B	608	CLA	C3C-C2C	5.24	1.47	1.36
24	B	616	CLA	C3B-C2B	5.24	1.47	1.40
24	B	603	CLA	CHC-C1C	5.24	1.48	1.35
24	b	615	CLA	C3D-C2D	5.23	1.48	1.39
24	c	513	CLA	C3C-C2C	5.23	1.47	1.36
24	c	516	CLA	C3C-C2C	5.22	1.47	1.36
24	C	505	CLA	CHC-C1C	5.21	1.48	1.35
24	c	509	CLA	C3C-C2C	5.21	1.47	1.36
24	d	404	CLA	C3C-C2C	5.20	1.47	1.36
24	A	407	CLA	CHC-C1C	5.20	1.48	1.35
24	c	517	CLA	CHC-C1C	5.20	1.48	1.35
24	B	616	CLA	O2D-CGD	5.20	1.45	1.33
24	C	502	CLA	C3B-C2B	5.20	1.47	1.40
24	d	404	CLA	O2D-CGD	5.19	1.45	1.33
24	c	506	CLA	C3C-C2C	5.19	1.47	1.36
24	C	509	CLA	O2D-CGD	5.19	1.45	1.33
24	B	606	CLA	CHC-C1C	5.19	1.48	1.35
24	B	605	CLA	C3D-C2D	5.19	1.48	1.39
24	c	507	CLA	C3C-C2C	5.19	1.47	1.36
24	b	623	CLA	C3C-C2C	5.19	1.47	1.36
24	A	409	CLA	CHC-C1C	5.19	1.48	1.35
24	a	409	CLA	C3D-C2D	5.18	1.48	1.39
24	C	512	CLA	C3C-C2C	5.18	1.47	1.36
24	b	615	CLA	C3C-C2C	5.18	1.47	1.36
24	B	617	CLA	CHC-C1C	5.18	1.48	1.35
24	b	624	CLA	C3C-C2C	5.17	1.47	1.36
24	a	410	CLA	CHC-C1C	5.17	1.48	1.35
24	b	620	CLA	O2D-CGD	5.17	1.45	1.33
24	C	508	CLA	C3C-C2C	5.17	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C3C-C2C	5.17	1.47	1.36
24	b	610	CLA	CHC-C1C	5.16	1.48	1.35
24	b	614	CLA	C3D-C2D	5.16	1.48	1.39
24	C	513	CLA	CHC-C1C	5.16	1.48	1.35
24	c	507	CLA	C3B-C2B	5.15	1.47	1.40
25	D	401	PHO	CHB-C1B	5.15	1.48	1.38
24	B	612	CLA	C3C-C2C	5.15	1.47	1.36
24	C	505	CLA	C3C-C2C	5.15	1.47	1.36
24	B	616	CLA	C3D-C2D	5.15	1.48	1.39
24	b	623	CLA	O2D-CGD	5.14	1.45	1.33
24	B	604	CLA	CHC-C1C	5.14	1.48	1.35
24	B	616	CLA	CHC-C1C	5.14	1.48	1.35
24	a	409	CLA	CHC-C1C	5.13	1.48	1.35
24	c	513	CLA	O2D-CGD	5.13	1.45	1.33
24	b	614	CLA	CHC-C1C	5.13	1.48	1.35
24	c	516	CLA	O2D-CGD	5.12	1.45	1.33
24	C	507	CLA	C3C-C2C	5.12	1.47	1.36
24	C	506	CLA	CHC-C1C	5.12	1.48	1.35
24	C	506	CLA	C3C-C2C	5.11	1.47	1.36
24	c	511	CLA	C3C-C2C	5.11	1.47	1.36
25	a	411	PHO	O2D-CGD	5.10	1.45	1.33
24	b	617	CLA	CHC-C1C	5.10	1.48	1.35
25	a	411	PHO	CHB-C1B	5.10	1.48	1.38
24	c	505	CLA	C3C-C2C	5.10	1.47	1.36
24	a	412	CLA	CHC-C1C	5.10	1.48	1.35
24	B	613	CLA	CHC-C1C	5.10	1.48	1.35
26	C	515	BCR	C23-C22	-5.09	1.35	1.45
24	B	606	CLA	C3C-C2C	5.09	1.47	1.36
24	b	621	CLA	C3C-C2C	5.09	1.47	1.36
24	B	614	CLA	C3C-C2C	5.08	1.47	1.36
26	Y	101	BCR	C23-C22	-5.08	1.35	1.45
24	A	407	CLA	OBD-CAD	5.08	1.29	1.22
24	B	617	CLA	O2D-CGD	5.08	1.45	1.33
24	B	608	CLA	C3D-C2D	5.08	1.48	1.39
24	C	511	CLA	O2D-CGD	5.07	1.45	1.33
24	d	403	CLA	C3C-C2C	5.07	1.47	1.36
24	A	409	CLA	C3C-C2C	5.07	1.47	1.36
24	c	513	CLA	CHC-C1C	5.07	1.48	1.35
24	B	610	CLA	C3C-C2C	5.06	1.47	1.36
24	B	602	CLA	CHC-C1C	5.05	1.47	1.35
24	b	618	CLA	C3C-C2C	5.05	1.47	1.36
24	c	509	CLA	CHC-C1C	5.05	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	CHC-C1C	5.05	1.47	1.35
24	C	510	CLA	CHC-C1C	5.05	1.47	1.35
24	A	409	CLA	O2D-CGD	5.05	1.45	1.33
24	b	618	CLA	O2D-CGD	5.05	1.45	1.33
25	a	411	PHO	CHD-C1D	5.05	1.48	1.38
24	b	616	CLA	O2D-CGD	5.04	1.45	1.33
24	a	412	CLA	O2D-CGD	5.04	1.45	1.33
24	B	605	CLA	C3C-C2C	5.04	1.47	1.36
24	A	405	CLA	C3C-C2C	5.04	1.47	1.36
24	B	609	CLA	C3C-C2C	5.04	1.47	1.36
24	b	625	CLA	O2D-CGD	5.03	1.45	1.33
24	C	514	CLA	CHC-C1C	5.03	1.47	1.35
24	c	508	CLA	O2D-CGD	5.03	1.45	1.33
24	B	607	CLA	CHC-C1C	5.03	1.47	1.35
24	B	603	CLA	O2D-CGD	5.03	1.45	1.33
24	c	508	CLA	CHC-C1C	5.03	1.47	1.35
24	B	607	CLA	C3C-C2C	5.03	1.47	1.36
24	d	402	CLA	O2D-CGD	5.02	1.45	1.33
24	B	613	CLA	C3C-C2C	5.02	1.47	1.36
24	B	607	CLA	C3D-C2D	5.02	1.48	1.39
24	b	611	CLA	CHC-C1C	5.01	1.47	1.35
26	B	620	BCR	C23-C22	-5.00	1.35	1.45
24	B	617	CLA	C3C-C2C	5.00	1.47	1.36
24	b	614	CLA	O2D-CGD	5.00	1.45	1.33
24	C	511	CLA	CHC-C1C	5.00	1.47	1.35
24	c	510	CLA	O2D-CGD	5.00	1.45	1.33
24	C	507	CLA	O2D-CGD	4.99	1.45	1.33
24	B	608	CLA	O2D-CGD	4.99	1.45	1.33
24	c	512	CLA	OBD-CAD	4.99	1.29	1.22
24	B	614	CLA	O2D-CGD	4.99	1.45	1.33
24	b	612	CLA	C3C-C2C	4.99	1.47	1.36
25	A	408	PHO	O2D-CGD	4.98	1.45	1.33
26	H	101	BCR	C23-C22	-4.98	1.35	1.45
24	B	603	CLA	OBD-CAD	4.97	1.29	1.22
24	c	517	CLA	O2D-CGD	4.97	1.45	1.33
24	c	515	CLA	C3C-C2C	4.97	1.47	1.36
24	a	410	CLA	C3C-C2C	4.96	1.47	1.36
24	d	404	CLA	CHC-C1C	4.96	1.47	1.35
24	C	510	CLA	O2D-CGD	4.96	1.45	1.33
24	C	512	CLA	O2D-CGD	4.95	1.45	1.33
25	A	408	PHO	CHC-C1C	4.95	1.48	1.38
24	c	514	CLA	OBD-CAD	4.95	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	619	CLA	CHC-C1C	4.95	1.47	1.35
24	b	623	CLA	CHC-C1C	4.95	1.47	1.35
24	C	514	CLA	O2D-CGD	4.95	1.45	1.33
24	c	506	CLA	O2D-CGD	4.95	1.45	1.33
24	b	616	CLA	CHC-C1C	4.94	1.47	1.35
26	T	103	BCR	C23-C22	-4.94	1.35	1.45
24	C	509	CLA	CHC-C1C	4.94	1.47	1.35
24	C	513	CLA	O2D-CGD	4.93	1.45	1.33
24	c	514	CLA	CHC-C1C	4.93	1.47	1.35
24	A	405	CLA	O2D-CGD	4.93	1.45	1.33
24	B	602	CLA	O2D-CGD	4.93	1.45	1.33
24	b	612	CLA	CHC-C1C	4.93	1.47	1.35
24	C	507	CLA	CHC-C1C	4.93	1.47	1.35
24	b	620	CLA	CHC-C1C	4.92	1.47	1.35
24	b	620	CLA	C3C-C2C	4.92	1.47	1.36
24	c	512	CLA	CHC-C1C	4.92	1.47	1.35
24	B	607	CLA	O2D-CGD	4.92	1.45	1.33
24	B	615	CLA	CHC-C1C	4.92	1.47	1.35
24	b	624	CLA	CHC-C1C	4.91	1.47	1.35
24	D	403	CLA	O2D-CGD	4.91	1.45	1.33
24	b	622	CLA	CHC-C1C	4.91	1.47	1.35
24	b	610	CLA	O2D-CGD	4.91	1.45	1.33
24	B	604	CLA	OBD-CAD	4.90	1.29	1.22
25	A	408	PHO	CHB-C1B	4.90	1.48	1.38
24	b	618	CLA	CHC-C1C	4.89	1.47	1.35
24	b	624	CLA	O2D-CGD	4.89	1.45	1.33
24	c	506	CLA	CHC-C1C	4.89	1.47	1.35
24	c	512	CLA	O2D-CGD	4.89	1.45	1.33
24	c	514	CLA	O2D-CGD	4.88	1.45	1.33
24	B	608	CLA	CHC-C1C	4.88	1.47	1.35
24	C	506	CLA	C3D-C2D	4.88	1.48	1.39
24	A	407	CLA	O2D-CGD	4.88	1.45	1.33
24	B	610	CLA	O2D-CGD	4.88	1.45	1.33
24	c	511	CLA	CHC-C1C	4.87	1.47	1.35
24	c	505	CLA	O2D-CGD	4.87	1.45	1.33
24	b	611	CLA	OBD-CAD	4.87	1.29	1.22
24	b	612	CLA	O2D-CGD	4.87	1.45	1.33
24	B	605	CLA	CHC-C1C	4.87	1.47	1.35
24	B	616	CLA	C3C-C2C	4.87	1.47	1.36
24	c	510	CLA	CHC-C1C	4.87	1.47	1.35
24	b	618	CLA	OBD-CAD	4.86	1.29	1.22
24	b	618	CLA	C3B-C2B	4.86	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	O2D-CGD	4.85	1.45	1.33
24	b	619	CLA	OBD-CAD	4.85	1.29	1.22
25	d	401	PHO	CHD-C1D	4.85	1.48	1.38
24	a	409	CLA	O2D-CGD	4.84	1.45	1.33
24	B	612	CLA	CHC-C1C	4.84	1.47	1.35
24	b	613	CLA	O2D-CGD	4.83	1.45	1.33
24	C	502	CLA	C3C-C2C	4.83	1.47	1.36
24	b	615	CLA	CHC-C1C	4.83	1.47	1.35
24	C	512	CLA	CHC-C1C	4.82	1.47	1.35
24	b	621	CLA	CHC-C1C	4.82	1.47	1.35
24	D	403	CLA	CHC-C1C	4.82	1.47	1.35
24	c	505	CLA	CHC-C1C	4.82	1.47	1.35
24	C	506	CLA	O2D-CGD	4.81	1.44	1.33
24	b	617	CLA	O2D-CGD	4.81	1.44	1.33
24	b	619	CLA	O2D-CGD	4.81	1.44	1.33
24	B	611	CLA	CHC-C1C	4.81	1.47	1.35
24	c	515	CLA	CHC-C1C	4.81	1.47	1.35
24	C	510	CLA	OBD-CAD	4.80	1.29	1.22
24	B	615	CLA	OBD-CAD	4.80	1.29	1.22
24	C	502	CLA	O2D-CGD	4.80	1.44	1.33
24	c	509	CLA	O2D-CGD	4.80	1.44	1.33
24	b	613	CLA	CHC-C1C	4.80	1.47	1.35
24	B	611	CLA	OBD-CAD	4.80	1.29	1.22
24	d	403	CLA	OBD-CAD	4.79	1.29	1.22
24	A	406	CLA	O2D-CGD	4.79	1.44	1.33
24	D	403	CLA	OBD-CAD	4.79	1.29	1.22
26	t	101	BCR	C23-C22	-4.78	1.35	1.45
24	b	621	CLA	OBD-CAD	4.78	1.29	1.22
24	B	606	CLA	C3B-C2B	4.78	1.47	1.40
24	C	503	CLA	O2D-CGD	4.77	1.44	1.33
24	D	402	CLA	O2D-CGD	4.77	1.44	1.33
24	B	606	CLA	OBD-CAD	4.76	1.29	1.22
24	c	516	CLA	OBD-CAD	4.76	1.29	1.22
24	c	513	CLA	OBD-CAD	4.76	1.29	1.22
24	a	410	CLA	O2D-CGD	4.76	1.44	1.33
24	b	617	CLA	OBD-CAD	4.76	1.29	1.22
26	y	101	BCR	C23-C22	-4.75	1.35	1.45
26	C	516	BCR	C23-C22	-4.75	1.35	1.45
24	a	410	CLA	OBD-CAD	4.75	1.28	1.22
26	c	527	BCR	C23-C22	-4.74	1.35	1.45
24	B	610	CLA	C3B-C2B	4.74	1.46	1.40
24	a	412	CLA	OBD-CAD	4.73	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	O2D-CGD	4.73	1.44	1.33
24	C	505	CLA	OBD-CAD	4.72	1.28	1.22
26	K	101	BCR	C23-C22	-4.71	1.35	1.45
24	B	614	CLA	OBD-CAD	4.71	1.28	1.22
24	B	615	CLA	O2D-CGD	4.71	1.44	1.33
24	B	602	CLA	OBD-CAD	4.71	1.28	1.22
26	d	405	BCR	C23-C22	-4.71	1.35	1.45
24	B	609	CLA	CHC-C1C	4.71	1.47	1.35
25	D	401	PHO	O2D-CGD	4.71	1.44	1.33
26	h	101	BCR	C23-C22	-4.70	1.35	1.45
24	b	624	CLA	OBD-CAD	4.70	1.28	1.22
24	c	507	CLA	OBD-CAD	4.70	1.28	1.22
24	B	602	CLA	O2A-CGA	4.70	1.47	1.33
24	b	625	CLA	OBD-CAD	4.69	1.28	1.22
24	b	611	CLA	O2D-CGD	4.69	1.44	1.33
25	d	401	PHO	O2D-CGD	4.69	1.44	1.33
25	a	411	PHO	CHC-C1C	4.69	1.47	1.38
24	B	609	CLA	O2D-CGD	4.69	1.44	1.33
24	D	402	CLA	CHC-C1C	4.68	1.47	1.35
24	B	611	CLA	O2D-CGD	4.68	1.44	1.33
24	c	507	CLA	O2D-CGD	4.66	1.44	1.33
24	d	402	CLA	CHC-C1C	4.66	1.46	1.35
24	c	511	CLA	O2D-CGD	4.66	1.44	1.33
24	c	515	CLA	O2D-CGD	4.66	1.44	1.33
24	C	511	CLA	OBD-CAD	4.65	1.28	1.22
24	A	409	CLA	OBD-CAD	4.65	1.28	1.22
25	D	401	PHO	CHC-C1C	4.65	1.47	1.38
26	D	404	BCR	C23-C22	-4.64	1.36	1.45
24	b	625	CLA	CHC-C1C	4.63	1.46	1.35
24	B	610	CLA	OBD-CAD	4.62	1.28	1.22
24	B	613	CLA	O2D-CGD	4.62	1.44	1.33
24	c	511	CLA	OBD-CAD	4.62	1.28	1.22
24	d	402	CLA	OBD-CAD	4.62	1.28	1.22
25	A	408	PHO	CHD-C1D	4.62	1.47	1.38
24	A	406	CLA	OBD-CAD	4.61	1.28	1.22
27	A	415	SQD	O48-C23	4.61	1.46	1.33
24	C	512	CLA	OBD-CAD	4.60	1.28	1.22
24	B	604	CLA	O2D-CGD	4.59	1.44	1.33
24	B	614	CLA	CHC-C1C	4.59	1.46	1.35
24	B	617	CLA	OBD-CAD	4.59	1.28	1.22
24	b	625	CLA	C3C-C2C	4.59	1.46	1.36
27	a	405	SQD	O48-C23	4.57	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	OBD-CAD	4.57	1.28	1.22
24	d	403	CLA	O2D-CGD	4.56	1.44	1.33
24	b	612	CLA	OBD-CAD	4.56	1.28	1.22
24	a	409	CLA	OBD-CAD	4.56	1.28	1.22
26	a	413	BCR	C23-C22	-4.56	1.36	1.45
24	c	508	CLA	OBD-CAD	4.55	1.28	1.22
24	C	513	CLA	OBD-CAD	4.54	1.28	1.22
24	C	504	CLA	O2D-CGD	4.54	1.44	1.33
24	C	510	CLA	O2A-CGA	4.54	1.46	1.33
24	c	505	CLA	OBD-CAD	4.54	1.28	1.22
24	b	620	CLA	OBD-CAD	4.53	1.28	1.22
27	f	102	SQD	O47-C7	4.53	1.47	1.34
24	B	609	CLA	OBD-CAD	4.53	1.28	1.22
36	D	406	DGD	O1G-C1A	4.53	1.46	1.33
24	C	505	CLA	O2D-CGD	4.52	1.44	1.33
24	B	607	CLA	OBD-CAD	4.51	1.28	1.22
24	B	612	CLA	OBD-CAD	4.51	1.28	1.22
24	B	605	CLA	O2D-CGD	4.51	1.44	1.33
26	c	518	BCR	C23-C22	-4.51	1.36	1.45
24	B	613	CLA	OBD-CAD	4.47	1.28	1.22
24	b	615	CLA	O2D-CGD	4.46	1.44	1.33
24	c	515	CLA	OBD-CAD	4.46	1.28	1.22
24	c	512	CLA	O2A-CGA	4.45	1.46	1.33
26	B	618	BCR	C23-C22	-4.45	1.36	1.45
24	A	406	CLA	CHC-C1C	4.45	1.46	1.35
35	z	101	LMG	O8-C28	4.45	1.46	1.33
24	B	616	CLA	OBD-CAD	4.44	1.28	1.22
26	b	626	BCR	C23-C22	-4.44	1.36	1.45
24	b	624	CLA	O2A-CGA	4.43	1.46	1.33
24	C	502	CLA	OBD-CAD	4.43	1.28	1.22
24	c	517	CLA	OBD-CAD	4.43	1.28	1.22
24	C	509	CLA	O2A-CGA	4.43	1.46	1.33
24	C	509	CLA	OBD-CAD	4.43	1.28	1.22
24	c	515	CLA	O2A-CGA	4.41	1.46	1.33
26	B	619	BCR	C23-C22	-4.41	1.36	1.45
24	b	616	CLA	OBD-CAD	4.40	1.28	1.22
24	b	610	CLA	OBD-CAD	4.40	1.28	1.22
27	F	103	SQD	O47-C7	4.40	1.46	1.34
36	e	101	DGD	O2G-C1B	4.39	1.46	1.34
24	c	513	CLA	O2A-CGA	4.39	1.46	1.33
24	C	504	CLA	OBD-CAD	4.39	1.28	1.22
24	C	508	CLA	O2A-CGA	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	410	BCR	C23-C22	-4.38	1.36	1.45
36	D	406	DGD	O2G-C1B	4.38	1.46	1.34
37	E	101	LHG	O8-C23	4.37	1.46	1.33
24	b	610	CLA	O2A-CGA	4.37	1.46	1.33
24	b	622	CLA	OBD-CAD	4.37	1.28	1.22
24	c	511	CLA	O2A-CGA	4.37	1.46	1.33
24	C	514	CLA	OBD-CAD	4.37	1.28	1.22
24	C	513	CLA	O2A-CGA	4.36	1.46	1.33
35	C	520	LMG	O8-C28	4.36	1.46	1.33
24	B	610	CLA	O2A-CGA	4.35	1.46	1.33
24	A	405	CLA	OBD-CAD	4.35	1.28	1.22
27	B	621	SQD	O47-C7	4.34	1.46	1.34
27	a	405	SQD	O47-C7	4.32	1.46	1.34
24	B	609	CLA	O2A-CGA	4.32	1.46	1.33
35	C	501	LMG	O7-C10	4.32	1.46	1.34
24	C	512	CLA	O2A-CGA	4.32	1.46	1.33
24	c	510	CLA	OBD-CAD	4.31	1.28	1.22
35	C	521	LMG	O7-C10	4.31	1.46	1.34
37	l	101	LHG	O8-C23	4.30	1.45	1.33
36	e	101	DGD	O1G-C1A	4.29	1.45	1.33
24	b	623	CLA	OBD-CAD	4.28	1.28	1.22
24	d	402	CLA	O2A-CGA	4.28	1.45	1.33
24	c	509	CLA	OBD-CAD	4.28	1.28	1.22
37	D	409	LHG	O7-C7	4.27	1.46	1.34
37	e	102	LHG	O8-C23	4.27	1.45	1.33
24	d	404	CLA	O2A-CGA	4.26	1.45	1.33
24	B	606	CLA	O2A-CGA	4.26	1.45	1.33
37	d	409	LHG	O8-C23	4.26	1.45	1.33
35	c	523	LMG	O7-C10	4.25	1.46	1.34
24	b	617	CLA	O2A-CGA	4.24	1.45	1.33
24	C	503	CLA	OBD-CAD	4.24	1.28	1.22
36	C	518	DGD	O1G-C1A	4.24	1.45	1.33
24	C	507	CLA	O2A-CGA	4.24	1.45	1.33
27	f	102	SQD	O48-C23	4.24	1.45	1.33
35	C	501	LMG	O8-C28	4.24	1.45	1.33
24	B	617	CLA	O2A-CGA	4.24	1.45	1.33
24	b	615	CLA	O2A-CGA	4.23	1.45	1.33
24	c	517	CLA	O2A-CGA	4.23	1.45	1.33
24	c	516	CLA	O2A-CGA	4.23	1.45	1.33
24	A	406	CLA	O2A-CGA	4.23	1.45	1.33
35	c	523	LMG	O8-C28	4.22	1.45	1.33
26	b	627	BCR	C23-C22	-4.21	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	O2A-CGA	4.21	1.45	1.33
24	c	506	CLA	OBD-CAD	4.21	1.28	1.22
24	C	514	CLA	O2A-CGA	4.21	1.45	1.33
35	M	101	LMG	O8-C28	4.20	1.45	1.33
27	a	414	SQD	O48-C23	4.20	1.45	1.33
24	b	613	CLA	OBD-CAD	4.19	1.28	1.22
24	b	625	CLA	O2A-CGA	4.19	1.45	1.33
24	A	409	CLA	O2A-CGA	4.18	1.45	1.33
24	a	410	CLA	O2A-CGA	4.18	1.45	1.33
35	a	415	LMG	O8-C28	4.18	1.45	1.33
36	c	521	DGD	O1G-C1A	4.17	1.45	1.33
24	C	507	CLA	OBD-CAD	4.17	1.28	1.22
24	D	402	CLA	O2A-CGA	4.17	1.45	1.33
35	c	522	LMG	O8-C28	4.17	1.45	1.33
27	L	102	SQD	O47-C7	4.16	1.46	1.34
24	d	404	CLA	OBD-CAD	4.16	1.28	1.22
36	C	517	DGD	O1G-C1A	4.16	1.45	1.33
24	b	623	CLA	O2A-CGA	4.16	1.45	1.33
24	B	608	CLA	OBD-CAD	4.16	1.28	1.22
24	C	502	CLA	O2A-CGA	4.16	1.45	1.33
34	B	623	HTG	C1'-S1	-4.16	1.76	1.81
35	C	521	LMG	O8-C28	4.15	1.45	1.33
36	h	102	DGD	O1G-C1A	4.15	1.45	1.33
37	e	102	LHG	O7-C7	4.15	1.46	1.34
36	H	102	DGD	O1G-C1A	4.15	1.45	1.33
24	B	616	CLA	O2A-CGA	4.15	1.45	1.33
37	L	101	LHG	O8-C23	4.14	1.45	1.33
36	h	102	DGD	O2G-C1B	4.13	1.46	1.34
24	B	615	CLA	O2A-CGA	4.13	1.45	1.33
24	C	505	CLA	O2A-CGA	4.13	1.45	1.33
27	A	415	SQD	O47-C7	4.13	1.45	1.34
24	b	620	CLA	O2A-CGA	4.12	1.45	1.33
36	C	519	DGD	O1G-C1A	4.12	1.45	1.33
25	d	401	PHO	O2A-CGA	4.12	1.45	1.33
24	C	504	CLA	O2A-CGA	4.12	1.45	1.33
24	C	506	CLA	OBD-CAD	4.11	1.28	1.22
35	b	629	LMG	O8-C28	4.11	1.45	1.33
35	Z	101	LMG	O7-C10	4.11	1.45	1.34
24	b	615	CLA	OBD-CAD	4.11	1.28	1.22
27	L	102	SQD	O48-C23	4.10	1.45	1.33
24	C	508	CLA	OBD-CAD	4.10	1.28	1.22
24	b	611	CLA	O2A-CGA	4.10	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	O2A-CGA	4.09	1.45	1.33
24	b	612	CLA	O2A-CGA	4.09	1.45	1.33
36	c	520	DGD	O1G-C1A	4.09	1.45	1.33
27	F	103	SQD	O48-C23	4.08	1.45	1.33
35	M	101	LMG	O7-C10	4.08	1.45	1.34
37	d	409	LHG	O7-C7	4.08	1.45	1.34
35	j	101	LMG	O8-C28	4.08	1.45	1.33
24	C	511	CLA	O2A-CGA	4.08	1.45	1.33
24	b	618	CLA	O2A-CGA	4.06	1.45	1.33
35	z	101	LMG	O7-C10	4.05	1.45	1.34
24	c	505	CLA	O2A-CGA	4.04	1.45	1.33
24	B	604	CLA	O2A-CGA	4.04	1.45	1.33
34	b	632	HTG	C1'-S1	-4.04	1.76	1.81
37	D	408	LHG	O7-C7	4.03	1.45	1.34
24	a	412	CLA	O2A-CGA	4.03	1.45	1.33
24	B	608	CLA	O2A-CGA	4.02	1.45	1.33
24	b	613	CLA	O2A-CGA	4.02	1.45	1.33
24	c	507	CLA	O2A-CGA	4.02	1.45	1.33
37	E	101	LHG	O7-C7	4.00	1.45	1.34
24	d	403	CLA	O2A-CGA	3.99	1.45	1.33
35	j	101	LMG	O7-C10	3.99	1.45	1.34
27	B	621	SQD	O48-C23	3.99	1.45	1.33
24	B	603	CLA	O2A-CGA	3.99	1.45	1.33
25	D	401	PHO	O2A-CGA	3.99	1.45	1.33
36	c	521	DGD	O2G-C1B	3.98	1.45	1.34
24	b	614	CLA	O2A-CGA	3.98	1.45	1.33
24	B	614	CLA	O2A-CGA	3.98	1.45	1.33
35	C	520	LMG	O7-C10	3.98	1.45	1.34
24	c	508	CLA	O2A-CGA	3.97	1.44	1.33
24	c	506	CLA	O2A-CGA	3.97	1.44	1.33
25	A	408	PHO	O2A-CGA	3.96	1.44	1.33
24	A	407	CLA	O2A-CGA	3.95	1.44	1.33
36	C	519	DGD	O2G-C1B	3.95	1.45	1.34
37	D	409	LHG	O8-C23	3.95	1.44	1.33
25	A	408	PHO	C3D-C2D	3.95	1.49	1.39
35	c	522	LMG	O7-C10	3.95	1.45	1.34
24	b	619	CLA	O2A-CGA	3.94	1.44	1.33
24	b	616	CLA	O2A-CGA	3.93	1.44	1.33
34	d	412	HTG	C1'-S1	-3.93	1.76	1.81
24	C	506	CLA	O2A-CGA	3.93	1.44	1.33
36	c	520	DGD	O2G-C1B	3.92	1.45	1.34
36	C	517	DGD	O2G-C1B	3.91	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	O2A-CGA	3.90	1.44	1.33
36	H	102	DGD	O2G-C1B	3.90	1.45	1.34
35	a	415	LMG	O7-C10	3.90	1.45	1.34
24	c	510	CLA	O2A-CGA	3.89	1.44	1.33
27	a	414	SQD	O47-C7	3.89	1.45	1.34
24	B	611	CLA	O2A-CGA	3.89	1.44	1.33
24	b	621	CLA	O2A-CGA	3.88	1.44	1.33
24	C	503	CLA	O2A-CGA	3.88	1.44	1.33
34	b	607	HTG	C1'-S1	-3.88	1.76	1.81
24	b	622	CLA	O2A-CGA	3.87	1.44	1.33
27	A	411	SQD	O48-C23	3.86	1.44	1.33
24	c	514	CLA	O2A-CGA	3.86	1.44	1.33
36	C	518	DGD	O2G-C1B	3.85	1.45	1.34
25	a	411	PHO	OBD-CAD	3.85	1.29	1.22
27	A	411	SQD	O47-C7	3.85	1.45	1.34
35	b	629	LMG	O7-C10	3.83	1.45	1.34
37	D	407	LHG	O8-C23	3.83	1.44	1.33
36	c	519	DGD	O1G-C1A	3.82	1.44	1.33
37	d	408	LHG	O7-C7	3.82	1.45	1.34
36	c	519	DGD	O2G-C1B	3.82	1.45	1.34
37	l	101	LHG	O7-C7	3.81	1.45	1.34
35	J	101	LMG	O8-C28	3.80	1.44	1.33
24	A	405	CLA	O2A-CGA	3.79	1.44	1.33
37	d	407	LHG	O8-C23	3.79	1.44	1.33
37	d	408	LHG	O8-C23	3.79	1.44	1.33
24	B	605	CLA	OBD-CAD	3.78	1.27	1.22
25	a	411	PHO	C3D-C2D	3.76	1.49	1.39
37	D	408	LHG	O8-C23	3.76	1.44	1.33
24	D	402	CLA	OBD-CAD	3.75	1.27	1.22
34	V	206	HTG	C1'-S1	-3.74	1.76	1.81
37	L	101	LHG	O7-C7	3.71	1.44	1.34
25	D	401	PHO	OBD-CAD	3.71	1.28	1.22
24	c	509	CLA	O2A-CGA	3.70	1.44	1.33
24	B	605	CLA	O2A-CGA	3.70	1.44	1.33
25	d	401	PHO	C3D-C2D	3.69	1.49	1.39
25	D	401	PHO	C3D-C2D	3.69	1.49	1.39
35	J	101	LMG	O7-C10	3.66	1.44	1.34
34	b	608	HTG	C1'-S1	-3.65	1.76	1.81
24	B	612	CLA	O2A-CGA	3.64	1.44	1.33
34	B	633	HTG	C1'-S1	-3.61	1.76	1.81
34	B	625	HTG	C1'-S1	-3.60	1.76	1.81
25	A	408	PHO	CHC-C4B	3.59	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	632	HTG	C1'-S1	-3.58	1.76	1.81
34	c	525	HTG	C1'-S1	-3.55	1.76	1.81
34	c	524	HTG	C1'-S1	-3.55	1.76	1.81
25	a	411	PHO	O2A-CGA	3.54	1.43	1.33
37	D	407	LHG	O7-C7	3.52	1.44	1.34
24	a	409	CLA	O2A-CGA	3.52	1.43	1.33
34	D	412	HTG	C1'-S1	-3.51	1.76	1.81
34	C	524	HTG	C1'-S1	-3.51	1.76	1.81
25	A	408	PHO	C4A-NA	-3.48	1.26	1.35
25	D	401	PHO	CHD-C4C	3.48	1.48	1.40
37	d	407	LHG	O7-C7	3.46	1.44	1.34
25	a	411	PHO	C4A-NA	-3.44	1.27	1.35
25	a	411	PHO	CHC-C4B	3.43	1.48	1.40
25	a	411	PHO	CHD-C4C	3.42	1.48	1.40
34	b	601	HTG	C1'-S1	-3.36	1.77	1.81
25	D	401	PHO	C4A-NA	-3.36	1.27	1.35
34	C	523	HTG	C1'-S1	-3.34	1.77	1.81
25	D	401	PHO	CHB-C4A	3.29	1.48	1.40
24	B	613	CLA	C1C-C2C	3.23	1.50	1.44
25	d	401	PHO	CHC-C4B	3.20	1.47	1.40
25	A	408	PHO	OBD-CAD	3.18	1.28	1.22
24	b	611	CLA	C1D-C2D	3.12	1.49	1.42
24	C	508	CLA	C1C-C2C	3.12	1.50	1.44
24	d	404	CLA	C1D-C2D	3.12	1.49	1.42
25	A	408	PHO	CHD-C4C	3.07	1.47	1.40
25	d	401	PHO	C4A-NA	-3.05	1.27	1.35
24	b	622	CLA	C4C-C3C	3.05	1.50	1.45
25	D	401	PHO	CHC-C4B	3.05	1.47	1.40
25	d	401	PHO	CHD-C4C	3.04	1.47	1.40
25	d	401	PHO	C3B-C4B	3.02	1.49	1.43
27	f	102	SQD	C6-S	-3.02	1.66	1.77
25	A	408	PHO	C3B-C4B	3.01	1.49	1.43
24	B	602	CLA	C1D-C2D	3.01	1.49	1.42
24	B	613	CLA	C1B-NB	-3.01	1.32	1.35
25	a	411	PHO	C3B-C4B	3.01	1.49	1.43
25	d	401	PHO	OBD-CAD	2.99	1.27	1.22
24	b	619	CLA	C1D-C2D	2.99	1.49	1.42
24	B	608	CLA	C4C-C3C	2.97	1.50	1.45
24	C	509	CLA	C4C-C3C	2.97	1.50	1.45
24	B	603	CLA	C1D-C2D	2.97	1.49	1.42
24	c	507	CLA	C1C-C2C	2.96	1.50	1.44
27	A	415	SQD	C6-S	-2.96	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C1C-C2C	2.94	1.50	1.44
24	B	615	CLA	C1D-C2D	2.93	1.49	1.42
24	b	614	CLA	C1D-C2D	2.92	1.49	1.42
24	b	618	CLA	C1D-C2D	2.92	1.49	1.42
25	a	411	PHO	CHB-C4A	2.91	1.47	1.40
24	C	507	CLA	C1D-C2D	2.91	1.49	1.42
24	d	403	CLA	C1D-C2D	2.90	1.49	1.42
24	c	515	CLA	C1D-C2D	2.88	1.49	1.42
24	b	610	CLA	C1D-C2D	2.88	1.49	1.42
24	b	612	CLA	C1C-C2C	2.88	1.50	1.44
24	B	611	CLA	C1D-C2D	2.87	1.49	1.42
24	c	517	CLA	C1D-C2D	2.86	1.49	1.42
24	b	614	CLA	C1C-C2C	2.86	1.50	1.44
24	D	403	CLA	C1D-C2D	2.86	1.49	1.42
24	B	616	CLA	C1D-C2D	2.86	1.49	1.42
24	b	621	CLA	C1B-CHB	2.85	1.48	1.41
24	B	614	CLA	C4C-C3C	2.84	1.49	1.45
25	d	401	PHO	CHB-C4A	2.84	1.47	1.40
24	C	511	CLA	C1B-CHB	2.84	1.48	1.41
24	B	608	CLA	C1D-C2D	2.84	1.49	1.42
24	D	403	CLA	C4C-C3C	2.83	1.49	1.45
34	b	631	HTG	C1'-S1	-2.83	1.77	1.81
24	b	625	CLA	C1B-CHB	2.83	1.48	1.41
24	C	509	CLA	C1C-C2C	2.82	1.50	1.44
24	c	517	CLA	C1C-C2C	2.81	1.50	1.44
24	b	624	CLA	C1D-C2D	2.81	1.48	1.42
24	A	407	CLA	C1D-C2D	2.80	1.48	1.42
24	A	405	CLA	C4C-C3C	2.80	1.49	1.45
24	C	508	CLA	C4B-CHC	2.80	1.48	1.41
24	c	509	CLA	C4C-C3C	2.79	1.49	1.45
24	B	614	CLA	C1B-CHB	2.79	1.48	1.41
27	a	405	SQD	C6-S	-2.78	1.67	1.77
24	C	514	CLA	C1D-C2D	2.78	1.48	1.42
24	b	625	CLA	C1D-C2D	2.78	1.48	1.42
34	B	624	HTG	C1'-S1	-2.78	1.77	1.81
24	B	604	CLA	C1C-C2C	2.78	1.49	1.44
24	C	502	CLA	C1D-C2D	2.78	1.48	1.42
24	a	409	CLA	CHD-C4C	2.77	1.49	1.41
24	C	510	CLA	C4C-C3C	2.77	1.49	1.45
24	c	509	CLA	C1C-C2C	2.77	1.49	1.44
24	C	505	CLA	C1D-C2D	2.76	1.48	1.42
24	a	409	CLA	C1D-C2D	2.76	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C1C-C2C	2.76	1.49	1.44
24	C	512	CLA	C4C-C3C	2.76	1.49	1.45
24	a	409	CLA	C4C-C3C	2.75	1.49	1.45
24	B	616	CLA	C4B-CHC	2.75	1.48	1.41
24	c	507	CLA	C1D-C2D	2.74	1.48	1.42
27	F	103	SQD	C6-S	-2.74	1.67	1.77
24	c	512	CLA	C1D-C2D	2.73	1.48	1.42
24	c	508	CLA	C1D-C2D	2.73	1.48	1.42
24	c	505	CLA	C1D-C2D	2.72	1.48	1.42
24	c	510	CLA	C1D-C2D	2.72	1.48	1.42
24	C	512	CLA	C1B-CHB	2.72	1.48	1.41
24	A	409	CLA	C4B-CHC	2.72	1.48	1.41
24	c	511	CLA	C1C-C2C	2.72	1.49	1.44
24	c	514	CLA	C1D-C2D	2.72	1.48	1.42
24	B	612	CLA	C1B-CHB	2.72	1.48	1.41
24	B	611	CLA	C4C-C3C	2.72	1.49	1.45
27	A	411	SQD	C6-S	-2.71	1.67	1.77
24	B	612	CLA	C1D-C2D	2.70	1.48	1.42
24	B	610	CLA	C1D-C2D	2.70	1.48	1.42
24	C	504	CLA	CHD-C4C	2.70	1.48	1.41
24	B	607	CLA	C1D-C2D	2.70	1.48	1.42
24	C	504	CLA	C4B-CHC	2.69	1.48	1.41
24	B	612	CLA	C1C-C2C	2.69	1.49	1.44
24	C	504	CLA	C1D-C2D	2.69	1.48	1.42
24	B	604	CLA	C4B-CHC	2.69	1.48	1.41
24	b	615	CLA	C1D-C2D	2.69	1.48	1.42
24	C	510	CLA	C1D-C2D	2.69	1.48	1.42
24	C	509	CLA	C1D-C2D	2.68	1.48	1.42
24	a	410	CLA	C1D-C2D	2.68	1.48	1.42
24	a	412	CLA	CHD-C4C	2.68	1.48	1.41
24	b	616	CLA	C1B-NB	-2.68	1.32	1.35
24	B	607	CLA	C1C-C2C	2.68	1.49	1.44
24	B	613	CLA	C1D-C2D	2.68	1.48	1.42
24	C	505	CLA	C1B-CHB	2.67	1.48	1.41
24	c	513	CLA	C1B-CHB	2.67	1.48	1.41
24	c	512	CLA	C1B-CHB	2.67	1.48	1.41
25	A	408	PHO	CHB-C4A	2.67	1.46	1.40
24	C	512	CLA	C1D-C2D	2.66	1.48	1.42
24	C	511	CLA	C1D-C2D	2.66	1.48	1.42
24	b	617	CLA	C4B-CHC	2.65	1.48	1.41
24	B	609	CLA	C4C-C3C	2.65	1.49	1.45
24	c	511	CLA	C1D-C2D	2.65	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C1C-C2C	2.65	1.49	1.44
24	B	606	CLA	C1D-C2D	2.65	1.48	1.42
24	d	402	CLA	C1D-C2D	2.64	1.48	1.42
24	B	615	CLA	C1C-C2C	2.64	1.49	1.44
24	C	507	CLA	CHD-C4C	2.64	1.48	1.41
24	a	410	CLA	C1C-C2C	2.64	1.49	1.44
24	c	517	CLA	C4B-CHC	2.63	1.48	1.41
24	C	503	CLA	C1C-C2C	2.63	1.49	1.44
24	a	409	CLA	C1C-C2C	2.63	1.49	1.44
24	b	616	CLA	C1B-CHB	2.63	1.48	1.41
24	d	403	CLA	CHD-C4C	2.63	1.48	1.41
24	b	617	CLA	CHD-C4C	2.63	1.48	1.41
24	d	403	CLA	C4C-C3C	2.62	1.49	1.45
27	B	621	SQD	C6-S	-2.62	1.67	1.77
24	C	502	CLA	C4B-CHC	2.62	1.48	1.41
24	c	505	CLA	C4C-C3C	2.62	1.49	1.45
24	C	505	CLA	C1C-C2C	2.61	1.49	1.44
24	c	509	CLA	C1B-CHB	2.61	1.48	1.41
24	C	513	CLA	C1D-C2D	2.61	1.48	1.42
24	B	607	CLA	C4C-C3C	2.60	1.49	1.45
24	b	615	CLA	C1C-C2C	2.60	1.49	1.44
35	Z	101	LMG	O8-C28	2.60	1.46	1.33
24	c	516	CLA	C1C-C2C	2.60	1.49	1.44
24	A	407	CLA	C1C-C2C	2.60	1.49	1.44
24	A	409	CLA	C1C-C2C	2.59	1.49	1.44
24	c	507	CLA	C4B-CHC	2.59	1.48	1.41
24	c	513	CLA	C1C-C2C	2.59	1.49	1.44
31	a	416	PL9	C6-C5	2.59	1.48	1.35
24	B	614	CLA	C1C-C2C	2.59	1.49	1.44
24	b	616	CLA	C1D-C2D	2.59	1.48	1.42
24	b	622	CLA	C1B-CHB	2.59	1.48	1.41
24	b	613	CLA	C1B-CHB	2.59	1.48	1.41
24	a	410	CLA	C1B-CHB	2.59	1.48	1.41
24	b	612	CLA	C1D-C2D	2.59	1.48	1.42
24	B	608	CLA	C4B-CHC	2.59	1.48	1.41
27	a	414	SQD	C6-S	-2.59	1.67	1.77
24	b	623	CLA	CHD-C4C	2.58	1.48	1.41
27	L	102	SQD	C6-S	-2.58	1.67	1.77
24	C	514	CLA	C1C-C2C	2.58	1.49	1.44
24	b	622	CLA	C1C-C2C	2.58	1.49	1.44
24	C	503	CLA	C4B-CHC	2.58	1.48	1.41
24	B	610	CLA	C1B-CHB	2.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	CHD-C4C	2.57	1.48	1.41
24	b	611	CLA	C4C-C3C	2.57	1.49	1.45
24	c	517	CLA	CHD-C4C	2.57	1.48	1.41
31	A	418	PL9	C6-C5	2.56	1.48	1.35
24	c	516	CLA	C4B-CHC	2.56	1.48	1.41
24	b	611	CLA	CHD-C4C	2.56	1.48	1.41
24	b	610	CLA	CHD-C4C	2.56	1.48	1.41
24	A	406	CLA	C1D-C2D	2.56	1.48	1.42
24	c	513	CLA	C1D-C2D	2.56	1.48	1.42
24	c	516	CLA	C1D-C2D	2.56	1.48	1.42
24	B	615	CLA	C1B-CHB	2.56	1.48	1.41
24	C	506	CLA	C1B-CHB	2.56	1.48	1.41
24	C	502	CLA	C1C-C2C	2.56	1.49	1.44
24	b	616	CLA	C4B-CHC	2.56	1.48	1.41
24	d	403	CLA	C1B-CHB	2.56	1.48	1.41
24	b	620	CLA	C1B-CHB	2.56	1.48	1.41
24	c	508	CLA	C1B-CHB	2.55	1.48	1.41
24	a	412	CLA	C1D-C2D	2.55	1.48	1.42
24	c	507	CLA	CHD-C4C	2.55	1.48	1.41
24	B	609	CLA	C1B-CHB	2.55	1.48	1.41
24	B	613	CLA	C4B-CHC	2.55	1.48	1.41
24	c	506	CLA	CHD-C4C	2.55	1.48	1.41
24	a	412	CLA	C1B-CHB	2.55	1.48	1.41
24	B	606	CLA	C4B-CHC	2.55	1.48	1.41
24	B	612	CLA	C4B-CHC	2.55	1.48	1.41
24	B	615	CLA	C4C-C3C	2.55	1.49	1.45
24	C	508	CLA	C1D-C2D	2.54	1.48	1.42
24	C	512	CLA	CHD-C4C	2.54	1.48	1.41
24	d	402	CLA	C1B-CHB	2.54	1.48	1.41
24	C	510	CLA	C1C-C2C	2.54	1.49	1.44
24	B	607	CLA	CHD-C4C	2.54	1.48	1.41
24	A	405	CLA	CHD-C4C	2.53	1.48	1.41
24	C	514	CLA	C4B-CHC	2.53	1.48	1.41
24	c	513	CLA	CHD-C4C	2.53	1.48	1.41
24	C	513	CLA	C1C-C2C	2.53	1.49	1.44
24	b	613	CLA	C4C-C3C	2.53	1.49	1.45
25	D	401	PHO	C3B-C4B	2.53	1.48	1.43
24	b	617	CLA	C1B-CHB	2.53	1.48	1.41
24	C	506	CLA	C1C-C2C	2.53	1.49	1.44
24	A	407	CLA	C4B-CHC	2.53	1.48	1.41
24	a	409	CLA	C4B-CHC	2.53	1.48	1.41
24	b	619	CLA	C4C-C3C	2.52	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	CHD-C4C	2.52	1.48	1.41
31	d	406	PL9	C6-C5	2.52	1.48	1.35
24	C	505	CLA	CHD-C4C	2.52	1.48	1.41
24	C	510	CLA	CHD-C4C	2.52	1.48	1.41
24	b	612	CLA	C1B-CHB	2.52	1.48	1.41
24	c	510	CLA	C1B-CHB	2.52	1.48	1.41
24	b	617	CLA	C1D-C2D	2.51	1.48	1.42
24	A	405	CLA	C1B-CHB	2.51	1.48	1.41
24	B	616	CLA	C1C-C2C	2.51	1.49	1.44
24	b	615	CLA	CHD-C4C	2.51	1.48	1.41
24	B	602	CLA	C1B-CHB	2.51	1.48	1.41
24	B	613	CLA	C1B-CHB	2.51	1.48	1.41
24	c	514	CLA	C1B-CHB	2.51	1.48	1.41
24	c	509	CLA	C4B-CHC	2.51	1.48	1.41
24	C	503	CLA	C1B-CHB	2.50	1.48	1.41
24	b	617	CLA	C1C-C2C	2.50	1.49	1.44
24	A	409	CLA	C1B-CHB	2.50	1.47	1.41
24	c	517	CLA	C4C-C3C	2.50	1.49	1.45
24	d	404	CLA	C1C-C2C	2.50	1.49	1.44
24	B	610	CLA	C4B-CHC	2.50	1.47	1.41
34	d	412	HTG	C1-S1	-2.50	1.76	1.80
24	B	614	CLA	C1D-C2D	2.50	1.48	1.42
24	A	409	CLA	C1D-C2D	2.49	1.48	1.42
24	B	603	CLA	C1C-C2C	2.49	1.49	1.44
24	B	602	CLA	CHD-C4C	2.49	1.48	1.41
24	b	619	CLA	C4B-CHC	2.49	1.47	1.41
24	C	511	CLA	C1C-C2C	2.49	1.49	1.44
24	b	623	CLA	C1D-C2D	2.49	1.48	1.42
24	b	618	CLA	C1B-CHB	2.49	1.47	1.41
24	B	615	CLA	CHD-C4C	2.49	1.48	1.41
24	c	515	CLA	CHD-C4C	2.48	1.48	1.41
24	C	514	CLA	C4C-C3C	2.48	1.49	1.45
24	c	515	CLA	C1B-CHB	2.48	1.47	1.41
24	b	614	CLA	C1B-CHB	2.48	1.47	1.41
24	b	624	CLA	C1B-CHB	2.48	1.47	1.41
25	d	401	PHO	C1A-NA	-2.48	1.32	1.37
24	A	406	CLA	CHD-C4C	2.47	1.48	1.41
24	C	514	CLA	CHD-C4C	2.47	1.48	1.41
24	c	516	CLA	CHD-C4C	2.47	1.48	1.41
34	b	607	HTG	C1-S1	-2.47	1.76	1.80
24	C	503	CLA	C1D-C2D	2.47	1.48	1.42
24	C	506	CLA	C4B-CHC	2.47	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C1C-C2C	2.47	1.49	1.44
24	b	620	CLA	C1D-C2D	2.47	1.48	1.42
24	c	510	CLA	CHD-C4C	2.47	1.48	1.41
24	D	403	CLA	CHD-C4C	2.47	1.48	1.41
24	C	502	CLA	CHD-C4C	2.46	1.48	1.41
24	b	615	CLA	C1B-CHB	2.46	1.47	1.41
24	B	615	CLA	C4B-CHC	2.46	1.47	1.41
24	B	609	CLA	C1D-C2D	2.46	1.48	1.42
24	b	619	CLA	C1B-CHB	2.46	1.47	1.41
24	c	508	CLA	CHD-C4C	2.46	1.48	1.41
24	b	610	CLA	C4B-CHC	2.46	1.47	1.41
24	b	612	CLA	C4B-CHC	2.46	1.47	1.41
24	b	616	CLA	C1C-C2C	2.46	1.49	1.44
24	B	617	CLA	C4B-CHC	2.46	1.47	1.41
24	c	507	CLA	C4C-C3C	2.45	1.49	1.45
24	B	605	CLA	C1B-CHB	2.45	1.47	1.41
24	c	509	CLA	C1D-C2D	2.45	1.48	1.42
24	B	608	CLA	CHD-C4C	2.45	1.48	1.41
24	d	404	CLA	C4B-CHC	2.45	1.47	1.41
25	a	411	PHO	C1A-NA	-2.45	1.32	1.37
24	C	511	CLA	C4C-C3C	2.45	1.49	1.45
24	c	508	CLA	C4B-CHC	2.45	1.47	1.41
24	B	617	CLA	C1B-CHB	2.44	1.47	1.41
31	D	405	PL9	C6-C5	2.44	1.48	1.35
24	c	505	CLA	C1B-CHB	2.44	1.47	1.41
24	b	625	CLA	CHD-C4C	2.44	1.48	1.41
24	B	604	CLA	CHD-C4C	2.44	1.48	1.41
25	a	411	PHO	C4C-C3C	2.44	1.49	1.45
25	A	408	PHO	C4D-CHA	2.44	1.50	1.43
24	B	604	CLA	C1B-NB	-2.43	1.33	1.35
24	b	613	CLA	C1C-C2C	2.43	1.49	1.44
29	A	416	LMT	O1'-C1'	2.43	1.44	1.40
24	b	618	CLA	CHD-C4C	2.43	1.48	1.41
34	c	524	HTG	C1-S1	-2.43	1.77	1.80
24	C	507	CLA	C1B-CHB	2.43	1.47	1.41
24	B	603	CLA	CHD-C4C	2.43	1.48	1.41
24	B	614	CLA	CHD-C4C	2.43	1.48	1.41
24	B	613	CLA	C4C-C3C	2.42	1.49	1.45
24	C	512	CLA	C1C-C2C	2.42	1.49	1.44
24	d	404	CLA	C4C-C3C	2.42	1.49	1.45
24	c	514	CLA	C4C-C3C	2.42	1.49	1.45
24	B	609	CLA	C1C-C2C	2.42	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C4B-CHC	2.42	1.47	1.41
38	v	205	HEM	C3B-C2B	-2.42	1.37	1.40
24	C	513	CLA	CHD-C4C	2.41	1.48	1.41
24	C	511	CLA	C4B-CHC	2.41	1.47	1.41
24	B	610	CLA	C1C-C2C	2.41	1.49	1.44
24	d	402	CLA	CHD-C4C	2.41	1.48	1.41
24	A	405	CLA	C1D-C2D	2.41	1.48	1.42
25	D	401	PHO	C4C-C3C	2.41	1.49	1.45
24	b	620	CLA	C4B-CHC	2.41	1.47	1.41
24	C	513	CLA	C4B-CHC	2.41	1.47	1.41
24	C	510	CLA	C1B-CHB	2.40	1.47	1.41
24	b	613	CLA	C1D-C2D	2.40	1.48	1.42
24	B	604	CLA	C4C-C3C	2.40	1.49	1.45
24	d	403	CLA	C4B-CHC	2.40	1.47	1.41
24	B	612	CLA	CHD-C4C	2.40	1.48	1.41
24	C	513	CLA	C1B-CHB	2.40	1.47	1.41
24	c	514	CLA	C1C-C2C	2.40	1.49	1.44
24	D	403	CLA	C1B-CHB	2.40	1.47	1.41
24	B	611	CLA	CHD-C4C	2.39	1.48	1.41
24	d	402	CLA	C4B-CHC	2.39	1.47	1.41
24	B	604	CLA	C1B-CHB	2.39	1.47	1.41
24	C	506	CLA	C4C-C3C	2.39	1.49	1.45
24	C	503	CLA	CHD-C4C	2.39	1.48	1.41
24	b	621	CLA	C4B-CHC	2.39	1.47	1.41
24	c	513	CLA	C4C-C3C	2.39	1.49	1.45
24	C	511	CLA	CHD-C4C	2.39	1.48	1.41
24	b	617	CLA	C4C-C3C	2.39	1.49	1.45
24	A	409	CLA	CHD-C4C	2.39	1.47	1.41
24	C	509	CLA	CHD-C4C	2.38	1.47	1.41
24	c	505	CLA	CHD-C4C	2.38	1.47	1.41
34	b	632	HTG	C1-S1	-2.38	1.77	1.80
24	b	614	CLA	C4B-CHC	2.38	1.47	1.41
25	A	408	PHO	C1A-NA	-2.38	1.32	1.37
24	A	407	CLA	CHD-C4C	2.38	1.47	1.41
38	V	205	HEM	C4D-C3D	2.38	1.48	1.42
24	b	622	CLA	CHD-C4C	2.38	1.47	1.41
38	e	103	HEM	C3B-C2B	-2.38	1.37	1.40
34	c	525	HTG	C1-S1	-2.38	1.77	1.80
34	D	412	HTG	C1-S1	-2.37	1.77	1.80
24	b	625	CLA	C1C-NC	-2.37	1.34	1.37
24	a	412	CLA	C4B-CHC	2.37	1.47	1.41
24	c	506	CLA	C1B-CHB	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C4B-CHC	2.37	1.47	1.41
24	C	510	CLA	C4B-CHC	2.36	1.47	1.41
24	b	614	CLA	CHD-C4C	2.36	1.47	1.41
24	c	506	CLA	C1D-C2D	2.36	1.47	1.42
24	c	511	CLA	CHD-C4C	2.36	1.47	1.41
24	B	603	CLA	C4B-CHC	2.36	1.47	1.41
24	d	404	CLA	C1B-CHB	2.36	1.47	1.41
24	b	621	CLA	C1C-C2C	2.35	1.49	1.44
24	c	511	CLA	C1B-CHB	2.35	1.47	1.41
24	B	603	CLA	C4C-C3C	2.35	1.49	1.45
36	D	406	DGD	O3G-C1D	2.35	1.44	1.40
24	B	606	CLA	C1B-CHB	2.35	1.47	1.41
24	B	607	CLA	C1B-CHB	2.35	1.47	1.41
38	E	102	HEM	C3B-C2B	-2.35	1.37	1.40
24	D	402	CLA	C1B-CHB	2.35	1.47	1.41
24	B	605	CLA	CHD-C4C	2.35	1.47	1.41
34	C	523	HTG	C1-S1	-2.35	1.77	1.80
24	B	611	CLA	C1B-CHB	2.34	1.47	1.41
24	b	624	CLA	C4B-CHC	2.34	1.47	1.41
24	C	509	CLA	C4B-CHC	2.34	1.47	1.41
24	b	616	CLA	CHD-C4C	2.34	1.47	1.41
24	b	620	CLA	CHD-C4C	2.34	1.47	1.41
24	b	619	CLA	CHD-C4C	2.34	1.47	1.41
24	C	508	CLA	C1B-CHB	2.34	1.47	1.41
34	b	608	HTG	C1-S1	-2.34	1.77	1.80
24	B	606	CLA	CHD-C4C	2.33	1.47	1.41
24	c	513	CLA	C4B-CHC	2.33	1.47	1.41
24	d	404	CLA	CHD-C4C	2.33	1.47	1.41
24	B	609	CLA	CHD-C4C	2.33	1.47	1.41
24	A	407	CLA	C4C-C3C	2.33	1.49	1.45
24	B	616	CLA	C1B-CHB	2.33	1.47	1.41
24	B	607	CLA	C4B-CHC	2.32	1.47	1.41
24	c	508	CLA	C4C-C3C	2.32	1.49	1.45
24	A	405	CLA	C1C-C2C	2.32	1.49	1.44
24	c	511	CLA	C4C-C3C	2.32	1.49	1.45
24	B	616	CLA	CHD-C4C	2.32	1.47	1.41
24	B	617	CLA	CHD-C4C	2.32	1.47	1.41
24	C	508	CLA	C4C-C3C	2.31	1.49	1.45
34	B	632	HTG	C1-S1	-2.31	1.77	1.80
24	C	507	CLA	C4C-C3C	2.31	1.49	1.45
24	B	602	CLA	C1C-C2C	2.31	1.49	1.44
24	b	611	CLA	C4B-CHC	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	CHD-C4C	2.31	1.47	1.41
24	b	620	CLA	C4C-C3C	2.31	1.49	1.45
24	B	605	CLA	C1D-C2D	2.31	1.47	1.42
34	V	206	HTG	C1-S1	-2.30	1.77	1.80
24	c	506	CLA	C1C-C2C	2.30	1.49	1.44
24	C	507	CLA	C1C-C2C	2.30	1.49	1.44
24	c	511	CLA	C4B-CHC	2.29	1.47	1.41
24	A	405	CLA	C4B-CHC	2.29	1.47	1.41
24	B	612	CLA	C4C-C3C	2.29	1.49	1.45
24	d	402	CLA	C1C-C2C	2.29	1.49	1.44
24	D	403	CLA	C4B-CHC	2.28	1.47	1.41
25	a	411	PHO	C4D-CHA	2.28	1.49	1.43
24	D	403	CLA	C1C-C2C	2.28	1.49	1.44
24	a	412	CLA	C1C-C2C	2.28	1.49	1.44
24	C	505	CLA	C4B-CHC	2.28	1.47	1.41
24	c	515	CLA	C4C-C3C	2.28	1.49	1.45
24	C	502	CLA	C1B-CHB	2.28	1.47	1.41
24	C	506	CLA	CHD-C4C	2.27	1.47	1.41
24	d	403	CLA	C1B-NB	-2.27	1.33	1.35
24	C	514	CLA	C1B-CHB	2.27	1.47	1.41
24	b	622	CLA	C1D-C2D	2.27	1.47	1.42
24	B	605	CLA	C1C-C2C	2.27	1.48	1.44
24	C	503	CLA	C4C-C3C	2.25	1.48	1.45
24	A	409	CLA	C4C-C3C	2.25	1.48	1.45
24	b	611	CLA	C1B-CHB	2.25	1.47	1.41
24	b	624	CLA	CHD-C4C	2.25	1.47	1.41
24	c	514	CLA	C4B-CHC	2.24	1.47	1.41
24	B	603	CLA	C1B-CHB	2.24	1.47	1.41
24	B	604	CLA	C1D-C2D	2.24	1.47	1.42
24	D	402	CLA	C1D-C2D	2.24	1.47	1.42
24	a	410	CLA	CHD-C4C	2.24	1.47	1.41
24	c	517	CLA	C1B-CHB	2.24	1.47	1.41
24	b	624	CLA	C1C-C2C	2.23	1.48	1.44
25	D	401	PHO	C4D-CHA	2.23	1.49	1.43
24	A	405	CLA	C4B-NB	-2.23	1.33	1.35
24	b	611	CLA	C1C-C2C	2.23	1.48	1.44
24	A	406	CLA	C1C-C2C	2.22	1.48	1.44
24	c	510	CLA	C1C-C2C	2.22	1.48	1.44
24	C	504	CLA	C1B-CHB	2.21	1.47	1.41
24	C	507	CLA	C4B-CHC	2.21	1.47	1.41
24	b	623	CLA	C4B-CHC	2.21	1.47	1.41
24	a	409	CLA	C1B-CHB	2.20	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C1D-C2D	2.20	1.47	1.42
24	b	610	CLA	C1C-C2C	2.20	1.48	1.44
24	c	515	CLA	C1C-C2C	2.20	1.48	1.44
24	B	610	CLA	CHD-C4C	2.20	1.47	1.41
24	A	406	CLA	C1B-CHB	2.20	1.47	1.41
24	b	618	CLA	C4B-CHC	2.20	1.47	1.41
24	b	621	CLA	C1D-C2D	2.20	1.47	1.42
24	b	621	CLA	C1C-NC	-2.20	1.34	1.37
24	b	623	CLA	C1B-CHB	2.19	1.47	1.41
24	D	402	CLA	CHD-C4C	2.19	1.47	1.41
24	b	614	CLA	C4C-C3C	2.19	1.48	1.45
24	C	508	CLA	CHD-C4C	2.19	1.47	1.41
24	C	513	CLA	C4C-C3C	2.19	1.48	1.45
24	b	615	CLA	C4B-CHC	2.19	1.47	1.41
24	b	612	CLA	CHD-C4C	2.19	1.47	1.41
34	B	633	HTG	C1-S1	-2.19	1.77	1.80
24	D	402	CLA	C4C-C3C	2.18	1.48	1.45
24	B	611	CLA	C4B-NB	-2.18	1.33	1.35
24	B	608	CLA	C1B-CHB	2.18	1.47	1.41
24	c	506	CLA	C1C-NC	-2.18	1.34	1.37
24	c	510	CLA	C4B-CHC	2.18	1.47	1.41
24	B	608	CLA	C1C-C2C	2.18	1.48	1.44
24	b	621	CLA	CHD-C4C	2.18	1.47	1.41
24	B	610	CLA	C4C-C3C	2.17	1.48	1.45
24	C	504	CLA	C4C-C3C	2.17	1.48	1.45
24	b	610	CLA	C1B-CHB	2.17	1.47	1.41
24	B	608	CLA	C1B-NB	-2.16	1.33	1.35
24	c	510	CLA	C1B-NB	-2.16	1.33	1.35
24	b	619	CLA	C1C-C2C	2.16	1.48	1.44
24	B	617	CLA	C1C-C2C	2.16	1.48	1.44
31	d	406	PL9	C2-C3	2.15	1.40	1.34
25	A	408	PHO	C1B-NB	-2.15	1.34	1.38
24	B	605	CLA	C4C-C3C	2.15	1.48	1.45
24	B	614	CLA	C4B-CHC	2.15	1.47	1.41
36	h	102	DGD	O5D-C1E	2.15	1.43	1.40
24	a	410	CLA	C4B-CHC	2.15	1.47	1.41
24	c	508	CLA	C1B-NB	-2.15	1.33	1.35
24	B	605	CLA	C1A-CHA	2.15	1.52	1.43
24	c	512	CLA	C4B-CHC	2.15	1.47	1.41
25	d	401	PHO	C4D-CHA	2.14	1.49	1.43
24	b	623	CLA	C1C-C2C	2.14	1.48	1.44
24	A	406	CLA	C4B-CHC	2.14	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C1B-CHB	2.14	1.46	1.41
24	D	403	CLA	C1C-NC	-2.14	1.34	1.37
31	a	416	PL9	C2-C3	2.13	1.40	1.34
24	c	515	CLA	C4B-CHC	2.13	1.46	1.41
24	c	507	CLA	C1B-CHB	2.12	1.46	1.41
24	a	410	CLA	C4C-C3C	2.12	1.48	1.45
29	B	635	LMT	O1'-C1'	2.12	1.43	1.40
24	b	618	CLA	C1C-C2C	2.12	1.48	1.44
24	b	612	CLA	C4C-C3C	2.12	1.48	1.45
24	d	404	CLA	C1B-NB	-2.12	1.33	1.35
24	c	510	CLA	C4C-C3C	2.12	1.48	1.45
24	B	609	CLA	C4B-CHC	2.11	1.46	1.41
24	b	625	CLA	C4B-CHC	2.11	1.46	1.41
24	c	506	CLA	C4C-C3C	2.11	1.48	1.45
24	c	506	CLA	C4B-CHC	2.11	1.46	1.41
24	b	621	CLA	C1A-CHA	2.11	1.51	1.43
24	b	613	CLA	C4B-CHC	2.11	1.46	1.41
29	M	104	LMT	O1'-C1'	2.10	1.43	1.40
24	C	505	CLA	C4C-C3C	2.09	1.48	1.45
24	C	506	CLA	C1D-C2D	2.09	1.47	1.42
24	A	407	CLA	C1B-CHB	2.09	1.46	1.41
24	A	406	CLA	C4C-C3C	2.09	1.48	1.45
29	a	404	LMT	O1'-C1'	2.09	1.43	1.40
24	D	402	CLA	C4B-CHC	2.09	1.46	1.41
24	c	516	CLA	C1B-CHB	2.09	1.46	1.41
31	A	418	PL9	C2-C3	2.08	1.40	1.34
24	c	512	CLA	C4C-C3C	2.08	1.48	1.45
38	V	205	HEM	C3B-C2B	-2.07	1.37	1.40
24	B	603	CLA	C1B-NB	-2.06	1.33	1.35
24	c	505	CLA	C1C-C2C	2.06	1.48	1.44
24	B	617	CLA	C4C-C3C	2.05	1.48	1.45
24	c	505	CLA	C4B-CHC	2.05	1.46	1.41
24	B	605	CLA	C4B-CHC	2.05	1.46	1.41
24	b	610	CLA	C4C-C3C	2.05	1.48	1.45
25	d	401	PHO	C1C-NC	-2.05	1.34	1.38
24	a	410	CLA	C1B-NB	-2.04	1.33	1.35
34	B	625	HTG	C1-S1	-2.04	1.77	1.80
24	b	615	CLA	C4C-C3C	2.04	1.48	1.45
37	d	407	LHG	O7-C5	-2.04	1.41	1.46
24	b	625	CLA	C4C-C3C	2.04	1.48	1.45
24	d	402	CLA	C1C-NC	-2.03	1.34	1.37
24	b	624	CLA	C4C-C3C	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	621	CLA	C4C-C3C	2.03	1.48	1.45
24	B	602	CLA	C4C-C3C	2.03	1.48	1.45
24	b	613	CLA	CHD-C4C	2.03	1.46	1.41
24	c	512	CLA	C1C-C2C	2.02	1.48	1.44
24	a	412	CLA	C4C-C3C	2.02	1.48	1.45
24	b	616	CLA	C4C-C3C	2.01	1.48	1.45
25	D	401	PHO	C1A-NA	-2.01	1.33	1.37
34	C	524	HTG	C1-S1	-2.01	1.77	1.80
24	b	619	CLA	C1B-NB	-2.00	1.33	1.35

All (2203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	C4A-NA-C1A	-7.42	103.37	106.71
24	b	615	CLA	C4A-NA-C1A	-7.24	103.45	106.71
24	d	403	CLA	C4A-NA-C1A	-7.05	103.54	106.71
24	B	606	CLA	CHD-C4C-C3C	-6.99	114.56	124.84
24	c	509	CLA	C4A-NA-C1A	-6.95	103.58	106.71
38	E	102	HEM	CAD-CBD-CGD	6.92	124.28	112.67
24	b	614	CLA	CHD-C4C-C3C	-6.84	114.78	124.84
25	a	411	PHO	CMD-C2D-C1D	6.84	135.59	125.06
24	A	405	CLA	C4A-NA-C1A	-6.73	103.68	106.71
25	D	401	PHO	CMD-C2D-C1D	6.72	135.41	125.06
24	b	613	CLA	C2C-C1C-NC	6.70	116.25	109.97
24	b	617	CLA	C4A-NA-C1A	-6.62	103.73	106.71
24	c	516	CLA	C4A-NA-C1A	-6.59	103.75	106.71
24	c	511	CLA	O2D-CGD-CBD	6.56	122.93	111.27
24	b	614	CLA	C4A-NA-C1A	-6.53	103.77	106.71
24	b	621	CLA	CHD-C4C-C3C	-6.51	115.26	124.84
24	b	623	CLA	O2D-CGD-CBD	6.46	122.75	111.27
24	b	624	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
24	C	508	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
24	B	616	CLA	CHD-C4C-C3C	-6.41	115.41	124.84
25	d	401	PHO	CMD-C2D-C1D	6.41	134.93	125.06
24	B	613	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
34	d	412	HTG	C1'-S1-C1	6.39	112.05	100.09
24	a	410	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
24	c	517	CLA	C4A-NA-C1A	-6.37	103.84	106.71
24	B	614	CLA	C2C-C1C-NC	6.37	115.94	109.97
24	B	612	CLA	C4A-NA-C1A	-6.36	103.85	106.71
24	B	603	CLA	C4A-NA-C1A	-6.35	103.85	106.71
24	c	509	CLA	C2C-C1C-NC	6.34	115.92	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	B	616	CLA	C4A-NA-C1A	-6.34	103.86	106.71
24	D	402	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
24	C	506	CLA	C4A-NA-C1A	-6.31	103.87	106.71
34	C	523	HTG	C1'-S1-C1	6.30	111.88	100.09
24	C	504	CLA	CHD-C4C-C3C	-6.29	115.58	124.84
24	C	513	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
24	B	607	CLA	C4A-NA-C1A	-6.26	103.89	106.71
24	B	605	CLA	C2C-C1C-NC	6.26	115.83	109.97
24	b	612	CLA	CHD-C4C-C3C	-6.25	115.65	124.84
24	b	610	CLA	O2D-CGD-CBD	6.24	122.36	111.27
24	c	511	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
24	C	502	CLA	O2D-CGD-CBD	6.23	122.35	111.27
24	B	612	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
25	A	408	PHO	CMD-C2D-C1D	6.23	134.65	125.06
24	b	619	CLA	C4A-NA-C1A	-6.18	103.93	106.71
24	c	516	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
24	B	610	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
24	C	503	CLA	CHD-C4C-C3C	-6.15	115.79	124.84
24	B	602	CLA	O2D-CGD-CBD	6.15	122.20	111.27
24	B	617	CLA	O2D-CGD-CBD	6.14	122.18	111.27
24	c	505	CLA	C2C-C1C-NC	6.14	115.72	109.97
24	b	615	CLA	CHD-C4C-C3C	-6.13	115.82	124.84
24	d	402	CLA	C2C-C1C-NC	6.13	115.71	109.97
24	b	622	CLA	C2C-C1C-NC	6.12	115.70	109.97
24	b	613	CLA	O2D-CGD-CBD	6.11	122.13	111.27
24	B	617	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
24	b	616	CLA	C2C-C1C-NC	6.10	115.68	109.97
24	d	402	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
24	B	603	CLA	CHD-C4C-C3C	-6.07	115.91	124.84
24	C	512	CLA	C2C-C1C-NC	6.06	115.65	109.97
24	A	406	CLA	C2C-C1C-NC	6.06	115.65	109.97
24	b	610	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
24	b	616	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
24	b	612	CLA	C4A-NA-C1A	-6.02	104.00	106.71
24	c	513	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
24	B	609	CLA	C2C-C1C-NC	6.00	115.59	109.97
24	b	625	CLA	O2D-CGD-CBD	5.98	121.89	111.27
24	c	507	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
24	b	613	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
24	B	602	CLA	CHD-C4C-C3C	-5.95	116.10	124.84
24	C	511	CLA	CHD-C4C-C3C	-5.95	116.10	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	412	CLA	CHD-C4C-C3C	-5.94	116.10	124.84
24	A	409	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
24	b	618	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
24	d	404	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
24	c	507	CLA	C4A-NA-C1A	-5.91	104.05	106.71
24	c	511	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	B	612	CLA	C2C-C1C-NC	5.90	115.50	109.97
24	C	513	CLA	O2D-CGD-CBD	5.87	121.70	111.27
24	B	604	CLA	O2D-CGD-CBD	5.86	121.68	111.27
24	D	402	CLA	C2C-C1C-NC	5.86	115.46	109.97
24	B	604	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
24	c	510	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
24	b	623	CLA	CHD-C4C-C3C	-5.83	116.26	124.84
24	c	510	CLA	C2C-C1C-NC	5.83	115.43	109.97
24	A	406	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
24	B	614	CLA	CHD-C4C-C3C	-5.81	116.29	124.84
24	B	617	CLA	C4A-NA-C1A	-5.81	104.09	106.71
24	c	516	CLA	O2D-CGD-CBD	5.81	121.58	111.27
24	A	407	CLA	C4A-NA-C1A	-5.80	104.10	106.71
24	B	605	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
24	c	515	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
24	B	611	CLA	C2C-C1C-NC	5.78	115.39	109.97
24	C	506	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
34	D	412	HTG	C1'-S1-C1	5.77	110.89	100.09
24	B	615	CLA	CHD-C4C-C3C	-5.76	116.37	124.84
24	c	509	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
24	c	512	CLA	C2C-C1C-NC	5.75	115.36	109.97
24	a	409	CLA	C4A-NA-C1A	-5.74	104.12	106.71
24	C	512	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
24	c	514	CLA	C2C-C1C-NC	5.73	115.34	109.97
24	B	608	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	b	620	CLA	C2C-C1C-NC	5.72	115.33	109.97
24	c	517	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
24	b	625	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
24	c	509	CLA	O2D-CGD-CBD	5.69	121.38	111.27
34	c	524	HTG	C1'-S1-C1	5.68	110.72	100.09
24	B	607	CLA	CHD-C4C-C3C	-5.68	116.50	124.84
24	c	512	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
24	B	615	CLA	O2D-CGD-CBD	5.66	121.33	111.27
24	C	502	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
24	C	506	CLA	C2C-C1C-NC	5.65	115.27	109.97
24	c	508	CLA	CHD-C4C-C3C	-5.65	116.53	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	c	514	CLA	CHD-C4C-C3C	-5.65	116.54	124.84
24	b	617	CLA	CHD-C4C-C3C	-5.64	116.54	124.84
24	B	607	CLA	C2C-C1C-NC	5.64	115.25	109.97
24	b	619	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
24	b	618	CLA	C2C-C1C-NC	5.62	115.24	109.97
24	b	621	CLA	C2C-C1C-NC	5.61	115.23	109.97
34	B	633	HTG	C1'-S1-C1	5.61	110.59	100.09
24	B	613	CLA	O2D-CGD-CBD	5.61	121.23	111.27
24	c	506	CLA	C4A-NA-C1A	-5.60	104.19	106.71
24	a	409	CLA	C2C-C1C-NC	5.60	115.21	109.97
25	A	408	PHO	C3D-C2D-C1D	-5.59	97.72	105.87
24	B	604	CLA	C4A-NA-C1A	-5.59	104.19	106.71
24	c	506	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
24	B	609	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
24	b	612	CLA	O2D-CGD-CBD	5.58	121.19	111.27
24	C	509	CLA	CHD-C4C-C3C	-5.58	116.64	124.84
24	b	615	CLA	C2C-C1C-NC	5.56	115.19	109.97
24	a	412	CLA	C2C-C1C-NC	5.56	115.18	109.97
24	D	403	CLA	C2C-C1C-NC	5.56	115.18	109.97
24	C	507	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
24	C	514	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
24	b	620	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	c	513	CLA	C2C-C1C-NC	5.52	115.14	109.97
27	f	102	SQD	O47-C7-C8	5.51	123.37	111.50
24	C	505	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
24	D	402	CLA	C4A-NA-C1A	-5.50	104.23	106.71
24	A	405	CLA	C2C-C1C-NC	5.50	115.12	109.97
24	C	509	CLA	O2D-CGD-CBD	5.50	121.03	111.27
24	c	508	CLA	C2C-C1C-NC	5.49	115.11	109.97
24	C	510	CLA	C2C-C1C-NC	5.48	115.10	109.97
24	C	504	CLA	C4A-NA-C1A	-5.47	104.25	106.71
24	A	407	CLA	O2D-CGD-CBD	5.46	120.98	111.27
24	B	615	CLA	C4A-NA-C1A	-5.46	104.25	106.71
24	C	510	CLA	CHD-C4C-C3C	-5.45	116.82	124.84
24	B	604	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	C	507	CLA	C2C-C1C-NC	5.45	115.08	109.97
24	b	610	CLA	C4A-NA-C1A	-5.43	104.27	106.71
24	B	615	CLA	C2C-C1C-NC	5.42	115.05	109.97
24	c	505	CLA	O2D-CGD-CBD	5.41	120.88	111.27
24	C	509	CLA	C2C-C1C-NC	5.40	115.03	109.97
24	d	404	CLA	C4A-NA-C1A	-5.40	104.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	625	HTG	C1'-S1-C1	5.38	110.16	100.09
25	d	401	PHO	O2D-CGD-CBD	5.38	120.82	111.27
27	L	102	SQD	O6-C1-C2	5.37	116.69	108.30
24	b	612	CLA	C2C-C1C-NC	5.36	115.00	109.97
24	C	511	CLA	C2C-C1C-NC	5.35	114.98	109.97
24	B	610	CLA	C4A-NA-C1A	-5.33	104.31	106.71
24	a	409	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
24	b	624	CLA	C2C-C1C-NC	5.33	114.97	109.97
24	C	508	CLA	O2D-CGD-CBD	5.32	120.72	111.27
24	b	625	CLA	C2C-C1C-NC	5.31	114.95	109.97
24	D	403	CLA	C4A-NA-C1A	-5.30	104.32	106.71
25	A	408	PHO	C2D-C1D-ND	5.29	117.78	109.79
24	C	507	CLA	C4A-NA-C1A	-5.29	104.33	106.71
24	c	515	CLA	C2C-C1C-NC	5.29	114.92	109.97
34	c	525	HTG	C1'-S1-C1	5.28	109.97	100.09
24	C	509	CLA	C4A-NA-C1A	-5.28	104.33	106.71
24	B	611	CLA	CHD-C4C-C3C	-5.26	117.10	124.84
24	B	603	CLA	C2C-C1C-NC	5.26	114.90	109.97
27	B	621	SQD	O6-C1-C2	5.26	116.51	108.30
24	b	615	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	c	506	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	B	607	CLA	O2D-CGD-CBD	5.25	120.60	111.27
24	B	605	CLA	O2D-CGD-CBD	5.24	120.58	111.27
24	b	617	CLA	C2C-C1C-NC	5.23	114.88	109.97
24	b	614	CLA	C2C-C1C-NC	5.23	114.87	109.97
24	D	403	CLA	CHD-C4C-C3C	-5.22	117.17	124.84
27	a	414	SQD	O6-C1-C2	5.21	116.44	108.30
24	b	620	CLA	C4A-NA-C1A	-5.21	104.36	106.71
24	B	608	CLA	C4A-NA-C1A	-5.20	104.37	106.71
24	c	505	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
34	C	524	HTG	C1'-S1-C1	5.20	109.82	100.09
24	b	611	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
24	b	623	CLA	C2C-C1C-NC	5.19	114.83	109.97
25	d	401	PHO	C3D-C2D-C1D	-5.19	98.31	105.87
24	c	508	CLA	O2D-CGD-CBD	5.18	120.47	111.27
24	C	505	CLA	C2C-C1C-NC	5.17	114.82	109.97
24	C	506	CLA	O2D-CGD-CBD	5.17	120.45	111.27
24	a	410	CLA	C2C-C1C-NC	5.16	114.80	109.97
24	C	514	CLA	C2C-C1C-NC	5.15	114.80	109.97
24	b	625	CLA	C4A-NA-C1A	-5.14	104.39	106.71
24	A	406	CLA	O2D-CGD-CBD	5.13	120.39	111.27
24	C	502	CLA	C2C-C1C-NC	5.12	114.77	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	101	BCR	C33-C5-C6	-5.12	118.78	124.53
24	b	622	CLA	CHD-C4C-C3C	-5.12	117.32	124.84
24	A	409	CLA	C2C-C1C-NC	5.12	114.76	109.97
24	b	611	CLA	C2C-C1C-NC	5.10	114.75	109.97
24	d	404	CLA	C2C-C1C-NC	5.10	114.75	109.97
24	b	611	CLA	O2D-CGD-CBD	5.09	120.32	111.27
24	c	512	CLA	C4A-NA-C1A	-5.08	104.42	106.71
24	C	513	CLA	C2C-C1C-NC	5.07	114.72	109.97
24	B	610	CLA	C2C-C1C-NC	5.06	114.71	109.97
34	B	625	HTG	O5-C1-C2	5.05	116.67	110.31
25	A	408	PHO	C1-C2-C3	-5.05	117.31	126.04
24	B	602	CLA	C2C-C1C-NC	5.04	114.70	109.97
25	d	401	PHO	C1-C2-C3	-5.04	117.32	126.04
24	B	608	CLA	CHD-C4C-C3C	-5.02	117.46	124.84
24	C	511	CLA	O2D-CGD-CBD	5.01	120.18	111.27
24	c	512	CLA	O2D-CGD-CBD	5.01	120.17	111.27
24	b	621	CLA	C3C-C4C-NC	5.01	116.19	110.57
24	c	508	CLA	C4A-NA-C1A	-5.01	104.45	106.71
27	F	103	SQD	O47-C7-C8	5.01	122.29	111.50
25	a	411	PHO	C3D-C2D-C1D	-5.00	98.58	105.87
24	C	514	CLA	C4A-NA-C1A	-5.00	104.46	106.71
34	b	632	HTG	C1'-S1-C1	5.00	109.44	100.09
24	C	505	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	c	509	CLA	C3C-C4C-NC	4.99	116.17	110.57
24	c	513	CLA	O2D-CGD-CBD	4.98	120.11	111.27
25	d	401	PHO	C2D-C1D-ND	4.98	117.30	109.79
27	A	411	SQD	O47-C7-C8	4.97	122.21	111.50
26	t	101	BCR	C33-C5-C6	-4.96	118.96	124.53
24	b	622	CLA	C4A-NA-C1A	-4.96	104.48	106.71
24	C	513	CLA	C4A-NA-C1A	-4.95	104.48	106.71
24	A	405	CLA	CHD-C4C-C3C	-4.95	117.57	124.84
24	B	609	CLA	O2D-CGD-CBD	4.95	120.06	111.27
24	B	613	CLA	C3C-C4C-NC	4.94	116.11	110.57
24	c	513	CLA	C4A-NA-C1A	-4.93	104.49	106.71
24	B	616	CLA	C2C-C1C-NC	4.93	114.59	109.97
34	B	624	HTG	C1'-S1-C1	4.93	109.31	100.09
24	C	504	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	b	619	CLA	C2C-C1C-NC	4.92	114.58	109.97
24	C	503	CLA	C4A-NA-C1A	-4.92	104.50	106.71
24	b	616	CLA	O2D-CGD-CBD	4.92	120.00	111.27
24	A	406	CLA	C4A-NA-C1A	-4.92	104.50	106.71
24	C	510	CLA	C4A-NA-C1A	-4.92	104.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C1-C2-C3	-4.90	117.57	126.04
24	B	603	CLA	O2D-CGD-CBD	4.87	119.93	111.27
24	c	511	CLA	C3C-C4C-NC	4.86	116.02	110.57
24	D	403	CLA	O2D-CGD-CBD	4.86	119.90	111.27
24	b	624	CLA	C4A-NA-C1A	-4.83	104.53	106.71
24	A	409	CLA	C4A-NA-C1A	-4.83	104.53	106.71
24	c	517	CLA	C2C-C1C-NC	4.83	114.50	109.97
34	C	524	HTG	C1-O5-C5	4.82	121.48	112.58
24	B	617	CLA	C2C-C1C-NC	4.82	114.49	109.97
24	B	606	CLA	O2D-CGD-CBD	4.82	119.83	111.27
24	b	621	CLA	O2D-CGD-CBD	4.81	119.82	111.27
25	a	411	PHO	O2D-CGD-CBD	4.81	119.81	111.27
24	a	410	CLA	O2D-CGD-CBD	4.80	119.79	111.27
27	B	621	SQD	O47-C7-C8	4.79	121.83	111.50
24	c	514	CLA	O2D-CGD-CBD	4.79	119.78	111.27
24	B	613	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	503	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	b	610	CLA	C2C-C1C-NC	4.79	114.46	109.97
24	C	506	CLA	C3C-C4C-NC	4.78	115.94	110.57
25	D	401	PHO	C3D-C2D-C1D	-4.78	98.90	105.87
24	C	502	CLA	C4A-NA-C1A	-4.78	104.56	106.71
24	c	507	CLA	C2C-C1C-NC	4.78	114.45	109.97
25	a	411	PHO	C2D-C1D-ND	4.78	117.00	109.79
24	B	614	CLA	C3C-C4C-NC	4.77	115.92	110.57
25	d	401	PHO	C4C-C3C-C2C	-4.76	101.51	106.78
26	B	618	BCR	C33-C5-C6	-4.74	119.20	124.53
24	B	604	CLA	O2D-CGD-O1D	-4.73	114.59	123.84
26	b	626	BCR	C33-C5-C6	-4.72	119.23	124.53
36	C	517	DGD	O2G-C1B-C2B	4.72	121.67	111.50
24	b	614	CLA	O2D-CGD-CBD	4.72	119.65	111.27
29	A	416	LMT	C1'-O5'-C5'	4.71	122.93	113.69
26	y	101	BCR	C33-C5-C6	-4.71	119.24	124.53
24	A	407	CLA	C2C-C1C-NC	4.70	114.37	109.97
24	C	503	CLA	O2D-CGD-CBD	4.69	119.61	111.27
24	b	619	CLA	O2D-CGD-CBD	4.69	119.60	111.27
24	d	402	CLA	O2D-CGD-CBD	4.68	119.59	111.27
24	A	406	CLA	C1C-C2C-C3C	-4.68	102.04	106.96
26	D	404	BCR	C7-C8-C9	-4.67	119.18	126.23
24	b	613	CLA	C4A-NA-C1A	-4.66	104.61	106.71
34	b	632	HTG	O5-C1-C2	4.64	116.15	110.31
24	b	618	CLA	C4A-NA-C1A	-4.64	104.62	106.71
24	b	616	CLA	C1C-C2C-C3C	-4.63	102.09	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C3C-C4C-NC	4.62	115.76	110.57
24	b	612	CLA	C3C-C4C-NC	4.62	115.75	110.57
27	L	102	SQD	O47-C7-C8	4.62	121.46	111.50
24	b	623	CLA	C4A-NA-C1A	-4.62	104.63	106.71
24	d	403	CLA	CHD-C4C-C3C	-4.62	118.05	124.84
24	B	606	CLA	C3C-C4C-NC	4.62	115.75	110.57
24	C	505	CLA	C4A-NA-C1A	-4.59	104.64	106.71
24	c	507	CLA	C3C-C4C-NC	4.59	115.71	110.57
36	e	101	DGD	O2G-C1B-C2B	4.58	121.38	111.50
24	d	402	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
24	D	402	CLA	C3C-C4C-NC	4.58	115.70	110.57
24	B	614	CLA	C4A-NA-C1A	-4.58	104.65	106.71
24	c	506	CLA	O2D-CGD-CBD	4.57	119.39	111.27
25	D	401	PHO	C2D-C1D-ND	4.57	116.69	109.79
26	B	620	BCR	C15-C14-C13	-4.56	120.80	127.31
24	b	613	CLA	C3C-C4C-NC	4.56	115.69	110.57
24	C	510	CLA	O2D-CGD-CBD	4.55	119.35	111.27
24	B	608	CLA	O2D-CGD-CBD	4.55	119.35	111.27
35	C	521	LMG	O7-C10-C11	4.54	121.29	111.50
24	A	409	CLA	C3C-C4C-NC	4.54	115.66	110.57
24	C	504	CLA	C3C-C4C-NC	4.53	115.66	110.57
24	b	613	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
24	c	511	CLA	C4A-NA-C1A	-4.53	104.67	106.71
24	B	611	CLA	O2D-CGD-CBD	4.53	119.32	111.27
35	C	501	LMG	O7-C10-C11	4.53	121.26	111.50
24	a	412	CLA	O2D-CGD-CBD	4.52	119.31	111.27
24	C	508	CLA	C4A-NA-C1A	-4.52	104.67	106.71
24	b	612	CLA	C1D-CHD-C4C	-4.51	116.60	122.56
24	C	508	CLA	C3C-C4C-NC	4.50	115.62	110.57
35	a	415	LMG	O7-C10-C11	4.50	121.19	111.50
24	B	612	CLA	C3C-C4C-NC	4.49	115.61	110.57
35	c	523	LMG	O7-C10-C11	4.48	121.16	111.50
38	E	102	HEM	CBD-CAD-C3D	-4.48	104.23	112.48
24	C	508	CLA	C2C-C1C-NC	4.48	114.17	109.97
24	C	511	CLA	C1-C2-C3	-4.48	118.30	126.04
24	b	620	CLA	O2D-CGD-CBD	4.48	119.22	111.27
24	c	516	CLA	C2C-C1C-NC	4.47	114.16	109.97
34	b	631	HTG	C1'-S1-C1	4.47	108.44	100.09
24	b	621	CLA	C1D-CHD-C4C	-4.46	116.68	122.56
24	d	404	CLA	O2D-CGD-CBD	4.45	119.18	111.27
24	C	511	CLA	C4A-NA-C1A	-4.45	104.70	106.71
24	a	412	CLA	C1C-C2C-C3C	-4.45	102.28	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C1D-CHD-C4C	-4.44	116.69	122.56
24	b	615	CLA	C3C-C4C-NC	4.44	115.55	110.57
24	B	606	CLA	C2C-C1C-NC	4.44	114.13	109.97
24	a	410	CLA	C3C-C4C-NC	4.43	115.54	110.57
34	B	632	HTG	C1'-S1-C1	4.43	108.37	100.09
24	b	612	CLA	CAA-C2A-C3A	-4.42	100.66	112.78
24	B	611	CLA	C4A-NA-C1A	-4.42	104.72	106.71
24	b	623	CLA	C1-C2-C3	-4.42	118.40	126.04
24	B	615	CLA	C3C-C4C-NC	4.41	115.52	110.57
24	C	507	CLA	O2D-CGD-CBD	4.41	119.10	111.27
24	b	616	CLA	C3C-C4C-NC	4.40	115.51	110.57
24	a	412	CLA	C4A-NA-C1A	-4.40	104.73	106.71
24	B	605	CLA	C3C-C4C-NC	4.40	115.50	110.57
24	c	505	CLA	C4A-NA-C1A	-4.38	104.73	106.71
34	b	607	HTG	C1'-S1-C1	4.38	108.28	100.09
24	C	513	CLA	C3C-C4C-NC	4.36	115.47	110.57
24	C	503	CLA	C3C-C4C-NC	4.36	115.46	110.57
24	b	624	CLA	C3C-C4C-NC	4.34	115.44	110.57
24	B	609	CLA	C4A-NA-C1A	-4.34	104.76	106.71
36	e	101	DGD	O6E-C5E-C4E	4.33	117.56	109.69
24	D	402	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	B	604	CLA	C3C-C4C-NC	4.31	115.41	110.57
24	B	609	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
24	B	610	CLA	O2D-CGD-CBD	4.30	118.91	111.27
24	B	606	CLA	C4A-NA-C1A	-4.30	104.77	106.71
27	A	411	SQD	O6-C1-C2	4.29	115.00	108.30
24	B	617	CLA	C1D-CHD-C4C	-4.29	116.90	122.56
24	b	625	CLA	CAC-C3C-C4C	4.29	130.37	124.81
27	L	102	SQD	C3-C4-C5	4.28	117.88	110.24
24	b	618	CLA	O2D-CGD-CBD	4.28	118.87	111.27
24	c	514	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	B	612	CLA	O2D-CGD-CBD	4.27	118.86	111.27
24	B	616	CLA	C3C-C4C-NC	4.27	115.36	110.57
24	B	610	CLA	C3C-C4C-NC	4.26	115.35	110.57
26	H	101	BCR	C16-C17-C18	-4.26	121.23	127.31
24	B	605	CLA	C4A-NA-C1A	-4.25	104.80	106.71
24	b	623	CLA	O2D-CGD-O1D	-4.25	115.54	123.84
24	C	512	CLA	C3B-C4B-NB	4.24	114.69	109.21
24	B	612	CLA	CMC-C2C-C1C	4.23	131.47	125.04
24	c	510	CLA	O2D-CGD-CBD	4.22	118.77	111.27
24	c	513	CLA	C1D-CHD-C4C	-4.21	117.00	122.56
25	A	408	PHO	O2D-CGD-CBD	4.21	118.75	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	C4A-NA-C1A	-4.21	104.81	106.71
24	B	606	CLA	C1D-CHD-C4C	-4.19	117.03	122.56
24	b	622	CLA	C3B-C4B-NB	4.19	114.62	109.21
24	C	505	CLA	CBC-CAC-C3C	-4.19	100.88	112.43
24	B	607	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
24	A	405	CLA	CAC-C3C-C4C	4.19	130.24	124.81
24	B	604	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
24	A	406	CLA	CBC-CAC-C3C	-4.18	100.91	112.43
27	a	414	SQD	O47-C7-C8	4.18	120.51	111.50
24	B	617	CLA	C3C-C4C-NC	4.18	115.26	110.57
24	A	405	CLA	C1D-CHD-C4C	-4.17	117.05	122.56
24	c	513	CLA	C3C-C4C-NC	4.17	115.25	110.57
24	C	504	CLA	C1D-CHD-C4C	-4.17	117.05	122.56
24	c	512	CLA	C3C-C4C-NC	4.17	115.25	110.57
24	C	503	CLA	C1-C2-C3	-4.17	118.83	126.04
24	c	510	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
36	D	406	DGD	O2G-C1B-C2B	4.17	120.48	111.50
24	c	505	CLA	C3C-C4C-NC	4.14	115.22	110.57
24	c	506	CLA	C4D-C3D-CAD	-4.14	106.16	108.47
26	b	626	BCR	C7-C8-C9	-4.13	119.99	126.23
37	D	409	LHG	O7-C7-C8	4.13	120.40	111.50
24	C	511	CLA	C3C-C4C-NC	4.13	115.20	110.57
25	d	401	PHO	O2D-CGD-O1D	-4.13	115.77	123.84
24	C	509	CLA	C3C-C4C-NC	4.12	115.20	110.57
24	c	507	CLA	C1D-CHD-C4C	-4.12	117.12	122.56
24	C	514	CLA	C3C-C4C-NC	4.12	115.19	110.57
24	b	617	CLA	O2D-CGD-CBD	4.11	118.58	111.27
26	d	405	BCR	C24-C23-C22	-4.11	120.03	126.23
24	b	625	CLA	C3B-C4B-NB	4.11	114.52	109.21
24	D	403	CLA	C3C-C4C-NC	4.10	115.17	110.57
27	B	621	SQD	O7-S-C6	4.10	111.81	106.94
24	b	619	CLA	C1-C2-C3	-4.09	118.96	126.04
24	D	402	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	c	515	CLA	C4A-NA-C1A	-4.09	104.87	106.71
24	d	402	CLA	C1D-CHD-C4C	-4.09	117.16	122.56
24	d	403	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
24	C	506	CLA	C1D-CHD-C4C	-4.09	117.17	122.56
29	A	416	LMT	O5'-C5'-C4'	4.08	118.36	109.75
26	T	103	BCR	C11-C10-C9	-4.08	121.49	127.31
36	c	521	DGD	O2G-C1B-C2B	4.08	120.29	111.50
24	A	406	CLA	C3B-C4B-NB	4.07	114.48	109.21
24	d	402	CLA	C4A-NA-C1A	-4.06	104.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	c	520	DGD	O2G-C1B-C2B	4.06	120.25	111.50
24	c	515	CLA	C1D-CHD-C4C	-4.06	117.20	122.56
24	C	512	CLA	C1D-CHD-C4C	-4.05	117.21	122.56
38	e	103	HEM	CAD-CBD-CGD	4.05	119.47	112.67
24	b	625	CLA	C1D-CHD-C4C	-4.05	117.21	122.56
24	a	410	CLA	C4A-NA-C1A	-4.04	104.89	106.71
31	a	416	PL9	C7-C3-C4	4.04	120.16	116.88
24	C	505	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
24	b	610	CLA	C1D-CHD-C4C	-4.04	117.23	122.56
24	B	605	CLA	C1D-CHD-C4C	-4.04	117.23	122.56
24	b	619	CLA	C3C-C4C-NC	4.04	115.10	110.57
24	c	514	CLA	C4-C3-C5	4.03	122.06	115.27
24	B	614	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
24	a	409	CLA	C1-C2-C3	-4.03	119.07	126.04
24	B	605	CLA	C3B-C4B-NB	4.03	114.42	109.21
24	b	617	CLA	C3C-C4C-NC	4.03	115.08	110.57
24	B	612	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
24	B	615	CLA	O2D-CGD-O1D	-4.02	115.99	123.84
24	c	508	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
29	C	522	LMT	O1B-C4'-C3'	4.01	117.94	107.28
25	a	411	PHO	C4C-C3C-C2C	-4.01	102.35	106.78
24	B	603	CLA	C3C-C4C-NC	4.01	115.06	110.57
24	C	510	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	d	402	CLA	C3C-C4C-NC	4.00	115.06	110.57
24	B	603	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
24	b	622	CLA	C3C-C4C-NC	4.00	115.06	110.57
29	B	622	LMT	O1B-C4'-C3'	4.00	117.92	107.28
35	Z	101	LMG	O7-C10-C11	4.00	120.12	111.50
24	c	509	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
27	a	405	SQD	O47-C7-C8	4.00	120.11	111.50
24	b	620	CLA	CAC-C3C-C4C	3.99	129.99	124.81
31	a	416	PL9	C22-C23-C24	-3.99	118.06	127.66
24	B	613	CLA	C4A-NA-C1A	-3.99	104.91	106.71
24	c	508	CLA	C3C-C4C-NC	3.98	115.04	110.57
24	C	508	CLA	CMC-C2C-C1C	3.98	131.11	125.04
24	b	618	CLA	C3C-C4C-NC	3.98	115.04	110.57
24	B	604	CLA	CAA-C2A-C3A	-3.98	101.87	112.78
24	c	517	CLA	O2D-CGD-CBD	3.98	118.34	111.27
24	C	502	CLA	C1C-C2C-C3C	-3.98	102.77	106.96
24	C	505	CLA	C3B-C4B-NB	3.97	114.35	109.21
24	B	602	CLA	C4A-NA-C1A	-3.97	104.92	106.71
24	c	514	CLA	C1-C2-C3	-3.97	119.18	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C4C-C3C-C2C	-3.97	102.39	106.78
24	c	511	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
24	b	621	CLA	C4A-NA-C1A	-3.96	104.92	106.71
24	c	510	CLA	C3C-C4C-NC	3.96	115.01	110.57
24	B	615	CLA	CAC-C3C-C4C	3.96	129.94	124.81
26	D	404	BCR	C33-C5-C6	-3.96	120.08	124.53
24	B	605	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
24	C	512	CLA	C4A-NA-C1A	-3.95	104.93	106.71
31	a	416	PL9	C32-C33-C34	-3.95	118.15	127.66
27	A	415	SQD	O48-C23-C24	3.94	124.29	111.91
24	b	613	CLA	C3B-C4B-NB	3.94	114.31	109.21
24	C	512	CLA	C3C-C4C-NC	3.94	114.99	110.57
24	b	611	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
24	c	514	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
24	b	623	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
37	D	407	LHG	O7-C7-C8	3.93	119.98	111.50
24	b	622	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
24	b	618	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
24	B	613	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
36	D	406	DGD	C1D-C2D-C3D	3.93	118.18	110.00
24	c	516	CLA	C3C-C4C-NC	3.93	114.98	110.57
24	b	616	CLA	C4A-NA-C1A	-3.93	104.94	106.71
25	D	401	PHO	O2D-CGD-CBD	3.93	118.24	111.27
24	c	514	CLA	C3C-C4C-NC	3.93	114.97	110.57
24	b	611	CLA	C3C-C4C-NC	3.93	114.97	110.57
24	c	514	CLA	C3B-C4B-NB	3.92	114.28	109.21
24	c	512	CLA	C3B-C4B-NB	3.91	114.27	109.21
27	a	414	SQD	C44-O6-C1	-3.91	106.10	113.74
24	a	409	CLA	C1D-CHD-C4C	-3.91	117.40	122.56
24	D	403	CLA	CAC-C3C-C4C	3.91	129.88	124.81
26	C	515	BCR	C15-C14-C13	-3.90	121.74	127.31
24	B	607	CLA	C3C-C4C-NC	3.90	114.94	110.57
24	b	620	CLA	C3C-C4C-NC	3.89	114.94	110.57
26	C	515	BCR	C16-C17-C18	-3.89	121.76	127.31
24	A	406	CLA	C1D-CHD-C4C	-3.88	117.43	122.56
26	H	101	BCR	C38-C26-C25	-3.88	120.17	124.53
24	a	409	CLA	C3C-C4C-NC	3.88	114.92	110.57
24	b	624	CLA	C1D-CHD-C4C	-3.88	117.44	122.56
27	A	411	SQD	C45-O47-C7	-3.86	108.28	117.79
24	B	616	CLA	C1D-CHD-C4C	-3.86	117.46	122.56
26	k	101	BCR	C24-C23-C22	-3.86	120.40	126.23
26	d	405	BCR	C38-C26-C25	-3.86	120.19	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	101	LHG	O7-C7-C8	3.86	119.82	111.50
24	c	507	CLA	O2D-CGD-CBD	3.86	118.12	111.27
26	D	404	BCR	C24-C23-C22	-3.86	120.41	126.23
24	C	512	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
24	C	514	CLA	O2D-CGD-CBD	3.86	118.12	111.27
24	C	512	CLA	O2D-CGD-CBD	3.85	118.12	111.27
24	B	608	CLA	C1C-C2C-C3C	-3.85	102.90	106.96
24	a	409	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	B	611	CLA	C3C-C4C-NC	3.85	114.89	110.57
24	c	505	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	B	614	CLA	C3B-C4B-NB	3.85	114.18	109.21
24	b	611	CLA	CAC-C3C-C4C	3.85	129.80	124.81
24	B	613	CLA	CMC-C2C-C1C	3.84	130.89	125.04
24	d	402	CLA	C3B-C4B-NB	3.84	114.17	109.21
24	C	504	CLA	O2D-CGD-CBD	3.84	118.09	111.27
24	B	615	CLA	O2A-CGA-O1A	-3.83	113.92	123.59
24	B	611	CLA	CAA-C2A-C3A	-3.83	102.29	112.78
24	B	612	CLA	C1D-CHD-C4C	-3.83	117.51	122.56
24	b	614	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
24	a	410	CLA	C1D-CHD-C4C	-3.82	117.52	122.56
24	b	614	CLA	C1D-CHD-C4C	-3.82	117.52	122.56
24	A	405	CLA	C3C-C4C-NC	3.82	114.85	110.57
24	c	510	CLA	C3B-C4B-NB	3.81	114.14	109.21
36	e	101	DGD	C3E-C4E-C5E	3.81	117.04	110.24
37	L	101	LHG	O7-C7-C8	3.81	119.71	111.50
24	C	507	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	B	609	CLA	C3C-C4C-NC	3.81	114.84	110.57
24	B	608	CLA	C3C-C4C-NC	3.81	114.84	110.57
36	c	519	DGD	O2G-C1B-C2B	3.81	119.70	111.50
24	d	404	CLA	C3C-C4C-NC	3.80	114.83	110.57
27	A	415	SQD	O47-C7-C8	3.80	119.69	111.50
24	C	502	CLA	CMC-C2C-C1C	3.80	130.83	125.04
24	b	615	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
24	C	502	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
26	T	103	BCR	C15-C16-C17	-3.79	115.70	123.47
26	C	515	BCR	C7-C8-C9	-3.79	120.50	126.23
24	c	513	CLA	C1-C2-C3	-3.79	119.48	126.04
24	c	517	CLA	C3C-C4C-NC	3.79	114.82	110.57
26	k	101	BCR	C11-C10-C9	-3.79	121.91	127.31
24	b	610	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
24	C	511	CLA	C3B-C4B-NB	3.78	114.10	109.21
24	c	505	CLA	C3B-C4B-NB	3.78	114.10	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	C1D-CHD-C4C	-3.78	117.57	122.56
24	b	625	CLA	C3C-C4C-NC	3.78	114.81	110.57
24	b	623	CLA	C3C-C4C-NC	3.77	114.80	110.57
24	c	512	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	C	507	CLA	C1C-C2C-C3C	-3.76	103.00	106.96
24	A	407	CLA	C3C-C4C-NC	3.76	114.78	110.57
24	B	602	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	b	610	CLA	C3C-C4C-NC	3.75	114.78	110.57
24	A	405	CLA	O2D-CGD-CBD	3.75	117.93	111.27
24	c	505	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
24	c	517	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
24	c	506	CLA	C1D-CHD-C4C	-3.73	117.63	122.56
24	B	602	CLA	O2D-CGD-O1D	-3.73	116.54	123.84
24	C	505	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	515	CLA	C3C-C4C-NC	3.73	114.75	110.57
24	c	515	CLA	C3B-C4B-NB	3.72	114.03	109.21
24	b	611	CLA	CAA-C2A-C3A	-3.72	102.58	112.78
24	A	409	CLA	O2D-CGD-CBD	3.72	117.88	111.27
24	B	607	CLA	C1D-CHD-C4C	-3.72	117.65	122.56
31	d	406	PL9	C42-C43-C44	-3.72	118.71	127.66
24	B	608	CLA	CAA-C2A-C3A	-3.72	102.60	112.78
26	c	518	BCR	C7-C8-C9	-3.71	120.63	126.23
24	B	605	CLA	C1-C2-C3	-3.71	119.63	126.04
24	d	404	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
24	B	604	CLA	C1D-CHD-C4C	-3.70	117.67	122.56
27	a	405	SQD	O8-S-C6	3.70	111.64	105.74
24	b	620	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	b	612	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	c	506	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
24	c	508	CLA	C1D-CHD-C4C	-3.69	117.68	122.56
31	a	416	PL9	C15-C14-C16	3.69	121.48	115.27
24	a	412	CLA	C3C-C4C-NC	3.69	114.71	110.57
24	A	407	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	c	506	CLA	C3C-C4C-NC	3.69	114.70	110.57
24	a	410	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
24	C	502	CLA	C3C-C4C-NC	3.68	114.70	110.57
24	d	403	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	b	613	CLA	C1D-CHD-C4C	-3.67	117.71	122.56
24	d	403	CLA	O2D-CGD-CBD	3.67	117.79	111.27
24	c	512	CLA	C1D-CHD-C4C	-3.67	117.72	122.56
24	c	513	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
24	C	513	CLA	C1D-CHD-C4C	-3.67	117.72	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	SQD	C1-C2-C3	-3.67	102.36	110.00
24	D	403	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	B	611	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
24	C	503	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
24	B	609	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	A	405	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	b	622	CLA	C1-C2-C3	-3.64	119.75	126.04
24	C	502	CLA	CBC-CAC-C3C	-3.64	102.41	112.43
24	B	602	CLA	C1D-CHD-C4C	-3.64	117.76	122.56
26	y	101	BCR	C15-C14-C13	-3.63	122.13	127.31
24	C	509	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
24	c	513	CLA	C3B-C4B-NB	3.63	113.90	109.21
24	C	510	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
25	D	401	PHO	CMB-C2B-C1B	3.62	130.64	125.06
24	b	615	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	D	403	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
24	c	511	CLA	C1D-CHD-C4C	-3.62	117.79	122.56
24	B	602	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
24	b	612	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
24	b	621	CLA	C3B-C4B-NB	3.60	113.86	109.21
24	b	621	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
24	b	617	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
24	c	517	CLA	C1C-C2C-C3C	-3.59	103.19	106.96
24	C	503	CLA	C1D-CHD-C4C	-3.58	117.83	122.56
26	D	404	BCR	C38-C26-C25	-3.58	120.51	124.53
34	V	206	HTG	C1'-S1-C1	3.58	106.78	100.09
24	B	607	CLA	CMC-C2C-C1C	3.58	130.48	125.04
24	B	615	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
35	c	522	LMG	O7-C10-C11	3.57	119.20	111.50
24	a	412	CLA	C1-C2-C3	-3.57	119.86	126.04
24	C	513	CLA	C1-C2-C3	-3.57	119.86	126.04
24	A	405	CLA	C3B-C4B-NB	3.57	113.83	109.21
24	C	512	CLA	CAC-C3C-C4C	3.57	129.44	124.81
35	z	101	LMG	O7-C10-C11	3.57	119.19	111.50
24	D	402	CLA	C3B-C4B-NB	3.57	113.82	109.21
24	C	507	CLA	CBC-CAC-C3C	-3.57	102.60	112.43
36	C	518	DGD	O2G-C1B-C2B	3.56	119.18	111.50
24	b	619	CLA	CAC-C3C-C4C	3.56	129.43	124.81
24	C	511	CLA	C1D-CHD-C4C	-3.56	117.86	122.56
29	C	522	LMT	C1'-O5'-C5'	3.56	120.68	113.69
26	b	627	BCR	C29-C30-C25	3.56	115.96	110.48
24	c	505	CLA	CAC-C3C-C4C	3.56	129.43	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	405	SQD	O48-C23-C24	3.55	123.05	111.91
24	d	403	CLA	C3C-C4C-NC	3.55	114.55	110.57
24	b	620	CLA	C3B-C4B-NB	3.55	113.80	109.21
35	c	523	LMG	C3-C4-C5	3.55	116.57	110.24
31	a	416	PL9	C20-C19-C21	3.55	121.24	115.27
24	b	612	CLA	CMC-C2C-C1C	3.54	130.43	125.04
35	C	520	LMG	O7-C10-C11	3.54	119.13	111.50
24	b	614	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
24	c	511	CLA	CMC-C2C-C1C	3.54	130.43	125.04
24	B	616	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
26	t	101	BCR	C15-C14-C13	3.53	132.34	127.31
24	c	516	CLA	C1D-CHD-C4C	-3.52	117.91	122.56
24	A	407	CLA	C4-C3-C5	3.52	121.19	115.27
25	D	401	PHO	C1C-C2C-C3C	-3.52	102.47	106.51
25	d	401	PHO	C4-C3-C5	3.51	121.17	115.27
24	A	406	CLA	C3C-C4C-NC	3.51	114.50	110.57
26	C	516	BCR	C33-C5-C6	-3.51	120.59	124.53
24	B	616	CLA	CMC-C2C-C1C	3.51	130.38	125.04
24	c	516	CLA	C1-C2-C3	-3.51	119.98	126.04
24	C	514	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
27	a	414	SQD	O8-S-C6	3.50	111.32	105.74
24	d	403	CLA	CAC-C3C-C4C	3.50	129.35	124.81
24	d	404	CLA	C3B-C4B-NB	3.50	113.73	109.21
25	D	401	PHO	C2C-C1C-NC	3.50	115.07	109.79
35	c	523	LMG	O6-C5-C4	3.49	116.04	109.69
25	D	401	PHO	C4D-CHA-C1A	-3.49	117.51	125.37
24	b	624	CLA	O2D-CGD-CBD	3.49	117.47	111.27
24	C	505	CLA	C1D-CHD-C4C	-3.49	117.95	122.56
24	c	508	CLA	C4-C3-C5	3.49	121.14	115.27
24	B	612	CLA	CAC-C3C-C4C	3.49	129.34	124.81
24	C	509	CLA	C3B-C4B-NB	3.49	113.72	109.21
34	B	624	HTG	C1-O5-C5	3.49	119.01	112.58
29	a	404	LMT	O5'-C5'-C4'	3.48	117.09	109.75
24	B	606	CLA	CHD-C4C-NC	3.48	129.69	124.20
24	b	622	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	B	608	CLA	C3B-C4B-NB	3.47	113.70	109.21
24	b	615	CLA	CMC-C2C-C1C	3.47	130.33	125.04
24	c	511	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
24	C	506	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
24	C	513	CLA	C3B-C4B-NB	3.46	113.69	109.21
26	c	527	BCR	C11-C10-C9	-3.46	122.37	127.31
24	c	506	CLA	C3B-C4B-NB	3.46	113.68	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C7-C8-C9	-3.46	121.01	126.23
24	c	516	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
27	f	102	SQD	C1-O5-C5	3.46	120.48	113.69
24	c	507	CLA	CAC-C3C-C4C	3.46	129.29	124.81
24	b	619	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
24	b	618	CLA	C3B-C4B-NB	3.46	113.68	109.21
24	a	412	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
24	B	612	CLA	C3B-C4B-NB	3.45	113.68	109.21
36	h	102	DGD	O2G-C1B-C2B	3.45	118.94	111.50
24	B	615	CLA	CMC-C2C-C1C	3.45	130.30	125.04
34	B	623	HTG	C1'-S1-C1	3.45	106.54	100.09
26	c	527	BCR	C16-C17-C18	-3.45	122.39	127.31
34	b	608	HTG	C1'-S1-C1	3.45	106.54	100.09
24	b	614	CLA	C4-C3-C5	3.45	121.07	115.27
31	D	405	PL9	C40-C39-C41	3.45	121.07	115.27
24	C	510	CLA	C3B-C4B-NB	3.45	113.66	109.21
31	a	416	PL9	C7-C8-C9	-3.44	121.06	126.79
24	B	606	CLA	CMC-C2C-C1C	3.44	130.28	125.04
24	C	508	CLA	C1D-CHD-C4C	-3.44	118.01	122.56
24	d	403	CLA	C1-C2-C3	-3.44	120.09	126.04
24	c	515	CLA	C1C-C2C-C3C	-3.44	103.34	106.96
24	c	510	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
37	d	409	LHG	O7-C7-C8	3.44	118.91	111.50
24	C	514	CLA	C1D-CHD-C4C	-3.44	118.02	122.56
31	A	418	PL9	C20-C19-C21	3.44	121.05	115.27
24	D	402	CLA	C1-C2-C3	-3.44	120.10	126.04
26	b	627	BCR	C38-C26-C25	-3.43	120.67	124.53
24	C	505	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
26	t	101	BCR	C15-C16-C17	-3.43	116.45	123.47
35	b	629	LMG	O7-C10-C11	3.43	118.89	111.50
24	C	511	CLA	C4-C3-C5	3.43	121.04	115.27
26	C	516	BCR	C7-C8-C9	-3.43	121.06	126.23
24	B	617	CLA	C3B-C4B-NB	3.42	113.64	109.21
31	A	418	PL9	C37-C38-C39	-3.42	119.42	127.66
24	B	607	CLA	C3B-C4B-NB	3.42	113.63	109.21
24	B	610	CLA	CAC-C3C-C4C	3.42	129.25	124.81
24	c	507	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
24	B	613	CLA	C3B-C4B-NB	3.42	113.63	109.21
29	a	404	LMT	C1'-O5'-C5'	3.41	120.39	113.69
26	B	619	BCR	C28-C27-C26	-3.41	107.98	114.08
24	C	511	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	c	515	CLA	O2D-CGD-CBD	3.41	117.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	103	BCR	C33-C5-C6	-3.41	120.70	124.53
24	b	624	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
24	b	615	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
24	D	402	CLA	CMC-C2C-C1C	3.41	130.23	125.04
34	b	601	HTG	C1'-S1-C1	3.41	106.46	100.09
27	F	103	SQD	O6-C1-C2	3.40	113.61	108.30
24	D	403	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
24	B	604	CLA	CMC-C2C-C1C	3.40	130.22	125.04
31	D	405	PL9	C42-C43-C44	-3.40	119.47	127.66
24	d	403	CLA	CHC-C1C-C2C	-3.40	117.33	126.72
24	C	513	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
31	a	416	PL9	C17-C18-C19	-3.39	119.49	127.66
31	D	405	PL9	C7-C8-C9	-3.39	121.15	126.79
24	B	611	CLA	CAC-C3C-C4C	3.39	129.21	124.81
31	D	405	PL9	C10-C9-C11	3.39	120.97	115.27
24	c	515	CLA	CAC-C3C-C4C	3.39	129.21	124.81
24	a	409	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
24	c	508	CLA	C3B-C4B-NB	3.38	113.59	109.21
24	B	605	CLA	OBD-CAD-C3D	-3.38	122.36	127.98
24	B	602	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	B	613	CLA	CAC-C3C-C4C	3.38	129.20	124.81
24	B	614	CLA	OBD-CAD-C3D	-3.38	122.37	127.98
31	A	418	PL9	C32-C33-C34	-3.38	119.53	127.66
24	C	510	CLA	CAC-C3C-C4C	3.38	129.19	124.81
24	C	509	CLA	CMB-C2B-C3B	3.38	131.00	124.68
24	b	610	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
24	B	615	CLA	O2A-CGA-CBA	3.38	122.50	111.91
24	b	617	CLA	OBD-CAD-C3D	-3.37	122.38	127.98
24	A	409	CLA	CAC-C3C-C4C	3.37	129.18	124.81
24	D	402	CLA	C1D-CHD-C4C	-3.37	118.12	122.56
24	b	624	CLA	C3B-C4B-NB	3.36	113.56	109.21
24	c	509	CLA	C1D-CHD-C4C	-3.36	118.12	122.56
24	b	612	CLA	C3B-C4B-NB	3.36	113.55	109.21
24	B	607	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
35	c	522	LMG	O8-C28-C29	3.36	122.44	111.91
24	a	412	CLA	C3B-C4B-NB	3.35	113.54	109.21
25	D	401	PHO	CAC-C3C-C4C	3.35	128.88	125.22
37	d	408	LHG	O7-C7-C8	3.35	118.72	111.50
24	b	617	CLA	C1D-CHD-C4C	-3.35	118.14	122.56
24	B	611	CLA	O2A-CGA-CBA	3.34	122.40	111.91
24	c	510	CLA	C1-C2-C3	-3.34	120.26	126.04
24	c	514	CLA	C1D-CHD-C4C	-3.34	118.15	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	CLA	C1D-CHD-C4C	-3.34	118.15	122.56
24	A	406	CLA	CHC-C1C-C2C	-3.34	117.49	126.72
24	B	613	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
24	B	613	CLA	C4-C3-C5	3.33	120.88	115.27
24	B	609	CLA	C1D-CHD-C4C	-3.33	118.16	122.56
24	b	622	CLA	C4D-C3D-CAD	-3.33	106.61	108.47
24	b	614	CLA	CHD-C4C-NC	3.33	129.46	124.20
24	D	402	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
24	b	625	CLA	CHC-C1C-C2C	-3.33	117.51	126.72
24	c	508	CLA	CBC-CAC-C3C	-3.33	103.25	112.43
24	C	510	CLA	C1-O2A-CGA	3.33	125.18	116.44
24	C	506	CLA	CAC-C3C-C4C	3.33	129.13	124.81
24	B	611	CLA	C3B-C4B-NB	3.33	113.51	109.21
24	b	613	CLA	CMC-C2C-C1C	3.33	130.10	125.04
24	D	403	CLA	C1C-C2C-C3C	-3.32	103.46	106.96
24	b	622	CLA	CHC-C1C-C2C	-3.32	117.53	126.72
24	A	409	CLA	C1D-CHD-C4C	-3.32	118.17	122.56
24	B	604	CLA	O2A-CGA-O1A	-3.32	115.21	123.59
24	B	603	CLA	C1D-CHD-C4C	-3.32	118.18	122.56
25	A	408	PHO	C4-C3-C5	3.32	120.85	115.27
25	D	401	PHO	CHC-C1C-C2C	-3.32	117.39	125.73
24	B	610	CLA	C3B-C4B-NB	3.31	113.50	109.21
24	b	614	CLA	C2A-C1A-CHA	-3.31	118.06	123.86
24	b	611	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
24	A	407	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
26	b	627	BCR	C15-C14-C13	-3.31	122.58	127.31
24	C	508	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
26	B	618	BCR	C7-C8-C9	-3.31	121.24	126.23
24	C	504	CLA	C1C-C2C-C3C	-3.31	103.48	106.96
26	B	618	BCR	C24-C23-C22	-3.30	121.24	126.23
35	J	101	LMG	O7-C10-C11	3.30	118.62	111.50
24	D	403	CLA	C1D-CHD-C4C	-3.30	118.20	122.56
24	A	405	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
24	d	402	CLA	CBC-CAC-C3C	-3.30	103.33	112.43
35	a	415	LMG	C8-O7-C10	-3.30	109.67	117.79
26	C	515	BCR	C33-C5-C6	-3.29	120.83	124.53
24	B	614	CLA	O2D-CGD-CBD	3.29	117.12	111.27
24	B	613	CLA	C1-C2-C3	-3.29	120.35	126.04
31	d	406	PL9	C10-C9-C11	3.29	120.81	115.27
24	B	610	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
24	C	504	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
24	A	409	CLA	C4C-C3C-C2C	-3.28	102.11	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	625	CLA	CBC-CAC-C3C	-3.28	103.38	112.43
24	C	505	CLA	CMC-C2C-C1C	3.28	130.04	125.04
24	c	510	CLA	CBC-CAC-C3C	-3.28	103.39	112.43
24	C	509	CLA	C1D-CHD-C4C	-3.28	118.23	122.56
31	d	406	PL9	C40-C39-C41	3.27	120.77	115.27
24	C	507	CLA	C3B-C4B-NB	3.27	113.44	109.21
24	B	614	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
24	b	617	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
24	b	623	CLA	C3B-C4B-NB	3.26	113.43	109.21
24	A	406	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
24	B	613	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
35	M	101	LMG	O7-C10-C11	3.26	118.53	111.50
24	B	617	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
24	C	514	CLA	C1-C2-C3	-3.26	120.41	126.04
27	F	103	SQD	O7-S-C6	3.25	110.81	106.94
37	l	101	LHG	O7-C7-C8	3.25	118.51	111.50
38	V	205	HEM	CAD-CBD-CGD	3.25	118.13	112.67
24	C	506	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
31	A	418	PL9	C7-C3-C4	3.25	119.52	116.88
24	B	605	CLA	CAC-C3C-C4C	3.25	129.03	124.81
26	d	405	BCR	C7-C8-C9	-3.25	121.33	126.23
24	B	603	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	c	509	CLA	O2D-CGD-O1D	-3.24	117.51	123.84
24	b	616	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	b	615	CLA	CAC-C3C-C4C	3.24	129.01	124.81
24	C	507	CLA	C1D-CHD-C4C	-3.24	118.29	122.56
24	C	503	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
24	b	620	CLA	CHC-C1C-C2C	-3.24	117.77	126.72
24	c	509	CLA	CAC-C3C-C4C	3.23	129.01	124.81
24	B	606	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
26	B	619	BCR	C29-C30-C25	3.23	115.46	110.48
27	f	102	SQD	O5-C5-C4	3.23	115.56	109.69
24	b	615	CLA	CMB-C2B-C3B	3.23	130.72	124.68
26	y	101	BCR	C16-C17-C18	-3.23	122.70	127.31
24	d	404	CLA	C1D-CHD-C4C	-3.23	118.30	122.56
24	c	509	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
24	B	611	CLA	CHC-C1C-C2C	-3.22	117.81	126.72
24	b	621	CLA	C1C-C2C-C3C	-3.22	103.57	106.96
24	b	611	CLA	C1D-CHD-C4C	-3.22	118.31	122.56
24	b	610	CLA	CHD-C4C-NC	3.22	129.27	124.20
24	b	621	CLA	O2A-CGA-CBA	3.21	122.00	111.91
24	B	605	CLA	CHC-C1C-C2C	-3.21	117.84	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CHC-C1C-C2C	-3.21	117.84	126.72
24	c	516	CLA	CHD-C4C-NC	3.21	129.26	124.20
24	b	621	CLA	C1-C2-C3	-3.21	120.50	126.04
24	B	616	CLA	C3B-C4B-NB	3.21	113.36	109.21
24	C	512	CLA	CHC-C1C-C2C	-3.21	117.85	126.72
24	b	610	CLA	C3B-C4B-NB	3.20	113.35	109.21
24	C	513	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
24	B	611	CLA	CMA-C3A-C4A	-3.20	103.17	111.77
25	D	401	PHO	CBD-CHA-C1A	3.20	133.83	126.40
24	A	409	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
24	c	507	CLA	C1-C2-C3	-3.20	120.51	126.04
24	b	621	CLA	C4-C3-C5	3.20	120.65	115.27
26	k	101	BCR	C20-C21-C22	-3.20	122.75	127.31
24	A	409	CLA	C1-C2-C3	-3.19	120.52	126.04
24	c	506	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
24	B	616	CLA	CHD-C4C-NC	3.19	129.23	124.20
24	B	613	CLA	CMB-C2B-C3B	3.19	130.64	124.68
26	b	628	BCR	C38-C26-C25	-3.19	120.95	124.53
25	d	401	PHO	C4A-NA-C1A	-3.18	105.57	108.14
26	b	626	BCR	C15-C14-C13	-3.18	122.77	127.31
26	d	405	BCR	C33-C5-C6	-3.18	120.95	124.53
24	b	619	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
26	B	619	BCR	C2-C1-C6	3.18	115.38	110.48
24	C	510	CLA	C1D-CHD-C4C	-3.18	118.36	122.56
37	D	408	LHG	O7-C7-C8	3.18	118.35	111.50
24	b	616	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
24	A	406	CLA	CHD-C4C-NC	3.18	129.21	124.20
24	C	503	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	A	407	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
24	B	617	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
24	b	618	CLA	C1D-CHD-C4C	-3.17	118.37	122.56
24	A	405	CLA	O2A-CGA-CBA	3.17	121.85	111.91
31	a	416	PL9	C10-C9-C11	3.17	120.60	115.27
24	b	624	CLA	CHD-C4C-NC	3.17	129.19	124.20
24	b	624	CLA	C4-C3-C5	3.17	120.60	115.27
24	a	412	CLA	CHD-C4C-NC	3.17	129.19	124.20
31	A	418	PL9	C53-C6-C1	3.16	121.45	114.99
24	B	615	CLA	C3B-C4B-NB	3.16	113.30	109.21
24	b	620	CLA	C1D-CHD-C4C	-3.16	118.39	122.56
24	a	409	CLA	CMB-C2B-C3B	3.16	130.59	124.68
24	c	505	CLA	CHC-C1C-C2C	-3.16	117.98	126.72
38	e	103	HEM	CBD-CAD-C3D	-3.15	106.67	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	411	SQD	O8-S-C6	3.15	110.76	105.74
24	B	611	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	c	516	CLA	CMC-C2C-C1C	3.15	129.84	125.04
24	b	611	CLA	C3B-C4B-NB	3.15	113.28	109.21
24	C	503	CLA	O2A-CGA-O1A	-3.15	115.65	123.59
24	C	507	CLA	CAC-C3C-C4C	3.15	128.89	124.81
25	d	401	PHO	CHD-C1D-C2D	-3.15	117.82	125.73
24	b	624	CLA	C4C-C3C-C2C	-3.15	102.31	106.90
24	d	402	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
24	b	625	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
24	b	613	CLA	CHC-C1C-C2C	-3.14	118.03	126.72
31	a	416	PL9	C42-C43-C44	-3.14	120.09	127.66
25	A	408	PHO	CHC-C1C-C2C	-3.14	117.82	125.73
37	l	101	LHG	O8-C23-C24	3.14	121.77	111.91
24	b	625	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
24	C	506	CLA	C3B-C4B-NB	3.14	113.27	109.21
24	B	602	CLA	O2A-CGA-CBA	3.13	121.74	111.91
31	a	416	PL9	C27-C28-C29	-3.13	120.11	127.66
24	C	510	CLA	CMB-C2B-C3B	3.13	130.54	124.68
34	C	524	HTG	O5-C5-C4	3.13	115.38	109.69
31	A	418	PL9	C45-C44-C46	3.13	120.53	115.27
24	C	510	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
24	b	618	CLA	CBC-CAC-C3C	-3.12	103.82	112.43
24	b	617	CLA	C3B-C4B-NB	3.12	113.25	109.21
24	B	616	CLA	O2D-CGD-CBD	3.12	116.82	111.27
24	B	602	CLA	CHD-C4C-NC	3.12	129.12	124.20
24	B	610	CLA	C1D-CHD-C4C	-3.12	118.44	122.56
24	B	615	CLA	C4-C3-C5	3.12	120.52	115.27
24	B	608	CLA	C1-C2-C3	-3.12	120.65	126.04
24	D	403	CLA	C4-C3-C5	3.12	120.52	115.27
24	D	403	CLA	CHC-C1C-C2C	-3.12	118.10	126.72
24	b	610	CLA	C4-C3-C5	3.12	120.51	115.27
24	C	513	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
24	b	614	CLA	C4C-C3C-C2C	-3.11	102.37	106.90
26	D	404	BCR	C29-C30-C25	3.11	115.27	110.48
24	C	514	CLA	CAC-C3C-C4C	3.11	128.84	124.81
24	a	412	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
24	d	403	CLA	C2A-C1A-CHA	-3.11	118.43	123.86
35	Z	101	LMG	O6-C5-C4	3.11	115.33	109.69
26	h	101	BCR	C16-C17-C18	-3.11	122.88	127.31
24	A	409	CLA	C4-C3-C5	3.10	120.49	115.27
26	c	518	BCR	C33-C5-C6	-3.10	121.05	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
37	D	407	LHG	O8-C23-C24	3.10	121.63	111.91
24	a	410	CLA	CMC-C2C-C1C	3.09	129.75	125.04
26	T	103	BCR	C34-C9-C10	-3.09	118.59	122.92
24	B	604	CLA	O2A-CGA-CBA	3.09	121.61	111.91
24	B	606	CLA	C4-C3-C5	3.09	120.47	115.27
24	b	625	CLA	O2A-CGA-CBA	3.09	121.61	111.91
26	h	101	BCR	C38-C26-C25	-3.09	121.06	124.53
24	b	613	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
24	C	514	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
24	A	407	CLA	C2A-C1A-CHA	-3.09	118.46	123.86
24	B	606	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
24	C	511	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
31	A	418	PL9	C8-C7-C3	3.09	120.70	111.98
24	b	618	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
24	c	514	CLA	CHC-C1C-C2C	-3.08	118.19	126.72
24	C	503	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
24	b	620	CLA	CBC-CAC-C3C	-3.08	103.94	112.43
24	d	404	CLA	CAC-C3C-C4C	3.08	128.81	124.81
24	c	511	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
24	d	403	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	B	609	CLA	CHC-C1C-C2C	-3.08	118.21	126.72
26	B	620	BCR	C32-C1-C6	-3.08	105.31	110.30
24	c	506	CLA	CAC-C3C-C4C	3.08	128.80	124.81
27	F	103	SQD	C3-C4-C5	3.08	115.73	110.24
24	d	402	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	B	608	CLA	C1D-CHD-C4C	-3.07	118.50	122.56
24	c	510	CLA	CHC-C1C-C2C	-3.07	118.22	126.72
24	d	402	CLA	CHD-C4C-NC	3.07	129.04	124.20
24	C	509	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	d	402	CLA	CHC-C1C-C2C	-3.07	118.24	126.72
24	c	505	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
24	b	621	CLA	O2A-CGA-O1A	-3.06	115.86	123.59
24	B	615	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
36	H	102	DGD	O2G-C1B-C2B	3.06	118.10	111.50
29	T	104	LMT	C1'-O5'-C5'	3.06	119.70	113.69
24	B	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	d	401	PHO	CHC-C1C-C2C	-3.06	118.04	125.73
24	d	404	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	B	603	CLA	CHD-C4C-NC	3.06	129.02	124.20
24	B	603	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	C	507	CLA	C4-C3-C5	3.06	120.41	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	C4-C3-C5	3.06	120.41	115.27
24	C	507	CLA	C1-C2-C3	-3.06	120.76	126.04
24	b	611	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
35	j	101	LMG	O7-C10-C11	3.05	118.08	111.50
24	D	402	CLA	C4D-C3D-CAD	-3.05	106.77	108.47
27	L	102	SQD	O8-S-C6	3.05	110.60	105.74
31	D	405	PL9	C36-C37-C38	-3.05	101.87	111.88
24	a	410	CLA	CHD-C4C-NC	3.05	129.00	124.20
24	A	409	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
24	a	409	CLA	C3B-C4B-NB	3.04	113.15	109.21
31	D	405	PL9	C53-C6-C1	3.04	121.21	114.99
24	B	613	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
24	a	409	CLA	O2D-CGD-CBD	3.04	116.67	111.27
25	d	401	PHO	C4D-CHA-C1A	-3.04	118.53	125.37
24	a	412	CLA	CBC-CAC-C3C	-3.04	104.05	112.43
24	c	517	CLA	CMC-C2C-C1C	3.04	129.66	125.04
26	K	101	BCR	C33-C5-C6	-3.04	121.12	124.53
24	B	609	CLA	CMC-C2C-C1C	3.03	129.66	125.04
24	A	405	CLA	CMB-C2B-C3B	3.03	130.35	124.68
24	a	409	CLA	C2A-C1A-CHA	-3.03	118.56	123.86
26	c	527	BCR	C33-C5-C6	-3.03	121.12	124.53
24	c	514	CLA	CBC-CAC-C3C	-3.03	104.08	112.43
24	C	508	CLA	CHD-C4C-NC	3.03	128.98	124.20
24	c	515	CLA	C4-C3-C5	3.03	120.37	115.27
24	B	610	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
26	Y	101	BCR	C15-C14-C13	-3.03	122.99	127.31
24	b	621	CLA	CAC-C3C-C4C	3.03	128.74	124.81
25	a	411	PHO	C2B-C1B-NB	3.02	114.35	109.79
24	B	610	CLA	CHC-C1C-C2C	-3.02	118.36	126.72
24	B	606	CLA	C2A-C1A-CHA	-3.02	118.58	123.86
24	c	511	CLA	C4-C3-C5	3.02	120.35	115.27
24	b	616	CLA	C1D-CHD-C4C	-3.02	118.57	122.56
31	A	418	PL9	C22-C23-C24	-3.02	120.39	127.66
36	D	406	DGD	O1G-C1A-C2A	3.02	121.37	111.91
37	d	407	LHG	O8-C23-O10	-3.01	115.98	123.59
24	b	622	CLA	CED-O2D-CGD	3.01	122.75	115.94
24	b	624	CLA	CAC-C3C-C4C	3.01	128.72	124.81
24	B	616	CLA	CBC-CAC-C3C	-3.01	104.14	112.43
24	C	510	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
24	C	513	CLA	CHD-C4C-NC	3.01	128.94	124.20
34	b	608	HTG	C1-O5-C5	3.01	118.13	112.58
24	b	623	CLA	CHD-C4C-NC	3.01	128.94	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
35	C	520	LMG	O8-C28-C29	3.00	121.33	111.91
24	c	515	CLA	CMC-C2C-C1C	3.00	129.61	125.04
24	C	508	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
24	c	512	CLA	CHC-C1C-C2C	-3.00	118.43	126.72
24	D	402	CLA	O2A-CGA-CBA	3.00	121.32	111.91
24	b	623	CLA	CBC-CAC-C3C	-3.00	104.17	112.43
24	c	515	CLA	CHD-C4C-NC	3.00	128.92	124.20
24	A	406	CLA	CMB-C2B-C3B	2.99	130.28	124.68
24	b	611	CLA	CHC-C1C-C2C	-2.99	118.44	126.72
27	F	103	SQD	O5-C5-C4	2.99	115.13	109.69
24	C	507	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	B	608	CLA	CHC-C1C-C2C	-2.99	118.45	126.72
24	c	507	CLA	CMC-C2C-C1C	2.99	129.59	125.04
24	a	410	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
24	b	614	CLA	C3B-C4B-NB	2.99	113.07	109.21
24	C	509	CLA	CHC-C1C-C2C	-2.99	118.46	126.72
24	B	603	CLA	CHC-C1C-C2C	-2.98	118.47	126.72
24	A	409	CLA	C3B-C4B-NB	2.98	113.07	109.21
26	D	404	BCR	C28-C27-C26	-2.98	108.75	114.08
25	d	401	PHO	C2A-C1A-NA	2.98	115.28	111.86
24	b	625	CLA	C1C-C2C-C3C	-2.98	103.82	106.96
24	b	619	CLA	C4-C3-C5	2.98	120.28	115.27
24	b	622	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
24	B	607	CLA	C1-C2-C3	-2.98	120.90	126.04
25	a	411	PHO	O1D-CGD-CBD	-2.97	118.40	124.48
24	C	514	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	C	504	CLA	O2A-CGA-CBA	2.97	121.23	111.91
36	C	519	DGD	O2G-C1B-C2B	2.97	117.90	111.50
24	C	505	CLA	CAC-C3C-C4C	2.97	128.66	124.81
24	b	613	CLA	C1-C2-C3	-2.97	120.91	126.04
26	B	619	BCR	C37-C22-C21	-2.97	118.77	122.92
24	B	617	CLA	CHD-C4C-NC	2.96	128.88	124.20
24	B	610	CLA	CHD-C4C-NC	2.96	128.87	124.20
24	a	412	CLA	C4-C3-C5	2.96	120.25	115.27
31	a	416	PL9	C35-C34-C36	2.96	120.25	115.27
24	B	610	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
24	b	612	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	B	617	CLA	CAC-C3C-C4C	2.95	128.64	124.81
24	A	405	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
24	C	503	CLA	C4D-C3D-CAD	-2.95	106.82	108.47
24	c	513	CLA	C4C-C3C-C2C	-2.95	102.59	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	101	LHG	O8-C23-C24	2.95	121.17	111.91
26	B	620	BCR	C38-C26-C25	-2.95	121.22	124.53
24	b	610	CLA	CHC-C1C-C2C	-2.95	118.56	126.72
24	c	515	CLA	C1-C2-C3	-2.95	120.94	126.04
26	C	516	BCR	C24-C23-C22	-2.95	121.78	126.23
24	c	517	CLA	C1-C2-C3	-2.95	120.95	126.04
27	a	414	SQD	O9-S-C6	2.95	110.44	106.94
24	c	515	CLA	CHC-C1C-C2C	-2.95	118.57	126.72
25	D	401	PHO	C2A-C1A-NA	2.95	115.24	111.86
24	d	403	CLA	O2A-CGA-CBA	2.94	121.15	111.91
37	D	409	LHG	O8-C23-C24	2.94	121.15	111.91
24	A	405	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
24	c	506	CLA	CHC-C1C-C2C	-2.94	118.58	126.72
24	C	511	CLA	CAC-C3C-C4C	2.94	128.63	124.81
24	b	617	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
25	d	401	PHO	C3C-C4C-NC	2.94	114.84	110.28
24	d	402	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
25	D	401	PHO	C4-C3-C5	2.94	120.21	115.27
24	b	610	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
24	b	618	CLA	CHD-C4C-NC	2.94	128.83	124.20
24	c	512	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
24	b	619	CLA	C3B-C4B-NB	2.93	113.00	109.21
27	F	103	SQD	O48-C23-C24	2.93	121.11	111.91
31	a	416	PL9	C37-C38-C39	-2.93	120.60	127.66
35	j	101	LMG	O6-C5-C4	2.93	115.01	109.69
24	C	503	CLA	O2A-CGA-CBA	2.93	121.09	111.91
24	b	619	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
24	a	410	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
24	B	611	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
24	D	402	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
24	A	405	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
27	A	415	SQD	O48-C23-O10	-2.92	116.22	123.59
24	A	406	CLA	C4-C3-C5	2.92	120.18	115.27
37	L	101	LHG	C5-O7-C7	-2.92	110.61	117.79
24	b	624	CLA	CHC-C1C-C2C	-2.92	118.65	126.72
24	B	605	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
36	H	102	DGD	C3G-O3G-C1D	-2.92	108.04	113.74
24	d	404	CLA	CAA-C2A-C3A	-2.92	104.79	112.78
25	D	401	PHO	C4C-C3C-C2C	-2.92	103.56	106.78
24	B	606	CLA	C3B-C4B-NB	2.91	112.98	109.21
24	c	512	CLA	C1-C2-C3	-2.91	121.00	126.04
25	d	401	PHO	CAC-C3C-C4C	2.91	128.40	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	CMC-C2C-C1C	2.91	129.48	125.04
24	C	511	CLA	CHC-C1C-C2C	-2.91	118.67	126.72
24	B	603	CLA	C1-C2-C3	-2.91	121.01	126.04
31	A	418	PL9	C27-C28-C29	-2.91	120.65	127.66
24	c	512	CLA	CAC-C3C-C4C	2.91	128.59	124.81
25	d	401	PHO	C2B-C1B-NB	2.91	114.18	109.79
24	a	409	CLA	CHC-C1C-C2C	-2.91	118.68	126.72
24	B	607	CLA	CAC-C3C-C4C	2.91	128.58	124.81
24	C	502	CLA	CHD-C4C-NC	2.91	128.78	124.20
24	C	503	CLA	CAC-C3C-C4C	2.90	128.58	124.81
24	c	507	CLA	C4-C3-C5	2.90	120.16	115.27
24	c	509	CLA	CMC-C2C-C1C	2.90	129.46	125.04
24	a	410	CLA	C3B-C4B-NB	2.90	112.95	109.21
24	c	514	CLA	O2A-CGA-CBA	2.90	121.00	111.91
36	C	518	DGD	O1G-C1A-C2A	2.89	120.99	111.91
24	B	610	CLA	CBC-CAC-C3C	-2.89	104.45	112.43
24	d	404	CLA	CHC-C1C-C2C	-2.89	118.72	126.72
35	c	522	LMG	C8-O7-C10	-2.89	110.67	117.79
24	B	607	CLA	CHC-C1C-C2C	-2.89	118.73	126.72
24	C	505	CLA	C4-C3-C5	2.89	120.13	115.27
24	B	617	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
24	c	508	CLA	CHC-C1C-C2C	-2.89	118.74	126.72
24	b	611	CLA	C4-C3-C5	2.88	120.12	115.27
24	b	612	CLA	CAC-C3C-C4C	2.88	128.55	124.81
24	b	623	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
24	C	504	CLA	CHD-C4C-NC	2.88	128.75	124.20
24	C	503	CLA	CHD-C4C-NC	2.88	128.75	124.20
24	c	512	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
24	B	611	CLA	C1D-CHD-C4C	-2.88	118.76	122.56
24	b	622	CLA	O2D-CGD-CBD	2.88	116.38	111.27
24	B	614	CLA	C1D-CHD-C4C	-2.88	118.76	122.56
24	a	412	CLA	CHC-C1C-C2C	-2.88	118.76	126.72
24	c	513	CLA	CHD-C4C-NC	2.88	128.74	124.20
25	a	411	PHO	CHC-C1C-C2C	-2.88	118.49	125.73
24	c	510	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	b	623	CLA	O2A-CGA-CBA	2.88	120.93	111.91
24	b	612	CLA	CMA-C3A-C2A	-2.88	102.23	113.83
24	b	615	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
24	C	513	CLA	CHC-C1C-C2C	-2.87	118.77	126.72
24	a	409	CLA	CAA-C2A-C1A	-2.87	102.56	111.97
31	D	405	PL9	C32-C33-C34	-2.87	120.74	127.66
24	b	623	CLA	CMC-C2C-C1C	2.87	129.41	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	CBC-CAC-C3C	-2.87	104.52	112.43
24	c	517	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
24	b	615	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
24	D	402	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	b	625	CLA	CHD-C4C-NC	2.87	128.72	124.20
24	B	602	CLA	CHC-C1C-C2C	-2.87	118.79	126.72
36	h	102	DGD	O1G-C1A-C2A	2.86	120.89	111.91
24	B	610	CLA	CMC-C2C-C1C	2.86	129.40	125.04
24	A	409	CLA	CED-O2D-CGD	2.86	122.41	115.94
24	c	510	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
24	c	516	CLA	C4-C3-C5	2.86	120.08	115.27
24	B	612	CLA	CHD-C4C-NC	2.86	128.71	124.20
24	c	517	CLA	CHD-C4C-NC	2.86	128.71	124.20
26	y	101	BCR	C24-C23-C22	-2.86	121.92	126.23
24	B	616	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
24	B	612	CLA	CHC-C1C-C2C	-2.86	118.82	126.72
24	C	512	CLA	C4C-C3C-C2C	-2.86	102.74	106.90
24	C	506	CLA	CHC-C1C-C2C	-2.85	118.83	126.72
24	C	511	CLA	CHD-C4C-NC	2.85	128.70	124.20
24	c	506	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	a	409	CLA	CAC-C3C-C4C	2.85	128.51	124.81
24	B	617	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
26	h	101	BCR	C11-C10-C9	-2.85	123.24	127.31
31	D	405	PL9	C15-C14-C16	2.85	120.06	115.27
31	A	418	PL9	C7-C8-C9	-2.85	122.05	126.79
24	b	621	CLA	CED-O2D-CGD	2.85	122.38	115.94
24	B	617	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
24	c	513	CLA	CHC-C1C-C2C	-2.85	118.84	126.72
24	c	516	CLA	C3B-C4B-NB	2.85	112.89	109.21
24	C	510	CLA	CHC-C1C-C2C	-2.85	118.85	126.72
31	a	416	PL9	C53-C6-C1	2.85	120.81	114.99
27	F	103	SQD	C44-O6-C1	-2.85	108.18	113.74
24	b	619	CLA	CAA-C2A-C3A	-2.84	104.99	112.78
24	B	605	CLA	C4-C3-C5	2.84	120.05	115.27
24	b	621	CLA	CHC-C1C-C2C	-2.84	118.86	126.72
34	b	608	HTG	O5-C1-C2	2.84	113.89	110.31
25	a	411	PHO	CMB-C2B-C1B	2.84	129.44	125.06
24	A	407	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	B	612	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	C	506	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	c	527	BCR	C15-C14-C13	-2.84	123.26	127.31
26	d	405	BCR	C28-C27-C26	-2.84	109.00	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	CHC-C1C-C2C	-2.84	118.87	126.72
24	a	410	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
24	c	513	CLA	O2A-CGA-CBA	2.84	120.81	111.91
24	B	614	CLA	CHC-C1C-C2C	-2.84	118.88	126.72
24	C	502	CLA	CAC-C3C-C4C	2.84	128.49	124.81
24	c	505	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
24	c	506	CLA	CHD-C4C-NC	2.83	128.67	124.20
24	c	512	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
24	B	607	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
24	B	615	CLA	OBD-CAD-C3D	-2.83	123.28	127.98
24	a	410	CLA	CAA-C2A-C3A	-2.83	105.03	112.78
24	B	602	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
24	b	613	CLA	CAC-C3C-C4C	2.83	128.48	124.81
24	b	625	CLA	C4D-C3D-CAD	-2.83	106.89	108.47
24	c	513	CLA	CMC-C2C-C1C	2.83	129.34	125.04
26	T	103	BCR	C35-C13-C12	2.82	122.53	118.08
29	M	104	LMT	O5'-C5'-C4'	2.82	115.70	109.75
24	b	613	CLA	O2A-CGA-CBA	2.82	120.77	111.91
24	D	403	CLA	C2A-C1A-CHA	-2.82	118.92	123.86
31	A	418	PL9	C12-C13-C14	-2.82	120.87	127.66
37	D	407	LHG	C5-O7-C7	-2.82	110.85	117.79
37	d	407	LHG	O8-C23-C24	2.82	120.75	111.91
24	B	615	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
24	b	623	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
24	C	502	CLA	C1-O2A-CGA	2.82	123.83	116.44
24	c	506	CLA	O2A-CGA-CBA	2.82	120.75	111.91
25	d	401	PHO	C4D-ND-C1D	-2.82	101.70	106.76
24	C	505	CLA	CHC-C1C-C2C	-2.82	118.93	126.72
24	d	404	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
24	B	605	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	c	514	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
24	d	403	CLA	C4-C3-C5	2.81	120.00	115.27
31	D	405	PL9	C12-C13-C14	-2.81	120.89	127.66
24	B	608	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
36	H	102	DGD	O1G-C1A-C2A	2.81	120.72	111.91
24	c	507	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
36	c	519	DGD	O6D-C5D-C6D	2.81	112.33	106.67
24	C	509	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	b	615	CLA	CHD-C4C-NC	2.80	128.62	124.20
35	b	629	LMG	O8-C28-C29	2.80	120.71	111.91
35	M	101	LMG	O8-C28-C29	2.80	120.71	111.91
24	b	613	CLA	C4C-C3C-C2C	-2.80	102.81	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	c	505	CLA	OBD-CAD-C3D	-2.80	123.33	127.98
31	D	405	PL9	C7-C3-C4	2.80	119.15	116.88
25	A	408	PHO	C2B-C1B-NB	2.80	114.02	109.79
24	C	507	CLA	C4D-C3D-CAD	-2.80	106.91	108.47
24	B	603	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	c	517	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
26	c	518	BCR	C15-C14-C13	-2.80	123.32	127.31
24	c	517	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
24	c	505	CLA	C1D-CHD-C4C	-2.80	118.87	122.56
24	c	506	CLA	C1-C2-C3	-2.80	121.20	126.04
24	C	507	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
24	A	405	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
24	A	406	CLA	C4D-C3D-CAD	-2.79	106.91	108.47
25	a	411	PHO	CAC-C3C-C4C	2.79	128.27	125.22
24	b	616	CLA	CMC-C2C-C1C	2.79	129.29	125.04
24	A	407	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	C	512	CLA	CHD-C4C-NC	2.79	128.60	124.20
24	c	515	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	c	516	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
24	b	615	CLA	O2A-CGA-CBA	2.79	120.67	111.91
24	B	615	CLA	C1D-CHD-C4C	-2.79	118.88	122.56
24	C	512	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
24	c	516	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
35	z	101	LMG	O8-C28-C29	2.79	120.66	111.91
26	d	405	BCR	C29-C30-C25	2.79	114.77	110.48
24	b	612	CLA	O2A-CGA-CBA	2.79	120.65	111.91
29	f	103	LMT	C1B-O5B-C5B	2.79	119.16	113.69
24	b	612	CLA	CHD-C4C-NC	2.78	128.59	124.20
24	b	618	CLA	C4-C3-C5	2.78	119.95	115.27
26	c	518	BCR	C3-C4-C5	-2.78	109.11	114.08
24	C	502	CLA	C3B-C4B-NB	2.78	112.81	109.21
24	B	607	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	c	516	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	B	604	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
24	c	508	CLA	C1-C2-C3	-2.78	121.24	126.04
26	b	628	BCR	C24-C23-C22	-2.77	122.05	126.23
25	a	411	PHO	C2C-C1C-NC	2.77	113.97	109.79
26	b	627	BCR	C33-C5-C6	-2.77	121.42	124.53
24	B	607	CLA	CHD-C4C-NC	2.77	128.56	124.20
24	c	509	CLA	CHC-C1C-C2C	-2.77	119.07	126.72
24	C	512	CLA	CMC-C2C-C1C	2.77	129.25	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
24	B	603	CLA	CAA-C2A-C3A	-2.77	105.21	112.78
26	A	410	BCR	C38-C26-C25	-2.76	121.42	124.53
24	c	511	CLA	C1-C2-C3	-2.76	121.26	126.04
24	B	609	CLA	CBC-CAC-C3C	-2.76	104.81	112.43
24	B	617	CLA	C1-O2A-CGA	2.76	123.69	116.44
24	b	617	CLA	O2A-CGA-CBA	2.76	120.57	111.91
31	d	406	PL9	C20-C19-C21	2.76	119.92	115.27
24	D	402	CLA	CHC-C1C-C2C	-2.76	119.08	126.72
24	C	509	CLA	CAC-C3C-C4C	2.76	128.39	124.81
24	a	409	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
37	D	407	LHG	O8-C23-O10	-2.76	116.63	123.59
24	c	510	CLA	C4-C3-C5	2.76	119.91	115.27
26	k	101	BCR	C7-C8-C9	-2.76	122.07	126.23
36	C	519	DGD	O1G-C1A-C2A	2.75	120.55	111.91
25	A	408	PHO	C3C-C4C-NC	2.75	114.55	110.28
24	b	622	CLA	C1D-CHD-C4C	-2.75	118.93	122.56
24	C	510	CLA	O2A-CGA-CBA	2.75	120.54	111.91
24	b	621	CLA	CHD-C4C-NC	2.75	128.54	124.20
26	h	101	BCR	C10-C11-C12	-2.75	114.64	123.22
24	b	614	CLA	OBD-CAD-C3D	-2.75	123.42	127.98
26	y	101	BCR	C38-C26-C25	-2.75	121.44	124.53
37	L	101	LHG	O8-C23-C24	2.75	120.53	111.91
24	c	513	CLA	CAC-C3C-C4C	2.75	128.37	124.81
26	d	405	BCR	C3-C4-C5	-2.74	109.18	114.08
34	b	632	HTG	C1-O5-C5	2.74	117.64	112.58
24	B	609	CLA	CHD-C4C-NC	2.74	128.52	124.20
24	b	612	CLA	CMB-C2B-C3B	2.74	129.81	124.68
31	a	416	PL9	C40-C39-C41	2.74	119.88	115.27
24	B	611	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	b	616	CLA	CHD-C4C-NC	2.74	128.52	124.20
24	C	506	CLA	C4-C3-C5	2.74	119.88	115.27
24	B	603	CLA	CMA-C3A-C4A	-2.74	104.42	111.77
36	h	102	DGD	O1G-C1A-O1A	-2.74	116.68	123.59
37	d	407	LHG	O7-C7-C8	2.74	117.40	111.50
27	A	411	SQD	O9-S-C6	2.74	110.19	106.94
26	K	101	BCR	C24-C23-C22	-2.74	122.10	126.23
24	C	514	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
27	L	102	SQD	O48-C23-C24	2.73	120.48	111.91
24	B	604	CLA	C3B-C4B-NB	2.73	112.74	109.21
24	b	618	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
24	C	505	CLA	CHD-C4C-NC	2.73	128.50	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	CMB-C2B-C3B	2.73	129.78	124.68
24	B	605	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
24	c	512	CLA	CMC-C2C-C1C	2.73	129.19	125.04
24	b	619	CLA	CHC-C1C-C2C	-2.72	119.19	126.72
24	c	508	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	c	517	CLA	C4-C3-C5	2.72	119.85	115.27
24	c	517	CLA	O2A-CGA-CBA	2.72	120.45	111.91
24	d	403	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
24	B	610	CLA	C4D-C3D-CAD	-2.72	106.95	108.47
24	a	409	CLA	O2A-CGA-O1A	-2.72	116.73	123.59
24	B	613	CLA	C1D-CHD-C4C	-2.72	118.97	122.56
24	A	407	CLA	CMC-C2C-C1C	2.72	129.18	125.04
24	c	514	CLA	CHD-C4C-NC	2.72	128.49	124.20
24	C	508	CLA	O2A-CGA-CBA	2.72	120.44	111.91
24	B	609	CLA	O2A-CGA-CBA	2.72	120.43	111.91
24	C	509	CLA	OBD-CAD-C3D	-2.72	123.47	127.98
31	a	416	PL9	C25-C24-C26	2.71	119.84	115.27
26	Y	101	BCR	C37-C22-C23	2.71	122.35	118.08
24	d	404	CLA	CMC-C2C-C1C	2.71	129.17	125.04
26	B	620	BCR	C10-C11-C12	-2.71	114.75	123.22
24	b	623	CLA	CMB-C2B-C3B	2.71	129.75	124.68
24	C	507	CLA	CHD-C4C-NC	2.71	128.47	124.20
24	B	613	CLA	O2A-CGA-CBA	2.71	120.41	111.91
24	a	409	CLA	O2A-CGA-CBA	2.71	120.41	111.91
25	a	411	PHO	C2A-C1A-NA	2.71	114.97	111.86
24	C	502	CLA	C4-C3-C5	2.71	119.83	115.27
24	c	511	CLA	C3B-C4B-NB	2.71	112.71	109.21
24	b	619	CLA	O2A-CGA-CBA	2.71	120.40	111.91
24	B	604	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	A	407	CLA	C1-C2-C3	-2.71	121.36	126.04
37	e	102	LHG	O7-C7-C8	2.70	117.33	111.50
27	A	415	SQD	O8-S-C6	2.70	110.05	105.74
24	b	616	CLA	CED-O2D-CGD	2.70	122.05	115.94
24	B	606	CLA	O2A-CGA-CBA	2.70	120.38	111.91
24	c	510	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	B	613	CLA	CHD-C4C-NC	2.70	128.46	124.20
24	C	510	CLA	C4-C3-C5	2.70	119.81	115.27
24	b	612	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
31	a	416	PL9	C7-C3-C2	-2.70	119.75	123.30
24	C	509	CLA	C4-C3-C5	2.69	119.80	115.27
24	C	503	CLA	CHC-C1C-C2C	-2.69	119.27	126.72
24	B	612	CLA	C4C-C3C-C2C	-2.69	102.97	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	O2A-CGA-O1A	-2.69	116.80	123.59
27	L	102	SQD	C44-O6-C1	-2.69	108.48	113.74
24	c	508	CLA	CMB-C2B-C3B	2.69	129.71	124.68
26	B	619	BCR	C33-C5-C6	-2.69	121.51	124.53
24	c	516	CLA	O2A-CGA-CBA	2.69	120.34	111.91
27	B	621	SQD	O48-C23-C24	2.69	120.34	111.91
37	D	409	LHG	O8-C23-O10	-2.68	116.82	123.59
24	D	402	CLA	CAA-C2A-C3A	-2.68	105.43	112.78
24	c	515	CLA	O2A-CGA-CBA	2.68	120.32	111.91
24	c	508	CLA	CHD-C4C-NC	2.68	128.43	124.20
24	c	515	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
24	B	612	CLA	C4D-C3D-CAD	-2.68	106.98	108.47
34	V	206	HTG	C1-C2-C3	-2.68	105.30	110.59
24	C	504	CLA	C3B-C4B-NB	2.68	112.67	109.21
24	A	409	CLA	CMC-C2C-C1C	2.68	129.12	125.04
31	D	405	PL9	C22-C23-C24	-2.68	121.21	127.66
26	c	518	BCR	C38-C26-C25	-2.68	121.52	124.53
24	C	512	CLA	C4-C3-C5	2.67	119.77	115.27
24	B	614	CLA	C1-C2-C3	-2.67	121.42	126.04
24	D	403	CLA	CAA-C2A-C3A	-2.67	105.47	112.78
24	c	508	CLA	CMC-C2C-C1C	2.67	129.10	125.04
27	A	411	SQD	O48-C23-C24	2.67	120.28	111.91
25	A	408	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
27	a	405	SQD	C3-C4-C5	2.67	115.00	110.24
24	b	621	CLA	OBD-CAD-C3D	-2.67	123.55	127.98
24	b	612	CLA	CBC-CAC-C3C	-2.66	105.09	112.43
37	e	102	LHG	O8-C23-C24	2.66	120.25	111.91
29	m	102	LMT	O5'-C5'-C4'	2.66	115.36	109.75
24	C	510	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	b	620	CLA	CMC-C2C-C1C	2.66	129.09	125.04
24	C	511	CLA	O2A-CGA-CBA	2.66	120.24	111.91
24	C	507	CLA	CMC-C2C-C1C	2.65	129.08	125.04
24	c	507	CLA	C3B-C4B-NB	2.65	112.64	109.21
26	H	101	BCR	C15-C14-C13	-2.65	123.52	127.31
24	D	402	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
27	B	621	SQD	C3-C4-C5	2.65	114.97	110.24
24	a	410	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
24	C	514	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	b	622	CLA	C4-C3-C5	2.65	119.73	115.27
24	B	603	CLA	C4-C3-C5	2.65	119.73	115.27
31	d	406	PL9	C53-C6-C1	2.65	120.40	114.99
24	b	617	CLA	CHD-C4C-NC	2.65	128.37	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CAC-C3C-C4C	2.65	128.24	124.81
31	A	418	PL9	C25-C24-C26	2.65	119.72	115.27
36	e	101	DGD	O5D-C1E-C2E	2.65	112.43	108.30
24	B	603	CLA	CMB-C2B-C3B	2.65	129.63	124.68
26	T	103	BCR	C12-C13-C14	-2.64	114.88	118.94
24	A	409	CLA	CMA-C3A-C4A	-2.64	104.67	111.77
25	a	411	PHO	C3C-C4C-NC	2.64	114.37	110.28
24	b	614	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
24	c	513	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
24	b	618	CLA	O2A-CGA-CBA	2.64	120.19	111.91
36	H	102	DGD	O1G-C1A-O1A	-2.64	116.93	123.59
24	B	608	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
24	b	625	CLA	C1-C2-C3	-2.64	121.48	126.04
26	A	410	BCR	C37-C22-C21	-2.64	119.23	122.92
24	B	608	CLA	C4-C3-C5	2.63	119.70	115.27
24	C	507	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
24	b	619	CLA	CHD-C4C-NC	2.63	128.35	124.20
24	C	508	CLA	CAC-C3C-C4C	2.63	128.22	124.81
24	B	604	CLA	CHD-C4C-NC	2.63	128.35	124.20
26	b	627	BCR	C37-C22-C21	-2.63	119.24	122.92
37	d	409	LHG	O8-C23-C24	2.63	120.16	111.91
24	B	611	CLA	CAA-CBA-CGA	-2.63	105.58	113.25
24	B	606	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	y	101	BCR	C21-C20-C19	-2.63	115.02	123.22
24	C	506	CLA	CMC-C2C-C1C	2.62	129.04	125.04
24	b	615	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
24	c	515	CLA	C1-O2A-CGA	2.62	123.32	116.44
26	t	101	BCR	C1-C6-C7	2.62	123.19	115.78
24	b	620	CLA	CHD-C4C-NC	2.62	128.33	124.20
34	V	206	HTG	O5-C1-C2	-2.62	107.02	110.31
36	C	517	DGD	C2G-O2G-C1B	-2.62	111.34	117.79
24	b	615	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
24	b	624	CLA	CMC-C2C-C1C	2.62	129.03	125.04
24	b	622	CLA	O2A-CGA-CBA	2.62	120.12	111.91
24	c	510	CLA	CMB-C2B-C3B	2.62	129.57	124.68
26	y	101	BCR	C10-C11-C12	-2.61	115.06	123.22
24	C	512	CLA	C1-C2-C3	-2.61	121.52	126.04
24	b	623	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
24	b	612	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
38	E	102	HEM	CBA-CAA-C2A	-2.61	107.67	112.49
24	B	605	CLA	O2A-CGA-CBA	2.61	120.10	111.91
24	a	412	CLA	CMA-C3A-C2A	-2.61	103.29	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	521	LMG	O8-C28-C29	2.61	120.10	111.91
24	a	412	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	C	512	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
24	B	607	CLA	C4-C3-C5	2.61	119.66	115.27
27	f	102	SQD	O47-C7-O49	-2.61	117.40	123.70
24	c	508	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	a	412	CLA	OBD-CAD-C3D	-2.60	123.66	127.98
24	d	404	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
24	C	514	CLA	C4-C3-C5	2.60	119.64	115.27
27	a	414	SQD	C45-O47-C7	-2.60	111.39	117.79
24	c	517	CLA	CAC-C3C-C4C	2.60	128.18	124.81
24	B	604	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
24	b	614	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
24	d	404	CLA	C4-C3-C5	2.59	119.64	115.27
31	D	405	PL9	C25-C24-C26	2.59	119.63	115.27
24	c	511	CLA	CHD-C4C-NC	2.59	128.29	124.20
24	C	504	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
27	L	102	SQD	O7-S-C6	2.59	110.02	106.94
24	B	608	CLA	CAC-C3C-C4C	2.59	128.17	124.81
24	b	623	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
26	c	527	BCR	C28-C27-C26	-2.59	109.45	114.08
24	c	512	CLA	C4-C3-C5	2.59	119.62	115.27
24	a	410	CLA	C4-C3-C5	2.58	119.62	115.27
24	C	514	CLA	CMC-C2C-C1C	2.58	128.97	125.04
26	C	516	BCR	C28-C27-C26	-2.58	109.47	114.08
24	c	511	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
24	c	512	CLA	CMB-C2B-C3B	2.58	129.51	124.68
27	L	102	SQD	O47-C7-O49	-2.58	117.47	123.70
24	B	609	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
24	b	618	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
24	C	511	CLA	CMC-C2C-C1C	2.58	128.97	125.04
24	C	508	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
24	A	405	CLA	CAA-C2A-C1A	-2.58	103.53	111.97
31	a	416	PL9	C51-C49-C50	2.58	120.30	114.60
26	K	101	BCR	C15-C14-C13	-2.58	123.64	127.31
24	c	515	CLA	CMB-C2B-C3B	2.57	129.49	124.68
26	Y	101	BCR	C10-C11-C12	-2.57	115.19	123.22
24	C	502	CLA	CHC-C1C-C2C	-2.57	119.61	126.72
31	d	406	PL9	C27-C28-C29	-2.57	121.47	127.66
31	d	406	PL9	C37-C38-C39	-2.57	121.47	127.66
24	b	623	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
27	F	103	SQD	O9-S-C6	2.57	109.99	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	415	LMG	O8-C28-C29	2.57	119.97	111.91
24	C	505	CLA	OBD-CAD-C3D	-2.57	123.72	127.98
24	c	512	CLA	CHD-C4C-NC	2.56	128.24	124.20
24	C	507	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
26	C	516	BCR	C11-C10-C9	-2.56	123.65	127.31
24	A	409	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
24	A	406	CLA	OBD-CAD-C3D	-2.56	123.73	127.98
24	C	511	CLA	CBC-CAC-C3C	-2.56	105.37	112.43
24	b	618	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
24	b	617	CLA	C1-C2-C3	-2.56	121.62	126.04
24	B	602	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
24	B	609	CLA	CAC-C3C-C4C	2.56	128.13	124.81
24	b	613	CLA	CHD-C4C-NC	2.55	128.23	124.20
27	A	411	SQD	O48-C23-O10	-2.55	117.14	123.59
25	A	408	PHO	CAC-C3C-C4C	2.55	128.01	125.22
24	A	409	CLA	CHD-C4C-NC	2.55	128.23	124.20
24	A	405	CLA	CMC-C2C-C1C	2.55	128.93	125.04
24	C	512	CLA	O2A-CGA-CBA	2.55	119.92	111.91
24	b	613	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
35	C	521	LMG	C3-C4-C5	2.55	114.79	110.24
27	a	414	SQD	O48-C23-C24	2.55	119.91	111.91
26	h	101	BCR	C7-C8-C9	-2.55	122.38	126.23
24	c	511	CLA	CAC-C3C-C4C	2.55	128.12	124.81
24	c	507	CLA	O2A-CGA-CBA	2.55	119.91	111.91
34	B	625	HTG	C1-O5-C5	2.55	117.28	112.58
24	c	517	CLA	C3B-C4B-NB	2.55	112.50	109.21
24	C	505	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
27	f	102	SQD	O48-C23-C24	2.54	119.89	111.91
24	d	403	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
24	c	507	CLA	CHD-C4C-NC	2.54	128.21	124.20
24	d	404	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	A	418	PL9	C15-C14-C16	2.54	119.55	115.27
24	B	603	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
24	b	619	CLA	CMB-C2B-C3B	2.54	129.43	124.68
36	e	101	DGD	C1E-O6E-C5E	2.54	118.67	113.69
35	J	101	LMG	C9-C8-C7	-2.54	105.78	111.79
27	A	411	SQD	O47-C7-O49	-2.54	117.57	123.70
36	c	521	DGD	O1G-C1A-C2A	2.54	119.87	111.91
24	B	602	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
24	b	615	CLA	OBD-CAD-C3D	-2.54	123.77	127.98
24	a	409	CLA	OBD-CAD-C3D	-2.54	123.77	127.98
24	b	611	CLA	C1-C2-C3	-2.54	121.66	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
24	b	612	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
24	A	409	CLA	CHB-C4A-NA	2.53	128.02	124.51
34	c	525	HTG	C1-O5-C5	2.53	117.25	112.58
26	k	101	BCR	C10-C11-C12	-2.53	115.31	123.22
24	a	409	CLA	CMC-C2C-C1C	2.53	128.90	125.04
24	b	614	CLA	CMC-C2C-C1C	2.53	128.89	125.04
24	d	402	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
24	B	605	CLA	CHD-C4C-NC	2.53	128.19	124.20
24	c	516	CLA	CBA-CAA-C2A	-2.53	106.40	113.86
26	d	405	BCR	C2-C1-C6	2.53	114.37	110.48
24	c	516	CLA	O1D-CGD-CBD	-2.53	119.31	124.48
24	a	409	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
34	C	524	HTG	O5-C1-C2	2.52	113.49	110.31
25	D	401	PHO	C2B-C1B-NB	2.52	113.60	109.79
24	B	617	CLA	O2A-CGA-CBA	2.52	119.83	111.91
24	C	503	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	B	602	CLA	CMC-C2C-C1C	2.52	128.88	125.04
24	D	402	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
24	B	607	CLA	O2A-CGA-CBA	2.52	119.82	111.91
24	c	508	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
31	A	418	PL9	C30-C29-C31	2.52	119.51	115.27
24	C	506	CLA	C1-O2A-CGA	2.52	123.05	116.44
26	d	405	BCR	C15-C14-C13	-2.52	123.72	127.31
24	A	409	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
26	c	527	BCR	C29-C30-C25	2.52	114.36	110.48
24	C	513	CLA	C4-C3-C5	2.52	119.50	115.27
36	e	101	DGD	O1G-C1A-C2A	2.51	119.80	111.91
24	b	619	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
24	B	607	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
24	B	602	CLA	CAC-C3C-C4C	2.51	128.07	124.81
24	b	621	CLA	CMC-C2C-C1C	2.51	128.86	125.04
35	a	415	LMG	C7-O1-C1	-2.51	108.83	113.74
34	B	625	HTG	C1-C2-C3	2.51	115.54	110.59
29	M	104	LMT	O5B-C5B-C4B	2.51	114.25	109.69
24	C	509	CLA	CHD-C4C-NC	2.51	128.16	124.20
24	B	612	CLA	C1-C2-C3	-2.51	121.70	126.04
26	a	413	BCR	C3-C4-C5	-2.51	109.60	114.08
26	c	527	BCR	C7-C8-C9	-2.51	122.45	126.23
26	k	101	BCR	C39-C30-C25	-2.51	106.23	110.30
35	Z	101	LMG	C1-O6-C5	2.50	118.60	113.69
35	c	523	LMG	O8-C28-C29	2.50	119.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	O2A-CGA-O1A	-2.50	117.27	123.59
24	a	412	CLA	C4C-C3C-C2C	-2.50	103.25	106.90
24	b	610	CLA	CMB-C2B-C3B	2.50	129.36	124.68
24	b	617	CLA	CMB-C2B-C3B	2.50	129.35	124.68
25	A	408	PHO	C2C-C1C-NC	2.50	113.56	109.79
24	c	508	CLA	CAC-C3C-C4C	2.50	128.05	124.81
24	A	406	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
24	B	612	CLA	C2A-C1A-CHA	-2.50	119.50	123.86
24	c	517	CLA	CMB-C2B-C3B	2.50	129.35	124.68
24	B	608	CLA	OBD-CAD-C3D	-2.50	123.84	127.98
25	A	408	PHO	C1C-C2C-C3C	-2.49	103.64	106.51
24	b	613	CLA	OBD-CAD-C3D	-2.49	123.84	127.98
26	K	101	BCR	C29-C30-C25	2.49	114.32	110.48
24	C	505	CLA	CMB-C2B-C3B	2.49	129.34	124.68
24	c	513	CLA	OBD-CAD-C3D	-2.49	123.84	127.98
24	a	410	CLA	O2A-CGA-CBA	2.49	119.73	111.91
24	c	505	CLA	O2A-CGA-CBA	2.49	119.73	111.91
24	c	517	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
24	D	403	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	b	620	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
25	A	408	PHO	C4D-ND-C1D	-2.49	102.28	106.76
24	c	510	CLA	C4D-C3D-CAD	-2.49	107.08	108.47
24	C	513	CLA	C1-O2A-CGA	2.49	122.97	116.44
24	B	611	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	B	615	CLA	CMB-C2B-C3B	2.49	129.33	124.68
26	H	101	BCR	C24-C23-C22	-2.49	122.48	126.23
26	C	515	BCR	C20-C21-C22	-2.48	123.77	127.31
24	A	407	CLA	CHC-C1C-C2C	-2.48	119.85	126.72
36	c	519	DGD	C2G-O2G-C1B	-2.48	111.68	117.79
26	B	620	BCR	C3-C4-C5	-2.48	109.64	114.08
24	B	608	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
24	C	510	CLA	CHD-C4C-NC	2.48	128.12	124.20
36	D	406	DGD	C4D-C3D-C2D	2.48	115.16	110.82
24	a	410	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	C	514	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	B	606	CLA	CMB-C2B-C1B	2.48	132.27	128.46
26	h	101	BCR	C16-C15-C14	-2.48	118.40	123.47
34	d	412	HTG	C1-O5-C5	2.48	117.15	112.58
24	B	615	CLA	CHD-C4C-NC	2.48	128.11	124.20
24	d	402	CLA	C1-C2-C3	-2.48	121.76	126.04
24	c	516	CLA	CHC-C1C-C2C	-2.48	119.88	126.72
24	B	616	CLA	CED-O2D-CGD	2.47	121.53	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	C3B-C4B-NB	2.47	112.41	109.21
24	B	616	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
24	C	509	CLA	C1-C2-C3	-2.47	121.77	126.04
31	A	418	PL9	C10-C9-C11	2.47	119.43	115.27
24	C	511	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
24	C	504	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
27	A	411	SQD	C1-C2-C3	-2.47	104.85	110.00
24	B	606	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
24	A	407	CLA	C3B-C4B-NB	2.47	112.40	109.21
24	B	606	CLA	CAC-C3C-C4C	2.47	128.01	124.81
24	C	505	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
24	B	614	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	b	620	CLA	O2A-CGA-CBA	2.46	119.64	111.91
24	B	616	CLA	CHC-C1C-C2C	-2.46	119.91	126.72
24	C	508	CLA	OBD-CAD-C3D	-2.46	123.89	127.98
24	a	409	CLA	CHD-C4C-NC	2.46	128.08	124.20
24	B	611	CLA	C4-C3-C5	2.46	119.41	115.27
24	B	608	CLA	CMC-C2C-C1C	2.46	128.78	125.04
24	c	508	CLA	OBD-CAD-C3D	-2.45	123.91	127.98
26	t	101	BCR	C7-C6-C5	-2.45	115.52	121.46
31	D	405	PL9	C27-C28-C29	-2.45	121.75	127.66
24	C	512	CLA	C1-O2A-CGA	2.45	122.87	116.44
24	b	616	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
24	a	409	CLA	C4-C3-C5	2.45	119.39	115.27
24	b	617	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
37	d	408	LHG	O8-C23-C24	2.45	119.59	111.91
24	C	509	CLA	O2A-CGA-CBA	2.45	119.58	111.91
24	B	617	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
24	c	510	CLA	CMC-C2C-C1C	2.44	128.76	125.04
26	t	101	BCR	C21-C20-C19	-2.44	115.59	123.22
25	a	411	PHO	C1C-C2C-C3C	-2.44	103.70	106.51
24	b	625	CLA	C4-C3-C5	2.44	119.38	115.27
24	d	403	CLA	C1D-CHD-C4C	-2.44	119.33	122.56
24	C	510	CLA	OBD-CAD-C3D	-2.44	123.93	127.98
26	C	516	BCR	C21-C20-C19	-2.44	115.60	123.22
26	C	516	BCR	C15-C14-C13	-2.44	123.83	127.31
24	c	512	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	C	502	CLA	C1-C2-C3	-2.44	121.82	126.04
31	a	416	PL9	C30-C29-C31	2.44	119.37	115.27
24	A	407	CLA	C1D-CHD-C4C	-2.44	119.34	122.56
26	a	413	BCR	C33-C5-C6	-2.44	121.79	124.53
24	d	403	CLA	O2A-CGA-O1A	-2.44	117.44	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
24	c	507	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
24	B	607	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
26	t	101	BCR	C2-C1-C6	2.43	114.23	110.48
24	d	404	CLA	C4D-C3D-CAD	-2.43	107.11	108.47
24	C	503	CLA	OBD-CAD-C3D	-2.43	123.94	127.98
24	B	608	CLA	CBC-CAC-C3C	-2.43	105.73	112.43
24	B	606	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
26	K	101	BCR	C16-C17-C18	-2.43	123.84	127.31
24	B	610	CLA	C1-C2-C3	-2.43	121.85	126.04
24	b	624	CLA	C11-C10-C8	-2.42	108.08	115.92
25	D	401	PHO	C4D-ND-C1D	-2.42	102.40	106.76
24	a	412	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	b	615	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
24	c	516	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
37	d	408	LHG	O8-C23-O10	-2.42	117.48	123.59
35	C	521	LMG	C8-O7-C10	-2.42	111.83	117.79
24	b	617	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
24	B	611	CLA	CHD-C4C-NC	2.41	128.01	124.20
24	B	617	CLA	O1D-CGD-CBD	-2.41	119.54	124.48
24	d	402	CLA	C1-O2A-CGA	2.41	122.78	116.44
26	B	619	BCR	C31-C1-C6	-2.41	106.39	110.30
24	c	507	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
31	A	418	PL9	C42-C43-C44	-2.41	121.86	127.66
24	a	412	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	c	506	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
24	b	619	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
26	C	515	BCR	C37-C22-C23	2.41	121.87	118.08
25	A	408	PHO	C2A-C1A-NA	2.41	114.62	111.86
24	b	625	CLA	OBD-CAD-C3D	-2.41	123.99	127.98
24	B	614	CLA	CAC-C3C-C4C	2.41	127.93	124.81
24	b	614	CLA	CAC-C3C-C2C	2.41	131.64	127.53
26	b	626	BCR	C16-C17-C18	-2.40	123.88	127.31
24	B	610	CLA	C1-O2A-CGA	2.40	122.74	116.44
27	F	103	SQD	O47-C7-O49	-2.40	117.90	123.70
24	B	605	CLA	C11-C10-C8	-2.40	108.16	115.92
36	c	520	DGD	O1G-C1A-C2A	2.40	119.44	111.91
26	A	410	BCR	C33-C5-C6	-2.40	121.83	124.53
26	t	101	BCR	C12-C13-C14	-2.40	115.26	118.94
24	b	620	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
24	b	611	CLA	CMB-C2B-C3B	2.40	129.16	124.68
24	b	616	CLA	C2A-C1A-CHA	-2.40	119.67	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
24	D	402	CLA	C4-C3-C5	2.40	119.30	115.27
24	C	509	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
24	A	406	CLA	CAA-CBA-CGA	2.40	120.25	113.25
24	a	412	CLA	C2A-C1A-CHA	-2.40	119.67	123.86
25	d	401	PHO	C3A-C4A-CHB	-2.39	117.69	121.83
35	Z	101	LMG	C1-C2-C3	2.39	114.98	110.00
24	b	611	CLA	O2A-CGA-CBA	2.39	119.42	111.91
24	d	402	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
35	c	522	LMG	O8-C28-O10	-2.39	117.56	123.59
24	b	613	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
24	B	604	CLA	CMA-C3A-C2A	-2.39	104.19	113.83
24	a	412	CLA	O2A-CGA-CBA	2.39	119.41	111.91
24	b	621	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
24	d	403	CLA	CMA-C3A-C2A	-2.39	104.19	113.83
37	L	101	LHG	O7-C7-O9	-2.39	117.93	123.70
24	c	515	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
27	B	621	SQD	O47-C7-O49	-2.39	117.94	123.70
24	c	510	CLA	O2A-CGA-CBA	2.39	119.39	111.91
24	c	505	CLA	CMC-C2C-C1C	2.38	128.67	125.04
27	B	621	SQD	C44-O6-C1	-2.38	109.08	113.74
24	C	513	CLA	CMC-C2C-C1C	2.38	128.67	125.04
25	d	401	PHO	C2C-C1C-NC	2.38	113.39	109.79
24	b	616	CLA	C4-C3-C5	2.38	119.28	115.27
29	M	104	LMT	O1B-C1B-C2B	2.38	114.27	108.10
24	B	611	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
24	d	404	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	C	502	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
24	A	409	CLA	O2A-CGA-CBA	2.38	119.36	111.91
24	B	606	CLA	C1-C2-C3	-2.38	121.93	126.04
24	a	410	CLA	CAC-C3C-C4C	2.38	127.89	124.81
29	A	416	LMT	C4B-C3B-C2B	-2.37	106.68	110.82
24	B	612	CLA	CMB-C2B-C3B	2.37	129.12	124.68
24	C	513	CLA	O2A-CGA-CBA	2.37	119.35	111.91
24	b	610	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
24	d	402	CLA	CMA-C3A-C2A	-2.37	104.27	113.83
24	c	509	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
24	C	514	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
27	a	405	SQD	O48-C23-O10	-2.36	117.63	123.59
24	C	503	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
26	H	101	BCR	C10-C11-C12	-2.36	115.85	123.22
26	C	515	BCR	C38-C26-C25	-2.36	121.88	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
24	b	623	CLA	CHB-C4A-NA	2.36	127.77	124.51
29	C	522	LMT	O5'-C5'-C4'	2.36	114.72	109.75
24	C	508	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
26	T	103	BCR	C16-C15-C14	2.36	128.30	123.47
35	c	523	LMG	C8-O7-C10	-2.36	111.99	117.79
26	K	101	BCR	C3-C4-C5	-2.35	109.88	114.08
24	c	517	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
31	A	418	PL9	C17-C18-C19	-2.35	122.00	127.66
24	c	505	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
24	c	506	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
26	A	410	BCR	C24-C23-C22	-2.35	122.68	126.23
24	b	623	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
25	a	411	PHO	C4D-ND-C1D	-2.35	102.53	106.76
24	b	625	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
36	C	517	DGD	O1G-C1A-O1A	-2.35	117.66	123.59
24	B	604	CLA	CAC-C3C-C4C	2.35	127.86	124.81
31	d	406	PL9	O1-C4-C3	-2.35	118.13	120.72
26	c	518	BCR	C21-C20-C19	-2.35	115.88	123.22
24	a	409	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	D	402	CLA	CMB-C2B-C3B	2.35	129.07	124.68
24	c	510	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
36	D	406	DGD	O6D-C5D-C6D	2.35	111.40	106.67
34	B	632	HTG	C3-C4-C5	2.35	114.42	110.24
26	Y	101	BCR	C28-C27-C26	-2.35	109.89	114.08
26	t	101	BCR	C20-C21-C22	-2.35	123.96	127.31
24	c	513	CLA	CMB-C2B-C3B	2.34	129.06	124.68
36	C	518	DGD	O1G-C1A-O1A	-2.34	117.68	123.59
24	c	513	CLA	C4-C3-C5	2.34	119.21	115.27
24	A	407	CLA	CAC-C3C-C4C	2.34	127.85	124.81
24	b	625	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
24	B	608	CLA	CED-O2D-CGD	2.34	121.23	115.94
24	C	514	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
24	b	614	CLA	O2A-CGA-CBA	2.34	119.24	111.91
24	b	610	CLA	C2A-C1A-CHA	-2.34	119.78	123.86
34	B	624	HTG	O5-C1-C2	2.33	113.25	110.31
24	C	508	CLA	CHC-C1C-C2C	-2.33	120.26	126.72
24	B	604	CLA	C1-O2A-CGA	2.33	122.57	116.44
24	A	406	CLA	C4C-C3C-C2C	-2.33	103.50	106.90
29	M	102	LMT	O6'-C6'-C5'	-2.33	103.29	111.29
24	B	609	CLA	CHB-C4A-NA	2.33	127.74	124.51
29	F	102	LMT	C1B-O5B-C5B	2.33	118.26	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	Z	101	LMG	C9-O8-C28	2.33	122.95	117.10
24	B	613	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
24	c	511	CLA	O2A-CGA-CBA	2.33	119.21	111.91
26	B	620	BCR	C28-C27-C26	-2.33	109.92	114.08
24	B	609	CLA	CAA-C2A-C3A	-2.32	106.41	112.78
31	d	406	PL9	C36-C37-C38	-2.32	104.25	111.88
31	D	405	PL9	C37-C38-C39	-2.32	122.07	127.66
36	c	520	DGD	C3B-C2B-C1B	-2.32	105.18	113.62
24	a	410	CLA	C1-C2-C3	-2.32	122.03	126.04
24	a	412	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
27	L	102	SQD	C1-C2-C3	-2.32	105.17	110.00
24	b	621	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
24	b	611	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
24	c	510	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
24	c	509	CLA	C4-C3-C5	2.32	119.17	115.27
29	m	102	LMT	C1'-O5'-C5'	2.31	118.23	113.69
36	c	519	DGD	O2G-C1B-O1B	-2.31	118.11	123.70
26	t	101	BCR	C7-C8-C9	-2.31	122.74	126.23
24	b	612	CLA	OBD-CAD-C3D	-2.31	124.14	127.98
24	c	510	CLA	CAC-C3C-C4C	2.31	127.81	124.81
25	a	411	PHO	C4D-CHA-C1A	-2.31	120.17	125.37
24	c	512	CLA	O2A-CGA-CBA	2.31	119.15	111.91
24	A	406	CLA	C2A-C1A-CHA	-2.31	119.83	123.86
35	j	101	LMG	C1-O6-C5	2.31	118.22	113.69
24	C	512	CLA	CMB-C2B-C3B	2.31	128.99	124.68
24	C	508	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
27	a	405	SQD	O5-C5-C4	2.30	113.88	109.69
24	c	508	CLA	C11-C10-C8	-2.30	108.47	115.92
24	b	613	CLA	CHA-C1A-NA	-2.30	121.12	126.40
24	c	506	CLA	CMC-C2C-C1C	2.30	128.54	125.04
24	A	406	CLA	CMA-C3A-C2A	-2.30	104.55	113.83
31	D	405	PL9	C51-C49-C50	2.30	119.68	114.60
24	b	611	CLA	CHD-C4C-NC	2.30	127.83	124.20
24	b	618	CLA	CMA-C3A-C4A	-2.30	105.59	111.77
24	C	513	CLA	CAC-C3C-C4C	2.30	127.79	124.81
26	b	626	BCR	C33-C5-C4	2.29	118.02	113.62
24	B	610	CLA	O2A-CGA-CBA	2.29	119.10	111.91
24	C	509	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
24	c	508	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
24	c	506	CLA	C3D-CAD-CBD	2.29	110.62	107.61
24	B	603	CLA	CMC-C2C-C1C	2.29	128.53	125.04
24	C	504	CLA	O2A-CGA-O1A	-2.29	117.82	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	621	SQD	C1-C2-C3	-2.29	105.23	110.00
31	d	406	PL9	C25-C24-C26	2.29	119.12	115.27
24	B	609	CLA	C1-C2-C3	-2.29	122.09	126.04
24	A	406	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
26	T	103	BCR	C21-C20-C19	-2.28	116.09	123.22
24	C	511	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
26	Y	101	BCR	C40-C30-C25	-2.28	106.60	110.30
26	k	101	BCR	C15-C14-C13	-2.28	124.06	127.31
24	B	613	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
36	h	102	DGD	C2G-O2G-C1B	-2.28	112.19	117.79
24	A	407	CLA	CAA-CBA-CGA	2.28	119.91	113.25
24	b	620	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
36	C	517	DGD	C3G-C2G-C1G	-2.28	106.41	111.79
24	c	514	CLA	CAC-C3C-C4C	2.27	127.76	124.81
24	B	614	CLA	C2A-C1A-CHA	-2.27	119.88	123.86
24	B	614	CLA	CHD-C4C-NC	2.27	127.78	124.20
24	B	611	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
24	d	404	CLA	CMB-C2B-C3B	2.27	128.93	124.68
26	T	103	BCR	C36-C18-C19	2.27	121.65	118.08
31	d	406	PL9	C15-C14-C16	2.27	119.09	115.27
24	b	611	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
35	Z	101	LMG	C8-O7-C10	-2.27	112.21	117.79
24	C	505	CLA	C1-O2A-CGA	2.27	122.39	116.44
26	b	628	BCR	C2-C1-C6	2.27	113.97	110.48
27	B	621	SQD	O9-S-C6	2.26	109.63	106.94
24	b	623	CLA	C4-C3-C5	2.26	119.08	115.27
25	d	401	PHO	CMB-C2B-C1B	2.26	128.55	125.06
26	D	404	BCR	C21-C20-C19	-2.26	116.16	123.22
24	B	616	CLA	C4-C3-C5	2.26	119.08	115.27
26	b	628	BCR	C8-C7-C6	-2.26	120.85	127.20
24	d	402	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
24	B	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
24	C	502	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
27	L	102	SQD	O5-C5-C4	2.26	113.80	109.69
24	c	514	CLA	CMB-C2B-C3B	2.26	128.90	124.68
24	b	622	CLA	O2A-CGA-O1A	-2.26	117.90	123.59
24	D	403	CLA	O2A-CGA-CBA	2.26	118.99	111.91
24	C	507	CLA	C2A-C1A-CHA	-2.26	119.92	123.86
24	b	610	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	a	409	CLA	CHB-C4A-NA	2.25	127.63	124.51
24	B	604	CLA	CMB-C2B-C3B	2.25	128.89	124.68
25	D	401	PHO	C1-C2-C3	-2.25	122.15	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	d	408	LHG	C6-C5-C4	-2.25	106.46	111.79
26	B	620	BCR	C36-C18-C19	2.25	121.62	118.08
24	b	620	CLA	C1-C2-C3	-2.25	122.15	126.04
35	z	101	LMG	C8-O7-C10	-2.25	112.25	117.79
24	B	610	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	D	403	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
26	B	618	BCR	C16-C17-C18	-2.25	124.10	127.31
37	D	407	LHG	O7-C7-O9	-2.25	118.27	123.70
37	L	101	LHG	O8-C23-O10	-2.25	117.92	123.59
24	B	614	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
24	c	517	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
24	A	405	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	C	514	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
24	B	602	CLA	C1-C2-C3	-2.24	122.17	126.04
24	B	617	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
31	d	406	PL9	C12-C13-C14	-2.24	122.27	127.66
35	C	501	LMG	O8-C28-C29	2.24	118.93	111.91
24	b	613	CLA	C6-C5-C3	-2.24	107.59	113.45
26	H	101	BCR	C29-C30-C25	2.23	113.92	110.48
24	b	624	CLA	O2A-CGA-O1A	-2.23	117.95	123.59
27	a	414	SQD	O47-C7-O49	-2.23	118.31	123.70
24	b	614	CLA	C1-C2-C3	-2.23	122.18	126.04
24	C	506	CLA	CHD-C4C-NC	2.23	127.72	124.20
24	B	614	CLA	CMC-C2C-C1C	2.23	128.44	125.04
27	A	411	SQD	C1-O5-C5	-2.23	109.31	113.69
24	d	403	CLA	CMB-C2B-C3B	2.23	128.84	124.68
24	C	506	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
24	C	503	CLA	C4-C3-C5	2.23	119.02	115.27
37	D	408	LHG	O8-C23-O10	-2.22	117.98	123.59
24	C	504	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
24	d	402	CLA	O2A-CGA-CBA	2.22	118.87	111.91
24	B	608	CLA	CHD-C4C-NC	2.22	127.70	124.20
24	B	613	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
24	c	506	CLA	C4-C3-C5	2.22	119.00	115.27
26	T	103	BCR	C10-C11-C12	-2.22	116.30	123.22
24	b	617	CLA	C4-C3-C5	2.21	119.00	115.27
24	b	613	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
24	B	609	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
26	t	101	BCR	C35-C13-C12	2.21	121.56	118.08
24	B	614	CLA	C4-C3-C5	2.21	118.99	115.27
24	c	511	CLA	OBD-CAD-C3D	-2.21	124.31	127.98
26	B	618	BCR	C15-C14-C13	-2.21	124.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	CMB-C2B-C3B	2.21	128.82	124.68
26	D	404	BCR	C1-C6-C7	2.21	122.03	115.78
26	A	410	BCR	C3-C4-C5	-2.21	110.13	114.08
36	c	521	DGD	C2G-O2G-C1B	-2.21	112.35	117.79
29	B	635	LMT	C1'-O5'-C5'	2.21	118.02	113.69
24	B	616	CLA	O2A-CGA-CBA	2.21	118.83	111.91
24	A	406	CLA	O2A-CGA-CBA	2.21	118.83	111.91
26	b	626	BCR	C10-C11-C12	-2.21	116.33	123.22
38	v	205	HEM	CBA-CAA-C2A	-2.20	108.42	112.49
24	c	511	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
24	c	515	CLA	CED-O2D-CGD	2.20	120.92	115.94
24	A	407	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
24	A	409	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
24	B	608	CLA	O2A-CGA-CBA	2.20	118.82	111.91
24	b	625	CLA	CHC-C1C-NC	2.20	127.54	124.20
24	C	513	CLA	CHB-C4A-NA	2.20	127.56	124.51
26	D	404	BCR	C3-C4-C5	-2.20	110.15	114.08
24	b	615	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
24	b	619	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
29	B	622	LMT	C1-O1'-C1'	-2.20	110.19	113.84
24	A	409	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
24	b	619	CLA	CMC-C2C-C1C	2.20	128.39	125.04
25	D	401	PHO	CBA-CAA-C2A	-2.20	107.38	113.86
24	D	402	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
24	c	508	CLA	O2A-CGA-CBA	2.20	118.80	111.91
26	t	101	BCR	C11-C10-C9	-2.19	124.18	127.31
24	C	502	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
24	C	514	CLA	CMB-C2B-C3B	2.19	128.78	124.68
25	a	411	PHO	C1-O2A-CGA	2.19	122.20	116.44
24	b	621	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
24	b	623	CLA	CED-O2D-CGD	2.19	120.90	115.94
24	B	604	CLA	C4-C3-C5	2.19	118.96	115.27
24	b	611	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
34	b	631	HTG	C1-C2-C3	2.19	114.92	110.59
24	D	403	CLA	CHD-C4C-NC	2.19	127.66	124.20
24	A	405	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
26	k	101	BCR	C29-C30-C25	2.19	113.85	110.48
24	B	611	CLA	C1-C2-C3	-2.19	122.26	126.04
24	A	407	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
25	a	411	PHO	C4-C3-C5	2.19	118.95	115.27
35	c	523	LMG	O8-C28-O10	-2.19	118.07	123.59
24	d	404	CLA	O2A-CGA-O1A	-2.19	118.07	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	t	101	BCR	C29-C28-C27	-2.19	106.49	111.38
24	B	609	CLA	OBD-CAD-C3D	-2.19	124.35	127.98
24	b	624	CLA	C4D-C3D-CAD	-2.18	107.25	108.47
24	c	513	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	c	508	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
24	C	502	CLA	O2A-CGA-CBA	2.18	118.76	111.91
24	A	405	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
25	A	408	PHO	CHD-C1D-C2D	-2.18	120.25	125.73
26	D	404	BCR	C39-C30-C25	-2.18	106.76	110.30
25	D	401	PHO	C3A-C4A-CHB	-2.18	118.06	121.83
24	C	507	CLA	OBD-CAD-C3D	-2.18	124.37	127.98
35	b	629	LMG	O8-C28-O10	-2.18	118.10	123.59
26	K	101	BCR	C2-C1-C6	2.18	113.83	110.48
24	c	506	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
24	C	511	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
27	F	103	SQD	C1-C2-C3	-2.18	105.47	110.00
24	A	409	CLA	CMB-C2B-C3B	2.18	128.75	124.68
24	B	616	CLA	C1-C2-C3	-2.18	122.28	126.04
24	b	619	CLA	CMA-C3A-C4A	-2.17	105.93	111.77
24	D	402	CLA	OBD-CAD-C3D	-2.17	124.37	127.98
24	B	609	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
24	B	617	CLA	C4-C3-C5	2.17	118.92	115.27
24	c	516	CLA	CAC-C3C-C4C	2.17	127.63	124.81
24	C	511	CLA	C6-C7-C8	-2.17	108.90	115.92
24	b	618	CLA	CED-O2D-CGD	2.17	120.84	115.94
24	b	622	CLA	CHD-C4C-NC	2.17	127.62	124.20
24	b	616	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
26	h	101	BCR	C24-C23-C22	-2.17	122.96	126.23
24	b	610	CLA	O2A-CGA-CBA	2.17	118.71	111.91
26	b	626	BCR	C3-C4-C5	-2.17	110.21	114.08
24	b	616	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	c	514	CLA	C4-C3-C2	-2.17	118.12	123.68
25	D	401	PHO	C3C-C4C-NC	2.17	113.64	110.28
24	c	510	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
24	B	610	CLA	CMB-C2B-C1B	2.16	131.79	128.46
26	b	626	BCR	C29-C30-C25	2.16	113.81	110.48
27	a	414	SQD	C1-O5-C5	-2.16	109.44	113.69
26	T	103	BCR	C16-C17-C18	-2.16	124.23	127.31
26	B	618	BCR	C34-C9-C10	-2.16	119.90	122.92
26	c	518	BCR	C16-C17-C18	-2.16	124.23	127.31
26	t	101	BCR	C23-C24-C25	-2.16	121.14	127.20
24	b	617	CLA	CMC-C2C-C1C	2.16	128.32	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C10-C11-C12	-2.16	116.49	123.22
24	b	624	CLA	O2A-CGA-CBA	2.16	118.67	111.91
24	b	618	CLA	CMC-C2C-C1C	2.16	128.32	125.04
24	C	511	CLA	CMB-C2B-C3B	2.15	128.71	124.68
36	e	101	DGD	O2G-C1B-O1B	-2.15	118.50	123.70
24	B	612	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
36	H	102	DGD	C3E-C4E-C5E	-2.15	106.40	110.24
26	d	405	BCR	C29-C28-C27	-2.15	106.57	111.38
24	c	505	CLA	CHD-C4C-NC	2.15	127.59	124.20
26	B	620	BCR	C2-C1-C6	2.15	113.79	110.48
24	C	511	CLA	C4-C3-C2	-2.15	118.17	123.68
38	e	103	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
24	C	513	CLA	C4D-C3D-CAD	-2.15	107.27	108.47
24	C	504	CLA	CMC-C2C-C1C	2.15	128.31	125.04
24	C	509	CLA	CHB-C4A-NA	2.14	127.48	124.51
26	a	413	BCR	C8-C7-C6	-2.14	121.18	127.20
24	C	512	CLA	CED-O2D-CGD	2.14	120.78	115.94
24	B	613	CLA	OBD-CAD-C3D	-2.14	124.42	127.98
26	h	101	BCR	C36-C18-C17	-2.14	119.92	122.92
36	C	517	DGD	O1G-C1A-C2A	2.14	118.62	111.91
24	c	514	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
24	c	514	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
26	b	627	BCR	C32-C1-C6	-2.14	106.84	110.30
26	k	101	BCR	C34-C9-C10	-2.13	119.93	122.92
24	c	514	CLA	CHB-C4A-NA	2.13	127.46	124.51
24	C	504	CLA	C4-C3-C5	2.13	118.86	115.27
24	B	617	CLA	CMB-C2B-C3B	2.13	128.67	124.68
31	A	418	PL9	C7-C3-C2	-2.13	120.50	123.30
24	C	514	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	B	603	CLA	OBD-CAD-C3D	-2.13	124.44	127.98
25	D	401	PHO	CHD-C1D-C2D	-2.13	120.37	125.73
24	A	406	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
24	A	405	CLA	CHD-C4C-NC	2.13	127.56	124.20
31	D	405	PL9	C42-C41-C39	-2.13	105.98	112.98
26	C	516	BCR	C3-C4-C5	-2.13	110.28	114.08
24	B	606	CLA	CED-O2D-CGD	2.13	120.75	115.94
24	C	514	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	B	614	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
24	C	510	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
36	c	521	DGD	C1D-O6D-C5D	2.12	117.86	113.69
26	Y	101	BCR	C24-C23-C22	-2.12	123.03	126.23
24	c	507	CLA	O2A-CGA-O1A	-2.12	118.24	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
24	d	404	CLA	CGD-CBD-CAD	-2.12	103.87	110.73
26	H	101	BCR	C36-C18-C17	-2.12	119.95	122.92
24	c	510	CLA	OBD-CAD-C3D	-2.12	124.46	127.98
26	b	628	BCR	C21-C20-C19	-2.12	116.61	123.22
27	f	102	SQD	O48-C23-O10	-2.12	118.25	123.59
26	d	405	BCR	C10-C11-C12	-2.12	116.61	123.22
24	b	623	CLA	C4-C3-C2	-2.12	118.25	123.68
24	b	612	CLA	C4-C3-C5	2.11	118.83	115.27
26	t	101	BCR	C37-C22-C23	2.11	121.41	118.08
35	C	501	LMG	C8-O7-C10	-2.11	112.59	117.79
26	d	405	BCR	C38-C26-C27	2.11	117.68	113.62
26	A	410	BCR	C8-C7-C6	-2.11	121.27	127.20
26	T	103	BCR	C2-C1-C6	2.11	113.73	110.48
24	a	410	CLA	CAA-CBA-CGA	2.11	119.42	113.25
35	C	521	LMG	O6-C5-C4	2.11	113.52	109.69
24	b	617	CLA	CMA-C3A-C4A	-2.11	106.11	111.77
24	b	617	CLA	CAC-C3C-C4C	2.11	127.55	124.81
25	A	408	PHO	C4D-CHA-C1A	-2.11	120.63	125.37
36	C	517	DGD	O2G-C1B-O1B	-2.11	118.61	123.70
24	d	404	CLA	C6-C7-C8	-2.11	109.11	115.92
37	d	407	LHG	O7-C7-O9	-2.11	118.61	123.70
24	C	508	CLA	CED-O2D-CGD	2.11	120.70	115.94
25	a	411	PHO	CBD-CHA-C1A	2.11	131.28	126.40
24	c	505	CLA	C4-C3-C5	2.10	118.81	115.27
26	y	101	BCR	C40-C30-C25	-2.10	106.89	110.30
34	C	523	HTG	C1-O5-C5	2.10	116.46	112.58
26	H	101	BCR	C39-C30-C25	-2.10	106.89	110.30
24	B	611	CLA	CGD-CBD-CAD	-2.10	103.93	110.73
24	b	619	CLA	CMA-C3A-C2A	-2.10	105.35	113.83
24	B	614	CLA	CHB-C4A-NA	2.10	127.42	124.51
31	d	406	PL9	C40-C39-C38	-2.10	118.29	123.68
24	c	514	CLA	CMA-C3A-C4A	-2.10	106.13	111.77
24	C	512	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
24	B	610	CLA	C7-C6-C5	-2.10	107.66	113.36
27	f	102	SQD	O9-S-C6	2.10	109.43	106.94
24	C	508	CLA	C1-C2-C3	-2.10	122.42	126.04
24	C	513	CLA	OBD-CAD-C3D	-2.09	124.50	127.98
24	B	609	CLA	CMA-C3A-C2A	-2.09	105.38	113.83
25	a	411	PHO	CBA-CAA-C2A	-2.09	107.68	113.86
26	B	618	BCR	C21-C20-C19	-2.09	116.69	123.22
24	C	514	CLA	OBD-CAD-C3D	-2.09	124.51	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	CHB-C4A-NA	2.09	127.41	124.51
26	h	101	BCR	C29-C30-C25	2.09	113.70	110.48
31	D	405	PL9	C45-C44-C46	2.09	118.79	115.27
24	B	614	CLA	CMA-C3A-C2A	-2.09	105.40	113.83
26	D	404	BCR	C15-C14-C13	-2.09	124.33	127.31
24	c	515	CLA	C4D-C3D-CAD	-2.09	107.31	108.47
26	B	620	BCR	C23-C24-C25	-2.09	121.33	127.20
25	d	401	PHO	CBD-CHA-C1A	2.09	131.25	126.40
24	b	612	CLA	C7-C6-C5	-2.09	107.69	113.36
35	a	415	LMG	O7-C10-O9	-2.09	118.66	123.70
24	b	618	CLA	CAC-C3C-C4C	2.09	127.52	124.81
29	F	102	LMT	C2'-C3'-C4'	2.09	114.45	109.68
24	D	403	CLA	C1-C2-C3	-2.09	122.44	126.04
25	d	401	PHO	C1C-C2C-C3C	-2.08	104.12	106.51
26	d	405	BCR	C21-C20-C19	-2.08	116.72	123.22
24	B	609	CLA	CMA-C3A-C4A	-2.08	106.18	111.77
24	C	506	CLA	CHA-C1A-NA	-2.08	121.63	126.40
36	c	519	DGD	O1G-C1A-C2A	2.08	118.44	111.91
29	M	104	LMT	C1B-O5B-C5B	2.08	117.77	113.69
24	c	512	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
25	A	408	PHO	O2A-CGA-CBA	2.08	118.42	111.91
36	c	520	DGD	O1G-C1A-O1A	-2.08	118.35	123.59
25	a	411	PHO	CAA-CBA-CGA	-2.08	107.19	113.25
24	C	509	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
31	A	418	PL9	C40-C39-C41	2.08	118.76	115.27
27	f	102	SQD	O7-S-C6	2.07	109.41	106.94
24	C	511	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
27	a	414	SQD	O6-C44-C45	-2.07	105.89	110.90
24	c	510	CLA	CGD-CBD-CAD	-2.07	104.02	110.73
31	A	418	PL9	C51-C49-C50	2.07	119.18	114.60
36	C	517	DGD	O3G-C3G-C2G	-2.07	105.90	110.90
24	c	509	CLA	CED-O2D-CGD	2.07	120.62	115.94
24	B	607	CLA	OBD-CAD-C3D	-2.07	124.54	127.98
26	h	101	BCR	C20-C21-C22	-2.07	124.36	127.31
37	D	408	LHG	O8-C23-C24	2.07	118.40	111.91
26	k	101	BCR	C34-C9-C8	2.07	121.34	118.08
24	b	624	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
26	D	404	BCR	C38-C26-C27	2.07	117.59	113.62
24	b	622	CLA	CMC-C2C-C1C	2.07	128.19	125.04
35	C	501	LMG	C7-O1-C1	-2.07	109.70	113.74
26	Y	101	BCR	C16-C17-C18	-2.07	124.36	127.31
24	C	503	CLA	CBC-CAC-C3C	-2.07	106.73	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	SQD	O48-C23-O10	-2.07	118.38	123.59
27	A	411	SQD	C44-O6-C1	-2.06	109.70	113.74
24	A	406	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
25	a	411	PHO	CHD-C1D-C2D	-2.06	120.54	125.73
26	A	410	BCR	C20-C21-C22	-2.06	124.37	127.31
24	c	509	CLA	CHD-C4C-NC	2.06	127.45	124.20
36	c	519	DGD	O5D-C6D-C5D	-2.06	105.23	109.05
29	a	419	LMT	C1B-O1B-C4'	-2.06	112.87	117.96
27	a	414	SQD	O9-S-O7	-2.06	106.82	113.95
24	b	613	CLA	CMB-C2B-C3B	2.06	128.53	124.68
24	b	622	CLA	CMA-C3A-C4A	-2.06	106.25	111.77
35	J	101	LMG	O8-C28-O10	-2.06	118.40	123.59
26	T	103	BCR	C29-C28-C27	-2.05	106.79	111.38
29	f	103	LMT	C4B-C3B-C2B	-2.05	107.24	110.82
27	F	103	SQD	O48-C23-O10	-2.05	118.41	123.59
24	b	622	CLA	CHA-C1A-NA	-2.05	121.69	126.40
26	k	101	BCR	C2-C1-C6	2.05	113.64	110.48
26	c	518	BCR	C37-C22-C21	-2.05	120.05	122.92
34	c	525	HTG	O5-C5-C4	2.05	113.42	109.69
24	C	505	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
36	C	518	DGD	O2G-C1B-O1B	-2.05	118.75	123.70
24	C	504	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
24	c	514	CLA	CED-O2D-CGD	2.05	120.57	115.94
37	E	101	LHG	O8-C23-O10	-2.05	118.42	123.59
24	C	507	CLA	CED-O2D-CGD	2.05	120.57	115.94
26	B	620	BCR	C36-C18-C17	-2.05	120.05	122.92
31	D	405	PL9	C40-C39-C38	-2.05	118.42	123.68
24	c	517	CLA	CED-O2D-CGD	2.05	120.57	115.94
24	c	511	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
36	H	102	DGD	C2G-O2G-C1B	-2.05	112.75	117.79
24	b	618	CLA	CMB-C2B-C1B	2.05	131.61	128.46
24	C	505	CLA	C11-C10-C8	-2.04	109.31	115.92
24	A	405	CLA	C11-C10-C8	-2.04	109.31	115.92
24	D	402	CLA	C3D-CAD-CBD	2.04	110.30	107.61
24	b	616	CLA	CAA-CBA-CGA	2.04	119.22	113.25
24	B	603	CLA	C1-O2A-CGA	2.04	121.80	116.44
37	D	408	LHG	O7-C7-O9	-2.04	118.77	123.70
24	c	513	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
24	B	615	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
26	K	101	BCR	C36-C18-C17	-2.04	120.06	122.92
26	D	404	BCR	C16-C17-C18	-2.04	124.40	127.31
26	b	628	BCR	C16-C17-C18	-2.04	124.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	OBD-CAD-C3D	-2.04	124.59	127.98
24	C	512	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
31	d	406	PL9	C45-C44-C46	2.04	118.70	115.27
26	Y	101	BCR	C21-C20-C19	-2.04	116.86	123.22
24	B	605	CLA	CHA-C1A-NA	-2.04	121.73	126.40
35	C	520	LMG	O8-C28-O10	-2.04	118.45	123.59
26	a	413	BCR	C37-C22-C21	-2.04	120.07	122.92
24	A	407	CLA	CMA-C3A-C2A	-2.03	105.62	113.83
24	b	623	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
24	c	512	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	c	516	CLA	C1-O2A-CGA	2.03	121.78	116.44
26	b	627	BCR	C8-C7-C6	-2.03	121.49	127.20
24	c	517	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
24	b	613	CLA	C6-C7-C8	-2.03	109.35	115.92
25	a	411	PHO	O2A-CGA-CBA	2.03	118.28	111.91
24	b	611	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	B	602	CLA	C4-C3-C5	2.03	118.68	115.27
24	B	608	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
26	c	527	BCR	C11-C12-C13	-2.03	120.72	126.42
34	d	412	HTG	C4-C3-C2	-2.03	107.29	110.82
26	b	628	BCR	C15-C14-C13	-2.02	124.42	127.31
24	b	622	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
26	K	101	BCR	C32-C1-C6	-2.02	107.02	110.30
24	A	405	CLA	CMA-C3A-C2A	-2.02	105.67	113.83
24	d	403	CLA	CHD-C4C-NC	2.02	127.39	124.20
26	H	101	BCR	C7-C8-C9	-2.02	123.18	126.23
24	C	511	CLA	OBD-CAD-C3D	-2.02	124.63	127.98
24	b	620	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
26	D	404	BCR	C7-C6-C5	-2.02	116.58	121.46
24	c	506	CLA	OBD-CAD-C3D	-2.02	124.63	127.98
36	C	518	DGD	C3G-O3G-C1D	-2.02	109.80	113.74
24	D	402	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
24	b	621	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
24	C	502	CLA	C4D-C3D-CAD	-2.02	107.35	108.47
24	c	516	CLA	CMA-C3A-C4A	-2.02	106.36	111.77
24	a	412	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
34	B	632	HTG	C6-C5-C4	-2.01	108.28	113.00
24	B	616	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
26	C	516	BCR	C15-C16-C17	-2.01	119.35	123.47
26	C	516	BCR	C29-C28-C27	-2.01	106.88	111.38
24	C	513	CLA	C2A-C1A-CHA	-2.01	120.34	123.86
31	d	406	PL9	C11-C9-C8	-2.01	117.04	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C3D-CAD-CBD	2.01	110.26	107.61
26	h	101	BCR	C37-C22-C21	-2.01	120.10	122.92
35	M	101	LMG	C9-C8-C7	-2.01	107.03	111.79
24	a	410	CLA	CMB-C2B-C3B	2.01	128.44	124.68
24	d	402	CLA	CAA-CBA-CGA	2.01	119.13	113.25
24	b	613	CLA	C4-C3-C5	2.01	118.65	115.27
35	c	523	LMG	O7-C10-O9	-2.01	118.84	123.70
24	b	616	CLA	OBD-CAD-C3D	-2.01	124.64	127.98
24	b	616	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
24	B	606	CLA	OBD-CAD-C3D	-2.01	124.65	127.98
24	b	617	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
26	C	516	BCR	C36-C18-C19	2.01	121.24	118.08
24	d	402	CLA	CED-O2D-CGD	2.01	120.48	115.94
31	d	406	PL9	C30-C29-C31	2.01	118.64	115.27
24	C	508	CLA	C3B-C4B-NB	2.01	111.80	109.21
24	a	410	CLA	OBD-CAD-C3D	-2.01	124.65	127.98
24	b	612	CLA	C1-O2A-CGA	2.01	121.71	116.44
26	C	516	BCR	C37-C22-C23	2.00	121.24	118.08
26	C	516	BCR	C40-C30-C25	-2.00	107.05	110.30
26	t	101	BCR	C33-C5-C4	2.00	117.47	113.62
24	B	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
24	b	621	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	c	505	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
26	y	101	BCR	C11-C10-C9	-2.00	124.45	127.31
37	l	101	LHG	O8-C23-O10	-2.00	118.53	123.59
24	a	410	CLA	C4D-C3D-CAD	-2.00	107.35	108.47
35	J	101	LMG	C7-O1-C1	-2.00	109.83	113.74
25	d	401	PHO	C3A-C4A-NA	2.00	116.47	113.05
36	c	519	DGD	C4D-C3D-C2D	-2.00	107.33	110.82
25	D	401	PHO	O2A-CGA-CBA	2.00	118.19	111.91
24	c	515	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
37	d	407	LHG	O4-P-O5	2.00	122.13	112.24

All (188) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	609	CLA	NC
24	B	609	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	604	CLA	NA
24	a	412	CLA	NC
24	a	412	CLA	ND
24	a	412	CLA	NA
24	b	623	CLA	NC
24	b	623	CLA	ND
24	b	623	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	D	402	CLA	ND
24	c	515	CLA	NC
24	c	515	CLA	ND
24	c	515	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	c	505	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	b	622	CLA	NC
24	b	622	CLA	ND
24	b	622	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	514	CLA	NC
24	C	514	CLA	ND
24	C	514	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	c	509	CLA	ND
24	c	509	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	618	CLA	NA
24	d	402	CLA	NC
24	d	402	CLA	ND
24	d	402	CLA	NA
24	C	506	CLA	ND
24	c	516	CLA	NC
24	c	516	CLA	ND
24	c	516	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA
24	C	503	CLA	NC
24	C	503	CLA	NA
24	b	624	CLA	NA
24	b	624	CLA	NC
24	b	624	CLA	ND
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	505	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	b	621	CLA	NC
24	b	621	CLA	ND
24	b	621	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	A	407	CLA	NC
24	A	407	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	a	409	CLA	NC
24	a	409	CLA	ND
24	a	409	CLA	NA
24	c	514	CLA	NC
24	c	514	CLA	ND
24	c	514	CLA	NA
24	b	625	CLA	NA
24	b	625	CLA	NC
24	b	625	CLA	ND
24	B	617	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	D	403	CLA	NC
24	D	403	CLA	ND
24	D	403	CLA	NA
24	b	614	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	614	CLA	ND
24	b	611	CLA	NC
24	b	611	CLA	ND
24	d	403	CLA	ND
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	a	410	CLA	NC
24	a	410	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	d	404	CLA	NC
24	d	404	CLA	ND
24	d	404	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	ND
24	c	508	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	b	619	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	603	CLA	NA
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	c	506	CLA	NC

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Mol	Chain	Res	Type	Atom
24	c	506	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	c	517	CLA	NC
24	c	517	CLA	ND
24	c	517	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	b	620	CLA	NC
24	b	620	CLA	NA
24	A	409	CLA	NC
24	A	409	CLA	NA

All (1279) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	607	CLA	CHA-CBD-CGD-O2D
37	e	102	LHG	C3-O3-P-O5
37	e	102	LHG	C3-O3-P-O6
27	A	415	SQD	O6-C44-C45-O47
29	F	102	LMT	C2'-C1'-O1'-C1
29	F	102	LMT	O5'-C1'-O1'-C1
28	V	201	GOL	C1-C2-C3-O3
26	D	404	BCR	C7-C8-C9-C10
26	D	404	BCR	C7-C8-C9-C34
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C37-C22-C23-C24
24	b	623	CLA	CHA-CBD-CGD-O1D
24	b	623	CLA	CHA-CBD-CGD-O2D
24	b	623	CLA	CAD-CBD-CGD-O1D
24	b	623	CLA	CAD-CBD-CGD-O2D
24	b	623	CLA	C2-C3-C5-C6
24	b	623	CLA	C4-C3-C5-C6
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
35	Z	101	LMG	O6-C1-O1-C7
35	Z	101	LMG	O9-C10-O7-C8
35	Z	101	LMG	C11-C10-O7-C8
31	a	416	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	a	416	PL9	C20-C19-C21-C22
24	b	615	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O2D
37	L	101	LHG	C4-O6-P-O4
36	D	406	DGD	C2B-C1B-O2G-C2G
36	D	406	DGD	C2D-C1D-O3G-C3G
36	D	406	DGD	O6D-C1D-O3G-C3G
24	B	602	CLA	CHA-CBD-CGD-O1D
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
34	B	624	HTG	C2'-C1'-S1-C1
34	b	632	HTG	O5-C1-S1-C1'
34	b	632	HTG	C2'-C1'-S1-C1
24	C	508	CLA	CHA-CBD-CGD-O2D
28	a	402	GOL	O1-C1-C2-C3
24	A	406	CLA	CHA-CBD-CGD-O1D
24	A	406	CLA	CHA-CBD-CGD-O2D
37	d	408	LHG	O2-C2-C3-O3
37	d	408	LHG	C3-O3-P-O4
28	B	627	GOL	O1-C1-C2-C3
28	f	101	GOL	O1-C1-C2-C3
24	C	510	CLA	C2-C1-O2A-CGA
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
35	C	521	LMG	C11-C10-O7-C8
28	a	401	GOL	C1-C2-C3-O3
29	C	522	LMT	C2'-C1'-O1'-C1
29	C	522	LMT	O5'-C1'-O1'-C1
28	B	628	GOL	O1-C1-C2-C3
29	b	630	LMT	C2'-C1'-O1'-C1
29	b	630	LMT	O5'-C1'-O1'-C1
28	F	101	GOL	O1-C1-C2-C3
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
29	a	419	LMT	C2'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
34	c	524	HTG	C2'-C1'-S1-C1

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Mol	Chain	Res	Type	Atoms
24	B	606	CLA	C2-C3-C5-C6
24	B	606	CLA	C4-C3-C5-C6
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C37-C22-C23-C24
38	e	103	HEM	C2A-CAA-CBA-CGA
38	e	103	HEM	C3D-CAD-CBD-CGD
29	f	103	LMT	C2'-C1'-O1'-C1
29	f	103	LMT	O5'-C1'-O1'-C1
26	B	618	BCR	C1-C6-C7-C8
24	c	512	CLA	CHA-CBD-CGD-O1D
24	c	512	CLA	CHA-CBD-CGD-O2D
28	C	525	GOL	O1-C1-C2-C3
24	b	614	CLA	C2-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
29	T	104	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
28	B	630	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
26	d	405	BCR	C21-C22-C23-C24
26	d	405	BCR	C37-C22-C23-C24
26	d	405	BCR	C23-C24-C25-C30
37	E	101	LHG	C3-O3-P-O4
37	E	101	LHG	C3-O3-P-O5
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O5
28	T	102	GOL	O1-C1-C2-C3
29	B	635	LMT	C2'-C1'-O1'-C1
29	B	635	LMT	O5'-C1'-O1'-C1
29	A	416	LMT	C2'-C1'-O1'-C1
29	A	416	LMT	O5'-C1'-O1'-C1
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
29	M	104	LMT	O5'-C1'-O1'-C1
28	O	301	GOL	O1-C1-C2-C3
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
34	B	625	HTG	O5-C1-S1-C1'
28	A	414	GOL	C1-C2-C3-O3
37	D	408	LHG	C4-O6-P-O4
35	z	101	LMG	O6-C1-O1-C7
35	z	101	LMG	O9-C10-O7-C8
37	l	101	LHG	C4-O6-P-O4
37	l	101	LHG	C4-O6-P-O5
36	e	101	DGD	C2B-C1B-O2G-C2G
36	e	101	DGD	O1B-C1B-O2G-C2G
36	e	101	DGD	O6E-C1E-O5D-C6D
28	A	413	GOL	C1-C2-C3-O3
28	b	606	GOL	O1-C1-C2-C3
29	C	522	LMT	C3'-C4'-O1B-C1B
37	e	102	LHG	O10-C23-O8-C6
29	B	622	LMT	C3'-C4'-O1B-C1B
37	e	102	LHG	C24-C23-O8-C6
37	E	101	LHG	O10-C23-O8-C6
36	D	406	DGD	O1B-C1B-O2G-C2G
35	C	521	LMG	O9-C10-O7-C8
24	b	623	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	A	409	CLA	C3-C5-C6-C7
37	E	101	LHG	C24-C23-O8-C6
27	L	102	SQD	C8-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
35	z	101	LMG	C11-C10-O7-C8
31	a	416	PL9	C12-C11-C9-C10
24	c	511	CLA	C4-C3-C5-C6
31	a	416	PL9	C18-C19-C21-C22
24	c	511	CLA	C2-C3-C5-C6
24	B	607	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C3-C5-C6-C7
24	c	510	CLA	C3-C5-C6-C7
35	z	101	LMG	O6-C5-C6-O5
34	b	632	HTG	S1-C1'-C2'-C3'
26	T	103	BCR	C13-C14-C15-C16
29	M	104	LMT	O5'-C5'-C6'-O6'
37	E	101	LHG	O2-C2-C3-O3
24	B	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	CBD-CGD-O2D-CED
29	M	102	LMT	O5B-C5B-C6B-O6B
36	C	518	DGD	CBB-CCB-CDB-CEB
29	f	103	LMT	C4'-C5'-C6'-O6'
29	M	104	LMT	O5B-C5B-C6B-O6B
29	M	104	LMT	C4'-C5'-C6'-O6'
35	C	521	LMG	O6-C5-C6-O5
31	a	416	PL9	C15-C14-C16-C17
31	a	416	PL9	C25-C24-C26-C27
24	B	615	CLA	C4-C3-C5-C6
31	A	418	PL9	C25-C24-C26-C27
31	a	416	PL9	C13-C14-C16-C17
31	a	416	PL9	C23-C24-C26-C27
31	A	418	PL9	C23-C24-C26-C27
24	b	615	CLA	C2A-CAA-CBA-CGA
35	z	101	LMG	C4-C5-C6-O5
31	d	406	PL9	C39-C41-C42-C43
31	D	405	PL9	C39-C41-C42-C43
24	C	510	CLA	CBA-CGA-O2A-C1
29	f	103	LMT	O5'-C5'-C6'-O6'
37	l	101	LHG	C7-C8-C9-C10
34	B	625	HTG	O5-C5-C6-O6
35	M	101	LMG	C15-C16-C17-C18
36	C	517	DGD	C2A-C3A-C4A-C5A
24	b	624	CLA	C10-C11-C12-C13
24	A	409	CLA	C13-C15-C16-C17
36	e	101	DGD	C2E-C1E-O5D-C6D
24	B	602	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C10-C8-C9
24	C	502	CLA	C11-C12-C13-C14
24	B	617	CLA	C6-C7-C8-C9
24	B	603	CLA	C14-C13-C15-C16
24	c	510	CLA	C6-C7-C8-C9
34	B	632	HTG	C4-C5-C6-O6
35	Z	101	LMG	C10-C11-C12-C13
24	B	615	CLA	C10-C11-C12-C13
24	C	509	CLA	C5-C6-C7-C8
24	b	615	CLA	C13-C15-C16-C17
24	C	502	CLA	C15-C16-C17-C18
24	B	617	CLA	C10-C11-C12-C13
24	c	512	CLA	C15-C16-C17-C18
29	B	622	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
35	c	522	LMG	C10-C11-C12-C13
37	L	101	LHG	C7-C8-C9-C10
35	C	521	LMG	C28-C29-C30-C31
34	b	601	HTG	C1'-C2'-C3'-C4'
29	m	102	LMT	O5'-C5'-C6'-O6'
24	B	602	CLA	C10-C11-C12-C13
24	B	616	CLA	C8-C10-C11-C12
24	B	615	CLA	C5-C6-C7-C8
24	B	615	CLA	C8-C10-C11-C12
36	C	517	DGD	C4A-C5A-C6A-C7A
28	b	605	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-O2
28	f	101	GOL	O1-C1-C2-O2
28	B	628	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-O2
28	A	413	GOL	O2-C2-C3-O3
24	C	510	CLA	O1A-CGA-O2A-C1
27	A	415	SQD	C23-C24-C25-C26
37	D	407	LHG	C23-C24-C25-C26
36	C	518	DGD	C1B-C2B-C3B-C4B
35	j	101	LMG	O6-C5-C6-O5
24	a	412	CLA	C8-C10-C11-C12
24	C	505	CLA	C15-C16-C17-C18
24	C	507	CLA	C13-C15-C16-C17
24	C	510	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
35	a	415	LMG	C17-C18-C19-C20
29	A	416	LMT	O5B-C5B-C6B-O6B
24	b	610	CLA	C2-C1-O2A-CGA
36	c	521	DGD	C1A-C2A-C3A-C4A
29	C	522	LMT	O5B-C5B-C6B-O6B
24	b	615	CLA	C12-C13-C15-C16
24	b	625	CLA	C11-C12-C13-C15
35	a	415	LMG	C10-C11-C12-C13
29	T	104	LMT	O1'-C1-C2-C3
29	M	102	LMT	C4B-C5B-C6B-O6B
36	e	101	DGD	O6D-C1D-O3G-C3G
24	b	623	CLA	C5-C6-C7-C8
34	V	206	HTG	S1-C1'-C2'-C3'
24	a	412	CLA	C10-C11-C12-C13
24	c	513	CLA	C13-C15-C16-C17
35	C	521	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
35	C	501	LMG	C11-C10-O7-C8
37	e	102	LHG	C11-C12-C13-C14
24	C	509	CLA	C10-C11-C12-C13
24	c	511	CLA	C5-C6-C7-C8
24	C	507	CLA	C5-C6-C7-C8
37	L	101	LHG	C4-O6-P-O3
37	d	408	LHG	C3-O3-P-O6
37	l	101	LHG	C4-O6-P-O3
27	B	621	SQD	C7-C8-C9-C10
34	b	632	HTG	C1'-C2'-C3'-C4'
24	B	605	CLA	CBD-CGD-O2D-CED
37	E	101	LHG	C1-C2-C3-O3
35	C	501	LMG	O9-C10-O7-C8
24	B	615	CLA	C2-C3-C5-C6
24	b	623	CLA	C13-C15-C16-C17
24	b	622	CLA	CBD-CGD-O2D-CED
27	F	103	SQD	C26-C27-C28-C29
29	M	104	LMT	C4B-C5B-C6B-O6B
36	C	519	DGD	C8A-C9A-CAA-CBA
24	B	614	CLA	C13-C15-C16-C17
26	t	101	BCR	C13-C14-C15-C16
35	C	501	LMG	C11-C12-C13-C14
34	c	524	HTG	C1'-C2'-C3'-C4'
36	c	519	DGD	C5A-C6A-C7A-C8A
36	c	521	DGD	C6A-C7A-C8A-C9A
36	C	517	DGD	C4B-C5B-C6B-C7B
27	B	621	SQD	C31-C32-C33-C34
29	T	104	LMT	C4-C5-C6-C7
24	a	412	CLA	C16-C17-C18-C19
34	c	524	HTG	S1-C1'-C2'-C3'
37	e	102	LHG	C24-C25-C26-C27
27	A	411	SQD	C9-C10-C11-C12
36	C	518	DGD	C9A-CAA-CBA-CCA
37	L	101	LHG	C14-C15-C16-C17
36	D	406	DGD	C6A-C7A-C8A-C9A
34	B	624	HTG	C2'-C3'-C4'-C5'
36	c	520	DGD	C9A-CAA-CBA-CCA
29	T	104	LMT	C11-C10-C9-C8
35	j	101	LMG	C19-C20-C21-C22
27	A	415	SQD	C30-C31-C32-C33
36	e	101	DGD	CCA-CDA-CEA-CFA
36	e	101	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
37	D	408	LHG	O2-C2-C3-O3
36	H	102	DGD	CBB-CCB-CDB-CEB
29	M	104	LMT	C2-C3-C4-C5
27	A	415	SQD	C2-C1-O6-C44
36	c	520	DGD	C2E-C1E-O5D-C6D
29	B	622	LMT	C2'-C1'-O1'-C1
36	C	518	DGD	C2E-C1E-O5D-C6D
36	e	101	DGD	C2D-C1D-O3G-C3G
27	L	102	SQD	C12-C13-C14-C15
29	B	635	LMT	C3-C4-C5-C6
35	c	522	LMG	C34-C35-C36-C37
37	D	407	LHG	C24-C25-C26-C27
31	a	416	PL9	C12-C11-C9-C8
24	B	604	CLA	C6-C7-C8-C9
24	a	410	CLA	C11-C12-C13-C14
36	c	519	DGD	O6D-C5D-C6D-O5D
35	b	629	LMG	C32-C33-C34-C35
35	C	501	LMG	C14-C15-C16-C17
35	C	501	LMG	C30-C31-C32-C33
24	c	514	CLA	C8-C10-C11-C12
34	B	632	HTG	O5-C5-C6-O6
36	c	521	DGD	C7A-C8A-C9A-CAA
35	M	101	LMG	C36-C37-C38-C39
28	B	626	GOL	C1-C2-C3-O3
28	b	602	GOL	O1-C1-C2-C3
28	b	602	GOL	C1-C2-C3-O3
28	v	201	GOL	O1-C1-C2-C3
28	b	605	GOL	O1-C1-C2-C3
37	d	409	LHG	O1-C1-C2-C3
28	V	202	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
28	B	629	GOL	O1-C1-C2-C3
28	o	301	GOL	C1-C2-C3-O3
28	b	604	GOL	O1-C1-C2-C3
35	c	522	LMG	C11-C10-O7-C8
37	d	407	LHG	C32-C33-C34-C35
37	D	409	LHG	C29-C30-C31-C32
36	C	519	DGD	CAA-CBA-CCA-CDA
35	M	101	LMG	C29-C30-C31-C32
29	T	104	LMT	C7-C8-C9-C10
36	D	406	DGD	C2A-C3A-C4A-C5A
27	L	102	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
35	b	629	LMG	C38-C39-C40-C41
35	a	415	LMG	C21-C22-C23-C24
35	z	101	LMG	C12-C13-C14-C15
34	b	632	HTG	O5-C5-C6-O6
24	a	412	CLA	C16-C17-C18-C20
24	b	620	CLA	C16-C17-C18-C19
36	C	518	DGD	O6E-C1E-O5D-C6D
36	h	102	DGD	CAA-CBA-CCA-CDA
27	a	414	SQD	C11-C12-C13-C14
27	a	405	SQD	C31-C32-C33-C34
24	c	515	CLA	CBD-CGD-O2D-CED
35	C	520	LMG	C11-C12-C13-C14
35	J	101	LMG	C19-C20-C21-C22
27	L	102	SQD	C24-C23-O48-C46
27	a	414	SQD	C29-C30-C31-C32
29	M	104	LMT	C2-C1-O1'-C1'
35	M	101	LMG	C31-C32-C33-C34
36	C	517	DGD	C5B-C6B-C7B-C8B
27	a	405	SQD	C25-C26-C27-C28
37	l	101	LHG	C27-C28-C29-C30
37	D	407	LHG	C34-C35-C36-C37
36	c	521	DGD	C7B-C8B-C9B-CAB
29	a	404	LMT	C4B-C5B-C6B-O6B
36	C	517	DGD	C3B-C4B-C5B-C6B
27	B	621	SQD	C30-C31-C32-C33
35	j	101	LMG	C14-C15-C16-C17
36	C	517	DGD	O6D-C5D-C6D-O5D
36	e	101	DGD	O6D-C5D-C6D-O5D
34	C	524	HTG	O5-C5-C6-O6
27	A	415	SQD	C26-C27-C28-C29
36	c	520	DGD	C4A-C5A-C6A-C7A
24	C	511	CLA	C4-C3-C5-C6
31	D	405	PL9	C15-C14-C16-C17
24	c	516	CLA	CBA-CGA-O2A-C1
36	e	101	DGD	C2A-C1A-O1G-C1G
24	c	514	CLA	C2-C3-C5-C6
24	C	511	CLA	C2-C3-C5-C6
31	D	405	PL9	C13-C14-C16-C17
29	a	404	LMT	C2-C3-C4-C5
36	c	521	DGD	C6B-C7B-C8B-C9B
28	v	201	GOL	O1-C1-C2-O2
28	a	402	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	a	401	GOL	O2-C2-C3-O3
28	C	525	GOL	O1-C1-C2-O2
28	B	630	GOL	O1-C1-C2-O2
28	O	301	GOL	O1-C1-C2-O2
35	Z	101	LMG	C19-C20-C21-C22
36	c	519	DGD	C9A-CAA-CBA-CCA
36	c	519	DGD	C8B-C9B-CAB-CBB
29	C	522	LMT	O5'-C5'-C6'-O6'
27	A	411	SQD	C14-C15-C16-C17
29	T	104	LMT	C1-C2-C3-C4
29	B	635	LMT	C11-C10-C9-C8
36	C	518	DGD	C1A-C2A-C3A-C4A
37	d	408	LHG	C1-C2-C3-O3
35	b	629	LMG	C16-C17-C18-C19
35	a	415	LMG	C29-C30-C31-C32
24	c	513	CLA	C2-C1-O2A-CGA
24	B	617	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C10-C11-C12-C13
27	A	411	SQD	C13-C14-C15-C16
36	e	101	DGD	C2A-C3A-C4A-C5A
26	B	618	BCR	C5-C6-C7-C8
26	b	626	BCR	C1-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
34	B	625	HTG	C3'-C4'-C5'-C6'
27	L	102	SQD	C35-C36-C37-C38
24	c	516	CLA	O1A-CGA-O2A-C1
24	B	602	CLA	C8-C10-C11-C12
24	c	514	CLA	C4-C3-C5-C6
24	B	604	CLA	C6-C7-C8-C10
24	b	612	CLA	C6-C7-C8-C10
25	D	401	PHO	C2-C3-C5-C6
24	B	615	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	C	507	CLA	C6-C7-C8-C10
24	a	410	CLA	C11-C12-C13-C15
27	L	102	SQD	O10-C23-O48-C46
36	e	101	DGD	O1A-C1A-O1G-C1G
35	c	522	LMG	O9-C10-O7-C8
24	C	513	CLA	CBA-CGA-O2A-C1
35	a	415	LMG	C12-C13-C14-C15
37	d	409	LHG	C31-C32-C33-C34
29	a	419	LMT	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
35	a	415	LMG	C14-C15-C16-C17
27	L	102	SQD	C30-C31-C32-C33
35	z	101	LMG	C15-C16-C17-C18
36	e	101	DGD	C2B-C3B-C4B-C5B
35	j	101	LMG	C38-C39-C40-C41
36	c	519	DGD	C4D-C5D-C6D-O5D
24	b	623	CLA	C16-C17-C18-C19
27	A	415	SQD	O5-C1-O6-C44
36	c	520	DGD	O6E-C1E-O5D-C6D
34	b	631	HTG	C2'-C3'-C4'-C5'
36	H	102	DGD	C3B-C4B-C5B-C6B
29	A	416	LMT	C6-C7-C8-C9
35	z	101	LMG	C13-C14-C15-C16
37	e	102	LHG	C23-C24-C25-C26
36	C	517	DGD	C1B-C2B-C3B-C4B
36	c	519	DGD	C7B-C8B-C9B-CAB
37	E	101	LHG	C24-C25-C26-C27
27	F	103	SQD	C31-C32-C33-C34
37	d	409	LHG	C29-C30-C31-C32
27	F	103	SQD	C2-C1-O6-C44
35	Z	101	LMG	O6-C5-C6-O5
37	D	409	LHG	C24-C23-O8-C6
37	D	407	LHG	C25-C26-C27-C28
27	L	102	SQD	C29-C30-C31-C32
37	l	101	LHG	C33-C34-C35-C36
35	b	629	LMG	C33-C34-C35-C36
34	b	601	HTG	C2'-C3'-C4'-C5'
36	c	519	DGD	O6E-C5E-C6E-O5E
24	b	610	CLA	C8-C10-C11-C12
25	D	401	PHO	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
35	C	501	LMG	C10-C11-C12-C13
34	B	625	HTG	C4-C5-C6-O6
24	c	508	CLA	C2-C3-C5-C6
31	a	416	PL9	C4-C3-C7-C8
31	A	418	PL9	C4-C3-C7-C8
27	L	102	SQD	C28-C29-C30-C31
24	b	623	CLA	C11-C12-C13-C14
24	b	612	CLA	C6-C7-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	c	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C6-C7-C8-C9
24	b	625	CLA	C11-C12-C13-C14
24	b	619	CLA	C11-C12-C13-C14
36	D	406	DGD	C8B-C9B-CAB-CBB
36	h	102	DGD	C5B-C6B-C7B-C8B
34	b	631	HTG	C3'-C4'-C5'-C6'
24	c	512	CLA	C1A-C2A-CAA-CBA
24	b	623	CLA	C16-C17-C18-C20
24	b	620	CLA	C16-C17-C18-C20
37	d	408	LHG	C34-C35-C36-C37
24	a	409	CLA	C2C-C3C-CAC-CBC
36	C	518	DGD	C8A-C9A-CAA-CBA
36	e	101	DGD	C5A-C6A-C7A-C8A
35	c	523	LMG	C10-C11-C12-C13
36	c	519	DGD	CAB-CBB-CCB-CDB
35	C	501	LMG	C32-C33-C34-C35
24	B	616	CLA	C13-C15-C16-C17
35	C	501	LMG	C12-C13-C14-C15
34	C	524	HTG	S1-C1'-C2'-C3'
36	c	520	DGD	C3B-C4B-C5B-C6B
37	d	408	LHG	C24-C23-O8-C6
24	C	512	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C24-C23-O48-C46
35	j	101	LMG	C17-C18-C19-C20
29	f	103	LMT	C5-C6-C7-C8
24	C	513	CLA	O1A-CGA-O2A-C1
24	c	510	CLA	C16-C17-C18-C19
36	C	517	DGD	C4D-C5D-C6D-O5D
27	A	415	SQD	O6-C44-C45-C46
35	c	522	LMG	C7-C8-C9-O8
35	Z	101	LMG	C7-C8-C9-O8
36	D	406	DGD	O1G-C1G-C2G-C3G
27	F	103	SQD	C44-C45-C46-O48
27	a	414	SQD	O6-C44-C45-C46
27	B	621	SQD	C44-C45-C46-O48
27	B	621	SQD	C35-C36-C37-C38
37	E	101	LHG	C4-C5-C6-O8
35	a	415	LMG	C7-C8-C9-O8
27	a	405	SQD	O6-C44-C45-C46
36	e	101	DGD	O1G-C1G-C2G-C3G
37	d	408	LHG	O10-C23-O8-C6
24	C	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	c	520	DGD	C2G-C3G-O3G-C1D
36	c	520	DGD	C5D-C6D-O5D-C1E
35	C	521	LMG	C8-C7-O1-C1
36	C	518	DGD	C2G-C3G-O3G-C1D
29	C	522	LMT	C9-C10-C11-C12
36	H	102	DGD	CDB-CEB-CFB-CGB
36	D	406	DGD	C7A-C8A-C9A-CAA
35	b	629	LMG	C40-C41-C42-C43
36	C	517	DGD	O6E-C5E-C6E-O5E
37	E	101	LHG	C19-C20-C21-C22
29	B	622	LMT	O5'-C1'-O1'-C1
28	V	201	GOL	O2-C2-C3-O3
28	V	202	GOL	O1-C1-C2-O2
28	A	414	GOL	O2-C2-C3-O3
37	d	407	LHG	C29-C30-C31-C32
27	F	103	SQD	C30-C31-C32-C33
36	C	519	DGD	CDA-CEA-CFA-CGA
27	a	405	SQD	C28-C29-C30-C31
24	b	623	CLA	C10-C11-C12-C13
35	c	522	LMG	C20-C21-C22-C23
27	a	414	SQD	C9-C10-C11-C12
36	C	518	DGD	CAB-CBB-CCB-CDB
24	B	604	CLA	C5-C6-C7-C8
29	a	404	LMT	C7-C8-C9-C10
27	L	102	SQD	C24-C25-C26-C27
24	c	506	CLA	C16-C17-C18-C19
36	C	519	DGD	C2A-C1A-O1G-C1G
35	j	101	LMG	C36-C37-C38-C39
24	a	412	CLA	C15-C16-C17-C18
36	H	102	DGD	CDA-CEA-CFA-CGA
35	J	101	LMG	O6-C5-C6-O5
24	c	510	CLA	C15-C16-C17-C18
24	C	513	CLA	CBD-CGD-O2D-CED
24	D	403	CLA	C3-C5-C6-C7
36	H	102	DGD	C7B-C8B-C9B-CAB
24	c	509	CLA	O1D-CGD-O2D-CED
24	C	510	CLA	C5-C6-C7-C8
27	A	415	SQD	C24-C23-O48-C46
35	M	101	LMG	C16-C17-C18-C19
35	a	415	LMG	C33-C34-C35-C36
37	D	409	LHG	O10-C23-O8-C6
29	f	103	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	l	101	LHG	C12-C13-C14-C15
27	A	411	SQD	C7-C8-C9-C10
27	a	405	SQD	C23-C24-C25-C26
24	a	410	CLA	C10-C11-C12-C13
24	c	508	CLA	C15-C16-C17-C18
35	Z	101	LMG	C2-C1-O1-C7
35	c	522	LMG	O1-C7-C8-O7
27	f	102	SQD	O6-C44-C45-O47
37	L	101	LHG	C13-C14-C15-C16
27	a	414	SQD	C34-C35-C36-C37
36	e	101	DGD	C4D-C5D-C6D-O5D
24	b	623	CLA	C11-C12-C13-C15
24	B	602	CLA	C11-C10-C8-C7
24	B	616	CLA	C11-C12-C13-C15
24	B	616	CLA	C12-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C10
24	c	513	CLA	C12-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C7
24	B	603	CLA	C12-C13-C15-C16
24	b	610	CLA	C6-C7-C8-C10
35	j	101	LMG	C35-C36-C37-C38
24	b	615	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	c	513	CLA	C14-C13-C15-C16
24	C	513	CLA	C11-C10-C8-C9
24	a	410	CLA	C6-C7-C8-C9
24	a	410	CLA	C14-C13-C15-C16
24	c	510	CLA	C11-C10-C8-C9
24	b	610	CLA	C6-C7-C8-C9
24	b	610	CLA	C11-C10-C8-C9
37	e	102	LHG	C14-C15-C16-C17
36	c	521	DGD	C5B-C6B-C7B-C8B
35	j	101	LMG	C13-C14-C15-C16
24	b	613	CLA	C13-C15-C16-C17
27	A	415	SQD	C11-C12-C13-C14
29	B	635	LMT	C4-C5-C6-C7
24	c	515	CLA	O1D-CGD-O2D-CED
24	B	611	CLA	C16-C17-C18-C20
27	L	102	SQD	C11-C12-C13-C14
34	B	624	HTG	C1'-C2'-C3'-C4'
26	y	101	BCR	C21-C22-C23-C24
29	m	102	LMT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
29	b	630	LMT	C3'-C4'-O1B-C1B
24	B	602	CLA	CBA-CGA-O2A-C1
24	b	610	CLA	CBA-CGA-O2A-C1
35	C	501	LMG	C13-C14-C15-C16
36	H	102	DGD	C4E-C5E-C6E-O5E
35	a	415	LMG	C35-C36-C37-C38
24	c	516	CLA	C15-C16-C17-C18
37	l	101	LHG	O6-C4-C5-C6
31	a	416	PL9	C14-C16-C17-C18
29	a	404	LMT	O5B-C5B-C6B-O6B
24	c	514	CLA	CBA-CGA-O2A-C1
24	C	511	CLA	CBA-CGA-O2A-C1
29	M	105	LMT	O5'-C5'-C6'-O6'
35	c	523	LMG	O6-C5-C6-O5
27	a	414	SQD	C17-C18-C19-C20
36	H	102	DGD	C7A-C8A-C9A-CAA
27	B	621	SQD	C11-C10-C9-C8
31	a	416	PL9	C45-C44-C46-C47
31	A	418	PL9	C15-C14-C16-C17
27	B	621	SQD	O10-C23-O48-C46
34	B	632	HTG	C2'-C3'-C4'-C5'
24	B	611	CLA	C16-C17-C18-C19
37	L	101	LHG	C30-C31-C32-C33
36	c	521	DGD	C2A-C1A-O1G-C1G
24	C	514	CLA	C3A-C2A-CAA-CBA
24	b	617	CLA	C13-C15-C16-C17
36	D	406	DGD	C4B-C5B-C6B-C7B
27	L	102	SQD	C32-C33-C34-C35
29	B	635	LMT	C2-C3-C4-C5
35	C	520	LMG	C14-C15-C16-C17
35	c	522	LMG	C40-C41-C42-C43
27	F	103	SQD	C32-C33-C34-C35
24	c	515	CLA	CBA-CGA-O2A-C1
37	e	102	LHG	C4-C5-C6-O8
27	L	102	SQD	C44-C45-C46-O48
35	C	501	LMG	C7-C8-C9-O8
36	D	406	DGD	C1B-C2B-C3B-C4B
37	D	409	LHG	C12-C13-C14-C15
27	a	414	SQD	C15-C16-C17-C18
27	a	414	SQD	C19-C20-C21-C22
36	C	518	DGD	C6B-C7B-C8B-C9B
36	c	519	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
24	b	610	CLA	C16-C17-C18-C20
31	a	416	PL9	C43-C44-C46-C47
36	h	102	DGD	C9B-CAB-CBB-CCB
35	J	101	LMG	C13-C14-C15-C16
36	C	518	DGD	C4B-C5B-C6B-C7B
24	b	622	CLA	O1D-CGD-O2D-CED
28	b	602	GOL	O2-C2-C3-O3
28	v	203	GOL	O1-C1-C2-O2
28	F	101	GOL	O1-C1-C2-O2
28	B	630	GOL	O2-C2-C3-O3
28	b	604	GOL	O1-C1-C2-O2
27	f	102	SQD	C24-C25-C26-C27
36	C	519	DGD	O1A-C1A-O1G-C1G
36	c	520	DGD	C2A-C3A-C4A-C5A
35	j	101	LMG	C16-C17-C18-C19
36	c	521	DGD	CBA-CCA-CDA-CEA
29	B	622	LMT	O5B-C1B-O1B-C4'
35	Z	101	LMG	O1-C7-C8-O7
35	Z	101	LMG	O7-C8-C9-O8
36	D	406	DGD	O2G-C2G-C3G-O3G
27	a	414	SQD	O6-C44-C45-O47
29	a	404	LMT	C6-C7-C8-C9
29	M	105	LMT	O5'-C1'-O1'-C1
24	b	615	CLA	C10-C11-C12-C13
24	b	625	CLA	C10-C11-C12-C13
31	A	418	PL9	C13-C14-C16-C17
24	b	623	CLA	C11-C10-C8-C9
24	b	615	CLA	C11-C10-C8-C9
24	c	516	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C10-C8-C9
27	a	405	SQD	C19-C20-C21-C22
31	A	418	PL9	C2-C3-C7-C8
36	c	519	DGD	C3A-C4A-C5A-C6A
27	a	405	SQD	C27-C28-C29-C30
26	D	404	BCR	C1-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	C	516	BCR	C1-C6-C7-C8
26	C	516	BCR	C5-C6-C7-C8
26	b	627	BCR	C23-C24-C25-C26
26	b	627	BCR	C23-C24-C25-C30
24	b	610	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	Y	101	BCR	C37-C22-C23-C24
27	B	621	SQD	C17-C18-C19-C20
26	Y	101	BCR	C21-C22-C23-C24
29	m	102	LMT	C1-C2-C3-C4
35	a	415	LMG	O9-C10-O7-C8
37	E	101	LHG	C8-C7-O7-C5
27	a	414	SQD	C35-C36-C37-C38
24	c	510	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C20
37	L	101	LHG	C16-C17-C18-C19
27	A	415	SQD	O10-C23-O48-C46
24	c	514	CLA	O1A-CGA-O2A-C1
24	C	511	CLA	O1A-CGA-O2A-C1
24	b	610	CLA	O1A-CGA-O2A-C1
36	c	521	DGD	C4A-C5A-C6A-C7A
37	e	102	LHG	O6-C4-C5-C6
36	h	102	DGD	O2G-C1B-C2B-C3B
35	C	520	LMG	C30-C31-C32-C33
36	e	101	DGD	C4A-C5A-C6A-C7A
24	c	516	CLA	C11-C10-C8-C7
24	c	510	CLA	C6-C7-C8-C10
24	c	510	CLA	C11-C10-C8-C7
36	C	518	DGD	C4A-C5A-C6A-C7A
24	b	619	CLA	C16-C17-C18-C20
37	D	409	LHG	C28-C29-C30-C31
27	a	414	SQD	C12-C13-C14-C15
36	e	101	DGD	C6A-C7A-C8A-C9A
35	C	520	LMG	C31-C32-C33-C34
24	c	515	CLA	O1A-CGA-O2A-C1
29	M	105	LMT	C5-C6-C7-C8
35	a	415	LMG	C11-C10-O7-C8
35	j	101	LMG	C15-C16-C17-C18
24	a	409	CLA	C4C-C3C-CAC-CBC
37	D	408	LHG	C13-C14-C15-C16
37	d	407	LHG	C25-C26-C27-C28
36	e	101	DGD	C7B-C8B-C9B-CAB
24	A	405	CLA	C13-C15-C16-C17
25	D	401	PHO	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CAD-CBD-CGD-O2D
24	b	625	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	C	511	CLA	CAD-CBD-CGD-O2D
24	b	619	CLA	CAD-CBD-CGD-O2D
24	c	517	CLA	CAD-CBD-CGD-O2D
36	D	406	DGD	C5B-C6B-C7B-C8B
24	d	404	CLA	C15-C16-C17-C18
29	f	103	LMT	C9-C10-C11-C12
24	b	625	CLA	C4-C3-C5-C6
34	B	623	HTG	C3'-C4'-C5'-C6'
35	C	520	LMG	C29-C30-C31-C32
27	F	103	SQD	O5-C1-O6-C44
24	b	625	CLA	C2-C3-C5-C6
31	D	405	PL9	C9-C11-C12-C13
35	c	522	LMG	C36-C37-C38-C39
37	D	409	LHG	C24-C25-C26-C27
37	D	409	LHG	C2-C3-O3-P
37	d	409	LHG	C2-C3-O3-P
35	C	501	LMG	O1-C7-C8-C9
35	z	101	LMG	O1-C7-C8-C9
37	l	101	LHG	O6-C4-C5-O7
24	b	610	CLA	CAA-CBA-CGA-O2A
24	b	619	CLA	C2A-CAA-CBA-CGA
36	h	102	DGD	C6A-C7A-C8A-C9A
24	C	510	CLA	C16-C17-C18-C19
24	A	405	CLA	C16-C17-C18-C19
37	E	101	LHG	O9-C7-O7-C5
24	B	602	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
24	C	503	CLA	CHA-CBD-CGD-O1D
24	C	503	CLA	CHA-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O1D
24	b	610	CLA	CHA-CBD-CGD-O2D
24	c	506	CLA	CHA-CBD-CGD-O1D
27	A	411	SQD	C18-C19-C20-C21
24	B	602	CLA	O1A-CGA-O2A-C1
27	F	103	SQD	C33-C34-C35-C36
35	b	629	LMG	C39-C40-C41-C42
29	M	105	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
35	c	522	LMG	O7-C8-C9-O8
36	D	406	DGD	O1G-C1G-C2G-O2G
27	L	102	SQD	O47-C45-C46-O48
37	E	101	LHG	O7-C5-C6-O8
35	a	415	LMG	O7-C8-C9-O8
35	C	501	LMG	O7-C8-C9-O8
36	e	101	DGD	O1G-C1G-C2G-O2G
35	b	629	LMG	C37-C38-C39-C40
37	l	101	LHG	C17-C18-C19-C20
24	b	610	CLA	C16-C17-C18-C19
28	f	101	GOL	O2-C2-C3-O3
28	V	203	GOL	O2-C2-C3-O3
28	v	202	GOL	O1-C1-C2-O2
28	B	629	GOL	O1-C1-C2-O2
28	b	606	GOL	O1-C1-C2-O2
24	B	616	CLA	C4-C3-C5-C6
24	A	406	CLA	C2C-C3C-CAC-CBC
27	A	411	SQD	C16-C17-C18-C19
35	C	501	LMG	C36-C37-C38-C39
36	e	101	DGD	C9B-CAB-CBB-CCB
36	c	520	DGD	CCB-CDB-CEB-CFB
36	C	518	DGD	C3B-C4B-C5B-C6B
34	b	607	HTG	C4'-C5'-C6'-C7'
36	c	521	DGD	O1A-C1A-O1G-C1G
24	B	613	CLA	C8-C10-C11-C12
27	F	103	SQD	C5-C6-S-O8
26	C	516	BCR	C11-C12-C13-C35
26	b	628	BCR	C37-C22-C23-C24
28	o	301	GOL	O1-C1-C2-C3
28	b	606	GOL	C1-C2-C3-O3
36	c	520	DGD	C6A-C7A-C8A-C9A
24	b	621	CLA	C1A-C2A-CAA-CBA
24	B	616	CLA	C5-C6-C7-C8
34	b	601	HTG	C3'-C4'-C5'-C6'
37	E	101	LHG	C4-O6-P-O3
37	D	408	LHG	C3-O3-P-O6
36	H	102	DGD	O2G-C1B-C2B-C3B
24	b	612	CLA	C5-C6-C7-C8
35	C	520	LMG	C12-C13-C14-C15
36	C	518	DGD	C5A-C6A-C7A-C8A
35	C	520	LMG	O10-C28-O8-C9
37	L	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
27	F	103	SQD	C34-C35-C36-C37
24	c	513	CLA	C15-C16-C17-C18
24	B	612	CLA	C15-C16-C17-C18
24	b	621	CLA	C8-C10-C11-C12
31	a	416	PL9	C39-C41-C42-C43
37	d	407	LHG	C30-C31-C32-C33
29	M	105	LMT	C1-C2-C3-C4
37	d	407	LHG	C11-C10-C9-C8
35	M	101	LMG	C34-C35-C36-C37
36	c	520	DGD	C2B-C3B-C4B-C5B
24	b	619	CLA	C16-C17-C18-C19
27	a	405	SQD	C35-C36-C37-C38
27	A	415	SQD	O5-C5-C6-S
24	B	602	CLA	CAD-CBD-CGD-O1D
27	F	103	SQD	C5-C6-S-O9
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
27	f	102	SQD	C31-C32-C33-C34
35	C	520	LMG	C29-C28-O8-C9
37	e	102	LHG	O6-C4-C5-O7
24	b	623	CLA	C12-C13-C15-C16
24	B	616	CLA	C2-C3-C5-C6
24	c	513	CLA	C11-C10-C8-C7
24	B	612	CLA	C12-C13-C15-C16
24	A	407	CLA	C11-C10-C8-C7
24	B	617	CLA	C6-C7-C8-C10
24	a	410	CLA	C11-C10-C8-C7
24	A	409	CLA	C6-C7-C8-C10
34	V	206	HTG	C2-C1-S1-C1'
37	d	409	LHG	C9-C10-C11-C12
35	a	415	LMG	C19-C20-C21-C22
24	b	620	CLA	C8-C10-C11-C12
29	f	103	LMT	C2B-C1B-O1B-C4'
27	a	414	SQD	C27-C28-C29-C30
29	b	630	LMT	C6-C7-C8-C9
35	C	521	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	H	102	DGD	C5A-C6A-C7A-C8A
27	a	405	SQD	C24-C25-C26-C27
27	A	415	SQD	C24-C25-C26-C27
35	c	522	LMG	O1-C7-C8-C9
24	d	402	CLA	C2C-C3C-CAC-CBC
37	e	102	LHG	O7-C5-C6-O8
35	C	501	LMG	O1-C7-C8-O7
35	z	101	LMG	O1-C7-C8-O7
24	c	510	CLA	C10-C11-C12-C13
34	B	623	HTG	C4'-C5'-C6'-C7'
29	C	522	LMT	O1'-C1-C2-C3
36	e	101	DGD	CAA-CBA-CCA-CDA
36	C	518	DGD	C5D-C6D-O5D-C1E
24	C	510	CLA	C10-C11-C12-C13
24	C	510	CLA	C13-C15-C16-C17
24	B	614	CLA	C15-C16-C17-C18
24	C	502	CLA	C13-C15-C16-C17
31	d	406	PL9	C45-C44-C46-C47
29	B	622	LMT	C2B-C1B-O1B-C4'
31	d	406	PL9	C43-C44-C46-C47
29	F	102	LMT	C2-C3-C4-C5
24	D	403	CLA	C8-C10-C11-C12
24	B	612	CLA	C14-C13-C15-C16
35	a	415	LMG	C31-C32-C33-C34
24	C	514	CLA	C3-C5-C6-C7
29	a	404	LMT	C3-C4-C5-C6
24	d	402	CLA	C15-C16-C17-C18
35	C	520	LMG	C35-C36-C37-C38
27	L	102	SQD	C31-C32-C33-C34
36	D	406	DGD	C3B-C4B-C5B-C6B
37	D	407	LHG	C11-C10-C9-C8
29	A	416	LMT	O1'-C1-C2-C3
37	d	409	LHG	C30-C31-C32-C33
35	b	629	LMG	C17-C18-C19-C20
24	b	623	CLA	C15-C16-C17-C18
35	C	501	LMG	C18-C19-C20-C21
36	C	519	DGD	C9A-CAA-CBA-CCA
37	D	407	LHG	C33-C34-C35-C36
36	c	519	DGD	CBA-CCA-CDA-CEA
27	L	102	SQD	C46-C45-O47-C7
27	B	621	SQD	C46-C45-O47-C7
24	b	623	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	c	505	CLA	C2A-CAA-CBA-CGA
24	b	622	CLA	C2-C1-O2A-CGA
24	C	512	CLA	C2-C1-O2A-CGA
37	D	407	LHG	C7-C8-C9-C10
27	a	414	SQD	C7-C8-C9-C10
37	d	407	LHG	C33-C34-C35-C36
24	C	510	CLA	C8-C10-C11-C12
24	a	412	CLA	O1A-CGA-O2A-C1
37	D	407	LHG	O10-C23-O8-C6
29	m	102	LMT	C11-C10-C9-C8
24	C	513	CLA	O1D-CGD-O2D-CED
31	D	405	PL9	C35-C34-C36-C37
26	D	404	BCR	C5-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	b	626	BCR	C5-C6-C7-C8
37	E	101	LHG	C15-C16-C17-C18
24	b	624	CLA	C16-C17-C18-C19
36	C	517	DGD	O6E-C1E-O5D-C6D
24	B	611	CLA	C2A-CAA-CBA-CGA
36	C	517	DGD	C2E-C1E-O5D-C6D
29	M	104	LMT	C2'-C1'-O1'-C1
27	F	103	SQD	O47-C45-C46-O48
27	B	621	SQD	O47-C45-C46-O48
37	e	102	LHG	C4-O6-P-O3
37	D	408	LHG	C4-O6-P-O3
35	c	522	LMG	C39-C40-C41-C42
37	D	408	LHG	C11-C10-C9-C8
27	f	102	SQD	O6-C44-C45-C46
24	b	615	CLA	C11-C10-C8-C7
24	d	403	CLA	C11-C12-C13-C15
24	a	410	CLA	C12-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C7
24	A	407	CLA	C11-C10-C8-C9
24	a	410	CLA	C11-C10-C8-C9
26	h	101	BCR	C9-C10-C11-C12
36	D	406	DGD	C2B-C3B-C4B-C5B
37	e	102	LHG	C13-C14-C15-C16
34	B	625	HTG	C2'-C3'-C4'-C5'
37	d	407	LHG	C34-C35-C36-C37
36	H	102	DGD	CCA-CDA-CEA-CFA
37	D	409	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	a	405	SQD	C24-C23-O48-C46
28	v	202	GOL	C1-C2-C3-O3
25	a	411	PHO	C2C-C3C-CAC-CBC
36	c	519	DGD	C1A-C2A-C3A-C4A
28	B	626	GOL	O2-C2-C3-O3
27	f	102	SQD	C34-C35-C36-C37
24	b	611	CLA	C16-C17-C18-C19
24	a	412	CLA	CBA-CGA-O2A-C1
27	a	405	SQD	O10-C23-O48-C46
36	c	519	DGD	O6E-C1E-O5D-C6D
26	k	101	BCR	C9-C10-C11-C12
29	C	522	LMT	C1-C2-C3-C4
29	f	103	LMT	C1-C2-C3-C4
31	A	418	PL9	C19-C21-C22-C23
27	a	405	SQD	C29-C30-C31-C32
34	B	624	HTG	C3'-C4'-C5'-C6'
35	J	101	LMG	C20-C21-C22-C23
24	B	605	CLA	C4-C3-C5-C6
24	B	607	CLA	C10-C11-C12-C13
24	b	618	CLA	C2-C3-C5-C6
37	d	409	LHG	O10-C23-O8-C6
37	E	101	LHG	C25-C26-C27-C28
24	c	515	CLA	C2-C1-O2A-CGA
24	B	602	CLA	C2-C1-O2A-CGA
24	C	514	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C2-C1-O2A-CGA
27	L	102	SQD	C11-C10-C9-C8
29	B	622	LMT	O1'-C1-C2-C3
27	a	414	SQD	C10-C11-C12-C13
24	B	614	CLA	C10-C11-C12-C13
36	h	102	DGD	CCB-CDB-CEB-CFB
24	B	610	CLA	C3A-C2A-CAA-CBA
37	D	407	LHG	C17-C18-C19-C20
37	d	409	LHG	C33-C34-C35-C36
29	M	104	LMT	C9-C10-C11-C12
25	d	401	PHO	C2C-C3C-CAC-CBC
29	C	522	LMT	C2B-C1B-O1B-C4'
24	B	615	CLA	C6-C7-C8-C9
24	b	616	CLA	C6-C7-C8-C9
24	C	505	CLA	C11-C12-C13-C14
24	c	514	CLA	C11-C12-C13-C14
24	b	624	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	B	622	LMT	C5-C6-C7-C8
35	C	501	LMG	C17-C18-C19-C20
35	Z	101	LMG	O1-C7-C8-C9
36	h	102	DGD	O1G-C1G-C2G-C3G
37	e	102	LHG	C18-C19-C20-C21
34	b	631	HTG	C4-C5-C6-O6
27	f	102	SQD	C30-C31-C32-C33
37	L	101	LHG	C23-C24-C25-C26
37	l	101	LHG	C13-C14-C15-C16
24	a	412	CLA	C4-C3-C5-C6
31	A	418	PL9	C45-C44-C46-C47
24	c	505	CLA	C1A-C2A-CAA-CBA
24	d	402	CLA	C1A-C2A-CAA-CBA
24	C	507	CLA	C1A-C2A-CAA-CBA
37	D	407	LHG	C24-C23-O8-C6
24	B	604	CLA	C11-C10-C8-C7
24	C	508	CLA	C11-C10-C8-C7
24	C	507	CLA	C12-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C15
24	b	625	CLA	C12-C13-C15-C16
24	D	403	CLA	C11-C10-C8-C7
24	a	410	CLA	C6-C7-C8-C10
24	C	511	CLA	C8-C10-C11-C12
34	C	524	HTG	C1'-C2'-C3'-C4'
24	C	513	CLA	C3-C5-C6-C7
36	H	102	DGD	O6E-C5E-C6E-O5E
37	d	407	LHG	C26-C27-C28-C29
24	d	402	CLA	C4C-C3C-CAC-CBC
35	J	101	LMG	C16-C17-C18-C19
24	b	612	CLA	C2A-CAA-CBA-CGA
24	B	605	CLA	C13-C15-C16-C17
24	A	409	CLA	C8-C10-C11-C12
35	j	101	LMG	C29-C30-C31-C32
37	L	101	LHG	C28-C29-C30-C31
35	C	520	LMG	C16-C17-C18-C19
35	C	521	LMG	C18-C19-C20-C21
24	a	410	CLA	C16-C17-C18-C20
31	A	418	PL9	C30-C29-C31-C32
24	c	517	CLA	C4-C3-C5-C6
27	a	414	SQD	C30-C31-C32-C33
35	a	415	LMG	C28-C29-C30-C31
25	a	411	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	B	610	CLA	C2-C3-C5-C6
35	z	101	LMG	C16-C17-C18-C19
35	a	415	LMG	C22-C23-C24-C25
37	d	408	LHG	O7-C5-C6-O8
27	A	411	SQD	O6-C44-C45-O47
35	c	523	LMG	O7-C8-C9-O8
37	d	407	LHG	C1-C2-C3-O3
37	D	408	LHG	C1-C2-C3-O3
35	J	101	LMG	C30-C31-C32-C33
24	c	516	CLA	C2-C1-O2A-CGA
24	a	412	CLA	C2-C3-C5-C6
31	A	418	PL9	C43-C44-C46-C47
31	D	405	PL9	C33-C34-C36-C37
24	A	409	CLA	O1A-CGA-O2A-C1
27	A	415	SQD	C17-C18-C19-C20
36	c	520	DGD	C7A-C8A-C9A-CAA
27	A	411	SQD	C15-C16-C17-C18
24	B	615	CLA	C16-C17-C18-C19
37	L	101	LHG	C33-C34-C35-C36
37	D	408	LHG	C33-C34-C35-C36
36	C	517	DGD	O1A-C1A-O1G-C1G
29	B	635	LMT	C7-C8-C9-C10
24	B	606	CLA	O1A-CGA-O2A-C1
26	c	518	BCR	C1-C6-C7-C8
26	T	103	BCR	C5-C6-C7-C8
26	t	101	BCR	C5-C6-C7-C8
36	C	517	DGD	O2G-C1B-C2B-C3B
36	D	406	DGD	C1G-C2G-C3G-O3G
37	D	407	LHG	O1-C1-C2-C3
28	v	202	GOL	O1-C1-C2-C3
31	D	405	PL9	C45-C44-C46-C47
24	d	402	CLA	C13-C15-C16-C17
29	a	419	LMT	C7-C8-C9-C10
27	B	621	SQD	C34-C35-C36-C37
36	c	520	DGD	C9B-CAB-CBB-CCB
36	H	102	DGD	CBA-CCA-CDA-CEA
35	Z	101	LMG	C8-C7-O1-C1
36	c	519	DGD	C5D-C6D-O5D-C1E
27	L	102	SQD	C7-C8-C9-C10
36	C	517	DGD	C2A-C1A-O1G-C1G
24	B	602	CLA	CAA-CBA-CGA-O2A
35	C	501	LMG	O8-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	b	618	CLA	C16-C17-C18-C19
37	D	409	LHG	C33-C34-C35-C36
24	d	404	CLA	CBD-CGD-O2D-CED
37	e	102	LHG	C28-C29-C30-C31
35	J	101	LMG	C34-C35-C36-C37
24	C	505	CLA	C12-C13-C15-C16
24	c	514	CLA	C12-C13-C15-C16
24	c	517	CLA	C2-C3-C5-C6
24	A	405	CLA	C15-C16-C17-C18
36	h	102	DGD	CDA-CEA-CFA-CGA
28	o	301	GOL	O2-C2-C3-O3
24	C	514	CLA	O1A-CGA-O2A-C1
29	B	622	LMT	C4B-C5B-C6B-O6B
35	a	415	LMG	C30-C31-C32-C33
24	b	611	CLA	C16-C17-C18-C20
34	B	623	HTG	C2'-C1'-S1-C1
34	b	608	HTG	O5-C1-S1-C1'
34	V	206	HTG	O5-C1-S1-C1'
24	C	513	CLA	CAA-CBA-CGA-O2A
24	C	507	CLA	C4-C3-C5-C6
31	A	418	PL9	C20-C19-C21-C22
31	A	418	PL9	C40-C39-C41-C42
37	D	407	LHG	C11-C12-C13-C14
31	A	418	PL9	C28-C29-C31-C32
36	C	519	DGD	C6B-C7B-C8B-C9B
24	B	607	CLA	C11-C12-C13-C14
24	C	508	CLA	C11-C10-C8-C9
24	C	507	CLA	C14-C13-C15-C16
24	d	403	CLA	C11-C12-C13-C14
24	A	409	CLA	C6-C7-C8-C9
24	b	618	CLA	C3A-C2A-CAA-CBA
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	604	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	c	505	CLA	CAD-CBD-CGD-O2D
24	c	509	CLA	CAD-CBD-CGD-O2D
24	b	618	CLA	CAD-CBD-CGD-O2D
24	c	516	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	D	403	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	611	CLA	CAD-CBD-CGD-O2D
24	b	613	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	b	623	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA
37	E	101	LHG	C23-C24-C25-C26
35	Z	101	LMG	O7-C10-C11-C12
27	f	102	SQD	O47-C7-C8-C9
25	a	411	PHO	C4-C3-C5-C6
31	a	416	PL9	C30-C29-C31-C32
24	b	618	CLA	C4-C3-C5-C6
29	m	102	LMT	O5'-C1'-O1'-C1
37	e	102	LHG	O8-C23-C24-C25
37	d	407	LHG	O8-C23-C24-C25
36	D	406	DGD	O1G-C1A-C2A-C3A
29	M	102	LMT	C3-C4-C5-C6
26	b	628	BCR	C21-C22-C23-C24
35	j	101	LMG	C11-C12-C13-C14
36	H	102	DGD	C1G-C2G-C3G-O3G
36	D	406	DGD	CBA-CCA-CDA-CEA
37	D	408	LHG	C26-C27-C28-C29
24	B	605	CLA	O1D-CGD-O2D-CED
25	a	411	PHO	O2A-C1-C2-C3
25	D	401	PHO	O2A-C1-C2-C3
24	b	611	CLA	O2A-C1-C2-C3
24	B	614	CLA	O2A-C1-C2-C3
24	d	404	CLA	O2A-C1-C2-C3
24	b	613	CLA	O2A-C1-C2-C3
24	B	603	CLA	O2A-C1-C2-C3
25	a	411	PHO	C4B-C3B-CAB-CBB
29	a	404	LMT	C4'-C5'-C6'-O6'
37	l	101	LHG	O7-C7-C8-C9
35	b	629	LMG	C20-C21-C22-C23
37	L	101	LHG	C18-C19-C20-C21
24	C	510	CLA	CHA-CBD-CGD-O2D
24	d	402	CLA	CHA-CBD-CGD-O1D
24	d	402	CLA	CHA-CBD-CGD-O2D
24	B	606	CLA	CHA-CBD-CGD-O1D
25	A	408	PHO	CHA-CBD-CGD-O1D
25	A	408	PHO	CHA-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	B	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CHA-CBD-CGD-O2D
24	c	510	CLA	CHA-CBD-CGD-O1D
24	c	506	CLA	CHA-CBD-CGD-O2D
24	c	516	CLA	CAA-CBA-CGA-O2A
37	L	101	LHG	C26-C27-C28-C29
24	A	405	CLA	C16-C17-C18-C20
36	c	520	DGD	O2G-C1B-C2B-C3B
37	E	101	LHG	O8-C23-C24-C25
36	c	521	DGD	O6D-C5D-C6D-O5D
37	L	101	LHG	O7-C7-C8-C9
24	B	614	CLA	CAA-CBA-CGA-O2A
35	M	101	LMG	O8-C28-C29-C30
24	c	514	CLA	CAA-CBA-CGA-O2A
27	a	405	SQD	C34-C35-C36-C37
29	f	103	LMT	O5B-C1B-O1B-C4'
37	d	407	LHG	C7-C8-C9-C10
37	l	101	LHG	C28-C29-C30-C31
24	c	508	CLA	C12-C13-C15-C16
27	A	411	SQD	O49-C7-O47-C45
24	c	510	CLA	C13-C15-C16-C17
35	z	101	LMG	O7-C10-C11-C12
36	e	101	DGD	O2G-C1B-C2B-C3B
24	B	604	CLA	C11-C10-C8-C9
24	B	616	CLA	C11-C12-C13-C14
24	b	625	CLA	C14-C13-C15-C16
29	C	522	LMT	O5B-C1B-O1B-C4'
36	C	517	DGD	C6A-C7A-C8A-C9A
27	F	103	SQD	C7-C8-C9-C10
37	d	409	LHG	C24-C23-O8-C6
27	a	405	SQD	C32-C33-C34-C35
36	c	521	DGD	CCA-CDA-CEA-CFA
37	D	408	LHG	C32-C33-C34-C35
27	A	411	SQD	C8-C7-O47-C45
24	C	511	CLA	CAA-CBA-CGA-O2A
36	D	406	DGD	O1A-C1A-C2A-C3A
37	e	102	LHG	C25-C26-C27-C28
37	d	409	LHG	C25-C26-C27-C28
28	B	629	GOL	C1-C2-C3-O3
31	D	405	PL9	C43-C44-C46-C47
29	M	105	LMT	C9-C10-C11-C12
35	J	101	LMG	C14-C15-C16-C17
24	C	513	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	K	101	BCR	C7-C8-C9-C10
26	d	405	BCR	C7-C8-C9-C10
27	A	415	SQD	C28-C29-C30-C31
24	C	514	CLA	CBA-CGA-O2A-C1
24	A	409	CLA	CBA-CGA-O2A-C1
37	d	409	LHG	C11-C10-C9-C8
24	B	610	CLA	C1A-C2A-CAA-CBA
24	C	514	CLA	C1A-C2A-CAA-CBA
24	c	510	CLA	C1A-C2A-CAA-CBA
27	f	102	SQD	C35-C36-C37-C38
36	C	518	DGD	CAA-CBA-CCA-CDA
36	c	521	DGD	CBB-CCB-CDB-CEB
29	M	105	LMT	C11-C10-C9-C8
35	a	415	LMG	C34-C35-C36-C37
29	B	622	LMT	C4-C5-C6-C7
36	h	102	DGD	C4E-C5E-C6E-O5E
37	d	409	LHG	O8-C23-C24-C25
36	c	521	DGD	C8A-C9A-CAA-CBA
24	a	409	CLA	C2A-CAA-CBA-CGA
24	b	611	CLA	C2A-CAA-CBA-CGA
37	d	408	LHG	C26-C27-C28-C29
24	A	407	CLA	C16-C17-C18-C20
37	d	407	LHG	O10-C23-C24-C25
25	a	411	PHO	C10-C11-C12-C13
24	B	609	CLA	C13-C15-C16-C17
37	D	407	LHG	C27-C28-C29-C30
36	C	517	DGD	CAA-CBA-CCA-CDA
36	C	518	DGD	O2G-C1B-C2B-C3B
35	z	101	LMG	O9-C10-C11-C12
27	B	621	SQD	C15-C16-C17-C18
36	c	519	DGD	C2E-C1E-O5D-C6D
35	c	522	LMG	C33-C34-C35-C36
34	b	607	HTG	C2'-C3'-C4'-C5'
37	e	102	LHG	C4-O6-P-O5
37	D	409	LHG	C4-O6-P-O4
37	D	409	LHG	C4-O6-P-O5
37	D	408	LHG	C4-O6-P-O5
24	B	612	CLA	C16-C17-C18-C19
35	C	521	LMG	C13-C14-C15-C16
37	e	102	LHG	O10-C23-C24-C25
24	c	516	CLA	CAA-CBA-CGA-O1A
27	f	102	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	c	518	BCR	C5-C6-C7-C8
26	t	101	BCR	C1-C6-C7-C8
24	a	409	CLA	C13-C15-C16-C17
27	f	102	SQD	C7-C8-C9-C10
36	c	520	DGD	O1B-C1B-C2B-C3B
37	l	101	LHG	O9-C7-C8-C9
36	e	101	DGD	C3A-C4A-C5A-C6A
37	L	101	LHG	O9-C7-C8-C9
36	e	101	DGD	O1B-C1B-C2B-C3B
37	D	409	LHG	C10-C11-C12-C13
37	E	101	LHG	C10-C11-C12-C13
35	C	520	LMG	C28-C29-C30-C31
37	E	101	LHG	O10-C23-C24-C25
24	b	618	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CAD-CBD-CGD-O1D
27	A	411	SQD	O5-C5-C6-S
24	C	505	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
35	Z	101	LMG	O9-C10-C11-C12
24	c	513	CLA	C11-C12-C13-C14
24	C	505	CLA	C14-C13-C15-C16
24	B	611	CLA	C14-C13-C15-C16
24	c	508	CLA	C14-C13-C15-C16
28	b	602	GOL	O1-C1-C2-O2
25	D	401	PHO	C10-C11-C12-C13
36	e	101	DGD	CAB-CBB-CCB-CDB
35	b	629	LMG	O8-C28-C29-C30
35	J	101	LMG	O7-C10-C11-C12
36	D	406	DGD	C6B-C7B-C8B-C9B
27	B	621	SQD	C12-C13-C14-C15
24	b	624	CLA	C13-C15-C16-C17
24	b	623	CLA	C2A-CAA-CBA-CGA
34	B	624	HTG	C4'-C5'-C6'-C7'
36	C	519	DGD	CBA-CCA-CDA-CEA
36	c	521	DGD	O1G-C1A-C2A-C3A
24	C	508	CLA	C5-C6-C7-C8
24	a	409	CLA	C15-C16-C17-C18
24	b	619	CLA	C15-C16-C17-C18
36	h	102	DGD	CDB-CEB-CFB-CGB
24	c	510	CLA	C4-C3-C5-C6

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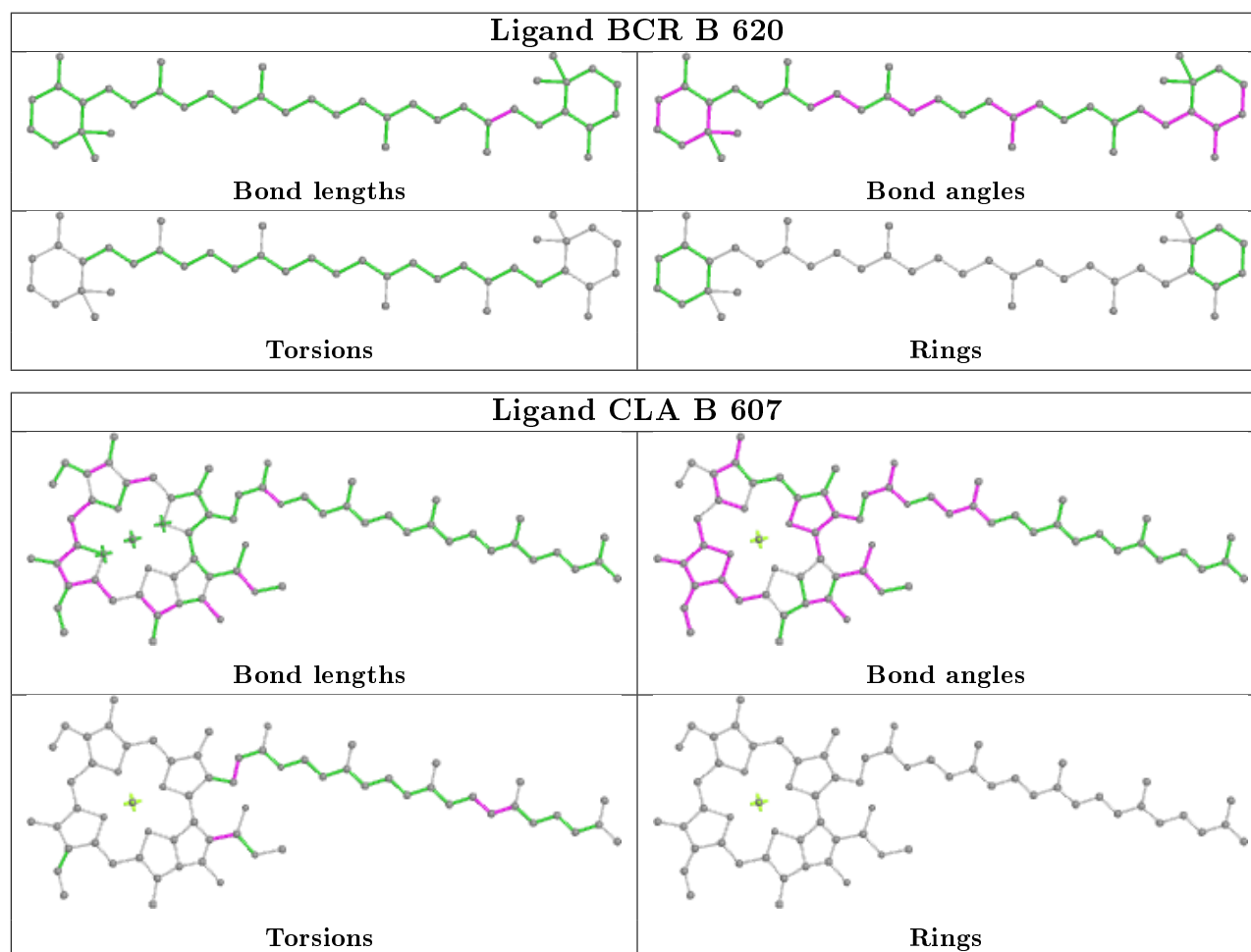
Mol	Chain	Res	Type	Atoms
24	b	610	CLA	C4-C3-C5-C6
24	A	409	CLA	C10-C11-C12-C13
24	B	611	CLA	C12-C13-C15-C16
24	b	617	CLA	C11-C10-C8-C7
24	B	605	CLA	C2-C3-C5-C6
37	d	409	LHG	O10-C23-C24-C25
36	C	518	DGD	O1B-C1B-C2B-C3B
36	c	520	DGD	C8A-C9A-CAA-CBA
37	E	101	LHG	C14-C15-C16-C17
24	b	622	CLA	CAA-CBA-CGA-O2A
24	c	509	CLA	CAA-CBA-CGA-O2A
24	C	506	CLA	CAA-CBA-CGA-O2A
37	D	409	LHG	C9-C10-C11-C12
37	D	409	LHG	C19-C20-C21-C22
26	C	516	BCR	C11-C12-C13-C14
24	B	614	CLA	CAA-CBA-CGA-O1A
29	M	102	LMT	C2-C1-O1'-C1'
34	D	412	HTG	C1'-C2'-C3'-C4'
29	M	102	LMT	O5'-C1'-O1'-C1
24	b	615	CLA	C8-C10-C11-C12
24	b	615	CLA	C15-C16-C17-C18
24	C	505	CLA	C13-C15-C16-C17
36	c	521	DGD	O1A-C1A-C2A-C3A
24	C	511	CLA	CAA-CBA-CGA-O1A
24	B	606	CLA	CBA-CGA-O2A-C1
24	C	509	CLA	C13-C15-C16-C17
24	A	406	CLA	C4C-C3C-CAC-CBC
29	a	419	LMT	C5-C6-C7-C8
24	c	514	CLA	CAA-CBA-CGA-O1A
24	c	507	CLA	C2A-CAA-CBA-CGA
24	a	409	CLA	C16-C17-C18-C19
34	V	206	HTG	C2'-C3'-C4'-C5'
24	B	614	CLA	CBD-CGD-O2D-CED
24	C	506	CLA	CAA-CBA-CGA-O1A
24	B	610	CLA	C4-C3-C5-C6
35	C	501	LMG	O7-C10-C11-C12
29	M	104	LMT	C2B-C1B-O1B-C4'

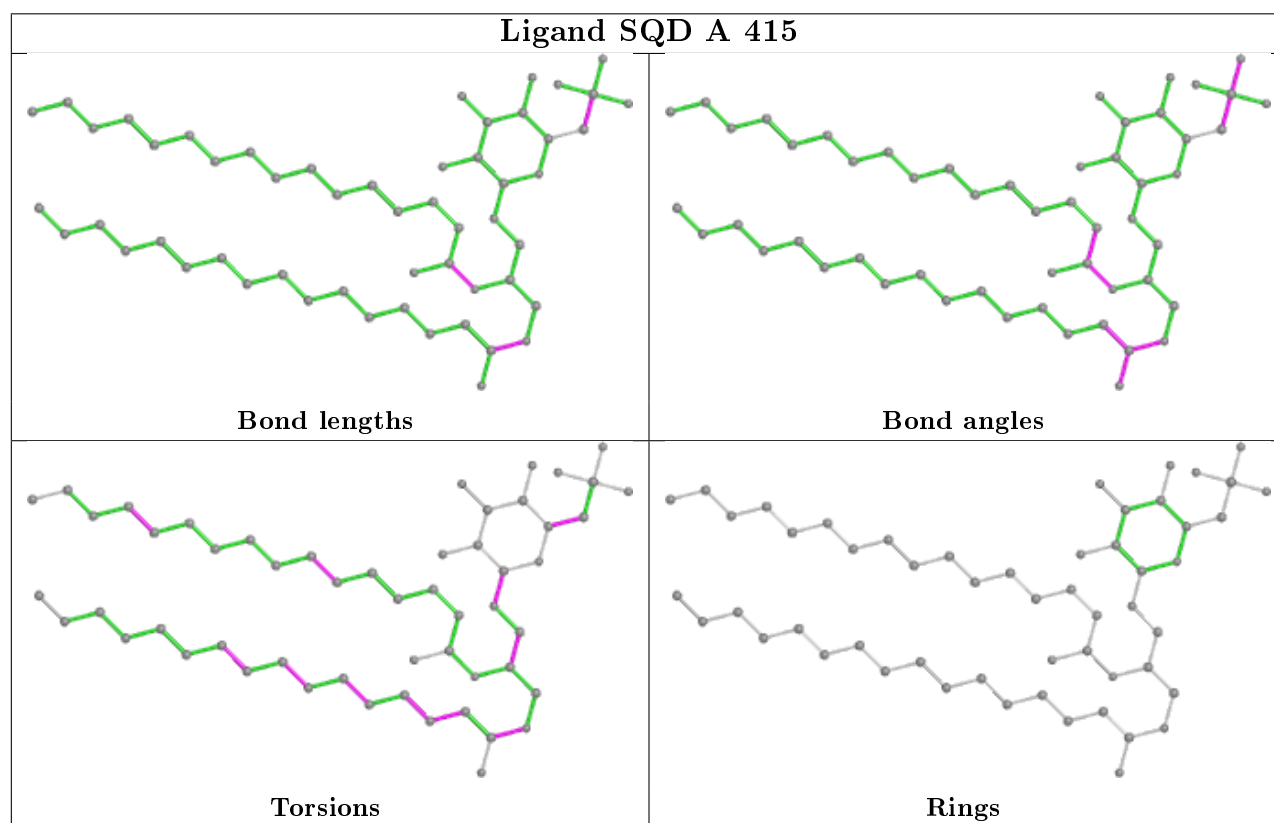
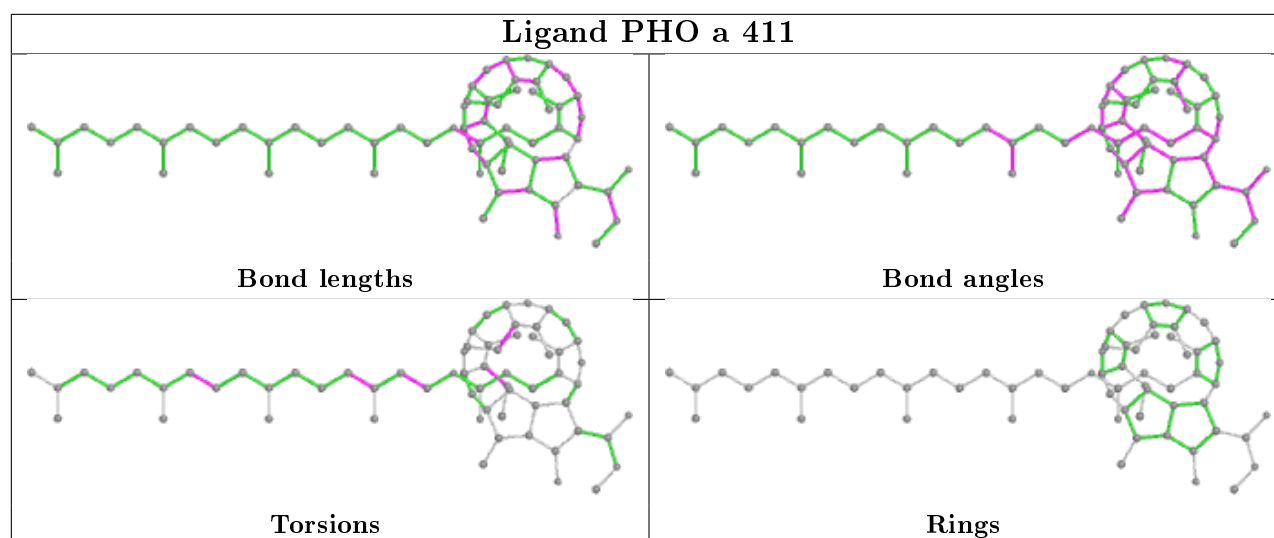
There are no ring outliers.

1 monomer is involved in 1 short contact:

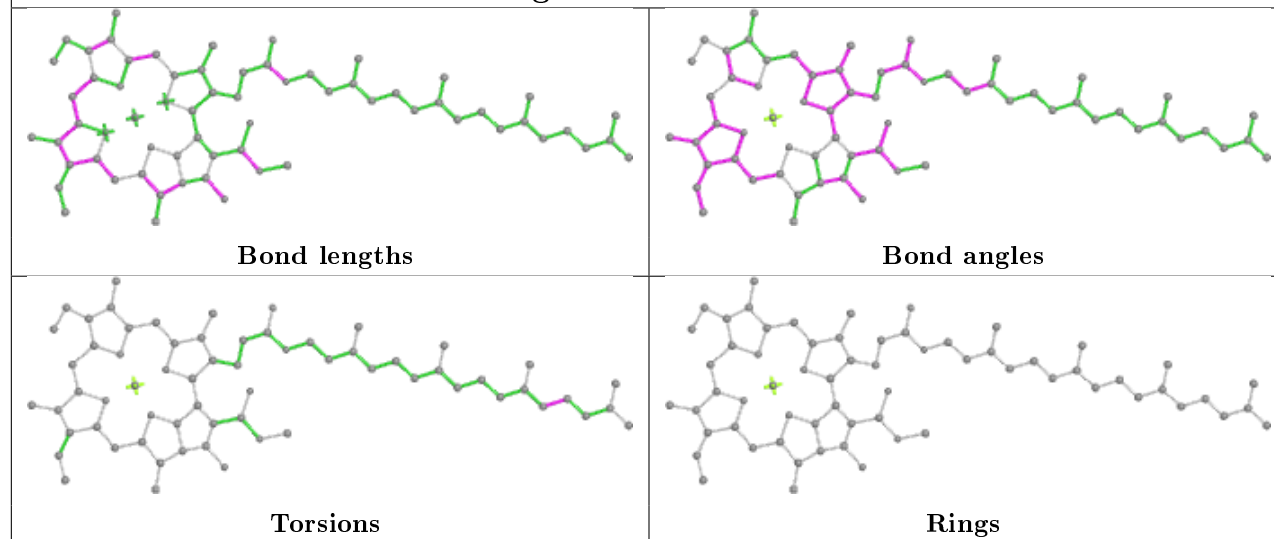
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	f	102	SQD	0	1

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

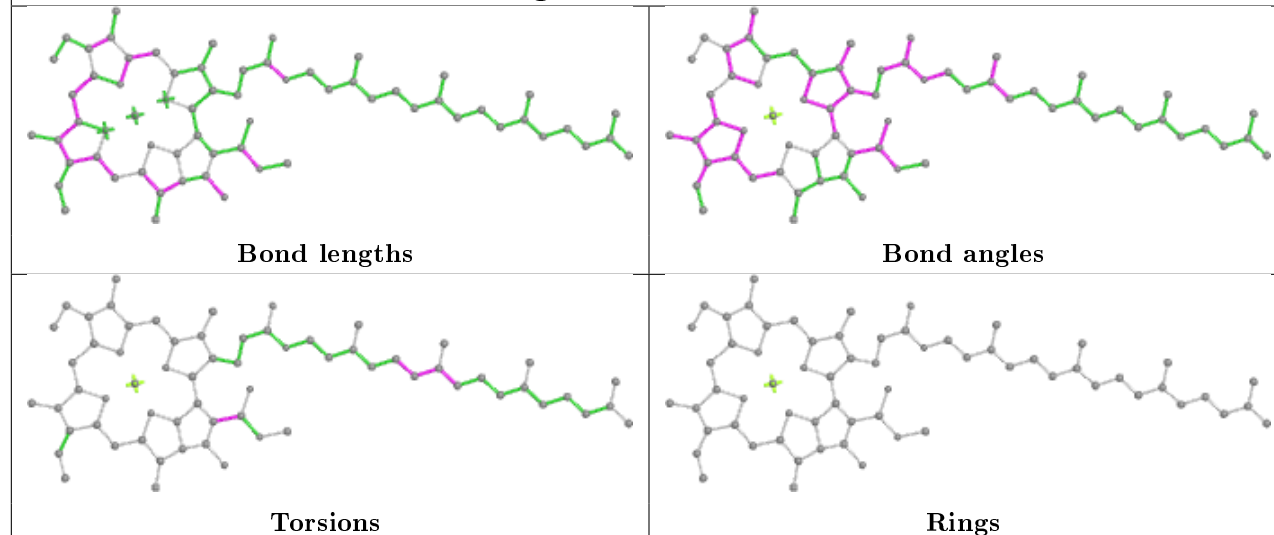




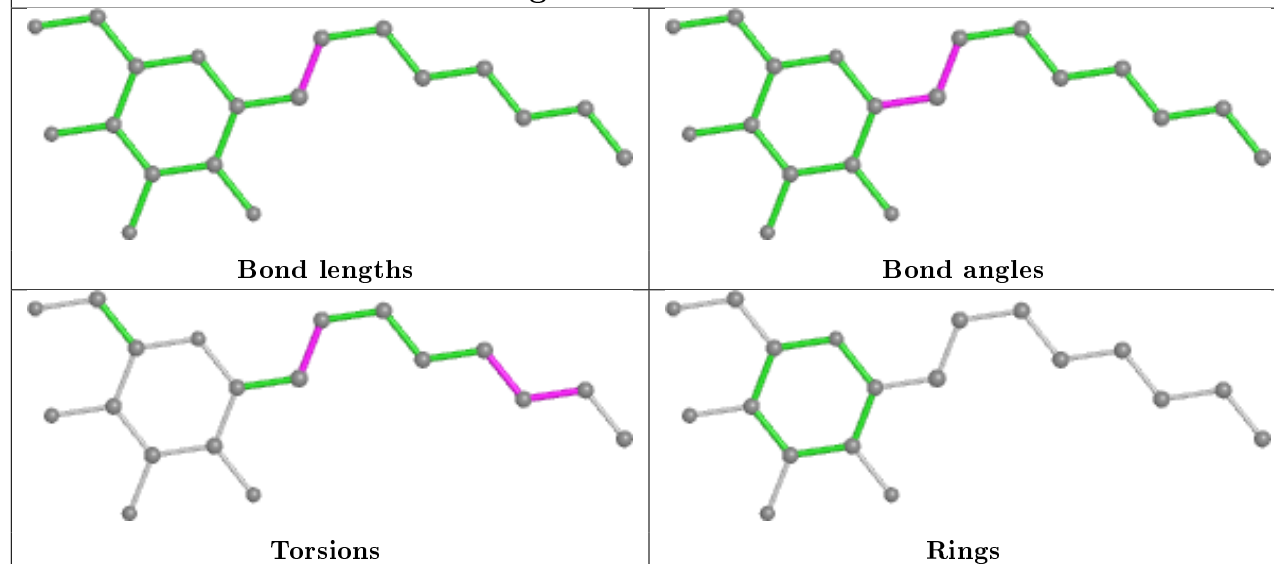
Ligand CLA B 609

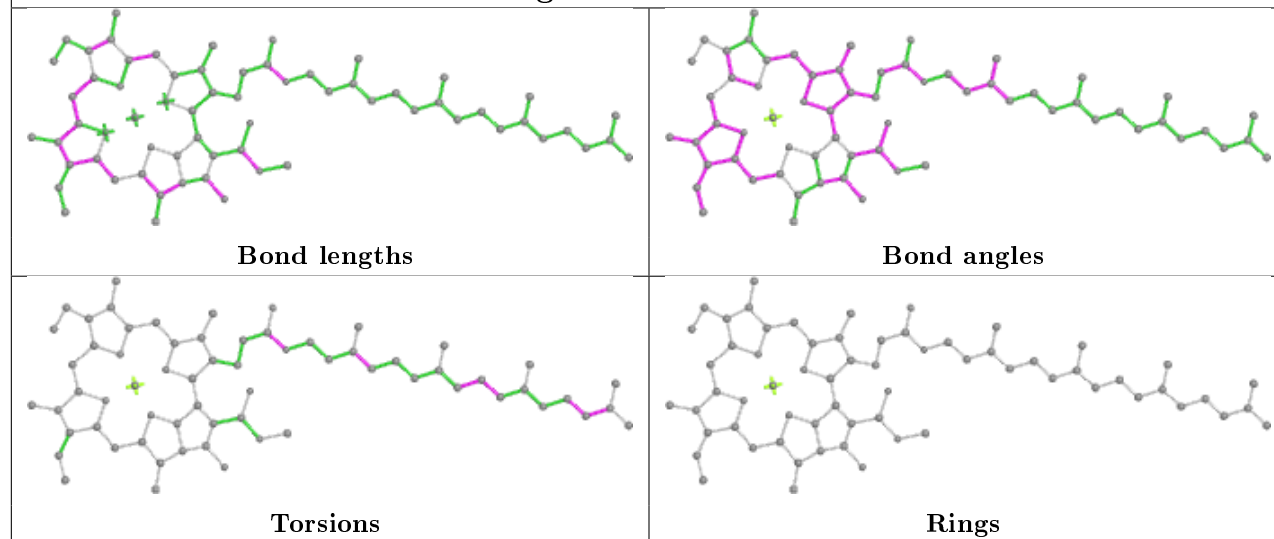
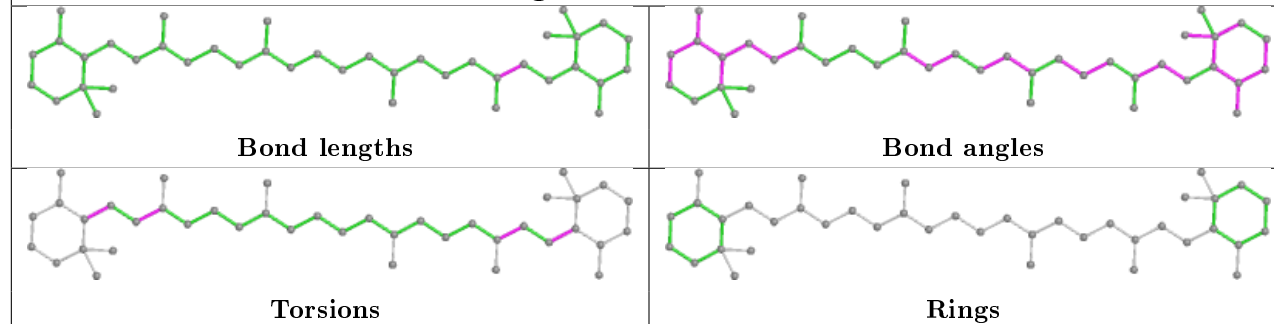


Ligand CLA B 604

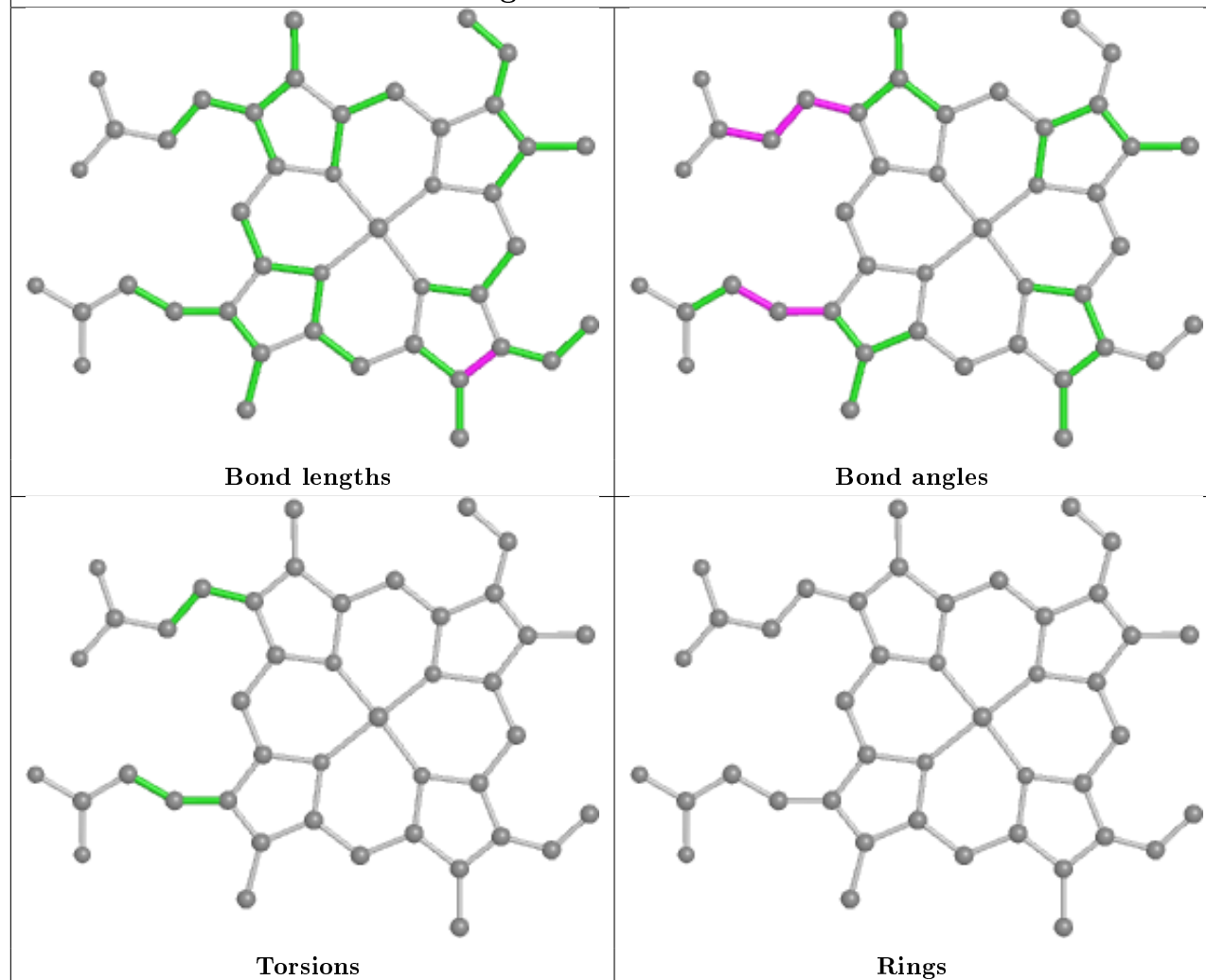


Ligand HTG B 623

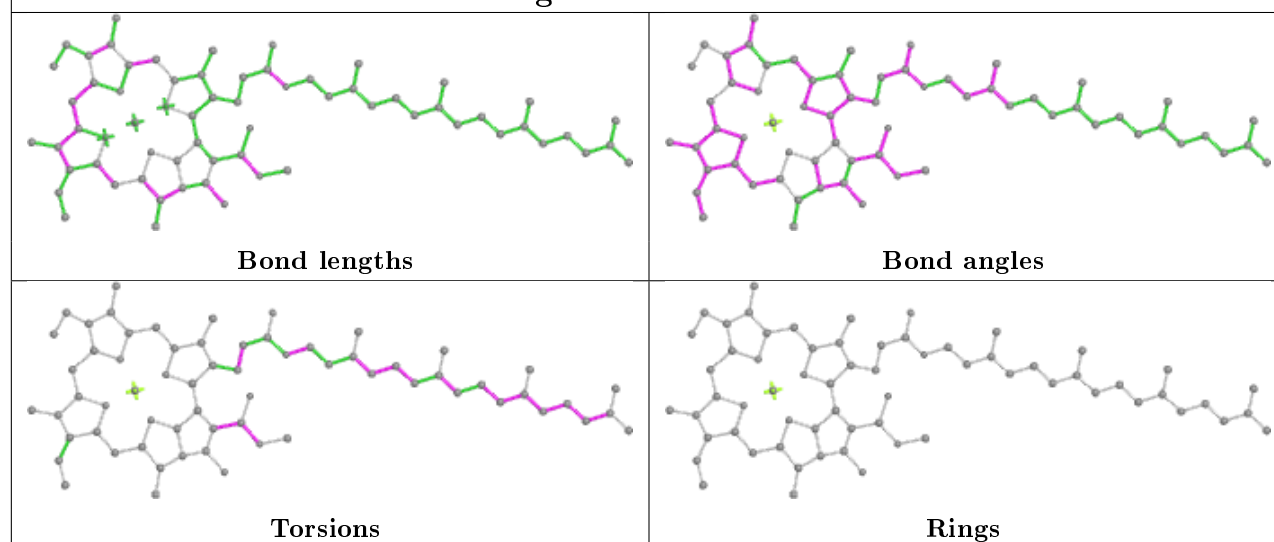


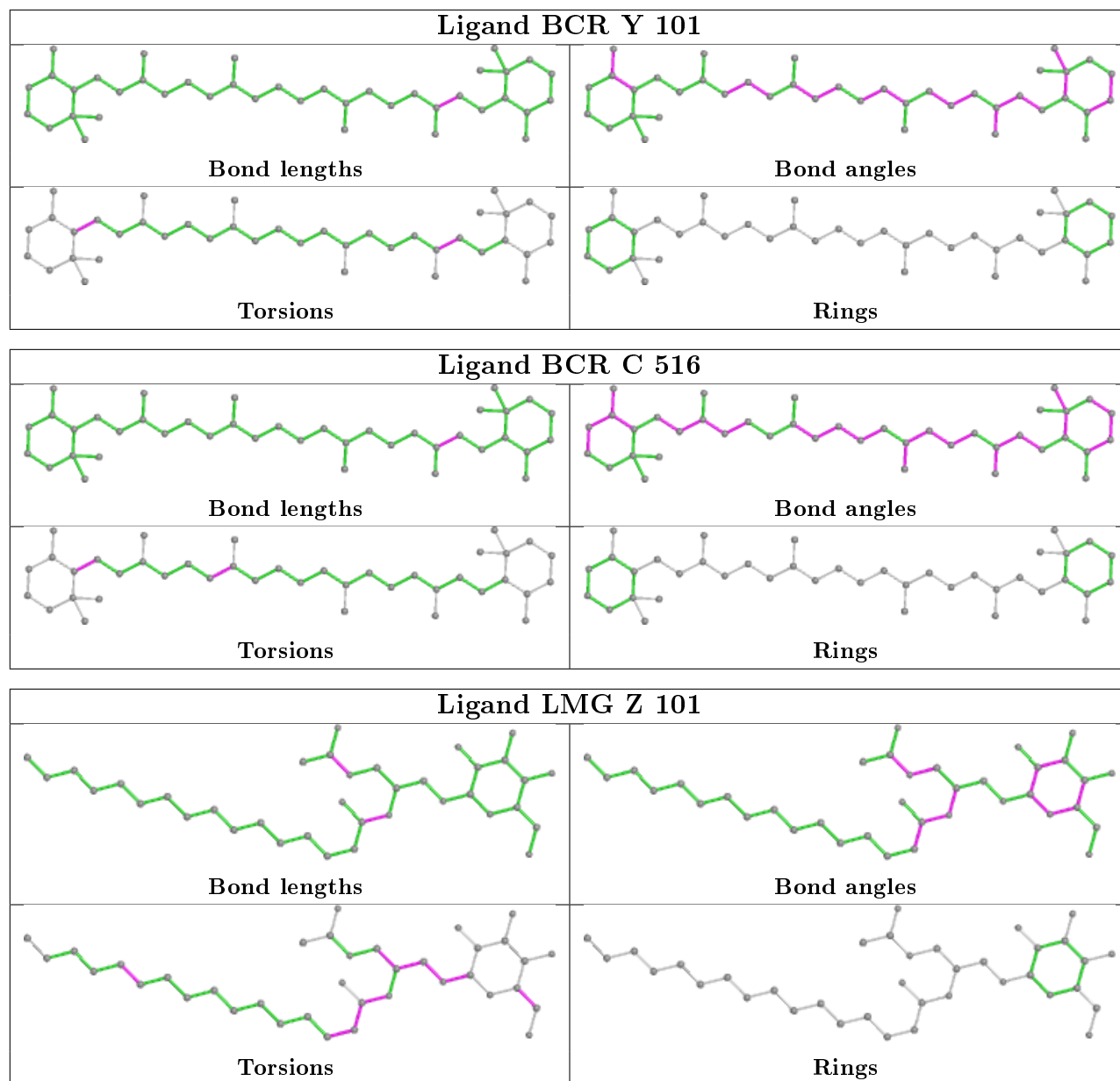
Ligand CLA a 412**Ligand BCR D 404**

Ligand HEM E 102

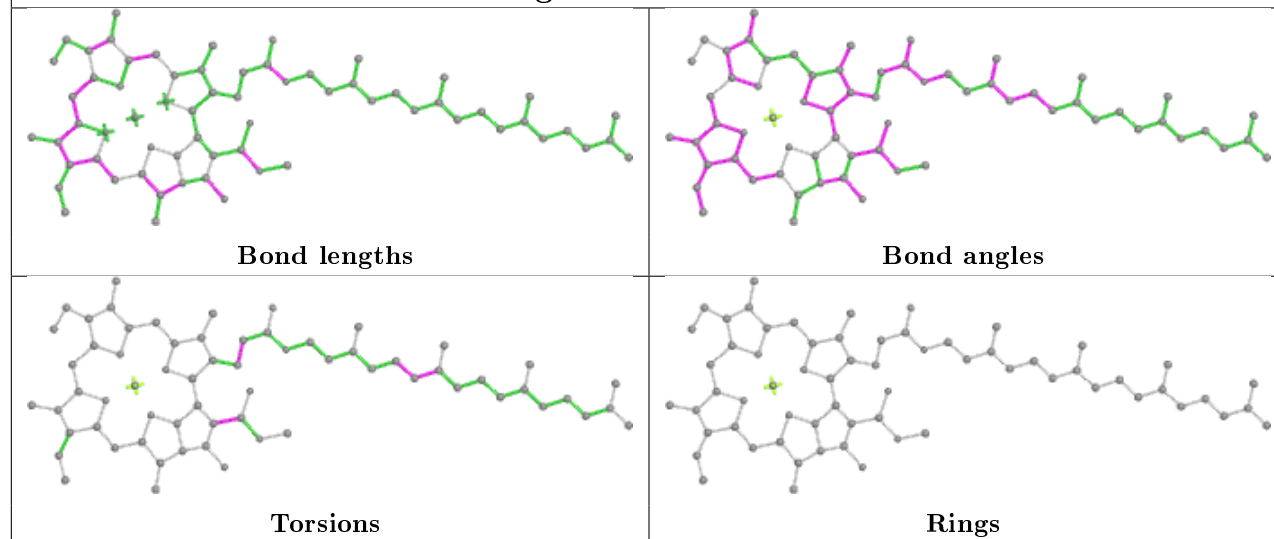


Ligand CLA b 623

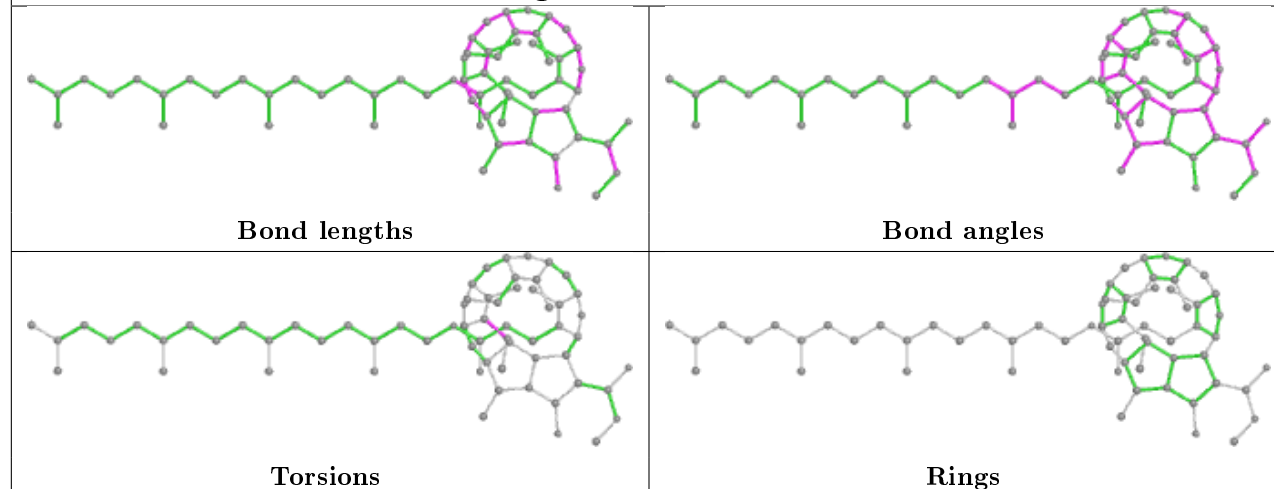




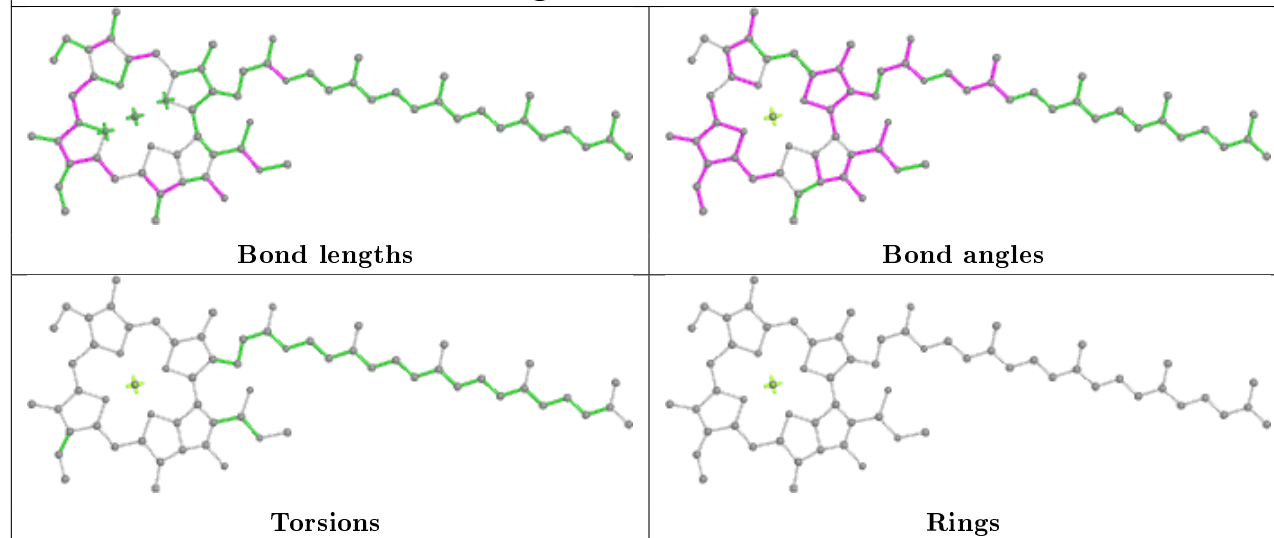
Ligand CLA b 612

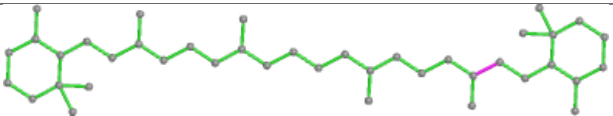
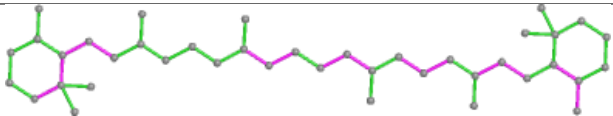
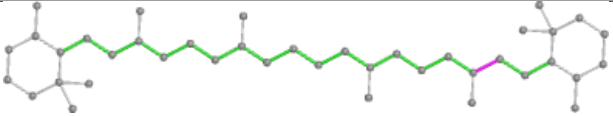
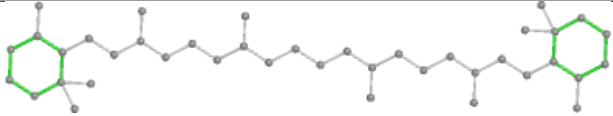


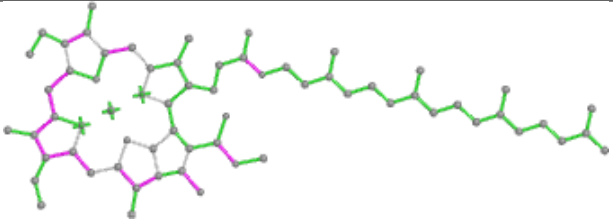
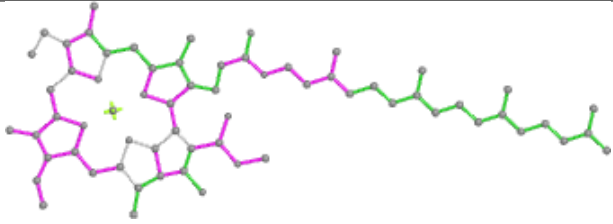
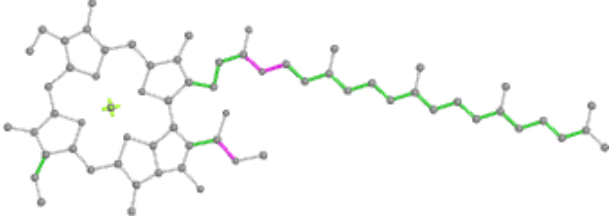
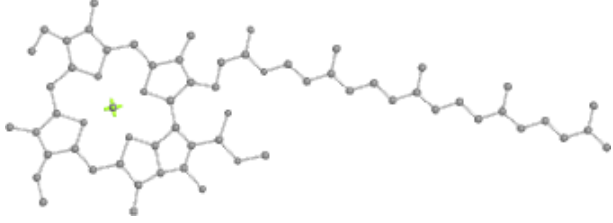
Ligand PHO d 401

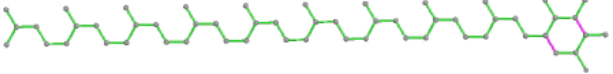
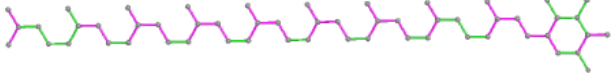
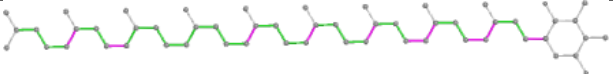
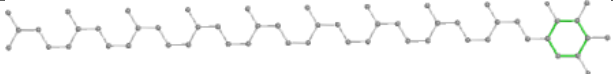


Ligand CLA D 402

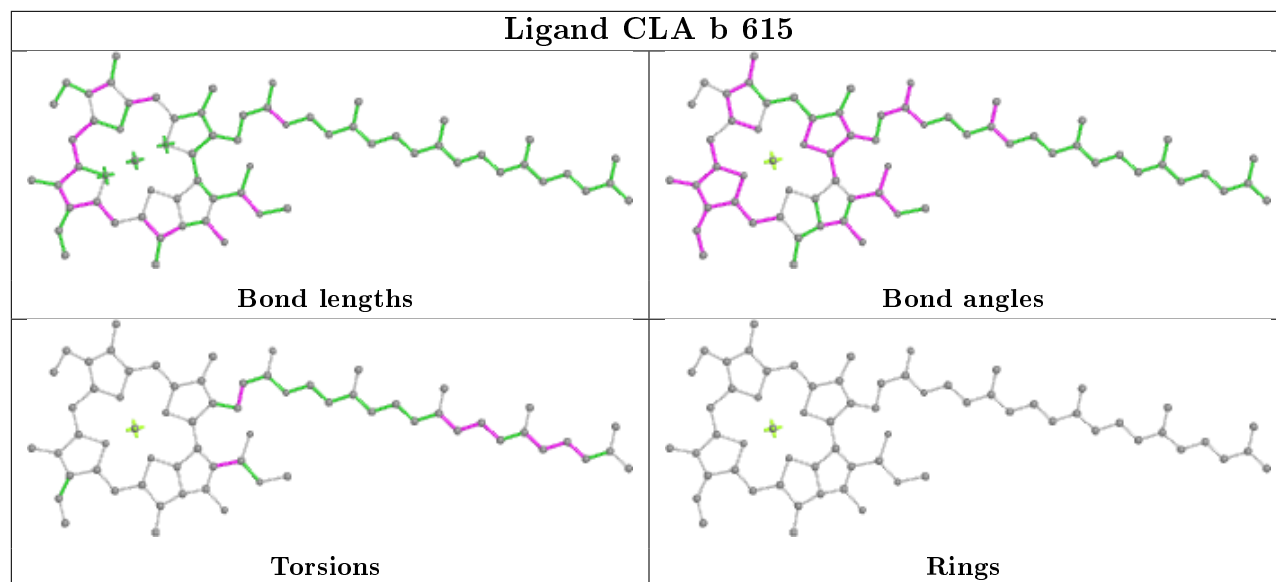


Ligand BCR b 628	
	
Bond lengths	Bond angles
	
Torsions	Rings

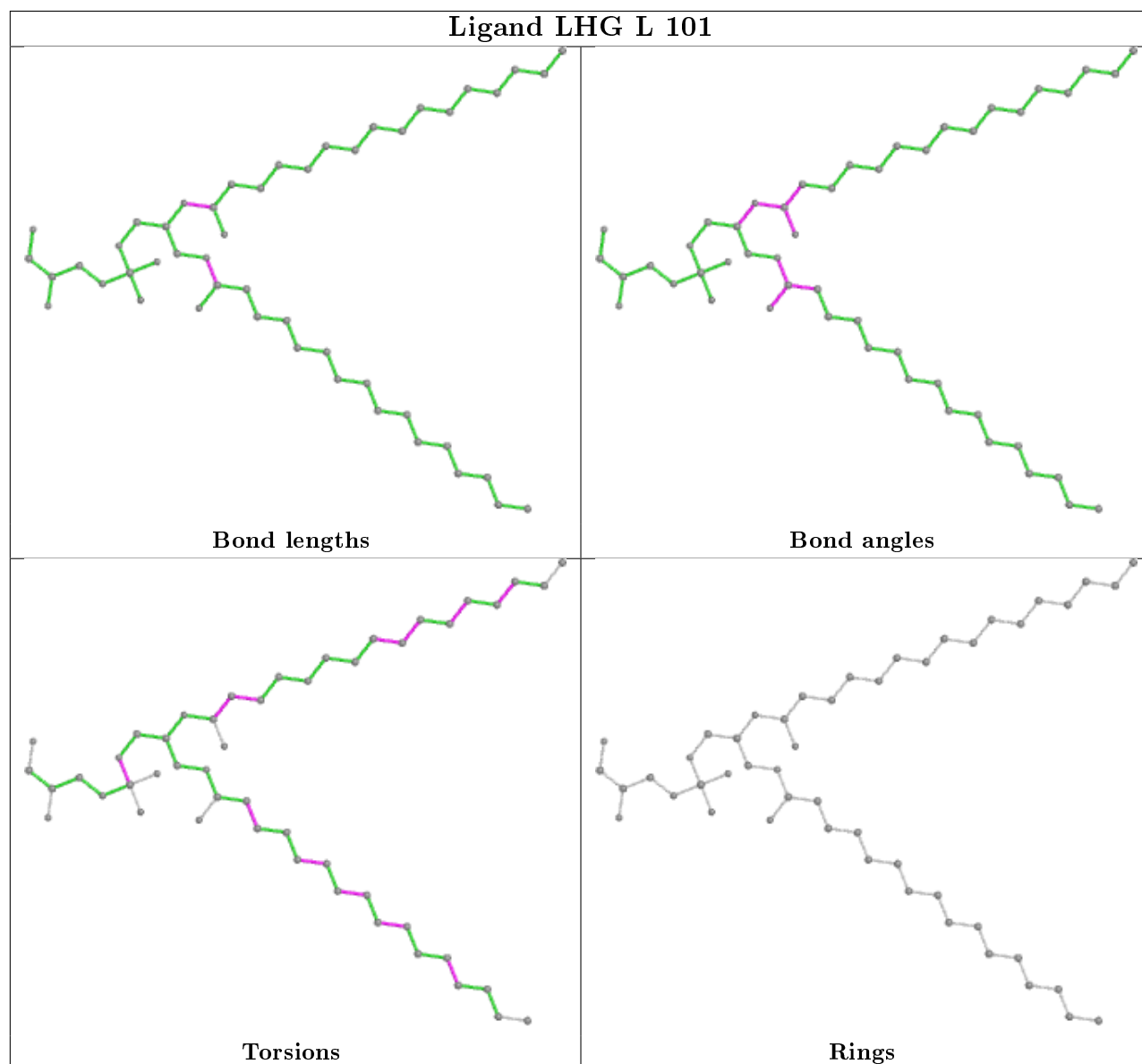
Ligand CLA c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

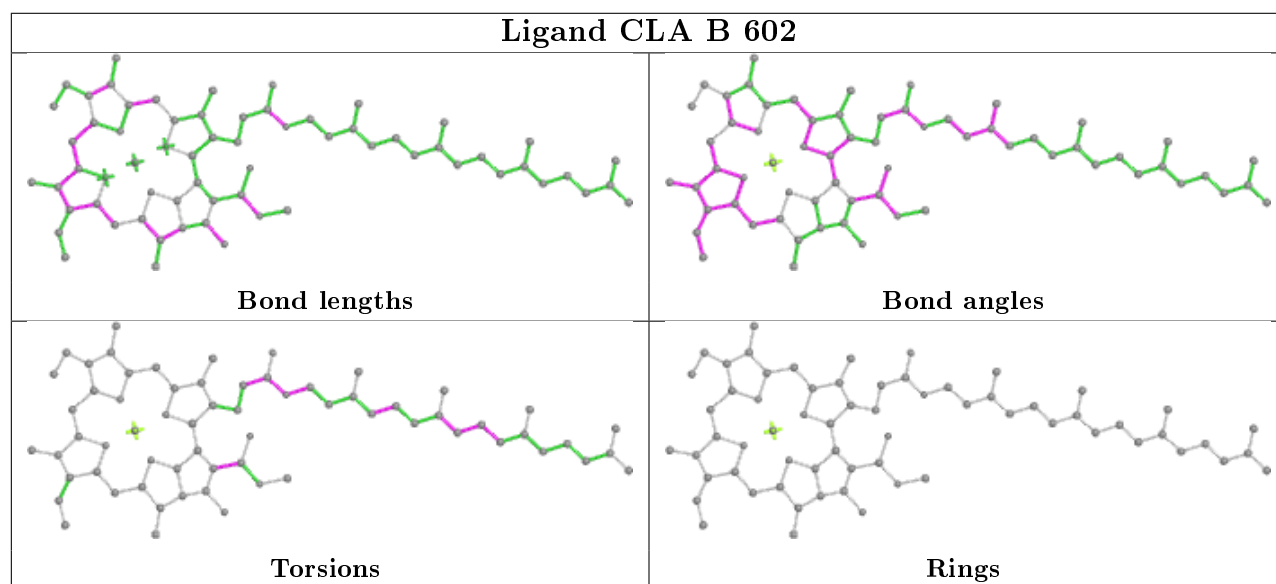
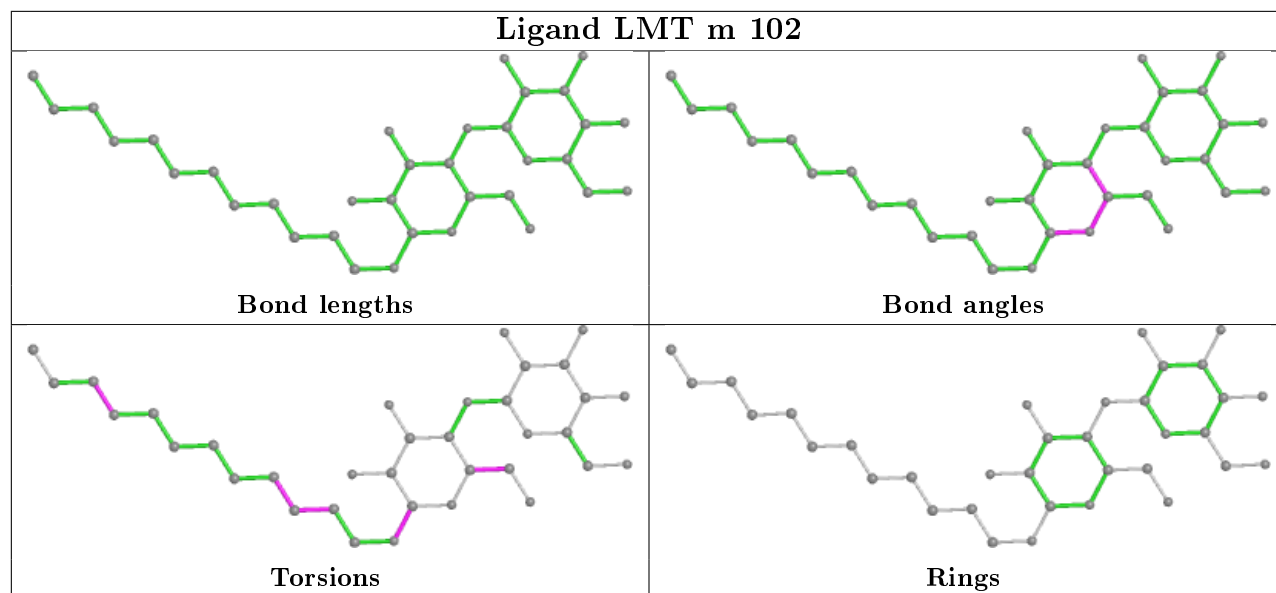
Ligand PL9 a 416	
	
Bond lengths	Bond angles
	
Torsions	Rings

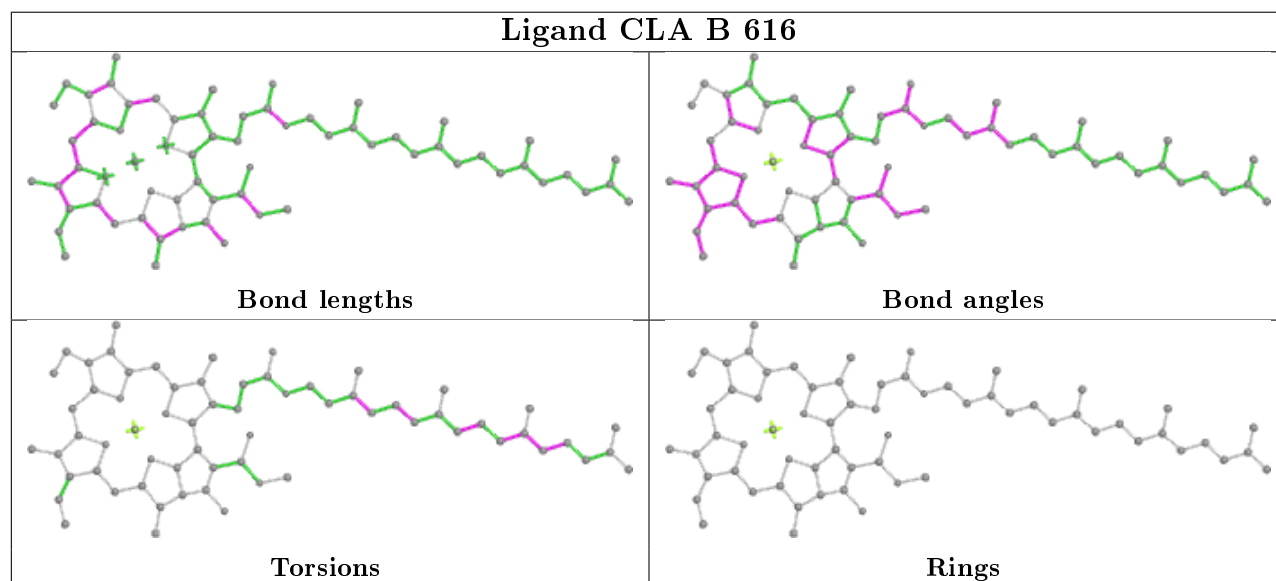
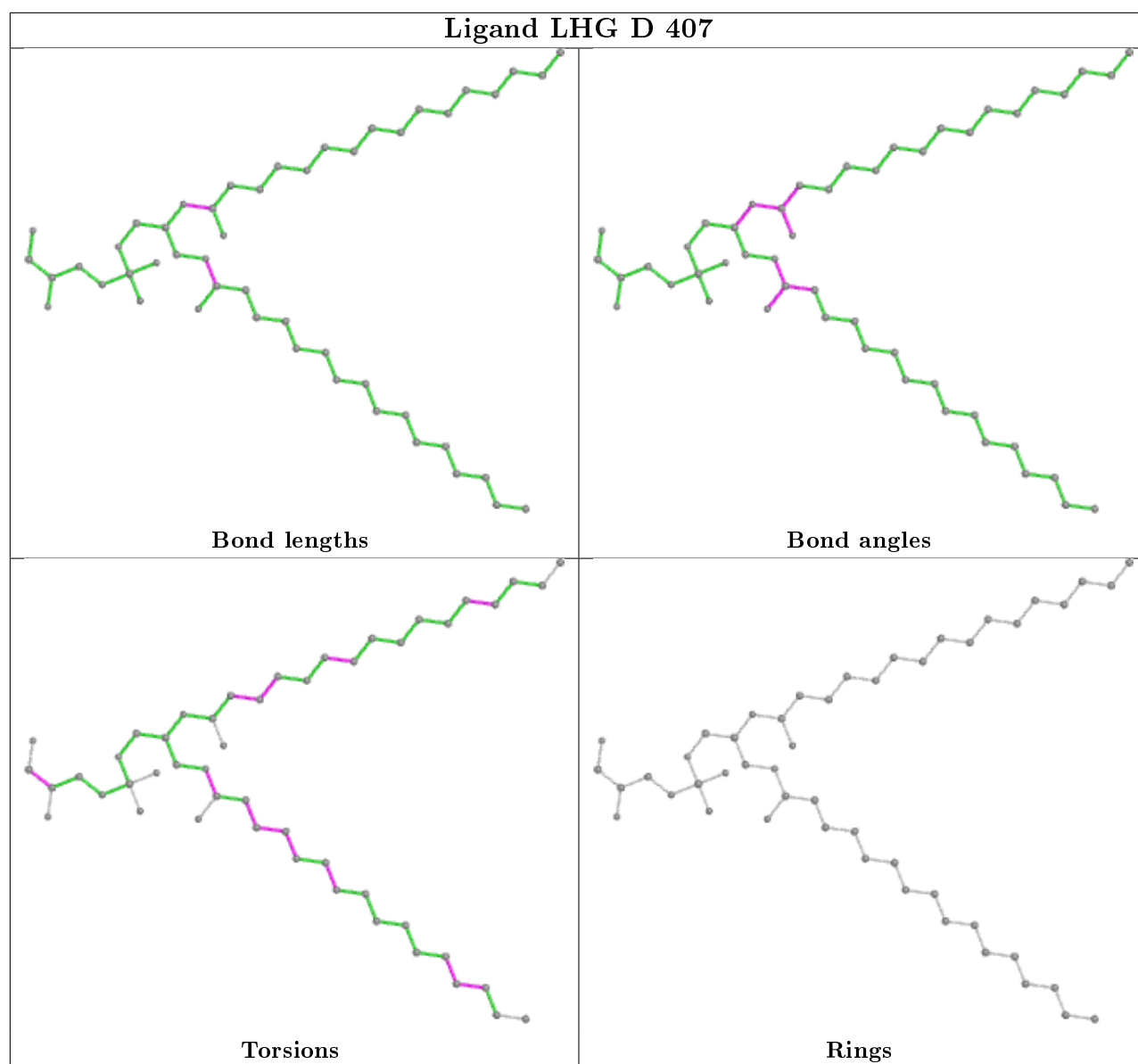
Ligand CLA b 615



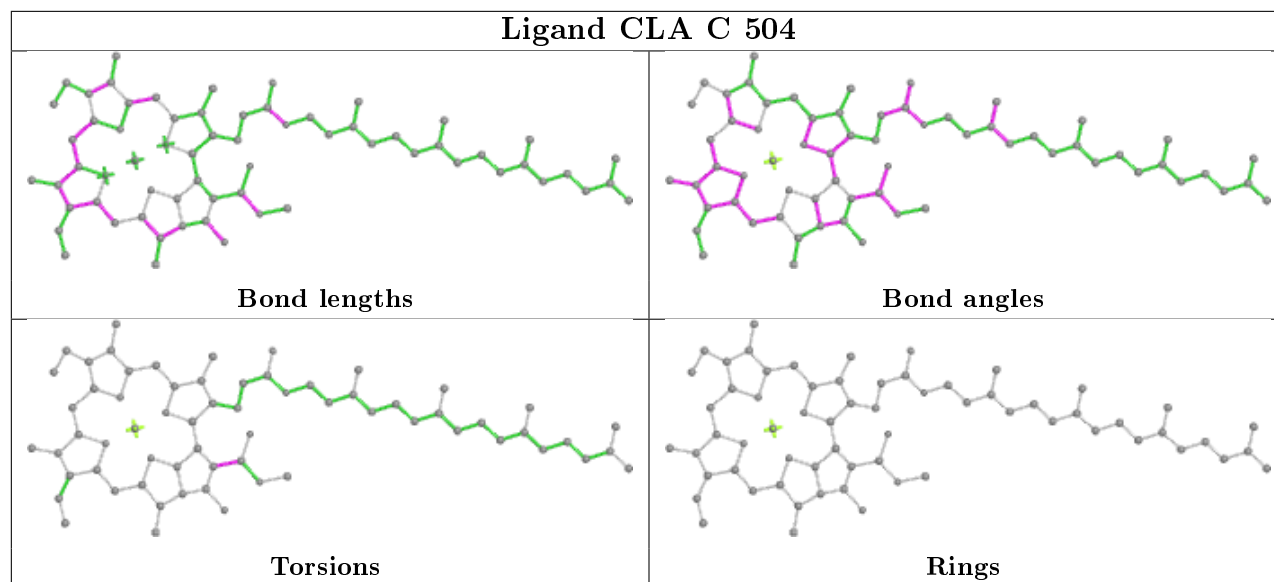
Ligand LHG L 101



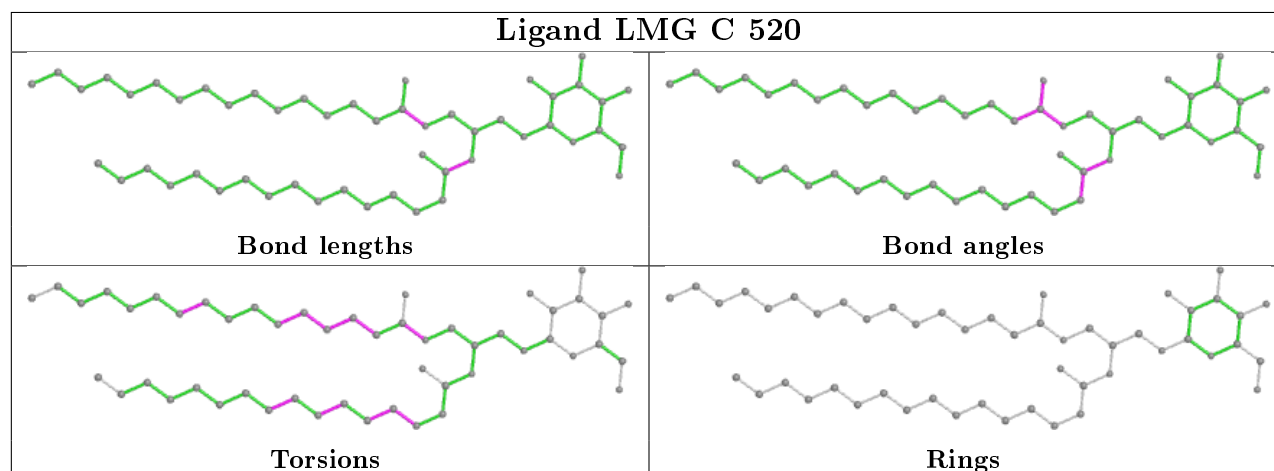




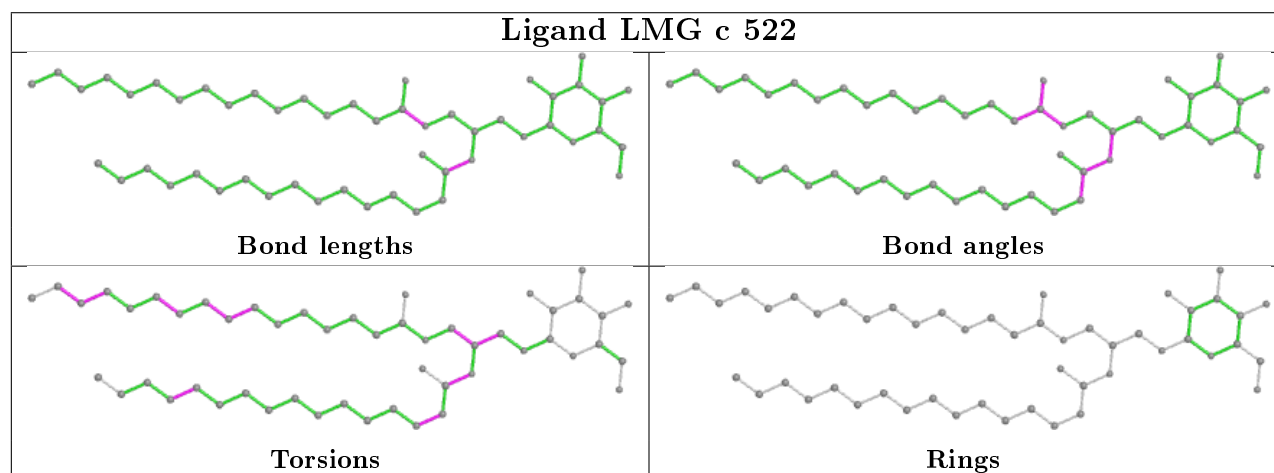
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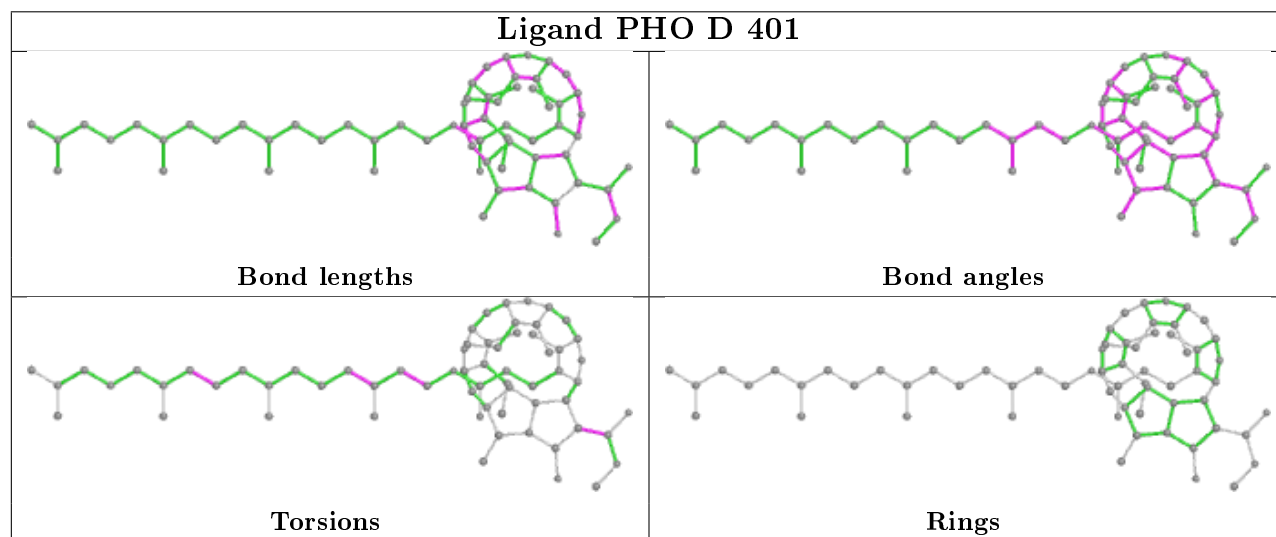
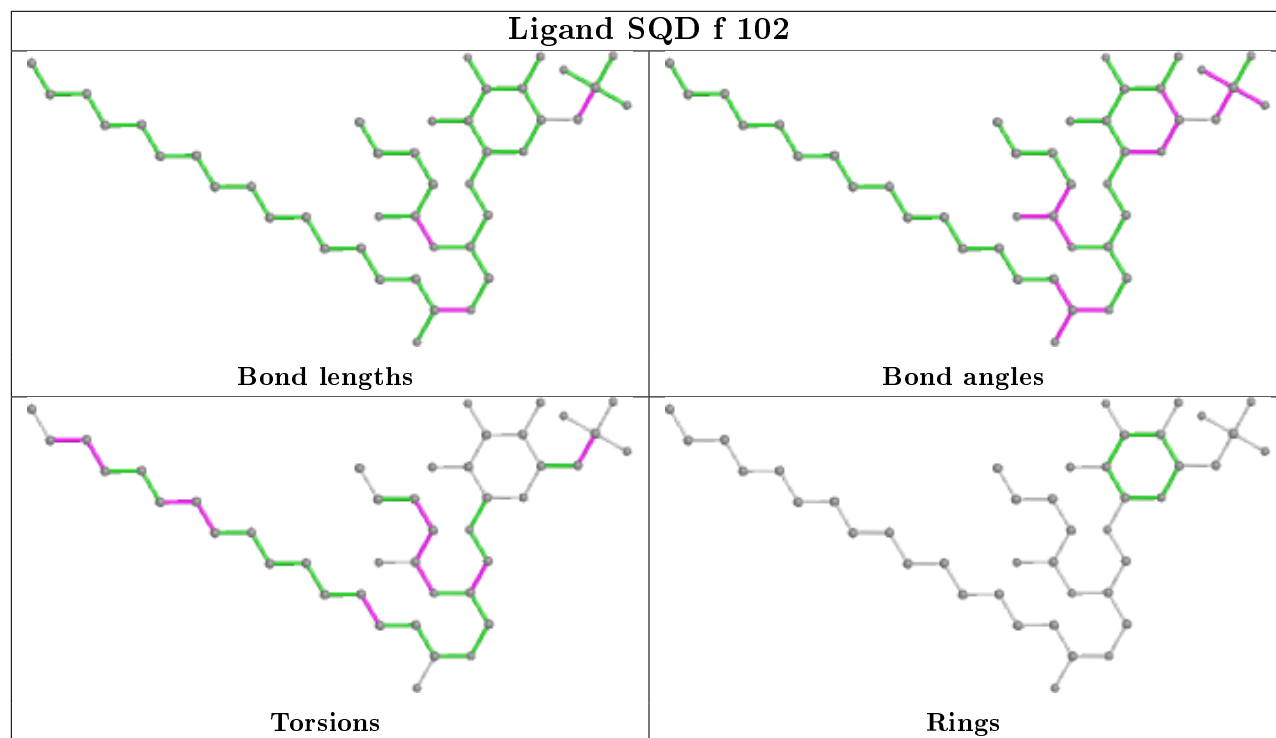
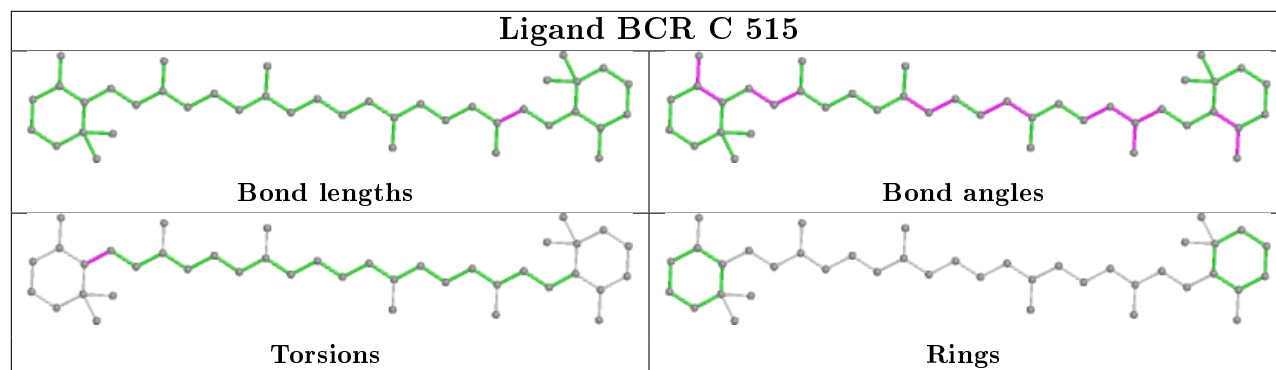


Ligand LMG C 520

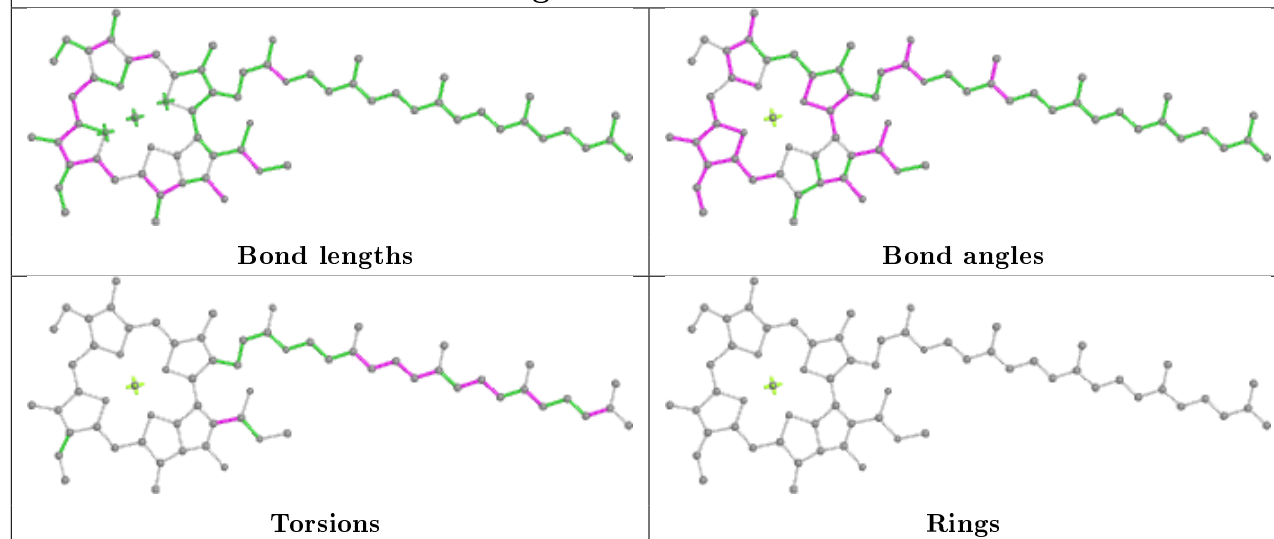


Ligand LMG c 522

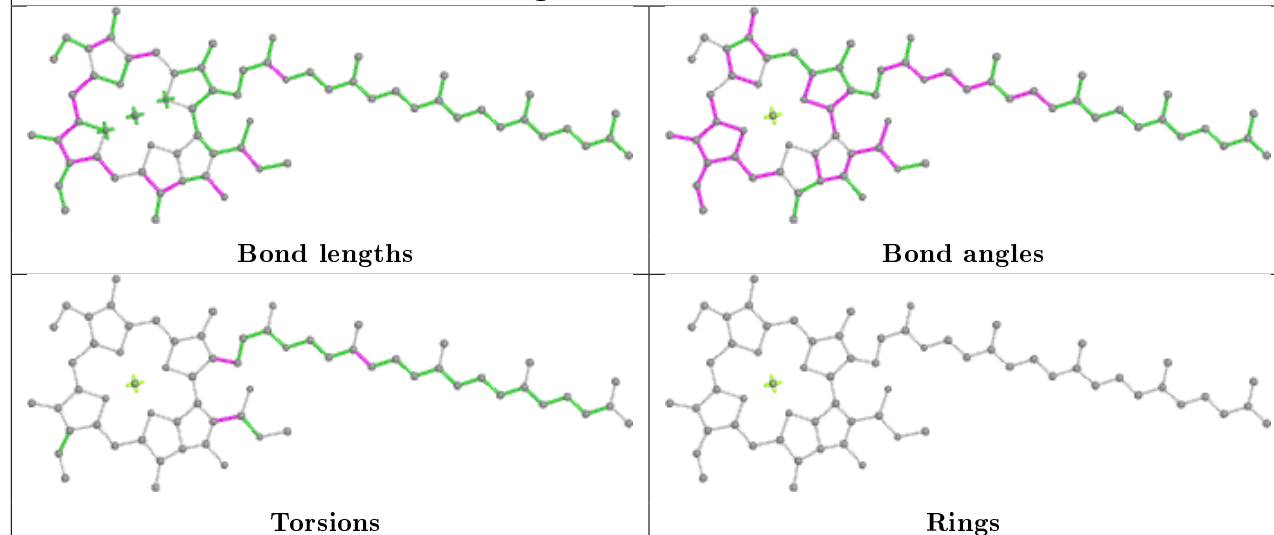




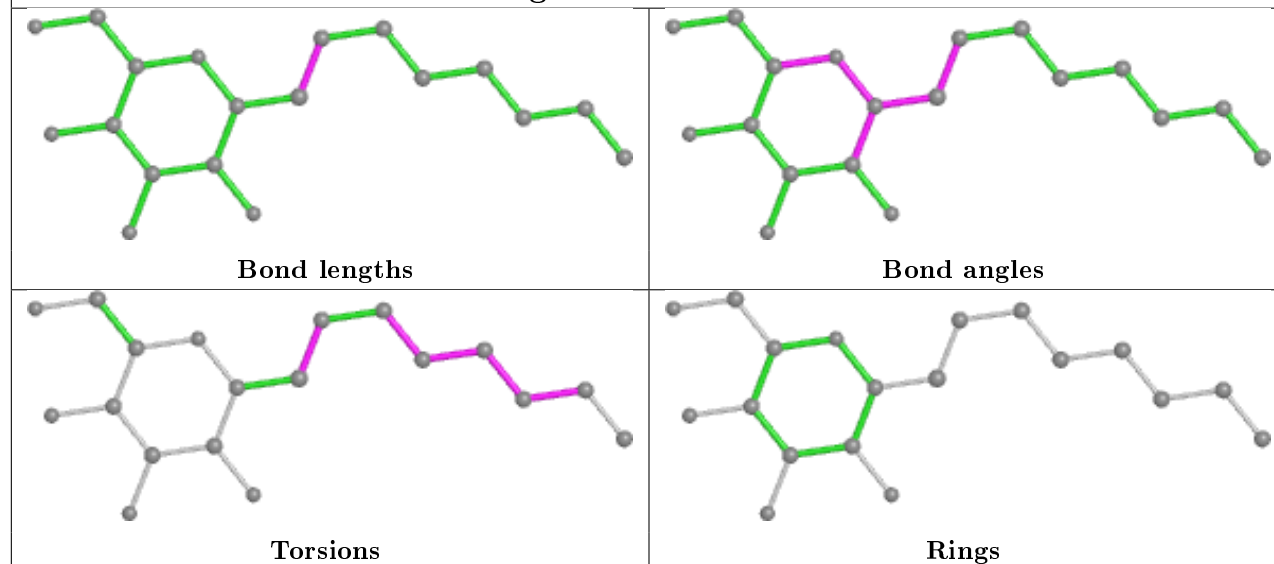
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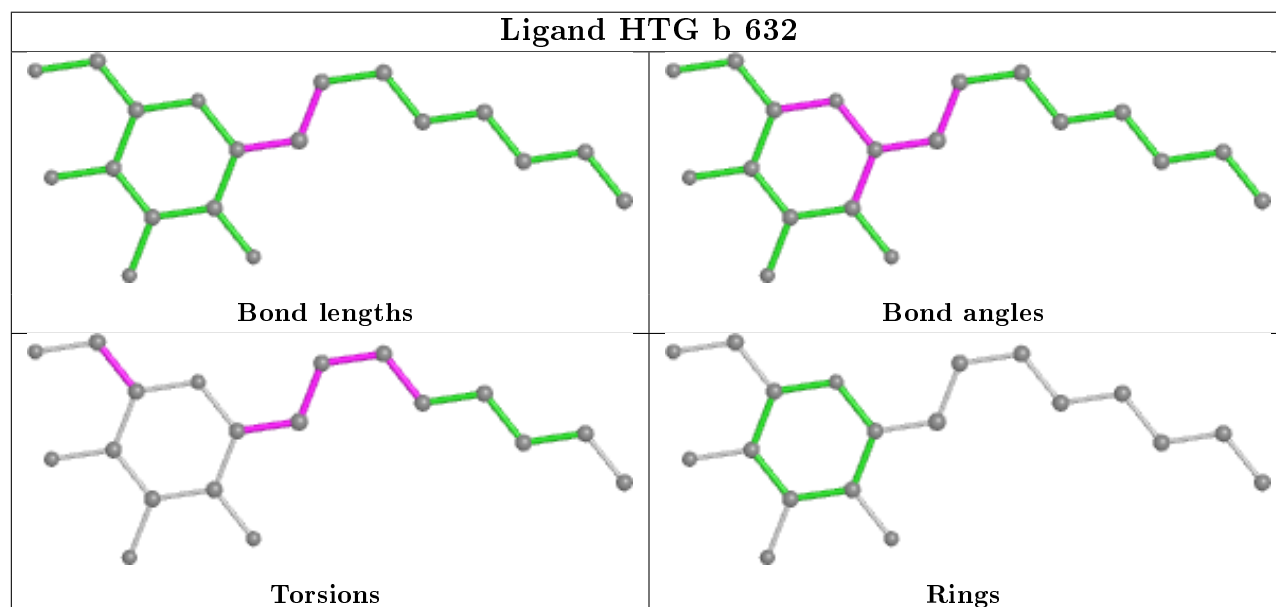
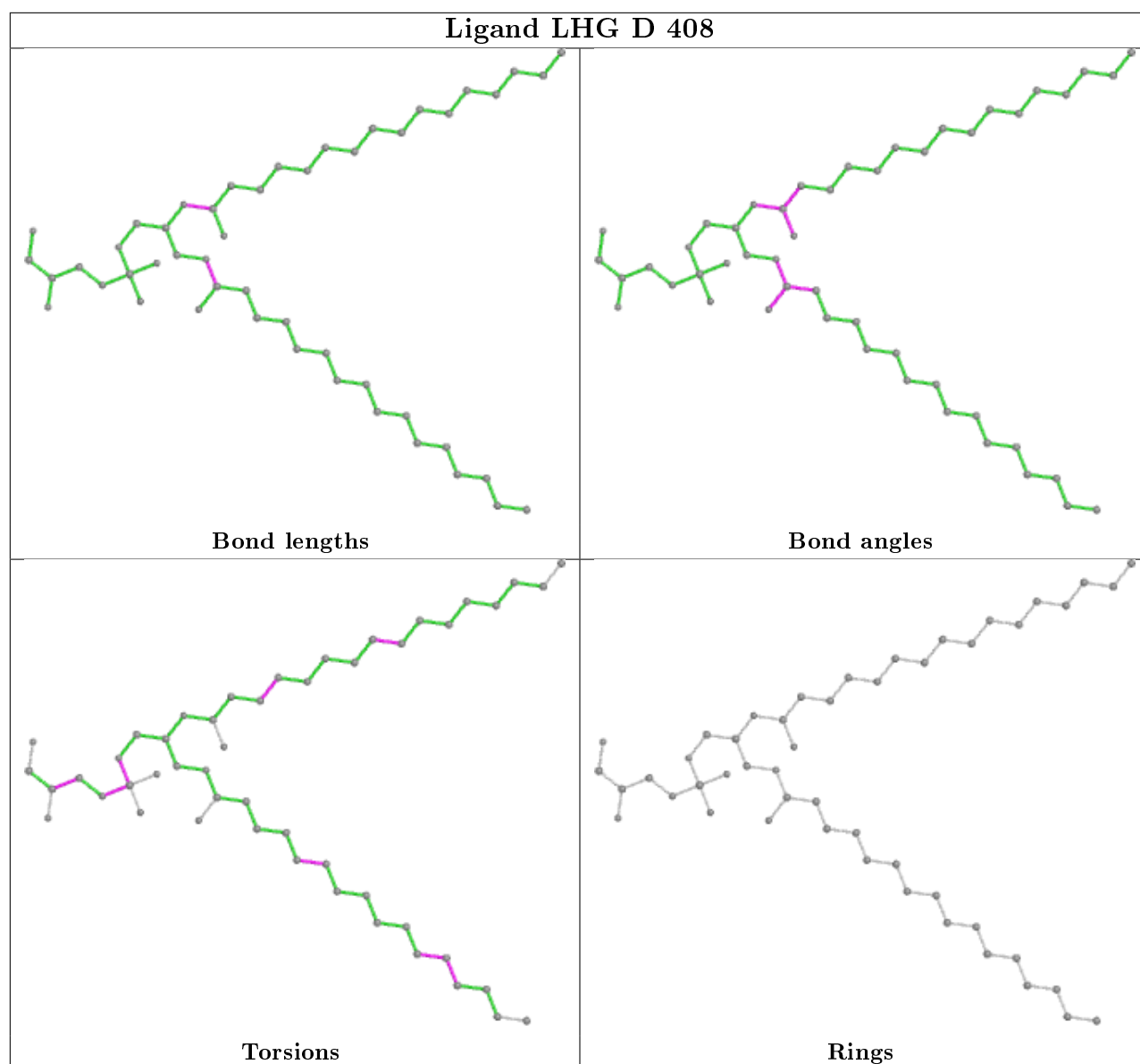


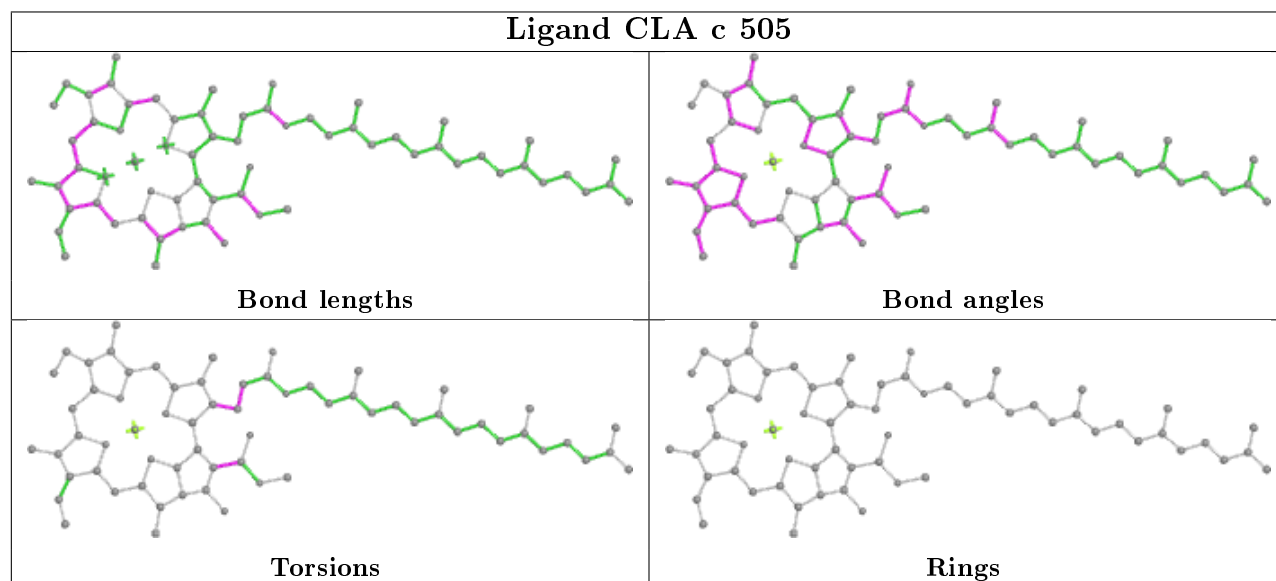
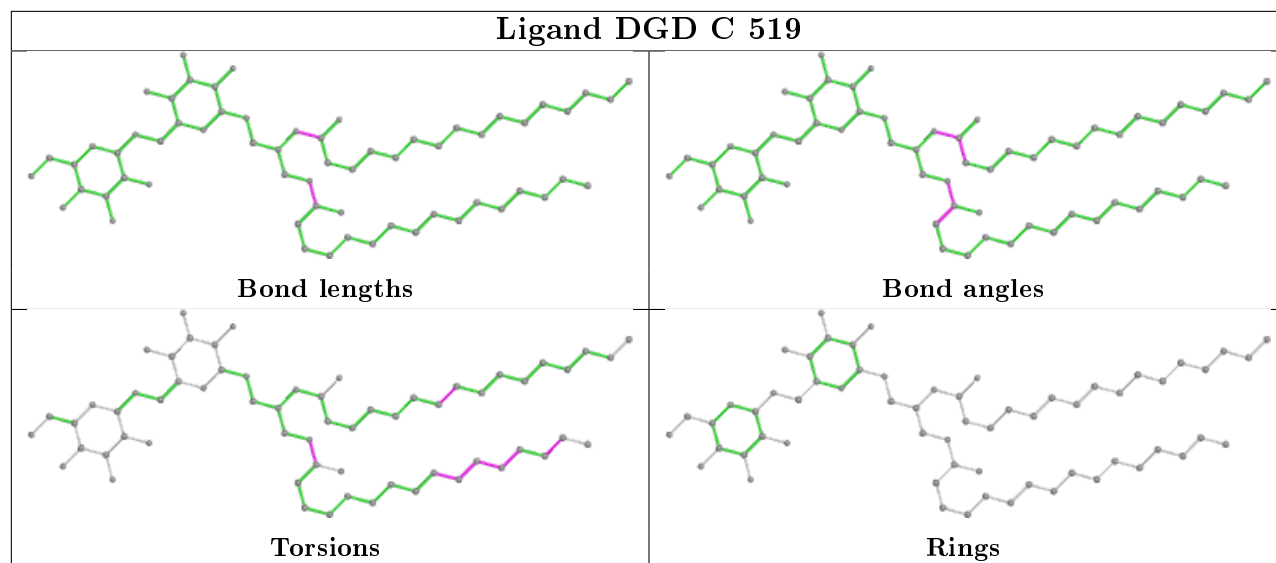
Ligand CLA B 610



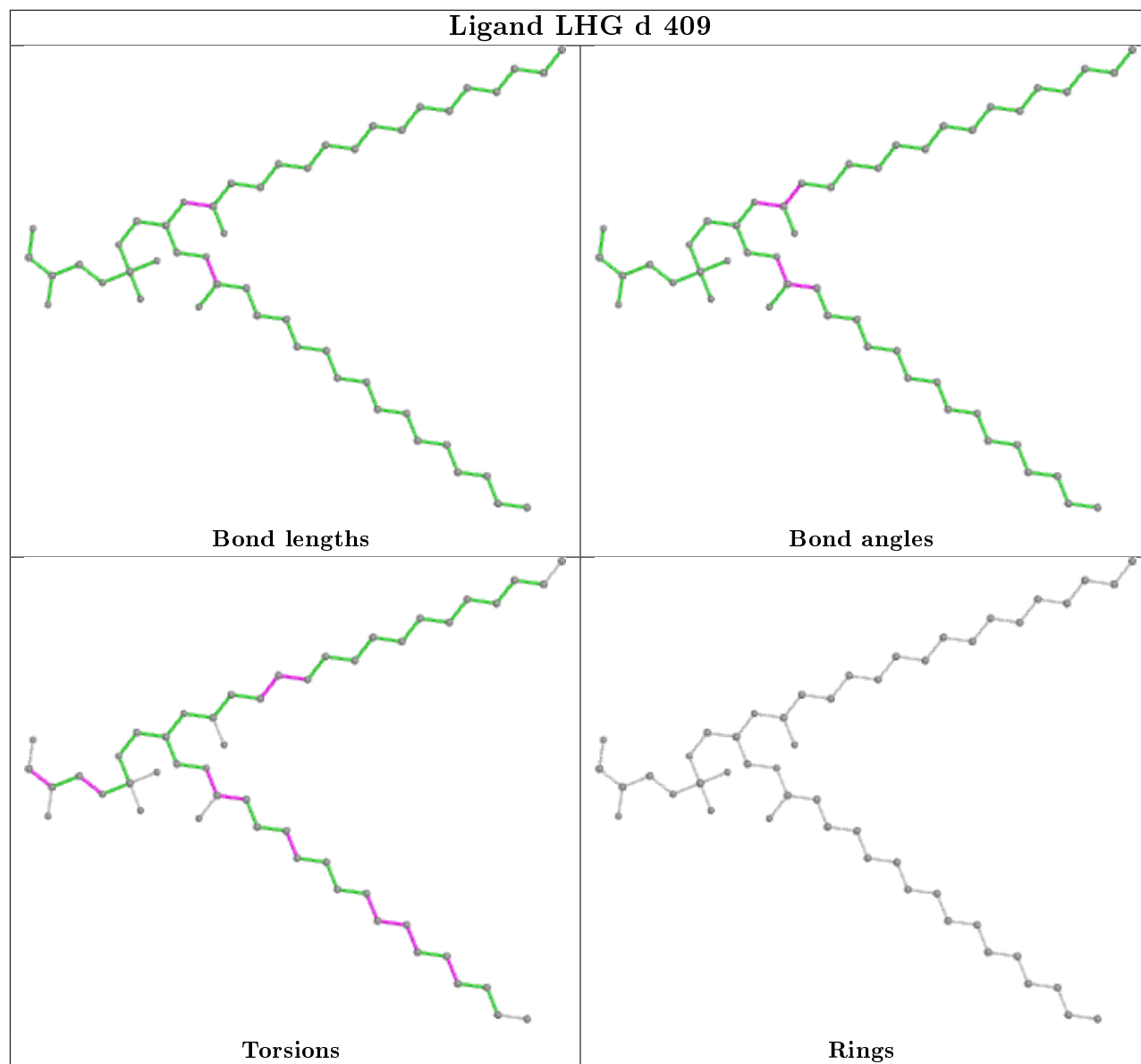
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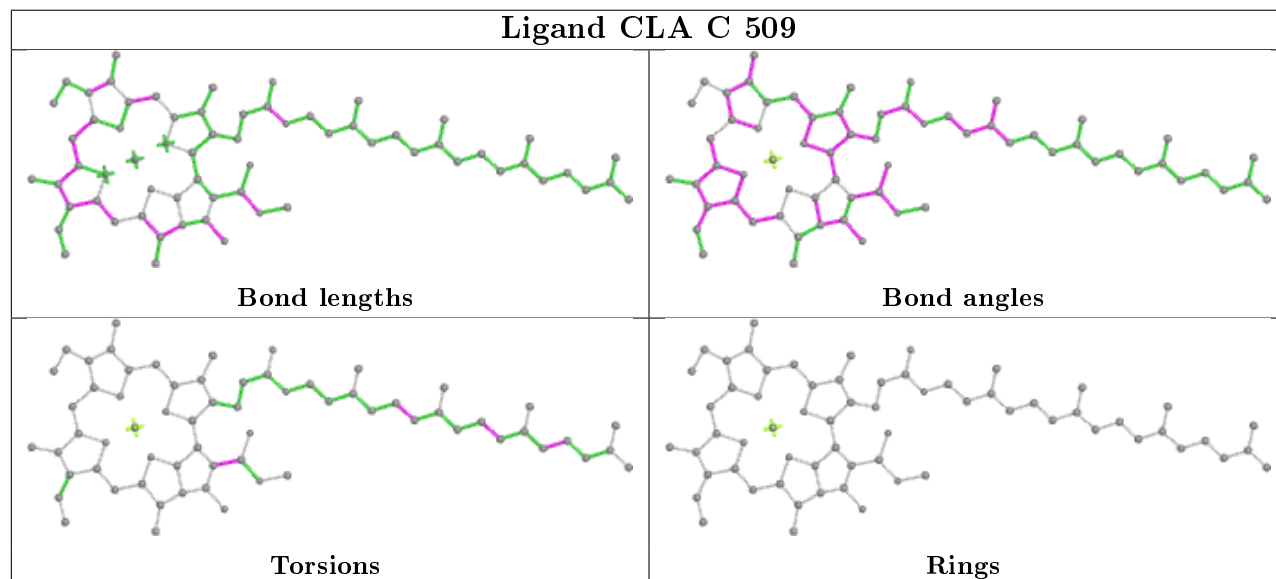




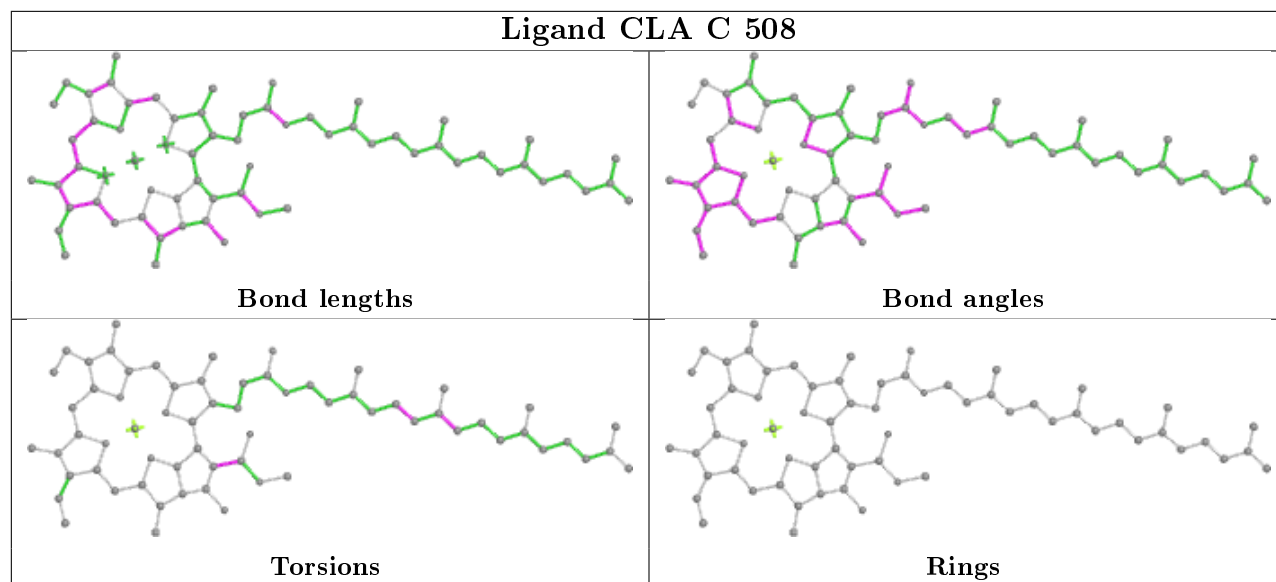
Ligand LHG d 409



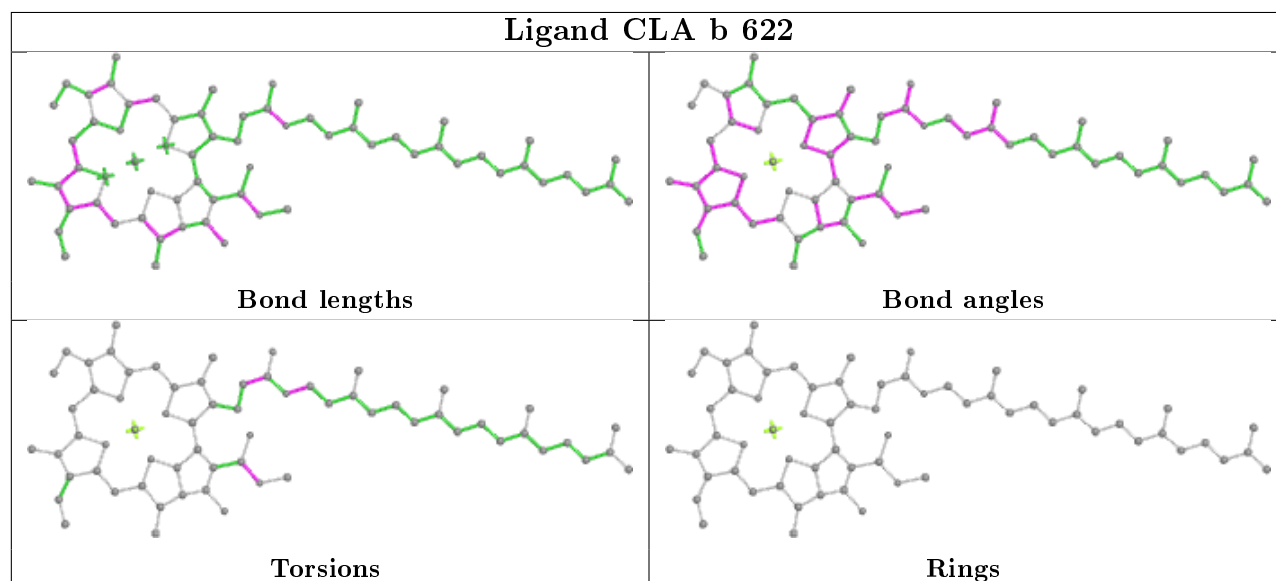
Ligand CLA C 509



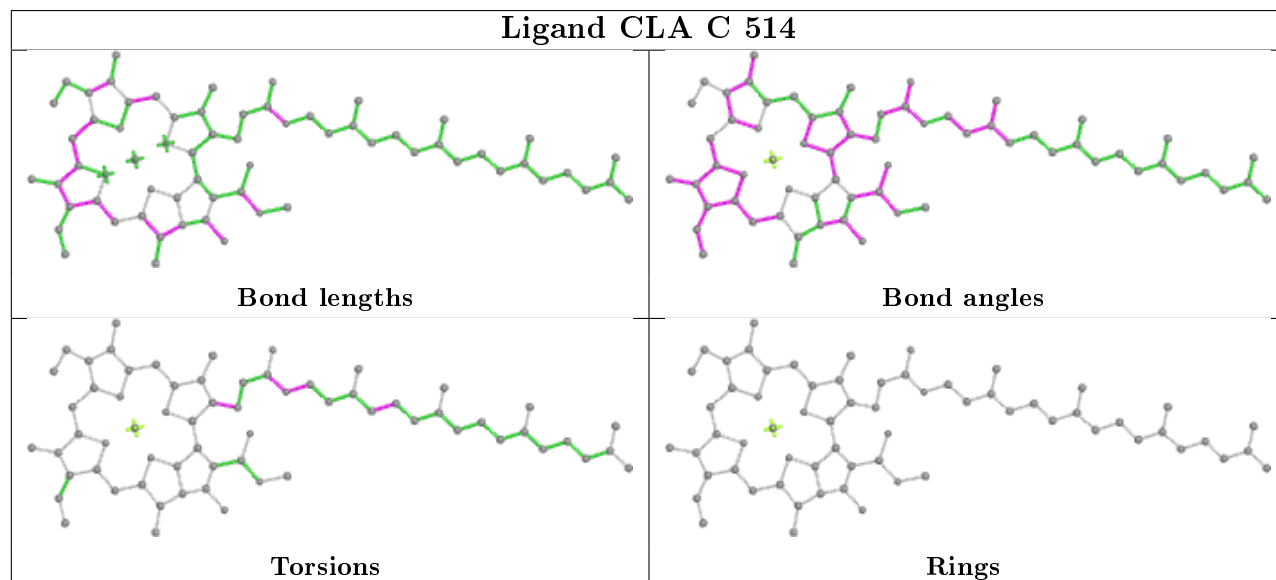
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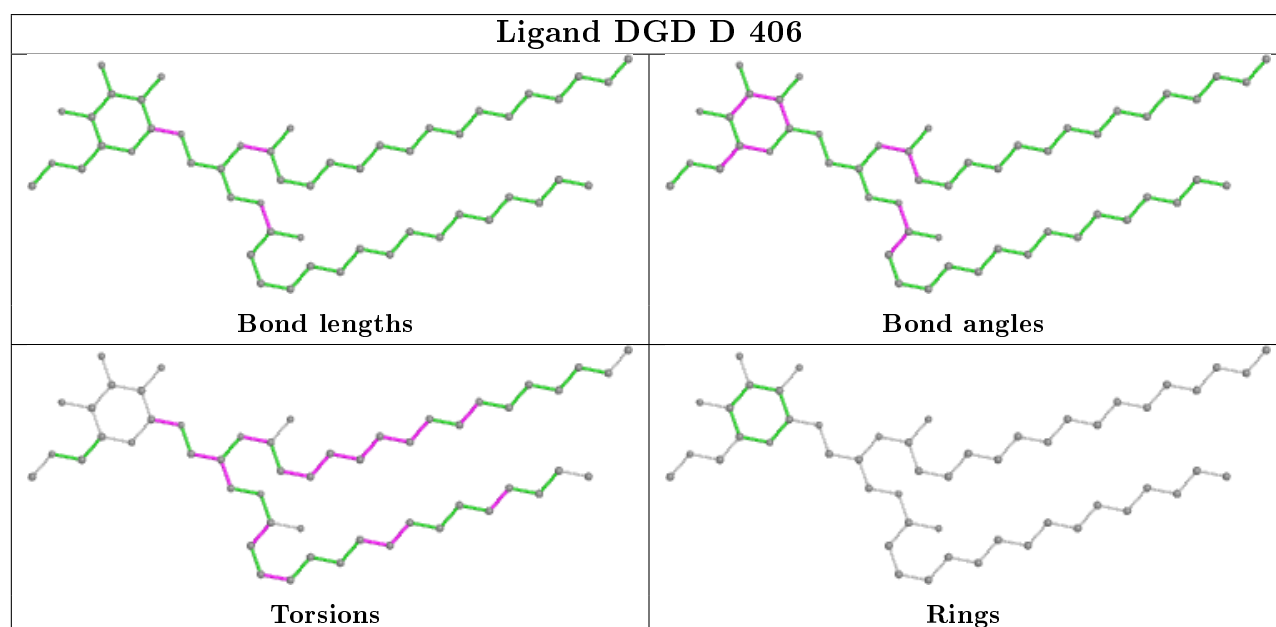
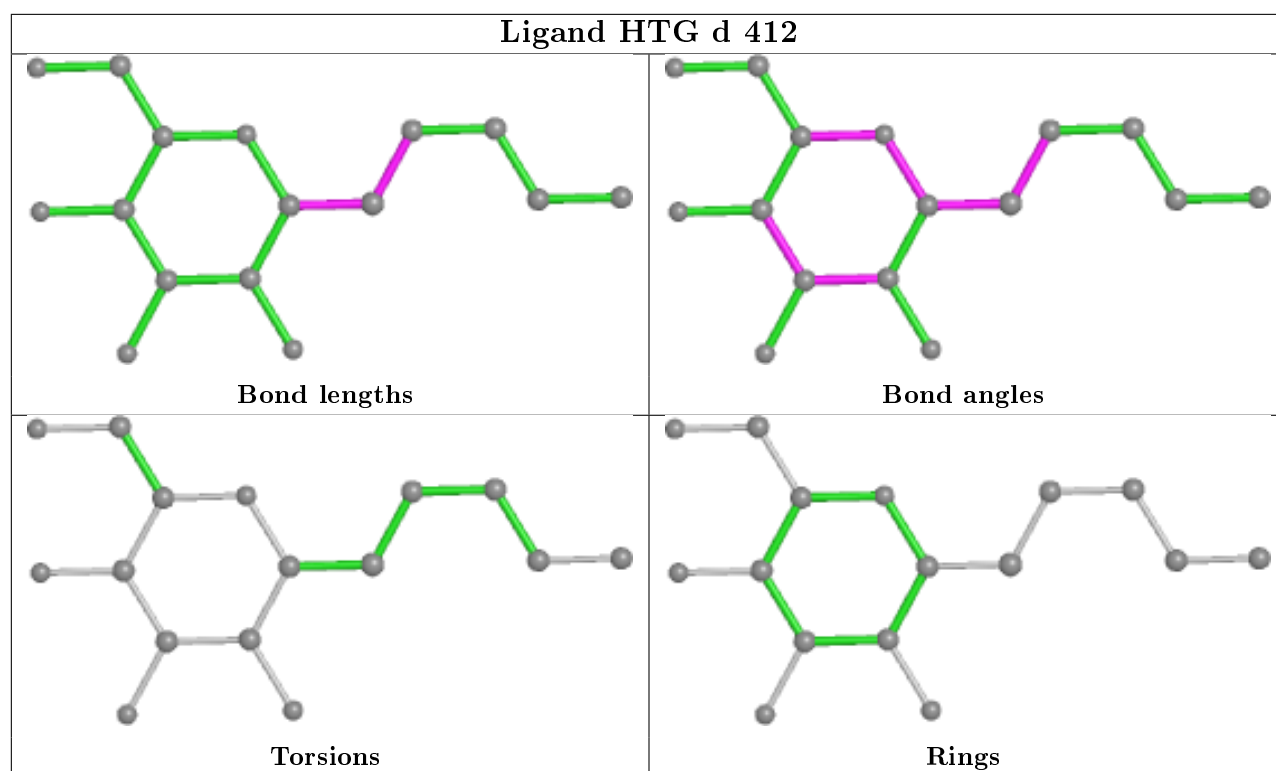


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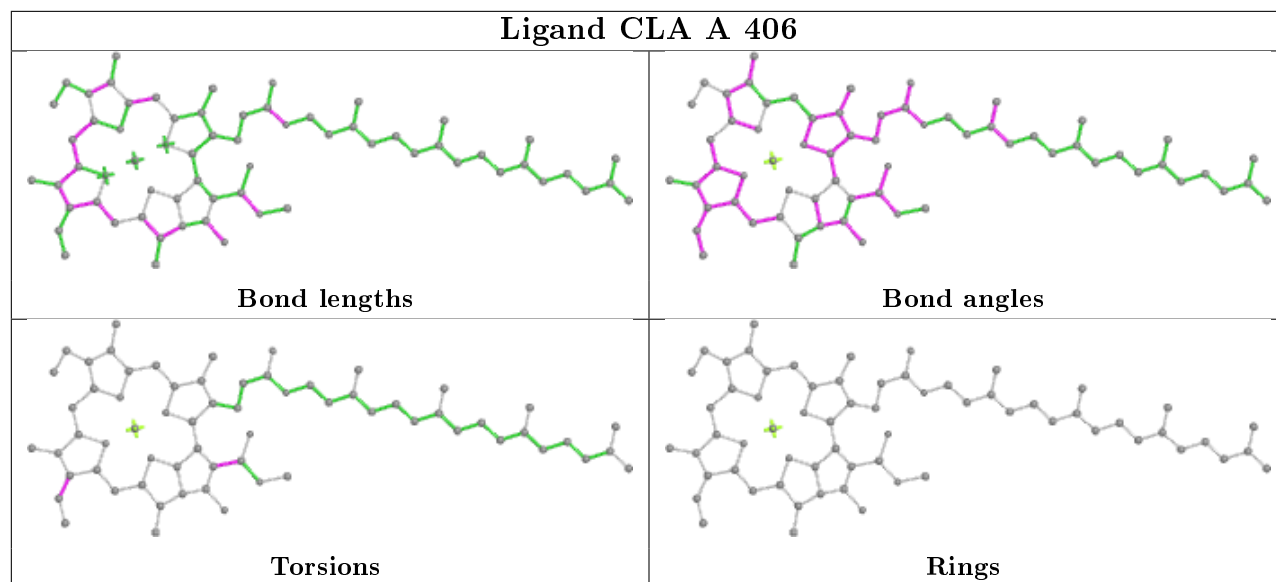


Ligand CLA C 514

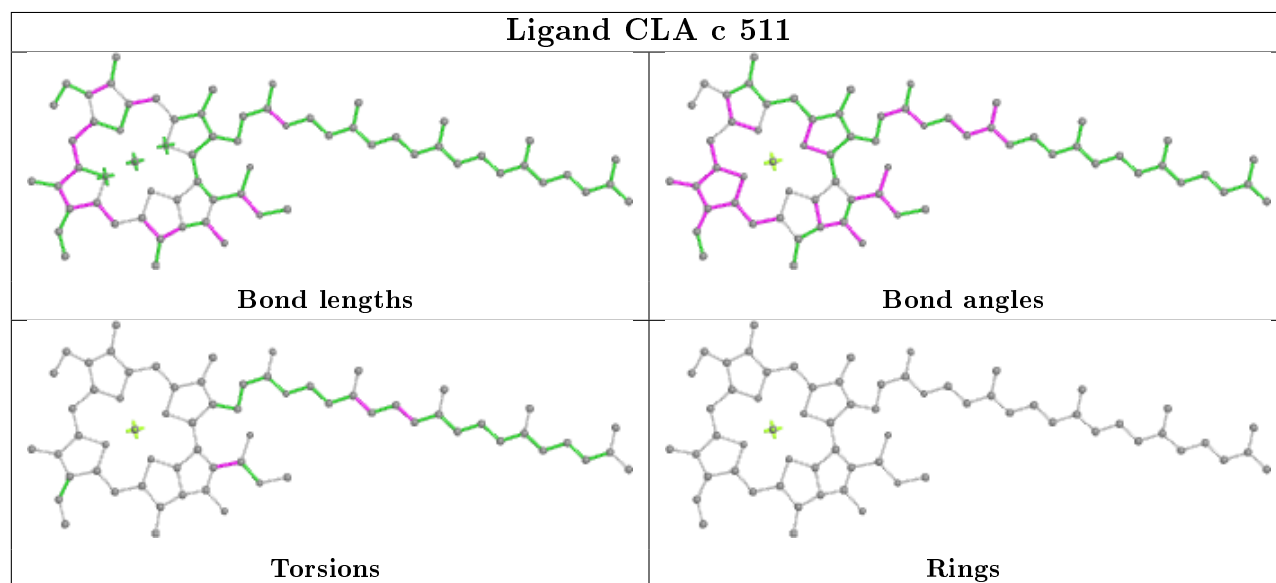


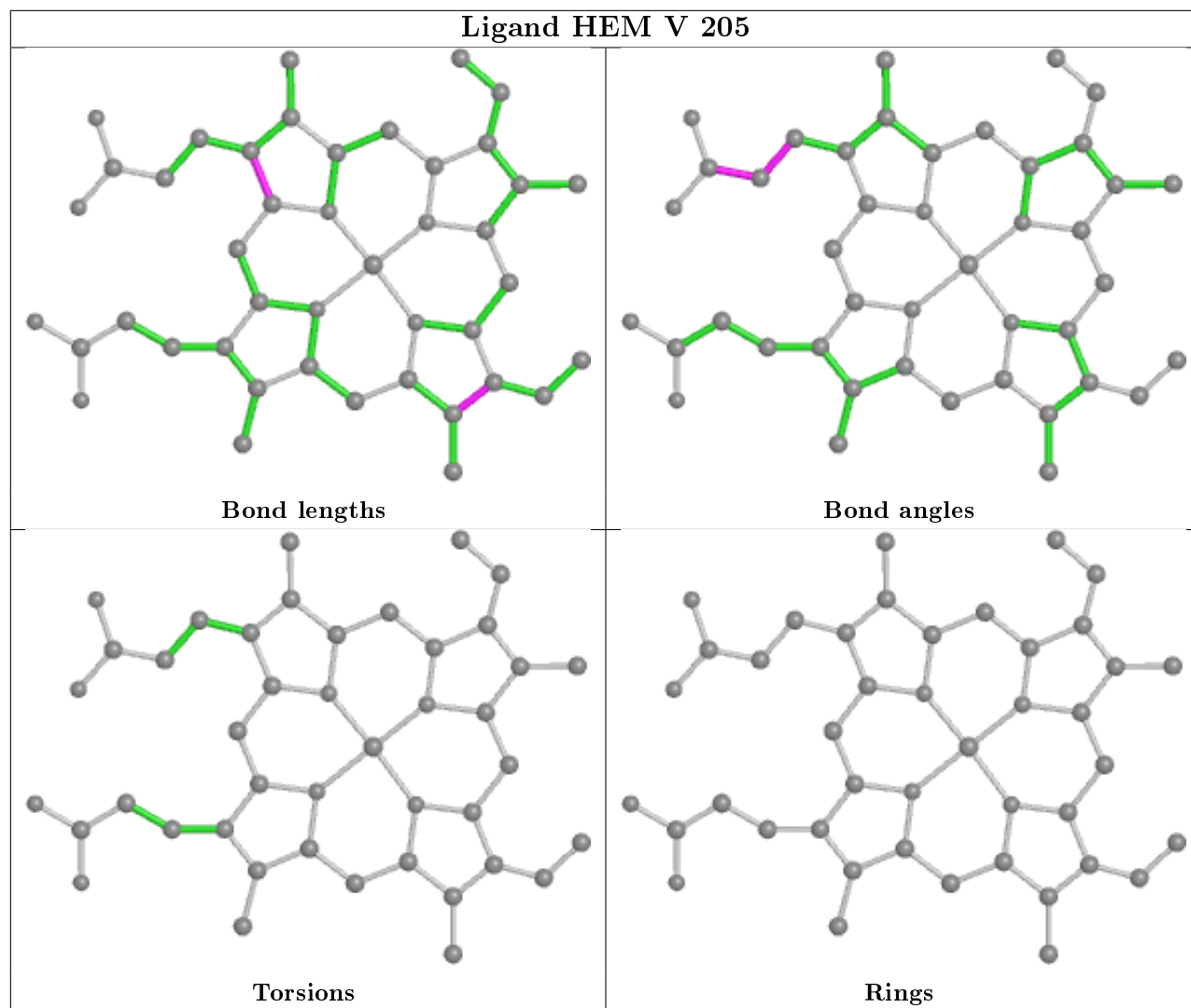


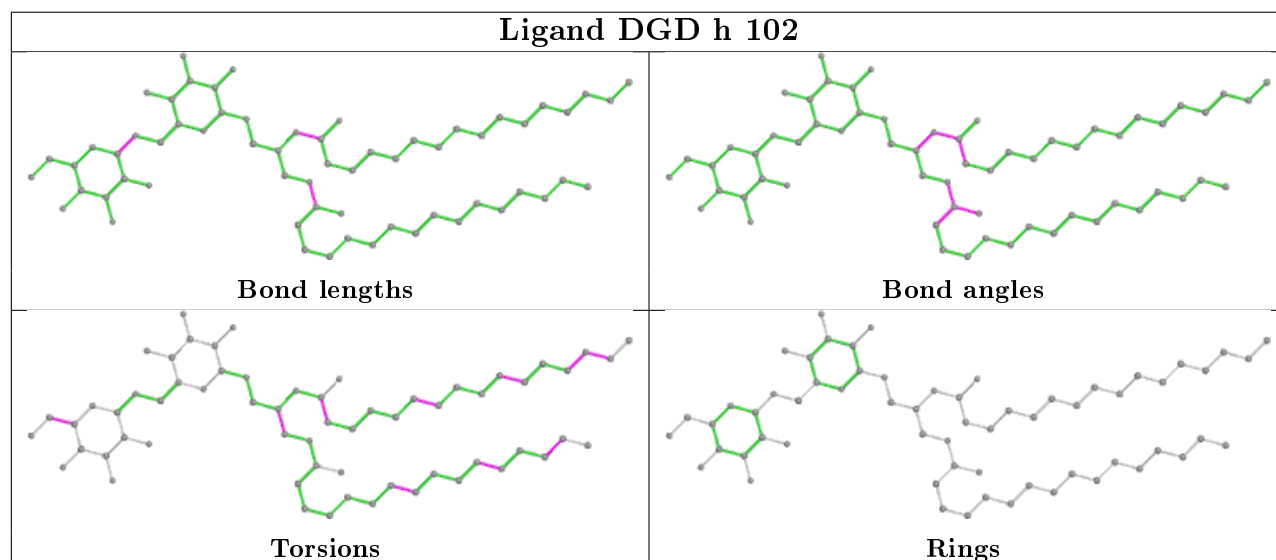
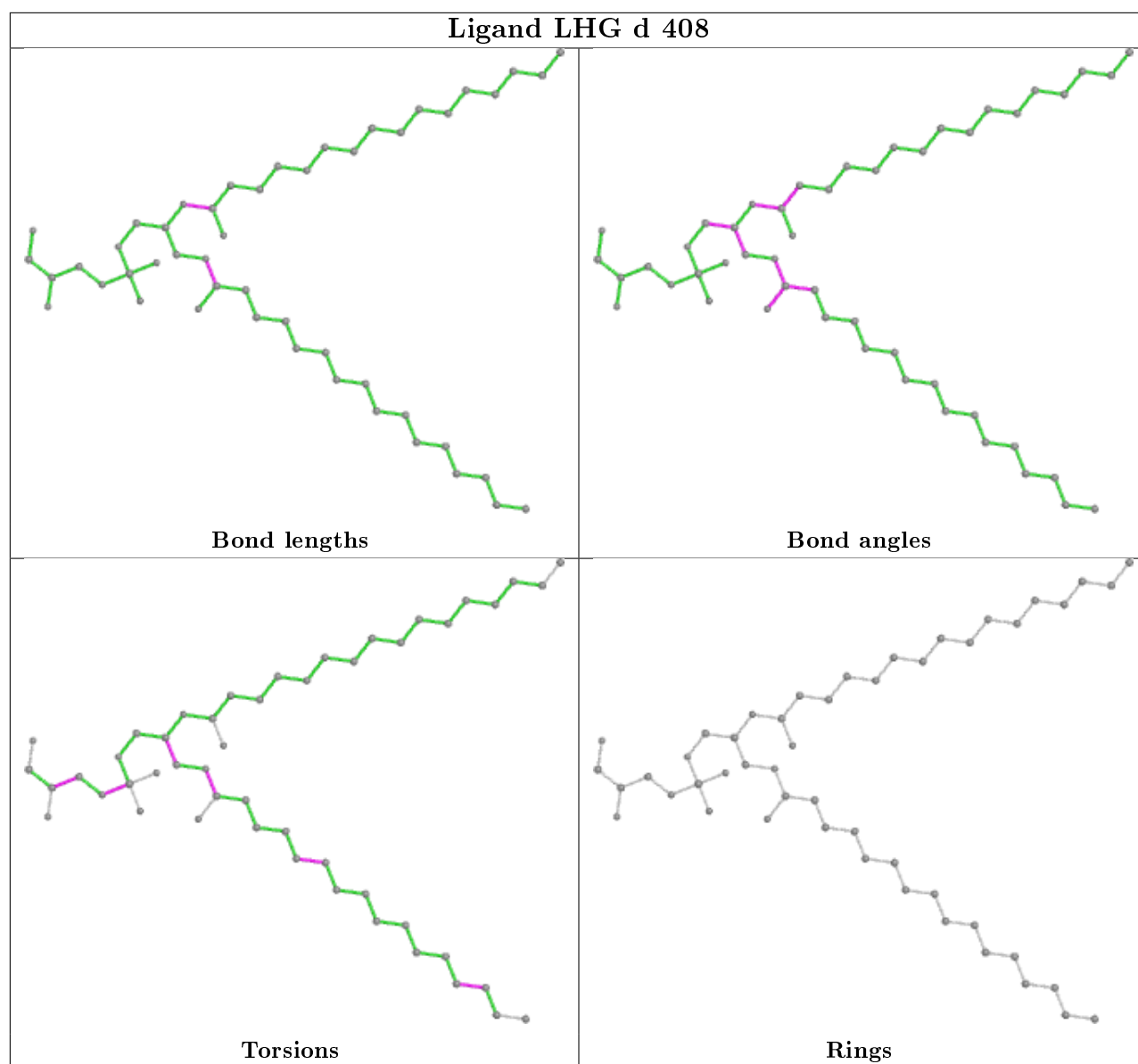
Ligand CLA A 406



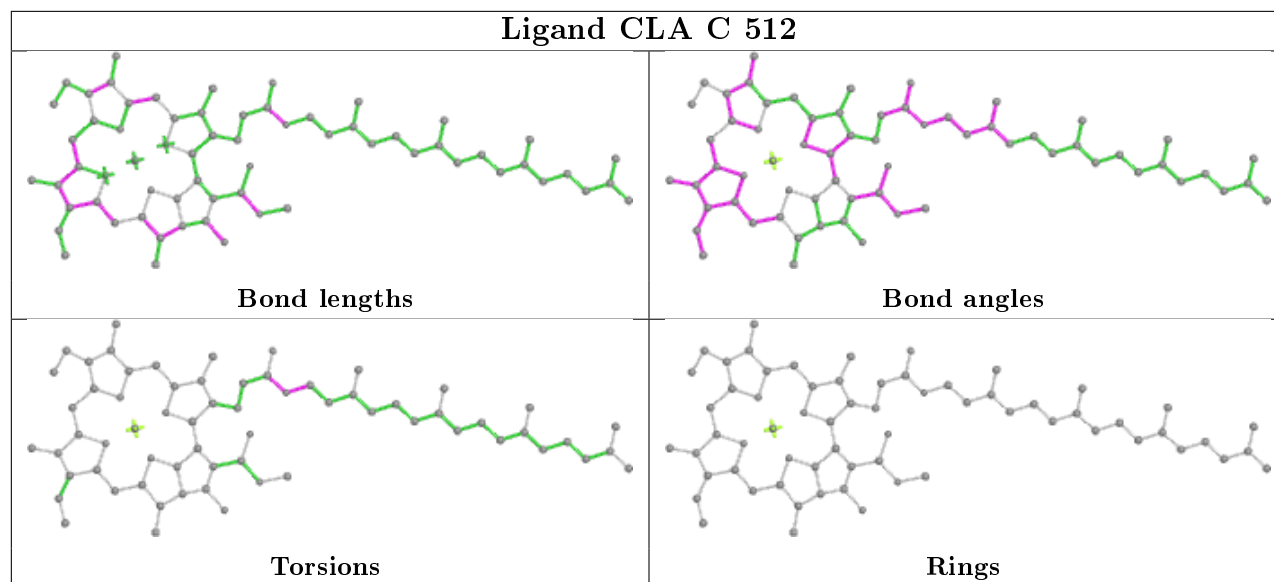
Ligand CLA c 511



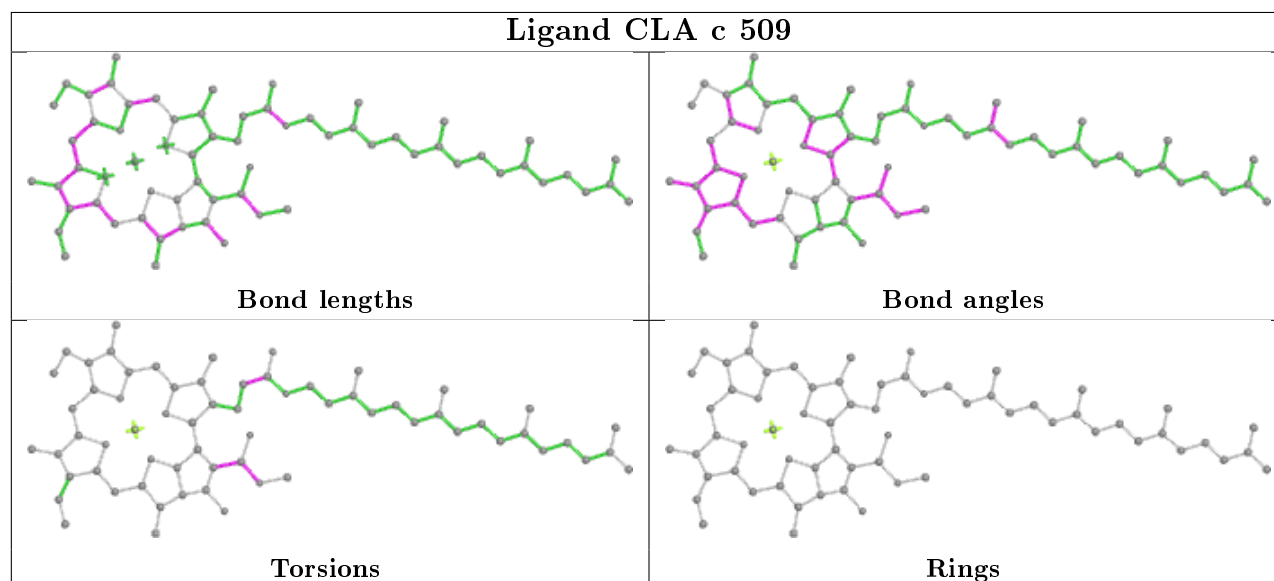




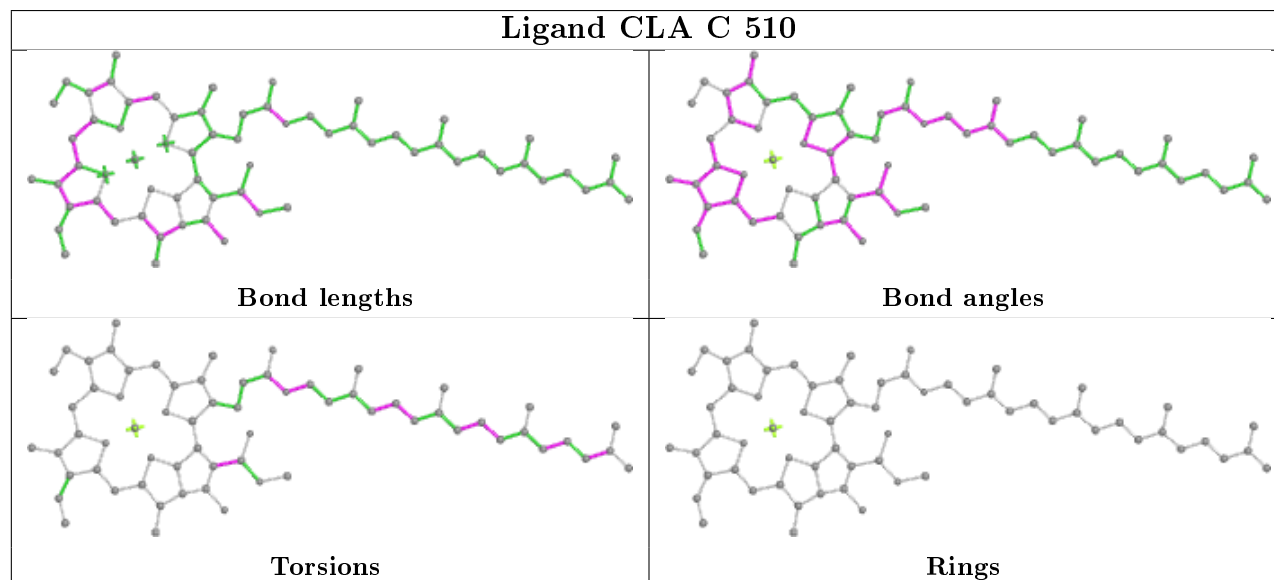
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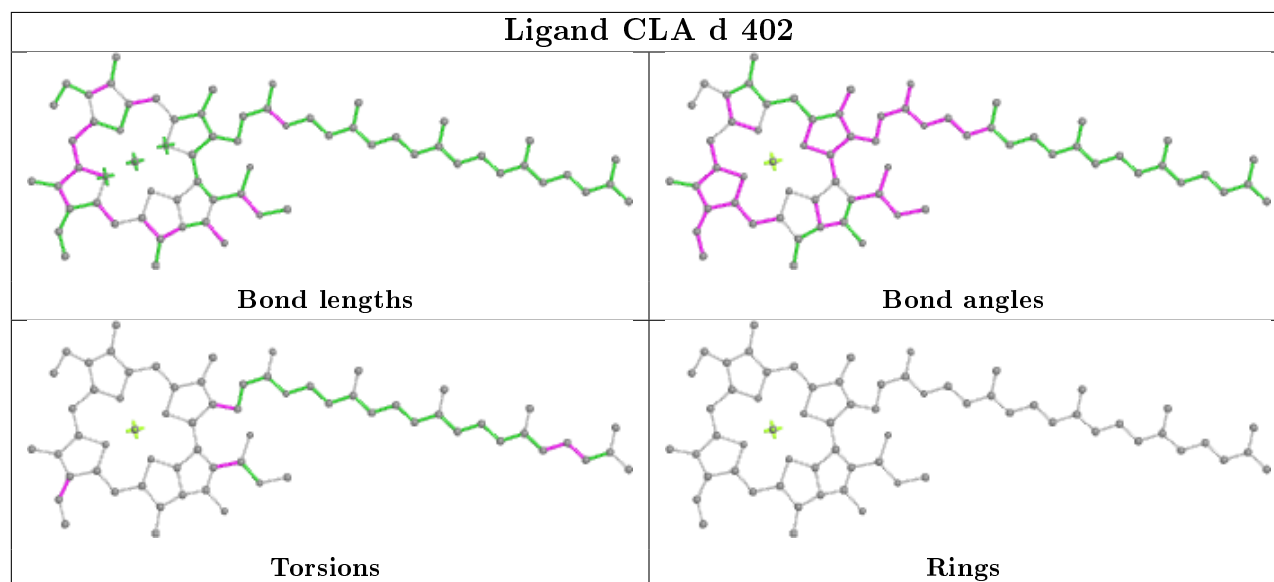
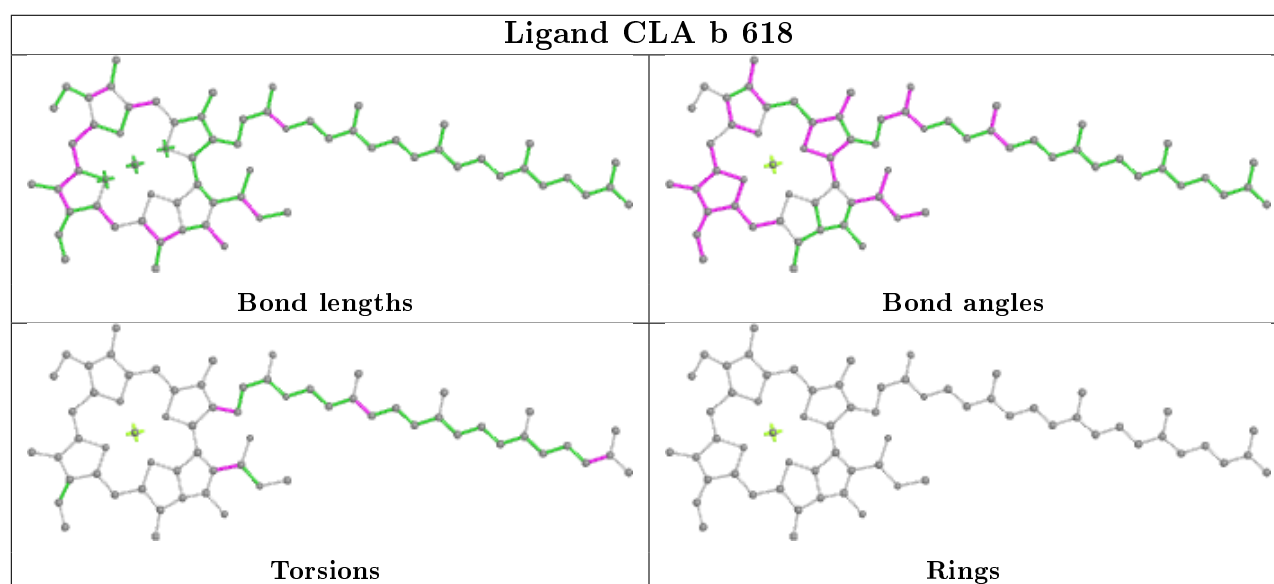
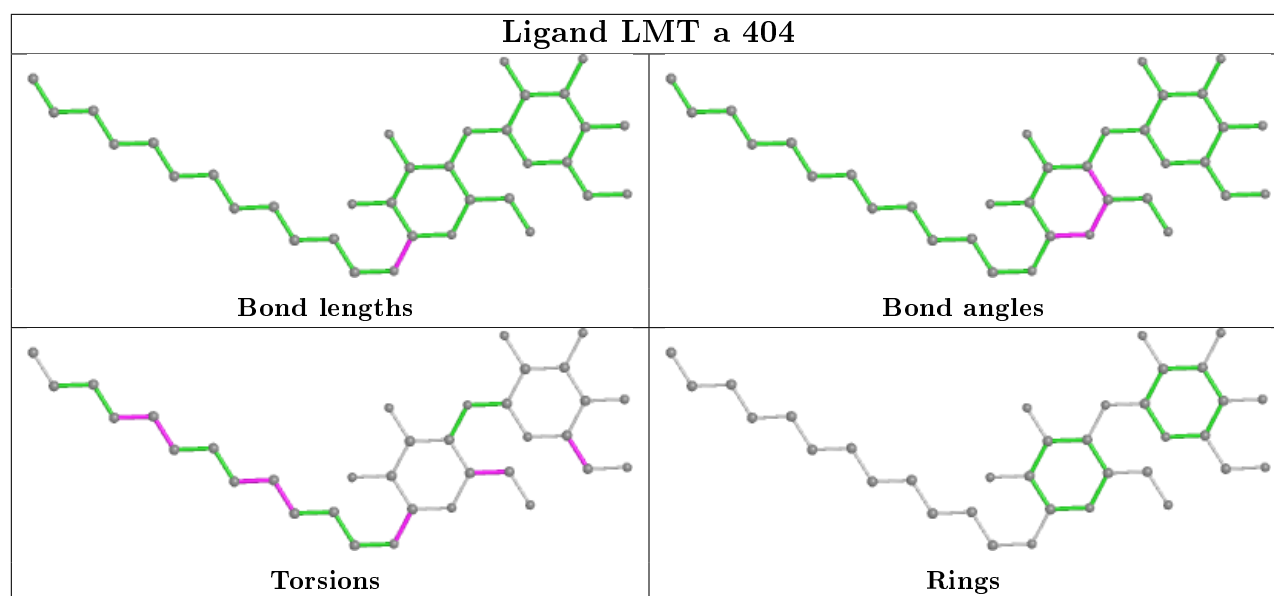


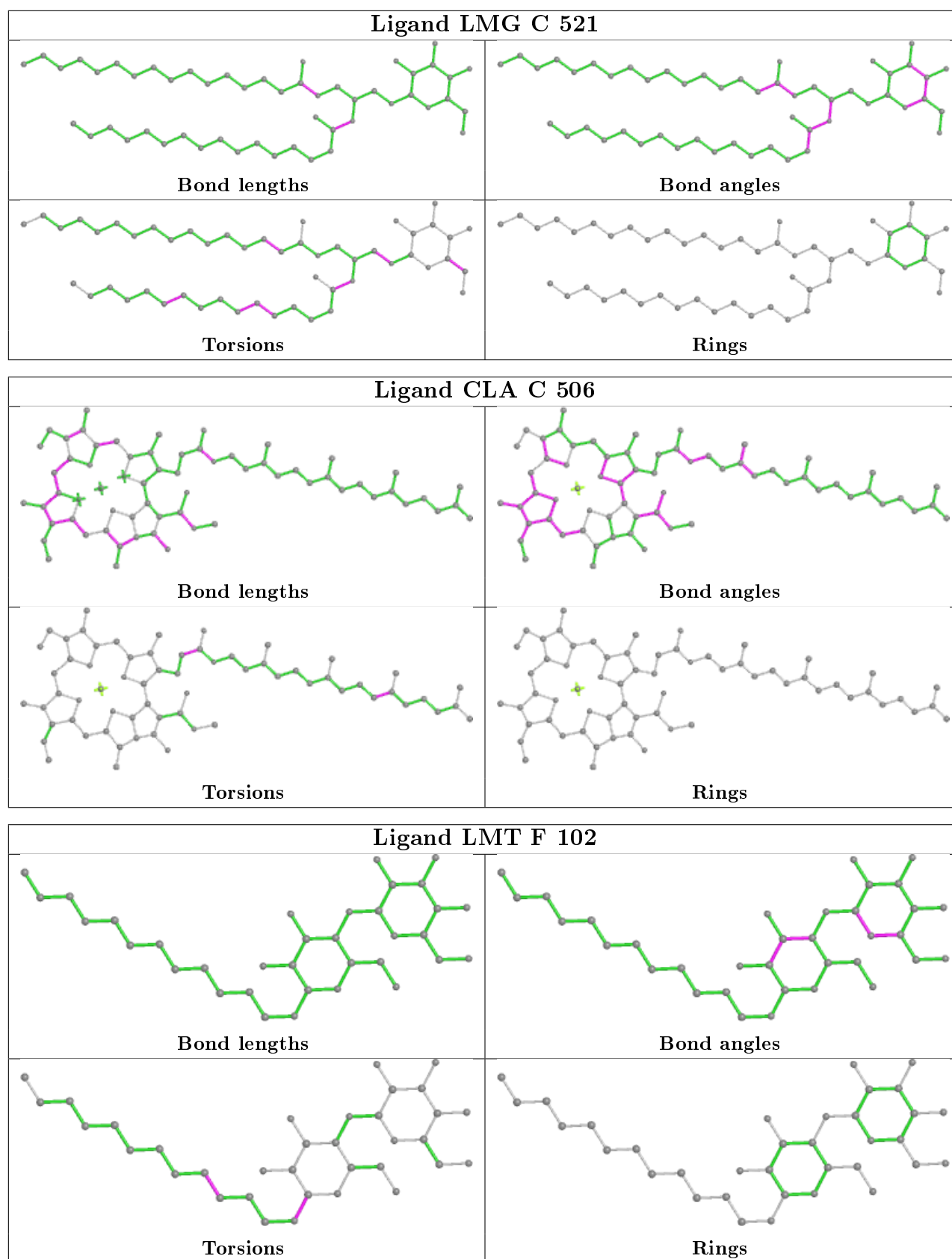
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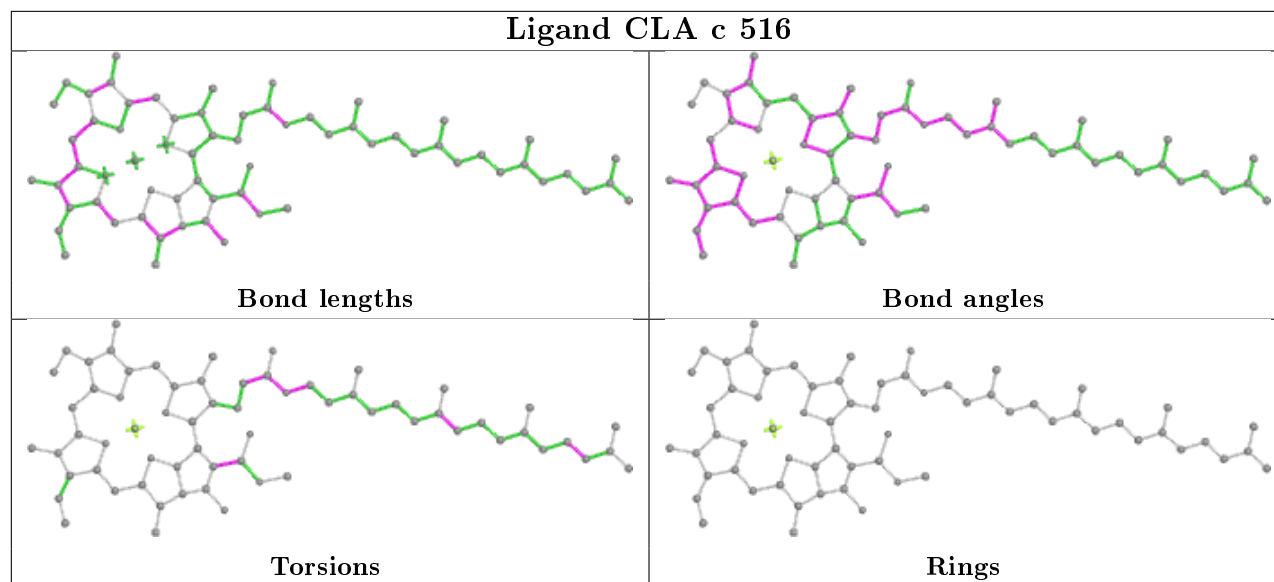
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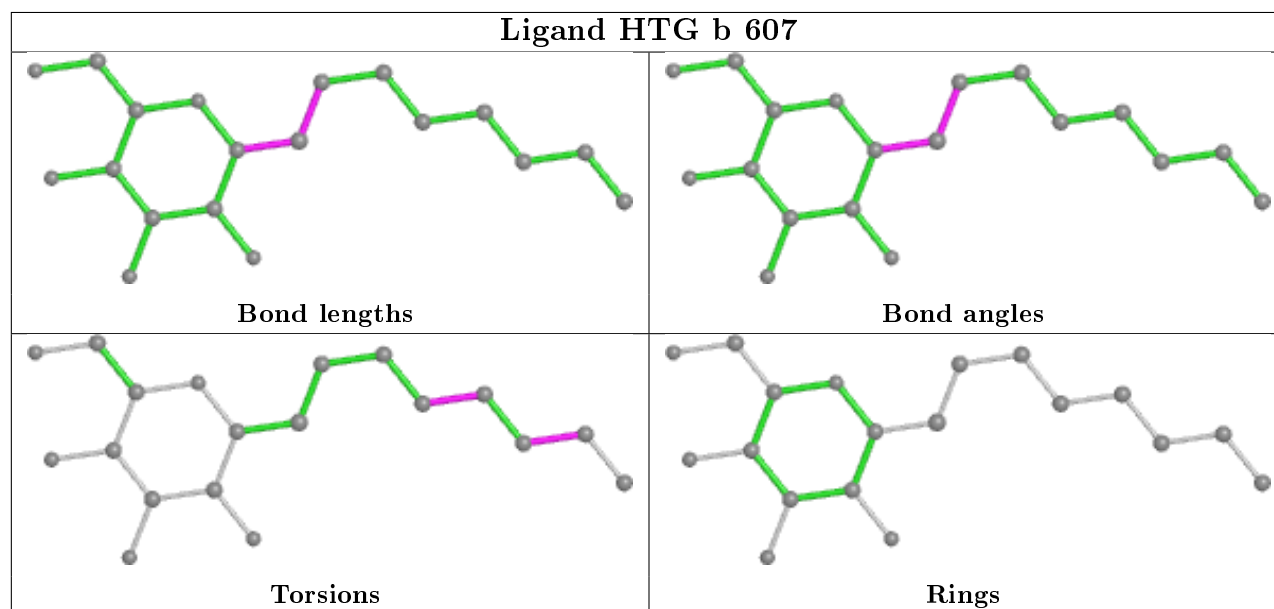




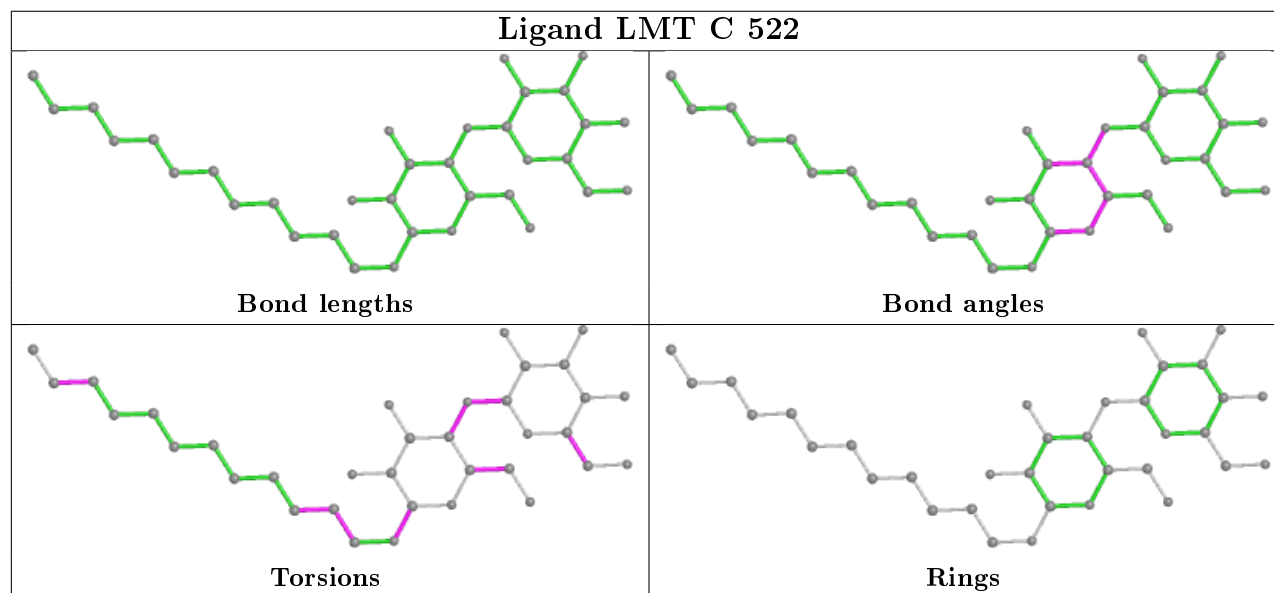
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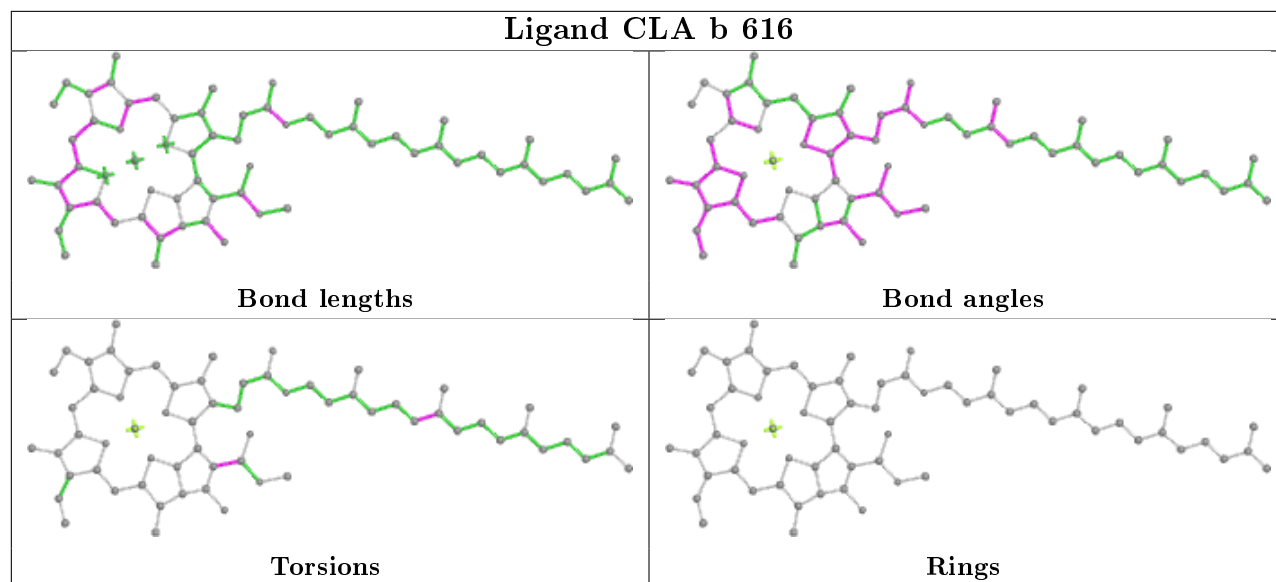
Ligand HTG b 607



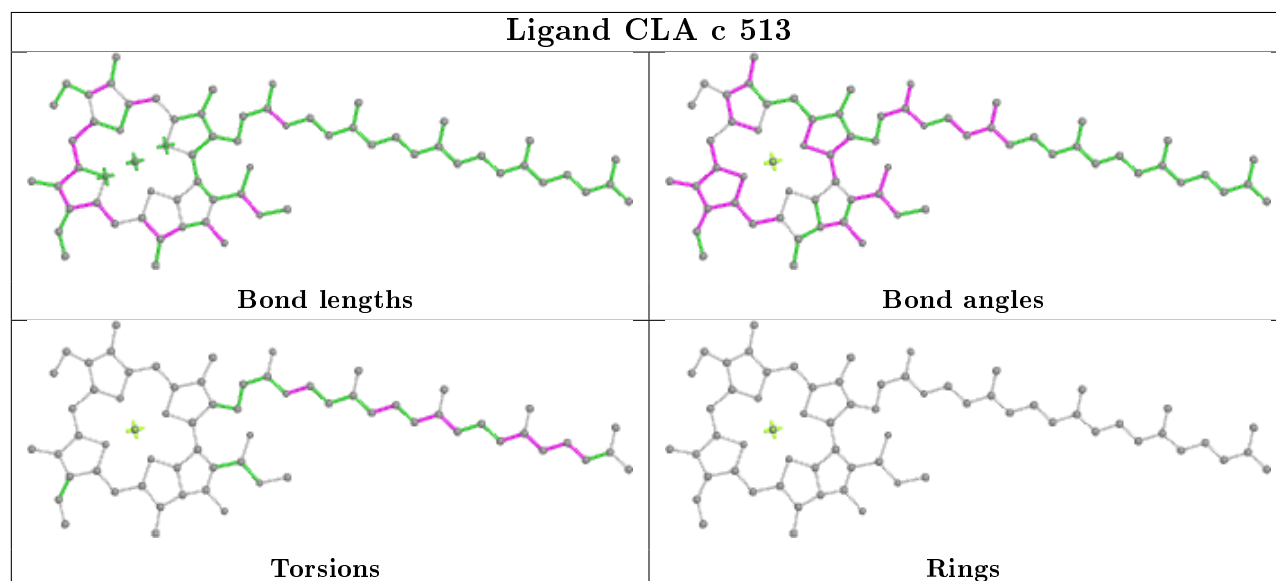
Ligand LMT C 522



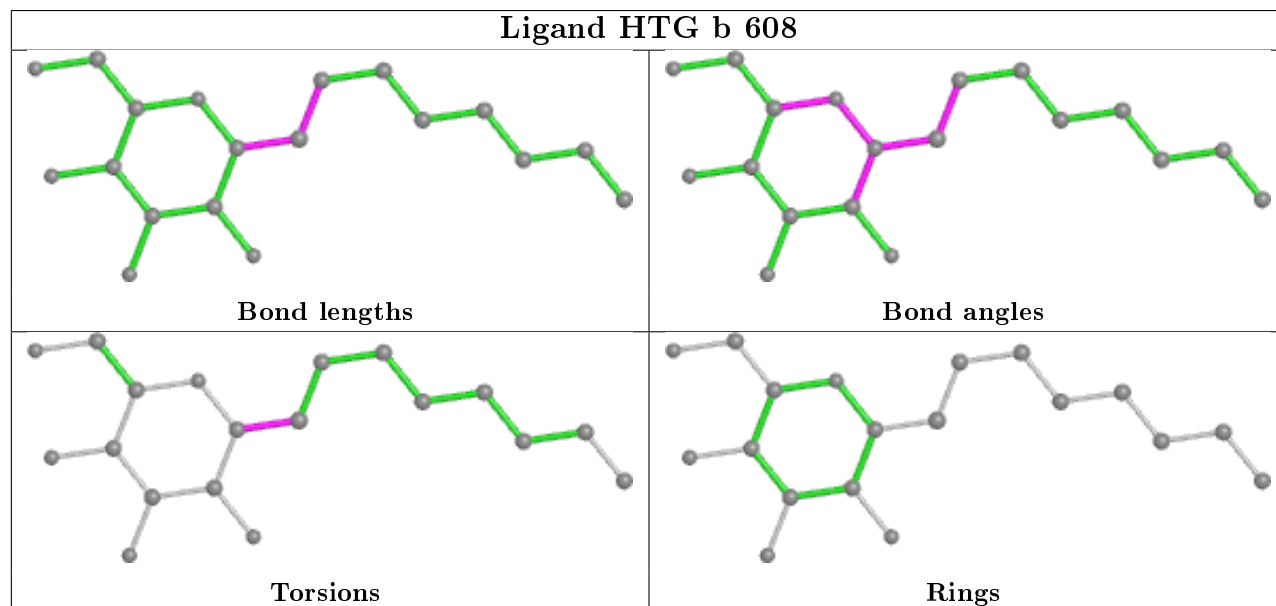
Ligand CLA b 616

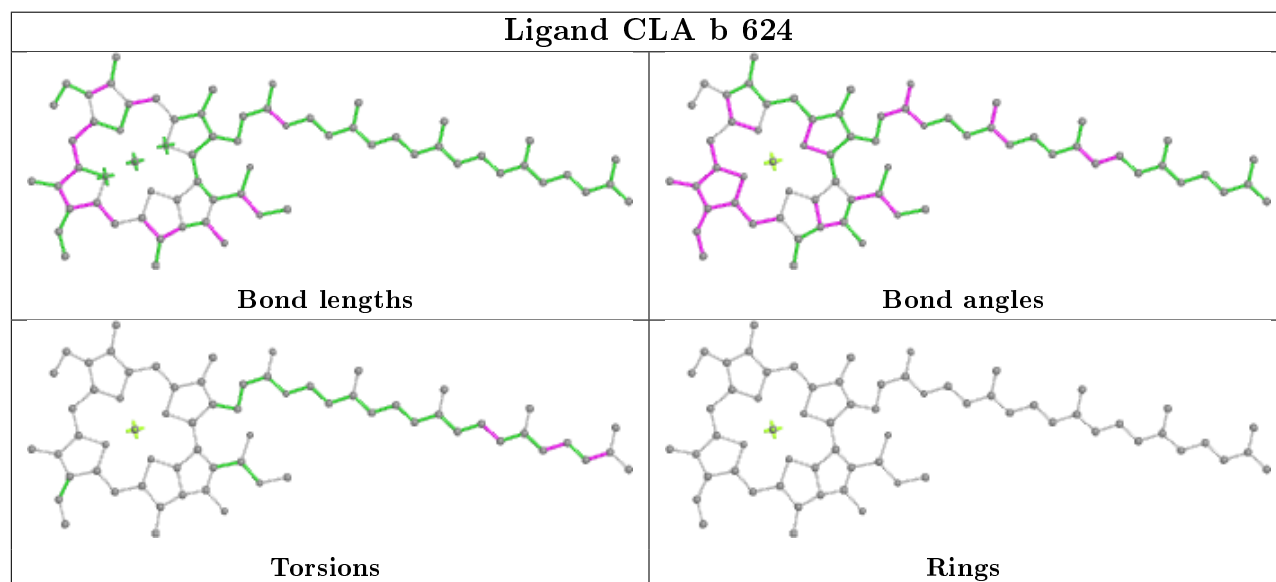
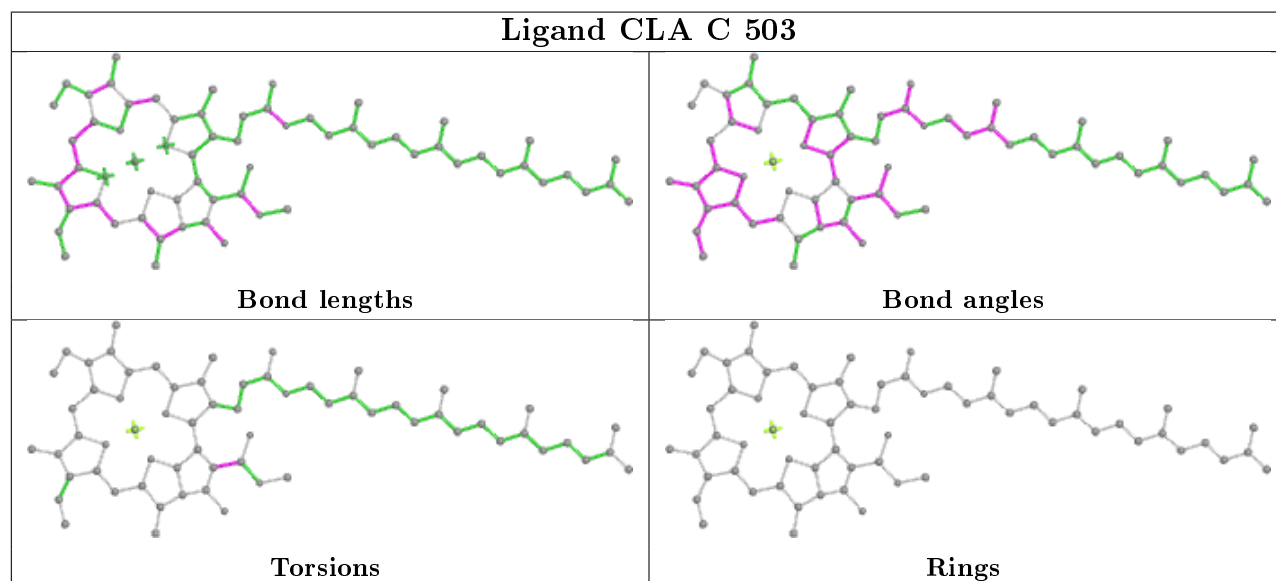
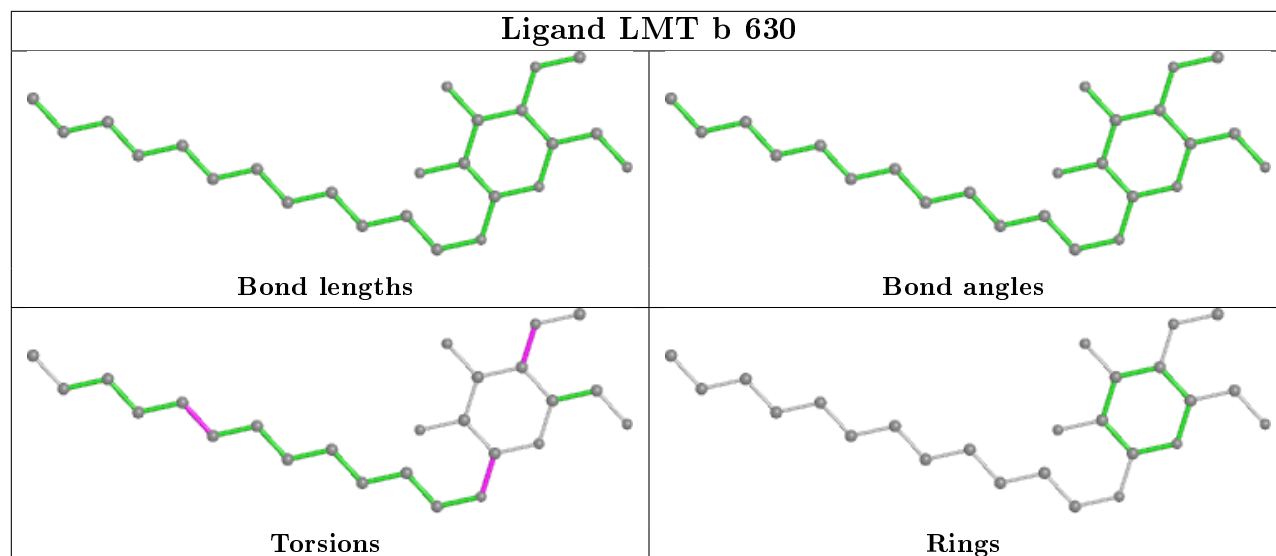


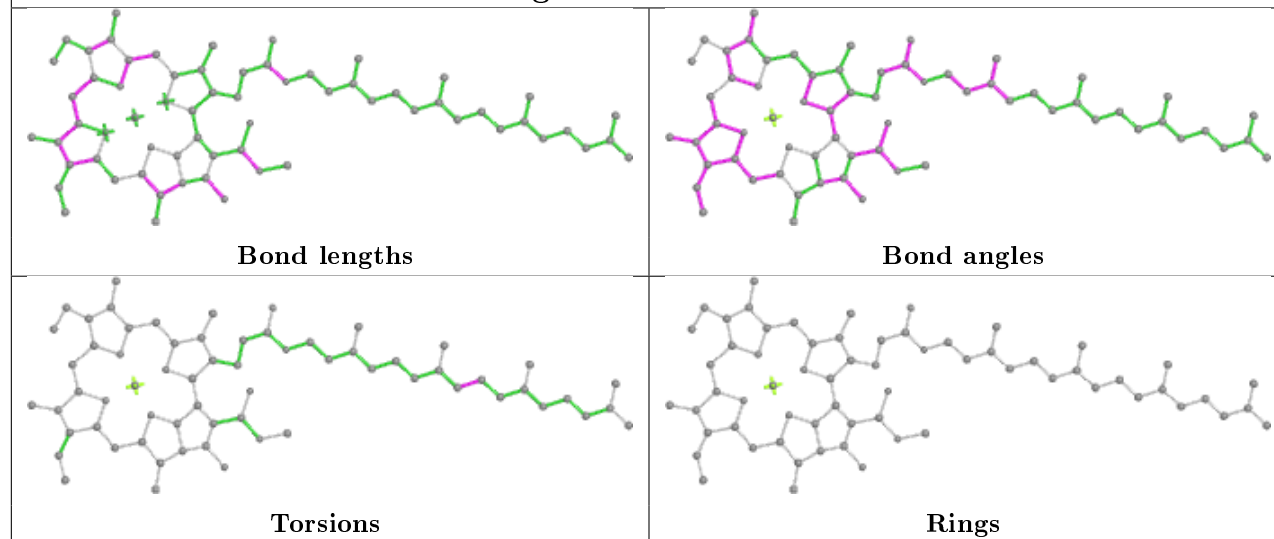
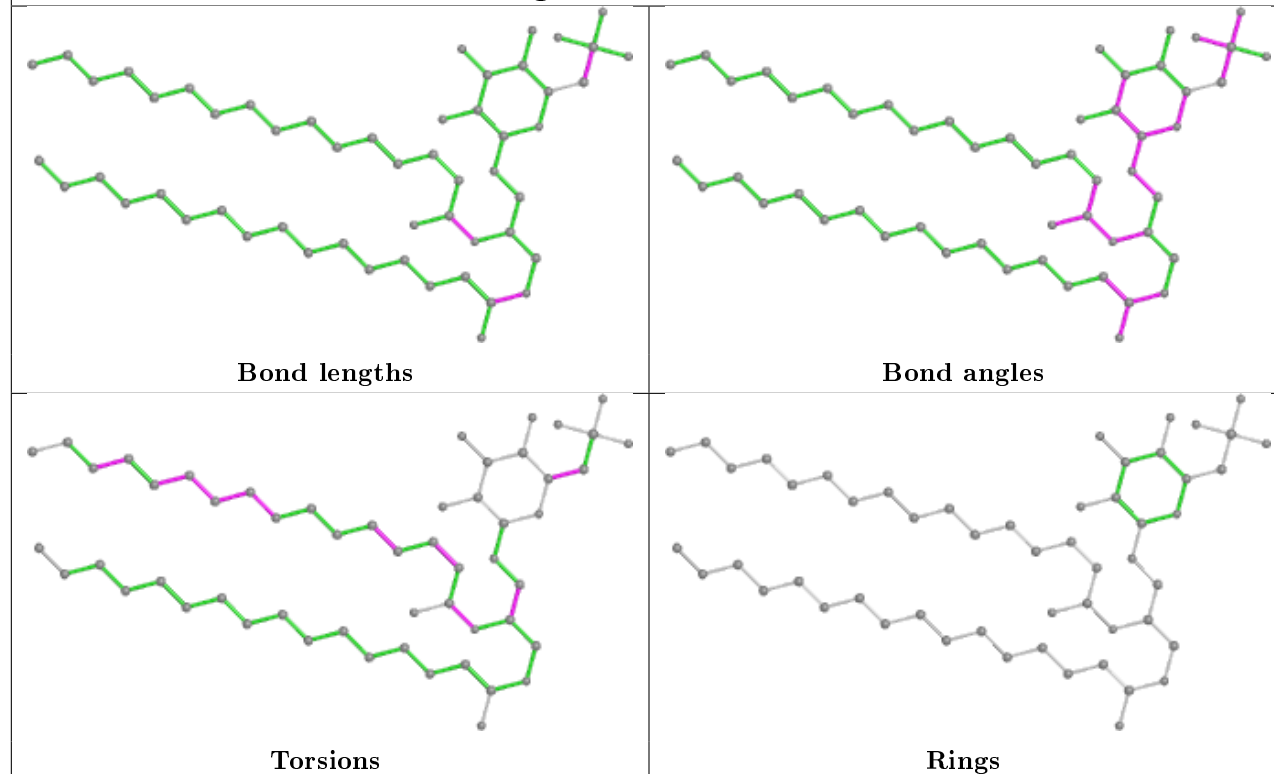
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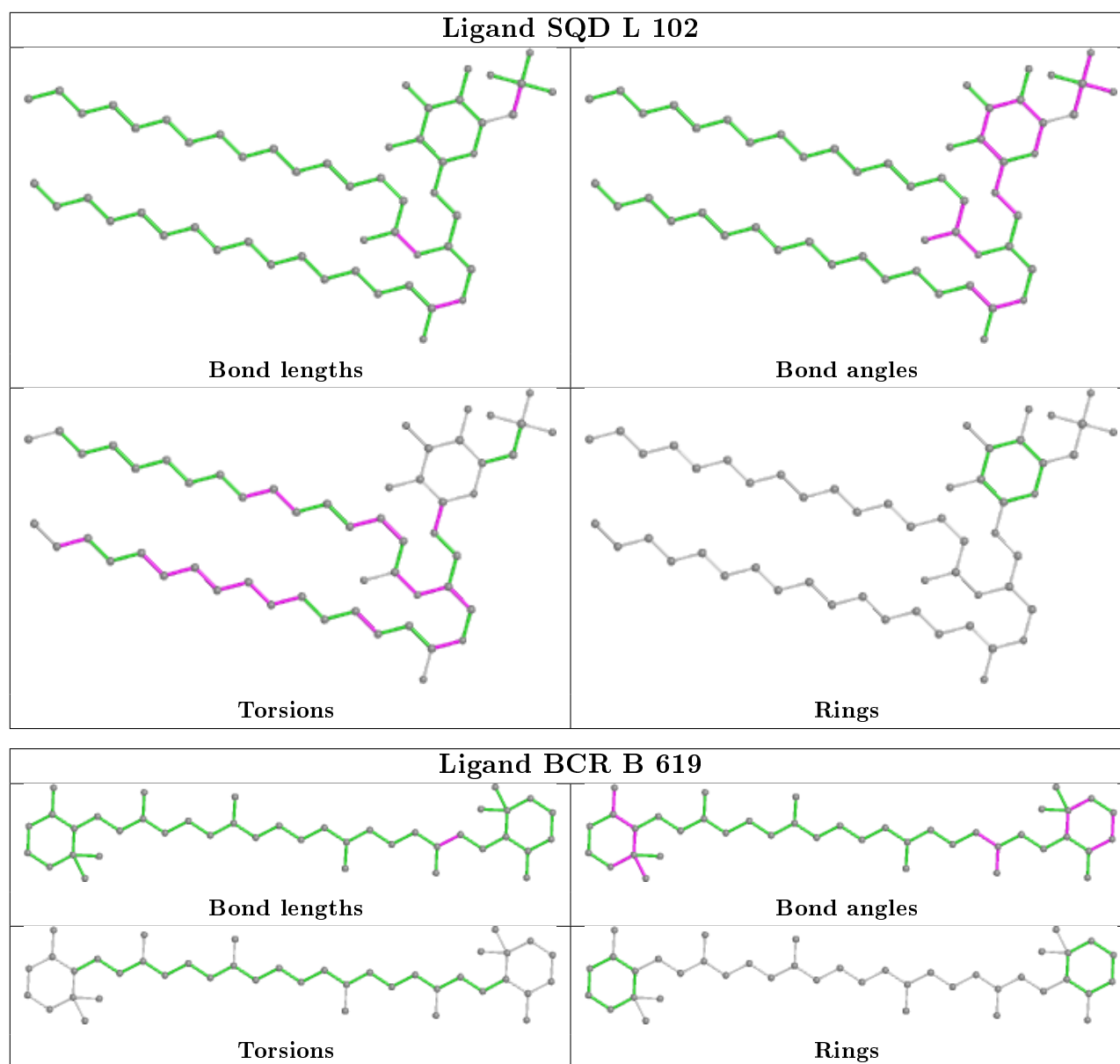


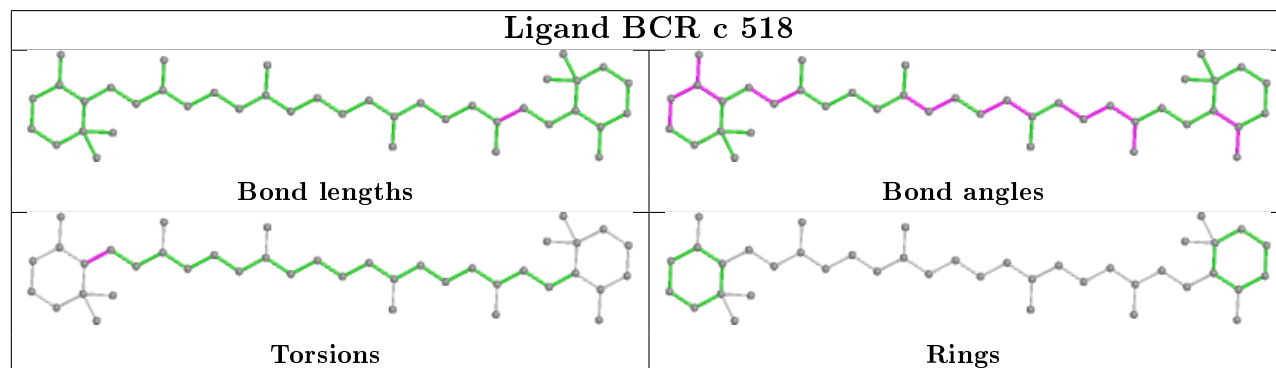
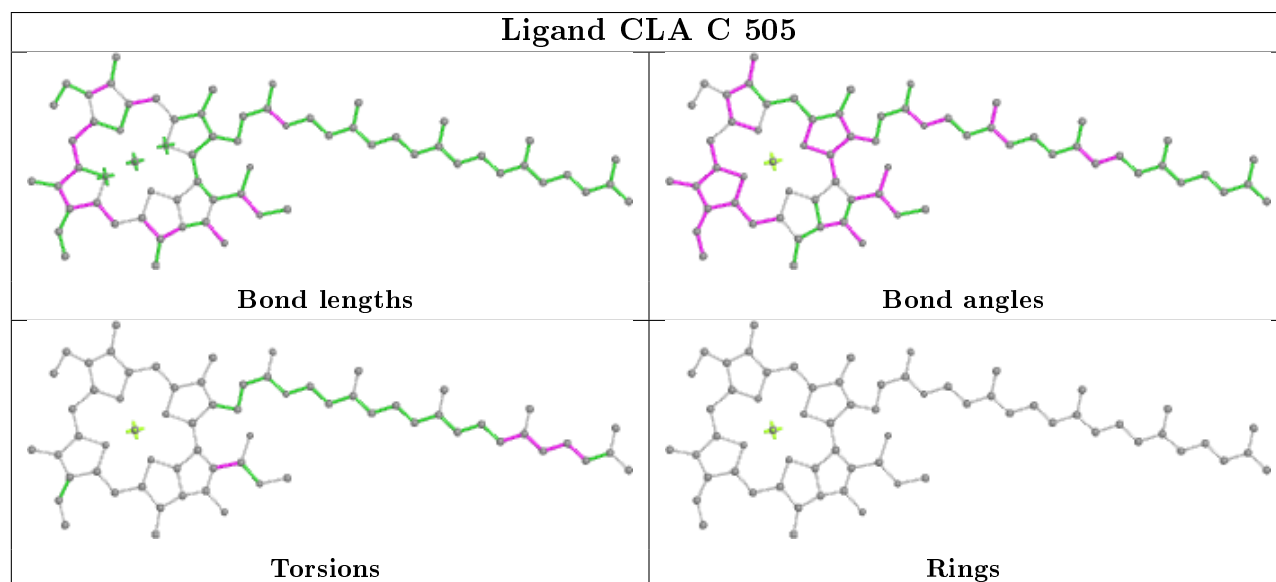
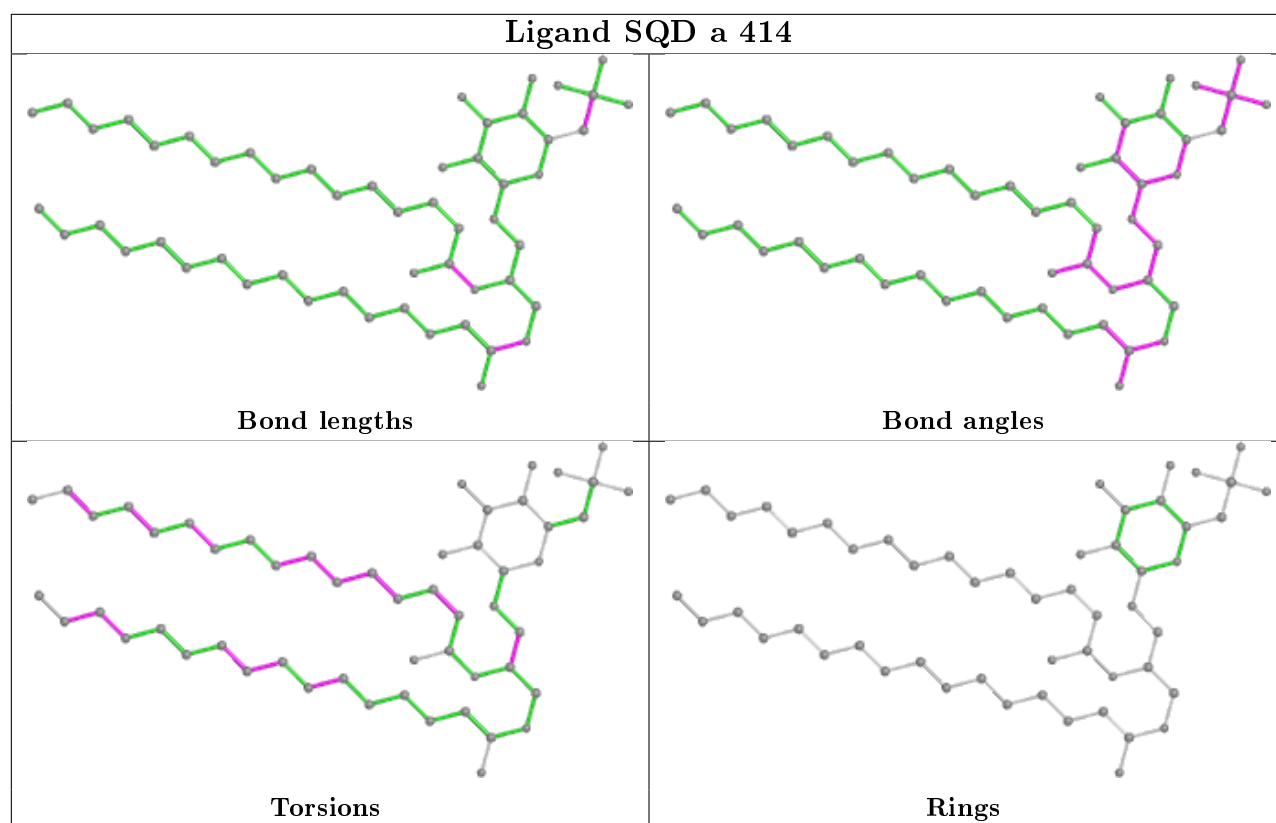
Ligand HTG b 608

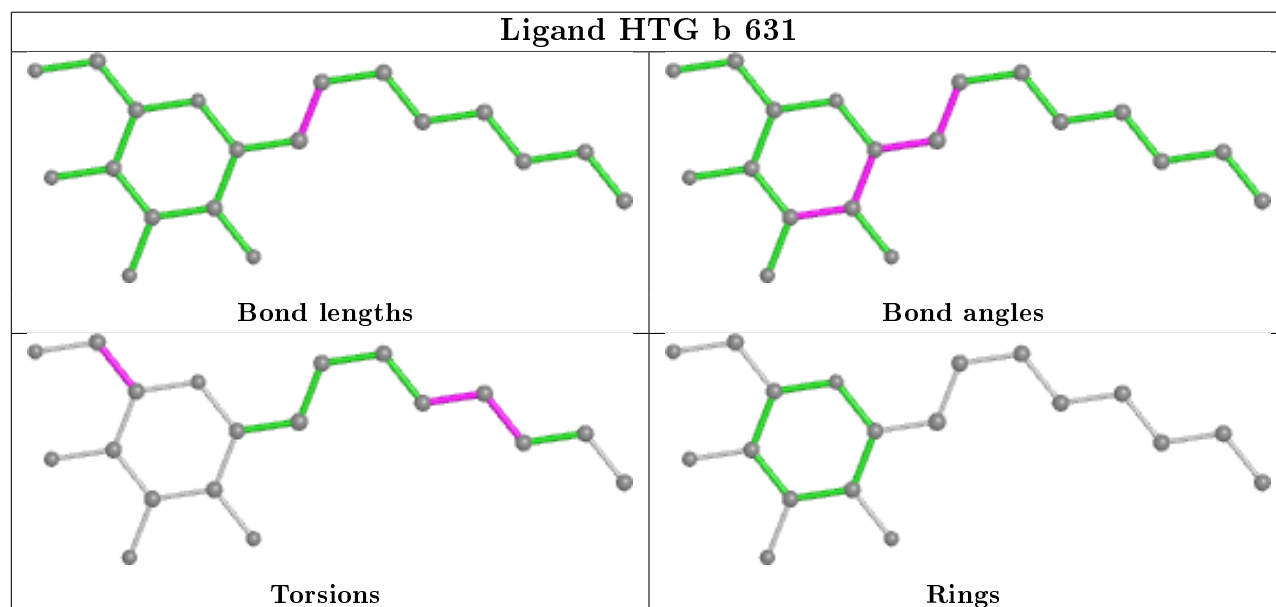
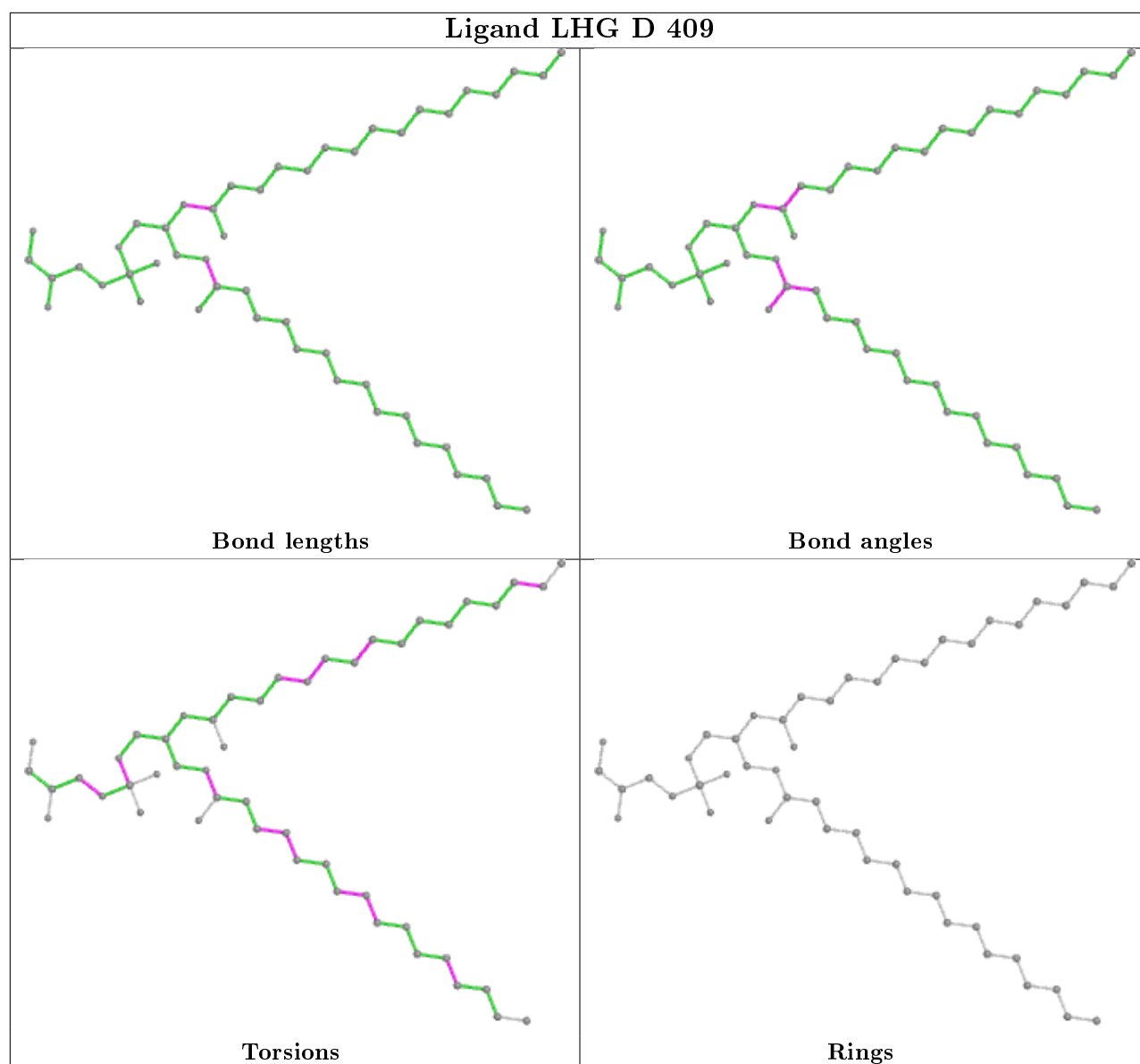




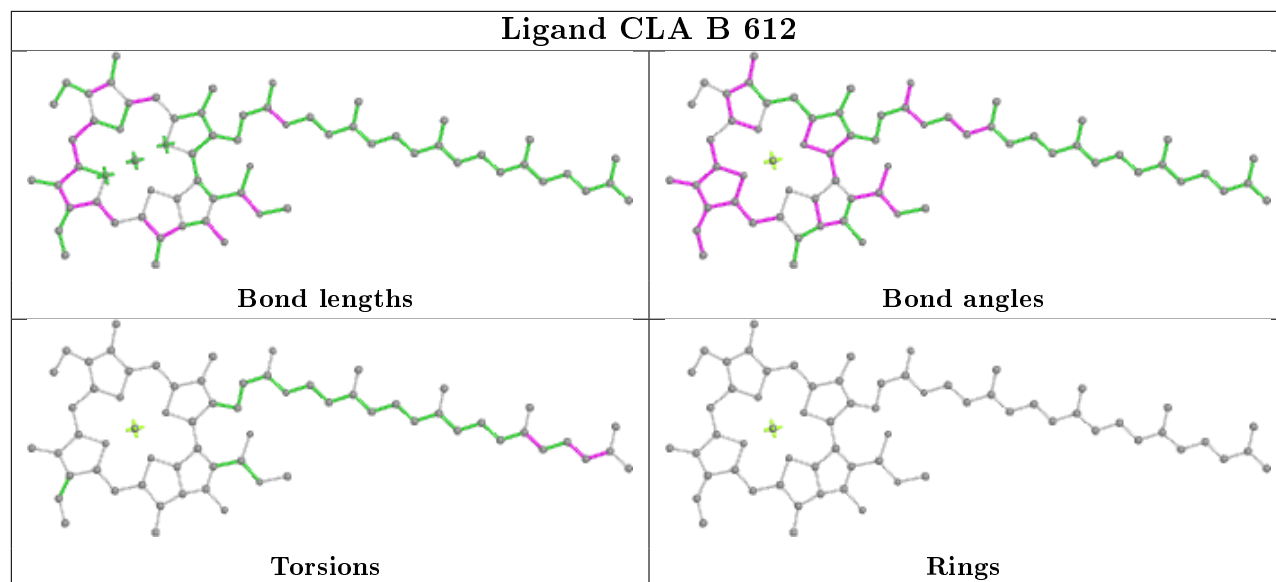
Ligand CLA B 613**Ligand SQD A 411**



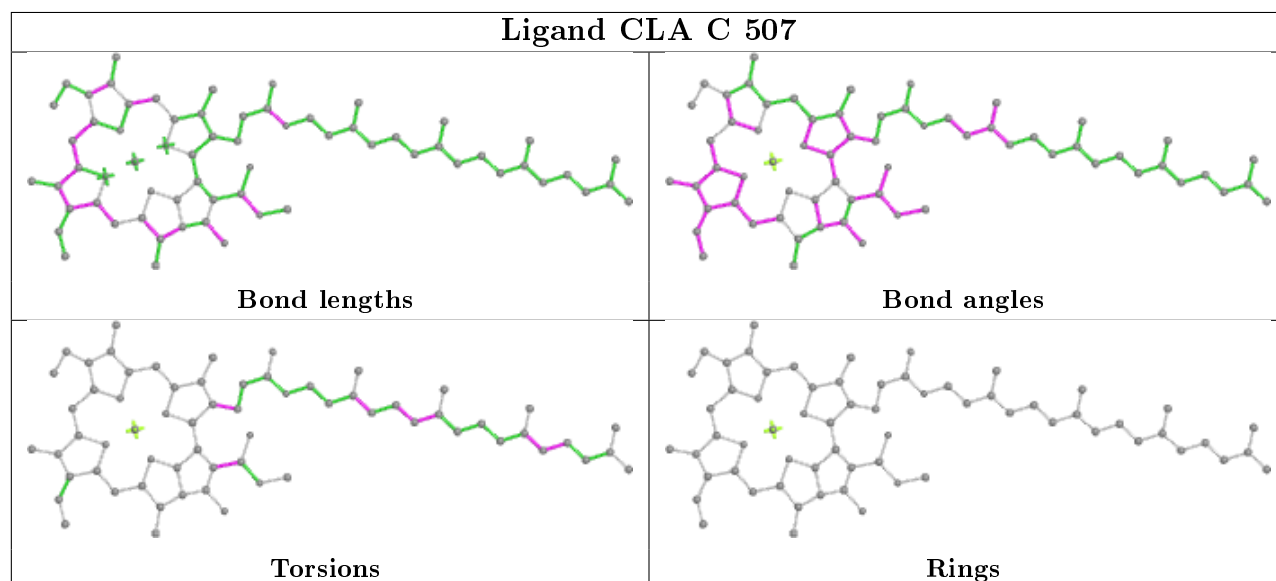




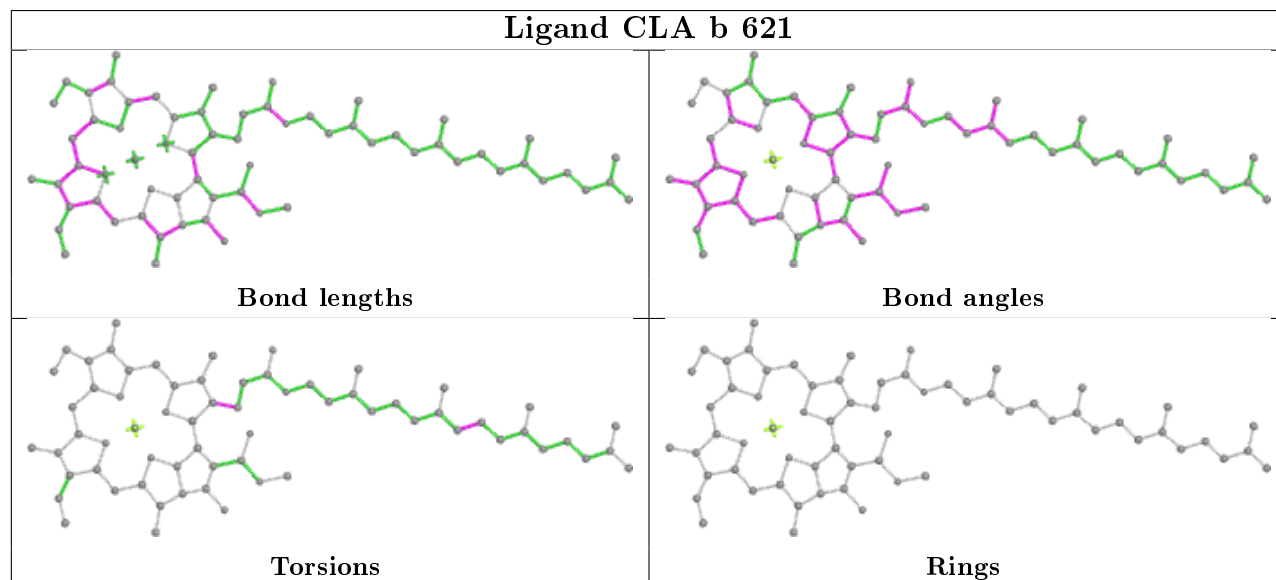
Ligand CLA B 612



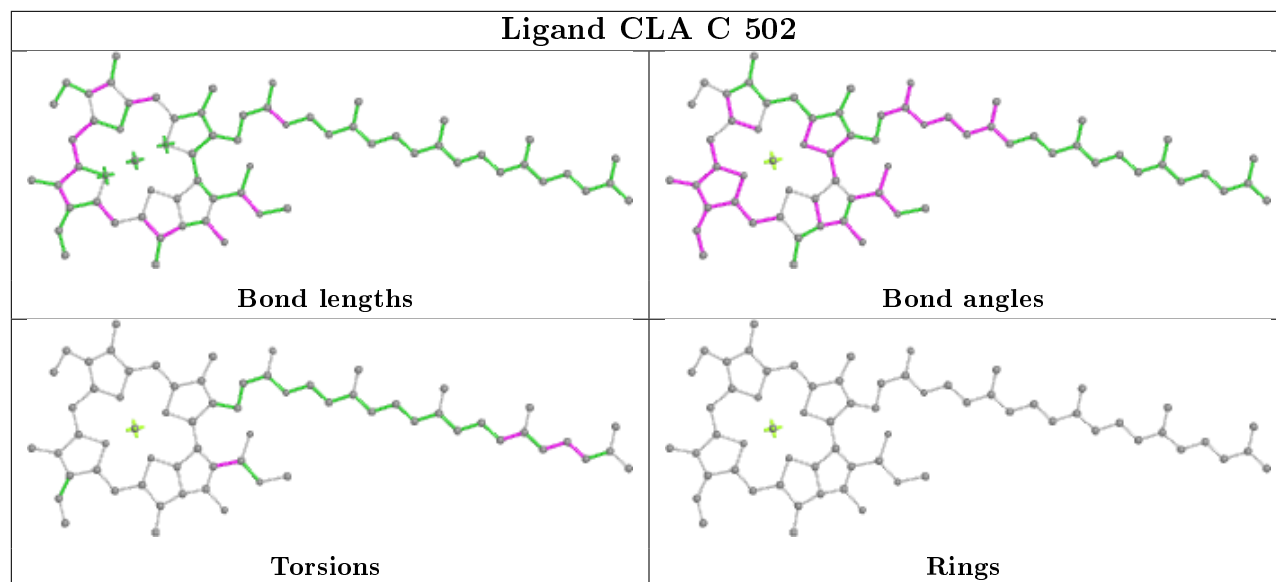
Ligand CLA C 507



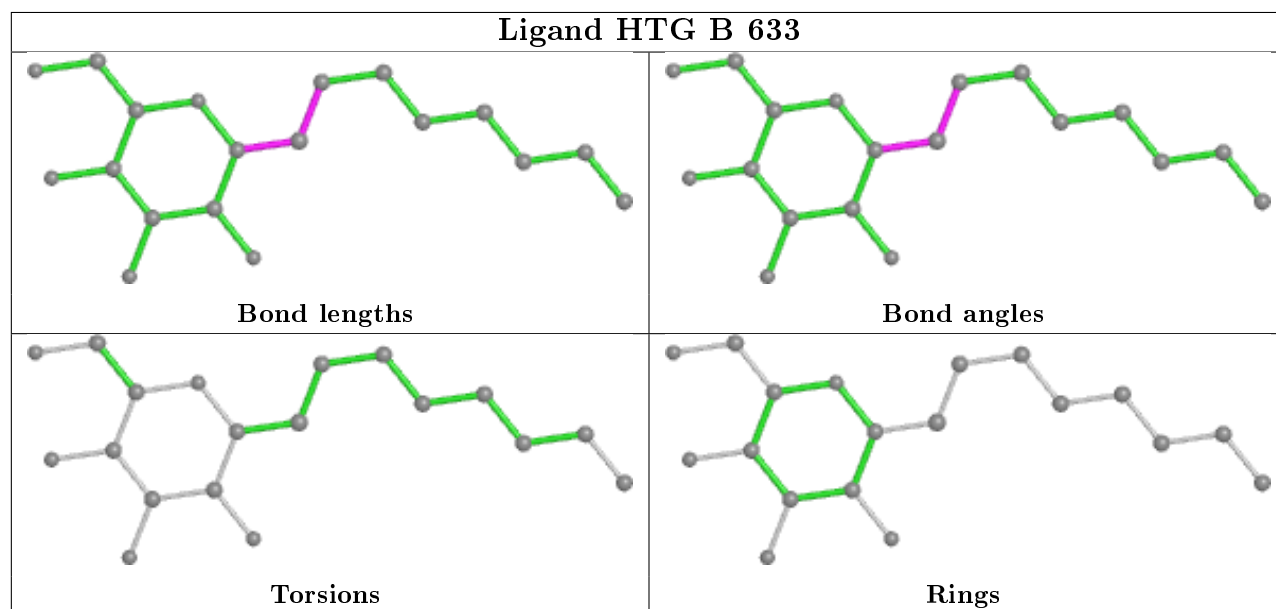
Ligand CLA b 621



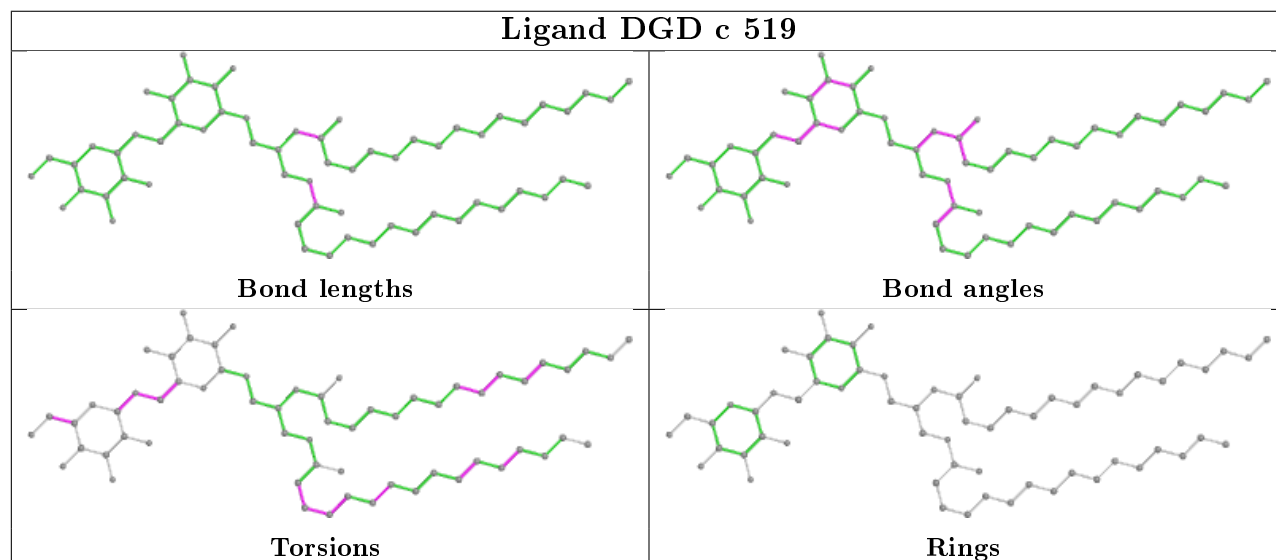
Ligand CLA C 502

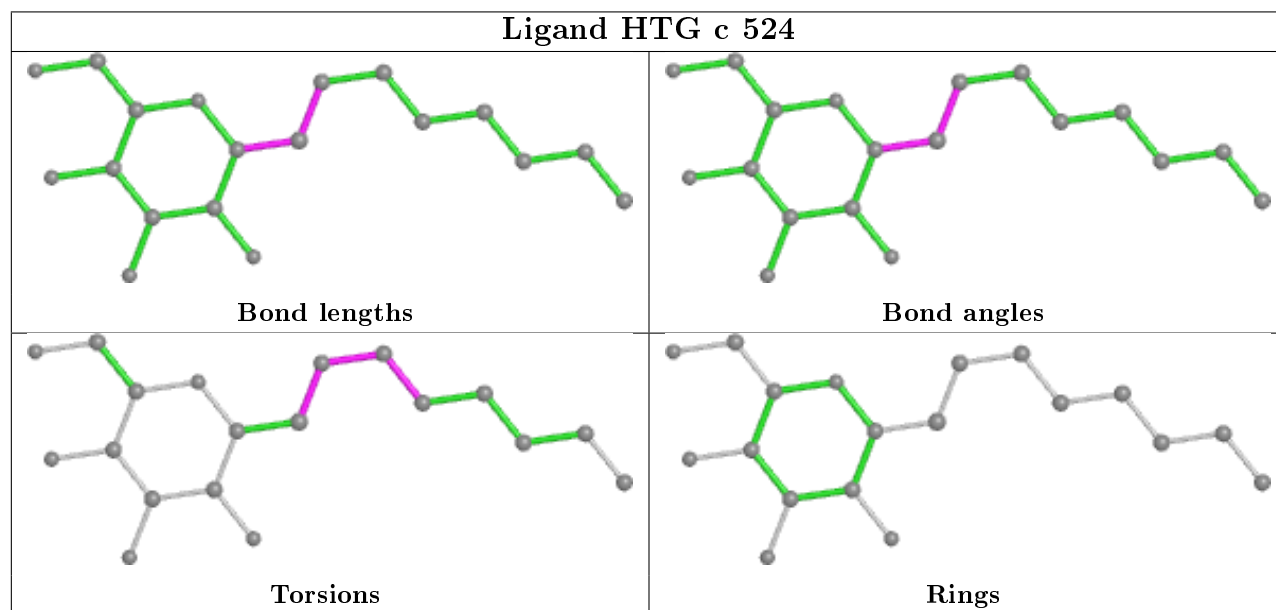
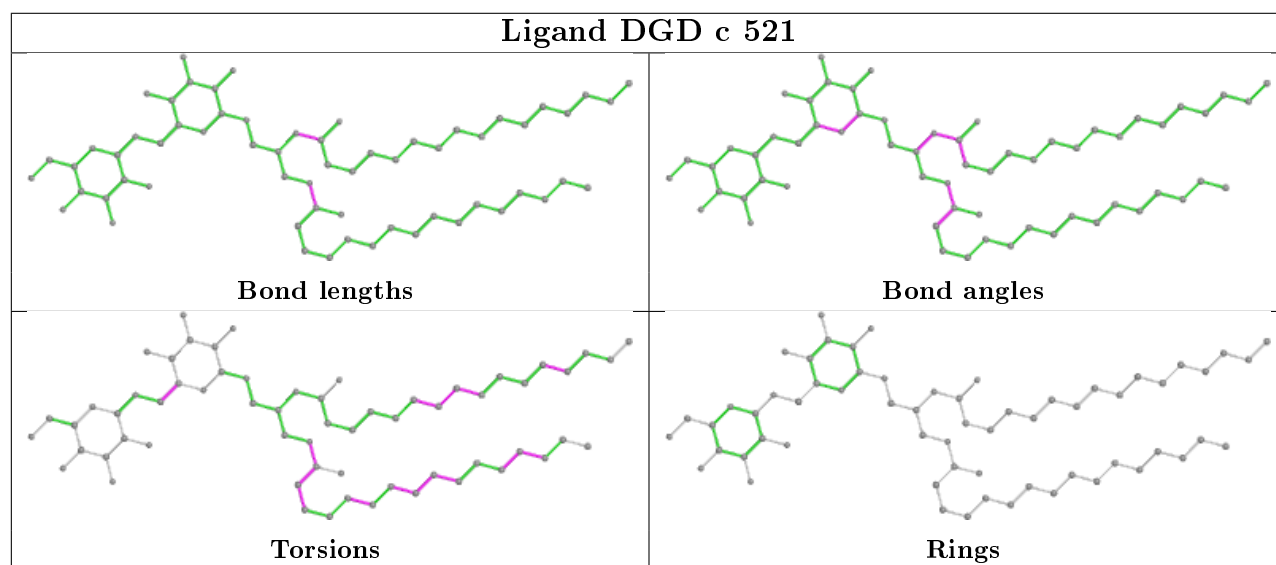
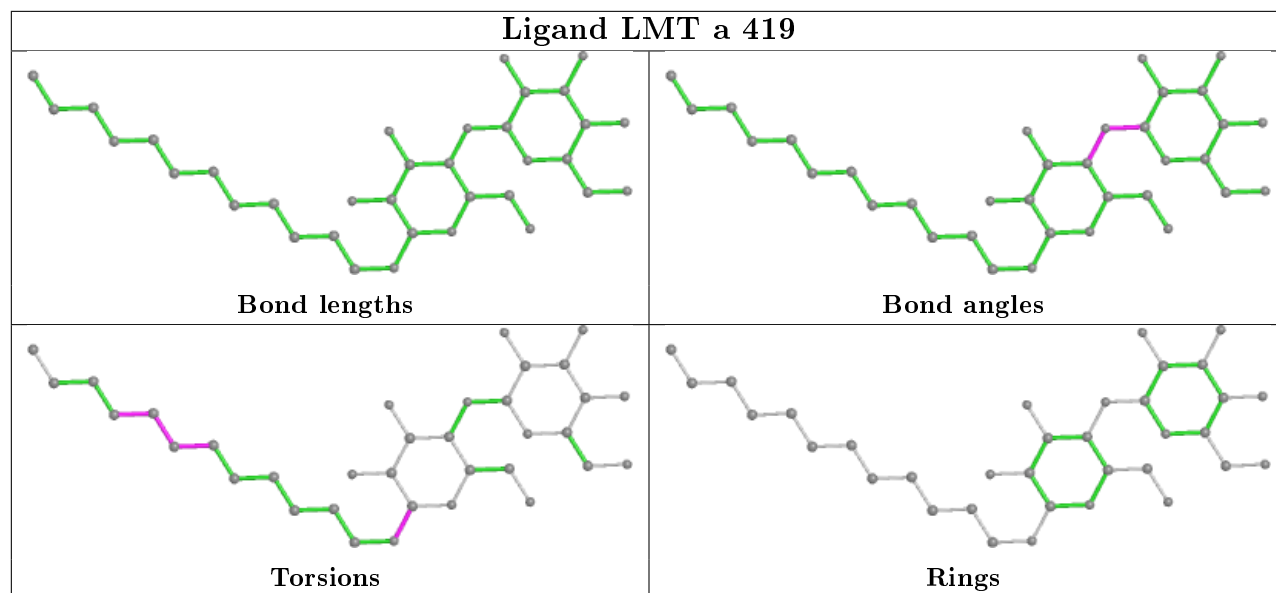


Ligand HTG B 633

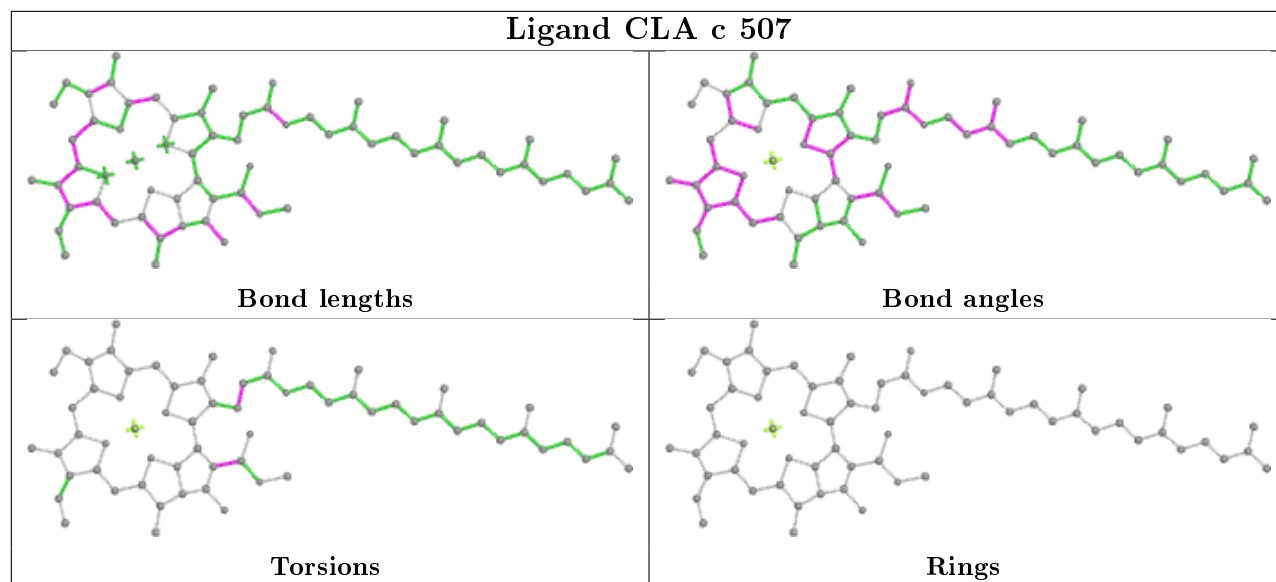


Ligand DGD c 519

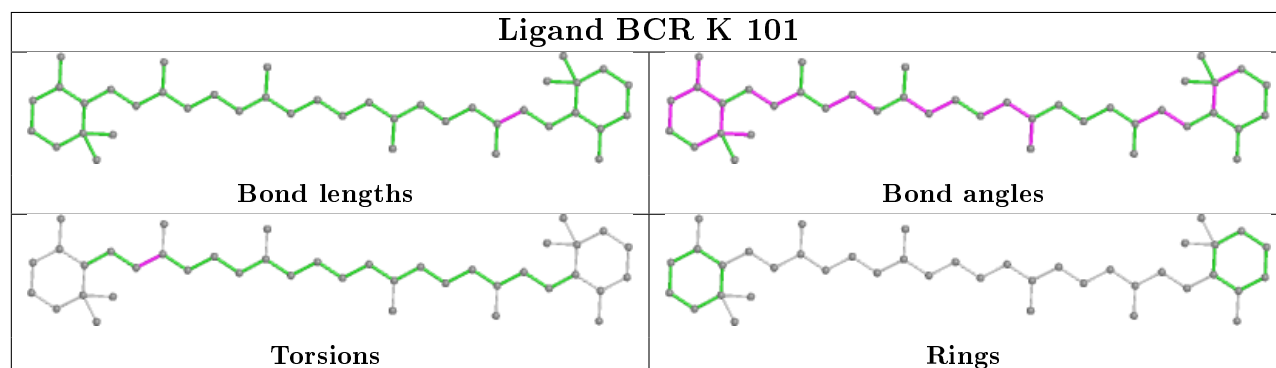




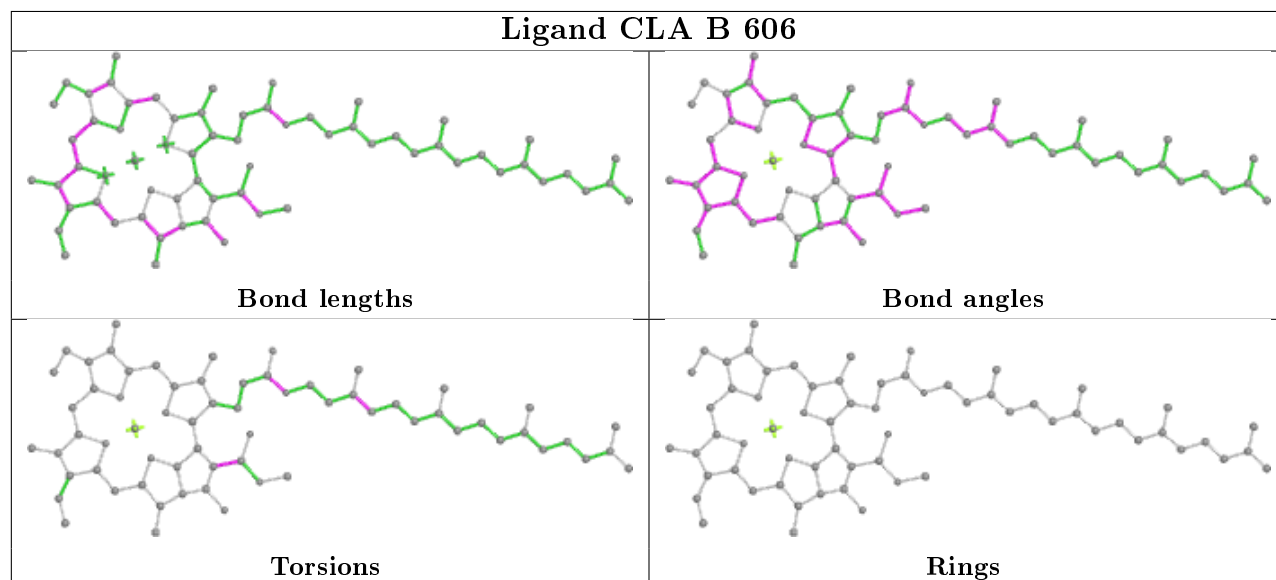
Ligand CLA c 507

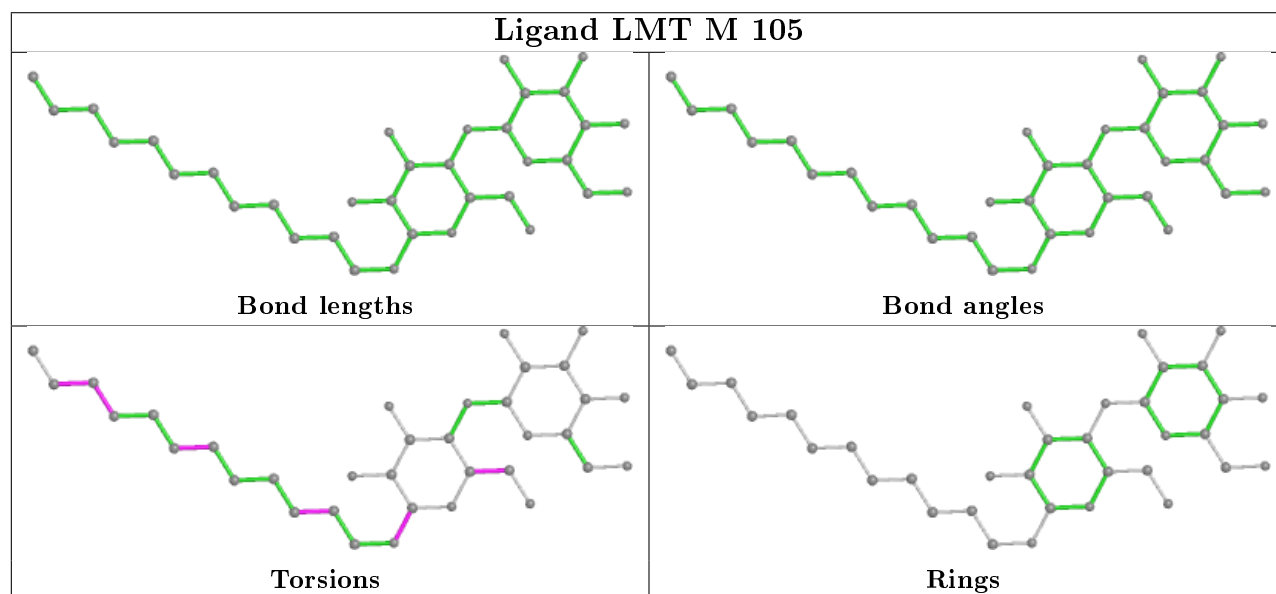
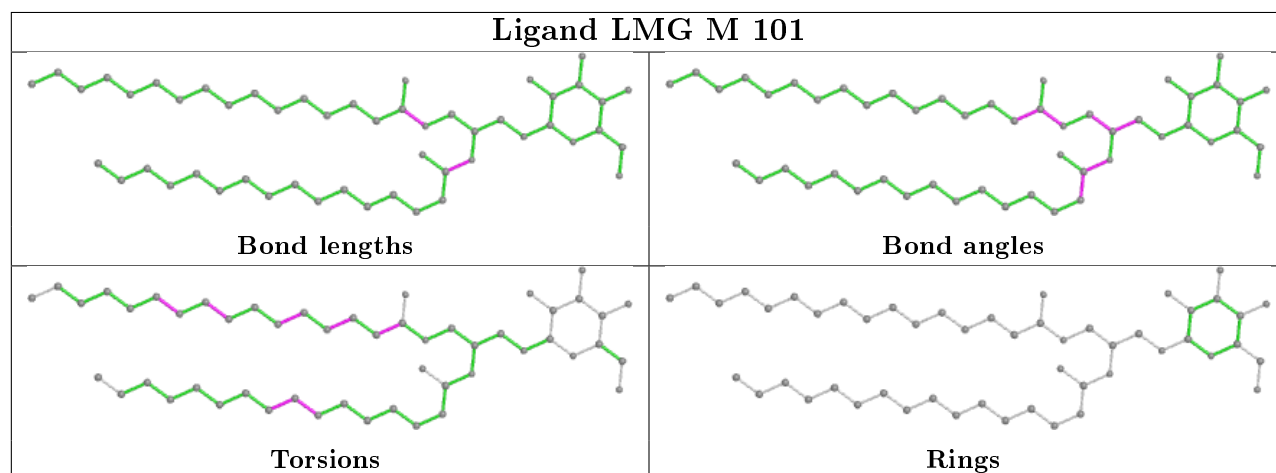
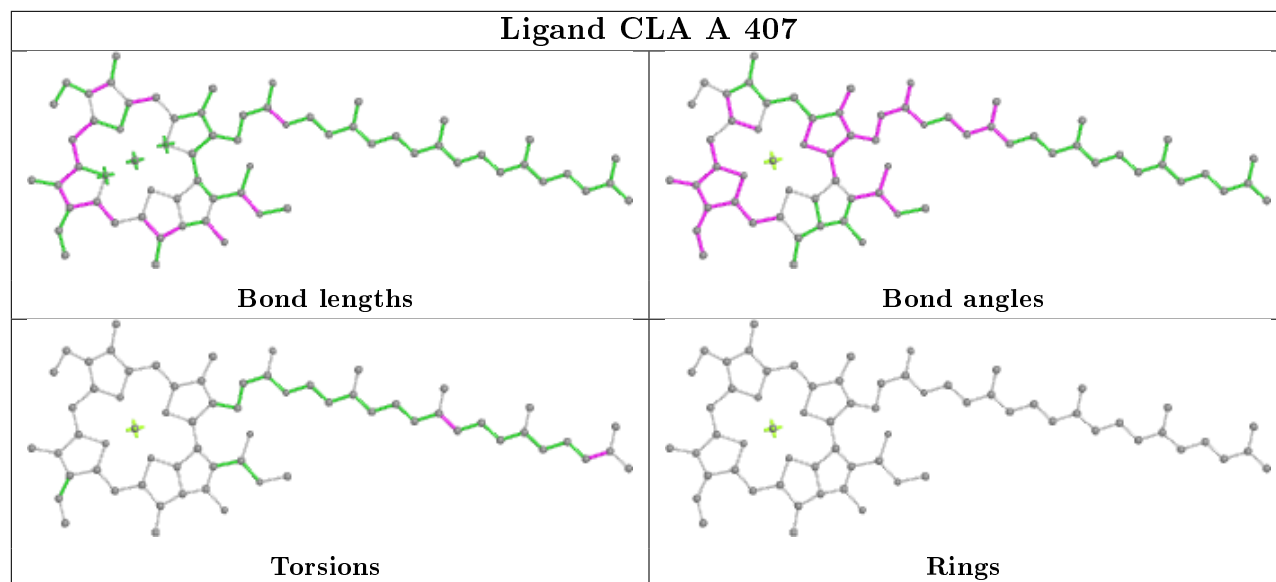


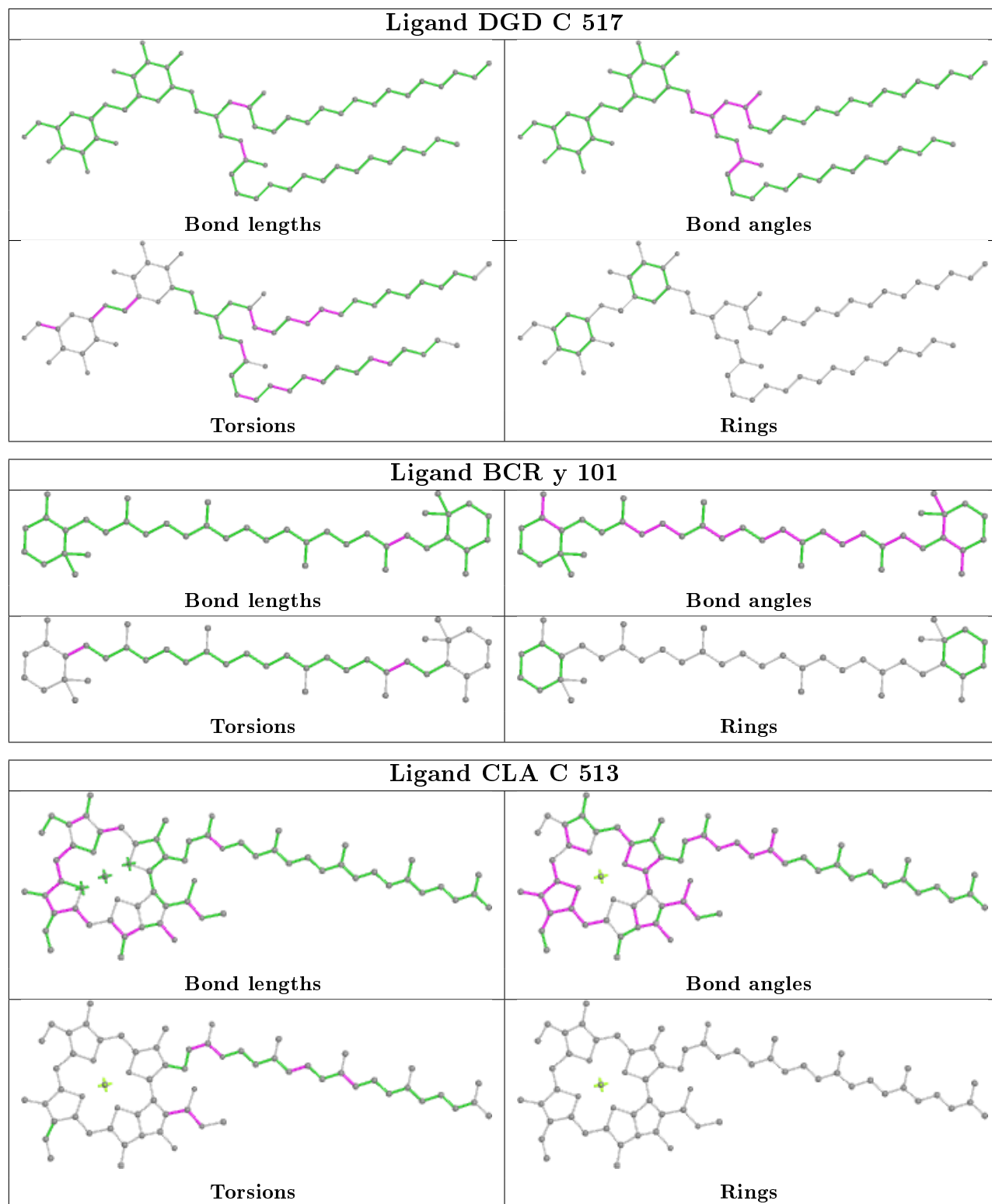
Ligand BCR K 101



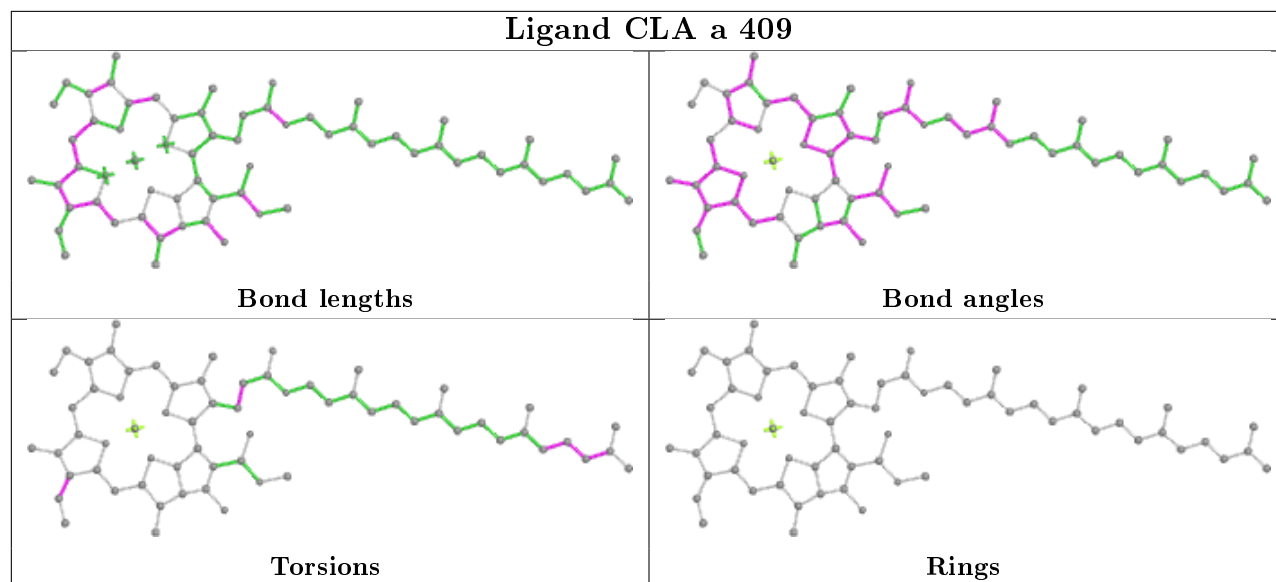
Ligand CLA B 606



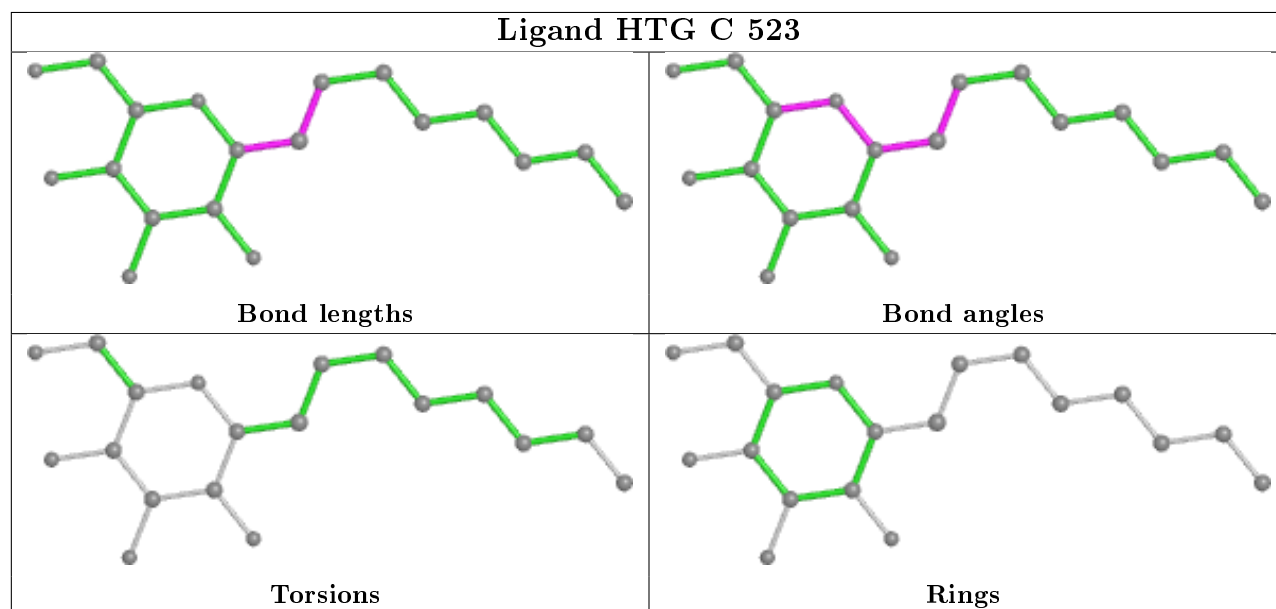




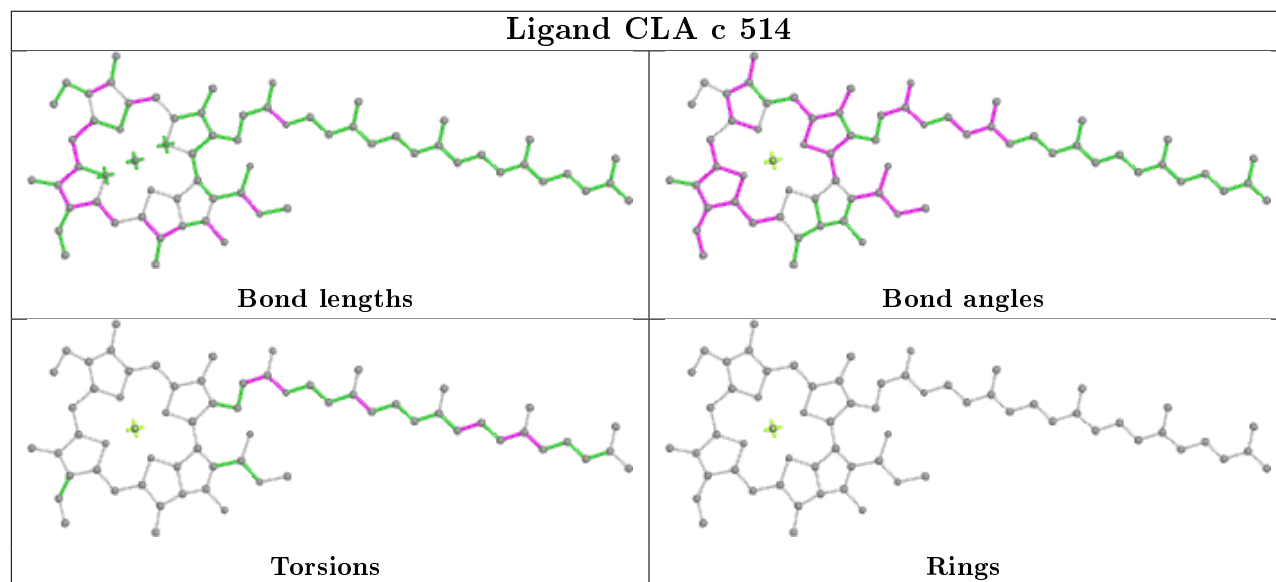
Ligand CLA a 409



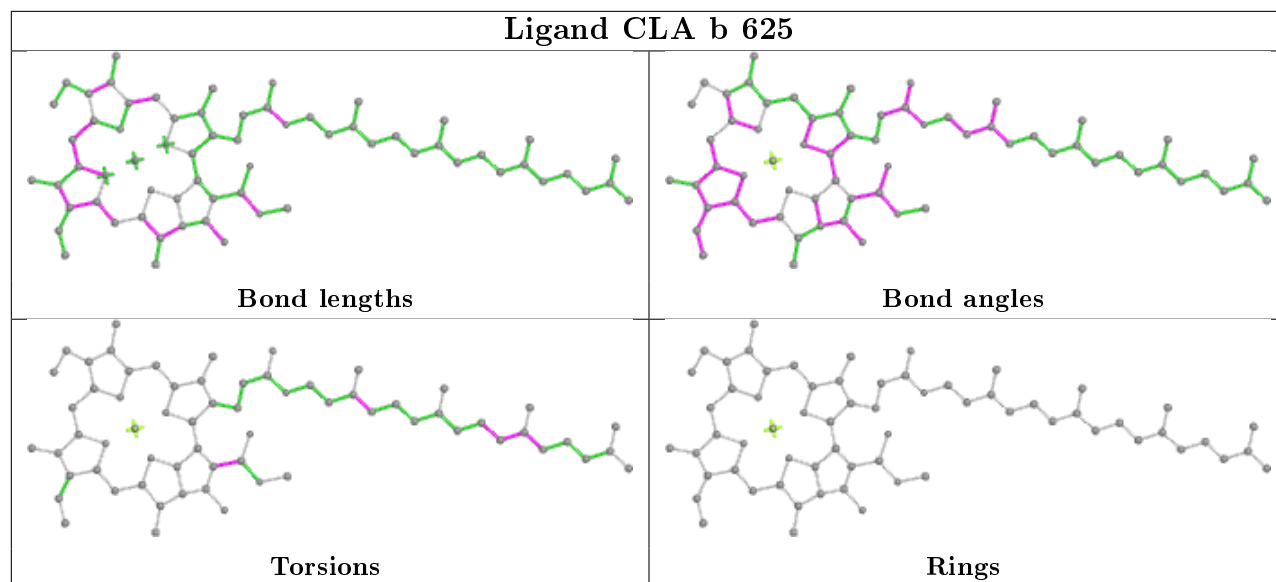
Ligand HTG C 523



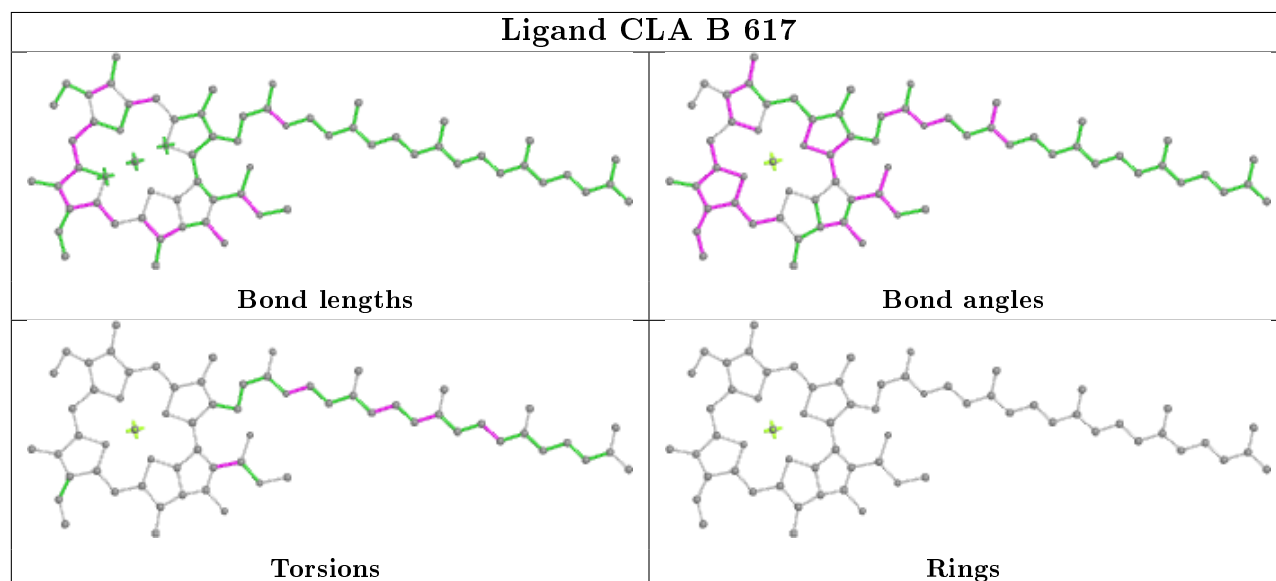
Ligand CLA c 514



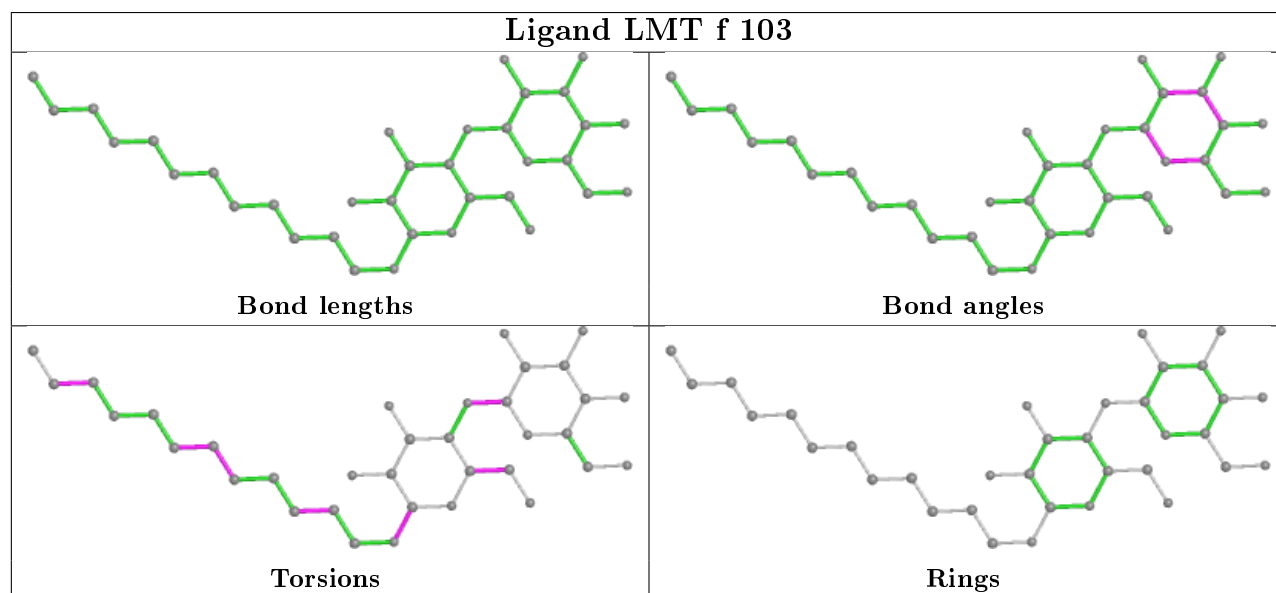
Ligand CLA b 625

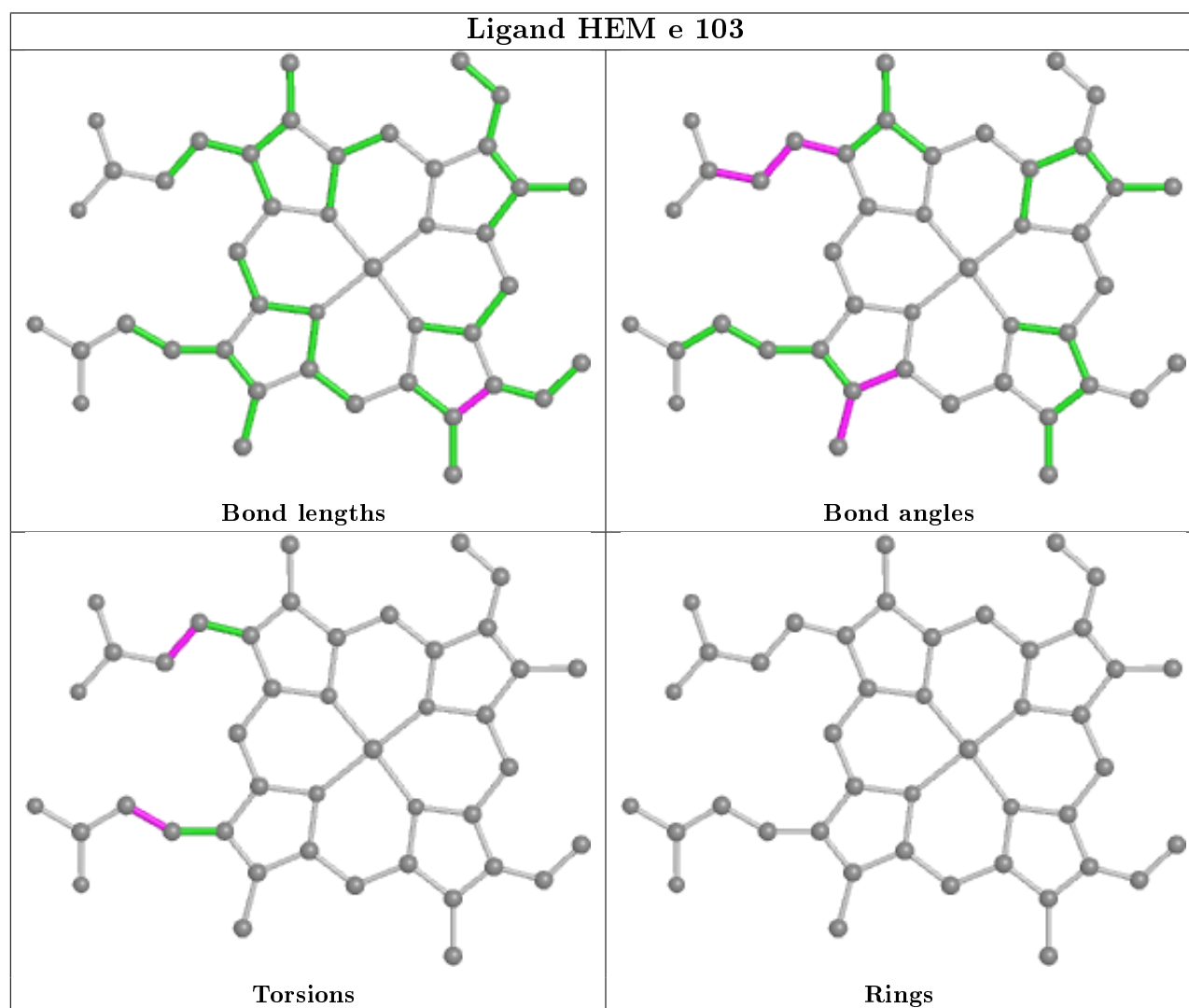
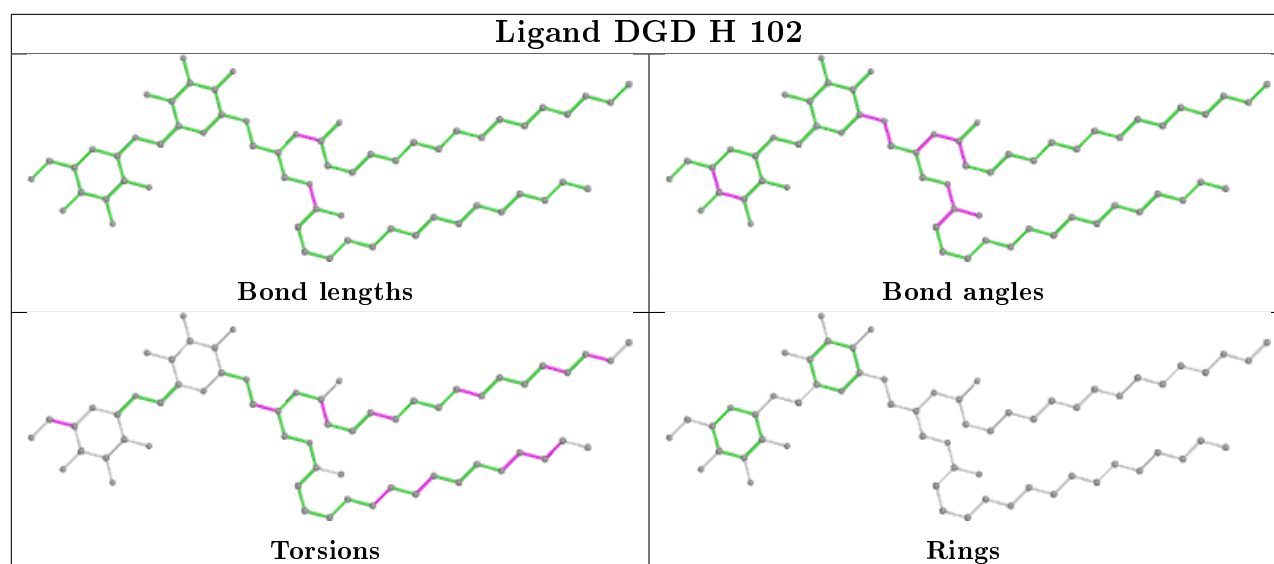


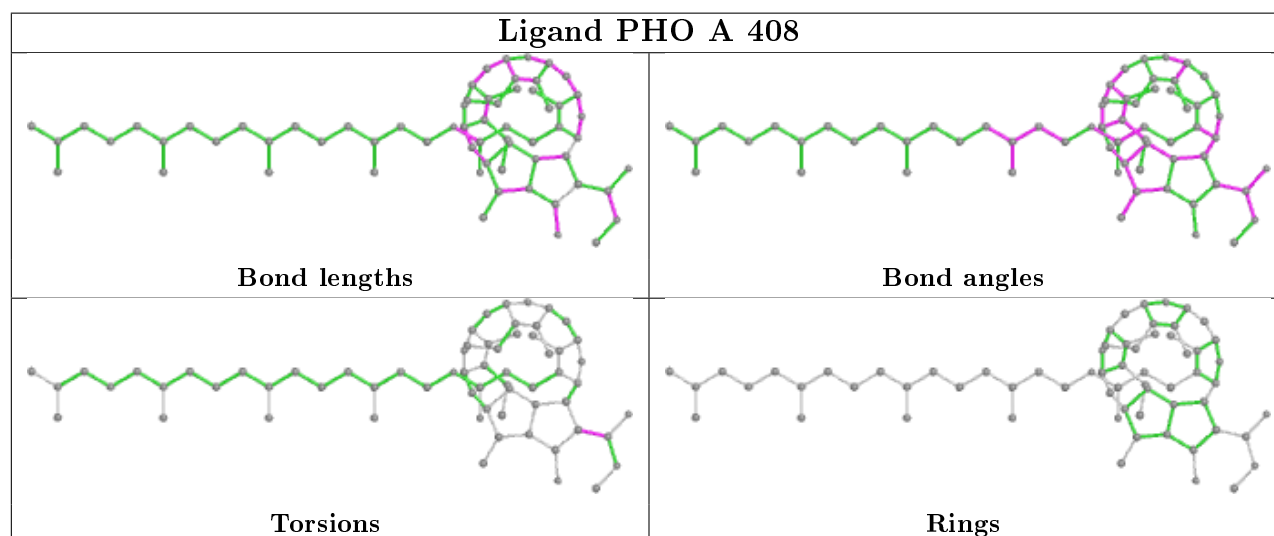
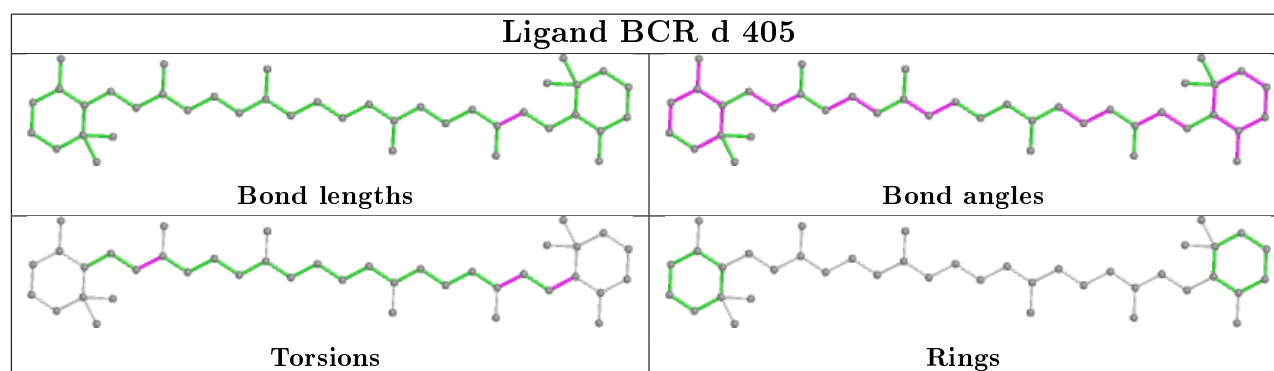
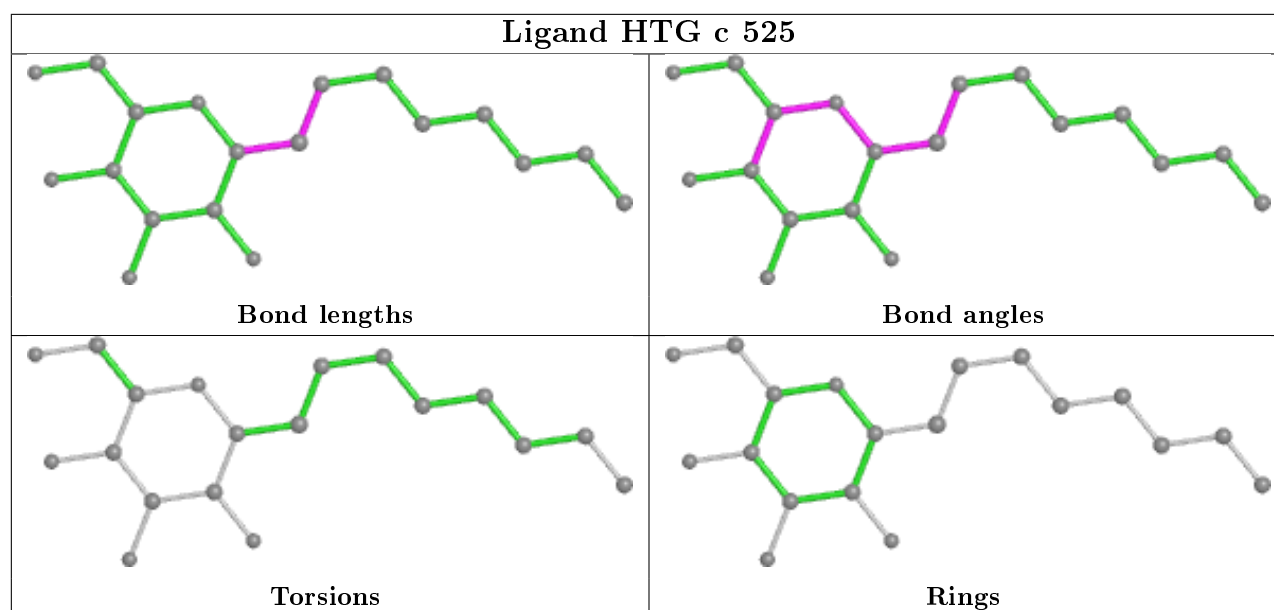
Ligand CLA B 617

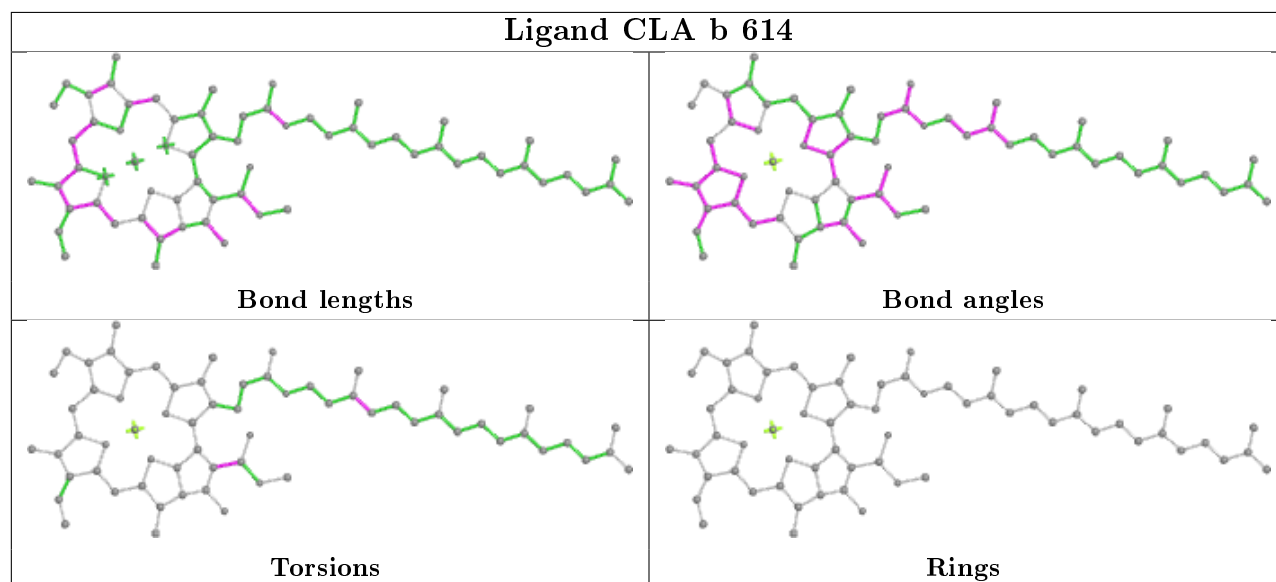
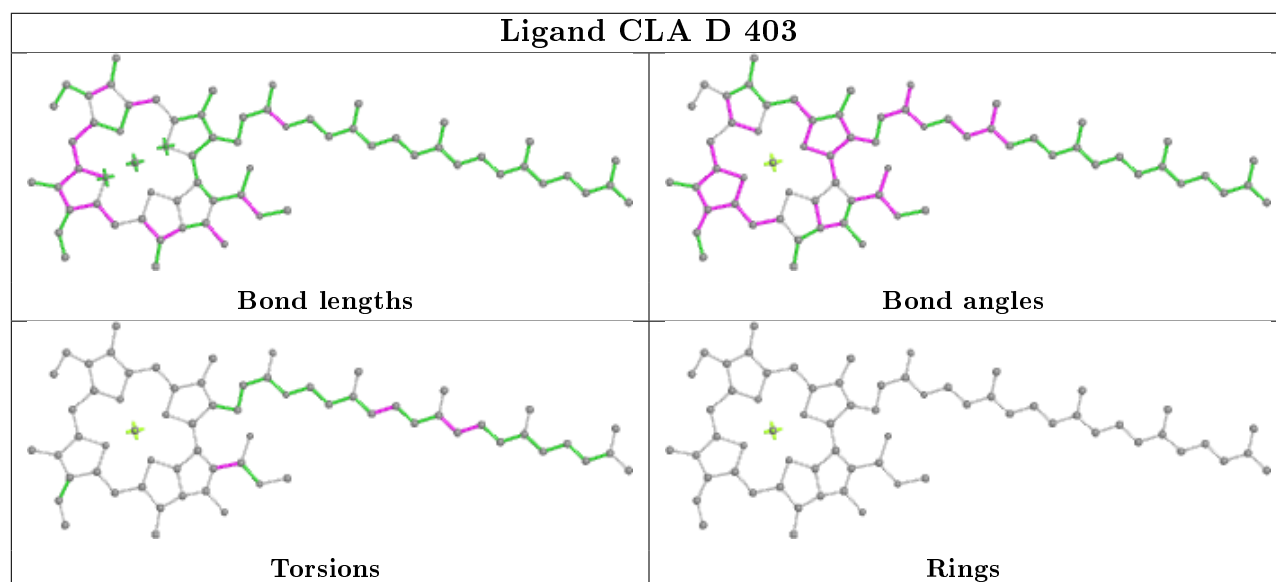
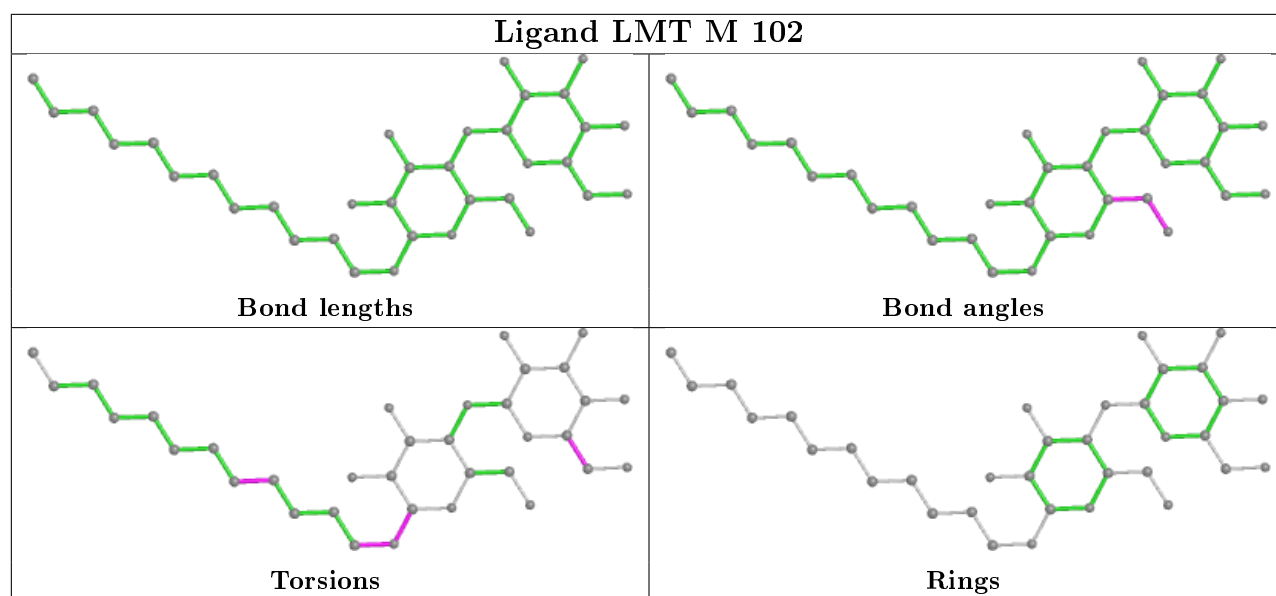


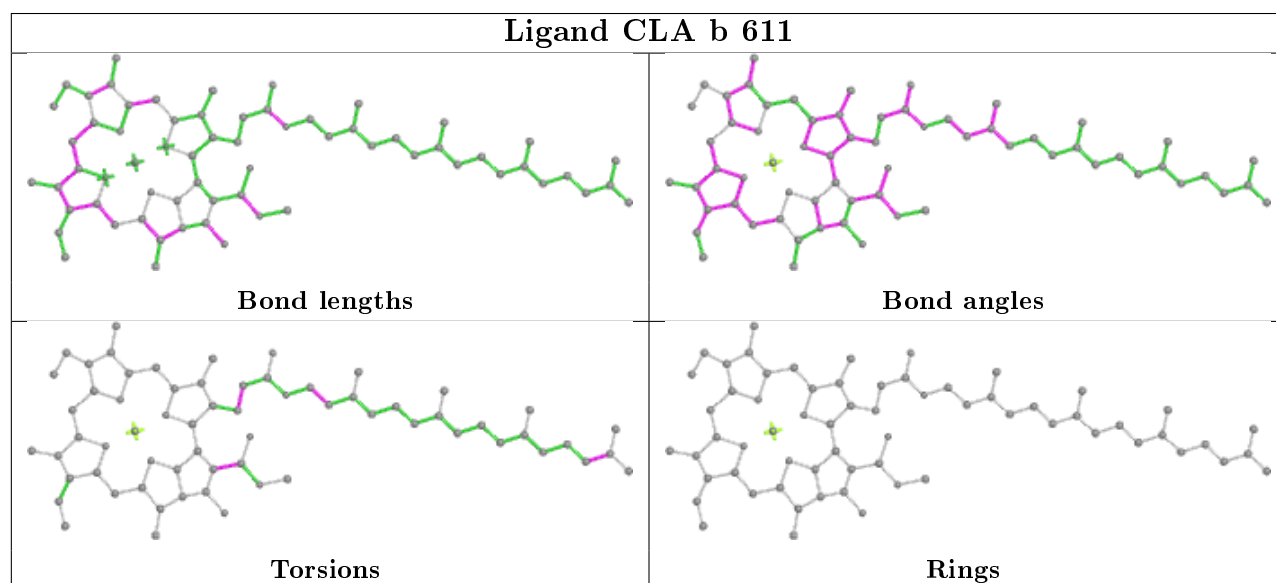
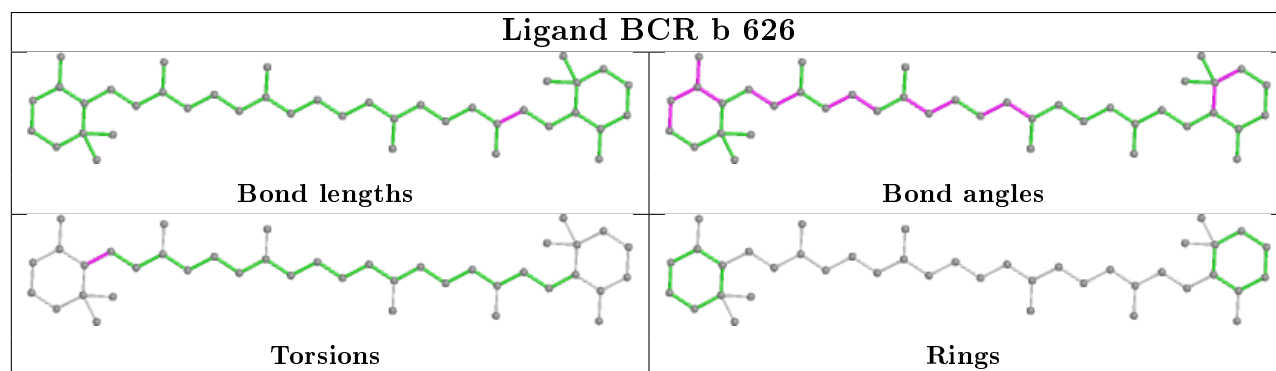
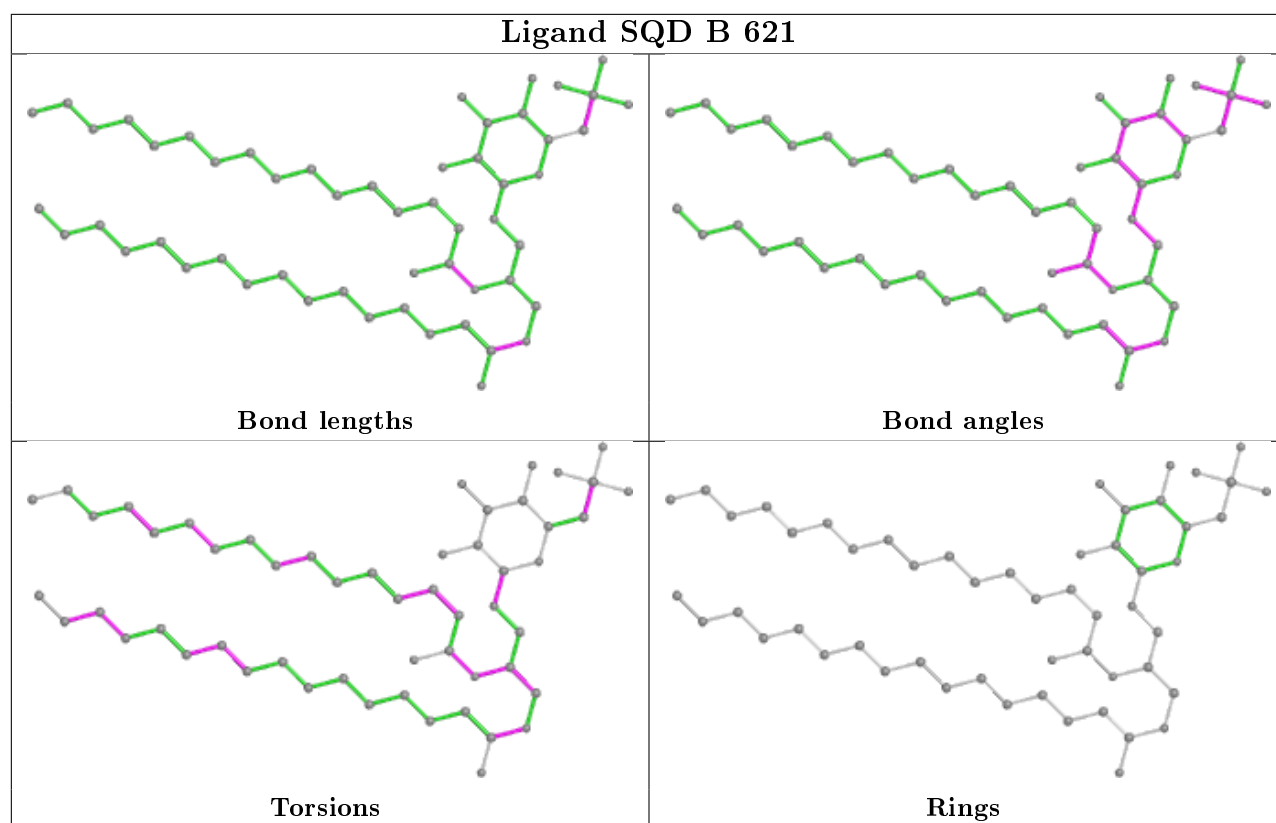
Ligand LMT f 103

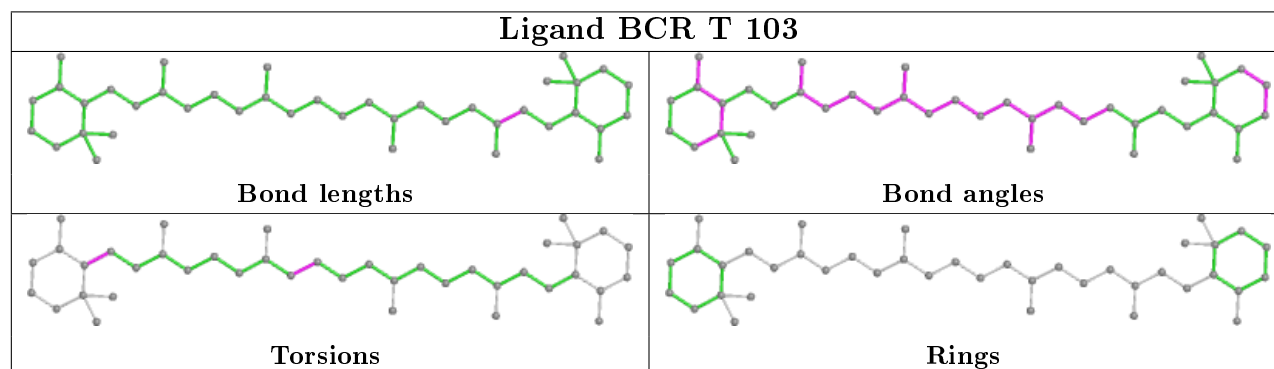
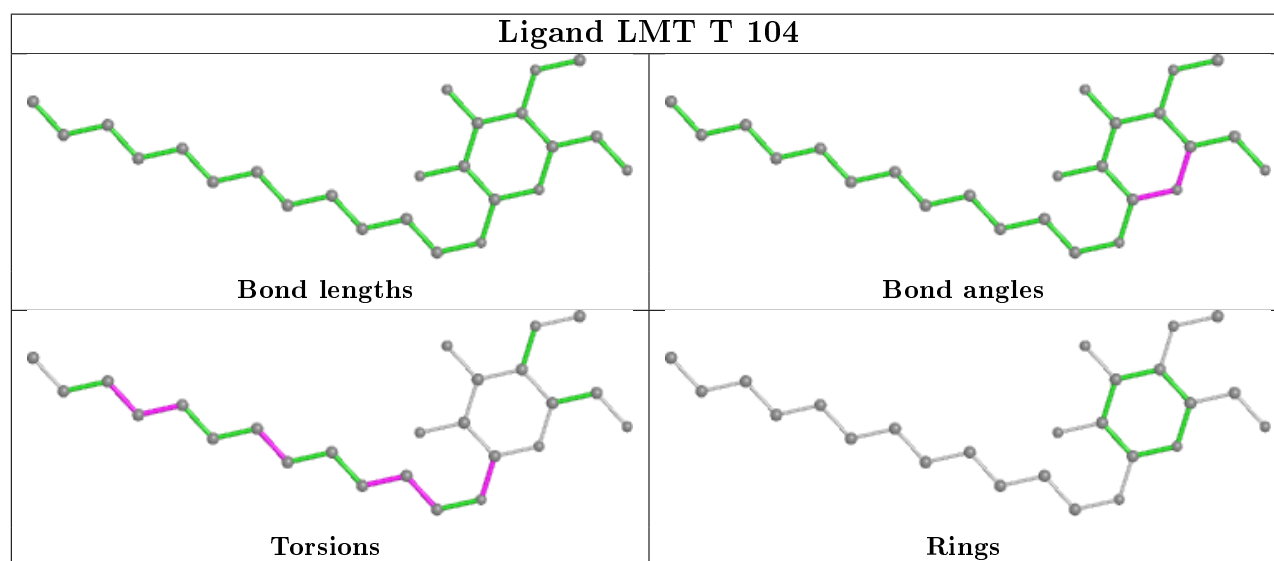
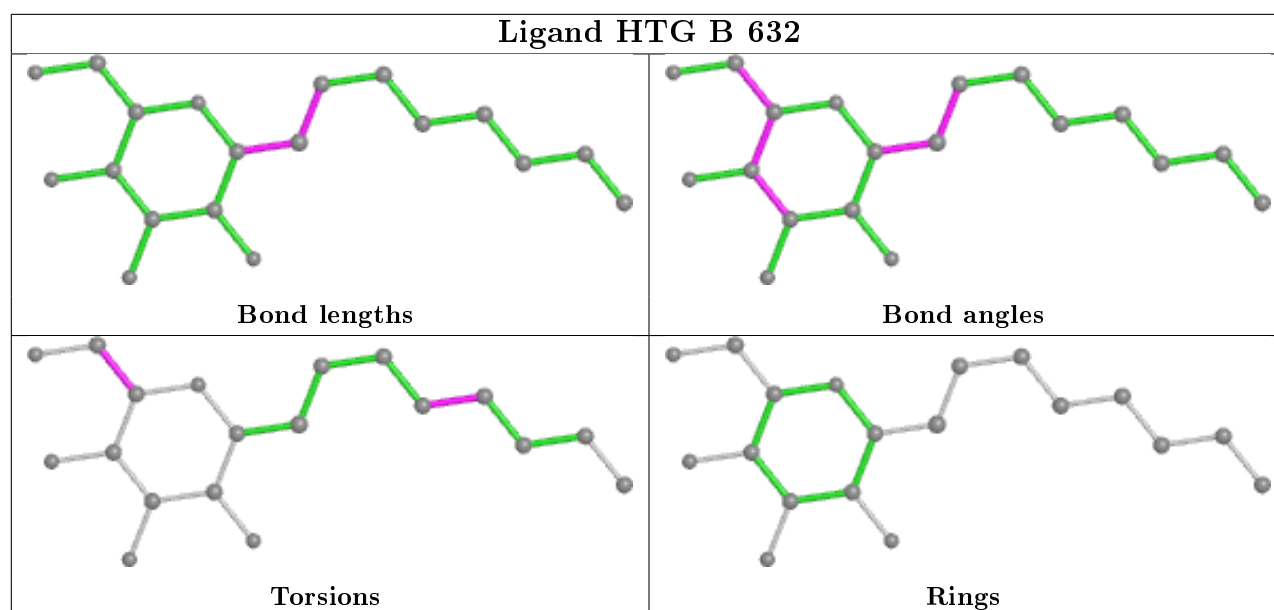


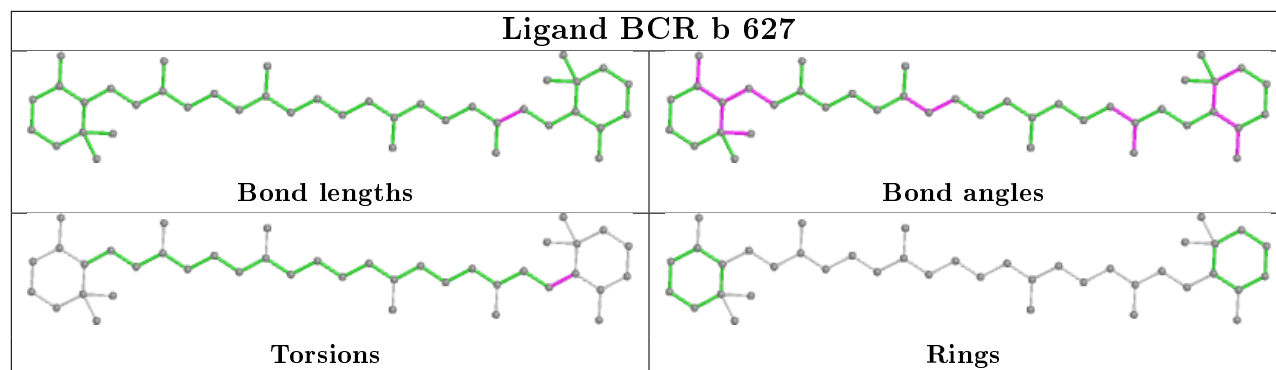
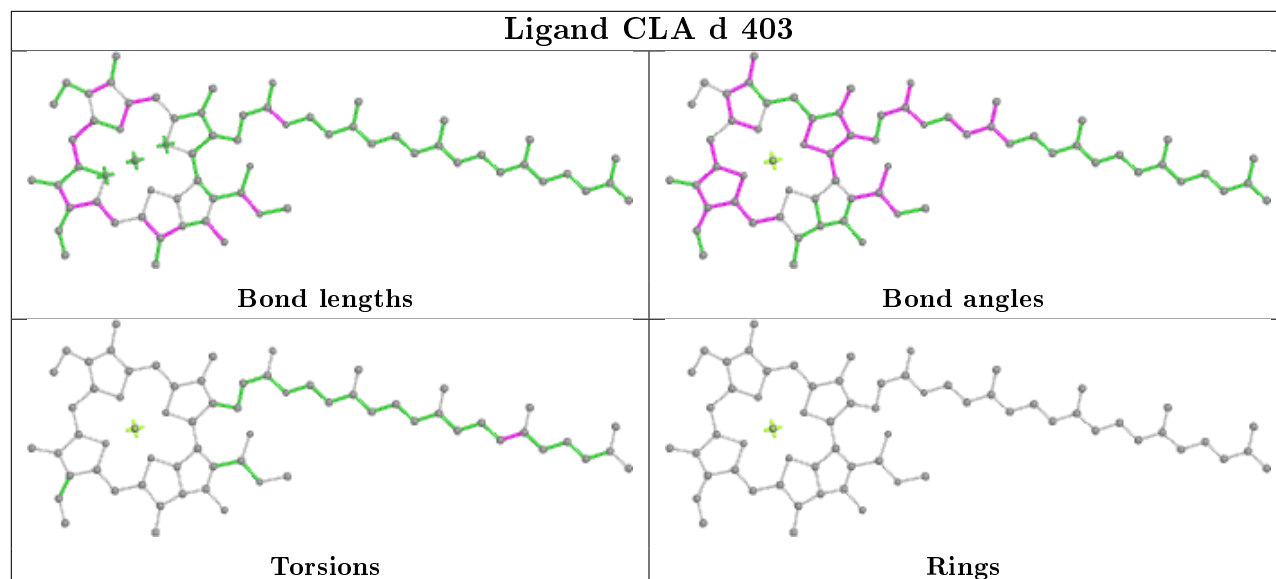
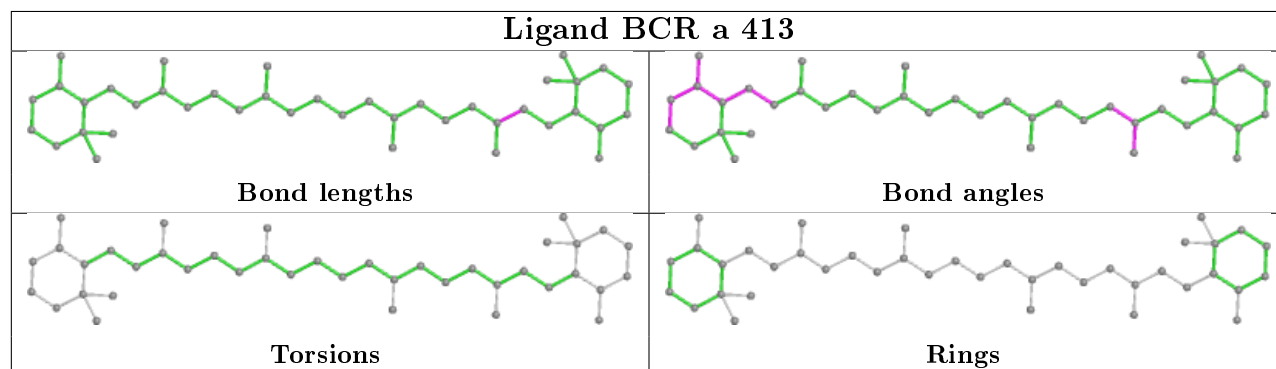


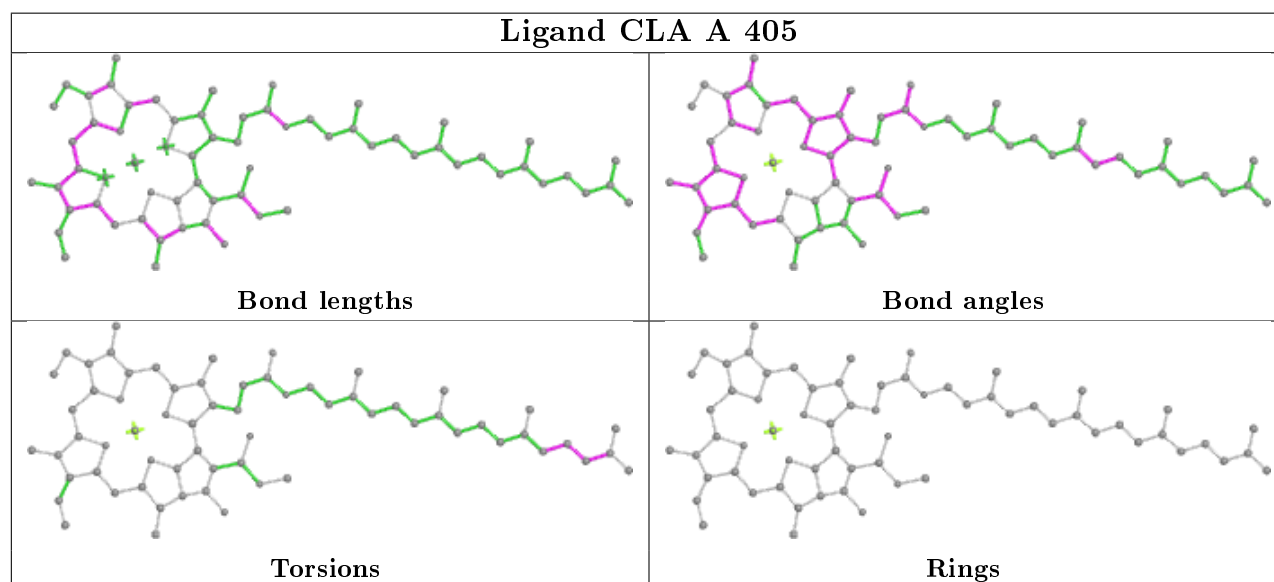
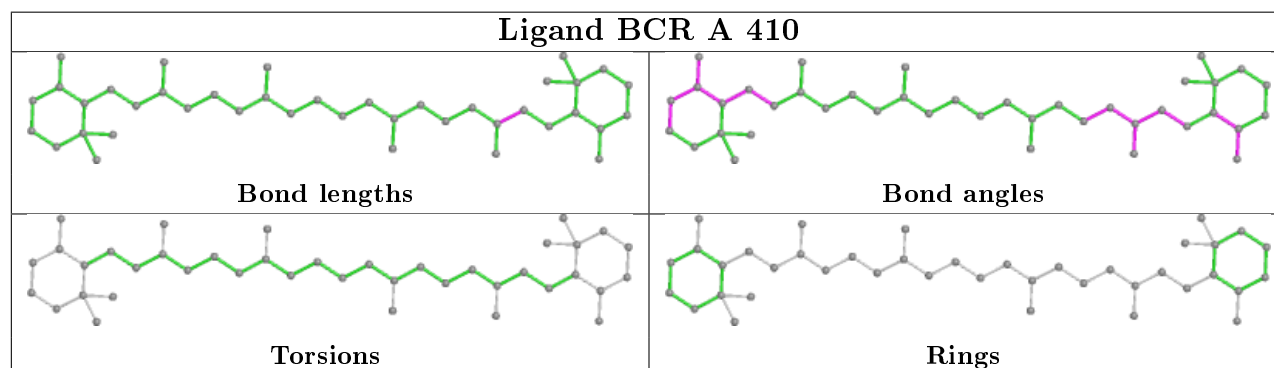
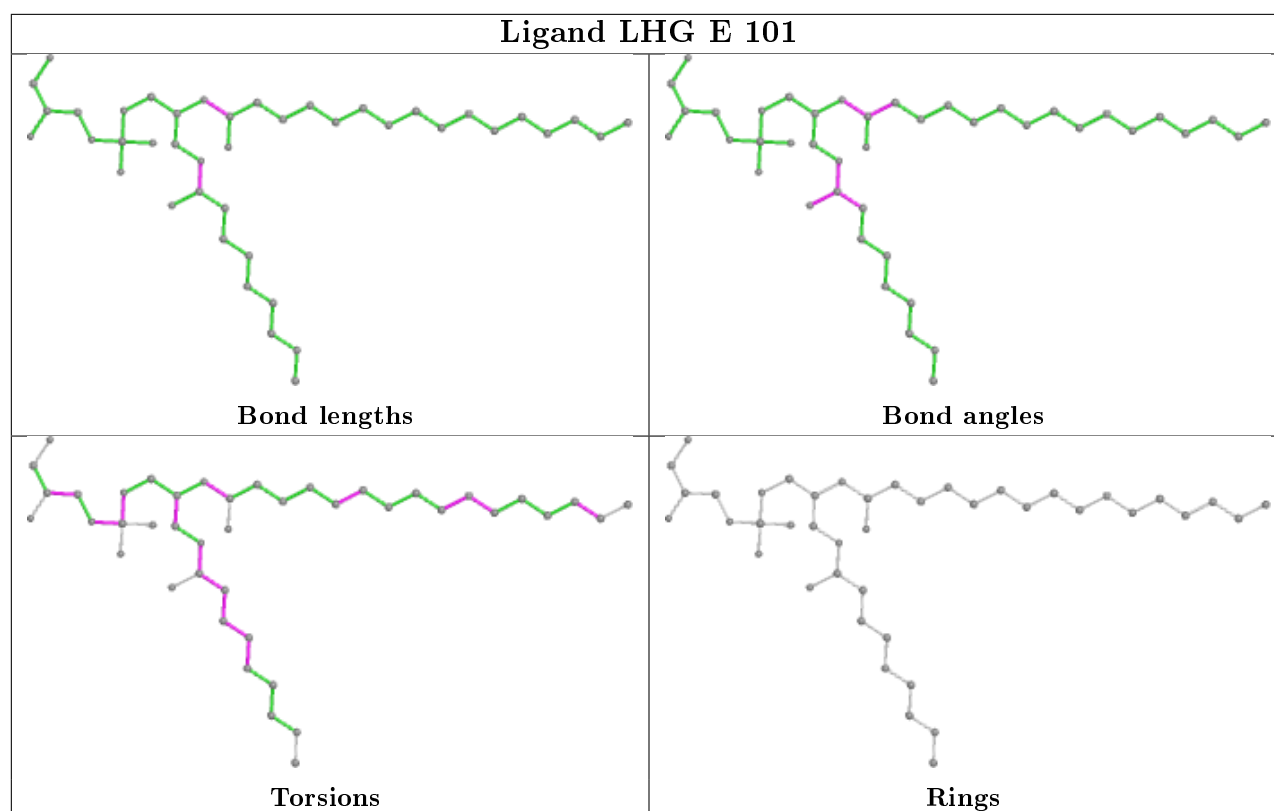


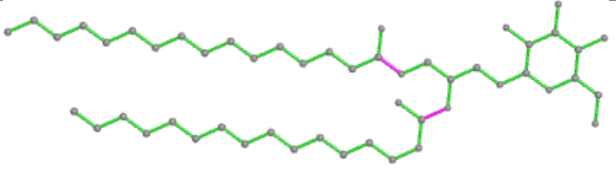
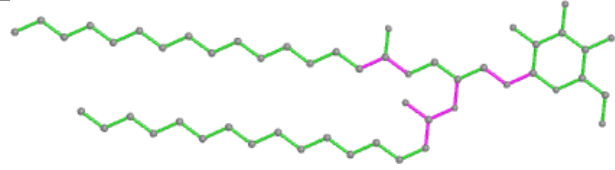
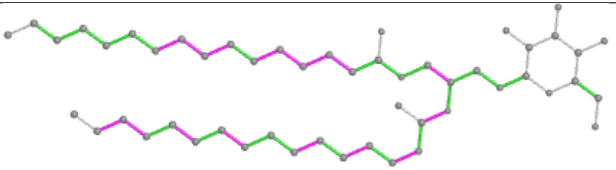
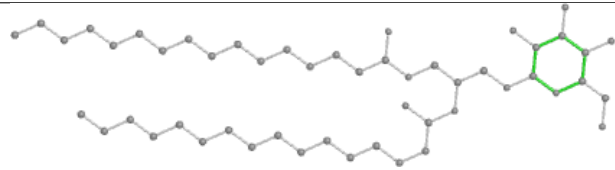


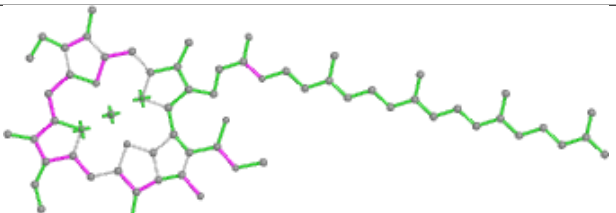
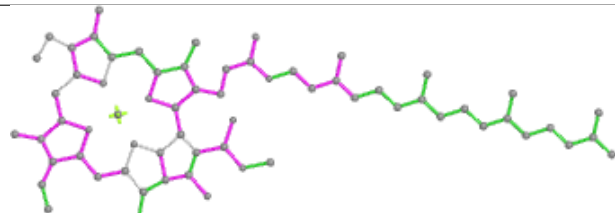
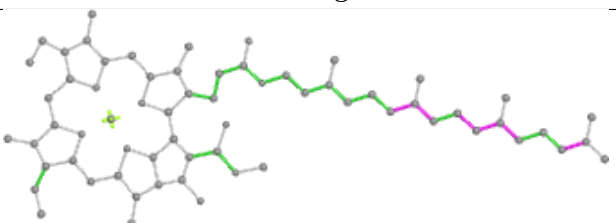
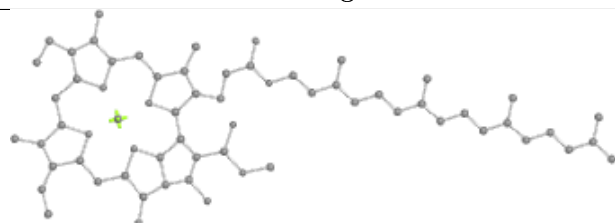



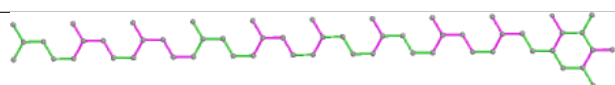
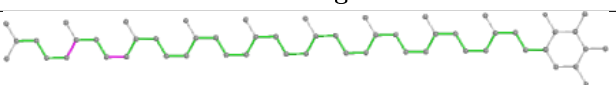
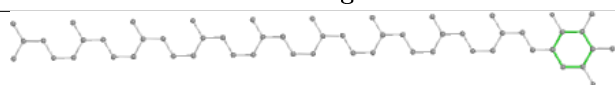


Ligand BCR b 627**Ligand CLA d 403****Ligand BCR a 413**

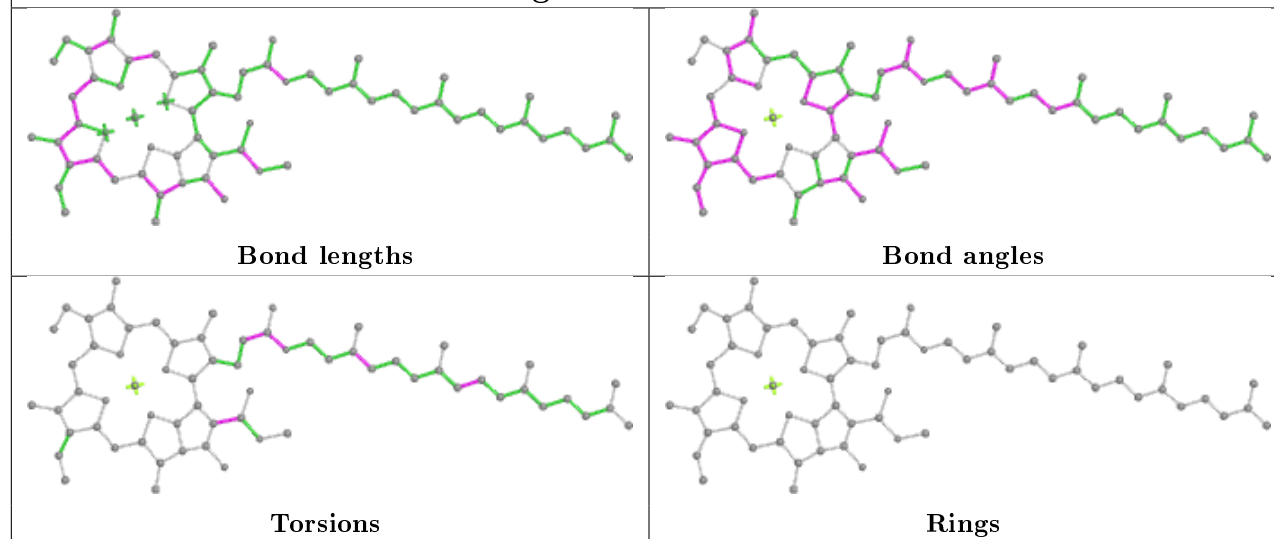


Ligand LMG a 415	
	
Bond lengths	Bond angles
	
Torsions	Rings

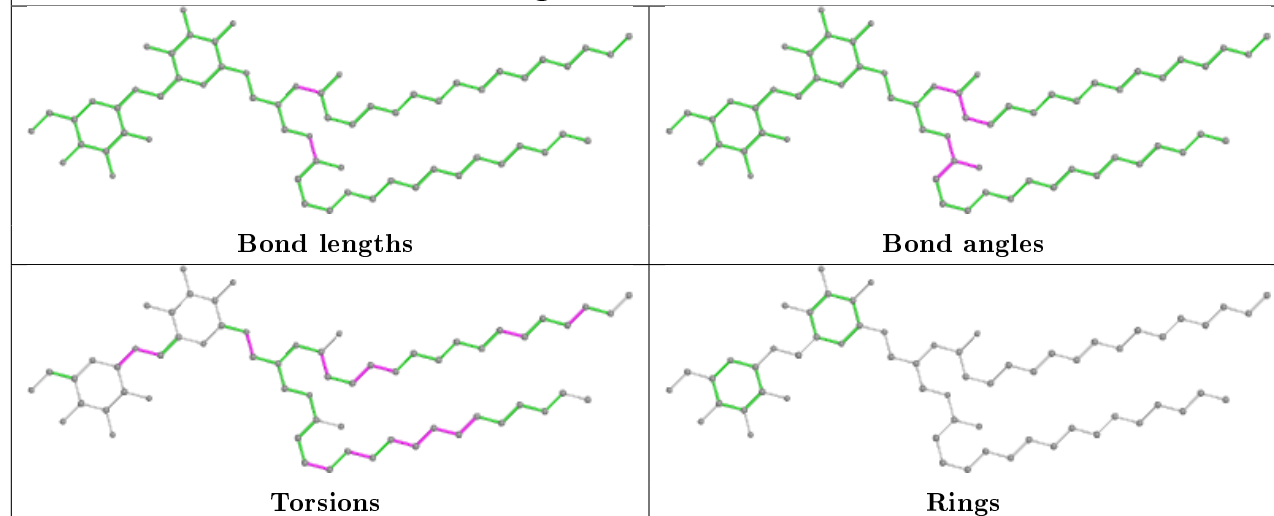
Ligand CLA a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PL9 d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

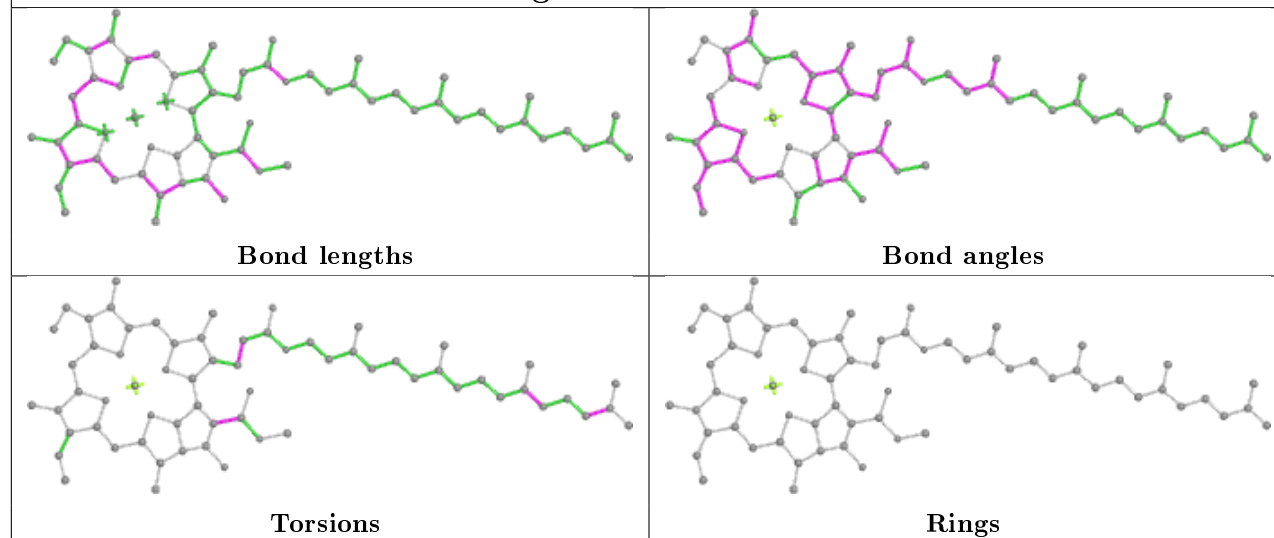
Ligand CLA C 511

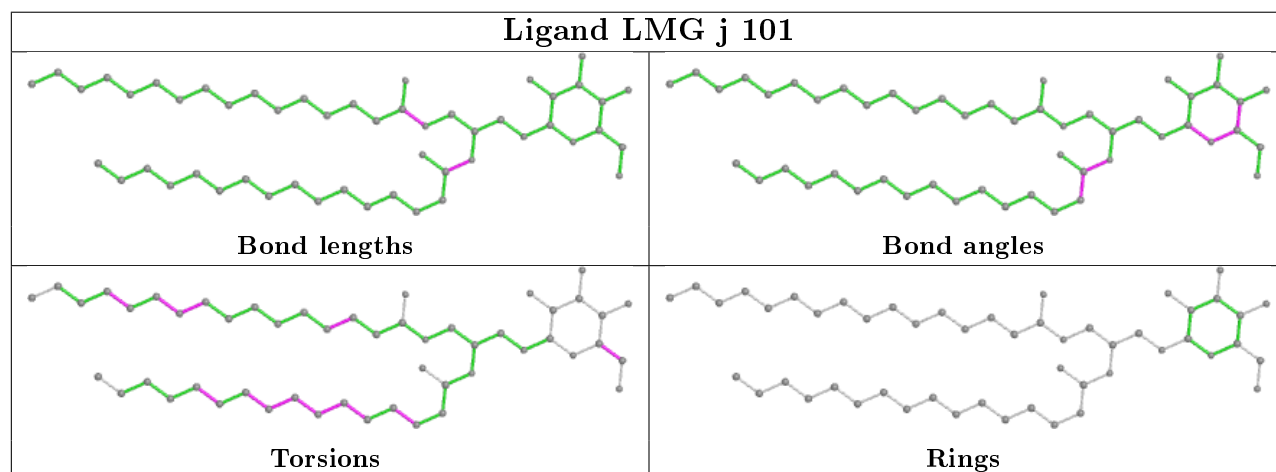
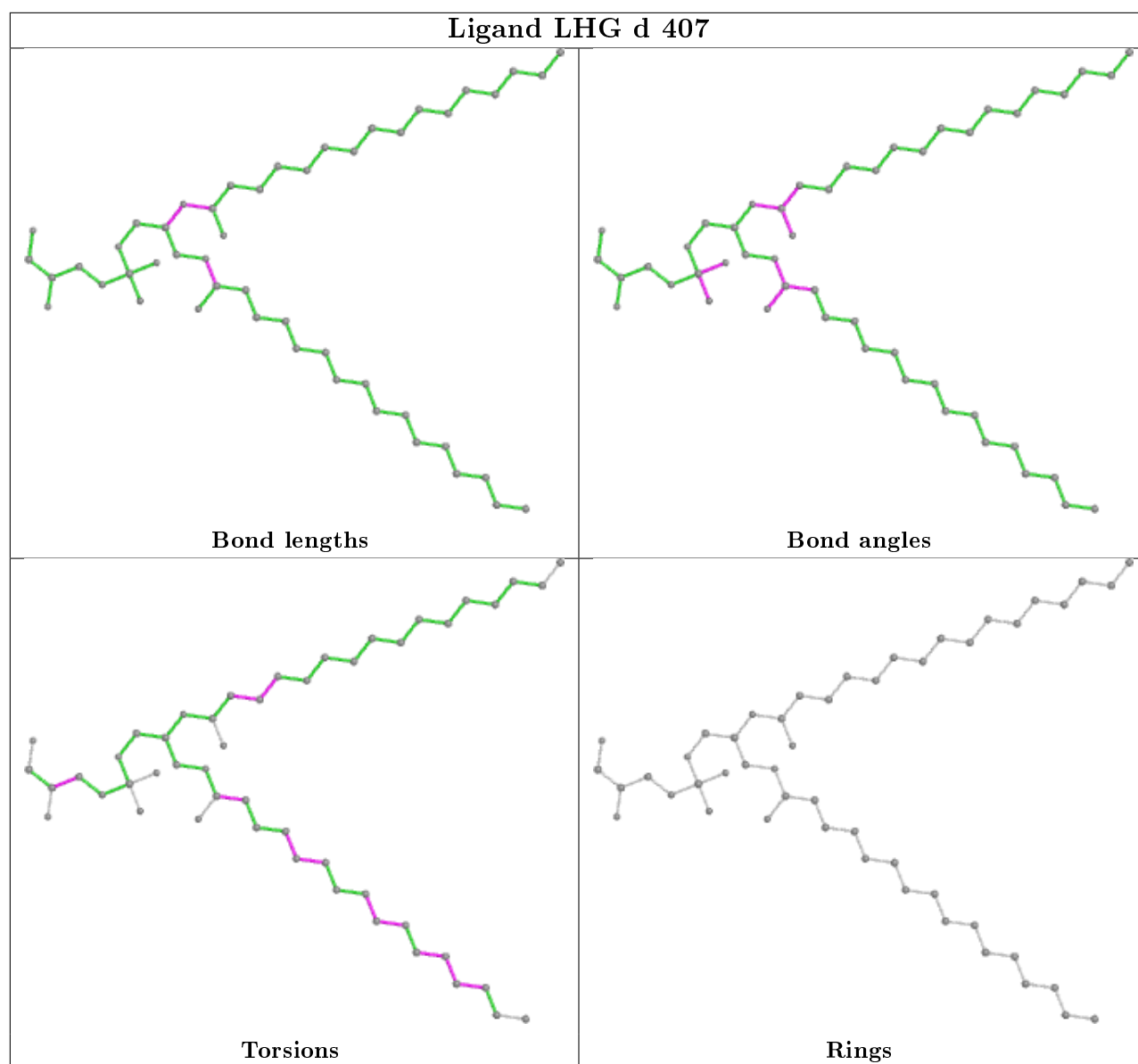


Ligand DGD c 520

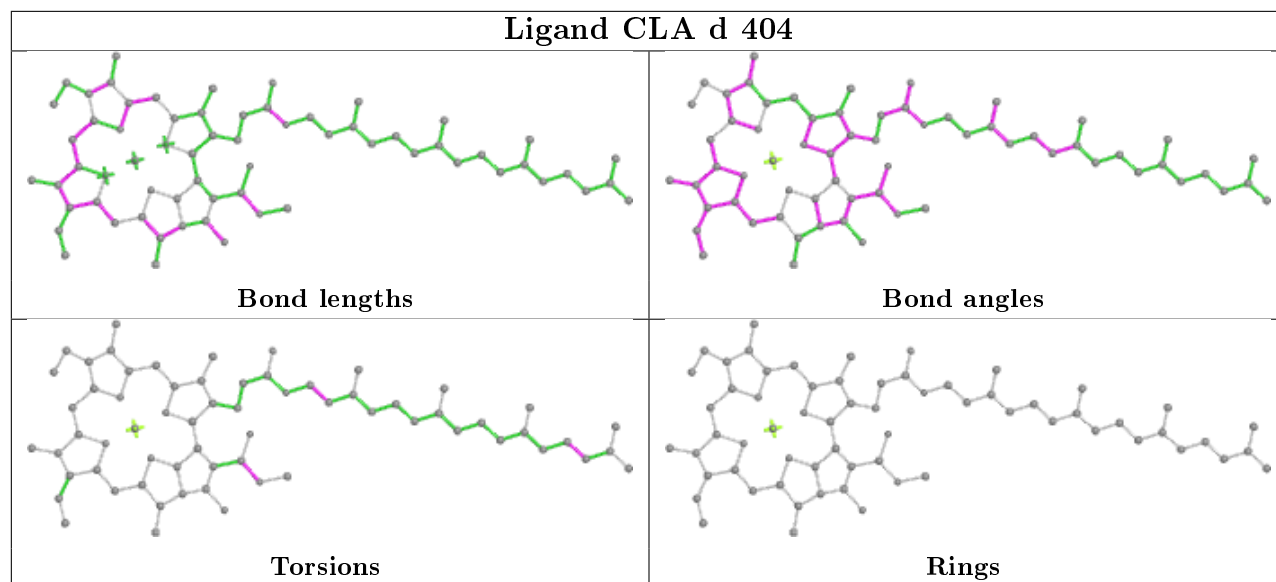


Ligand CLA B 611

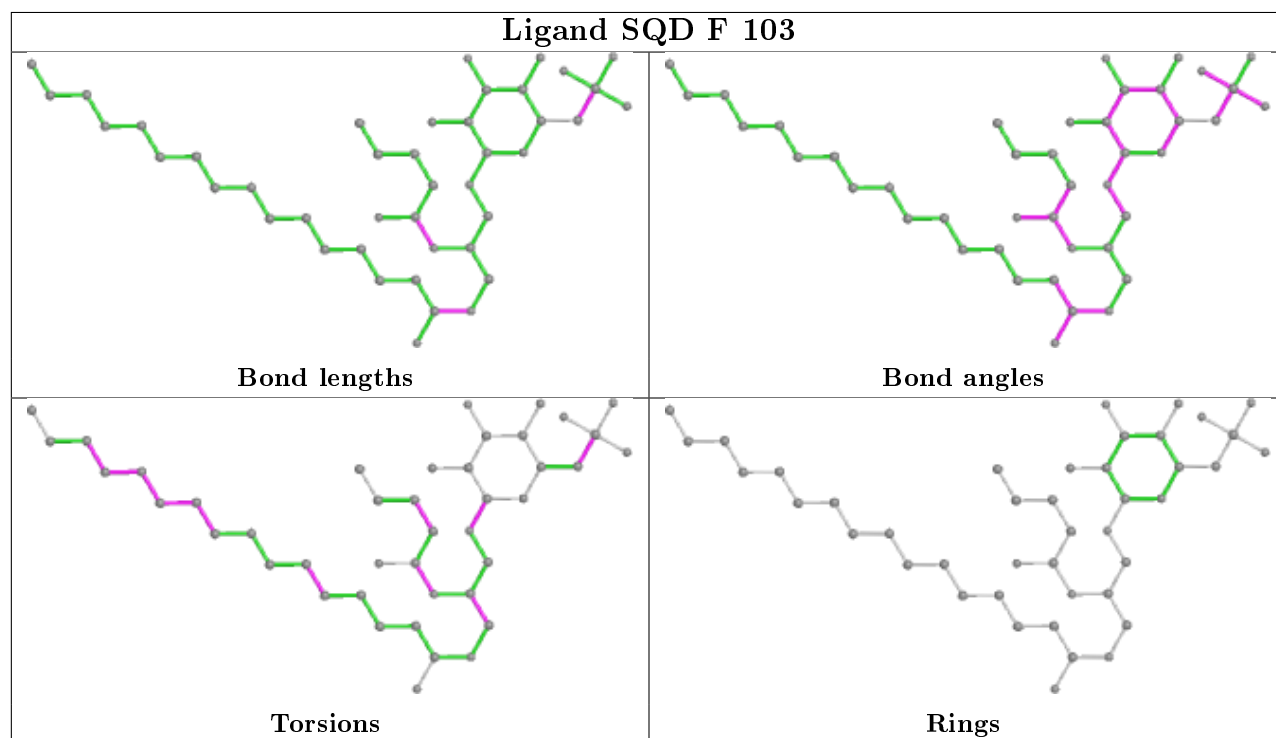


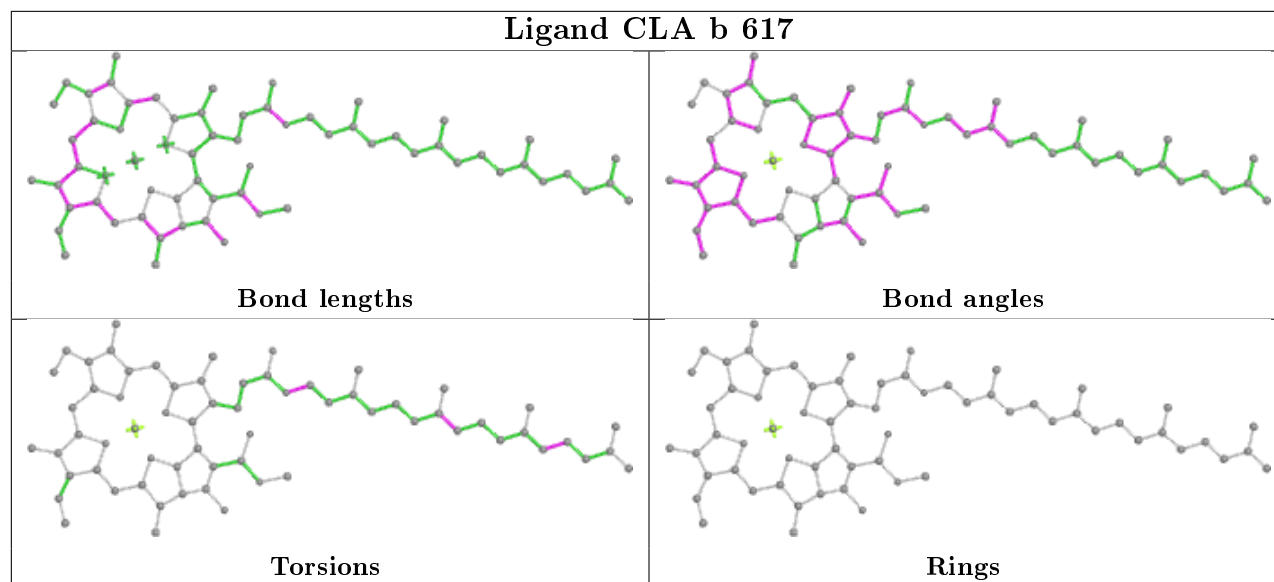
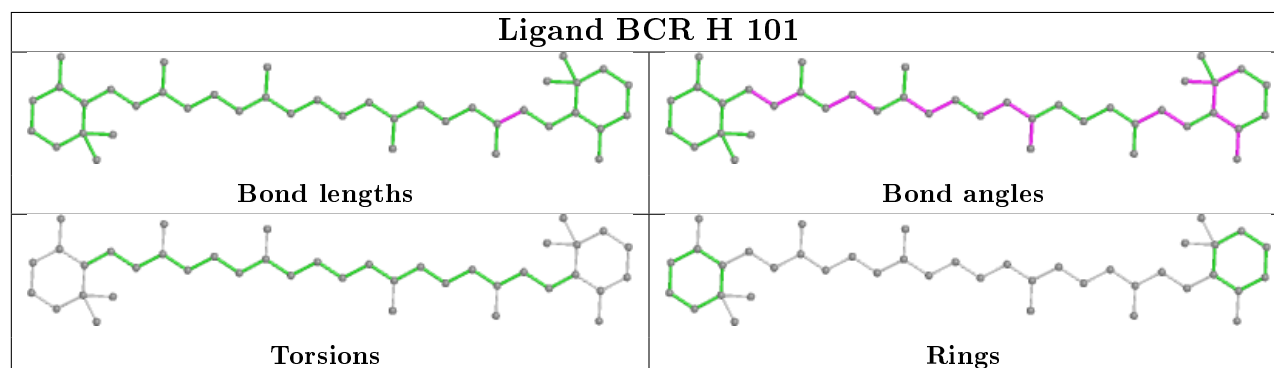
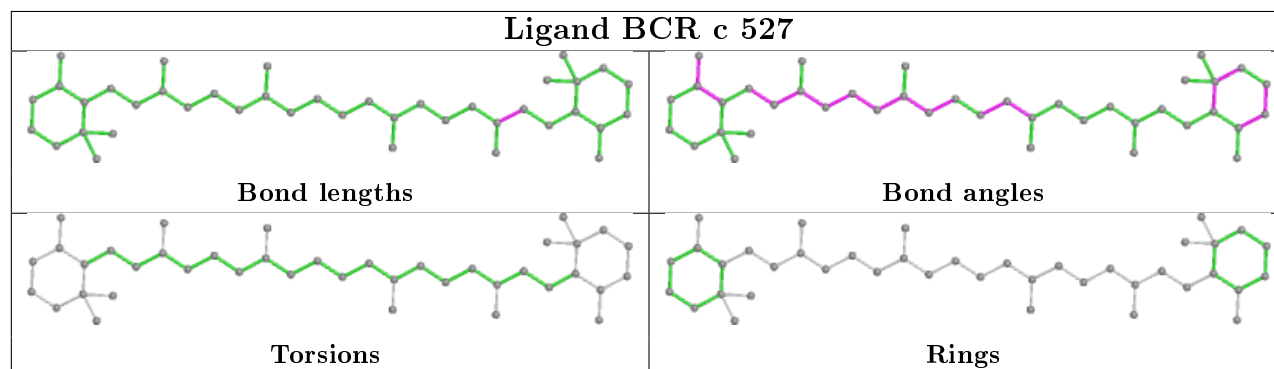


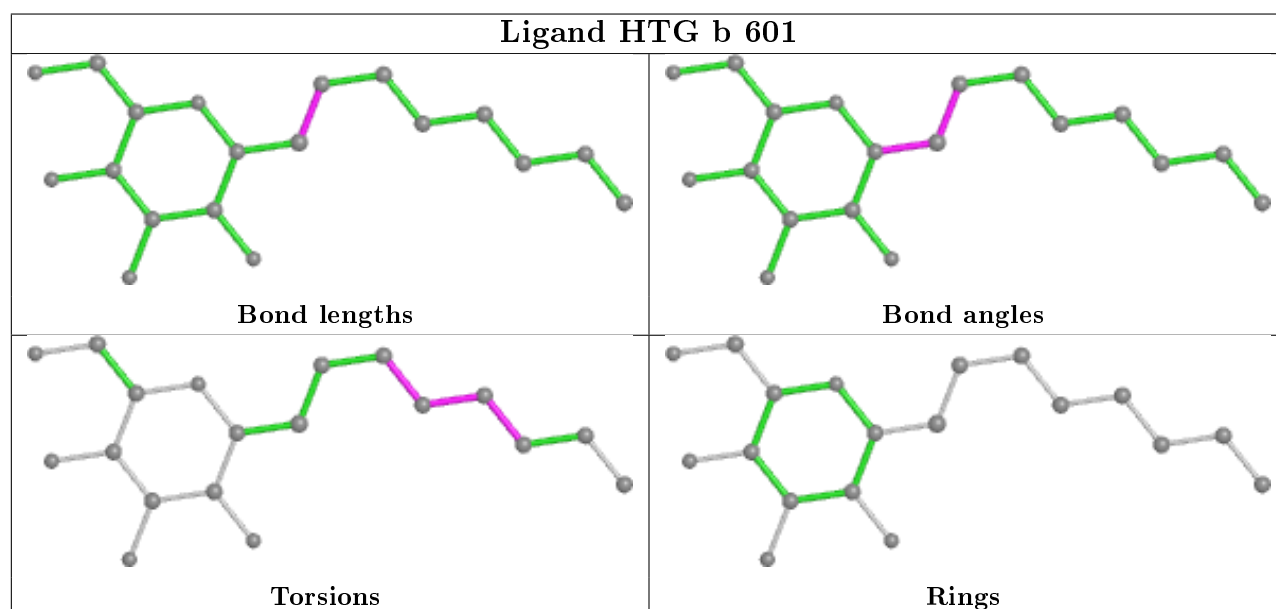
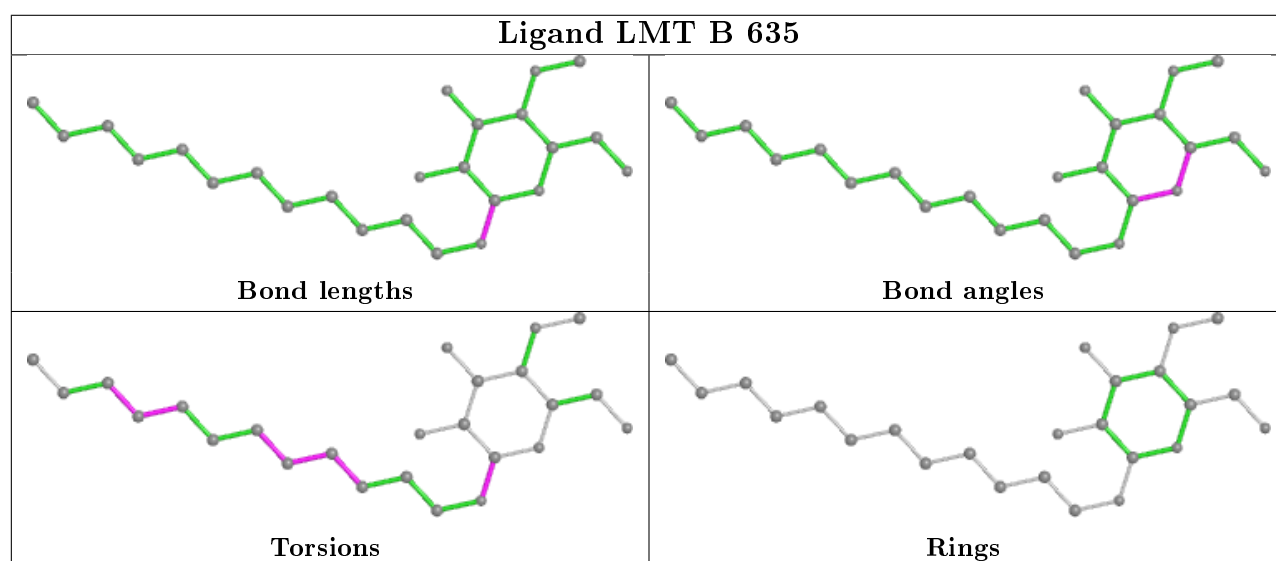
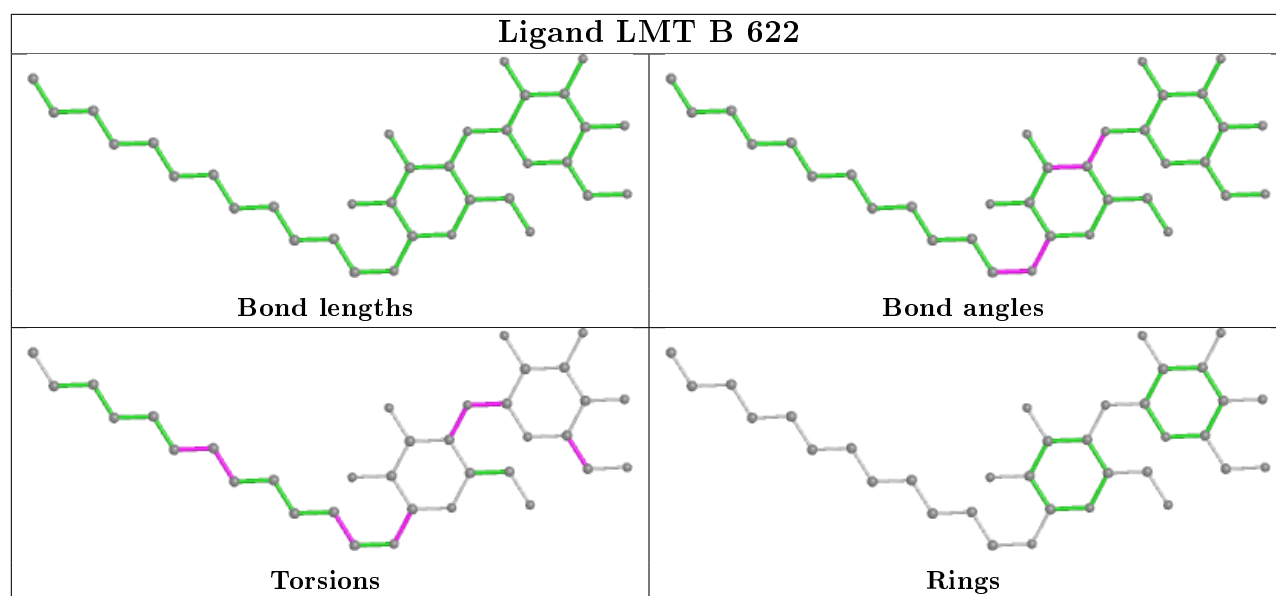
Ligand CLA d 404



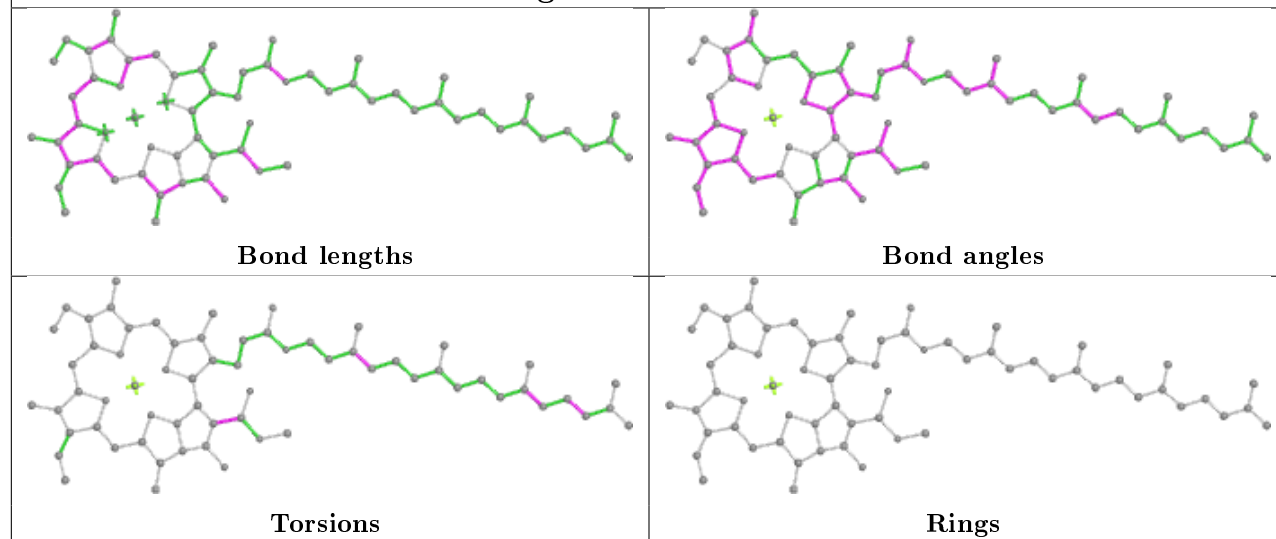
Ligand SQD F 103



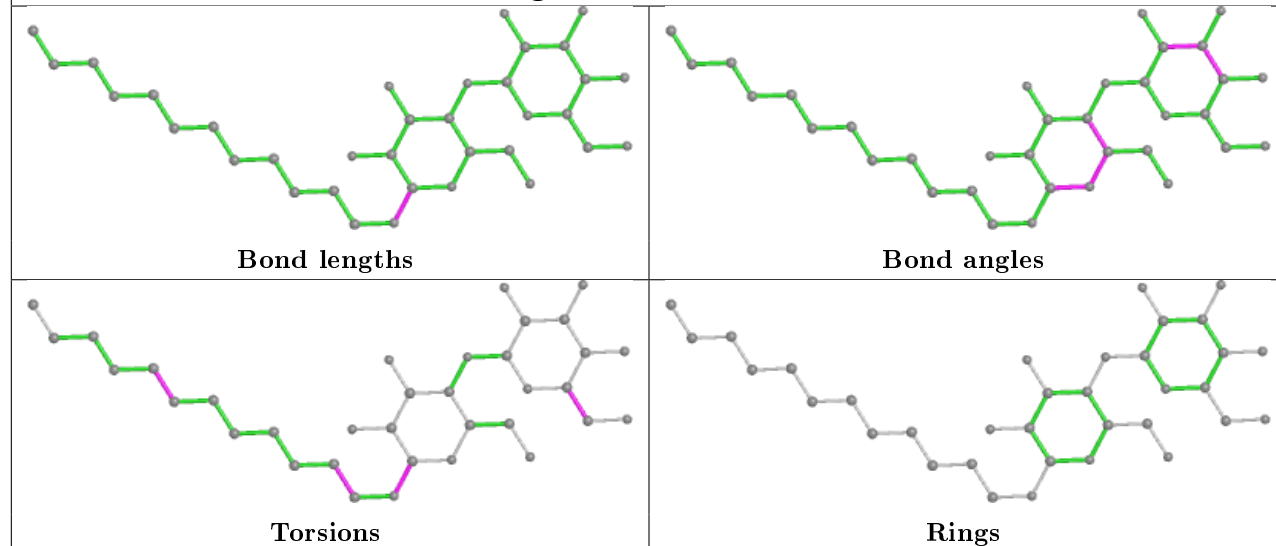
Ligand CLA b 617**Ligand BCR H 101****Ligand BCR c 527**



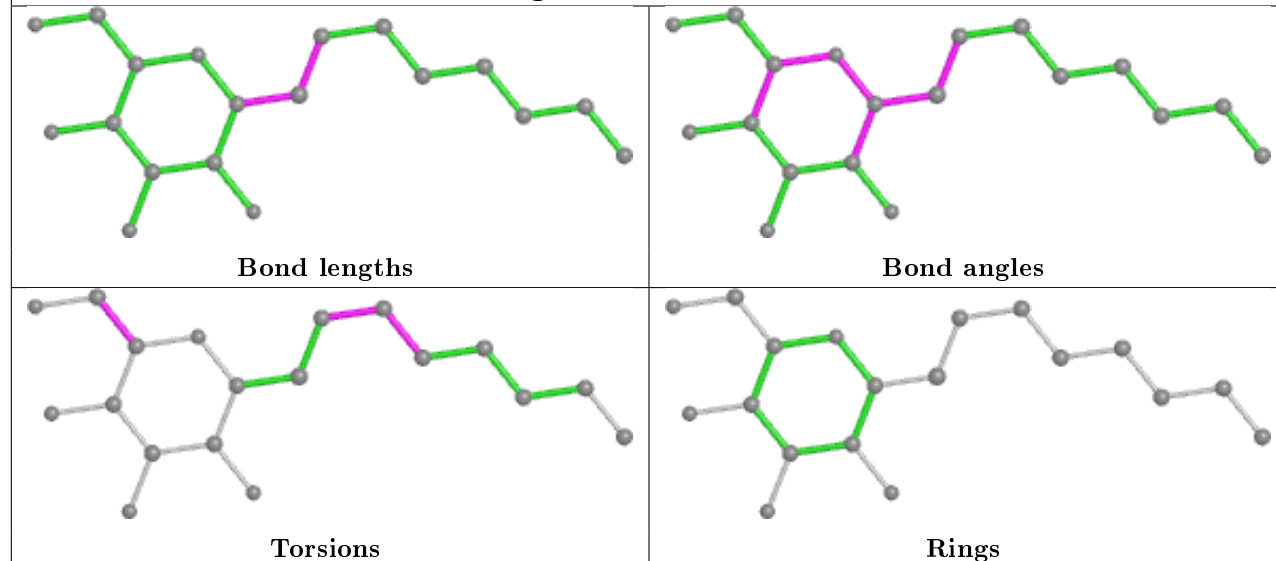
Ligand CLA c 508

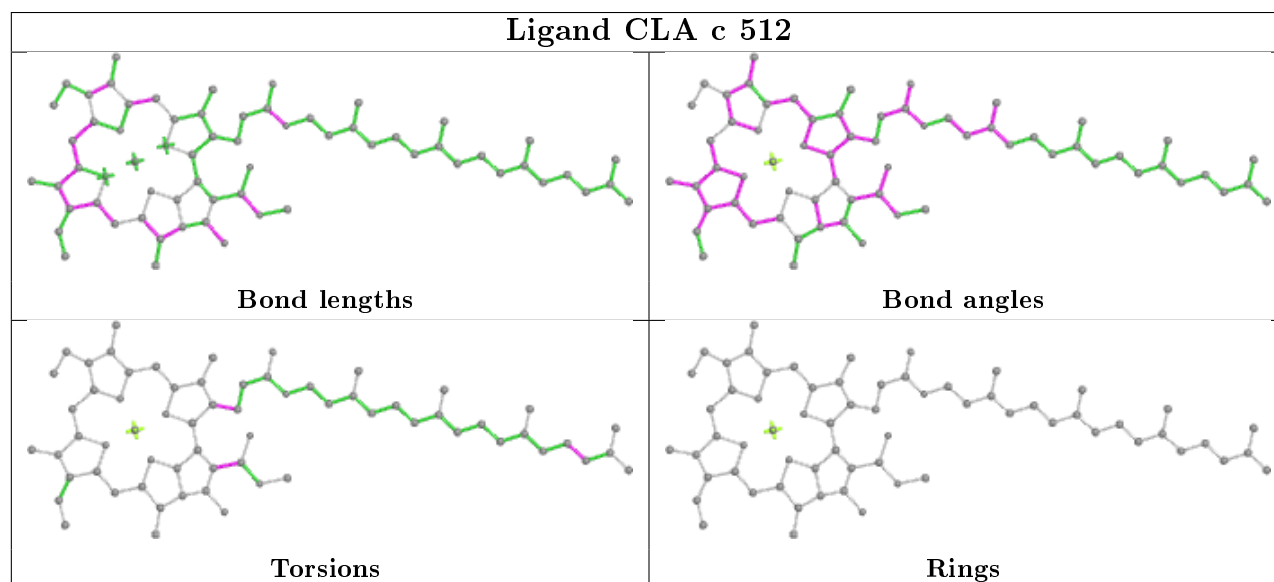
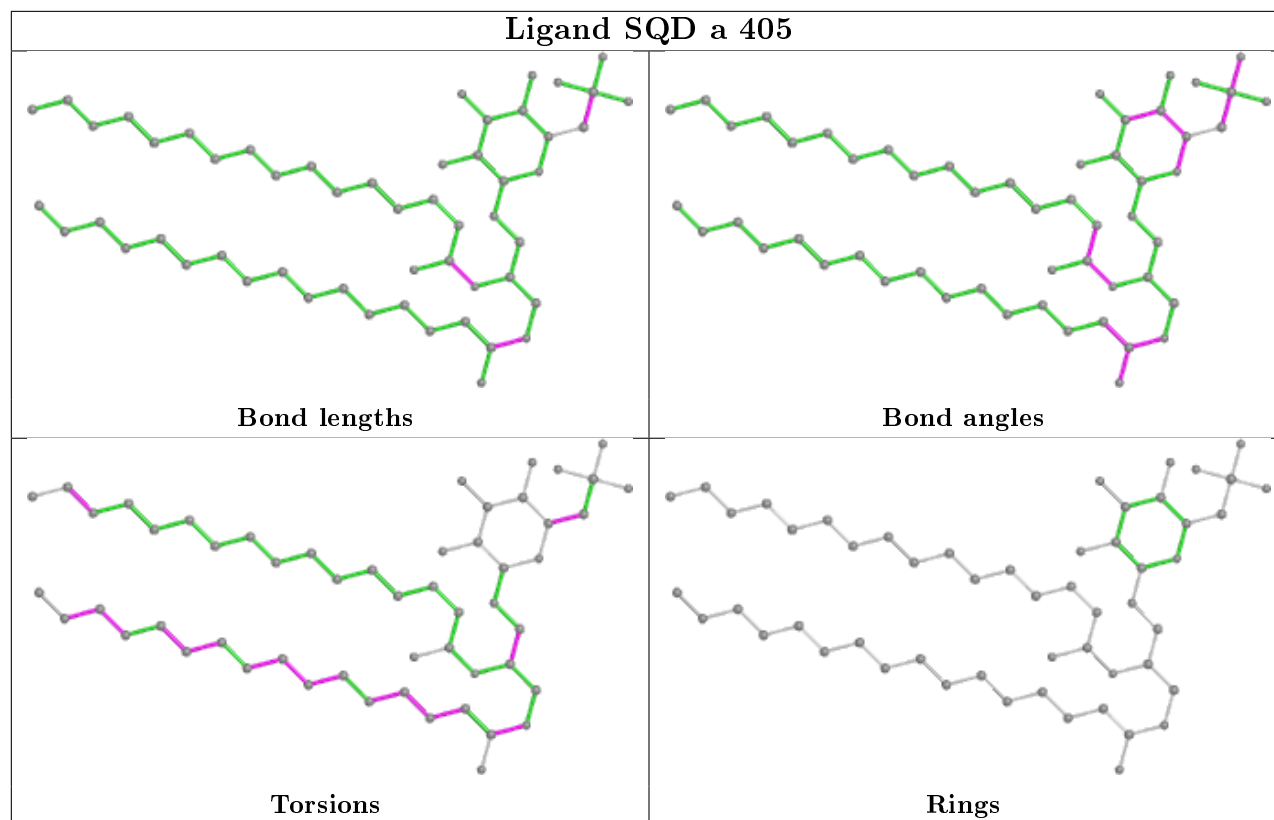


Ligand LMT A 416

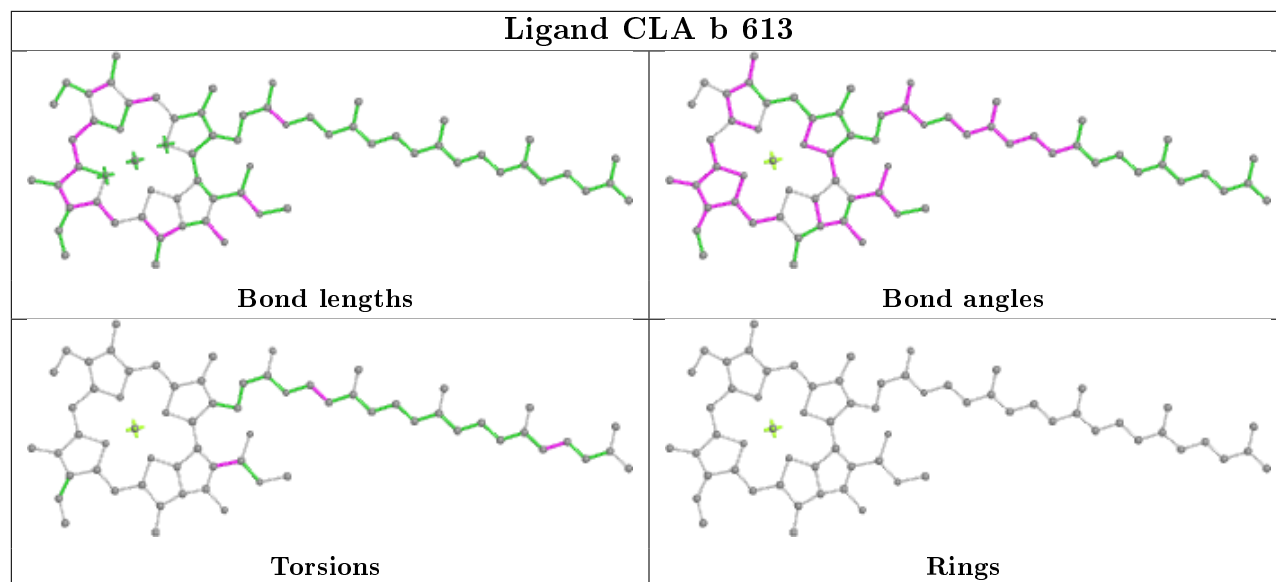


Ligand HTG C 524

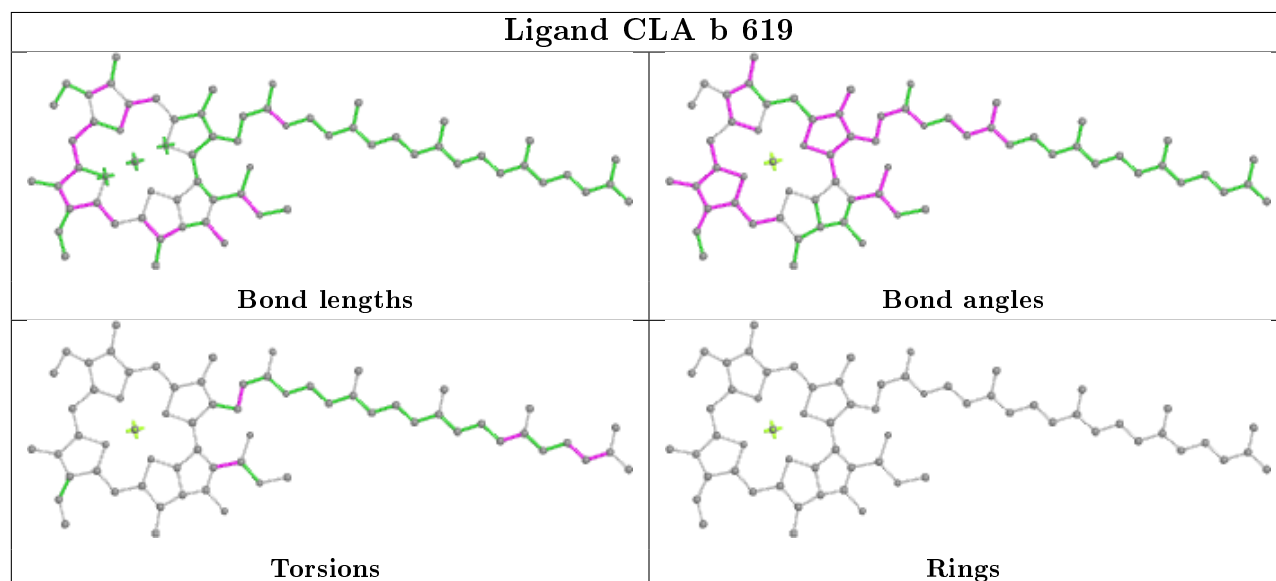




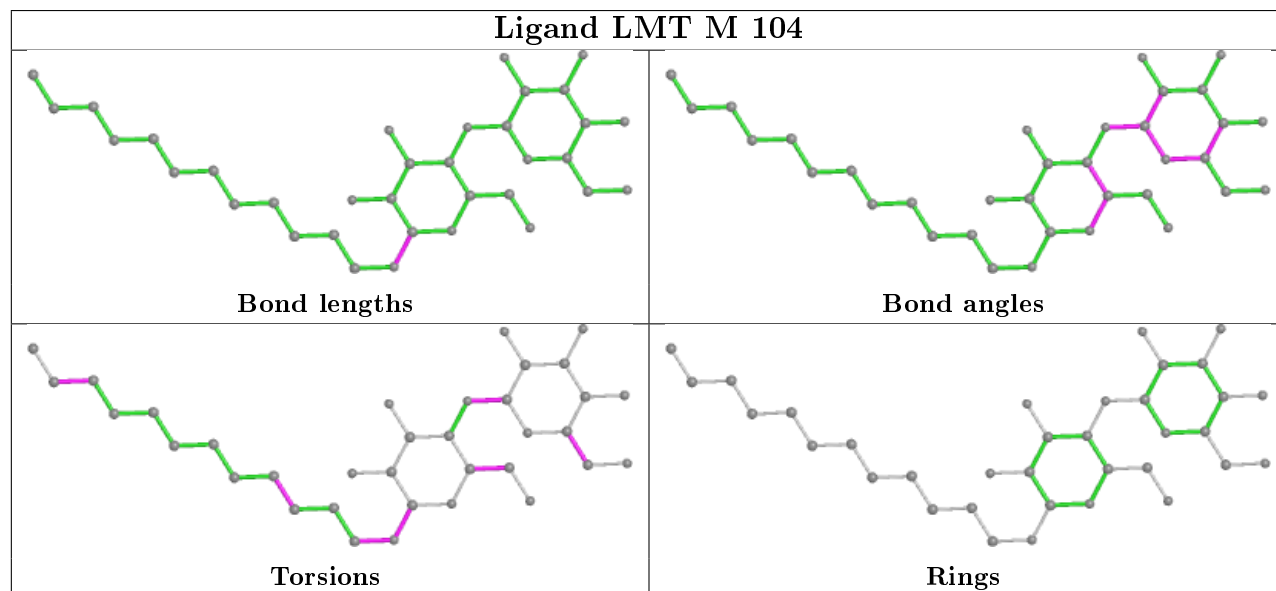
Ligand CLA b 613

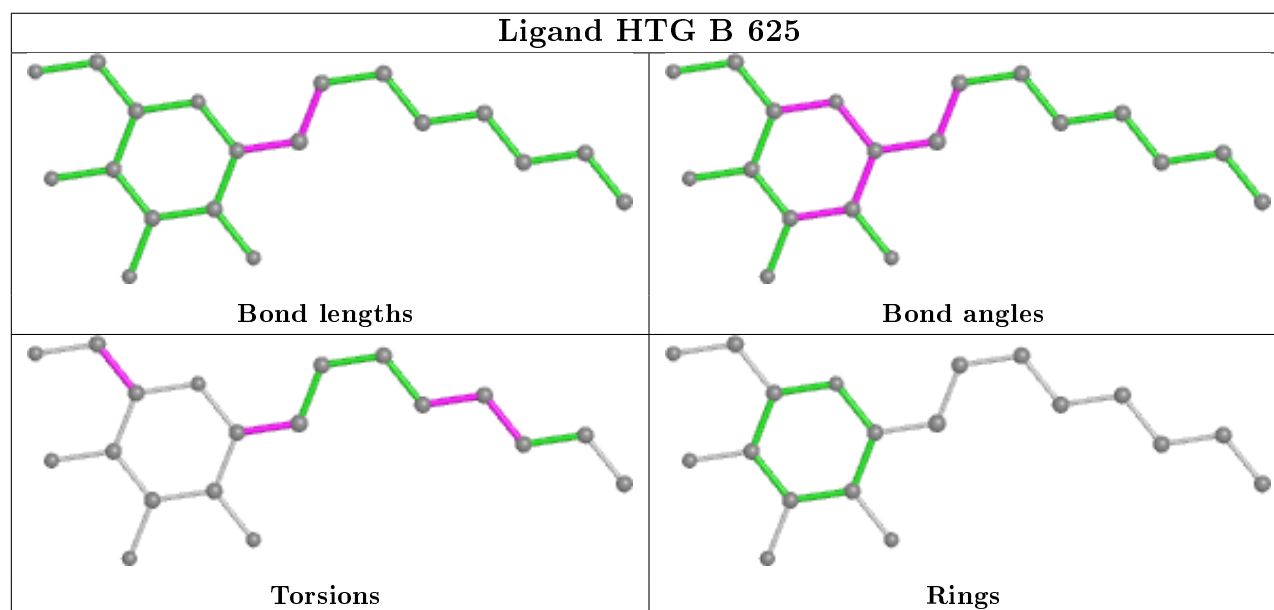
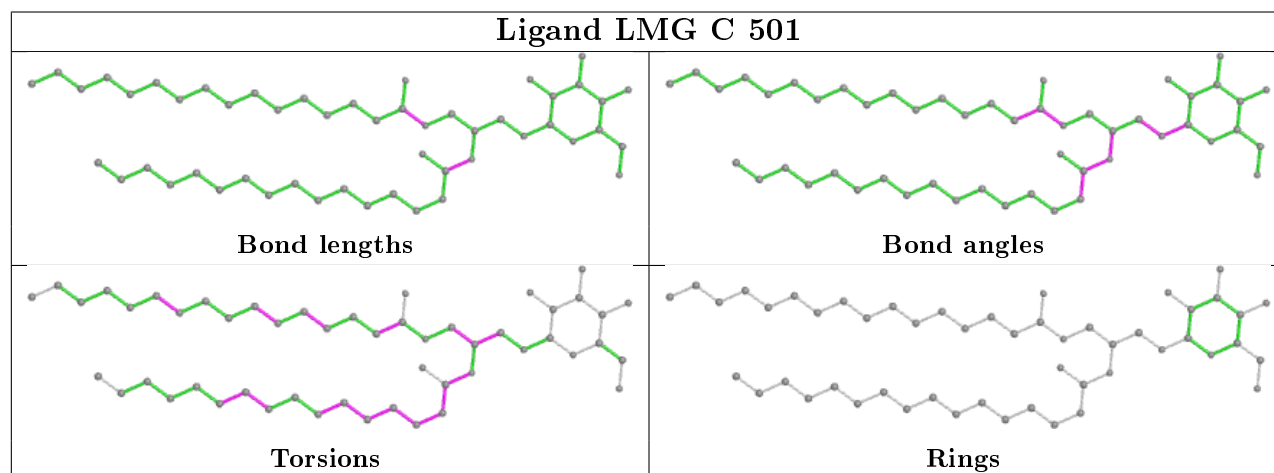
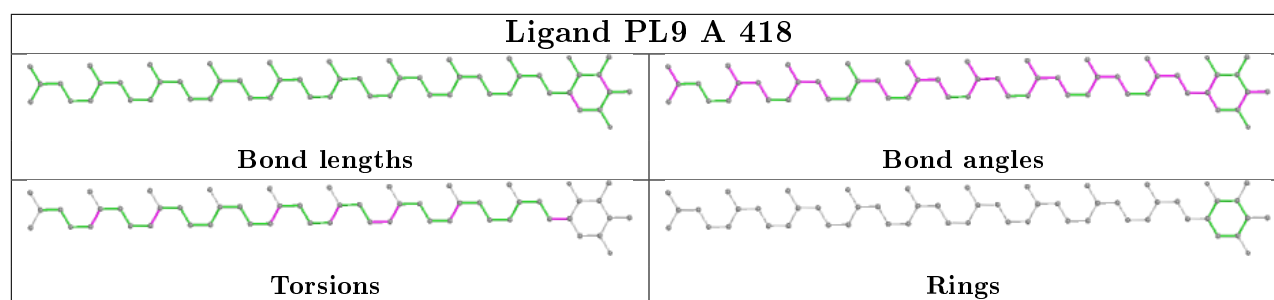


Ligand CLA b 619

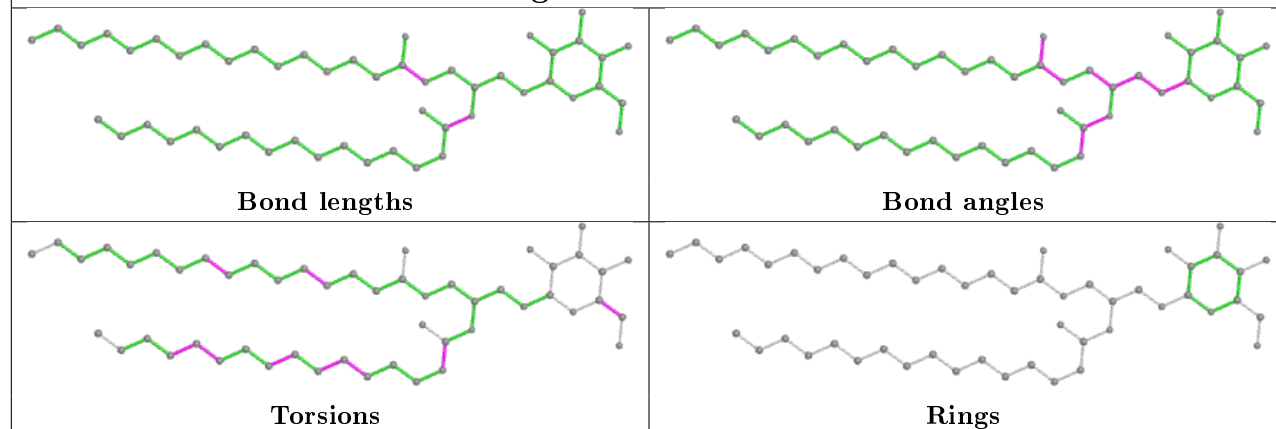


Ligand LMT M 104

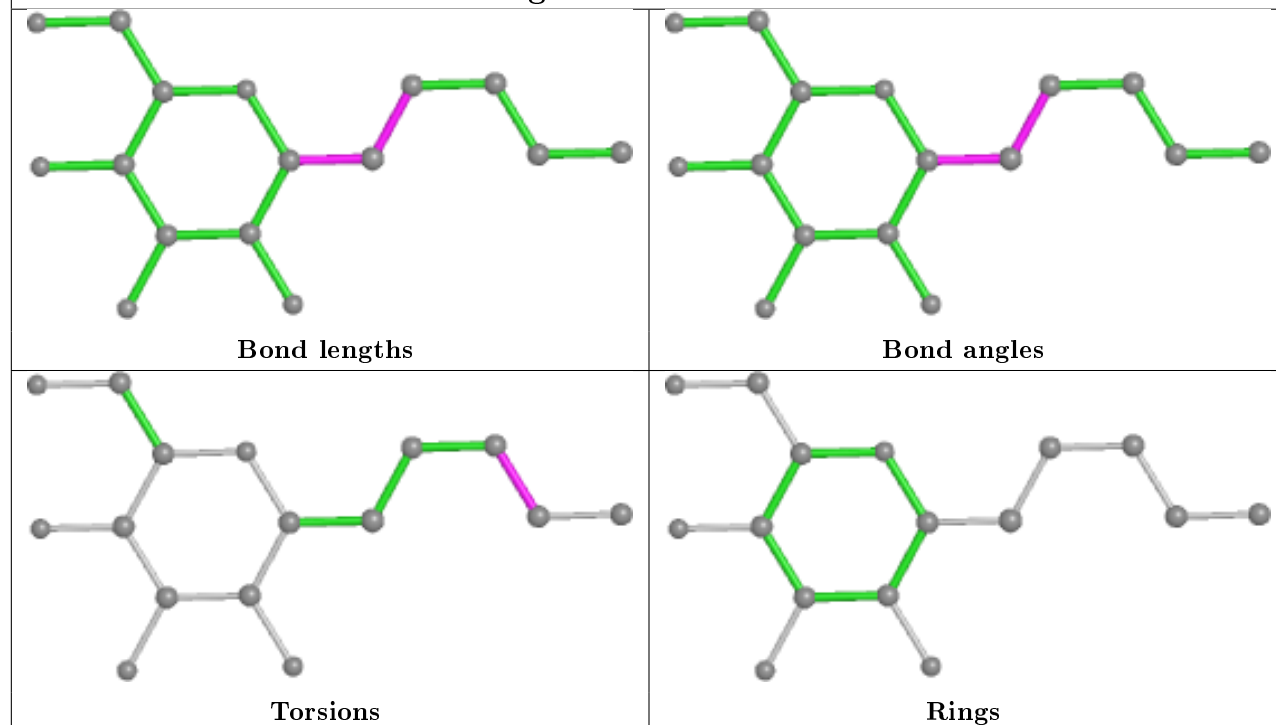




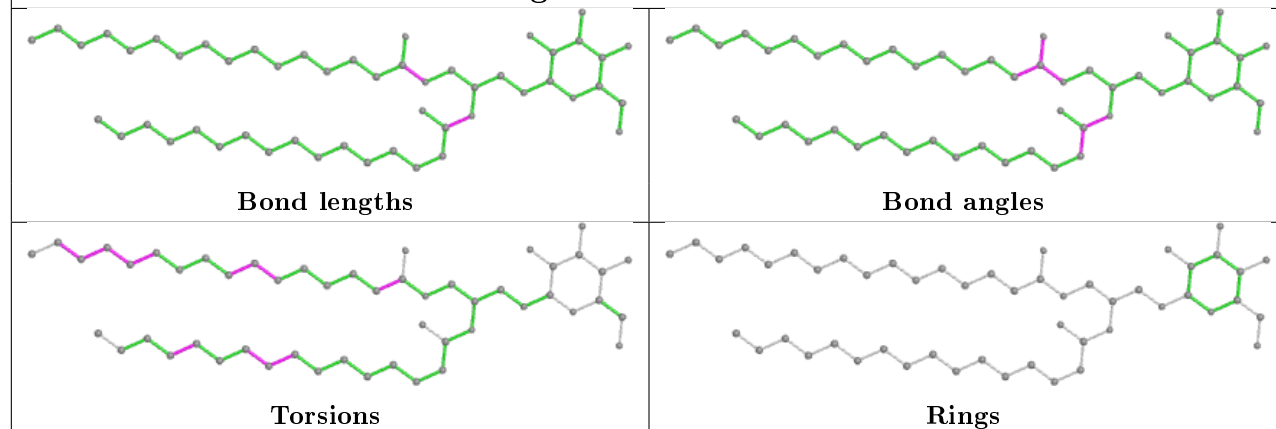
Ligand LMG J 101

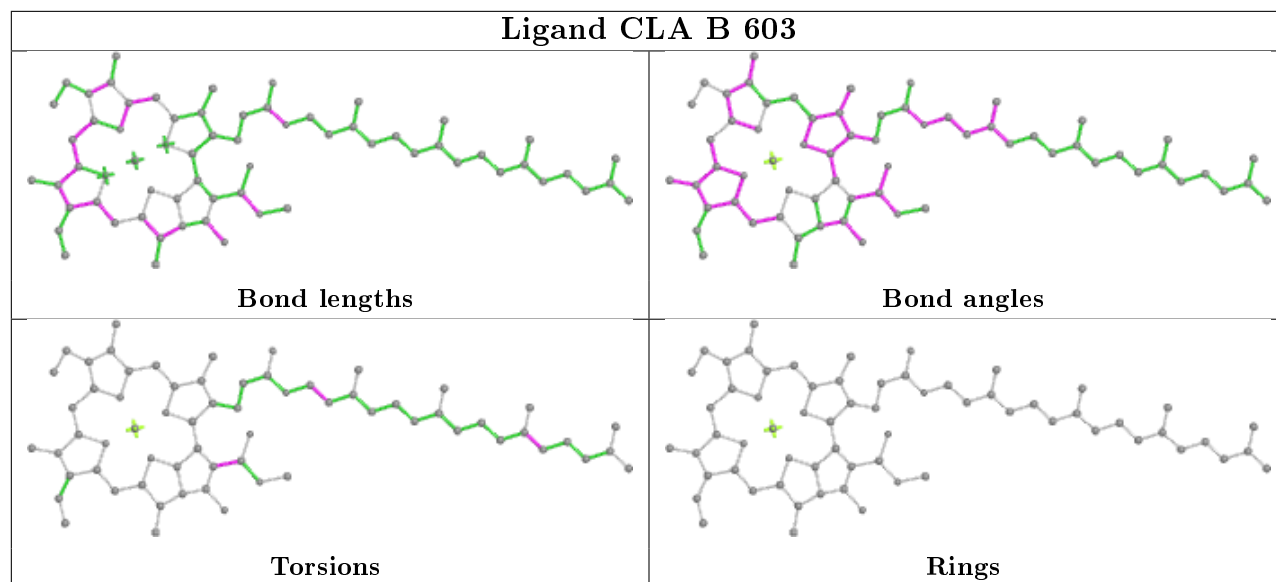
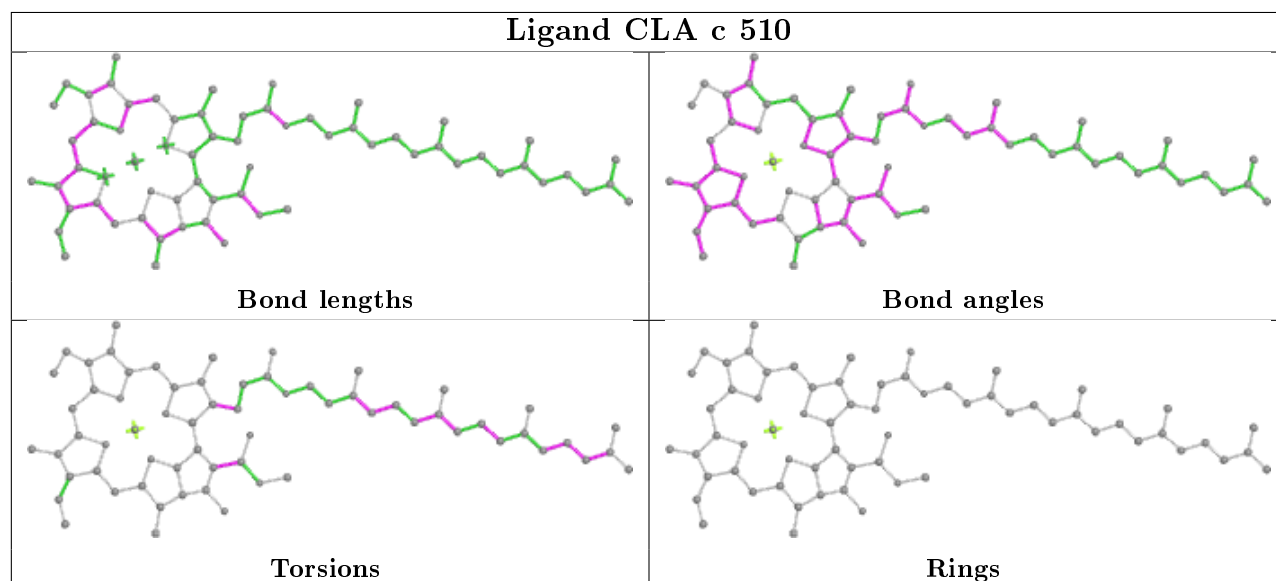
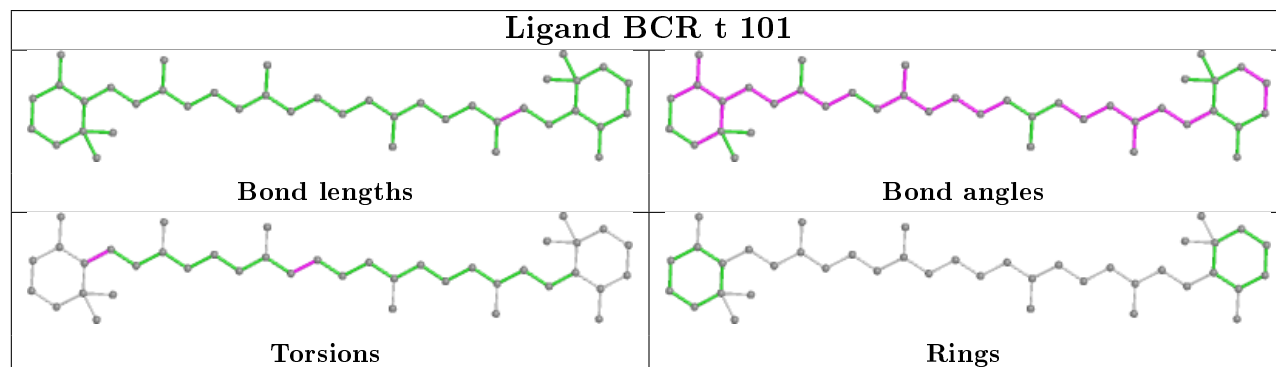


Ligand HTG D 412

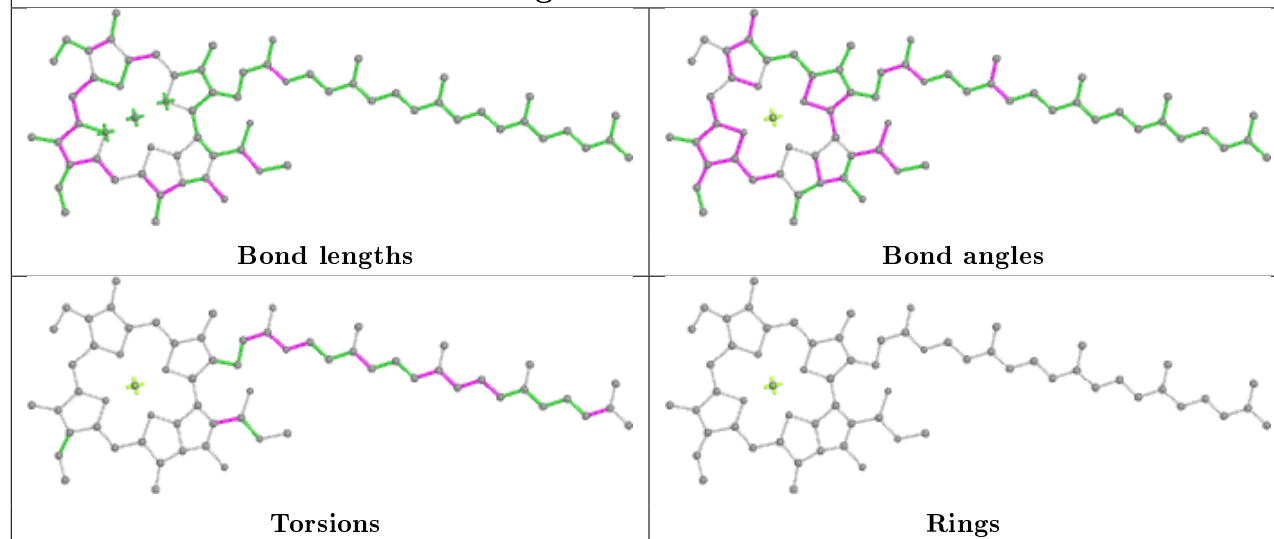


Ligand LMG b 629

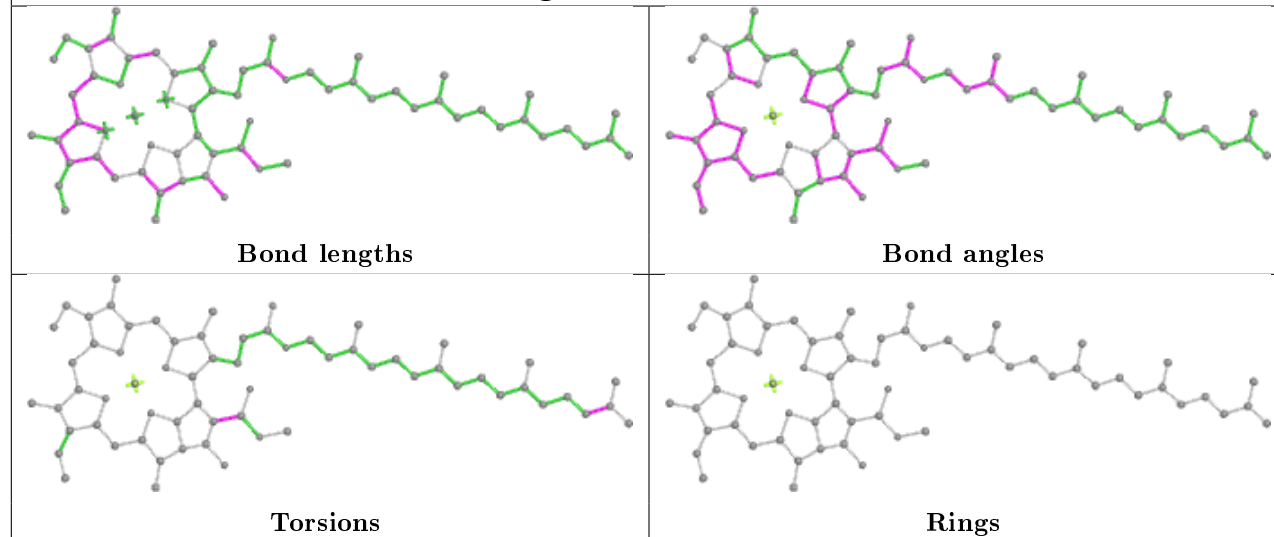


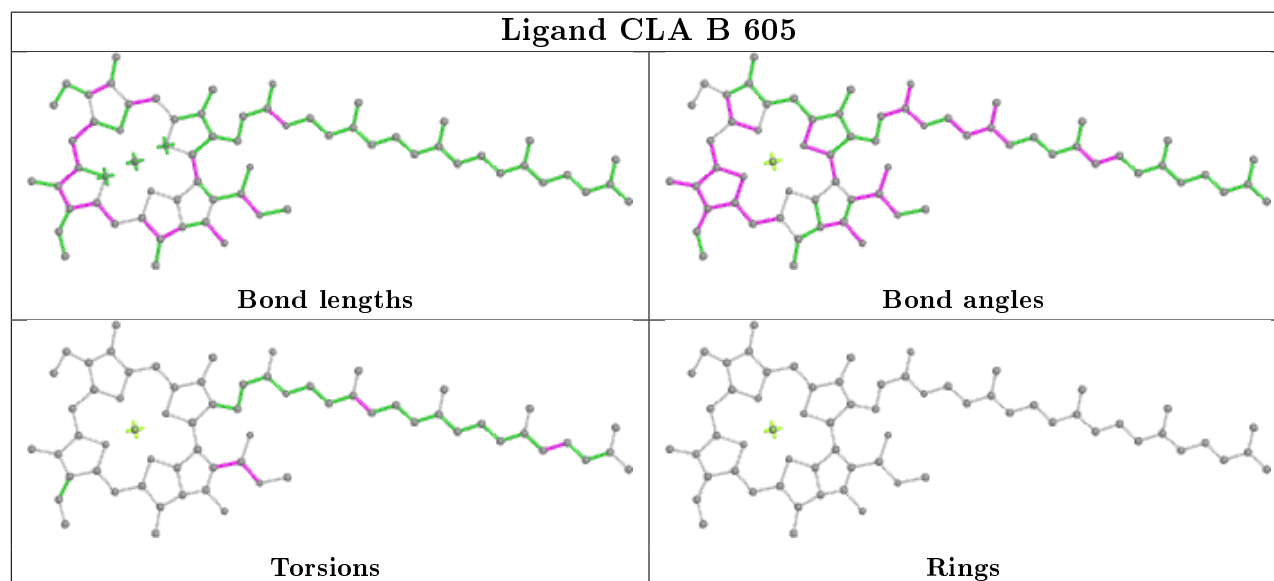
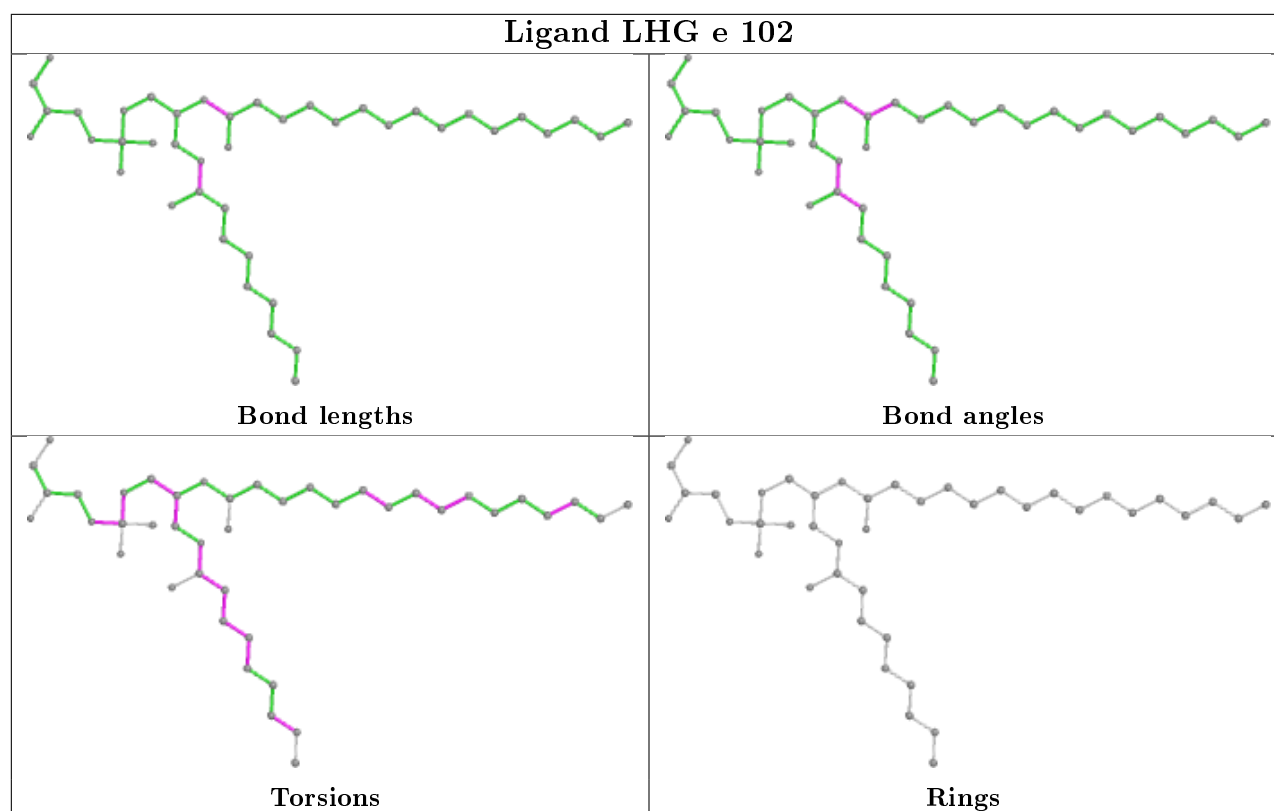
Ligand CLA B 603**Ligand CLA c 510****Ligand BCR t 101**

Ligand CLA b 610

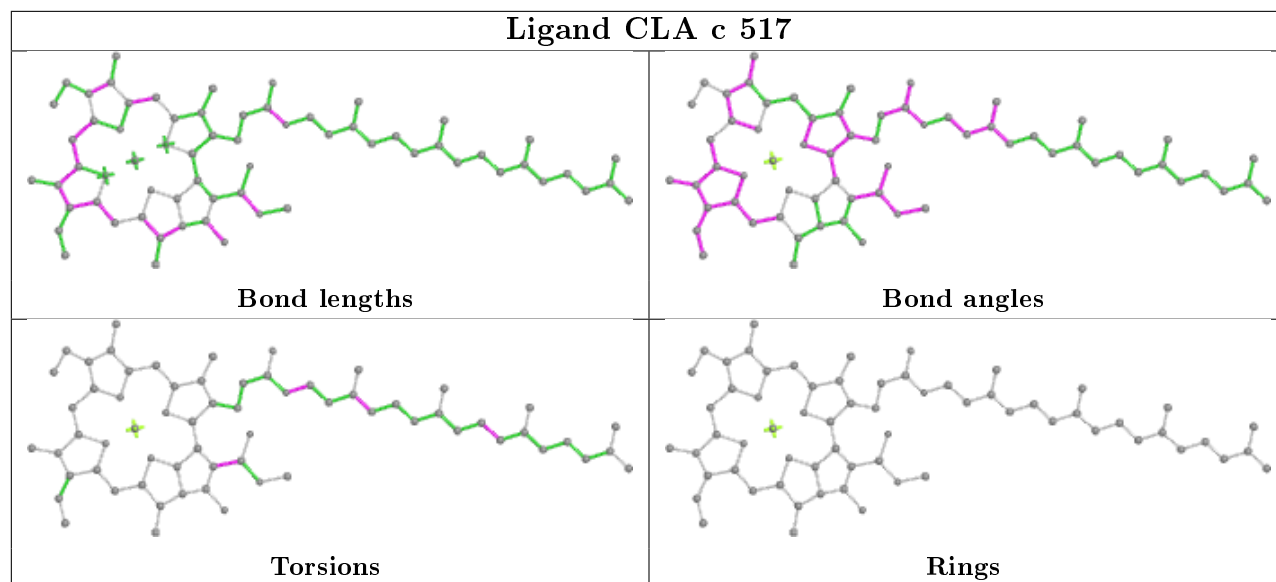


Ligand CLA c 506

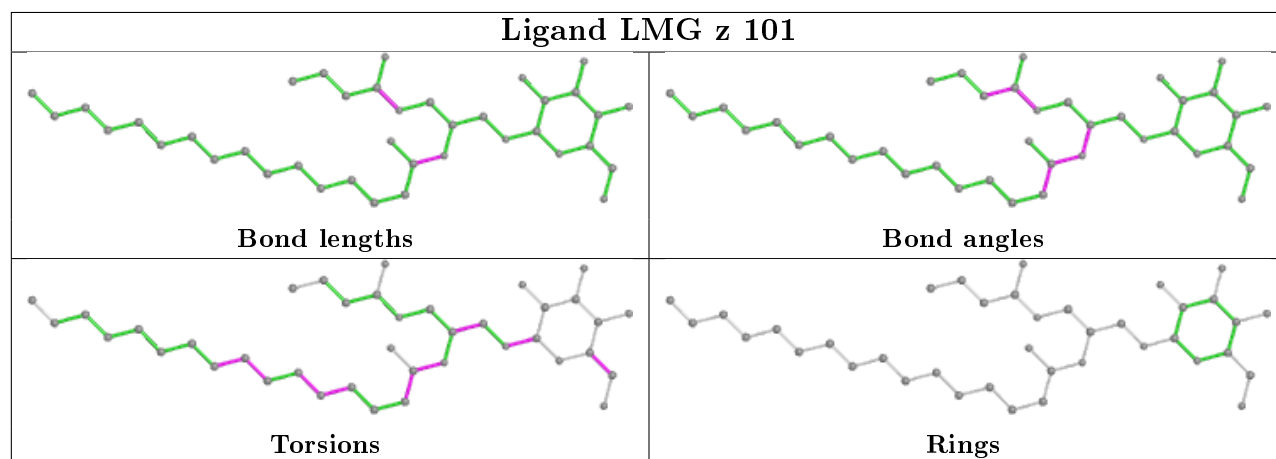




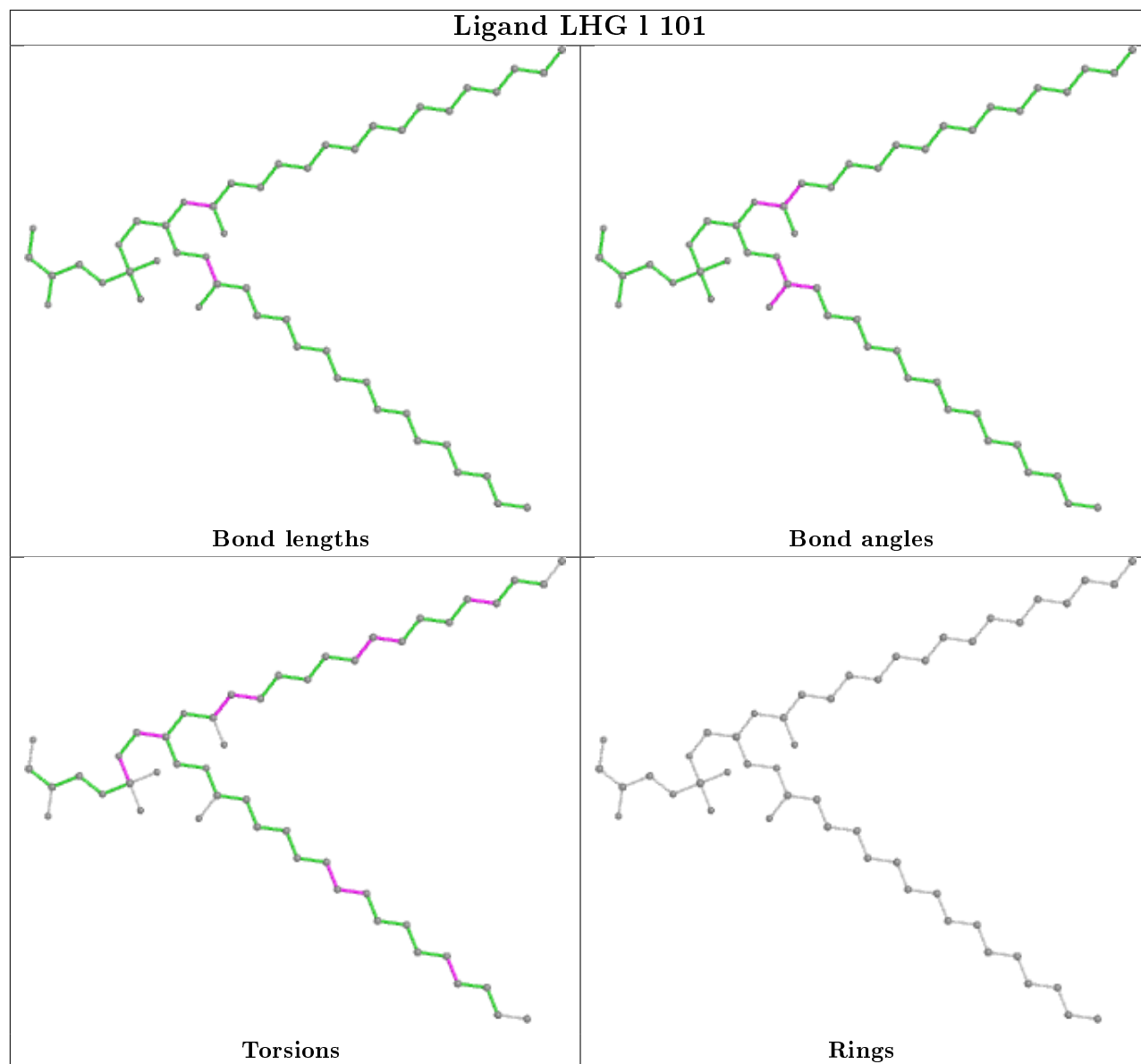
Ligand CLA c 517



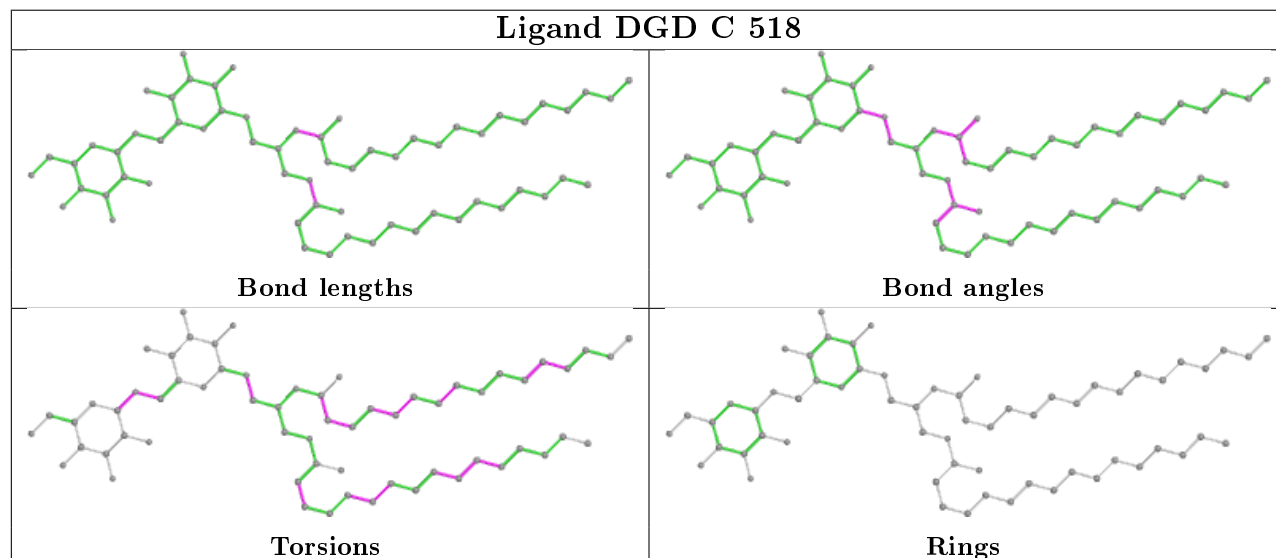
Ligand LMG z 101



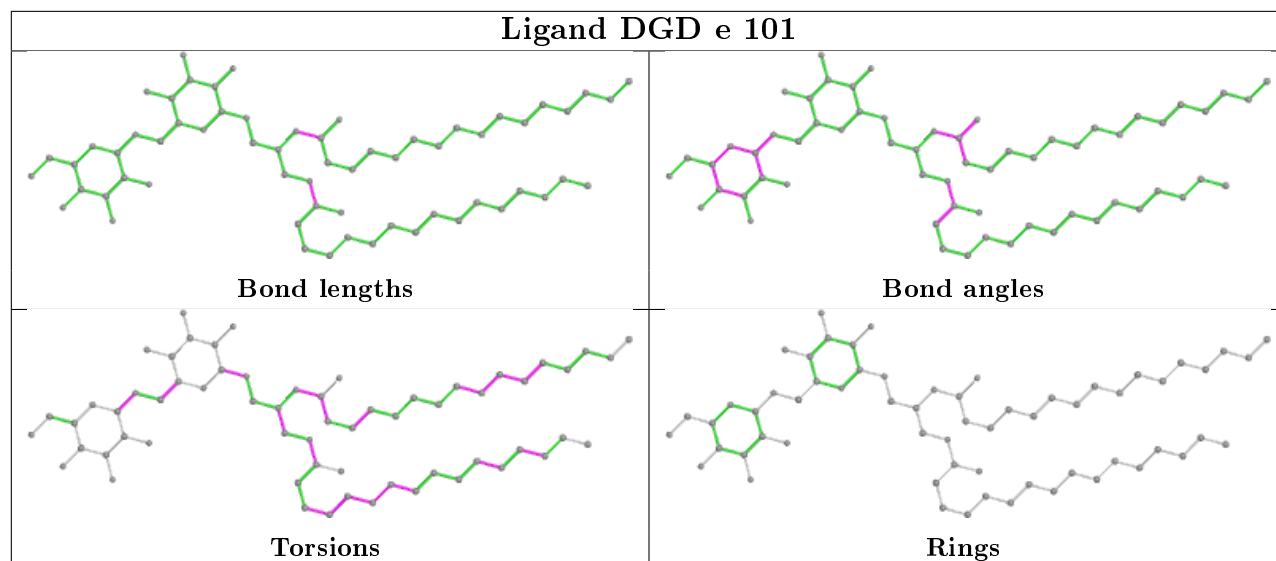
Ligand LHG 1 101



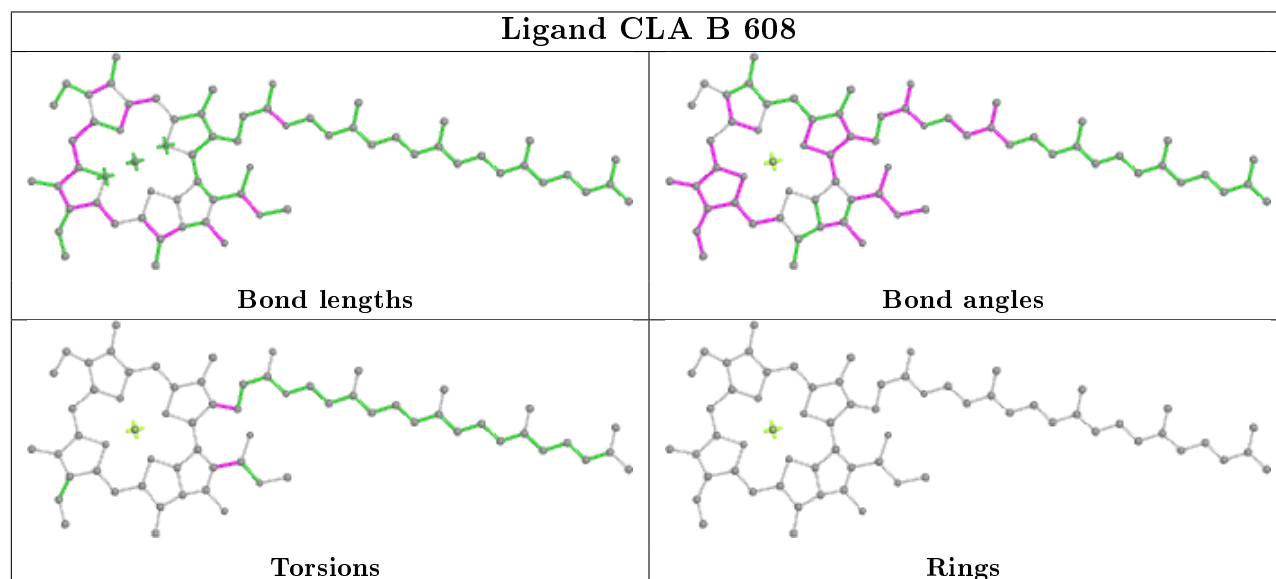
Ligand DGD C 518



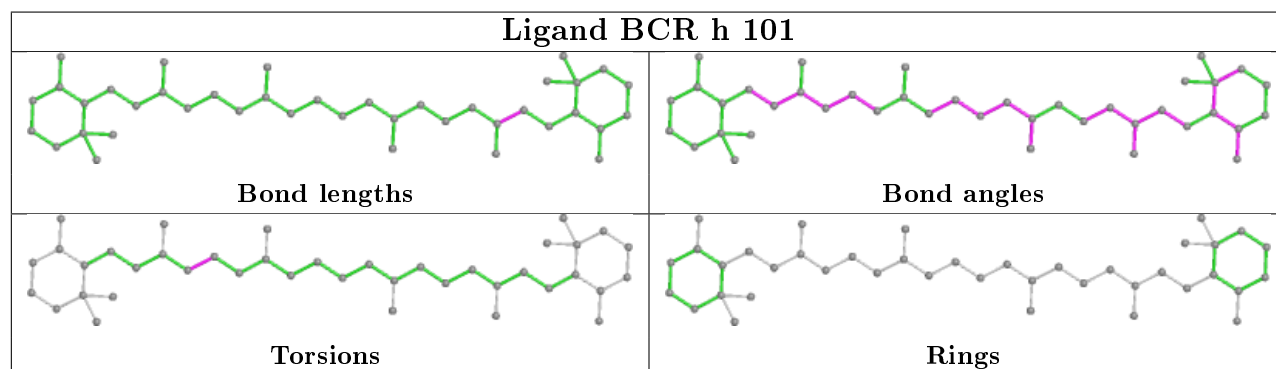
Ligand DGD e 101

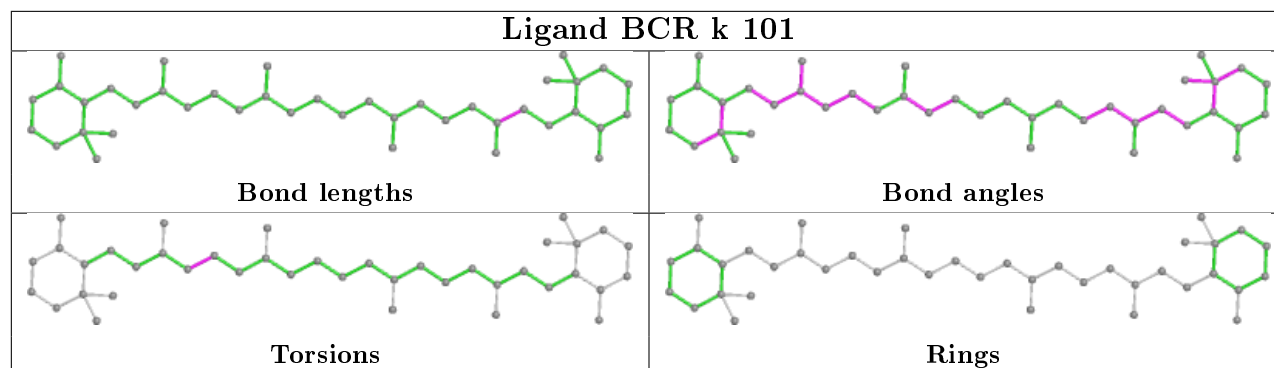
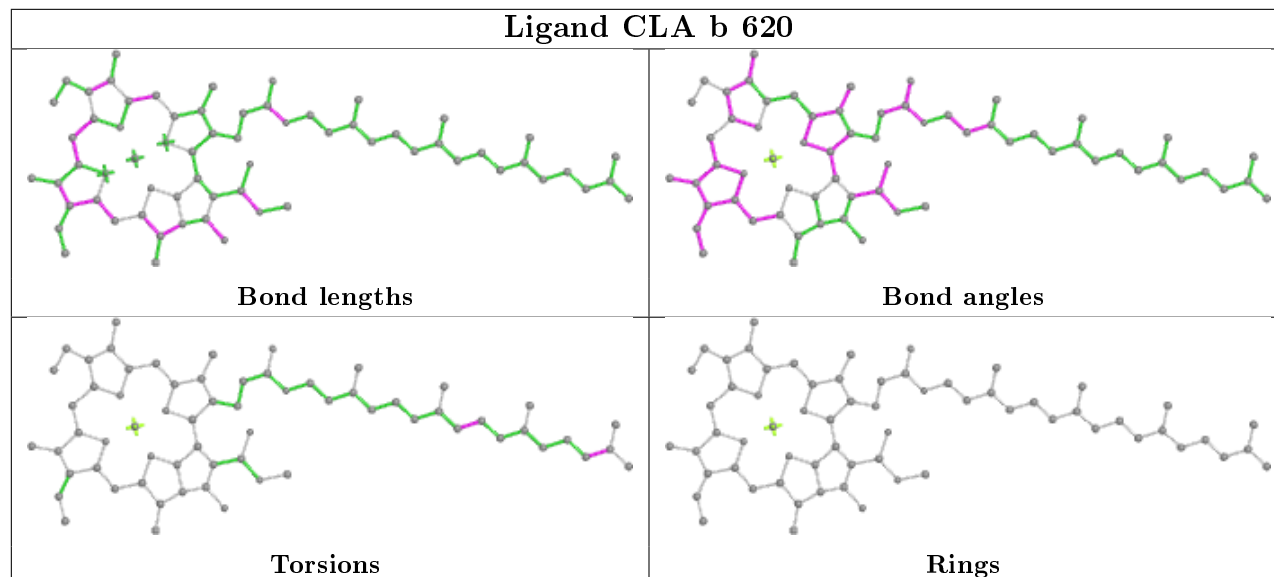
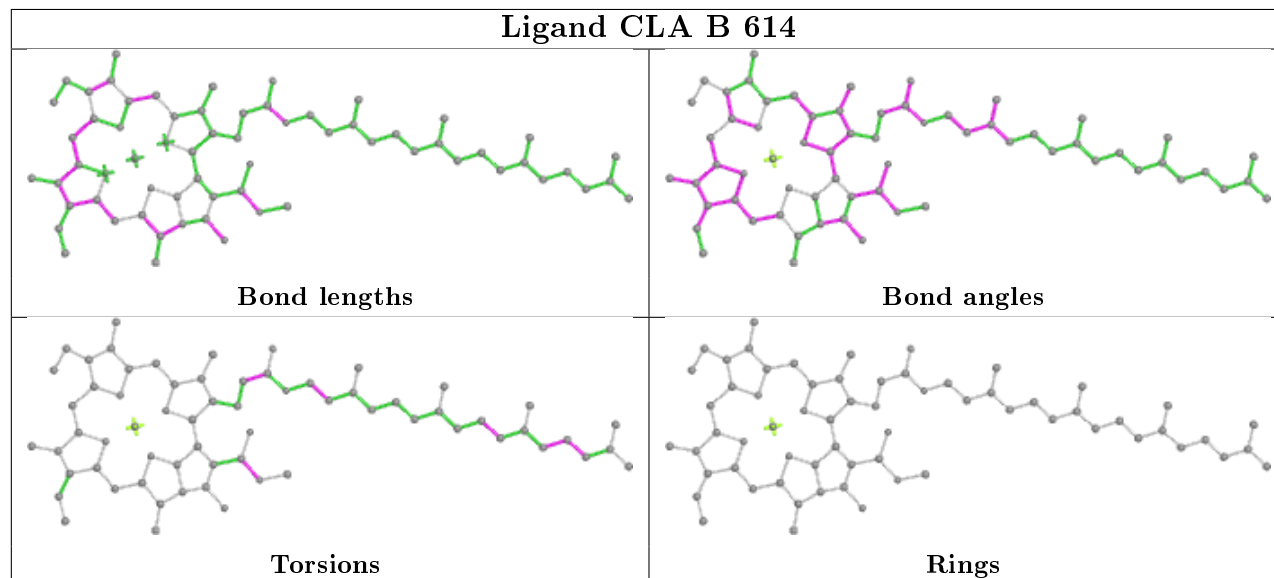


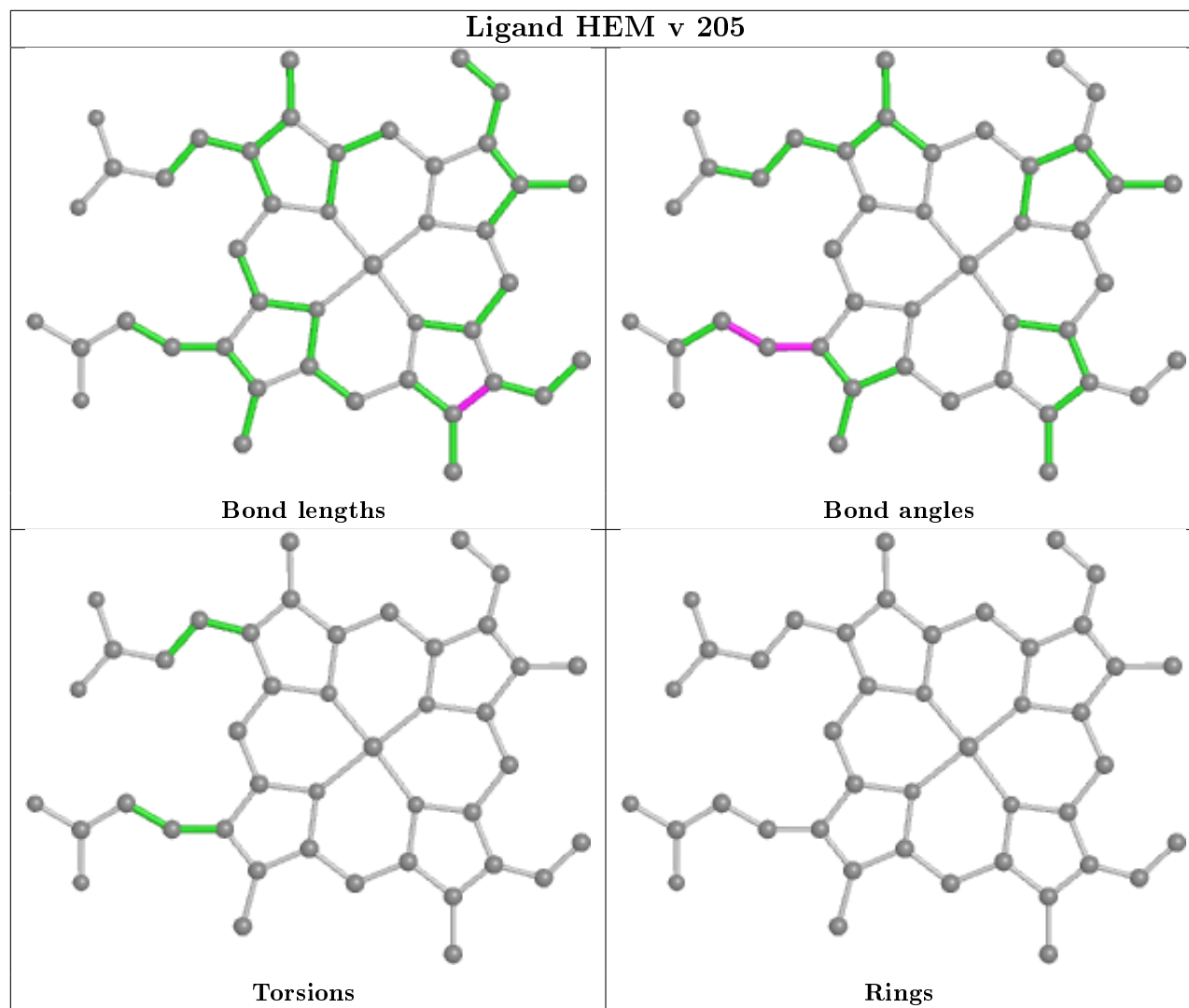
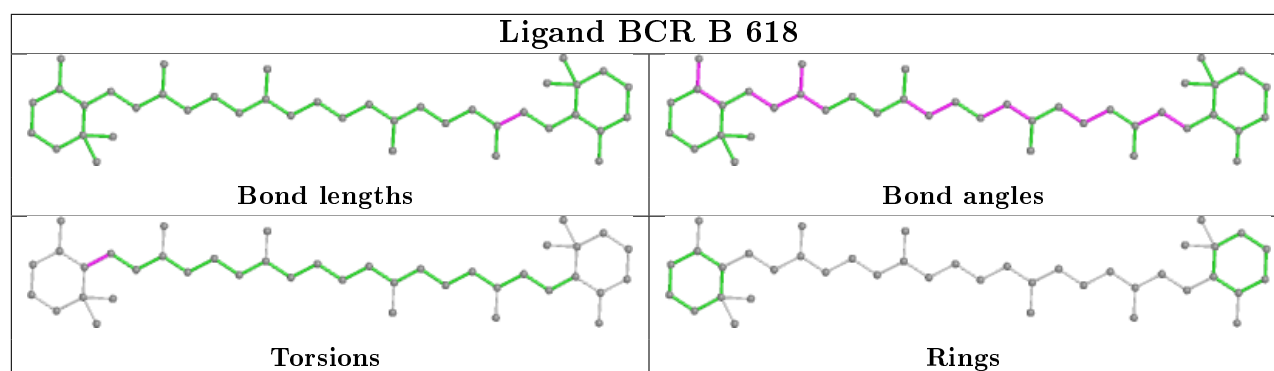
Ligand CLA B 608

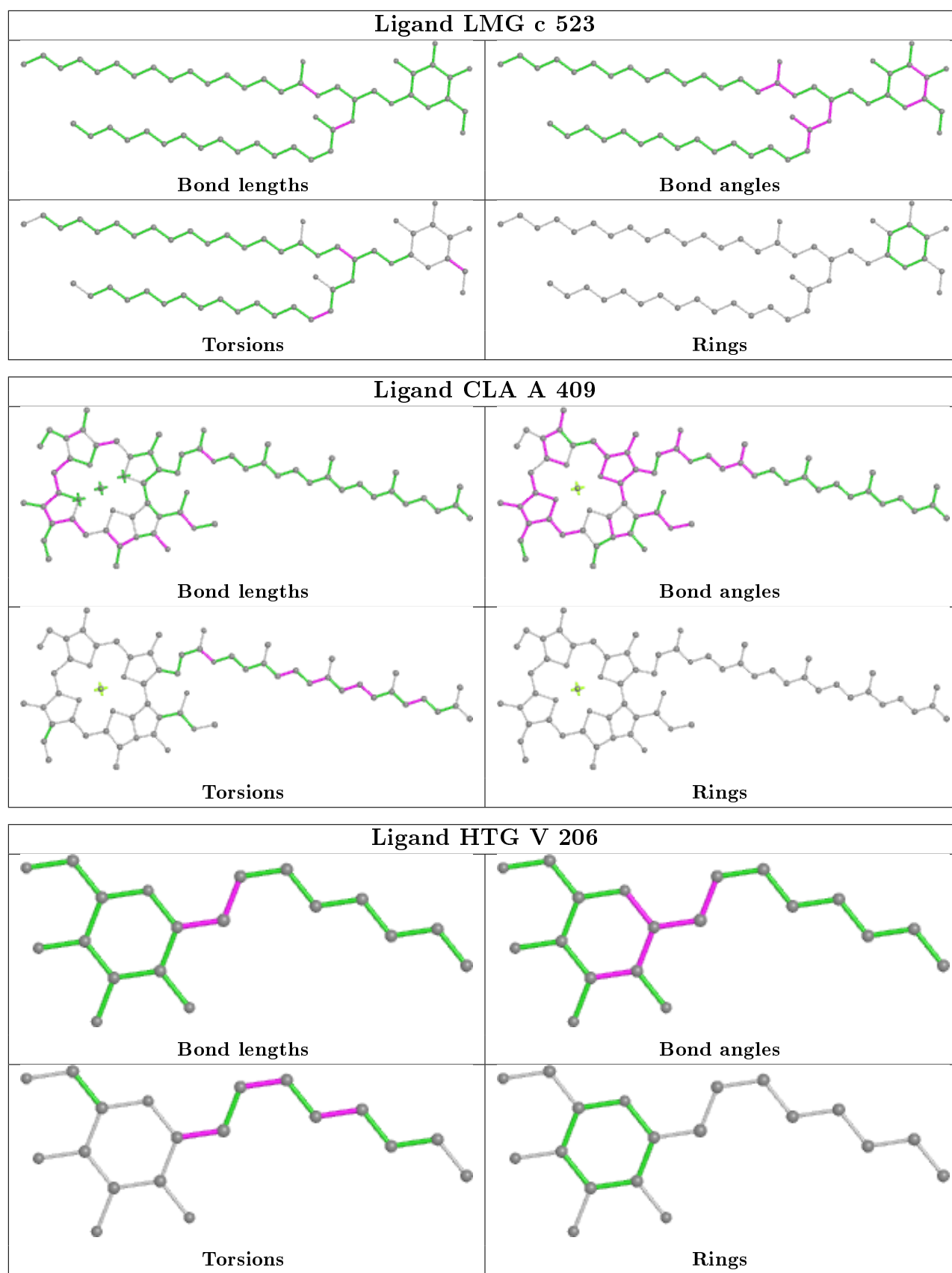


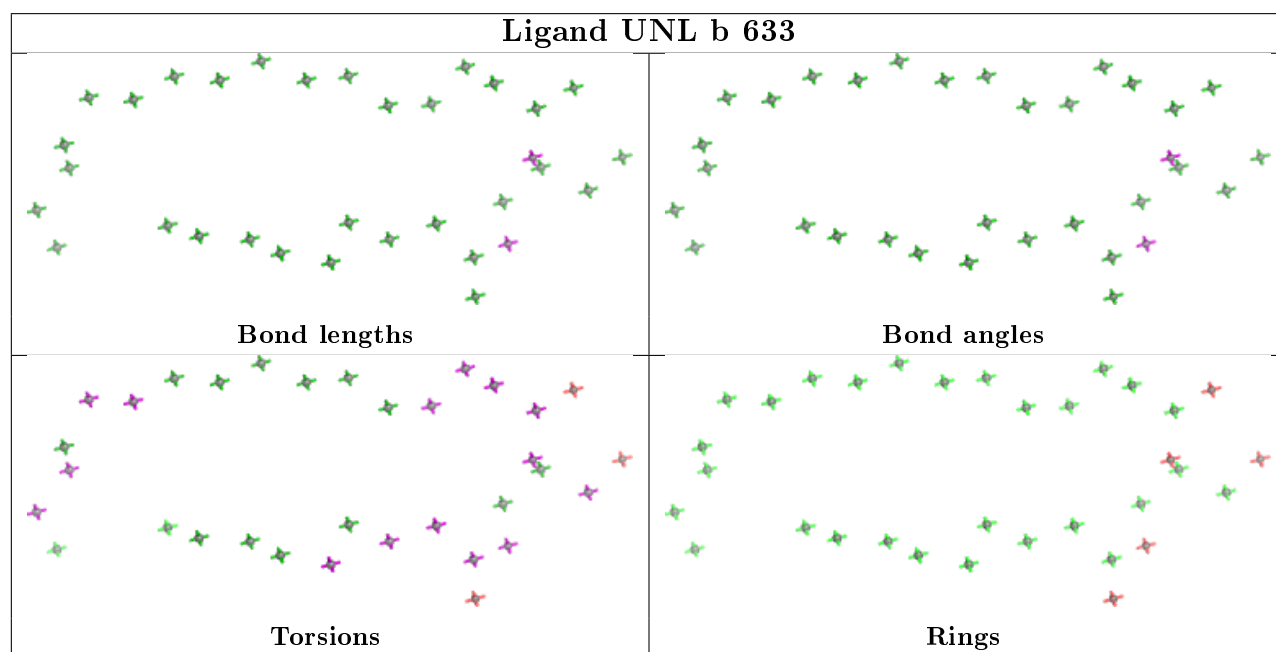
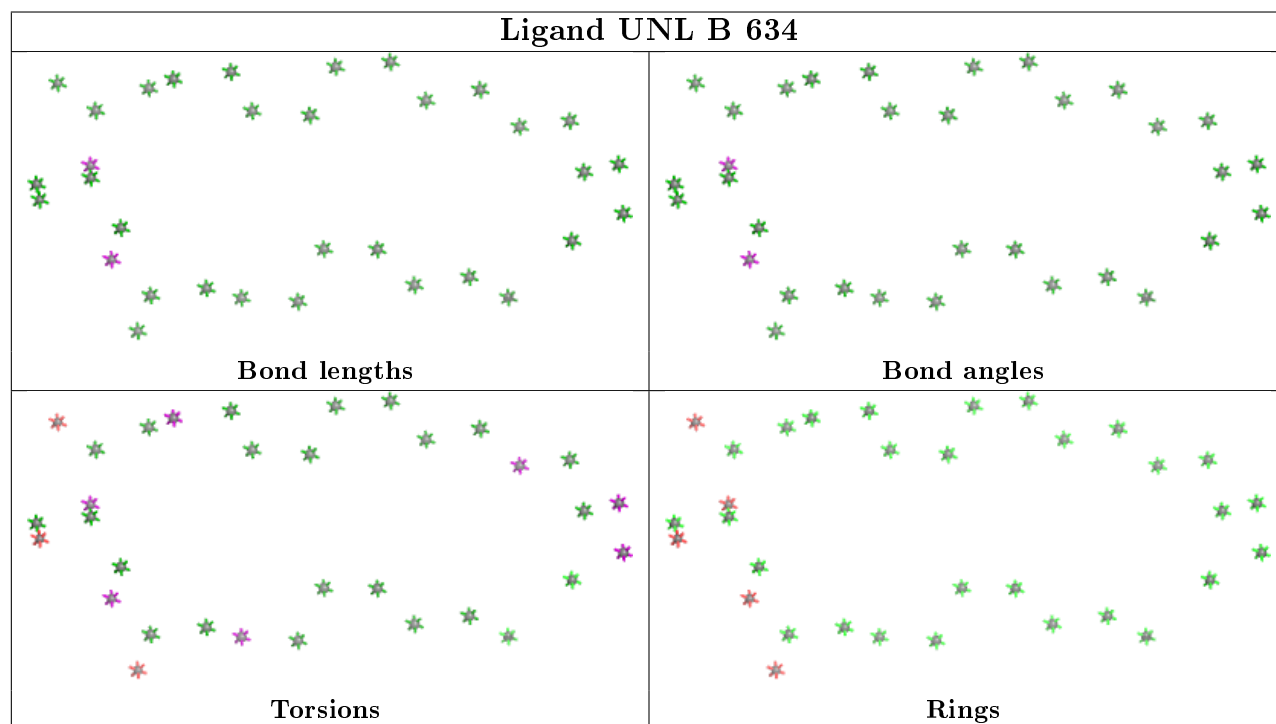
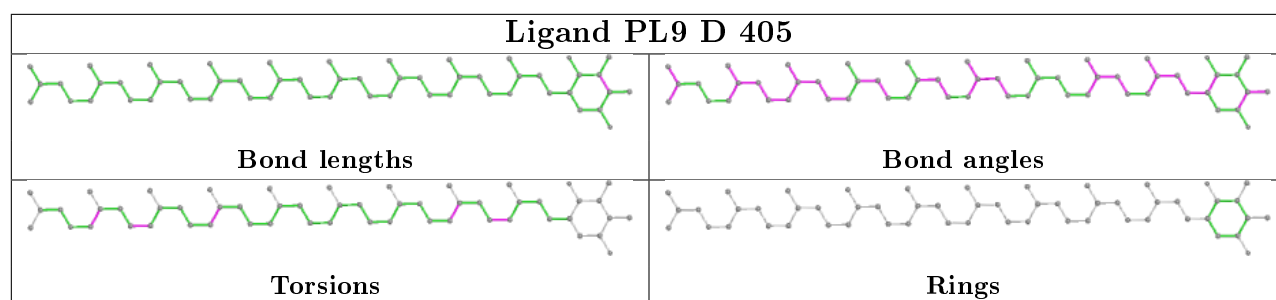
Ligand BCR h 101

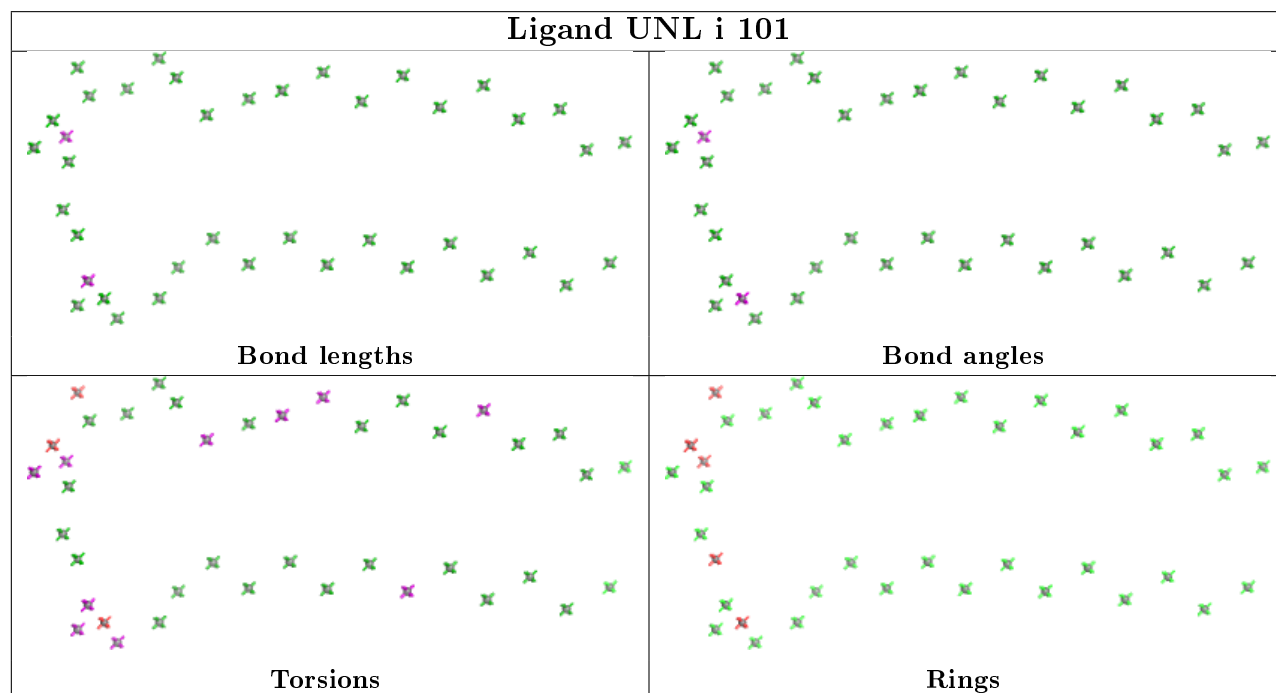
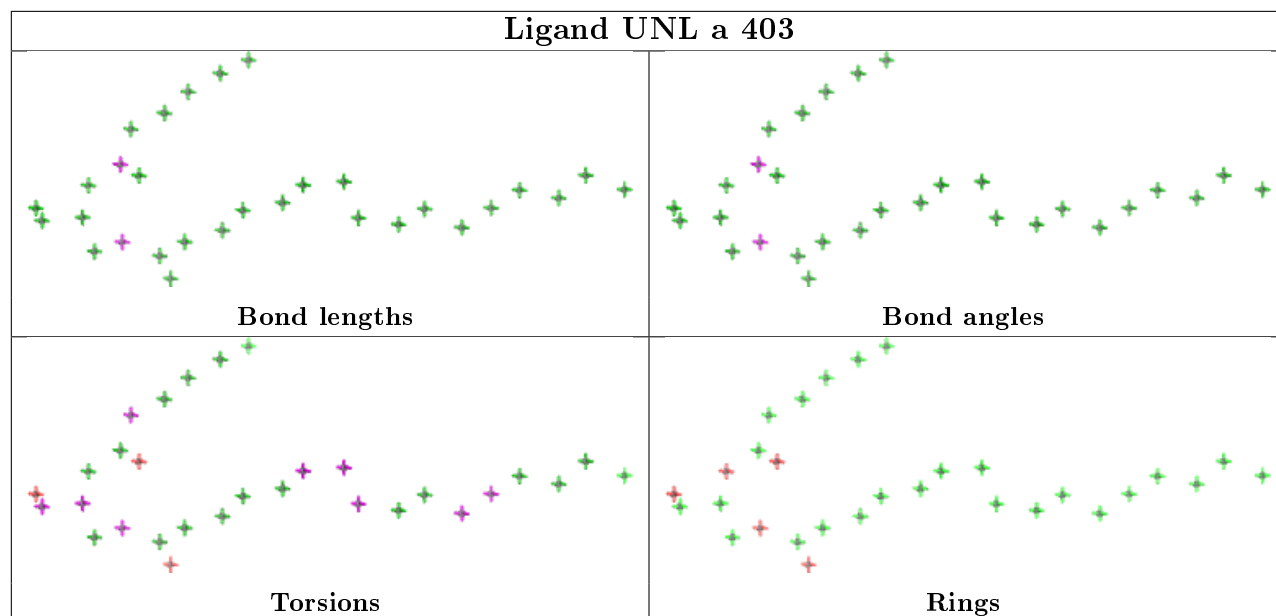


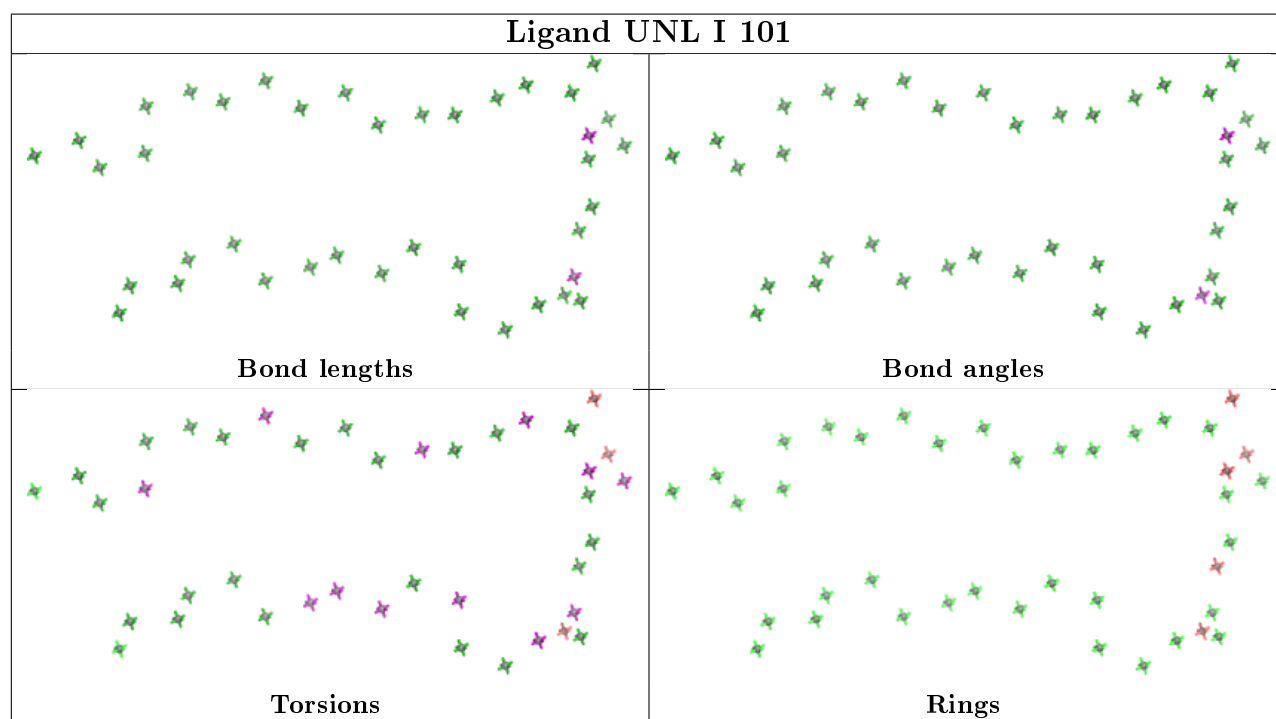
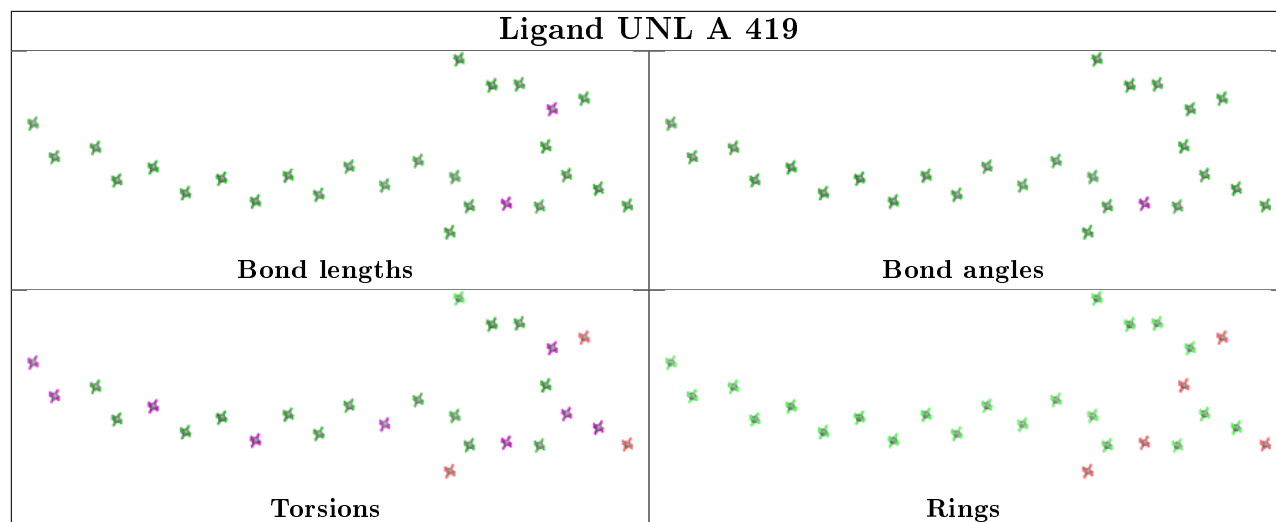
Ligand BCR k 101**Ligand CLA b 620****Ligand CLA B 614**

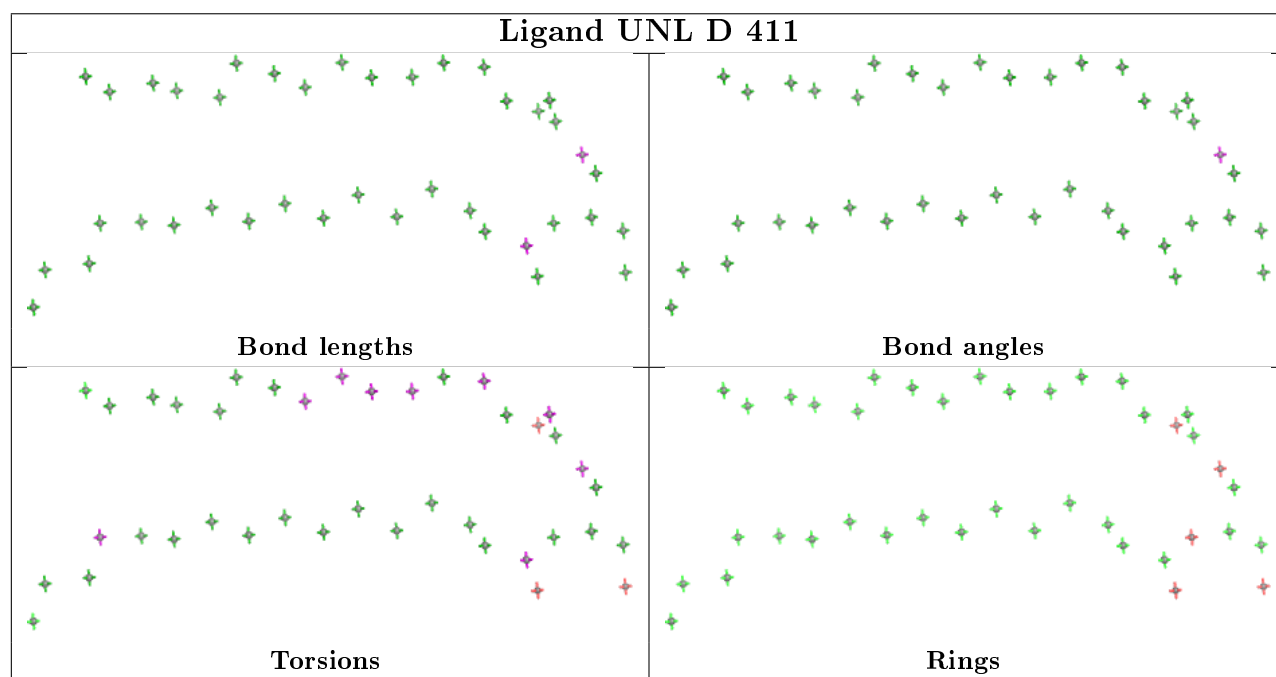
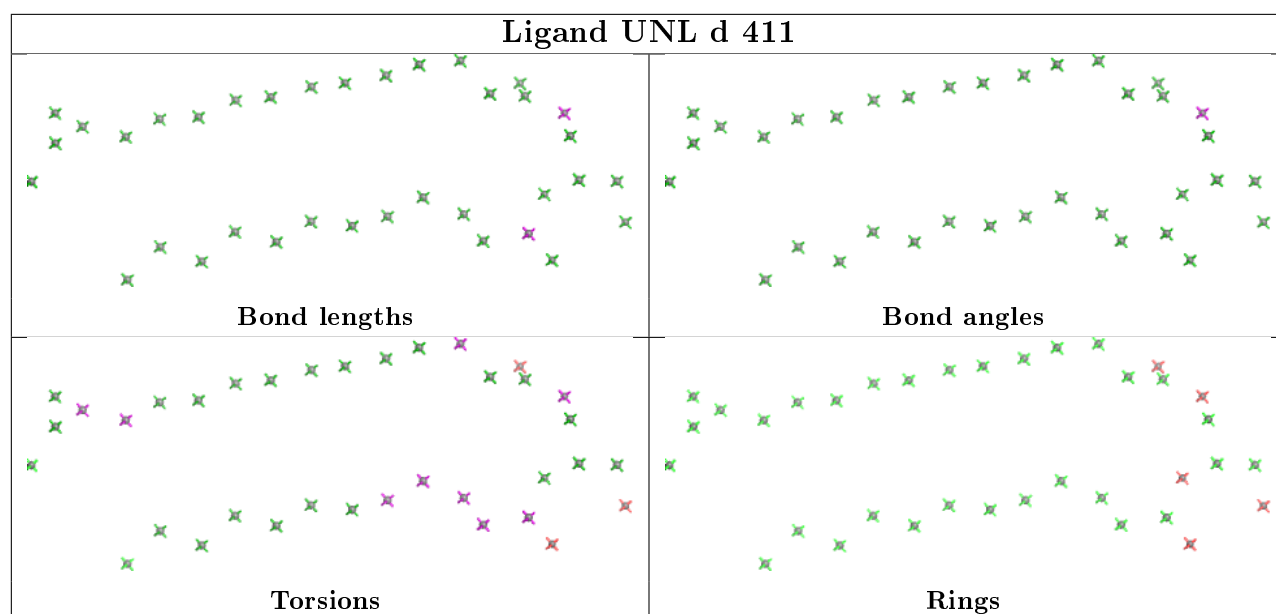


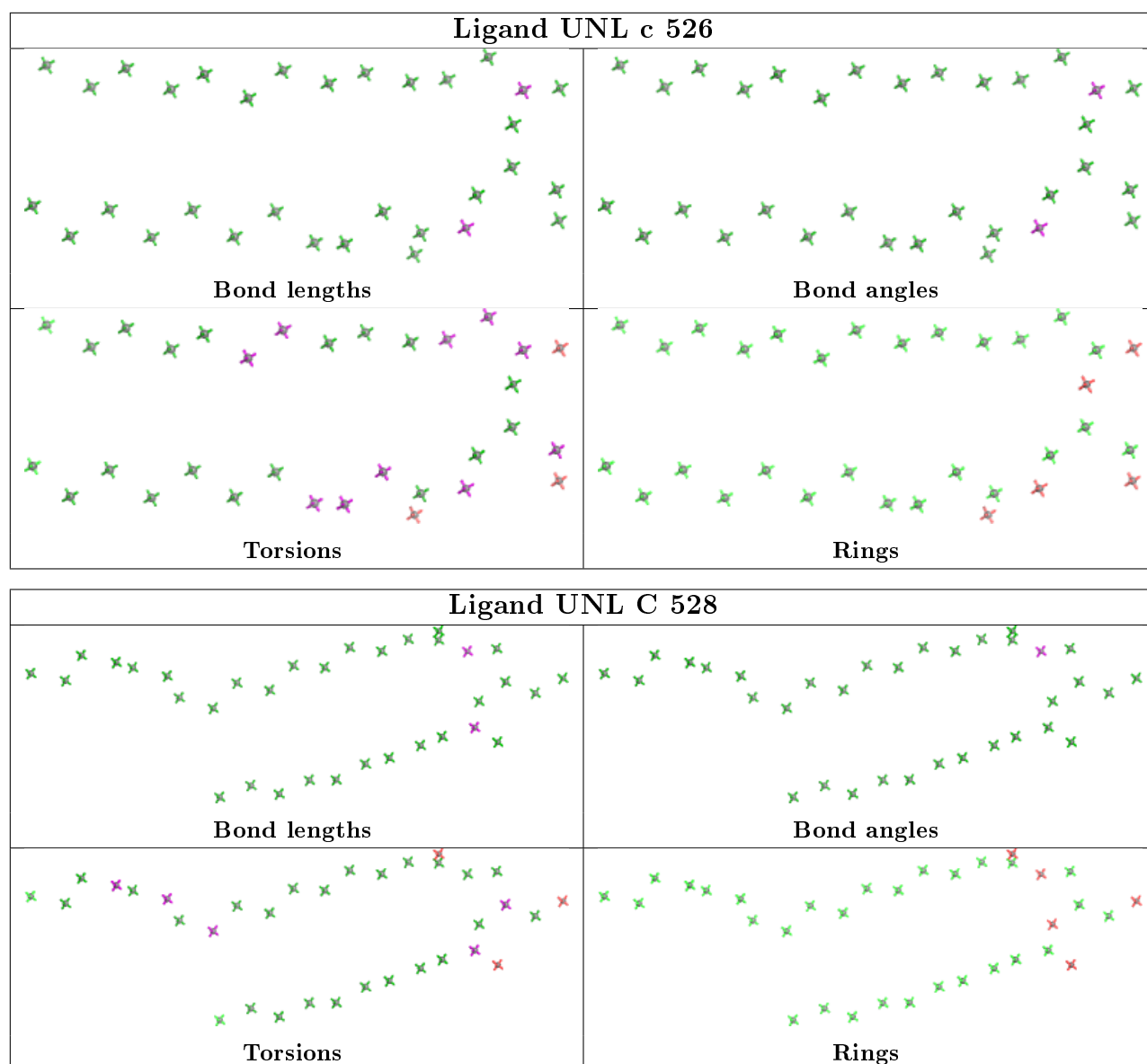












5.7 Other polymers [i](#)

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%)	0.07	2 (0%) 89 91	30, 39, 69, 112	0
1	a	334/344 (97%)	0.15	8 (2%) 59 67	31, 40, 74, 141	0
2	B	504/505 (99%)	0.11	8 (1%) 72 77	30, 44, 78, 119	0
2	b	503/505 (99%)	0.21	23 (4%) 32 42	32, 45, 83, 174	0
3	C	451/455 (99%)	0.06	2 (0%) 92 94	35, 52, 70, 120	0
3	c	455/455 (100%)	0.08	3 (0%) 87 91	37, 53, 71, 124	0
4	D	341/342 (99%)	0.05	2 (0%) 89 91	30, 41, 64, 131	0
4	d	341/342 (99%)	0.01	0 100 100	31, 42, 65, 122	0
5	E	81/84 (96%)	0.56	8 (9%) 7 11	46, 64, 95, 127	0
5	e	81/84 (96%)	0.86	9 (11%) 5 7	47, 66, 118, 172	0
6	F	34/44 (77%)	0.32	2 (5%) 22 30	46, 57, 91, 98	0
6	f	32/44 (72%)	0.35	2 (6%) 20 27	47, 57, 115, 139	0
7	H	65/65 (100%)	0.22	3 (4%) 32 42	40, 54, 71, 154	0
7	h	65/65 (100%)	0.07	2 (3%) 49 58	43, 56, 77, 165	0
8	I	37/38 (97%)	0.17	2 (5%) 25 34	43, 53, 107, 152	0
8	i	37/38 (97%)	0.19	2 (5%) 25 34	42, 53, 100, 129	0
9	J	38/39 (97%)	0.52	3 (7%) 12 17	43, 61, 133, 171	0
9	j	39/39 (100%)	0.65	5 (12%) 3 5	48, 61, 130, 168	0
10	K	37/37 (100%)	0.12	0 100 100	53, 62, 77, 105	0
10	k	37/37 (100%)	0.22	0 100 100	53, 62, 80, 105	0
11	L	37/37 (100%)	0.16	0 100 100	30, 37, 101, 123	0
11	l	37/37 (100%)	0.24	2 (5%) 25 34	31, 36, 99, 122	0
12	M	33/36 (91%)	0.27	2 (6%) 21 28	33, 38, 63, 116	0
12	m	33/36 (91%)	0.19	0 100 100	33, 38, 71, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.07	4 (1%) 72 77	32, 50, 95, 134	0
13	o	243/244 (99%)	0.08	4 (1%) 72 77	33, 51, 102, 167	0
14	T	29/32 (90%)	0.14	0 100 100	31, 38, 65, 135	0
14	t	29/32 (90%)	0.10	0 100 100	32, 38, 66, 135	0
15	U	97/104 (93%)	-0.05	0 100 100	37, 48, 75, 118	0
15	u	97/104 (93%)	-0.05	0 100 100	41, 49, 72, 118	0
16	V	137/137 (100%)	0.04	0 100 100	35, 49, 78, 121	0
16	v	137/137 (100%)	0.06	2 (1%) 73 79	40, 55, 82, 123	0
17	Y	29/30 (96%)	1.76	7 (24%) 0 0	64, 77, 135, 141	0
17	y	29/30 (96%)	0.62	2 (6%) 16 23	67, 80, 135, 142	0
18	X	39/40 (97%)	0.37	1 (2%) 56 64	53, 62, 114, 138	0
18	x	38/40 (95%)	0.63	5 (13%) 3 4	53, 62, 110, 130	0
19	Z	62/62 (100%)	0.64	6 (9%) 7 11	65, 77, 122, 164	0
19	z	62/62 (100%)	1.17	17 (27%) 0 0	68, 79, 122, 165	0
20	R	18/34 (52%)	7.25	18 (100%) 0 0	106, 139, 173, 174	0
All	All	5275/5384 (97%)	0.18	156 (2%) 50 59	30, 48, 91, 174	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Y	18	VAL	16.7
20	R	15	ALA	13.5
20	R	18	TRP	11.8
5	e	5	THR	11.8
20	R	9	LEU	10.4
20	R	6	LEU	9.5
2	b	496	TYR	9.5
2	b	494	GLY	8.8
20	R	16	ALA	8.6
2	b	495	PHE	8.5
19	z	3	ILE	8.2
17	Y	19	ILE	8.1
20	R	14	LEU	7.8
20	R	12	VAL	7.8
20	R	3	TRP	7.7
2	b	486	LEU	7.6
20	R	5	VAL	7.4

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Mol	Chain	Res	Type	RSRZ
20	R	17	GLY	7.3
9	j	1	MET	7.2
20	R	13	LEU	6.6
20	R	8	VAL	6.6
2	b	499	VAL	6.3
2	b	489	GLU	6.2
1	a	264	SER	6.1
5	e	6	GLY	6.0
19	Z	62	VAL	6.0
20	R	19	ALA	5.9
5	e	4	THR	5.9
17	Y	20	ALA	5.9
13	O	56	PRO	5.8
20	R	11	PRO	5.1
7	h	65	LEU	5.0
2	b	487	SER	5.0
2	B	479	PHE	4.9
3	C	23	ALA	4.8
2	b	493	TRP	4.8
18	x	37	VAL	4.8
19	z	62	VAL	4.7
5	E	6	GLY	4.7
13	o	58	ASN	4.7
18	x	2	THR	4.7
18	x	38	GLN	4.7
17	Y	22	LEU	4.5
19	z	32	ASP	4.4
19	Z	31	GLN	4.3
9	J	5	GLY	4.2
5	E	5	THR	4.2
1	a	262	TYR	4.1
2	b	500	GLY	4.1
2	b	504	THR	4.0
2	B	495	PHE	4.0
19	Z	33	TRP	4.0
13	o	59	LYS	3.9
19	z	5	PHE	3.9
20	R	4	ARG	3.9
9	j	3	GLU	3.9
17	y	20	ALA	3.8
17	Y	21	GLN	3.8
13	O	60	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
20	R	10	LEU	3.7
2	b	498	LYS	3.7
2	b	485	GLU	3.6
7	h	66	GLY	3.6
8	I	37	LEU	3.6
2	b	484	PRO	3.6
2	b	488	PRO	3.6
1	a	261	GLN	3.5
20	R	7	VAL	3.5
9	j	4	GLY	3.5
3	c	140	LEU	3.4
18	X	37	VAL	3.4
5	e	7	GLU	3.4
19	z	2	THR	3.4
11	l	3	PRO	3.4
20	R	2	ASP	3.3
2	b	497	GLN	3.3
5	e	10	PHE	3.3
16	v	106	ASN	3.3
5	E	4	THR	3.3
19	z	38	GLN	3.2
19	z	33	TRP	3.2
19	z	35	ARG	3.2
4	D	12	ARG	3.2
8	I	34	ARG	3.2
2	B	496	TYR	3.2
13	o	246	ALA	3.1
6	F	16	PHE	3.1
2	B	494	GLY	3.1
2	b	86[A]	ILE	3.1
13	O	62	GLU	3.1
7	H	65	LEU	3.1
6	f	16	PHE	3.0
19	Z	61	VAL	2.9
17	Y	25	ILE	2.9
5	E	83	LEU	2.9
6	f	14	PRO	2.9
1	a	265	PHE	2.9
5	e	61	ARG	2.9
2	b	503	THR	2.9
2	b	502	VAL	2.8
2	B	504	THR	2.8

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Mol	Chain	Res	Type	RSRZ
19	z	61	VAL	2.8
7	H	64	ALA	2.8
19	z	41	PHE	2.8
19	z	42	LEU	2.8
1	a	263	ALA	2.7
2	b	490	GLN	2.7
2	B	501	ASP	2.7
13	o	56	PRO	2.7
5	e	59	GLU	2.6
9	J	3	GLU	2.6
6	F	15	ILE	2.6
3	c	143	TYR	2.6
17	Y	26	ALA	2.5
19	z	28	ALA	2.5
5	E	84	LYS	2.5
2	B	486	LEU	2.5
2	b	491	VAL	2.5
1	A	12	ASN	2.5
9	j	2	SER	2.5
7	H	66	GLY	2.5
12	M	33	GLN	2.4
17	y	25	ILE	2.4
2	B	490	GLN	2.4
9	J	2	SER	2.4
2	b	85	GLY	2.4
2	b	483	ASP	2.4
5	E	79	PHE	2.4
1	A	13	LEU	2.4
1	a	260	PHE	2.4
18	x	39	ARG	2.3
3	c	50	LEU	2.3
19	z	29	SER	2.3
18	x	35	ASP	2.3
19	Z	30	PRO	2.3
3	C	145[A]	SER	2.3
5	E	19	TYR	2.2
2	b	501	ASP	2.2
9	j	5	GLY	2.2
13	O	246	ALA	2.2
1	a	252	HIS	2.2
12	M	34	LYS	2.2
19	z	4	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
19	z	39	LEU	2.1
8	i	36	ASP	2.1
5	E	82	GLN	2.1
5	e	8	ARG	2.1
19	Z	32	ASP	2.0
19	z	30	PRO	2.0
16	v	17	LYS	2.0
19	z	60	PHE	2.0
4	D	17	ILE	2.0
1	a	15	GLU	2.0
11	l	1	MET	2.0
5	e	72	ALA	2.0
8	i	37	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.95	0.11	33,38,60,72	0
12	FME	m	1	10/11	0.97	0.16	35,47,107,124	0
12	FME	M	1	10/11	0.97	0.14	33,52,85,91	0
8	FME	I	1	10/11	0.97	0.11	36,49,53,57	0
14	FME	t	1	10/11	0.97	0.11	28,40,49,83	0
8	FME	i	1	10/11	0.97	0.12	39,51,57,61	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	DGD	e	101	62/66	0.46	0.39	68,115,177,183	0
29	LMT	F	102	35/35	0.59	0.32	81,117,147,150	0
29	LMT	C	522	35/35	0.60	0.30	83,119,152,161	0
32	UNL	C	528	34/-	0.61	0.23	68,109,132,133	0
37	LHG	e	102	42/49	0.61	0.30	68,134,167,175	0
29	LMT	M	104	35/35	0.63	0.26	44,96,137,144	0
29	LMT	b	630	25/35	0.64	0.28	70,95,151,153	0
34	HTG	d	412	16/19	0.65	0.21	64,114,125,129	0
36	DGD	D	406	52/66	0.65	0.27	62,106,145,154	0
32	UNL	a	403	30/-	0.66	0.24	69,90,128,130	0
29	LMT	f	103	35/35	0.69	0.28	74,122,151,156	0
29	LMT	a	419	35/35	0.69	0.35	86,112,130,132	0
29	LMT	B	622	35/35	0.70	0.28	62,118,148,153	0
32	UNL	j	102	10/-	0.71	0.23	64,78,93,97	0
34	HTG	D	412	16/19	0.71	0.26	70,142,157,160	0
32	UNL	A	419	28/-	0.71	0.19	63,86,104,104	0
32	UNL	c	526	32/-	0.72	0.23	63,98,133,141	0
27	SQD	f	102	43/54	0.72	0.28	86,119,144,148	0
35	LMG	Z	101	37/55	0.73	0.27	50,111,133,137	0
32	UNL	J	102	10/-	0.74	0.21	47,71,94,97	0
29	LMT	m	102	35/35	0.75	0.22	35,98,128,134	0
34	HTG	B	633	19/19	0.75	0.20	53,105,137,170	0
34	HTG	c	525	19/19	0.76	0.33	56,109,121,130	0
37	LHG	E	101	42/49	0.76	0.21	67,98,120,121	0
28	GOL	V	201	6/6	0.76	0.40	69,78,89,95	0
34	HTG	b	608	19/19	0.78	0.21	56,113,148,151	0
34	HTG	B	625	19/19	0.78	0.26	72,118,144,148	0
29	LMT	M	105	35/35	0.78	0.21	41,84,106,116	0
32	UNL	B	634	33/-	0.78	0.24	57,82,136,141	0
29	LMT	a	404	35/35	0.79	0.22	44,83,115,132	0
32	UNL	b	633	33/-	0.79	0.24	41,94,159,162	0
28	GOL	v	201	6/6	0.79	0.27	71,93,96,100	0
31	PL9	a	416	55/55	0.80	0.25	64,103,126,128	0
34	HTG	C	524	19/19	0.80	0.20	82,92,128,134	0
27	SQD	L	102	54/54	0.81	0.18	46,74,126,143	0
29	LMT	M	102	35/35	0.81	0.21	41,85,110,112	0
31	PL9	A	418	55/55	0.81	0.23	56,99,114,133	0
27	SQD	B	621	54/54	0.81	0.19	52,88,144,153	0
35	LMG	C	520	51/55	0.82	0.20	50,77,108,118	0
27	SQD	A	415	54/54	0.82	0.18	48,74,114,132	0
32	UNL	m	101	10/-	0.82	0.23	54,59,86,88	0
29	LMT	A	416	35/35	0.82	0.19	40,84,106,133	0
32	UNL	i	101	40/-	0.83	0.22	49,77,144,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	UNL	M	103	10/-	0.83	0.20	48,61,72,79	0
27	SQD	a	405	54/54	0.83	0.17	43,78,123,126	0
33	CA	b	609	1/1	0.83	0.15	137,137,137,137	0
29	LMT	B	635	25/35	0.83	0.24	42,86,138,141	0
32	UNL	d	411	36/-	0.84	0.18	54,77,132,138	0
32	UNL	I	101	40/-	0.84	0.22	41,84,148,161	0
35	LMG	a	415	51/55	0.84	0.20	57,82,99,102	0
35	LMG	z	101	39/55	0.84	0.22	63,116,139,159	0
35	LMG	C	521	51/55	0.84	0.20	55,109,128,136	0
34	HTG	b	632	19/19	0.85	0.23	66,115,147,147	0
28	GOL	b	606	6/6	0.85	0.17	63,79,87,89	0
35	LMG	c	523	51/55	0.85	0.22	49,107,130,130	0
32	UNL	X	101	18/-	0.86	0.16	56,75,101,102	0
28	GOL	A	414	6/6	0.86	0.20	53,77,82,88	0
35	LMG	b	629	51/55	0.86	0.17	41,51,73,89	0
36	DGD	C	518	62/66	0.86	0.15	37,55,95,113	0
34	HTG	B	624	19/19	0.86	0.18	48,66,92,98	0
28	GOL	T	102	6/6	0.86	0.27	106,113,118,120	0
29	LMT	T	104	25/35	0.86	0.22	34,84,134,140	0
34	HTG	b	631	19/19	0.87	0.23	58,68,84,96	0
35	LMG	c	522	51/55	0.87	0.17	51,86,112,114	0
32	UNL	D	411	40/-	0.87	0.16	56,80,133,139	0
28	GOL	O	301	6/6	0.87	0.11	68,79,81,88	0
35	LMG	C	501	51/55	0.87	0.17	49,84,108,116	0
28	GOL	V	204	6/6	0.88	0.20	68,81,85,94	0
34	HTG	c	524	19/19	0.88	0.12	89,95,108,128	0
28	GOL	v	202	6/6	0.88	0.22	74,80,100,114	0
27	SQD	F	103	43/54	0.88	0.20	75,102,123,134	0
36	DGD	h	102	62/66	0.88	0.16	34,50,68,82	0
33	CA	f	104	1/1	0.89	0.07	104,104,104,104	0
28	GOL	t	102	6/6	0.89	0.44	54,82,93,98	0
35	LMG	M	101	51/55	0.89	0.17	35,52,78,95	0
28	GOL	T	101	6/6	0.89	0.41	51,78,96,104	0
28	GOL	B	630	6/6	0.89	0.29	51,67,75,83	0
24	CLA	c	517	65/65	0.89	0.17	57,80,96,104	0
33	CA	F	104	1/1	0.89	0.07	84,84,84,84	0
28	GOL	B	636	6/6	0.89	0.13	48,57,65,65	0
33	CA	B	601	1/1	0.89	0.10	143,143,143,143	0
32	UNL	d	413	18/-	0.89	0.18	52,71,109,110	0
24	CLA	C	514	65/65	0.89	0.17	51,65,99,109	0
28	GOL	c	502	6/6	0.89	0.41	75,86,99,108	0
36	DGD	H	102	62/66	0.90	0.16	32,49,69,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CL	v	204	1/1	0.90	0.08	94,94,94,94	0
28	GOL	A	412	6/6	0.90	0.14	43,50,53,61	0
27	SQD	A	411	54/54	0.90	0.17	45,78,99,103	0
36	DGD	c	520	62/66	0.90	0.15	38,55,107,128	0
34	HTG	B	632	19/19	0.90	0.14	48,69,99,103	0
24	CLA	c	511	65/65	0.91	0.14	42,55,70,76	0
28	GOL	C	525	6/6	0.91	0.25	54,60,75,81	0
27	SQD	a	414	54/54	0.91	0.15	49,79,106,110	0
34	HTG	b	607	19/19	0.91	0.15	46,75,81,82	0
36	DGD	c	521	62/66	0.91	0.15	38,52,94,99	0
37	LHG	D	407	49/49	0.91	0.19	31,49,67,73	0
36	DGD	C	519	62/66	0.91	0.14	36,48,73,86	0
34	HTG	V	206	19/19	0.91	0.23	61,91,114,204	0
28	GOL	a	402	6/6	0.92	0.24	73,83,89,92	0
34	HTG	B	623	19/19	0.92	0.15	40,54,75,76	0
35	LMG	j	101	51/55	0.92	0.16	46,58,105,117	0
24	CLA	b	618	65/65	0.92	0.14	36,48,60,71	0
24	CLA	C	507	65/65	0.92	0.14	46,64,107,116	0
24	CLA	b	616	65/65	0.92	0.14	24,36,48,52	0
28	GOL	A	413	6/6	0.92	0.27	51,54,63,67	0
34	HTG	C	523	19/19	0.92	0.15	72,86,102,106	0
35	LMG	J	101	51/55	0.92	0.17	38,58,111,127	0
24	CLA	C	505	65/65	0.92	0.15	34,48,82,94	0
28	GOL	o	301	6/6	0.93	0.18	71,80,88,106	0
24	CLA	b	615	65/65	0.93	0.14	31,45,89,103	0
24	CLA	C	502	65/65	0.93	0.13	38,51,77,91	0
24	CLA	B	602	65/65	0.93	0.15	43,60,100,128	0
24	CLA	C	508	65/65	0.93	0.14	42,54,68,76	0
24	CLA	b	625	65/65	0.93	0.14	35,54,102,112	0
28	GOL	B	628	6/6	0.93	0.14	52,71,84,87	0
36	DGD	c	519	62/66	0.93	0.13	38,48,98,105	0
24	CLA	c	510	65/65	0.93	0.13	44,63,92,115	0
28	GOL	f	101	6/6	0.93	0.21	76,84,86,91	0
24	CLA	c	512	65/65	0.93	0.13	36,49,116,129	0
37	LHG	d	408	49/49	0.93	0.17	32,41,57,86	0
37	LHG	l	101	49/49	0.93	0.16	37,46,58,66	0
26	BCR	b	627	40/40	0.93	0.15	31,41,60,69	0
37	LHG	D	409	49/49	0.93	0.18	36,54,115,128	0
34	HTG	b	601	19/19	0.93	0.12	40,50,74,83	0
28	GOL	B	626	6/6	0.93	0.17	44,52,59,85	0
24	CLA	c	507	65/65	0.93	0.14	41,53,65,83	0
24	CLA	b	611	65/65	0.93	0.15	33,45,55,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	512	65/65	0.93	0.13	41,57,68,83	0
32	UNL	d	410	17/-	0.93	0.18	48,69,97,101	0
24	CLA	D	403	65/65	0.94	0.14	38,52,104,119	0
24	CLA	C	504	65/65	0.94	0.14	39,50,60,64	0
24	CLA	b	623	65/65	0.94	0.14	27,41,88,115	0
24	CLA	c	505	65/65	0.94	0.12	42,55,66,70	0
28	GOL	b	605	6/6	0.94	0.23	67,80,108,110	0
37	LHG	d	409	49/49	0.94	0.18	34,55,108,115	0
36	DGD	C	517	62/66	0.94	0.14	32,47,94,98	0
26	BCR	y	101	40/40	0.94	0.14	44,61,74,84	0
24	CLA	C	513	65/65	0.94	0.11	46,63,85,92	0
24	CLA	c	509	65/65	0.94	0.13	36,47,70,78	0
24	CLA	B	603	65/65	0.94	0.13	33,44,51,54	0
24	CLA	c	514	65/65	0.94	0.12	41,53,63,77	0
24	CLA	C	509	65/65	0.94	0.13	36,50,110,126	0
24	CLA	b	610	65/65	0.94	0.15	43,69,104,133	0
24	CLA	B	614	65/65	0.94	0.14	26,37,63,84	0
37	LHG	L	101	49/49	0.94	0.16	31,44,56,61	0
32	UNL	D	410	17/-	0.94	0.15	37,68,83,91	0
24	CLA	B	615	65/65	0.94	0.14	27,41,91,103	0
26	BCR	c	527	40/40	0.94	0.12	57,74,86,89	0
28	GOL	B	629	6/6	0.94	0.14	48,57,63,72	0
24	CLA	b	620	65/65	0.94	0.13	28,40,52,59	0
24	CLA	B	610	65/65	0.94	0.14	34,47,56,66	0
24	CLA	c	515	65/65	0.94	0.13	43,54,75,87	0
24	CLA	c	508	65/65	0.94	0.13	38,55,73,80	0
24	CLA	B	607	65/65	0.94	0.14	31,43,93,105	0
24	CLA	c	516	65/65	0.94	0.13	47,65,83,91	0
26	BCR	T	103	40/40	0.95	0.12	28,47,64,68	0
37	LHG	d	407	49/49	0.95	0.17	37,51,64,71	0
26	BCR	B	620	40/40	0.95	0.14	32,46,59,65	0
26	BCR	d	405	40/40	0.95	0.15	40,55,77,83	0
28	GOL	v	203	6/6	0.95	0.19	47,53,61,71	0
24	CLA	b	612	65/65	0.95	0.13	34,44,57,62	0
24	CLA	A	405	65/65	0.95	0.15	25,33,49,67	0
26	BCR	C	515	40/40	0.95	0.13	49,65,78,83	0
31	PL9	d	406	55/55	0.95	0.15	26,38,48,58	0
24	CLA	c	513	65/65	0.95	0.13	42,54,74,88	0
24	CLA	B	616	65/65	0.95	0.13	34,47,65,76	0
24	CLA	C	510	65/65	0.95	0.14	41,54,76,80	0
37	LHG	D	408	49/49	0.95	0.16	27,42,64,86	0
26	BCR	K	101	40/40	0.95	0.14	43,55,63,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	GOL	V	203	6/6	0.95	0.14	59,61,61,68	0
24	CLA	d	404	65/65	0.95	0.13	37,52,101,114	0
24	CLA	b	617	65/65	0.95	0.13	34,45,55,58	0
26	BCR	H	101	40/40	0.95	0.13	36,51,67,73	0
26	BCR	D	404	40/40	0.95	0.14	38,51,93,99	0
24	CLA	B	608	65/65	0.95	0.14	24,36,50,55	0
26	BCR	k	101	40/40	0.95	0.15	45,62,73,75	0
24	CLA	b	621	65/65	0.95	0.13	29,42,50,56	0
24	CLA	b	614	65/65	0.95	0.14	29,39,49,58	0
31	PL9	D	405	55/55	0.95	0.16	26,38,51,69	0
28	GOL	F	101	6/6	0.95	0.21	70,74,77,77	0
24	CLA	b	624	65/65	0.95	0.12	34,46,60,73	0
28	GOL	V	202	6/6	0.95	0.14	40,47,51,59	0
24	CLA	d	402	65/65	0.95	0.13	27,35,43,55	0
24	CLA	a	409	65/65	0.95	0.14	28,35,51,55	0
38	HEM	e	103	43/43	0.96	0.17	55,78,123,153	0
24	CLA	d	403	65/65	0.96	0.14	27,38,59,62	0
26	BCR	c	518	40/40	0.96	0.14	40,55,67,69	0
26	BCR	Y	101	40/40	0.96	0.12	44,60,69,71	0
24	CLA	a	412	65/65	0.96	0.14	32,48,114,123	0
24	CLA	B	612	65/65	0.96	0.15	26,37,51,59	0
24	CLA	b	622	65/65	0.96	0.14	26,39,55,61	0
24	CLA	C	511	65/65	0.96	0.12	39,49,62,82	0
24	CLA	B	606	65/65	0.96	0.13	29,40,53,64	0
24	CLA	B	611	65/65	0.96	0.14	36,47,54,68	0
33	CA	o	302	1/1	0.96	0.07	91,91,91,91	0
26	BCR	t	101	40/40	0.96	0.14	31,46,62,64	0
25	PHO	A	408	64/64	0.96	0.14	29,42,52,56	0
26	BCR	B	619	40/40	0.96	0.15	29,41,56,60	0
24	CLA	c	506	65/65	0.96	0.13	39,54,67,74	0
24	CLA	B	605	65/65	0.96	0.13	26,37,70,75	0
23	BCT	A	404	4/4	0.96	0.13	52,54,73,86	0
24	CLA	B	604	65/65	0.96	0.13	34,44,53,61	0
22	CL	U	201	1/1	0.96	0.17	92,92,92,92	0
24	CLA	B	613	65/65	0.96	0.12	28,38,48,55	0
28	GOL	b	603	6/6	0.96	0.17	47,56,83,87	0
24	CLA	C	506	65/65	0.96	0.13	36,48,70,73	0
26	BCR	h	101	40/40	0.96	0.11	42,56,70,74	0
28	GOL	a	401	6/6	0.96	0.26	51,66,70,85	0
28	GOL	B	627	6/6	0.96	0.19	47,62,83,99	0
25	PHO	D	401	64/64	0.96	0.13	25,35,41,43	0
24	CLA	A	406	65/65	0.96	0.14	24,34,44,58	0

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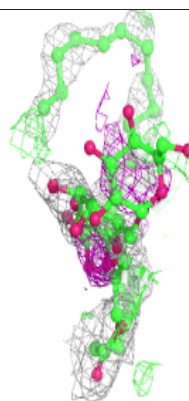
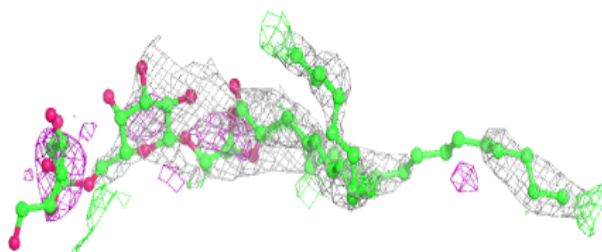
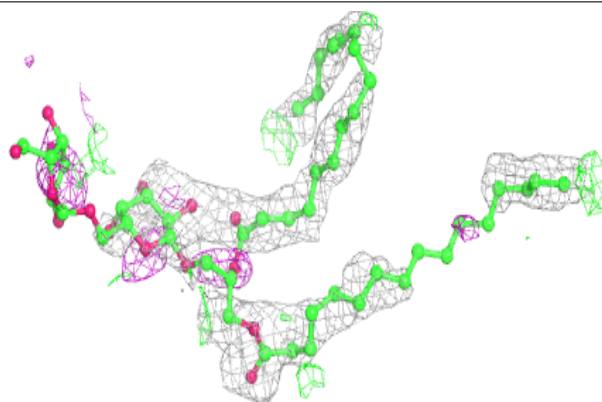
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	B	609	65/65	0.96	0.15	32,43,56,58	0
25	PHO	d	401	64/64	0.96	0.14	29,42,50,56	0
24	CLA	b	613	65/65	0.96	0.13	26,38,73,79	0
24	CLA	A	409	65/65	0.96	0.12	33,47,119,128	0
24	CLA	b	619	65/65	0.96	0.13	36,46,56,60	0
24	CLA	B	617	65/65	0.96	0.15	36,52,114,120	0
26	BCR	A	410	40/40	0.97	0.14	30,39,45,50	0
24	CLA	A	407	65/65	0.97	0.13	28,40,98,118	0
24	CLA	C	503	65/65	0.97	0.13	37,46,61,71	0
24	CLA	a	410	65/65	0.97	0.14	31,41,105,116	0
26	BCR	b	628	40/40	0.97	0.14	39,50,66,77	0
33	CA	O	302	1/1	0.97	0.04	84,84,84,84	0
28	GOL	b	602	6/6	0.97	0.21	56,60,69,93	0
28	GOL	b	604	6/6	0.97	0.21	60,73,79,90	0
26	BCR	B	618	40/40	0.97	0.15	27,40,47,52	0
28	GOL	B	631	6/6	0.97	0.29	40,73,74,83	0
26	BCR	C	516	40/40	0.97	0.15	39,54,64,65	0
25	PHO	a	411	64/64	0.97	0.14	28,36,44,47	0
38	HEM	E	102	43/43	0.97	0.14	44,64,81,93	0
24	CLA	D	402	65/65	0.97	0.14	24,35,54,58	0
26	BCR	a	413	40/40	0.97	0.12	30,41,52,56	0
26	BCR	b	626	40/40	0.97	0.15	30,42,49,49	0
33	CA	c	504	1/1	0.98	0.05	74,74,74,74	0
39	MG	j	103	1/1	0.98	0.18	57,57,57,57	0
38	HEM	v	205	43/43	0.98	0.12	42,52,61,62	0
38	HEM	V	205	43/43	0.98	0.11	35,41,50,53	0
23	BCT	a	418	4/4	0.98	0.17	60,63,70,83	0
22	CL	A	402	1/1	0.99	0.13	32,32,32,32	0
39	MG	J	103	1/1	0.99	0.08	53,53,53,53	0
33	CA	C	527	1/1	0.99	0.07	67,67,67,67	0
22	CL	a	408	1/1	0.99	0.11	41,41,41,41	0
33	CA	c	503	1/1	0.99	0.07	66,66,66,66	0
28	GOL	C	526	6/6	0.99	0.12	33,42,47,49	0
28	GOL	c	501	6/6	0.99	0.13	43,45,47,48	0
30	OEX	A	417	10/10	0.99	0.12	33,36,47,71	0
21	FE2	A	401	1/1	0.99	0.16	51,51,51,51	0
30	OEX	a	417	10/10	0.99	0.12	32,40,64,67	0
22	CL	A	403	1/1	0.99	0.11	35,35,35,35	0
21	FE2	a	406	1/1	0.99	0.18	49,49,49,49	0
22	CL	a	407	1/1	1.00	0.09	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

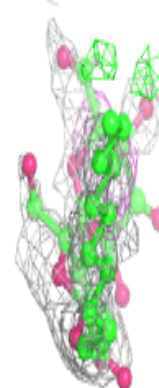
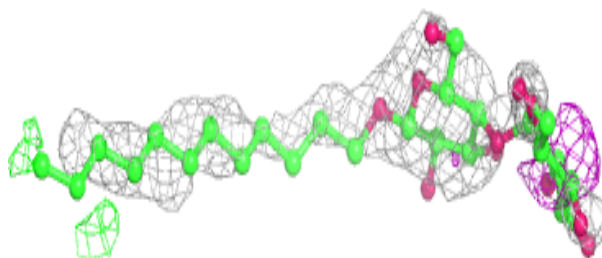
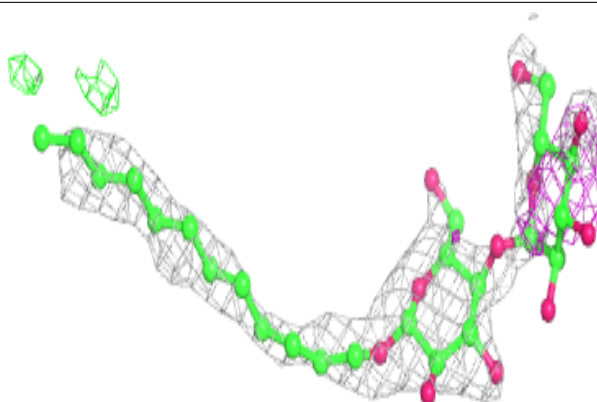
Electron density around DGD e 101:

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



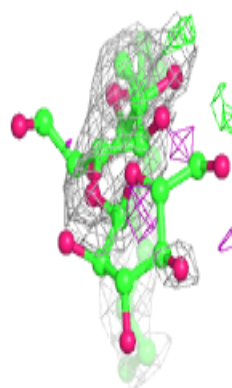
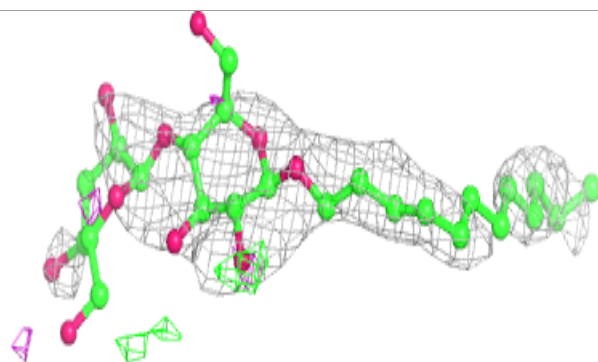
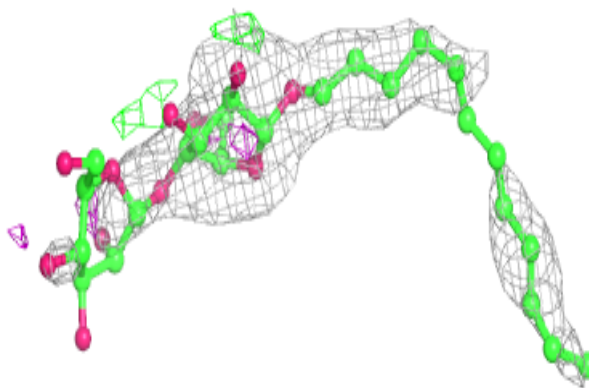
Electron density around LMT F 102:

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

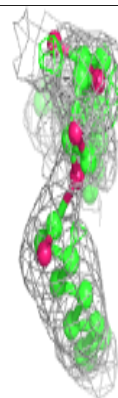
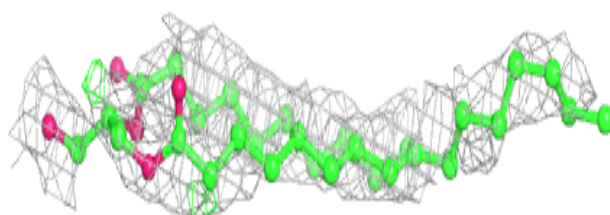
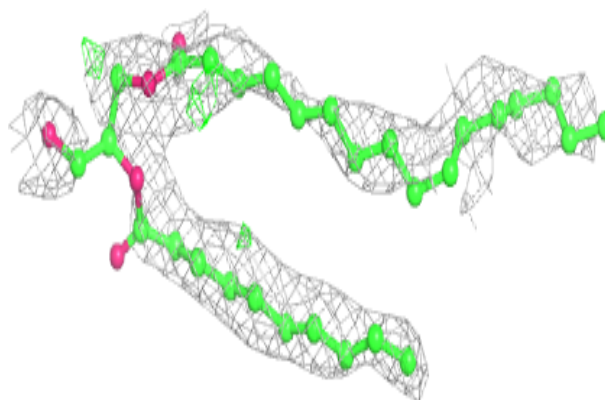


Electron density around LMT C 522:

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

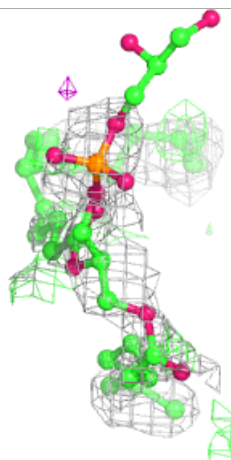
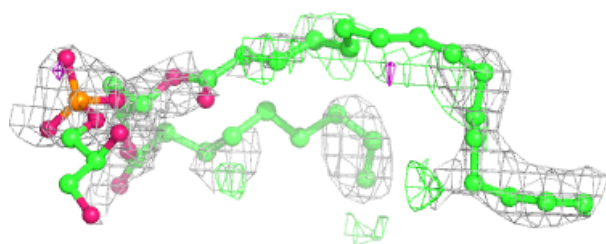
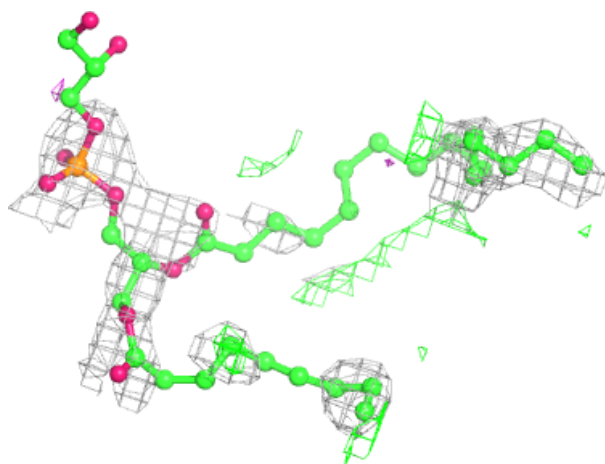
**Electron density around UNL C 528:**

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



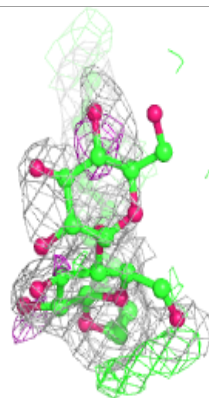
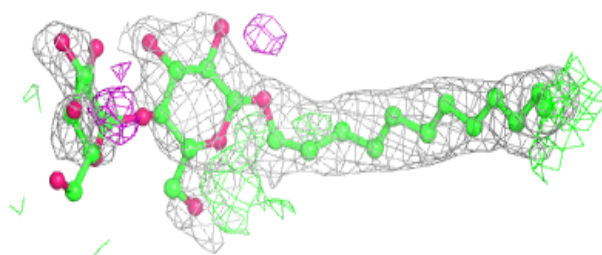
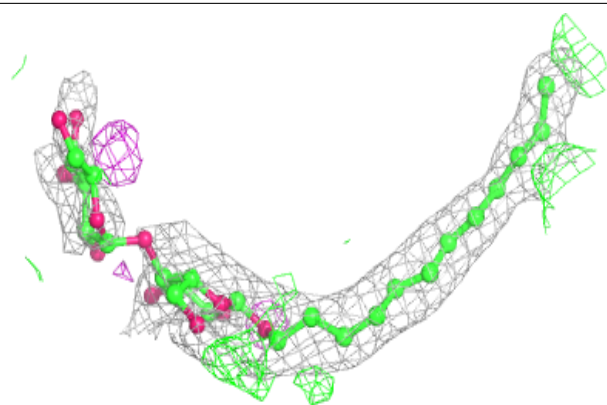
Electron density around LHG e 102:

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

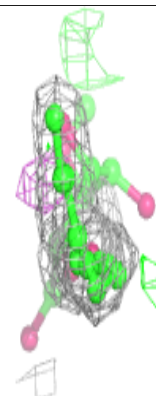
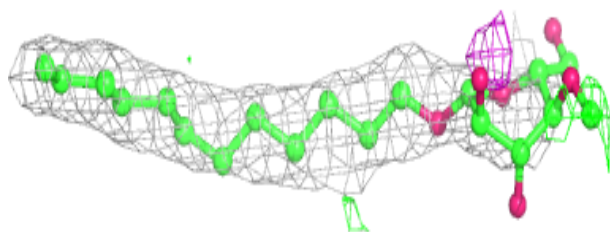
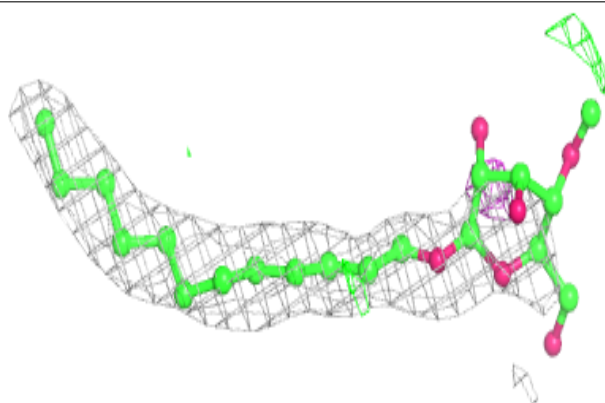


Electron density around LMT M 104:

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

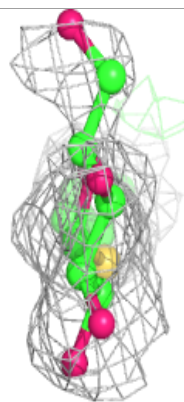
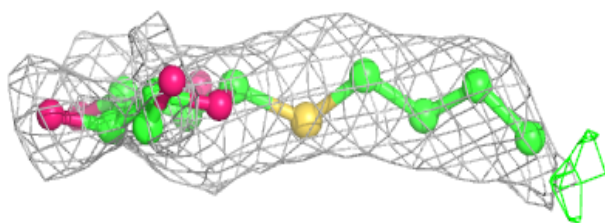
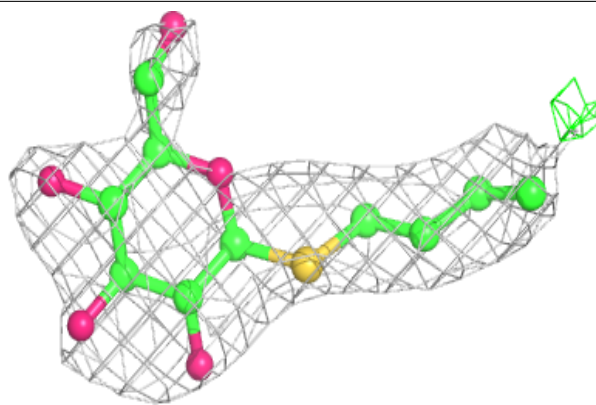
**Electron density around LMT b 630:**

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

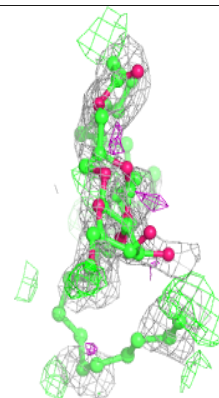
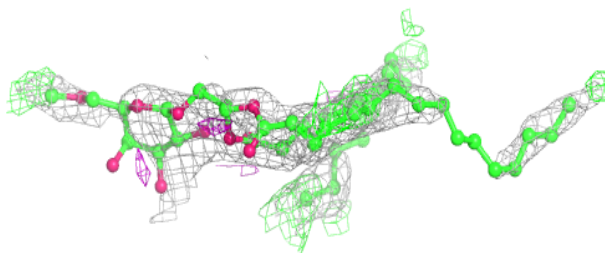
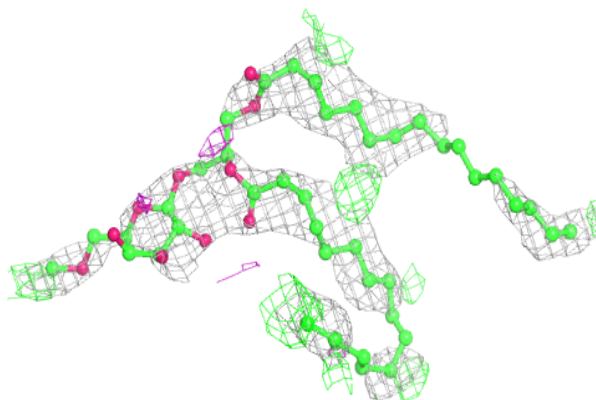


Electron density around HTG d 412:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

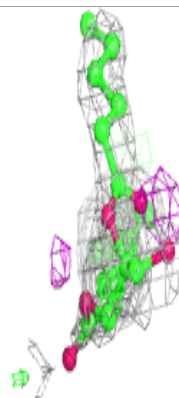
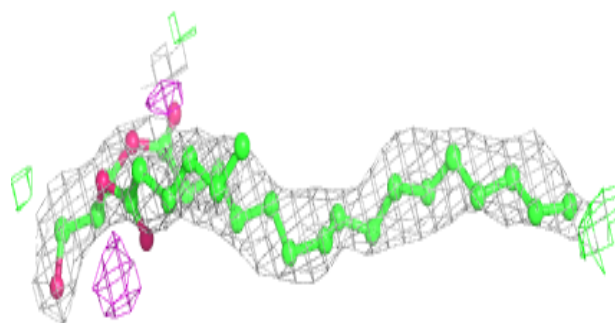
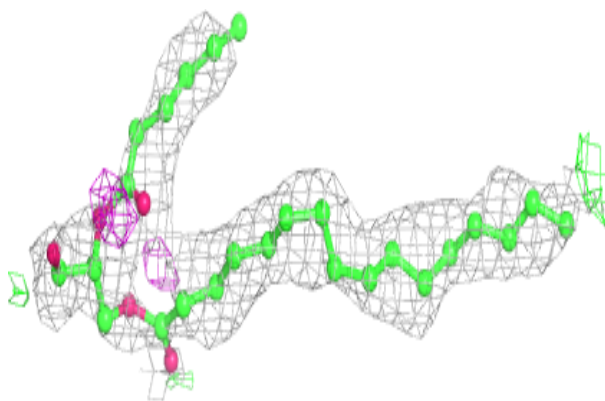
**Electron density around DGD D 406:**

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

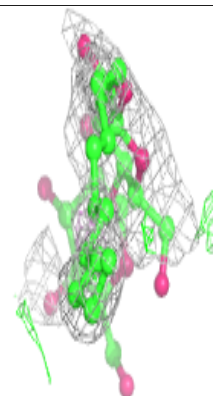
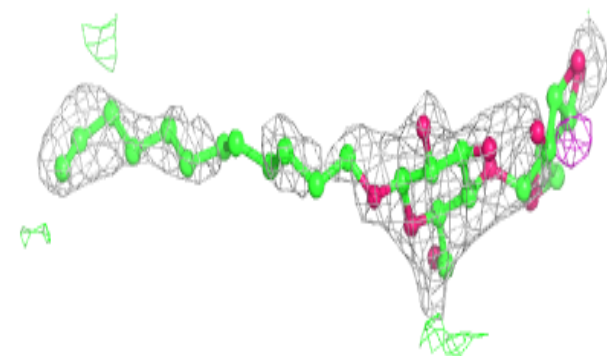
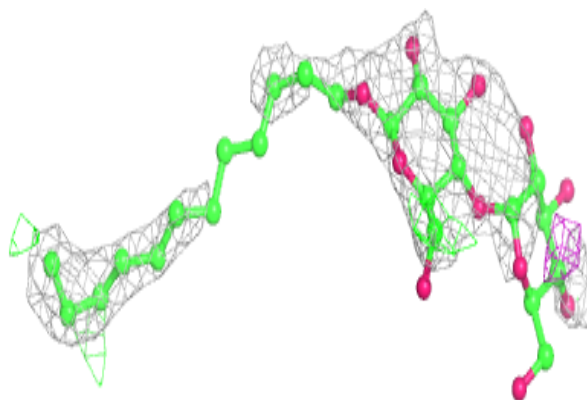


Electron density around UNL a 403:

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

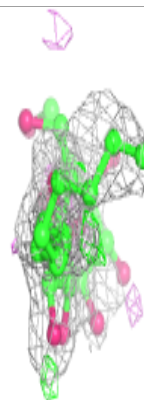
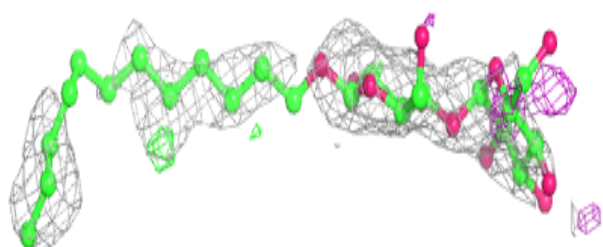
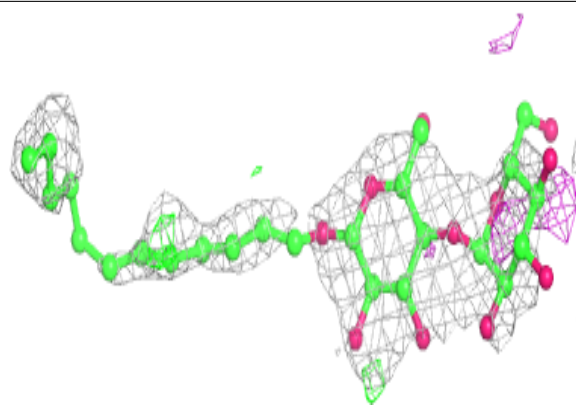
**Electron density around LMT f 103:**

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

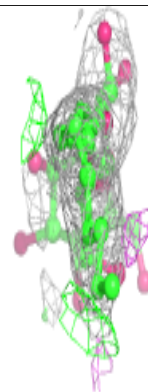
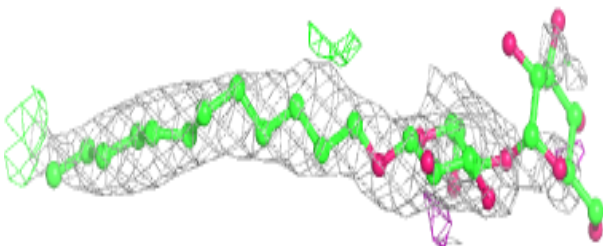
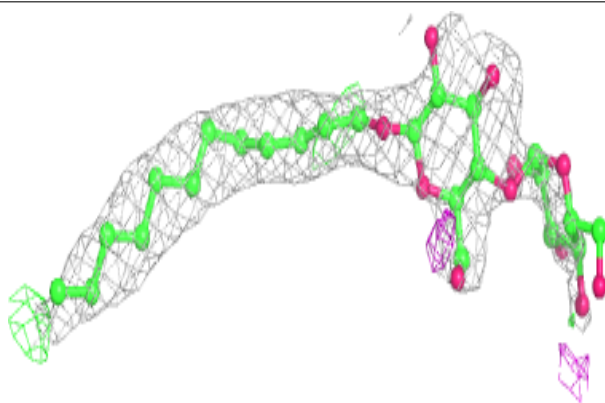


Electron density around LMT a 419:

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

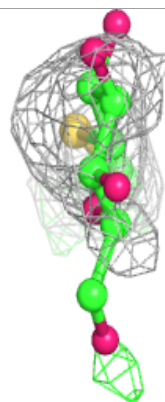
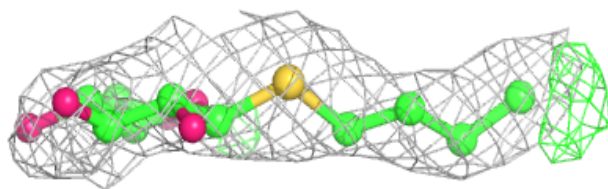
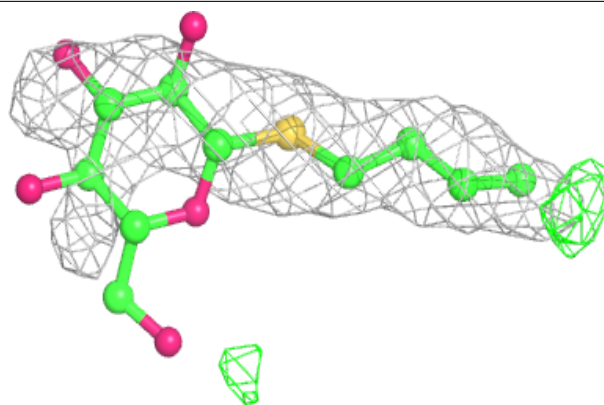
**Electron density around LMT B 622:**

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

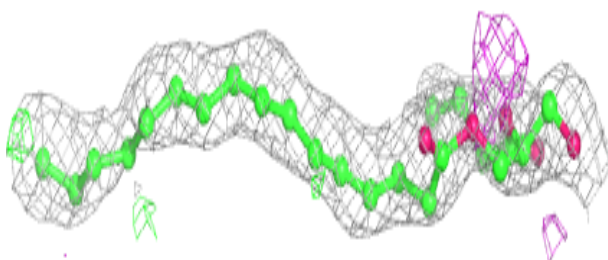
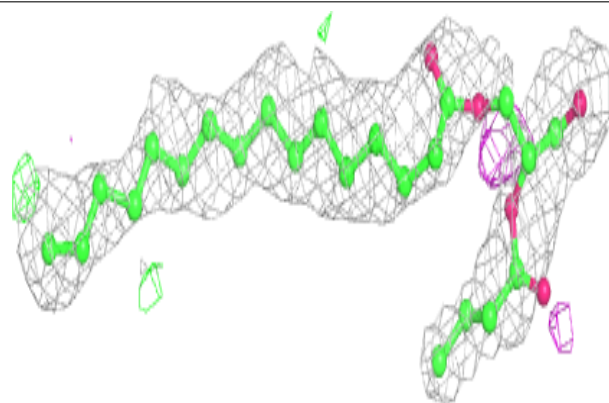


Electron density around HTG D 412:

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

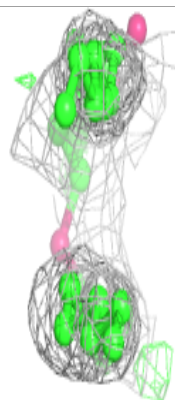
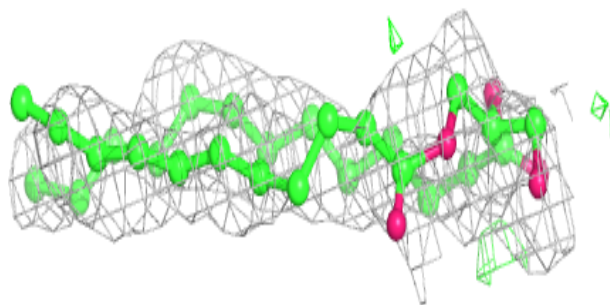
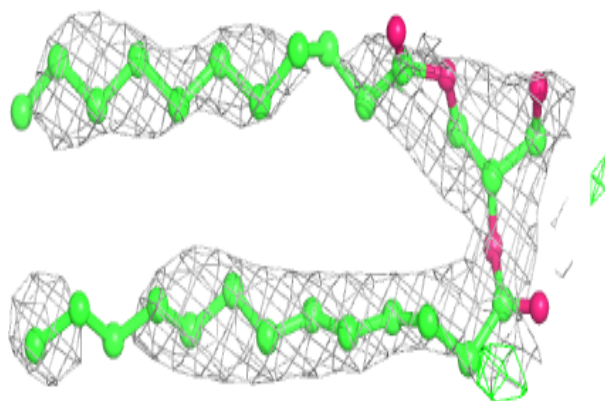
**Electron density around UNL A 419:**

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

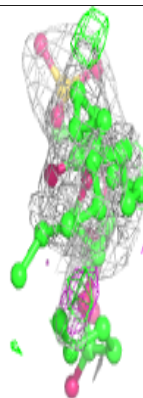
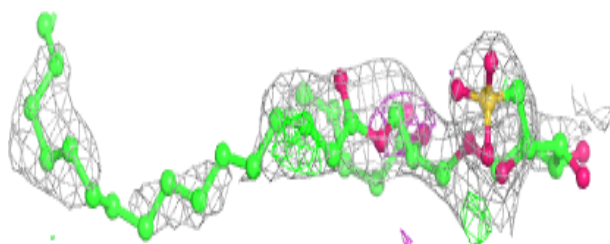
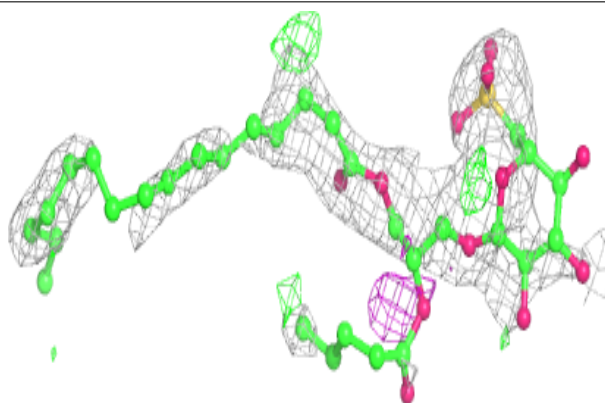


Electron density around UNL c 526:

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

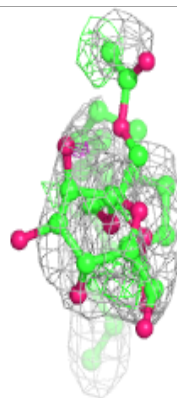
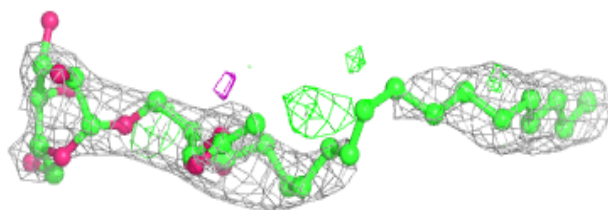
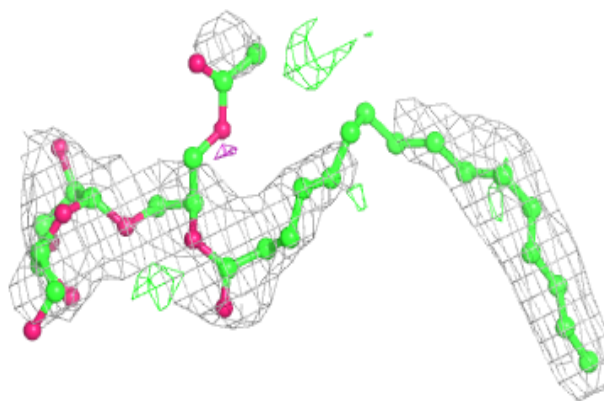
**Electron density around SQD f 102:**

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

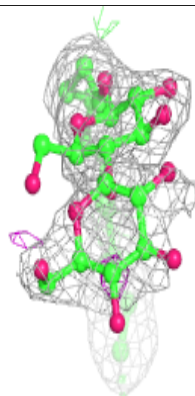
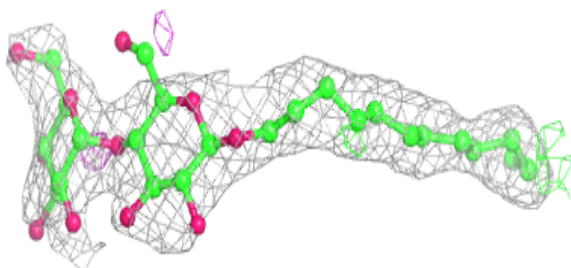
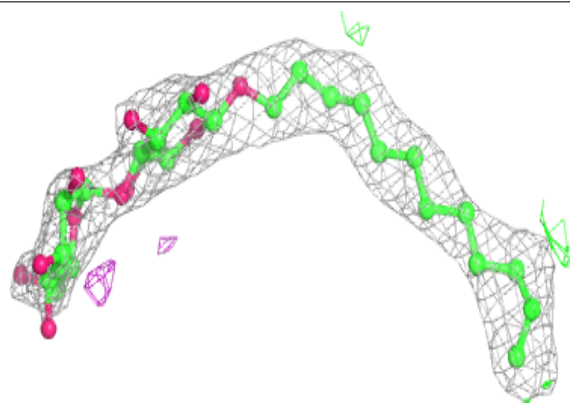


Electron density around LMG Z 101:

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

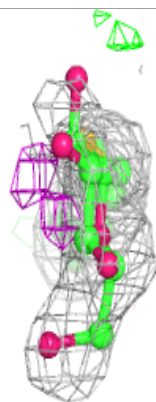
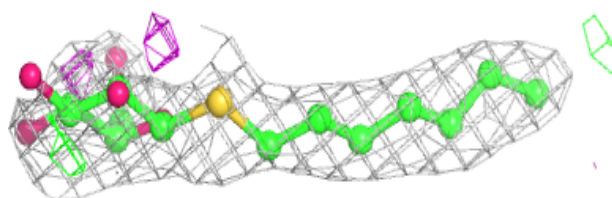
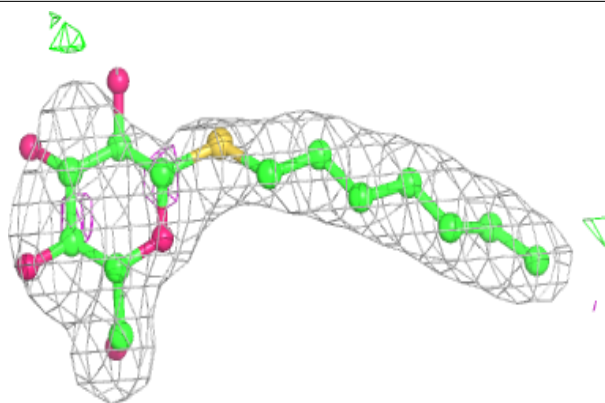
**Electron density around LMT m 102:**

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

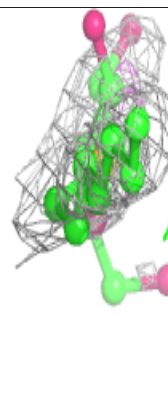
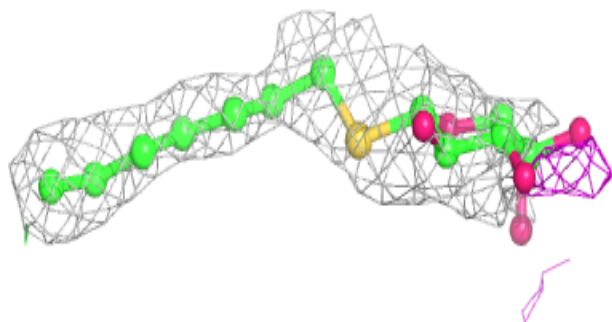
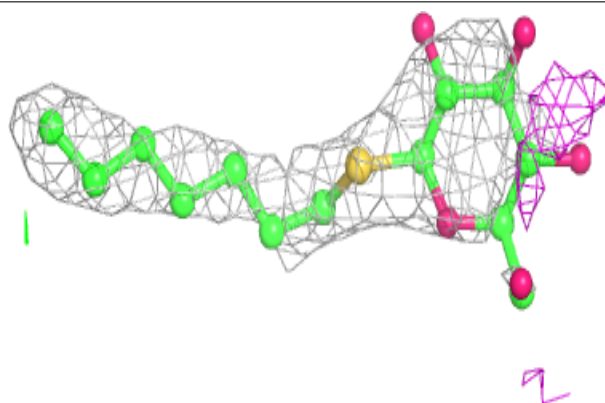


Electron density around HTG B 633:

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

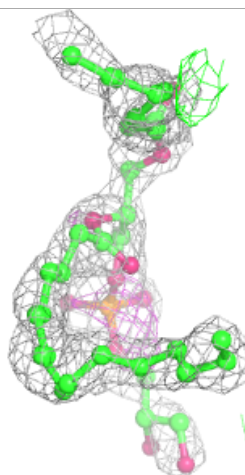
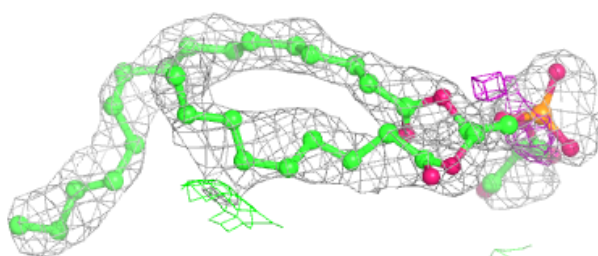
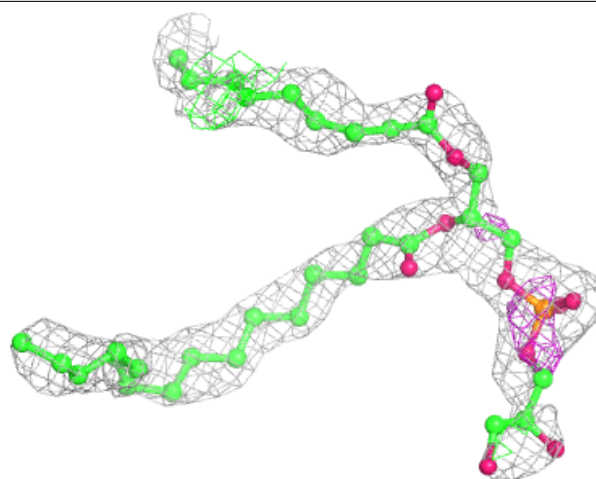
**Electron density around HTG c 525:**

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



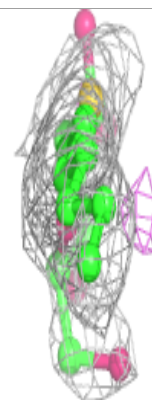
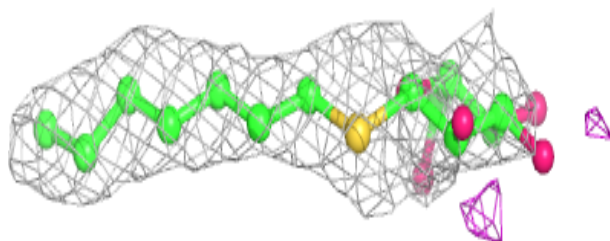
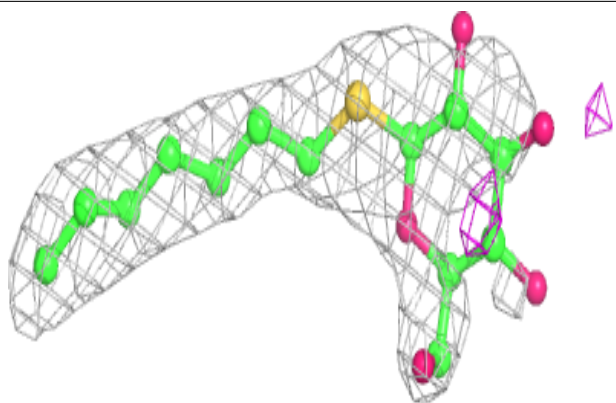
Electron density around LHG E 101:

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

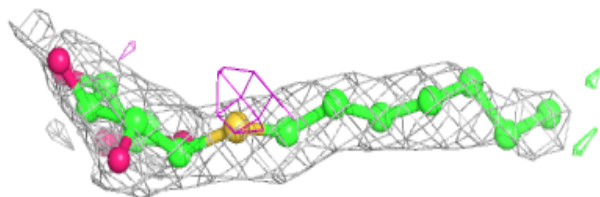
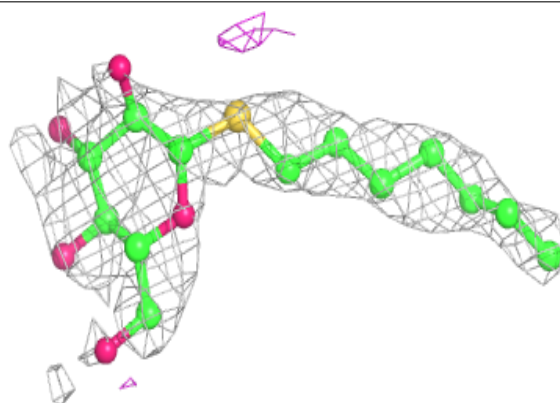


Electron density around HTG b 608:

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

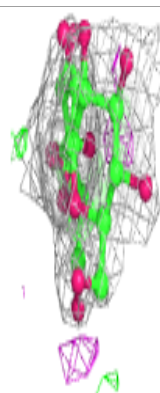
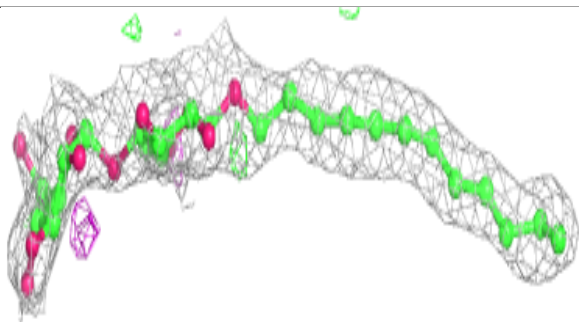
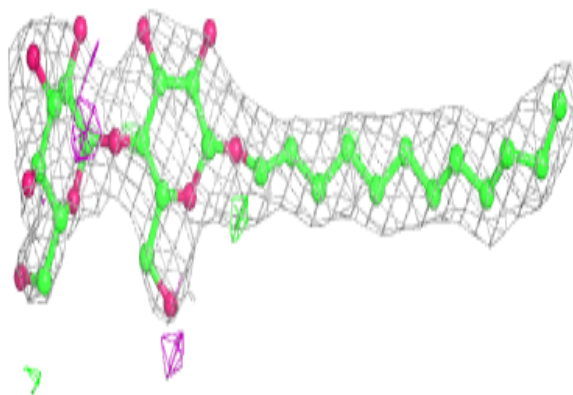
**Electron density around HTG B 625:**

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

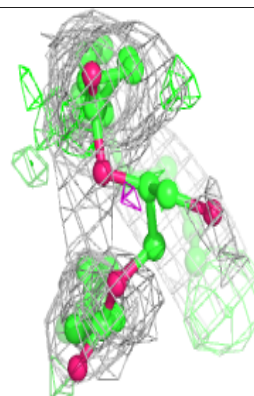
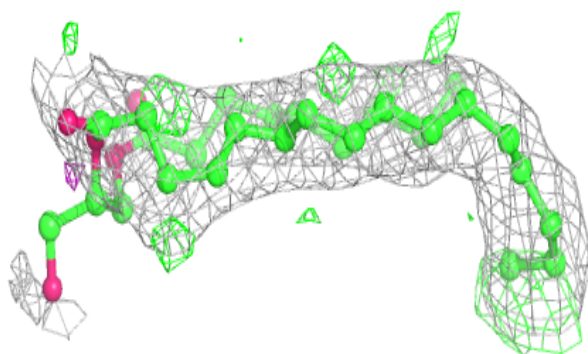
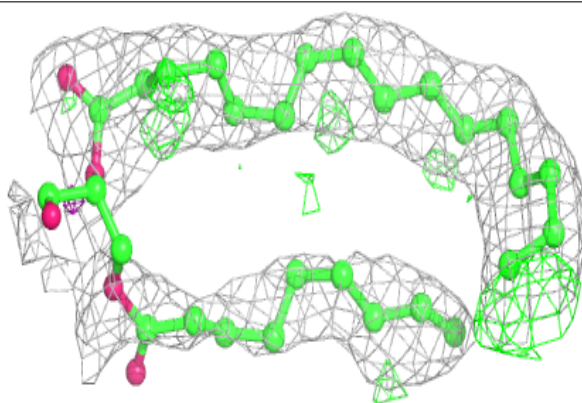


Electron density around LMT M 105:

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

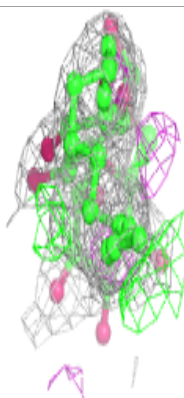
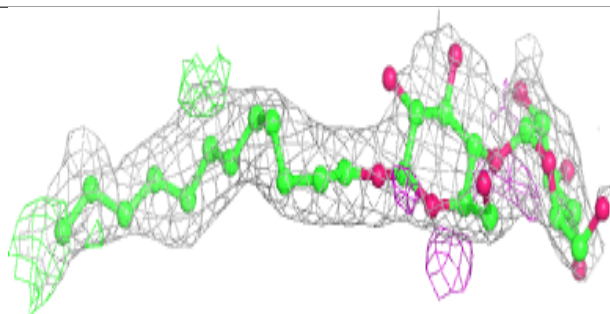
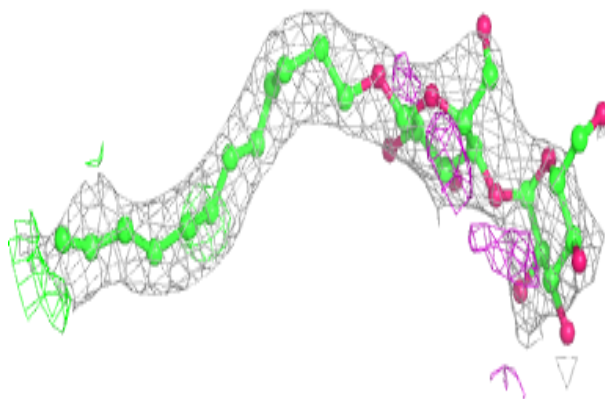
**Electron density around UNL B 634:**

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

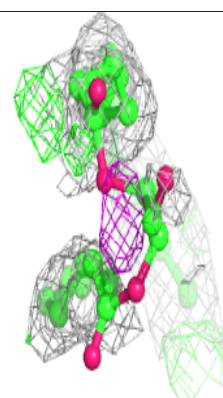
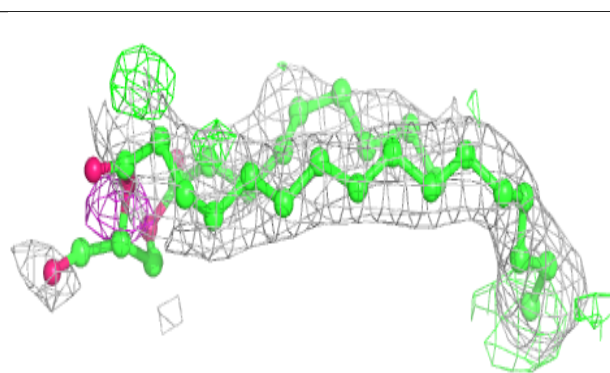
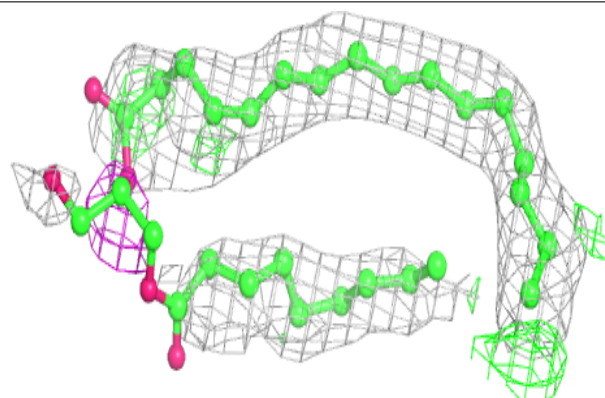


Electron density around LMT a 404:

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

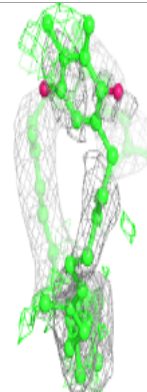
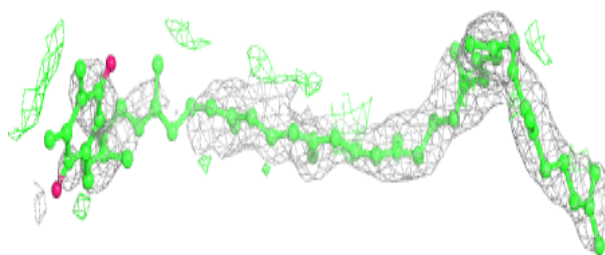
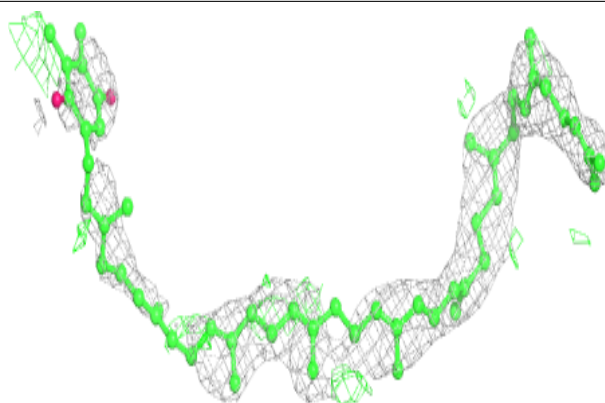
**Electron density around UNL b 633:**

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

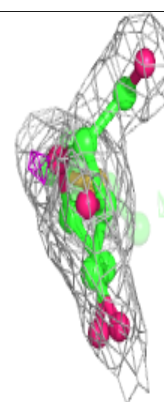
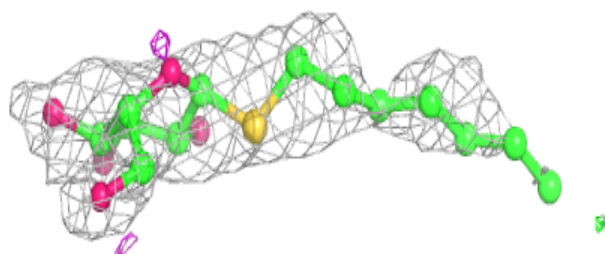
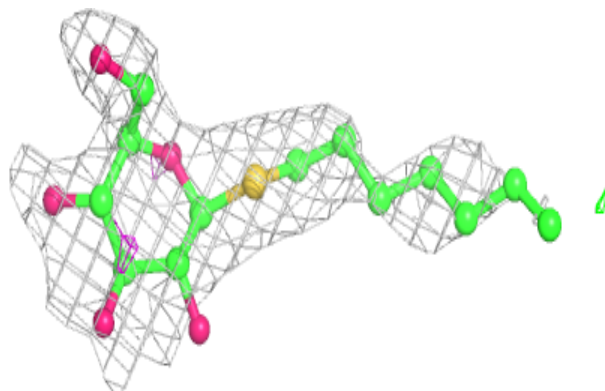


Electron density around PL9 a 416:

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

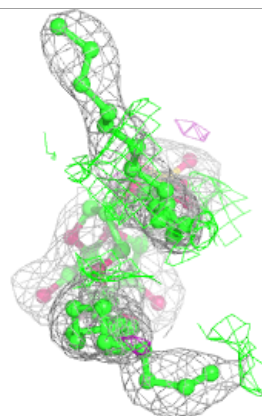
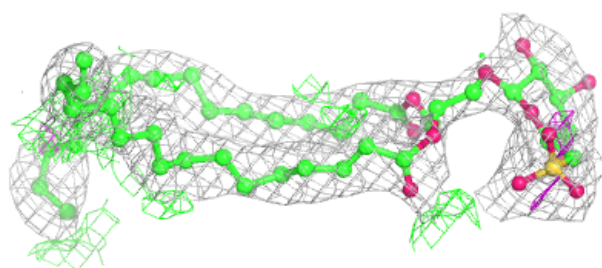
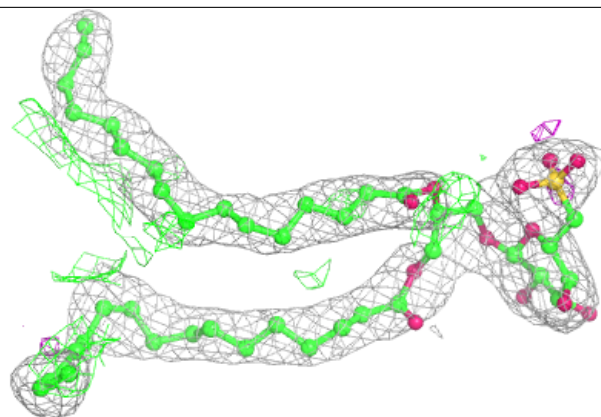
**Electron density around HTG C 524:**

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

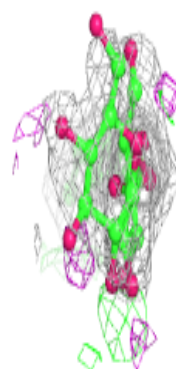
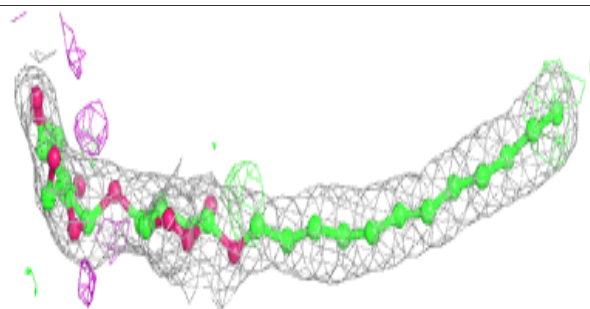
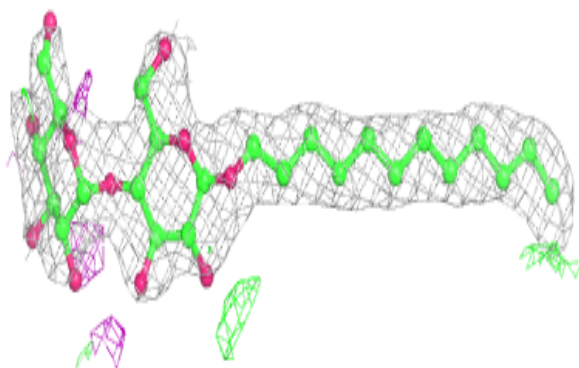


Electron density around SQD L 102:

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

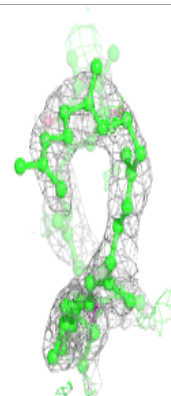
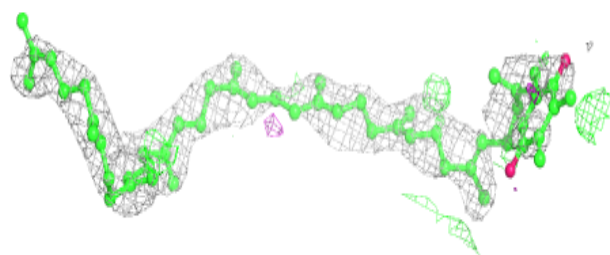
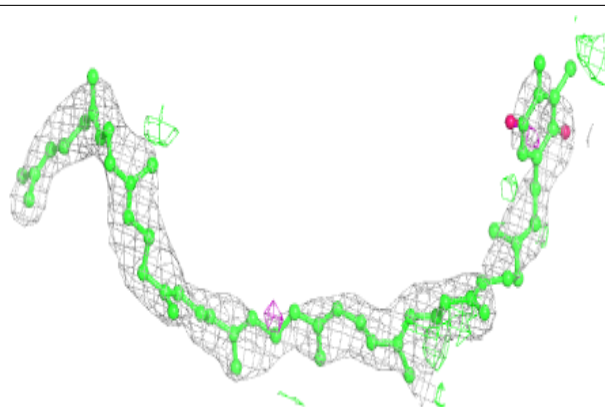
**Electron density around LMT M 102:**

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

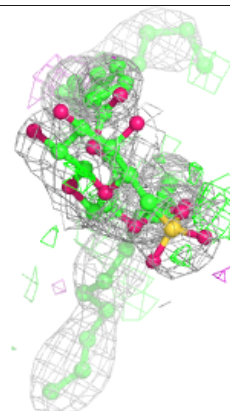
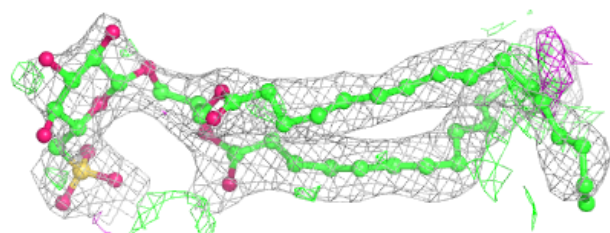
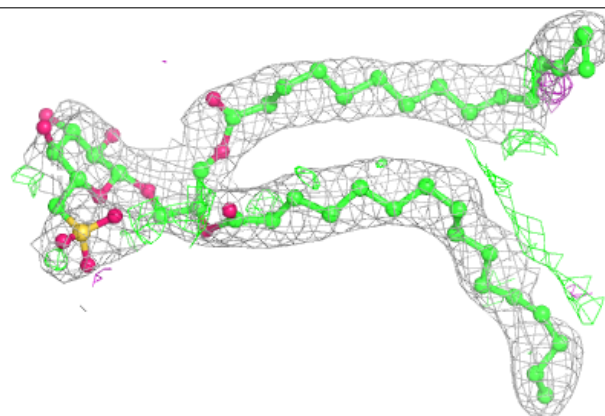


Electron density around PL9 A 418:

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

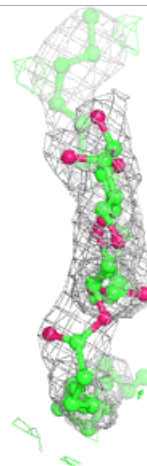
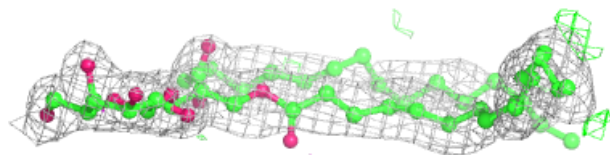
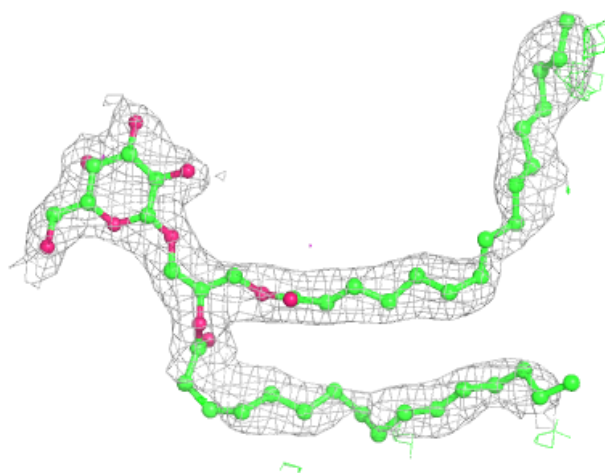
**Electron density around SQD B 621:**

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



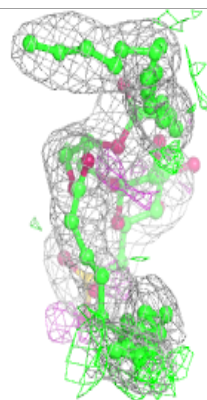
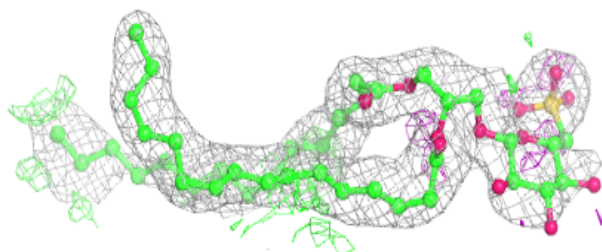
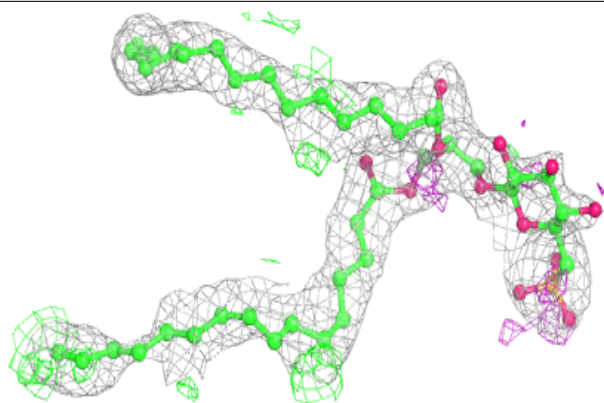
Electron density around LMG C 520:

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

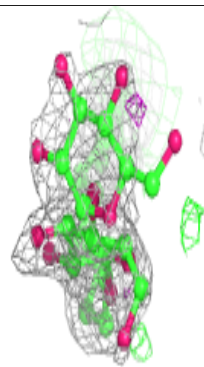
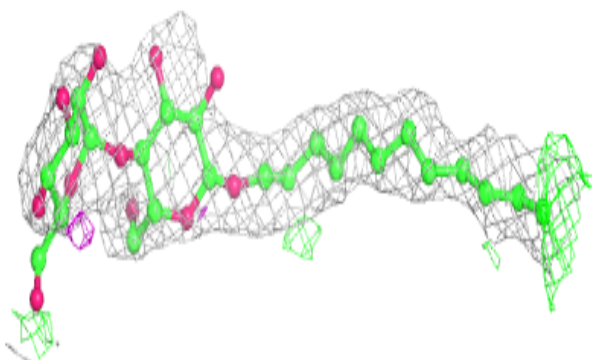
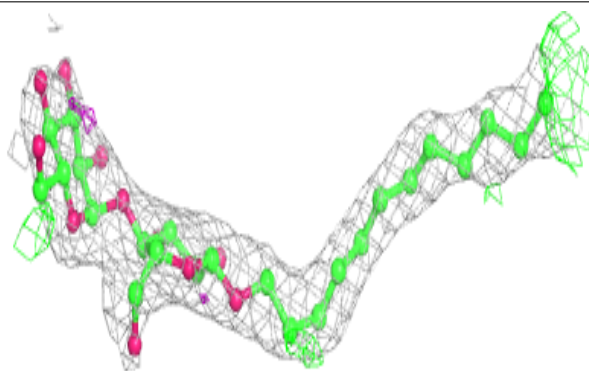


Electron density around SQD A 415:

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

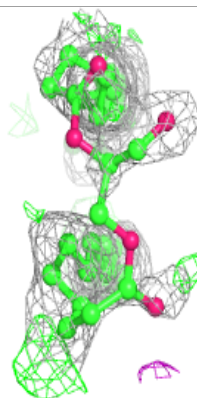
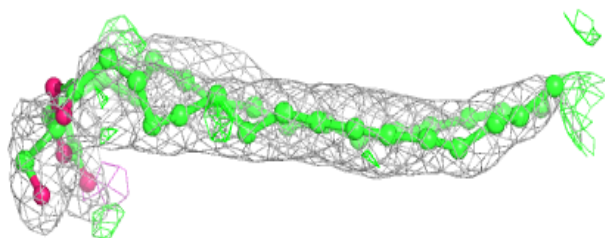
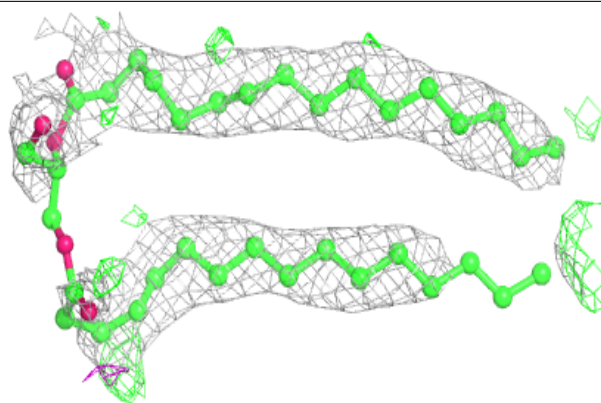
**Electron density around LMT A 416:**

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

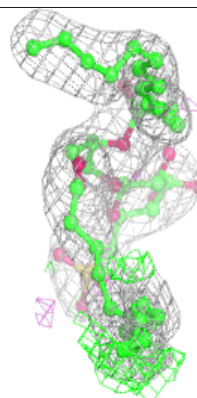
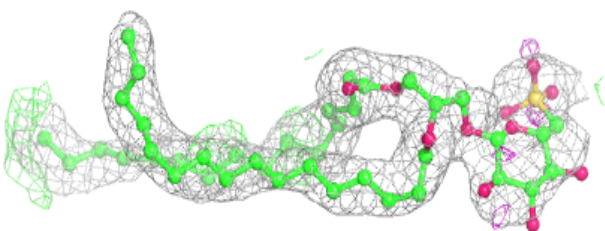
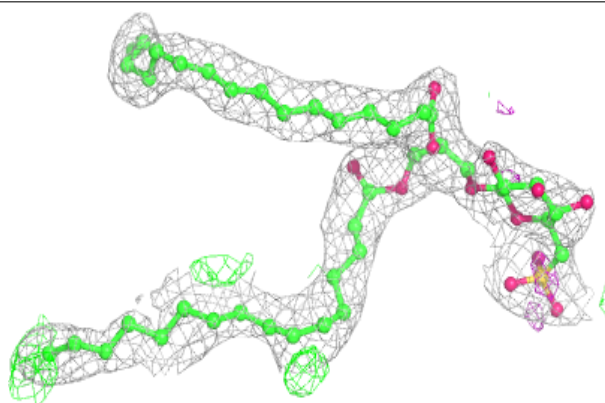


Electron density around UNL i 101:

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

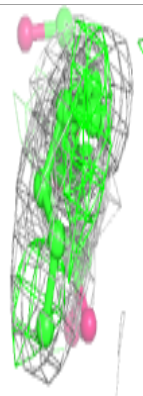
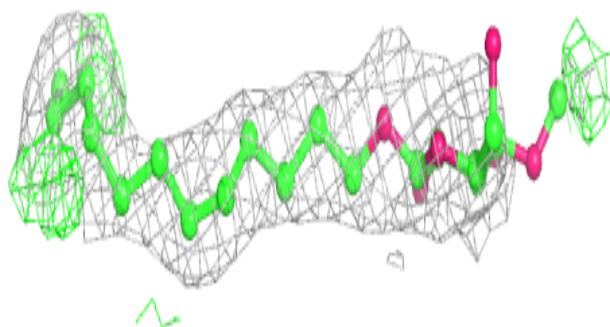
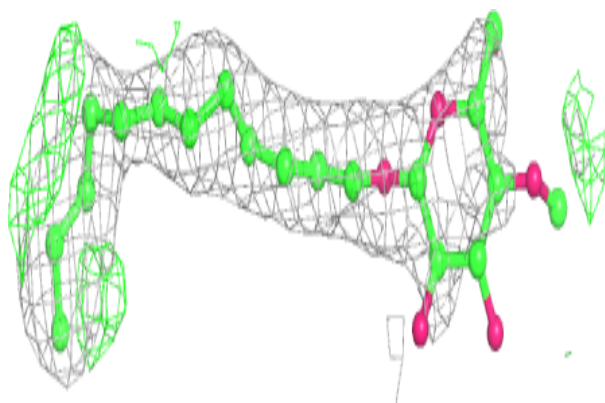
**Electron density around SQD a 405:**

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

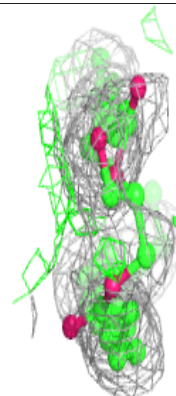
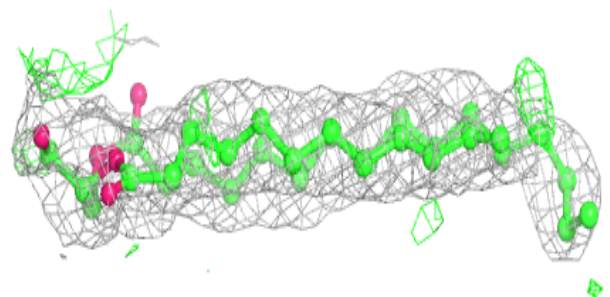
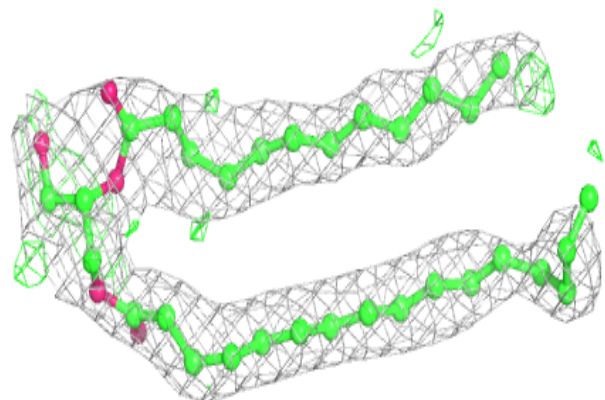


Electron density around LMT B 635:

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

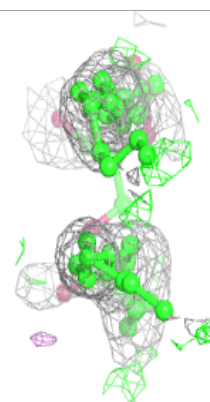
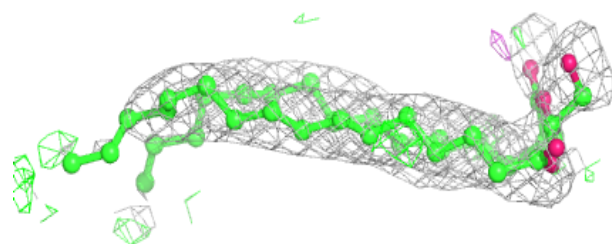
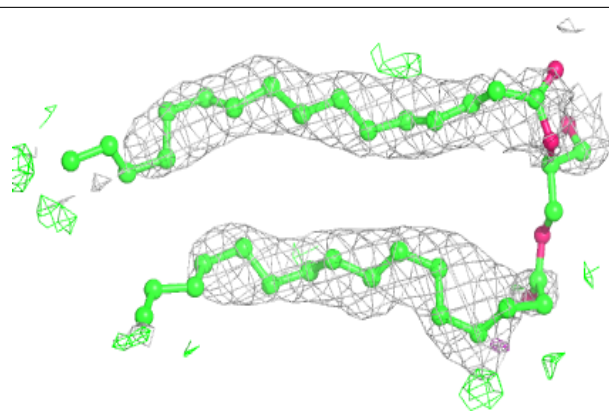
**Electron density around UNL d 411:**

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

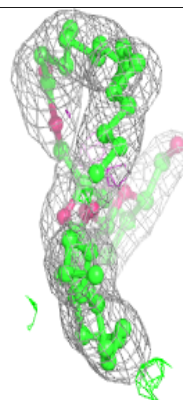
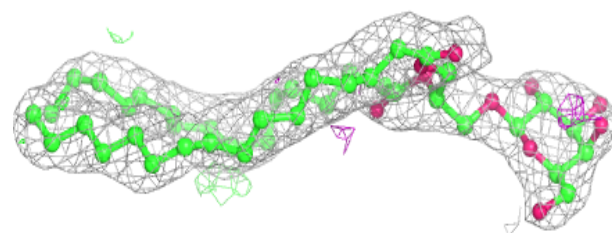
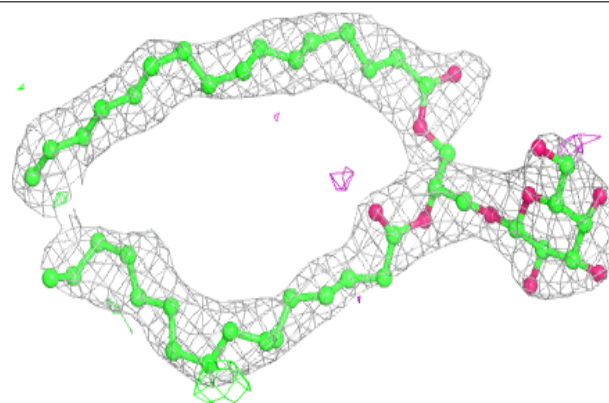


Electron density around UNL I 101:

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

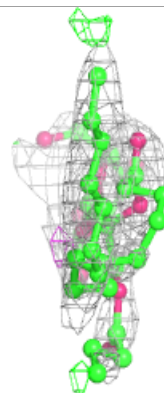
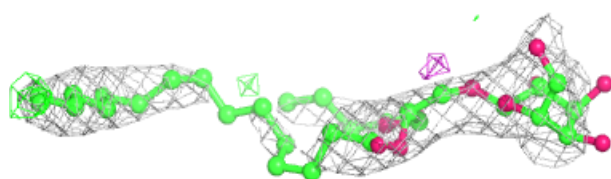
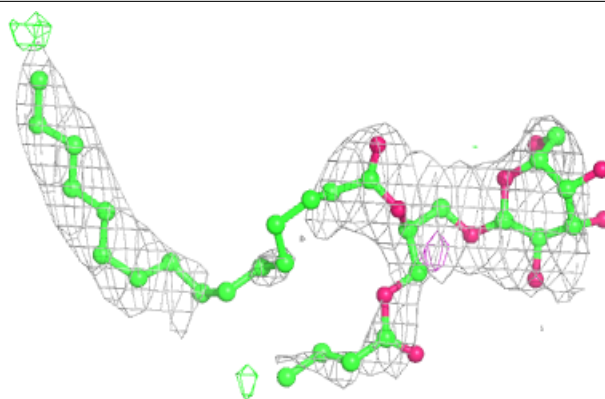
**Electron density around LMG a 415:**

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

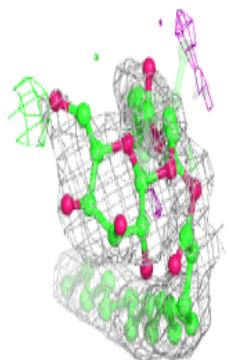
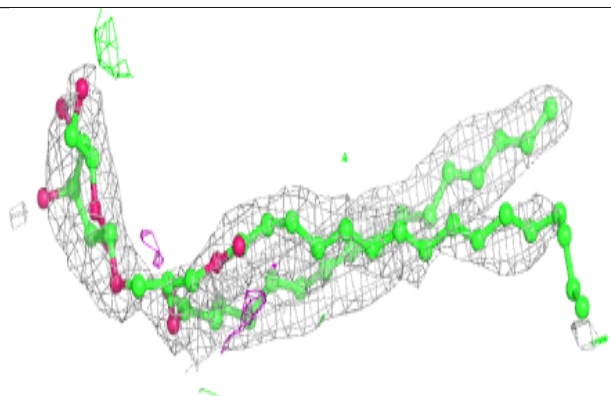
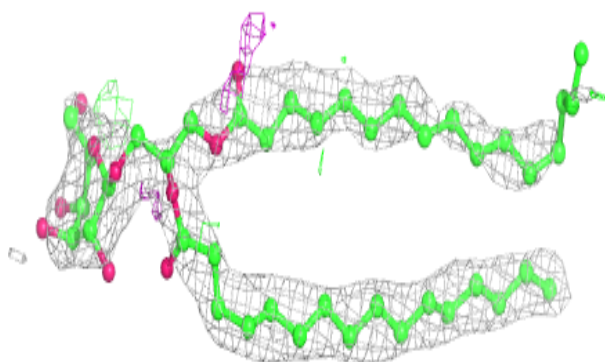


Electron density around LMG z 101:

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

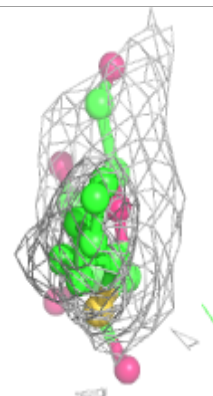
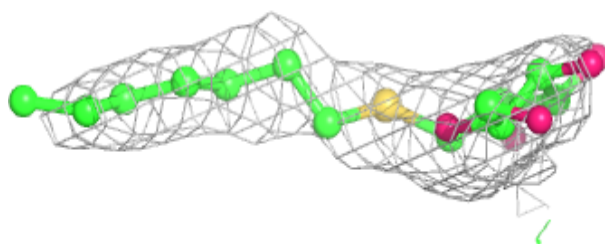
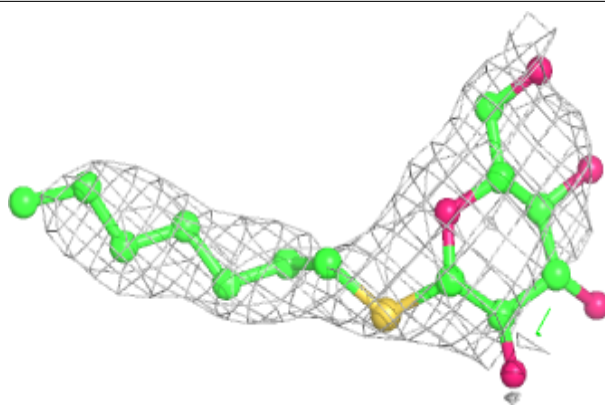
**Electron density around LMG C 521:**

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

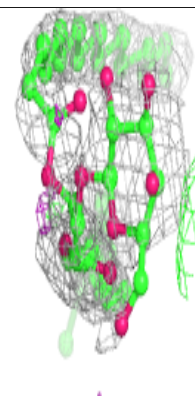
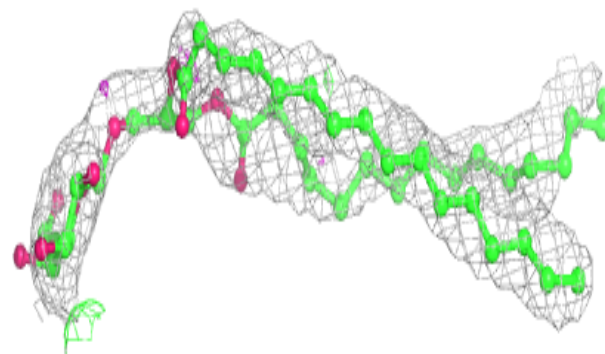
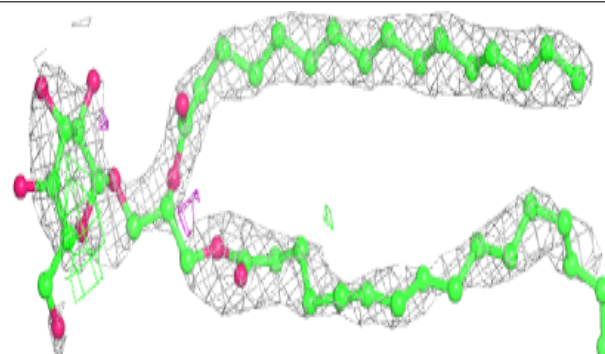


Electron density around HTG b 632:

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

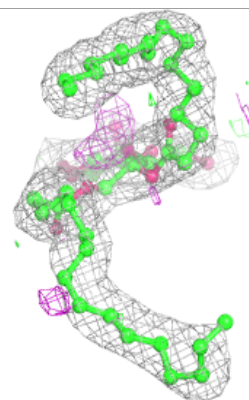
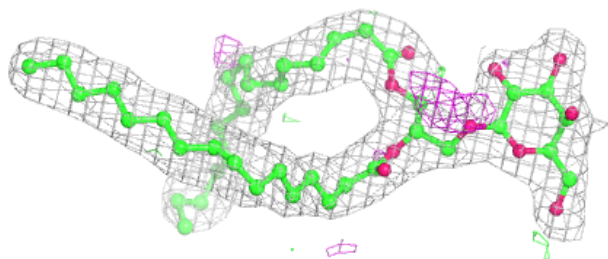
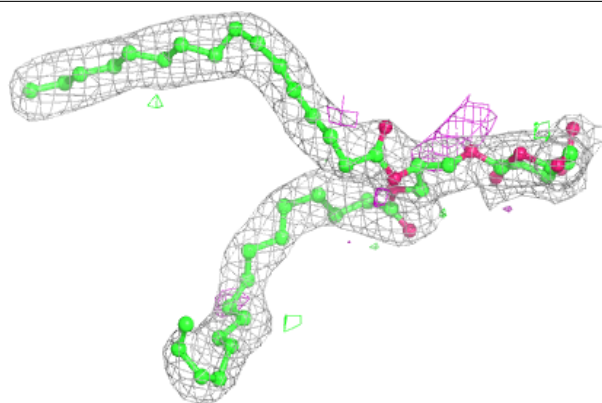
**Electron density around LMG c 523:**

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

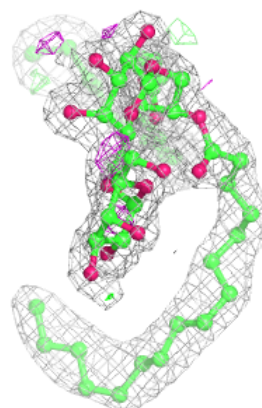
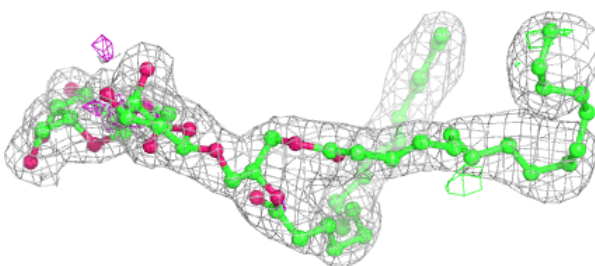
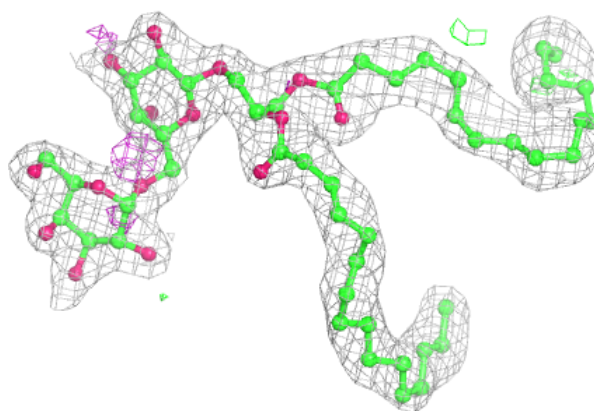


Electron density around LMG b 629:

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

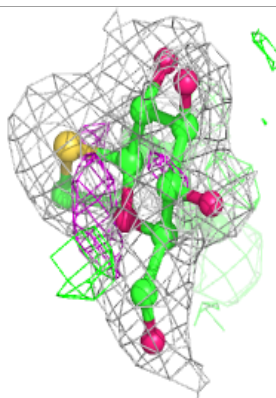
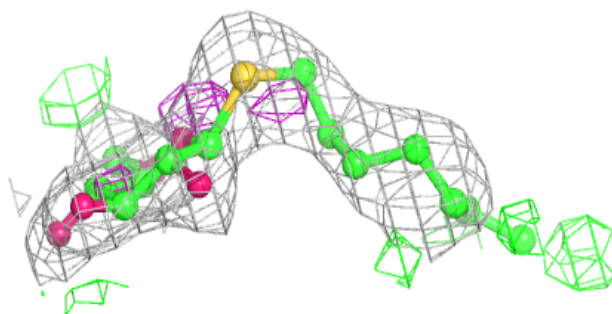
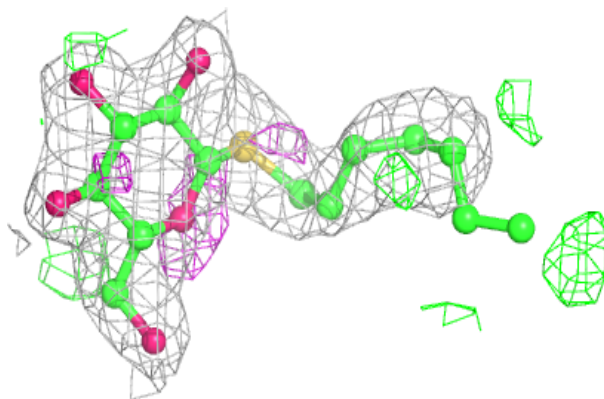
**Electron density around DGD C 518:**

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

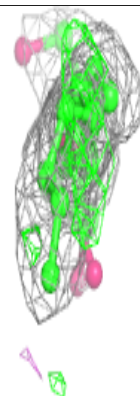
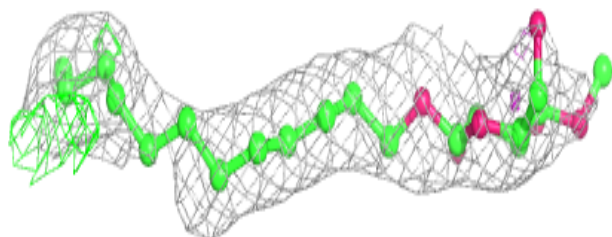
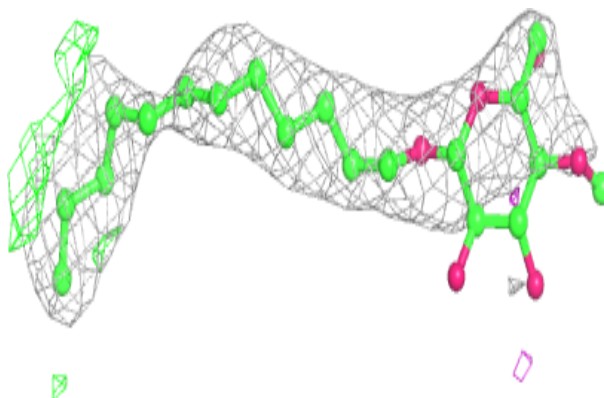


Electron density around HTG B 624:

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

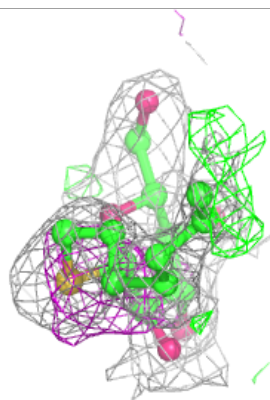
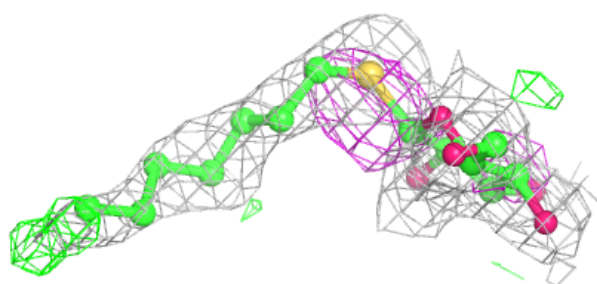
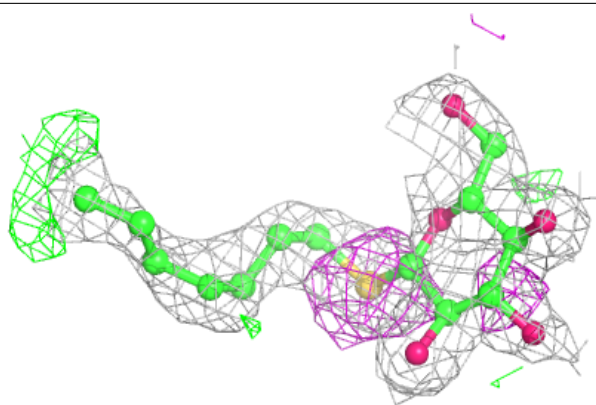
**Electron density around LMT T 104:**

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



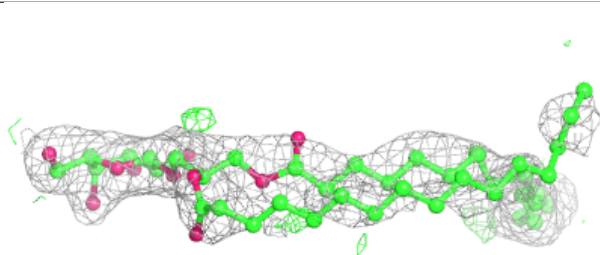
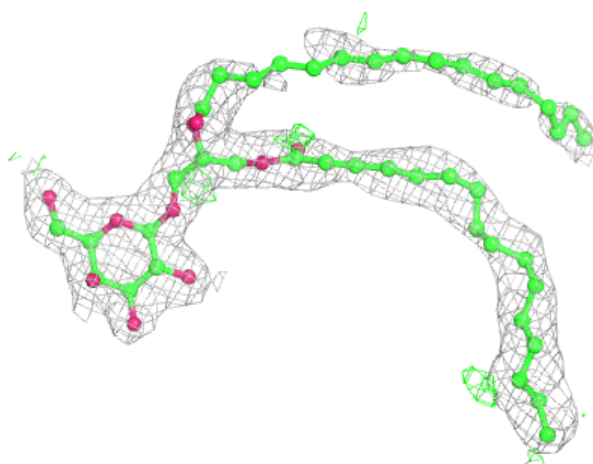
Electron density around HTG b 631:

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



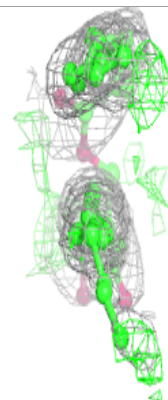
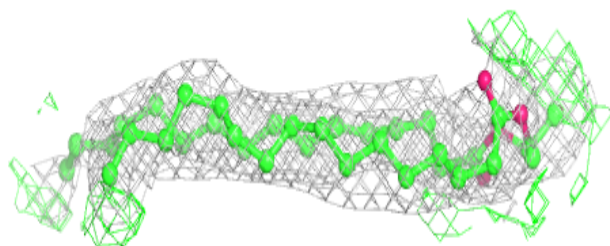
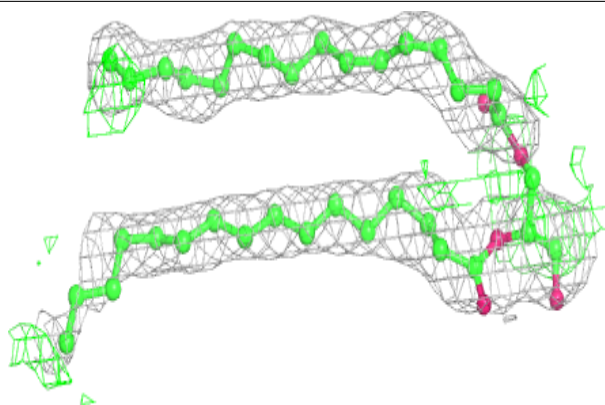
Electron density around LMG c 522:

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

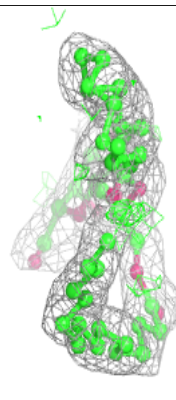
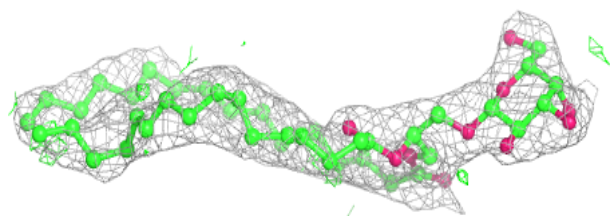
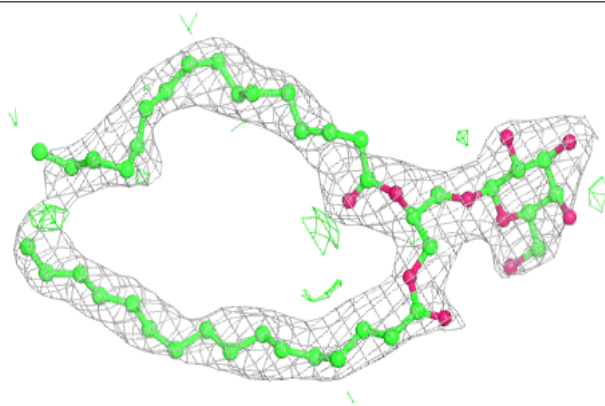


Electron density around UNL D 411:

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

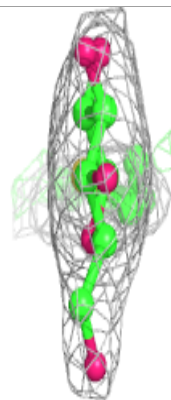
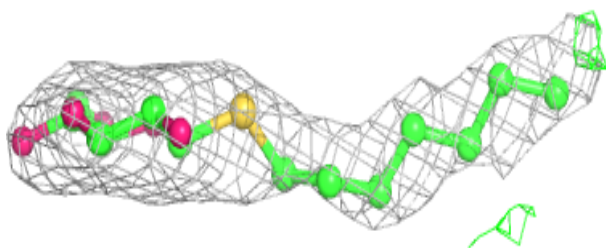
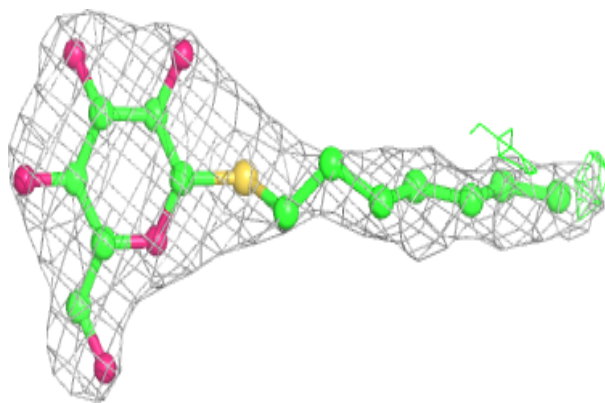
**Electron density around LMG C 501:**

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

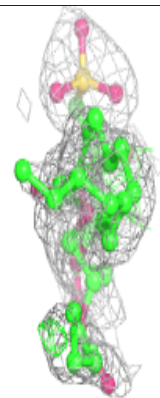
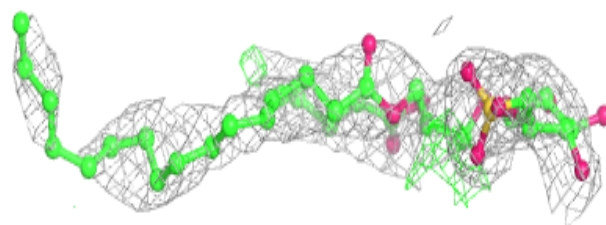
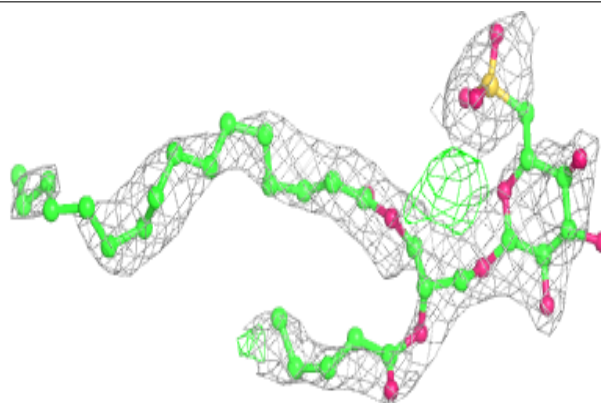


Electron density around HTG c 524:

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

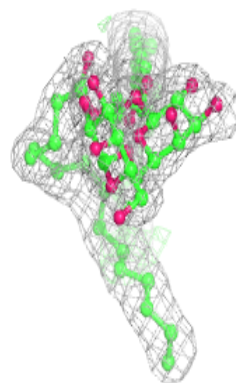
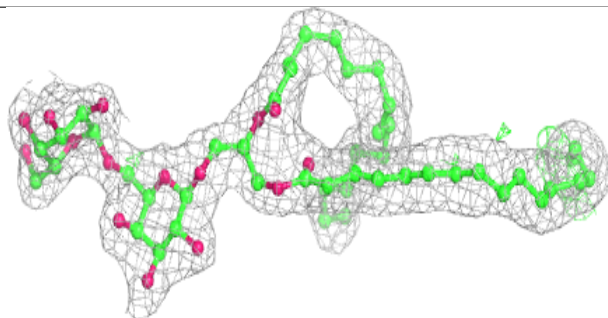
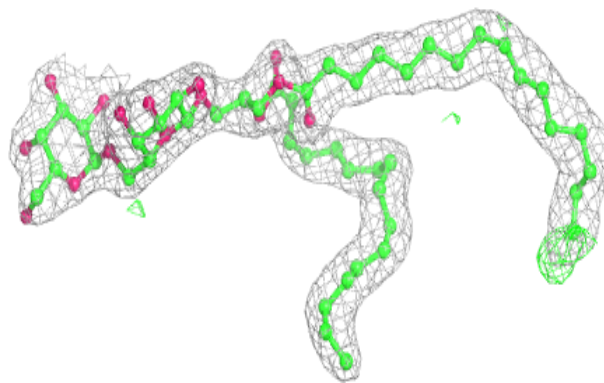
**Electron density around SQD F 103:**

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

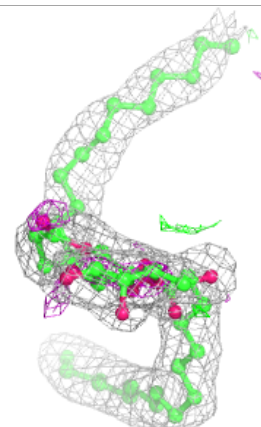
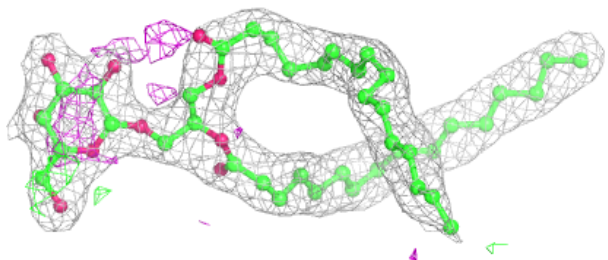
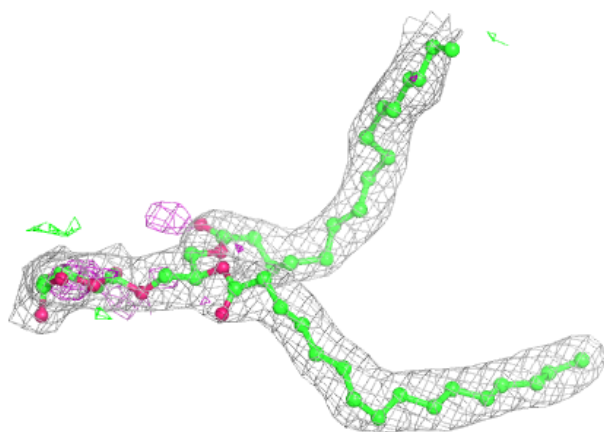


Electron density around DGD h 102:

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

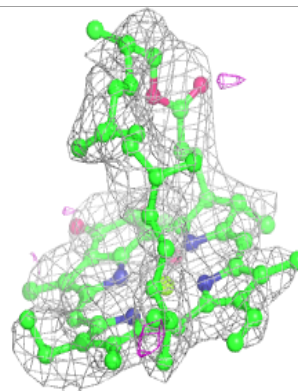
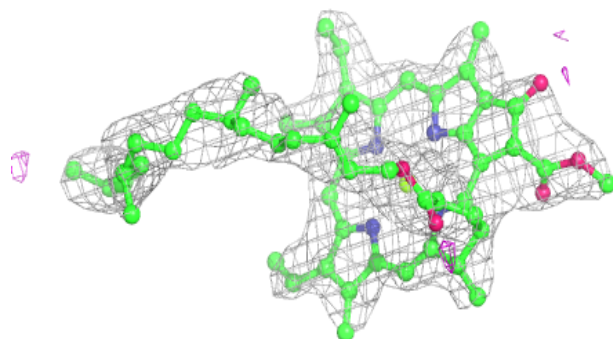
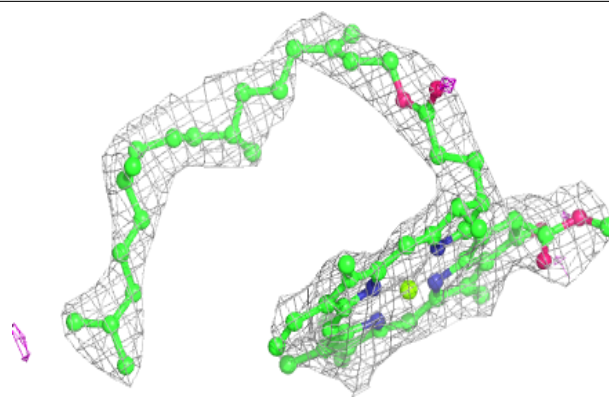
**Electron density around LMG M 101:**

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

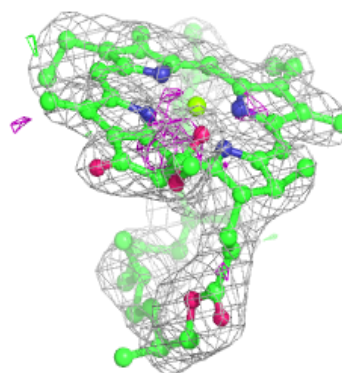
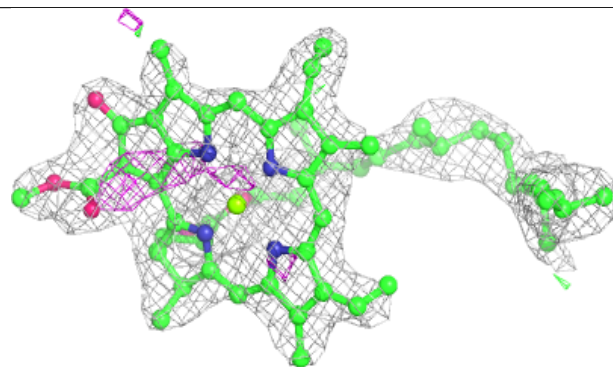
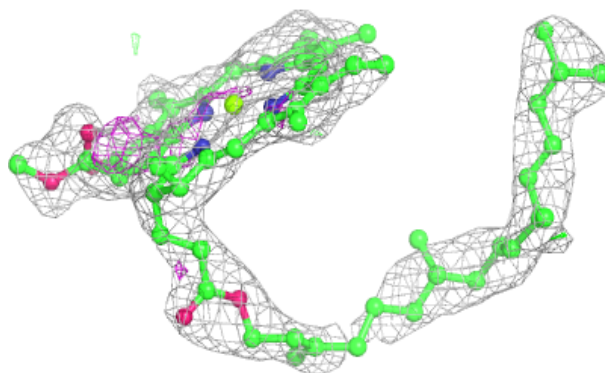


Electron density around CLA c 517:

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

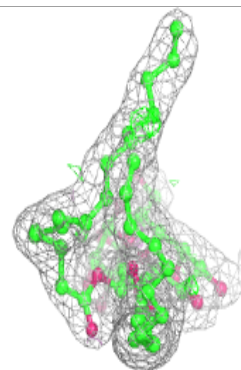
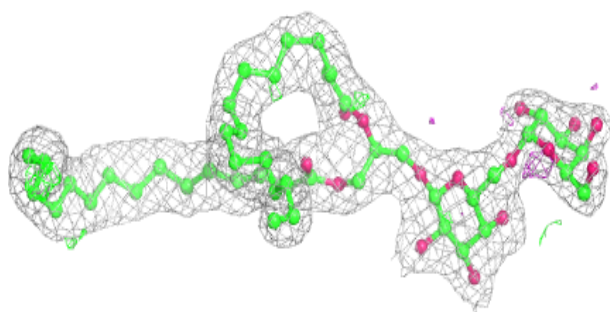
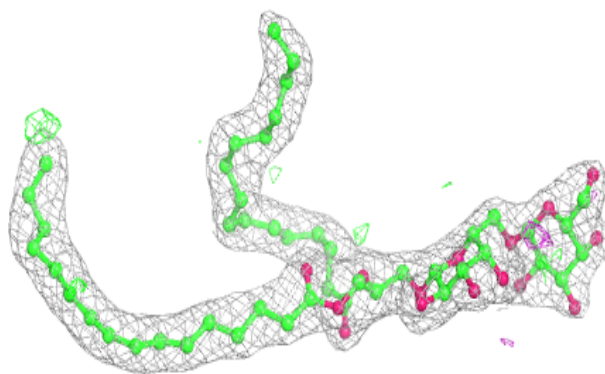
**Electron density around CLA C 514:**

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



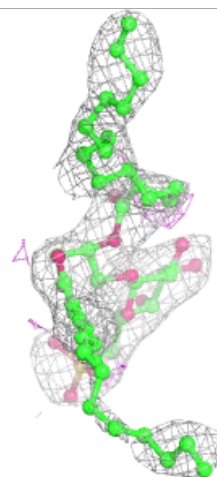
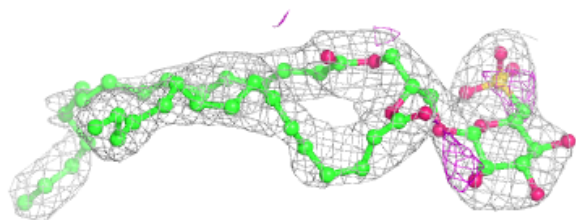
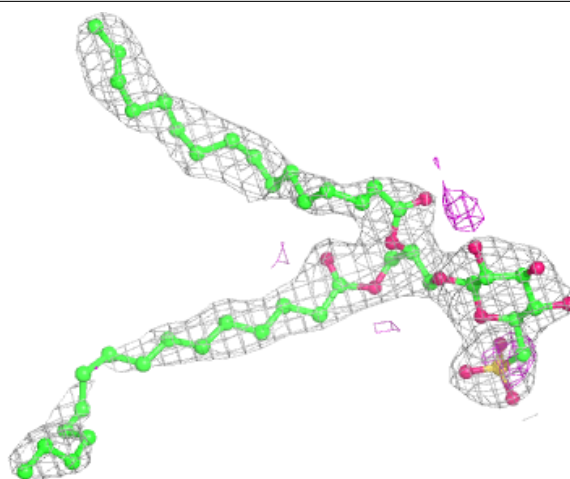
Electron density around DGD H 102:

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



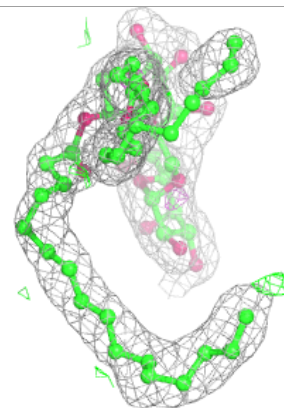
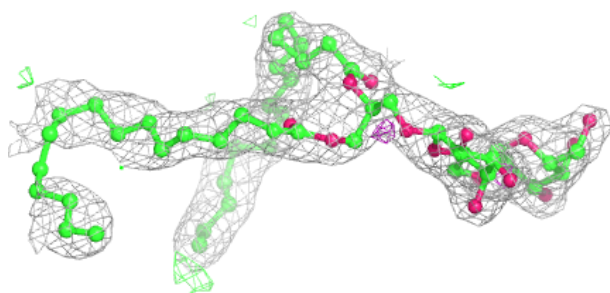
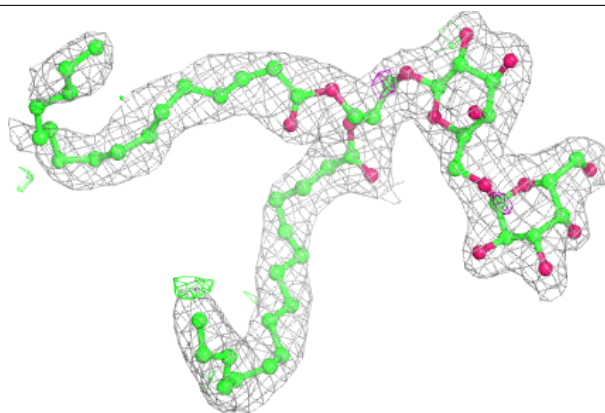
Electron density around SQD A 411:

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

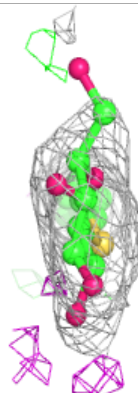
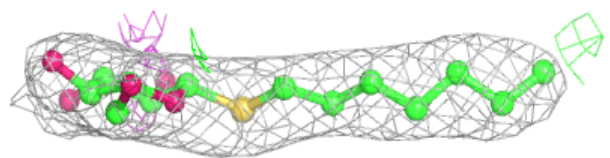
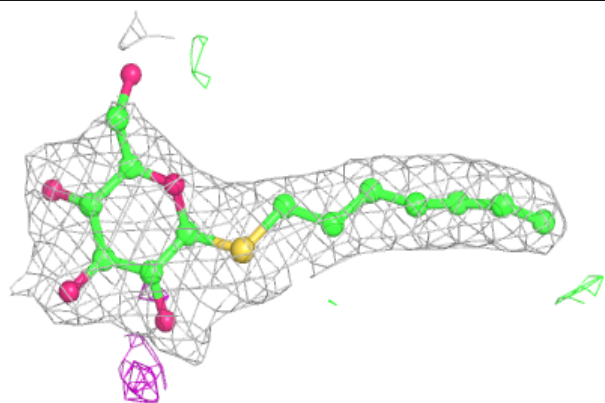


Electron density around DGD c 520:

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

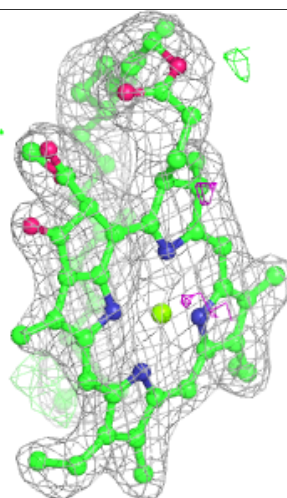
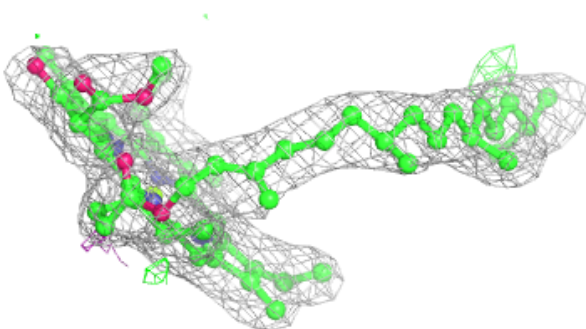
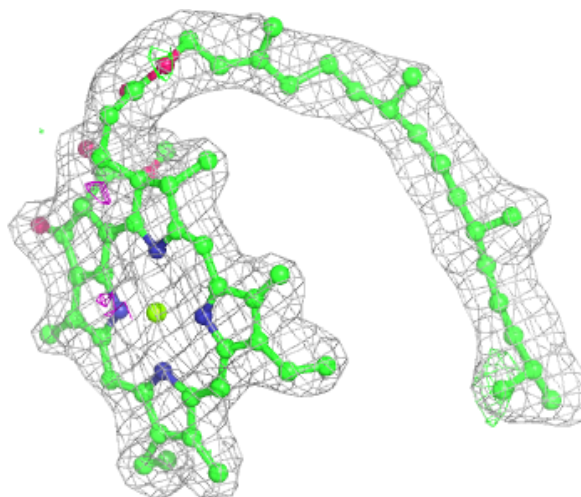
**Electron density around HTG B 632:**

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



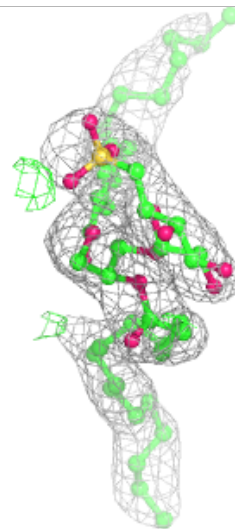
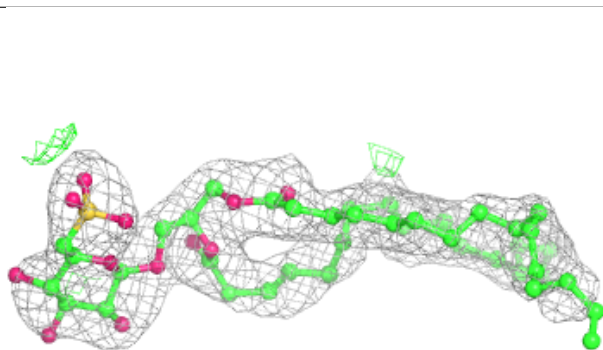
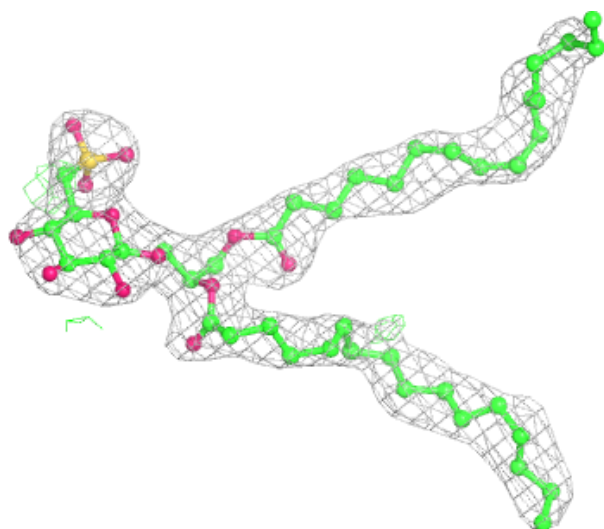
Electron density around CLA c 511:

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



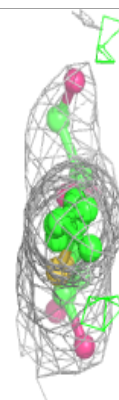
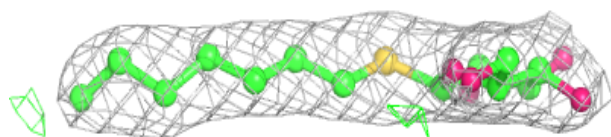
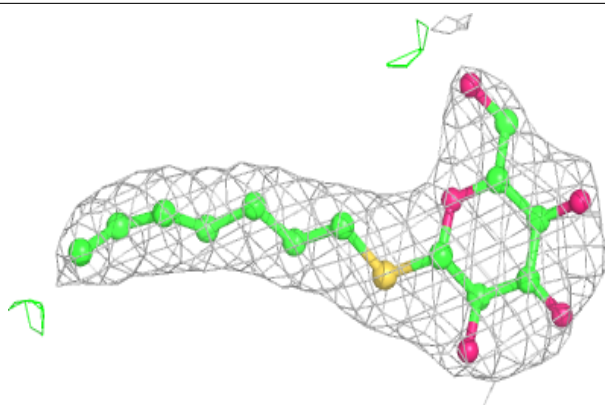
Electron density around SQD a 414:

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

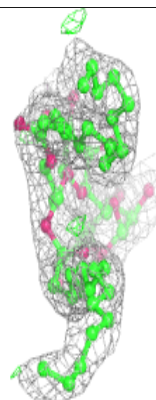
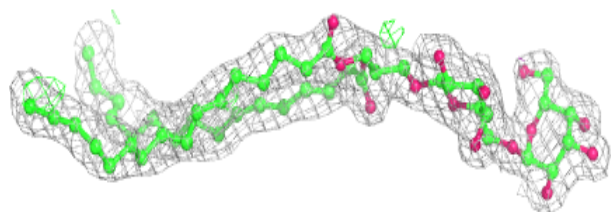
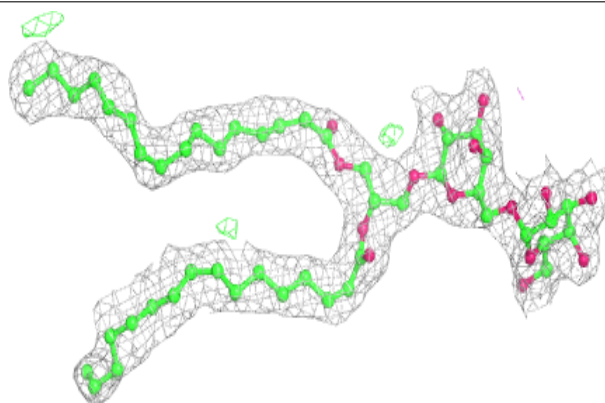


Electron density around HTG b 607:

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

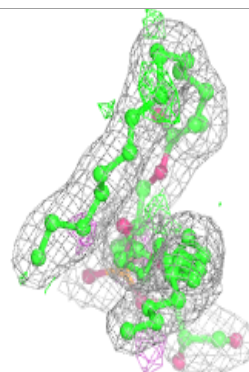
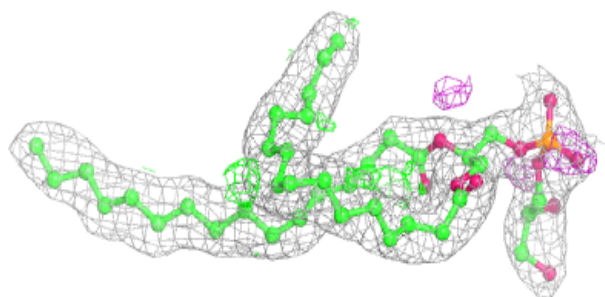
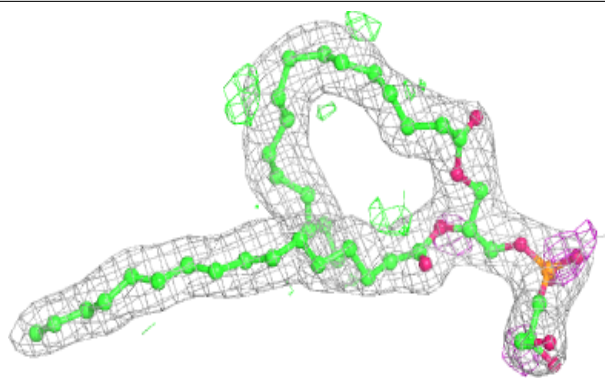
**Electron density around DGD c 521:**

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

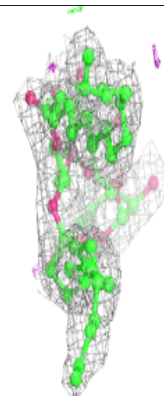
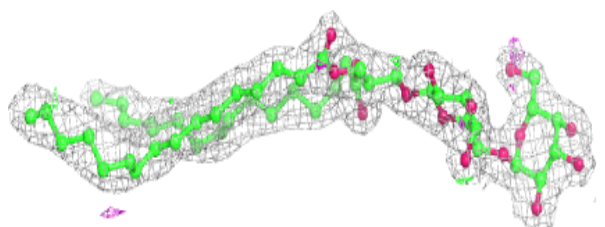
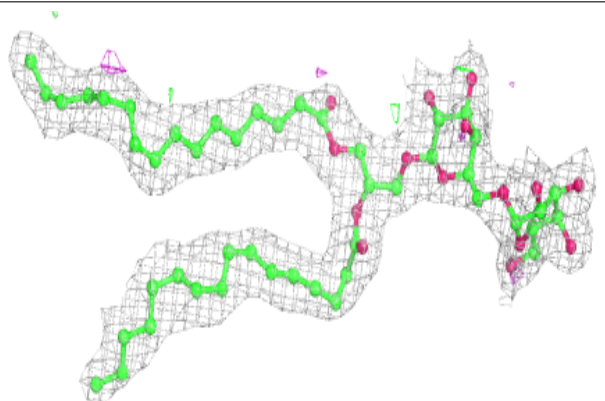


Electron density around LHG D 407:

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

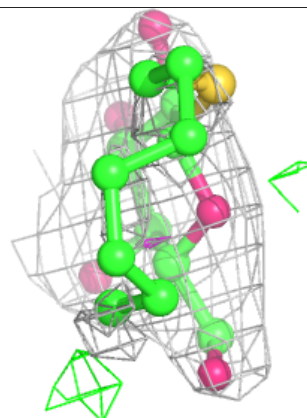
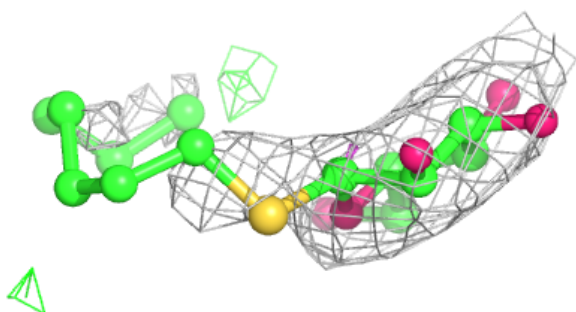
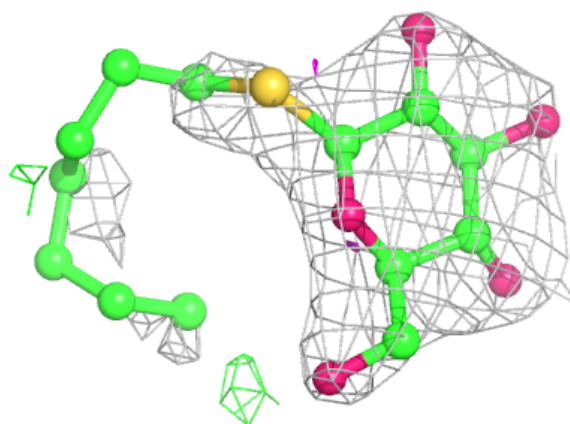
**Electron density around DGD C 519:**

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

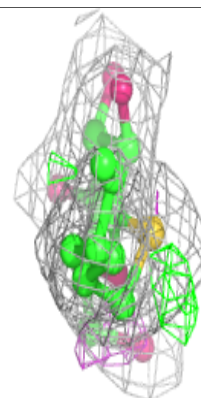
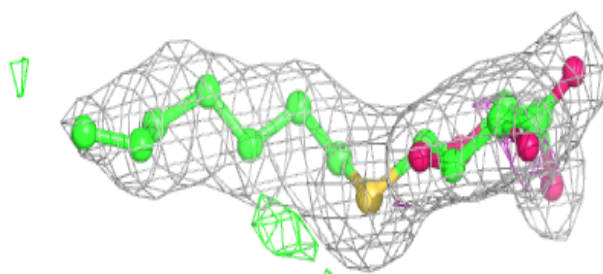
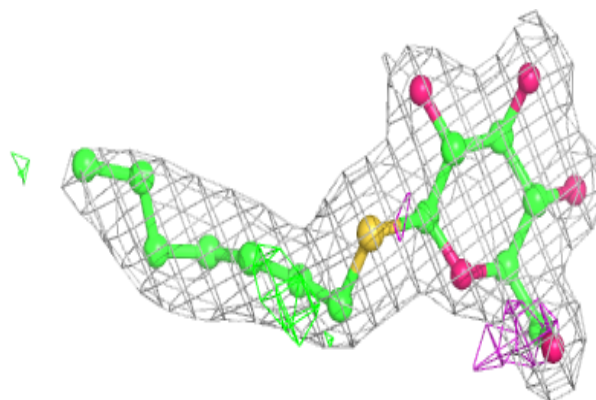


Electron density around HTG V 206:

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

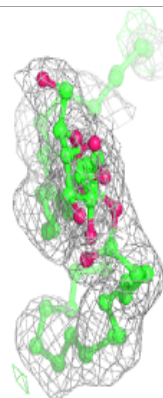
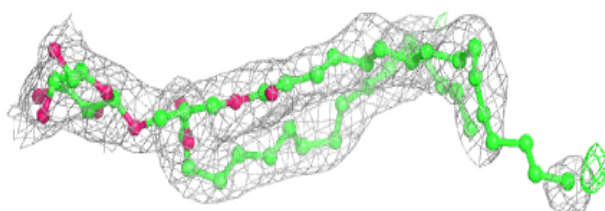
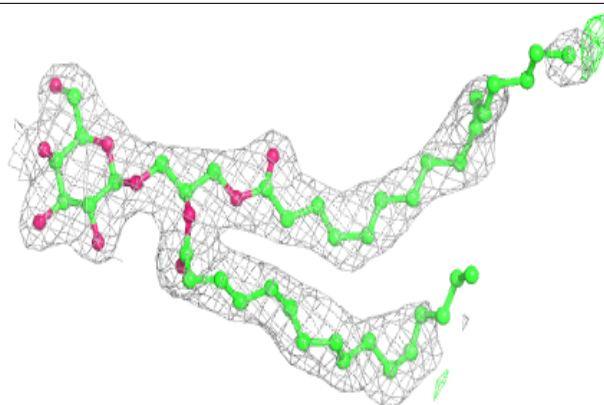
**Electron density around HTG B 623:**

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

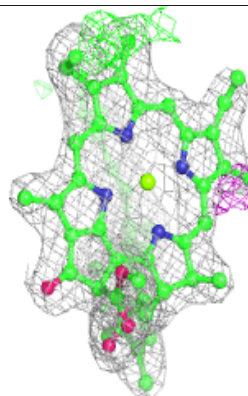
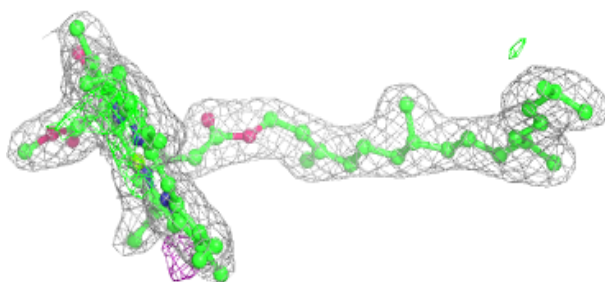
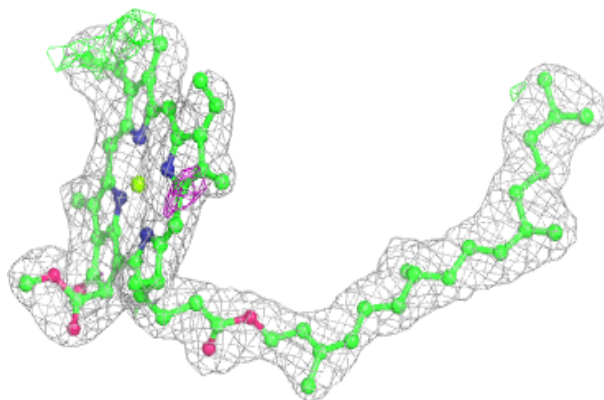


Electron density around LMG j 101:

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

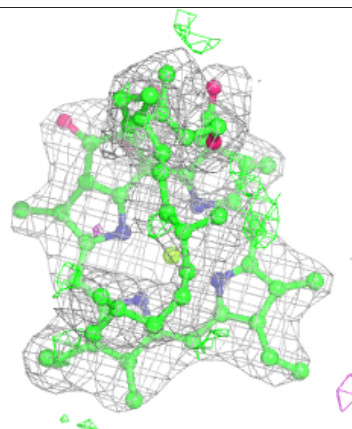
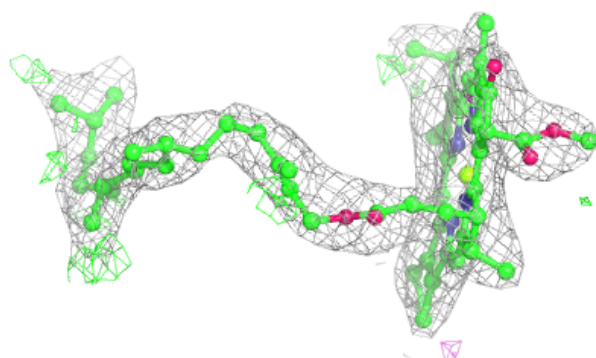
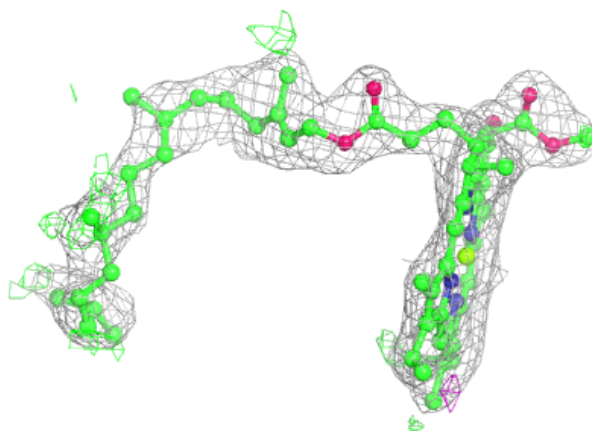
**Electron density around CLA b 618:**

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

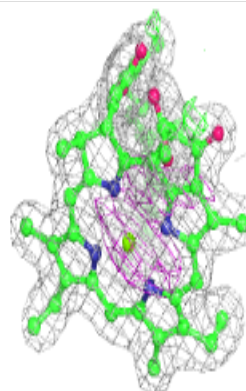
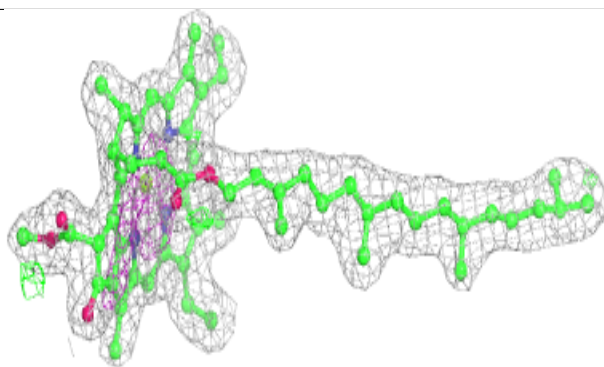
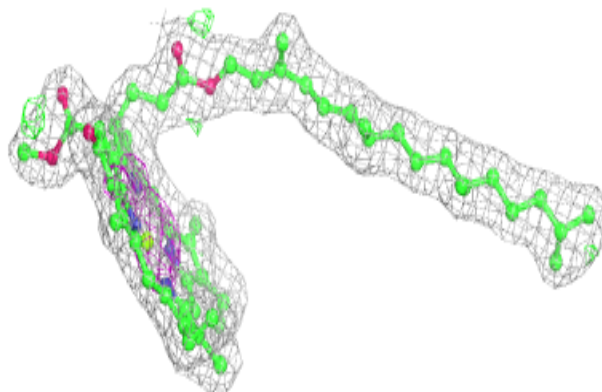


Electron density around CLA C 507:

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

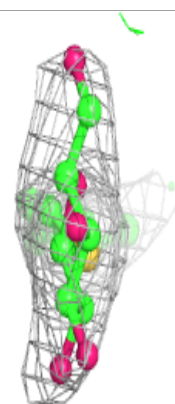
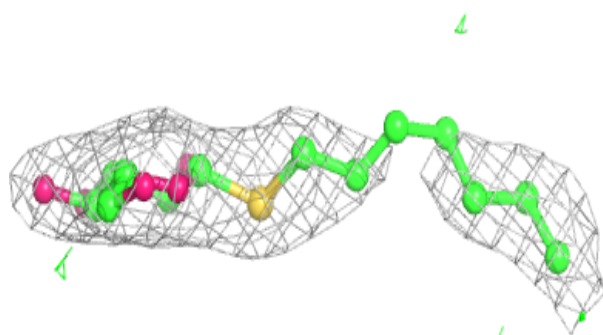
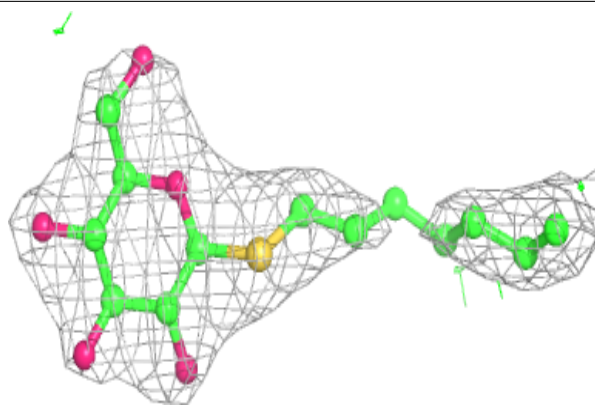
**Electron density around CLA b 616:**

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

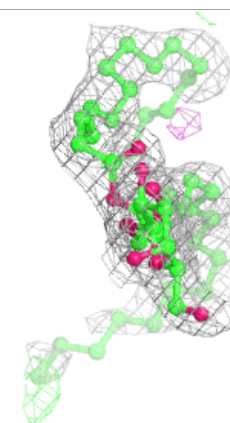
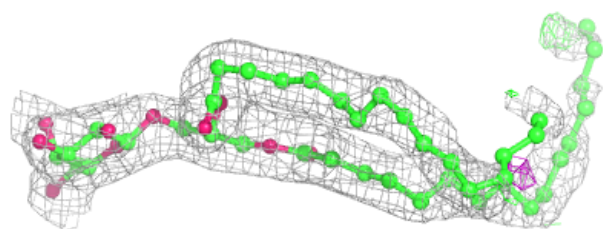
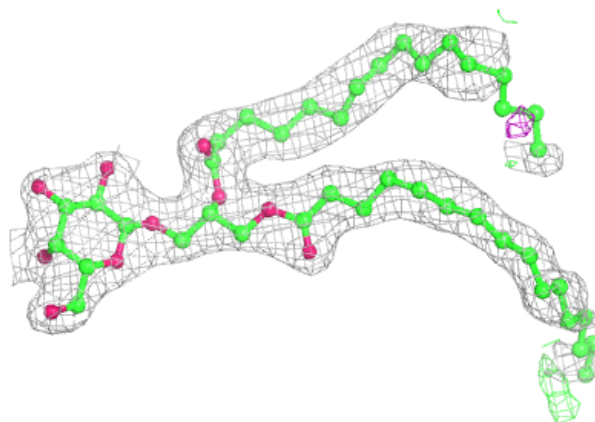


Electron density around HTG C 523:

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

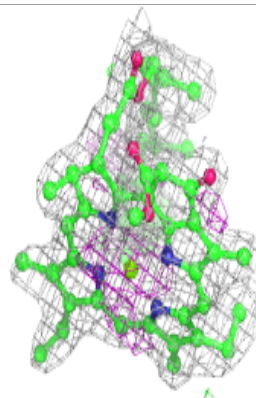
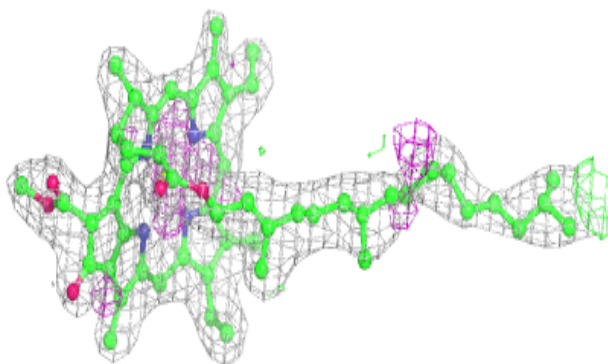
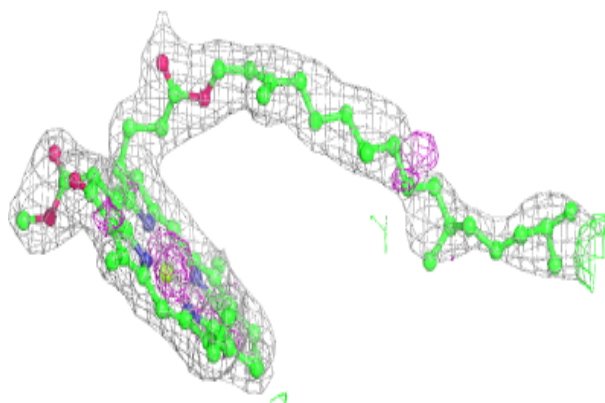
**Electron density around LMG J 101:**

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

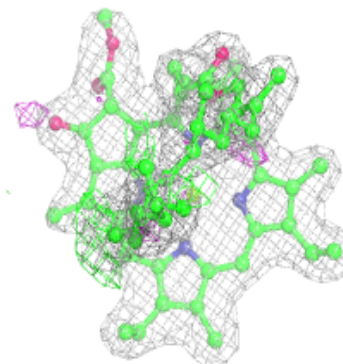
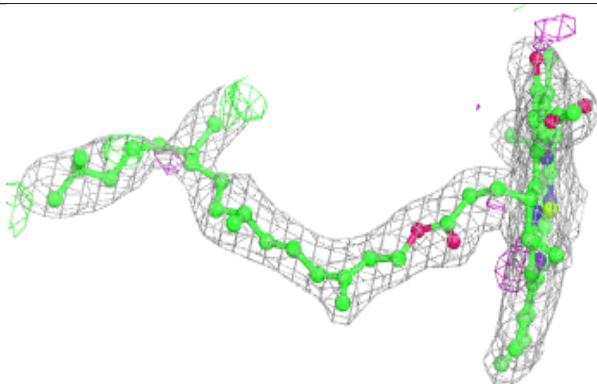
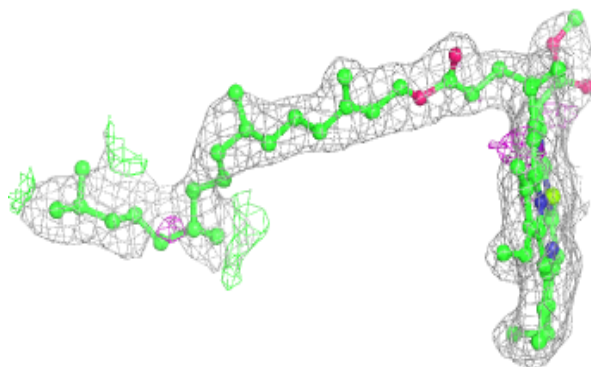


Electron density around CLA C 505:

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

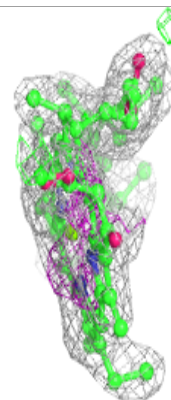
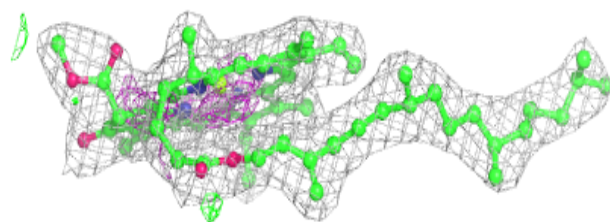
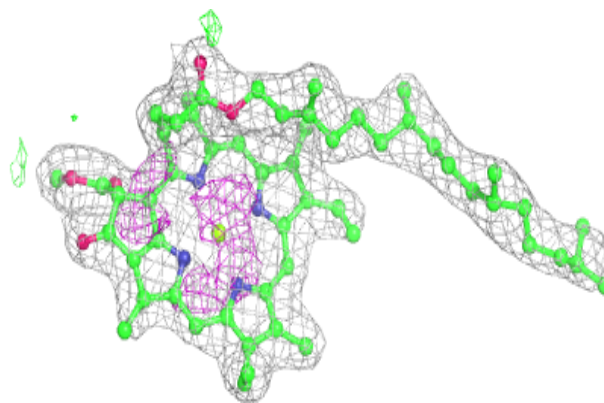
**Electron density around CLA b 615:**

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

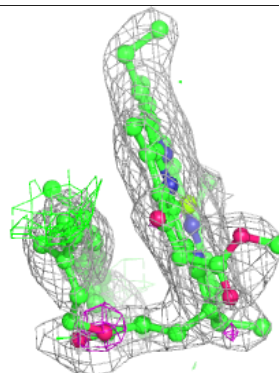
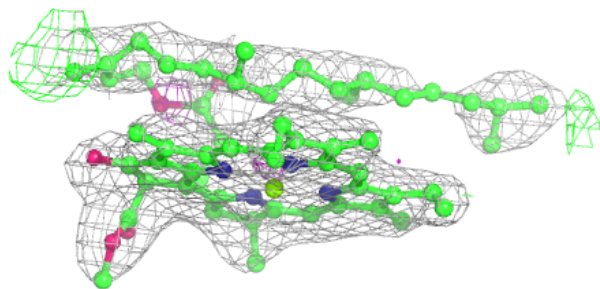
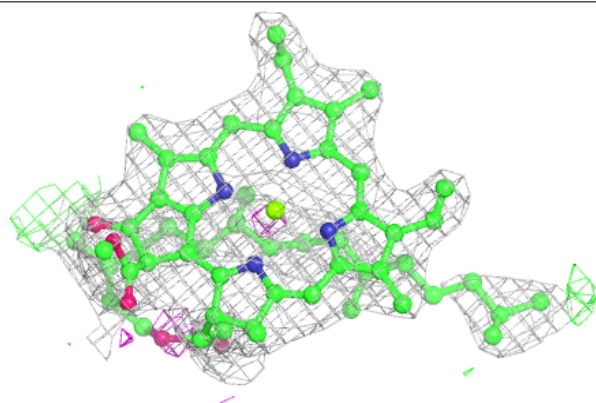


Electron density around CLA C 502:

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

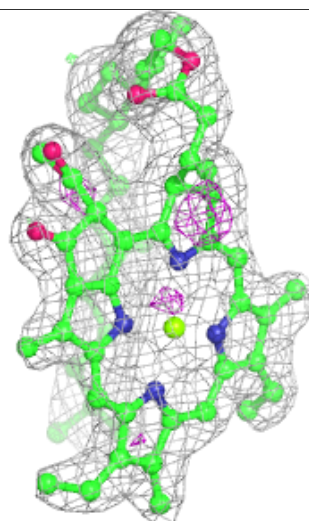
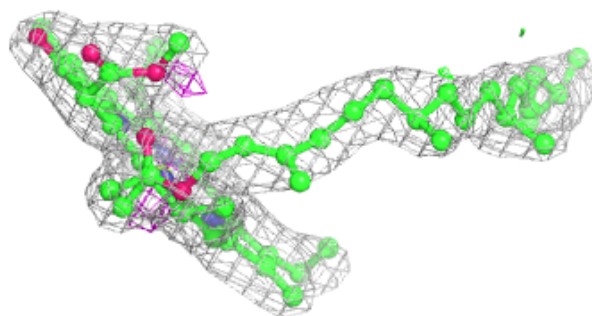
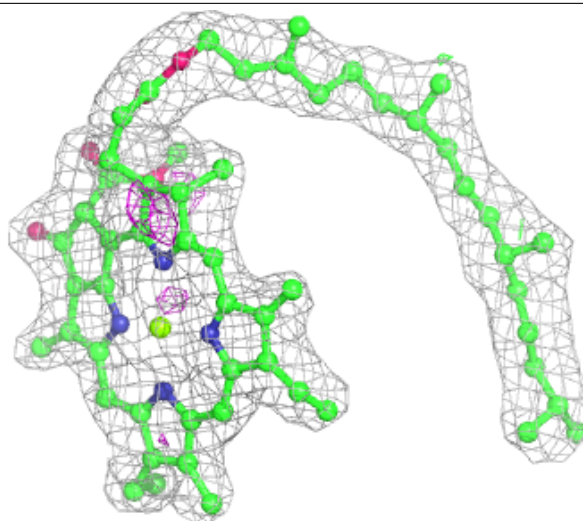
**Electron density around CLA B 602:**

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



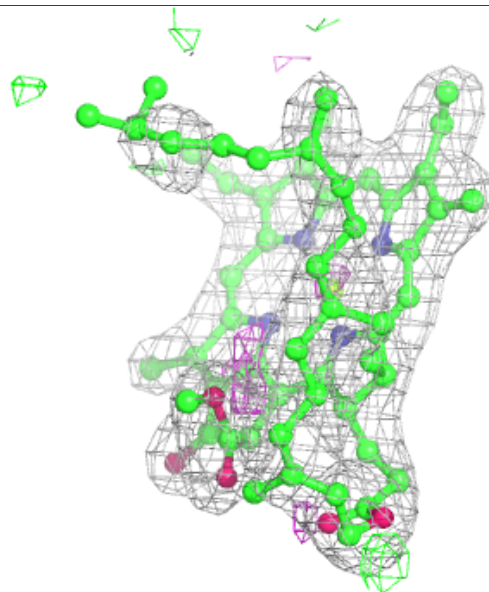
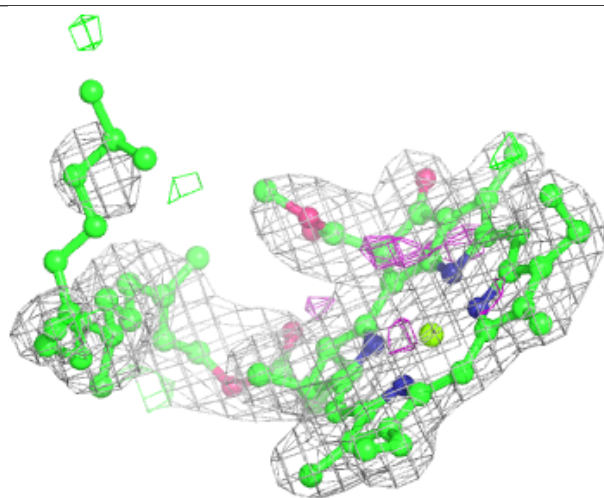
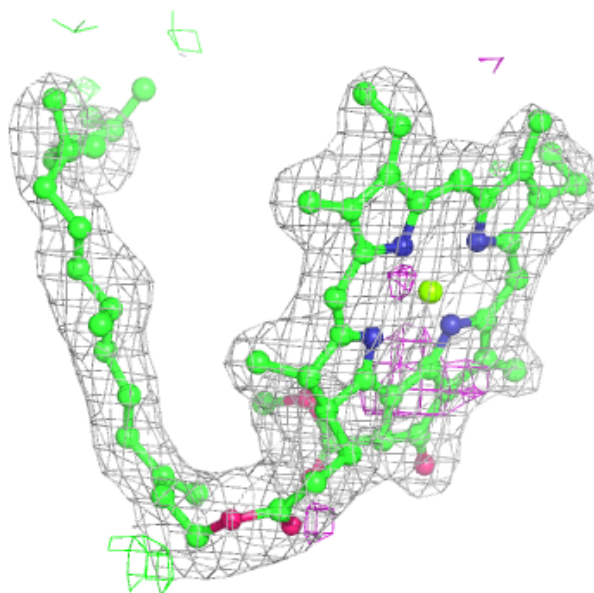
Electron density around CLA C 508:

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



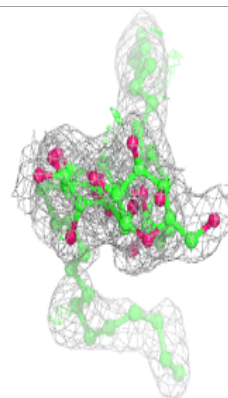
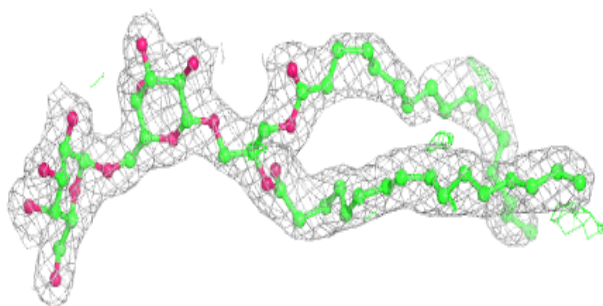
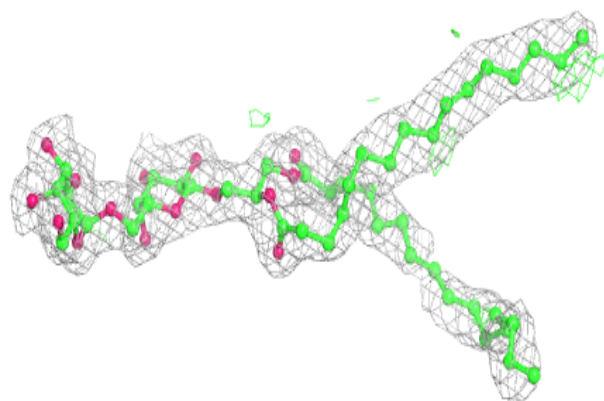
Electron density around CLA b 625:

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

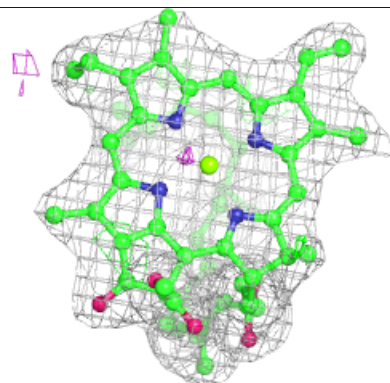
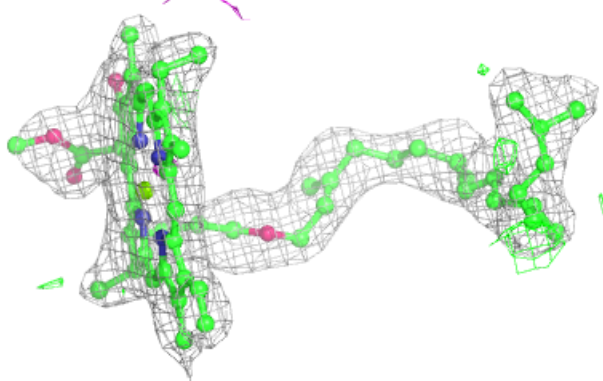
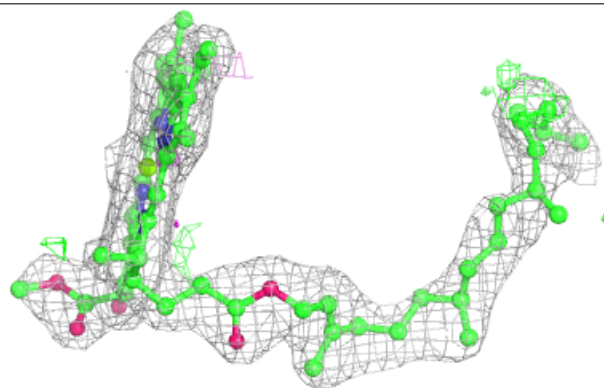


Electron density around DGD c 519:

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

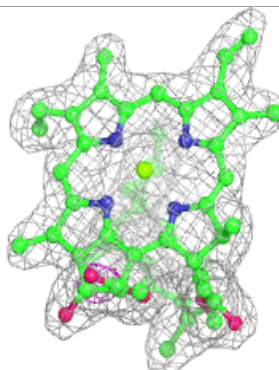
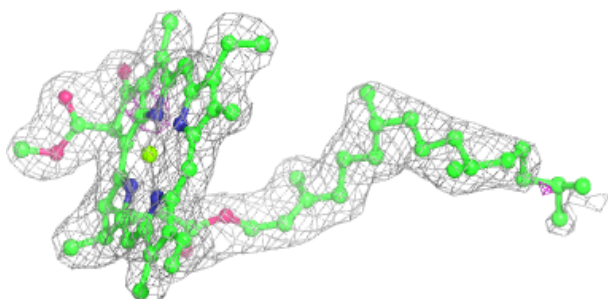
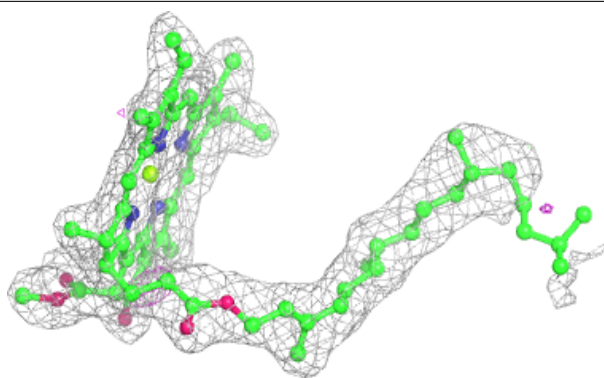
**Electron density around CLA c 510:**

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

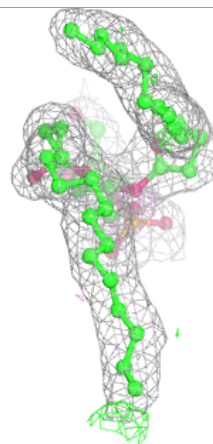
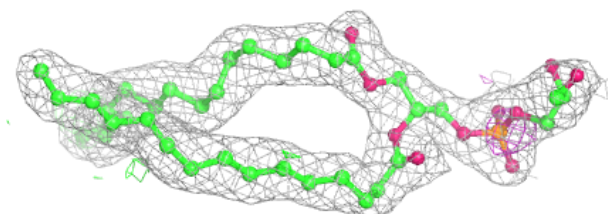
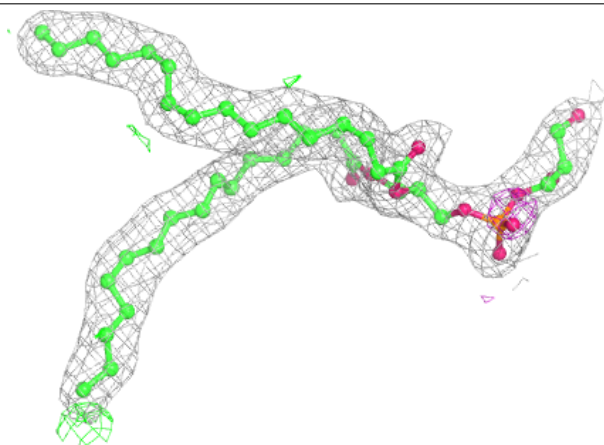


Electron density around CLA c 512:

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

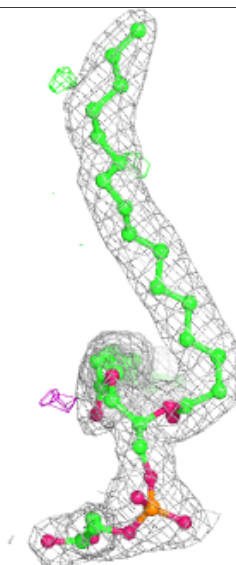
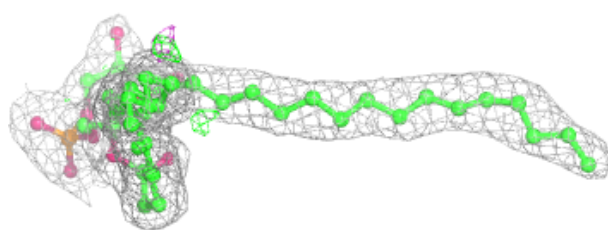
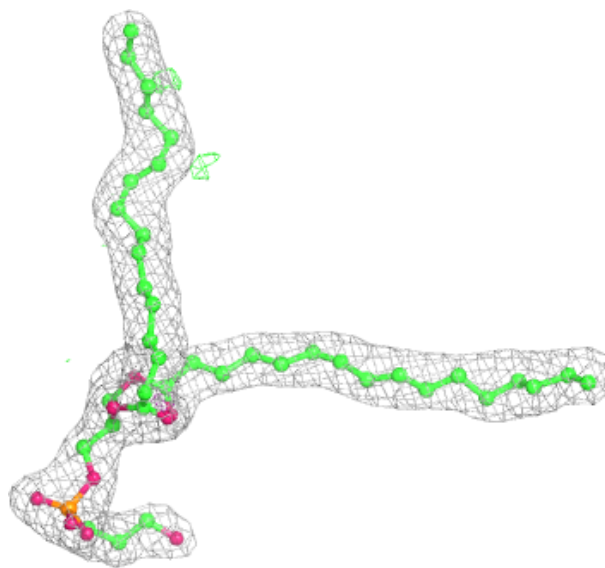
**Electron density around LHG d 408:**

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



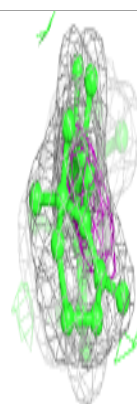
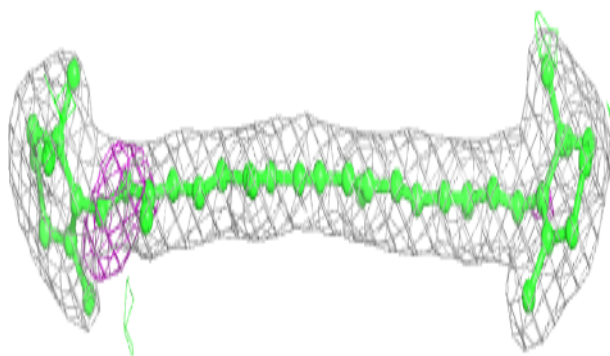
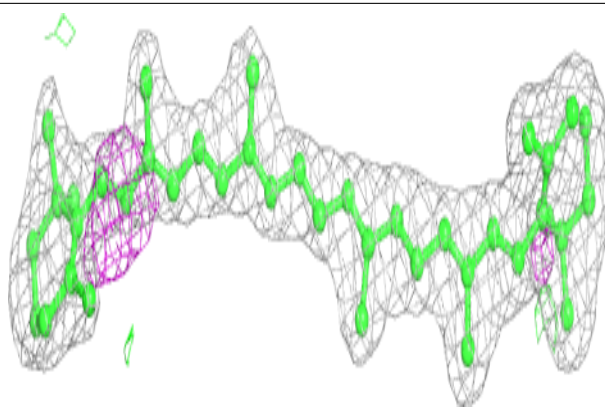
Electron density around LHG 1 101:

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

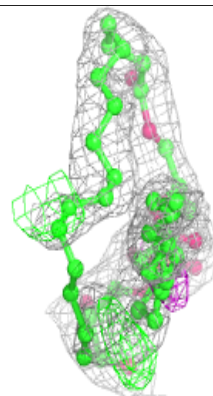
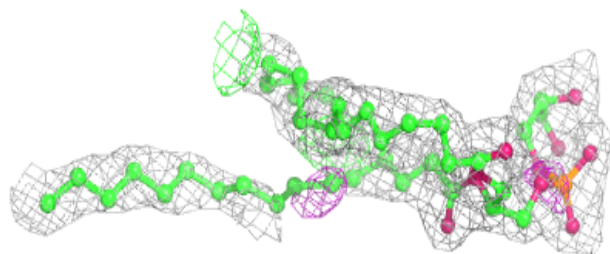
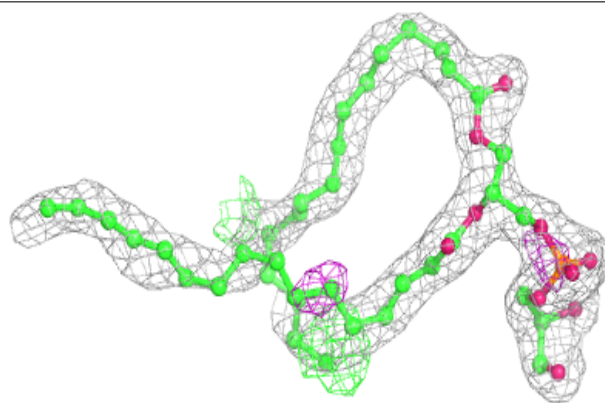


Electron density around BCR b 627:

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

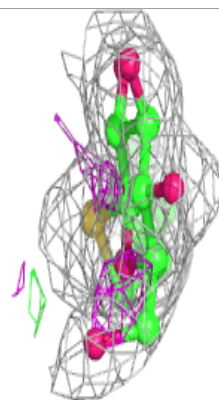
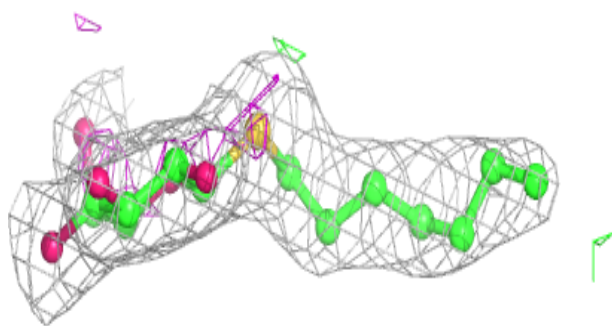
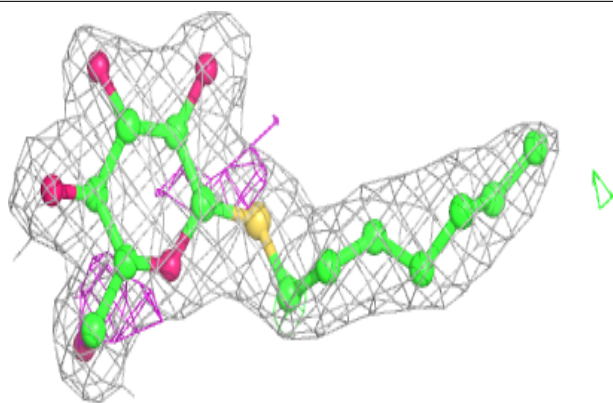
**Electron density around LHG D 409:**

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



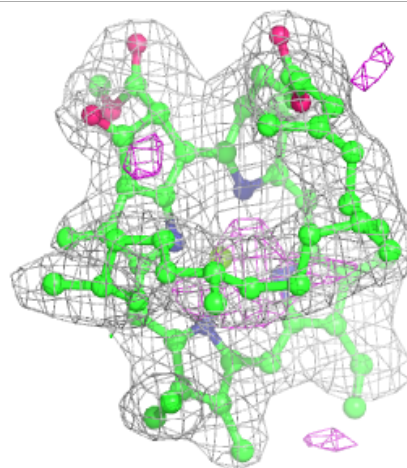
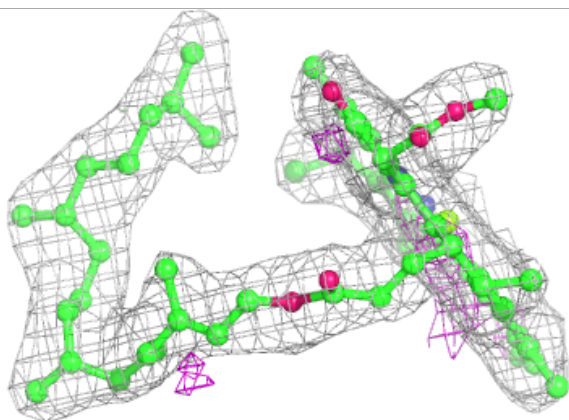
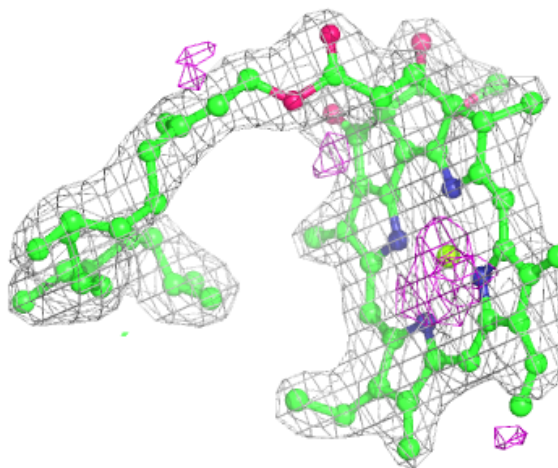
Electron density around HTG b 601:

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



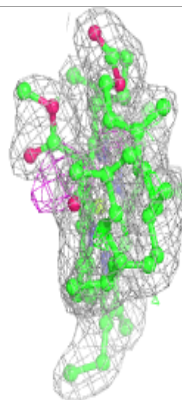
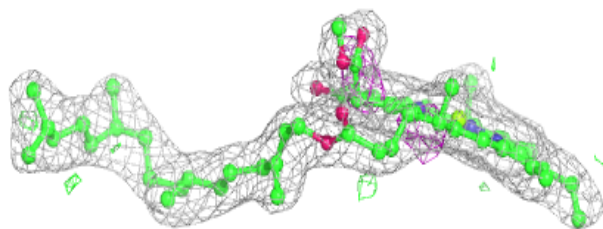
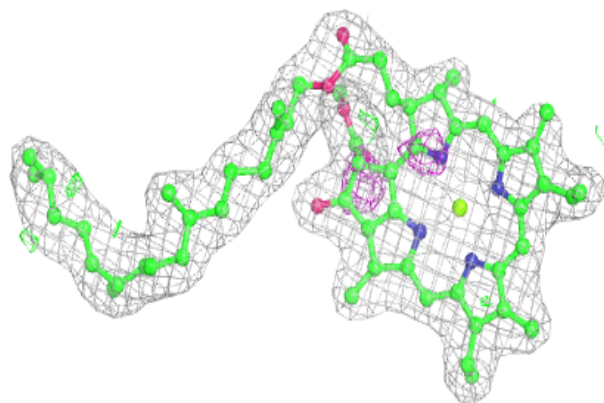
Electron density around CLA c 507:

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

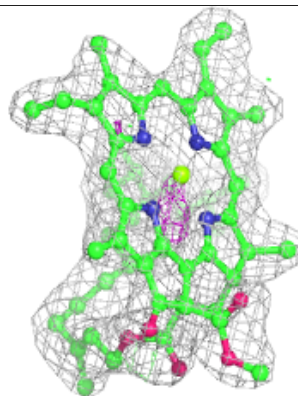
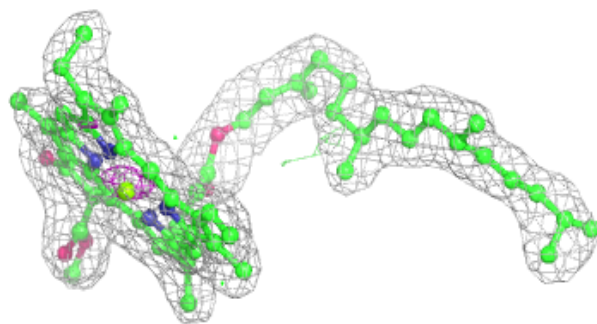
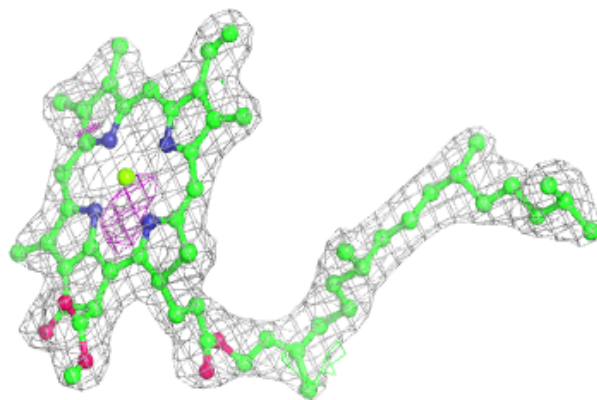


Electron density around CLA b 611:

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

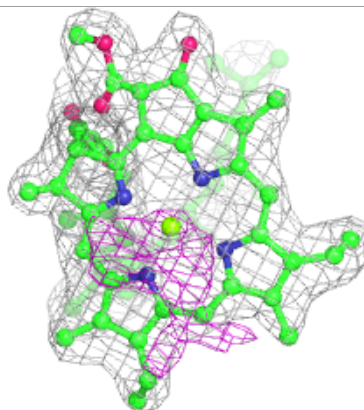
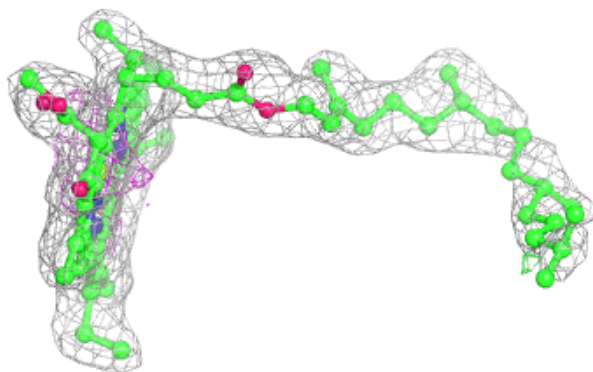
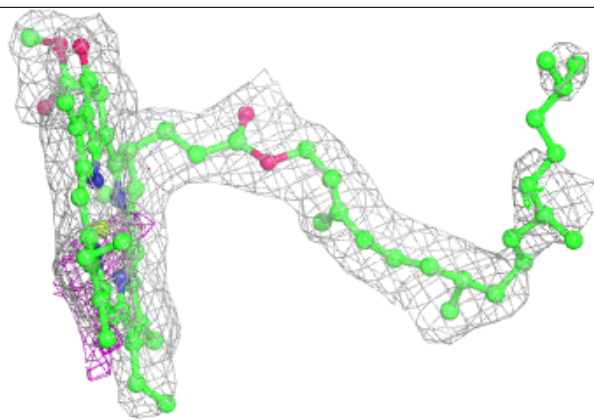
**Electron density around CLA C 512:**

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



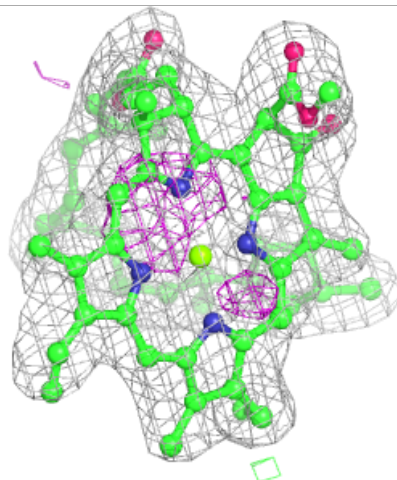
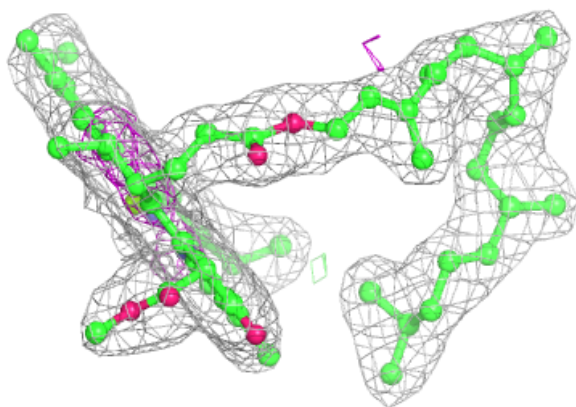
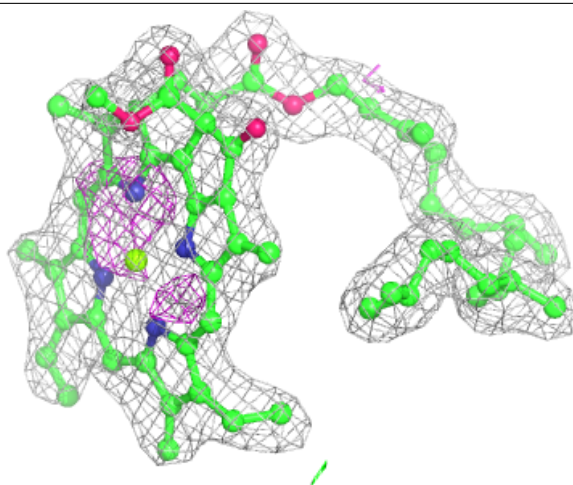
Electron density around CLA D 403:

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



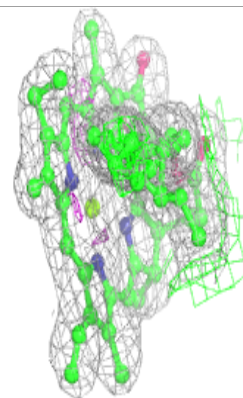
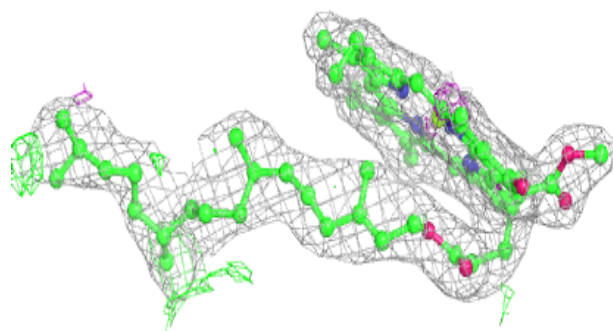
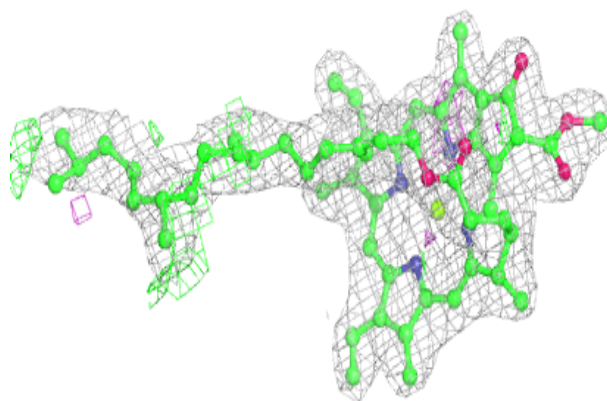
Electron density around CLA C 504:

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

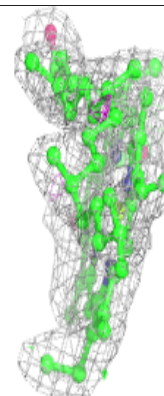
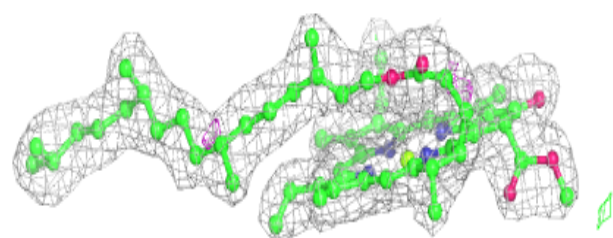
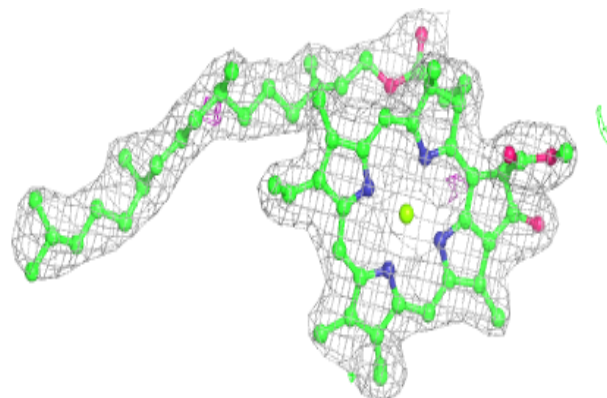


Electron density around CLA b 623:

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

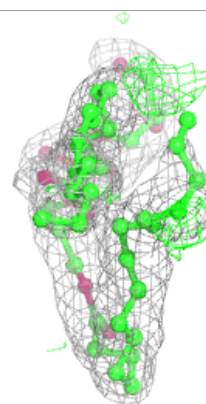
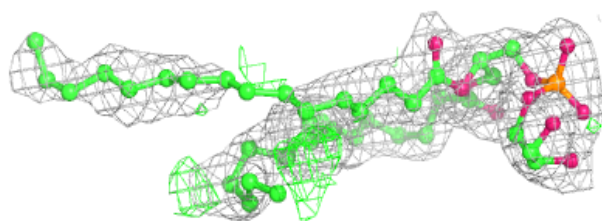
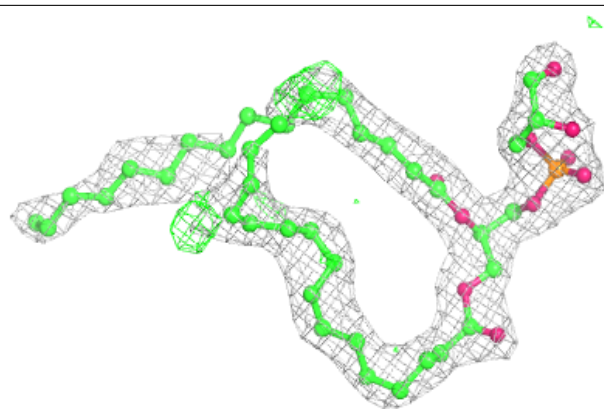
**Electron density around CLA c 505:**

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

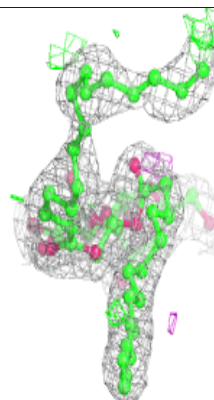
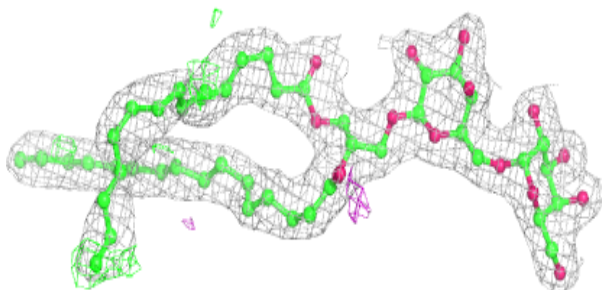
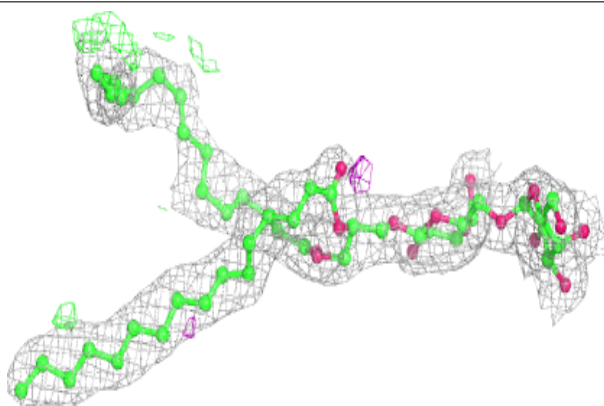


Electron density around LHG d 409:

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

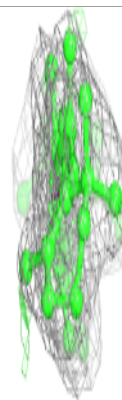
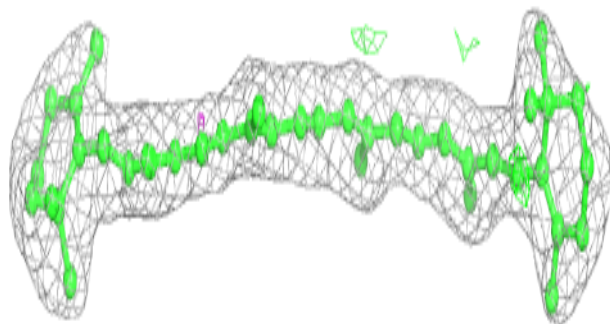
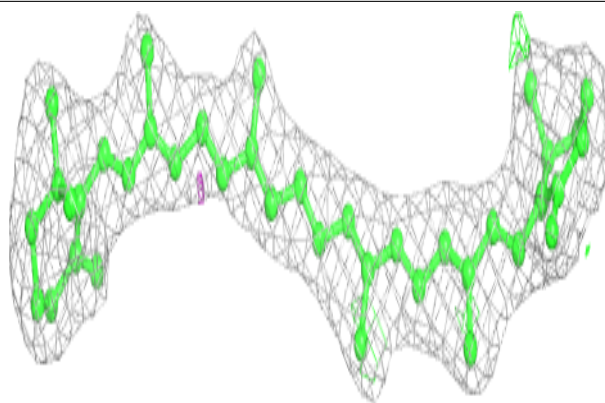
**Electron density around DGD C 517:**

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



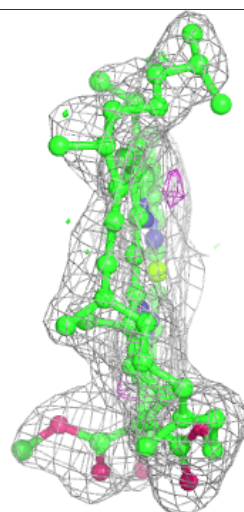
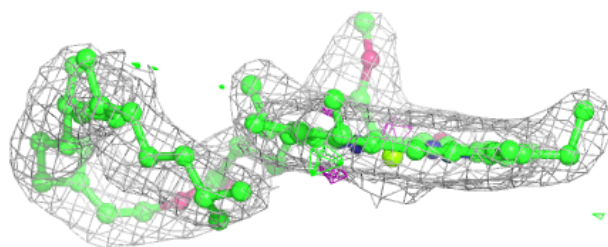
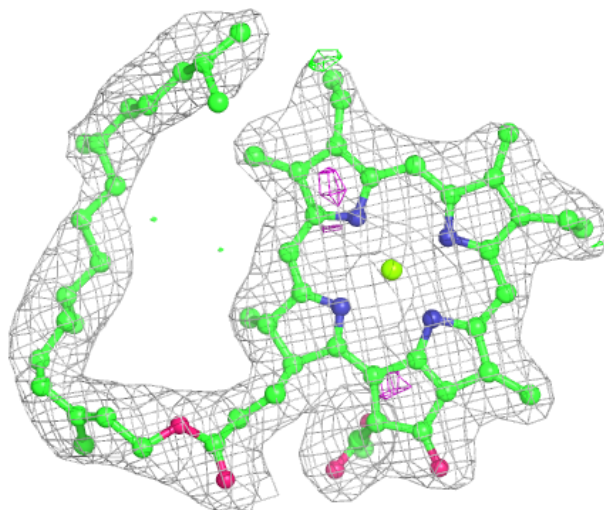
Electron density around BCR y 101:

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



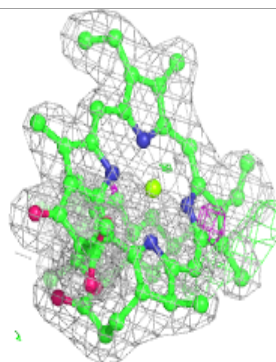
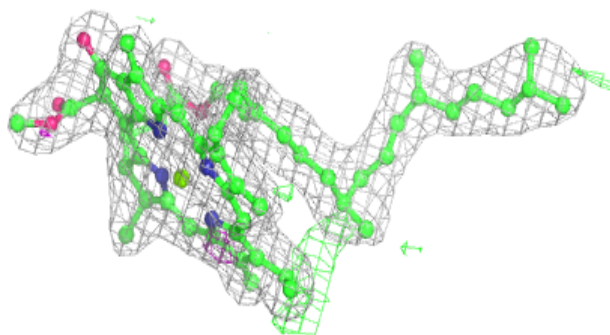
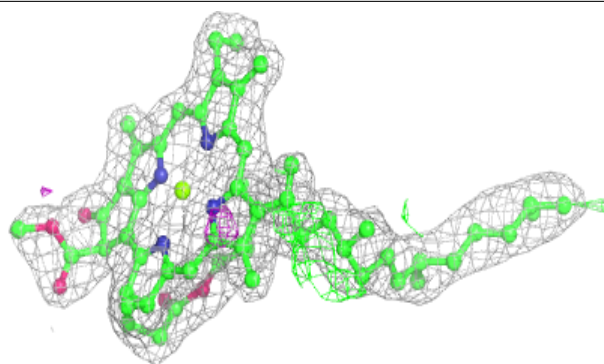
Electron density around CLA C 513:

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

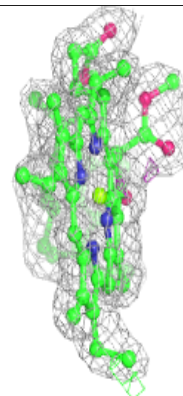
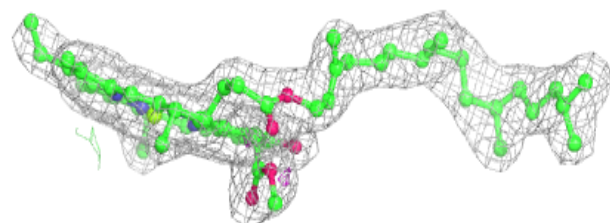
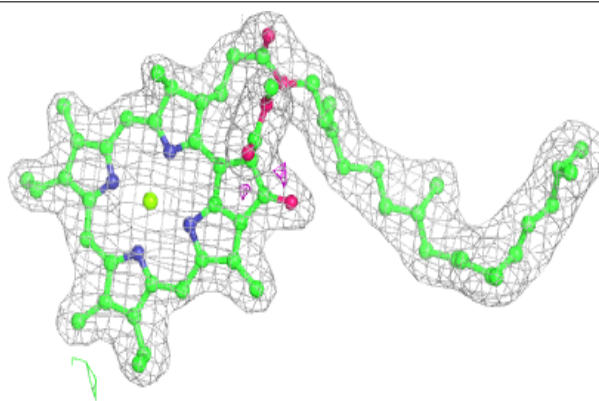


Electron density around CLA c 509:

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

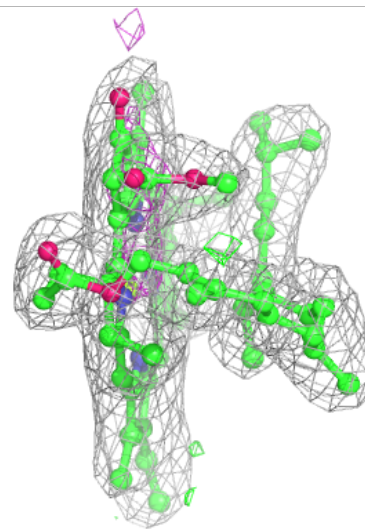
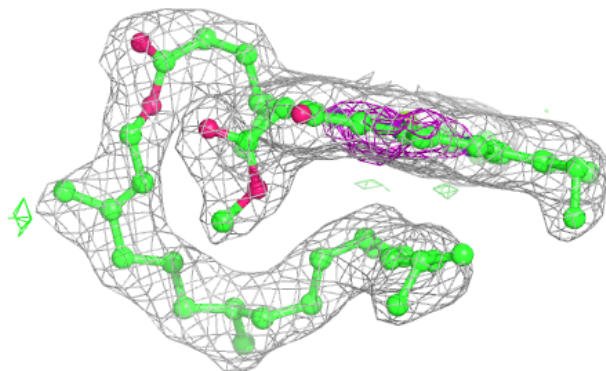
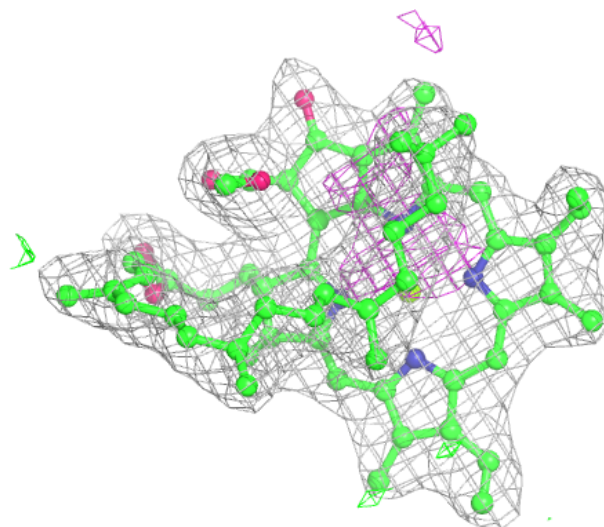
**Electron density around CLA B 603:**

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



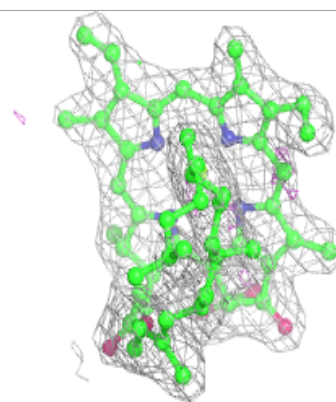
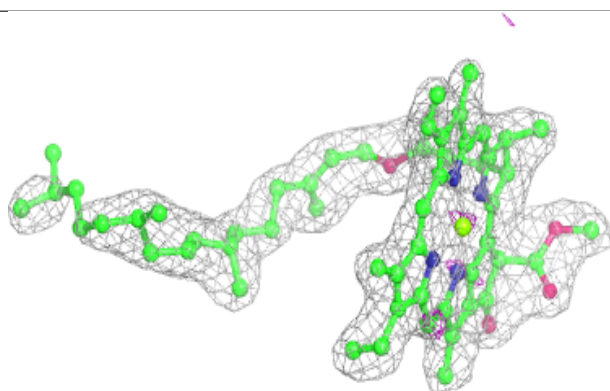
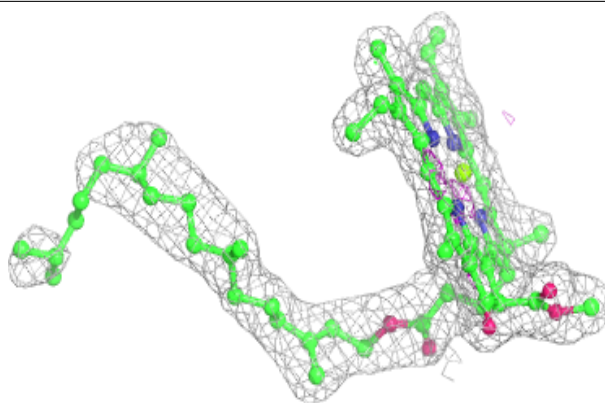
Electron density around CLA c 514:

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



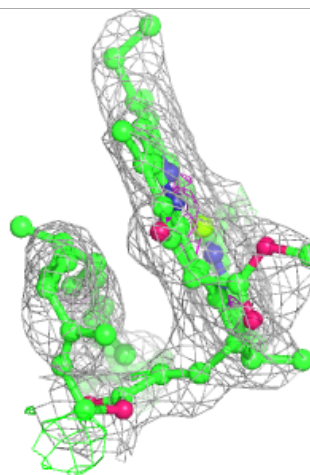
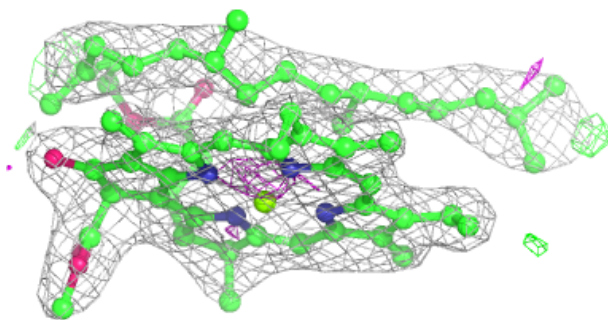
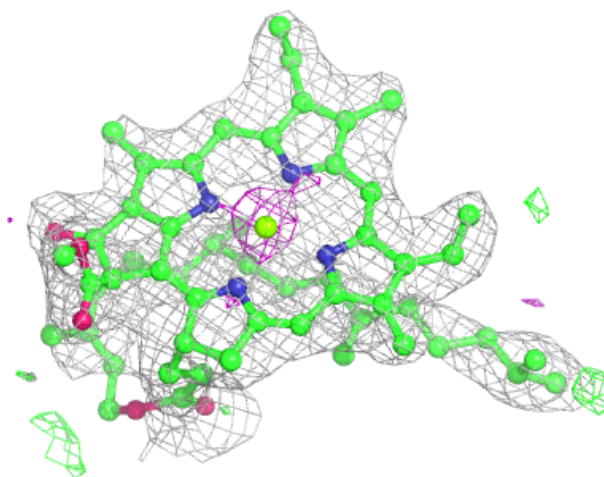
Electron density around CLA C 509:

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



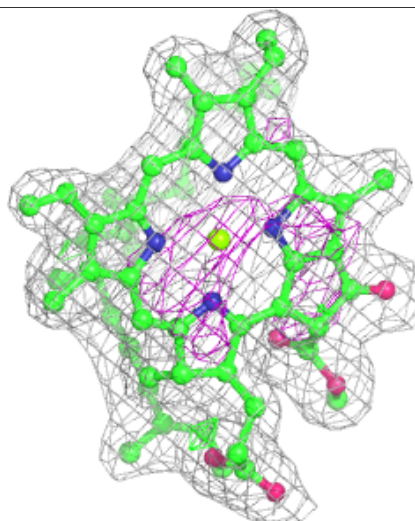
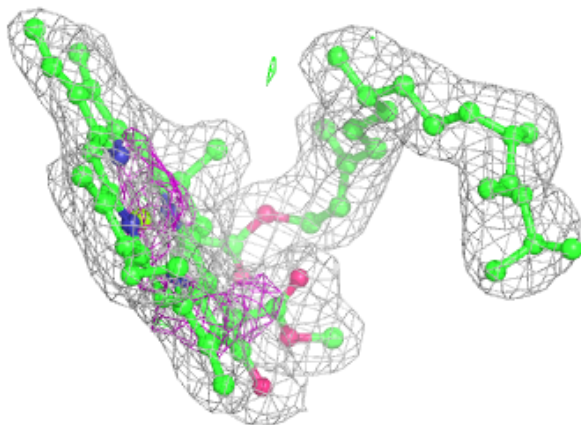
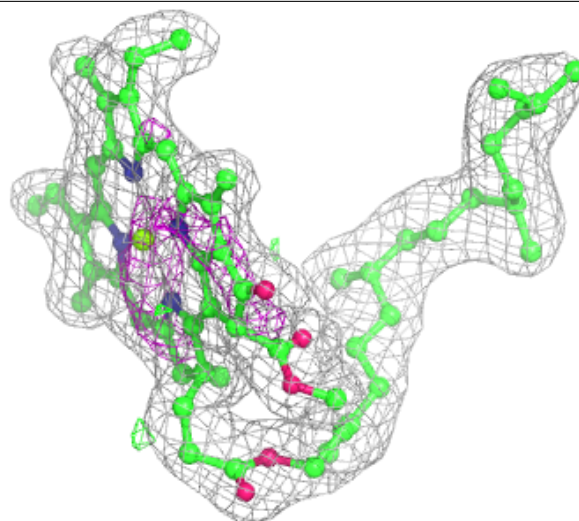
Electron density around CLA b 610:

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



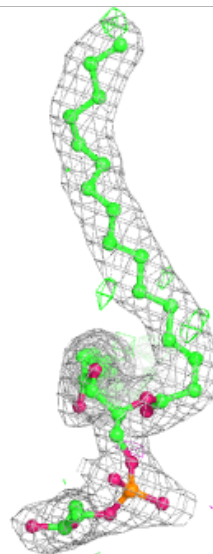
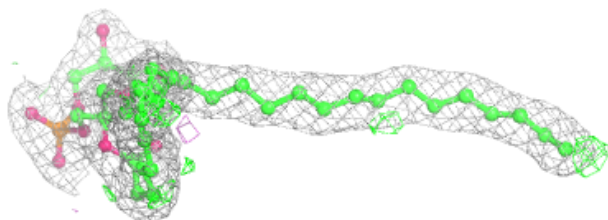
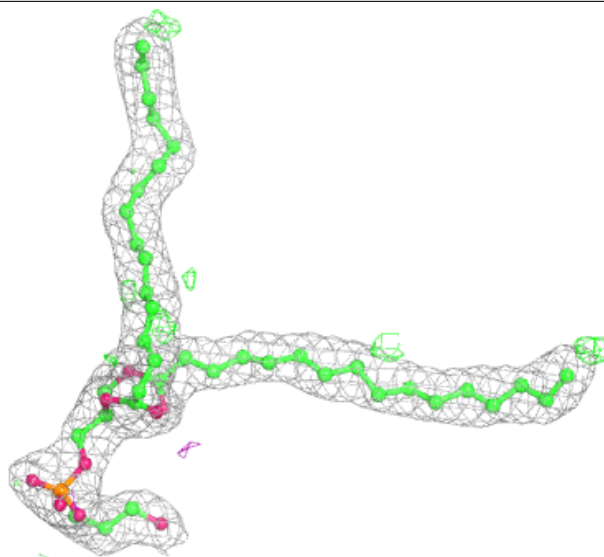
Electron density around CLA B 614:

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



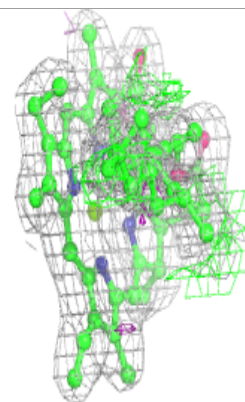
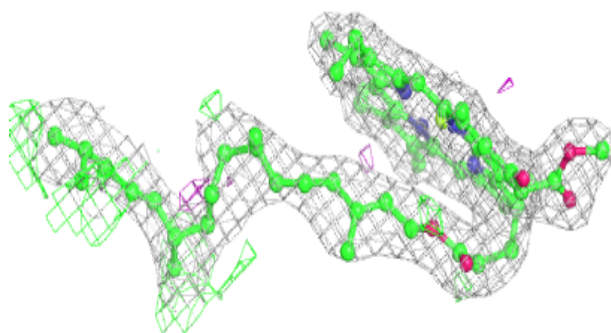
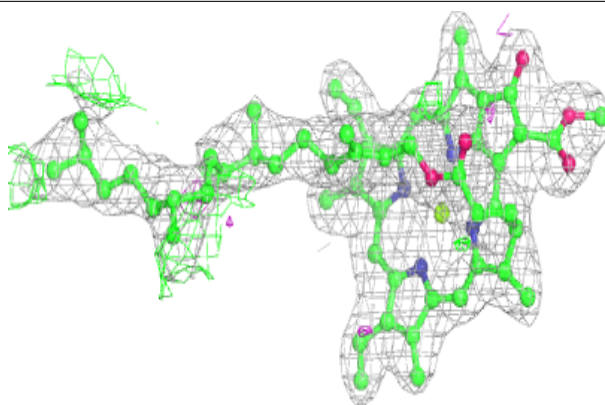
Electron density around LHG L 101:

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

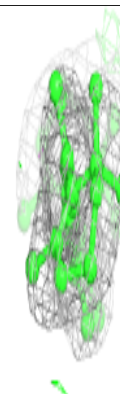
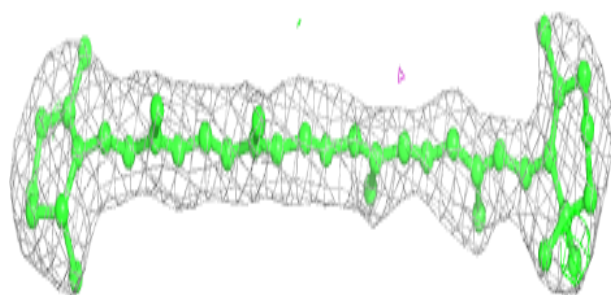
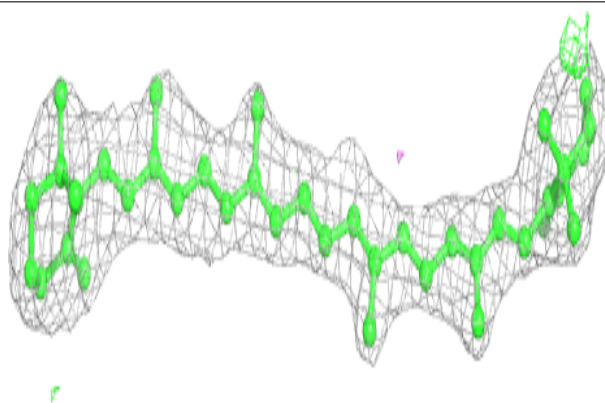


Electron density around CLA B 615:

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

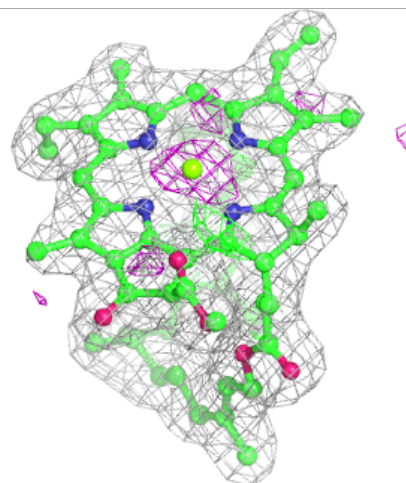
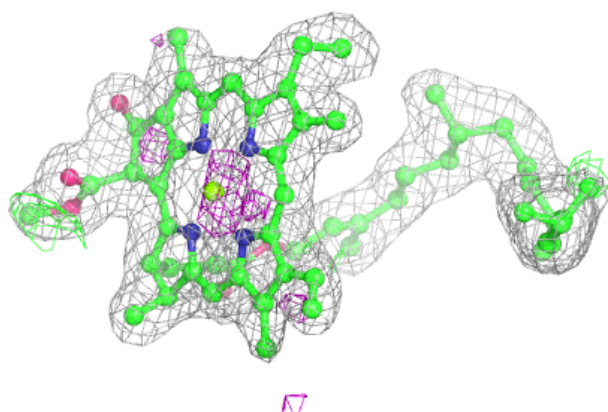
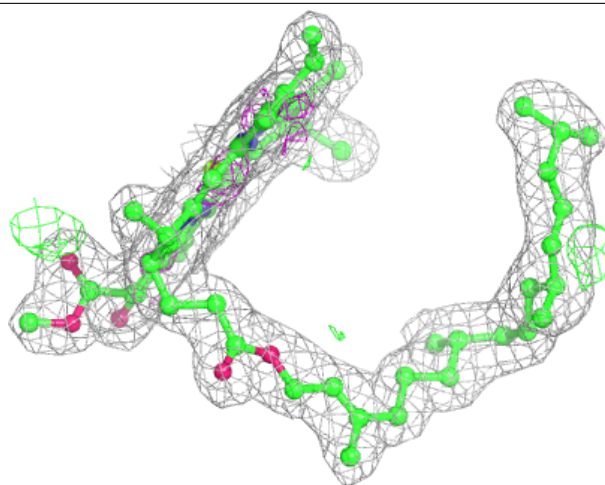
**Electron density around BCR c 527:**

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



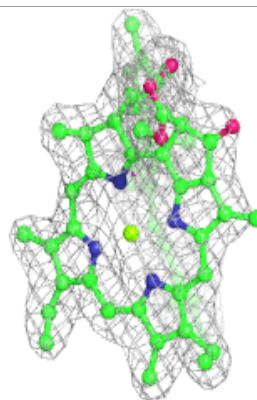
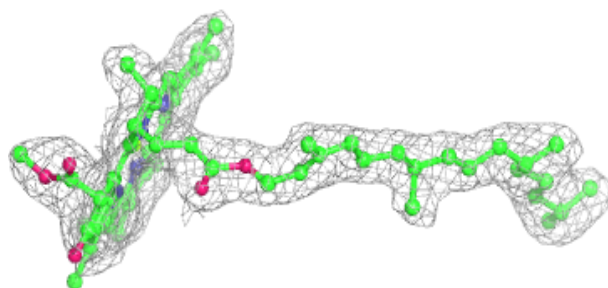
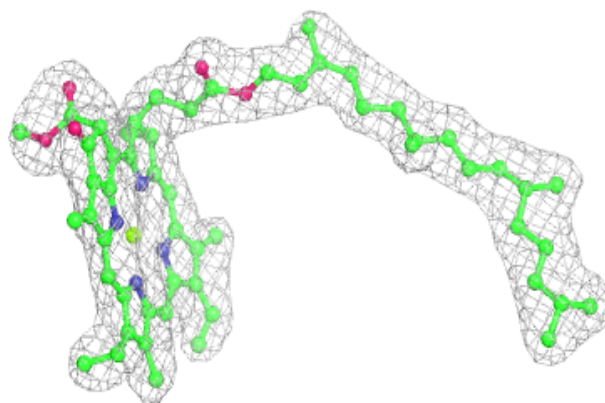
Electron density around CLA b 620:

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

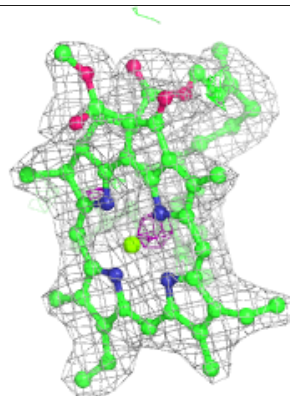
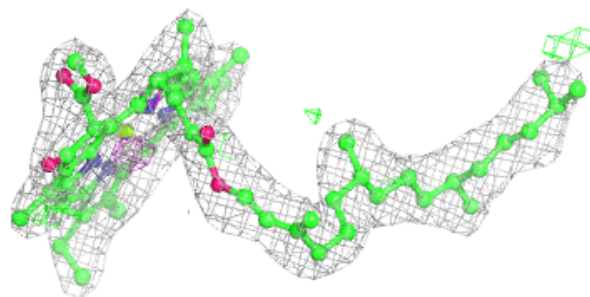
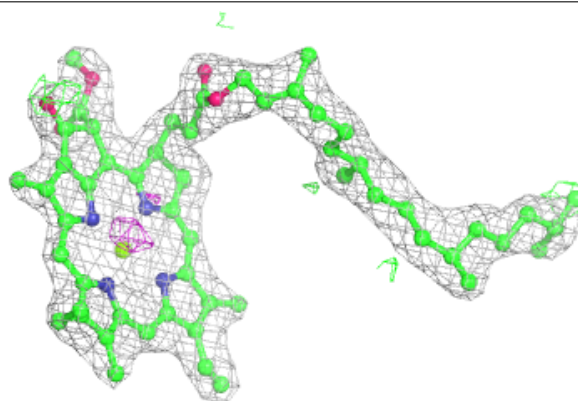


Electron density around CLA B 610:

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

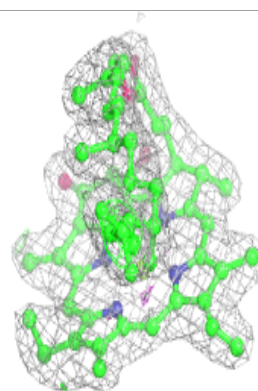
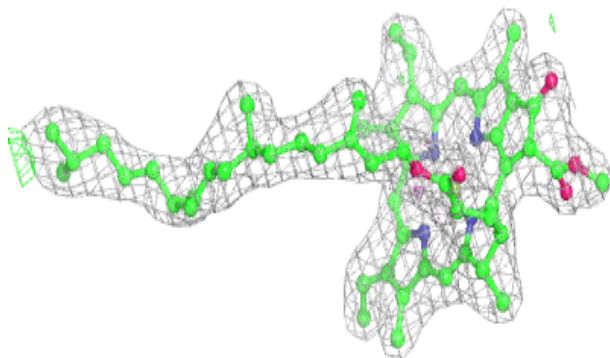
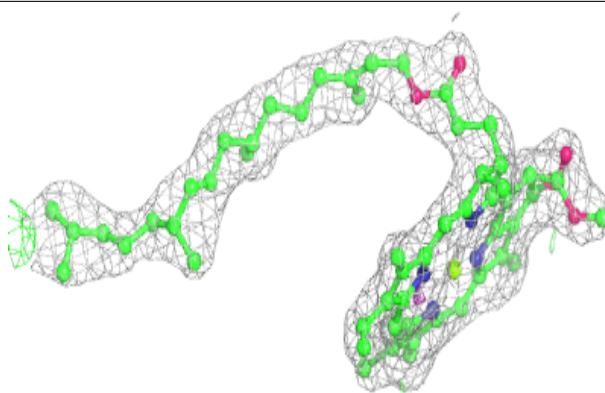
**Electron density around CLA c 515:**

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

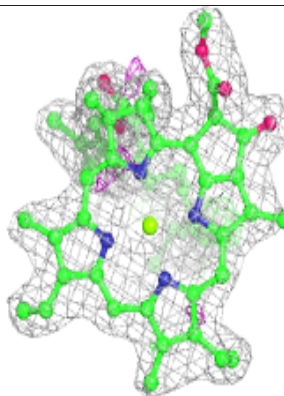
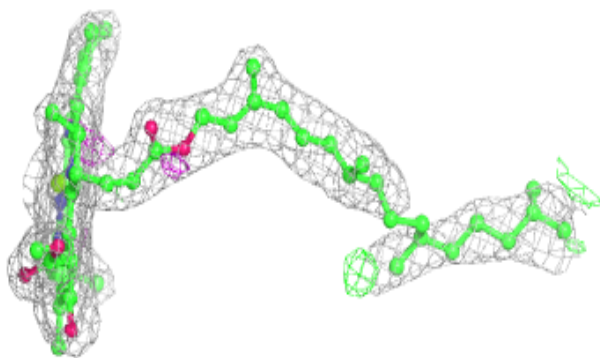
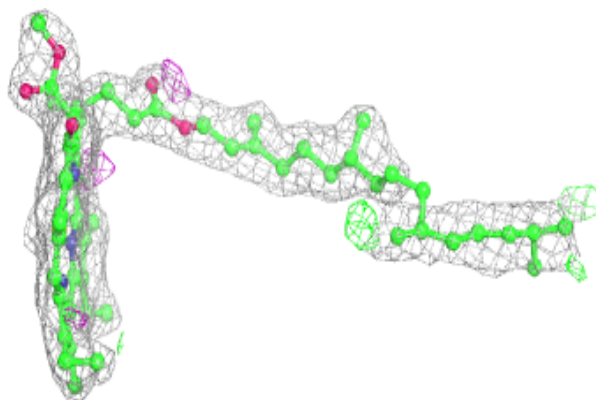


Electron density around CLA c 508:

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

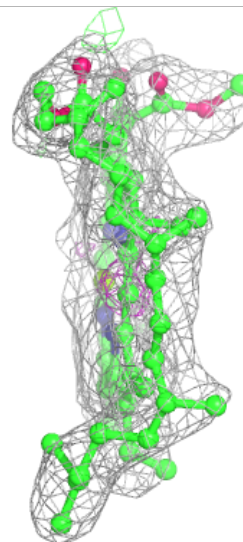
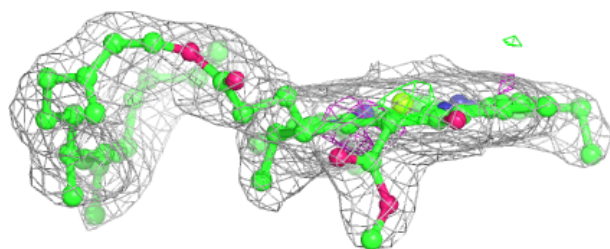
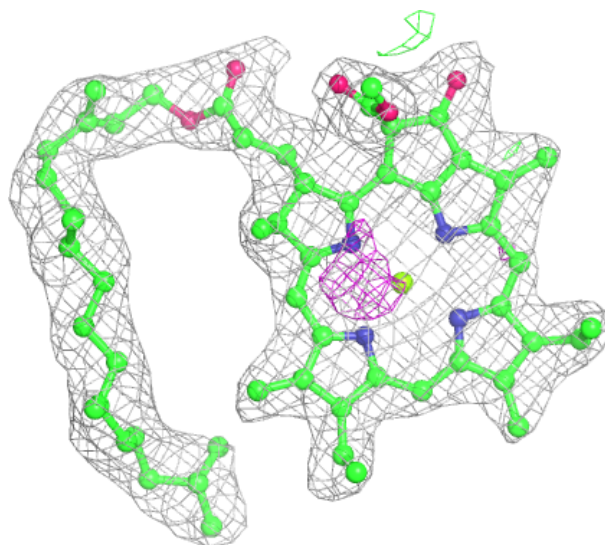
**Electron density around CLA B 607:**

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



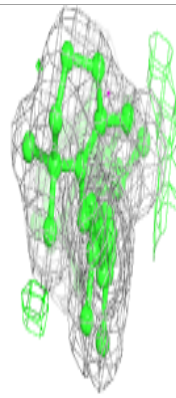
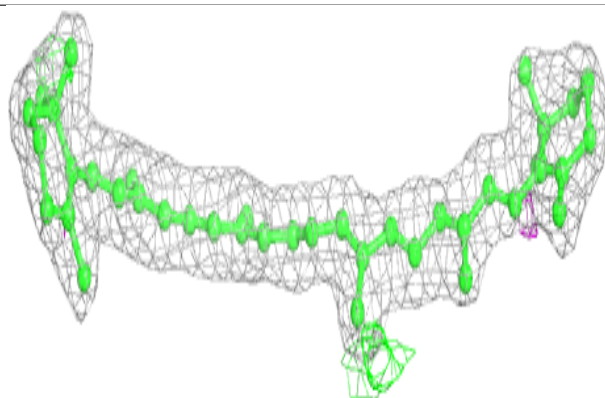
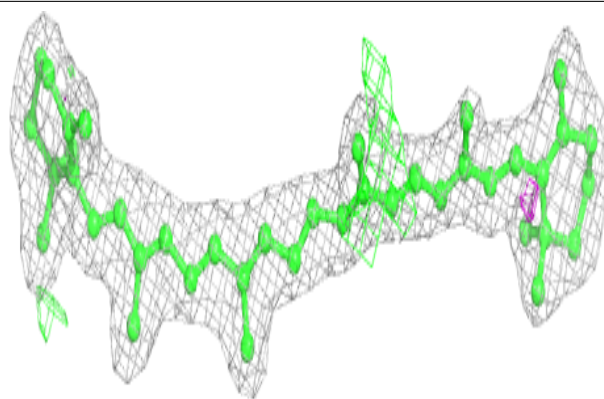
Electron density around CLA c 516:

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

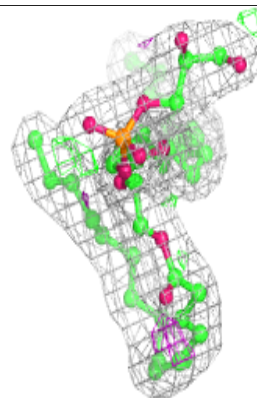
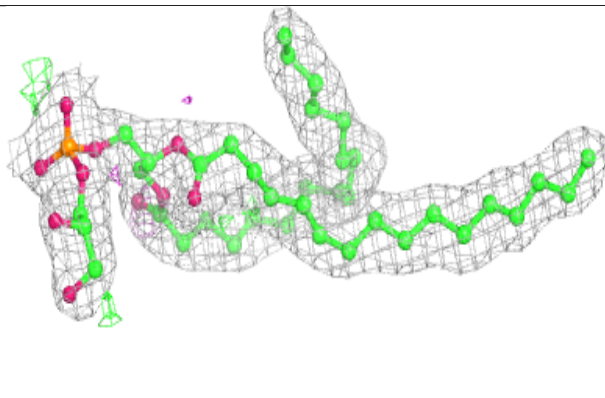
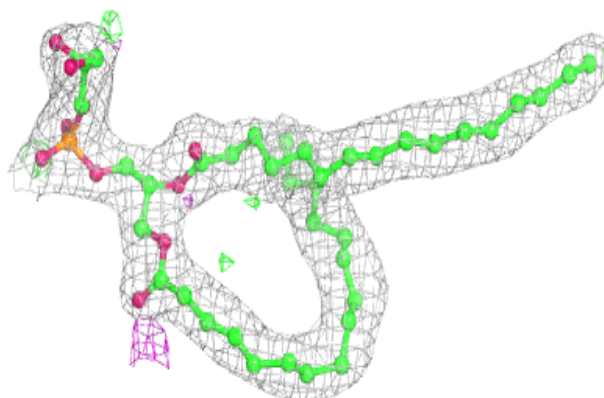


Electron density around BCR T 103:

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

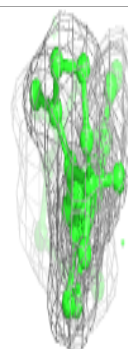
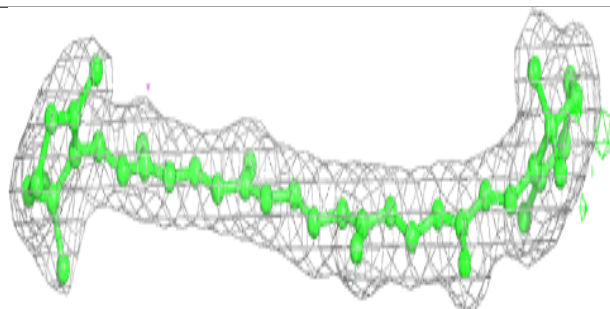
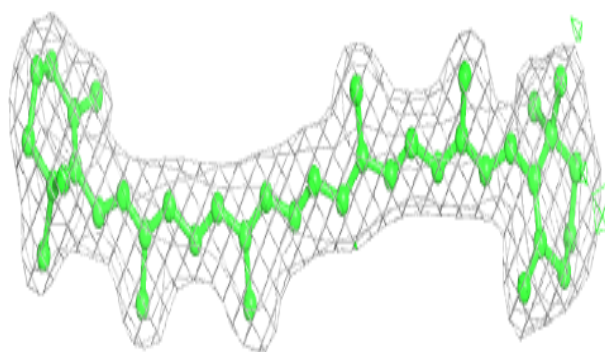
**Electron density around LHG d 407:**

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

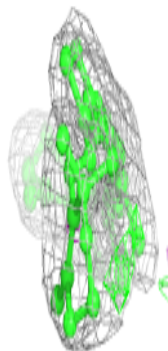
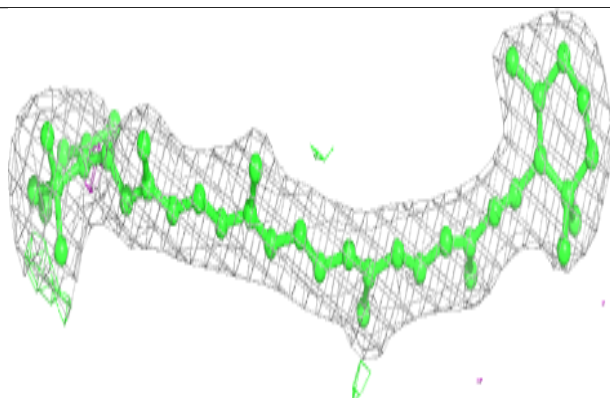
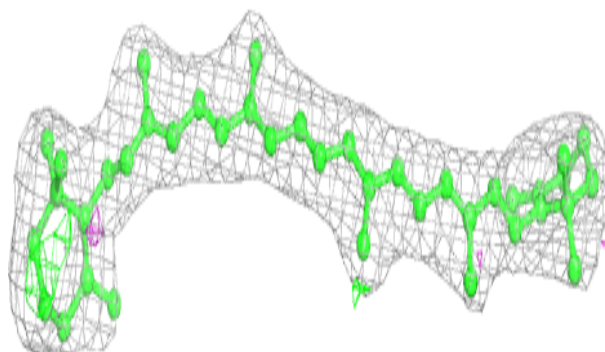


Electron density around BCR B 620:

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

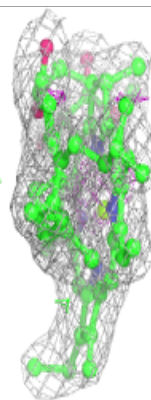
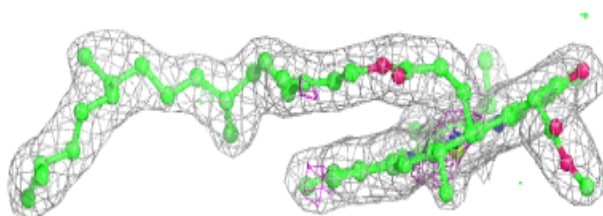
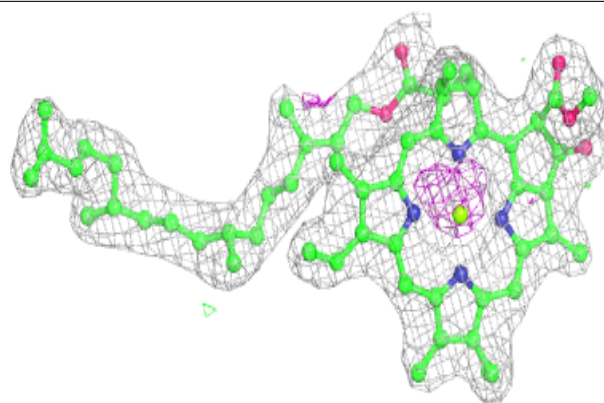
**Electron density around BCR d 405:**

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

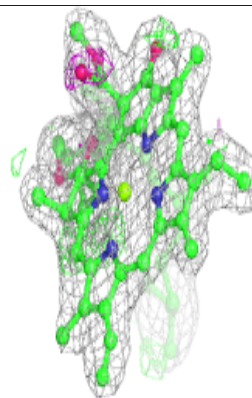
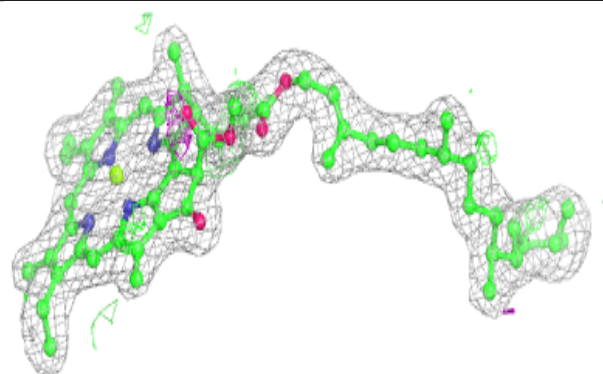
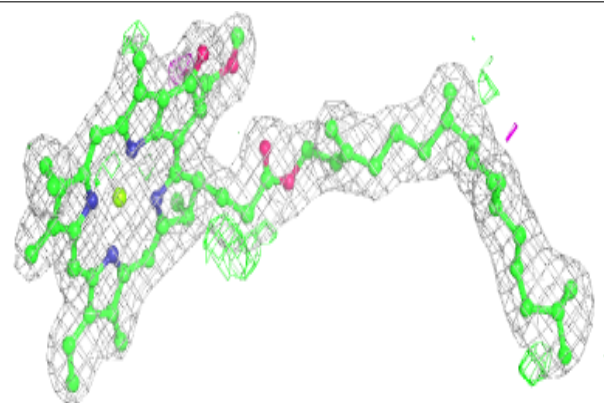


Electron density around CLA b 612:

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

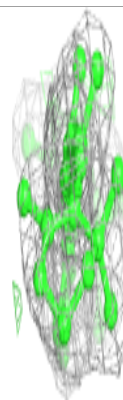
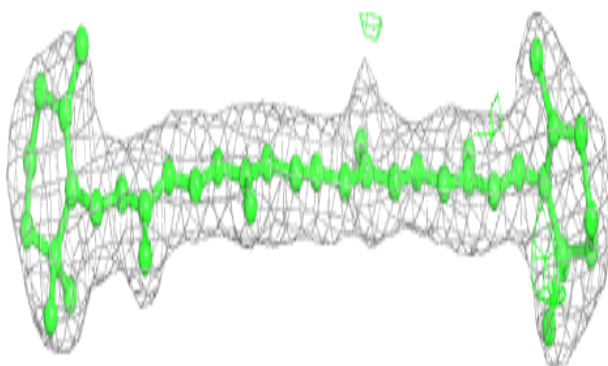
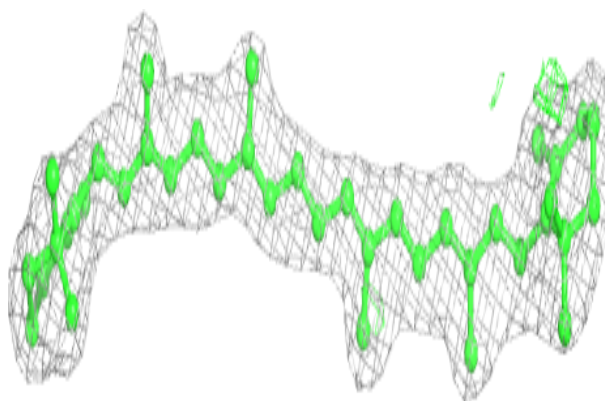
**Electron density around CLA A 405:**

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

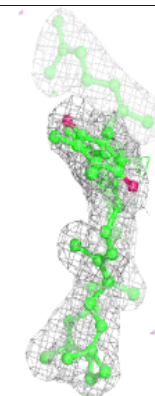
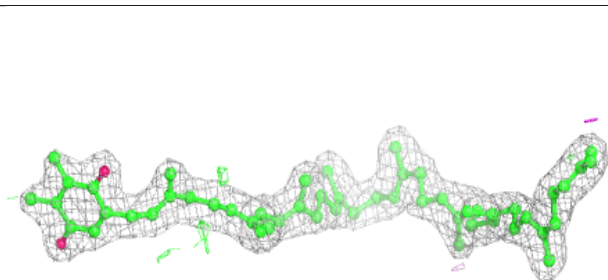
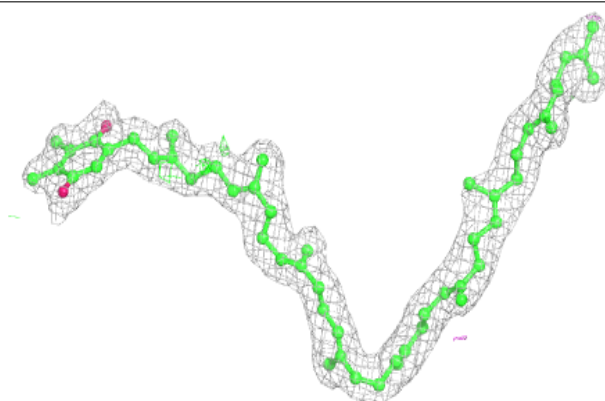


Electron density around BCR C 515:

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

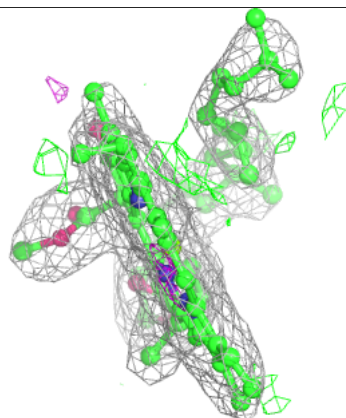
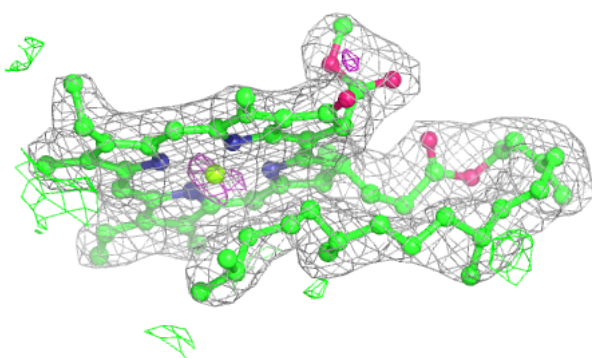
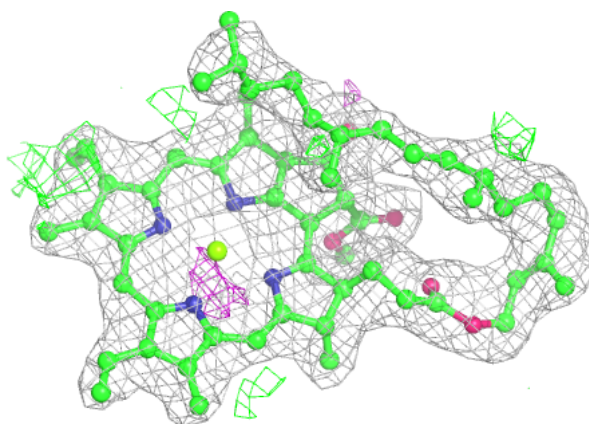
**Electron density around PL9 d 406:**

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



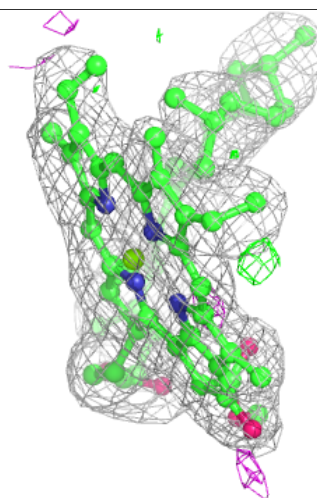
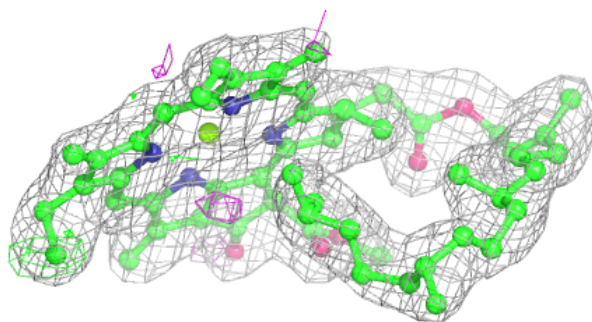
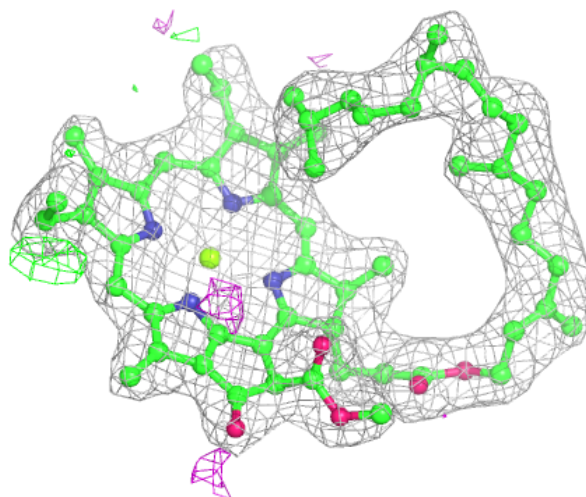
Electron density around CLA c 513:

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



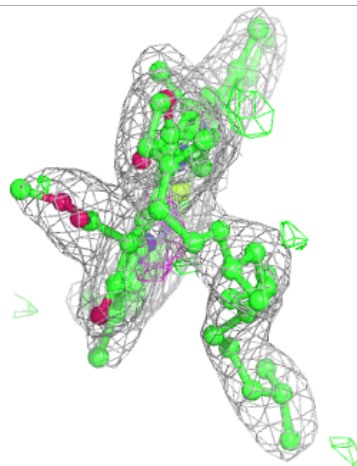
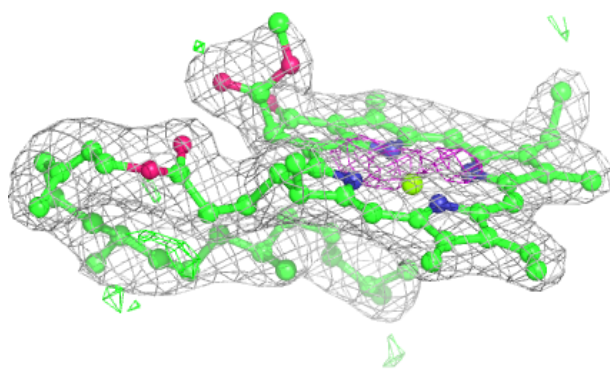
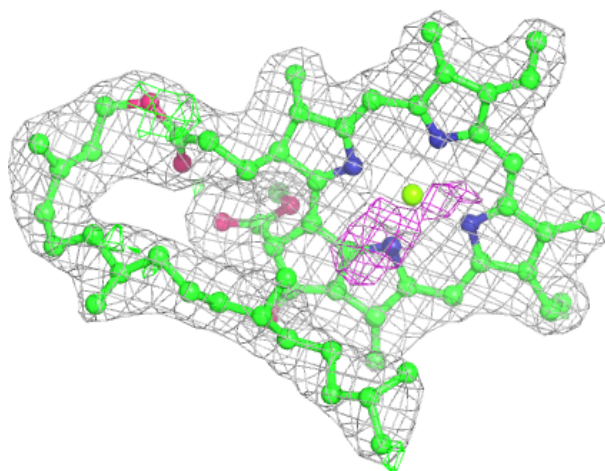
Electron density around CLA B 616:

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



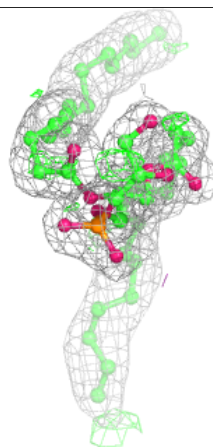
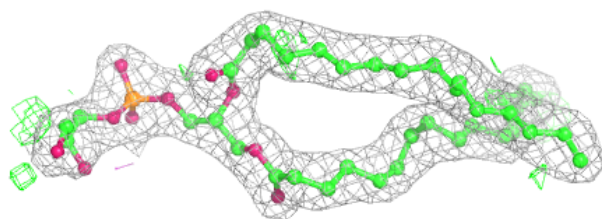
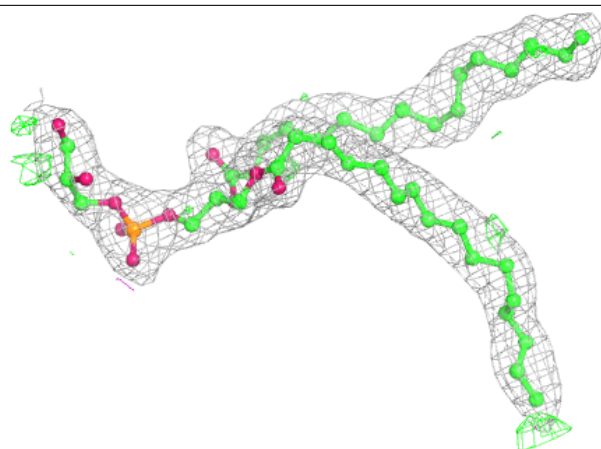
Electron density around CLA C 510:

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

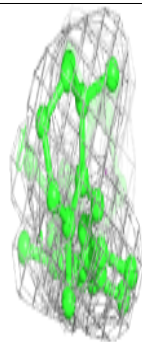
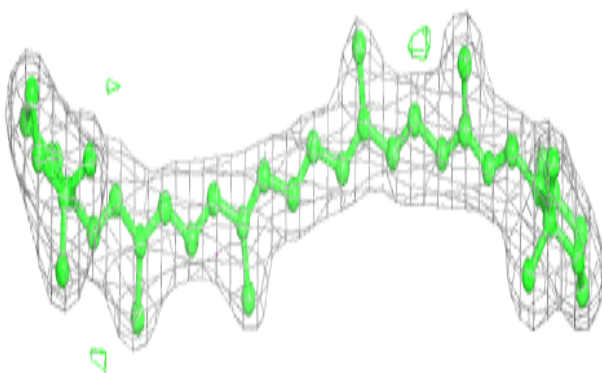
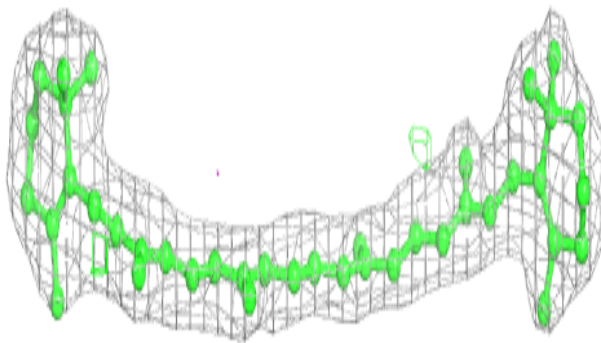


Electron density around LHG D 408:

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

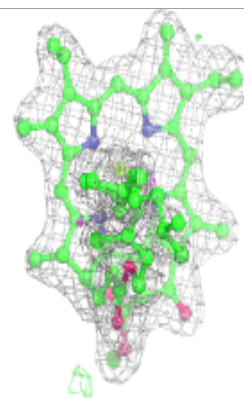
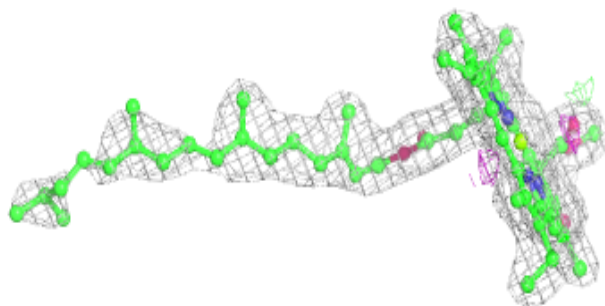
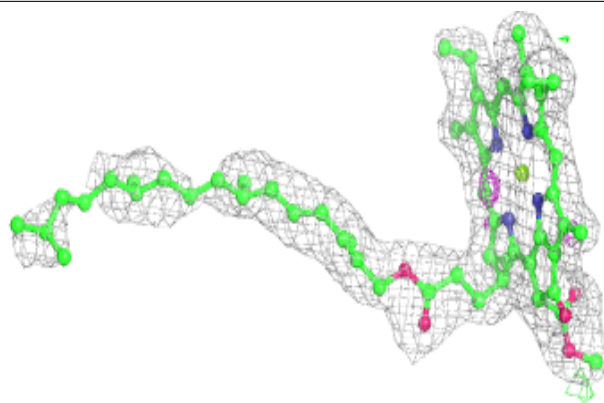
**Electron density around BCR K 101:**

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

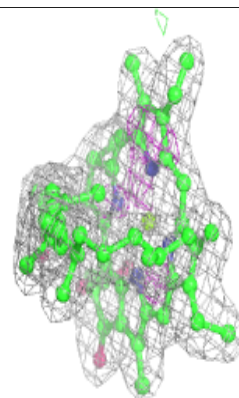
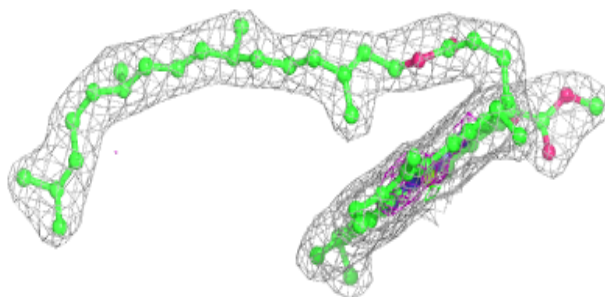
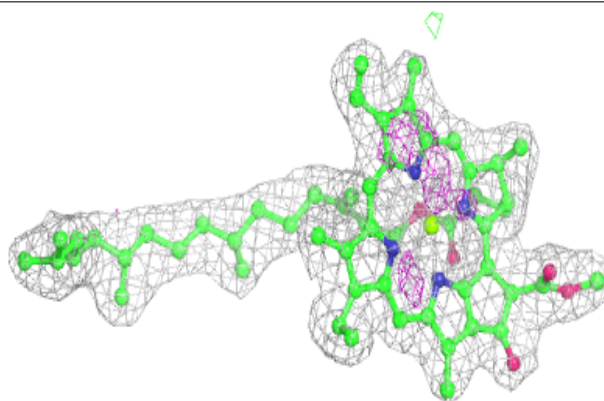


Electron density around CLA d 404:

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

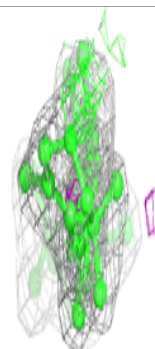
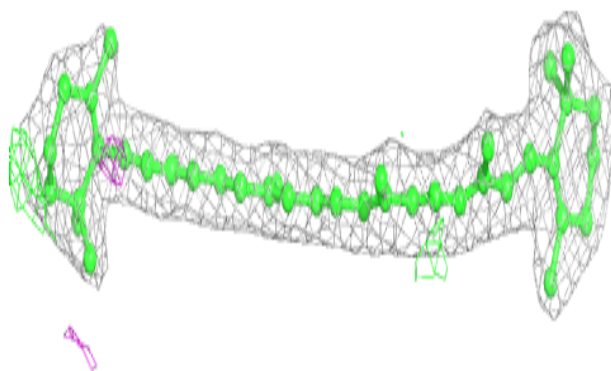
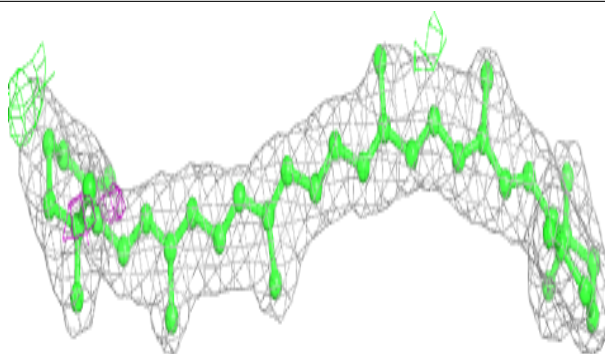
**Electron density around CLA b 617:**

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

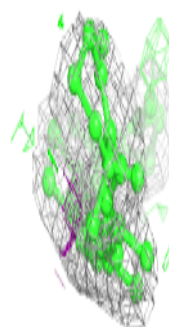
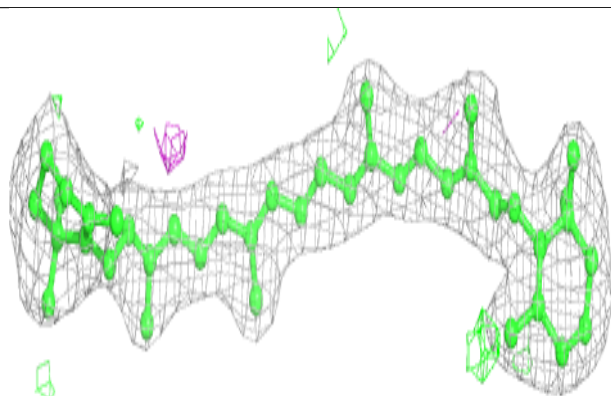
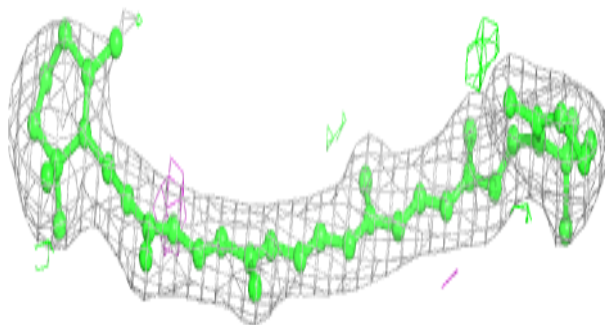


Electron density around BCR H 101:

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

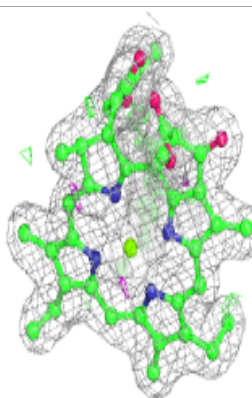
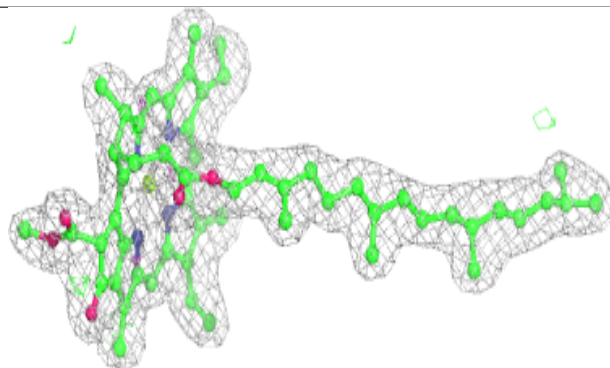
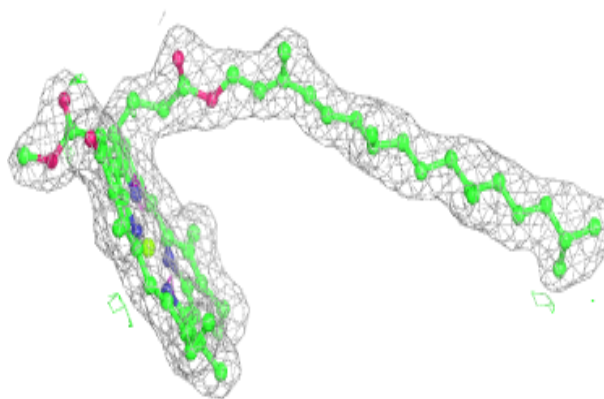
**Electron density around BCR D 404:**

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

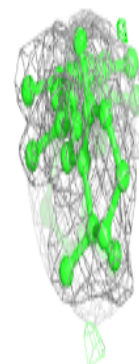
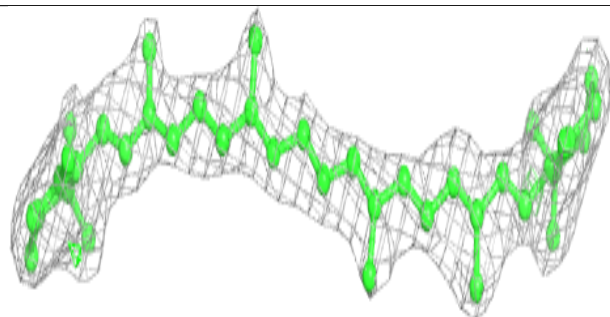
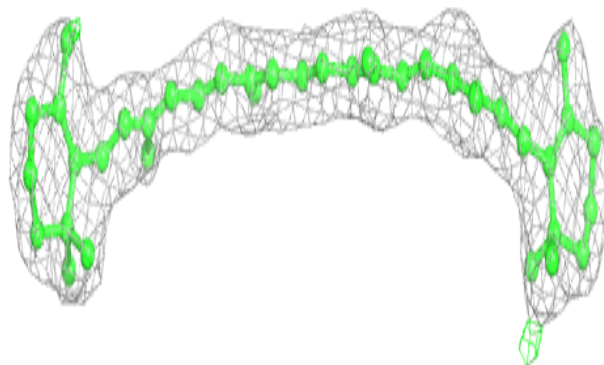


Electron density around CLA B 608:

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

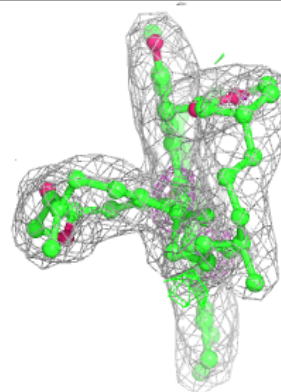
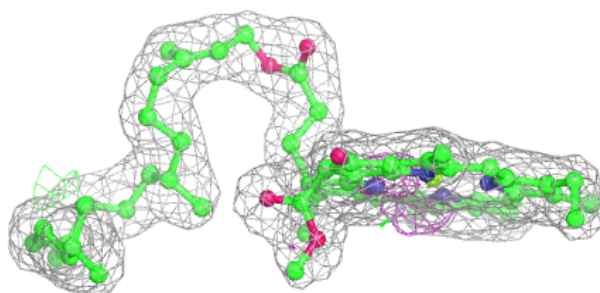
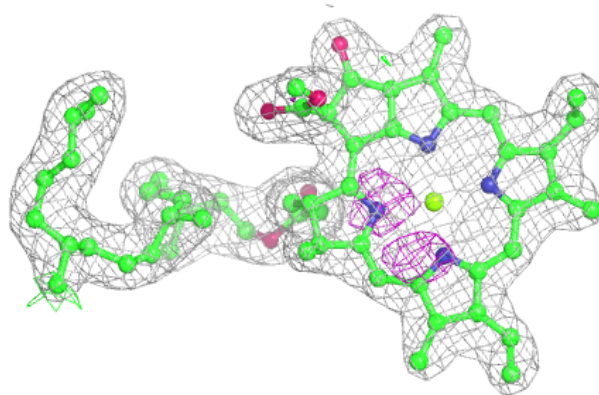
**Electron density around BCR k 101:**

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

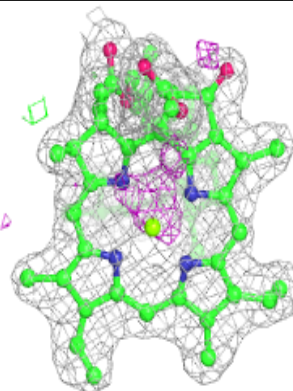
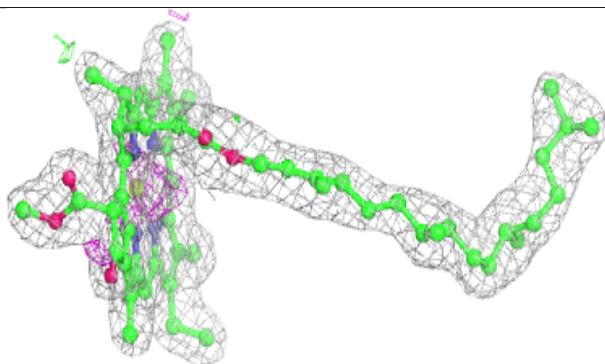
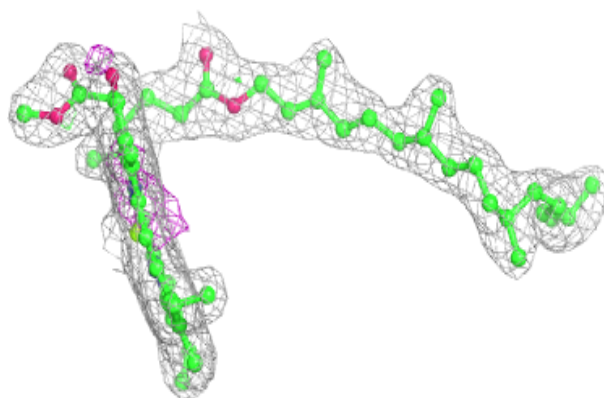


Electron density around CLA b 621:

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

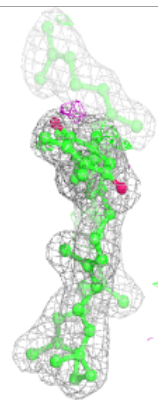
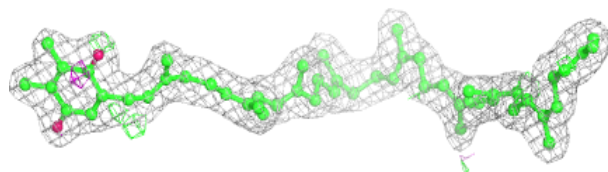
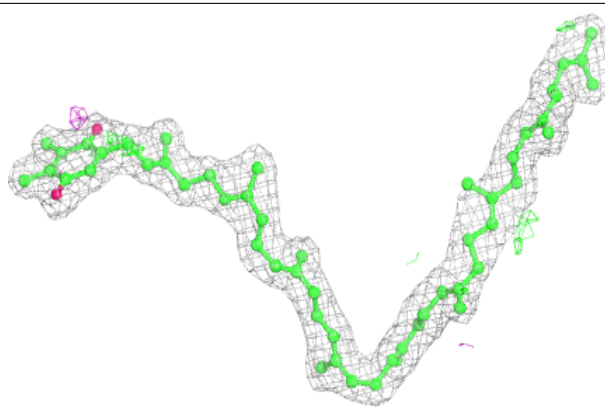
**Electron density around CLA b 614:**

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



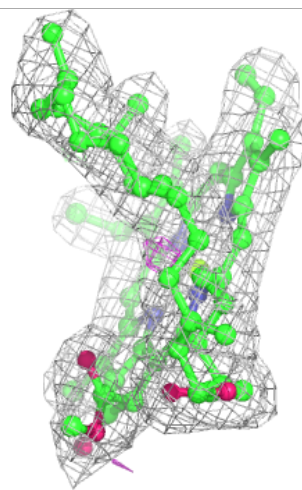
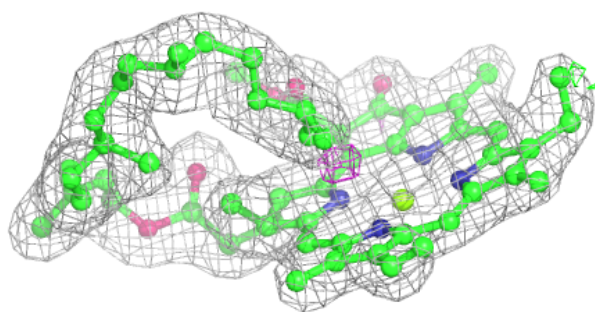
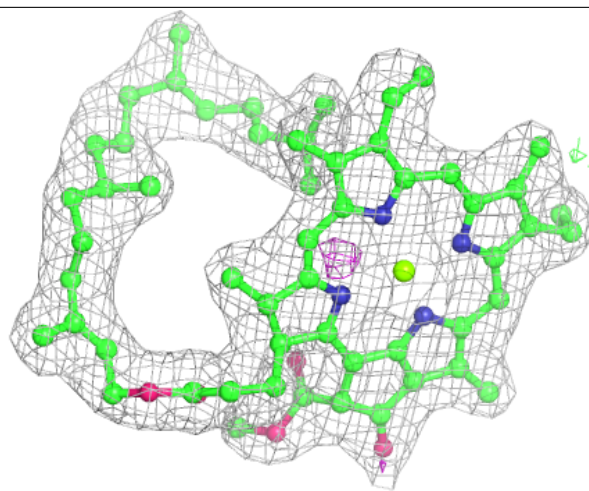
Electron density around PL9 D 405:

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



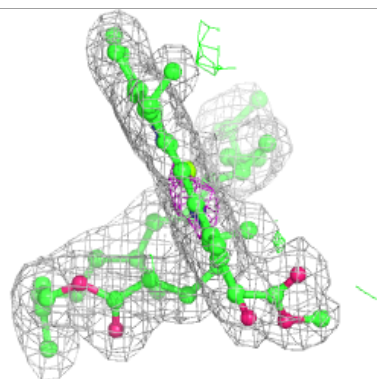
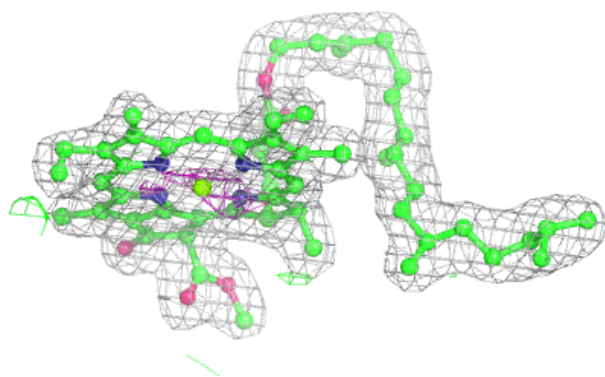
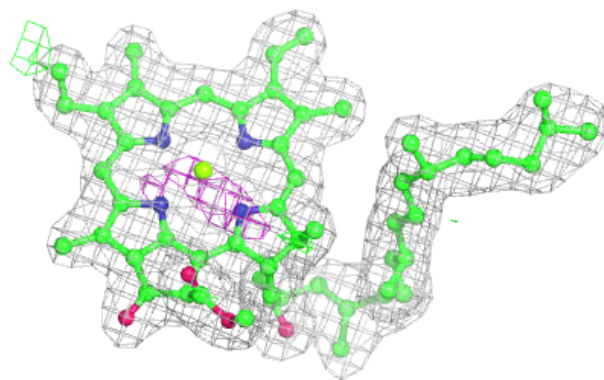
Electron density around CLA b 624:

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

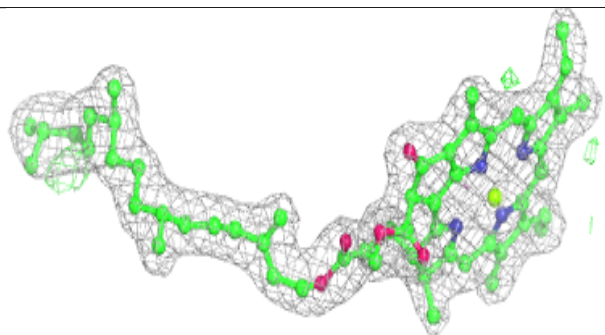
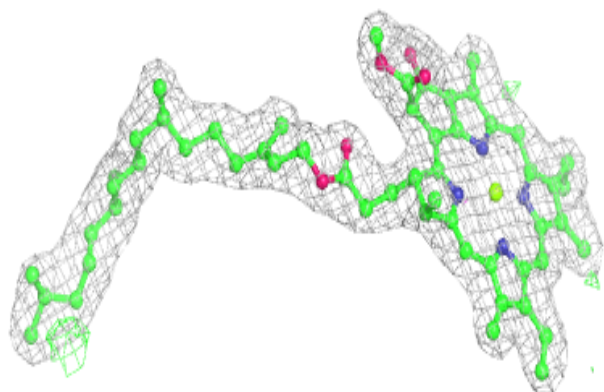


Electron density around CLA d 402:

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

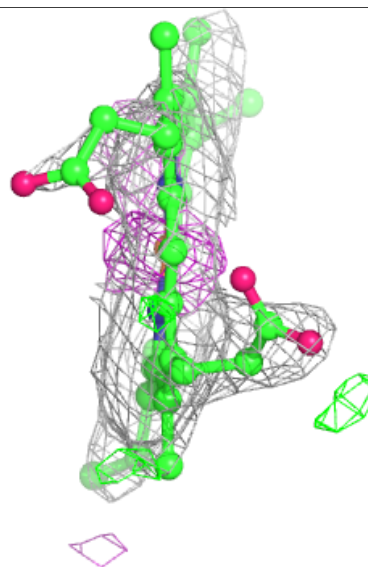
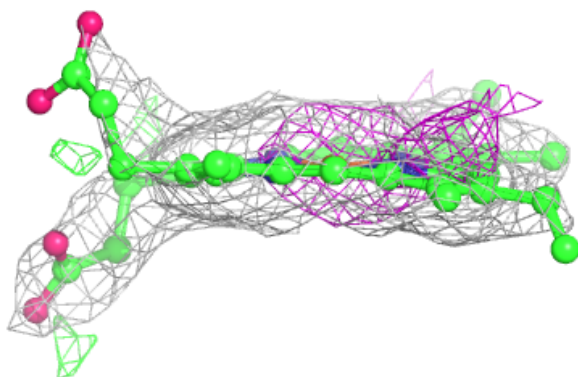
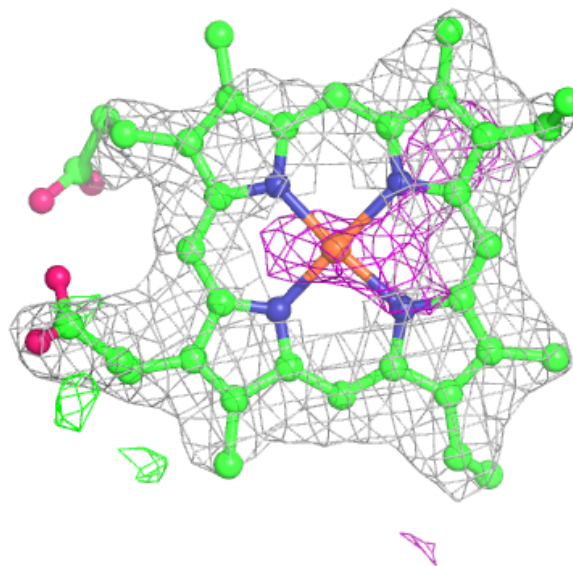
**Electron density around CLA a 409:**

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



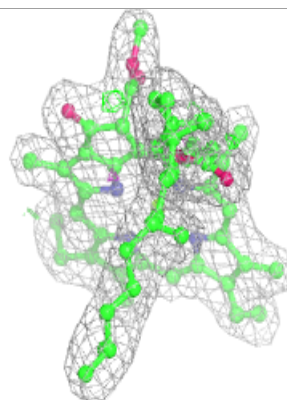
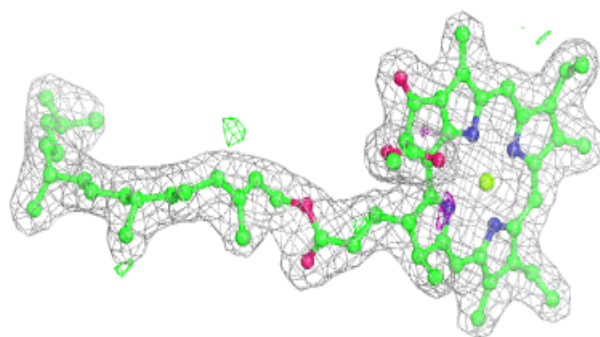
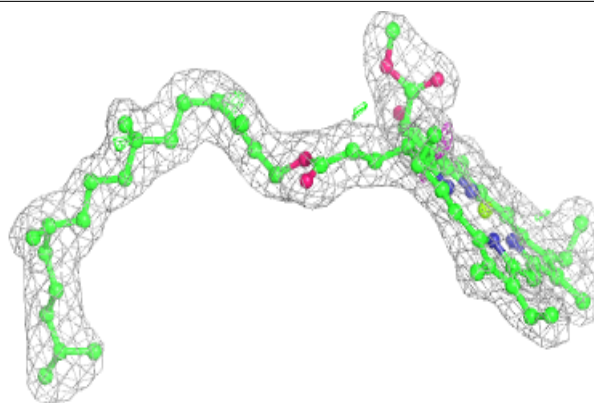
Electron density around HEM e 103:

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

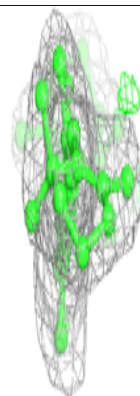
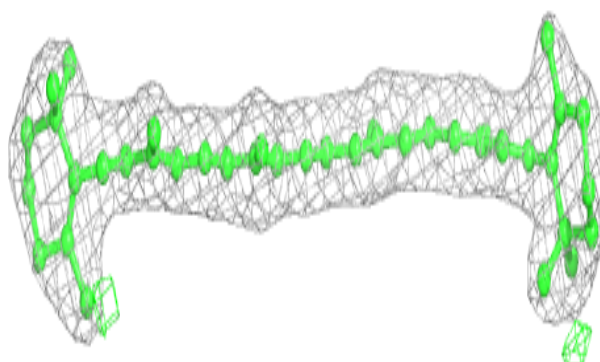
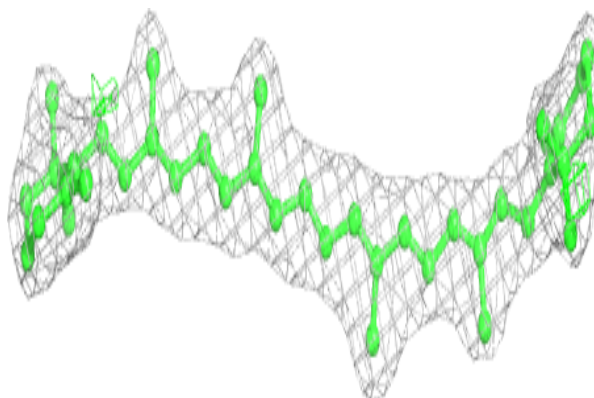


Electron density around CLA d 403:

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

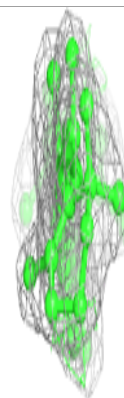
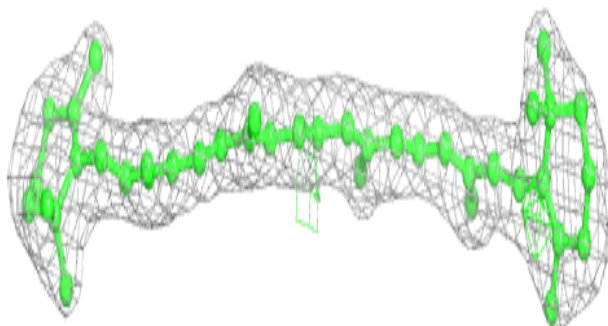
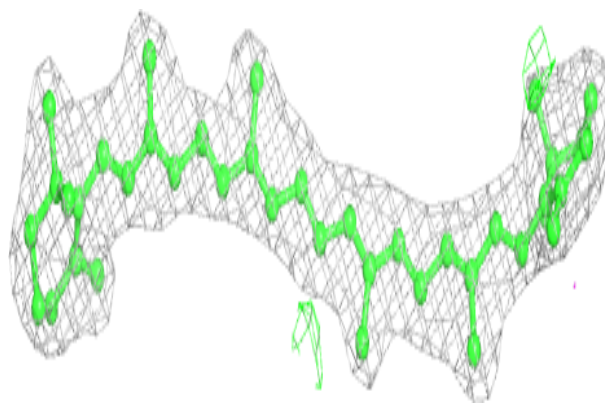
**Electron density around BCR c 518:**

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

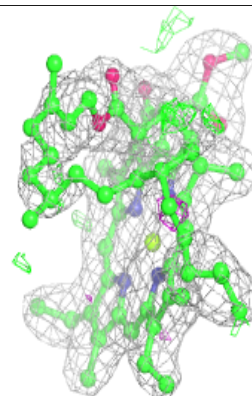
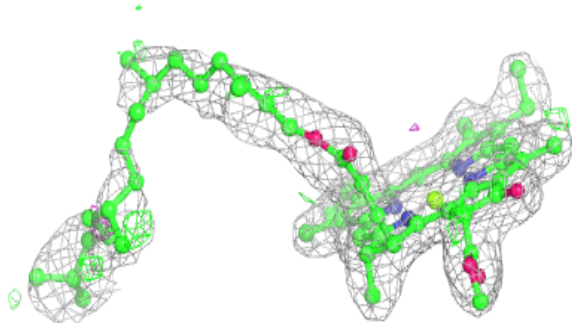
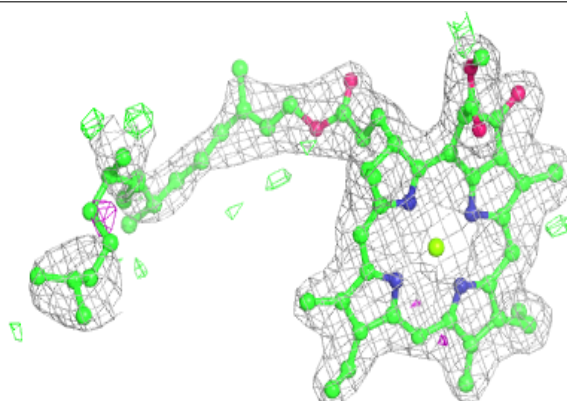


Electron density around BCR Y 101:

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

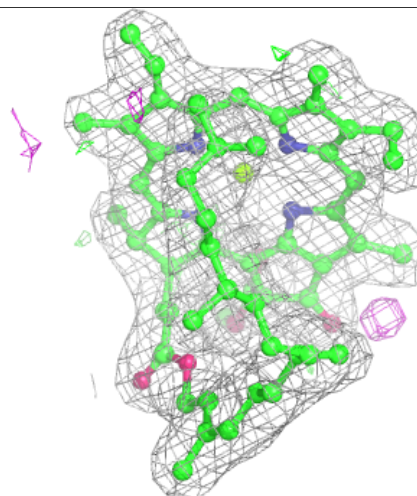
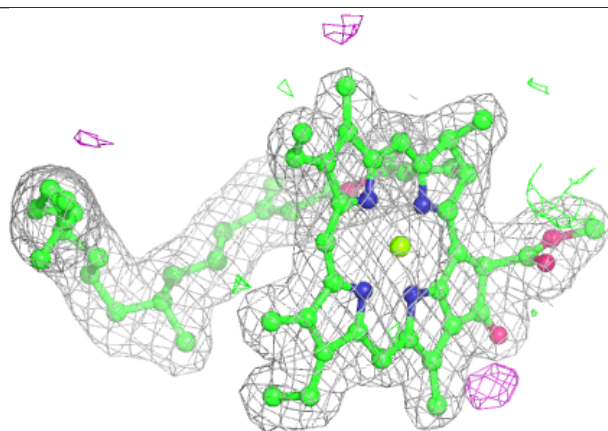
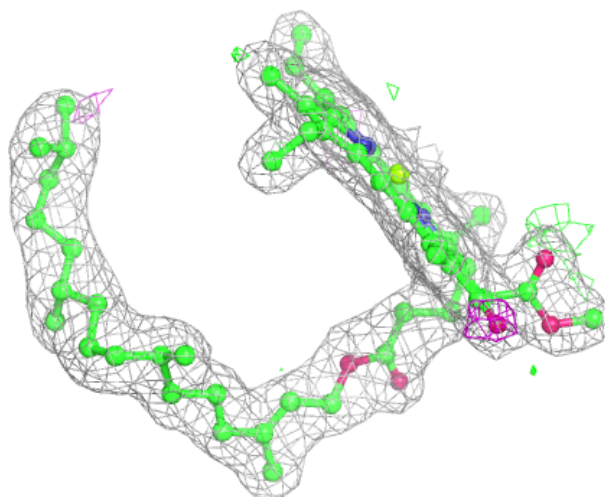
**Electron density around CLA a 412:**

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



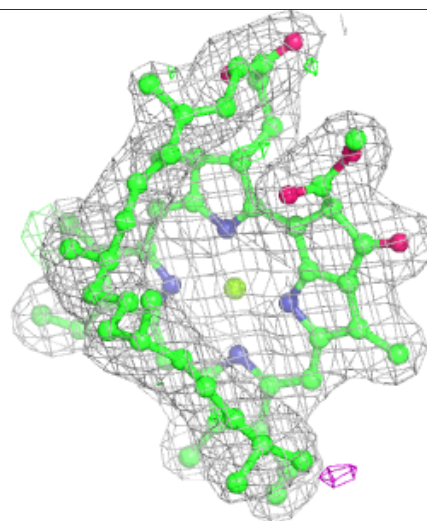
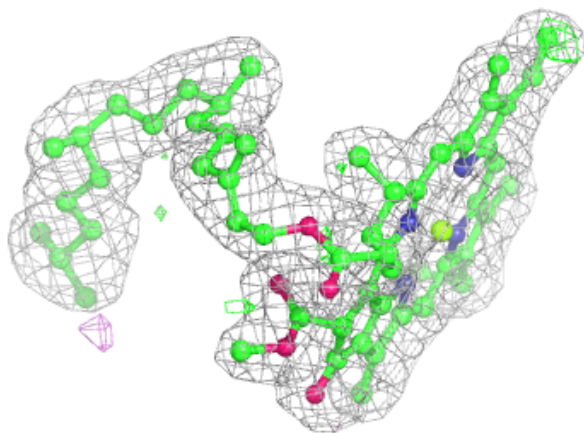
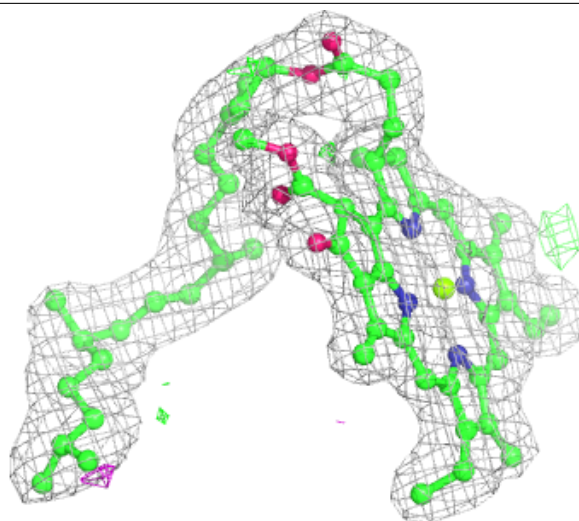
Electron density around CLA B 612:

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



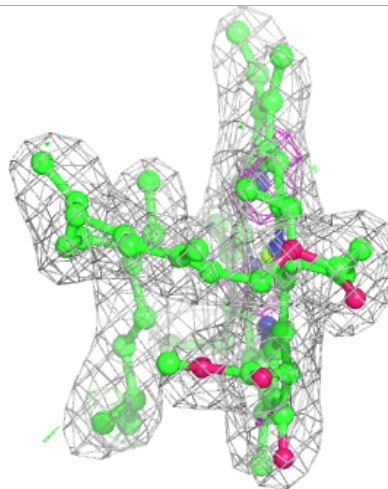
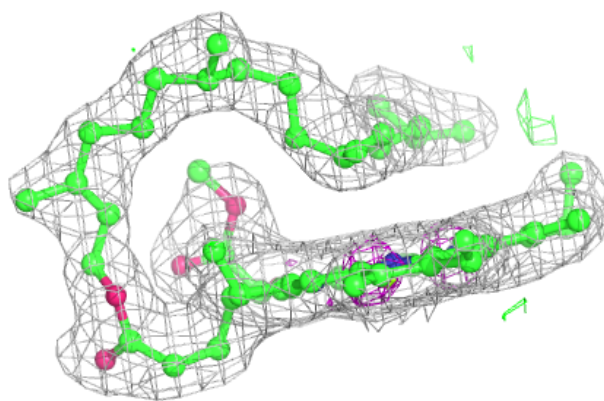
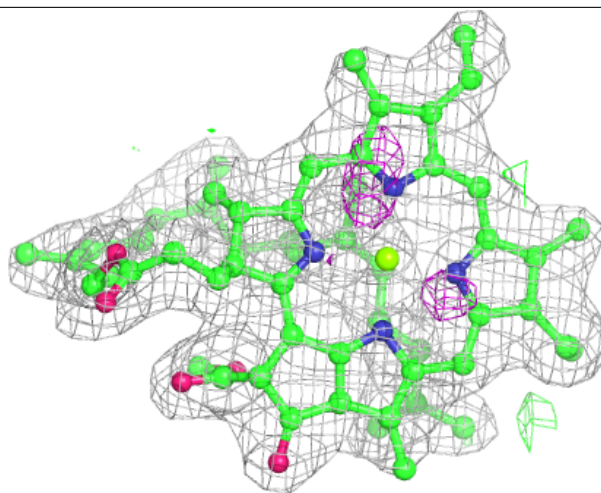
Electron density around CLA b 622:

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



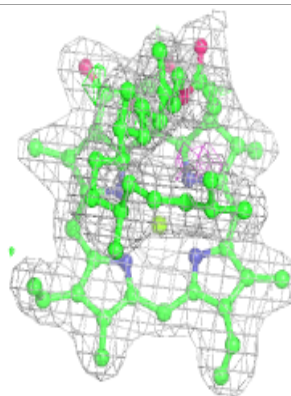
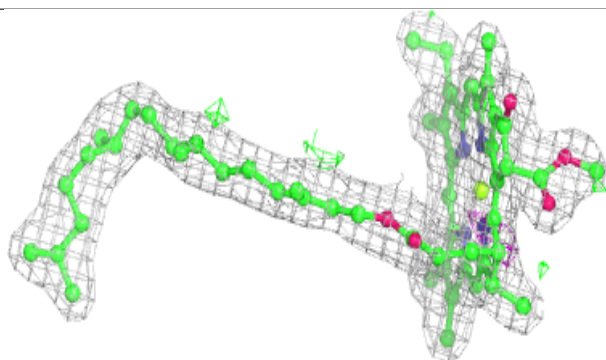
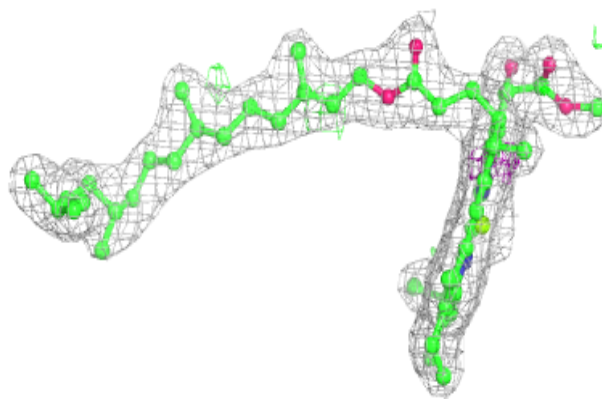
Electron density around CLA C 511:

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

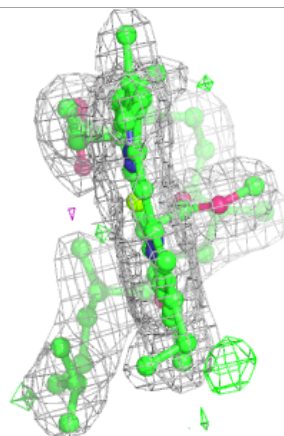
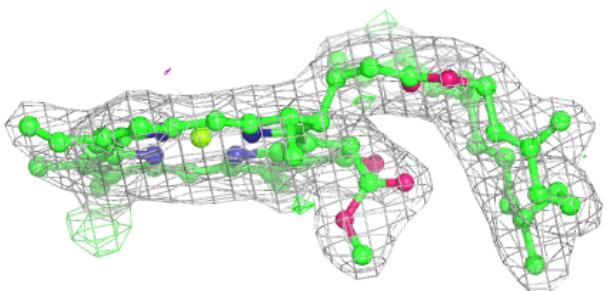
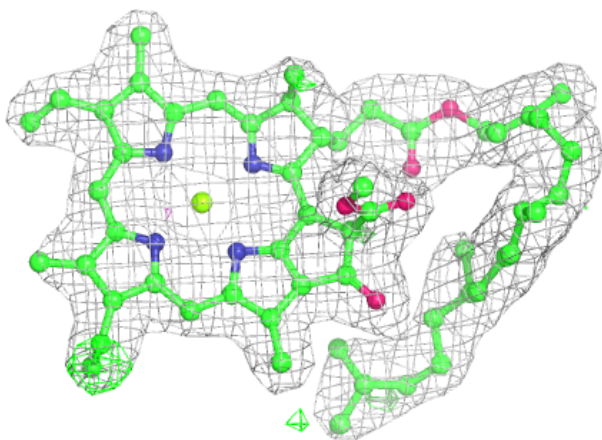


Electron density around CLA B 606:

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

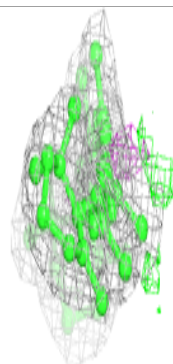
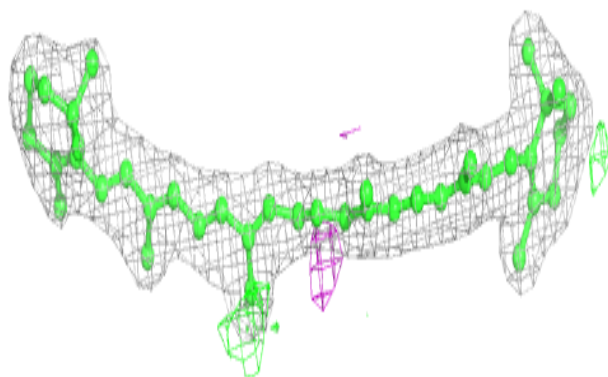
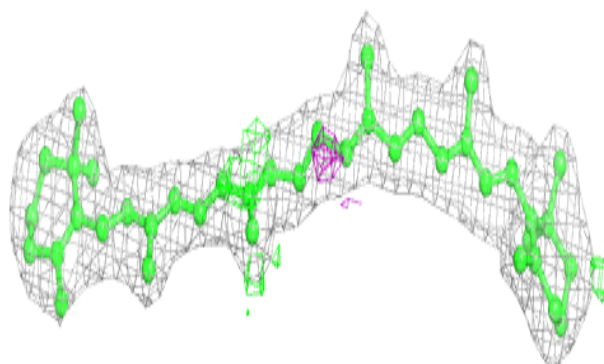
**Electron density around CLA B 611:**

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

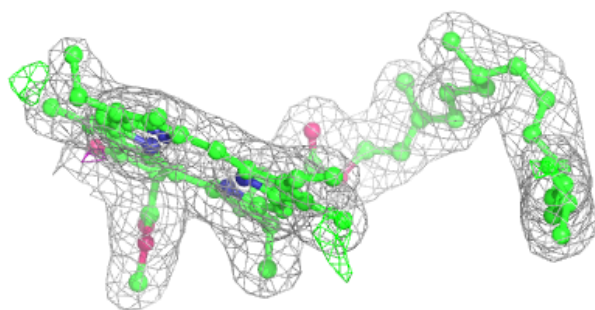
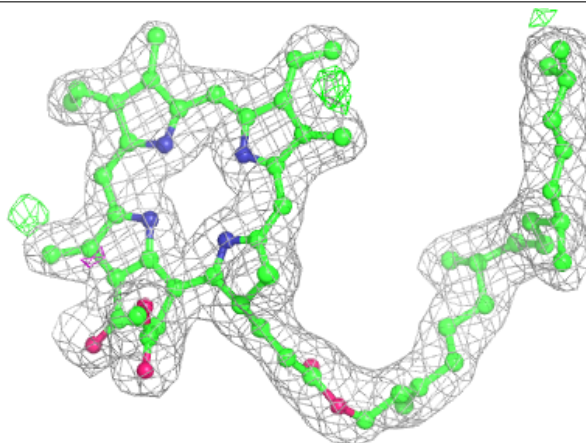


Electron density around BCR t 101:

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

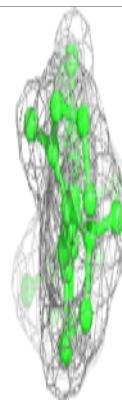
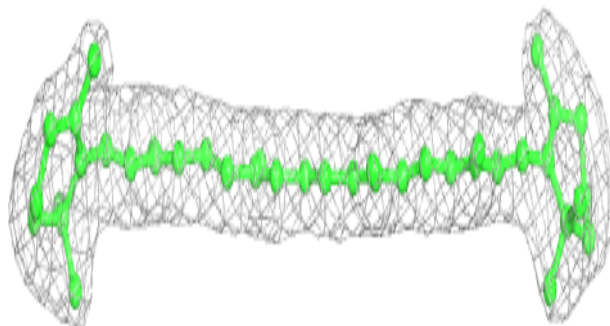
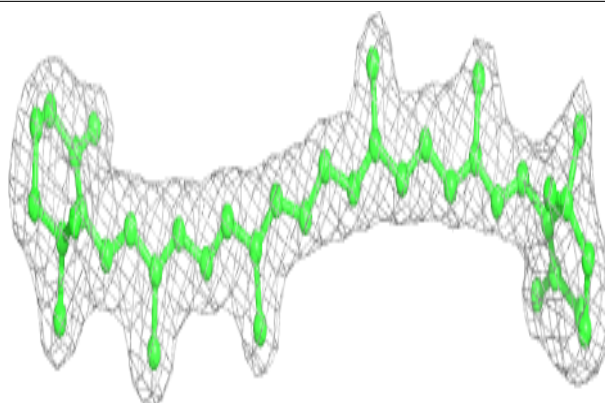
**Electron density around PHO A 408:**

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

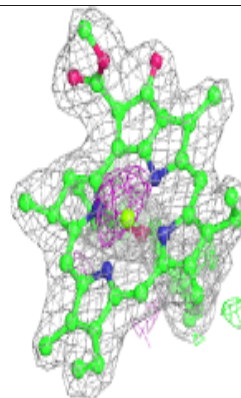
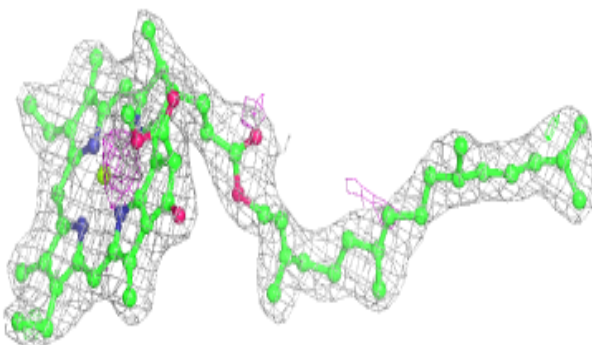
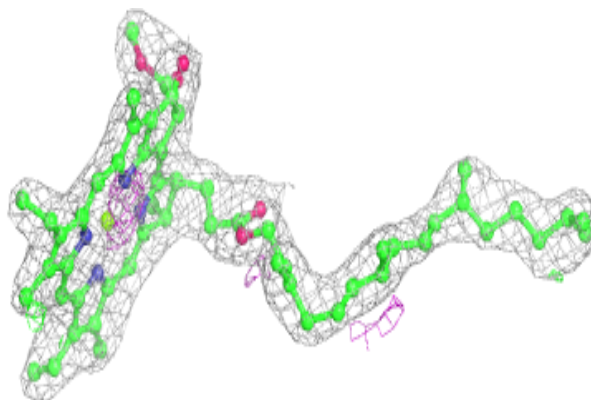


Electron density around BCR B 619:

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

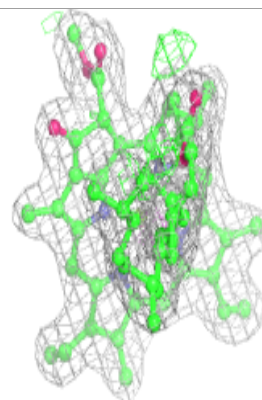
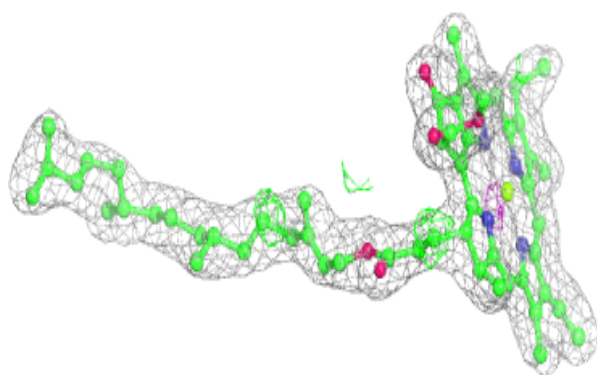
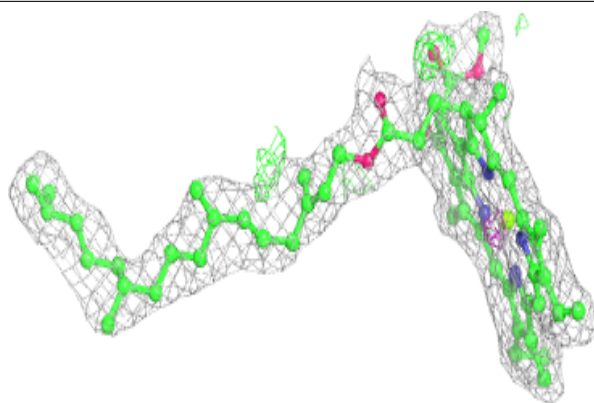
**Electron density around CLA c 506:**

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

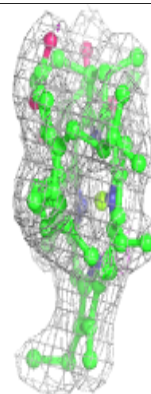
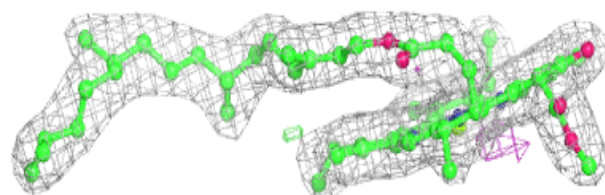
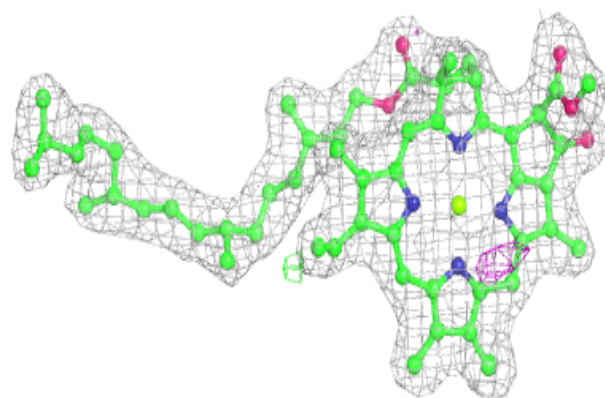


Electron density around CLA B 605:

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

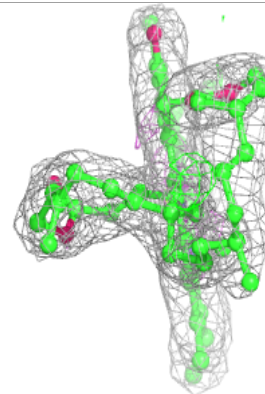
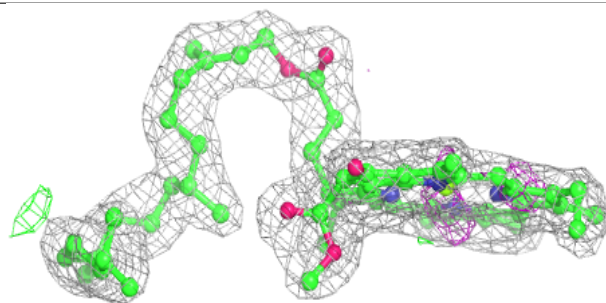
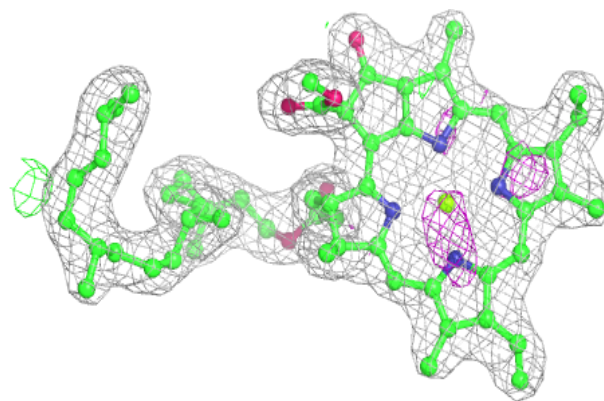
**Electron density around CLA B 604:**

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

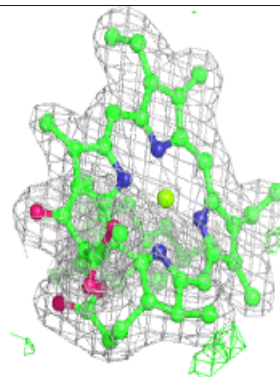
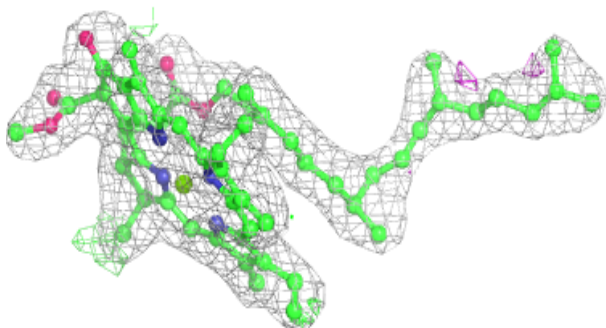
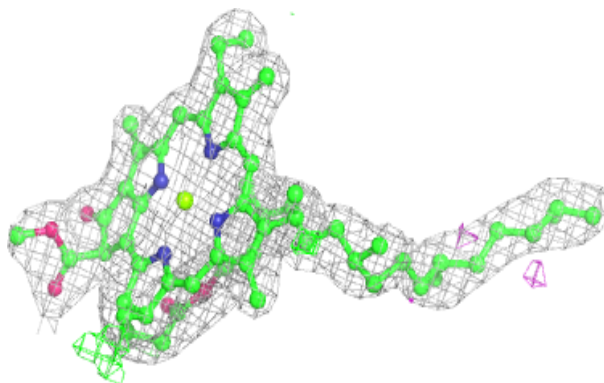


Electron density around CLA B 613:

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

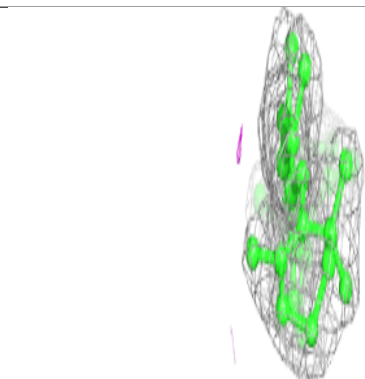
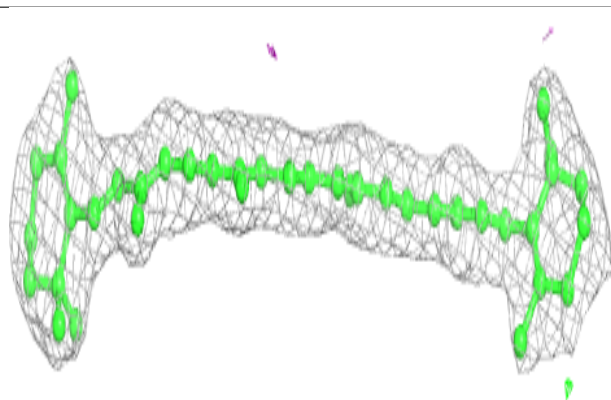
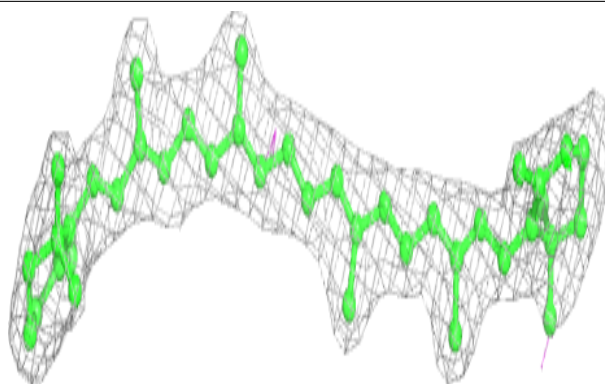
**Electron density around CLA C 506:**

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

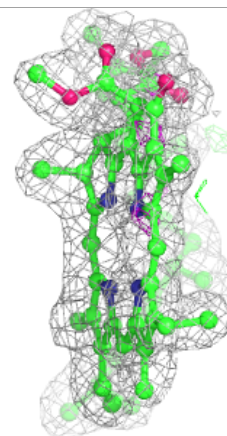
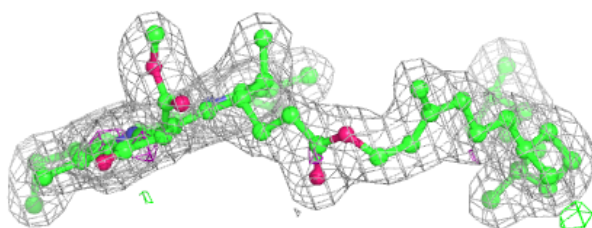
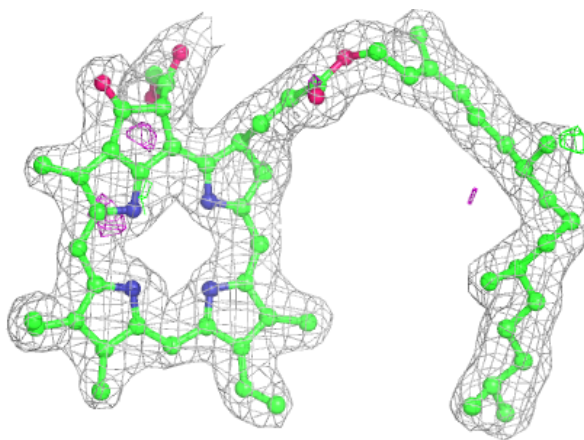


Electron density around BCR h 101:

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

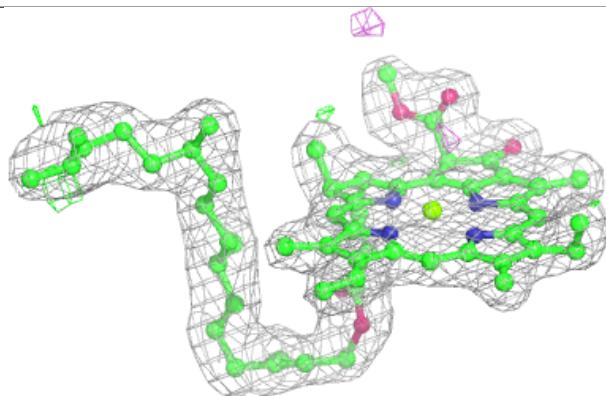
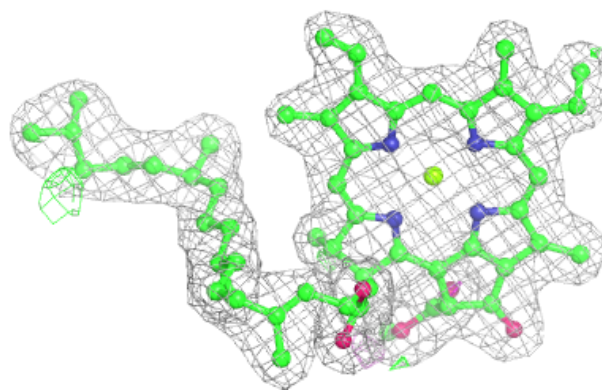
**Electron density around PHO D 401:**

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

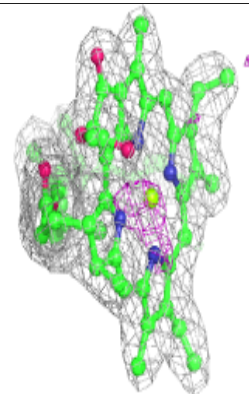
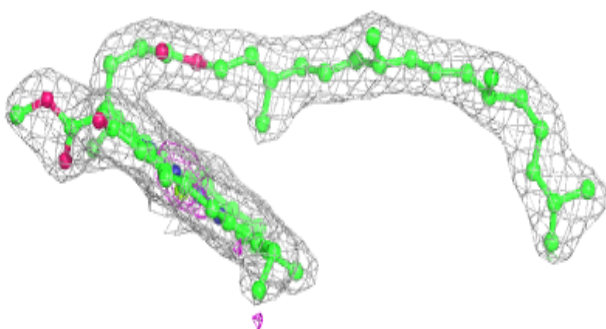
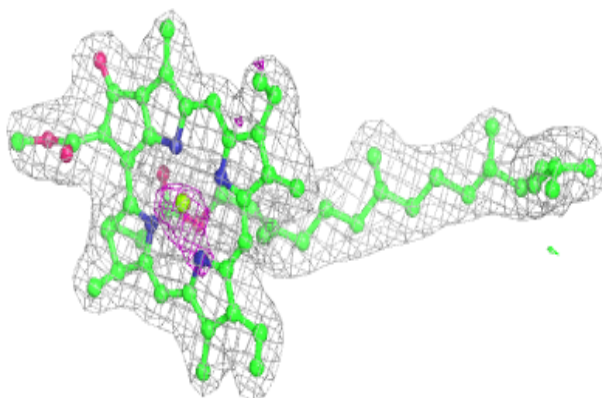


Electron density around CLA A 406:

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

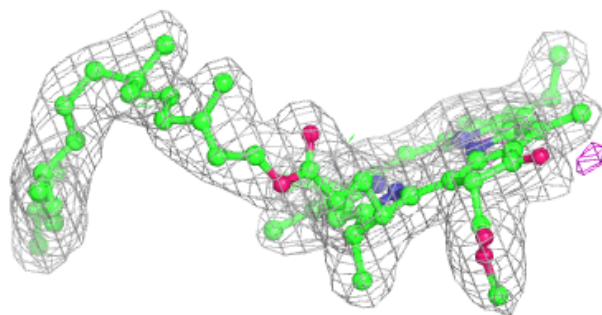
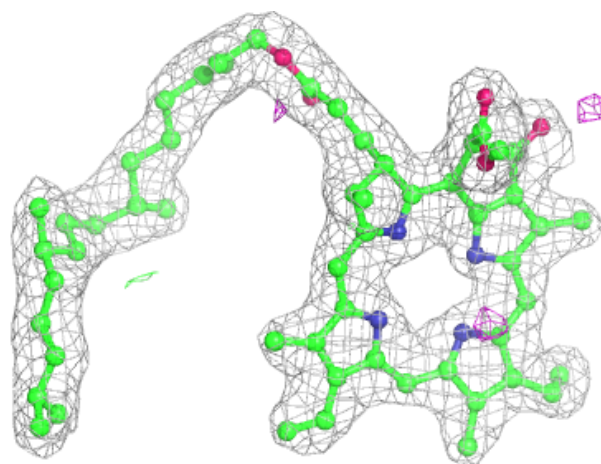
**Electron density around CLA B 609:**

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



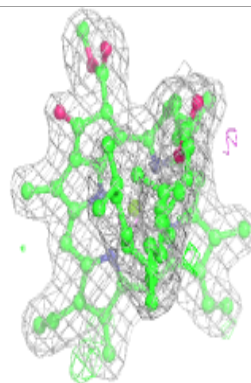
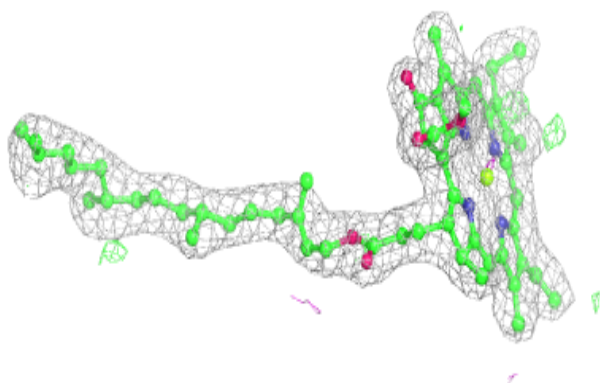
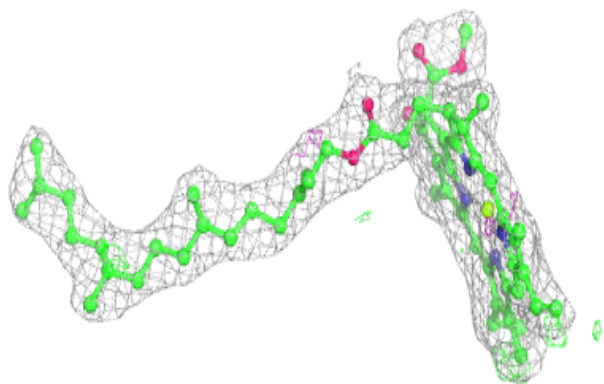
Electron density around PHO d 401:

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

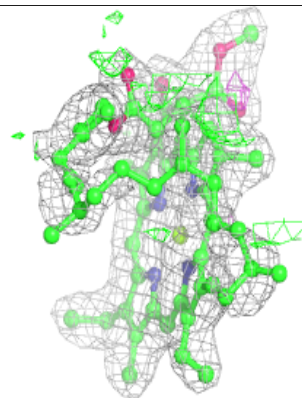
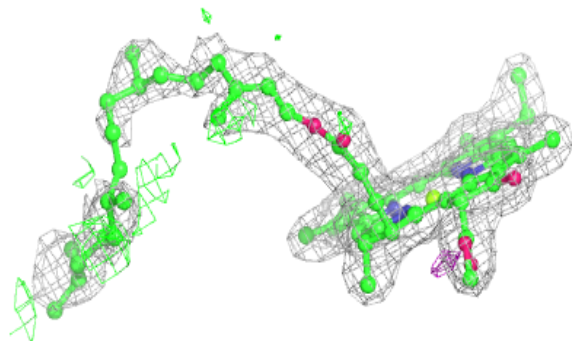
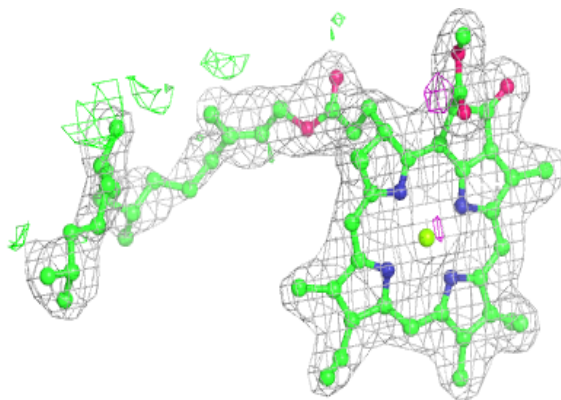


Electron density around CLA b 613:

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

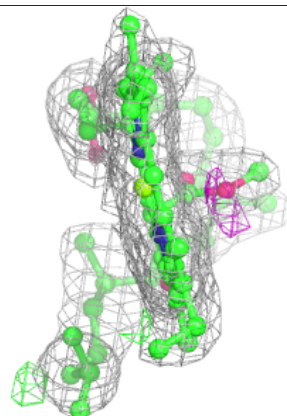
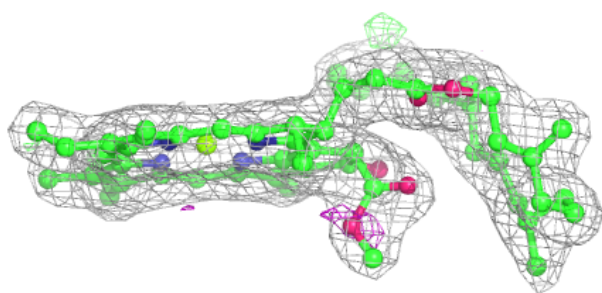
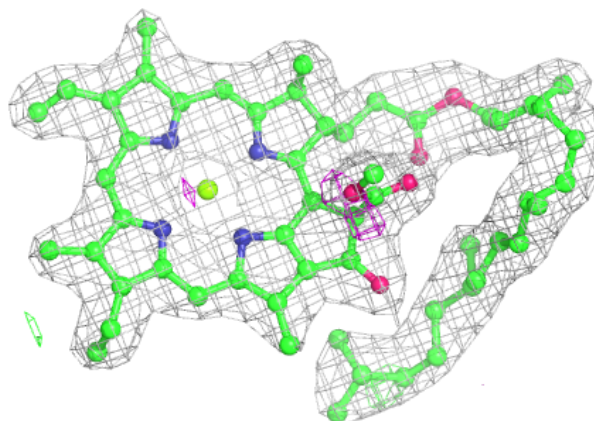
**Electron density around CLA A 409:**

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



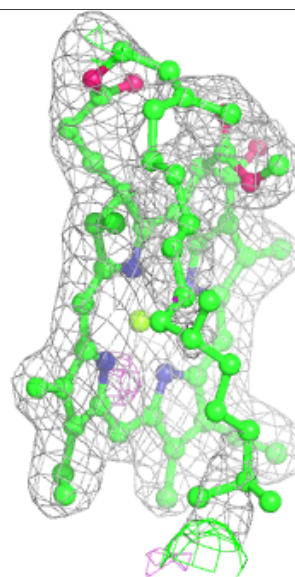
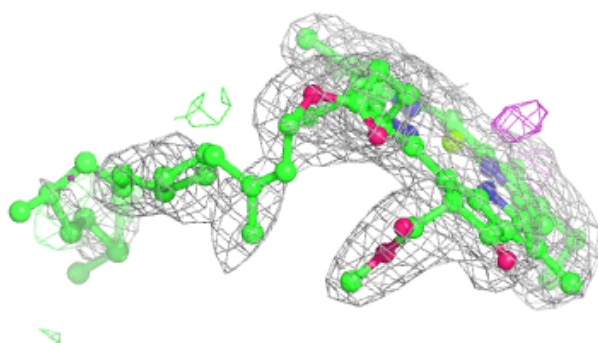
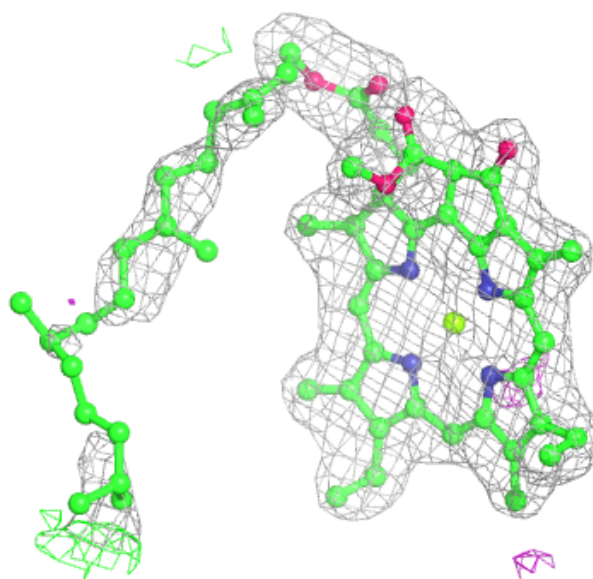
Electron density around CLA b 619:

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



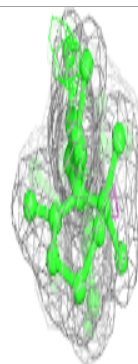
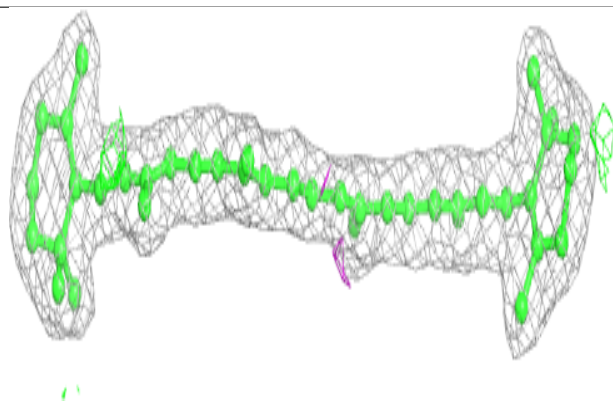
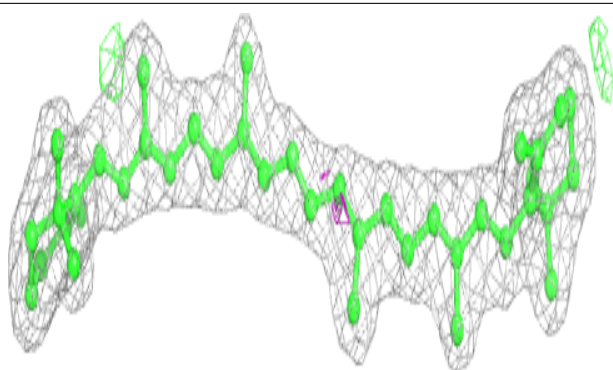
Electron density around CLA B 617:

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

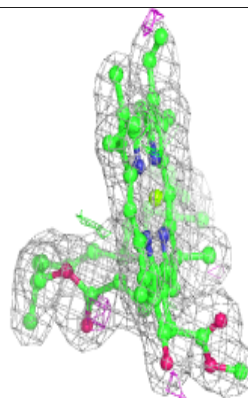
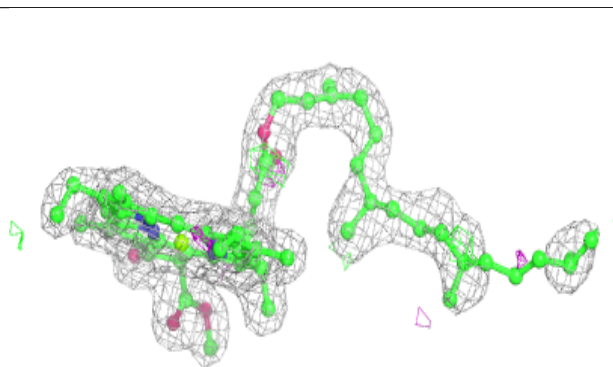
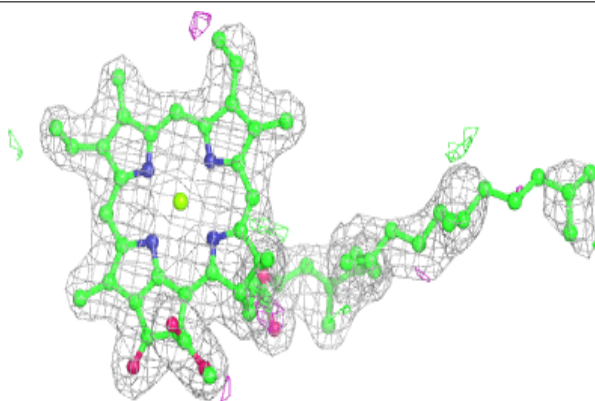


Electron density around BCR A 410:

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

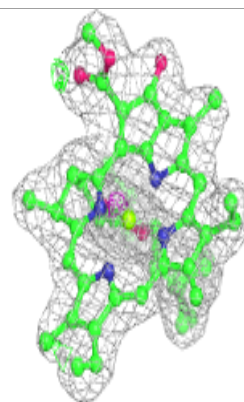
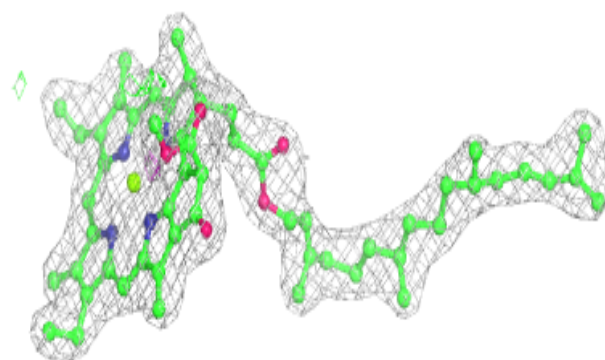
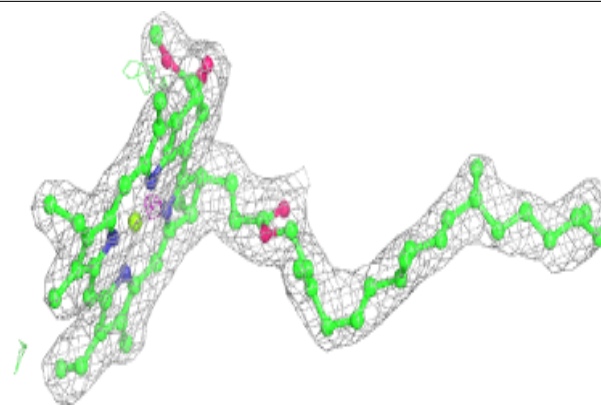
**Electron density around CLA A 407:**

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

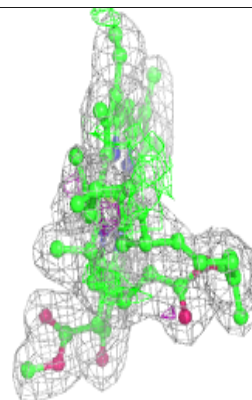
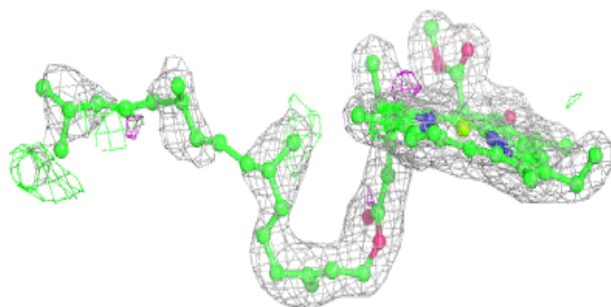
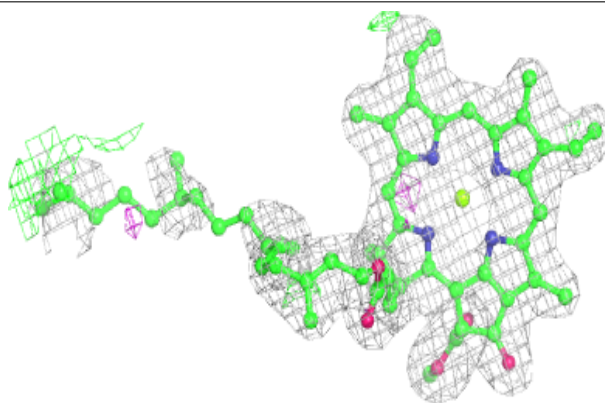


Electron density around CLA C 503:

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

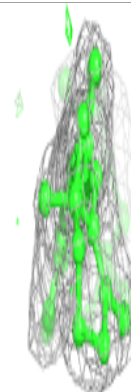
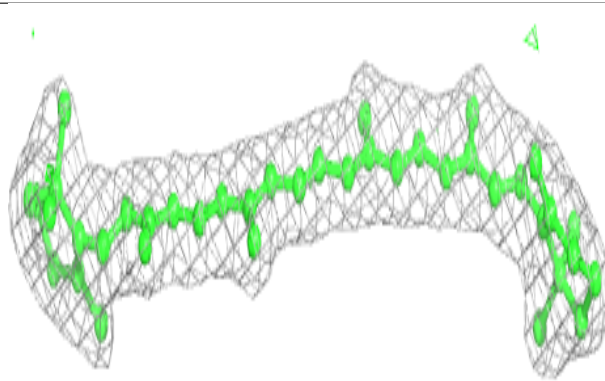
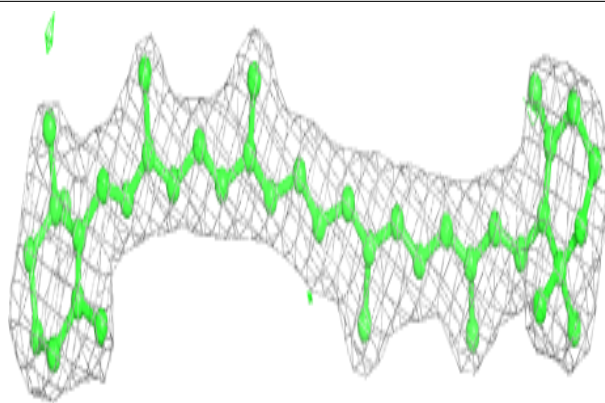
**Electron density around CLA a 410:**

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

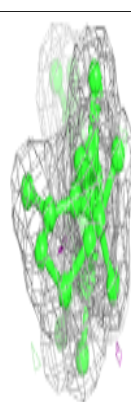
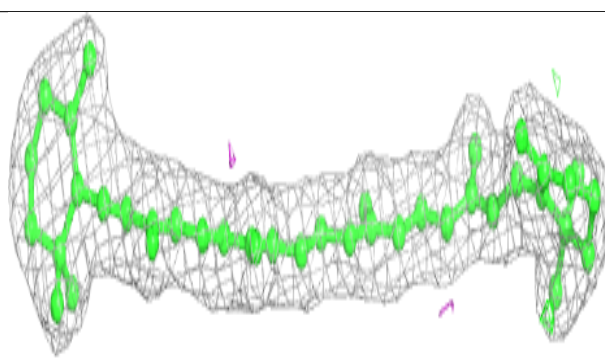
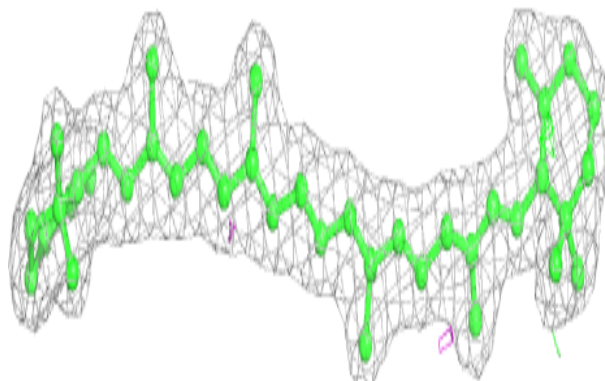


Electron density around BCR b 628:

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

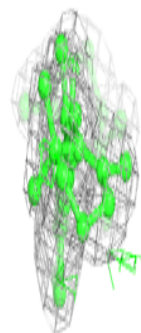
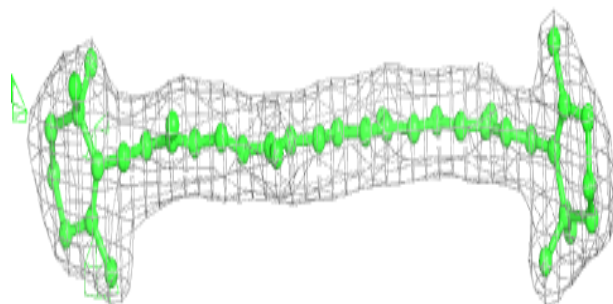
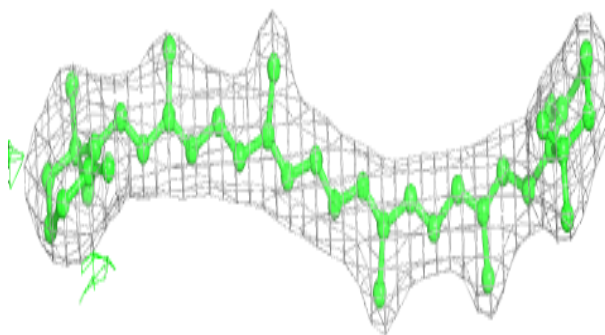
**Electron density around BCR B 618:**

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

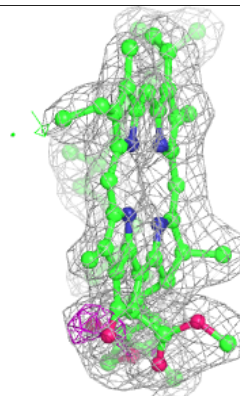
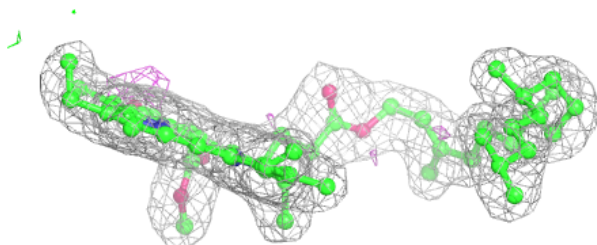
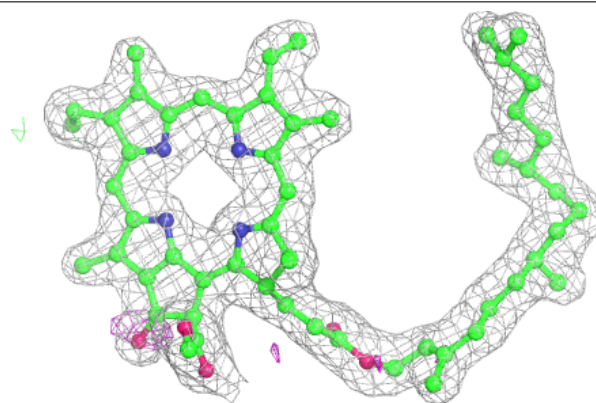


Electron density around BCR C 516:

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

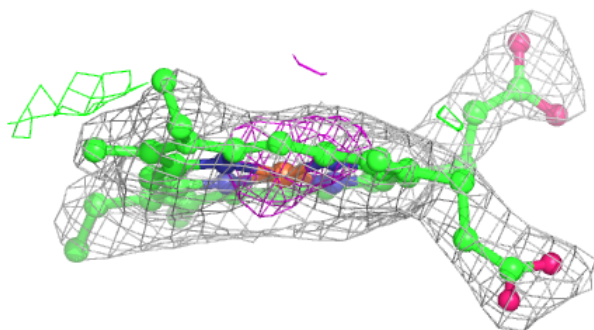
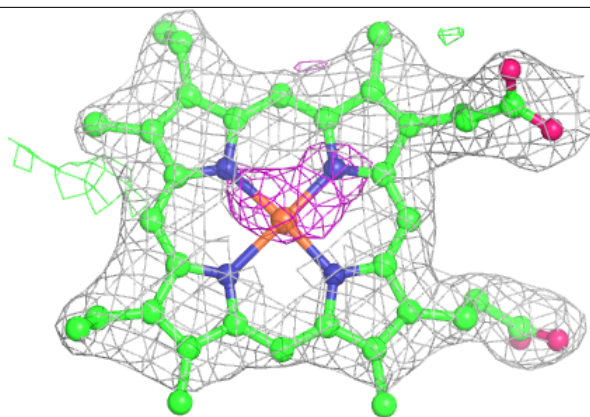
**Electron density around PHO a 411:**

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

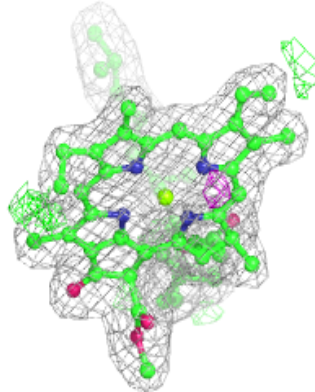
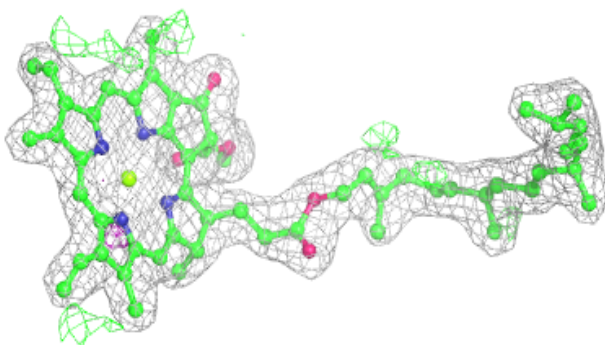
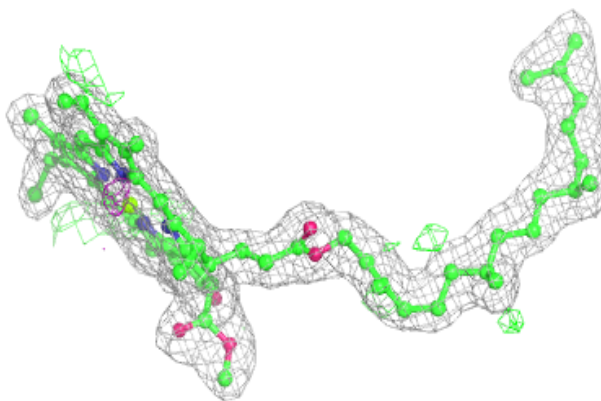


Electron density around HEM E 102:

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

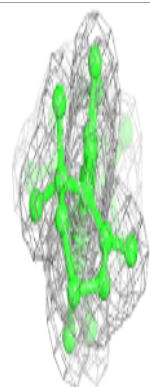
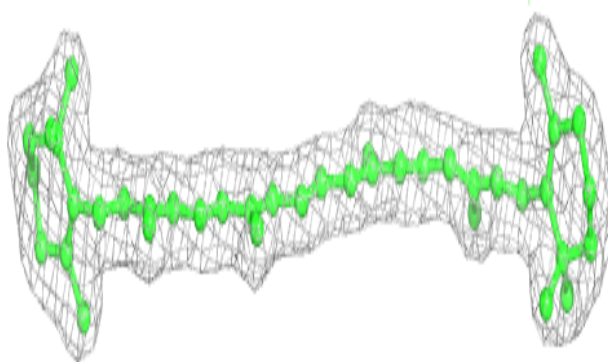
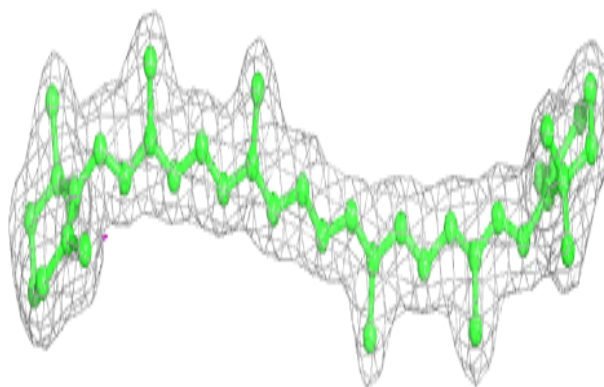
**Electron density around CLA D 402:**

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

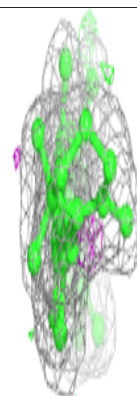
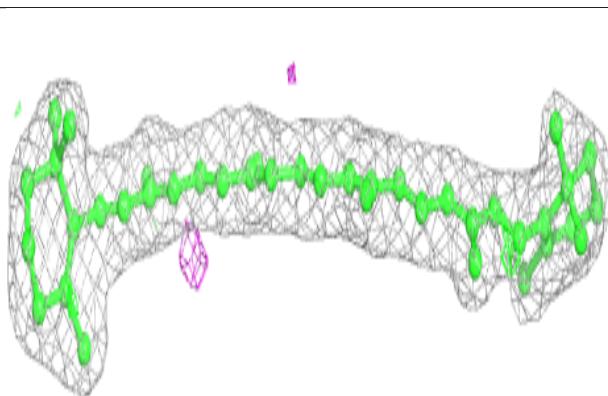
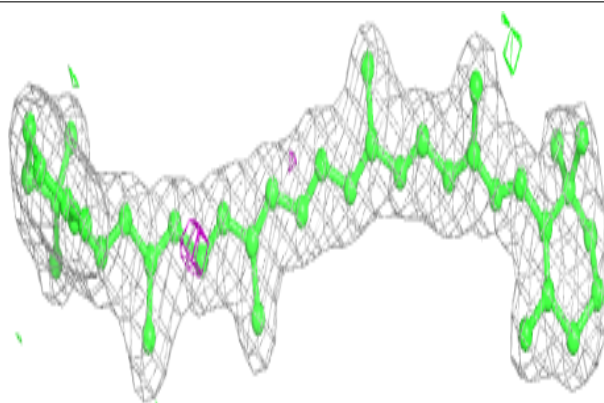


Electron density around BCR a 413:

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

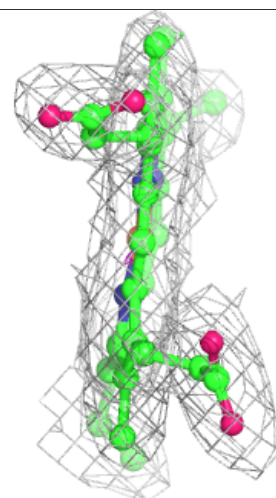
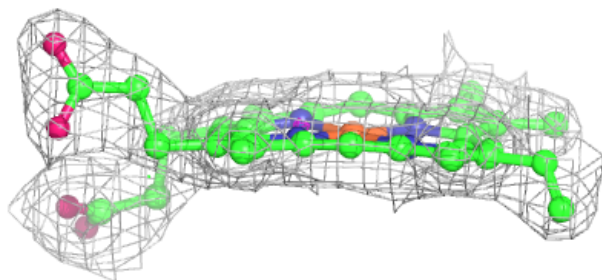
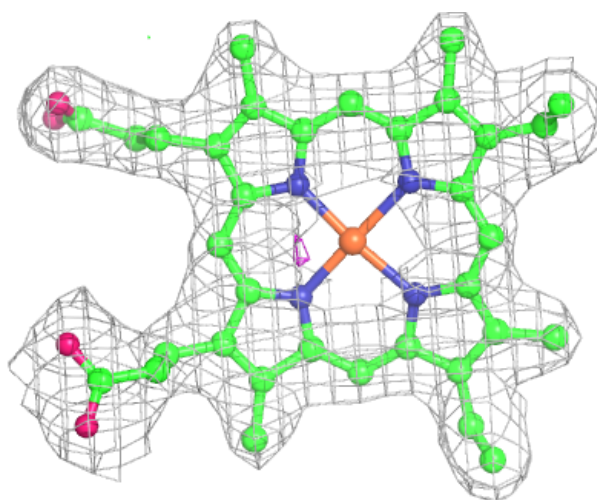
**Electron density around BCR b 626:**

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



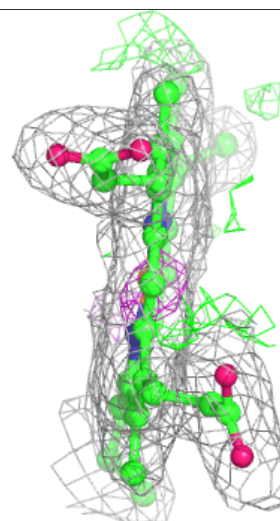
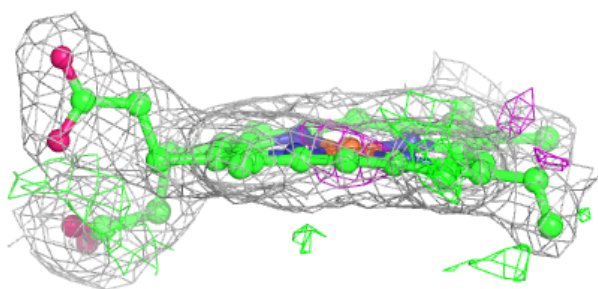
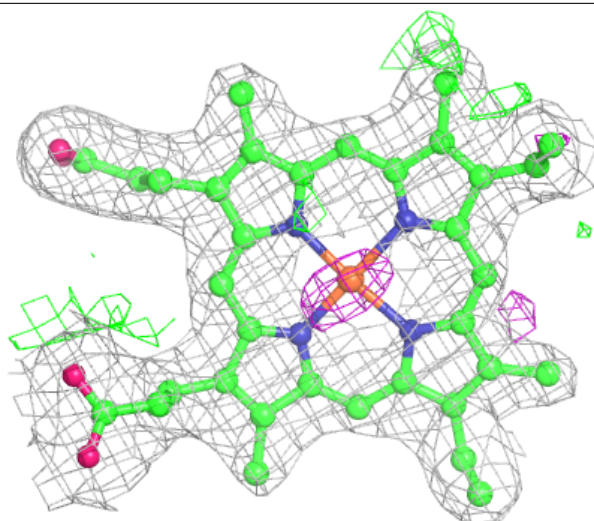
Electron density around HEM v 205:

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



Electron density around HEM V 205:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.