



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2020 – 01:55 PM BST

PDB ID : 5B66
Title : Crystal structure analysis of Photosystem II complex
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on : 2016-05-25
Resolution : 1.85 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
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

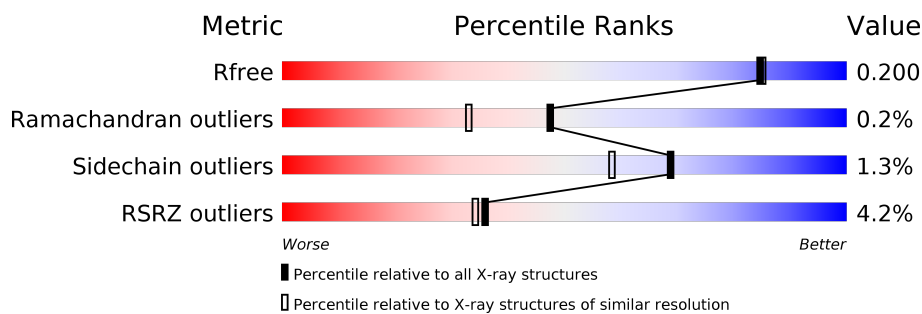
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
1	a	344	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
2	B	505	<div> <div>4%</div> <div>97%</div> <div>.</div> </div>
2	b	505	<div> <div>4%</div> <div>95%</div> <div>..</div> </div>
3	C	455	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
3	c	455	<div> <div>%</div> <div>97%</div> <div>.</div> </div>
4	D	342	<div> <div>%</div> <div>98%</div> <div>.</div> </div>

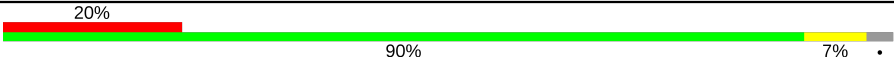
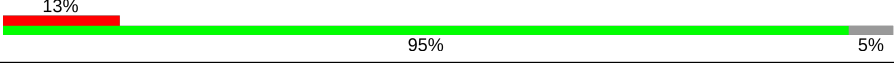

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Mol	Chain	Length	Quality of chain
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	
16	v	137	

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

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
20	CLA	A	401	X	-	-	-
20	CLA	A	402	X	-	-	-
20	CLA	A	404	X	-	-	-
20	CLA	B	601	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	609	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	C	501	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	C	504	X	-	-	-
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	511	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	C	513	X	-	-	-
20	CLA	D	401	X	-	-	-
20	CLA	D	402	X	-	-	-
20	CLA	D	404	X	-	-	-
20	CLA	a	403	X	-	-	-
20	CLA	a	404	X	-	-	-
20	CLA	a	407	X	-	-	-
20	CLA	b	603	X	-	-	-
20	CLA	b	604	X	-	-	-
20	CLA	b	605	X	-	-	-
20	CLA	b	606	X	-	-	-
20	CLA	b	607	X	-	-	-
20	CLA	b	608	X	-	-	-
20	CLA	b	609	X	-	-	-
20	CLA	b	610	X	-	-	-
20	CLA	b	611	X	-	-	-
20	CLA	b	612	X	-	-	-
20	CLA	b	613	X	-	-	-
20	CLA	b	614	X	-	-	-
20	CLA	b	615	X	-	-	-
20	CLA	b	616	X	-	-	-
20	CLA	b	617	X	-	-	-
20	CLA	b	618	X	-	-	-
20	CLA	c	501	X	-	-	-
20	CLA	c	502	X	-	-	-
20	CLA	c	503	X	-	-	-
20	CLA	c	504	X	-	-	-
20	CLA	c	505	X	-	-	-
20	CLA	c	506	X	-	-	-
20	CLA	c	507	X	-	-	-
20	CLA	c	508	X	-	-	-
20	CLA	c	509	X	-	-	-
20	CLA	c	510	X	-	-	-
20	CLA	c	511	X	-	-	-
20	CLA	c	512	X	-	-	-
20	CLA	c	513	X	-	-	-
20	CLA	d	402	X	-	-	-
20	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	d	404	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54996 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
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	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	505	Total	C	N	O	S	0	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	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	1	0
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	614	13			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	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	64	Total	C	N	O	S	0	1	0
			508	339	81	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			284	194	45	44	1			
8	i	36	Total	C	N	O	S	0	1	0
			300	203	49	47	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			272	183	41	47	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			285	199	42	44			

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	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	1	0
			296	200	45	51			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			259	175	37	46	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	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	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	0	0
			770	489	129	152				

- 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	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	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
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

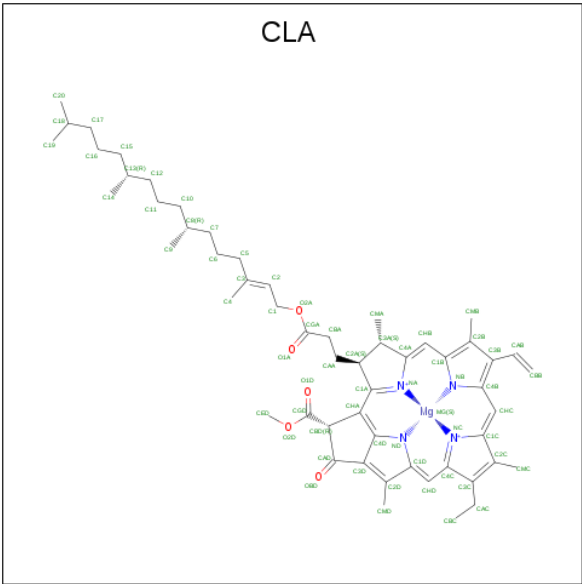
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			274	183	44	47				
18	x	35	Total	C	N	O		0	0	0
			252	171	38	43				

- 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
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	a	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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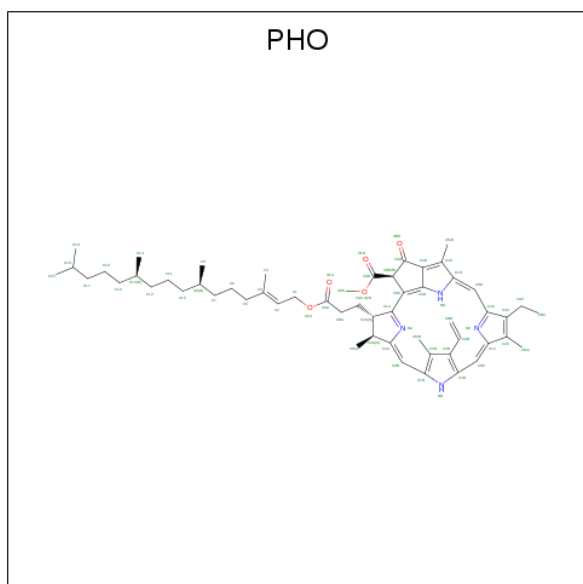
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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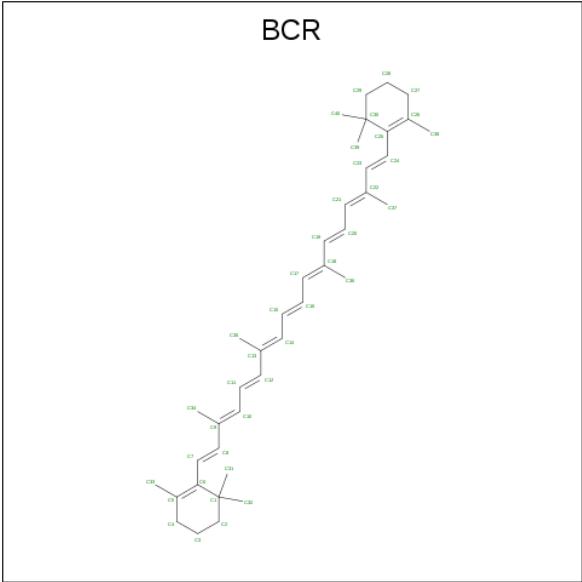
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



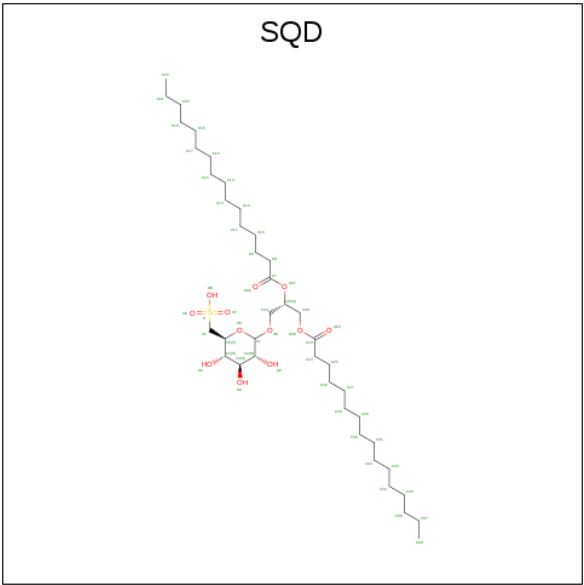
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	D	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	T	1	Total C 40 40	0	0
22	a	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C 40 40	0	0
22	d	1	Total C 40 40	0	0
22	j	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	t	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



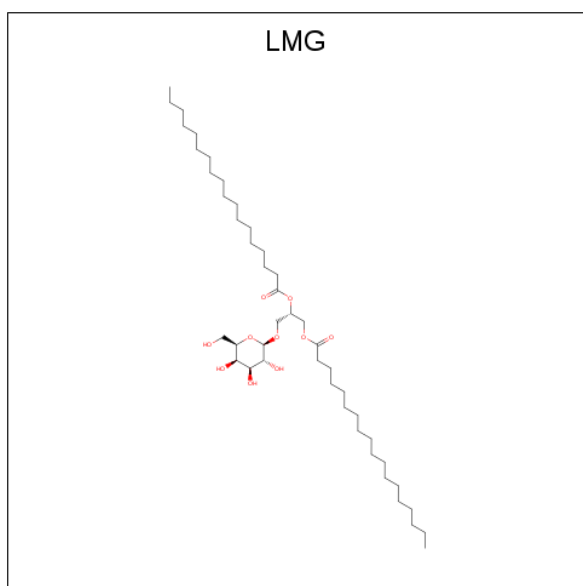
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	b	1	Total	C	O	S	0	0
			54	41	12	1		
23	f	1	Total	C	O	S	0	0
			40	27	12	1		
23	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			51	41	10			
24	B	1	Total	C	O		0	0
			51	41	10			
24	C	1	Total	C	O		0	0
			51	41	10			
24	C	1	Total	C	O		0	0
			45	35	10			
24	J	1	Total	C	O		0	0
			45	35	10			
24	a	1	Total	C	O		0	0
			51	41	10			
24	b	1	Total	C	O		0	0
			49	39	10			
24	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	c	1	Total	C	O	0	0
			51	41	10		
24	j	1	Total	C	O	0	0
			45	35	10		

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

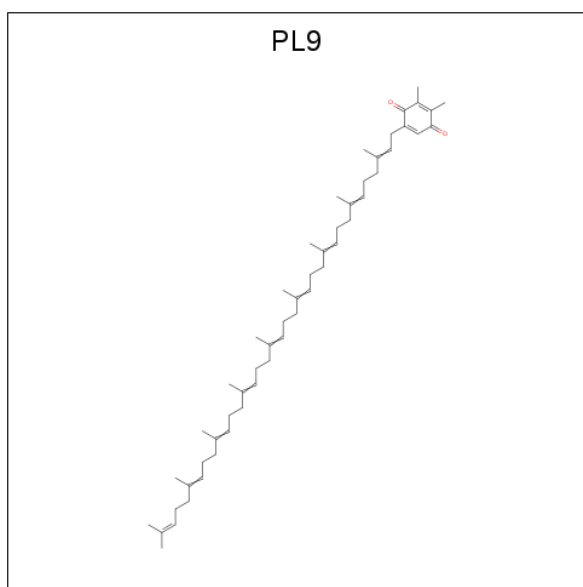
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	h	1	Total	C		0	0
			16	16			
26	B	6	Total	C		0	0
			84	84			
26	c	3	Total	C	O	0	0
			48	43	5		
26	t	1	Total	C		0	0
			16	16			
26	X	1	Total	C		0	0
			16	16			
26	J	4	Total	C		0	0
			33	33			
26	E	1	Total	C		0	0
			15	15			
26	b	7	Total	C		0	0
			68	68			
26	A	2	Total	C	O	0	0
			40	35	5		
26	x	1	Total	C		0	0
			9	9			
26	M	1	Total	C		0	0
			12	12			
26	j	2	Total	C		0	0
			22	22			
26	D	2	Total	C	O	0	0
			53	48	5		

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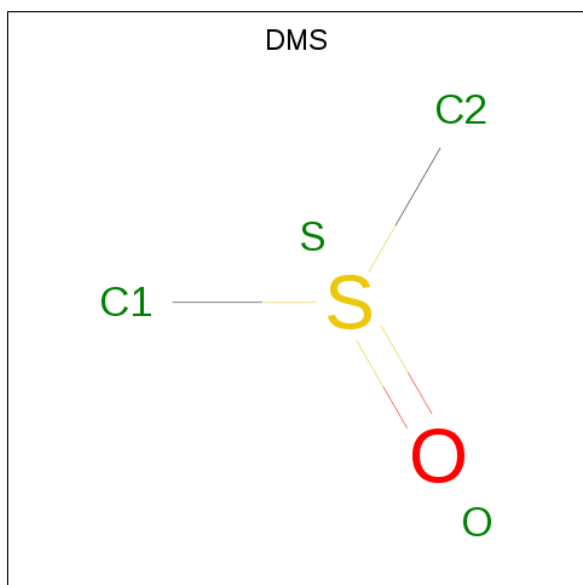
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	e	1	Total C 7 7	0	0
26	I	5	Total C 61 61	0	0
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	U	1	Total C 14 14	0	0
26	L	1	Total C 14 14	0	0
26	d	3	Total C O 68 63 5	0	0
26	H	2	Total C 10 10	0	0
26	i	3	Total C 38 38	0	0
26	C	1	Total C O 34 29 5	0	0
26	z	1	Total C 6 6	0	0
26	T	1	Total C 13 13	0	0

- Molecule 27 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: C₅₃H₈₀O₂).



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

- Molecule 28 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 8	C 4	O 2	S 2	0	1
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	F	1	Total 4	C 2	O 1	S 1	0	0
28	H	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 8	C 4	O 2	S 2	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	U	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	V	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	b	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	h	1	Total 4	C 2	O 1	S 1	0	0
28	i	1	Total 4	C 2	O 1	S 1	0	0
28	j	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	u	1	Total 4	C 2	O 1	S 1	0	0

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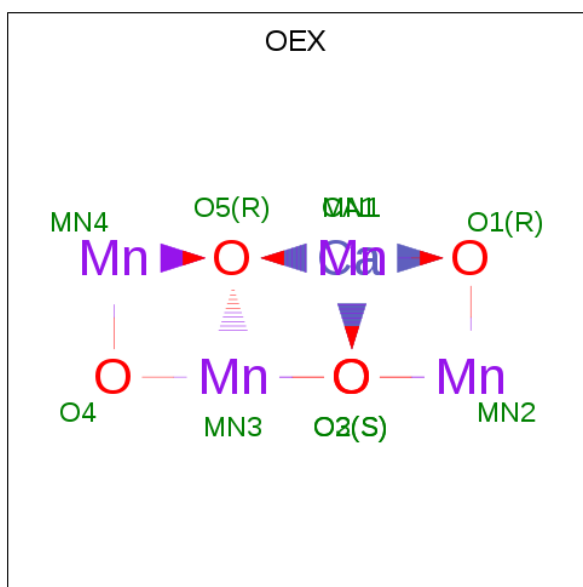
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	u	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0

- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

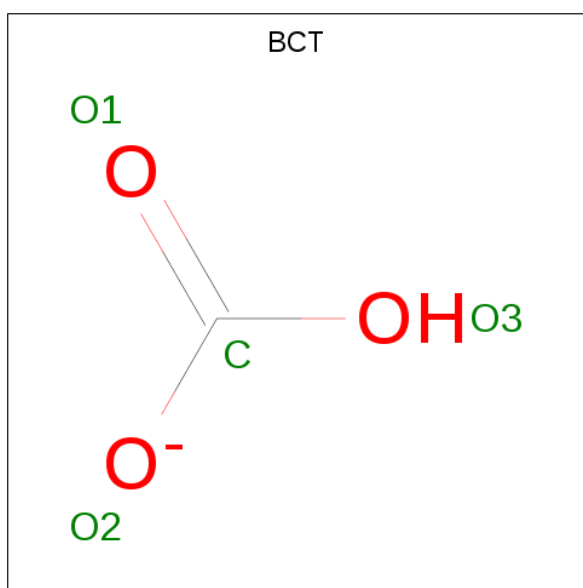
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Fe 1 1	0	0
29	a	1	Total Fe 1 1	0	0

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



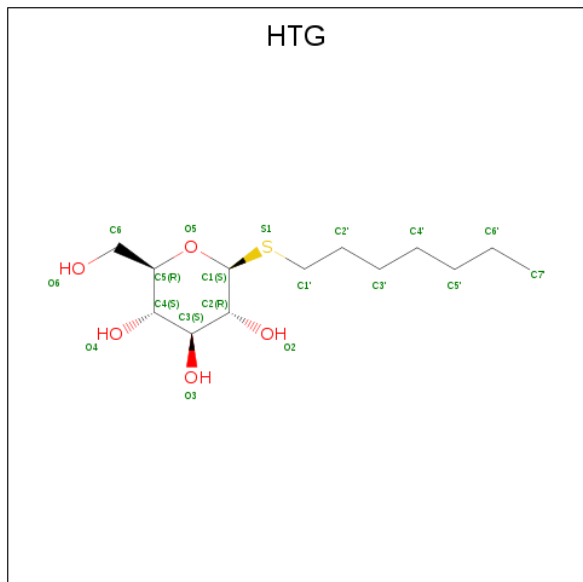
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			19	13	5	1		
32	O	1	Total	C	O	S	0	0
			19	13	5	1		
32	V	1	Total	C	O	S	0	0
			13	7	5	1		

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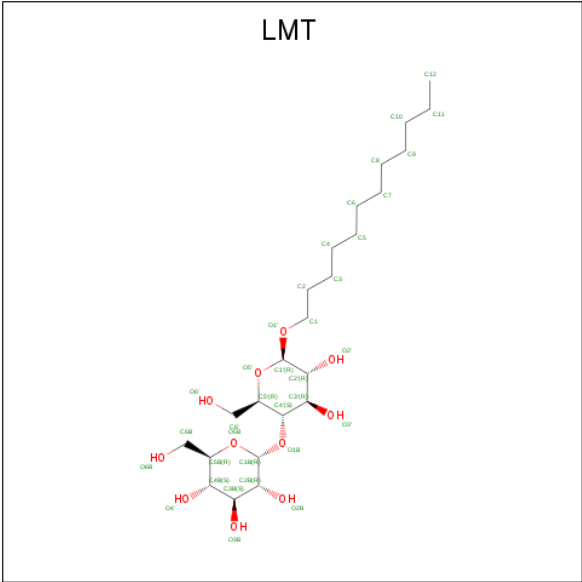
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	d	1	Total C O S 19 13 5 1	0	0
32	u	1	Total C S 8 7 1	0	0
32	v	1	Total C O S 14 8 5 1	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	V	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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



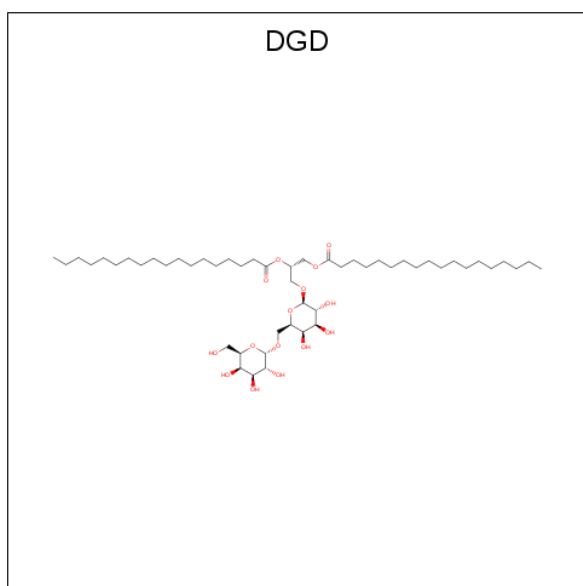
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			16	14	2		
34	E	1	Total	C	O	0	0
			24	18	6		
34	I	1	Total	C	O	0	0
			35	24	11		
34	J	1	Total	C	O	0	0
			24	18	6		
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			24	18	6		
34	Z	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			32	21	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	c	1	Total	C	O	0	0
			35	24	11		
34	f	1	Total	C	O	0	0
			24	18	6		

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

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



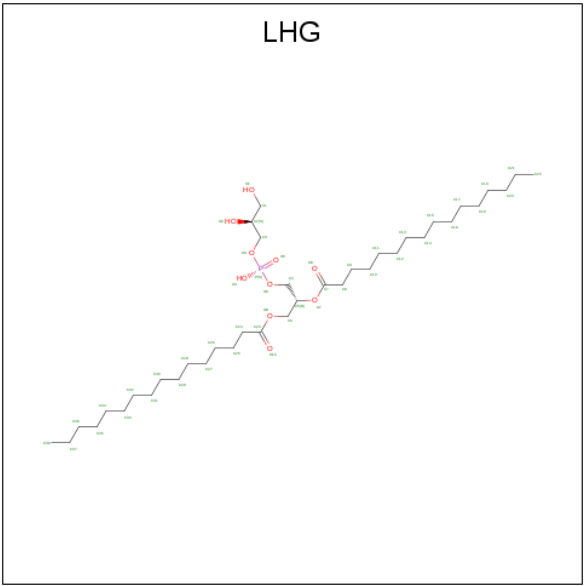
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			62	47	15		
35	C	1	Total	C	O	0	0
			55	40	15		
35	C	1	Total	C	O	0	0
			62	47	15		
35	D	1	Total	C	O	0	0
			51	41	10		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			57	42	15		
35	c	1	Total	C	O	0	0
			62	47	15		

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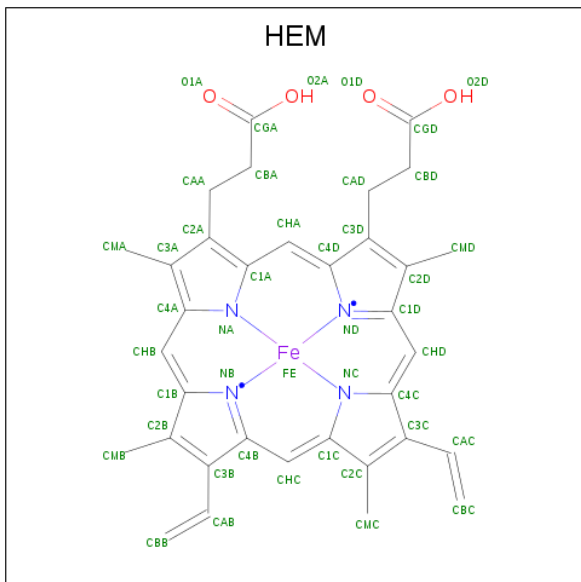
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			51	41	10		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



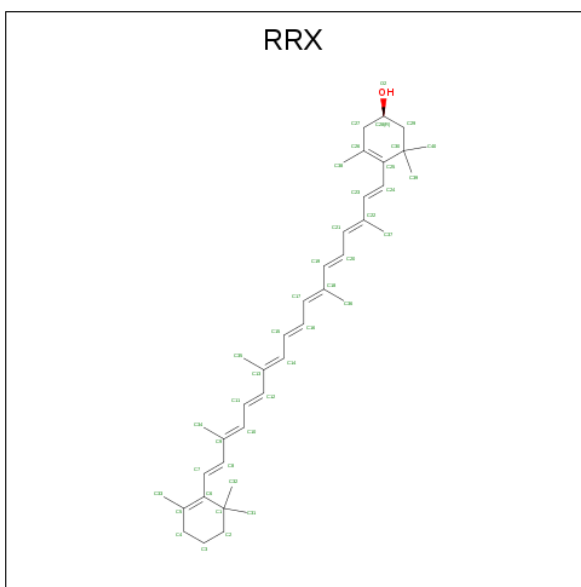
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			48	37	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

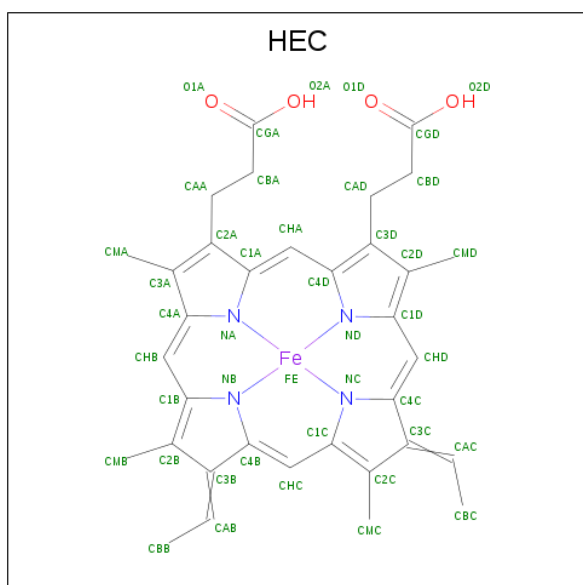


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

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

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

- Molecule 40 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	177	Total	O	0	5
			182	182		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	B	447	Total 473	O 473	0	25
41	C	317	Total 324	O 324	0	7
41	D	175	Total 180	O 180	0	5
41	E	62	Total 66	O 66	0	4
41	F	8	Total 8	O 8	0	0
41	H	62	Total 65	O 65	0	3
41	I	16	Total 16	O 16	0	0
41	J	23	Total 23	O 23	0	0
41	K	12	Total 12	O 12	0	0
41	L	19	Total 21	O 21	0	2
41	M	12	Total 12	O 12	0	0
41	O	263	Total 273	O 273	0	10
41	T	19	Total 20	O 20	0	1
41	U	133	Total 136	O 136	0	3
41	V	177	Total 183	O 183	0	6
41	Y	7	Total 7	O 7	0	0
41	X	22	Total 22	O 22	0	0
41	Z	5	Total 5	O 5	0	0
41	a	182	Total 185	O 185	0	3
41	b	451	Total 465	O 465	0	14
41	c	362	Total 374	O 374	0	12

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	d	176	Total 182	O 182	0	6
41	e	48	Total 49	O 49	0	1
41	f	15	Total 16	O 16	0	1
41	h	68	Total 70	O 70	0	2
41	i	19	Total 21	O 21	0	2
41	j	23	Total 24	O 24	0	1
41	k	11	Total 12	O 12	0	1
41	l	22	Total 24	O 24	0	2
41	m	23	Total 24	O 24	0	1
41	o	214	Total 230	O 230	0	15
41	t	19	Total 20	O 20	0	1
41	u	146	Total 150	O 150	0	4
41	v	144	Total 147	O 147	0	3
41	y	7	Total 7	O 7	0	0
41	x	25	Total 26	O 26	0	1
41	z	12	Total 12	O 12	0	0

3 Residue-property plots

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



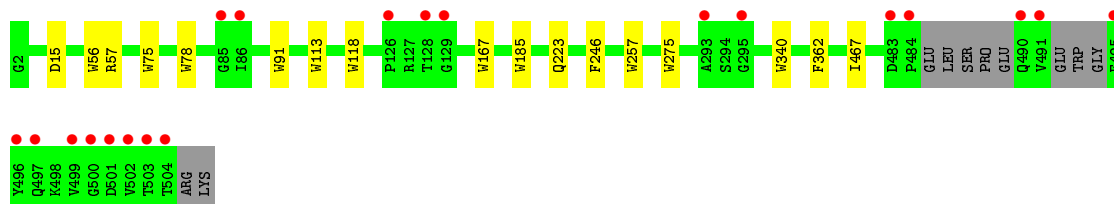
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein

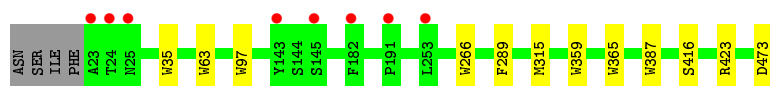


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein



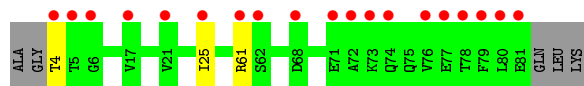
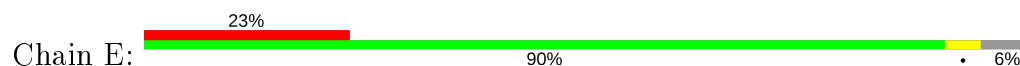
- Molecule 4: Photosystem II D2 protein



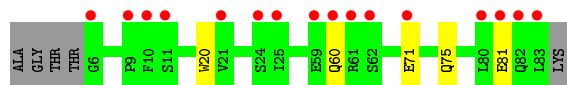
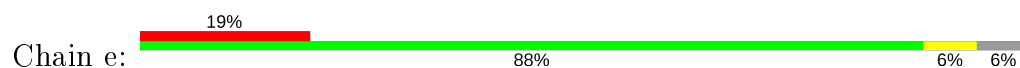
- Molecule 4: Photosystem II D2 protein



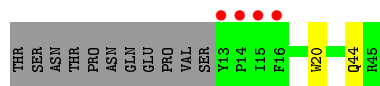
- Molecule 5: Cytochrome b559 subunit alpha



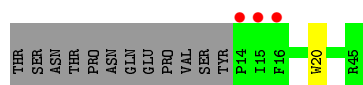
- Molecule 5: Cytochrome b559 subunit alpha



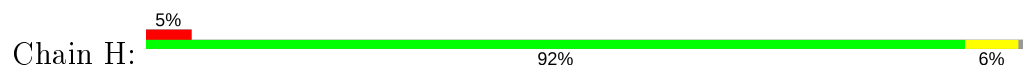
- Molecule 6: Cytochrome b559 subunit beta



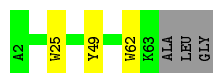
- Molecule 6: Cytochrome b559 subunit beta



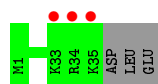
- Molecule 7: Photosystem II reaction center protein H



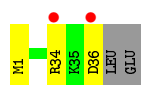
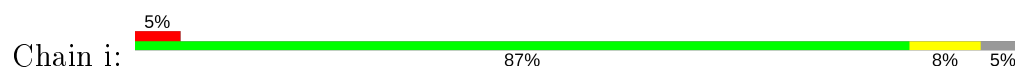
- Molecule 7: Photosystem II reaction center protein H



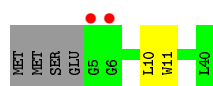
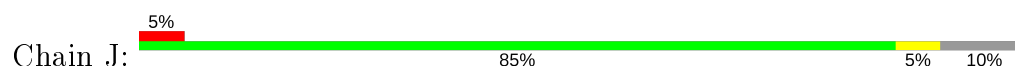
- Molecule 8: Photosystem II reaction center protein I



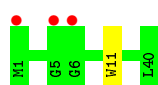
- Molecule 8: Photosystem II reaction center protein I



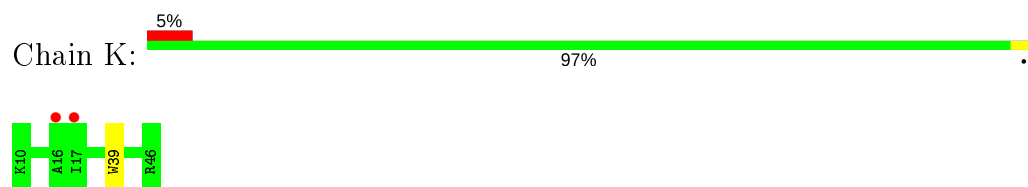
- Molecule 9: Photosystem II reaction center protein J



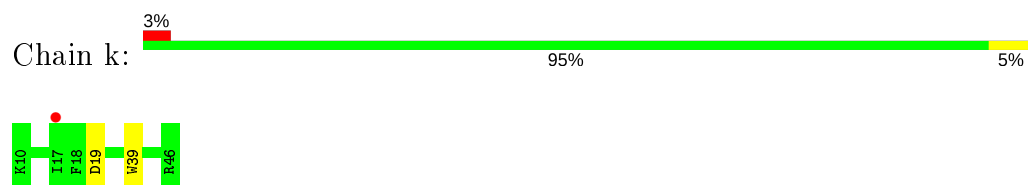
- Molecule 9: Photosystem II reaction center protein J



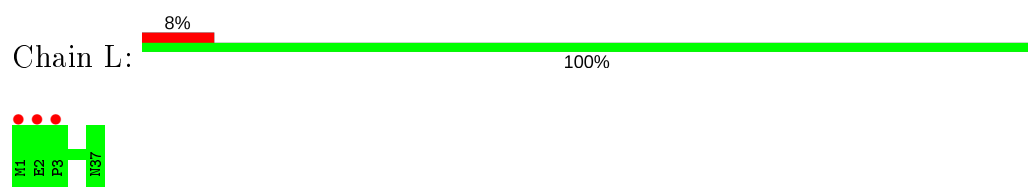
- Molecule 10: Photosystem II reaction center protein K



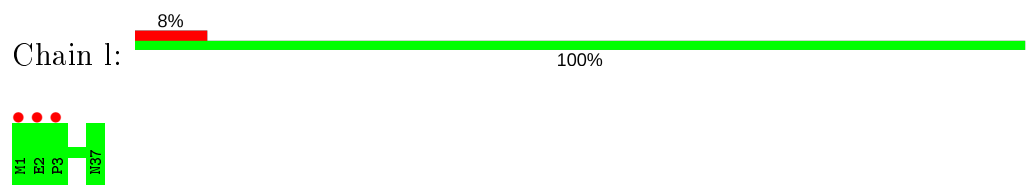
- Molecule 10: Photosystem II reaction center protein K



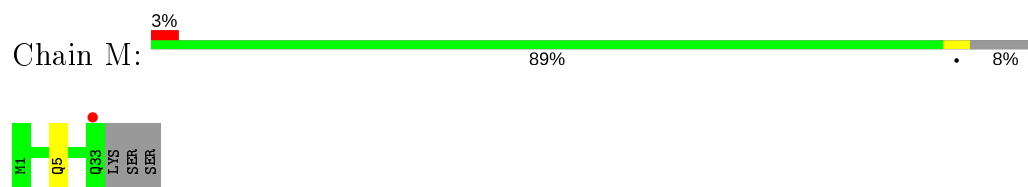
- Molecule 11: Photosystem II reaction center protein L



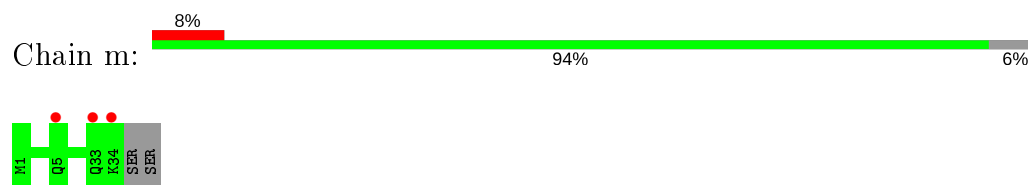
- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

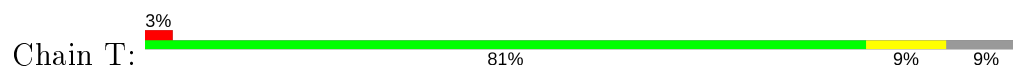




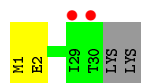
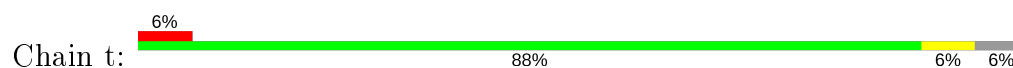
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



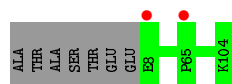
- Molecule 14: Photosystem II reaction center protein T



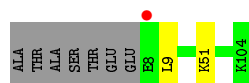
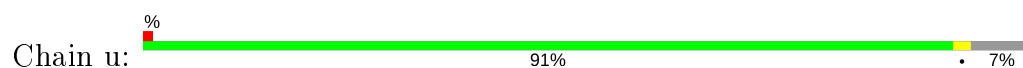
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



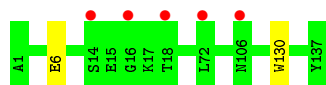
- Molecule 15: Photosystem II 12 kDa extrinsic protein



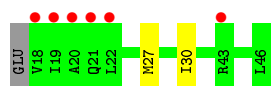
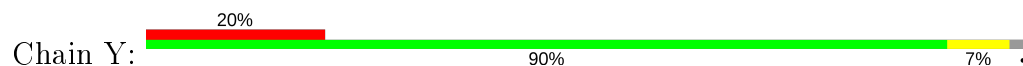
- Molecule 16: Cytochrome c-550



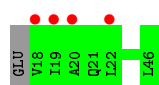
- Molecule 16: Cytochrome c-550



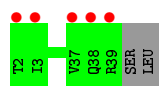
- Molecule 17: Photosystem II reaction center protein Ycf12



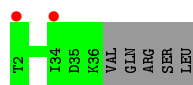
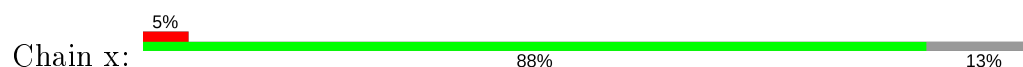
- Molecule 17: Photosystem II reaction center protein Ycf12



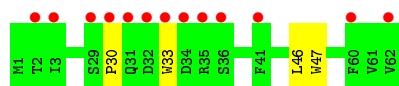
- Molecule 18: Photosystem II reaction center protein X



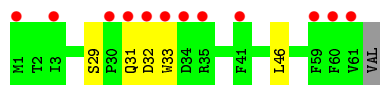
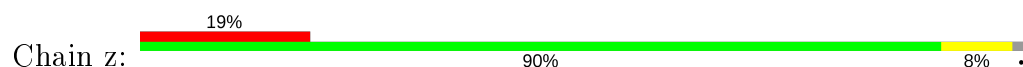
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 100.0 (19.99-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	33616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.95	5/2717 (0.2%)	0.77	1/3707 (0.0%)
1	a	0.93	4/2718 (0.1%)	0.79	2/3707 (0.1%)
2	B	0.90	9/4181 (0.2%)	0.77	1/5700 (0.0%)
2	b	0.91	11/4029 (0.3%)	0.78	2/5490 (0.0%)
3	C	0.87	7/3599 (0.2%)	0.74	2/4901 (0.0%)
3	c	0.86	8/3640 (0.2%)	0.72	2/4956 (0.0%)
4	D	0.95	3/2826 (0.1%)	0.78	1/3850 (0.0%)
4	d	0.95	8/2817 (0.3%)	0.78	1/3839 (0.0%)
5	E	0.71	0/654	0.68	0/896
5	e	0.69	1/661 (0.2%)	0.72	0/904
6	F	0.79	1/278 (0.4%)	0.60	0/379
6	f	0.81	1/265 (0.4%)	0.62	0/360
7	H	0.84	2/524 (0.4%)	0.75	0/715
7	h	0.86	2/517 (0.4%)	0.71	0/704
8	I	0.63	0/281	0.69	0/380
8	i	0.61	0/300	0.62	0/405
9	J	0.82	1/257 (0.4%)	0.61	0/349
9	j	0.81	1/278 (0.4%)	0.62	0/378
10	K	0.70	1/303 (0.3%)	0.65	0/416
10	k	0.72	1/295 (0.3%)	0.64	0/407
11	L	0.88	0/312	0.76	0/425
11	l	0.91	0/306	0.76	0/418
12	M	0.70	0/265	0.74	0/362
12	m	0.70	0/270	0.76	0/369
13	O	0.72	0/1919	0.80	1/2607 (0.0%)
13	o	0.69	0/1875	0.77	2/2548 (0.1%)
14	T	0.78	0/259	0.77	0/352
14	t	0.79	0/257	0.73	0/349
15	U	0.77	0/777	0.78	0/1055
15	u	0.76	0/781	0.77	0/1059
16	V	0.80	0/1110	0.80	1/1506 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.71	1/1073 (0.1%)	0.75	0/1461
17	Y	0.50	0/213	0.63	0/285
17	y	0.45	0/214	0.60	0/286
18	X	0.54	0/277	0.69	0/375
18	x	0.57	0/255	0.66	0/345
19	Z	0.70	2/461 (0.4%)	0.56	0/632
19	z	0.61	1/444 (0.2%)	0.57	0/611
All	All	0.85	70/42208 (0.2%)	0.75	16/57488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.13	1.50	1.41
1	A	343	LEU	C-N	6.74	1.49	1.34
1	a	131	TRP	CD2-CE2	6.46	1.49	1.41
3	C	266	TRP	CD2-CE2	6.43	1.49	1.41
2	B	33	TRP	CD2-CE2	6.27	1.48	1.41
9	j	11	TRP	CD2-CE2	6.26	1.48	1.41
10	k	39	TRP	CD2-CE2	6.25	1.48	1.41
2	B	56	TRP	CD2-CE2	6.21	1.48	1.41
3	c	35	TRP	CD2-CE2	6.21	1.48	1.41
2	B	78	TRP	CD2-CE2	6.18	1.48	1.41
4	D	280	TRP	CD2-CE2	6.11	1.48	1.41
2	b	113	TRP	CD2-CE2	6.08	1.48	1.41
1	a	284	TRP	CD2-CE2	6.00	1.48	1.41
16	v	130	TRP	CD2-CE2	5.96	1.48	1.41
3	c	443	TRP	CD2-CE2	5.93	1.48	1.41
1	A	278	TRP	CD2-CE2	5.90	1.48	1.41
2	b	56	TRP	CD2-CE2	5.90	1.48	1.41
19	Z	47	TRP	CD2-CE2	5.86	1.48	1.41
6	f	20	TRP	CD2-CE2	5.85	1.48	1.41
3	c	97	TRP	CD2-CE2	5.76	1.48	1.41
1	A	284	TRP	CD2-CE2	5.74	1.48	1.41
2	b	275	TRP	CD2-CE2	5.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	387	TRP	CD2-CE2	5.69	1.48	1.41
9	J	11	TRP	CD2-CE2	5.68	1.48	1.41
2	B	113	TRP	CD2-CE2	5.67	1.48	1.41
6	F	20	TRP	CD2-CE2	5.60	1.48	1.41
7	H	62	TRP	CD2-CE2	5.60	1.48	1.41
7	h	62	TRP	CD2-CE2	5.60	1.48	1.41
4	D	32	TRP	CD2-CE2	5.59	1.48	1.41
4	D	167	TRP	CD2-CE2	5.58	1.48	1.41
3	C	35	TRP	CD2-CE2	5.48	1.48	1.41
10	K	39	TRP	CD2-CE2	5.47	1.48	1.41
19	Z	33	TRP	CD2-CE2	5.47	1.48	1.41
4	d	48	TRP	CD2-CE2	5.45	1.47	1.41
4	d	111	TRP	CD2-CE2	5.44	1.47	1.41
2	b	185	TRP	CD2-CE2	5.44	1.47	1.41
1	A	20	TRP	CD2-CE2	5.43	1.47	1.41
1	a	32	TRP	CD2-CE2	5.42	1.47	1.41
2	b	340	TRP	CD2-CE2	5.41	1.47	1.41
1	a	317	TRP	CD2-CE2	5.41	1.47	1.41
3	c	250	TRP	CD2-CE2	5.40	1.47	1.41
2	b	78	TRP	CD2-CE2	5.37	1.47	1.41
3	C	365	TRP	CD2-CE2	5.37	1.47	1.41
2	B	302	TRP	CD2-CE2	5.35	1.47	1.41
7	h	25	TRP	CD2-CE2	5.35	1.47	1.41
3	C	97	TRP	CD2-CE2	5.32	1.47	1.41
4	d	93	TRP	CD2-CE2	5.32	1.47	1.41
4	d	58	TRP	CD2-CE2	5.32	1.47	1.41
19	z	33	TRP	CD2-CE2	5.29	1.47	1.41
2	b	91	TRP	CD2-CE2	5.29	1.47	1.41
3	c	365	TRP	CG-CD1	5.26	1.44	1.36
4	d	104	TRP	CD2-CE2	5.25	1.47	1.41
5	e	20	TRP	CD2-CE2	5.25	1.47	1.41
2	b	75	TRP	CD2-CE2	5.23	1.47	1.41
4	d	21	TRP	CD2-CE2	5.22	1.47	1.41
1	A	142	TRP	CD2-CE2	5.21	1.47	1.41
4	d	32	TRP	CD2-CE2	5.21	1.47	1.41
3	C	359	TRP	CD2-CE2	5.20	1.47	1.41
2	B	91	TRP	CD2-CE2	5.17	1.47	1.41
4	d	14	TRP	CD2-CE2	5.15	1.47	1.41
2	B	75	TRP	CD2-CE2	5.14	1.47	1.41
3	C	63	TRP	CD2-CE2	5.14	1.47	1.41
2	B	115	TRP	CD2-CE2	5.13	1.47	1.41
2	b	167	TRP	CD2-CE2	5.13	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	239	TRP	CD2-CE2	5.09	1.47	1.41
2	B	493	TRP	CD2-CE2	5.07	1.47	1.41
2	b	118	TRP	CD2-CE2	5.06	1.47	1.41
3	c	223	TRP	CD2-CE2	5.04	1.47	1.41
7	H	25	TRP	CD2-CE2	5.03	1.47	1.41
2	b	257	TRP	CD2-CE2	5.01	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	342	ASP	CB-CG-OD1	6.34	124.01	118.30
16	V	128	ASP	CB-CG-OD1	6.14	123.82	118.30
3	C	473	ASP	CB-CG-OD2	5.92	123.63	118.30
13	o	152	ARG	NE-CZ-NH1	-5.84	117.38	120.30
3	c	423	ARG	NE-CZ-NH2	-5.79	117.41	120.30
4	D	100	ASP	CB-CG-OD1	5.70	123.43	118.30
2	b	57	ARG	NE-CZ-NH1	5.47	123.04	120.30
13	O	158	ASP	CB-CG-OD1	5.38	123.14	118.30
2	B	15	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	131	TRP	CA-CB-CG	-5.31	103.61	113.70
3	c	423	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	b	15	ASP	CB-CG-OD1	5.21	122.98	118.30
3	C	423	ARG	NE-CZ-NH2	-5.11	117.75	120.30
13	o	223	ASP	CB-CG-OD1	5.04	122.84	118.30
1	a	151	LEU	CB-CG-CD2	-5.04	102.44	111.00
4	d	297	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

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%)	329 (98%)	5 (2%)	1 (0%)	41	26
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	26
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100	100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100	100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	47	33
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	47	33
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	41	26
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100
6	F	31/44 (70%)	31 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	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	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	34	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	13	3
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	9	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	47	33

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	GLN
3	c	416	SER
19	z	31	GLN
19	Z	30	PRO
13	o	34	SER
13	o	61	GLN
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	269/279 (96%)	268 (100%)	1 (0%)	91	89
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	405/403 (100%)	401 (99%)	4 (1%)	76	69
2	b	390/403 (97%)	386 (99%)	4 (1%)	76	69
3	C	351/356 (99%)	349 (99%)	2 (1%)	86	83
3	c	356/356 (100%)	351 (99%)	5 (1%)	67	55
4	D	277/277 (100%)	274 (99%)	3 (1%)	73	65
4	d	276/277 (100%)	272 (99%)	4 (1%)	67	55
5	E	68/72 (94%)	65 (96%)	3 (4%)	28	12
5	e	68/72 (94%)	63 (93%)	5 (7%)	13	3
6	F	27/38 (71%)	26 (96%)	1 (4%)	34	17
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	34	17
7	h	54/54 (100%)	53 (98%)	1 (2%)	57	43
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	32/34 (94%)	29 (91%)	3 (9%)	8	1
9	J	23/28 (82%)	22 (96%)	1 (4%)	29	12
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/30 (100%)	30 (100%)	0	100	100
10	k	28/30 (93%)	27 (96%)	1 (4%)	35	18
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	33/35 (94%)	33 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	38	21
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	207/207 (100%)	202 (98%)	5 (2%)	49	33
13	o	199/207 (96%)	197 (99%)	2 (1%)	76	69
14	T	26/28 (93%)	23 (88%)	3 (12%)	5	1
14	t	26/28 (93%)	25 (96%)	1 (4%)	33	16
15	U	82/89 (92%)	82 (100%)	0	100	100
15	u	83/89 (93%)	81 (98%)	2 (2%)	49	33
16	V	120/117 (103%)	119 (99%)	1 (1%)	81	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	v	114/117 (97%)	113 (99%)	1 (1%)	78	72
17	Y	21/23 (91%)	19 (90%)	2 (10%)	8	1
17	y	21/23 (91%)	21 (100%)	0	100	100
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	27/33 (82%)	27 (100%)	0	100	100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	50	34
19	z	39/52 (75%)	37 (95%)	2 (5%)	24	9
All	All	4223/4376 (96%)	4162 (99%)	61 (1%)	69	55

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

Mol	Chain	Res	Type
1	A	244	GLU
2	B	80	ILE
2	B	246	PHE
2	B	307[A]	GLU
2	B	307[B]	GLU
3	C	289	PHE
3	C	315	MET
4	D	26	ARG
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
5	E	25	ILE
5	E	61	ARG
6	F	44	GLN
7	H	49	TYR
7	H	63	LYS
9	J	10	LEU
12	M	5	GLN
13	O	23	ASP
13	O	24	ASP
13	O	118	LEU
13	O	130[A]	GLN
13	O	130[B]	GLN
14	T	2	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
16	V	86	GLN
17	Y	27	MET

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Mol	Chain	Res	Type
17	Y	30	ILE
19	Z	46	LEU
2	b	223	GLN
2	b	246	PHE
2	b	362	PHE
2	b	467	ILE
3	c	156	LYS
3	c	255	THR
3	c	289	PHE
3	c	355	THR
3	c	416	SER
4	d	180	ARG
4	d	233	ARG
4	d	237	PRO
4	d	329	MET
5	e	60[A]	GLN
5	e	60[B]	GLN
5	e	71	GLU
5	e	75	GLN
5	e	81	GLU
7	h	49	TYR
8	i	34[A]	ARG
8	i	34[B]	ARG
8	i	36	ASP
10	k	19	ASP
13	o	23	ASP
13	o	118	LEU
14	t	2	GLU
15	u	9	LEU
15	u	51	LYS
16	v	6	GLU
19	z	29	SER
19	z	46	LEU

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	261	GLN
1	A	315	ASN
2	B	53	ASN
2	B	179	GLN
2	B	331	ASN

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Mol	Chain	Res	Type
2	B	409	GLN
7	H	59	ASN
11	L	6	ASN
12	M	5	GLN
13	O	82	GLN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	331	ASN
4	d	332	GLN
13	o	82	GLN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN
16	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	1.11	0
14	FME	T	1	14	8,9,10	0.43	0	7,9,11	1.79	2 (28%)
8	FME	i	1	8	8,9,10	0.52	0	7,9,11	1.68	1 (14%)
14	FME	t	1	14	8,9,10	0.49	0	7,9,11	1.86	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	2/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.88	114.93	109.73
14	T	1	FME	CE-SD-CG	2.70	109.68	100.40
14	T	1	FME	O-C-CA	-2.46	118.34	124.78
14	t	1	FME	CG-CB-CA	2.44	119.72	112.95
14	t	1	FME	CE-SD-CG	2.32	108.38	100.40
14	t	1	FME	C-CA-N	2.28	113.84	109.73
14	t	1	FME	O-C-CA	-2.24	118.90	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O1-CN-N-CA
14	T	1	FME	N-CA-CB-CG
8	i	1	FME	O1-CN-N-CA
14	t	1	FME	N-CA-CB-CG
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
14	T	1	FME	C-CA-CB-CG
14	t	1	FME	C-CA-CB-CG
8	I	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 349 ligands modelled in this entry, 55 are unknown and 14 are monoatomic - leaving 280 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMG	B	620	-	51,51,55	1.02	2 (3%)	59,59,63	1.31	5 (8%)
28	DMS	O	305	-	3,3,3	2.63	1 (33%)	3,3,3	0.79	0
28	DMS	A	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.78	0
28	DMS	c	528	-	3,3,3	2.57	1 (33%)	3,3,3	0.44	0
28	DMS	c	536	-	3,3,3	2.84	1 (33%)	3,3,3	1.23	0
28	DMS	B	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.73	0
20	CLA	d	403	41	59,73,73	2.06	12 (20%)	67,113,113	2.07	16 (23%)
27	PL9	A	411	-	55,55,55	0.83	3 (5%)	68,69,69	1.69	18 (26%)
28	DMS	c	527	-	3,3,3	2.31	1 (33%)	3,3,3	0.49	0
35	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	3 (3%)
28	DMS	V	209	-	3,3,3	2.61	1 (33%)	3,3,3	0.64	0
32	HTG	b	602	-	19,19,19	1.00	2 (10%)	23,24,24	1.15	1 (4%)
20	CLA	B	604	-	59,73,73	1.92	14 (23%)	67,113,113	2.20	17 (25%)
28	DMS	b	639	-	3,3,3	2.81	1 (33%)	3,3,3	0.57	0
30	OEX	A	420	1,3,41	0,15,15	0.00	-	-	-	-
28	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.83	0
24	LMG	C	519	-	51,51,55	1.03	2 (3%)	59,59,63	1.23	8 (13%)
20	CLA	C	503	-	59,73,73	2.29	13 (22%)	67,113,113	1.85	18 (26%)
28	DMS	V	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
21	PHO	A	403	-	67,69,69	1.69	11 (16%)	85,99,99	2.04	20 (23%)
23	SQD	f	101	-	39,40,54	1.37	3 (7%)	48,51,65	3.70	12 (25%)
32	HTG	b	601	-	19,19,19	1.04	2 (10%)	23,24,24	1.27	2 (8%)
20	CLA	c	504	41	59,73,73	2.14	13 (22%)	67,113,113	2.30	15 (22%)
35	DGD	D	406	-	51,51,67	1.11	2 (3%)	59,59,81	1.21	5 (8%)
28	DMS	C	526	-	3,3,3	2.56	1 (33%)	3,3,3	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DMS	c	530	-	3,3,3	2.80	1 (33%)	3,3,3	1.01	0
28	DMS	C	525[A]	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
22	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.23	5 (8%)
34	LMT	B	626	-	24,24,36	0.54	0	29,29,47	1.14	3 (10%)
40	HEC	v	201	16	26,50,50	2.25	8 (30%)	18,82,82	2.26	6 (33%)
20	CLA	C	507	41	59,73,73	2.42	16 (27%)	67,113,113	2.26	17 (25%)
20	CLA	c	502	-	59,73,73	2.18	12 (20%)	67,113,113	2.28	20 (29%)
20	CLA	b	614	-	59,73,73	1.88	12 (20%)	67,113,113	2.14	18 (26%)
28	DMS	C	528	-	3,3,3	2.31	1 (33%)	3,3,3	0.59	0
20	CLA	A	404	-	59,73,73	2.00	14 (23%)	67,113,113	1.92	16 (23%)
24	LMG	A	407	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	3 (5%)
28	DMS	V	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.67	0
28	DMS	c	532	-	3,3,3	2.60	1 (33%)	3,3,3	0.47	0
20	CLA	D	402	41	59,73,73	1.86	15 (25%)	67,113,113	2.14	16 (23%)
20	CLA	C	504	41	59,73,73	2.14	11 (18%)	67,113,113	2.07	19 (28%)
20	CLA	a	404	41	54,68,73	1.86	12 (22%)	61,107,113	2.13	18 (29%)
28	DMS	C	529	-	3,3,3	2.69	1 (33%)	3,3,3	0.81	0
34	LMT	f	102	-	24,24,36	0.79	1 (4%)	29,29,47	0.96	2 (6%)
28	DMS	b	635	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
22	BCR	t	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.74	19 (33%)
20	CLA	D	404	-	59,73,73	2.12	15 (25%)	67,113,113	1.97	21 (31%)
28	DMS	V	207	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
36	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
20	CLA	B	603	-	59,73,73	2.19	14 (23%)	67,113,113	2.17	21 (31%)
32	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	1 (4%)
34	LMT	b	628	-	25,25,36	0.55	0	30,30,47	1.20	2 (6%)
27	PL9	D	412	-	55,55,55	1.06	3 (5%)	68,69,69	1.51	12 (17%)
28	DMS	D	413	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0
20	CLA	c	513	-	59,73,73	2.50	14 (23%)	67,113,113	2.03	18 (26%)
20	CLA	b	609	41	59,73,73	2.01	13 (22%)	67,113,113	1.90	21 (31%)
22	BCR	B	617	-	41,41,41	0.98	0	56,56,56	1.62	11 (19%)
28	DMS	b	634	-	3,3,3	2.67	1 (33%)	3,3,3	0.68	0
28	DMS	b	637	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
21	PHO	a	405	-	67,69,69	1.81	12 (17%)	85,99,99	1.84	17 (20%)
20	CLA	C	511	3	59,73,73	2.35	15 (25%)	67,113,113	2.29	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	b	606	-	59,73,73	1.96	11 (18%)	67,113,113	2.26	20 (29%)
20	CLA	C	501	-	59,73,73	1.98	14 (23%)	67,113,113	1.98	13 (19%)
28	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
20	CLA	D	401	-	59,73,73	1.79	11 (18%)	67,113,113	2.22	20 (29%)
28	DMS	A	414	-	3,3,3	1.97	1 (33%)	3,3,3	0.54	0
20	CLA	a	407	-	41,55,73	2.30	9 (21%)	45,91,113	2.44	18 (40%)
32	HTG	u	201	-	7,7,19	0.43	0	6,6,24	0.70	0
35	DGD	C	516	-	63,63,67	0.89	2 (3%)	77,77,81	1.20	7 (9%)
28	DMS	A	415	-	3,3,3	2.75	1 (33%)	3,3,3	1.01	0
23	SQD	F	101	-	34,35,54	1.01	2 (5%)	42,45,65	1.59	7 (16%)
28	DMS	b	640	-	3,3,3	2.76	1 (33%)	3,3,3	1.38	1 (33%)
37	HEM	e	102	5,6	27,50,50	2.06	8 (29%)	17,82,82	2.69	8 (47%)
28	DMS	v	207	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
32	HTG	b	624	-	19,19,19	1.15	2 (10%)	23,24,24	1.60	2 (8%)
35	DGD	C	517	-	56,56,67	0.98	2 (3%)	70,70,81	0.93	4 (5%)
28	DMS	B	644	-	3,3,3	2.87	1 (33%)	3,3,3	1.26	0
20	CLA	B	610	-	59,73,73	2.14	13 (22%)	67,113,113	2.09	19 (28%)
28	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.81	0
28	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
28	DMS	d	414	-	3,3,3	2.50	1 (33%)	3,3,3	0.24	0
20	CLA	b	610	-	59,73,73	1.99	12 (20%)	67,113,113	2.09	19 (28%)
28	DMS	c	535	-	3,3,3	2.78	1 (33%)	3,3,3	0.79	0
28	DMS	j	105	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
35	DGD	H	102	-	63,63,67	1.04	3 (4%)	77,77,81	1.27	8 (10%)
32	HTG	d	401	-	19,19,19	1.08	1 (5%)	23,24,24	2.36	4 (17%)
36	LHG	L	101	-	48,48,48	0.90	3 (6%)	51,54,54	0.90	1 (1%)
20	CLA	B	602	41	59,73,73	2.54	17 (28%)	67,113,113	2.37	20 (29%)
22	BCR	C	515	-	41,41,41	0.97	0	56,56,56	1.19	6 (10%)
28	DMS	O	309	-	3,3,3	2.67	1 (33%)	3,3,3	1.16	0
20	CLA	C	505	-	59,73,73	2.09	16 (27%)	67,113,113	1.93	15 (22%)
28	DMS	V	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
22	BCR	A	405	-	41,41,41	0.95	3 (7%)	56,56,56	1.27	7 (12%)
22	BCR	C	514	-	41,41,41	0.85	0	56,56,56	1.31	7 (12%)
28	DMS	o	304	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
20	CLA	B	605	-	59,73,73	2.02	12 (20%)	67,113,113	1.89	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DMS	u	203	-	3,3,3	2.57	1 (33%)	3,3,3	0.78	0
20	CLA	b	618	-	59,73,73	2.14	14 (23%)	67,113,113	2.21	21 (31%)
31	BCT	a	413	29	0,3,3	0.00	-	0,3,3	0.00	-
22	BCR	j	102	-	41,41,41	0.85	0	56,56,56	1.38	9 (16%)
28	DMS	b	638	-	3,3,3	2.78	1 (33%)	3,3,3	0.94	0
28	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.74	0
28	DMS	B	635	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
28	DMS	F	102	-	3,3,3	2.63	1 (33%)	3,3,3	0.61	0
32	HTG	B	621	-	19,19,19	1.45	3 (15%)	23,24,24	1.79	6 (26%)
28	DMS	B	640	-	3,3,3	2.55	1 (33%)	3,3,3	0.97	0
28	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.76	0
28	DMS	H	103	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
20	CLA	b	603	41	59,73,73	2.45	16 (27%)	67,113,113	2.11	19 (28%)
32	HTG	c	521	-	19,19,19	0.96	1 (5%)	23,24,24	2.03	3 (13%)
35	DGD	c	515	-	63,63,67	0.85	3 (4%)	77,77,81	1.19	8 (10%)
34	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.93	2 (4%)
28	DMS	v	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
20	CLA	b	613	-	59,73,73	2.03	9 (15%)	67,113,113	1.97	19 (28%)
28	DMS	U	903[B]	-	3,3,3	2.44	1 (33%)	3,3,3	0.17	0
28	DMS	B	642	-	3,3,3	2.79	1 (33%)	3,3,3	0.75	0
20	CLA	d	402	-	59,73,73	1.90	12 (20%)	67,113,113	1.89	19 (28%)
28	DMS	o	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.77	0
28	DMS	o	306	-	3,3,3	2.79	1 (33%)	3,3,3	1.03	0
28	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
36	LHG	D	407	-	48,48,48	0.86	1 (2%)	51,54,54	1.26	5 (9%)
34	LMT	Z	101	-	36,36,36	0.68	1 (2%)	47,47,47	0.98	3 (6%)
20	CLA	A	401	-	59,73,73	1.85	13 (22%)	67,113,113	2.01	18 (26%)
28	DMS	U	903[A]	-	3,3,3	2.56	1 (33%)	3,3,3	0.75	0
22	BCR	k	102	-	41,41,41	0.79	0	56,56,56	1.29	9 (16%)
32	HTG	C	521	-	19,19,19	0.98	2 (10%)	23,24,24	1.97	4 (17%)
20	CLA	c	507	41	59,73,73	2.31	13 (22%)	67,113,113	2.11	16 (23%)
20	CLA	B	606	-	59,73,73	1.85	10 (16%)	67,113,113	2.11	19 (28%)
34	LMT	m	101	-	36,36,36	0.61	1 (2%)	47,47,47	0.96	1 (2%)
20	CLA	b	608	-	59,73,73	2.43	16 (27%)	67,113,113	1.99	16 (23%)
20	CLA	a	403	-	59,73,73	1.86	13 (22%)	67,113,113	2.05	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PL9	d	412	-	55,55,55	1.09	3 (5%)	68,69,69	1.59	16 (23%)
28	DMS	v	203	-	3,3,3	2.59	1 (33%)	3,3,3	0.85	0
28	DMS	O	311	-	3,3,3	2.87	1 (33%)	3,3,3	0.92	0
23	SQD	a	409	-	53,54,54	1.01	4 (7%)	62,65,65	2.11	11 (17%)
28	DMS	O	306	-	3,3,3	2.53	1 (33%)	3,3,3	0.64	0
32	HTG	B	631	-	19,19,19	0.94	2 (10%)	23,24,24	2.09	6 (26%)
21	PHO	D	403	-	67,69,69	1.92	14 (20%)	85,99,99	1.90	19 (22%)
22	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
20	CLA	c	508	-	54,68,73	2.45	16 (29%)	61,107,113	2.05	19 (31%)
22	BCR	K	102	-	41,41,41	0.92	1 (2%)	56,56,56	1.48	6 (10%)
20	CLA	C	506	-	59,73,73	2.38	14 (23%)	67,113,113	2.17	19 (28%)
20	CLA	c	510	-	59,73,73	1.77	13 (22%)	67,113,113	1.98	20 (29%)
20	CLA	C	509	-	59,73,73	2.24	11 (18%)	67,113,113	2.11	18 (26%)
28	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
20	CLA	B	601	-	59,73,73	2.02	13 (22%)	67,113,113	1.90	19 (28%)
28	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.73	0
20	CLA	b	617	-	59,73,73	2.23	14 (23%)	67,113,113	2.18	22 (32%)
28	DMS	d	413	-	3,3,3	2.57	1 (33%)	3,3,3	0.91	0
24	LMG	J	101	39	45,45,55	1.01	2 (4%)	53,53,63	0.98	3 (5%)
28	DMS	C	525[B]	-	3,3,3	2.59	1 (33%)	3,3,3	0.79	0
28	DMS	b	632	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
35	DGD	d	416	-	51,51,67	1.11	3 (5%)	59,59,81	1.20	6 (10%)
34	LMT	J	103	-	24,24,36	0.65	1 (4%)	29,29,47	1.12	1 (3%)
28	DMS	C	530	-	3,3,3	2.61	1 (33%)	3,3,3	1.00	0
34	LMT	c	523	-	36,36,36	0.81	1 (2%)	47,47,47	1.60	6 (12%)
28	DMS	B	636	-	3,3,3	2.76	1 (33%)	3,3,3	0.78	0
22	BCR	D	405	-	41,41,41	1.03	3 (7%)	56,56,56	1.73	13 (23%)
28	DMS	B	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.63	0
37	HEM	E	104	5,6	27,50,50	2.12	8 (29%)	17,82,82	2.43	6 (35%)
20	CLA	c	512	-	59,73,73	2.32	15 (25%)	67,113,113	2.09	16 (23%)
23	SQD	l	101	-	53,54,54	1.08	4 (7%)	62,65,65	1.68	8 (12%)
32	HTG	c	520	-	19,19,19	0.89	2 (10%)	23,24,24	1.32	2 (8%)
34	LMT	a	418	-	36,36,36	0.68	2 (5%)	47,47,47	1.54	6 (12%)
32	HTG	v	210	-	14,14,19	0.62	0	18,19,24	2.19	4 (22%)
22	BCR	K	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.48	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	b	621	-	41,41,41	0.80	1 (2%)	56,56,56	1.47	8 (14%)
20	CLA	B	616	-	59,73,73	2.15	14 (23%)	67,113,113	1.97	19 (28%)
28	DMS	c	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
32	HTG	B	622	-	19,19,19	1.34	3 (15%)	23,24,24	1.93	6 (26%)
32	HTG	C	522	-	19,19,19	1.06	2 (10%)	23,24,24	1.56	1 (4%)
28	DMS	D	415	-	3,3,3	2.92	1 (33%)	3,3,3	0.73	0
20	CLA	c	505	-	59,73,73	2.07	14 (23%)	67,113,113	1.95	16 (23%)
34	LMT	B	627	-	15,15,36	0.48	0	14,14,47	0.67	0
24	LMG	j	101	39	45,45,55	1.00	3 (6%)	53,53,63	1.02	6 (11%)
36	LHG	l	102	-	48,48,48	0.78	2 (4%)	51,54,54	1.00	2 (3%)
28	DMS	O	304	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
23	SQD	b	622	-	53,54,54	1.10	3 (5%)	62,65,65	1.55	11 (17%)
24	LMG	C	524	-	45,45,55	1.10	3 (6%)	53,53,63	1.36	5 (9%)
35	DGD	c	516	-	58,58,67	0.86	2 (3%)	72,72,81	1.13	6 (8%)
28	DMS	b	636	-	3,3,3	2.71	1 (33%)	3,3,3	0.75	0
36	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	5 (9%)
23	SQD	A	406	-	53,54,54	1.00	3 (5%)	62,65,65	1.75	14 (22%)
22	BCR	a	408	-	41,41,41	1.21	2 (4%)	56,56,56	1.44	7 (12%)
28	DMS	B	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.82	0
32	HTG	C	534	-	19,19,19	1.08	1 (5%)	23,24,24	1.47	5 (21%)
35	DGD	c	517	-	63,63,67	1.04	4 (6%)	77,77,81	1.19	8 (10%)
27	PL9	a	415	-	55,55,55	0.83	3 (5%)	68,69,69	1.67	16 (23%)
32	HTG	b	625	-	19,19,19	1.21	2 (10%)	23,24,24	1.34	4 (17%)
22	BCR	b	619	-	41,41,41	0.95	0	56,56,56	1.77	11 (19%)
34	LMT	z	102	-	36,36,36	0.76	1 (2%)	47,47,47	1.49	8 (17%)
32	HTG	O	302	-	19,19,19	1.29	2 (10%)	23,24,24	1.18	2 (8%)
28	DMS	b	633	-	3,3,3	2.55	1 (33%)	3,3,3	1.05	0
28	DMS	u	202	-	3,3,3	2.65	1 (33%)	3,3,3	1.29	0
34	LMT	b	627	-	33,33,36	0.88	1 (3%)	44,44,47	1.80	10 (22%)
30	OEX	a	419	1,3,41	0,15,15	0.00	-	-	-	-
28	DMS	U	902	-	3,3,3	2.66	1 (33%)	3,3,3	1.63	1 (33%)
28	DMS	U	904	-	3,3,3	2.85	1 (33%)	3,3,3	0.70	0
22	BCR	T	101	-	41,41,41	0.81	0	56,56,56	1.50	11 (19%)
28	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.74	0
24	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.17	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	C	512	-	49,63,73	2.69	15 (30%)	55,101,113	2.35	17 (30%)
34	LMT	T	102	-	24,24,36	0.45	0	29,29,47	1.15	2 (6%)
21	PHO	a	406	-	67,69,69	1.89	14 (20%)	85,99,99	1.92	22 (25%)
20	CLA	C	508	-	54,68,73	2.47	15 (27%)	61,107,113	2.01	18 (29%)
32	HTG	B	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.56	2 (8%)
20	CLA	B	609	-	59,73,73	1.90	13 (22%)	67,113,113	2.07	20 (29%)
31	BCT	A	421	29	0,3,3	0.00	-	0,3,3	0.00	-
28	DMS	B	634	-	3,3,3	1.94	1 (33%)	3,3,3	0.29	0
28	DMS	O	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.42	0
28	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
36	LHG	d	407	-	48,48,48	0.73	2 (4%)	51,54,54	0.99	4 (7%)
20	CLA	b	607	-	59,73,73	1.79	9 (15%)	67,113,113	2.13	17 (25%)
20	CLA	b	615	-	59,73,73	1.87	13 (22%)	67,113,113	2.13	18 (26%)
32	HTG	B	632	-	19,19,19	1.02	1 (5%)	23,24,24	1.26	2 (8%)
20	CLA	c	501	-	59,73,73	2.15	13 (22%)	67,113,113	2.44	17 (25%)
28	DMS	v	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
28	DMS	h	102	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
20	CLA	C	502	-	59,73,73	2.26	14 (23%)	67,113,113	2.02	16 (23%)
20	CLA	B	611	41	59,73,73	2.27	15 (25%)	67,113,113	2.18	16 (23%)
38	RRX	H	101	-	42,42,42	0.77	1 (2%)	57,58,58	1.49	8 (14%)
36	LHG	E	103	-	46,46,48	1.03	2 (4%)	49,50,54	1.14	5 (10%)
28	DMS	v	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.66	0
28	DMS	C	532	-	3,3,3	3.28	1 (33%)	3,3,3	1.29	1 (33%)
22	BCR	B	618	-	41,41,41	1.05	0	56,56,56	1.26	7 (12%)
20	CLA	A	402	41	53,67,73	1.76	10 (18%)	59,105,113	2.38	16 (27%)
28	DMS	o	302	-	3,3,3	2.75	1 (33%)	3,3,3	0.90	0
20	CLA	c	511	3	59,73,73	2.56	17 (28%)	67,113,113	2.18	16 (23%)
24	LMG	b	623	-	49,49,55	0.96	2 (4%)	57,57,63	1.31	6 (10%)
34	LMT	B	625	-	24,24,36	0.53	0	29,29,47	1.26	4 (13%)
38	RRX	x	101	-	42,42,42	0.82	0	57,58,58	1.22	6 (10%)
20	CLA	B	607	-	59,73,73	2.39	15 (25%)	67,113,113	2.09	19 (28%)
23	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.71	10 (16%)
28	DMS	o	307	-	3,3,3	2.65	1 (33%)	3,3,3	0.85	0
34	LMT	I	101	-	36,36,36	0.65	1 (2%)	47,47,47	1.28	6 (12%)
28	DMS	i	104	-	3,3,3	2.62	1 (33%)	3,3,3	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	c	506	-	59,73,73	1.99	14 (23%)	67,113,113	1.91	19 (28%)
28	DMS	A	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
34	LMT	m	102	-	36,36,36	0.58	0	47,47,47	1.14	4 (8%)
20	CLA	c	509	-	59,73,73	2.32	15 (25%)	67,113,113	2.25	20 (29%)
20	CLA	c	503	-	59,73,73	2.42	16 (27%)	67,113,113	2.17	15 (22%)
20	CLA	b	605	-	59,73,73	2.04	11 (18%)	67,113,113	2.18	22 (32%)
28	DMS	B	641	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
28	DMS	u	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
36	LHG	D	408	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	1 (1%)
20	CLA	C	513	-	59,73,73	2.48	15 (25%)	67,113,113	2.01	14 (20%)
32	HTG	V	202	-	12,13,19	0.76	1 (8%)	16,18,24	2.50	6 (37%)
28	DMS	C	531	-	3,3,3	2.66	1 (33%)	3,3,3	0.97	0
28	DMS	D	416	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
20	CLA	b	611	-	59,73,73	2.64	15 (25%)	67,113,113	1.70	15 (22%)
32	HTG	D	417	-	19,19,19	1.05	1 (5%)	23,24,24	1.49	3 (13%)
28	DMS	O	303	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
23	SQD	a	401	-	53,54,54	1.12	3 (5%)	62,65,65	1.40	7 (11%)
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.84	11 (19%)
40	HEC	V	201	16	26,50,50	1.99	8 (30%)	18,82,82	1.88	4 (22%)
28	DMS	D	414	-	3,3,3	2.53	1 (33%)	3,3,3	0.25	0
28	DMS	B	645	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
22	BCR	k	101	-	41,41,41	0.94	0	56,56,56	1.12	6 (10%)
28	DMS	v	202	-	3,3,3	2.50	1 (33%)	3,3,3	0.58	0
28	DMS	b	641	-	3,3,3	2.79	1 (33%)	3,3,3	1.11	0
28	DMS	b	631	-	3,3,3	2.88	1 (33%)	3,3,3	1.24	0
20	CLA	b	612	41	59,73,73	1.97	13 (22%)	67,113,113	1.86	17 (25%)
28	DMS	v	208	-	3,3,3	2.63	1 (33%)	3,3,3	0.66	0
24	LMG	c	518	-	51,51,55	1.11	3 (5%)	59,59,63	1.31	7 (11%)
22	BCR	c	514	-	41,41,41	0.85	1 (2%)	56,56,56	1.49	7 (12%)
28	DMS	O	310	-	3,3,3	2.70	1 (33%)	3,3,3	0.70	0
20	CLA	B	608	41	59,73,73	1.95	12 (20%)	67,113,113	1.92	14 (20%)
20	CLA	B	614	-	59,73,73	1.96	16 (27%)	67,113,113	1.90	17 (25%)
28	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.49	0
24	LMG	a	410	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	2 (3%)
36	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	b	604	-	59,73,73	1.92	14 (23%)	67,113,113	2.16	25 (37%)
20	CLA	b	616	-	59,73,73	2.03	13 (22%)	67,113,113	2.22	23 (34%)
20	CLA	C	510	-	59,73,73	2.13	13 (22%)	67,113,113	2.07	17 (25%)
20	CLA	d	404	-	59,73,73	1.98	14 (23%)	67,113,113	1.93	17 (25%)
28	DMS	o	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.81	0
34	LMT	E	101	-	24,24,36	0.62	1 (4%)	29,29,47	1.01	3 (10%)
20	CLA	B	613	-	59,73,73	2.07	12 (20%)	67,113,113	2.08	18 (26%)
20	CLA	B	612	-	59,73,73	1.86	13 (22%)	67,113,113	2.10	19 (28%)
35	DGD	h	101	-	63,63,67	0.98	3 (4%)	77,77,81	1.04	4 (5%)
20	CLA	B	615	-	59,73,73	1.97	13 (22%)	67,113,113	2.13	19 (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
24	LMG	B	620	-	-	19/46/66/70	0/1/1/1
22	BCR	k	101	-	-	4/29/63/63	0/2/2/2
20	CLA	d	403	41	1/1/20/25	5/37/135/135	-
27	PL9	A	411	-	-	10/53/73/73	0/1/1/1
20	CLA	a	404	41	2/2/19/25	6/31/129/135	-
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
32	HTG	b	602	-	-	3/10/30/30	0/1/1/1
20	CLA	B	604	-	3/3/20/25	3/37/135/135	-
24	LMG	C	519	-	-	19/46/66/70	0/1/1/1
20	CLA	C	503	-	2/2/20/25	4/37/135/135	-
21	PHO	A	403	-	-	2/53/103/103	0/5/6/6
23	SQD	f	101	-	-	16/34/54/69	0/1/1/1
32	HTG	b	601	-	-	2/10/30/30	0/1/1/1
20	CLA	c	504	41	3/3/20/25	5/37/135/135	-
35	DGD	D	406	-	-	26/46/66/95	0/1/1/2
34	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
34	LMT	B	626	-	-	7/15/35/61	0/1/1/2
40	HEC	v	201	16	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	502	-	2/2/20/25	6/37/135/135	-
20	CLA	b	606	-	3/3/20/25	3/37/135/135	-
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
24	LMG	A	407	-	-	28/46/66/70	0/1/1/1
20	CLA	D	402	41	1/1/20/25	5/37/135/135	-
34	LMT	f	102	-	-	8/15/35/61	0/1/1/2
22	BCR	t	101	-	-	3/29/63/63	0/2/2/2
20	CLA	D	404	-	3/3/20/25	13/37/135/135	-
36	LHG	D	409	-	-	14/53/53/53	-
34	LMT	m	102	-	-	3/21/61/61	0/2/2/2
32	HTG	C	520	-	-	4/10/30/30	0/1/1/1
34	LMT	b	628	-	-	9/17/37/61	0/1/1/2
27	PL9	D	412	-	-	3/53/73/73	0/1/1/1
20	CLA	c	513	-	1/1/20/25	14/37/135/135	-
20	CLA	b	609	41	3/3/20/25	2/37/135/135	-
22	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	PL9	a	415	-	-	11/53/73/73	0/1/1/1
21	PHO	a	405	-	-	4/53/103/103	0/5/6/6
20	CLA	C	501	-	3/3/20/25	3/37/135/135	-
36	LHG	l	102	-	-	19/53/53/53	-
20	CLA	D	401	-	1/1/20/25	7/37/135/135	-
20	CLA	a	407	-	1/1/16/25	0/16/114/135	-
32	HTG	u	201	-	-	1/5/5/30	-
35	DGD	C	516	-	-	18/51/91/95	0/2/2/2
23	SQD	F	101	-	-	17/28/48/69	0/1/1/1
20	CLA	B	606	-	3/3/20/25	4/37/135/135	-
35	DGD	C	517	-	-	14/44/84/95	0/2/2/2
23	SQD	b	622	-	-	23/49/69/69	0/1/1/1
35	DGD	h	101	-	-	15/51/91/95	0/2/2/2
20	CLA	b	610	-	1/1/20/25	1/37/135/135	-
32	HTG	d	401	-	-	9/10/30/30	0/1/1/1
36	LHG	L	101	-	-	17/53/53/53	-
20	CLA	B	602	41	2/2/20/25	21/37/135/135	-
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
20	CLA	C	505	-	2/2/20/25	1/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	615	-	3/3/20/25	10/37/135/135	-
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
22	BCR	C	514	-	-	5/29/63/63	0/2/2/2
20	CLA	B	605	-	3/3/20/25	8/37/135/135	-
22	BCR	j	102	-	-	2/29/63/63	0/2/2/2
20	CLA	b	614	-	3/3/20/25	4/37/135/135	-
22	BCR	K	101	-	-	4/29/63/63	0/2/2/2
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
20	CLA	b	603	41	3/3/20/25	18/37/135/135	-
23	SQD	l	101	-	-	28/49/69/69	0/1/1/1
35	DGD	c	515	-	-	18/51/91/95	0/2/2/2
34	LMT	M	101	-	-	1/21/61/61	0/2/2/2
20	CLA	b	613	-	1/1/20/25	7/37/135/135	-
20	CLA	b	608	-	3/3/20/25	9/37/135/135	-
20	CLA	d	402	-	2/2/20/25	3/37/135/135	-
36	LHG	D	407	-	-	9/53/53/53	-
20	CLA	A	404	-	1/1/20/25	10/37/135/135	-
20	CLA	A	401	-	3/3/20/25	4/37/135/135	-
32	HTG	c	521	-	-	5/10/30/30	0/1/1/1
22	BCR	k	102	-	-	1/29/63/63	0/2/2/2
32	HTG	C	521	-	-	6/10/30/30	0/1/1/1
20	CLA	c	507	41	3/3/20/25	6/37/135/135	-
32	HTG	B	623	-	-	6/10/30/30	0/1/1/1
34	LMT	m	101	-	-	15/21/61/61	0/2/2/2
20	CLA	a	403	-	3/3/20/25	4/37/135/135	-
20	CLA	B	608	41	3/3/20/25	1/37/135/135	-
23	SQD	a	409	-	-	20/49/69/69	0/1/1/1
32	HTG	B	631	-	-	5/10/30/30	0/1/1/1
21	PHO	D	403	-	-	5/53/103/103	0/5/6/6
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2
20	CLA	c	508	-	2/2/19/25	2/31/129/135	-
22	BCR	K	102	-	-	1/29/63/63	0/2/2/2
20	CLA	C	506	-	3/3/20/25	12/37/135/135	-
20	CLA	c	510	-	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	C	509	-	3/3/20/25	8/37/135/135	-
20	CLA	B	601	-	3/3/20/25	18/37/135/135	-
20	CLA	b	617	-	3/3/20/25	8/37/135/135	-
37	HEM	e	102	5,6	-	0/6/54/54	-
24	LMG	J	101	39	-	9/40/60/70	0/1/1/1
35	DGD	d	416	-	-	30/46/66/95	0/1/1/2
34	LMT	J	103	-	-	7/15/35/61	0/1/1/2
34	LMT	c	523	-	-	8/21/61/61	0/2/2/2
22	BCR	D	405	-	-	4/29/63/63	0/2/2/2
37	HEM	E	104	5,6	-	0/6/54/54	-
20	CLA	c	512	-	3/3/20/25	7/37/135/135	-
32	HTG	c	520	-	-	5/10/30/30	0/1/1/1
34	LMT	a	418	-	-	11/21/61/61	0/2/2/2
32	HTG	v	210	-	-	3/5/25/30	0/1/1/1
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
20	CLA	B	616	-	3/3/20/25	5/37/135/135	-
20	CLA	A	402	41	2/2/18/25	3/30/128/135	-
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
20	CLA	c	505	-	2/2/20/25	1/37/135/135	-
34	LMT	B	627	-	-	7/13/13/61	-
20	CLA	C	511	3	2/2/20/25	0/37/135/135	-
24	LMG	C	524	-	-	22/40/60/70	0/1/1/1
35	DGD	c	516	-	-	13/46/86/95	0/2/2/2
36	LHG	d	408	-	-	14/53/53/53	-
23	SQD	A	406	-	-	21/49/69/69	0/1/1/1
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
32	HTG	C	534	-	-	6/10/30/30	0/1/1/1
35	DGD	c	517	-	-	14/51/91/95	0/2/2/2
20	CLA	B	611	41	3/3/20/25	4/37/135/135	-
32	HTG	b	625	-	-	4/10/30/30	0/1/1/1
22	BCR	b	619	-	-	2/29/63/63	0/2/2/2
34	LMT	z	102	-	-	13/21/61/61	0/2/2/2
20	CLA	B	603	-	3/3/20/25	3/37/135/135	-
34	LMT	b	627	-	-	10/18/58/61	0/2/2/2
21	PHO	a	406	-	-	4/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	T	101	-	-	1/29/63/63	0/2/2/2
27	PL9	d	412	-	-	3/53/73/73	0/1/1/1
24	LMG	c	519	-	-	26/46/66/70	0/1/1/1
34	LMT	T	102	-	-	11/15/35/61	0/1/1/2
20	CLA	C	504	41	2/2/20/25	11/37/135/135	-
20	CLA	B	609	-	1/1/20/25	1/37/135/135	-
36	LHG	d	407	-	-	11/53/53/53	-
20	CLA	b	607	-	3/3/20/25	4/37/135/135	-
20	CLA	b	615	-	3/3/20/25	6/37/135/135	-
32	HTG	B	632	-	-	2/10/30/30	0/1/1/1
20	CLA	c	501	-	3/3/20/25	3/37/135/135	-
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
20	CLA	C	502	-	1/1/20/25	5/37/135/135	-
24	LMG	b	623	-	-	14/44/64/70	0/1/1/1
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
36	LHG	E	103	-	-	27/45/45/53	-
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
20	CLA	b	616	-	3/3/20/25	18/37/135/135	-
20	CLA	c	511	3	3/3/20/25	0/37/135/135	-
34	LMT	B	625	-	-	4/15/35/61	0/1/1/2
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
20	CLA	B	607	-	3/3/20/25	11/37/135/135	-
23	SQD	A	412	-	-	24/49/69/69	0/1/1/1
20	CLA	c	506	-	2/2/20/25	10/37/135/135	-
20	CLA	B	610	-	2/2/20/25	1/37/135/135	-
20	CLA	C	507	41	3/3/20/25	11/37/135/135	-
20	CLA	c	509	-	3/3/20/25	10/37/135/135	-
20	CLA	c	503	-	1/1/20/25	3/37/135/135	-
20	CLA	b	605	-	3/3/20/25	1/37/135/135	-
36	LHG	D	408	-	-	10/53/53/53	-
20	CLA	C	513	-	1/1/20/25	10/37/135/135	-
32	HTG	V	202	-	-	1/4/24/30	0/1/1/1
20	CLA	b	611	-	2/2/20/25	0/37/135/135	-
32	HTG	D	417	-	-	5/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	618	-	3/3/20/25	17/37/135/135	-
23	SQD	a	401	-	-	20/49/69/69	0/1/1/1
22	BCR	d	405	-	-	4/29/63/63	0/2/2/2
40	HEC	V	201	16	-	0/6/54/54	-
20	CLA	B	614	-	3/3/20/25	6/37/135/135	-
20	CLA	b	612	41	3/3/20/25	5/37/135/135	-
24	LMG	c	518	-	-	8/46/66/70	0/1/1/1
24	LMG	j	101	39	-	15/40/60/70	0/1/1/1
32	HTG	O	302	-	-	5/10/30/30	0/1/1/1
20	CLA	C	512	-	3/3/18/25	6/25/123/135	-
20	CLA	C	508	-	3/3/19/25	6/31/129/135	-
24	LMG	a	410	-	-	18/46/66/70	0/1/1/1
36	LHG	d	406	-	-	11/53/53/53	-
20	CLA	b	604	-	3/3/20/25	7/37/135/135	-
34	LMT	I	101	-	-	8/21/61/61	0/2/2/2
20	CLA	C	510	-	3/3/20/25	2/37/135/135	-
20	CLA	d	404	-	1/1/20/25	8/37/135/135	-
34	LMT	E	101	-	-	8/15/35/61	0/1/1/2
20	CLA	B	613	-	3/3/20/25	0/37/135/135	-
20	CLA	B	612	-	3/3/20/25	3/37/135/135	-

All (1283) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	MG-NA	12.91	2.36	2.06
20	c	513	CLA	MG-NA	12.66	2.36	2.06
20	B	602	CLA	MG-NA	11.66	2.34	2.06
20	c	507	CLA	MG-NA	10.98	2.32	2.06
20	c	511	CLA	MG-NC	10.70	2.31	2.06
20	C	502	CLA	MG-NA	10.10	2.30	2.06
20	C	506	CLA	MG-NA	10.02	2.30	2.06
20	b	608	CLA	MG-NA	9.93	2.29	2.06
20	c	502	CLA	MG-NA	9.90	2.29	2.06
20	C	511	CLA	MG-NA	9.62	2.29	2.06
20	C	508	CLA	MG-NA	9.57	2.29	2.06
20	B	605	CLA	MG-NA	9.52	2.28	2.06
20	c	503	CLA	MG-NA	9.50	2.28	2.06
20	b	603	CLA	MG-NC	9.40	2.28	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	617	CLA	MG-NA	9.30	2.28	2.06
20	B	613	CLA	MG-NA	9.26	2.28	2.06
20	c	509	CLA	MG-NA	9.07	2.27	2.06
20	C	509	CLA	MG-NA	9.01	2.27	2.06
20	C	503	CLA	MG-NA	8.95	2.27	2.06
20	b	613	CLA	MG-NA	8.84	2.27	2.06
20	c	508	CLA	MG-NA	8.69	2.26	2.06
20	d	403	CLA	MG-NA	8.65	2.26	2.06
20	C	507	CLA	MG-NC	8.62	2.26	2.06
20	C	513	CLA	MG-NA	8.51	2.26	2.06
20	B	610	CLA	MG-NA	8.45	2.26	2.06
20	C	512	CLA	MG-NA	8.34	2.26	2.06
20	B	608	CLA	MG-NA	8.25	2.25	2.06
20	C	504	CLA	MG-NA	8.16	2.25	2.06
20	c	501	CLA	MG-NA	8.12	2.25	2.06
20	c	504	CLA	MG-NA	8.10	2.25	2.06
20	c	512	CLA	MG-NA	8.09	2.25	2.06
20	b	605	CLA	MG-NA	8.07	2.25	2.06
20	B	607	CLA	MG-NA	7.94	2.25	2.06
20	C	510	CLA	MG-NA	7.85	2.24	2.06
20	B	603	CLA	MG-NA	7.84	2.24	2.06
20	B	616	CLA	MG-NA	7.81	2.24	2.06
20	b	606	CLA	MG-NA	7.76	2.24	2.06
20	b	618	CLA	MG-NA	7.73	2.24	2.06
20	C	507	CLA	MG-NA	7.70	2.24	2.06
20	b	616	CLA	MG-NA	7.66	2.24	2.06
20	C	513	CLA	MG-NC	7.30	2.23	2.06
20	c	505	CLA	MG-NA	7.26	2.23	2.06
20	B	611	CLA	MG-NA	7.15	2.23	2.06
20	c	503	CLA	MG-NC	7.01	2.22	2.06
20	B	614	CLA	MG-NA	6.94	2.22	2.06
20	D	401	CLA	MG-NA	6.93	2.22	2.06
20	C	512	CLA	MG-NC	6.85	2.22	2.06
20	B	612	CLA	MG-NA	6.73	2.22	2.06
20	D	404	CLA	MG-NC	6.62	2.22	2.06
20	B	611	CLA	MG-NC	6.61	2.22	2.06
20	B	601	CLA	MG-NA	6.58	2.21	2.06
20	B	607	CLA	MG-NC	6.52	2.21	2.06
20	c	506	CLA	MG-NA	6.46	2.21	2.06
20	b	614	CLA	MG-NA	6.41	2.21	2.06
20	b	608	CLA	C3B-C2B	6.32	1.49	1.40
20	d	404	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	607	CLA	MG-NA	6.30	2.21	2.06
20	c	501	CLA	OBD-CAD	6.24	1.31	1.22
20	C	507	CLA	C3B-C2B	6.22	1.49	1.40
20	A	402	CLA	MG-NA	6.14	2.20	2.06
20	C	509	CLA	OBD-CAD	6.05	1.30	1.22
20	c	509	CLA	OBD-CAD	6.05	1.30	1.22
20	D	404	CLA	MG-NA	6.03	2.20	2.06
20	B	607	CLA	C3C-C2C	6.01	1.49	1.36
20	c	512	CLA	C3B-C2B	5.97	1.48	1.40
20	B	607	CLA	CHC-C1C	5.96	1.50	1.35
20	d	402	CLA	CHC-C1C	5.94	1.50	1.35
20	b	610	CLA	CHC-C1C	5.93	1.50	1.35
20	C	513	CLA	C3B-C2B	5.93	1.48	1.40
20	C	512	CLA	C3B-C2B	5.93	1.48	1.40
20	a	403	CLA	MG-NA	5.91	2.20	2.06
20	b	609	CLA	MG-NC	5.90	2.20	2.06
20	b	604	CLA	MG-NA	5.88	2.20	2.06
20	a	404	CLA	MG-NA	5.88	2.20	2.06
20	a	407	CLA	CHC-C1C	5.88	1.50	1.35
20	b	617	CLA	C3B-C2B	5.87	1.48	1.40
20	b	605	CLA	CHC-C1C	5.84	1.49	1.35
20	B	609	CLA	MG-NA	5.83	2.20	2.06
20	C	512	CLA	C3C-C2C	5.82	1.49	1.36
20	b	609	CLA	MG-NA	5.81	2.20	2.06
20	C	503	CLA	CHC-C1C	5.79	1.49	1.35
20	b	610	CLA	C3C-C2C	5.77	1.49	1.36
20	c	503	CLA	C3C-C2C	5.75	1.49	1.36
20	b	615	CLA	CHC-C1C	5.74	1.49	1.35
20	B	601	CLA	CHC-C1C	5.72	1.49	1.35
20	C	513	CLA	C3C-C2C	5.69	1.48	1.36
21	a	406	PHO	CHB-C1B	5.67	1.49	1.38
21	D	403	PHO	C3B-C2B	5.66	1.48	1.37
20	b	608	CLA	MG-NC	5.65	2.19	2.06
20	B	603	CLA	OBD-CAD	5.64	1.30	1.22
20	b	611	CLA	CHC-C1C	5.62	1.49	1.35
20	A	402	CLA	CHC-C1C	5.62	1.49	1.35
20	C	506	CLA	CHC-C1C	5.61	1.49	1.35
20	b	606	CLA	C3C-C2C	5.61	1.48	1.36
20	C	513	CLA	C3D-C2D	5.58	1.49	1.39
20	c	509	CLA	C3B-C2B	5.58	1.48	1.40
20	B	614	CLA	CHC-C1C	5.57	1.49	1.35
28	C	532	DMS	O-S	5.56	1.87	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	509	CLA	C3D-C2D	5.55	1.49	1.39
20	B	610	CLA	CHC-C1C	5.55	1.49	1.35
20	b	612	CLA	CHC-C1C	5.54	1.49	1.35
20	d	402	CLA	C3B-C2B	5.54	1.48	1.40
20	b	618	CLA	CHC-C1C	5.54	1.49	1.35
20	C	505	CLA	C3C-C2C	5.53	1.48	1.36
20	C	508	CLA	C3B-C2B	5.52	1.48	1.40
20	c	511	CLA	OBD-CAD	5.52	1.30	1.22
20	c	512	CLA	CHC-C1C	5.50	1.49	1.35
20	B	606	CLA	MG-NA	5.50	2.19	2.06
20	b	612	CLA	O2D-CGD	5.50	1.46	1.33
20	c	505	CLA	CHC-C1C	5.50	1.49	1.35
20	c	508	CLA	C3D-C2D	5.49	1.49	1.39
20	B	615	CLA	MG-NA	5.48	2.19	2.06
20	C	509	CLA	C3C-C2C	5.47	1.48	1.36
20	c	502	CLA	CHC-C1C	5.47	1.49	1.35
20	c	512	CLA	C3C-C2C	5.47	1.48	1.36
20	c	511	CLA	O2D-CGD	5.46	1.46	1.33
20	b	603	CLA	CHC-C1C	5.45	1.48	1.35
20	C	503	CLA	C3C-C2C	5.44	1.48	1.36
20	b	608	CLA	C3D-C2D	5.44	1.49	1.39
20	b	611	CLA	C3B-C2B	5.43	1.47	1.40
20	b	615	CLA	MG-NA	5.43	2.19	2.06
20	C	501	CLA	CHC-C1C	5.42	1.48	1.35
20	c	501	CLA	C3B-C2B	5.42	1.47	1.40
37	e	102	HEM	C3D-C2D	5.42	1.53	1.37
20	c	504	CLA	C3C-C2C	5.42	1.48	1.36
20	b	611	CLA	C3C-C2C	5.42	1.48	1.36
20	c	503	CLA	CHC-C1C	5.41	1.48	1.35
20	b	603	CLA	C3B-C2B	5.41	1.47	1.40
20	c	503	CLA	C3B-C2B	5.39	1.47	1.40
20	c	511	CLA	C3D-C2D	5.39	1.49	1.39
20	B	606	CLA	CHC-C1C	5.39	1.48	1.35
20	C	512	CLA	O2D-CGD	5.39	1.46	1.33
20	b	609	CLA	C3D-C2D	5.38	1.49	1.39
20	b	611	CLA	C3D-C2D	5.37	1.49	1.39
23	f	101	SQD	O47-C7	5.37	1.47	1.35
20	C	504	CLA	C3C-C2C	5.34	1.48	1.36
20	c	511	CLA	MG-NA	5.33	2.18	2.06
20	b	604	CLA	C3C-C2C	5.32	1.48	1.36
20	D	402	CLA	MG-NA	5.32	2.18	2.06
20	B	601	CLA	C3C-C2C	5.31	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	CLA	C3C-C2C	5.30	1.48	1.36
20	C	506	CLA	C3B-C2B	5.29	1.47	1.40
20	c	511	CLA	CHC-C1C	5.29	1.48	1.35
20	C	503	CLA	C3B-C2B	5.29	1.47	1.40
20	c	507	CLA	C3C-C2C	5.28	1.48	1.36
20	B	602	CLA	C3C-C2C	5.27	1.47	1.36
21	A	403	PHO	CHB-C1B	5.26	1.48	1.38
20	d	403	CLA	C3C-C2C	5.25	1.47	1.36
20	a	403	CLA	CHC-C1C	5.25	1.48	1.35
20	b	610	CLA	OBD-CAD	5.24	1.29	1.22
20	C	501	CLA	MG-NC	5.23	2.18	2.06
20	C	511	CLA	MG-NC	5.23	2.18	2.06
20	b	607	CLA	CHC-C1C	5.23	1.48	1.35
20	C	505	CLA	CHC-C1C	5.23	1.48	1.35
20	b	605	CLA	C3C-C2C	5.22	1.47	1.36
20	b	603	CLA	O2A-CGA	5.21	1.48	1.33
37	E	104	HEM	C3D-C2D	5.20	1.53	1.37
20	A	401	CLA	OBD-CAD	5.20	1.29	1.22
20	C	510	CLA	O2D-CGD	5.20	1.45	1.33
20	b	603	CLA	O2D-CGD	5.20	1.45	1.33
20	c	511	CLA	C3B-C2B	5.19	1.47	1.40
20	C	508	CLA	CHC-C1C	5.19	1.48	1.35
20	B	613	CLA	CHC-C1C	5.19	1.48	1.35
20	C	508	CLA	C3C-C2C	5.18	1.47	1.36
20	C	510	CLA	C3D-C2D	5.17	1.48	1.39
20	C	512	CLA	CHC-C1C	5.17	1.48	1.35
20	A	404	CLA	MG-NC	5.17	2.18	2.06
20	b	616	CLA	CHC-C1C	5.16	1.48	1.35
20	B	611	CLA	CHC-C1C	5.15	1.48	1.35
20	b	603	CLA	C3C-C2C	5.15	1.47	1.36
20	a	404	CLA	CHC-C1C	5.13	1.48	1.35
20	b	609	CLA	C3C-C2C	5.13	1.47	1.36
20	c	509	CLA	CHC-C1C	5.13	1.48	1.35
20	C	502	CLA	CHC-C1C	5.13	1.48	1.35
20	c	506	CLA	CHC-C1C	5.12	1.48	1.35
32	B	621	HTG	C1'-S1	-5.11	1.74	1.81
20	C	508	CLA	O2D-CGD	5.11	1.45	1.33
20	b	607	CLA	C3C-C2C	5.11	1.47	1.36
20	B	602	CLA	O2A-CGA	5.10	1.48	1.33
20	c	508	CLA	C3C-C2C	5.10	1.47	1.36
20	c	504	CLA	O2D-CGD	5.09	1.45	1.33
20	B	615	CLA	CHC-C1C	5.09	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	504	CLA	C3D-C2D	5.07	1.48	1.39
24	B	620	LMG	O8-C28	5.07	1.48	1.33
20	D	404	CLA	C3C-C2C	5.07	1.47	1.36
21	a	405	PHO	CHB-C1B	5.06	1.48	1.38
20	A	404	CLA	CHC-C1C	5.06	1.47	1.35
20	b	606	CLA	CHC-C1C	5.06	1.47	1.35
20	c	513	CLA	C3C-C2C	5.05	1.47	1.36
20	C	513	CLA	O2D-CGD	5.05	1.45	1.33
20	c	506	CLA	O2D-CGD	5.04	1.45	1.33
20	b	613	CLA	CHC-C1C	5.04	1.47	1.35
20	B	615	CLA	MG-NC	5.04	2.18	2.06
20	C	502	CLA	O2D-CGD	5.03	1.45	1.33
20	c	513	CLA	O2D-CGD	5.03	1.45	1.33
20	B	603	CLA	C3B-C2B	5.02	1.47	1.40
20	C	507	CLA	C3C-C2C	5.02	1.47	1.36
20	B	604	CLA	C3C-C2C	5.01	1.47	1.36
20	a	403	CLA	C3C-C2C	5.01	1.47	1.36
20	c	505	CLA	C3C-C2C	5.01	1.47	1.36
20	b	614	CLA	C3C-C2C	5.01	1.47	1.36
20	C	506	CLA	C3C-C2C	5.01	1.47	1.36
20	a	407	CLA	C3B-C2B	5.00	1.47	1.40
20	A	404	CLA	C3B-C2B	5.00	1.47	1.40
20	C	511	CLA	O2D-CGD	5.00	1.45	1.33
40	v	201	HEC	C3C-C2C	-5.00	1.35	1.40
20	B	602	CLA	CHC-C1C	4.99	1.47	1.35
20	C	506	CLA	O2D-CGD	4.99	1.45	1.33
20	C	508	CLA	C3D-C2D	4.99	1.48	1.39
20	C	504	CLA	O2D-CGD	4.98	1.45	1.33
20	b	618	CLA	C3D-C2D	4.98	1.48	1.39
21	D	403	PHO	CHB-C1B	4.97	1.48	1.38
20	C	501	CLA	C3D-C2D	4.96	1.48	1.39
20	B	604	CLA	O2D-CGD	4.96	1.45	1.33
20	a	407	CLA	OBD-CAD	4.95	1.29	1.22
20	c	512	CLA	O2D-CGD	4.95	1.45	1.33
20	B	611	CLA	C3C-C2C	4.95	1.47	1.36
21	D	403	PHO	C3C-C2C	4.95	1.47	1.36
20	b	617	CLA	CHC-C1C	4.94	1.47	1.35
20	B	607	CLA	C3B-C2B	4.92	1.47	1.40
28	b	631	DMS	O-S	4.92	1.83	1.50
20	B	604	CLA	CHC-C1C	4.91	1.47	1.35
20	c	508	CLA	MG-NC	4.90	2.17	2.06
20	C	511	CLA	C3C-C2C	4.90	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	504	CLA	CHC-C1C	4.90	1.47	1.35
20	b	604	CLA	CHC-C1C	4.90	1.47	1.35
20	B	612	CLA	CHC-C1C	4.90	1.47	1.35
20	C	513	CLA	CHC-C1C	4.90	1.47	1.35
28	D	415	DMS	O-S	4.89	1.83	1.50
20	c	508	CLA	CHC-C1C	4.88	1.47	1.35
20	B	608	CLA	C3D-C2D	4.88	1.48	1.39
20	B	606	CLA	C3C-C2C	4.88	1.47	1.36
20	D	404	CLA	C3B-C2B	4.87	1.47	1.40
20	C	507	CLA	CHC-C1C	4.86	1.47	1.35
20	B	602	CLA	O2D-CGD	4.86	1.45	1.33
20	b	618	CLA	C3C-C2C	4.86	1.47	1.36
20	B	610	CLA	C3C-C2C	4.86	1.47	1.36
20	b	616	CLA	C3C-C2C	4.86	1.47	1.36
21	A	403	PHO	C3B-C2B	4.85	1.47	1.37
35	d	416	DGD	O2G-C1B	4.85	1.48	1.34
20	b	612	CLA	C3C-C2C	4.84	1.47	1.36
20	A	404	CLA	C3C-C2C	4.84	1.47	1.36
20	B	604	CLA	MG-NA	4.84	2.17	2.06
20	C	509	CLA	CHC-C1C	4.83	1.47	1.35
20	C	510	CLA	CHC-C1C	4.83	1.47	1.35
20	C	508	CLA	OBD-CAD	4.83	1.29	1.22
20	b	617	CLA	C3C-C2C	4.83	1.47	1.36
20	C	511	CLA	C3D-C2D	4.83	1.48	1.39
20	B	616	CLA	O2D-CGD	4.83	1.45	1.33
20	B	611	CLA	C3D-C2D	4.82	1.48	1.39
20	b	611	CLA	O2D-CGD	4.81	1.44	1.33
28	c	536	DMS	O-S	4.81	1.82	1.50
35	D	406	DGD	O2G-C1B	4.81	1.47	1.34
20	b	615	CLA	O2D-CGD	4.80	1.44	1.33
20	B	603	CLA	C3C-C2C	4.80	1.46	1.36
20	C	504	CLA	C3B-C2B	4.80	1.47	1.40
20	C	511	CLA	C3B-C2B	4.80	1.47	1.40
20	C	507	CLA	C3D-C2D	4.80	1.48	1.39
28	B	644	DMS	O-S	4.80	1.82	1.50
20	B	612	CLA	OBD-CAD	4.80	1.29	1.22
20	B	609	CLA	C3B-C2B	4.79	1.47	1.40
35	D	406	DGD	O1G-C1A	4.78	1.47	1.33
28	O	311	DMS	O-S	4.78	1.82	1.50
20	b	603	CLA	OBD-CAD	4.78	1.29	1.22
20	B	602	CLA	OBD-CAD	4.77	1.29	1.22
20	c	513	CLA	CHC-C1C	4.77	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	639	DMS	O-S	4.77	1.82	1.50
28	o	308	DMS	O-S	4.77	1.82	1.50
40	v	201	HEC	C3D-C2D	4.76	1.51	1.37
20	b	617	CLA	OBD-CAD	4.76	1.29	1.22
20	B	607	CLA	O2D-CGD	4.75	1.44	1.33
20	B	605	CLA	CHC-C1C	4.75	1.47	1.35
28	U	904	DMS	O-S	4.75	1.82	1.50
20	c	508	CLA	C3B-C2B	4.75	1.47	1.40
20	C	502	CLA	C3C-C2C	4.75	1.46	1.36
20	D	401	CLA	C3C-C2C	4.74	1.46	1.36
20	B	610	CLA	C3D-C2D	4.74	1.47	1.39
20	B	616	CLA	C3B-C2B	4.73	1.46	1.40
24	c	518	LMG	O8-C28	4.73	1.47	1.33
20	d	403	CLA	CHC-C1C	4.73	1.47	1.35
20	c	507	CLA	CHC-C1C	4.72	1.47	1.35
20	c	512	CLA	OBD-CAD	4.72	1.28	1.22
20	D	402	CLA	C3B-C2B	4.72	1.46	1.40
20	C	502	CLA	C3D-C2D	4.72	1.47	1.39
24	C	519	LMG	O8-C28	4.72	1.47	1.33
20	C	502	CLA	C3B-C2B	4.72	1.46	1.40
28	c	530	DMS	O-S	4.72	1.82	1.50
20	C	509	CLA	O2D-CGD	4.72	1.44	1.33
20	B	603	CLA	CHC-C1C	4.71	1.47	1.35
24	C	524	LMG	O8-C28	4.71	1.47	1.33
24	J	101	LMG	O7-C10	4.71	1.47	1.34
35	d	416	DGD	O1G-C1A	4.71	1.47	1.33
20	b	618	CLA	O2D-CGD	4.70	1.44	1.33
21	a	406	PHO	C3B-C2B	4.70	1.46	1.37
20	b	608	CLA	C3C-C2C	4.70	1.46	1.36
20	b	613	CLA	C3C-C2C	4.70	1.46	1.36
20	b	608	CLA	O2D-CGD	4.70	1.44	1.33
20	c	501	CLA	CHC-C1C	4.70	1.47	1.35
20	b	611	CLA	OBD-CAD	4.70	1.28	1.22
20	C	505	CLA	C3D-C2D	4.69	1.47	1.39
23	a	401	SQD	O48-C23	4.69	1.47	1.33
28	C	525[A]	DMS	O-S	4.69	1.81	1.50
20	c	510	CLA	CHC-C1C	4.69	1.47	1.35
20	c	502	CLA	C3D-C2D	4.68	1.47	1.39
20	c	504	CLA	OBD-CAD	4.68	1.28	1.22
20	A	404	CLA	OBD-CAD	4.68	1.28	1.22
20	C	512	CLA	C3D-C2D	4.68	1.47	1.39
28	o	302	DMS	O-S	4.68	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	B	642	DMS	O-S	4.68	1.81	1.50
20	b	614	CLA	CHC-C1C	4.68	1.47	1.35
28	B	643	DMS	O-S	4.68	1.81	1.50
28	A	418	DMS	O-S	4.68	1.81	1.50
20	C	510	CLA	OBD-CAD	4.67	1.28	1.22
20	B	609	CLA	O2D-CGD	4.67	1.44	1.33
20	C	503	CLA	C3D-C2D	4.67	1.47	1.39
20	B	616	CLA	CHC-C1C	4.66	1.46	1.35
28	j	105	DMS	O-S	4.66	1.81	1.50
28	b	638	DMS	O-S	4.66	1.81	1.50
20	a	407	CLA	C3D-C2D	4.66	1.47	1.39
20	A	401	CLA	CHC-C1C	4.65	1.46	1.35
21	a	406	PHO	CHC-C1C	4.65	1.47	1.38
20	d	404	CLA	CHC-C1C	4.65	1.46	1.35
20	c	510	CLA	C3C-C2C	4.65	1.46	1.36
20	D	404	CLA	CHC-C1C	4.64	1.46	1.35
28	o	306	DMS	O-S	4.64	1.81	1.50
20	c	513	CLA	C3B-C2B	4.64	1.46	1.40
20	c	511	CLA	C3C-C2C	4.64	1.46	1.36
21	a	405	PHO	C3C-C2C	4.64	1.46	1.36
20	b	603	CLA	C3D-C2D	4.64	1.47	1.39
24	c	518	LMG	O7-C10	4.63	1.47	1.34
20	B	615	CLA	C3C-C2C	4.63	1.46	1.36
28	A	415	DMS	O-S	4.63	1.81	1.50
23	b	622	SQD	O47-C7	4.63	1.47	1.34
21	a	406	PHO	C3C-C2C	4.63	1.46	1.36
20	B	603	CLA	C3D-C2D	4.63	1.47	1.39
28	O	308	DMS	O-S	4.62	1.81	1.50
20	B	614	CLA	C3C-C2C	4.61	1.46	1.36
28	b	641	DMS	O-S	4.61	1.81	1.50
28	B	638	DMS	O-S	4.61	1.81	1.50
20	c	512	CLA	C3D-C2D	4.61	1.47	1.39
20	B	613	CLA	C3C-C2C	4.61	1.46	1.36
20	B	601	CLA	C3D-C2D	4.61	1.47	1.39
20	C	510	CLA	C3C-C2C	4.60	1.46	1.36
28	B	636	DMS	O-S	4.60	1.81	1.50
21	a	405	PHO	O2D-CGD	4.60	1.44	1.33
28	v	207	DMS	O-S	4.60	1.81	1.50
20	B	608	CLA	CHC-C1C	4.60	1.46	1.35
28	c	535	DMS	O-S	4.60	1.81	1.50
20	d	404	CLA	C3C-C2C	4.60	1.46	1.36
28	b	640	DMS	O-S	4.60	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	h	102	DMS	O-S	4.59	1.81	1.50
20	c	509	CLA	C3D-C2D	4.58	1.47	1.39
20	B	616	CLA	C3C-C2C	4.58	1.46	1.36
28	H	103	DMS	O-S	4.58	1.81	1.50
28	D	413	DMS	O-S	4.58	1.81	1.50
20	c	501	CLA	C3C-C2C	4.58	1.46	1.36
28	c	533	DMS	O-S	4.57	1.81	1.50
20	c	508	CLA	O2D-CGD	4.57	1.44	1.33
20	b	609	CLA	CHC-C1C	4.57	1.46	1.35
20	b	603	CLA	MG-NA	4.57	2.17	2.06
28	o	305	DMS	O-S	4.56	1.81	1.50
28	B	645	DMS	O-S	4.56	1.81	1.50
20	b	616	CLA	OBD-CAD	4.55	1.28	1.22
20	C	511	CLA	CHC-C1C	4.55	1.46	1.35
28	B	639	DMS	O-S	4.55	1.81	1.50
20	c	505	CLA	C3D-C2D	4.55	1.47	1.39
28	V	205	DMS	O-S	4.55	1.81	1.50
20	b	612	CLA	C1B-NB	-4.55	1.31	1.35
20	B	606	CLA	OBD-CAD	4.55	1.28	1.22
20	b	610	CLA	MG-NA	4.55	2.17	2.06
28	O	310	DMS	O-S	4.54	1.80	1.50
28	b	636	DMS	O-S	4.54	1.80	1.50
20	c	502	CLA	C3B-C2B	4.54	1.46	1.40
28	d	415	DMS	O-S	4.53	1.80	1.50
20	c	504	CLA	CHC-C1C	4.53	1.46	1.35
28	b	632	DMS	O-S	4.53	1.80	1.50
28	A	416	DMS	O-S	4.52	1.80	1.50
20	a	407	CLA	C3C-C2C	4.52	1.46	1.36
28	O	307	DMS	O-S	4.52	1.80	1.50
28	o	303	DMS	O-S	4.52	1.80	1.50
28	b	635	DMS	O-S	4.52	1.80	1.50
20	B	602	CLA	C3B-C2B	4.51	1.46	1.40
20	d	402	CLA	MG-NA	4.51	2.17	2.06
20	c	509	CLA	C3C-C2C	4.51	1.46	1.36
20	B	607	CLA	OBD-CAD	4.51	1.28	1.22
20	b	606	CLA	C3D-C2D	4.50	1.47	1.39
40	v	201	HEC	C3B-C2B	-4.50	1.36	1.40
36	E	103	LHG	O8-C23	4.49	1.46	1.33
20	c	506	CLA	C3C-C2C	4.49	1.46	1.36
23	l	101	SQD	O47-C7	4.49	1.47	1.34
28	C	529	DMS	O-S	4.49	1.80	1.50
20	c	503	CLA	C3D-C2D	4.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	416	DMS	O-S	4.48	1.80	1.50
28	V	206	DMS	O-S	4.48	1.80	1.50
28	v	206	DMS	O-S	4.48	1.80	1.50
20	b	606	CLA	O2D-CGD	4.48	1.44	1.33
28	B	641	DMS	O-S	4.48	1.80	1.50
28	c	531	DMS	O-S	4.48	1.80	1.50
20	d	402	CLA	OBD-CAD	4.48	1.28	1.22
36	E	103	LHG	O7-C7	4.47	1.46	1.33
28	b	637	DMS	O-S	4.47	1.80	1.50
20	C	505	CLA	O2D-CGD	4.47	1.44	1.33
28	c	529	DMS	O-S	4.47	1.80	1.50
28	c	534	DMS	O-S	4.46	1.80	1.50
20	C	505	CLA	MG-NA	4.46	2.16	2.06
20	D	404	CLA	C3D-C2D	4.46	1.47	1.39
20	B	611	CLA	O2D-CGD	4.46	1.44	1.33
28	o	307	DMS	O-S	4.46	1.80	1.50
20	c	507	CLA	OBD-CAD	4.46	1.28	1.22
20	b	608	CLA	CHC-C1C	4.46	1.46	1.35
28	v	204	DMS	O-S	4.46	1.80	1.50
20	c	504	CLA	C3D-C2D	4.46	1.47	1.39
20	c	502	CLA	O2D-CGD	4.46	1.44	1.33
20	b	613	CLA	O2D-CGD	4.45	1.44	1.33
20	B	603	CLA	O2D-CGD	4.45	1.44	1.33
20	c	510	CLA	O2D-CGD	4.45	1.44	1.33
20	b	618	CLA	C3B-C2B	4.45	1.46	1.40
21	a	405	PHO	CHC-C1C	4.44	1.47	1.38
28	C	531	DMS	O-S	4.44	1.80	1.50
28	F	102	DMS	O-S	4.44	1.80	1.50
23	b	622	SQD	O48-C23	4.44	1.46	1.33
28	b	634	DMS	O-S	4.44	1.80	1.50
28	i	104	DMS	O-S	4.44	1.80	1.50
28	u	204	DMS	O-S	4.44	1.80	1.50
20	c	509	CLA	O2D-CGD	4.44	1.44	1.33
28	V	208	DMS	O-S	4.43	1.80	1.50
21	a	406	PHO	O2D-CGD	4.43	1.44	1.33
20	C	511	CLA	OBD-CAD	4.42	1.28	1.22
20	C	505	CLA	C3B-C2B	4.42	1.46	1.40
28	O	305	DMS	O-S	4.42	1.80	1.50
28	V	204	DMS	O-S	4.42	1.80	1.50
28	v	205	DMS	O-S	4.42	1.80	1.50
40	V	201	HEC	C3C-C2C	-4.42	1.36	1.40
28	B	635	DMS	O-S	4.41	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	524	LMG	O7-C10	4.41	1.46	1.34
28	O	309	DMS	O-S	4.41	1.80	1.50
28	A	417	DMS	O-S	4.41	1.80	1.50
23	a	401	SQD	O47-C7	4.41	1.46	1.34
23	F	101	SQD	O48-C23	4.41	1.46	1.33
28	C	533	DMS	O-S	4.40	1.80	1.50
28	v	208	DMS	O-S	4.40	1.79	1.50
20	a	407	CLA	O2D-CGD	4.40	1.43	1.33
20	c	513	CLA	C3D-C2D	4.39	1.47	1.39
20	c	506	CLA	C3B-C2B	4.39	1.46	1.40
28	o	304	DMS	O-S	4.39	1.79	1.50
20	B	606	CLA	O2D-CGD	4.39	1.43	1.33
28	v	209	DMS	O-S	4.38	1.79	1.50
20	b	613	CLA	C3D-C2D	4.37	1.47	1.39
20	C	503	CLA	O2D-CGD	4.37	1.43	1.33
20	C	505	CLA	MG-NC	4.36	2.16	2.06
20	C	506	CLA	O2A-CGA	4.36	1.46	1.33
24	A	407	LMG	O7-C10	4.35	1.46	1.34
28	c	532	DMS	O-S	4.34	1.79	1.50
21	a	406	PHO	CHD-C1D	4.34	1.47	1.38
23	f	101	SQD	O48-C23	4.34	1.46	1.33
28	V	209	DMS	O-S	4.34	1.79	1.50
28	O	303	DMS	O-S	4.34	1.79	1.50
20	C	506	CLA	C3D-C2D	4.34	1.47	1.39
28	C	525[B]	DMS	O-S	4.34	1.79	1.50
20	d	404	CLA	C3B-C2B	4.34	1.46	1.40
28	O	304	DMS	O-S	4.34	1.79	1.50
28	V	207	DMS	O-S	4.33	1.79	1.50
28	v	203	DMS	O-S	4.32	1.79	1.50
28	u	202	DMS	O-S	4.32	1.79	1.50
28	c	528	DMS	O-S	4.32	1.79	1.50
23	A	412	SQD	O48-C23	4.31	1.45	1.33
23	l	101	SQD	O48-C23	4.31	1.45	1.33
20	B	613	CLA	C3B-C2B	4.31	1.46	1.40
21	a	406	PHO	C1A-NA	-4.30	1.29	1.37
20	c	502	CLA	OBD-CAD	4.30	1.28	1.22
28	U	903[A]	DMS	O-S	4.30	1.79	1.50
20	d	404	CLA	C3D-C2D	4.30	1.47	1.39
28	C	526	DMS	O-S	4.29	1.79	1.50
28	C	527	DMS	O-S	4.29	1.79	1.50
28	D	414	DMS	O-S	4.29	1.79	1.50
20	c	504	CLA	C3B-C2B	4.29	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	507	CLA	C3B-C2B	4.29	1.46	1.40
20	b	605	CLA	C3D-C2D	4.28	1.47	1.39
20	C	507	CLA	OBD-CAD	4.28	1.28	1.22
20	b	605	CLA	O2D-CGD	4.28	1.43	1.33
36	D	407	LHG	O8-C23	4.28	1.45	1.33
20	a	407	CLA	O2A-CGA	4.27	1.45	1.33
28	b	633	DMS	O-S	4.27	1.79	1.50
28	U	902	DMS	O-S	4.27	1.79	1.50
28	d	413	DMS	O-S	4.26	1.79	1.50
24	c	519	LMG	O8-C28	4.26	1.45	1.33
28	C	530	DMS	O-S	4.26	1.79	1.50
20	b	613	CLA	C3B-C2B	4.25	1.46	1.40
24	b	623	LMG	O8-C28	4.25	1.45	1.33
28	B	637	DMS	O-S	4.25	1.78	1.50
28	d	414	DMS	O-S	4.25	1.78	1.50
20	d	404	CLA	OBD-CAD	4.24	1.28	1.22
21	D	403	PHO	O2D-CGD	4.23	1.43	1.33
23	A	406	SQD	O47-C7	4.23	1.46	1.34
20	C	512	CLA	O2A-CGA	4.22	1.45	1.33
28	u	203	DMS	O-S	4.22	1.78	1.50
20	b	605	CLA	OBD-CAD	4.22	1.28	1.22
20	B	607	CLA	C3D-C2D	4.21	1.47	1.39
20	b	610	CLA	C3D-C2D	4.21	1.47	1.39
20	c	513	CLA	OBD-CAD	4.20	1.28	1.22
28	O	306	DMS	O-S	4.20	1.78	1.50
20	B	616	CLA	OBD-CAD	4.19	1.28	1.22
20	c	507	CLA	C3D-C2D	4.19	1.46	1.39
20	B	608	CLA	C3C-C2C	4.18	1.45	1.36
20	b	616	CLA	C3D-C2D	4.18	1.46	1.39
20	B	611	CLA	C3B-C2B	4.17	1.46	1.40
20	C	509	CLA	O2A-CGA	4.17	1.45	1.33
20	a	404	CLA	OBD-CAD	4.17	1.28	1.22
24	A	407	LMG	O8-C28	4.17	1.45	1.33
20	c	505	CLA	OBD-CAD	4.17	1.28	1.22
28	v	202	DMS	O-S	4.16	1.78	1.50
20	c	507	CLA	O2D-CGD	4.16	1.43	1.33
20	c	501	CLA	C3D-C2D	4.16	1.46	1.39
20	b	614	CLA	C3D-C2D	4.15	1.46	1.39
20	a	403	CLA	C3B-C2B	4.14	1.46	1.40
24	j	101	LMG	O8-C28	4.14	1.45	1.33
20	b	617	CLA	O2D-CGD	4.14	1.43	1.33
20	c	506	CLA	C3D-C2D	4.14	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	613	CLA	O2D-CGD	4.14	1.43	1.33
24	b	623	LMG	O7-C10	4.13	1.45	1.34
24	a	410	LMG	O7-C10	4.13	1.45	1.34
20	d	403	CLA	C3B-C2B	4.12	1.46	1.40
20	B	615	CLA	OBD-CAD	4.12	1.28	1.22
28	U	903[B]	DMS	O-S	4.12	1.78	1.50
24	c	519	LMG	O7-C10	4.12	1.45	1.34
20	D	402	CLA	CHC-C1C	4.12	1.45	1.35
36	D	409	LHG	O8-C23	4.11	1.45	1.33
20	D	402	CLA	MG-NC	4.11	2.16	2.06
35	c	517	DGD	O1G-C1A	4.11	1.45	1.33
20	b	615	CLA	C3C-C2C	4.11	1.45	1.36
20	B	601	CLA	C3B-C2B	4.11	1.46	1.40
20	C	501	CLA	C3B-C2B	4.09	1.46	1.40
23	A	412	SQD	O47-C7	4.09	1.45	1.34
20	B	601	CLA	O2D-CGD	4.09	1.43	1.33
20	C	510	CLA	C3B-C2B	4.09	1.46	1.40
28	B	640	DMS	O-S	4.09	1.77	1.50
20	c	506	CLA	O2A-CGA	4.08	1.45	1.33
21	A	403	PHO	C3C-C2C	4.08	1.45	1.36
20	a	404	CLA	C3D-C2D	4.07	1.46	1.39
20	B	609	CLA	CHC-C1C	4.07	1.45	1.35
20	D	402	CLA	C3C-C2C	4.07	1.45	1.36
20	c	513	CLA	O2A-CGA	4.06	1.45	1.33
20	d	402	CLA	C3C-C2C	4.06	1.45	1.36
20	c	510	CLA	OBD-CAD	4.05	1.28	1.22
20	B	611	CLA	C4C-C3C	4.05	1.52	1.45
24	a	410	LMG	O8-C28	4.04	1.45	1.33
20	b	611	CLA	O2A-CGA	4.04	1.45	1.33
35	h	101	DGD	O2G-C1B	4.03	1.45	1.34
35	H	102	DGD	O2G-C1B	4.02	1.45	1.34
20	b	618	CLA	O2A-CGA	4.02	1.45	1.33
20	B	610	CLA	OBD-CAD	4.01	1.27	1.22
20	c	508	CLA	OBD-CAD	4.00	1.27	1.22
21	a	405	PHO	C3B-C2B	4.00	1.45	1.37
24	C	519	LMG	O7-C10	4.00	1.45	1.34
20	b	612	CLA	MG-NC	4.00	2.15	2.06
20	b	607	CLA	O2D-CGD	4.00	1.42	1.33
20	C	507	CLA	O2D-CGD	3.99	1.42	1.33
20	C	505	CLA	O2A-CGA	3.99	1.45	1.33
20	A	402	CLA	C3D-C2D	3.99	1.46	1.39
36	d	406	LHG	O8-C23	3.99	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	503	CLA	O2D-CGD	3.99	1.42	1.33
20	C	505	CLA	OBD-CAD	3.98	1.27	1.22
20	c	507	CLA	O2A-CGA	3.98	1.45	1.33
23	a	409	SQD	O48-C23	3.98	1.45	1.33
20	B	612	CLA	C3D-C2D	3.97	1.46	1.39
20	C	501	CLA	O2D-CGD	3.97	1.42	1.33
20	A	401	CLA	O2D-CGD	3.97	1.42	1.33
20	C	513	CLA	O2A-CGA	3.96	1.44	1.33
20	B	609	CLA	C3D-C2D	3.96	1.46	1.39
20	c	501	CLA	O2D-CGD	3.95	1.42	1.33
20	B	609	CLA	C3C-C2C	3.94	1.45	1.36
20	B	614	CLA	O2A-CGA	3.94	1.44	1.33
21	a	405	PHO	CHD-C4C	3.93	1.49	1.40
20	C	508	CLA	O2A-CGA	3.93	1.44	1.33
20	B	616	CLA	MG-NC	3.92	2.15	2.06
35	C	516	DGD	O2G-C1B	3.92	1.45	1.34
20	C	501	CLA	MG-NA	3.91	2.15	2.06
20	b	610	CLA	O2D-CGD	3.90	1.42	1.33
20	c	512	CLA	O2A-CGA	3.90	1.44	1.33
20	B	616	CLA	C3D-C2D	3.90	1.46	1.39
21	D	403	PHO	CHD-C1D	3.90	1.46	1.38
20	c	506	CLA	OBD-CAD	3.89	1.27	1.22
20	B	613	CLA	C3D-C2D	3.89	1.46	1.39
20	B	602	CLA	C4B-NB	3.88	1.38	1.35
20	a	403	CLA	O2D-CGD	3.88	1.42	1.33
35	c	517	DGD	O2G-C1B	3.88	1.45	1.34
35	C	517	DGD	O1G-C1A	3.87	1.44	1.33
20	B	604	CLA	C3D-C2D	3.87	1.46	1.39
28	c	527	DMS	O-S	3.87	1.76	1.50
20	C	506	CLA	OBD-CAD	3.87	1.27	1.22
20	B	605	CLA	C3C-C2C	3.87	1.44	1.36
20	C	503	CLA	O2A-CGA	3.86	1.44	1.33
20	b	609	CLA	O2D-CGD	3.86	1.42	1.33
20	B	608	CLA	C3B-C2B	3.85	1.45	1.40
20	d	404	CLA	O2A-CGA	3.85	1.44	1.33
20	d	404	CLA	C4C-C3C	3.84	1.51	1.45
20	B	605	CLA	C3B-C2B	3.84	1.45	1.40
20	C	503	CLA	MG-NC	3.84	2.15	2.06
32	B	622	HTG	C1'-S1	-3.84	1.76	1.81
21	D	403	PHO	CHC-C4B	3.83	1.49	1.40
20	B	602	CLA	C3D-C2D	3.83	1.46	1.39
35	C	518	DGD	O1G-C1A	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	505	CLA	C3B-C2B	3.83	1.45	1.40
20	B	605	CLA	O2D-CGD	3.82	1.42	1.33
20	b	617	CLA	C3D-C2D	3.82	1.46	1.39
20	C	513	CLA	OBD-CAD	3.81	1.27	1.22
37	E	104	HEM	C3B-CAB	3.81	1.55	1.47
20	B	601	CLA	MG-NC	3.80	2.15	2.06
37	E	104	HEM	C3C-CAC	3.80	1.55	1.47
20	B	606	CLA	C3B-C2B	3.80	1.45	1.40
20	A	404	CLA	MG-NA	3.79	2.15	2.06
32	D	417	HTG	C1'-S1	-3.79	1.76	1.81
20	d	403	CLA	C4B-NB	3.79	1.38	1.35
20	B	612	CLA	C3C-C2C	3.79	1.44	1.36
20	D	401	CLA	CHC-C1C	3.79	1.44	1.35
20	b	614	CLA	O2D-CGD	3.79	1.42	1.33
20	C	504	CLA	MG-NC	3.79	2.15	2.06
20	b	613	CLA	O2A-CGA	3.79	1.44	1.33
28	C	528	DMS	O-S	3.78	1.75	1.50
20	C	502	CLA	O2A-CGA	3.77	1.44	1.33
20	b	610	CLA	C3B-C2B	3.77	1.45	1.40
20	b	606	CLA	C3B-C2B	3.76	1.45	1.40
32	b	624	HTG	C1'-S1	-3.76	1.76	1.81
20	b	616	CLA	O2D-CGD	3.75	1.42	1.33
32	O	302	HTG	C1'-S1	-3.74	1.76	1.81
23	a	409	SQD	O47-C7	3.74	1.44	1.34
20	A	401	CLA	C4C-C3C	3.74	1.51	1.45
20	b	605	CLA	C3B-C2B	3.74	1.45	1.40
20	b	612	CLA	C3B-C2B	3.74	1.45	1.40
24	j	101	LMG	O7-C10	3.74	1.44	1.34
20	D	404	CLA	O2D-CGD	3.73	1.42	1.33
20	C	512	CLA	OBD-CAD	3.72	1.27	1.22
24	J	101	LMG	O8-C28	3.72	1.44	1.33
20	B	614	CLA	C3B-C2B	3.72	1.45	1.40
20	B	603	CLA	C4C-C3C	3.72	1.51	1.45
21	D	403	PHO	O2A-CGA	3.72	1.44	1.33
21	A	403	PHO	CHC-C1C	3.71	1.45	1.38
20	A	401	CLA	C3D-C2D	3.71	1.46	1.39
20	c	504	CLA	O2A-CGA	3.70	1.44	1.33
20	A	404	CLA	C3D-C2D	3.70	1.46	1.39
20	a	403	CLA	C3D-C2D	3.69	1.46	1.39
20	c	510	CLA	O2A-CGA	3.69	1.44	1.33
20	B	609	CLA	OBD-CAD	3.69	1.27	1.22
35	c	516	DGD	O1G-C1A	3.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	501	CLA	OBD-CAD	3.68	1.27	1.22
20	b	604	CLA	C3D-C2D	3.68	1.46	1.39
20	b	615	CLA	O2A-CGA	3.68	1.44	1.33
20	D	404	CLA	OBD-CAD	3.68	1.27	1.22
32	C	534	HTG	C1'-S1	-3.68	1.76	1.81
20	B	612	CLA	O2D-CGD	3.67	1.42	1.33
21	D	403	PHO	C1A-NA	-3.67	1.30	1.37
32	d	401	HTG	C1'-S1	-3.67	1.76	1.81
20	c	501	CLA	O2A-CGA	3.67	1.44	1.33
20	b	612	CLA	MG-NA	3.66	2.15	2.06
35	h	101	DGD	O5D-C1E	3.66	1.46	1.40
37	e	102	HEM	C3C-CAC	3.66	1.55	1.47
21	A	403	PHO	O2A-CGA	3.65	1.44	1.33
20	b	614	CLA	OBD-CAD	3.65	1.27	1.22
20	c	510	CLA	MG-NA	3.64	2.14	2.06
20	B	607	CLA	O2A-CGA	3.64	1.44	1.33
37	e	102	HEM	C3B-CAB	3.64	1.55	1.47
20	b	604	CLA	C3B-C2B	3.63	1.45	1.40
37	E	104	HEM	C3B-C2B	-3.63	1.35	1.40
40	V	201	HEC	C3B-C2B	-3.63	1.37	1.40
20	d	403	CLA	OBD-CAD	3.62	1.27	1.22
20	B	615	CLA	C3B-C2B	3.61	1.45	1.40
23	A	406	SQD	O48-C23	3.61	1.43	1.33
20	B	601	CLA	O2A-CGA	3.60	1.43	1.33
20	B	607	CLA	C1C-C2C	3.60	1.51	1.44
20	A	401	CLA	MG-NC	3.60	2.14	2.06
20	B	616	CLA	O2A-CGA	3.59	1.43	1.33
20	c	505	CLA	O2A-CGA	3.58	1.43	1.33
20	a	407	CLA	MG-NA	3.58	2.14	2.06
20	C	504	CLA	O2A-CGA	3.58	1.43	1.33
20	D	404	CLA	O2A-CGA	3.58	1.43	1.33
21	A	403	PHO	C1A-NA	-3.57	1.30	1.37
20	A	404	CLA	O2A-CGA	3.57	1.43	1.33
35	c	515	DGD	O1G-C1A	3.57	1.43	1.33
20	B	615	CLA	C3D-C2D	3.57	1.45	1.39
20	c	508	CLA	C1C-NC	-3.57	1.32	1.37
20	b	616	CLA	O2A-CGA	3.56	1.43	1.33
20	B	610	CLA	O2D-CGD	3.56	1.41	1.33
20	B	610	CLA	C3B-C2B	3.56	1.45	1.40
20	b	612	CLA	C3D-C2D	3.56	1.45	1.39
35	C	518	DGD	O2G-C1B	3.55	1.44	1.34
20	C	503	CLA	OBD-CAD	3.55	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	615	CLA	C3B-C2B	3.54	1.45	1.40
20	B	603	CLA	MG-NC	3.54	2.14	2.06
20	c	509	CLA	O2A-CGA	3.54	1.43	1.33
20	B	615	CLA	O2A-CGA	3.54	1.43	1.33
20	B	611	CLA	OBD-CAD	3.54	1.27	1.22
34	c	523	LMT	O1'-C1'	3.54	1.46	1.40
20	d	403	CLA	C3D-C2D	3.53	1.45	1.39
20	C	506	CLA	MG-NC	3.53	2.14	2.06
20	a	404	CLA	C3C-C2C	3.53	1.44	1.36
32	C	522	HTG	C1'-S1	-3.53	1.76	1.81
20	B	605	CLA	C3D-C2D	3.52	1.45	1.39
20	c	512	CLA	C4C-C3C	3.51	1.51	1.45
35	H	102	DGD	O1G-C1A	3.51	1.43	1.33
24	B	620	LMG	O7-C10	3.51	1.44	1.34
20	B	601	CLA	OBD-CAD	3.51	1.27	1.22
20	b	616	CLA	C3B-C2B	3.50	1.45	1.40
20	C	507	CLA	O2A-CGA	3.50	1.43	1.33
21	a	406	PHO	O2A-CGA	3.49	1.43	1.33
32	B	632	HTG	C1'-S1	-3.48	1.77	1.81
20	c	502	CLA	C3C-C2C	3.48	1.44	1.36
21	D	403	PHO	CHC-C1C	3.47	1.45	1.38
20	A	402	CLA	C3C-C2C	3.47	1.44	1.36
20	b	604	CLA	O2A-CGA	3.47	1.43	1.33
20	D	401	CLA	C3B-C2B	3.47	1.45	1.40
20	b	614	CLA	C4B-NB	-3.47	1.32	1.35
20	C	501	CLA	O2A-CGA	3.47	1.43	1.33
35	H	102	DGD	O5D-C1E	3.46	1.46	1.40
20	D	402	CLA	O2D-CGD	3.45	1.41	1.33
20	b	607	CLA	OBD-CAD	3.45	1.27	1.22
20	b	615	CLA	OBD-CAD	3.45	1.27	1.22
22	b	620	BCR	C5-C6	3.45	1.40	1.34
20	C	505	CLA	C1B-NB	-3.44	1.32	1.35
20	D	401	CLA	O2A-CGA	3.44	1.43	1.33
36	d	408	LHG	O8-C23	3.44	1.43	1.33
20	c	510	CLA	C3D-C2D	3.44	1.45	1.39
20	A	404	CLA	O2D-CGD	3.43	1.41	1.33
20	c	508	CLA	O2A-CGA	3.43	1.43	1.33
20	C	502	CLA	OBD-CAD	3.43	1.27	1.22
40	V	201	HEC	C3D-C2D	3.42	1.47	1.37
20	B	614	CLA	C3D-C2D	3.42	1.45	1.39
20	B	604	CLA	MG-NC	3.41	2.14	2.06
27	d	412	PL9	C7-C3	3.41	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	201	HEC	CBC-CAC	-3.41	1.36	1.49
20	C	510	CLA	O2A-CGA	3.41	1.43	1.33
20	B	614	CLA	C4C-C3C	3.41	1.50	1.45
20	b	612	CLA	C4C-C3C	3.41	1.50	1.45
20	B	610	CLA	O2A-CGA	3.40	1.43	1.33
20	b	609	CLA	C3B-C2B	3.40	1.45	1.40
20	B	606	CLA	C3D-C2D	3.40	1.45	1.39
20	A	401	CLA	C1D-C2D	3.40	1.50	1.42
20	b	615	CLA	C3D-C2D	3.40	1.45	1.39
35	C	516	DGD	O1G-C1A	3.40	1.43	1.33
20	c	511	CLA	O2A-CGA	3.39	1.43	1.33
20	a	404	CLA	O2A-CGA	3.38	1.43	1.33
20	B	604	CLA	OBD-CAD	3.38	1.27	1.22
20	c	502	CLA	O2A-CGA	3.38	1.43	1.33
20	B	615	CLA	O2D-CGD	3.37	1.41	1.33
20	B	616	CLA	C1B-NB	-3.35	1.32	1.35
20	b	618	CLA	MG-NC	3.35	2.14	2.06
36	D	408	LHG	O8-C23	3.35	1.43	1.33
36	L	101	LHG	O7-C7	3.35	1.43	1.34
32	B	631	HTG	C1'-S1	-3.35	1.77	1.81
20	d	402	CLA	C1B-CHB	3.33	1.50	1.41
36	L	101	LHG	O8-C23	3.33	1.43	1.33
20	c	510	CLA	C3B-C2B	3.32	1.45	1.40
20	d	404	CLA	MG-NC	3.32	2.14	2.06
20	B	611	CLA	O2A-CGA	3.31	1.43	1.33
20	d	402	CLA	O2A-CGA	3.31	1.43	1.33
20	B	607	CLA	C4B-CHC	3.31	1.50	1.41
20	b	607	CLA	C3D-C2D	3.31	1.45	1.39
20	a	404	CLA	O2D-CGD	3.31	1.41	1.33
20	C	511	CLA	O2A-CGA	3.31	1.43	1.33
20	b	604	CLA	OBD-CAD	3.31	1.26	1.22
34	b	627	LMT	O1'-C1'	3.30	1.45	1.40
32	b	601	HTG	C1'-S1	-3.30	1.77	1.81
20	C	509	CLA	C3B-C2B	3.30	1.44	1.40
21	A	403	PHO	O2D-CGD	3.29	1.41	1.33
20	d	402	CLA	C3D-C2D	3.28	1.45	1.39
20	C	512	CLA	C4C-C3C	3.28	1.50	1.45
20	B	613	CLA	OBD-CAD	3.28	1.26	1.22
21	a	405	PHO	CHD-C1D	3.28	1.45	1.38
20	B	610	CLA	MG-NC	3.27	2.14	2.06
20	B	615	CLA	C1C-NC	-3.26	1.32	1.37
36	l	102	LHG	O8-C23	3.25	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	604	CLA	C4C-C3C	3.25	1.50	1.45
20	c	503	CLA	O2A-CGA	3.25	1.42	1.33
20	C	502	CLA	C1B-CHB	3.24	1.50	1.41
20	B	609	CLA	O2A-CGA	3.24	1.42	1.33
20	c	505	CLA	C1D-C2D	3.24	1.49	1.42
35	C	517	DGD	O2G-C1B	3.23	1.43	1.34
28	A	414	DMS	O-S	3.23	1.72	1.50
21	A	403	PHO	CHD-C1D	3.21	1.44	1.38
40	v	201	HEC	CBC-CAC	-3.20	1.37	1.49
21	D	403	PHO	C3D-C2D	3.20	1.47	1.39
20	D	401	CLA	C3D-C2D	3.20	1.45	1.39
20	B	604	CLA	O2A-CGA	3.19	1.42	1.33
20	D	401	CLA	O2D-CGD	3.19	1.41	1.33
20	c	511	CLA	C1B-CHB	3.19	1.49	1.41
20	C	512	CLA	C1B-CHB	3.18	1.49	1.41
20	b	618	CLA	OBD-CAD	3.18	1.26	1.22
21	D	403	PHO	C3D-C4D	-3.18	1.33	1.43
20	c	508	CLA	C4C-C3C	3.18	1.50	1.45
36	D	408	LHG	O7-C7	3.17	1.43	1.34
20	B	605	CLA	OBD-CAD	3.17	1.26	1.22
20	A	402	CLA	OBD-CAD	3.17	1.26	1.22
36	d	406	LHG	O7-C7	3.16	1.43	1.34
32	b	602	HTG	C1'-S1	-3.15	1.77	1.81
20	A	404	CLA	C1B-CHB	3.15	1.49	1.41
20	B	612	CLA	C3B-C2B	3.14	1.44	1.40
23	a	409	SQD	C6-S	-3.14	1.65	1.77
20	C	513	CLA	C4C-C3C	3.12	1.50	1.45
20	C	506	CLA	C1B-CHB	3.12	1.49	1.41
20	a	404	CLA	C3B-C2B	3.12	1.44	1.40
20	B	606	CLA	O2A-CGA	3.10	1.42	1.33
20	B	615	CLA	C1B-CHB	3.10	1.49	1.41
20	d	404	CLA	O2D-CGD	3.10	1.40	1.33
20	b	608	CLA	OBD-CAD	3.10	1.26	1.22
21	a	405	PHO	C1A-NA	-3.10	1.31	1.37
32	B	623	HTG	C1'-S1	-3.09	1.77	1.81
20	B	605	CLA	O2A-CGA	3.08	1.42	1.33
20	d	402	CLA	C1D-C2D	3.08	1.49	1.42
36	D	409	LHG	O7-C7	3.07	1.43	1.34
20	b	614	CLA	O2A-CGA	3.07	1.42	1.33
35	c	516	DGD	O2G-C1B	3.06	1.42	1.34
22	a	408	BCR	C26-C25	3.06	1.39	1.34
20	b	604	CLA	O2D-CGD	3.06	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	521	HTG	C1'-S1	-3.05	1.77	1.81
20	B	614	CLA	O2D-CGD	3.05	1.40	1.33
21	a	406	PHO	C3D-C2D	3.05	1.47	1.39
20	B	604	CLA	C1B-CHB	3.05	1.49	1.41
37	e	102	HEM	C3C-C2C	-3.04	1.36	1.40
20	B	608	CLA	OBD-CAD	3.04	1.26	1.22
32	b	625	HTG	C1-S1	3.03	1.85	1.80
20	C	511	CLA	C4C-C3C	3.03	1.50	1.45
20	B	613	CLA	O2A-CGA	3.03	1.42	1.33
20	b	608	CLA	C4B-CHC	3.03	1.49	1.41
20	b	617	CLA	C4B-NB	3.03	1.37	1.35
20	C	513	CLA	C1B-CHB	3.02	1.49	1.41
20	A	401	CLA	C3C-C2C	3.02	1.43	1.36
36	d	408	LHG	O7-C7	3.02	1.42	1.34
20	b	610	CLA	C4B-NB	-3.02	1.32	1.35
20	C	511	CLA	C1B-CHB	3.01	1.49	1.41
20	A	402	CLA	C3B-C2B	3.01	1.44	1.40
35	h	101	DGD	O1G-C1A	3.00	1.42	1.33
28	B	634	DMS	O-S	3.00	1.70	1.50
20	B	614	CLA	OBD-CAD	3.00	1.26	1.22
37	E	104	HEM	C1D-ND	2.99	1.42	1.36
20	C	503	CLA	CHD-C4C	2.99	1.49	1.41
20	b	608	CLA	O2A-CGA	2.99	1.42	1.33
21	a	405	PHO	C3D-C2D	2.98	1.47	1.39
20	b	604	CLA	C1B-NB	-2.98	1.32	1.35
20	D	402	CLA	C3D-C2D	2.98	1.44	1.39
20	c	503	CLA	C1B-CHB	2.97	1.49	1.41
21	D	403	PHO	OBD-CAD	2.97	1.27	1.22
20	b	612	CLA	OBD-CAD	2.97	1.26	1.22
20	C	508	CLA	C4C-C3C	2.97	1.50	1.45
20	a	403	CLA	O2A-CGA	2.97	1.42	1.33
20	B	615	CLA	C4C-C3C	2.96	1.50	1.45
32	C	520	HTG	C1'-S1	-2.96	1.77	1.81
20	c	505	CLA	C1B-NB	-2.96	1.32	1.35
20	b	604	CLA	C1D-C2D	2.95	1.49	1.42
20	D	402	CLA	CHD-C4C	2.95	1.49	1.41
27	a	415	PL9	C7-C3	2.95	1.54	1.51
32	C	521	HTG	C1'-S1	-2.94	1.77	1.81
20	a	407	CLA	C1B-CHB	2.94	1.49	1.41
20	c	511	CLA	C4C-C3C	2.94	1.50	1.45
20	b	609	CLA	OBD-CAD	2.94	1.26	1.22
20	B	608	CLA	C1D-C2D	2.94	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	509	CLA	C1B-CHB	2.92	1.49	1.41
20	c	505	CLA	C1B-CHB	2.92	1.49	1.41
20	b	608	CLA	C1B-CHB	2.92	1.49	1.41
21	a	405	PHO	OBD-CAD	2.92	1.27	1.22
20	c	512	CLA	MG-NC	2.91	2.13	2.06
20	c	501	CLA	C4B-CHC	2.91	1.49	1.41
20	b	614	CLA	C3B-C2B	2.91	1.44	1.40
20	c	504	CLA	MG-NC	2.90	2.13	2.06
20	C	505	CLA	CHD-C4C	2.89	1.49	1.41
37	e	102	HEM	C3B-C2B	-2.89	1.36	1.40
21	A	403	PHO	CHD-C4C	2.89	1.47	1.40
20	C	506	CLA	C4B-CHC	2.89	1.49	1.41
32	b	624	HTG	C1-S1	-2.89	1.76	1.80
20	c	504	CLA	C4C-C3C	2.89	1.50	1.45
34	Z	101	LMT	O1'-C1'	2.88	1.45	1.40
20	b	611	CLA	C1D-C2D	2.86	1.49	1.42
20	a	403	CLA	O2A-C1	-2.86	1.38	1.46
20	c	505	CLA	O2D-CGD	2.86	1.40	1.33
20	B	610	CLA	C1B-NB	-2.85	1.32	1.35
20	C	505	CLA	C4C-C3C	2.85	1.50	1.45
20	b	613	CLA	C1B-CHB	2.85	1.48	1.41
20	D	404	CLA	C4C-C3C	2.85	1.49	1.45
20	c	503	CLA	OBD-CAD	2.85	1.26	1.22
20	C	507	CLA	C4C-C3C	2.84	1.49	1.45
20	B	609	CLA	MG-NC	2.84	2.13	2.06
20	A	402	CLA	C1C-NC	-2.84	1.33	1.37
20	B	608	CLA	C1B-CHB	2.83	1.48	1.41
20	C	510	CLA	C1C-NC	-2.83	1.33	1.37
20	b	616	CLA	C4C-C3C	2.82	1.49	1.45
20	B	605	CLA	C1D-C2D	2.81	1.48	1.42
20	b	609	CLA	O2A-CGA	2.81	1.41	1.33
20	b	617	CLA	C1B-CHB	2.81	1.48	1.41
20	c	513	CLA	C1B-CHB	2.81	1.48	1.41
20	B	613	CLA	C1B-CHB	2.80	1.48	1.41
20	D	402	CLA	C1D-C2D	2.80	1.48	1.42
20	B	603	CLA	C1B-CHB	2.80	1.48	1.41
20	D	404	CLA	C1B-CHB	2.80	1.48	1.41
20	A	401	CLA	C4B-CHC	2.79	1.48	1.41
20	b	617	CLA	O2A-CGA	2.79	1.41	1.33
20	b	606	CLA	O2A-CGA	2.79	1.41	1.33
20	a	404	CLA	CHD-C4C	2.78	1.49	1.41
23	A	412	SQD	C6-S	-2.78	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	404	CLA	C4B-CHC	2.78	1.48	1.41
20	b	617	CLA	MG-NC	2.78	2.12	2.06
20	b	610	CLA	C1B-CHB	2.78	1.48	1.41
20	A	401	CLA	CHD-C4C	2.78	1.49	1.41
20	c	512	CLA	C4B-CHC	2.76	1.48	1.41
23	a	401	SQD	C6-S	-2.76	1.67	1.77
40	v	201	HEC	CBB-CAB	-2.76	1.39	1.49
20	b	608	CLA	C1D-C2D	2.76	1.48	1.42
20	b	615	CLA	C1C-NC	-2.75	1.33	1.37
21	a	406	PHO	CHC-C4B	2.75	1.46	1.40
20	C	507	CLA	C1B-CHB	2.75	1.48	1.41
20	d	404	CLA	C4B-CHC	2.75	1.48	1.41
20	b	612	CLA	O2A-CGA	2.75	1.41	1.33
20	B	608	CLA	O2A-CGA	2.74	1.41	1.33
40	V	201	HEC	CMD-C2D	2.74	1.57	1.51
27	A	411	PL9	C7-C3	2.74	1.54	1.51
20	C	510	CLA	C1B-CHB	2.74	1.48	1.41
20	C	507	CLA	CHD-C4C	2.74	1.49	1.41
27	D	412	PL9	C6-C5	2.74	1.49	1.35
20	B	608	CLA	C4B-CHC	2.73	1.48	1.41
20	B	602	CLA	C1D-C2D	2.73	1.48	1.42
32	B	622	HTG	O5-C1	2.73	1.46	1.42
20	C	510	CLA	C4C-C3C	2.73	1.49	1.45
20	c	507	CLA	C1B-CHB	2.71	1.48	1.41
20	b	607	CLA	O2A-CGA	2.71	1.41	1.33
20	B	607	CLA	C4C-C3C	2.71	1.49	1.45
20	b	618	CLA	C1B-CHB	2.70	1.48	1.41
20	b	603	CLA	C4B-CHC	2.69	1.48	1.41
20	c	509	CLA	C4C-C3C	2.69	1.49	1.45
20	C	505	CLA	C4B-CHC	2.69	1.48	1.41
32	c	520	HTG	C1'-S1	-2.69	1.78	1.81
20	b	607	CLA	C3B-C2B	2.69	1.44	1.40
20	A	402	CLA	O2D-CGD	2.69	1.39	1.33
20	C	501	CLA	C4B-CHC	2.69	1.48	1.41
20	C	503	CLA	C4B-CHC	2.69	1.48	1.41
20	c	513	CLA	C1D-C2D	2.69	1.48	1.42
20	d	404	CLA	C1B-CHB	2.67	1.48	1.41
20	C	508	CLA	C1B-CHB	2.67	1.48	1.41
20	b	604	CLA	CHD-C4C	2.67	1.48	1.41
20	B	603	CLA	C4B-NB	2.66	1.37	1.35
20	B	609	CLA	C4B-NB	2.66	1.37	1.35
20	C	504	CLA	CHD-C4C	2.66	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	515	DGD	O2G-C1B	2.65	1.41	1.34
20	C	504	CLA	C1D-C2D	2.65	1.48	1.42
20	b	610	CLA	O2A-CGA	2.65	1.41	1.33
20	C	506	CLA	C4C-C3C	2.65	1.49	1.45
20	D	402	CLA	O2A-CGA	2.65	1.41	1.33
20	c	510	CLA	C1B-CHB	2.65	1.48	1.41
40	V	201	HEC	CBB-CAB	-2.64	1.39	1.49
20	D	402	CLA	C1C-NC	-2.64	1.33	1.37
20	b	615	CLA	MG-NC	2.64	2.12	2.06
20	B	610	CLA	C1B-CHB	2.64	1.48	1.41
21	a	406	PHO	CHD-C4C	2.63	1.46	1.40
20	c	513	CLA	C1C-C2C	2.63	1.49	1.44
20	c	512	CLA	CHD-C4C	2.63	1.48	1.41
20	B	602	CLA	C4B-CHC	2.63	1.48	1.41
20	b	603	CLA	C1C-NC	-2.63	1.33	1.37
23	A	406	SQD	C6-S	-2.63	1.67	1.77
20	B	612	CLA	C4B-CHC	2.63	1.48	1.41
20	b	608	CLA	C4B-NB	2.63	1.37	1.35
20	c	512	CLA	C1D-C2D	2.62	1.48	1.42
20	B	612	CLA	C4B-NB	2.62	1.37	1.35
20	a	403	CLA	C1B-CHB	2.62	1.48	1.41
27	a	415	PL9	C2-C3	2.62	1.41	1.34
36	l	102	LHG	O7-C7	2.62	1.41	1.34
27	a	415	PL9	C6-C5	2.61	1.48	1.35
20	D	402	CLA	C4C-C3C	2.61	1.49	1.45
20	c	510	CLA	MG-NC	2.60	2.12	2.06
20	b	618	CLA	C1C-C2C	2.60	1.49	1.44
20	C	513	CLA	CHD-C4C	2.60	1.48	1.41
27	A	411	PL9	C6-C5	2.60	1.48	1.35
20	c	508	CLA	C1B-NB	2.60	1.37	1.35
20	b	610	CLA	CHD-C4C	2.60	1.48	1.41
32	O	302	HTG	O5-C1	2.59	1.46	1.42
20	D	401	CLA	OBD-CAD	2.59	1.25	1.22
20	B	604	CLA	C3B-C2B	2.59	1.44	1.40
20	B	614	CLA	C1D-C2D	2.59	1.48	1.42
20	D	402	CLA	C4B-CHC	2.59	1.48	1.41
20	c	503	CLA	C4C-C3C	2.59	1.49	1.45
20	B	616	CLA	C4C-C3C	2.58	1.49	1.45
20	B	602	CLA	C1B-CHB	2.58	1.48	1.41
20	C	508	CLA	C1D-C2D	2.58	1.48	1.42
20	b	617	CLA	CHD-C4C	2.58	1.48	1.41
20	b	611	CLA	C1B-CHB	2.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	404	CLA	C4C-C3C	2.58	1.49	1.45
20	B	611	CLA	C1C-C2C	2.57	1.49	1.44
21	a	405	PHO	C1C-NC	-2.57	1.33	1.38
20	c	507	CLA	C4B-CHC	2.57	1.48	1.41
20	b	611	CLA	C4B-CHC	2.57	1.48	1.41
20	B	602	CLA	MG-NC	2.56	2.12	2.06
20	B	606	CLA	C1B-CHB	2.56	1.48	1.41
32	b	601	HTG	C1-S1	-2.56	1.76	1.80
20	c	502	CLA	C1B-CHB	2.55	1.48	1.41
24	c	519	LMG	O1-C1	2.55	1.44	1.40
20	C	503	CLA	C1C-C2C	2.55	1.49	1.44
20	c	504	CLA	C1C-NC	-2.54	1.34	1.37
20	b	605	CLA	O2A-CGA	2.54	1.40	1.33
34	f	102	LMT	O1'-C1'	2.54	1.44	1.40
20	b	603	CLA	C1B-CHB	2.54	1.48	1.41
20	c	505	CLA	CHD-C4C	2.54	1.48	1.41
21	a	406	PHO	C3D-C4D	-2.54	1.35	1.43
20	C	512	CLA	CHD-C4C	2.54	1.48	1.41
20	C	508	CLA	C4B-CHC	2.53	1.48	1.41
20	B	611	CLA	C4B-CHC	2.53	1.48	1.41
21	a	405	PHO	O2A-CGA	2.53	1.40	1.33
20	b	615	CLA	C1D-C2D	2.53	1.48	1.42
34	z	102	LMT	O1'-C1'	2.52	1.44	1.40
22	a	408	BCR	C40-C30	2.52	1.58	1.53
20	b	608	CLA	C4C-C3C	2.52	1.49	1.45
20	A	401	CLA	O2A-CGA	2.52	1.40	1.33
20	B	604	CLA	C1C-NC	-2.52	1.34	1.37
20	C	513	CLA	C4B-CHC	2.51	1.48	1.41
27	d	412	PL9	C6-C5	2.51	1.48	1.35
20	B	614	CLA	C1B-CHB	2.51	1.48	1.41
20	A	404	CLA	C1B-NB	2.51	1.37	1.35
23	b	622	SQD	C6-S	-2.51	1.68	1.77
20	B	609	CLA	CHD-C4C	2.51	1.48	1.41
20	b	612	CLA	C4B-CHC	2.51	1.48	1.41
21	A	403	PHO	C1D-C2D	2.50	1.51	1.45
20	c	509	CLA	MG-NC	2.49	2.12	2.06
20	c	507	CLA	C1C-C2C	2.49	1.49	1.44
20	c	505	CLA	C4C-C3C	2.49	1.49	1.45
35	c	515	DGD	O5D-C1E	2.49	1.44	1.40
36	d	407	LHG	O8-C23	2.49	1.40	1.33
22	D	405	BCR	C12-C13	2.49	1.51	1.45
20	B	608	CLA	C4C-C3C	2.48	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	606	CLA	CHD-C4C	2.48	1.48	1.41
37	E	104	HEM	C3C-C2C	-2.48	1.36	1.40
20	d	402	CLA	C4C-C3C	2.48	1.49	1.45
20	D	402	CLA	C4B-NB	-2.48	1.33	1.35
20	B	616	CLA	C1D-C2D	2.48	1.48	1.42
20	b	617	CLA	C4C-C3C	2.48	1.49	1.45
20	c	511	CLA	C4B-CHC	2.47	1.47	1.41
20	c	511	CLA	C1C-C2C	2.47	1.49	1.44
20	b	604	CLA	C3B-CAB	2.47	1.53	1.47
20	B	601	CLA	C4B-CHC	2.47	1.47	1.41
20	a	404	CLA	C1B-CHB	2.47	1.47	1.41
20	B	604	CLA	C4C-C3C	2.46	1.49	1.45
20	B	602	CLA	C1C-C2C	2.46	1.49	1.44
20	B	610	CLA	C1D-C2D	2.46	1.48	1.42
20	c	506	CLA	C1C-NC	-2.46	1.34	1.37
23	l	101	SQD	O6-C1	2.46	1.44	1.40
20	C	509	CLA	C4C-C3C	2.45	1.49	1.45
20	C	512	CLA	C1C-C2C	2.45	1.49	1.44
20	c	512	CLA	C1B-CHB	2.45	1.47	1.41
20	c	513	CLA	CHD-C4C	2.45	1.48	1.41
27	A	411	PL9	C2-C3	2.45	1.41	1.34
20	b	616	CLA	C4B-CHC	2.45	1.47	1.41
20	b	615	CLA	CHD-C4C	2.45	1.48	1.41
21	a	406	PHO	OBD-CAD	2.45	1.26	1.22
20	c	508	CLA	C4B-CHC	2.44	1.47	1.41
20	B	604	CLA	CHD-C4C	2.44	1.48	1.41
20	D	404	CLA	C1C-NC	-2.44	1.34	1.37
24	c	518	LMG	O1-C1	2.44	1.44	1.40
27	D	412	PL9	C2-C3	2.43	1.41	1.34
20	c	509	CLA	C4B-NB	2.43	1.37	1.35
20	D	401	CLA	CHD-C4C	2.43	1.48	1.41
20	D	404	CLA	C4B-CHC	2.43	1.47	1.41
20	d	403	CLA	O2A-CGA	2.43	1.40	1.33
32	b	625	HTG	O5-C1	2.43	1.46	1.42
20	C	506	CLA	C1C-C2C	2.43	1.49	1.44
20	c	508	CLA	C1B-CHB	2.43	1.47	1.41
20	b	608	CLA	C1C-C2C	2.42	1.49	1.44
37	E	104	HEM	C4B-NB	2.42	1.41	1.36
24	C	524	LMG	O1-C1	2.42	1.44	1.40
21	A	403	PHO	C3D-C4D	-2.42	1.36	1.43
20	d	403	CLA	O2D-CGD	2.41	1.39	1.33
20	c	501	CLA	C1B-CHB	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	416	DGD	O3G-C1D	2.41	1.44	1.40
20	C	501	CLA	C1B-CHB	2.40	1.47	1.41
20	B	605	CLA	C1B-CHB	2.40	1.47	1.41
20	C	512	CLA	C4B-CHC	2.40	1.47	1.41
20	C	506	CLA	CHD-C4C	2.39	1.48	1.41
20	c	507	CLA	C1B-NB	2.39	1.37	1.35
32	B	621	HTG	C1-C2	2.39	1.57	1.53
20	b	606	CLA	C1B-CHB	2.39	1.47	1.41
20	b	604	CLA	C1B-CHB	2.39	1.47	1.41
20	C	511	CLA	C1C-NC	-2.39	1.34	1.37
20	c	501	CLA	C4C-C3C	2.39	1.49	1.45
20	d	402	CLA	MG-NC	2.39	2.11	2.06
20	d	403	CLA	MG-NC	-2.38	2.00	2.06
34	E	101	LMT	O1'-C1'	2.38	1.44	1.40
20	a	403	CLA	CHD-C4C	2.38	1.47	1.41
21	D	403	PHO	CHD-C4C	2.38	1.46	1.40
32	C	522	HTG	C1-S1	-2.38	1.77	1.80
20	B	609	CLA	C1B-CHB	2.38	1.47	1.41
23	f	101	SQD	C6-S	-2.37	1.68	1.77
20	d	404	CLA	C1C-C2C	2.37	1.49	1.44
20	b	614	CLA	C1B-NB	-2.37	1.33	1.35
20	C	501	CLA	CHD-C4C	2.37	1.47	1.41
20	B	605	CLA	C4C-C3C	2.36	1.49	1.45
20	B	612	CLA	O2A-CGA	2.36	1.40	1.33
20	C	505	CLA	C1D-C2D	2.35	1.47	1.42
20	B	611	CLA	C1B-CHB	2.35	1.47	1.41
20	B	616	CLA	C1B-CHB	2.35	1.47	1.41
20	c	512	CLA	C1C-C2C	2.35	1.49	1.44
20	c	509	CLA	C1C-NC	-2.35	1.34	1.37
20	b	611	CLA	C4C-C3C	2.34	1.49	1.45
20	b	606	CLA	C4C-C3C	2.34	1.49	1.45
20	d	403	CLA	C1D-C2D	2.34	1.47	1.42
20	c	502	CLA	C4C-C3C	2.34	1.49	1.45
20	c	513	CLA	C4B-CHC	2.33	1.47	1.41
20	B	616	CLA	CHD-C4C	2.33	1.47	1.41
27	d	412	PL9	C43-C44	2.33	1.38	1.33
20	C	507	CLA	C1D-C2D	2.33	1.47	1.42
20	B	607	CLA	C1D-C2D	2.32	1.47	1.42
23	F	101	SQD	C6-S	-2.32	1.68	1.77
20	D	402	CLA	OBD-CAD	2.32	1.25	1.22
20	b	605	CLA	CHD-C4C	2.32	1.47	1.41
20	B	602	CLA	CHD-C4C	2.31	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	610	CLA	MG-NC	2.31	2.11	2.06
20	b	618	CLA	C4B-CHC	2.30	1.47	1.41
20	b	616	CLA	MG-NC	2.30	2.11	2.06
20	B	604	CLA	C1D-C2D	2.30	1.47	1.42
35	c	517	DGD	O5D-C1E	2.29	1.44	1.40
20	c	503	CLA	C4B-CHC	2.29	1.47	1.41
20	A	401	CLA	C3B-C2B	2.29	1.43	1.40
20	c	511	CLA	C1D-C2D	2.29	1.47	1.42
20	b	605	CLA	C1B-CHB	2.29	1.47	1.41
20	C	505	CLA	C1B-CHB	2.29	1.47	1.41
36	d	407	LHG	O7-C7	2.29	1.40	1.34
20	c	504	CLA	C1D-C2D	2.28	1.47	1.42
20	B	605	CLA	CHD-C4C	2.28	1.47	1.41
20	b	611	CLA	C1C-C2C	2.28	1.49	1.44
36	L	101	LHG	O7-C5	-2.28	1.40	1.46
20	B	614	CLA	C1C-C2C	2.27	1.49	1.44
20	A	402	CLA	O2A-CGA	2.27	1.40	1.33
20	B	601	CLA	C4C-C3C	2.26	1.48	1.45
34	J	103	LMT	O1'-C1'	2.26	1.44	1.40
20	c	511	CLA	C4B-NB	2.26	1.37	1.35
20	c	503	CLA	CHD-C4C	2.26	1.47	1.41
20	b	605	CLA	C4C-C3C	2.26	1.48	1.45
20	b	603	CLA	C4C-C3C	2.26	1.48	1.45
20	A	401	CLA	MG-NA	2.25	2.11	2.06
20	c	506	CLA	CHD-C4C	2.25	1.47	1.41
20	b	611	CLA	CHD-C4C	2.25	1.47	1.41
35	c	517	DGD	O2G-C2G	-2.25	1.41	1.46
20	B	615	CLA	C4B-CHC	2.24	1.47	1.41
20	C	513	CLA	C1C-C2C	2.24	1.48	1.44
20	b	609	CLA	CHD-C4C	2.24	1.47	1.41
32	c	520	HTG	C1-S1	-2.24	1.77	1.80
20	a	404	CLA	C1D-C2D	2.24	1.47	1.42
22	D	405	BCR	C21-C22	2.24	1.38	1.35
20	B	608	CLA	CHD-C4C	2.24	1.47	1.41
20	C	509	CLA	C1B-CHB	2.24	1.47	1.41
20	C	508	CLA	MG-NC	2.24	2.11	2.06
32	B	621	HTG	O5-C1	2.23	1.45	1.42
20	b	616	CLA	C1B-CHB	2.23	1.47	1.41
20	c	509	CLA	CHD-C4C	2.23	1.47	1.41
20	C	501	CLA	C1D-C2D	2.23	1.47	1.42
20	B	611	CLA	CHD-C4C	2.23	1.47	1.41
22	b	621	BCR	C26-C25	2.23	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	508	CLA	C1C-NC	-2.23	1.34	1.37
20	C	511	CLA	C4B-CHC	2.23	1.47	1.41
20	C	507	CLA	C4B-CHC	2.23	1.47	1.41
20	c	501	CLA	C1C-C2C	2.23	1.48	1.44
20	c	511	CLA	CHD-C4C	2.22	1.47	1.41
32	b	602	HTG	C1-S1	-2.22	1.77	1.80
20	d	403	CLA	CHD-C4C	2.22	1.47	1.41
20	B	611	CLA	C1C-NC	-2.21	1.34	1.37
20	a	403	CLA	OBD-CAD	2.21	1.25	1.22
20	c	506	CLA	C4B-CHC	2.21	1.47	1.41
22	A	405	BCR	C19-C18	2.21	1.50	1.45
20	c	502	CLA	CHD-C4C	2.21	1.47	1.41
20	B	610	CLA	C4B-CHC	2.21	1.47	1.41
20	B	602	CLA	C1C-NC	-2.21	1.34	1.37
20	B	609	CLA	C4B-CHC	2.21	1.47	1.41
20	A	404	CLA	C1C-NC	-2.21	1.34	1.37
37	E	104	HEM	CMD-C2D	2.20	1.56	1.51
20	D	404	CLA	CHD-C4C	2.20	1.47	1.41
20	B	612	CLA	C1B-NB	2.20	1.37	1.35
20	C	507	CLA	C1C-C2C	2.20	1.48	1.44
20	C	507	CLA	C1A-CHA	2.20	1.52	1.43
20	B	603	CLA	CHD-C4C	2.20	1.47	1.41
20	B	602	CLA	C4C-C3C	2.19	1.48	1.45
20	C	502	CLA	MG-NC	2.19	2.11	2.06
34	a	418	LMT	O5B-C1B	2.18	1.47	1.41
20	C	511	CLA	C1D-C2D	2.18	1.47	1.42
20	b	609	CLA	C1B-CHB	2.18	1.47	1.41
37	e	102	HEM	CAA-C2A	2.18	1.55	1.52
20	b	614	CLA	C4C-C3C	2.18	1.48	1.45
20	b	614	CLA	CHD-C4C	2.18	1.47	1.41
20	C	504	CLA	C1B-CHB	2.18	1.47	1.41
20	c	506	CLA	C1C-C2C	2.17	1.48	1.44
20	a	403	CLA	C1D-C2D	2.17	1.47	1.42
20	c	503	CLA	C1D-C2D	2.17	1.47	1.42
20	B	613	CLA	C1D-C2D	2.17	1.47	1.42
20	B	607	CLA	C1B-CHB	2.17	1.47	1.41
20	b	606	CLA	MG-NC	2.17	2.11	2.06
20	b	603	CLA	C1D-C2D	2.17	1.47	1.42
20	c	503	CLA	C1C-NC	-2.16	1.34	1.37
20	d	402	CLA	O2D-CGD	2.16	1.38	1.33
34	I	101	LMT	O1'-C1'	2.16	1.43	1.40
20	b	613	CLA	OBD-CAD	2.16	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	511	CLA	CHD-C4C	2.15	1.47	1.41
20	b	603	CLA	CHD-C4C	2.15	1.47	1.41
20	b	609	CLA	C1C-NC	-2.14	1.34	1.37
20	B	614	CLA	CHD-C4C	2.14	1.47	1.41
20	c	511	CLA	C3D-CAD	2.14	1.51	1.46
20	D	401	CLA	C4C-C3C	2.14	1.48	1.45
20	C	502	CLA	CAA-C2A	2.14	1.58	1.54
20	c	505	CLA	C4B-CHC	2.14	1.46	1.41
20	b	612	CLA	CHD-C4C	2.13	1.47	1.41
24	j	101	LMG	O7-C8	-2.13	1.41	1.46
32	C	521	HTG	O5-C1	2.13	1.45	1.42
32	B	622	HTG	C1-S1	2.13	1.84	1.80
20	c	503	CLA	C1C-C2C	2.13	1.48	1.44
20	b	603	CLA	C1C-C2C	2.13	1.48	1.44
20	B	601	CLA	C1B-CHB	2.13	1.46	1.41
20	a	404	CLA	C4B-NB	-2.13	1.33	1.35
20	c	506	CLA	MG-NC	2.12	2.11	2.06
40	v	201	HEC	C1D-ND	2.12	1.40	1.36
20	b	607	CLA	C4B-NB	-2.12	1.33	1.35
20	C	501	CLA	C4C-C3C	2.12	1.48	1.45
20	c	508	CLA	C4B-NB	2.12	1.37	1.35
20	c	507	CLA	CHD-C4C	2.12	1.47	1.41
21	a	406	PHO	C3B-C4B	2.12	1.47	1.43
20	C	512	CLA	C1D-C2D	2.11	1.47	1.42
20	c	509	CLA	C4B-CHC	2.11	1.46	1.41
20	C	509	CLA	C4B-CHC	2.11	1.46	1.41
20	a	403	CLA	C4C-C3C	2.10	1.48	1.45
20	C	502	CLA	C1C-C2C	2.10	1.48	1.44
20	B	603	CLA	C4B-CHC	2.10	1.46	1.41
20	b	616	CLA	CHD-C4C	2.10	1.47	1.41
22	K	101	BCR	C12-C13	2.09	1.50	1.45
20	c	504	CLA	C4B-CHC	2.09	1.46	1.41
20	B	614	CLA	C3B-CAB	2.09	1.52	1.47
22	A	405	BCR	C8-C9	2.09	1.50	1.45
20	B	614	CLA	C1-C2	2.09	1.55	1.49
22	t	101	BCR	C23-C22	2.09	1.50	1.45
20	B	612	CLA	C1B-CHB	2.08	1.46	1.41
20	C	502	CLA	C4B-CHC	2.08	1.46	1.41
34	a	418	LMT	O1'-C1'	2.08	1.43	1.40
20	b	618	CLA	C1D-C2D	2.08	1.47	1.42
20	C	510	CLA	CHD-C4C	2.08	1.47	1.41
20	b	609	CLA	C4C-C3C	2.08	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	613	CLA	CHD-C4C	2.07	1.47	1.41
23	a	409	SQD	O47-C45	-2.07	1.41	1.46
20	b	617	CLA	C1D-C2D	2.07	1.47	1.42
23	l	101	SQD	C6-S	-2.06	1.69	1.77
37	e	102	HEM	C1C-C2C	2.06	1.47	1.42
20	b	618	CLA	C1C-NC	-2.06	1.34	1.37
20	C	503	CLA	C4C-C3C	2.06	1.48	1.45
20	B	612	CLA	C1D-C2D	2.06	1.47	1.42
40	v	201	HEC	CMC-C2C	2.06	1.56	1.51
20	b	606	CLA	CHD-C4C	2.06	1.47	1.41
20	B	603	CLA	O2A-CGA	2.06	1.39	1.33
20	c	510	CLA	C5-C3	2.06	1.55	1.51
20	c	510	CLA	C4B-CHC	2.05	1.46	1.41
22	t	101	BCR	C20-C21	2.05	1.49	1.43
20	b	615	CLA	C1B-CHB	2.05	1.46	1.41
20	c	510	CLA	CHD-C4C	2.05	1.47	1.41
21	D	403	PHO	CHB-C4A	-2.05	1.34	1.40
20	b	611	CLA	C1A-CHA	2.05	1.51	1.43
20	D	404	CLA	C1C-C2C	2.05	1.48	1.44
27	D	412	PL9	C28-C29	2.05	1.37	1.33
20	C	510	CLA	C4B-CHC	2.05	1.46	1.41
22	D	405	BCR	C20-C21	2.04	1.49	1.43
22	c	514	BCR	C12-C13	2.04	1.50	1.45
20	B	613	CLA	C4C-C3C	2.04	1.48	1.45
40	V	201	HEC	CMC-C2C	2.04	1.56	1.51
20	c	513	CLA	MG-NC	2.04	2.11	2.06
20	C	508	CLA	CHD-C4C	2.04	1.46	1.41
20	b	608	CLA	CHD-C4C	2.04	1.46	1.41
20	B	601	CLA	C1D-C2D	2.03	1.47	1.42
20	C	513	CLA	C1D-C2D	2.03	1.47	1.42
22	B	619	BCR	C20-C21	2.03	1.49	1.43
20	c	506	CLA	C1B-CHB	2.03	1.46	1.41
20	d	404	CLA	C1D-C2D	2.03	1.47	1.42
40	v	201	HEC	CMD-C2D	2.03	1.55	1.51
20	C	505	CLA	C1C-C2C	2.03	1.48	1.44
32	B	631	HTG	C1-S1	-2.02	1.77	1.80
40	V	201	HEC	CMA-C3A	2.02	1.56	1.51
20	c	508	CLA	C1D-C2D	2.02	1.47	1.42
37	e	102	HEM	CMA-C3A	2.02	1.55	1.51
38	H	101	RRX	C5-C6	2.02	1.37	1.34
20	B	607	CLA	CHD-C4C	2.01	1.46	1.41
32	V	202	HTG	O5-C1	2.01	1.45	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	102	BCR	C23-C22	2.01	1.50	1.45
22	A	405	BCR	C15-C14	2.01	1.49	1.43
34	m	101	LMT	O1'-C1'	2.01	1.43	1.40
20	B	614	CLA	C4B-NB	2.01	1.37	1.35
20	c	501	CLA	CHD-C4C	2.01	1.46	1.41
20	C	502	CLA	CHD-C4C	2.01	1.46	1.41
20	c	502	CLA	C1C-NC	-2.01	1.34	1.37
20	A	402	CLA	C1B-CHB	2.01	1.46	1.41
20	D	401	CLA	C1C-C2C	2.01	1.48	1.44

All (1978) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	f	101	SQD	O9-S-C6	-14.05	90.24	106.94
20	c	504	CLA	C4A-NA-C1A	12.19	112.19	106.71
20	C	511	CLA	C4A-NA-C1A	11.76	111.99	106.71
20	c	501	CLA	C4A-NA-C1A	11.42	111.84	106.71
20	c	509	CLA	C4A-NA-C1A	10.78	111.55	106.71
23	f	101	SQD	O8-S-O9	-10.52	85.57	111.27
20	C	507	CLA	C4A-NA-C1A	10.48	111.42	106.71
20	c	503	CLA	C4A-NA-C1A	10.40	111.38	106.71
20	c	502	CLA	C4A-NA-C1A	10.20	111.29	106.71
23	f	101	SQD	O7-S-C6	10.17	119.03	106.94
32	d	401	HTG	C1'-S1-C1	9.92	118.65	100.09
20	B	611	CLA	C4A-NA-C1A	9.65	111.05	106.71
20	C	506	CLA	C4A-NA-C1A	9.63	111.04	106.71
23	f	101	SQD	O9-S-O7	-9.49	81.11	113.95
20	C	512	CLA	C4A-NA-C1A	9.49	110.97	106.71
20	c	511	CLA	C4A-NA-C1A	9.47	110.96	106.71
23	a	409	SQD	O6-C1-C2	9.27	122.78	108.30
20	b	606	CLA	C4A-NA-C1A	9.18	110.83	106.71
20	B	602	CLA	C4A-NA-C1A	8.77	110.65	106.71
20	b	616	CLA	C4A-NA-C1A	8.71	110.62	106.71
20	b	615	CLA	C4A-NA-C1A	8.61	110.58	106.71
20	A	402	CLA	C4A-NA-C1A	8.41	110.49	106.71
20	B	615	CLA	C4A-NA-C1A	8.32	110.45	106.71
20	C	502	CLA	C4A-NA-C1A	8.09	110.34	106.71
20	C	509	CLA	C4A-NA-C1A	7.86	110.24	106.71
20	c	508	CLA	C4A-NA-C1A	7.86	110.24	106.71
20	C	508	CLA	C4A-NA-C1A	7.78	110.20	106.71
23	a	409	SQD	O9-S-C6	7.70	116.09	106.94
20	B	603	CLA	C4A-NA-C1A	7.68	110.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	512	CLA	C4A-NA-C1A	7.63	110.14	106.71
20	B	607	CLA	C4A-NA-C1A	7.53	110.09	106.71
20	b	605	CLA	C2C-C1C-NC	7.53	117.02	109.97
20	B	604	CLA	C2C-C1C-NC	7.51	117.00	109.97
32	c	521	HTG	C1'-S1-C1	7.37	113.87	100.09
20	d	403	CLA	C2C-C1C-NC	7.36	116.87	109.97
20	C	513	CLA	C4A-NA-C1A	7.33	110.00	106.71
20	c	507	CLA	C4A-NA-C1A	7.28	109.98	106.71
20	D	401	CLA	C4A-NA-C1A	7.21	109.95	106.71
20	b	617	CLA	C4A-NA-C1A	7.20	109.94	106.71
20	D	404	CLA	C4A-NA-C1A	7.13	109.91	106.71
20	b	603	CLA	C4A-NA-C1A	7.08	109.89	106.71
20	b	614	CLA	C2C-C1C-NC	7.05	116.58	109.97
20	b	607	CLA	C2C-C1C-NC	7.05	116.57	109.97
20	c	513	CLA	C4A-NA-C1A	7.02	109.86	106.71
20	A	404	CLA	C4A-NA-C1A	7.01	109.86	106.71
37	E	104	HEM	CBD-CAD-C3D	-6.99	99.61	112.48
32	B	631	HTG	C1'-S1-C1	6.86	112.92	100.09
20	b	618	CLA	C4A-NA-C1A	6.84	109.78	106.71
20	a	404	CLA	C2C-C1C-NC	6.80	116.34	109.97
22	d	405	BCR	C24-C23-C22	-6.80	115.96	126.23
20	B	613	CLA	C4A-NA-C1A	6.78	109.75	106.71
20	B	612	CLA	CHD-C4C-C3C	-6.76	114.89	124.84
20	B	602	CLA	O2D-CGD-CBD	6.74	123.25	111.27
20	b	618	CLA	O2D-CGD-CBD	6.74	123.24	111.27
32	C	522	HTG	C1'-S1-C1	6.74	112.70	100.09
20	B	606	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
20	C	505	CLA	C4A-NA-C1A	6.58	109.67	106.71
20	D	401	CLA	C2C-C1C-NC	6.57	116.12	109.97
20	C	510	CLA	C2C-C1C-NC	6.55	116.11	109.97
20	b	613	CLA	C4A-NA-C1A	6.54	109.65	106.71
20	b	606	CLA	C2C-C1C-NC	6.53	116.09	109.97
20	B	608	CLA	C2C-C1C-NC	6.52	116.08	109.97
20	C	501	CLA	O2D-CGD-CBD	6.50	122.82	111.27
20	B	616	CLA	C4A-NA-C1A	6.49	109.62	106.71
20	B	605	CLA	C2C-C1C-NC	6.48	116.04	109.97
20	b	608	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	B	609	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	C	504	CLA	C2C-C1C-NC	6.42	115.98	109.97
20	B	610	CLA	C4A-NA-C1A	6.39	109.58	106.71
20	B	615	CLA	O2D-CGD-O1D	-6.38	111.37	123.84
20	B	613	CLA	CAC-C3C-C4C	6.35	133.04	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	406	PHO	CMD-C2D-C1D	6.28	134.74	125.06
32	C	521	HTG	C1'-S1-C1	6.26	111.80	100.09
20	A	402	CLA	CAC-C3C-C4C	6.25	132.92	124.81
20	C	509	CLA	C2C-C1C-NC	6.23	115.81	109.97
37	e	102	HEM	CBA-CAA-C2A	-6.21	101.04	112.49
20	B	614	CLA	C2C-C1C-NC	6.21	115.79	109.97
20	D	402	CLA	C2C-C1C-NC	6.19	115.78	109.97
23	f	101	SQD	O47-C7-C8	6.18	122.47	111.09
21	A	403	PHO	CMD-C2D-C1D	6.13	134.50	125.06
20	C	510	CLA	C4A-NA-C1A	6.12	109.46	106.71
32	V	202	HTG	O5-C1-C2	-6.09	102.65	110.31
23	l	101	SQD	O7-S-C6	6.09	114.17	106.94
32	B	623	HTG	C1'-S1-C1	6.09	111.47	100.09
32	C	520	HTG	C1'-S1-C1	6.03	111.36	100.09
20	c	505	CLA	C4A-NA-C1A	6.02	109.41	106.71
20	A	401	CLA	CMD-C2D-C3D	6.02	135.94	124.68
20	B	607	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	b	603	CLA	O2D-CGD-CBD	5.99	121.91	111.27
21	D	403	PHO	CMD-C2D-C1D	5.98	134.28	125.06
20	B	603	CLA	C2C-C1C-NC	5.96	115.56	109.97
20	a	403	CLA	C4A-NA-C1A	5.92	109.37	106.71
20	B	613	CLA	C2C-C1C-NC	5.90	115.50	109.97
20	C	510	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
20	A	402	CLA	C2C-C1C-NC	5.88	115.48	109.97
20	c	507	CLA	C2C-C1C-NC	5.85	115.46	109.97
20	C	504	CLA	C4A-NA-C1A	5.85	109.34	106.71
23	f	101	SQD	O8-S-C6	5.84	115.04	105.74
20	b	618	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
20	d	402	CLA	C2C-C1C-NC	5.81	115.41	109.97
20	c	510	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
22	b	619	BCR	C7-C8-C9	-5.78	117.50	126.23
20	a	407	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	b	615	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	b	614	CLA	C4A-NA-C1A	5.76	109.30	106.71
20	c	501	CLA	CHD-C4C-C3C	-5.75	116.38	124.84
20	b	605	CLA	C1C-C2C-C3C	-5.74	100.92	106.96
20	a	404	CLA	C1C-C2C-C3C	-5.73	100.93	106.96
21	A	403	PHO	C3D-C2D-C1D	-5.73	97.52	105.87
20	b	610	CLA	C2C-C1C-NC	5.73	115.34	109.97
20	C	511	CLA	C2C-C1C-NC	5.71	115.33	109.97
20	C	505	CLA	C2C-C1C-NC	5.71	115.32	109.97
20	B	604	CLA	C1C-C2C-C3C	-5.69	100.97	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	609	CLA	C2C-C1C-NC	5.68	115.29	109.97
20	B	616	CLA	C2C-C1C-NC	5.68	115.29	109.97
32	b	624	HTG	C1'-S1-C1	5.68	110.71	100.09
20	B	602	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
20	B	610	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	A	412	SQD	O9-S-C6	5.67	113.67	106.94
20	d	404	CLA	C2C-C1C-NC	5.65	115.26	109.97
20	b	605	CLA	O2D-CGD-O1D	-5.58	112.93	123.84
20	c	513	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
37	e	102	HEM	CBD-CAD-C3D	-5.55	102.25	112.48
20	b	614	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
20	b	609	CLA	C2C-C1C-NC	5.54	115.16	109.97
34	c	523	LMT	C1'-O5'-C5'	5.53	124.55	113.69
20	d	403	CLA	C4A-NA-C1A	5.51	109.18	106.71
23	a	409	SQD	C1-O5-C5	-5.51	102.88	113.69
20	b	611	CLA	C2C-C1C-NC	5.50	115.12	109.97
20	C	507	CLA	O2D-CGD-CBD	5.50	121.04	111.27
38	H	101	RRX	C24-C23-C22	-5.50	117.93	126.23
23	l	101	SQD	O6-C1-C2	5.48	116.86	108.30
20	b	607	CLA	CAC-C3C-C4C	5.48	131.91	124.81
20	c	501	CLA	C2C-C1C-NC	5.47	115.10	109.97
20	B	612	CLA	C4A-NA-C1A	5.46	109.16	106.71
20	C	504	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
20	B	611	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
20	B	604	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
20	c	506	CLA	C4A-NA-C1A	5.42	109.14	106.71
32	C	521	HTG	C1-O5-C5	5.41	122.56	112.58
23	A	406	SQD	O6-C1-C2	5.40	116.73	108.30
20	b	614	CLA	CAC-C3C-C4C	5.40	131.81	124.81
32	v	210	HTG	C1'-S1-C1	5.39	110.47	100.16
20	D	402	CLA	C4A-NA-C1A	5.39	109.13	106.71
24	C	524	LMG	O7-C10-C11	5.36	123.04	111.50
35	D	406	DGD	O2G-C1B-C2B	5.35	123.04	111.50
32	B	622	HTG	C1'-S1-C1	5.35	110.09	100.09
20	b	608	CLA	C2C-C1C-NC	5.35	114.98	109.97
21	a	405	PHO	C3D-C2D-C1D	-5.35	98.08	105.87
20	a	407	CLA	O2D-CGD-CBD	5.33	120.74	111.27
20	b	612	CLA	O2D-CGD-CBD	5.33	120.73	111.27
20	b	613	CLA	C2C-C1C-NC	5.32	114.95	109.97
20	c	503	CLA	C2C-C1C-NC	5.31	114.94	109.97
20	C	502	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
20	a	407	CLA	CAC-C3C-C4C	5.26	131.63	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	f	101	SQD	O8-S-O7	5.24	124.09	111.27
34	b	627	LMT	C3B-C4B-C5B	5.23	119.58	110.24
20	B	609	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
22	D	405	BCR	C24-C23-C22	-5.22	118.35	126.23
20	B	606	CLA	C2C-C1C-NC	5.21	114.85	109.97
20	C	501	CLA	O2D-CGD-O1D	-5.21	113.66	123.84
20	c	505	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
20	C	506	CLA	O2D-CGD-CBD	5.19	120.50	111.27
23	A	412	SQD	O6-C1-C2	5.19	116.40	108.30
20	c	502	CLA	CAC-C3C-C4C	5.19	131.54	124.81
40	V	201	HEC	CBD-CAD-C3D	-5.18	102.93	112.49
20	b	606	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
21	D	403	PHO	C3D-C2D-C1D	-5.18	98.32	105.87
20	c	507	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
20	c	507	CLA	O2D-CGD-CBD	5.18	120.47	111.27
22	B	617	BCR	C7-C8-C9	-5.16	118.44	126.23
22	D	405	BCR	C7-C8-C9	-5.16	118.44	126.23
20	A	401	CLA	C1D-CHD-C4C	-5.16	115.75	122.56
20	B	611	CLA	C2C-C1C-NC	5.15	114.80	109.97
34	c	523	LMT	C1B-O5B-C5B	5.15	123.80	113.69
20	D	402	CLA	CAC-C3C-C4C	5.15	131.49	124.81
20	d	404	CLA	C4A-NA-C1A	5.15	109.02	106.71
20	C	505	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
20	a	403	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
20	B	610	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
20	b	610	CLA	CAC-C3C-C4C	5.13	131.46	124.81
20	C	501	CLA	C2C-C1C-NC	5.12	114.77	109.97
20	d	404	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
20	c	512	CLA	O2D-CGD-CBD	5.11	120.35	111.27
20	B	601	CLA	C2C-C1C-NC	5.11	114.76	109.97
20	b	604	CLA	C2C-C1C-NC	5.10	114.75	109.97
20	b	604	CLA	CMB-C2B-C3B	5.06	134.15	124.68
34	I	101	LMT	O1B-C4'-C3'	5.06	120.75	107.28
20	c	506	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
20	b	607	CLA	C1C-C2C-C3C	-5.01	101.69	106.96
20	c	505	CLA	C2C-C1C-NC	5.01	114.67	109.97
21	A	403	PHO	C2C-C1C-NC	5.01	117.34	109.79
32	v	210	HTG	O5-C1-C2	-4.99	104.03	110.31
20	b	607	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
20	c	507	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
20	C	509	CLA	C1C-C2C-C3C	-4.98	101.73	106.96
20	D	402	CLA	CHD-C4C-C3C	-4.96	117.55	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	513	CLA	C2C-C1C-NC	4.93	114.59	109.97
32	D	417	HTG	C1'-S1-C1	4.92	109.30	100.09
20	B	604	CLA	O2D-CGD-CBD	4.92	120.01	111.27
20	B	607	CLA	O2D-CGD-O1D	-4.92	114.22	123.84
20	a	407	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
20	B	614	CLA	CHD-C4C-C3C	-4.91	117.63	124.84
34	a	418	LMT	C3'-C4'-C5'	-4.89	99.72	110.93
20	a	407	CLA	CMD-C2D-C3D	4.88	133.81	124.68
20	c	501	CLA	O2D-CGD-CBD	4.87	119.93	111.27
20	c	502	CLA	C2C-C1C-NC	4.87	114.54	109.97
21	A	403	PHO	C2D-C1D-ND	4.87	117.13	109.79
20	B	605	CLA	C4A-NA-C1A	4.86	108.89	106.71
20	b	608	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
21	a	405	PHO	CMD-C2D-C1D	4.86	132.55	125.06
40	v	201	HEC	CBD-CAD-C3D	-4.85	103.54	112.49
20	b	615	CLA	C1-C2-C3	-4.85	117.65	126.04
23	A	406	SQD	C1-C2-C3	-4.84	99.91	110.00
20	c	506	CLA	C2C-C1C-NC	4.84	114.51	109.97
21	a	405	PHO	C2C-C1C-NC	4.83	117.08	109.79
27	D	412	PL9	C40-C39-C41	4.83	123.39	115.27
20	d	403	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
20	b	610	CLA	CHD-C4C-C3C	-4.82	117.76	124.84
20	b	605	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
20	b	615	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
20	B	611	CLA	O2D-CGD-CBD	4.78	119.76	111.27
20	D	401	CLA	C3C-C4C-NC	4.77	115.92	110.57
20	C	506	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
20	B	614	CLA	C4A-NA-C1A	4.76	108.85	106.71
20	D	402	CLA	C1C-C2C-C3C	-4.76	101.95	106.96
20	b	612	CLA	C2C-C1C-NC	4.75	114.42	109.97
20	B	608	CLA	C1C-C2C-C3C	-4.75	101.96	106.96
34	z	102	LMT	O1B-C4'-C3'	4.74	119.89	107.28
22	b	619	BCR	C24-C23-C22	-4.74	119.07	126.23
20	C	503	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
20	a	403	CLA	C1D-CHD-C4C	-4.73	116.31	122.56
20	c	512	CLA	CHD-C4C-C3C	-4.73	117.88	124.84
20	b	617	CLA	C2C-C1C-NC	4.73	114.41	109.97
20	C	501	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
20	b	610	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
36	D	407	LHG	O8-C23-O10	-4.71	111.72	123.59
20	a	404	CLA	O2D-CGD-CBD	4.70	119.62	111.27
20	b	613	CLA	CHD-C4C-C3C	-4.70	117.93	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	507	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
20	C	503	CLA	C2C-C1C-NC	4.70	114.38	109.97
22	c	514	BCR	C24-C23-C22	-4.69	119.14	126.23
20	B	604	CLA	C4A-NA-C1A	4.69	108.81	106.71
20	c	503	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
20	b	615	CLA	CHD-C4C-C3C	-4.68	117.96	124.84
20	c	508	CLA	C2C-C1C-NC	4.67	114.35	109.97
20	A	402	CLA	O2D-CGD-CBD	4.66	119.55	111.27
20	c	501	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
20	A	402	CLA	C3B-C4B-NB	4.66	115.23	109.21
21	a	405	PHO	C4C-C3C-C2C	-4.65	101.63	106.78
23	A	406	SQD	O47-C7-C8	4.63	121.49	111.50
20	c	501	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
20	D	402	CLA	CMD-C2D-C3D	4.60	133.29	124.68
21	a	406	PHO	C3D-C2D-C1D	-4.59	99.18	105.87
20	c	511	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
20	b	610	CLA	CMD-C2D-C3D	4.58	133.24	124.68
20	c	504	CLA	C2C-C1C-NC	4.58	114.26	109.97
20	b	617	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
20	C	513	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
20	C	508	CLA	C2C-C1C-NC	4.56	114.24	109.97
23	a	409	SQD	C1-C2-C3	-4.55	100.52	110.00
20	b	608	CLA	O2D-CGD-CBD	4.55	119.35	111.27
20	c	503	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
20	c	511	CLA	C2C-C1C-NC	4.55	114.23	109.97
21	a	405	PHO	C3C-C4C-NC	4.54	117.32	110.28
36	D	407	LHG	O8-C23-C24	4.54	126.15	111.91
20	C	512	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	A	404	CLA	C4-C3-C5	4.54	122.90	115.27
20	D	401	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
20	C	504	CLA	CHD-C4C-C3C	-4.54	118.17	124.84
20	b	617	CLA	CMD-C2D-C3D	4.53	133.15	124.68
22	b	621	BCR	C24-C23-C22	-4.52	119.40	126.23
20	c	511	CLA	O2D-CGD-CBD	4.52	119.30	111.27
20	d	403	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
20	B	602	CLA	CHD-C4C-NC	4.51	131.31	124.20
20	c	509	CLA	CHD-C4C-C3C	-4.51	118.21	124.84
20	a	404	CLA	CAC-C3C-C4C	4.51	130.66	124.81
22	B	619	BCR	C38-C26-C25	-4.50	119.48	124.53
24	c	518	LMG	O7-C10-C11	4.49	121.18	111.50
20	b	609	CLA	C4-C3-C5	4.48	122.81	115.27
20	B	601	CLA	CAC-C3C-C4C	4.48	130.62	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	613	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
20	b	603	CLA	CHD-C4C-C3C	-4.48	118.26	124.84
20	a	403	CLA	CHD-C4C-NC	4.48	131.26	124.20
20	b	603	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
20	C	510	CLA	O2D-CGD-CBD	4.47	119.21	111.27
21	A	403	PHO	C3C-C4C-NC	4.46	117.19	110.28
20	b	614	CLA	C3C-C4C-NC	4.46	115.57	110.57
20	b	606	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
20	C	510	CLA	CHD-C4C-NC	4.45	131.21	124.20
20	b	616	CLA	C1-C2-C3	-4.44	118.36	126.04
20	C	505	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
21	a	405	PHO	C2D-C1D-ND	4.44	116.49	109.79
20	D	404	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
20	B	612	CLA	C1D-CHD-C4C	-4.42	116.72	122.56
20	c	511	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
32	b	602	HTG	C1'-S1-C1	4.42	108.35	100.09
35	d	416	DGD	O2G-C1B-C2B	4.41	121.02	111.50
32	b	601	HTG	C1'-S1-C1	4.41	108.35	100.09
20	c	504	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
20	c	513	CLA	C2C-C1C-NC	4.41	114.11	109.97
20	d	404	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
20	c	502	CLA	CMD-C2D-C3D	4.41	132.93	124.68
20	A	402	CLA	CHD-C4C-C3C	-4.40	118.36	124.84
20	C	503	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
20	B	614	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
27	A	411	PL9	C53-C6-C1	4.40	123.98	114.99
20	B	616	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
20	b	609	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
20	C	501	CLA	C4A-NA-C1A	4.38	108.68	106.71
20	B	607	CLA	O2D-CGD-CBD	4.38	119.05	111.27
20	C	502	CLA	C2C-C1C-NC	4.37	114.07	109.97
20	C	507	CLA	C2C-C1C-NC	4.37	114.07	109.97
20	B	602	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
23	A	412	SQD	C1-O5-C5	-4.37	105.10	113.69
20	d	402	CLA	C4-C3-C5	4.37	122.62	115.27
20	c	510	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
20	b	612	CLA	C4A-NA-C1A	4.36	108.66	106.71
20	B	608	CLA	CHD-C4C-C3C	-4.35	118.44	124.84
20	a	403	CLA	CAC-C3C-C4C	4.35	130.46	124.81
20	C	511	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	b	622	SQD	O47-C7-C8	4.34	120.86	111.50
20	b	616	CLA	O2D-CGD-CBD	4.34	118.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	617	BCR	C15-C14-C13	-4.34	121.12	127.31
40	v	201	HEC	CMB-C2B-C1B	-4.34	121.80	128.46
20	C	508	CLA	CAC-C3C-C4C	4.33	130.43	124.81
20	b	606	CLA	O2D-CGD-CBD	4.33	118.96	111.27
32	c	520	HTG	C1'-S1-C1	4.33	108.19	100.09
20	B	606	CLA	CMD-C2D-C3D	4.32	132.76	124.68
20	A	401	CLA	CAC-C3C-C4C	4.32	130.41	124.81
20	b	617	CLA	CAC-C3C-C4C	4.32	130.41	124.81
20	C	503	CLA	O2D-CGD-CBD	4.31	118.93	111.27
20	D	401	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	K	101	BCR	C33-C5-C6	-4.31	119.69	124.53
20	d	402	CLA	C4A-NA-C1A	4.31	108.64	106.71
20	b	604	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
20	B	603	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
20	C	503	CLA	C4A-NA-C1A	4.30	108.64	106.71
20	B	601	CLA	CHD-C4C-C3C	-4.30	118.52	124.84
20	C	501	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
21	D	403	PHO	C2D-C1D-ND	4.28	116.25	109.79
20	C	504	CLA	O2D-CGD-CBD	4.28	118.87	111.27
20	c	509	CLA	C2C-C1C-NC	4.28	113.98	109.97
20	c	506	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
20	B	604	CLA	C3B-C4B-NB	4.27	114.73	109.21
24	B	620	LMG	O7-C10-C11	4.27	120.70	111.50
20	b	616	CLA	C2C-C1C-NC	4.27	113.97	109.97
22	t	101	BCR	C29-C28-C27	-4.26	101.86	111.38
23	A	412	SQD	O47-C7-C8	4.26	120.68	111.50
20	c	510	CLA	C2C-C1C-NC	4.26	113.96	109.97
20	B	612	CLA	CHD-C4C-NC	4.25	130.91	124.20
32	V	202	HTG	C1-C2-C3	-4.25	102.19	110.59
21	a	406	PHO	C1-C2-C3	-4.25	118.69	126.04
32	c	521	HTG	C1-O5-C5	4.25	120.41	112.58
20	B	605	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
20	D	404	CLA	C2C-C1C-NC	4.24	113.95	109.97
20	b	613	CLA	O2D-CGD-CBD	4.24	118.80	111.27
20	b	607	CLA	CMC-C2C-C1C	4.23	131.48	125.04
20	c	512	CLA	C2C-C1C-NC	4.23	113.94	109.97
32	V	202	HTG	C1-O5-C5	-4.23	104.78	112.58
20	B	612	CLA	C2C-C1C-NC	4.22	113.92	109.97
20	A	401	CLA	C4-C3-C5	4.21	122.36	115.27
21	A	403	PHO	C4D-ND-C1D	-4.21	99.19	106.76
34	z	102	LMT	C1B-O1B-C4'	4.21	128.38	117.96
20	c	512	CLA	C1-C2-C3	-4.21	118.77	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	508	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
20	A	404	CLA	C2C-C1C-NC	4.20	113.91	109.97
20	b	612	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
20	C	506	CLA	C2C-C1C-NC	4.20	113.91	109.97
20	C	509	CLA	O2D-CGD-CBD	4.20	118.72	111.27
20	D	401	CLA	CMC-C2C-C1C	4.19	131.42	125.04
20	b	608	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
20	B	605	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
35	C	516	DGD	O3G-C3G-C2G	-4.18	100.82	110.90
20	C	512	CLA	CHD-C4C-C3C	-4.17	118.70	124.84
20	B	615	CLA	O2D-CGD-CBD	4.17	118.68	111.27
34	b	627	LMT	O5'-C5'-C4'	4.16	118.53	109.75
22	K	102	BCR	C7-C8-C9	-4.15	119.96	126.23
20	b	617	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
20	C	512	CLA	C1-O2A-CGA	4.14	127.31	116.44
21	A	403	PHO	C2B-C1B-NB	4.14	116.04	109.79
20	c	513	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
20	B	606	CLA	C1D-CHD-C4C	-4.14	117.10	122.56
35	H	102	DGD	O1G-C1A-O1A	-4.14	113.15	123.59
22	d	405	BCR	C11-C10-C9	-4.14	121.41	127.31
20	b	606	CLA	C3C-C4C-NC	4.14	115.21	110.57
23	b	622	SQD	O7-S-C6	4.13	111.85	106.94
20	b	617	CLA	C1D-CHD-C4C	-4.13	117.11	122.56
20	b	611	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
20	A	402	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
20	B	606	CLA	CAC-C3C-C4C	4.11	130.15	124.81
20	B	602	CLA	O2A-CGA-CBA	4.11	124.81	111.91
22	B	619	BCR	C24-C23-C22	-4.10	120.03	126.23
20	b	611	CLA	CAC-C3C-C4C	4.10	130.13	124.81
20	B	610	CLA	CAC-C3C-C4C	4.10	130.13	124.81
23	a	401	SQD	O47-C7-C8	4.10	120.34	111.50
20	c	502	CLA	O2D-CGD-CBD	4.10	118.55	111.27
24	b	623	LMG	O7-C10-C11	4.10	120.33	111.50
23	F	101	SQD	O9-S-C6	4.10	111.81	106.94
20	c	510	CLA	C4D-C3D-CAD	4.09	110.75	108.47
20	B	603	CLA	CMB-C2B-C3B	4.09	132.33	124.68
35	C	516	DGD	O2G-C1B-C2B	4.09	120.31	111.50
23	F	101	SQD	O6-C1-C2	4.08	114.68	108.30
20	b	603	CLA	C2C-C1C-NC	4.08	113.80	109.97
20	C	512	CLA	CMD-C2D-C3D	4.08	132.31	124.68
21	D	403	PHO	C2B-C1B-NB	4.06	115.92	109.79
23	A	406	SQD	O9-S-C6	4.05	111.75	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	616	CLA	CMD-C2D-C3D	4.05	132.25	124.68
20	B	608	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
20	b	614	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
20	a	404	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
20	a	403	CLA	C2C-C1C-NC	4.04	113.76	109.97
20	C	508	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
20	c	511	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
34	b	627	LMT	C1'-O5'-C5'	4.04	121.61	113.69
20	b	607	CLA	C4-C3-C5	4.04	122.06	115.27
34	a	418	LMT	O5B-C5B-C6B	4.03	116.46	106.44
20	A	402	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
20	C	507	CLA	CHD-C4C-C3C	-4.01	118.94	124.84
20	b	618	CLA	C4-C3-C5	4.01	122.02	115.27
20	D	401	CLA	CMB-C2B-C3B	4.01	132.18	124.68
20	B	606	CLA	CHD-C4C-NC	4.01	130.52	124.20
20	c	513	CLA	CMD-C2D-C3D	4.00	132.16	124.68
20	b	605	CLA	O2D-CGD-CBD	4.00	118.37	111.27
20	B	616	CLA	C1D-CHD-C4C	-4.00	117.28	122.56
20	D	402	CLA	O2D-CGD-CBD	3.99	118.36	111.27
20	b	609	CLA	CAC-C3C-C4C	3.99	129.99	124.81
20	d	404	CLA	CHD-C4C-NC	3.99	130.49	124.20
20	B	616	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
20	B	609	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
21	a	406	PHO	C2D-C1D-ND	3.98	115.80	109.79
20	b	616	CLA	CHB-C4A-NA	3.98	130.02	124.51
20	B	615	CLA	C2C-C1C-NC	3.98	113.70	109.97
23	a	401	SQD	C1-O5-C5	-3.98	105.89	113.69
20	B	610	CLA	C3C-C4C-NC	3.97	115.03	110.57
20	b	604	CLA	C1-C2-C3	-3.97	119.17	126.04
20	C	512	CLA	C2C-C1C-NC	3.97	113.69	109.97
20	b	616	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
20	C	513	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
20	b	607	CLA	C3C-C4C-NC	3.95	115.00	110.57
20	C	509	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
24	b	623	LMG	C9-C8-C7	-3.95	102.45	111.79
20	b	606	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
20	c	504	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	c	509	CLA	C4D-C3D-CAD	3.94	110.67	108.47
20	b	610	CLA	O2A-CGA-O1A	-3.93	113.69	123.59
20	A	404	CLA	CHD-C4C-C3C	-3.92	119.07	124.84
20	b	604	CLA	CMD-C2D-C3D	3.92	132.02	124.68
32	B	621	HTG	C1'-S1-C1	3.92	107.43	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	406	PHO	C4C-C3C-C2C	-3.92	102.44	106.78
34	c	523	LMT	O5B-C5B-C4B	3.92	116.81	109.69
20	C	513	CLA	O2A-CGA-CBA	3.91	124.18	111.91
22	D	405	BCR	C29-C30-C25	3.91	116.50	110.48
20	A	401	CLA	C3B-C4B-NB	3.91	114.26	109.21
20	C	510	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
27	A	411	PL9	C20-C19-C21	3.91	121.84	115.27
20	b	607	CLA	O2D-CGD-CBD	3.91	118.21	111.27
34	b	628	LMT	O5'-C5'-C4'	3.91	117.99	109.75
20	b	618	CLA	C2C-C1C-NC	3.90	113.63	109.97
20	c	504	CLA	C3B-C4B-NB	3.90	114.25	109.21
20	B	607	CLA	CHD-C4C-NC	3.89	130.34	124.20
36	D	409	LHG	O4-P-O5	3.89	131.46	112.24
20	B	609	CLA	CMD-C2D-C3D	3.89	131.95	124.68
20	b	616	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
23	a	401	SQD	O6-C1-C2	3.88	114.35	108.30
20	d	403	CLA	C1D-CHD-C4C	-3.87	117.45	122.56
21	A	403	PHO	O2D-CGD-CBD	3.87	118.15	111.27
21	A	403	PHO	C4C-C3C-C2C	-3.87	102.50	106.78
20	C	513	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
23	l	101	SQD	O48-C23-C24	3.86	124.01	111.91
21	a	405	PHO	CAC-C3C-C4C	3.85	129.43	125.22
32	B	631	HTG	C3-C4-C5	3.85	117.11	110.24
27	d	412	PL9	C40-C39-C41	3.85	121.75	115.27
32	B	632	HTG	C1'-S1-C1	3.85	107.28	100.09
20	c	512	CLA	CHD-C4C-NC	3.84	130.26	124.20
20	D	401	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
20	c	512	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
20	B	610	CLA	OBD-CAD-C3D	-3.84	121.61	127.98
20	b	617	CLA	O2D-CGD-CBD	3.83	118.07	111.27
35	H	102	DGD	O1G-C1A-C2A	3.83	123.91	111.91
20	b	611	CLA	CHD-C4C-C3C	-3.82	119.22	124.84
20	c	505	CLA	O2D-CGD-CBD	3.82	118.05	111.27
20	C	505	CLA	O2D-CGD-CBD	3.82	118.05	111.27
20	c	510	CLA	CHD-C4C-NC	3.82	130.22	124.20
20	b	610	CLA	O2D-CGD-CBD	3.81	118.04	111.27
20	C	512	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
27	a	415	PL9	C53-C6-C1	3.81	122.78	114.99
20	B	615	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
20	c	506	CLA	O2D-CGD-CBD	3.80	118.03	111.27
23	A	406	SQD	C1-O5-C5	-3.80	106.23	113.69
20	B	601	CLA	O2D-CGD-O1D	-3.80	116.41	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	603	CLA	CHD-C4C-C3C	-3.80	119.26	124.84
20	B	610	CLA	C1-C2-C3	-3.80	119.48	126.04
20	B	612	CLA	C1-C2-C3	-3.80	119.48	126.04
24	a	410	LMG	O7-C10-C11	3.79	119.67	111.50
21	a	406	PHO	O2D-CGD-CBD	3.79	117.99	111.27
32	B	622	HTG	C1-C2-C3	3.78	118.06	110.59
21	a	406	PHO	C2B-C1B-NB	3.78	115.50	109.79
27	a	415	PL9	C30-C29-C31	3.78	121.63	115.27
21	D	403	PHO	CED-O2D-CGD	3.78	124.49	115.94
20	B	602	CLA	O2A-C1-C2	3.77	118.53	108.64
20	B	602	CLA	C2C-C1C-NC	3.75	113.49	109.97
20	B	601	CLA	O2D-CGD-CBD	3.74	117.91	111.27
20	B	605	CLA	O2D-CGD-CBD	3.73	117.90	111.27
20	c	510	CLA	O2D-CGD-CBD	3.73	117.89	111.27
20	a	403	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
20	c	501	CLA	CHD-C4C-NC	3.72	130.07	124.20
21	A	403	PHO	C1C-C2C-C3C	-3.72	102.24	106.51
20	B	603	CLA	O2D-CGD-CBD	3.72	117.87	111.27
20	C	506	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
20	C	502	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
34	c	523	LMT	O5'-C5'-C4'	3.71	117.58	109.75
35	c	515	DGD	O5D-C6D-C5D	-3.71	102.18	109.05
20	A	401	CLA	C7-C6-C5	-3.71	103.28	113.36
23	l	101	SQD	O47-C7-C8	3.70	119.48	111.50
24	c	519	LMG	O7-C10-C11	3.70	119.48	111.50
20	b	604	CLA	OBD-CAD-C3D	-3.70	121.83	127.98
20	B	614	CLA	C3B-C4B-NB	3.70	113.99	109.21
20	B	610	CLA	CMD-C2D-C3D	3.70	131.60	124.68
20	C	507	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
20	B	612	CLA	O2D-CGD-CBD	3.69	117.83	111.27
20	b	614	CLA	CMC-C2C-C1C	3.68	130.65	125.04
20	b	609	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	A	404	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	A	401	CLA	CHD-C4C-C3C	-3.68	119.44	124.84
20	B	601	CLA	CMD-C2D-C3D	3.67	131.55	124.68
20	c	504	CLA	O2D-CGD-CBD	3.67	117.79	111.27
21	D	403	PHO	C4C-C3C-C2C	-3.66	102.73	106.78
23	b	622	SQD	C3-C4-C5	3.66	116.77	110.24
20	a	407	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
22	d	405	BCR	C39-C30-C25	-3.65	104.38	110.30
22	t	101	BCR	C33-C5-C6	-3.65	120.43	124.53
20	b	613	CLA	C1C-C2C-C3C	-3.65	103.12	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	510	CLA	C4-C3-C5	3.65	121.41	115.27
20	B	610	CLA	CED-O2D-CGD	3.64	124.17	115.94
20	B	615	CLA	C4D-C3D-CAD	3.64	110.50	108.47
21	a	405	PHO	O2D-CGD-O1D	-3.64	116.72	123.84
20	b	617	CLA	CMC-C2C-C1C	3.64	130.58	125.04
20	b	615	CLA	CAC-C3C-C4C	3.63	129.52	124.81
22	B	617	BCR	C24-C23-C22	-3.62	120.76	126.23
35	c	515	DGD	O2G-C1B-C2B	3.62	119.31	111.50
35	h	101	DGD	O2G-C1B-C2B	3.62	119.31	111.50
27	a	415	PL9	O1-C4-C3	-3.62	116.73	120.72
20	C	513	CLA	O2D-CGD-CBD	3.62	117.69	111.27
20	d	402	CLA	C2A-C1A-CHA	-3.61	117.54	123.86
20	b	618	CLA	C3B-C4B-NB	3.61	113.88	109.21
20	c	503	CLA	C4-C3-C5	3.61	121.34	115.27
20	B	608	CLA	CBC-CAC-C3C	-3.61	102.49	112.43
32	B	621	HTG	C1-O5-C5	3.60	119.22	112.58
20	D	402	CLA	CHD-C4C-NC	3.60	129.88	124.20
20	c	501	CLA	C3B-C4B-NB	3.59	113.86	109.21
22	b	619	BCR	C33-C5-C6	-3.59	120.50	124.53
20	b	605	CLA	C4-C3-C5	3.59	121.31	115.27
20	C	509	CLA	C1-C2-C3	-3.59	119.84	126.04
20	C	506	CLA	C1-C2-C3	-3.59	119.84	126.04
20	a	404	CLA	C4A-NA-C1A	3.59	108.32	106.71
20	C	511	CLA	CHD-C4C-C3C	-3.58	119.57	124.84
20	c	509	CLA	CAC-C3C-C4C	3.58	129.46	124.81
20	d	402	CLA	C3B-C4B-NB	3.58	113.83	109.21
21	D	403	PHO	CAC-C3C-C4C	3.57	129.12	125.22
21	A	403	PHO	O2D-CGD-O1D	-3.57	116.86	123.84
20	B	602	CLA	O1D-CGD-CBD	-3.57	117.19	124.48
35	c	517	DGD	O1G-C1A-O1A	-3.56	114.60	123.59
32	C	534	HTG	C1'-S1-C1	3.56	106.75	100.09
20	d	404	CLA	C4-C3-C5	3.56	121.26	115.27
23	A	412	SQD	O48-C23-C24	3.56	123.08	111.91
20	B	606	CLA	CMB-C2B-C3B	3.56	131.34	124.68
20	A	401	CLA	C2C-C1C-NC	3.56	113.31	109.97
20	C	511	CLA	CMD-C2D-C3D	3.56	131.34	124.68
21	D	403	PHO	C4D-ND-C1D	-3.55	100.38	106.76
20	b	617	CLA	CHD-C4C-NC	3.55	129.79	124.20
20	d	404	CLA	C3B-C4B-NB	3.54	113.79	109.21
24	B	620	LMG	O8-C28-C29	3.54	123.02	111.91
20	B	601	CLA	C4A-NA-C1A	3.54	108.30	106.71
20	C	513	CLA	CMD-C2D-C3D	3.53	131.29	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	403	PHO	C1-C2-C3	-3.53	119.94	126.04
20	B	608	CLA	CMD-C2D-C3D	3.53	131.28	124.68
20	d	402	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
20	c	508	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
21	D	403	PHO	C2C-C1C-NC	3.53	115.11	109.79
20	B	605	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
20	D	404	CLA	CAC-C3C-C4C	3.52	129.38	124.81
20	B	606	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
22	C	514	BCR	C38-C26-C25	-3.51	120.59	124.53
22	b	620	BCR	C29-C30-C25	3.51	115.88	110.48
20	b	618	CLA	CAC-C3C-C4C	3.50	129.36	124.81
20	B	610	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
36	d	406	LHG	O8-C23-O10	-3.50	114.77	123.59
20	D	404	CLA	O2D-CGD-CBD	3.50	117.48	111.27
20	B	611	CLA	C3C-C4C-NC	3.50	114.49	110.57
20	b	618	CLA	CBC-CAC-C3C	-3.50	102.79	112.43
20	d	402	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
20	B	613	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
20	c	511	CLA	CMC-C2C-C1C	3.49	130.35	125.04
22	k	101	BCR	C7-C8-C9	-3.48	120.97	126.23
20	B	611	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
20	C	507	CLA	CHD-C4C-NC	3.48	129.68	124.20
38	H	101	RRX	C7-C8-C9	-3.48	120.98	126.23
21	a	405	PHO	C2B-C1B-NB	3.47	115.03	109.79
20	b	617	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
34	J	103	LMT	C3'-C4'-C5'	-3.47	104.05	110.24
36	d	406	LHG	O8-C23-C24	3.47	122.79	111.91
20	B	607	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
20	B	606	CLA	C3C-C4C-NC	3.46	114.45	110.57
21	a	406	PHO	C3C-C4C-NC	3.46	115.64	110.28
20	a	404	CLA	CMC-C2C-C1C	3.46	130.30	125.04
20	d	403	CLA	C3C-C4C-NC	3.46	114.45	110.57
20	b	605	CLA	CMC-C2C-C1C	3.45	130.30	125.04
20	B	615	CLA	C2A-C1A-CHA	-3.45	117.82	123.86
20	b	610	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
20	b	610	CLA	C1D-CHD-C4C	-3.45	118.00	122.56
20	B	608	CLA	C2A-C1A-CHA	-3.45	117.83	123.86
20	c	505	CLA	CAC-C3C-C4C	3.45	129.28	124.81
20	c	502	CLA	CHD-C4C-C3C	-3.45	119.77	124.84
22	b	619	BCR	C23-C22-C21	-3.44	113.66	118.94
20	b	618	CLA	CMD-C2D-C3D	3.44	131.12	124.68
20	b	604	CLA	C1-O2A-CGA	3.44	125.47	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	606	CLA	C1-C2-C3	-3.44	120.09	126.04
20	A	404	CLA	CHB-C4A-NA	3.44	129.27	124.51
23	b	622	SQD	O6-C1-C2	3.44	113.67	108.30
23	b	622	SQD	O5-C1-C2	-3.44	103.07	110.35
36	E	103	LHG	O7-C7-C8	3.44	122.69	111.91
22	b	620	BCR	C38-C26-C25	-3.44	120.67	124.53
20	b	608	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
20	b	604	CLA	C1B-CHB-C4A	-3.43	123.32	130.12
20	c	506	CLA	CHD-C4C-NC	3.43	129.61	124.20
23	l	101	SQD	C1-O5-C5	-3.43	106.96	113.69
40	v	201	HEC	CMB-C2B-C3B	3.43	129.85	125.82
24	B	620	LMG	O7-C10-O9	-3.42	115.43	123.70
20	b	616	CLA	C3B-C4B-NB	3.42	113.64	109.21
20	b	612	CLA	CMD-C2D-C3D	3.42	131.08	124.68
22	d	405	BCR	C29-C30-C25	3.42	115.75	110.48
20	b	608	CLA	CMD-C2D-C3D	3.42	131.07	124.68
20	b	603	CLA	C1D-CHD-C4C	-3.42	118.05	122.56
20	d	403	CLA	CBC-CAC-C3C	-3.41	103.03	112.43
40	v	201	HEC	C1D-C2D-C3D	-3.41	104.62	107.00
20	b	611	CLA	C4A-NA-C1A	3.41	108.24	106.71
23	A	406	SQD	O8-S-C6	3.41	111.17	105.74
21	A	403	PHO	CMB-C2B-C1B	3.41	130.31	125.06
34	b	627	LMT	O5B-C5B-C6B	3.40	114.90	106.44
20	c	502	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
22	B	618	BCR	C29-C30-C25	3.40	115.72	110.48
20	c	503	CLA	CMD-C2D-C3D	3.40	131.04	124.68
20	c	510	CLA	C4A-NA-C1A	3.40	108.23	106.71
20	a	407	CLA	CMB-C2B-C3B	3.40	131.03	124.68
23	F	101	SQD	C1-C2-C3	-3.39	102.93	110.00
20	C	502	CLA	C3B-C4B-NB	3.39	113.59	109.21
20	c	505	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
20	b	608	CLA	C1-O2A-CGA	3.38	125.32	116.44
27	A	411	PL9	C30-C29-C31	3.38	120.96	115.27
24	C	519	LMG	O7-C10-C11	3.38	118.79	111.50
20	B	609	CLA	O2D-CGD-CBD	3.38	117.27	111.27
20	c	510	CLA	C1D-CHD-C4C	-3.38	118.10	122.56
20	c	509	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
20	B	610	CLA	O2D-CGD-CBD	3.37	117.26	111.27
20	c	504	CLA	C4D-C3D-CAD	3.37	110.35	108.47
20	B	603	CLA	CMD-C2D-C3D	3.37	130.97	124.68
20	C	504	CLA	CHD-C4C-NC	3.36	129.50	124.20
24	C	519	LMG	O8-C28-C29	3.36	122.46	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	618	CLA	CHD-C4C-NC	3.36	129.49	124.20
20	B	608	CLA	CAC-C3C-C4C	3.36	129.16	124.81
20	C	507	CLA	C4-C3-C5	3.36	120.92	115.27
20	c	513	CLA	O2D-CGD-CBD	3.35	117.23	111.27
20	C	503	CLA	CMD-C2D-C3D	3.35	130.95	124.68
20	c	513	CLA	CHD-C4C-NC	3.35	129.49	124.20
20	B	609	CLA	C3B-C4B-NB	3.35	113.54	109.21
20	c	509	CLA	CHD-C4C-NC	3.35	129.48	124.20
32	b	624	HTG	O5-C1-C2	-3.34	106.11	110.31
20	D	402	CLA	CMB-C2B-C3B	3.34	130.94	124.68
20	C	505	CLA	CHD-C4C-NC	3.34	129.47	124.20
20	b	603	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
20	B	612	CLA	CMD-C2D-C3D	3.34	130.93	124.68
20	b	613	CLA	OBD-CAD-CBD	-3.34	121.13	125.89
22	b	621	BCR	C38-C26-C25	-3.33	120.78	124.53
32	B	631	HTG	O5-C5-C4	3.33	115.75	109.69
21	D	403	PHO	C3C-C4C-NC	3.33	115.45	110.28
20	B	604	CLA	CHC-C1C-NC	-3.33	119.15	124.20
20	a	404	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
24	c	518	LMG	C4-C3-C2	3.33	116.63	110.82
23	f	101	SQD	O48-C23-C24	3.32	122.33	111.91
38	H	101	RRX	C16-C15-C14	-3.32	116.67	123.47
20	b	604	CLA	CMC-C2C-C1C	3.32	130.09	125.04
20	c	509	CLA	C3B-C4B-NB	3.31	113.49	109.21
27	a	415	PL9	C25-C24-C26	3.31	120.84	115.27
20	B	615	CLA	CHB-C4A-NA	3.31	129.09	124.51
20	B	601	CLA	C3C-C4C-NC	3.31	114.28	110.57
34	B	625	LMT	O5'-C5'-C4'	3.31	115.70	109.69
22	K	102	BCR	C38-C26-C25	-3.30	120.82	124.53
20	c	511	CLA	CMD-C2D-C3D	3.30	130.86	124.68
20	B	604	CLA	C2A-C1A-CHA	-3.30	118.09	123.86
21	a	405	PHO	C1C-C2C-C3C	-3.30	102.72	106.51
20	c	505	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	b	622	SQD	O9-S-C6	3.30	110.86	106.94
22	K	102	BCR	C24-C23-C22	-3.30	121.26	126.23
20	a	403	CLA	CMD-C2D-C3D	3.30	130.84	124.68
20	b	618	CLA	CMB-C2B-C3B	3.29	130.84	124.68
20	c	512	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	c	504	CLA	CHD-C4C-NC	3.29	129.39	124.20
20	a	407	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
20	b	604	CLA	OBD-CAD-CBD	3.29	130.60	125.89
20	B	604	CLA	CHD-C4C-NC	3.29	129.38	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	101	BCR	C35-C13-C12	3.29	123.26	118.08
21	a	406	PHO	C2C-C1C-NC	3.29	114.75	109.79
20	C	509	CLA	C4-C3-C5	3.28	120.80	115.27
20	B	605	CLA	C3C-C4C-NC	3.28	114.25	110.57
24	c	519	LMG	O8-C28-C29	3.28	122.20	111.91
22	c	514	BCR	C32-C1-C6	-3.28	104.98	110.30
22	C	515	BCR	C7-C8-C9	-3.28	121.28	126.23
20	C	502	CLA	O2D-CGD-CBD	3.28	117.09	111.27
20	C	508	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
20	c	505	CLA	CMC-C2C-C1C	3.28	130.03	125.04
20	C	504	CLA	CMD-C2D-C3D	3.27	130.80	124.68
20	B	614	CLA	C2A-C1A-CHA	-3.27	118.14	123.86
20	c	504	CLA	CAC-C3C-C4C	3.27	129.05	124.81
27	D	412	PL9	C10-C9-C11	3.27	120.77	115.27
20	c	507	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
20	b	609	CLA	CMD-C2D-C3D	3.27	130.79	124.68
22	B	619	BCR	C2-C1-C6	3.27	115.51	110.48
20	b	616	CLA	CHD-C4C-NC	3.27	129.35	124.20
20	B	609	CLA	CMB-C2B-C3B	3.26	130.78	124.68
35	C	517	DGD	O2G-C1B-C2B	3.26	118.52	111.50
20	B	616	CLA	CMB-C2B-C3B	3.25	130.77	124.68
24	b	623	LMG	O8-C28-C29	3.25	122.12	111.91
20	c	508	CLA	CMD-C2D-C3D	3.25	130.75	124.68
20	B	613	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
22	T	101	BCR	C38-C26-C25	-3.24	120.89	124.53
20	b	607	CLA	CMB-C2B-C3B	3.24	130.75	124.68
20	b	618	CLA	C3C-C4C-NC	3.24	114.21	110.57
20	B	615	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	C	508	CLA	C4-C3-C5	3.24	120.72	115.27
35	c	516	DGD	O2G-C1B-C2B	3.24	118.48	111.50
20	b	603	CLA	CMD-C2D-C3D	3.24	130.73	124.68
20	c	513	CLA	CMB-C2B-C3B	3.24	130.73	124.68
22	a	408	BCR	C15-C16-C17	-3.23	116.85	123.47
20	C	501	CLA	CHD-C4C-NC	3.23	129.30	124.20
20	B	612	CLA	C3C-C4C-NC	3.23	114.20	110.57
20	c	508	CLA	O2D-CGD-CBD	3.23	117.01	111.27
20	b	612	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
21	A	403	PHO	C4A-NA-C1A	3.23	110.75	108.14
20	b	606	CLA	CMD-C2D-C3D	3.23	130.72	124.68
34	m	101	LMT	C1'-O5'-C5'	3.23	120.03	113.69
20	d	403	CLA	O2D-CGD-CBD	3.23	117.00	111.27
20	B	611	CLA	O2D-CGD-O1D	-3.23	117.53	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	401	CLA	C2A-C1A-CHA	-3.22	118.22	123.86
24	C	519	LMG	O1-C7-C8	-3.22	103.12	110.90
38	H	101	RRX	C10-C11-C12	-3.22	113.16	123.22
20	B	606	CLA	C3B-C4B-NB	3.22	113.38	109.21
20	b	610	CLA	CED-O2D-CGD	3.22	123.22	115.94
20	C	503	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	A	412	SQD	C1-C2-C3	-3.21	103.31	110.00
20	B	607	CLA	C4D-C3D-CAD	3.21	110.26	108.47
20	C	507	CLA	CBC-CAC-C3C	-3.21	103.59	112.43
20	A	401	CLA	OBD-CAD-C3D	-3.21	122.66	127.98
20	c	513	CLA	CMC-C2C-C1C	3.20	129.92	125.04
20	c	509	CLA	CMC-C2C-C1C	3.20	129.91	125.04
20	C	502	CLA	CHD-C4C-NC	3.20	129.25	124.20
20	c	503	CLA	CHD-C4C-NC	3.20	129.24	124.20
27	d	412	PL9	C7-C8-C9	-3.20	121.47	126.79
22	B	617	BCR	C33-C5-C6	-3.19	120.95	124.53
20	D	401	CLA	C3B-C4B-NB	3.19	113.33	109.21
20	B	607	CLA	C2C-C1C-NC	3.19	112.96	109.97
21	a	406	PHO	C4D-ND-C1D	-3.19	101.03	106.76
20	B	604	CLA	CMD-C2D-C3D	3.18	130.63	124.68
20	c	511	CLA	C1-O2A-CGA	3.18	124.80	116.44
20	C	504	CLA	CAC-C3C-C4C	3.18	128.94	124.81
20	B	607	CLA	CMB-C2B-C1B	3.18	133.35	128.46
23	b	622	SQD	O48-C23-C24	3.18	121.88	111.91
22	a	408	BCR	C29-C30-C25	3.18	115.37	110.48
20	C	501	CLA	C2A-C1A-CHA	-3.18	118.31	123.86
20	B	614	CLA	O2A-CGA-CBA	3.17	121.87	111.91
20	b	604	CLA	CMB-C2B-C1B	-3.17	123.58	128.46
20	B	609	CLA	CHD-C4C-NC	3.17	129.20	124.20
20	C	509	CLA	C3B-C4B-NB	3.17	113.31	109.21
22	D	405	BCR	C38-C26-C25	-3.17	120.97	124.53
21	A	403	PHO	C1C-NC-C4C	-3.17	100.54	106.51
20	C	502	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
20	C	512	CLA	C4-C3-C5	3.17	120.60	115.27
20	c	511	CLA	C4-C3-C5	3.17	120.60	115.27
20	B	603	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
20	B	602	CLA	C4D-C3D-CAD	3.16	110.23	108.47
20	b	616	CLA	C4D-C3D-CAD	3.16	110.23	108.47
20	b	612	CLA	C3B-C4B-NB	3.15	113.28	109.21
32	v	210	HTG	C1-C2-C3	-3.15	104.37	110.59
20	b	613	CLA	C3C-C4C-NC	3.15	114.10	110.57
35	c	517	DGD	O1G-C1A-C2A	3.15	121.79	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	619	BCR	C23-C24-C25	-3.15	118.36	127.20
22	T	101	BCR	C23-C24-C25	-3.15	118.36	127.20
27	d	412	PL9	O1-C4-C3	-3.14	117.26	120.72
20	b	606	CLA	C3B-C4B-NB	3.14	113.27	109.21
22	b	620	BCR	C8-C7-C6	-3.14	118.39	127.20
22	t	101	BCR	C12-C13-C14	-3.14	114.13	118.94
34	b	627	LMT	C4B-C3B-C2B	3.13	116.30	110.82
22	K	102	BCR	C34-C9-C8	3.13	123.01	118.08
20	b	618	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
22	B	619	BCR	C33-C5-C6	-3.13	121.01	124.53
20	a	403	CLA	C4-C3-C5	3.13	120.53	115.27
20	B	609	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	B	611	CLA	C1D-CHD-C4C	-3.13	118.43	122.56
20	B	612	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	b	603	CLA	CHD-C4C-NC	3.13	129.13	124.20
20	b	616	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
20	c	509	CLA	C1-C2-C3	-3.12	120.64	126.04
20	b	604	CLA	C16-C17-C18	-3.12	101.28	115.98
21	a	406	PHO	CMB-C2B-C1B	3.12	129.87	125.06
20	D	402	CLA	C3B-C4B-NB	3.12	113.24	109.21
20	C	510	CLA	C3B-C4B-NB	3.12	113.24	109.21
20	c	511	CLA	CHD-C4C-NC	3.11	129.11	124.20
34	B	625	LMT	C1-O1'-C1'	-3.11	108.68	113.84
27	a	415	PL9	C3-C4-C5	3.11	122.65	118.60
20	C	511	CLA	O2D-CGD-CBD	3.11	116.79	111.27
20	b	604	CLA	C4-C3-C5	3.10	120.49	115.27
20	b	603	CLA	C4D-C3D-CAD	3.10	110.20	108.47
20	B	603	CLA	C4D-C3D-CAD	3.10	110.20	108.47
32	b	625	HTG	C1-O5-C5	3.10	118.29	112.58
21	a	406	PHO	O2D-CGD-O1D	-3.09	117.79	123.84
20	D	402	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
20	C	502	CLA	CAC-C3C-C4C	3.09	128.82	124.81
22	C	514	BCR	C15-C14-C13	-3.09	122.90	127.31
20	b	616	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
27	d	412	PL9	C3-C4-C5	3.09	122.62	118.60
20	c	512	CLA	CBC-CAC-C3C	-3.08	103.93	112.43
20	c	505	CLA	CHD-C4C-NC	3.08	129.06	124.20
38	x	101	RRX	C16-C17-C18	-3.08	122.91	127.31
20	A	401	CLA	C3C-C4C-NC	3.08	114.02	110.57
20	b	612	CLA	CAC-C3C-C4C	3.08	128.80	124.81
27	d	412	PL9	C36-C37-C38	-3.08	101.77	111.88
20	D	402	CLA	CBC-CAC-C3C	-3.08	103.95	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	608	CLA	CMB-C2B-C3B	3.08	130.43	124.68
20	B	613	CLA	C2A-C1A-CHA	-3.08	118.48	123.86
21	D	403	PHO	O2D-CGD-O1D	-3.07	117.83	123.84
22	B	617	BCR	C20-C21-C22	-3.07	122.92	127.31
22	T	101	BCR	C7-C8-C9	-3.07	121.59	126.23
20	C	505	CLA	CMD-C2D-C3D	3.07	130.43	124.68
40	v	201	HEC	CMC-C2C-C1C	-3.07	123.74	128.46
20	b	612	CLA	C1D-CHD-C4C	-3.07	118.51	122.56
20	b	618	CLA	O1D-CGD-CBD	-3.07	118.20	124.48
34	T	102	LMT	C1'-C2'-C3'	3.07	116.38	110.00
34	b	627	LMT	C3'-C4'-C5'	3.07	117.96	110.93
22	b	621	BCR	C33-C5-C6	-3.07	121.08	124.53
20	D	404	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	j	101	LMG	O2-C2-C1	-3.06	102.60	110.05
20	a	407	CLA	C3C-C4C-NC	3.06	114.00	110.57
20	b	603	CLA	C1-O2A-CGA	3.06	124.48	116.44
20	d	403	CLA	C3B-C4B-NB	3.06	113.17	109.21
35	c	517	DGD	O2G-C1B-C2B	3.06	118.10	111.50
20	A	404	CLA	C3B-C4B-NB	3.06	113.17	109.21
24	c	518	LMG	O1-C1-C2	3.06	113.08	108.30
20	b	604	CLA	C2A-C1A-CHA	-3.06	118.52	123.86
24	B	620	LMG	C9-C8-C7	-3.05	104.57	111.79
20	d	402	CLA	CMD-C2D-C3D	3.05	130.38	124.68
22	d	405	BCR	C38-C26-C25	-3.05	121.10	124.53
20	C	510	CLA	C4-C3-C5	3.05	120.40	115.27
20	C	511	CLA	C4D-C3D-CAD	3.05	110.17	108.47
20	c	505	CLA	CMB-C2B-C3B	3.05	130.38	124.68
22	t	101	BCR	C15-C16-C17	-3.04	117.24	123.47
20	d	402	CLA	C4D-C3D-CAD	3.04	110.17	108.47
20	C	506	CLA	CAC-C3C-C4C	3.04	128.76	124.81
23	A	412	SQD	O6-C44-C45	-3.04	103.56	110.90
36	L	101	LHG	O4-P-O5	3.04	127.26	112.24
20	b	615	CLA	CHD-C4C-NC	3.03	128.98	124.20
20	c	502	CLA	OBD-CAD-C3D	-3.03	122.94	127.98
37	E	104	HEM	CMA-C3A-C4A	-3.03	123.80	128.46
20	B	603	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
20	a	403	CLA	CHC-C1C-C2C	-3.03	118.34	126.72
20	B	604	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	C	515	BCR	C23-C24-C25	-3.02	118.71	127.20
20	c	507	CLA	O2A-CGA-CBA	3.02	121.39	111.91
24	A	407	LMG	O7-C10-C11	3.02	118.01	111.50
20	B	601	CLA	C4C-C3C-C2C	-3.02	102.49	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	609	CLA	CMC-C2C-C1C	3.02	129.64	125.04
20	C	505	CLA	CMB-C2B-C3B	3.02	130.33	124.68
37	E	104	HEM	C1D-C2D-C3D	-3.02	104.89	107.00
20	b	610	CLA	CMB-C2B-C3B	3.02	130.33	124.68
20	b	606	CLA	CAC-C3C-C4C	3.02	128.73	124.81
35	C	517	DGD	O5D-C6D-C5D	3.02	114.63	109.05
20	b	614	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
20	C	512	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
20	c	507	CLA	CHD-C4C-NC	3.02	128.96	124.20
36	d	408	LHG	O7-C7-O9	-3.02	116.41	123.70
23	A	406	SQD	C44-O6-C1	-3.02	107.85	113.74
20	C	506	CLA	C4-C3-C5	3.01	120.34	115.27
22	b	619	BCR	C11-C10-C9	-3.01	123.01	127.31
20	b	617	CLA	C1-O2A-CGA	3.01	124.34	116.44
20	a	404	CLA	C3C-C4C-NC	3.01	113.94	110.57
32	C	521	HTG	O5-C5-C4	3.01	115.16	109.69
20	B	611	CLA	CAA-CBA-CGA	-3.01	104.47	113.25
20	c	501	CLA	C4D-C3D-CAD	3.01	110.15	108.47
20	C	506	CLA	CMC-C2C-C1C	3.00	129.61	125.04
22	A	405	BCR	C38-C26-C25	-3.00	121.16	124.53
20	C	507	CLA	C1-O2A-CGA	3.00	124.31	116.44
20	D	404	CLA	CMA-C3A-C4A	-3.00	103.72	111.77
20	b	605	CLA	C3C-C4C-NC	3.00	113.93	110.57
20	B	601	CLA	C1-O2A-CGA	3.00	124.31	116.44
20	C	508	CLA	CHB-C4A-NA	2.99	128.65	124.51
20	B	602	CLA	C2A-C1A-CHA	-2.99	118.62	123.86
22	a	408	BCR	C7-C8-C9	-2.99	121.71	126.23
20	d	402	CLA	CAC-C3C-C4C	2.99	128.69	124.81
20	C	508	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
20	B	615	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
20	b	604	CLA	C4D-C3D-CAD	2.99	110.14	108.47
20	b	613	CLA	CBC-CAC-C3C	-2.98	104.20	112.43
24	b	623	LMG	O8-C28-O10	-2.98	116.06	123.59
22	K	101	BCR	C38-C26-C25	-2.98	121.18	124.53
35	d	416	DGD	O1G-C1A-C2A	2.98	121.26	111.91
20	B	613	CLA	O2D-CGD-CBD	2.98	116.56	111.27
23	a	409	SQD	O47-C7-C8	2.98	117.92	111.50
20	B	614	CLA	C3C-C4C-NC	2.98	113.91	110.57
20	B	613	CLA	C4-C3-C5	2.98	120.28	115.27
20	b	614	CLA	O2D-CGD-CBD	2.98	116.56	111.27
36	E	103	LHG	O8-C23-C24	2.98	121.25	111.91
20	C	509	CLA	O2A-CGA-CBA	2.98	121.24	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	621	BCR	C7-C8-C9	-2.97	121.74	126.23
27	a	415	PL9	C7-C8-C9	-2.97	121.84	126.79
20	C	511	CLA	C3B-C4B-NB	2.97	113.05	109.21
20	c	510	CLA	C2A-C1A-CHA	-2.97	118.66	123.86
20	C	506	CLA	CMB-C2B-C3B	2.97	130.24	124.68
20	D	404	CLA	CMB-C2B-C3B	2.97	130.23	124.68
20	c	509	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
35	d	416	DGD	C3D-C4D-C5D	2.97	115.53	110.24
20	a	407	CLA	CMC-C2C-C1C	2.96	129.55	125.04
20	b	608	CLA	CHD-C4C-NC	2.96	128.87	124.20
34	a	418	LMT	C1B-O5B-C5B	2.96	119.50	113.69
20	b	616	CLA	CAC-C3C-C4C	2.95	128.64	124.81
20	c	513	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
32	B	621	HTG	O5-C5-C6	2.95	113.77	106.44
20	c	504	CLA	C4-C3-C5	2.95	120.23	115.27
20	B	606	CLA	O2D-CGD-CBD	2.95	116.51	111.27
20	c	508	CLA	C2A-C1A-CHA	-2.94	118.71	123.86
34	m	102	LMT	C3'-C4'-C5'	-2.94	104.18	110.93
20	b	611	CLA	C3C-C4C-NC	2.94	113.87	110.57
20	B	606	CLA	OBD-CAD-C3D	-2.94	123.10	127.98
35	c	515	DGD	O2G-C1B-O1B	-2.94	116.60	123.70
20	B	615	CLA	CHD-C4C-NC	2.94	128.83	124.20
27	D	412	PL9	C22-C23-C24	-2.94	120.59	127.66
20	c	502	CLA	C1D-CHD-C4C	-2.94	118.68	122.56
20	C	503	CLA	CHD-C4C-NC	2.93	128.83	124.20
34	a	418	LMT	O1'-C1'-C2'	2.93	112.88	108.30
20	B	601	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
27	A	411	PL9	C3-C4-C5	2.93	122.42	118.60
20	B	601	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
20	c	508	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	f	101	SQD	C1-O5-C5	2.93	119.43	113.69
20	B	612	CLA	C3B-C4B-NB	2.92	112.99	109.21
20	b	610	CLA	CHD-C4C-NC	2.92	128.81	124.20
20	b	614	CLA	CMD-C2D-C3D	2.92	130.15	124.68
27	A	411	PL9	C45-C44-C46	2.92	120.19	115.27
34	b	628	LMT	C1'-O5'-C5'	2.92	119.42	113.69
20	C	508	CLA	C5-C3-C2	-2.92	115.22	121.12
32	V	202	HTG	O5-C1-S1	2.92	117.24	110.14
20	c	505	CLA	CMD-C2D-C3D	2.91	130.13	124.68
20	C	504	CLA	C3B-C4B-NB	2.91	112.98	109.21
20	B	610	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
20	b	611	CLA	CBC-CAC-C3C	-2.91	104.40	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	513	CLA	C3C-C4C-NC	2.91	113.84	110.57
20	B	611	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
35	c	515	DGD	O3G-C3G-C2G	-2.91	103.88	110.90
34	b	627	LMT	O2'-C2'-C3'	-2.91	103.62	110.35
20	C	510	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
20	B	606	CLA	CMC-C2C-C1C	2.91	129.47	125.04
21	A	403	PHO	CAC-C3C-C4C	2.91	128.39	125.22
24	C	524	LMG	O8-C28-C29	2.91	121.03	111.91
32	D	417	HTG	O5-C5-C6	2.91	113.66	106.44
27	d	412	PL9	C36-C34-C33	-2.91	115.24	121.12
22	T	101	BCR	C15-C16-C17	-2.91	117.52	123.47
20	C	501	CLA	CMD-C2D-C3D	2.90	130.11	124.68
20	C	512	CLA	OBD-CAD-C3D	-2.90	123.16	127.98
20	c	509	CLA	CHB-C4A-NA	2.90	128.53	124.51
20	a	403	CLA	C5-C3-C2	-2.90	115.25	121.12
20	D	404	CLA	C6-C7-C8	-2.90	106.56	115.92
20	C	507	CLA	CMC-C2C-C1C	2.90	129.45	125.04
20	c	507	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
34	E	101	LMT	C1'-C2'-C3'	2.89	116.02	110.00
37	e	102	HEM	CAD-CBD-CGD	2.89	117.52	112.67
20	b	604	CLA	O2D-CGD-CBD	2.89	116.40	111.27
20	b	605	CLA	CAC-C3C-C4C	2.89	128.56	124.81
20	C	510	CLA	CMD-C2D-C3D	2.89	130.08	124.68
23	a	401	SQD	O48-C23-C24	2.89	120.97	111.91
22	t	101	BCR	C28-C27-C26	-2.89	108.92	114.08
32	B	631	HTG	C1-O5-C5	2.89	117.90	112.58
22	B	619	BCR	C32-C1-C6	-2.88	105.62	110.30
35	c	517	DGD	O3G-C3G-C2G	-2.88	103.94	110.90
21	a	406	PHO	C4-C3-C5	2.88	120.11	115.27
20	D	404	CLA	CHD-C4C-C3C	-2.88	120.61	124.84
20	b	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
20	c	502	CLA	C1-C2-C3	-2.88	121.06	126.04
38	x	101	RRX	C33-C5-C6	-2.88	121.30	124.53
20	c	504	CLA	CHB-C4A-NA	2.88	128.49	124.51
23	a	409	SQD	C44-O6-C1	-2.88	108.12	113.74
22	B	618	BCR	C11-C10-C9	-2.88	123.21	127.31
20	a	407	CLA	CED-O2D-CGD	2.88	122.44	115.94
35	c	516	DGD	O6E-C5E-C6E	2.87	113.58	106.44
22	k	102	BCR	C33-C5-C6	-2.87	121.30	124.53
20	c	503	CLA	OBD-CAD-C3D	-2.87	123.22	127.98
22	b	619	BCR	C15-C16-C17	-2.87	117.60	123.47
20	C	513	CLA	CMB-C2B-C3B	2.87	130.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	e	102	HEM	CMC-C2C-C3C	2.87	130.04	124.68
20	c	507	CLA	C3C-C4C-NC	2.87	113.78	110.57
20	c	502	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
20	B	606	CLA	C4-C3-C5	2.86	120.09	115.27
34	Z	101	LMT	C1'-O5'-C5'	2.86	119.31	113.69
20	b	618	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
20	D	402	CLA	C4-C3-C5	2.86	120.08	115.27
20	B	608	CLA	C3B-C4B-NB	2.86	112.91	109.21
27	D	412	PL9	C40-C39-C38	-2.86	116.34	123.68
20	C	506	CLA	C1D-CHD-C4C	-2.85	118.79	122.56
20	c	507	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
20	B	607	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
27	A	411	PL9	C17-C18-C19	-2.85	120.81	127.66
34	B	625	LMT	C1'-O5'-C5'	2.84	119.27	113.69
20	b	616	CLA	OBD-CAD-CBD	2.84	129.95	125.89
20	b	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
21	D	403	PHO	O2D-CGD-CBD	2.84	116.31	111.27
20	B	612	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	t	101	BCR	C11-C10-C9	-2.83	123.27	127.31
20	B	602	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
20	c	511	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
32	O	302	HTG	C1-O5-C5	2.83	117.80	112.58
22	D	405	BCR	C36-C18-C19	2.83	122.54	118.08
20	b	607	CLA	C1-C2-C3	-2.83	121.15	126.04
20	b	612	CLA	CMC-C2C-C1C	2.83	129.34	125.04
23	a	409	SQD	O8-S-C6	2.83	110.24	105.74
20	B	604	CLA	C3C-C4C-NC	2.82	113.74	110.57
20	c	505	CLA	C3C-C4C-NC	2.82	113.73	110.57
20	D	404	CLA	C3B-C4B-NB	2.82	112.86	109.21
21	a	405	PHO	C1C-NC-C4C	-2.82	101.20	106.51
32	v	210	HTG	O5-C1-S1	2.82	116.57	109.82
20	A	401	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
20	C	510	CLA	CAC-C3C-C4C	2.82	128.47	124.81
20	C	504	CLA	C1-C2-C3	-2.82	121.17	126.04
32	b	625	HTG	C1-C2-C3	2.82	116.15	110.59
20	b	608	CLA	CAC-C3C-C4C	2.82	128.46	124.81
22	k	101	BCR	C3-C4-C5	-2.82	109.05	114.08
20	b	605	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
20	c	511	CLA	C4D-C3D-CAD	2.81	110.04	108.47
20	a	404	CLA	C3B-C4B-NB	2.81	112.85	109.21
32	C	534	HTG	O5-C5-C4	2.81	114.80	109.69
21	D	403	PHO	CMB-C2B-C1B	2.81	129.39	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	609	CLA	CHD-C4C-NC	2.81	128.63	124.20
27	d	412	PL9	C21-C19-C18	-2.81	115.44	121.12
24	c	518	LMG	C3-C4-C5	2.81	115.25	110.24
34	B	626	LMT	O1'-C1'-C2'	2.81	112.68	108.30
20	c	512	CLA	C1-O2A-CGA	2.81	123.81	116.44
24	C	519	LMG	O8-C28-O10	-2.81	116.51	123.59
20	b	614	CLA	CMB-C2B-C3B	2.80	129.92	124.68
22	c	514	BCR	C21-C20-C19	-2.80	114.47	123.22
20	C	502	CLA	C16-C17-C18	-2.80	102.78	115.98
20	C	512	CLA	CED-O2D-CGD	2.80	122.27	115.94
20	B	602	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	A	406	SQD	O48-C23-O10	-2.80	116.53	123.59
20	B	611	CLA	C3B-C4B-NB	2.80	112.83	109.21
20	C	503	CLA	C5-C3-C2	-2.80	115.46	121.12
35	c	516	DGD	O1G-C1A-O1A	-2.80	116.53	123.59
22	B	619	BCR	C21-C20-C19	-2.80	114.49	123.22
20	b	613	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
20	B	611	CLA	CHD-C4C-NC	2.79	128.60	124.20
20	A	404	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
34	z	102	LMT	O5'-C1'-C2'	-2.79	104.44	110.35
20	C	511	CLA	C1-O2A-CGA	2.79	123.76	116.44
22	t	101	BCR	C34-C9-C8	2.78	122.46	118.08
20	C	510	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
21	A	403	PHO	CBC-CAC-C3C	-2.78	104.76	112.43
20	C	513	CLA	CHD-C4C-NC	2.78	128.59	124.20
20	B	603	CLA	C1-O2A-CGA	2.78	123.73	116.44
20	a	404	CLA	C1-C2-C3	-2.77	121.25	126.04
38	H	101	RRX	C16-C17-C18	-2.77	123.35	127.31
27	a	415	PL9	C40-C39-C41	2.77	119.93	115.27
35	c	517	DGD	O6D-C1D-O3G	-2.76	103.43	109.97
20	B	607	CLA	CAC-C3C-C2C	2.76	132.26	127.53
27	a	415	PL9	C42-C43-C44	-2.76	121.00	127.66
20	b	616	CLA	CMB-C2B-C1B	2.76	132.71	128.46
35	C	516	DGD	C3D-C4D-C5D	-2.76	105.31	110.24
38	x	101	RRX	C38-C26-C25	-2.76	121.43	124.53
22	K	101	BCR	C7-C8-C9	-2.76	122.07	126.23
20	b	618	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
20	b	605	CLA	CMD-C2D-C3D	2.76	129.84	124.68
20	B	606	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
20	c	506	CLA	CED-O2D-CGD	2.76	122.17	115.94
22	t	101	BCR	C21-C20-C19	-2.75	114.62	123.22
20	C	506	CLA	CHD-C4C-NC	2.75	128.54	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	412	PL9	C15-C14-C16	2.75	119.90	115.27
20	b	617	CLA	CMB-C2B-C3B	2.75	129.83	124.68
37	E	104	HEM	CMC-C2C-C3C	2.75	129.82	124.68
20	c	504	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
20	c	508	CLA	C3B-C4B-NB	2.75	112.77	109.21
20	B	605	CLA	CAC-C3C-C4C	2.75	128.38	124.81
20	c	506	CLA	C1D-CHD-C4C	-2.75	118.93	122.56
27	D	412	PL9	C36-C37-C38	-2.75	102.85	111.88
38	H	101	RRX	C34-C9-C8	2.74	122.40	118.08
32	B	632	HTG	C1-O5-C5	2.74	117.64	112.58
22	k	102	BCR	C11-C10-C9	-2.74	123.40	127.31
20	C	509	CLA	C3C-C4C-NC	2.74	113.64	110.57
20	c	508	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
20	A	404	CLA	CHD-C4C-NC	2.74	128.52	124.20
20	b	604	CLA	CHD-C4C-C3C	-2.74	120.81	124.84
38	x	101	RRX	C24-C23-C22	-2.74	122.10	126.23
23	F	101	SQD	O48-C23-C24	2.74	120.50	111.91
20	B	607	CLA	C3C-C4C-NC	2.74	113.64	110.57
20	D	401	CLA	CAC-C3C-C4C	2.73	128.36	124.81
20	B	610	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	b	622	SQD	C4-C3-C2	2.73	115.59	110.82
20	b	603	CLA	O2A-CGA-CBA	2.73	120.48	111.91
21	a	406	PHO	C4A-NA-C1A	2.73	110.35	108.14
21	a	406	PHO	CMA-C3A-C4A	-2.73	104.24	112.36
34	f	102	LMT	O5'-C5'-C6'	2.73	113.22	106.44
20	B	611	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
20	C	502	CLA	C3C-C4C-NC	2.72	113.63	110.57
27	D	412	PL9	C36-C34-C33	-2.72	115.60	121.12
20	A	401	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
20	c	513	CLA	O2A-CGA-CBA	2.72	120.45	111.91
34	B	626	LMT	O5'-C5'-C6'	2.72	113.20	106.44
20	B	604	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
20	b	609	CLA	C4D-C3D-CAD	-2.72	106.95	108.47
20	b	605	CLA	C3B-C4B-NB	2.72	112.73	109.21
22	c	514	BCR	C38-C26-C25	-2.72	121.47	124.53
20	C	501	CLA	C1-O2A-CGA	2.72	123.58	116.44
35	D	406	DGD	O1G-C1A-C2A	2.72	120.44	111.91
20	b	614	CLA	C3B-C4B-NB	2.72	112.73	109.21
20	C	506	CLA	C3C-C4C-NC	2.72	113.62	110.57
20	b	616	CLA	C4-C3-C5	2.72	119.84	115.27
20	b	616	CLA	OBD-CAD-C3D	-2.72	123.47	127.98
20	b	617	CLA	C4-C3-C5	2.72	119.84	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	609	CLA	C3C-C4C-NC	2.72	113.62	110.57
22	B	617	BCR	C21-C20-C19	-2.71	114.75	123.22
20	b	609	CLA	O2D-CGD-CBD	2.71	116.09	111.27
20	D	404	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
34	c	523	LMT	O1'-C1'-C2'	2.71	112.53	108.30
20	C	504	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	c	512	CLA	CBA-CAA-C2A	-2.71	105.87	113.86
36	d	406	LHG	C6-O8-C23	2.71	127.14	117.12
20	b	606	CLA	C4-C3-C5	2.71	119.82	115.27
20	c	503	CLA	C1-C2-C3	-2.70	121.36	126.04
20	A	404	CLA	CMD-C2D-C3D	2.70	129.74	124.68
20	c	508	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	B	606	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
23	a	409	SQD	O5-C1-C2	-2.70	104.63	110.35
20	B	614	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	B	603	CLA	CMA-C3A-C4A	-2.70	104.52	111.77
20	D	404	CLA	CBC-CAC-C3C	-2.70	105.00	112.43
22	t	101	BCR	C35-C13-C12	2.70	122.33	118.08
21	D	403	PHO	C1C-C2C-C3C	-2.69	103.42	106.51
24	C	519	LMG	C8-O7-C10	-2.69	111.17	117.79
20	C	504	CLA	C1-O2A-CGA	2.69	123.50	116.44
20	b	612	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	c	512	CLA	CMC-C2C-C1C	2.69	129.13	125.04
20	a	404	CLA	CMB-C2B-C3B	2.69	129.71	124.68
20	C	513	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
21	a	405	PHO	CMC-C2C-C1C	2.69	129.20	125.06
20	b	608	CLA	C1-C2-C3	-2.69	121.40	126.04
20	d	404	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
20	A	402	CLA	CAC-C3C-C2C	-2.68	122.94	127.53
22	K	102	BCR	C20-C21-C22	-2.68	123.48	127.31
20	c	508	CLA	C1-C2-C3	-2.68	121.40	126.04
20	b	617	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
20	B	605	CLA	C6-C5-C3	-2.68	106.42	113.45
24	C	524	LMG	O1-C1-C2	2.68	112.49	108.30
22	A	405	BCR	C15-C16-C17	-2.68	117.98	123.47
20	C	512	CLA	CHD-C4C-NC	2.68	128.43	124.20
32	c	521	HTG	O5-C5-C4	2.68	114.56	109.69
36	D	407	LHG	C11-C10-C9	-2.68	100.83	114.42
35	H	102	DGD	O3G-C3G-C2G	-2.68	104.44	110.90
22	t	101	BCR	C23-C24-C25	-2.67	119.69	127.20
20	C	504	CLA	OBD-CAD-C3D	-2.67	123.54	127.98
20	D	404	CLA	C4-C3-C5	2.67	119.77	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	401	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
20	c	512	CLA	O2A-CGA-CBA	2.67	120.29	111.91
20	d	403	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
22	B	618	BCR	C24-C23-C22	-2.67	122.20	126.23
20	C	506	CLA	CMD-C2D-C3D	2.67	129.67	124.68
20	b	614	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
21	D	403	PHO	OBD-CAD-C3D	-2.66	122.11	128.52
20	B	616	CLA	C4D-C3D-CAD	2.66	109.95	108.47
20	B	602	CLA	C4-C3-C2	-2.66	116.85	123.68
27	A	411	PL9	C25-C24-C26	2.66	119.75	115.27
20	c	501	CLA	C3C-C4C-NC	2.66	113.55	110.57
21	A	403	PHO	CHC-C1C-C2C	-2.66	119.05	125.73
22	t	101	BCR	C38-C26-C25	-2.66	121.54	124.53
20	d	403	CLA	CMD-C2D-C3D	2.66	129.65	124.68
35	h	101	DGD	O1G-C1A-O1A	-2.66	116.89	123.59
20	C	504	CLA	CMC-C2C-C1C	2.66	129.08	125.04
20	A	402	CLA	C4-C3-C5	2.66	119.74	115.27
20	b	616	CLA	C4-C3-C2	-2.65	116.87	123.68
20	b	612	CLA	CHD-C4C-NC	2.65	128.38	124.20
20	A	401	CLA	OBD-CAD-CBD	2.65	129.69	125.89
20	C	503	CLA	CAC-C3C-C4C	2.65	128.25	124.81
20	a	407	CLA	CHD-C4C-NC	2.65	128.38	124.20
20	b	604	CLA	C1D-CHD-C4C	-2.65	119.06	122.56
20	C	503	CLA	CMB-C2B-C3B	2.65	129.63	124.68
32	B	622	HTG	O2-C2-C3	-2.64	104.24	110.35
20	C	513	CLA	C4-C3-C5	2.64	119.72	115.27
20	b	605	CLA	C4A-NA-C1A	2.64	107.89	106.71
21	D	403	PHO	C4-C3-C5	2.64	119.71	115.27
27	a	415	PL9	C10-C9-C11	2.64	119.71	115.27
20	C	505	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
20	b	609	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
20	B	609	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	A	402	CLA	CHD-C4C-NC	2.63	128.34	124.20
20	D	401	CLA	C4-C3-C5	2.63	119.69	115.27
22	a	408	BCR	C35-C13-C12	2.63	122.22	118.08
20	C	505	CLA	C7-C6-C5	-2.63	106.22	113.36
20	b	606	CLA	C6-C5-C3	-2.63	106.57	113.45
20	a	403	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
36	D	408	LHG	C13-C12-C11	-2.63	101.10	114.42
20	b	609	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
20	b	615	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
21	a	406	PHO	CED-O2D-CGD	2.62	121.87	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	612	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
20	B	613	CLA	CMB-C2B-C3B	2.62	129.58	124.68
20	B	604	CLA	CMC-C2C-C1C	2.62	129.03	125.04
20	a	403	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
20	C	509	CLA	CMB-C2B-C1B	2.62	132.49	128.46
27	a	415	PL9	C37-C38-C39	-2.62	121.36	127.66
23	A	406	SQD	O3-C3-C4	2.62	116.40	110.35
20	d	402	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
23	b	622	SQD	O47-C7-O49	-2.61	117.39	123.70
20	B	613	CLA	CAC-C3C-C2C	-2.61	123.06	127.53
20	a	404	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	b	615	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
35	C	517	DGD	O2G-C1B-O1B	-2.60	117.41	123.70
20	c	508	CLA	C7-C6-C5	-2.60	106.30	113.36
20	B	607	CLA	C1-O2A-CGA	2.60	123.27	116.44
20	A	401	CLA	CHC-C1C-C2C	-2.60	119.53	126.72
22	j	102	BCR	C16-C17-C18	-2.60	123.60	127.31
35	H	102	DGD	C2G-O2G-C1B	-2.60	111.40	117.79
24	c	518	LMG	O8-C28-C29	2.60	120.06	111.91
23	F	101	SQD	O6-C44-C45	2.60	113.73	108.76
20	A	402	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
22	j	102	BCR	C33-C5-C6	-2.59	121.62	124.53
20	b	605	CLA	CHD-C4C-NC	2.59	128.29	124.20
20	b	618	CLA	O2A-CGA-CBA	2.59	120.04	111.91
20	b	606	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
20	B	607	CLA	C4-C3-C5	2.59	119.63	115.27
20	d	403	CLA	CAC-C3C-C4C	2.59	128.17	124.81
20	A	404	CLA	O2D-CGD-CBD	2.59	115.87	111.27
20	D	401	CLA	C1D-CHD-C4C	-2.59	119.14	122.56
20	C	507	CLA	C7-C6-C5	-2.59	106.33	113.36
20	B	613	CLA	CHD-C4C-NC	2.59	128.28	124.20
20	C	504	CLA	CMB-C2B-C3B	2.59	129.52	124.68
20	D	401	CLA	CAA-CBA-CGA	-2.59	105.69	113.25
22	A	405	BCR	C24-C23-C22	-2.59	122.33	126.23
24	c	519	LMG	O5-C6-C5	-2.59	102.42	111.29
20	B	614	CLA	C16-C15-C13	-2.58	107.56	115.92
20	B	605	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
40	V	201	HEC	CBA-CAA-C2A	-2.58	107.72	112.48
20	b	605	CLA	CHC-C1C-NC	-2.58	120.28	124.20
20	c	510	CLA	C3B-C4B-NB	2.58	112.55	109.21
20	C	508	CLA	O2D-CGD-CBD	2.58	115.86	111.27
20	c	506	CLA	C2A-C1A-CHA	-2.58	119.35	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	603	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
20	B	608	CLA	C3C-C4C-NC	2.58	113.46	110.57
20	B	613	CLA	C3C-C4C-NC	2.58	113.46	110.57
20	b	607	CLA	CMD-C2D-C3D	2.58	129.50	124.68
22	B	617	BCR	C34-C9-C10	-2.57	119.32	122.92
20	d	404	CLA	O2D-CGD-CBD	2.57	115.84	111.27
20	c	510	CLA	C3C-C4C-NC	2.57	113.46	110.57
22	k	101	BCR	C20-C21-C22	-2.57	123.64	127.31
32	b	601	HTG	C2'-C1'-S1	-2.57	104.09	112.40
20	c	503	CLA	CMC-C2C-C1C	2.57	128.96	125.04
32	C	534	HTG	C1-O5-C5	2.57	117.32	112.58
21	a	406	PHO	CHD-C4C-C3C	-2.57	119.28	124.49
20	B	614	CLA	O2A-CGA-O1A	-2.57	117.12	123.59
20	c	510	CLA	CMC-C2C-C1C	2.57	128.95	125.04
20	b	610	CLA	C3B-C4B-NB	2.56	112.53	109.21
20	b	607	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
20	c	503	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
34	E	101	LMT	C4'-C3'-C2'	2.56	115.30	110.82
35	C	518	DGD	O2G-C1B-C2B	2.56	117.02	111.50
20	b	607	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
20	C	506	CLA	C4D-C3D-CAD	2.56	109.90	108.47
20	b	608	CLA	C3C-C4C-NC	2.56	113.44	110.57
35	d	416	DGD	O6D-C5D-C4D	2.56	114.34	109.69
20	c	509	CLA	O2D-CGD-CBD	2.56	115.81	111.27
20	A	404	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
22	d	405	BCR	C10-C11-C12	-2.55	115.25	123.22
20	B	605	CLA	C3B-C4B-NB	2.55	112.51	109.21
20	B	612	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
24	C	524	LMG	O7-C10-O9	-2.55	117.54	123.70
22	C	515	BCR	C33-C5-C6	-2.55	121.67	124.53
22	t	101	BCR	C7-C6-C5	-2.55	115.29	121.46
20	d	404	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	B	605	CLA	CGD-CBD-CAD	-2.55	102.48	110.73
20	b	614	CLA	C4-C3-C5	2.55	119.56	115.27
20	b	603	CLA	O2A-C1-C2	2.54	115.32	108.64
20	b	603	CLA	OBD-CAD-C3D	-2.54	123.76	127.98
20	C	511	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
20	b	615	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
20	B	609	CLA	C1-O2A-CGA	2.54	123.11	116.44
20	B	607	CLA	O2A-CGA-CBA	2.54	119.88	111.91
20	D	401	CLA	O2D-CGD-CBD	2.54	115.78	111.27
22	D	405	BCR	C10-C11-C12	-2.54	115.29	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	610	CLA	OBD-CAD-CBD	2.54	129.52	125.89
20	b	613	CLA	CMB-C2B-C3B	2.54	129.42	124.68
20	A	404	CLA	CAC-C3C-C4C	2.54	128.10	124.81
20	C	502	CLA	CED-O2D-CGD	2.54	121.67	115.94
21	D	403	PHO	C4A-NA-C1A	2.54	110.19	108.14
34	I	101	LMT	C3'-C4'-C5'	-2.54	105.11	110.93
20	b	605	CLA	CMB-C2B-C3B	2.53	129.42	124.68
20	a	403	CLA	O2A-CGA-CBA	2.53	119.86	111.91
20	C	509	CLA	CAC-C3C-C4C	2.53	128.10	124.81
23	A	412	SQD	O48-C46-C45	2.53	115.80	108.43
24	B	620	LMG	O6-C5-C6	2.53	112.73	106.44
20	D	402	CLA	CMC-C2C-C1C	2.53	128.89	125.04
20	B	606	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	b	610	CLA	C3C-C4C-NC	2.53	113.41	110.57
20	B	616	CLA	OBD-CAD-C3D	-2.53	123.78	127.98
20	c	507	CLA	C3B-C4B-NB	2.53	112.48	109.21
20	B	603	CLA	CHD-C4C-NC	2.53	128.19	124.20
20	D	404	CLA	CED-O2D-CGD	2.53	121.65	115.94
24	A	407	LMG	O1-C1-C2	2.52	112.24	108.30
20	B	604	CLA	C4-C3-C5	2.52	119.52	115.27
20	B	614	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
20	c	504	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
20	b	611	CLA	C1-O2A-CGA	2.52	123.06	116.44
21	a	405	PHO	O2D-CGD-CBD	2.52	115.75	111.27
22	j	102	BCR	C38-C26-C25	-2.52	121.70	124.53
20	B	608	CLA	C4A-NA-C1A	2.52	107.84	106.71
20	D	404	CLA	C4D-C3D-CAD	2.52	109.88	108.47
20	a	404	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
20	b	614	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
20	b	605	CLA	C5-C3-C2	-2.52	116.02	121.12
20	c	512	CLA	CAC-C3C-C4C	2.52	128.08	124.81
22	c	514	BCR	C11-C10-C9	-2.52	123.72	127.31
34	T	102	LMT	O1'-C1'-C2'	-2.51	104.38	108.30
27	A	411	PL9	C15-C14-C16	2.51	119.50	115.27
20	C	507	CLA	OBD-CAD-C3D	-2.51	123.81	127.98
20	d	402	CLA	O2A-CGA-CBA	2.51	119.79	111.91
20	b	615	CLA	O2D-CGD-CBD	2.51	115.72	111.27
20	C	509	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
20	c	501	CLA	C2A-C1A-CHA	-2.51	119.48	123.86
20	c	508	CLA	C4-C3-C5	2.51	119.49	115.27
20	c	502	CLA	C16-C17-C18	-2.50	104.18	115.98
36	D	407	LHG	O4-P-O5	2.50	124.62	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	403	CLA	CMB-C2B-C3B	2.50	129.36	124.68
20	C	508	CLA	C3B-C4B-NB	2.50	112.44	109.21
20	b	609	CLA	C3B-C4B-NB	2.50	112.44	109.21
20	D	404	CLA	O2A-C1-C2	-2.50	102.07	108.64
20	b	610	CLA	C6-C5-C3	-2.50	106.91	113.45
20	C	510	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
22	d	405	BCR	C2-C1-C6	2.49	114.32	110.48
20	B	613	CLA	C3B-C4B-NB	2.49	112.43	109.21
20	b	607	CLA	CHC-C1C-NC	-2.49	120.42	124.20
22	t	101	BCR	C1-C6-C7	2.49	122.82	115.78
24	J	101	LMG	O8-C28-O10	-2.49	117.31	123.59
20	C	512	CLA	CAC-C3C-C4C	2.49	128.04	124.81
22	d	405	BCR	C34-C9-C10	-2.49	119.44	122.92
23	F	101	SQD	C1-O5-C5	-2.49	108.81	113.69
23	F	101	SQD	C3-C4-C5	2.49	114.67	110.24
20	c	505	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
20	B	616	CLA	O2D-CGD-CBD	2.49	115.69	111.27
20	B	610	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
23	a	409	SQD	C45-O47-C7	-2.48	111.67	117.79
22	j	102	BCR	C37-C22-C23	2.48	121.99	118.08
20	c	507	CLA	C4-C3-C5	2.48	119.45	115.27
20	c	505	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	K	101	BCR	C37-C22-C23	2.48	121.99	118.08
20	B	614	CLA	C7-C6-C5	-2.48	106.62	113.36
20	c	513	CLA	C4-C3-C5	2.48	119.44	115.27
20	c	502	CLA	CMB-C2B-C3B	2.48	129.32	124.68
20	B	615	CLA	CMA-C3A-C4A	-2.48	105.11	111.77
34	m	102	LMT	C1'-O5'-C5'	-2.48	108.82	113.69
24	c	518	LMG	C8-O7-C10	-2.48	111.69	117.79
20	B	607	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
22	T	101	BCR	C33-C5-C6	-2.47	121.75	124.53
34	Z	101	LMT	O1B-C4'-C3'	2.47	113.86	107.28
32	C	534	HTG	C1-C2-C3	-2.47	105.71	110.59
20	b	608	CLA	O2A-CGA-CBA	2.47	119.67	111.91
27	a	415	PL9	C45-C44-C46	2.47	119.43	115.27
20	c	502	CLA	C3B-C4B-NB	2.47	112.40	109.21
20	B	616	CLA	C11-C10-C8	-2.47	107.94	115.92
27	d	412	PL9	C31-C32-C33	-2.47	103.77	111.88
20	b	617	CLA	C11-C10-C8	-2.47	107.94	115.92
20	a	407	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
20	C	508	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
20	B	615	CLA	OBD-CAD-C3D	-2.46	123.89	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	608	CLA	CHD-C4C-NC	2.46	128.09	124.20
23	A	406	SQD	C45-O47-C7	-2.46	111.73	117.79
20	c	511	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
21	a	405	PHO	C4D-ND-C1D	-2.46	102.34	106.76
20	c	510	CLA	CMD-C2D-C3D	2.46	129.28	124.68
22	K	101	BCR	C24-C23-C22	-2.46	122.52	126.23
34	z	102	LMT	O1B-C1B-C2B	2.46	114.47	108.10
20	b	615	CLA	O2A-CGA-CBA	2.46	119.61	111.91
20	C	505	CLA	CAC-C3C-C4C	2.46	128.00	124.81
20	B	615	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
35	C	518	DGD	O3G-C3G-C2G	-2.45	104.98	110.90
20	b	618	CLA	C4-C3-C2	-2.45	117.39	123.68
36	E	103	LHG	O7-C7-O9	-2.45	117.40	123.59
27	A	411	PL9	C7-C3-C4	2.45	118.87	116.88
20	b	616	CLA	CMC-C2C-C1C	2.45	128.77	125.04
20	a	404	CLA	CHC-C1C-C2C	-2.45	119.95	126.72
27	d	412	PL9	C25-C24-C26	2.45	119.39	115.27
24	a	410	LMG	O8-C28-C29	2.45	119.59	111.91
20	B	601	CLA	C4-C3-C5	2.45	119.39	115.27
22	K	101	BCR	C8-C9-C10	-2.45	115.19	118.94
20	C	510	CLA	C1-C2-C3	-2.44	121.82	126.04
20	d	404	CLA	CAC-C3C-C4C	2.44	127.98	124.81
22	k	101	BCR	C38-C26-C25	-2.44	121.78	124.53
20	D	401	CLA	CMB-C2B-C1B	-2.44	124.71	128.46
20	b	604	CLA	CAC-C3C-C4C	2.44	127.98	124.81
20	B	602	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
34	I	101	LMT	O3'-C3'-C4'	2.44	116.41	109.94
20	C	506	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
20	a	403	CLA	C1-C2-C3	-2.44	121.83	126.04
20	b	609	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
22	C	515	BCR	C38-C26-C25	-2.44	121.79	124.53
20	A	402	CLA	C1-O2A-CGA	2.44	122.83	116.44
32	c	520	HTG	C3-C4-C5	2.44	114.58	110.24
20	B	616	CLA	OBD-CAD-CBD	2.44	129.37	125.89
23	A	412	SQD	O5-C1-C2	-2.43	105.20	110.35
20	b	612	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
20	c	506	CLA	CAC-C3C-C4C	2.43	127.97	124.81
20	a	404	CLA	O2A-CGA-CBA	2.43	119.53	111.91
35	D	406	DGD	C3D-C4D-C5D	2.43	114.57	110.24
20	C	507	CLA	CMB-C2B-C3B	2.43	129.22	124.68
35	H	102	DGD	C6D-C5D-C4D	2.43	117.16	112.09
20	a	407	CLA	CBC-CAC-C3C	-2.43	105.74	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	505	CLA	O2A-CGA-CBA	2.43	119.52	111.91
22	b	621	BCR	C16-C15-C14	-2.43	118.50	123.47
27	D	412	PL9	C35-C34-C36	2.43	119.35	115.27
20	B	609	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
20	B	616	CLA	CHD-C4C-NC	2.42	128.02	124.20
20	c	507	CLA	CMD-C2D-C3D	2.42	129.21	124.68
22	B	617	BCR	C8-C7-C6	-2.42	120.40	127.20
20	b	609	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
20	b	615	CLA	C7-C6-C5	-2.42	106.79	113.36
38	H	101	RRX	C38-C26-C25	-2.42	121.81	124.53
23	A	406	SQD	O48-C23-C24	2.41	119.49	111.91
20	c	502	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
22	B	619	BCR	C23-C22-C21	-2.41	115.24	118.94
20	b	611	CLA	CMD-C2D-C3D	2.41	129.19	124.68
20	c	511	CLA	O2A-CGA-CBA	2.41	119.48	111.91
27	A	411	PL9	C32-C33-C34	-2.41	121.85	127.66
35	D	406	DGD	O2G-C1B-O1B	-2.41	117.87	123.70
32	d	401	HTG	C1-C2-C3	2.41	115.35	110.59
20	B	614	CLA	CMB-C2B-C3B	2.41	129.19	124.68
37	e	102	HEM	C4C-C3C-C2C	2.41	108.58	106.90
27	D	412	PL9	C53-C6-C1	2.41	119.92	114.99
36	E	103	LHG	O4-P-O5	2.41	120.11	110.68
20	B	601	CLA	C3B-C4B-NB	2.41	112.32	109.21
22	D	405	BCR	C15-C14-C13	-2.41	123.87	127.31
27	d	412	PL9	C42-C41-C39	-2.41	105.06	112.98
20	b	613	CLA	C1-C2-C3	-2.41	121.88	126.04
35	h	101	DGD	C6D-C5D-C4D	2.41	117.12	112.09
20	B	603	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
20	B	607	CLA	C3B-C4B-NB	2.41	112.32	109.21
27	d	412	PL9	C20-C19-C21	2.40	119.32	115.27
22	B	617	BCR	C16-C15-C14	-2.40	118.56	123.47
20	B	612	CLA	C4C-C3C-C2C	-2.40	103.41	106.90
22	B	618	BCR	C28-C27-C26	-2.40	109.80	114.08
23	l	101	SQD	O48-C23-O10	-2.40	117.55	123.59
20	B	603	CLA	O2A-CGA-CBA	2.40	119.42	111.91
35	c	516	DGD	O1G-C1A-C2A	2.40	119.42	111.91
20	B	616	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	c	519	LMG	O3-C3-C4	-2.39	104.81	110.35
24	j	101	LMG	C9-C8-C7	-2.39	106.13	111.79
35	H	102	DGD	O4D-C4D-C3D	-2.39	104.82	110.35
27	a	415	PL9	C20-C19-C21	2.39	119.29	115.27
20	B	611	CLA	CAC-C3C-C2C	2.39	131.62	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	403	CLA	CHC-C1C-NC	2.39	127.83	124.20
22	T	101	BCR	C12-C13-C14	-2.39	115.28	118.94
20	C	505	CLA	C3C-C4C-NC	2.39	113.25	110.57
22	K	102	BCR	C37-C22-C21	-2.39	119.58	122.92
20	b	609	CLA	O2A-CGA-CBA	2.39	119.39	111.91
23	A	412	SQD	O48-C23-O10	-2.39	117.57	123.59
20	C	513	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
27	a	415	PL9	C15-C14-C16	2.38	119.28	115.27
20	b	614	CLA	CHC-C1C-NC	-2.38	120.59	124.20
22	d	405	BCR	C2-C3-C4	2.38	116.70	111.38
20	c	501	CLA	CMD-C2D-C3D	2.38	129.14	124.68
27	A	411	PL9	O2-C1-C2	-2.38	116.32	121.78
28	b	640	DMS	C2-S-C1	2.38	110.69	98.44
20	b	611	CLA	CED-O2D-CGD	2.38	121.32	115.94
20	C	505	CLA	CMC-C2C-C1C	2.38	128.66	125.04
35	c	517	DGD	C3A-C2A-C1A	2.38	122.27	113.62
23	a	401	SQD	O9-S-C6	2.38	109.76	106.94
20	c	512	CLA	CMB-C2B-C3B	2.38	129.12	124.68
23	A	406	SQD	O9-S-O7	-2.37	105.73	113.95
20	b	608	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
20	c	513	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
20	B	612	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
22	d	405	BCR	C7-C8-C9	-2.37	122.65	126.23
20	d	403	CLA	CHC-C1C-C2C	-2.37	120.16	126.72
20	B	607	CLA	C1-C2-C3	-2.37	121.94	126.04
20	B	609	CLA	C6-C5-C3	-2.37	107.23	113.45
32	C	534	HTG	C3-C4-C5	2.37	114.47	110.24
20	A	402	CLA	C3C-C4C-NC	2.37	113.23	110.57
20	c	510	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
20	b	611	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
20	C	502	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
24	c	519	LMG	O7-C10-O9	-2.37	117.99	123.70
20	b	611	CLA	O2D-CGD-CBD	2.36	115.47	111.27
20	c	509	CLA	O2A-CGA-CBA	2.36	119.33	111.91
20	b	607	CLA	OBD-CAD-C3D	-2.36	124.06	127.98
20	B	611	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	B	616	CLA	C1-O2A-CGA	2.36	122.64	116.44
20	b	613	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
20	C	503	CLA	C4-C3-C5	2.36	119.24	115.27
20	b	605	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
34	Z	101	LMT	O1B-C4'-C5'	2.36	115.91	109.45
20	d	404	CLA	CMB-C2B-C1B	2.36	132.09	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	412	PL9	C11-C9-C8	-2.36	116.35	121.12
34	b	627	LMT	C2'-C3'-C4'	2.36	115.06	109.68
20	d	402	CLA	O1D-CGD-CBD	2.35	129.30	124.48
20	B	612	CLA	CMC-C2C-C1C	2.35	128.62	125.04
27	A	411	PL9	C16-C14-C13	-2.35	116.36	121.12
20	b	606	CLA	CMC-C2C-C1C	2.35	128.62	125.04
20	C	511	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	a	408	BCR	C8-C7-C6	-2.35	120.60	127.20
20	C	502	CLA	O2A-CGA-CBA	2.35	119.29	111.91
20	B	615	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
22	D	405	BCR	C28-C27-C26	-2.35	109.89	114.08
20	c	509	CLA	CMB-C2B-C3B	2.34	129.06	124.68
20	C	511	CLA	C4-C3-C5	2.34	119.21	115.27
22	B	618	BCR	C33-C5-C6	-2.34	121.90	124.53
22	B	619	BCR	C37-C22-C21	2.34	126.20	122.92
20	b	612	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
32	V	202	HTG	O2-C2-C1	2.34	114.56	110.27
20	C	501	CLA	CAC-C3C-C4C	2.34	127.84	124.81
36	d	408	LHG	O8-C23-O10	-2.34	117.69	123.59
24	c	519	LMG	O1-C7-C8	-2.34	105.26	110.90
20	D	404	CLA	O2A-CGA-CBA	2.34	119.25	111.91
20	c	506	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
20	b	605	CLA	O2A-CGA-CBA	2.34	119.24	111.91
36	d	408	LHG	O8-C23-C24	2.34	119.24	111.91
20	A	401	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
20	B	615	CLA	C4-C3-C5	2.33	119.19	115.27
37	e	102	HEM	CMB-C2B-C3B	2.33	129.04	124.68
23	a	409	SQD	O9-S-O7	-2.33	105.89	113.95
20	c	503	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
20	b	604	CLA	CMA-C3A-C4A	-2.33	105.52	111.77
20	b	605	CLA	C7-C6-C5	-2.33	107.04	113.36
20	b	616	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
21	a	406	PHO	CAA-C2A-C1A	-2.32	106.33	112.33
20	B	602	CLA	C1-O2A-CGA	2.32	122.54	116.44
27	A	411	PL9	O1-C4-C3	-2.32	118.16	120.72
20	B	614	CLA	CAC-C3C-C4C	2.32	127.82	124.81
36	d	408	LHG	O7-C7-C8	2.32	116.50	111.50
20	b	613	CLA	CHD-C4C-NC	2.32	127.86	124.20
22	C	514	BCR	C23-C24-C25	-2.32	120.69	127.20
27	D	412	PL9	C27-C28-C29	-2.31	122.09	127.66
20	C	504	CLA	C4-C3-C5	2.31	119.17	115.27
22	A	405	BCR	C37-C22-C21	2.31	126.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	514	BCR	C34-C9-C10	-2.31	119.68	122.92
21	a	405	PHO	C4A-NA-C1A	2.31	110.01	108.14
35	c	516	DGD	C6D-O5D-C1E	2.31	118.26	113.74
35	H	102	DGD	O2G-C1B-C2B	2.31	116.48	111.50
20	B	615	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
20	D	401	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
20	d	404	CLA	C6-C7-C8	-2.31	108.45	115.92
22	t	101	BCR	C33-C5-C4	2.31	118.06	113.62
24	J	101	LMG	O7-C10-C11	2.31	116.48	111.50
22	B	618	BCR	C30-C25-C26	-2.31	119.36	122.61
20	A	404	CLA	C5-C3-C2	-2.31	116.44	121.12
27	a	415	PL9	C35-C34-C36	2.31	119.16	115.27
20	b	617	CLA	OBD-CAD-C3D	-2.31	124.15	127.98
20	C	503	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
20	b	603	CLA	CED-O2D-CGD	2.31	121.16	115.94
34	z	102	LMT	O2'-C2'-C3'	2.31	115.68	110.35
27	A	411	PL9	C40-C39-C41	2.31	119.15	115.27
38	x	101	RRX	C16-C15-C14	-2.31	118.75	123.47
20	b	609	CLA	C4C-C3C-C2C	-2.31	103.54	106.90
23	A	406	SQD	O47-C7-O49	-2.30	118.14	123.70
20	b	617	CLA	C3B-C4B-NB	2.30	112.18	109.21
20	d	402	CLA	CMC-C2C-C1C	2.30	128.54	125.04
20	b	617	CLA	C6-C5-C3	-2.30	107.43	113.45
20	b	611	CLA	CHC-C1C-NC	-2.30	120.72	124.20
40	V	201	HEC	C3B-C4B-NB	-2.30	106.61	110.94
32	V	202	HTG	O5-C5-C6	2.30	112.14	106.44
20	B	613	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
34	M	101	LMT	C3'-C4'-C5'	-2.30	105.66	110.93
20	b	606	CLA	CMB-C2B-C3B	2.30	128.97	124.68
20	C	508	CLA	CHD-C4C-NC	2.29	127.82	124.20
35	d	416	DGD	O3G-C1D-C2D	2.29	111.88	108.30
32	d	401	HTG	C2'-C1'-S1	-2.29	104.99	112.40
20	c	506	CLA	C3B-C4B-NB	2.29	112.17	109.21
22	k	101	BCR	C8-C7-C6	-2.29	120.77	127.20
20	C	506	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
20	b	610	CLA	C4A-NA-C1A	2.29	107.73	106.71
21	A	403	PHO	CHD-C4C-NC	-2.29	120.15	124.93
22	k	102	BCR	C37-C22-C23	2.29	121.68	118.08
20	c	502	CLA	OBD-CAD-CBD	2.29	129.16	125.89
20	C	503	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
34	a	418	LMT	O1B-C4'-C5'	2.28	115.71	109.45
34	m	102	LMT	O1'-C1'-C2'	2.28	111.87	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	513	CLA	CHC-C1C-NC	-2.28	120.74	124.20
20	c	509	CLA	C4-C3-C5	2.28	119.11	115.27
20	B	603	CLA	CHB-C4A-NA	2.28	127.67	124.51
20	d	402	CLA	C1D-CHD-C4C	-2.28	119.55	122.56
24	C	519	LMG	O6-C5-C6	2.28	112.10	106.44
20	C	506	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
20	b	608	CLA	C3B-C4B-NB	2.28	112.15	109.21
20	c	501	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
20	B	603	CLA	C4-C3-C5	2.27	119.10	115.27
24	C	519	LMG	C9-C8-C7	-2.27	106.41	111.79
20	C	503	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
20	b	605	CLA	C1-O2A-CGA	2.27	122.40	116.44
35	c	515	DGD	O1G-C1G-C2G	-2.27	101.83	108.43
20	b	611	CLA	CMC-C2C-C1C	2.27	128.50	125.04
37	e	102	HEM	CMA-C3A-C4A	-2.27	124.97	128.46
20	C	509	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
20	B	606	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
20	c	509	CLA	CMD-C2D-C3D	2.27	128.92	124.68
20	c	503	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	D	405	BCR	C40-C30-C25	-2.27	106.62	110.30
20	c	509	CLA	C1-O2A-CGA	2.26	122.39	116.44
32	B	622	HTG	C1-O5-C5	2.26	116.75	112.58
20	b	616	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
20	C	510	CLA	CMC-C2C-C3C	2.26	132.26	126.12
36	d	407	LHG	O8-C23-O10	-2.26	117.88	123.59
20	B	601	CLA	O2A-CGA-CBA	2.26	119.00	111.91
22	j	102	BCR	C8-C9-C10	-2.26	115.48	118.94
20	B	610	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
20	d	403	CLA	CHD-C4C-NC	2.26	127.76	124.20
24	A	407	LMG	O8-C28-C29	2.26	118.99	111.91
21	D	403	PHO	CHD-C4C-C3C	-2.26	119.91	124.49
20	C	511	CLA	O2A-C1-C2	-2.26	102.70	108.64
20	c	511	CLA	CHC-C1C-NC	-2.26	120.78	124.20
20	C	503	CLA	CHC-C1C-NC	-2.26	120.78	124.20
22	t	101	BCR	C7-C8-C9	-2.26	122.83	126.23
20	B	602	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
20	C	507	CLA	CMD-C2D-C3D	2.25	128.90	124.68
20	c	506	CLA	C4D-C3D-CAD	2.25	109.73	108.47
20	b	610	CLA	O2A-CGA-CBA	2.25	118.98	111.91
24	c	519	LMG	O8-C28-O10	-2.25	117.91	123.59
20	b	616	CLA	CMD-C2D-C3D	2.25	128.89	124.68
20	c	506	CLA	C1B-CHB-C4A	-2.25	125.66	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	614	CLA	O2A-CGA-CBA	2.25	118.98	111.91
20	c	510	CLA	O2A-C1-C2	-2.25	102.72	108.64
20	B	616	CLA	C3B-C4B-NB	2.25	112.12	109.21
20	B	609	CLA	OBD-CAD-C3D	-2.25	124.24	127.98
20	B	611	CLA	O2A-CGA-CBA	2.25	118.97	111.91
21	a	405	PHO	CHD-C4C-C3C	-2.25	119.92	124.49
20	c	510	CLA	C4-C3-C2	-2.25	117.91	123.68
20	D	404	CLA	CHD-C4C-NC	2.25	127.75	124.20
23	l	101	SQD	O5-C5-C4	-2.25	105.61	109.69
20	c	501	CLA	CMC-C2C-C1C	2.25	128.46	125.04
35	C	516	DGD	O1G-C1A-O1A	-2.25	117.92	123.59
27	A	411	PL9	C37-C38-C39	-2.24	122.26	127.66
20	b	612	CLA	C4-C3-C5	2.24	119.04	115.27
37	E	104	HEM	CBA-CAA-C2A	-2.24	108.36	112.49
22	C	515	BCR	C24-C23-C22	-2.24	122.85	126.23
24	b	623	LMG	C13-C12-C11	2.24	121.24	113.19
36	d	407	LHG	O7-C7-O9	-2.24	118.29	123.70
20	B	616	CLA	C1-C2-C3	-2.24	122.17	126.04
34	a	418	LMT	O3'-C3'-C2'	2.24	115.52	110.35
20	C	511	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
20	C	511	CLA	CBC-CAC-C3C	-2.24	106.27	112.43
36	D	409	LHG	O8-C23-O10	-2.24	117.95	123.59
20	B	601	CLA	CMC-C2C-C3C	2.23	132.18	126.12
21	A	403	PHO	C7-C6-C5	-2.23	107.30	113.36
32	B	631	HTG	O5-C1-C2	-2.23	107.51	110.31
20	c	508	CLA	CHB-C4A-NA	2.23	127.59	124.51
40	V	201	HEC	CMB-C2B-C1B	-2.23	125.04	128.46
22	C	514	BCR	C29-C30-C25	2.22	113.91	110.48
35	C	517	DGD	O1G-C1A-O1A	-2.22	117.98	123.59
20	a	403	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
20	C	512	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
20	B	604	CLA	CMB-C2B-C3B	2.22	128.84	124.68
20	b	604	CLA	CHC-C1C-NC	-2.22	120.83	124.20
22	T	101	BCR	C20-C21-C22	-2.22	124.14	127.31
32	D	417	HTG	C1-C2-C3	2.22	114.97	110.59
36	d	406	LHG	O4-P-O5	2.22	123.22	112.24
35	c	517	DGD	C3E-C4E-C5E	-2.22	106.28	110.24
34	b	627	LMT	O2'-C2'-C1'	2.22	115.44	110.05
32	B	621	HTG	O4-C4-C3	-2.22	105.22	110.35
20	b	614	CLA	CHD-C4C-NC	2.22	127.70	124.20
20	C	510	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
22	k	102	BCR	C20-C21-C22	-2.22	124.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	101	LMG	O7-C10-C11	2.22	116.28	111.50
27	D	412	PL9	C11-C9-C8	-2.22	116.63	121.12
22	K	101	BCR	C10-C11-C12	-2.21	116.31	123.22
27	A	411	PL9	C51-C49-C50	2.21	119.49	114.60
20	b	603	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
20	d	404	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
35	C	516	DGD	C4A-C3A-C2A	-2.21	105.23	113.19
20	B	610	CLA	C7-C6-C5	-2.21	107.35	113.36
32	B	621	HTG	O3-C3-C4	-2.21	105.24	110.35
20	c	502	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	K	101	BCR	C7-C6-C5	-2.21	116.11	121.46
20	D	402	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
20	b	609	CLA	CGD-CBD-CAD	-2.21	103.59	110.73
20	B	610	CLA	CHD-C4C-NC	2.21	127.68	124.20
20	C	505	CLA	O2D-CGD-O1D	-2.21	119.53	123.84
20	c	513	CLA	C1D-CHD-C4C	-2.20	119.65	122.56
20	C	501	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
22	A	405	BCR	C39-C30-C25	-2.20	106.72	110.30
22	k	102	BCR	C24-C23-C22	-2.20	122.91	126.23
36	E	103	LHG	O7-C5-C6	2.20	115.12	108.61
24	c	518	LMG	O7-C10-O9	-2.20	118.38	123.70
32	b	625	HTG	C4-C3-C2	2.20	114.67	110.82
20	C	504	CLA	C4D-C3D-CAD	-2.20	107.24	108.47
34	z	102	LMT	C1B-O5B-C5B	2.20	118.00	113.69
22	K	101	BCR	C1-C6-C7	2.20	122.00	115.78
20	c	504	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
20	B	610	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
36	l	102	LHG	O4-P-O5	2.20	123.10	112.24
22	K	101	BCR	C21-C20-C19	-2.19	116.37	123.22
21	a	406	PHO	CHB-C1B-C2B	-2.19	120.21	125.73
34	z	102	LMT	O1'-C1'-C2'	2.19	111.73	108.30
23	f	101	SQD	O48-C23-O10	-2.19	118.06	123.59
20	C	503	CLA	C1D-CHD-C4C	-2.19	119.67	122.56
20	B	612	CLA	C4D-C3D-CAD	2.19	109.69	108.47
20	D	404	CLA	C6-C5-C3	-2.19	107.72	113.45
21	a	406	PHO	C1C-C2C-C3C	-2.19	104.00	106.51
20	B	608	CLA	CMC-C2C-C3C	2.19	132.05	126.12
20	b	613	CLA	O2A-C1-C2	-2.19	102.89	108.64
20	b	615	CLA	C3C-C4C-NC	2.18	113.02	110.57
20	C	507	CLA	CED-O2D-CGD	2.18	120.88	115.94
20	B	605	CLA	C4-C3-C5	2.18	118.94	115.27
22	t	101	BCR	C2-C1-C6	2.18	113.84	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	405	BCR	C29-C28-C27	-2.18	106.50	111.38
20	B	601	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
20	c	506	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
35	D	406	DGD	O6D-C5D-C4D	2.18	113.65	109.69
20	c	508	CLA	C1-O2A-CGA	2.18	122.16	116.44
22	b	620	BCR	C33-C5-C6	2.18	126.97	124.53
20	b	612	CLA	OBD-CAD-C3D	-2.18	124.36	127.98
27	A	411	PL9	C10-C9-C11	2.18	118.93	115.27
20	B	603	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
36	d	408	LHG	O4-P-O5	2.18	123.00	112.24
20	a	403	CLA	C3B-C4B-NB	2.18	112.03	109.21
20	B	612	CLA	C16-C15-C13	2.18	122.95	115.92
20	c	502	CLA	C6-C5-C3	-2.17	107.75	113.45
35	d	416	DGD	C4D-C3D-C2D	2.17	114.62	110.82
22	k	101	BCR	C24-C23-C22	-2.17	122.95	126.23
22	b	621	BCR	C23-C24-C25	-2.17	121.10	127.20
20	b	615	CLA	C3B-C4B-NB	2.17	112.02	109.21
20	b	611	CLA	C4-C3-C5	2.17	118.92	115.27
20	c	506	CLA	O2A-CGA-CBA	2.17	118.72	111.91
20	d	402	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
32	b	625	HTG	C3-C4-C5	-2.17	106.37	110.24
22	c	514	BCR	C29-C30-C25	2.17	113.82	110.48
21	a	406	PHO	CHD-C1D-ND	-2.17	120.07	124.58
32	B	621	HTG	O3-C3-C2	2.16	115.35	110.35
20	D	404	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
20	c	509	CLA	C4C-C3C-C2C	-2.16	103.74	106.90
20	c	503	CLA	CHC-C1C-NC	-2.16	120.92	124.20
32	B	622	HTG	C3-C4-C5	-2.16	106.38	110.24
34	B	625	LMT	C3'-C4'-C5'	2.16	114.09	110.24
20	b	618	CLA	C1-O2A-CGA	2.16	122.11	116.44
20	b	606	CLA	CGD-CBD-CAD	-2.16	103.74	110.73
20	C	513	CLA	C3B-C4B-NB	2.16	112.00	109.21
23	a	401	SQD	C44-O6-C1	-2.16	109.52	113.74
20	b	604	CLA	O2A-CGA-CBA	2.16	118.68	111.91
21	a	405	PHO	CHD-C1D-ND	-2.16	120.08	124.58
22	D	405	BCR	C30-C25-C24	2.16	121.88	115.78
20	C	509	CLA	CMD-C2D-C3D	2.16	128.72	124.68
22	b	619	BCR	C21-C20-C19	-2.16	116.48	123.22
20	d	402	CLA	C3C-C4C-NC	2.16	112.99	110.57
20	a	404	CLA	C4-C3-C5	2.16	118.90	115.27
22	b	621	BCR	C24-C25-C26	-2.16	116.24	121.46
20	c	501	CLA	CMB-C2B-C3B	2.16	128.71	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	BCR	C3-C4-C5	-2.15	110.23	114.08
22	k	102	BCR	C16-C17-C18	-2.15	124.24	127.31
20	b	613	CLA	CAC-C3C-C4C	2.15	127.60	124.81
20	a	407	CLA	C3B-C4B-NB	2.15	111.99	109.21
20	b	609	CLA	C3C-C4C-NC	2.15	112.98	110.57
20	b	604	CLA	C3C-C4C-NC	2.15	112.98	110.57
40	v	201	HEC	CMC-C2C-C3C	2.15	128.35	125.82
24	C	524	LMG	O6-C5-C6	2.15	111.78	106.44
20	c	501	CLA	O2A-CGA-CBA	2.15	118.64	111.91
36	l	102	LHG	O7-C7-C8	2.15	116.13	111.50
20	c	506	CLA	C1-C2-C3	-2.14	122.33	126.04
22	B	617	BCR	C40-C30-C25	-2.14	106.83	110.30
20	C	508	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	B	616	CLA	C3C-C4C-NC	2.14	112.97	110.57
32	B	623	HTG	O5-C1-C2	2.14	113.00	110.31
20	B	604	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
20	b	610	CLA	CHC-C1C-C2C	-2.14	120.81	126.72
20	C	509	CLA	CHC-C1C-NC	-2.14	120.96	124.20
22	t	101	BCR	C8-C9-C10	-2.14	115.66	118.94
20	B	602	CLA	C5-C3-C2	2.14	125.44	121.12
28	U	902	DMS	O-S-C1	2.14	117.44	106.54
20	c	510	CLA	CED-O2D-CGD	2.13	120.76	115.94
23	b	622	SQD	O48-C23-O10	-2.13	118.21	123.59
20	B	607	CLA	C7-C6-C5	-2.13	107.57	113.36
20	c	506	CLA	C3C-C4C-NC	2.13	112.96	110.57
20	D	402	CLA	CAC-C3C-C2C	-2.13	123.88	127.53
20	B	601	CLA	C4-C3-C2	-2.13	118.21	123.68
20	A	402	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
20	C	507	CLA	C3B-C4B-NB	2.13	111.97	109.21
20	B	603	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
23	f	101	SQD	O47-C7-O49	-2.13	118.73	122.96
20	C	504	CLA	C3D-CAD-CBD	2.13	110.41	107.61
27	a	415	PL9	C26-C24-C23	-2.13	116.81	121.12
20	b	609	CLA	CMB-C2B-C3B	2.13	128.66	124.68
27	d	412	PL9	C22-C23-C24	-2.13	122.54	127.66
23	a	401	SQD	C1-C2-C3	-2.13	105.57	110.00
24	j	101	LMG	O8-C28-O10	-2.13	118.23	123.59
24	J	101	LMG	O7-C10-O9	-2.12	118.57	123.70
27	D	412	PL9	C2-C3-C4	2.12	121.72	118.80
27	d	412	PL9	C35-C34-C36	2.12	118.84	115.27
20	c	510	CLA	O2A-CGA-CBA	2.12	118.56	111.91
20	C	502	CLA	C1-C2-C3	-2.12	122.38	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	408	BCR	C38-C26-C25	-2.12	122.15	124.53
20	B	602	CLA	C1D-CHD-C4C	-2.12	119.76	122.56
20	c	505	CLA	C7-C6-C5	-2.12	107.61	113.36
20	b	609	CLA	C5-C3-C2	-2.12	116.83	121.12
22	a	408	BCR	C33-C5-C6	-2.12	122.15	124.53
20	C	512	CLA	CHB-C4A-NA	2.12	127.44	124.51
32	C	521	HTG	O5-C1-C2	2.12	112.97	110.31
35	H	102	DGD	O5E-C6E-C5E	-2.12	104.03	111.29
20	C	502	CLA	C4C-C3C-C2C	-2.11	103.81	106.90
20	B	613	CLA	O2A-CGA-CBA	2.11	118.54	111.91
20	D	401	CLA	C14-C13-C15	-2.11	103.64	111.29
20	b	612	CLA	C3C-C4C-NC	2.11	112.94	110.57
20	B	609	CLA	C11-C10-C8	-2.11	109.09	115.92
20	C	508	CLA	O2A-CGA-CBA	2.11	118.54	111.91
20	b	606	CLA	CHD-C4C-NC	2.11	127.53	124.20
24	b	623	LMG	O7-C10-O9	-2.11	118.60	123.70
35	c	516	DGD	O2G-C1B-O1B	-2.11	118.60	123.70
20	c	513	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
20	d	404	CLA	C1-C2-C3	-2.11	122.39	126.04
20	c	505	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
35	c	515	DGD	C6D-O5D-C1E	-2.11	109.62	113.74
20	B	614	CLA	CMD-C2D-C3D	2.11	128.62	124.68
20	C	508	CLA	CMB-C2B-C3B	2.11	128.62	124.68
23	l	101	SQD	O8-S-C6	2.11	109.10	105.74
22	K	101	BCR	C15-C16-C17	-2.11	119.16	123.47
20	B	605	CLA	C4D-C3D-CAD	2.11	109.64	108.47
35	h	101	DGD	O3G-C3G-C2G	-2.11	105.82	110.90
20	b	617	CLA	C5-C3-C2	-2.11	116.86	121.12
20	A	401	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	c	507	CLA	CMC-C2C-C3C	2.10	131.83	126.12
20	b	615	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
22	T	101	BCR	C21-C20-C19	-2.10	116.65	123.22
22	k	102	BCR	C35-C13-C12	2.10	121.39	118.08
20	a	407	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
36	D	409	LHG	O8-C23-C24	2.10	118.50	111.91
20	B	615	CLA	CMD-C2D-C3D	2.10	128.61	124.68
34	E	101	LMT	O5'-C5'-C6'	2.10	111.66	106.44
20	B	605	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
20	b	613	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
20	d	404	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	C	511	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	j	102	BCR	C10-C11-C12	-2.10	116.67	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	101	BCR	C7-C6-C5	-2.10	116.38	121.46
20	c	504	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
20	A	401	CLA	C5-C3-C2	-2.10	116.88	121.12
20	C	511	CLA	CHD-C4C-NC	2.09	127.50	124.20
20	B	605	CLA	O2A-CGA-CBA	2.09	118.47	111.91
20	B	614	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
20	c	509	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	a	407	CLA	O2A-CGA-CBA	2.09	118.47	111.91
20	C	504	CLA	C7-C6-C5	-2.09	107.68	113.36
20	b	608	CLA	C7-C6-C5	-2.09	107.68	113.36
24	j	101	LMG	O8-C28-C29	2.09	118.47	111.91
27	a	415	PL9	C17-C18-C19	-2.09	122.62	127.66
21	A	403	PHO	CHD-C1D-ND	-2.09	120.23	124.58
20	B	609	CLA	C2A-C3A-C4A	-2.09	98.49	101.87
35	c	515	DGD	CDB-CCB-CBB	-2.09	103.82	114.42
22	B	618	BCR	C8-C7-C6	-2.09	121.34	127.20
35	C	518	DGD	O1G-C1A-C2A	2.09	118.46	111.91
37	e	102	HEM	CAA-CBA-CGA	2.09	116.17	112.67
20	b	607	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
20	b	618	CLA	CED-O2D-CGD	2.08	120.65	115.94
38	x	101	RRX	O2-C28-C27	-2.08	105.21	109.68
20	C	508	CLA	C4C-C3C-C2C	-2.08	103.86	106.90
20	C	509	CLA	CED-O2D-CGD	2.08	120.65	115.94
34	I	101	LMT	C2'-C3'-C4'	-2.08	104.93	109.68
34	z	102	LMT	O2B-C2B-C3B	2.08	115.16	110.35
34	m	102	LMT	O5B-C5B-C6B	2.07	111.59	106.44
22	b	619	BCR	C15-C14-C13	-2.07	124.35	127.31
20	c	501	CLA	C4-C3-C5	2.07	118.76	115.27
34	M	101	LMT	O5B-C5B-C6B	2.07	111.59	106.44
22	B	617	BCR	C16-C17-C18	-2.07	124.35	127.31
22	b	619	BCR	C37-C22-C21	2.07	125.82	122.92
36	d	407	LHG	O7-C7-C8	2.07	115.96	111.50
22	C	514	BCR	C11-C10-C9	-2.07	124.36	127.31
20	b	607	CLA	CHD-C4C-NC	2.07	127.46	124.20
20	A	401	CLA	C4D-C3D-CAD	2.07	109.62	108.47
20	B	613	CLA	C4C-C3C-C2C	-2.07	103.89	106.90
20	C	508	CLA	CMD-C2D-C3D	2.07	128.54	124.68
20	b	609	CLA	O2A-C1-C2	-2.07	103.21	108.64
20	b	617	CLA	OBD-CAD-CBD	2.07	128.85	125.89
20	d	402	CLA	CHD-C4C-C3C	-2.07	121.80	124.84
34	c	523	LMT	O5B-C1B-C2B	2.06	114.72	110.35
20	C	506	CLA	OBD-CAD-C3D	-2.06	124.55	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	609	CLA	O2A-CGA-CBA	2.06	118.39	111.91
35	c	515	DGD	O2D-C2D-C1D	-2.06	105.03	110.05
24	j	101	LMG	O1-C7-C8	-2.06	105.92	110.90
20	c	513	CLA	C1-O2A-CGA	2.06	121.85	116.44
20	b	613	CLA	C7-C6-C5	-2.06	107.76	113.36
20	b	618	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
20	B	613	CLA	CMD-C2D-C3D	2.06	128.53	124.68
20	c	508	CLA	C3C-C4C-NC	2.06	112.88	110.57
20	B	603	CLA	OBD-CAD-C3D	-2.06	124.57	127.98
20	C	510	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
22	T	101	BCR	C29-C30-C25	2.05	113.64	110.48
22	K	101	BCR	C20-C21-C22	-2.05	124.38	127.31
22	D	405	BCR	C32-C1-C6	2.05	113.63	110.30
20	b	613	CLA	C6-C5-C3	2.05	118.84	113.45
27	D	412	PL9	C31-C32-C33	-2.05	105.13	111.88
23	a	409	SQD	O48-C23-C24	2.05	118.35	111.91
23	f	101	SQD	O5-C5-C4	2.05	113.42	109.69
22	t	101	BCR	C40-C30-C25	-2.05	106.97	110.30
22	j	102	BCR	C1-C6-C7	2.05	121.58	115.78
22	b	619	BCR	C23-C24-C25	-2.05	121.44	127.20
22	C	514	BCR	C33-C5-C6	-2.05	122.23	124.53
23	b	622	SQD	O9-S-O7	-2.05	106.86	113.95
20	d	404	CLA	CMD-C2D-C3D	2.05	128.51	124.68
20	C	511	CLA	CAC-C3C-C4C	2.05	127.47	124.81
20	C	511	CLA	C3C-C4C-NC	2.05	112.87	110.57
38	H	101	RRX	C34-C9-C10	-2.05	120.06	122.92
28	C	532	DMS	O-S-C2	2.05	116.98	106.54
32	d	401	HTG	C1-O5-C5	2.05	116.35	112.58
22	b	619	BCR	C35-C13-C12	2.05	121.30	118.08
34	I	101	LMT	O1B-C4'-C5'	2.05	115.05	109.45
22	j	102	BCR	C35-C13-C14	-2.05	120.06	122.92
20	B	615	CLA	O2A-CGA-CBA	2.04	118.33	111.91
20	b	605	CLA	C2A-C3A-C4A	-2.04	98.57	101.87
20	a	404	CLA	C7-C6-C5	-2.04	107.81	113.36
35	C	516	DGD	O1G-C1G-C2G	-2.04	102.48	108.43
34	f	102	LMT	O1B-C4'-C5'	2.04	114.37	109.30
20	b	615	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	d	403	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
20	C	509	CLA	C1-O2A-CGA	2.04	121.80	116.44
20	c	502	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	B	603	CLA	C3B-C4B-NB	2.04	111.85	109.21
20	D	401	CLA	CHC-C1C-C2C	-2.04	121.08	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	407	LHG	O7-C7-O9	-2.04	118.78	123.70
20	b	603	CLA	CMC-C2C-C1C	2.04	128.14	125.04
32	O	302	HTG	C4-C3-C2	2.04	114.38	110.82
20	B	601	CLA	O2A-C1-C2	2.04	113.99	108.64
22	k	102	BCR	C15-C14-C13	-2.04	124.40	127.31
20	c	508	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
34	B	626	LMT	O3'-C3'-C4'	-2.04	105.64	110.35
24	C	519	LMG	O7-C10-O9	-2.04	118.78	123.70
22	C	514	BCR	C20-C21-C22	-2.03	124.41	127.31
34	I	101	LMT	C1B-O1B-C4'	2.03	123.00	117.96
21	a	406	PHO	CHC-C1C-C2C	-2.03	120.61	125.73
35	c	517	DGD	C3D-C4D-C5D	-2.03	106.61	110.24
20	c	506	CLA	O2A-C1-C2	2.03	113.98	108.64
27	d	412	PL9	C37-C36-C34	-2.03	106.29	112.98
22	j	102	BCR	C21-C20-C19	-2.03	116.87	123.22
22	A	405	BCR	C8-C7-C6	-2.03	121.50	127.20
22	b	621	BCR	C23-C22-C21	-2.03	115.83	118.94
20	b	616	CLA	O2A-CGA-CBA	2.03	118.27	111.91
20	c	503	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
22	d	405	BCR	C34-C9-C8	2.03	121.27	118.08
27	A	411	PL9	C7-C8-C9	-2.03	123.42	126.79
20	A	402	CLA	CHB-C4A-NA	2.03	127.31	124.51
20	c	508	CLA	OBD-CAD-C3D	-2.02	124.62	127.98
22	b	620	BCR	C15-C16-C17	-2.02	119.33	123.47
20	C	501	CLA	CHC-C1C-NC	-2.02	121.14	124.20
36	d	407	LHG	C13-C12-C11	-2.02	104.17	114.42
20	A	404	CLA	CBC-CAC-C3C	-2.02	106.86	112.43
20	C	512	CLA	C3C-C4C-NC	2.02	112.83	110.57
34	b	627	LMT	C1-O1'-C1'	2.02	117.19	113.84
22	k	102	BCR	C7-C8-C9	-2.02	123.19	126.23
32	B	622	HTG	O4-C4-C5	2.02	114.31	109.30
20	A	404	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
20	b	606	CLA	C1D-CHD-C4C	-2.02	119.90	122.56
22	t	101	BCR	C3-C4-C5	-2.02	110.48	114.08
20	c	512	CLA	CMD-C2D-C3D	2.01	128.45	124.68
20	b	606	CLA	CHB-C4A-NA	2.01	127.30	124.51
20	b	610	CLA	C5-C3-C2	-2.01	117.05	121.12
20	B	602	CLA	CED-O2D-CGD	2.01	120.49	115.94
22	K	101	BCR	C23-C22-C21	-2.01	115.86	118.94
36	d	406	LHG	C11-C10-C9	-2.01	104.22	114.42
37	E	104	HEM	C3C-C4C-NC	-2.01	107.15	110.94
22	C	515	BCR	C3-C4-C5	-2.01	110.49	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	502	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
32	B	631	HTG	C6-C5-C4	-2.01	108.30	113.00
22	D	405	BCR	C30-C25-C26	-2.01	119.79	122.61
20	c	510	CLA	CHB-C4A-NA	2.01	127.29	124.51
35	C	516	DGD	C1E-O6E-C5E	2.01	117.63	113.69
20	b	603	CLA	C1-C2-C3	-2.01	122.57	126.04
20	b	615	CLA	C12-C11-C10	-2.01	104.02	113.24
20	b	606	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
20	b	617	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	A	406	SQD	O5-C1-C2	-2.00	106.11	110.35
20	b	604	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
20	C	503	CLA	C7-C6-C5	-2.00	107.92	113.36
20	B	616	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
20	C	512	CLA	CMB-C2B-C3B	2.00	128.42	124.68
20	c	507	CLA	CED-O2D-CGD	2.00	120.46	115.94
20	a	407	CLA	C1-O2A-CGA	2.00	122.54	116.73
20	d	402	CLA	C5-C3-C2	-2.00	117.07	121.12

All (170) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	c	502	CLA	NC
20	c	502	CLA	NA
20	b	614	CLA	NA
20	b	614	CLA	NC
20	b	614	CLA	ND
20	D	404	CLA	NC
20	D	404	CLA	ND
20	D	404	CLA	NA
20	C	505	CLA	ND
20	C	505	CLA	NA
20	B	605	CLA	NC
20	B	605	CLA	ND
20	B	605	CLA	NA
20	a	407	CLA	NC
20	c	507	CLA	NC
20	c	507	CLA	ND
20	c	507	CLA	NA
20	A	401	CLA	NC
20	A	401	CLA	ND
20	A	401	CLA	NA
20	C	504	CLA	NC

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Mol	Chain	Res	Type	Atom
20	C	504	CLA	NA
20	B	608	CLA	NC
20	B	608	CLA	ND
20	B	608	CLA	NA
20	C	506	CLA	NC
20	C	506	CLA	ND
20	C	506	CLA	NA
20	B	616	CLA	NC
20	B	616	CLA	ND
20	B	616	CLA	NA
20	B	603	CLA	NC
20	B	603	CLA	ND
20	B	603	CLA	NA
20	c	509	CLA	NC
20	c	509	CLA	ND
20	c	509	CLA	NA
20	c	503	CLA	NC
20	C	513	CLA	NC
20	b	611	CLA	NC
20	b	611	CLA	NA
20	C	508	CLA	NC
20	C	508	CLA	ND
20	C	508	CLA	NA
20	d	403	CLA	NA
20	a	404	CLA	NC
20	a	404	CLA	NA
20	c	504	CLA	NC
20	c	504	CLA	ND
20	c	504	CLA	NA
20	D	402	CLA	NA
20	c	513	CLA	NC
20	B	606	CLA	NC
20	B	606	CLA	ND
20	B	606	CLA	NA
20	b	603	CLA	NC
20	b	603	CLA	ND
20	b	603	CLA	NA
20	b	608	CLA	NC
20	b	608	CLA	ND
20	b	608	CLA	NA
20	d	402	CLA	ND
20	d	402	CLA	NA

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Mol	Chain	Res	Type	Atom
20	B	601	CLA	NC
20	B	601	CLA	ND
20	B	601	CLA	NA
20	b	617	CLA	NC
20	b	617	CLA	ND
20	b	617	CLA	NA
20	A	402	CLA	NC
20	A	402	CLA	NA
20	c	505	CLA	ND
20	c	505	CLA	NA
20	C	511	CLA	NC
20	C	511	CLA	NA
20	B	611	CLA	NC
20	B	611	CLA	ND
20	B	611	CLA	NA
20	c	512	CLA	NC
20	c	512	CLA	ND
20	c	512	CLA	NA
20	C	502	CLA	NA
20	B	610	CLA	NC
20	B	610	CLA	ND
20	C	510	CLA	NC
20	C	510	CLA	ND
20	C	510	CLA	NA
20	C	512	CLA	NC
20	C	512	CLA	NA
20	C	512	CLA	ND
20	c	511	CLA	NC
20	c	511	CLA	ND
20	c	511	CLA	NA
20	B	613	CLA	NA
20	B	613	CLA	NC
20	B	613	CLA	ND
20	b	606	CLA	NC
20	b	606	CLA	ND
20	b	606	CLA	NA
20	b	609	CLA	NC
20	b	609	CLA	ND
20	b	609	CLA	NA
20	C	501	CLA	NC
20	C	501	CLA	ND
20	C	501	CLA	NA

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Mol	Chain	Res	Type	Atom
20	D	401	CLA	ND
20	B	602	CLA	NC
20	B	602	CLA	ND
20	A	404	CLA	NC
20	a	403	CLA	NC
20	a	403	CLA	ND
20	a	403	CLA	NA
20	c	510	CLA	NC
20	c	510	CLA	ND
20	c	510	CLA	NA
20	b	607	CLA	NC
20	b	607	CLA	ND
20	b	607	CLA	NA
20	b	615	CLA	NC
20	b	615	CLA	ND
20	b	615	CLA	NA
20	b	616	CLA	NC
20	b	616	CLA	ND
20	b	616	CLA	NA
20	B	607	CLA	NC
20	B	607	CLA	ND
20	B	607	CLA	NA
20	B	614	CLA	NC
20	B	614	CLA	NA
20	B	614	CLA	ND
20	b	604	CLA	NC
20	b	604	CLA	ND
20	b	604	CLA	NA
20	d	404	CLA	NA
20	B	604	CLA	NC
20	B	604	CLA	ND
20	B	604	CLA	NA
20	C	503	CLA	NC
20	C	503	CLA	NA
20	b	610	CLA	NC
20	B	615	CLA	NC
20	B	615	CLA	ND
20	B	615	CLA	NA
20	b	618	CLA	NC
20	b	618	CLA	ND
20	b	618	CLA	NA
20	b	613	CLA	NC

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Mol	Chain	Res	Type	Atom
20	c	508	CLA	NC
20	c	508	CLA	NA
20	b	605	CLA	NC
20	b	605	CLA	ND
20	b	605	CLA	NA
20	C	509	CLA	NC
20	C	509	CLA	ND
20	C	509	CLA	NA
20	B	609	CLA	NC
20	c	501	CLA	NC
20	c	501	CLA	ND
20	c	501	CLA	NA
20	c	506	CLA	ND
20	c	506	CLA	NA
20	C	507	CLA	NC
20	C	507	CLA	ND
20	C	507	CLA	NA
20	b	612	CLA	NC
20	b	612	CLA	ND
20	b	612	CLA	NA
20	B	612	CLA	NC
20	B	612	CLA	ND
20	B	612	CLA	NA

All (1383) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	k	101	BCR	C7-C8-C9-C10
22	k	101	BCR	C7-C8-C9-C34
20	c	502	CLA	CHA-CBD-CGD-O2D
32	C	520	HTG	C2'-C1'-S1-C1
23	F	101	SQD	C44-C45-C46-O48
36	L	101	LHG	C4-O6-P-O3
36	L	101	LHG	C4-O6-P-O4
36	L	101	LHG	C4-O6-P-O5
32	C	522	HTG	O5-C1-S1-C1'
36	E	103	LHG	O1-C1-C2-C3
36	E	103	LHG	C6-C5-O7-C7
23	a	401	SQD	C2-C1-O6-C44
23	a	401	SQD	O6-C44-C45-O47
20	C	508	CLA	CHA-CBD-CGD-O1D
27	A	411	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	f	101	SQD	C8-C7-O47-C45
23	f	101	SQD	C5-C6-S-O8
20	D	402	CLA	CHA-CBD-CGD-O1D
20	B	606	CLA	C2-C3-C5-C6
20	b	603	CLA	CHA-CBD-CGD-O2D
20	b	603	CLA	C11-C10-C8-C9
23	l	101	SQD	C8-C7-O47-C45
23	l	101	SQD	O10-C23-O48-C46
23	l	101	SQD	C24-C23-O48-C46
23	l	101	SQD	O5-C5-C6-S
20	b	608	CLA	CHA-CBD-CGD-O1D
20	b	608	CLA	CHA-CBD-CGD-O2D
20	b	608	CLA	C6-C7-C8-C10
32	C	521	HTG	C2-C1-S1-C1'
34	m	101	LMT	O5'-C1'-O1'-C1
34	m	101	LMT	C2-C1-O1'-C1'
20	B	601	CLA	C11-C10-C8-C9
36	l	102	LHG	C4-O6-P-O3
36	l	102	LHG	C4-O6-P-O4
36	l	102	LHG	C4-O6-P-O5
20	C	502	CLA	CHA-CBD-CGD-O1D
20	C	502	CLA	CAD-CBD-CGD-O1D
23	A	412	SQD	C2-C1-O6-C44
23	A	412	SQD	O5-C1-O6-C44
22	K	101	BCR	C36-C18-C19-C20
23	b	622	SQD	O5-C1-O6-C44
23	b	622	SQD	C46-C45-O47-C7
23	b	622	SQD	O49-C7-O47-C45
23	b	622	SQD	C8-C7-O47-C45
20	B	602	CLA	CBA-CGA-O2A-C1
20	B	602	CLA	O1A-CGA-O2A-C1
20	B	602	CLA	CHA-CBD-CGD-O1D
20	B	602	CLA	CHA-CBD-CGD-O2D
20	B	602	CLA	CAD-CBD-CGD-O2D
35	D	406	DGD	C2B-C1B-O2G-C2G
35	D	406	DGD	C2D-C1D-O3G-C3G
35	D	406	DGD	O6D-C1D-O3G-C3G
34	a	418	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
32	B	622	HTG	C2'-C1'-S1-C1
32	B	623	HTG	C2-C1-S1-C1'
32	B	623	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
36	d	407	LHG	O1-C1-C2-C3
36	d	407	LHG	C3-O3-P-O5
20	b	616	CLA	CHA-CBD-CGD-O1D
20	b	616	CLA	CHA-CBD-CGD-O2D
20	b	616	CLA	CAD-CBD-CGD-O1D
20	b	616	CLA	CAD-CBD-CGD-O2D
20	b	616	CLA	C4-C3-C5-C6
20	B	607	CLA	C11-C12-C13-C14
36	D	408	LHG	C4-O6-P-O4
22	d	405	BCR	C37-C22-C23-C24
20	b	604	CLA	CHA-CBD-CGD-O1D
34	f	102	LMT	C2'-C1'-O1'-C1
34	f	102	LMT	O5'-C1'-O1'-C1
22	t	101	BCR	C11-C12-C13-C14
22	t	101	BCR	C11-C12-C13-C35
32	d	401	HTG	C2-C1-S1-C1'
32	d	401	HTG	O5-C1-S1-C1'
20	B	615	CLA	CHA-CBD-CGD-O2D
20	B	615	CLA	CAD-CBD-CGD-O1D
20	b	618	CLA	C2-C3-C5-C6
20	b	618	CLA	C4-C3-C5-C6
32	c	521	HTG	C2'-C1'-S1-C1
20	c	508	CLA	CHA-CBD-CGD-O1D
20	C	509	CLA	C11-C10-C8-C9
22	D	405	BCR	C21-C22-C23-C24
22	D	405	BCR	C37-C22-C23-C24
22	D	405	BCR	C23-C24-C25-C30
32	c	520	HTG	C2-C1-S1-C1'
32	c	520	HTG	O5-C1-S1-C1'
34	B	627	LMT	C2-C1-O1'-C1'
24	C	524	LMG	C11-C10-O7-C8
32	C	534	HTG	C2'-C1'-S1-C1
27	a	415	PL9	C9-C11-C12-C13
27	a	415	PL9	C14-C16-C17-C18
27	a	415	PL9	C23-C24-C26-C27
27	a	415	PL9	C25-C24-C26-C27
32	V	202	HTG	C2-C1-S1-C1'
20	B	611	CLA	C15-C16-C17-C18
23	f	101	SQD	O49-C7-O47-C45
23	F	101	SQD	O10-C23-O48-C46
36	E	103	LHG	O10-C23-O8-C6
34	z	102	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
36	E	103	LHG	C8-C7-O7-C5
36	E	103	LHG	C24-C23-O8-C6
36	E	103	LHG	O9-C7-O7-C5
35	d	416	DGD	O1A-C1A-O1G-C1G
20	b	617	CLA	C13-C15-C16-C17
34	b	627	LMT	C2B-C1B-O1B-C4'
23	l	101	SQD	O49-C7-O47-C45
24	C	524	LMG	O9-C10-O7-C8
34	I	101	LMT	C3'-C4'-O1B-C1B
20	b	603	CLA	C3-C5-C6-C7
20	B	601	CLA	C3-C5-C6-C7
20	B	602	CLA	C3-C5-C6-C7
23	F	101	SQD	C24-C23-O48-C46
20	B	606	CLA	C4-C3-C5-C6
20	A	404	CLA	C4-C3-C5-C6
20	A	404	CLA	C2-C3-C5-C6
20	b	616	CLA	C2-C3-C5-C6
20	C	513	CLA	CBD-CGD-O2D-CED
20	B	615	CLA	C3-C5-C6-C7
23	b	622	SQD	C24-C23-O48-C46
35	d	416	DGD	C2A-C1A-O1G-C1G
32	v	210	HTG	O5-C5-C6-O6
34	Z	101	LMT	O5B-C5B-C6B-O6B
32	c	521	HTG	O5-C5-C6-O6
32	C	520	HTG	S1-C1'-C2'-C3'
32	D	417	HTG	S1-C1'-C2'-C3'
35	D	406	DGD	O1B-C1B-O2G-C2G
34	m	101	LMT	O5'-C5'-C6'-O6'
32	C	534	HTG	O5-C5-C6-O6
34	z	102	LMT	C4'-C5'-C6'-O6'
20	B	605	CLA	C3-C5-C6-C7
20	b	618	CLA	CBD-CGD-O2D-CED
34	c	523	LMT	O5'-C5'-C6'-O6'
34	b	627	LMT	O5'-C5'-C6'-O6'
36	D	409	LHG	C31-C32-C33-C34
35	c	515	DGD	C2A-C3A-C4A-C5A
32	B	622	HTG	C3'-C4'-C5'-C6'
24	a	410	LMG	C37-C38-C39-C40
23	b	622	SQD	C31-C32-C33-C34
32	c	520	HTG	C4-C5-C6-O6
24	b	623	LMG	C10-C11-C12-C13
23	l	101	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
34	z	102	LMT	C3'-C4'-O1B-C1B
34	J	103	LMT	O5'-C5'-C6'-O6'
34	a	418	LMT	O5'-C5'-C6'-O6'
32	B	623	HTG	O5-C5-C6-O6
35	d	416	DGD	O6D-C5D-C6D-O5D
32	v	210	HTG	C4-C5-C6-O6
34	b	627	LMT	C4B-C5B-C6B-O6B
23	b	622	SQD	O10-C23-O48-C46
34	B	627	LMT	O1'-C1'-O5'-C5'
32	D	417	HTG	O5-C5-C6-O6
34	z	102	LMT	O5'-C5'-C6'-O6'
32	c	520	HTG	O5-C5-C6-O6
20	B	601	CLA	C4-C3-C5-C6
27	a	415	PL9	C30-C29-C31-C32
20	B	601	CLA	C2-C3-C5-C6
20	b	607	CLA	C2-C3-C5-C6
27	a	415	PL9	C28-C29-C31-C32
24	j	101	LMG	C10-C11-C12-C13
34	T	102	LMT	O5'-C5'-C6'-O6'
34	f	102	LMT	O5'-C5'-C6'-O6'
32	B	631	HTG	O5-C5-C6-O6
24	A	407	LMG	O10-C28-O8-C9
34	Z	101	LMT	C4B-C5B-C6B-O6B
24	a	410	LMG	O6-C1-O1-C7
34	z	102	LMT	O5'-C1'-O1'-C1
27	A	411	PL9	C24-C26-C27-C28
24	A	407	LMG	C29-C28-O8-C9
20	C	513	CLA	CBA-CGA-O2A-C1
34	f	102	LMT	C4'-C5'-C6'-O6'
24	A	407	LMG	C15-C16-C17-C18
34	T	102	LMT	C4'-C5'-C6'-O6'
20	C	513	CLA	O1A-CGA-O2A-C1
24	c	519	LMG	O10-C28-O8-C9
23	f	101	SQD	C24-C23-O48-C46
24	c	519	LMG	C29-C28-O8-C9
35	c	516	DGD	C1A-C2A-C3A-C4A
36	d	408	LHG	C11-C12-C13-C14
34	b	627	LMT	C4'-C5'-C6'-O6'
32	B	631	HTG	C4-C5-C6-O6
32	D	417	HTG	C4-C5-C6-O6
20	B	602	CLA	C10-C11-C12-C13
20	b	618	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	d	407	LHG	O2-C2-C3-O3
23	A	412	SQD	O6-C44-C45-O47
23	a	409	SQD	C9-C10-C11-C12
24	B	620	LMG	C37-C38-C39-C40
34	J	103	LMT	C4'-C5'-C6'-O6'
20	C	504	CLA	C11-C12-C13-C14
20	c	513	CLA	C11-C10-C8-C9
20	c	513	CLA	C14-C13-C15-C16
20	b	603	CLA	C14-C13-C15-C16
20	B	602	CLA	C11-C10-C8-C9
20	b	604	CLA	C14-C13-C15-C16
20	c	506	CLA	C6-C7-C8-C9
35	D	406	DGD	C7B-C8B-C9B-CAB
32	C	521	HTG	S1-C1'-C2'-C3'
22	d	405	BCR	C21-C22-C23-C24
23	F	101	SQD	O47-C45-C46-O48
35	C	517	DGD	C1B-C2B-C3B-C4B
23	f	101	SQD	O10-C23-O48-C46
20	C	506	CLA	C10-C11-C12-C13
32	B	623	HTG	C4-C5-C6-O6
32	c	521	HTG	C4-C5-C6-O6
20	c	513	CLA	C8-C10-C11-C12
20	A	404	CLA	C13-C15-C16-C17
20	A	404	CLA	C15-C16-C17-C18
20	b	616	CLA	C10-C11-C12-C13
20	B	612	CLA	C15-C16-C17-C18
20	D	404	CLA	C8-C10-C11-C12
20	c	509	CLA	C13-C15-C16-C17
20	b	616	CLA	C8-C10-C11-C12
20	B	615	CLA	C5-C6-C7-C8
20	b	618	CLA	C15-C16-C17-C18
23	a	409	SQD	C7-C8-C9-C10
23	A	412	SQD	C23-C24-C25-C26
23	b	622	SQD	C23-C24-C25-C26
24	c	519	LMG	C10-C11-C12-C13
24	c	519	LMG	C28-C29-C30-C31
20	B	601	CLA	C10-C11-C12-C13
34	m	101	LMT	O1'-C1-C2-C3
23	a	401	SQD	C23-C24-C25-C26
24	a	410	LMG	C10-C11-C12-C13
32	B	621	HTG	C4-C5-C6-O6
20	b	614	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	615	CLA	C8-C10-C11-C12
20	c	506	CLA	C10-C11-C12-C13
20	D	401	CLA	C12-C13-C15-C16
20	A	404	CLA	C12-C13-C15-C16
20	b	615	CLA	C11-C12-C13-C15
22	T	101	BCR	C13-C14-C15-C16
22	t	101	BCR	C13-C14-C15-C16
20	B	607	CLA	C2A-CAA-CBA-CGA
20	B	602	CLA	O1D-CGD-O2D-CED
34	a	418	LMT	C4'-C5'-C6'-O6'
23	a	401	SQD	O5-C1-O6-C44
34	B	626	LMT	O5'-C1'-O1'-C1
27	A	411	PL9	C19-C21-C22-C23
34	T	102	LMT	O1'-C1-C2-C3
32	b	625	HTG	S1-C1'-C2'-C3'
32	B	621	HTG	O5-C5-C6-O6
36	D	408	LHG	O2-C2-C3-O3
20	A	404	CLA	C3-C5-C6-C7
20	a	404	CLA	C8-C10-C11-C12
20	C	507	CLA	C5-C6-C7-C8
24	A	407	LMG	C10-C11-C12-C13
35	d	416	DGD	C4D-C5D-C6D-O5D
20	c	513	CLA	C10-C11-C12-C13
20	c	513	CLA	C13-C15-C16-C17
20	B	601	CLA	C13-C15-C16-C17
20	C	503	CLA	O1D-CGD-O2D-CED
32	C	534	HTG	C4-C5-C6-O6
20	b	608	CLA	C15-C16-C17-C18
20	b	606	CLA	C15-C16-C17-C18
35	D	406	DGD	C2A-C1A-O1G-C1G
32	C	522	HTG	C1'-C2'-C3'-C4'
20	c	506	CLA	C15-C16-C17-C18
32	B	622	HTG	S1-C1'-C2'-C3'
36	d	406	LHG	C23-C24-C25-C26
35	c	517	DGD	C1A-C2A-C3A-C4A
36	d	407	LHG	C1-C2-C3-O3
36	D	408	LHG	C1-C2-C3-O3
36	E	103	LHG	C11-C10-C9-C8
20	B	616	CLA	C10-C11-C12-C13
20	b	605	CLA	C5-C6-C7-C8
20	C	503	CLA	CBD-CGD-O2D-CED
20	b	608	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	C	524	LMG	O6-C5-C6-O5
35	C	517	DGD	C8B-C9B-CAB-CBB
34	Z	101	LMT	C5'-C4'-O1B-C1B
20	B	602	CLA	C13-C15-C16-C17
32	B	622	HTG	C1'-C2'-C3'-C4'
24	A	407	LMG	C11-C12-C13-C14
24	A	407	LMG	C18-C19-C20-C21
23	F	101	SQD	C28-C29-C30-C31
23	l	101	SQD	C15-C16-C17-C18
34	m	101	LMT	C7-C8-C9-C10
23	A	412	SQD	C28-C29-C30-C31
35	C	518	DGD	CBB-CCB-CDB-CEB
24	a	410	LMG	C34-C35-C36-C37
35	c	515	DGD	C5A-C6A-C7A-C8A
24	c	519	LMG	C16-C17-C18-C19
24	c	519	LMG	C32-C33-C34-C35
24	c	519	LMG	C39-C40-C41-C42
36	d	406	LHG	C29-C30-C31-C32
35	h	101	DGD	C6B-C7B-C8B-C9B
35	d	416	DGD	C2A-C3A-C4A-C5A
35	d	416	DGD	C7A-C8A-C9A-CAA
20	c	502	CLA	C16-C17-C18-C19
20	C	502	CLA	C16-C17-C18-C20
36	L	101	LHG	C27-C28-C29-C30
34	b	628	LMT	C5-C6-C7-C8
36	E	103	LHG	C28-C29-C30-C31
23	a	401	SQD	C15-C16-C17-C18
23	a	401	SQD	C29-C30-C31-C32
23	A	412	SQD	C27-C28-C29-C30
24	B	620	LMG	C31-C32-C33-C34
24	B	620	LMG	C32-C33-C34-C35
35	D	406	DGD	C5A-C6A-C7A-C8A
35	D	406	DGD	C8B-C9B-CAB-CBB
36	d	408	LHG	C10-C11-C12-C13
23	l	101	SQD	C46-C45-O47-C7
24	C	524	LMG	C9-C8-O7-C10
24	J	101	LMG	O6-C5-C6-O5
24	A	407	LMG	O9-C10-O7-C8
36	l	102	LHG	C27-C28-C29-C30
35	D	406	DGD	C6A-C7A-C8A-C9A
35	C	516	DGD	C7A-C8A-C9A-CAA
36	D	407	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
36	d	408	LHG	C28-C29-C30-C31
23	A	406	SQD	C11-C12-C13-C14
23	A	412	SQD	C26-C27-C28-C29
24	B	620	LMG	C15-C16-C17-C18
24	a	410	LMG	C17-C18-C19-C20
24	a	410	LMG	C35-C36-C37-C38
36	D	409	LHG	C15-C16-C17-C18
35	c	515	DGD	C7A-C8A-C9A-CAA
35	D	406	DGD	C2A-C3A-C4A-C5A
35	d	416	DGD	C3B-C4B-C5B-C6B
23	A	406	SQD	C18-C19-C20-C21
34	I	101	LMT	O1'-C1-C2-C3
34	z	102	LMT	C5-C6-C7-C8
24	C	519	LMG	C17-C18-C19-C20
35	d	416	DGD	CAB-CBB-CCB-CDB
24	C	524	LMG	C33-C34-C35-C36
24	J	101	LMG	C10-C11-C12-C13
36	D	407	LHG	C23-C24-C25-C26
20	c	501	CLA	O1D-CGD-O2D-CED
24	A	407	LMG	C2-C1-O1-C7
23	b	622	SQD	C2-C1-O6-C44
34	B	626	LMT	C2'-C1'-O1'-C1
24	A	407	LMG	C21-C22-C23-C24
24	A	407	LMG	C36-C37-C38-C39
23	l	101	SQD	C29-C30-C31-C32
35	d	416	DGD	C7B-C8B-C9B-CAB
20	d	404	CLA	C13-C15-C16-C17
20	C	506	CLA	C16-C17-C18-C20
20	b	615	CLA	C16-C17-C18-C19
20	b	618	CLA	C16-C17-C18-C20
20	B	607	CLA	O1D-CGD-O2D-CED
34	b	627	LMT	O5B-C5B-C6B-O6B
23	F	101	SQD	C32-C33-C34-C35
23	A	406	SQD	C34-C35-C36-C37
36	D	409	LHG	C28-C29-C30-C31
23	b	622	SQD	C24-C25-C26-C27
24	C	519	LMG	C34-C35-C36-C37
35	h	101	DGD	C6A-C7A-C8A-C9A
36	D	407	LHG	C28-C29-C30-C31
34	B	627	LMT	C11-C10-C9-C8
20	D	404	CLA	C11-C10-C8-C9
20	b	608	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	604	CLA	C6-C7-C8-C9
20	b	612	CLA	C14-C13-C15-C16
35	C	517	DGD	C1A-C2A-C3A-C4A
24	c	518	LMG	C10-C11-C12-C13
24	C	519	LMG	C10-C11-C12-C13
24	A	407	LMG	C17-C18-C19-C20
23	f	101	SQD	C25-C26-C27-C28
35	C	517	DGD	C3A-C4A-C5A-C6A
34	c	523	LMT	C5-C6-C7-C8
20	A	402	CLA	C10-C11-C12-C13
24	a	410	LMG	C30-C31-C32-C33
35	c	515	DGD	C8A-C9A-CAA-CBA
35	D	406	DGD	C9B-CAB-CBB-CCB
35	C	516	DGD	C8B-C9B-CAB-CBB
24	C	524	LMG	C19-C20-C21-C22
20	D	402	CLA	O1D-CGD-O2D-CED
34	b	628	LMT	C2-C3-C4-C5
23	a	401	SQD	C24-C25-C26-C27
23	l	101	SQD	C11-C12-C13-C14
23	A	412	SQD	C9-C10-C11-C12
24	C	519	LMG	C14-C15-C16-C17
24	C	519	LMG	C39-C40-C41-C42
35	c	517	DGD	C8A-C9A-CAA-CBA
36	d	406	LHG	O1-C1-C2-C3
24	A	407	LMG	C11-C10-O7-C8
24	c	519	LMG	C11-C10-O7-C8
23	A	406	SQD	C31-C32-C33-C34
24	B	620	LMG	C17-C18-C19-C20
24	a	410	LMG	C16-C17-C18-C19
35	D	406	DGD	CCB-CDB-CEB-CFB
24	C	519	LMG	C20-C21-C22-C23
34	f	102	LMT	C3-C4-C5-C6
24	C	524	LMG	C34-C35-C36-C37
36	d	408	LHG	C17-C18-C19-C20
23	F	101	SQD	C23-C24-C25-C26
24	A	407	LMG	C13-C14-C15-C16
32	C	520	HTG	C3'-C4'-C5'-C6'
23	F	101	SQD	C27-C28-C29-C30
23	a	409	SQD	C30-C31-C32-C33
23	A	406	SQD	C30-C31-C32-C33
24	b	623	LMG	C32-C33-C34-C35
23	a	401	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	C4B-C5B-C6B-C7B
32	B	632	HTG	C3'-C4'-C5'-C6'
34	I	101	LMT	C5-C6-C7-C8
24	B	620	LMG	C35-C36-C37-C38
35	C	518	DGD	CCB-CDB-CEB-CFB
35	D	406	DGD	C6B-C7B-C8B-C9B
32	B	623	HTG	C3'-C4'-C5'-C6'
24	C	519	LMG	C33-C34-C35-C36
35	d	416	DGD	CCB-CDB-CEB-CFB
24	C	524	LMG	C18-C19-C20-C21
20	B	605	CLA	C16-C17-C18-C20
20	C	506	CLA	C16-C17-C18-C19
20	c	509	CLA	C16-C17-C18-C19
20	b	608	CLA	C16-C17-C18-C19
20	b	617	CLA	C16-C17-C18-C19
20	b	617	CLA	C16-C17-C18-C20
20	C	507	CLA	C16-C17-C18-C20
24	A	407	LMG	O6-C1-O1-C7
20	b	617	CLA	C10-C11-C12-C13
23	a	409	SQD	C26-C27-C28-C29
24	j	101	LMG	C18-C19-C20-C21
23	a	401	SQD	C25-C26-C27-C28
23	A	412	SQD	C25-C26-C27-C28
24	B	620	LMG	C34-C35-C36-C37
36	D	407	LHG	C25-C26-C27-C28
35	d	416	DGD	C6A-C7A-C8A-C9A
34	B	625	LMT	C7-C8-C9-C10
34	b	627	LMT	C1-C2-C3-C4
24	b	623	LMG	C35-C36-C37-C38
36	E	103	LHG	C34-C35-C36-C37
35	C	518	DGD	C9A-CAA-CBA-CCA
35	D	406	DGD	CBB-CCB-CDB-CEB
34	J	103	LMT	C5-C6-C7-C8
20	b	603	CLA	C10-C11-C12-C13
35	D	406	DGD	O1A-C1A-O1G-C1G
35	H	102	DGD	C8A-C9A-CAA-CBA
24	j	101	LMG	C32-C33-C34-C35
24	b	623	LMG	C33-C34-C35-C36
23	a	401	SQD	C28-C29-C30-C31
34	E	101	LMT	C2-C3-C4-C5
23	b	622	SQD	C33-C34-C35-C36
24	c	519	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	B	623	HTG	C2'-C3'-C4'-C5'
34	z	102	LMT	C6-C7-C8-C9
24	c	519	LMG	C15-C16-C17-C18
24	c	519	LMG	C35-C36-C37-C38
34	z	102	LMT	C5'-C4'-O1B-C1B
32	B	621	HTG	C3'-C4'-C5'-C6'
20	C	512	CLA	O1D-CGD-O2D-CED
23	a	409	SQD	C29-C30-C31-C32
32	b	601	HTG	C3'-C4'-C5'-C6'
36	D	408	LHG	C11-C10-C9-C8
32	B	631	HTG	C2'-C3'-C4'-C5'
20	B	605	CLA	C16-C17-C18-C19
20	b	618	CLA	C16-C17-C18-C19
20	C	507	CLA	C16-C17-C18-C19
23	a	409	SQD	C11-C10-C9-C8
23	a	409	SQD	C27-C28-C29-C30
23	l	101	SQD	C17-C18-C19-C20
23	A	412	SQD	C11-C10-C9-C8
35	c	516	DGD	C3A-C4A-C5A-C6A
36	d	406	LHG	C27-C28-C29-C30
35	c	517	DGD	C8B-C9B-CAB-CBB
34	z	102	LMT	C2B-C1B-O1B-C4'
20	C	510	CLA	O1D-CGD-O2D-CED
24	A	407	LMG	C20-C21-C22-C23
23	A	412	SQD	C10-C11-C12-C13
34	I	101	LMT	C4-C5-C6-C7
32	d	401	HTG	C3'-C4'-C5'-C6'
23	a	409	SQD	C18-C19-C20-C21
23	l	101	SQD	C28-C29-C30-C31
34	T	102	LMT	C6-C7-C8-C9
34	I	101	LMT	C11-C10-C9-C8
36	E	103	LHG	O1-C1-C2-O2
34	B	627	LMT	O5'-C1'-O1'-C1
20	B	616	CLA	C5-C6-C7-C8
24	A	407	LMG	C29-C30-C31-C32
32	C	520	HTG	C2'-C3'-C4'-C5'
35	H	102	DGD	C9B-CAB-CBB-CCB
36	E	103	LHG	C29-C30-C31-C32
23	f	101	SQD	C24-C25-C26-C27
32	O	302	HTG	C3'-C4'-C5'-C6'
23	b	622	SQD	C18-C19-C20-C21
35	c	515	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
20	a	403	CLA	C2C-C3C-CAC-CBC
35	C	516	DGD	C3B-C4B-C5B-C6B
32	C	521	HTG	O5-C5-C6-O6
24	b	623	LMG	C14-C15-C16-C17
23	A	412	SQD	C31-C32-C33-C34
32	D	417	HTG	C2'-C3'-C4'-C5'
23	l	101	SQD	C14-C15-C16-C17
34	m	101	LMT	C6-C7-C8-C9
24	c	519	LMG	C29-C30-C31-C32
23	a	409	SQD	C17-C18-C19-C20
36	E	103	LHG	C26-C27-C28-C29
36	l	102	LHG	C28-C29-C30-C31
23	b	622	SQD	C27-C28-C29-C30
24	c	519	LMG	C34-C35-C36-C37
24	B	620	LMG	C33-C34-C35-C36
24	c	519	LMG	O9-C10-O7-C8
34	J	103	LMT	C1-C2-C3-C4
35	c	515	DGD	O6D-C5D-C6D-O5D
20	C	509	CLA	C2-C1-O2A-CGA
32	c	521	HTG	C1'-C2'-C3'-C4'
35	h	101	DGD	CBB-CCB-CDB-CEB
20	B	601	CLA	C15-C16-C17-C18
24	c	518	LMG	C39-C40-C41-C42
24	B	620	LMG	C12-C13-C14-C15
20	c	509	CLA	C16-C17-C18-C20
35	C	516	DGD	C1B-C2B-C3B-C4B
22	B	617	BCR	C1-C6-C7-C8
22	B	617	BCR	C5-C6-C7-C8
22	C	514	BCR	C23-C24-C25-C26
22	C	514	BCR	C23-C24-C25-C30
22	d	405	BCR	C23-C24-C25-C26
22	d	405	BCR	C23-C24-C25-C30
22	D	405	BCR	C23-C24-C25-C26
36	L	101	LHG	C31-C32-C33-C34
34	b	628	LMT	C7-C8-C9-C10
20	d	403	CLA	C2C-C3C-CAC-CBC
24	a	410	LMG	C18-C19-C20-C21
24	c	519	LMG	C18-C19-C20-C21
35	c	517	DGD	C7B-C8B-C9B-CAB
20	b	608	CLA	C10-C11-C12-C13
20	B	607	CLA	C15-C16-C17-C18
23	l	101	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	C2A-C3A-C4A-C5A
24	C	519	LMG	C19-C20-C21-C22
34	f	102	LMT	C4-C5-C6-C7
35	c	517	DGD	CAA-CBA-CCA-CDA
23	b	622	SQD	C7-C8-C9-C10
35	C	517	DGD	C5B-C6B-C7B-C8B
35	C	517	DGD	C6B-C7B-C8B-C9B
34	b	627	LMT	C6-C7-C8-C9
35	c	516	DGD	C5A-C6A-C7A-C8A
35	d	416	DGD	C3A-C4A-C5A-C6A
20	b	607	CLA	C4-C3-C5-C6
20	C	504	CLA	C11-C12-C13-C15
20	c	509	CLA	C12-C13-C15-C16
20	B	601	CLA	C12-C13-C15-C16
20	b	616	CLA	C11-C10-C8-C7
20	b	604	CLA	C12-C13-C15-C16
20	b	613	CLA	C12-C13-C15-C16
20	b	612	CLA	C12-C13-C15-C16
23	a	401	SQD	C33-C34-C35-C36
32	d	401	HTG	C2'-C3'-C4'-C5'
34	B	625	LMT	C11-C10-C9-C8
35	d	416	DGD	O1B-C1B-O2G-C2G
34	b	628	LMT	O1'-C1-C2-C3
35	C	518	DGD	CAA-CBA-CCA-CDA
35	C	518	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CCA-CDA-CEA-CFA
20	b	608	CLA	C2A-CAA-CBA-CGA
20	C	504	CLA	C13-C15-C16-C17
20	b	610	CLA	C13-C15-C16-C17
24	j	101	LMG	C34-C35-C36-C37
35	C	516	DGD	C6B-C7B-C8B-C9B
34	B	627	LMT	C4-C5-C6-C7
36	d	408	LHG	C30-C31-C32-C33
23	b	622	SQD	C29-C30-C31-C32
34	B	626	LMT	C7-C8-C9-C10
36	d	408	LHG	C32-C33-C34-C35
20	c	509	CLA	C15-C16-C17-C18
20	B	607	CLA	C13-C15-C16-C17
24	j	101	LMG	C13-C14-C15-C16
24	a	410	LMG	C19-C20-C21-C22
32	b	625	HTG	C3'-C4'-C5'-C6'
35	c	515	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
24	c	519	LMG	C20-C21-C22-C23
34	E	101	LMT	C1-C2-C3-C4
20	b	609	CLA	C3-C5-C6-C7
34	c	523	LMT	C7-C8-C9-C10
20	b	616	CLA	C16-C17-C18-C19
20	B	607	CLA	C8-C10-C11-C12
23	f	101	SQD	C26-C27-C28-C29
34	I	101	LMT	C6-C7-C8-C9
34	T	102	LMT	C2-C3-C4-C5
34	z	102	LMT	C2-C3-C4-C5
35	d	416	DGD	C2B-C1B-O2G-C2G
32	v	210	HTG	C2'-C1'-S1-C1
20	b	615	CLA	C8-C10-C11-C12
24	C	524	LMG	C20-C21-C22-C23
24	J	101	LMG	C12-C13-C14-C15
24	b	623	LMG	C29-C30-C31-C32
23	l	101	SQD	C26-C27-C28-C29
35	c	516	DGD	CBB-CCB-CDB-CEB
23	A	406	SQD	O6-C44-C45-O47
35	C	518	DGD	C7B-C8B-C9B-CAB
23	f	101	SQD	C27-C28-C29-C30
23	l	101	SQD	C11-C10-C9-C8
36	l	102	LHG	C11-C10-C9-C8
20	c	504	CLA	C13-C15-C16-C17
20	C	510	CLA	C8-C10-C11-C12
20	C	507	CLA	C4-C3-C5-C6
20	C	507	CLA	C2-C3-C5-C6
27	a	415	PL9	C4-C3-C7-C8
23	a	401	SQD	C18-C19-C20-C21
34	T	102	LMT	C1-C2-C3-C4
34	a	418	LMT	C1-C2-C3-C4
20	c	509	CLA	C14-C13-C15-C16
20	a	404	CLA	C6-C7-C8-C9
20	B	601	CLA	C14-C13-C15-C16
20	c	506	CLA	C14-C13-C15-C16
24	c	519	LMG	C33-C34-C35-C36
35	h	101	DGD	C8A-C9A-CAA-CBA
20	b	618	CLA	C3-C5-C6-C7
34	B	627	LMT	C1-C2-C3-C4
24	a	410	LMG	C36-C37-C38-C39
34	T	102	LMT	C3-C4-C5-C6
23	A	406	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
35	C	516	DGD	CBA-CCA-CDA-CEA
20	C	506	CLA	C1A-C2A-CAA-CBA
20	C	502	CLA	C16-C17-C18-C19
20	b	615	CLA	C16-C17-C18-C20
23	A	406	SQD	C28-C29-C30-C31
23	l	101	SQD	C27-C28-C29-C30
24	B	620	LMG	C18-C19-C20-C21
34	m	101	LMT	C4'-C5'-C6'-O6'
34	f	102	LMT	C1-C2-C3-C4
23	a	409	SQD	C33-C34-C35-C36
23	b	622	SQD	C30-C31-C32-C33
36	D	407	LHG	C34-C35-C36-C37
36	E	103	LHG	C23-C24-C25-C26
23	b	622	SQD	C34-C35-C36-C37
20	D	404	CLA	C13-C15-C16-C17
34	T	102	LMT	C9-C10-C11-C12
24	B	620	LMG	C10-C11-C12-C13
35	D	406	DGD	CCA-CDA-CEA-CFA
23	A	412	SQD	C16-C17-C18-C19
23	b	622	SQD	C11-C10-C9-C8
36	d	408	LHG	C16-C17-C18-C19
20	B	615	CLA	O1D-CGD-O2D-CED
36	D	409	LHG	C17-C18-C19-C20
35	c	517	DGD	C7A-C8A-C9A-CAA
32	O	302	HTG	C2'-C3'-C4'-C5'
35	C	516	DGD	C5B-C6B-C7B-C8B
24	j	101	LMG	O6-C5-C6-O5
27	a	415	PL9	C15-C14-C16-C17
24	c	518	LMG	C38-C39-C40-C41
36	d	407	LHG	C34-C35-C36-C37
23	a	409	SQD	C14-C15-C16-C17
23	l	101	SQD	C10-C11-C12-C13
36	l	102	LHG	C32-C33-C34-C35
34	E	101	LMT	C6-C7-C8-C9
20	b	604	CLA	C16-C17-C18-C19
24	A	407	LMG	C32-C33-C34-C35
23	F	101	SQD	C30-C31-C32-C33
23	a	409	SQD	O6-C44-C45-C46
23	A	412	SQD	O6-C44-C45-C46
24	c	519	LMG	C7-C8-C9-O8
35	c	517	DGD	C9A-CAA-CBA-CCA
23	a	409	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	b	601	HTG	C4'-C5'-C6'-C7'
23	a	401	SQD	C19-C20-C21-C22
35	D	406	DGD	C4B-C5B-C6B-C7B
23	F	101	SQD	C45-C44-O6-C1
35	C	517	DGD	C2G-C3G-O3G-C1D
35	C	517	DGD	C5D-C6D-O5D-C1E
24	c	518	LMG	C8-C7-O1-C1
24	C	524	LMG	C8-C7-O1-C1
23	l	101	SQD	C16-C17-C18-C19
34	J	103	LMT	C7-C8-C9-C10
35	h	101	DGD	C7A-C8A-C9A-CAA
23	a	401	SQD	C26-C27-C28-C29
24	A	407	LMG	C40-C41-C42-C43
36	L	101	LHG	C33-C34-C35-C36
35	H	102	DGD	CDB-CEB-CFB-CGB
21	D	403	PHO	C2C-C3C-CAC-CBC
35	C	518	DGD	CAB-CBB-CCB-CDB
23	a	409	SQD	C31-C32-C33-C34
23	A	406	SQD	C15-C16-C17-C18
36	E	103	LHG	C9-C10-C11-C12
24	c	519	LMG	C40-C41-C42-C43
35	h	101	DGD	CDB-CEB-CFB-CGB
36	d	406	LHG	O1-C1-C2-O2
24	j	101	LMG	C12-C13-C14-C15
21	a	405	PHO	C8-C10-C11-C12
34	m	101	LMT	C9-C10-C11-C12
35	c	515	DGD	O6E-C5E-C6E-O5E
35	D	406	DGD	O6D-C5D-C6D-O5D
32	B	631	HTG	C1'-C2'-C3'-C4'
21	a	405	PHO	C4-C3-C5-C6
23	f	101	SQD	C35-C36-C37-C38
20	c	513	CLA	C16-C17-C18-C19
20	b	603	CLA	CBA-CGA-O2A-C1
24	C	519	LMG	C21-C22-C23-C24
24	C	519	LMG	C22-C23-C24-C25
24	C	524	LMG	C17-C18-C19-C20
34	b	628	LMT	C1-C2-C3-C4
35	H	102	DGD	CAA-CBA-CCA-CDA
23	a	401	SQD	C31-C32-C33-C34
34	a	418	LMT	C9-C10-C11-C12
24	c	519	LMG	C22-C23-C24-C25
36	D	408	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
32	B	632	HTG	O5-C5-C6-O6
20	c	509	CLA	C2-C1-O2A-CGA
20	B	601	CLA	C2-C1-O2A-CGA
35	H	102	DGD	CDA-CEA-CFA-CGA
36	d	406	LHG	C31-C32-C33-C34
34	I	101	LMT	O5B-C5B-C6B-O6B
35	C	516	DGD	O6E-C5E-C6E-O5E
24	b	623	LMG	C12-C13-C14-C15
34	b	627	LMT	O5B-C1B-O1B-C4'
36	E	103	LHG	C3-O3-P-O5
32	B	631	HTG	C4'-C5'-C6'-C7'
35	h	101	DGD	O2G-C1B-C2B-C3B
20	B	602	CLA	C16-C17-C18-C20
24	A	407	LMG	C12-C13-C14-C15
23	F	101	SQD	C33-C34-C35-C36
36	d	408	LHG	C35-C36-C37-C38
20	C	509	CLA	C15-C16-C17-C18
23	a	401	SQD	C35-C36-C37-C38
35	D	406	DGD	C4A-C5A-C6A-C7A
34	Z	101	LMT	C3'-C4'-O1B-C1B
35	d	416	DGD	CBB-CCB-CDB-CEB
23	a	409	SQD	O6-C44-C45-O47
21	a	406	PHO	C2C-C3C-CAC-CBC
24	B	620	LMG	C19-C20-C21-C22
35	d	416	DGD	C4A-C5A-C6A-C7A
34	B	625	LMT	C6-C7-C8-C9
23	A	406	SQD	C27-C28-C29-C30
23	a	401	SQD	C16-C17-C18-C19
20	D	404	CLA	C6-C7-C8-C10
20	c	507	CLA	C11-C10-C8-C7
20	C	506	CLA	C11-C12-C13-C15
20	C	513	CLA	C11-C10-C8-C7
20	C	508	CLA	C11-C10-C8-C7
20	a	404	CLA	C6-C7-C8-C10
20	c	513	CLA	C11-C10-C8-C7
20	b	603	CLA	C12-C13-C15-C16
20	B	601	CLA	C11-C10-C8-C7
20	B	602	CLA	C11-C12-C13-C15
20	A	404	CLA	C6-C7-C8-C10
20	B	607	CLA	C11-C12-C13-C15
20	c	506	CLA	C12-C13-C15-C16
20	C	507	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
34	I	101	LMT	C9-C10-C11-C12
32	b	625	HTG	C2'-C3'-C4'-C5'
20	C	506	CLA	C11-C12-C13-C14
20	C	508	CLA	C11-C10-C8-C9
20	D	401	CLA	C14-C13-C15-C16
20	B	602	CLA	C11-C12-C13-C14
20	B	602	CLA	C14-C13-C15-C16
20	A	404	CLA	C6-C7-C8-C9
20	b	615	CLA	C11-C12-C13-C14
20	B	607	CLA	C11-C10-C8-C9
20	C	507	CLA	C11-C10-C8-C9
34	B	625	LMT	C4'-C5'-C6'-O6'
35	c	515	DGD	C4A-C5A-C6A-C7A
20	B	615	CLA	C10-C11-C12-C13
35	C	517	DGD	C5A-C6A-C7A-C8A
22	C	514	BCR	C37-C22-C23-C24
20	d	404	CLA	C16-C17-C18-C20
23	A	406	SQD	C9-C10-C11-C12
36	d	407	LHG	C11-C10-C9-C8
36	d	407	LHG	C32-C33-C34-C35
23	F	101	SQD	O6-C44-C45-O47
24	A	407	LMG	C22-C23-C24-C25
23	a	401	SQD	C34-C35-C36-C37
36	D	409	LHG	C35-C36-C37-C38
35	d	416	DGD	C8A-C9A-CAA-CBA
36	d	408	LHG	C19-C20-C21-C22
35	C	518	DGD	CDB-CEB-CFB-CGB
20	C	506	CLA	C5-C6-C7-C8
24	J	101	LMG	C36-C37-C38-C39
36	l	102	LHG	O6-C4-C5-C6
35	c	515	DGD	CAA-CBA-CCA-CDA
34	a	418	LMT	C4-C5-C6-C7
35	c	516	DGD	C6A-C7A-C8A-C9A
20	B	605	CLA	C13-C15-C16-C17
34	M	101	LMT	O5'-C5'-C6'-O6'
35	C	516	DGD	C8A-C9A-CAA-CBA
34	c	523	LMT	C4'-C5'-C6'-O6'
27	a	415	PL9	C13-C14-C16-C17
23	A	412	SQD	C7-C8-C9-C10
24	c	519	LMG	C21-C22-C23-C24
20	d	404	CLA	C8-C10-C11-C12
23	A	406	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
34	m	101	LMT	C5-C6-C7-C8
36	l	102	LHG	C31-C32-C33-C34
34	T	102	LMT	C7-C8-C9-C10
36	d	406	LHG	C25-C26-C27-C28
24	C	524	LMG	C31-C32-C33-C34
23	a	409	SQD	C13-C14-C15-C16
24	j	101	LMG	C36-C37-C38-C39
20	a	403	CLA	C4C-C3C-CAC-CBC
20	c	513	CLA	CBA-CGA-O2A-C1
24	C	519	LMG	C29-C28-O8-C9
36	E	103	LHG	C13-C14-C15-C16
34	m	102	LMT	C2-C1-O1'-C1'
34	T	102	LMT	C2-C1-O1'-C1'
34	z	102	LMT	C2-C1-O1'-C1'
24	J	101	LMG	C35-C36-C37-C38
24	c	519	LMG	C14-C15-C16-C17
20	b	616	CLA	C16-C17-C18-C20
23	A	406	SQD	C32-C33-C34-C35
24	C	519	LMG	C30-C31-C32-C33
35	d	416	DGD	C4B-C5B-C6B-C7B
24	A	407	LMG	O1-C7-C8-C9
24	A	407	LMG	C7-C8-C9-O8
23	A	406	SQD	O6-C44-C45-C46
23	f	101	SQD	C44-C45-C46-O48
35	d	416	DGD	O1G-C1G-C2G-C3G
34	Z	101	LMT	C2-C3-C4-C5
24	B	620	LMG	C11-C12-C13-C14
23	F	101	SQD	O6-C44-C45-C46
34	B	626	LMT	C11-C10-C9-C8
24	C	524	LMG	C21-C22-C23-C24
27	D	412	PL9	C30-C29-C31-C32
20	B	602	CLA	C4-C3-C5-C6
20	c	502	CLA	C16-C17-C18-C20
35	H	102	DGD	C3B-C4B-C5B-C6B
20	d	402	CLA	C2C-C3C-CAC-CBC
34	c	523	LMT	C4B-C5B-C6B-O6B
32	d	401	HTG	C4-C5-C6-O6
36	D	408	LHG	C4-O6-P-O3
20	b	603	CLA	O1A-CGA-O2A-C1
20	B	601	CLA	C8-C10-C11-C12
20	b	618	CLA	C13-C15-C16-C17
35	H	102	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
24	j	101	LMG	C31-C32-C33-C34
23	A	406	SQD	C12-C13-C14-C15
35	d	416	DGD	C9A-CAA-CBA-CCA
35	c	515	DGD	C4D-C5D-C6D-O5D
20	B	602	CLA	C16-C17-C18-C19
34	m	101	LMT	C1-C2-C3-C4
34	b	628	LMT	C2'-C1'-O1'-C1
23	l	101	SQD	O6-C44-C45-O47
23	b	622	SQD	O47-C45-C46-O48
35	D	406	DGD	O2G-C2G-C3G-O3G
24	c	519	LMG	O7-C8-C9-O8
35	d	416	DGD	O1G-C1G-C2G-O2G
24	C	524	LMG	O7-C8-C9-O8
23	A	406	SQD	C35-C36-C37-C38
34	T	102	LMT	C5-C6-C7-C8
34	B	626	LMT	C6-C7-C8-C9
24	b	623	LMG	C31-C32-C33-C34
20	b	617	CLA	C5-C6-C7-C8
20	c	510	CLA	C8-C10-C11-C12
20	b	616	CLA	C2-C1-O2A-CGA
20	b	618	CLA	C10-C11-C12-C13
20	B	605	CLA	C6-C7-C8-C9
20	C	513	CLA	C11-C10-C8-C9
20	B	614	CLA	C14-C13-C15-C16
20	b	618	CLA	C11-C10-C8-C9
20	b	612	CLA	C11-C12-C13-C14
20	a	404	CLA	C11-C12-C13-C15
20	C	513	CLA	C3-C5-C6-C7
38	x	101	RRX	C23-C24-C25-C30
38	x	101	RRX	C23-C24-C25-C26
24	a	410	LMG	C29-C30-C31-C32
22	C	514	BCR	C21-C22-C23-C24
20	b	613	CLA	C13-C15-C16-C17
34	E	101	LMT	O1'-C1-C2-C3
23	b	622	SQD	C28-C29-C30-C31
35	C	516	DGD	O6D-C5D-C6D-O5D
36	d	407	LHG	C26-C27-C28-C29
20	D	404	CLA	C16-C17-C18-C19
20	c	513	CLA	C16-C17-C18-C20
20	b	604	CLA	C16-C17-C18-C20
20	b	613	CLA	C16-C17-C18-C20
36	L	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	b	602	HTG	C4-C5-C6-O6
35	c	515	DGD	CCA-CDA-CEA-CFA
32	B	621	HTG	C4'-C5'-C6'-C7'
24	j	101	LMG	C15-C16-C17-C18
20	B	605	CLA	C6-C7-C8-C10
20	C	504	CLA	C11-C10-C8-C7
20	C	504	CLA	C12-C13-C15-C16
20	c	513	CLA	C12-C13-C15-C16
20	b	603	CLA	C11-C12-C13-C15
20	b	617	CLA	C12-C13-C15-C16
20	c	512	CLA	C11-C10-C8-C7
20	B	607	CLA	C11-C10-C8-C7
20	B	614	CLA	C12-C13-C15-C16
20	d	404	CLA	C6-C7-C8-C10
20	b	618	CLA	C11-C10-C8-C7
20	C	509	CLA	C11-C10-C8-C7
23	a	409	SQD	C28-C29-C30-C31
20	B	612	CLA	C16-C17-C18-C20
23	A	412	SQD	C15-C16-C17-C18
32	C	521	HTG	O5-C1-S1-C1'
32	d	401	HTG	C2'-C1'-S1-C1
32	C	534	HTG	O5-C1-S1-C1'
32	O	302	HTG	C1'-C2'-C3'-C4'
35	d	416	DGD	C5B-C6B-C7B-C8B
20	d	404	CLA	C16-C17-C18-C19
20	B	614	CLA	C10-C11-C12-C13
24	j	101	LMG	C17-C18-C19-C20
35	c	515	DGD	CDA-CEA-CFA-CGA
23	a	409	SQD	C12-C13-C14-C15
34	c	523	LMT	C4-C5-C6-C7
32	d	401	HTG	S1-C1'-C2'-C3'
20	B	611	CLA	C8-C10-C11-C12
20	c	506	CLA	C5-C6-C7-C8
34	m	101	LMT	C2-C3-C4-C5
20	D	404	CLA	CAD-CBD-CGD-O2D
20	B	605	CLA	CAD-CBD-CGD-O2D
20	A	401	CLA	CAD-CBD-CGD-O2D
20	c	513	CLA	CAD-CBD-CGD-O2D
21	a	406	PHO	CAD-CBD-CGD-O2D
20	C	512	CLA	CAD-CBD-CGD-O2D
20	b	606	CLA	CAD-CBD-CGD-O2D
20	a	403	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	C	503	CLA	CAD-CBD-CGD-O2D
20	B	615	CLA	CAD-CBD-CGD-O2D
20	C	509	CLA	CAD-CBD-CGD-O2D
20	b	612	CLA	CAD-CBD-CGD-O2D
23	A	412	SQD	C17-C18-C19-C20
35	c	516	DGD	C2B-C3B-C4B-C5B
35	c	517	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CCB-CDB-CEB-CFB
35	d	416	DGD	O6D-C1D-O3G-C3G
20	c	512	CLA	C15-C16-C17-C18
23	a	401	SQD	O6-C44-C45-C46
35	C	516	DGD	C9A-CAA-CBA-CCA
36	L	101	LHG	O6-C4-C5-O7
36	l	102	LHG	O6-C4-C5-O7
35	H	102	DGD	O2G-C1B-C2B-C3B
24	j	101	LMG	C14-C15-C16-C17
24	B	620	LMG	C30-C31-C32-C33
20	a	404	CLA	C11-C12-C13-C14
20	c	502	CLA	CHA-CBD-CGD-O1D
20	c	507	CLA	CHA-CBD-CGD-O1D
20	C	504	CLA	CHA-CBD-CGD-O1D
20	B	608	CLA	CHA-CBD-CGD-O2D
20	C	506	CLA	CHA-CBD-CGD-O1D
20	B	603	CLA	CHA-CBD-CGD-O2D
20	c	509	CLA	CHA-CBD-CGD-O1D
20	C	508	CLA	CHA-CBD-CGD-O2D
20	c	504	CLA	CHA-CBD-CGD-O1D
20	b	603	CLA	CHA-CBD-CGD-O1D
21	D	403	PHO	CHA-CBD-CGD-O1D
20	b	607	CLA	CHA-CBD-CGD-O1D
20	B	607	CLA	CHA-CBD-CGD-O1D
20	c	508	CLA	CHA-CBD-CGD-O2D
20	C	507	CLA	CHA-CBD-CGD-O1D
20	C	507	CLA	CHA-CBD-CGD-O2D
20	C	509	CLA	C13-C15-C16-C17
20	c	513	CLA	O1A-CGA-O2A-C1
24	A	407	LMG	O1-C7-C8-O7
24	A	407	LMG	O7-C8-C9-O8
23	f	101	SQD	O47-C45-C46-O48
23	l	101	SQD	O47-C45-C46-O48
35	d	416	DGD	O2G-C2G-C3G-O3G
20	D	404	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	C	519	LMG	O10-C28-O8-C9
34	m	102	LMT	O5'-C5'-C6'-O6'
23	l	101	SQD	C35-C36-C37-C38
20	D	401	CLA	C2C-C3C-CAC-CBC
27	A	411	PL9	C4-C3-C7-C8
20	C	504	CLA	C11-C10-C8-C9
20	B	601	CLA	C11-C12-C13-C14
20	c	512	CLA	C11-C10-C8-C9
20	C	502	CLA	C14-C13-C15-C16
23	b	622	SQD	C11-C12-C13-C14
24	A	407	LMG	C39-C40-C41-C42
34	m	101	LMT	C4-C5-C6-C7
36	l	102	LHG	C30-C31-C32-C33
35	C	516	DGD	CDA-CEA-CFA-CGA
20	c	506	CLA	C13-C15-C16-C17
24	a	410	LMG	C20-C21-C22-C23
35	C	516	DGD	CBB-CCB-CDB-CEB
20	c	507	CLA	C5-C6-C7-C8
24	C	524	LMG	C29-C28-O8-C9
34	E	101	LMT	C7-C8-C9-C10
32	C	534	HTG	C4'-C5'-C6'-C7'
36	D	409	LHG	C2-C3-O3-P
36	d	408	LHG	C2-C3-O3-P
35	H	102	DGD	C6A-C7A-C8A-C9A
34	c	523	LMT	C11-C10-C9-C8
36	D	408	LHG	C4-O6-P-O5
20	b	603	CLA	C16-C17-C18-C19
34	b	628	LMT	O5'-C1'-O1'-C1
35	D	406	DGD	CAB-CBB-CCB-CDB
24	C	524	LMG	O10-C28-O8-C9
20	c	502	CLA	CAD-CBD-CGD-O1D
20	C	504	CLA	CAD-CBD-CGD-O1D
20	C	506	CLA	CAD-CBD-CGD-O1D
20	c	504	CLA	CAD-CBD-CGD-O1D
20	B	606	CLA	CAD-CBD-CGD-O1D
20	b	603	CLA	CAD-CBD-CGD-O1D
20	B	602	CLA	CAD-CBD-CGD-O1D
20	b	607	CLA	CAD-CBD-CGD-O1D
20	c	501	CLA	CAD-CBD-CGD-O1D
36	E	103	LHG	C7-C8-C9-C10
36	D	409	LHG	C34-C35-C36-C37
35	c	515	DGD	CBA-CCA-CDA-CEA

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Mol	Chain	Res	Type	Atoms
36	l	102	LHG	C10-C11-C12-C13
34	m	101	LMT	O5B-C5B-C6B-O6B
35	c	515	DGD	C5B-C6B-C7B-C8B
20	C	508	CLA	C11-C12-C13-C14
20	D	404	CLA	C11-C12-C13-C15
32	C	522	HTG	C2-C1-S1-C1'
20	c	513	CLA	C11-C12-C13-C15
20	b	603	CLA	C11-C10-C8-C7
23	l	101	SQD	C7-C8-C9-C10
20	B	601	CLA	C6-C7-C8-C10
20	B	601	CLA	C11-C12-C13-C15
32	D	417	HTG	C2-C1-S1-C1'
21	a	405	PHO	C2-C3-C5-C6
20	d	404	CLA	C11-C12-C13-C15
20	C	509	CLA	C6-C7-C8-C10
32	C	534	HTG	C2-C1-S1-C1'
23	l	101	SQD	C25-C26-C27-C28
34	Z	101	LMT	O5'-C5'-C6'-O6'
32	O	302	HTG	C4'-C5'-C6'-C7'
20	C	503	CLA	C8-C10-C11-C12
36	D	409	LHG	C12-C13-C14-C15
36	L	101	LHG	C30-C31-C32-C33
34	m	101	LMT	C4B-C5B-C6B-O6B
34	m	102	LMT	C5-C6-C7-C8
24	a	410	LMG	C7-C8-C9-O8
35	d	416	DGD	C1G-C2G-C3G-O3G
24	a	410	LMG	O7-C8-C9-O8
36	L	101	LHG	C28-C29-C30-C31
36	D	409	LHG	C10-C11-C12-C13
35	h	101	DGD	C7B-C8B-C9B-CAB
24	J	101	LMG	C34-C35-C36-C37
32	C	521	HTG	C2'-C3'-C4'-C5'
24	B	620	LMG	C14-C15-C16-C17
35	c	516	DGD	C2G-C3G-O3G-C1D
35	c	516	DGD	C5D-C6D-O5D-C1E
35	d	416	DGD	CDB-CEB-CFB-CGB
20	c	507	CLA	C11-C10-C8-C9
20	c	513	CLA	C11-C12-C13-C14
20	b	603	CLA	C11-C12-C13-C14
20	d	404	CLA	C6-C7-C8-C9
20	d	404	CLA	C11-C12-C13-C14
24	C	519	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
23	b	622	SQD	C9-C10-C11-C12
36	d	406	LHG	C15-C16-C17-C18
23	A	406	SQD	C11-C10-C9-C8
24	B	620	LMG	O8-C28-C29-C30
35	d	416	DGD	CAA-CBA-CCA-CDA
36	D	408	LHG	C14-C15-C16-C17
32	B	622	HTG	C4'-C5'-C6'-C7'
24	b	623	LMG	C13-C14-C15-C16
20	B	609	CLA	C13-C15-C16-C17
34	B	626	LMT	C4-C5-C6-C7
36	d	408	LHG	C33-C34-C35-C36
23	A	412	SQD	C24-C25-C26-C27
35	h	101	DGD	C9B-CAB-CBB-CCB
35	D	406	DGD	CBA-CCA-CDA-CEA
36	L	101	LHG	O6-C4-C5-C6
20	b	618	CLA	CBA-CGA-O2A-C1
20	d	402	CLA	C2-C1-O2A-CGA
20	D	401	CLA	C2-C1-O2A-CGA
36	L	101	LHG	C11-C12-C13-C14
24	C	524	LMG	C32-C33-C34-C35
35	D	406	DGD	C8A-C9A-CAA-CBA
24	C	519	LMG	C12-C13-C14-C15
20	b	618	CLA	O1A-CGA-O2A-C1
22	b	619	BCR	C1-C6-C7-C8
32	u	201	HTG	C3'-C4'-C5'-C6'
34	a	418	LMT	C11-C10-C9-C8
24	C	519	LMG	C11-C12-C13-C14
34	J	103	LMT	C2-C3-C4-C5
24	c	519	LMG	O1-C7-C8-O7
21	D	403	PHO	C4C-C3C-CAC-CBC
34	b	627	LMT	C3-C4-C5-C6
35	h	101	DGD	C5B-C6B-C7B-C8B
36	d	407	LHG	C3-O3-P-O6
36	D	408	LHG	C3-O3-P-O6
24	c	518	LMG	C11-C12-C13-C14
24	A	407	LMG	C37-C38-C39-C40
23	F	101	SQD	C24-C25-C26-C27
36	l	102	LHG	C5-C6-O8-C23
24	B	620	LMG	C28-C29-C30-C31
20	d	403	CLA	C4C-C3C-CAC-CBC
35	C	516	DGD	C5A-C6A-C7A-C8A
36	D	407	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	O6D-C5D-C6D-O5D
23	b	622	SQD	C44-C45-C46-O48
35	D	406	DGD	C1G-C2G-C3G-O3G
24	C	524	LMG	C7-C8-C9-O8
34	E	101	LMT	C11-C10-C9-C8
20	D	404	CLA	C11-C10-C8-C7
20	B	602	CLA	C2-C3-C5-C6
20	B	602	CLA	C11-C10-C8-C7
20	B	602	CLA	C12-C13-C15-C16
20	b	616	CLA	C12-C13-C15-C16
20	B	604	CLA	C6-C7-C8-C10
20	B	615	CLA	C12-C13-C15-C16
24	C	524	LMG	C29-C30-C31-C32
35	c	517	DGD	CBB-CCB-CDB-CEB
20	D	404	CLA	C6-C7-C8-C9
20	D	404	CLA	C11-C12-C13-C14
20	C	504	CLA	C14-C13-C15-C16
20	b	617	CLA	C14-C13-C15-C16
20	A	404	CLA	C14-C13-C15-C16
20	D	404	CLA	C16-C17-C18-C20
35	H	102	DGD	C5B-C6B-C7B-C8B
32	c	521	HTG	C2'-C3'-C4'-C5'
36	L	101	LHG	C17-C18-C19-C20
23	A	412	SQD	C24-C23-O48-C46
20	D	401	CLA	C15-C16-C17-C18
32	b	602	HTG	C3'-C4'-C5'-C6'
23	f	101	SQD	C31-C32-C33-C34
24	b	623	LMG	C30-C31-C32-C33
36	d	406	LHG	C11-C10-C9-C8
34	c	523	LMT	O1'-C1-C2-C3
20	b	614	CLA	C10-C11-C12-C13
20	b	616	CLA	C15-C16-C17-C18
23	l	101	SQD	C32-C33-C34-C35
34	a	418	LMT	C7-C8-C9-C10
36	E	103	LHG	C1-C2-C3-O3
27	D	412	PL9	C28-C29-C31-C32
23	A	406	SQD	C10-C11-C12-C13
20	b	613	CLA	C16-C17-C18-C19
32	d	401	HTG	O5-C5-C6-O6
24	c	519	LMG	C31-C32-C33-C34
20	C	508	CLA	CBD-CGD-O2D-CED
35	d	416	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
35	c	516	DGD	O6E-C1E-O5D-C6D
27	A	411	PL9	C14-C16-C17-C18
27	D	412	PL9	C39-C41-C42-C43
36	d	406	LHG	C7-C8-C9-C10
35	c	517	DGD	O6D-C5D-C6D-O5D
20	C	513	CLA	C8-C10-C11-C12
20	b	617	CLA	C8-C10-C11-C12
35	h	101	DGD	CCB-CDB-CEB-CFB
20	C	504	CLA	C5-C6-C7-C8
24	J	101	LMG	C30-C31-C32-C33
27	d	412	PL9	C43-C44-C46-C47
36	D	409	LHG	C29-C30-C31-C32
20	b	603	CLA	C13-C15-C16-C17
20	c	506	CLA	C8-C10-C11-C12
24	a	410	LMG	C31-C32-C33-C34
34	b	627	LMT	C2-C3-C4-C5
36	E	103	LHG	C32-C33-C34-C35
36	D	409	LHG	C11-C12-C13-C14
34	Z	101	LMT	C3-C4-C5-C6
24	C	524	LMG	O1-C7-C8-O7
24	C	524	LMG	C11-C12-C13-C14
36	E	103	LHG	C2-C3-O3-P
35	C	518	DGD	CCA-CDA-CEA-CFA
32	C	521	HTG	C4-C5-C6-O6
36	l	102	LHG	C17-C18-C19-C20
20	c	504	CLA	C11-C12-C13-C14
20	d	402	CLA	C4C-C3C-CAC-CBC
34	f	102	LMT	C5-C6-C7-C8
20	A	401	CLA	C2C-C3C-CAC-CBC
36	E	103	LHG	O2-C2-C3-O3
23	a	409	SQD	C11-C12-C13-C14
36	D	409	LHG	C14-C15-C16-C17
32	B	621	HTG	S1-C1'-C2'-C3'
20	c	503	CLA	C10-C11-C12-C13
24	b	623	LMG	C36-C37-C38-C39
20	C	506	CLA	C6-C7-C8-C10
20	C	507	CLA	C11-C12-C13-C15
20	b	615	CLA	C15-C16-C17-C18
34	E	101	LMT	C5-C6-C7-C8
23	A	412	SQD	O10-C23-O48-C46
20	b	616	CLA	O1D-CGD-O2D-CED
36	d	407	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
36	l	102	LHG	C29-C30-C31-C32
35	d	416	DGD	C5A-C6A-C7A-C8A
27	A	411	PL9	C3-C7-C8-C9
36	d	408	LHG	C13-C14-C15-C16
20	D	402	CLA	C2C-C3C-CAC-CBC
20	B	614	CLA	C15-C16-C17-C18
20	C	513	CLA	C4-C3-C5-C6
27	A	411	PL9	C15-C14-C16-C17
36	D	407	LHG	C29-C30-C31-C32
34	a	418	LMT	C6-C7-C8-C9
32	O	302	HTG	O5-C5-C6-O6
34	z	102	LMT	O5B-C5B-C6B-O6B
23	A	412	SQD	C11-C12-C13-C14
24	a	410	LMG	C39-C40-C41-C42
35	D	406	DGD	CDA-CEA-CFA-CGA
35	H	102	DGD	O1G-C1G-C2G-O2G
20	a	403	CLA	O1D-CGD-O2D-CED
22	k	101	BCR	C19-C20-C21-C22
38	x	101	RRX	C9-C10-C11-C12
36	E	103	LHG	C30-C31-C32-C33
32	c	520	HTG	C2'-C3'-C4'-C5'
36	d	408	LHG	C14-C15-C16-C17
36	E	103	LHG	C5-C6-O8-C23
20	c	503	CLA	C8-C10-C11-C12
27	A	411	PL9	C39-C41-C42-C43
23	F	101	SQD	C25-C26-C27-C28
24	b	623	LMG	C38-C39-C40-C41
35	D	406	DGD	C5B-C6B-C7B-C8B
20	A	402	CLA	C6-C7-C8-C9
20	b	616	CLA	C14-C13-C15-C16
36	l	102	LHG	C11-C12-C13-C14
24	a	410	LMG	C11-C12-C13-C14
27	a	415	PL9	C2-C3-C7-C8
34	J	103	LMT	C6-C7-C8-C9
24	J	101	LMG	C32-C33-C34-C35
35	C	516	DGD	C4D-C5D-C6D-O5D
35	h	101	DGD	O1B-C1B-C2B-C3B
20	b	603	CLA	CAA-CBA-CGA-O2A
36	D	407	LHG	C17-C18-C19-C20
20	C	504	CLA	C15-C16-C17-C18
20	A	404	CLA	C8-C10-C11-C12
22	b	619	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	k	102	BCR	C1-C6-C7-C8
23	l	101	SQD	O6-C44-C45-C46
24	C	519	LMG	C32-C33-C34-C35
34	E	101	LMT	C3-C4-C5-C6
35	c	515	DGD	C5D-C6D-O5D-C1E
24	B	620	LMG	C20-C21-C22-C23
34	B	626	LMT	C4'-C5'-C6'-O6'
24	c	518	LMG	C14-C15-C16-C17
20	B	616	CLA	C13-C15-C16-C17
23	f	101	SQD	C30-C31-C32-C33
27	a	415	PL9	C39-C41-C42-C43
35	C	517	DGD	C2E-C1E-O5D-C6D
35	c	517	DGD	C6A-C7A-C8A-C9A
36	D	409	LHG	C33-C34-C35-C36
20	b	612	CLA	C16-C17-C18-C20
20	C	513	CLA	C10-C11-C12-C13
20	c	509	CLA	O1D-CGD-O2D-CED
27	A	411	PL9	C20-C19-C21-C22
20	d	403	CLA	C13-C15-C16-C17
27	A	411	PL9	C13-C14-C16-C17
34	Z	101	LMT	C11-C10-C9-C8
32	b	602	HTG	O5-C5-C6-O6
23	A	406	SQD	O47-C7-C8-C9
24	A	407	LMG	C38-C39-C40-C41
20	B	616	CLA	C14-C13-C15-C16
20	B	601	CLA	C6-C7-C8-C9
20	b	616	CLA	C11-C10-C8-C9
20	C	509	CLA	C6-C7-C8-C9
20	C	507	CLA	C11-C12-C13-C14
20	D	401	CLA	C4C-C3C-CAC-CBC
24	j	101	LMG	C35-C36-C37-C38
36	d	408	LHG	C31-C32-C33-C34
20	c	509	CLA	CAD-CBD-CGD-O2D
20	c	503	CLA	CAD-CBD-CGD-O2D
20	b	603	CLA	CAD-CBD-CGD-O2D
21	D	403	PHO	CAD-CBD-CGD-O2D
20	B	601	CLA	CAD-CBD-CGD-O2D
20	B	611	CLA	CAD-CBD-CGD-O2D
20	c	512	CLA	CAD-CBD-CGD-O2D
21	A	403	PHO	CAD-CBD-CGD-O2D
21	a	405	PHO	CAD-CBD-CGD-O2D
20	C	501	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	601	CLA	C16-C17-C18-C19
23	A	412	SQD	C14-C15-C16-C17
20	C	506	CLA	C15-C16-C17-C18
23	F	101	SQD	O48-C23-C24-C25
20	C	512	CLA	CAA-CBA-CGA-O2A
36	L	101	LHG	C32-C33-C34-C35
32	b	625	HTG	C4'-C5'-C6'-C7'
24	C	519	LMG	C15-C16-C17-C18
20	C	513	CLA	C2-C3-C5-C6
36	E	103	LHG	O7-C5-C6-O8
35	d	416	DGD	CCA-CDA-CEA-CFA
23	l	101	SQD	C44-C45-C46-O48
24	c	519	LMG	O1-C7-C8-C9
20	B	612	CLA	C16-C17-C18-C19
36	d	407	LHG	C31-C32-C33-C34
20	B	605	CLA	O2A-C1-C2-C3
20	C	512	CLA	O2A-C1-C2-C3
21	A	403	PHO	O2A-C1-C2-C3
20	b	606	CLA	O2A-C1-C2-C3
20	D	401	CLA	O2A-C1-C2-C3
20	B	614	CLA	O2A-C1-C2-C3
20	b	618	CLA	O2A-C1-C2-C3
20	B	611	CLA	C4C-C3C-CAC-CBC
36	l	102	LHG	C9-C10-C11-C12
36	E	103	LHG	O8-C23-C24-C25
24	C	524	LMG	C4-C5-C6-O5
20	c	510	CLA	C16-C17-C18-C19
34	b	628	LMT	C6-C7-C8-C9
20	c	507	CLA	CHA-CBD-CGD-O2D
20	B	603	CLA	CHA-CBD-CGD-O1D
20	d	403	CLA	CHA-CBD-CGD-O1D
20	d	403	CLA	CHA-CBD-CGD-O2D
20	D	402	CLA	CHA-CBD-CGD-O2D
20	B	606	CLA	CHA-CBD-CGD-O1D
21	D	403	PHO	CHA-CBD-CGD-O2D
20	A	402	CLA	CHA-CBD-CGD-O1D
21	a	406	PHO	CHA-CBD-CGD-O1D
20	B	607	CLA	CHA-CBD-CGD-O2D
20	b	618	CLA	CHA-CBD-CGD-O1D
20	b	613	CLA	CHA-CBD-CGD-O2D
20	c	512	CLA	CAA-CBA-CGA-O2A
20	A	401	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
20	b	614	CLA	C8-C10-C11-C12
32	d	401	HTG	C4'-C5'-C6'-C7'
24	j	101	LMG	O7-C10-C11-C12
23	f	101	SQD	O48-C23-C24-C25
36	L	101	LHG	C25-C26-C27-C28
24	b	623	LMG	C17-C18-C19-C20
34	b	628	LMT	C11-C10-C9-C8
20	D	404	CLA	C12-C13-C15-C16
20	B	616	CLA	C12-C13-C15-C16
27	d	412	PL9	C28-C29-C31-C32
20	B	615	CLA	C14-C13-C15-C16
20	b	613	CLA	C14-C13-C15-C16
38	H	101	RRX	C9-C10-C11-C12
36	L	101	LHG	C13-C14-C15-C16
23	A	412	SQD	C33-C34-C35-C36
20	b	616	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	C6B-C7B-C8B-C9B
21	a	406	PHO	C4C-C3C-CAC-CBC
35	h	101	DGD	CDA-CEA-CFA-CGA
23	a	401	SQD	C30-C31-C32-C33
22	K	101	BCR	C17-C18-C19-C20
22	K	102	BCR	C7-C8-C9-C10
34	a	418	LMT	O1'-C1-C2-C3
20	c	512	CLA	C1A-C2A-CAA-CBA
23	A	406	SQD	O49-C7-C8-C9
36	E	103	LHG	O10-C23-C24-C25
36	l	102	LHG	C26-C27-C28-C29
35	C	516	DGD	C7B-C8B-C9B-CAB
20	b	604	CLA	C8-C10-C11-C12
23	F	101	SQD	O10-C23-C24-C25
22	C	514	BCR	C9-C10-C11-C12
35	c	516	DGD	C4E-C5E-C6E-O5E
35	C	517	DGD	C4A-C5A-C6A-C7A
20	C	501	CLA	C2A-CAA-CBA-CGA
20	b	604	CLA	C2A-CAA-CBA-CGA
35	C	518	DGD	C4B-C5B-C6B-C7B
20	c	512	CLA	CAA-CBA-CGA-O1A
35	c	516	DGD	C2E-C1E-O5D-C6D
36	D	408	LHG	C3-O3-P-O5
20	C	512	CLA	CAA-CBA-CGA-O1A
24	A	407	LMG	C19-C20-C21-C22
22	k	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
20	b	614	CLA	C3-C5-C6-C7
22	j	102	BCR	C1-C6-C7-C8
22	j	102	BCR	C5-C6-C7-C8
22	K	101	BCR	C1-C6-C7-C8
22	K	101	BCR	C5-C6-C7-C8
35	H	102	DGD	CCB-CDB-CEB-CFB
35	h	101	DGD	C9A-CAA-CBA-CCA
20	A	401	CLA	C15-C16-C17-C18
20	B	604	CLA	C5-C6-C7-C8
20	b	613	CLA	C8-C10-C11-C12
35	H	102	DGD	CCA-CDA-CEA-CFA
23	A	412	SQD	C13-C14-C15-C16
20	a	404	CLA	CAD-CBD-CGD-O1D
20	B	610	CLA	CAD-CBD-CGD-O1D
20	C	512	CLA	CAD-CBD-CGD-O1D
20	b	609	CLA	CAD-CBD-CGD-O1D
20	c	506	CLA	CAD-CBD-CGD-O1D
35	H	102	DGD	O1B-C1B-C2B-C3B
20	C	505	CLA	CAA-CBA-CGA-O2A
20	C	506	CLA	C6-C7-C8-C9
36	d	406	LHG	C32-C33-C34-C35
24	c	518	LMG	C32-C33-C34-C35
35	C	516	DGD	C2A-C3A-C4A-C5A
24	j	101	LMG	O9-C10-C11-C12
34	z	102	LMT	C4-C5-C6-C7
20	B	614	CLA	C13-C15-C16-C17
24	B	620	LMG	C36-C37-C38-C39
35	c	515	DGD	C6A-C7A-C8A-C9A
34	B	627	LMT	C2-C3-C4-C5
34	m	101	LMT	C11-C10-C9-C8
35	h	101	DGD	CAA-CBA-CCA-CDA
24	b	623	LMG	O8-C28-C29-C30
35	c	516	DGD	C4A-C5A-C6A-C7A
20	c	510	CLA	C16-C17-C18-C20
23	A	406	SQD	C33-C34-C35-C36
20	c	502	CLA	C11-C12-C13-C15
20	c	507	CLA	C11-C12-C13-C15
20	B	603	CLA	C11-C12-C13-C15
20	c	504	CLA	C12-C13-C15-C16
20	b	618	CLA	C12-C13-C15-C16
20	c	506	CLA	C11-C10-C8-C7
23	f	101	SQD	O10-C23-C24-C25

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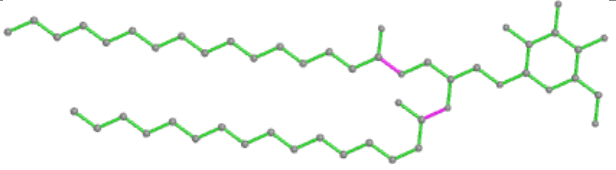
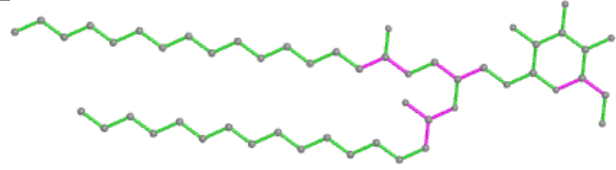
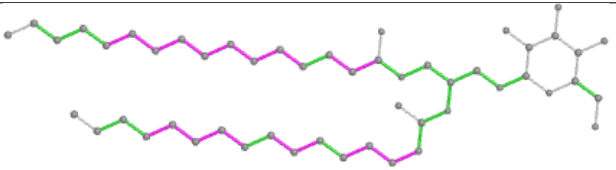
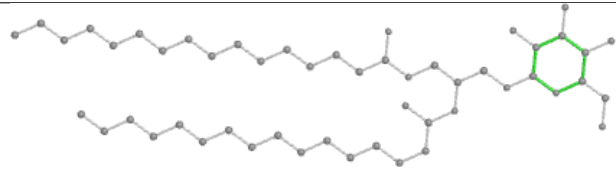
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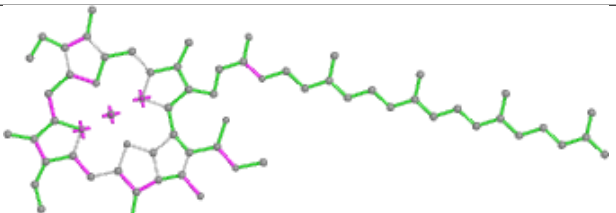
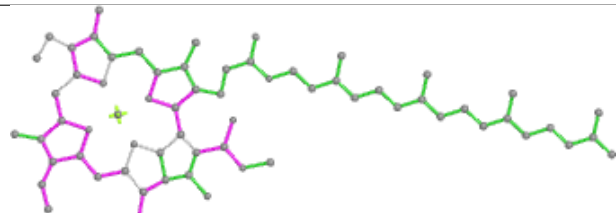
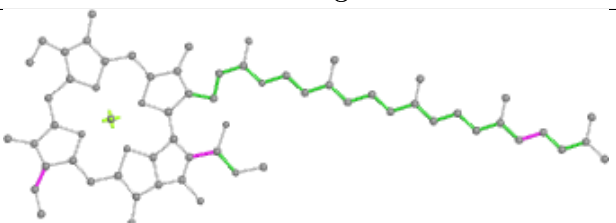
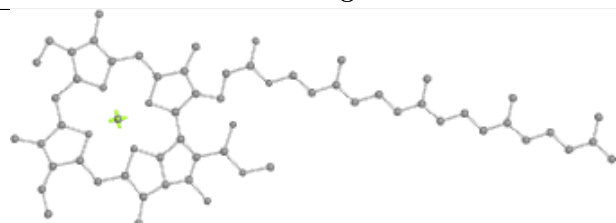
Mol	Chain	Res	Type	Atoms
24	J	101	LMG	O7-C10-C11-C12
35	C	517	DGD	O2G-C1B-C2B-C3B
20	c	505	CLA	CAA-CBA-CGA-O2A
35	c	516	DGD	C7A-C8A-C9A-CAA
24	C	519	LMG	C16-C17-C18-C19
36	l	102	LHG	C7-C8-C9-C10
24	c	518	LMG	O6-C5-C6-O5
36	L	101	LHG	C26-C27-C28-C29
35	C	517	DGD	O6E-C1E-O5D-C6D
35	c	515	DGD	O6E-C1E-O5D-C6D
35	C	516	DGD	O6E-C1E-O5D-C6D
20	B	602	CLA	C5-C6-C7-C8
36	D	407	LHG	C11-C10-C9-C8
32	C	522	HTG	C4-C5-C6-O6
20	C	501	CLA	CAA-CBA-CGA-O2A
35	c	517	DGD	O1G-C1A-C2A-C3A
20	c	501	CLA	CAA-CBA-CGA-O2A
36	E	103	LHG	C24-C25-C26-C27
20	b	603	CLA	C8-C10-C11-C12
20	D	402	CLA	C15-C16-C17-C18
23	l	101	SQD	C19-C20-C21-C22
27	d	412	PL9	C45-C44-C46-C47
23	a	409	SQD	O47-C7-C8-C9
36	D	409	LHG	O8-C23-C24-C25


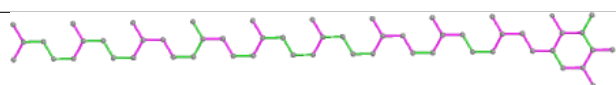
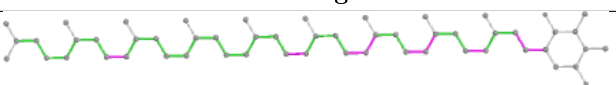
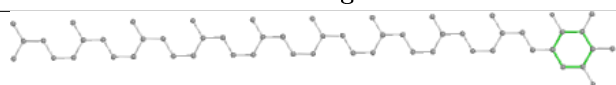
There are no ring outliers.

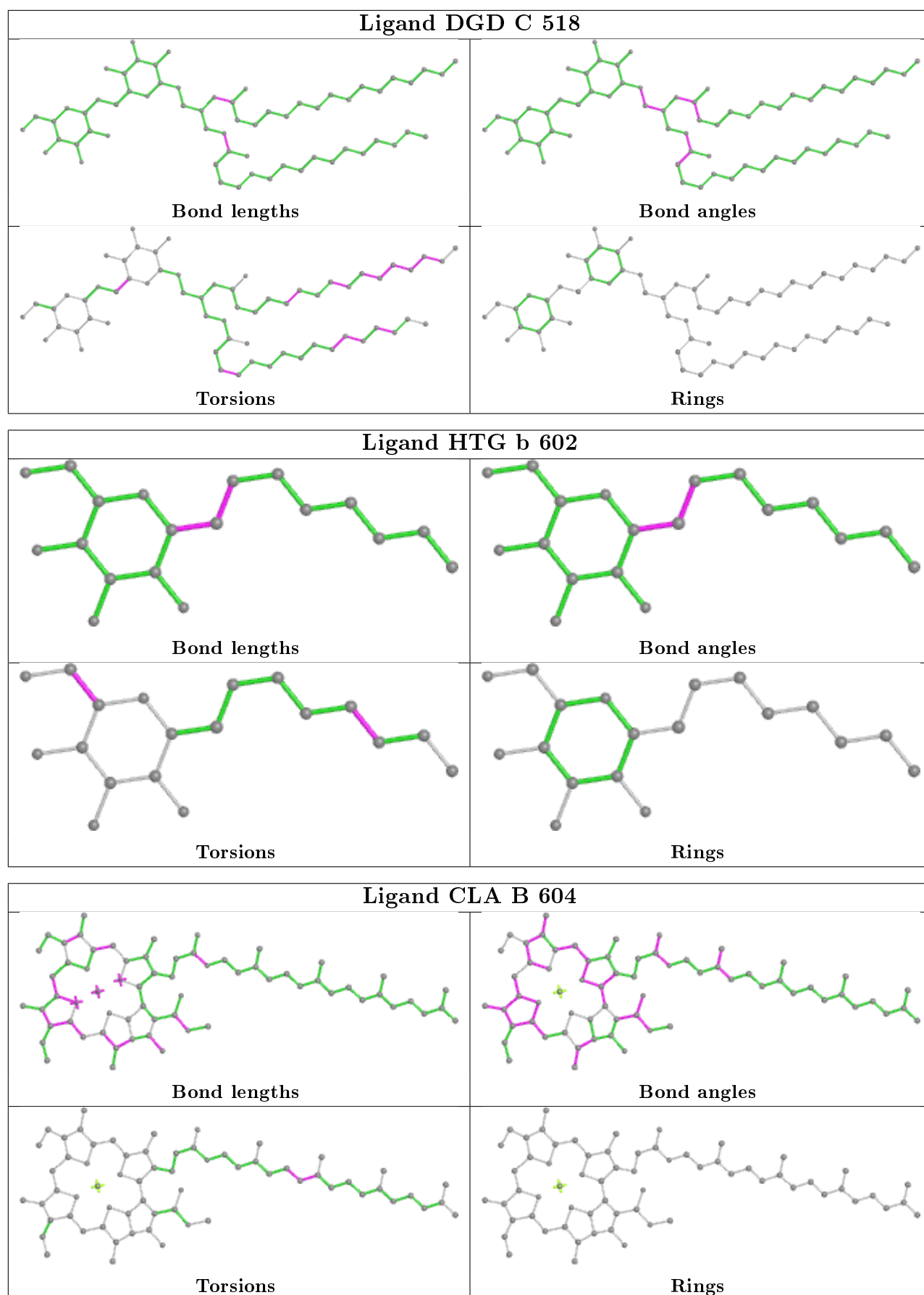
No monomer is involved in short contacts.

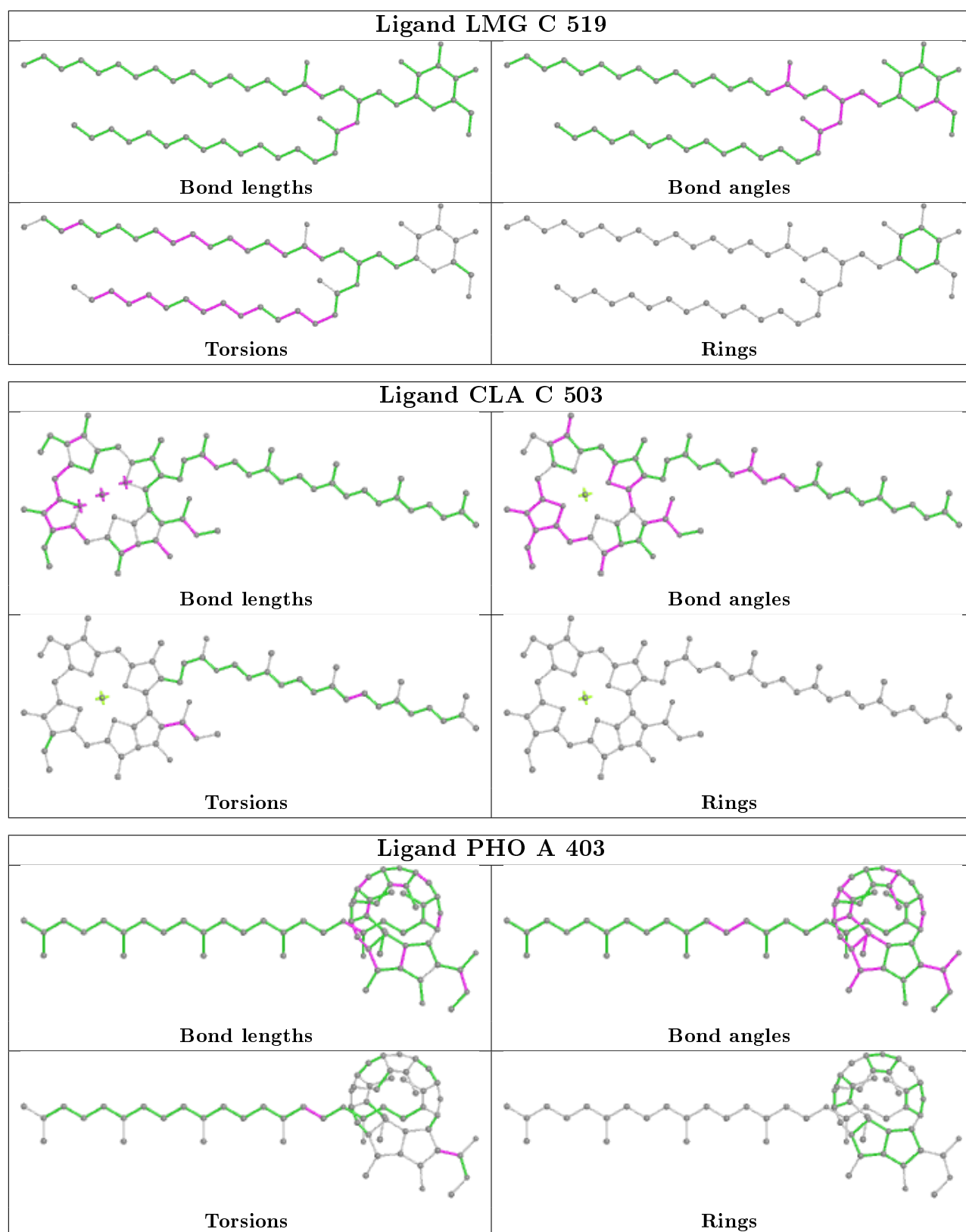
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

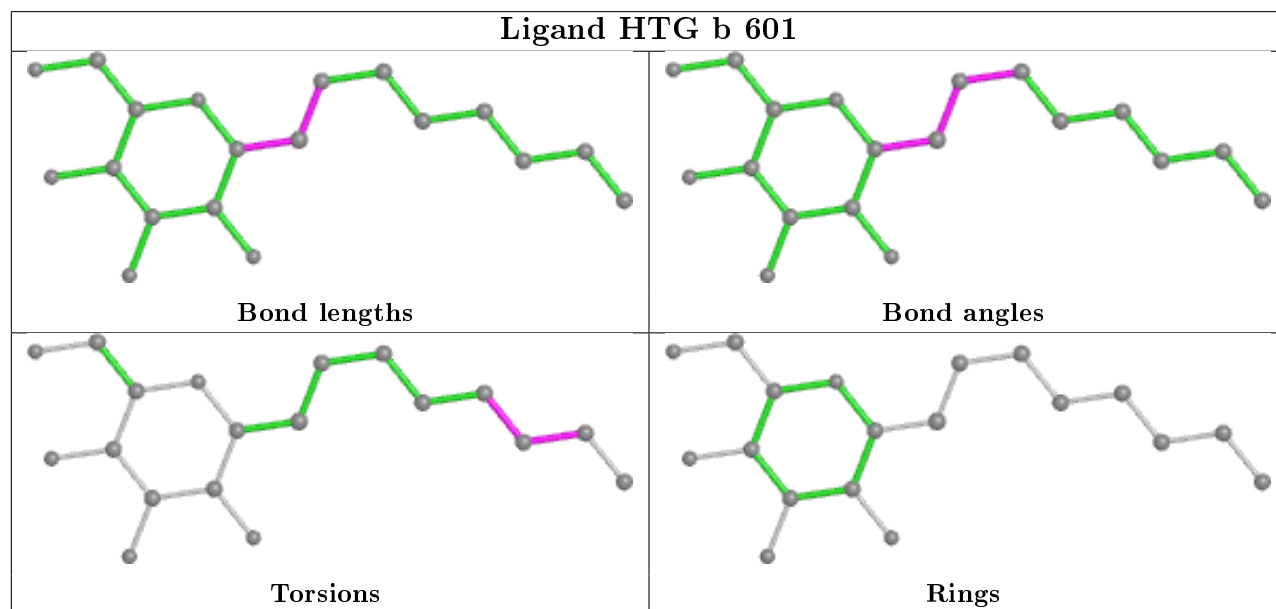
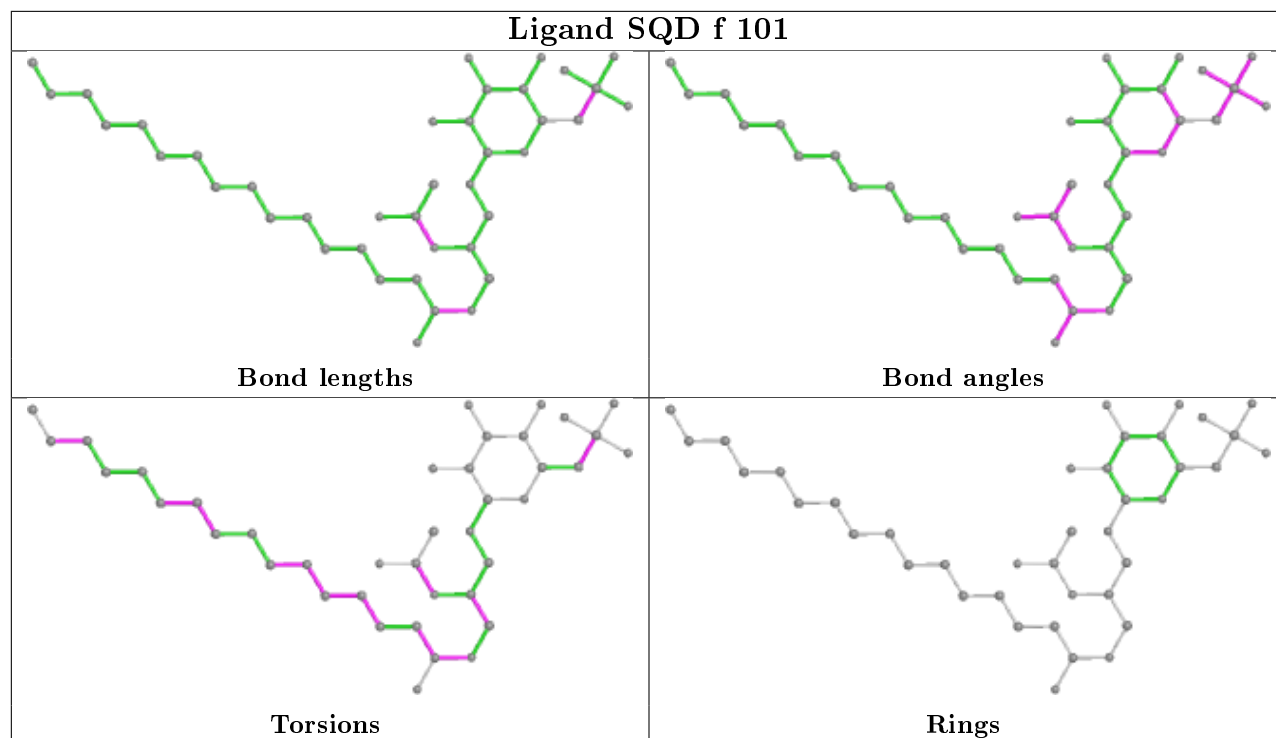
Ligand LMG B 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA d 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

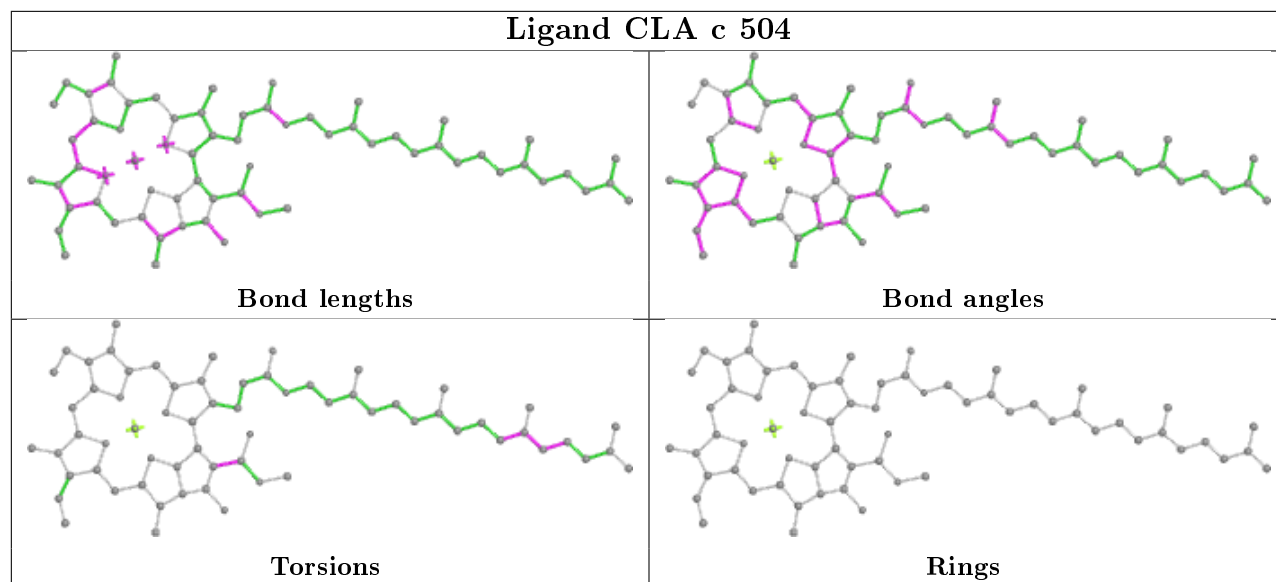
Ligand PL9 A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings



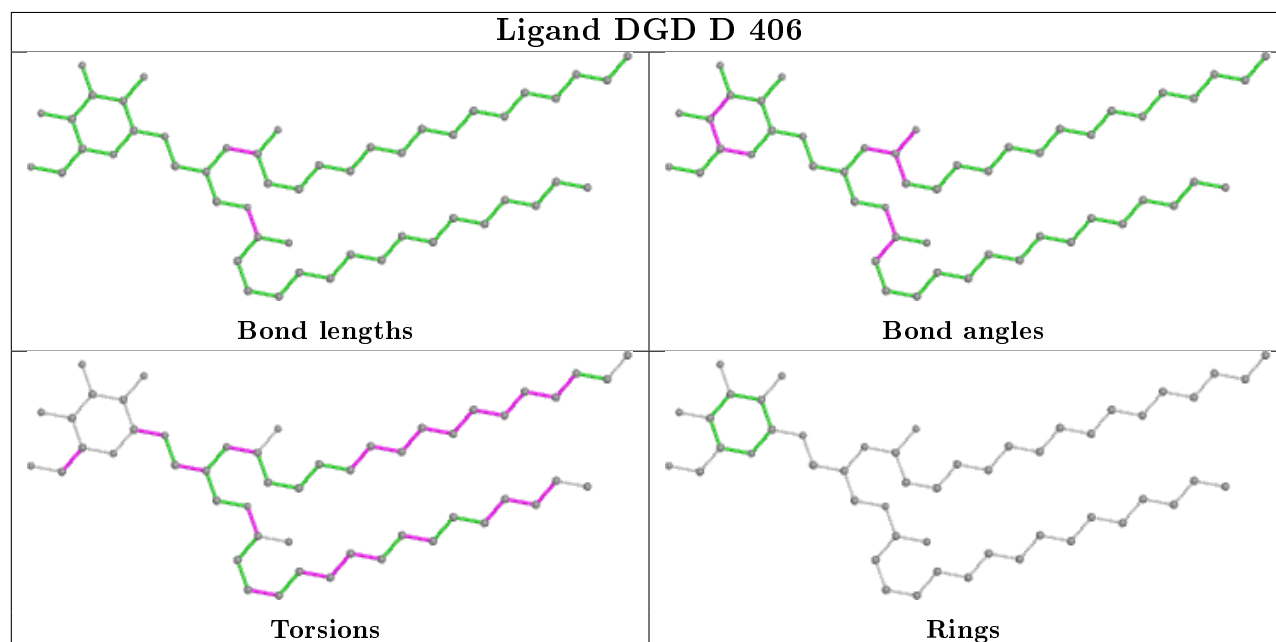




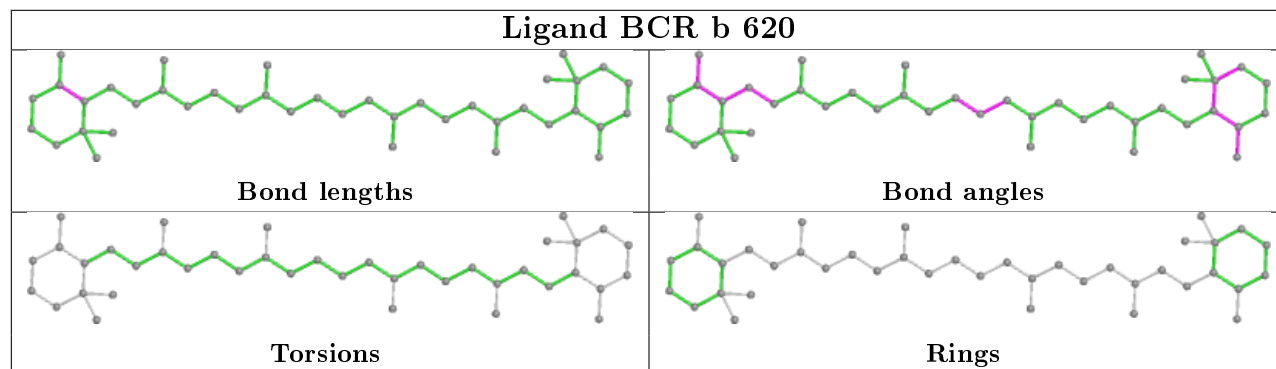
Ligand CLA c 504

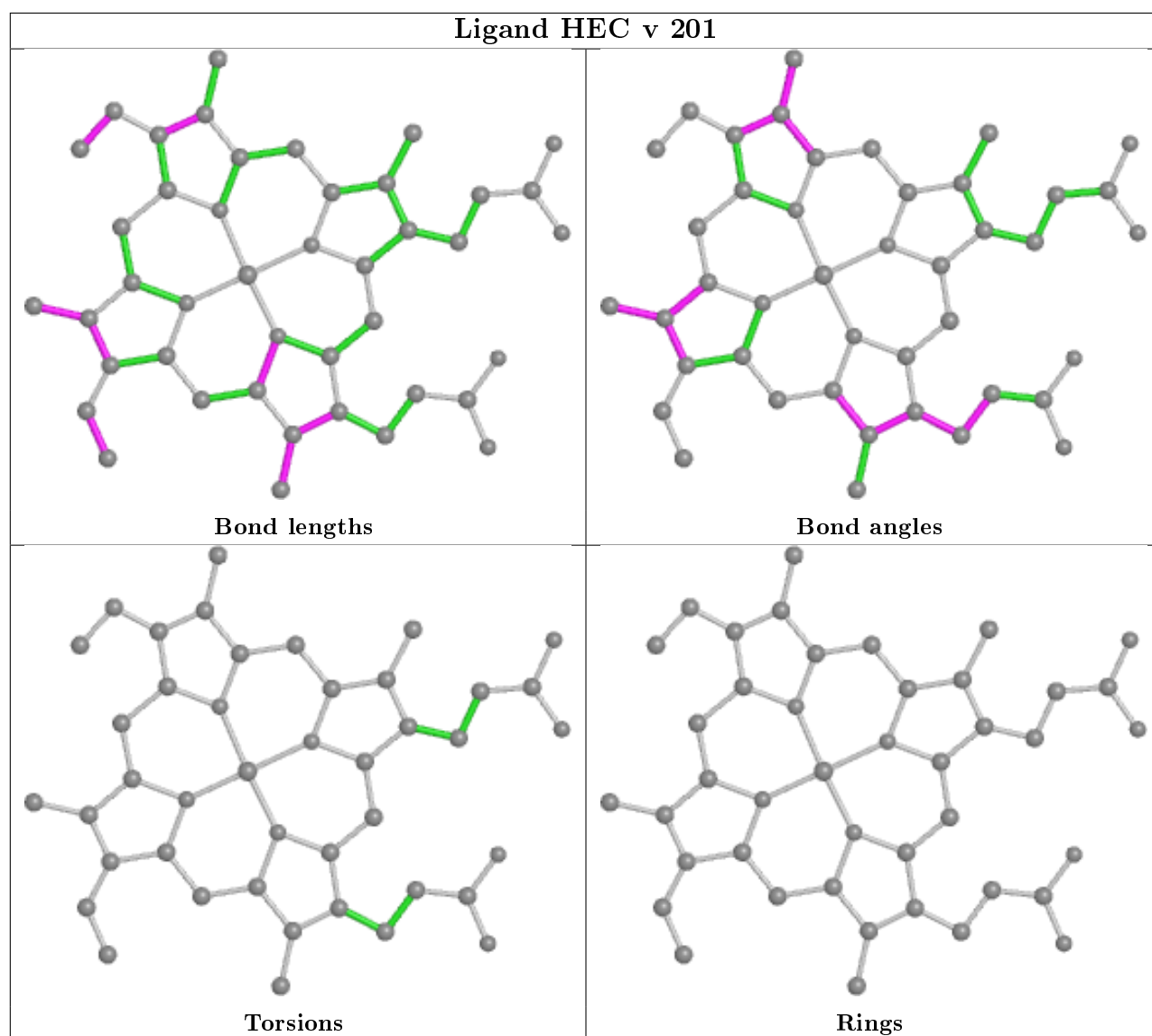
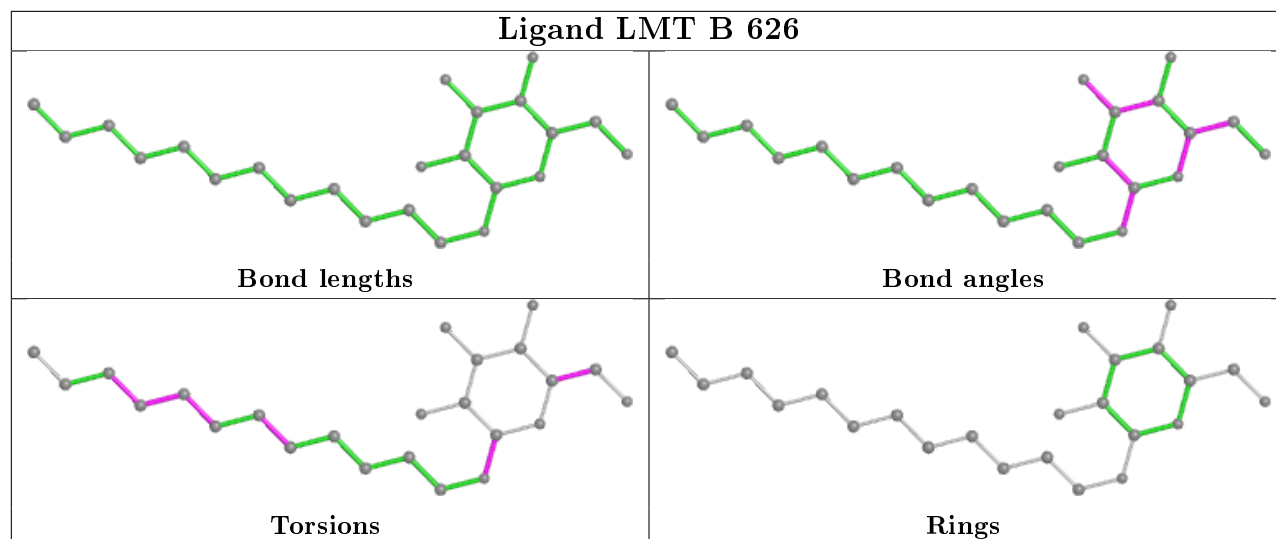


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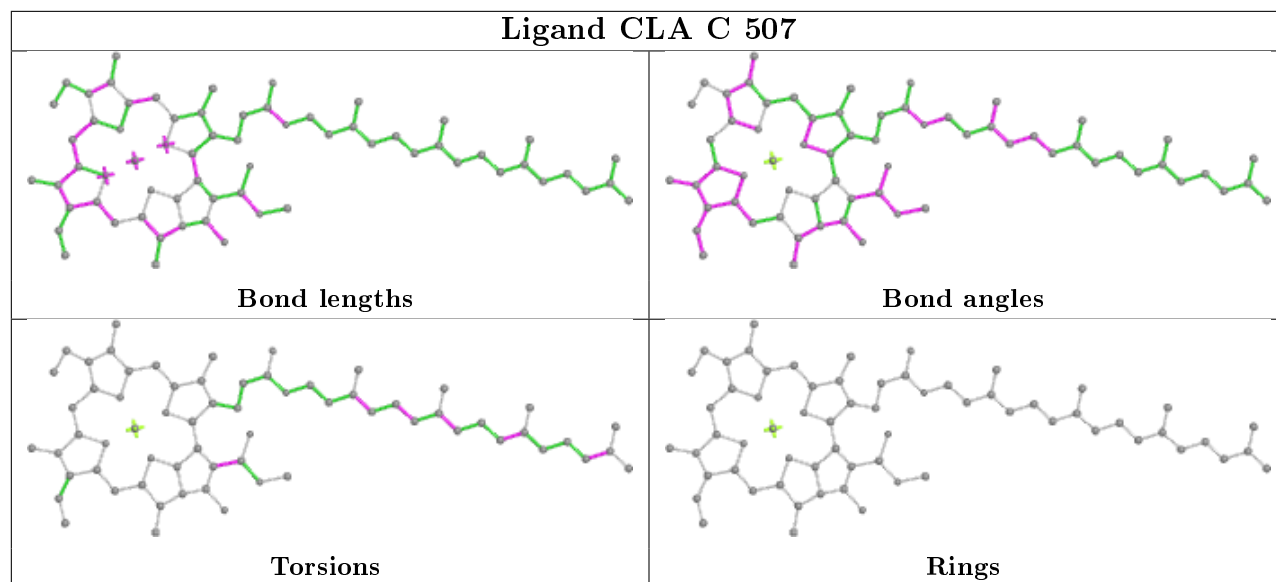


Ligand BCR b 620

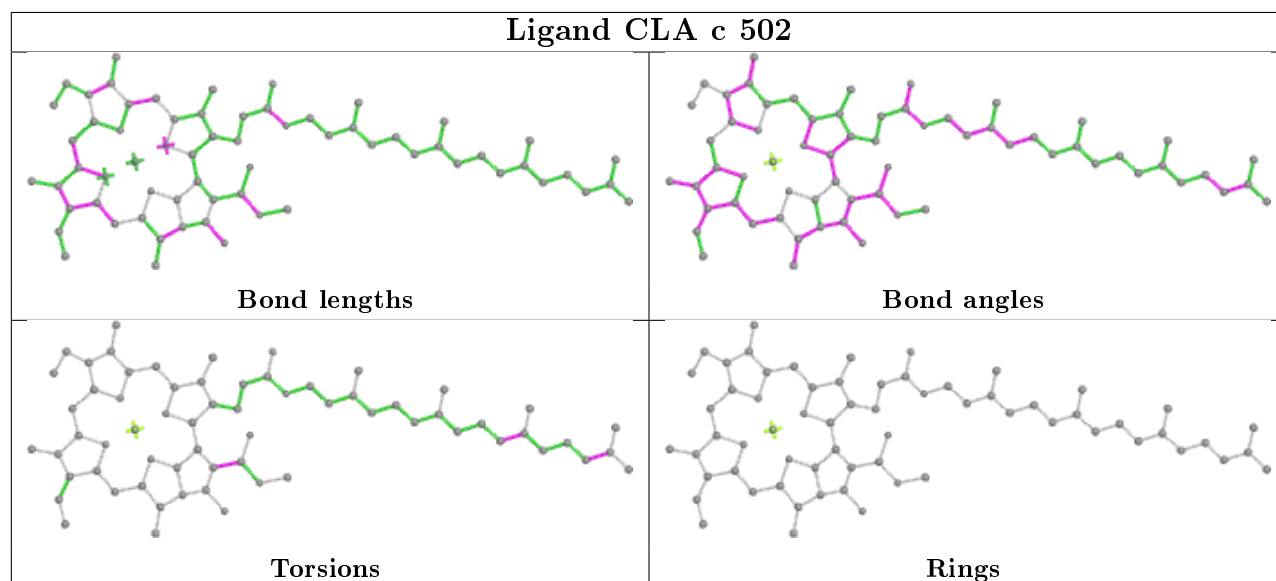




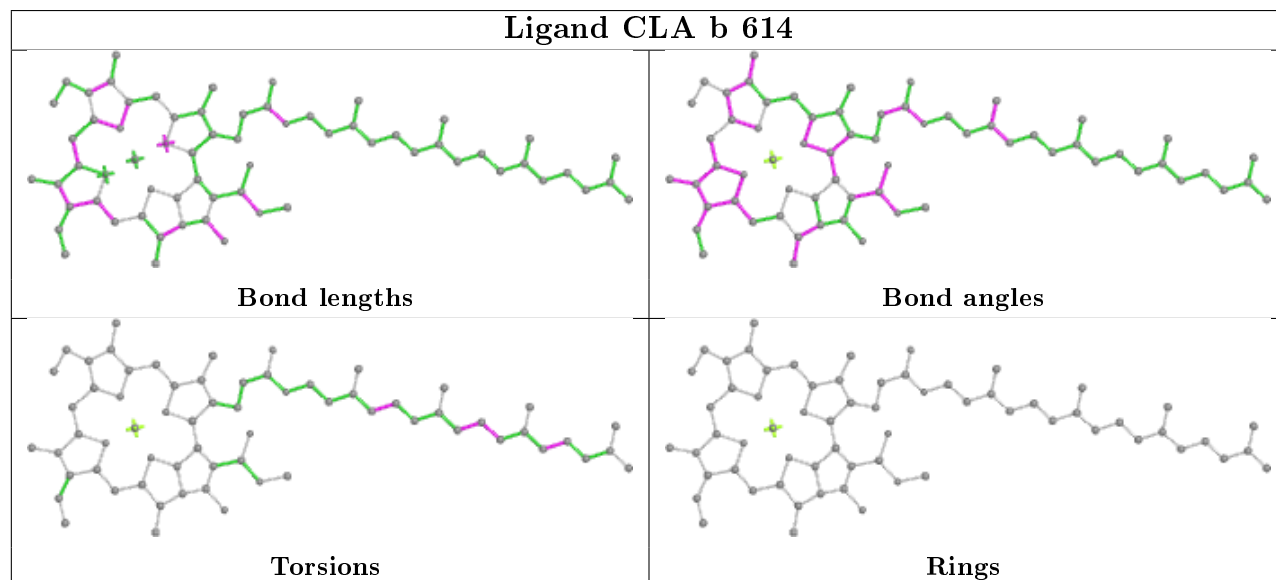
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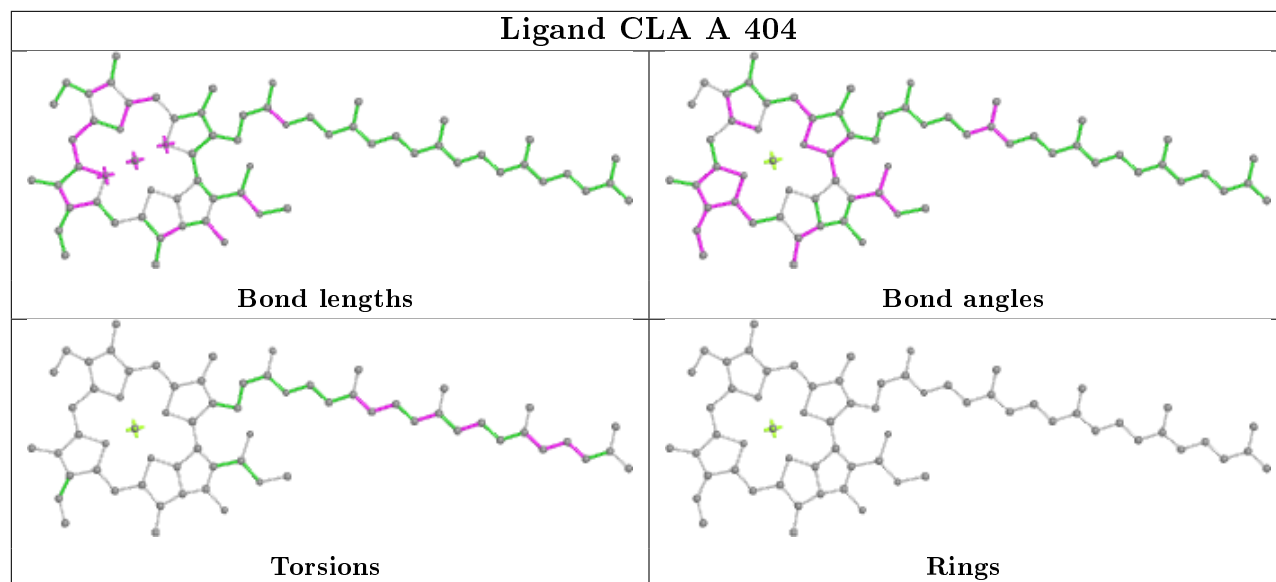
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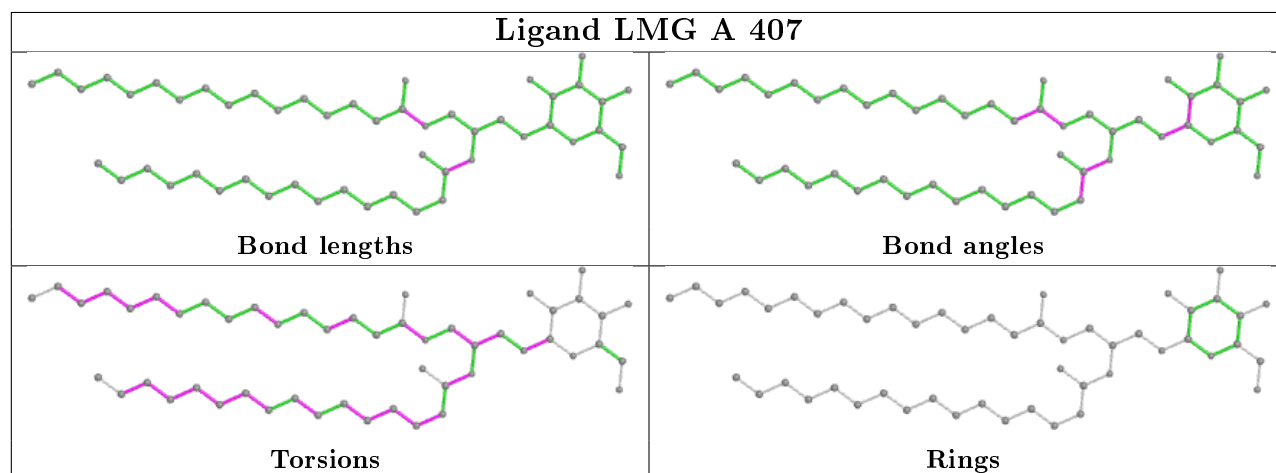
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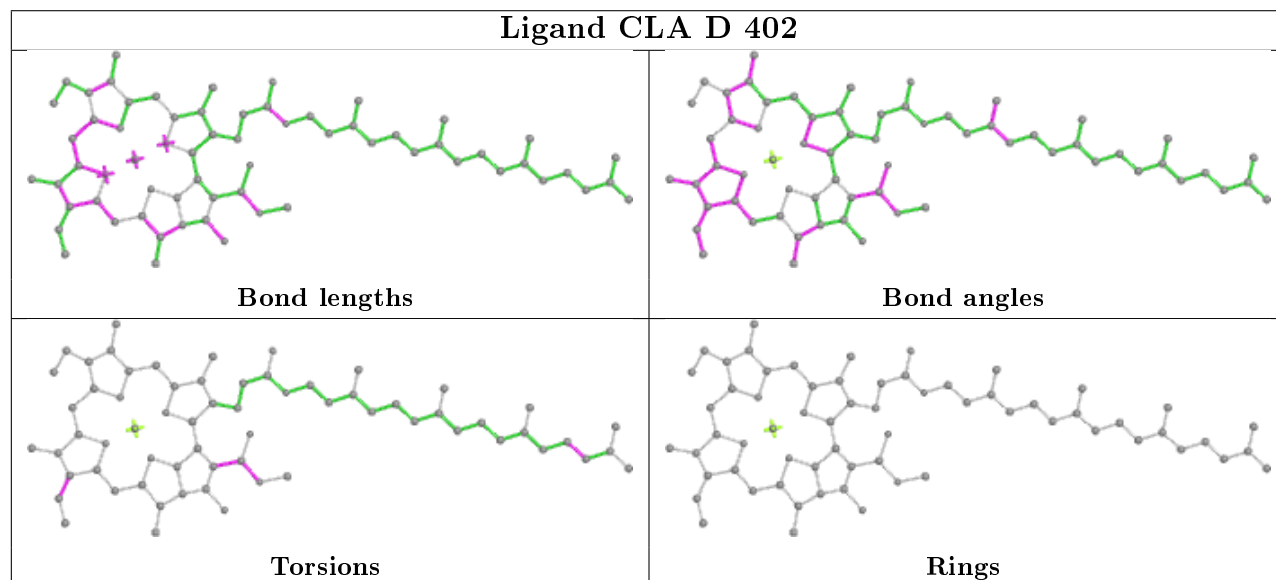
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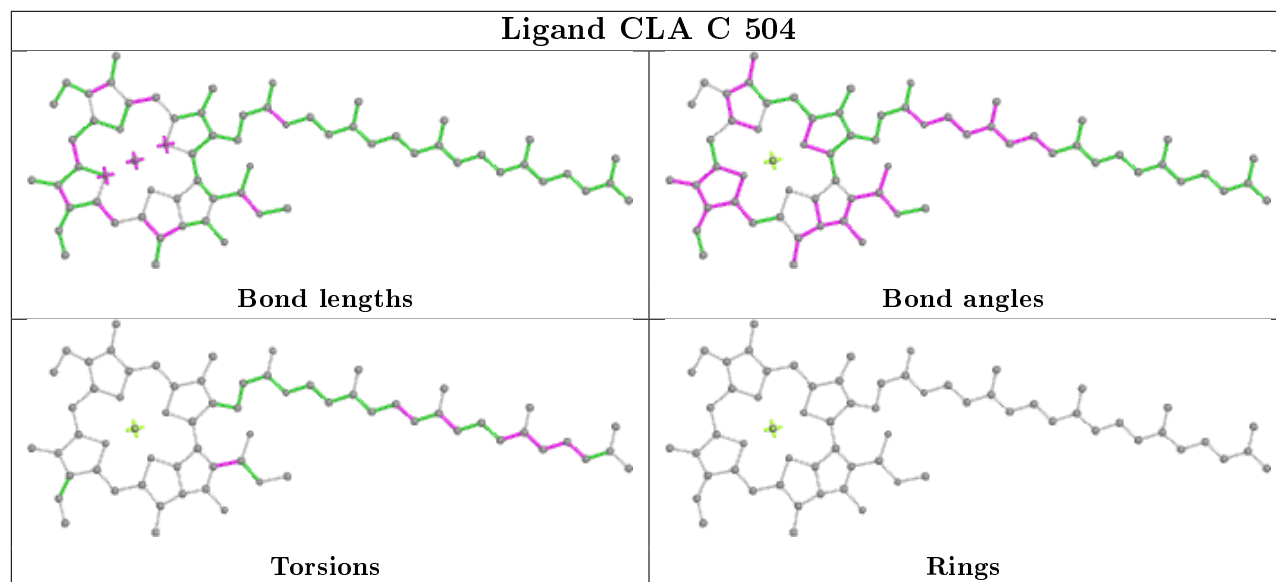
Ligand LMG A 407



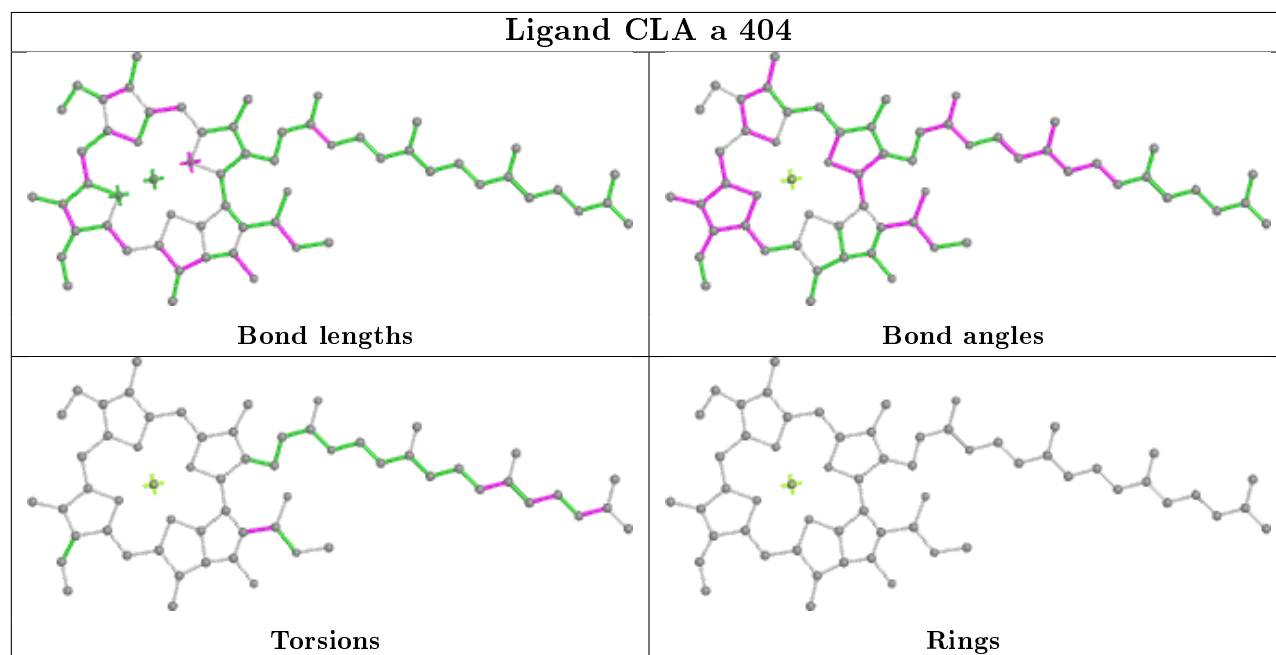
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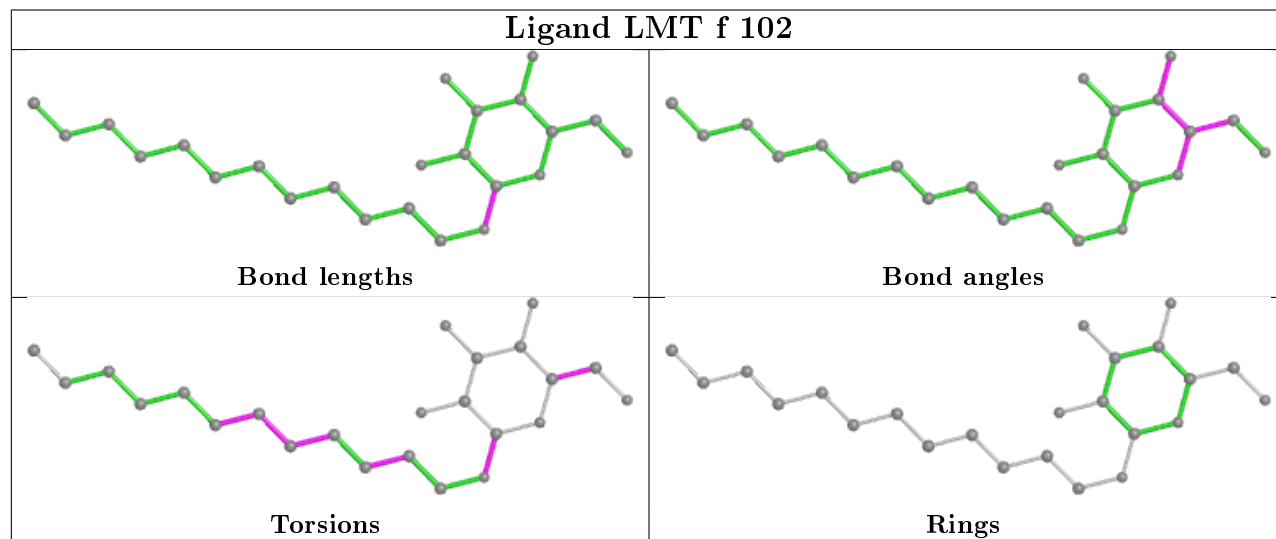
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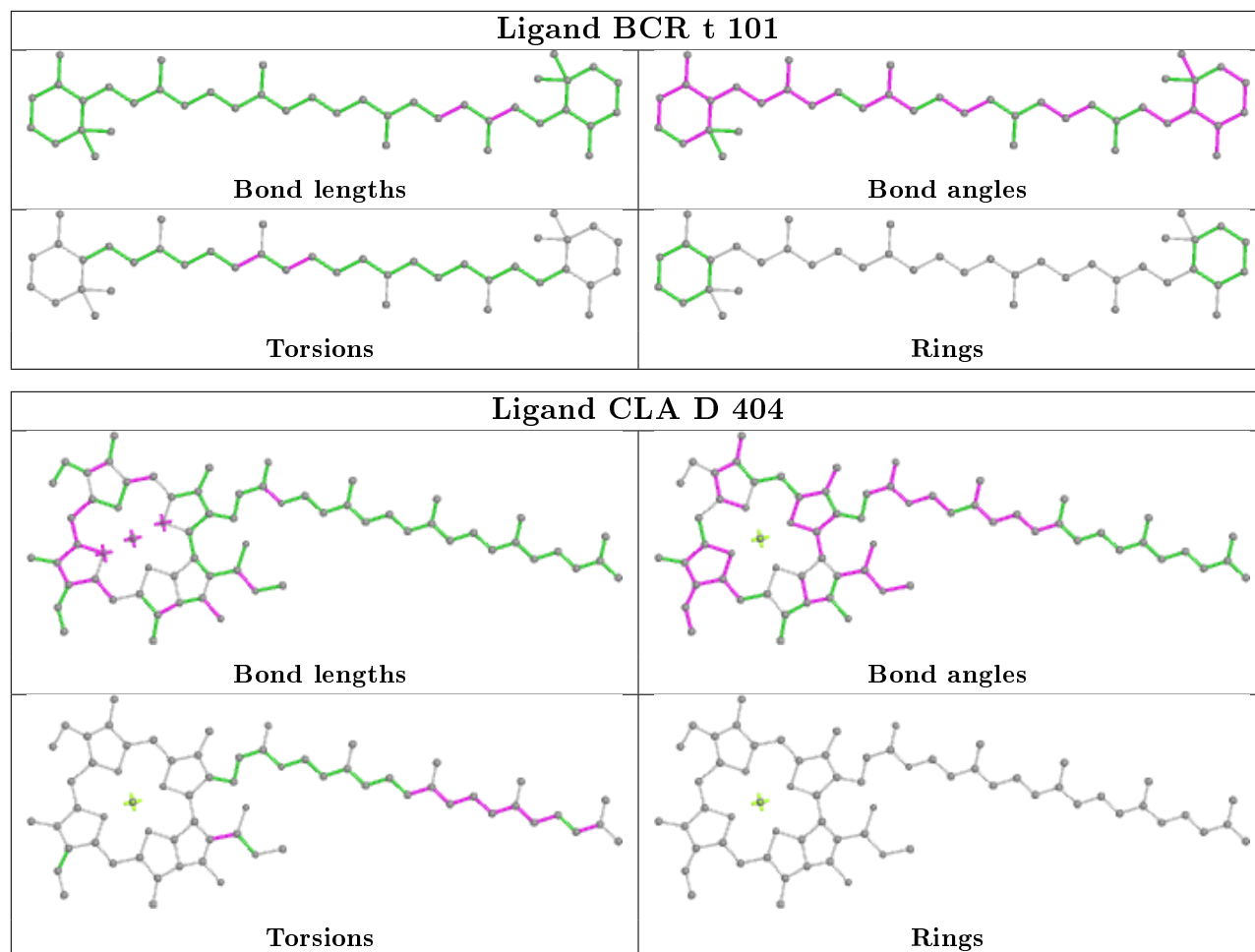


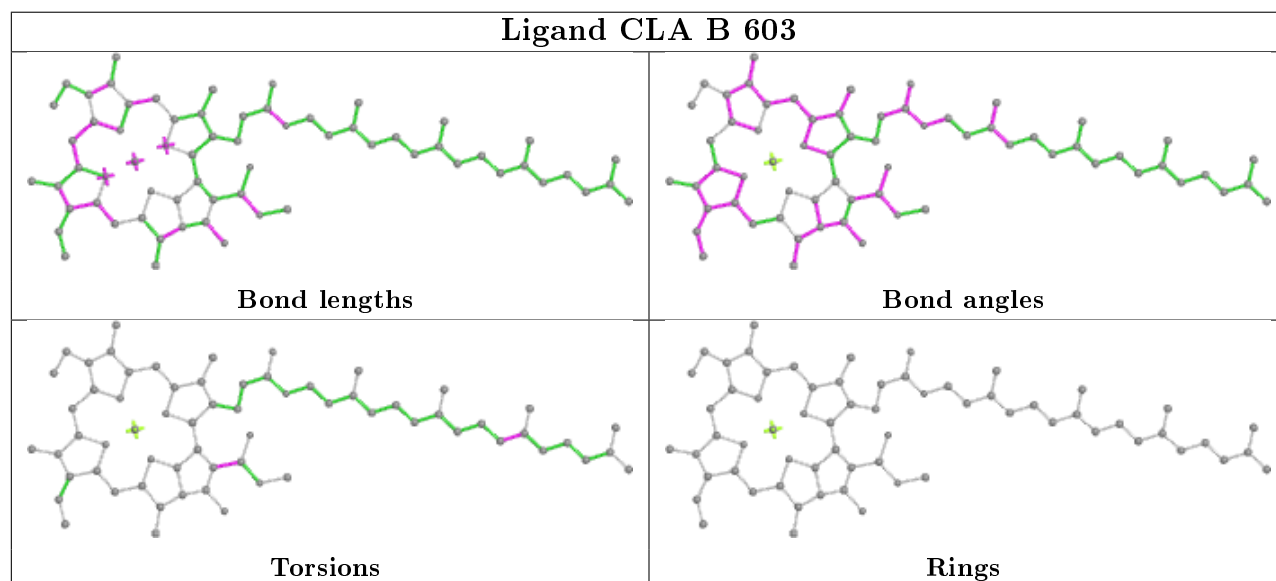
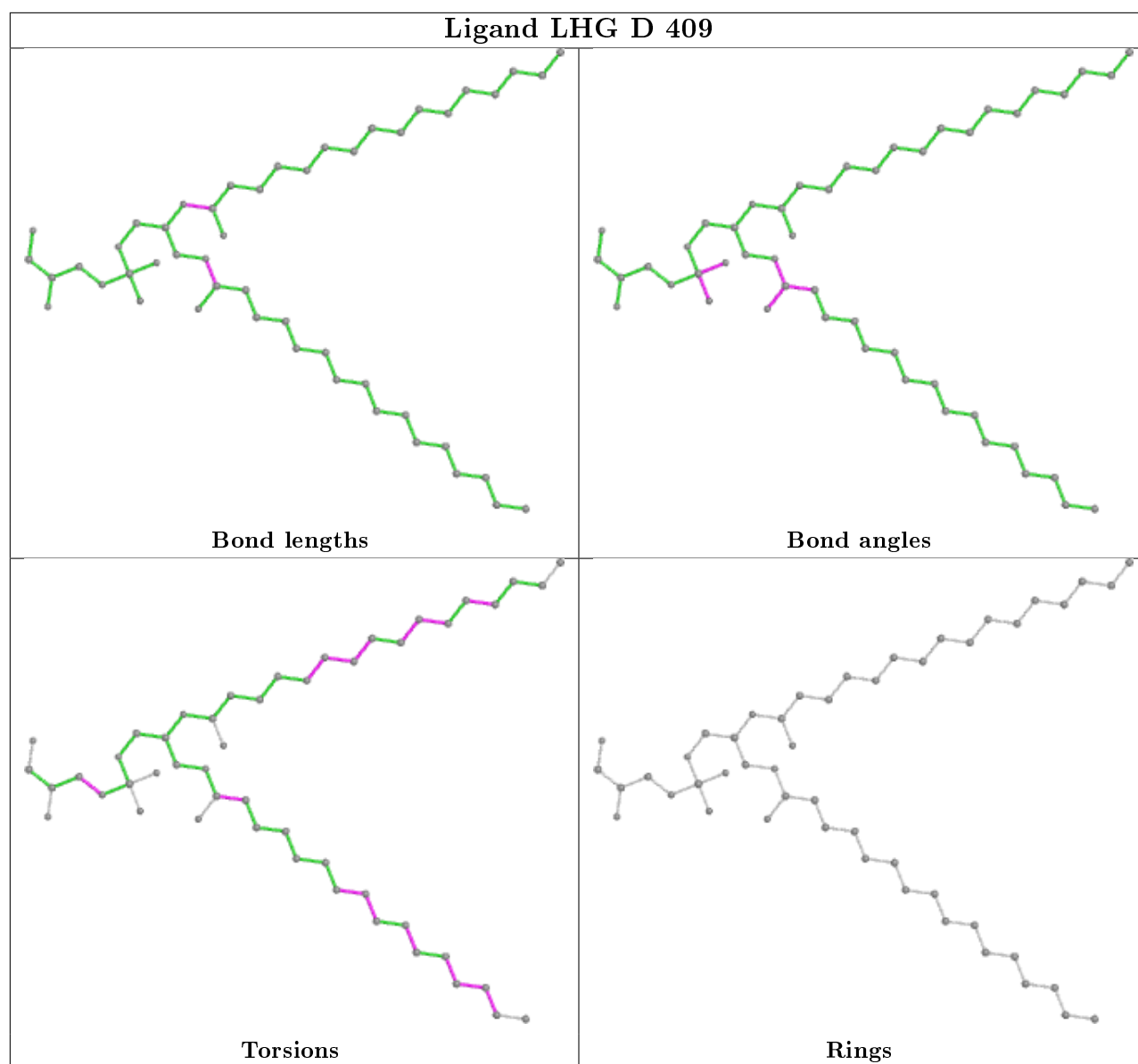
Ligand CLA a 404

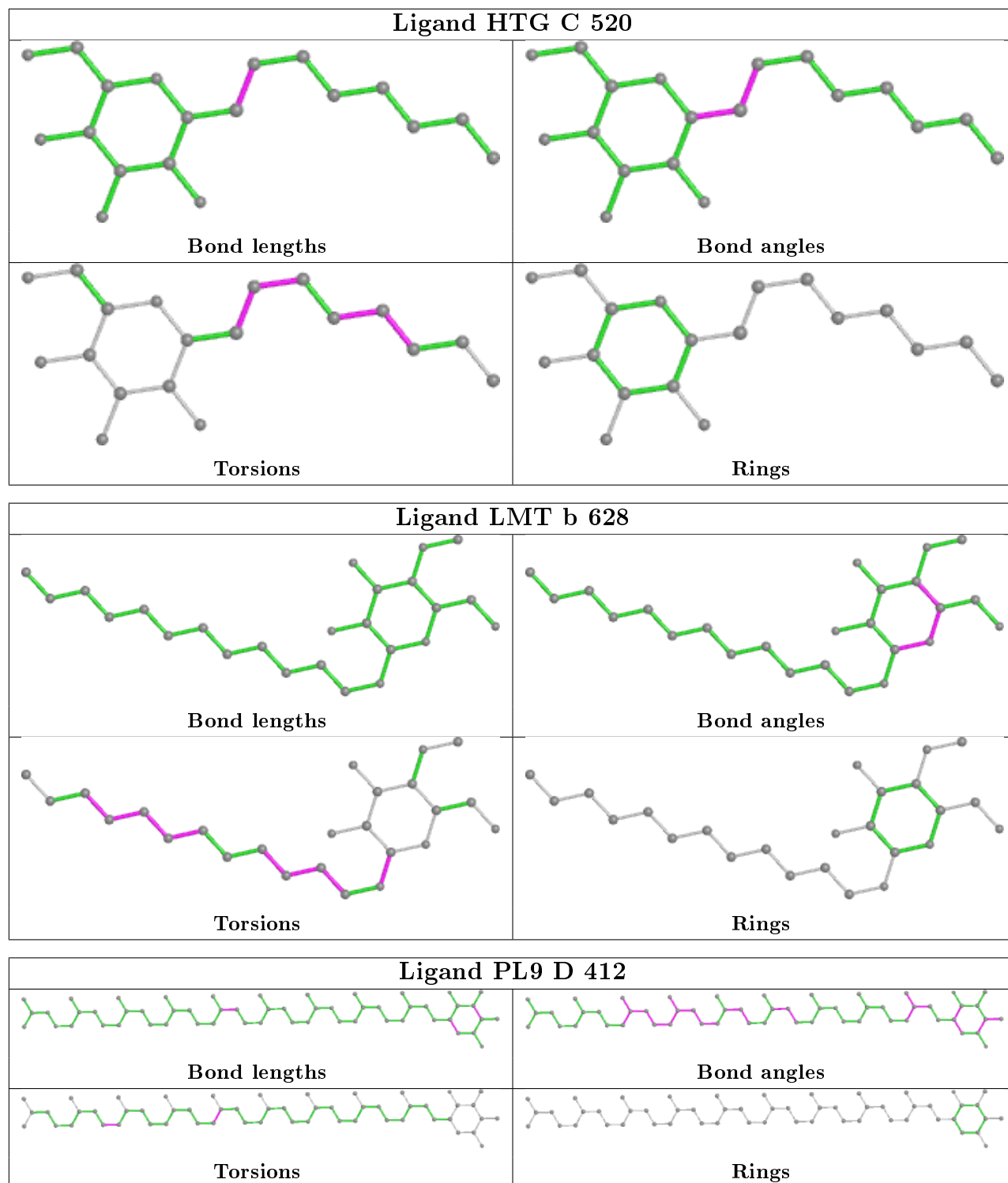


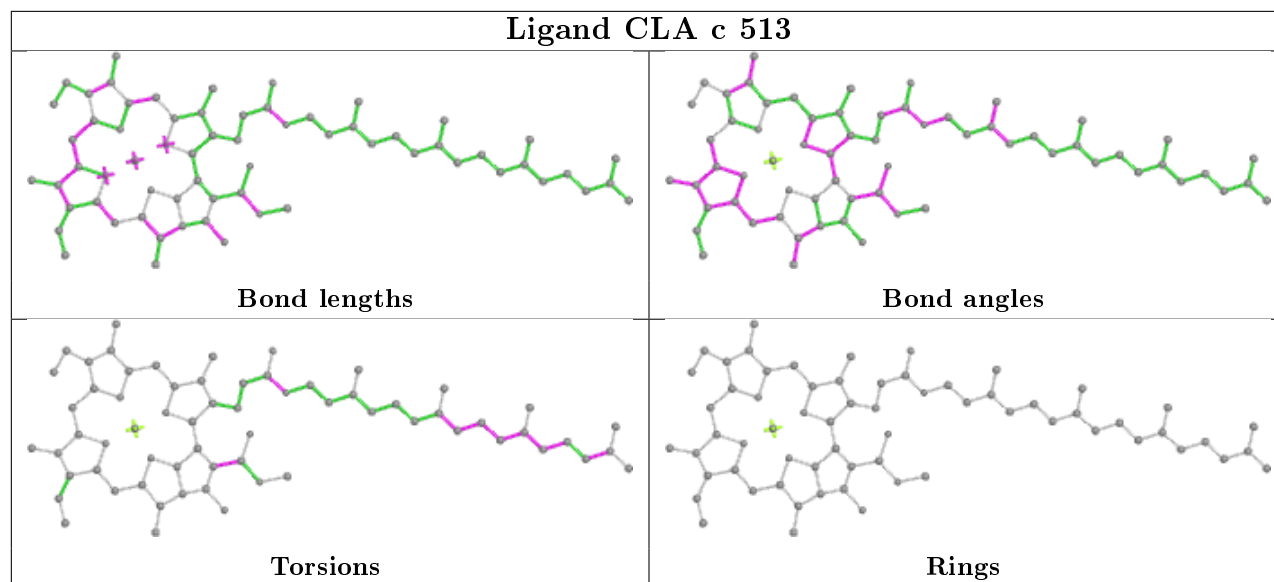
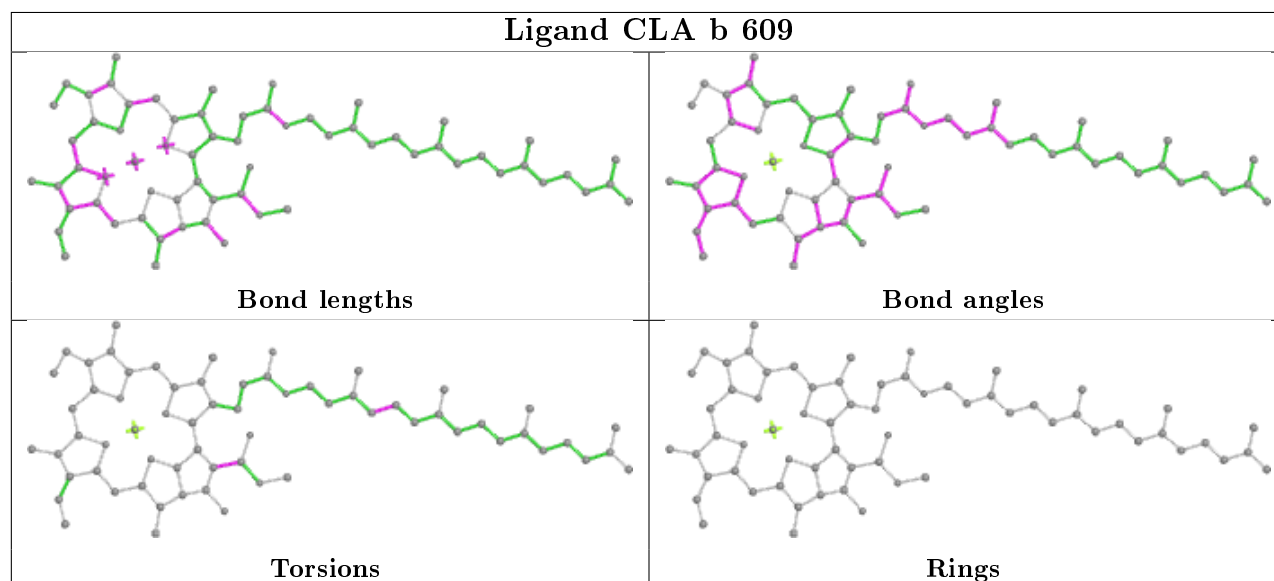
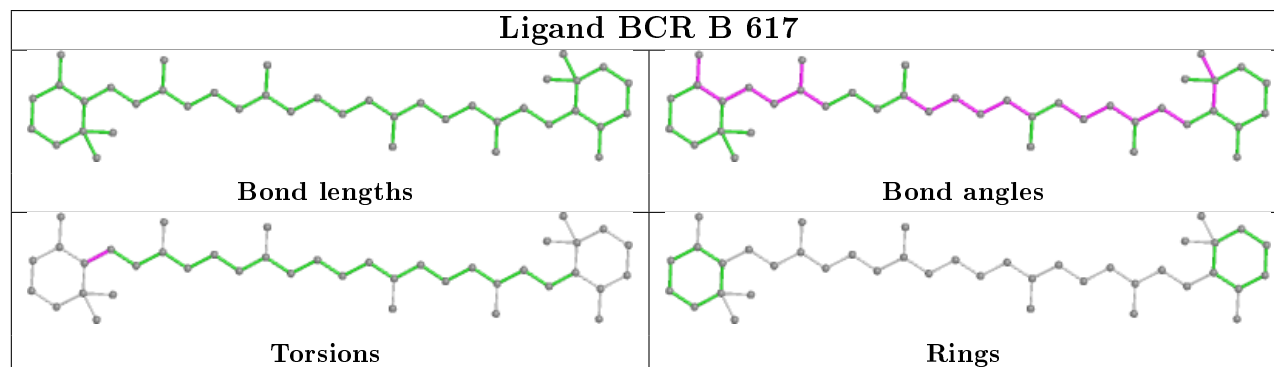
Ligand LMT f 102

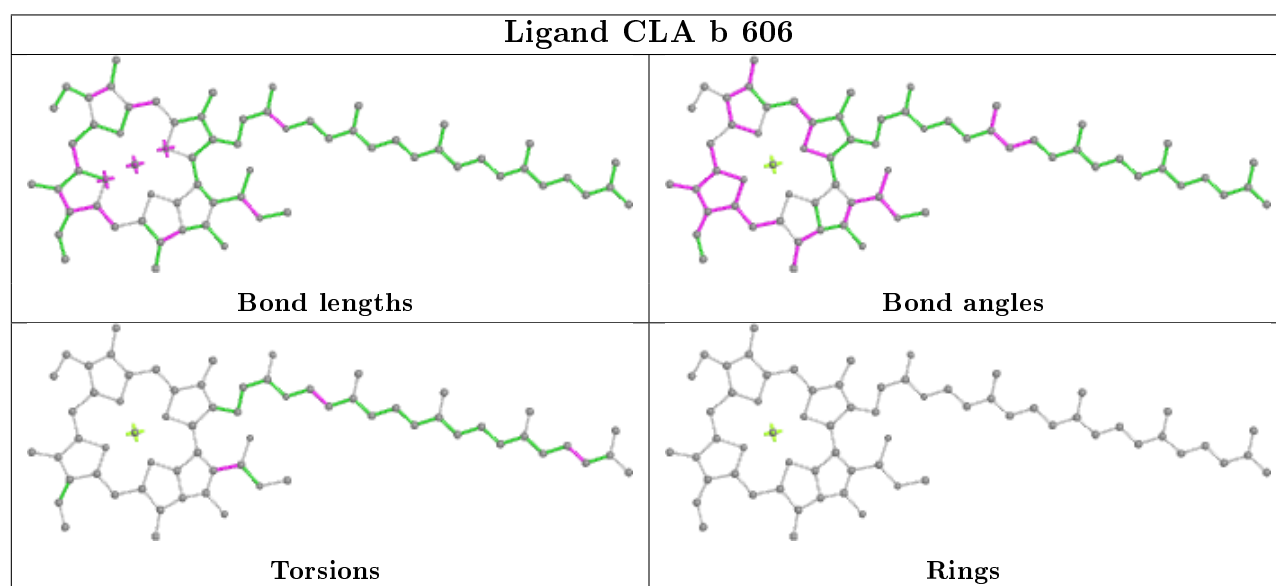
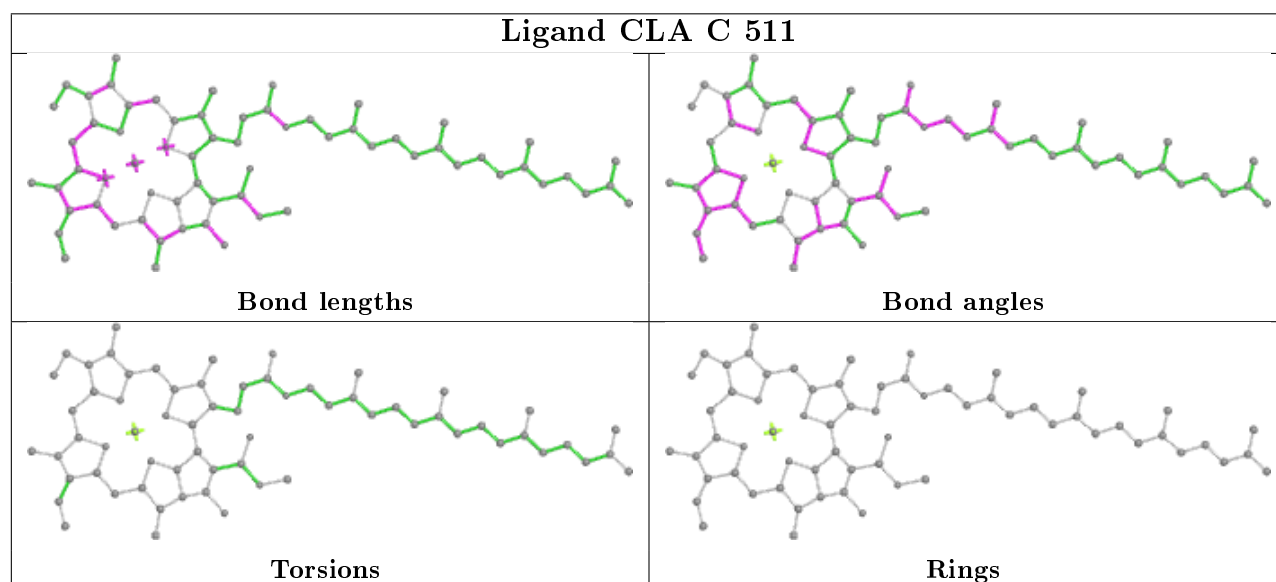
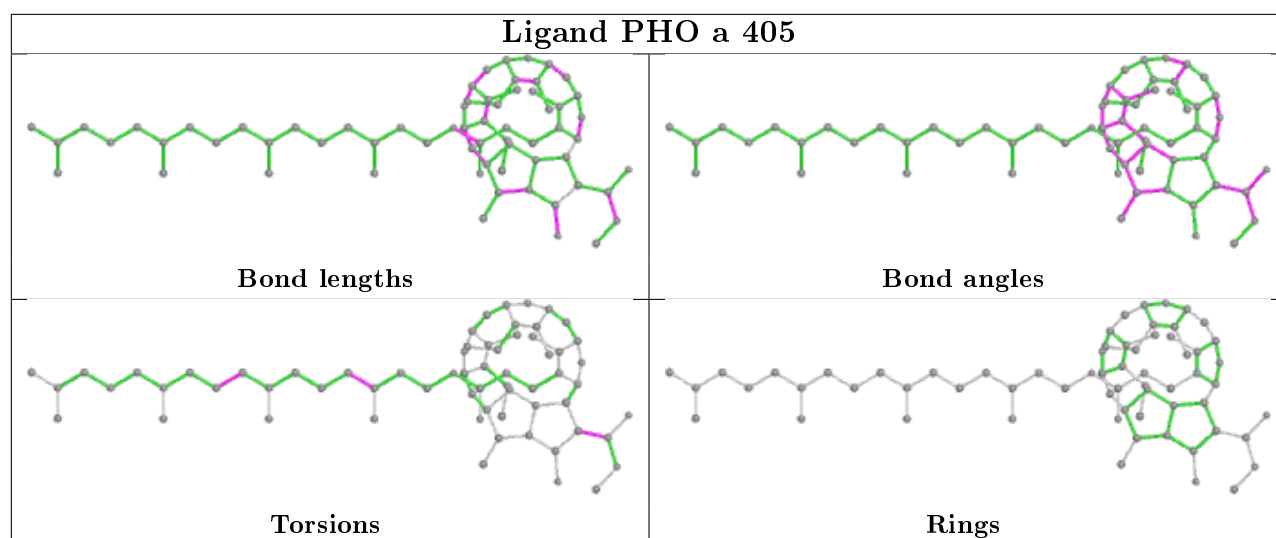




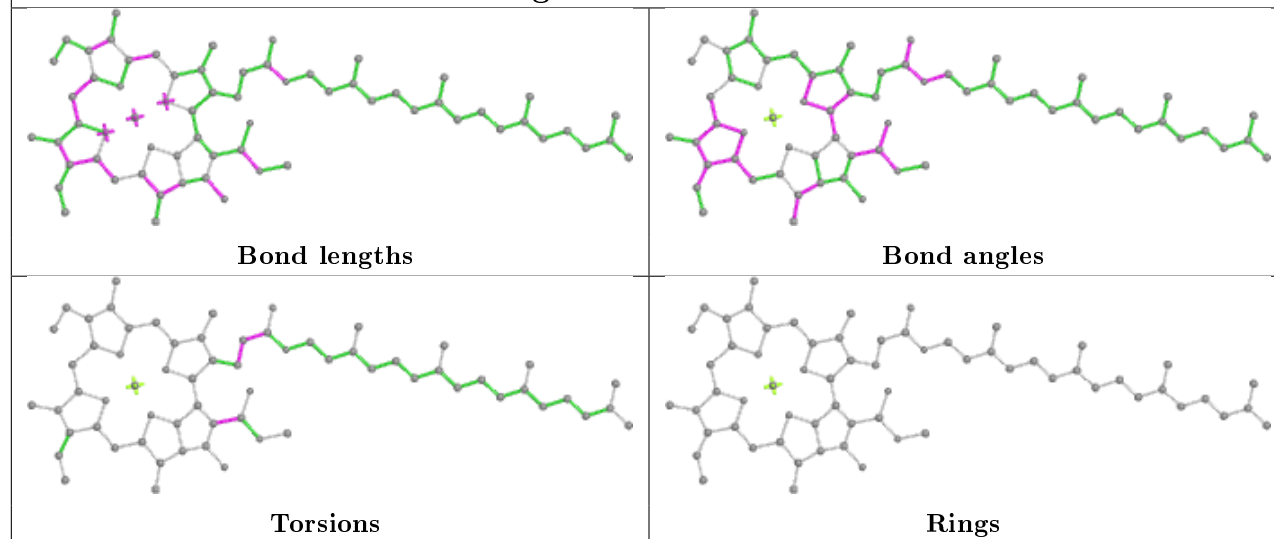




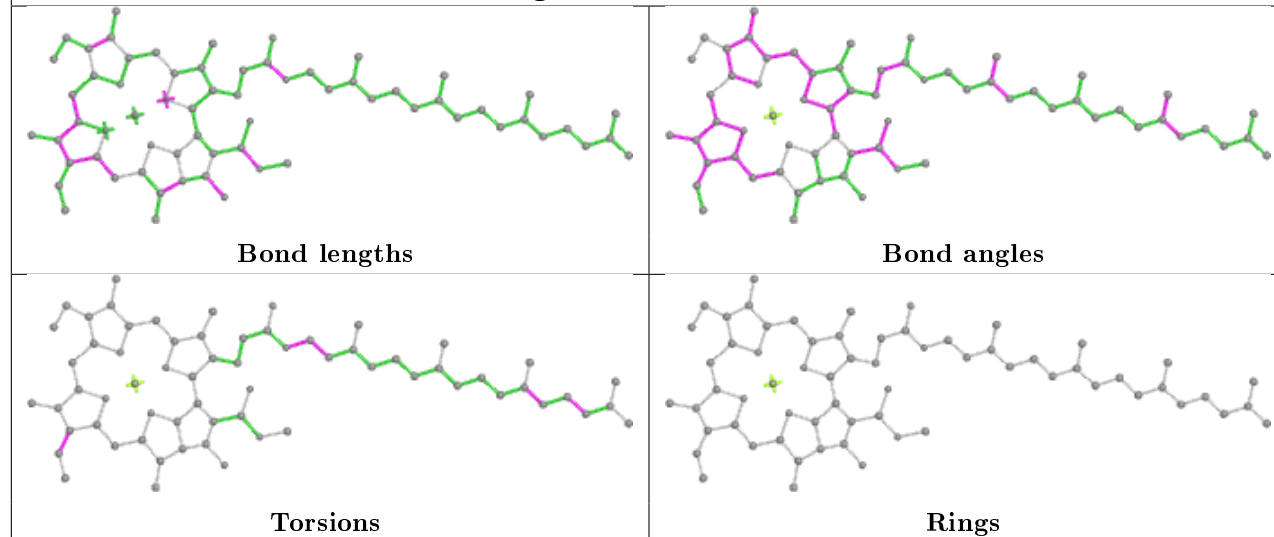
Ligand CLA c 513**Ligand CLA b 609****Ligand BCR B 617**



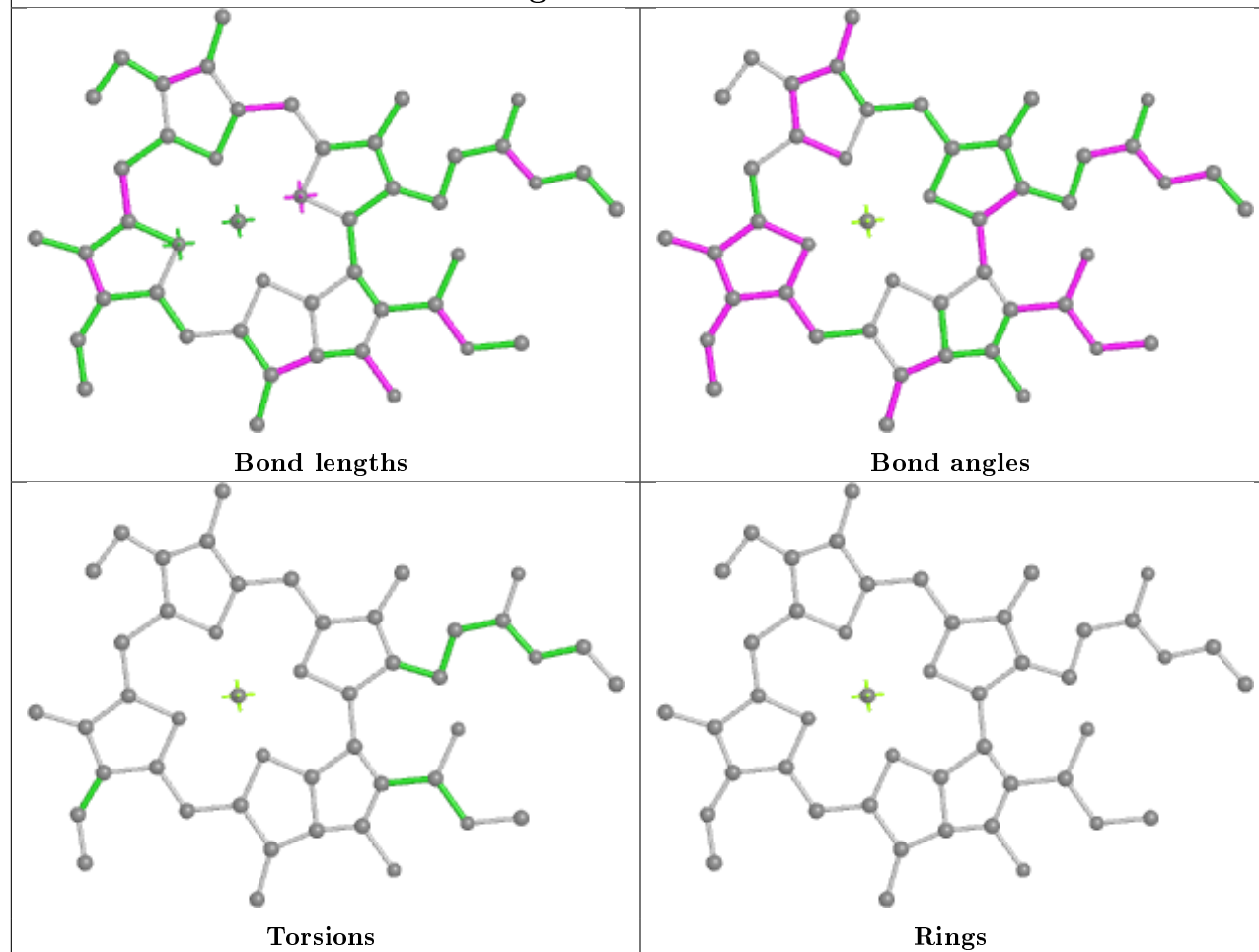
Ligand CLA C 501



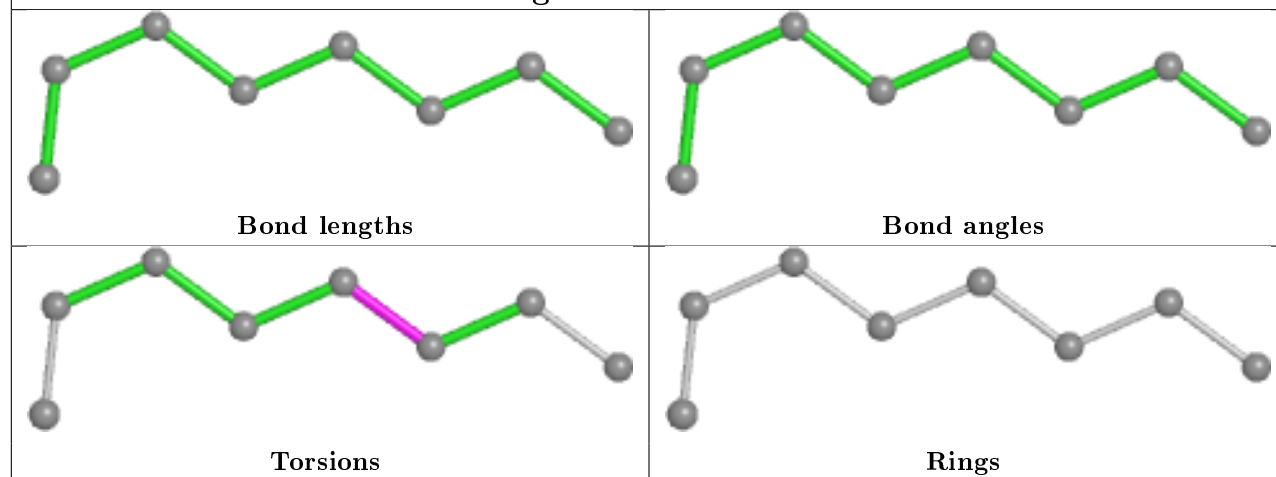
Ligand CLA D 401

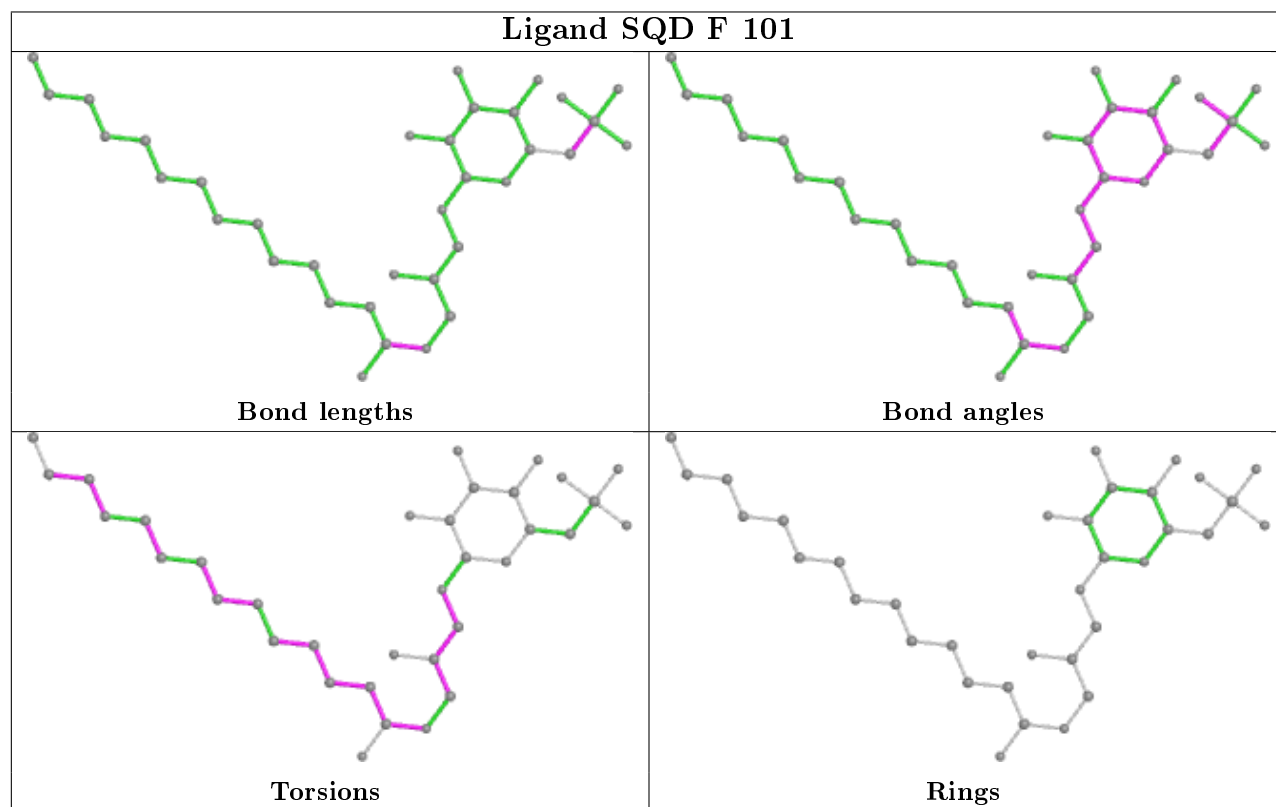
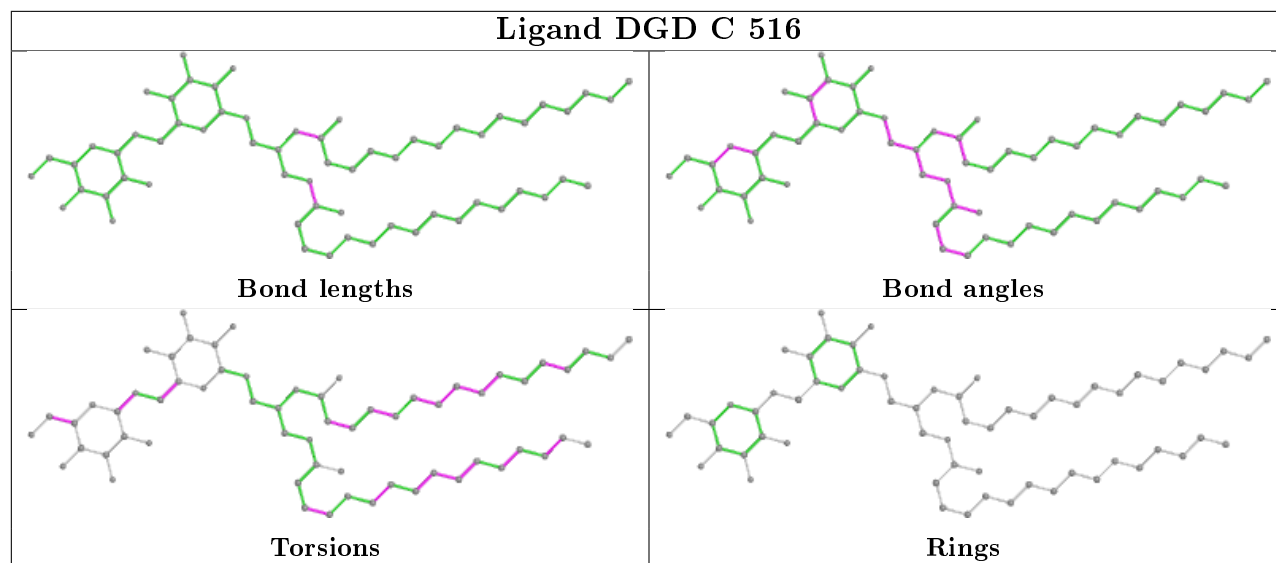


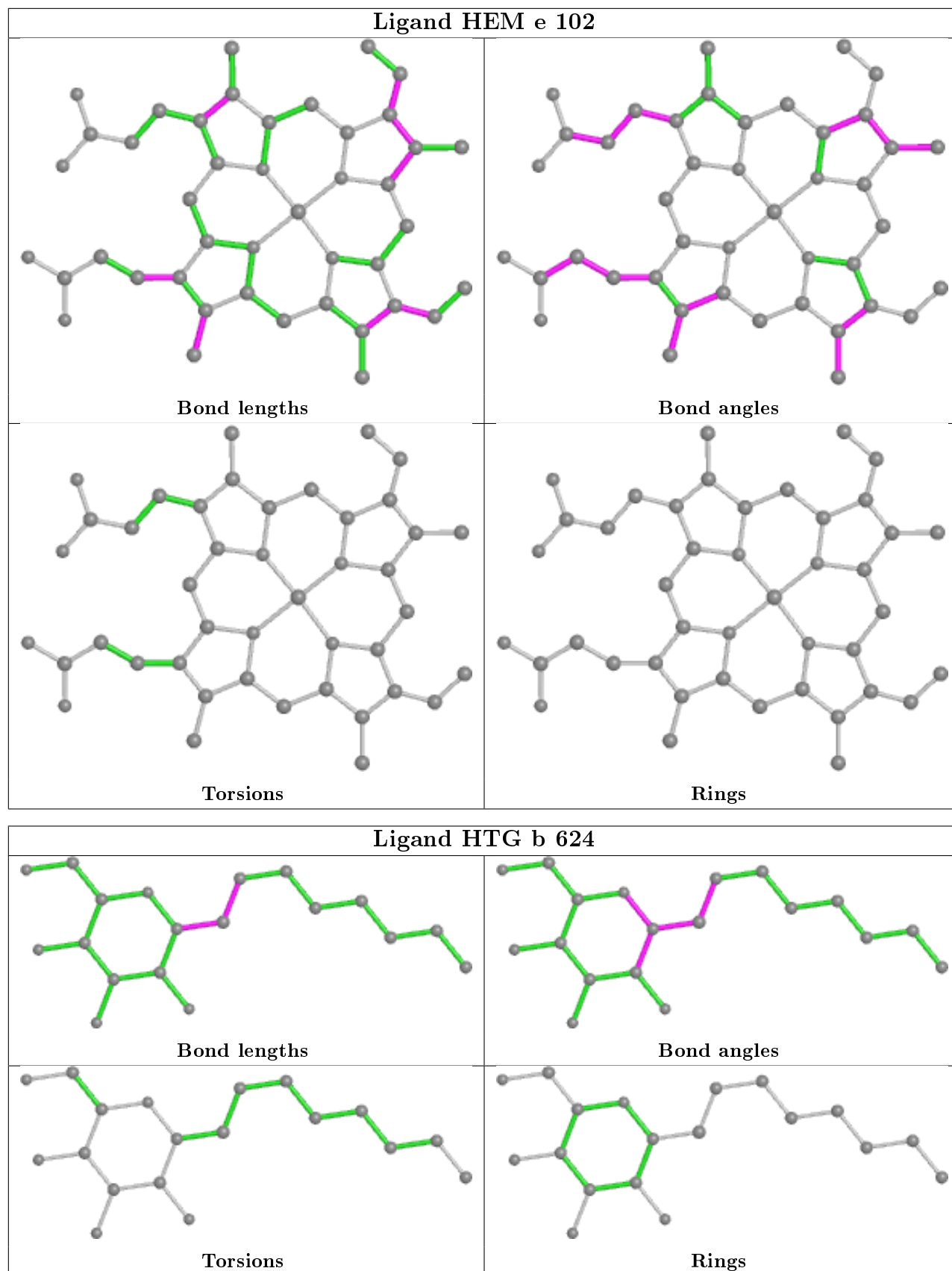
Ligand CLA a 407

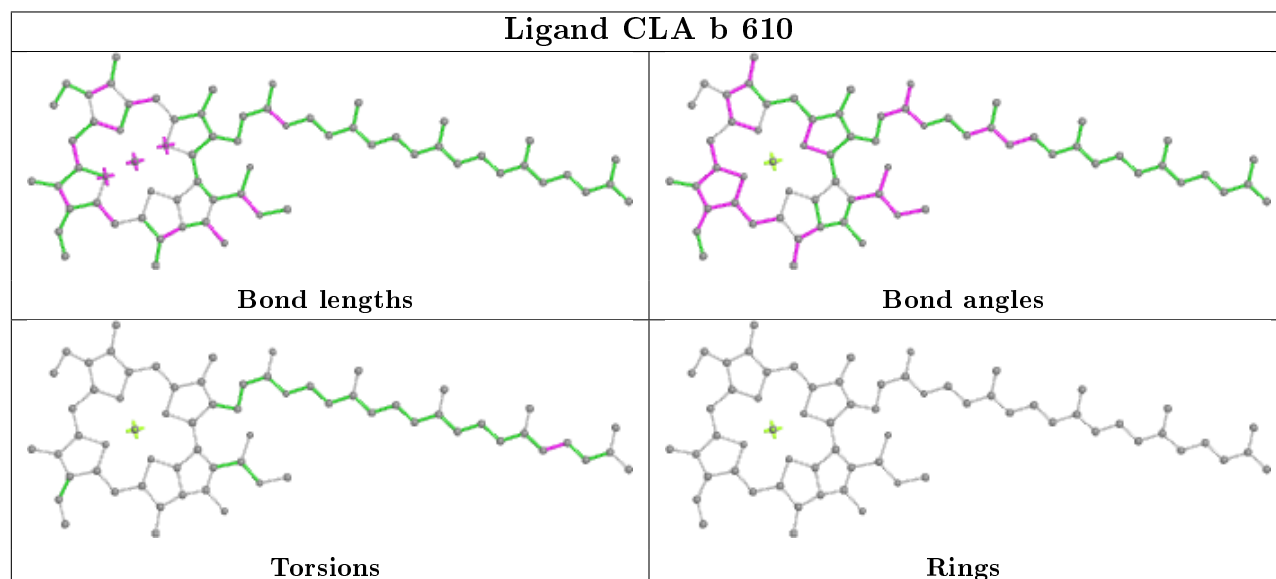
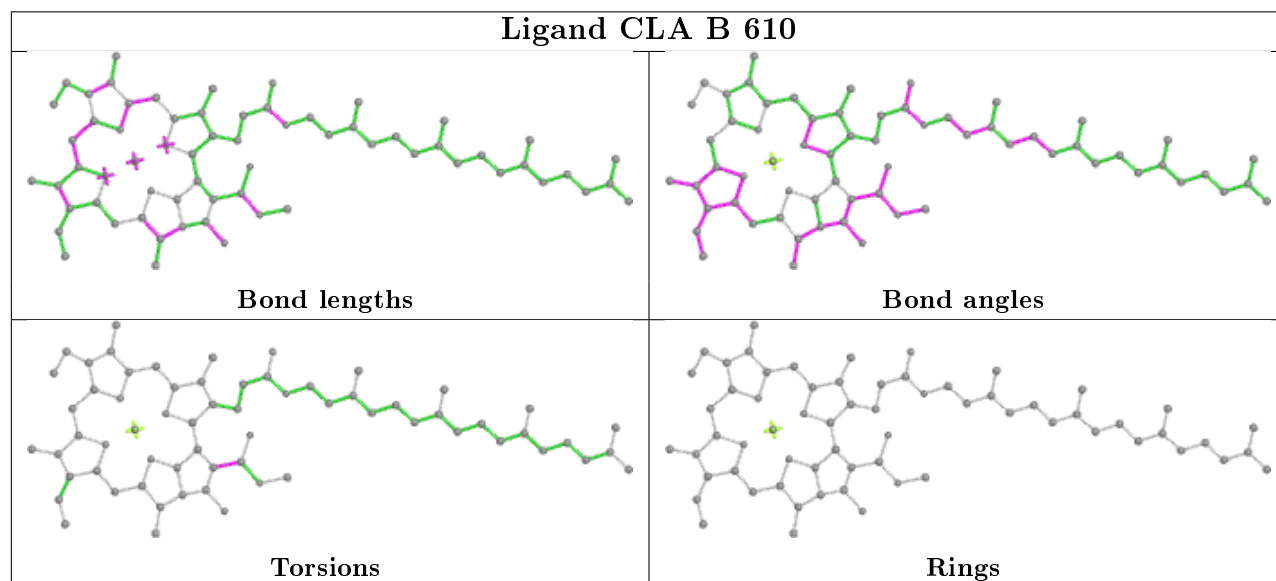
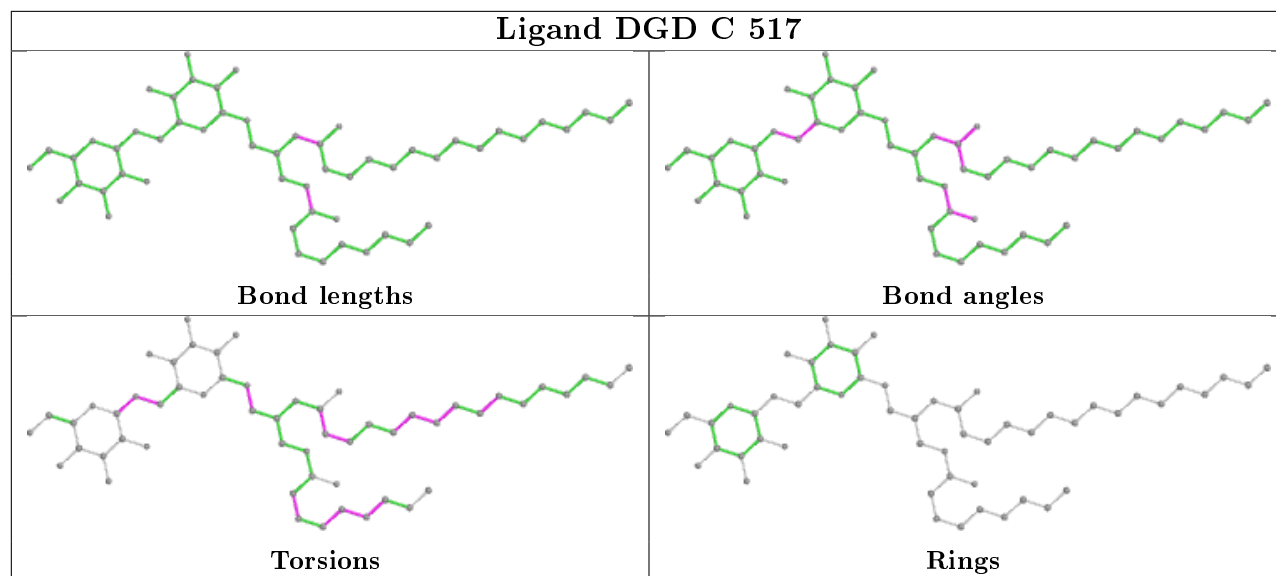


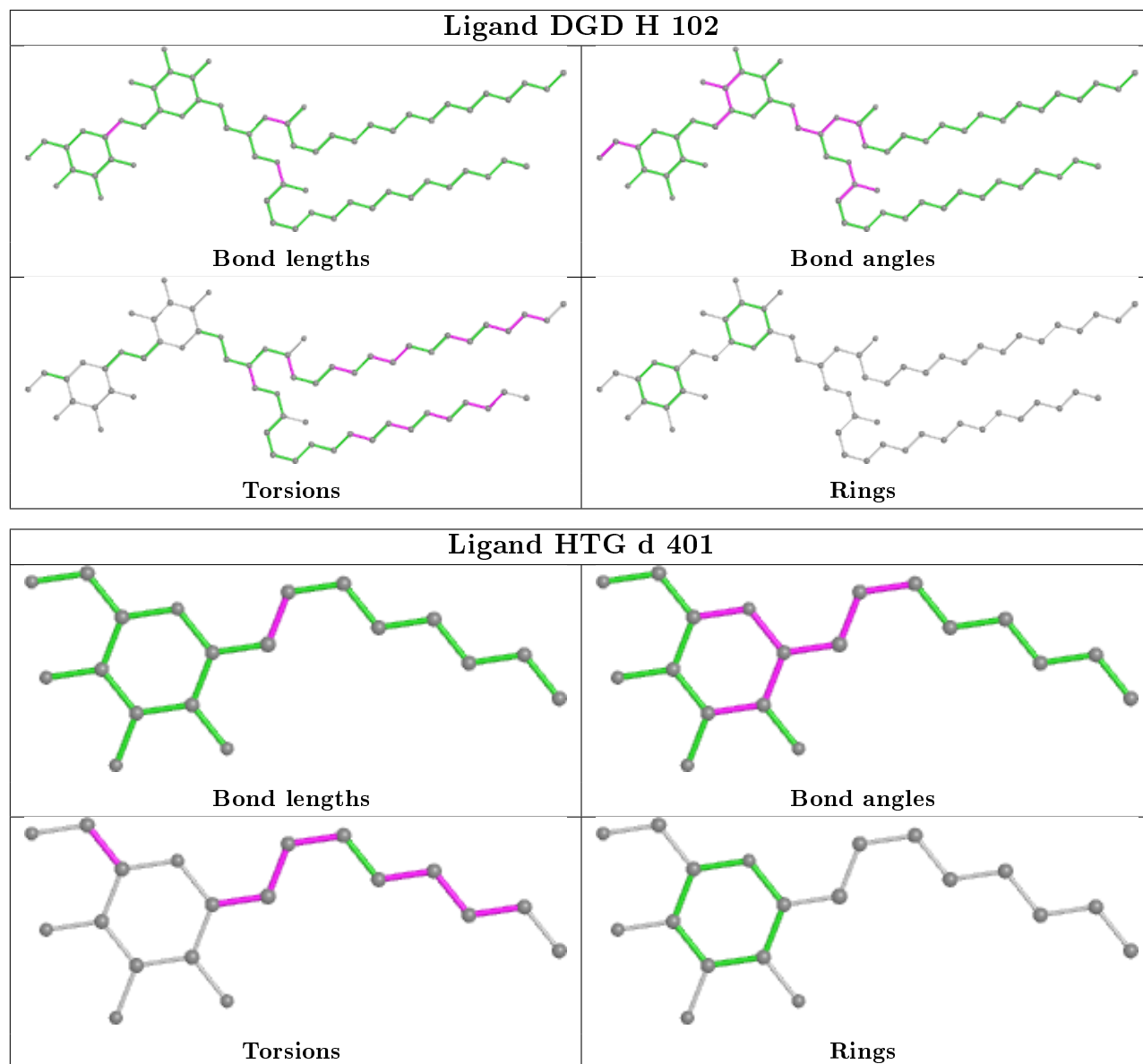
Ligand HTG u 201

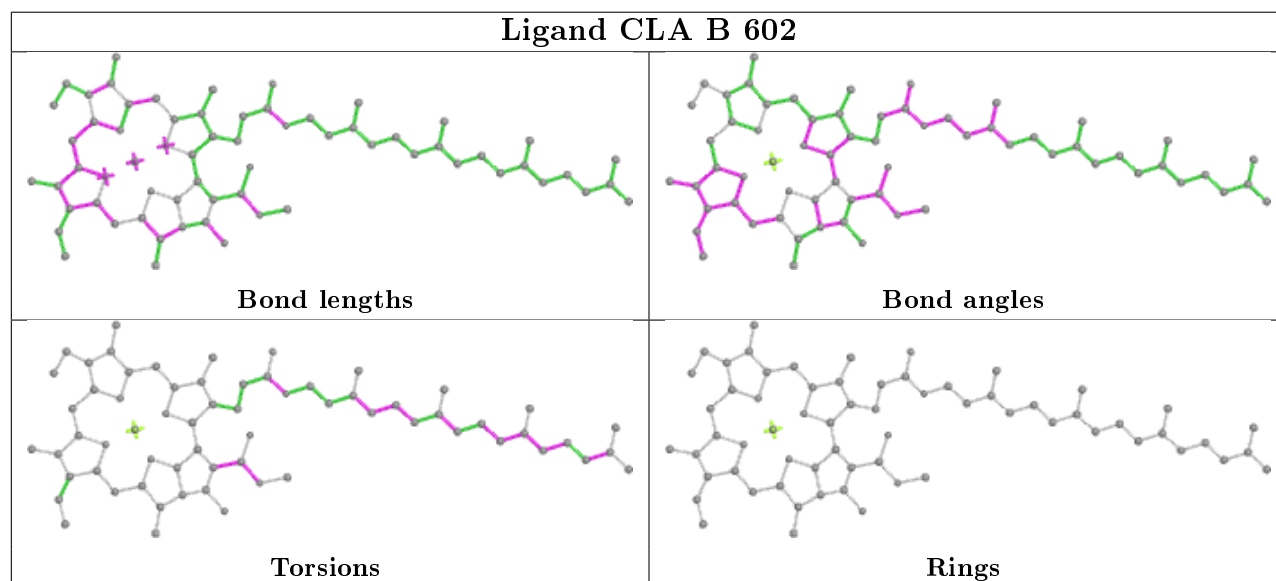
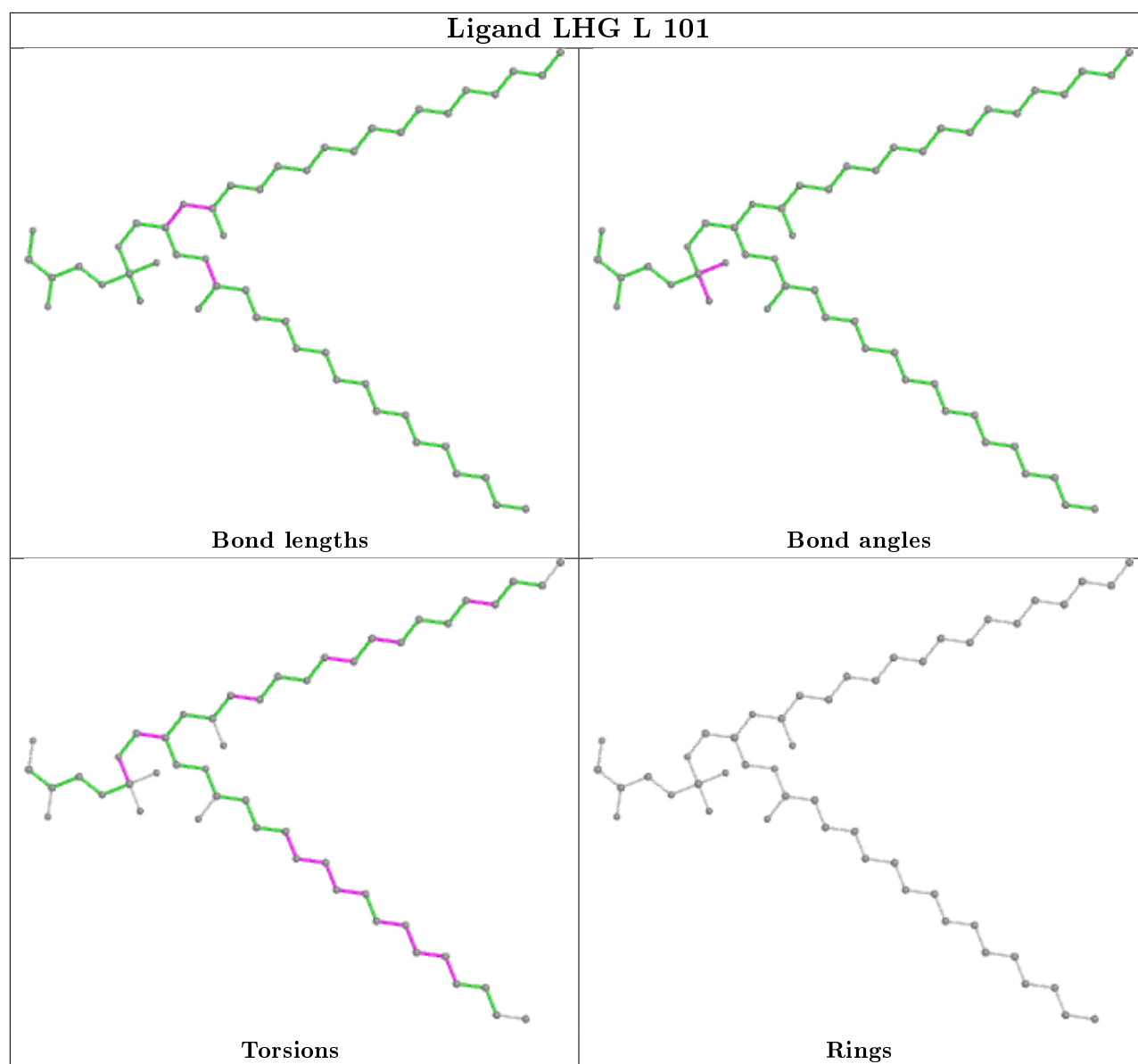


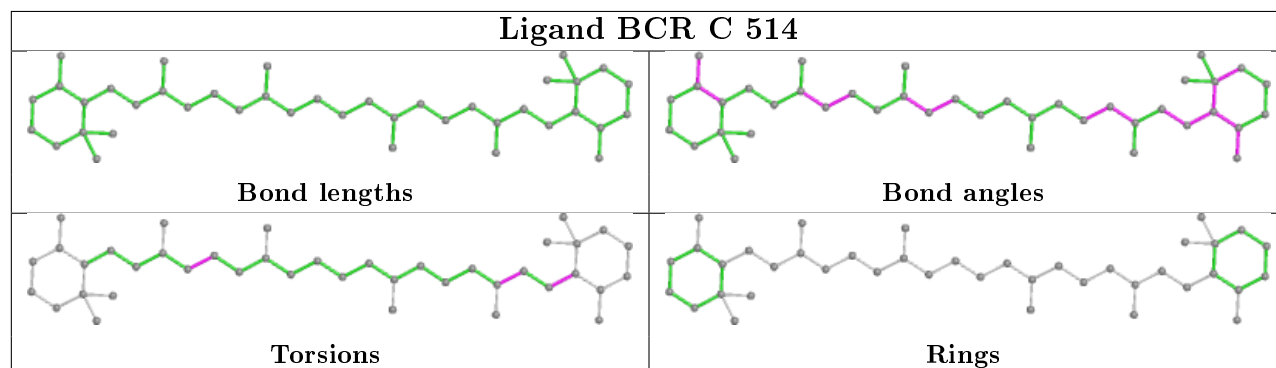
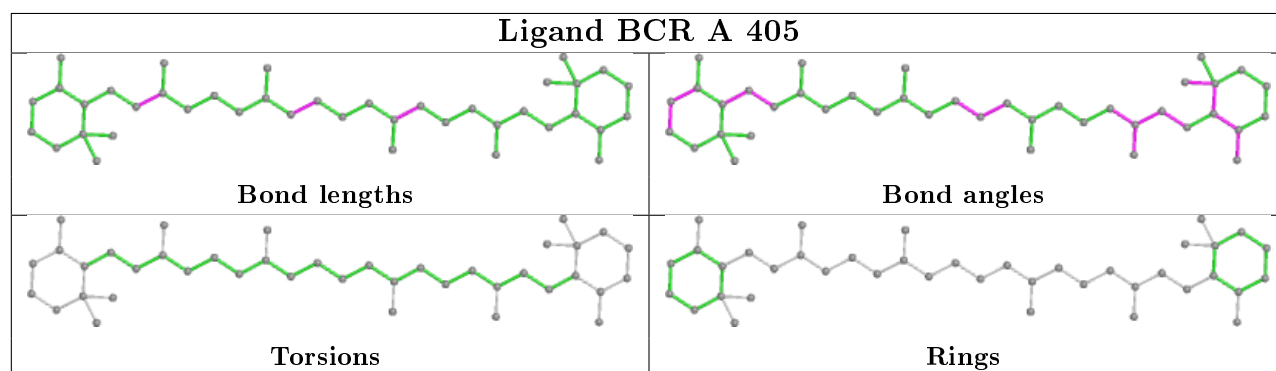
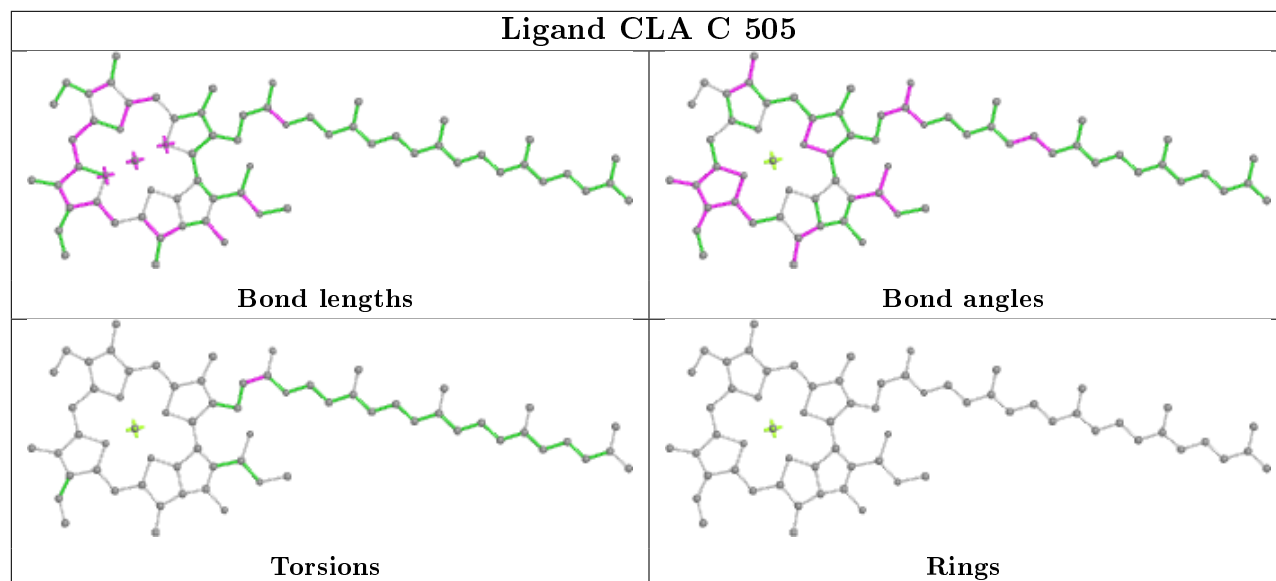
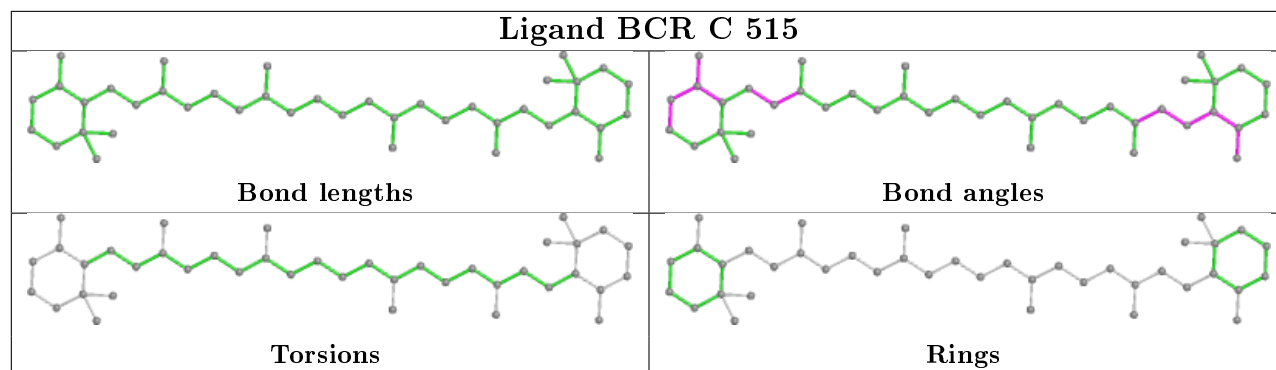




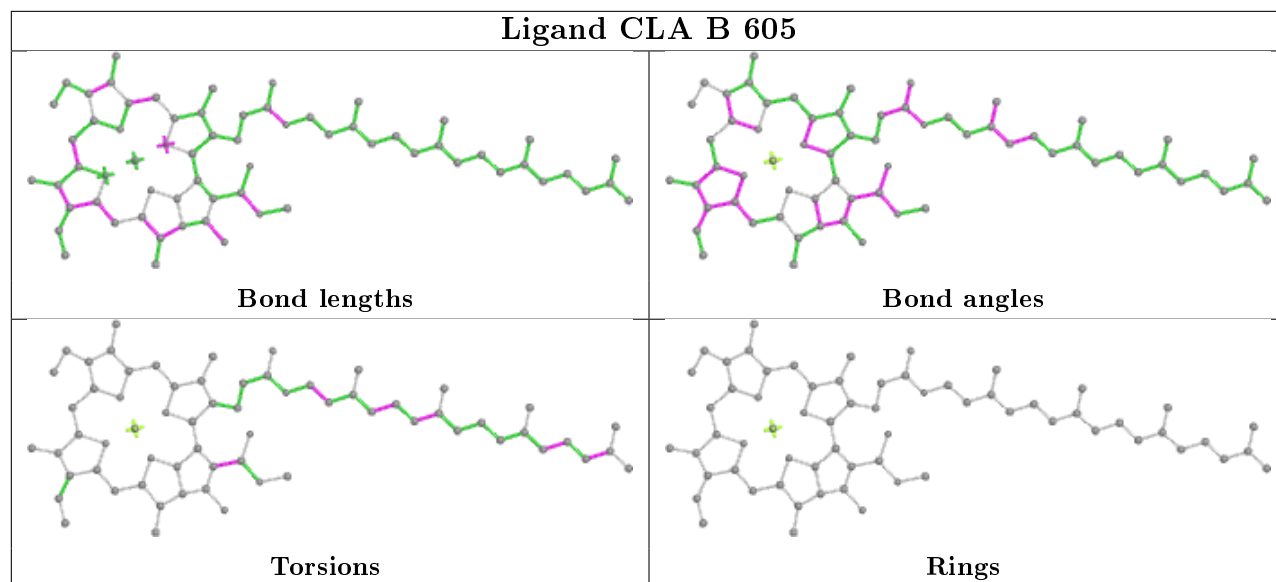




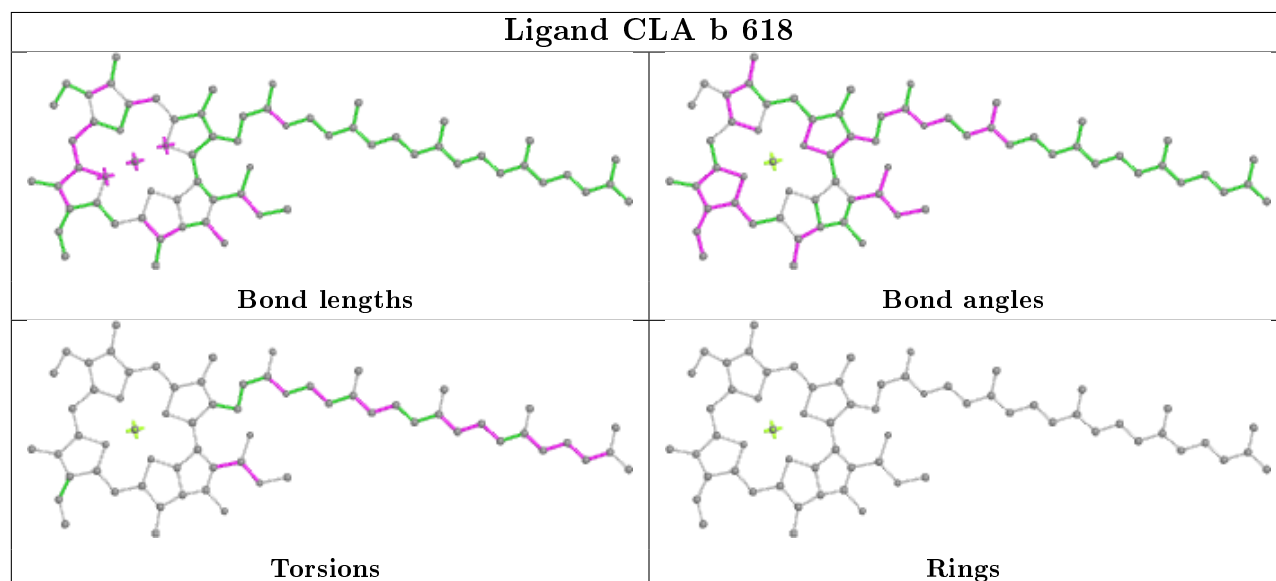




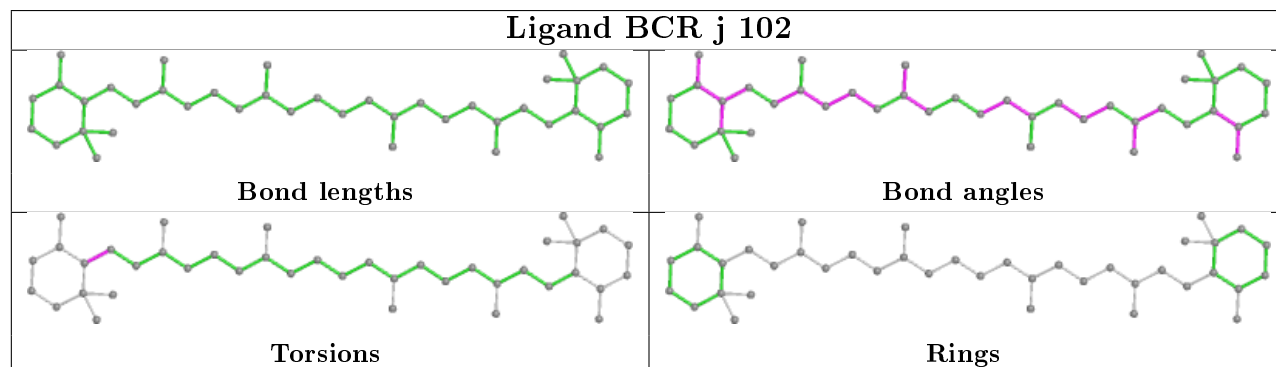
Ligand CLA B 605

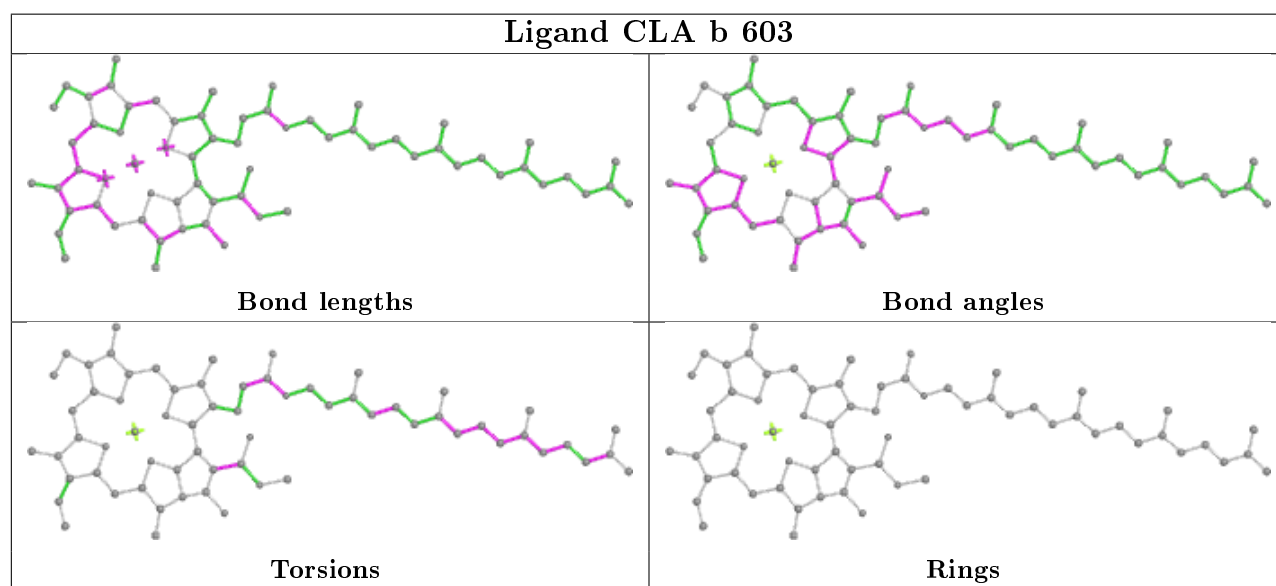
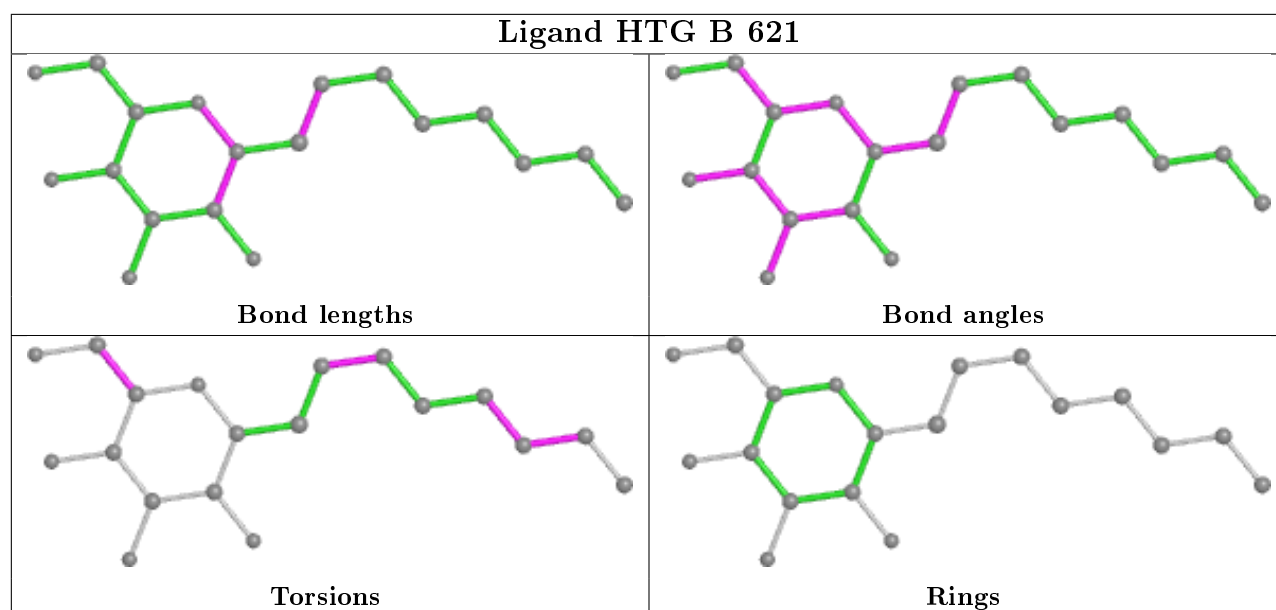


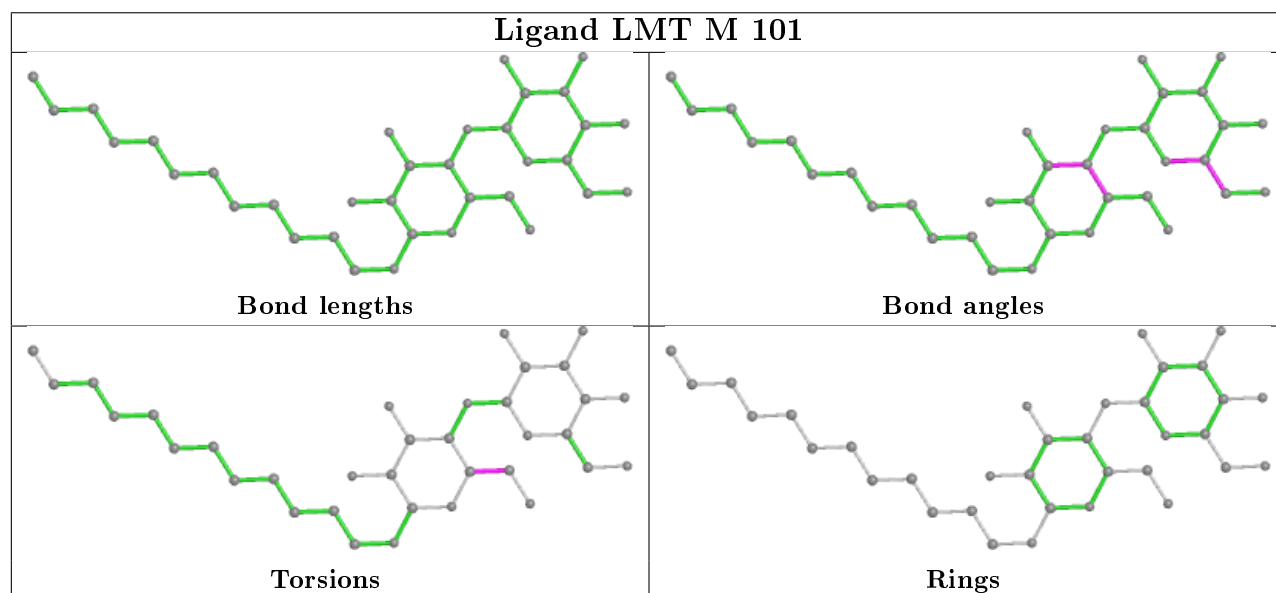
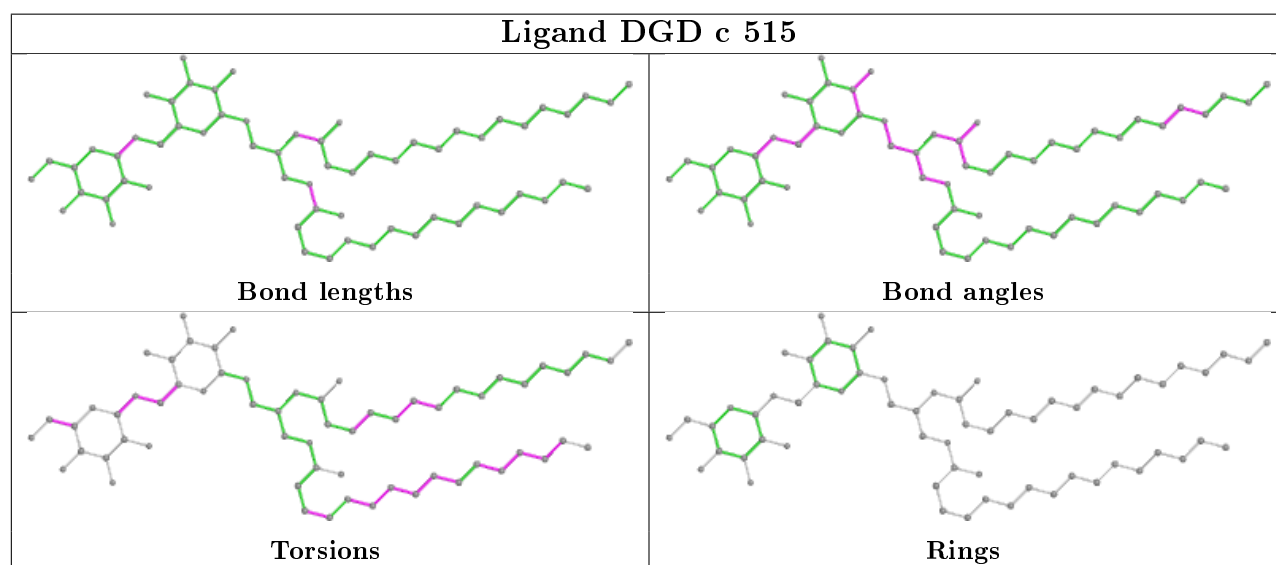
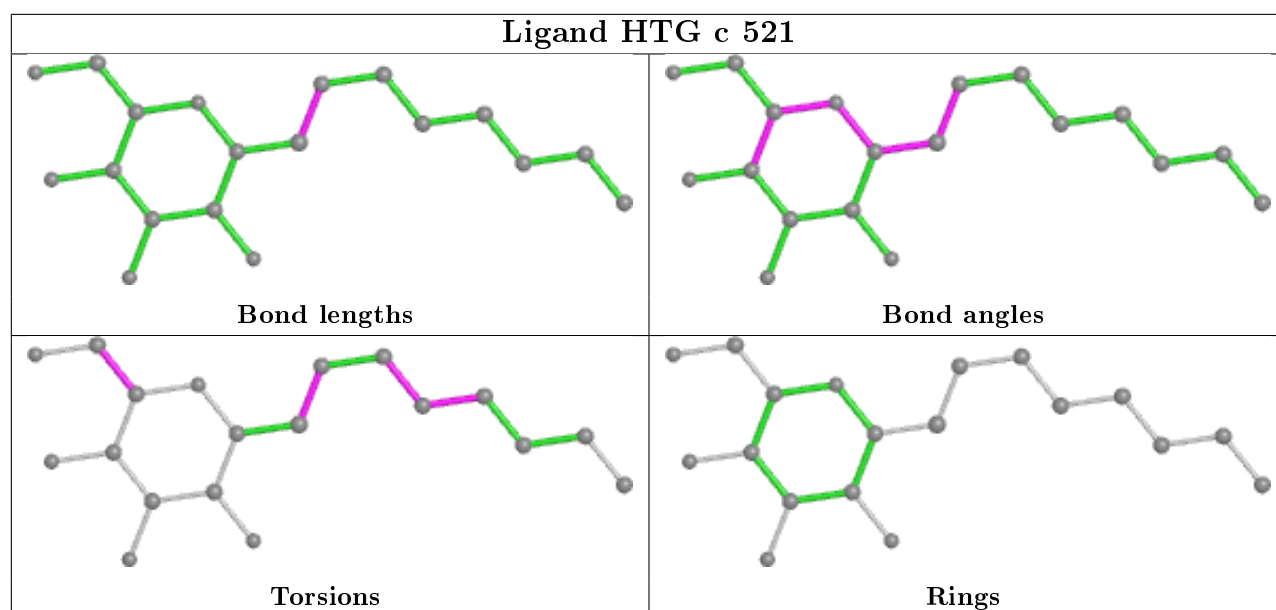
Ligand CLA b 618

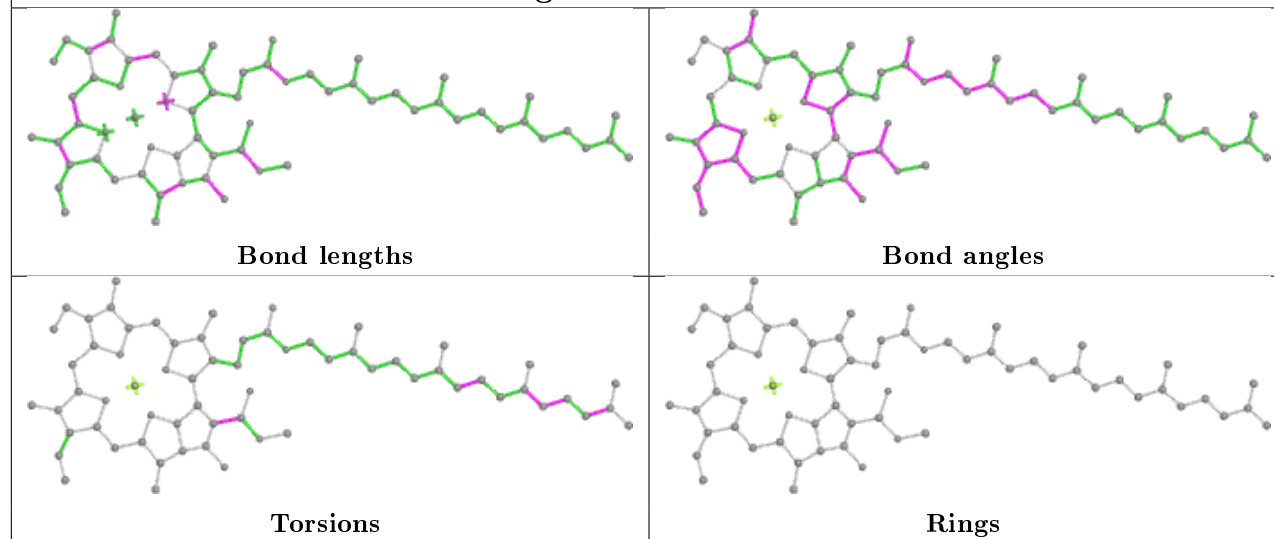
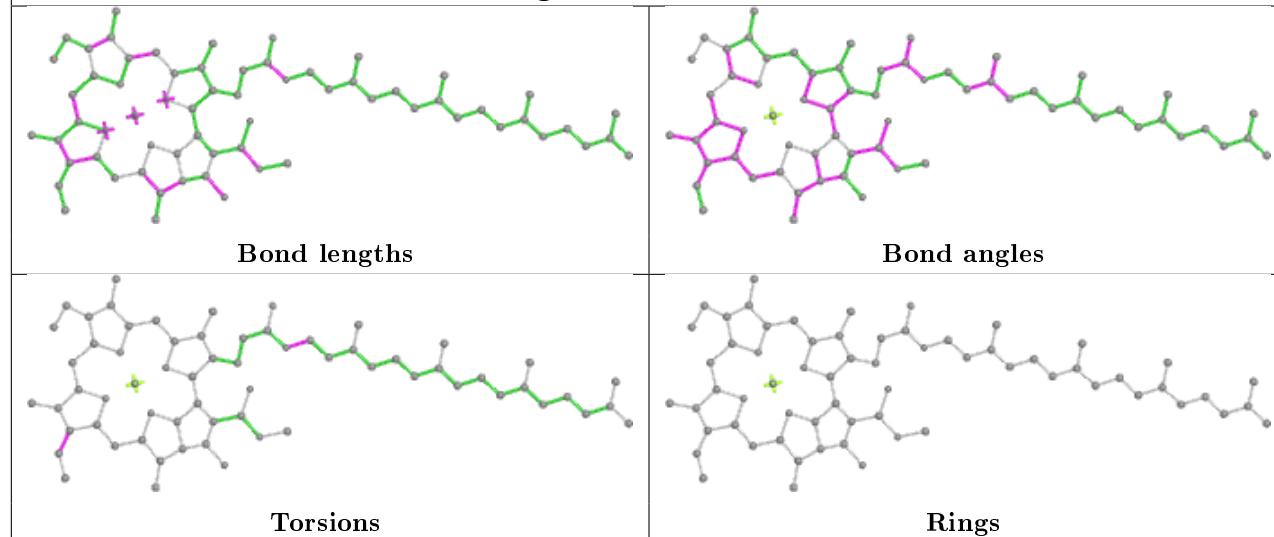


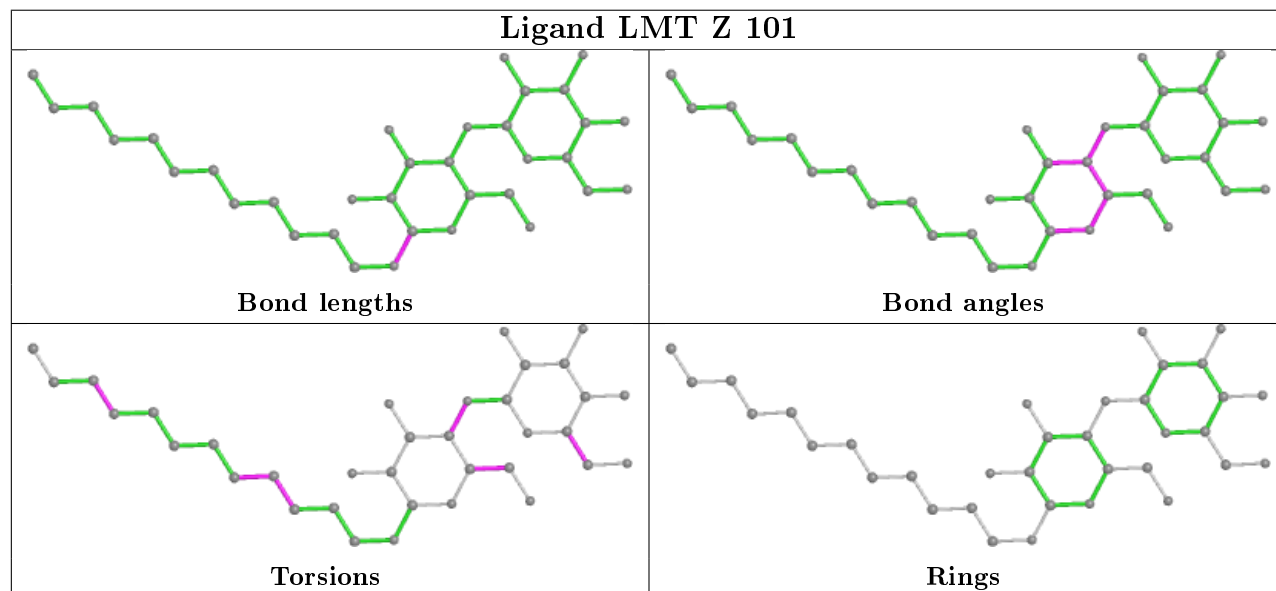
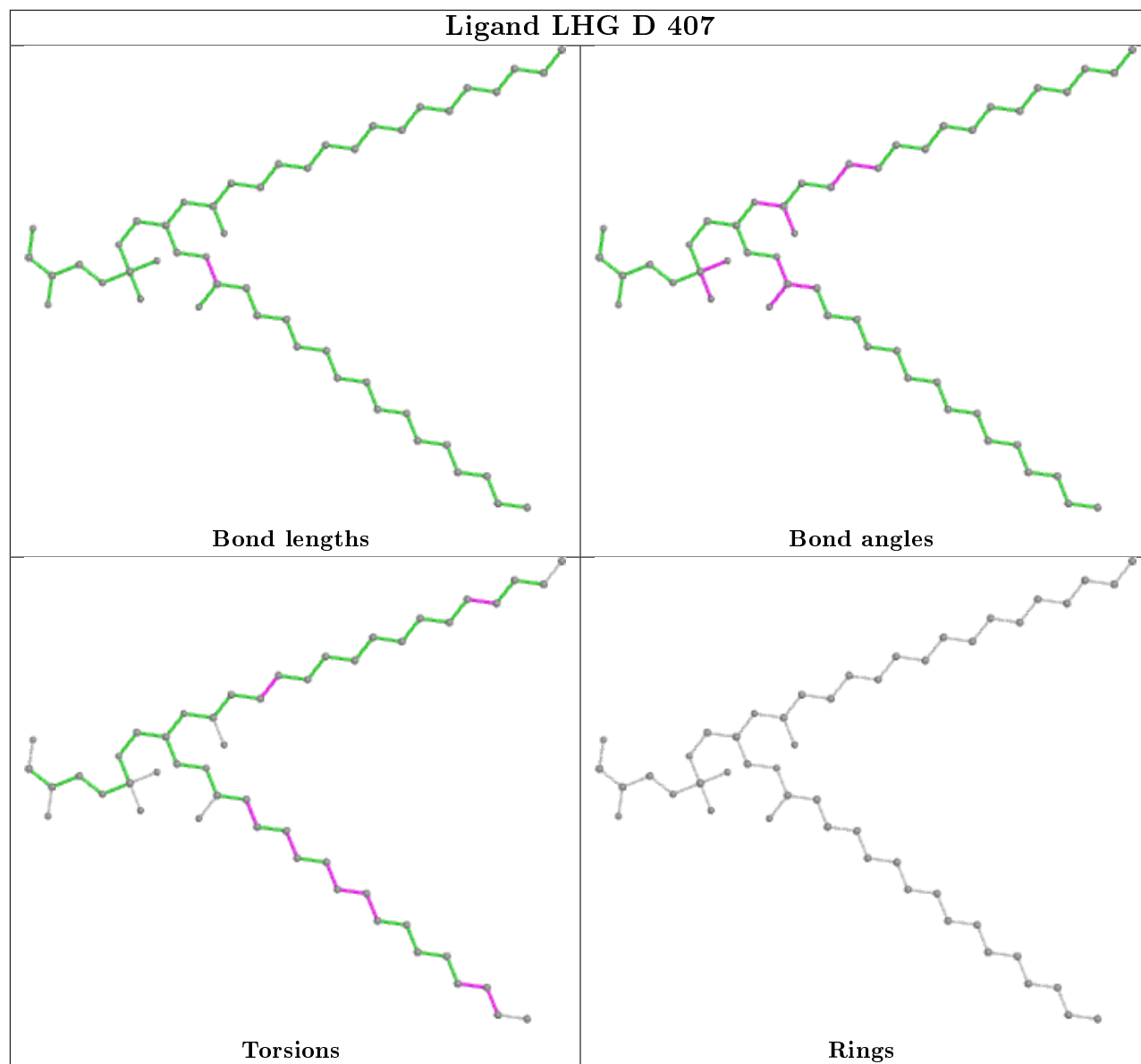
Ligand BCR j 102

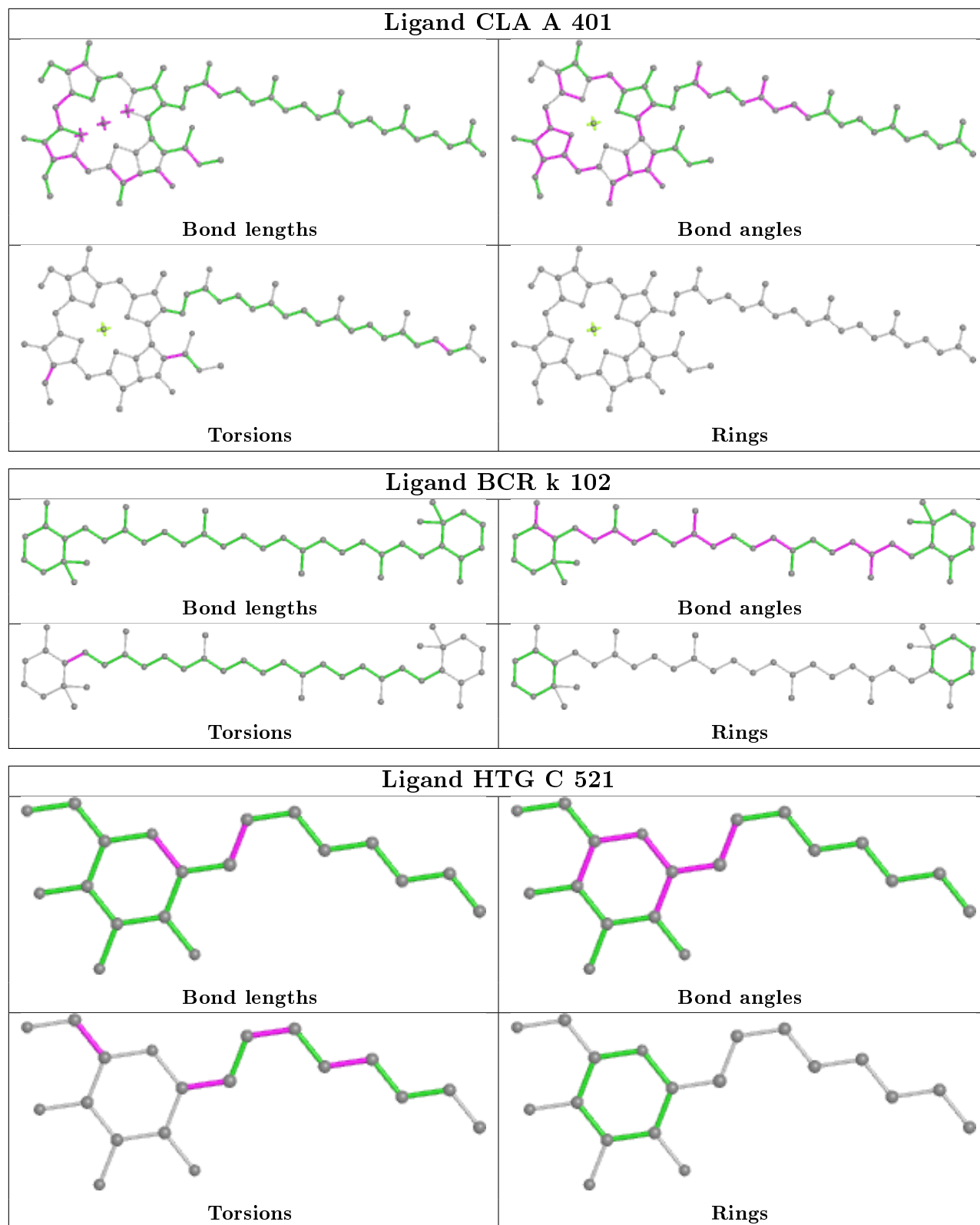




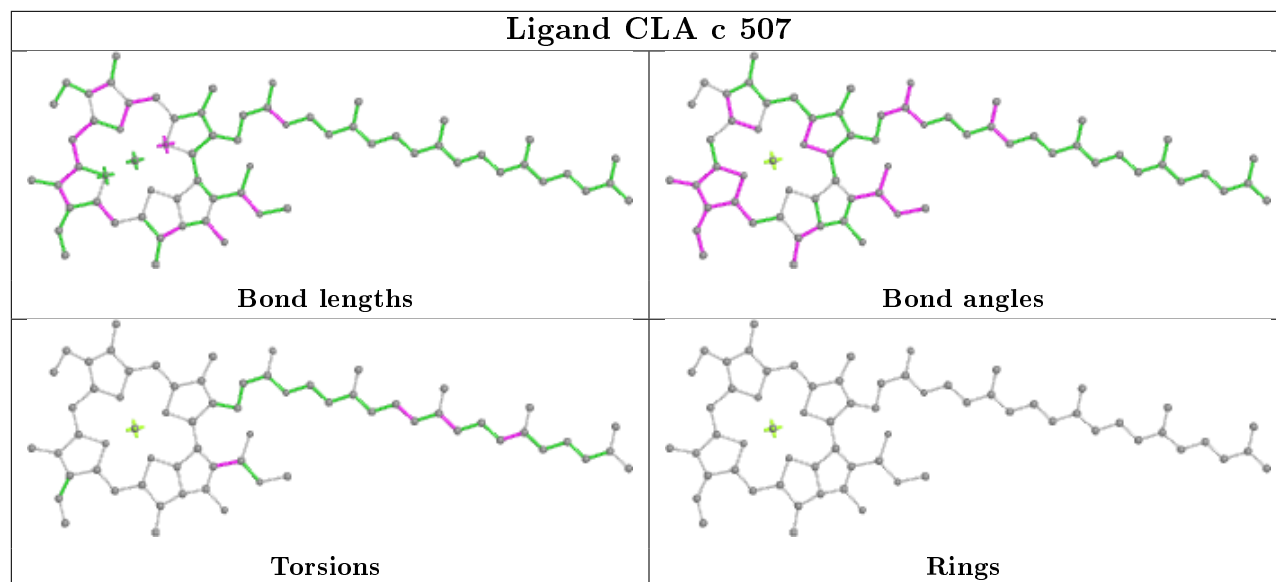


Ligand CLA b 613**Ligand CLA d 402**

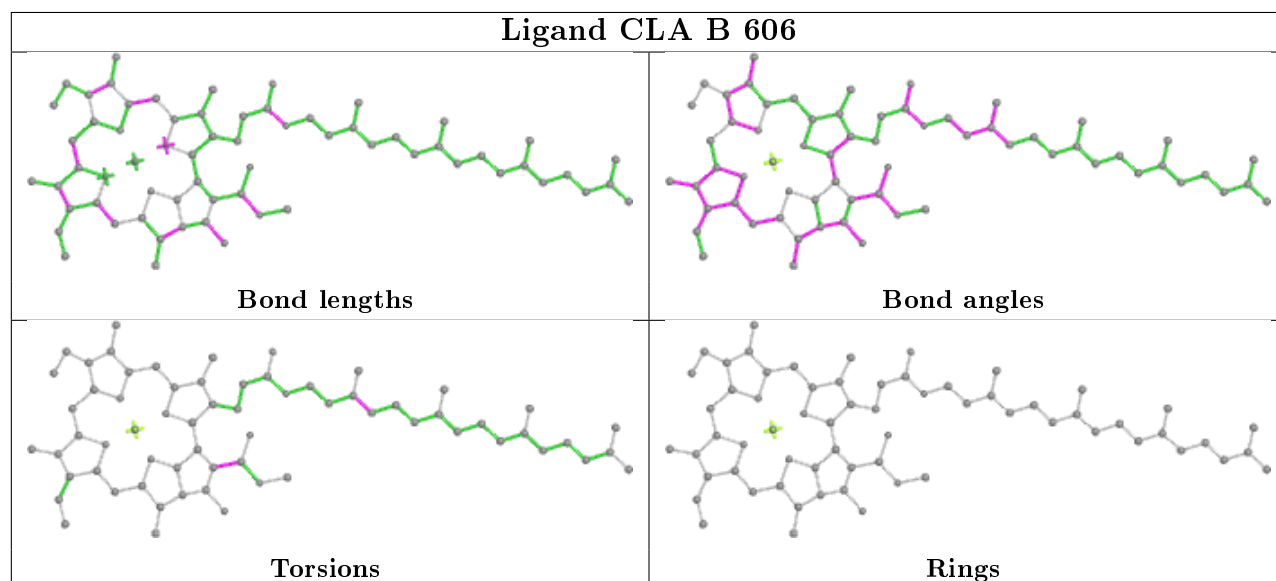




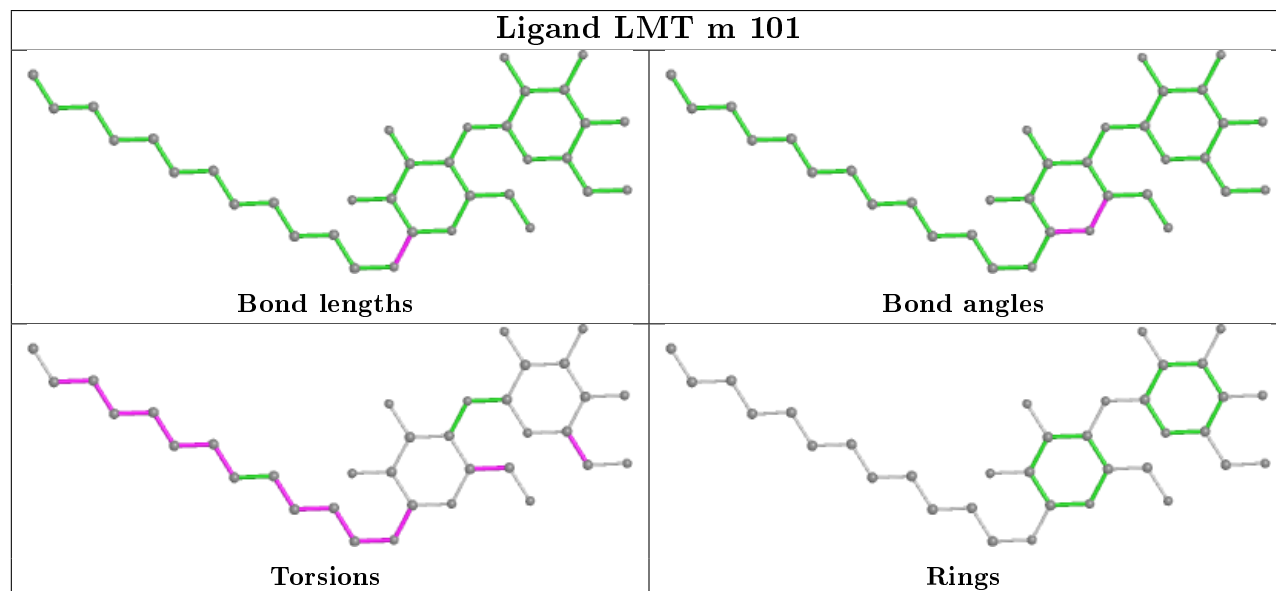
Ligand CLA c 507

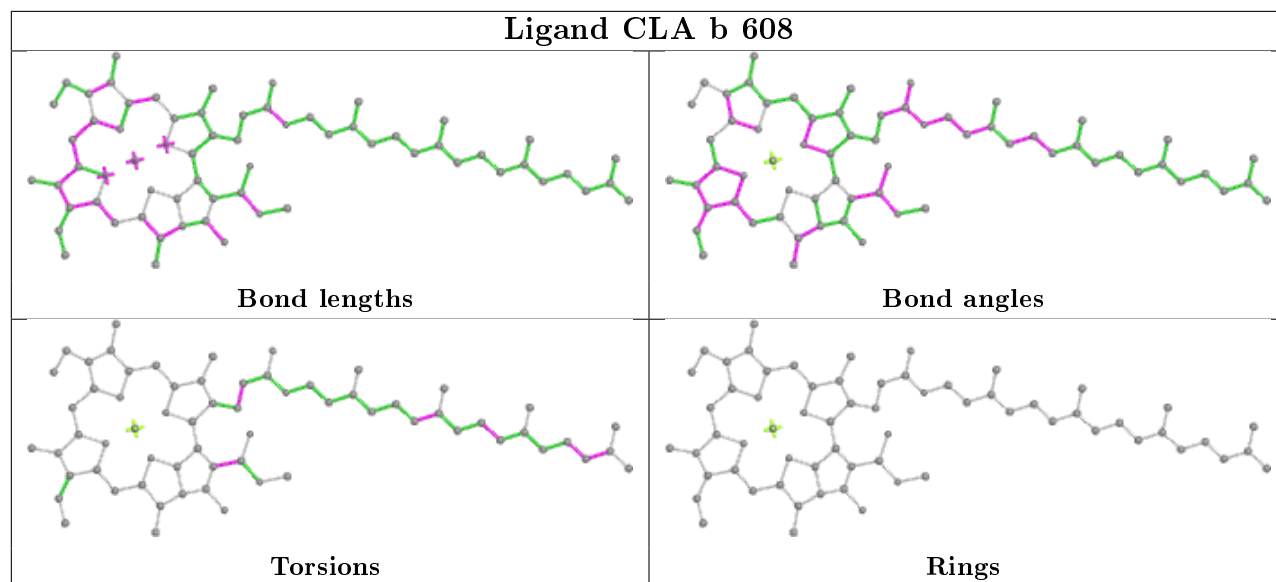
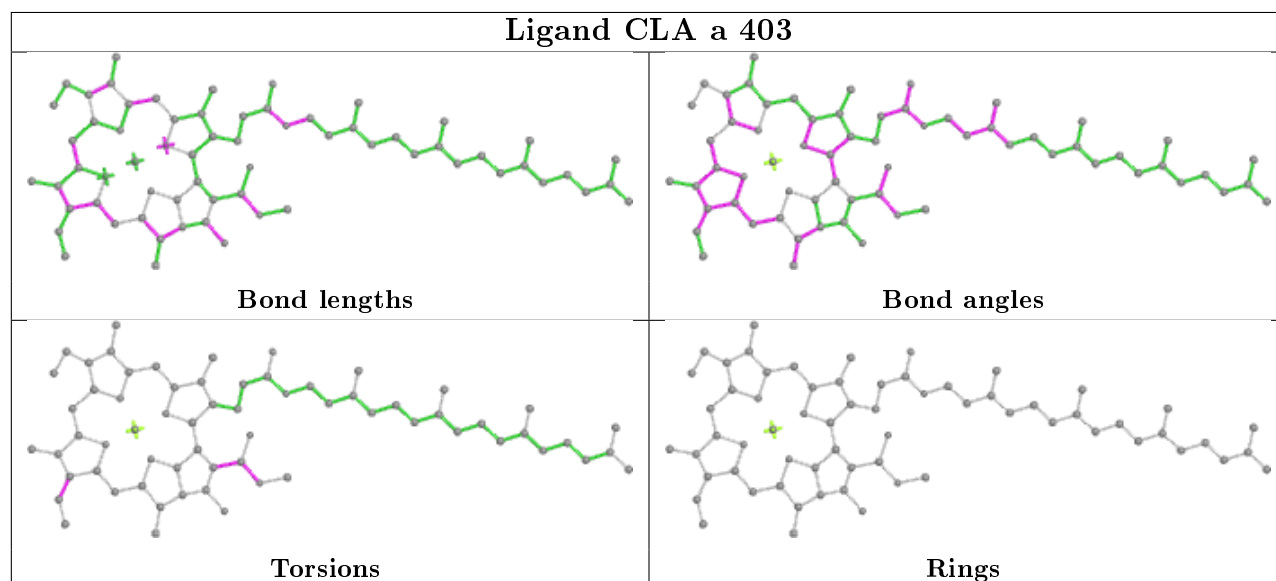
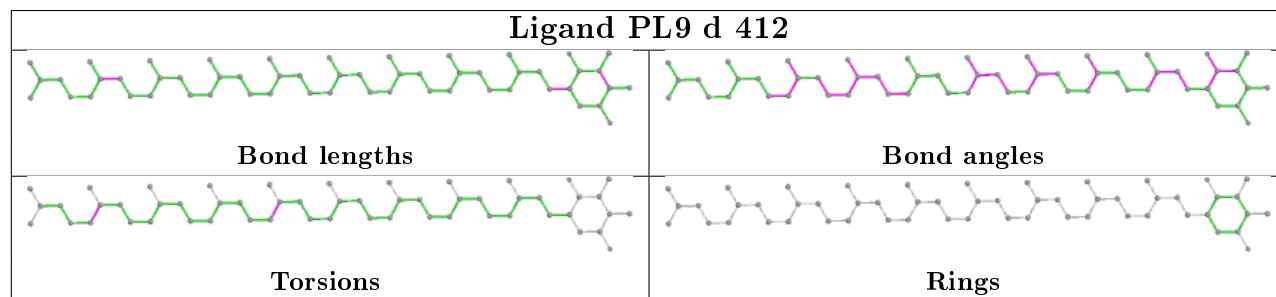


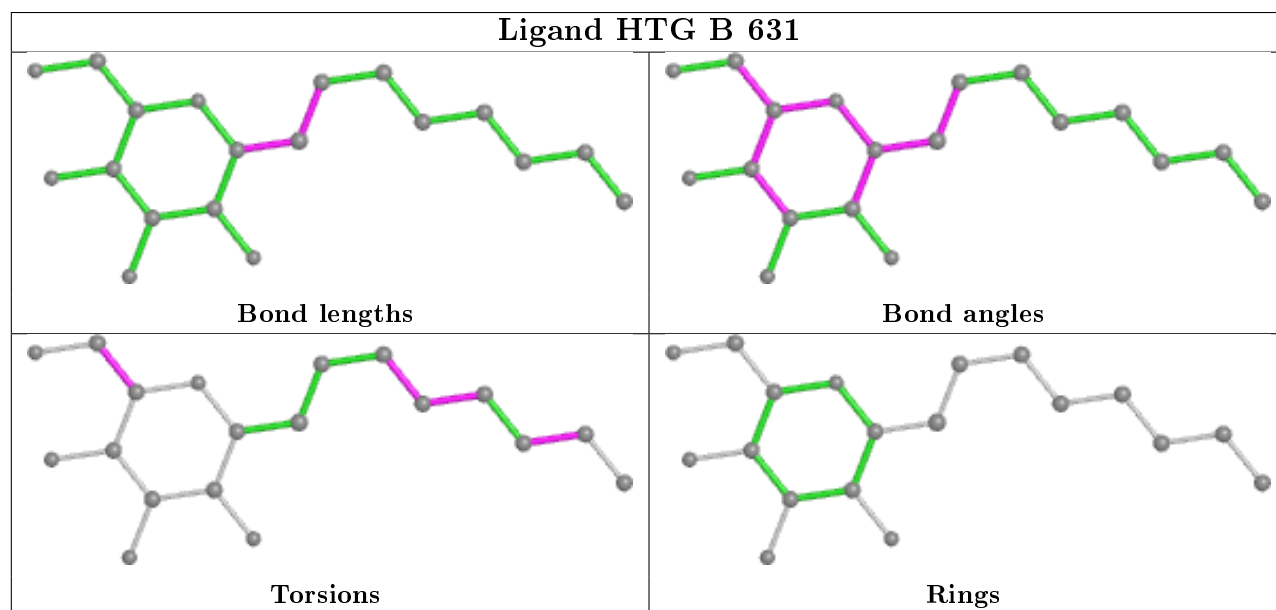
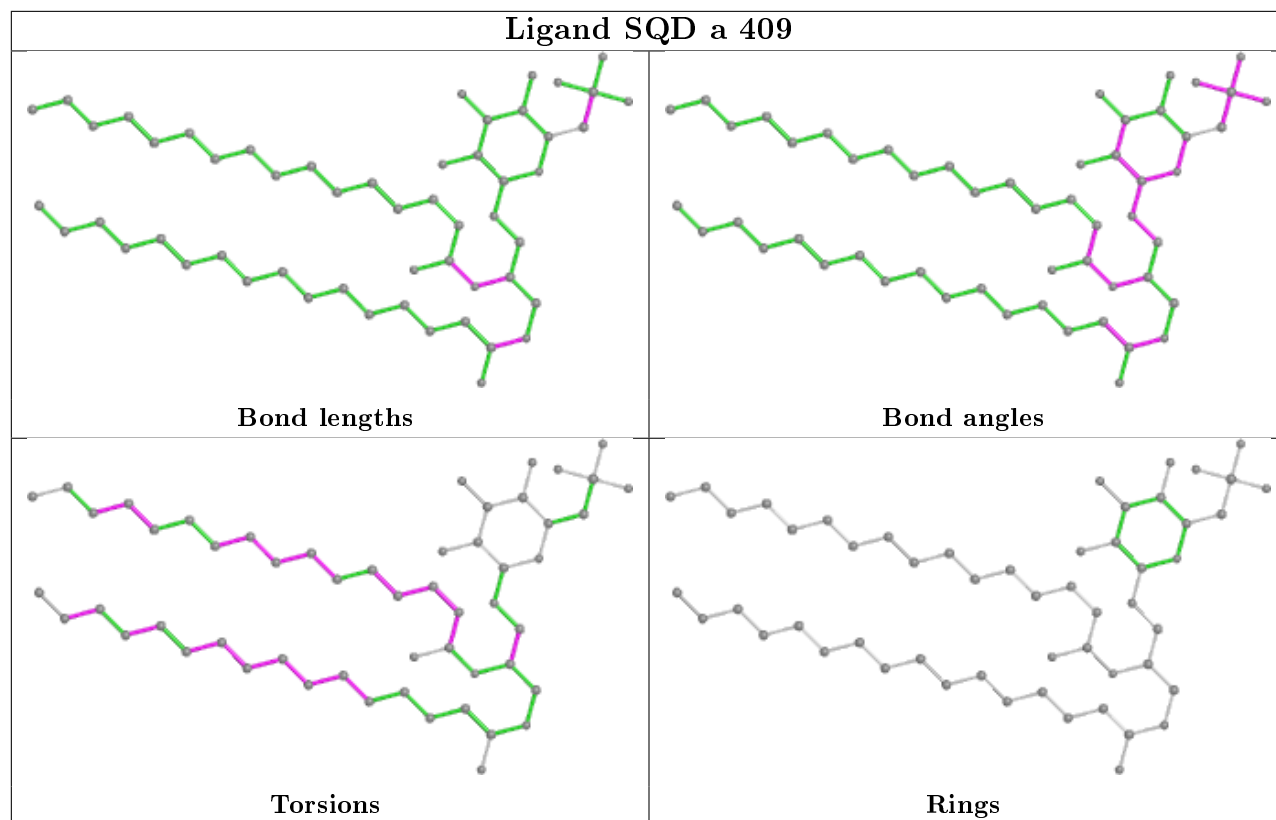
Ligand CLA B 606

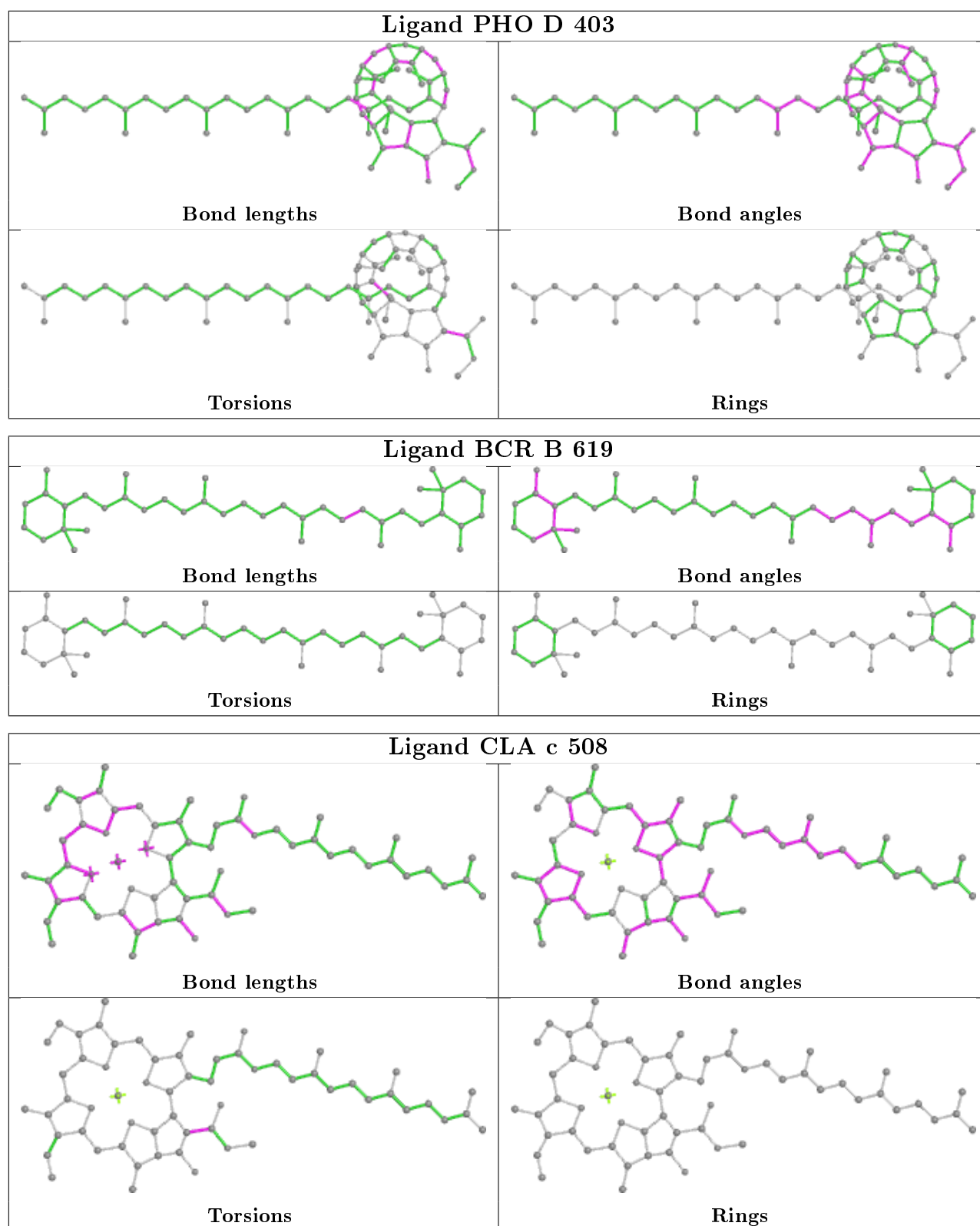


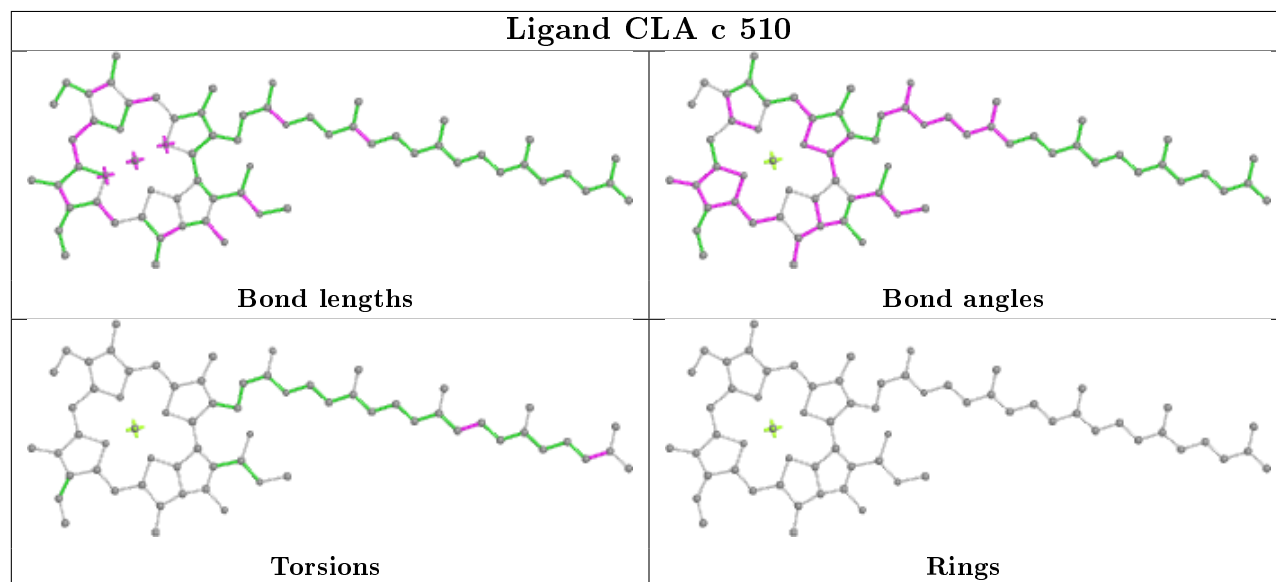
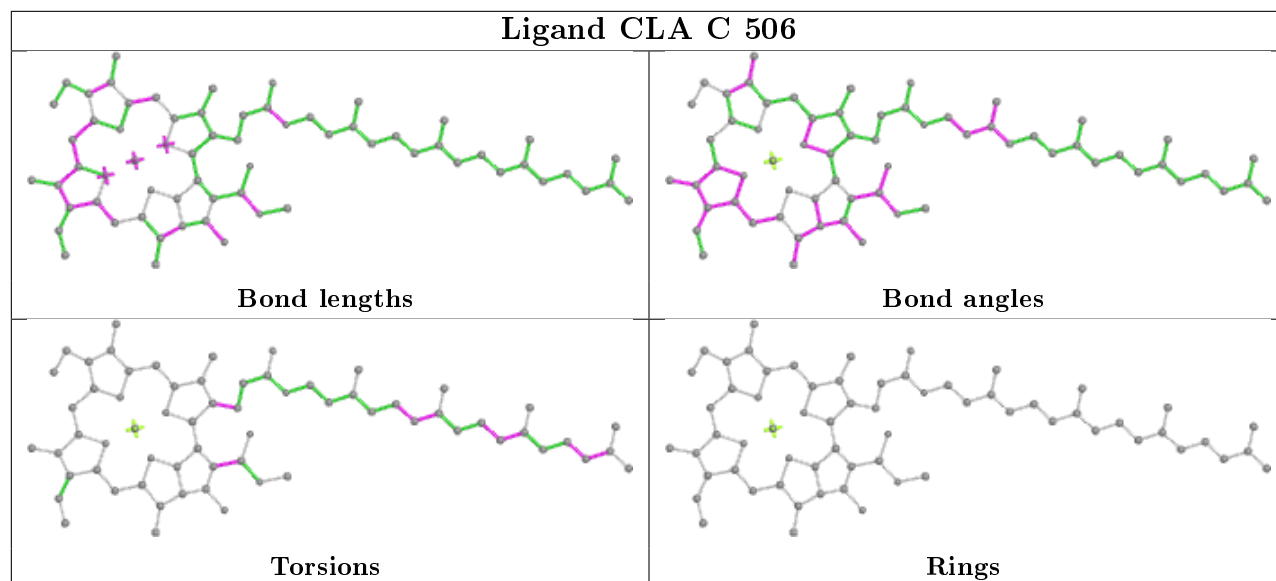
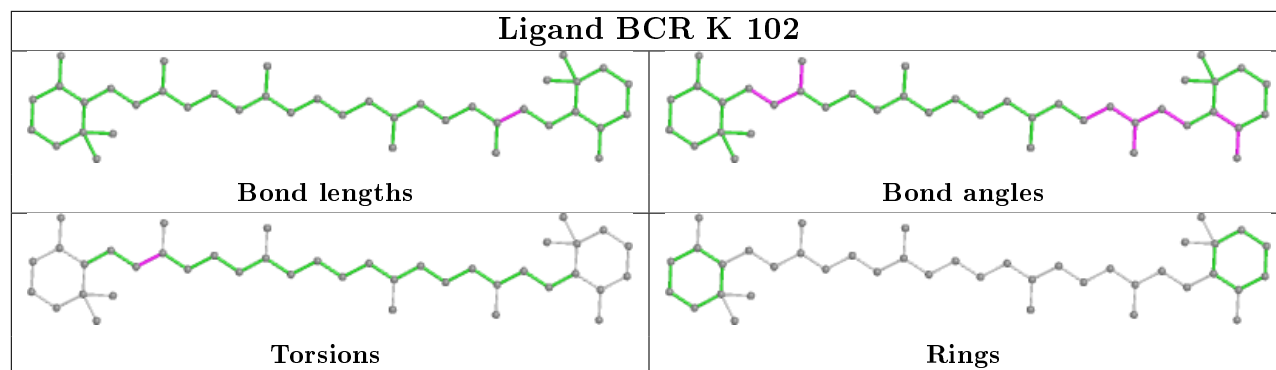
Ligand LMT m 101



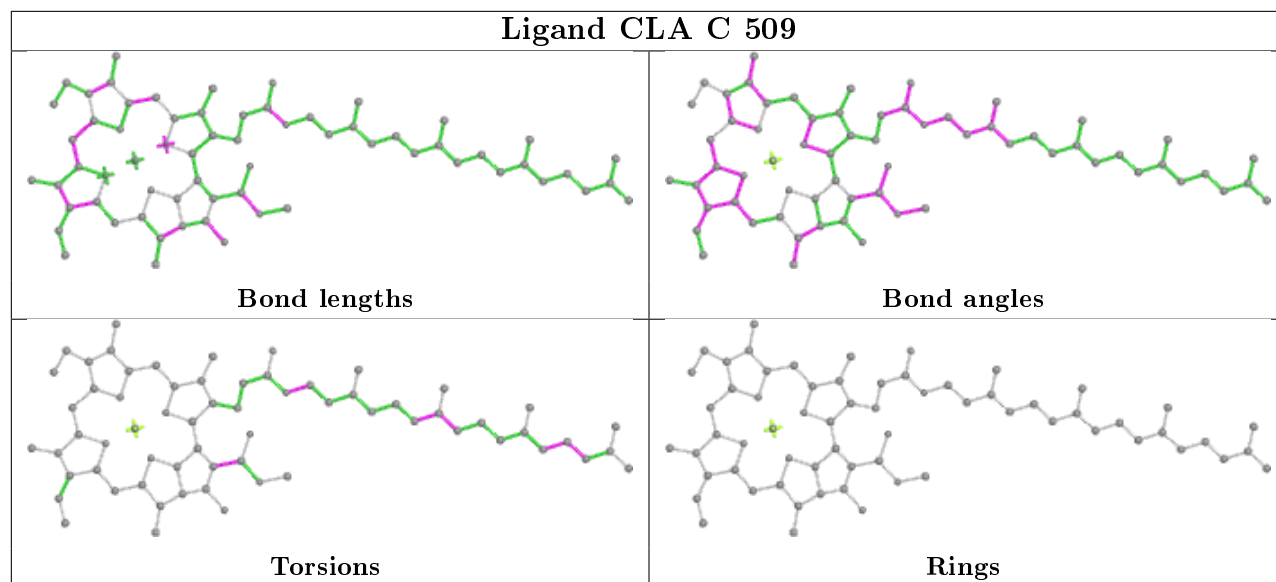
Ligand CLA b 608**Ligand CLA a 403****Ligand PL9 d 412**



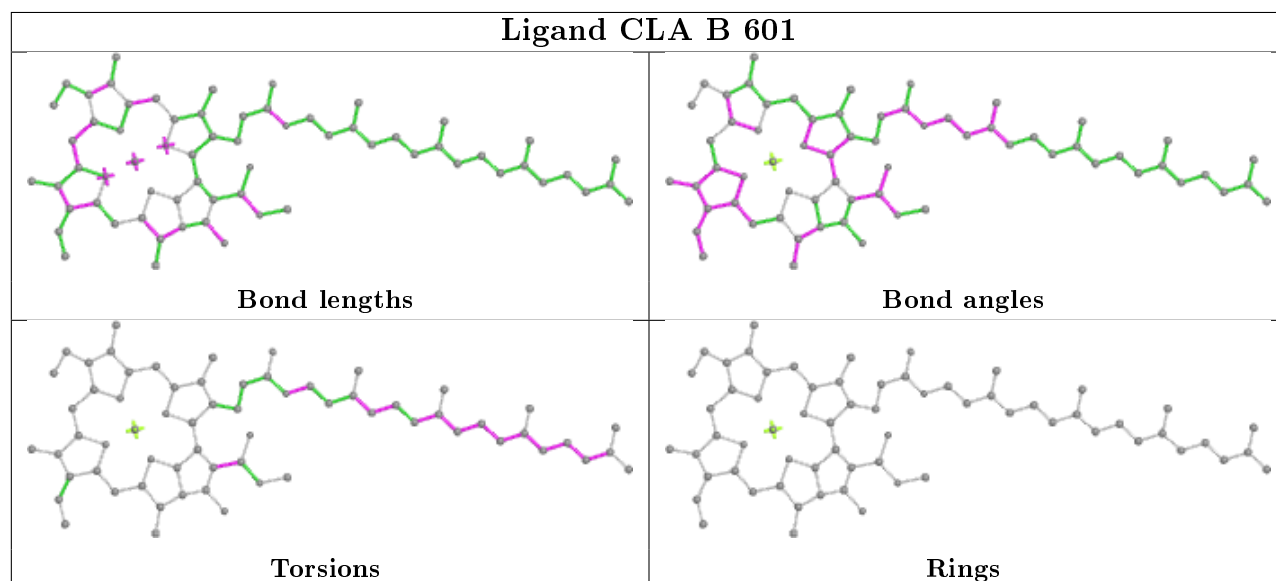




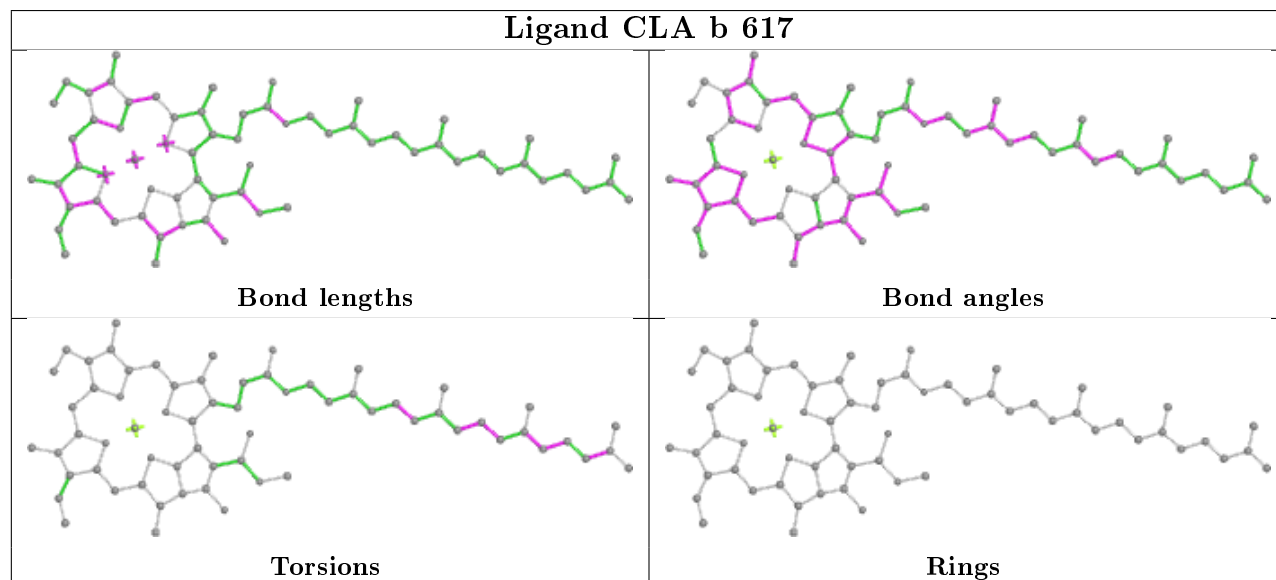
Ligand CLA C 509

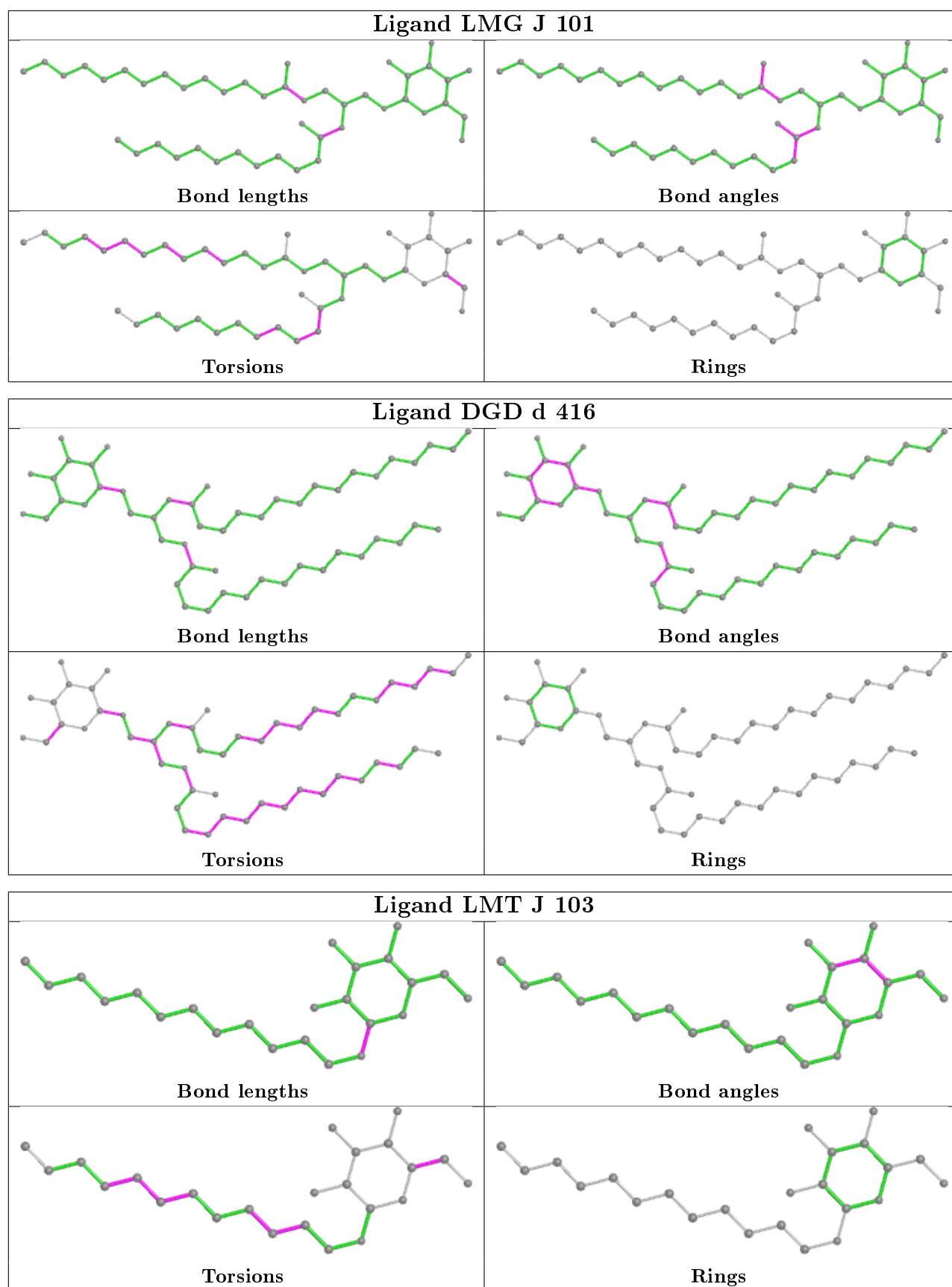


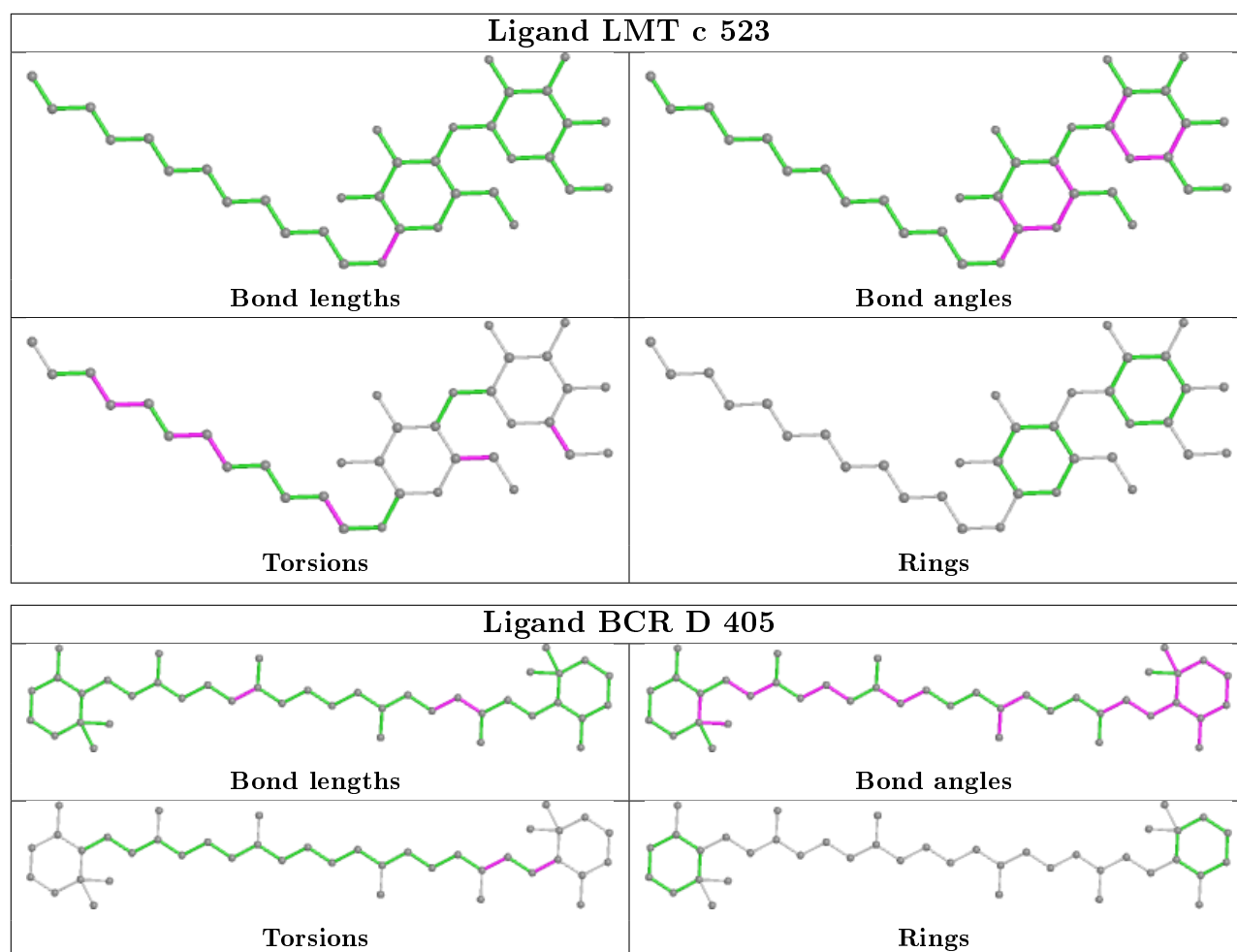
Ligand CLA B 601

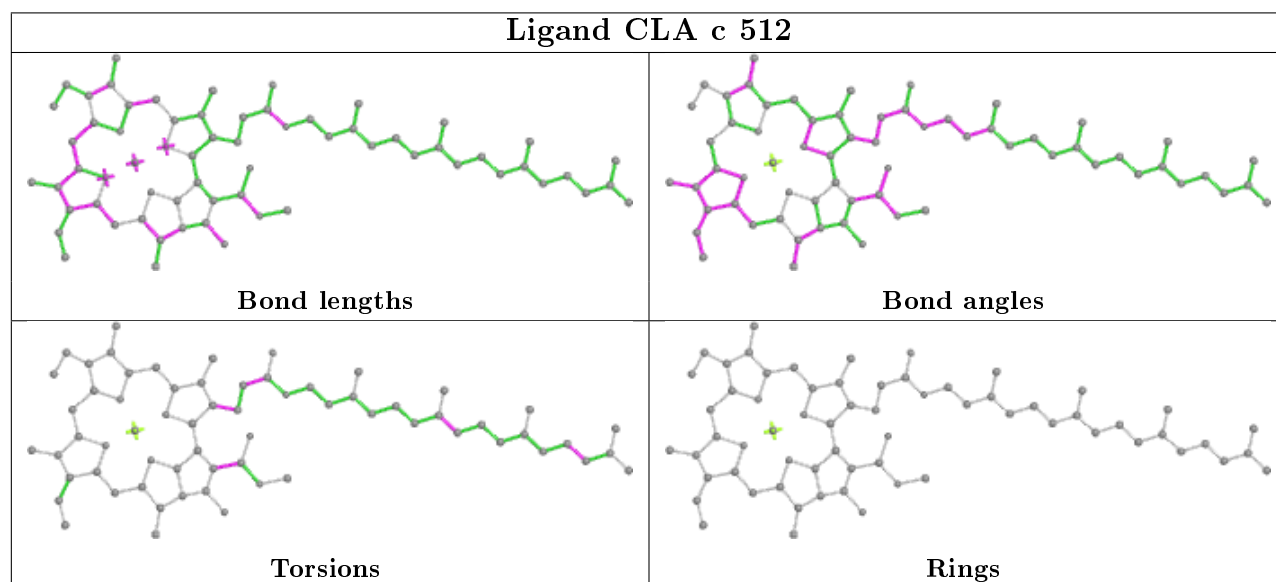
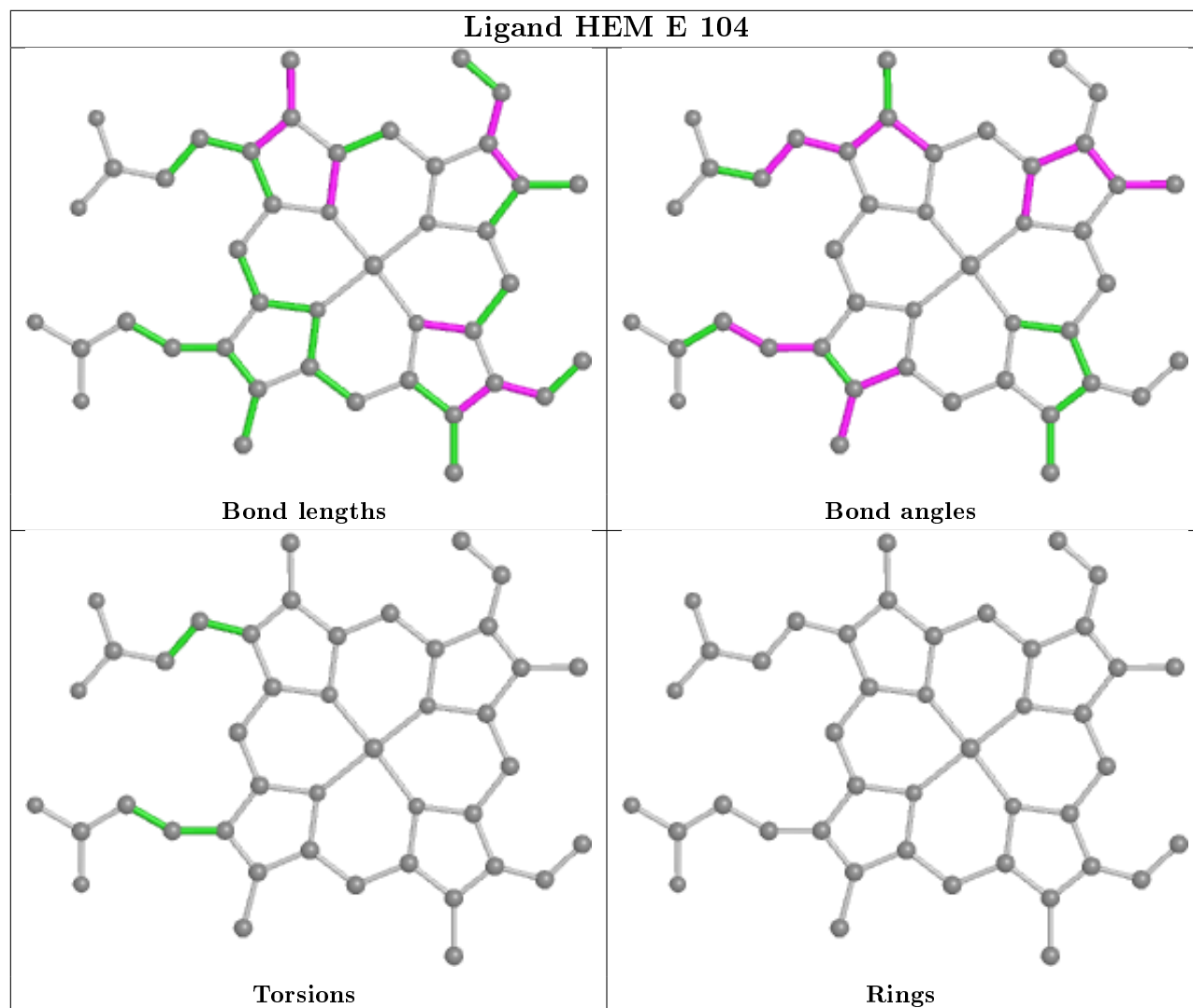


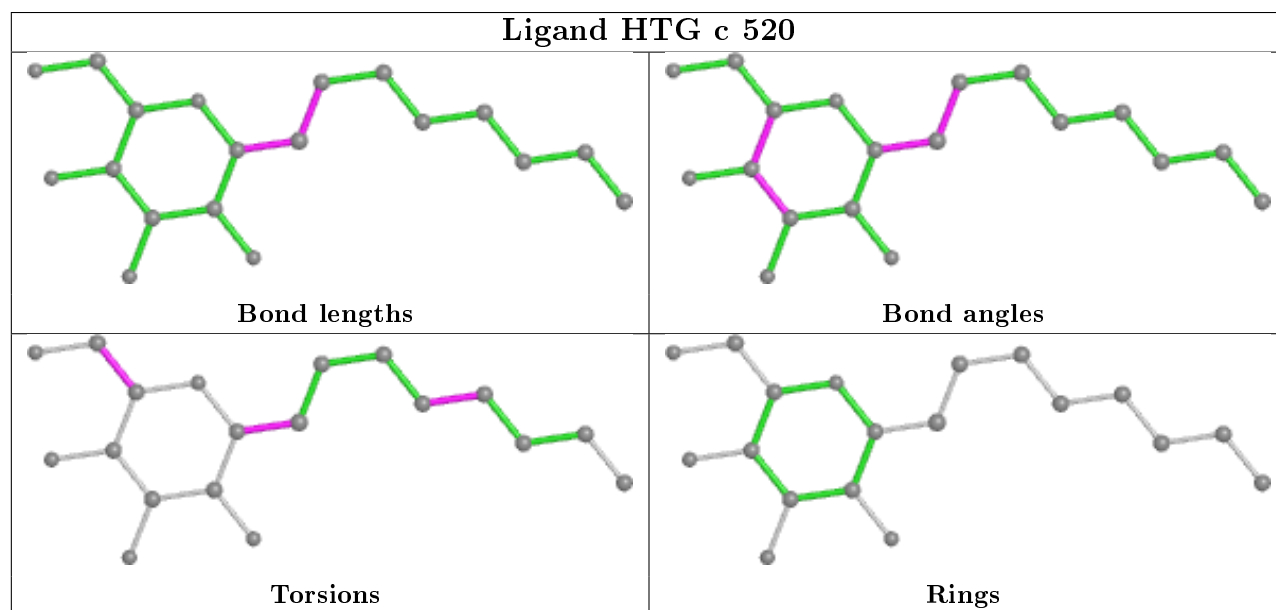
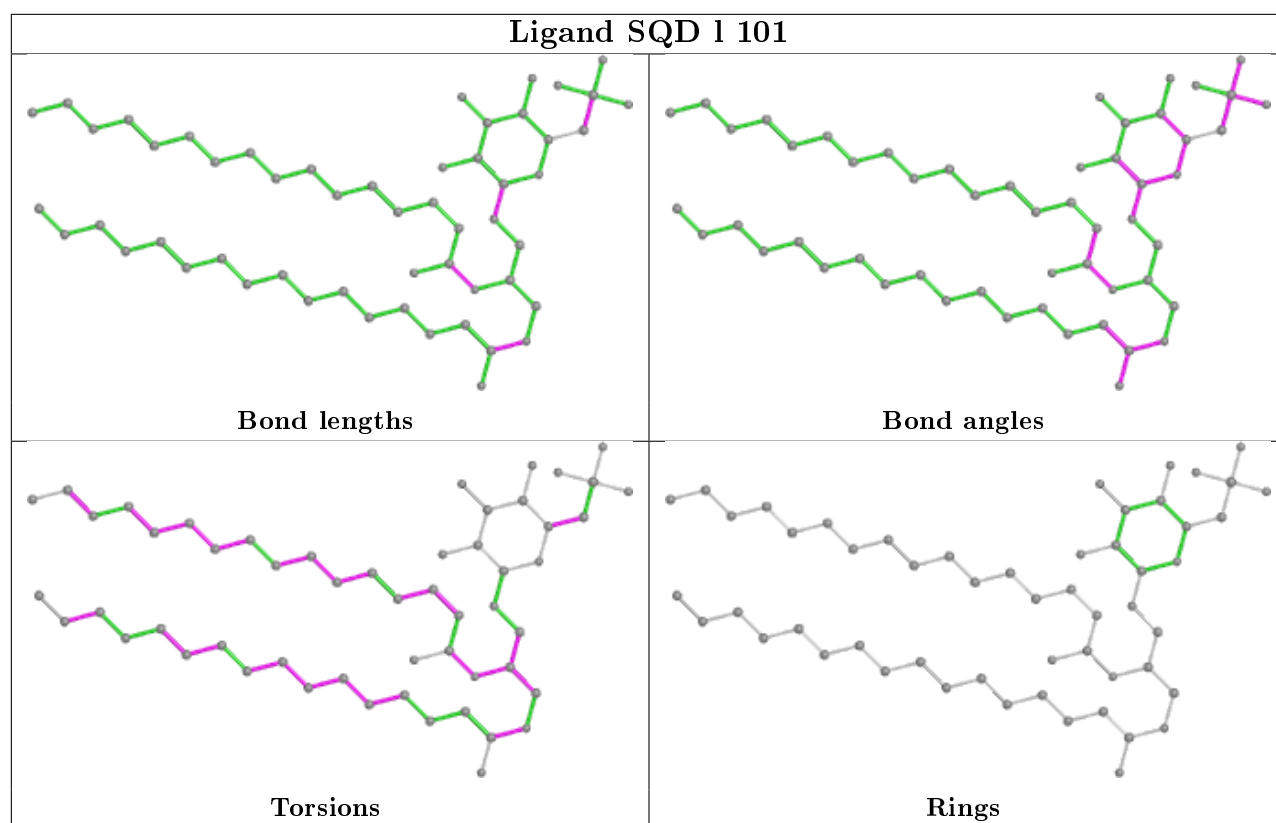
Ligand CLA b 617

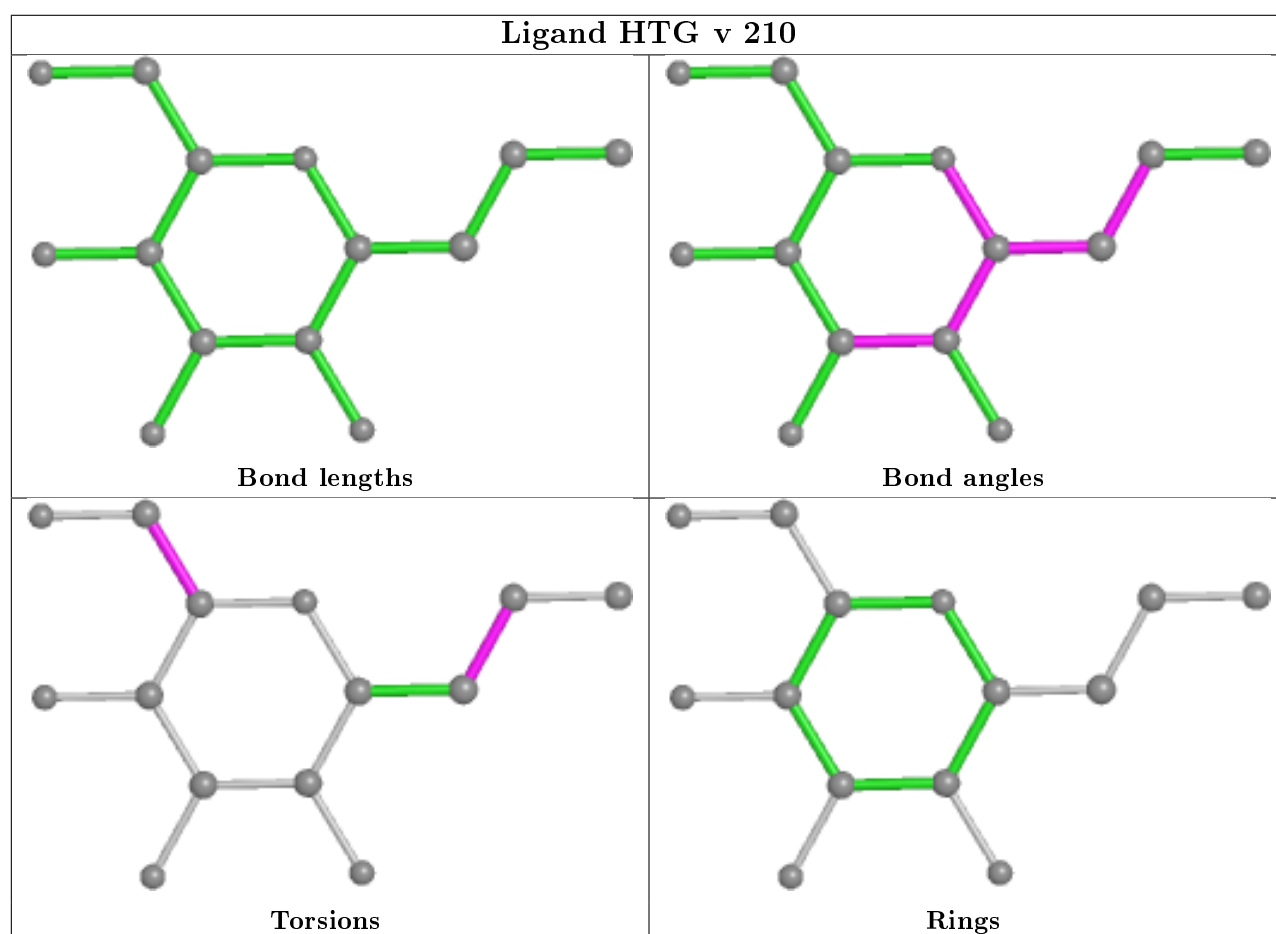
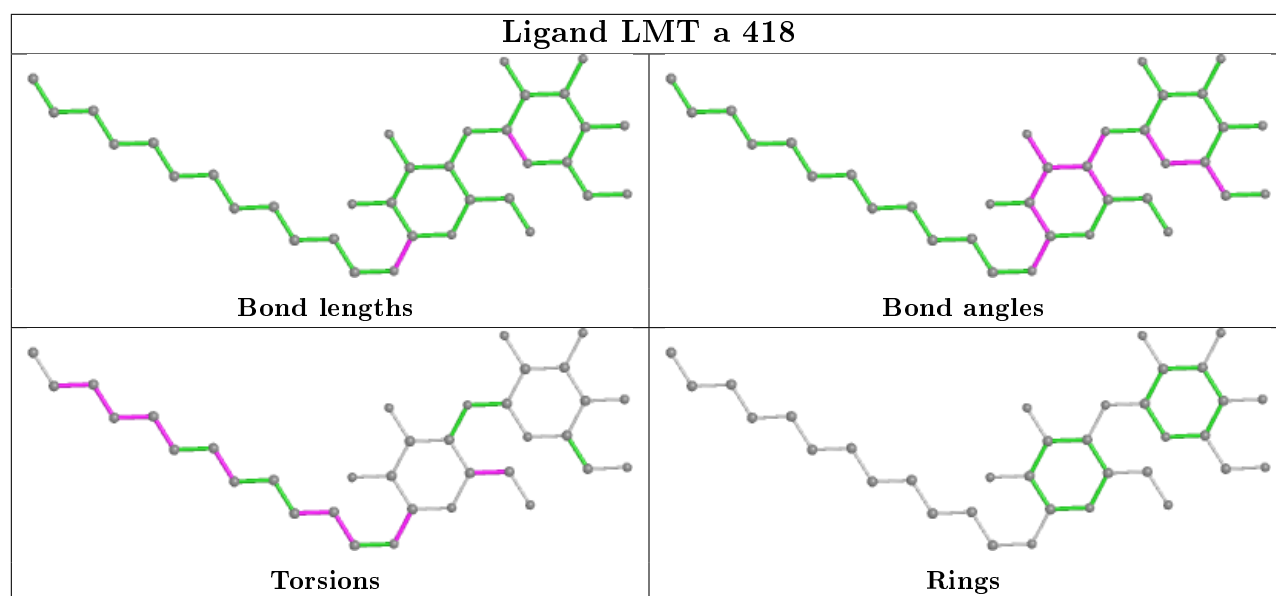


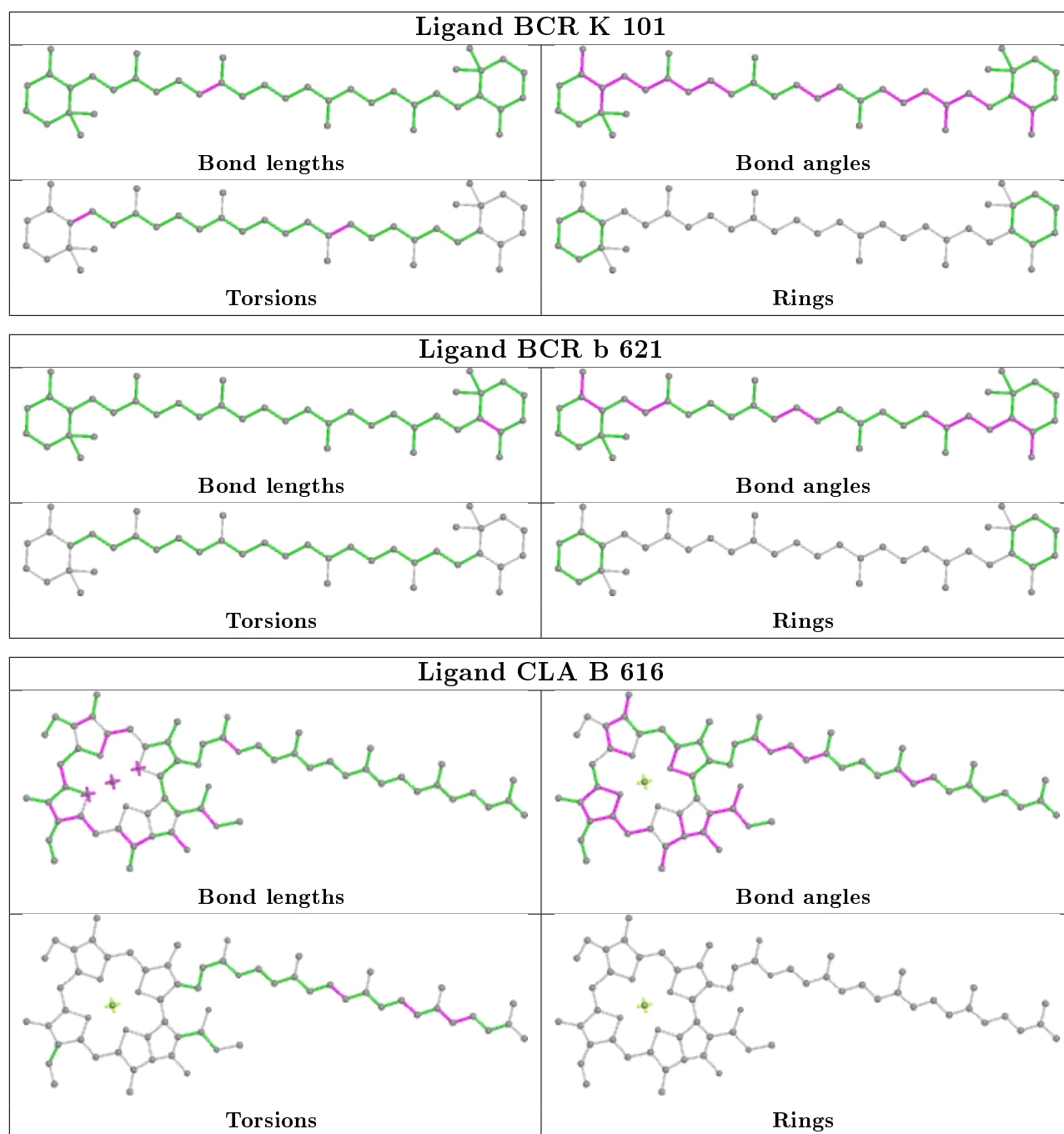


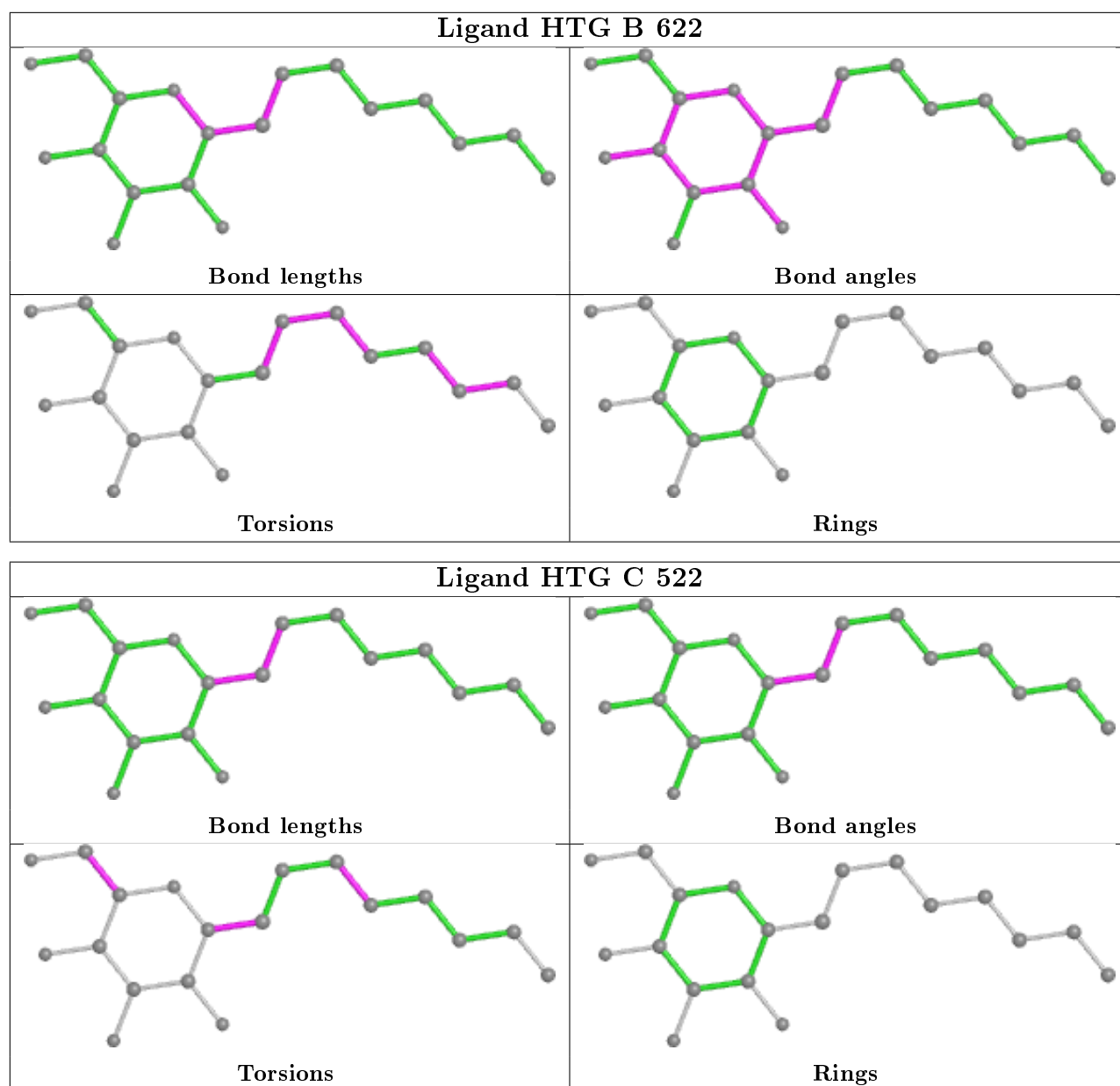




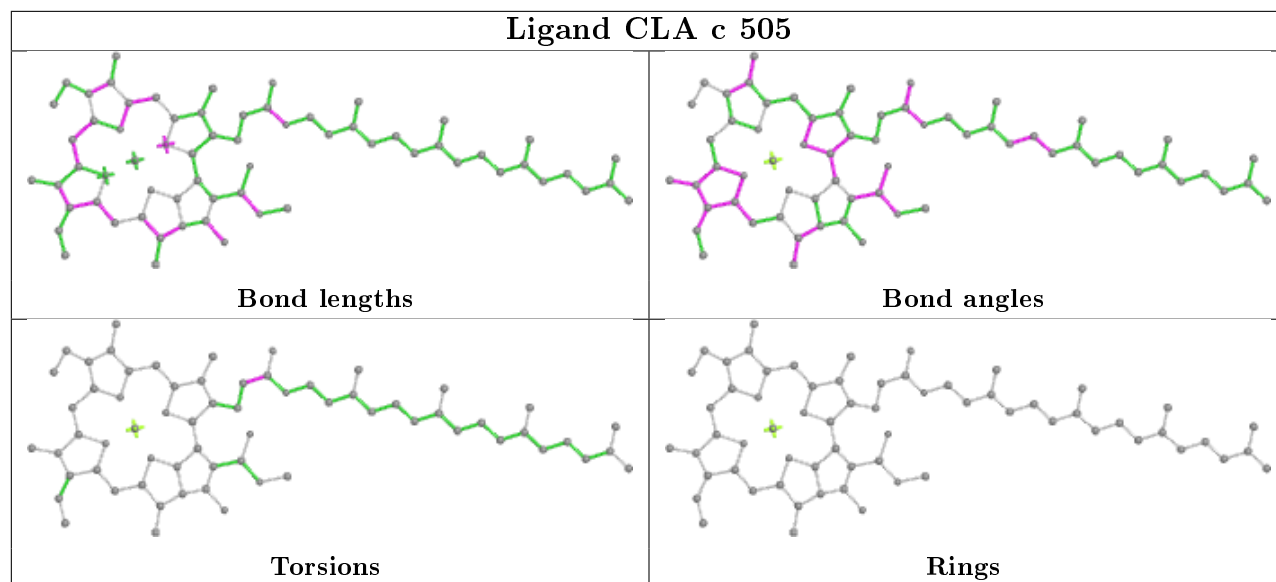




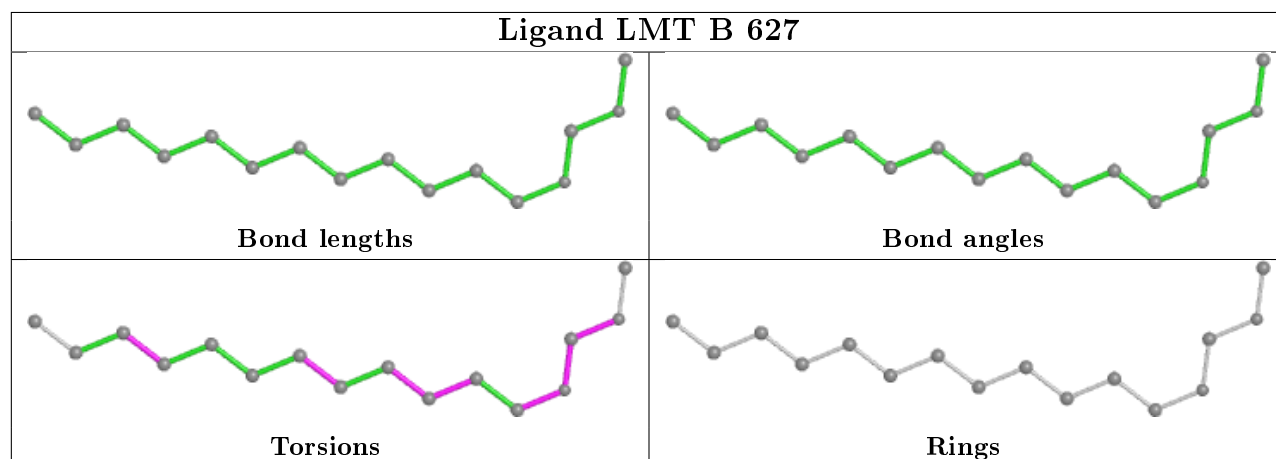




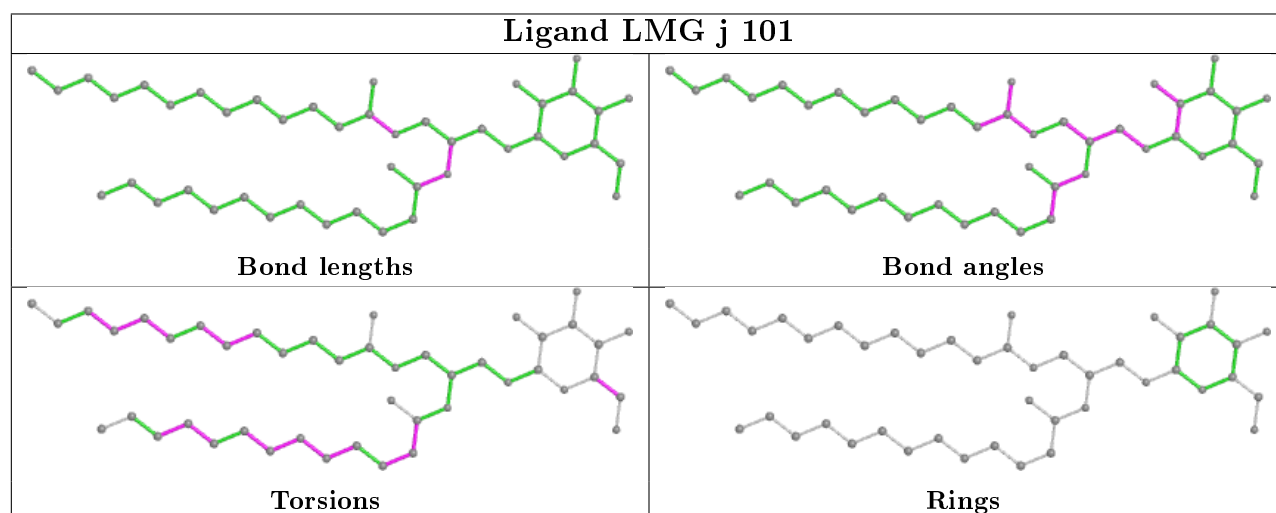
Ligand CLA c 505

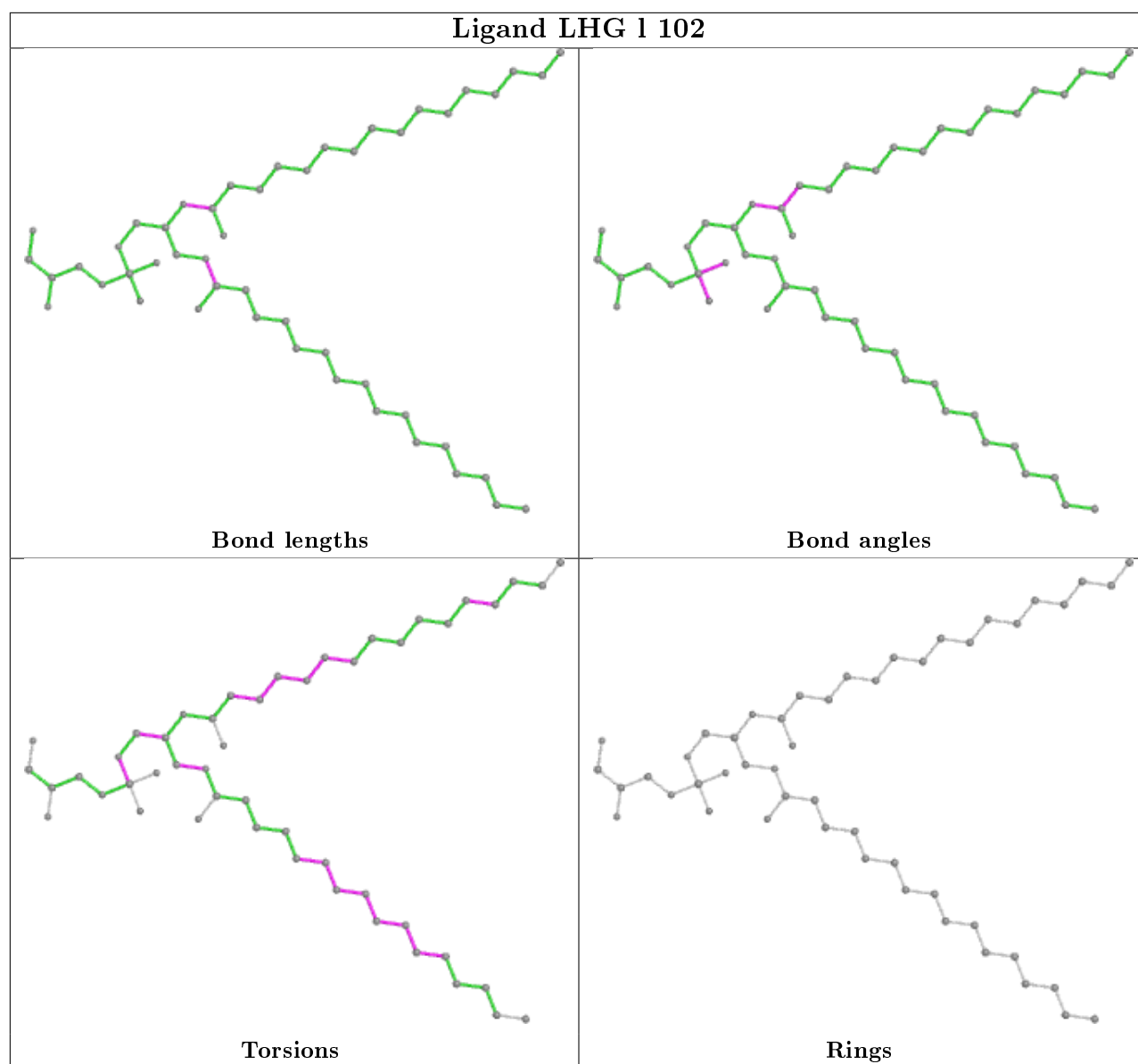


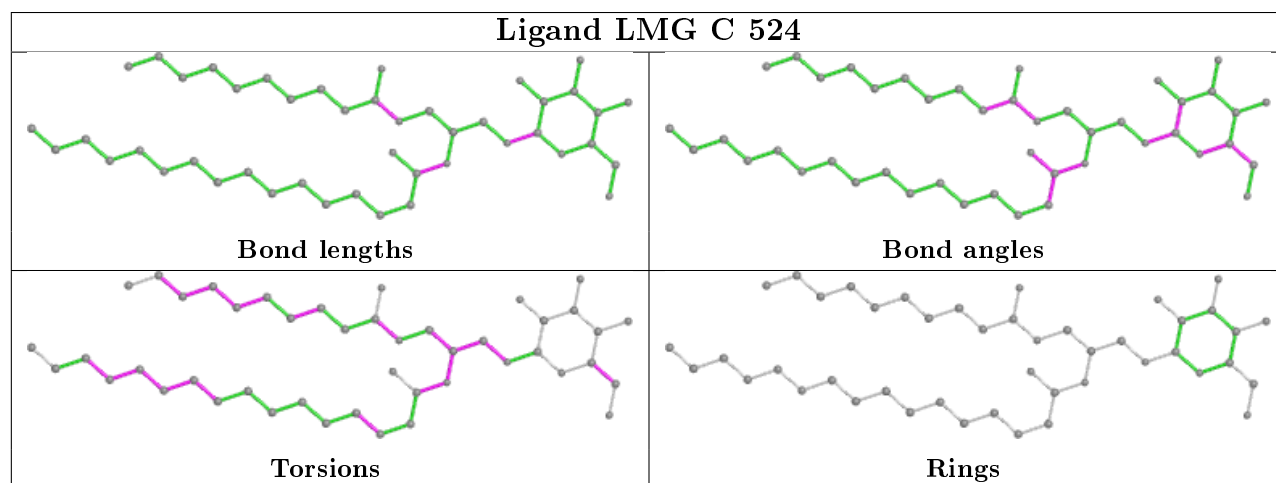
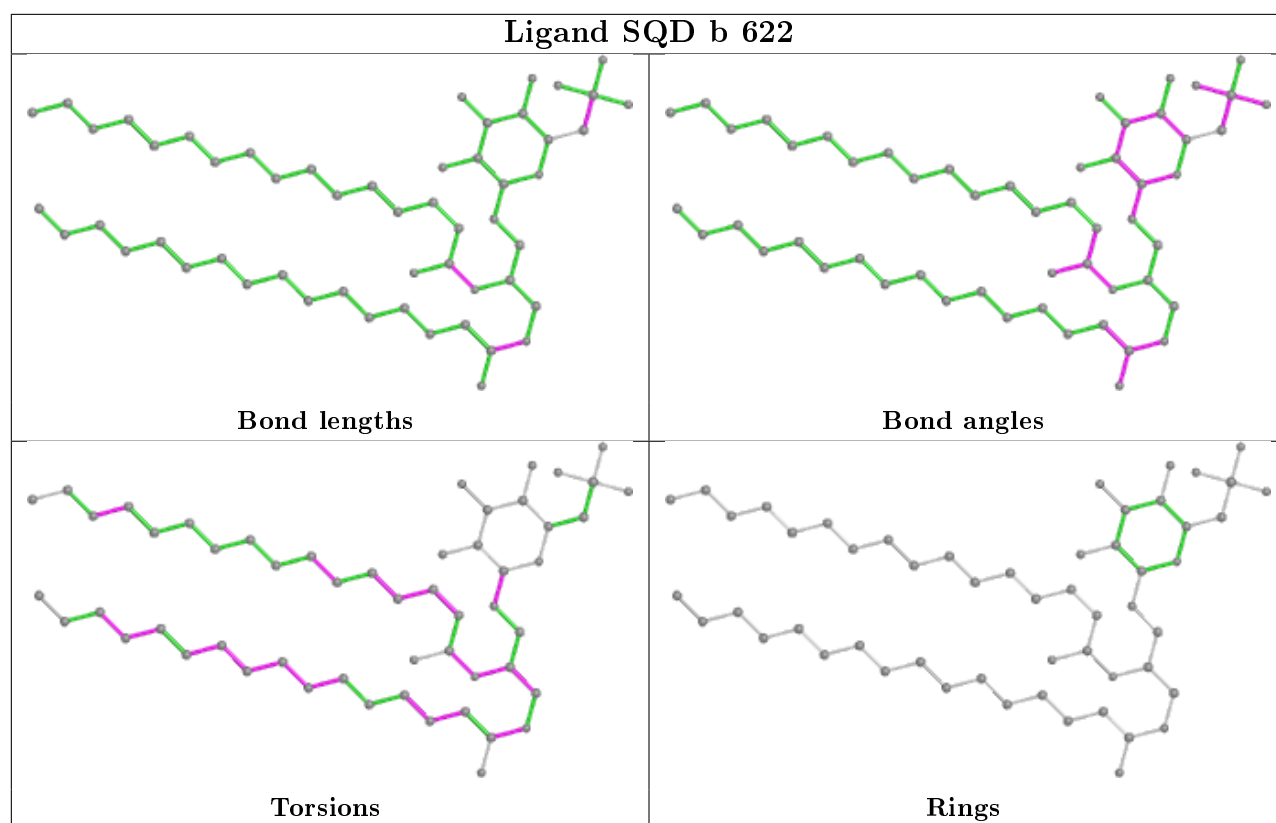
Ligand LMT B 627

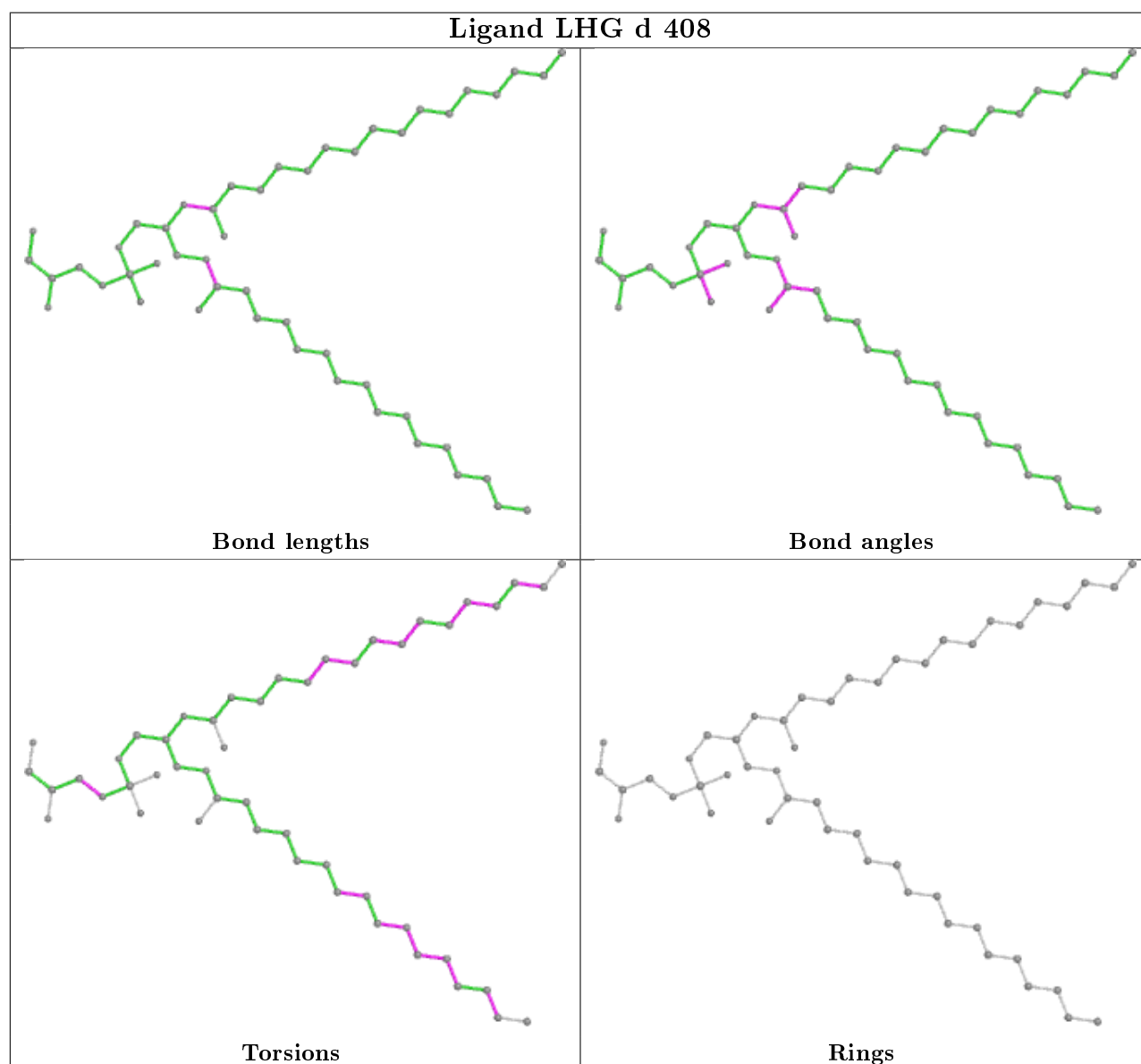
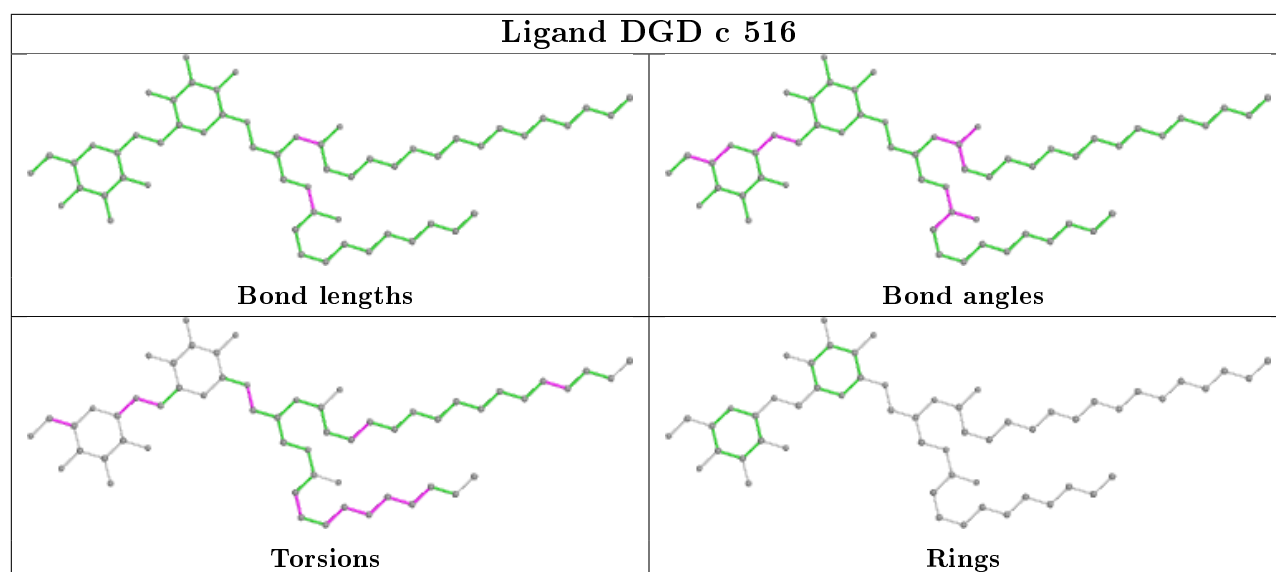


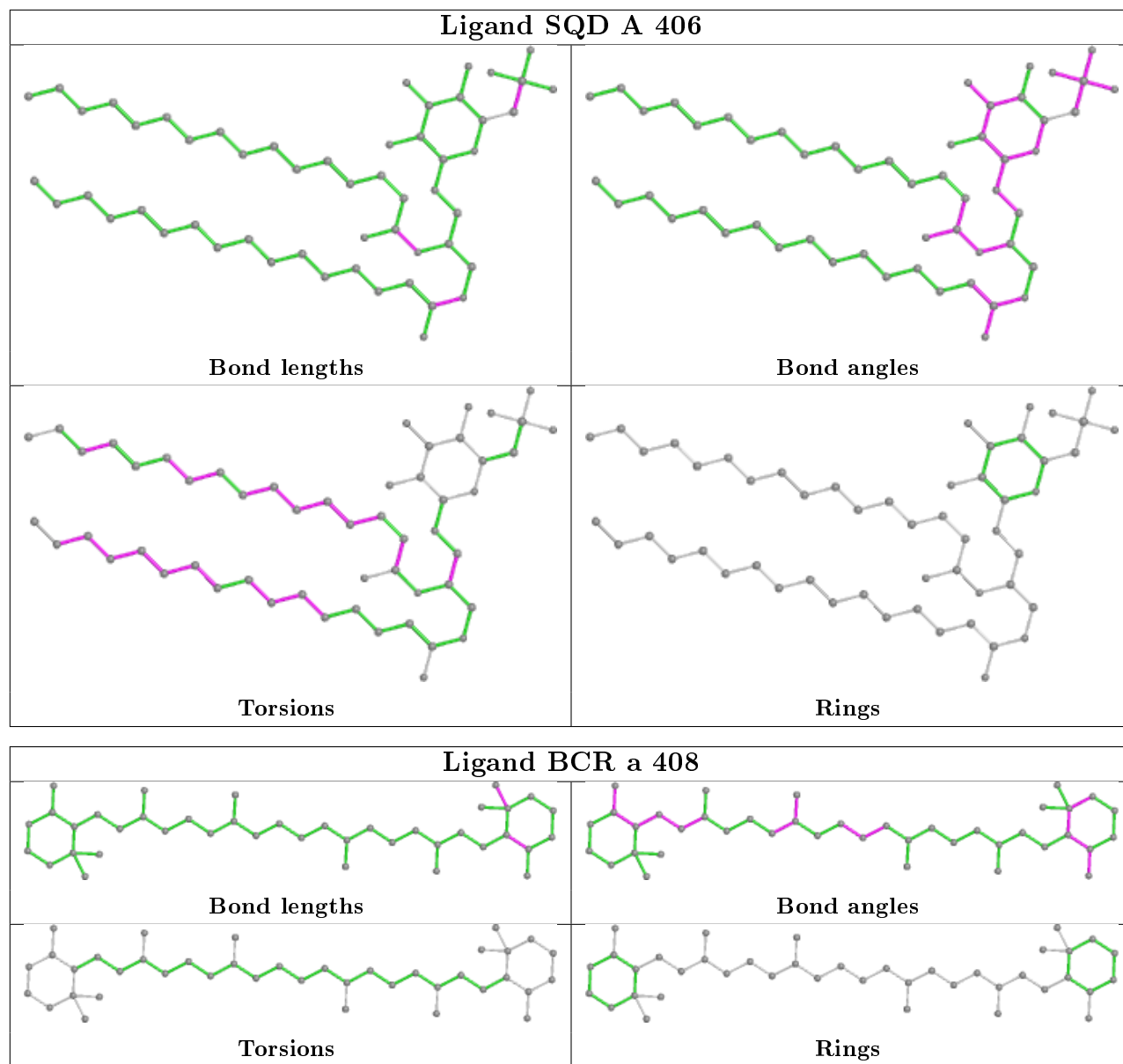
Ligand LMG j 101

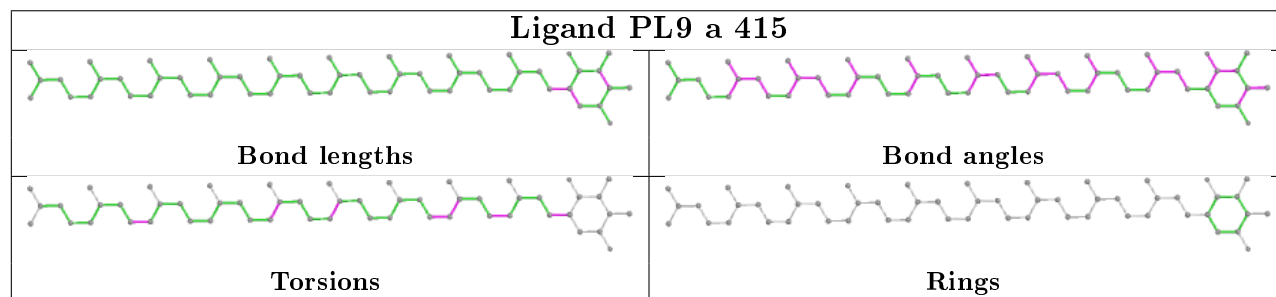
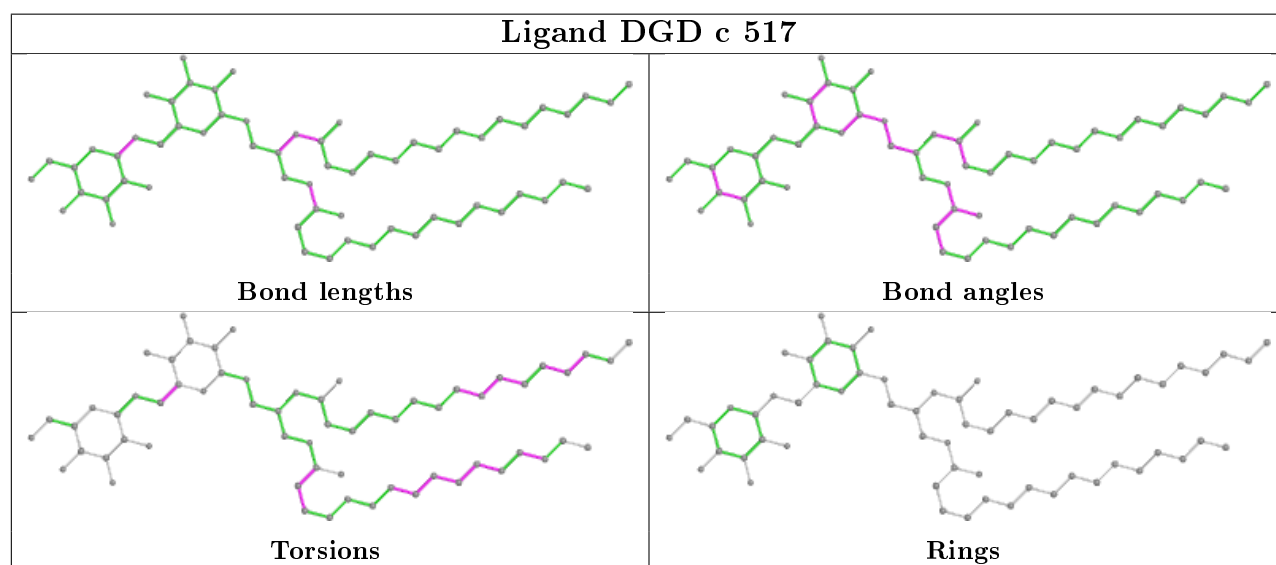
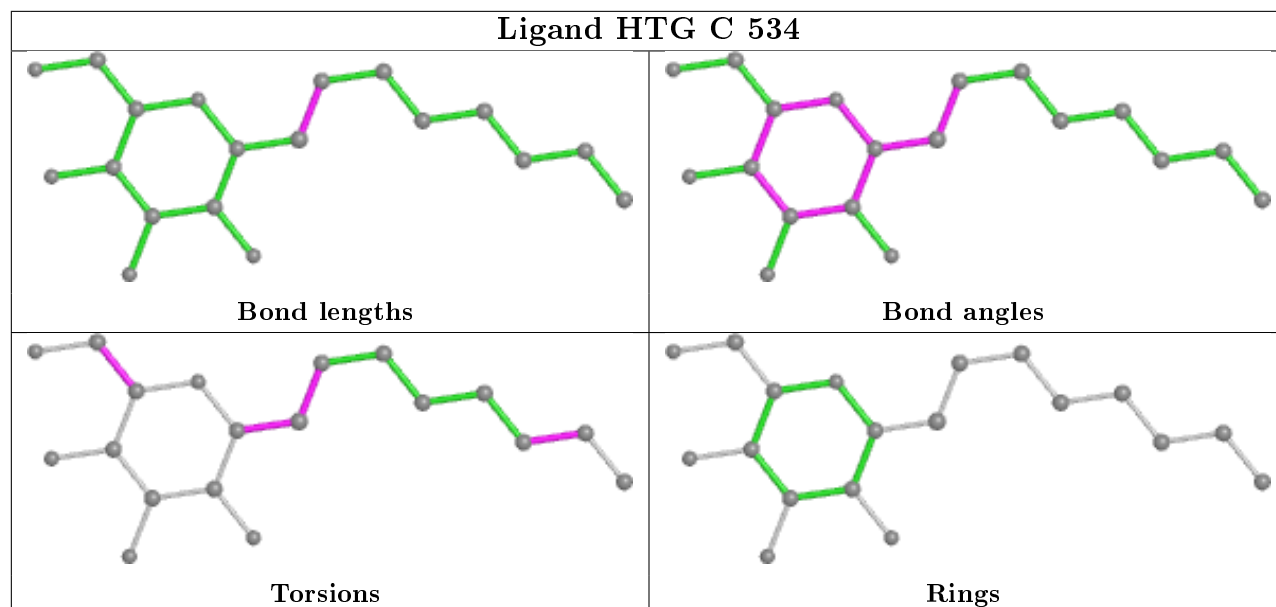


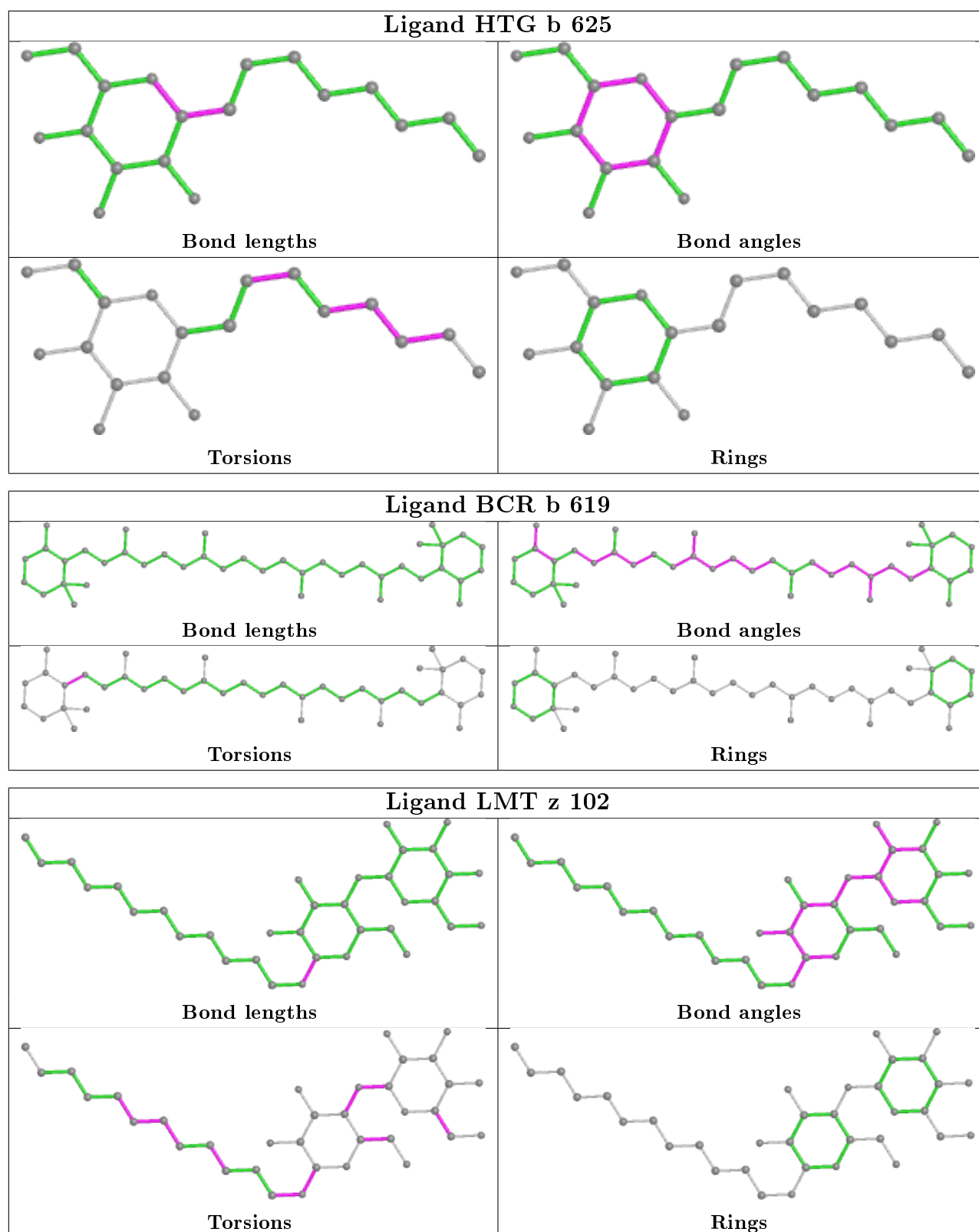


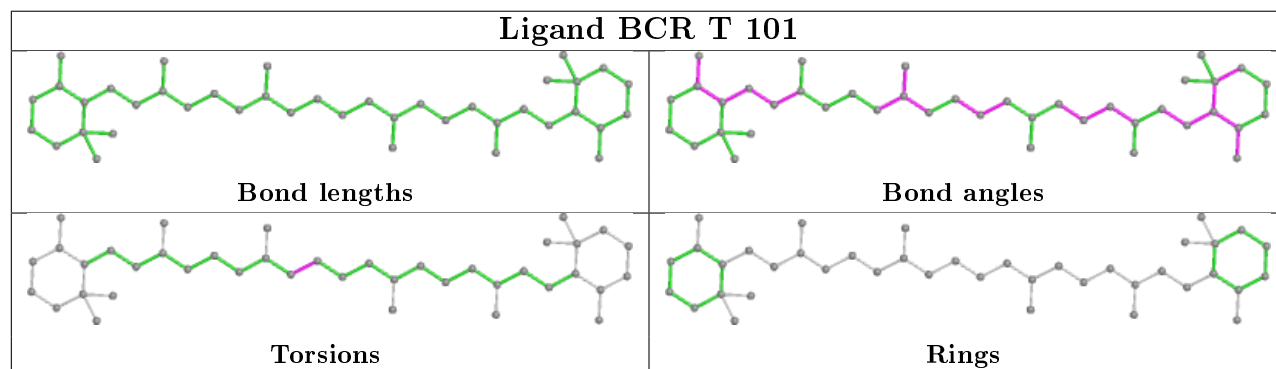
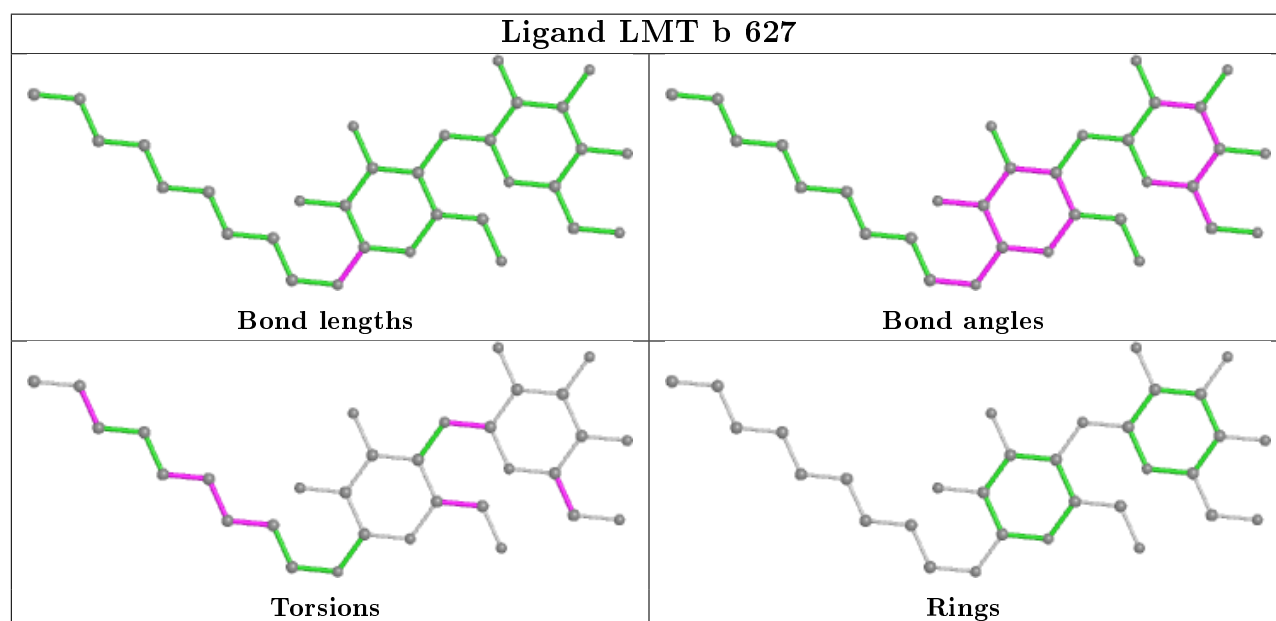
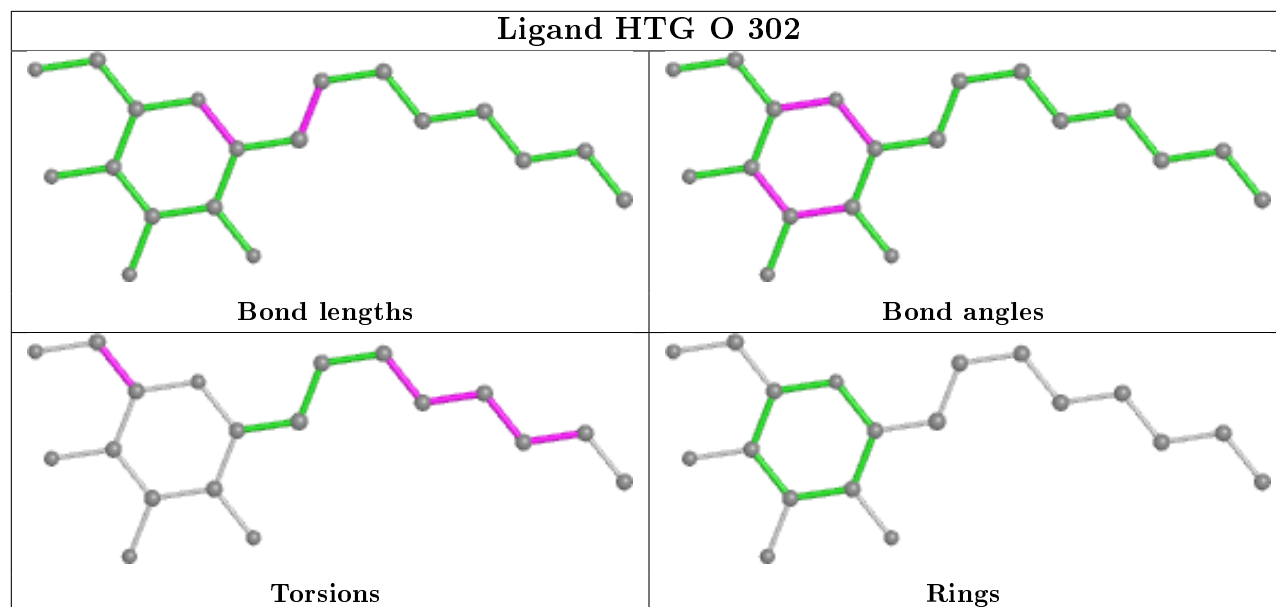


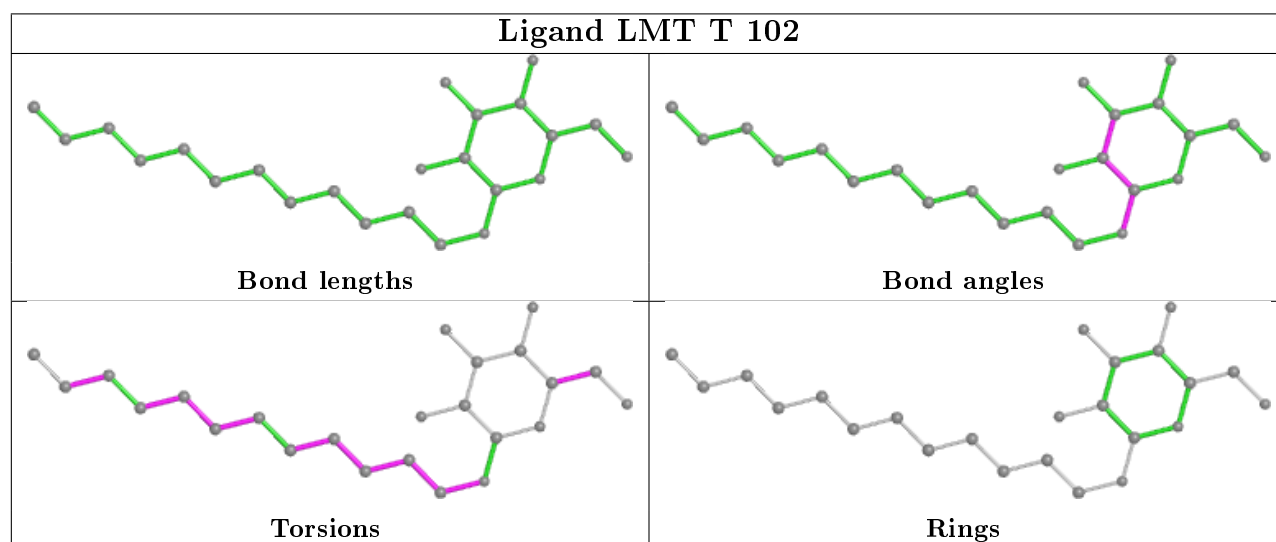
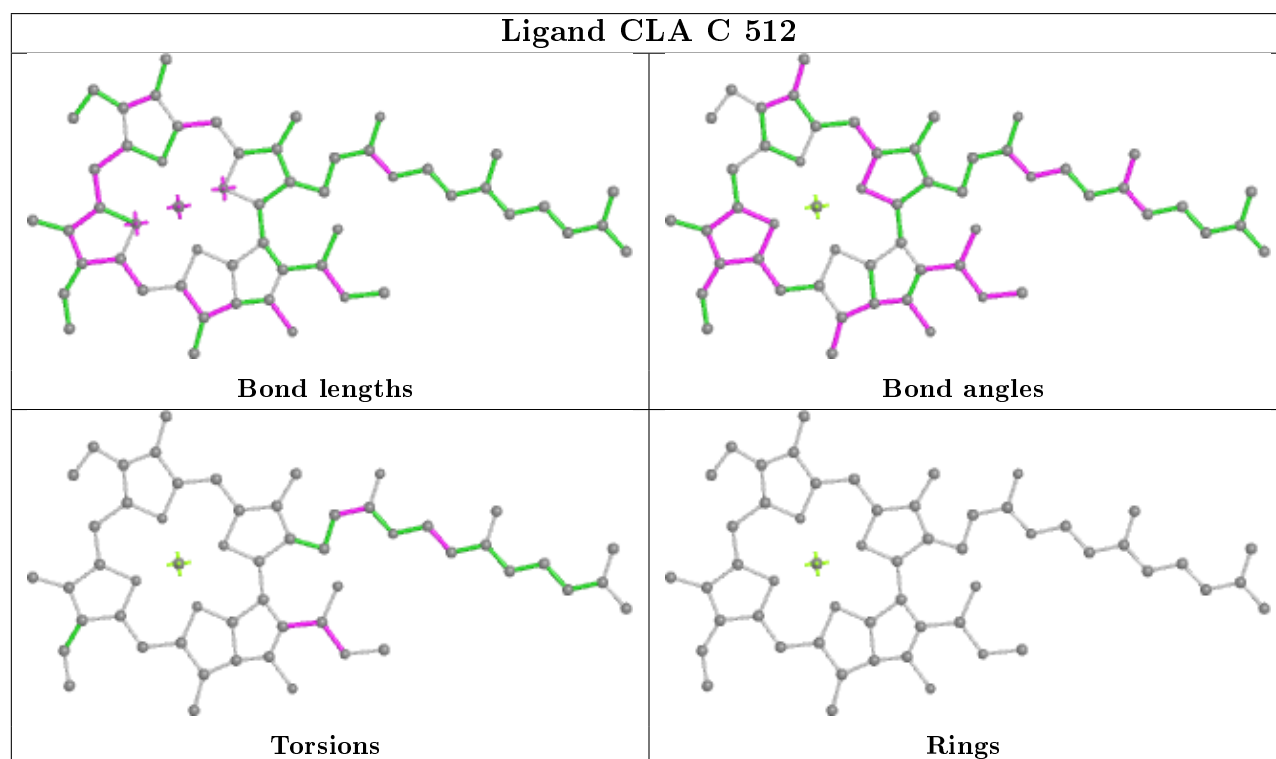
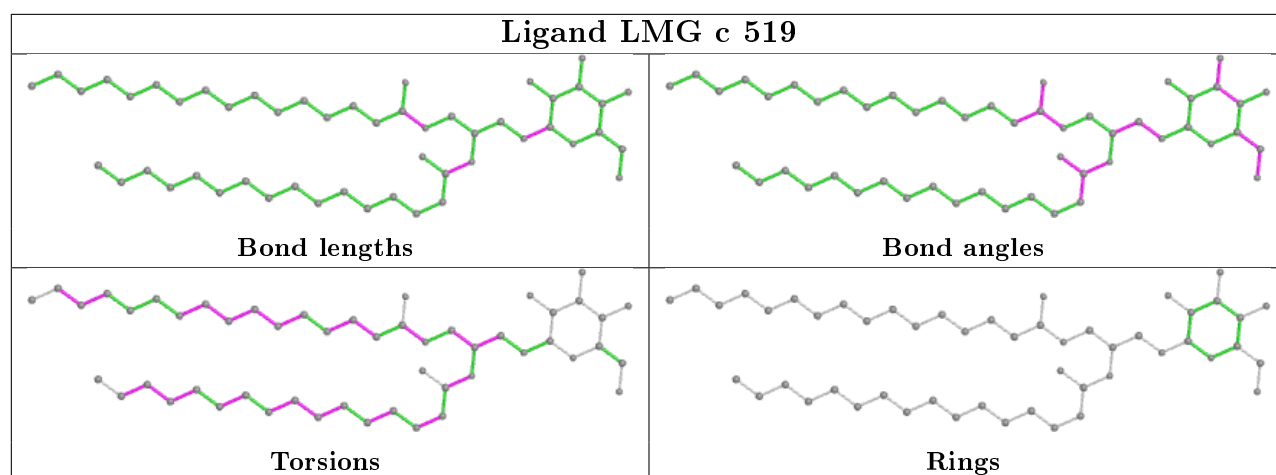


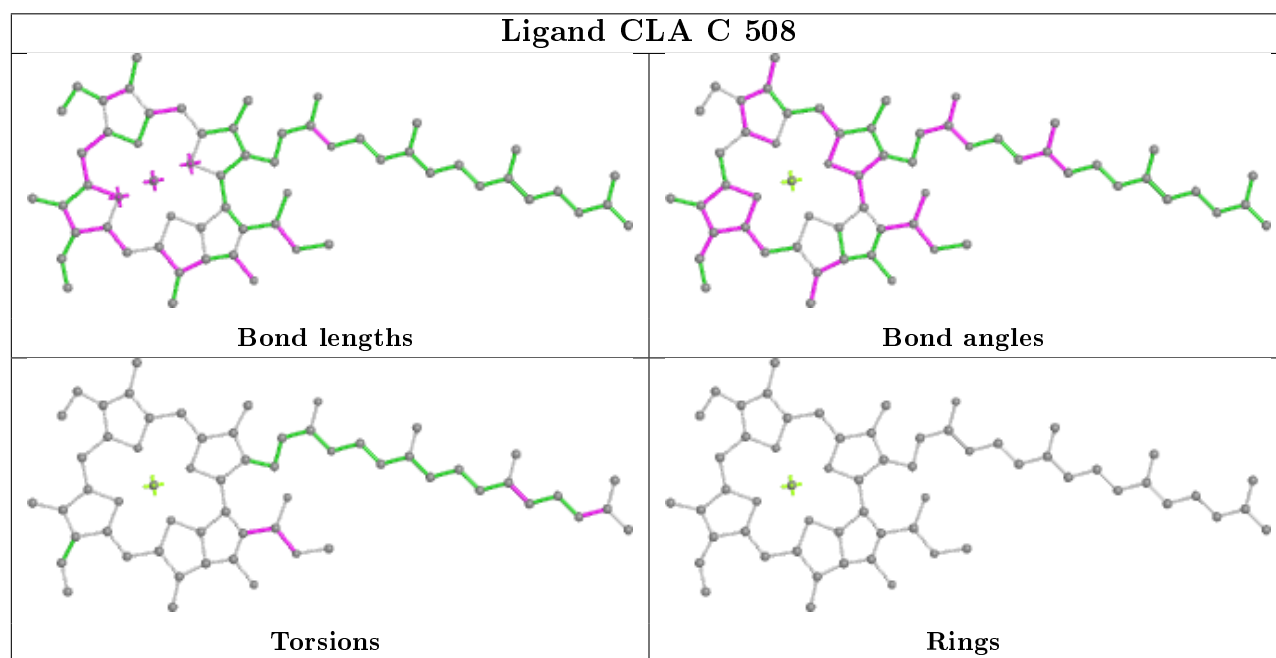
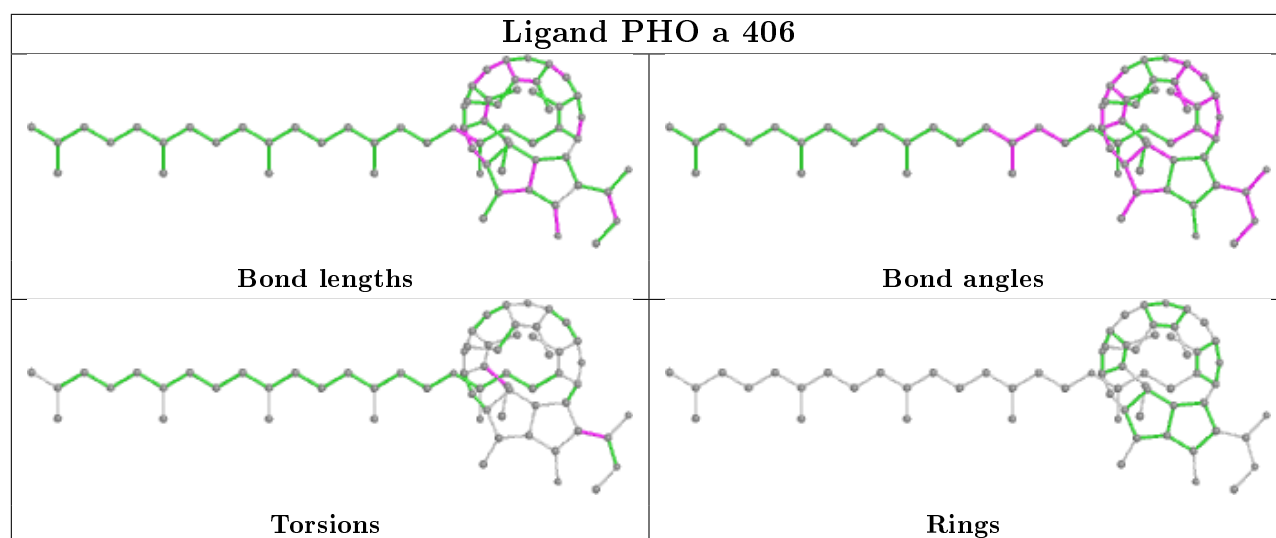


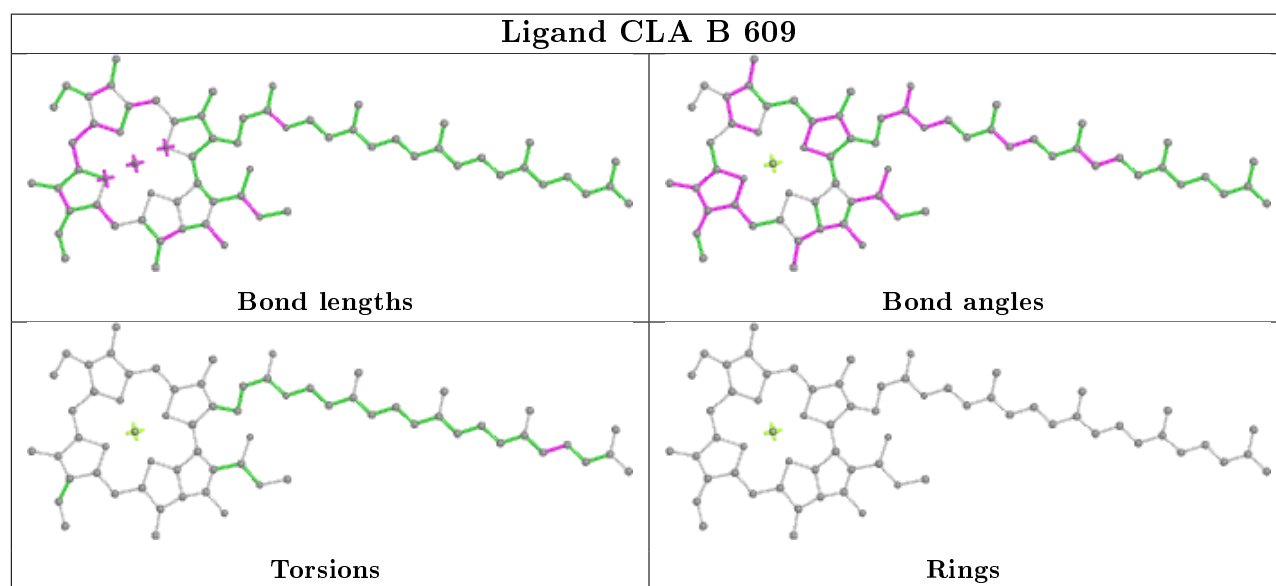
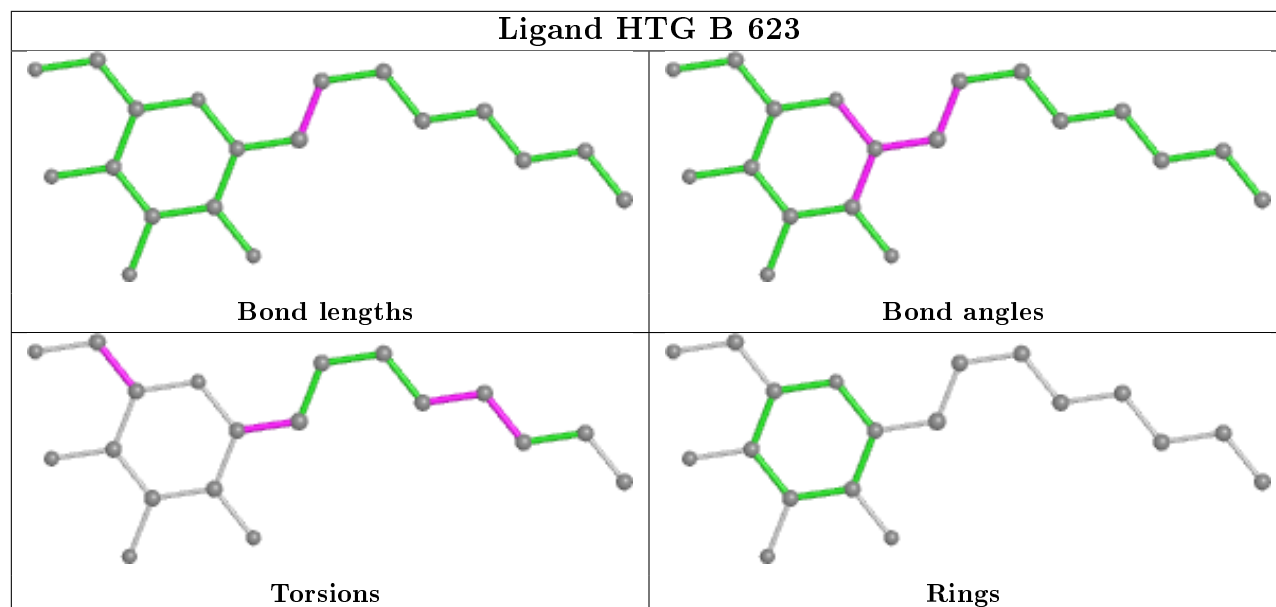


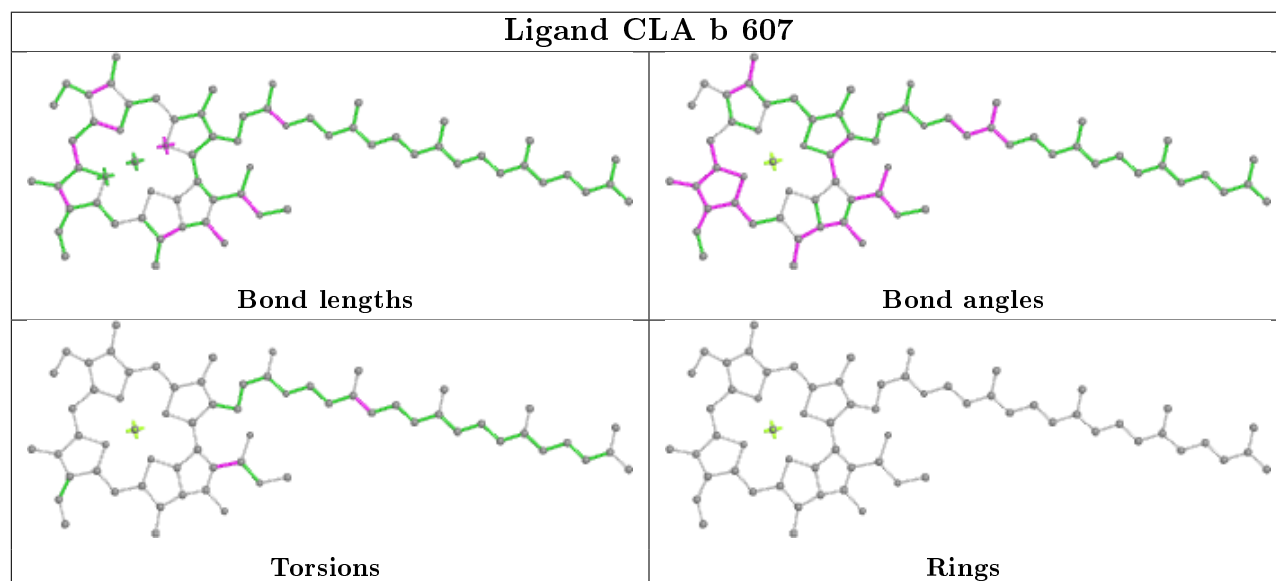
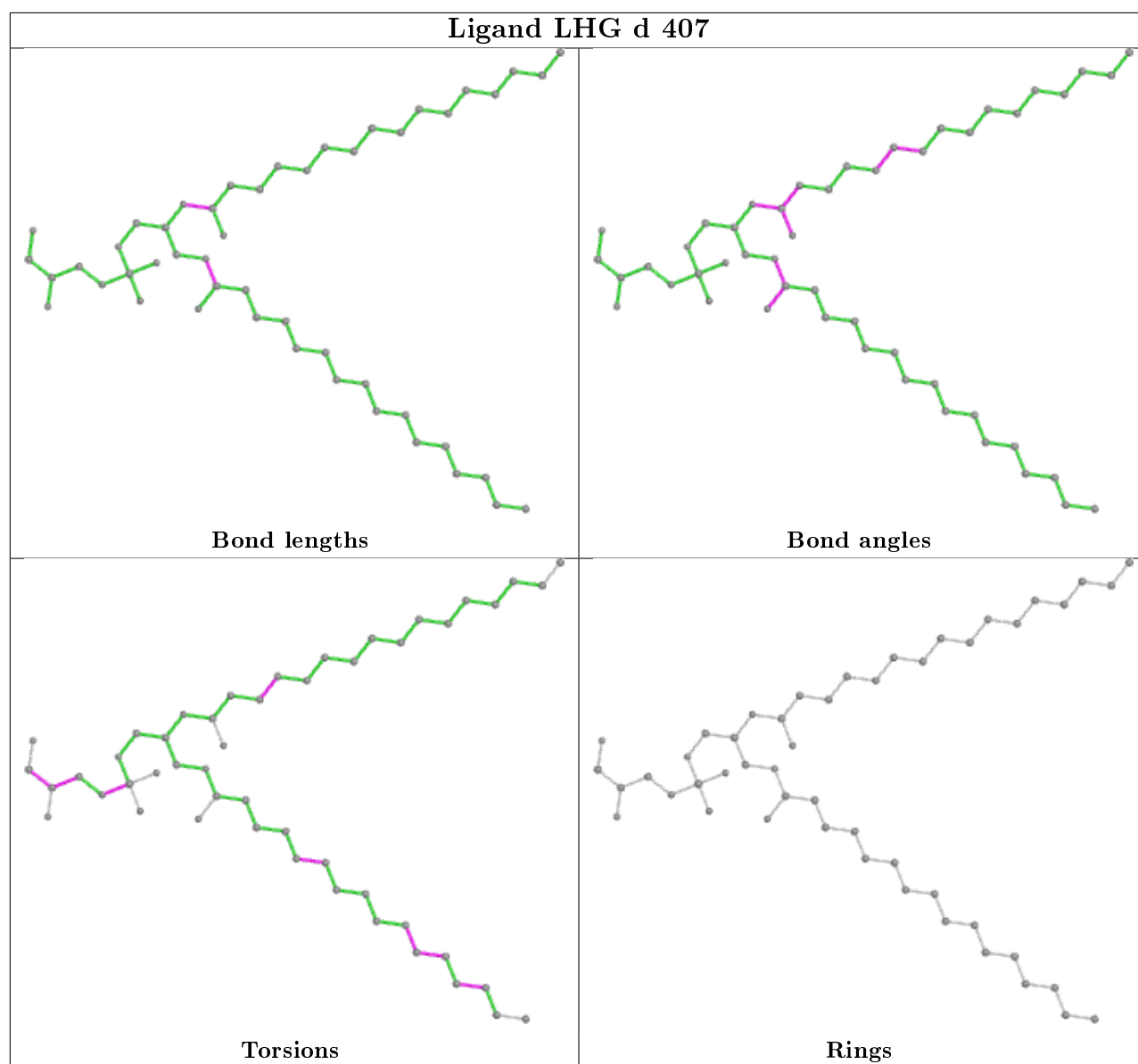




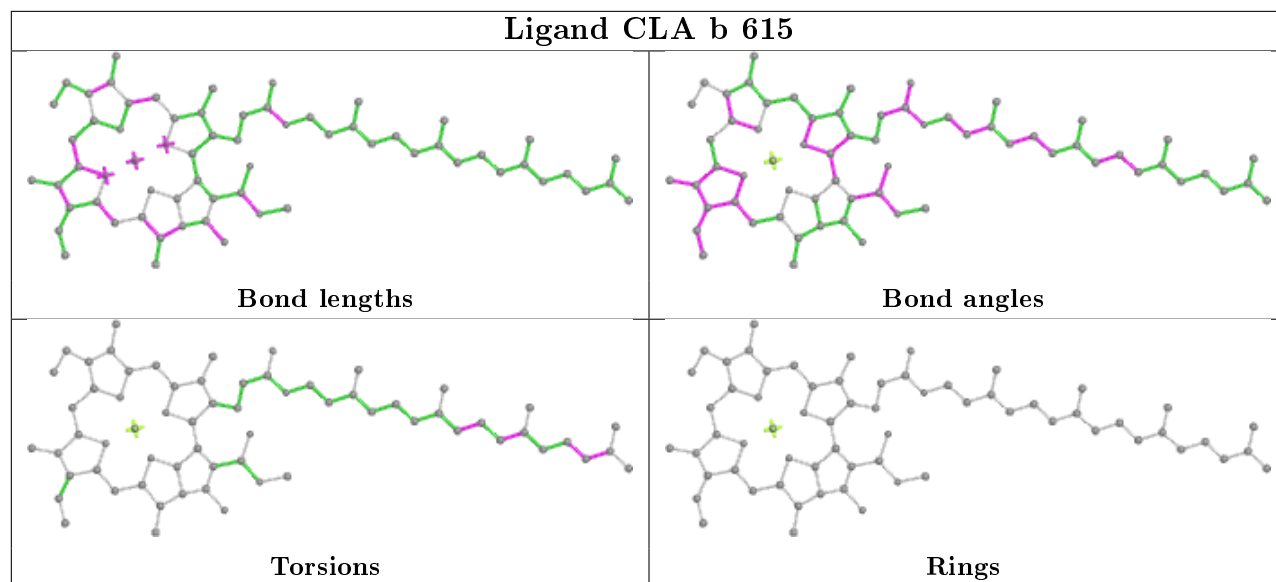




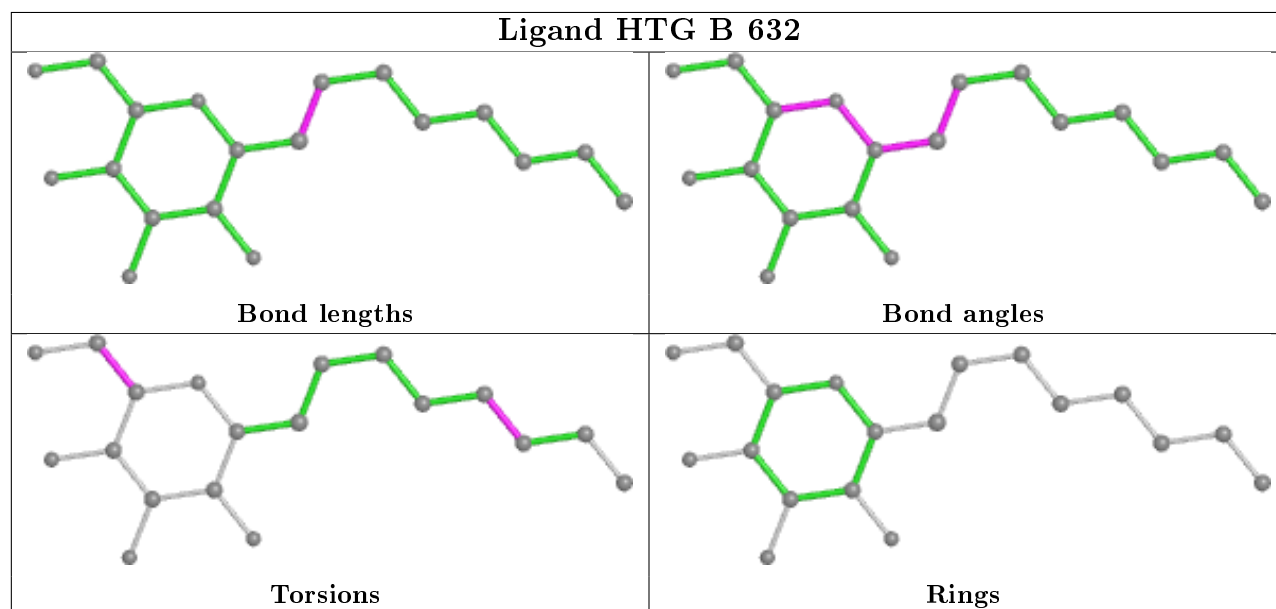




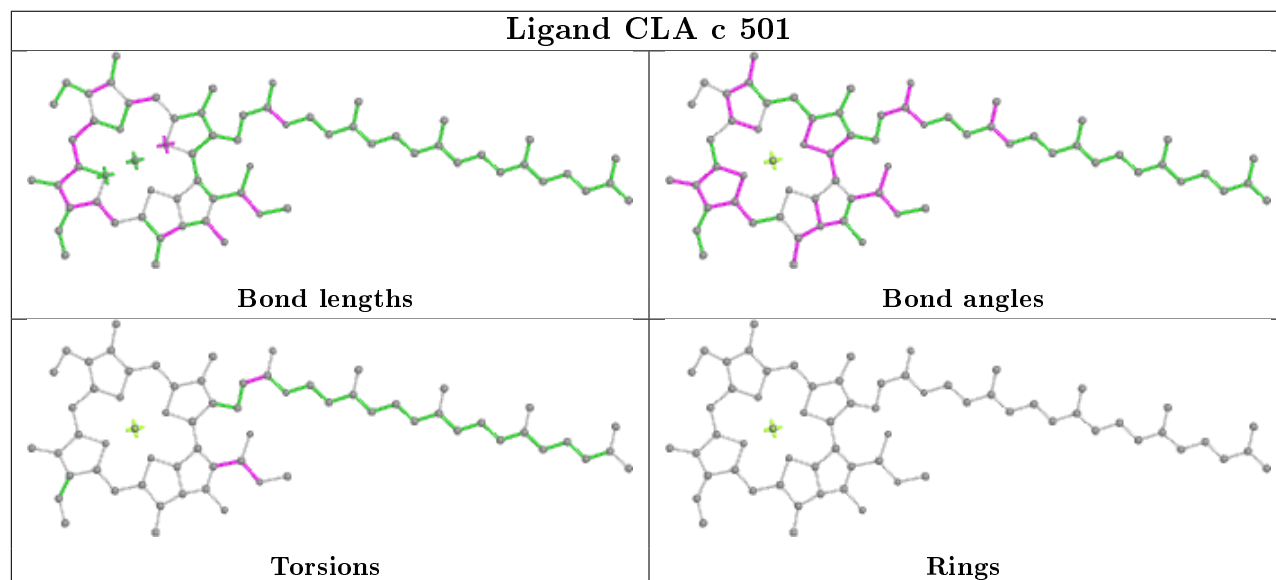
Ligand CLA b 615

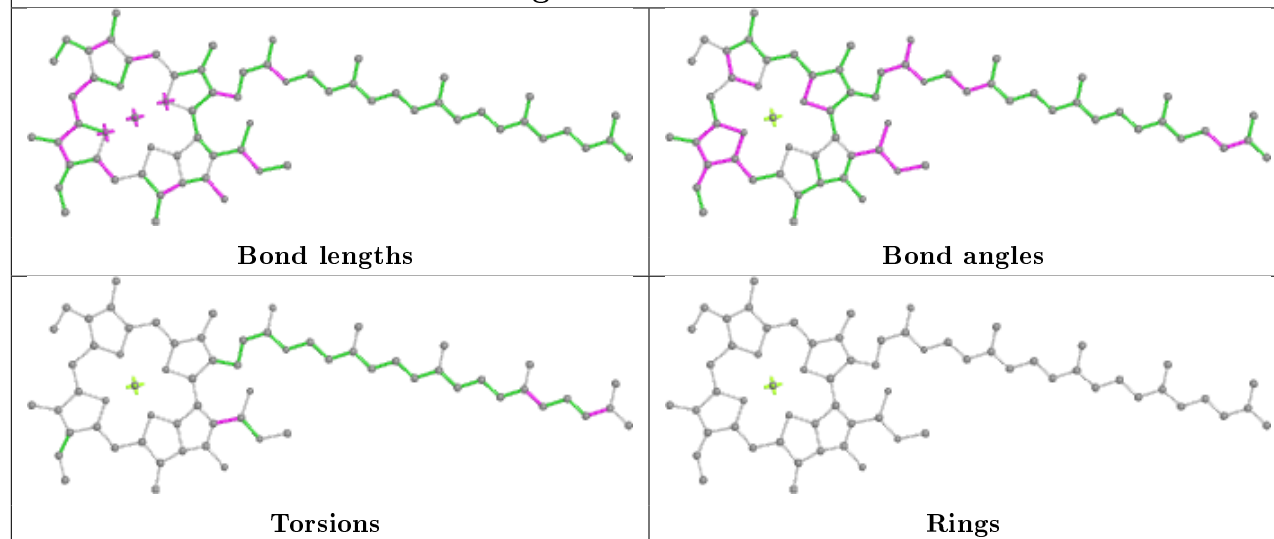
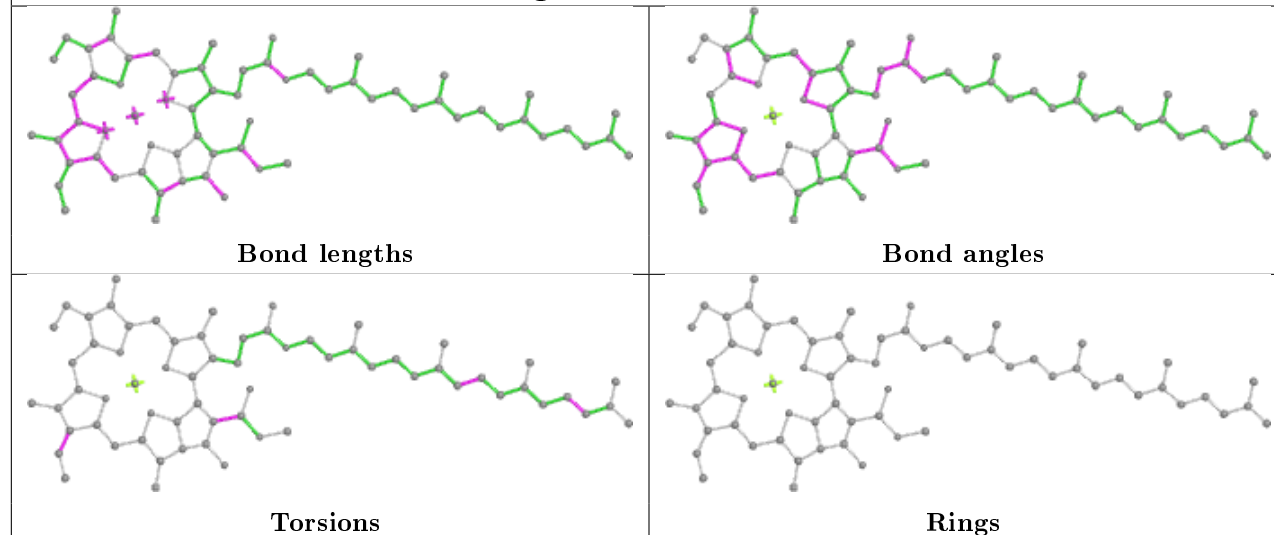
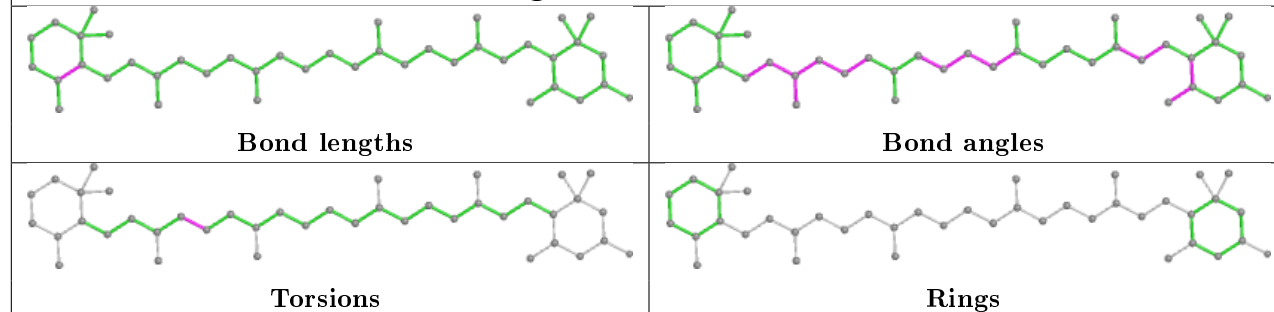


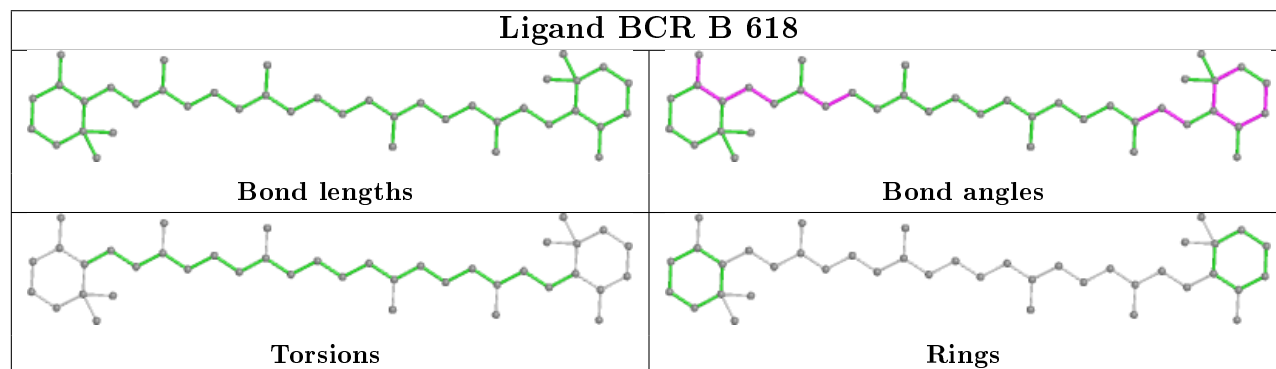
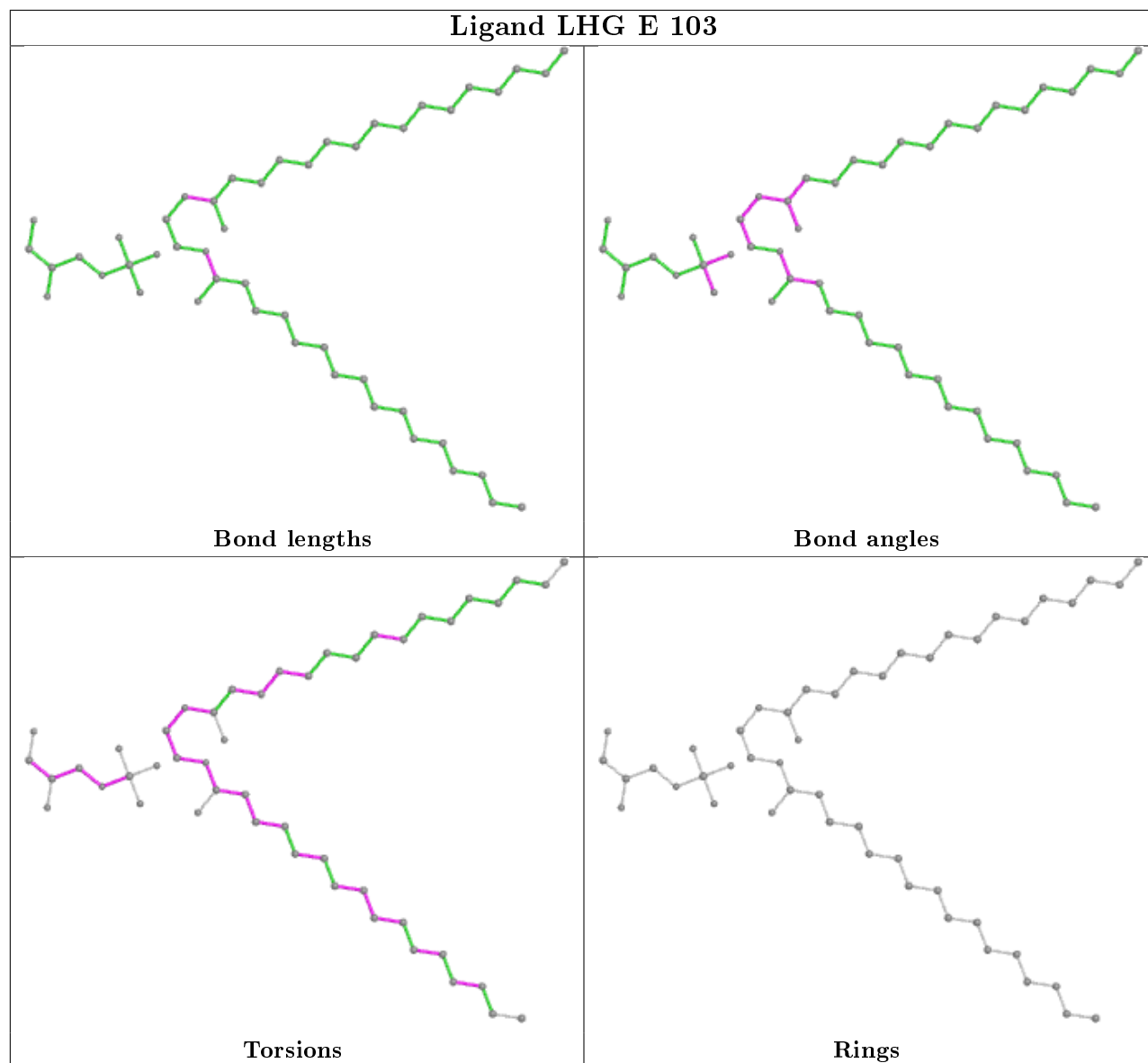
Ligand HTG B 632



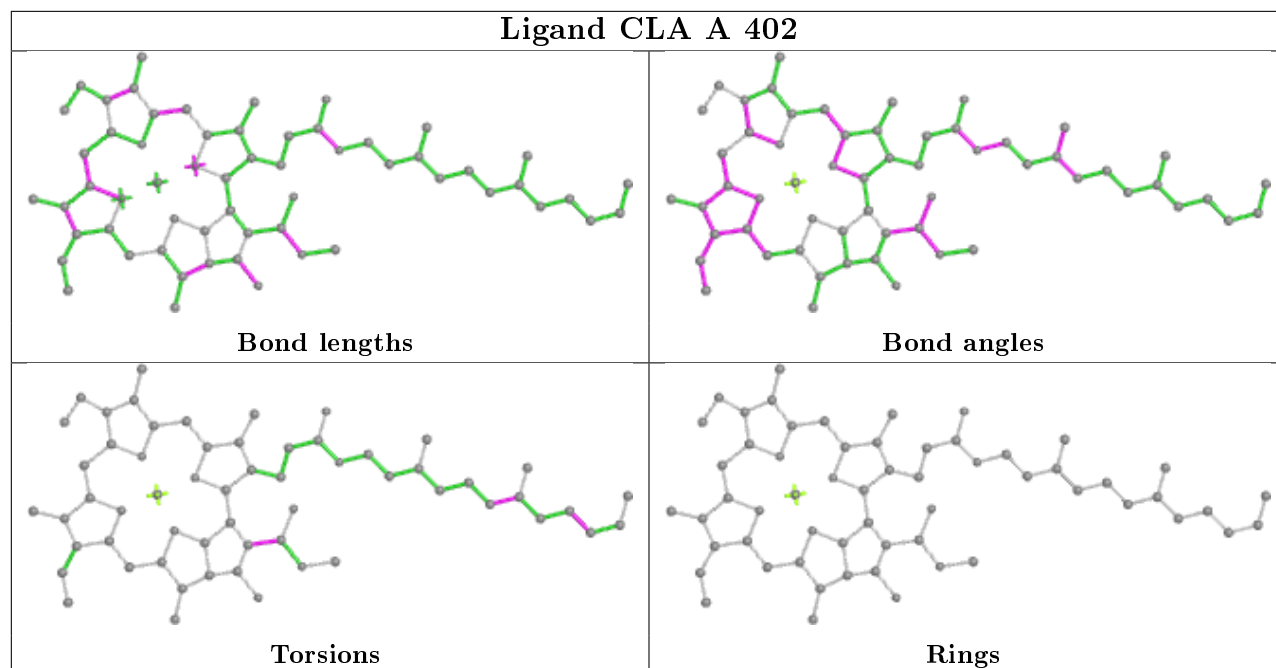
Ligand CLA c 501



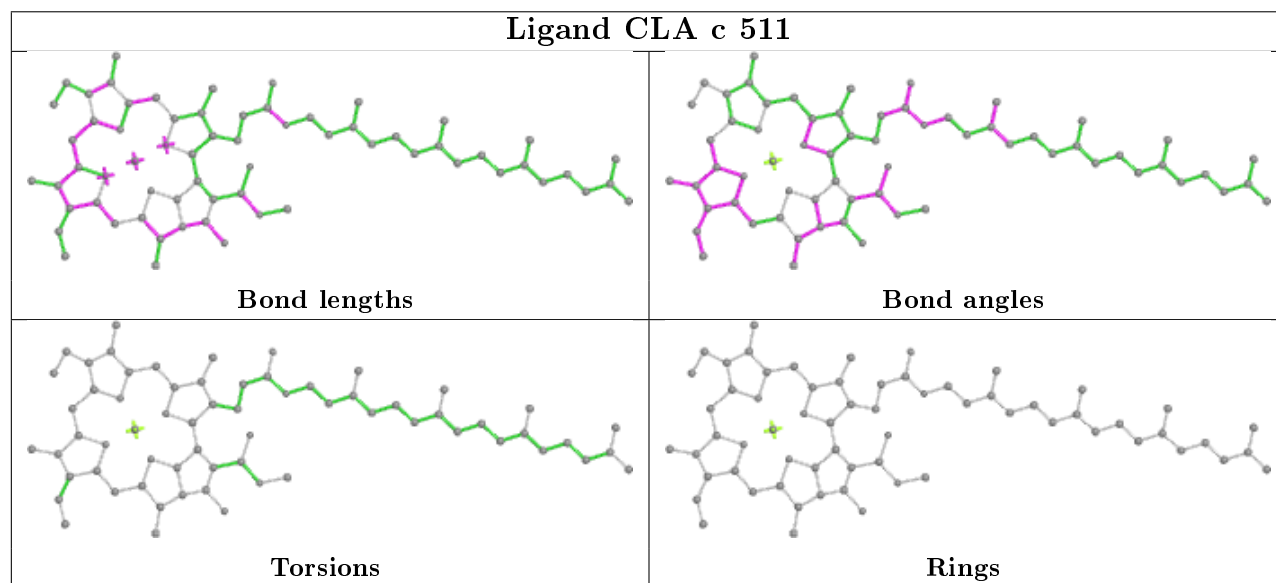
Ligand CLA C 502**Ligand CLA B 611****Ligand RRX H 101**



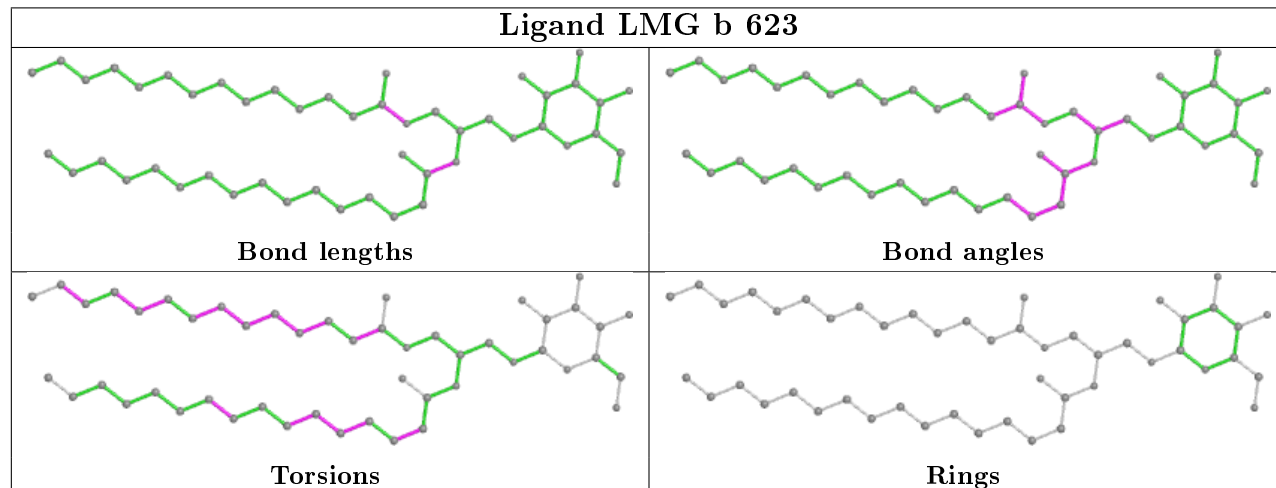
Ligand CLA A 402

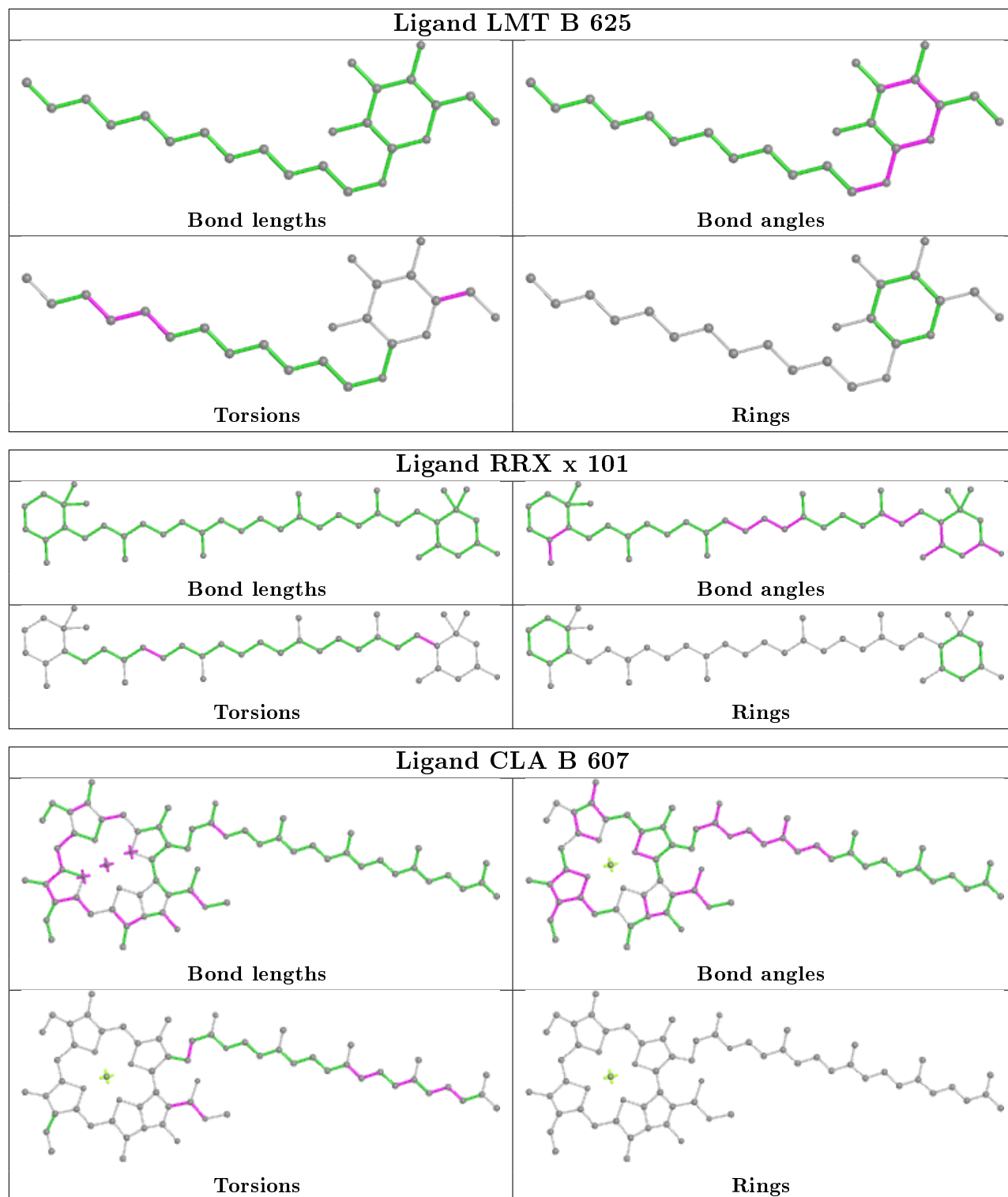


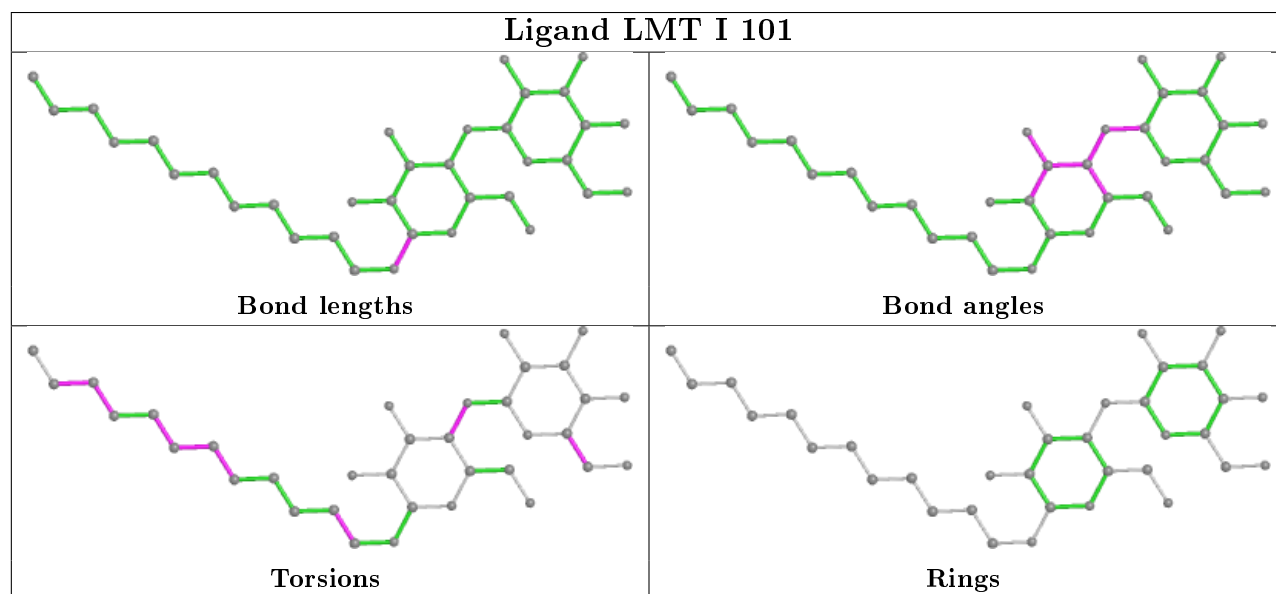
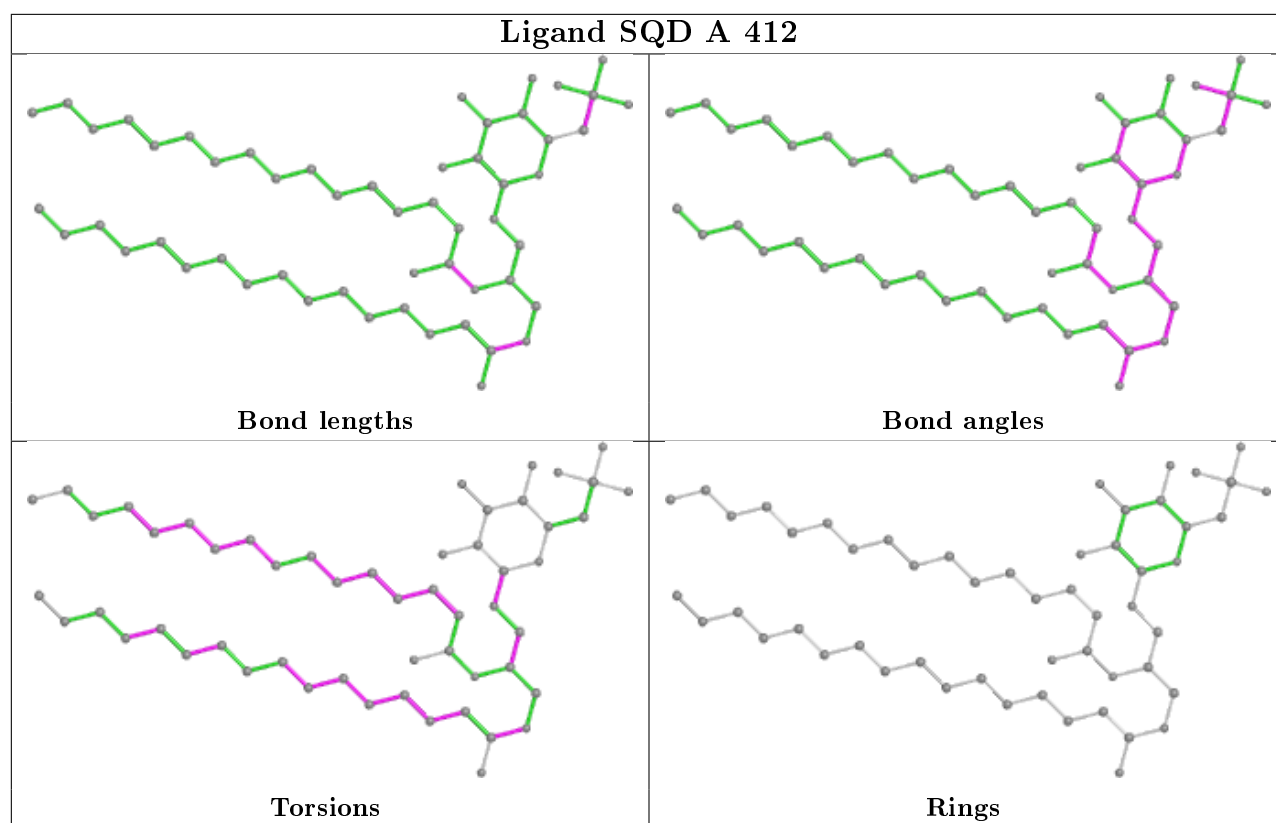
Ligand CLA c 511



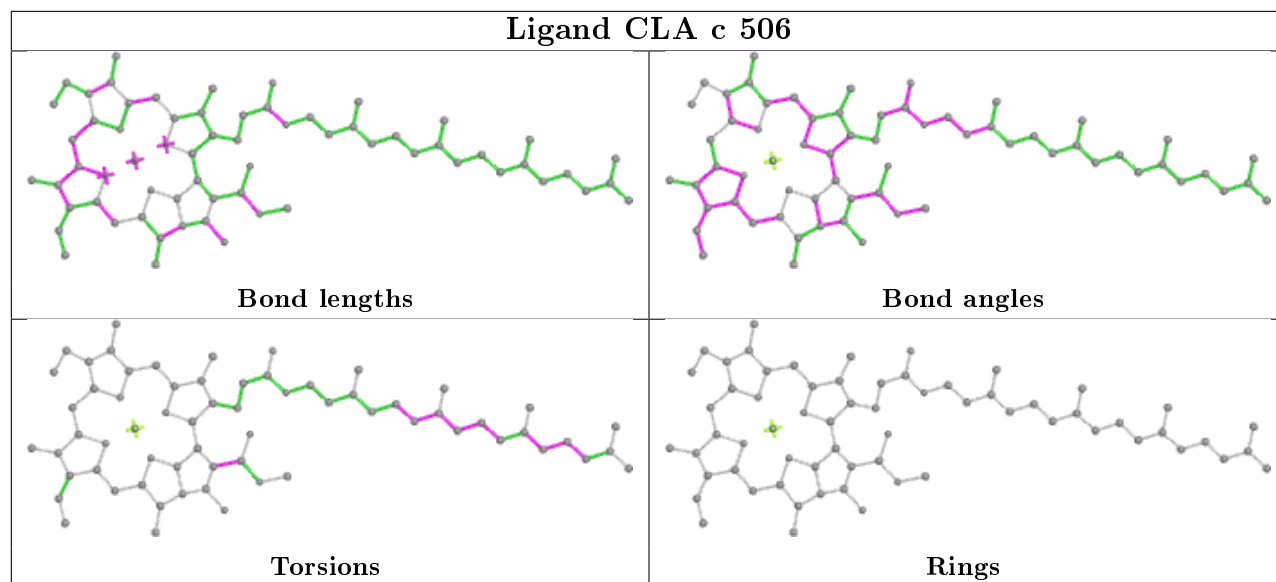
Ligand LMG b 623



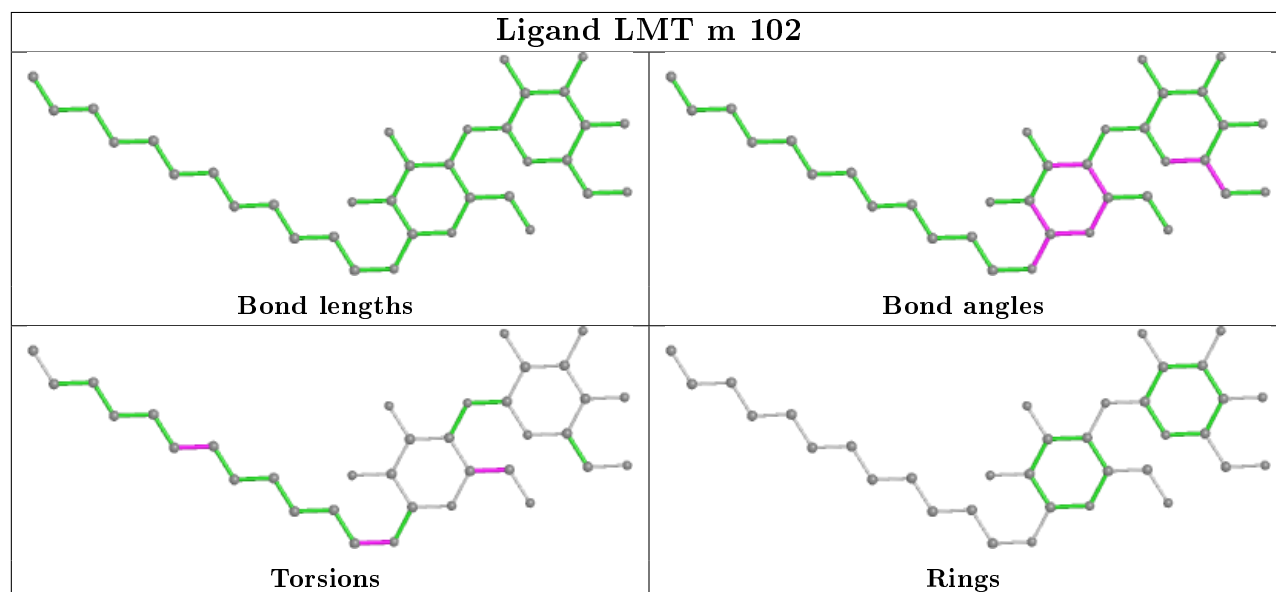




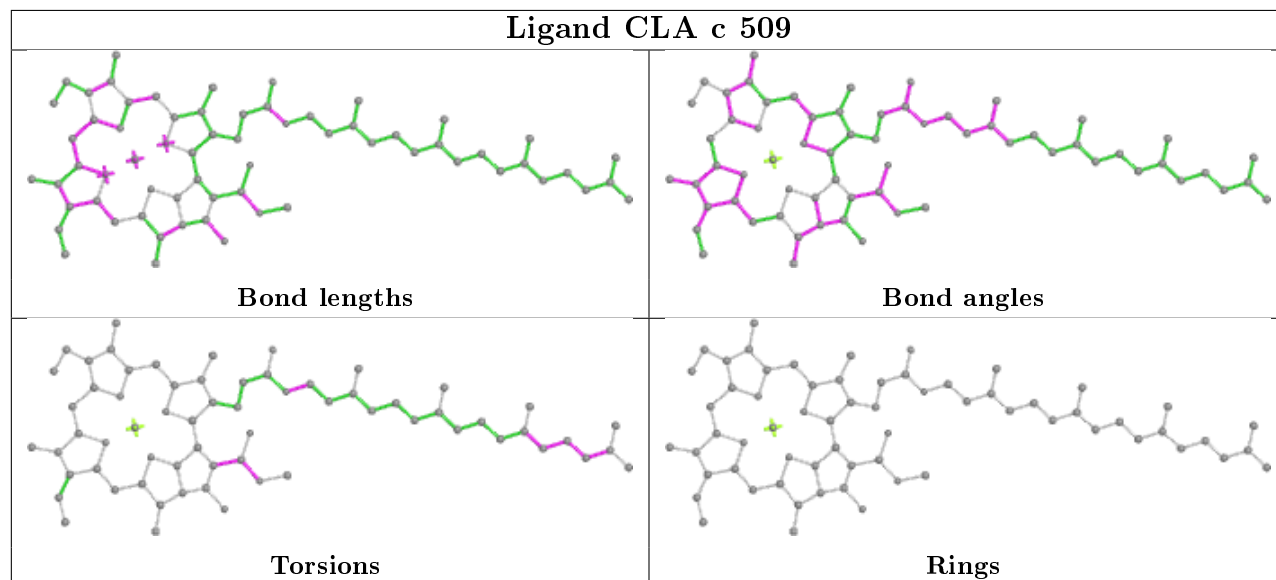
Ligand CLA c 506

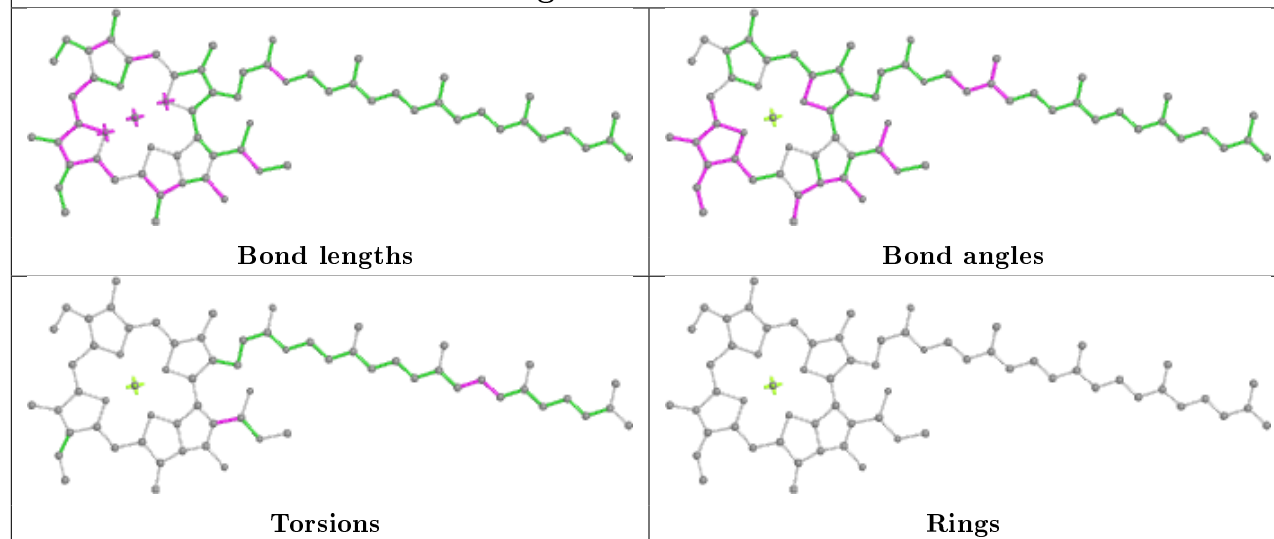
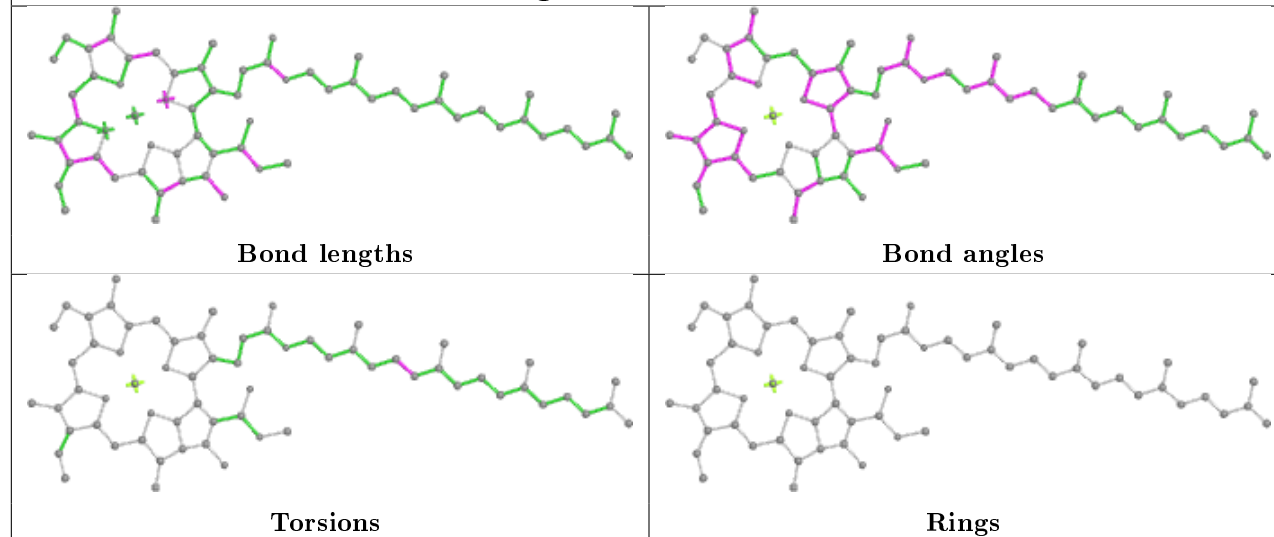


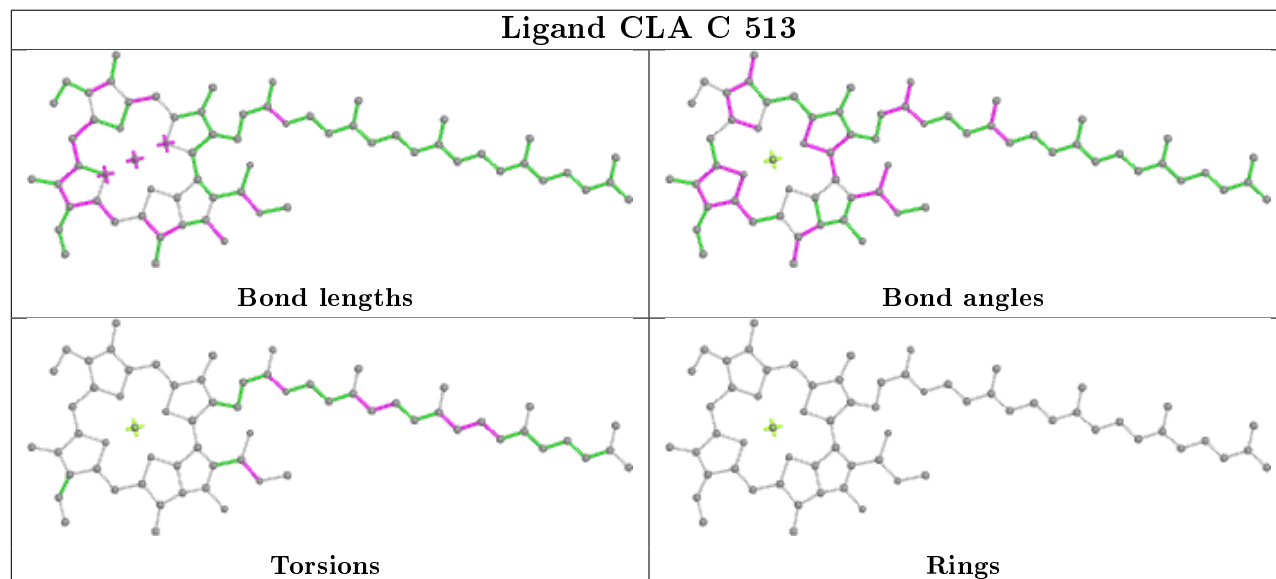
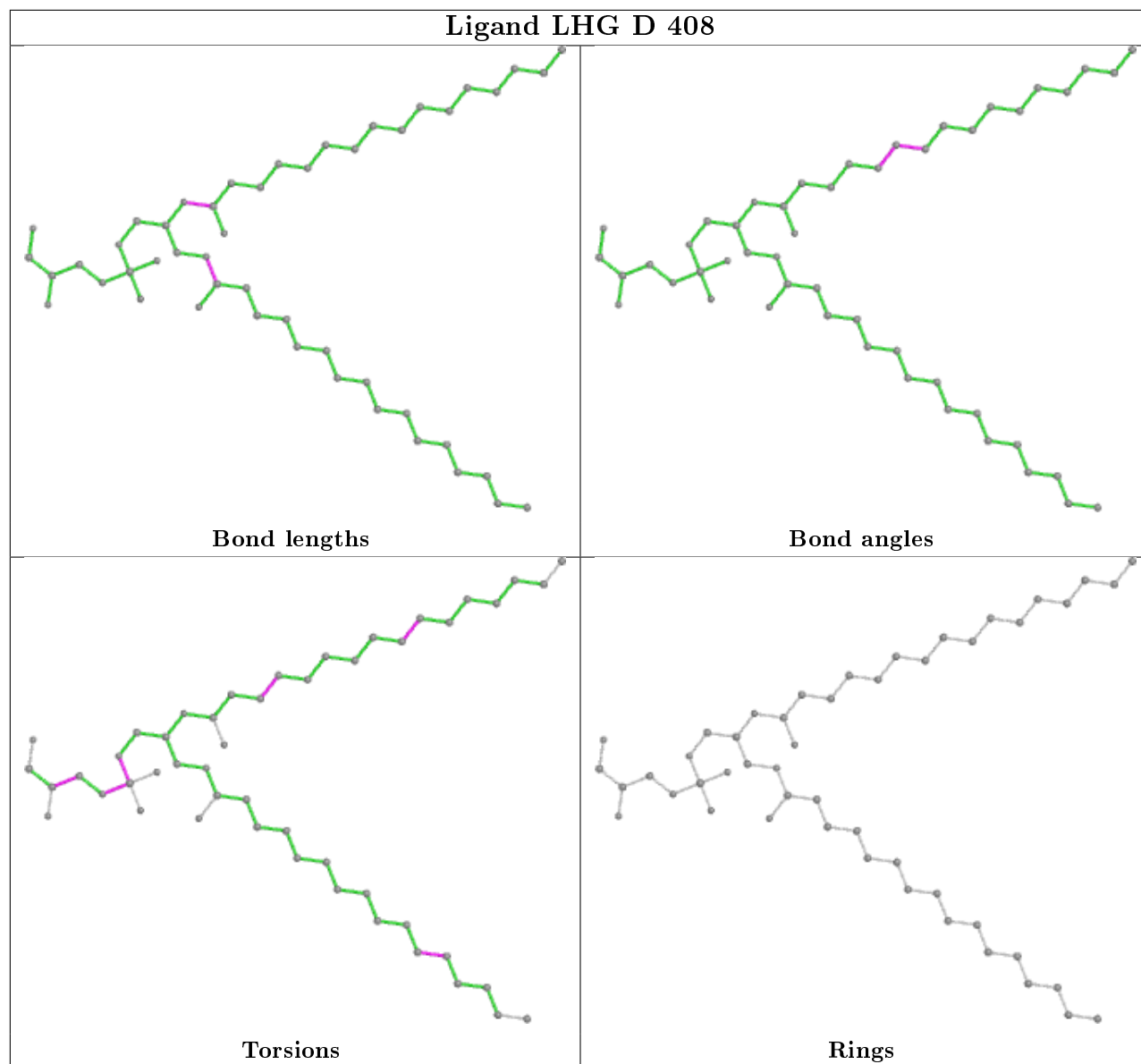
Ligand LMT m 102

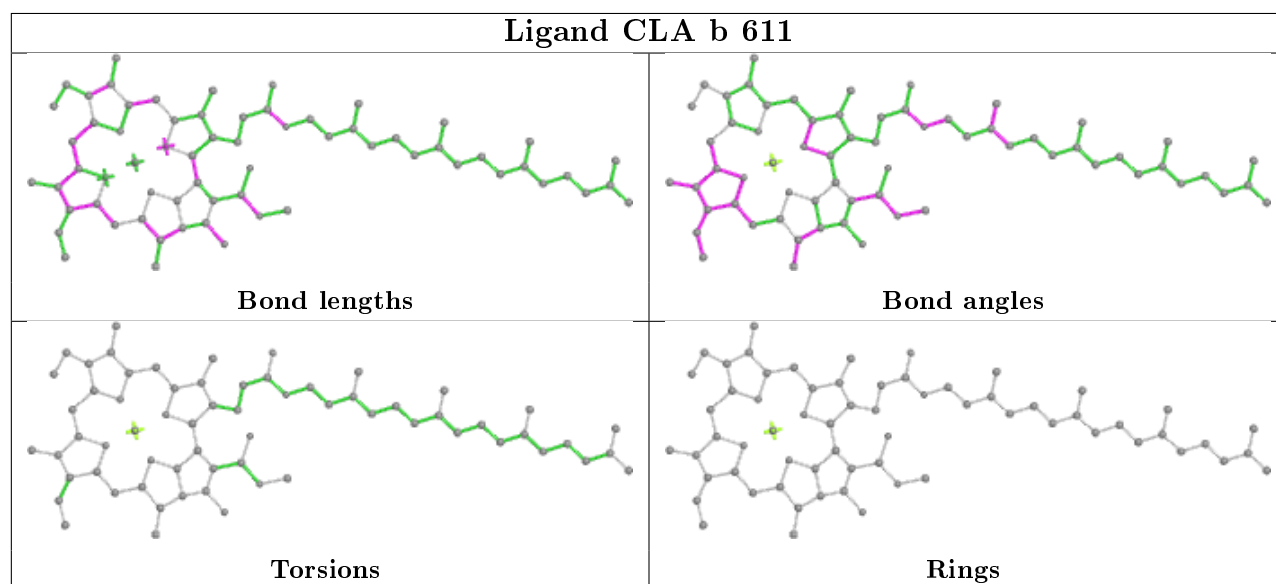
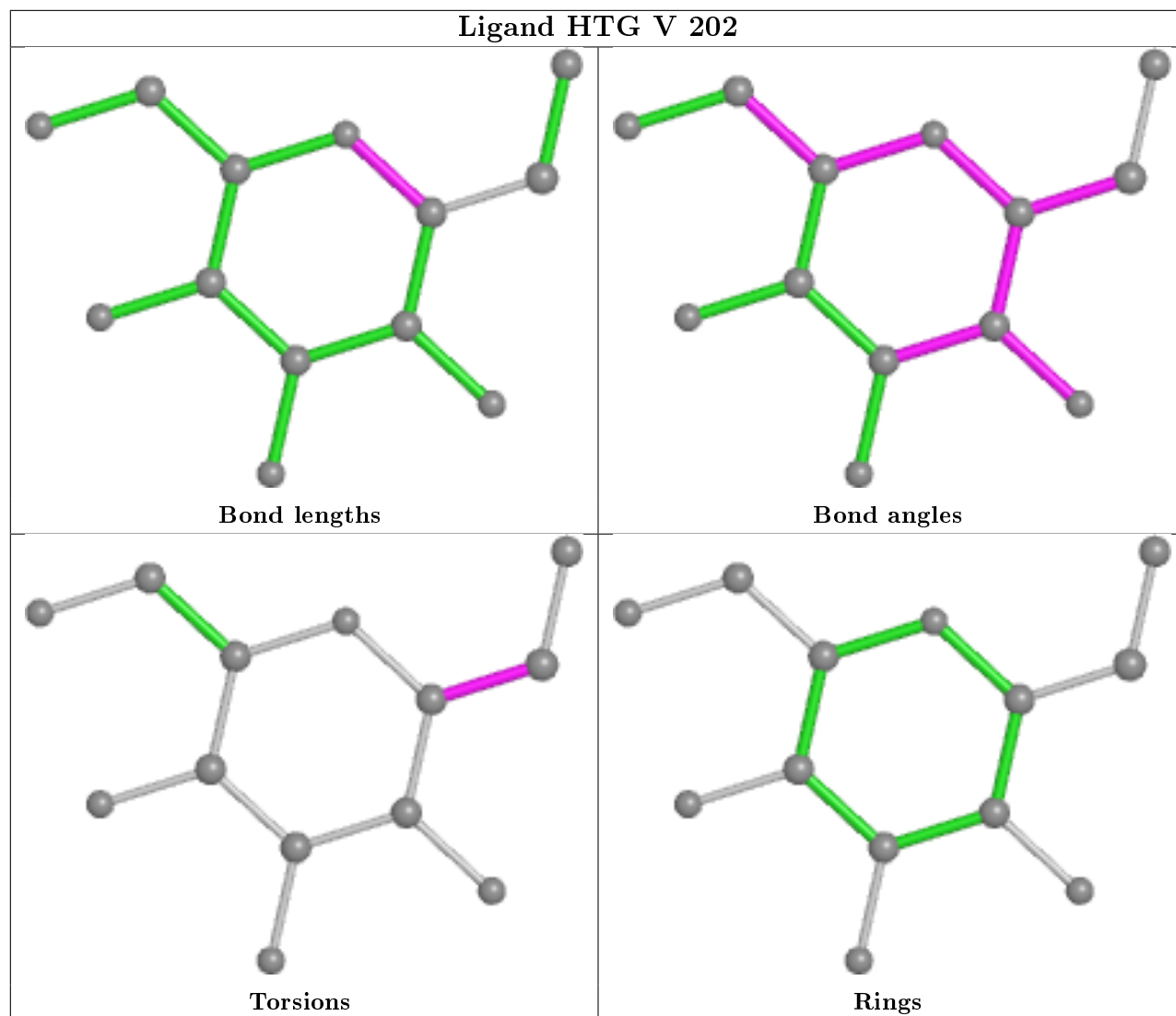


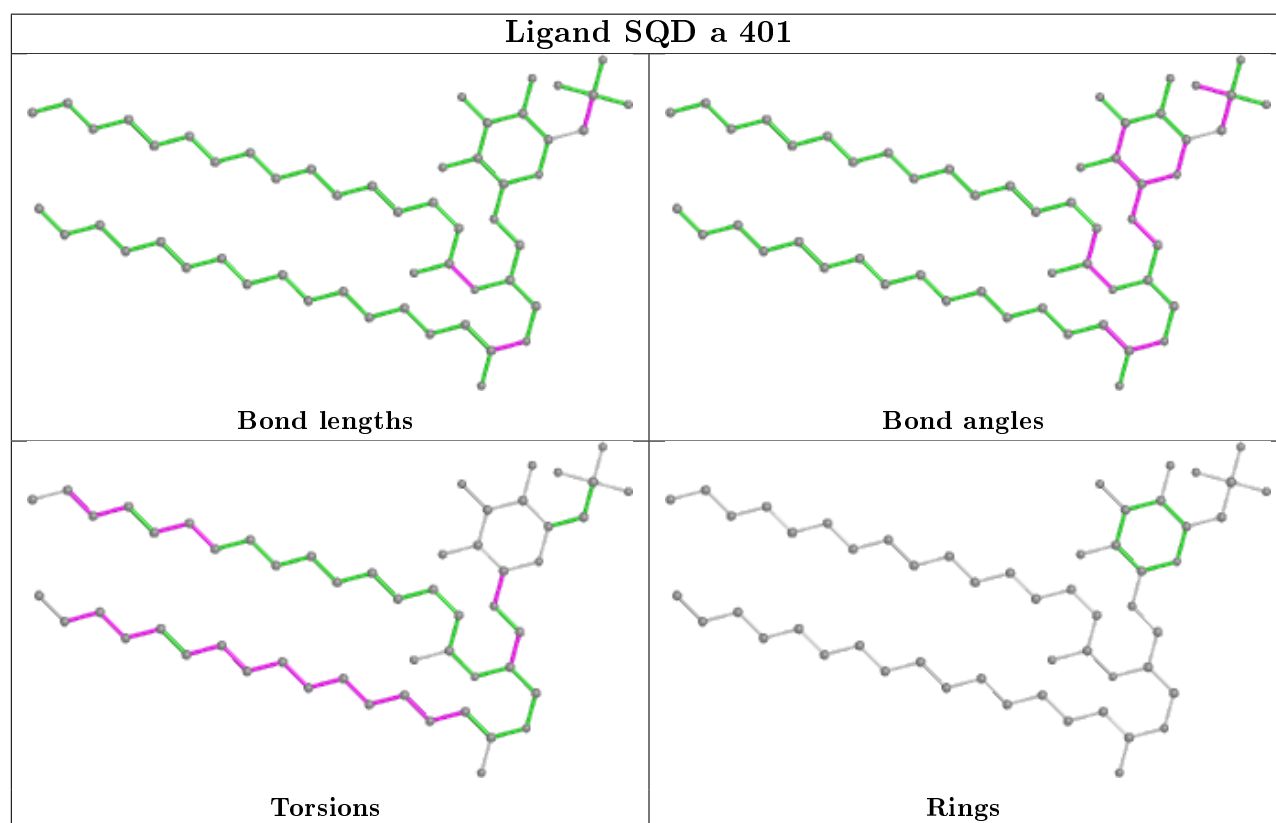
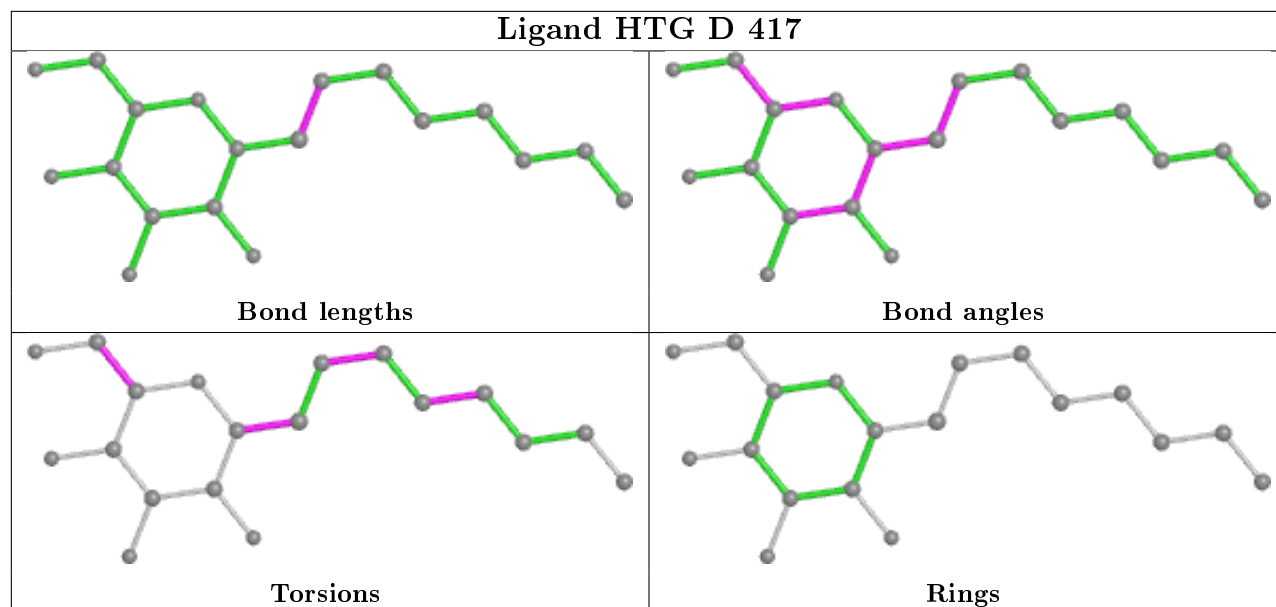
Ligand CLA c 509



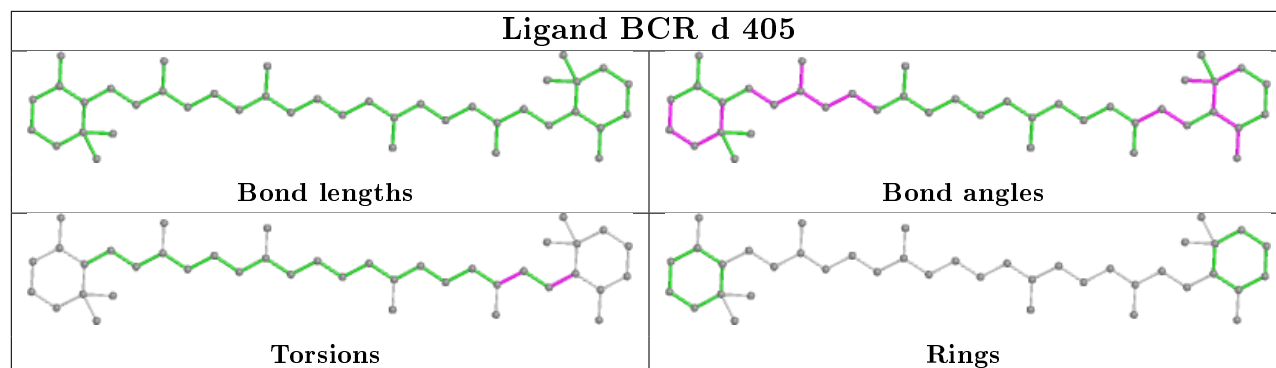
Ligand CLA c 503**Ligand CLA b 605**



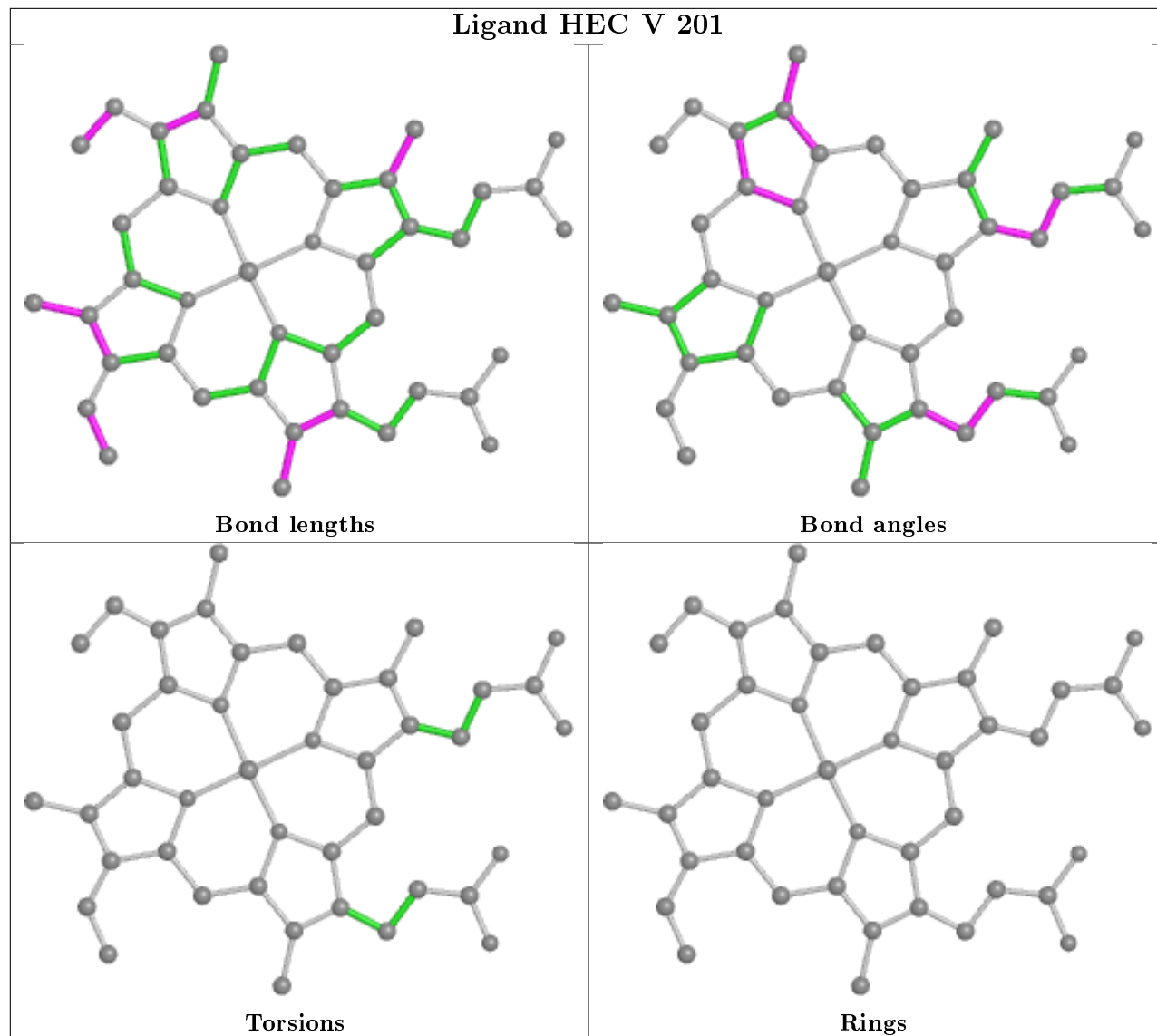


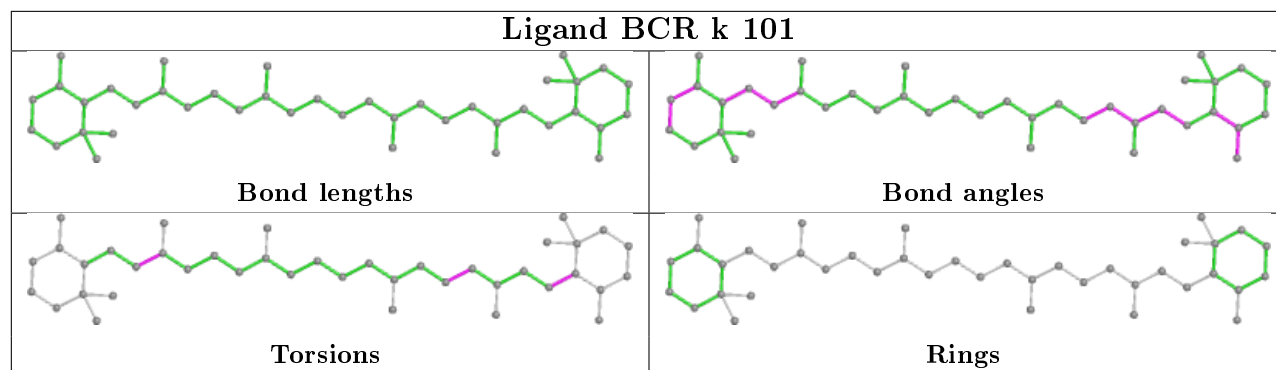
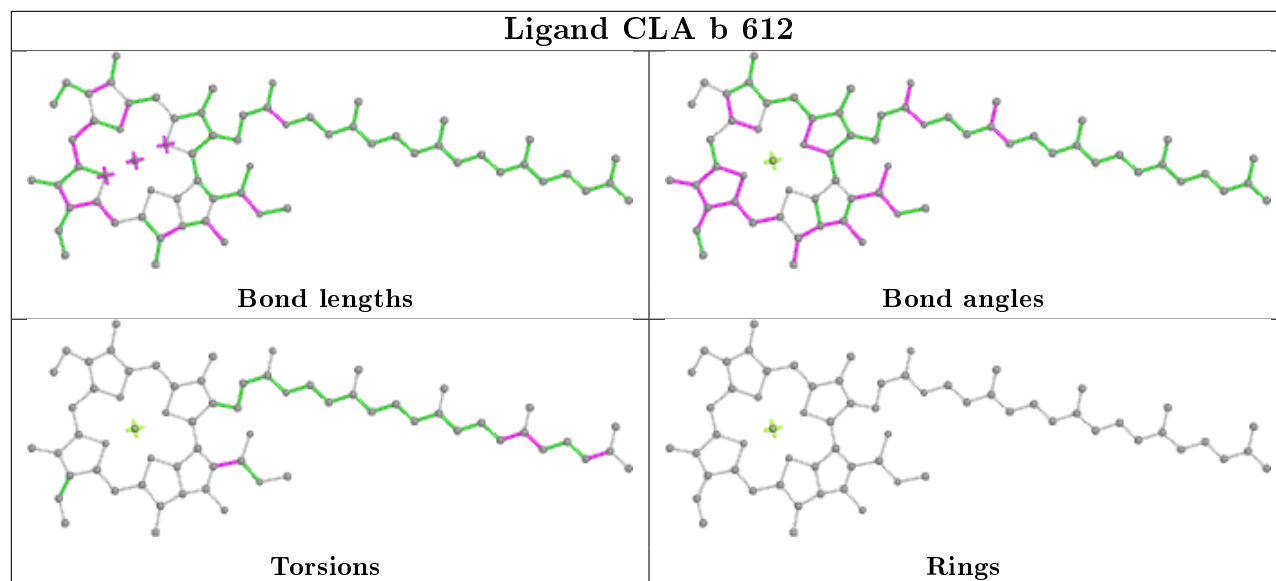
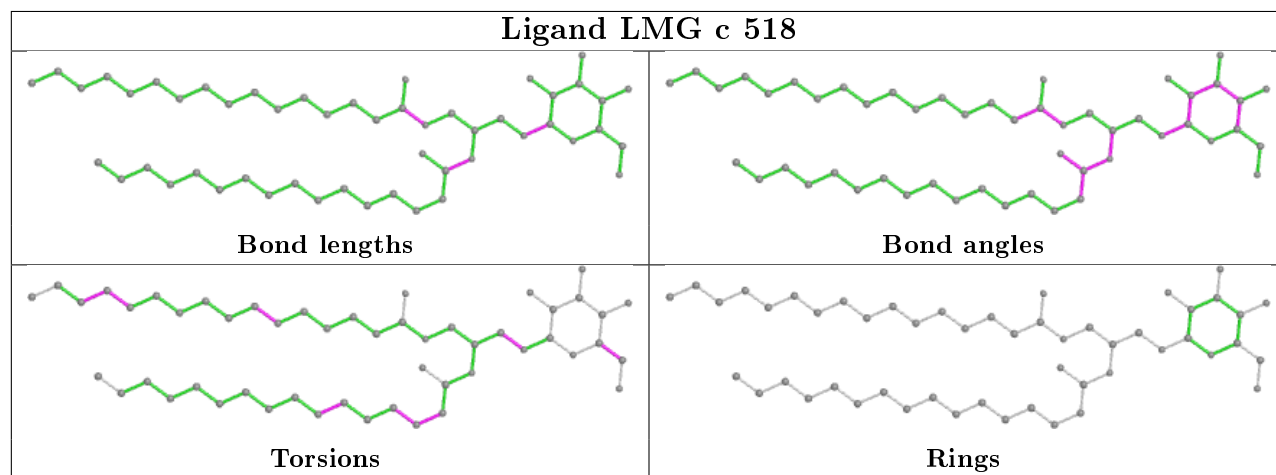


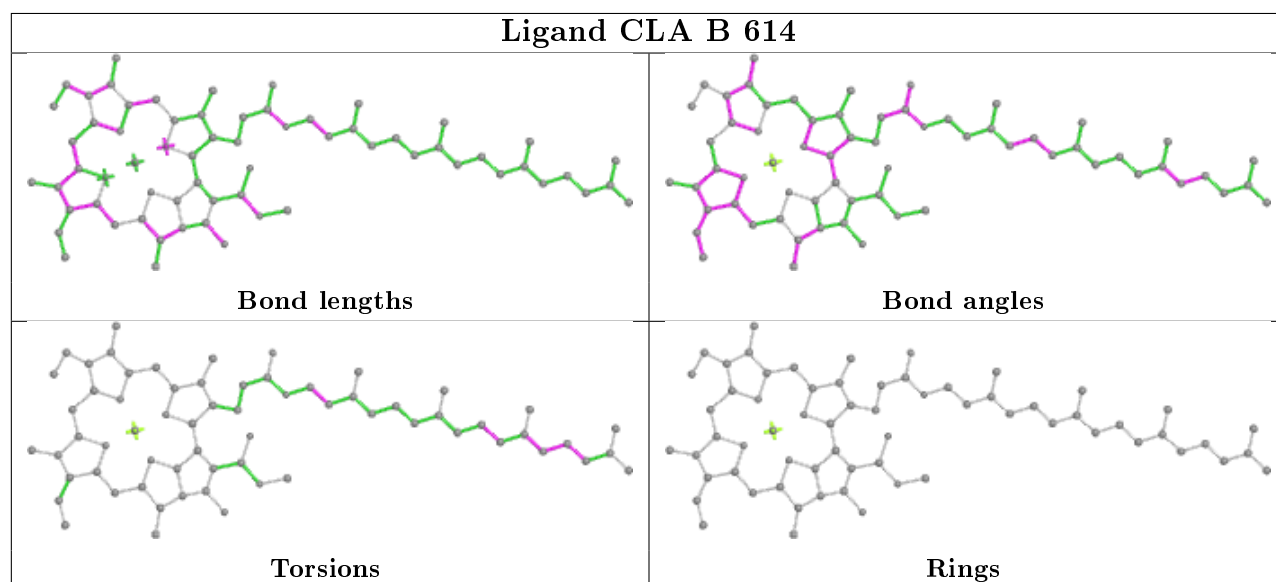
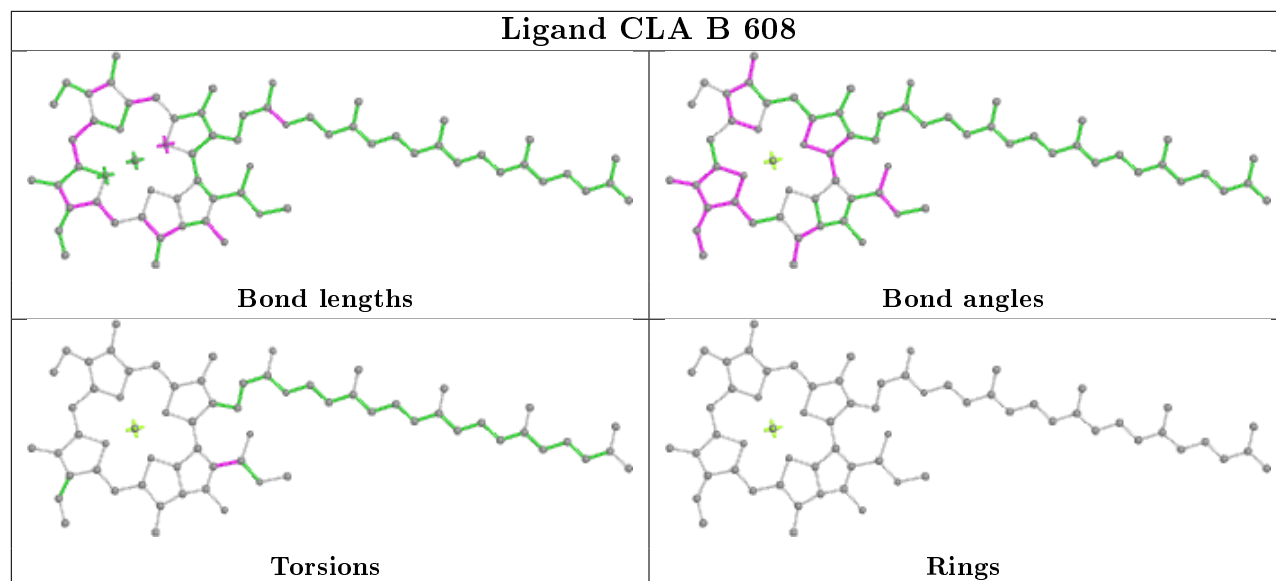
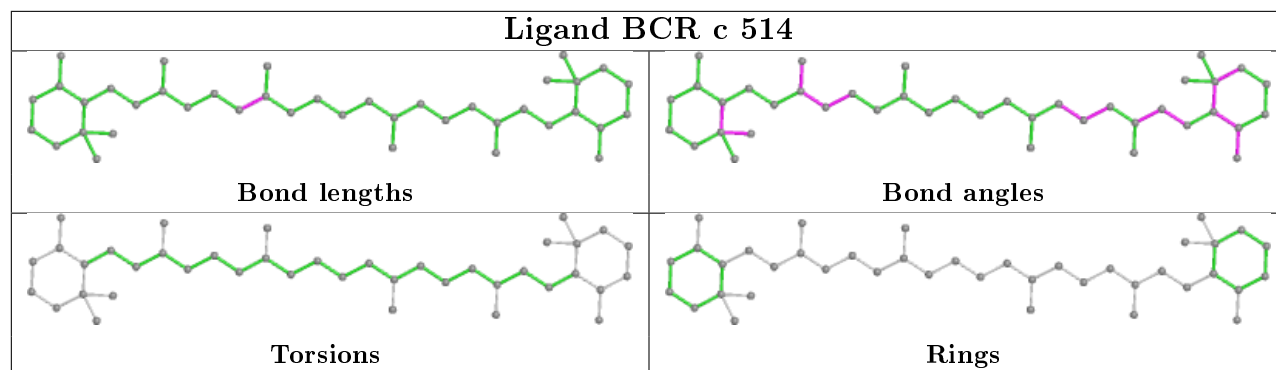
Ligand BCR d 405

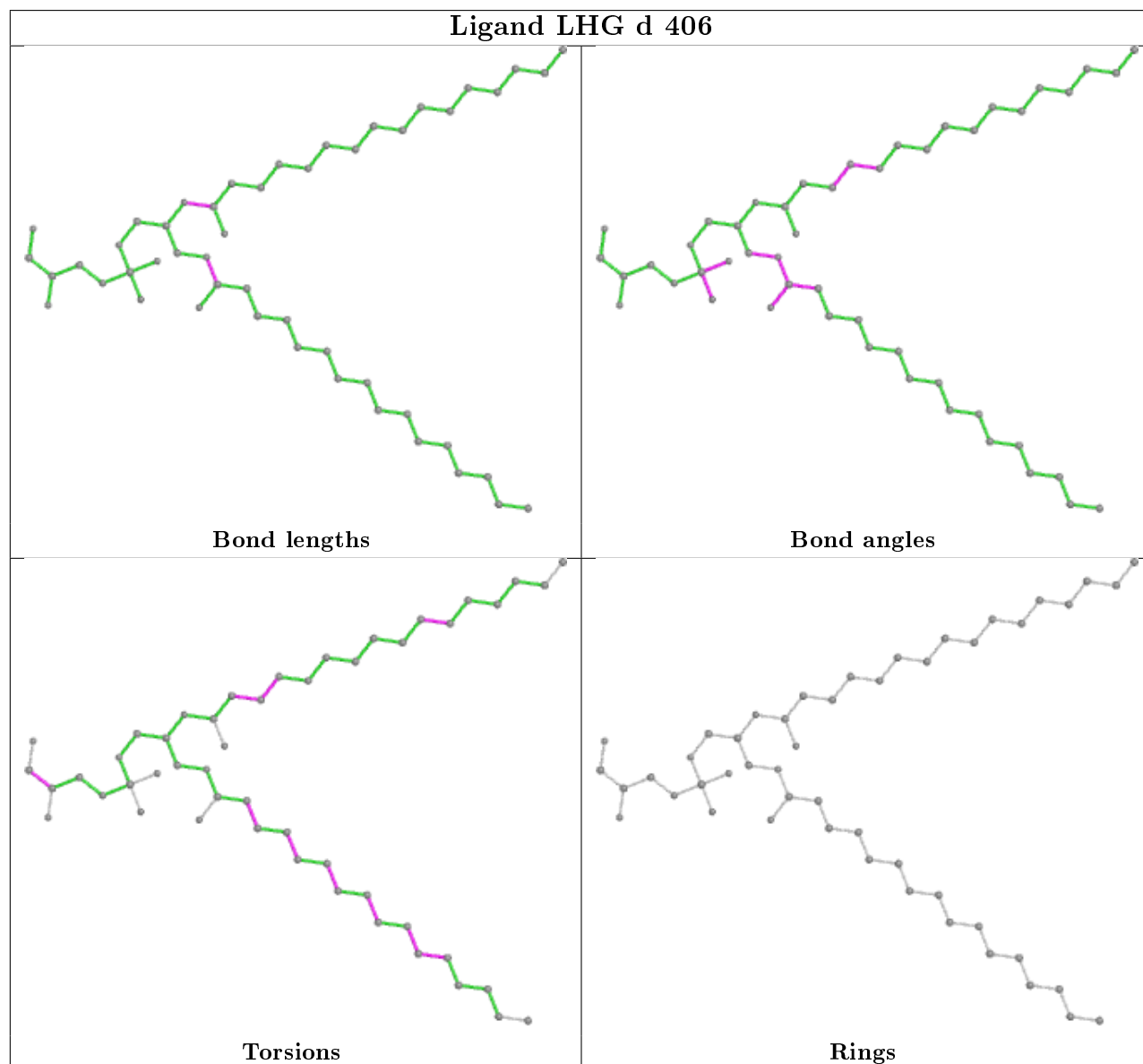
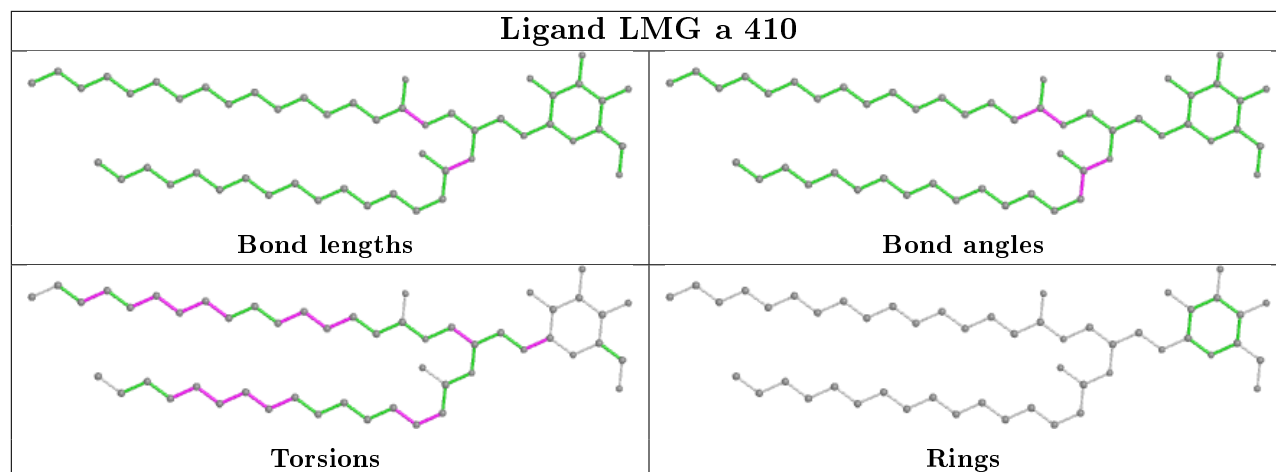


Ligand HEC V 201

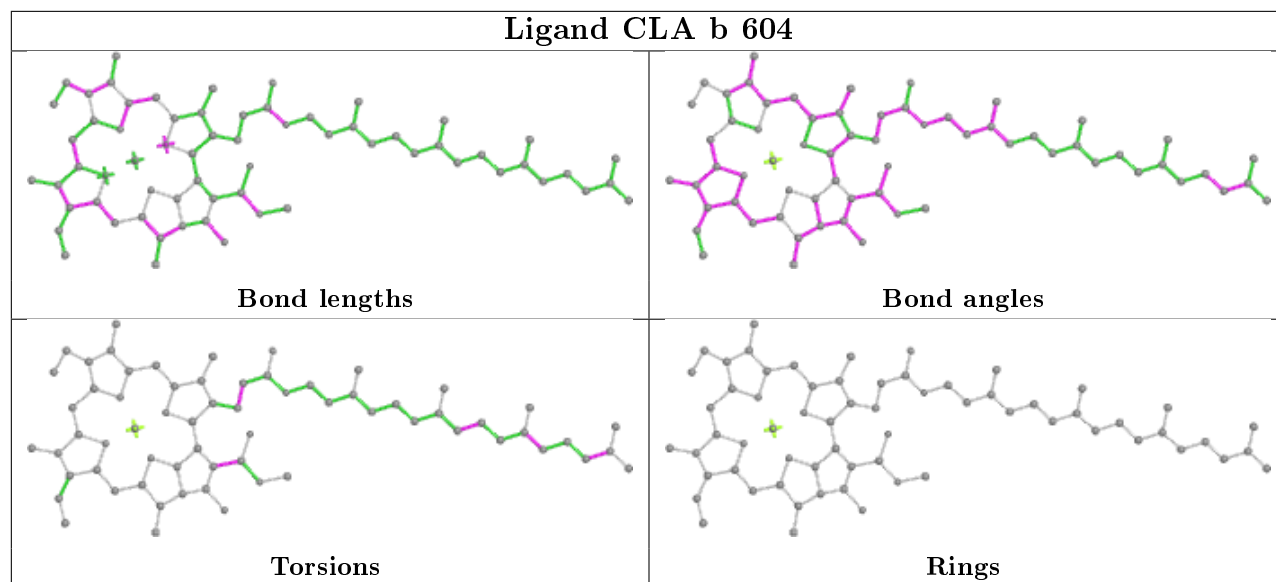


Ligand BCR k 101**Ligand CLA b 612****Ligand LMG c 518**

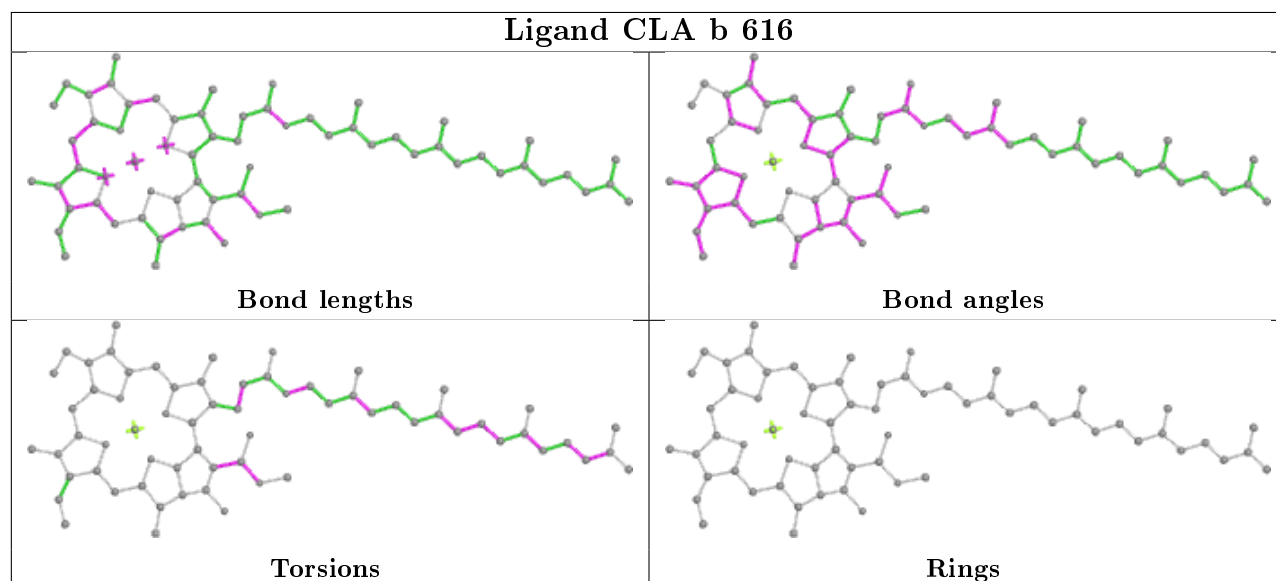




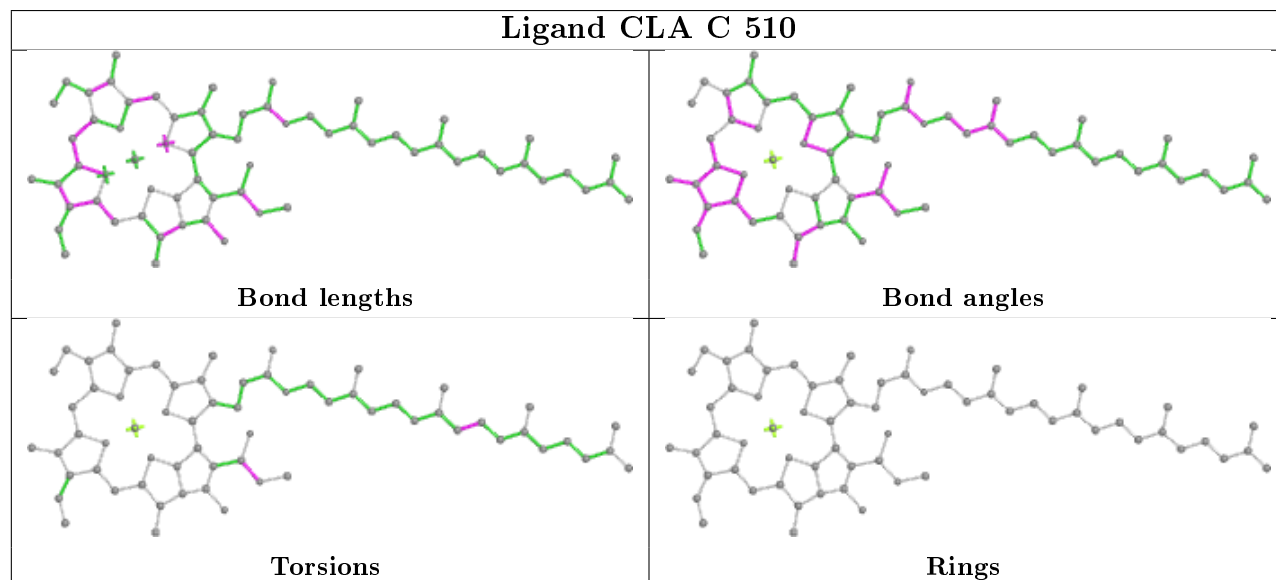
Ligand CLA b 604



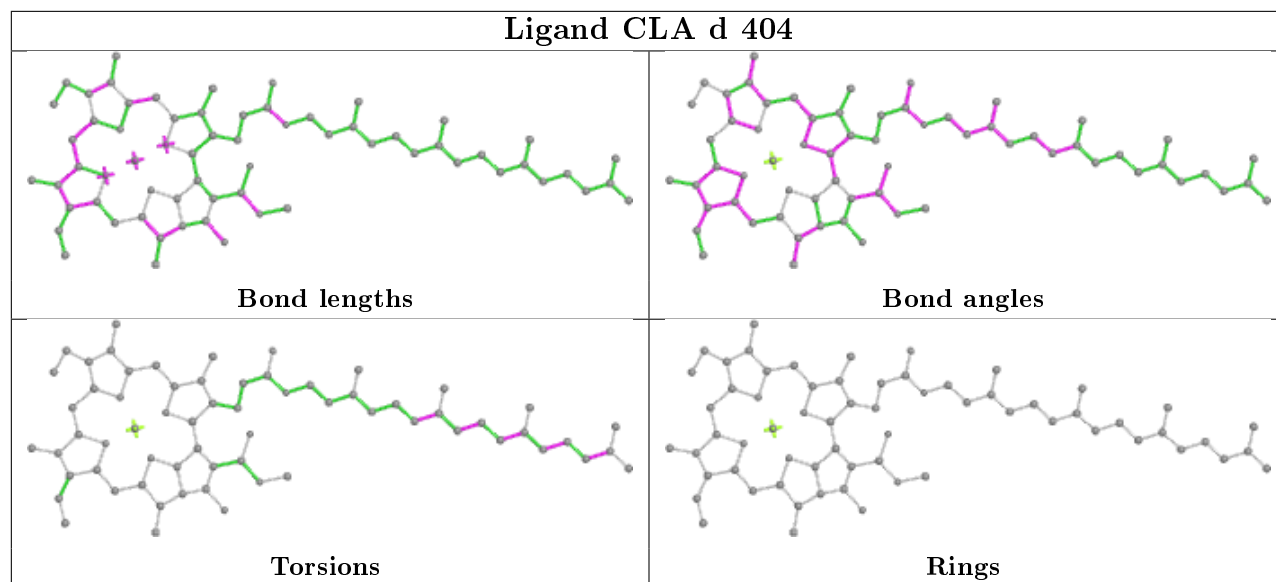
Ligand CLA b 616



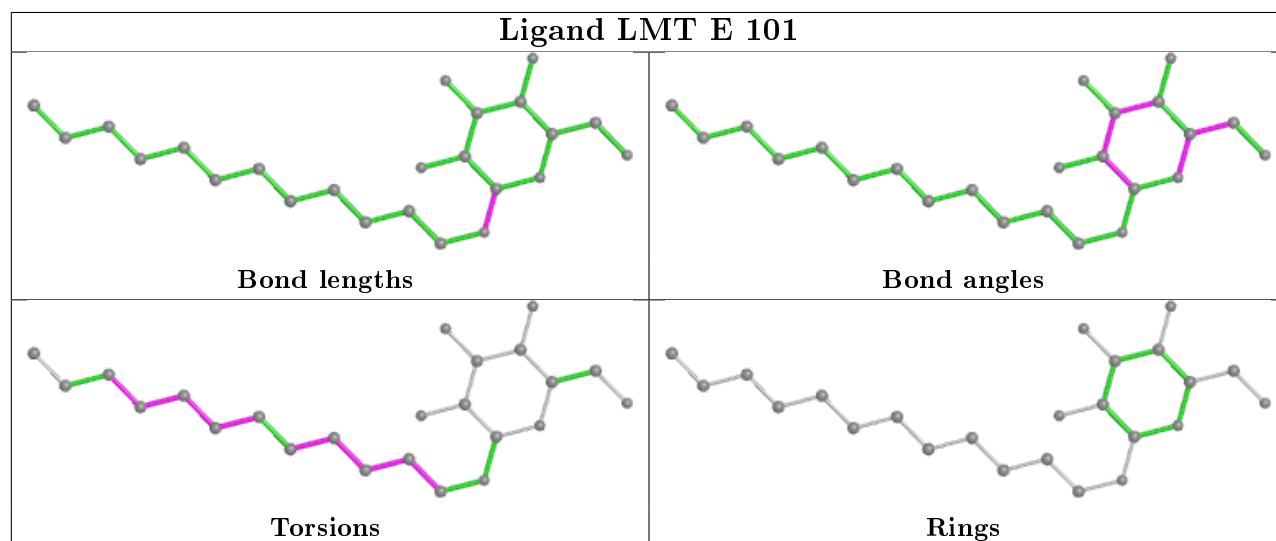
Ligand CLA C 510



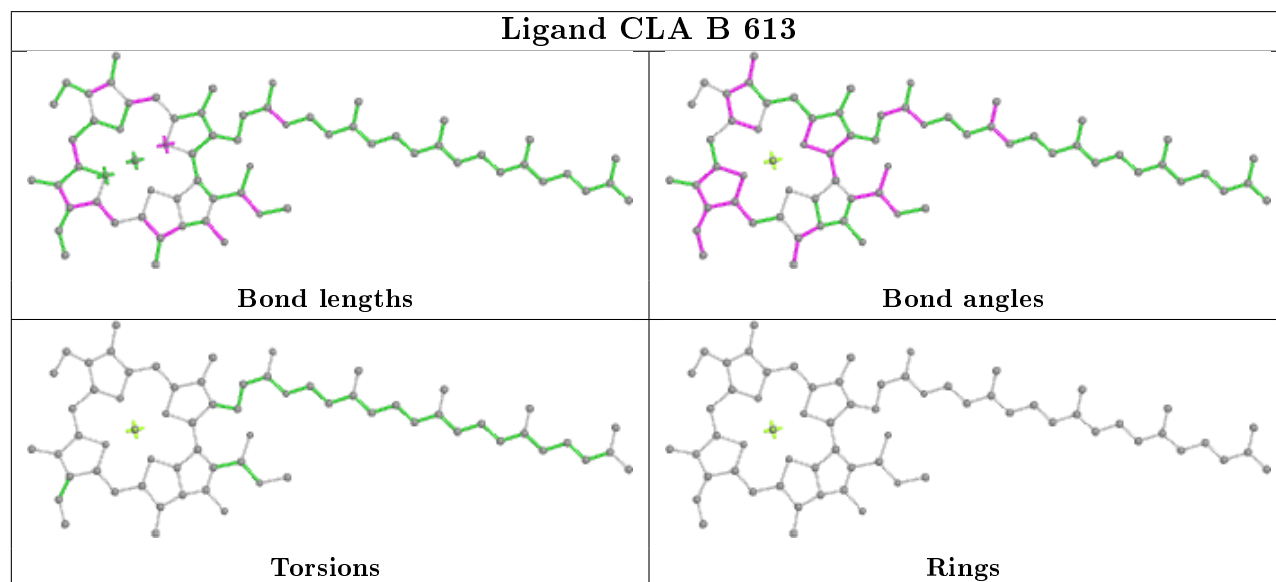
Ligand CLA d 404



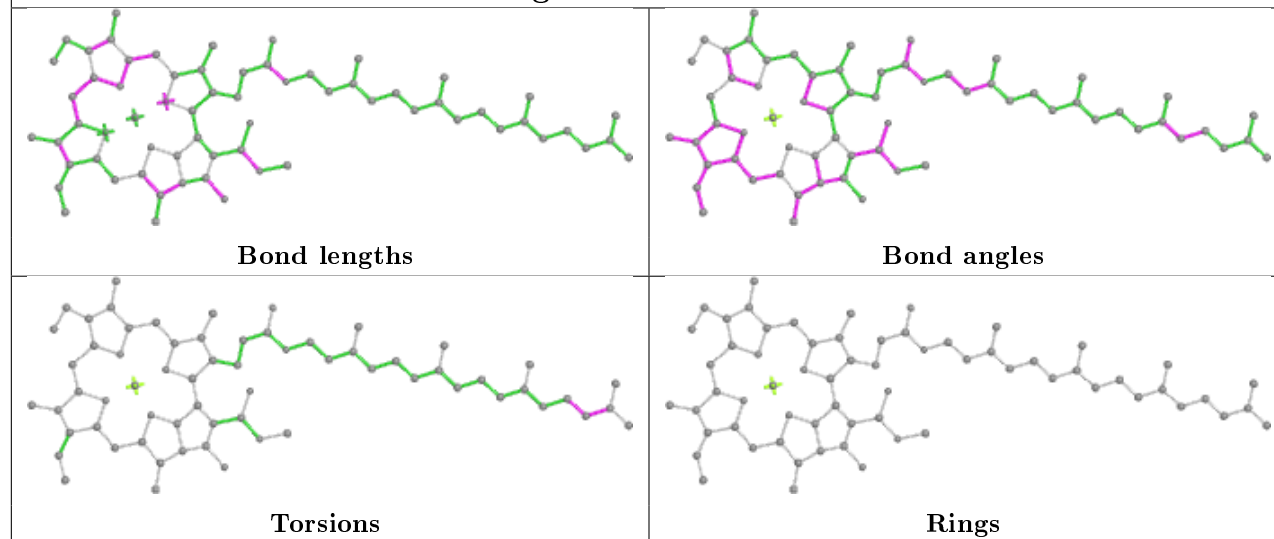
Ligand LMT E 101



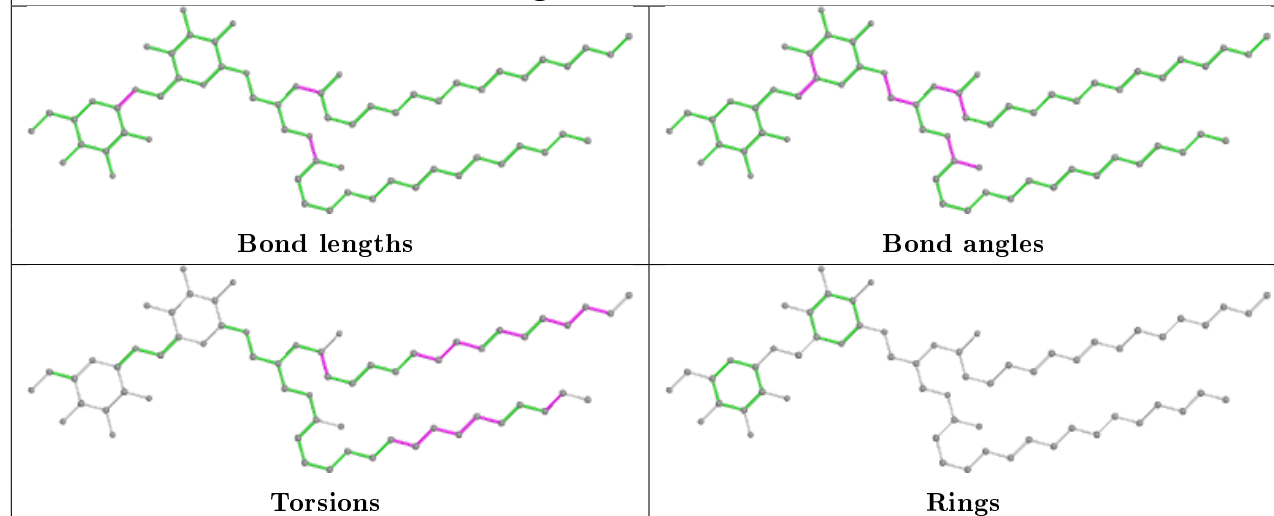
Ligand CLA B 613



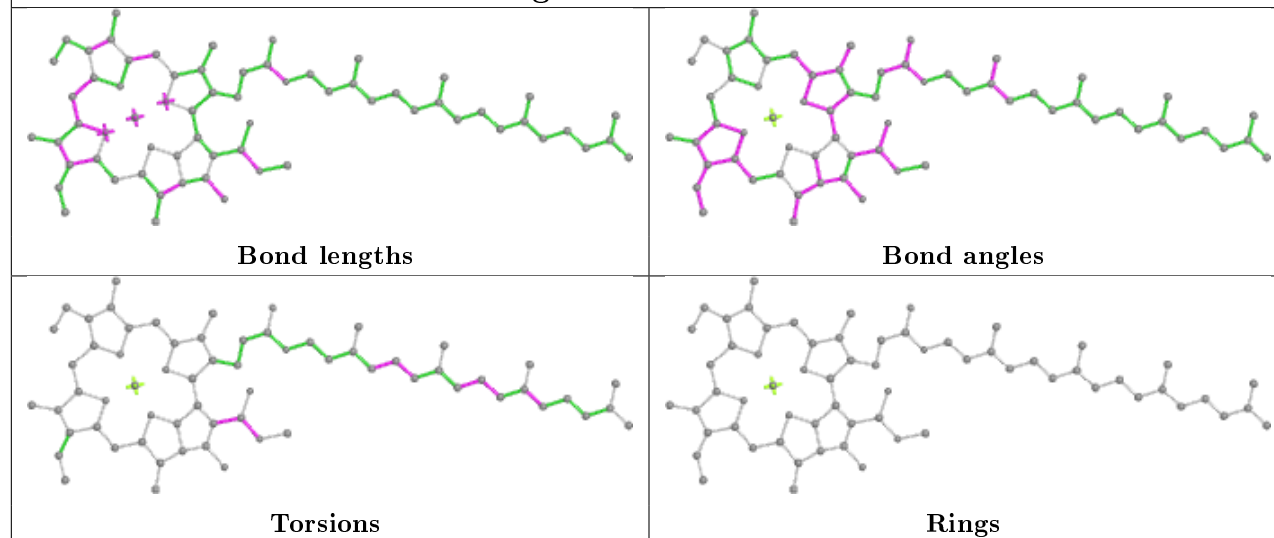
Ligand CLA B 612

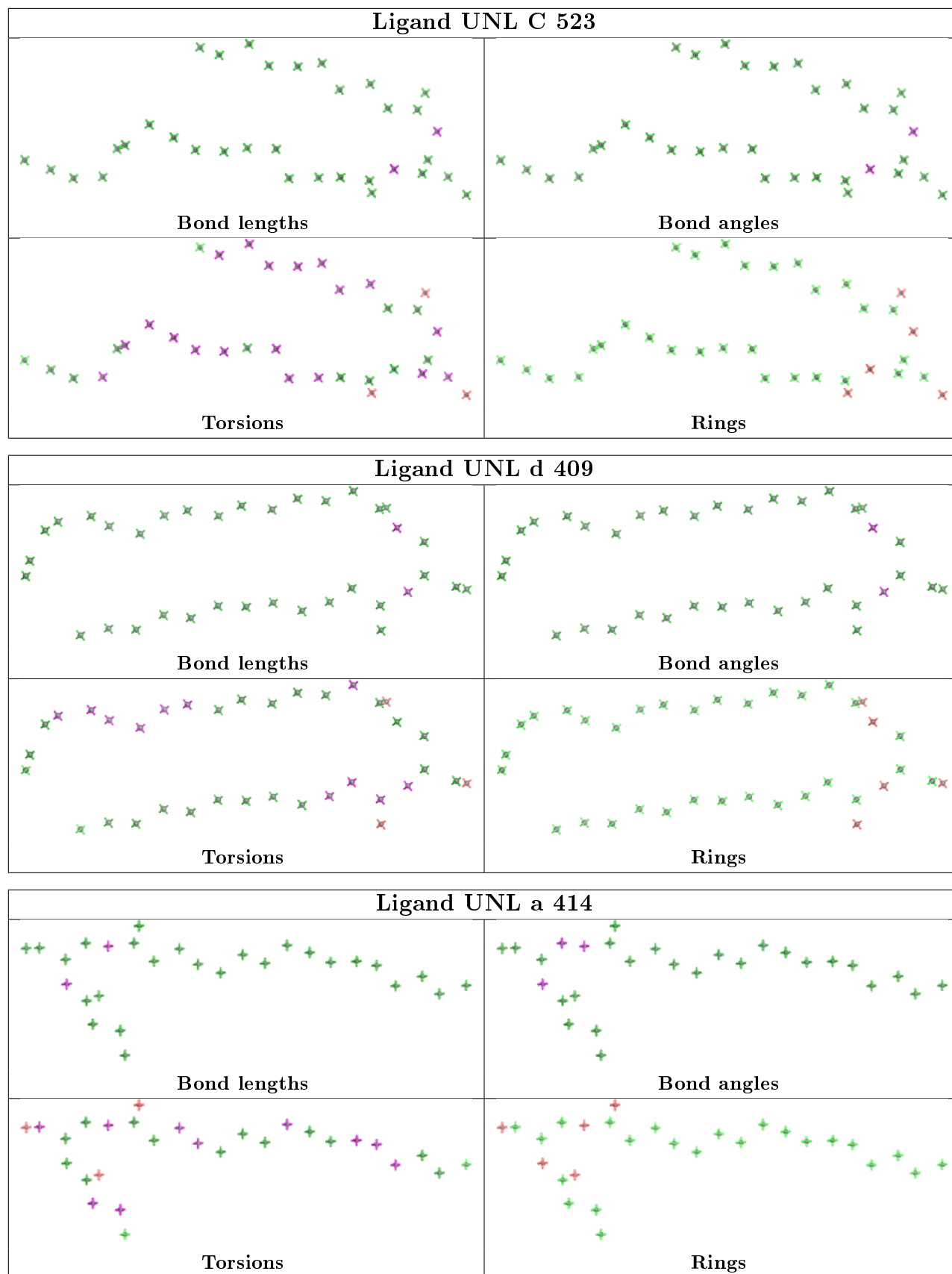


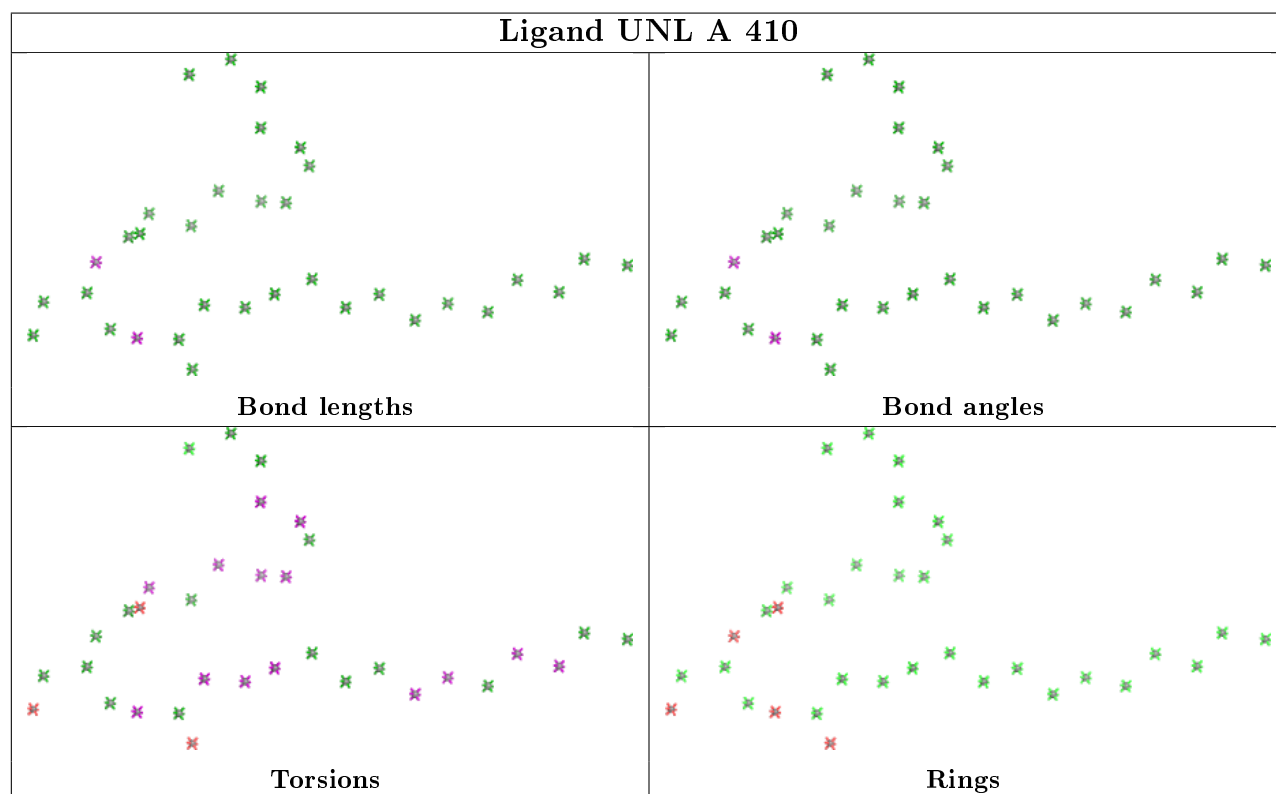
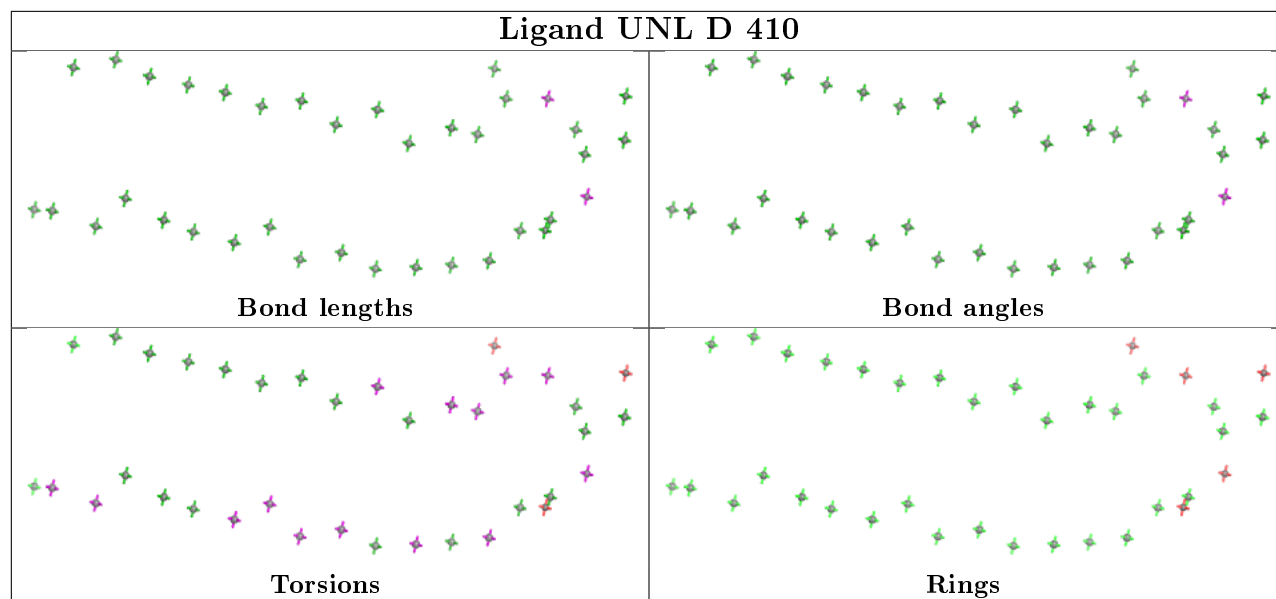
Ligand DGD h 101

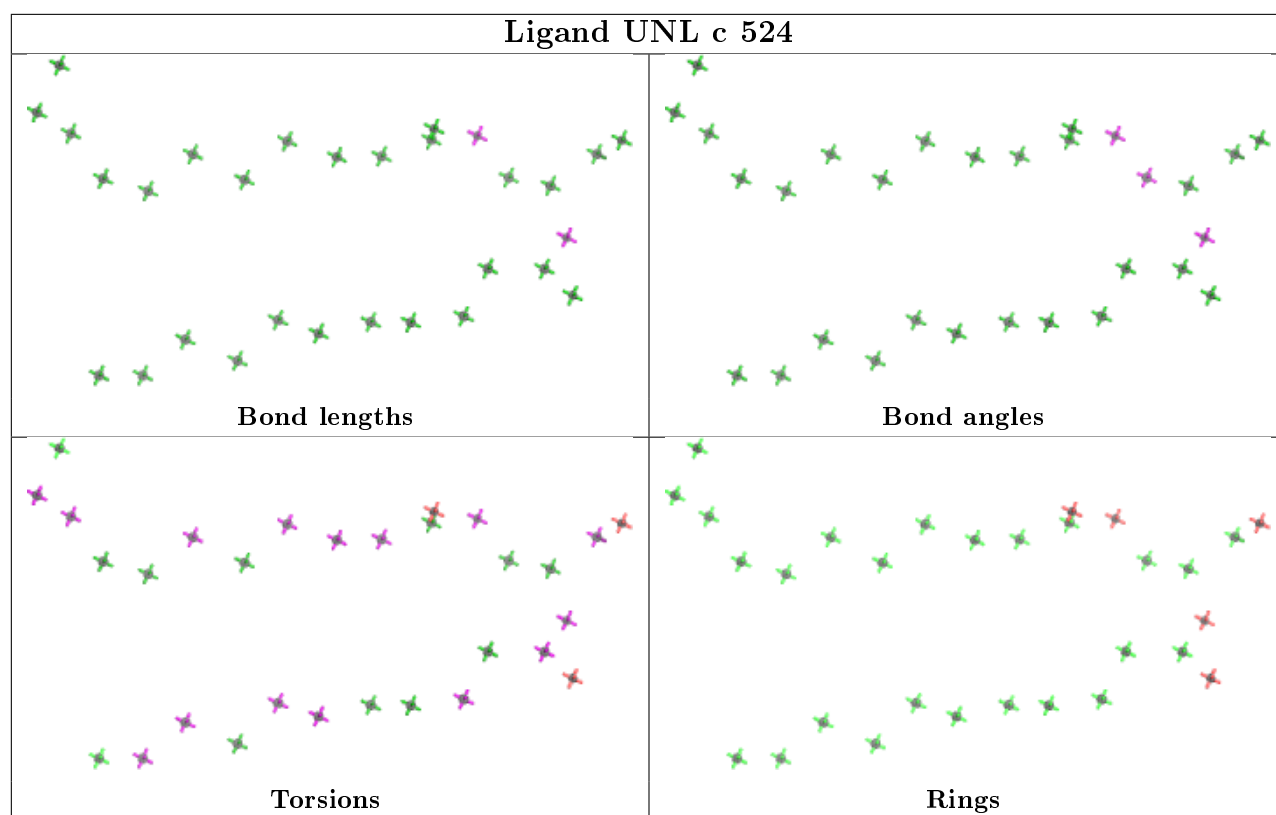


Ligand CLA B 615









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%)	-0.70	3 (0%) 84 84	16, 23, 46, 68	0
1	a	334/344 (97%)	-0.63	7 (2%) 63 63	18, 23, 48, 78	0
2	B	505/505 (100%)	-0.47	19 (3%) 40 38	19, 28, 54, 85	0
2	b	495/505 (98%)	-0.40	20 (4%) 38 36	19, 28, 53, 95	0
3	C	451/455 (99%)	-0.45	8 (1%) 68 68	21, 33, 49, 83	0
3	c	455/455 (100%)	-0.47	6 (1%) 77 78	22, 33, 46, 79	0
4	D	342/342 (100%)	-0.67	4 (1%) 79 79	17, 24, 44, 90	0
4	d	342/342 (100%)	-0.73	5 (1%) 73 74	18, 25, 42, 86	0
5	E	78/83 (93%)	0.76	19 (24%) 0 0	28, 47, 75, 87	0
5	e	78/83 (93%)	0.64	16 (20%) 1 1	29, 44, 67, 81	0
6	F	33/44 (75%)	-0.09	4 (12%) 4 4	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.04	3 (9%) 8 8	28, 34, 72, 90	0
7	H	64/65 (98%)	0.08	3 (4%) 31 30	26, 37, 50, 78	0
7	h	62/65 (95%)	-0.24	0 100 100	25, 36, 48, 58	0
8	I	34/38 (89%)	-0.11	3 (8%) 10 9	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.15	2 (5%) 23 23	29, 34, 52, 85	0
9	J	36/40 (90%)	-0.04	2 (5%) 24 23	26, 41, 74, 90	0
9	j	40/40 (100%)	-0.03	3 (7%) 14 14	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.27	2 (5%) 25 24	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.22	1 (2%) 54 53	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.36	3 (8%) 12 12	18, 22, 65, 81	0
11	l	37/37 (100%)	-0.22	3 (8%) 12 12	18, 22, 76, 91	0
12	M	33/36 (91%)	-0.65	1 (3%) 50 48	21, 25, 39, 57	0
12	m	34/36 (94%)	-0.55	3 (8%) 10 9	20, 26, 53, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.23	8 (3%) 46 44	18, 32, 56, 85	0
13	o	243/244 (99%)	-0.09	19 (7%) 13 13	19, 35, 67, 89	0
14	T	28/32 (87%)	-0.69	1 (3%) 42 40	19, 24, 37, 54	0
14	t	29/32 (90%)	-0.36	2 (6%) 16 16	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.34	2 (2%) 63 63	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.36	1 (1%) 82 82	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.62	0 100 100	22, 28, 43, 60	0
16	v	137/137 (100%)	-0.25	5 (3%) 42 40	25, 36, 53, 74	0
17	Y	29/30 (96%)	1.08	6 (20%) 1 0	41, 51, 72, 79	0
17	y	29/30 (96%)	0.76	4 (13%) 2 3	41, 50, 66, 70	0
18	X	38/40 (95%)	0.26	5 (13%) 3 3	32, 42, 68, 72	0
18	x	35/40 (87%)	-0.09	2 (5%) 23 23	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.66	13 (20%) 1 0	38, 48, 86, 98	0
19	z	61/62 (98%)	0.71	12 (19%) 1 1	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.37	220 (4%) 36 34	16, 30, 57, 98	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	9.7
2	b	495	PHE	9.2
2	b	503	THR	8.4
13	o	246	ALA	8.3
2	b	502	VAL	7.4
6	f	14	PRO	7.2
2	b	504	THR	7.1
5	e	61	ARG	6.9
13	o	4	THR	6.9
7	H	64	ALA	6.8
3	C	23	ALA	6.3
11	l	3	PRO	6.1
2	b	484	PRO	5.9
17	y	19	ILE	5.9
1	a	11	ALA	5.9
17	Y	19	ILE	5.9
17	Y	18	VAL	5.5
5	e	59[A]	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
13	O	60	ARG	5.3
5	E	4	THR	5.2
2	b	500	GLY	5.1
2	B	486	LEU	5.1
15	u	8	GLU	5.1
2	B	494	GLY	5.1
11	l	1	MET	5.0
4	D	240	ALA	4.9
19	z	32	ASP	4.9
14	t	30	THR	4.8
7	H	65	LEU	4.8
18	X	2	THR	4.8
19	Z	32	ASP	4.7
13	O	4	THR	4.7
4	D	11	GLU	4.7
19	Z	33	TRP	4.6
9	J	5	GLY	4.6
19	Z	30	PRO	4.6
2	b	499	VAL	4.5
1	A	11	ALA	4.5
2	b	501	ASP	4.5
19	z	30	PRO	4.4
19	z	3	ILE	4.4
4	D	12	ARG	4.4
9	j	6	GLY	4.4
19	Z	31	GLN	4.3
16	v	16	GLY	4.3
3	c	21	ILE	4.3
2	B	485	GLU	4.3
11	L	1	MET	4.3
4	d	11	GLU	4.3
13	o	35	SER	4.2
5	E	17	VAL	4.2
19	z	60	PHE	4.2
1	A	262	TYR	4.2
6	F	16	PHE	4.2
11	l	2	GLU	4.1
6	F	13	TYR	4.1
5	E	78	THR	4.1
11	L	3	PRO	4.0
1	a	262	TYR	3.9
5	E	79	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	487	SER	3.9
5	e	25	ILE	3.9
2	B	506	LYS	3.8
2	B	502	VAL	3.8
8	I	34	ARG	3.8
6	f	16	PHE	3.7
2	B	503	THR	3.7
19	z	33	TRP	3.7
19	z	34	ASP	3.7
3	C	143	TYR	3.7
5	E	6	GLY	3.6
12	M	33	GLN	3.6
2	B	495	PHE	3.6
2	b	483	ASP	3.6
19	Z	35	ARG	3.6
18	x	2	THR	3.6
5	e	62	SER	3.6
5	e	81	GLU	3.5
2	b	491	VAL	3.5
11	L	2	GLU	3.5
8	i	36	ASP	3.5
17	Y	20	ALA	3.5
14	t	29	ILE	3.5
19	Z	34	ASP	3.5
5	E	74	GLN	3.5
1	a	263	ALA	3.4
4	d	238	THR	3.4
19	z	1	MET	3.4
17	Y	22	LEU	3.4
7	H	6	TRP	3.4
3	c	20	SER	3.4
2	b	490	GLN	3.4
3	c	207	ARG	3.3
2	B	293	ALA	3.3
19	Z	60	PHE	3.3
3	c	19	ASN	3.3
19	z	31	GLN	3.3
13	o	60	ARG	3.2
17	y	18	VAL	3.2
9	j	1	MET	3.2
5	E	81	GLU	3.2
9	J	6	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
17	y	20	ALA	3.2
19	Z	3	ILE	3.2
5	e	60[A]	GLN	3.1
13	o	5	LEU	3.1
17	y	22	LEU	3.1
4	D	238	THR	3.1
5	E	62	SER	3.1
2	B	501	ASP	3.1
2	B	496	TYR	3.1
2	b	295	GLY	3.1
5	E	61	ARG	3.0
4	d	236	ASN	3.0
9	j	5	GLY	3.0
2	b	129	GLY	2.9
5	E	25	ILE	2.9
5	e	10	PHE	2.9
1	a	260	PHE	2.9
13	o	25	THR	2.9
5	E	21	VAL	2.9
2	B	504	THR	2.8
8	i	34[A]	ARG	2.8
10	k	17	ILE	2.8
5	e	6	GLY	2.8
4	d	240	ALA	2.8
13	O	25	THR	2.8
13	O	59	LYS	2.8
3	C	25	ASN	2.8
13	O	61	GLN	2.8
13	o	36	GLN	2.8
17	Y	43	ARG	2.8
3	C	191	PRO	2.8
12	m	34	LYS	2.8
13	O	62	GLU	2.8
1	a	261	GLN	2.8
19	z	61	VAL	2.8
18	x	34	ILE	2.7
1	A	12	ASN	2.7
2	b	85	GLY	2.7
5	E	5	THR	2.7
5	e	11	SER	2.7
13	o	24	ASP	2.7
2	B	85	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	a	13	LEU	2.7
13	o	27	ARG	2.6
5	E	80	LEU	2.6
12	m	33	GLN	2.6
19	Z	41	PHE	2.6
19	z	41	PHE	2.6
19	z	59	PHE	2.6
10	K	17	ILE	2.6
18	X	3	ILE	2.6
5	e	71	GLU	2.6
18	X	37	VAL	2.6
1	a	242	GLU	2.5
2	b	86	ILE	2.5
6	f	15	ILE	2.5
8	I	35	LYS	2.5
2	b	497	GLN	2.5
5	E	73	LYS	2.5
19	Z	62	VAL	2.5
15	U	8	GLU	2.5
16	v	14	SER	2.5
2	B	488	PRO	2.5
4	d	237	PRO	2.5
2	B	374	ASN	2.5
19	Z	29	SER	2.5
3	C	24	THR	2.4
19	z	35	ARG	2.4
2	b	126	PRO	2.4
6	F	14	PRO	2.4
6	F	15	ILE	2.4
12	m	5	GLN	2.4
13	o	23	ASP	2.4
5	E	72	ALA	2.4
5	e	82	GLN	2.4
16	v	106	ASN	2.3
16	v	72	LEU	2.3
5	e	9	PRO	2.3
14	T	29	ILE	2.3
13	O	56	PRO	2.3
13	o	132	ASN	2.3
13	o	34	SER	2.3
13	o	136	ILE	2.2
13	o	61	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
8	I	33	LYS	2.2
13	o	131	PRO	2.2
19	Z	2	THR	2.2
19	Z	36	SER	2.2
5	e	21	VAL	2.2
2	B	505	ARG	2.2
2	B	484	PRO	2.2
13	O	132[A]	ASN	2.2
2	B	483	ASP	2.2
2	b	128	THR	2.2
3	C	182	PHE	2.2
13	o	130	GLN	2.2
18	X	38	GLN	2.2
5	e	24	SER	2.1
13	o	56	PRO	2.1
18	X	39	ARG	2.1
13	o	59	LYS	2.1
3	c	143	TYR	2.1
15	U	65	PRO	2.1
16	v	18	THR	2.1
3	c	23	ALA	2.1
5	e	83	LEU	2.1
10	K	16	ALA	2.1
3	C	253	LEU	2.1
5	e	80	LEU	2.1
5	E	68	ASP	2.1
5	E	71	GLU	2.1
13	o	62	GLU	2.1
17	Y	21	GLN	2.0
5	E	76	VAL	2.0
2	b	293	ALA	2.0
5	E	77	GLU	2.0
2	B	86	ILE	2.0
3	C	145	SER	2.0

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

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
14	FME	T	1	10/11	0.97	0.07	23,29,48,51	0
14	FME	t	1	10/11	0.97	0.06	23,27,49,50	0
8	FME	i	1	10/11	0.98	0.09	30,31,34,35	0
8	FME	I	1	10/11	0.98	0.07	26,32,36,37	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
32	HTG	C	534	19/19	0.39	0.39	68,110,128,130	0
24	LMG	C	524	45/55	0.52	0.32	22,46,51,56	45
26	UNL	Z	102	4/-	0.52	0.17	59,61,62,63	0
32	HTG	D	417	19/19	0.53	0.31	67,105,119,120	0
28	DMS	U	904	4/4	0.55	0.22	58,66,66,83	0
32	HTG	c	521	19/19	0.56	0.35	57,85,102,105	0
26	UNL	b	642	13/-	0.57	0.22	71,80,87,90	0
32	HTG	d	401	19/19	0.58	0.29	58,99,111,120	0
26	UNL	b	645	6/-	0.58	0.24	57,65,76,76	0
32	HTG	B	623	19/19	0.59	0.35	53,88,93,94	0
34	LMT	f	102	24/35	0.59	0.26	62,77,94,98	0
35	DGD	D	406	51/66	0.59	0.30	57,74,100,108	0
26	UNL	J	104	14/-	0.60	0.24	67,77,80,81	0
34	LMT	J	103	24/35	0.60	0.23	53,61,81,85	0
28	DMS	H	103	4/4	0.61	0.40	84,101,109,112	0
28	DMS	B	636	4/4	0.61	0.40	77,86,90,96	0
34	LMT	m	101	35/35	0.63	0.25	48,94,110,114	0
26	UNL	A	410	36/-	0.64	0.25	57,78,84,91	0
34	LMT	b	628	25/35	0.64	0.22	54,79,95,96	0
35	DGD	d	416	51/66	0.64	0.27	56,75,96,103	0
32	HTG	B	632	19/19	0.65	0.23	51,97,108,114	0
36	LHG	E	103	48/49	0.66	0.29	44,99,108,119	0
28	DMS	v	207	4/4	0.67	0.20	53,66,72,87	0
26	UNL	a	414	28/-	0.67	0.23	59,68,84,87	0
32	HTG	C	521	19/19	0.67	0.26	46,78,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	UNL	B	646	16/-	0.68	0.24	85,89,93,94	0
26	UNL	b	643	9/-	0.68	0.18	67,67,74,74	0
26	UNL	E	102	15/-	0.68	0.28	55,62,76,77	0
28	DMS	O	305	4/4	0.69	0.30	64,66,77,86	0
28	DMS	j	105	4/4	0.69	0.19	70,74,75,88	0
26	UNL	T	103	13/-	0.69	0.17	64,68,72,72	0
32	HTG	v	210	14/19	0.69	0.27	60,80,92,100	0
26	UNL	a	402	6/-	0.69	0.17	50,57,62,63	0
26	UNL	B	630	14/-	0.70	0.20	67,74,83,84	0
34	LMT	Z	101	35/35	0.70	0.23	44,90,107,109	0
32	HTG	b	602	19/19	0.70	0.20	51,103,117,118	0
34	LMT	b	627	32/35	0.71	0.24	42,67,84,87	0
24	LMG	c	518	51/55	0.72	0.21	37,72,84,87	0
26	UNL	B	629	10/-	0.72	0.27	54,69,74,74	0
26	UNL	c	524	30/-	0.72	0.19	59,74,86,87	0
26	UNL	J	107	3/-	0.73	0.21	61,61,63,64	0
34	LMT	a	418	35/35	0.73	0.21	45,69,78,81	0
26	UNL	U	901	14/-	0.74	0.27	40,49,59,59	0
26	UNL	h	103	16/-	0.74	0.29	61,69,73,76	0
34	LMT	B	626	24/35	0.74	0.20	37,54,86,95	0
32	HTG	u	201	8/19	0.74	0.21	45,52,69,89	0
34	LMT	m	102	35/35	0.74	0.20	34,53,58,59	0
28	DMS	b	638	4/4	0.75	0.28	67,75,77,86	0
23	SQD	l	101	54/54	0.75	0.20	47,68,101,106	0
26	UNL	a	416	11/-	0.75	0.16	66,68,76,78	0
34	LMT	M	101	35/35	0.75	0.20	34,53,63,64	0
26	UNL	C	523	34/-	0.75	0.22	59,80,92,101	0
26	UNL	I	106	11/-	0.76	0.19	61,73,81,81	0
34	LMT	B	625	24/35	0.76	0.16	48,67,86,89	0
28	DMS	b	640	4/4	0.76	0.27	49,58,71,73	0
26	UNL	B	647	13/-	0.76	0.24	71,81,90,91	0
27	PL9	a	415	55/55	0.77	0.23	52,67,89,94	0
28	DMS	B	642	4/4	0.77	0.31	43,51,68,71	0
34	LMT	I	101	35/35	0.77	0.24	67,82,91,92	0
28	DMS	O	308	4/4	0.77	0.24	66,74,76,87	0
26	UNL	t	102	16/-	0.77	0.17	61,71,80,80	0
32	HTG	c	520	19/19	0.78	0.21	77,88,99,100	0
26	UNL	c	526	8/-	0.78	0.15	54,59,64,65	0
34	LMT	z	102	35/35	0.78	0.19	46,85,99,101	0
26	UNL	H	105	6/-	0.78	0.14	51,55,63,65	0
26	UNL	J	105	12/-	0.79	0.23	63,67,71,71	0
26	UNL	d	409	36/-	0.79	0.18	36,60,91,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	PL9	A	411	55/55	0.79	0.20	43,67,89,92	0
26	UNL	B	633	16/-	0.80	0.25	53,61,69,70	0
26	UNL	i	102	11/-	0.80	0.16	48,54,64,65	0
23	SQD	b	622	54/54	0.80	0.17	46,63,95,100	0
32	HTG	C	522	19/19	0.80	0.27	66,83,104,107	0
34	LMT	T	102	24/35	0.80	0.19	36,53,78,85	0
23	SQD	a	401	54/54	0.81	0.16	39,58,82,86	0
34	LMT	E	101	24/35	0.81	0.26	64,78,84,90	0
28	DMS	V	205	4/4	0.81	0.25	67,76,77,79	0
32	HTG	b	624	19/19	0.81	0.23	49,74,80,85	0
26	UNL	b	630	11/-	0.81	0.21	55,60,67,68	0
28	DMS	O	309	4/4	0.81	0.23	58,65,72,73	0
34	LMT	c	523	35/35	0.81	0.23	67,77,83,85	0
26	UNL	X	101	16/-	0.81	0.17	37,40,59,59	0
26	UNL	d	410	16/-	0.82	0.18	33,45,63,63	0
34	LMT	B	627	16/35	0.82	0.18	52,60,78,78	0
23	SQD	A	412	54/54	0.82	0.16	41,60,78,81	0
26	UNL	j	106	6/-	0.82	0.19	52,55,58,59	0
28	DMS	O	303	4/4	0.82	0.29	63,72,77,78	0
26	UNL	e	101	7/-	0.82	0.24	54,58,64,65	0
26	UNL	J	106	4/-	0.83	0.16	57,60,61,67	0
26	UNL	I	104	11/-	0.83	0.18	53,56,59,62	0
28	DMS	u	204	4/4	0.83	0.20	71,78,83,86	0
26	UNL	D	410	37/-	0.83	0.15	42,57,93,98	0
23	SQD	f	101	40/54	0.83	0.25	57,86,102,107	0
26	UNL	x	102	9/-	0.83	0.28	56,68,72,72	0
28	DMS	b	641	4/4	0.83	0.17	63,65,75,80	0
28	DMS	o	308	4/4	0.83	0.21	60,61,62,63	0
26	UNL	c	525	10/-	0.84	0.15	58,65,66,67	0
26	UNL	I	105	10/-	0.84	0.15	60,66,71,72	0
32	HTG	B	622	19/19	0.84	0.16	28,46,54,54	0
26	UNL	M	102	12/-	0.84	0.22	49,53,95,98	0
28	DMS	O	310	4/4	0.84	0.32	76,78,82,94	0
28	DMS	o	306	4/4	0.84	0.25	55,58,65,77	0
26	UNL	I	102	16/-	0.85	0.19	38,47,63,64	0
26	UNL	L	102	14/-	0.85	0.22	56,60,84,84	0
28	DMS	D	415	4/4	0.85	0.25	57,58,63,65	0
28	DMS	c	533	4/4	0.85	0.27	73,75,77,87	0
26	UNL	i	101	16/-	0.85	0.18	41,45,65,65	0
32	HTG	b	625	19/19	0.85	0.20	30,44,66,70	0
23	SQD	F	101	35/54	0.86	0.23	51,76,89,90	0
28	DMS	B	635	4/4	0.86	0.24	90,94,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
26	UNL	b	646	6/-	0.86	0.14	54,58,60,62	0
26	UNL	B	628	15/-	0.86	0.15	45,50,60,66	0
32	HTG	V	202	13/19	0.86	0.21	45,49,70,82	0
28	DMS	o	304	4/4	0.86	0.32	68,79,82,83	0
28	DMS	v	209	4/4	0.86	0.31	71,78,79,79	0
26	UNL	A	413	4/-	0.86	0.19	64,64,64,66	0
32	HTG	C	520	19/19	0.86	0.21	64,70,76,79	0
28	DMS	B	644	4/4	0.87	0.32	52,53,61,69	0
28	DMS	b	637	4/4	0.87	0.17	77,79,84,93	0
32	HTG	b	601	19/19	0.87	0.15	45,61,67,80	0
24	LMG	B	620	51/55	0.87	0.12	33,43,55,58	0
20	CLA	C	513	65/65	0.87	0.14	40,48,72,77	0
28	DMS	C	532	4/4	0.87	0.19	33,40,41,48	0
24	LMG	A	407	51/55	0.87	0.13	40,55,70,78	0
28	DMS	B	638	4/4	0.87	0.19	53,61,63,68	0
26	UNL	H	104	4/-	0.88	0.20	60,62,65,67	0
32	HTG	B	631	19/19	0.88	0.12	41,57,69,73	0
24	LMG	a	410	51/55	0.88	0.15	44,55,65,67	0
33	CA	V	203	1/1	0.88	0.11	63,63,63,63	0
28	DMS	U	902	4/4	0.88	0.23	35,44,49,58	0
20	CLA	B	602	65/65	0.88	0.14	29,42,77,81	0
26	UNL	I	103	13/-	0.88	0.13	47,53,84,87	0
24	LMG	C	519	51/55	0.89	0.15	31,67,83,84	0
28	DMS	O	306	4/4	0.89	0.29	66,73,73,75	0
26	UNL	D	411	16/-	0.89	0.16	39,45,58,62	0
22	BCR	d	405	40/40	0.89	0.12	24,30,56,58	0
26	UNL	j	104	16/-	0.89	0.11	49,58,64,66	0
24	LMG	c	519	51/55	0.89	0.13	29,59,86,88	0
28	DMS	C	527	4/4	0.89	0.17	73,76,79,87	0
20	CLA	b	603	65/65	0.89	0.15	30,45,75,82	0
24	LMG	b	623	49/55	0.89	0.12	33,42,54,61	0
26	UNL	b	644	7/-	0.90	0.18	64,65,70,70	0
28	DMS	b	632	4/4	0.90	0.15	55,58,66,70	0
26	UNL	z	101	6/-	0.90	0.13	49,55,55,57	0
28	DMS	c	534	4/4	0.90	0.24	70,71,75,81	0
28	DMS	O	311	4/4	0.90	0.26	57,65,69,72	0
28	DMS	A	418	4/4	0.90	0.31	68,74,80,85	0
28	DMS	b	636	4/4	0.90	0.14	66,71,72,79	0
22	BCR	D	405	40/40	0.90	0.11	26,30,58,60	0
22	BCR	C	514	40/40	0.90	0.10	36,45,49,50	0
28	DMS	B	639	4/4	0.90	0.24	65,70,71,76	0
28	DMS	V	204	4/4	0.91	0.32	58,64,64,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	DMS	c	535	4/4	0.91	0.18	58,59,65,68	0
26	UNL	b	629	16/-	0.91	0.14	41,48,60,60	0
26	UNL	i	103	11/-	0.91	0.27	58,61,65,66	0
28	DMS	u	203	4/4	0.91	0.29	47,55,56,65	0
28	DMS	d	415	4/4	0.91	0.26	68,71,71,72	0
28	DMS	A	416	4/4	0.91	0.23	59,60,69,77	0
28	DMS	V	209	4/4	0.91	0.20	57,73,77,81	0
28	DMS	o	305	4/4	0.91	0.23	73,75,77,87	0
28	DMS	b	634	4/4	0.91	0.29	59,67,67,75	0
20	CLA	b	618	65/65	0.91	0.13	23,33,92,98	0
28	DMS	u	202	4/4	0.91	0.18	40,46,52,54	0
28	DMS	v	208	4/4	0.91	0.26	89,92,92,95	0
28	DMS	o	303	4/4	0.92	0.38	66,69,75,79	0
26	UNL	d	411	16/-	0.92	0.12	33,42,55,55	0
28	DMS	b	635	4/4	0.92	0.27	58,62,69,73	0
28	DMS	c	536	4/4	0.92	0.15	33,33,45,46	0
20	CLA	c	512	65/65	0.92	0.11	28,41,70,72	0
20	CLA	C	506	65/65	0.92	0.10	32,45,86,87	0
38	RRX	x	101	41/41	0.92	0.09	26,32,47,58	0
28	DMS	O	304	4/4	0.92	0.28	63,68,72,73	0
22	BCR	K	101	40/40	0.92	0.10	33,37,42,45	0
20	CLA	c	513	65/65	0.92	0.11	36,46,81,87	0
22	BCR	K	102	40/40	0.92	0.13	31,36,40,41	0
28	DMS	C	529	4/4	0.92	0.19	70,73,74,74	0
28	DMS	B	640	4/4	0.93	0.33	45,48,49,50	0
28	DMS	O	307	4/4	0.93	0.16	69,76,77,88	0
32	HTG	B	621	19/19	0.93	0.12	36,41,48,52	0
28	DMS	A	417	4/4	0.93	0.17	70,72,77,81	0
20	CLA	B	601	65/65	0.93	0.12	23,29,82,86	0
35	DGD	H	102	62/66	0.93	0.11	25,33,40,43	0
28	DMS	c	529	4/4	0.93	0.23	79,82,86,87	0
28	DMS	C	531	4/4	0.93	0.24	53,54,58,74	0
22	BCR	k	102	40/40	0.93	0.09	41,46,51,51	0
28	DMS	v	204	4/4	0.93	0.15	48,54,57,69	0
20	CLA	C	512	55/65	0.93	0.09	37,44,49,54	0
20	CLA	c	506	65/65	0.93	0.10	24,39,71,74	0
35	DGD	h	101	62/66	0.93	0.10	25,34,41,49	0
28	DMS	v	203	4/4	0.93	0.16	67,69,76,79	0
38	RRX	H	101	41/41	0.93	0.10	27,31,41,46	0
28	DMS	D	416	4/4	0.93	0.17	83,87,89,91	0
23	SQD	A	406	54/54	0.93	0.13	34,59,71,76	0
24	LMG	j	101	45/55	0.94	0.09	27,32,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	d	404	65/65	0.94	0.10	24,29,78,87	0
32	HTG	O	302	19/19	0.94	0.10	34,42,50,53	0
23	SQD	a	409	54/54	0.94	0.12	33,56,75,78	0
28	DMS	v	206	4/4	0.94	0.20	52,53,61,66	0
28	DMS	B	643	4/4	0.94	0.14	51,53,62,71	0
28	DMS	c	531	4/4	0.94	0.15	73,78,85,86	0
33	CA	O	301	1/1	0.94	0.06	47,47,47,47	0
33	CA	o	301	1/1	0.94	0.07	48,48,48,48	0
24	LMG	J	101	45/55	0.94	0.10	27,32,64,70	0
28	DMS	A	415	4/4	0.94	0.20	55,58,65,71	0
28	DMS	c	532	4/4	0.94	0.23	65,70,76,77	0
28	DMS	C	533	4/4	0.94	0.28	72,73,73,74	0
20	CLA	B	607	65/65	0.95	0.09	22,29,55,62	0
22	BCR	t	101	40/40	0.95	0.07	22,29,41,43	0
28	DMS	B	641	4/4	0.95	0.31	68,69,75,80	0
20	CLA	D	404	65/65	0.95	0.10	26,29,77,81	0
31	BCT	A	421	4/4	0.95	0.10	31,34,40,44	0
28	DMS	V	208	4/4	0.95	0.12	75,77,82,85	0
28	DMS	d	413	4/4	0.95	0.17	47,53,55,57	0
35	DGD	c	517	62/66	0.95	0.09	23,30,56,71	0
22	BCR	B	619	40/40	0.95	0.07	22,30,42,44	0
28	DMS	b	639	4/4	0.95	0.20	46,49,49,50	0
35	DGD	C	517	55/66	0.95	0.07	26,34,59,62	0
33	CA	b	626	1/1	0.95	0.07	42,42,42,42	0
36	LHG	D	409	49/49	0.95	0.12	27,33,81,83	0
28	DMS	o	307	4/4	0.95	0.16	53,58,63,65	0
22	BCR	k	101	40/40	0.95	0.09	28,36,41,42	0
20	CLA	b	608	65/65	0.95	0.09	24,31,59,63	0
20	CLA	c	511	65/65	0.95	0.09	27,33,40,43	0
20	CLA	C	503	65/65	0.95	0.08	28,33,37,42	0
20	CLA	C	507	65/65	0.95	0.09	28,37,52,57	0
28	DMS	d	414	4/4	0.95	0.16	57,62,64,68	0
22	BCR	C	515	40/40	0.95	0.09	31,37,43,45	0
20	CLA	C	511	65/65	0.95	0.08	30,37,42,45	0
22	BCR	j	102	40/40	0.95	0.09	30,35,42,45	0
35	DGD	c	515	62/66	0.95	0.10	23,32,71,75	0
22	BCR	c	514	40/40	0.96	0.07	28,36,39,39	0
20	CLA	b	611	65/65	0.96	0.09	24,30,34,41	0
36	LHG	D	407	49/49	0.96	0.09	28,37,44,52	0
27	PL9	d	412	55/55	0.96	0.08	18,23,29,35	0
20	CLA	b	604	65/65	0.96	0.08	23,27,33,35	0
20	CLA	C	509	65/65	0.96	0.09	29,34,52,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	DGD	c	516	57/66	0.96	0.08	27,32,62,68	0
31	BCT	a	413	4/4	0.96	0.07	32,32,38,42	0
35	DGD	C	518	62/66	0.96	0.09	24,30,62,73	0
20	CLA	C	504	65/65	0.96	0.08	27,30,59,61	0
28	DMS	V	206	4/4	0.96	0.21	59,61,63,65	0
22	BCR	T	101	40/40	0.96	0.07	24,32,43,45	0
20	CLA	B	610	65/65	0.96	0.10	26,31,35,38	0
20	CLA	A	404	65/65	0.96	0.10	20,25,88,90	0
22	BCR	b	620	40/40	0.96	0.07	22,27,43,46	0
20	CLA	C	510	65/65	0.96	0.08	26,31,38,44	0
20	CLA	B	603	65/65	0.96	0.08	23,28,35,39	0
37	HEM	E	104	43/43	0.96	0.10	39,44,52,56	0
20	CLA	C	508	60/65	0.96	0.07	23,31,47,51	0
20	CLA	C	501	65/65	0.96	0.08	27,33,45,52	0
28	DMS	h	102	4/4	0.96	0.17	50,51,53,62	0
28	DMS	c	528	4/4	0.96	0.18	58,62,63,65	0
20	CLA	c	501	65/65	0.96	0.08	26,30,41,48	0
28	DMS	v	205	4/4	0.96	0.18	67,70,72,73	0
22	BCR	B	618	40/40	0.96	0.08	21,28,42,45	0
28	DMS	B	637	4/4	0.96	0.17	53,53,54,60	0
20	CLA	c	509	65/65	0.96	0.09	25,30,53,58	0
20	CLA	b	616	65/65	0.96	0.09	20,26,73,80	0
28	DMS	V	207	4/4	0.96	0.10	62,63,63,70	0
22	BCR	a	408	40/40	0.96	0.07	21,25,30,31	0
20	CLA	a	404	60/65	0.96	0.09	18,22,66,75	0
20	CLA	c	503	65/65	0.96	0.08	25,35,40,43	0
28	DMS	D	413	4/4	0.96	0.11	50,56,60,61	0
28	DMS	B	645	4/4	0.96	0.11	56,59,64,71	0
20	CLA	b	612	65/65	0.96	0.08	21,27,36,41	0
20	CLA	C	505	65/65	0.96	0.08	28,33,44,48	0
28	DMS	C	530	4/4	0.96	0.16	44,44,46,50	0
20	CLA	b	609	65/65	0.97	0.07	19,22,33,37	0
28	DMS	i	104	4/4	0.97	0.21	63,66,67,71	0
20	CLA	c	510	65/65	0.97	0.07	23,29,39,42	0
20	CLA	B	608	65/65	0.97	0.07	18,21,34,39	0
22	BCR	A	405	40/40	0.97	0.08	21,26,32,35	0
20	CLA	b	613	65/65	0.97	0.07	20,22,38,44	0
21	PHO	a	405	64/64	0.97	0.07	17,20,22,25	0
20	CLA	a	407	47/65	0.97	0.08	19,22,41,48	0
37	HEM	e	102	43/43	0.97	0.09	34,41,56,68	0
20	CLA	b	617	65/65	0.97	0.07	23,30,44,50	0
28	DMS	b	631	4/4	0.97	0.10	23,24,27,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	CLA	c	508	60/65	0.97	0.07	24,28,52,54	0
20	CLA	b	605	65/65	0.97	0.07	21,25,34,37	0
28	DMS	b	633	4/4	0.97	0.13	45,48,49,53	0
36	LHG	d	406	49/49	0.97	0.10	29,36,43,48	0
20	CLA	c	504	65/65	0.97	0.07	25,29,55,60	0
28	DMS	C	525[B]	4/4	0.97	0.19	32,33,35,35	4
20	CLA	b	614	65/65	0.97	0.07	21,25,31,37	0
28	DMS	C	525[A]	4/4	0.97	0.19	48,49,51,57	4
28	DMS	D	414	4/4	0.97	0.14	55,56,57,58	0
28	DMS	c	530	4/4	0.97	0.16	36,43,45,49	0
20	CLA	A	402	59/65	0.97	0.07	18,22,52,58	0
22	BCR	b	621	40/40	0.97	0.07	27,32,42,44	0
20	CLA	c	505	65/65	0.97	0.06	25,30,46,50	0
20	CLA	B	604	65/65	0.97	0.07	21,24,33,39	0
28	DMS	U	903[B]	4/4	0.97	0.17	26,28,29,32	4
36	LHG	d	408	49/49	0.97	0.10	24,31,83,88	0
28	DMS	U	903[A]	4/4	0.97	0.17	32,34,40,41	4
20	CLA	c	507	65/65	0.97	0.08	25,30,49,57	0
39	MG	J	102	1/1	0.97	0.05	33,33,33,33	0
28	DMS	F	102	4/4	0.97	0.11	51,52,56,64	0
28	DMS	C	526	4/4	0.97	0.15	59,60,63,65	0
36	LHG	L	101	49/49	0.97	0.09	24,31,49,53	0
20	CLA	B	611	65/65	0.97	0.08	21,26,34,40	0
36	LHG	l	102	49/49	0.97	0.08	22,30,51,54	0
22	BCR	b	619	40/40	0.97	0.07	23,26,32,35	0
36	LHG	d	407	49/49	0.97	0.12	22,27,46,50	0
20	CLA	B	616	65/65	0.97	0.07	25,29,48,52	0
22	BCR	B	617	40/40	0.97	0.07	22,26,32,33	0
20	CLA	c	502	65/65	0.97	0.07	22,26,39,48	0
20	CLA	C	502	65/65	0.97	0.07	24,29,41,48	0
35	DGD	C	516	62/66	0.97	0.09	22,32,74,79	0
20	CLA	a	403	65/65	0.97	0.09	17,20,29,38	0
20	CLA	b	610	65/65	0.97	0.07	20,26,31,33	0
20	CLA	B	605	65/65	0.97	0.08	19,23,55,58	0
21	PHO	D	403	64/64	0.97	0.07	18,24,29,35	0
20	CLA	B	615	65/65	0.97	0.08	20,24,70,79	0
27	PL9	D	412	55/55	0.97	0.08	19,23,29,34	0
20	CLA	b	606	65/65	0.97	0.07	20,24,54,59	0
20	CLA	b	607	65/65	0.98	0.08	20,24,33,35	0
36	LHG	D	408	49/49	0.98	0.09	23,30,44,49	0
20	CLA	B	609	65/65	0.98	0.07	22,25,31,33	0
20	CLA	b	615	65/65	0.98	0.06	18,22,53,59	0

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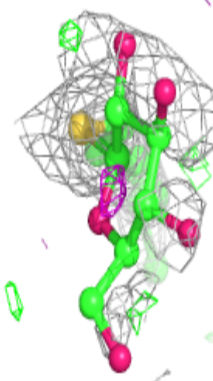
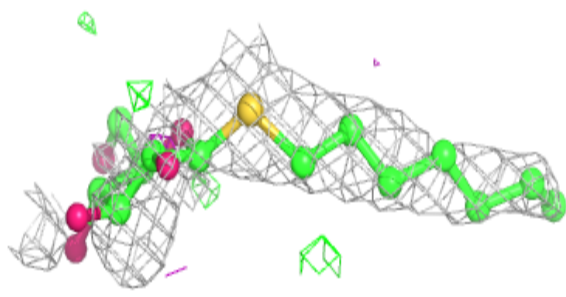
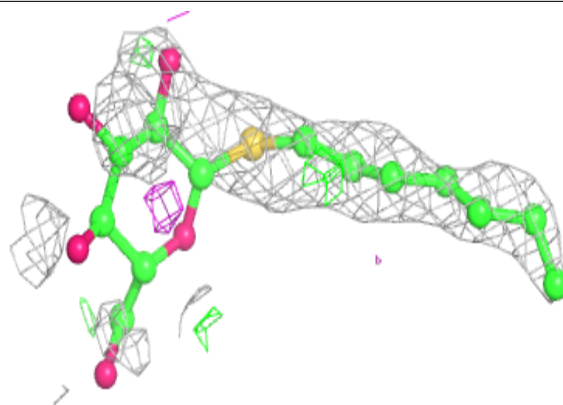
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	PHO	A	403	64/64	0.98	0.07	18,22,24,25	0
33	CA	c	522	1/1	0.98	0.04	41,41,41,41	0
20	CLA	B	614	65/65	0.98	0.06	19,22,48,53	0
40	HEC	v	201	43/43	0.98	0.08	25,29,34,37	0
28	DMS	v	202	4/4	0.98	0.15	50,51,53,55	0
20	CLA	D	401	65/65	0.98	0.08	16,20,35,41	0
21	PHO	a	406	64/64	0.98	0.08	19,24,29,32	0
28	DMS	B	634	4/4	0.98	0.08	23,24,25,26	0
20	CLA	B	613	65/65	0.98	0.07	21,25,30,34	0
20	CLA	B	606	65/65	0.98	0.09	19,24,35,37	0
20	CLA	d	402	65/65	0.98	0.08	16,20,35,41	0
20	CLA	A	401	65/65	0.98	0.08	16,19,30,36	0
28	DMS	o	302	4/4	0.98	0.07	20,28,31,36	0
20	CLA	D	402	65/65	0.98	0.06	15,19,30,36	0
20	CLA	d	403	65/65	0.98	0.07	17,19,27,34	0
20	CLA	B	612	65/65	0.98	0.07	19,22,36,42	0
29	FE2	A	419	1/1	0.99	0.03	29,29,29,29	0
28	DMS	C	528	4/4	0.99	0.09	33,37,39,41	0
33	CA	B	624	1/1	0.99	0.16	43,43,43,43	0
40	HEC	V	201	43/43	0.99	0.08	21,23,27,31	0
29	FE2	a	417	1/1	0.99	0.05	27,27,27,27	0
25	CL	a	412	1/1	0.99	0.06	24,24,24,24	0
28	DMS	A	414	4/4	0.99	0.07	25,28,28,29	0
28	DMS	c	527	4/4	0.99	0.05	33,33,34,38	0
25	CL	A	409	1/1	0.99	0.03	22,22,22,22	0
25	CL	A	408	1/1	1.00	0.05	22,22,22,22	0
30	OEX	A	420	10/10	1.00	0.04	21,23,24,24	0
25	CL	a	411	1/1	1.00	0.02	22,22,22,22	0
30	OEX	a	419	10/10	1.00	0.04	21,24,26,26	0
39	MG	j	103	1/1	1.00	0.08	31,31,31,31	0

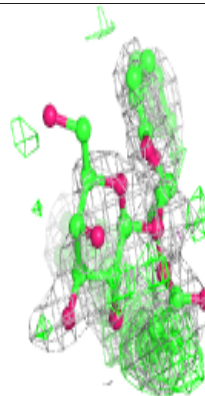
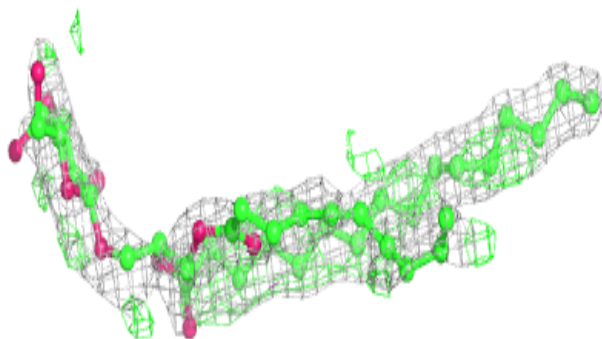
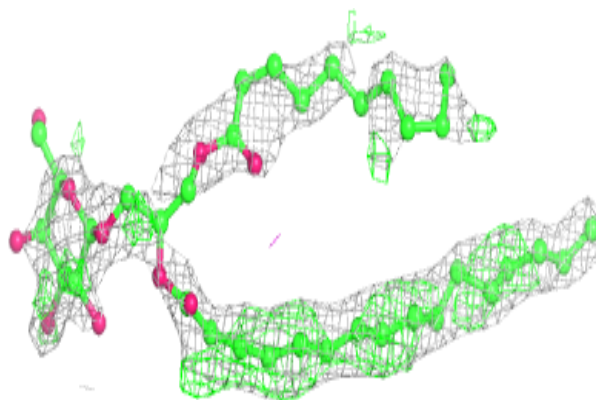
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG C 534:

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

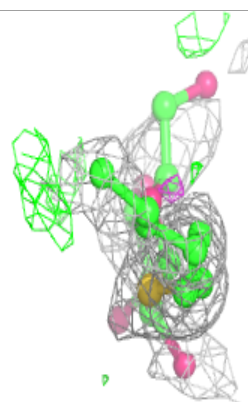
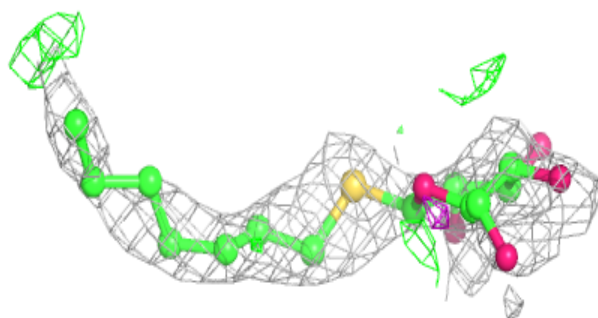
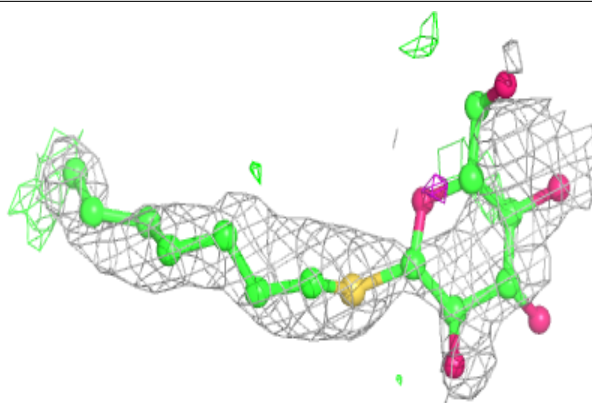
**Electron density around LMG C 524:**

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

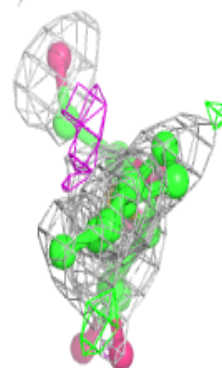
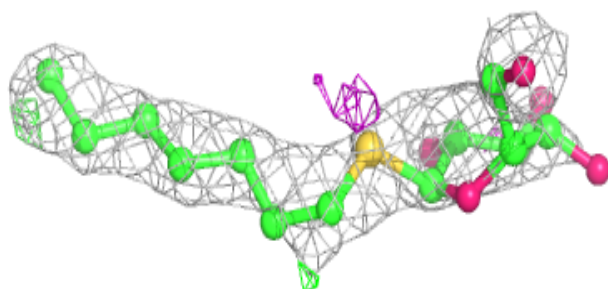
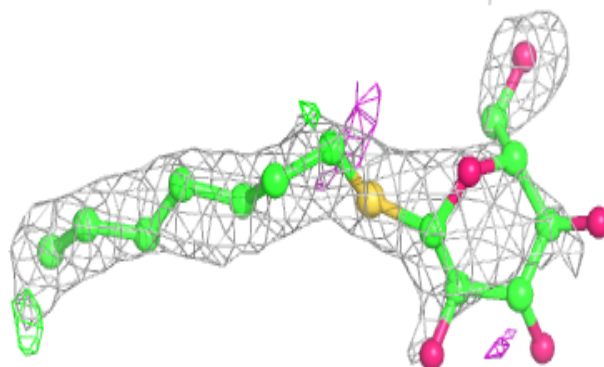


Electron density around HTG D 417:

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

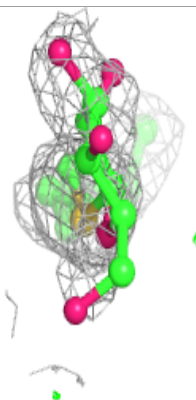
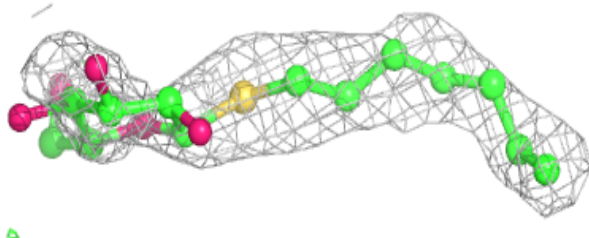
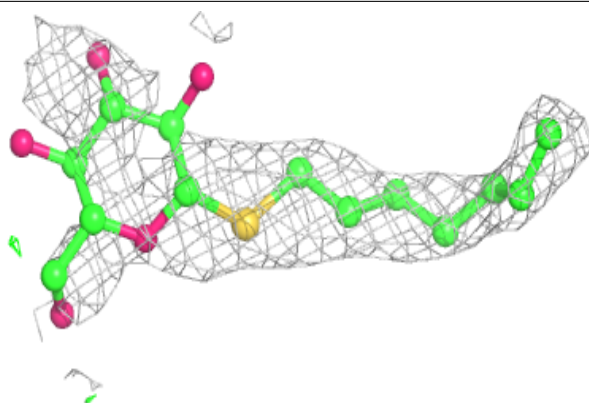
**Electron density around HTG c 521:**

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

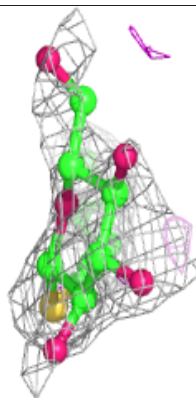
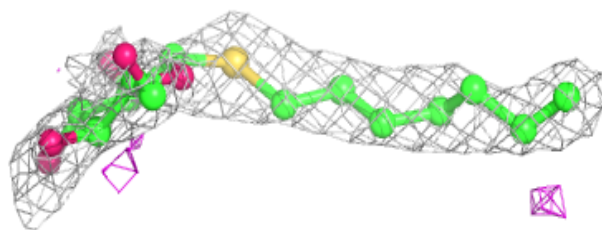
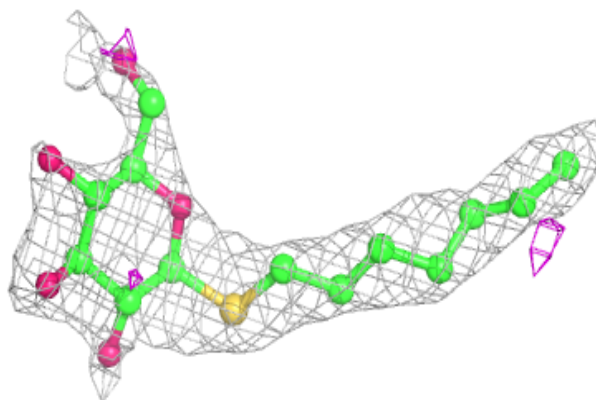


Electron density around HTG d 401:

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

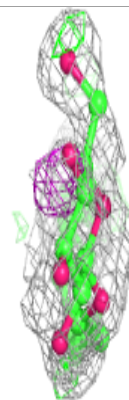
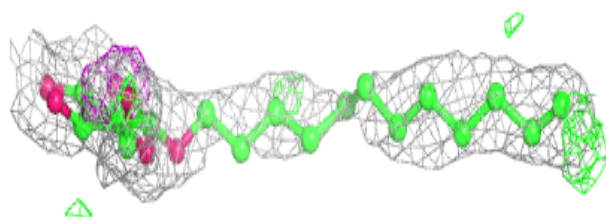
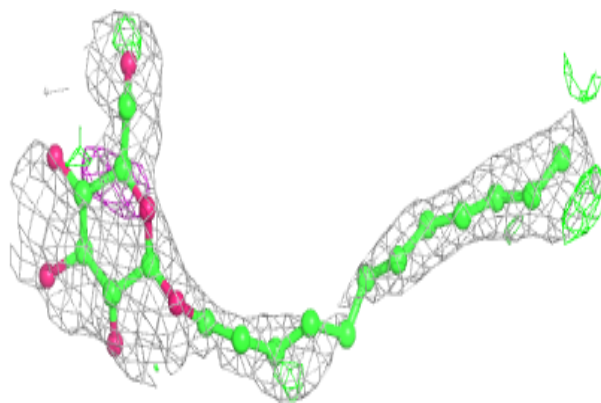
**Electron density around HTG B 623:**

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

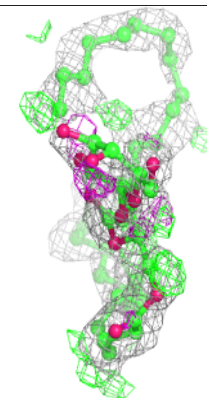
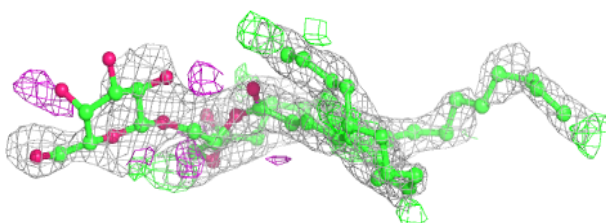
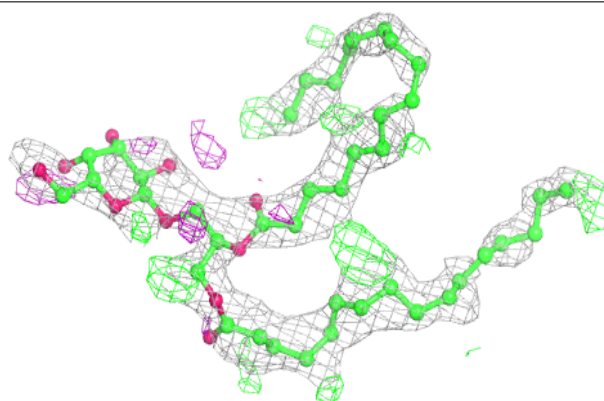


Electron density around LMT f 102:

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

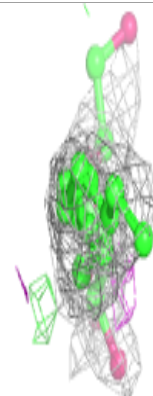
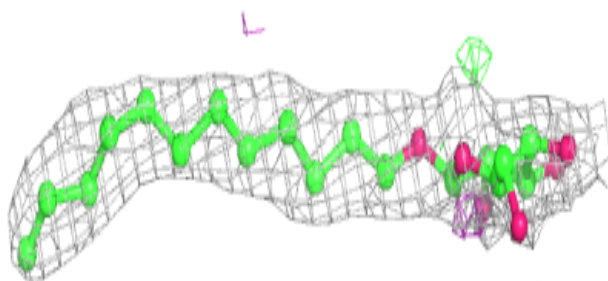
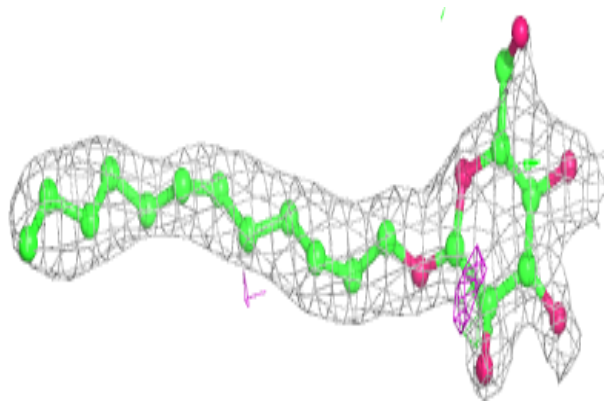
**Electron density around DGD D 406:**

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

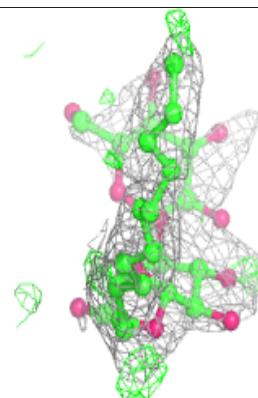
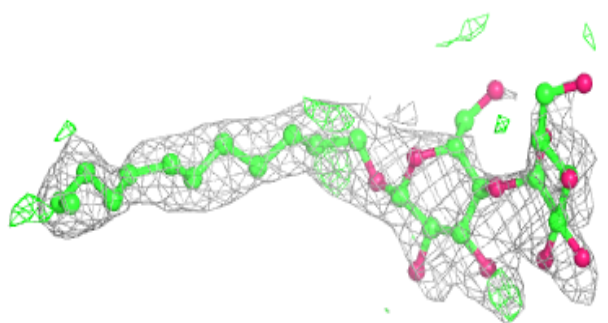
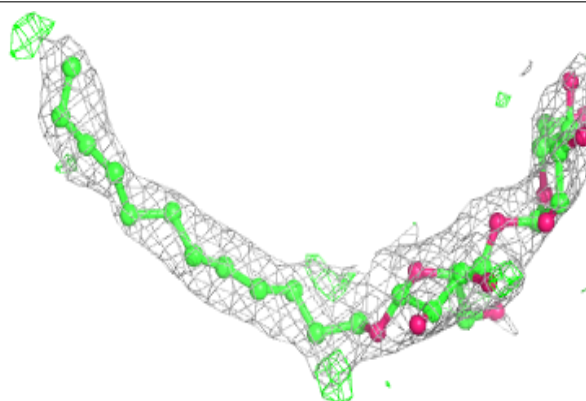


Electron density around LMT J 103:

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

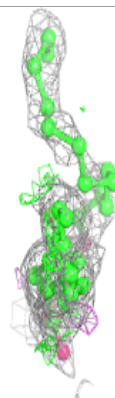
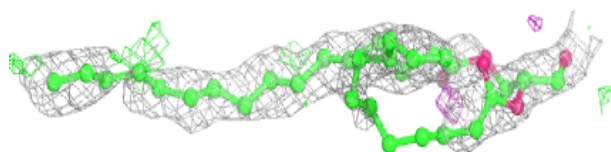
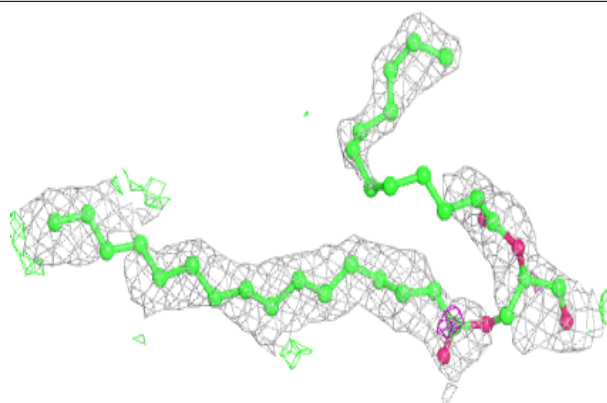
**Electron density around LMT m 101:**

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

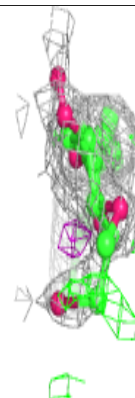
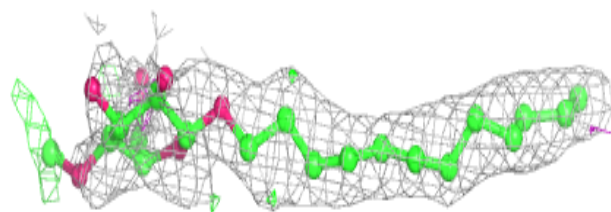
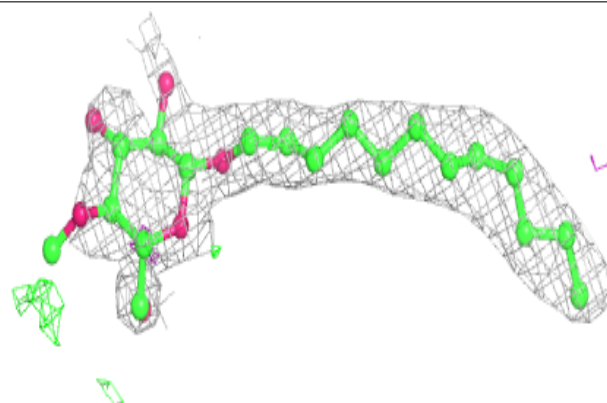


Electron density around UNL A 410:

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

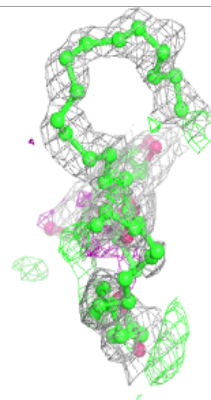
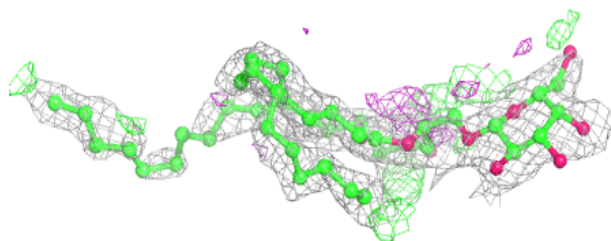
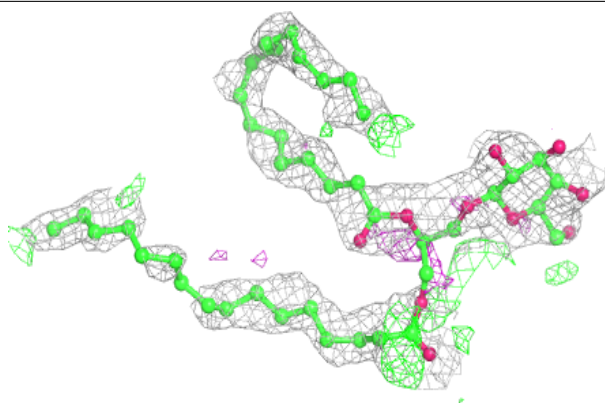
**Electron density around LMT b 628:**

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

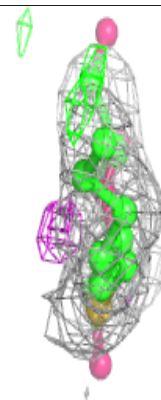
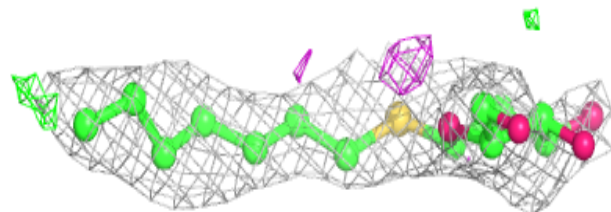
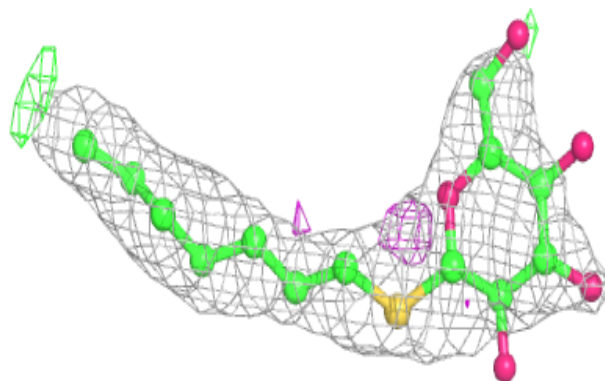


Electron density around DGD d 416:

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

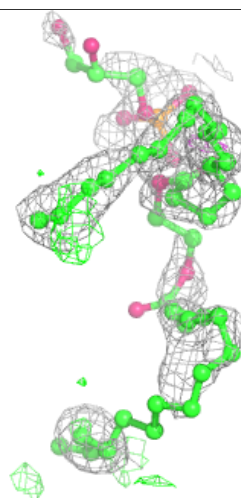
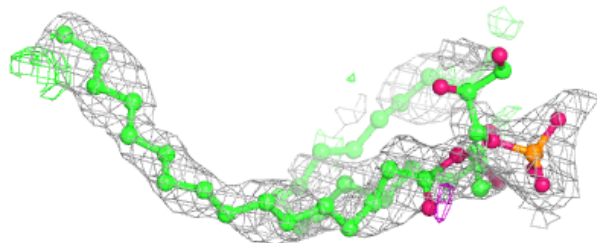
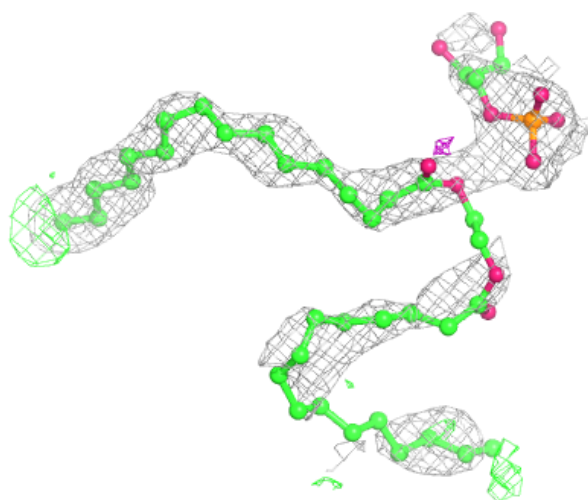
**Electron density around HTG B 632:**

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



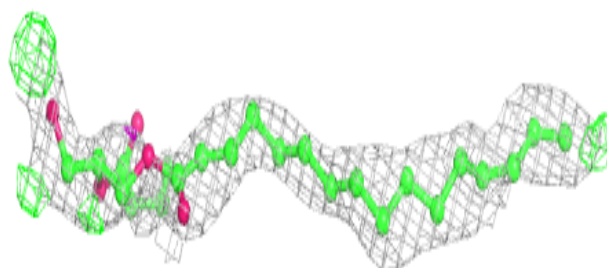
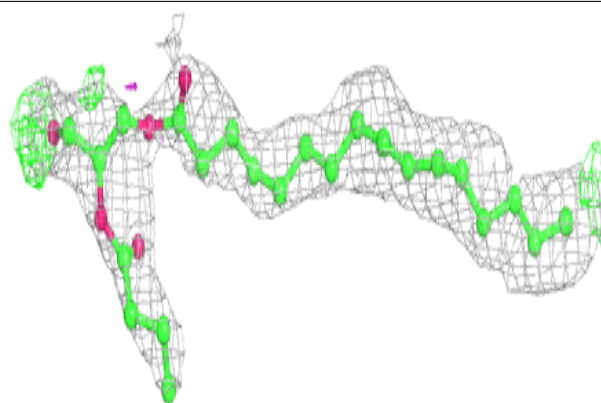
Electron density around LHG E 103:

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

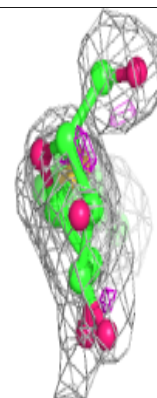
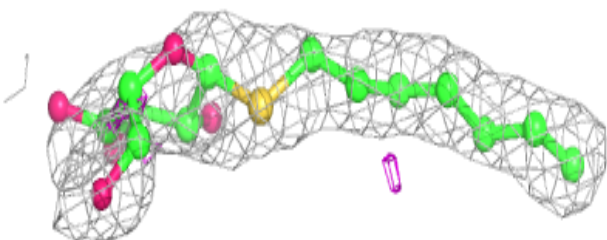
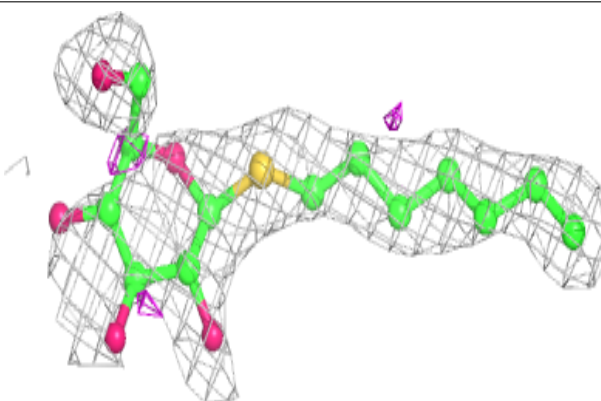


Electron density around UNL a 414:

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

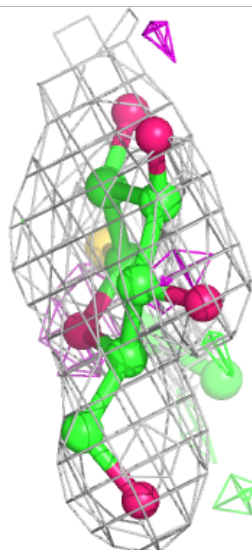
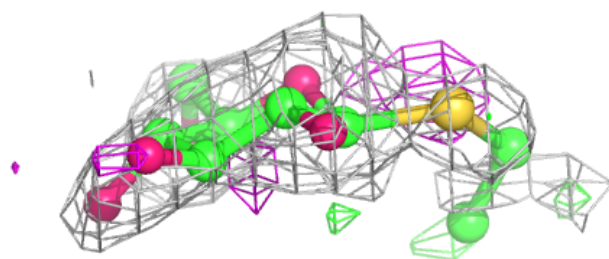
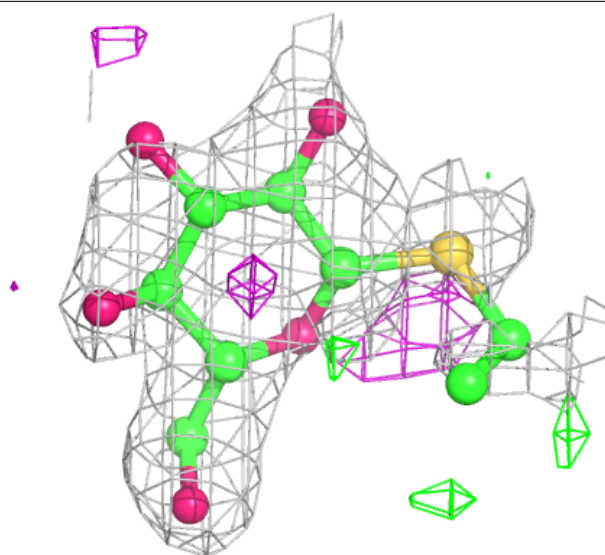
**Electron density around HTG C 521:**

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



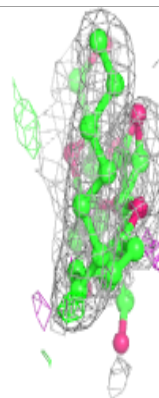
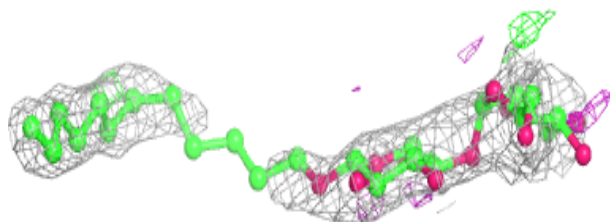
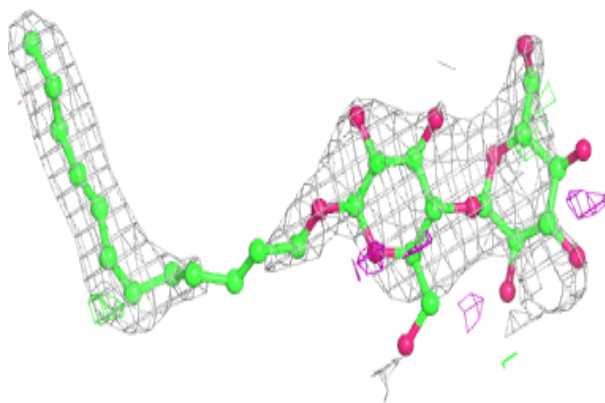
Electron density around HTG v 210:

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

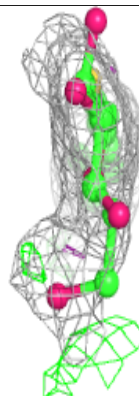
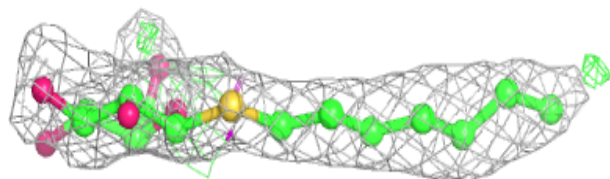
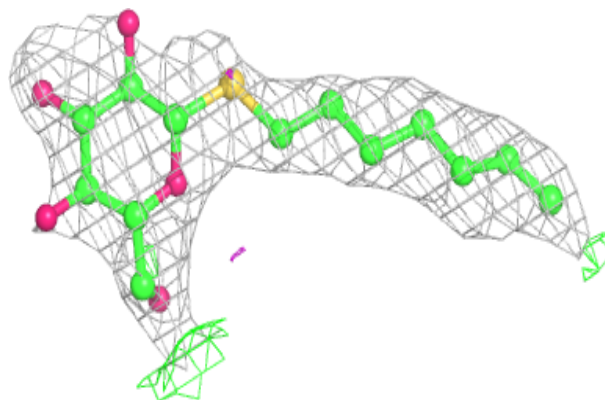


Electron density around LMT Z 101:

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

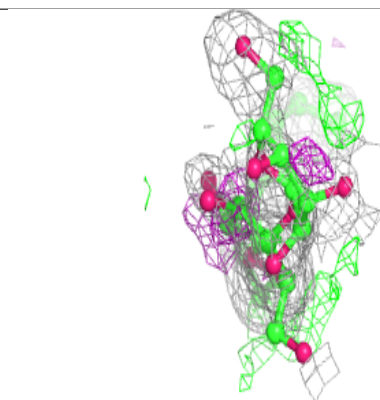
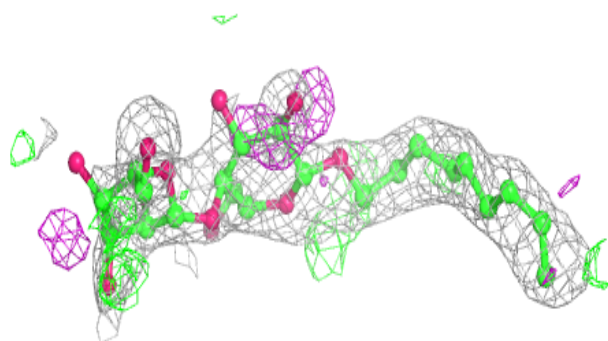
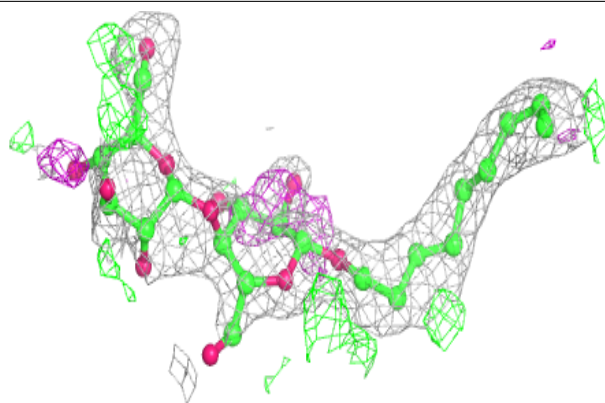
**Electron density around HTG b 602:**

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

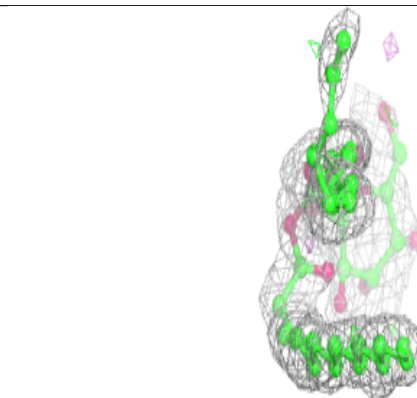
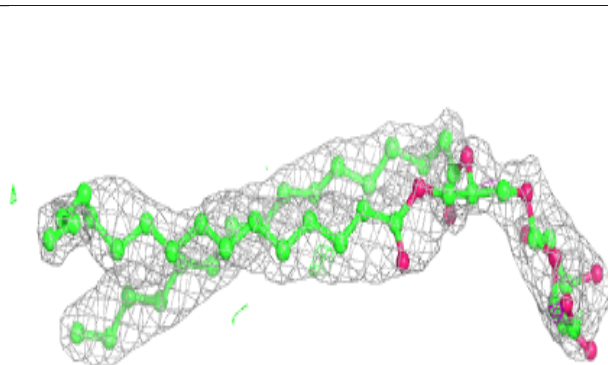
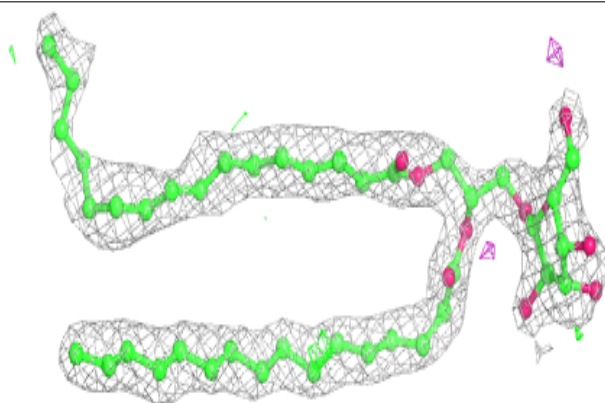


Electron density around LMT b 627:

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

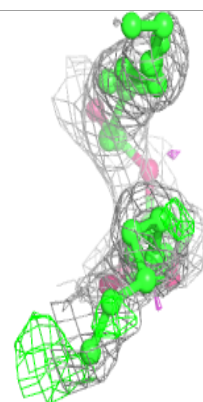
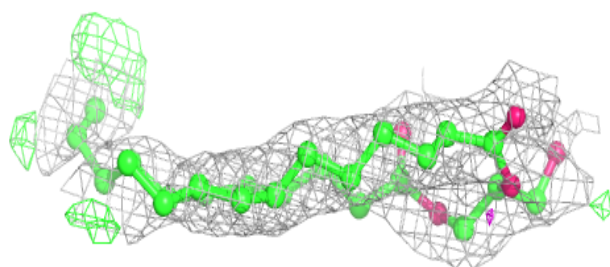
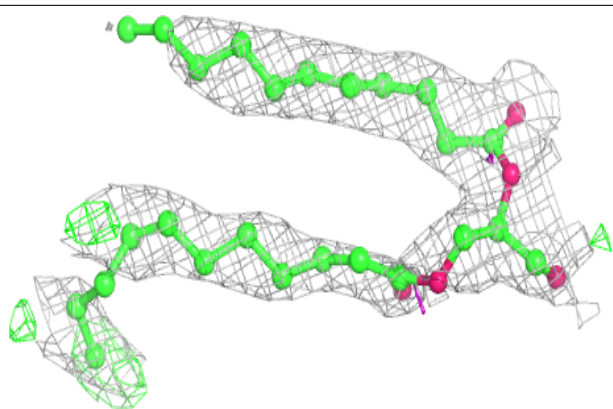
**Electron density around LMG c 518:**

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

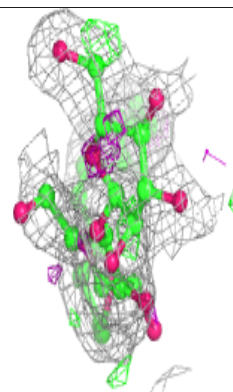
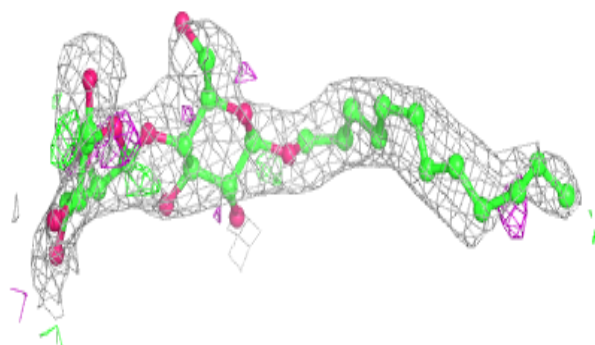
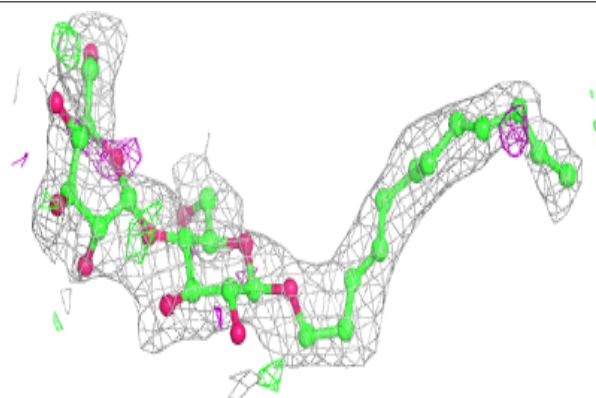


Electron density around UNL c 524:

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

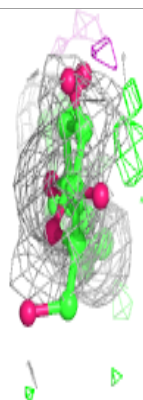
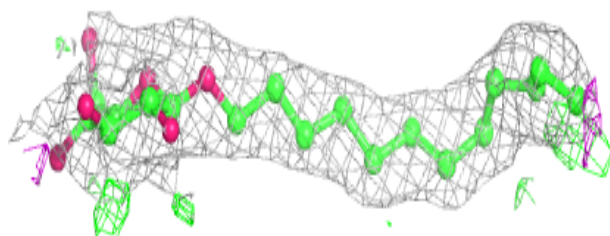
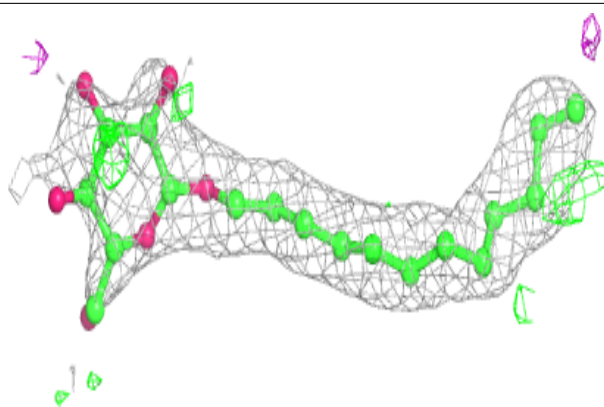
**Electron density around LMT a 418:**

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

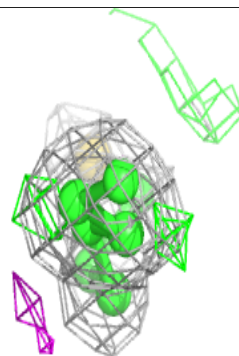
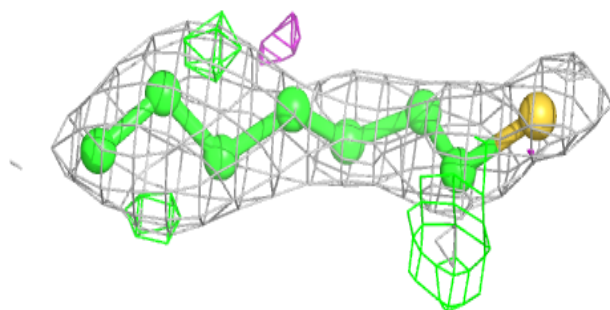
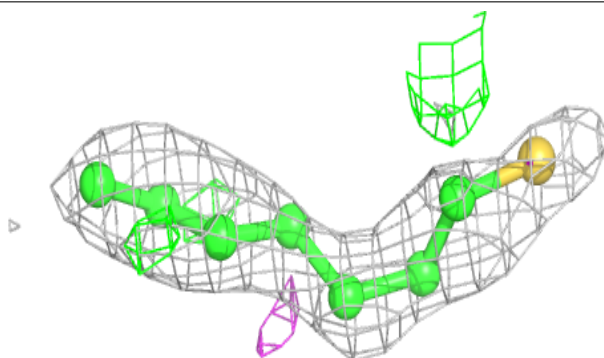


Electron density around LMT B 626:

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

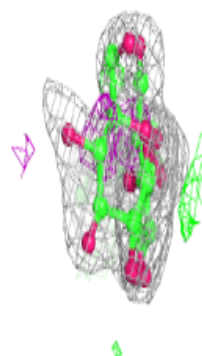
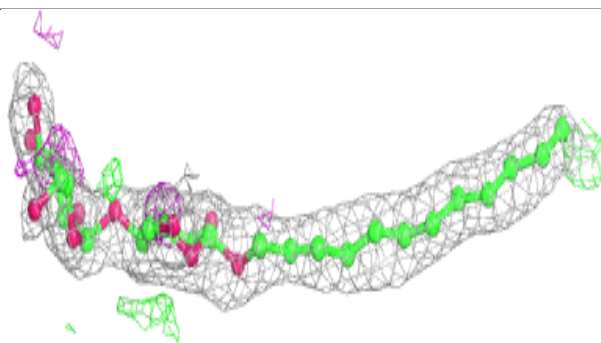
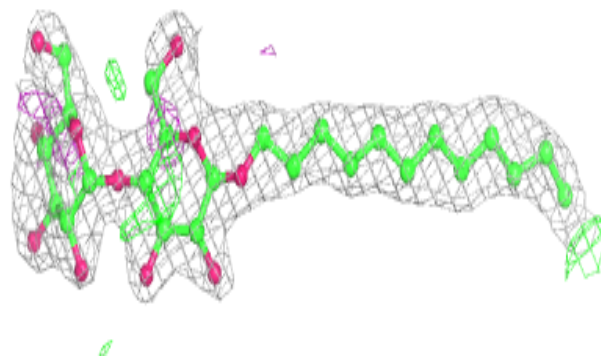
**Electron density around HTG u 201:**

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

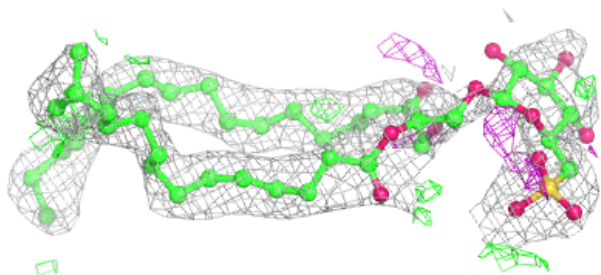
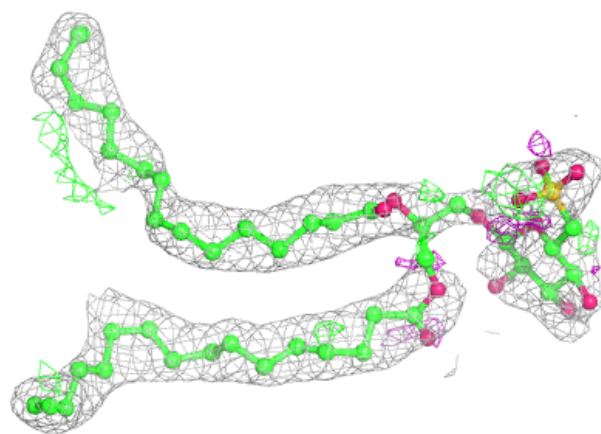


Electron density around LMT m 102:

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

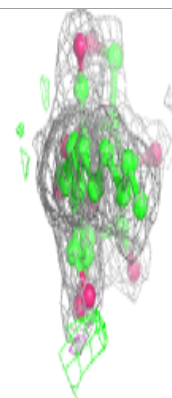
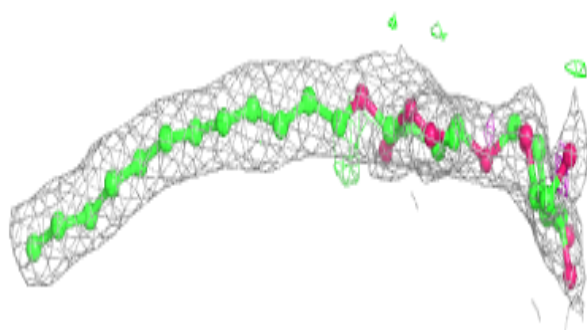
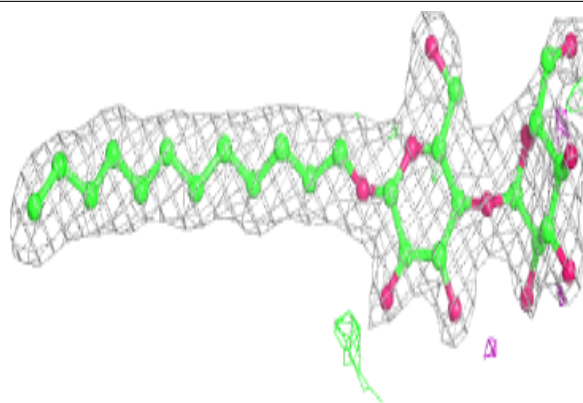
**Electron density around SQD l 101:**

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

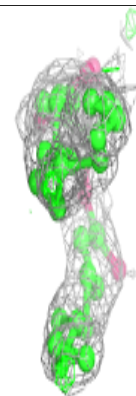
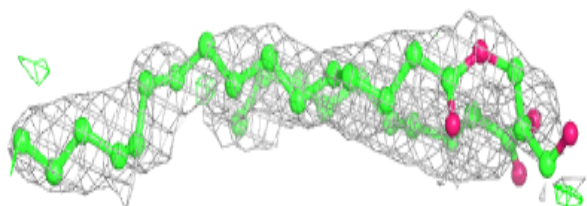
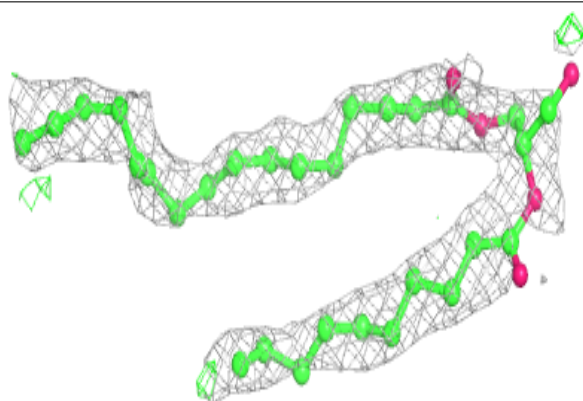


Electron density around LMT M 101:

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

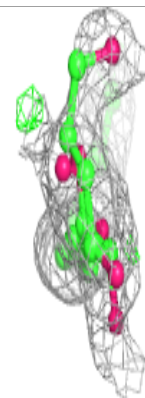
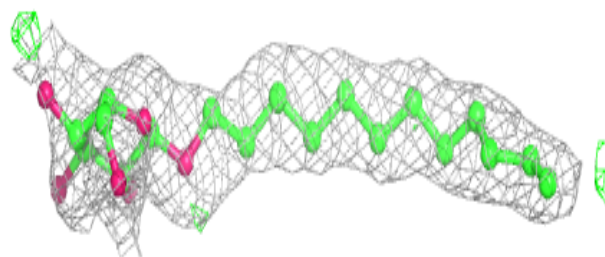
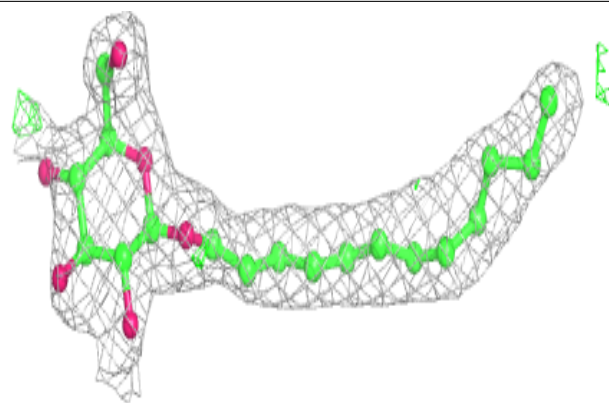
**Electron density around UNL C 523:**

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

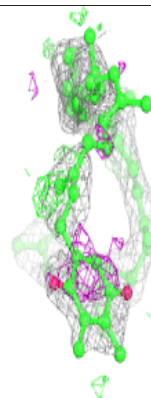
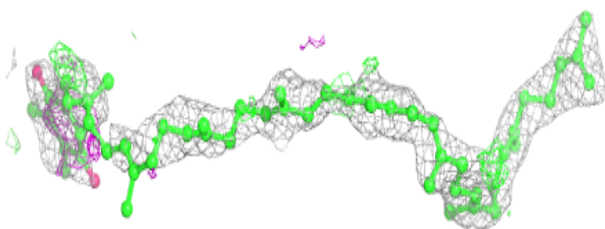
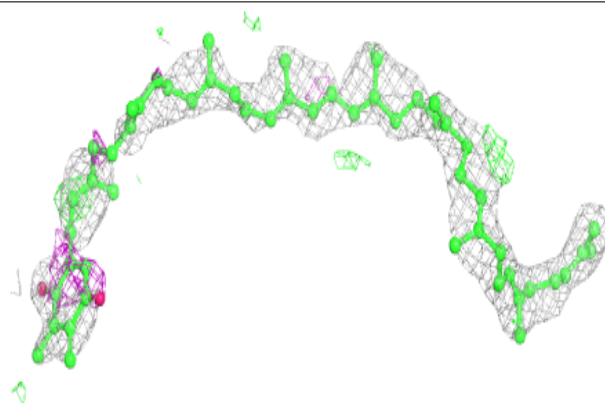


Electron density around LMT B 625:

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

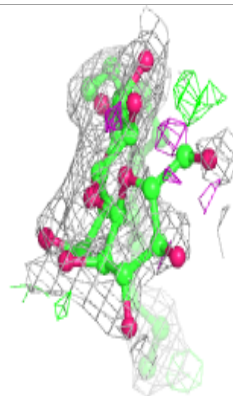
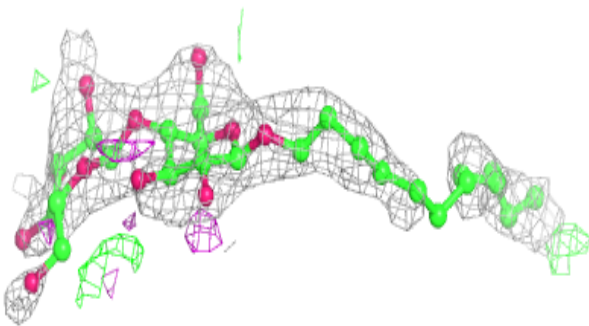
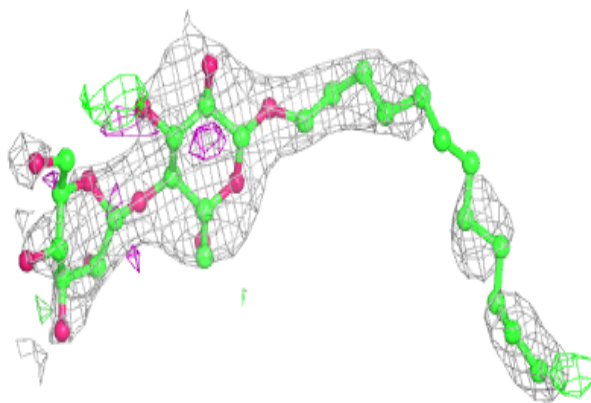
**Electron density around PL9 a 415:**

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

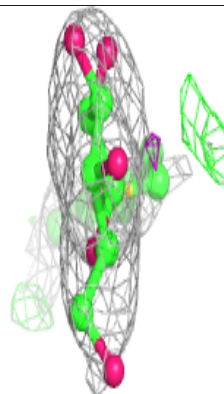
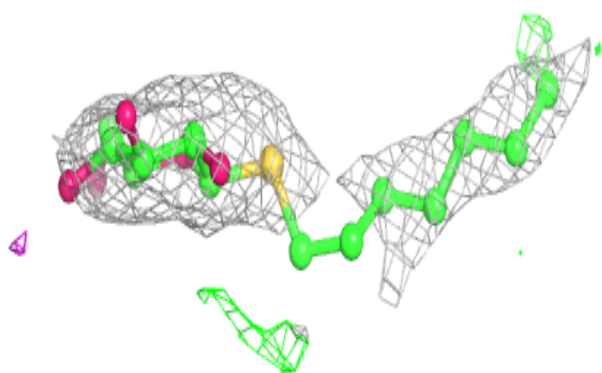
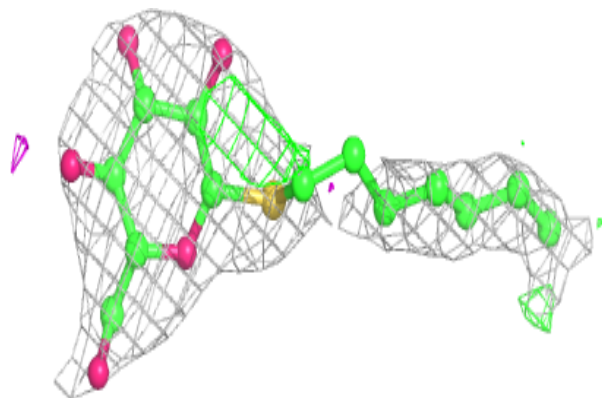


Electron density around LMT I 101:

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

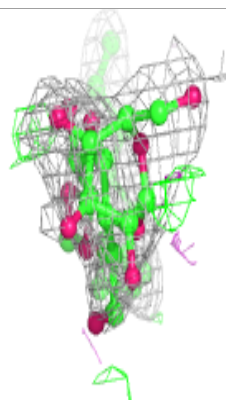
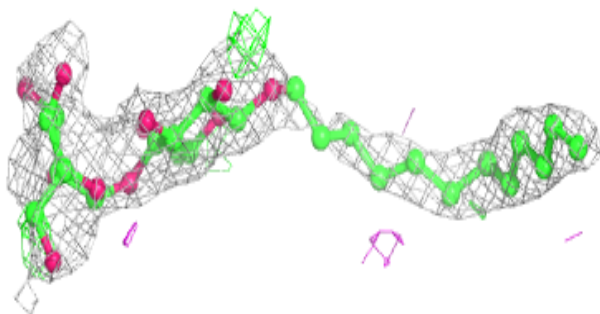
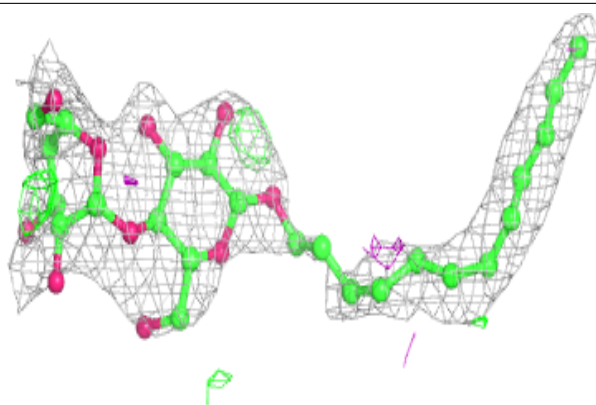
**Electron density around HTG c 520:**

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

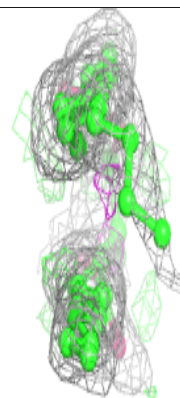
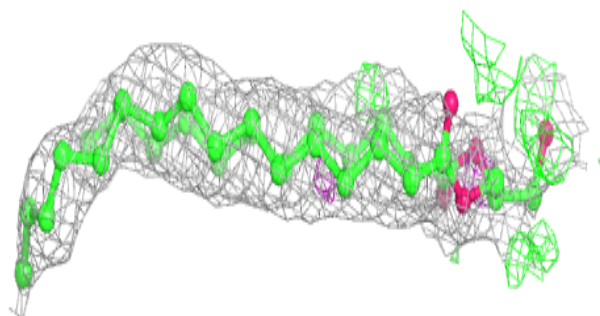
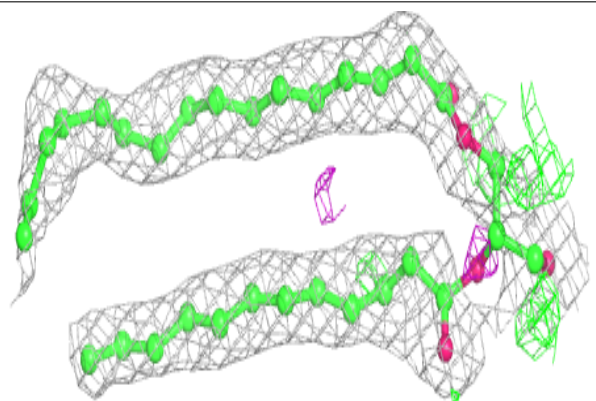


Electron density around LMT z 102:

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

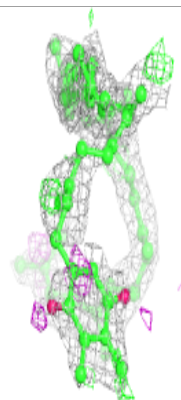
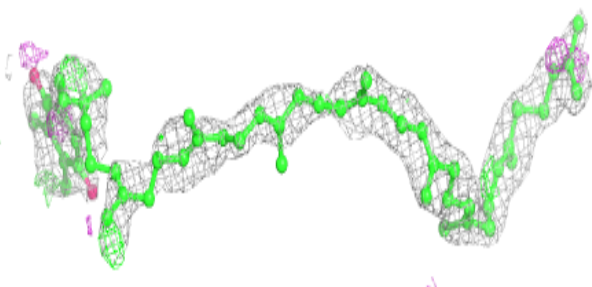
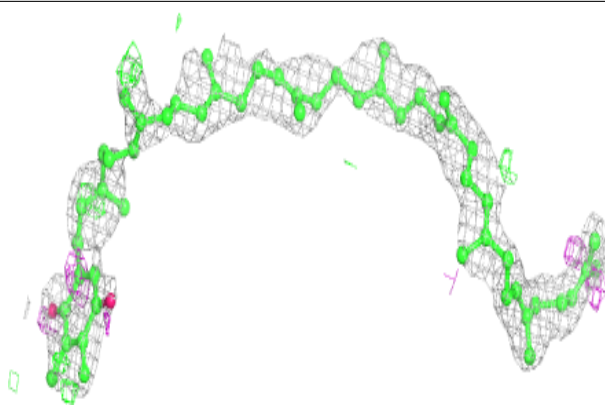
**Electron density around UNL d 409:**

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

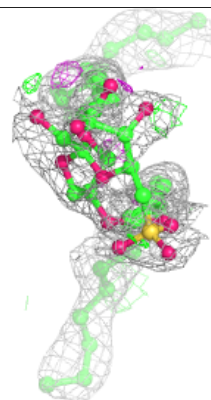
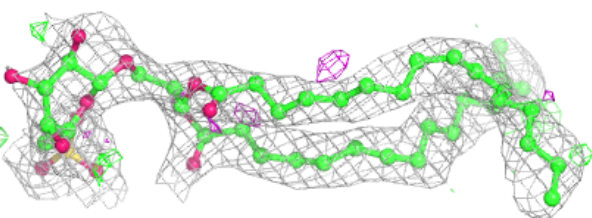
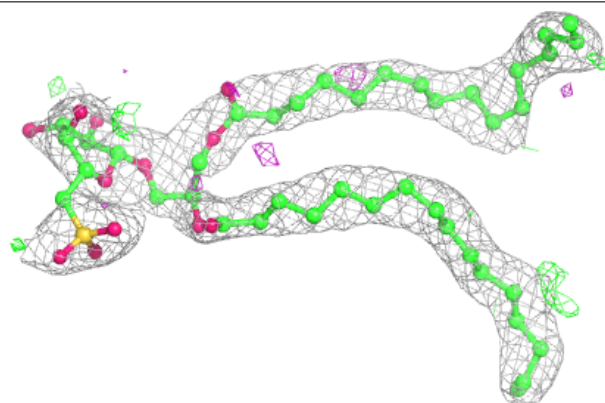


Electron density around PL9 A 411:

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

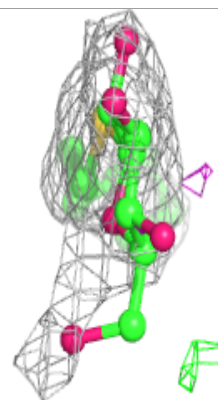
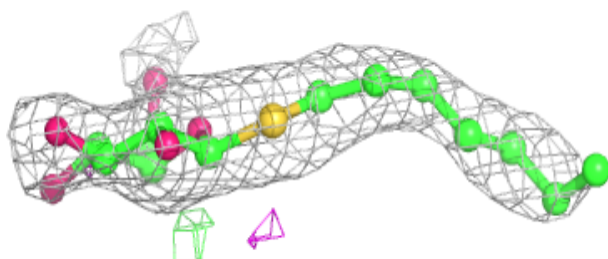
**Electron density around SQD b 622:**

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

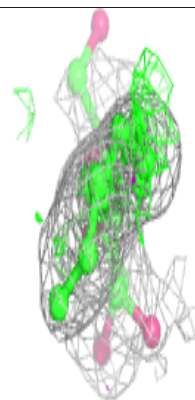
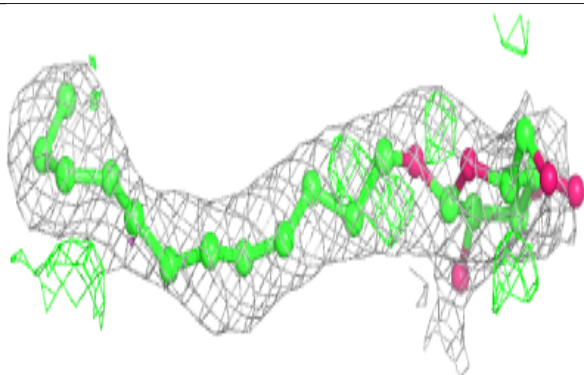
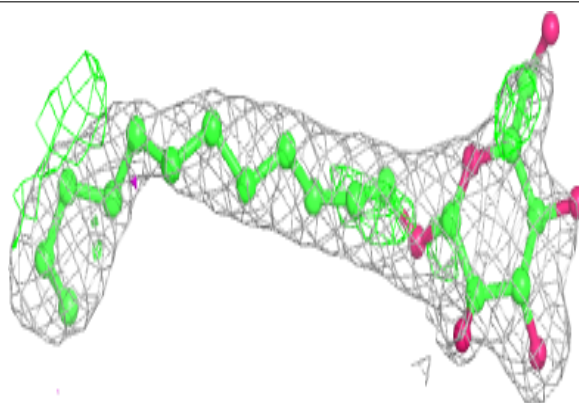


Electron density around HTG C 522:

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

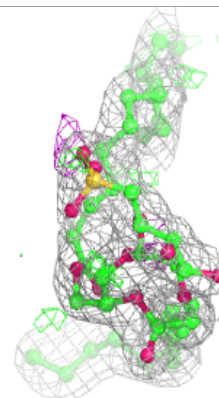
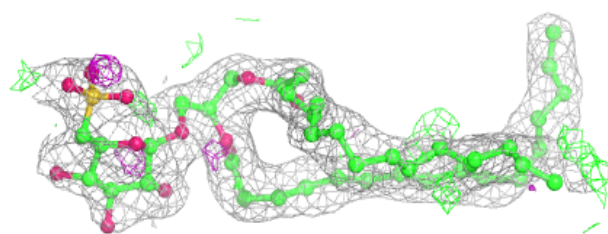
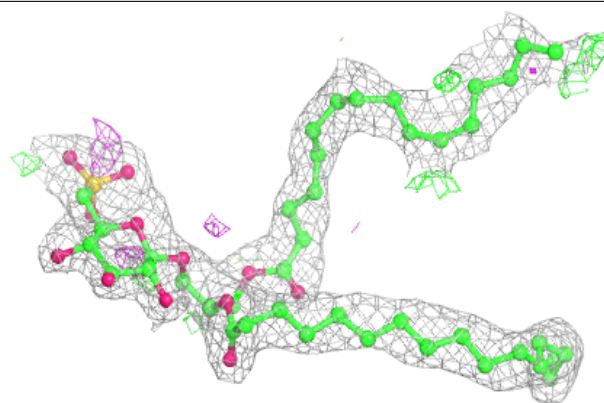
**Electron density around LMT T 102:**

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

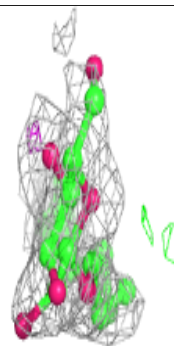
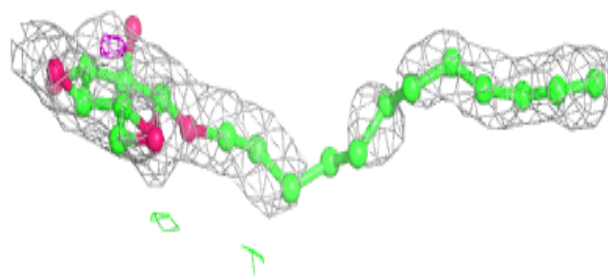
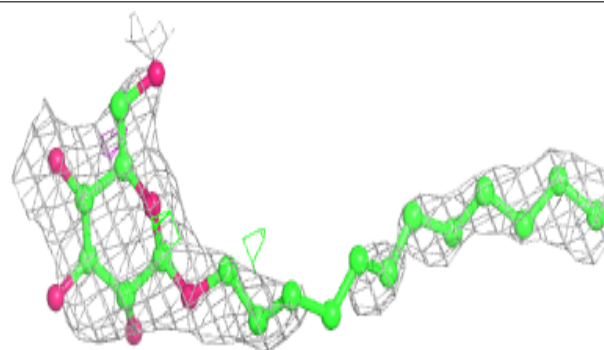


Electron density around SQD a 401:

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

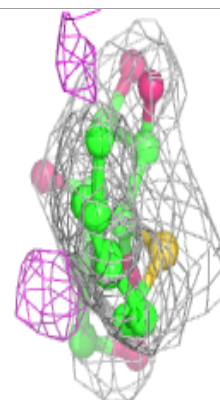
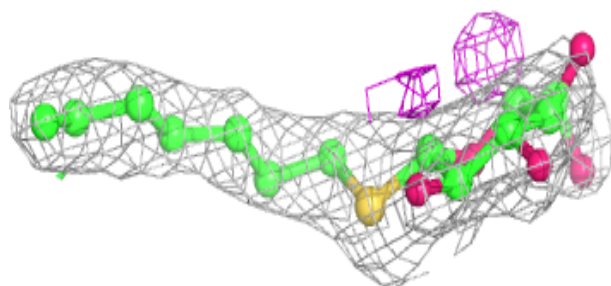
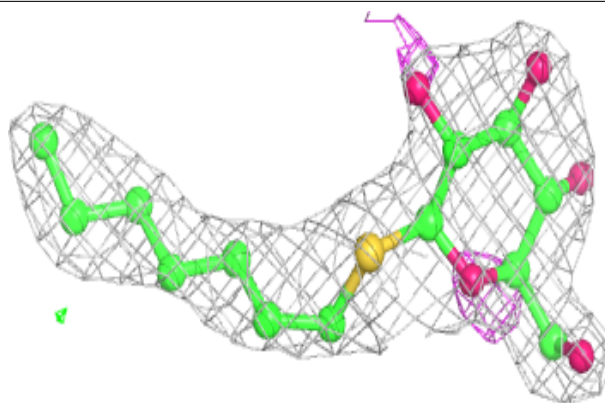
**Electron density around LMT E 101:**

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

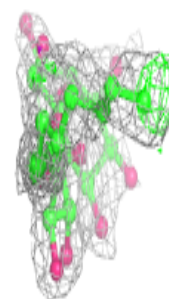
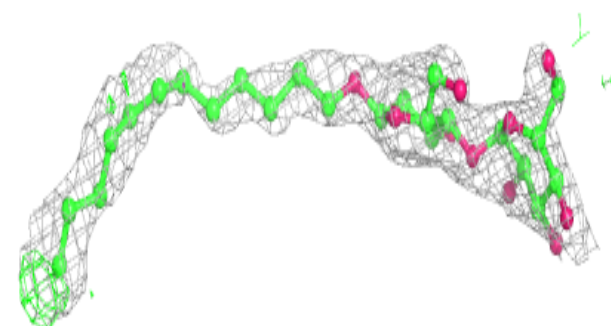
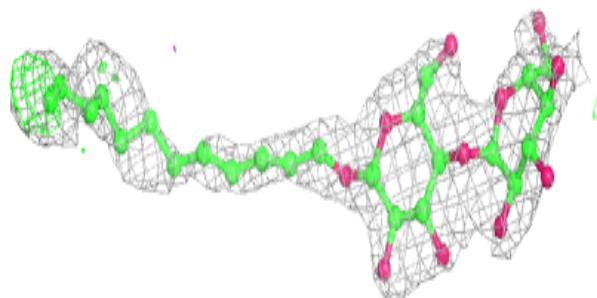


Electron density around HTG b 624:

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

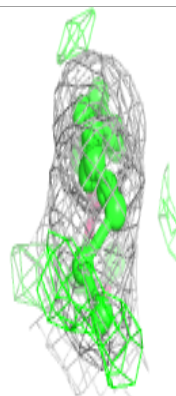
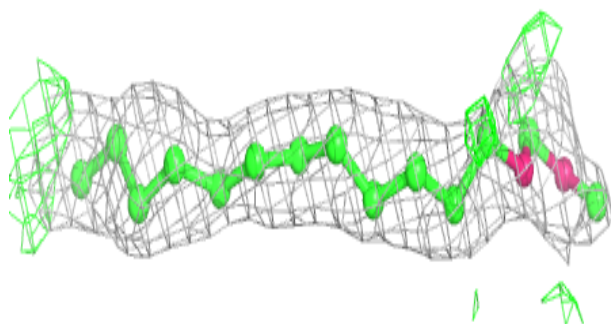
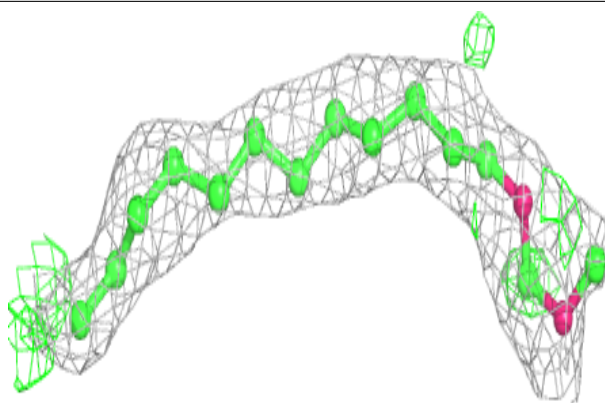
**Electron density around LMT c 523:**

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

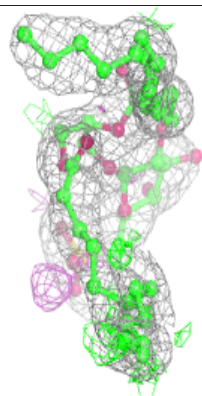
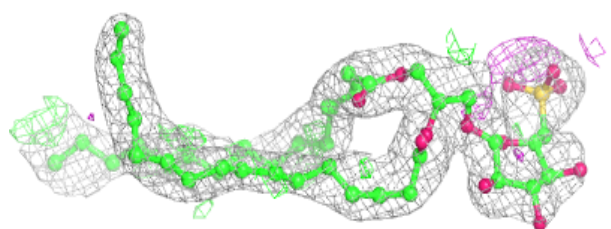
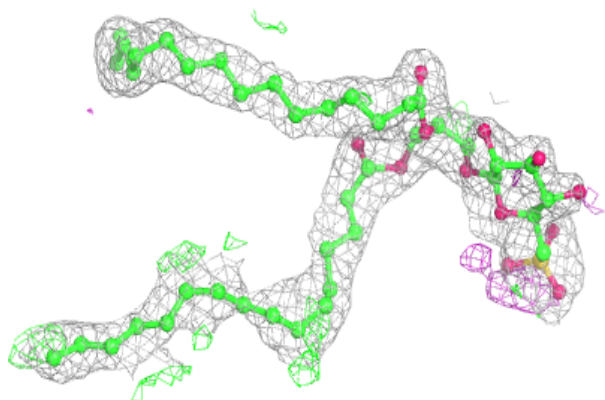


Electron density around LMT B 627:

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

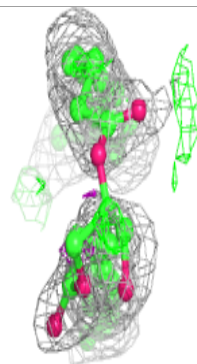
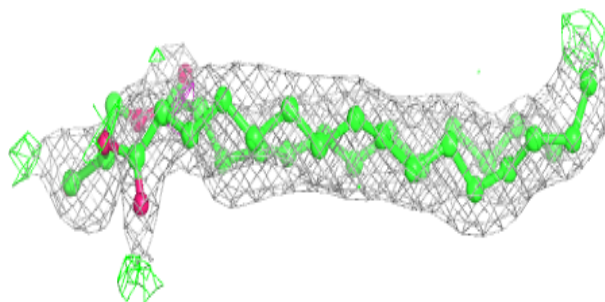
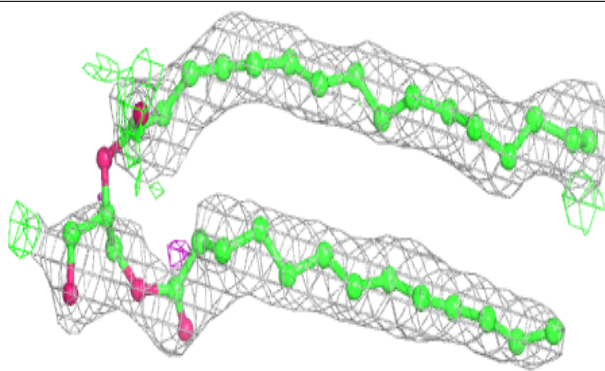
**Electron density around SQD A 412:**

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

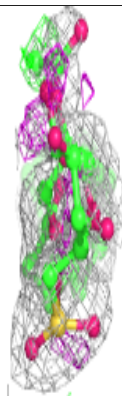
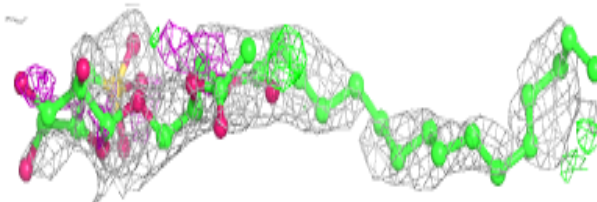
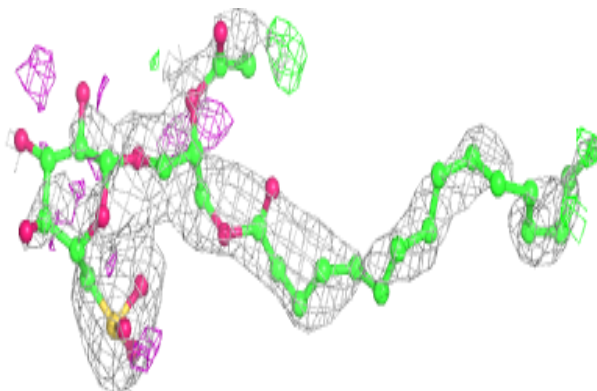


Electron density around UNL D 410:

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

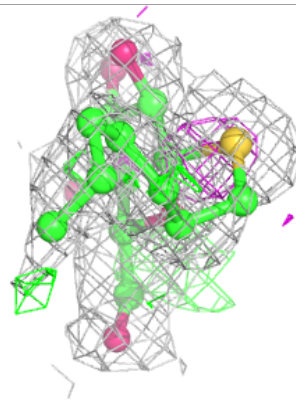
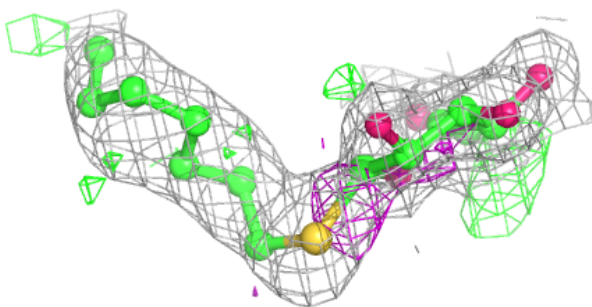
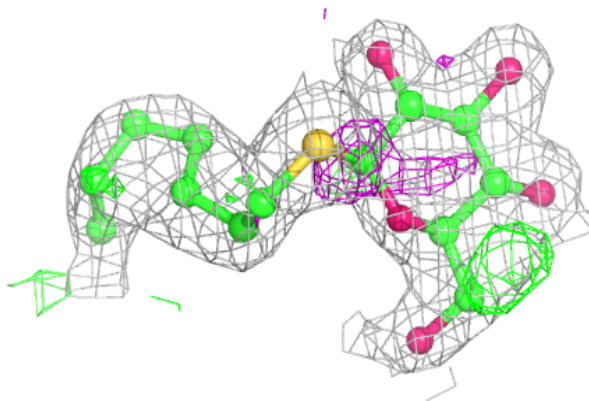
**Electron density around SQD f 101:**

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

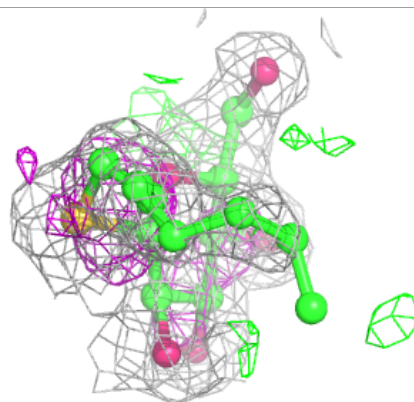
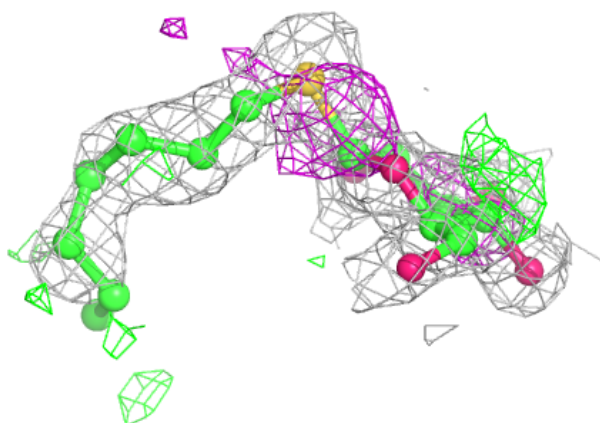
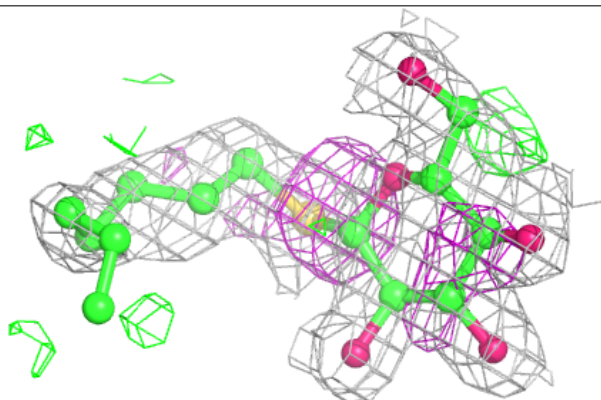


Electron density around HTG B 622:

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

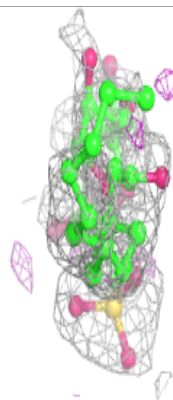
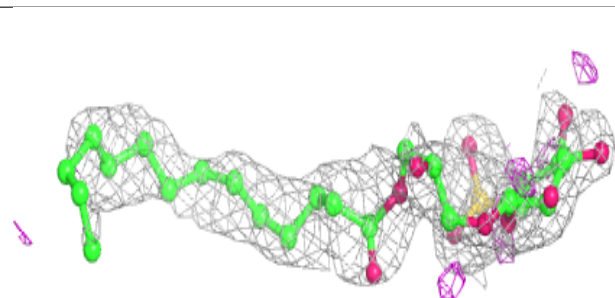
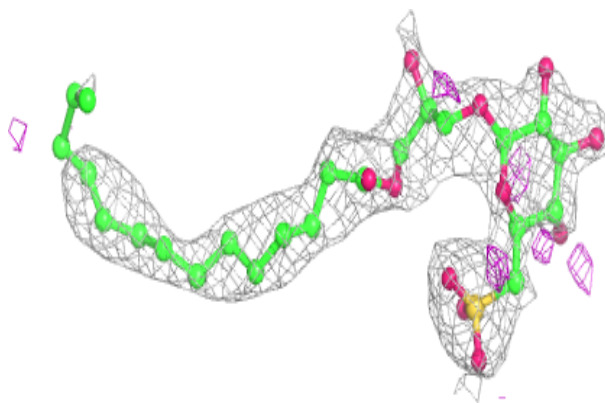
**Electron density around HTG b 625:**

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



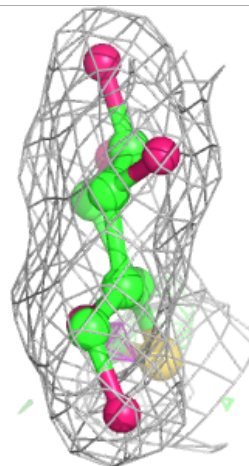
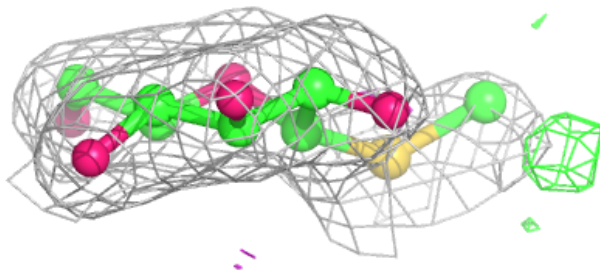
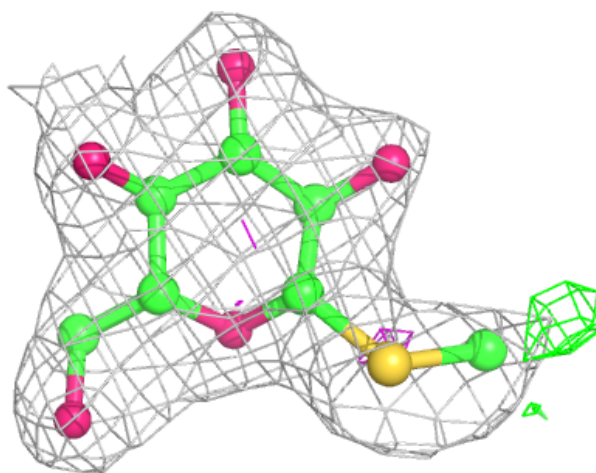
Electron density around SQD F 101:

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



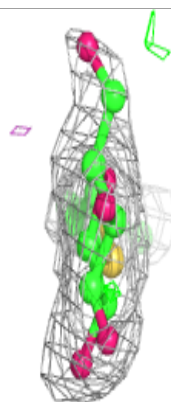
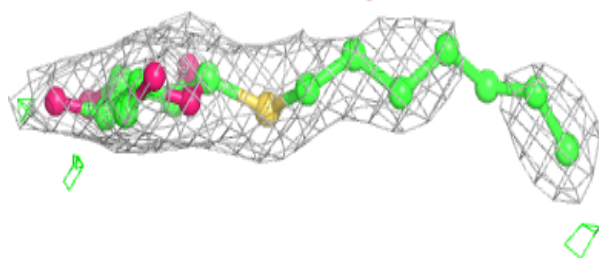
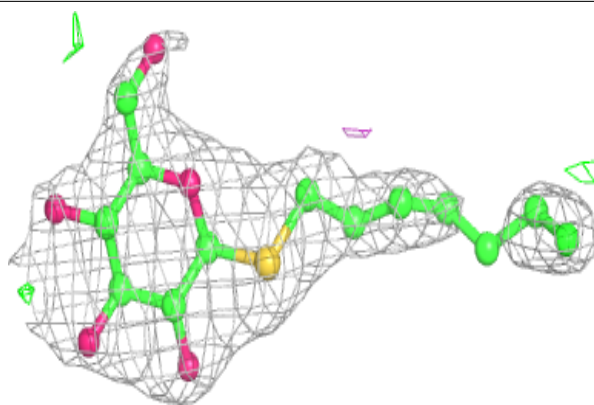
Electron density around HTG V 202:

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

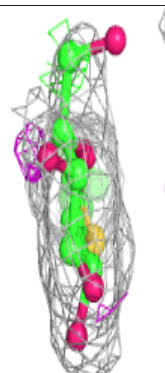
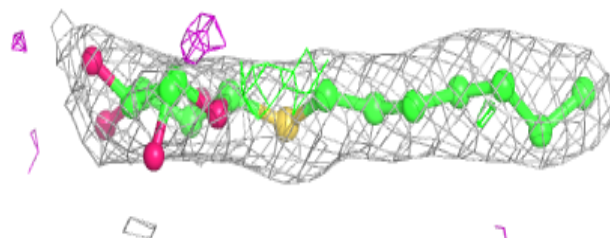
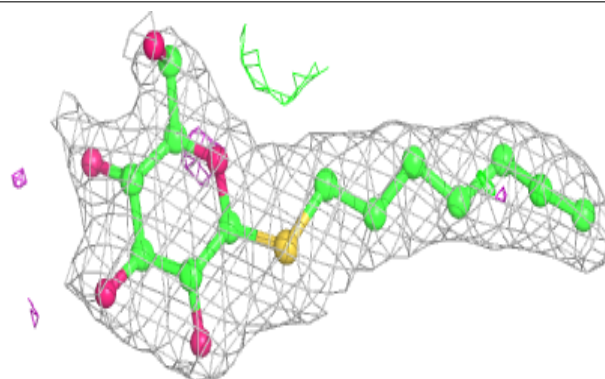


Electron density around HTG C 520:

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

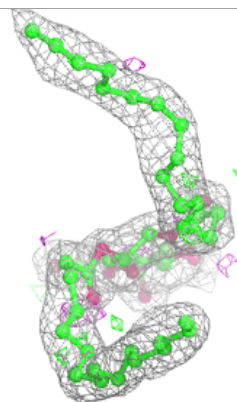
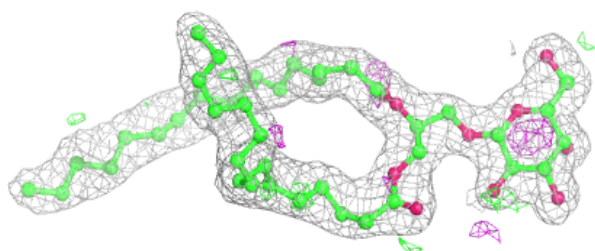
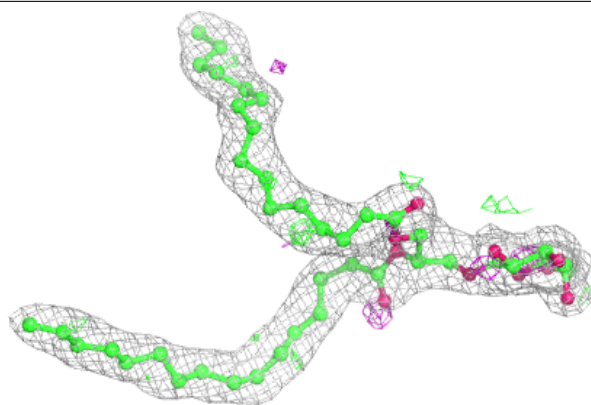
**Electron density around HTG b 601:**

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

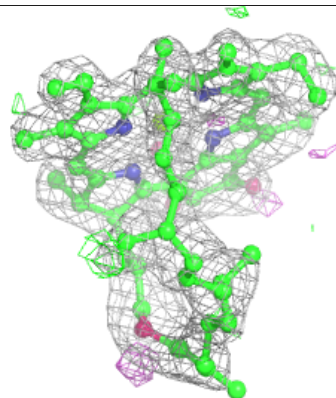
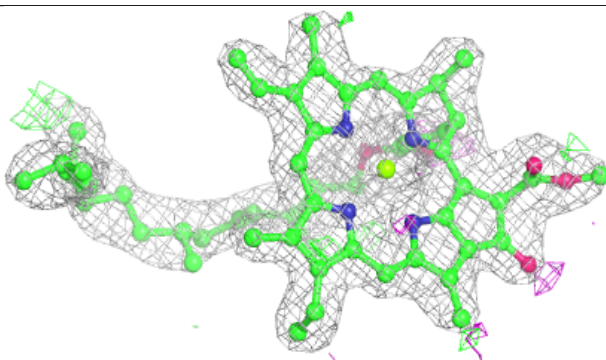
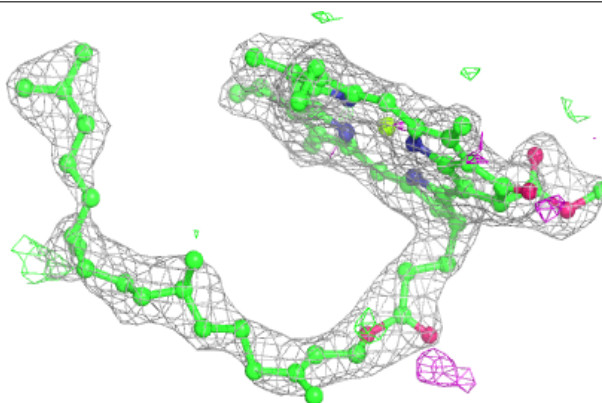


Electron density around LMG B 620:

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

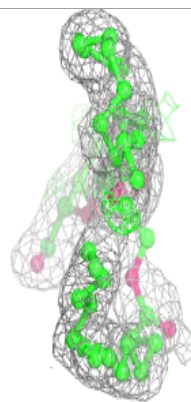
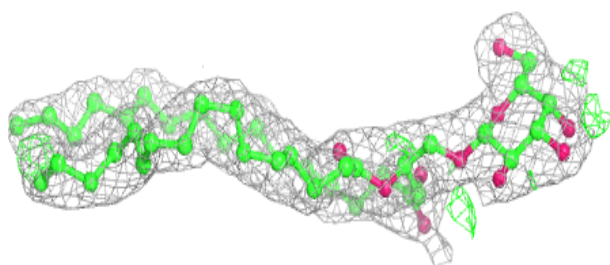
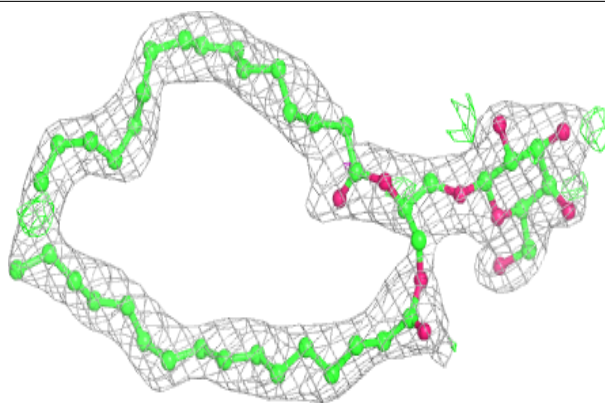
**Electron density around CLA C 513:**

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

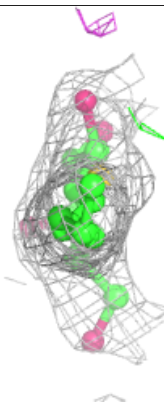
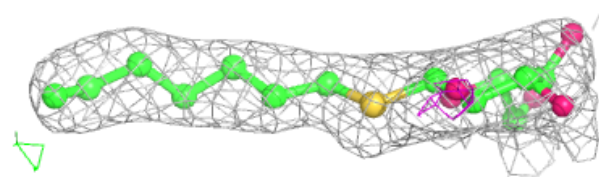
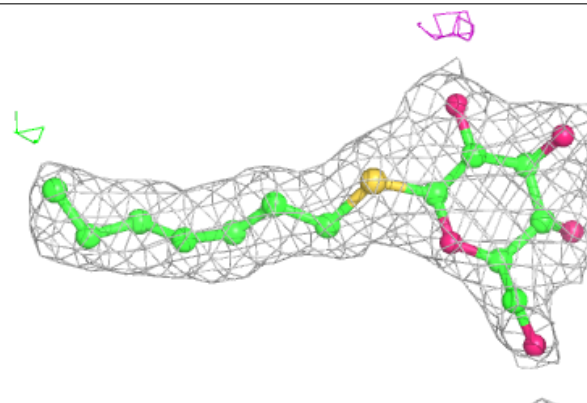


Electron density around LMG A 407:

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

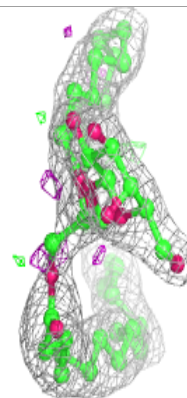
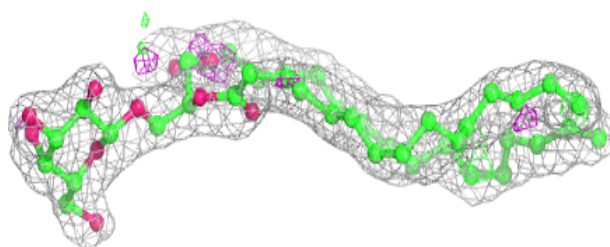
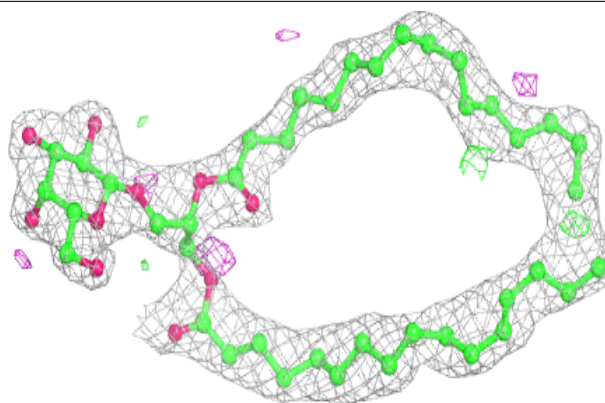
**Electron density around HTG B 631:**

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

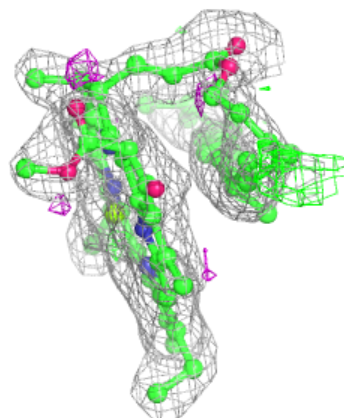
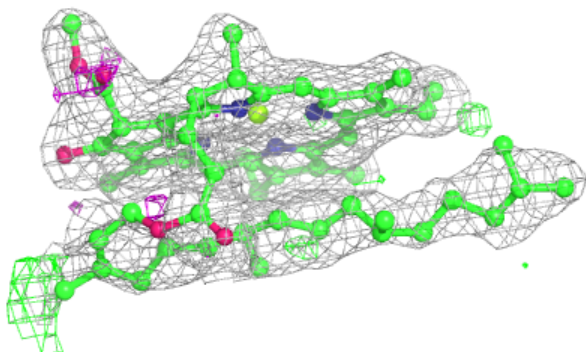
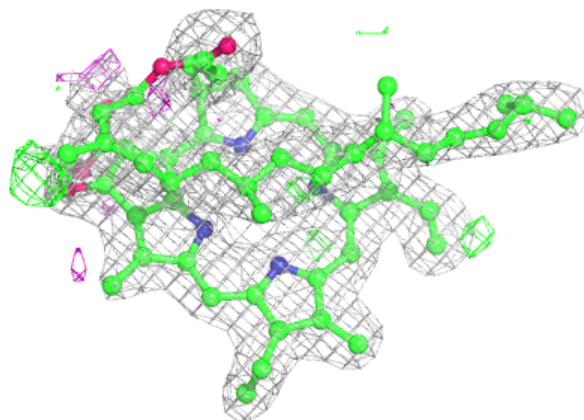


Electron density around LMG a 410:

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

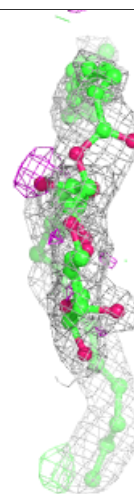
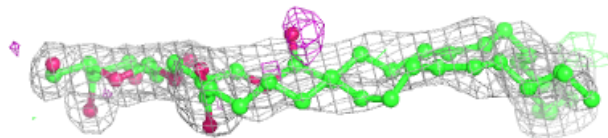
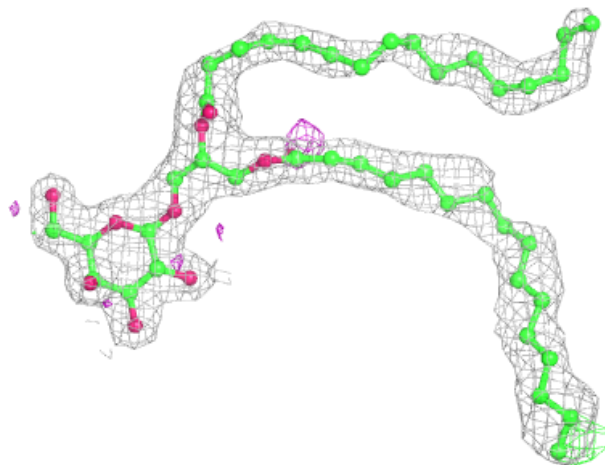
**Electron density around CLA B 602:**

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



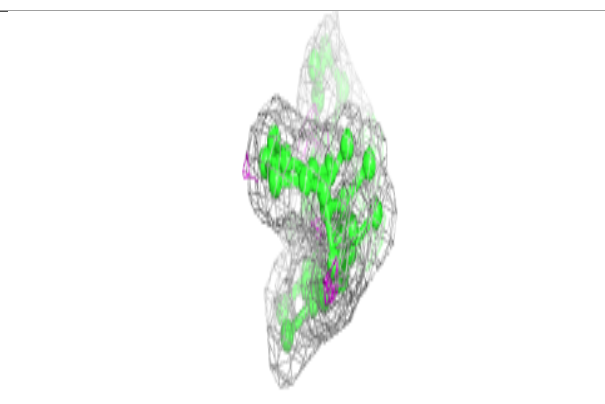
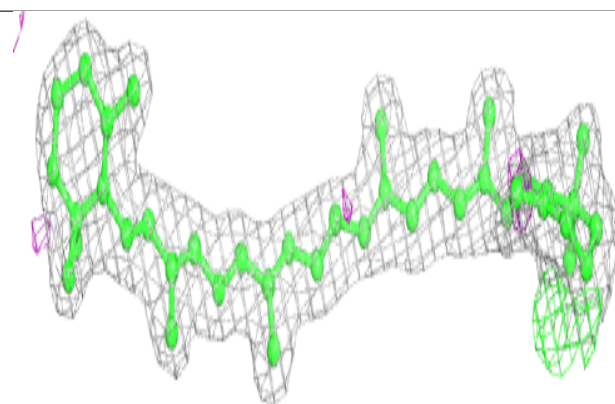
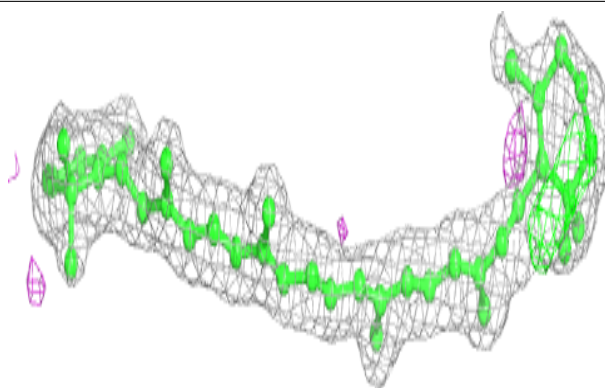
Electron density around LMG C 519:

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

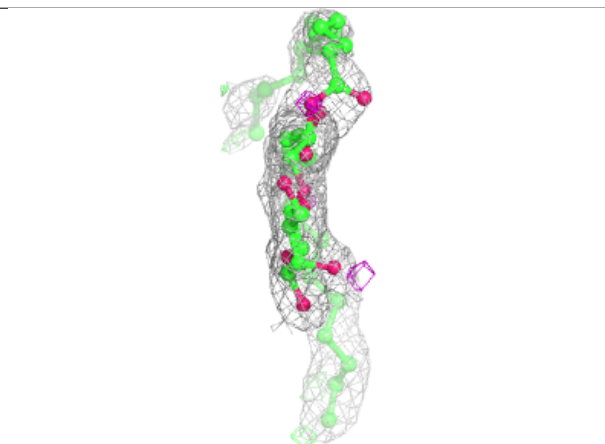
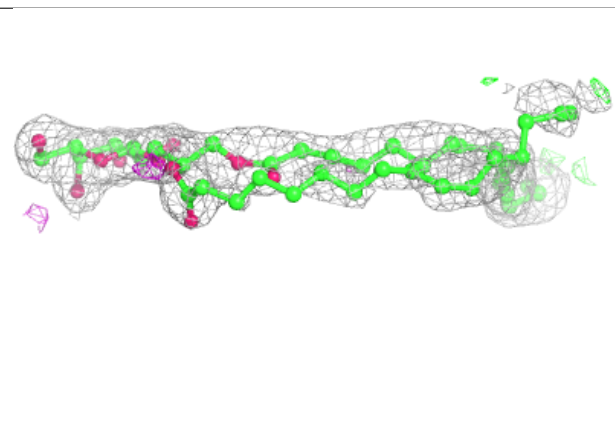
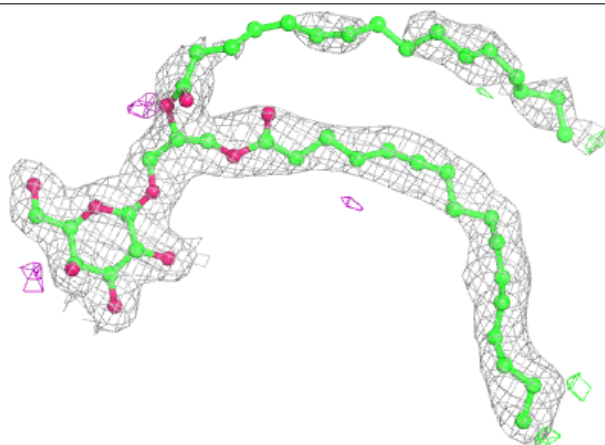


Electron density around BCR d 405:

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

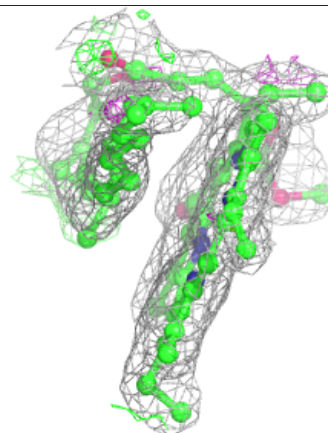
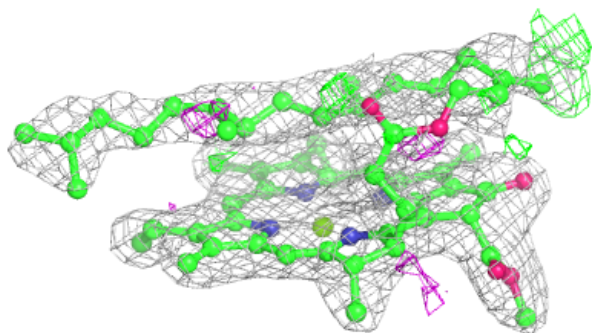
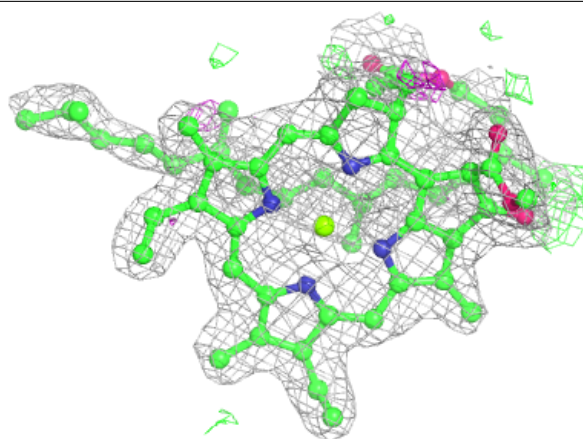
**Electron density around LMG c 519:**

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

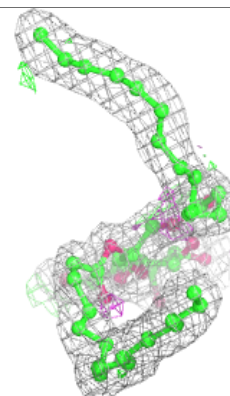
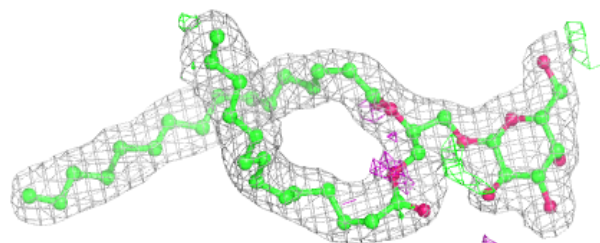
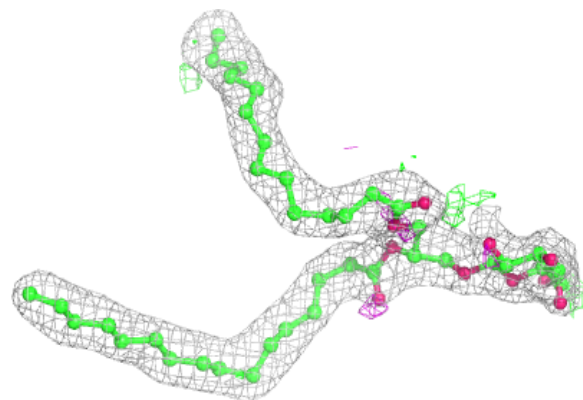


Electron density around CLA b 603:

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

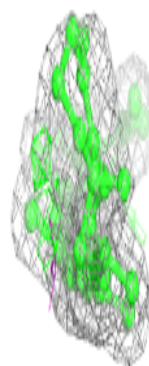
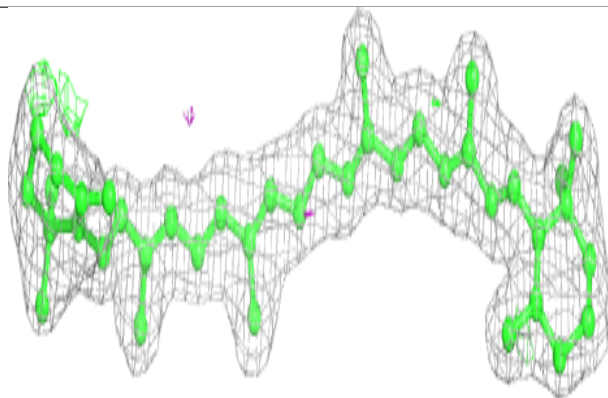
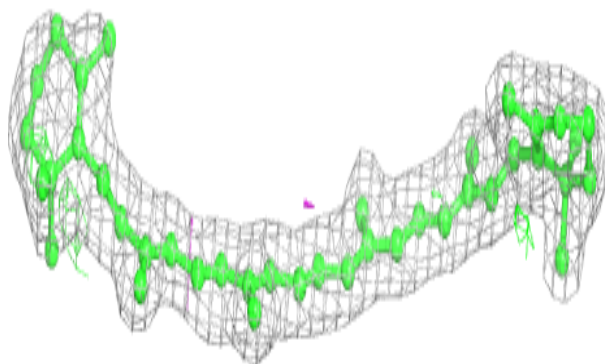
**Electron density around LMG b 623:**

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

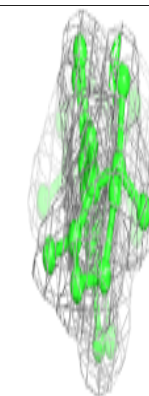
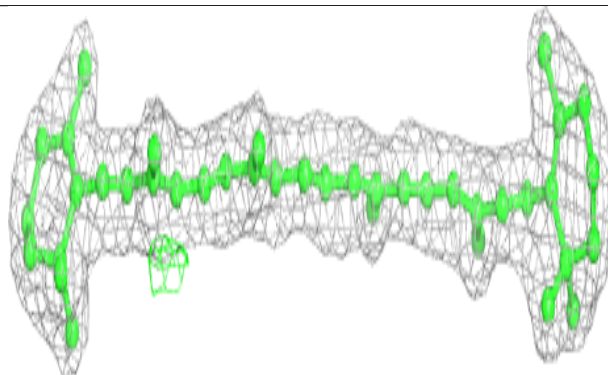
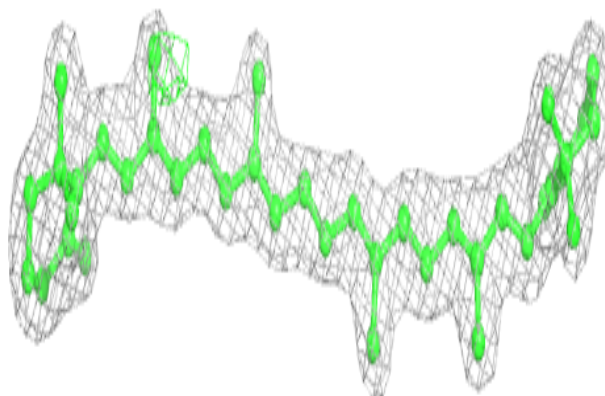


Electron density around BCR D 405:

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

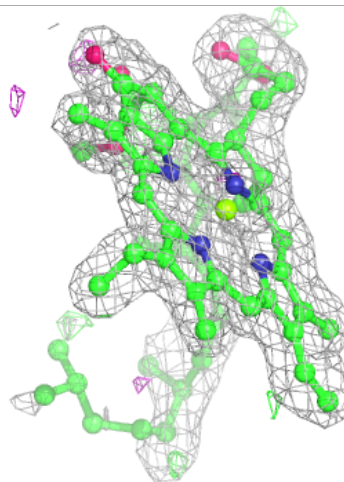
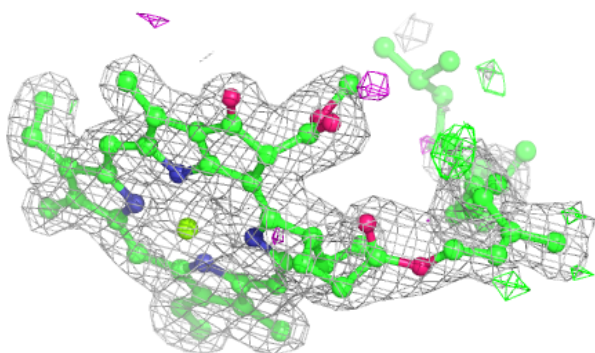
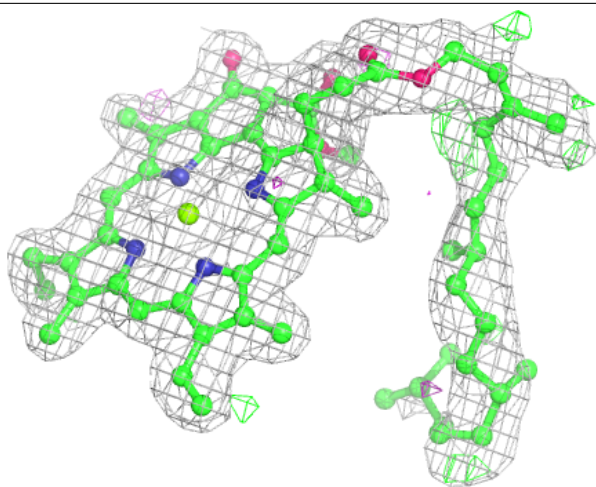
**Electron density around BCR C 514:**

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



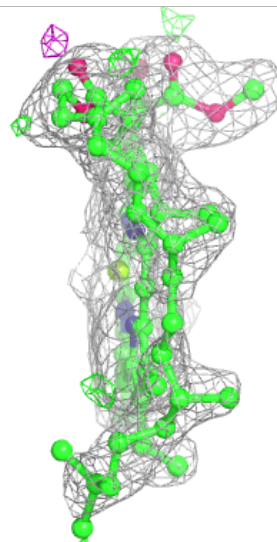
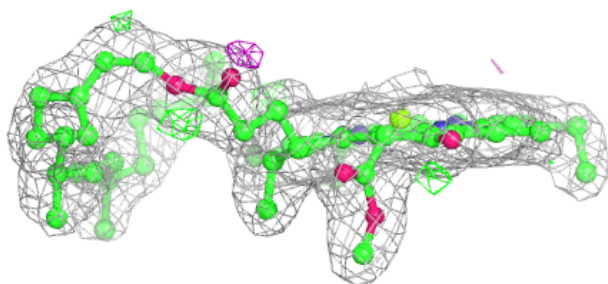
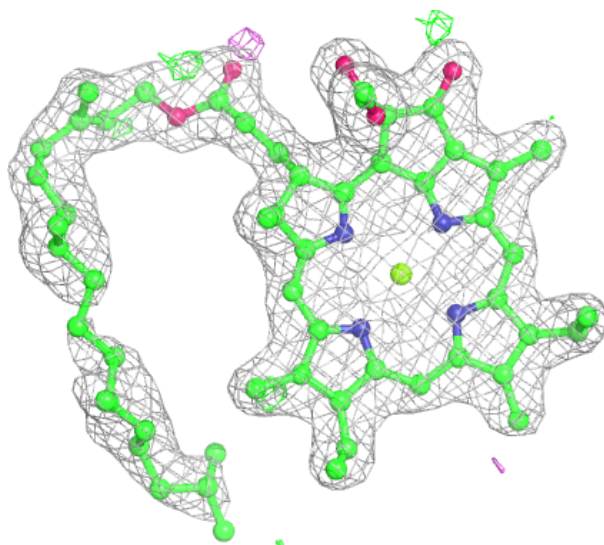
Electron density around CLA b 618:

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



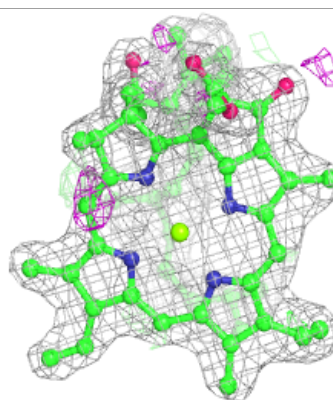
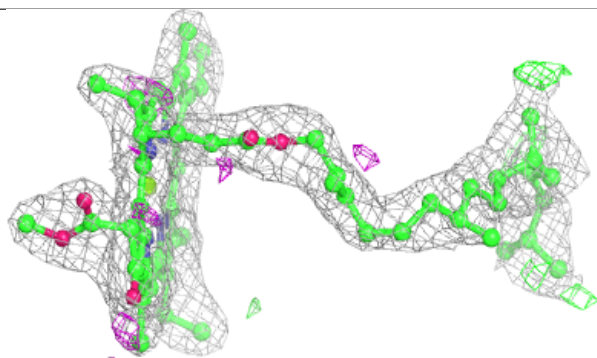
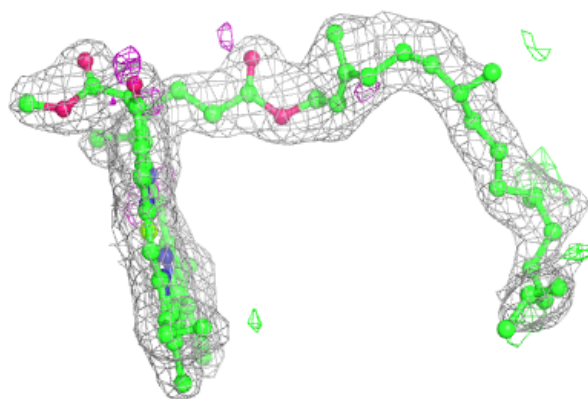
Electron density around CLA c 512:

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

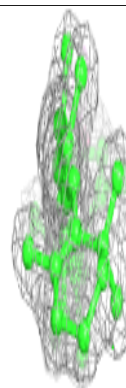
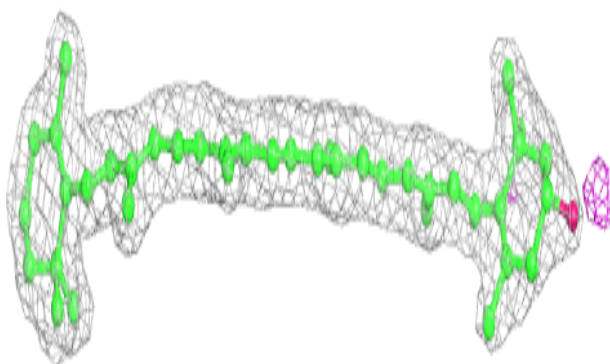
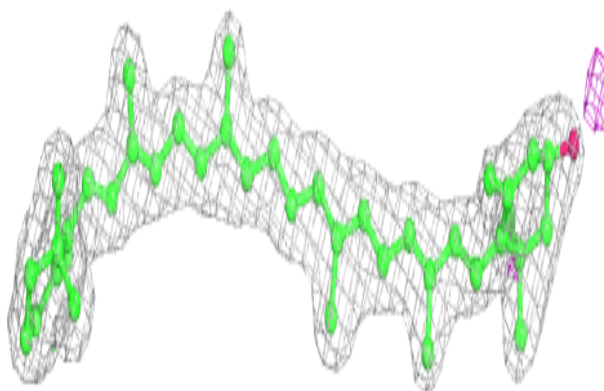


Electron density around CLA C 506:

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

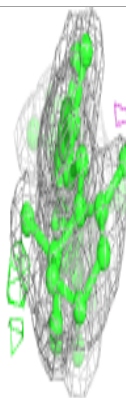
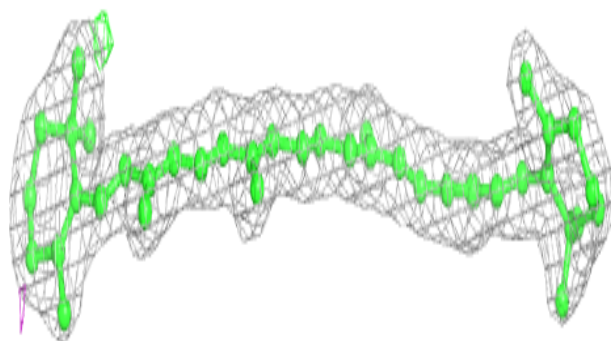
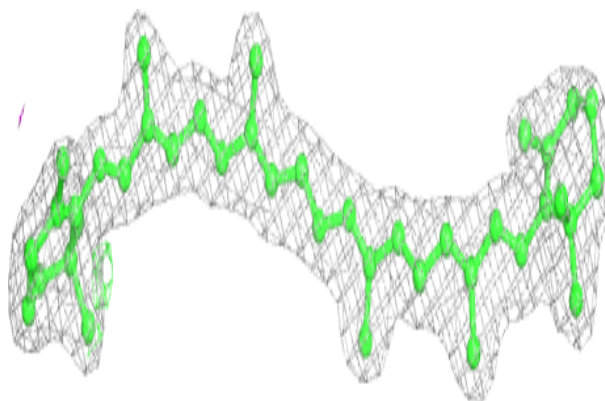
**Electron density around RRX x 101:**

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

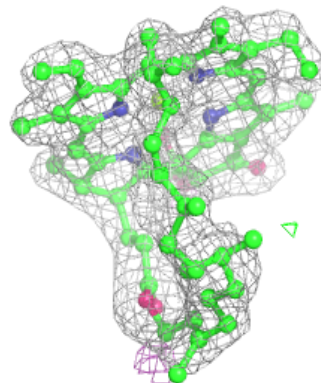
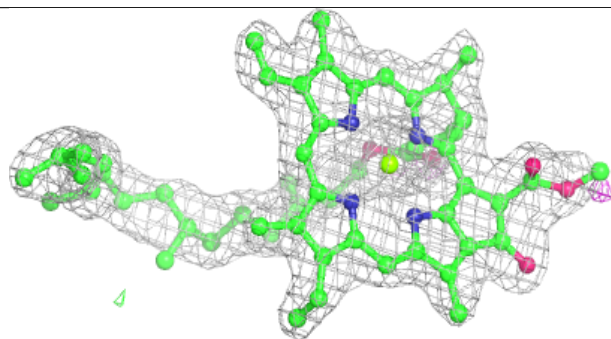
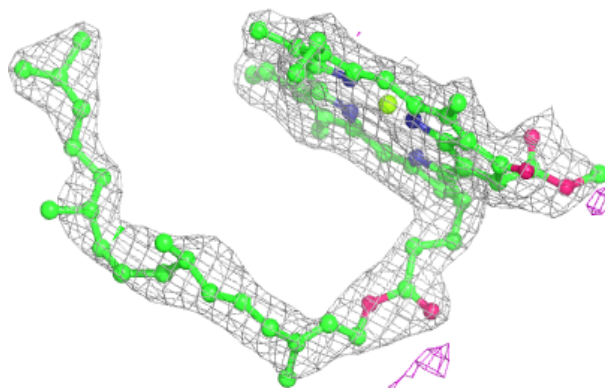


Electron density around BCR K 101:

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

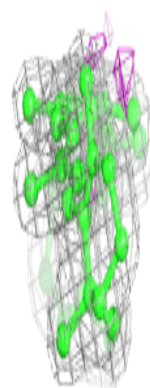
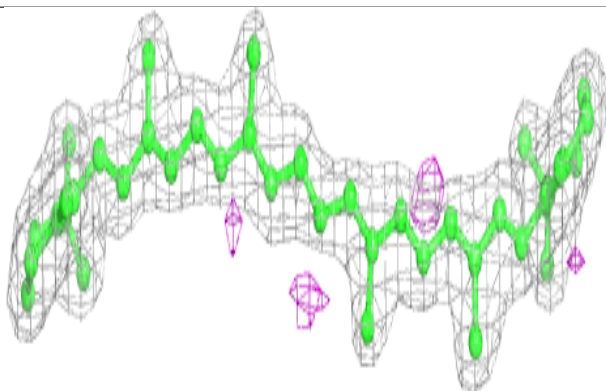
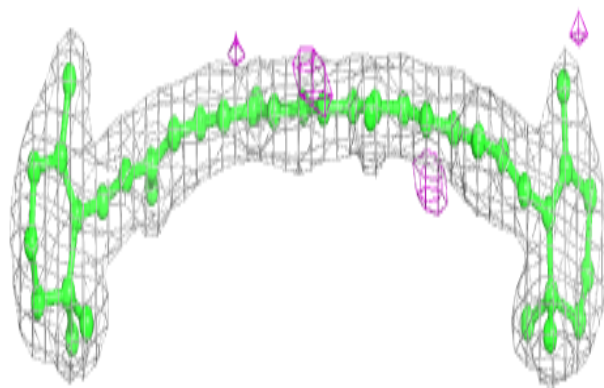
**Electron density around CLA c 513:**

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

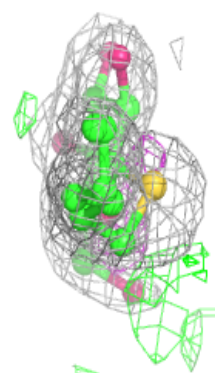
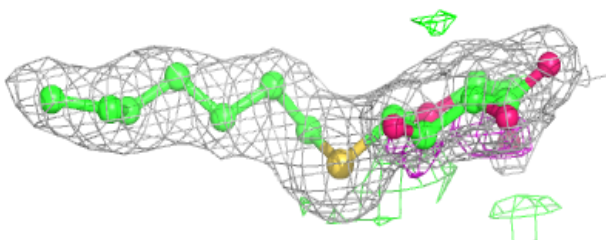
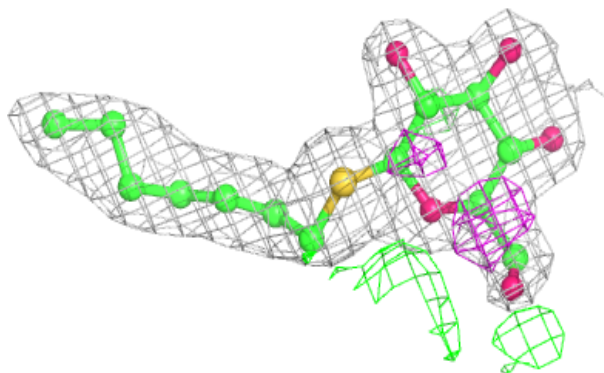


Electron density around BCR K 102:

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

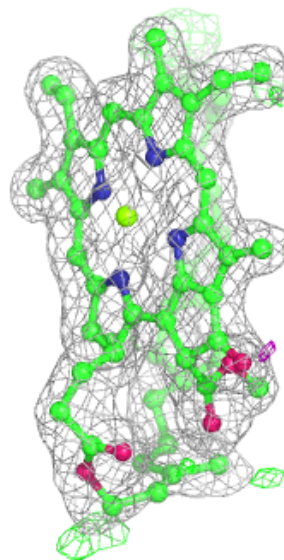
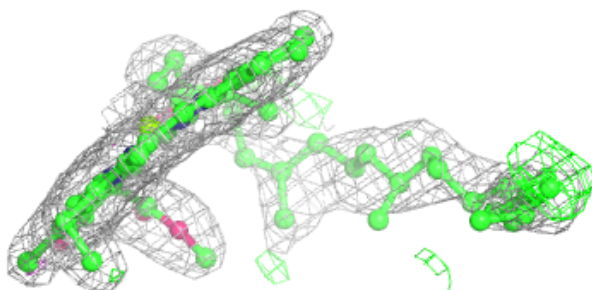
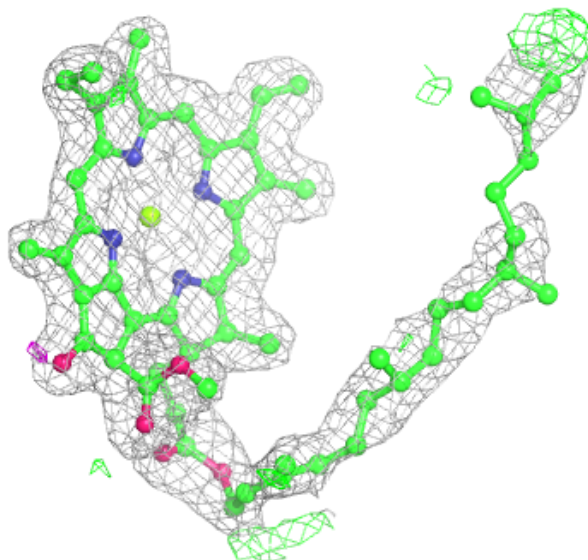
**Electron density around HTG B 621:**

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



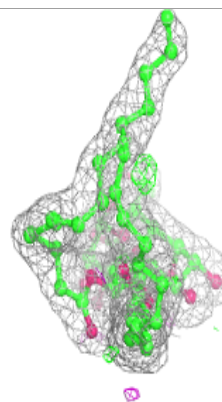
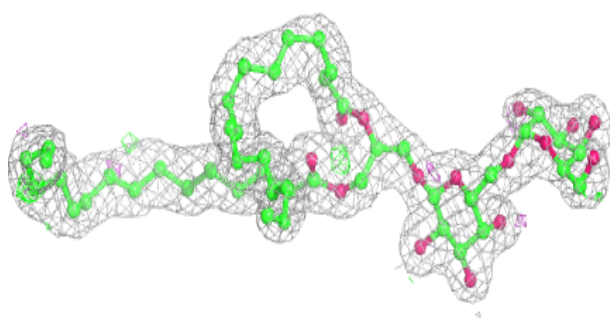
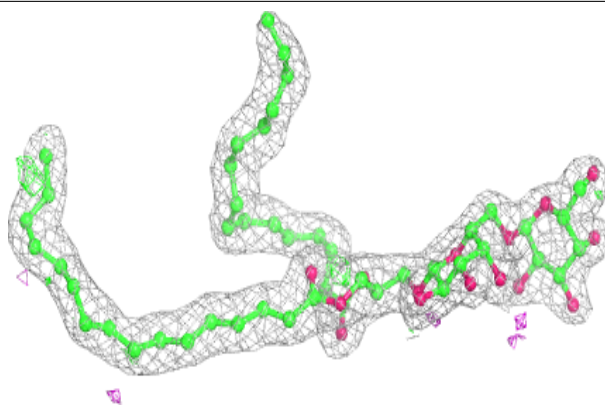
Electron density around CLA B 601:

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

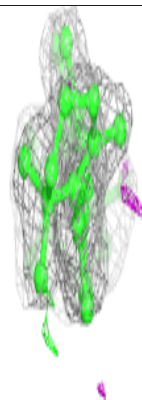
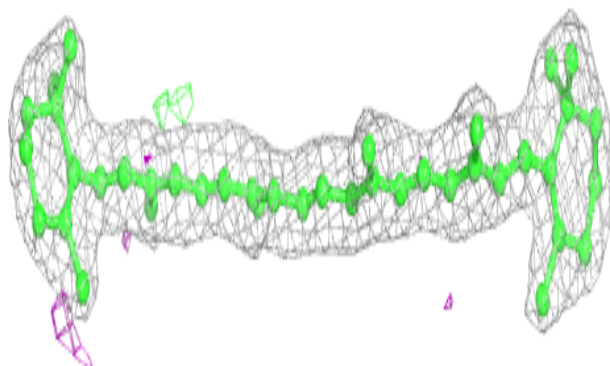
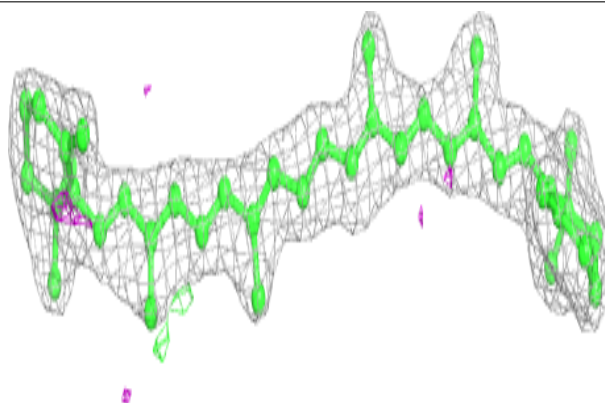


Electron density around DGD H 102:

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

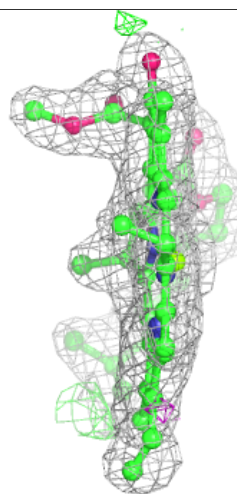
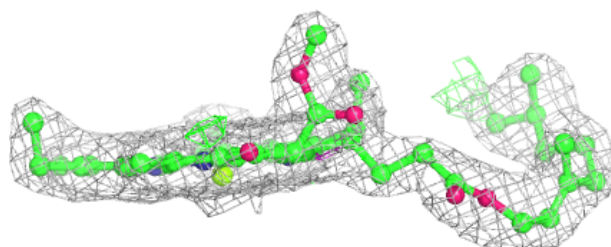
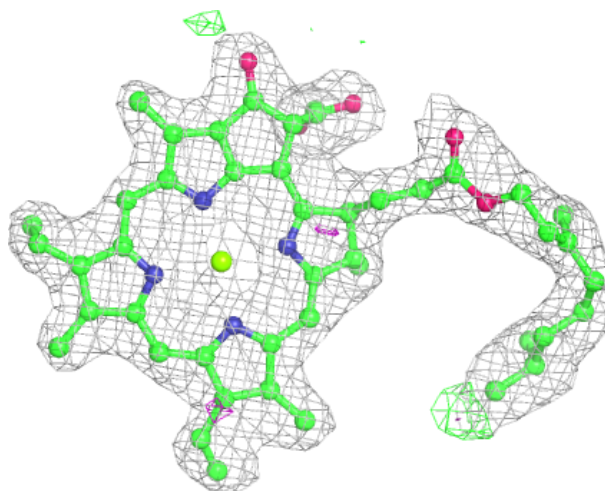
**Electron density around BCR k 102:**

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



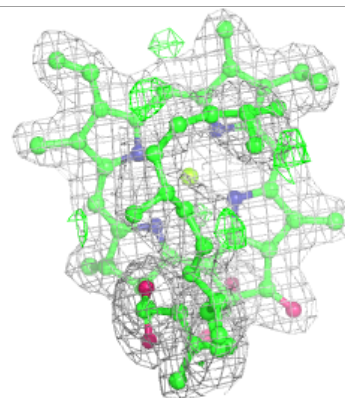
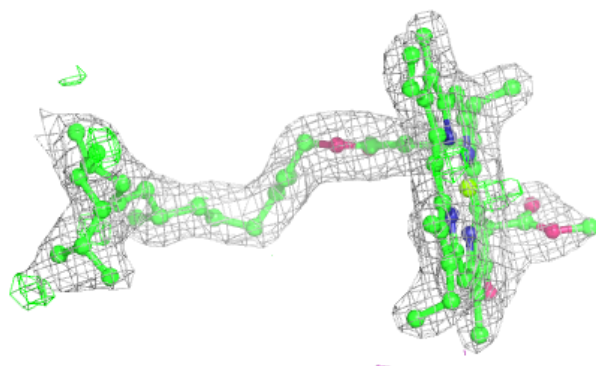
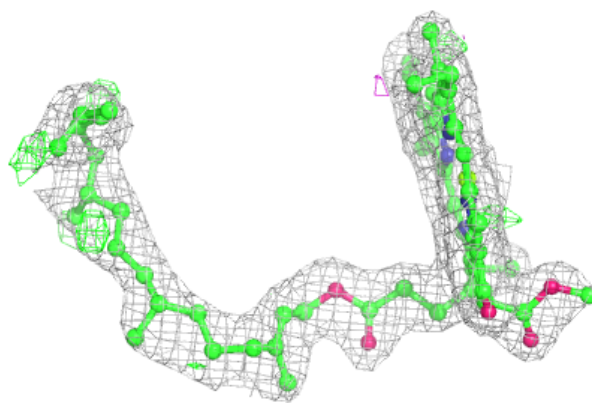
Electron density around CLA C 512:

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

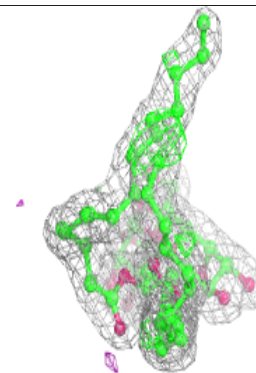
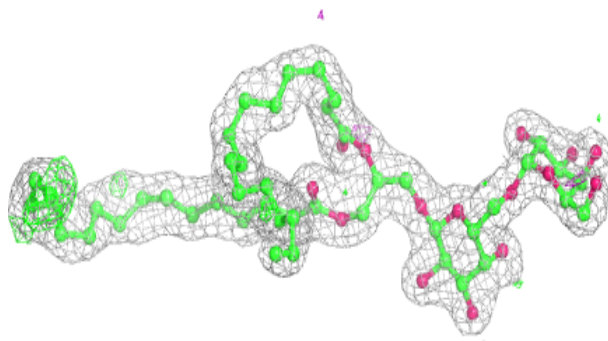
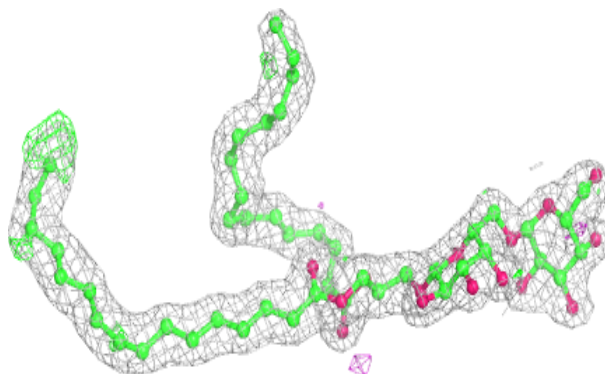


Electron density around CLA c 506:

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

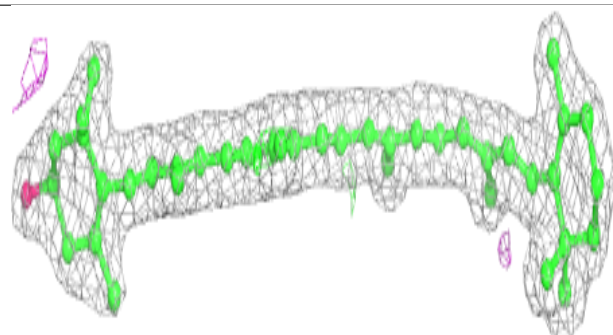
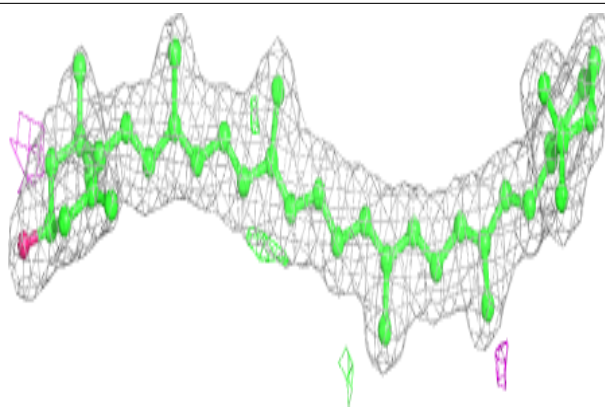
**Electron density around DGD h 101:**

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



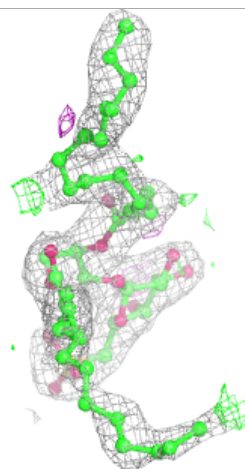
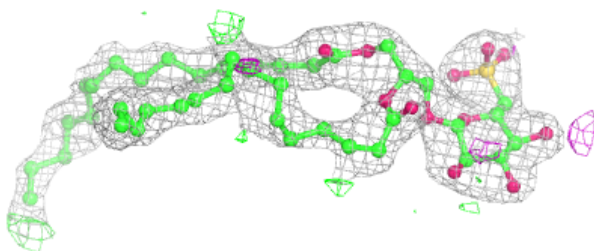
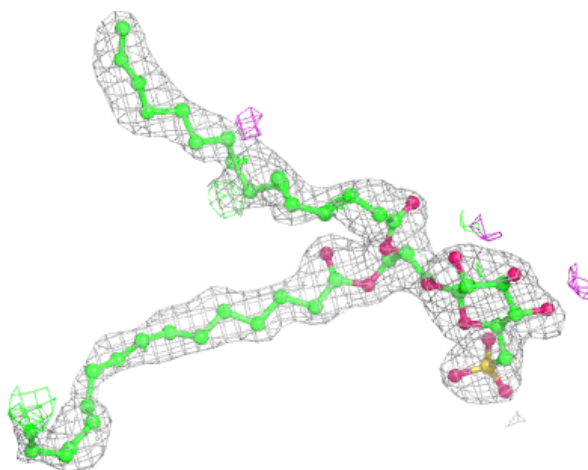
Electron density around RRX H 101:

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



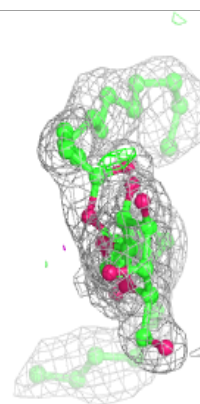
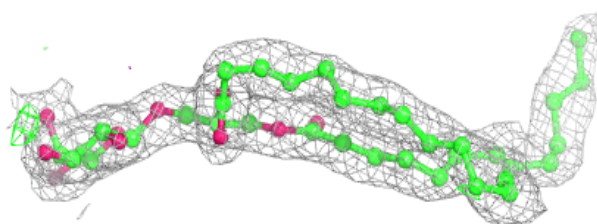
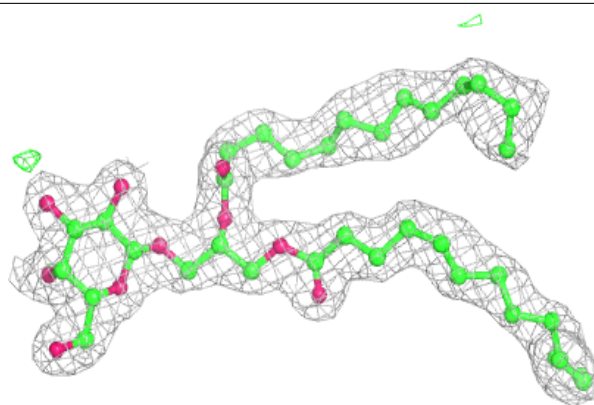
Electron density around SQD A 406:

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

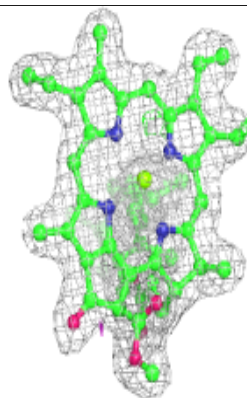
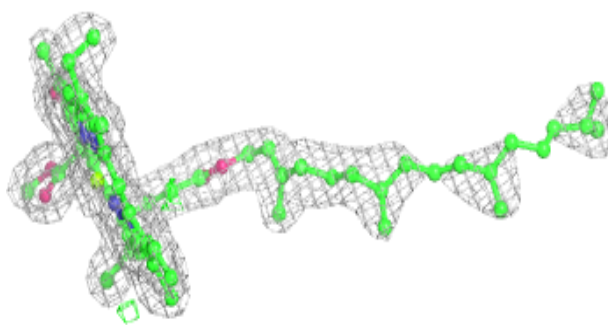
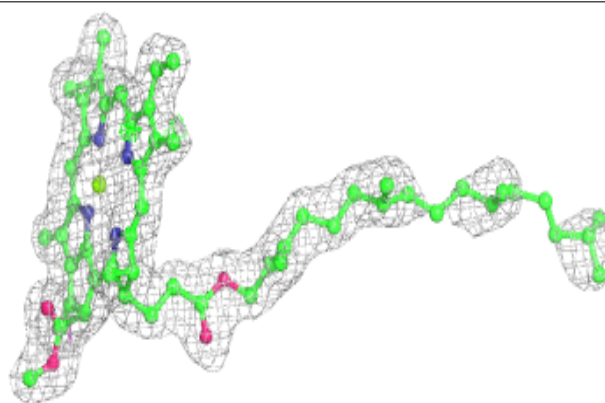


Electron density around LMG j 101:

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

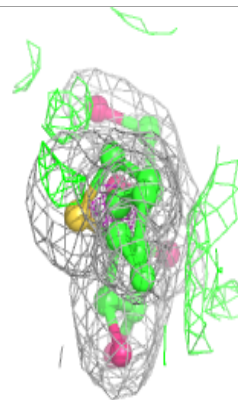
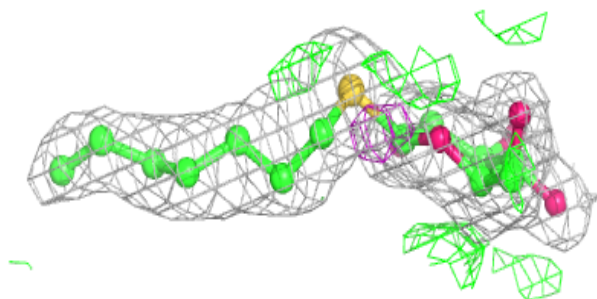
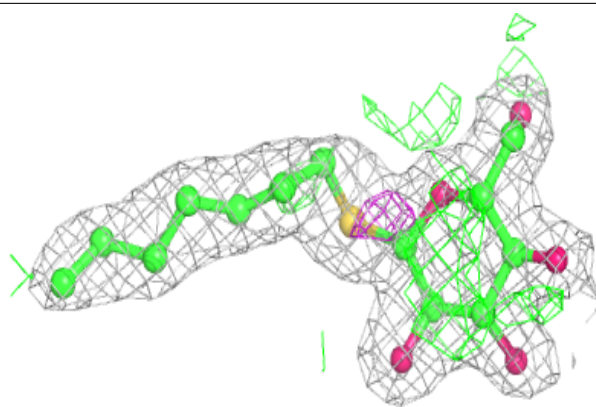
**Electron density around CLA d 404:**

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



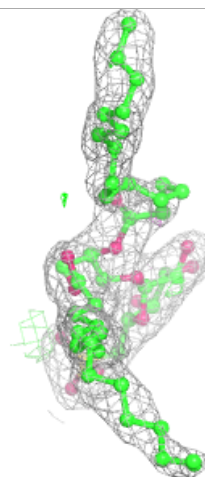
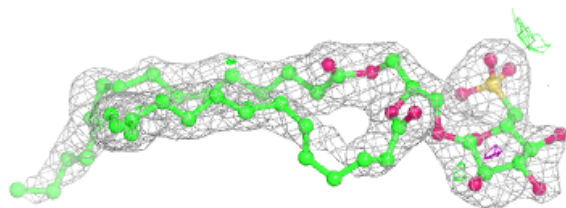
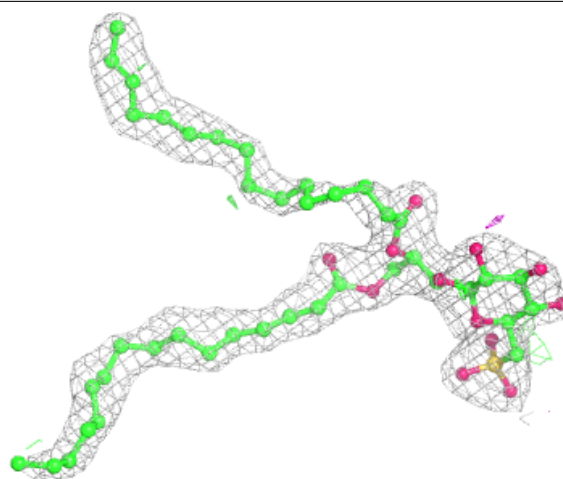
Electron density around HTG O 302:

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



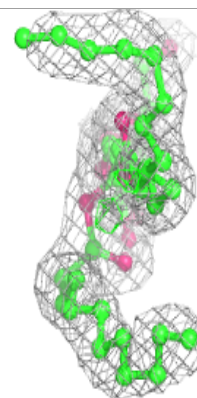
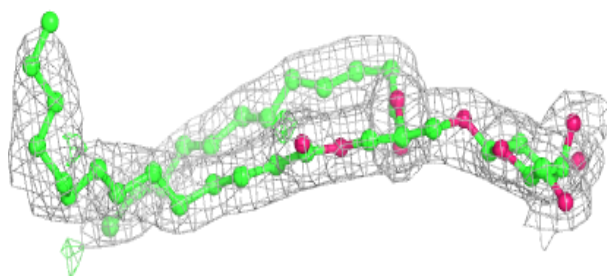
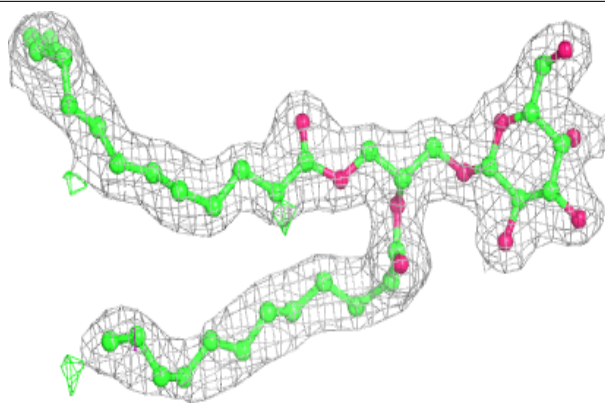
Electron density around SQD a 409:

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

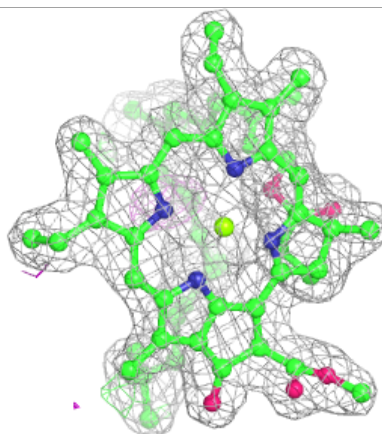
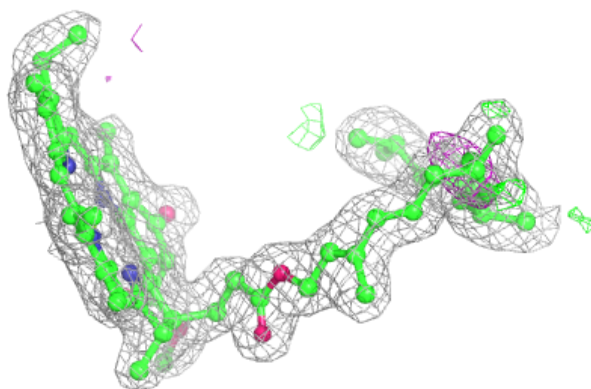
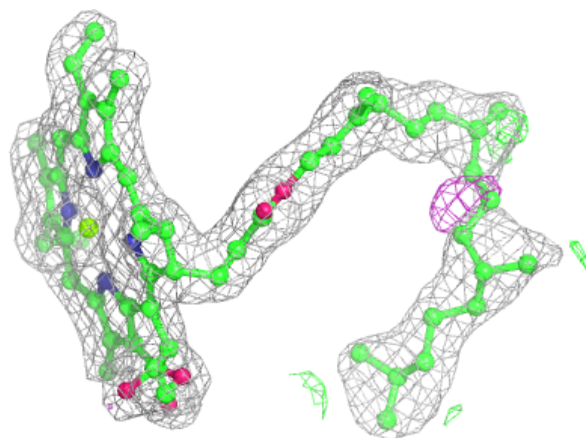


Electron density around LMG J 101:

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

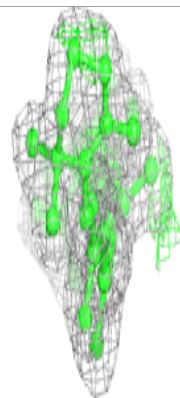
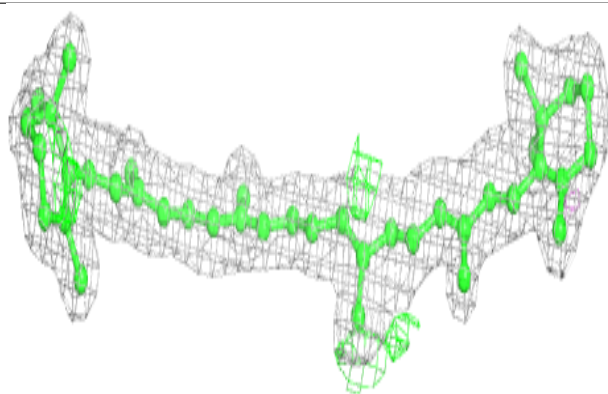
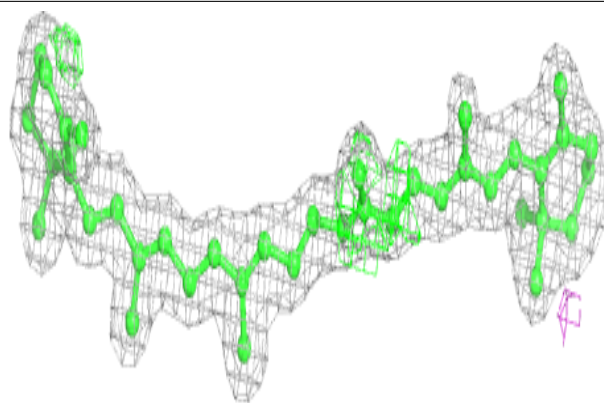
**Electron density around CLA B 607:**

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



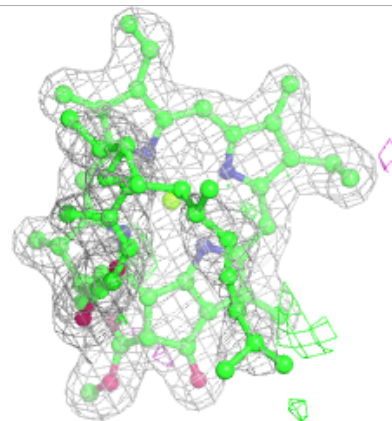
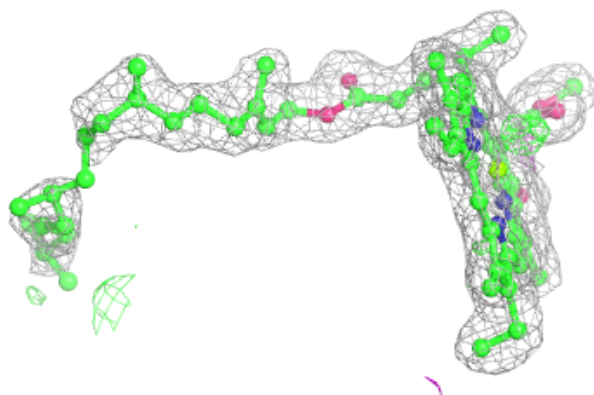
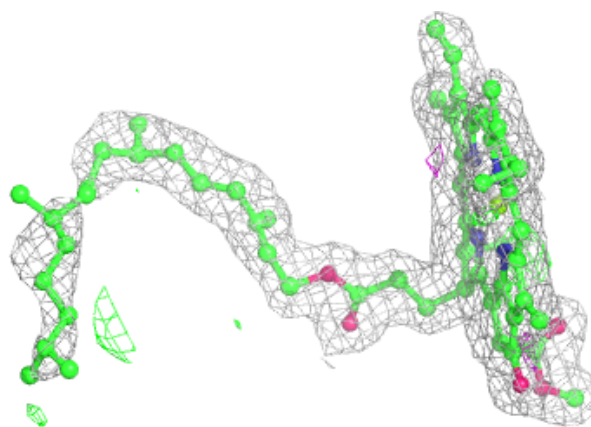
Electron density around BCR t 101:

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



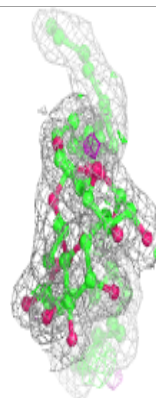
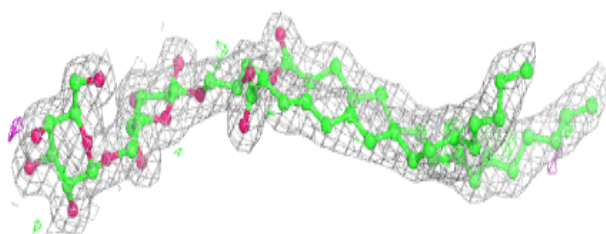
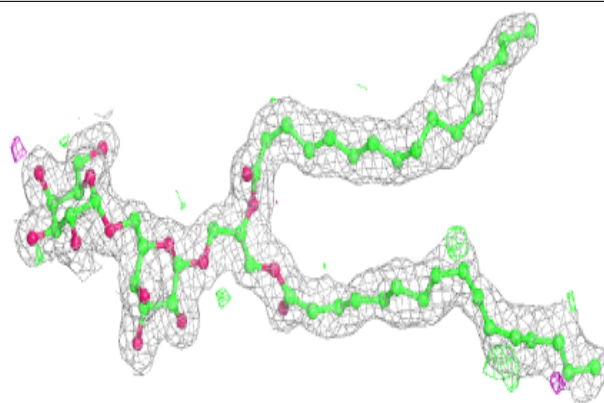
Electron density around CLA D 404:

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

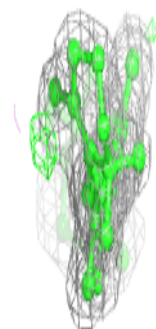
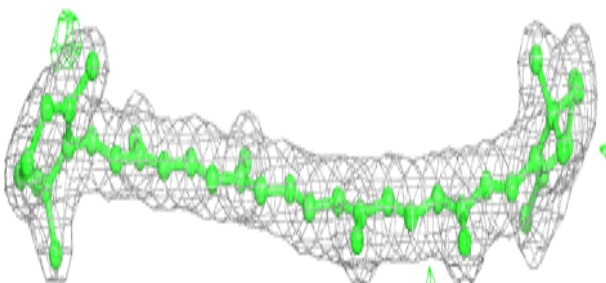
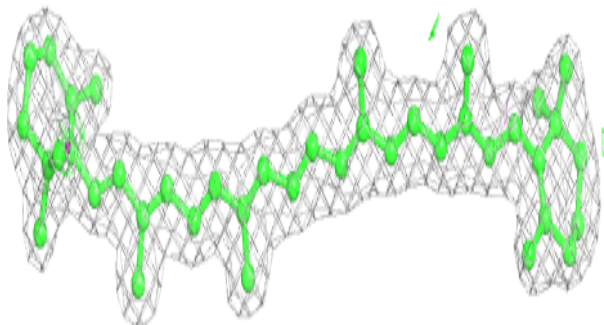


Electron density around DGD c 517:

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

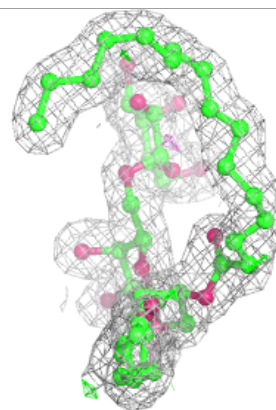
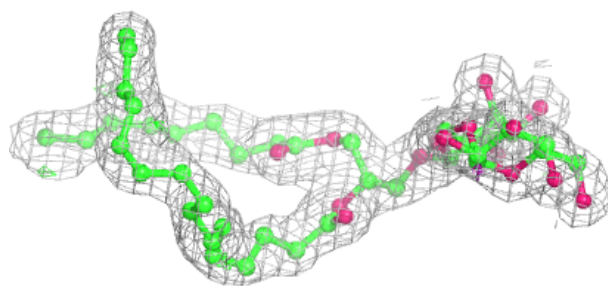
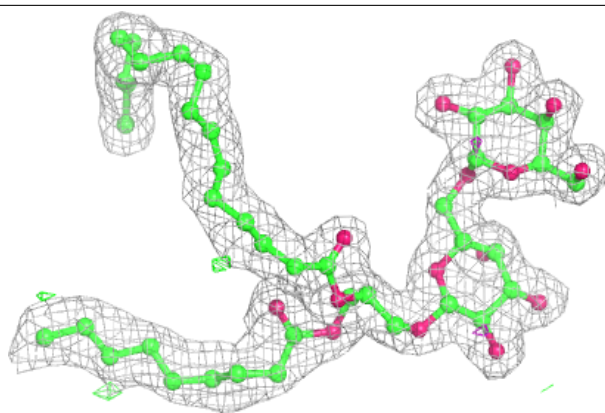
**Electron density around BCR B 619:**

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

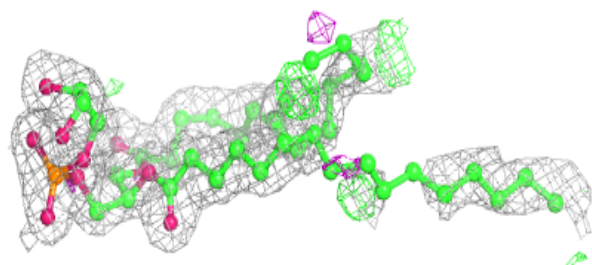
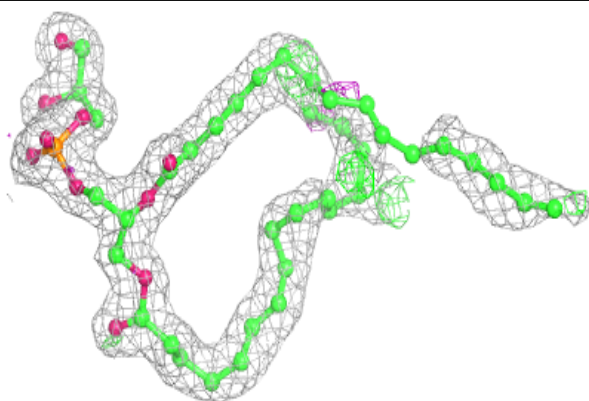


Electron density around DGD C 517:

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

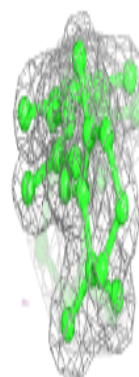
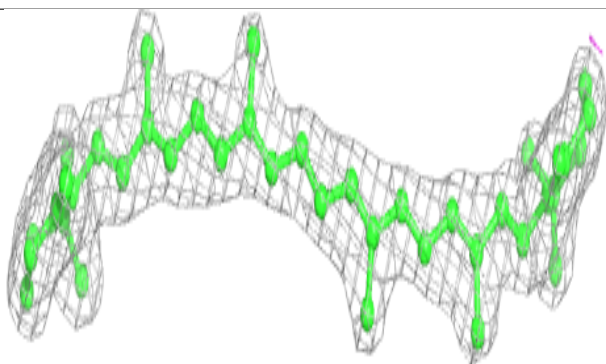
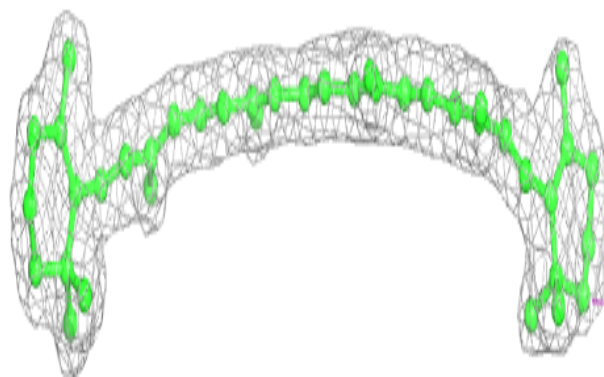
**Electron density around LHG D 409:**

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



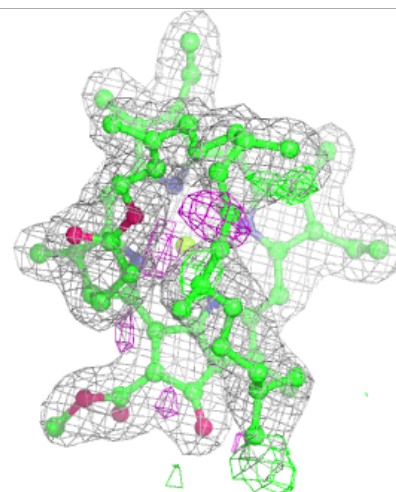
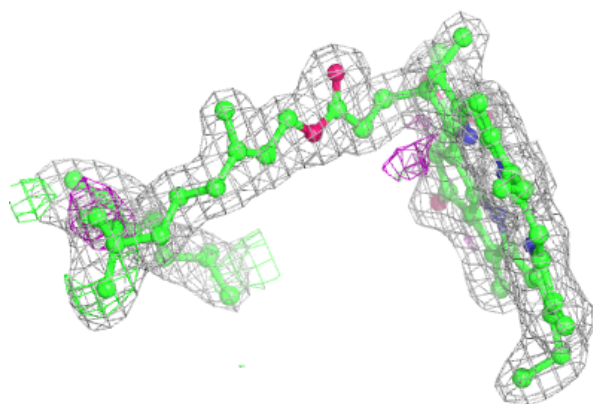
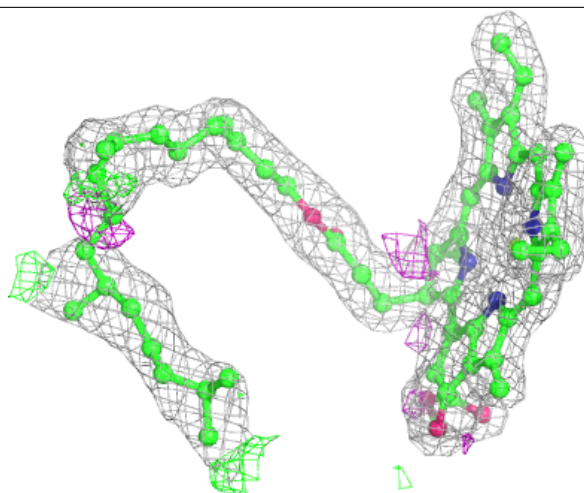
Electron density around BCR k 101:

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



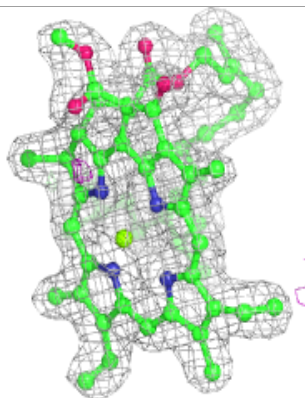
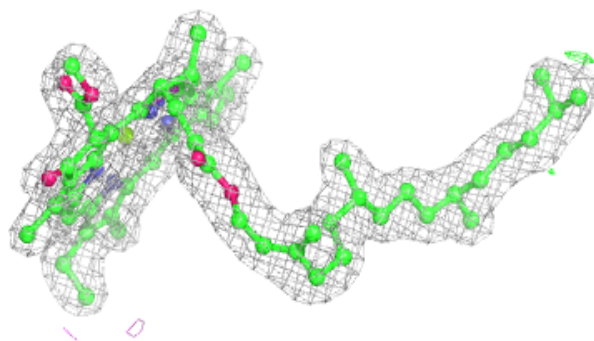
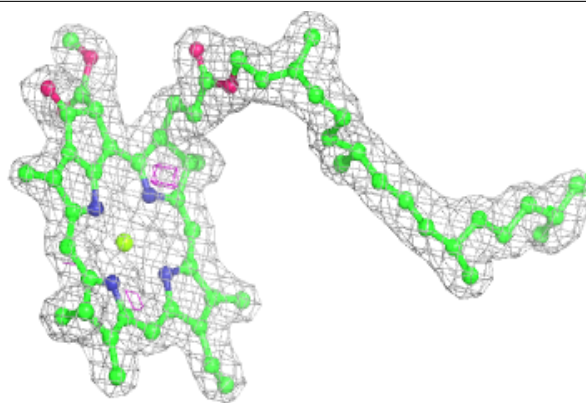
Electron density around CLA b 608:

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



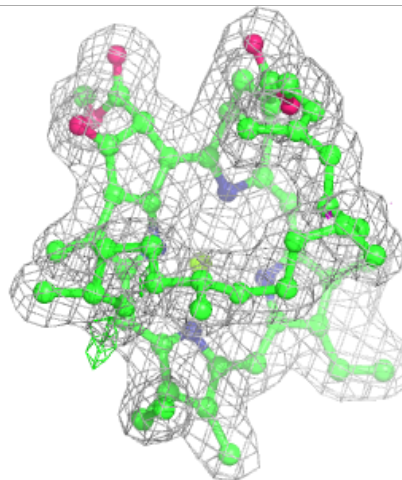
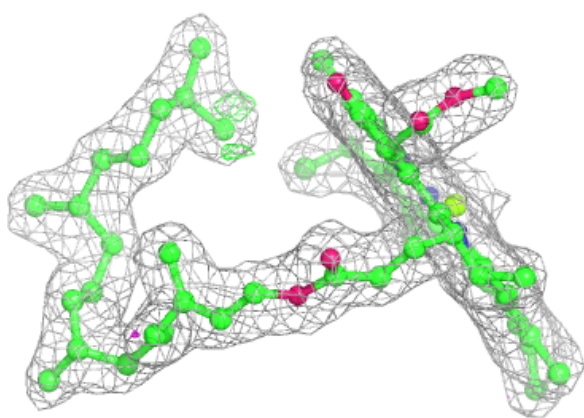
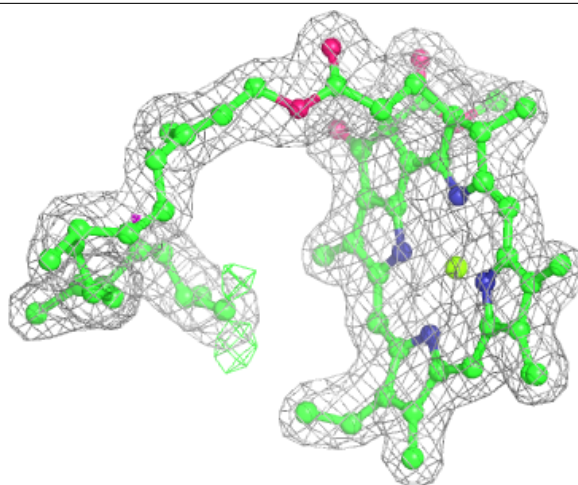
Electron density around CLA c 511:

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



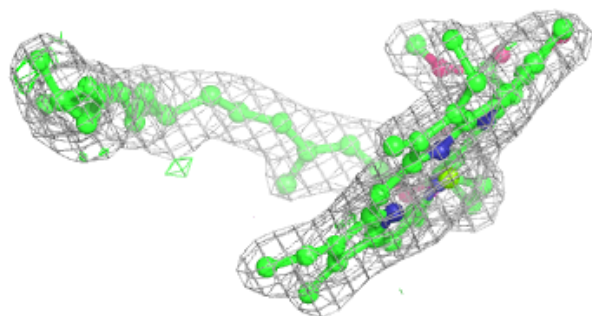
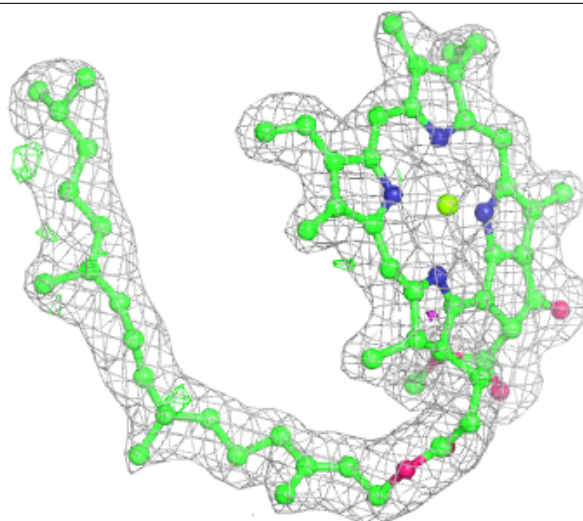
Electron density around CLA C 503:

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



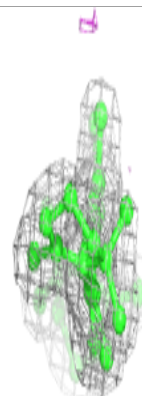
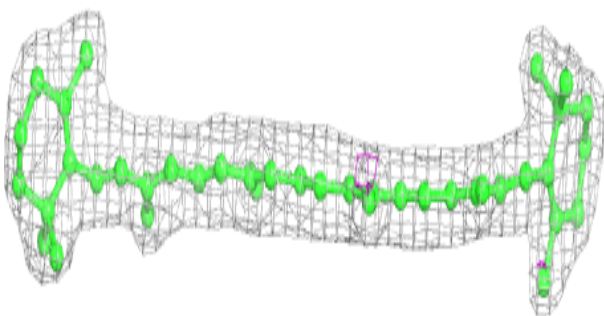
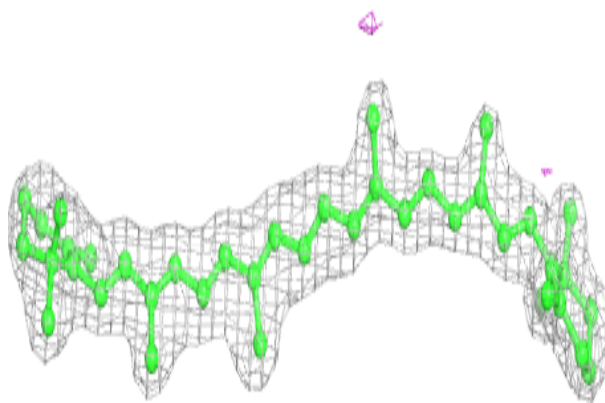
Electron density around CLA C 507:

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

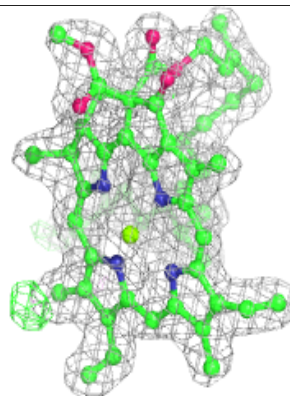
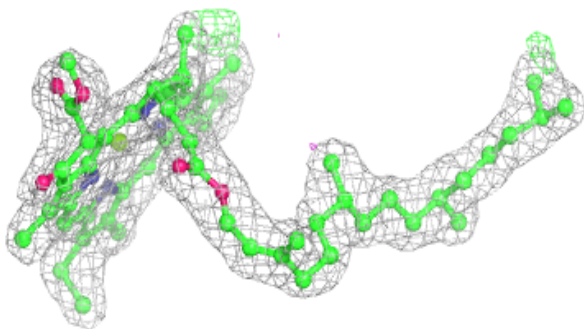
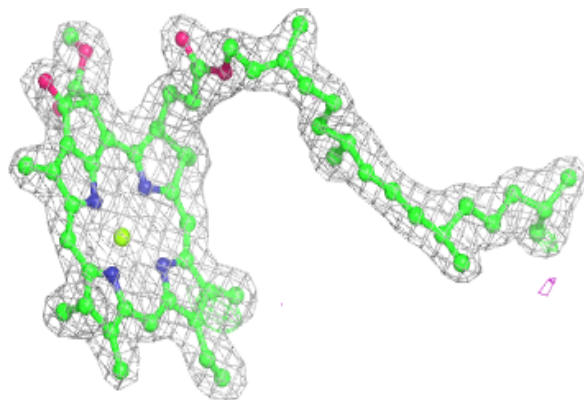


Electron density around BCR C 515:

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

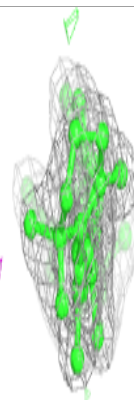
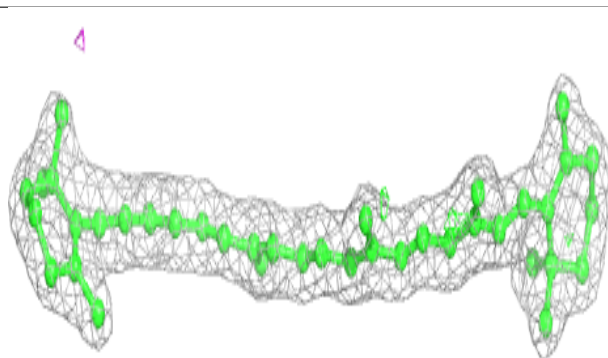
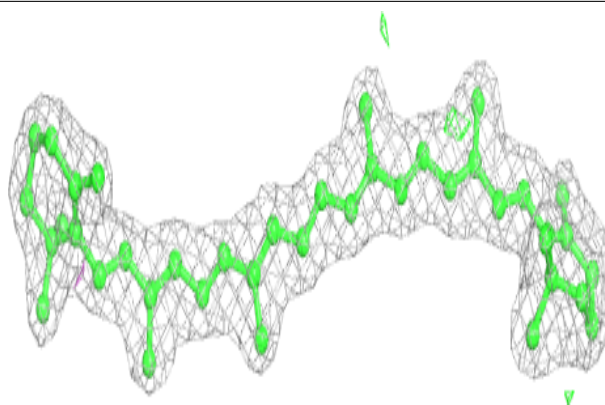
**Electron density around CLA C 511:**

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

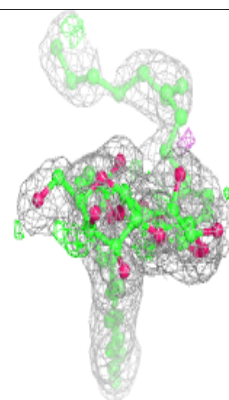
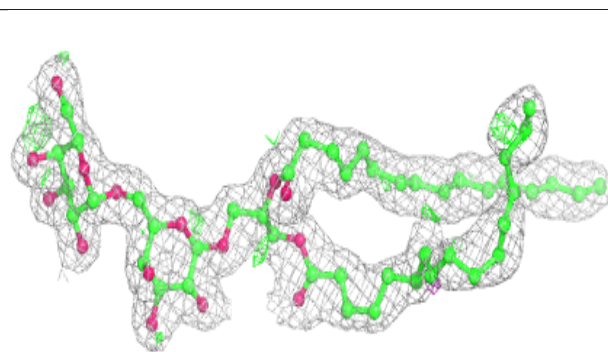
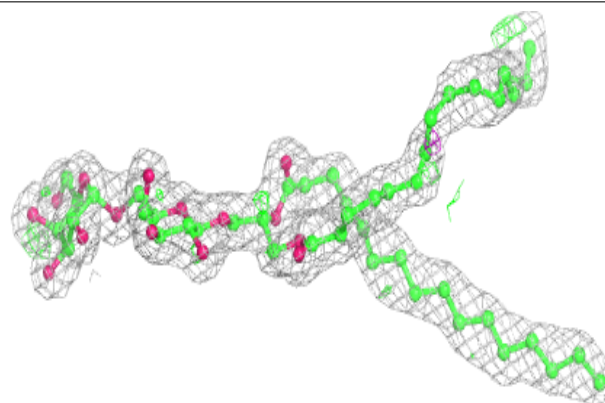


Electron density around BCR j 102:

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

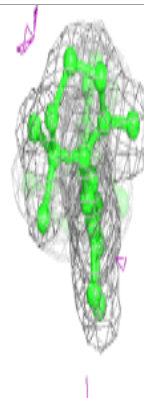
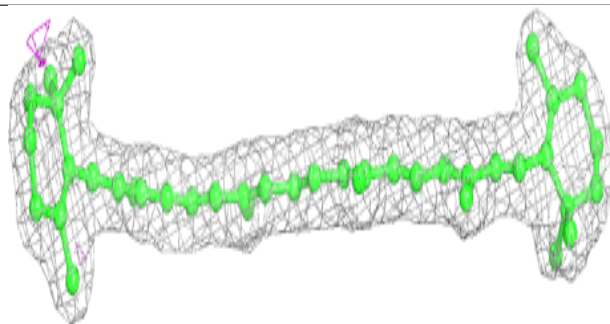
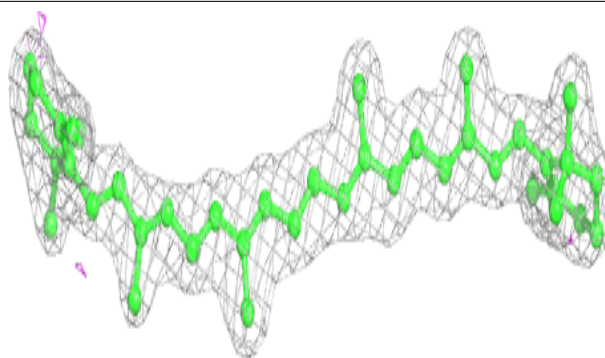
**Electron density around DGD c 515:**

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

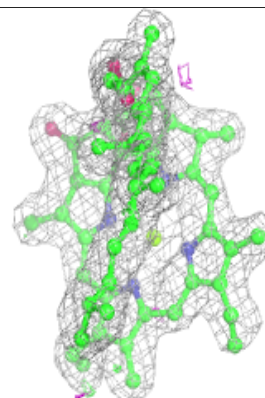
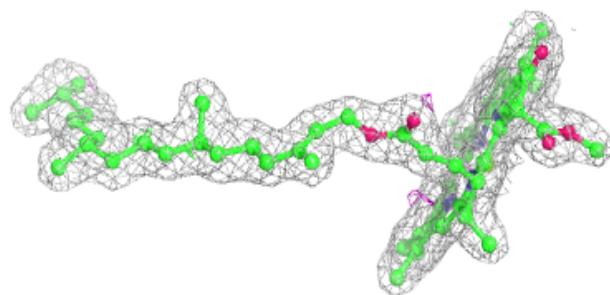
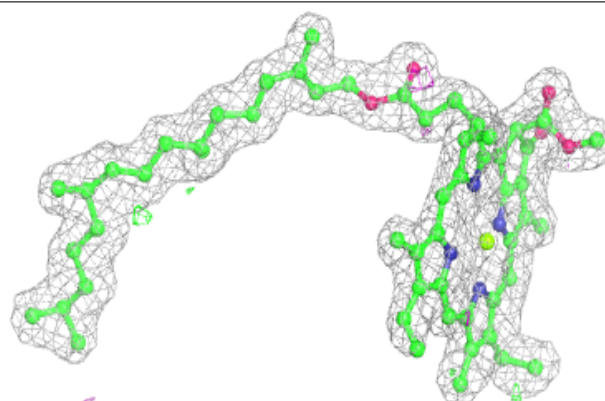


Electron density around BCR c 514:

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

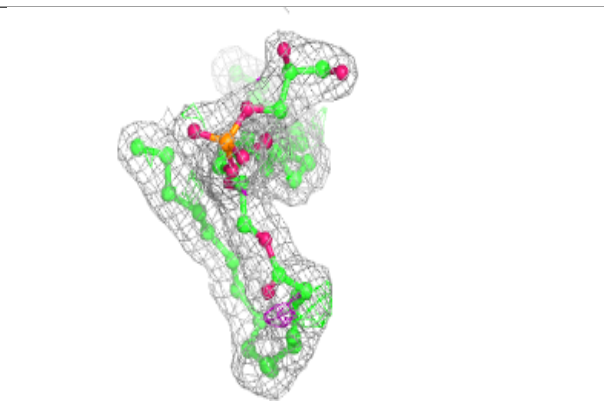
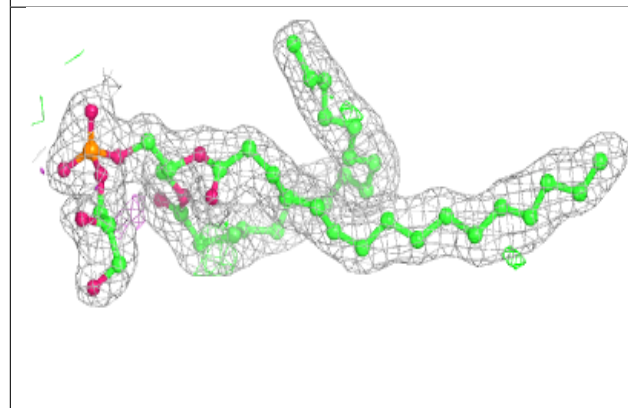
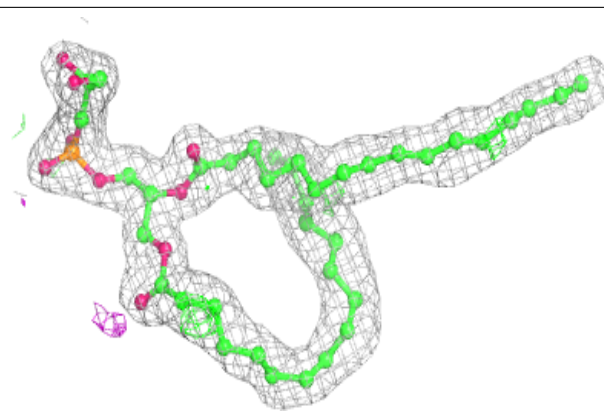
**Electron density around CLA b 611:**

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

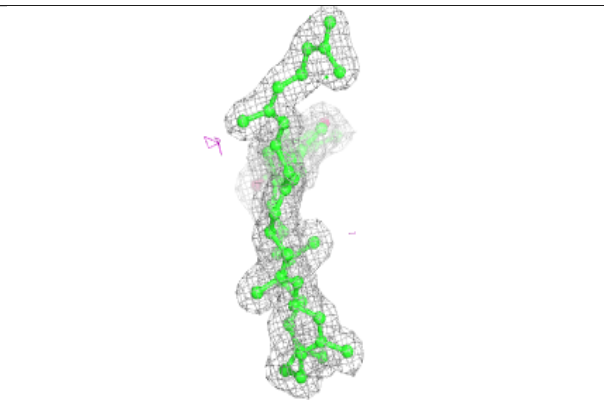
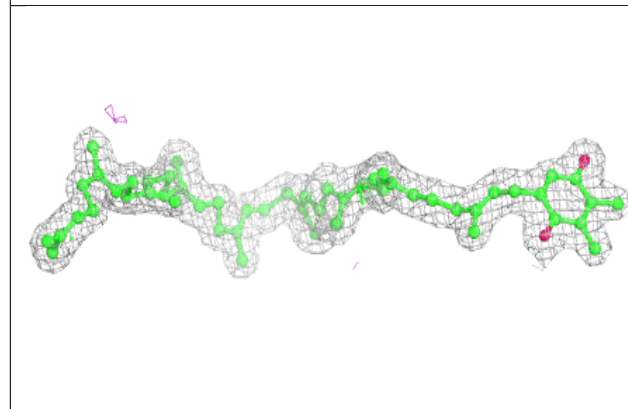
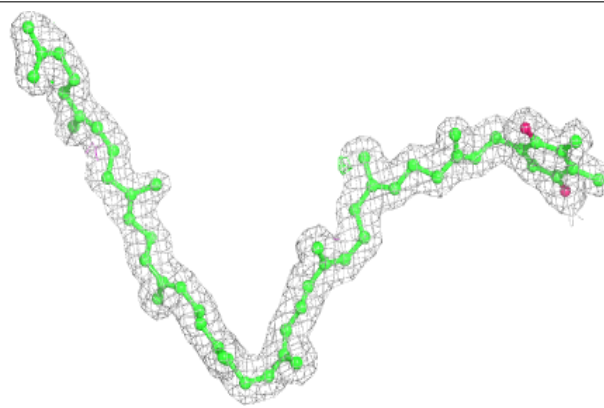


Electron density around LHG D 407:

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

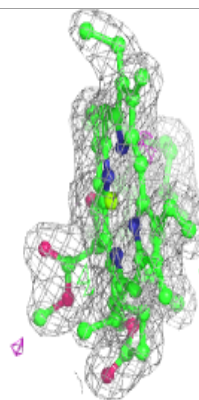
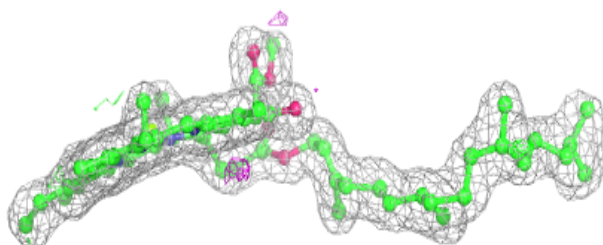
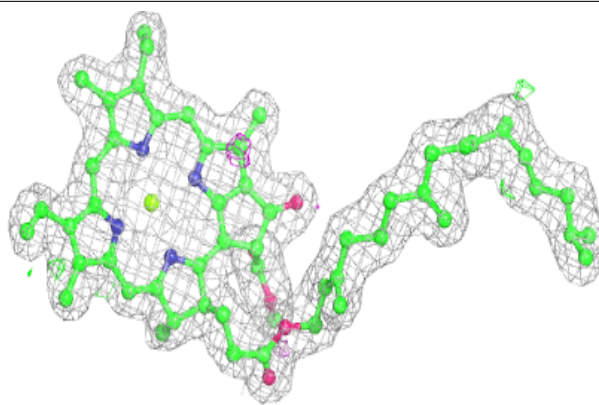
**Electron density around PL9 d 412:**

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



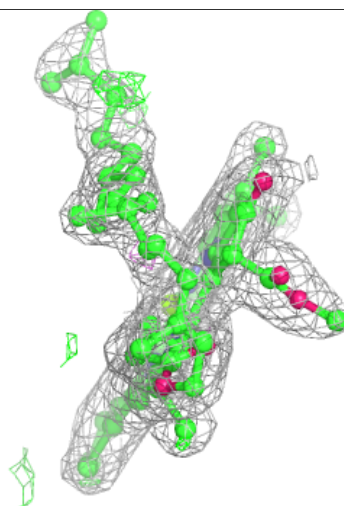
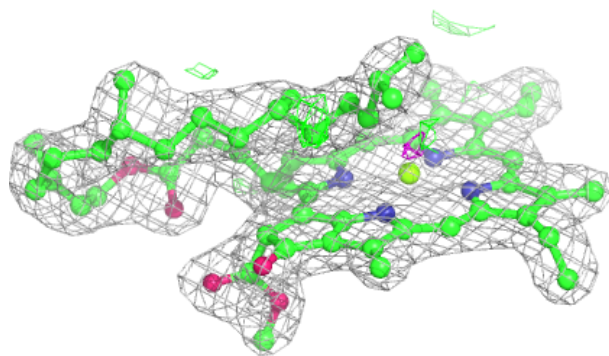
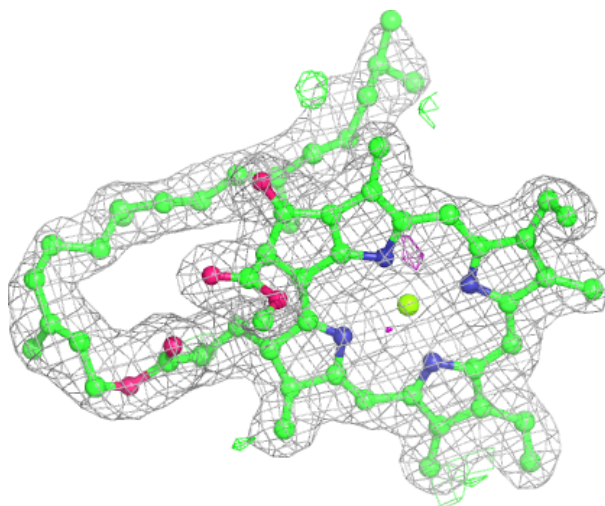
Electron density around CLA b 604:

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



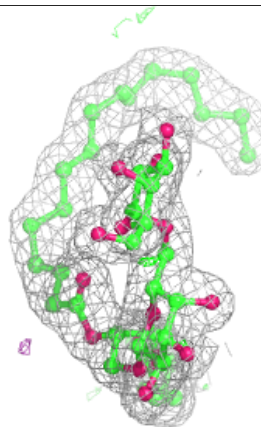
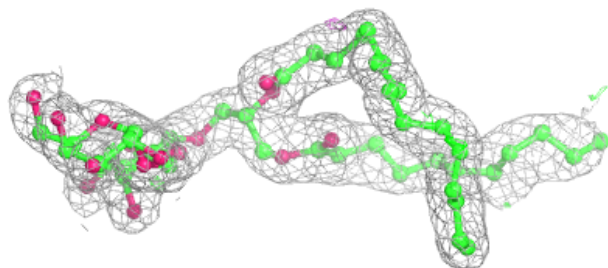
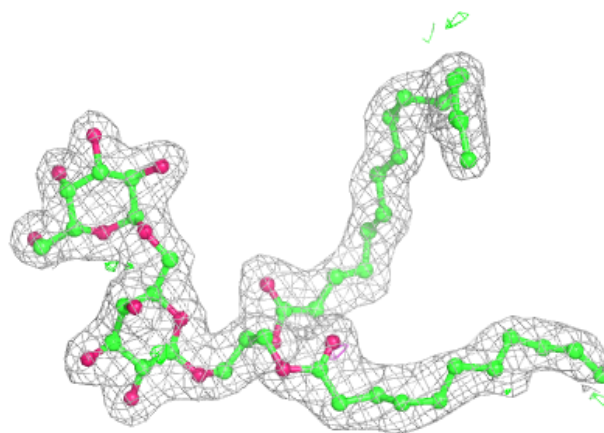
Electron density around CLA C 509:

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

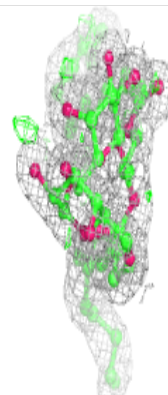
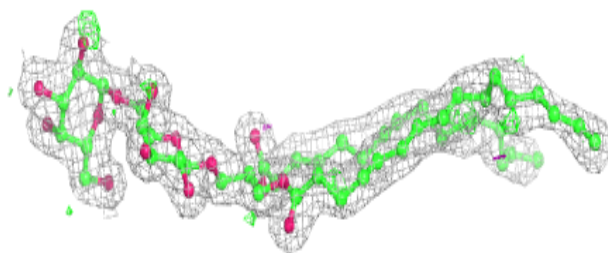
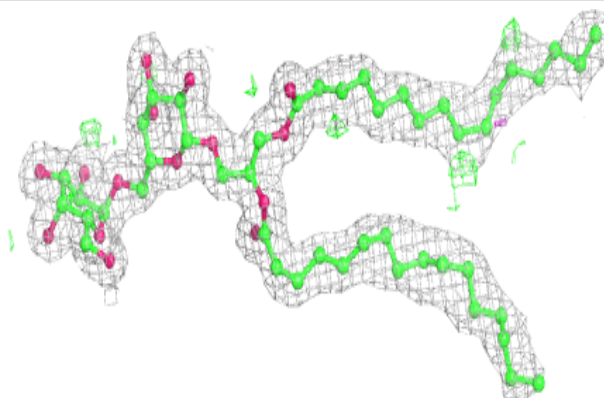


Electron density around DGD c 516:

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

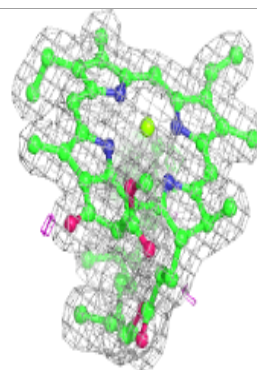
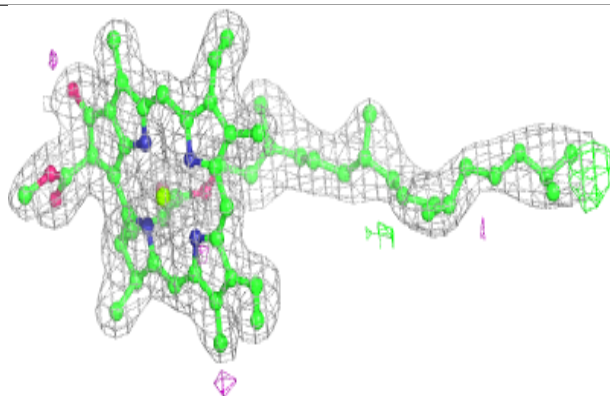
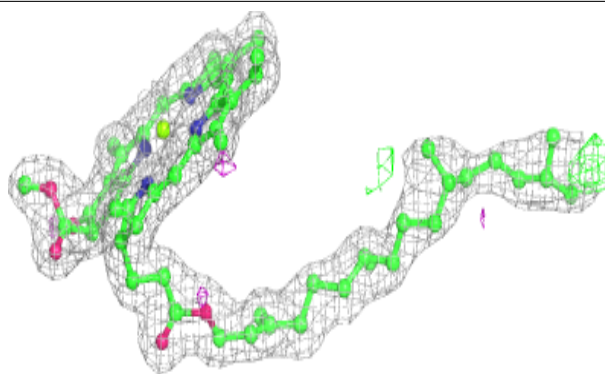
**Electron density around DGD C 518:**

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

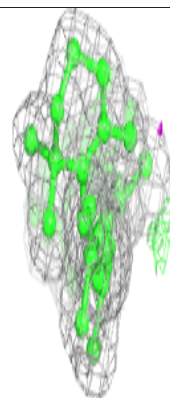
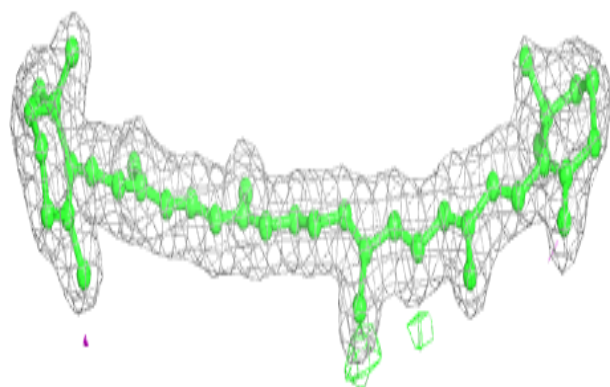
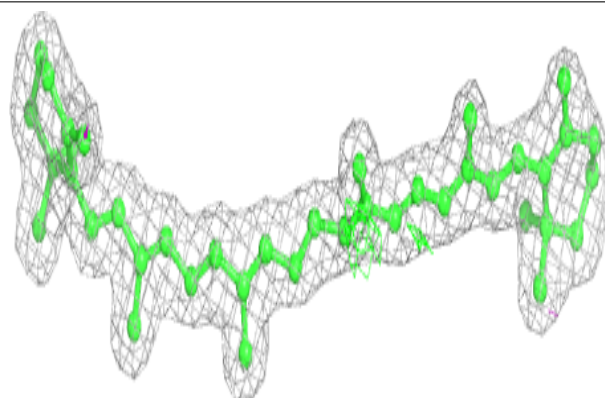


Electron density around CLA C 504:

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

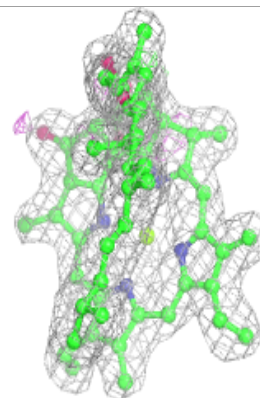
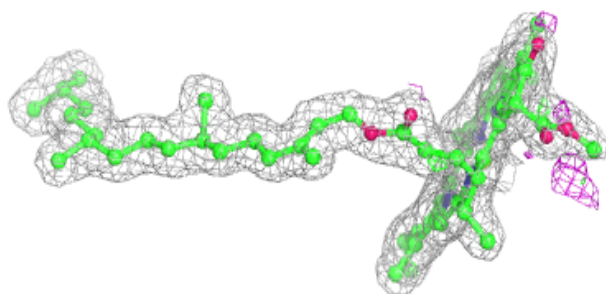
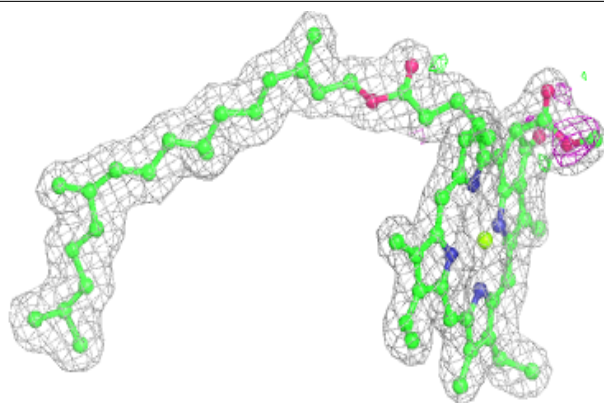
**Electron density around BCR T 101:**

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

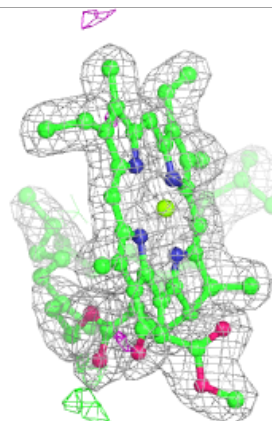
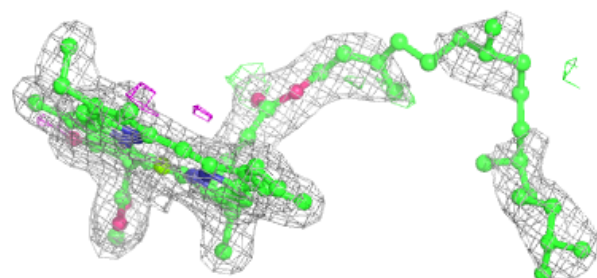
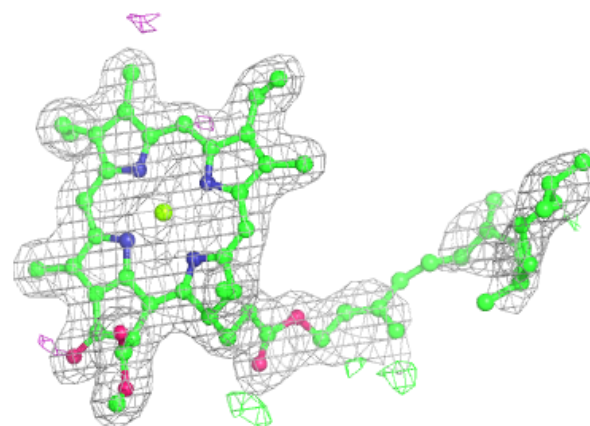


Electron density around CLA B 610:

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

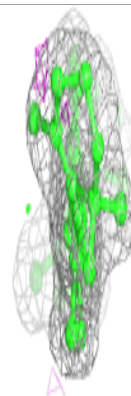
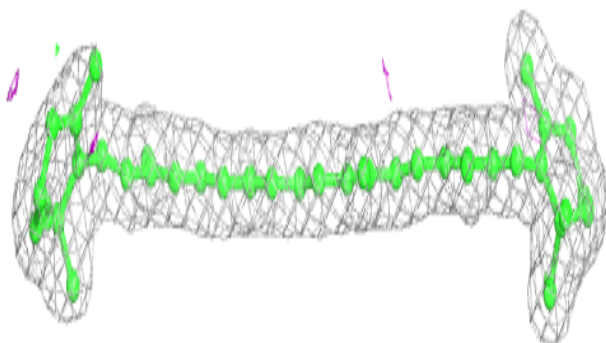
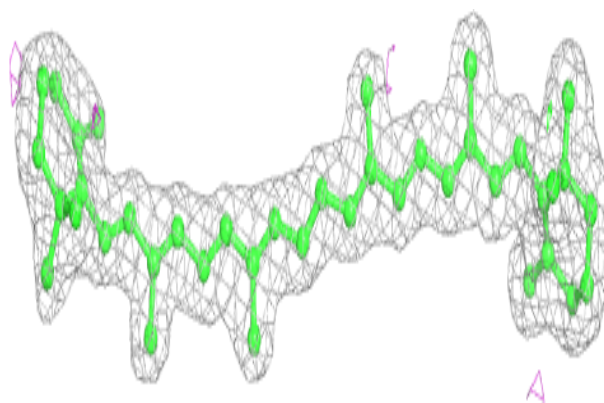
**Electron density around CLA A 404:**

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



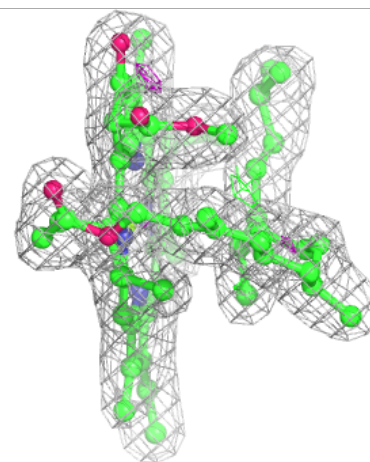
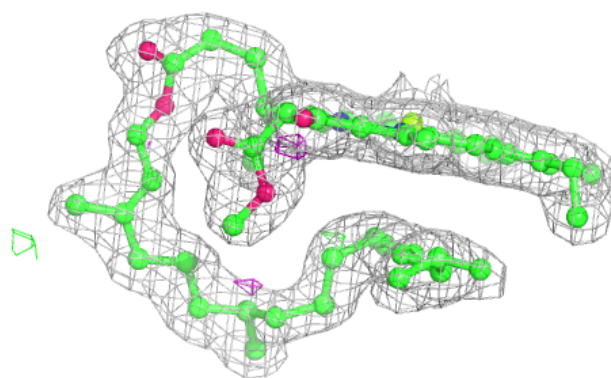
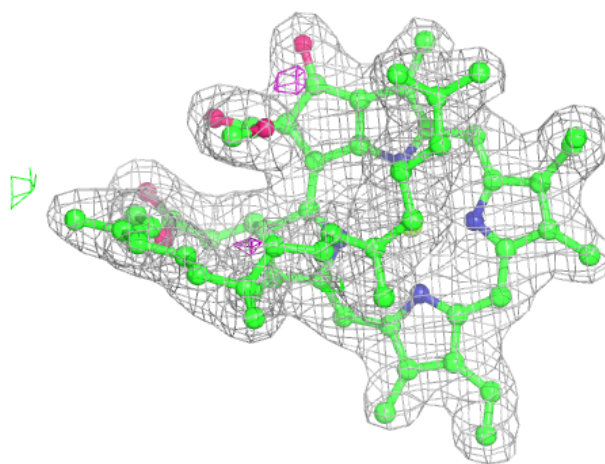
Electron density around BCR b 620:

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



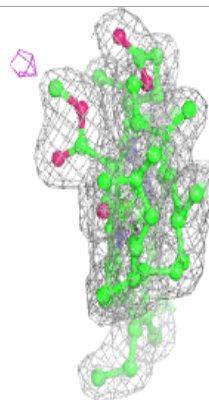
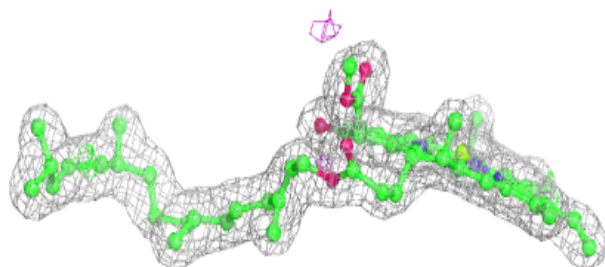
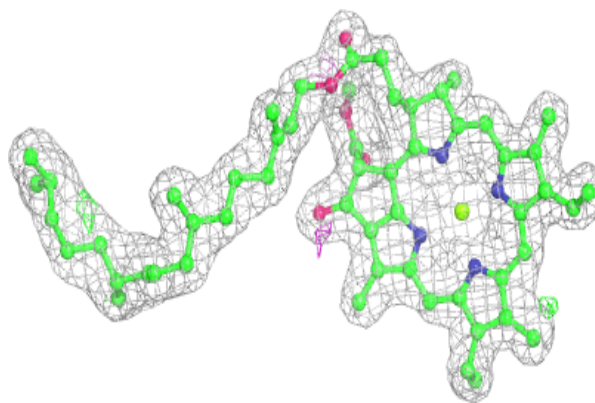
Electron density around CLA C 510:

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



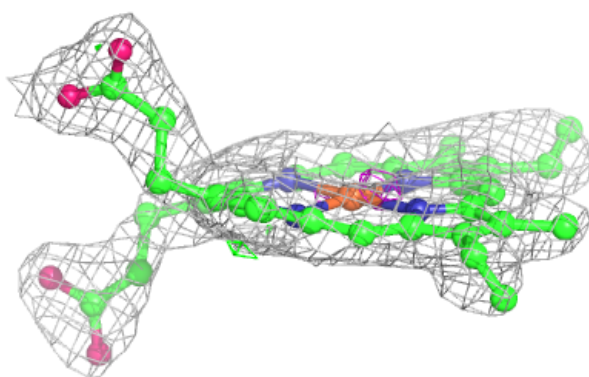
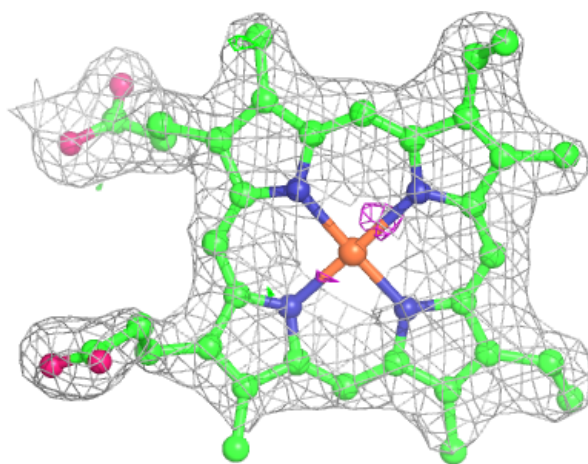
Electron density around CLA B 603:

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



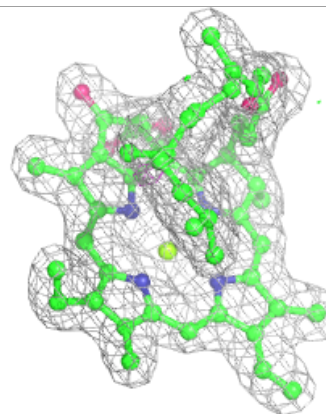
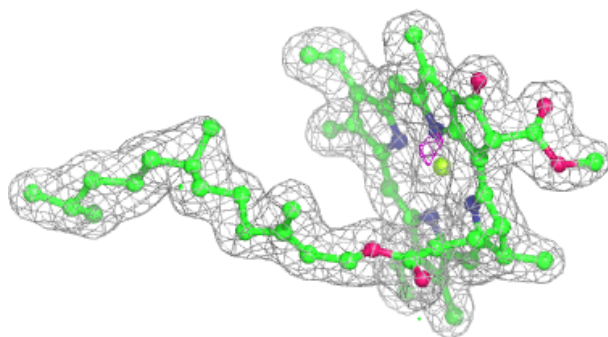
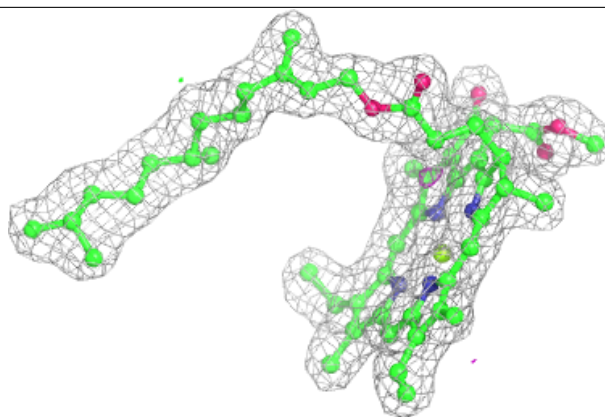
Electron density around HEM E 104:

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

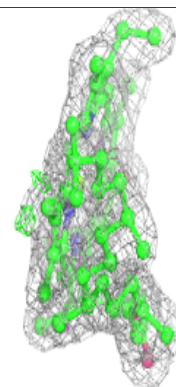
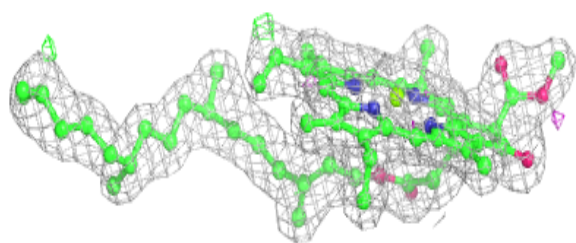
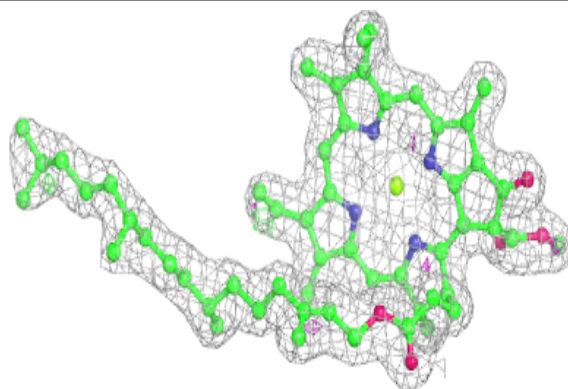


Electron density around CLA C 508:

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

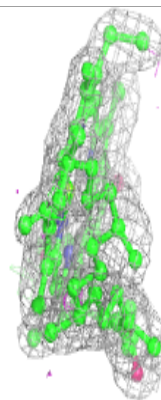
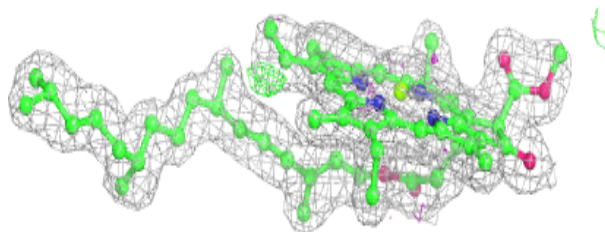
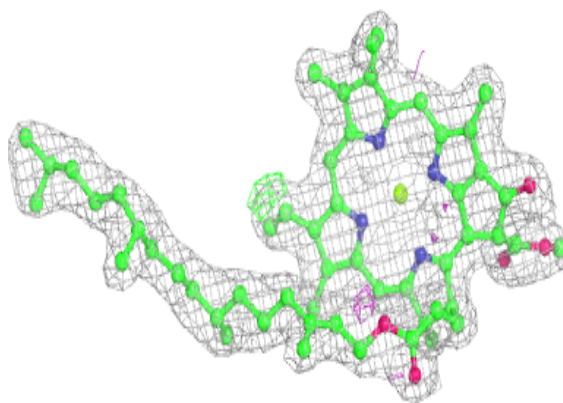
**Electron density around CLA C 501:**

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

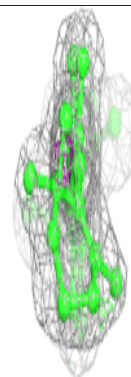
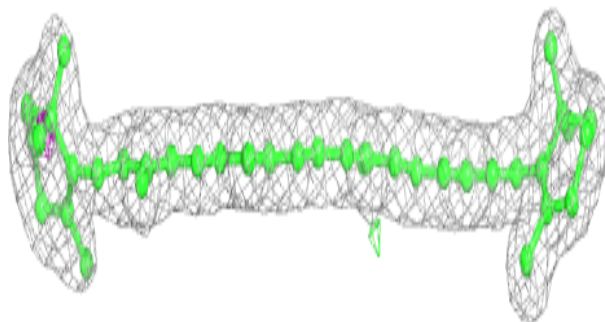
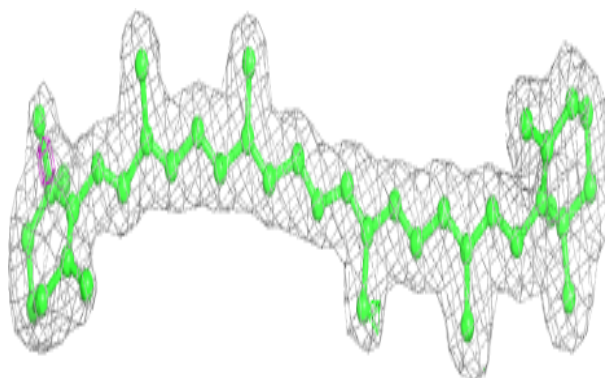


Electron density around CLA c 501:

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

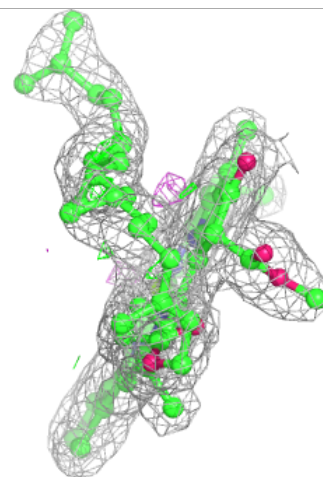
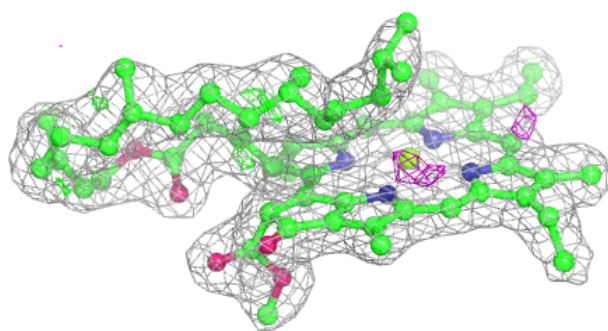
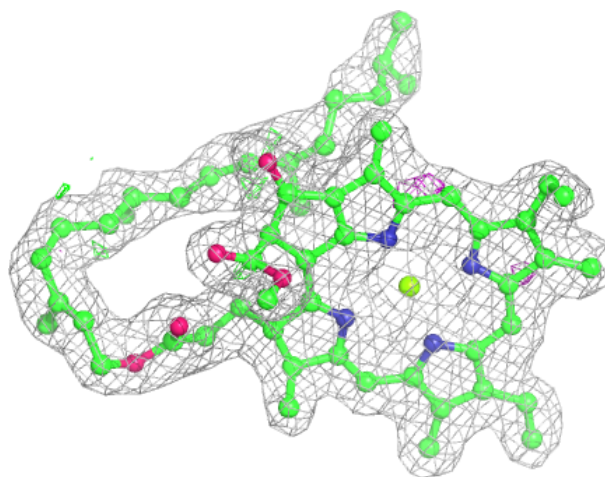
**Electron density around BCR B 618:**

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



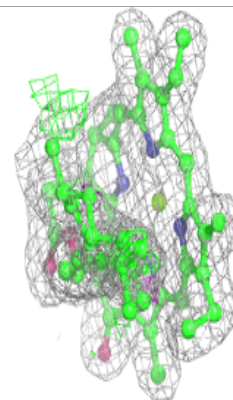
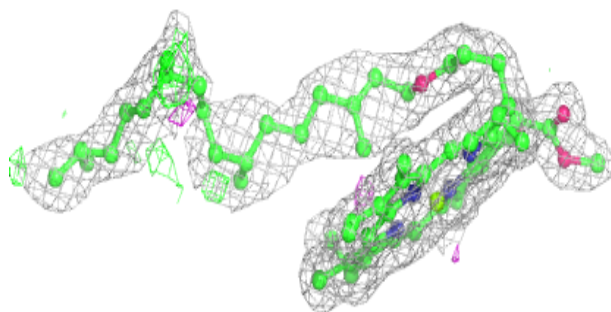
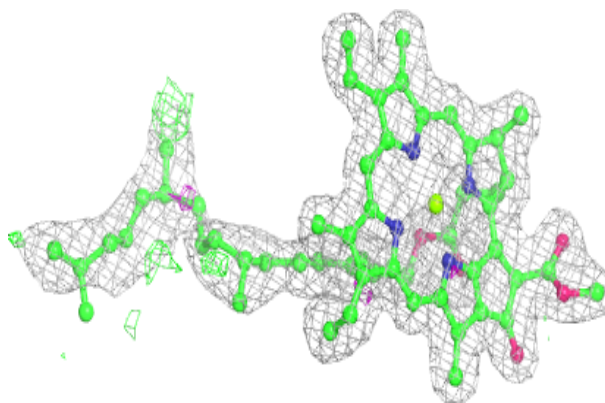
Electron density around CLA c 509:

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

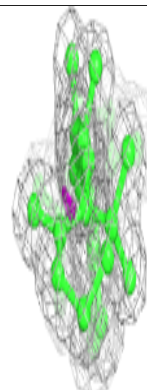
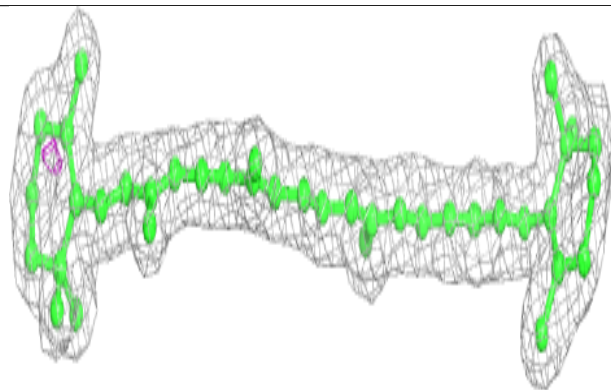
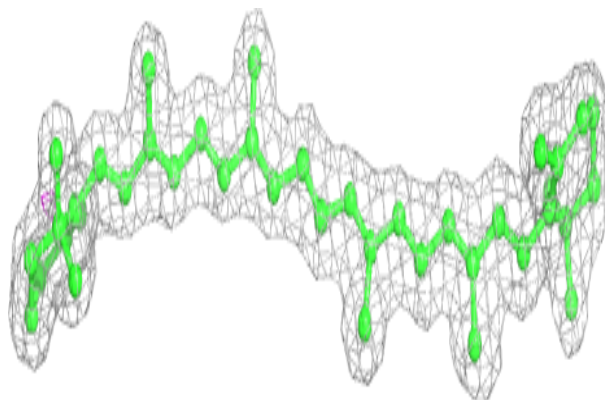


Electron density around CLA b 616:

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

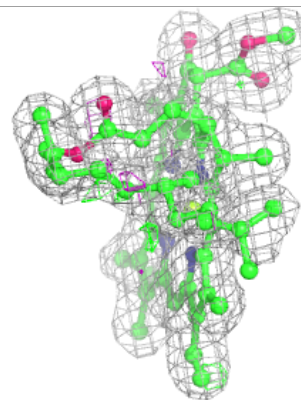
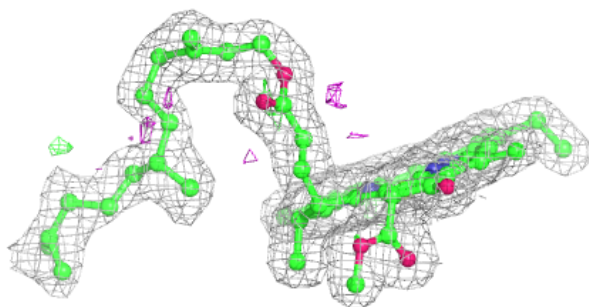
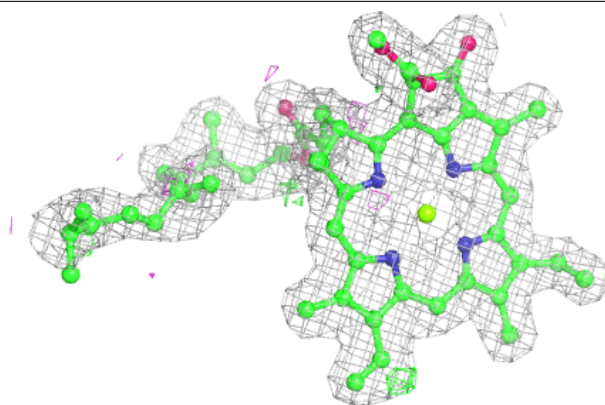
**Electron density around BCR a 408:**

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



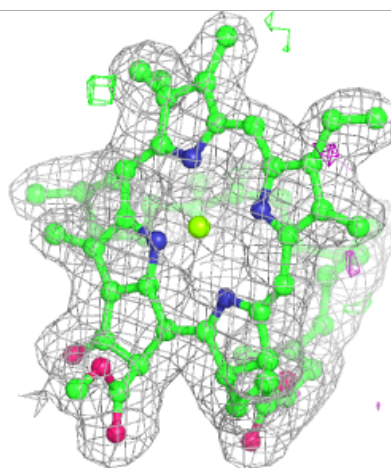
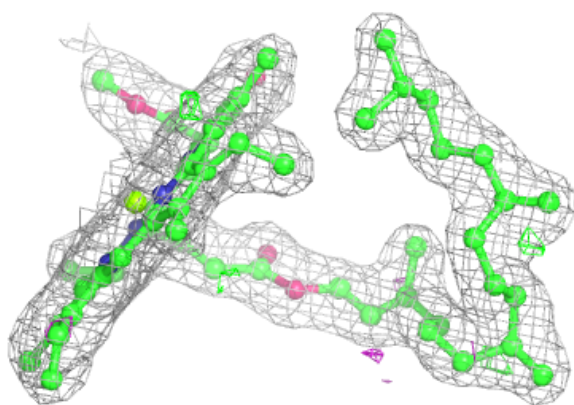
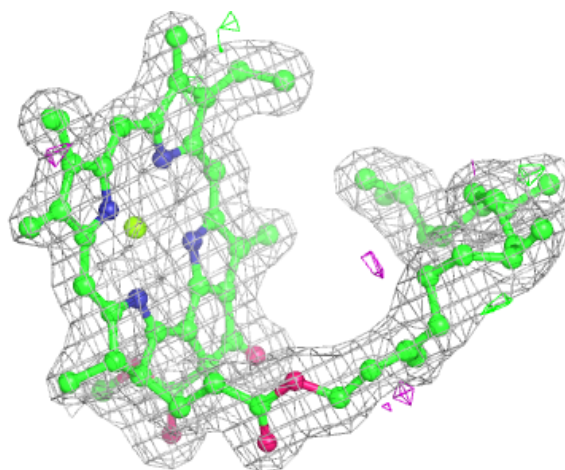
Electron density around CLA a 404:

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



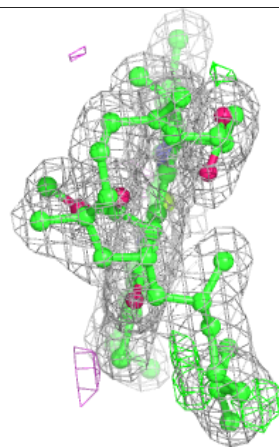
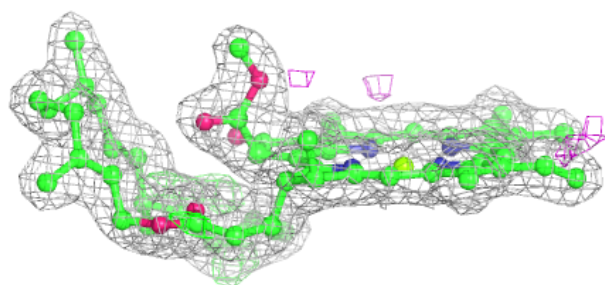
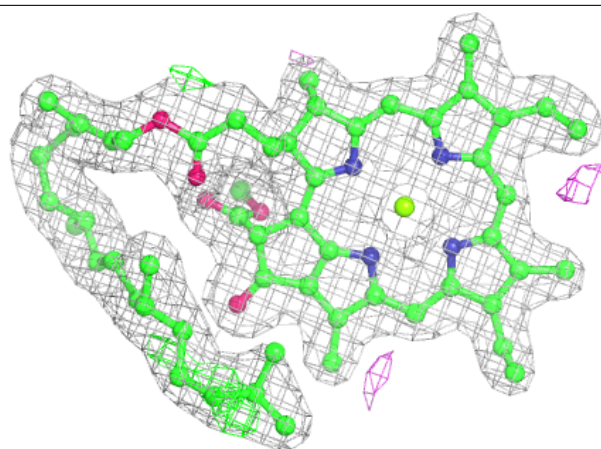
Electron density around CLA c 503:

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

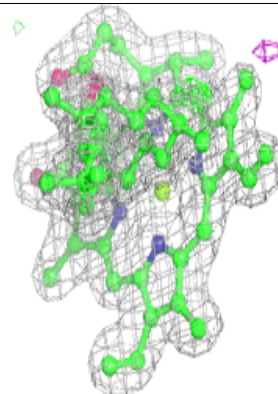
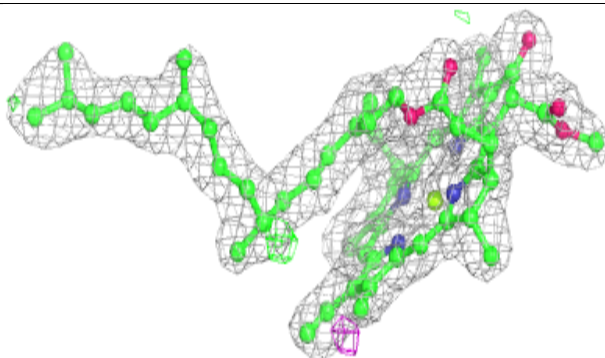
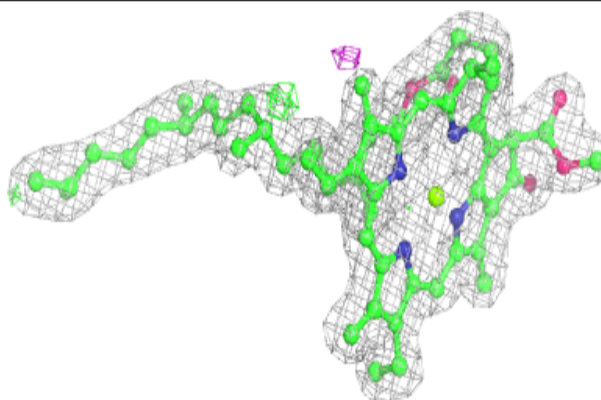


Electron density around CLA b 612:

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

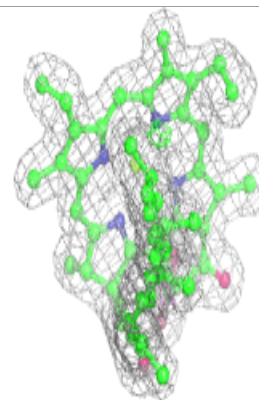
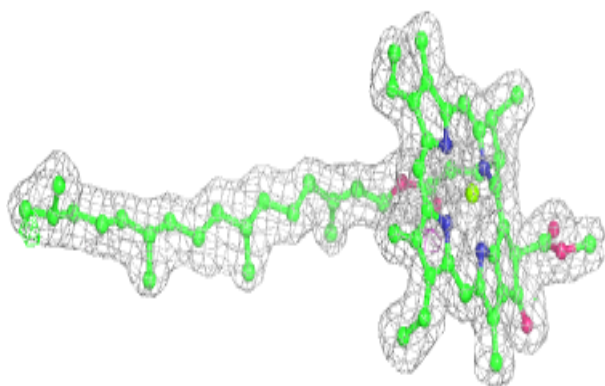
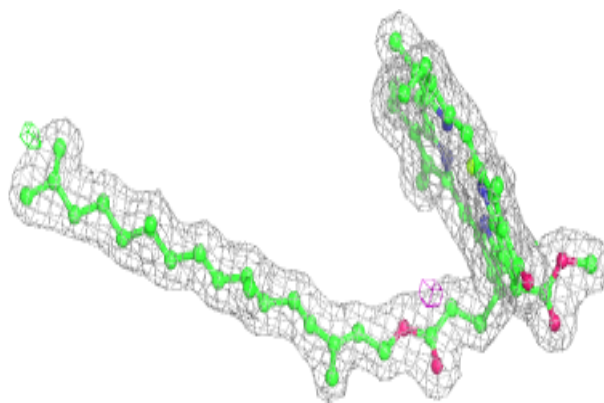
**Electron density around CLA C 505:**

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



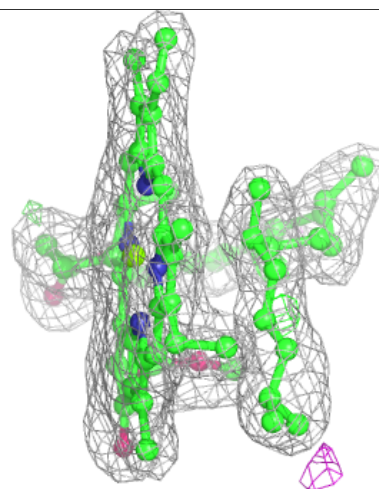
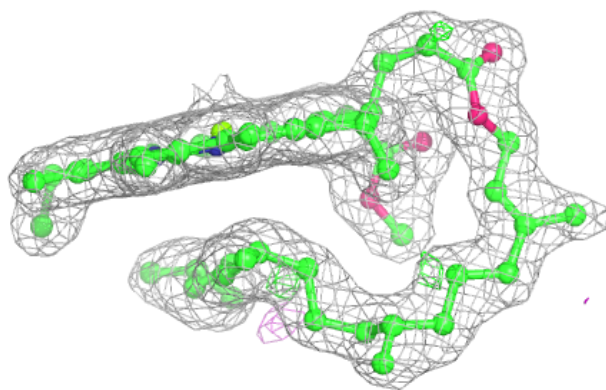
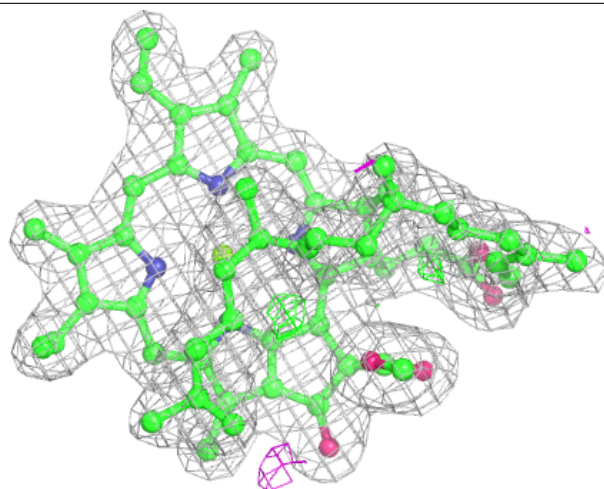
Electron density around CLA b 609:

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



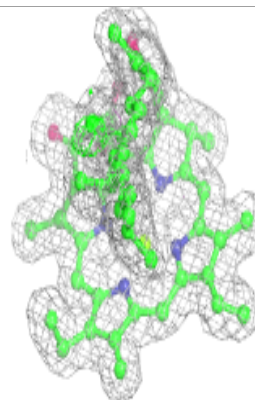
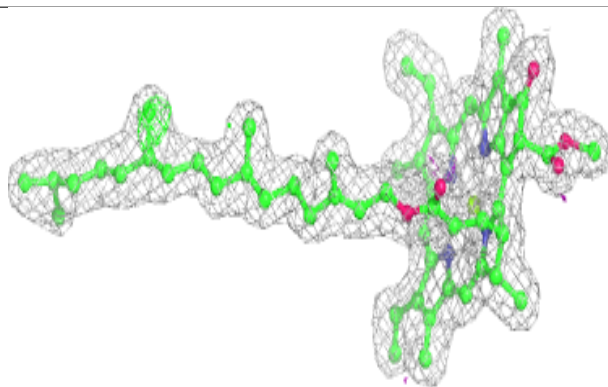
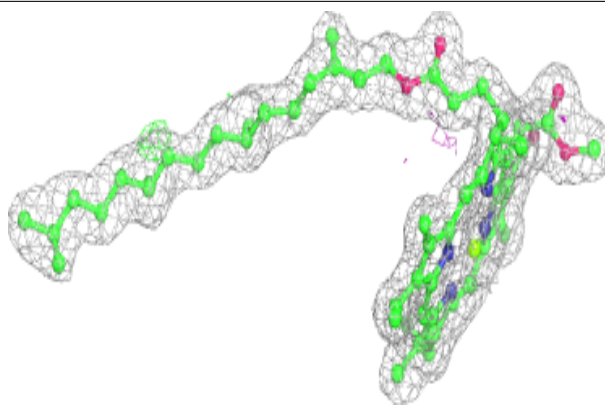
Electron density around CLA c 510:

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

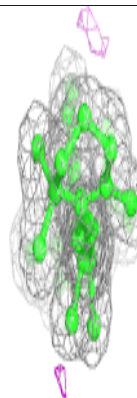
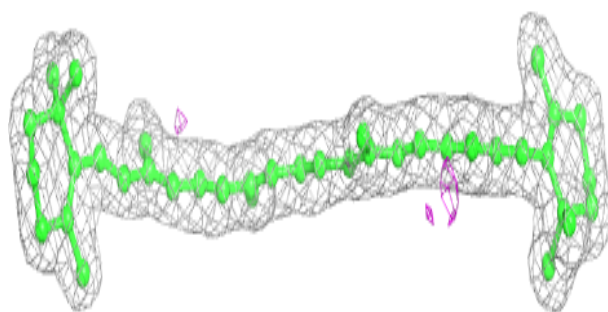
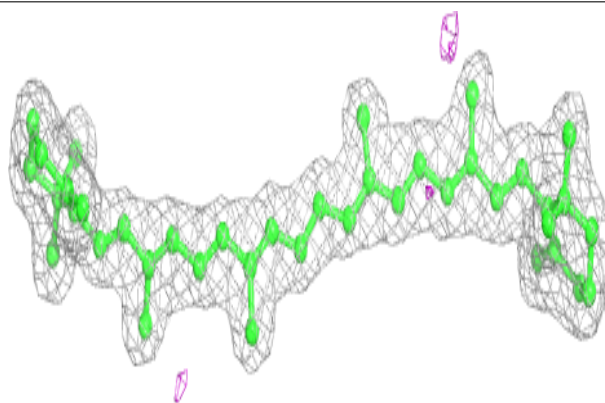


Electron density around CLA B 608:

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

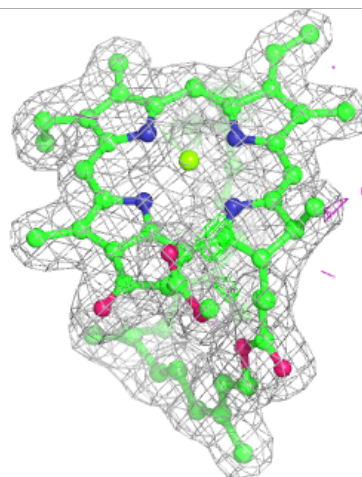
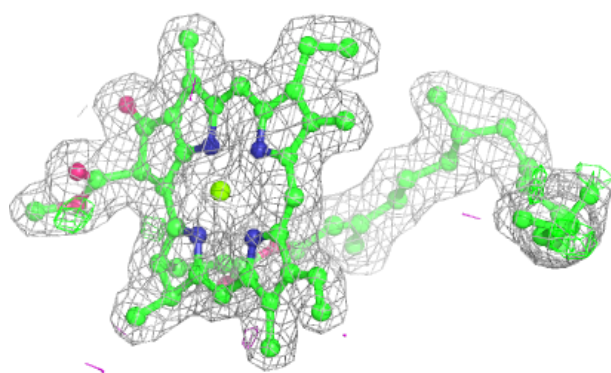
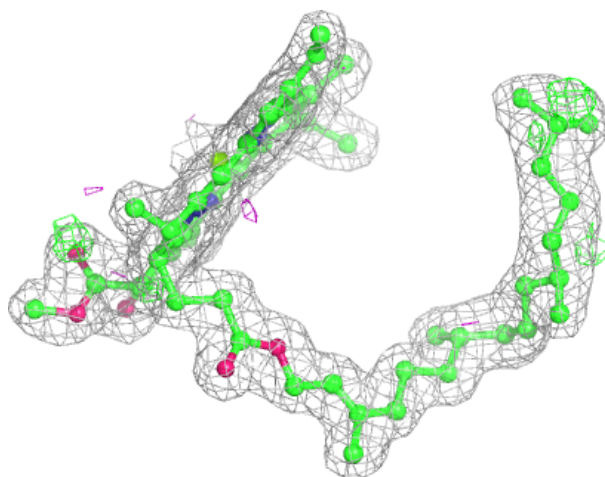
**Electron density around BCR A 405:**

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



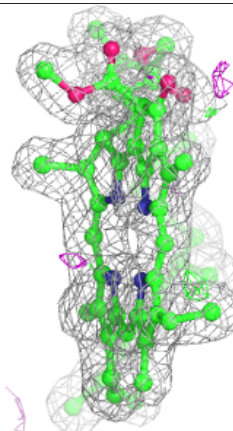
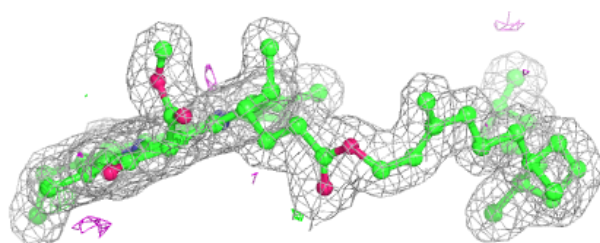
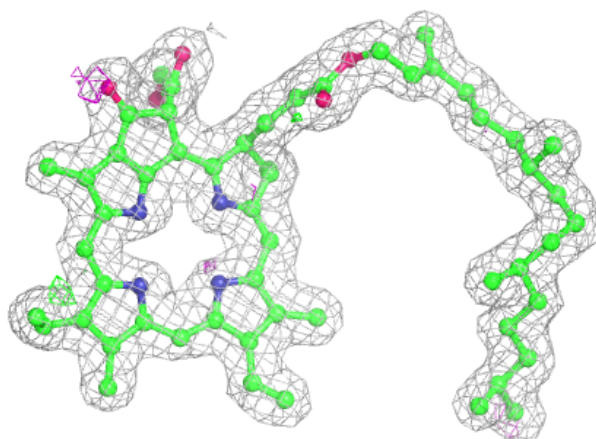
Electron density around CLA b 613:

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



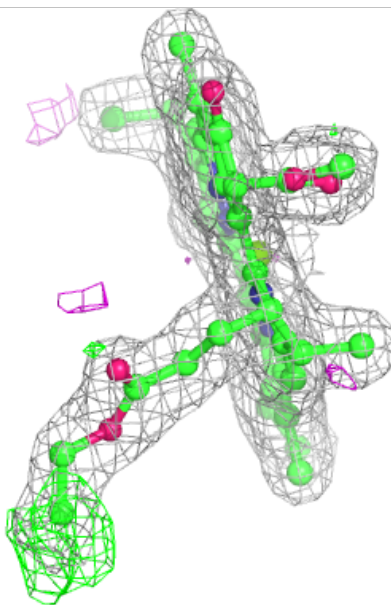
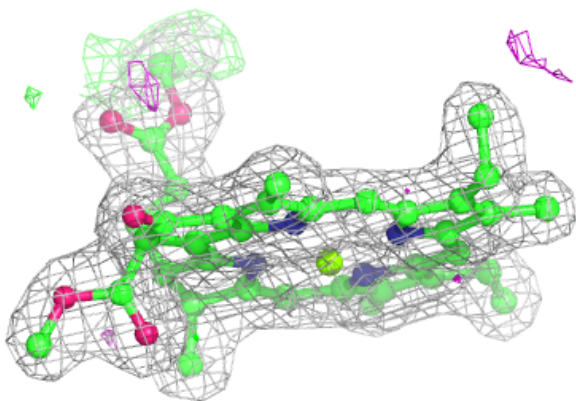
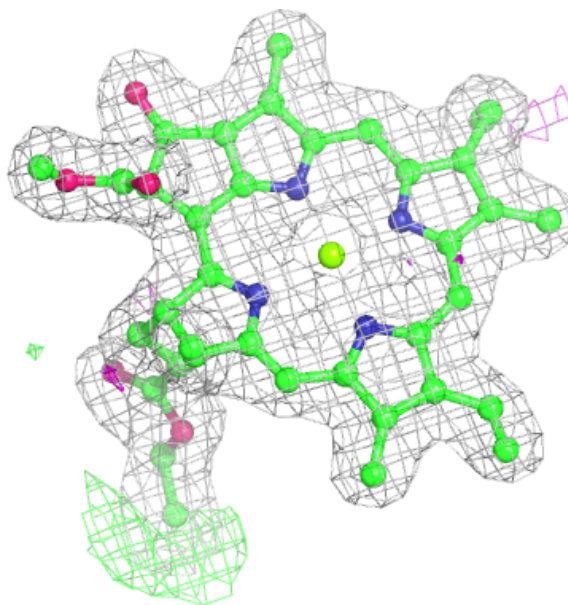
Electron density around PHO a 405:

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



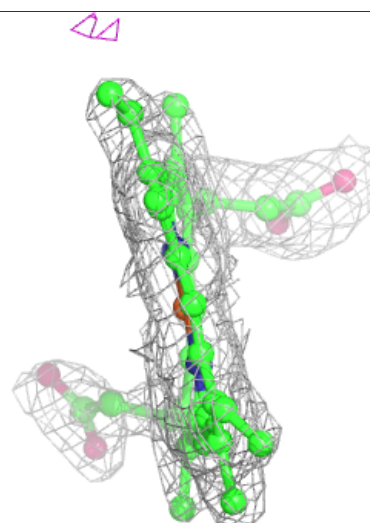
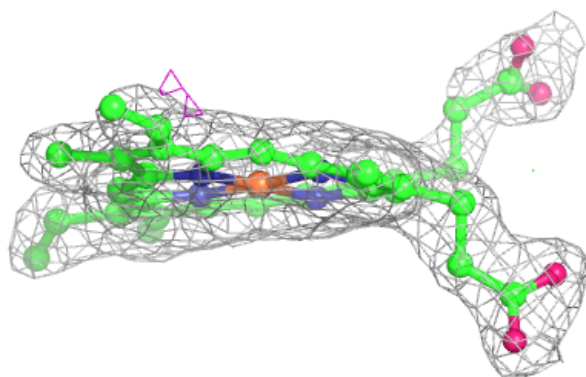
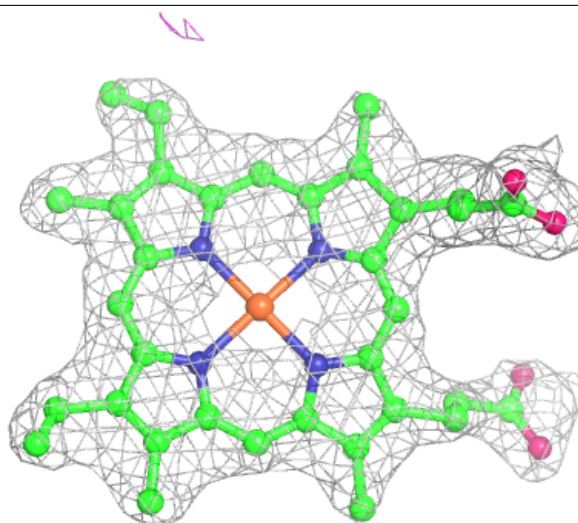
Electron density around CLA a 407:

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



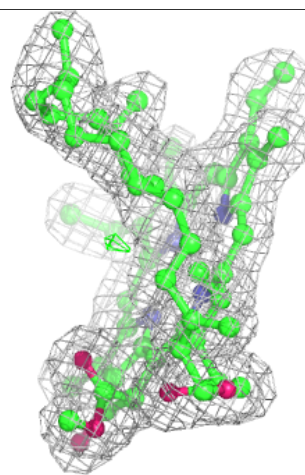
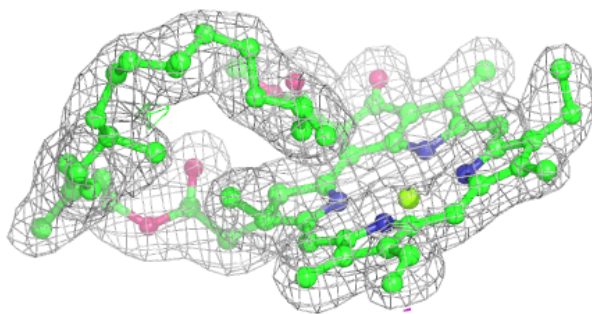
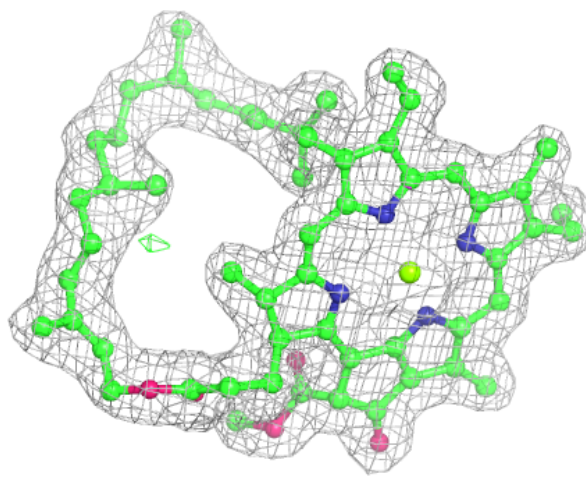
Electron density around HEM e 102:

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



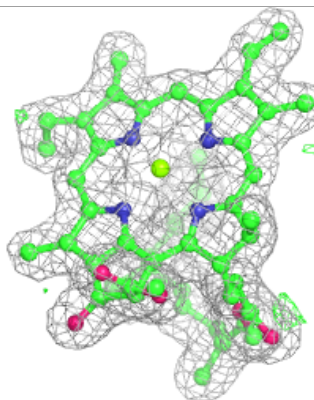
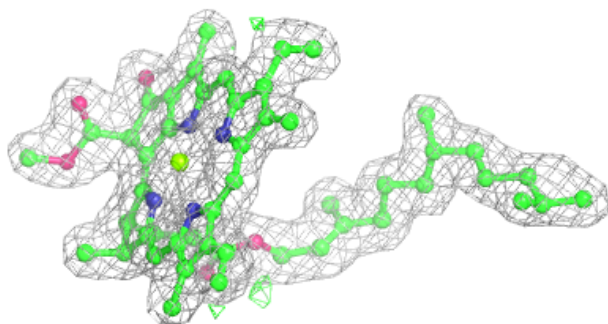
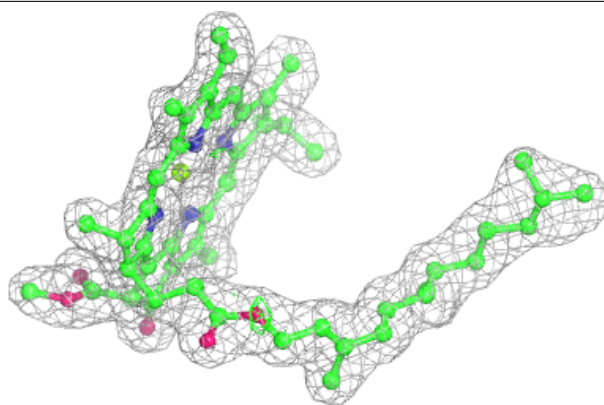
Electron density around CLA b 617:

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

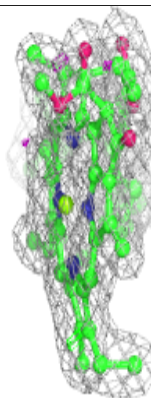
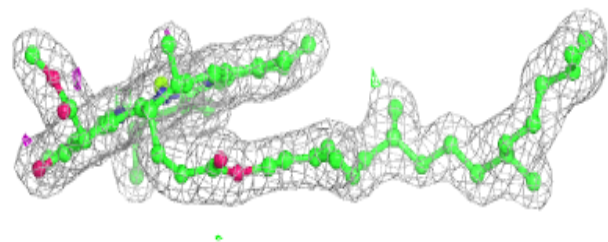
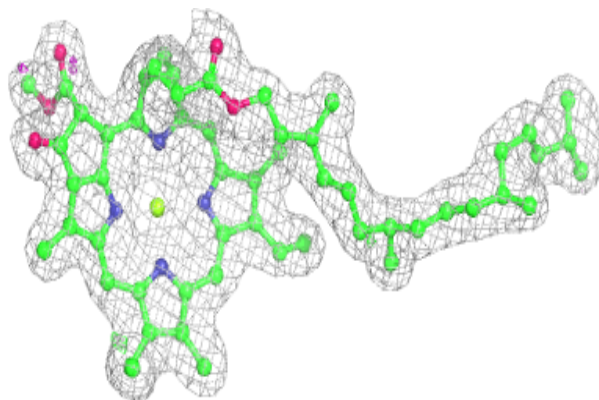


Electron density around CLA c 508:

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

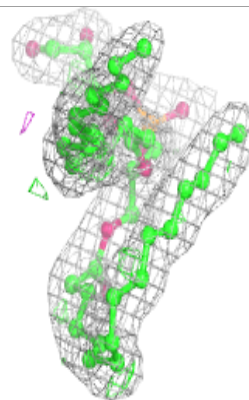
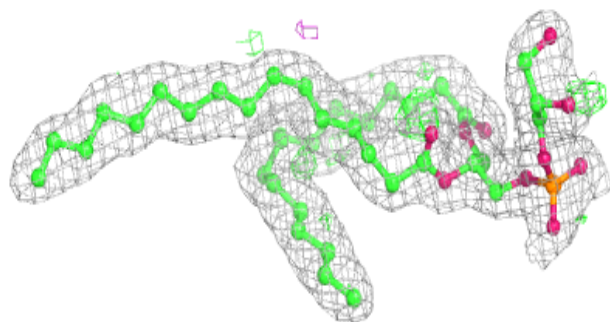
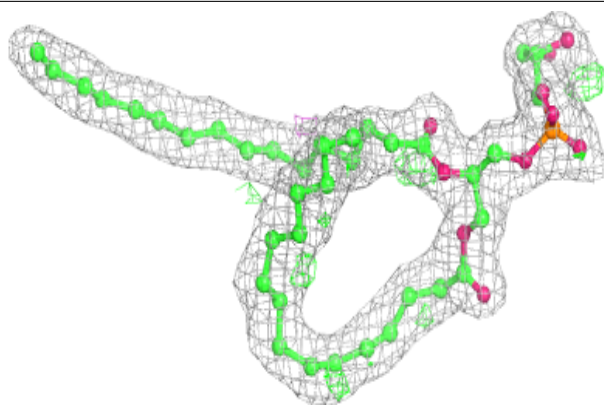
**Electron density around CLA b 605:**

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

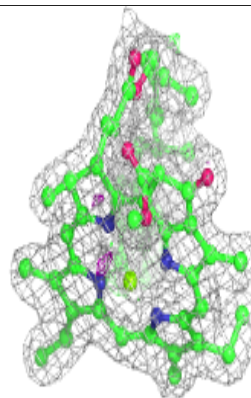
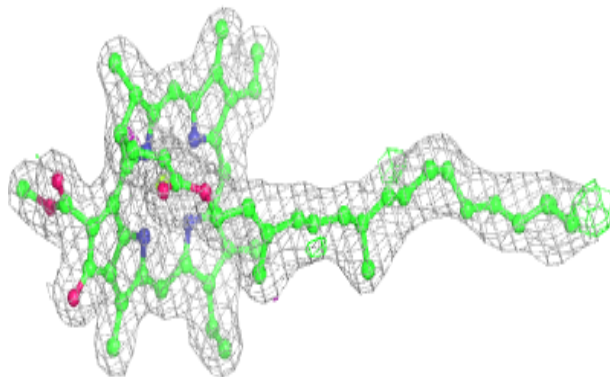
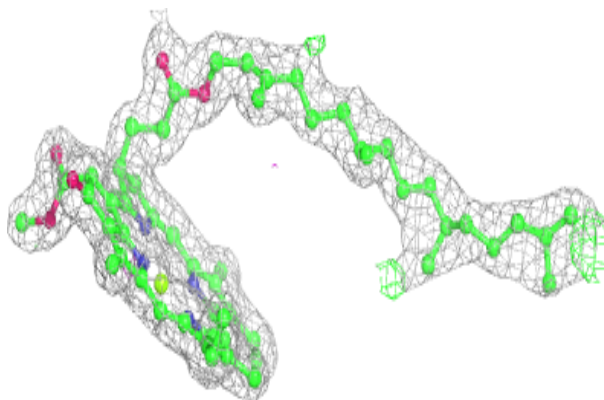


Electron density around LHG d 406:

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

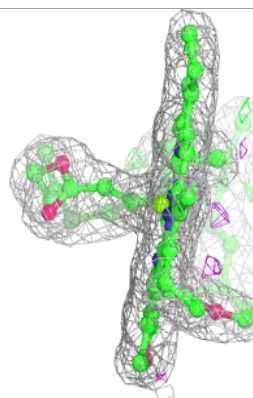
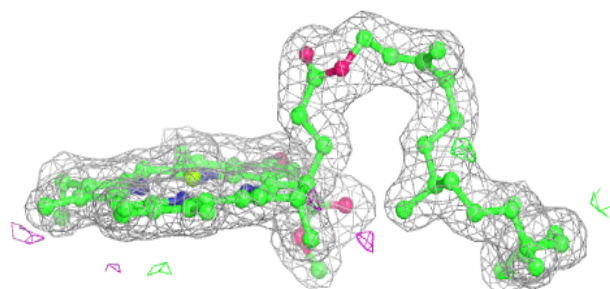
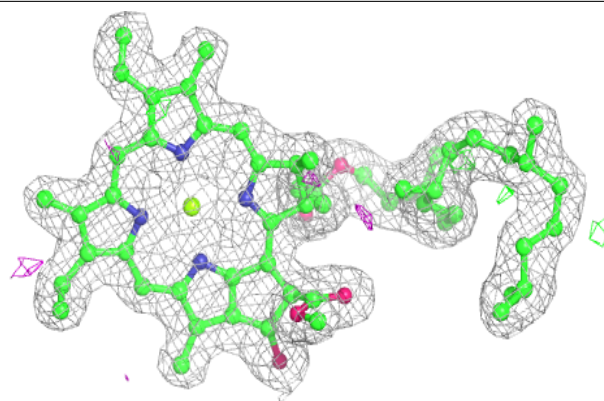
**Electron density around CLA c 504:**

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

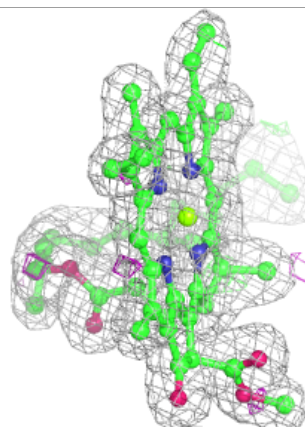
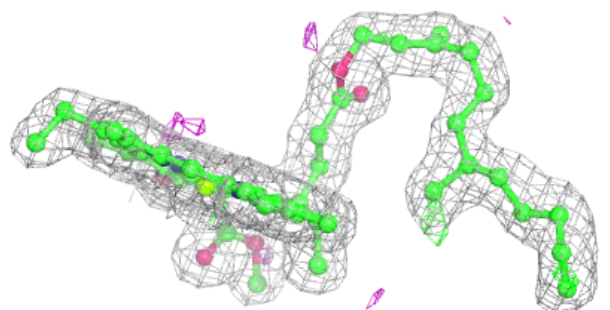
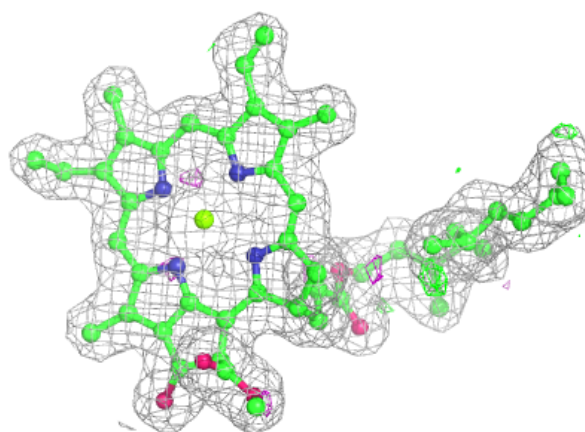


Electron density around CLA b 614:

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

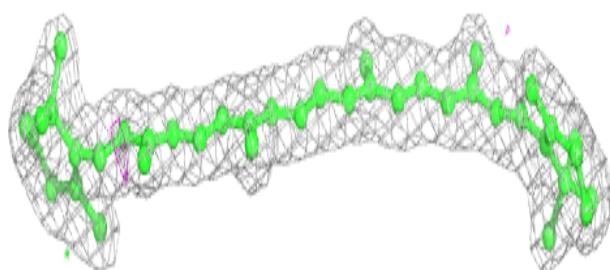
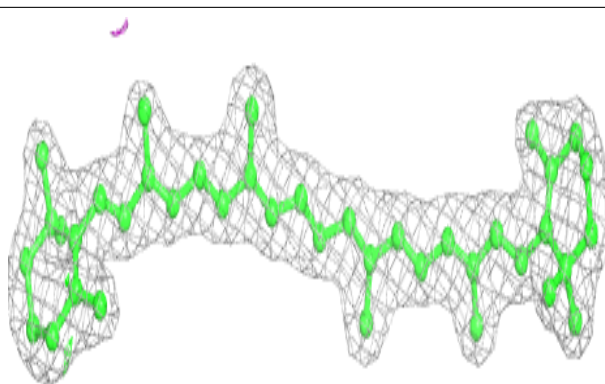
**Electron density around CLA A 402:**

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

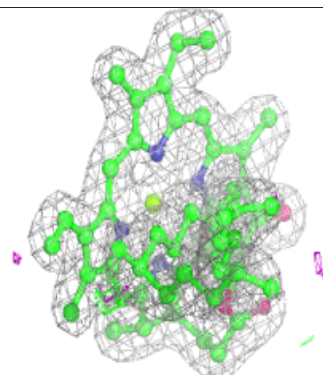
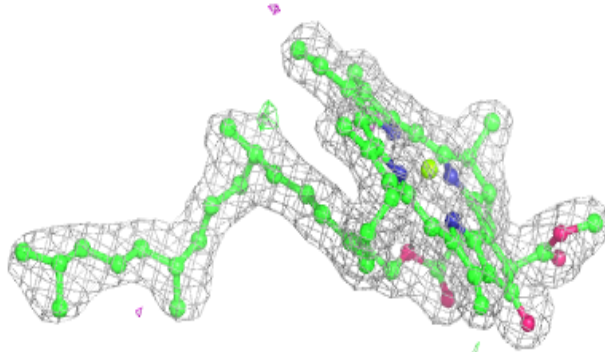
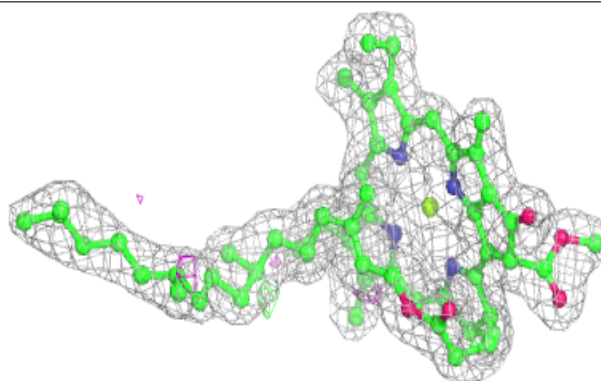


Electron density around BCR b 621:

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

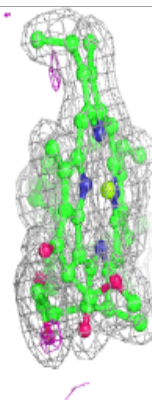
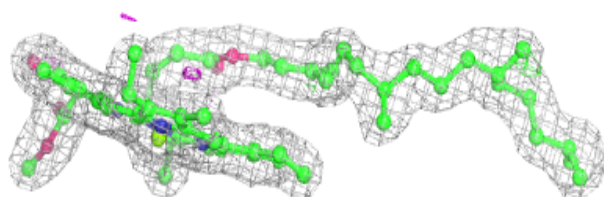
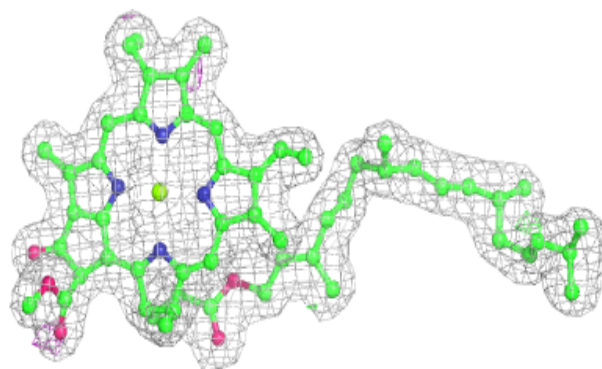
**Electron density around CLA c 505:**

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

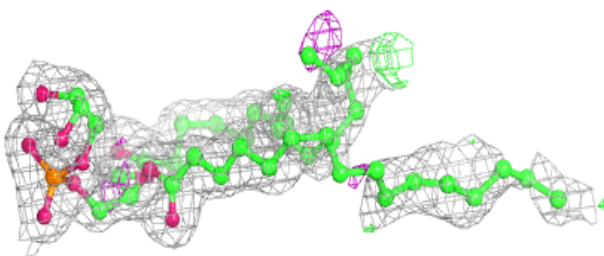
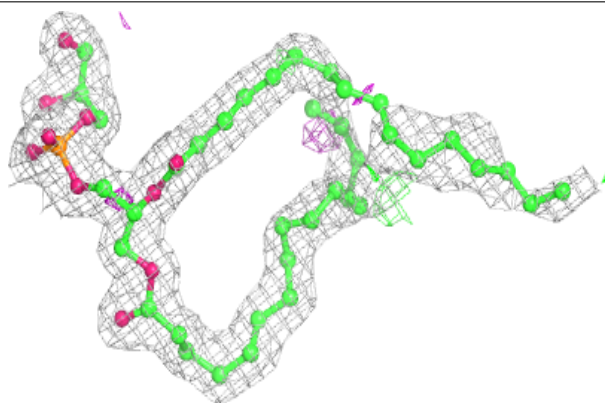


Electron density around CLA B 604:

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

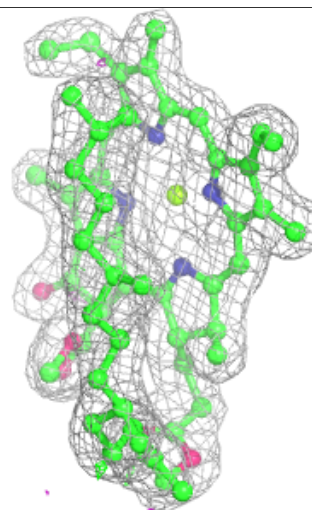
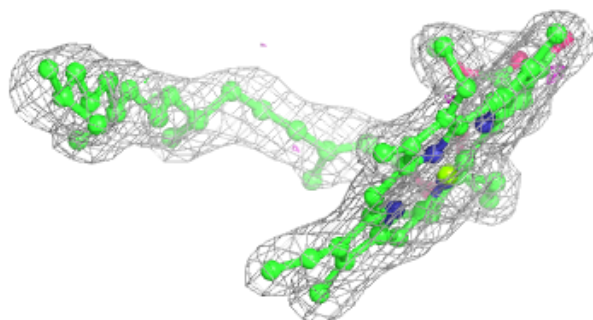
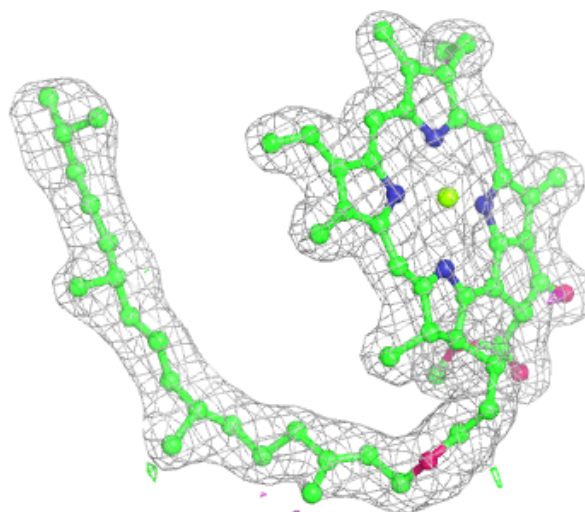
**Electron density around LHG d 408:**

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



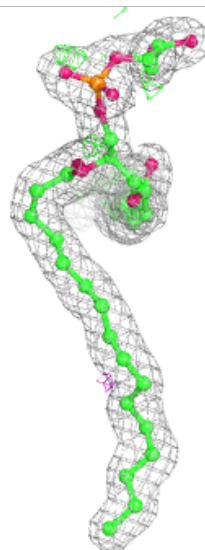
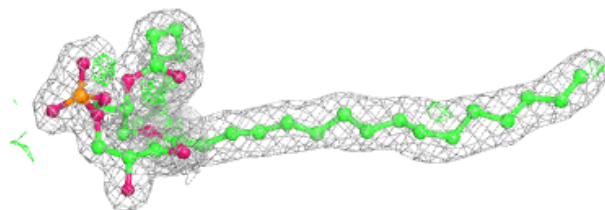
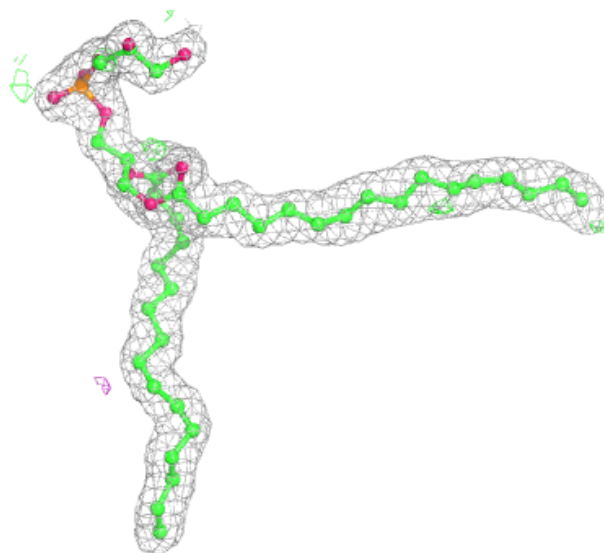
Electron density around CLA c 507:

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



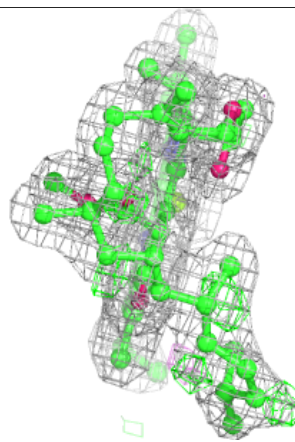
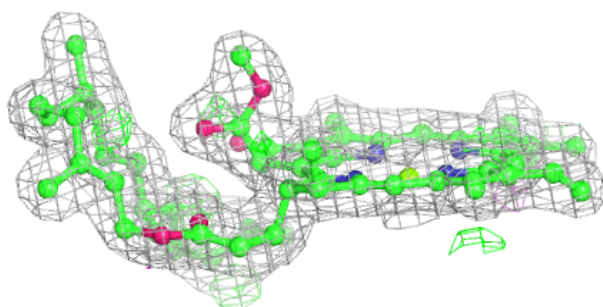
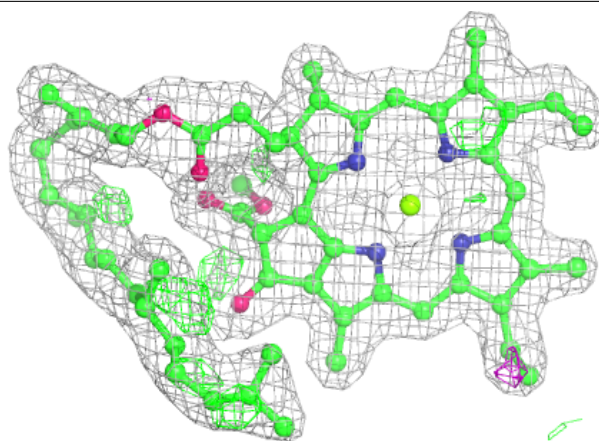
Electron density around LHG L 101:

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



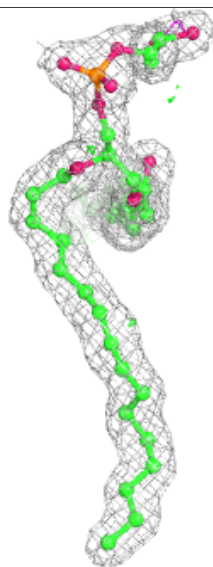
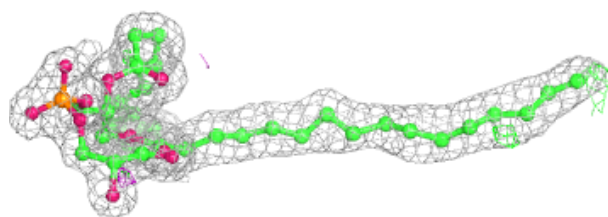
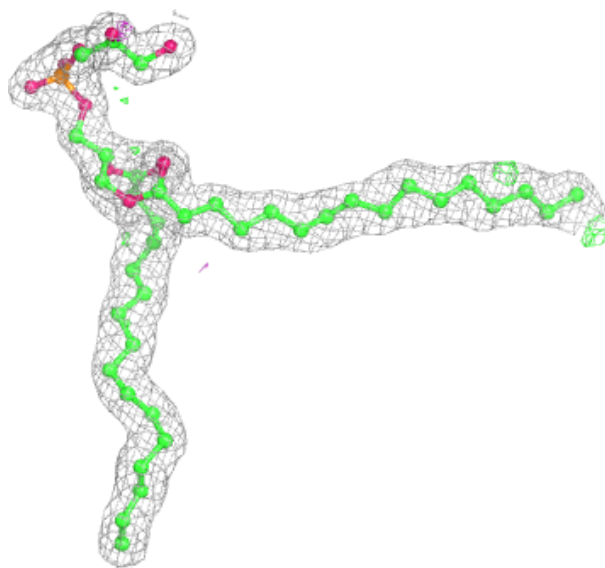
Electron density around CLA B 611:

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



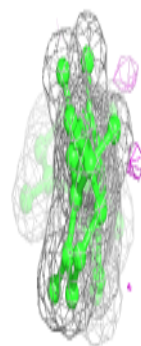
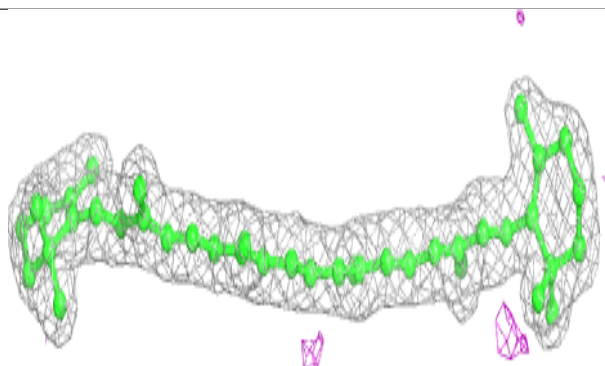
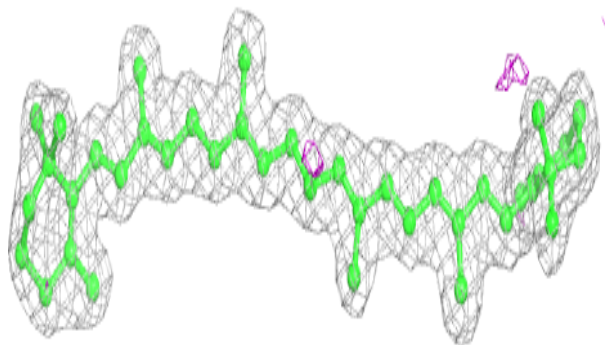
Electron density around LHG 1 102:

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

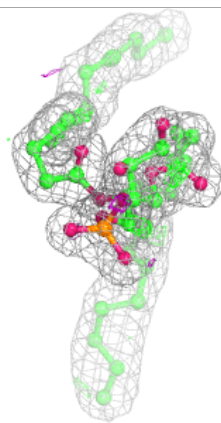
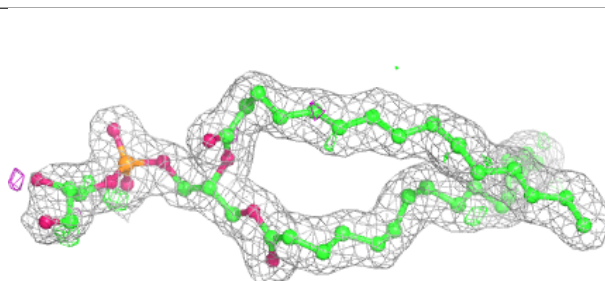
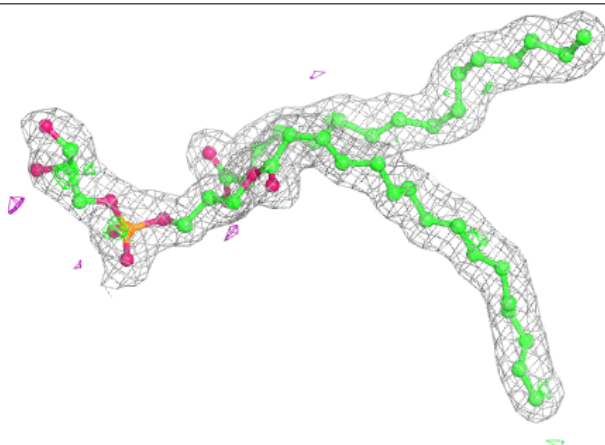


Electron density around BCR b 619:

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

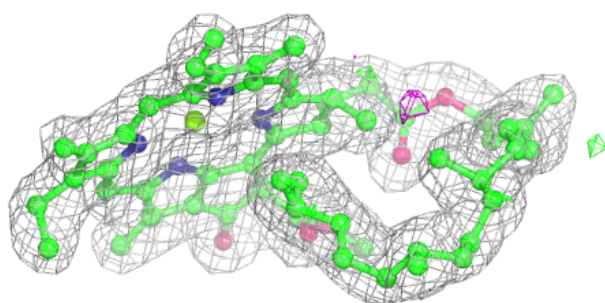
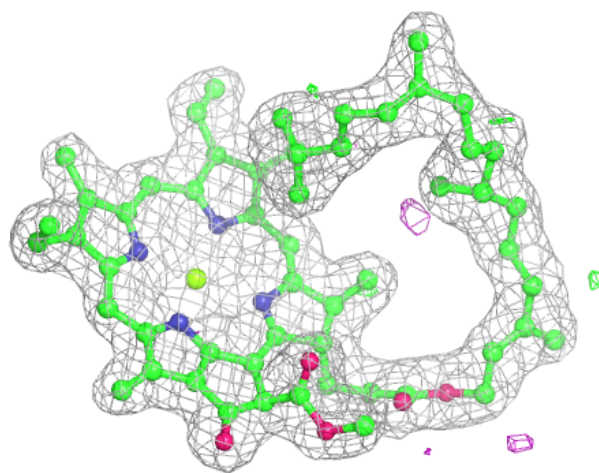
**Electron density around LHG d 407:**

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



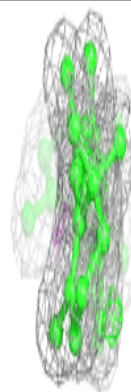
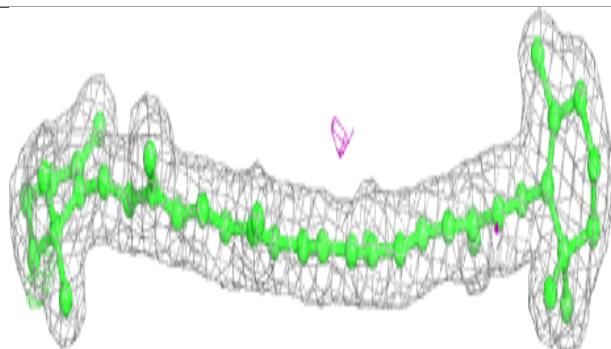
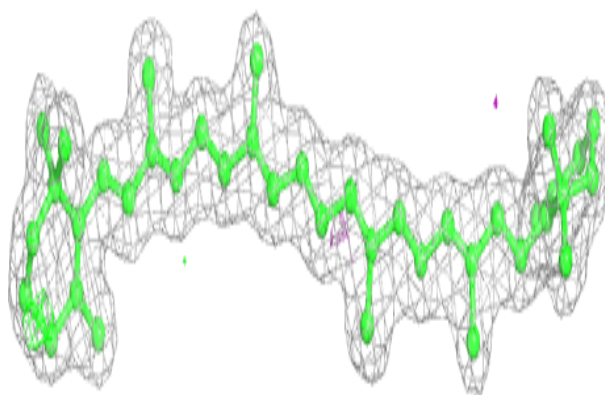
Electron density around CLA B 616:

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

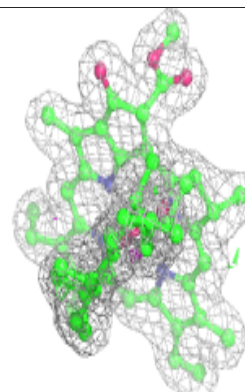
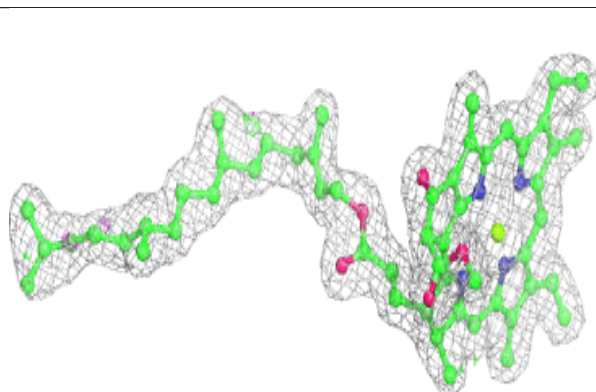
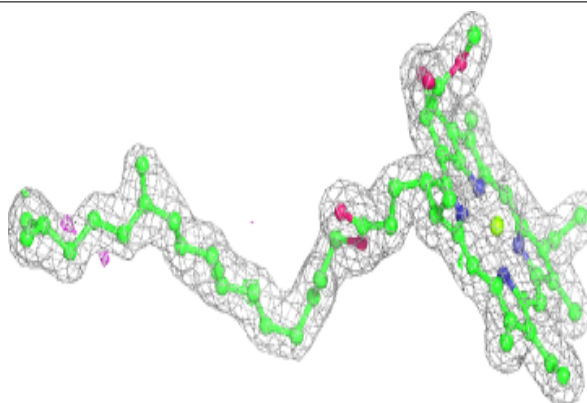


Electron density around BCR B 617:

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

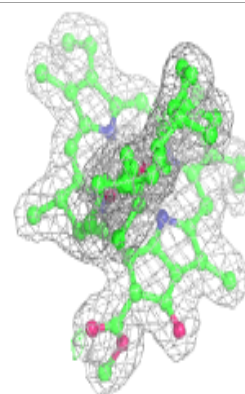
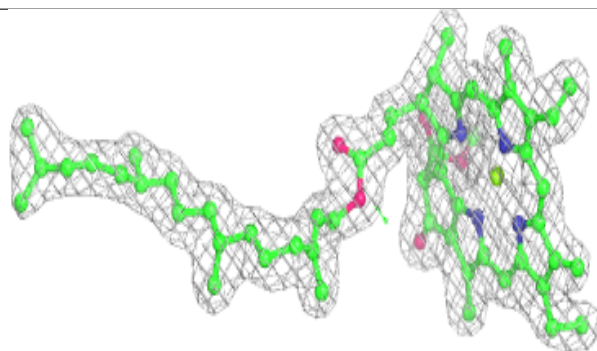
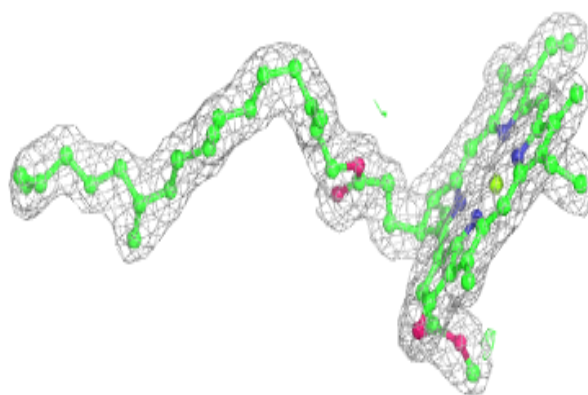
**Electron density around CLA c 502:**

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

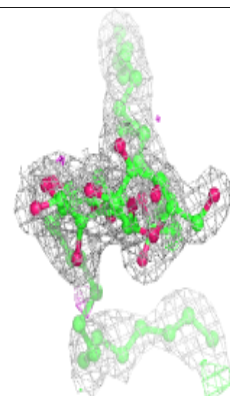
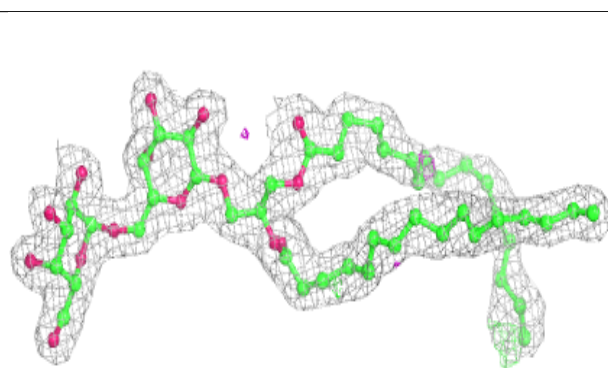
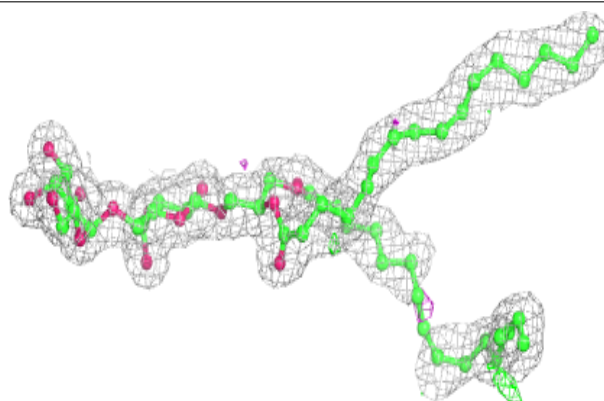


Electron density around CLA C 502:

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

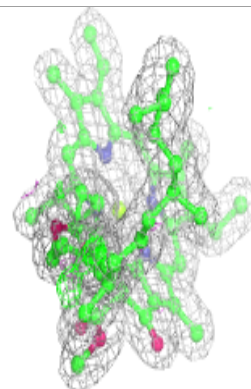
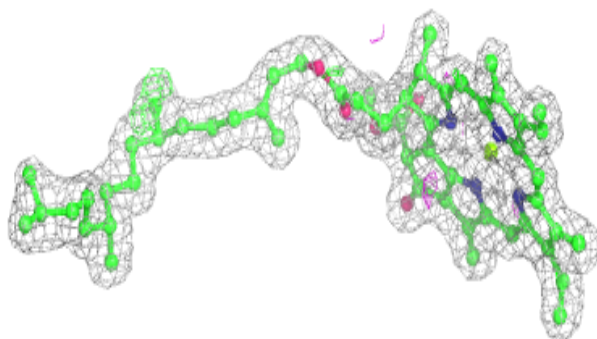
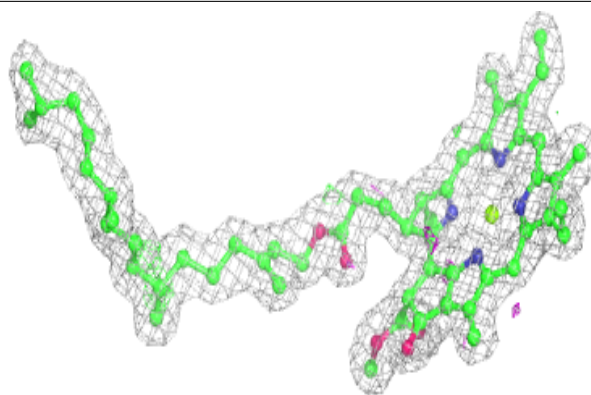
**Electron density around DGD C 516:**

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

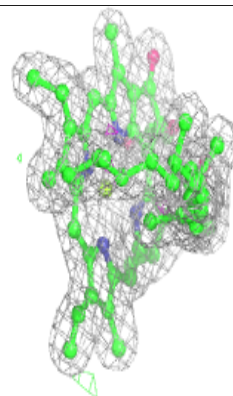
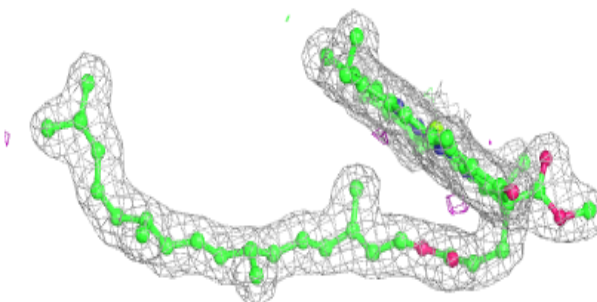
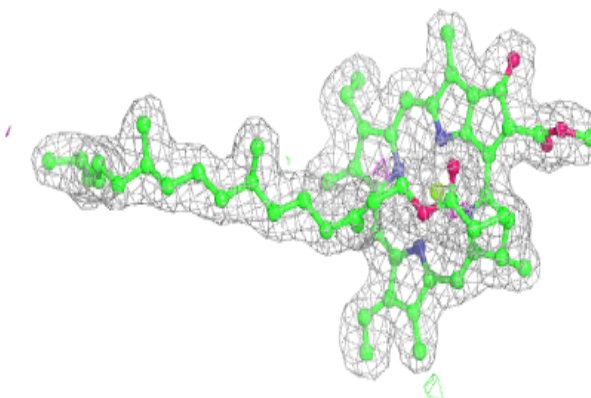


Electron density around CLA a 403:

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

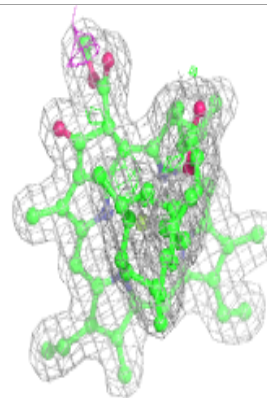
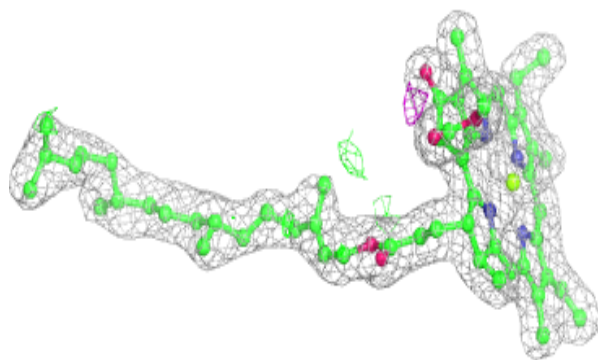
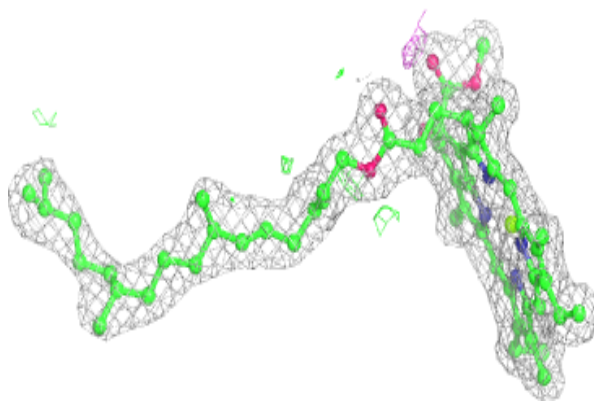
**Electron density around CLA b 610:**

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



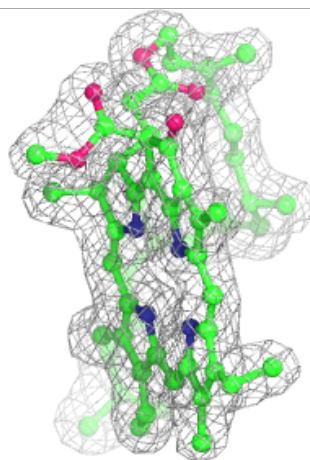
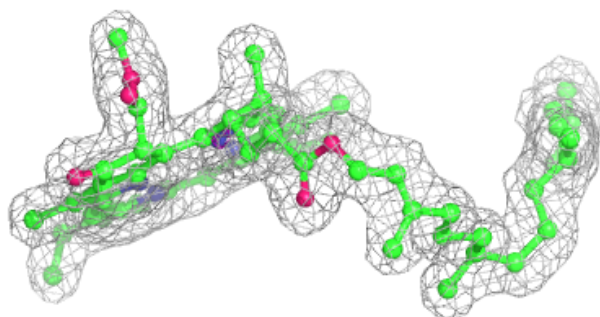
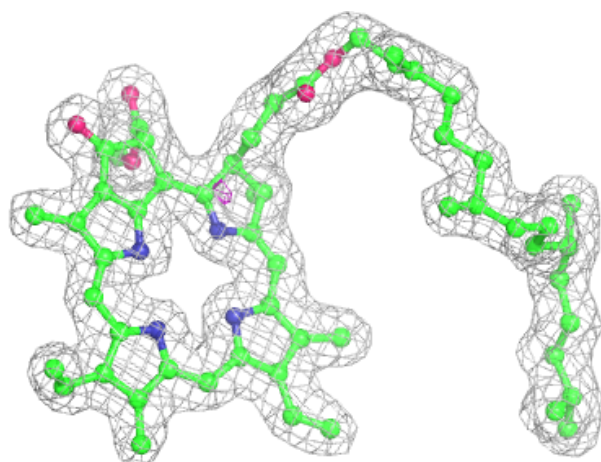
Electron density around CLA B 605:

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



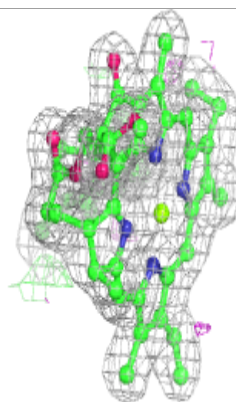
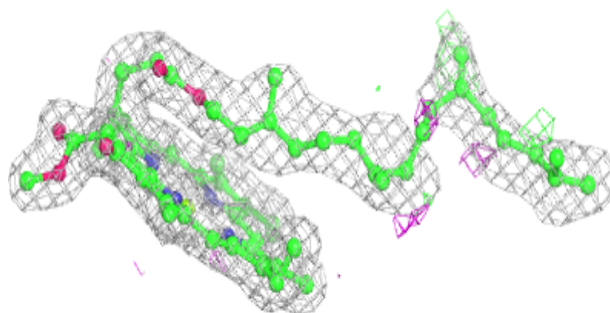
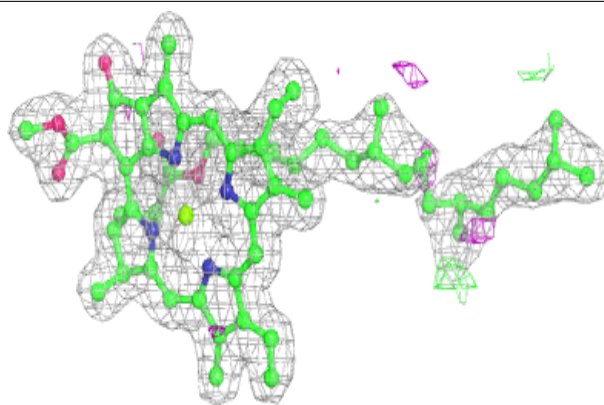
Electron density around PHO D 403:

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

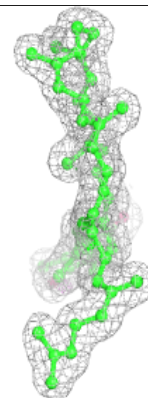
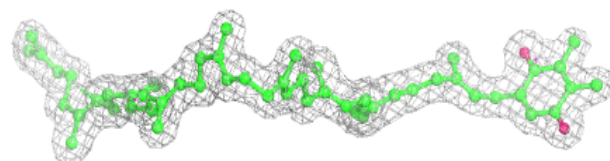
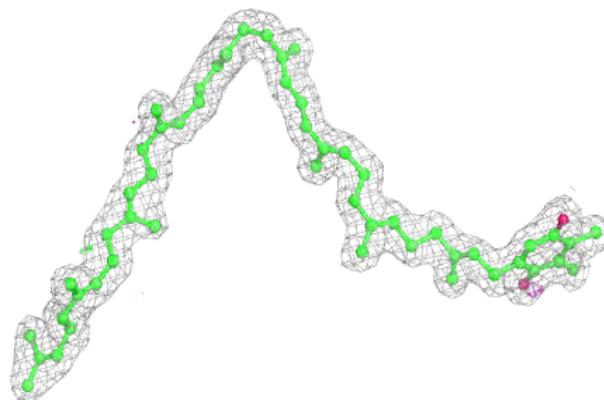


Electron density around CLA B 615:

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

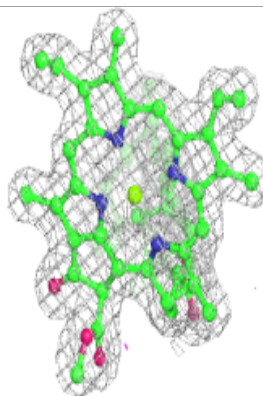
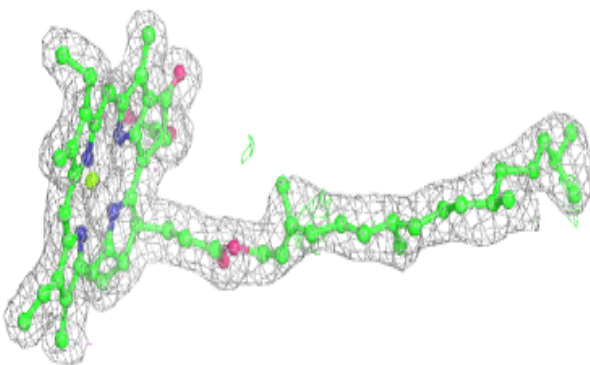
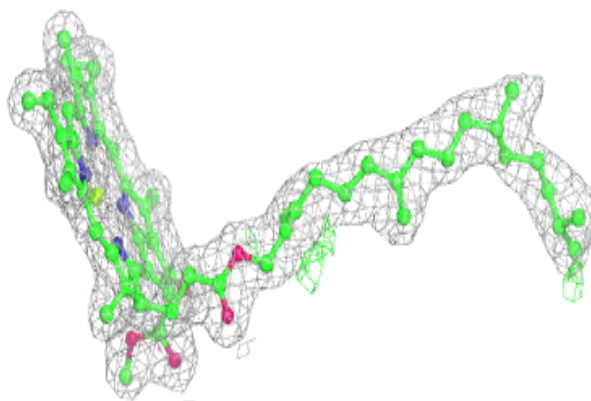
**Electron density around PL9 D 412:**

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

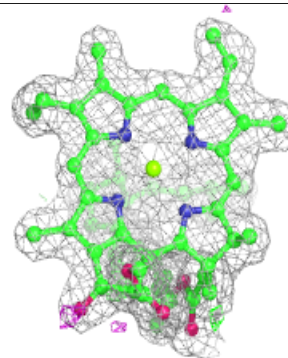
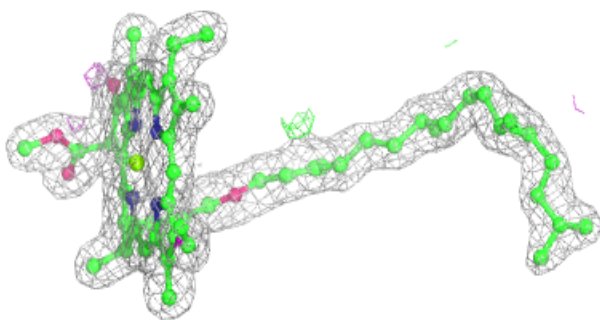
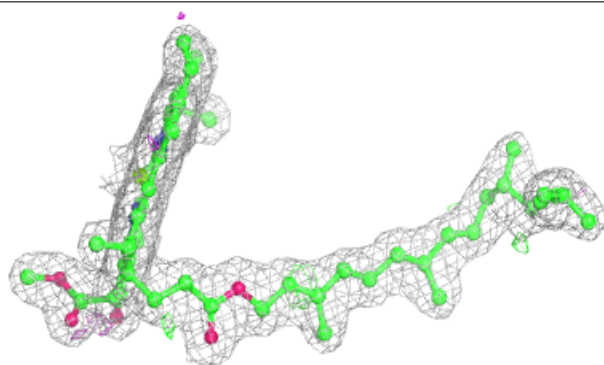


Electron density around CLA b 606:

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

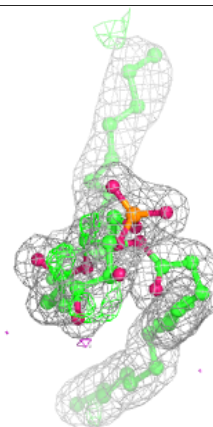
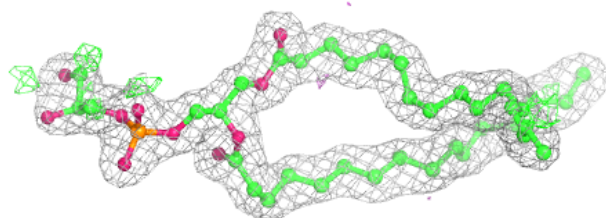
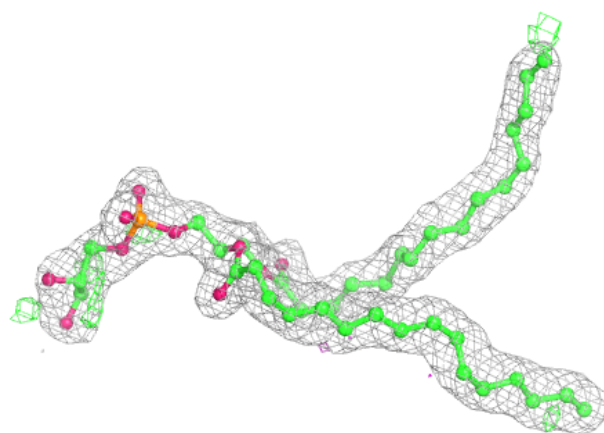
**Electron density around CLA b 607:**

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

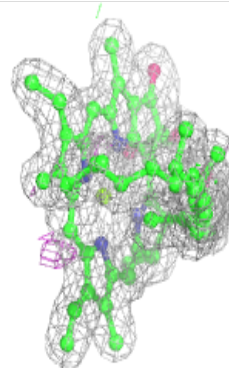
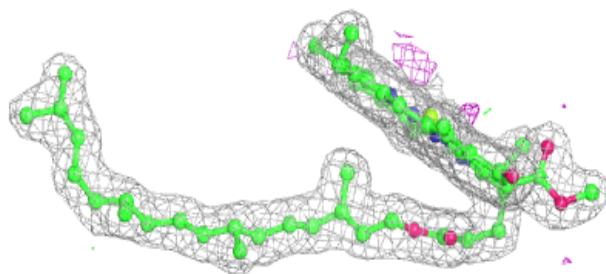
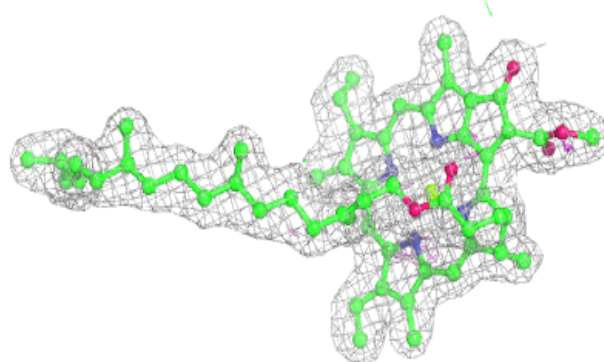


Electron density around LHG D 408:

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

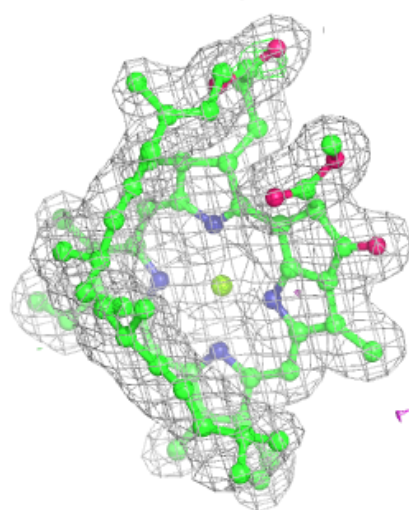
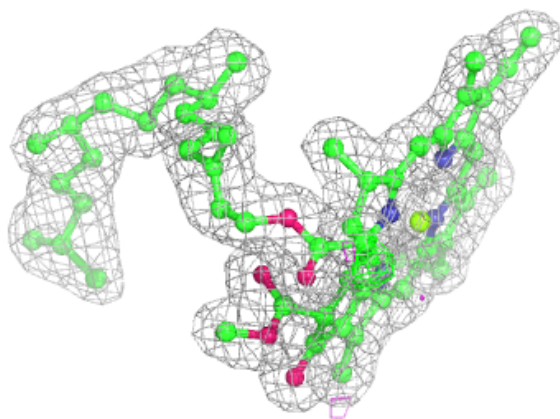
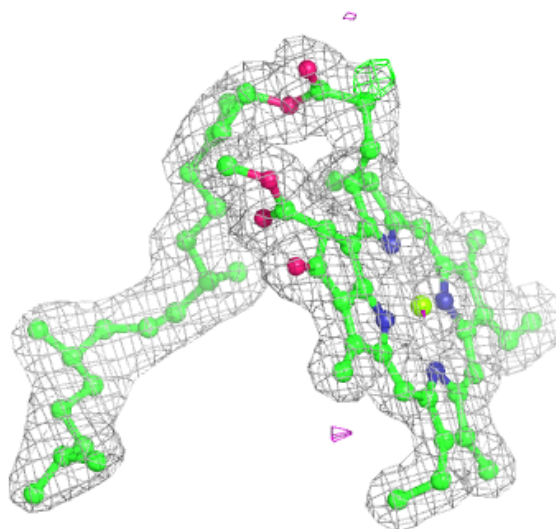
**Electron density around CLA B 609:**

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



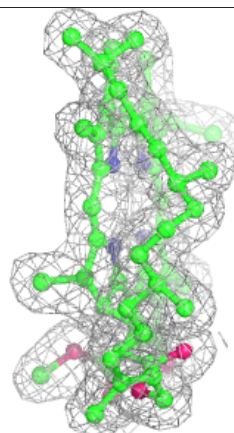
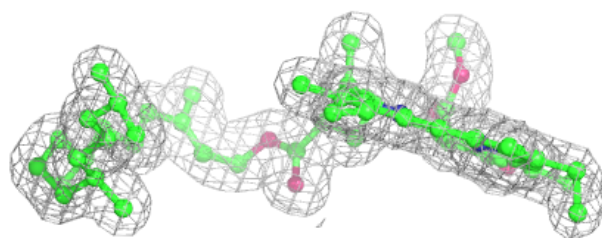
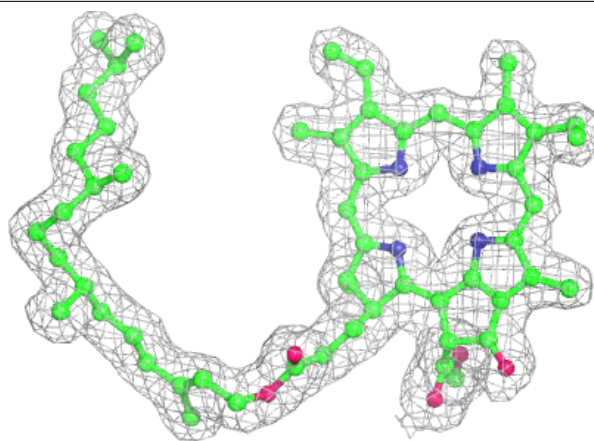
Electron density around CLA b 615:

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



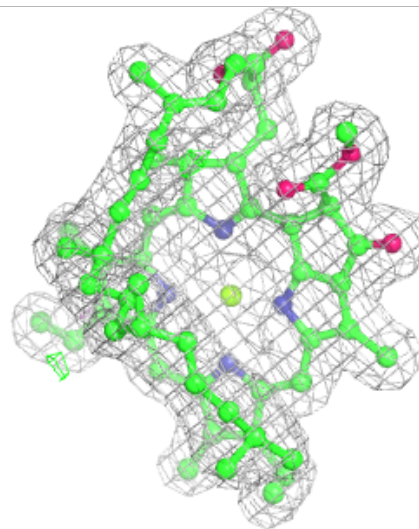
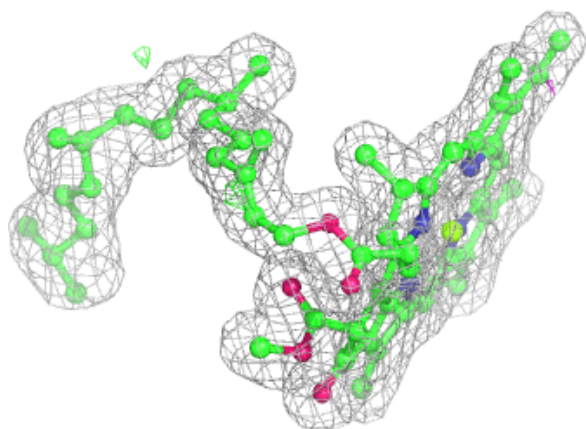
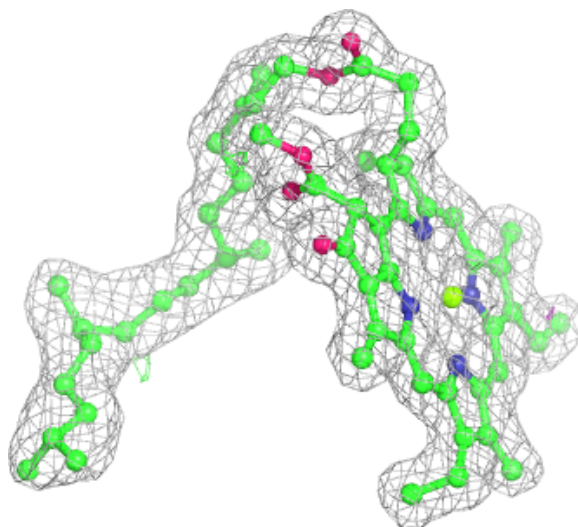
Electron density around PHO A 403:

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



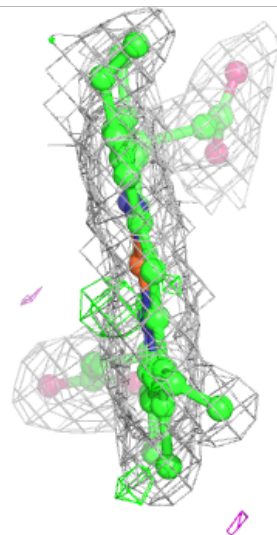
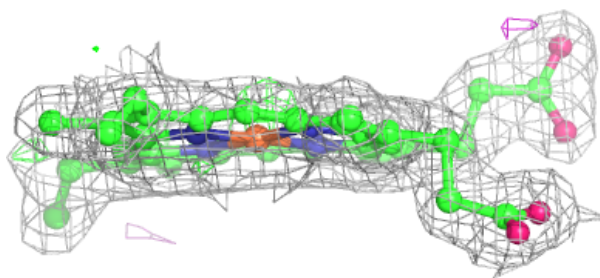
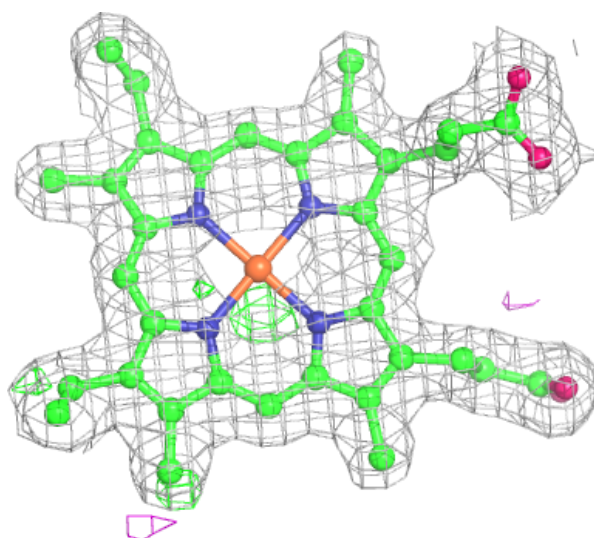
Electron density around CLA B 614:

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



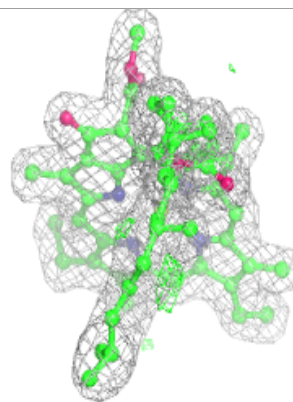
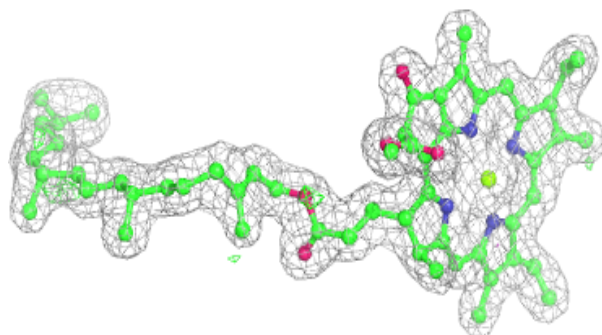
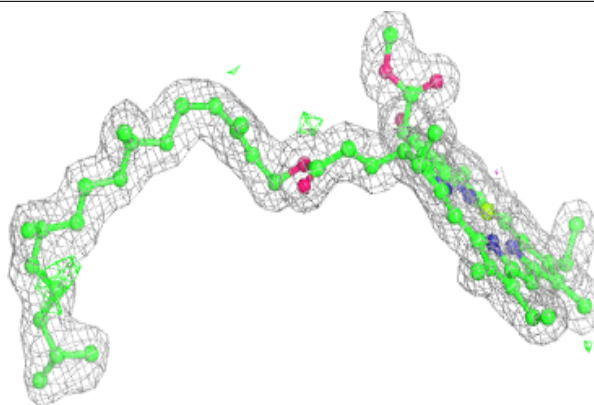
Electron density around HEC v 201:

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



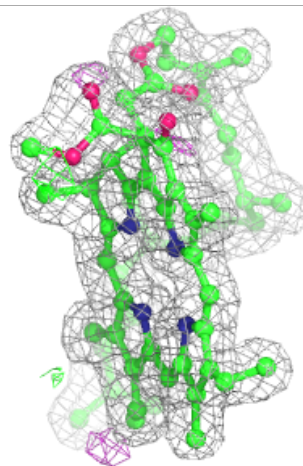
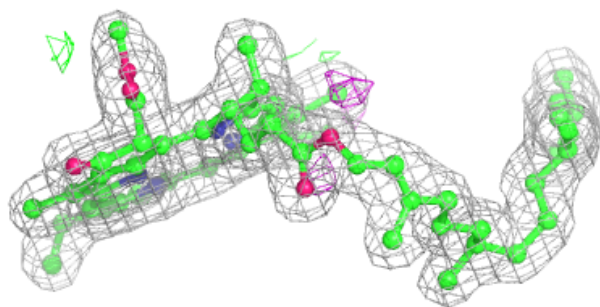
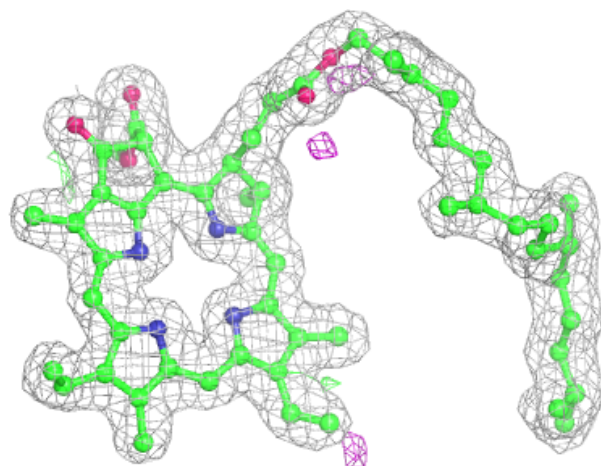
Electron density around CLA D 401:

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



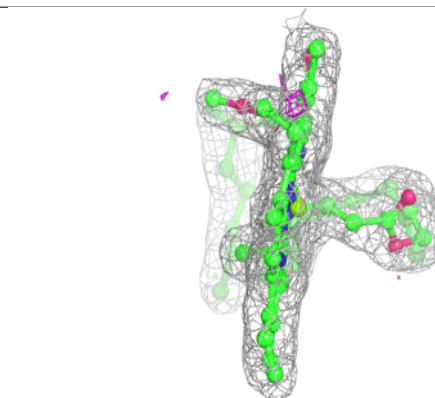
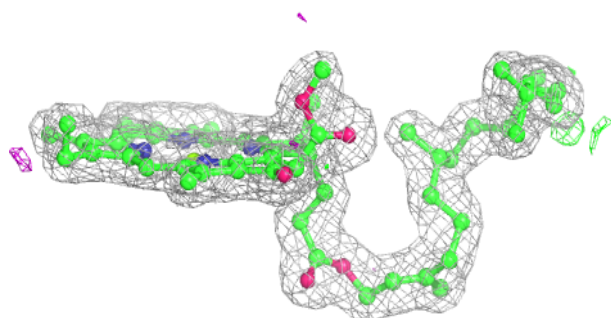
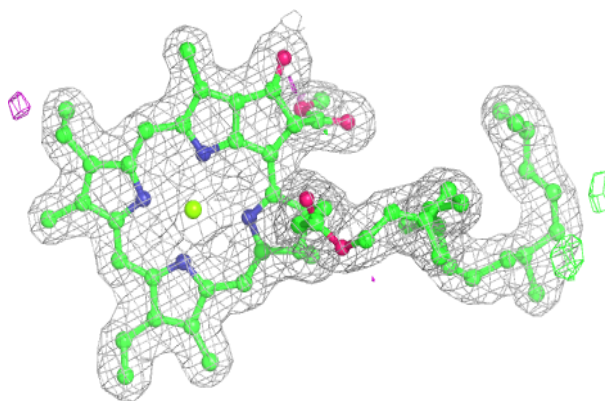
Electron density around PHO a 406:

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

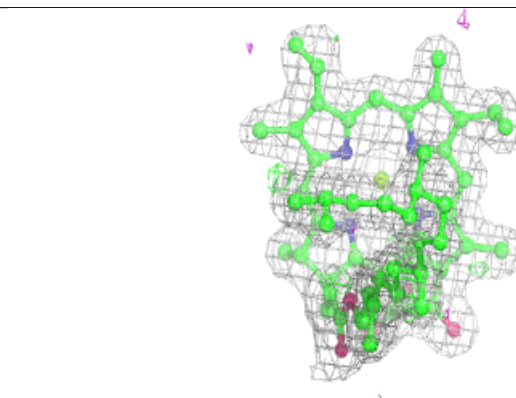
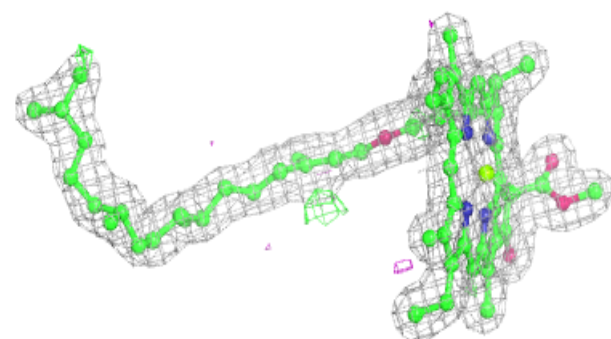
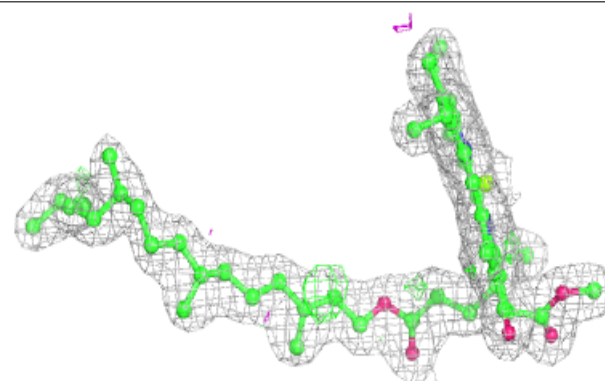


Electron density around CLA B 613:

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

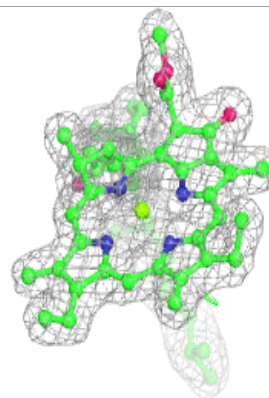
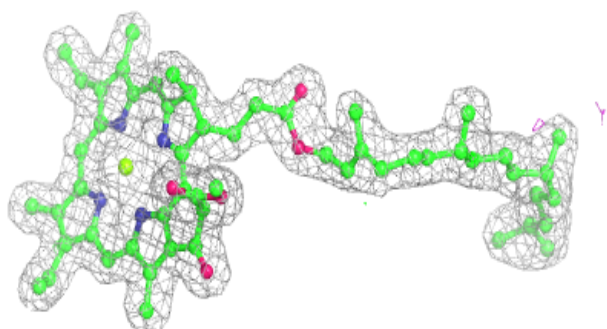
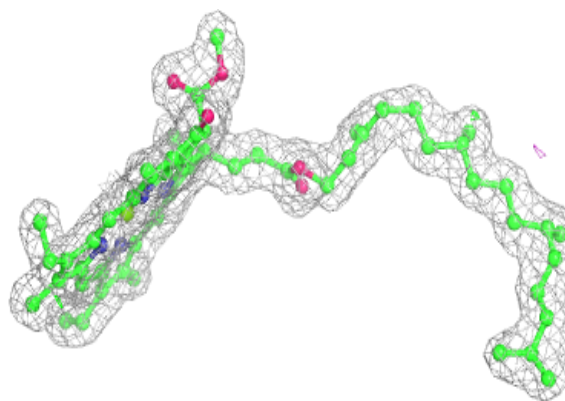
**Electron density around CLA B 606:**

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

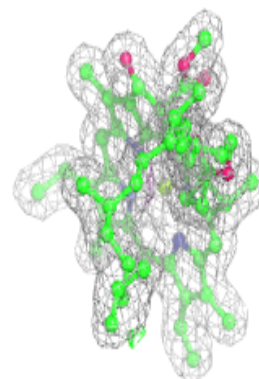
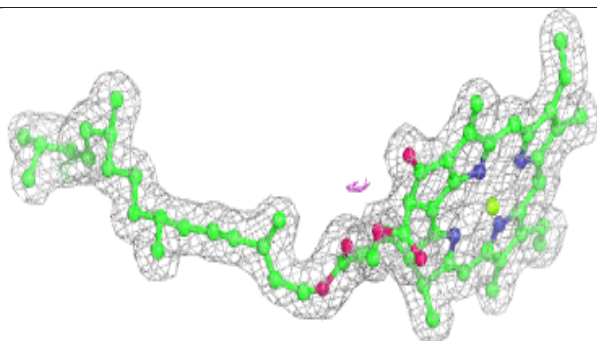
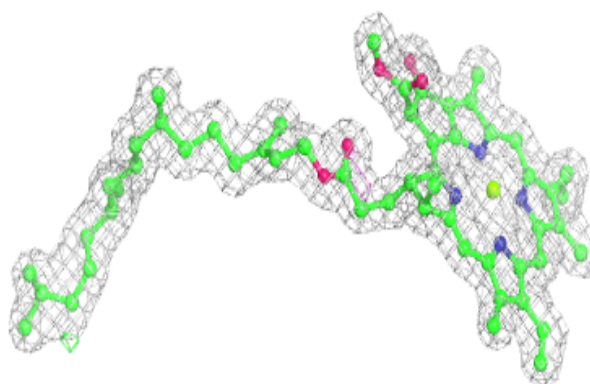


Electron density around CLA d 402:

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

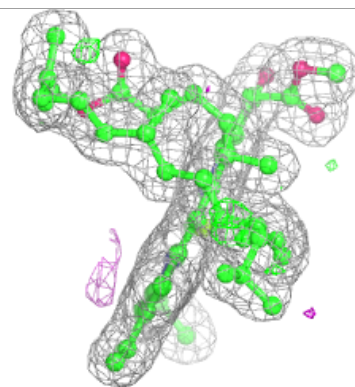
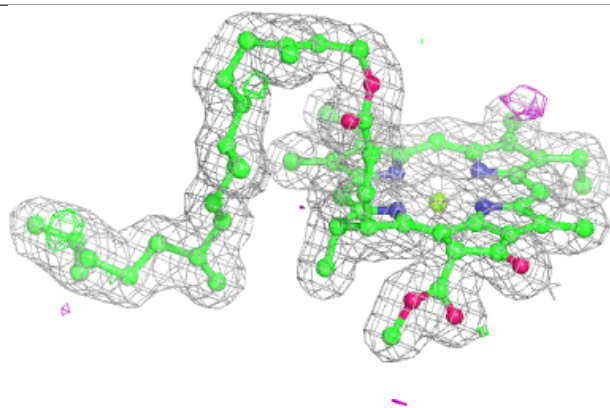
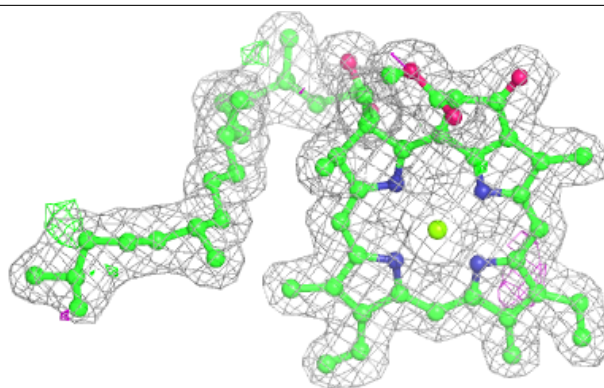
**Electron density around CLA A 401:**

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

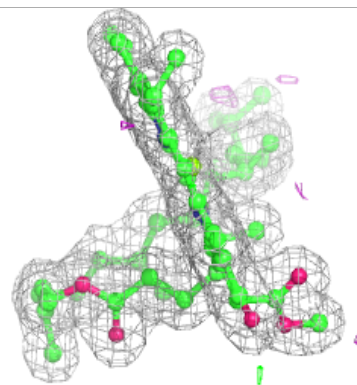
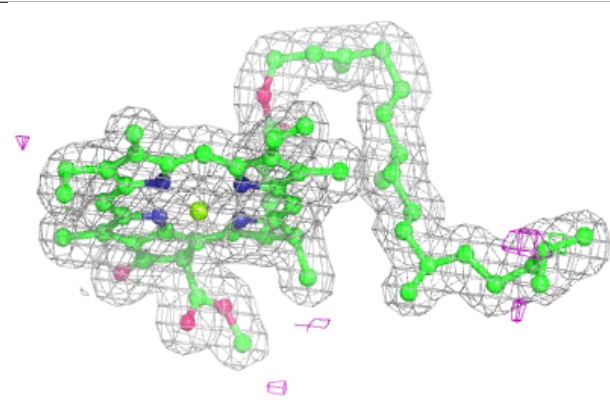
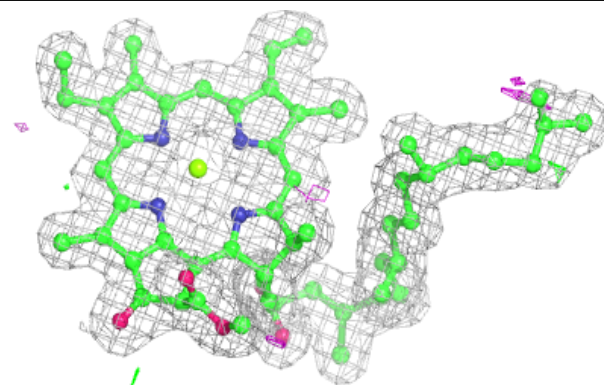


Electron density around CLA D 402:

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

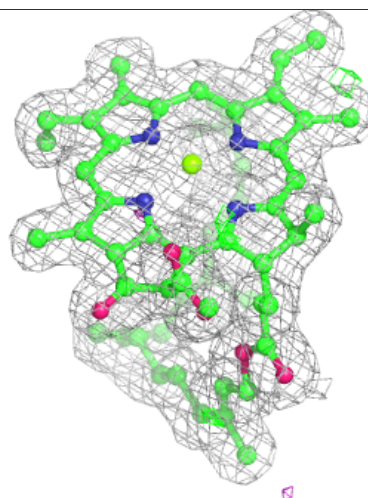
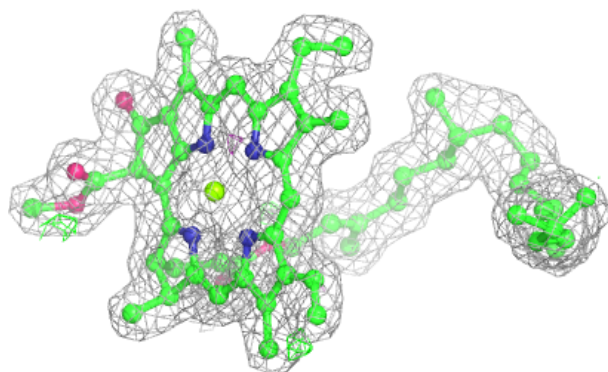
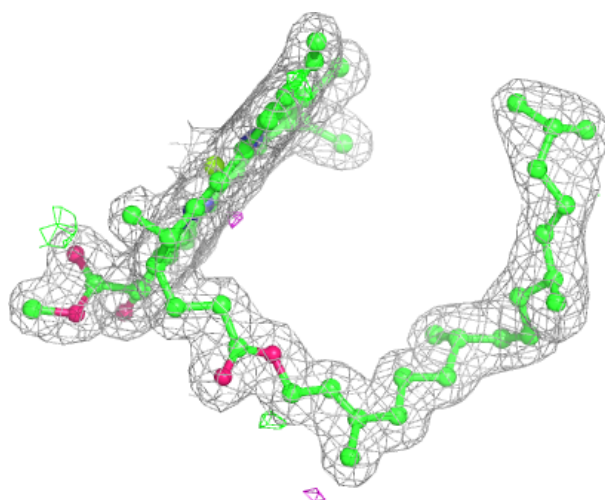
**Electron density around CLA d 403:**

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



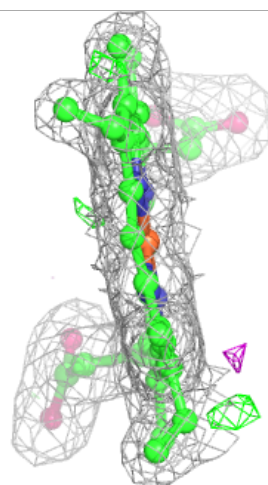
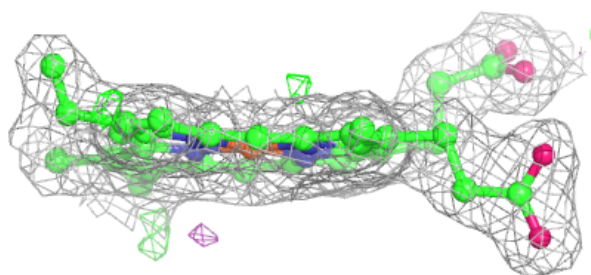
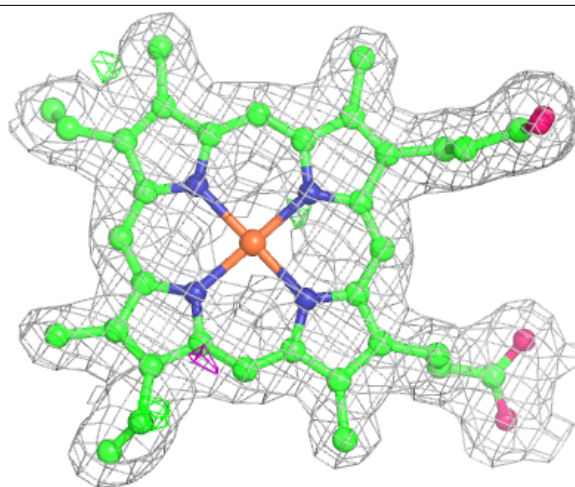
Electron density around CLA B 612:

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



Electron density around HEC V 201:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.