



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2020 – 05:09 PM BST

PDB ID : 5MX2
Title : Photosystem II depleted of the Mn₄CaO₅ cluster at 2.55 Å resolution
Authors : Zhang, M.; Bommer, M.; Chatterjee, R.; Hussain, R.; Kern, J.; Yano, J.; Dau, H.; Dobbek, H.; Zouni, A.
Deposited on : 2017-01-20
Resolution : 2.20 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

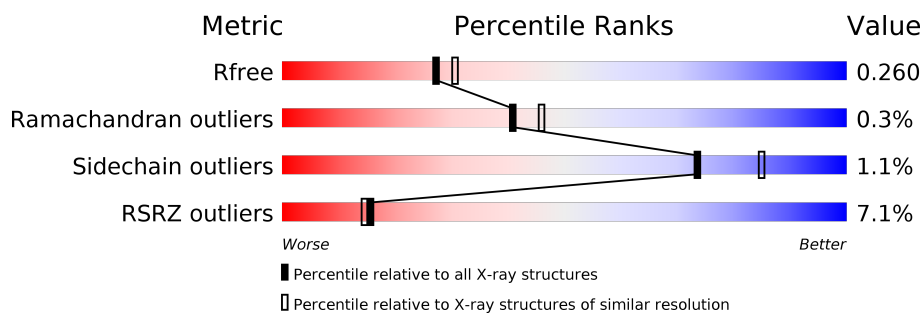
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



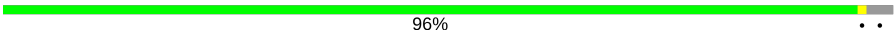

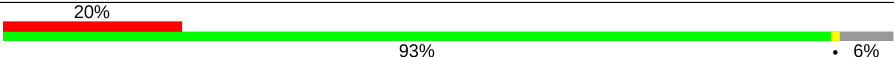
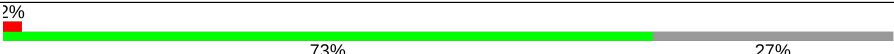
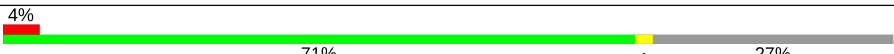
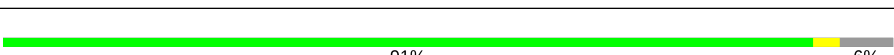
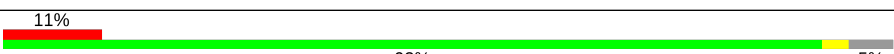
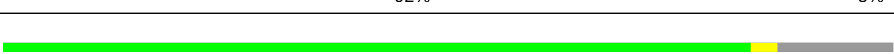

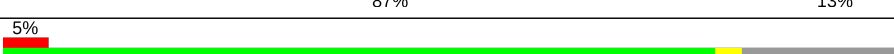

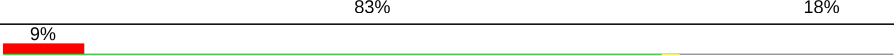
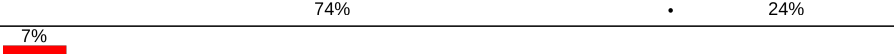
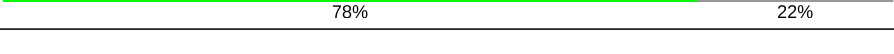
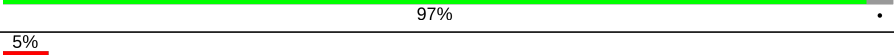
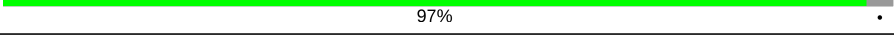





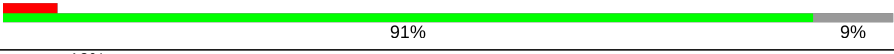



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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>4%</div> <div>96%</div> <div>..</div> </div>
1	a	344	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
2	B	510	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
2	b	510	<div> <div>7%</div> <div>98%</div> <div>..</div> </div>
3	C	461	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
3	c	461	<div> <div>3%</div> <div>95%</div> <div>..</div> </div>
4	D	352	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	
15	u	134	
16	V	163	
16	v	163	

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Mol	Chain	Length	Quality of chain
17	Y	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	R	41	
20	r	41	

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
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	412	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 50407 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			
1	a	333	Total	C	N	O	S	0	0	0
			2617	1714	430	458	15			

- 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	0	0
			3980	2611	665	691	13			
2	b	503	Total	C	N	O	S	0	0	0
			3958	2599	657	689	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3455	2264	576	602	13			
3	c	448	Total	C	N	O	S	0	0	0
			3466	2270	580	603	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			656	428	106	122			
5	e	79	Total	C	N	O	0	0	0
			645	422	104	119			

- 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	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	62	Total	C	N	O	S	0	0	0
			493	330	79	82	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			
8	i	33	Total	C	N	O	S	0	0	0
			266	183	39	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			
9	j	33	Total	C	N	O	S	0	0	0
			238	164	34	39	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	35	Total	C	N	O	0	0	0
			272	192	37	43			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	36	Total	C	N	O	0	0	0
			284	198	41	45			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			
12	m	32	Total	C	N	O	S	0	0	0
			249	167	36	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1859	1162	314	379	4			
13	o	241	Total	C	N	O	S	0	0	0
			1852	1158	313	377	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	28	Total	C	N	O	S	0	0	0
			241	170	34	35	2			
14	t	29	Total	C	N	O	S	0	0	0
			249	176	35	36	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	96	Total	C	N	O	0	0	0
			765	486	128	151			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	21	Total	C	N	O	S	0	0	0
			155	102	28	23	2			
17	y	23	Total	C	N	O	S	0	0	0
			171	113	30	25	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	S	0	0	0
			270	182	41	47				
18	x	38	Total	C	N	O	S	0	0	0
			281	188	45	48				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			471	323	71	75	2			

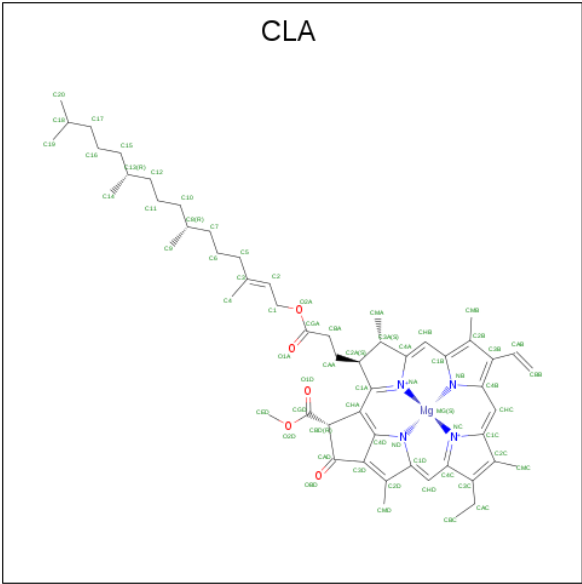
- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	35	Total	C	N	O	S	0	0	0
			282	191	49	42				
20	r	32	Total	C	N	O	S	0	0	0
			257	176	45	36				

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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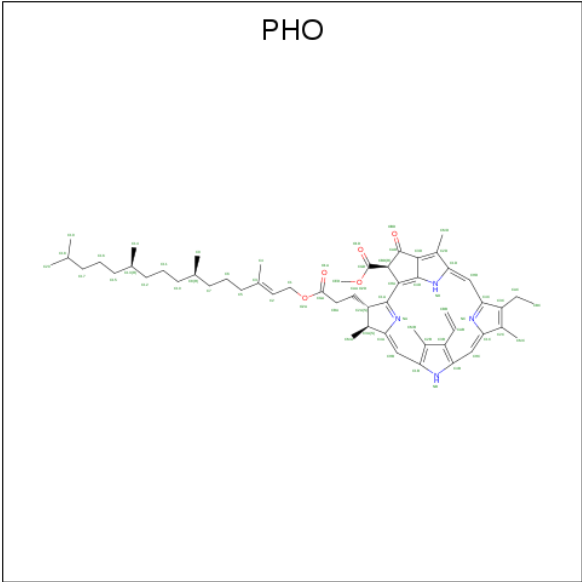
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22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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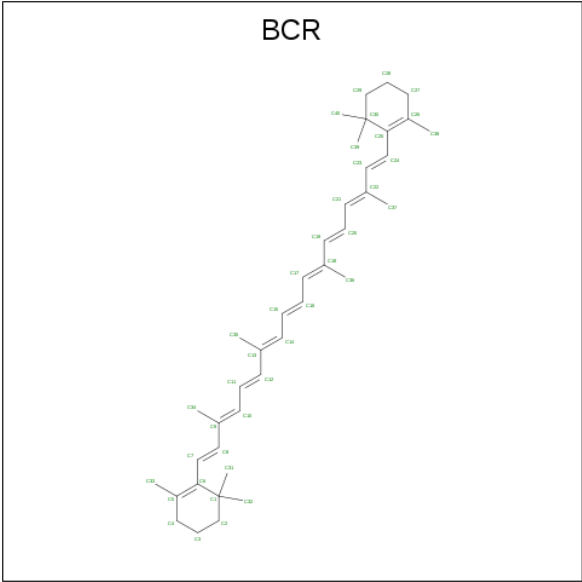
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



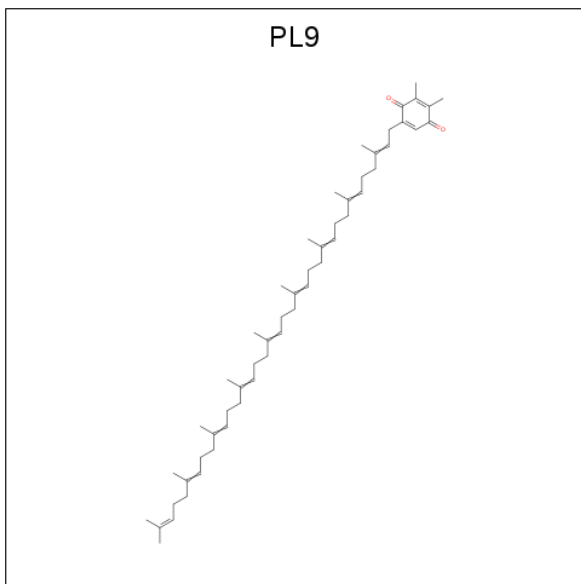
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



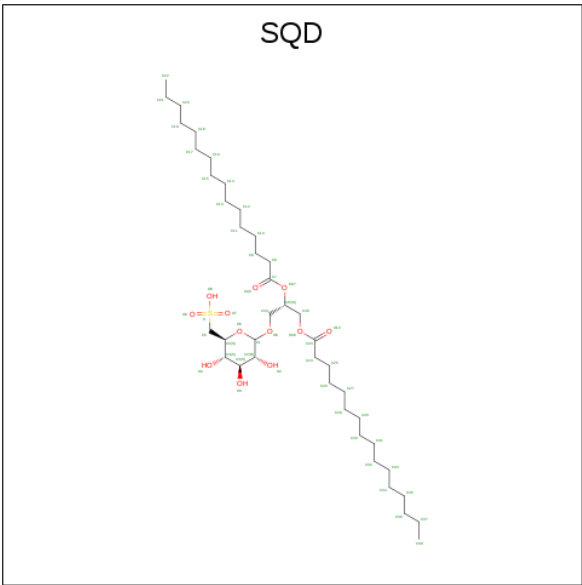
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total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

- Molecule 25 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



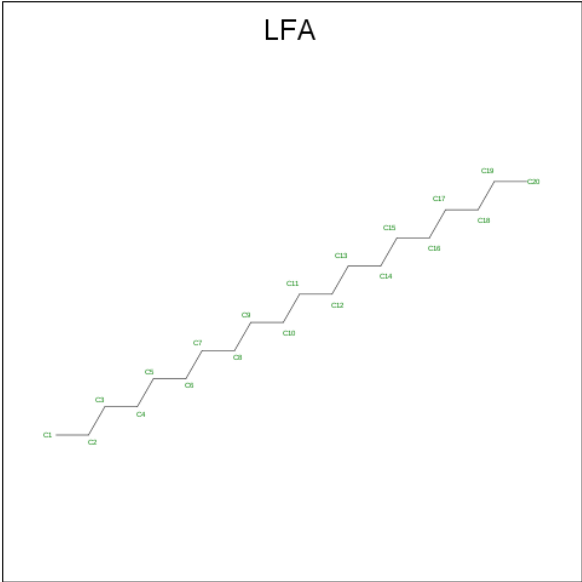
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			55	53	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	a	1	Total	C	O	0	0
			55	53	2		
25	d	1	Total	C	O	0	0
			55	53	2		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			48	35	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O		0	0
			50	41	9			
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is EICOSANE (three-letter code: LFA) (formula: C₂₀H₄₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	1	Total	C	0	0
			14	14		
27	A	1	Total	C	0	0
			11	11		
27	B	1	Total	C	0	0
			10	10		
27	B	1	Total	C	0	0
			16	16		
27	B	1	Total	C	0	0
			13	13		
27	B	1	Total	C	0	0
			15	15		
27	B	1	Total	C	0	0
			9	9		
27	B	1	Total	C	0	0
			10	10		
27	B	1	Total	C	0	0
			14	14		
27	B	1	Total	C	0	0
			12	12		
27	C	1	Total	C	0	0
			15	15		
27	D	1	Total	C	0	0
			15	15		
27	D	1	Total	C	0	0
			8	8		
27	D	1	Total	C	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C 14 14	0	0
27	J	1	Total C 11 11	0	0
27	M	1	Total C 10 10	0	0
27	M	1	Total C 16 16	0	0
27	T	1	Total C 12 12	0	0
27	a	1	Total C 7 7	0	0
27	b	1	Total C 15 15	0	0
27	b	1	Total C 10 10	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 16 16	0	0
27	b	1	Total C 12 12	0	0
27	b	1	Total C 11 11	0	0
27	b	1	Total C 9 9	0	0
27	b	1	Total C 15 15	0	0
27	c	1	Total C 9 9	0	0
27	c	1	Total C 15 15	0	0
27	d	1	Total C 15 15	0	0
27	d	1	Total C 9 9	0	0
27	d	1	Total C 16 16	0	0
27	i	1	Total C 16 16	0	0
27	i	1	Total C 7 7	0	0

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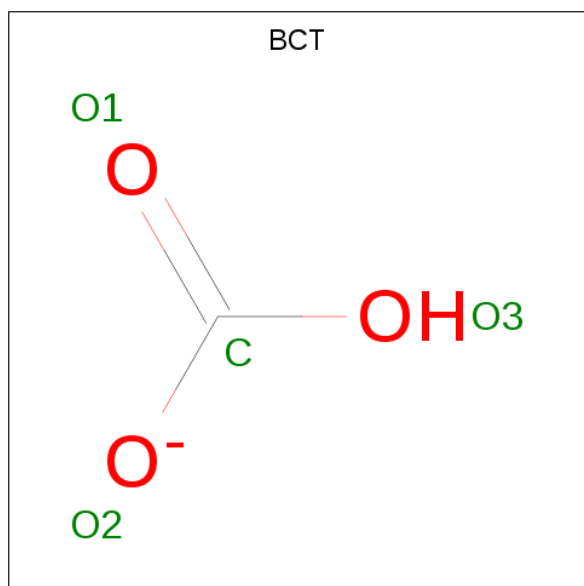
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	j	1	Total C 15 15	0	0
27	m	1	Total C 10 10	0	0
27	m	1	Total C 15 15	0	0
27	t	1	Total C 15 15	0	0

- Molecule 28 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

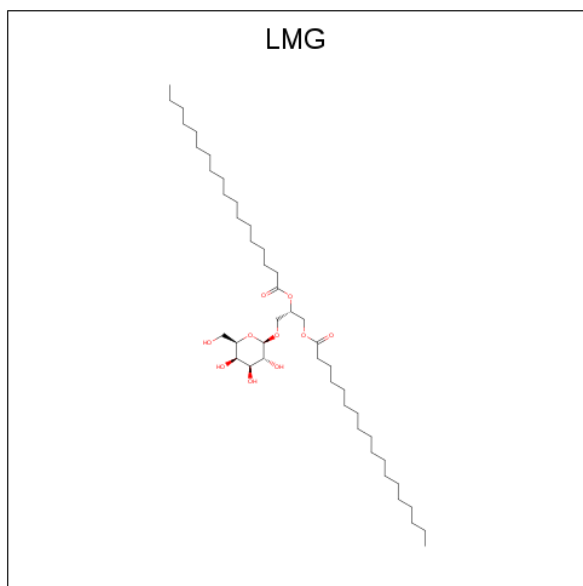
- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

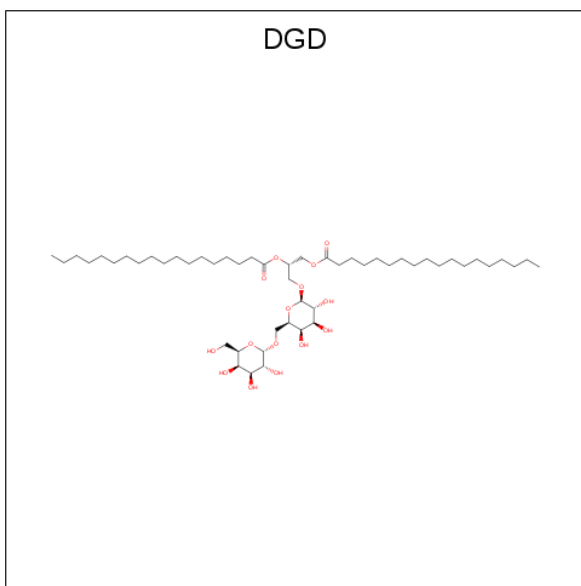
code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			51	41	10		
30	B	1	Total	C	O	0	0
			36	26	10		
30	C	1	Total	C	O	0	0
			51	41	10		
30	C	1	Total	C	O	0	0
			48	38	10		
30	C	1	Total	C	O	0	0
			44	34	10		
30	D	1	Total	C	O	0	0
			51	41	10		
30	b	1	Total	C	O	0	0
			39	29	10		
30	c	1	Total	C	O	0	0
			51	41	10		
30	c	1	Total	C	O	0	0
			51	41	10		
30	c	1	Total	C	O	0	0
			41	31	10		
30	f	1	Total	C	O	0	0
			51	41	10		
30	m	1	Total	C	O	0	0
			51	41	10		

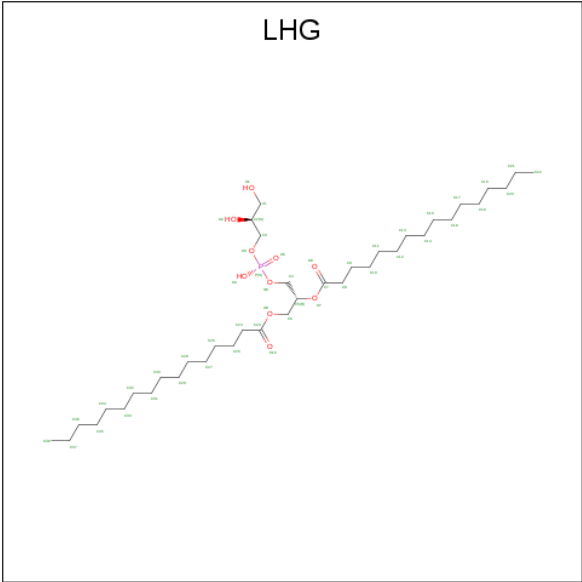
- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: C₅₁H₉₆O₁₅).



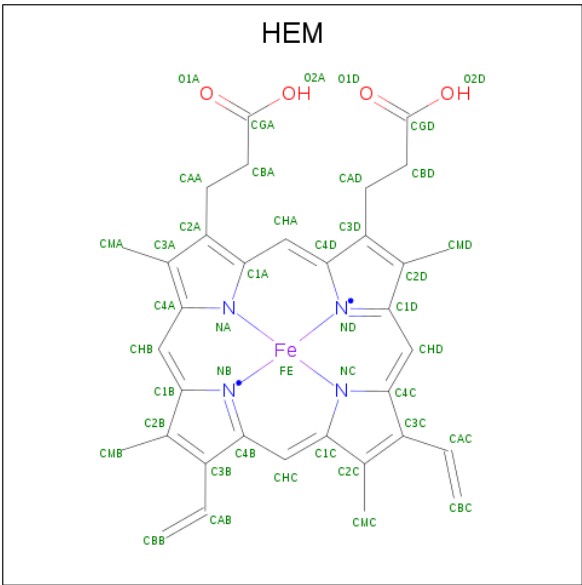
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	C	1	Total	C	O	0	0
			62	47	15		
31	C	1	Total	C	O	0	0
			56	41	15		
31	C	1	Total	C	O	0	0
			62	47	15		
31	H	1	Total	C	O	0	0
			60	45	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	c	1	Total	C	O	0	0
			55	40	15		
31	c	1	Total	C	O	0	0
			62	47	15		
31	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	70	Total	O	0	0
			70	70		
34	B	84	Total	O	0	0
			84	84		
34	C	62	Total	O	0	0
			62	62		
34	D	72	Total	O	0	0
			72	72		
34	E	5	Total	O	0	0
			5	5		
34	F	1	Total	O	0	0
			1	1		
34	H	17	Total	O	0	0
			17	17		
34	J	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	O 1	0	0
34	L	5	Total 5	O 5	0	0
34	M	3	Total 3	O 3	0	0
34	O	30	Total 30	O 30	0	0
34	T	2	Total 2	O 2	0	0
34	U	2	Total 2	O 2	0	0
34	V	12	Total 12	O 12	0	0
34	X	3	Total 3	O 3	0	0
34	a	77	Total 77	O 77	0	0
34	b	72	Total 72	O 72	0	0
34	c	65	Total 65	O 65	0	0
34	d	51	Total 51	O 51	0	0
34	e	5	Total 5	O 5	0	0
34	f	2	Total 2	O 2	0	0
34	h	3	Total 3	O 3	0	0
34	l	5	Total 5	O 5	0	0
34	m	2	Total 2	O 2	0	0
34	o	25	Total 25	O 25	0	0
34	t	3	Total 3	O 3	0	0
34	u	12	Total 12	O 12	0	0
34	v	11	Total 11	O 11	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 1



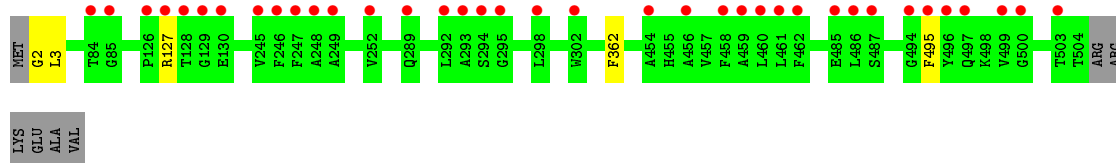
- Molecule 1: Photosystem II protein D1 1



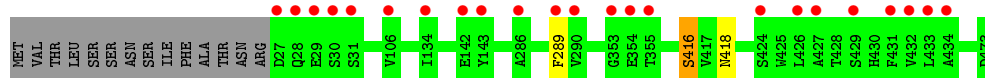
- Molecule 2: Photosystem II CP47 reaction center protein



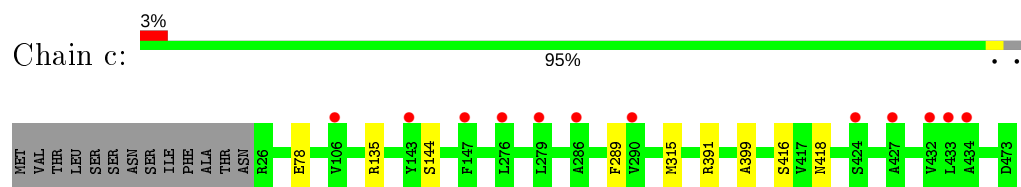
- Molecule 2: Photosystem II CP47 reaction center protein



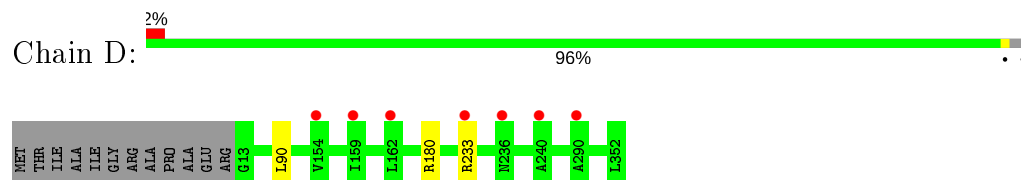
- Molecule 3: Photosystem II CP43 reaction center protein



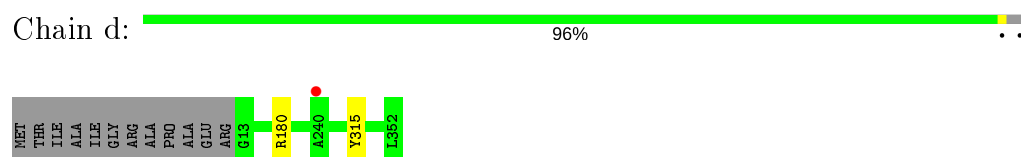
- Molecule 3: Photosystem II CP43 reaction center protein



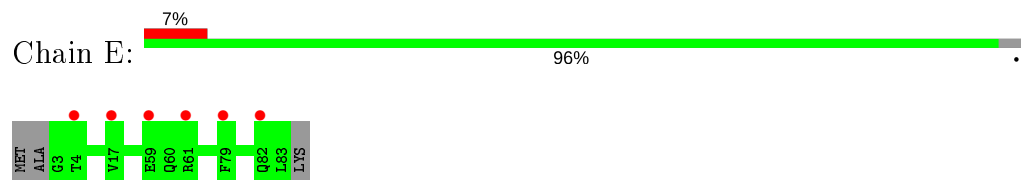
- Molecule 4: Photosystem II D2 protein



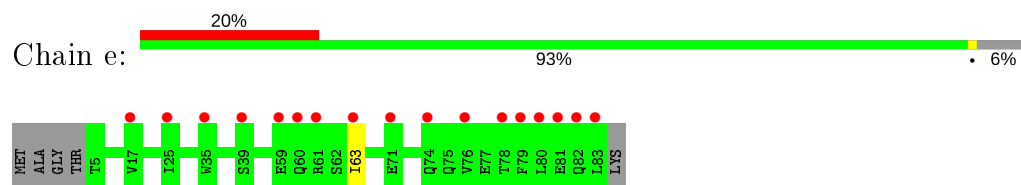
- Molecule 4: Photosystem II D2 protein



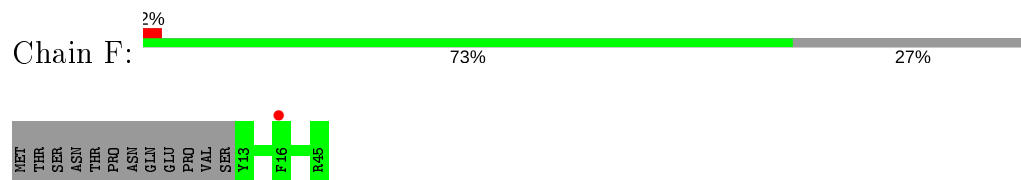
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha

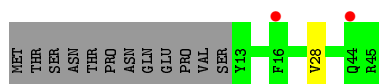


- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta





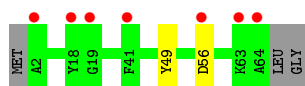
- Molecule 7: Photosystem II reaction center protein H

Chain H: 91% 6%



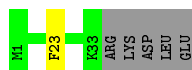
- Molecule 7: Photosystem II reaction center protein H

Chain h: 11% 92% 5%



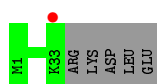
- Molecule 8: Photosystem II reaction center protein I

Chain I: 84% 13%



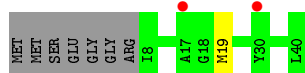
- Molecule 8: Photosystem II reaction center protein I

Chain i: 3% 87% 13%



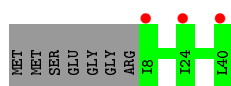
- Molecule 9: Photosystem II reaction center protein J

Chain J: 5% 80% 18%

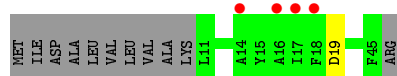
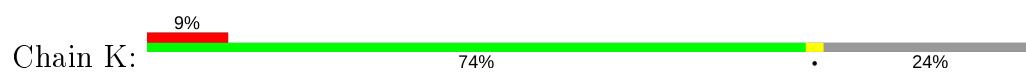


- Molecule 9: Photosystem II reaction center protein J

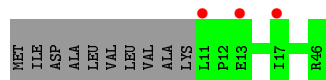
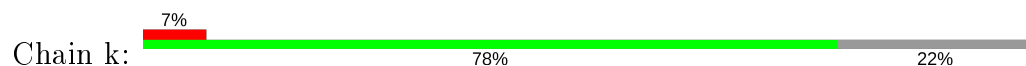
Chain j: 8% 83% 18%



- Molecule 10: Photosystem II reaction center protein K



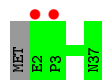
- Molecule 10: Photosystem II reaction center protein K



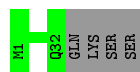
- Molecule 11: Photosystem II reaction center protein L



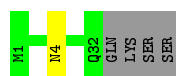
- Molecule 11: Photosystem II reaction center protein L



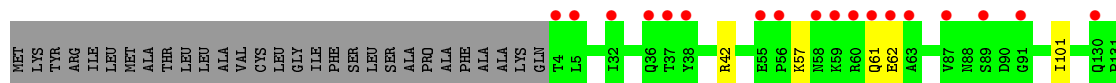
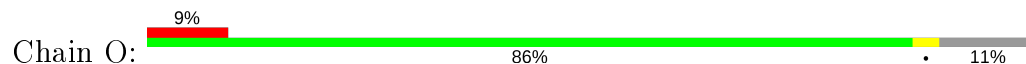
- Molecule 12: Photosystem II reaction center protein M

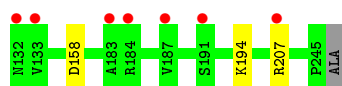


- Molecule 12: Photosystem II reaction center protein M

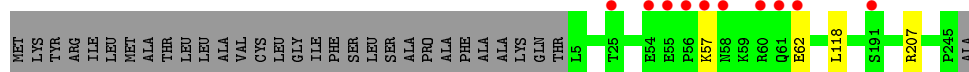
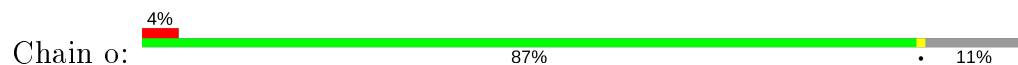


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

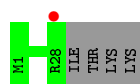
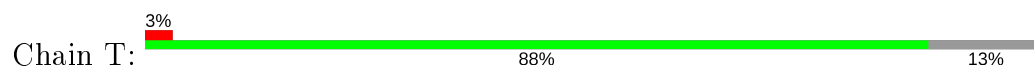




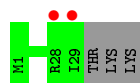
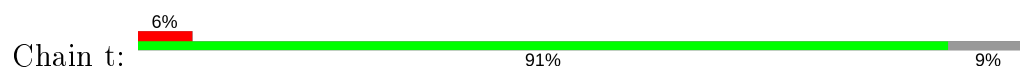
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



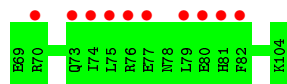
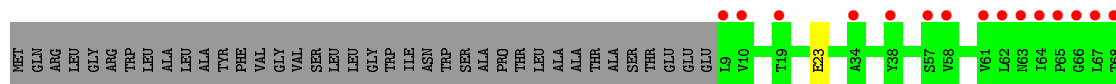
- Molecule 14: Photosystem II reaction center protein T



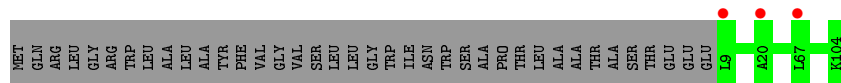
- Molecule 14: Photosystem II reaction center protein T



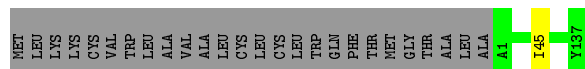
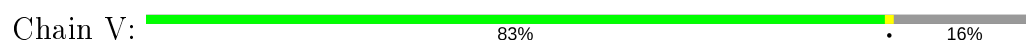
- Molecule 15: Photosystem II 12 kDa extrinsic protein



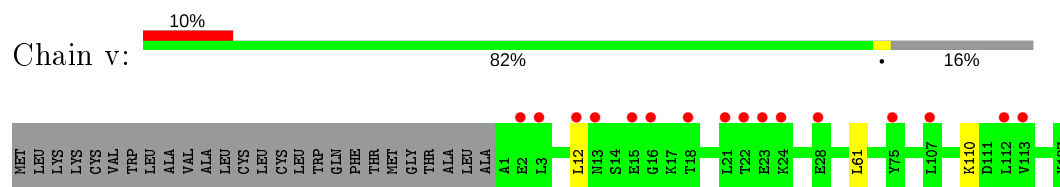
- Molecule 15: Photosystem II 12 kDa extrinsic protein



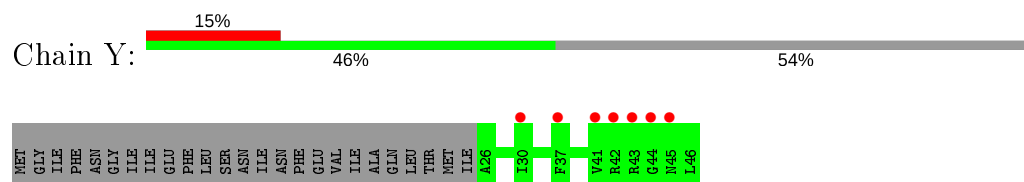
- Molecule 16: Cytochrome c-550



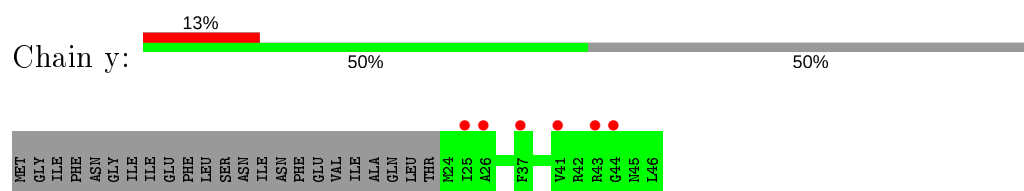
- Molecule 16: Cytochrome c-550



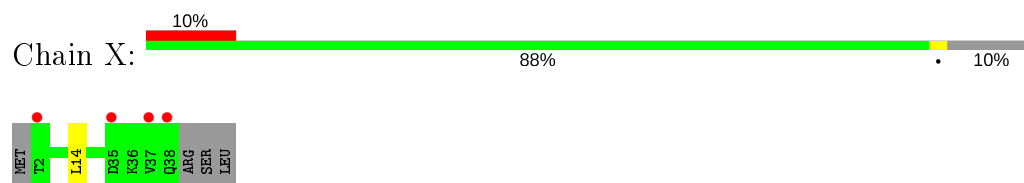
- Molecule 17: Photosystem II reaction center protein Ycf12



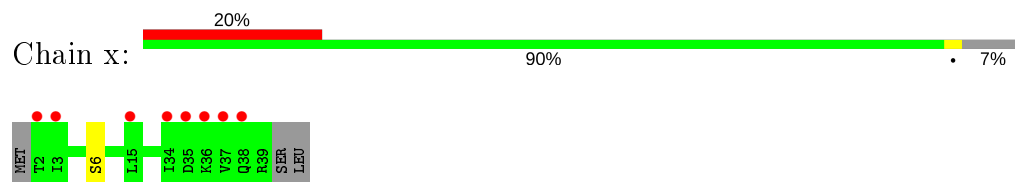
- Molecule 17: Photosystem II reaction center protein Ycf12



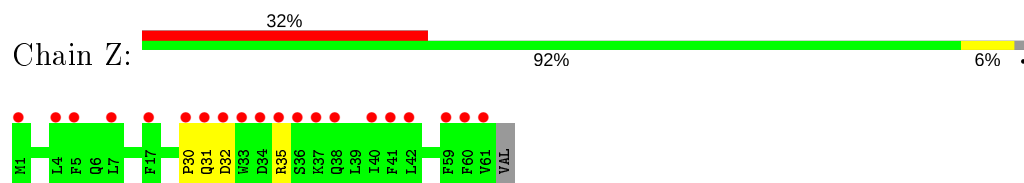
- Molecule 18: Photosystem II reaction center X protein



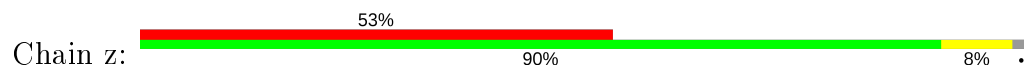
- Molecule 18: Photosystem II reaction center X protein

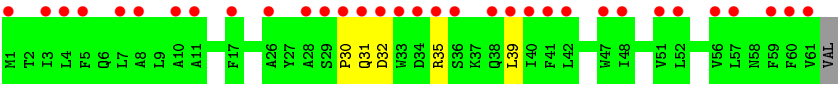


- Molecule 19: Photosystem II reaction center protein Z

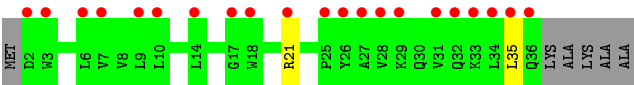
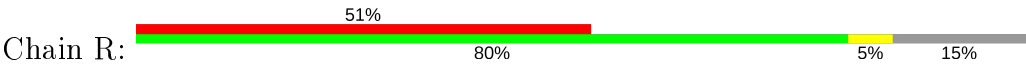


- Molecule 19: Photosystem II reaction center protein Z

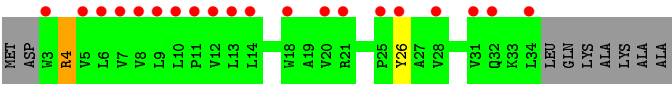




● Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.33Å 219.62Å 304.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 2.20 49.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.65-2.20) 92.6 (49.65-2.20)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.211 , 0.260 0.212 , 0.260	Depositor DCC
R_{free} test set	18229 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.673	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	50407	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LFA, DGD, CL, CLA, PL9, FE, HEM, BCT, PHO, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/2702	0.52	0/3685
1	a	0.53	0/2702	0.51	0/3685
2	B	0.54	0/4120	0.54	1/5614 (0.0%)
2	b	0.51	1/4098 (0.0%)	0.53	2/5586 (0.0%)
3	C	0.48	0/3568	0.51	0/4858
3	c	0.50	2/3579 (0.1%)	0.54	1/4872 (0.0%)
4	D	0.57	0/2801	0.54	1/3818 (0.0%)
4	d	0.52	0/2801	0.53	0/3818
5	E	0.41	0/675	0.48	0/922
5	e	0.58	1/664 (0.2%)	0.52	0/907
6	F	0.41	0/278	0.44	0/379
6	f	0.40	0/278	0.44	0/379
7	H	0.50	0/506	0.51	0/690
7	h	0.43	0/511	0.50	0/697
8	I	0.48	0/273	0.49	0/370
8	i	0.47	0/273	0.48	0/370
9	J	0.51	0/244	0.46	0/332
9	j	0.38	0/244	0.47	0/332
10	K	0.38	0/282	0.46	0/391
10	k	0.42	0/294	0.48	0/405
11	L	0.55	0/303	0.55	0/412
11	l	0.56	0/303	0.50	0/412
12	M	0.52	0/252	0.50	0/344
12	m	0.45	0/252	0.47	0/344
13	O	0.45	0/1890	0.56	1/2564 (0.0%)
13	o	0.46	0/1883	0.54	0/2554
14	T	0.60	0/250	0.41	0/338
14	t	0.51	0/258	0.45	0/349
15	U	0.33	0/776	0.49	0/1052
15	u	0.45	0/776	0.52	0/1052
16	V	0.43	0/1085	0.50	0/1473
16	v	0.40	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.28	0/156	0.43	0/207
17	y	0.31	0/172	0.47	0/228
18	X	0.38	0/273	0.45	0/370
18	x	0.31	0/284	0.43	0/384
19	Z	0.31	0/482	0.49	0/659
19	z	0.36	0/482	0.66	1/659 (0.2%)
20	R	0.31	0/288	0.44	0/395
20	r	0.37	0/263	0.69	1/361 (0.3%)
All	All	0.49	4/42406 (0.0%)	0.52	8/57740 (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
1	a	0	1
19	z	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	63	ILE	C-N	-10.84	1.13	1.34
3	c	399	ALA	C-N	-7.65	1.19	1.34
2	b	2	GLY	C-N	-5.82	1.20	1.34
3	c	78	GLU	C-N	-5.37	1.21	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	135	ARG	NE-CZ-NH1	9.25	124.93	120.30
19	z	39	LEU	CA-CB-CG	9.14	136.31	115.30
2	B	476	ARG	NE-CZ-NH2	6.77	123.69	120.30
4	D	233	ARG	NE-CZ-NH1	6.47	123.54	120.30
20	r	4	ARG	NE-CZ-NH2	6.45	123.53	120.30
2	b	127	ARG	NE-CZ-NH2	5.37	122.99	120.30
13	O	42	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	b	3	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	81	ALA	Peptide
19	z	35	ARG	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	331/344 (96%)	321 (97%)	9 (3%)	1 (0%)	41	46
1	a	331/344 (96%)	319 (96%)	11 (3%)	1 (0%)	41	46
2	B	503/510 (99%)	478 (95%)	25 (5%)	0	100	100
2	b	501/510 (98%)	479 (96%)	22 (4%)	0	100	100
3	C	445/461 (96%)	433 (97%)	11 (2%)	1 (0%)	47	55
3	c	446/461 (97%)	430 (96%)	15 (3%)	1 (0%)	47	55
4	D	338/352 (96%)	327 (97%)	11 (3%)	0	100	100
4	d	338/352 (96%)	321 (95%)	17 (5%)	0	100	100
5	E	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
5	e	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
6	F	31/45 (69%)	31 (100%)	0	0	100	100
6	f	31/45 (69%)	30 (97%)	1 (3%)	0	100	100
7	H	60/66 (91%)	56 (93%)	4 (7%)	0	100	100
7	h	61/66 (92%)	55 (90%)	6 (10%)	0	100	100
8	I	31/38 (82%)	30 (97%)	1 (3%)	0	100	100
8	i	31/38 (82%)	31 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
9	j	31/40 (78%)	30 (97%)	1 (3%)	0	100	100
10	K	33/46 (72%)	32 (97%)	1 (3%)	0	100	100
10	k	34/46 (74%)	33 (97%)	1 (3%)	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	30/36 (83%)	30 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	240/272 (88%)	222 (92%)	15 (6%)	3 (1%)	12	9
13	o	239/272 (88%)	223 (93%)	14 (6%)	2 (1%)	19	19
14	T	26/32 (81%)	26 (100%)	0	0	100	100
14	t	27/32 (84%)	25 (93%)	2 (7%)	0	100	100
15	U	94/134 (70%)	90 (96%)	4 (4%)	0	100	100
15	u	94/134 (70%)	89 (95%)	5 (5%)	0	100	100
16	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	22
16	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
17	Y	19/46 (41%)	18 (95%)	1 (5%)	0	100	100
17	y	21/46 (46%)	21 (100%)	0	0	100	100
18	X	35/41 (85%)	34 (97%)	1 (3%)	0	100	100
18	x	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
19	Z	59/62 (95%)	54 (92%)	2 (3%)	3 (5%)	2	0
19	z	59/62 (95%)	53 (90%)	3 (5%)	3 (5%)	2	0
20	R	33/41 (80%)	32 (97%)	0	1 (3%)	4	2
20	r	30/41 (73%)	30 (100%)	0	0	100	100
All	All	5173/5700 (91%)	4951 (96%)	205 (4%)	17 (0%)	41	46

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	57	LYS
19	Z	32	ASP
19	Z	35	ARG
3	c	416	SER
19	z	30	PRO

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Mol	Chain	Res	Type
19	z	32	ASP
3	C	416	SER
19	Z	30	PRO
19	z	31	GLN
13	O	62	GLU
13	o	62	GLU
13	o	57	LYS
20	R	35	LEU
1	a	259	ILE
13	O	101	ILE
16	V	45	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	270/280 (96%)	268 (99%)	2 (1%)	84	91
1	a	270/280 (96%)	268 (99%)	2 (1%)	84	91
2	B	403/407 (99%)	400 (99%)	3 (1%)	84	91
2	b	401/407 (98%)	399 (100%)	2 (0%)	88	94
3	C	349/362 (96%)	346 (99%)	3 (1%)	78	88
3	c	350/362 (97%)	345 (99%)	5 (1%)	67	80
4	D	275/283 (97%)	273 (99%)	2 (1%)	84	91
4	d	275/283 (97%)	273 (99%)	2 (1%)	84	91
5	E	71/73 (97%)	71 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	100	100
6	f	27/39 (69%)	26 (96%)	1 (4%)	34	43
7	H	53/55 (96%)	51 (96%)	2 (4%)	33	42
7	h	53/55 (96%)	51 (96%)	2 (4%)	33	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	30/35 (86%)	29 (97%)	1 (3%)	38	49
8	i	30/35 (86%)	30 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	29	36
9	j	23/28 (82%)	23 (100%)	0	100	100
10	K	28/37 (76%)	27 (96%)	1 (4%)	35	45
10	k	29/37 (78%)	29 (100%)	0	100	100
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/33 (88%)	29 (100%)	0	100	100
12	m	29/33 (88%)	28 (97%)	1 (3%)	37	47
13	O	206/228 (90%)	202 (98%)	4 (2%)	57	71
13	o	205/228 (90%)	203 (99%)	2 (1%)	76	86
14	T	25/29 (86%)	25 (100%)	0	100	100
14	t	26/29 (90%)	26 (100%)	0	100	100
15	U	83/112 (74%)	82 (99%)	1 (1%)	71	83
15	u	83/112 (74%)	83 (100%)	0	100	100
16	V	117/138 (85%)	117 (100%)	0	100	100
16	v	117/138 (85%)	114 (97%)	3 (3%)	46	58
17	Y	15/37 (40%)	15 (100%)	0	100	100
17	y	17/37 (46%)	17 (100%)	0	100	100
18	X	30/34 (88%)	29 (97%)	1 (3%)	38	49
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	50
19	Z	51/52 (98%)	50 (98%)	1 (2%)	55	69
19	z	51/52 (98%)	51 (100%)	0	100	100
20	R	30/33 (91%)	29 (97%)	1 (3%)	38	49
20	r	27/33 (82%)	25 (93%)	2 (7%)	13	14
All	All	4297/4660 (92%)	4251 (99%)	46 (1%)	73	85

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	SER
1	A	270	SER

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Mol	Chain	Res	Type
2	B	362	PHE
2	B	476	ARG
2	B	479	PHE
3	C	289	PHE
3	C	416	SER
3	C	418	ASN
4	D	90	LEU
4	D	180	ARG
7	H	3	ARG
7	H	49	TYR
8	I	23	PHE
9	J	19	MET
10	K	19	ASP
13	O	61	GLN
13	O	158	ASP
13	O	194	LYS
13	O	207	ARG
15	U	23	GLU
18	X	14	LEU
19	Z	31	GLN
1	a	222	SER
1	a	332	HIS
2	b	362	PHE
2	b	495	PHE
3	c	144	SER
3	c	289	PHE
3	c	315	MET
3	c	391	ARG
3	c	418	ASN
4	d	180	ARG
4	d	315	TYR
6	f	28	VAL
7	h	49	TYR
7	h	56	ASP
12	m	4	ASN
13	o	118	LEU
13	o	207	ARG
16	v	12	LEU
16	v	61	LEU
16	v	110	LYS
18	x	6	SER
20	R	21	ARG

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Mol	Chain	Res	Type
20	r	4	ARG
20	r	26	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
2	B	394	GLN
2	B	497	GLN
3	C	155	ASN
3	C	311	GLN
3	C	327	ASN
4	D	106	GLN
4	D	236	ASN
10	K	40	GLN
13	O	58	ASN
15	U	73	GLN
15	U	78	ASN
17	Y	45	ASN
1	a	252	HIS
1	a	312	ASN
2	b	282	GLN
3	c	201	ASN
3	c	332	GLN
3	c	418	ASN
4	d	224	GLN
5	e	82	GLN
6	f	44	GLN
12	m	4	ASN
12	m	32	GLN
13	o	36	GLN
13	o	58	ASN
13	o	80	GLN
13	o	124	ASN
13	o	200	ASN
13	o	236	GLN
16	v	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 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	BCR	C	515	-	41,41,41	0.83	1 (2%)	56,56,56	1.80	17 (30%)
25	PL9	a	409	-	55,55,55	0.59	2 (3%)	68,69,69	1.78	18 (26%)
27	LFA	b	622	-	9,9,19	0.12	0	8,8,18	0.32	0
27	LFA	B	620	-	9,9,19	0.14	0	8,8,18	0.43	0
22	CLA	b	606	-	59,73,73	1.75	6 (10%)	67,113,113	1.53	9 (13%)
22	CLA	b	614	-	59,73,73	1.54	7 (11%)	67,113,113	1.39	8 (11%)
24	BCR	K	102	-	41,41,41	0.85	1 (2%)	56,56,56	1.90	12 (21%)
26	SQD	a	410	-	53,54,54	1.13	4 (7%)	62,65,65	1.37	11 (17%)
30	LMG	D	409	-	51,51,55	0.95	2 (3%)	59,59,63	0.94	2 (3%)
23	PHO	A	405	-	67,69,69	0.79	3 (4%)	85,99,99	1.02	5 (5%)
22	CLA	b	617	-	59,73,73	1.72	6 (10%)	67,113,113	1.31	7 (10%)
24	BCR	c	515	-	41,41,41	0.85	2 (4%)	56,56,56	1.39	6 (10%)
24	BCR	k	101	-	41,41,41	0.86	1 (2%)	56,56,56	1.83	13 (23%)
27	LFA	T	102	-	11,11,19	0.11	0	10,10,18	0.42	0
26	SQD	D	411	-	42,43,54	1.27	4 (9%)	51,54,65	1.80	10 (19%)
22	CLA	B	606	34	59,73,73	1.68	8 (13%)	67,113,113	1.54	9 (13%)
31	DGD	C	517	-	63,63,67	0.83	2 (3%)	77,77,81	1.23	8 (10%)
25	PL9	A	408	-	55,55,55	0.63	2 (3%)	68,69,69	1.98	19 (27%)
27	LFA	b	602	-	14,14,19	0.10	0	13,13,18	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	512	3	59,73,73	1.71	7 (11%)	67,113,113	1.35	8 (11%)
33	HEM	v	201	16	27,50,50	1.60	2 (7%)	17,82,82	2.21	4 (23%)
22	CLA	B	611	-	59,73,73	1.67	5 (8%)	67,113,113	1.31	7 (10%)
27	LFA	d	409	-	8,8,19	0.12	0	7,7,18	0.26	0
31	DGD	c	517	-	56,56,67	0.88	2 (3%)	70,70,81	1.10	5 (7%)
22	CLA	C	510	-	59,73,73	1.64	7 (11%)	67,113,113	1.33	8 (11%)
22	CLA	C	503	-	59,73,73	1.69	6 (10%)	67,113,113	1.28	11 (16%)
22	CLA	b	610	-	59,73,73	1.65	9 (15%)	67,113,113	1.45	7 (10%)
27	LFA	B	624	-	14,14,19	0.08	0	13,13,18	0.31	0
25	PL9	D	405	-	55,55,55	0.70	3 (5%)	68,69,69	1.64	17 (25%)
33	HEM	V	201	16	27,50,50	1.58	2 (7%)	17,82,82	2.02	5 (29%)
22	CLA	B	615	-	59,73,73	1.78	7 (11%)	67,113,113	1.53	6 (8%)
24	BCR	B	617	-	41,41,41	0.86	2 (4%)	56,56,56	1.61	12 (21%)
33	HEM	e	102	5,6	27,50,50	1.50	2 (7%)	17,82,82	1.47	3 (17%)
22	CLA	b	613	-	59,73,73	1.67	6 (10%)	67,113,113	1.39	6 (8%)
22	CLA	d	403	-	59,73,73	1.60	6 (10%)	67,113,113	1.35	8 (11%)
30	LMG	C	522	-	44,44,55	1.05	3 (6%)	52,52,63	1.59	8 (15%)
24	BCR	t	102	-	41,41,41	0.86	1 (2%)	56,56,56	1.93	14 (25%)
30	LMG	C	501	-	51,51,55	0.88	2 (3%)	59,59,63	1.09	3 (5%)
27	LFA	J	101	-	10,10,19	0.11	0	9,9,18	0.37	0
30	LMG	f	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	5 (8%)
22	CLA	b	605	-	59,73,73	1.75	8 (13%)	67,113,113	1.36	6 (8%)
32	LHG	D	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.19	4 (7%)
27	LFA	B	625	-	8,8,19	0.10	0	7,7,18	0.31	0
22	CLA	B	612	-	59,73,73	1.68	8 (13%)	67,113,113	1.35	7 (10%)
24	BCR	H	102	-	41,41,41	0.76	0	56,56,56	1.87	14 (25%)
22	CLA	B	613	-	59,73,73	1.95	8 (13%)	67,113,113	1.40	6 (8%)
27	LFA	b	623	-	11,11,19	0.10	0	10,10,18	0.39	0
22	CLA	b	603	34	59,73,73	1.82	7 (11%)	67,113,113	1.30	8 (11%)
22	CLA	H	101	34	59,73,73	1.81	7 (11%)	67,113,113	1.28	5 (7%)
27	LFA	A	410	-	13,13,19	0.10	0	12,12,18	0.33	0
27	LFA	C	521	-	14,14,19	0.08	0	13,13,18	0.33	0
22	CLA	c	505	34	59,73,73	1.49	5 (8%)	67,113,113	1.27	10 (14%)
22	CLA	B	605	-	59,73,73	1.81	6 (10%)	67,113,113	1.45	6 (8%)
29	BCT	A	415	28	0,3,3	0.00	-	0,3,3	0.00	-
31	DGD	c	516	-	63,63,67	0.83	3 (4%)	77,77,81	1.13	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SQD	A	409	-	53,54,54	1.12	4 (7%)	62,65,65	1.65	11 (17%)
22	CLA	C	513	-	59,73,73	1.80	8 (13%)	67,113,113	1.25	9 (13%)
27	LFA	d	408	-	14,14,19	0.10	0	13,13,18	0.42	0
22	CLA	c	514	-	59,73,73	1.69	8 (13%)	67,113,113	1.36	9 (13%)
24	BCR	A	407	-	41,41,41	0.83	0	56,56,56	1.57	13 (23%)
27	LFA	b	629	-	8,8,19	0.11	0	7,7,18	0.32	0
24	BCR	K	101	-	41,41,41	0.79	0	56,56,56	1.64	12 (21%)
24	BCR	D	404	-	41,41,41	0.90	2 (4%)	56,56,56	1.89	13 (23%)
22	CLA	a	407	-	59,73,73	1.63	7 (11%)	67,113,113	1.31	9 (13%)
22	CLA	b	615	-	59,73,73	1.90	10 (16%)	67,113,113	1.36	8 (11%)
27	LFA	i	101	-	15,15,19	0.10	0	14,14,18	0.38	0
24	BCR	h	101	-	41,41,41	0.78	0	56,56,56	1.83	14 (25%)
27	LFA	M	101	-	9,9,19	0.15	0	8,8,18	0.64	0
24	BCR	b	620	-	41,41,41	0.78	0	56,56,56	1.51	9 (16%)
30	LMG	B	619	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	2 (3%)
22	CLA	c	507	-	59,73,73	1.77	8 (13%)	67,113,113	1.48	7 (10%)
22	CLA	A	406	-	59,73,73	1.75	8 (13%)	67,113,113	1.29	8 (11%)
30	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.16	6 (10%)
22	CLA	c	504	-	59,73,73	1.91	7 (11%)	67,113,113	1.32	8 (11%)
24	BCR	C	516	-	41,41,41	0.98	3 (7%)	56,56,56	1.73	10 (17%)
22	CLA	b	607	-	59,73,73	2.00	8 (13%)	67,113,113	1.31	7 (10%)
22	CLA	b	608	-	59,73,73	1.78	8 (13%)	67,113,113	1.39	8 (11%)
23	PHO	a	414	-	67,69,69	0.76	2 (2%)	85,99,99	0.96	4 (4%)
23	PHO	D	401	-	67,69,69	0.79	2 (2%)	85,99,99	0.98	5 (5%)
24	BCR	B	616	-	41,41,41	0.85	1 (2%)	56,56,56	1.71	12 (21%)
22	CLA	c	502	-	59,73,73	1.73	7 (11%)	67,113,113	1.44	8 (11%)
27	LFA	c	521	-	14,14,19	0.08	0	13,13,18	0.35	0
30	LMG	c	501	-	51,51,55	0.86	2 (3%)	59,59,63	1.24	4 (6%)
22	CLA	a	404	-	59,73,73	1.60	7 (11%)	67,113,113	1.47	7 (10%)
33	HEM	E	102	5,6	27,50,50	1.57	2 (7%)	17,82,82	2.03	5 (29%)
22	CLA	a	405	34	59,73,73	1.70	8 (13%)	67,113,113	1.29	8 (11%)
22	CLA	B	607	-	59,73,73	1.89	7 (11%)	67,113,113	1.24	6 (8%)
22	CLA	C	507	-	59,73,73	1.76	8 (13%)	67,113,113	1.46	7 (10%)
26	SQD	a	412	-	50,50,54	0.89	2 (4%)	58,58,65	1.17	6 (10%)
27	LFA	a	411	-	6,6,19	0.11	0	5,5,18	0.21	0
27	LFA	M	102	-	15,15,19	0.17	0	14,14,18	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PHO	a	406	-	67,69,69	0.74	2 (2%)	85,99,99	1.02	6 (7%)
32	LHG	d	406	-	48,48,48	0.92	4 (8%)	51,54,54	1.16	4 (7%)
26	SQD	A	411	-	53,54,54	1.14	4 (7%)	62,65,65	1.34	8 (12%)
22	CLA	b	611	-	59,73,73	1.79	9 (15%)	67,113,113	1.38	7 (10%)
27	LFA	b	625	-	15,15,19	0.09	0	14,14,18	0.39	0
22	CLA	B	601	-	59,73,73	1.94	6 (10%)	67,113,113	1.41	6 (8%)
31	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.04	2 (2%)
22	CLA	C	514	-	59,73,73	1.62	7 (11%)	67,113,113	1.35	9 (13%)
27	LFA	c	520	-	8,8,19	0.11	0	7,7,18	0.37	0
22	CLA	B	603	-	59,73,73	1.71	4 (6%)	67,113,113	1.45	8 (11%)
27	LFA	b	627	-	10,10,19	0.10	0	9,9,18	0.35	0
22	CLA	B	614	-	59,73,73	1.77	7 (11%)	67,113,113	1.45	8 (11%)
27	LFA	D	410	-	14,14,19	0.09	0	13,13,18	0.25	0
26	SQD	b	601	-	53,54,54	1.14	4 (7%)	62,65,65	1.53	13 (20%)
22	CLA	B	604	-	59,73,73	1.99	5 (8%)	67,113,113	1.33	6 (8%)
22	CLA	A	403	-	59,73,73	1.73	7 (11%)	67,113,113	1.54	6 (8%)
22	CLA	d	402	-	59,73,73	1.63	6 (10%)	67,113,113	1.25	5 (7%)
22	CLA	c	513	-	59,73,73	1.72	7 (11%)	67,113,113	1.28	8 (11%)
22	CLA	c	510	-	59,73,73	1.67	7 (11%)	67,113,113	1.31	7 (10%)
31	DGD	H	103	-	61,61,67	0.84	2 (3%)	75,75,81	1.19	5 (6%)
22	CLA	C	502	-	59,73,73	1.67	8 (13%)	67,113,113	1.49	8 (11%)
22	CLA	c	512	3	59,73,73	1.64	7 (11%)	67,113,113	1.40	9 (13%)
32	LHG	D	407	-	48,48,48	0.86	3 (6%)	51,54,54	1.17	4 (7%)
24	BCR	d	404	-	41,41,41	0.90	1 (2%)	56,56,56	2.20	18 (32%)
30	LMG	C	520	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	5 (8%)
22	CLA	C	511	-	59,73,73	1.72	6 (10%)	67,113,113	1.36	8 (11%)
22	CLA	b	612	34	59,73,73	1.89	8 (13%)	67,113,113	1.59	8 (11%)
22	CLA	C	504	-	59,73,73	1.84	6 (10%)	67,113,113	1.24	8 (11%)
22	CLA	b	609	34	59,73,73	1.65	10 (16%)	67,113,113	1.52	11 (16%)
27	LFA	m	101	-	9,9,19	0.12	0	8,8,18	0.44	0
22	CLA	A	412	34	59,73,73	1.49	8 (13%)	67,113,113	1.31	7 (10%)
27	LFA	B	623	-	12,12,19	0.09	0	11,11,18	0.23	0
27	LFA	B	622	-	15,15,19	0.10	0	14,14,18	0.33	0
32	LHG	l	101	-	48,48,48	0.87	3 (6%)	51,54,54	1.22	5 (9%)
25	PL9	d	405	-	55,55,55	0.63	3 (5%)	68,69,69	1.73	14 (20%)
32	LHG	d	407	-	48,48,48	0.91	3 (6%)	51,54,54	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	509	-	59,73,73	1.71	7 (11%)	67,113,113	1.41	7 (10%)
30	LMG	b	624	-	39,39,55	1.11	3 (7%)	47,47,63	1.12	6 (12%)
22	CLA	B	609	34	59,73,73	1.91	8 (13%)	67,113,113	1.49	8 (11%)
30	LMG	B	621	-	36,36,55	1.05	2 (5%)	44,44,63	1.22	4 (9%)
22	CLA	c	511	-	59,73,73	1.75	8 (13%)	67,113,113	1.36	6 (8%)
27	LFA	B	627	-	13,13,19	0.10	0	12,12,18	0.51	0
27	LFA	b	630	-	14,14,19	0.08	0	13,13,18	0.37	0
27	LFA	j	101	-	14,14,19	0.09	0	13,13,18	0.43	0
24	BCR	B	618	-	41,41,41	0.91	1 (2%)	56,56,56	1.97	16 (28%)
26	SQD	f	102	-	42,43,54	1.27	4 (9%)	51,54,65	1.68	10 (19%)
32	LHG	E	101	-	41,41,48	1.00	2 (4%)	44,47,54	1.08	3 (6%)
27	LFA	d	410	-	15,15,19	0.08	0	14,14,18	0.37	0
31	DGD	h	102	-	63,63,67	0.81	2 (3%)	77,77,81	1.01	4 (5%)
22	CLA	b	604	-	59,73,73	1.62	8 (13%)	67,113,113	1.45	7 (10%)
27	LFA	b	626	-	11,11,19	0.11	0	10,10,18	0.30	0
27	LFA	I	101	-	13,13,19	0.09	0	12,12,18	0.36	0
24	BCR	a	408	-	41,41,41	0.87	1 (2%)	56,56,56	1.45	12 (21%)
22	CLA	b	616	-	59,73,73	1.81	8 (13%)	67,113,113	1.17	6 (8%)
27	LFA	B	628	-	11,11,19	0.09	0	10,10,18	0.38	0
22	CLA	C	506	-	59,73,73	1.91	6 (10%)	67,113,113	1.26	7 (10%)
24	BCR	c	524	-	41,41,41	0.79	0	56,56,56	1.74	13 (23%)
24	BCR	c	523	-	41,41,41	0.84	1 (2%)	56,56,56	1.84	12 (21%)
24	BCR	T	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.03	16 (28%)
24	BCR	b	621	-	41,41,41	0.84	1 (2%)	56,56,56	1.86	13 (23%)
30	LMG	m	103	-	51,51,55	0.83	2 (3%)	59,59,63	1.36	8 (13%)
31	DGD	C	518	-	57,57,67	0.85	2 (3%)	71,71,81	1.28	10 (14%)
31	DGD	C	519	-	63,63,67	0.82	3 (4%)	77,77,81	1.09	7 (9%)
27	LFA	A	413	-	10,10,19	0.08	0	9,9,18	0.43	0
22	CLA	D	403	-	59,73,73	1.74	8 (13%)	67,113,113	1.34	8 (11%)
27	LFA	i	102	-	6,6,19	0.12	0	5,5,18	0.16	0
32	LHG	e	101	-	41,41,48	0.97	2 (4%)	44,47,54	1.06	3 (6%)
22	CLA	b	618	-	59,73,73	1.72	7 (11%)	67,113,113	1.44	8 (11%)
30	LMG	c	522	-	41,41,55	1.04	2 (4%)	49,49,63	1.60	11 (22%)
22	CLA	C	508	34	59,73,73	1.71	7 (11%)	67,113,113	1.39	8 (11%)
26	SQD	L	101	-	47,48,54	1.22	4 (8%)	56,59,65	3.78	10 (17%)
22	CLA	c	506	-	59,73,73	1.78	7 (11%)	67,113,113	1.24	7 (10%)
29	BCT	a	413	28	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	D	408	-	48,48,48	0.86	3 (6%)	51,54,54	1.02	2 (3%)
22	CLA	A	404	34	59,73,73	1.68	7 (11%)	67,113,113	1.30	7 (10%)
27	LFA	m	102	-	14,14,19	0.11	0	13,13,18	0.40	0
22	CLA	C	509	-	59,73,73	1.65	8 (13%)	67,113,113	1.27	8 (11%)
32	LHG	b	628	-	48,48,48	0.89	3 (6%)	51,54,54	1.11	5 (9%)
27	LFA	t	101	-	14,14,19	0.12	0	13,13,18	0.52	0
27	LFA	D	412	-	7,7,19	0.12	0	6,6,18	0.33	0
27	LFA	D	413	-	9,9,19	0.16	0	8,8,18	0.52	0
22	CLA	c	503	-	59,73,73	1.66	8 (13%)	67,113,113	1.33	8 (11%)
22	CLA	c	508	34	59,73,73	1.68	8 (13%)	67,113,113	1.57	7 (10%)
22	CLA	B	610	-	59,73,73	1.57	7 (11%)	67,113,113	1.56	8 (11%)
22	CLA	D	402	-	59,73,73	1.78	6 (10%)	67,113,113	1.56	8 (11%)
22	CLA	B	602	-	59,73,73	1.79	7 (11%)	67,113,113	1.41	7 (10%)
22	CLA	C	505	34	59,73,73	1.64	8 (13%)	67,113,113	1.36	9 (13%)
22	CLA	d	401	34	59,73,73	1.61	8 (13%)	67,113,113	1.28	8 (11%)
24	BCR	b	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.79	12 (21%)
27	LFA	B	626	-	9,9,19	0.11	0	8,8,18	0.45	0
32	LHG	L	102	-	48,48,48	0.95	2 (4%)	51,54,54	1.11	2 (3%)
22	CLA	B	608	-	59,73,73	1.72	7 (11%)	67,113,113	1.36	7 (10%)

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	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	PL9	a	409	-	-	17/53/73/73	0/1/1/1
27	LFA	b	622	-	-	3/7/7/17	-
27	LFA	B	620	-	-	5/7/7/17	-
22	CLA	b	606	-	3/3/20/25	8/37/135/135	-
22	CLA	b	614	-	3/3/20/25	4/37/135/135	-
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
26	SQD	a	410	-	-	14/49/69/69	0/1/1/1
30	LMG	D	409	-	-	4/46/66/70	0/1/1/1
23	PHO	A	405	-	-	1/53/103/103	0/5/6/6
22	CLA	b	617	-	3/3/20/25	3/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	507	-	3/3/20/25	6/37/135/135	-
24	BCR	k	101	-	-	5/29/63/63	0/2/2/2
22	CLA	b	613	-	3/3/20/25	6/37/135/135	-
26	SQD	D	411	-	-	6/38/58/69	0/1/1/1
22	CLA	B	606	34	3/3/20/25	7/37/135/135	-
31	DGD	C	517	-	-	14/51/91/95	0/2/2/2
25	PL9	A	408	-	-	9/53/73/73	0/1/1/1
27	LFA	b	602	-	-	5/12/12/17	-
22	CLA	C	512	3	3/3/20/25	1/37/135/135	-
33	HEM	v	201	16	-	0/6/54/54	-
22	CLA	B	611	-	3/3/20/25	4/37/135/135	-
27	LFA	d	409	-	-	2/6/6/17	-
31	DGD	c	517	-	-	14/44/84/95	0/2/2/2
22	CLA	C	510	-	3/3/20/25	6/37/135/135	-
22	CLA	C	503	-	3/3/20/25	4/37/135/135	-
22	CLA	b	610	-	3/3/20/25	3/37/135/135	-
27	LFA	B	624	-	-	8/12/12/17	-
25	PL9	D	405	-	-	13/53/73/73	0/1/1/1
33	HEM	V	201	16	-	0/6/54/54	-
22	CLA	B	615	-	3/3/20/25	6/37/135/135	-
24	BCR	B	617	-	-	0/29/63/63	0/2/2/2
33	HEM	e	102	5,6	-	1/6/54/54	-
27	LFA	T	102	-	-	2/9/9/17	-
22	CLA	d	403	-	3/3/20/25	8/37/135/135	-
30	LMG	C	522	-	-	16/39/59/70	0/1/1/1
24	BCR	t	102	-	-	6/29/63/63	0/2/2/2
30	LMG	C	501	-	-	15/46/66/70	0/1/1/1
27	LFA	J	101	-	-	1/8/8/17	-
30	LMG	f	101	-	-	8/46/66/70	0/1/1/1
22	CLA	b	605	-	3/3/20/25	5/37/135/135	-
32	LHG	D	406	-	-	15/53/53/53	-
27	LFA	B	625	-	-	0/6/6/17	-
22	CLA	B	612	-	3/3/20/25	2/37/135/135	-
22	CLA	c	504	-	3/3/20/25	2/37/135/135	-
22	CLA	B	613	-	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LFA	b	623	-	-	0/9/9/17	-
22	CLA	b	603	34	3/3/20/25	8/37/135/135	-
22	CLA	H	101	34	3/3/20/25	7/37/135/135	-
22	CLA	C	514	-	3/3/20/25	2/37/135/135	-
27	LFA	C	521	-	-	5/12/12/17	-
22	CLA	c	505	34	3/3/20/25	5/37/135/135	-
22	CLA	B	605	-	3/3/20/25	6/37/135/135	-
30	LMG	c	522	-	-	10/36/56/70	0/1/1/1
31	DGD	c	516	-	-	13/51/91/95	0/2/2/2
26	SQD	A	409	-	-	10/49/69/69	0/1/1/1
22	CLA	C	513	-	3/3/20/25	5/37/135/135	-
27	LFA	d	408	-	-	5/12/12/17	-
22	CLA	c	514	-	3/3/20/25	2/37/135/135	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
27	LFA	b	629	-	-	0/6/6/17	-
24	BCR	K	101	-	-	4/29/63/63	0/2/2/2
24	BCR	D	404	-	-	6/29/63/63	0/2/2/2
22	CLA	a	407	-	3/3/20/25	4/37/135/135	-
22	CLA	b	615	-	3/3/20/25	5/37/135/135	-
27	LFA	i	101	-	-	6/13/13/17	-
24	BCR	h	101	-	-	4/29/63/63	0/2/2/2
27	LFA	M	101	-	-	2/7/7/17	-
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	LMG	B	619	-	-	15/46/66/70	0/1/1/1
24	BCR	c	515	-	-	1/29/63/63	0/2/2/2
22	CLA	A	406	-	3/3/20/25	2/37/135/135	-
30	LMG	c	519	-	-	12/46/66/70	0/1/1/1
27	LFA	c	520	-	-	0/6/6/17	-
24	BCR	H	102	-	-	3/29/63/63	0/2/2/2
24	BCR	C	516	-	-	1/29/63/63	0/2/2/2
22	CLA	b	607	-	3/3/20/25	6/37/135/135	-
22	CLA	b	608	-	3/3/20/25	4/37/135/135	-
22	CLA	c	510	-	3/3/20/25	4/37/135/135	-
23	PHO	D	401	-	-	6/53/103/103	0/5/6/6
22	CLA	C	511	-	3/3/20/25	2/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	502	-	3/3/20/25	2/37/135/135	-
27	LFA	c	521	-	-	4/12/12/17	-
30	LMG	c	501	-	-	17/46/66/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	2/37/135/135	-
33	HEM	E	102	5,6	-	2/6/54/54	-
22	CLA	a	405	34	3/3/20/25	5/37/135/135	-
22	CLA	B	607	-	3/3/20/25	2/37/135/135	-
22	CLA	C	507	-	3/3/20/25	6/37/135/135	-
26	SQD	a	412	-	-	15/44/64/69	0/1/1/1
27	LFA	a	411	-	-	1/4/4/17	-
27	LFA	M	102	-	-	5/13/13/17	-
23	PHO	a	406	-	-	4/53/103/103	0/5/6/6
32	LHG	d	406	-	-	16/53/53/53	-
26	SQD	A	411	-	-	23/49/69/69	0/1/1/1
22	CLA	b	611	-	3/3/20/25	7/37/135/135	-
27	LFA	b	625	-	-	6/13/13/17	-
22	CLA	B	601	-	3/3/20/25	6/37/135/135	-
31	DGD	c	518	-	-	17/51/91/95	0/2/2/2
27	LFA	A	410	-	-	6/11/11/17	-
22	CLA	b	618	-	3/3/20/25	5/37/135/135	-
22	CLA	B	603	-	3/3/20/25	2/37/135/135	-
27	LFA	b	627	-	-	3/8/8/17	-
22	CLA	B	614	-	3/3/20/25	7/37/135/135	-
27	LFA	D	410	-	-	5/12/12/17	-
26	SQD	b	601	-	-	11/49/69/69	0/1/1/1
22	CLA	B	604	-	3/3/20/25	9/37/135/135	-
22	CLA	A	403	-	3/3/20/25	1/37/135/135	-
24	BCR	B	618	-	-	4/29/63/63	0/2/2/2
22	CLA	c	513	-	3/3/20/25	2/37/135/135	-
23	PHO	a	414	-	-	0/53/103/103	0/5/6/6
31	DGD	H	103	-	-	12/49/89/95	0/2/2/2
22	CLA	C	502	-	3/3/20/25	0/37/135/135	-
22	CLA	c	512	3	3/3/20/25	0/37/135/135	-
32	LHG	D	407	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	d	404	-	-	6/29/63/63	0/2/2/2
30	LMG	C	520	-	-	10/43/63/70	0/1/1/1
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
22	CLA	b	612	34	3/3/20/25	6/37/135/135	-
22	CLA	C	504	-	3/3/20/25	6/37/135/135	-
22	CLA	b	609	34	3/3/20/25	7/37/135/135	-
27	LFA	m	101	-	-	1/7/7/17	-
22	CLA	A	412	34	3/3/20/25	2/37/135/135	-
27	LFA	B	623	-	-	6/10/10/17	-
27	LFA	B	622	-	-	2/13/13/17	-
32	LHG	l	101	-	-	20/53/53/53	-
25	PL9	d	405	-	-	11/53/73/73	0/1/1/1
32	LHG	d	407	-	-	25/53/53/53	-
22	CLA	c	509	-	3/3/20/25	5/37/135/135	-
30	LMG	b	624	-	-	13/34/54/70	0/1/1/1
22	CLA	B	609	34	3/3/20/25	4/37/135/135	-
30	LMG	B	621	-	-	7/31/51/70	0/1/1/1
22	CLA	c	511	-	3/3/20/25	4/37/135/135	-
27	LFA	B	627	-	-	8/11/11/17	-
27	LFA	b	630	-	-	6/12/12/17	-
27	LFA	j	101	-	-	3/12/12/17	-
22	CLA	d	402	-	3/3/20/25	1/37/135/135	-
26	SQD	f	102	-	-	18/38/58/69	0/1/1/1
32	LHG	E	101	-	-	20/46/46/53	-
27	LFA	d	410	-	-	5/13/13/17	-
31	DGD	h	102	-	-	18/51/91/95	0/2/2/2
22	CLA	b	604	-	3/3/20/25	8/37/135/135	-
27	LFA	b	626	-	-	6/9/9/17	-
27	LFA	I	101	-	-	6/11/11/17	-
24	BCR	a	408	-	-	2/29/63/63	0/2/2/2
22	CLA	b	616	-	3/3/20/25	11/37/135/135	-
27	LFA	B	628	-	-	2/9/9/17	-
22	CLA	C	506	-	3/3/20/25	6/37/135/135	-
24	BCR	c	524	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	523	-	-	2/29/63/63	0/2/2/2
24	BCR	T	101	-	-	8/29/63/63	0/2/2/2
24	BCR	b	621	-	-	8/29/63/63	0/2/2/2
30	LMG	m	103	-	-	17/46/66/70	0/1/1/1
31	DGD	C	518	-	-	16/45/85/95	0/2/2/2
31	DGD	C	519	-	-	6/51/91/95	0/2/2/2
27	LFA	A	413	-	-	5/8/8/17	-
22	CLA	D	403	-	3/3/20/25	6/37/135/135	-
27	LFA	i	102	-	-	1/4/4/17	-
32	LHG	e	101	-	-	13/46/46/53	-
22	CLA	c	506	-	3/3/20/25	6/37/135/135	-
22	CLA	C	508	34	3/3/20/25	1/37/135/135	-
26	SQD	L	101	-	-	18/43/63/69	0/1/1/1
32	LHG	D	408	-	-	17/53/53/53	-
22	CLA	A	404	34	3/3/20/25	2/37/135/135	-
27	LFA	m	102	-	-	4/12/12/17	-
22	CLA	C	509	-	3/3/20/25	4/37/135/135	-
32	LHG	b	628	-	-	12/53/53/53	-
27	LFA	t	101	-	-	3/12/12/17	-
27	LFA	D	412	-	-	2/5/5/17	-
27	LFA	D	413	-	-	0/7/7/17	-
22	CLA	c	503	-	3/3/20/25	3/37/135/135	-
22	CLA	c	508	34	3/3/20/25	4/37/135/135	-
22	CLA	B	610	-	3/3/20/25	4/37/135/135	-
22	CLA	D	402	-	3/3/20/25	3/37/135/135	-
22	CLA	B	602	-	3/3/20/25	4/37/135/135	-
22	CLA	C	505	34	3/3/20/25	7/37/135/135	-
22	CLA	d	401	34	3/3/20/25	4/37/135/135	-
24	BCR	b	619	-	-	2/29/63/63	0/2/2/2
27	LFA	B	626	-	-	4/7/7/17	-
32	LHG	L	102	-	-	16/53/53/53	-
22	CLA	B	608	-	3/3/20/25	7/37/135/135	-

All (655) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C4B-NB	11.88	1.45	1.35
22	B	613	CLA	C4B-NB	11.43	1.45	1.35
22	B	601	CLA	C4B-NB	11.36	1.45	1.35
22	c	504	CLA	C4B-NB	11.36	1.45	1.35
22	b	607	CLA	C4B-NB	11.25	1.45	1.35
22	C	504	CLA	C4B-NB	11.18	1.45	1.35
22	b	603	CLA	C4B-NB	11.03	1.45	1.35
22	c	507	CLA	C4B-NB	10.89	1.44	1.35
22	B	608	CLA	C4B-NB	10.78	1.44	1.35
22	b	616	CLA	C4B-NB	10.63	1.44	1.35
22	C	506	CLA	C4B-NB	10.62	1.44	1.35
22	H	101	CLA	C4B-NB	10.36	1.44	1.35
22	C	513	CLA	C4B-NB	10.34	1.44	1.35
22	B	602	CLA	C4B-NB	10.34	1.44	1.35
22	B	607	CLA	C4B-NB	10.17	1.44	1.35
22	C	511	CLA	C4B-NB	10.05	1.44	1.35
22	b	611	CLA	C4B-NB	10.03	1.44	1.35
22	B	603	CLA	C4B-NB	10.02	1.44	1.35
22	B	609	CLA	C4B-NB	10.00	1.44	1.35
22	c	506	CLA	C4B-NB	9.96	1.44	1.35
22	b	606	CLA	C4B-NB	9.90	1.44	1.35
22	D	402	CLA	C4B-NB	9.79	1.43	1.35
22	C	512	CLA	C4B-NB	9.77	1.43	1.35
22	c	502	CLA	C4B-NB	9.70	1.43	1.35
22	b	615	CLA	C4B-NB	9.70	1.43	1.35
22	B	614	CLA	C4B-NB	9.67	1.43	1.35
22	c	508	CLA	C4B-NB	9.52	1.43	1.35
22	B	615	CLA	C4B-NB	9.52	1.43	1.35
22	c	509	CLA	C4B-NB	9.46	1.43	1.35
22	A	404	CLA	C4B-NB	9.41	1.43	1.35
22	c	511	CLA	C4B-NB	9.37	1.43	1.35
22	C	509	CLA	C4B-NB	9.35	1.43	1.35
22	B	605	CLA	C4B-NB	9.29	1.43	1.35
22	C	507	CLA	C4B-NB	9.23	1.43	1.35
22	B	611	CLA	C4B-NB	9.21	1.43	1.35
22	A	403	CLA	C4B-NB	9.20	1.43	1.35
22	c	513	CLA	C4B-NB	9.19	1.43	1.35
22	b	617	CLA	C4B-NB	9.12	1.43	1.35
22	b	605	CLA	C4B-NB	9.09	1.43	1.35
22	b	608	CLA	C4B-NB	9.07	1.43	1.35
22	c	512	CLA	C4B-NB	8.99	1.43	1.35
22	C	514	CLA	C4B-NB	8.99	1.43	1.35
22	c	514	CLA	C4B-NB	8.92	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	C4B-NB	8.90	1.43	1.35
22	C	503	CLA	C4B-NB	8.79	1.43	1.35
22	b	613	CLA	C4B-NB	8.77	1.43	1.35
22	c	510	CLA	C4B-NB	8.75	1.43	1.35
22	C	505	CLA	C4B-NB	8.64	1.42	1.35
22	c	503	CLA	C4B-NB	8.58	1.42	1.35
22	b	610	CLA	C4B-NB	8.51	1.42	1.35
22	a	405	CLA	C4B-NB	8.48	1.42	1.35
22	B	612	CLA	C4B-NB	8.42	1.42	1.35
22	C	510	CLA	C4B-NB	8.38	1.42	1.35
22	C	508	CLA	C4B-NB	8.36	1.42	1.35
22	b	604	CLA	C4B-NB	8.35	1.42	1.35
22	d	401	CLA	C4B-NB	8.22	1.42	1.35
22	D	403	CLA	C4B-NB	8.15	1.42	1.35
22	B	610	CLA	C4B-NB	7.97	1.42	1.35
22	C	502	CLA	C4B-NB	7.84	1.42	1.35
22	a	404	CLA	C4B-NB	7.65	1.42	1.35
22	d	402	CLA	C4B-NB	7.43	1.41	1.35
22	c	505	CLA	C4B-NB	7.43	1.41	1.35
22	a	407	CLA	C4B-NB	7.40	1.41	1.35
22	b	618	CLA	C4B-NB	7.36	1.41	1.35
22	b	609	CLA	C4B-NB	7.01	1.41	1.35
22	d	403	CLA	C4B-NB	6.99	1.41	1.35
22	B	606	CLA	C3B-C2B	-6.57	1.31	1.40
22	b	614	CLA	C4B-NB	6.30	1.40	1.35
22	A	412	CLA	C4B-NB	6.27	1.40	1.35
33	v	201	HEM	C3C-C2C	-6.22	1.31	1.40
22	A	406	CLA	C3B-C2B	-6.12	1.31	1.40
33	V	201	HEM	C3C-C2C	-6.10	1.31	1.40
22	B	607	CLA	C3B-C2B	-5.99	1.32	1.40
22	B	606	CLA	C4B-NB	5.85	1.40	1.35
22	C	506	CLA	C3B-C2B	-5.75	1.32	1.40
22	B	605	CLA	C1B-NB	5.71	1.40	1.35
33	E	102	HEM	C3C-C2C	-5.66	1.32	1.40
22	B	606	CLA	MG-NC	-5.63	1.92	2.06
22	b	607	CLA	C3B-C2B	-5.58	1.32	1.40
22	A	406	CLA	C4B-NB	5.56	1.40	1.35
22	d	402	CLA	C3B-C2B	-5.54	1.32	1.40
33	e	102	HEM	C3C-C2C	-5.48	1.32	1.40
22	b	612	CLA	C3B-C2B	-5.47	1.32	1.40
22	A	404	CLA	C1B-NB	5.35	1.40	1.35
22	b	618	CLA	MG-NC	-5.34	1.93	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	MG-NC	-5.33	1.93	2.06
22	a	407	CLA	MG-NC	-5.30	1.93	2.06
22	C	507	CLA	MG-NC	-5.29	1.93	2.06
22	B	614	CLA	C3B-C2B	-5.19	1.33	1.40
22	C	508	CLA	MG-NC	-5.19	1.94	2.06
22	A	406	CLA	MG-NC	-5.18	1.94	2.06
22	B	605	CLA	C3B-C2B	-5.12	1.33	1.40
22	B	613	CLA	C3B-C2B	-5.11	1.33	1.40
22	b	612	CLA	MG-NC	-5.09	1.94	2.06
22	b	615	CLA	MG-NC	-5.09	1.94	2.06
22	B	609	CLA	C3B-C2B	-5.07	1.33	1.40
22	B	615	CLA	MG-NC	-5.05	1.94	2.06
22	A	406	CLA	MG-NA	-5.04	1.94	2.06
22	D	403	CLA	MG-NC	-5.04	1.94	2.06
22	c	504	CLA	C1B-NB	4.98	1.39	1.35
22	D	402	CLA	MG-NC	-4.98	1.94	2.06
22	b	613	CLA	C3B-C2B	-4.97	1.33	1.40
22	b	613	CLA	MG-NC	-4.94	1.94	2.06
22	C	506	CLA	MG-NC	-4.93	1.94	2.06
22	C	507	CLA	C3B-C2B	-4.91	1.33	1.40
22	b	608	CLA	C3B-C2B	-4.89	1.33	1.40
22	C	512	CLA	C1B-NB	4.89	1.39	1.35
22	b	617	CLA	MG-NC	-4.89	1.94	2.06
22	B	607	CLA	MG-NC	-4.89	1.94	2.06
22	b	618	CLA	C3B-C2B	-4.86	1.33	1.40
22	c	503	CLA	MG-NC	-4.85	1.94	2.06
22	B	604	CLA	C3B-C2B	-4.84	1.33	1.40
22	c	505	CLA	MG-NC	-4.82	1.94	2.06
22	D	403	CLA	C3B-C2B	-4.82	1.33	1.40
26	L	101	SQD	O8-S	4.81	1.64	1.47
22	B	604	CLA	MG-NC	-4.79	1.94	2.06
22	C	503	CLA	MG-NC	-4.79	1.94	2.06
22	c	509	CLA	MG-NC	-4.77	1.94	2.06
22	C	502	CLA	C3B-C2B	-4.75	1.33	1.40
22	a	405	CLA	C1B-NB	4.74	1.39	1.35
22	H	101	CLA	C3B-C2B	-4.73	1.33	1.40
22	d	403	CLA	MG-NC	-4.70	1.95	2.06
22	b	614	CLA	MG-NA	-4.70	1.95	2.06
22	A	412	CLA	MG-NC	-4.67	1.95	2.06
22	b	604	CLA	MG-NC	-4.67	1.95	2.06
22	B	601	CLA	C1B-NB	4.66	1.39	1.35
22	c	506	CLA	C3B-C2B	-4.65	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	C1B-NB	4.64	1.39	1.35
22	B	611	CLA	MG-NA	-4.64	1.95	2.06
22	B	601	CLA	MG-NC	-4.62	1.95	2.06
22	c	513	CLA	MG-NC	-4.62	1.95	2.06
22	c	502	CLA	MG-NC	-4.61	1.95	2.06
22	b	612	CLA	C3A-C2A	-4.57	1.41	1.54
22	C	513	CLA	MG-NC	-4.55	1.95	2.06
26	A	411	SQD	O8-S	4.55	1.63	1.47
22	b	616	CLA	C3B-C2B	-4.53	1.34	1.40
22	b	614	CLA	MG-NC	-4.53	1.95	2.06
22	b	606	CLA	MG-NC	-4.53	1.95	2.06
22	c	514	CLA	MG-NC	-4.53	1.95	2.06
22	b	605	CLA	MG-NC	-4.52	1.95	2.06
22	B	609	CLA	C3A-C2A	-4.52	1.41	1.54
30	b	624	LMG	O8-C28	4.52	1.46	1.33
22	C	502	CLA	MG-NC	-4.51	1.95	2.06
22	b	611	CLA	C3B-C2B	-4.47	1.34	1.40
22	B	609	CLA	MG-NC	-4.47	1.95	2.06
22	d	402	CLA	MG-NA	-4.45	1.95	2.06
22	b	609	CLA	C3B-C2B	-4.43	1.34	1.40
22	B	610	CLA	MG-NC	-4.42	1.95	2.06
22	B	613	CLA	MG-NC	-4.42	1.95	2.06
22	C	509	CLA	MG-NC	-4.42	1.95	2.06
22	b	617	CLA	C3B-C2B	-4.40	1.34	1.40
22	b	606	CLA	C3B-C2B	-4.39	1.34	1.40
22	b	608	CLA	MG-NC	-4.38	1.95	2.06
22	d	403	CLA	C3B-C2B	-4.38	1.34	1.40
22	d	403	CLA	MG-NA	-4.38	1.95	2.06
26	b	601	SQD	O8-S	4.38	1.63	1.47
22	a	404	CLA	C1B-NB	4.38	1.39	1.35
22	B	611	CLA	C3B-C2B	-4.35	1.34	1.40
32	L	102	LHG	O8-C23	4.35	1.46	1.33
22	b	607	CLA	MG-NC	-4.35	1.95	2.06
22	b	605	CLA	C3B-C2B	-4.35	1.34	1.40
22	B	602	CLA	C1B-NB	4.35	1.39	1.35
22	B	614	CLA	MG-NC	-4.34	1.96	2.06
22	a	404	CLA	MG-NC	-4.33	1.96	2.06
22	c	506	CLA	MG-NC	-4.32	1.96	2.06
22	C	510	CLA	MG-NC	-4.31	1.96	2.06
22	b	603	CLA	C1B-NB	4.31	1.39	1.35
22	B	603	CLA	C3B-C2B	-4.28	1.34	1.40
22	c	514	CLA	MG-NA	-4.28	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	409	LMG	O8-C28	4.27	1.45	1.33
33	E	102	HEM	C3B-C2B	-4.27	1.34	1.40
22	d	402	CLA	MG-NC	-4.27	1.96	2.06
26	D	411	SQD	O47-C7	4.27	1.46	1.34
30	C	522	LMG	O7-C10	4.26	1.46	1.34
22	C	514	CLA	MG-NC	-4.26	1.96	2.06
22	C	503	CLA	C1B-NB	4.25	1.39	1.35
22	c	511	CLA	MG-NC	-4.25	1.96	2.06
30	C	520	LMG	O8-C28	4.24	1.45	1.33
22	c	508	CLA	MG-NC	-4.24	1.96	2.06
30	D	409	LMG	O7-C10	4.24	1.46	1.34
22	b	610	CLA	MG-NC	-4.23	1.96	2.06
26	a	410	SQD	O8-S	4.23	1.62	1.47
22	B	610	CLA	C3B-C2B	-4.23	1.34	1.40
32	E	101	LHG	O8-C23	4.22	1.45	1.33
30	c	522	LMG	O7-C10	4.20	1.46	1.34
22	H	101	CLA	C1B-NB	4.19	1.38	1.35
22	d	401	CLA	MG-NC	-4.19	1.96	2.06
22	C	511	CLA	C1B-NB	4.18	1.38	1.35
22	b	615	CLA	C3B-C2B	-4.18	1.34	1.40
22	c	512	CLA	C1B-NB	4.17	1.38	1.35
22	B	612	CLA	MG-NC	-4.17	1.96	2.06
30	B	619	LMG	O7-C10	4.17	1.46	1.34
30	c	519	LMG	O8-C28	4.16	1.45	1.33
22	C	505	CLA	MG-NC	-4.16	1.96	2.06
26	A	409	SQD	O8-S	4.16	1.62	1.47
26	f	102	SQD	O8-S	4.15	1.62	1.47
22	A	412	CLA	MG-NA	-4.15	1.96	2.06
22	C	511	CLA	MG-NC	-4.12	1.96	2.06
22	C	502	CLA	C1B-NB	4.11	1.38	1.35
22	c	511	CLA	C1B-NB	4.10	1.38	1.35
22	c	504	CLA	MG-NC	-4.10	1.96	2.06
22	B	602	CLA	MG-NC	-4.10	1.96	2.06
22	B	612	CLA	C3B-C2B	-4.09	1.34	1.40
22	a	407	CLA	C3B-C2B	-4.08	1.34	1.40
22	c	513	CLA	C3B-C2B	-4.07	1.34	1.40
30	C	501	LMG	O8-C28	4.06	1.45	1.33
26	a	410	SQD	O48-C23	4.06	1.45	1.33
22	c	502	CLA	C1B-NB	4.06	1.38	1.35
31	H	103	DGD	O1G-C1A	4.06	1.45	1.33
32	E	101	LHG	O7-C7	4.05	1.45	1.34
22	A	403	CLA	MG-NC	-4.05	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	MG-NC	-4.05	1.96	2.06
22	b	618	CLA	C1B-NB	4.05	1.38	1.35
22	c	510	CLA	MG-NA	-4.04	1.96	2.06
26	f	102	SQD	O48-C23	4.04	1.45	1.33
22	b	615	CLA	C3A-C2A	-4.04	1.43	1.54
22	a	407	CLA	MG-NA	-4.03	1.96	2.06
30	f	101	LMG	O8-C28	4.03	1.45	1.33
22	B	605	CLA	MG-NC	-4.03	1.96	2.06
31	c	518	DGD	O2G-C1B	4.03	1.45	1.34
22	c	510	CLA	MG-NC	-4.03	1.96	2.06
22	c	507	CLA	MG-NC	-4.02	1.96	2.06
22	a	405	CLA	MG-NC	-4.02	1.96	2.06
22	C	510	CLA	MG-NA	-4.01	1.96	2.06
26	D	411	SQD	O8-S	4.01	1.61	1.47
30	c	522	LMG	O8-C28	3.99	1.45	1.33
22	D	402	CLA	C3B-C2B	-3.99	1.34	1.40
30	B	619	LMG	O8-C28	3.98	1.45	1.33
31	c	516	DGD	O1G-C1A	3.98	1.45	1.33
31	c	517	DGD	O1G-C1A	3.98	1.45	1.33
30	b	624	LMG	O7-C10	3.98	1.45	1.34
32	e	101	LHG	O8-C23	3.97	1.44	1.33
22	b	608	CLA	C1B-NB	3.97	1.38	1.35
26	L	101	SQD	O47-C7	3.96	1.45	1.34
22	B	612	CLA	C3A-C2A	-3.95	1.43	1.54
22	b	604	CLA	C1B-NB	3.95	1.38	1.35
32	d	406	LHG	O7-C7	3.95	1.45	1.34
22	C	512	CLA	MG-NC	-3.94	1.96	2.06
22	b	616	CLA	MG-NC	-3.94	1.96	2.06
32	e	101	LHG	O7-C7	3.93	1.45	1.34
22	B	603	CLA	MG-NC	-3.93	1.96	2.06
22	C	508	CLA	MG-NA	-3.93	1.96	2.06
22	B	614	CLA	C1B-NB	3.91	1.38	1.35
30	C	522	LMG	O8-C28	3.91	1.44	1.33
30	c	501	LMG	O8-C28	3.90	1.44	1.33
26	a	412	SQD	O47-C7	3.90	1.45	1.34
22	D	402	CLA	C3A-C2A	-3.89	1.43	1.54
22	A	403	CLA	MG-NA	-3.89	1.97	2.06
22	a	405	CLA	C3B-C2B	-3.89	1.35	1.40
33	e	102	HEM	C3B-C2B	-3.88	1.35	1.40
26	L	101	SQD	O48-C23	3.87	1.44	1.33
22	A	403	CLA	C1B-NB	3.86	1.38	1.35
30	B	621	LMG	O7-C10	3.86	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	h	102	DGD	O1G-C1A	3.85	1.44	1.33
31	C	518	DGD	O1G-C1A	3.84	1.44	1.33
26	A	409	SQD	O48-C23	3.84	1.44	1.33
22	B	601	CLA	C3B-C2B	-3.84	1.35	1.40
30	C	520	LMG	O7-C10	3.84	1.45	1.34
31	c	518	DGD	O1G-C1A	3.84	1.44	1.33
33	V	201	HEM	C3B-C2B	-3.83	1.35	1.40
22	B	615	CLA	C3B-C2B	-3.83	1.35	1.40
26	D	411	SQD	O48-C23	3.83	1.44	1.33
22	C	508	CLA	C3A-C2A	-3.82	1.43	1.54
22	B	612	CLA	C1B-NB	3.81	1.38	1.35
22	A	412	CLA	C3B-C2B	-3.81	1.35	1.40
26	A	411	SQD	O48-C23	3.81	1.44	1.33
32	b	628	LHG	O8-C23	3.80	1.44	1.33
26	b	601	SQD	O48-C23	3.80	1.44	1.33
22	b	612	CLA	MG-NA	-3.80	1.97	2.06
30	c	519	LMG	O7-C10	3.80	1.45	1.34
22	H	101	CLA	MG-NC	-3.80	1.97	2.06
31	C	518	DGD	O2G-C1B	3.79	1.45	1.34
22	A	403	CLA	C3A-C2A	-3.79	1.43	1.54
30	C	501	LMG	O7-C10	3.78	1.45	1.34
31	C	517	DGD	O1G-C1A	3.77	1.44	1.33
30	B	621	LMG	O8-C28	3.77	1.44	1.33
26	a	412	SQD	O48-C23	3.76	1.44	1.33
22	B	609	CLA	MG-NA	-3.76	1.97	2.06
22	b	607	CLA	C1B-NB	3.75	1.38	1.35
22	b	614	CLA	C3B-C2B	-3.75	1.35	1.40
22	b	605	CLA	C1B-NB	3.75	1.38	1.35
26	A	411	SQD	O47-C7	3.74	1.44	1.34
26	f	102	SQD	O47-C7	3.74	1.44	1.34
26	b	601	SQD	O47-C7	3.74	1.44	1.34
31	c	517	DGD	O2G-C1B	3.73	1.44	1.34
26	A	409	SQD	O47-C7	3.73	1.44	1.34
32	d	407	LHG	O7-C7	3.73	1.44	1.34
22	c	509	CLA	C3B-C2B	-3.73	1.35	1.40
22	c	513	CLA	MG-NA	-3.73	1.97	2.06
22	D	403	CLA	C3B-CAB	-3.72	1.40	1.47
22	b	610	CLA	MG-NA	-3.72	1.97	2.06
22	B	607	CLA	MG-NA	-3.72	1.97	2.06
30	f	101	LMG	O7-C10	3.70	1.44	1.34
22	c	510	CLA	C1B-NB	3.70	1.38	1.35
26	a	410	SQD	O47-C7	3.70	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	MG-NA	-3.69	1.97	2.06
22	C	513	CLA	C1B-NB	3.68	1.38	1.35
22	c	511	CLA	C3A-C2A	-3.67	1.44	1.54
22	c	503	CLA	C1B-NB	3.67	1.38	1.35
22	C	503	CLA	C3B-C2B	-3.66	1.35	1.40
30	m	103	LMG	O8-C28	3.66	1.44	1.33
22	B	608	CLA	C3B-C2B	-3.66	1.35	1.40
22	c	509	CLA	MG-NA	-3.65	1.97	2.06
22	c	511	CLA	C3B-C2B	-3.65	1.35	1.40
22	A	404	CLA	C3B-C2B	-3.65	1.35	1.40
22	C	504	CLA	MG-NC	-3.64	1.97	2.06
22	b	610	CLA	C3B-C2B	-3.63	1.35	1.40
33	v	201	HEM	C3B-C2B	-3.62	1.35	1.40
22	b	616	CLA	C1B-NB	3.62	1.38	1.35
22	B	608	CLA	MG-NC	-3.60	1.97	2.06
22	C	513	CLA	MG-NA	-3.59	1.97	2.06
22	d	401	CLA	MG-NA	-3.58	1.97	2.06
22	b	610	CLA	C3A-C2A	-3.58	1.44	1.54
31	C	519	DGD	O1G-C1A	3.58	1.43	1.33
22	c	503	CLA	C3B-C2B	-3.57	1.35	1.40
22	B	604	CLA	MG-NA	-3.57	1.97	2.06
22	B	606	CLA	MG-NA	-3.57	1.97	2.06
22	d	401	CLA	C3B-C2B	-3.57	1.35	1.40
31	h	102	DGD	O2G-C1B	3.56	1.44	1.34
22	c	507	CLA	C3B-C2B	-3.56	1.35	1.40
31	C	519	DGD	O2G-C1B	3.56	1.44	1.34
22	C	505	CLA	C1B-NB	3.55	1.38	1.35
22	C	505	CLA	MG-NA	-3.55	1.97	2.06
22	B	604	CLA	C1B-NB	3.54	1.38	1.35
32	D	408	LHG	O8-C23	3.54	1.43	1.33
32	D	406	LHG	O8-C23	3.54	1.43	1.33
30	c	501	LMG	O7-C10	3.53	1.44	1.34
22	d	401	CLA	C1B-NB	3.53	1.38	1.35
22	a	404	CLA	C3A-C2A	-3.53	1.44	1.54
31	C	517	DGD	O2G-C1B	3.53	1.44	1.34
22	c	512	CLA	MG-NC	-3.52	1.97	2.06
32	L	102	LHG	O7-C7	3.52	1.44	1.34
22	C	514	CLA	MG-NA	-3.52	1.97	2.06
31	H	103	DGD	O2G-C1B	3.51	1.44	1.34
22	D	403	CLA	MG-NA	-3.50	1.98	2.06
22	B	613	CLA	C1B-NB	3.50	1.38	1.35
22	c	504	CLA	C3B-C2B	-3.49	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	MG-NA	-3.49	1.98	2.06
32	l	101	LHG	O8-C23	3.48	1.43	1.33
32	d	407	LHG	O8-C23	3.48	1.43	1.33
22	c	505	CLA	MG-NA	-3.48	1.98	2.06
32	D	407	LHG	O8-C23	3.45	1.43	1.33
22	b	603	CLA	MG-NC	-3.45	1.98	2.06
22	B	610	CLA	MG-NA	-3.45	1.98	2.06
22	b	603	CLA	C3B-C2B	-3.42	1.35	1.40
22	C	504	CLA	C3B-C2B	-3.41	1.35	1.40
22	b	618	CLA	MG-NA	-3.38	1.98	2.06
22	c	512	CLA	C3B-C2B	-3.38	1.35	1.40
32	l	101	LHG	O7-C7	3.38	1.43	1.34
22	b	617	CLA	MG-NA	-3.38	1.98	2.06
22	B	602	CLA	C3B-C2B	-3.37	1.35	1.40
22	B	611	CLA	MG-NC	-3.36	1.98	2.06
22	b	617	CLA	C1B-NB	3.36	1.38	1.35
32	D	408	LHG	O7-C7	3.36	1.43	1.34
22	B	601	CLA	MG-NA	-3.34	1.98	2.06
22	C	508	CLA	C3B-C2B	-3.34	1.35	1.40
22	b	615	CLA	MG-NA	-3.32	1.98	2.06
32	b	628	LHG	O7-C7	3.32	1.43	1.34
32	D	406	LHG	O7-C7	3.31	1.43	1.34
22	c	513	CLA	C1B-NB	3.31	1.38	1.35
30	m	103	LMG	O7-C10	3.31	1.43	1.34
22	a	404	CLA	MG-NA	-3.30	1.98	2.06
22	A	406	CLA	C3A-C2A	-3.30	1.45	1.54
22	a	405	CLA	C3A-C2A	-3.27	1.45	1.54
22	A	403	CLA	C3B-C2B	-3.27	1.35	1.40
22	B	615	CLA	C3A-C2A	-3.26	1.45	1.54
22	a	404	CLA	C3B-C2B	-3.26	1.35	1.40
22	C	509	CLA	C3B-C2B	-3.26	1.35	1.40
22	b	604	CLA	MG-NA	-3.25	1.98	2.06
22	b	611	CLA	C1B-NB	3.24	1.38	1.35
22	C	509	CLA	MG-NA	-3.24	1.98	2.06
22	C	502	CLA	C3A-C2A	-3.23	1.45	1.54
22	c	503	CLA	MG-NA	-3.23	1.98	2.06
22	c	514	CLA	C3B-C2B	-3.23	1.35	1.40
22	c	511	CLA	MG-NA	-3.22	1.98	2.06
22	C	511	CLA	MG-NA	-3.22	1.98	2.06
22	A	406	CLA	C3B-CAB	-3.21	1.41	1.47
22	C	510	CLA	C1B-NB	3.21	1.38	1.35
22	C	514	CLA	C3B-C2B	-3.20	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	C3B-CAB	-3.19	1.41	1.47
22	C	514	CLA	C1B-NB	3.15	1.38	1.35
22	b	607	CLA	MG-NA	-3.14	1.98	2.06
26	D	411	SQD	C6-S	-3.12	1.65	1.77
22	D	402	CLA	MG-NA	-3.12	1.98	2.06
26	f	102	SQD	C6-S	-3.12	1.65	1.77
22	c	510	CLA	C3B-C2B	-3.11	1.36	1.40
22	c	508	CLA	MG-NA	-3.10	1.98	2.06
22	B	603	CLA	C1B-NB	3.09	1.38	1.35
22	b	613	CLA	MG-NA	-3.08	1.98	2.06
22	c	505	CLA	C3B-C2B	-3.07	1.36	1.40
22	b	614	CLA	C3A-C2A	-3.06	1.45	1.54
22	C	510	CLA	C3B-C2B	-3.06	1.36	1.40
22	c	512	CLA	MG-NA	-3.05	1.99	2.06
22	B	606	CLA	CHD-C4C	-3.05	1.32	1.41
24	C	516	BCR	C1-C6	-3.05	1.49	1.53
26	a	410	SQD	C6-S	-3.04	1.66	1.77
22	C	505	CLA	C3B-C2B	-3.04	1.36	1.40
31	c	516	DGD	O2G-C1B	3.03	1.42	1.34
22	c	506	CLA	MG-NA	-3.02	1.99	2.06
32	D	407	LHG	O7-C7	3.01	1.42	1.34
22	c	508	CLA	C3A-C2A	-2.99	1.46	1.54
22	B	615	CLA	C1B-NB	2.99	1.37	1.35
22	b	606	CLA	C1B-NB	2.98	1.37	1.35
26	b	601	SQD	C6-S	-2.98	1.66	1.77
22	b	607	CLA	C3B-CAB	-2.97	1.41	1.47
22	A	406	CLA	CHD-C4C	-2.97	1.32	1.41
22	b	603	CLA	MG-NA	-2.97	1.99	2.06
22	b	615	CLA	C1B-NB	2.96	1.37	1.35
22	d	402	CLA	C1B-NB	2.95	1.37	1.35
22	b	607	CLA	C3A-C2A	-2.95	1.46	1.54
22	b	612	CLA	C1B-NB	2.94	1.37	1.35
32	d	406	LHG	O8-C23	2.94	1.41	1.33
26	A	409	SQD	C6-S	-2.94	1.66	1.77
22	B	606	CLA	C3B-CAB	-2.92	1.42	1.47
22	b	611	CLA	C3B-CAB	-2.91	1.42	1.47
26	A	411	SQD	C6-S	-2.90	1.66	1.77
22	b	606	CLA	C3A-C2A	-2.90	1.46	1.54
22	b	611	CLA	MG-NA	-2.88	1.99	2.06
22	b	608	CLA	MG-NA	-2.88	1.99	2.06
22	D	402	CLA	C1B-NB	2.87	1.37	1.35
22	H	101	CLA	MG-NA	-2.87	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C3B-CAB	-2.86	1.42	1.47
22	b	609	CLA	MG-NA	-2.84	1.99	2.06
22	b	605	CLA	C3B-CAB	-2.83	1.42	1.47
22	C	505	CLA	C3A-C2A	-2.82	1.46	1.54
22	B	615	CLA	MG-NA	-2.82	1.99	2.06
22	b	609	CLA	C1B-NB	2.82	1.37	1.35
22	C	504	CLA	MG-NA	-2.82	1.99	2.06
22	b	609	CLA	CHD-C4C	-2.81	1.32	1.41
22	C	511	CLA	C3B-C2B	-2.81	1.36	1.40
22	D	403	CLA	C1B-NB	2.81	1.37	1.35
23	A	405	PHO	C1D-C2D	-2.80	1.39	1.45
22	c	504	CLA	MG-NA	-2.80	1.99	2.06
22	b	615	CLA	C4C-C3C	-2.78	1.40	1.45
22	c	514	CLA	C1B-NB	2.77	1.37	1.35
22	c	506	CLA	C1B-NB	2.77	1.37	1.35
22	b	618	CLA	CHD-C4C	-2.76	1.33	1.41
22	C	513	CLA	C3B-C2B	-2.76	1.36	1.40
22	a	405	CLA	MG-NA	-2.76	1.99	2.06
22	d	401	CLA	C4C-C3C	2.75	1.49	1.45
22	C	512	CLA	MG-NA	-2.75	1.99	2.06
22	b	618	CLA	C3A-C2A	-2.75	1.46	1.54
22	c	508	CLA	C3B-C2B	-2.74	1.36	1.40
22	c	510	CLA	C3A-C2A	-2.73	1.46	1.54
22	b	610	CLA	C1B-NB	2.73	1.37	1.35
22	c	502	CLA	C3A-C2A	-2.73	1.46	1.54
26	L	101	SQD	C6-S	-2.72	1.67	1.77
22	C	508	CLA	CHD-C4C	-2.70	1.33	1.41
22	B	613	CLA	C3B-CAB	-2.70	1.42	1.47
22	A	406	CLA	C1C-NC	-2.69	1.33	1.37
23	a	414	PHO	C1D-C2D	-2.68	1.40	1.45
24	K	102	BCR	C30-C25	-2.68	1.50	1.53
32	D	406	LHG	O7-C5	-2.68	1.39	1.46
24	B	618	BCR	C1-C6	-2.68	1.50	1.53
30	C	522	LMG	O1-C1	2.67	1.44	1.40
22	C	507	CLA	C3B-CAB	-2.67	1.42	1.47
23	D	401	PHO	C4A-NA	-2.67	1.28	1.35
22	a	407	CLA	CHD-C4C	-2.67	1.33	1.41
23	D	401	PHO	C1D-C2D	-2.65	1.40	1.45
22	b	605	CLA	CHD-C4C	-2.65	1.33	1.41
22	d	403	CLA	CHD-C4C	-2.65	1.33	1.41
22	C	508	CLA	C1B-NB	2.62	1.37	1.35
22	C	507	CLA	C3A-C2A	-2.62	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	605	CLA	MG-NA	-2.61	2.00	2.06
24	k	101	BCR	C1-C6	-2.61	1.50	1.53
22	C	510	CLA	C3A-C2A	-2.61	1.47	1.54
22	A	404	CLA	C3A-C2A	-2.60	1.47	1.54
22	b	605	CLA	C3A-C2A	-2.60	1.47	1.54
22	b	609	CLA	C3B-CAB	-2.59	1.42	1.47
24	c	523	BCR	C1-C6	-2.59	1.50	1.53
22	C	513	CLA	C3A-C2A	-2.57	1.47	1.54
22	c	508	CLA	C1B-NB	2.57	1.37	1.35
22	c	513	CLA	C3A-C2A	-2.57	1.47	1.54
22	c	502	CLA	C3B-C2B	-2.57	1.36	1.40
22	b	608	CLA	CHD-C4C	-2.56	1.33	1.41
22	a	407	CLA	C3A-C2A	-2.55	1.47	1.54
22	B	602	CLA	CHD-C4C	-2.55	1.33	1.41
32	D	407	LHG	O7-C5	-2.55	1.40	1.46
32	d	406	LHG	O8-C6	-2.54	1.39	1.45
22	A	404	CLA	MG-NC	-2.53	2.00	2.06
23	a	414	PHO	C4A-NA	-2.53	1.29	1.35
24	t	102	BCR	C30-C25	-2.52	1.50	1.53
22	B	609	CLA	CBC-CAC	-2.52	1.40	1.51
22	c	506	CLA	CHD-C4C	-2.52	1.33	1.41
24	B	617	BCR	C1-C6	-2.52	1.50	1.53
22	c	514	CLA	CHD-C4C	-2.52	1.33	1.41
22	c	502	CLA	CHD-C4C	-2.52	1.33	1.41
22	C	513	CLA	CHD-C4C	-2.51	1.33	1.41
22	C	509	CLA	C1B-NB	2.50	1.37	1.35
24	c	515	BCR	C1-C6	-2.50	1.50	1.53
22	b	609	CLA	C4C-C3C	-2.49	1.40	1.45
22	C	502	CLA	CHD-C4C	-2.49	1.33	1.41
23	a	406	PHO	C1D-C2D	-2.49	1.40	1.45
22	C	507	CLA	MG-NA	-2.48	2.00	2.06
24	T	101	BCR	C30-C25	-2.48	1.50	1.53
22	b	614	CLA	C1C-NC	-2.48	1.34	1.37
22	c	509	CLA	C3A-C2A	-2.48	1.47	1.54
22	C	505	CLA	CHD-C4C	-2.48	1.33	1.41
22	b	615	CLA	CHD-C4C	-2.48	1.33	1.41
22	c	502	CLA	MG-NA	-2.47	2.00	2.06
22	B	608	CLA	C3B-CAB	-2.47	1.42	1.47
22	c	503	CLA	CHD-C4C	-2.47	1.33	1.41
22	c	507	CLA	MG-NA	-2.45	2.00	2.06
22	D	403	CLA	CHD-C4C	-2.44	1.34	1.41
22	b	611	CLA	CHD-C4C	-2.43	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	CHD-C4C	-2.42	1.34	1.41
31	c	516	DGD	O2G-C2G	-2.42	1.40	1.46
22	C	506	CLA	CHD-C4C	-2.42	1.34	1.41
22	B	612	CLA	MG-NA	-2.41	2.00	2.06
22	c	514	CLA	C3B-CAB	-2.41	1.43	1.47
32	b	628	LHG	O7-C5	-2.40	1.40	1.46
22	C	510	CLA	CHD-C4C	-2.40	1.34	1.41
22	B	606	CLA	C4C-C3C	-2.40	1.40	1.45
22	b	612	CLA	C3B-CAB	-2.40	1.43	1.47
22	B	605	CLA	CHD-C4C	-2.39	1.34	1.41
22	b	614	CLA	CHD-C4C	-2.38	1.34	1.41
22	B	602	CLA	C3A-C2A	-2.38	1.47	1.54
22	b	611	CLA	C3A-C2A	-2.38	1.47	1.54
22	B	613	CLA	MG-NA	-2.38	2.00	2.06
22	B	602	CLA	MG-NA	-2.37	2.00	2.06
22	B	608	CLA	CHD-C4C	-2.35	1.34	1.41
22	c	512	CLA	C3A-C2A	-2.35	1.47	1.54
22	C	514	CLA	CHD-C4C	-2.34	1.34	1.41
22	a	407	CLA	C1B-NB	2.34	1.37	1.35
22	A	412	CLA	C3A-C2A	-2.33	1.47	1.54
22	b	616	CLA	C3B-CAB	-2.33	1.43	1.47
22	B	612	CLA	CHD-C4C	-2.33	1.34	1.41
22	B	605	CLA	C3B-CAB	-2.33	1.43	1.47
22	b	608	CLA	C3A-C2A	-2.32	1.48	1.54
22	C	507	CLA	CHD-C4C	-2.32	1.34	1.41
24	a	408	BCR	C30-C25	-2.32	1.50	1.53
22	B	607	CLA	CHD-C4C	-2.31	1.34	1.41
22	c	509	CLA	CHD-C4C	-2.31	1.34	1.41
23	A	405	PHO	C4A-NA	-2.31	1.29	1.35
25	A	408	PL9	C6-C5	2.31	1.47	1.35
31	C	519	DGD	O2G-C2G	-2.31	1.40	1.46
25	D	405	PL9	C3-C4	-2.31	1.45	1.49
22	B	615	CLA	CHD-C4C	-2.30	1.34	1.41
24	B	616	BCR	C1-C6	-2.30	1.50	1.53
22	A	412	CLA	C1B-NB	2.30	1.37	1.35
22	B	607	CLA	C3B-CAB	-2.30	1.43	1.47
22	c	510	CLA	CHD-C4C	-2.30	1.34	1.41
22	c	513	CLA	CHD-C4C	-2.30	1.34	1.41
22	B	614	CLA	C3A-C2A	-2.30	1.48	1.54
22	C	509	CLA	CHD-C4C	-2.29	1.34	1.41
22	B	609	CLA	C1B-NB	2.29	1.37	1.35
23	a	406	PHO	CHB-C4A	2.29	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	CHD-C4C	-2.29	1.34	1.41
24	d	404	BCR	C30-C25	-2.29	1.50	1.53
22	B	613	CLA	CHD-C4C	-2.29	1.34	1.41
24	b	621	BCR	C1-C6	-2.28	1.50	1.53
22	b	612	CLA	CHD-C4C	-2.28	1.34	1.41
25	D	405	PL9	C6-C5	2.28	1.47	1.35
22	b	604	CLA	C3B-C2B	-2.28	1.37	1.40
22	B	601	CLA	C3A-C2A	-2.28	1.48	1.54
22	B	610	CLA	C1B-NB	2.27	1.37	1.35
22	B	614	CLA	MG-NA	-2.27	2.00	2.06
22	b	617	CLA	CHD-C4C	-2.27	1.34	1.41
22	C	512	CLA	CHD-C4C	-2.27	1.34	1.41
22	b	604	CLA	C1C-NC	-2.27	1.34	1.37
22	B	610	CLA	C3A-C2A	-2.27	1.48	1.54
22	A	412	CLA	C4C-C3C	2.27	1.48	1.45
22	C	503	CLA	CHD-C4C	-2.26	1.34	1.41
32	D	408	LHG	O7-C5	-2.26	1.40	1.46
22	b	606	CLA	CHD-C4C	-2.25	1.34	1.41
22	a	405	CLA	C3B-CAB	-2.25	1.43	1.47
22	a	405	CLA	C3D-C2D	2.24	1.43	1.39
22	c	504	CLA	CHD-C4C	-2.24	1.34	1.41
22	c	511	CLA	CHD-C4C	-2.24	1.34	1.41
22	H	101	CLA	CHD-C4C	-2.23	1.34	1.41
22	b	604	CLA	CHD-C4C	-2.23	1.34	1.41
24	C	516	BCR	C21-C22	-2.23	1.32	1.35
22	b	616	CLA	MG-NA	-2.22	2.01	2.06
25	a	409	PL9	C6-C5	2.22	1.46	1.35
22	C	502	CLA	C3B-CAB	-2.22	1.43	1.47
30	b	624	LMG	O1-C1	2.21	1.44	1.40
22	C	507	CLA	C3D-C2D	2.21	1.43	1.39
22	b	613	CLA	C1B-NB	2.20	1.37	1.35
22	B	611	CLA	CHD-C4C	-2.20	1.34	1.41
22	c	512	CLA	CHD-C4C	-2.20	1.34	1.41
22	c	503	CLA	C3A-C2A	-2.20	1.48	1.54
22	C	506	CLA	C3B-CAB	-2.19	1.43	1.47
22	b	613	CLA	C3D-C2D	2.19	1.43	1.39
22	C	512	CLA	C3B-C2B	-2.19	1.37	1.40
32	l	101	LHG	O7-C5	-2.19	1.41	1.46
22	c	514	CLA	C3A-C2A	-2.18	1.48	1.54
22	B	607	CLA	C3D-C2D	2.18	1.43	1.39
22	C	502	CLA	MG-NA	-2.18	2.01	2.06
22	c	508	CLA	C3B-CAB	-2.17	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	516	BCR	C30-C25	-2.17	1.50	1.53
22	B	614	CLA	C3B-CAB	-2.17	1.43	1.47
24	D	404	BCR	C30-C25	-2.17	1.50	1.53
22	b	603	CLA	CHD-C4C	-2.17	1.34	1.41
22	A	404	CLA	MG-NA	-2.17	2.01	2.06
22	b	616	CLA	CHD-C4C	-2.16	1.34	1.41
25	d	405	PL9	C6-C5	2.16	1.46	1.35
25	A	408	PL9	C2-C1	-2.16	1.38	1.44
22	b	609	CLA	C3A-C2A	-2.15	1.48	1.54
22	B	613	CLA	C3A-C2A	-2.15	1.48	1.54
22	b	616	CLA	C3D-C2D	2.15	1.43	1.39
22	b	609	CLA	C1B-CHB	-2.15	1.35	1.41
25	d	405	PL9	C2-C1	-2.14	1.38	1.44
22	C	504	CLA	CHD-C4C	-2.13	1.34	1.41
22	c	507	CLA	C3A-C2A	-2.13	1.48	1.54
22	b	610	CLA	C3D-C2D	2.12	1.43	1.39
22	A	404	CLA	C3D-C2D	2.12	1.43	1.39
22	c	503	CLA	C3D-C2D	2.12	1.43	1.39
24	D	404	BCR	C1-C6	-2.11	1.50	1.53
22	b	603	CLA	C3D-C2D	2.11	1.43	1.39
22	c	507	CLA	C1B-NB	2.11	1.37	1.35
22	a	404	CLA	CHD-C4C	-2.10	1.34	1.41
31	c	518	DGD	O2G-C2G	-2.10	1.41	1.46
25	D	405	PL9	C2-C1	-2.10	1.39	1.44
22	b	610	CLA	C3B-CAB	-2.09	1.43	1.47
22	c	509	CLA	C3B-CAB	-2.09	1.43	1.47
23	A	405	PHO	C3D-C4D	-2.09	1.36	1.43
22	C	511	CLA	CHD-C4C	-2.09	1.35	1.41
22	C	509	CLA	C3B-CAB	-2.09	1.43	1.47
22	H	101	CLA	C3A-C2A	-2.08	1.48	1.54
22	b	615	CLA	C3B-CAB	-2.08	1.43	1.47
24	B	617	BCR	C30-C25	-2.08	1.50	1.53
22	B	612	CLA	C3D-C2D	2.08	1.43	1.39
22	d	402	CLA	CHD-C4C	-2.08	1.35	1.41
22	b	607	CLA	CHD-C4C	-2.07	1.35	1.41
32	d	406	LHG	O7-C5	-2.07	1.41	1.46
22	b	604	CLA	C3A-C2A	-2.06	1.48	1.54
32	d	407	LHG	O7-C5	-2.06	1.41	1.46
22	d	401	CLA	CHD-C4C	-2.06	1.35	1.41
22	B	608	CLA	C1B-NB	2.06	1.37	1.35
22	C	505	CLA	C3D-C2D	2.06	1.43	1.39
22	b	610	CLA	CHD-C4C	-2.06	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	CHD-C4C	-2.06	1.35	1.41
25	d	405	PL9	C3-C4	-2.05	1.46	1.49
24	C	515	BCR	C30-C25	-2.05	1.50	1.53
22	c	507	CLA	CHD-C4C	-2.05	1.35	1.41
22	A	403	CLA	C1C-NC	-2.05	1.34	1.37
22	b	611	CLA	C3D-C2D	2.04	1.43	1.39
22	D	403	CLA	C3A-C2A	-2.04	1.48	1.54
25	a	409	PL9	C2-C1	-2.04	1.39	1.44
24	c	515	BCR	C30-C25	-2.04	1.51	1.53
22	C	512	CLA	C3D-C2D	2.04	1.43	1.39
22	B	608	CLA	C3D-C2D	2.04	1.43	1.39
22	c	511	CLA	C3D-C2D	2.03	1.43	1.39
22	b	615	CLA	C1C-NC	-2.03	1.34	1.37
22	c	504	CLA	C3A-C2A	-2.02	1.48	1.54
22	c	506	CLA	C3D-C2D	2.02	1.43	1.39
22	B	610	CLA	CHD-C4C	-2.02	1.35	1.41
22	c	507	CLA	C3D-C2D	2.02	1.43	1.39
24	b	619	BCR	C1-C6	-2.01	1.51	1.53
22	C	513	CLA	C3D-C2D	2.01	1.43	1.39
22	A	412	CLA	C3D-C2D	2.01	1.43	1.39
22	C	509	CLA	C3D-C2D	2.01	1.43	1.39
22	d	401	CLA	C3D-C2D	2.01	1.43	1.39
22	B	606	CLA	C1B-CHB	-2.01	1.35	1.41
22	C	514	CLA	C3B-CAB	-2.00	1.43	1.47

All (1142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	101	SQD	O9-S-C6	-18.70	84.72	106.94
26	L	101	SQD	O8-S-O9	-10.90	84.64	111.27
26	L	101	SQD	O7-S-C6	10.80	119.78	106.94
26	L	101	SQD	O9-S-O7	-9.72	80.32	113.95
22	A	403	CLA	C4A-NA-C1A	-8.71	102.79	106.71
22	B	615	CLA	C4A-NA-C1A	-8.28	102.98	106.71
22	b	610	CLA	C4A-NA-C1A	-8.27	102.99	106.71
22	C	507	CLA	C4A-NA-C1A	-8.20	103.02	106.71
22	b	612	CLA	C4A-NA-C1A	-8.12	103.06	106.71
22	b	606	CLA	C4A-NA-C1A	-7.90	103.16	106.71
22	C	502	CLA	C4A-NA-C1A	-7.86	103.17	106.71
22	c	508	CLA	C4D-C3D-CAD	7.66	112.74	108.47
22	B	606	CLA	C4D-C3D-CAD	7.51	112.66	108.47
22	c	507	CLA	C4A-NA-C1A	-7.49	103.34	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	402	CLA	C4A-NA-C1A	-7.41	103.38	106.71
22	b	611	CLA	C4A-NA-C1A	-7.24	103.45	106.71
22	B	613	CLA	C4A-NA-C1A	-7.17	103.48	106.71
22	c	502	CLA	C4A-NA-C1A	-7.14	103.50	106.71
22	a	404	CLA	C4A-NA-C1A	-7.02	103.55	106.71
22	b	605	CLA	C4A-NA-C1A	-7.02	103.55	106.71
22	B	609	CLA	C4A-NA-C1A	-7.00	103.56	106.71
22	b	608	CLA	C4A-NA-C1A	-6.89	103.61	106.71
22	b	609	CLA	C4A-NA-C1A	-6.89	103.61	106.71
22	c	511	CLA	C4A-NA-C1A	-6.89	103.61	106.71
22	a	405	CLA	C4A-NA-C1A	-6.81	103.65	106.71
22	B	614	CLA	C4A-NA-C1A	-6.74	103.68	106.71
22	B	610	CLA	C4A-NA-C1A	-6.66	103.71	106.71
22	b	604	CLA	C4A-NA-C1A	-6.64	103.72	106.71
22	C	508	CLA	C4A-NA-C1A	-6.63	103.72	106.71
22	c	509	CLA	C4A-NA-C1A	-6.62	103.73	106.71
22	A	404	CLA	C4A-NA-C1A	-6.56	103.75	106.71
22	b	615	CLA	C4A-NA-C1A	-6.55	103.76	106.71
22	B	610	CLA	C4D-C3D-CAD	6.55	112.12	108.47
22	B	601	CLA	C4A-NA-C1A	-6.54	103.76	106.71
22	B	602	CLA	C4A-NA-C1A	-6.54	103.77	106.71
22	B	612	CLA	C4A-NA-C1A	-6.53	103.77	106.71
22	D	402	CLA	C4D-C3D-CAD	6.52	112.11	108.47
22	c	503	CLA	C4A-NA-C1A	-6.42	103.82	106.71
25	A	408	PL9	C7-C8-C9	-6.40	116.14	126.79
22	c	508	CLA	C4A-NA-C1A	-6.39	103.83	106.71
22	B	605	CLA	C4D-C3D-CAD	6.30	111.98	108.47
22	B	604	CLA	C4A-NA-C1A	-6.29	103.88	106.71
22	B	603	CLA	C4D-C3D-CAD	6.24	111.95	108.47
22	a	404	CLA	C4D-C3D-CAD	6.22	111.94	108.47
22	C	505	CLA	C4A-NA-C1A	-6.21	103.91	106.71
22	b	618	CLA	C4D-C3D-CAD	6.19	111.92	108.47
22	H	101	CLA	C4D-C3D-CAD	6.19	111.92	108.47
26	L	101	SQD	O8-S-C6	6.19	115.60	105.74
22	b	618	CLA	C4A-NA-C1A	-6.18	103.93	106.71
22	b	607	CLA	C4A-NA-C1A	-6.13	103.95	106.71
22	B	603	CLA	C4A-NA-C1A	-6.11	103.96	106.71
33	v	201	HEM	CBD-CAD-C3D	-6.11	101.23	112.48
22	b	609	CLA	C4D-C3D-CAD	6.08	111.86	108.47
22	C	506	CLA	C4A-NA-C1A	-6.06	103.98	106.71
24	d	404	BCR	C28-C27-C26	-6.04	103.30	114.08
22	b	617	CLA	C4A-NA-C1A	-6.01	104.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4D-C3D-CAD	6.00	111.81	108.47
22	c	512	CLA	C4D-C3D-CAD	5.99	111.81	108.47
22	B	605	CLA	C4A-NA-C1A	-5.99	104.01	106.71
22	c	502	CLA	C4D-C3D-CAD	5.96	111.79	108.47
22	b	614	CLA	C4A-NA-C1A	-5.94	104.04	106.71
22	B	614	CLA	C4D-C3D-CAD	5.94	111.78	108.47
22	C	514	CLA	C4D-C3D-CAD	5.93	111.78	108.47
22	b	603	CLA	C4D-C3D-CAD	5.89	111.76	108.47
22	B	607	CLA	C4A-NA-C1A	-5.89	104.06	106.71
25	a	409	PL9	C7-C8-C9	-5.88	117.00	126.79
22	b	613	CLA	C4A-NA-C1A	-5.86	104.07	106.71
22	B	608	CLA	C4A-NA-C1A	-5.84	104.08	106.71
22	C	508	CLA	C4D-C3D-CAD	5.83	111.72	108.47
22	C	511	CLA	C4D-C3D-CAD	5.83	111.72	108.47
24	T	101	BCR	C20-C21-C22	-5.80	119.03	127.31
24	h	101	BCR	C11-C10-C9	-5.80	119.03	127.31
30	m	103	LMG	O7-C10-C11	5.79	123.99	111.50
22	b	606	CLA	C4D-C3D-CAD	5.78	111.69	108.47
22	b	612	CLA	C4D-C3D-CAD	5.77	111.69	108.47
22	B	611	CLA	C4D-C3D-CAD	5.76	111.68	108.47
24	K	102	BCR	C7-C8-C9	-5.73	117.58	126.23
22	B	609	CLA	C4D-C3D-CAD	5.73	111.66	108.47
22	c	504	CLA	C4A-NA-C1A	-5.72	104.13	106.71
24	H	102	BCR	C7-C8-C9	-5.72	117.60	126.23
22	d	403	CLA	C4D-C3D-CAD	5.68	111.64	108.47
24	D	404	BCR	C24-C23-C22	-5.67	117.66	126.23
24	T	101	BCR	C33-C5-C6	-5.65	118.18	124.53
22	b	604	CLA	C4D-C3D-CAD	5.65	111.62	108.47
22	c	514	CLA	C4D-C3D-CAD	5.64	111.62	108.47
22	c	512	CLA	C4A-NA-C1A	-5.64	104.17	106.71
22	b	616	CLA	C4A-NA-C1A	-5.64	104.17	106.71
22	D	403	CLA	C4D-C3D-CAD	5.56	111.57	108.47
22	C	509	CLA	C4A-NA-C1A	-5.56	104.21	106.71
22	d	402	CLA	C4D-C3D-CAD	5.54	111.56	108.47
22	c	510	CLA	C4A-NA-C1A	-5.53	104.22	106.71
22	B	602	CLA	C4D-C3D-CAD	5.52	111.55	108.47
24	d	404	BCR	C24-C23-C22	-5.51	117.91	126.23
24	c	523	BCR	C28-C27-C26	-5.50	104.25	114.08
24	K	101	BCR	C33-C5-C6	-5.50	118.35	124.53
22	B	601	CLA	C4D-C3D-CAD	5.49	111.53	108.47
24	H	102	BCR	C11-C10-C9	-5.49	119.48	127.31
22	D	403	CLA	C4A-NA-C1A	-5.48	104.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	BCR	C24-C23-C22	-5.44	118.01	126.23
22	A	406	CLA	C4A-NA-C1A	-5.42	104.27	106.71
22	C	512	CLA	C4D-C3D-CAD	5.41	111.49	108.47
26	D	411	SQD	O9-S-C6	5.37	113.32	106.94
24	h	101	BCR	C7-C8-C9	-5.35	118.14	126.23
22	c	513	CLA	C4D-C3D-CAD	5.34	111.45	108.47
22	c	506	CLA	C4D-C3D-CAD	5.34	111.45	108.47
22	c	504	CLA	C4D-C3D-CAD	5.33	111.44	108.47
25	d	405	PL9	C7-C8-C9	-5.33	117.92	126.79
30	c	522	LMG	O7-C10-C11	5.31	122.94	111.50
22	C	513	CLA	C4A-NA-C1A	-5.30	104.32	106.71
22	B	606	CLA	C4A-NA-C1A	-5.29	104.33	106.71
24	d	404	BCR	C15-C14-C13	-5.28	119.78	127.31
22	b	608	CLA	C4D-C3D-CAD	5.28	111.41	108.47
24	C	516	BCR	C7-C8-C9	-5.27	118.28	126.23
24	c	523	BCR	C33-C5-C6	-5.26	118.62	124.53
22	d	401	CLA	C4A-NA-C1A	-5.26	104.34	106.71
22	c	507	CLA	C4D-C3D-CAD	5.24	111.39	108.47
22	C	503	CLA	C4D-C3D-CAD	5.24	111.39	108.47
22	C	514	CLA	C4A-NA-C1A	-5.22	104.36	106.71
30	C	522	LMG	O1-C1-C2	5.21	116.44	108.30
22	B	613	CLA	C4D-C3D-CAD	5.18	111.36	108.47
22	c	505	CLA	C4A-NA-C1A	-5.17	104.38	106.71
24	k	101	BCR	C24-C23-C22	-5.15	118.46	126.23
22	C	502	CLA	C4D-C3D-CAD	5.14	111.34	108.47
22	A	412	CLA	C4A-NA-C1A	-5.14	104.39	106.71
22	C	504	CLA	C4A-NA-C1A	-5.11	104.41	106.71
22	C	510	CLA	C4A-NA-C1A	-5.09	104.42	106.71
24	B	617	BCR	C28-C27-C26	-5.09	104.99	114.08
24	B	618	BCR	C7-C8-C9	-5.08	118.56	126.23
22	c	513	CLA	C4A-NA-C1A	-5.08	104.42	106.71
22	C	504	CLA	C4D-C3D-CAD	5.06	111.29	108.47
22	a	407	CLA	C4A-NA-C1A	-5.06	104.43	106.71
31	C	517	DGD	O2G-C1B-C2B	5.00	122.27	111.50
22	B	608	CLA	C4D-C3D-CAD	4.97	111.24	108.47
24	K	102	BCR	C15-C14-C13	-4.94	120.26	127.31
22	A	403	CLA	C4D-C3D-CAD	4.94	111.22	108.47
22	c	514	CLA	C4A-NA-C1A	-4.90	104.50	106.71
22	C	505	CLA	C4D-C3D-CAD	4.90	111.20	108.47
24	t	102	BCR	C33-C5-C6	-4.89	119.03	124.53
22	B	604	CLA	C4D-C3D-CAD	4.89	111.20	108.47
22	d	402	CLA	C4A-NA-C1A	-4.89	104.51	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C4D-C3D-CAD	4.88	111.19	108.47
22	C	510	CLA	C4D-C3D-CAD	4.87	111.19	108.47
22	b	603	CLA	C4A-NA-C1A	-4.85	104.52	106.71
22	a	407	CLA	C4D-C3D-CAD	4.83	111.16	108.47
22	C	512	CLA	C4A-NA-C1A	-4.82	104.54	106.71
24	D	404	BCR	C38-C26-C25	-4.82	119.12	124.53
22	c	505	CLA	C4D-C3D-CAD	4.81	111.16	108.47
26	f	102	SQD	C45-O47-C7	-4.79	106.00	117.79
24	c	524	BCR	C28-C27-C26	-4.78	105.55	114.08
26	A	409	SQD	O6-C1-C2	4.76	115.74	108.30
24	c	515	BCR	C33-C5-C6	-4.76	119.19	124.53
26	D	411	SQD	O6-C1-C2	4.72	115.68	108.30
31	H	103	DGD	O2G-C1B-C2B	4.72	121.68	111.50
22	C	511	CLA	C4A-NA-C1A	-4.72	104.59	106.71
24	t	102	BCR	C24-C23-C22	-4.70	119.13	126.23
22	c	511	CLA	C4D-C3D-CAD	4.69	111.08	108.47
33	V	201	HEM	CBD-CAD-C3D	-4.68	103.86	112.48
24	d	404	BCR	C33-C5-C6	-4.67	119.28	124.53
22	d	403	CLA	C4A-NA-C1A	-4.67	104.61	106.71
30	c	501	LMG	C8-O7-C10	-4.66	106.33	117.79
22	b	607	CLA	C4D-C3D-CAD	4.62	111.05	108.47
22	b	617	CLA	C4D-C3D-CAD	4.62	111.05	108.47
33	E	102	HEM	CBA-CAA-C2A	-4.62	103.97	112.49
30	B	619	LMG	O7-C10-C11	4.61	121.44	111.50
30	C	522	LMG	O6-C5-C6	4.61	117.89	106.44
22	c	506	CLA	C4A-NA-C1A	-4.59	104.64	106.71
22	B	611	CLA	C4A-NA-C1A	-4.58	104.65	106.71
22	b	613	CLA	C4D-C3D-CAD	4.57	111.02	108.47
22	H	101	CLA	C4A-NA-C1A	-4.54	104.66	106.71
26	D	411	SQD	C44-O6-C1	-4.53	104.89	113.74
30	B	621	LMG	O7-C10-C11	4.51	121.22	111.50
30	C	522	LMG	O7-C10-C11	4.50	121.19	111.50
23	D	401	PHO	CBD-CHA-C4D	-4.47	103.51	108.54
24	B	618	BCR	C15-C14-C13	-4.47	120.94	127.31
32	d	406	LHG	O7-C7-C8	4.46	121.12	111.50
22	B	615	CLA	C4D-C3D-CAD	4.46	110.95	108.47
24	C	516	BCR	C24-C23-C22	-4.44	119.52	126.23
22	B	612	CLA	C4D-C3D-CAD	4.41	110.93	108.47
22	A	406	CLA	C4D-C3D-CAD	4.41	110.93	108.47
22	c	510	CLA	C4D-C3D-CAD	4.41	110.93	108.47
30	c	519	LMG	O7-C10-C11	4.40	120.97	111.50
22	A	404	CLA	C4D-C3D-CAD	4.39	110.92	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	414	PHO	CBD-CHA-C4D	-4.37	103.62	108.54
26	A	409	SQD	C1-O5-C5	-4.32	105.21	113.69
24	D	404	BCR	C7-C8-C9	-4.31	119.72	126.23
22	A	412	CLA	C4D-C3D-CAD	4.29	110.86	108.47
30	C	520	LMG	O7-C10-C11	4.29	120.76	111.50
30	f	101	LMG	O7-C10-C11	4.29	120.76	111.50
26	f	102	SQD	O9-S-C6	4.28	112.03	106.94
22	C	513	CLA	C4D-C3D-CAD	4.28	110.85	108.47
22	b	611	CLA	C4D-C3D-CAD	4.26	110.85	108.47
24	c	524	BCR	C16-C17-C18	-4.26	121.23	127.31
22	b	612	CLA	C1-C2-C3	-4.26	118.67	126.04
22	b	614	CLA	C4D-C3D-CAD	4.25	110.84	108.47
24	B	618	BCR	C1-C6-C5	-4.24	116.64	122.61
26	A	409	SQD	O47-C7-C8	4.22	120.59	111.50
24	b	621	BCR	C15-C14-C13	-4.18	121.34	127.31
32	d	407	LHG	C6-C5-C4	-4.18	101.90	111.79
24	C	516	BCR	C33-C5-C6	-4.18	119.84	124.53
33	V	201	HEM	CAD-CBD-CGD	4.18	119.68	112.67
22	c	507	CLA	C1-C2-C3	-4.17	118.83	126.04
24	b	619	BCR	C29-C30-C25	4.17	116.90	110.48
23	a	406	PHO	CBD-CHA-C4D	-4.16	103.85	108.54
26	b	601	SQD	O6-C1-C2	4.16	114.80	108.30
24	C	515	BCR	C7-C8-C9	-4.15	119.96	126.23
22	B	605	CLA	C1-C2-C3	-4.15	118.87	126.04
25	d	405	PL9	C37-C38-C39	-4.13	117.72	127.66
22	C	506	CLA	C4D-C3D-CAD	4.12	110.77	108.47
22	C	509	CLA	C4D-C3D-CAD	4.12	110.77	108.47
24	t	102	BCR	C7-C8-C9	-4.10	120.04	126.23
26	b	601	SQD	O47-C7-C8	4.09	120.31	111.50
26	f	102	SQD	C44-O6-C1	-4.09	105.75	113.74
26	D	411	SQD	C1-C2-C3	-4.07	101.52	110.00
24	t	102	BCR	C3-C4-C5	-4.07	106.81	114.08
22	B	607	CLA	C4D-C3D-CAD	4.06	110.73	108.47
22	b	615	CLA	C4D-C3D-CAD	4.05	110.73	108.47
24	k	101	BCR	C20-C21-C22	-4.05	121.53	127.31
23	A	405	PHO	CBD-CHA-C4D	-4.05	103.98	108.54
24	k	101	BCR	C7-C8-C9	-4.04	120.13	126.23
22	b	613	CLA	C1-C2-C3	-4.04	119.06	126.04
26	D	411	SQD	O47-C7-C8	4.02	120.17	111.50
22	C	503	CLA	C4A-NA-C1A	-3.99	104.91	106.71
32	E	101	LHG	O7-C7-C8	3.99	120.09	111.50
24	c	524	BCR	C15-C14-C13	-3.98	121.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C16-C17-C18	-3.98	121.63	127.31
26	A	411	SQD	O47-C7-C8	3.98	120.07	111.50
24	b	621	BCR	C7-C8-C9	-3.95	120.27	126.23
26	A	409	SQD	O5-C1-C2	-3.95	101.99	110.35
23	A	405	PHO	C1-C2-C3	-3.94	119.23	126.04
24	B	618	BCR	C28-C27-C26	-3.93	107.05	114.08
33	v	201	HEM	CAD-CBD-CGD	3.92	119.25	112.67
24	b	619	BCR	C33-C5-C6	-3.92	120.13	124.53
22	b	610	CLA	C4D-C3D-CAD	3.92	110.65	108.47
25	A	408	PL9	C37-C38-C39	-3.92	118.23	127.66
24	c	523	BCR	C16-C17-C18	-3.91	121.72	127.31
22	d	401	CLA	C2C-C1C-NC	3.89	113.61	109.97
32	D	406	LHG	O8-C23-C24	3.88	124.10	111.91
24	b	621	BCR	C28-C27-C26	-3.87	107.17	114.08
22	C	507	CLA	C4D-C3D-CAD	3.85	110.62	108.47
32	D	408	LHG	O7-C7-C8	3.82	119.74	111.50
24	K	102	BCR	C38-C26-C25	-3.82	120.24	124.53
30	b	624	LMG	O7-C10-C11	3.80	119.69	111.50
25	d	405	PL9	C27-C28-C29	-3.79	118.53	127.66
22	d	403	CLA	C2C-C1C-NC	3.78	113.52	109.97
22	b	616	CLA	C4D-C3D-CAD	3.77	110.57	108.47
25	a	409	PL9	C32-C33-C34	-3.77	118.58	127.66
30	C	501	LMG	O7-C10-C11	3.77	119.62	111.50
24	b	621	BCR	C16-C17-C18	-3.77	121.93	127.31
26	f	102	SQD	O47-C7-C8	3.76	119.61	111.50
32	b	628	LHG	O7-C7-C8	3.76	119.60	111.50
30	c	501	LMG	O7-C10-C11	3.76	119.60	111.50
26	L	101	SQD	O8-S-O7	3.75	120.45	111.27
25	A	408	PL9	C53-C6-C1	3.74	122.64	114.99
24	k	101	BCR	C33-C5-C6	-3.74	120.33	124.53
22	a	405	CLA	C4D-C3D-CAD	3.74	110.56	108.47
24	t	102	BCR	C15-C14-C13	-3.74	121.97	127.31
32	D	407	LHG	O7-C7-C8	3.74	119.55	111.50
24	A	407	BCR	C29-C30-C25	3.72	116.22	110.48
24	d	404	BCR	C38-C26-C27	3.72	120.77	113.62
24	K	102	BCR	C24-C23-C22	-3.72	120.62	126.23
25	A	408	PL9	C22-C23-C24	-3.71	118.73	127.66
30	c	522	LMG	O8-C28-C29	3.70	123.52	111.91
32	l	101	LHG	O7-C7-C8	3.70	119.47	111.50
24	H	102	BCR	C24-C23-C22	-3.66	120.71	126.23
25	D	405	PL9	C25-C24-C26	3.64	121.39	115.27
31	c	516	DGD	O2G-C1B-C2B	3.64	119.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C20-C21-C22	-3.63	122.13	127.31
30	c	522	LMG	C8-O7-C10	-3.63	108.86	117.79
24	B	616	BCR	C15-C14-C13	-3.62	122.14	127.31
24	b	620	BCR	C15-C14-C13	-3.62	122.15	127.31
31	C	518	DGD	O2G-C1B-C2B	3.61	119.29	111.50
22	d	401	CLA	C4D-C3D-CAD	3.61	110.48	108.47
22	b	614	CLA	C1-C2-C3	-3.60	119.82	126.04
24	t	102	BCR	C16-C17-C18	-3.59	122.19	127.31
24	B	616	BCR	C33-C5-C6	-3.58	120.50	124.53
31	c	517	DGD	O2G-C1B-C2B	3.57	119.20	111.50
26	a	410	SQD	O47-C7-C8	3.56	119.17	111.50
32	L	102	LHG	O7-C7-C8	3.55	119.16	111.50
24	b	619	BCR	C7-C8-C9	-3.55	120.86	126.23
26	a	410	SQD	O9-S-C6	3.55	111.16	106.94
22	c	503	CLA	C4D-C3D-CAD	3.55	110.45	108.47
25	D	405	PL9	C20-C19-C21	3.54	121.23	115.27
24	b	621	BCR	C33-C5-C6	-3.53	120.56	124.53
25	D	405	PL9	C45-C44-C46	3.52	121.19	115.27
32	e	101	LHG	O7-C7-C8	3.51	119.07	111.50
24	C	515	BCR	C11-C10-C9	-3.50	122.32	127.31
24	k	101	BCR	C16-C17-C18	-3.50	122.32	127.31
24	b	619	BCR	C28-C27-C26	-3.49	107.84	114.08
24	B	617	BCR	C24-C23-C22	-3.49	120.97	126.23
26	A	411	SQD	O7-S-C6	3.49	111.08	106.94
22	B	606	CLA	C3D-CAD-CBD	-3.47	103.04	107.61
24	K	102	BCR	C33-C5-C6	-3.46	120.64	124.53
24	B	616	BCR	C11-C10-C9	-3.46	122.37	127.31
24	b	620	BCR	C33-C5-C6	-3.46	120.65	124.53
23	a	414	PHO	C1-C2-C3	-3.44	120.09	126.04
26	A	409	SQD	C1-C2-C3	-3.43	102.84	110.00
32	d	407	LHG	O7-C7-C8	3.43	118.89	111.50
22	b	613	CLA	C2C-C1C-NC	3.42	113.18	109.97
24	H	102	BCR	C16-C17-C18	-3.42	122.43	127.31
24	D	404	BCR	C33-C5-C6	-3.42	120.69	124.53
24	b	621	BCR	C1-C6-C5	-3.42	117.80	122.61
24	t	102	BCR	C20-C21-C22	-3.42	122.43	127.31
22	a	407	CLA	C2C-C1C-NC	3.42	113.17	109.97
22	B	608	CLA	C2C-C1C-NC	3.41	113.17	109.97
26	b	601	SQD	C3-C4-C5	3.41	116.32	110.24
22	A	412	CLA	C2C-C1C-NC	3.40	113.16	109.97
26	b	601	SQD	C1-O5-C5	-3.40	107.01	113.69
22	c	508	CLA	C3D-CAD-CBD	-3.40	103.13	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	404	BCR	C15-C14-C13	-3.40	122.46	127.31
24	C	515	BCR	C38-C26-C25	-3.40	120.72	124.53
24	B	616	BCR	C16-C17-C18	-3.39	122.47	127.31
25	A	408	PL9	C30-C29-C31	3.38	120.96	115.27
24	B	618	BCR	C29-C30-C25	3.38	115.69	110.48
26	b	601	SQD	O7-S-C6	3.38	110.96	106.94
22	C	510	CLA	C1-C2-C3	-3.38	120.20	126.04
24	b	619	BCR	C11-C10-C9	-3.37	122.50	127.31
24	B	616	BCR	C34-C9-C10	-3.37	118.20	122.92
25	A	408	PL9	C17-C18-C19	-3.37	119.56	127.66
24	b	620	BCR	C28-C27-C26	-3.37	108.07	114.08
24	k	101	BCR	C38-C26-C25	-3.37	120.75	124.53
22	C	506	CLA	C1-C2-C3	-3.35	120.25	126.04
30	c	522	LMG	O6-C5-C6	3.34	114.75	106.44
24	b	621	BCR	C29-C30-C25	3.34	115.62	110.48
33	E	102	HEM	CAA-CBA-CGA	3.34	118.27	112.67
26	A	409	SQD	C44-O6-C1	-3.32	107.25	113.74
22	B	610	CLA	C1-C2-C3	-3.30	120.33	126.04
22	B	610	CLA	C2C-C1C-NC	3.30	113.07	109.97
24	B	616	BCR	C24-C23-C22	-3.30	121.25	126.23
26	A	409	SQD	C45-O47-C7	-3.29	109.69	117.79
30	c	519	LMG	C8-O7-C10	-3.29	109.69	117.79
22	C	512	CLA	C2C-C1C-NC	3.28	113.04	109.97
24	c	515	BCR	C7-C8-C9	-3.27	121.29	126.23
24	h	101	BCR	C34-C9-C10	-3.27	118.34	122.92
26	f	102	SQD	O6-C1-C2	3.27	113.40	108.30
26	A	411	SQD	C45-O47-C7	-3.27	109.75	117.79
30	m	103	LMG	C8-O7-C10	-3.26	109.76	117.79
24	B	618	BCR	C16-C17-C18	-3.26	122.66	127.31
30	C	520	LMG	O8-C28-C29	3.26	122.14	111.91
25	d	405	PL9	C53-C6-C1	3.26	121.65	114.99
25	a	409	PL9	C17-C18-C19	-3.26	119.82	127.66
24	H	102	BCR	C29-C30-C25	3.25	115.49	110.48
22	C	511	CLA	C1-C2-C3	-3.23	120.45	126.04
24	T	101	BCR	C15-C14-C13	-3.23	122.70	127.31
26	L	101	SQD	O47-C7-C8	3.23	118.45	111.50
24	t	102	BCR	C33-C5-C4	3.22	119.80	113.62
25	D	405	PL9	C17-C18-C19	-3.22	119.91	127.66
25	a	409	PL9	C45-C44-C46	3.21	120.68	115.27
24	H	102	BCR	C28-C27-C26	-3.21	108.34	114.08
25	D	405	PL9	C12-C13-C14	-3.21	119.93	127.66
22	A	406	CLA	C2C-C1C-NC	3.21	112.98	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	409	PL9	C22-C23-C24	-3.20	119.94	127.66
32	l	101	LHG	O8-C23-C24	3.20	121.96	111.91
25	a	409	PL9	C53-C6-C1	3.20	121.54	114.99
30	c	519	LMG	O8-C28-C29	3.20	121.94	111.91
31	C	517	DGD	O1G-C1A-C2A	3.20	121.94	111.91
26	A	411	SQD	O48-C23-C24	3.19	121.91	111.91
30	m	103	LMG	O7-C10-O9	-3.18	116.01	123.70
25	A	408	PL9	C32-C33-C34	-3.18	120.00	127.66
23	a	406	PHO	C4A-NA-C1A	3.18	110.71	108.14
24	k	101	BCR	C15-C14-C13	-3.18	122.78	127.31
24	K	101	BCR	C38-C26-C25	-3.17	120.97	124.53
24	B	617	BCR	C33-C5-C6	-3.17	120.97	124.53
22	D	402	CLA	C3D-CAD-CBD	-3.16	103.44	107.61
24	d	404	BCR	C27-C26-C25	-3.15	118.15	122.73
25	D	405	PL9	C37-C38-C39	-3.15	120.08	127.66
24	B	617	BCR	C15-C14-C13	-3.14	122.83	127.31
24	h	101	BCR	C16-C17-C18	-3.14	122.83	127.31
24	d	404	BCR	C38-C26-C25	-3.13	121.02	124.53
30	D	409	LMG	O7-C10-C11	3.13	118.24	111.50
25	d	405	PL9	C40-C39-C41	3.13	120.53	115.27
24	K	101	BCR	C24-C23-C22	-3.13	121.51	126.23
22	B	603	CLA	C2C-C1C-NC	3.12	112.90	109.97
22	C	507	CLA	C1-C2-C3	-3.12	120.65	126.04
25	d	405	PL9	C17-C18-C19	-3.12	120.16	127.66
24	C	515	BCR	C20-C21-C22	-3.11	122.87	127.31
24	C	516	BCR	C21-C20-C19	-3.11	113.51	123.22
24	C	516	BCR	C15-C14-C13	-3.11	122.87	127.31
22	a	404	CLA	C3D-CAD-CBD	-3.10	103.52	107.61
22	D	403	CLA	C2C-C1C-NC	3.10	112.88	109.97
22	c	510	CLA	C2C-C1C-NC	3.10	112.88	109.97
26	a	412	SQD	O47-C7-C8	3.10	118.18	111.50
25	a	409	PL9	C12-C13-C14	-3.10	120.21	127.66
31	h	102	DGD	O2G-C1B-C2B	3.09	118.17	111.50
24	d	404	BCR	C7-C8-C9	-3.09	121.56	126.23
32	D	406	LHG	O8-C23-O10	-3.09	115.79	123.59
32	l	101	LHG	C6-C5-C4	-3.09	104.49	111.79
24	a	408	BCR	C15-C14-C13	-3.09	122.91	127.31
24	h	101	BCR	C15-C14-C13	-3.08	122.91	127.31
31	H	103	DGD	O1G-C1A-C2A	3.08	121.56	111.91
32	D	406	LHG	O7-C7-C8	3.07	118.13	111.50
31	C	519	DGD	O2G-C1B-C2B	3.07	118.13	111.50
22	b	614	CLA	C2C-C1C-NC	3.05	112.83	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	SQD	O7-S-C6	3.04	110.56	106.94
31	H	103	DGD	C1D-O6D-C5D	-3.04	107.72	113.69
31	c	516	DGD	C2G-O2G-C1B	-3.04	110.31	117.79
31	h	102	DGD	O1G-C1A-C2A	3.04	121.43	111.91
31	c	518	DGD	O2G-C1B-C2B	3.03	118.04	111.50
24	T	101	BCR	C33-C5-C4	3.03	119.44	113.62
24	A	407	BCR	C7-C8-C9	-3.03	121.66	126.23
33	e	102	HEM	CMA-C3A-C4A	-3.03	123.81	128.46
26	a	412	SQD	O48-C23-C24	3.02	121.39	111.91
33	E	102	HEM	CMC-C2C-C3C	3.02	130.32	124.68
24	C	516	BCR	C15-C16-C17	-3.02	117.30	123.47
22	C	510	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	B	608	CLA	CHA-C1A-NA	-3.02	119.49	126.40
26	a	410	SQD	O6-C1-C2	3.01	113.01	108.30
22	C	514	CLA	C2C-C1C-NC	3.01	112.80	109.97
32	b	628	LHG	O8-C23-C24	3.01	121.34	111.91
22	d	402	CLA	C3D-CAD-CBD	-3.00	103.65	107.61
22	b	610	CLA	C1-C2-C3	-3.00	120.86	126.04
25	D	405	PL9	C7-C8-C9	-3.00	121.80	126.79
24	B	618	BCR	C4-C5-C6	-2.99	118.39	122.73
25	A	408	PL9	C15-C14-C16	2.99	120.30	115.27
22	C	507	CLA	C2C-C1C-NC	2.99	112.77	109.97
24	c	523	BCR	C29-C30-C25	2.98	115.07	110.48
25	d	405	PL9	C42-C43-C44	-2.98	120.48	127.66
24	B	618	BCR	C33-C5-C4	2.98	119.34	113.62
24	K	102	BCR	C10-C11-C12	-2.98	113.92	123.22
26	A	411	SQD	O8-S-C6	2.98	110.49	105.74
25	d	405	PL9	C12-C13-C14	-2.98	120.49	127.66
25	a	409	PL9	C37-C38-C39	-2.98	120.49	127.66
22	D	402	CLA	C1-C2-C3	-2.96	120.92	126.04
22	C	512	CLA	C1-C2-C3	-2.96	120.92	126.04
31	c	516	DGD	C4E-C3E-C2E	-2.96	105.66	110.82
24	C	515	BCR	C15-C14-C13	-2.95	123.10	127.31
25	A	408	PL9	C12-C13-C14	-2.94	120.57	127.66
30	C	520	LMG	C8-O7-C10	-2.94	110.54	117.79
32	E	101	LHG	O8-C23-C24	2.93	121.11	111.91
31	C	519	DGD	O3G-C3G-C2G	-2.93	103.83	110.90
24	K	102	BCR	C39-C30-C25	-2.93	105.55	110.30
31	C	518	DGD	C6D-C5D-C4D	2.93	118.20	112.09
22	b	609	CLA	C1-C2-C3	-2.92	121.00	126.04
30	c	501	LMG	C7-O1-C1	-2.92	108.04	113.74
22	B	611	CLA	C1-C2-C3	-2.91	121.01	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C3D-CAD-CBD	-2.91	103.78	107.61
31	C	518	DGD	O1G-C1A-O1A	-2.91	116.25	123.59
22	b	617	CLA	C1-C2-C3	-2.91	121.02	126.04
31	c	517	DGD	O1G-C1A-C2A	2.91	121.03	111.91
26	A	409	SQD	O9-S-C6	2.90	110.39	106.94
24	c	524	BCR	C11-C10-C9	-2.90	123.17	127.31
24	C	515	BCR	C24-C23-C22	-2.90	121.85	126.23
24	C	515	BCR	C33-C5-C6	-2.90	121.27	124.53
22	C	509	CLA	C1-C2-C3	-2.90	121.03	126.04
22	C	502	CLA	C2C-C1C-NC	2.90	112.69	109.97
22	H	101	CLA	C3D-CAD-CBD	-2.90	103.79	107.61
22	c	512	CLA	C2C-C1C-NC	2.90	112.69	109.97
24	c	523	BCR	C15-C14-C13	-2.89	123.18	127.31
24	b	619	BCR	C34-C9-C10	-2.89	118.87	122.92
24	b	621	BCR	C33-C5-C4	2.89	119.17	113.62
22	a	407	CLA	CHC-C1C-C2C	-2.88	118.77	126.72
31	C	518	DGD	O1G-C1A-C2A	2.87	120.91	111.91
22	c	504	CLA	C2C-C1C-NC	2.86	112.66	109.97
22	C	505	CLA	C2C-C1C-NC	2.86	112.65	109.97
32	b	628	LHG	C5-O7-C7	-2.86	110.75	117.79
24	T	101	BCR	C20-C19-C18	-2.86	118.39	126.42
22	C	509	CLA	C2C-C1C-NC	2.85	112.64	109.97
24	c	523	BCR	C27-C26-C25	-2.85	118.59	122.73
33	E	102	HEM	CAD-CBD-CGD	2.85	117.45	112.67
24	B	616	BCR	C28-C27-C26	-2.84	109.00	114.08
24	t	102	BCR	C39-C30-C25	-2.84	105.69	110.30
22	B	605	CLA	C3D-CAD-CBD	-2.84	103.86	107.61
30	C	522	LMG	O2-C2-C3	-2.84	103.78	110.35
30	m	103	LMG	O8-C28-C29	2.84	120.83	111.91
26	A	409	SQD	O8-S-C6	2.84	110.27	105.74
22	B	601	CLA	C1-C2-C3	-2.84	121.13	126.04
25	D	405	PL9	C27-C28-C29	-2.84	120.83	127.66
24	b	620	BCR	C24-C23-C22	-2.83	121.95	126.23
24	K	102	BCR	C16-C17-C18	-2.83	123.27	127.31
24	K	101	BCR	C23-C24-C25	-2.83	119.25	127.20
22	b	608	CLA	C1-C2-C3	-2.83	121.15	126.04
22	d	401	CLA	CHC-C1C-C2C	-2.82	118.91	126.72
24	C	515	BCR	C16-C17-C18	-2.82	123.28	127.31
24	k	101	BCR	C10-C11-C12	-2.82	114.42	123.22
24	b	619	BCR	C37-C22-C21	-2.81	118.98	122.92
22	d	403	CLA	CHC-C1C-C2C	-2.80	118.98	126.72
24	c	524	BCR	C29-C30-C25	2.80	114.79	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PL9	C20-C19-C21	2.80	119.97	115.27
24	C	516	BCR	C11-C10-C9	-2.80	123.32	127.31
25	A	408	PL9	C27-C28-C29	-2.79	120.93	127.66
33	e	102	HEM	CAD-CBD-CGD	2.79	117.35	112.67
24	A	407	BCR	C36-C18-C17	-2.79	119.02	122.92
30	f	101	LMG	C8-O7-C10	-2.79	110.93	117.79
24	k	101	BCR	C15-C16-C17	-2.78	117.78	123.47
32	D	407	LHG	O8-C23-C24	2.78	120.63	111.91
24	c	523	BCR	C21-C20-C19	-2.78	114.55	123.22
22	B	611	CLA	C2C-C1C-NC	2.78	112.57	109.97
22	B	614	CLA	CHC-C1C-NC	2.77	128.41	124.20
22	B	614	CLA	CHC-C1C-C2C	-2.77	119.06	126.72
22	c	503	CLA	C1-C2-C3	-2.77	121.25	126.04
33	E	102	HEM	CMA-C3A-C4A	-2.77	124.21	128.46
31	C	519	DGD	O1G-C1A-C2A	2.76	120.58	111.91
26	D	411	SQD	O48-C23-C24	2.76	120.57	111.91
32	d	406	LHG	O8-C23-C24	2.75	120.54	111.91
25	A	408	PL9	C45-C44-C46	2.75	119.89	115.27
22	A	412	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
22	c	514	CLA	C2C-C1C-NC	2.74	112.54	109.97
24	A	407	BCR	C16-C17-C18	-2.74	123.40	127.31
22	b	613	CLA	CHC-C1C-C2C	-2.74	119.15	126.72
31	C	517	DGD	C2G-O2G-C1B	-2.73	111.06	117.79
22	c	513	CLA	C2C-C1C-NC	2.73	112.53	109.97
24	D	404	BCR	C38-C26-C27	2.73	118.86	113.62
24	d	404	BCR	C29-C30-C25	2.72	114.67	110.48
24	D	404	BCR	C35-C13-C14	-2.71	119.12	122.92
22	C	511	CLA	C2C-C1C-NC	2.70	112.50	109.97
24	a	408	BCR	C3-C4-C5	-2.70	109.26	114.08
26	a	410	SQD	C1-C2-C3	-2.70	104.38	110.00
24	A	407	BCR	C33-C5-C6	-2.70	121.50	124.53
22	c	508	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
22	B	613	CLA	C1-C2-C3	-2.69	121.39	126.04
22	d	401	CLA	C1-C2-C3	-2.69	121.39	126.04
25	a	409	PL9	C35-C34-C36	2.69	119.80	115.27
22	B	610	CLA	CHC-C1C-C2C	-2.69	119.29	126.72
25	a	409	PL9	C10-C9-C11	2.69	119.79	115.27
25	a	409	PL9	C40-C39-C41	2.68	119.79	115.27
24	d	404	BCR	C30-C25-C26	-2.68	118.83	122.61
24	D	404	BCR	C16-C17-C18	-2.68	123.48	127.31
30	c	522	LMG	O8-C28-O10	-2.68	116.82	123.59
25	d	405	PL9	C35-C34-C36	2.68	119.78	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	C1-C2-C3	-2.68	121.41	126.04
22	c	514	CLA	CGD-CBD-CAD	-2.68	102.06	110.73
24	a	408	BCR	C40-C30-C25	-2.68	105.96	110.30
24	T	101	BCR	C37-C22-C21	-2.67	119.18	122.92
22	c	512	CLA	C3D-CAD-CBD	-2.67	104.09	107.61
24	c	523	BCR	C38-C26-C27	2.67	118.74	113.62
24	B	617	BCR	C7-C8-C9	-2.67	122.21	126.23
22	B	602	CLA	C2C-C1C-NC	2.66	112.47	109.97
24	c	523	BCR	C8-C7-C6	-2.66	119.72	127.20
24	b	620	BCR	C7-C8-C9	-2.66	122.21	126.23
22	b	618	CLA	C3D-CAD-CBD	-2.66	104.11	107.61
22	C	514	CLA	C3D-CAD-CBD	-2.65	104.11	107.61
24	t	102	BCR	C35-C13-C14	-2.65	119.21	122.92
24	B	617	BCR	C39-C30-C25	-2.65	106.00	110.30
26	a	412	SQD	C45-O47-C7	-2.65	111.27	117.79
26	f	102	SQD	O8-S-C6	2.65	109.96	105.74
22	b	611	CLA	C2C-C1C-NC	2.65	112.45	109.97
24	b	620	BCR	C38-C26-C25	-2.65	121.55	124.53
30	c	522	LMG	O1-C7-C8	2.64	117.28	110.90
24	a	408	BCR	C37-C22-C21	-2.64	119.22	122.92
31	C	518	DGD	O3G-C1D-C2D	2.64	112.43	108.30
24	D	404	BCR	C30-C25-C26	-2.64	118.89	122.61
24	A	407	BCR	C38-C26-C25	-2.64	121.56	124.53
24	B	618	BCR	C10-C11-C12	-2.63	115.00	123.22
31	C	518	DGD	O5D-C6D-C5D	2.63	113.92	109.05
24	B	617	BCR	C38-C26-C25	-2.63	121.57	124.53
32	d	406	LHG	O8-C23-O10	-2.63	116.95	123.59
26	b	601	SQD	C45-O47-C7	-2.63	111.32	117.79
30	c	522	LMG	O7-C10-O9	-2.63	117.35	123.70
22	b	617	CLA	CHC-C1C-NC	2.62	128.19	124.20
22	c	508	CLA	C1-C2-C3	-2.62	121.50	126.04
22	b	616	CLA	C1-C2-C3	-2.62	121.52	126.04
22	B	614	CLA	C2C-C1C-NC	2.62	112.42	109.97
26	a	412	SQD	C9-C8-C7	-2.62	104.11	113.62
22	B	608	CLA	CHC-C1C-C2C	-2.61	119.49	126.72
24	B	618	BCR	C3-C4-C5	-2.61	109.41	114.08
24	T	101	BCR	C11-C10-C9	-2.61	123.58	127.31
31	C	518	DGD	O5D-C1E-C2E	2.61	112.38	108.30
24	K	101	BCR	C15-C14-C13	-2.61	123.59	127.31
22	b	607	CLA	C3D-CAD-CBD	-2.60	104.18	107.61
25	d	405	PL9	C15-C14-C16	2.60	119.65	115.27
33	v	201	HEM	CBA-CAA-C2A	-2.60	107.70	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	501	LMG	O8-C28-C29	2.60	120.05	111.91
26	A	409	SQD	O48-C23-C24	2.59	120.05	111.91
32	L	102	LHG	C6-C5-C4	-2.59	105.66	111.79
24	H	102	BCR	C34-C9-C10	-2.59	119.29	122.92
31	c	518	DGD	O1G-C1A-C2A	2.59	120.02	111.91
24	d	404	BCR	C36-C18-C17	-2.58	119.30	122.92
22	c	504	CLA	C3D-CAD-CBD	-2.58	104.20	107.61
22	B	615	CLA	CHC-C1C-NC	2.58	128.12	124.20
25	D	405	PL9	C53-C6-C1	2.58	120.27	114.99
22	B	603	CLA	CHA-C1A-NA	-2.58	120.49	126.40
24	c	524	BCR	C7-C8-C9	-2.57	122.34	126.23
22	b	606	CLA	CHA-C1A-NA	-2.57	120.50	126.40
22	c	505	CLA	CMB-C2B-C1B	-2.57	124.51	128.46
22	c	509	CLA	C3D-CAD-CBD	-2.57	104.22	107.61
31	C	517	DGD	C4D-C3D-C2D	-2.57	106.33	110.82
24	D	404	BCR	C21-C20-C19	-2.57	115.19	123.22
32	D	408	LHG	O8-C23-C24	2.57	119.98	111.91
22	C	513	CLA	C2C-C1C-NC	2.57	112.38	109.97
22	c	506	CLA	C3D-CAD-CBD	-2.57	104.22	107.61
22	b	604	CLA	C2C-C1C-NC	2.57	112.38	109.97
24	K	101	BCR	C16-C17-C18	-2.57	123.65	127.31
24	k	101	BCR	C21-C20-C19	-2.56	115.22	123.22
22	c	514	CLA	C3D-CAD-CBD	-2.56	104.24	107.61
31	C	518	DGD	C3G-O3G-C1D	-2.55	108.75	113.74
24	C	515	BCR	C35-C13-C12	2.55	122.10	118.08
22	A	404	CLA	C2C-C1C-NC	2.55	112.36	109.97
22	b	604	CLA	C1-C2-C3	-2.55	121.63	126.04
22	C	512	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
24	h	101	BCR	C8-C9-C10	2.55	122.85	118.94
22	C	509	CLA	C3D-CAD-CBD	-2.55	104.25	107.61
22	B	603	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
30	c	519	LMG	O8-C28-O10	-2.54	117.18	123.59
22	a	404	CLA	C2C-C1C-NC	2.54	112.35	109.97
24	b	621	BCR	C39-C30-C25	-2.54	106.18	110.30
24	k	101	BCR	C11-C10-C9	-2.54	123.69	127.31
22	B	612	CLA	C2C-C1C-NC	2.54	112.35	109.97
22	B	603	CLA	C3D-CAD-CBD	-2.54	104.26	107.61
24	t	102	BCR	C1-C6-C7	2.54	122.95	115.78
22	b	607	CLA	CHC-C1C-NC	2.54	128.05	124.20
22	B	615	CLA	C1-C2-C3	-2.53	121.66	126.04
22	B	609	CLA	C3D-CAD-CBD	-2.53	104.27	107.61
24	H	102	BCR	C31-C1-C6	-2.53	106.19	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	101	LMG	O8-C28-C29	2.53	119.85	111.91
24	H	102	BCR	C16-C15-C14	-2.53	118.29	123.47
22	c	505	CLA	C1-C2-C3	-2.53	121.67	126.04
22	c	509	CLA	C2C-C1C-NC	2.52	112.34	109.97
24	a	408	BCR	C7-C8-C9	-2.52	122.42	126.23
25	A	408	PL9	C25-C24-C26	2.52	119.52	115.27
24	K	102	BCR	C15-C16-C17	-2.52	118.31	123.47
22	c	503	CLA	C2C-C1C-NC	2.52	112.33	109.97
24	h	101	BCR	C31-C1-C6	-2.52	106.22	110.30
22	A	406	CLA	C1-C2-C3	-2.52	121.69	126.04
22	B	606	CLA	CHC-C1C-NC	2.52	128.02	124.20
26	b	601	SQD	O9-S-C6	2.51	109.93	106.94
25	d	405	PL9	C45-C44-C46	2.51	119.50	115.27
22	a	407	CLA	CHC-C1C-NC	2.51	128.01	124.20
22	b	614	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
30	c	522	LMG	C6-C5-C4	-2.51	107.13	113.00
24	B	617	BCR	C29-C30-C25	2.51	114.34	110.48
22	B	601	CLA	CHC-C1C-NC	2.51	128.01	124.20
26	f	102	SQD	C1-C2-C3	-2.51	104.78	110.00
25	D	405	PL9	C15-C14-C16	2.51	119.49	115.27
24	C	516	BCR	C10-C11-C12	-2.51	115.40	123.22
26	D	411	SQD	C45-O47-C7	-2.51	111.62	117.79
22	c	510	CLA	CHC-C1C-C2C	-2.51	119.79	126.72
22	b	603	CLA	C3D-CAD-CBD	-2.50	104.31	107.61
30	c	522	LMG	C7-O1-C1	-2.50	108.85	113.74
22	C	511	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
25	A	408	PL9	C37-C36-C34	-2.50	104.76	112.98
24	A	407	BCR	C28-C27-C26	-2.50	109.62	114.08
22	B	612	CLA	C3D-CAD-CBD	-2.50	104.32	107.61
22	B	611	CLA	O2A-C1-C2	-2.49	102.08	108.64
22	b	609	CLA	C3D-CAD-CBD	-2.49	104.33	107.61
22	b	603	CLA	C2C-C1C-NC	2.49	112.31	109.97
24	c	515	BCR	C15-C16-C17	-2.49	118.38	123.47
33	V	201	HEM	C4C-C3C-C2C	2.48	108.63	106.90
22	c	514	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
22	b	605	CLA	CMA-C3A-C4A	2.48	118.44	111.77
23	a	406	PHO	CBD-CHA-C1A	2.48	132.15	126.40
24	B	616	BCR	C29-C30-C25	2.47	114.29	110.48
22	C	514	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
22	B	604	CLA	CHC-C1C-NC	2.47	127.95	124.20
22	D	402	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
22	A	403	CLA	C2C-C1C-NC	2.47	112.28	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C2-C3-C4	-2.47	105.87	111.38
30	C	501	LMG	C8-O7-C10	-2.47	111.72	117.79
31	H	103	DGD	O2G-C1B-O1B	-2.46	117.76	123.70
22	B	602	CLA	C1-C2-C3	-2.46	121.79	126.04
23	a	406	PHO	C1-C2-C3	-2.46	121.79	126.04
24	K	101	BCR	C11-C10-C9	-2.46	123.80	127.31
22	b	611	CLA	CMB-C2B-C1B	-2.46	124.69	128.46
24	t	102	BCR	C36-C18-C17	-2.46	119.48	122.92
30	b	624	LMG	O8-C28-C29	2.45	119.61	111.91
26	A	411	SQD	O48-C23-O10	-2.45	117.40	123.59
23	D	401	PHO	C4A-NA-C1A	2.45	110.12	108.14
22	C	503	CLA	C3D-CAD-CBD	-2.45	104.38	107.61
32	d	406	LHG	O8-C6-C5	-2.45	101.30	108.43
22	b	618	CLA	CHC-C1C-NC	2.45	127.92	124.20
22	b	617	CLA	CHC-C1C-C2C	-2.44	119.96	126.72
31	C	519	DGD	O5E-C6E-C5E	-2.44	102.92	111.29
23	D	401	PHO	C3D-C4D-CHA	2.44	116.07	109.49
22	C	507	CLA	CHA-C1A-NA	-2.44	120.81	126.40
25	D	405	PL9	C35-C34-C36	2.44	119.37	115.27
26	D	411	SQD	O48-C23-O10	-2.43	117.45	123.59
22	C	507	CLA	CMB-C2B-C1B	-2.43	124.72	128.46
22	b	604	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
30	b	624	LMG	C1-C2-C3	2.43	115.06	110.00
24	a	408	BCR	C38-C26-C25	-2.43	121.80	124.53
26	L	101	SQD	O6-C44-C45	-2.43	105.04	110.90
22	B	608	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
24	K	101	BCR	C8-C7-C6	-2.43	120.38	127.20
22	c	503	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
24	C	515	BCR	C21-C20-C19	-2.43	115.65	123.22
22	A	404	CLA	CHA-C1A-NA	-2.42	120.84	126.40
22	C	507	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
22	B	606	CLA	C1-C2-C3	-2.42	121.85	126.04
33	v	201	HEM	CMA-C3A-C4A	-2.42	124.75	128.46
31	C	517	DGD	O1G-C1A-O1A	-2.42	117.49	123.59
22	b	604	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
22	D	403	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
22	B	615	CLA	CHC-C1C-C2C	-2.41	120.04	126.72
26	A	411	SQD	C3-C4-C5	2.41	114.54	110.24
25	A	408	PL9	C42-C43-C44	-2.41	121.86	127.66
22	b	609	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
24	T	101	BCR	C3-C4-C5	-2.41	109.78	114.08
22	C	512	CLA	C3D-CAD-CBD	-2.41	104.44	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
26	b	601	SQD	O48-C23-C24	2.40	119.45	111.91
22	c	514	CLA	CMB-C2B-C1B	-2.40	124.77	128.46
30	B	621	LMG	O8-C28-C29	2.40	119.45	111.91
32	l	101	LHG	O8-C23-O10	-2.40	117.53	123.59
24	c	523	BCR	C16-C15-C14	-2.40	118.55	123.47
22	c	505	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
24	c	524	BCR	C36-C18-C17	-2.40	119.56	122.92
22	B	607	CLA	C2C-C1C-NC	2.40	112.22	109.97
22	b	606	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
24	A	407	BCR	C3-C4-C5	-2.40	109.80	114.08
22	C	504	CLA	C2C-C1C-NC	2.39	112.22	109.97
24	C	515	BCR	C34-C9-C10	-2.39	119.57	122.92
25	d	405	PL9	C30-C29-C31	2.39	119.29	115.27
26	D	411	SQD	C1-O5-C5	-2.39	109.00	113.69
24	T	101	BCR	C32-C1-C6	-2.39	106.42	110.30
22	C	514	CLA	C1-C2-C3	-2.39	121.91	126.04
24	C	515	BCR	C3-C4-C5	-2.39	109.81	114.08
23	A	405	PHO	CBD-CHA-C1A	2.39	131.94	126.40
24	d	404	BCR	C10-C11-C12	-2.38	115.78	123.22
22	b	611	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
22	b	618	CLA	CHC-C1C-C2C	-2.38	120.14	126.72
30	c	519	LMG	O7-C10-O9	-2.38	117.95	123.70
26	a	412	SQD	O48-C23-O10	-2.37	117.60	123.59
22	b	611	CLA	CHA-C1A-NA	-2.37	120.96	126.40
22	b	610	CLA	C2C-C1C-NC	2.37	112.19	109.97
22	A	406	CLA	CHC-C1C-C2C	-2.37	120.17	126.72
22	c	513	CLA	CHC-C1C-C2C	-2.37	120.17	126.72
24	b	621	BCR	C24-C23-C22	-2.37	122.66	126.23
22	c	507	CLA	CHA-C1A-NA	-2.37	120.97	126.40
26	a	410	SQD	C45-O47-C7	-2.37	111.96	117.79
22	D	403	CLA	CHC-C1C-C2C	-2.37	120.17	126.72
22	C	513	CLA	CHC-C1C-C2C	-2.37	120.18	126.72
22	c	512	CLA	C1-C2-C3	-2.37	121.95	126.04
30	B	621	LMG	O7-C10-O9	-2.36	117.99	123.70
22	C	503	CLA	O2A-C1-C2	2.36	114.84	108.64
24	t	102	BCR	C7-C6-C5	-2.36	115.74	121.46
22	b	606	CLA	C3D-CAD-CBD	-2.36	104.50	107.61
25	D	405	PL9	C10-C9-C11	2.36	119.24	115.27
22	B	606	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
22	c	506	CLA	C2C-C1C-NC	2.36	112.18	109.97
24	c	524	BCR	C23-C24-C25	-2.36	120.57	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	CHC-C1C-C2C	-2.36	120.19	126.72
22	c	504	CLA	CHC-C1C-C2C	-2.36	120.20	126.72
32	E	101	LHG	O8-C23-O10	-2.36	117.64	123.59
22	b	607	CLA	C1-C2-C3	-2.35	121.97	126.04
25	A	408	PL9	C35-C34-C36	2.35	119.23	115.27
22	C	514	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
22	a	407	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
30	C	522	LMG	O1-C7-C8	2.35	116.56	110.90
24	K	101	BCR	C10-C11-C12	-2.35	115.89	123.22
32	D	407	LHG	O8-C23-O10	-2.35	117.67	123.59
22	C	503	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
22	C	505	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
24	h	101	BCR	C38-C26-C25	-2.35	121.89	124.53
22	B	602	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
22	B	602	CLA	CMA-C3A-C4A	2.34	118.06	111.77
24	c	524	BCR	C27-C26-C25	-2.34	119.33	122.73
24	b	621	BCR	C3-C4-C5	-2.34	109.90	114.08
23	a	406	PHO	C2B-C1B-NB	-2.34	106.26	109.79
22	C	504	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
24	D	404	BCR	C3-C4-C5	-2.34	109.91	114.08
30	C	522	LMG	O8-C28-C29	2.33	119.23	111.91
24	A	407	BCR	C2-C1-C6	2.33	114.07	110.48
24	c	524	BCR	C38-C26-C27	2.33	118.10	113.62
24	B	617	BCR	C32-C1-C6	-2.33	106.51	110.30
23	D	401	PHO	C2B-C1B-NB	-2.33	106.27	109.79
26	f	102	SQD	O48-C23-C24	2.33	119.22	111.91
25	a	409	PL9	C15-C14-C16	2.33	119.19	115.27
22	B	613	CLA	C3D-CAD-CBD	-2.33	104.54	107.61
22	b	608	CLA	C3D-CAD-CBD	-2.33	104.54	107.61
22	b	607	CLA	CHC-C1C-C2C	-2.33	120.28	126.72
22	b	609	CLA	CHA-C1A-NA	-2.33	121.06	126.40
22	b	616	CLA	C2C-C1C-NC	2.33	112.15	109.97
30	B	619	LMG	O8-C28-C29	2.33	119.21	111.91
22	c	502	CLA	CHA-C1A-NA	-2.32	121.07	126.40
22	b	606	CLA	C2C-C1C-NC	2.32	112.15	109.97
24	b	620	BCR	C29-C30-C25	2.32	114.06	110.48
22	B	614	CLA	C3D-CAD-CBD	-2.32	104.55	107.61
31	C	517	DGD	O2G-C1B-O1B	-2.32	118.09	123.70
22	c	504	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
26	a	410	SQD	O48-C23-C24	2.32	119.19	111.91
24	H	102	BCR	C20-C21-C22	-2.32	124.00	127.31
22	c	509	CLA	CHC-C1C-C2C	-2.32	120.31	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
22	C	504	CLA	C3D-CAD-CBD	-2.32	104.55	107.61
22	H	101	CLA	C2C-C1C-NC	2.32	112.14	109.97
22	C	513	CLA	CMB-C2B-C1B	-2.32	124.91	128.46
22	c	512	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
22	c	510	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
22	B	610	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
24	A	407	BCR	C36-C18-C19	2.31	121.72	118.08
22	A	412	CLA	CHC-C1C-NC	2.31	127.71	124.20
22	C	504	CLA	CHA-C1A-NA	-2.31	121.11	126.40
22	c	502	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
22	B	611	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
22	C	510	CLA	CHC-C1C-C2C	-2.31	120.34	126.72
22	a	404	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
25	A	408	PL9	C10-C9-C11	2.30	119.14	115.27
24	C	515	BCR	C16-C15-C14	-2.30	118.76	123.47
24	h	101	BCR	C33-C5-C6	-2.30	121.94	124.53
22	C	511	CLA	CHC-C1C-NC	2.30	127.69	124.20
32	e	101	LHG	C5-O7-C7	-2.30	112.13	117.79
22	C	505	CLA	C3D-CAD-CBD	-2.30	104.58	107.61
22	d	401	CLA	CHA-C1A-NA	-2.30	121.13	126.40
24	H	102	BCR	C15-C14-C13	-2.30	124.03	127.31
22	C	506	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
30	m	103	LMG	O1-C7-C8	-2.30	105.36	110.90
22	D	403	CLA	C3D-CAD-CBD	-2.29	104.58	107.61
32	d	407	LHG	O8-C23-C24	2.29	119.10	111.91
24	K	102	BCR	C2-C1-C6	2.29	114.01	110.48
22	B	607	CLA	CHC-C1C-C2C	-2.29	120.39	126.72
25	D	405	PL9	C41-C42-C43	-2.29	104.36	111.88
24	B	617	BCR	C38-C26-C27	2.29	118.01	113.62
32	e	101	LHG	O8-C23-C24	2.29	119.08	111.91
22	c	507	CLA	C2C-C1C-NC	2.29	112.11	109.97
25	A	408	PL9	C22-C21-C19	-2.29	105.46	112.98
22	B	606	CLA	CMB-C2B-C1B	-2.28	124.95	128.46
22	B	609	CLA	CHA-C1A-NA	-2.28	121.17	126.40
31	H	103	DGD	C2G-O2G-C1B	-2.28	112.17	117.79
22	b	610	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
26	L	101	SQD	O48-C23-C24	2.28	119.06	111.91
31	C	519	DGD	O1G-C1A-O1A	-2.28	117.84	123.59
22	C	503	CLA	CHC-C1C-C2C	-2.28	120.42	126.72
22	c	502	CLA	C3D-CAD-CBD	-2.28	104.61	107.61
22	c	505	CLA	CHC-C1C-C2C	-2.28	120.43	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
22	b	614	CLA	C2A-C3A-C4A	2.27	105.54	101.87
30	C	520	LMG	O7-C10-O9	-2.27	118.21	123.70
22	b	611	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	b	609	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	b	606	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
22	B	609	CLA	CHC-C1C-C2C	-2.27	120.45	126.72
24	H	102	BCR	C2-C1-C6	2.27	113.97	110.48
22	A	403	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
24	b	619	BCR	C36-C18-C19	2.27	121.65	118.08
22	B	609	CLA	C2C-C1C-NC	2.27	112.09	109.97
22	d	403	CLA	CHA-C1A-NA	-2.26	121.21	126.40
22	b	608	CLA	C2C-C1C-NC	2.26	112.09	109.97
24	a	408	BCR	C34-C9-C10	-2.26	119.76	122.92
22	b	612	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
24	a	408	BCR	C2-C1-C6	2.26	113.96	110.48
22	B	601	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
22	A	403	CLA	CHC-C1C-C2C	-2.26	120.48	126.72
22	b	614	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
33	V	201	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
31	h	102	DGD	O1G-C1A-O1A	-2.25	117.91	123.59
25	d	405	PL9	C25-C24-C26	2.25	119.06	115.27
22	C	503	CLA	C1-C2-C3	-2.25	122.15	126.04
22	B	606	CLA	CAA-CBA-CGA	2.25	119.83	113.25
22	C	512	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
30	C	522	LMG	C1-O6-C5	-2.25	109.28	113.69
22	C	513	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	A	405	PHO	C2B-C1B-NB	-2.25	106.40	109.79
33	e	102	HEM	CMC-C2C-C3C	2.25	128.88	124.68
22	b	603	CLA	CHC-C1C-C2C	-2.25	120.51	126.72
23	A	405	PHO	C3D-C4D-CHA	2.25	115.55	109.49
22	C	503	CLA	CHC-C1C-NC	2.24	127.61	124.20
22	C	509	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
22	c	508	CLA	CHA-C1A-NA	-2.24	121.27	126.40
22	C	508	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
22	c	511	CLA	C2C-C1C-NC	2.24	112.07	109.97
24	d	404	BCR	C39-C30-C25	-2.24	106.67	110.30
24	T	101	BCR	C35-C13-C14	-2.24	119.79	122.92
22	b	612	CLA	C2C-C1C-NC	2.23	112.06	109.97
22	a	407	CLA	C3D-CAD-CBD	-2.23	104.66	107.61
22	C	511	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
23	a	414	PHO	C3D-C4D-CHA	2.23	115.51	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	409	PL9	C30-C29-C31	2.23	119.03	115.27
22	A	406	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
22	d	401	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
22	B	615	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
22	b	613	CLA	CHC-C1C-NC	2.23	127.58	124.20
22	c	503	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	C	508	CLA	CHC-C1C-NC	2.23	127.58	124.20
22	B	606	CLA	CHA-C1A-NA	-2.23	121.30	126.40
30	c	522	LMG	C1-O6-C5	-2.23	109.32	113.69
22	B	604	CLA	CHC-C1C-C2C	-2.23	120.56	126.72
30	m	103	LMG	C4-C3-C2	-2.22	106.94	110.82
22	B	612	CLA	CHA-C1A-NA	-2.22	121.30	126.40
22	b	605	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
22	b	615	CLA	C2C-C1C-NC	2.22	112.05	109.97
25	A	408	PL9	C40-C39-C41	2.22	119.01	115.27
22	c	504	CLA	CHA-C1A-NA	-2.22	121.31	126.40
22	b	608	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
26	f	102	SQD	O47-C7-O49	-2.22	118.34	123.70
22	c	507	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
22	b	604	CLA	CHC-C1C-C2C	-2.22	120.58	126.72
25	a	409	PL9	C10-C9-C8	-2.22	117.99	123.68
22	c	509	CLA	CMB-C2B-C1B	-2.22	125.06	128.46
24	B	618	BCR	C21-C20-C19	-2.22	116.30	123.22
24	T	101	BCR	C28-C27-C26	-2.21	110.12	114.08
22	C	506	CLA	CHA-C1A-NA	-2.21	121.33	126.40
22	c	502	CLA	CHC-C1C-C2C	-2.21	120.61	126.72
22	c	505	CLA	C2C-C1C-NC	2.21	112.04	109.97
32	b	628	LHG	O8-C23-O10	-2.21	118.02	123.59
24	B	616	BCR	C37-C22-C21	-2.21	119.83	122.92
26	a	410	SQD	C44-O6-C1	-2.21	109.42	113.74
30	b	624	LMG	C6-C5-C4	-2.21	107.84	113.00
31	h	102	DGD	O5D-C6D-C5D	-2.20	104.97	109.05
22	b	615	CLA	C3D-CAD-CBD	-2.20	104.70	107.61
22	B	604	CLA	C1-C2-C3	-2.20	122.23	126.04
24	k	101	BCR	C8-C7-C6	-2.20	121.02	127.20
22	C	508	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
22	c	514	CLA	C1-C2-C3	-2.20	122.24	126.04
23	a	414	PHO	C2B-C1B-NB	-2.20	106.47	109.79
22	b	609	CLA	CHC-C1C-C2C	-2.20	120.64	126.72
24	C	516	BCR	C29-C30-C25	2.20	113.87	110.48
30	c	522	LMG	O6-C1-O1	2.20	115.18	109.97
31	c	516	DGD	O2G-C1B-O1B	-2.20	118.39	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	BCR	C15-C14-C13	-2.20	124.18	127.31
24	c	523	BCR	C23-C24-C25	-2.19	121.04	127.20
22	d	403	CLA	CMB-C2B-C1B	-2.19	125.09	128.46
22	B	609	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
32	D	406	LHG	O3-P-O5	-2.19	100.51	109.07
23	a	406	PHO	C3D-C4D-CHA	2.19	115.39	109.49
24	B	616	BCR	C21-C20-C19	-2.19	116.39	123.22
25	a	409	PL9	C51-C49-C50	2.19	119.44	114.60
31	C	518	DGD	C1D-O6D-C5D	-2.19	109.39	113.69
24	c	515	BCR	C15-C14-C13	-2.19	124.19	127.31
22	a	404	CLA	CHC-C1C-C2C	-2.19	120.67	126.72
22	C	503	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
22	B	605	CLA	C2C-C1C-NC	2.19	112.02	109.97
26	a	410	SQD	O48-C23-O10	-2.19	118.08	123.59
24	T	101	BCR	C30-C25-C26	-2.18	119.54	122.61
26	a	412	SQD	O6-C1-C2	2.18	111.71	108.30
24	c	515	BCR	C29-C30-C25	2.18	113.84	110.48
33	V	201	HEM	CBA-CAA-C2A	-2.18	108.46	112.49
24	B	616	BCR	C7-C8-C9	-2.18	122.94	126.23
22	C	508	CLA	C3D-CAD-CBD	-2.18	104.73	107.61
22	c	514	CLA	CHC-C1C-NC	2.18	127.51	124.20
24	c	524	BCR	C33-C5-C6	-2.18	122.08	124.53
25	a	409	PL9	C27-C28-C29	-2.18	122.41	127.66
24	b	619	BCR	C30-C25-C26	-2.18	119.54	122.61
22	c	511	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
22	C	510	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	D	403	CLA	CHA-C1A-NA	-2.18	121.41	126.40
22	b	606	CLA	CHC-C1C-NC	2.18	127.51	124.20
30	m	103	LMG	O8-C28-O10	-2.18	118.10	123.59
24	c	515	BCR	C23-C24-C25	-2.18	121.09	127.20
31	C	519	DGD	C2G-O2G-C1B	-2.17	112.44	117.79
22	b	612	CLA	C3D-CAD-CBD	-2.17	104.74	107.61
22	B	614	CLA	CHA-C1A-NA	-2.17	121.42	126.40
24	h	101	BCR	C2-C1-C6	2.17	113.83	110.48
22	c	503	CLA	CHC-C1C-C2C	-2.17	120.71	126.72
22	c	506	CLA	C1-C2-C3	-2.17	122.29	126.04
24	t	102	BCR	C2-C1-C6	2.17	113.83	110.48
22	c	513	CLA	C3D-CAD-CBD	-2.17	104.75	107.61
22	A	404	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
24	C	515	BCR	C37-C22-C23	2.17	121.50	118.08
22	b	603	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
23	D	401	PHO	CBD-CHA-C1A	2.17	131.43	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	624	LMG	C9-O8-C28	2.17	125.15	117.12
31	c	517	DGD	O3G-C1D-C2D	2.17	111.69	108.30
22	C	506	CLA	CHC-C1C-NC	2.17	127.49	124.20
32	D	407	LHG	O7-C7-O9	-2.16	118.47	123.70
26	f	102	SQD	C3-C4-C5	2.16	114.10	110.24
30	c	501	LMG	O8-C28-C29	2.16	118.70	111.91
22	b	609	CLA	CHC-C1C-NC	2.16	127.48	124.20
22	A	412	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
22	c	510	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	C	509	CLA	CHA-C1A-NA	-2.16	121.45	126.40
24	K	101	BCR	C21-C20-C19	-2.16	116.47	123.22
24	T	101	BCR	C38-C26-C27	2.16	117.77	113.62
22	D	402	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
22	B	601	CLA	C3D-CAD-CBD	-2.16	104.76	107.61
22	c	508	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
22	c	505	CLA	CHC-C1C-NC	2.16	127.48	124.20
22	C	505	CLA	CHC-C1C-C2C	-2.16	120.76	126.72
24	T	101	BCR	C27-C26-C25	-2.16	119.60	122.73
22	d	403	CLA	CHC-C1C-NC	2.15	127.47	124.20
24	C	516	BCR	C36-C18-C19	2.15	121.47	118.08
22	B	610	CLA	CHC-C1C-NC	2.15	127.47	124.20
32	b	628	LHG	O7-C7-O9	-2.15	118.51	123.70
22	D	403	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
25	d	405	PL9	C10-C9-C11	2.15	118.88	115.27
22	C	504	CLA	CHC-C1C-NC	2.14	127.46	124.20
22	C	514	CLA	CHA-C1A-NA	-2.14	121.49	126.40
26	A	411	SQD	C4-C3-C2	2.14	114.56	110.82
26	b	601	SQD	O47-C7-O49	-2.14	118.53	123.70
22	a	407	CLA	CHA-C1A-NA	-2.14	121.49	126.40
24	d	404	BCR	C34-C9-C10	-2.14	119.92	122.92
31	C	519	DGD	C3G-C2G-C1G	-2.14	106.72	111.79
26	L	101	SQD	C4-C3-C2	-2.14	107.09	110.82
22	b	610	CLA	CHC-C1C-C2C	-2.14	120.82	126.72
31	c	517	DGD	C3G-O3G-C1D	-2.14	109.57	113.74
26	A	409	SQD	O47-C7-O49	-2.13	118.54	123.70
22	b	608	CLA	CMB-C2B-C1B	-2.13	125.18	128.46
22	d	401	CLA	CHC-C1C-NC	2.13	127.44	124.20
22	b	617	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
22	c	512	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
24	k	101	BCR	C33-C5-C4	2.13	117.71	113.62
22	c	512	CLA	CHA-C1A-NA	-2.13	121.52	126.40
24	b	619	BCR	C39-C30-C25	-2.13	106.84	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	BCR	C35-C13-C14	-2.13	119.94	122.92
22	b	618	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
30	D	409	LMG	O8-C28-C29	2.13	118.59	111.91
22	C	502	CLA	C1-C2-C3	-2.13	122.36	126.04
22	b	603	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
24	K	102	BCR	C21-C20-C19	-2.13	116.57	123.22
24	C	515	BCR	C28-C27-C26	-2.13	110.28	114.08
22	C	505	CLA	C1-C2-C3	-2.13	122.36	126.04
32	l	101	LHG	C25-C24-C23	-2.13	105.88	113.62
22	H	101	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
26	a	410	SQD	C1-O5-C5	-2.13	109.51	113.69
22	C	509	CLA	CHC-C1C-C2C	-2.13	120.84	126.72
22	C	502	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
22	b	612	CLA	CHC-C1C-C2C	-2.12	120.85	126.72
24	D	404	BCR	C30-C25-C24	2.12	121.79	115.78
22	b	616	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
30	b	624	LMG	O6-C5-C6	2.12	111.71	106.44
24	A	407	BCR	C37-C22-C21	-2.12	119.95	122.92
24	d	404	BCR	C3-C4-C5	-2.12	110.29	114.08
24	B	618	BCR	C11-C10-C9	-2.12	124.29	127.31
31	c	517	DGD	O1G-C1A-O1A	-2.12	118.25	123.59
22	B	607	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
22	A	403	CLA	C3D-CAD-CBD	-2.12	104.82	107.61
30	f	101	LMG	O7-C10-O9	-2.12	118.58	123.70
22	b	609	CLA	C1-O2A-CGA	2.12	122.00	116.44
22	a	404	CLA	CMB-C2B-C1B	-2.11	125.21	128.46
24	B	618	BCR	C34-C9-C10	-2.11	119.96	122.92
22	c	502	CLA	C2C-C1C-NC	2.11	111.95	109.97
22	B	612	CLA	CAA-CBA-CGA	2.11	119.43	113.25
24	a	408	BCR	C10-C11-C12	-2.11	116.62	123.22
22	C	503	CLA	C2C-C1C-NC	2.11	111.95	109.97
22	b	617	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
22	d	403	CLA	C3D-CAD-CBD	-2.11	104.83	107.61
24	B	616	BCR	C34-C9-C8	2.11	121.40	118.08
22	B	611	CLA	CHC-C1C-C2C	-2.11	120.89	126.72
24	h	101	BCR	C20-C21-C22	-2.11	124.30	127.31
26	b	601	SQD	O5-C1-C2	-2.11	105.89	110.35
22	c	506	CLA	CHA-C1A-NA	-2.11	121.58	126.40
22	b	615	CLA	CMB-C2B-C1B	-2.11	125.23	128.46
24	T	101	BCR	C1-C6-C7	2.11	121.73	115.78
22	b	610	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
22	B	609	CLA	CHC-C1C-NC	2.10	127.39	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	404	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
30	m	103	LMG	C9-C8-C7	-2.10	106.82	111.79
22	C	502	CLA	CHA-C1A-NA	-2.10	121.59	126.40
24	B	617	BCR	C8-C7-C6	-2.10	121.31	127.20
24	c	524	BCR	C24-C23-C22	-2.10	123.07	126.23
25	D	405	PL9	C22-C23-C24	-2.10	122.61	127.66
22	B	613	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
22	b	615	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
24	D	404	BCR	C34-C9-C10	-2.09	119.99	122.92
24	a	408	BCR	C35-C13-C14	-2.09	119.99	122.92
30	C	522	LMG	C3-C4-C5	-2.09	106.50	110.24
24	b	619	BCR	C38-C26-C27	2.09	117.64	113.62
22	c	513	CLA	C3A-C2A-C1A	2.09	104.47	101.34
22	c	513	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
24	C	515	BCR	C2-C1-C6	2.09	113.69	110.48
24	B	617	BCR	C21-C20-C19	-2.09	116.70	123.22
22	c	503	CLA	CHA-C1A-NA	-2.09	121.62	126.40
25	D	405	PL9	C51-C49-C50	2.09	119.21	114.60
22	b	614	CLA	CHC-C1C-NC	2.09	127.37	124.20
22	b	616	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
24	c	523	BCR	C34-C9-C8	2.08	121.36	118.08
22	D	402	CLA	O2A-C1-C2	2.08	114.11	108.64
22	c	504	CLA	CMB-C2B-C1B	-2.08	125.26	128.46
22	C	508	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
26	a	410	SQD	O5-C1-C2	-2.08	105.95	110.35
22	C	513	CLA	C3A-C2A-C1A	2.08	104.45	101.34
22	a	405	CLA	C1-C2-C3	-2.08	122.45	126.04
22	C	508	CLA	CHA-C1A-NA	-2.08	121.64	126.40
24	K	101	BCR	C16-C15-C14	-2.08	119.22	123.47
22	C	513	CLA	CHC-C1C-NC	2.08	127.35	124.20
22	b	612	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
22	C	504	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
24	K	101	BCR	C33-C5-C4	2.07	117.60	113.62
22	c	509	CLA	CHC-C1C-NC	2.07	127.35	124.20
24	h	101	BCR	C28-C27-C26	-2.07	110.38	114.08
22	c	506	CLA	CHC-C1C-C2C	-2.07	120.99	126.72
26	b	601	SQD	C1-C2-C3	-2.07	105.68	110.00
24	c	524	BCR	C15-C16-C17	-2.07	119.23	123.47
22	b	618	CLA	C2C-C1C-NC	2.07	111.91	109.97
31	C	518	DGD	C2G-O2G-C1B	-2.07	112.69	117.79
24	B	618	BCR	C33-C5-C6	-2.07	122.21	124.53
24	a	408	BCR	C37-C22-C23	2.07	121.33	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	C2A-C3A-C4A	2.07	105.21	101.87
22	c	512	CLA	C2A-C3A-C4A	2.07	105.21	101.87
25	D	405	PL9	C32-C33-C34	-2.06	122.69	127.66
22	c	502	CLA	CHC-C1C-NC	2.06	127.33	124.20
22	c	510	CLA	CHC-C1C-NC	2.06	127.33	124.20
22	b	605	CLA	CHC-C1C-C2C	-2.06	121.03	126.72
22	c	507	CLA	C3D-CAD-CBD	-2.06	104.90	107.61
22	c	505	CLA	C3D-CAD-CBD	-2.06	104.90	107.61
22	A	412	CLA	C1-C2-C3	-2.06	122.49	126.04
26	b	601	SQD	O48-C23-O10	-2.06	118.40	123.59
22	B	603	CLA	CHC-C1C-NC	2.05	127.32	124.20
24	b	619	BCR	C38-C26-C25	-2.05	122.22	124.53
24	b	620	BCR	C21-C20-C19	-2.05	116.81	123.22
22	a	407	CLA	C1-C2-C3	-2.05	122.49	126.04
22	C	502	CLA	CMA-C3A-C4A	2.05	117.29	111.77
22	C	514	CLA	CHC-C1C-NC	2.05	127.32	124.20
24	b	620	BCR	C8-C7-C6	-2.05	121.44	127.20
25	a	409	PL9	C37-C36-C34	-2.05	106.23	112.98
22	a	405	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
24	B	618	BCR	C16-C15-C14	-2.05	119.28	123.47
22	A	406	CLA	CHA-C1A-NA	-2.05	121.70	126.40
24	a	408	BCR	C29-C30-C25	2.05	113.63	110.48
22	C	510	CLA	C3D-CAD-CBD	-2.05	104.91	107.61
24	h	101	BCR	C2-C3-C4	-2.05	106.80	111.38
22	B	607	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	d	402	CLA	C2C-C1C-NC	2.04	111.89	109.97
30	c	519	LMG	C4-C3-C2	-2.04	107.26	110.82
22	a	405	CLA	CHC-C1C-C2C	-2.04	121.07	126.72
22	d	402	CLA	O2A-C1-C2	2.04	114.00	108.64
30	B	621	LMG	C8-O7-C10	-2.04	112.77	117.79
22	C	502	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
22	A	404	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
22	C	513	CLA	C3D-CAD-CBD	-2.04	104.92	107.61
22	a	405	CLA	CHA-C1A-NA	-2.04	121.74	126.40
22	B	603	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
25	a	409	PL9	C47-C48-C49	-2.03	120.80	127.75
22	b	615	CLA	C3A-C2A-C1A	2.03	104.38	101.34
31	C	517	DGD	C3G-O3G-C1D	-2.03	109.77	113.74
25	D	405	PL9	C30-C29-C31	2.03	118.69	115.27
22	b	605	CLA	C2C-C1C-NC	2.03	111.87	109.97
22	C	506	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
22	C	512	CLA	CHA-C1A-NA	-2.03	121.75	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	101	LMG	O8-C28-O10	-2.03	118.47	123.59
22	C	511	CLA	C3D-CAD-CBD	-2.03	104.94	107.61
22	b	608	CLA	CHA-C1A-NA	-2.03	121.75	126.40
22	c	511	CLA	C3D-CAD-CBD	-2.03	104.94	107.61
22	c	505	CLA	CMB-C2B-C3B	2.03	128.47	124.68
31	C	517	DGD	C4E-C3E-C2E	-2.02	107.29	110.82
22	A	406	CLA	C3D-CAD-CBD	-2.02	104.94	107.61
22	a	405	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
22	b	603	CLA	CHA-C1A-NA	-2.02	121.76	126.40
22	B	604	CLA	C3D-CAD-CBD	-2.02	104.94	107.61
30	C	520	LMG	O8-C28-O10	-2.02	118.49	123.59
22	b	615	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	C	505	CLA	CMA-C3A-C4A	2.02	117.20	111.77
26	b	601	SQD	O5-C5-C4	2.02	113.36	109.69
24	h	101	BCR	C24-C23-C22	-2.02	123.19	126.23
22	D	402	CLA	C3A-C2A-C1A	2.01	104.36	101.34
24	H	102	BCR	C3-C4-C5	-2.01	110.48	114.08
22	B	608	CLA	C3D-CAD-CBD	-2.01	104.95	107.61
22	C	503	CLA	CHA-C1A-NA	-2.01	121.79	126.40
24	b	621	BCR	C11-C10-C9	-2.01	124.44	127.31
24	b	621	BCR	C37-C22-C23	2.01	121.25	118.08
22	B	605	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
22	c	513	CLA	CHC-C1C-NC	2.01	127.25	124.20
22	a	405	CLA	C2C-C1C-NC	2.01	111.86	109.97
24	C	515	BCR	C23-C24-C25	-2.01	121.56	127.20
22	b	606	CLA	C2A-C3A-C4A	2.01	105.11	101.87
24	B	618	BCR	C37-C22-C23	2.01	121.24	118.08
22	b	609	CLA	C2C-C1C-NC	2.01	111.85	109.97
22	B	612	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
22	b	607	CLA	CHA-C1A-NA	-2.00	121.81	126.40
22	B	613	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
31	c	516	DGD	O6D-C5D-C6D	2.00	110.71	106.67
26	D	411	SQD	O5-C1-C2	-2.00	106.11	110.35
24	A	407	BCR	C2-C3-C4	-2.00	106.90	111.38
24	H	102	BCR	C8-C9-C10	2.00	122.01	118.94
31	c	516	DGD	O1G-C1A-C2A	2.00	118.19	111.91

All (210) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	614	CLA	NC
22	b	614	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	614	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	d	403	CLA	NC
22	d	403	CLA	ND
22	d	403	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	612	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	C	514	CLA	NC
22	C	514	CLA	ND
22	C	514	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	513	CLA	NC
22	C	513	CLA	ND
22	C	513	CLA	NA
22	c	514	CLA	NC
22	c	514	CLA	ND
22	c	514	CLA	NA
22	a	407	CLA	NC
22	a	407	CLA	ND
22	a	407	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	A	406	CLA	NC
22	A	406	CLA	ND
22	A	406	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	608	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	d	402	CLA	NC
22	d	402	CLA	ND
22	d	402	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	513	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	A	412	CLA	NC
22	A	412	CLA	ND
22	A	412	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	506	CLA	NA
22	D	403	CLA	NC
22	D	403	CLA	ND
22	D	403	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	D	402	CLA	NC
22	D	402	CLA	ND
22	D	402	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	d	401	CLA	NC
22	d	401	CLA	ND
22	d	401	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA

All (1127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	a	409	PL9	C45-C44-C46-C47
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
25	A	408	PL9	C9-C11-C12-C13
25	A	408	PL9	C13-C14-C16-C17
25	A	408	PL9	C15-C14-C16-C17
30	C	522	LMG	O6-C1-O1-C7
24	t	102	BCR	C7-C8-C9-C34
22	b	605	CLA	C2-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	B	613	CLA	CHA-CBD-CGD-O1D
22	B	613	CLA	CHA-CBD-CGD-O2D
22	B	613	CLA	CAD-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O1D
22	b	603	CLA	CHA-CBD-CGD-O2D
22	b	603	CLA	CAD-CBD-CGD-O1D
22	b	603	CLA	CAD-CBD-CGD-O2D
22	H	101	CLA	CAD-CBD-CGD-O1D
22	H	101	CLA	CAD-CBD-CGD-O2D
24	D	404	BCR	C1-C6-C7-C8
24	D	404	BCR	C7-C8-C9-C10
24	D	404	BCR	C7-C8-C9-C34
24	D	404	BCR	C21-C22-C23-C24
24	D	404	BCR	C37-C22-C23-C24
24	h	101	BCR	C7-C8-C9-C10
24	h	101	BCR	C7-C8-C9-C34
22	b	607	CLA	C2-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
33	E	102	HEM	C3D-CAD-CBD-CGD
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
32	d	406	LHG	C3-O3-P-O4
32	d	406	LHG	C4-O6-P-O4
26	A	411	SQD	O6-C44-C45-O47
26	A	411	SQD	O5-C5-C6-S
26	A	411	SQD	C5-C6-S-O7
26	A	411	SQD	C5-C6-S-O8
26	A	411	SQD	C5-C6-S-O9
22	B	601	CLA	CHA-CBD-CGD-O1D
22	B	601	CLA	CHA-CBD-CGD-O2D
32	D	407	LHG	C4-O6-P-O4
24	d	404	BCR	C21-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	A	412	CLA	CHA-CBD-CGD-O1D
22	A	412	CLA	CHA-CBD-CGD-O2D
32	l	101	LHG	C3-O3-P-O4
32	l	101	LHG	C4-O6-P-O4
32	l	101	LHG	C4-O6-P-O5
32	d	407	LHG	C3-O3-P-O5
32	d	407	LHG	C4-O6-P-O5
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
30	b	624	LMG	C11-C10-O7-C8
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	C8-C7-O47-C45
22	b	604	CLA	CHA-CBD-CGD-O1D
22	b	604	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O1D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	C2-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	T	101	BCR	C17-C18-C19-C20
24	T	101	BCR	C36-C18-C19-C20
24	T	101	BCR	C21-C22-C23-C24
24	T	101	BCR	C37-C22-C23-C24
24	b	621	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C34
32	e	101	LHG	C3-O3-P-O4
32	e	101	LHG	C3-O3-P-O5
26	L	101	SQD	C46-C45-O47-C7
26	L	101	SQD	C5-C6-S-O7
26	L	101	SQD	C5-C6-S-O8
32	D	408	LHG	C4-O6-P-O4
22	A	404	CLA	CHA-CBD-CGD-O1D
22	A	404	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
32	b	628	LHG	C3-O3-P-O4
22	d	401	CLA	CHA-CBD-CGD-O1D
22	d	401	CLA	CHA-CBD-CGD-O2D
32	L	102	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
32	L	102	LHG	C4-O6-P-O4
32	L	102	LHG	C4-O6-P-O5
30	b	624	LMG	O9-C10-O7-C8
26	f	102	SQD	O49-C7-O47-C45
26	L	101	SQD	O49-C7-O47-C45
22	B	613	CLA	C3-C5-C6-C7
22	b	616	CLA	C3-C5-C6-C7
22	B	609	CLA	C2A-CAA-CBA-CGA
22	d	403	CLA	C3-C5-C6-C7
32	E	101	LHG	O2-C2-C3-O3
26	L	101	SQD	C24-C23-O48-C46
26	L	101	SQD	C8-C7-O47-C45
32	D	408	LHG	C24-C25-C26-C27
31	c	516	DGD	O6E-C5E-C6E-O5E
22	a	407	CLA	C4-C3-C5-C6
22	B	604	CLA	C4-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
25	a	409	PL9	C43-C44-C46-C47
22	a	407	CLA	C2-C3-C5-C6
22	B	604	CLA	C2-C3-C5-C6
22	b	604	CLA	C2-C3-C5-C6
22	b	608	CLA	C2A-CAA-CBA-CGA
27	D	412	LFA	C3-C4-C5-C6
26	L	101	SQD	O10-C23-O48-C46
25	a	409	PL9	C19-C21-C22-C23
25	A	408	PL9	C14-C16-C17-C18
31	c	517	DGD	C9B-CAB-CBB-CCB
30	c	501	LMG	C11-C12-C13-C14
31	h	102	DGD	C4B-C5B-C6B-C7B
31	c	516	DGD	C6A-C7A-C8A-C9A
32	E	101	LHG	C1-C2-C3-O3
30	C	522	LMG	C29-C28-O8-C9
26	f	102	SQD	C33-C34-C35-C36
22	B	615	CLA	C13-C15-C16-C17
31	c	517	DGD	O6E-C5E-C6E-O5E
31	C	518	DGD	O6E-C5E-C6E-O5E
22	H	101	CLA	C10-C11-C12-C13
30	b	624	LMG	C10-C11-C12-C13
30	c	522	LMG	C2-C1-O1-C7
31	c	517	DGD	C4E-C5E-C6E-O5E
31	C	518	DGD	C4E-C5E-C6E-O5E
22	B	615	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	B	604	CLA	C14-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C14
22	B	608	CLA	C14-C13-C15-C16
32	d	407	LHG	C24-C25-C26-C27
24	k	101	BCR	C11-C12-C13-C35
24	t	102	BCR	C37-C22-C23-C24
24	d	404	BCR	C7-C8-C9-C34
24	c	524	BCR	C7-C8-C9-C34
24	T	101	BCR	C7-C8-C9-C34
24	b	621	BCR	C37-C22-C23-C24
24	t	102	BCR	C21-C22-C23-C24
24	T	101	BCR	C7-C8-C9-C10
30	c	519	LMG	C10-C11-C12-C13
26	A	409	SQD	C7-C8-C9-C10
22	a	404	CLA	C15-C16-C17-C18
22	d	403	CLA	C8-C10-C11-C12
22	b	607	CLA	C15-C16-C17-C18
22	B	601	CLA	C15-C16-C17-C18
22	C	504	CLA	C5-C6-C7-C8
22	B	613	CLA	C5-C6-C7-C8
31	c	516	DGD	C1B-C2B-C3B-C4B
30	B	619	LMG	C10-C11-C12-C13
30	c	522	LMG	C28-C29-C30-C31
31	C	518	DGD	C1A-C2A-C3A-C4A
22	b	613	CLA	C13-C15-C16-C17
26	b	601	SQD	C7-C8-C9-C10
30	B	621	LMG	C10-C11-C12-C13
26	L	101	SQD	C23-C24-C25-C26
27	M	102	LFA	C12-C13-C14-C15
31	C	517	DGD	O6E-C5E-C6E-O5E
22	b	615	CLA	C11-C10-C8-C7
22	c	509	CLA	C11-C10-C8-C7
22	D	402	CLA	C12-C13-C15-C16
30	C	522	LMG	O10-C28-O8-C9
22	b	612	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C5-C6-C7-C8
31	c	518	DGD	O6D-C1D-O3G-C3G
22	c	507	CLA	C13-C15-C16-C17
25	a	409	PL9	C34-C36-C37-C38
30	C	501	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C3-C5-C6-C7
22	b	604	CLA	C13-C15-C16-C17
22	b	610	CLA	C13-C15-C16-C17
32	d	406	LHG	C3-O3-P-O6
32	l	101	LHG	C4-O6-P-O3
32	E	101	LHG	C3-O3-P-O6
32	e	101	LHG	C3-O3-P-O6
32	b	628	LHG	C3-O3-P-O6
32	L	102	LHG	C4-O6-P-O3
25	D	405	PL9	C30-C29-C31-C32
22	b	603	CLA	C8-C10-C11-C12
22	B	601	CLA	C13-C15-C16-C17
30	B	619	LMG	C32-C33-C34-C35
22	B	605	CLA	C2A-CAA-CBA-CGA
31	c	517	DGD	C3B-C4B-C5B-C6B
30	C	501	LMG	C15-C16-C17-C18
26	a	410	SQD	C33-C34-C35-C36
27	b	602	LFA	C11-C10-C9-C8
27	b	630	LFA	C9-C10-C11-C12
27	d	408	LFA	C2-C3-C4-C5
30	c	501	LMG	C18-C19-C20-C21
30	C	520	LMG	C31-C32-C33-C34
27	B	623	LFA	C5-C6-C7-C8
32	d	407	LHG	C16-C17-C18-C19
27	B	627	LFA	C9-C10-C11-C12
30	C	501	LMG	C18-C19-C20-C21
27	C	521	LFA	C6-C7-C8-C9
27	C	521	LFA	C7-C8-C9-C10
27	i	101	LFA	C10-C11-C12-C13
30	c	501	LMG	C36-C37-C38-C39
26	a	412	SQD	C15-C16-C17-C18
26	A	411	SQD	C34-C35-C36-C37
27	D	410	LFA	C3-C4-C5-C6
32	d	407	LHG	C31-C32-C33-C34
26	f	102	SQD	C29-C30-C31-C32
26	A	409	SQD	C10-C11-C12-C13
31	h	102	DGD	C3B-C4B-C5B-C6B
32	b	628	LHG	C15-C16-C17-C18
27	t	101	LFA	C5-C6-C7-C8
30	D	409	LMG	C20-C21-C22-C23
27	B	624	LFA	C6-C7-C8-C9
26	f	102	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
32	L	102	LHG	C13-C14-C15-C16
32	d	406	LHG	C11-C10-C9-C8
32	D	407	LHG	C14-C15-C16-C17
27	B	623	LFA	C3-C4-C5-C6
32	l	101	LHG	C13-C14-C15-C16
27	B	627	LFA	C11-C10-C9-C8
32	e	101	LHG	C12-C13-C14-C15
26	L	101	SQD	C7-C8-C9-C10
31	c	518	DGD	C2D-C1D-O3G-C3G
30	m	103	LMG	C31-C32-C33-C34
22	b	604	CLA	C8-C10-C11-C12
25	a	409	PL9	C30-C29-C31-C32
25	A	408	PL9	C12-C11-C9-C10
25	D	405	PL9	C15-C14-C16-C17
25	D	405	PL9	C40-C39-C41-C42
25	d	405	PL9	C15-C14-C16-C17
25	d	405	PL9	C45-C44-C46-C47
22	c	506	CLA	C4-C3-C5-C6
26	a	410	SQD	C14-C15-C16-C17
27	d	409	LFA	C5-C6-C7-C8
30	C	520	LMG	C35-C36-C37-C38
32	d	407	LHG	C30-C31-C32-C33
32	d	407	LHG	C32-C33-C34-C35
30	m	103	LMG	C32-C33-C34-C35
22	b	617	CLA	C11-C12-C13-C14
22	C	510	CLA	C14-C13-C15-C16
22	b	613	CLA	C11-C12-C13-C14
22	b	613	CLA	C14-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C9
22	B	614	CLA	C11-C12-C13-C14
26	A	411	SQD	C7-C8-C9-C10
30	C	522	LMG	C32-C33-C34-C35
32	D	406	LHG	C18-C19-C20-C21
32	D	406	LHG	C34-C35-C36-C37
30	B	619	LMG	C38-C39-C40-C41
27	D	410	LFA	C11-C10-C9-C8
27	B	627	LFA	C5-C6-C7-C8
27	j	101	LFA	C3-C4-C5-C6
32	e	101	LHG	C14-C15-C16-C17
32	e	101	LHG	C27-C28-C29-C30
22	b	616	CLA	C8-C10-C11-C12
24	H	102	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
26	b	601	SQD	C16-C17-C18-C19
30	m	103	LMG	C18-C19-C20-C21
26	L	101	SQD	C16-C17-C18-C19
32	D	408	LHG	C12-C13-C14-C15
32	d	407	LHG	O1-C1-C2-C3
32	D	408	LHG	O1-C1-C2-C3
24	H	102	BCR	C7-C8-C9-C10
22	A	403	CLA	C15-C16-C17-C18
26	A	411	SQD	C31-C32-C33-C34
32	D	407	LHG	C11-C10-C9-C8
32	L	102	LHG	C16-C17-C18-C19
32	D	406	LHG	C7-C8-C9-C10
26	a	410	SQD	C26-C27-C28-C29
26	a	410	SQD	C27-C28-C29-C30
27	C	521	LFA	C5-C6-C7-C8
27	c	521	LFA	C4-C5-C6-C7
27	a	411	LFA	C6-C7-C8-C9
27	D	412	LFA	C5-C6-C7-C8
27	B	626	LFA	C5-C6-C7-C8
30	c	522	LMG	O6-C1-O1-C7
25	D	405	PL9	C39-C41-C42-C43
30	C	501	LMG	C36-C37-C38-C39
27	b	625	LFA	C7-C8-C9-C10
26	b	601	SQD	C10-C11-C12-C13
30	b	624	LMG	C29-C30-C31-C32
32	l	101	LHG	C18-C19-C20-C21
32	l	101	LHG	C28-C29-C30-C31
31	c	517	DGD	C1A-C2A-C3A-C4A
27	b	602	LFA	C2-C3-C4-C5
30	m	103	LMG	C15-C16-C17-C18
31	C	519	DGD	C2A-C1A-O1G-C1G
30	c	519	LMG	C17-C18-C19-C20
30	B	619	LMG	C19-C20-C21-C22
30	c	501	LMG	C39-C40-C41-C42
26	A	411	SQD	C27-C28-C29-C30
31	H	103	DGD	C3B-C4B-C5B-C6B
27	B	623	LFA	C4-C5-C6-C7
30	b	624	LMG	C14-C15-C16-C17
32	D	407	LHG	C16-C17-C18-C19
30	D	409	LMG	C14-C15-C16-C17
26	a	412	SQD	C28-C29-C30-C31
22	c	513	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	m	103	LMG	C10-C11-C12-C13
25	D	405	PL9	C45-C44-C46-C47
22	b	611	CLA	C4-C3-C5-C6
22	B	608	CLA	C4-C3-C5-C6
25	a	409	PL9	C28-C29-C31-C32
25	d	405	PL9	C13-C14-C16-C17
25	d	405	PL9	C43-C44-C46-C47
22	c	506	CLA	C2-C3-C5-C6
30	B	621	LMG	C29-C30-C31-C32
32	L	102	LHG	C27-C28-C29-C30
30	C	520	LMG	C39-C40-C41-C42
32	E	101	LHG	C9-C10-C11-C12
27	D	410	LFA	C7-C8-C9-C10
27	B	628	LFA	C9-C10-C11-C12
22	C	504	CLA	C15-C16-C17-C18
32	D	407	LHG	C30-C31-C32-C33
27	B	622	LFA	C3-C4-C5-C6
31	c	516	DGD	C4E-C5E-C6E-O5E
31	H	103	DGD	C6A-C7A-C8A-C9A
26	L	101	SQD	C27-C28-C29-C30
30	c	519	LMG	C13-C14-C15-C16
27	B	620	LFA	C5-C6-C7-C8
27	c	521	LFA	C6-C7-C8-C9
26	b	601	SQD	C28-C29-C30-C31
24	t	102	BCR	C1-C6-C7-C8
24	t	102	BCR	C5-C6-C7-C8
24	D	404	BCR	C5-C6-C7-C8
24	B	616	BCR	C1-C6-C7-C8
24	B	616	BCR	C5-C6-C7-C8
24	K	101	BCR	C1-C6-C7-C8
24	K	101	BCR	C5-C6-C7-C8
24	c	523	BCR	C1-C6-C7-C8
24	c	523	BCR	C5-C6-C7-C8
24	b	621	BCR	C5-C6-C7-C8
24	b	619	BCR	C1-C6-C7-C8
24	b	619	BCR	C5-C6-C7-C8
26	a	410	SQD	C16-C17-C18-C19
31	C	517	DGD	C8A-C9A-CAA-CBA
22	b	616	CLA	C13-C15-C16-C17
26	a	412	SQD	C8-C7-O47-C45
32	d	407	LHG	C25-C26-C27-C28
31	C	519	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C27-C28-C29-C30
27	I	101	LFA	C10-C11-C12-C13
27	A	413	LFA	C9-C10-C11-C12
27	b	630	LFA	C10-C11-C12-C13
27	d	408	LFA	C4-C5-C6-C7
26	f	102	SQD	C32-C33-C34-C35
31	h	102	DGD	C2B-C3B-C4B-C5B
22	b	618	CLA	C4-C3-C5-C6
25	a	409	PL9	C12-C11-C9-C8
22	b	617	CLA	C11-C12-C13-C15
25	D	405	PL9	C13-C14-C16-C17
25	D	405	PL9	C28-C29-C31-C32
25	D	405	PL9	C38-C39-C41-C42
25	D	405	PL9	C43-C44-C46-C47
22	b	613	CLA	C12-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C10
22	b	611	CLA	C2-C3-C5-C6
22	b	618	CLA	C2-C3-C5-C6
22	B	614	CLA	C11-C12-C13-C15
22	B	602	CLA	C6-C7-C8-C10
22	B	608	CLA	C2-C3-C5-C6
30	C	501	LMG	C17-C18-C19-C20
26	A	411	SQD	C13-C14-C15-C16
31	h	102	DGD	CDB-CEB-CFB-CGB
22	b	613	CLA	C15-C16-C17-C18
30	C	522	LMG	O6-C5-C6-O5
32	b	628	LHG	C25-C26-C27-C28
27	b	602	LFA	C11-C12-C13-C14
27	B	624	LFA	C5-C6-C7-C8
27	b	626	LFA	C6-C7-C8-C9
27	I	101	LFA	C3-C4-C5-C6
32	b	628	LHG	C13-C14-C15-C16
27	C	521	LFA	C2-C3-C4-C5
32	E	101	LHG	C17-C18-C19-C20
26	a	410	SQD	C7-C8-C9-C10
31	C	518	DGD	CAB-CBB-CCB-CDB
26	L	101	SQD	C12-C13-C14-C15
26	A	411	SQD	C25-C26-C27-C28
31	c	517	DGD	O6E-C1E-O5D-C6D
22	B	609	CLA	C13-C15-C16-C17
27	b	626	LFA	C5-C6-C7-C8
26	L	101	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
31	c	518	DGD	C1B-C2B-C3B-C4B
30	c	501	LMG	C11-C10-O7-C8
26	b	601	SQD	C8-C7-O47-C45
27	b	625	LFA	C10-C11-C12-C13
30	m	103	LMG	C35-C36-C37-C38
30	c	501	LMG	O9-C10-O7-C8
26	b	601	SQD	O49-C7-O47-C45
27	B	624	LFA	C2-C3-C4-C5
27	i	102	LFA	C6-C7-C8-C9
26	D	411	SQD	C2-C1-O6-C44
31	c	517	DGD	C2E-C1E-O5D-C6D
26	a	410	SQD	O6-C44-C45-O47
30	C	522	LMG	O7-C8-C9-O8
26	A	411	SQD	O47-C45-C46-O48
32	d	407	LHG	O7-C5-C6-O8
32	e	101	LHG	O7-C5-C6-O8
27	b	602	LFA	C3-C4-C5-C6
30	B	619	LMG	C20-C21-C22-C23
26	b	601	SQD	C32-C33-C34-C35
30	c	522	LMG	O6-C5-C6-O5
25	a	409	PL9	C12-C11-C9-C10
25	A	408	PL9	C12-C11-C9-C8
25	D	405	PL9	C4-C3-C7-C8
25	d	405	PL9	C4-C3-C7-C8
26	A	411	SQD	C15-C16-C17-C18
22	b	609	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C10-C8-C9
30	c	519	LMG	C38-C39-C40-C41
22	b	606	CLA	C3-C5-C6-C7
32	e	101	LHG	C17-C18-C19-C20
22	b	604	CLA	C5-C6-C7-C8
32	D	406	LHG	C9-C10-C11-C12
32	l	101	LHG	C32-C33-C34-C35
32	d	407	LHG	C27-C28-C29-C30
24	t	102	BCR	C7-C8-C9-C10
22	D	403	CLA	C16-C17-C18-C20
26	A	409	SQD	C17-C18-C19-C20
22	C	507	CLA	C10-C11-C12-C13
32	d	406	LHG	C4-O6-P-O3
32	l	101	LHG	C3-O3-P-O6
32	E	101	LHG	C4-O6-P-O3
32	L	102	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
31	C	517	DGD	C4B-C5B-C6B-C7B
30	B	619	LMG	C31-C32-C33-C34
27	m	102	LFA	C5-C6-C7-C8
27	b	622	LFA	C2-C3-C4-C5
30	c	501	LMG	C32-C33-C34-C35
30	m	103	LMG	C39-C40-C41-C42
31	c	516	DGD	CAB-CBB-CCB-CDB
27	b	627	LFA	C11-C10-C9-C8
30	b	624	LMG	C11-C12-C13-C14
30	c	501	LMG	C21-C22-C23-C24
30	c	519	LMG	C14-C15-C16-C17
31	C	519	DGD	CBA-CCA-CDA-CEA
27	M	101	LFA	C7-C8-C9-C10
26	A	409	SQD	O6-C44-C45-C46
26	b	601	SQD	C26-C27-C28-C29
27	B	623	LFA	C11-C10-C9-C8
32	d	407	LHG	C4-C5-C6-O8
26	f	102	SQD	O6-C44-C45-C46
32	e	101	LHG	C4-C5-C6-O8
30	B	621	LMG	O6-C5-C6-O5
30	c	501	LMG	C28-C29-C30-C31
31	c	517	DGD	C5D-C6D-O5D-C1E
26	a	410	SQD	C24-C25-C26-C27
27	B	627	LFA	C6-C7-C8-C9
32	l	101	LHG	C14-C15-C16-C17
30	B	621	LMG	C34-C35-C36-C37
22	B	603	CLA	C3-C5-C6-C7
25	a	409	PL9	C24-C26-C27-C28
30	D	409	LMG	O6-C5-C6-O5
30	c	522	LMG	C19-C20-C21-C22
26	A	409	SQD	C11-C12-C13-C14
30	f	101	LMG	O6-C5-C6-O5
27	B	624	LFA	C1-C2-C3-C4
32	D	406	LHG	C23-C24-C25-C26
31	c	518	DGD	C2A-C1A-O1G-C1G
27	I	101	LFA	C6-C7-C8-C9
22	B	604	CLA	C13-C15-C16-C17
31	c	517	DGD	C2A-C3A-C4A-C5A
27	M	102	LFA	C6-C7-C8-C9
30	b	624	LMG	O6-C5-C6-O5
27	b	630	LFA	C2-C3-C4-C5
26	A	411	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	t	101	LFA	C12-C13-C14-C15
22	c	504	CLA	C15-C16-C17-C18
27	M	102	LFA	C2-C3-C4-C5
32	d	406	LHG	C25-C26-C27-C28
27	B	627	LFA	C2-C3-C4-C5
31	C	518	DGD	CDB-CEB-CFB-CGB
32	d	407	LHG	C24-C23-O8-C6
30	c	501	LMG	C31-C32-C33-C34
31	C	518	DGD	O6D-C5D-C6D-O5D
31	C	518	DGD	C5B-C6B-C7B-C8B
32	d	406	LHG	O2-C2-C3-O3
31	h	102	DGD	C1B-C2B-C3B-C4B
22	b	612	CLA	C13-C15-C16-C17
30	C	522	LMG	C2-C1-O1-C7
26	a	412	SQD	C9-C10-C11-C12
26	A	409	SQD	O6-C44-C45-O47
27	i	101	LFA	C3-C4-C5-C6
27	d	410	LFA	C4-C5-C6-C7
26	a	412	SQD	O49-C7-O47-C45
30	m	103	LMG	C36-C37-C38-C39
22	B	615	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	H	101	CLA	C11-C10-C8-C7
22	B	605	CLA	C6-C7-C8-C10
22	b	608	CLA	C6-C7-C8-C10
22	b	618	CLA	C11-C10-C8-C7
22	B	602	CLA	C11-C12-C13-C15
22	d	403	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C9
30	f	101	LMG	C10-C11-C12-C13
26	a	410	SQD	C25-C26-C27-C28
31	H	103	DGD	C4B-C5B-C6B-C7B
22	d	401	CLA	C16-C17-C18-C20
30	c	501	LMG	C33-C34-C35-C36
22	C	511	CLA	C8-C10-C11-C12
31	c	516	DGD	CAA-CBA-CCA-CDA
27	b	625	LFA	C12-C13-C14-C15
27	I	101	LFA	C9-C10-C11-C12
27	b	625	LFA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
27	d	410	LFA	C11-C10-C9-C8
22	c	507	CLA	C15-C16-C17-C18
25	a	409	PL9	C25-C24-C26-C27
25	D	405	PL9	C35-C34-C36-C37
30	B	619	LMG	C28-C29-C30-C31
27	D	410	LFA	C9-C10-C11-C12
30	C	520	LMG	C30-C31-C32-C33
26	a	412	SQD	C12-C13-C14-C15
30	c	522	LMG	C13-C14-C15-C16
27	A	410	LFA	C7-C8-C9-C10
32	D	408	LHG	C29-C30-C31-C32
32	D	406	LHG	C17-C18-C19-C20
22	b	603	CLA	C10-C11-C12-C13
31	h	102	DGD	C5B-C6B-C7B-C8B
22	c	511	CLA	C8-C10-C11-C12
26	a	410	SQD	O6-C44-C45-C46
30	C	522	LMG	C7-C8-C9-O8
30	C	501	LMG	C7-C8-C9-O8
26	A	411	SQD	O6-C44-C45-C46
26	A	411	SQD	C44-C45-C46-O48
26	f	102	SQD	C44-C45-C46-O48
26	L	101	SQD	C44-C45-C46-O48
31	C	519	DGD	CCB-CDB-CEB-CFB
32	d	406	LHG	C23-C24-C25-C26
31	h	102	DGD	C4E-C5E-C6E-O5E
26	L	101	SQD	C29-C30-C31-C32
32	b	628	LHG	C16-C17-C18-C19
26	D	411	SQD	C31-C32-C33-C34
27	m	102	LFA	C4-C5-C6-C7
22	B	601	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C19
26	A	411	SQD	C18-C19-C20-C21
32	E	101	LHG	C11-C10-C9-C8
32	D	408	LHG	C28-C29-C30-C31
27	m	102	LFA	C6-C7-C8-C9
32	D	407	LHG	C4-O6-P-O3
30	f	101	LMG	C15-C16-C17-C18
32	d	407	LHG	O1-C1-C2-O2
32	D	408	LHG	O1-C1-C2-O2
32	D	406	LHG	C28-C29-C30-C31
27	A	410	LFA	C2-C3-C4-C5
26	a	412	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	h	102	DGD	O2G-C1B-C2B-C3B
31	H	103	DGD	CBB-CCB-CDB-CEB
30	C	520	LMG	C12-C13-C14-C15
32	L	102	LHG	C32-C33-C34-C35
22	C	510	CLA	C13-C15-C16-C17
22	B	615	CLA	C8-C10-C11-C12
31	c	518	DGD	O1A-C1A-O1G-C1G
32	d	407	LHG	O10-C23-O8-C6
27	B	620	LFA	C7-C8-C9-C10
30	c	501	LMG	C40-C41-C42-C43
31	c	518	DGD	CCB-CDB-CEB-CFB
31	c	518	DGD	O1G-C1G-C2G-O2G
30	b	624	LMG	O1-C7-C8-O7
31	c	516	DGD	C2A-C1A-O1G-C1G
22	b	615	CLA	C13-C15-C16-C17
27	d	408	LFA	C1-C2-C3-C4
32	l	101	LHG	C12-C13-C14-C15
32	E	101	LHG	C28-C29-C30-C31
31	C	517	DGD	C7B-C8B-C9B-CAB
31	C	518	DGD	C5A-C6A-C7A-C8A
22	c	507	CLA	C5-C6-C7-C8
22	d	403	CLA	C10-C11-C12-C13
27	J	101	LFA	C5-C6-C7-C8
27	m	101	LFA	C7-C8-C9-C10
30	m	103	LMG	C34-C35-C36-C37
32	L	102	LHG	C33-C34-C35-C36
22	b	610	CLA	C2-C1-O2A-CGA
22	D	402	CLA	C2-C1-O2A-CGA
27	B	624	LFA	C7-C8-C9-C10
31	H	103	DGD	CAB-CBB-CCB-CDB
22	C	510	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	609	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
26	L	101	SQD	C25-C26-C27-C28
27	C	521	LFA	C1-C2-C3-C4
32	e	101	LHG	C28-C29-C30-C31
22	H	101	CLA	C8-C10-C11-C12
32	D	408	LHG	C2-C3-O3-P
32	E	101	LHG	C18-C19-C20-C21
31	C	519	DGD	C6B-C7B-C8B-C9B
24	A	407	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	A	407	BCR	C23-C24-C25-C30
24	a	408	BCR	C1-C6-C7-C8
24	a	408	BCR	C5-C6-C7-C8
24	b	621	BCR	C1-C6-C7-C8
24	b	621	BCR	C23-C24-C25-C26
30	b	624	LMG	C34-C35-C36-C37
32	D	408	LHG	C30-C31-C32-C33
24	k	101	BCR	C7-C8-C9-C34
24	B	618	BCR	C7-C8-C9-C34
30	c	522	LMG	C18-C19-C20-C21
24	d	404	BCR	C7-C8-C9-C10
27	B	627	LFA	C7-C8-C9-C10
27	i	101	LFA	C1-C2-C3-C4
26	a	412	SQD	C17-C18-C19-C20
22	B	601	CLA	C16-C17-C18-C19
32	D	406	LHG	C19-C20-C21-C22
32	D	406	LHG	C32-C33-C34-C35
30	C	501	LMG	C35-C36-C37-C38
30	m	103	LMG	C11-C12-C13-C14
22	B	606	CLA	C12-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C10
22	B	614	CLA	C12-C13-C15-C16
22	B	604	CLA	C12-C13-C15-C16
22	c	508	CLA	C12-C13-C15-C16
27	T	102	LFA	C9-C10-C11-C12
22	b	609	CLA	C16-C17-C18-C20
22	B	610	CLA	C16-C17-C18-C20
30	B	619	LMG	C37-C38-C39-C40
27	c	521	LFA	C3-C4-C5-C6
30	m	103	LMG	C11-C10-O7-C8
30	C	501	LMG	C16-C17-C18-C19
30	f	101	LMG	C30-C31-C32-C33
30	B	619	LMG	C17-C18-C19-C20
31	C	517	DGD	C2A-C3A-C4A-C5A
27	i	101	LFA	C7-C8-C9-C10
22	C	505	CLA	C13-C15-C16-C17
31	c	516	DGD	C2A-C3A-C4A-C5A
23	A	405	PHO	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	510	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CAD-CBD-CGD-O2D
22	B	613	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	D	401	PHO	CAD-CBD-CGD-O2D
22	a	404	CLA	CAD-CBD-CGD-O2D
23	a	406	PHO	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	c	511	CLA	CAD-CBD-CGD-O2D
32	d	406	LHG	C16-C17-C18-C19
22	a	405	CLA	C15-C16-C17-C18
31	H	103	DGD	C6B-C7B-C8B-C9B
26	D	411	SQD	O5-C1-O6-C44
31	C	518	DGD	O6E-C1E-O5D-C6D
22	C	506	CLA	C2-C3-C5-C6
30	c	519	LMG	C18-C19-C20-C21
30	C	522	LMG	C28-C29-C30-C31
26	D	411	SQD	C44-C45-C46-O48
30	C	501	LMG	O1-C7-C8-C9
31	h	102	DGD	O1G-C1G-C2G-C3G
32	l	101	LHG	O6-C4-C5-O7
26	b	601	SQD	O47-C7-C8-C9
32	E	101	LHG	C25-C26-C27-C28
32	L	102	LHG	C14-C15-C16-C17
32	l	101	LHG	C26-C27-C28-C29
30	b	624	LMG	C31-C32-C33-C34
32	E	101	LHG	C24-C25-C26-C27
22	b	611	CLA	C16-C17-C18-C19
22	B	606	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
26	f	102	SQD	C35-C36-C37-C38
27	B	620	LFA	C1-C2-C3-C4
30	c	501	LMG	C35-C36-C37-C38
30	C	501	LMG	C22-C23-C24-C25
27	I	101	LFA	C7-C8-C9-C10
31	H	103	DGD	O1G-C1G-C2G-O2G
26	f	102	SQD	O47-C45-C46-O48
31	h	102	DGD	O1G-C1G-C2G-O2G
26	L	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
27	b	622	LFA	C7-C8-C9-C10
26	A	409	SQD	C13-C14-C15-C16
22	B	613	CLA	C4-C3-C5-C6
27	b	630	LFA	C1-C2-C3-C4
30	m	103	LMG	O9-C10-O7-C8
22	B	606	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C14-C13-C15-C16
22	D	402	CLA	C14-C13-C15-C16
31	C	517	DGD	C4D-C5D-C6D-O5D
31	c	516	DGD	O1A-C1A-O1G-C1G
31	H	103	DGD	C5B-C6B-C7B-C8B
27	B	627	LFA	C11-C12-C13-C14
22	b	607	CLA	C10-C11-C12-C13
27	b	630	LFA	C6-C7-C8-C9
32	e	101	LHG	C19-C20-C21-C22
24	K	101	BCR	C37-C22-C23-C24
31	c	516	DGD	C9A-CAA-CBA-CCA
30	c	519	LMG	C12-C13-C14-C15
24	k	101	BCR	C7-C8-C9-C10
24	c	524	BCR	C7-C8-C9-C10
22	H	101	CLA	C3-C5-C6-C7
23	a	406	PHO	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C19
22	c	505	CLA	C13-C15-C16-C17
27	b	627	LFA	C10-C11-C12-C13
22	b	616	CLA	C2-C1-O2A-CGA
32	d	407	LHG	C4-O6-P-O3
32	D	408	LHG	C4-O6-P-O3
32	b	628	LHG	C24-C25-C26-C27
27	B	626	LFA	C7-C8-C9-C10
27	B	623	LFA	C9-C10-C11-C12
32	d	407	LHG	C9-C10-C11-C12
27	i	101	LFA	C12-C13-C14-C15
32	d	406	LHG	C4-O6-P-O5
32	D	407	LHG	C4-O6-P-O5
32	l	101	LHG	C3-O3-P-O5
32	d	407	LHG	C4-O6-P-O4
32	E	101	LHG	C3-O3-P-O4
32	E	101	LHG	C4-O6-P-O4
32	E	101	LHG	C4-O6-P-O5
32	D	408	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
32	L	102	LHG	C3-O3-P-O5
22	B	611	CLA	C16-C17-C18-C20
30	C	522	LMG	C10-C11-C12-C13
32	l	101	LHG	C15-C16-C17-C18
32	l	101	LHG	O6-C4-C5-C6
32	l	101	LHG	C11-C12-C13-C14
27	A	410	LFA	C11-C10-C9-C8
22	C	507	CLA	C3-C5-C6-C7
31	H	103	DGD	C2B-C3B-C4B-C5B
26	L	101	SQD	C24-C25-C26-C27
26	f	102	SQD	C11-C10-C9-C8
31	h	102	DGD	C2B-C1B-O2G-C2G
22	B	606	CLA	CAD-CBD-CGD-O1D
22	b	606	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
27	m	102	LFA	C2-C3-C4-C5
30	C	501	LMG	C13-C14-C15-C16
31	c	517	DGD	C6B-C7B-C8B-C9B
26	f	102	SQD	C25-C26-C27-C28
30	c	522	LMG	C14-C15-C16-C17
22	C	506	CLA	C4-C3-C5-C6
22	a	407	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
26	A	411	SQD	C33-C34-C35-C36
32	d	407	LHG	C12-C13-C14-C15
27	b	626	LFA	C7-C8-C9-C10
31	C	518	DGD	C9B-CAB-CBB-CCB
31	H	103	DGD	O2G-C1B-C2B-C3B
32	D	406	LHG	C30-C31-C32-C33
27	B	624	LFA	C10-C11-C12-C13
31	c	518	DGD	O1G-C1G-C2G-C3G
30	b	624	LMG	O1-C7-C8-C9
26	D	411	SQD	O47-C45-C46-O48
30	C	522	LMG	O1-C7-C8-O7
30	C	501	LMG	O1-C7-C8-O7
30	C	501	LMG	O7-C8-C9-O8
30	C	522	LMG	C20-C21-C22-C23
30	c	501	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	a	412	SQD	C29-C30-C31-C32
32	d	406	LHG	C34-C35-C36-C37
27	A	413	LFA	C6-C7-C8-C9
22	B	606	CLA	C13-C15-C16-C17
26	a	412	SQD	C18-C19-C20-C21
30	c	522	LMG	C29-C28-O8-C9
27	T	102	LFA	C6-C7-C8-C9
25	D	405	PL9	C33-C34-C36-C37
22	a	407	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C10-C8-C9
22	b	618	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	d	401	CLA	C16-C17-C18-C19
27	A	413	LFA	C7-C8-C9-C10
32	e	101	LHG	C15-C16-C17-C18
27	M	102	LFA	C7-C8-C9-C10
27	B	626	LFA	C2-C3-C4-C5
27	M	102	LFA	C11-C12-C13-C14
22	a	405	CLA	C16-C17-C18-C20
32	d	406	LHG	C30-C31-C32-C33
26	A	409	SQD	C30-C31-C32-C33
24	K	101	BCR	C21-C22-C23-C24
24	b	621	BCR	C21-C22-C23-C24
27	b	626	LFA	C11-C12-C13-C14
23	D	401	PHO	C16-C17-C18-C19
27	b	622	LFA	C4-C5-C6-C7
27	d	409	LFA	C4-C5-C6-C7
31	c	518	DGD	C9B-CAB-CBB-CCB
30	f	101	LMG	C39-C40-C41-C42
30	B	619	LMG	C13-C14-C15-C16
22	B	612	CLA	C13-C15-C16-C17
22	B	610	CLA	C8-C10-C11-C12
31	C	517	DGD	O6D-C5D-C6D-O5D
30	B	621	LMG	C31-C32-C33-C34
22	c	504	CLA	C10-C11-C12-C13
26	A	411	SQD	O10-C23-O48-C46
22	c	507	CLA	C2-C1-O2A-CGA
30	C	501	LMG	C11-C12-C13-C14
32	l	101	LHG	C16-C17-C18-C19
27	d	410	LFA	C3-C4-C5-C6
26	A	409	SQD	C18-C19-C20-C21
32	d	407	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
26	A	411	SQD	C24-C23-O48-C46
30	b	624	LMG	C29-C28-O8-C9
22	B	607	CLA	C16-C17-C18-C19
27	B	620	LFA	C6-C7-C8-C9
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C30
24	b	621	BCR	C23-C24-C25-C30
30	b	624	LMG	O10-C28-O8-C9
32	D	406	LHG	C31-C32-C33-C34
30	C	520	LMG	C10-C11-C12-C13
32	D	408	LHG	C11-C12-C13-C14
25	d	405	PL9	C24-C26-C27-C28
31	C	518	DGD	C2E-C1E-O5D-C6D
32	D	406	LHG	C15-C16-C17-C18
32	D	407	LHG	C3-O3-P-O6
32	b	628	LHG	C27-C28-C29-C30
22	c	514	CLA	C16-C17-C18-C20
27	I	101	LFA	C5-C6-C7-C8
31	H	103	DGD	O1G-C1G-C2G-C3G
30	c	519	LMG	C19-C20-C21-C22
30	c	501	LMG	C17-C18-C19-C20
27	b	627	LFA	C5-C6-C7-C8
22	b	606	CLA	C6-C7-C8-C9
22	B	608	CLA	C11-C10-C8-C9
26	a	412	SQD	C27-C28-C29-C30
27	M	101	LFA	C6-C7-C8-C9
32	E	101	LHG	C14-C15-C16-C17
30	D	409	LMG	C10-C11-C12-C13
30	c	519	LMG	C29-C30-C31-C32
26	a	412	SQD	C19-C20-C21-C22
30	f	101	LMG	C14-C15-C16-C17
27	B	623	LFA	C2-C3-C4-C5
32	d	407	LHG	C29-C30-C31-C32
22	C	510	CLA	C16-C17-C18-C20
32	d	406	LHG	C24-C23-O8-C6
32	D	408	LHG	C24-C23-O8-C6
26	f	102	SQD	O10-C23-O48-C46
27	A	410	LFA	C10-C11-C12-C13
26	f	102	SQD	C24-C23-O48-C46
32	E	101	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	k	101	BCR	C19-C20-C21-C22
27	b	626	LFA	C9-C10-C11-C12
25	d	405	PL9	C39-C41-C42-C43
31	C	517	DGD	C5A-C6A-C7A-C8A
27	j	101	LFA	C5-C6-C7-C8
32	d	407	LHG	C15-C16-C17-C18
32	d	406	LHG	C28-C29-C30-C31
31	c	516	DGD	C4D-C5D-C6D-O5D
27	b	630	LFA	C11-C10-C9-C8
30	B	619	LMG	C33-C34-C35-C36
31	C	519	DGD	CDB-CEB-CFB-CGB
22	B	611	CLA	C16-C17-C18-C19
32	E	101	LHG	O7-C5-C6-O8
30	m	103	LMG	C37-C38-C39-C40
22	D	403	CLA	C3A-C2A-CAA-CBA
27	b	625	LFA	C9-C10-C11-C12
26	f	102	SQD	C24-C25-C26-C27
27	b	626	LFA	C4-C5-C6-C7
25	a	409	PL9	C35-C34-C36-C37
27	B	628	LFA	C10-C11-C12-C13
25	a	409	PL9	C4-C3-C7-C8
22	c	507	CLA	C11-C10-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	b	615	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C10-C8-C9
23	D	401	PHO	C14-C13-C15-C16
22	b	611	CLA	C14-C13-C15-C16
32	L	102	LHG	C11-C10-C9-C8
32	D	407	LHG	C26-C27-C28-C29
27	t	101	LFA	C4-C5-C6-C7
30	c	522	LMG	O10-C28-O8-C9
32	d	407	LHG	C35-C36-C37-C38
22	B	614	CLA	C16-C17-C18-C19
22	C	513	CLA	O2A-C1-C2-C3
30	C	501	LMG	O6-C1-O1-C7
32	L	102	LHG	C26-C27-C28-C29
31	h	102	DGD	O1B-C1B-C2B-C3B
27	B	624	LFA	C11-C10-C9-C8
27	A	410	LFA	C4-C5-C6-C7
22	B	607	CLA	C15-C16-C17-C18
22	b	614	CLA	C12-C13-C15-C16
22	B	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
27	d	410	LFA	C7-C8-C9-C10
31	C	517	DGD	CDA-CEA-CFA-CGA
27	i	101	LFA	C2-C3-C4-C5
22	B	604	CLA	C10-C11-C12-C13
32	d	406	LHG	C26-C27-C28-C29
32	D	408	LHG	C9-C10-C11-C12
27	c	521	LFA	C12-C13-C14-C15
27	A	413	LFA	C10-C11-C12-C13
25	d	405	PL9	C30-C29-C31-C32
25	d	405	PL9	C40-C39-C41-C42
22	B	605	CLA	C8-C10-C11-C12
31	C	517	DGD	C8B-C9B-CAB-CBB
32	l	101	LHG	C27-C28-C29-C30
31	h	102	DGD	C5A-C6A-C7A-C8A
27	B	626	LFA	C3-C4-C5-C6
31	c	517	DGD	O1G-C1G-C2G-O2G
31	C	518	DGD	C4D-C5D-C6D-O5D
27	B	622	LFA	C4-C5-C6-C7
31	h	102	DGD	O6E-C5E-C6E-O5E
32	D	408	LHG	O10-C23-O8-C6
27	d	410	LFA	C6-C7-C8-C9
31	h	102	DGD	C2A-C3A-C4A-C5A
27	A	410	LFA	C3-C4-C5-C6
32	D	408	LHG	C25-C26-C27-C28
30	C	522	LMG	C29-C30-C31-C32
30	C	522	LMG	C14-C15-C16-C17
25	a	409	PL9	C33-C34-C36-C37
30	B	619	LMG	C12-C13-C14-C15
32	d	406	LHG	O10-C23-O8-C6
22	b	603	CLA	CAA-CBA-CGA-O2A
22	c	506	CLA	C11-C10-C8-C9
27	b	625	LFA	C13-C14-C15-C16
27	B	620	LFA	C2-C3-C4-C5
31	c	518	DGD	C7B-C8B-C9B-CAB
26	a	410	SQD	C9-C10-C11-C12
27	D	410	LFA	C11-C12-C13-C14
22	a	405	CLA	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C19
27	B	627	LFA	C10-C11-C12-C13
24	H	102	BCR	C1-C6-C7-C8
24	c	515	BCR	C1-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
26	a	410	SQD	C18-C19-C20-C21
30	m	103	LMG	C30-C31-C32-C33
26	D	411	SQD	O48-C23-C24-C25
27	B	624	LFA	C9-C10-C11-C12
31	c	518	DGD	C1G-C2G-C3G-O3G
22	C	505	CLA	C4-C3-C5-C6
26	b	601	SQD	C29-C30-C31-C32
25	a	409	PL9	C23-C24-C26-C27
22	B	613	CLA	C2-C3-C5-C6
27	d	408	LFA	C3-C4-C5-C6
31	c	516	DGD	O6D-C5D-C6D-O5D
30	C	522	LMG	C8-C7-O1-C1
22	A	406	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
26	A	411	SQD	C26-C27-C28-C29
22	C	504	CLA	C10-C11-C12-C13
32	b	628	LHG	O6-C4-C5-O7
33	e	102	HEM	C3D-CAD-CBD-CGD
33	E	102	HEM	C2A-CAA-CBA-CGA
31	c	516	DGD	C1A-C2A-C3A-C4A
31	C	517	DGD	CAB-CBB-CCB-CDB
27	A	413	LFA	C4-C5-C6-C7
25	A	408	PL9	C28-C29-C31-C32
22	b	613	CLA	C2-C3-C5-C6
22	C	504	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
30	f	101	LMG	C29-C30-C31-C32
32	b	628	LHG	C14-C15-C16-C17
31	h	102	DGD	O1B-C1B-O2G-C2G
31	c	517	DGD	CAB-CBB-CCB-CDB
22	b	614	CLA	CAA-CBA-CGA-O2A
23	a	406	PHO	C15-C16-C17-C18
32	E	101	LHG	O8-C23-C24-C25
22	B	615	CLA	C3-C5-C6-C7
22	b	617	CLA	C4-C3-C5-C6
22	D	403	CLA	C4-C3-C5-C6
25	d	405	PL9	C28-C29-C31-C32
25	d	405	PL9	C38-C39-C41-C42
22	b	607	CLA	C14-C13-C15-C16
22	B	604	CLA	C6-C7-C8-C9
22	d	402	CLA	C11-C12-C13-C14
22	c	513	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	C	520	LMG	C17-C18-C19-C20
22	b	614	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CAD-CBD-CGD-O2D
22	b	618	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	D	403	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	B	608	CLA	CAD-CBD-CGD-O2D
31	c	518	DGD	C7A-C8A-C9A-CAA
30	B	621	LMG	O7-C10-C11-C12
22	B	614	CLA	C4-C3-C5-C6
26	a	410	SQD	O47-C7-C8-C9
24	k	101	BCR	C11-C12-C13-C14
24	B	618	BCR	C7-C8-C9-C10
27	j	101	LFA	C1-C2-C3-C4
32	d	407	LHG	C2-C3-O3-P
22	B	604	CLA	C15-C16-C17-C18
30	m	103	LMG	O8-C28-C29-C30
22	C	507	CLA	C16-C17-C18-C19
32	L	102	LHG	C18-C19-C20-C21
22	b	606	CLA	O2A-C1-C2-C3
22	c	514	CLA	O2A-C1-C2-C3
23	D	401	PHO	O2A-C1-C2-C3
23	a	406	PHO	O2A-C1-C2-C3
22	c	510	CLA	O2A-C1-C2-C3
23	D	401	PHO	C4B-C3B-CAB-CBB
27	d	408	LFA	C5-C6-C7-C8
22	c	507	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O2D
22	B	605	CLA	CHA-CBD-CGD-O1D
22	B	605	CLA	CHA-CBD-CGD-O2D
22	b	608	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	CHA-CBD-CGD-O2D
22	b	609	CLA	CHA-CBD-CGD-O1D
22	b	609	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
26	a	412	SQD	C26-C27-C28-C29
31	c	517	DGD	CDB-CEB-CFB-CGB
26	A	411	SQD	C16-C17-C18-C19
32	D	406	LHG	C33-C34-C35-C36
31	C	517	DGD	O2G-C1B-C2B-C3B
32	D	406	LHG	O7-C5-C6-O8
31	c	518	DGD	O6D-C5D-C6D-O5D
30	c	519	LMG	C20-C21-C22-C23
26	a	412	SQD	C33-C34-C35-C36
31	c	518	DGD	C2B-C3B-C4B-C5B
32	l	101	LHG	C30-C31-C32-C33
25	a	409	PL9	C13-C14-C16-C17
22	b	609	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C7
30	c	501	LMG	C10-C11-C12-C13
31	C	518	DGD	C7B-C8B-C9B-CAB
30	C	520	LMG	C29-C28-O8-C9
26	A	411	SQD	C4-C5-C6-S
22	B	614	CLA	C16-C17-C18-C20
31	C	517	DGD	C3A-C4A-C5A-C6A
25	A	408	PL9	C26-C27-C28-C29
25	D	405	PL9	C11-C12-C13-C14
30	B	621	LMG	O9-C10-C11-C12
27	b	602	LFA	C1-C2-C3-C4
30	B	619	LMG	O8-C28-C29-C30
22	B	602	CLA	C13-C15-C16-C17
26	b	601	SQD	C33-C34-C35-C36
32	e	101	LHG	C13-C14-C15-C16
32	L	102	LHG	O1-C1-C2-C3
30	m	103	LMG	C16-C17-C18-C19
31	c	517	DGD	O6D-C5D-C6D-O5D
32	b	628	LHG	C24-C23-O8-C6
32	D	406	LHG	C26-C27-C28-C29
23	D	401	PHO	C1A-C2A-CAA-CBA
22	D	403	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C2-C1-O2A-CGA
22	C	505	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
32	D	408	LHG	C33-C34-C35-C36
32	E	101	LHG	O10-C23-C24-C25
31	h	102	DGD	C1G-C2G-C3G-O3G
32	d	407	LHG	C14-C15-C16-C17
32	b	628	LHG	C26-C27-C28-C29
22	A	406	CLA	C16-C17-C18-C20
22	b	612	CLA	C16-C17-C18-C20
22	b	614	CLA	CAA-CBA-CGA-O1A
31	h	102	DGD	C8A-C9A-CAA-CBA
22	C	513	CLA	CAA-CBA-CGA-O2A
31	c	518	DGD	C1A-C2A-C3A-C4A
22	b	610	CLA	C16-C17-C18-C19
22	C	507	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
30	B	619	LMG	C30-C31-C32-C33
30	B	619	LMG	O10-C28-C29-C30
24	d	404	BCR	C1-C6-C7-C8
24	d	404	BCR	C5-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C26
25	a	409	PL9	C29-C31-C32-C33
22	B	611	CLA	C10-C11-C12-C13
22	C	504	CLA	C8-C10-C11-C12
22	C	510	CLA	C16-C17-C18-C19
31	H	103	DGD	C4E-C5E-C6E-O5E
22	C	514	CLA	C8-C10-C11-C12
26	a	412	SQD	O49-C7-C8-C9
22	C	514	CLA	CAD-CBD-CGD-O1D
22	C	513	CLA	CAD-CBD-CGD-O1D
22	b	609	CLA	CAD-CBD-CGD-O1D
30	m	103	LMG	O10-C28-C29-C30
26	A	409	SQD	O47-C7-C8-C9
22	c	510	CLA	C5-C6-C7-C8
22	C	503	CLA	C14-C13-C15-C16
22	B	613	CLA	C11-C12-C13-C14
22	B	603	CLA	C6-C7-C8-C9
22	b	604	CLA	C6-C7-C8-C9
30	C	522	LMG	C17-C18-C19-C20
30	f	101	LMG	C20-C21-C22-C23
22	c	511	CLA	CAA-CBA-CGA-O2A
31	C	518	DGD	O2G-C1B-C2B-C3B
22	c	505	CLA	C15-C16-C17-C18
22	C	509	CLA	C13-C15-C16-C17

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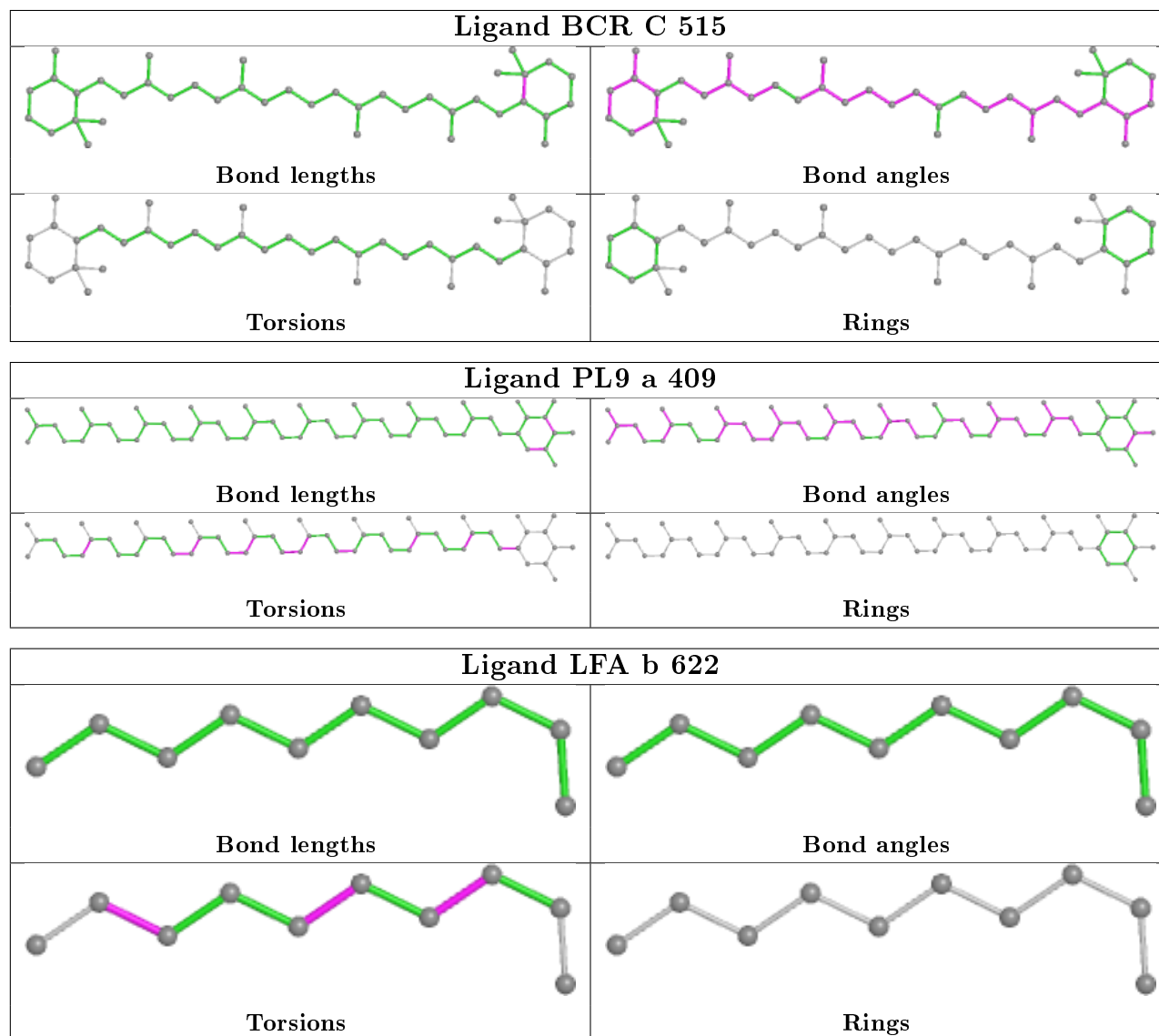
Mol	Chain	Res	Type	Atoms
30	C	520	LMG	O10-C28-O8-C9
22	C	506	CLA	CAA-CBA-CGA-O2A
22	c	506	CLA	CAA-CBA-CGA-O2A
32	D	407	LHG	O10-C23-O8-C6
22	d	403	CLA	C13-C15-C16-C17
31	C	518	DGD	C6B-C7B-C8B-C9B
25	a	409	PL9	C15-C14-C16-C17
25	A	408	PL9	C30-C29-C31-C32
22	b	603	CLA	C4-C3-C5-C6
22	c	502	CLA	C11-C10-C8-C7
22	b	612	CLA	C11-C12-C13-C15
22	c	509	CLA	C12-C13-C15-C16
22	b	616	CLA	C12-C13-C15-C16
22	B	610	CLA	C2-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
22	B	608	CLA	C11-C12-C13-C15
22	C	513	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
26	a	410	SQD	C11-C12-C13-C14
30	c	519	LMG	O7-C10-C11-C12
30	C	520	LMG	O7-C10-C11-C12
26	f	102	SQD	O47-C7-C8-C9
32	D	407	LHG	C32-C33-C34-C35
24	C	516	BCR	C7-C8-C9-C10
31	C	518	DGD	O1B-C1B-C2B-C3B
32	E	101	LHG	C12-C13-C14-C15
30	c	501	LMG	C13-C14-C15-C16
31	c	518	DGD	CAA-CBA-CCA-CDA
31	C	517	DGD	O1B-C1B-C2B-C3B
30	c	519	LMG	O9-C10-C11-C12
22	C	512	CLA	C16-C17-C18-C20
22	b	606	CLA	C13-C15-C16-C17
31	c	518	DGD	C8B-C9B-CAB-CBB
22	C	511	CLA	C4-C3-C5-C6

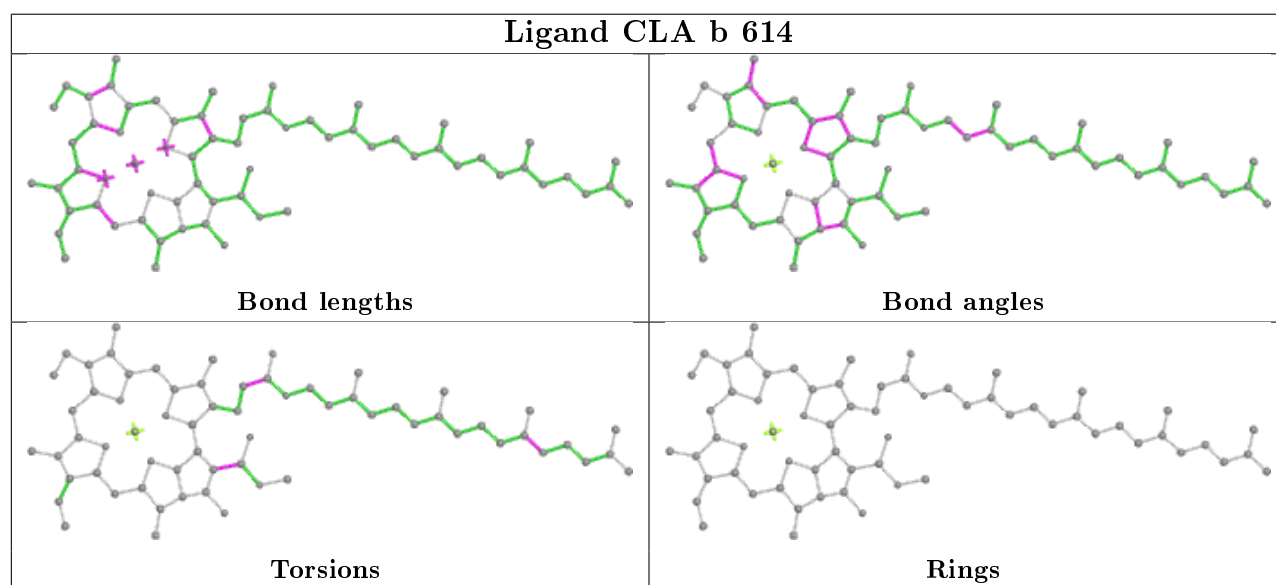
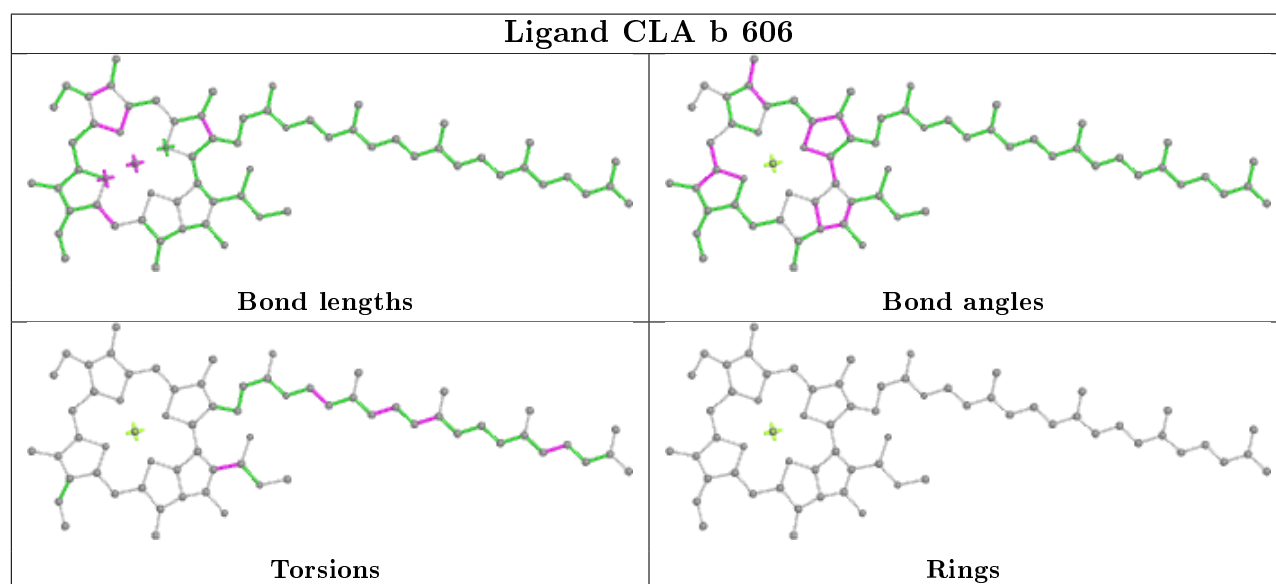
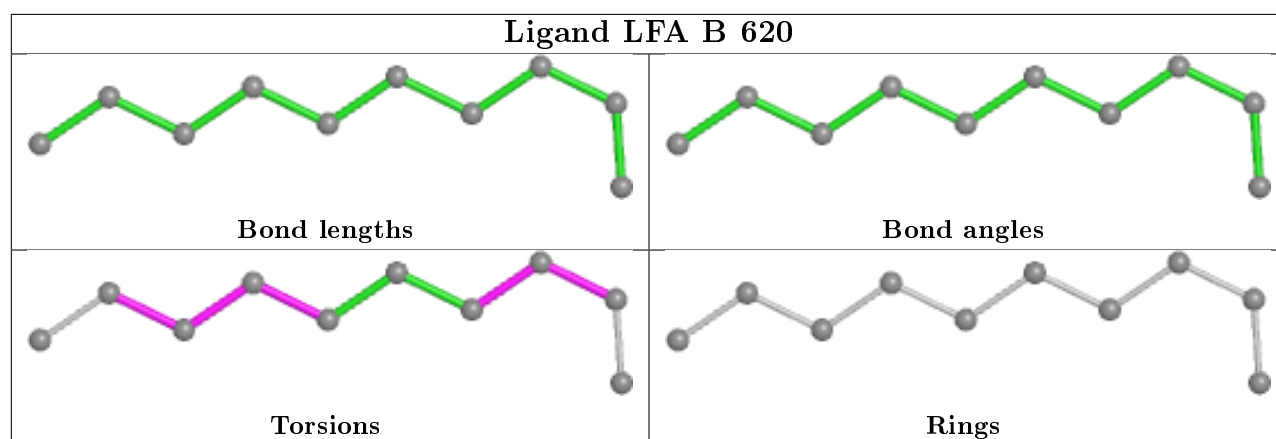
There are no ring outliers.

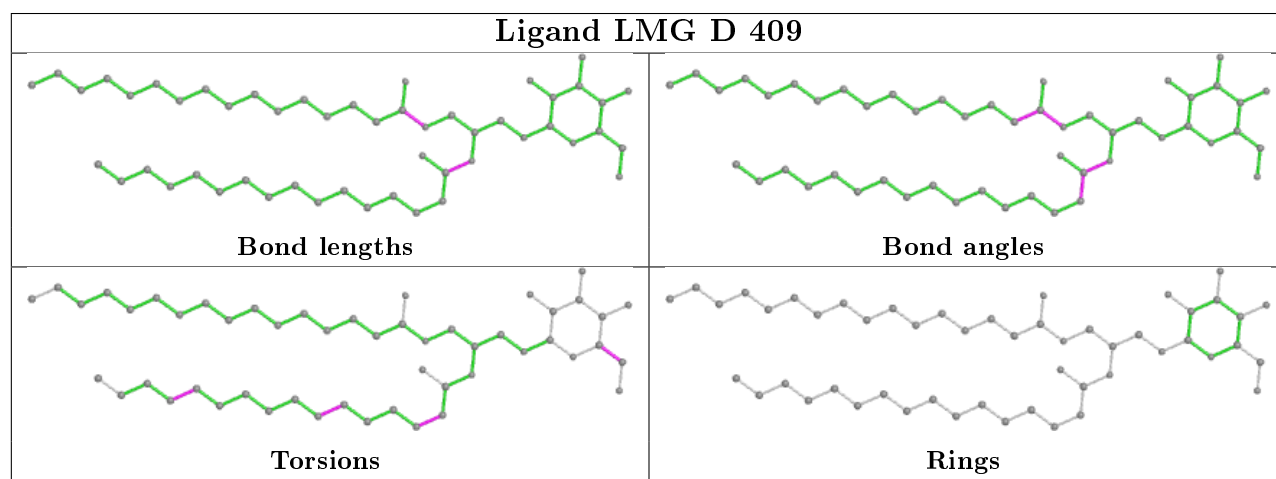
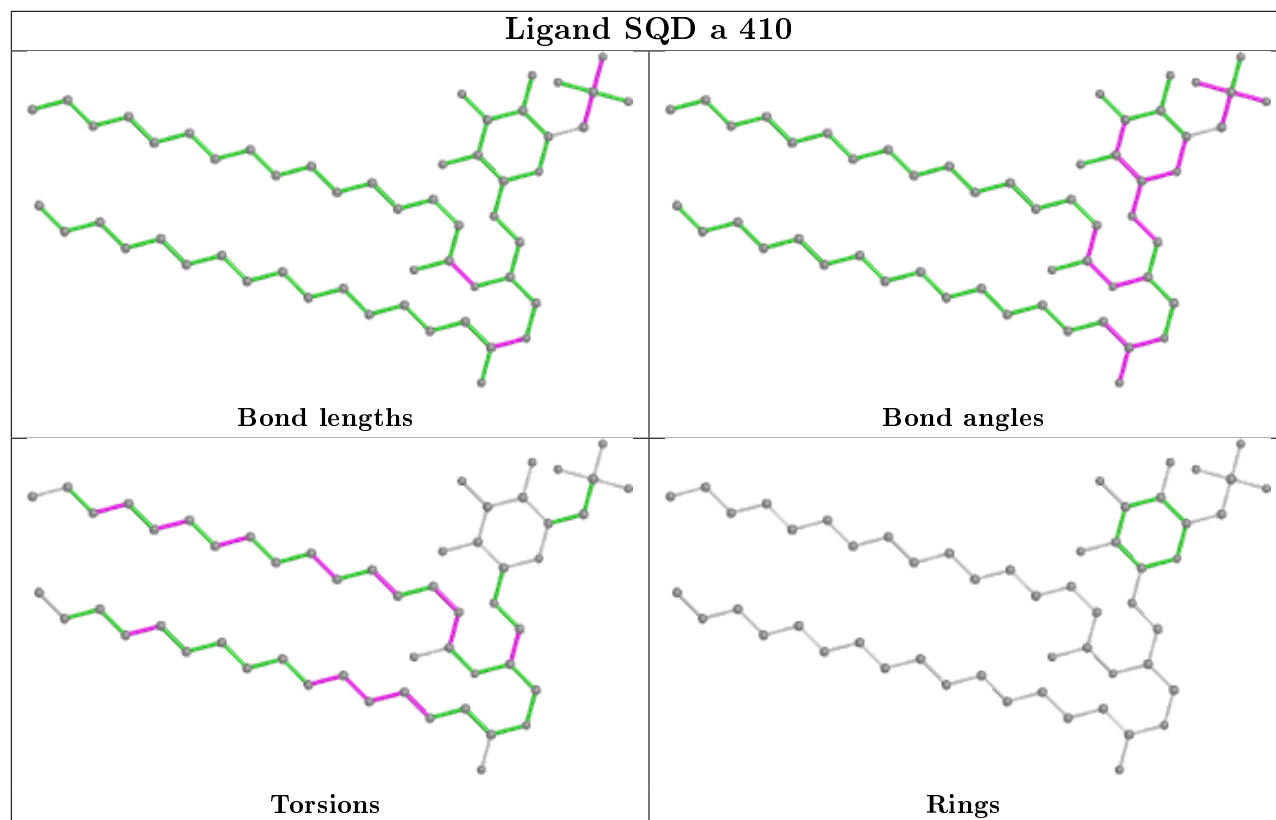
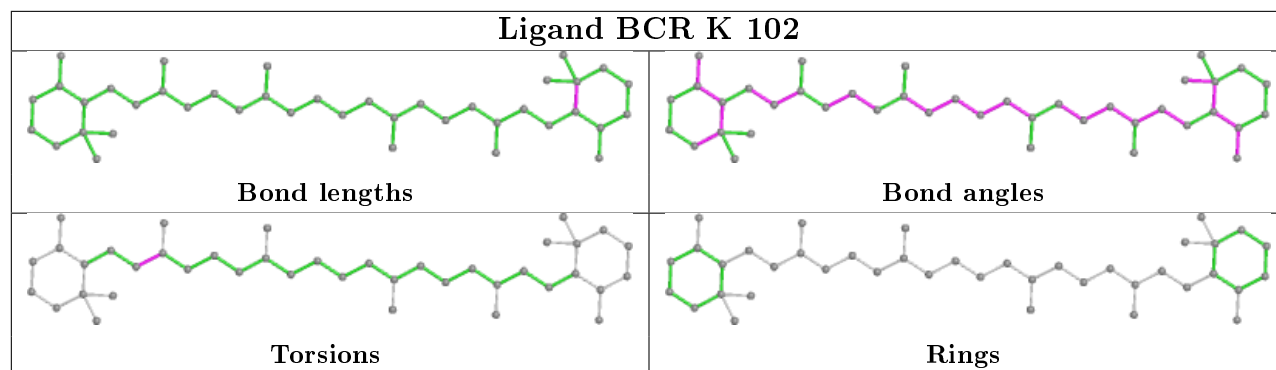
No monomer is involved in short contacts.

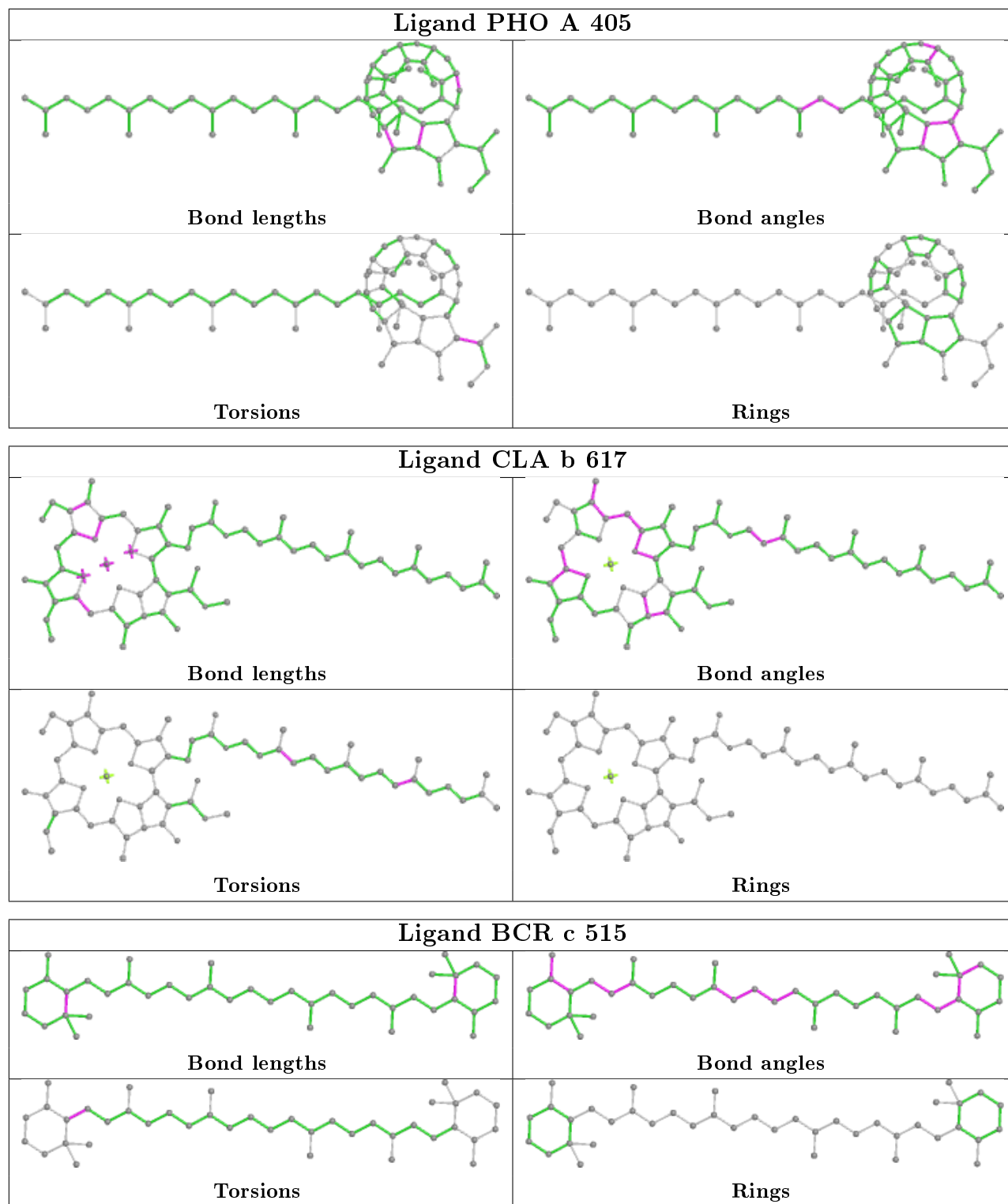
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

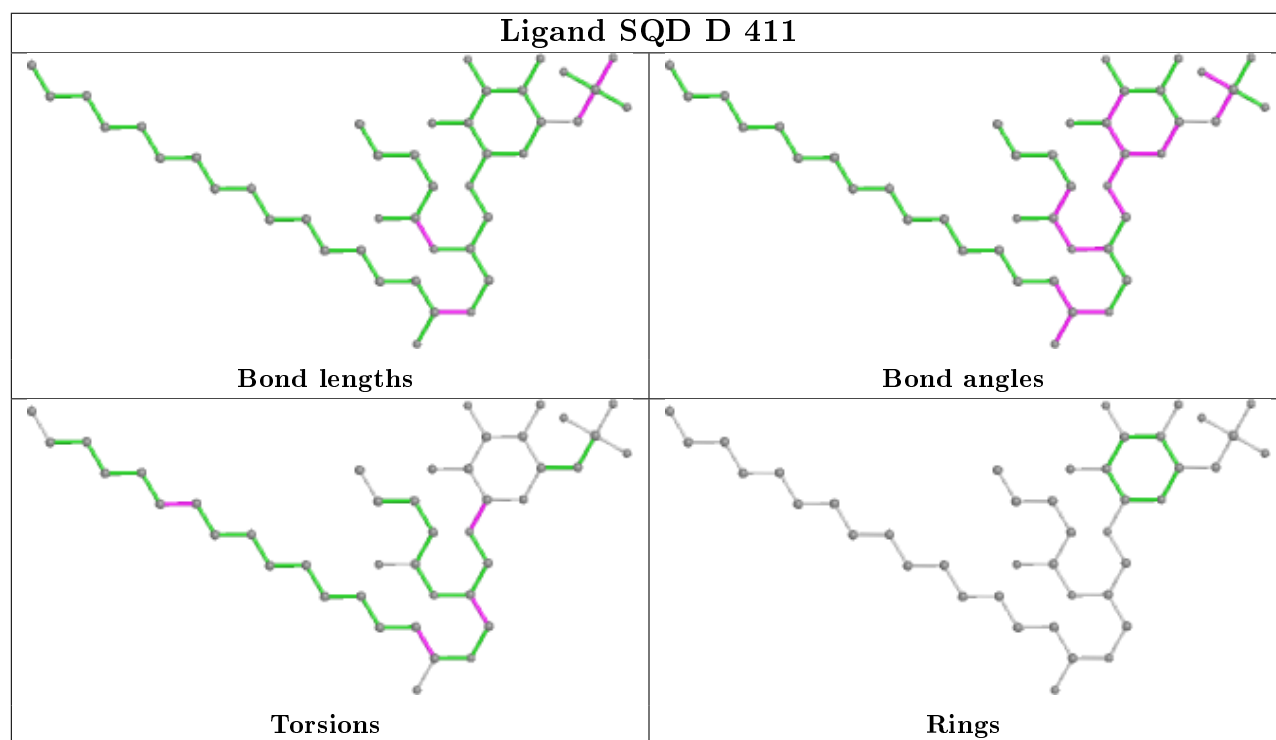
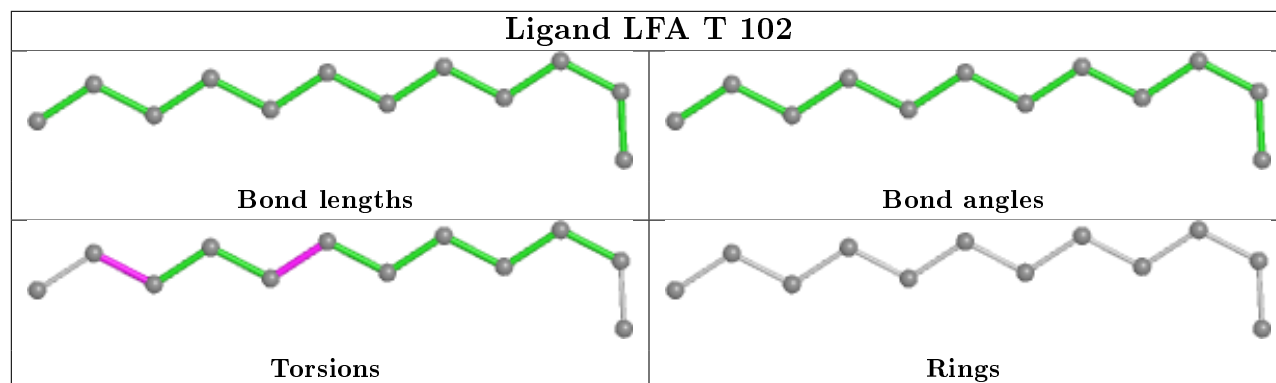
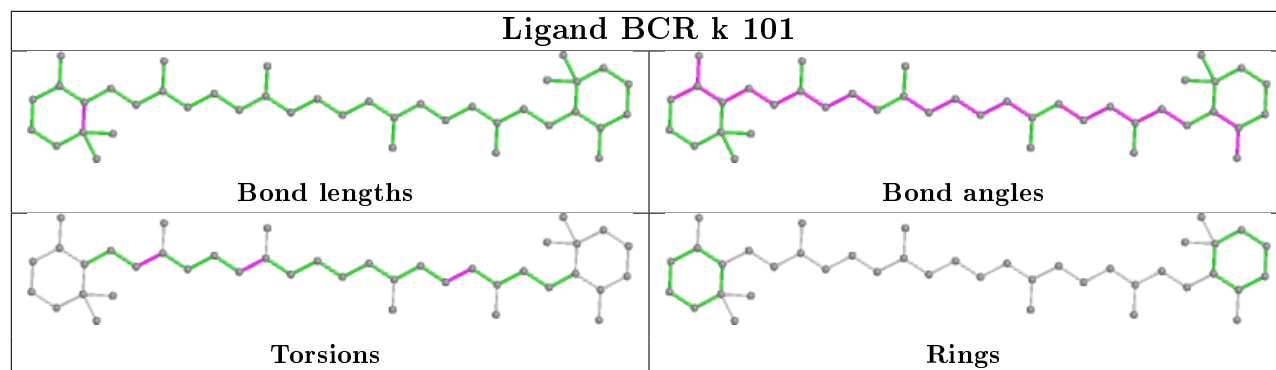
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

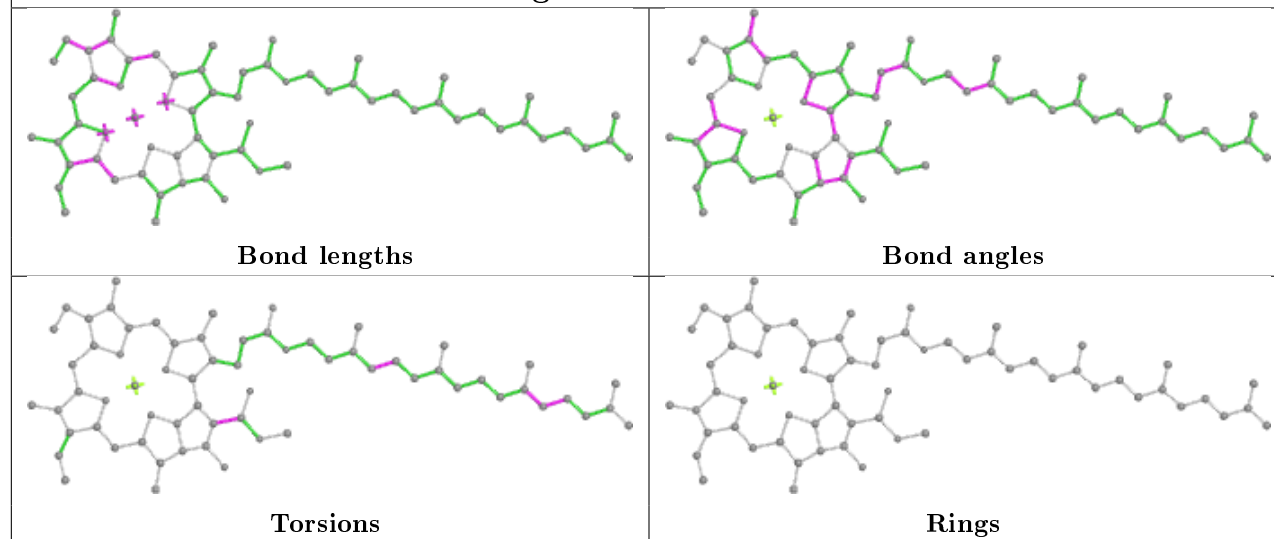
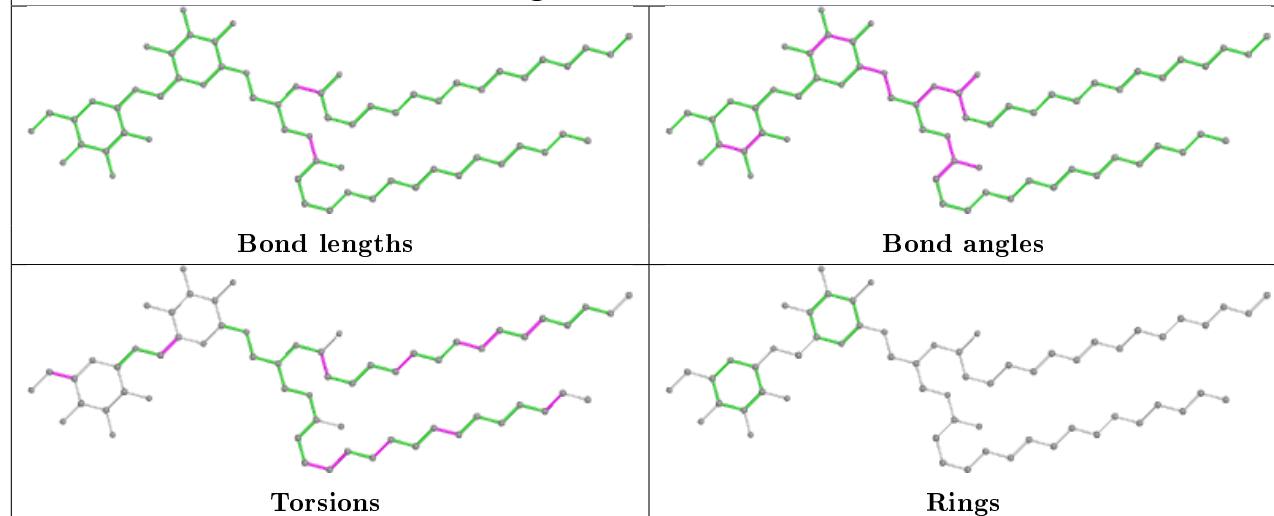
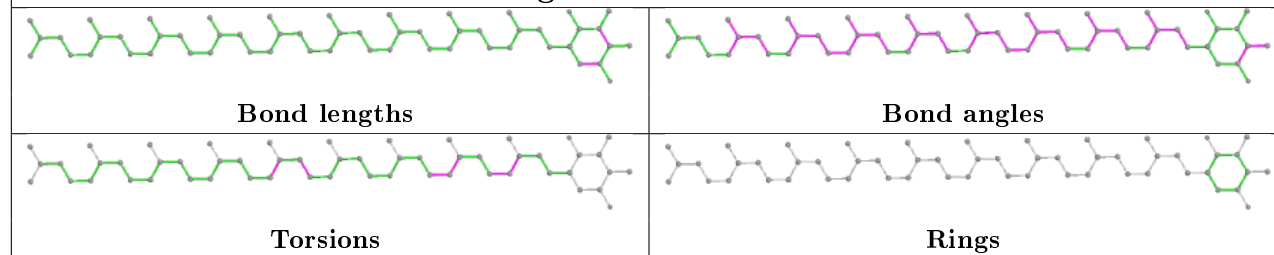


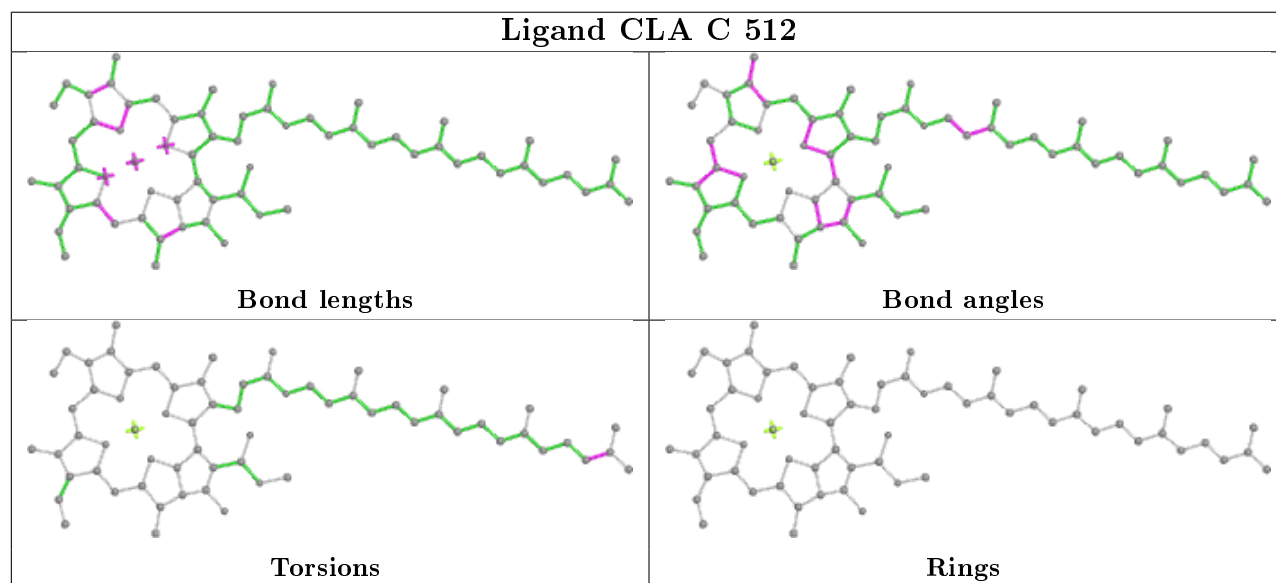
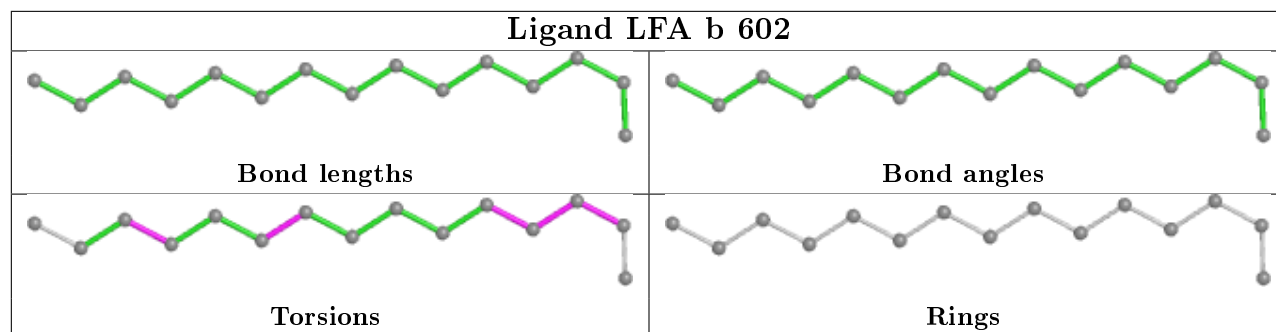




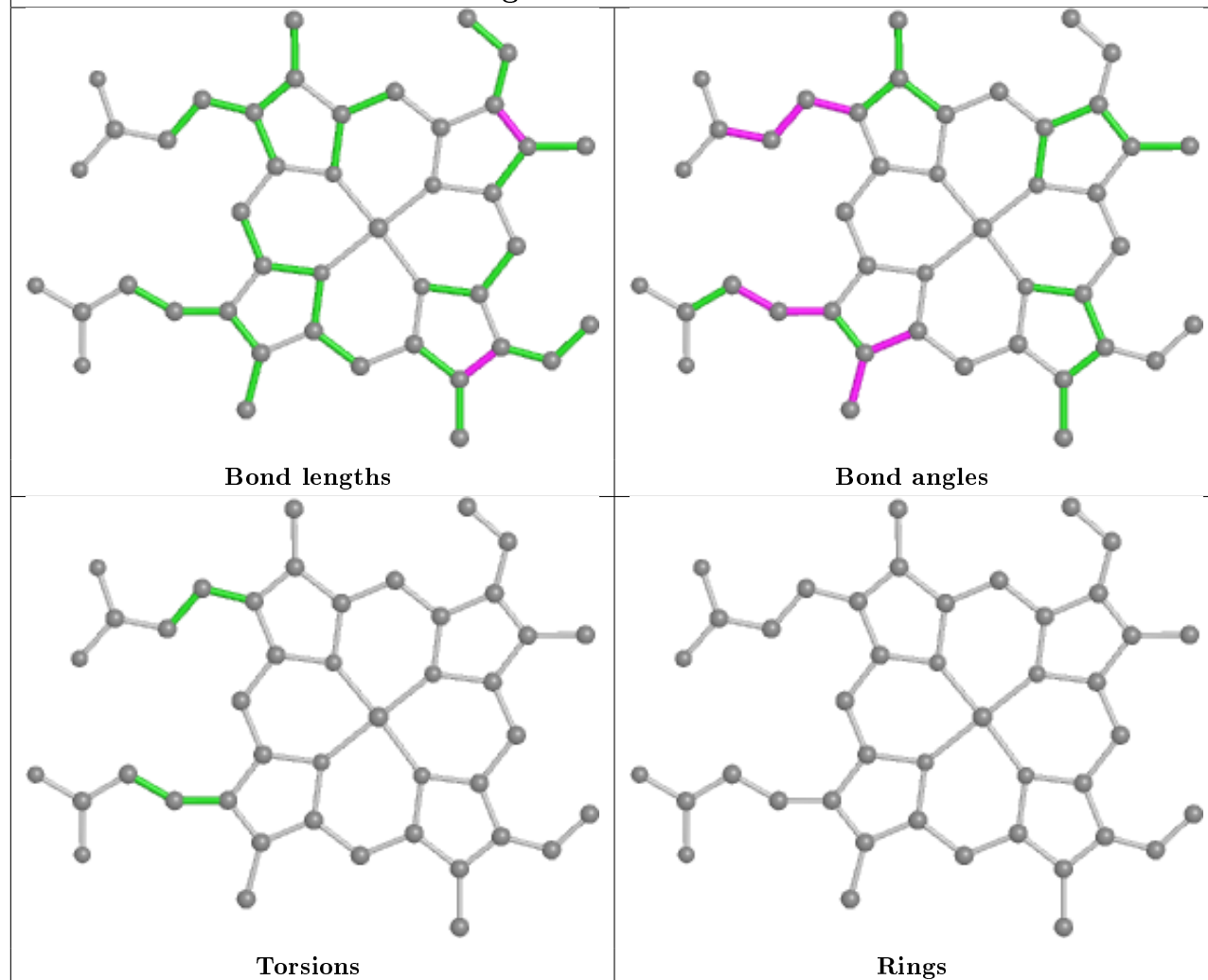




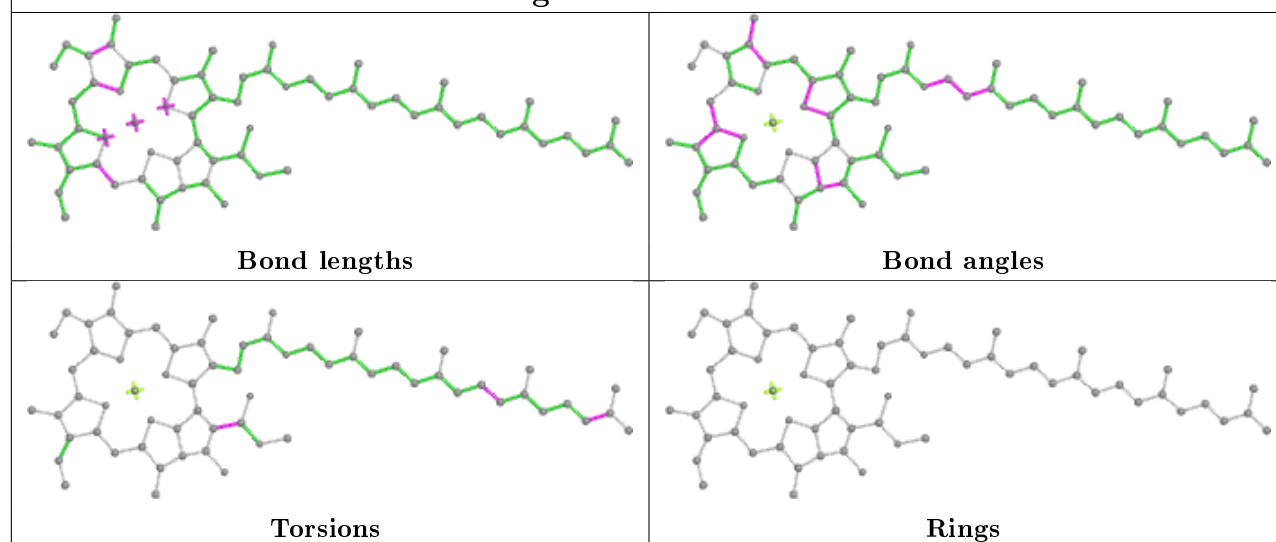
Ligand CLA B 606**Ligand DGD C 517****Ligand PL9 A 408**

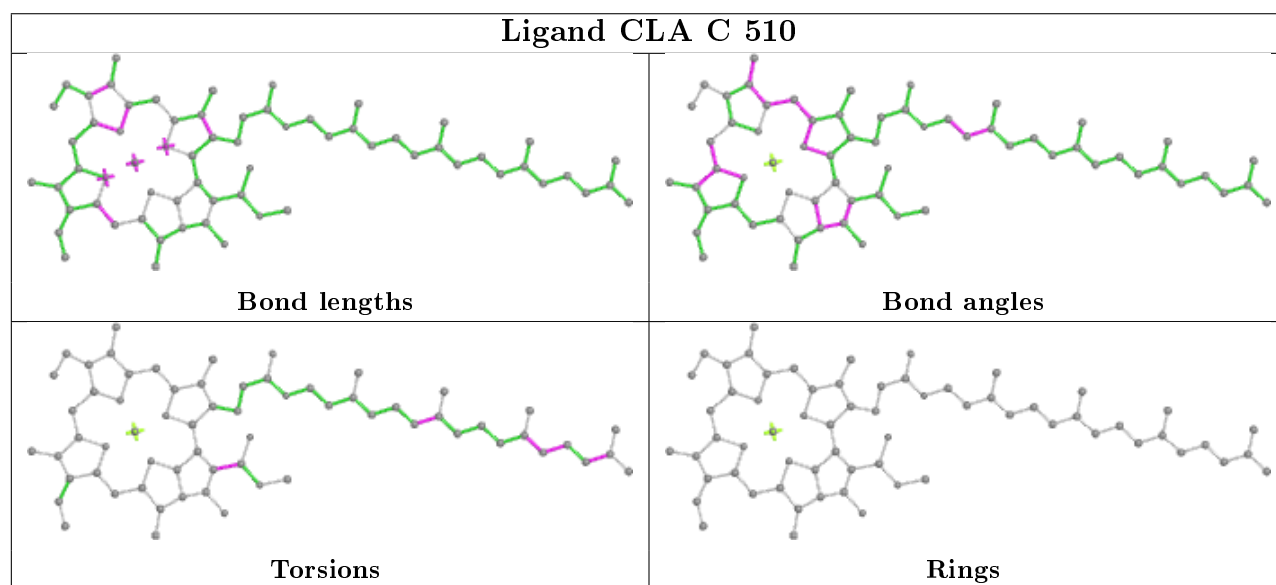
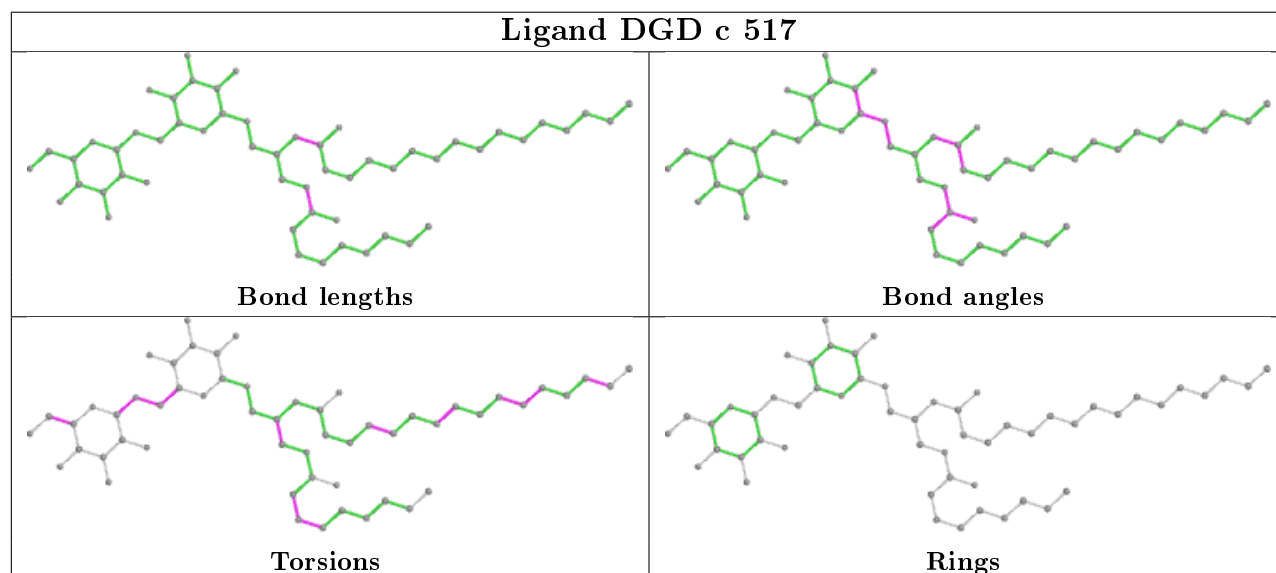
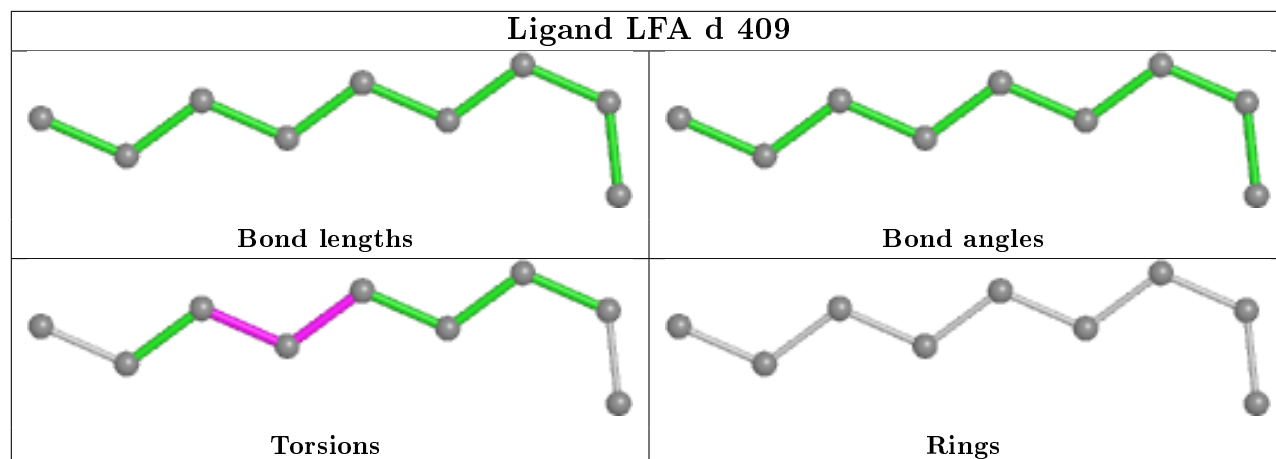


Ligand HEM v 201

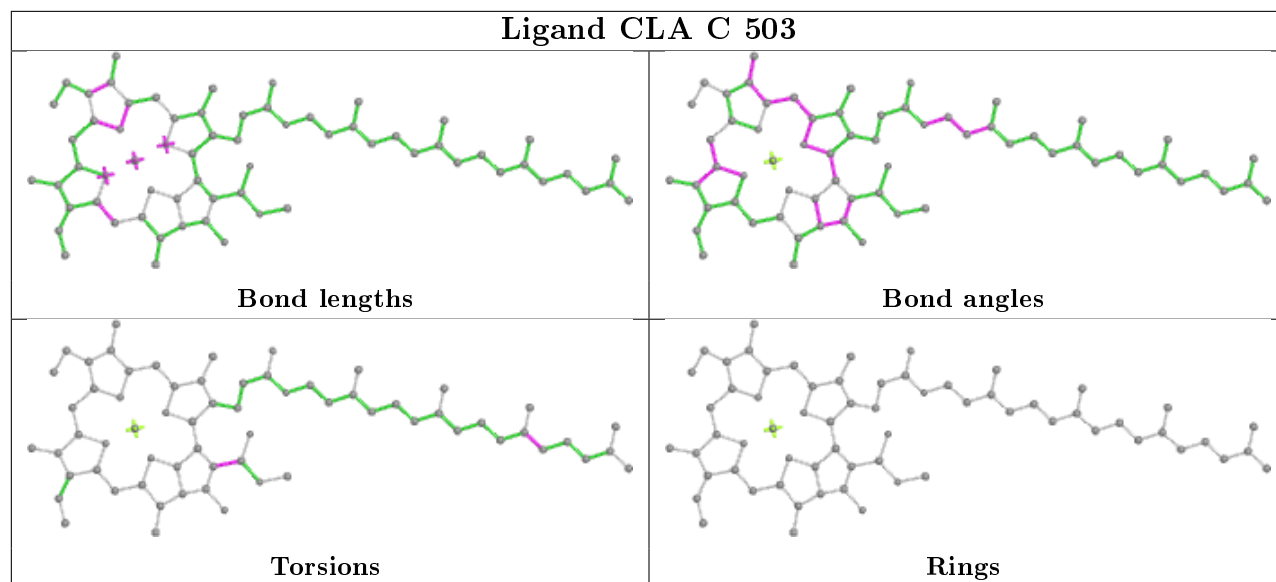


Ligand CLA B 611

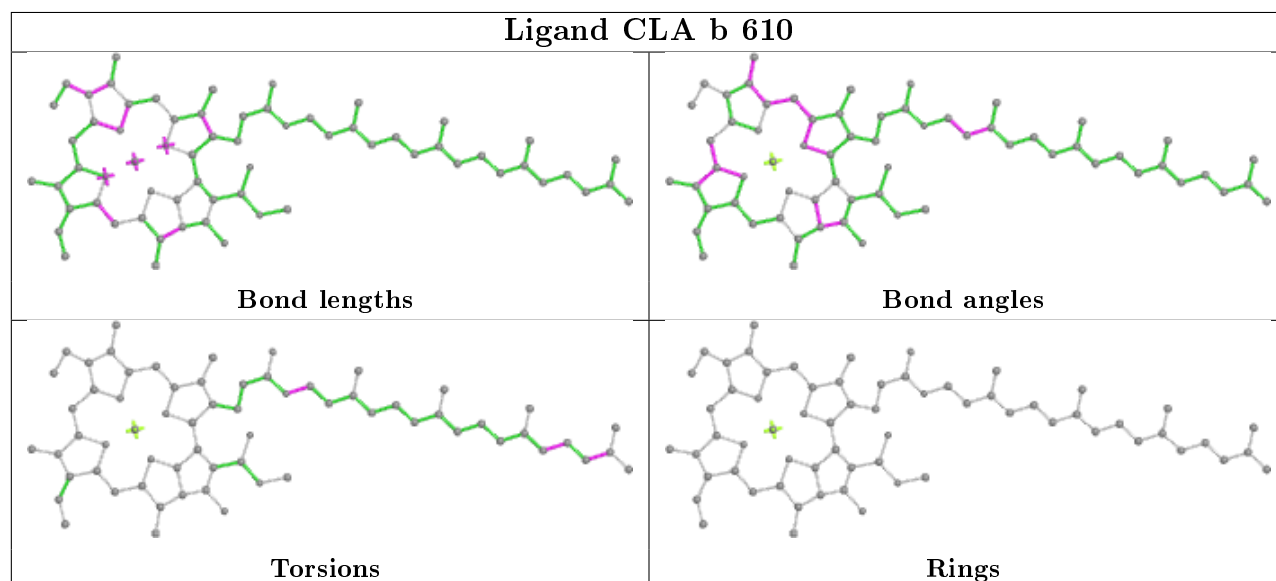




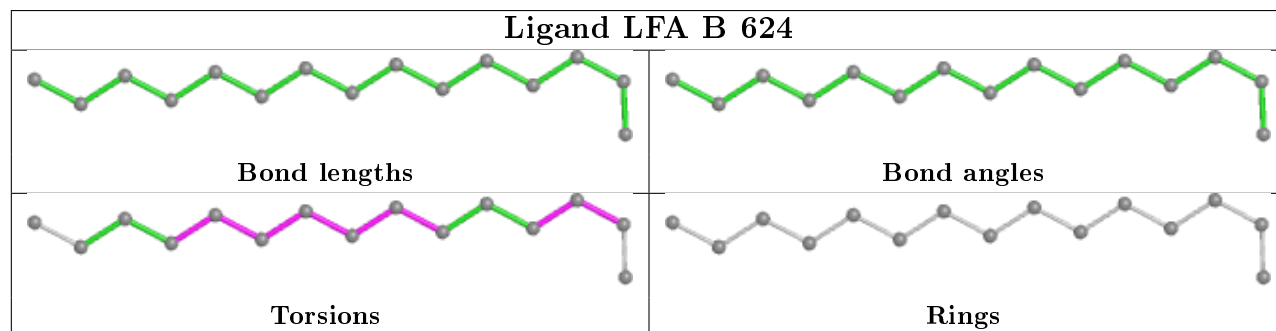
Ligand CLA C 503

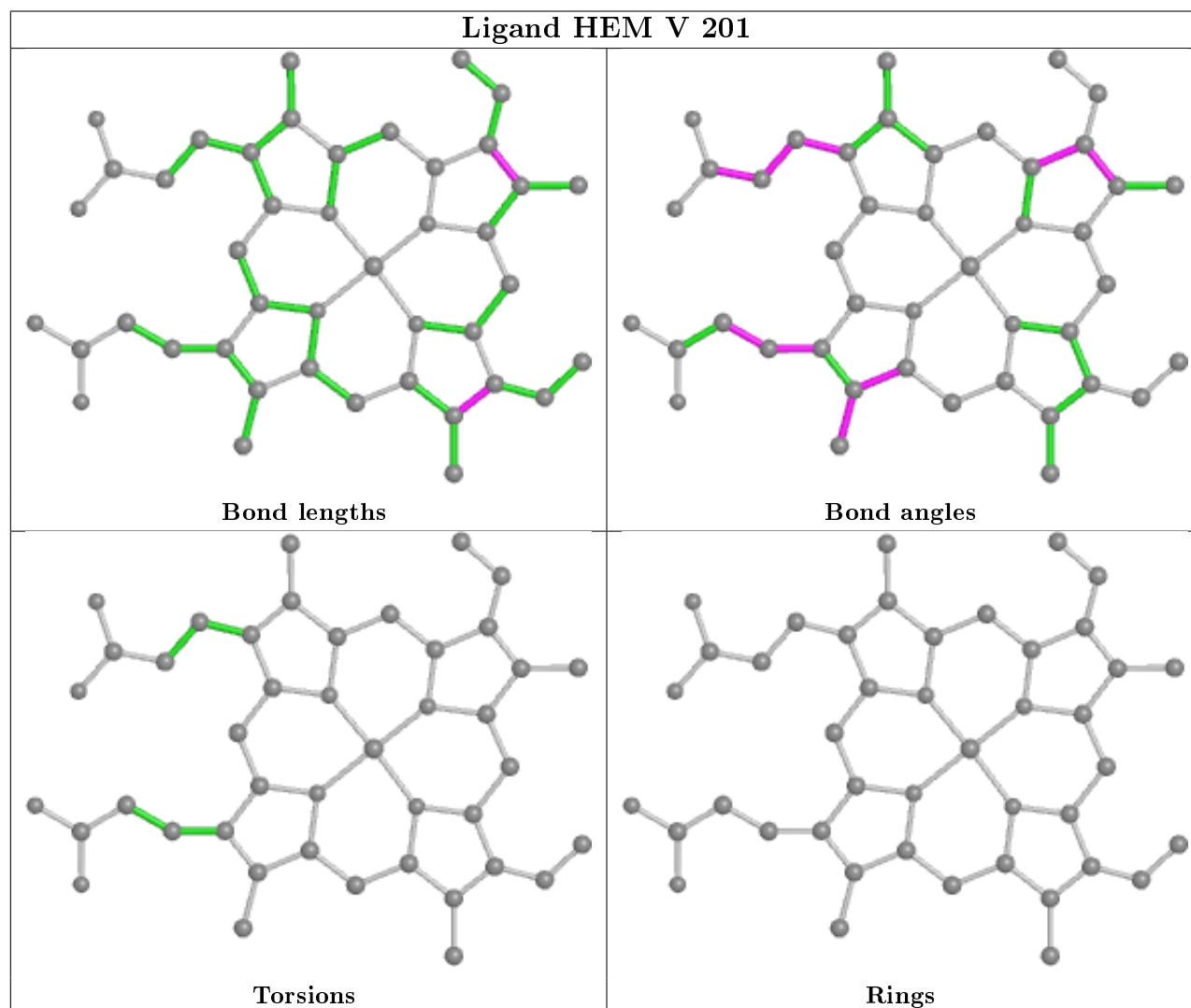
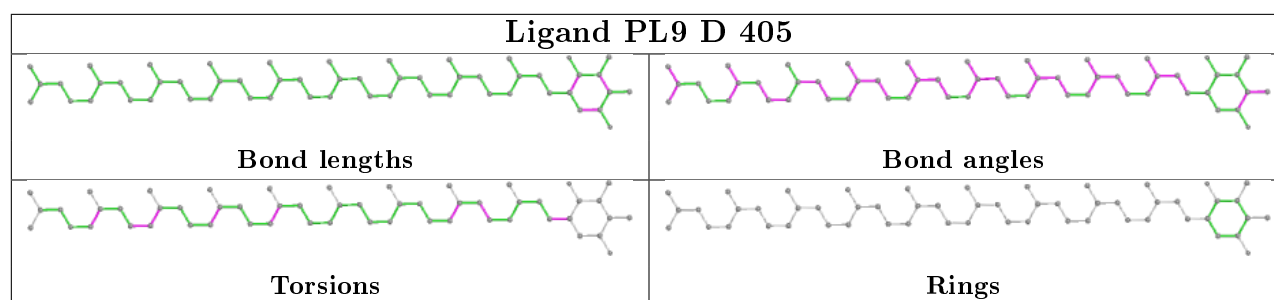


Ligand CLA b 610

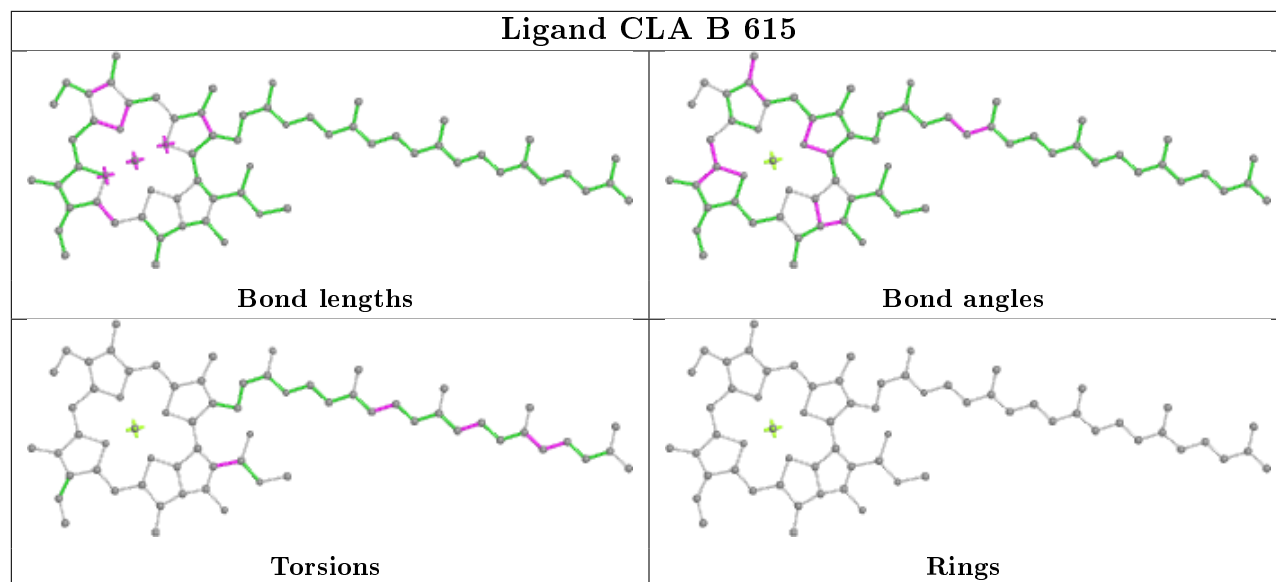


Ligand LFA B 624

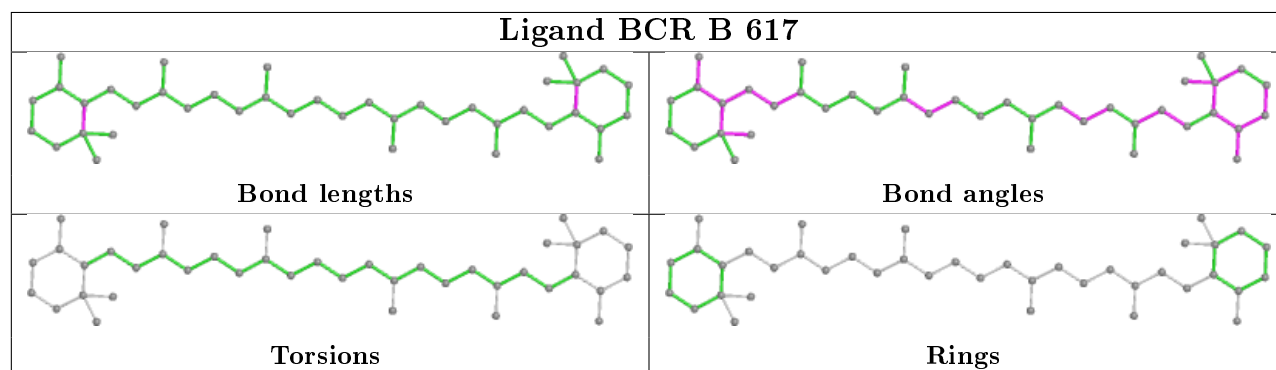




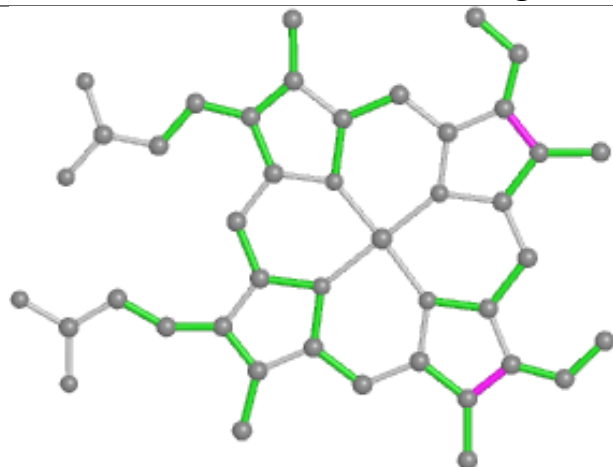
Ligand CLA B 615



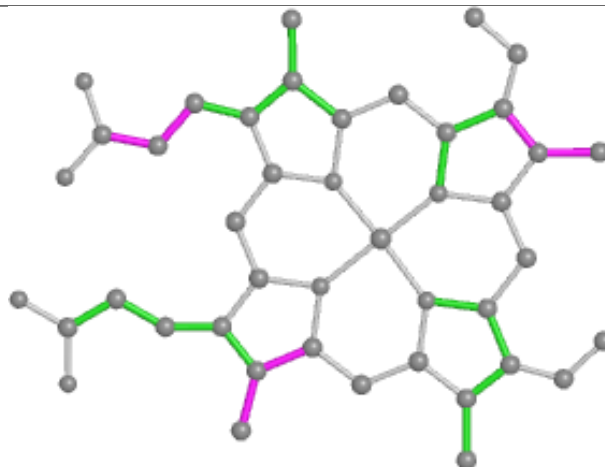
Ligand BCR B 617



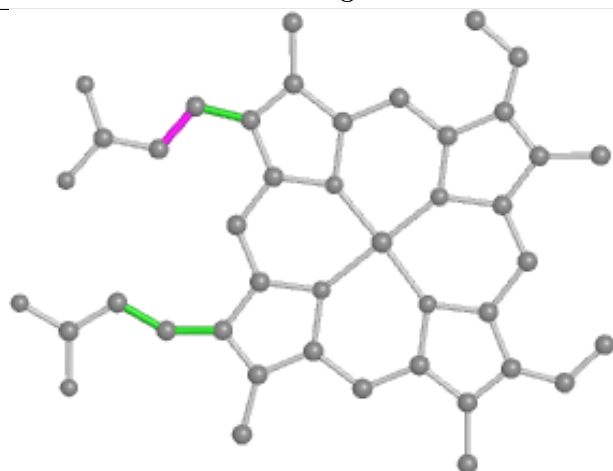
Ligand HEM e 102



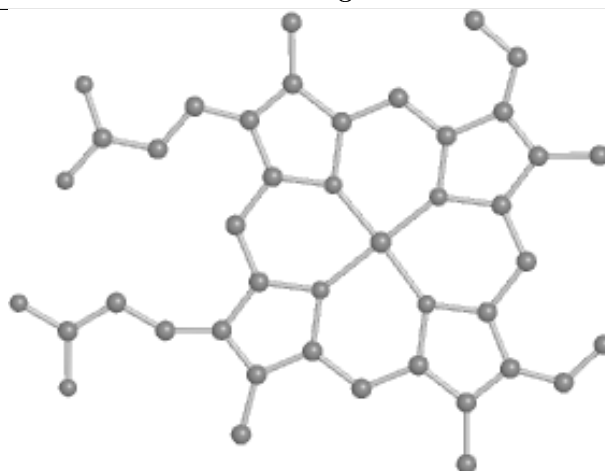
Bond lengths



Bond angles

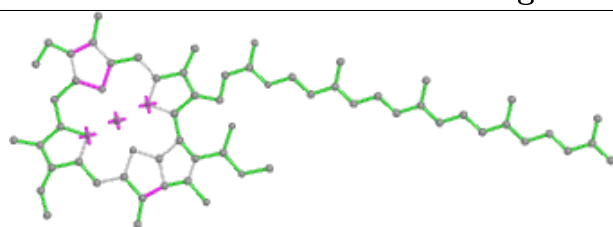


Torsions

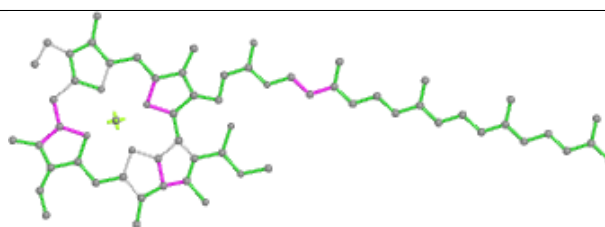


Rings

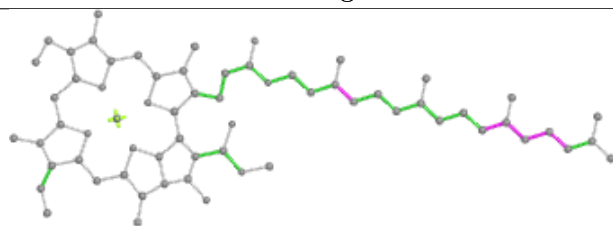
Ligand CLA b 613



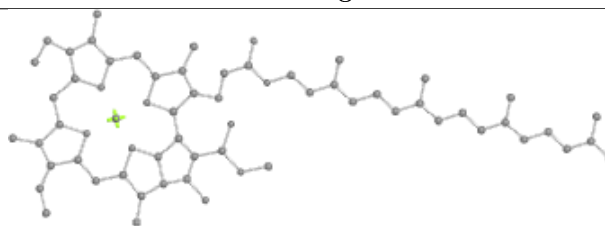
Bond lengths



Bond angles

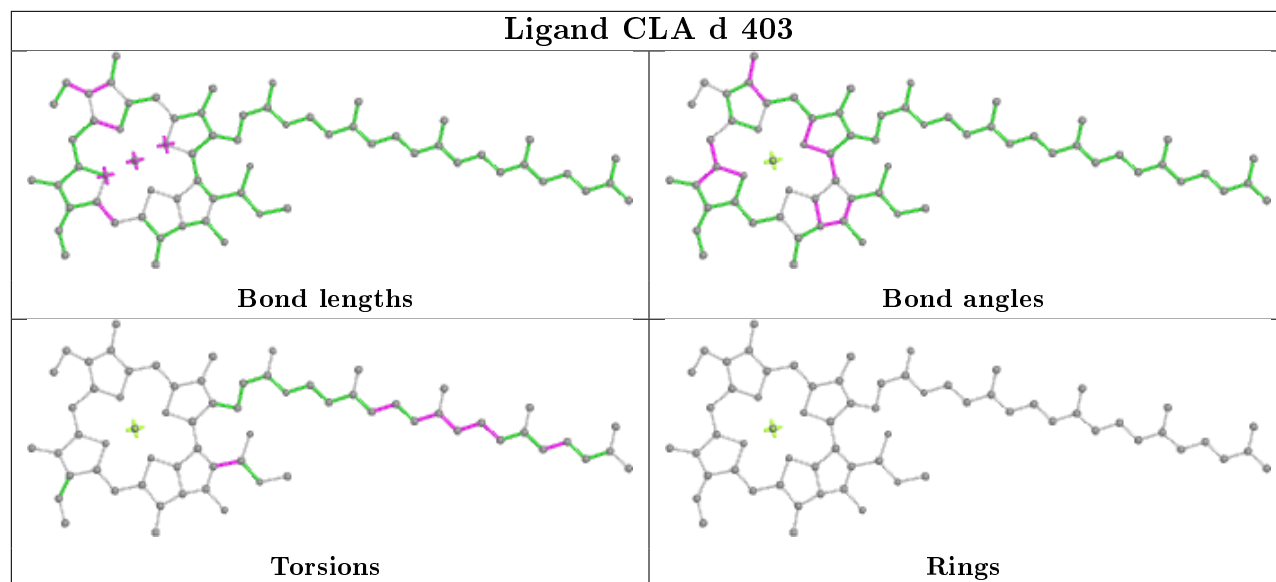


Torsions

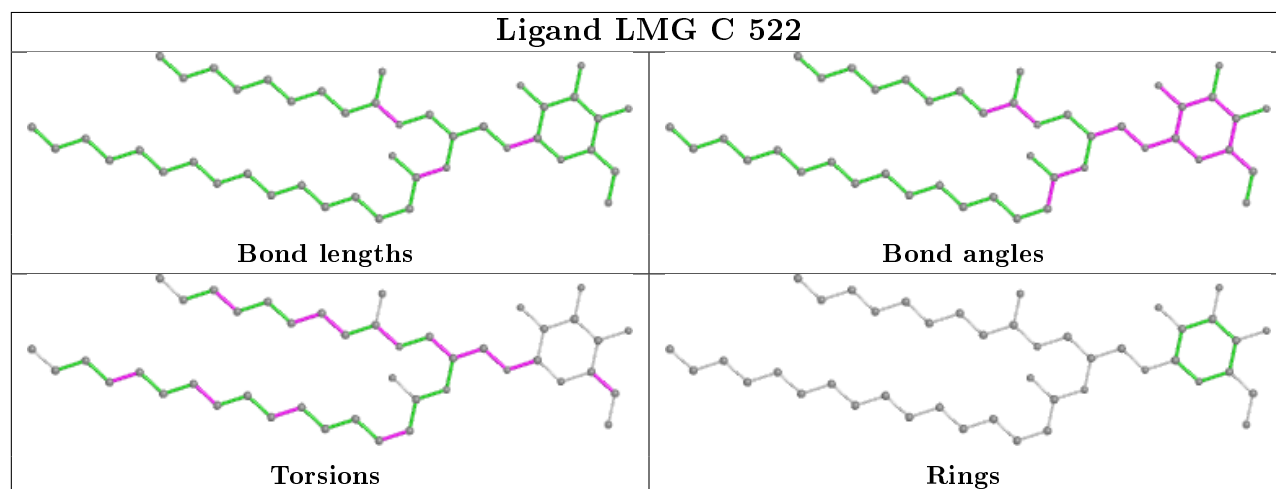


Rings

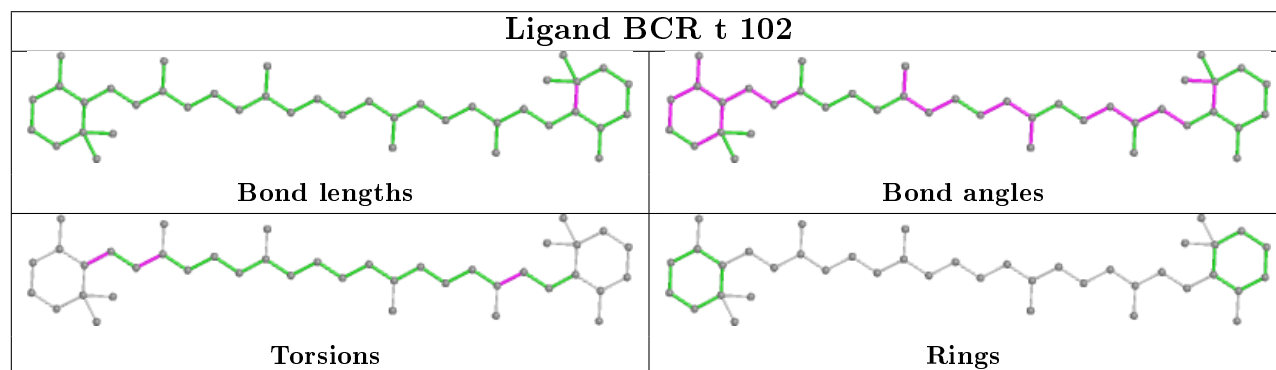
Ligand CLA d 403

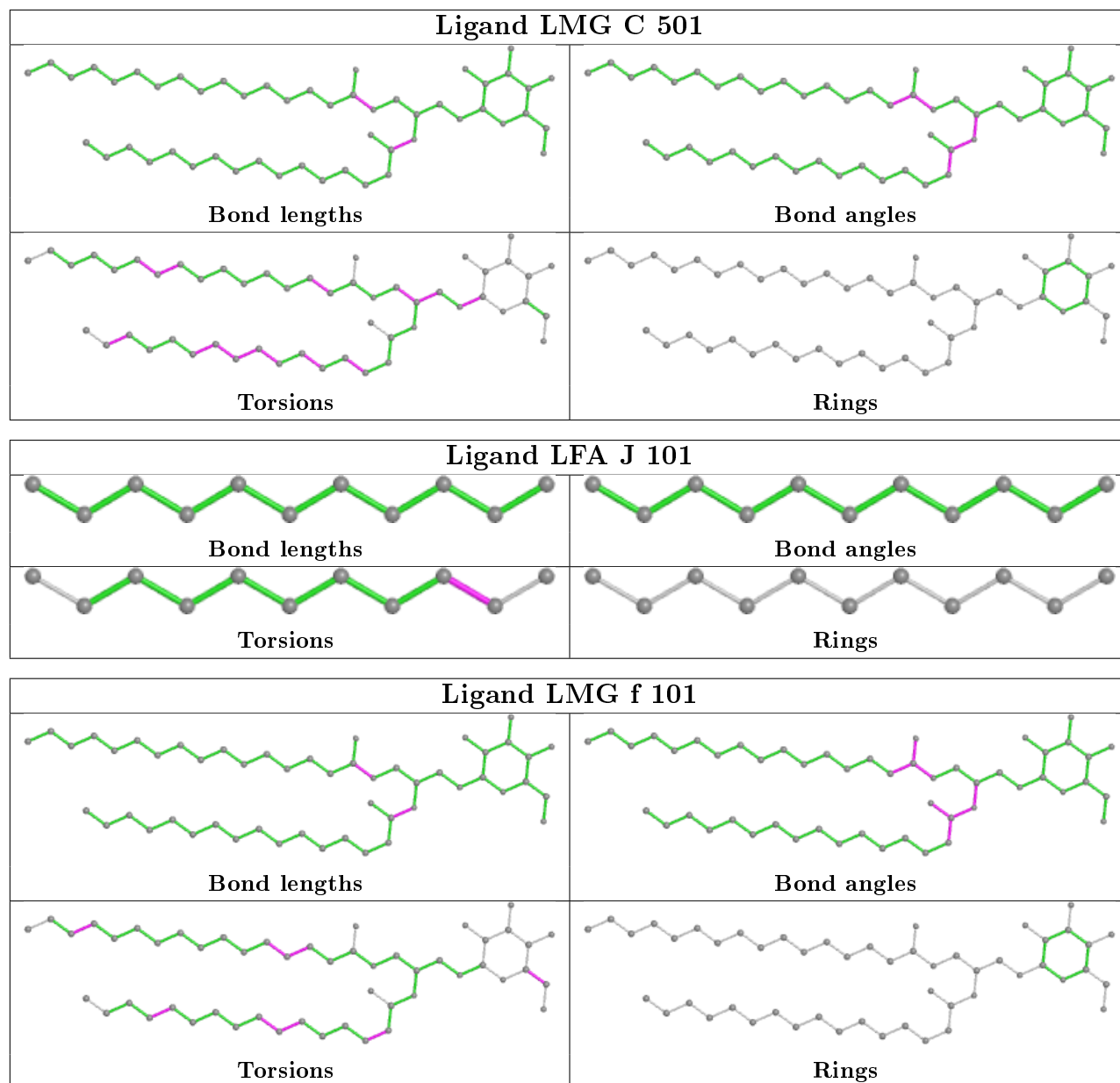


Ligand LMG C 522

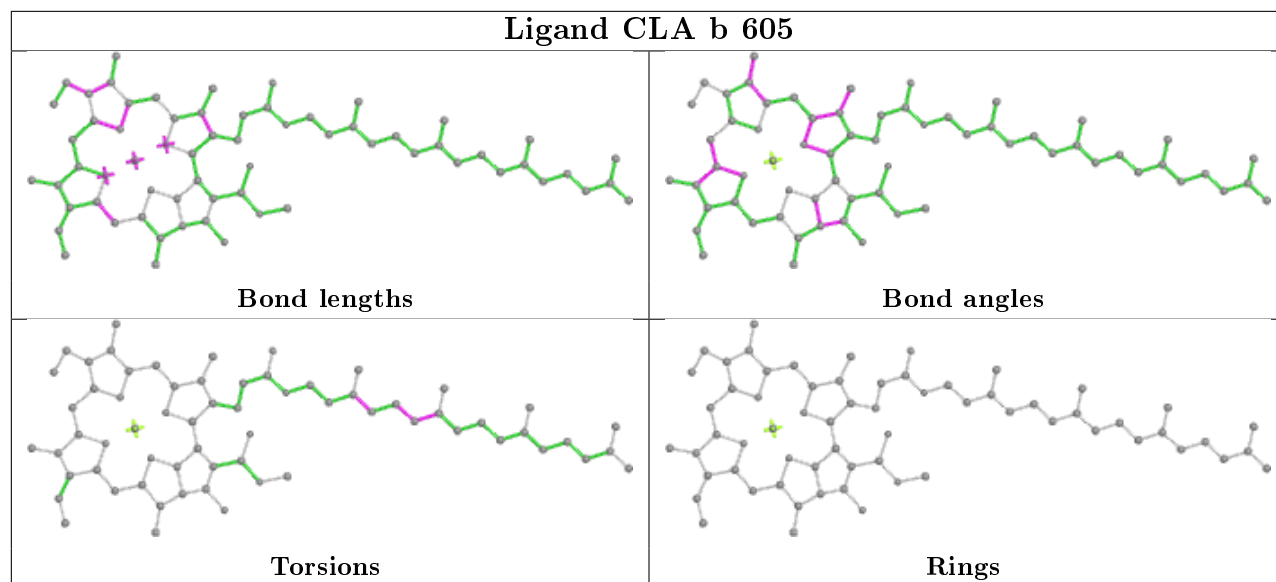


Ligand BCR t 102

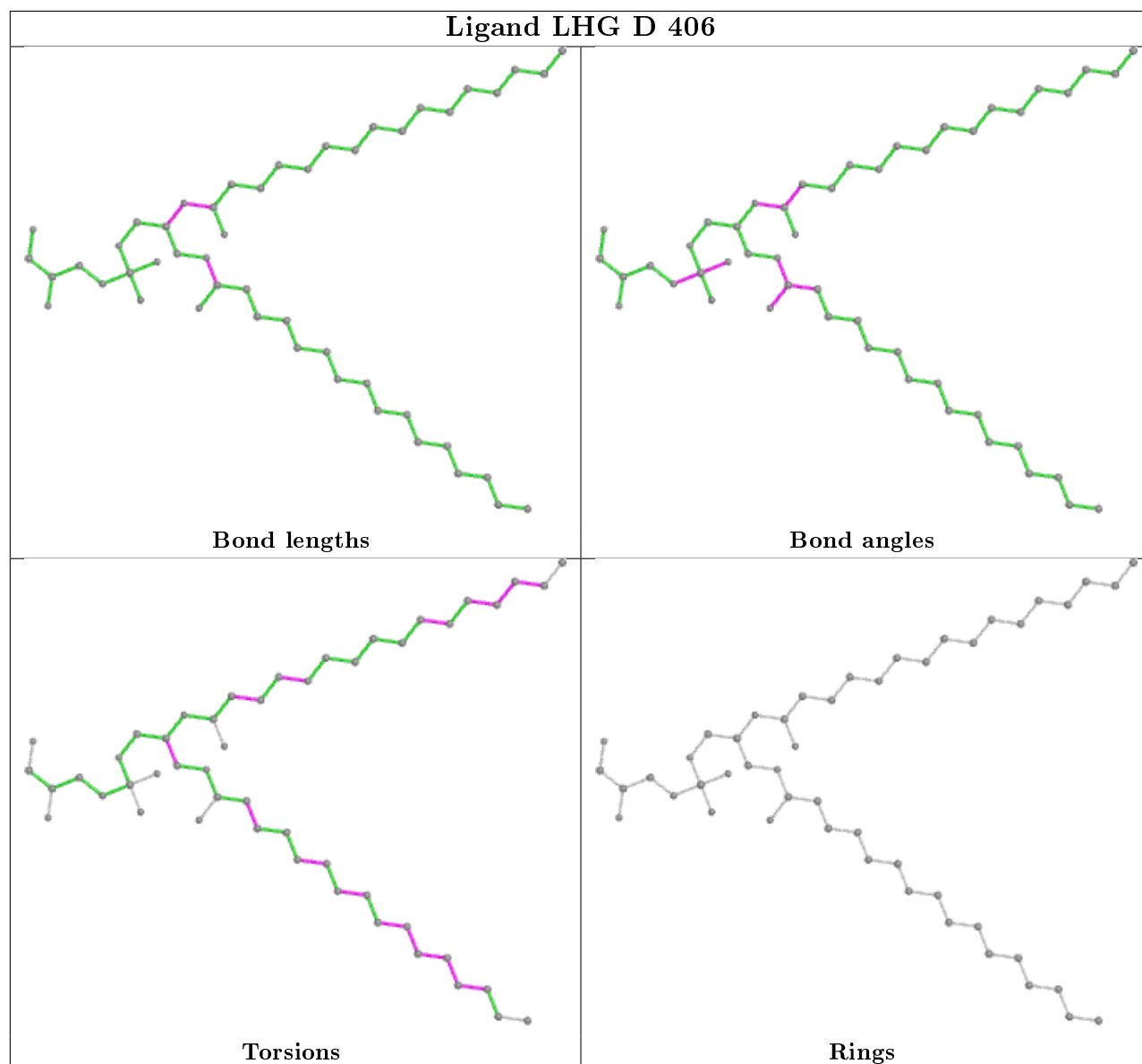


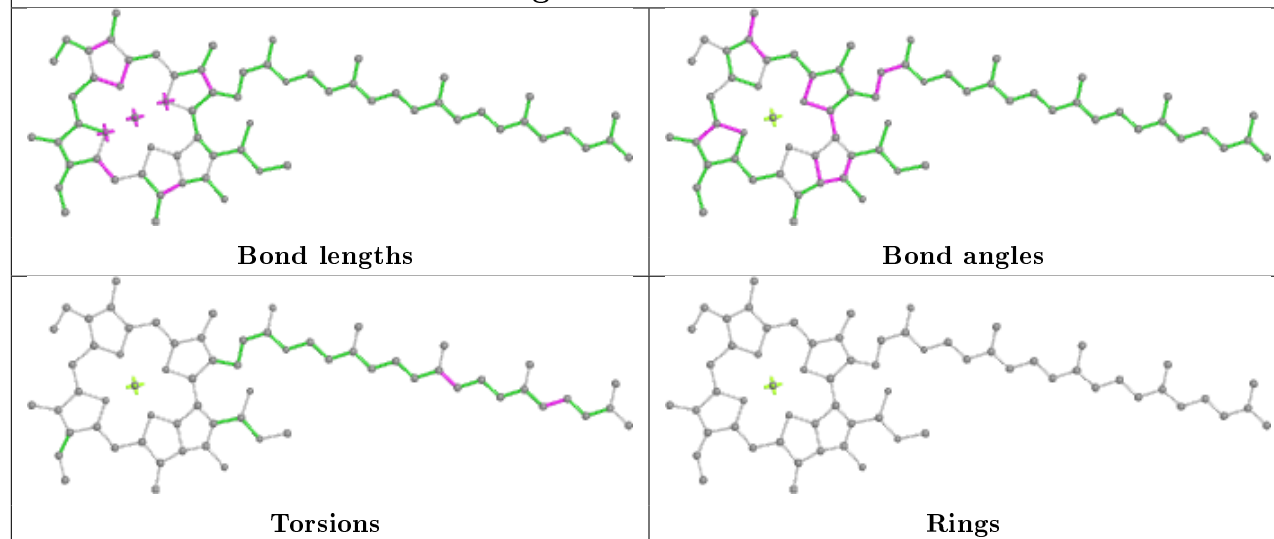
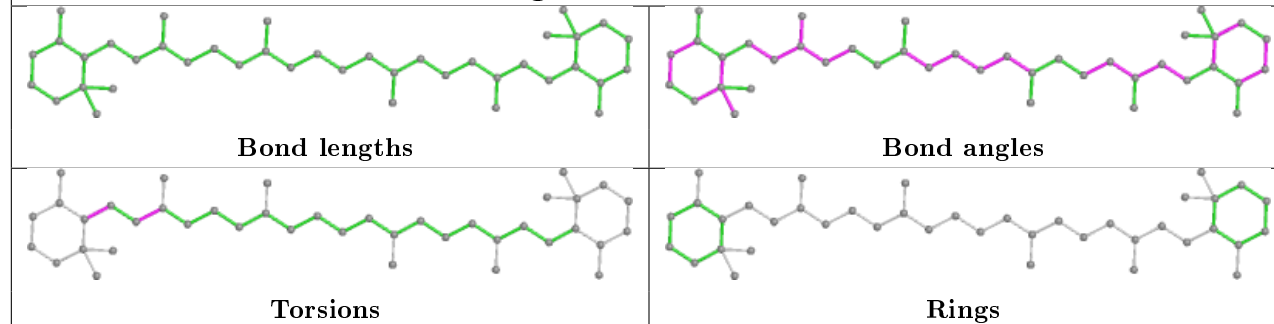
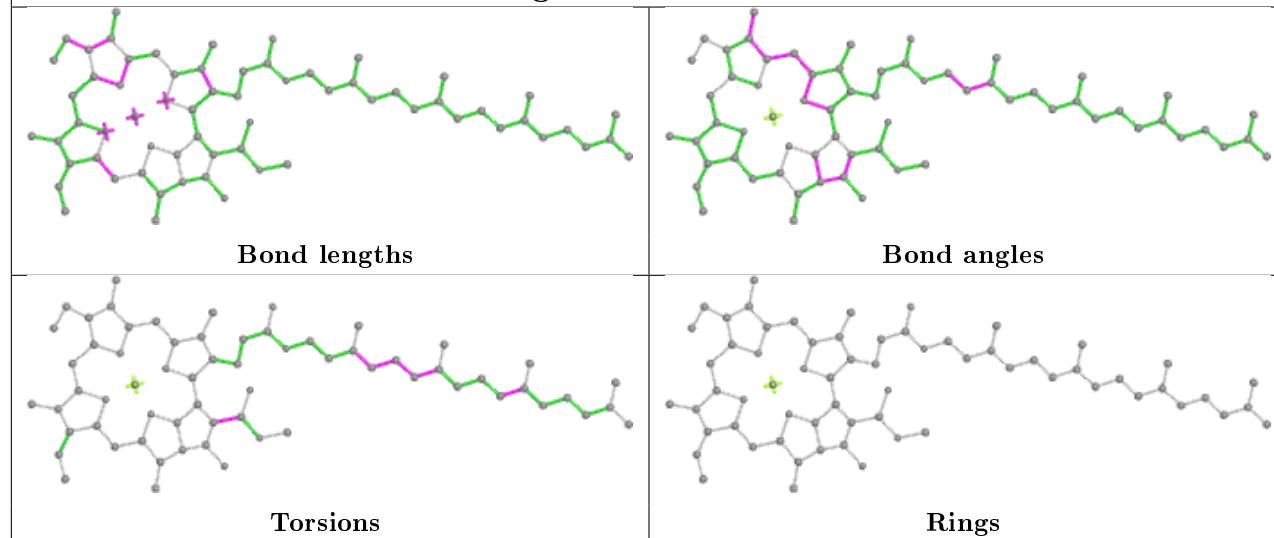


Ligand CLA b 605

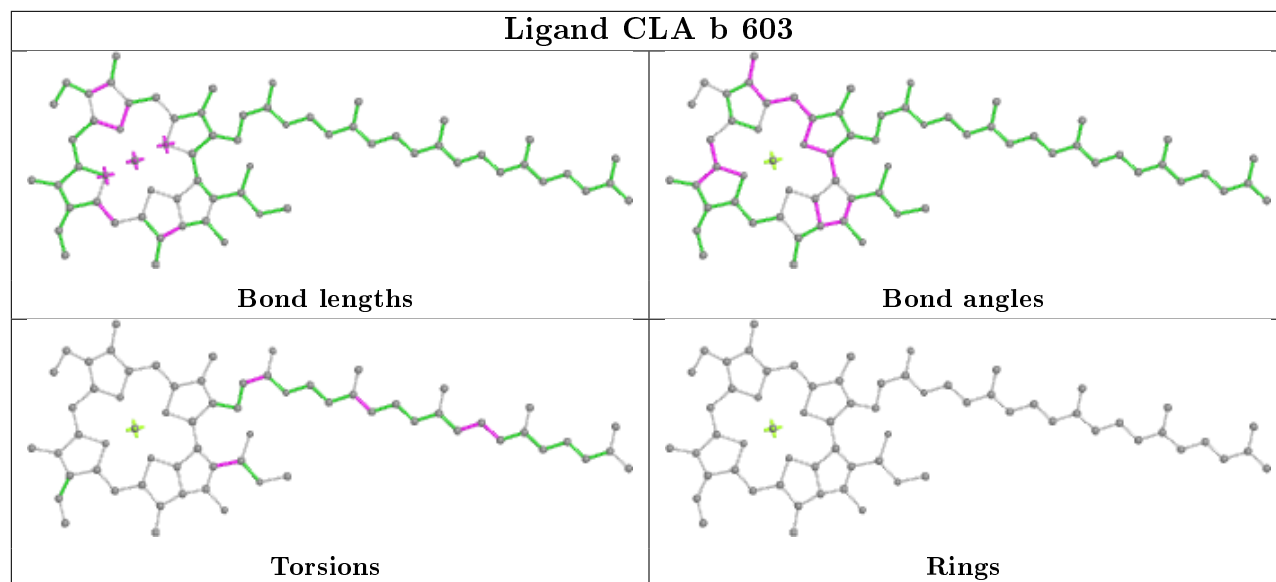


Ligand LHG D 406

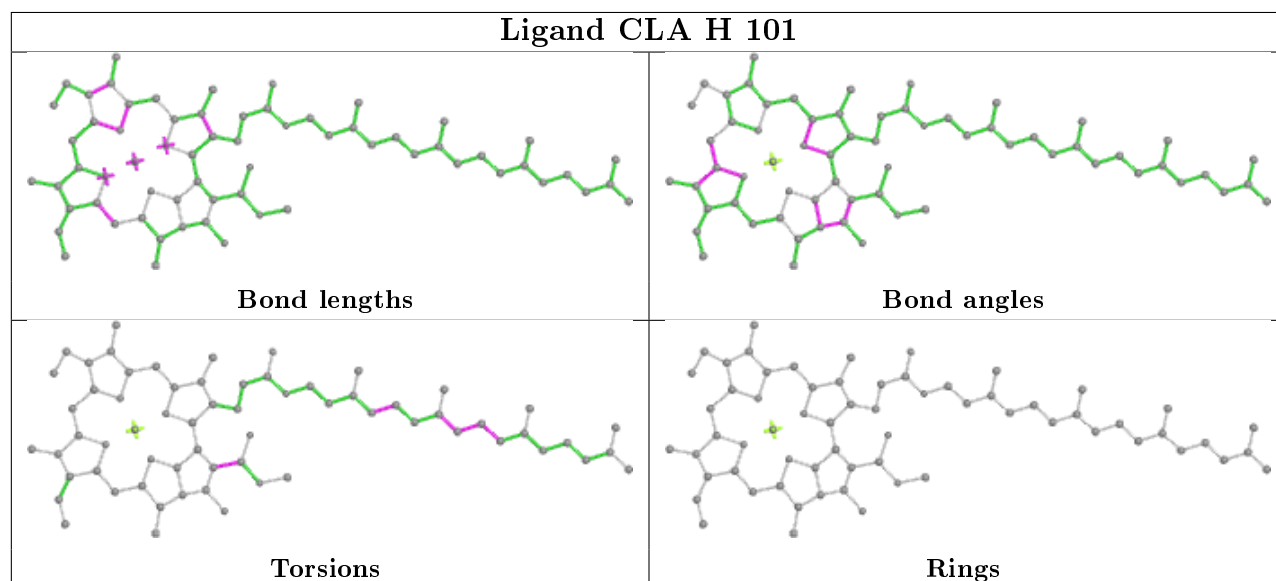


Ligand CLA B 612**Ligand BCR H 102****Ligand CLA B 613**

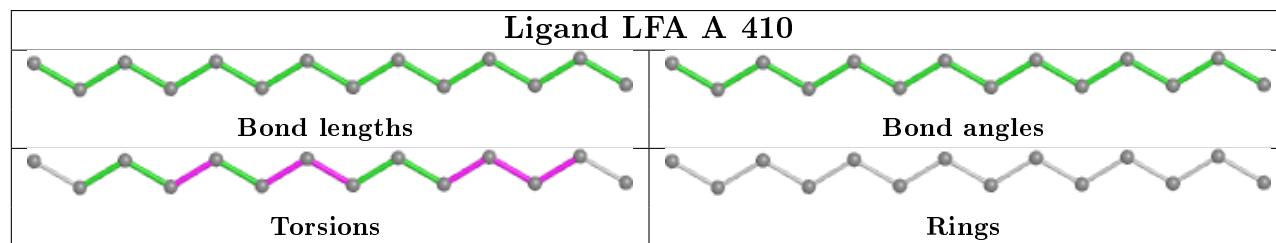
Ligand CLA b 603



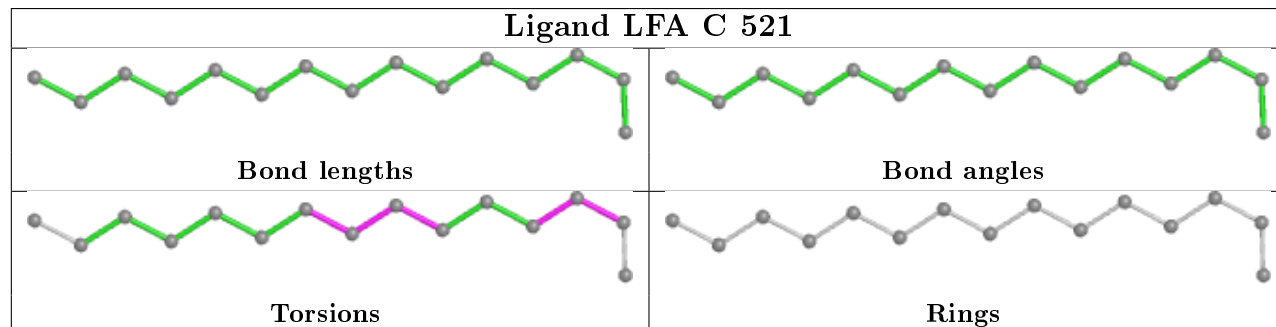
Ligand CLA H 101



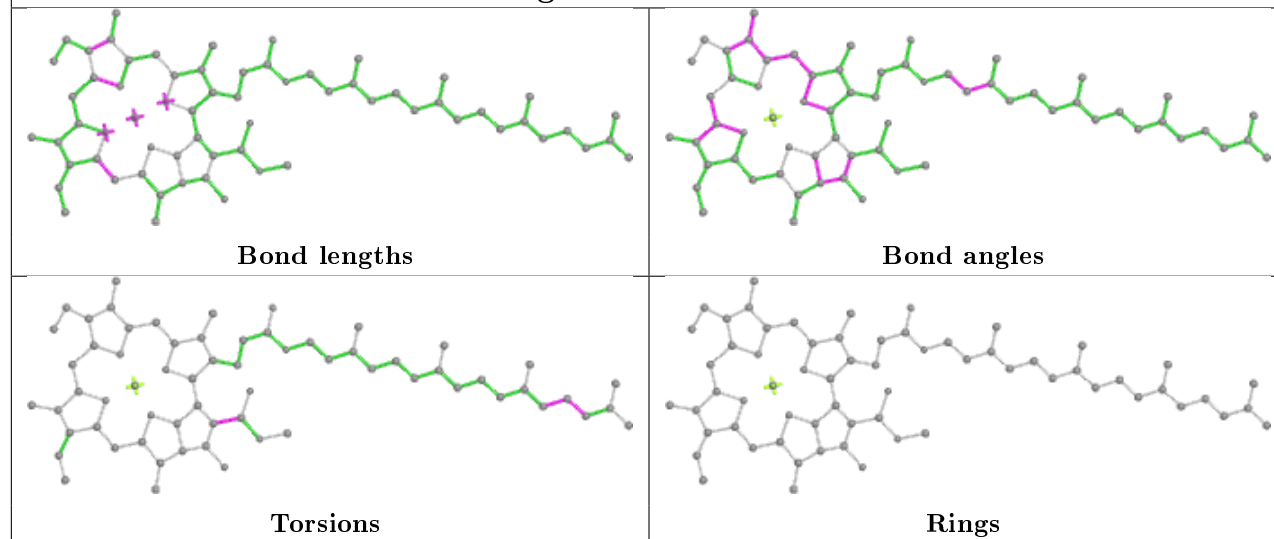
Ligand LFA A 410



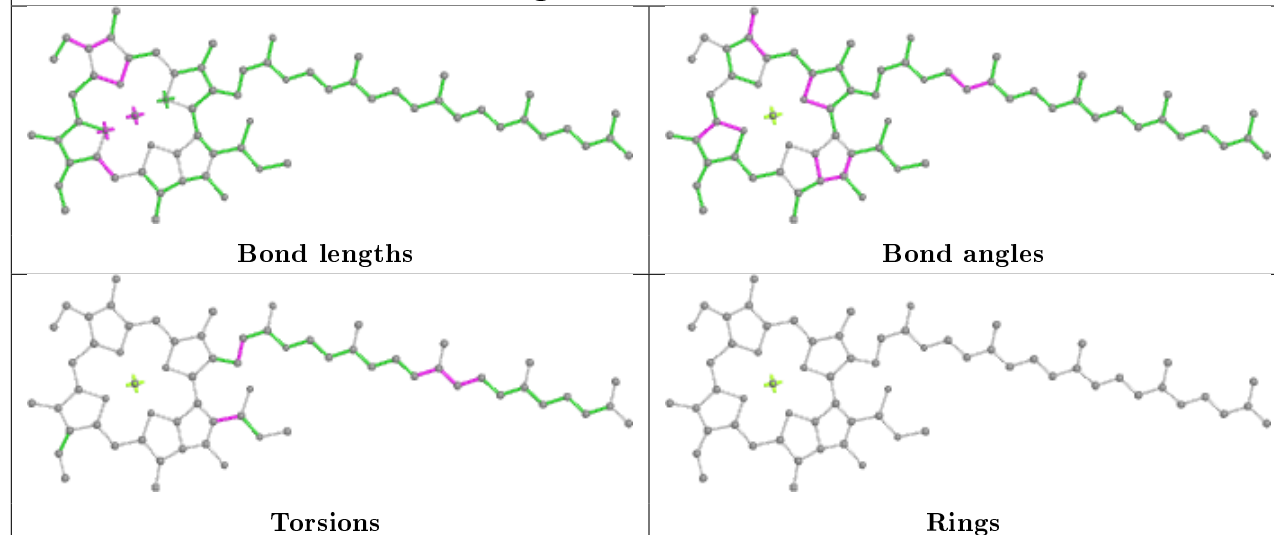
Ligand LFA C 521



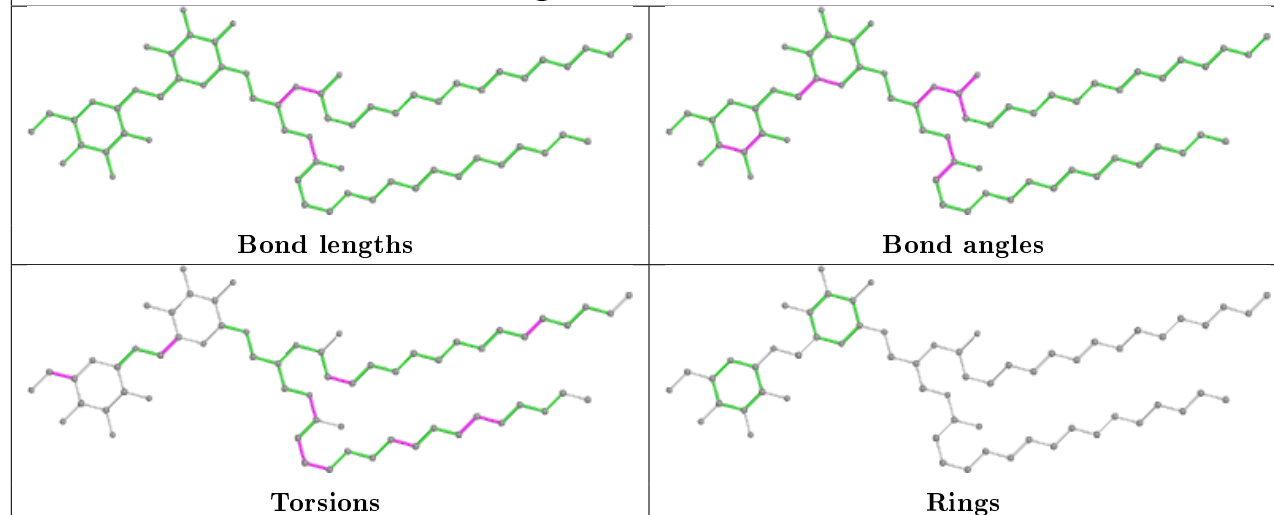
Ligand CLA c 505

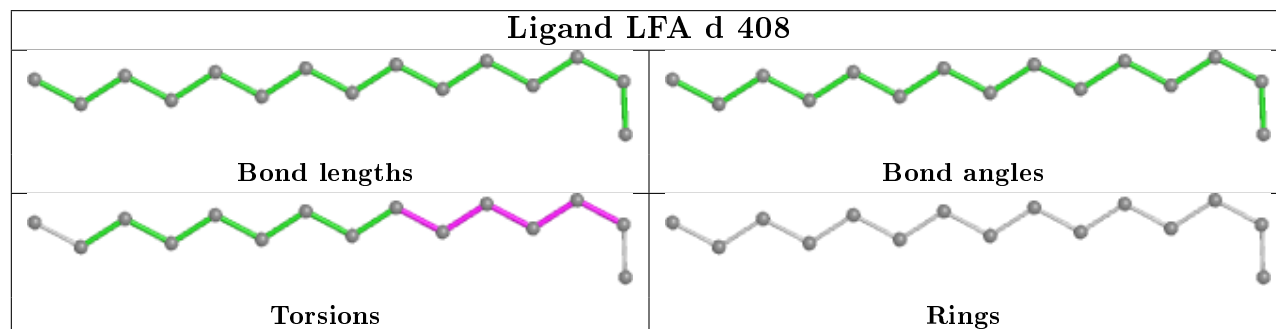
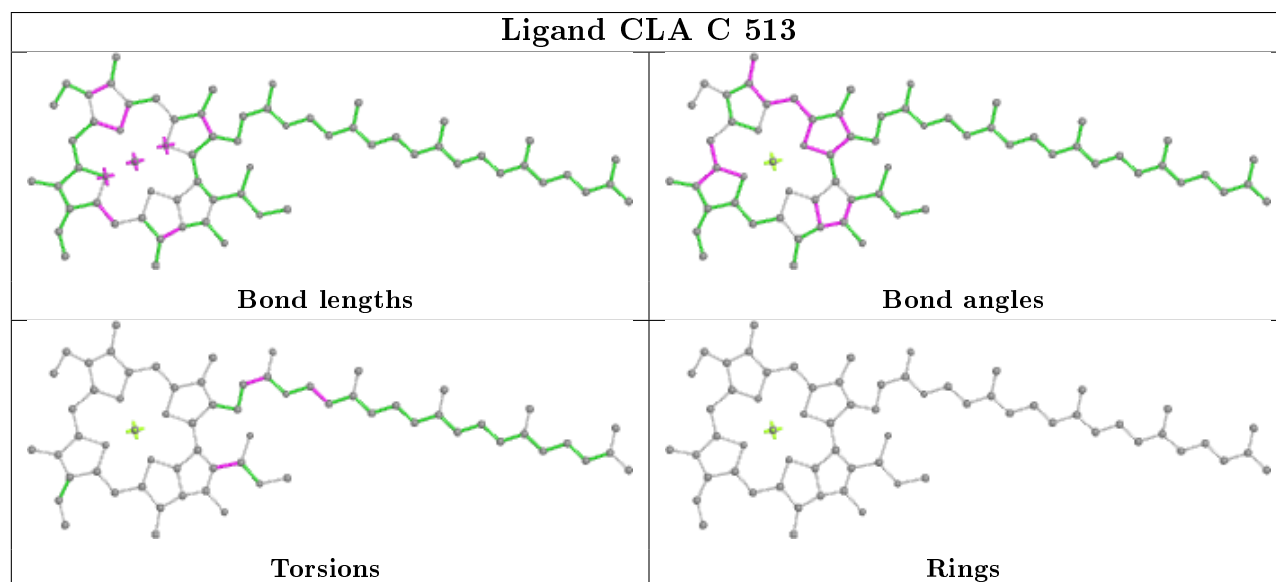
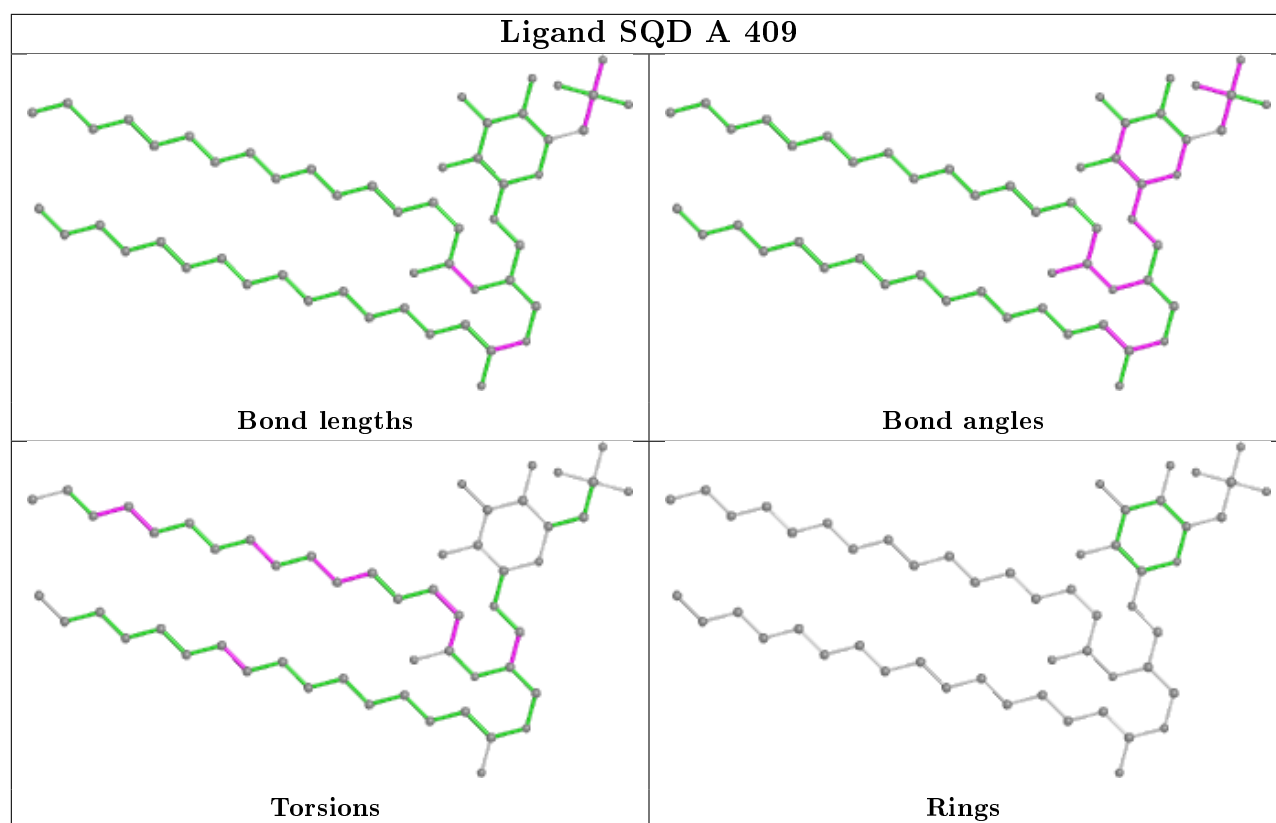


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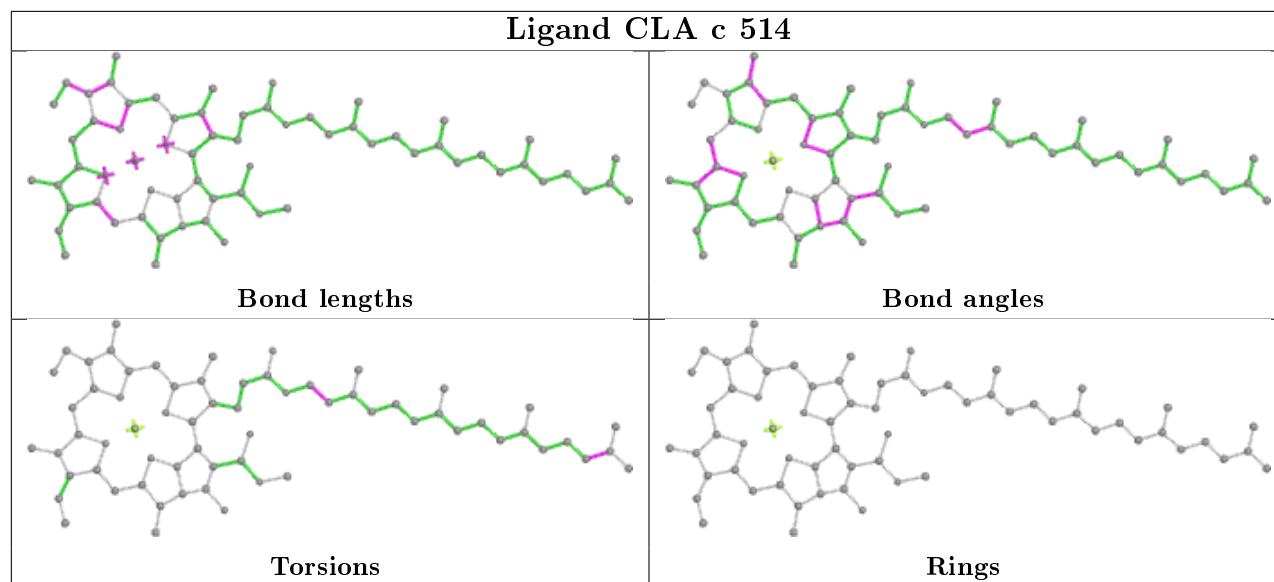


Ligand DGD c 516

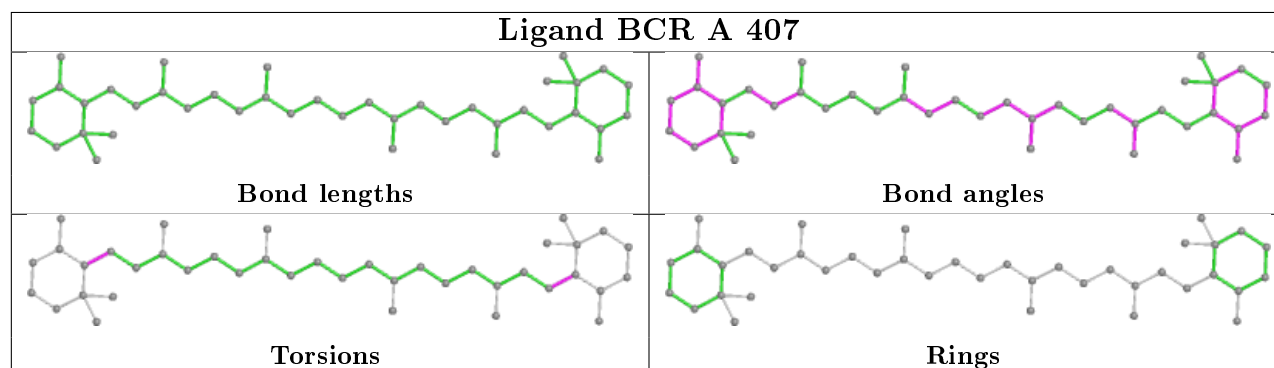




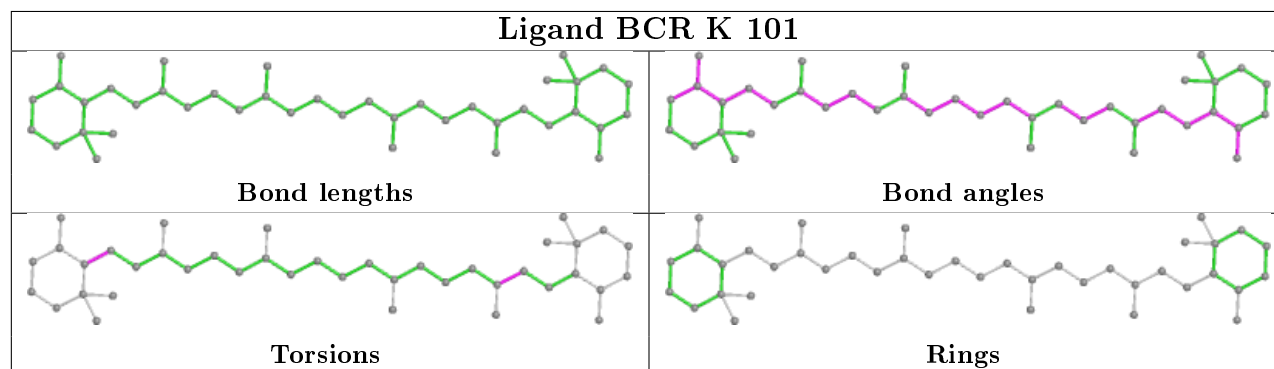
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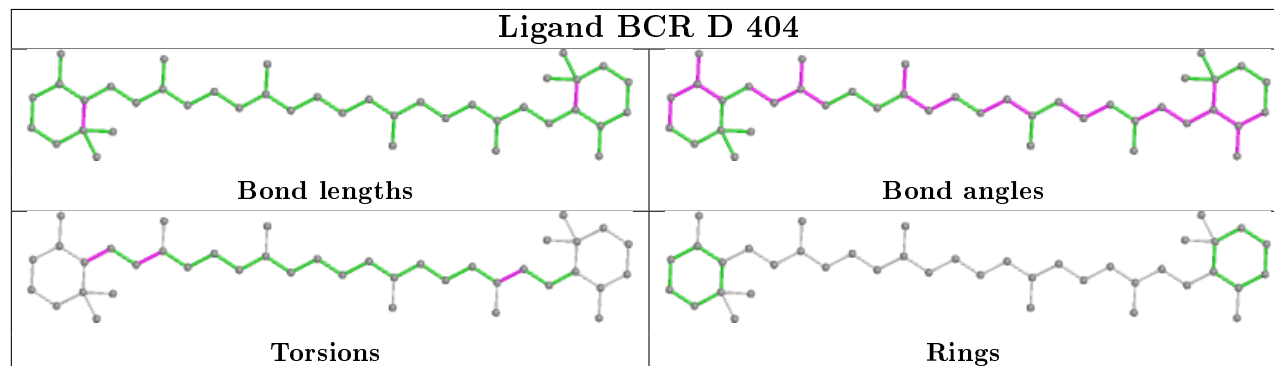
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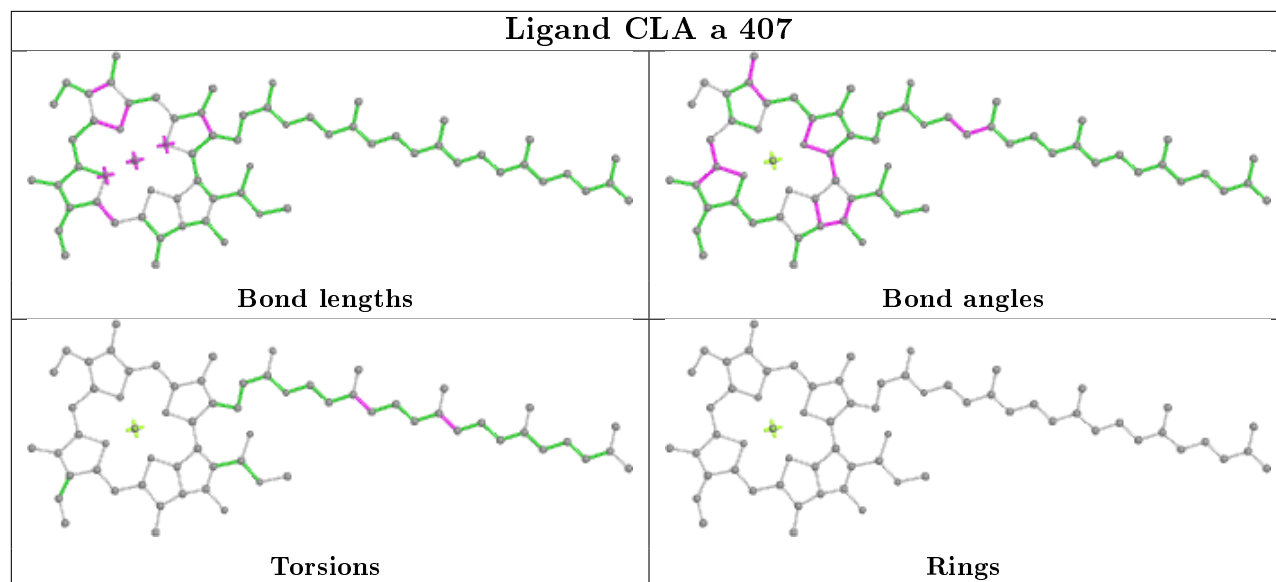
Ligand BCR K 101



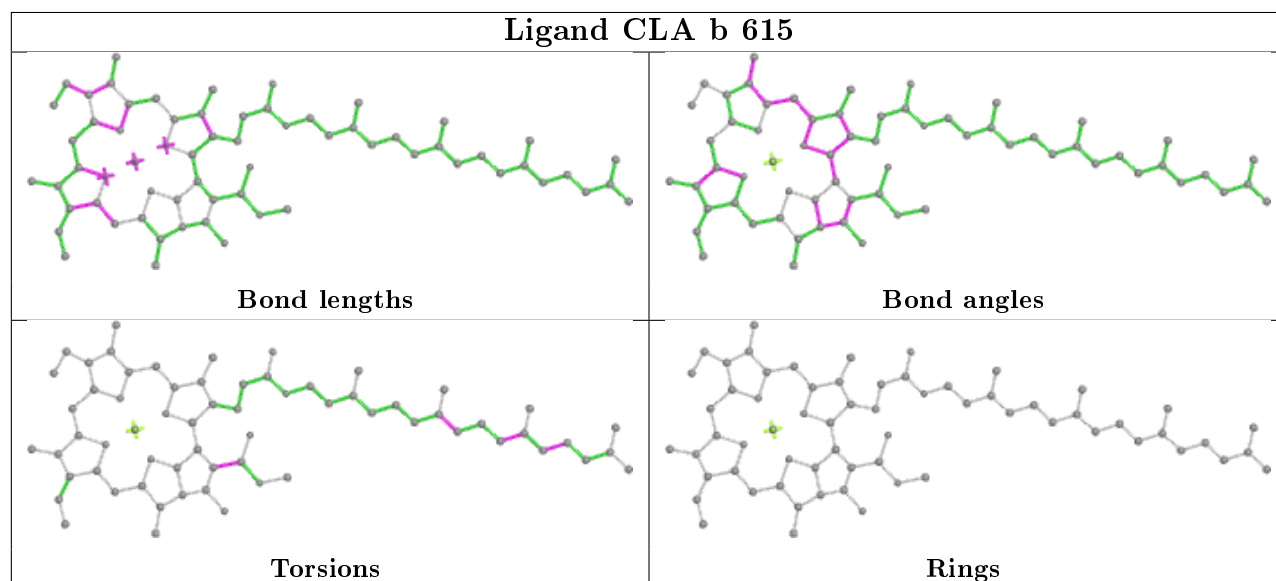
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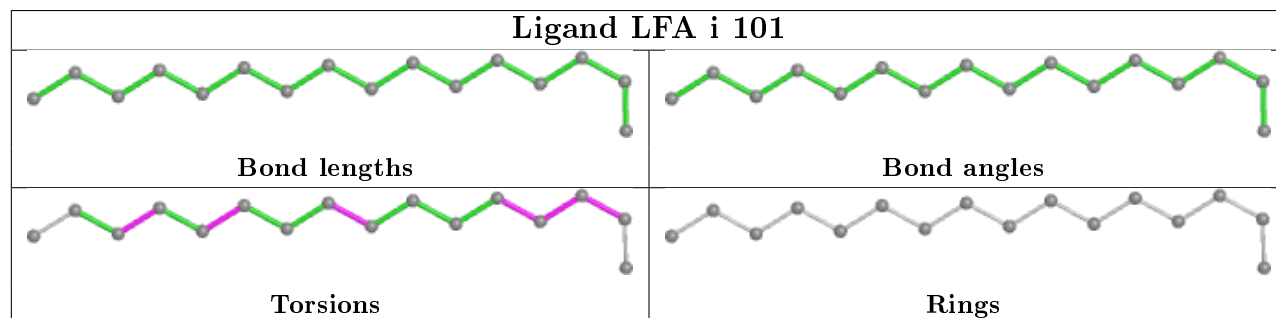
Ligand CLA a 407

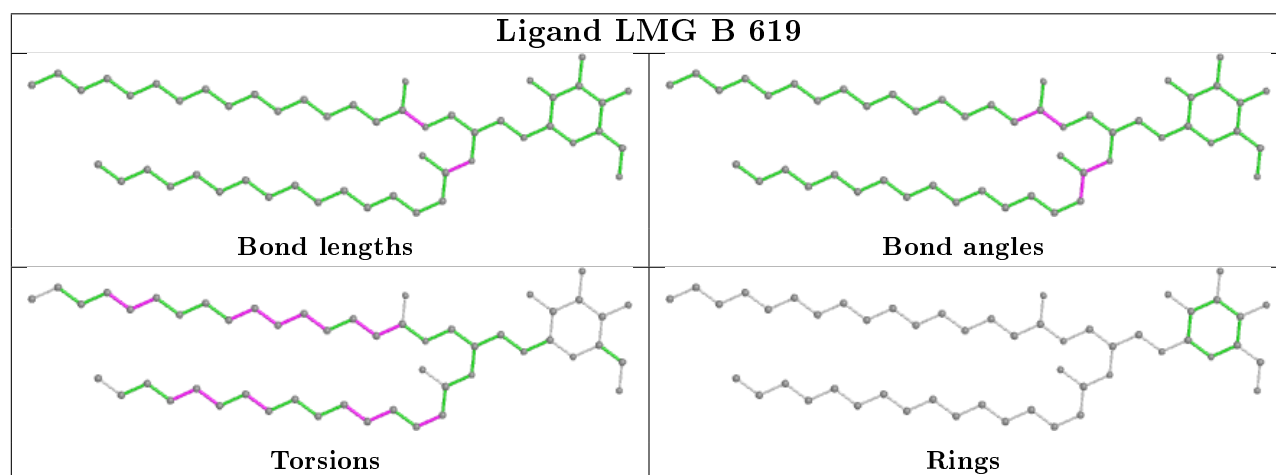
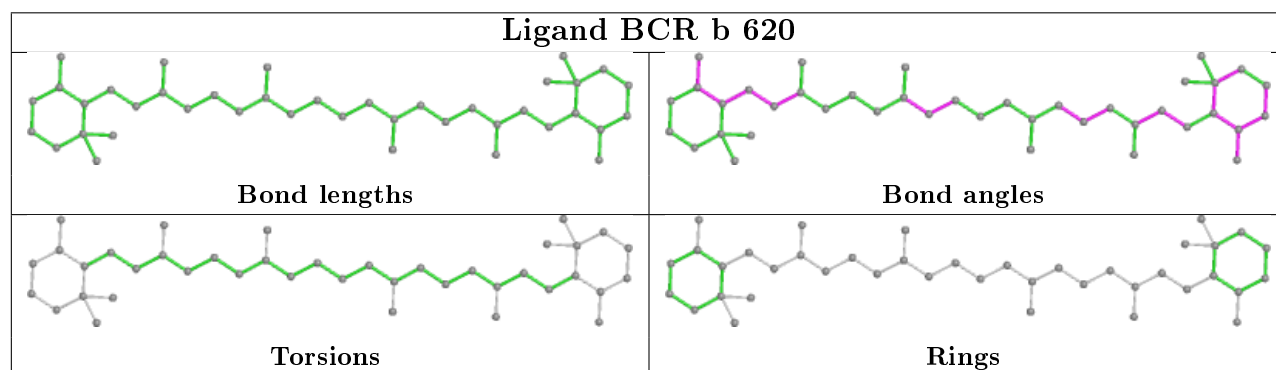
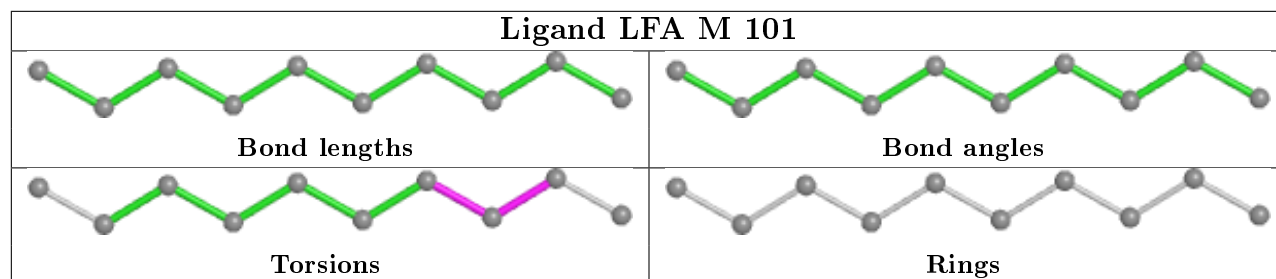
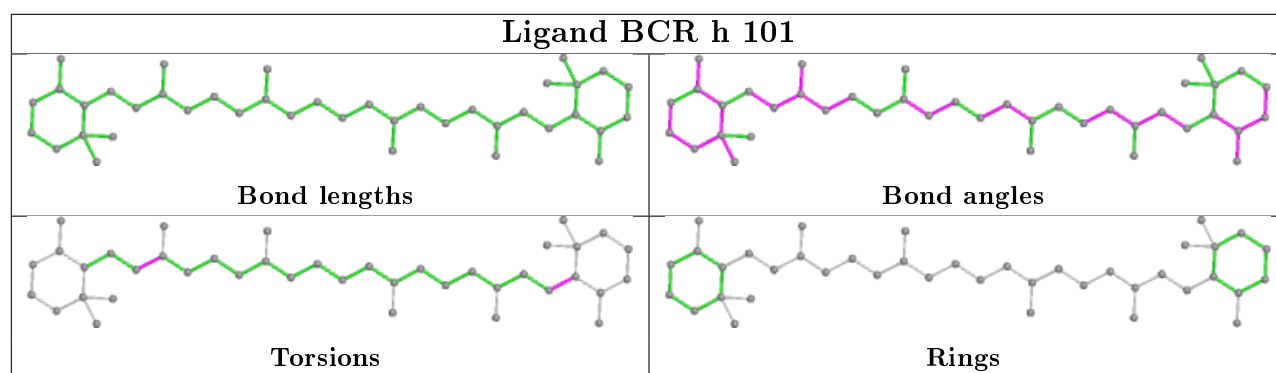


Ligand CLA b 615

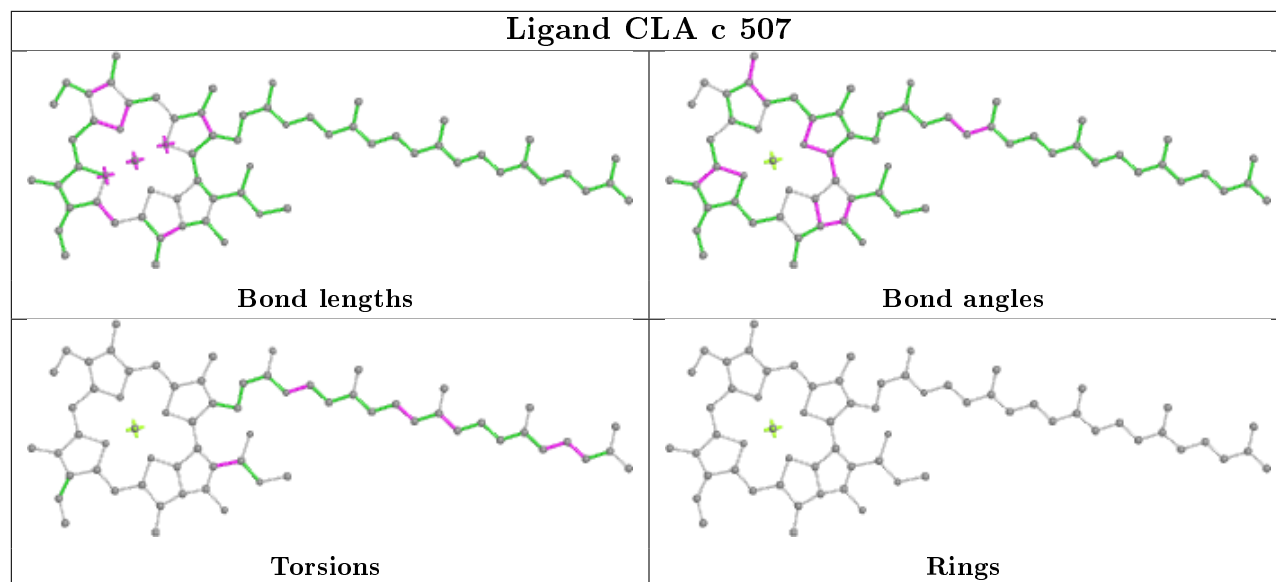


Ligand LFA i 101

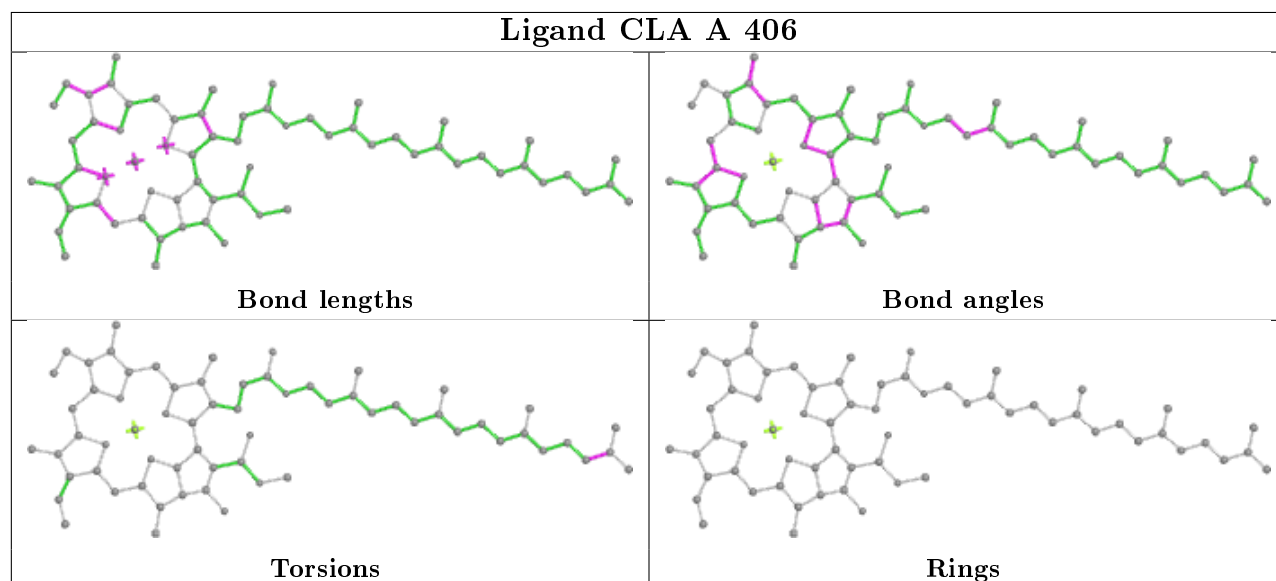




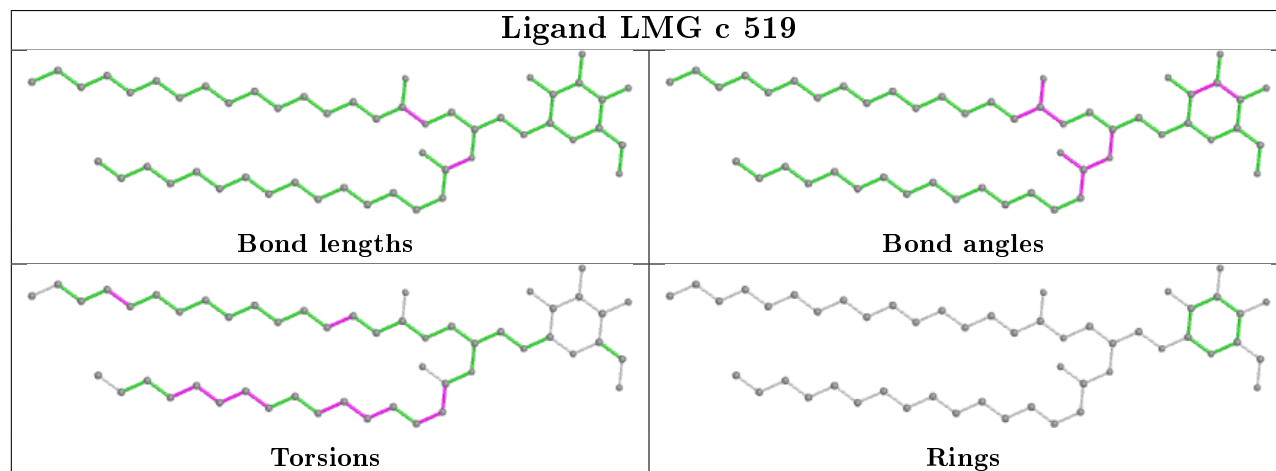
Ligand CLA c 507



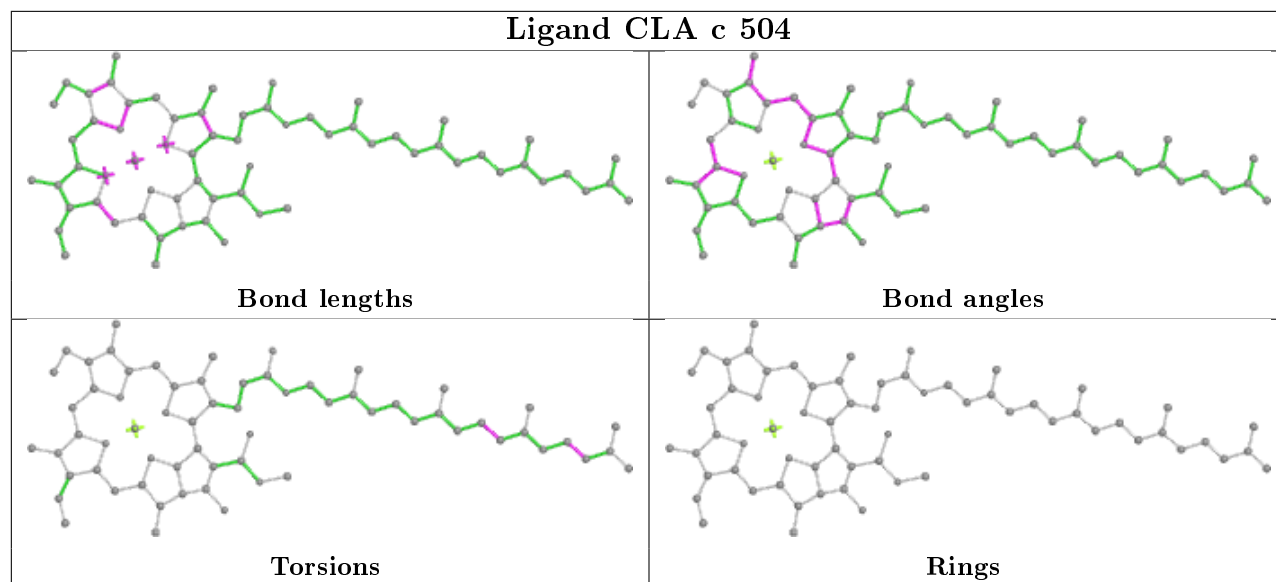
Ligand CLA A 406



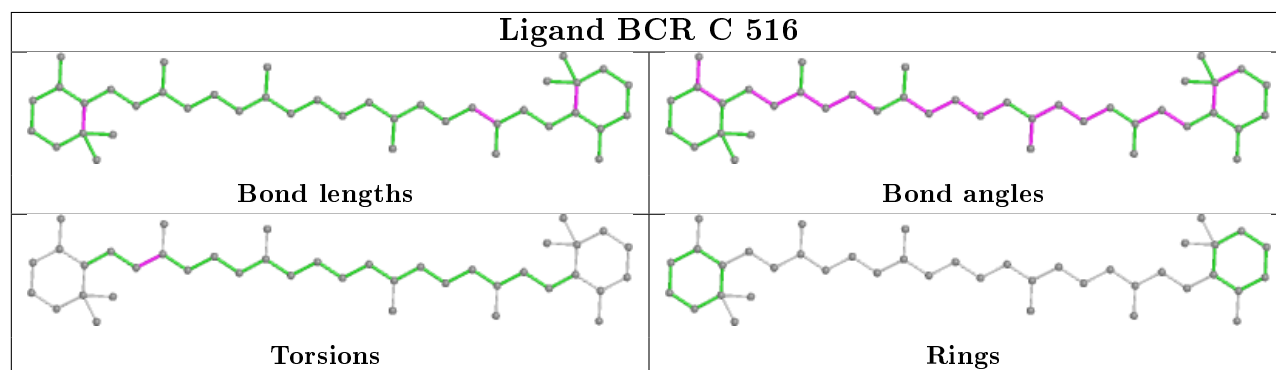
Ligand LMG c 519



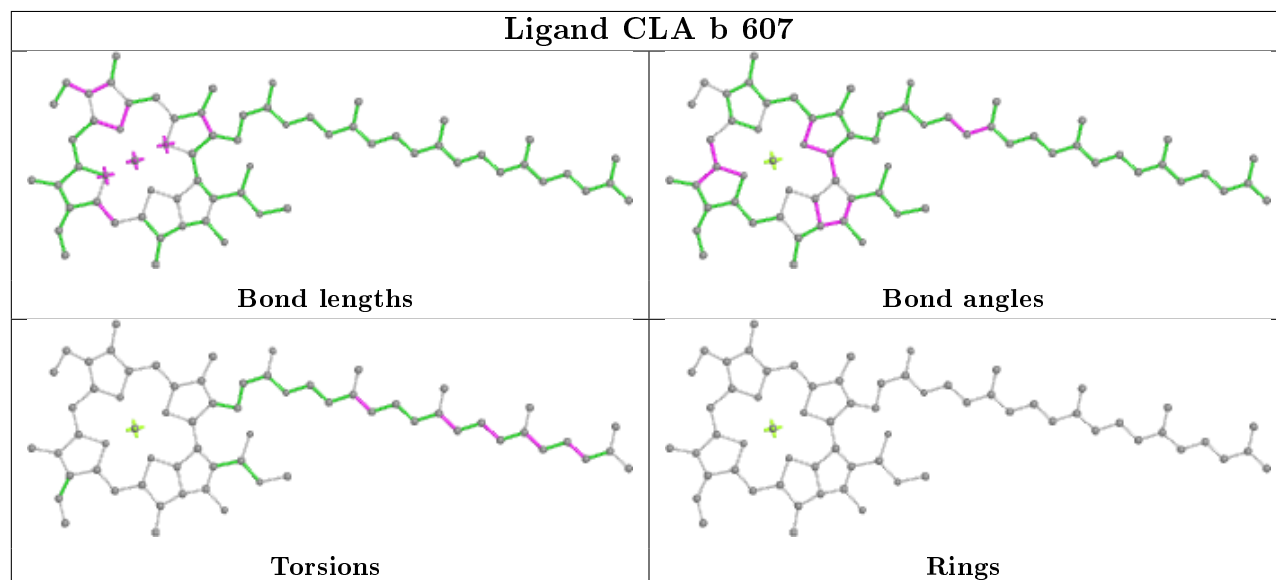
Ligand CLA c 504



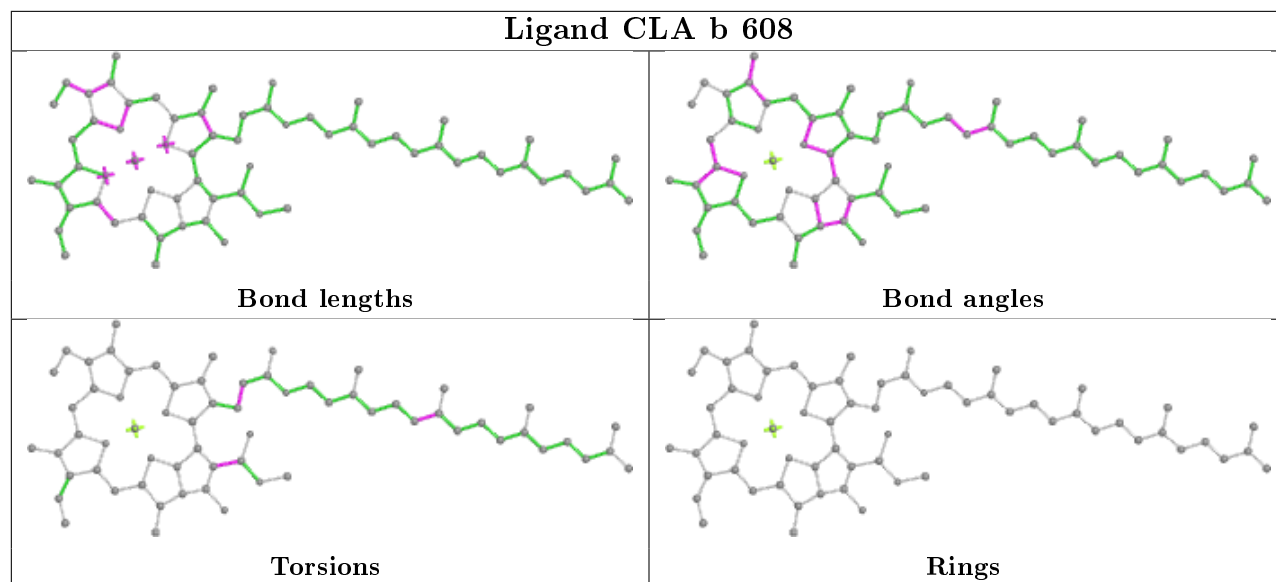
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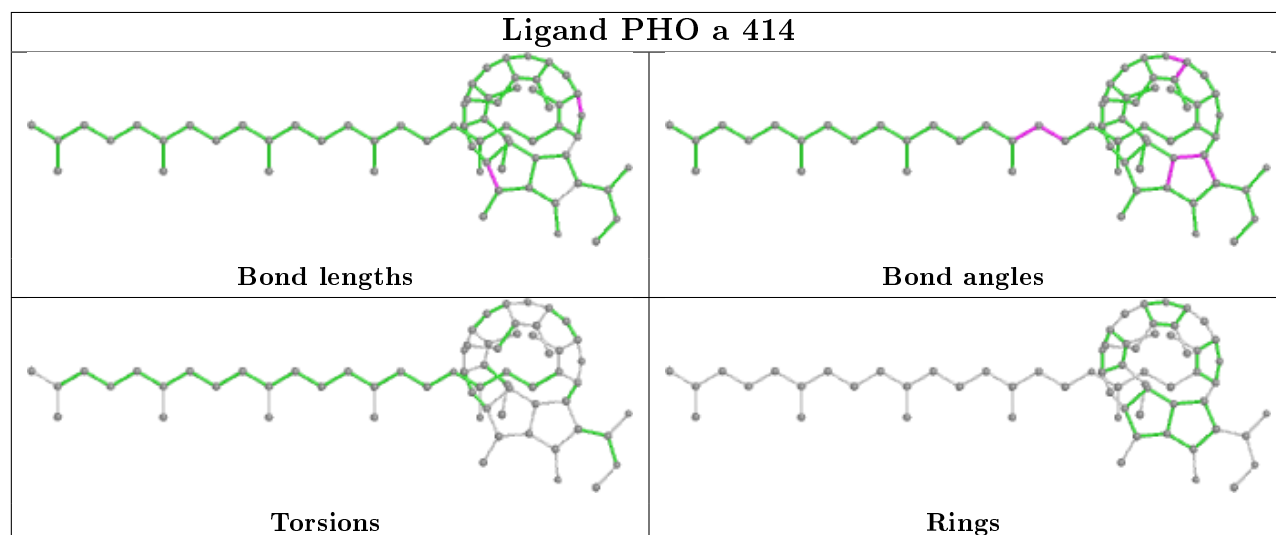
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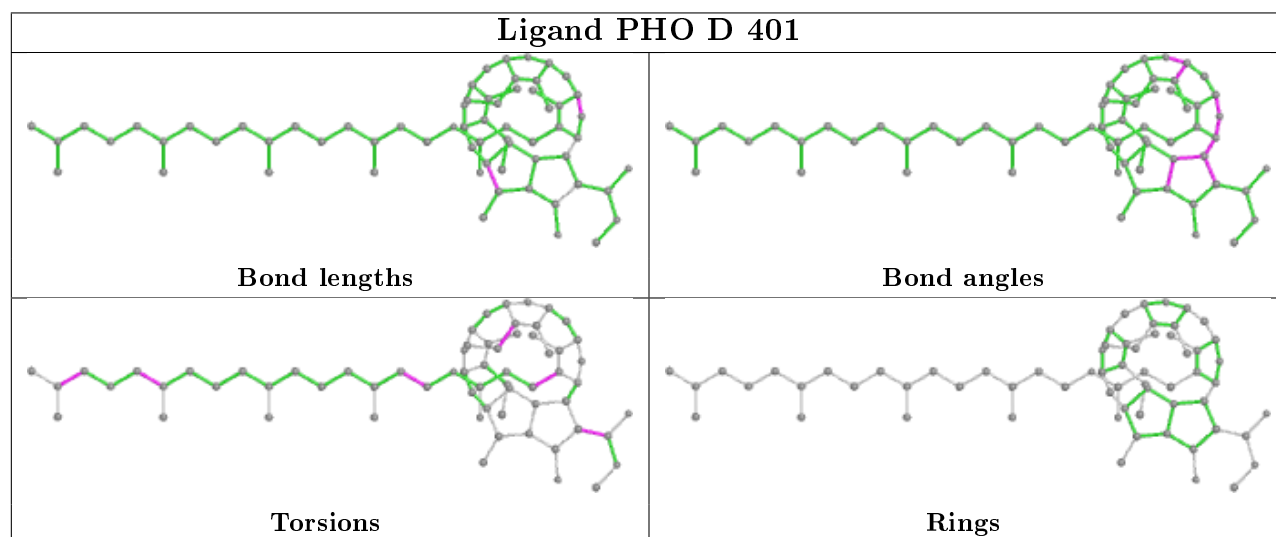
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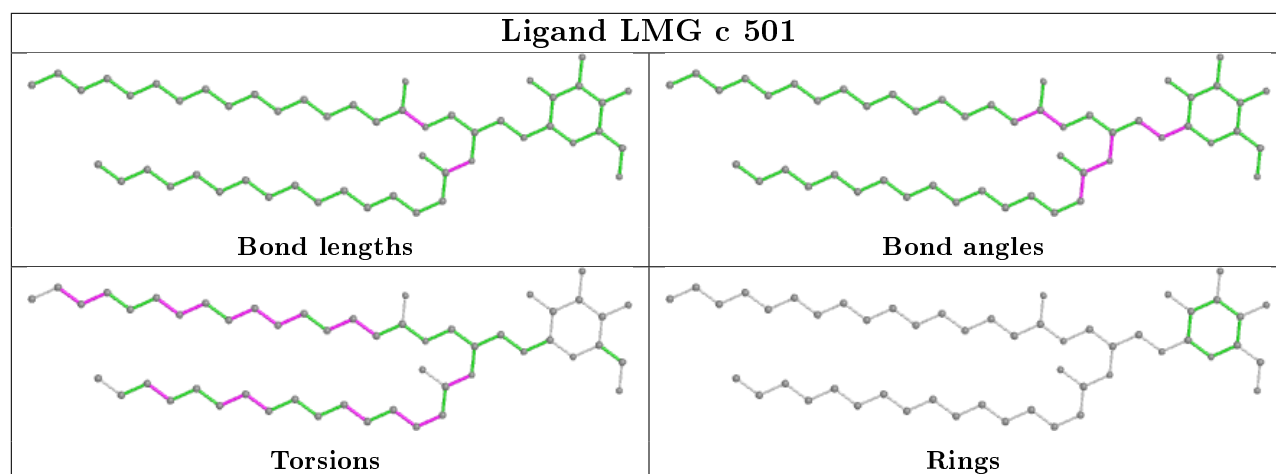
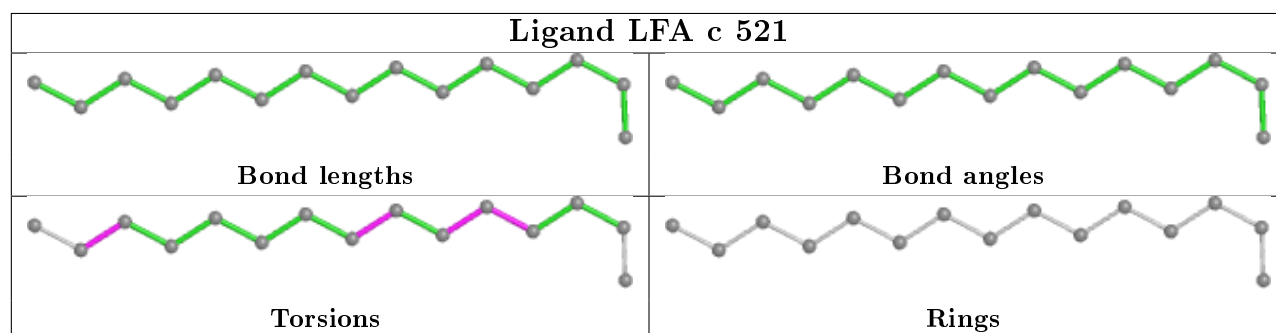
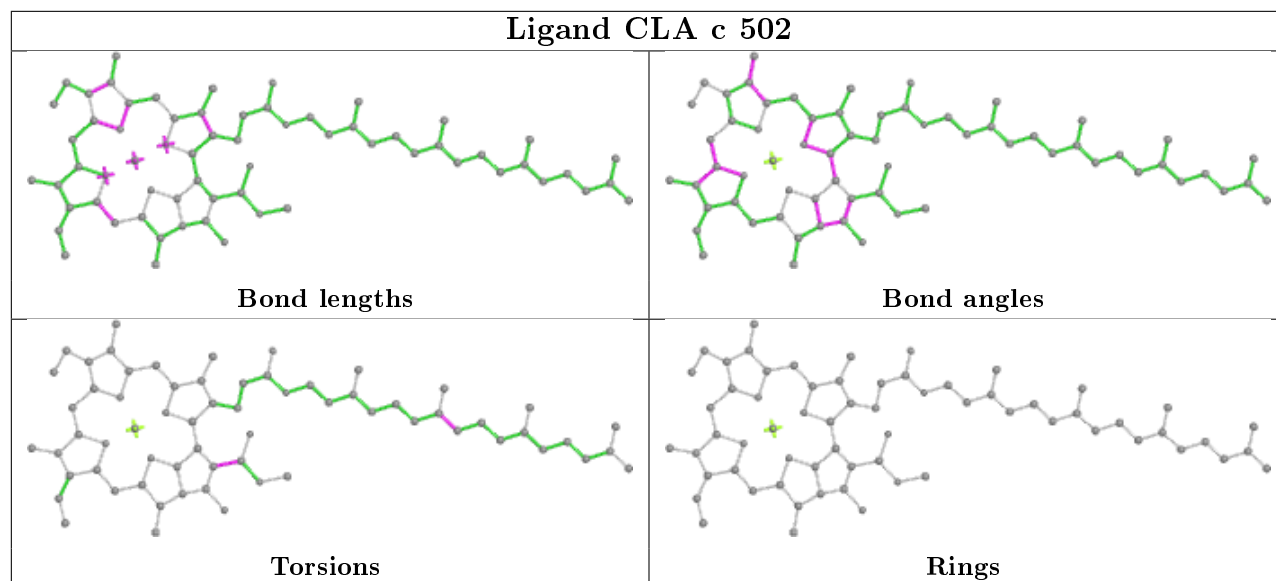
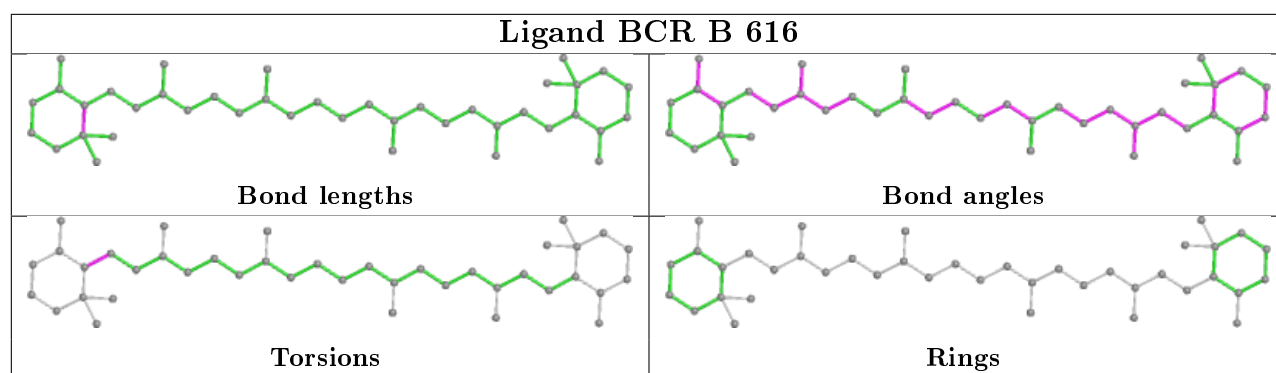


Ligand PHO a 414

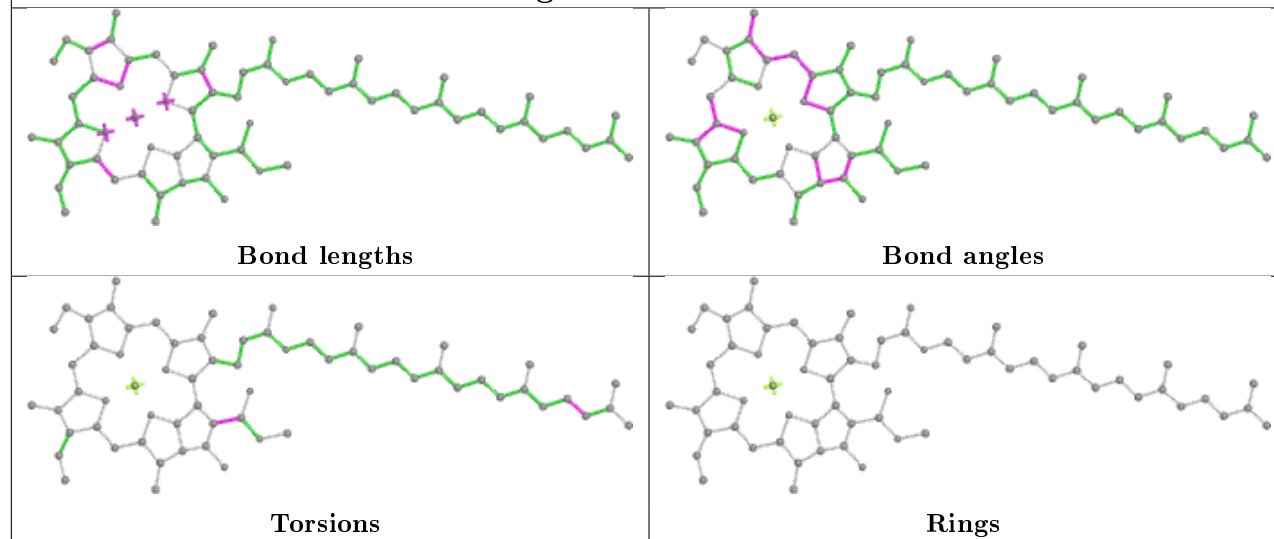


Ligand PHO D 401

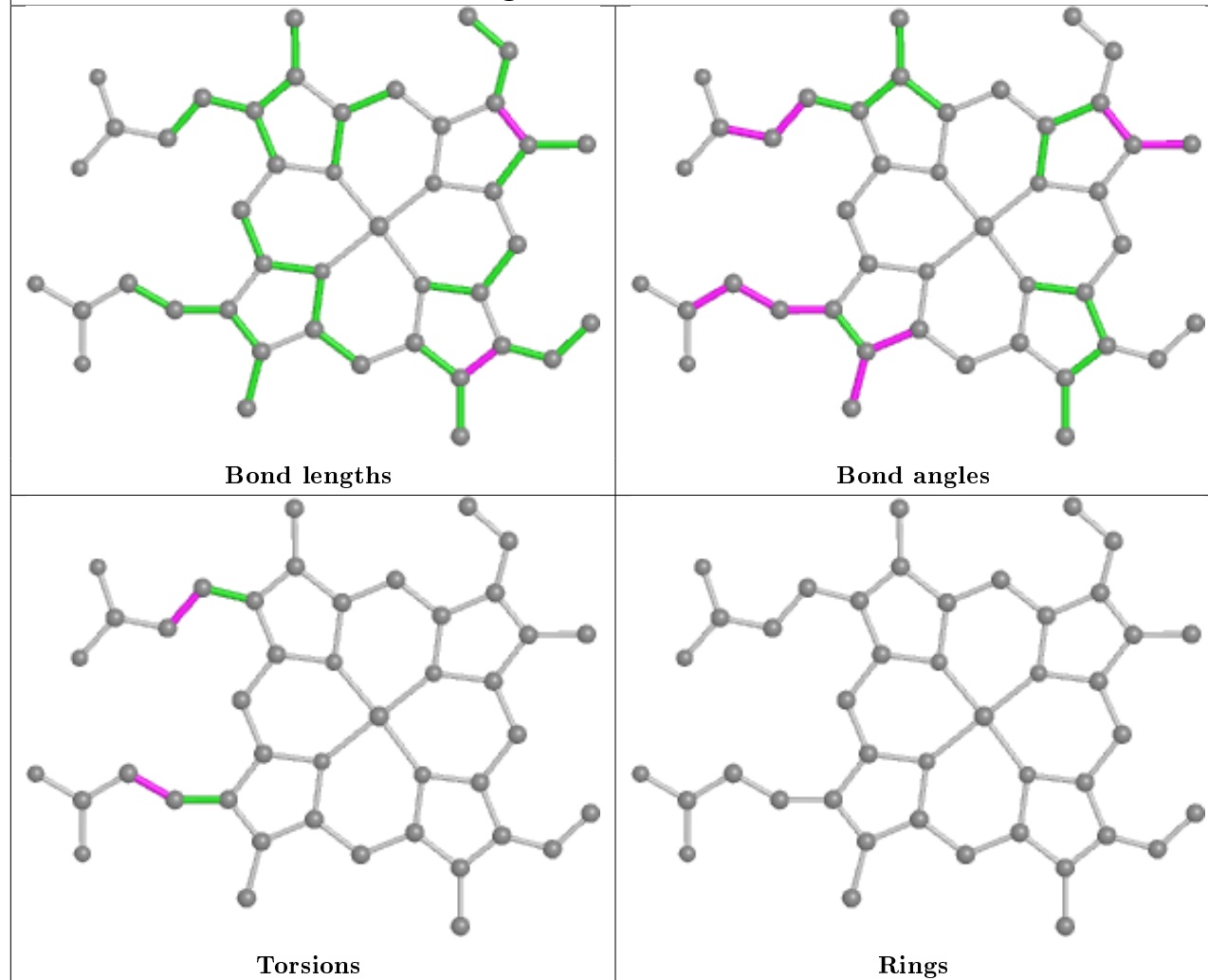




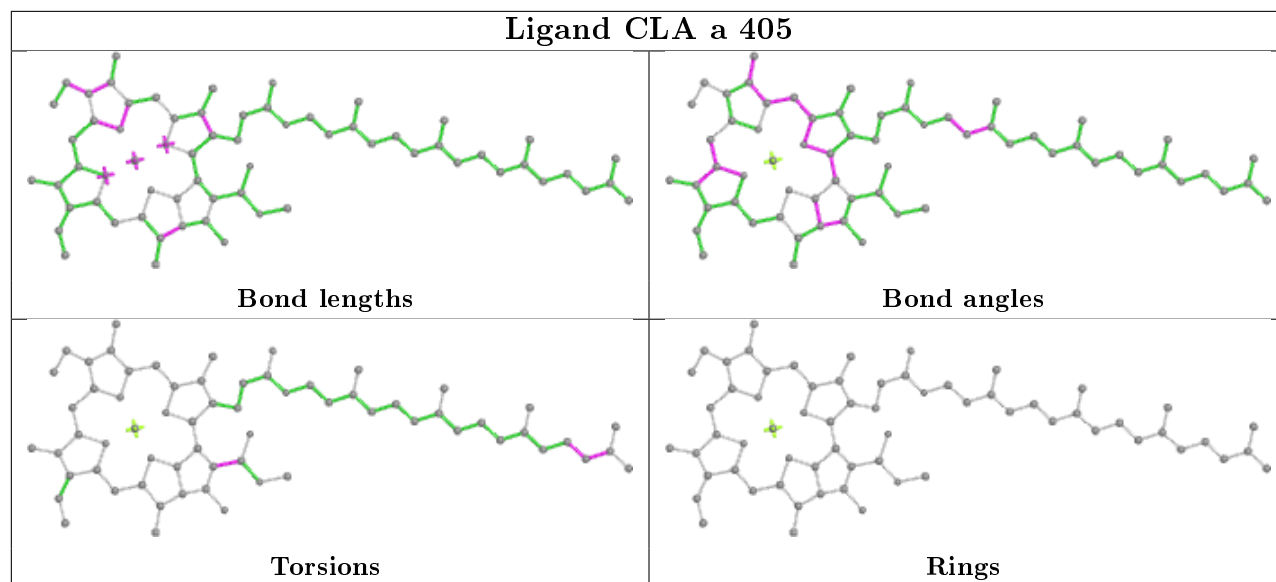
Ligand CLA a 404



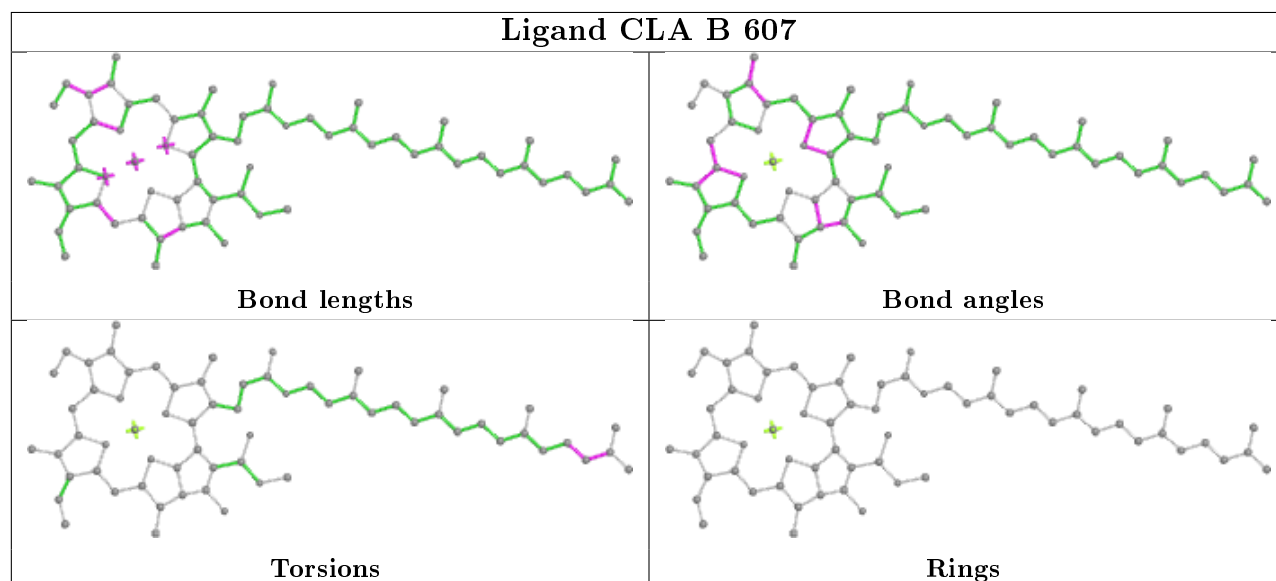
Ligand HEM E 102



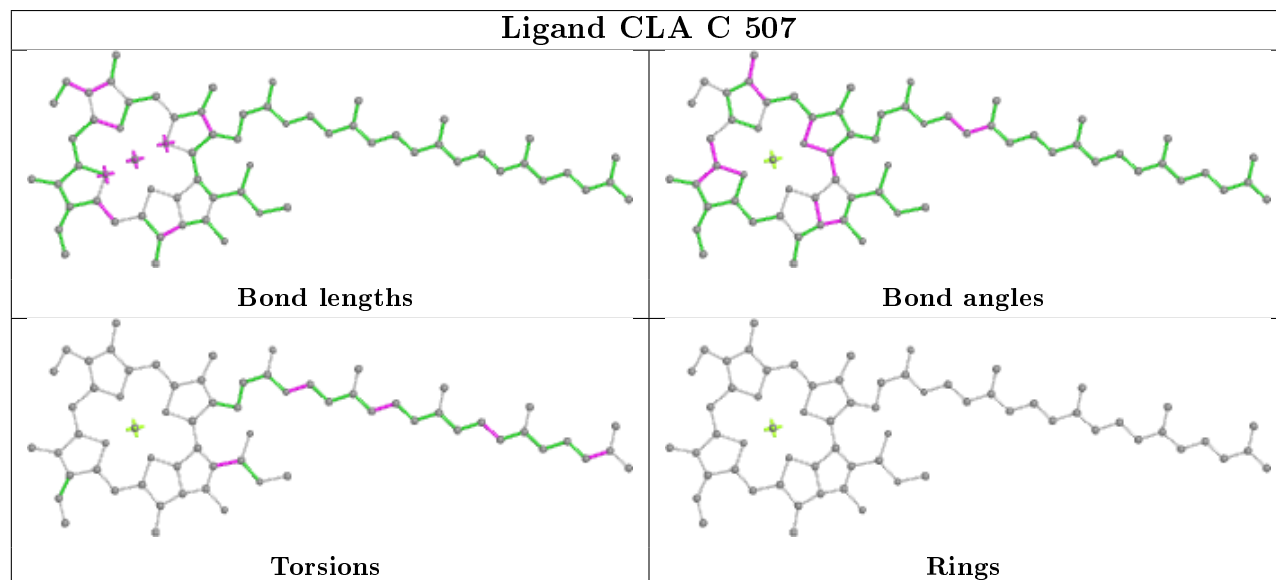
Ligand CLA a 405

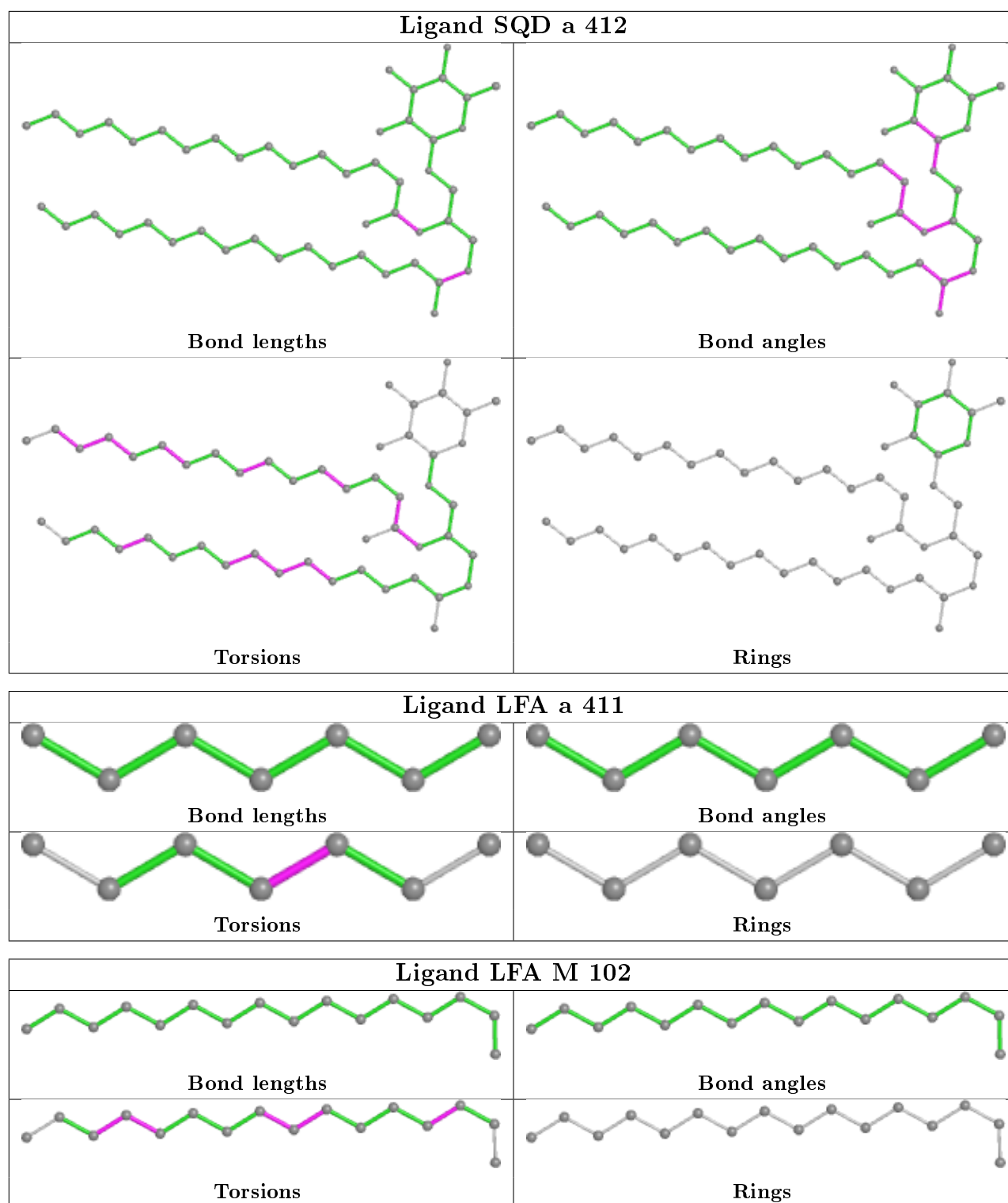


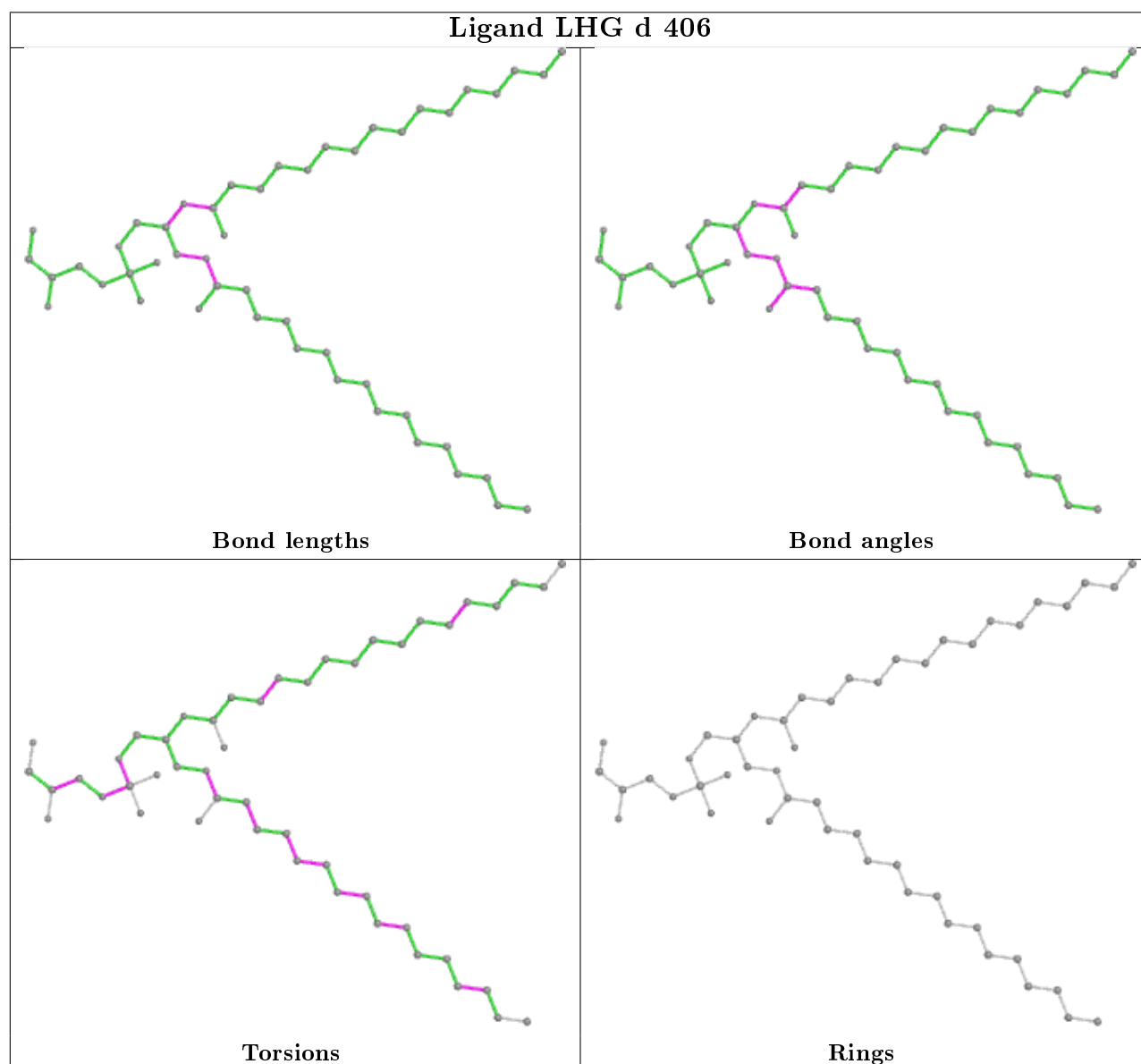
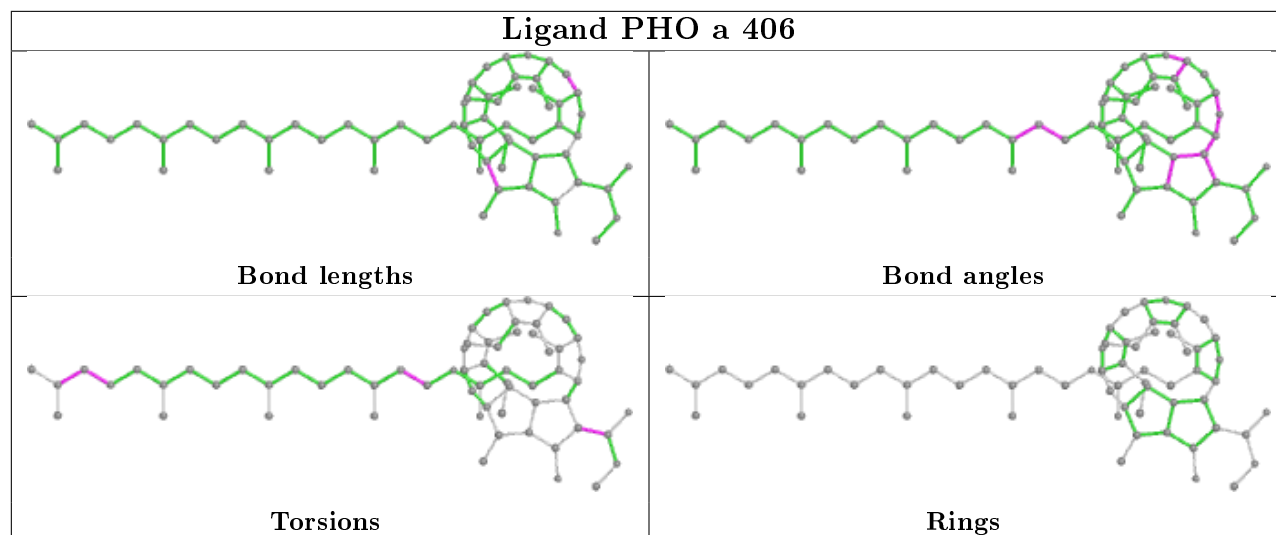
Ligand CLA B 607

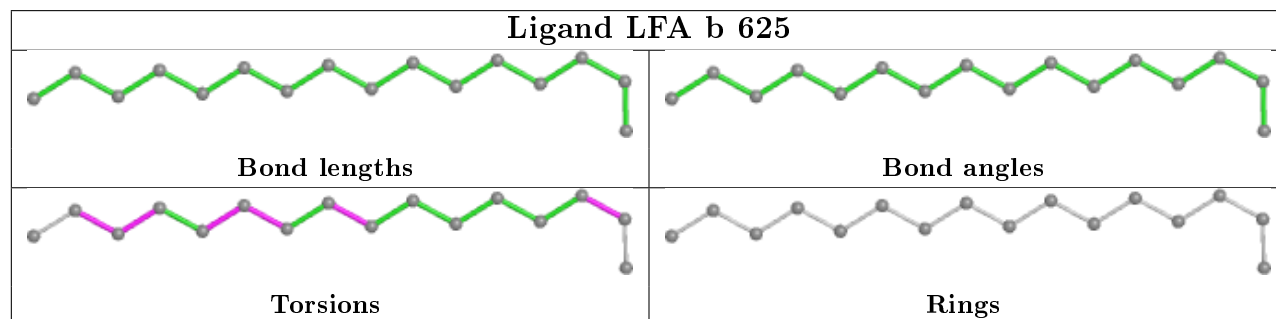
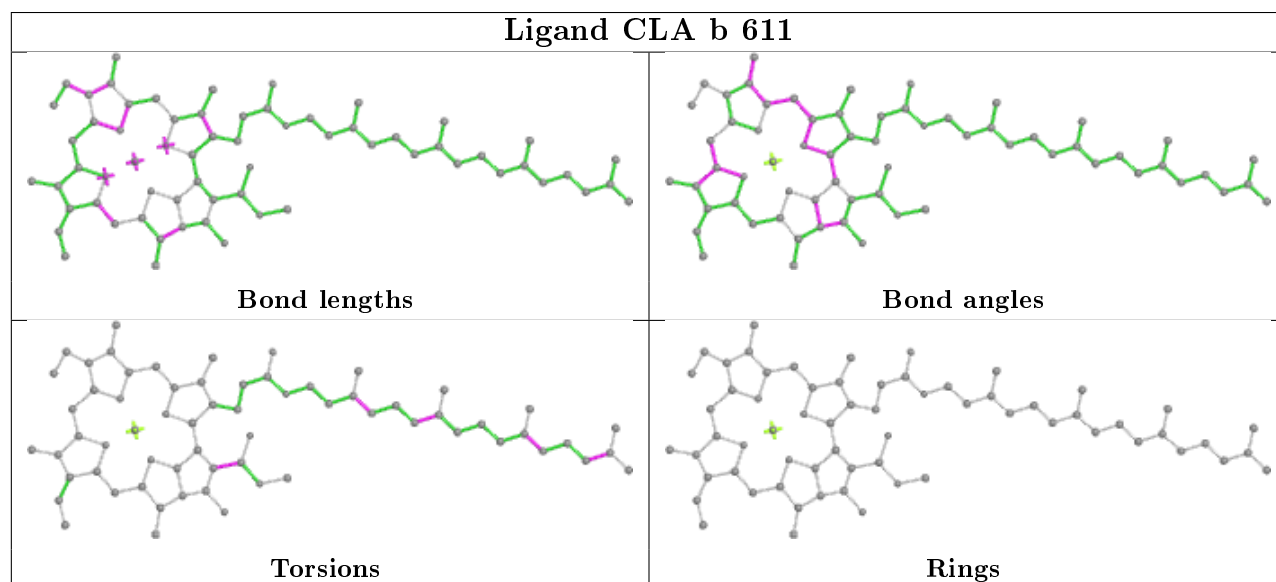
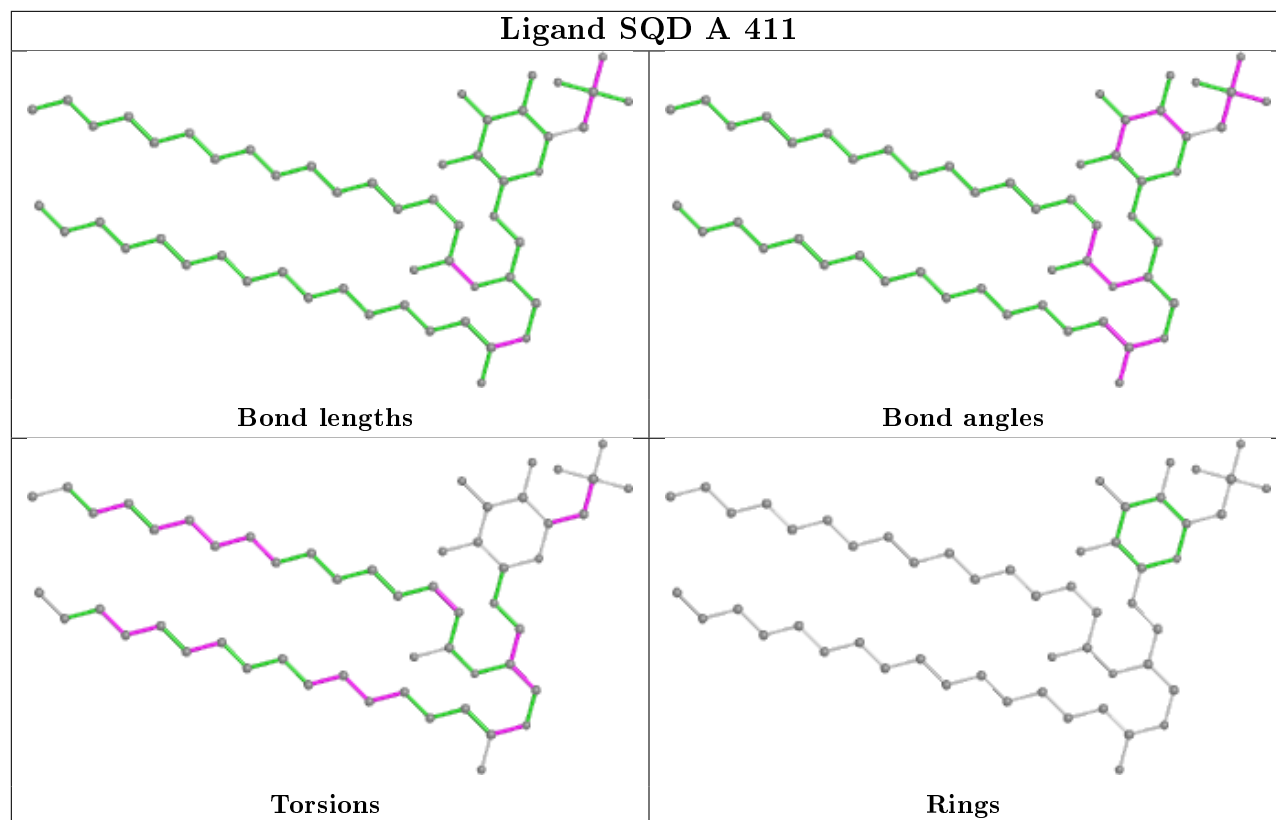


Ligand CLA C 507

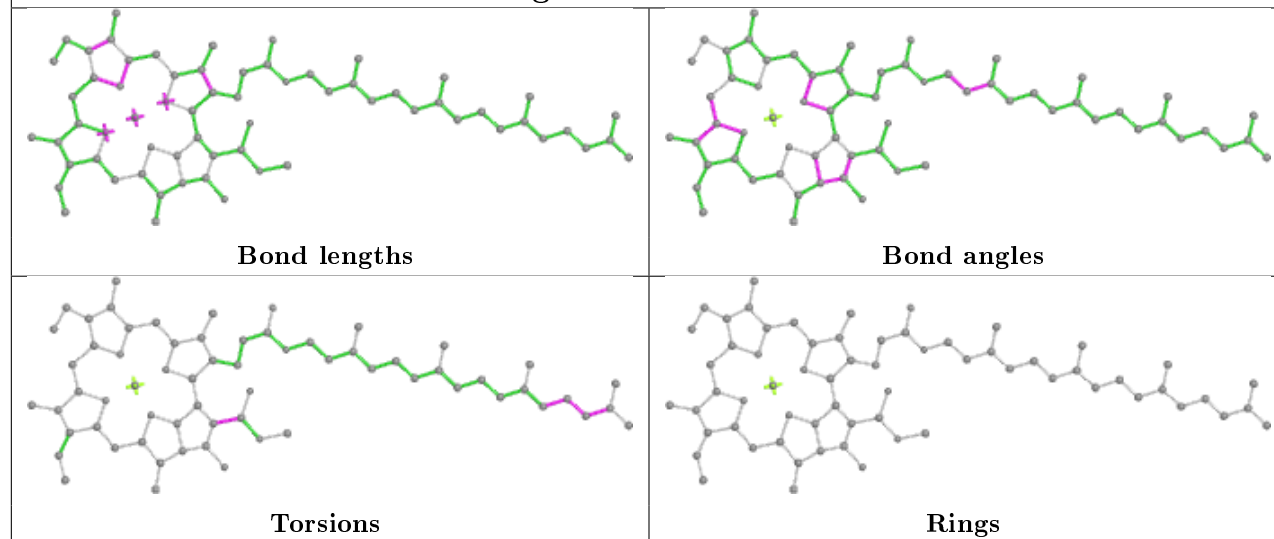




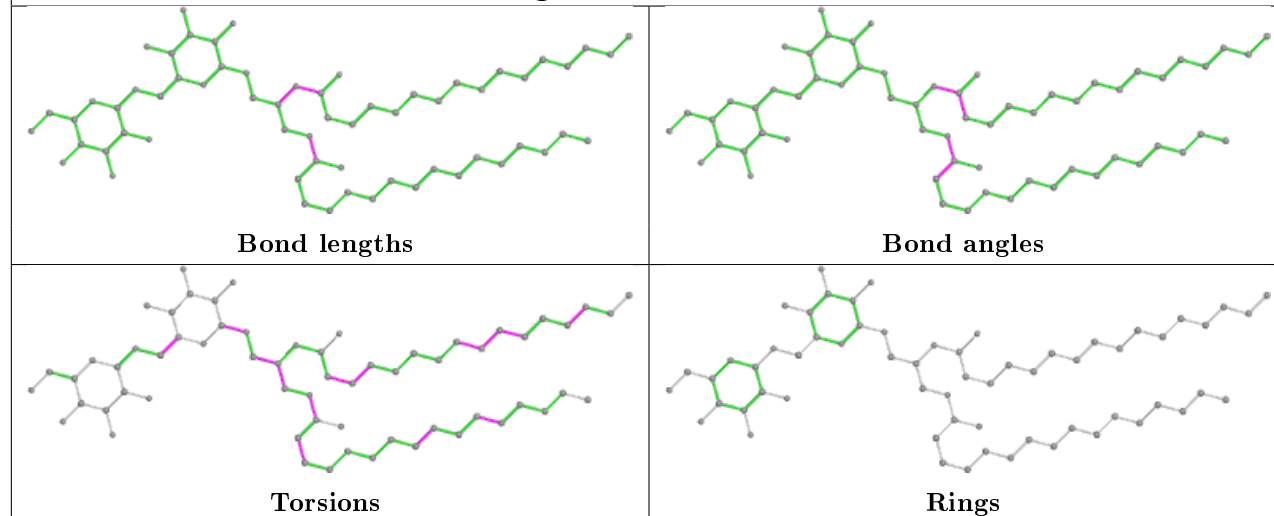




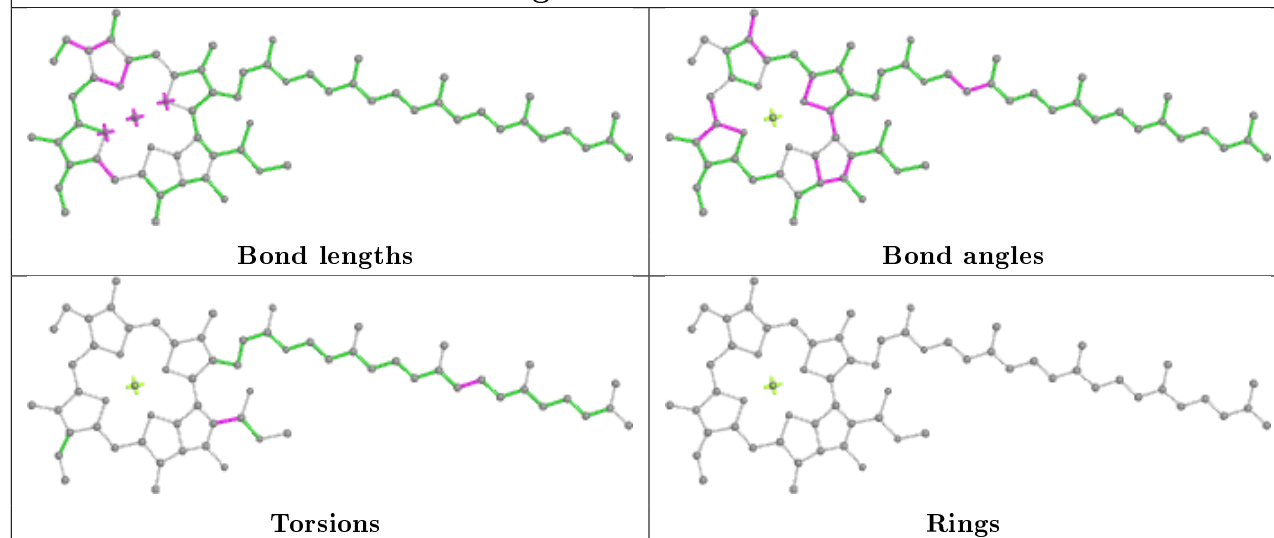
Ligand CLA B 601



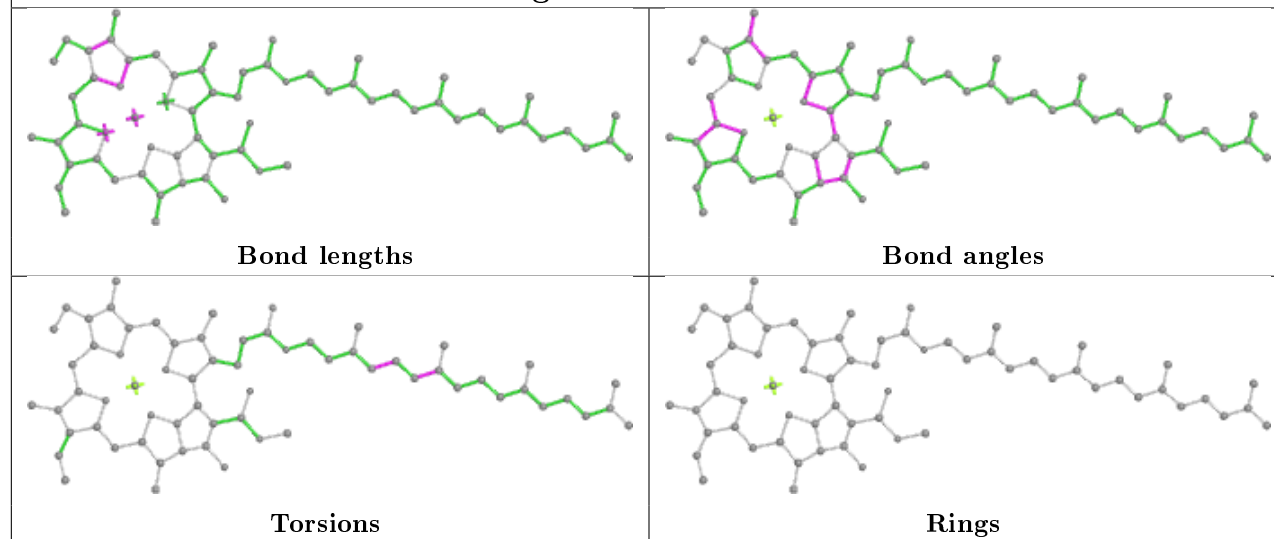
Ligand DGD c 518



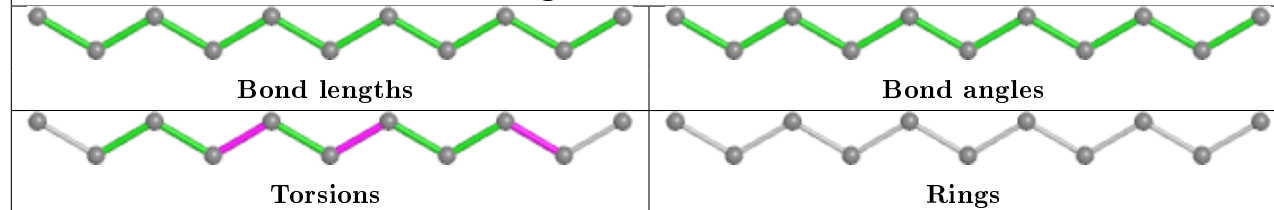
Ligand CLA C 514



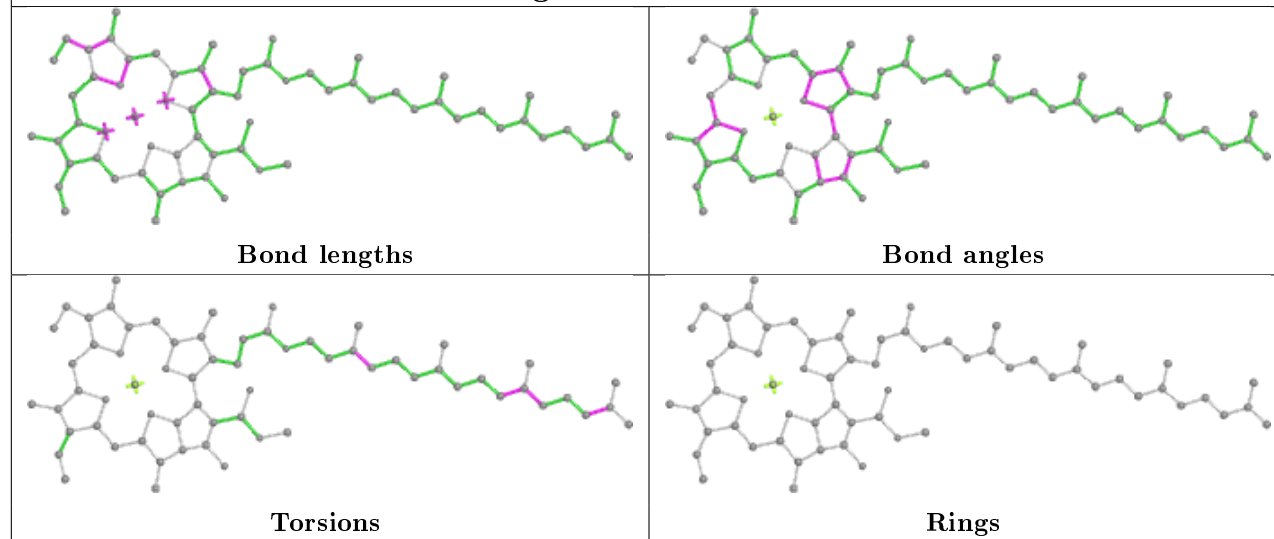
Ligand CLA B 603



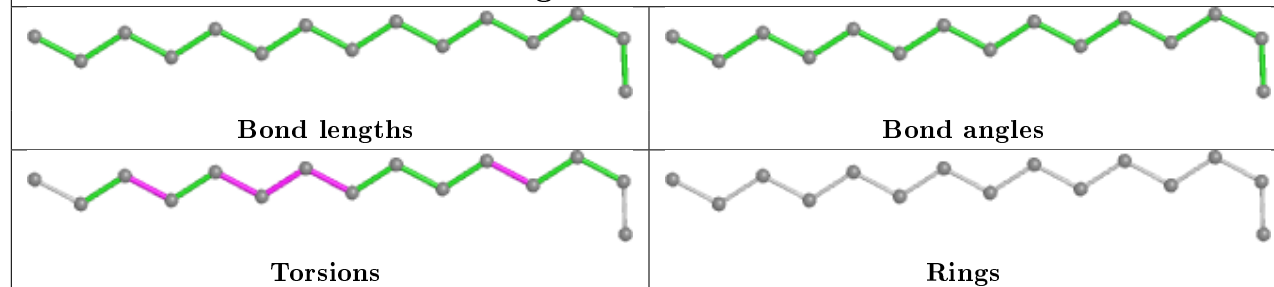
Ligand LFA b 627

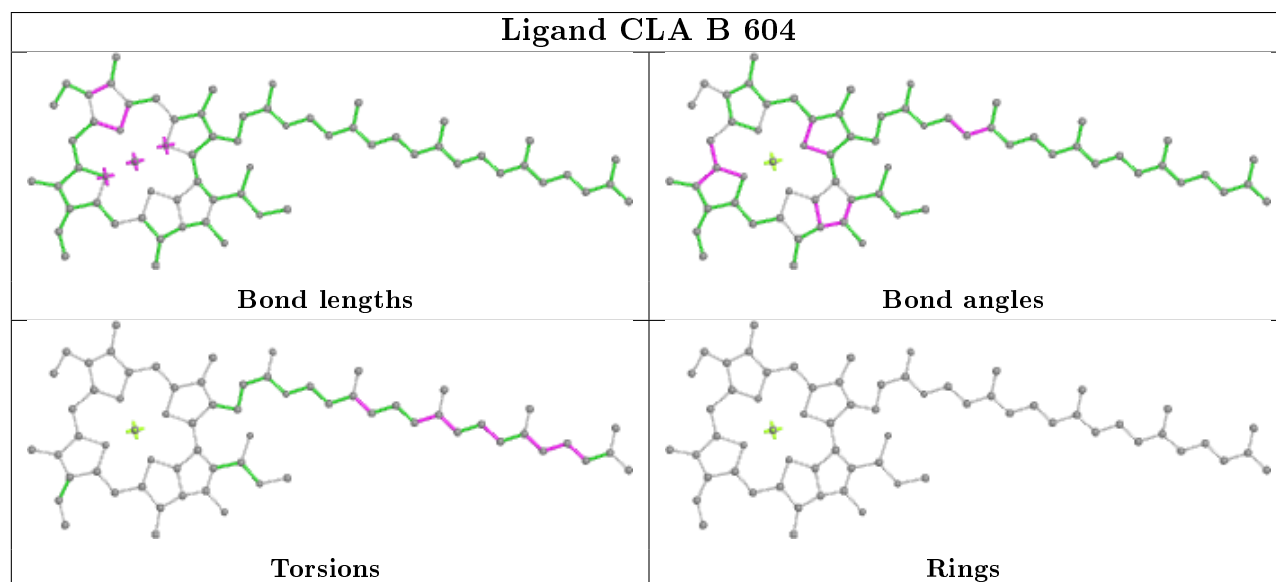
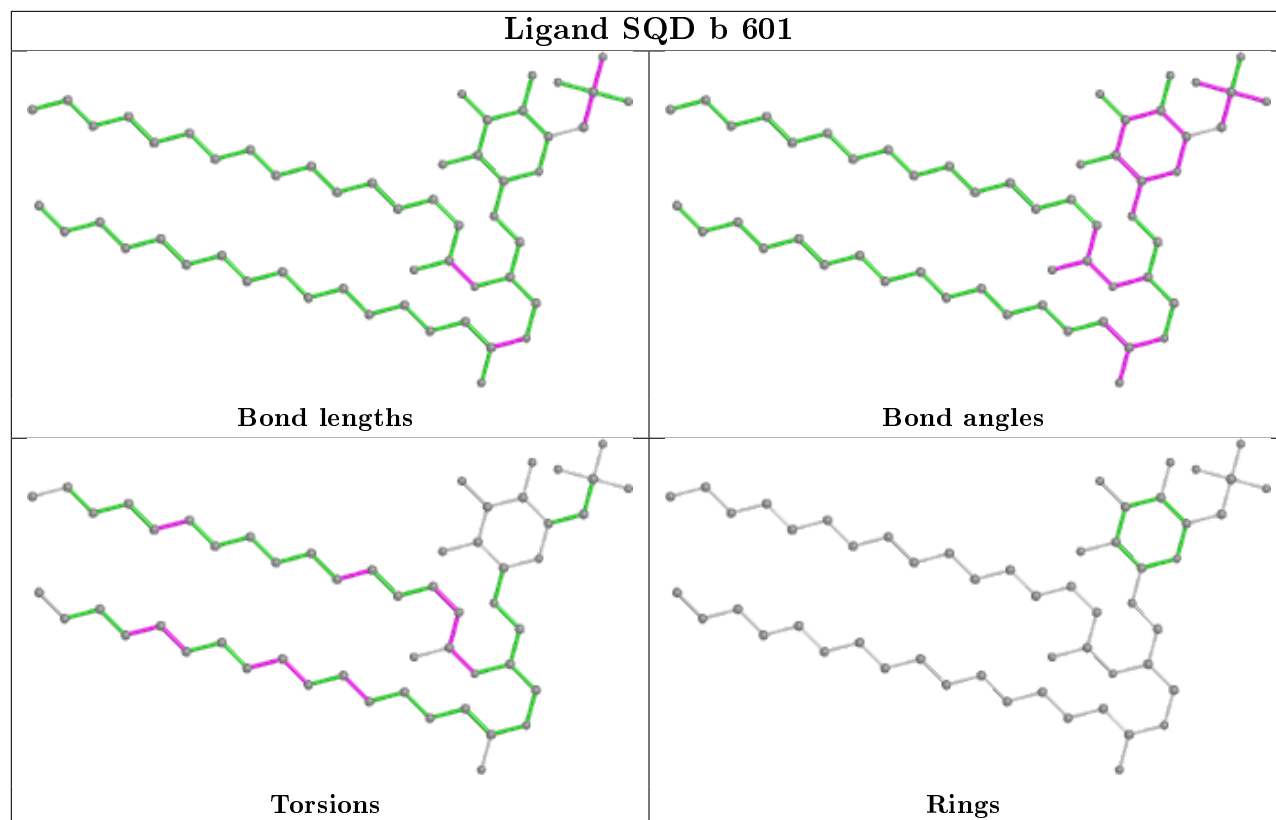


Ligand CLA B 614

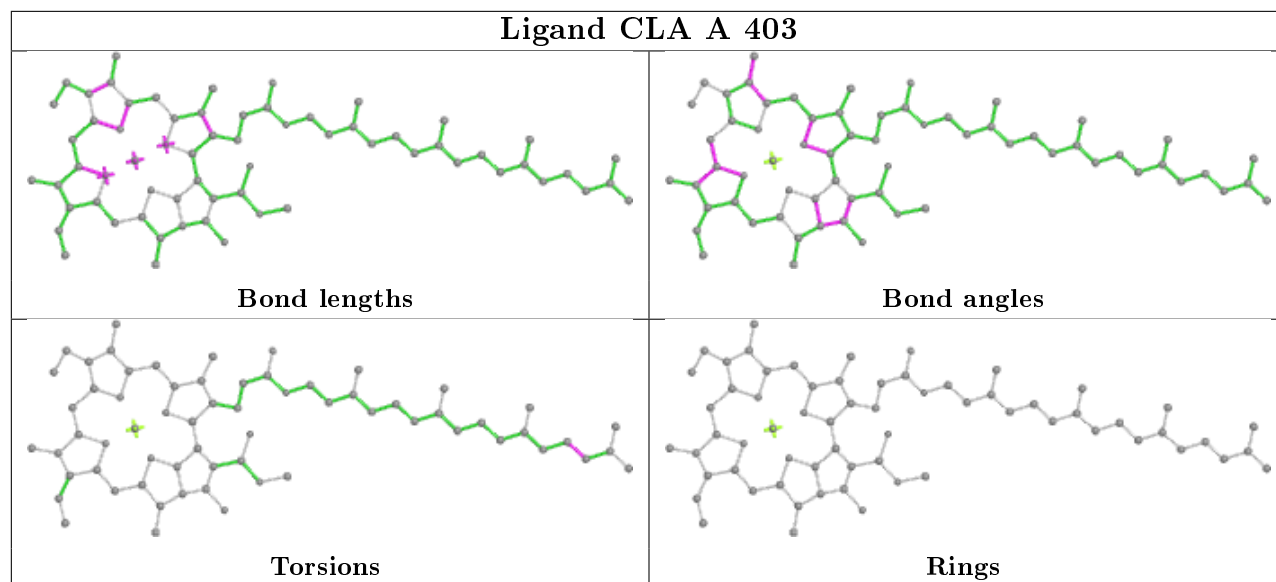


Ligand LFA D 410

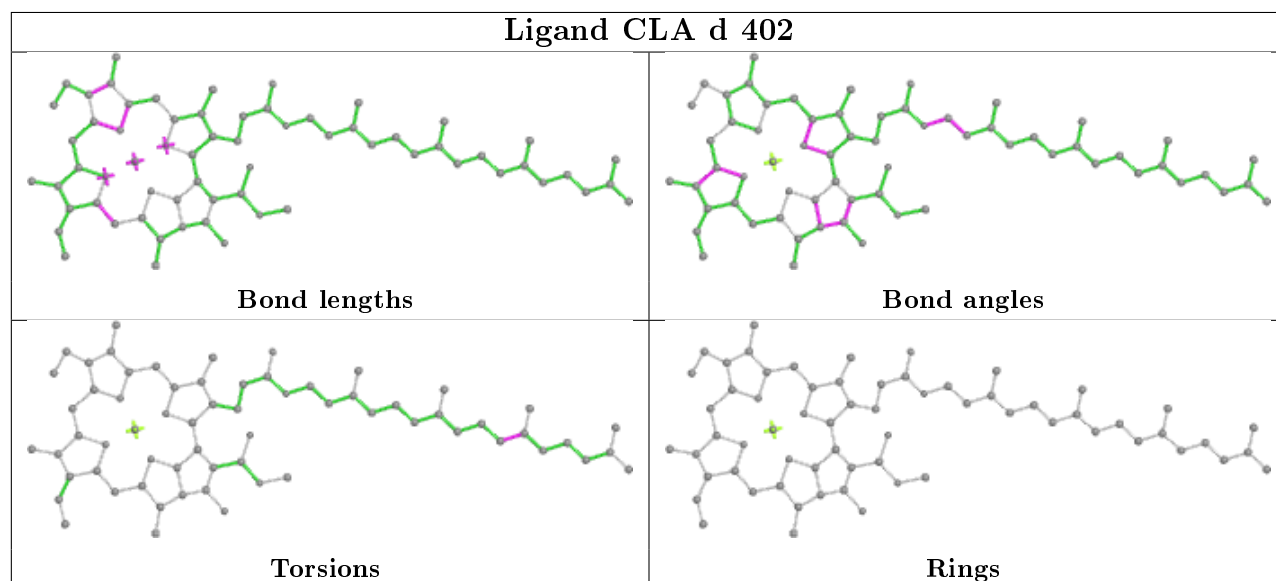




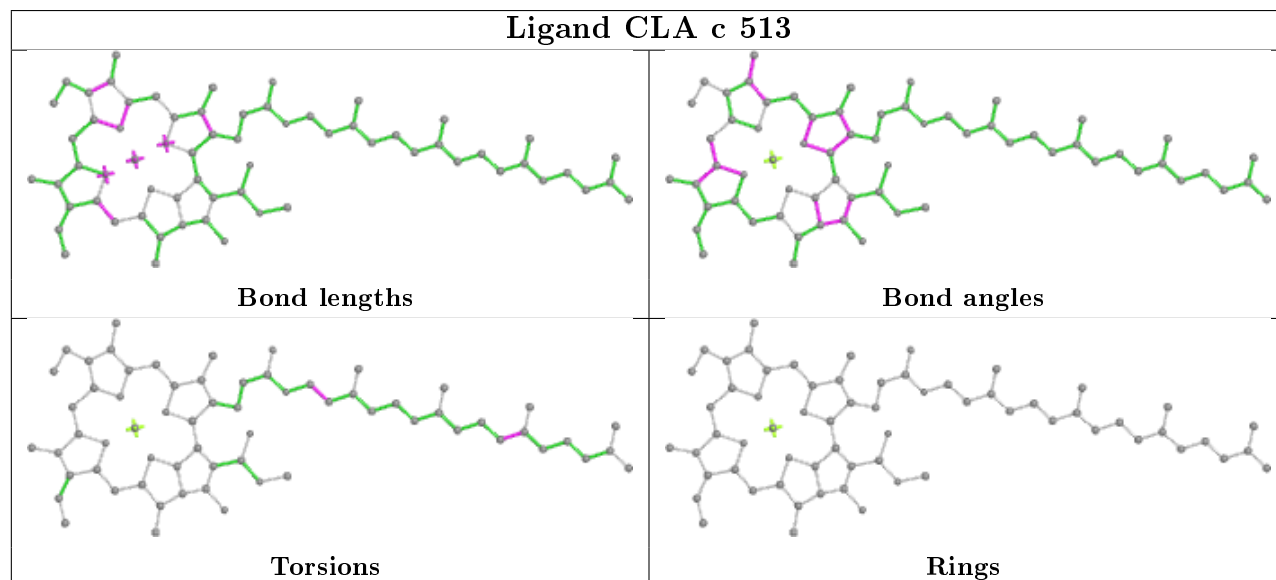
Ligand CLA A 403



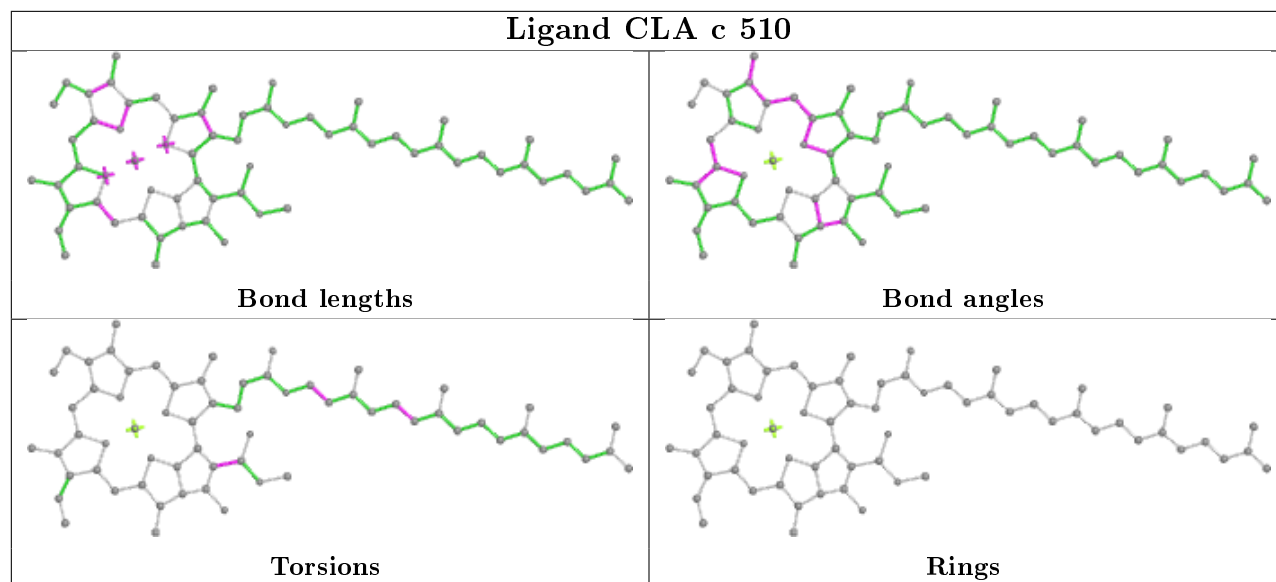
Ligand CLA d 402



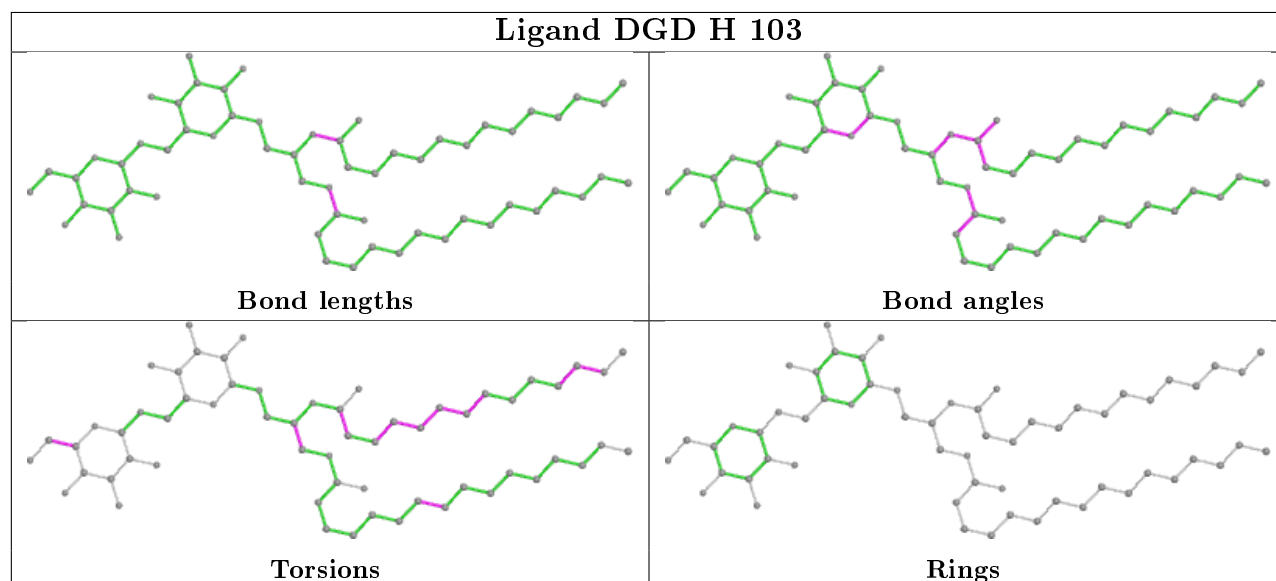
Ligand CLA c 513



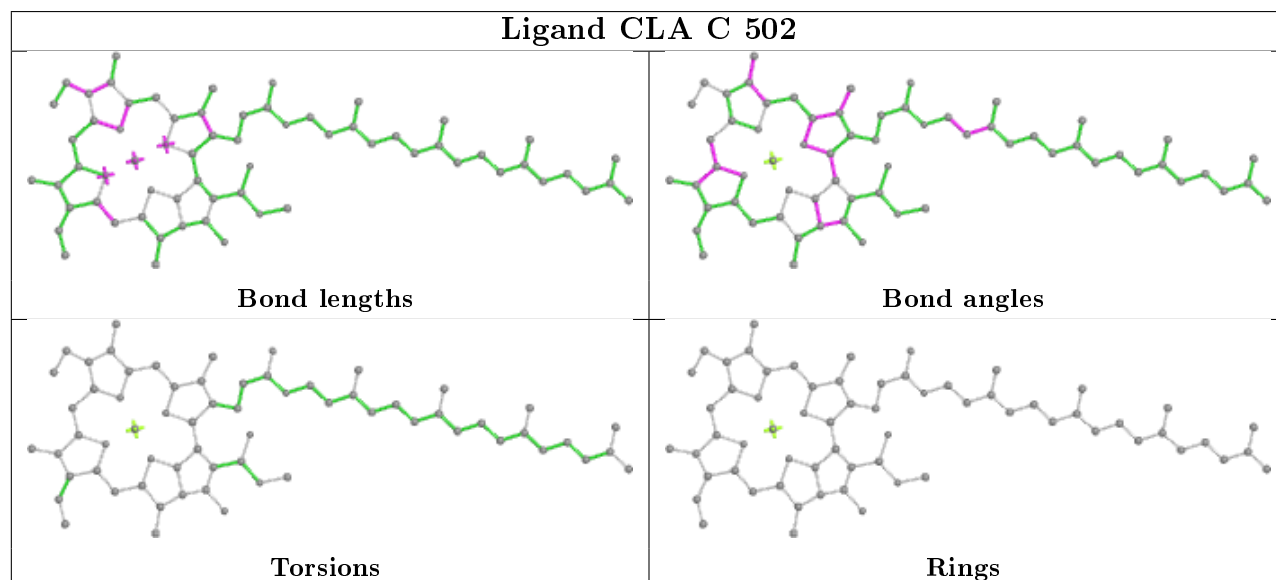
Ligand CLA c 510



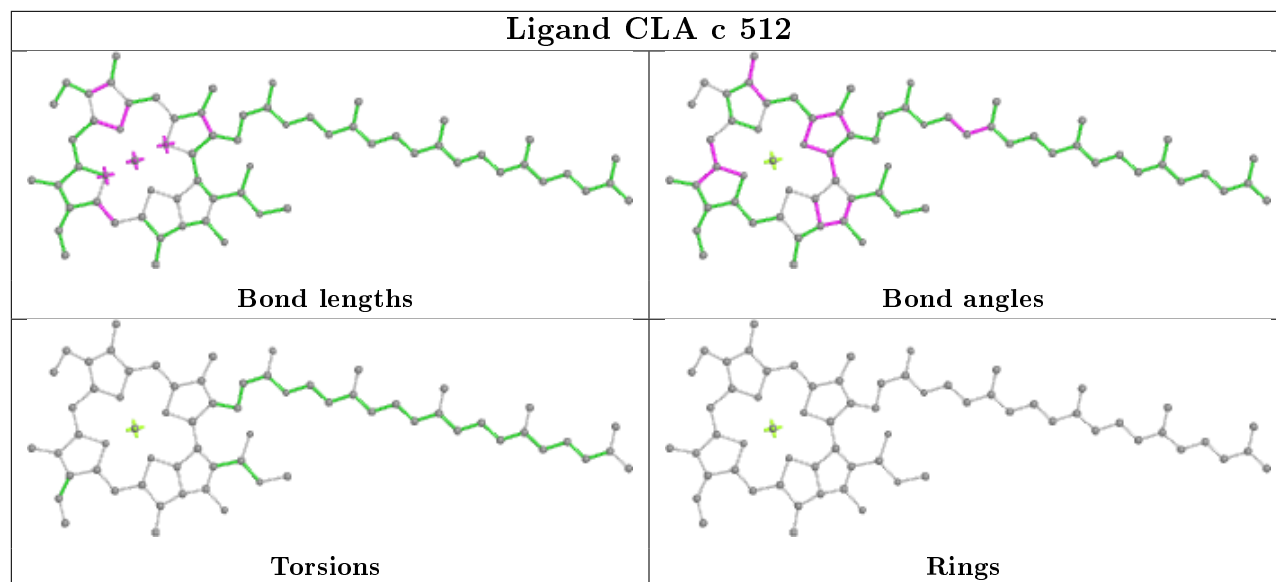
Ligand DGD H 103



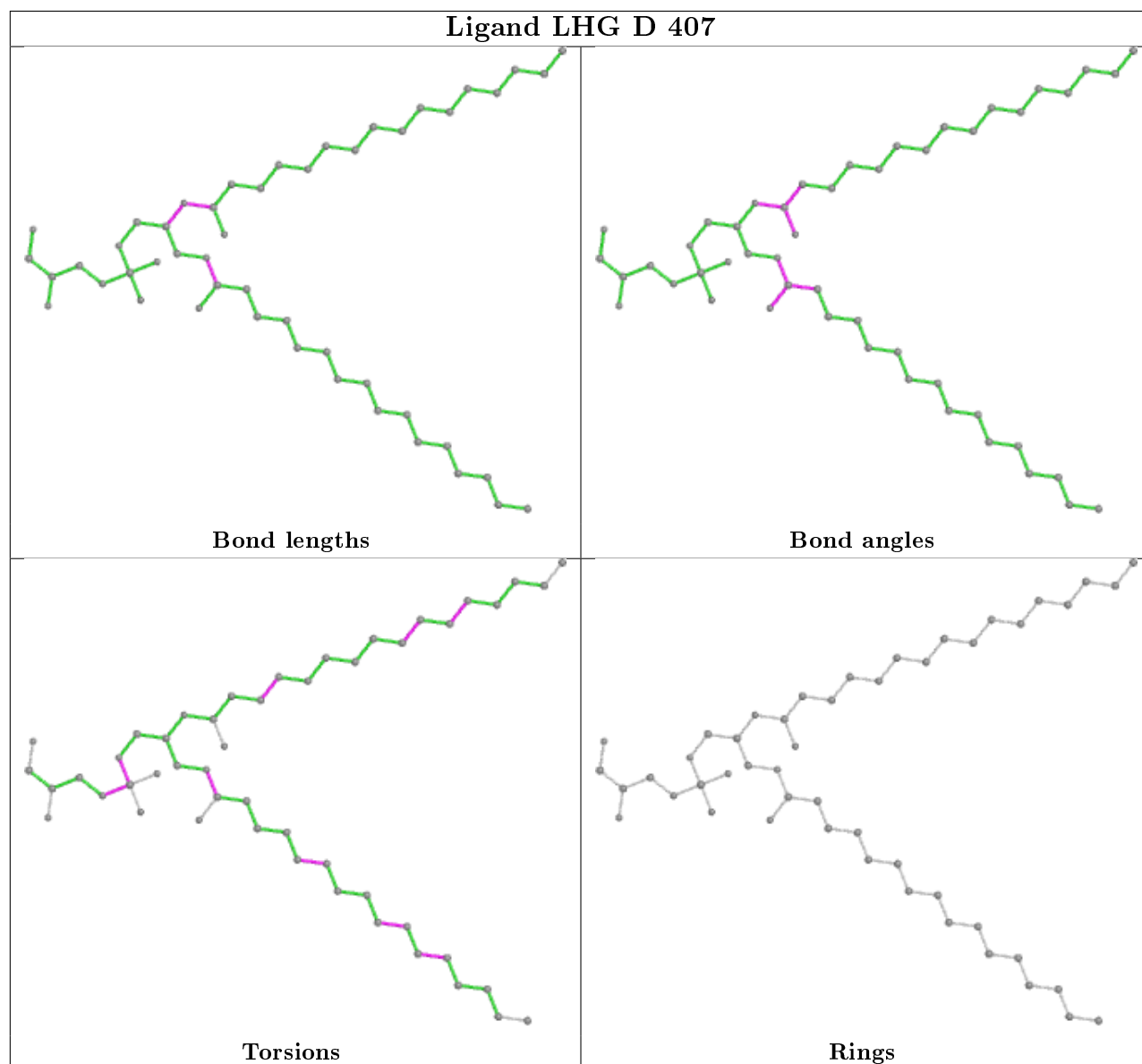
Ligand CLA C 502



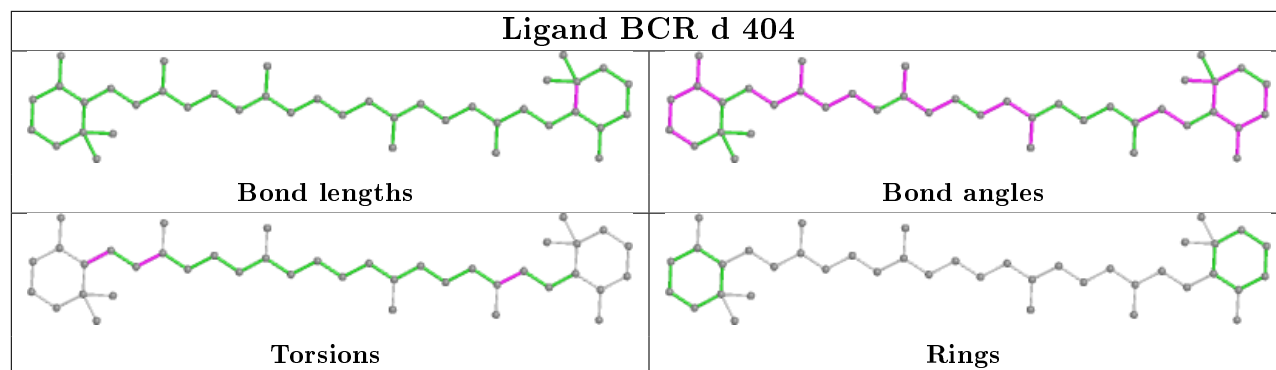
Ligand CLA c 512



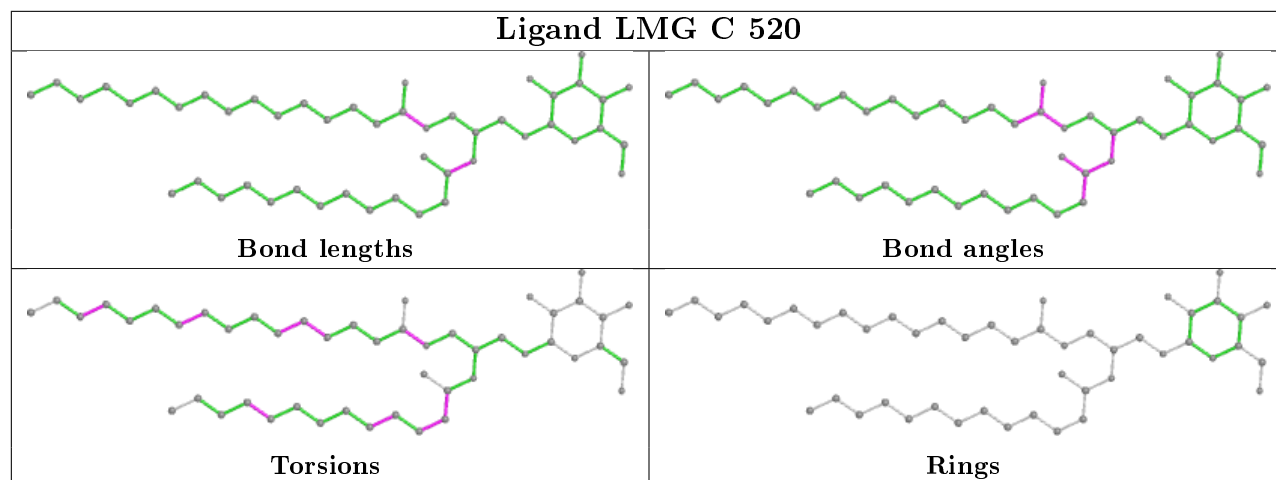
Ligand LHG D 407



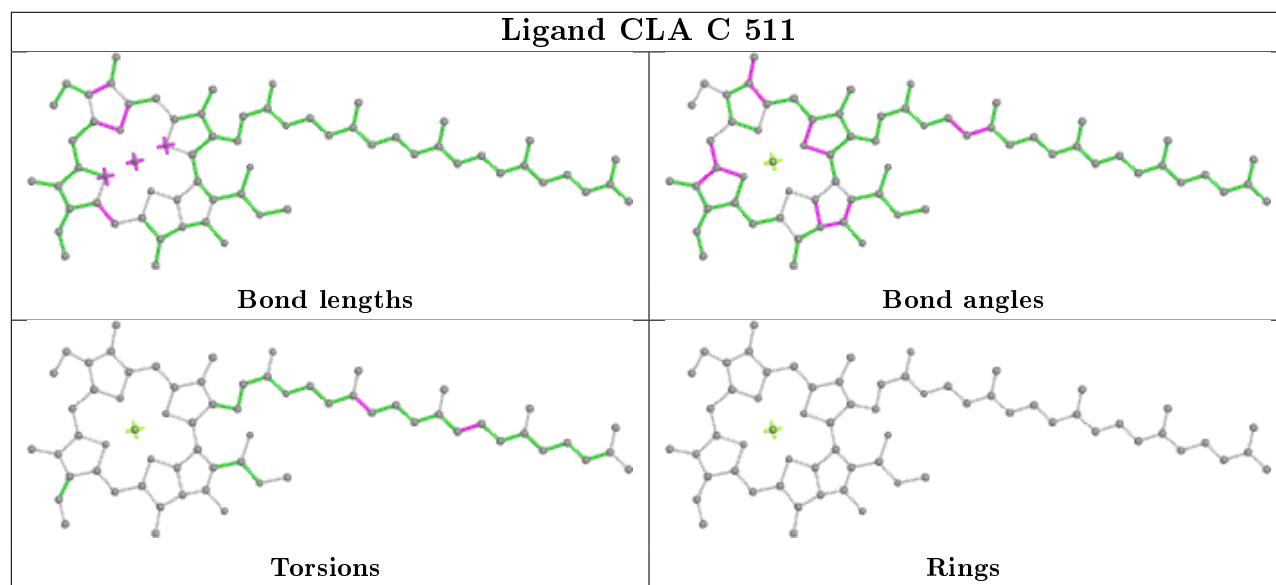
Ligand BCR d 404



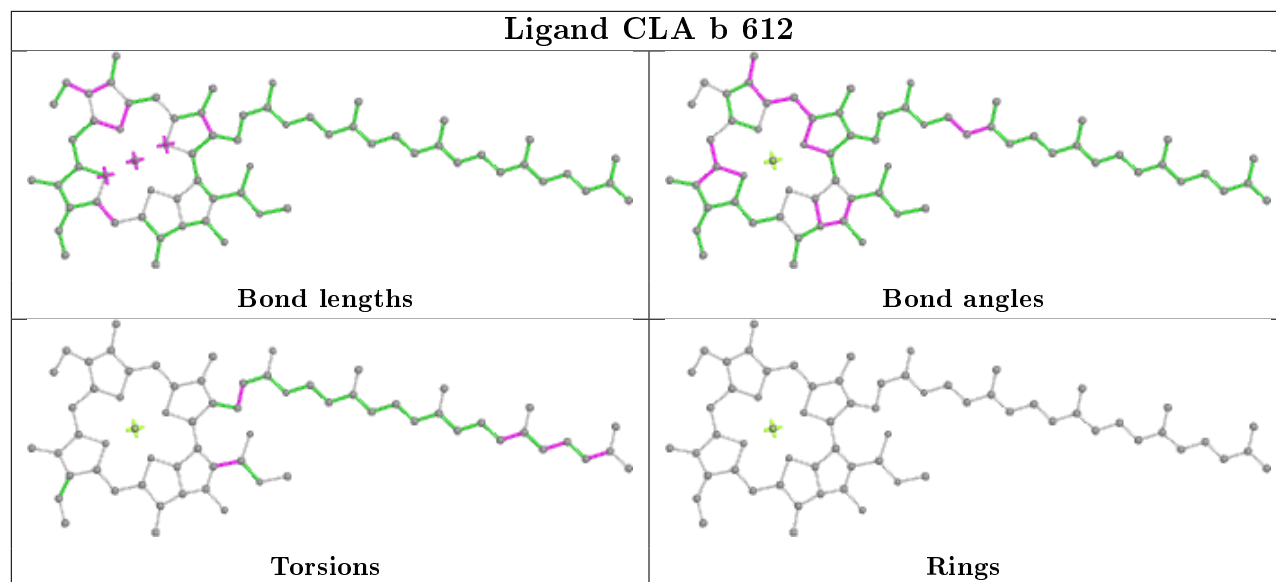
Ligand LMG C 520



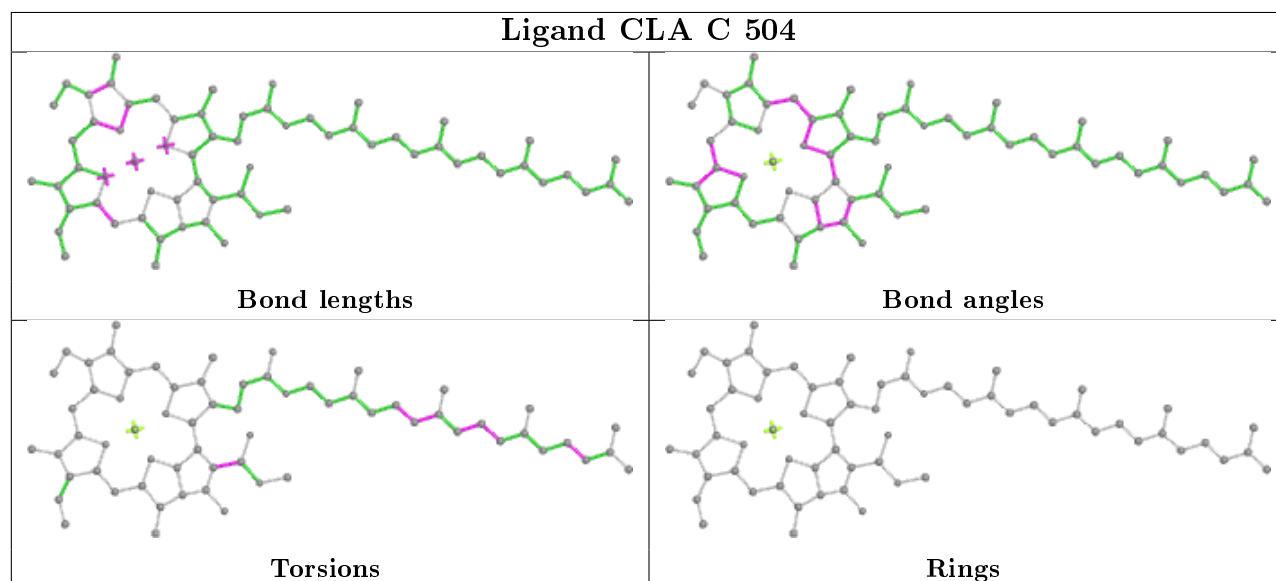
Ligand CLA C 511



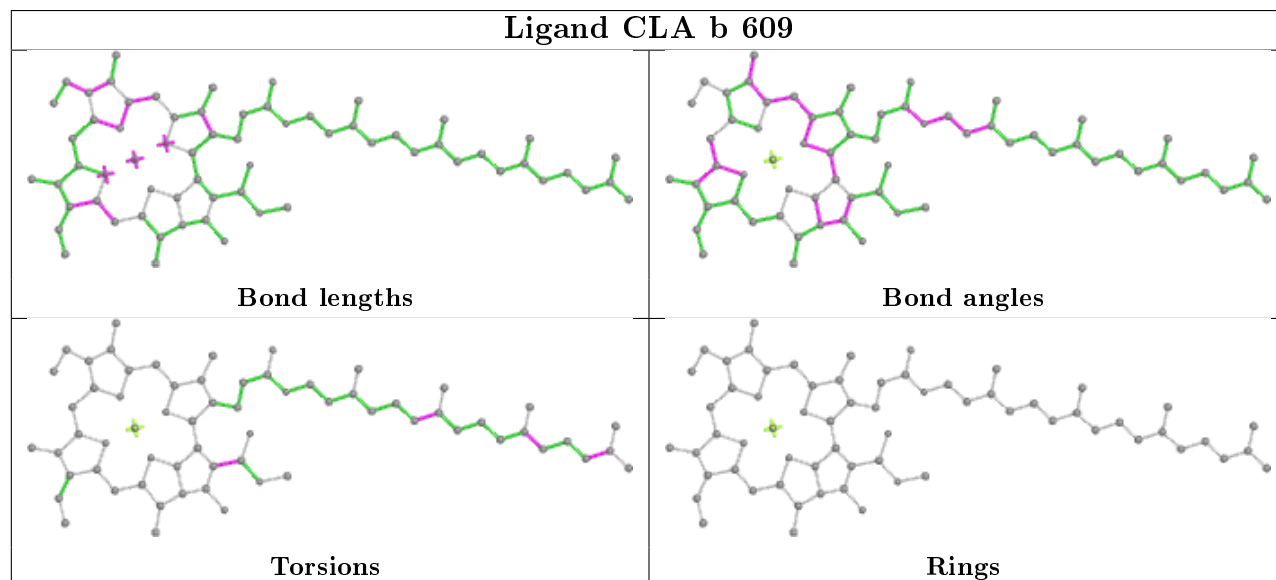
Ligand CLA b 612

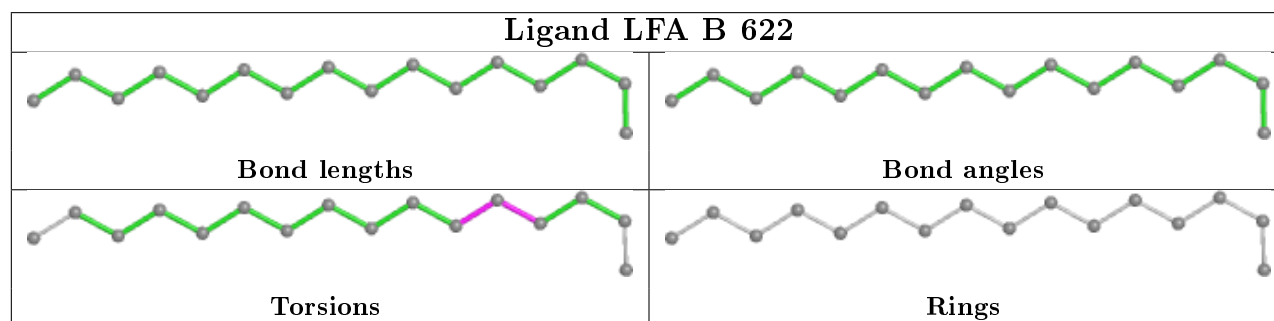
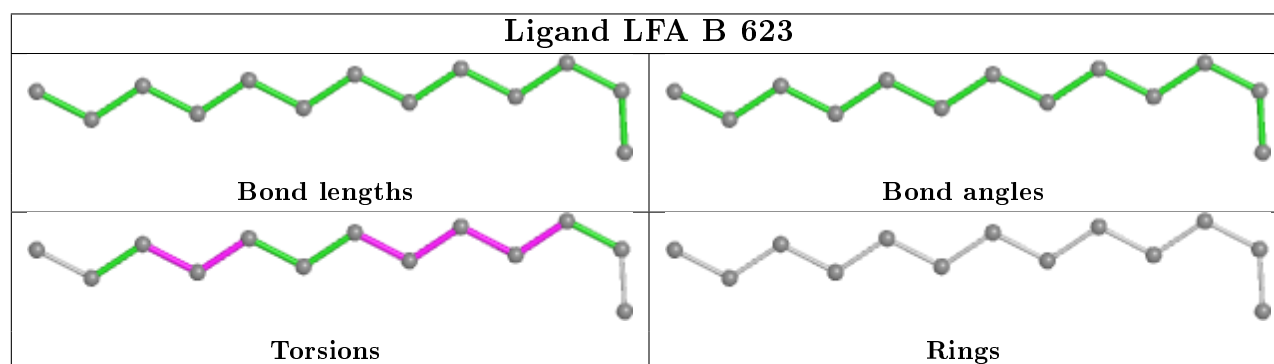
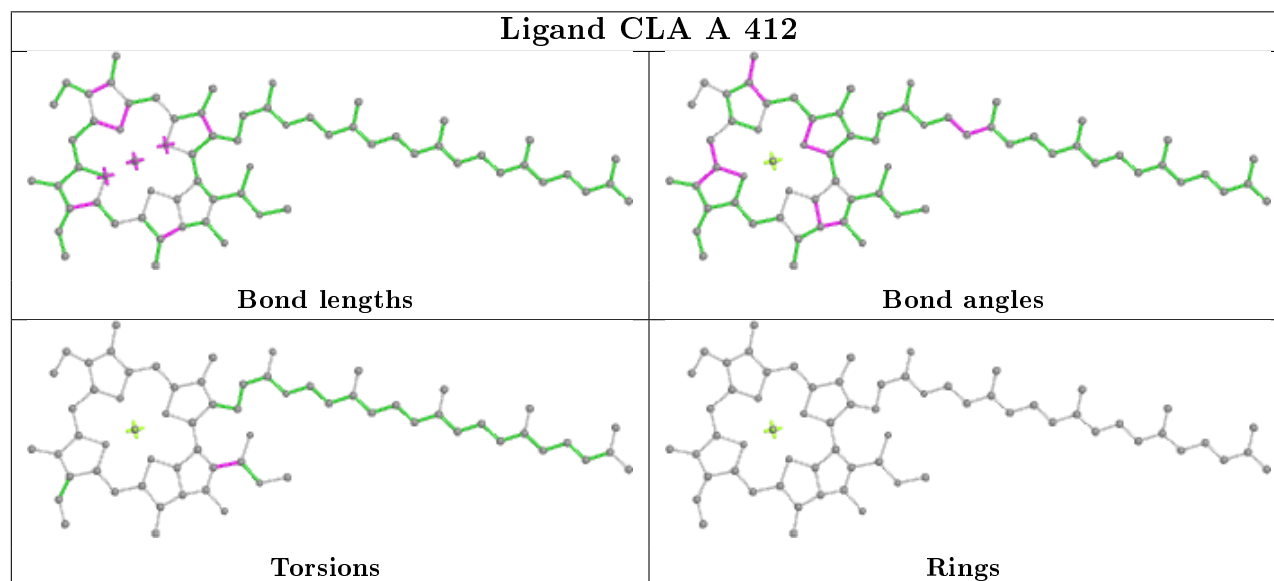
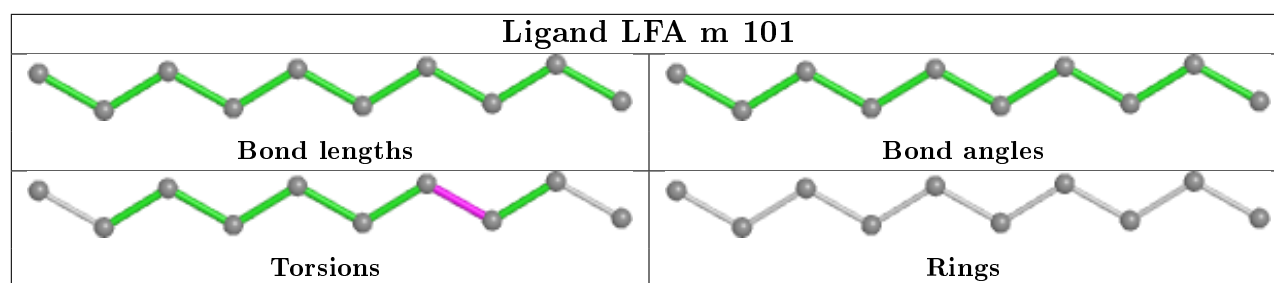


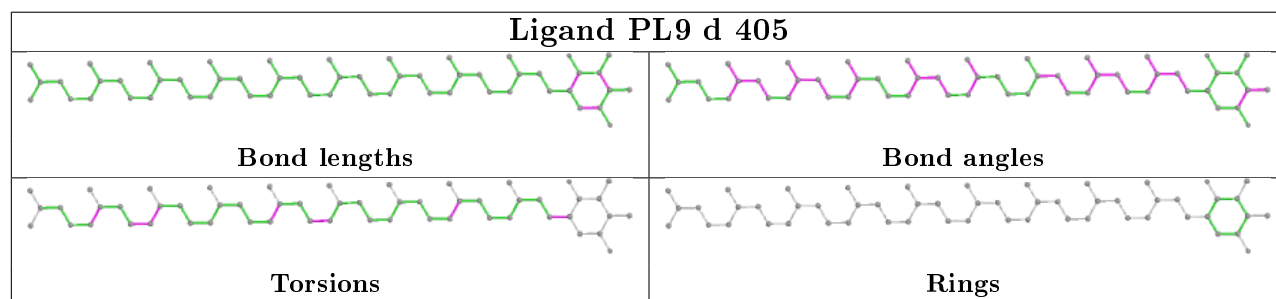
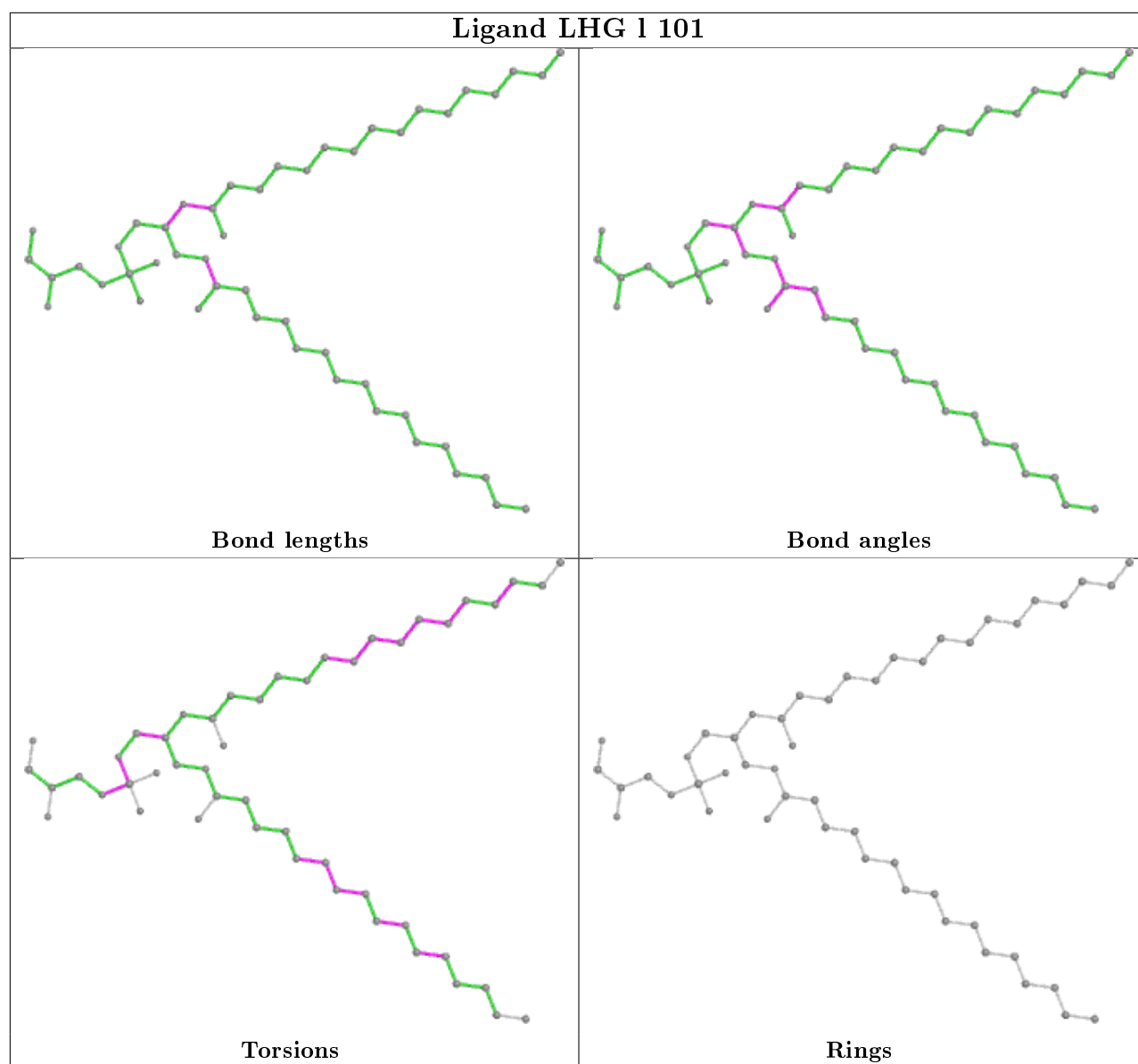
Ligand CLA C 504

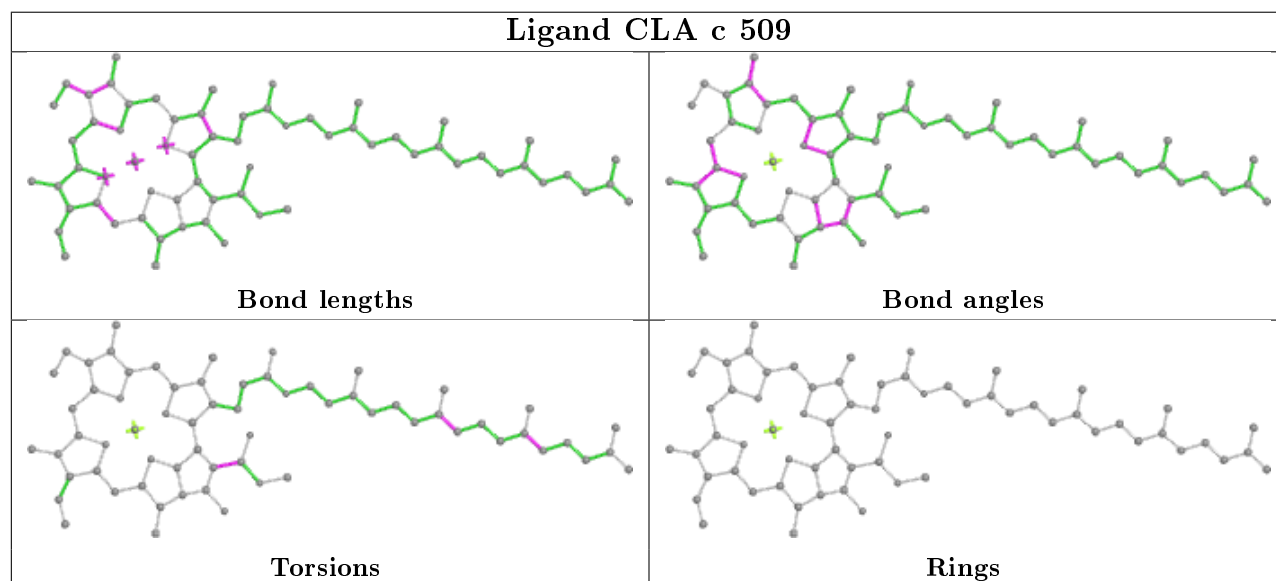
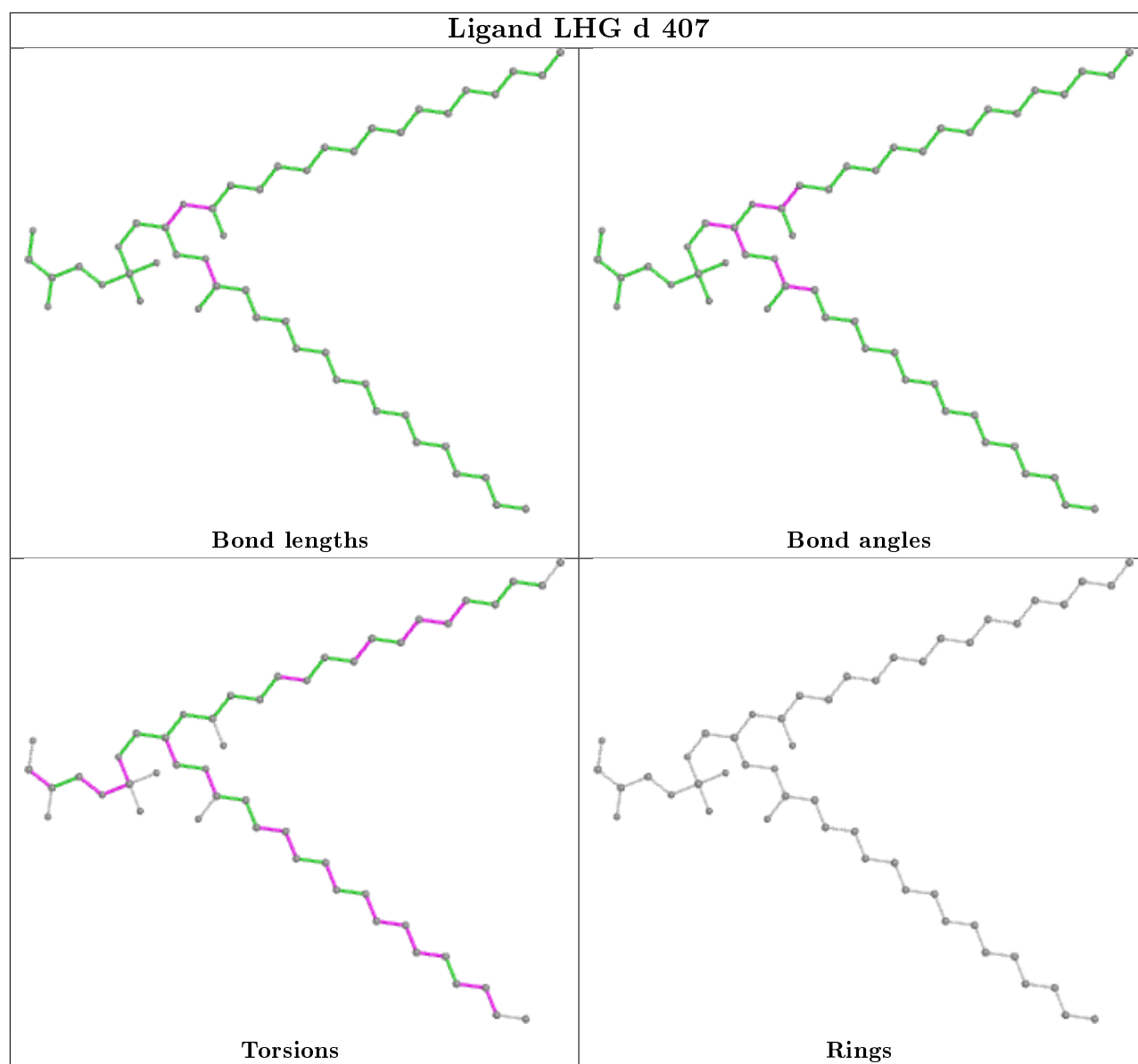


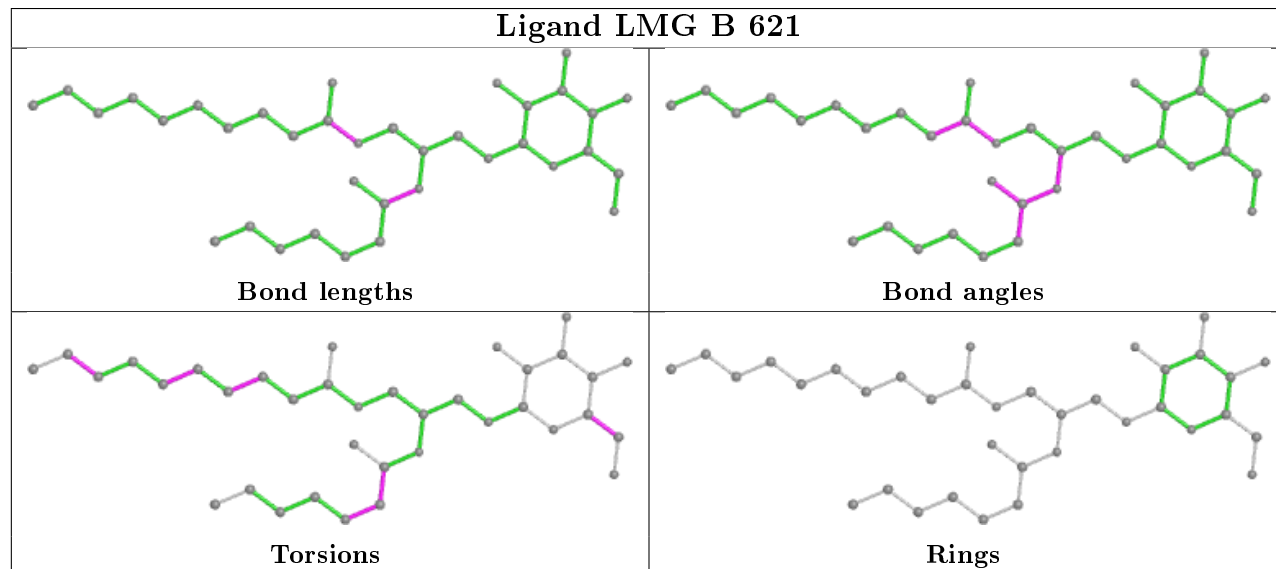
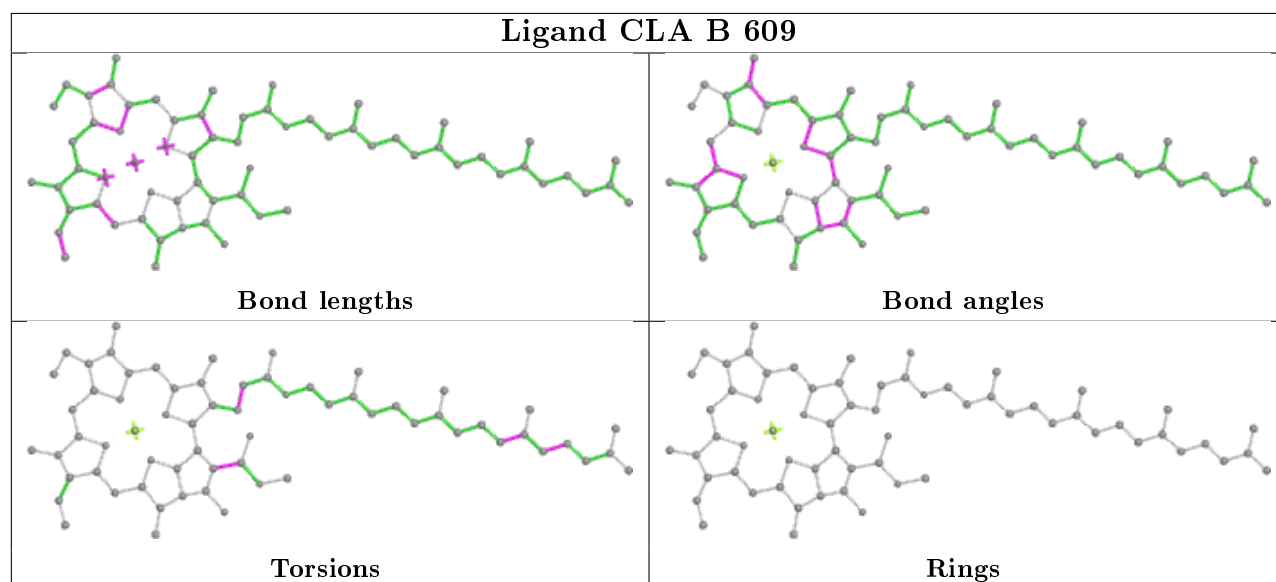
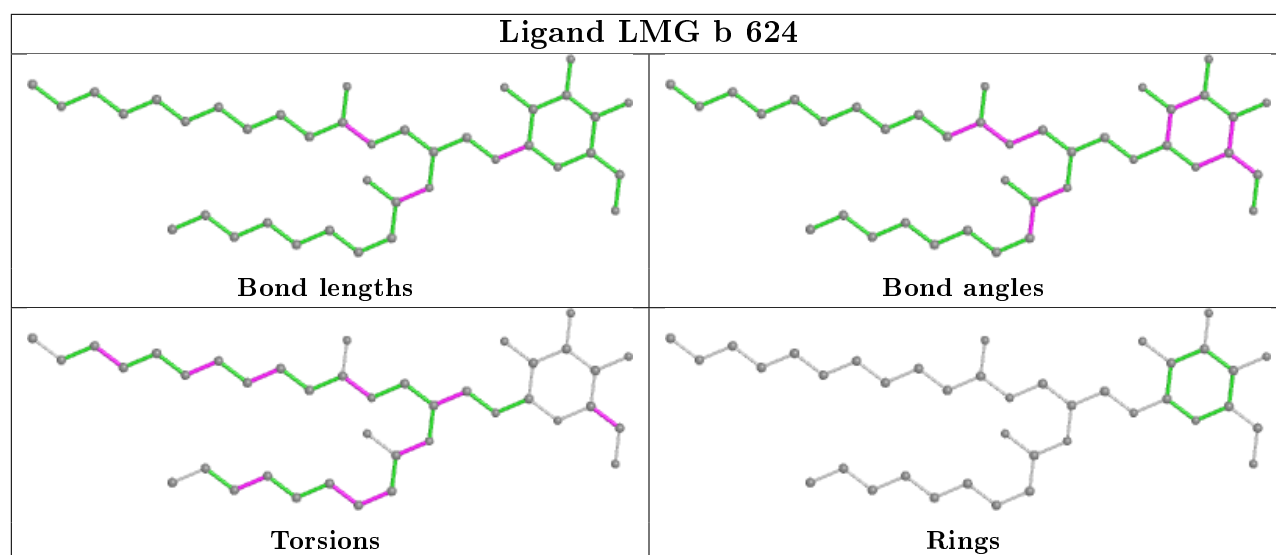
Ligand CLA b 609



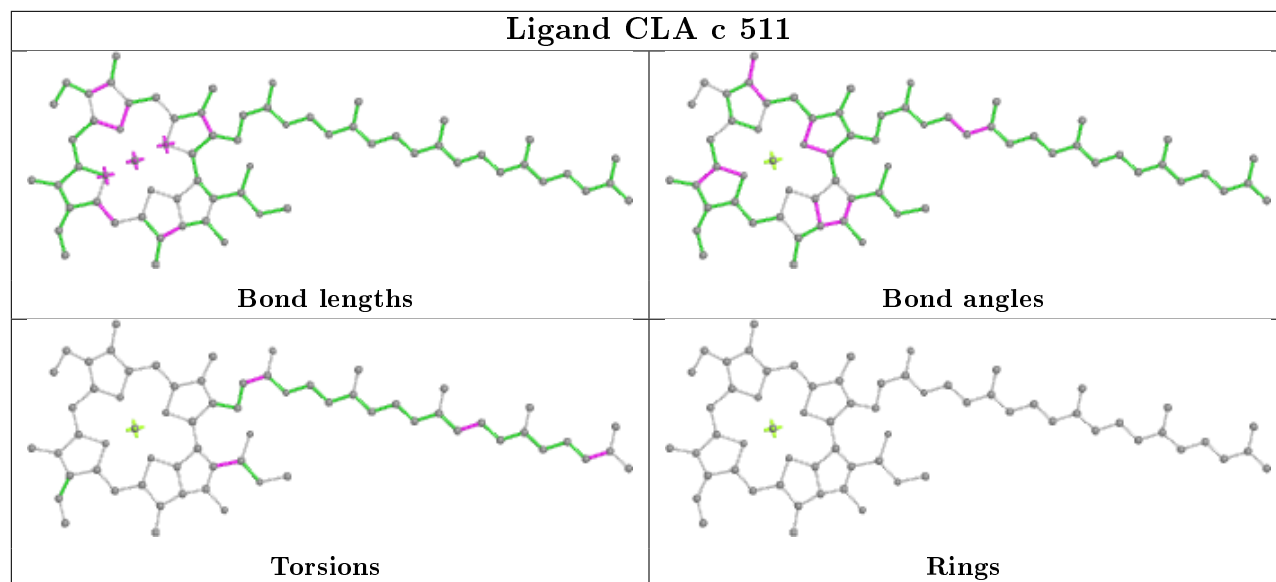




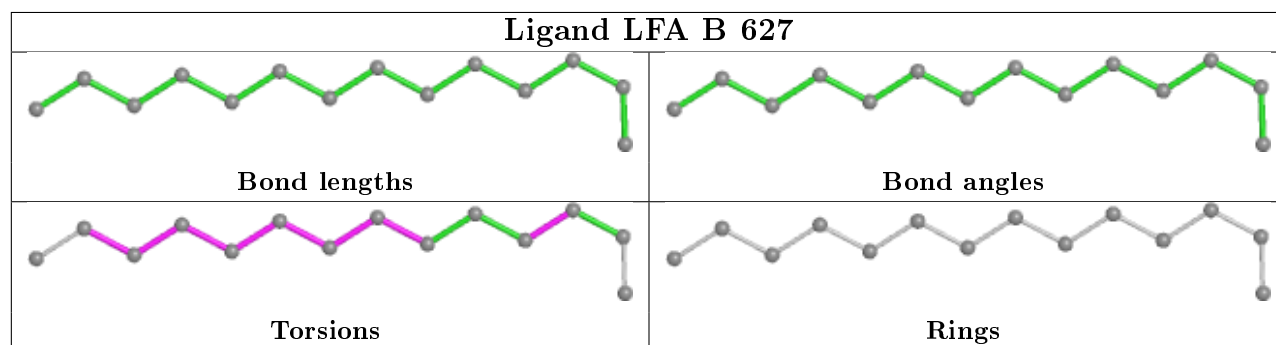




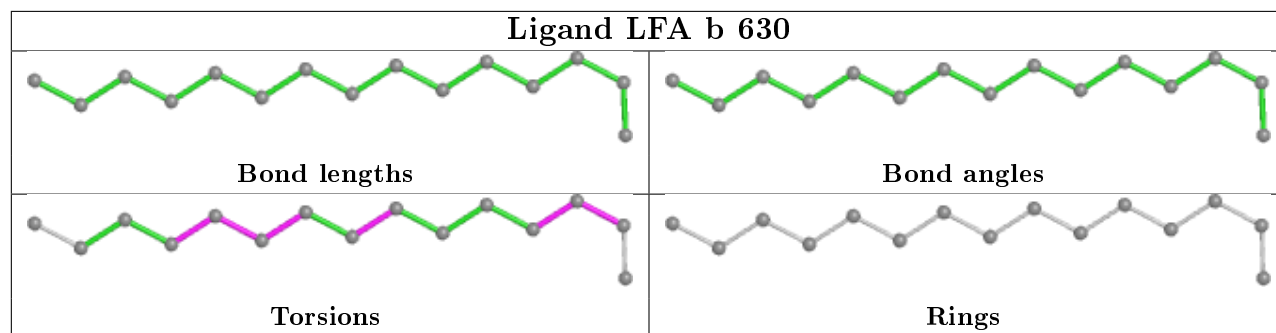
Ligand CLA c 511



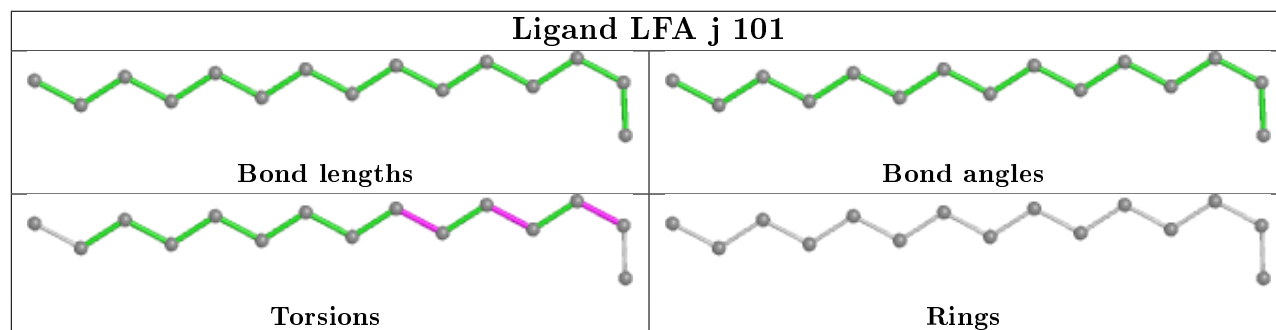
Ligand LFA B 627

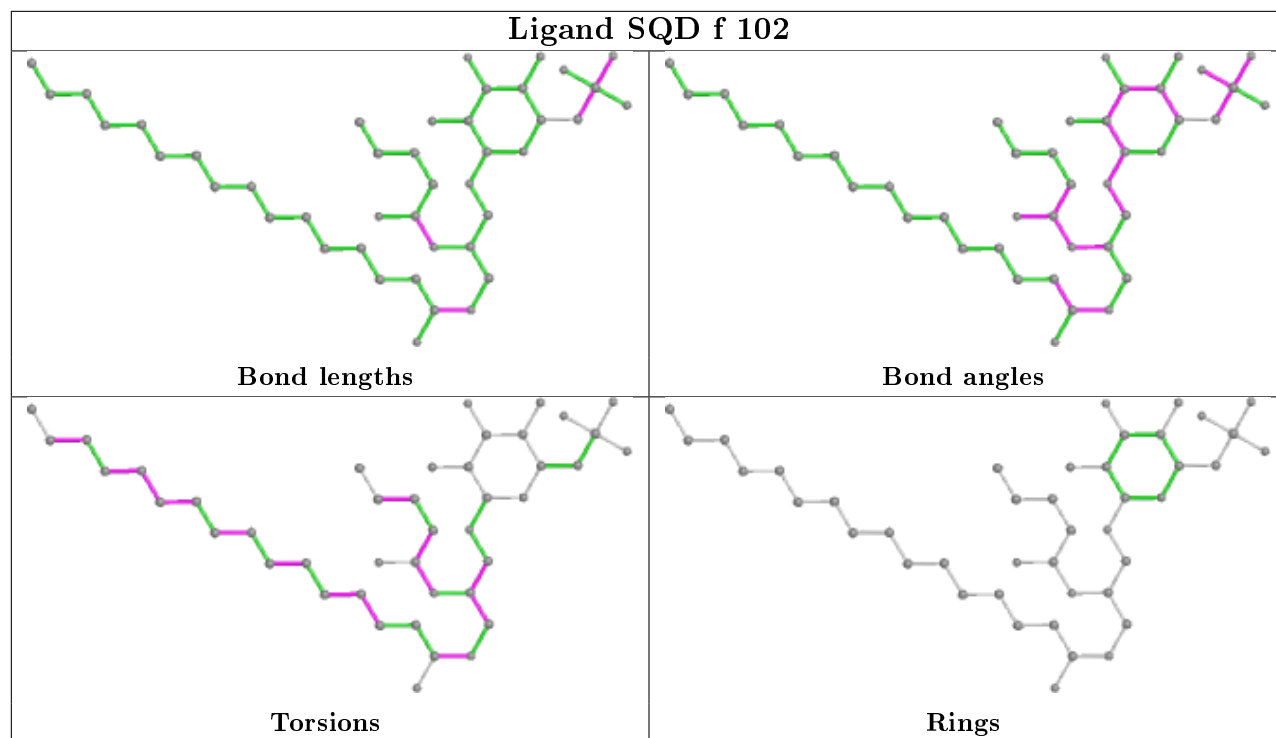
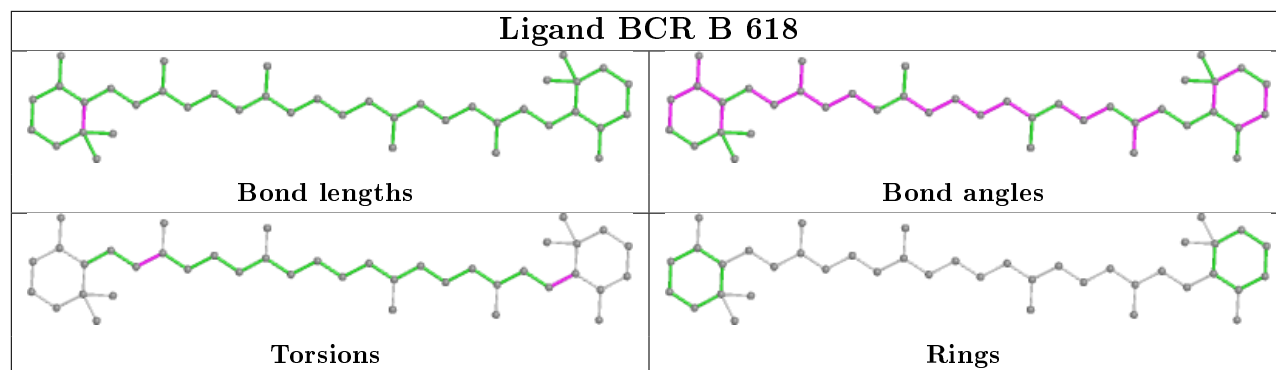


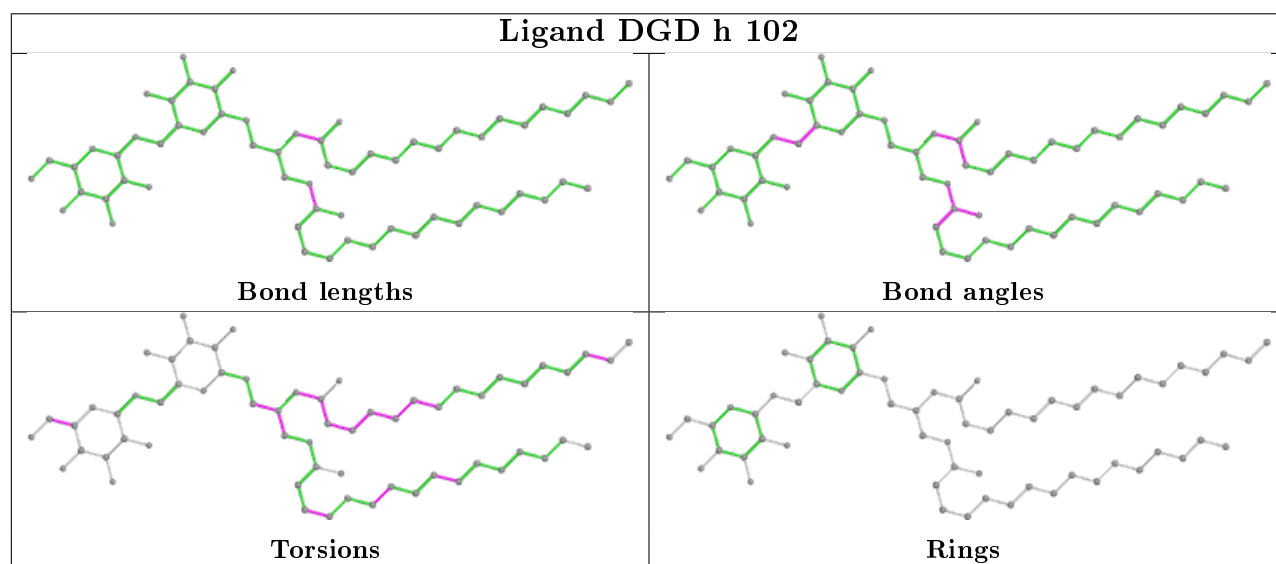
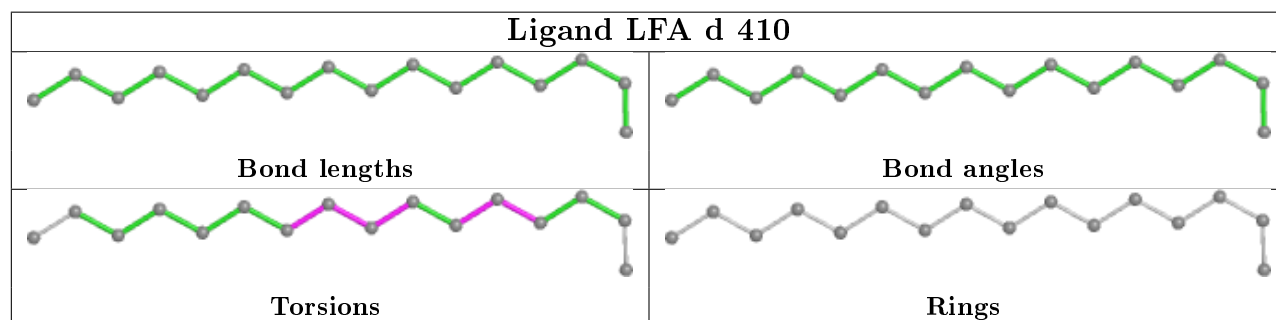
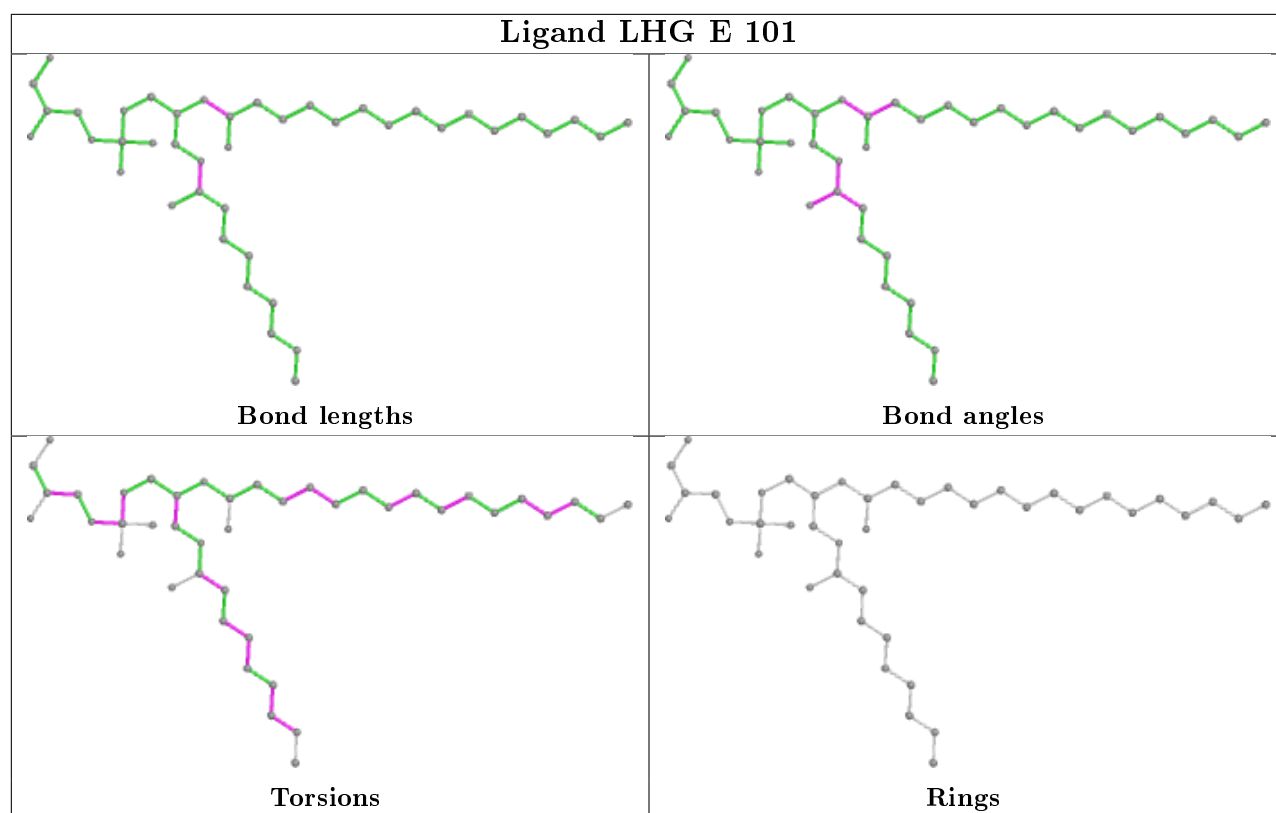
Ligand LFA b 630



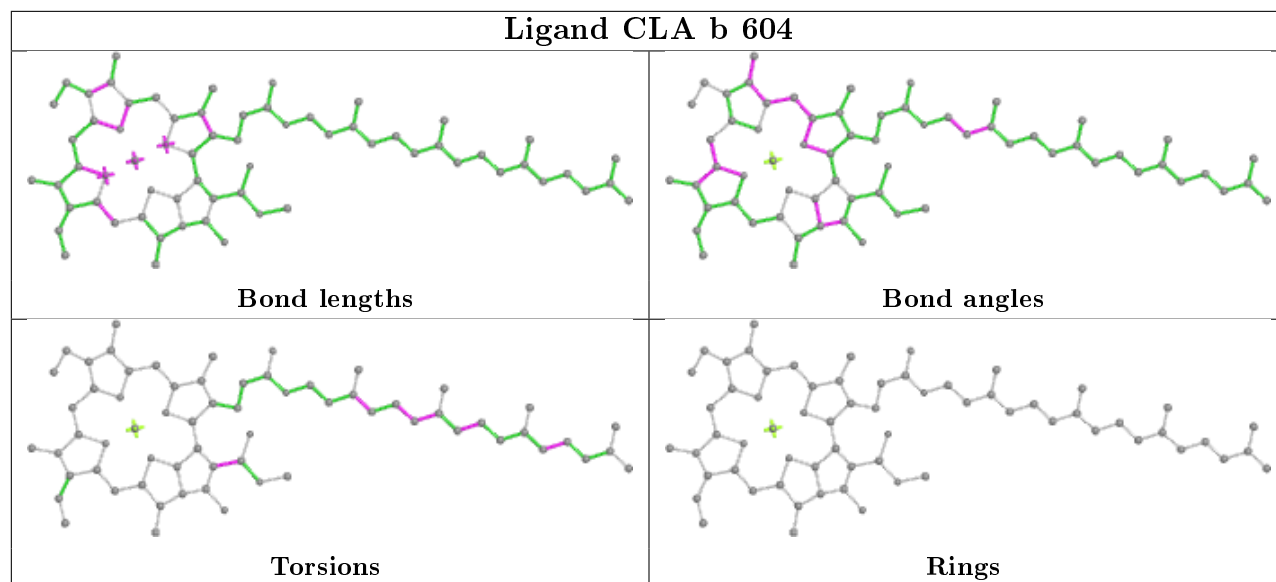
Ligand LFA j 101



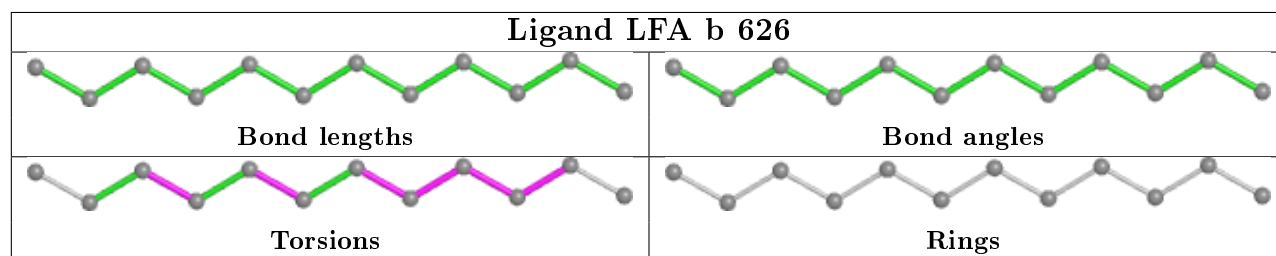




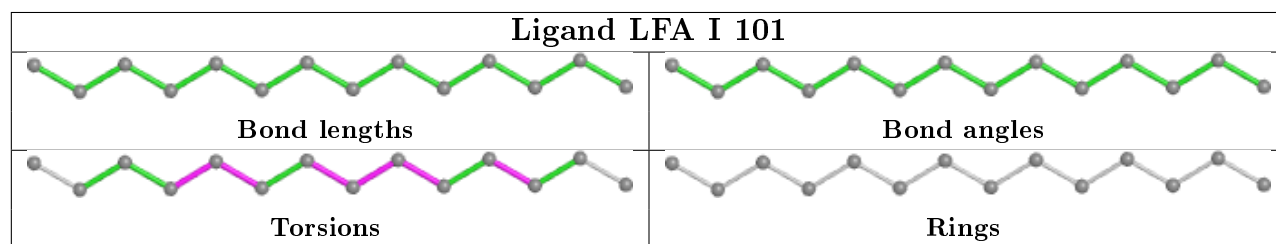
Ligand CLA b 604



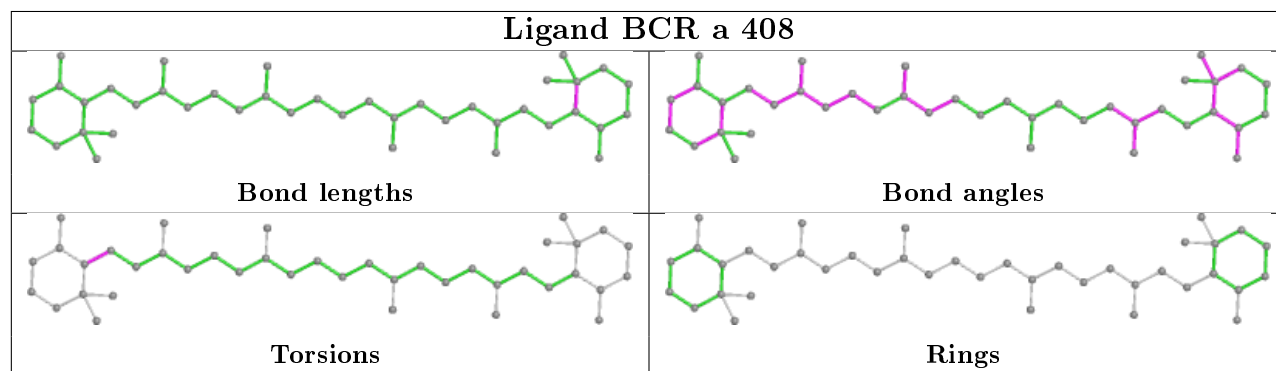
Ligand LFA b 626



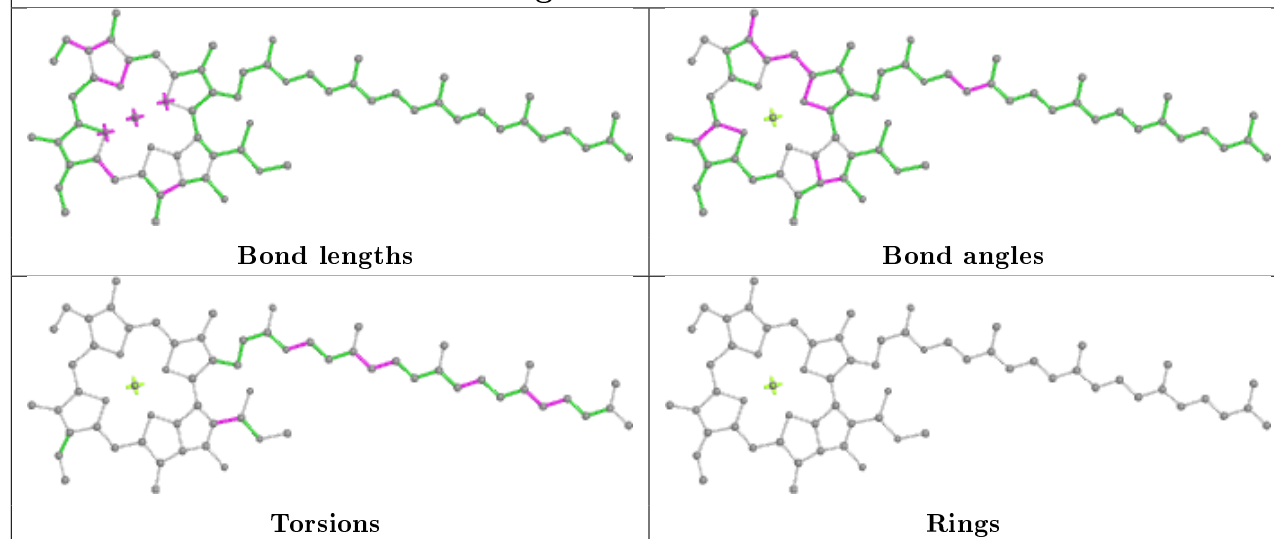
Ligand LFA I 101



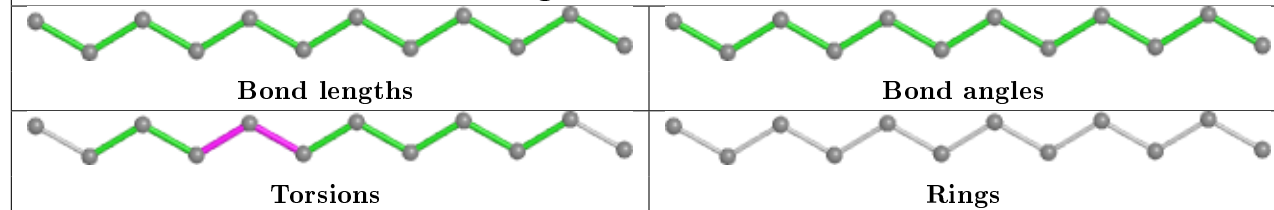
Ligand BCR a 408



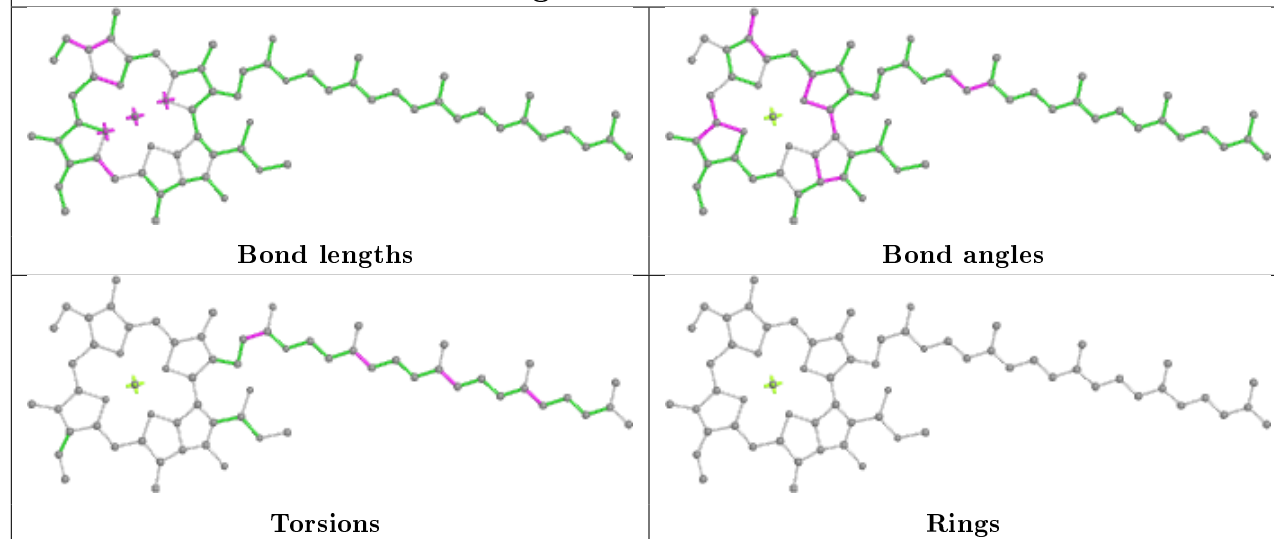
Ligand CLA b 616

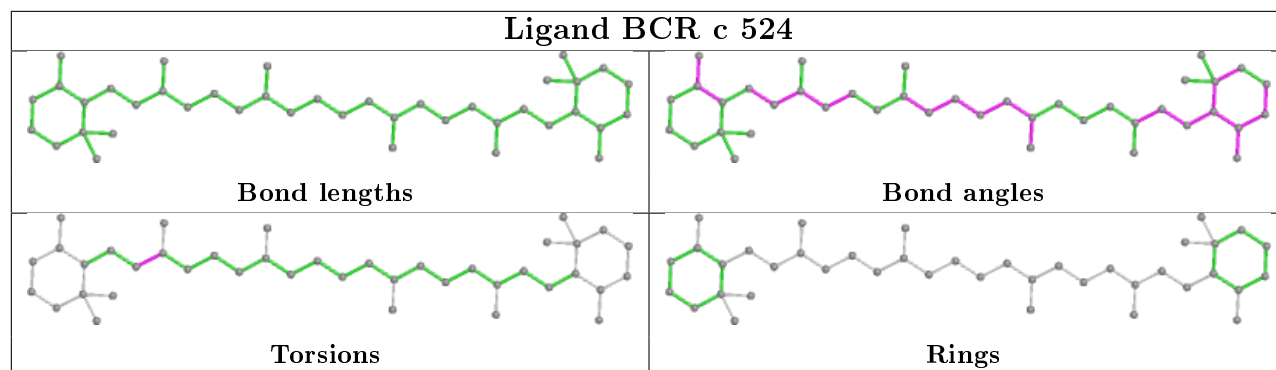
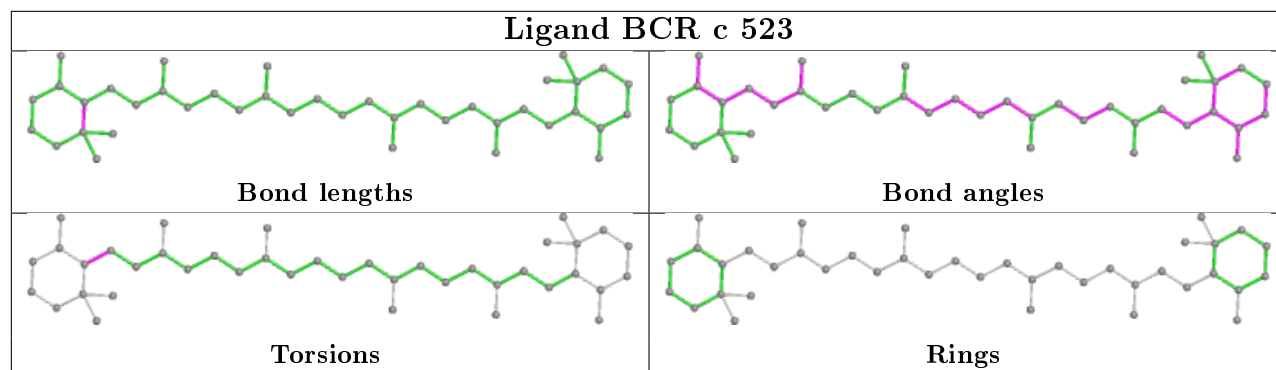
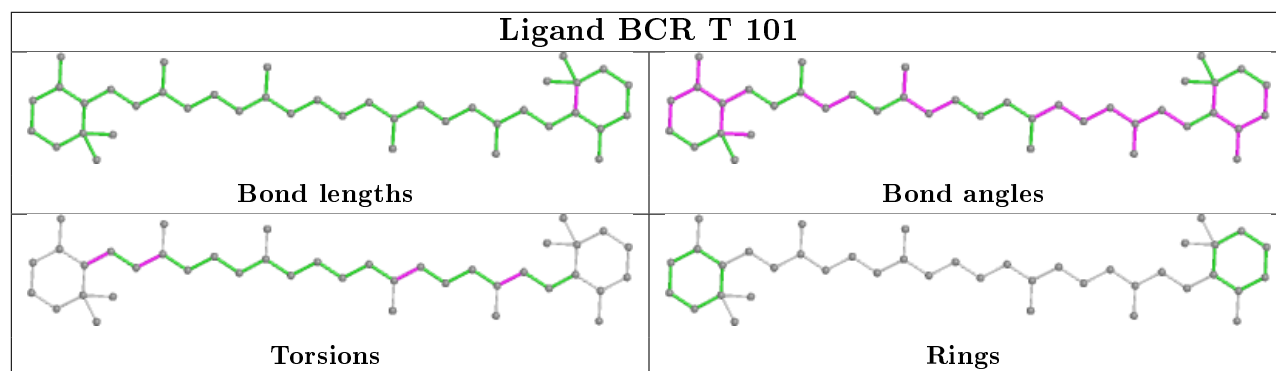
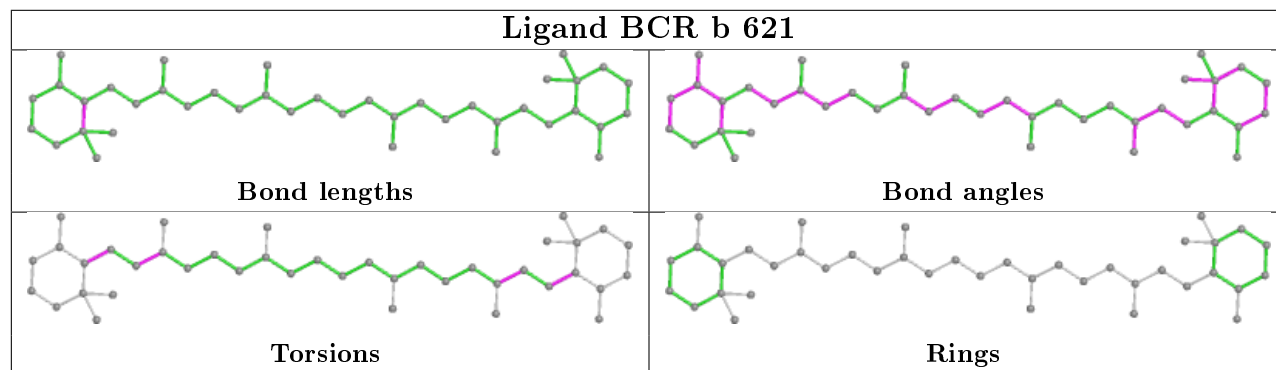


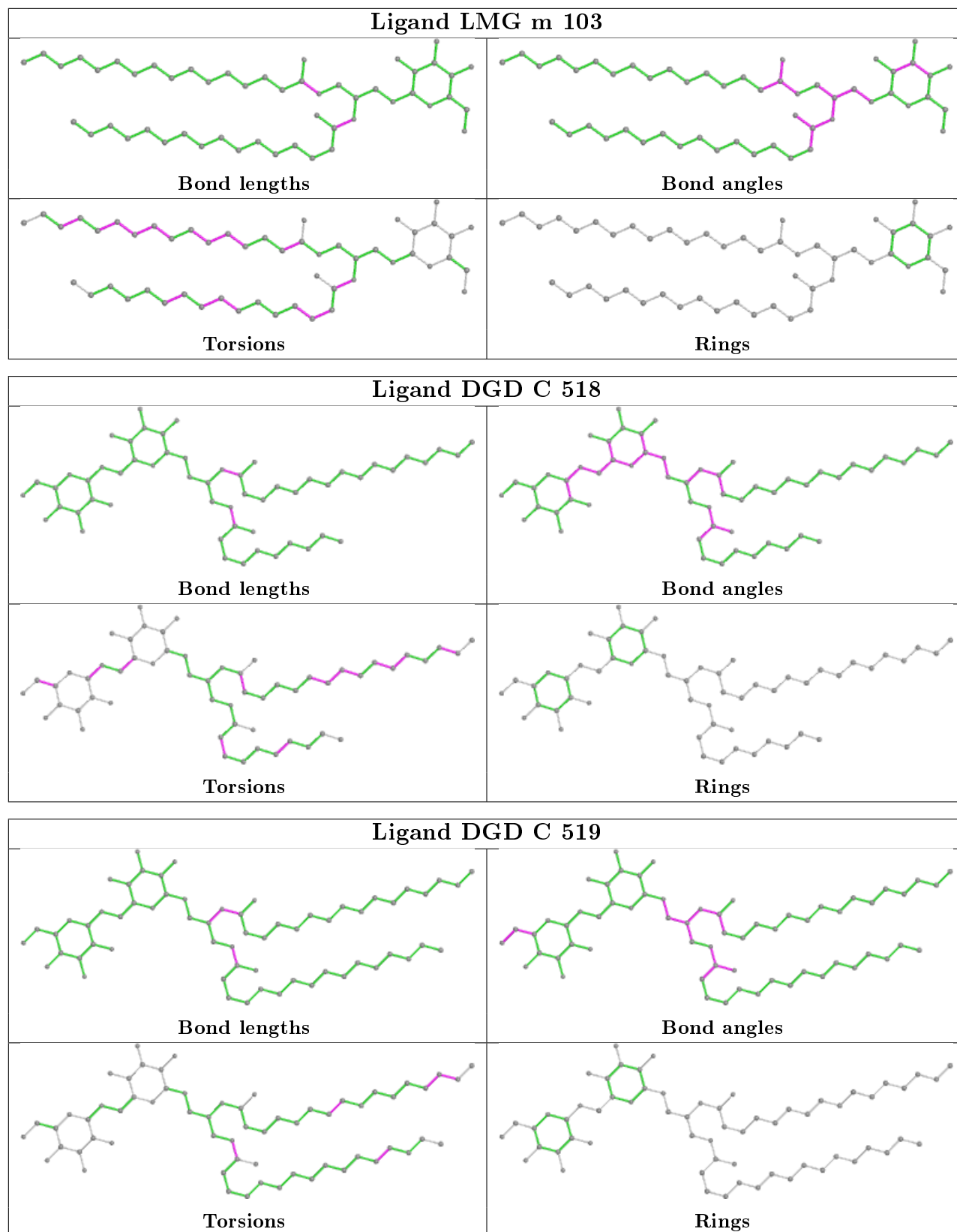
Ligand LFA B 628

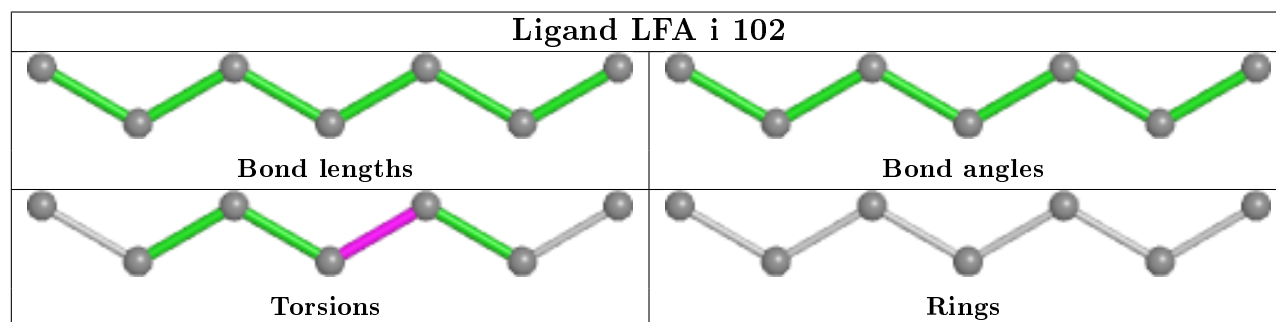
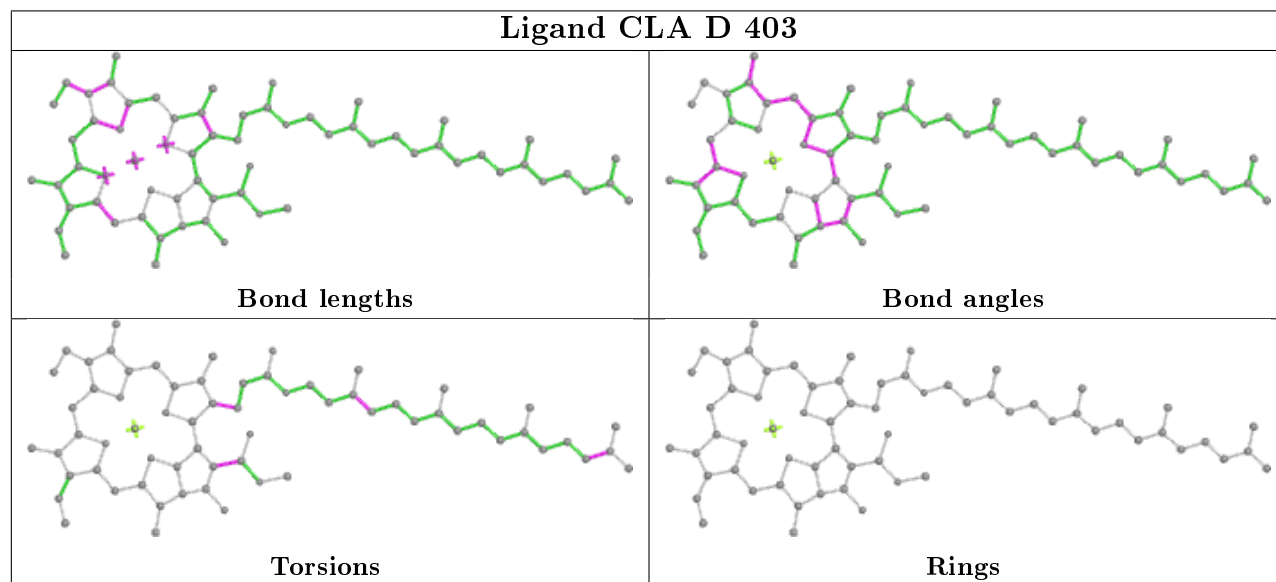
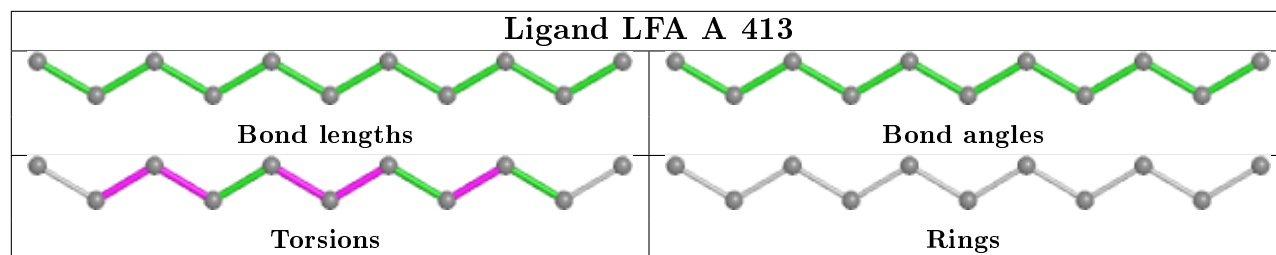


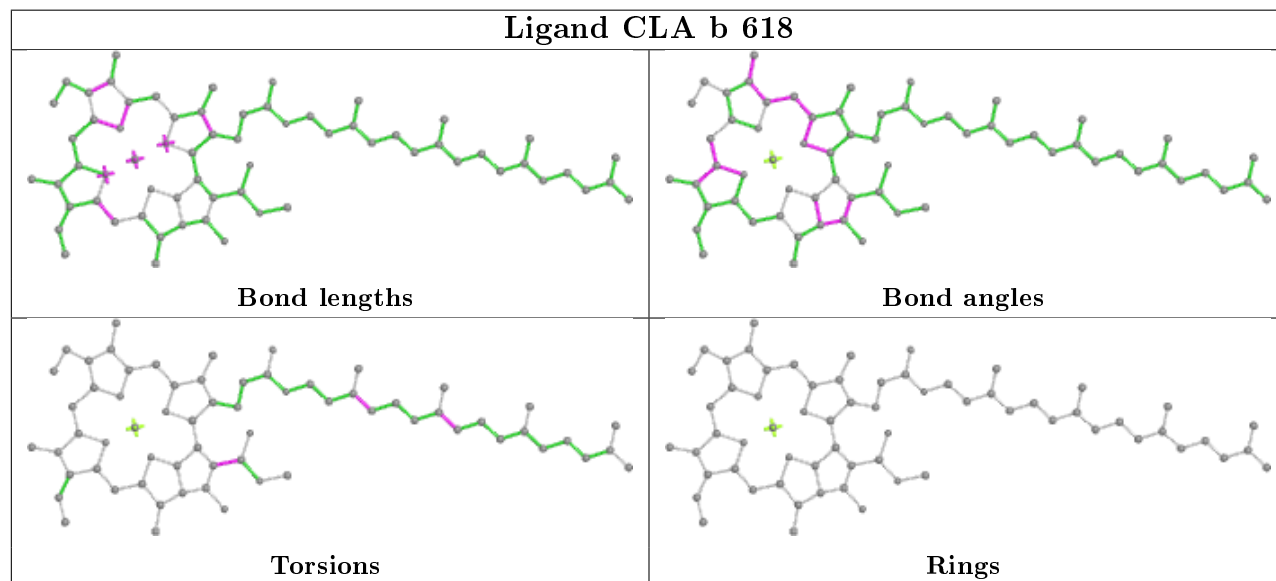
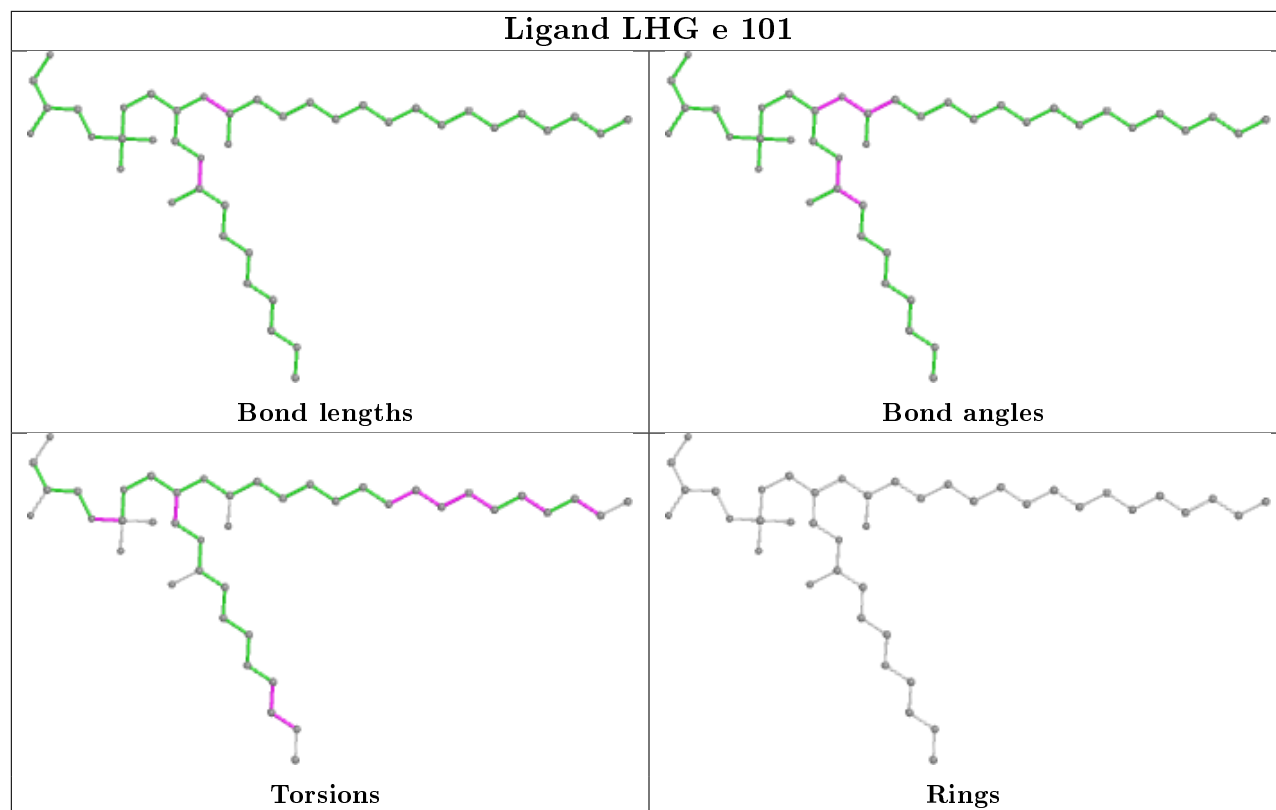
Ligand CLA C 506

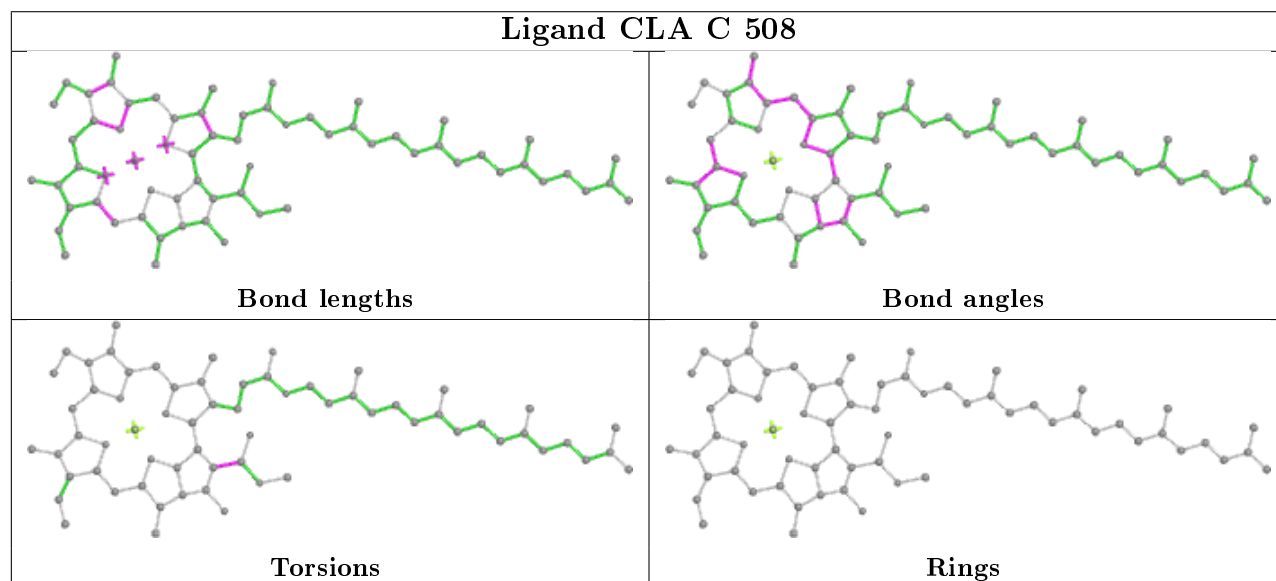
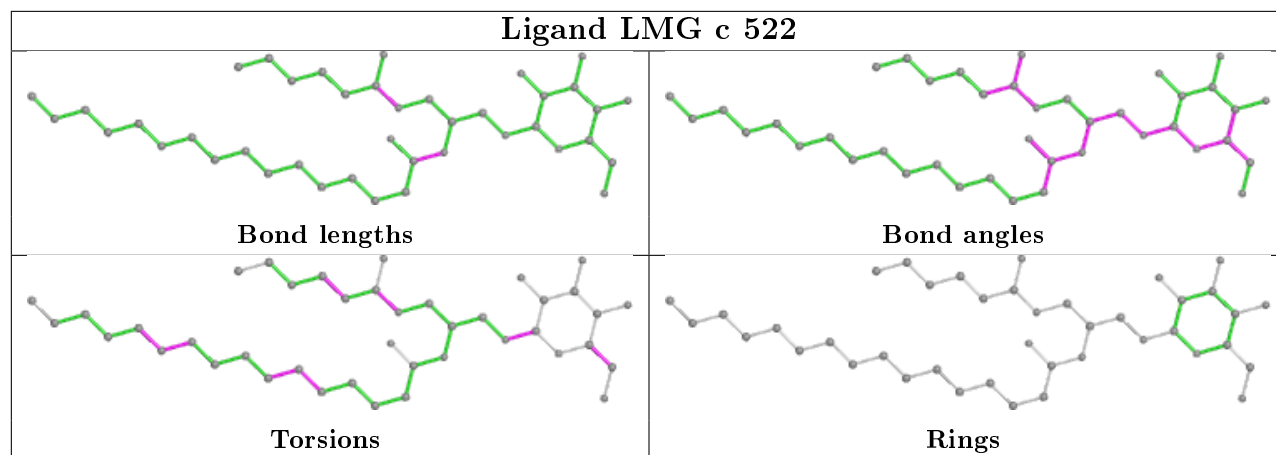


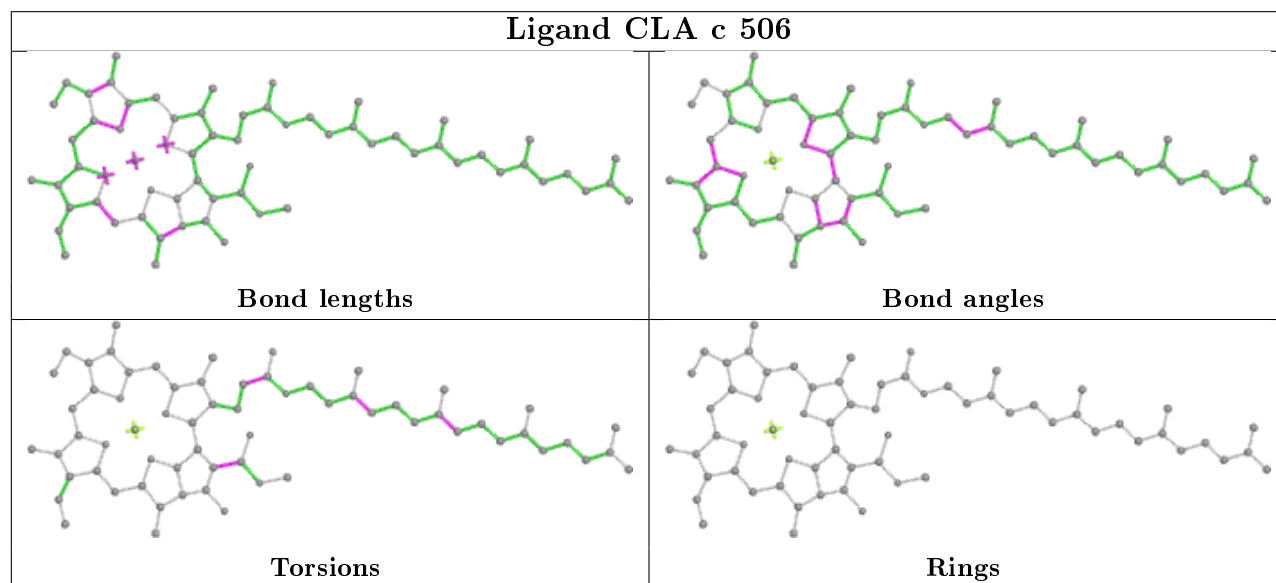
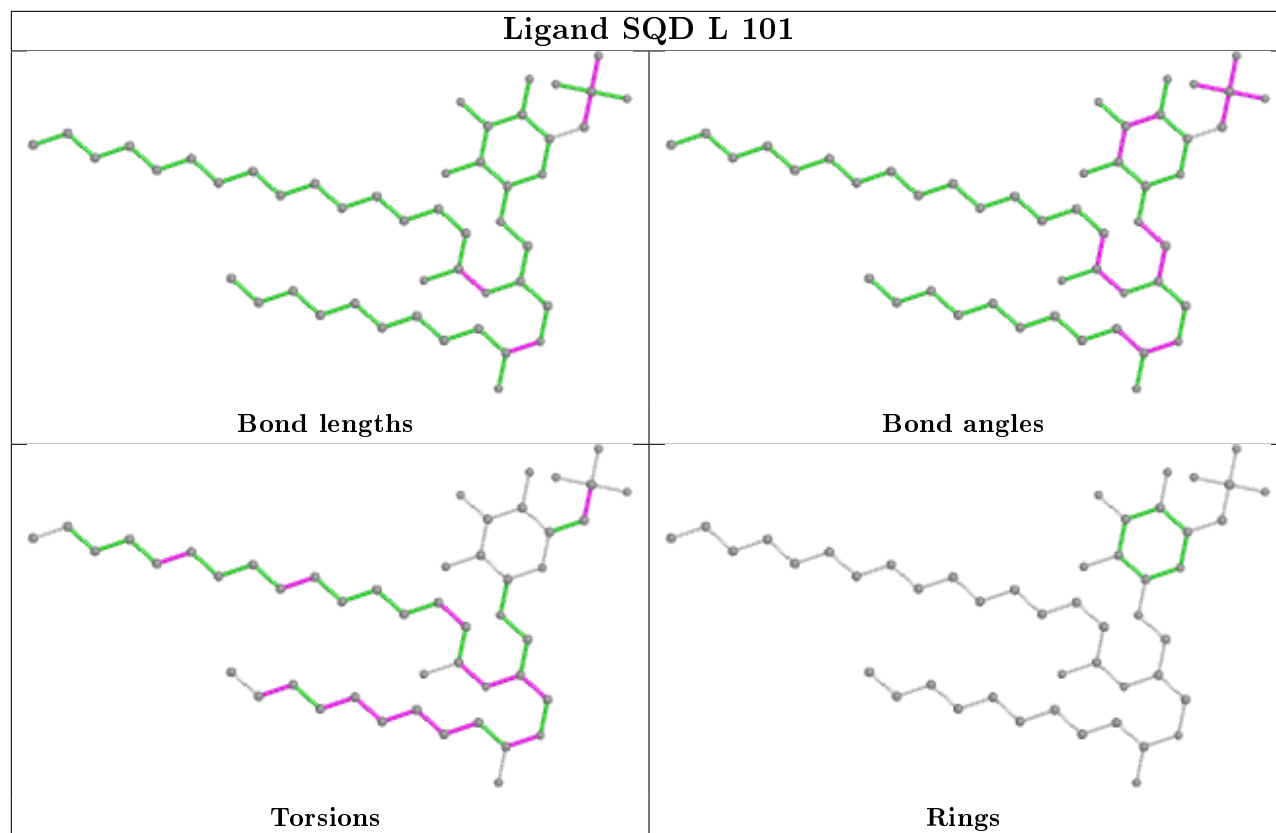
Ligand BCR c 524**Ligand BCR c 523****Ligand BCR T 101****Ligand BCR b 621**

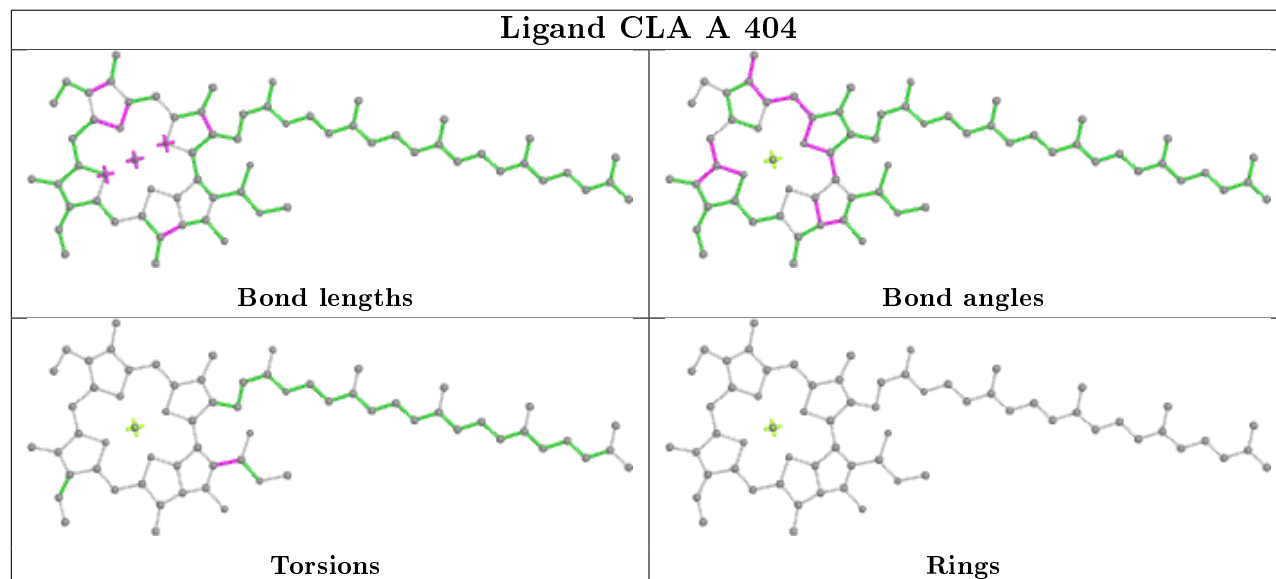
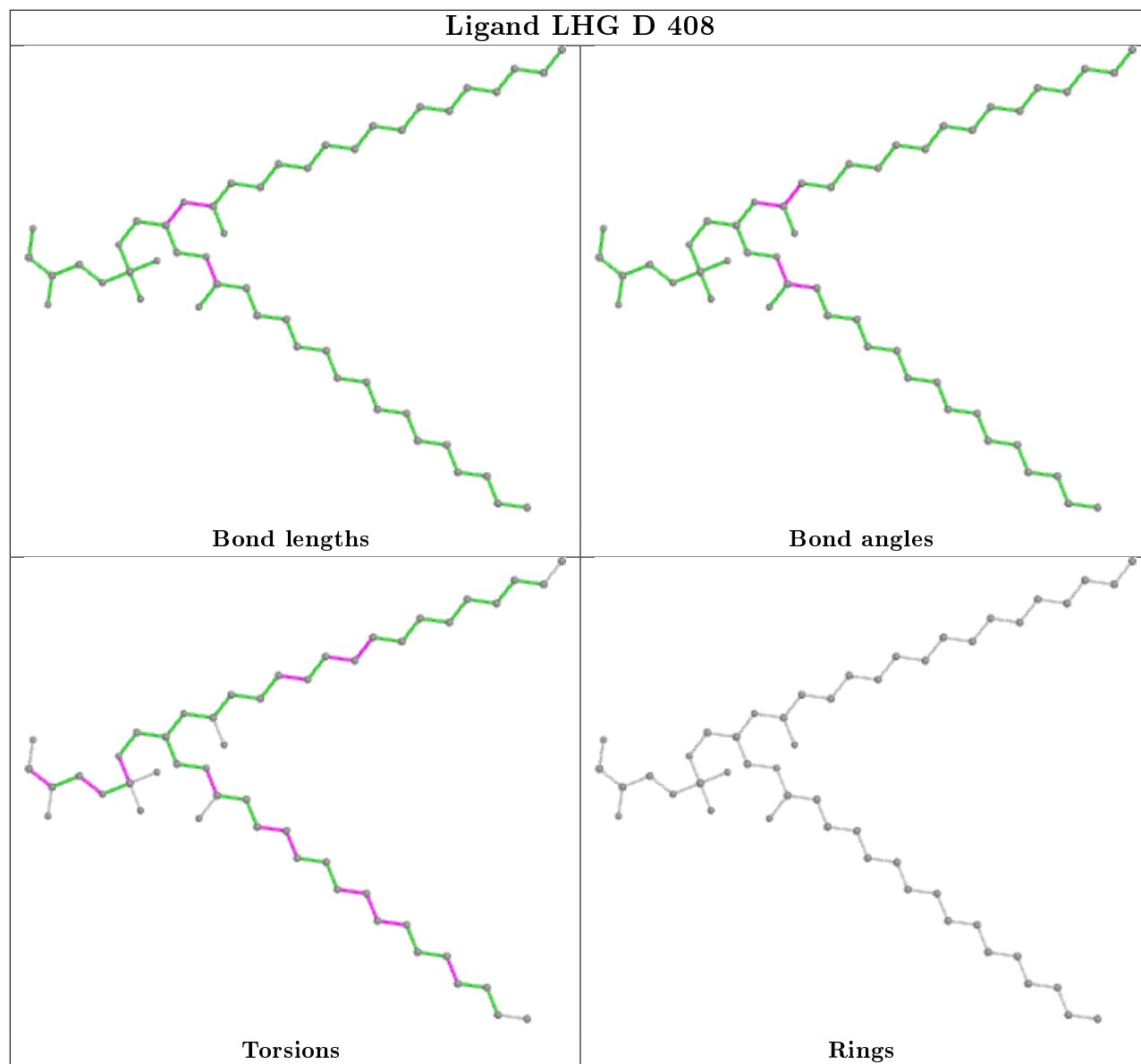


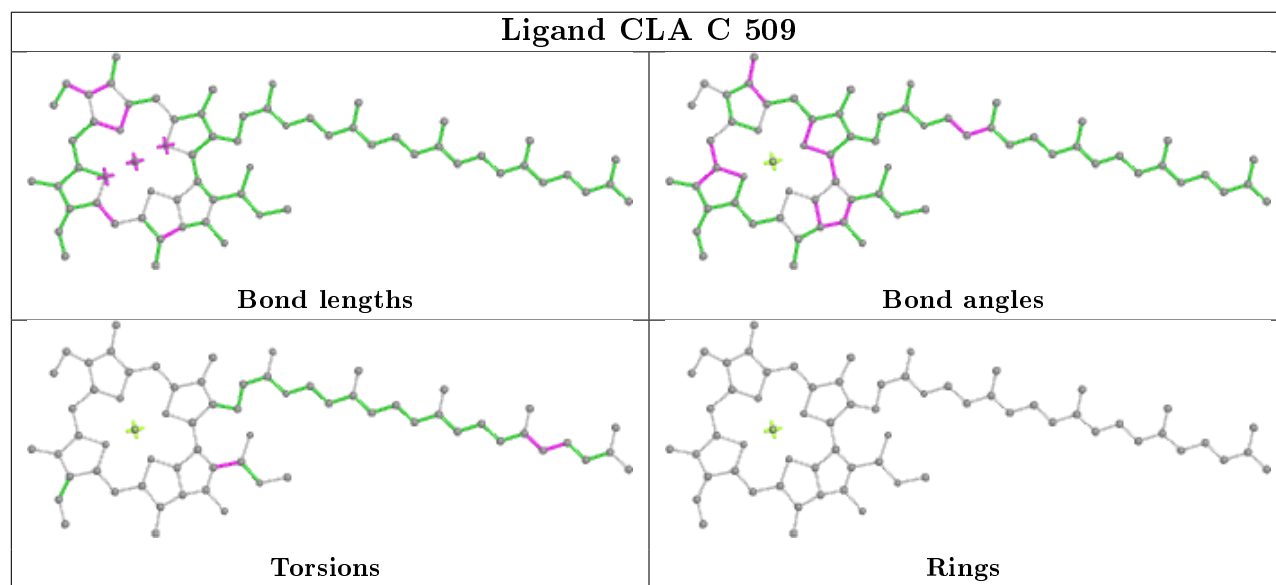
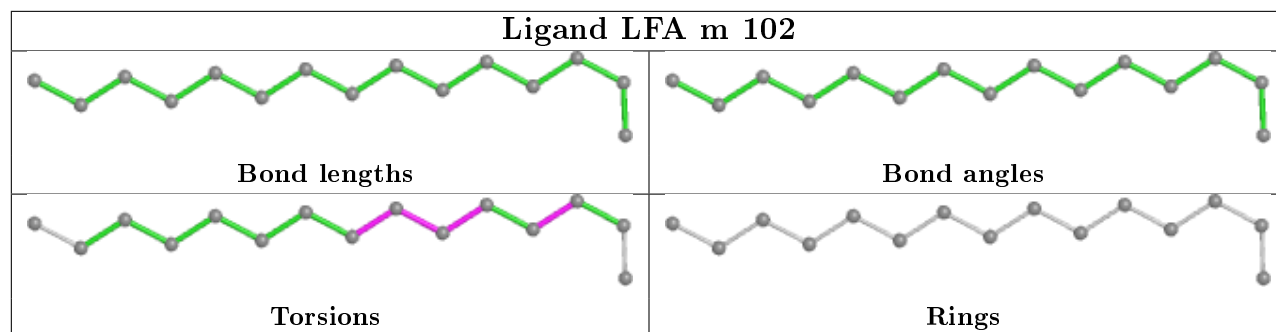


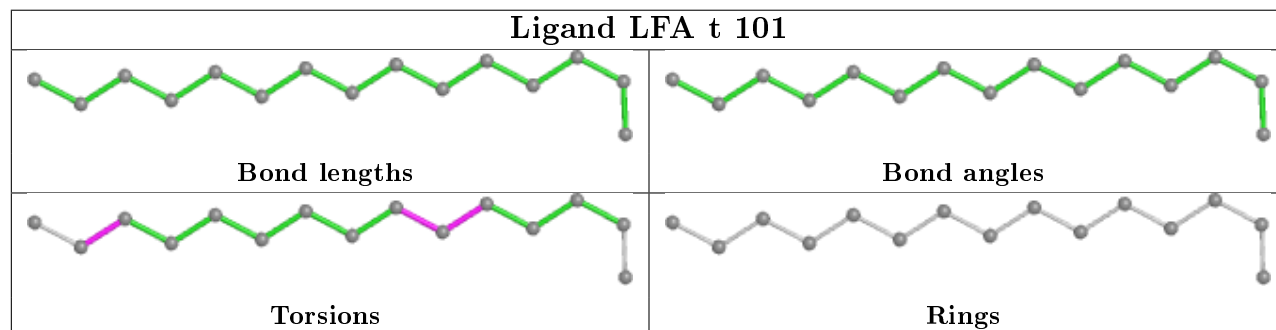
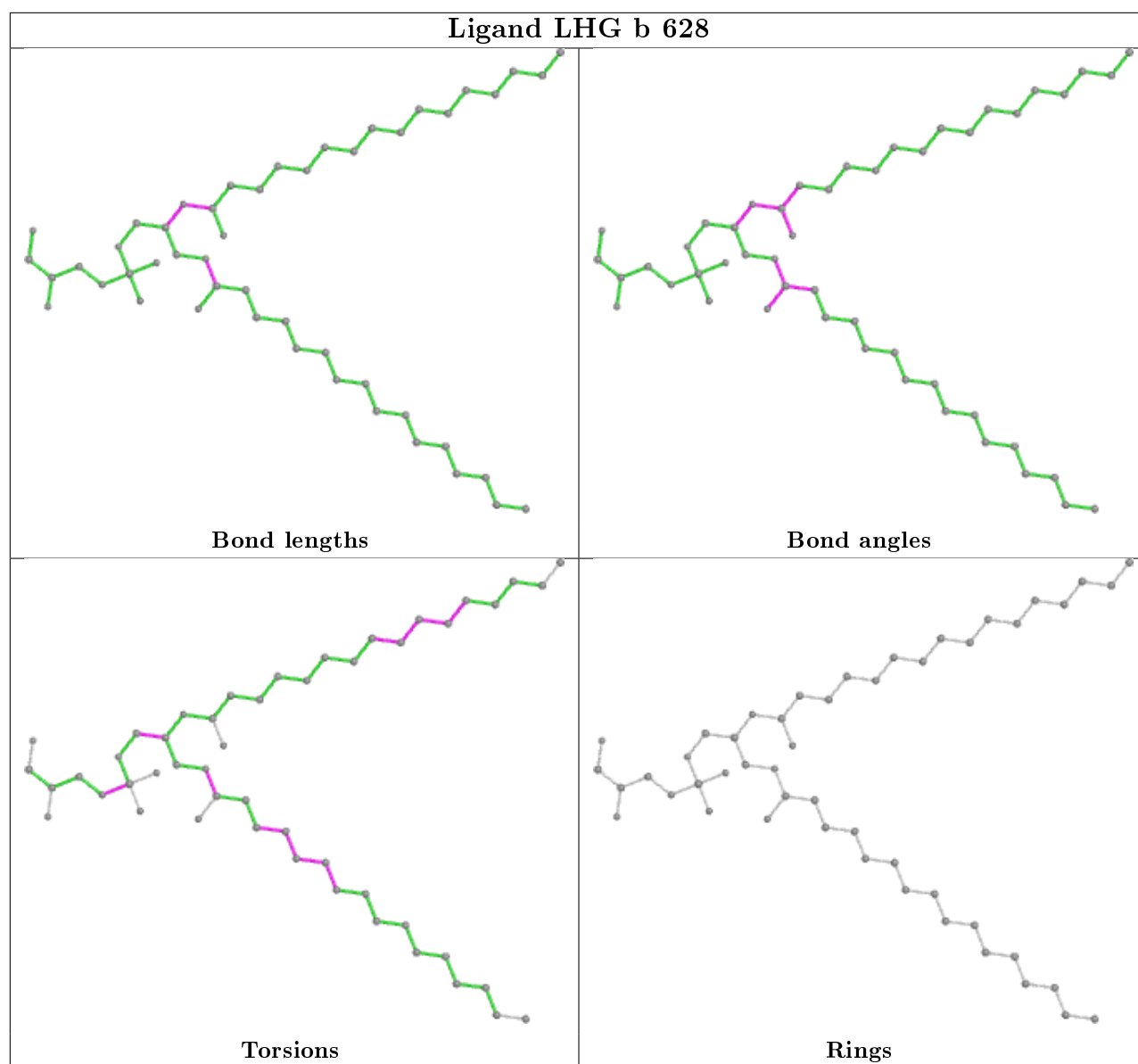


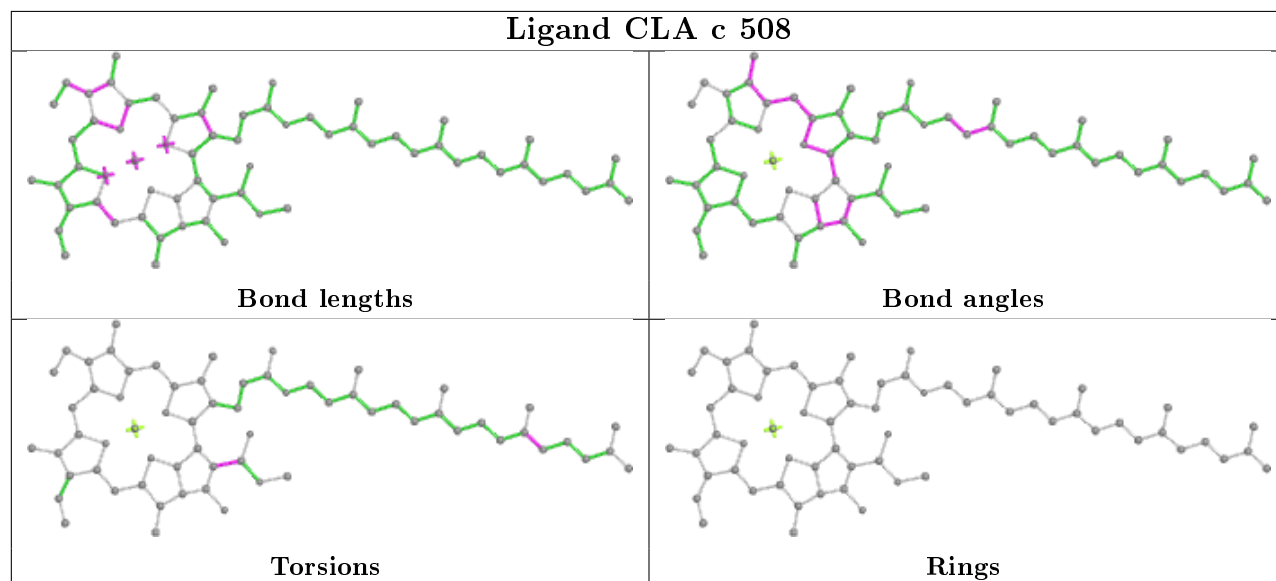
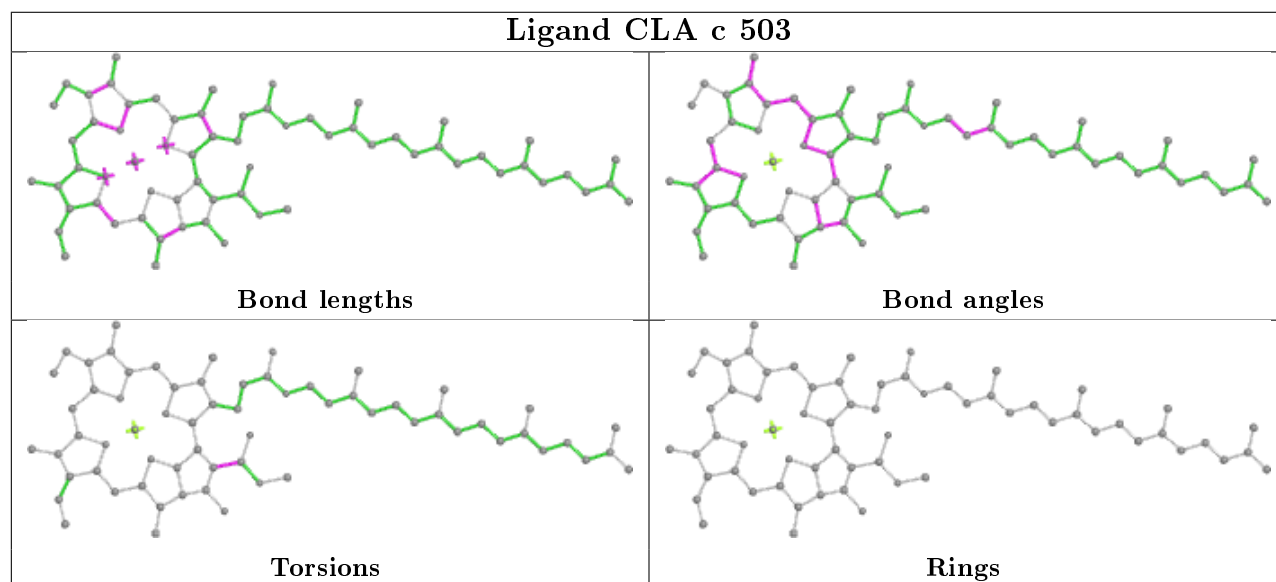
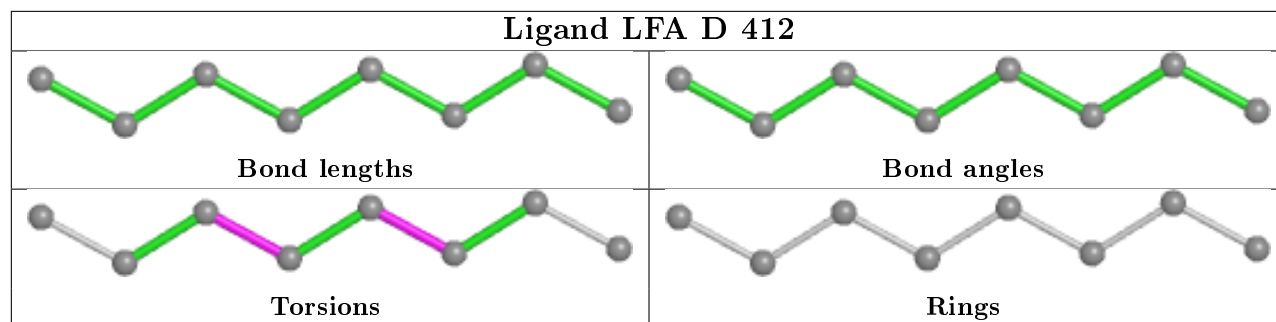




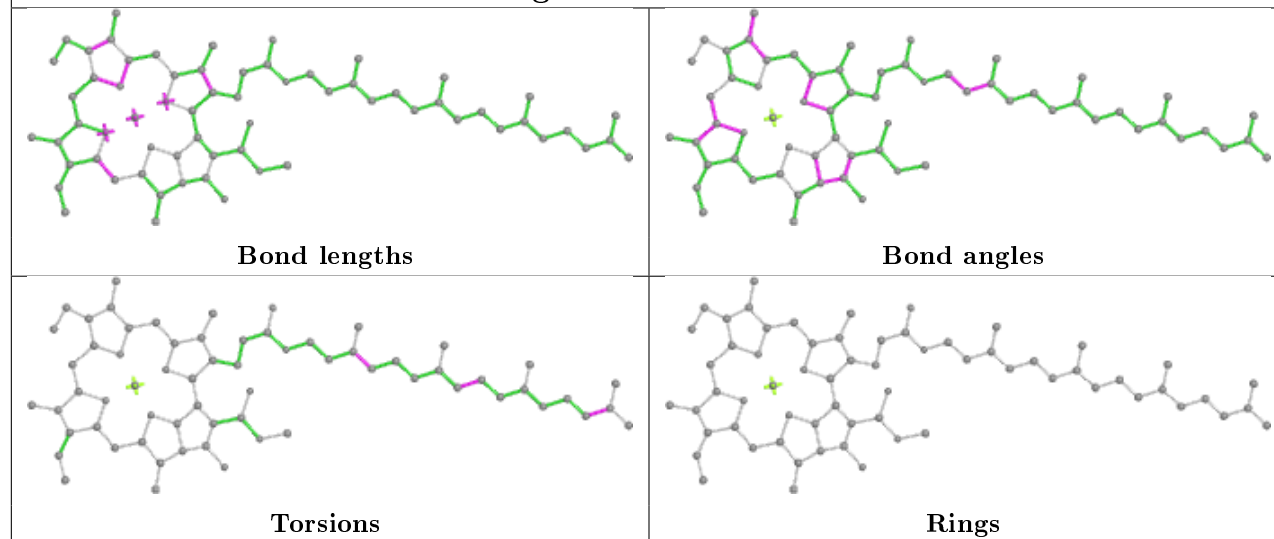




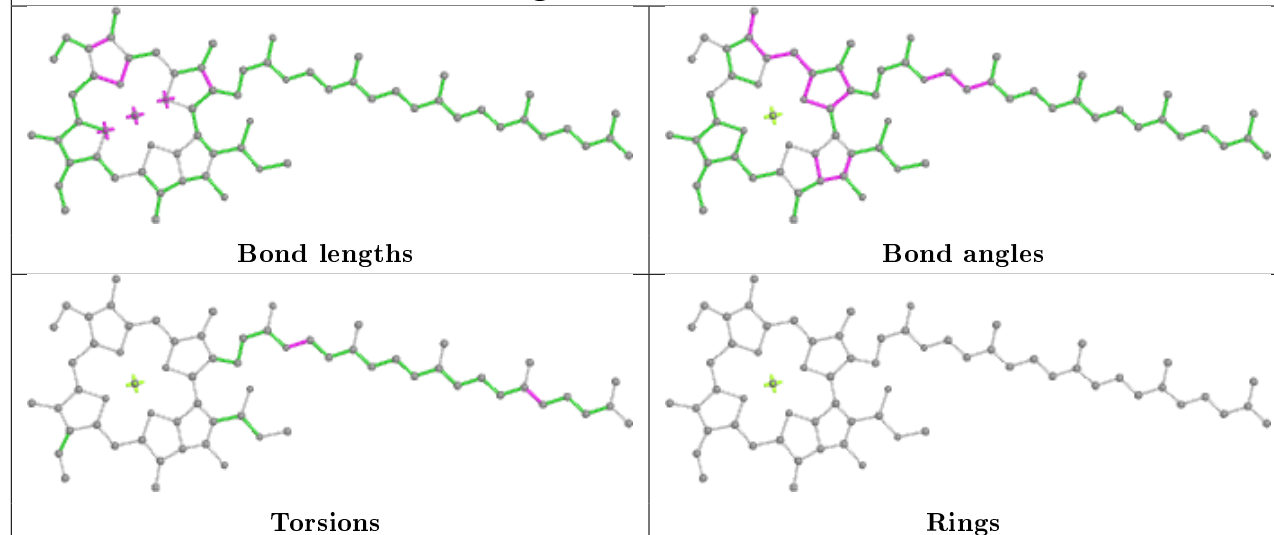




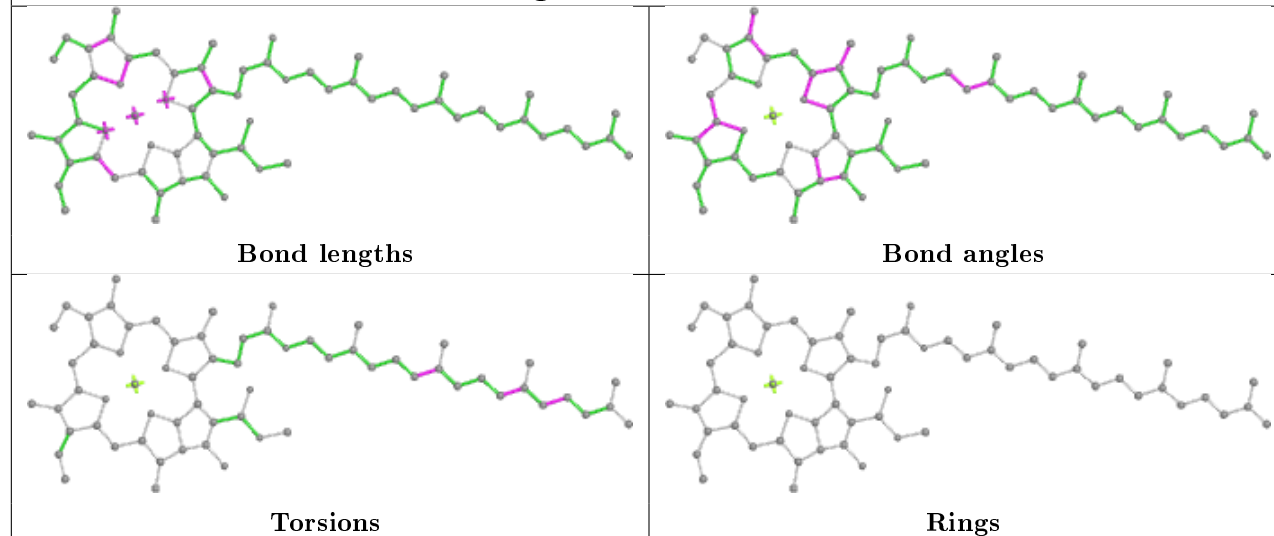
Ligand CLA B 610



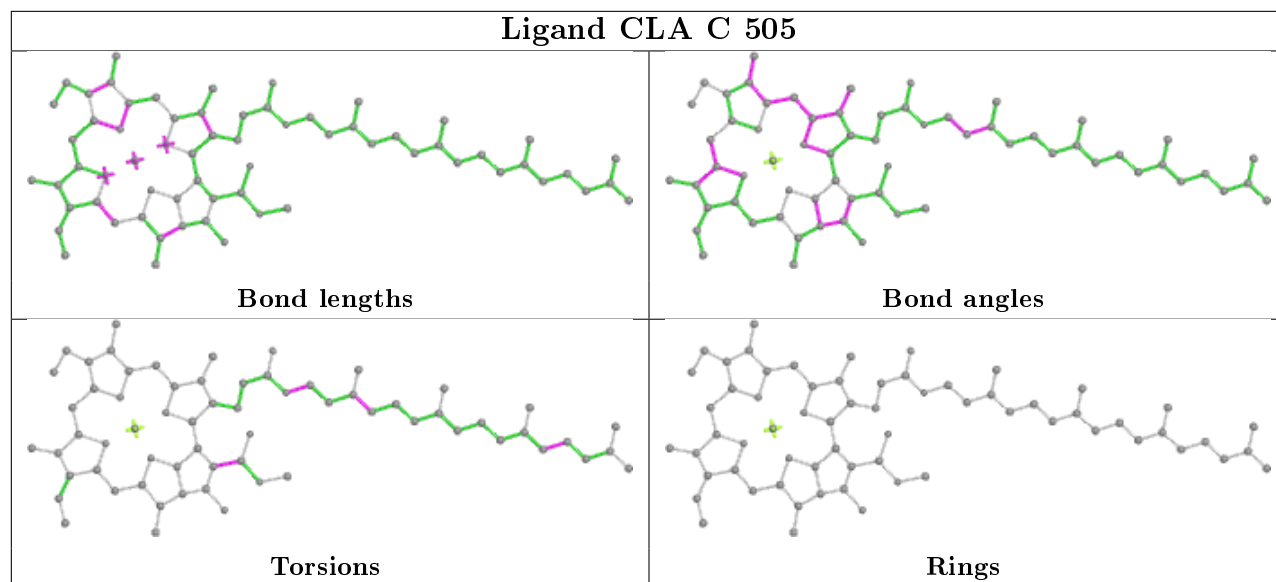
Ligand CLA D 402



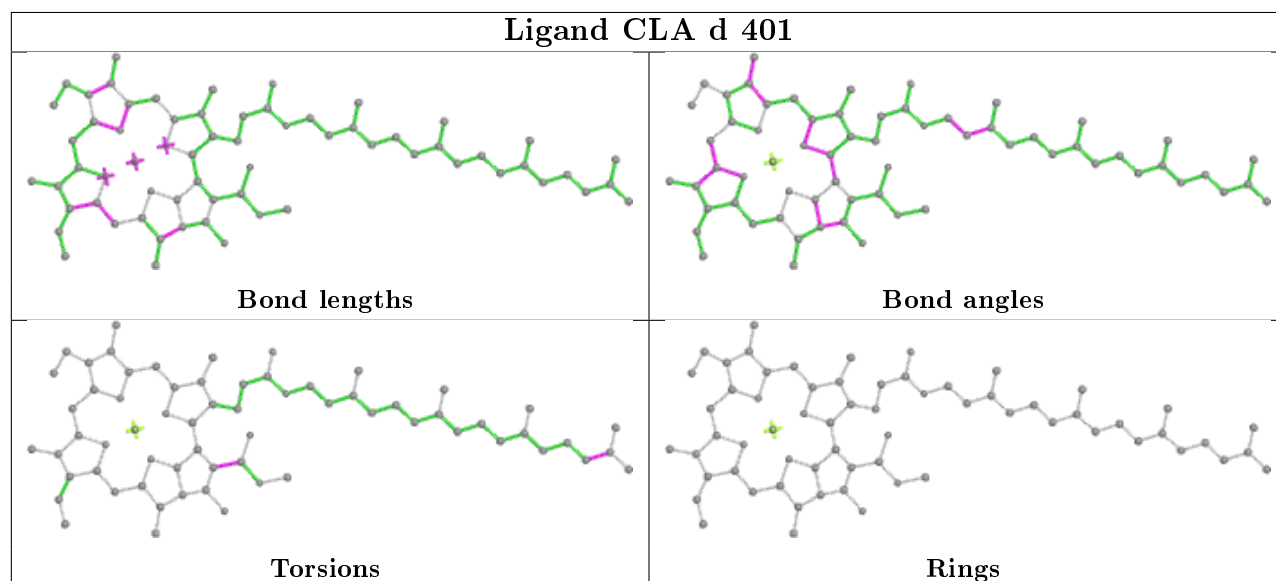
Ligand CLA B 602



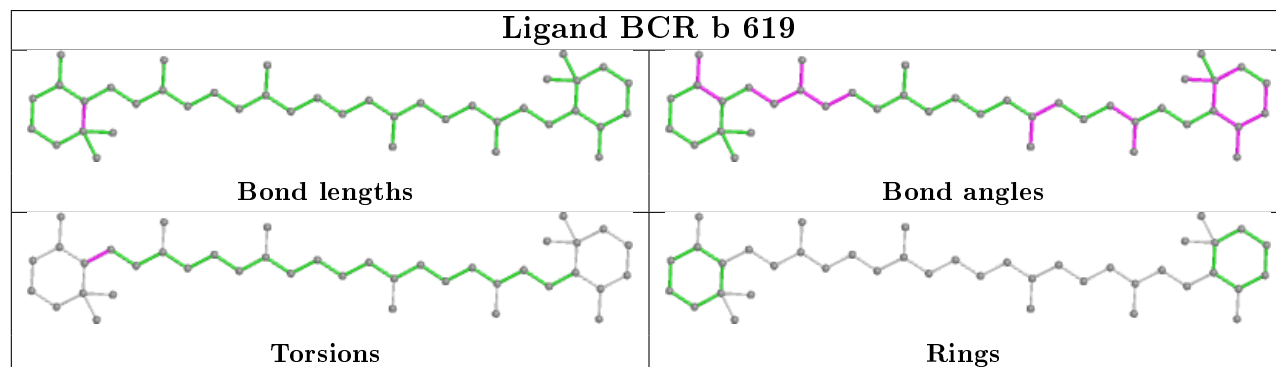
Ligand CLA C 505

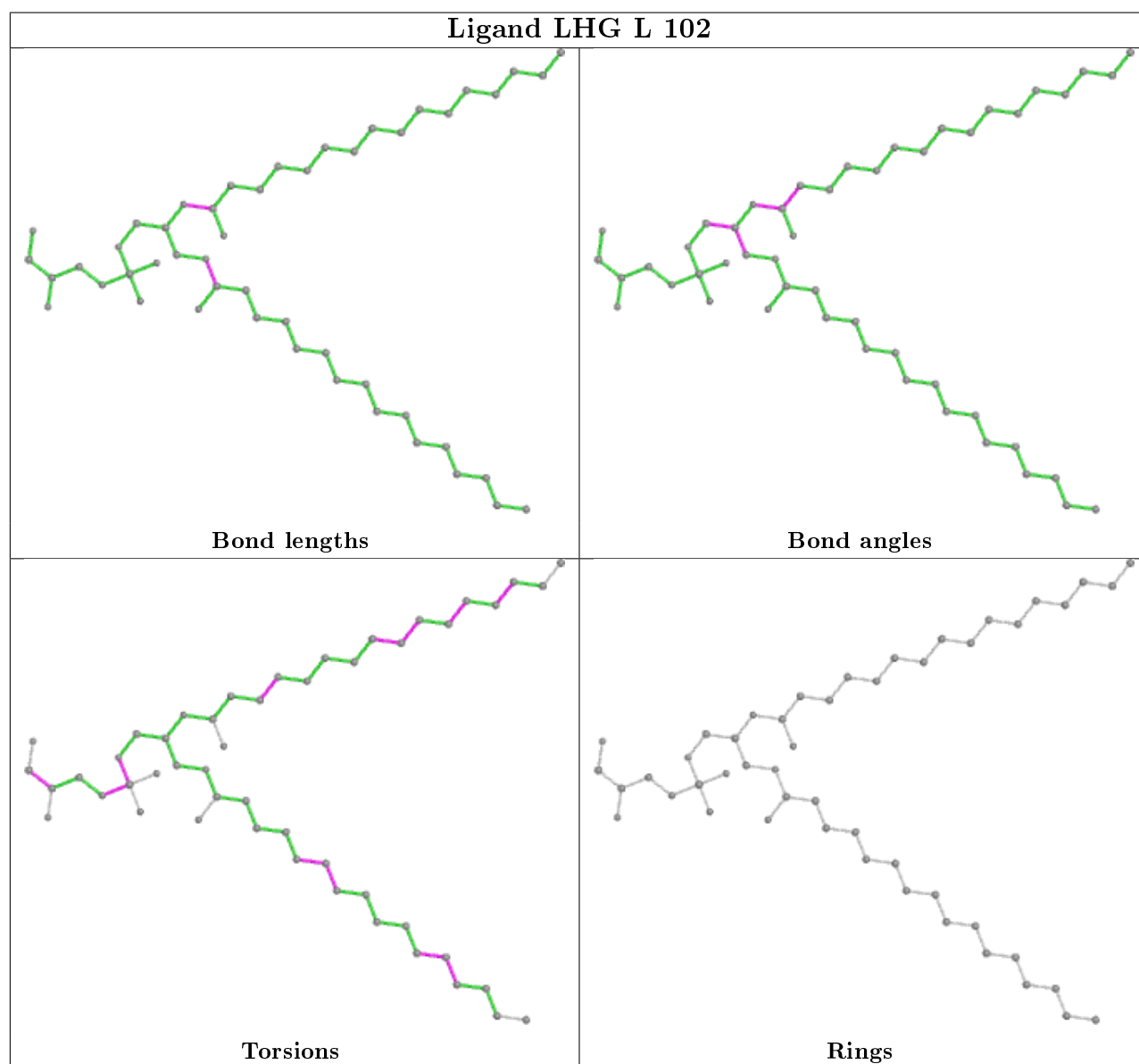
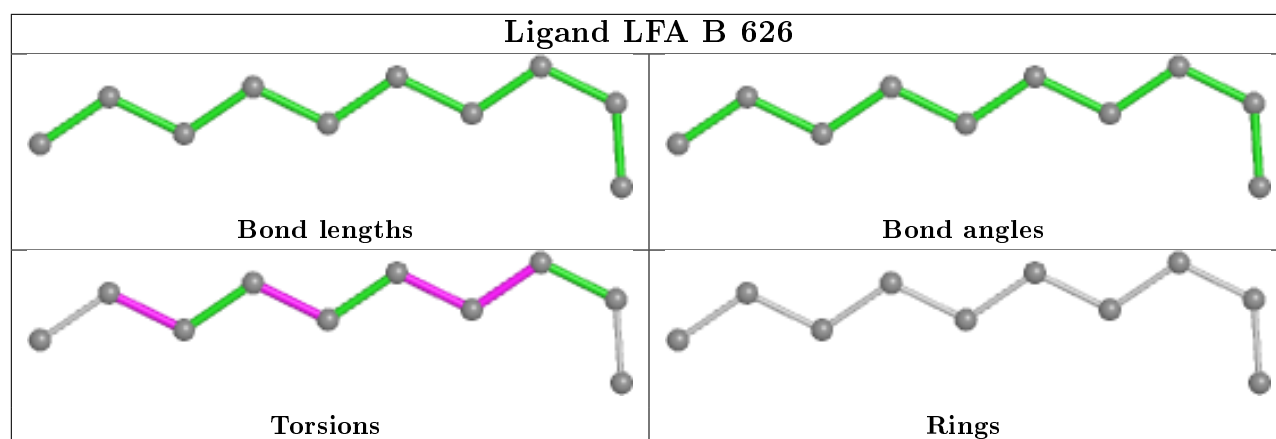


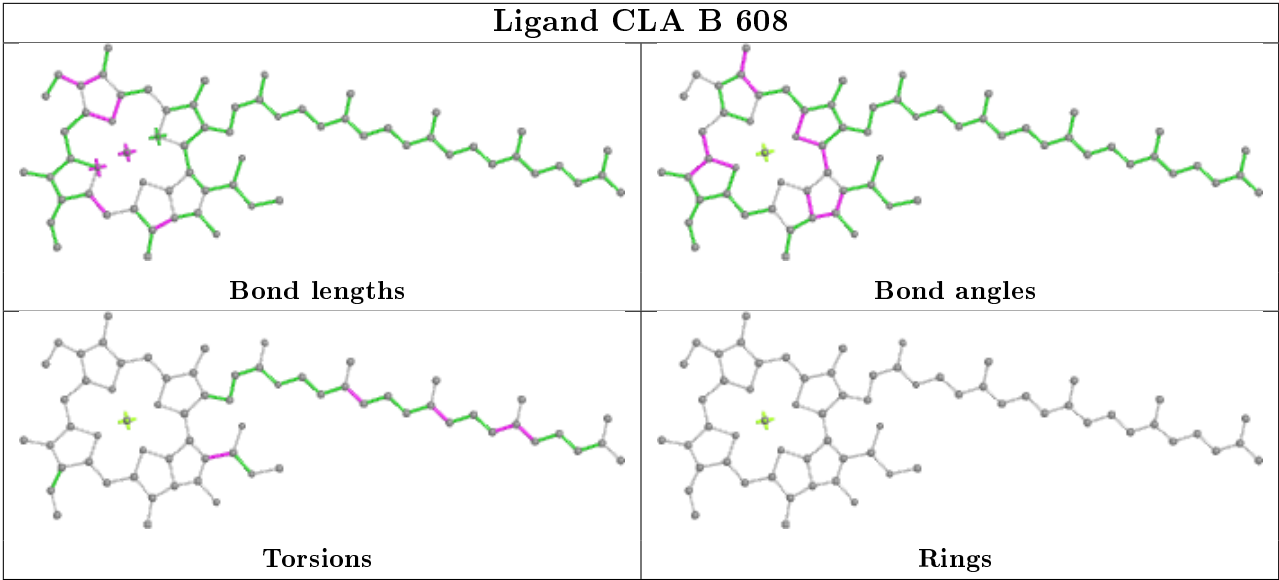
Ligand CLA d 401



Ligand BCR b 619







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	c	1
5	e	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	c	399:ALA	C	400:PRO	N	1.19
1	e	63:ILE	C	64:PRO	N	1.13

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	333/344 (96%)	0.33	15 (4%) 33 32	17, 24, 47, 70	0
1	a	333/344 (96%)	0.15	7 (2%) 63 61	16, 24, 48, 66	0
2	B	505/510 (99%)	0.16	23 (4%) 32 31	16, 25, 55, 73	0
2	b	503/510 (98%)	0.20	37 (7%) 14 13	19, 30, 59, 90	0
3	C	447/461 (96%)	0.23	23 (5%) 28 26	20, 32, 50, 83	0
3	c	448/461 (97%)	0.08	12 (2%) 54 52	21, 32, 46, 67	0
4	D	340/352 (96%)	0.08	7 (2%) 63 61	16, 25, 42, 62	0
4	d	340/352 (96%)	0.06	1 (0%) 94 93	17, 28, 48, 67	0
5	E	81/84 (96%)	0.60	6 (7%) 14 13	29, 46, 59, 76	0
5	e	79/84 (94%)	0.92	17 (21%) 0 0	34, 50, 68, 87	0
6	F	33/45 (73%)	0.02	1 (3%) 50 48	32, 39, 49, 58	0
6	f	33/45 (73%)	-0.03	2 (6%) 21 20	39, 44, 61, 63	0
7	H	62/66 (93%)	0.00	0 100 100	25, 30, 36, 45	0
7	h	63/66 (95%)	0.46	7 (11%) 5 4	34, 39, 50, 55	0
8	I	33/38 (86%)	-0.16	0 100 100	23, 28, 35, 43	0
8	i	33/38 (86%)	-0.22	1 (3%) 50 48	21, 28, 39, 45	0
9	J	33/40 (82%)	0.41	2 (6%) 21 20	33, 41, 49, 54	0
9	j	33/40 (82%)	0.34	3 (9%) 9 8	33, 41, 49, 56	0
10	K	35/46 (76%)	0.52	4 (11%) 5 4	41, 47, 69, 76	0
10	k	36/46 (78%)	0.17	3 (8%) 11 10	35, 45, 66, 77	0
11	L	36/37 (97%)	-0.30	0 100 100	18, 22, 46, 54	0
11	l	36/37 (97%)	-0.15	2 (5%) 24 23	17, 23, 43, 55	0
12	M	32/36 (88%)	-0.09	0 100 100	19, 24, 45, 51	0
12	m	32/36 (88%)	0.02	0 100 100	20, 25, 48, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/272 (88%)	0.48	25 (10%) 6 5	24, 43, 69, 124	0
13	o	241/272 (88%)	0.11	10 (4%) 37 35	25, 39, 68, 122	0
14	T	28/32 (87%)	0.06	1 (3%) 42 41	19, 23, 42, 72	0
14	t	29/32 (90%)	0.09	2 (6%) 16 15	20, 24, 46, 57	0
15	U	96/134 (71%)	1.33	25 (26%) 0 0	45, 61, 83, 90	0
15	u	96/134 (71%)	0.31	3 (3%) 49 47	32, 40, 51, 54	0
16	V	137/163 (84%)	0.00	0 100 100	32, 40, 50, 61	0
16	v	137/163 (84%)	0.56	16 (11%) 4 4	34, 43, 59, 75	0
17	Y	21/46 (45%)	1.76	7 (33%) 0 0	54, 65, 81, 85	0
17	y	23/46 (50%)	1.19	6 (26%) 0 0	50, 58, 79, 82	0
18	X	37/41 (90%)	0.33	4 (10%) 5 5	32, 38, 53, 65	0
18	x	38/41 (92%)	0.93	8 (21%) 1 1	38, 49, 68, 84	0
19	Z	61/62 (98%)	1.79	20 (32%) 0 0	50, 64, 121, 133	0
19	z	61/62 (98%)	2.46	33 (54%) 0 0	51, 72, 114, 128	0
20	R	35/41 (85%)	2.23	21 (60%) 0 0	49, 61, 81, 84	0
20	r	32/41 (78%)	2.40	20 (62%) 0 0	56, 65, 90, 97	0
All	All	5253/5700 (92%)	0.30	374 (7%) 16 14	16, 33, 65, 133	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	Z	33	TRP	12.4
19	z	31	GLN	9.6
19	Z	30	PRO	8.4
13	O	58	ASN	7.9
3	C	29	GLU	7.6
19	z	39	LEU	6.5
19	Z	34	ASP	6.4
19	z	36	SER	6.2
13	o	57	LYS	6.2
3	C	30	SER	6.1
15	U	75	LEU	6.0
13	o	60	ARG	6.0
19	Z	38	GLN	5.7
13	O	61	GLN	5.6
13	O	191	SER	5.6

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Mol	Chain	Res	Type	RSRZ
2	b	485	GLU	5.6
19	Z	31	GLN	5.5
19	z	1	MET	5.5
15	U	62	LEU	5.5
20	r	9	LEU	5.3
10	K	17	ILE	5.3
19	Z	60	PHE	5.3
5	e	78	THR	5.1
13	o	58	ASN	5.1
17	Y	45	ASN	5.1
15	U	61	VAL	5.1
18	x	2	THR	5.1
19	z	33	TRP	5.1
13	O	62	GLU	5.0
18	X	37	VAL	5.0
13	O	60	ARG	5.0
19	Z	7	LEU	4.9
15	U	80	GLU	4.9
5	e	79	PHE	4.9
3	C	354	GLU	4.8
15	U	82	PHE	4.8
15	U	64	ILE	4.8
19	z	4	LEU	4.7
20	r	28	VAL	4.7
19	z	35	ARG	4.6
19	z	32	ASP	4.6
17	Y	43	ARG	4.6
19	Z	42	LEU	4.6
2	b	127	ARG	4.5
19	z	10	ALA	4.4
18	X	2	THR	4.3
15	U	10	VAL	4.3
18	x	38	GLN	4.3
19	z	41	PHE	4.3
20	R	35	LEU	4.3
2	B	503	THR	4.2
5	e	82	GLN	4.2
19	z	30	PRO	4.2
13	O	4	THR	4.2
7	h	19	GLY	4.1
7	h	64	ALA	4.1
2	b	130	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
20	r	26	TYR	4.1
2	B	485	GLU	4.0
5	E	82	GLN	4.0
20	R	32	GLN	4.0
20	R	18	TRP	4.0
20	R	3	TRP	3.9
2	b	293	ALA	3.9
19	z	34	ASP	3.9
1	A	230	THR	3.9
20	R	28	VAL	3.8
20	r	14	LEU	3.8
2	b	503	THR	3.8
17	y	41	VAL	3.8
2	B	487	SER	3.8
13	O	63	ALA	3.8
16	v	3	LEU	3.8
13	O	59	LYS	3.8
19	z	52	LEU	3.7
5	E	17	VAL	3.7
13	o	62	GLU	3.7
18	x	34	ILE	3.7
20	R	34	LEU	3.7
3	C	27	ASP	3.7
11	l	2	GLU	3.7
1	A	344	ALA	3.6
1	A	235	TYR	3.6
19	z	56	VAL	3.6
15	U	77	GLU	3.6
20	r	18	TRP	3.6
19	z	40	ILE	3.6
19	z	60	PHE	3.5
1	A	227	THR	3.5
19	z	3	ILE	3.5
20	r	10	LEU	3.5
5	e	61	ARG	3.5
19	Z	36	SER	3.5
15	U	74	ILE	3.4
19	Z	32	ASP	3.4
17	Y	44	GLY	3.4
20	R	10	LEU	3.4
15	U	76	ARG	3.4
20	r	34	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
20	R	31	VAL	3.4
20	R	29	LYS	3.4
2	B	294	SER	3.3
3	C	427	ALA	3.3
2	B	84	THR	3.3
13	o	61	GLN	3.3
2	b	126	PRO	3.3
13	O	56	PRO	3.3
19	z	28	ALA	3.3
15	u	67	LEU	3.3
20	R	6	LEU	3.3
2	B	127	ARG	3.2
2	B	506	ARG	3.2
13	o	54	GLU	3.2
18	x	37	VAL	3.2
2	b	499	VAL	3.2
2	B	490	GLN	3.2
2	b	302	TRP	3.2
13	o	191	SER	3.2
19	z	42	LEU	3.2
2	B	484	PRO	3.2
7	h	63	LYS	3.2
20	r	8	VAL	3.2
19	z	5	PHE	3.1
20	R	21	ARG	3.1
2	b	461	LEU	3.1
5	E	61	ARG	3.1
16	v	18	THR	3.1
17	y	43	ARG	3.1
9	J	30	TYR	3.1
15	U	79	LEU	3.1
2	B	502	VAL	3.1
2	b	129	GLY	3.0
20	r	12	VAL	3.0
20	R	27	ALA	3.0
5	e	60	GLN	3.0
4	D	236	ASN	3.0
2	b	298	LEU	3.0
5	E	59	GLU	3.0
5	e	81	GLU	3.0
2	b	459	ALA	3.0
17	Y	30	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
17	Y	42	ARG	3.0
2	B	486	LEU	3.0
5	e	76	VAL	3.0
13	O	36	GLN	3.0
19	z	8	ALA	3.0
17	Y	37	PHE	3.0
2	B	504	THR	3.0
3	C	28	GLN	3.0
2	b	295	GLY	3.0
19	Z	1	MET	3.0
20	r	5	VAL	2.9
19	z	47	TRP	2.9
2	b	454	ALA	2.9
16	v	107	LEU	2.9
20	r	6	LEU	2.9
15	U	70	ARG	2.9
15	U	81	HIS	2.9
20	R	14	LEU	2.9
2	b	495	PHE	2.9
20	r	11	PRO	2.9
3	C	143	TYR	2.9
3	C	429	SER	2.9
13	O	91	GLY	2.9
2	B	505	ARG	2.9
19	z	11	ALA	2.9
5	e	83	LEU	2.9
15	U	67	LEU	2.9
2	b	84	THR	2.8
20	r	3	TRP	2.8
13	O	132	ASN	2.8
15	U	38	TYR	2.8
16	v	21	LEU	2.8
1	A	236	GLY	2.8
9	J	17	ALA	2.8
10	K	16	ALA	2.8
17	y	25	ILE	2.8
14	t	28	ARG	2.8
3	c	143	TYR	2.8
2	b	245	VAL	2.8
2	b	294	SER	2.8
15	U	57	SER	2.8
1	A	189	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
13	O	5	LEU	2.8
13	O	130	GLN	2.8
3	c	286	ALA	2.8
7	h	18	TYR	2.8
10	k	13	GLU	2.7
15	U	19	THR	2.7
15	U	68	THR	2.7
2	b	487	SER	2.7
16	v	23	GLU	2.7
1	A	188	ALA	2.7
3	C	434	ALA	2.7
15	U	66	GLY	2.7
19	Z	4	LEU	2.7
1	A	243	GLU	2.7
2	B	295	GLY	2.7
19	Z	41	PHE	2.7
20	r	25	PRO	2.7
19	z	7	LEU	2.7
2	B	496	TYR	2.6
1	A	343	LEU	2.6
5	E	4	THR	2.6
3	c	433	LEU	2.6
18	x	15	LEU	2.6
20	R	9	LEU	2.6
13	O	89	SER	2.6
13	O	133	VAL	2.6
9	j	8	ILE	2.6
3	C	355	THR	2.6
20	r	20	VAL	2.6
20	r	21	ARG	2.6
2	B	459	ALA	2.6
19	z	48	ILE	2.6
3	c	147	PHE	2.6
5	E	79	PHE	2.6
19	z	59	PHE	2.6
3	C	432	VAL	2.5
3	c	279	LEU	2.5
19	Z	17	PHE	2.5
3	C	353	GLY	2.5
14	T	28	ARG	2.5
2	b	247	PHE	2.5
3	C	433	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	a	294	ALA	2.5
13	O	87	VAL	2.5
16	v	113	VAL	2.5
3	C	134	ILE	2.5
5	e	74	GLN	2.5
3	c	106	VAL	2.5
11	l	3	PRO	2.5
2	b	249	ALA	2.5
5	e	80	LEU	2.4
5	e	17	VAL	2.4
16	v	16	GLY	2.4
3	c	434	ALA	2.4
2	B	480	SER	2.4
17	Y	41	VAL	2.4
19	Z	37	LYS	2.4
10	K	14	ALA	2.4
16	v	22	THR	2.4
6	F	16	PHE	2.4
16	v	2	GLU	2.4
19	Z	61	VAL	2.4
1	A	160	ILE	2.4
19	z	38	GLN	2.4
2	b	486	LEU	2.4
16	v	12	LEU	2.4
20	r	13	LEU	2.4
13	o	56	PRO	2.4
1	a	230	THR	2.4
2	b	289	GLN	2.4
13	O	207	ARG	2.4
2	b	494	GLY	2.4
1	a	13	LEU	2.3
5	e	71	GLU	2.3
15	U	9	LEU	2.3
16	v	112	LEU	2.3
13	O	183	ALA	2.3
2	b	85	GLY	2.3
17	y	44	GLY	2.3
4	D	159	ILE	2.3
2	b	462	PHE	2.3
3	C	431	PHE	2.3
4	D	233	ARG	2.3
18	X	38	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
13	o	25	THR	2.3
16	v	15	GLU	2.3
2	b	496	TYR	2.3
5	e	25	ILE	2.3
20	R	2	ASP	2.3
1	A	164	GLY	2.3
10	k	11	LEU	2.3
19	Z	5	PHE	2.3
2	b	248	ALA	2.3
3	c	432	VAL	2.3
20	R	7	VAL	2.3
18	x	35	ASP	2.3
3	C	426	LEU	2.3
2	b	128	THR	2.3
20	r	7	VAL	2.3
15	U	65	PRO	2.3
1	A	242	GLU	2.3
1	a	297	LEU	2.2
2	B	296	ALA	2.2
18	x	36	LYS	2.2
2	B	491	VAL	2.2
3	C	290	VAL	2.2
13	O	184	ARG	2.2
20	r	32	GLN	2.2
14	t	29	ILE	2.2
13	O	37	THR	2.2
3	c	290	VAL	2.2
20	R	36	GLN	2.2
15	U	63	ASN	2.2
1	a	242	GLU	2.2
9	j	24	ILE	2.2
2	B	248	ALA	2.2
4	d	240	ALA	2.2
3	c	276	LEU	2.2
19	Z	35	ARG	2.2
4	D	162	LEU	2.2
3	c	424	SER	2.2
2	b	458	PHE	2.2
3	C	289	PHE	2.2
7	h	41	PHE	2.2
17	y	37	PHE	2.2
20	r	31	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
8	i	33	LYS	2.2
5	e	59	GLU	2.2
4	D	154	VAL	2.2
16	v	75	TYR	2.2
2	B	243	ALA	2.2
3	C	31	SER	2.2
5	e	39	SER	2.2
2	b	497	GLN	2.1
10	k	17	ILE	2.1
2	b	460	LEU	2.1
2	B	462	PHE	2.1
2	b	246	PHE	2.1
13	O	187	VAL	2.1
2	B	249	ALA	2.1
4	D	290	ALA	2.1
2	b	292	LEU	2.1
1	A	332	HIS	2.1
3	C	106	VAL	2.1
15	U	58	VAL	2.1
19	Z	59	PHE	2.1
13	O	38	TYR	2.1
3	C	424	SER	2.1
17	y	26	ALA	2.1
20	R	33	LYS	2.1
16	v	13	ASN	2.1
3	C	142	GLU	2.1
15	U	73	GLN	2.1
18	x	3	ILE	2.1
16	v	24	LYS	2.1
19	z	61	VAL	2.1
4	D	240	ALA	2.1
15	U	34	ALA	2.1
20	R	25	PRO	2.1
13	o	55	GLU	2.1
19	Z	40	ILE	2.1
19	z	51	VAL	2.1
2	b	456	ALA	2.1
1	A	197	PHE	2.1
6	f	16	PHE	2.1
16	v	28	GLU	2.0
9	j	40	LEU	2.0
7	h	2	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
15	u	20	ALA	2.0
19	z	17	PHE	2.0
1	a	226	GLU	2.0
1	a	225	ARG	2.0
5	e	63	ILE	2.0
15	u	9	LEU	2.0
19	z	57	LEU	2.0
3	C	286	ALA	2.0
19	z	26	ALA	2.0
13	O	55	GLU	2.0
2	b	500	GLY	2.0
10	K	18	PHE	2.0
20	R	17	GLY	2.0
7	h	56	ASP	2.0
18	X	35	ASP	2.0
19	z	29	SER	2.0
20	R	26	TYR	2.0
5	e	35	TRP	2.0
1	A	226	GLU	2.0
3	c	427	ALA	2.0
13	O	32	ILE	2.0
2	b	252	VAL	2.0
6	f	44	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LFA	A	410	14/20	0.72	0.20	37,39,43,45	0
27	LFA	i	102	7/20	0.74	0.17	26,32,34,39	0
27	LFA	b	626	12/20	0.74	0.24	29,36,43,47	0
30	LMG	C	520	48/55	0.75	0.22	38,53,67,71	0
27	LFA	b	623	12/20	0.76	0.22	25,36,38,39	0
27	LFA	A	413	11/20	0.76	0.17	27,32,46,47	0
30	LMG	c	522	41/55	0.78	0.30	21,46,54,60	0
27	LFA	m	101	10/20	0.78	0.17	28,36,44,50	0
30	LMG	b	624	39/55	0.78	0.23	34,53,60,66	0
27	LFA	B	624	15/20	0.78	0.15	28,37,47,48	0
26	SQD	A	411	54/54	0.79	0.20	27,47,71,83	0
27	LFA	B	626	10/20	0.79	0.20	20,29,38,40	0
26	SQD	b	601	54/54	0.80	0.18	25,39,62,65	0
27	LFA	b	627	11/20	0.80	0.19	36,46,49,53	0
30	LMG	B	621	36/55	0.80	0.25	28,50,59,63	0
27	LFA	C	521	15/20	0.81	0.16	26,34,39,42	0
30	LMG	B	619	51/55	0.81	0.18	15,31,42,47	0
30	LMG	C	501	51/55	0.81	0.21	26,40,50,53	0
27	LFA	b	625	16/20	0.82	0.17	27,32,41,45	0
27	LFA	b	629	9/20	0.82	0.26	29,31,33,39	0
22	CLA	b	603	65/65	0.82	0.24	33,57,78,85	0
27	LFA	d	410	16/20	0.82	0.16	28,35,44,45	0
26	SQD	L	101	48/54	0.82	0.17	21,42,66,69	0
30	LMG	C	522	44/55	0.82	0.29	32,42,53,58	0
30	LMG	c	501	51/55	0.83	0.18	25,39,51,60	0
25	PL9	A	408	55/55	0.84	0.20	34,43,53,56	0
32	LHG	E	101	42/49	0.84	0.17	31,54,67,71	0
26	SQD	a	412	50/54	0.85	0.16	28,43,70,76	0
31	DGD	H	103	60/66	0.85	0.22	22,29,40,45	0
31	DGD	h	102	62/66	0.85	0.20	23,33,40,45	0
24	BCR	h	101	40/40	0.85	0.17	28,40,45,49	0
27	LFA	m	102	15/20	0.85	0.20	25,29,37,37	0
27	LFA	j	101	15/20	0.85	0.21	41,45,51,56	0
24	BCR	K	101	40/40	0.86	0.17	37,48,53,55	0
30	LMG	c	519	51/55	0.86	0.20	38,52,64,67	0
27	LFA	d	409	9/20	0.86	0.19	24,35,40,46	0
30	LMG	m	103	51/55	0.86	0.18	17,30,41,45	0
27	LFA	b	630	15/20	0.86	0.13	31,39,42,42	0
27	LFA	B	623	13/20	0.87	0.16	21,31,34,36	0
27	LFA	B	627	14/20	0.87	0.17	20,31,36,39	0
27	LFA	B	622	16/20	0.87	0.14	27,32,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PL9	a	409	55/55	0.87	0.20	38,48,59,65	0
26	SQD	D	411	43/54	0.88	0.21	38,50,58,69	0
27	LFA	i	101	16/20	0.88	0.16	23,32,40,41	0
27	LFA	D	410	15/20	0.88	0.17	23,28,40,47	0
27	LFA	T	102	12/20	0.88	0.13	22,28,32,32	0
27	LFA	d	408	15/20	0.88	0.18	25,32,37,37	0
31	DGD	C	518	56/66	0.88	0.17	29,38,48,53	0
22	CLA	C	513	65/65	0.89	0.16	34,41,54,63	0
32	LHG	e	101	42/49	0.89	0.16	40,62,80,94	0
27	LFA	M	102	16/20	0.89	0.13	25,27,46,47	0
27	LFA	b	622	10/20	0.89	0.13	27,31,37,38	0
22	CLA	H	101	65/65	0.89	0.15	30,45,64,72	0
27	LFA	t	101	15/20	0.89	0.18	25,31,42,43	0
24	BCR	t	102	40/40	0.89	0.17	21,26,38,40	0
24	BCR	c	523	40/40	0.90	0.15	39,46,52,55	0
24	BCR	T	101	40/40	0.90	0.14	22,29,34,37	0
22	CLA	c	513	65/65	0.90	0.15	36,42,55,62	0
26	SQD	A	409	54/54	0.90	0.15	24,42,54,56	0
22	CLA	b	618	65/65	0.90	0.15	23,32,58,64	0
22	CLA	C	511	65/65	0.90	0.18	25,34,41,49	0
22	CLA	C	504	65/65	0.90	0.14	20,35,38,42	0
22	CLA	B	603	65/65	0.90	0.17	14,21,35,44	0
22	CLA	c	504	65/65	0.90	0.16	26,34,39,40	0
24	BCR	H	102	40/40	0.90	0.13	22,28,42,43	0
22	CLA	b	606	65/65	0.90	0.20	16,23,38,45	0
24	BCR	c	524	40/40	0.90	0.18	36,43,53,53	0
24	BCR	d	404	40/40	0.91	0.14	25,36,53,56	0
27	LFA	I	101	14/20	0.91	0.10	21,29,32,32	0
24	BCR	B	616	40/40	0.91	0.15	19,25,31,32	0
27	LFA	B	620	10/20	0.91	0.14	22,24,28,33	0
22	CLA	B	605	65/65	0.91	0.12	17,25,38,44	0
21	CL	A	401	1/1	0.91	0.13	57,57,57,57	0
22	CLA	C	512	65/65	0.91	0.13	35,44,52,56	0
22	CLA	c	514	65/65	0.91	0.17	33,45,61,67	0
31	DGD	C	519	62/66	0.91	0.15	27,33,46,60	0
24	BCR	K	102	40/40	0.91	0.14	39,44,47,48	0
24	BCR	D	404	40/40	0.91	0.13	23,33,49,50	0
27	LFA	J	101	11/20	0.91	0.15	38,43,49,49	0
24	BCR	k	101	40/40	0.91	0.16	29,43,51,54	0
22	CLA	C	503	65/65	0.91	0.16	24,32,36,38	0
24	BCR	C	515	40/40	0.91	0.14	36,45,52,55	0
25	PL9	D	405	55/55	0.91	0.15	12,21,26,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LFA	D	412	8/20	0.91	0.15	25,30,37,40	0
27	LFA	D	413	10/20	0.91	0.17	22,23,26,28	0
22	CLA	c	503	65/65	0.91	0.20	23,30,38,39	0
24	BCR	b	619	40/40	0.91	0.16	18,28,34,35	0
22	CLA	b	608	65/65	0.91	0.13	22,29,42,53	0
22	CLA	c	502	65/65	0.92	0.14	17,28,35,38	0
27	LFA	B	628	12/20	0.92	0.20	23,28,37,37	0
27	LFA	c	521	15/20	0.92	0.11	31,35,41,41	0
22	CLA	c	507	65/65	0.92	0.13	25,32,52,58	0
22	CLA	B	615	65/65	0.92	0.15	19,25,70,79	0
24	BCR	b	621	40/40	0.92	0.12	23,34,42,47	0
24	BCR	B	617	40/40	0.92	0.15	15,24,30,30	0
31	DGD	c	517	55/66	0.92	0.18	25,34,50,63	0
22	CLA	C	514	65/65	0.92	0.14	37,49,63,67	0
31	DGD	c	518	62/66	0.92	0.15	26,32,52,58	0
22	CLA	D	403	65/65	0.92	0.16	17,24,62,66	0
24	BCR	b	620	40/40	0.92	0.15	18,25,30,32	0
27	LFA	b	602	15/20	0.92	0.12	29,33,42,42	0
26	SQD	a	410	54/54	0.92	0.15	30,48,58,62	0
27	LFA	c	520	9/20	0.92	0.17	31,39,46,47	0
24	BCR	B	618	40/40	0.92	0.12	18,26,34,36	0
22	CLA	C	509	65/65	0.92	0.17	22,31,62,66	0
26	SQD	f	102	43/54	0.92	0.23	51,66,77,86	0
31	DGD	c	516	62/66	0.92	0.15	23,28,49,52	0
24	BCR	C	516	40/40	0.92	0.12	21,30,37,38	0
31	DGD	C	517	62/66	0.92	0.17	20,26,49,52	0
22	CLA	c	508	65/65	0.92	0.15	22,30,34,37	0
22	CLA	C	505	65/65	0.92	0.19	28,35,48,61	0
27	LFA	B	625	9/20	0.92	0.17	20,25,27,33	0
22	CLA	c	512	65/65	0.92	0.11	28,39,47,50	0
22	CLA	d	403	65/65	0.93	0.15	22,30,57,63	0
24	BCR	c	515	40/40	0.93	0.12	19,29,38,41	0
22	CLA	a	404	65/65	0.93	0.15	14,20,27,36	0
22	CLA	a	405	65/65	0.93	0.13	14,19,25,31	0
22	CLA	C	507	65/65	0.93	0.12	22,30,55,57	0
22	CLA	c	510	65/65	0.93	0.15	22,31,38,40	0
30	LMG	f	101	51/55	0.93	0.13	31,38,55,61	0
27	LFA	a	411	7/20	0.93	0.09	26,32,35,35	0
22	CLA	c	506	65/65	0.93	0.12	21,26,37,40	0
22	CLA	C	508	65/65	0.93	0.13	21,26,35,45	0
32	LHG	D	406	49/49	0.93	0.14	17,24,30,33	0
32	LHG	D	408	49/49	0.93	0.16	16,33,53,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	b	604	65/65	0.93	0.15	25,30,41,46	0
23	PHO	a	406	64/64	0.93	0.14	13,17,25,27	0
22	CLA	b	610	65/65	0.93	0.17	22,28,37,45	0
22	CLA	b	616	65/65	0.93	0.13	20,26,39,42	0
22	CLA	b	611	65/65	0.93	0.12	23,30,40,52	0
22	CLA	C	510	65/65	0.93	0.14	25,31,39,40	0
21	CL	a	403	1/1	0.93	0.10	40,40,40,40	0
22	CLA	B	613	65/65	0.93	0.14	18,25,46,57	0
32	LHG	l	101	49/49	0.93	0.13	17,25,34,39	0
22	CLA	B	611	65/65	0.93	0.16	14,19,25,28	0
32	LHG	L	102	49/49	0.93	0.13	18,24,31,34	0
22	CLA	C	506	65/65	0.94	0.12	17,27,32,40	0
22	CLA	b	615	65/65	0.94	0.20	16,21,36,39	0
23	PHO	a	414	64/64	0.94	0.14	21,28,33,39	0
22	CLA	c	505	65/65	0.94	0.23	21,33,49,53	0
22	CLA	A	412	65/65	0.94	0.12	16,20,25,27	0
22	CLA	B	601	65/65	0.94	0.15	17,26,32,36	0
22	CLA	b	617	65/65	0.94	0.11	21,27,39,50	0
27	LFA	M	101	10/20	0.94	0.17	26,31,41,42	0
25	PL9	d	405	55/55	0.94	0.12	16,23,27,30	0
22	CLA	c	509	65/65	0.94	0.18	24,30,59,66	0
33	HEM	e	102	43/43	0.94	0.13	37,48,57,60	0
21	CL	a	402	1/1	0.94	0.16	52,52,52,52	0
22	CLA	c	511	65/65	0.94	0.21	27,32,38,44	0
22	CLA	b	613	65/65	0.94	0.15	18,23,29,31	0
22	CLA	B	614	65/65	0.94	0.10	15,22,32,47	0
33	HEM	E	102	43/43	0.94	0.12	34,43,52,54	0
22	CLA	b	614	65/65	0.94	0.17	16,23,28,32	0
22	CLA	A	404	65/65	0.94	0.15	15,23,61,72	0
22	CLA	B	604	65/65	0.94	0.16	15,21,25,29	0
22	CLA	d	402	65/65	0.94	0.13	17,20,37,40	0
32	LHG	b	628	49/49	0.94	0.13	22,27,35,49	0
22	CLA	B	607	65/65	0.94	0.17	13,19,26,34	0
24	BCR	A	407	40/40	0.94	0.10	14,23,30,31	0
30	LMG	D	409	51/55	0.94	0.13	25,36,51,54	0
22	CLA	C	502	65/65	0.94	0.13	18,24,33,35	0
22	CLA	B	612	65/65	0.94	0.17	13,18,40,43	0
22	CLA	B	610	65/65	0.94	0.17	12,18,24,29	0
22	CLA	B	602	65/65	0.94	0.15	18,21,35,38	0
24	BCR	a	408	40/40	0.94	0.10	18,22,29,31	0
22	CLA	d	401	65/65	0.94	0.15	18,27,63,69	0
32	LHG	D	407	49/49	0.94	0.13	18,24,30,37	0

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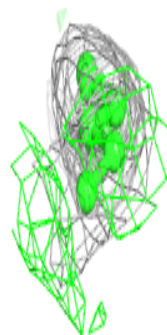
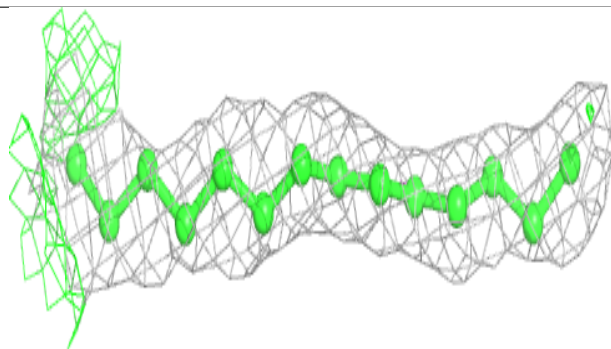
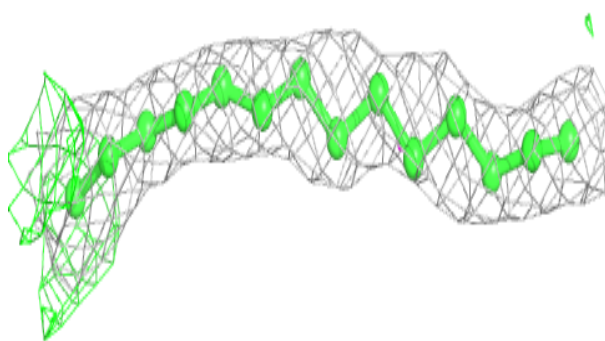
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	a	407	65/65	0.94	0.13	13,19,56,60	0
22	CLA	b	607	65/65	0.94	0.14	18,23,30,32	0
22	CLA	B	608	65/65	0.94	0.11	15,24,33,36	0
23	PHO	D	401	64/64	0.95	0.15	14,18,25,28	0
33	HEM	V	201	43/43	0.95	0.12	28,36,41,45	0
22	CLA	B	606	65/65	0.95	0.15	10,18,33,37	0
22	CLA	A	403	65/65	0.95	0.14	12,18,23,30	0
32	LHG	d	406	49/49	0.95	0.12	18,24,32,36	0
22	CLA	D	402	65/65	0.95	0.14	13,18,26,35	0
32	LHG	d	407	49/49	0.95	0.16	21,37,60,63	0
22	CLA	A	406	65/65	0.95	0.13	11,20,54,60	0
22	CLA	b	612	65/65	0.95	0.14	16,25,31,33	0
22	CLA	B	609	65/65	0.95	0.15	15,20,27,29	0
22	CLA	b	605	65/65	0.95	0.17	18,22,37,49	0
22	CLA	b	609	65/65	0.95	0.16	11,21,29,32	0
23	PHO	A	405	64/64	0.95	0.17	15,21,28,31	0
29	BCT	a	413	4/4	0.96	0.11	31,33,34,40	0
21	CL	A	402	1/1	0.96	0.12	57,57,57,57	0
33	HEM	v	201	43/43	0.97	0.09	28,34,38,41	0
29	BCT	A	415	4/4	0.97	0.09	25,29,31,32	0
28	FE	A	414	1/1	0.98	0.04	26,26,26,26	0
28	FE	a	401	1/1	0.99	0.10	39,39,39,39	0

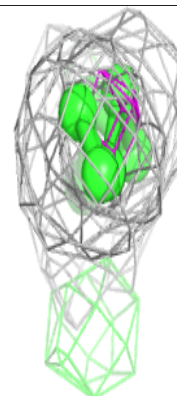
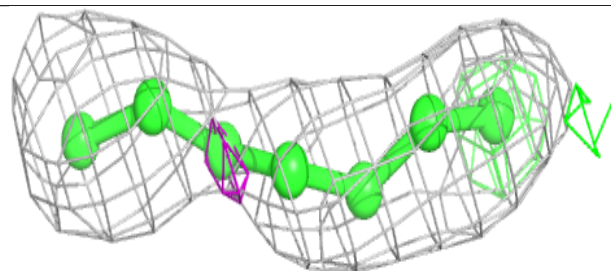
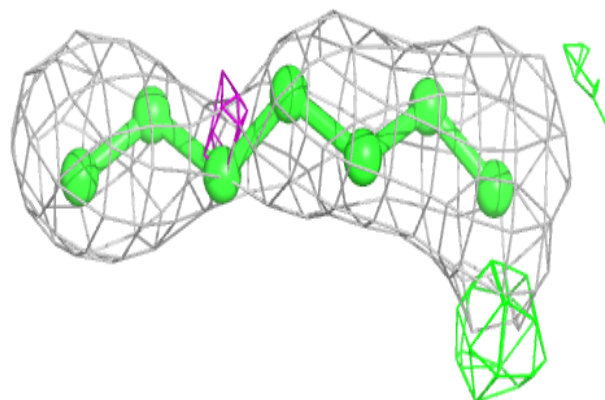
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFA 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)

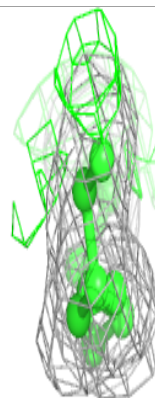
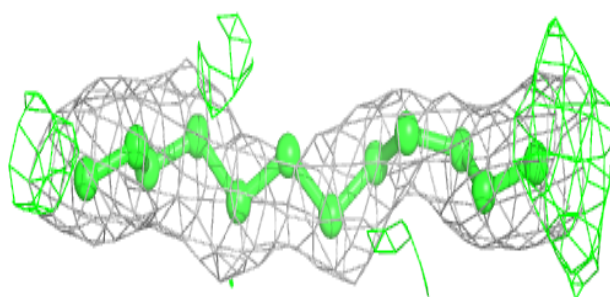
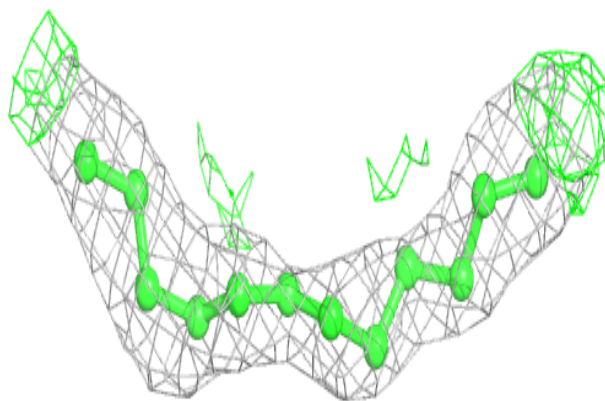
**Electron density around LFA i 102:**

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

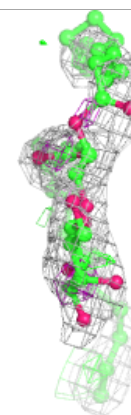
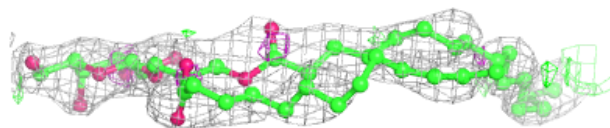
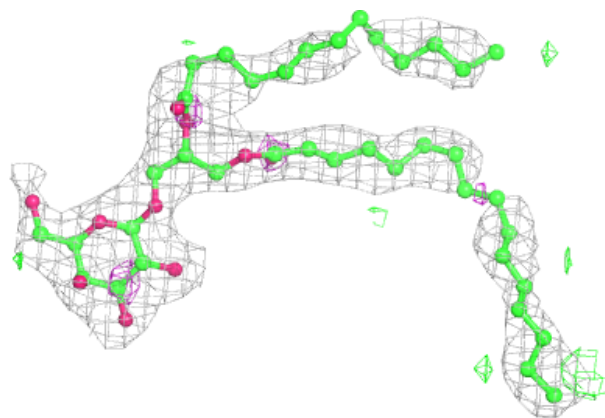


Electron density around LFA b 626:

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

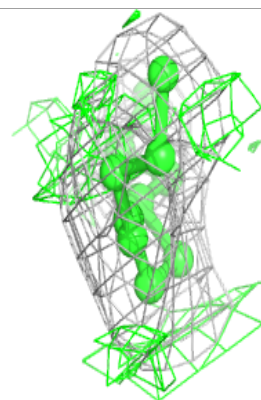
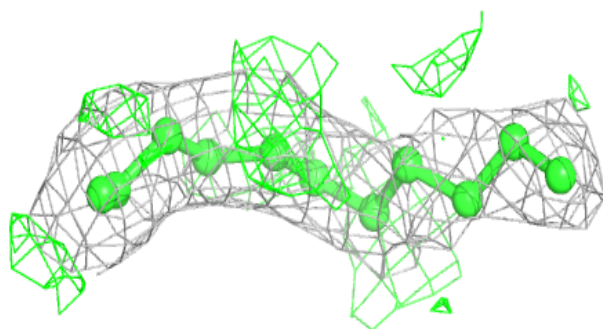
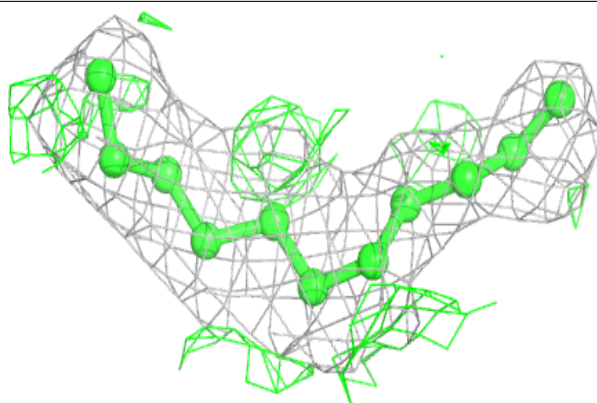
**Electron density around LMG C 520:**

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

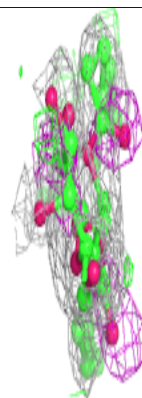
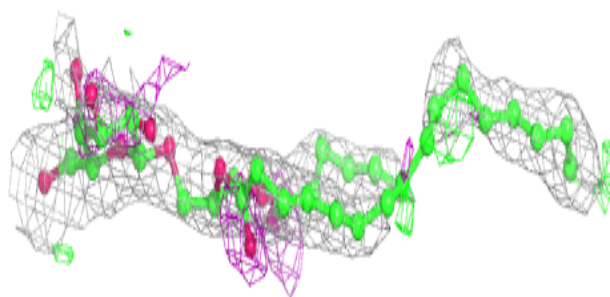
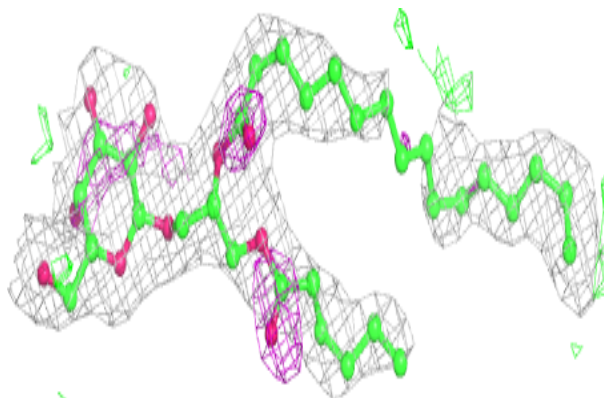


Electron density around LFA A 413:

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

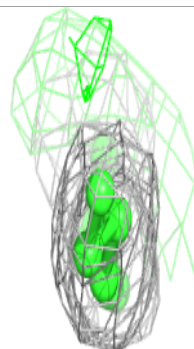
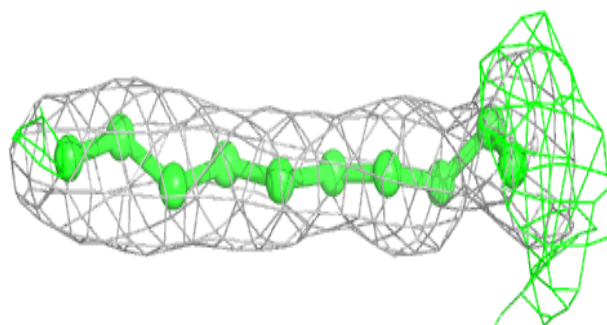
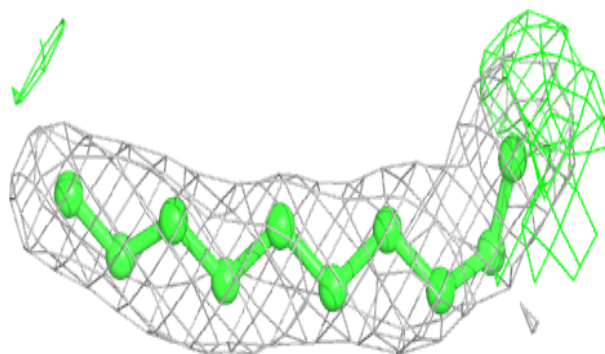
**Electron density around LMG c 522:**

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

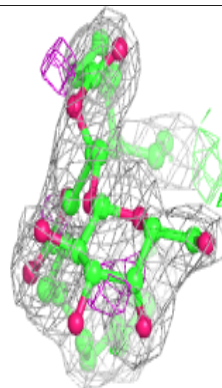
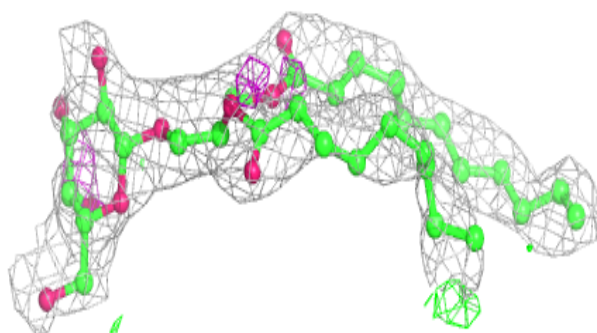
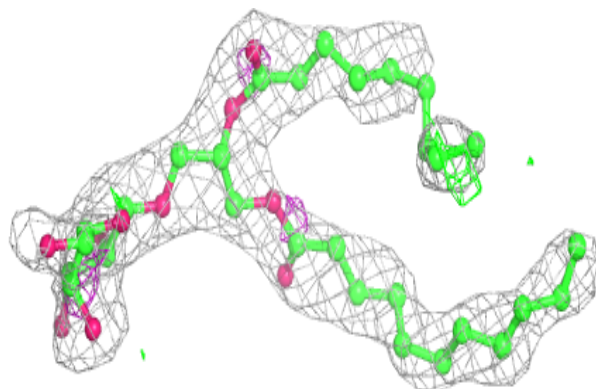


Electron density around LFA m 101:

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

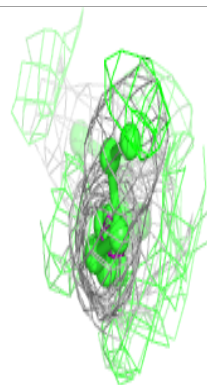
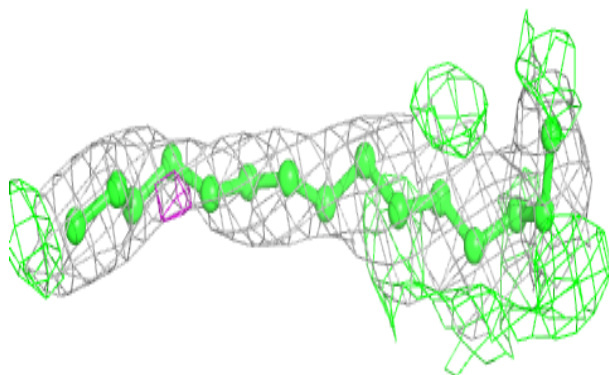
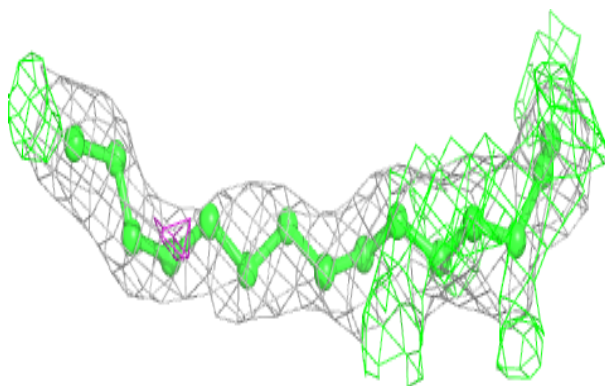
**Electron density around LMG b 624:**

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

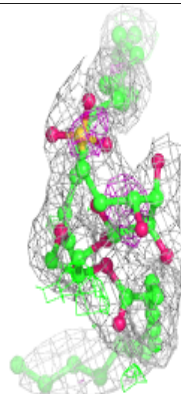
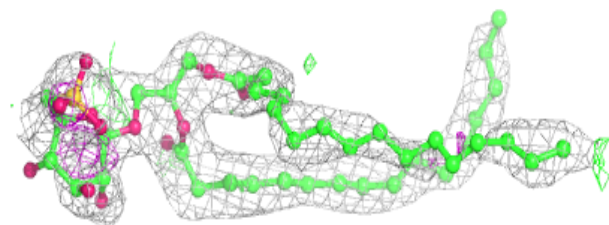
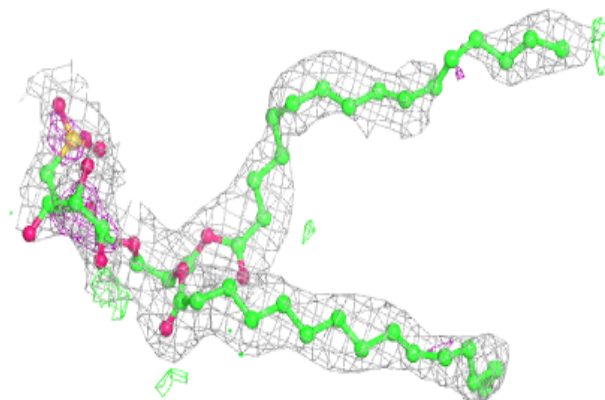


Electron density around LFA B 624:

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

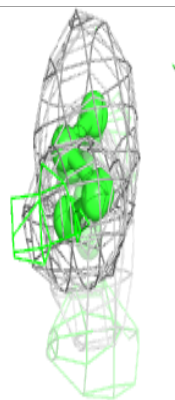
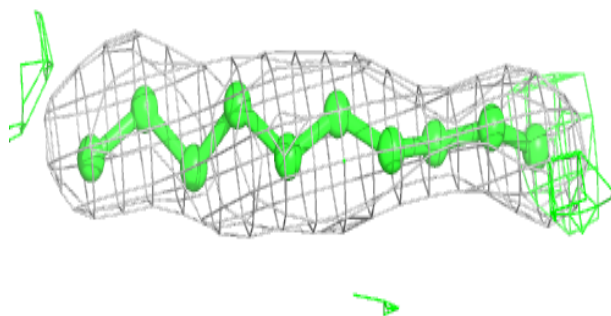
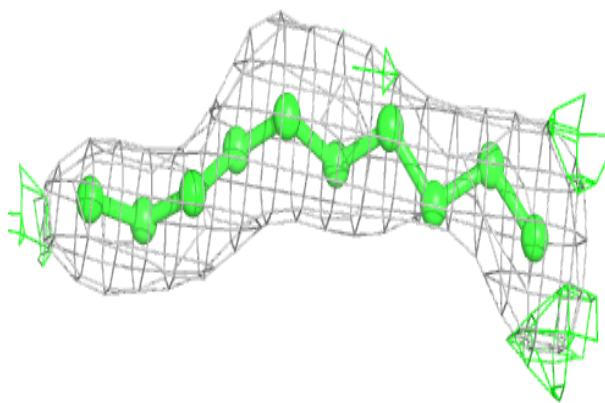
**Electron density around SQD A 411:**

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

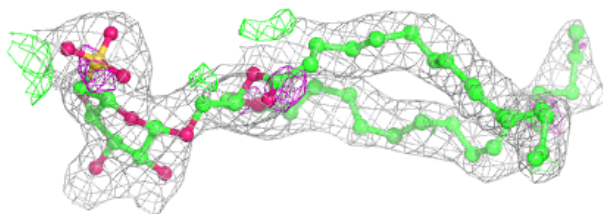
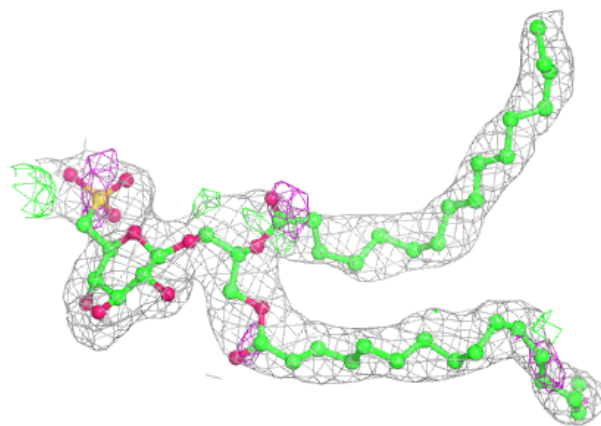


Electron density around LFA B 626:

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

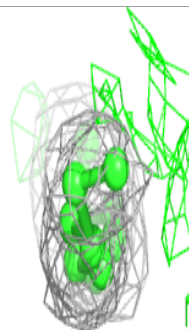
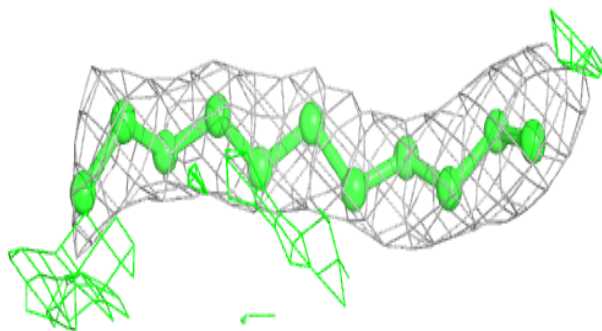
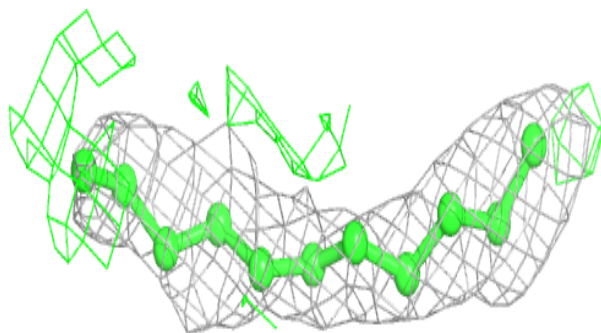
**Electron density around SQD b 601:**

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

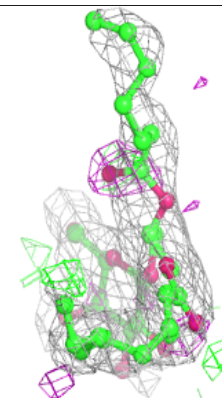
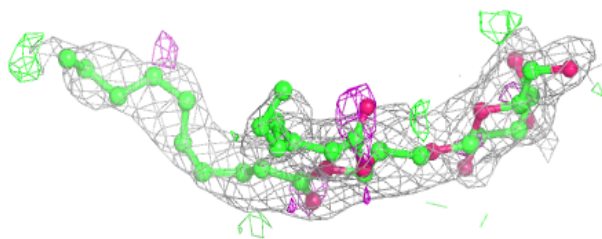
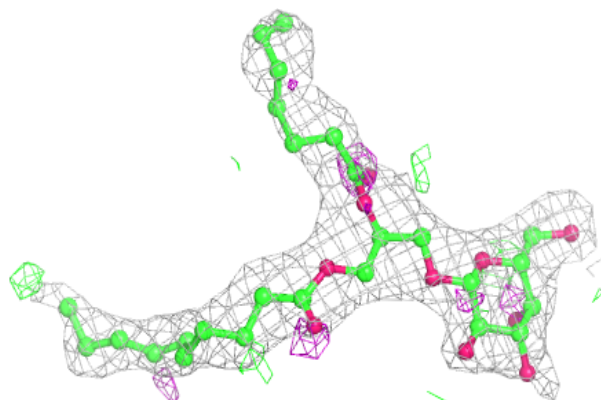


Electron density around LFA b 627:

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

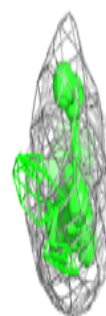
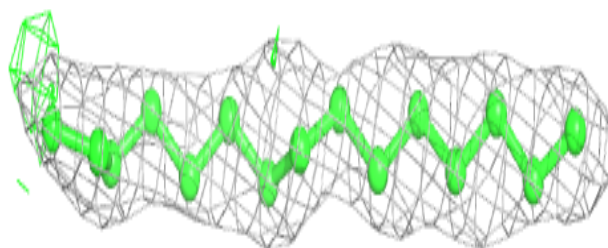
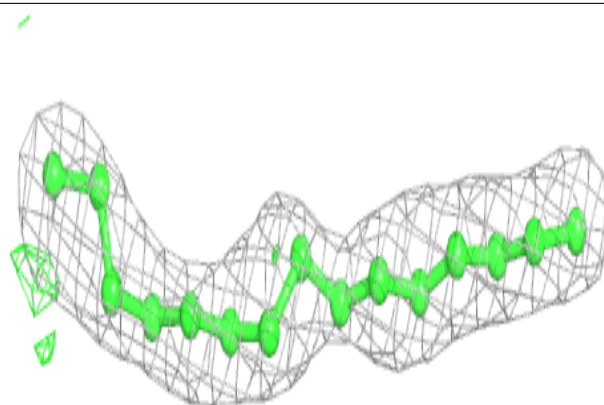
**Electron density around LMG B 621:**

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

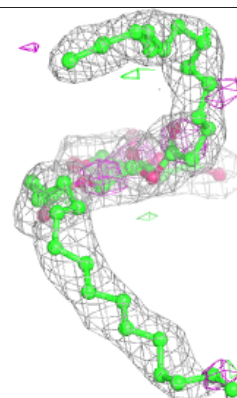
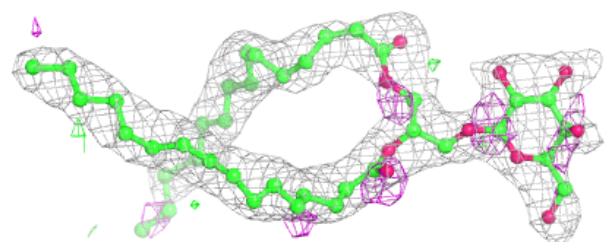
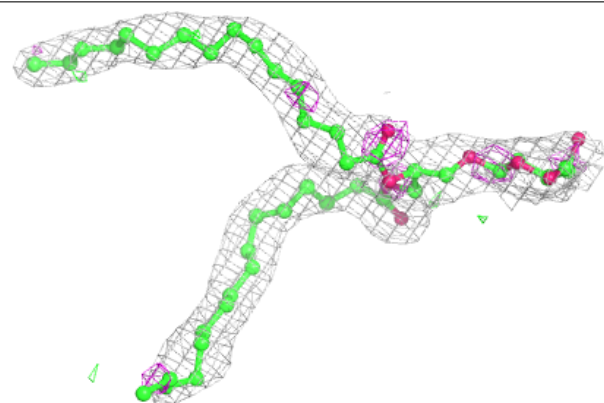


Electron density around LFA C 521:

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

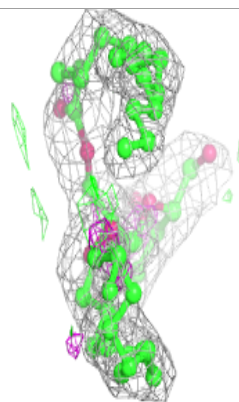
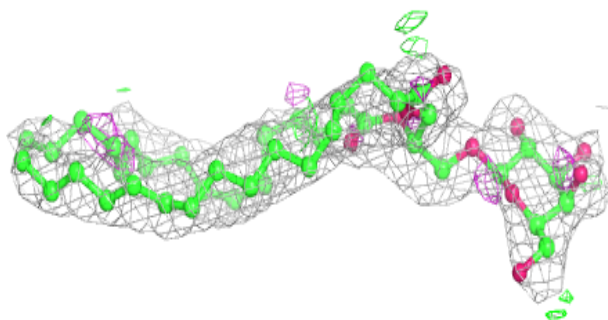
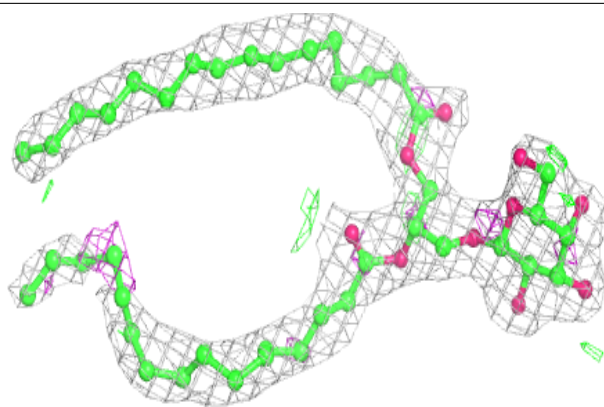
**Electron density around LMG B 619:**

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

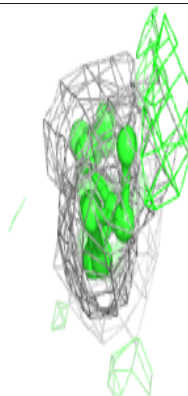
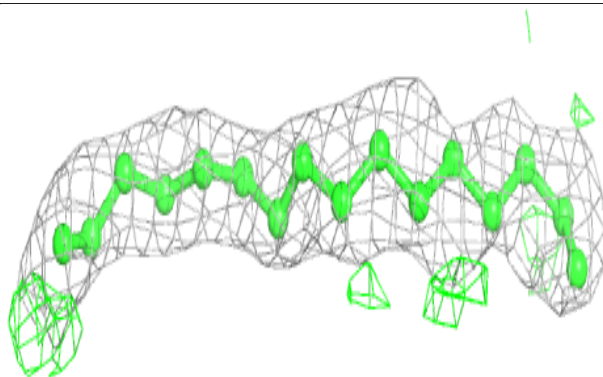
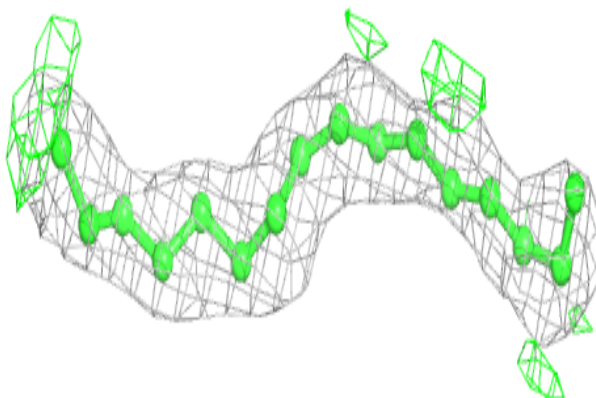


Electron density around LMG C 501:

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

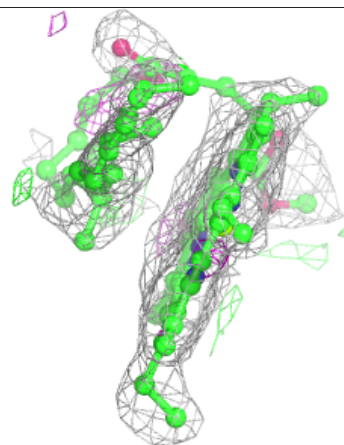
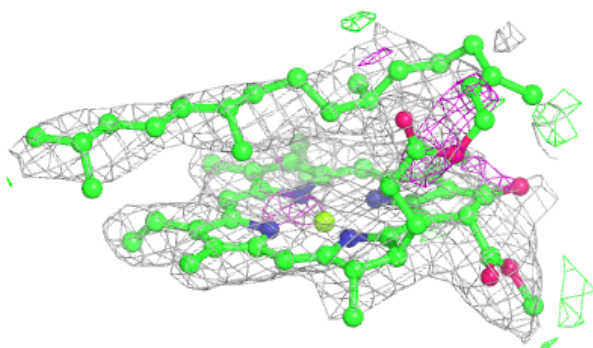
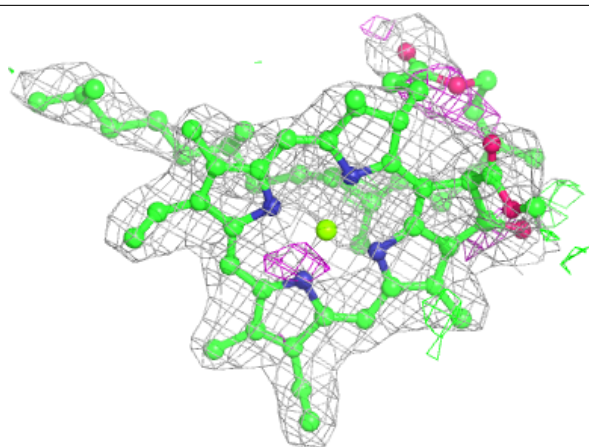
**Electron density around LFA b 625:**

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

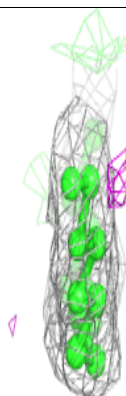
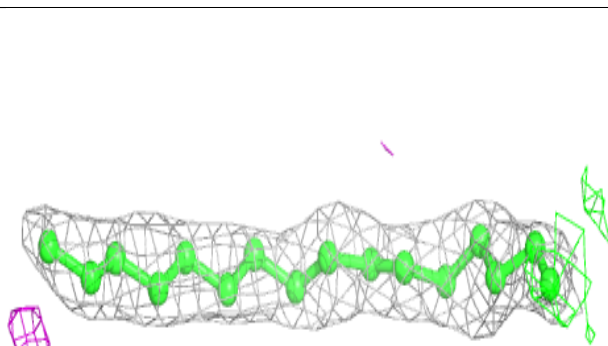
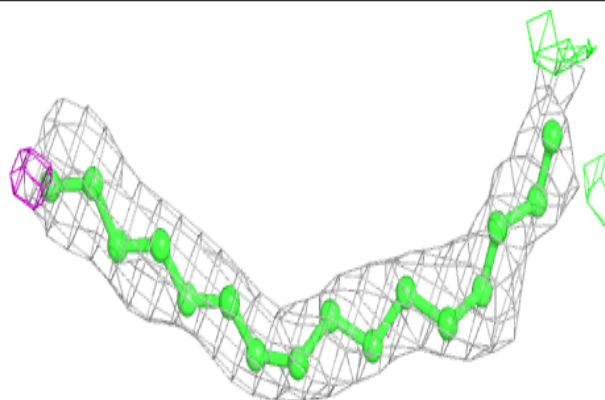


Electron density around CLA b 603:

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

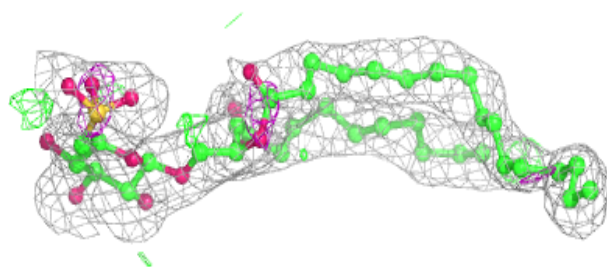
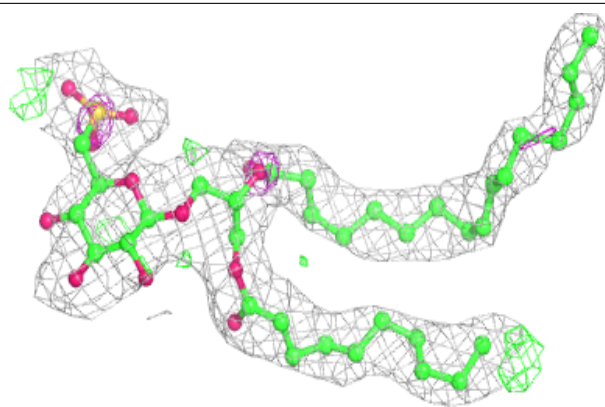
**Electron density around LFA d 410:**

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

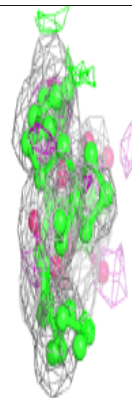
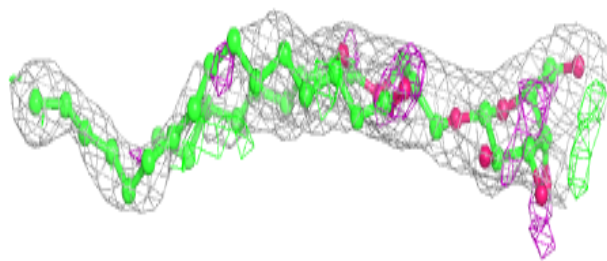
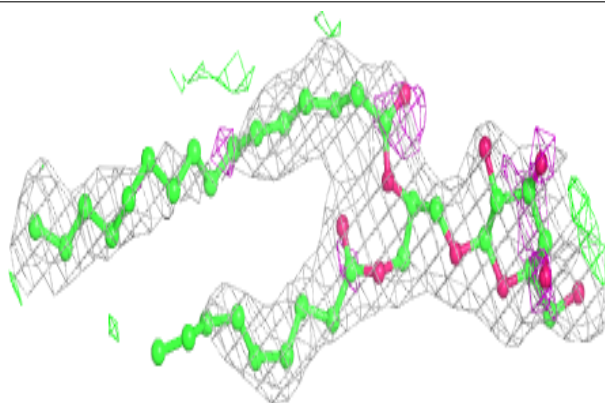


Electron density around SQD L 101:

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

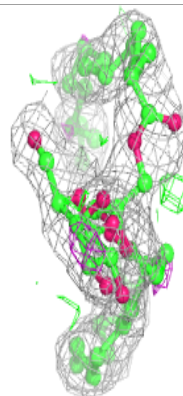
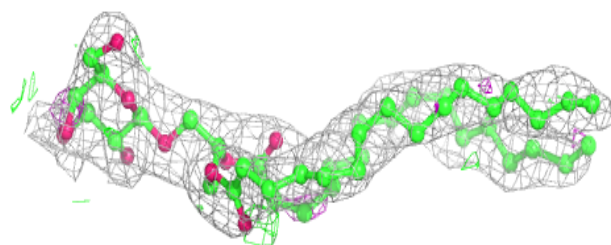
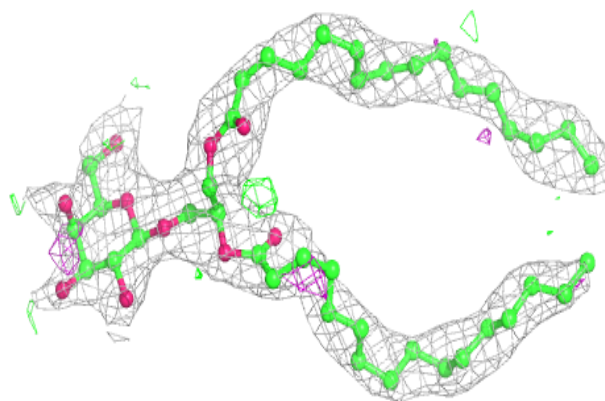
**Electron density around LMG C 522:**

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

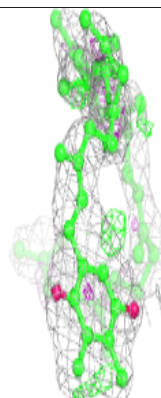
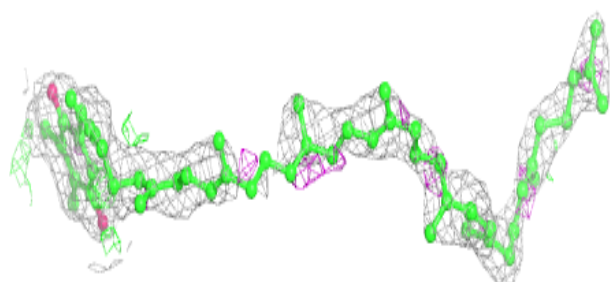
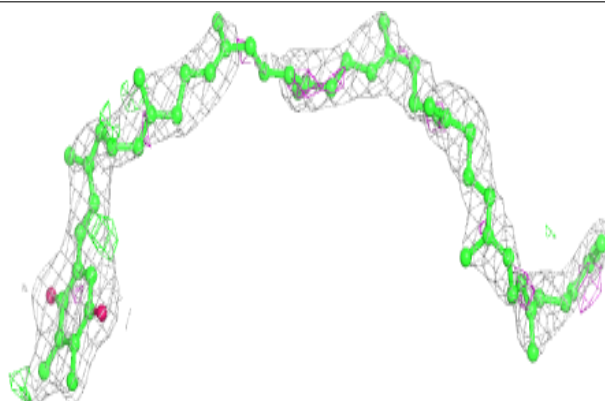


Electron density around LMG c 501:

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

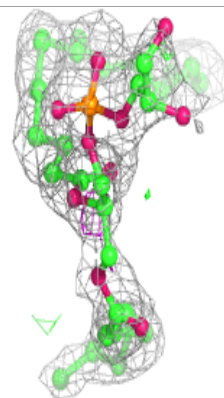
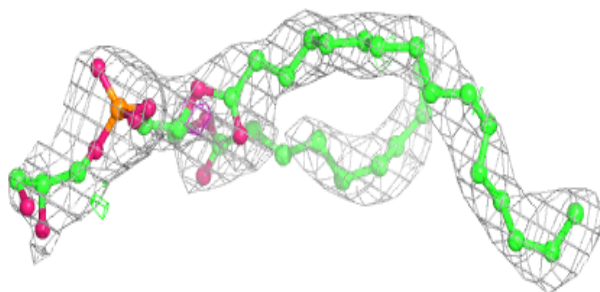
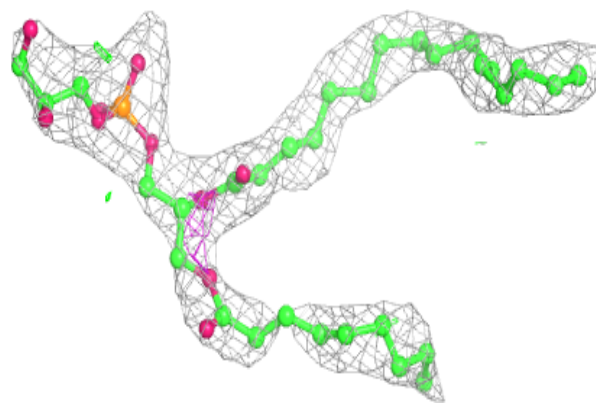
**Electron density around PL9 A 408:**

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

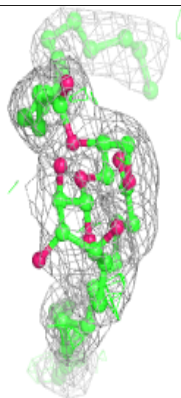
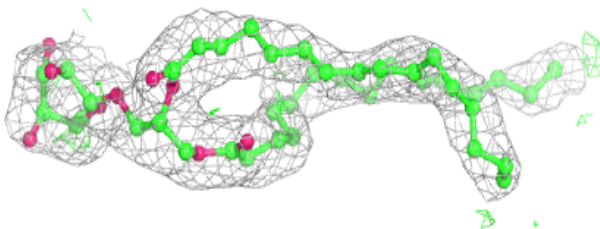
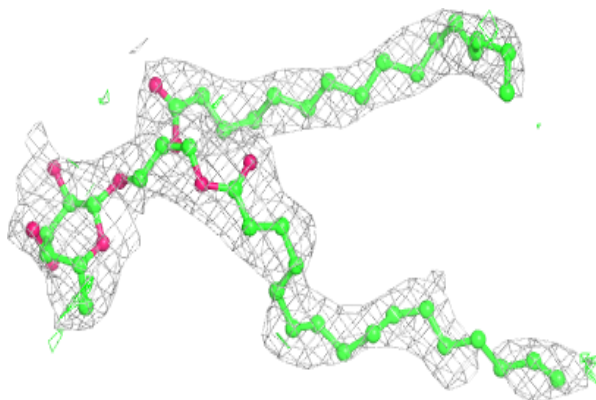


Electron density around LHG E 101:

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

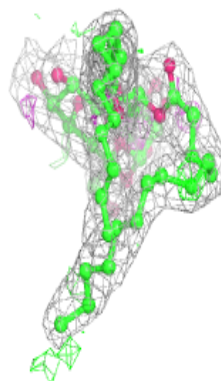
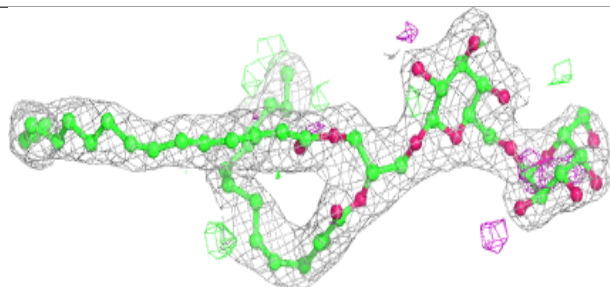
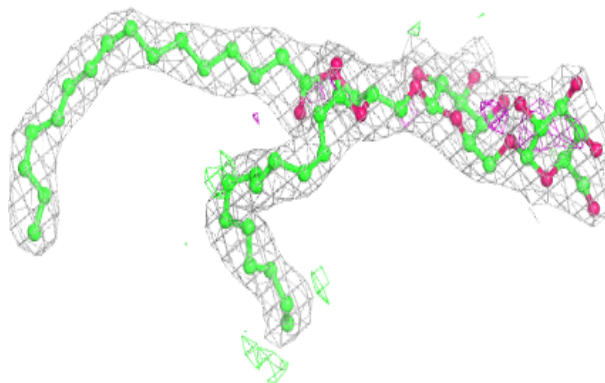
**Electron density around SQD a 412:**

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

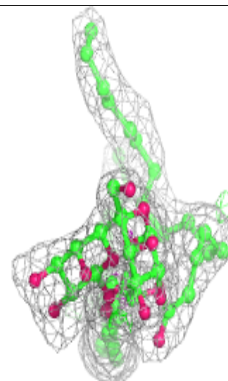
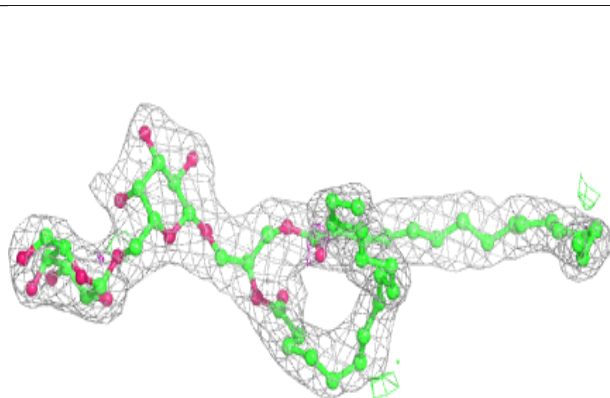
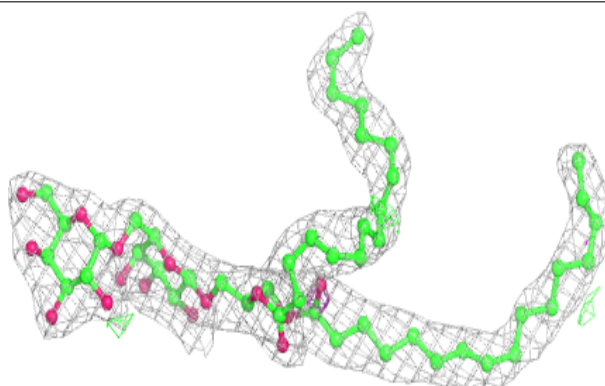


Electron density around DGD H 103:

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

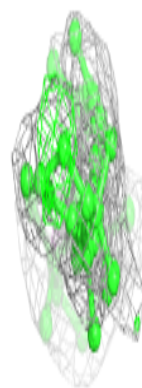
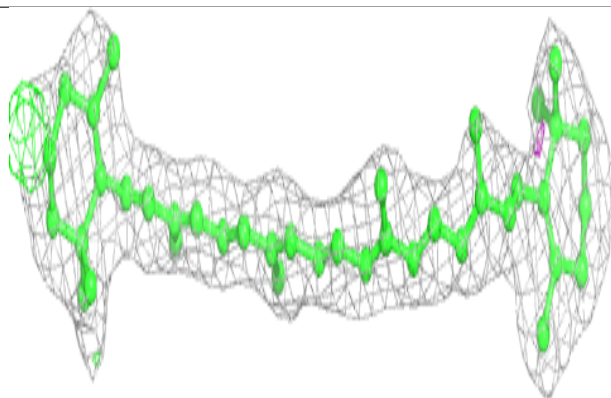
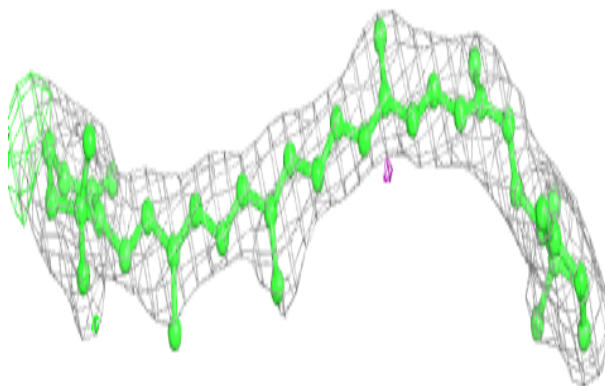
**Electron density around DGD h 102:**

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

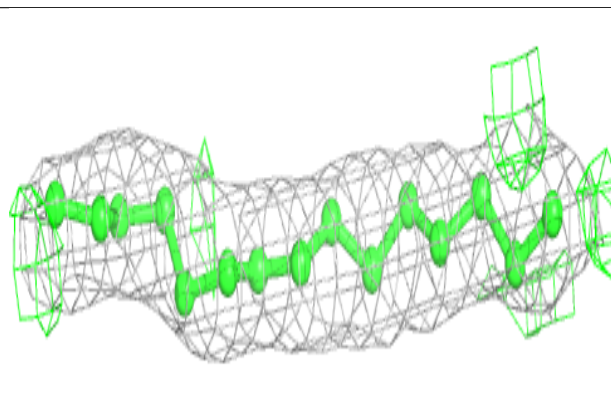
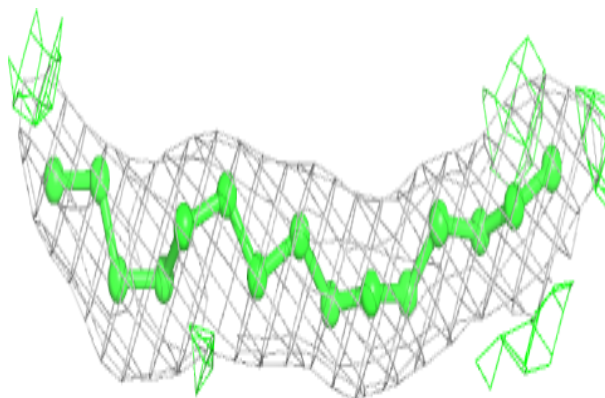


Electron density around BCR h 101:

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

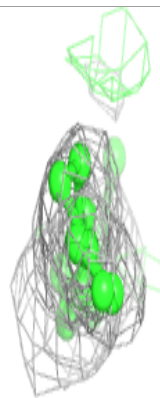
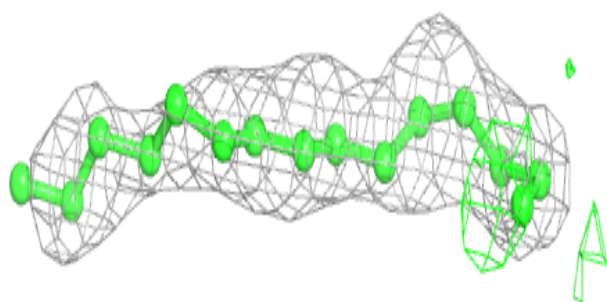
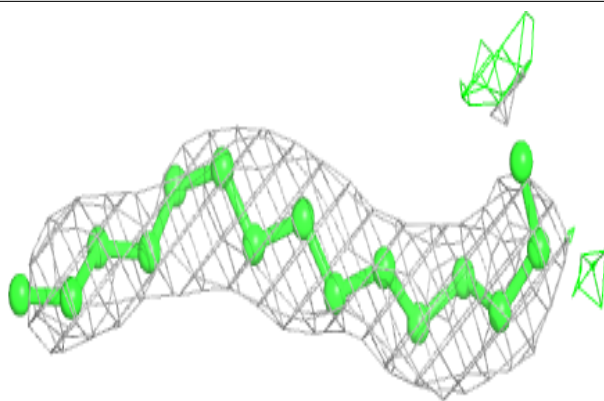
**Electron density around LFA m 102:**

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

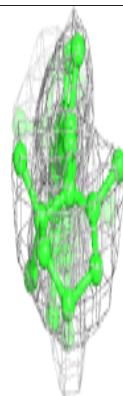
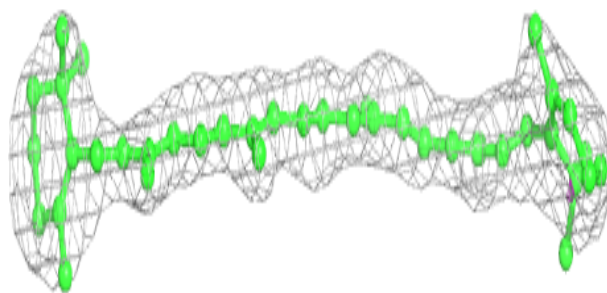
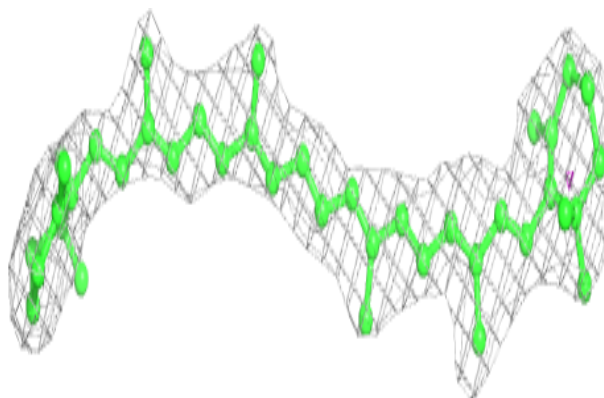


Electron density around LFA j 101:

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

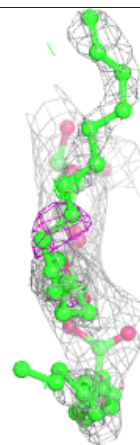
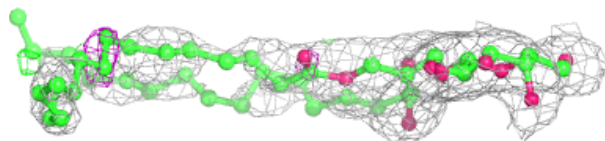
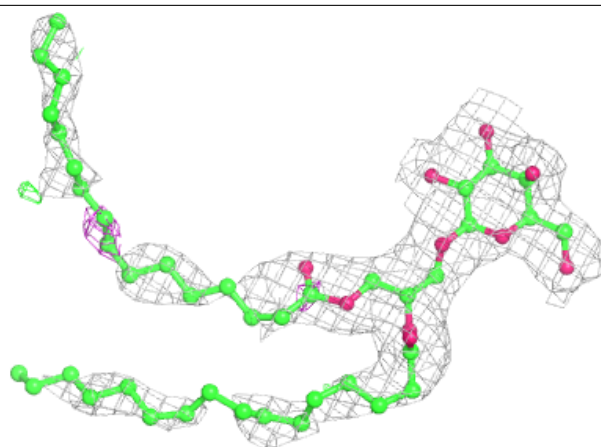
**Electron density around BCR K 101:**

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

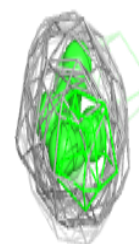
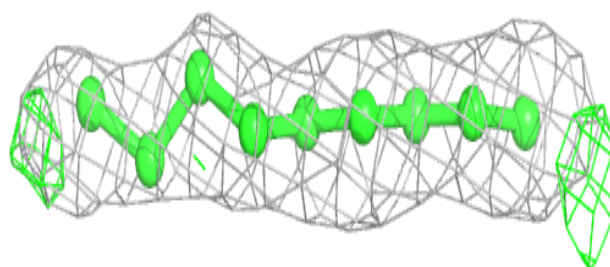
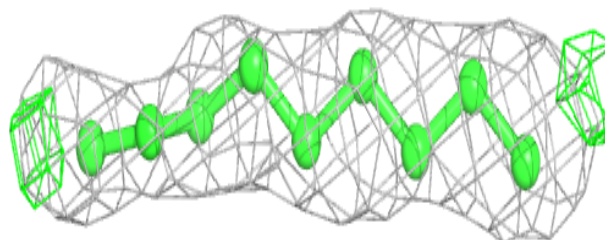


Electron density around LMG c 519:

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

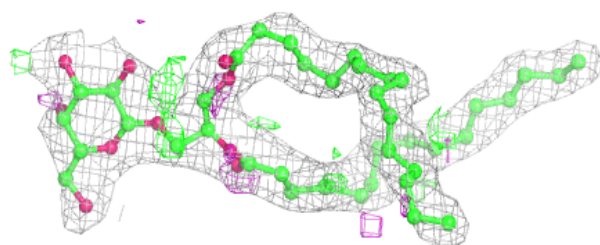
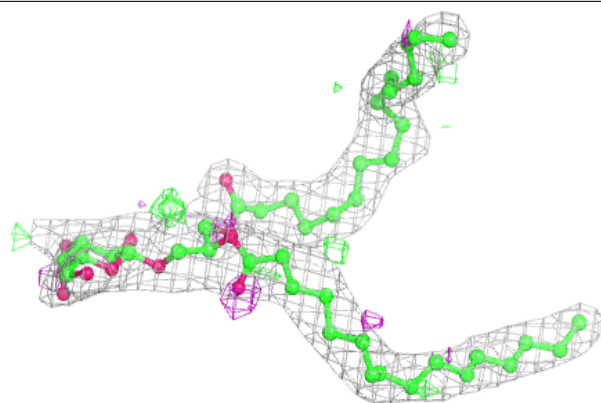
**Electron density around LFA d 409:**

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

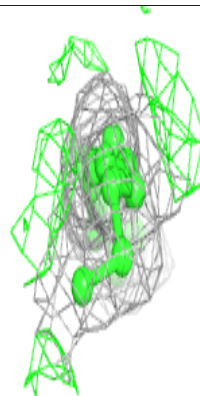
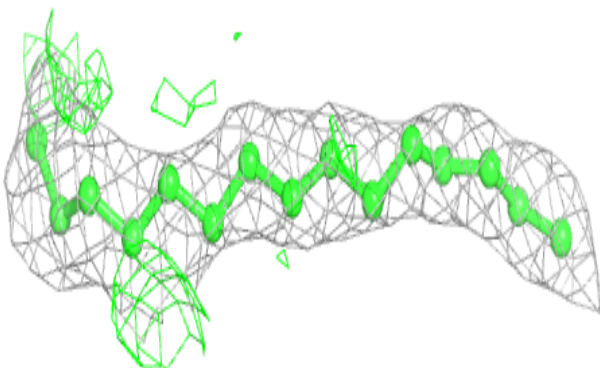
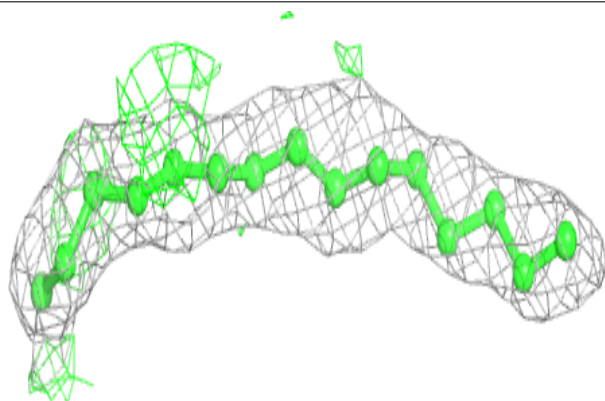


Electron density around LMG m 103:

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

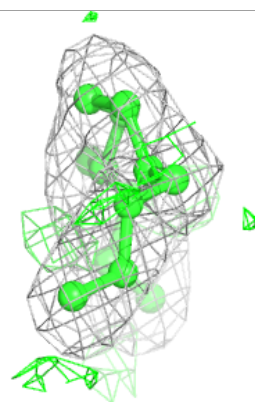
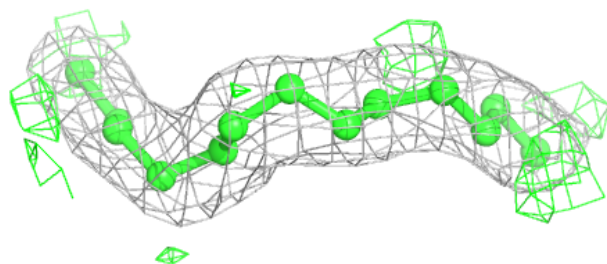
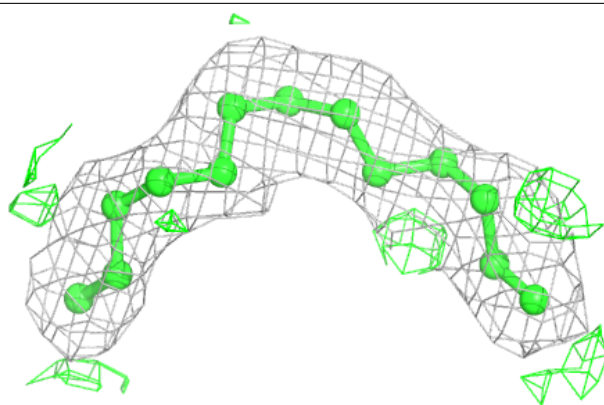
**Electron density around LFA b 630:**

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

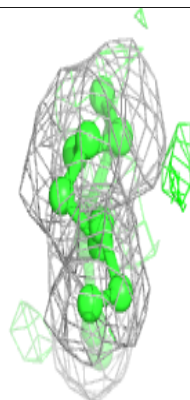
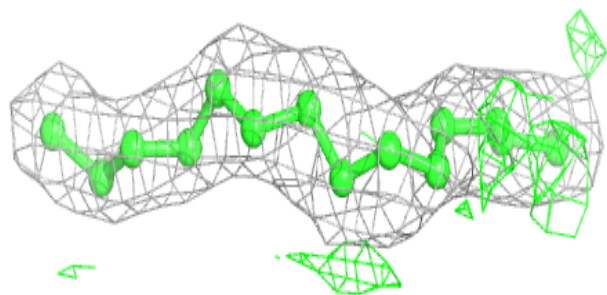
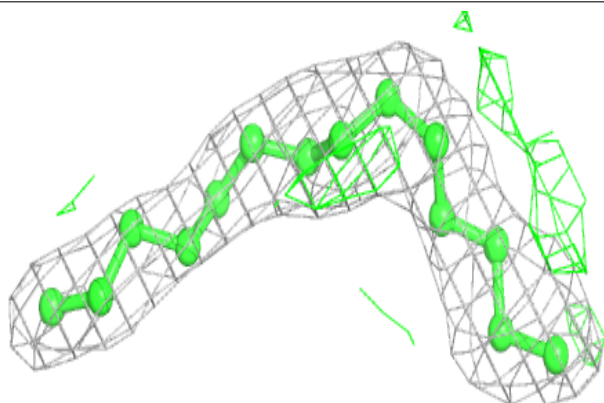


Electron density around LFA B 623:

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

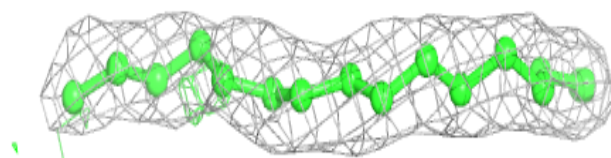
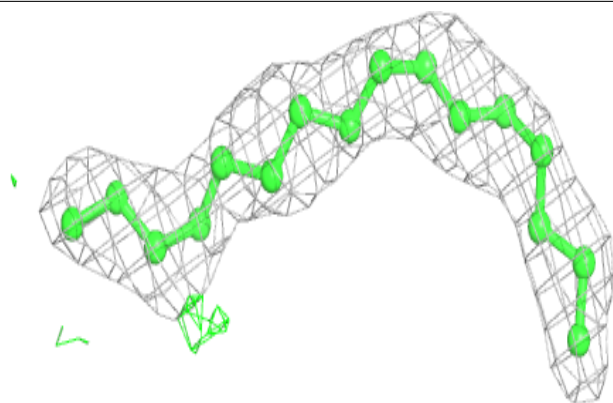
**Electron density around LFA B 627:**

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

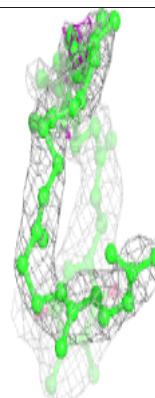
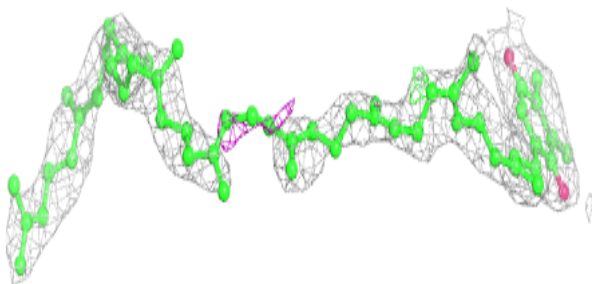
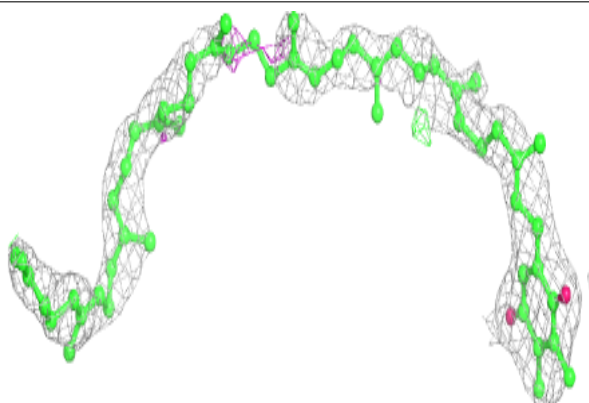


Electron density around LFA B 622:

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

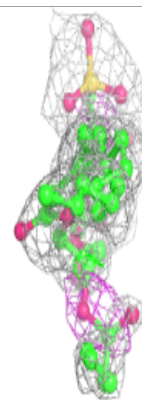
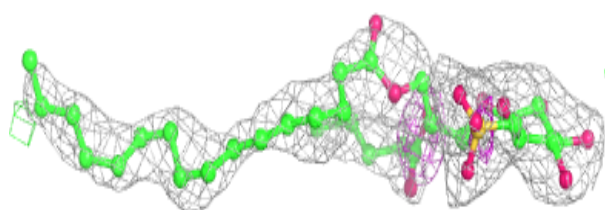
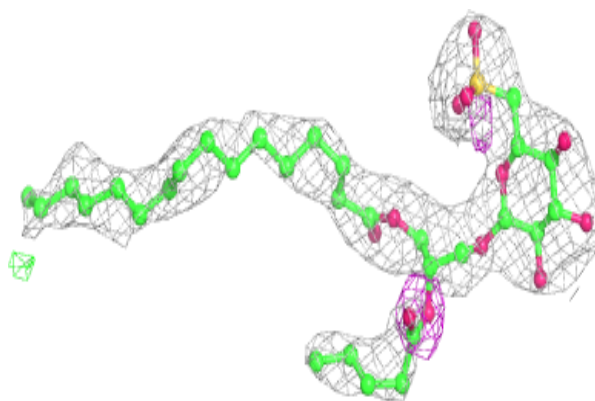
**Electron density around PL9 a 409:**

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

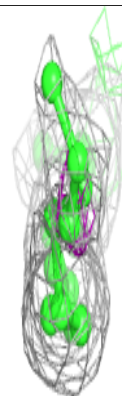
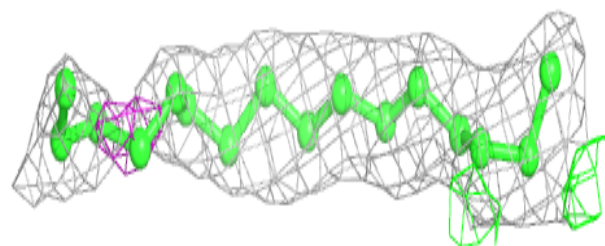
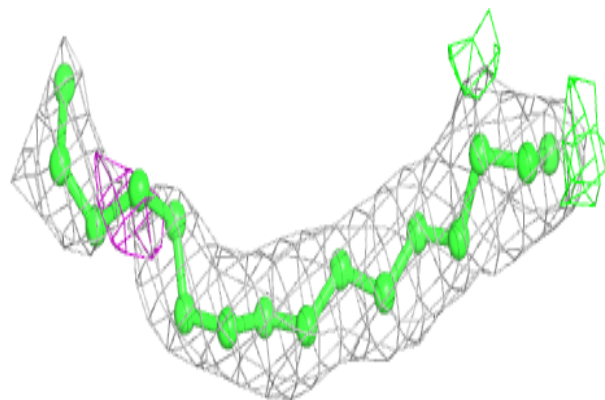


Electron density around SQD D 411:

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

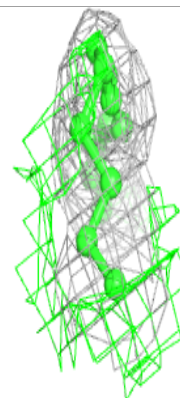
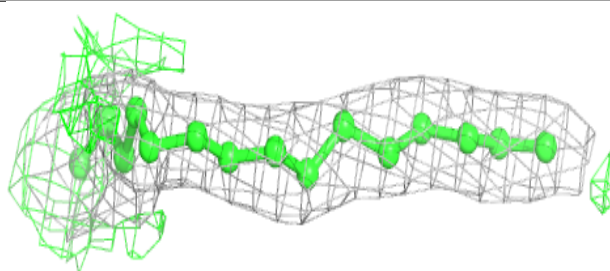
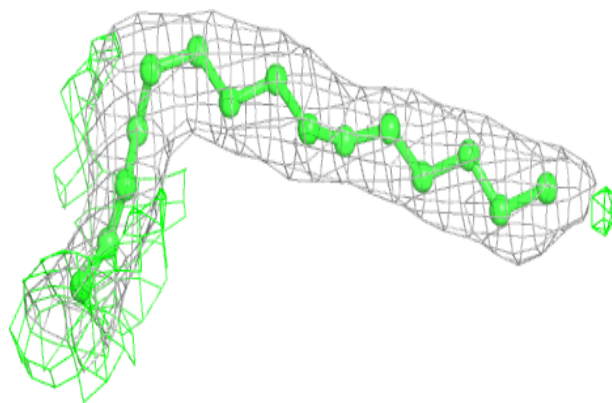
**Electron density around LFA i 101:**

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

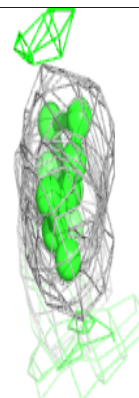
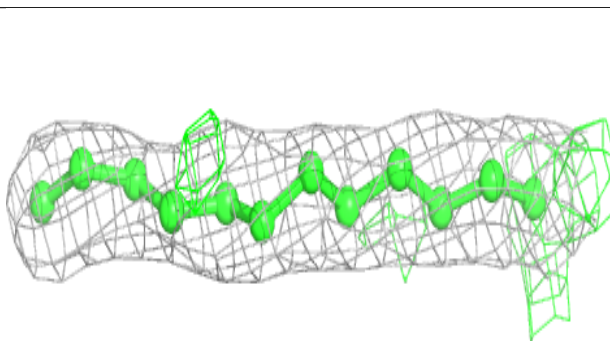
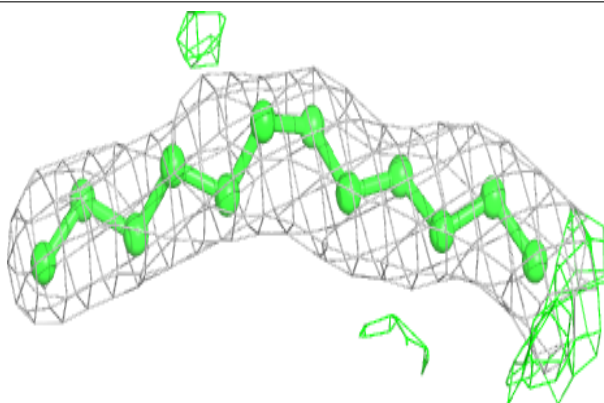


Electron density around LFA D 410:

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

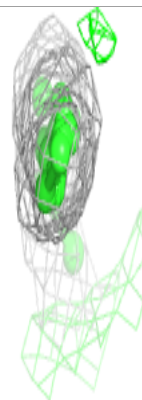
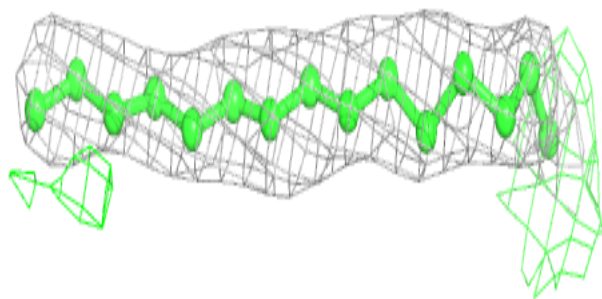
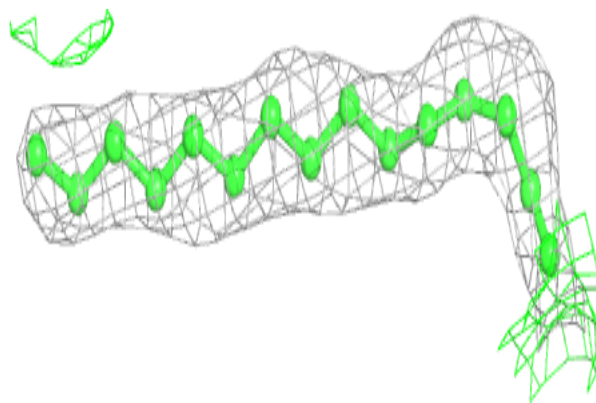
**Electron density around LFA T 102:**

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

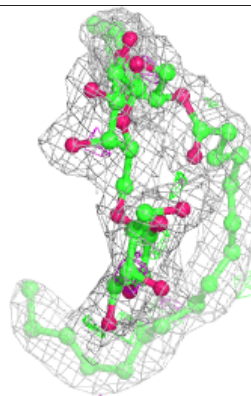
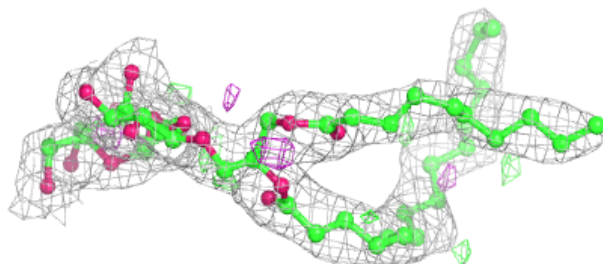
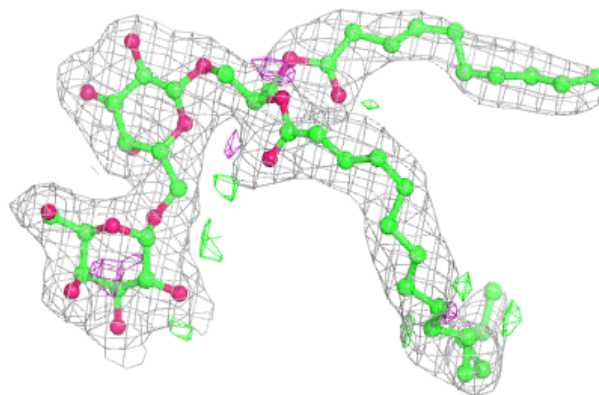


Electron density around LFA d 408:

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

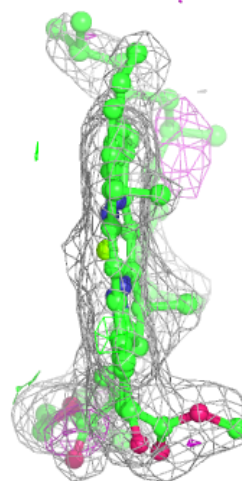
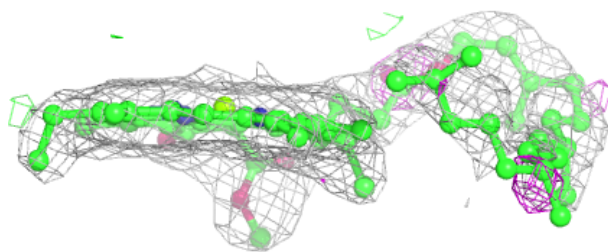
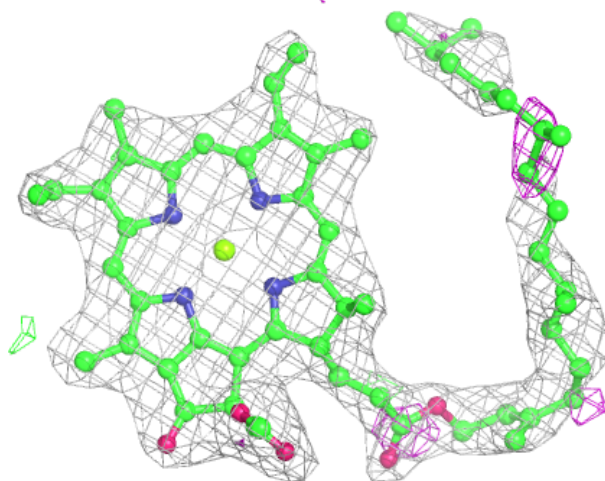
**Electron density around DGD C 518:**

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



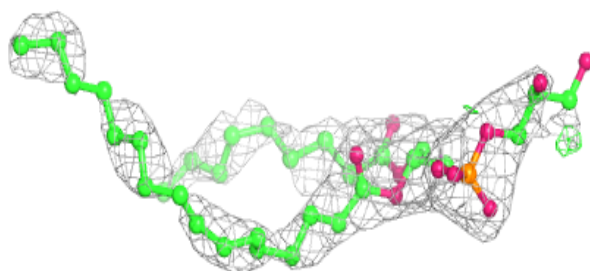
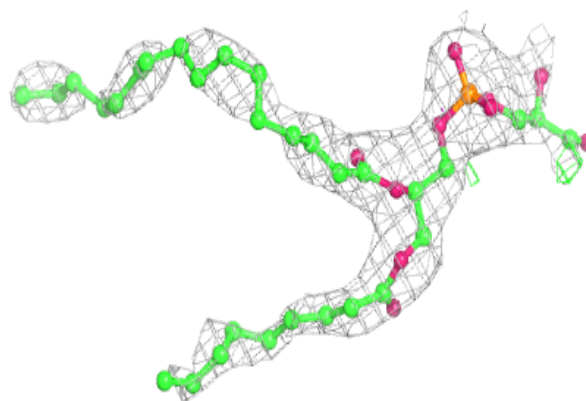
Electron density around CLA C 513:

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

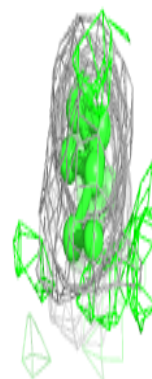
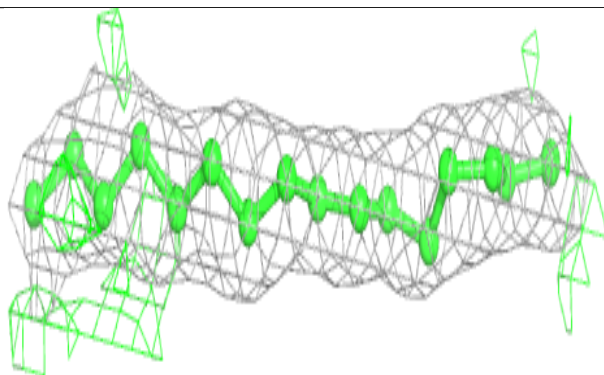
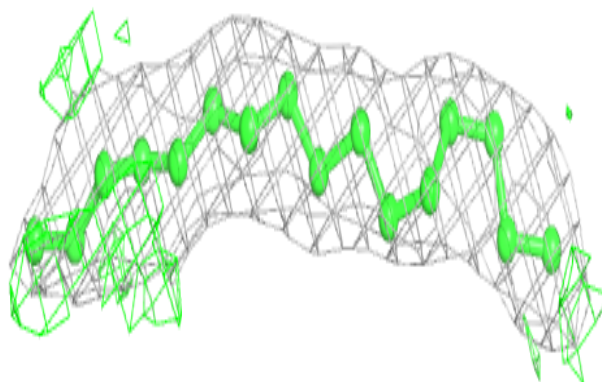


Electron density around LHG e 101:

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

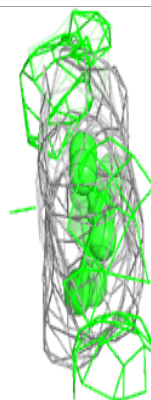
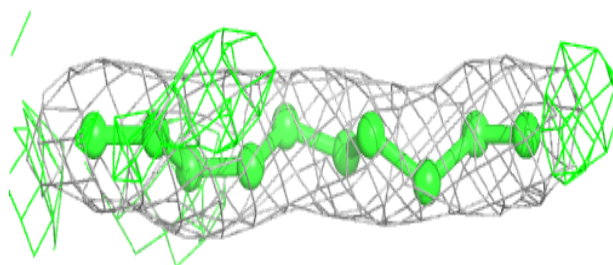
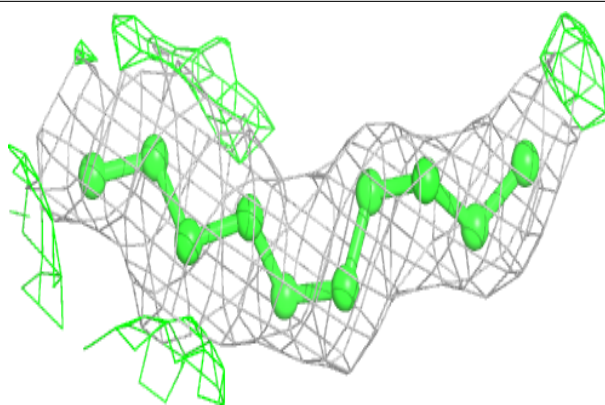
**Electron density around LFA M 102:**

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

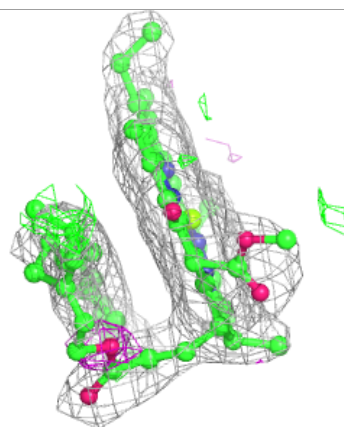
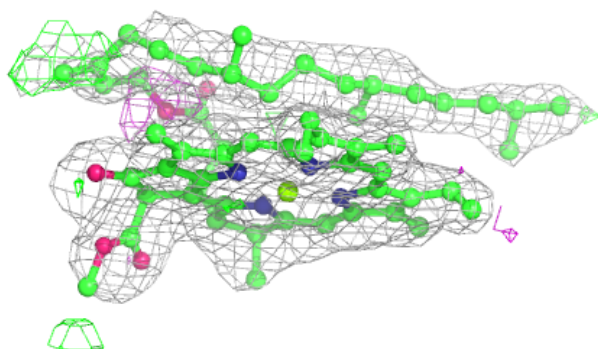
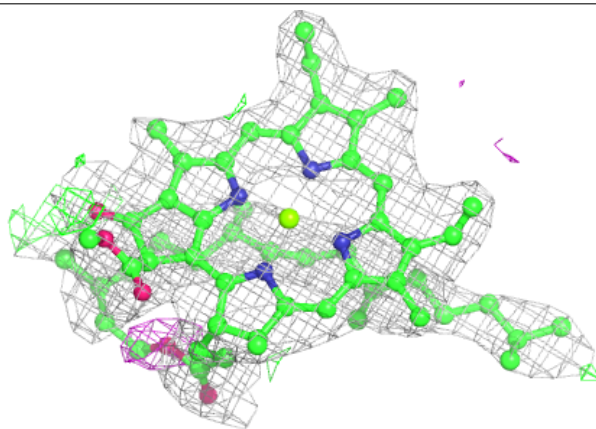


Electron density around LFA b 622:

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

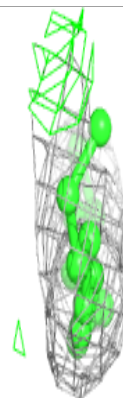
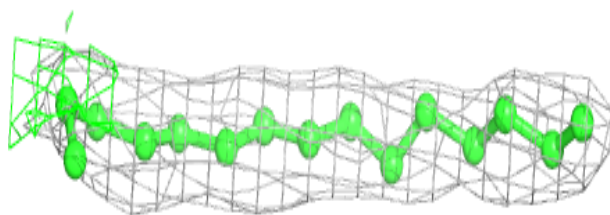
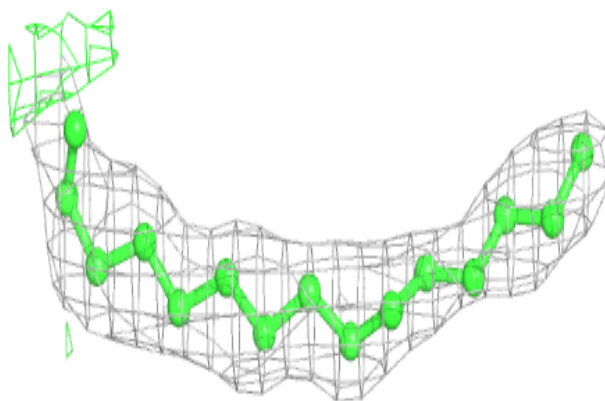
**Electron density around CLA H 101:**

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

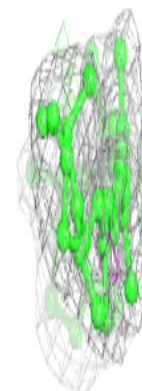
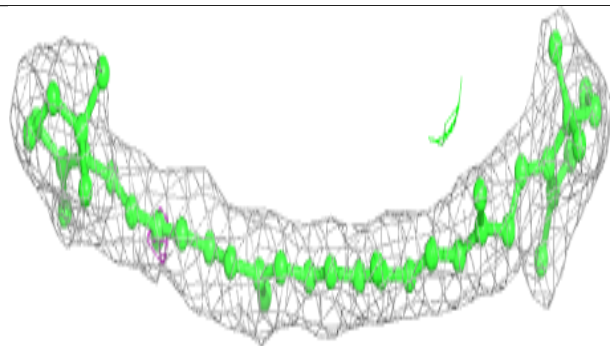
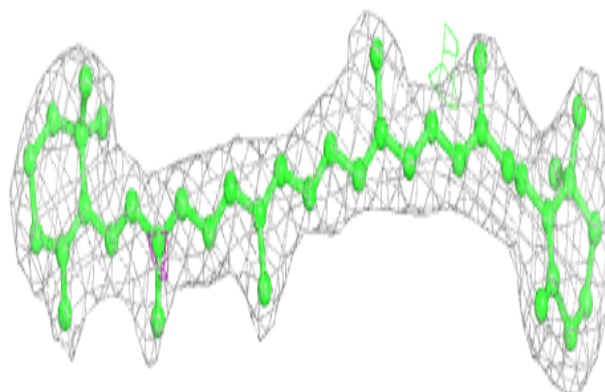


Electron density around LFA t 101:

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

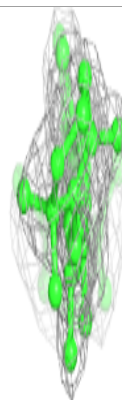
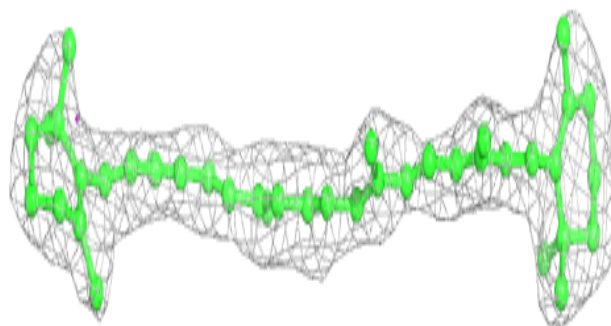
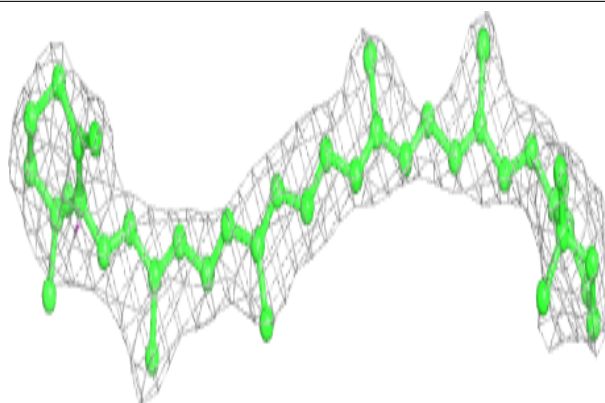
**Electron density around BCR t 102:**

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

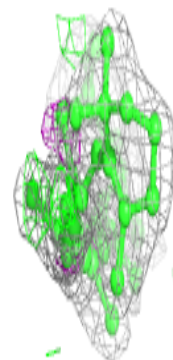
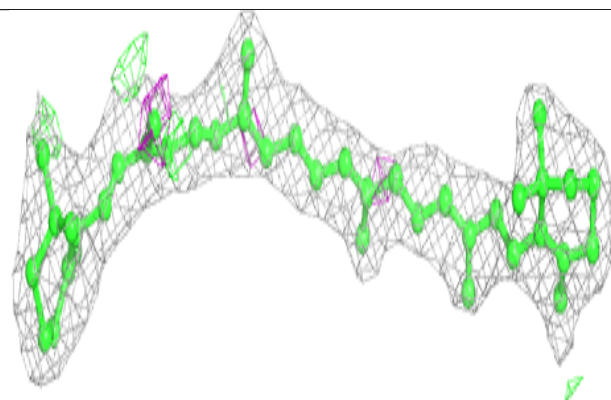
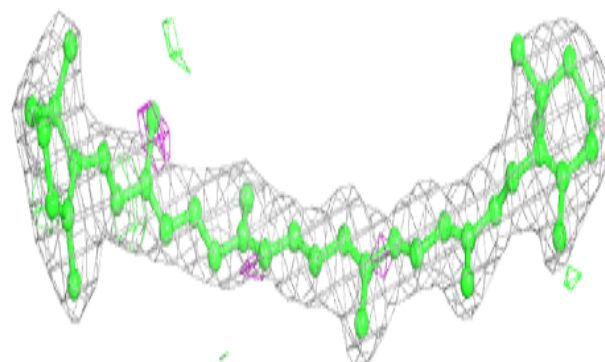


Electron density around BCR c 523:

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

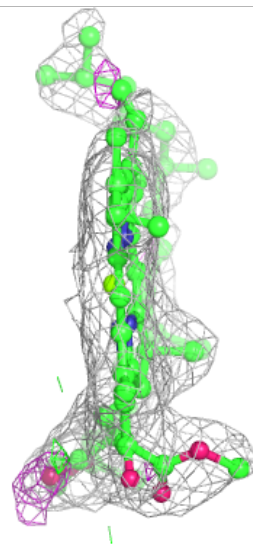
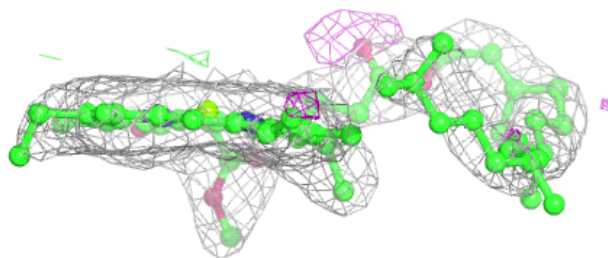
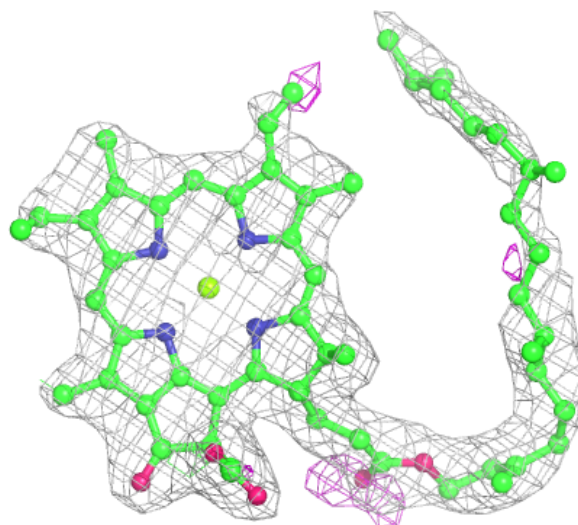
**Electron density around BCR T 101:**

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



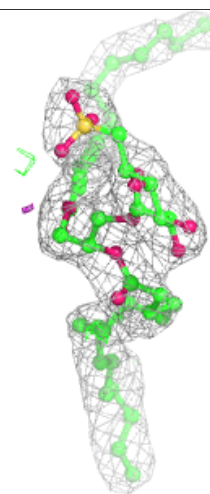
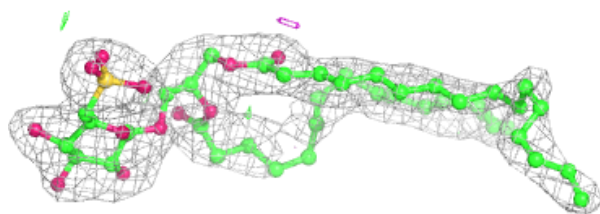
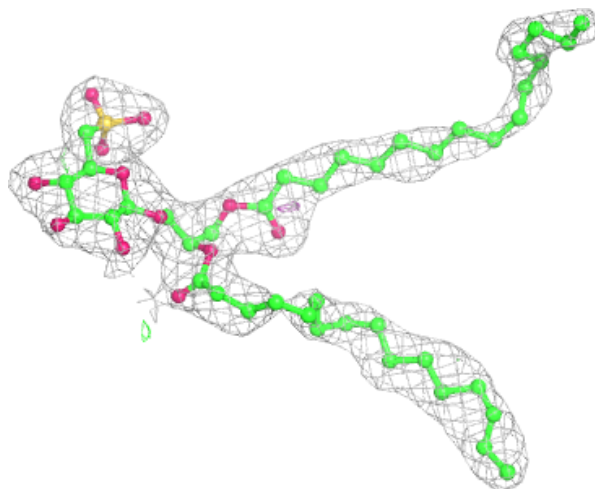
Electron density around CLA c 513:

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



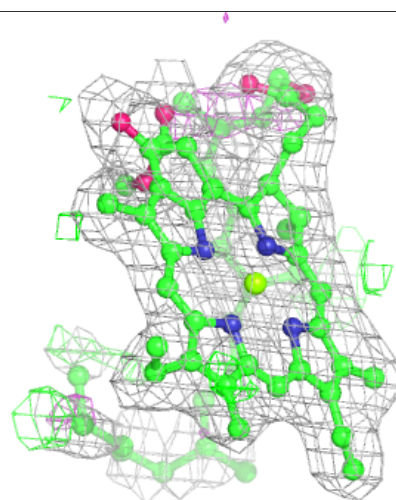
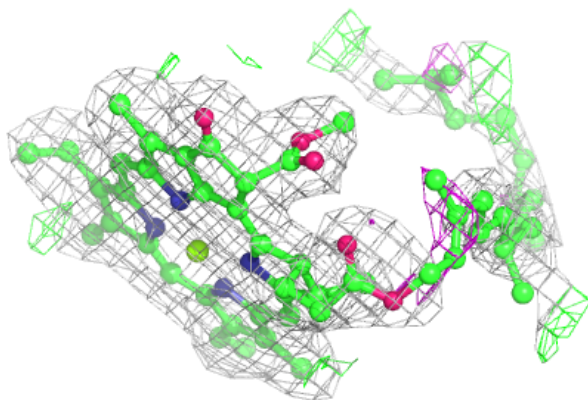
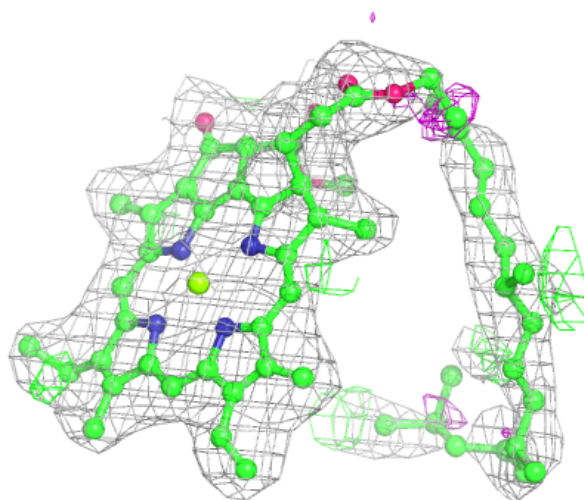
Electron density around SQD A 409:

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



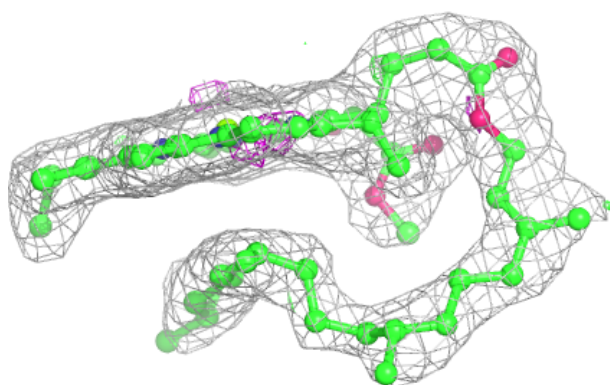
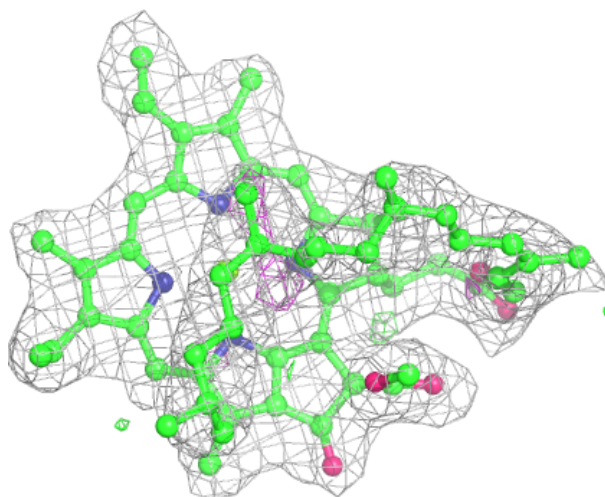
Electron density around CLA b 618:

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



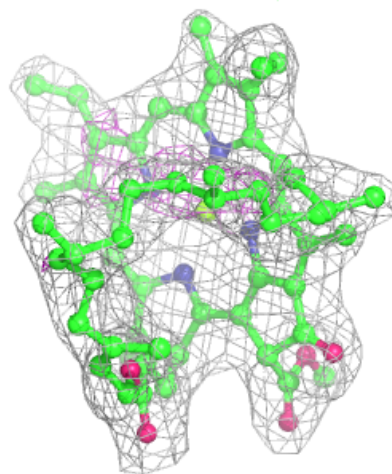
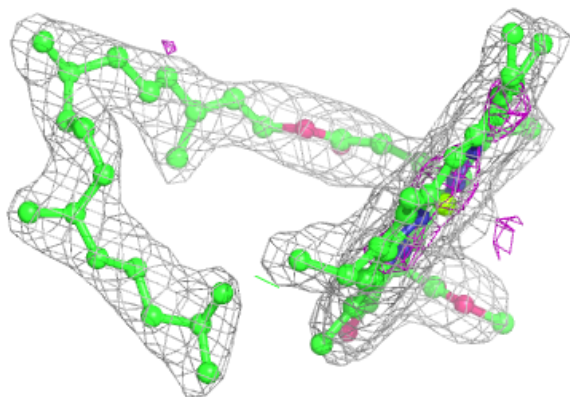
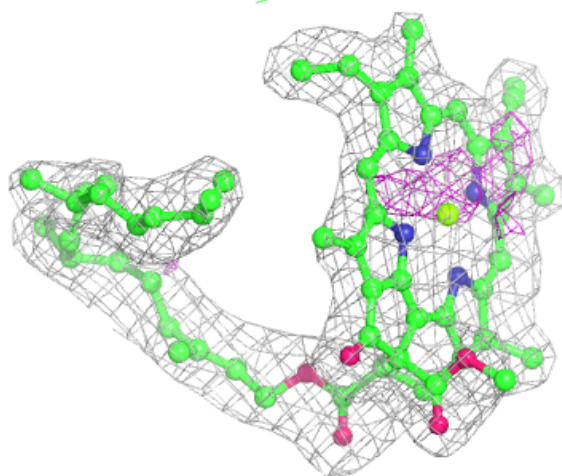
Electron density around CLA C 511:

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



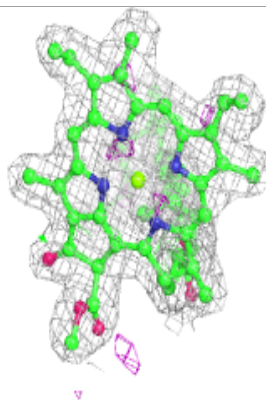
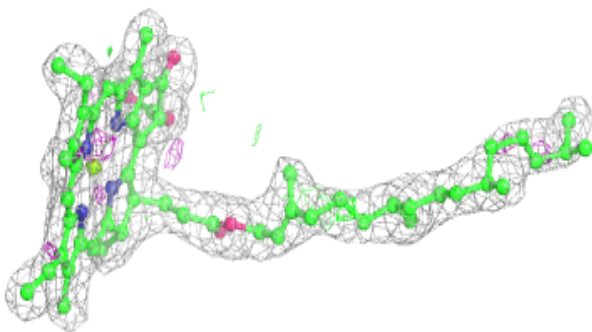
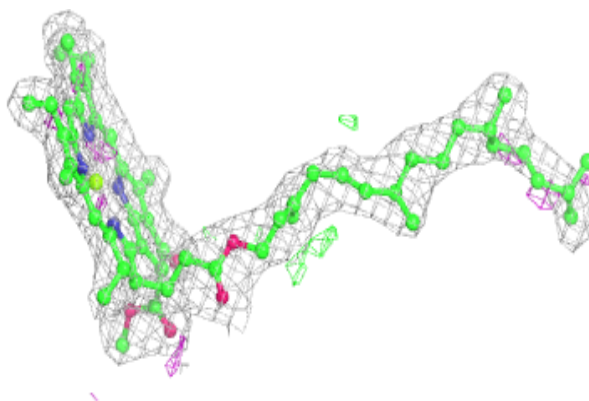
Electron density around CLA C 504:

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



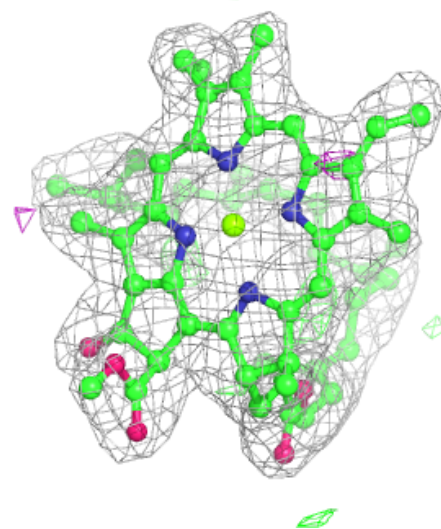
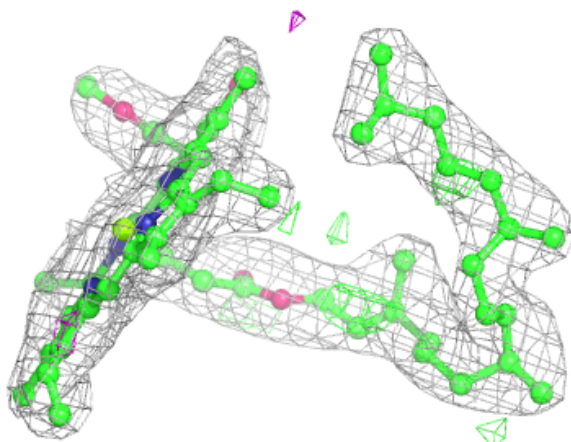
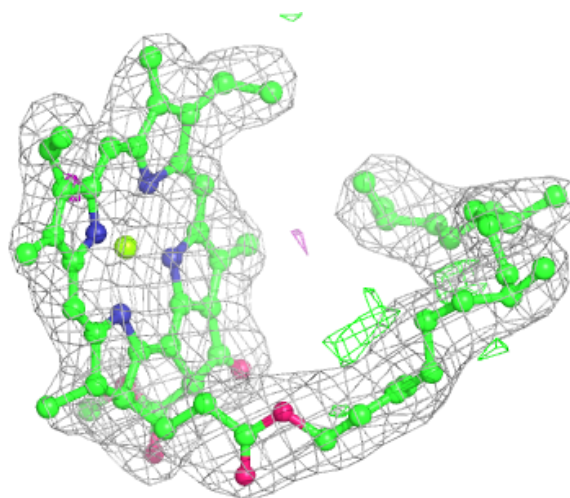
Electron density around CLA B 603:

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



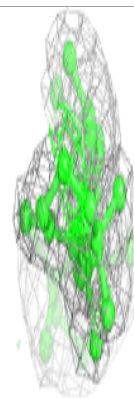
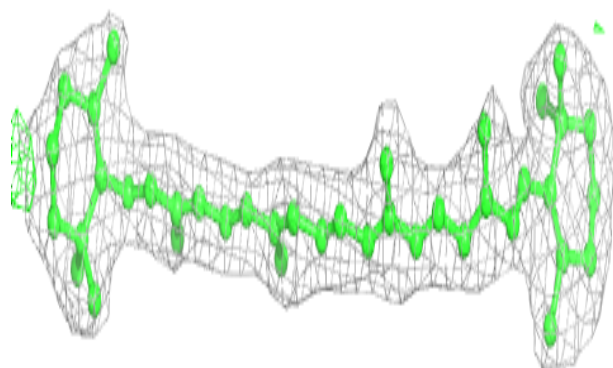
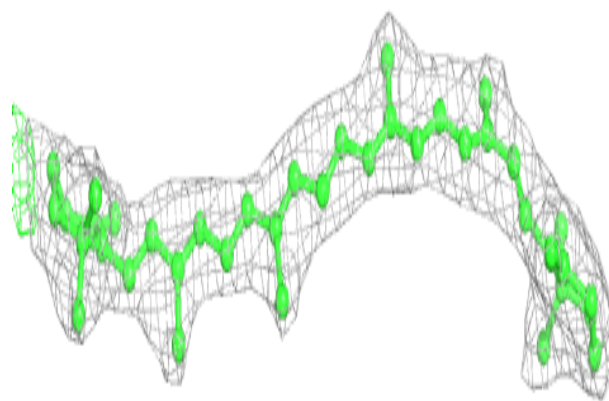
Electron density around CLA c 504:

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

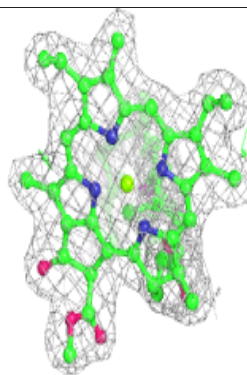
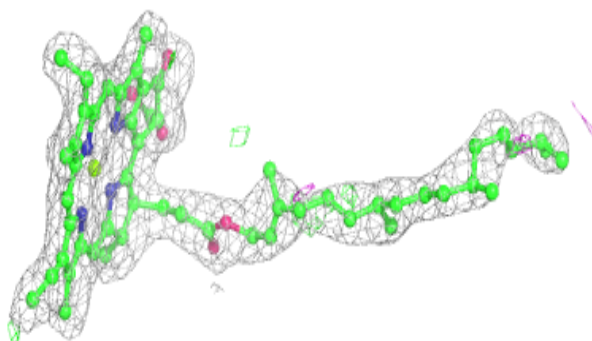
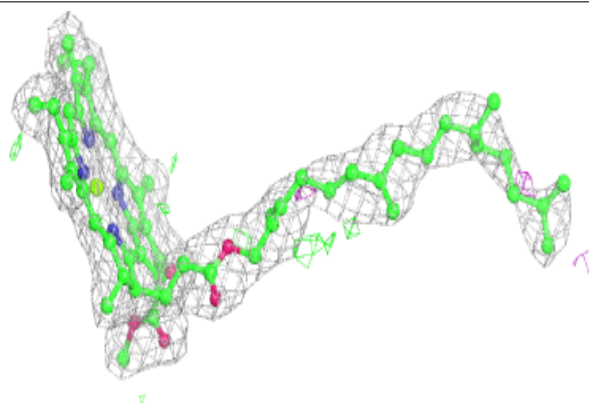


Electron density around BCR H 102:

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

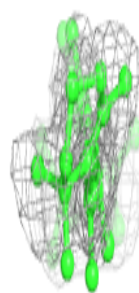
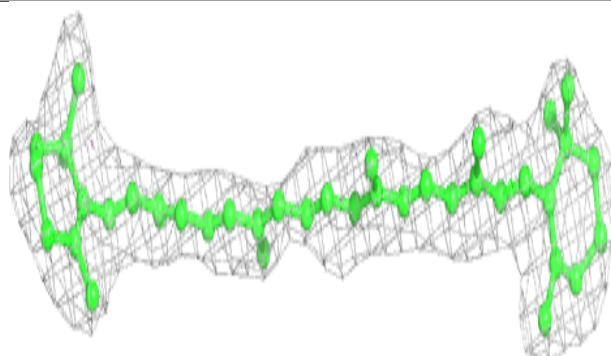
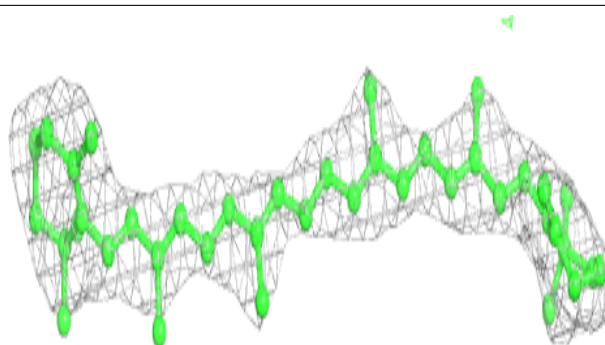
**Electron density around CLA b 606:**

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

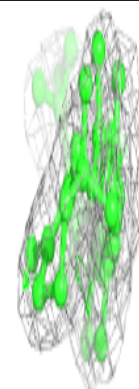
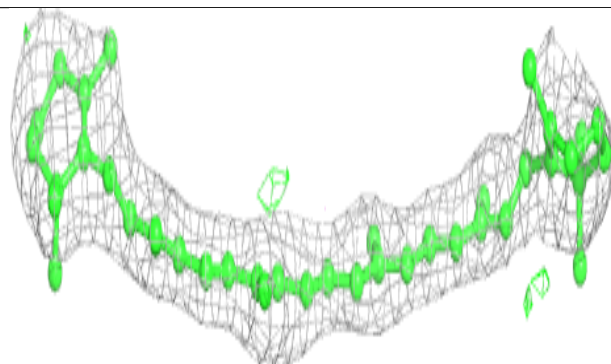
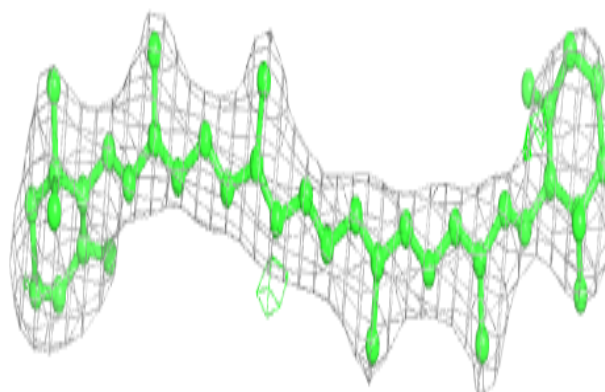


Electron density around BCR c 524:

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

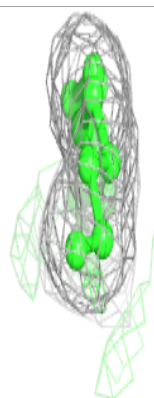
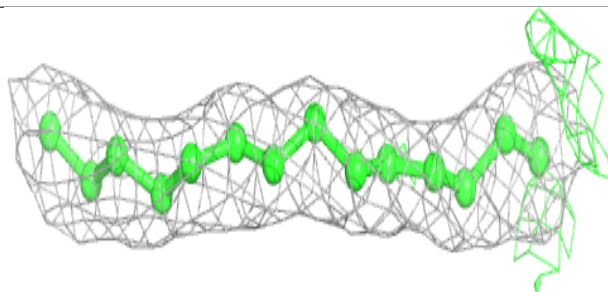
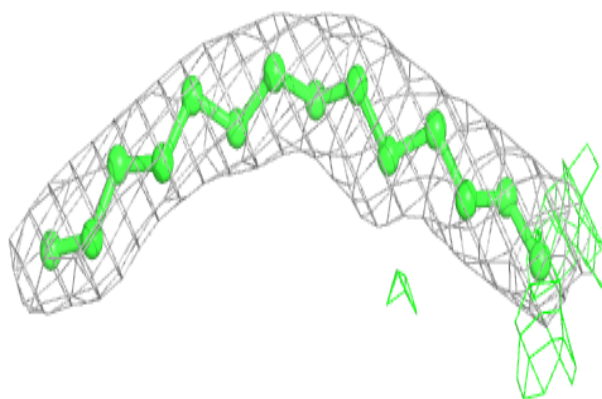
**Electron density around BCR d 404:**

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

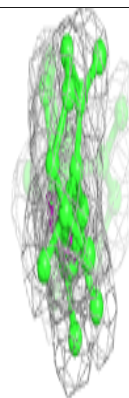
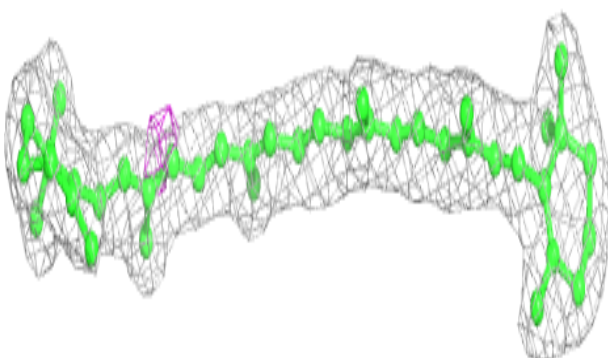
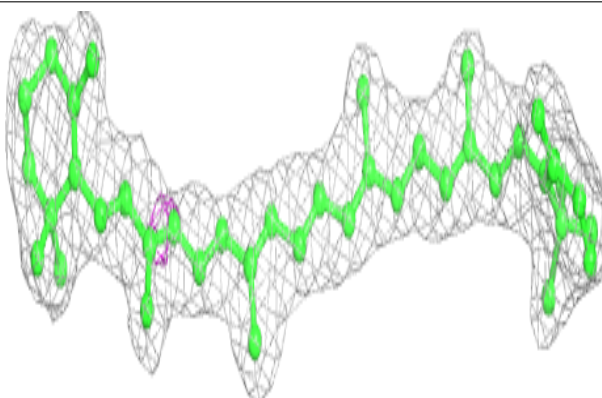


Electron density around LFA I 101:

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

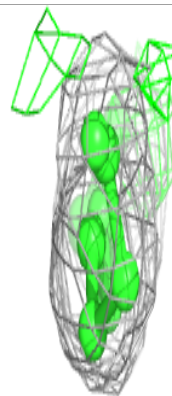
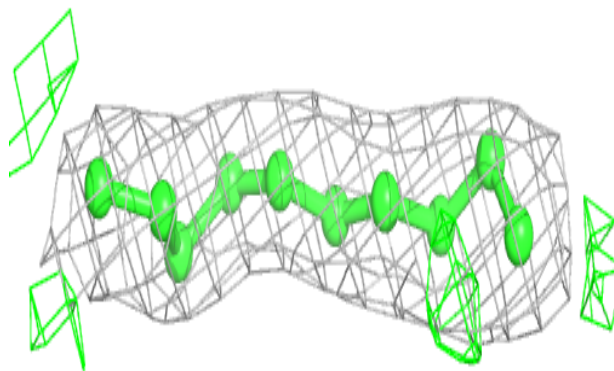
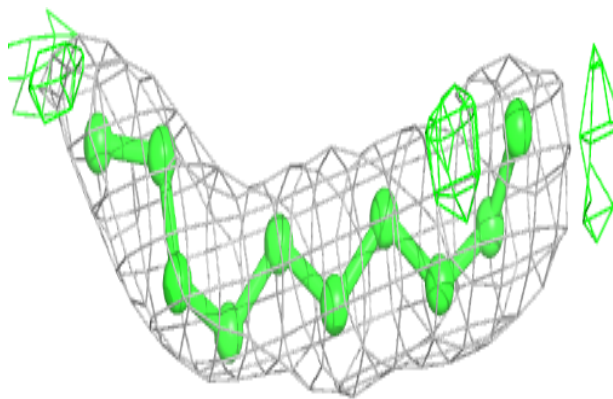
**Electron density around BCR B 616:**

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



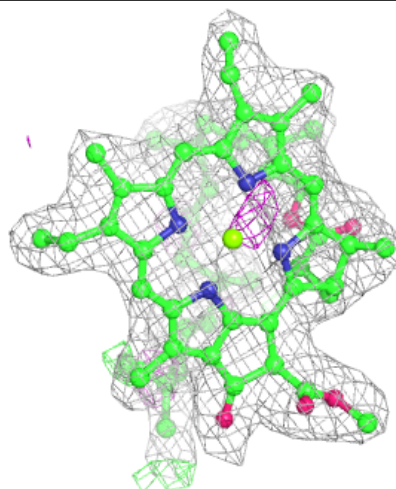
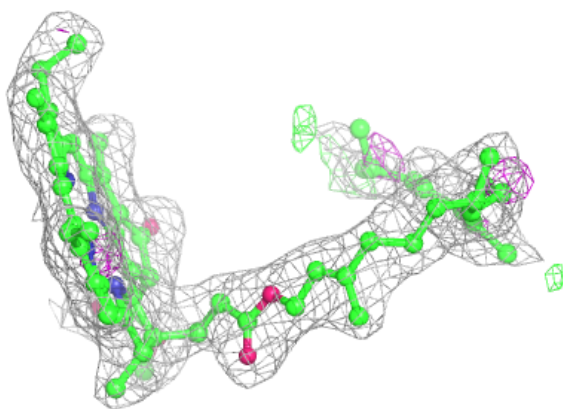
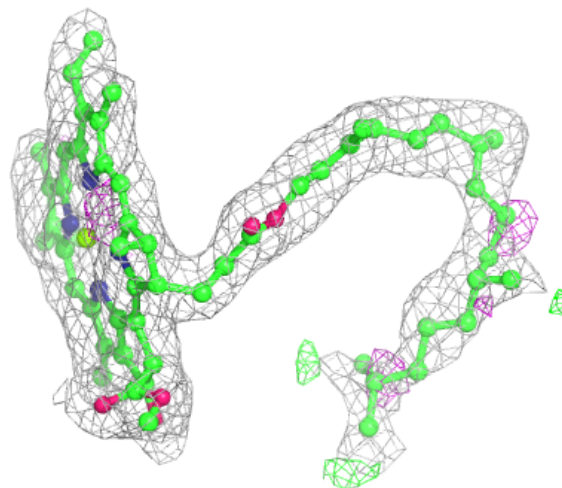
Electron density around LFA B 620:

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



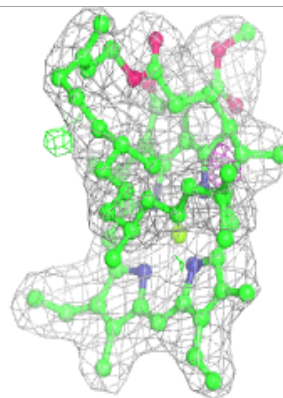
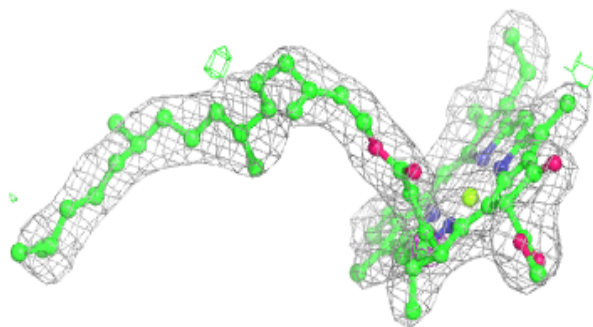
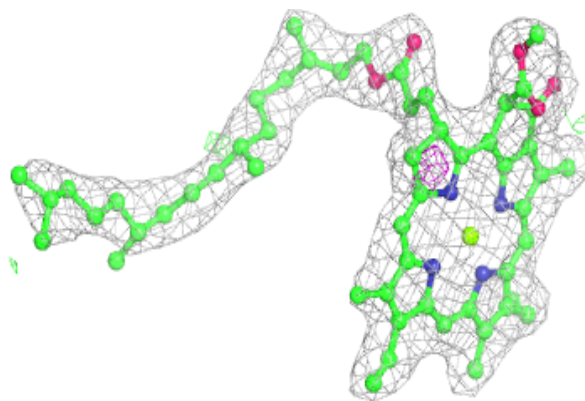
Electron density around CLA B 605:

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

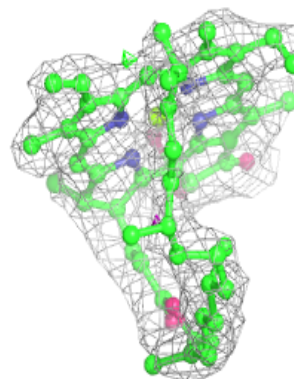
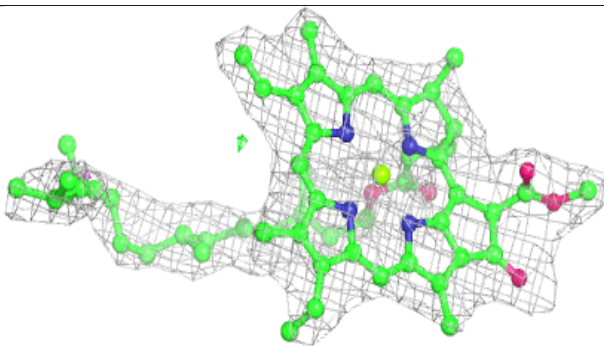
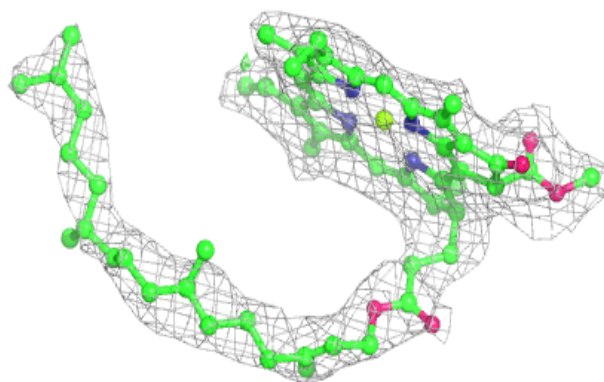


Electron density around CLA C 512:

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

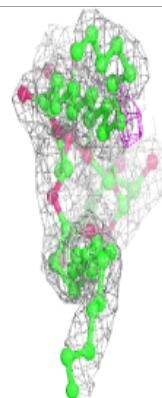
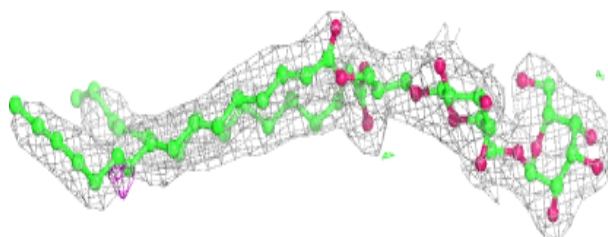
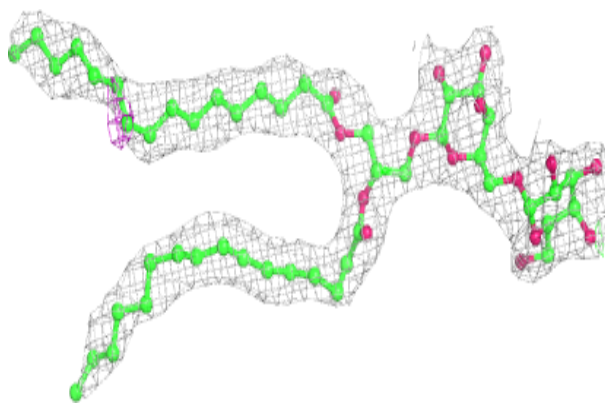
**Electron density around CLA c 514:**

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

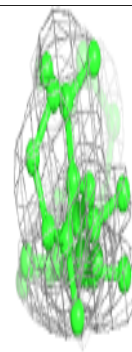
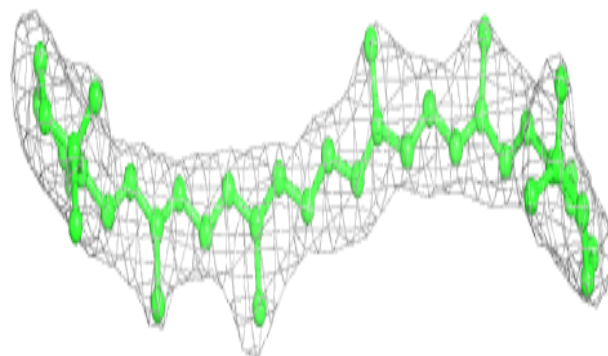
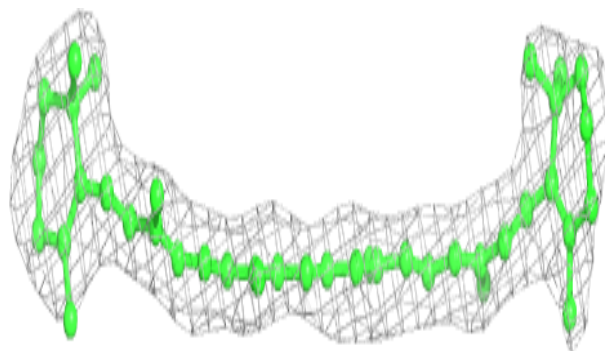


Electron density around DGD C 519:

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

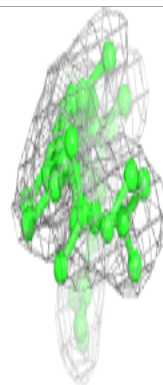
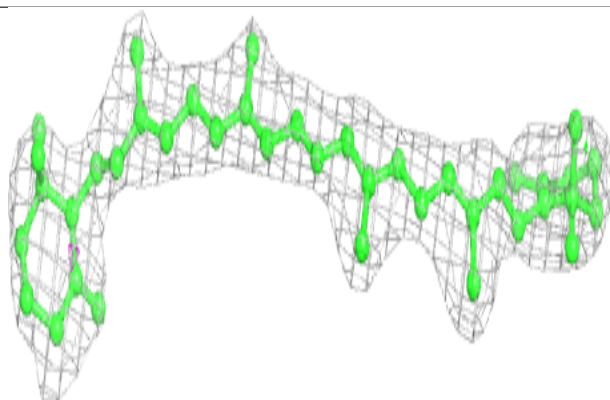
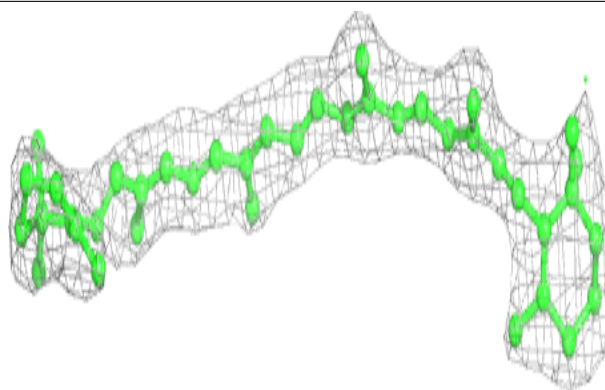
**Electron density around BCR K 102:**

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

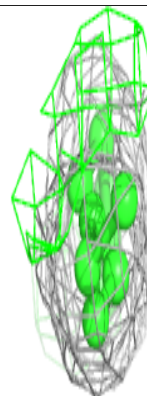
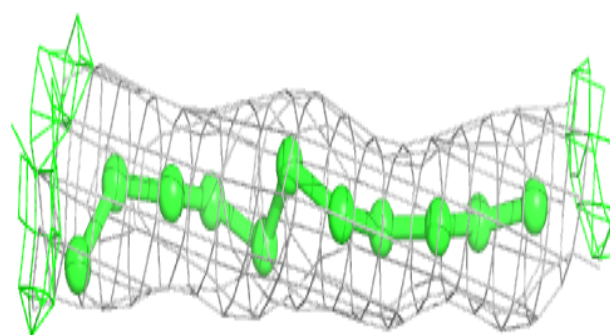
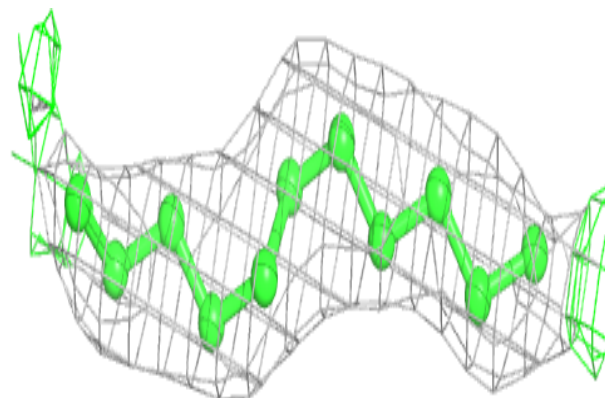


Electron density around BCR D 404:

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

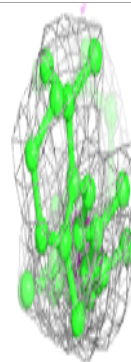
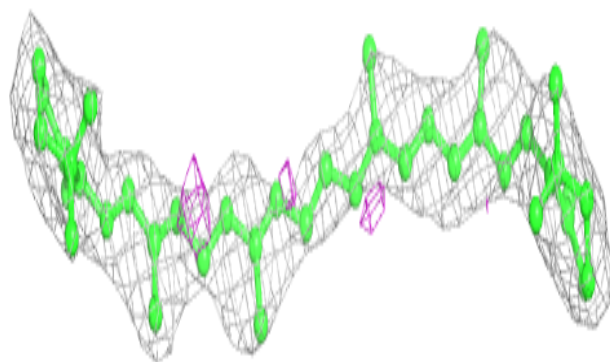
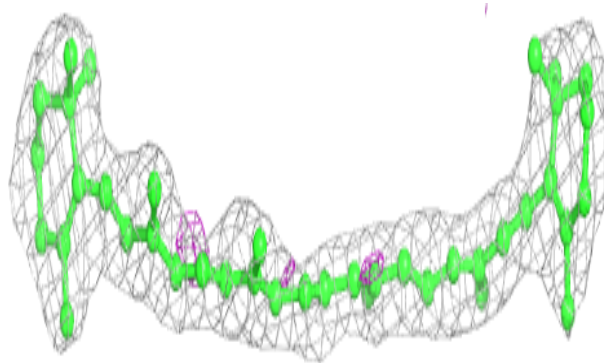
**Electron density around LFA J 101:**

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

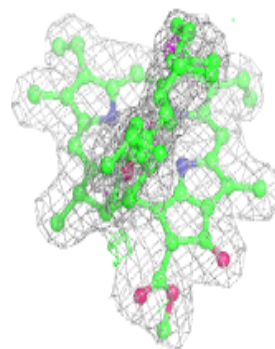
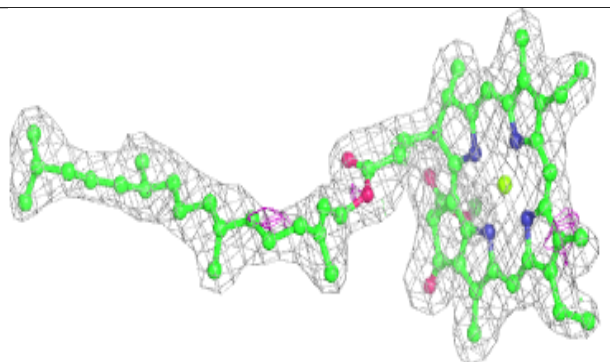
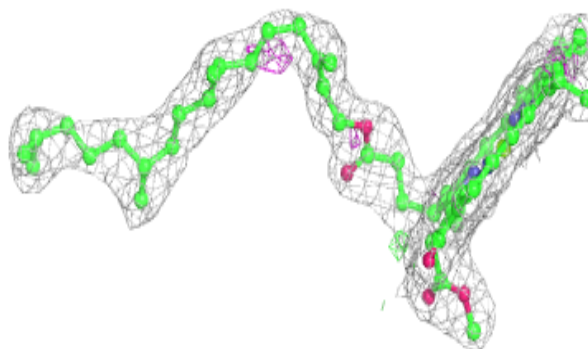


Electron density around BCR k 101:

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

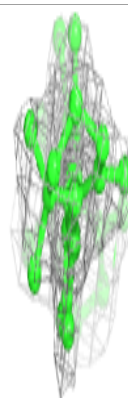
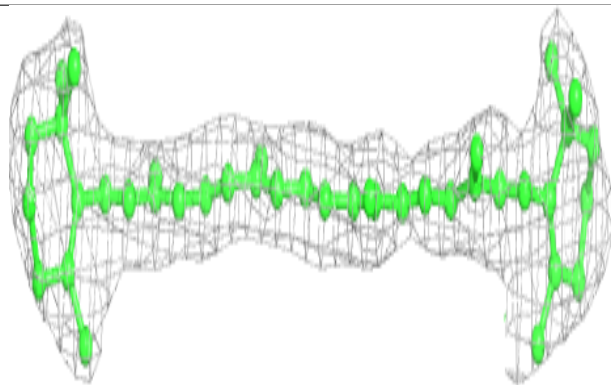
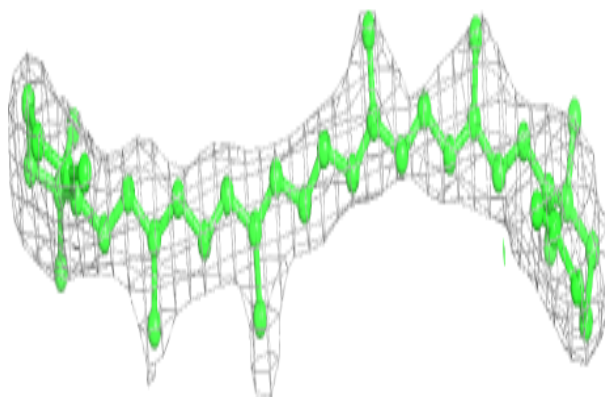
**Electron density around CLA C 503:**

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

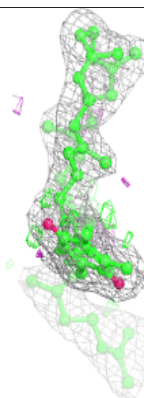
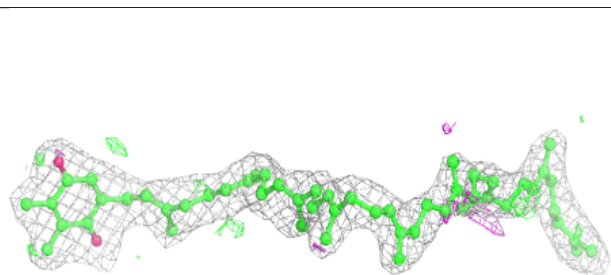
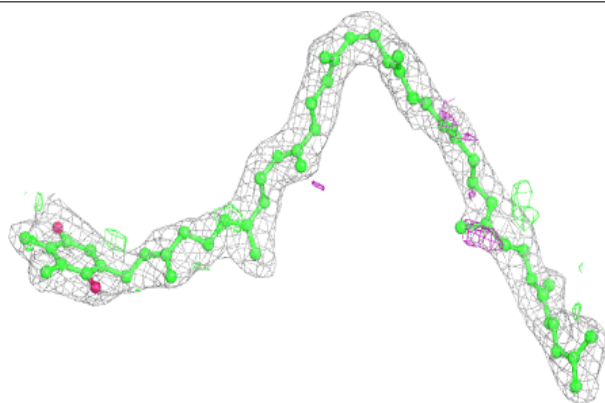


Electron density around BCR C 515:

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

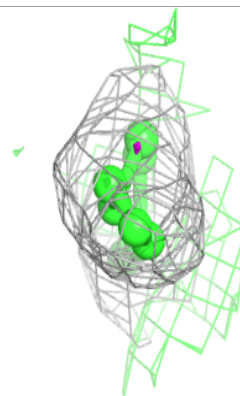
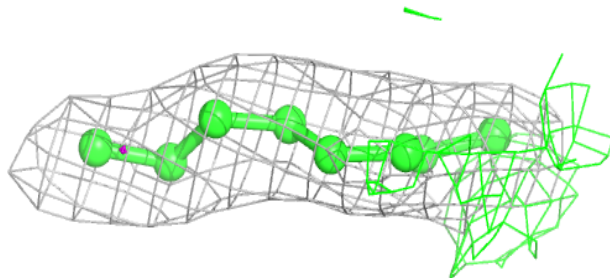
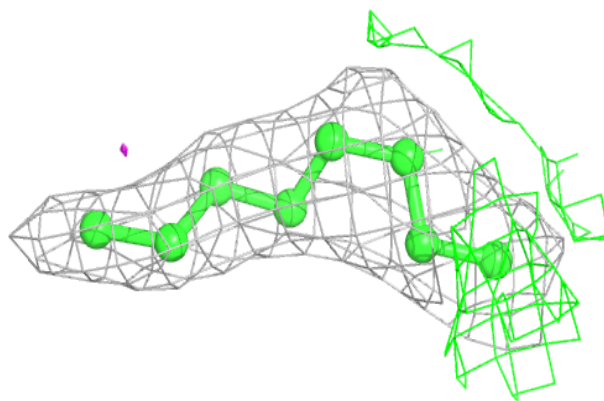
**Electron density around PL9 D 405:**

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

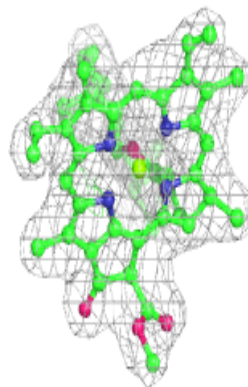
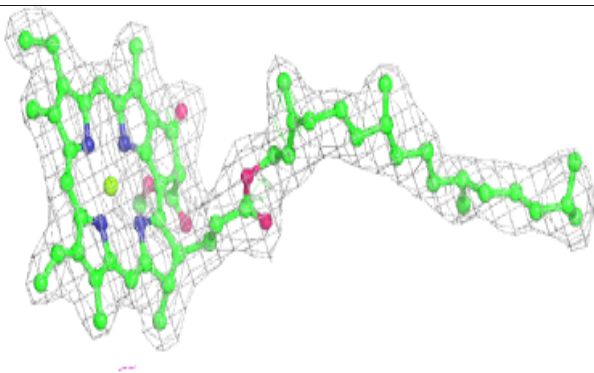
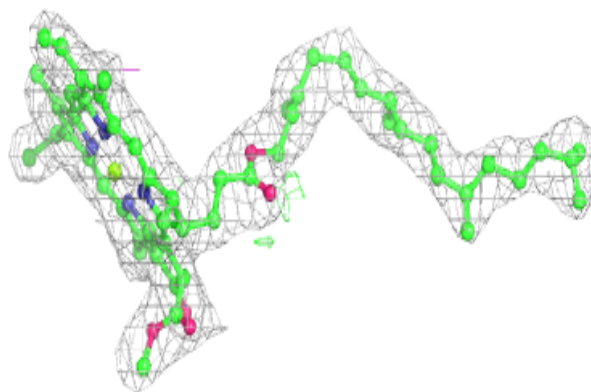


Electron density around LFA D 412:

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

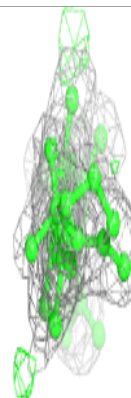
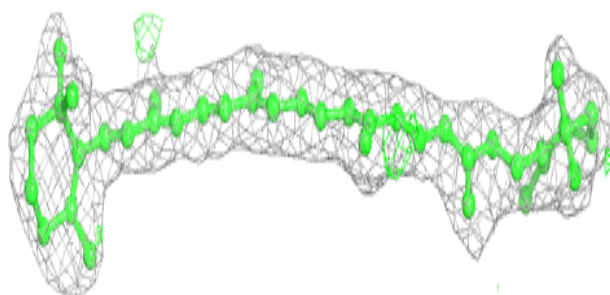
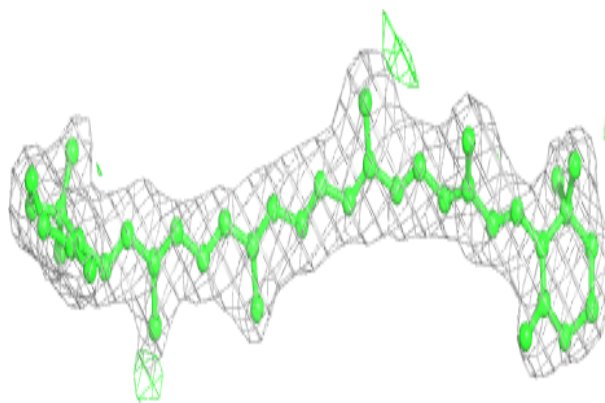
**Electron density around CLA c 503:**

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

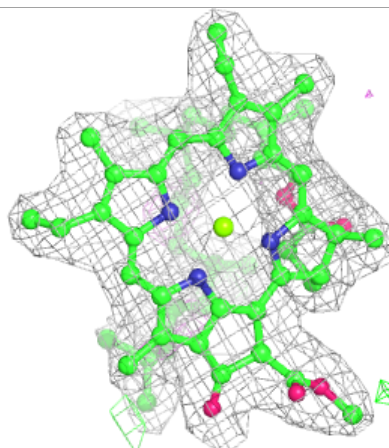
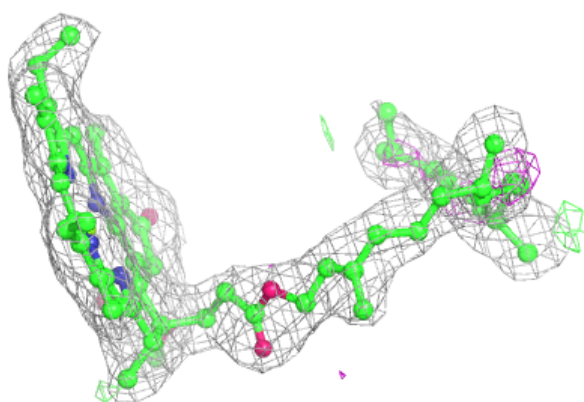
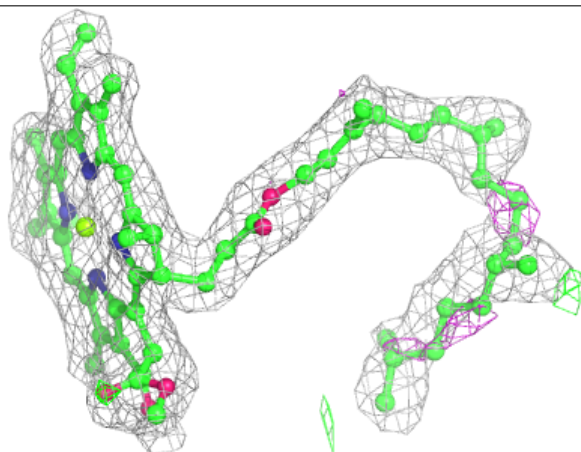


Electron density around BCR b 619:

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

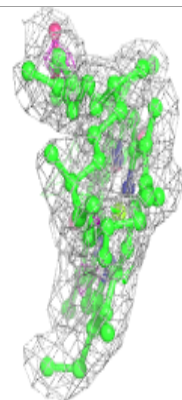
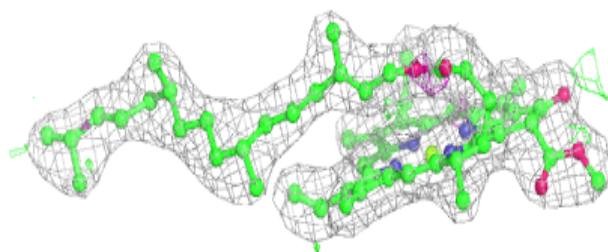
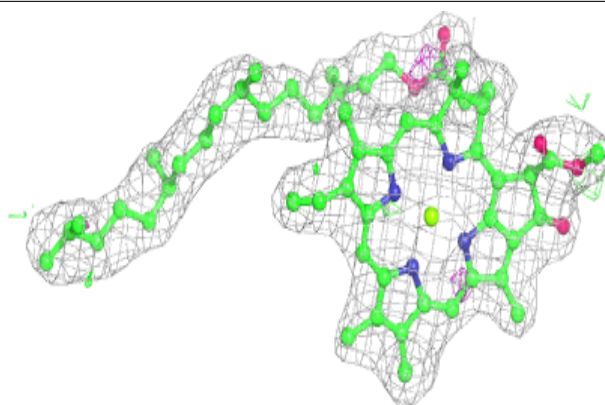
**Electron density around CLA b 608:**

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

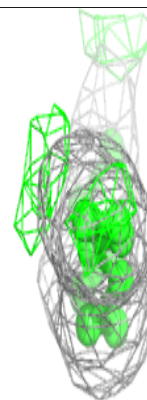
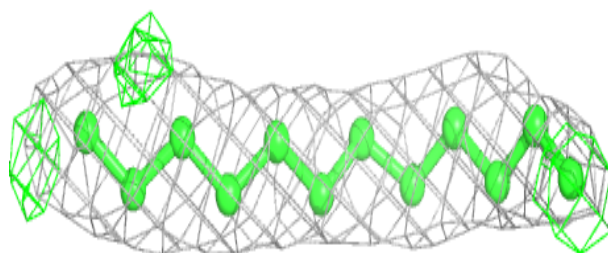
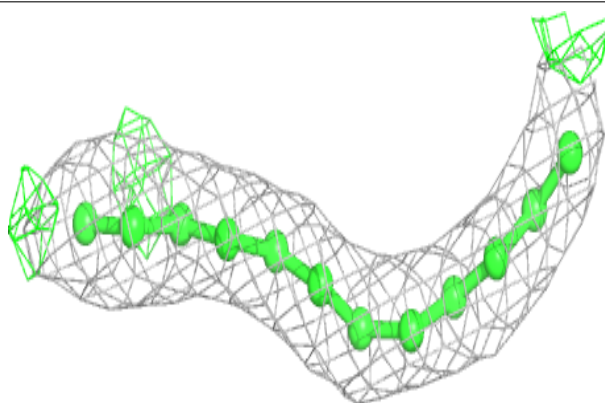


Electron density around CLA c 502:

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

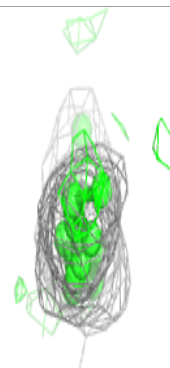
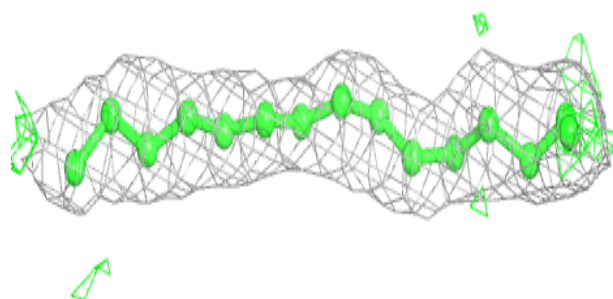
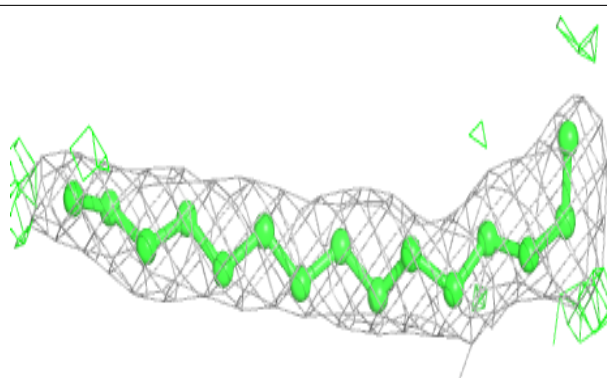
**Electron density around LFA B 628:**

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

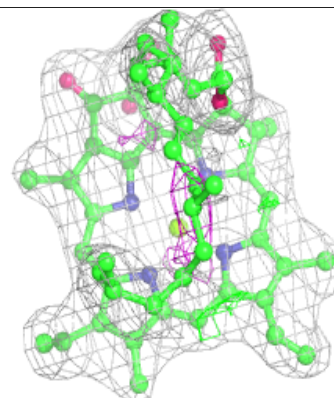
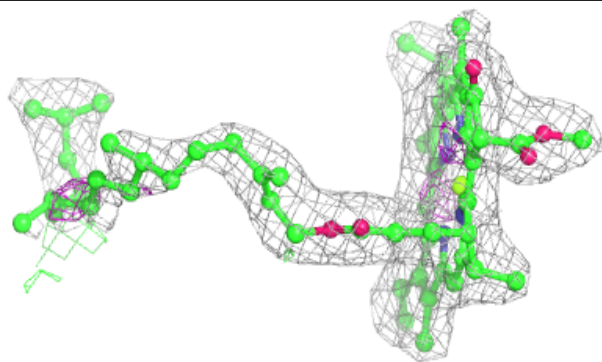
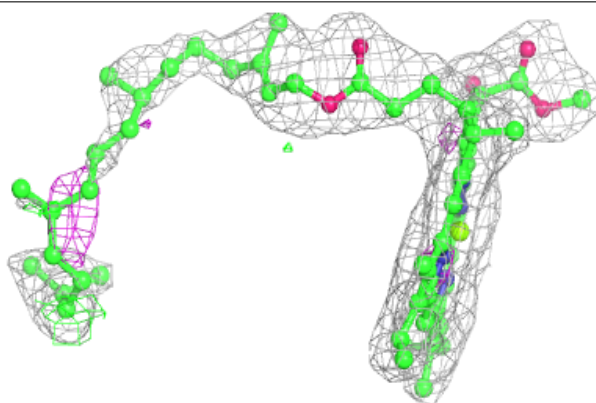


Electron density around LFA c 521:

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

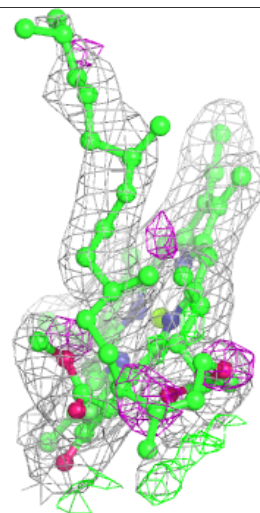
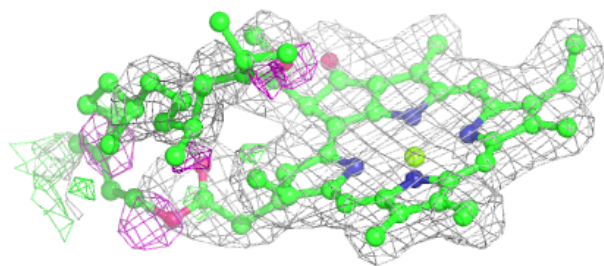
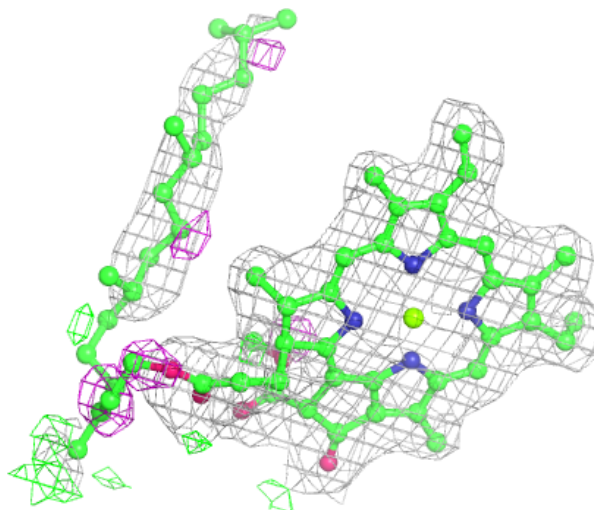
**Electron density around CLA c 507:**

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



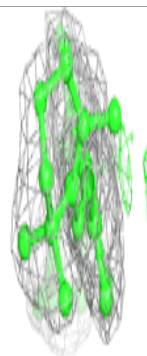
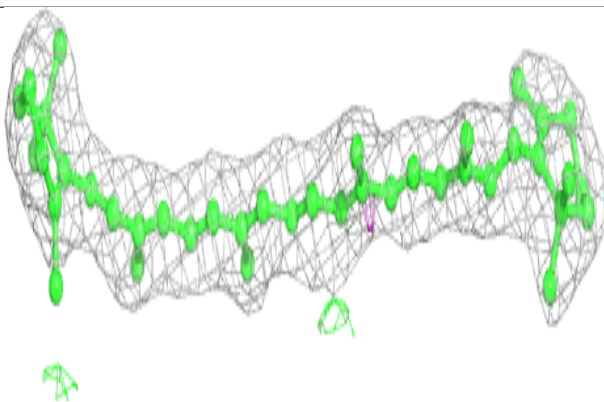
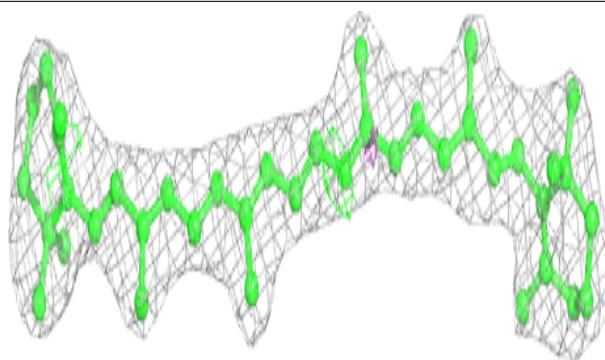
Electron density around CLA B 615:

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

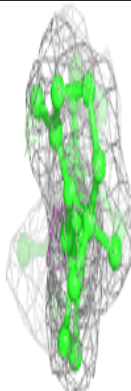
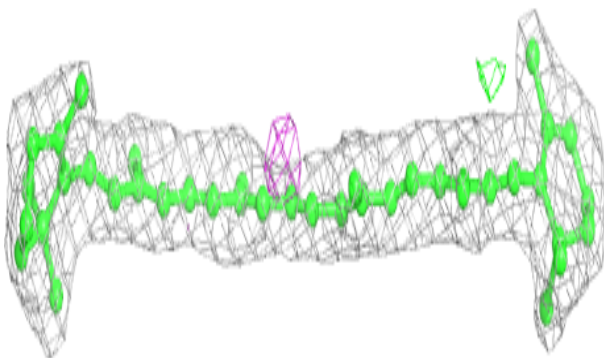
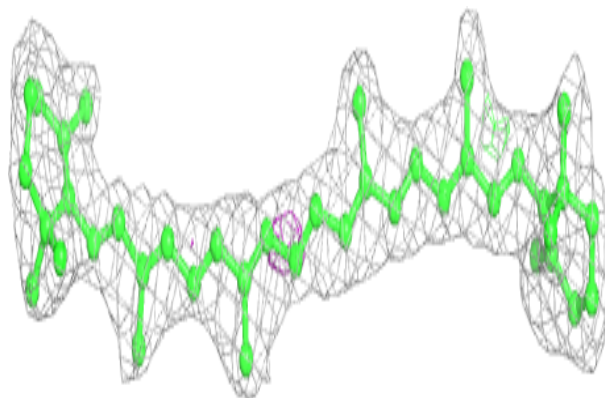


Electron density around BCR b 621:

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

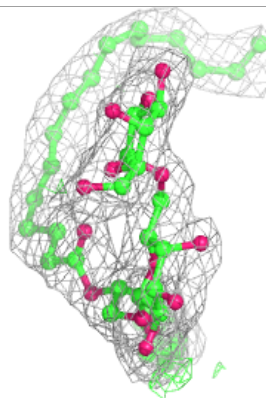
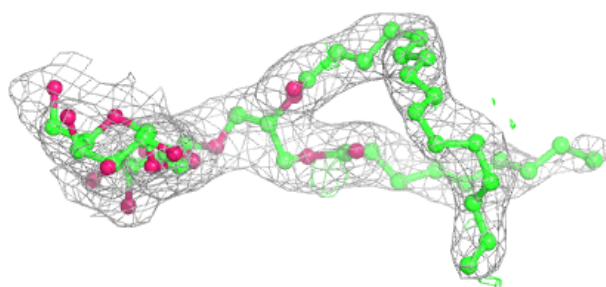
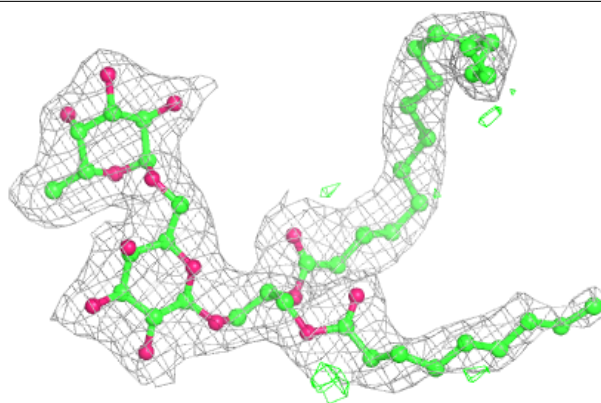
**Electron density around BCR B 617:**

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

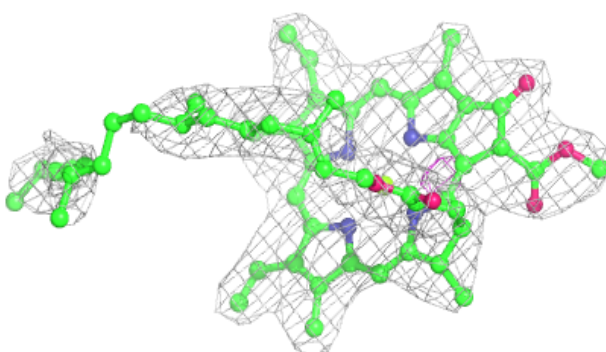
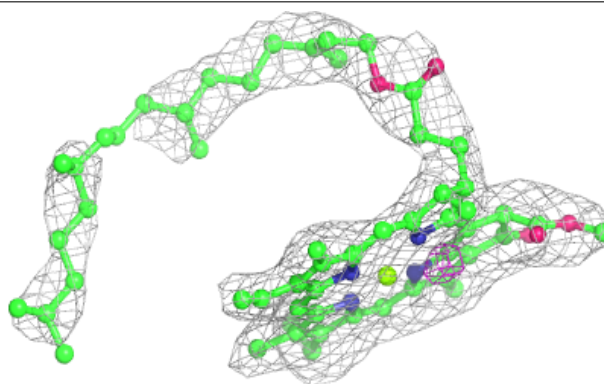


Electron density around DGD c 517:

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

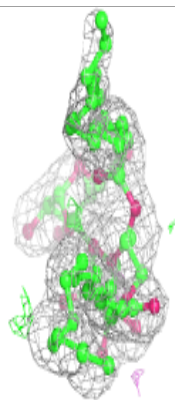
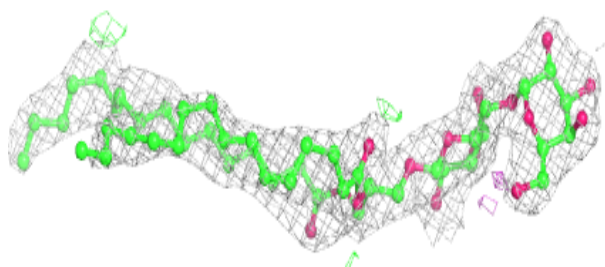
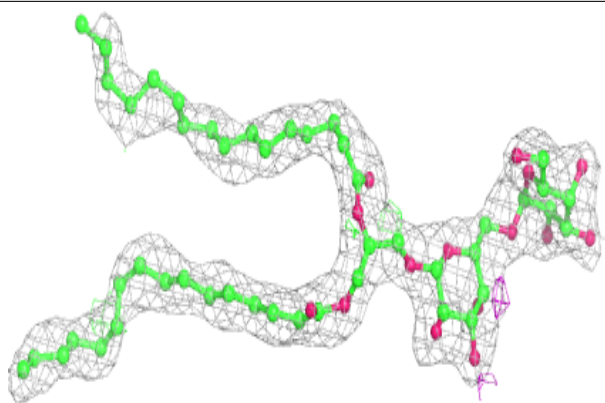
**Electron density around CLA C 514:**

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

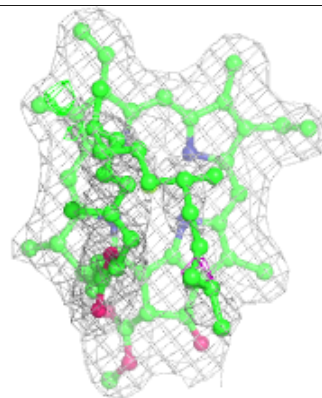
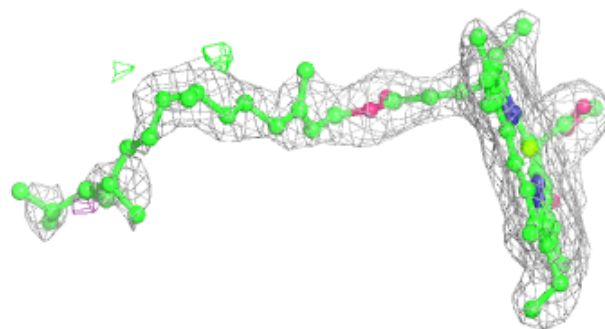
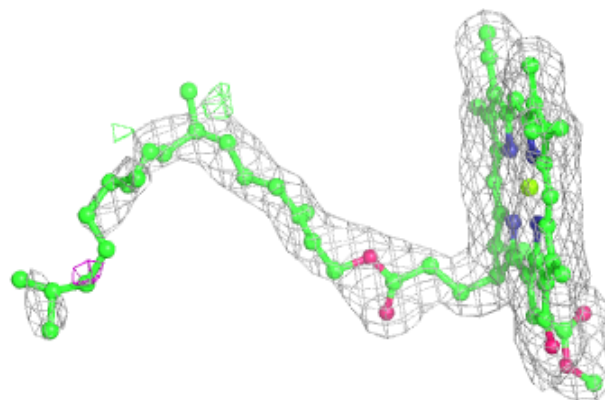


Electron density around DGD c 518:

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

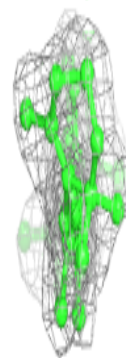
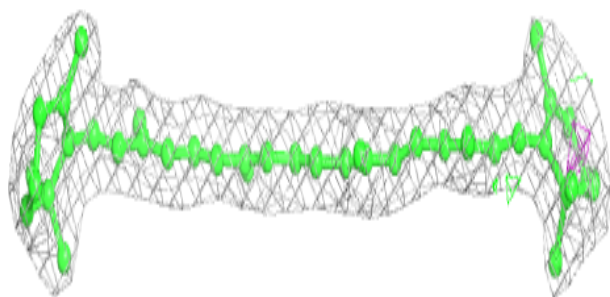
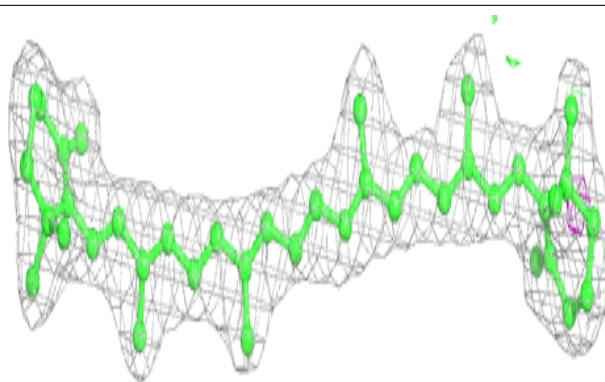
**Electron density around CLA D 403:**

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

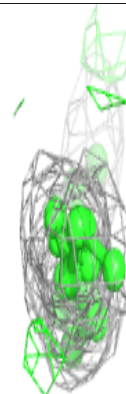
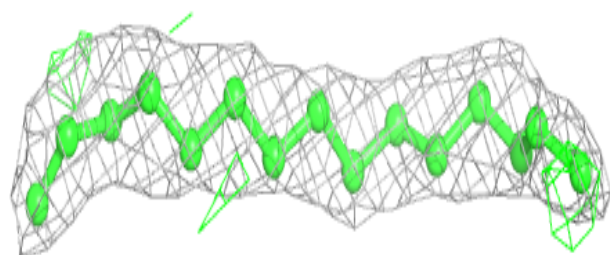
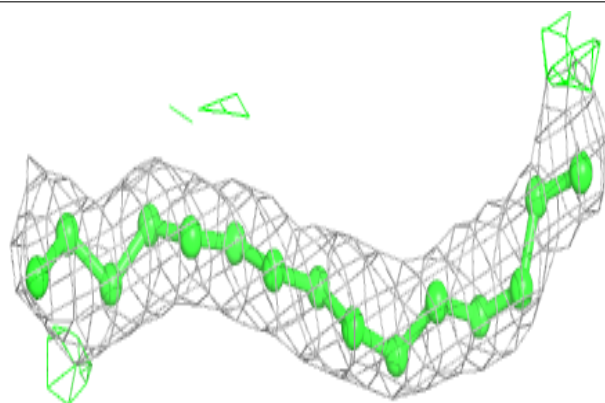


Electron density around BCR b 620:

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

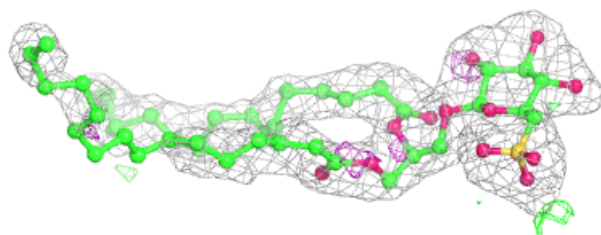
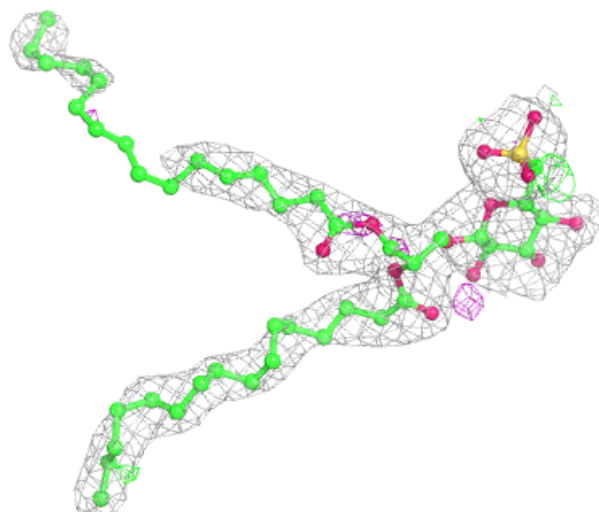
**Electron density around LFA b 602:**

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



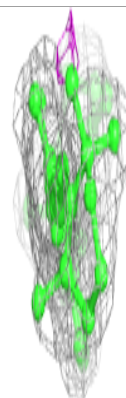
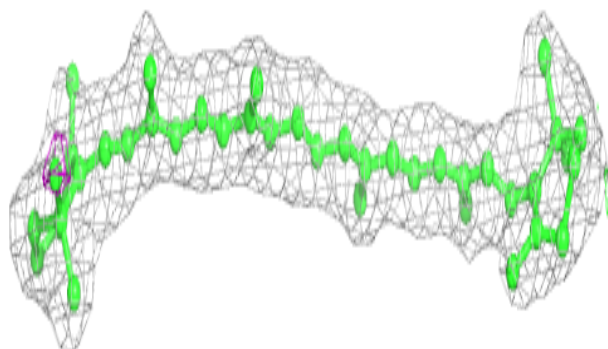
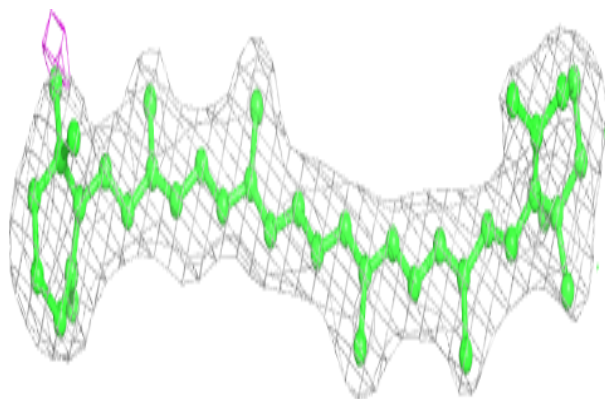
Electron density around SQD a 410:

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

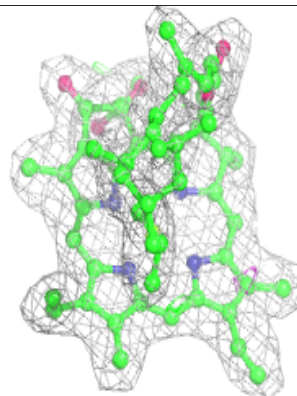
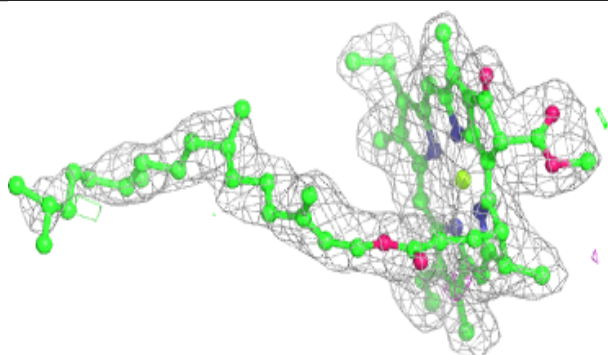
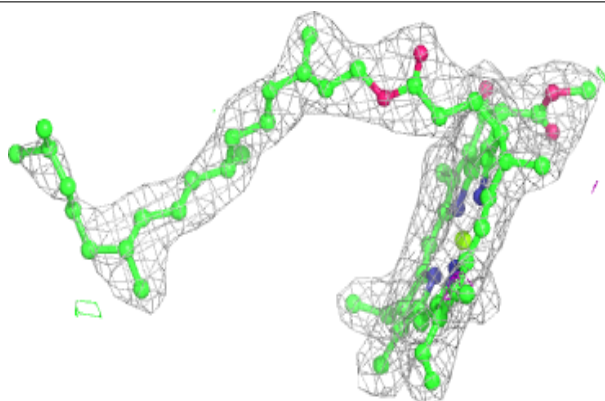


Electron density around BCR B 618:

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

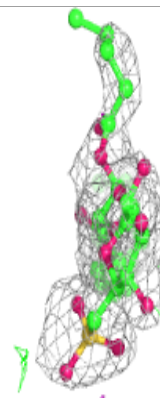
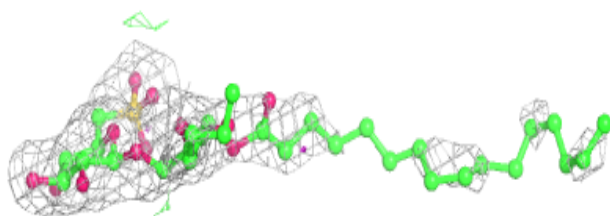
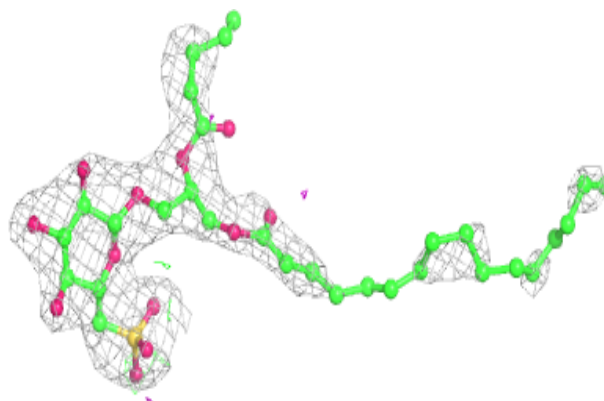
**Electron density around CLA C 509:**

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

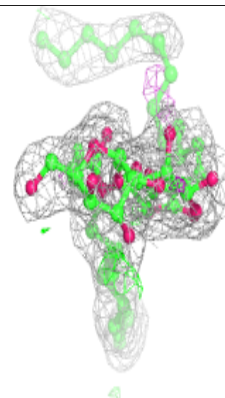
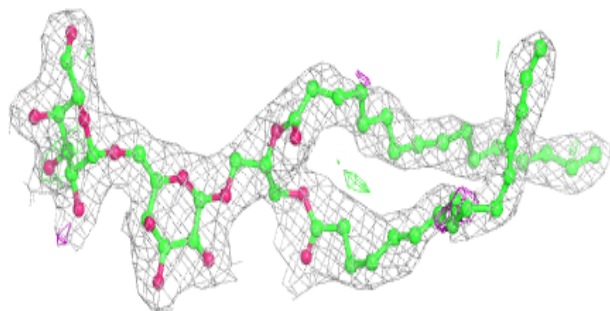
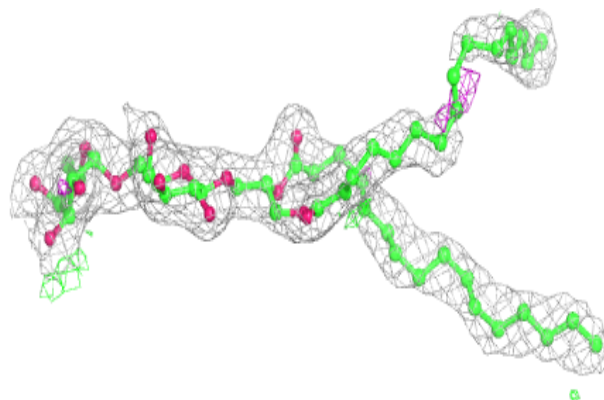


Electron density around SQD f 102:

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

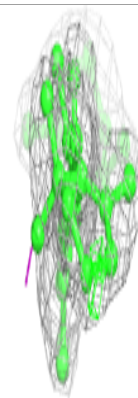
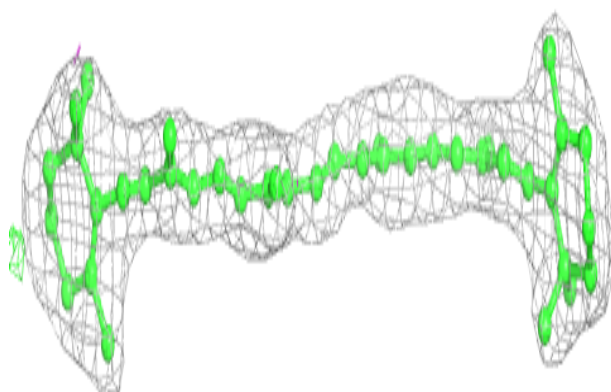
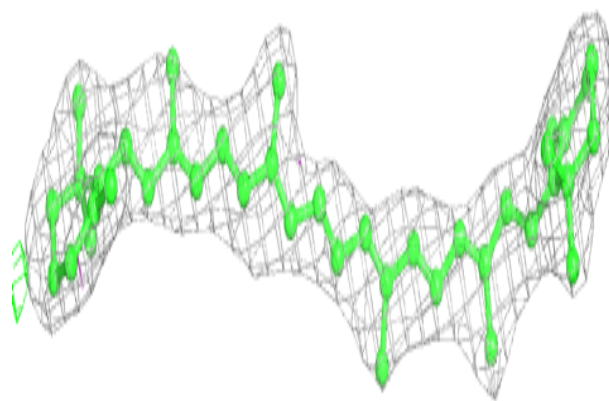
**Electron density around DGD c 516:**

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

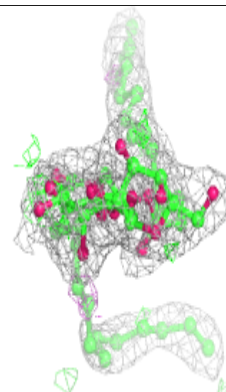
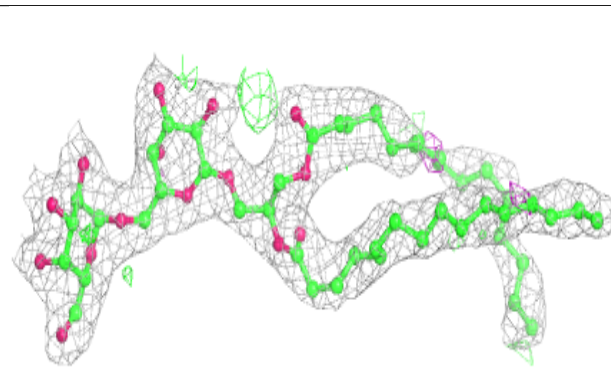
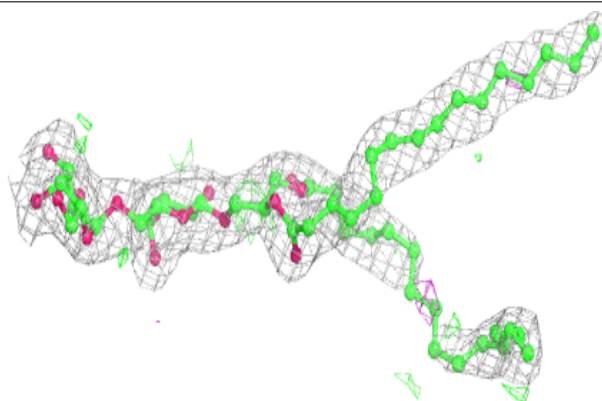


Electron density around BCR C 516:

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

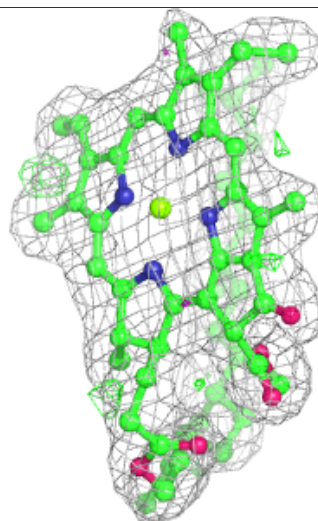
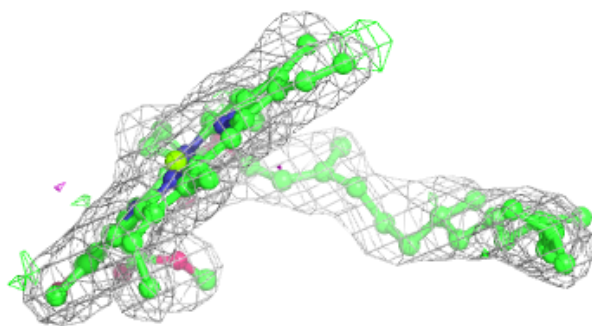
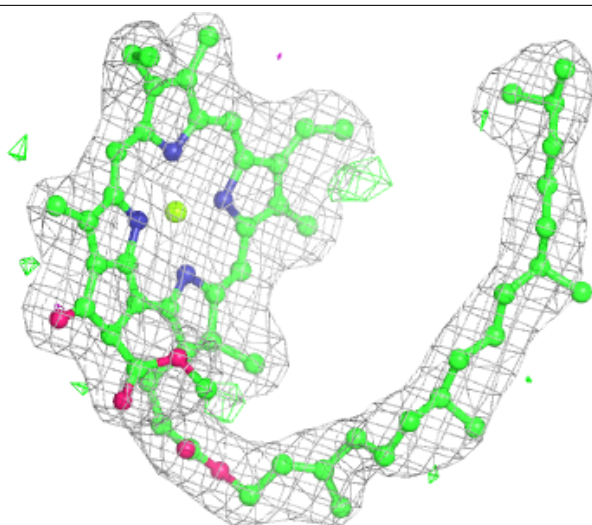
**Electron density around DGD C 517:**

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



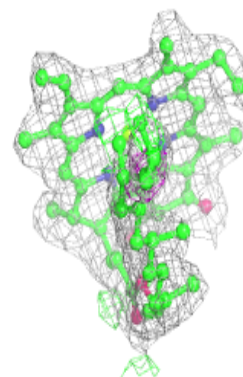
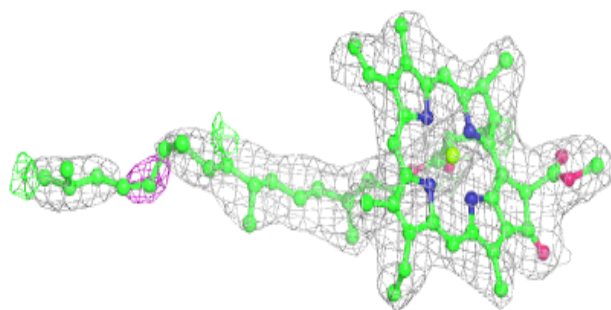
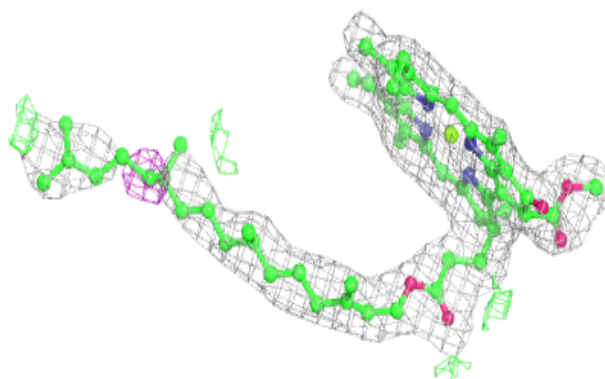
Electron density around CLA c 508:

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

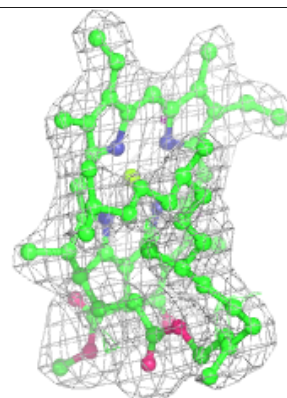
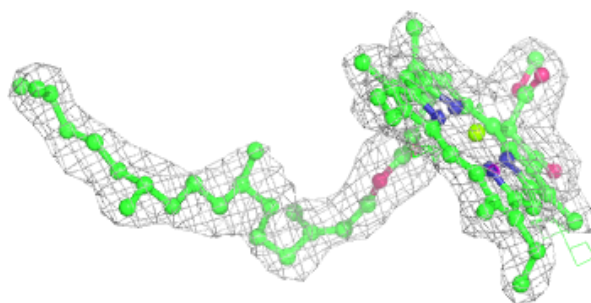
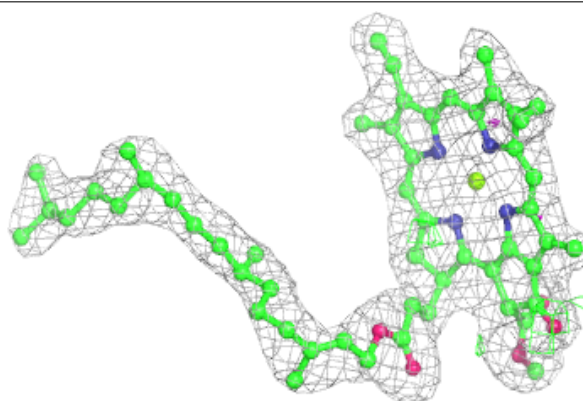


Electron density around CLA C 505:

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

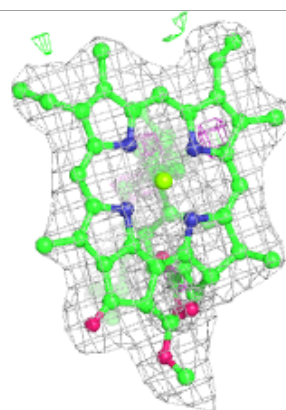
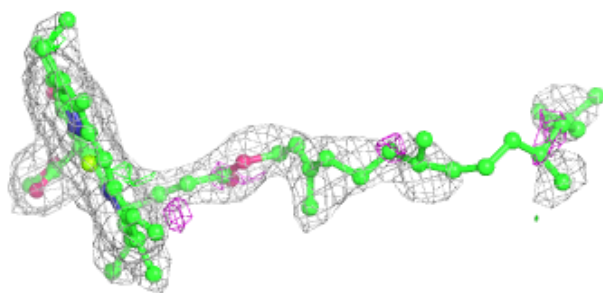
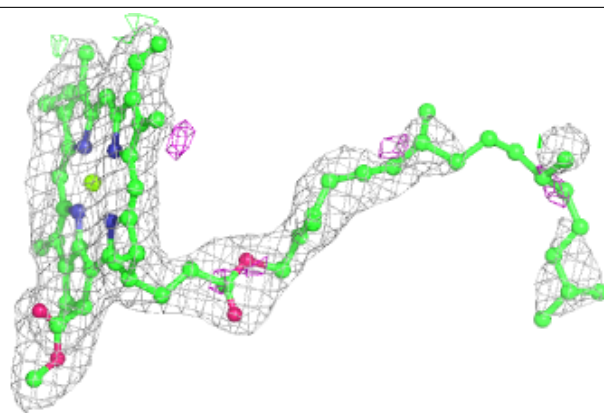
**Electron density around CLA c 512:**

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

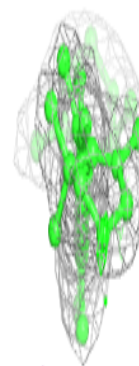
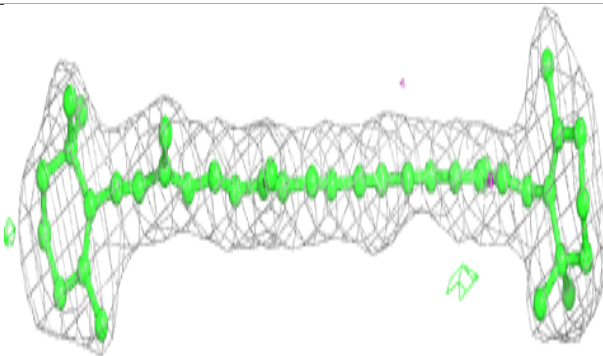
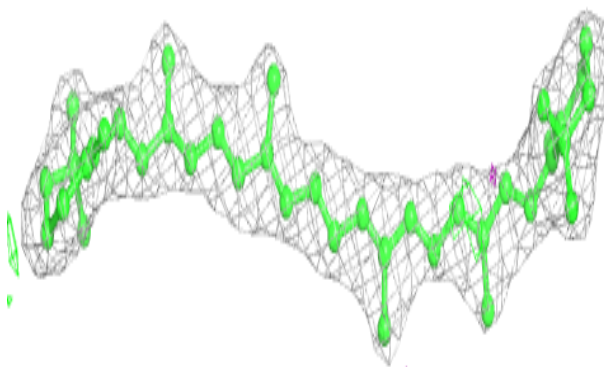


Electron density around CLA d 403:

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

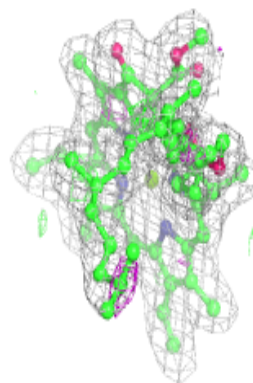
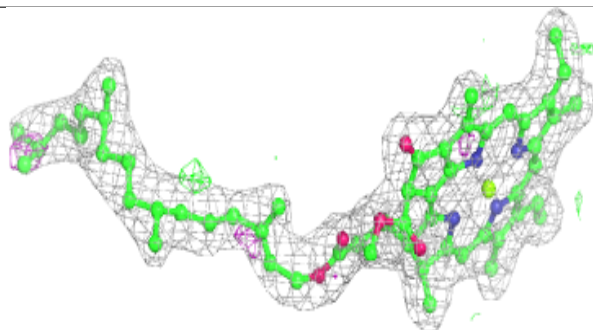
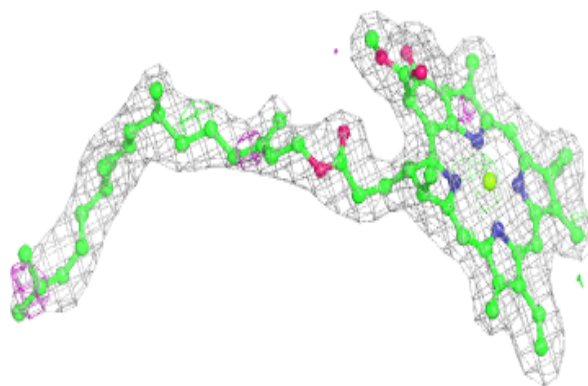
**Electron density around BCR c 515:**

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

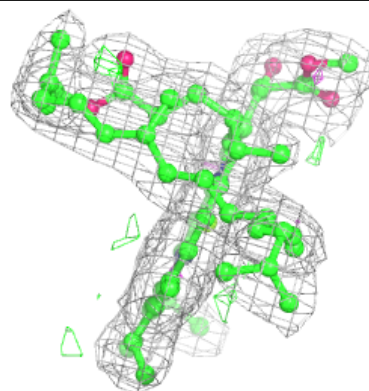
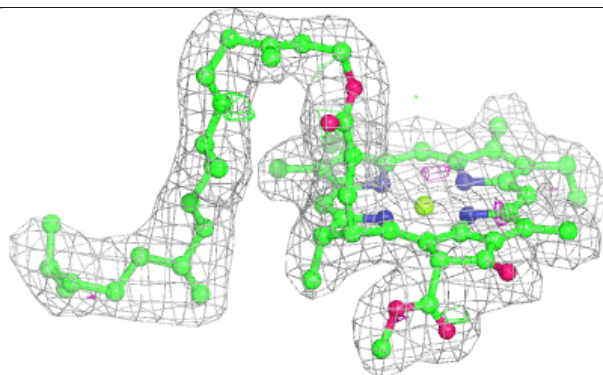
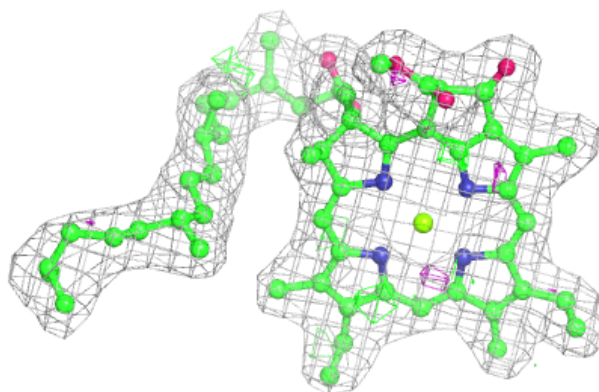


Electron density around CLA a 404:

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

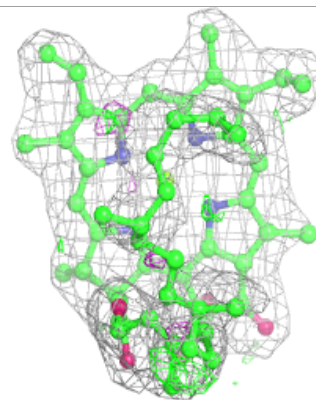
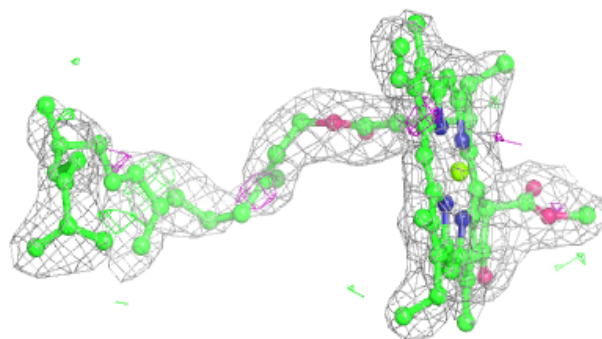
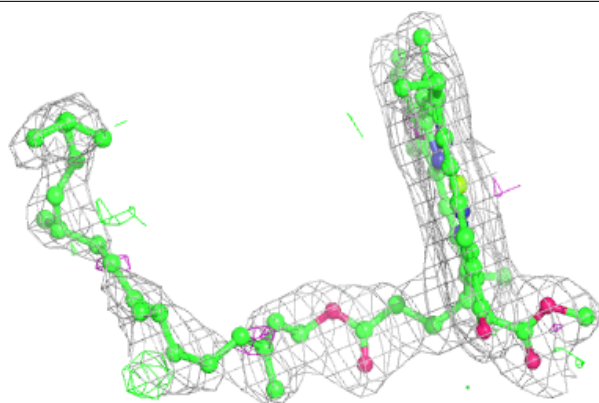
**Electron density around CLA a 405:**

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



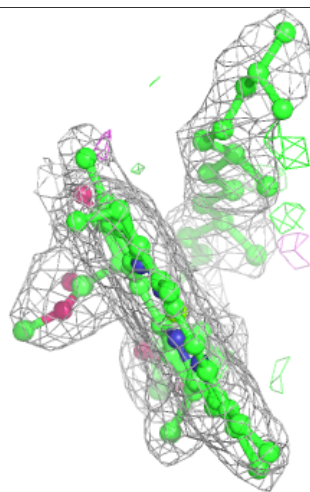
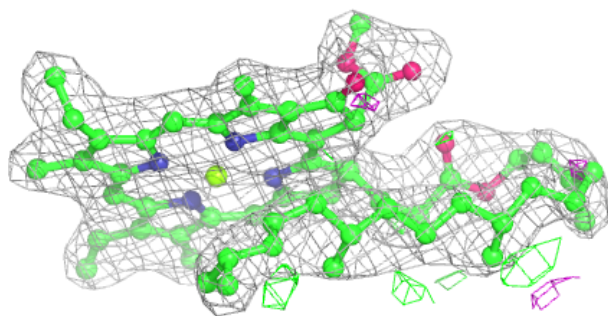
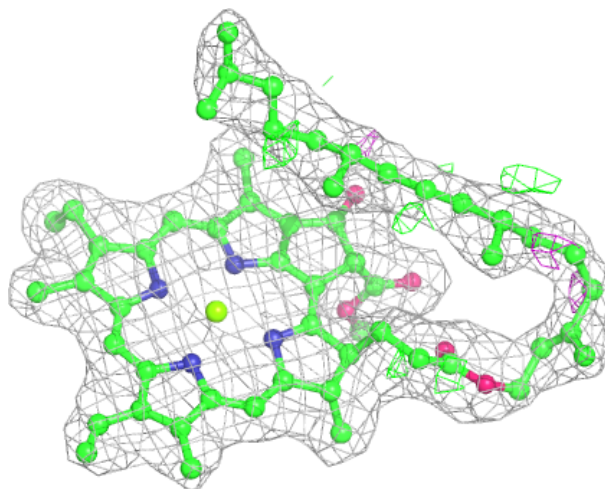
Electron density around CLA C 507:

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



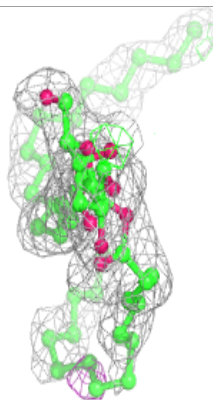
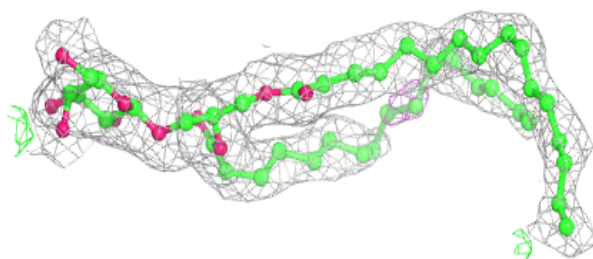
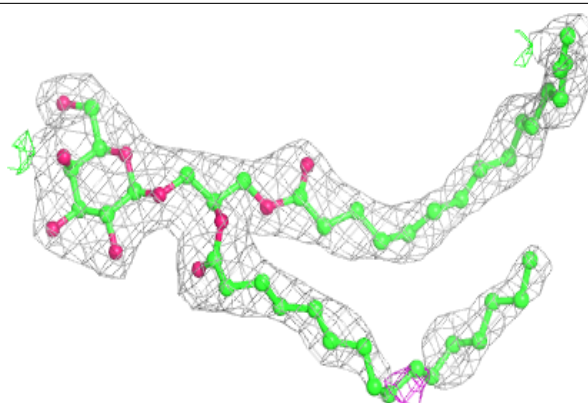
Electron density around CLA c 510:

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

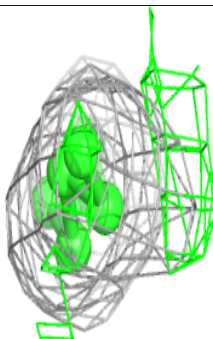
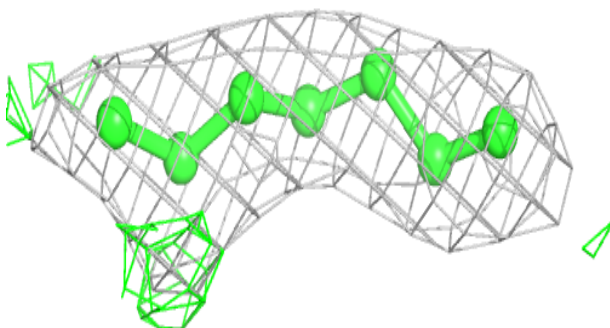
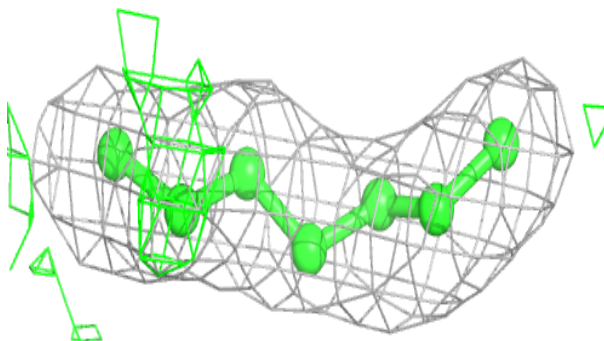


Electron density around LMG f 101:

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

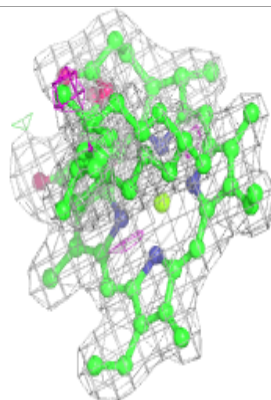
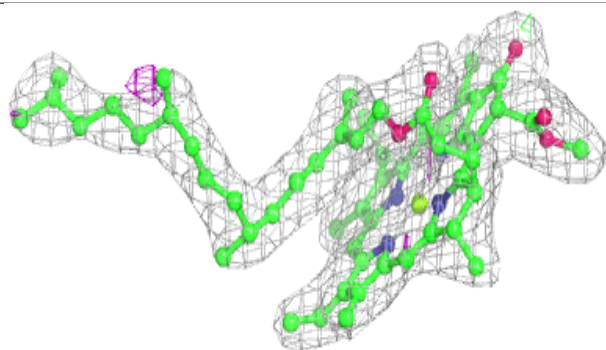
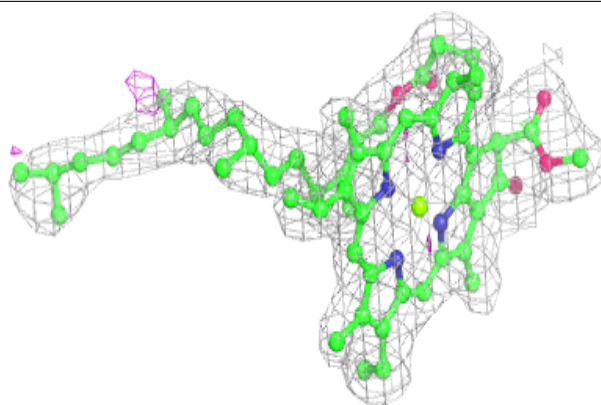
**Electron density around LFA a 411:**

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



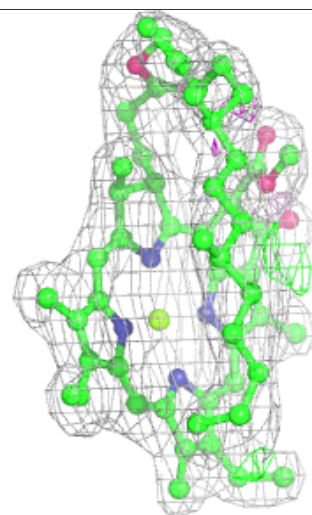
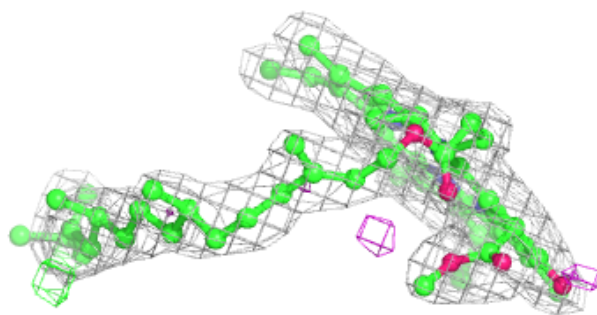
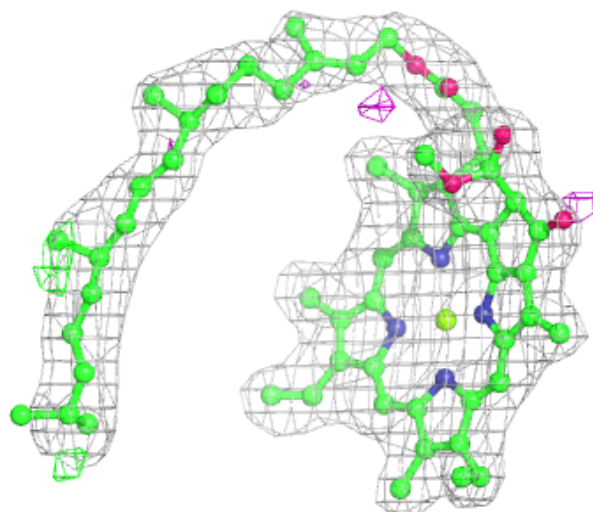
Electron density around CLA c 506:

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



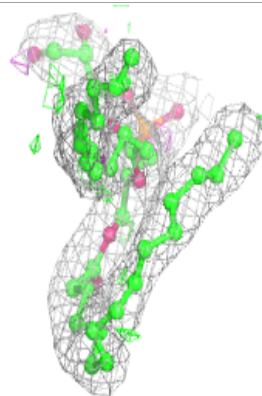
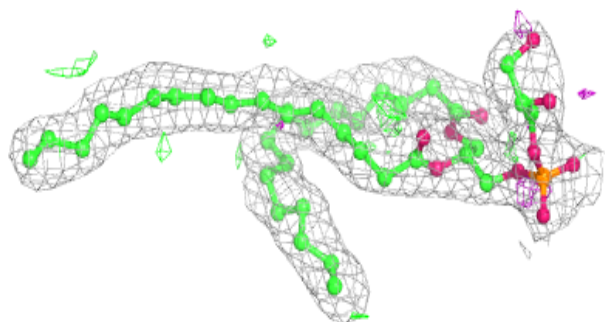
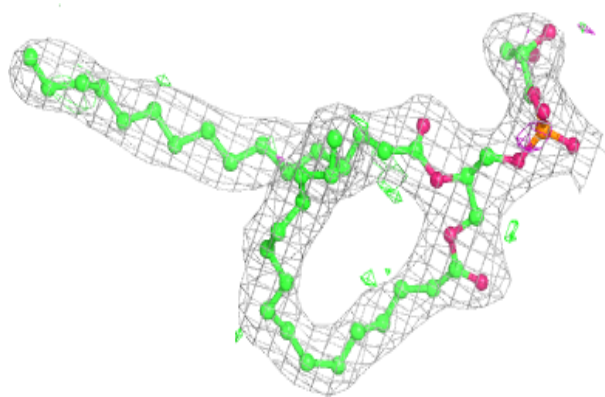
Electron density around CLA C 508:

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

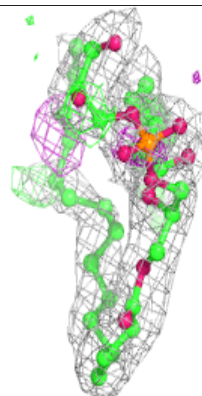
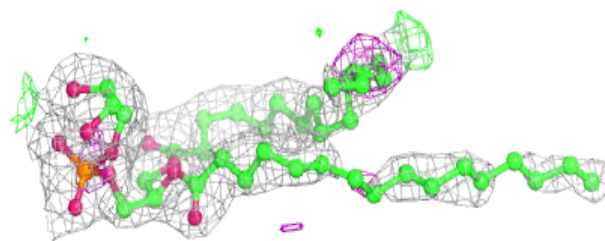
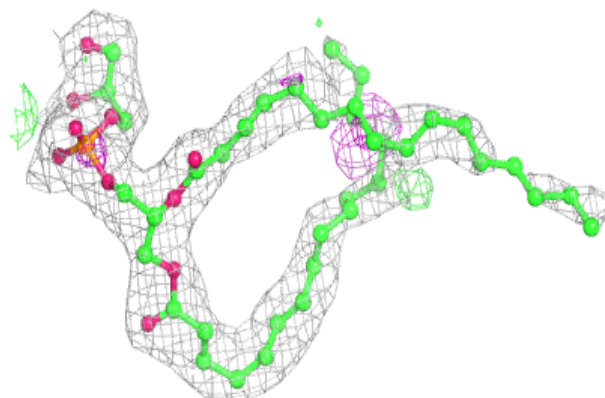


Electron density around LHG D 406:

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

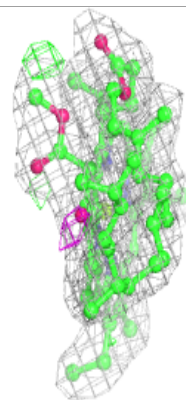
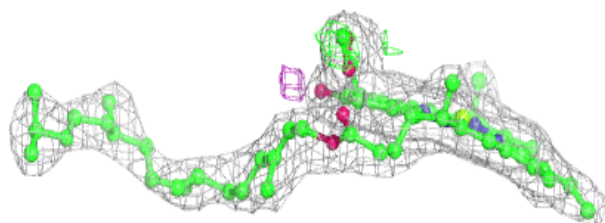
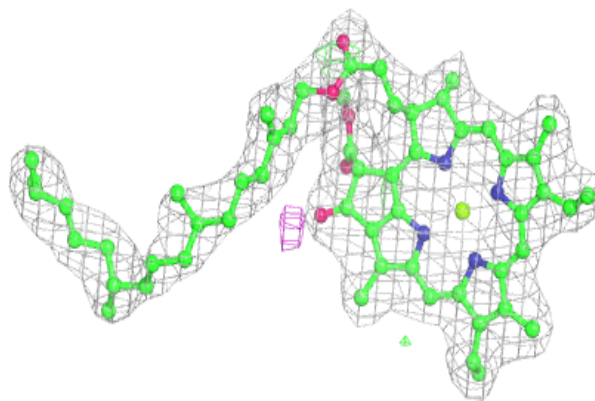
**Electron density around LHG D 408:**

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



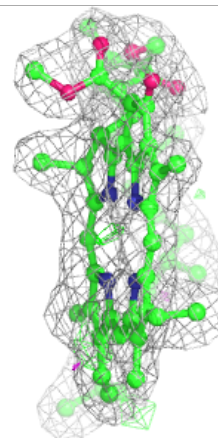
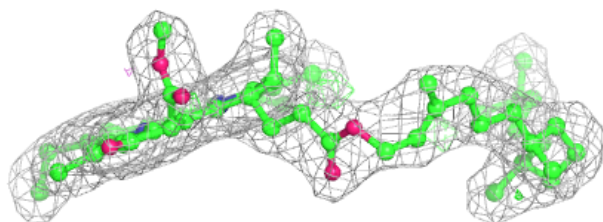
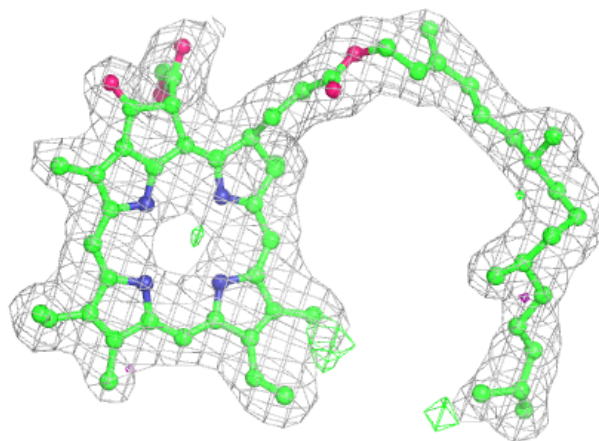
Electron density around CLA b 604:

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



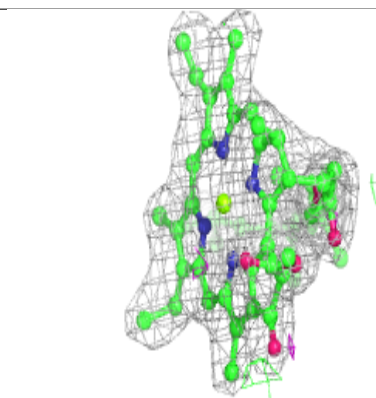
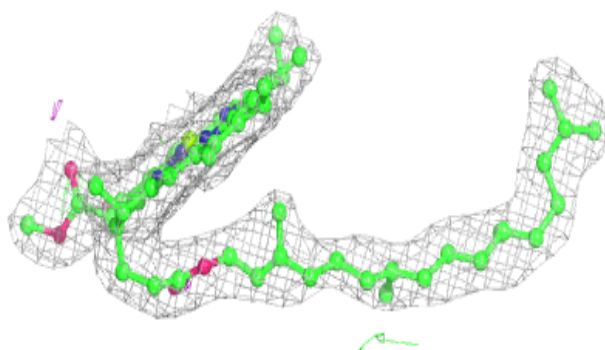
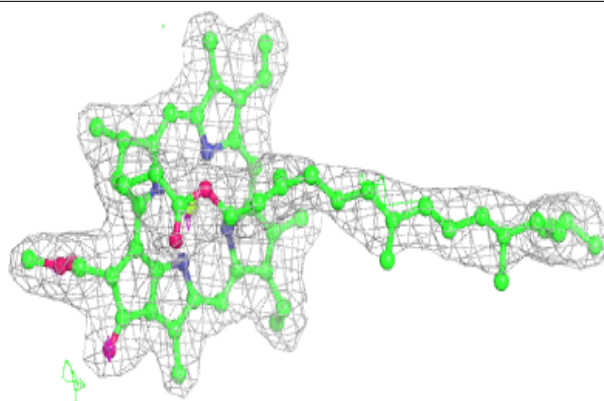
Electron density around PHO a 406:

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

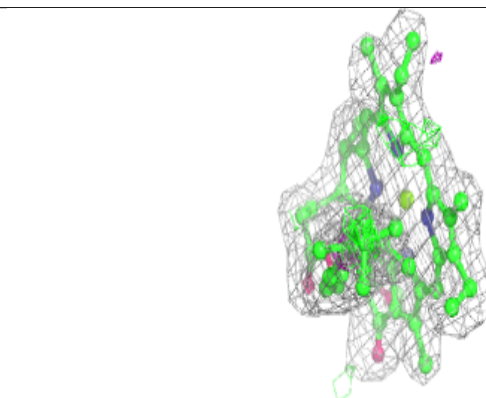
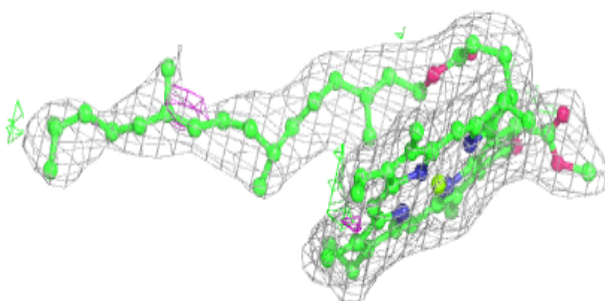
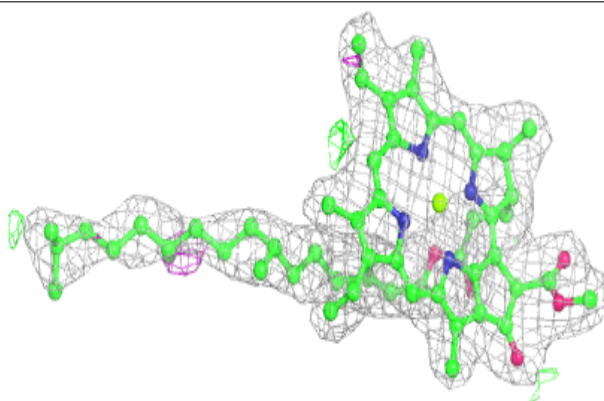


Electron density around CLA b 610:

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

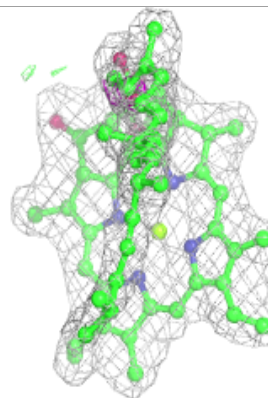
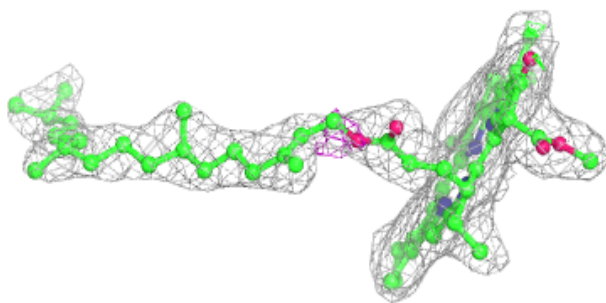
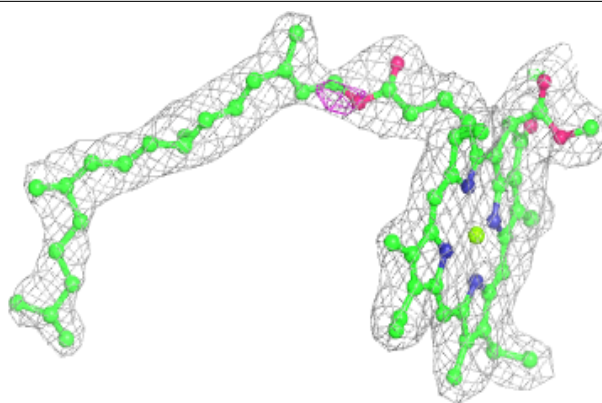
**Electron density around CLA b 616:**

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

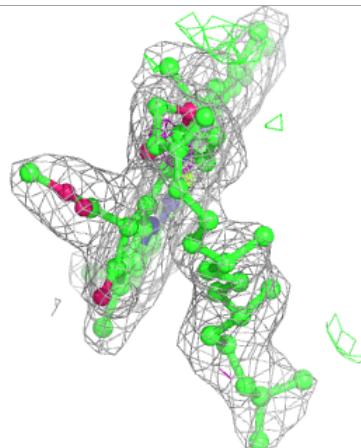
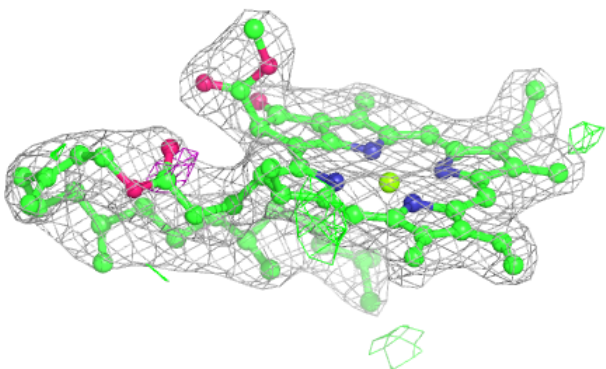
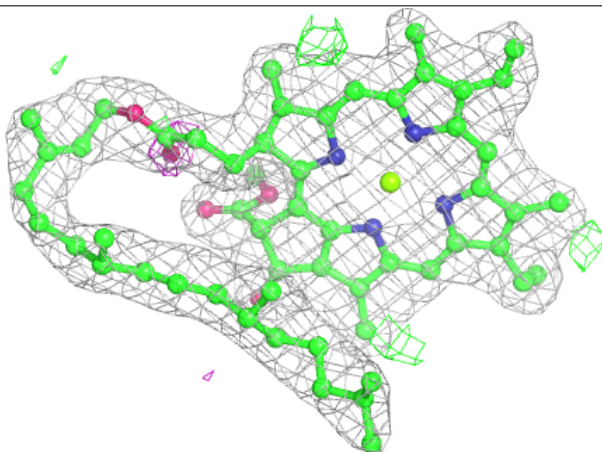


Electron density around CLA b 611:

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

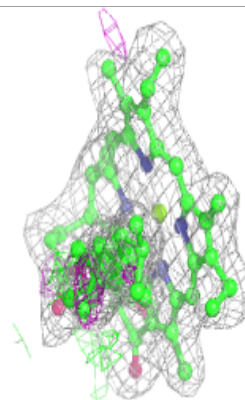
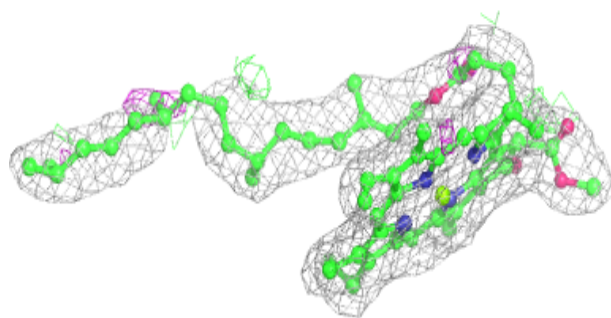
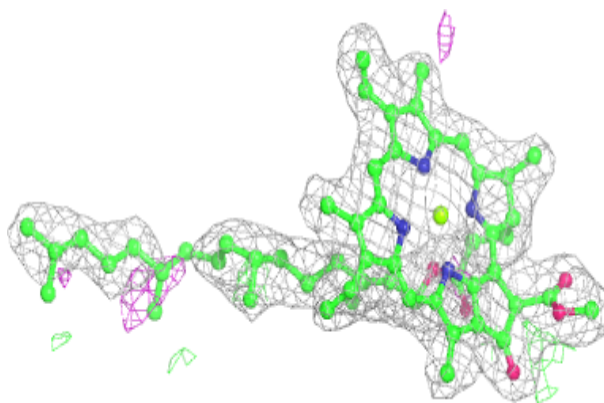
**Electron density around CLA C 510:**

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



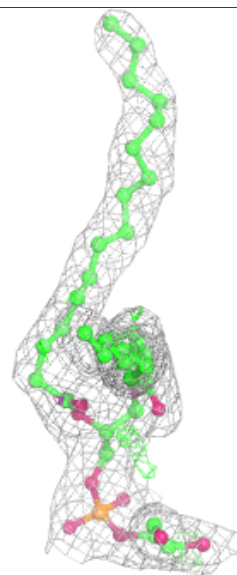
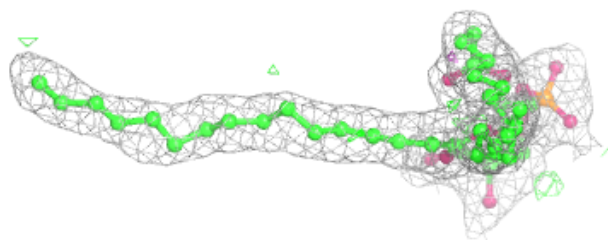
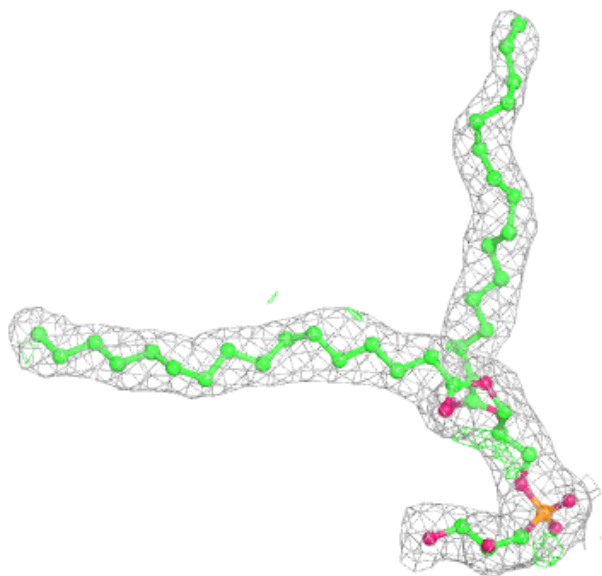
Electron density around CLA B 613:

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



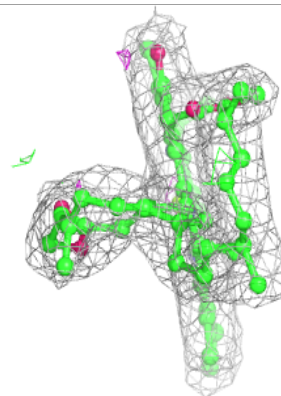
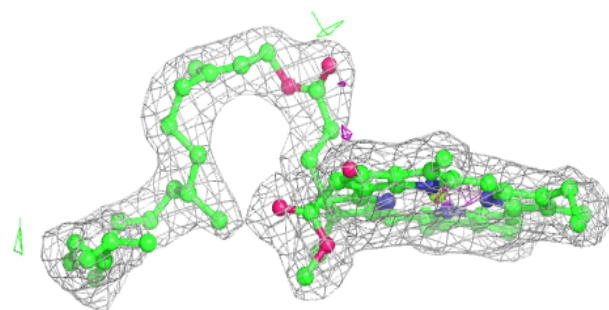
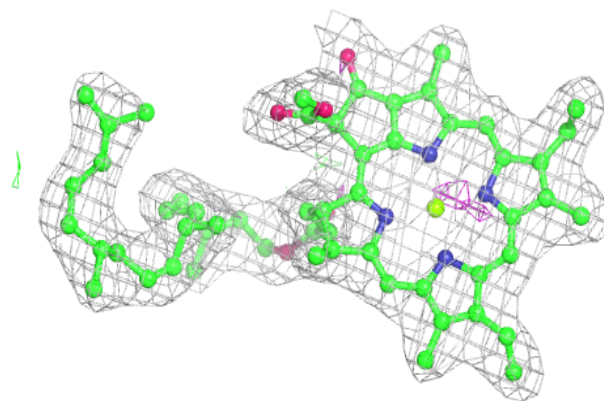
Electron density around LHG 1 101:

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



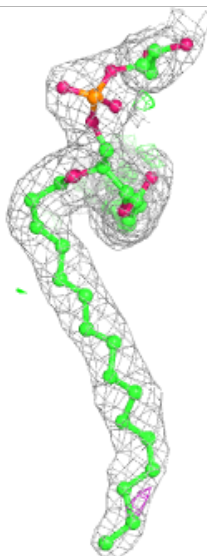
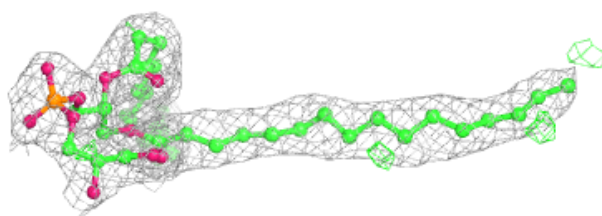
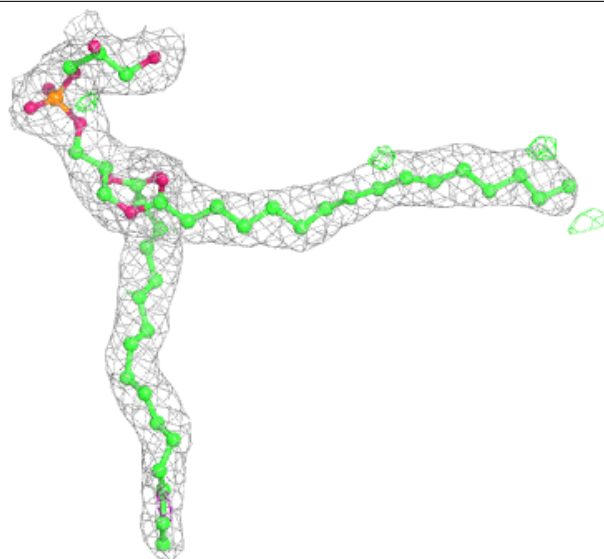
Electron density around CLA B 611:

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



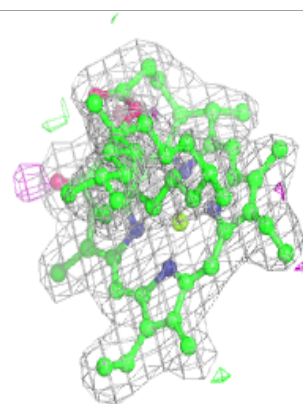
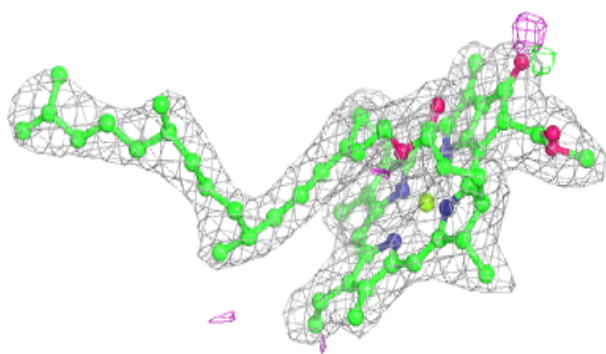
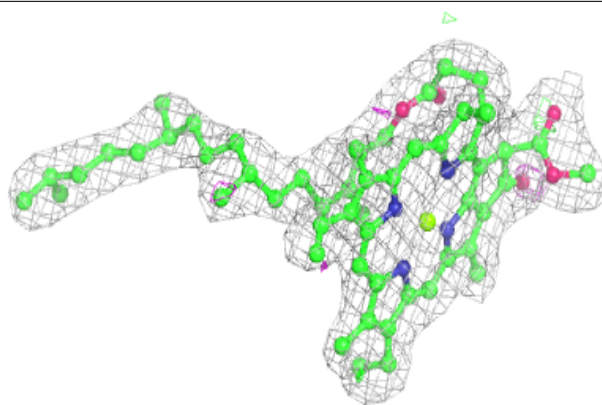
Electron density around LHG L 102:

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



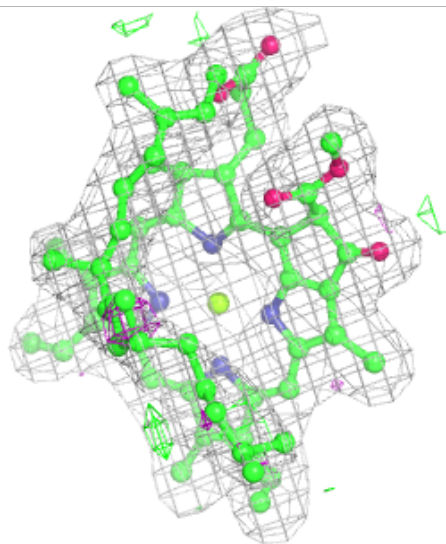
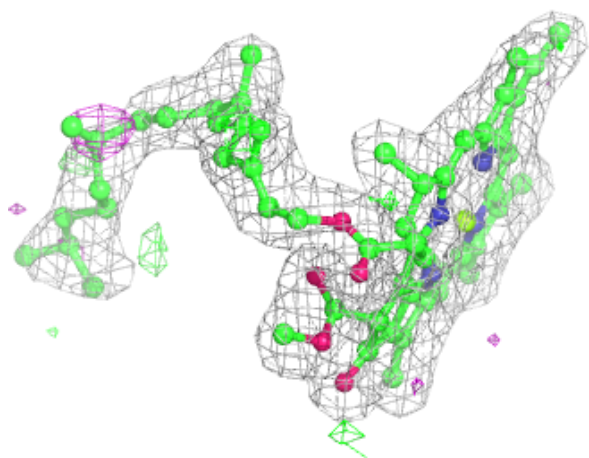
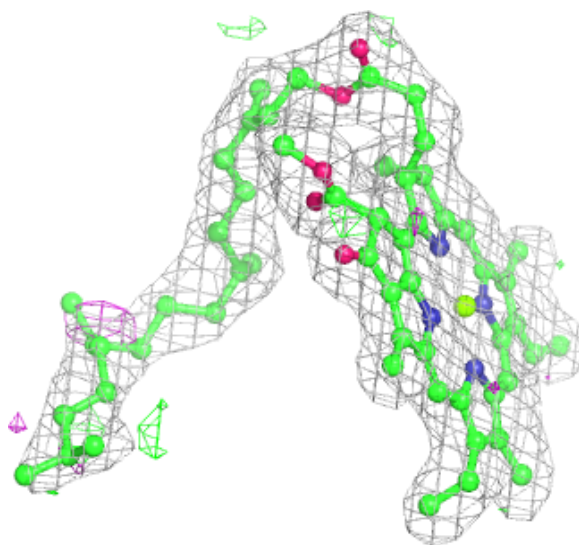
Electron density around CLA C 506:

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



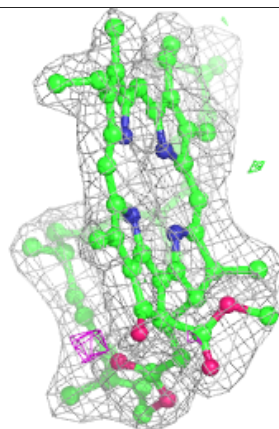
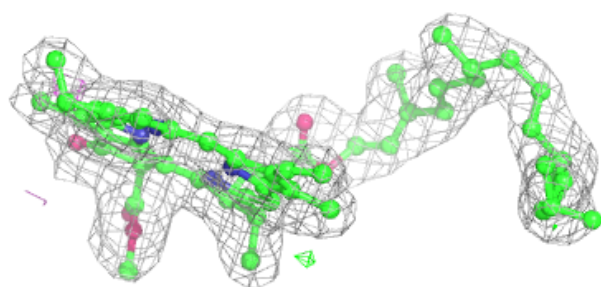
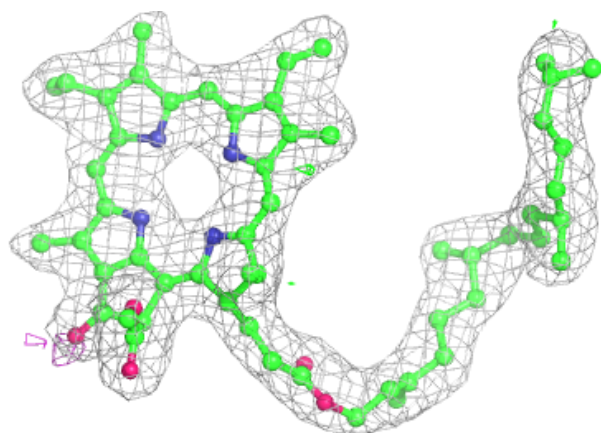
Electron density around CLA b 615:

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

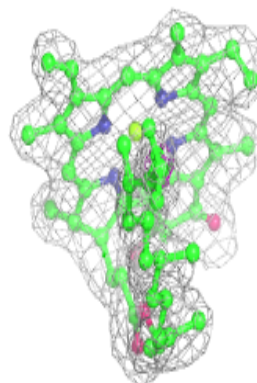
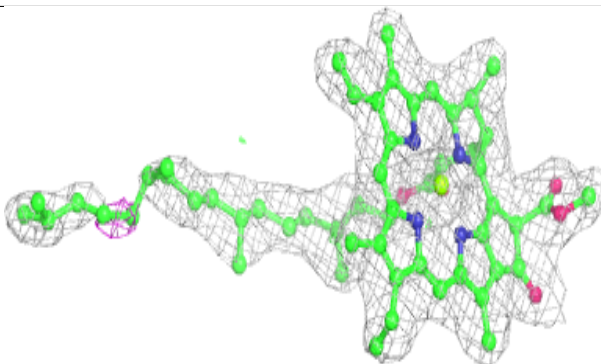
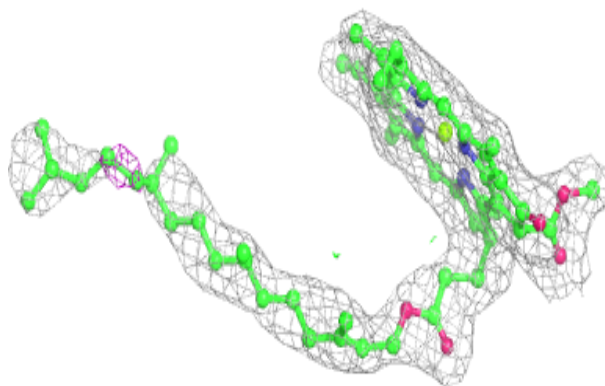


Electron density around PHO a 414:

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

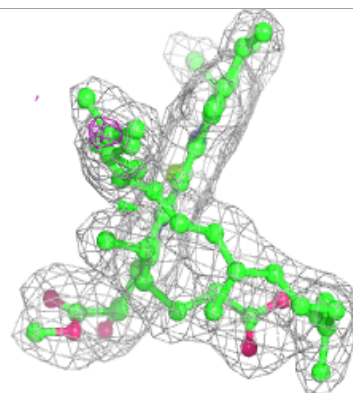
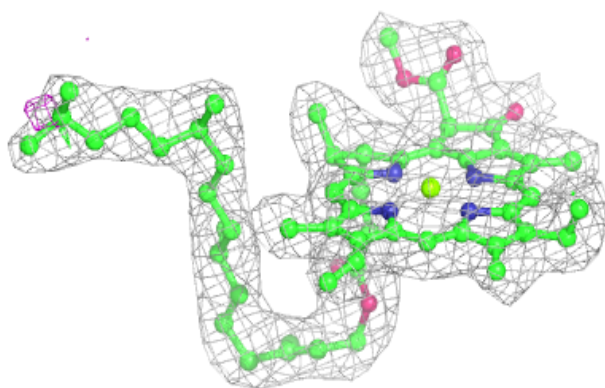
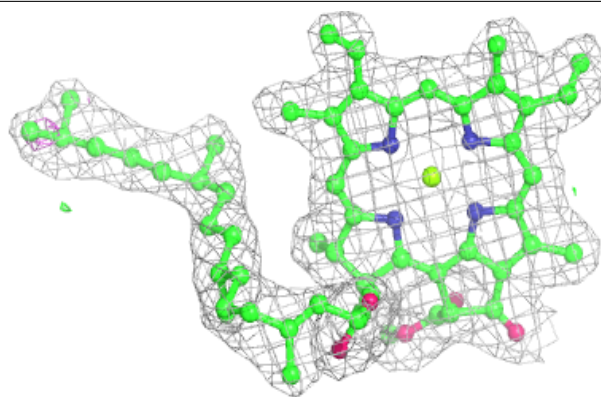
**Electron density around CLA c 505:**

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

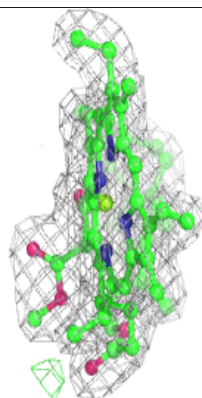
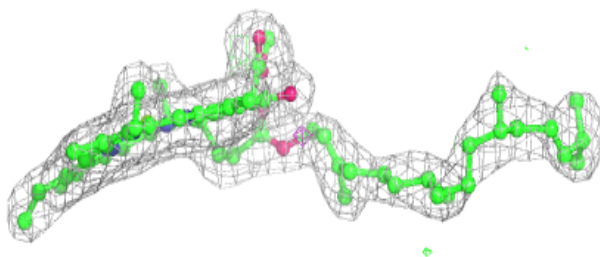
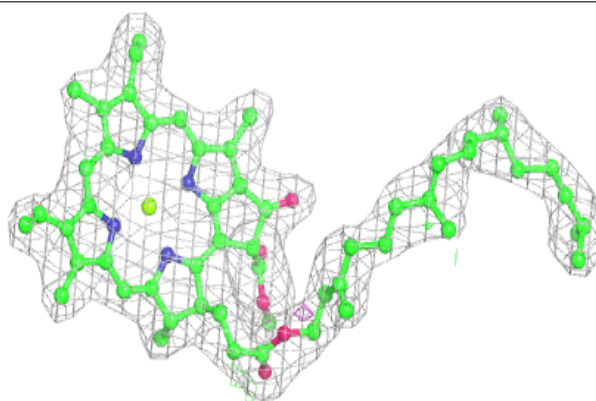


Electron density around CLA A 412:

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

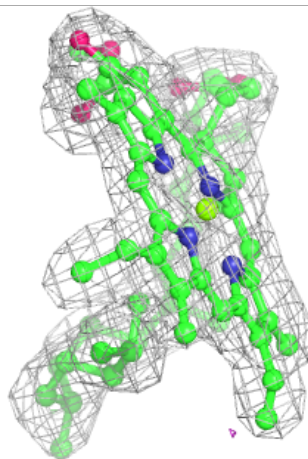
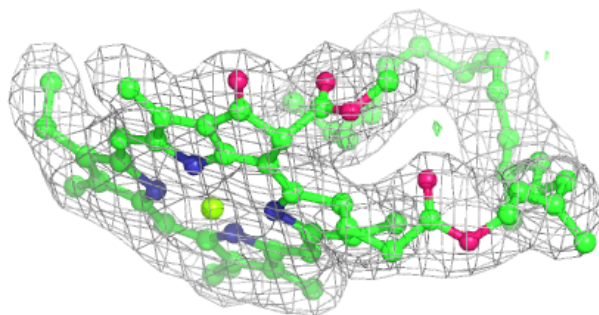
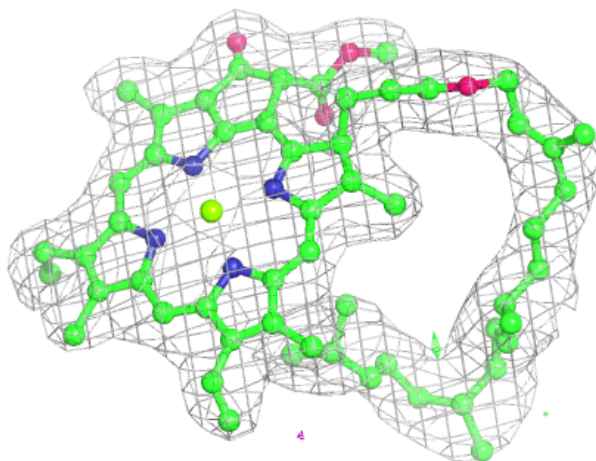
**Electron density around CLA B 601:**

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



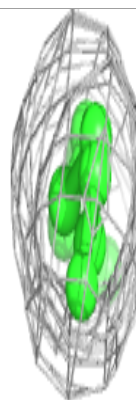
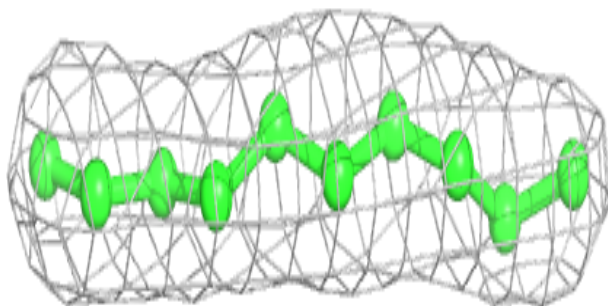
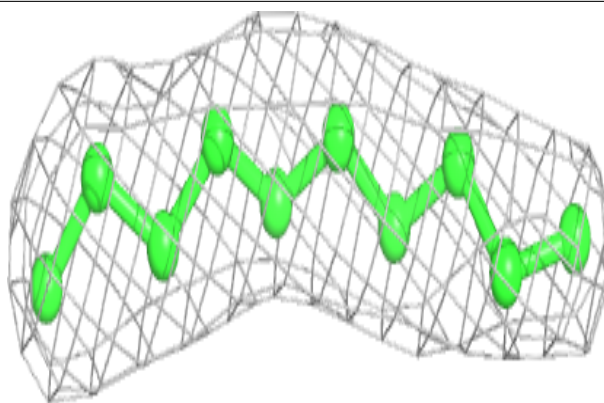
Electron density around CLA b 617:

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

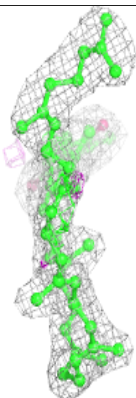
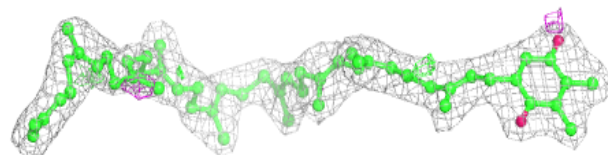
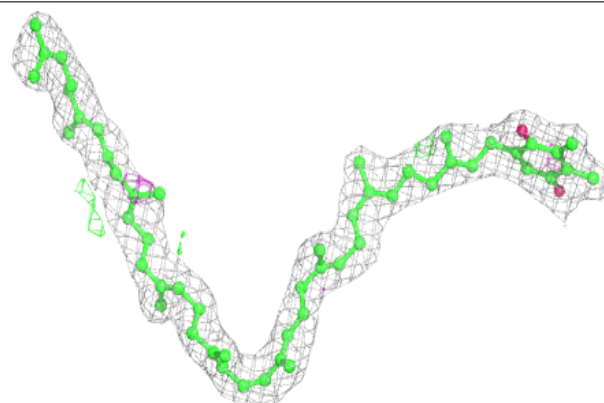


Electron density around LFA M 101:

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

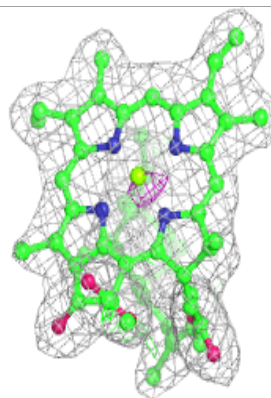
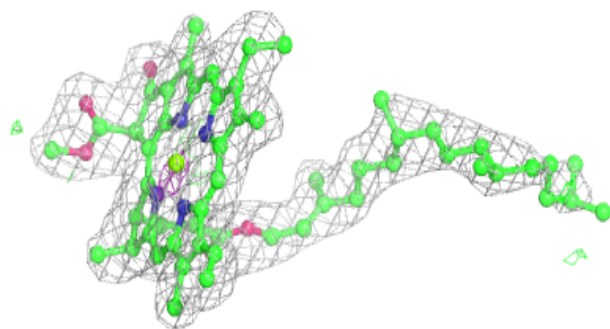
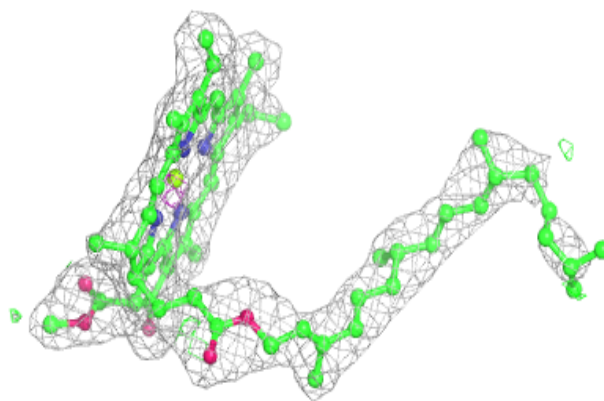
**Electron density around PL9 d 405:**

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



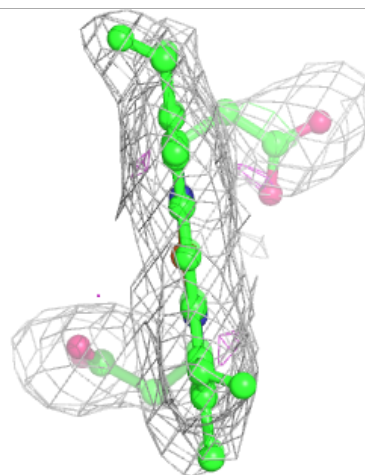
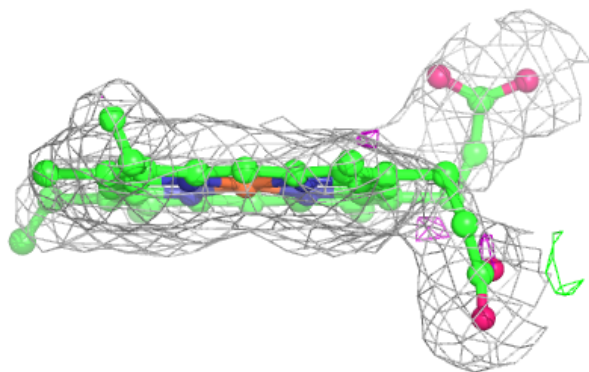
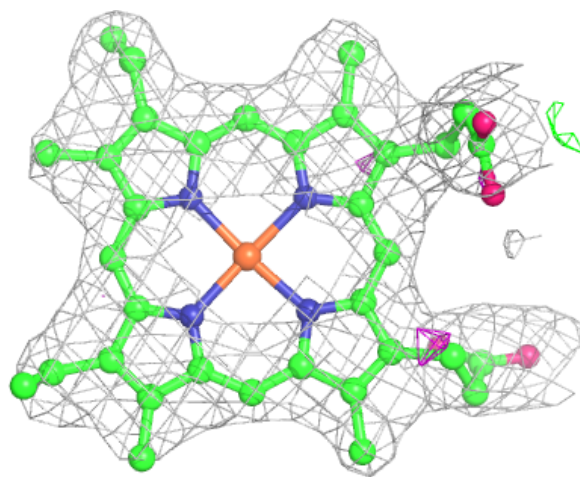
Electron density around CLA c 509:

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



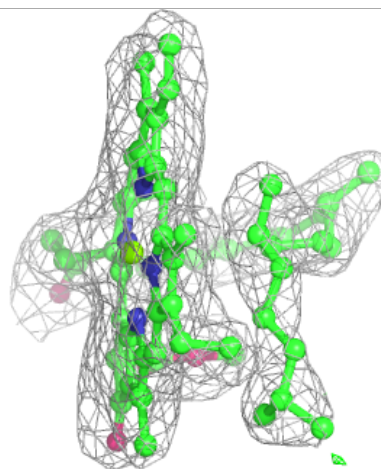
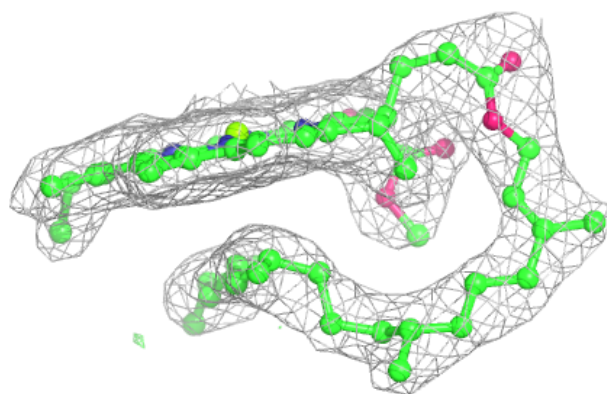
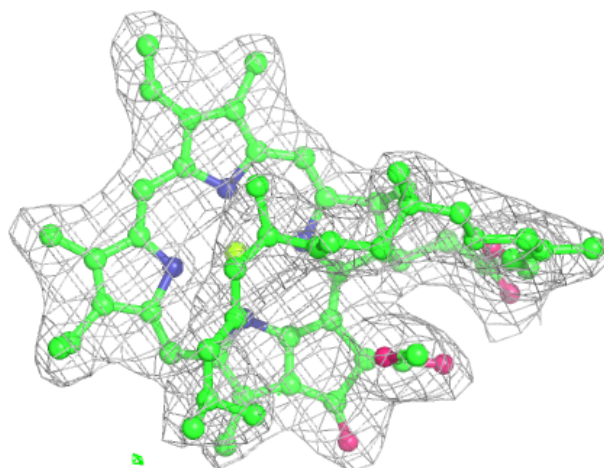
Electron density around HEM e 102:

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



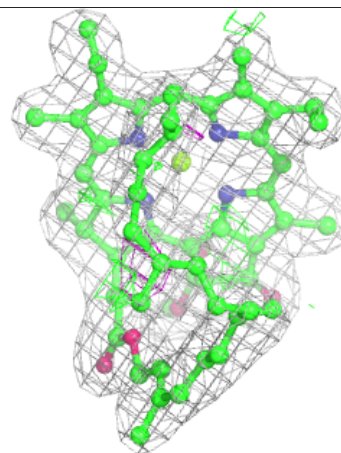
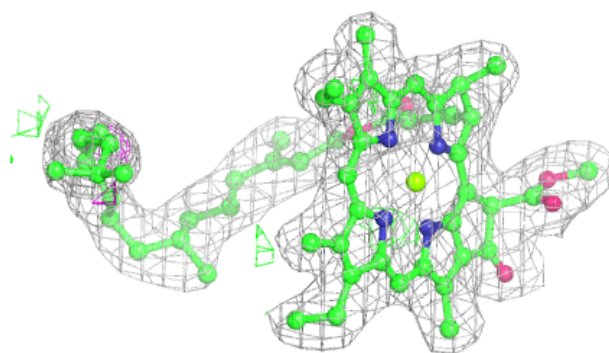
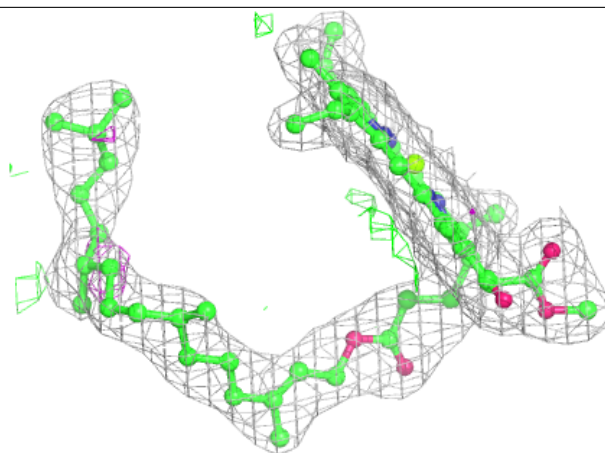
Electron density around CLA c 511:

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



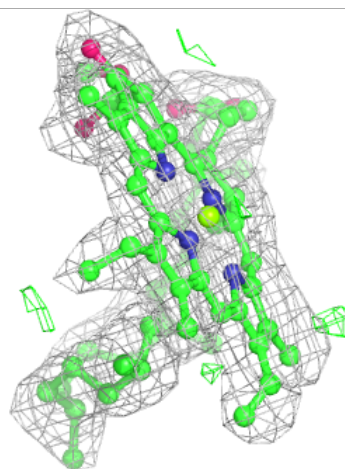
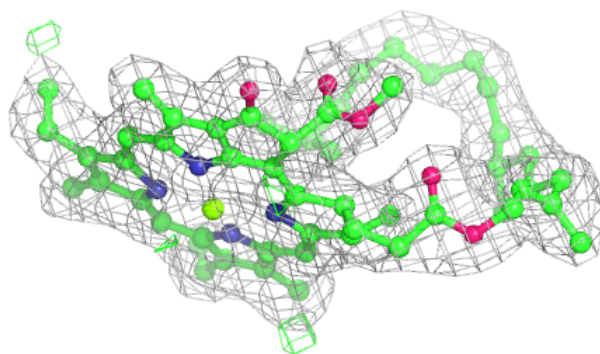
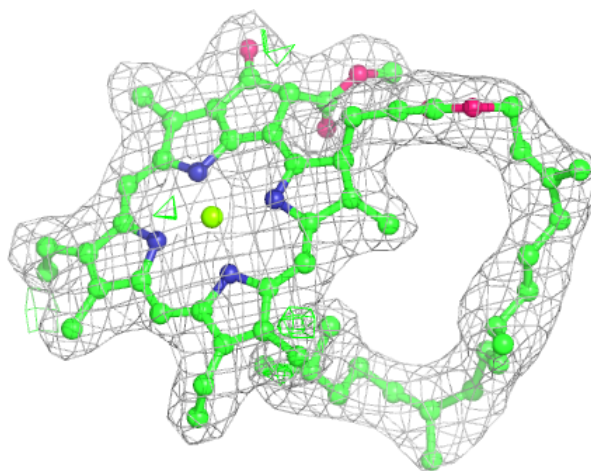
Electron density around CLA b 613:

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



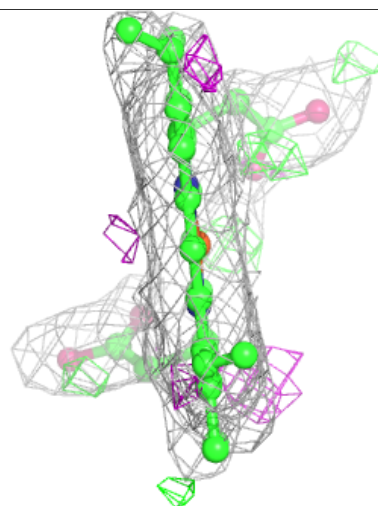
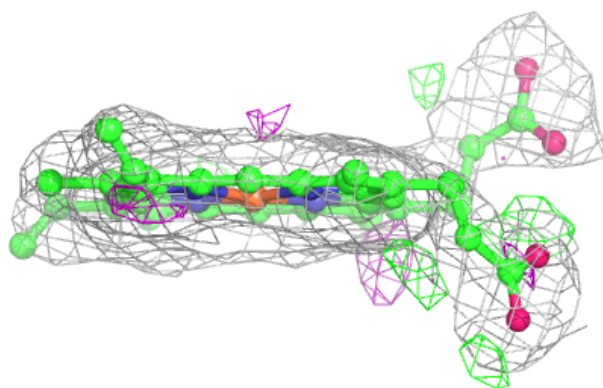
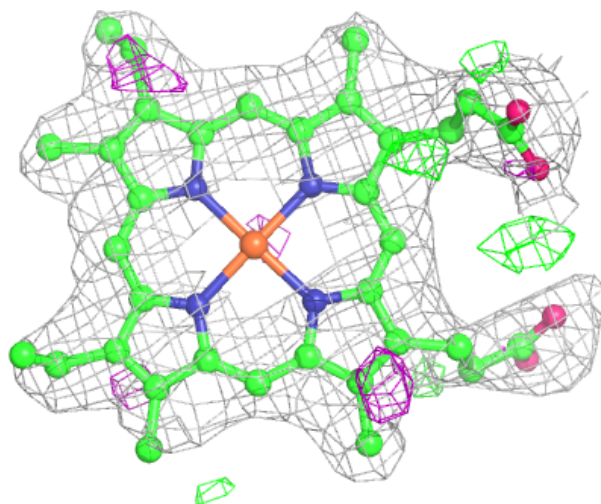
Electron density around CLA B 614:

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



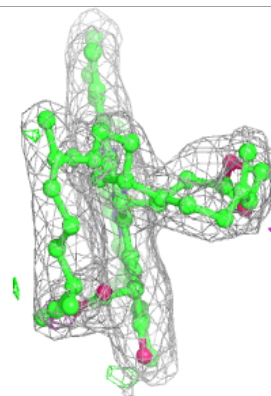
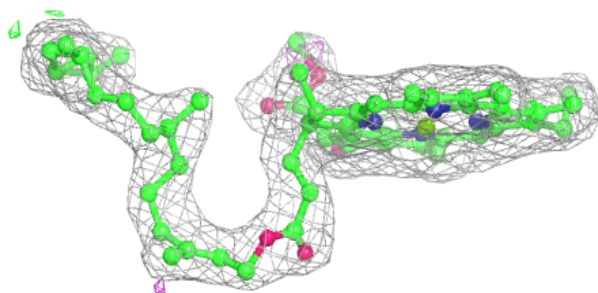
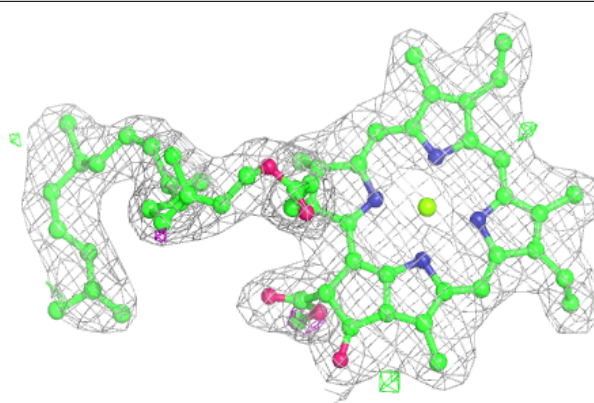
Electron density around HEM E 102:

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

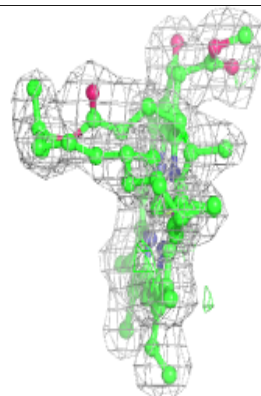
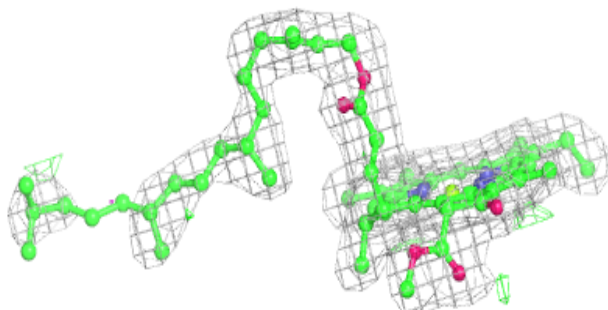
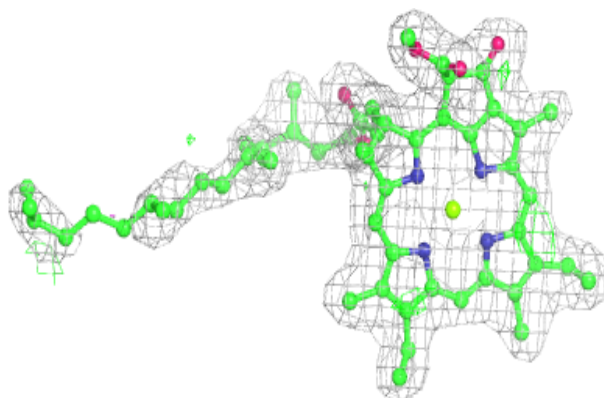


Electron density around CLA b 614:

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

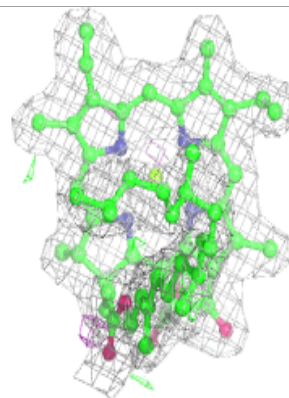
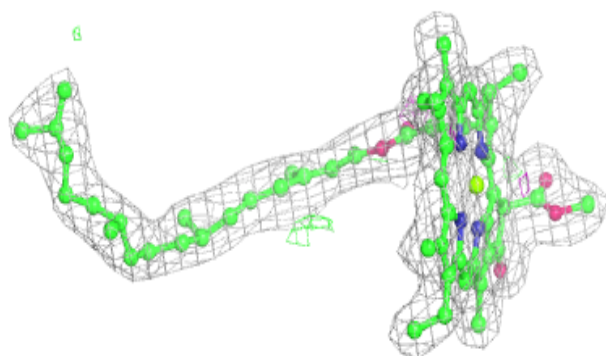
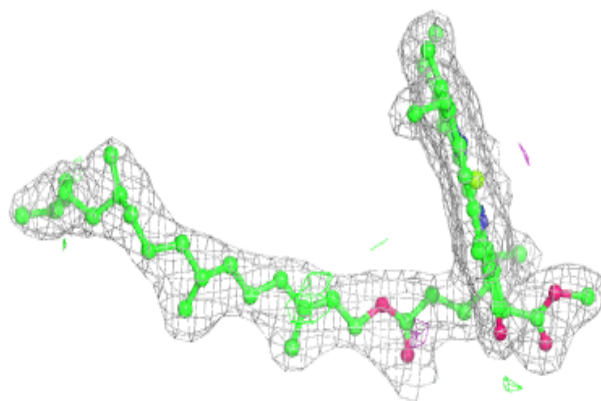
**Electron density around CLA A 404:**

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

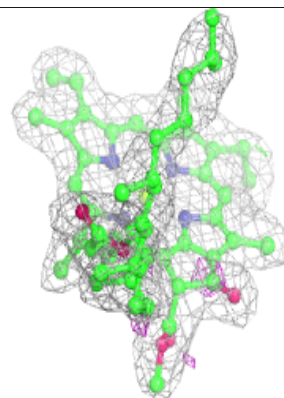
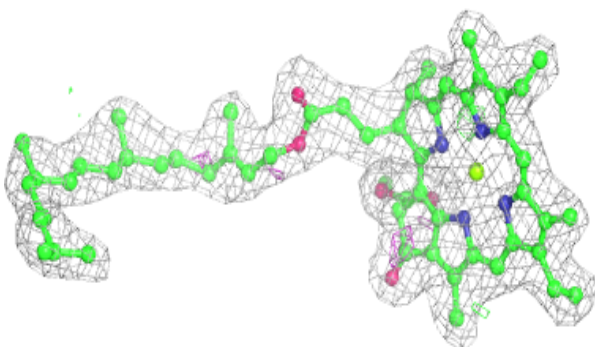
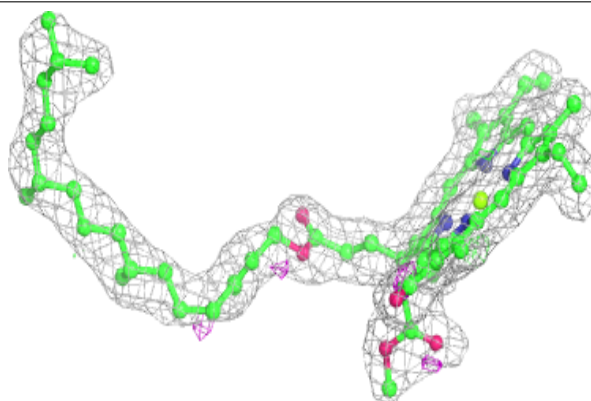


Electron density around CLA B 604:

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

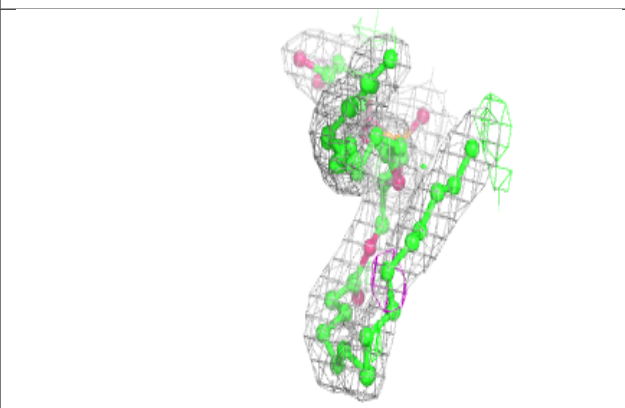
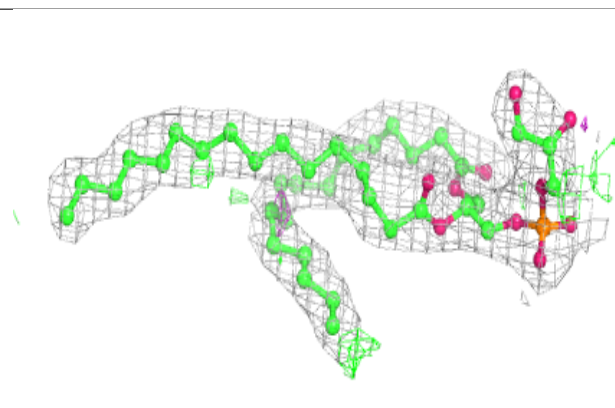
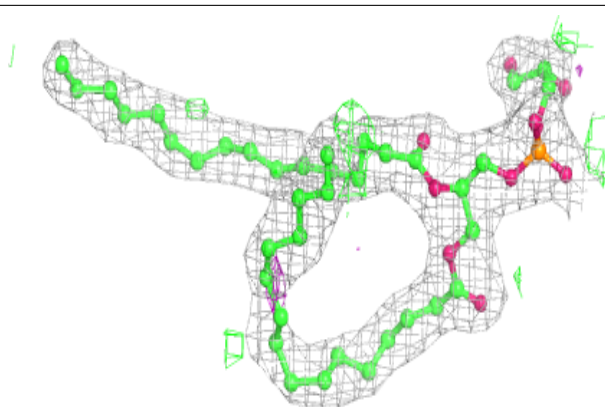
**Electron density around CLA d 402:**

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

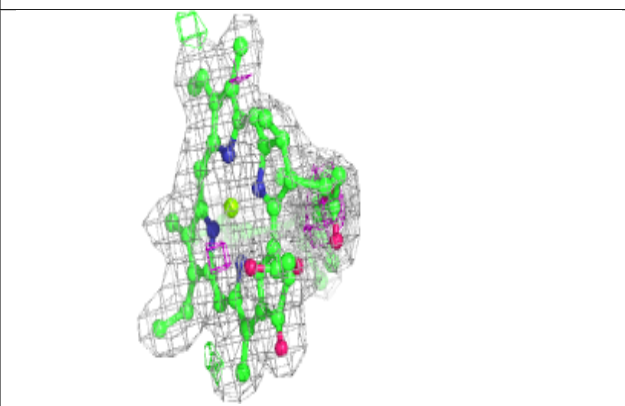
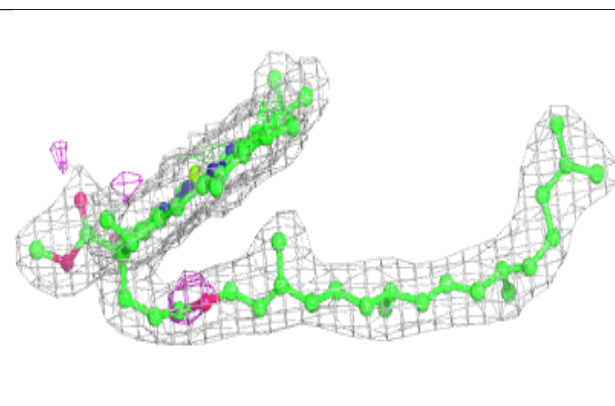
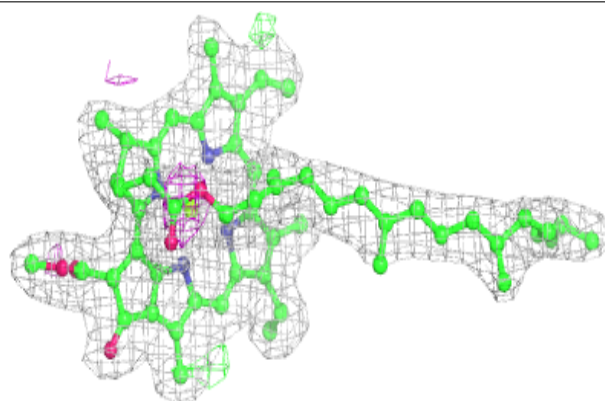


Electron density around LHG b 628:

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

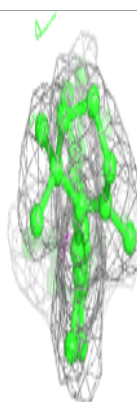
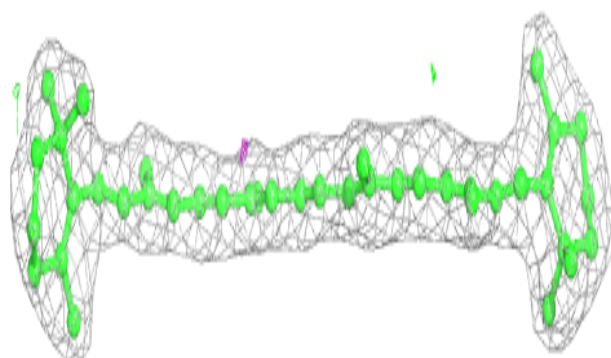
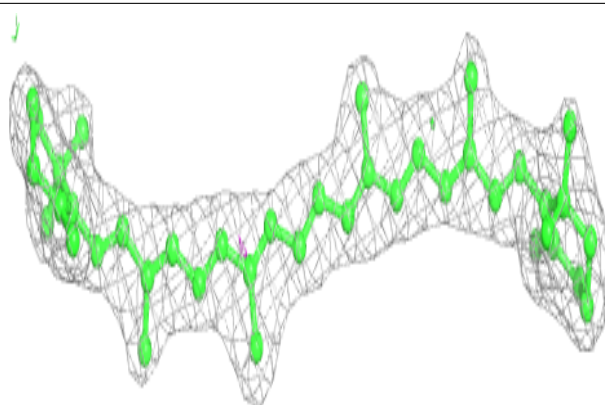
**Electron density around CLA B 607:**

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

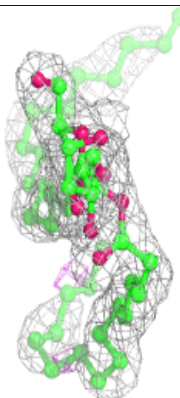
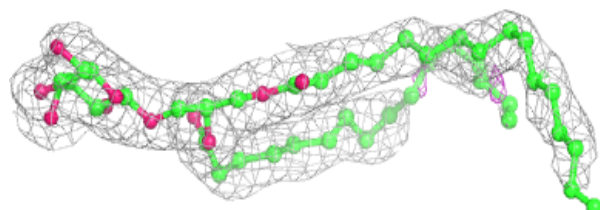
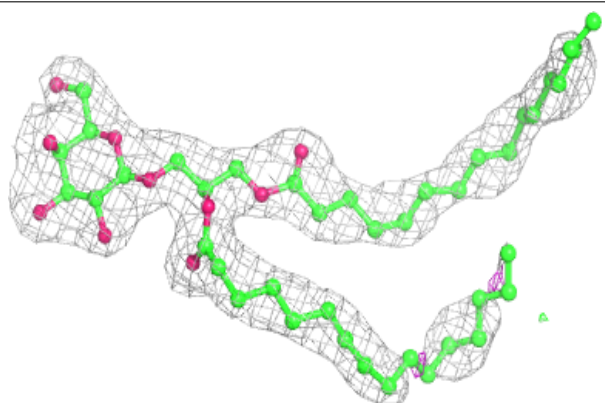


Electron density around BCR A 407:

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

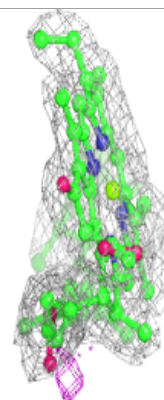
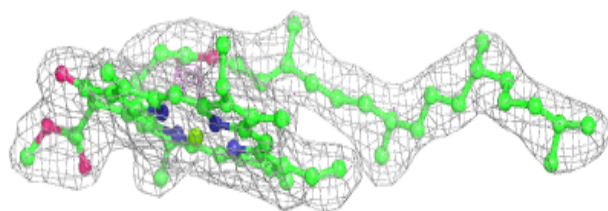
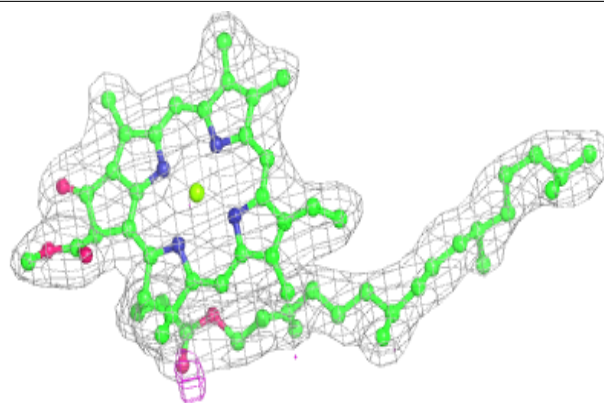
**Electron density around LMG D 409:**

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



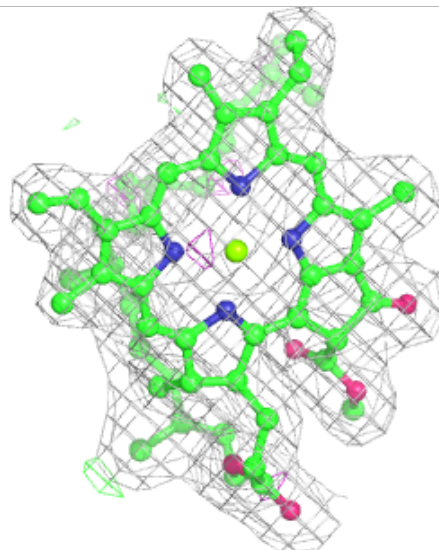
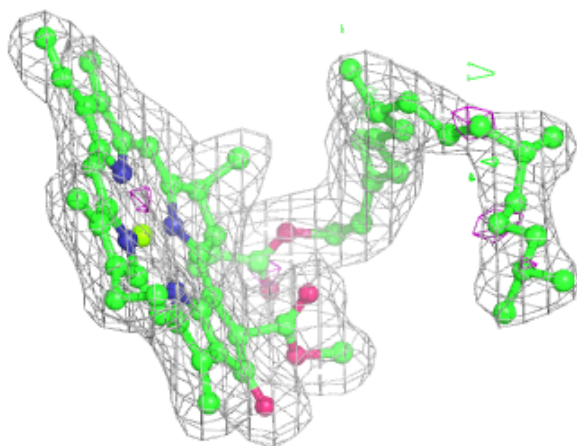
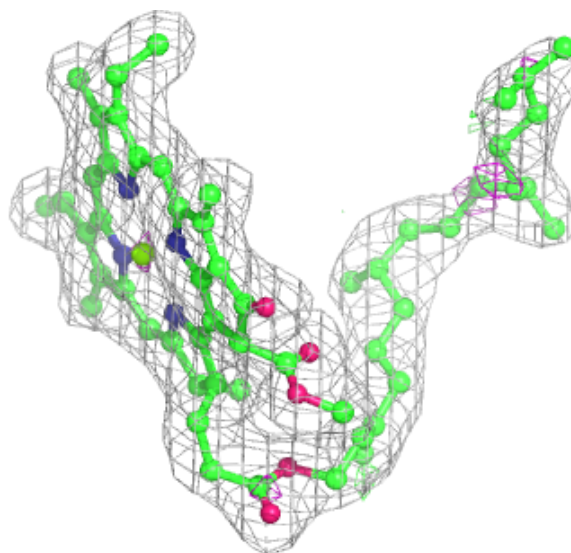
Electron density around CLA C 502:

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



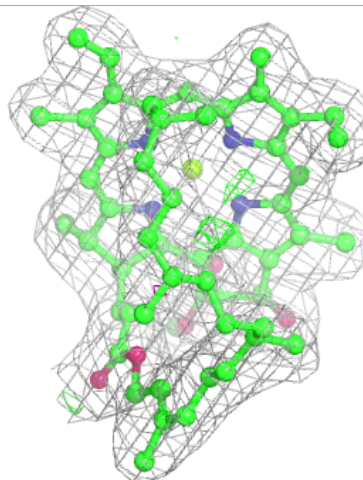
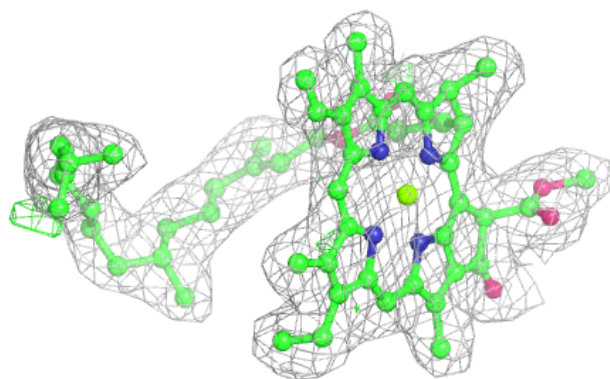
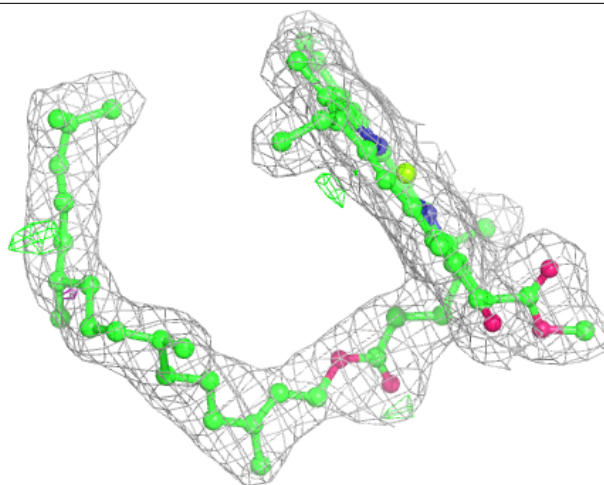
Electron density around CLA B 612:

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



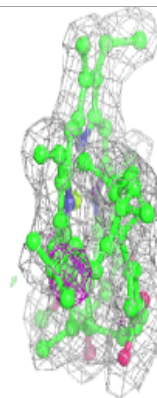
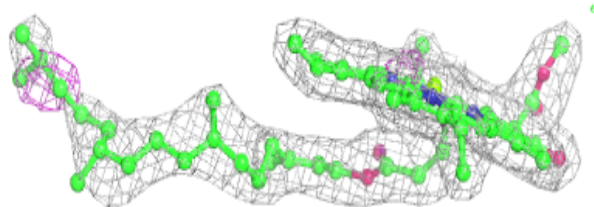
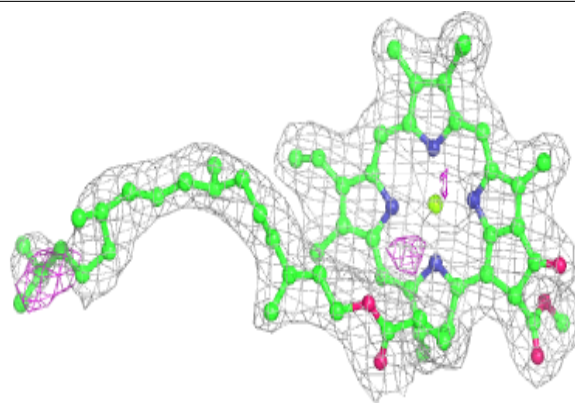
Electron density around CLA B 610:

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

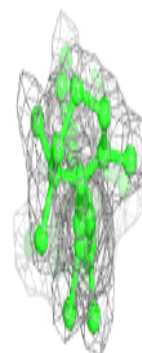
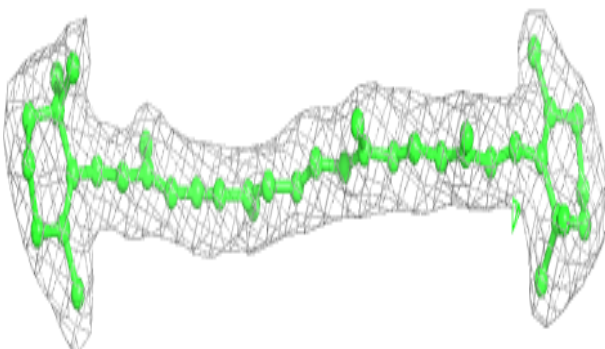
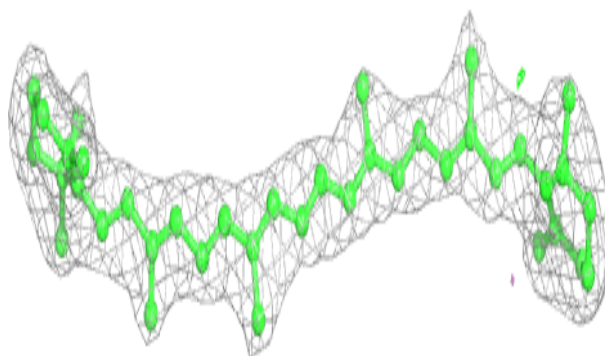


Electron density around CLA B 602:

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

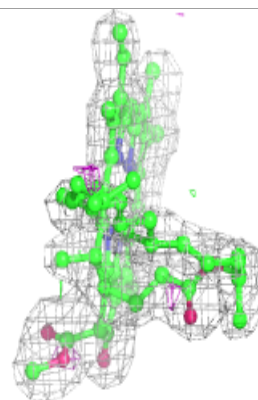
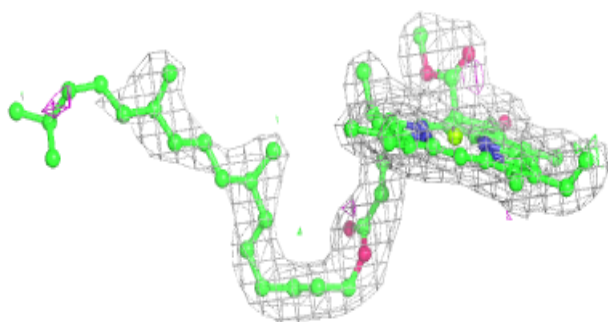
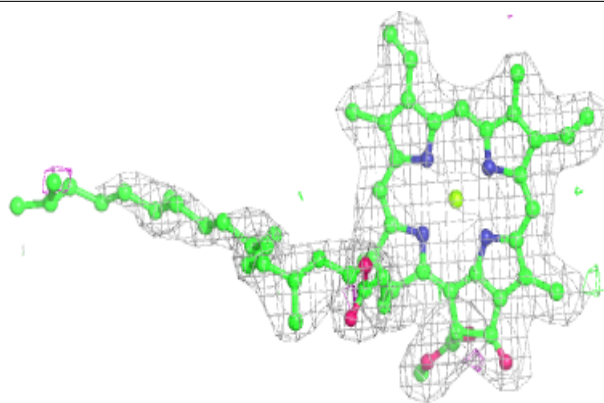
**Electron density around BCR a 408:**

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

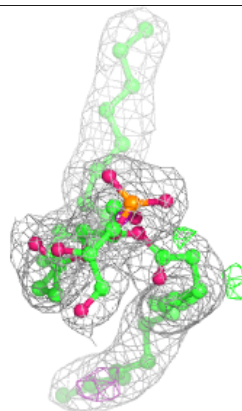
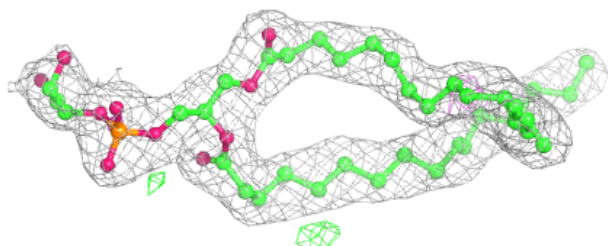
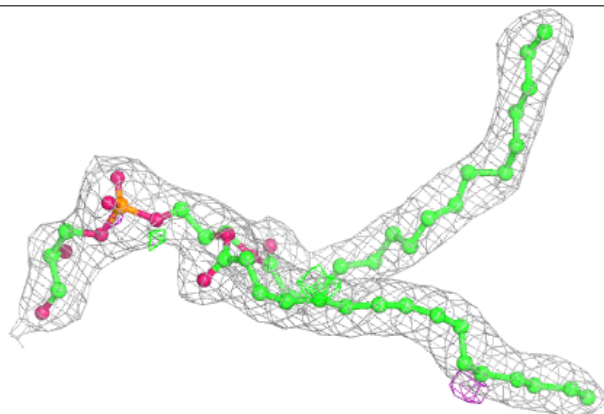


Electron density around CLA d 401:

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

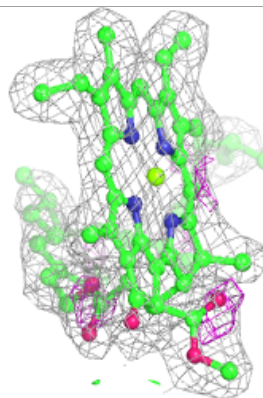
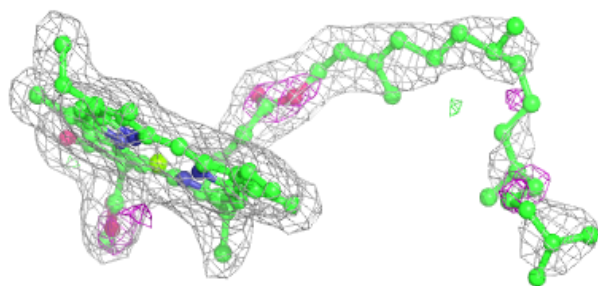
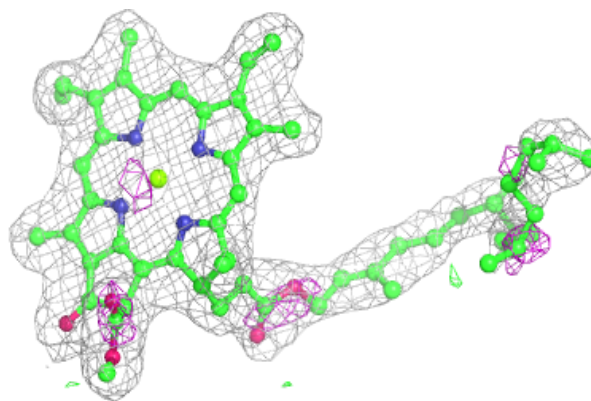
**Electron density around LHG D 407:**

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

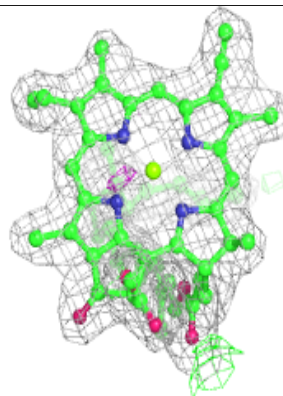
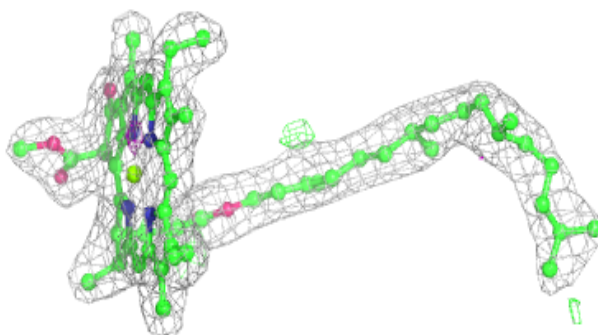
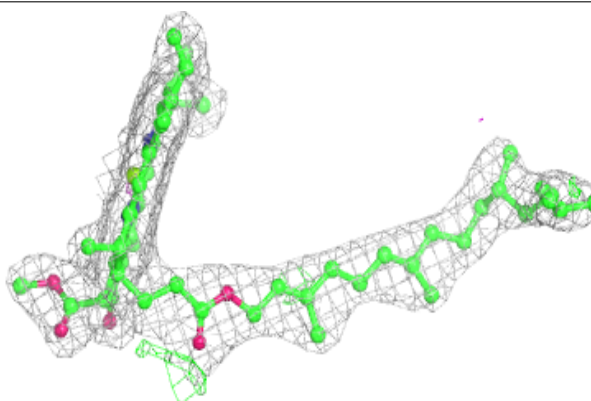


Electron density around CLA a 407:

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

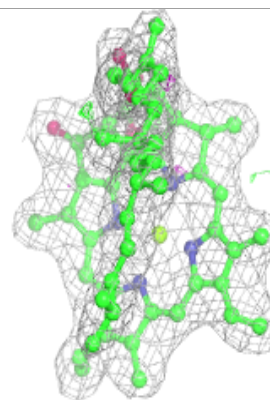
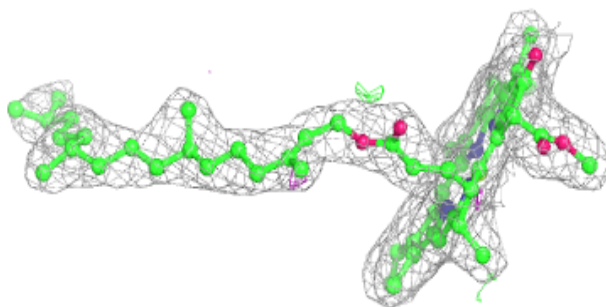
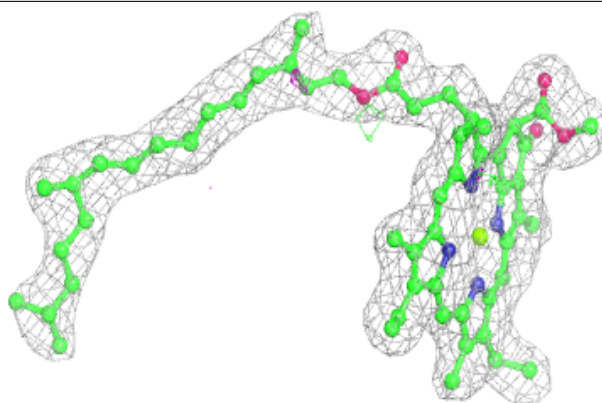
**Electron density around CLA b 607:**

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

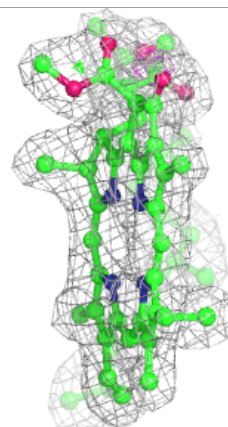
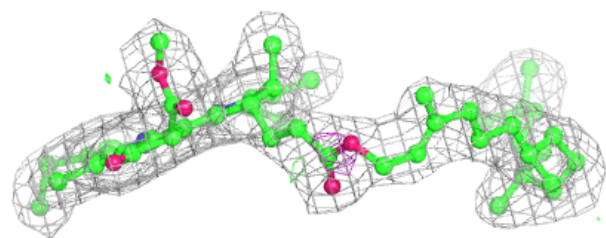
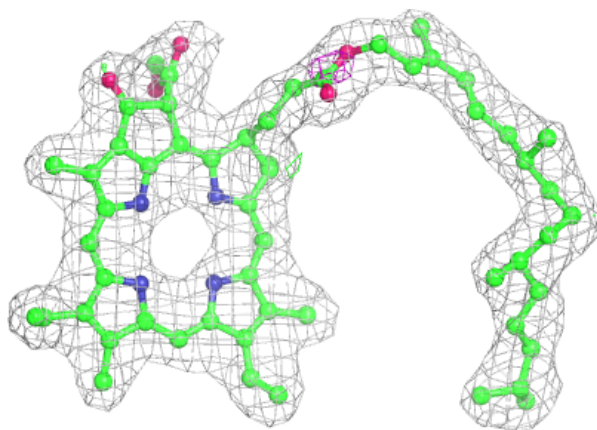


Electron density around CLA B 608:

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

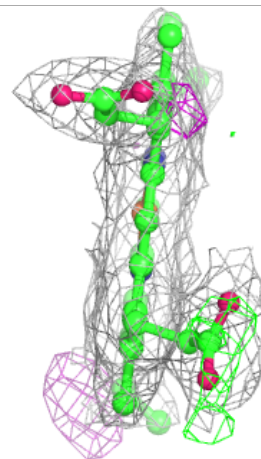
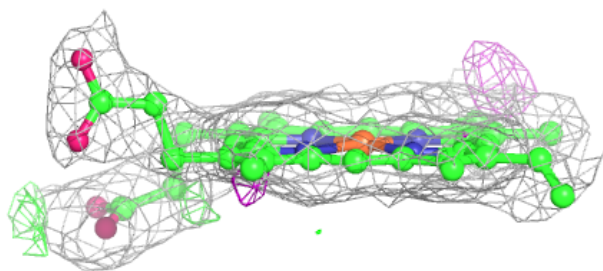
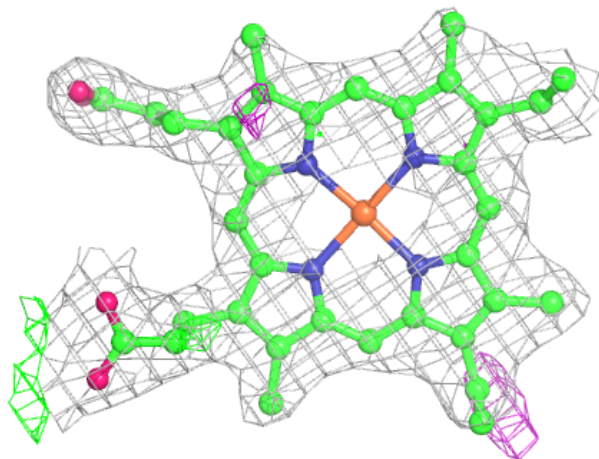
**Electron density around PHO D 401:**

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



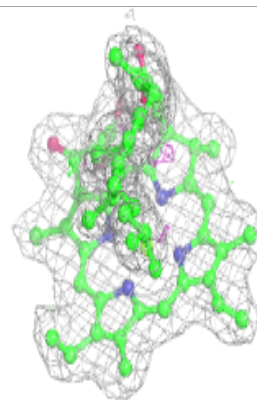
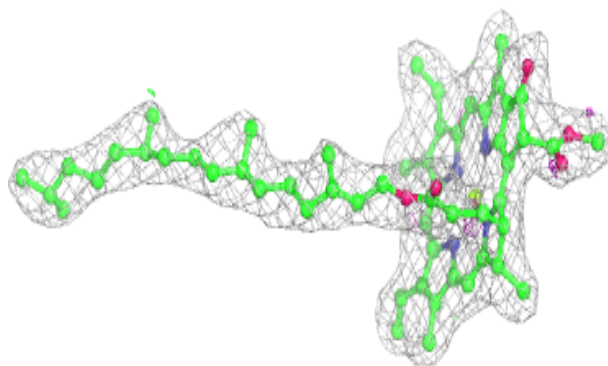
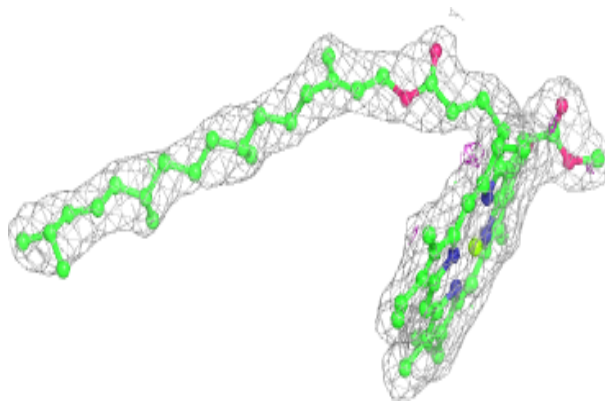
Electron density around HEM V 201:

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

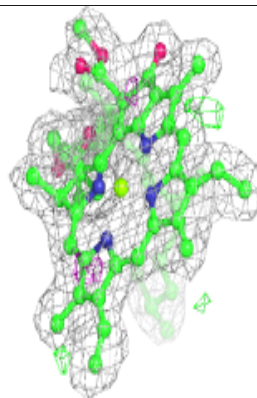
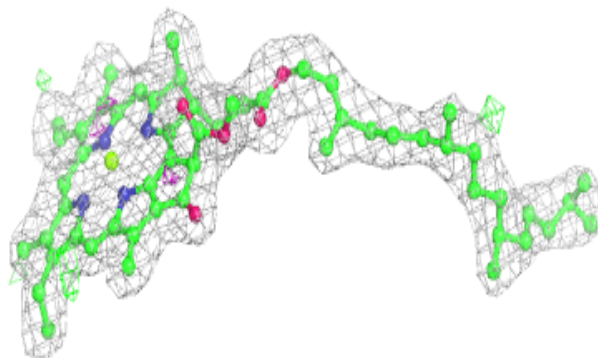
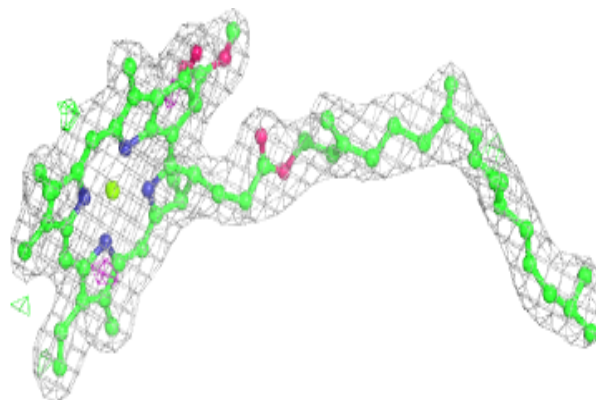


Electron density around CLA B 606:

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

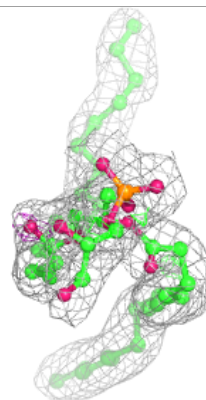
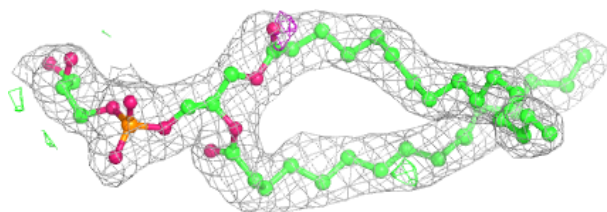
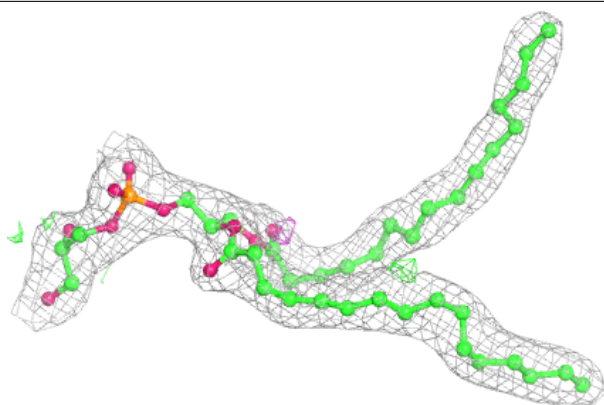
**Electron density around CLA A 403:**

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

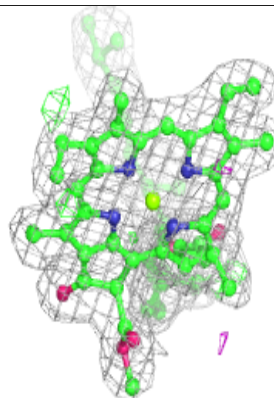
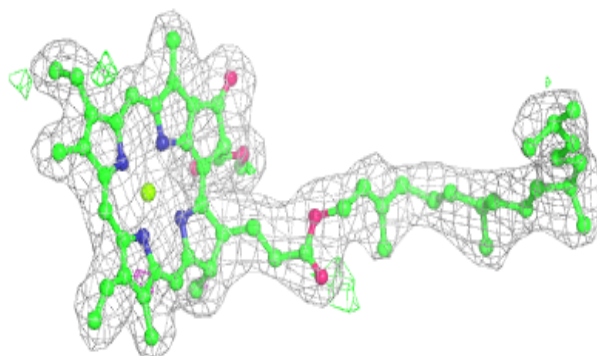
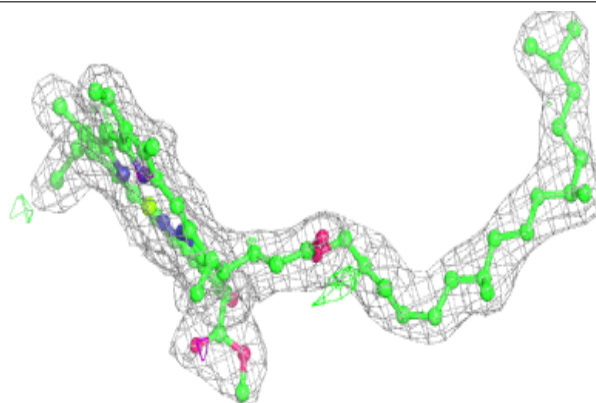


Electron density around LHG d 406:

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

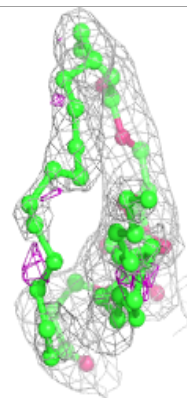
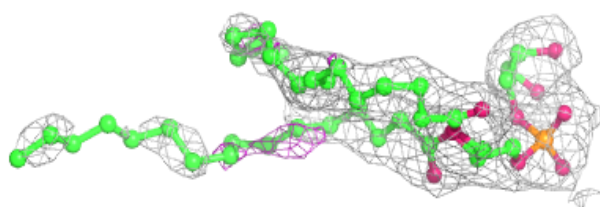
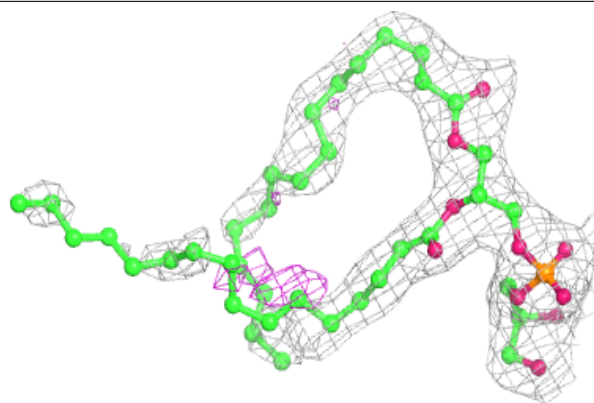
**Electron density around CLA D 402:**

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

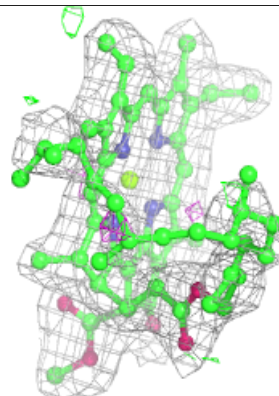
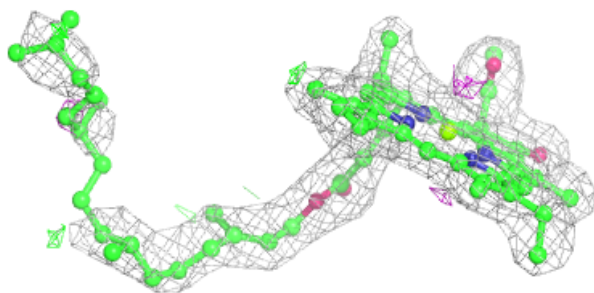
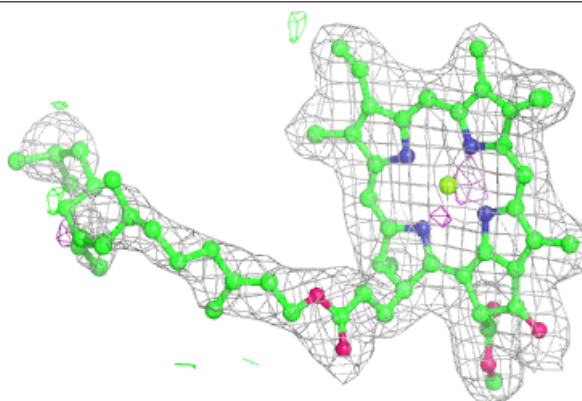


Electron density around LHG d 407:

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

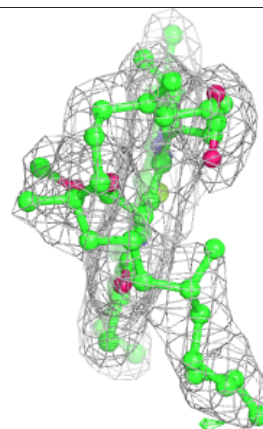
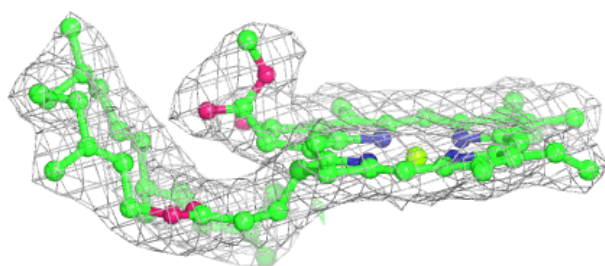
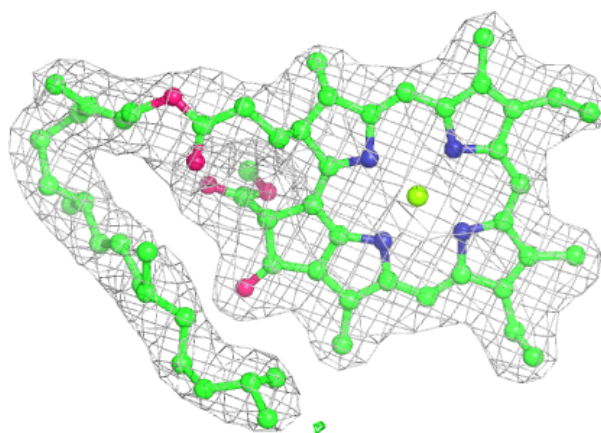
**Electron density around CLA A 406:**

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



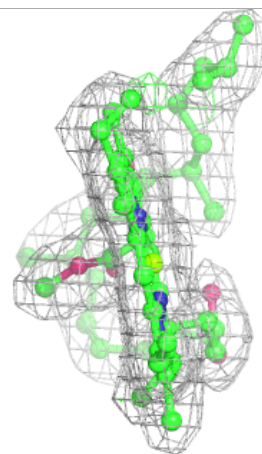
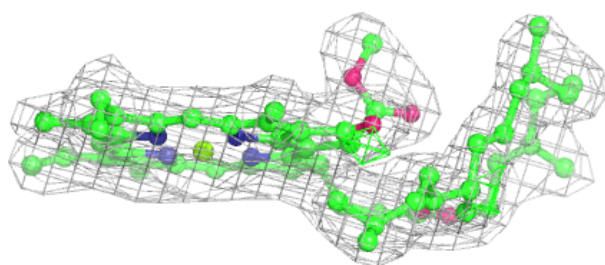
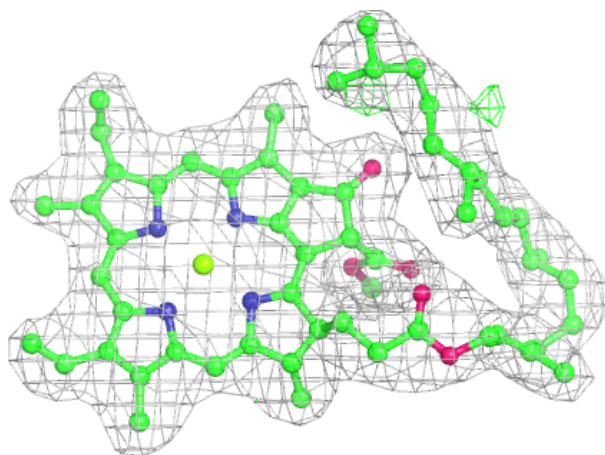
Electron density around CLA b 612:

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



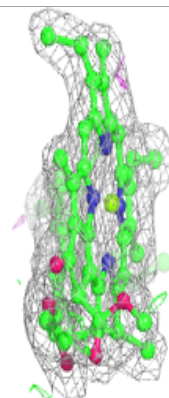
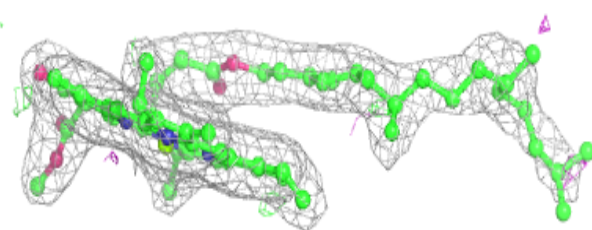
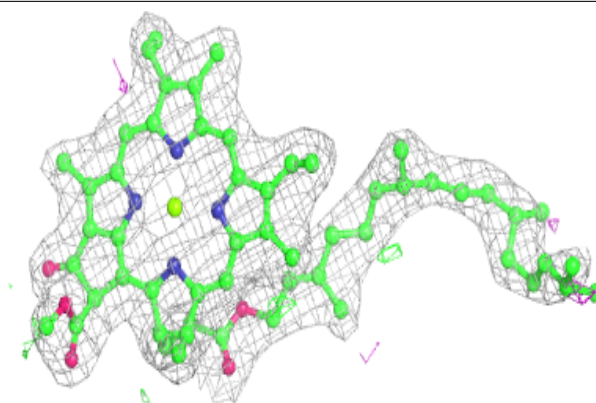
Electron density around CLA B 609:

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

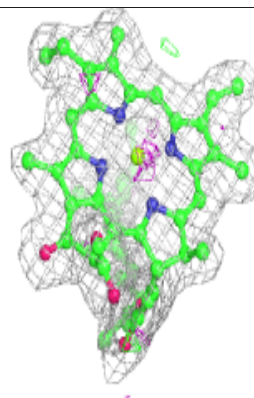
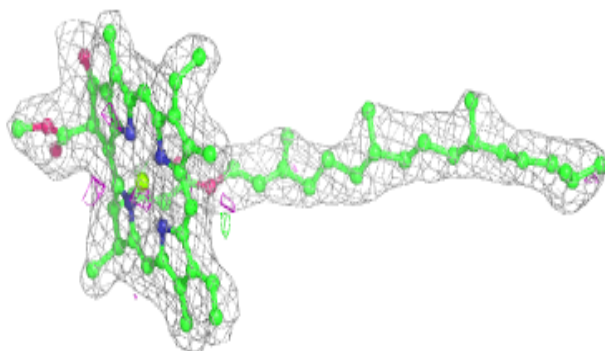
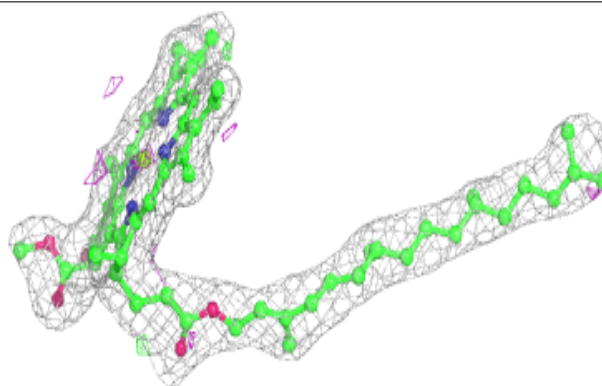


Electron density around CLA b 605:

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

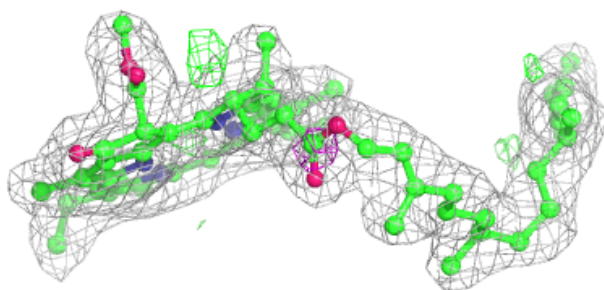
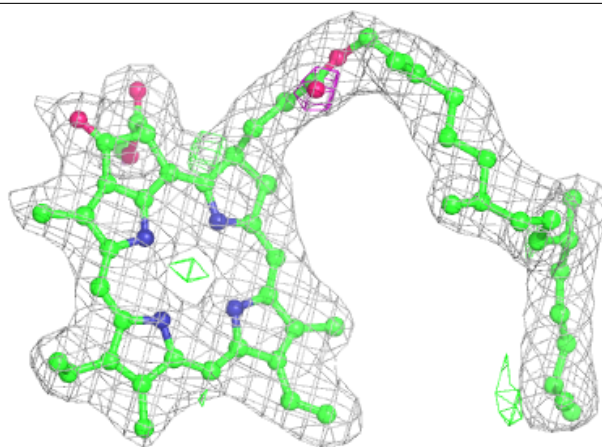
**Electron density around CLA b 609:**

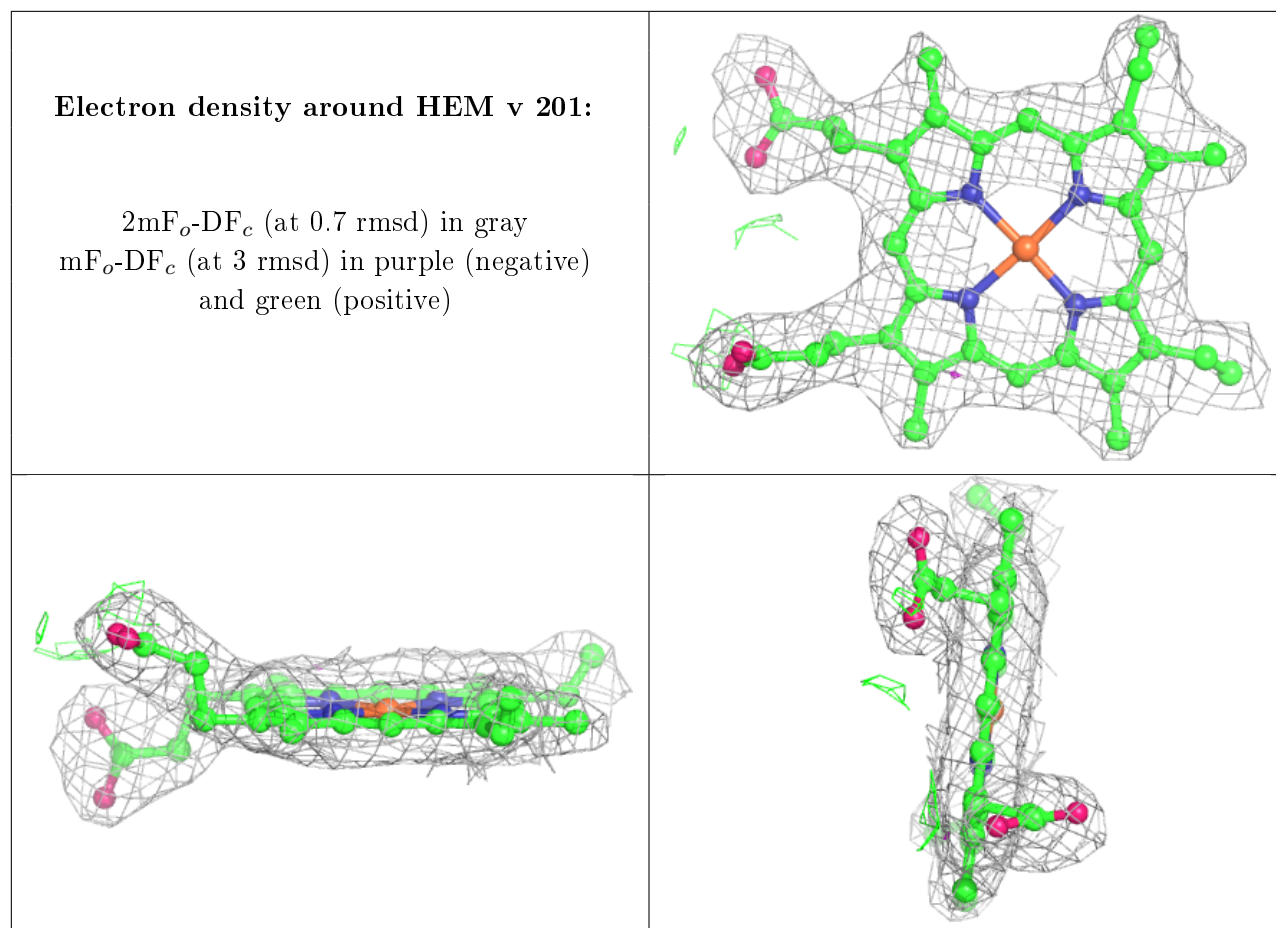
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PHO 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.