



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 12:44 am BST

PDB ID : 4TNI  
Title : RT XFEL structure of Photosystem II 500 ms after the third illumination at 4.6 Å resolution  
Authors : Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.  
Deposited on : 2014-06-04  
Resolution : 4.60 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](mailto: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.

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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 : 2.11  
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)

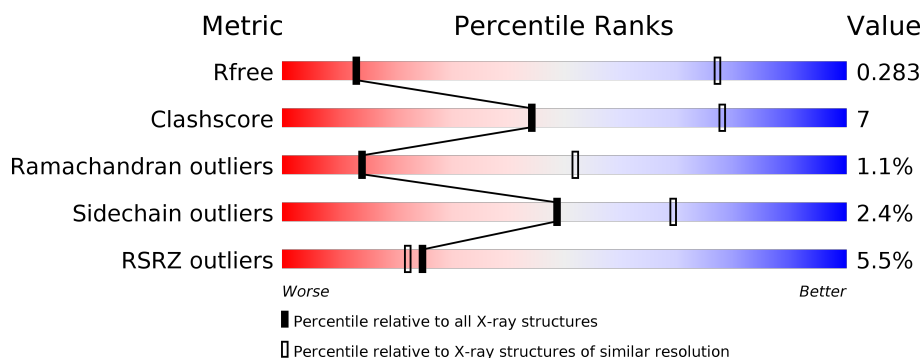
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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  $\geq 3$ , 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	
1	a	344	
2	B	510	

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Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
2	b	510	
3	C	461	
3	c	461	
4	D	352	
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	

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Mol	Chain	Length	Quality of chain
15	U	134	
15	u	134	
16	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	G	28	
19	Y	28	
20	Z	62	
20	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	X
22	CLA	B	601	X	-	-	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	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	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	-	-	X
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	X
22	CLA	C	520	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	407	X	-	-	X
22	CLA	b	605	X	-	-	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	b	619	X	-	-	X
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	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	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	405	X	-	-	-
22	CLA	d	406	X	-	-	-
22	CLA	h	101	X	-	-	-
23	PL9	A	406	-	-	-	X
23	PL9	D	407	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	d	407	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	F	102	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	409	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	g	101	-	-	-	X
24	BCR	x	101	-	-	-	X
24	BCR	y	101	-	-	-	X
25	DGD	A	408	-	-	-	X
25	DGD	B	625	-	-	-	X
25	DGD	D	410	-	-	-	X
25	DGD	a	410	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	410	-	-	-	X
27	LMG	A	414	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	I	101	-	-	-	X
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	c	518	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	m	101	-	-	-	X
29	SQD	B	626	-	-	-	X
29	SQD	b	602	-	-	-	X
29	SQD	d	403	-	-	-	X
30	LMT	B	623	-	-	-	X
30	LMT	B	624	-	-	-	X
30	LMT	B	627	-	-	-	X
30	LMT	B	628	-	-	-	X
30	LMT	D	411	-	-	-	X
30	LMT	I	102	-	-	-	X
30	LMT	M	103	-	-	-	X
30	LMT	b	603	-	-	-	X
30	LMT	b	604	-	-	-	X
30	LMT	b	626	-	-	-	X
30	LMT	b	627	-	-	-	X
30	LMT	d	411	-	-	-	X
30	LMT	i	102	-	-	-	X
31	PHO	d	401	-	-	-	X
35	CA	K	101	-	-	-	X
35	CA	O	301	-	-	-	X
35	CA	o	301	-	-	-	X

## 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 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 Q(B) protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	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	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	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		0	0	0
			270	182	41	47				
18	x	37	Total	C	N	O		0	0	0
			270	182	41	47				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	G	28	Total	C	N	O		0	0	0
			140	84	28	28				

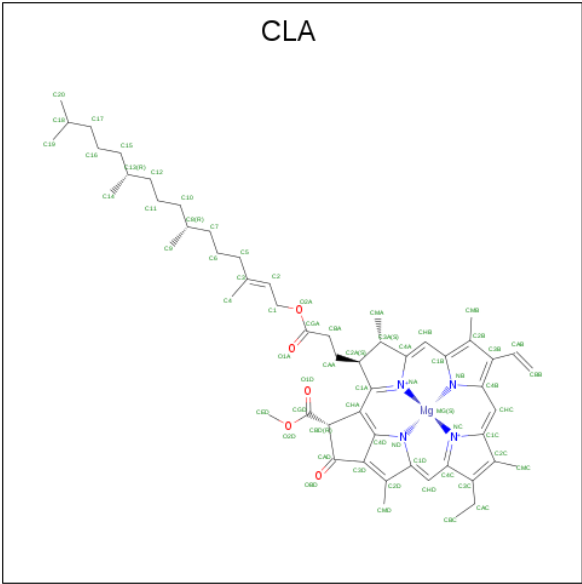
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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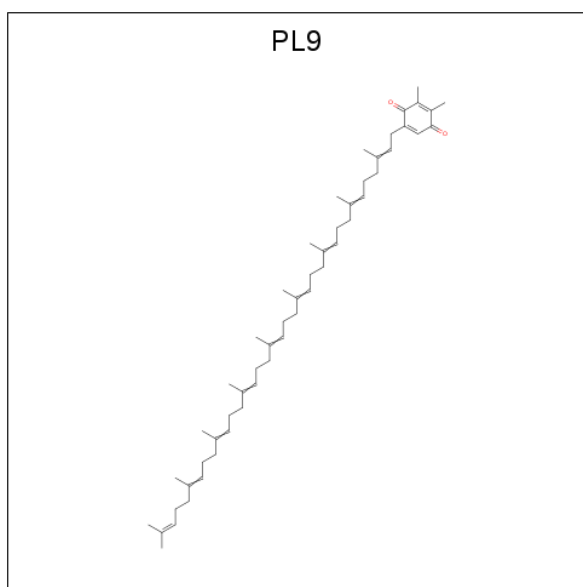
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22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55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

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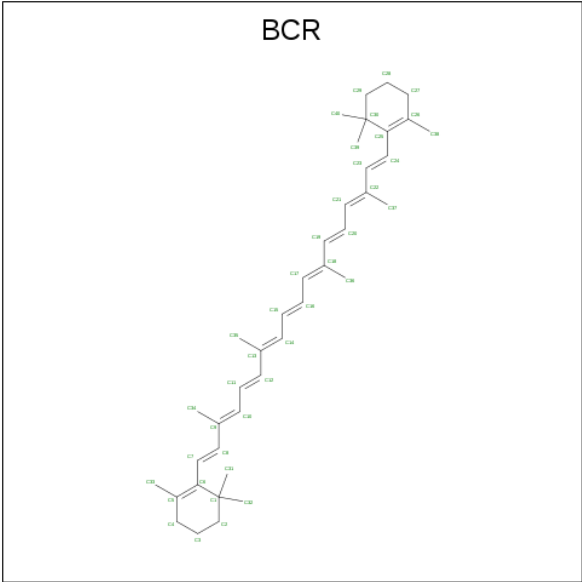
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 23 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<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	a	1	Total	C	O	0	0
			45	43	2		
23	d	1	Total	C	O	0	0
			55	53	2		
23	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



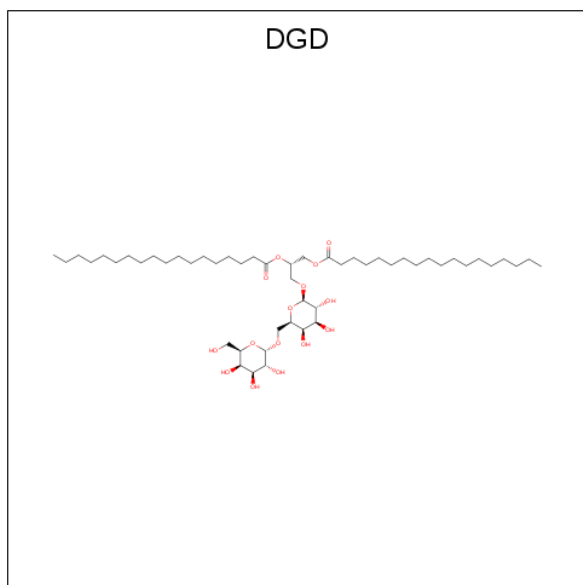
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	f	1	Total C 40 40	0	0
24	j	1	Total C 40 40	0	0
24	g	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



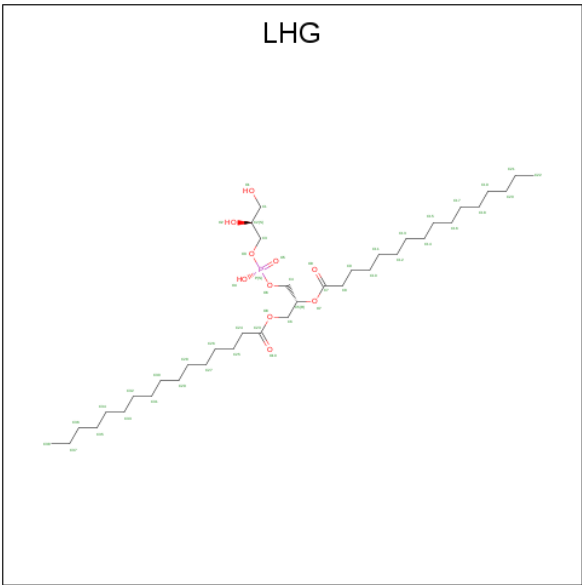
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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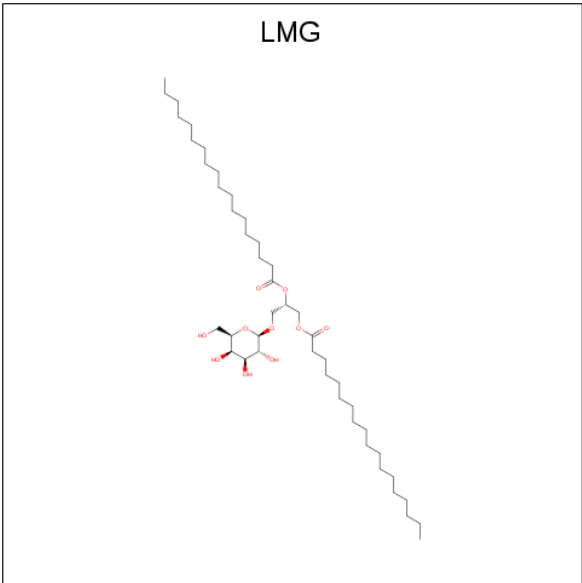
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total	C	O	0	0
			52	37	15		
25	b	1	Total	C	O	0	0
			58	43	15		
25	c	1	Total	C	O	0	0
			53	38	15		
25	c	1	Total	C	O	0	0
			62	47	15		
25	c	1	Total	C	O	0	0
			66	51	15		
25	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	P	0	0
			39	28	10	1		
26	C	1	Total	C	O	P	0	0
			37	26	10	1		
26	a	1	Total	C	O	P	0	0
			39	28	10	1		
26	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).

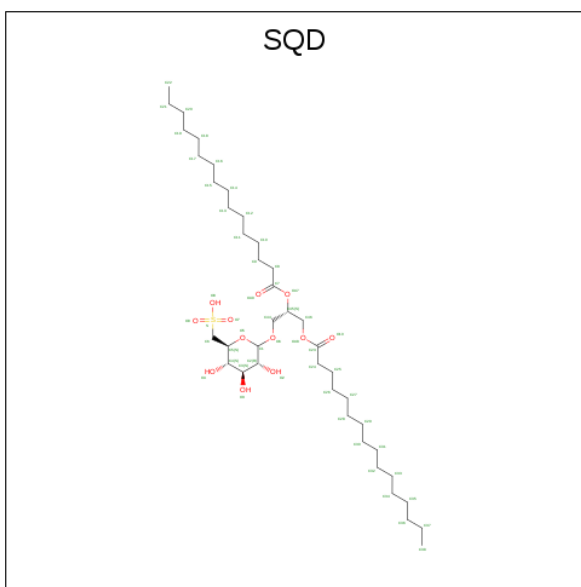




Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	E	1	Total	C	O	0	0
			44	34	10		
27	I	1	Total	C	O	0	0
			43	33	10		
27	M	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			42	32	10		
27	a	1	Total	C	O	0	0
			51	41	10		
27	b	1	Total	C	O	0	0
			49	39	10		
27	c	1	Total	C	O	0	0
			45	35	10		
27	c	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			49	39	10		
27	d	1	Total	C	O	0	0
			48	38	10		
27	d	1	Total	C	O	0	0
			46	36	10		
27	e	1	Total	C	O	0	0
			44	34	10		
27	i	1	Total	C	O	0	0
			43	33	10		
27	m	1	Total	C	O	0	0
			42	32	10		

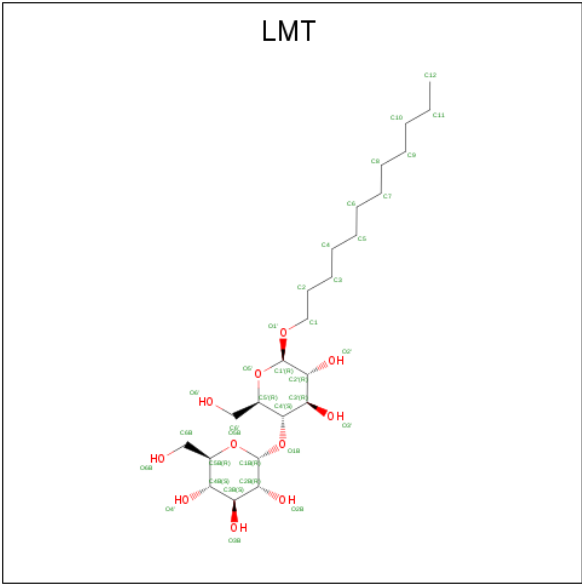
- 

- Molecule 29 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
29	A	1	Total	C	O	S	0	0
			51	38	12	1		
29	A	1	Total	C	O	S	0	0
			54	41	12	1		
29	B	1	Total	C	O	S	0	0
			43	30	12	1		
29	B	1	Total	C	O	S	0	0
			47	34	12	1		
29	F	1	Total	C	O	S	0	0
			45	32	12	1		
29	a	1	Total	C	O	S	0	0
			54	41	12	1		
29	a	1	Total	C	O	S	0	0
			51	38	12	1		
29	b	1	Total	C	O	S	0	0
			47	34	12	1		
29	d	1	Total	C	O	S	0	0
			43	30	12	1		
29	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



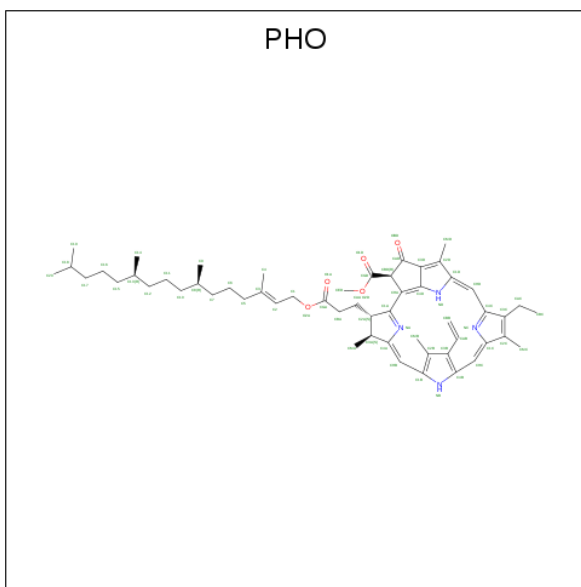
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	D	1	Total	C	O	0	0
			31	20	11		
30	I	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	M	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			35	24	11		
30	d	1	Total	C	O	0	0
			31	20	11		
30	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 31 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).

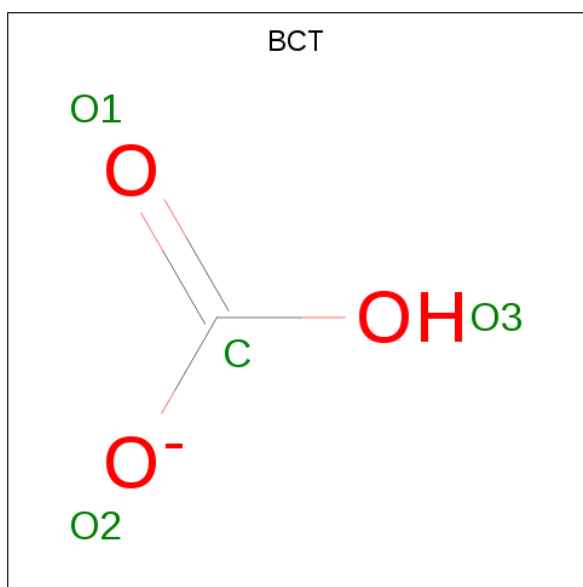


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	D	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		
31	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

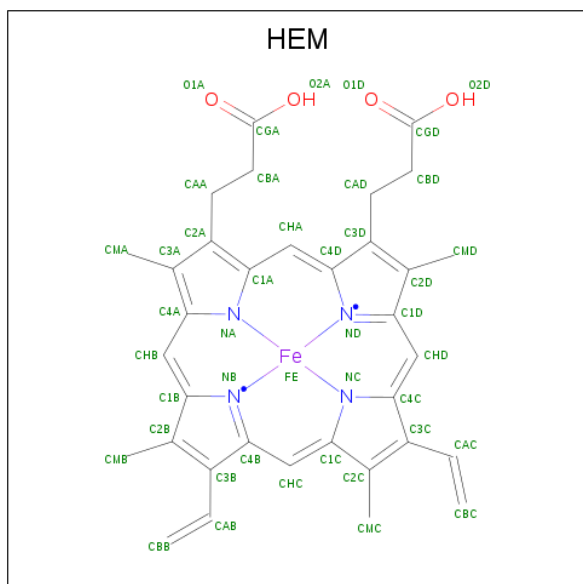
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	a	1	Total	Cl	0	0
			1	1		
32	D	1	Total	Cl	0	0
			1	1		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	D	1	Total	C	O	0	0
			4	1	3		
33	d	1	Total	C	O	0	0
			4	1	3		

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



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

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

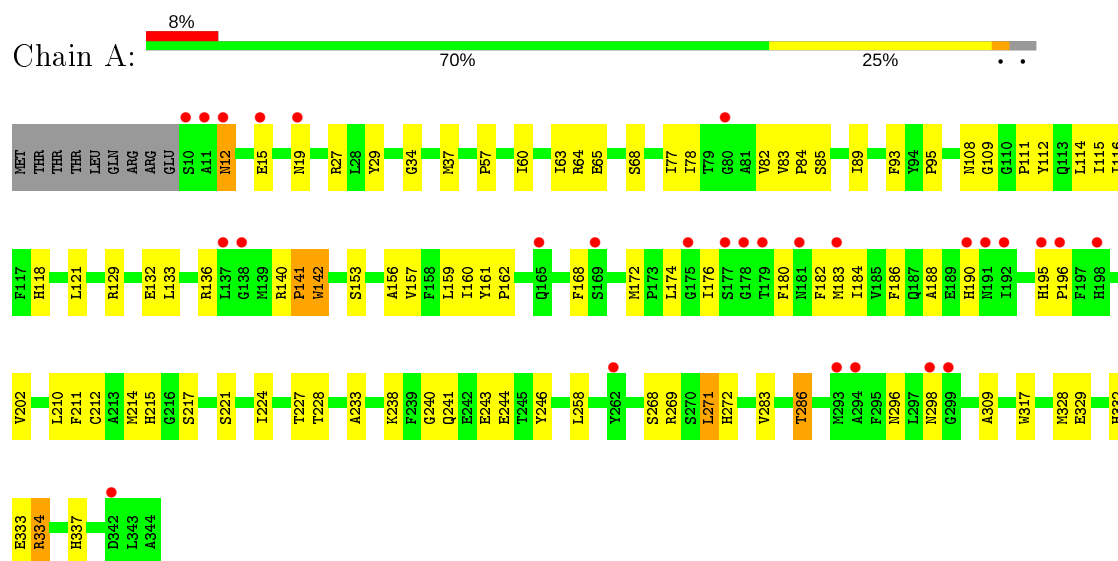
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total 1	Ca 1	0	0
35	O	1	Total 1	Ca 1	0	0
35	K	1	Total 1	Ca 1	0	0
35	k	1	Total 1	Ca 1	0	0

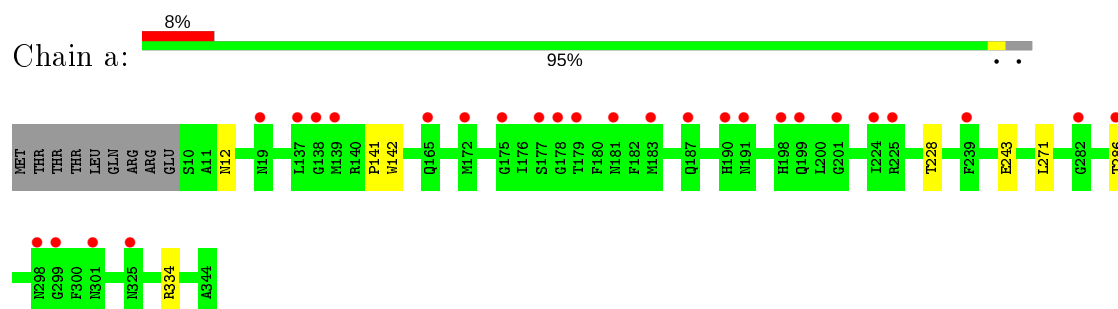
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

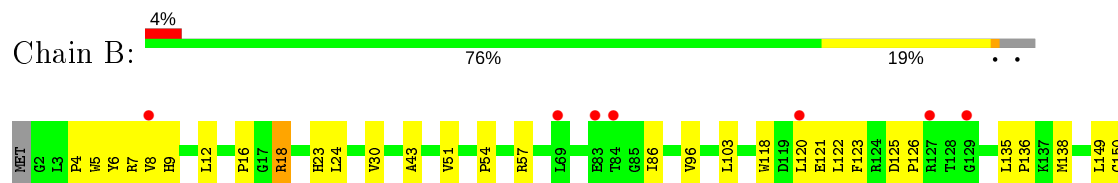
#### • Molecule 1: Photosystem Q(B) protein 1



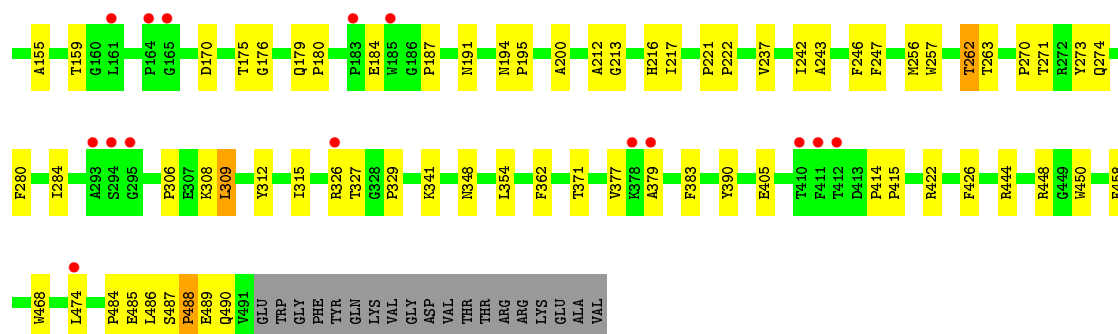
#### • Molecule 1: Photosystem Q(B) protein 1



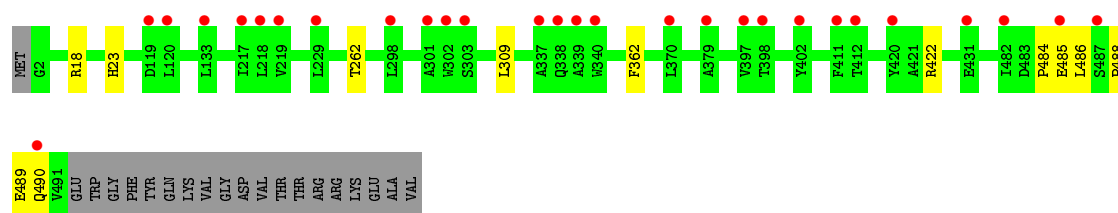
#### • Molecule 2: Photosystem II core light harvesting protein



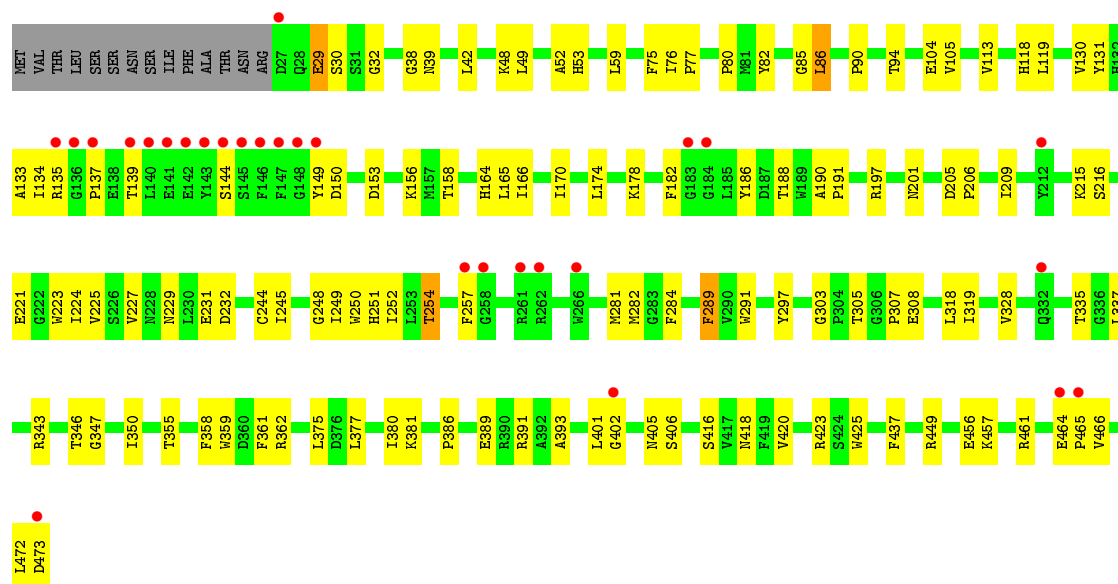




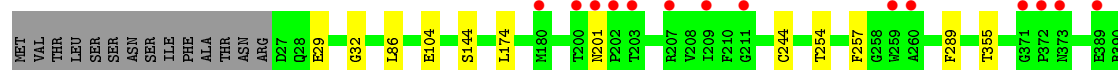
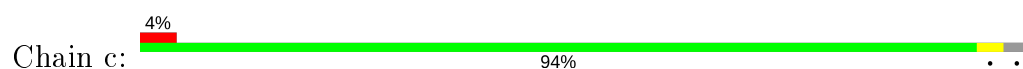
• Molecule 2: Photosystem II core light harvesting protein

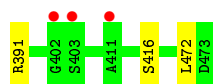


• Molecule 3: Photosystem II CP43 protein

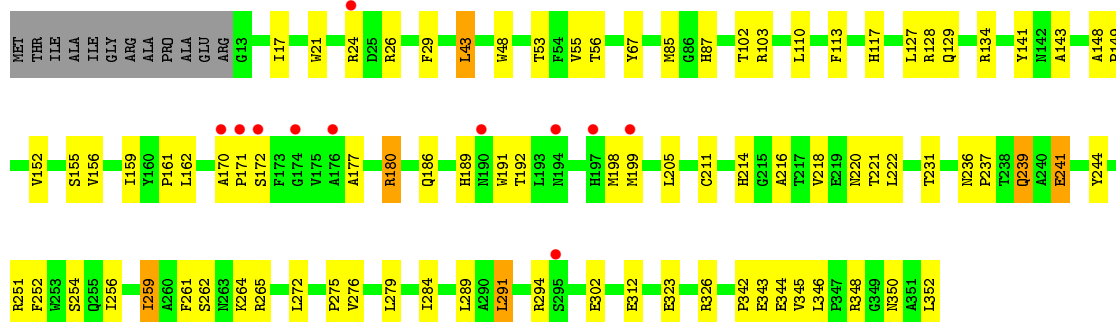


• Molecule 3: Photosystem II CP43 protein

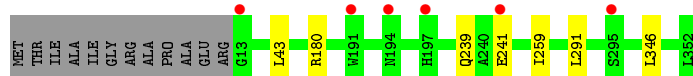




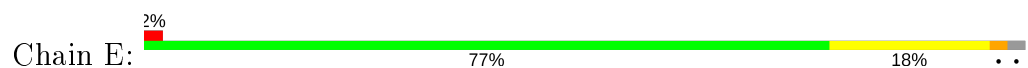
- Molecule 4: Photosystem II D2 protein



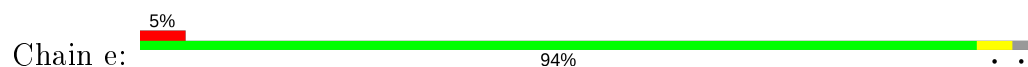
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha




- Molecule 5: Cytochrome b559 subunit alpha

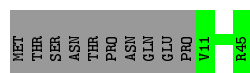


- Molecule 6: Cytochrome b559 subunit beta



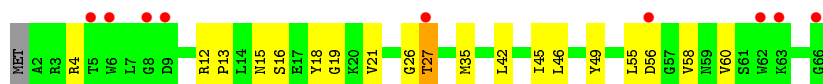
- Molecule 6: Cytochrome b559 subunit beta

Chain f:  78% 22%




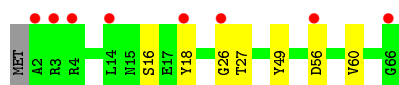
• Molecule 7: Photosystem II reaction center protein H

Chain H:  14% 70% 27% ..




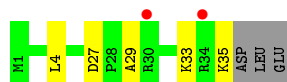
• Molecule 7: Photosystem II reaction center protein H

Chain h:  12% 88% 11% .




• Molecule 8: Photosystem II reaction center protein I

Chain I:  5% 79% 13% 8%



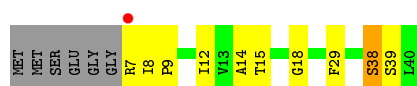
• Molecule 8: Photosystem II reaction center protein I

Chain i:  89% . 8%




• Molecule 9: Photosystem II reaction center protein J

Chain J:  3% 60% 23% . 15%



• Molecule 9: Photosystem II reaction center protein J

Chain j:  80% 5% 15%




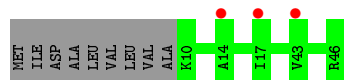
• Molecule 10: Photosystem II reaction center protein K

Chain K:  59% 22% 20%




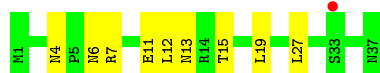
- Molecule 10: Photosystem II reaction center protein K

Chain k:  7% 80% 20%



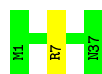
- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 76% 24%




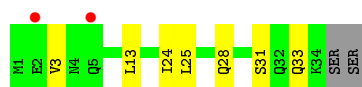
- Molecule 11: Photosystem II reaction center protein L

Chain l:  97% .



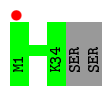
- Molecule 12: Photosystem II reaction center protein M

Chain M:  6% 75% 19% 6%



- Molecule 12: Photosystem II reaction center protein M

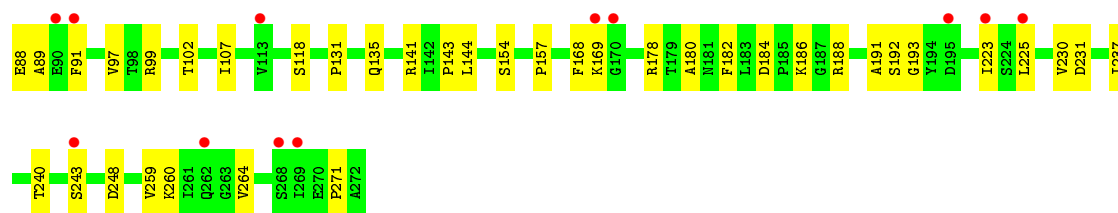
Chain m:  3% 94% 6%



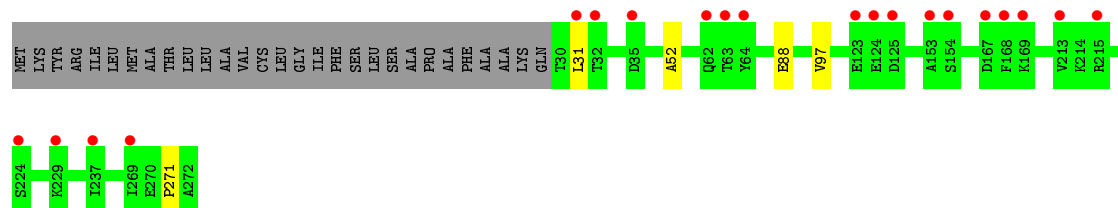
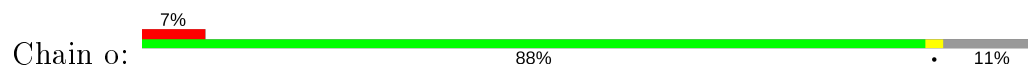
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  7% 71% 18% 11%

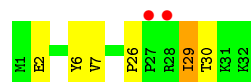
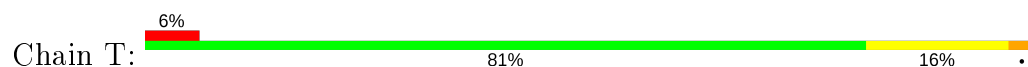




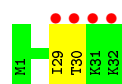
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



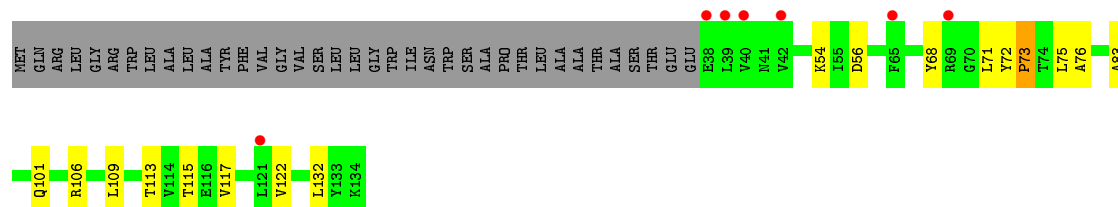
- Molecule 14: Photosystem II reaction center protein T



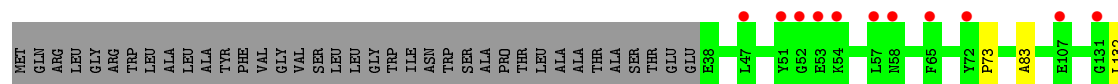
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein




- Molecule 15: Photosystem II 12 kDa extrinsic protein




Y133  
K134

- Molecule 16: Cytochrome c-550

Chain V: 

MET LEU LYS LYS CYS VAL TRP LEU ALA VAL ALA LEU CYS CYS LEU TRP GLN PHE THR MET GLY THR ALA LEU ALA A27 A43 A47 V68 I71 R81 P90 P91 R92 D93 R94 I98 M102 E116 R122 G157 K160 V161 Y162 Y163

- Molecule 16: Cytochrome c-550

Chain v: 

MET LEU LYS LYS CYS VAL TRP LEU ALA VAL ALA LEU CYS CYS LEU TRP GLN PHE THR MET GLY THR ALA LEU ALA A27 A47 Q51 R92 R122 R131 R132 L133 L138 A142 I145 Y163

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 

MET GLY ILE PHE ASN GLY ILE ILE GLU PHE LEU SER ASN ILE PHE LEU GLU VAL I19 I28 R43 L46

- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g: 


MET GLY ILE PHE ASN GLY ILE ILE GLU PHE LEU SER ASN ILE PHE LEU VAL I19 I27 I28 G29 I30 R43 L46

- Molecule 18: Photosystem II reaction center X protein

Chain X: 

MET T11 T12 T13 L16 K17 I21 G22 L23 G26 T33 F34 A35 V36 L37 L38 Q42 I43 D44 K45 V46 Q47 ARG SER LEU

- Molecule 18: Photosystem II reaction center X protein

Chain x: 

MET T11 T12 L16 Q42 K45 V46 Q47 ARG SER LEU

- Molecule 19: Photosystem II reaction center protein Y

Chain Y: 


There are no outlier residues recorded for this chain.

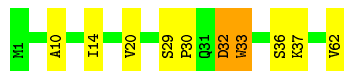
- Molecule 19: Photosystem II reaction center protein Y

Chain G:  100%

There are no outlier residues recorded for this chain.

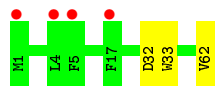
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  84% 13%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  6% 95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.43Å 228.81Å 307.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.96 – 4.60 72.96 – 4.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (72.96-4.60) 97.7 (72.96-4.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 4.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, $R_{free}$	0.278 , 0.284 0.279 , 0.283	Depositor DCC
$R_{free}$ test set	2522 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	159.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 127.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, BCT, HEM, LMG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/2713	0.41	0/3700
1	a	0.24	0/2713	0.41	0/3700
2	B	0.23	0/3986	0.40	0/5433
2	b	0.23	0/3986	0.40	0/5433
3	C	0.22	0/3556	0.41	0/4842
3	c	0.22	0/3556	0.41	0/4842
4	D	0.23	0/2801	0.40	0/3818
4	d	0.24	0/2801	0.40	0/3818
5	E	0.23	0/685	0.42	0/933
5	e	0.22	0/685	0.43	0/933
6	F	0.22	0/291	0.40	0/397
6	f	0.22	0/291	0.40	0/397
7	H	0.23	0/520	0.45	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.21	0/255	0.39	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.48	0/416
11	L	0.22	0/311	0.39	0/422
11	l	0.22	0/311	0.39	0/422
12	M	0.23	0/270	0.43	0/367
12	m	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.42	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.40	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.21	0/202	0.45	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.25	0/273	0.43	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	78	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	85	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	83	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	74	0
4	d	2706	0	2608	0	0
5	E	666	0	651	13	0
5	e	666	0	651	0	0
6	F	282	0	291	6	0
6	f	282	0	291	0	0
7	H	507	0	521	17	0
7	h	507	0	521	0	0
8	I	286	0	308	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	0
9	j	249	0	262	0	0
10	K	293	0	305	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	7	0
11	l	304	0	316	0	0
12	M	267	0	289	7	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	5	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	8	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	44	0
22	B	975	0	1080	90	0
22	C	845	0	936	47	0
22	D	130	0	144	11	0
22	H	65	0	72	9	0
22	a	260	0	288	0	0
22	b	975	0	1080	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
22	h	65	0	72	0	0
23	A	45	0	61	4	0
23	D	55	0	80	12	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	3	0
24	B	160	0	224	10	0
24	C	80	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	40	0	56	4	0
24	H	40	0	56	2	0
24	J	40	0	56	1	0
24	K	40	0	56	3	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	11	0
25	D	63	0	87	2	0
25	a	56	0	70	0	0
25	b	110	0	136	0	0
25	c	181	0	245	0	0
25	d	63	0	87	0	0
26	A	39	0	51	3	0
26	C	37	0	44	2	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	4	0
27	D	143	0	196	11	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	93	0	126	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	m	42	0	54	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	105	0	147	6	0
29	B	90	0	111	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F	45	0	54	3	0
29	a	105	0	147	0	0
29	b	47	0	61	0	0
29	d	43	0	50	0	0
29	f	45	0	54	0	0
30	B	140	0	184	6	0
30	D	31	0	35	0	0
30	I	35	0	46	1	0
30	M	70	0	91	0	0
30	b	140	0	183	0	0
30	d	31	0	35	0	0
30	i	35	0	46	0	0
31	D	128	0	148	15	0
31	d	128	0	148	0	0
32	D	1	0	0	0	0
32	a	1	0	0	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	4	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51372	579	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (579) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.51	0.81
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.61	0.80
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.66	0.77
4:D:199:MET:HG2	23:D:407:PL9:H322	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.72	0.74
22:B:605:CLA:H72	24:B:619:BCR:H311	1.70	0.73
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.70	0.72
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.72	0.71
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.70
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.70
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.74	0.70
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.70
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.73	0.70
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
3:C:250:TRP:O	3:C:254:THR:OG1	2.10	0.69
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.68
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.28	0.68
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.76	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
4:D:259:ILE:HG12	27:D:409:LMG:H292	1.78	0.67
1:A:63:ILE:HB	3:C:335:THR:HG21	1.77	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.67
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.76	0.67
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.76	0.66
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.77	0.66
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.66
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.95	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
22:C:506:CLA:H112	24:C:514:BCR:H362	1.77	0.66
4:D:236:ASN:ND2	4:D:239:GLN:O	2.30	0.66
1:A:15:GLU:O	1:A:19:ASN:ND2	2.27	0.66
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.69	0.65
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.65
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.79	0.65
1:A:174:LEU:HD22	31:D:401:PHO:H151	1.82	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.81	0.64
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.78	0.64
22:A:404:CLA:H142	22:D:405:CLA:H151	1.79	0.64
22:B:607:CLA:HBA2	29:B:622:SQD:H101	1.80	0.64
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.79	0.64
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.89	0.63
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.63
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:406:SER:O	3:C:418:ASN:ND2	2.32	0.63
31:D:402:PHO:H151	22:D:405:CLA:H172	1.89	0.63
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.80	0.63
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.63
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
27:D:409:LMG:HO4	27:D:409:LMG:HO5	1.52	0.62
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.87	0.62
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.59	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.32	0.62
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.91	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.62
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.81	0.62
1:A:329:GLU:O	1:A:332:HIS:ND1	2.36	0.61
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.61
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.87	0.61
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.61
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.61
22:A:404:CLA:H122	31:D:401:PHO:H3A	32.56	0.61
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.83	0.61
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.82	0.61
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.61
29:A:412:SQD:H172	26:C:519:LHG:H172	1.84	0.60
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.60
22:A:404:CLA:H71	22:A:405:CLA:HAB	46.99	0.60
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.67	0.60
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.61	0.60
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.84	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.67	0.59
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.24	0.59
4:D:24:ARG:NH2	18:X:44:ASP:O	2.36	0.59
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.90	0.59
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.84	0.59
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.41	0.59
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.59
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.84	0.58
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.86	0.58
29:B:622:SQD:H171	29:B:622:SQD:H301	1.86	0.58
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.58
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.39	0.57
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.57
27:D:409:LMG:O6	11:L:15:THR:HG21	2.05	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.88	0.57
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.57
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.87	0.57
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.86	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.34	0.57
1:A:268:SER:O	1:A:272:HIS:ND1	2.35	0.57
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.57
1:A:64:ARG:O	13:O:178:ARG:NH2	2.41	0.56
22:A:402:CLA:H122	31:D:401:PHO:H3A	1.87	0.56
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.56
22:A:404:CLA:H93	22:D:405:CLA:H152	1.87	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.91	0.56
27:D:412:LMG:H171	24:F:102:BCR:H383	1.95	0.56
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.45	0.56
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.88	0.56
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.88	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.27	0.55
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.18	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.88	0.55
22:B:606:CLA:C2D	22:B:608:CLA:H2	40.02	0.55
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.40	0.55
22:A:403:CLA:H203	31:D:401:PHO:H71	1.87	0.55
27:A:410:LMG:H231	23:D:407:PL9:H352	1.89	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.92	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.55
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.41	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.39	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
1:A:29:TYR:O	1:A:129:ARG:NH1	2.55	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.92	0.55
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.55
22:B:611:CLA:H151	22:B:612:CLA:H203	19.95	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.54
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.37	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.96	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.91	0.54
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.89	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.38	0.54
22:A:405:CLA:HED1	23:D:407:PL9:H372	28.93	0.54
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.90	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.90	0.54
24:A:407:BCR:H342	29:A:413:SQD:H311	1.90	0.54
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.85	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.25	0.54
26:C:519:LHG:H101	26:C:519:LHG:H271	1.90	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
13:O:73:PRO:HG2	13:O:102:THR:HB	1.90	0.54
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.90	0.53
22:A:405:CLA:H203	31:D:401:PHO:H71	33.12	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.53
29:F:103:SQD:H131	18:X:36:VAL:HG11	1.96	0.53
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.94	0.53
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.53
29:B:626:SQD:H1	29:B:626:SQD:H462	1.90	0.53
2:B:474:LEU:O	4:D:134:ARG:NH1	2.50	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.90	0.53
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.53
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.53
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.63	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.53
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.44	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.90	0.53
22:B:605:CLA:OBD	30:B:623:LMT:O6'	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:407:BCR:H321	29:A:413:SQD:H321	1.91	0.52
2:B:271:THR:HB	2:B:274:GLN:HG3	1.91	0.52
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
1:A:244:GLU:HG3	1:A:246:TYR:H	1.76	0.52
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.25	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.74	0.52
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.93	0.52
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.52
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.91	0.52
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.17	0.51
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.92	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.91	0.51
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.35	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.92	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.51
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
22:A:405:CLA:H42	23:D:407:PL9:H162	36.95	0.51
29:A:412:SQD:H311	22:C:507:CLA:H71	1.93	0.51
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.92	0.51
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.94	0.51
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.94	0.51
3:C:85:GLY:N	25:C:516:DGD:HE4	2.26	0.51
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.54	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.11	0.51
2:B:135:LEU:HA	2:B:138:MET:HE3	2.02	0.51
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.05	0.50
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.94	0.50
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.50
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.94	0.50
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.92	0.50
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.88	0.50
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.97	0.50
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.93	0.50
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.83	0.50
4:D:85:MET:HA	5:E:69:ARG:HB3	2.03	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.50
29:A:412:SQD:H223	25:C:517:DGD:HAE1	1.93	0.50
4:D:279:LEU:HG	31:D:402:PHO:HBC3	1.96	0.50
25:D:410:DGD:O5E	25:D:410:DGD:O4E	2.25	0.50
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.83	0.50
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.27	0.49
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.49
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.94	0.49
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.51	0.49
4:D:348:ARG:NH2	4:D:352:LEU:O	2.39	0.49
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.49
2:B:327:THR:HG22	22:B:606:CLA:H12	1.94	0.49
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.77	0.49
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.00	0.49
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.49
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.42	0.49
27:D:409:LMG:H111	11:L:19:LEU:HD21	1.97	0.49
1:A:210:LEU:HG	31:D:402:PHO:NC	2.28	0.49
29:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.49
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.94	0.49
22:B:611:CLA:H51	22:B:612:CLA:H101	18.01	0.49
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.95	0.49
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.49
2:B:222:PRO:HG3	7:H:27:THR:H	1.78	0.48
22:B:612:CLA:H51	27:D:408:LMG:H231	1.95	0.48
29:B:622:SQD:H111	29:B:622:SQD:H241	1.96	0.48
30:B:627:LMT:H62	8:I:4:LEU:HD22	82.08	0.48
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.95	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.48	0.48
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.48
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.94	0.48
2:B:327:THR:HG22	22:B:610:CLA:H12	26.92	0.48
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.95	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48
25:B:625:DGD:HD1	30:B:627:LMT:H32	1.95	0.48
27:A:414:LMG:H112	2:B:43:ALA:HA	42.29	0.48
4:D:102:THR:OG1	25:D:410:DGD:HD62	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.48
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.48
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	1.99	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.70	0.48
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
27:C:518:LMG:H292	27:C:518:LMG:H111	1.95	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
22:A:405:CLA:HMA2	23:D:407:PL9:H411	24.71	0.47
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.96	0.47
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.52	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.47
3:C:158:THR:O	3:C:251:HIS:HB3	2.14	0.47
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.47
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.63	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.80	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.97	0.47
22:B:615:CLA:H72	22:B:615:CLA:H12	1.97	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.98	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.97	0.47
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.47
22:C:501:CLA:H193	22:C:506:CLA:H111	2.04	0.47
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.47
4:D:262:SER:N	27:D:409:LMG:O3	2.46	0.47
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.47
22:A:405:CLA:H162	22:A:405:CLA:H141	1.71	0.46
22:B:607:CLA:H18	22:B:608:CLA:H192	1.97	0.46
27:I:101:LMG:H181	30:I:102:LMT:H42	2.04	0.46
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.98	0.46
1:A:202:VAL:HB	22:A:404:CLA:HMB3	12.99	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.01	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.99	0.46
4:D:48:TRP:CE2	31:D:402:PHO:H161	2.50	0.46
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.05	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:101:CLA:H62	22:H:101:CLA:H41	1.56	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.52	0.46
22:H:101:CLA:H162	22:H:101:CLA:H122	1.50	0.46
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.46
22:A:404:CLA:H161	23:A:406:PL9:H253	1.96	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
4:D:261:PHE:HB2	23:D:407:PL9:H522	1.98	0.46
2:B:170:ASP:OD1	2:B:175:THR:N	2.50	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.51	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.18	0.46
31:D:401:PHO:H41	31:D:401:PHO:H62	1.47	0.46
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.51	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.01	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.98	0.46
24:B:616:BCR:H20C	24:B:616:BCR:H361	1.76	0.46
22:C:510:CLA:H61	22:C:510:CLA:H93	1.81	0.46
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.79	0.46
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.46
27:D:409:LMG:HC1	27:D:409:LMG:O9	2.18	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.52	0.45
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.82	0.45
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.45
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.45
12:M:24:ILE:HG21	27:M:101:LMG:H322	9.39	0.45
22:B:607:CLA:H51	22:B:608:CLA:H101	1.98	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.48	0.45
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.99	0.45
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.99	0.45
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.77	0.45
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.82	0.45
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.45
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.57	0.45
1:A:114:LEU:O	1:A:118:HIS:ND1	2.46	0.45
22:A:402:CLA:HBA1	22:A:402:CLA:H3A	1.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.19	0.45
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.45
22:B:614:CLA:H172	22:B:614:CLA:H111	1.99	0.45
24:C:514:BCR:H361	24:C:514:BCR:H20C	1.83	0.45
13:O:143:PRO:HG2	13:O:248:ASP:HB3	1.98	0.45
22:A:402:CLA:H51	31:D:401:PHO:C3B	2.47	0.45
22:B:611:CLA:H162	22:B:611:CLA:H122	1.76	0.45
30:B:628:LMT:H122	14:T:7:VAL:HG12	34.40	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.45
16:V:98:LEU:O	16:V:102:MET:HG3	2.22	0.45
1:A:224:ILE:O	4:D:265:ARG:NH2	2.49	0.45
22:A:405:CLA:H162	22:A:405:CLA:H202	3.78	0.45
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.45
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.17	0.45
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.45
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.04	0.45
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.31	0.45
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.03	0.45
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.57	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.27	0.44
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.26	0.44
22:C:508:CLA:H11	22:C:508:CLA:H51	1.82	0.44
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.42	0.44
22:C:504:CLA:H11	24:C:514:BCR:H312	2.01	0.44
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.44
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.44
22:B:613:CLA:H51	24:B:616:BCR:H372	1.98	0.44
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.44
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.78	0.44
1:A:240:GLY:HA3	14:T:29:ILE:HG22	1.99	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.18	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.44
3:C:149:TYR:HA	3:C:156:LYS:HD3	1.99	0.44
22:C:501:CLA:H141	22:C:501:CLA:H162	1.78	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.71	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.01	0.44
3:C:224:ILE:O	3:C:227:VAL:HG23	2.18	0.44
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.00	0.44
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.44
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.18	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	2.00	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.53	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.92	0.44
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.00	0.44
22:C:512:CLA:HBA2	22:C:512:CLA:H3A	1.72	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.43
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.81	0.43
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.06	0.43
3:C:245:ILE:O	3:C:249:ILE:HG12	2.17	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.43
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:605:CLA:C3D	30:B:623:LMT:H11	2.49	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
1:A:271:LEU:HD21	23:A:406:PL9:HC71	1.99	0.43
22:C:503:CLA:H201	22:C:503:CLA:HMD2	2.02	0.43
31:D:401:PHO:H13	31:D:401:PHO:H102	1.82	0.43
22:D:405:CLA:H62	22:D:405:CLA:H92	1.79	0.43
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.58	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
22:B:606:CLA:H2	22:B:608:CLA:H93	34.06	0.43
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.78	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.43
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.43
22:A:404:CLA:H143	22:A:404:CLA:H161	1.86	0.43
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.06	0.43
30:B:628:LMT:H3'	30:B:628:LMT:H1B	1.53	0.43
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.58	0.43
11:L:4:ASN:OD1	11:L:6:ASN:ND2	2.49	0.43
2:B:468:TRP:HH2	27:D:408:LMG:HO2	1.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:615:CLA:H162	22:B:615:CLA:H122	5.18	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.64	0.43
6:F:16:PHE:HB3	29:F:103:SQD:H241	2.07	0.43
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.03	0.43
22:B:611:CLA:H171	22:B:612:CLA:HBB2	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.84	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.35	0.43
26:A:409:LHG:H382	22:C:509:CLA:H93	2.01	0.43
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.01	0.43
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.01	0.43
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.76	0.43
22:D:405:CLA:H3A	22:D:405:CLA:HBA1	1.82	0.43
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.67	0.43
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.12	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.42
22:B:606:CLA:H41	22:B:606:CLA:H61	2.89	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.78	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
7:H:12:ARG:HD3	7:H:12:ARG:O	2.19	0.42
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.04	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
23:D:407:PL9:H421	23:D:407:PL9:H401	1.86	0.42
24:F:102:BCR:H15C	24:F:102:BCR:H351	1.91	0.42
15:U:72:TYR:O	15:U:76:ALA:HB3	2.19	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
25:B:620:DGD:HAW2	22:H:101:CLA:H152	2.02	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.42
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.88	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.01	0.42
22:C:511:CLA:H61	22:C:511:CLA:H13	2.05	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.53	0.42
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.32	0.42
1:A:140:ARG:HH22	26:A:409:LHG:P	2.41	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.42
22:A:404:CLA:H51	31:D:401:PHO:C3B	21.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.91	0.42
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.86	0.42
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.02	0.42
3:C:377:LEU:O	3:C:381:LYS:HB2	2.20	0.42
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.42
22:C:511:CLA:H143	22:C:512:CLA:H162	2.02	0.42
22:B:612:CLA:H171	27:D:408:LMG:H401	2.01	0.42
22:A:403:CLA:H42	23:D:407:PL9:H162	2.01	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.04	0.42
22:B:613:CLA:H12	22:B:613:CLA:H51	4.48	0.42
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.84	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.42
3:C:456:GLU:N	3:C:456:GLU:OE1	2.52	0.42
22:C:520:CLA:H112	22:C:520:CLA:H142	1.77	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.02	0.42
22:A:405:CLA:H11	22:A:405:CLA:H51	4.35	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.88	0.42
31:D:401:PHO:H202	31:D:401:PHO:H162	1.87	0.42
13:O:192:SER:OG	13:O:193:GLY:N	2.52	0.42
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.21	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.02	0.42
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.05	0.42
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.63	0.41
22:D:406:CLA:H41	22:D:406:CLA:H61	1.86	0.41
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.83	0.41
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.50	0.41
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.41
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.48	0.41
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.02	0.41
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.41
22:A:403:CLA:H202	22:A:403:CLA:H162	1.76	0.41
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.41
22:B:611:CLA:H18	22:B:612:CLA:H192	22.27	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.85	0.41
1:A:238:LYS:O	1:A:241:GLN:HG3	2.21	0.41
22:A:403:CLA:H41	22:A:403:CLA:H62	1.76	0.41
22:B:602:CLA:H92	22:B:602:CLA:HBB2	2.03	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.79	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.84	0.41
24:F:102:BCR:H11C	24:F:102:BCR:H341	1.94	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
3:C:282:MET:HG2	22:C:501:CLA:H61	2.09	0.41
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.54	0.41
1:A:269:ARG:NH1	4:D:231:THR:HB	2.38	0.41
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.54	0.41
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.37	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.41
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.04	0.41
1:A:153:SER:HB2	22:A:404:CLA:H43	19.16	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.97	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.88	0.41
31:D:402:PHO:CHB	22:D:405:CLA:H101	2.51	0.41
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.41
1:A:258:LEU:O	4:D:128:ARG:NH1	2.54	0.41
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.10	0.41
24:A:407:BCR:H341	24:A:407:BCR:H11C	1.94	0.41
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.02	0.41
22:B:611:CLA:H161	22:B:611:CLA:H143	4.42	0.41
3:C:303:GLY:O	3:C:423:ARG:NE	2.41	0.41
3:C:119:LEU:HG	24:C:513:BCR:H10C	2.15	0.41
4:D:342:PRO:O	4:D:345:VAL:HG12	2.22	0.41
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.02	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.21	0.41
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.21	0.41
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:602:CLA:H162	22:B:602:CLA:H192	1.77	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41
7:H:35:MET:HB2	7:H:35:MET:HE3	1.87	0.41
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.26	0.41
22:A:404:CLA:H62	22:A:404:CLA:H102	4.12	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.94	0.41
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.21	0.41
24:H:102:BCR:HC31	24:H:102:BCR:H323	1.89	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.40
22:B:605:CLA:H41	22:B:605:CLA:H62	1.86	0.40
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.03	0.40
2:B:179:GLN:HA	2:B:180:PRO:HD3	1.97	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
3:C:375:LEU:HB3	3:C:380:ILE:HD11	2.04	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
24:K:102:BCR:H361	24:K:102:BCR:H20C	1.81	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.90	0.40
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.04	0.40
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.08	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.61	0.40
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.04	0.40
1:A:180:PHE:O	1:A:184:ILE:HG13	2.26	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.40
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.52	0.40
22:B:606:CLA:H161	22:B:606:CLA:H141	2.05	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.51	0.40
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.86	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.96	0.40
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.40
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.59	0.40
29:A:413:SQD:H332	22:B:609:CLA:H203	66.25	0.40
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.40
2:B:6:TYR:OH	27:D:408:LMG:HC5	2.26	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	13	50
1	a	333/344 (97%)	309 (93%)	20 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	17	56
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	26 (79%)	7 (21%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	31
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100	100
13	O	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	13	50
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	30
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	38
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	38
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	27
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	27
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	1	20
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	43
All	All	5138/5618 (92%)	4675 (91%)	408 (8%)	55 (1%)	14	52

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
7	H	26	GLY
9	J	38	SER
13	O	52	ALA
14	T	30	THR
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO

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Mol	Chain	Res	Type
3	c	257	PHE
3	c	416	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
2	B	489	GLU
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
18	X	12	ILE
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN
7	h	26	GLY
9	j	38	SER
13	o	88	GLU
1	A	142	TRP
3	C	32	GLY
5	E	82	GLN
1	a	142	TRP
1	a	334	ARG
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
7	H	16	SER
15	U	73	PRO
3	c	144	SER
7	h	16	SER
15	u	73	PRO
3	C	144	SER
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

### 5.3.2 Protein sidechains [i](#)

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	271/280 (97%)	267 (98%)	4 (2%)	65	80
1	a	271/280 (97%)	267 (98%)	4 (2%)	65	80
2	B	390/407 (96%)	381 (98%)	9 (2%)	50	70
2	b	390/407 (96%)	381 (98%)	9 (2%)	50	70
3	C	347/362 (96%)	336 (97%)	11 (3%)	39	62
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	62
4	D	275/283 (97%)	269 (98%)	6 (2%)	52	71
4	d	275/283 (97%)	269 (98%)	6 (2%)	52	71
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	65
5	e	72/73 (99%)	70 (97%)	2 (3%)	43	65
6	F	29/39 (74%)	29 (100%)	0	100	100
6	f	29/39 (74%)	29 (100%)	0	100	100
7	H	53/55 (96%)	49 (92%)	4 (8%)	13	40
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	40
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	55
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	55
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	116/138 (84%)	114 (98%)	2 (2%)	60	78
16	v	116/138 (84%)	114 (98%)	2 (2%)	60	78
17	g	20/37 (54%)	18 (90%)	2 (10%)	7	28
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	28
18	X	30/34 (88%)	28 (93%)	2 (7%)	16	43
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	43
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	58
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	58
All	All	4244/4594 (92%)	4142 (98%)	102 (2%)	49	69

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG

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Mol	Chain	Res	Type
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU
16	V	92	ARG
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU

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Mol	Chain	Res	Type
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	346	LEU
5	e	18	ARG
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	132	LEU
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

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

Mol	Chain	Res	Type
3	C	118	HIS
4	D	117	HIS
4	d	117	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\# Z  > 2$
27	LMG	a	412	-	51,51,55	0.75	1 (1%)	59,59,63	1.34	6 (10%)
23	PL9	D	407	-	55,55,55	1.07	3 (5%)	68,69,69	1.52	13 (19%)
30	LMT	M	102	-	36,36,36	1.15	6 (16%)	47,47,47	1.00	2 (4%)
24	BCR	b	623	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	9 (16%)
22	CLA	C	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
24	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	8 (14%)
29	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
30	LMT	B	624	-	36,36,36	1.11	4 (11%)	47,47,47	1.01	2 (4%)
24	BCR	J	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.61	12 (21%)
26	LHG	C	519	-	36,36,48	0.71	1 (2%)	39,42,54	1.27	4 (10%)
22	CLA	C	510	3	59,73,73	1.41	5 (8%)	67,113,113	1.52	7 (10%)
22	CLA	b	616	-	59,73,73	1.40	5 (8%)	67,113,113	1.51	8 (11%)
22	CLA	c	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	c	520	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	c	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	7 (10%)
27	LMG	d	412	-	46,46,55	0.77	1 (2%)	54,54,63	1.30	5 (9%)
34	HEM	V	201	16	27,50,50	2.19	5 (18%)	17,82,82	1.46	2 (11%)
29	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.74	10 (16%)
22	CLA	b	606	-	59,73,73	1.40	5 (8%)	67,113,113	1.44	9 (13%)
31	PHO	d	402	-	67,69,69	1.26	8 (11%)	85,99,99	1.00	5 (5%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
22	CLA	B	613	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	7 (10%)
29	SQD	A	413	-	53,54,54	0.95	4 (7%)	62,65,65	1.54	9 (14%)
22	CLA	B	604	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	7 (10%)
24	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	6 (10%)
24	BCR	F	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
30	LMT	i	102	-	36,36,36	1.11	4 (11%)	47,47,47	0.99	2 (4%)
22	CLA	B	601	-	59,73,73	1.45	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	c	509	-	59,73,73	1.45	5 (8%)	67,113,113	1.42	8 (11%)
22	CLA	b	605	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	9 (13%)
25	DGD	c	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.43	11 (14%)
24	BCR	j	102	-	41,41,41	1.08	2 (4%)	56,56,56	1.59	12 (21%)
24	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	8 (14%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.31	7 (10%)
25	DGD	a	410	-	57,57,67	0.93	1 (1%)	71,71,81	1.40	8 (11%)
29	SQD	F	103	-	44,45,54	1.03	4 (9%)	53,56,65	1.64	10 (18%)
24	BCR	c	513	-	41,41,41	1.10	2 (4%)	56,56,56	1.34	9 (16%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	10 (17%)
22	CLA	C	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	9 (13%)
25	DGD	c	517	-	67,67,67	0.87	1 (1%)	81,81,81	1.41	10 (12%)
26	LHG	c	519	-	36,36,48	0.72	1 (2%)	39,42,54	1.27	4 (10%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.31	7 (12%)
25	DGD	d	410	-	64,64,67	0.92	1 (1%)	78,78,81	1.33	9 (11%)
22	CLA	c	508	-	59,73,73	1.46	5 (8%)	67,113,113	1.43	9 (13%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-
31	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.03	6 (7%)
24	BCR	c	514	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	8 (14%)
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.33	7 (9%)
29	SQD	B	626	-	46,47,54	1.01	5 (10%)	55,58,65	1.75	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	B	609	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
22	CLA	C	504	-	59,73,73	1.42	5 (8%)	67,113,113	1.53	8 (11%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	5 (8%)
27	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.28	4 (7%)
22	CLA	b	615	-	59,73,73	1.41	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	d	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.42	9 (13%)
22	CLA	B	602	-	59,73,73	1.39	5 (8%)	67,113,113	1.46	9 (13%)
30	LMT	M	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
27	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.27	5 (9%)
29	SQD	A	412	-	50,51,54	0.96	4 (8%)	59,62,65	1.73	10 (16%)
23	PL9	d	407	-	55,55,55	1.07	2 (3%)	68,69,69	1.53	14 (20%)
24	BCR	x	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	3 (5%)
27	LMG	d	409	-	48,48,55	0.77	0	56,56,63	1.36	4 (7%)
30	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.04	1 (2%)
34	HEM	f	101	5,6	27,50,50	2.16	5 (18%)	17,82,82	1.48	3 (17%)
22	CLA	D	406	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	9 (13%)
22	CLA	C	511	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	8 (11%)
27	LMG	I	101	-	43,43,55	0.79	0	51,51,63	1.26	4 (7%)
22	CLA	b	608	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	7 (10%)
29	SQD	a	401	-	53,54,54	0.95	3 (5%)	62,65,65	1.55	10 (16%)
22	CLA	A	405	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	7 (10%)
24	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	8 (14%)
28	OEX	a	414	1,3	0,15,15	0.00	-	-	-	-
27	LMG	M	101	-	42,42,55	0.85	2 (4%)	50,50,63	1.22	4 (8%)
22	CLA	A	402	-	59,73,73	1.45	5 (8%)	67,113,113	1.44	7 (10%)
27	LMG	C	521	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
22	CLA	d	406	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)
28	OEX	A	411	1,3	0,15,15	0.00	-	-	-	-
27	LMG	i	101	-	43,43,55	0.81	0	51,51,63	1.27	6 (11%)
23	PL9	A	406	-	45,45,55	1.02	4 (8%)	56,57,69	1.57	9 (16%)
22	CLA	c	503	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	8 (11%)
23	PL9	j	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.57	7 (15%)
22	CLA	b	609	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	H	101	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	7 (10%)
24	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.28	4 (7%)
22	CLA	B	605	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	8 (11%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.26	6 (8%)
34	HEM	F	101	5,6	27,50,50	2.17	5 (18%)	17,82,82	1.45	4 (23%)
22	CLA	C	506	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	b	617	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	7 (10%)
26	LHG	A	409	-	38,38,48	0.69	1 (2%)	41,44,54	1.19	3 (7%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.26	6 (8%)
25	DGD	B	620	-	59,59,67	0.91	1 (1%)	73,73,81	1.34	8 (10%)
22	CLA	B	612	-	59,73,73	1.39	5 (8%)	67,113,113	1.50	8 (11%)
25	DGD	b	601	-	53,53,67	1.05	4 (7%)	67,67,81	1.31	7 (10%)
22	CLA	C	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.51	8 (11%)
24	BCR	b	621	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	9 (16%)
22	CLA	b	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
34	HEM	v	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.41	2 (11%)
22	CLA	c	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	7 (10%)
30	LMT	D	411	-	32,32,36	1.19	5 (15%)	43,43,47	1.02	2 (4%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
22	CLA	b	613	-	59,73,73	1.41	5 (8%)	67,113,113	1.45	7 (10%)
31	PHO	D	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.02	5 (5%)
22	CLA	c	504	-	59,73,73	1.44	5 (8%)	67,113,113	1.51	8 (11%)
30	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	1 (2%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.42	8 (11%)
22	CLA	B	615	-	59,73,73	1.43	6 (10%)	67,113,113	1.45	7 (10%)
30	LMT	b	627	-	36,36,36	1.11	5 (13%)	47,47,47	0.99	2 (4%)
27	LMG	A	414	-	42,42,55	0.83	1 (2%)	50,50,63	1.24	4 (8%)
22	CLA	b	614	-	59,73,73	1.49	5 (8%)	67,113,113	1.54	9 (13%)
22	CLA	B	610	-	59,73,73	1.48	6 (10%)	67,113,113	1.54	9 (13%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	8 (14%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.27	5 (9%)
30	LMT	B	623	-	36,36,36	1.13	5 (13%)	47,47,47	0.96	1 (2%)
22	CLA	C	509	-	59,73,73	1.46	5 (8%)	67,113,113	1.43	8 (11%)
22	CLA	c	510	3	59,73,73	1.42	5 (8%)	67,113,113	1.49	7 (10%)
27	LMG	D	409	-	48,48,55	0.77	0	56,56,63	1.37	4 (7%)
24	BCR	y	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	BCR	a	409	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	7 (12%)
27	LMG	D	412	-	46,46,55	0.76	1 (2%)	54,54,63	1.30	5 (9%)
23	PL9	a	408	-	45,45,55	1.07	3 (6%)	56,57,69	1.56	10 (17%)
22	CLA	a	406	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	8 (11%)
22	CLA	c	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)
22	CLA	B	608	-	59,73,73	1.44	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	B	607	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	8 (11%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	C	507	-	59,73,73	1.43	5 (8%)	67,113,113	1.52	9 (13%)
30	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	D	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.42	8 (11%)
24	BCR	C	514	-	41,41,41	1.12	3 (7%)	56,56,56	1.29	9 (16%)
22	CLA	b	619	-	59,73,73	1.44	6 (10%)	67,113,113	1.43	7 (10%)
24	BCR	B	616	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	7 (12%)
23	PL9	J	101	-	35,35,55	1.02	2 (5%)	44,45,69	1.56	7 (15%)
24	BCR	g	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.27	7 (12%)
22	CLA	c	507	-	59,73,73	1.42	5 (8%)	67,113,113	1.52	9 (13%)
22	CLA	C	503	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	7 (10%)
24	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	5 (8%)
29	SQD	B	622	-	42,43,54	1.05	4 (9%)	51,54,65	1.74	11 (21%)
22	CLA	A	404	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
22	CLA	C	520	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	8 (11%)
30	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.01	2 (4%)
29	SQD	f	103	-	44,45,54	1.03	4 (9%)	53,56,65	1.64	10 (18%)
24	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	4 (7%)
22	CLA	b	610	-	59,73,73	1.44	5 (8%)	67,113,113	1.44	10 (14%)
22	CLA	c	506	-	59,73,73	1.40	5 (8%)	67,113,113	1.48	8 (11%)
22	CLA	B	603	-	59,73,73	1.40	5 (8%)	67,113,113	1.55	10 (14%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.43	12 (15%)
22	CLA	C	508	-	59,73,73	1.45	5 (8%)	67,113,113	1.42	8 (11%)
27	LMG	m	101	-	42,42,55	0.85	1 (2%)	50,50,63	1.22	4 (8%)
22	CLA	a	404	-	59,73,73	1.45	5 (8%)	67,113,113	1.44	7 (10%)
30	LMT	b	626	-	36,36,36	1.13	4 (11%)	47,47,47	0.95	1 (2%)
22	CLA	A	403	-	59,73,73	1.42	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	B	611	-	59,73,73	1.41	5 (8%)	67,113,113	1.51	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	a	402	-	42,42,55	0.83	1 (2%)	50,50,63	1.25	3 (6%)
22	CLA	b	607	-	59,73,73	1.41	5 (8%)	67,113,113	1.52	10 (14%)
25	DGD	D	410	-	64,64,67	0.92	0	78,78,81	1.32	9 (11%)
27	LMG	D	408	-	49,49,55	0.76	1 (2%)	57,57,63	1.30	5 (8%)
25	DGD	C	517	-	67,67,67	0.87	1 (1%)	81,81,81	1.42	10 (12%)
22	CLA	h	101	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
22	CLA	C	512	-	59,73,73	1.42	4 (6%)	67,113,113	1.47	8 (11%)
22	CLA	a	407	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	7 (10%)
27	LMG	d	408	-	49,49,55	0.76	0	57,57,63	1.30	4 (7%)
22	CLA	B	606	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	10 (14%)
31	PHO	D	402	-	67,69,69	1.27	10 (14%)	85,99,99	1.03	6 (7%)
26	LHG	a	411	-	38,38,48	0.68	1 (2%)	41,44,54	1.20	3 (7%)
29	SQD	d	403	-	42,43,54	1.05	4 (9%)	51,54,65	1.76	11 (21%)
22	CLA	a	405	-	59,73,73	1.42	5 (8%)	67,113,113	1.49	8 (11%)
30	LMT	d	411	-	32,32,36	1.19	5 (15%)	43,43,47	0.99	2 (4%)
22	CLA	b	612	-	59,73,73	1.45	5 (8%)	67,113,113	1.42	8 (11%)
22	CLA	c	512	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	9 (13%)
22	CLA	B	614	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
24	BCR	C	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.33	9 (16%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	7 (12%)
30	LMT	B	628	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	1 (2%)
22	CLA	b	618	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)

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
27	LMG	a	412	-	-	26/46/66/70	0/1/1/1
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
30	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
22	CLA	C	501	-	3/3/20/25	15/37/135/135	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
29	SQD	b	602	-	-	14/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LMT	B	624	-	-	4/21/61/61	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
26	LHG	C	519	-	-	17/41/41/53	-
22	CLA	C	510	3	3/3/20/25	15/37/135/135	-
22	CLA	b	616	-	3/3/20/25	15/37/135/135	-
30	LMT	B	623	-	-	3/21/61/61	0/2/2/2
22	CLA	c	501	-	3/3/20/25	13/37/135/135	-
22	CLA	c	520	-	3/3/20/25	11/37/135/135	-
22	CLA	c	505	-	3/3/20/25	17/37/135/135	-
27	LMG	d	412	-	-	15/41/61/70	0/1/1/1
34	HEM	V	201	16	-	2/6/54/54	-
29	SQD	a	415	-	-	19/46/66/69	0/1/1/1
22	CLA	b	606	-	3/3/20/25	14/37/135/135	-
31	PHO	d	402	-	-	12/53/103/103	0/5/6/6
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
22	CLA	B	613	-	3/3/20/25	16/37/135/135	-
29	SQD	A	413	-	-	13/49/69/69	0/1/1/1
22	CLA	B	604	-	3/3/20/25	15/37/135/135	-
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
24	BCR	F	102	-	-	6/29/63/63	0/2/2/2
30	LMT	i	102	-	-	3/21/61/61	0/2/2/2
22	CLA	B	601	-	3/3/20/25	16/37/135/135	-
22	CLA	B	614	-	3/3/20/25	10/37/135/135	-
22	CLA	b	605	-	3/3/20/25	15/37/135/135	-
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
25	DGD	a	410	-	-	15/45/85/95	0/2/2/2
29	SQD	F	103	-	-	11/40/60/69	0/1/1/1
30	LMT	b	604	-	-	5/21/61/61	0/2/2/2
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
22	CLA	C	502	-	3/3/20/25	9/37/135/135	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	c	519	-	-	17/41/41/53	-
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
25	DGD	d	410	-	-	35/52/92/95	0/2/2/2
29	SQD	a	401	-	-	14/49/69/69	0/1/1/1
31	PHO	d	401	-	-	13/53/103/103	0/5/6/6
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
29	SQD	B	626	-	-	14/42/62/69	0/1/1/1
22	CLA	B	609	-	3/3/20/25	18/37/135/135	-
22	CLA	C	504	-	3/3/20/25	19/37/135/135	-
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
22	CLA	b	615	-	3/3/20/25	12/37/135/135	-
22	CLA	d	405	-	3/3/20/25	12/37/135/135	-
22	CLA	B	602	-	3/3/20/25	15/37/135/135	-
30	LMT	M	103	-	-	0/21/61/61	0/2/2/2
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
29	SQD	A	412	-	-	19/46/66/69	0/1/1/1
23	PL9	d	407	-	-	12/53/73/73	0/1/1/1
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
27	LMG	d	409	-	-	20/43/63/70	0/1/1/1
24	BCR	c	513	-	-	5/29/63/63	0/2/2/2
34	HEM	f	101	5,6	-	0/6/54/54	-
22	CLA	D	406	-	2/2/20/25	7/37/135/135	-
22	CLA	C	511	-	3/3/20/25	18/37/135/135	-
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
22	CLA	b	608	-	3/3/20/25	15/37/135/135	-
22	CLA	c	508	-	3/3/20/25	15/37/135/135	-
22	CLA	A	405	-	3/3/20/25	8/37/135/135	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
22	CLA	A	402	-	3/3/20/25	8/37/135/135	-
27	LMG	C	521	-	-	20/43/63/70	0/1/1/1
22	CLA	d	406	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	i	101	-	-	17/38/58/70	0/1/1/1
23	PL9	A	406	-	-	18/41/61/73	0/1/1/1
22	CLA	c	503	-	3/3/20/25	14/37/135/135	-
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
22	CLA	b	609	-	3/3/20/25	15/37/135/135	-
22	CLA	H	101	-	3/3/20/25	19/37/135/135	-
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
27	LMG	E	101	-	-	19/39/59/70	0/1/1/1
22	CLA	B	605	-	3/3/20/25	12/37/135/135	-
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
34	HEM	F	101	5,6	-	0/6/54/54	-
22	CLA	C	506	-	3/3/20/25	13/37/135/135	-
22	CLA	b	617	-	3/3/20/25	16/37/135/135	-
26	LHG	A	409	-	-	13/43/43/53	-
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
22	CLA	B	612	-	3/3/20/25	15/37/135/135	-
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
22	CLA	C	505	-	3/3/20/25	17/37/135/135	-
24	BCR	b	621	-	-	9/29/63/63	0/2/2/2
22	CLA	b	611	-	3/3/20/25	12/37/135/135	-
34	HEM	v	201	16	-	2/6/54/54	-
22	CLA	c	502	-	3/3/20/25	10/37/135/135	-
30	LMT	D	411	-	-	0/17/57/61	0/2/2/2
27	LMG	B	621	-	-	15/44/64/70	0/1/1/1
22	CLA	b	613	-	3/3/20/25	17/37/135/135	-
31	PHO	D	401	-	-	13/53/103/103	0/5/6/6
22	CLA	c	504	-	3/3/20/25	19/37/135/135	-
30	LMT	b	603	-	-	3/21/61/61	0/2/2/2
25	DGD	A	408	-	-	13/45/85/95	0/2/2/2
22	CLA	B	615	-	3/3/20/25	18/37/135/135	-
30	LMT	b	627	-	-	3/21/61/61	0/2/2/2
27	LMG	A	414	-	-	15/37/57/70	0/1/1/1
22	CLA	b	614	-	3/3/20/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	610	-	3/3/20/25	10/37/135/135	-
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
27	LMG	C	518	-	-	21/40/60/70	0/1/1/1
22	CLA	C	503	-	3/3/20/25	14/37/135/135	-
22	CLA	C	509	-	3/3/20/25	16/37/135/135	-
22	CLA	c	510	3	3/3/20/25	17/37/135/135	-
27	LMG	D	409	-	-	21/43/63/70	0/1/1/1
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
24	BCR	a	409	-	-	4/29/63/63	0/2/2/2
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
23	PL9	a	408	-	-	17/41/61/73	0/1/1/1
22	CLA	a	406	-	3/3/20/25	8/37/135/135	-
22	CLA	c	511	-	3/3/20/25	19/37/135/135	-
22	CLA	B	608	-	3/3/20/25	11/37/135/135	-
22	CLA	B	607	-	3/3/20/25	12/37/135/135	-
22	CLA	c	509	-	3/3/20/25	17/37/135/135	-
22	CLA	C	507	-	3/3/20/25	14/37/135/135	-
30	LMT	B	627	-	-	3/21/61/61	0/2/2/2
22	CLA	D	405	-	3/3/20/25	13/37/135/135	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	b	619	-	3/3/20/25	19/37/135/135	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
22	CLA	c	507	-	3/3/20/25	14/37/135/135	-
24	BCR	f	102	-	-	7/29/63/63	0/2/2/2
29	SQD	B	622	-	-	13/38/58/69	0/1/1/1
22	CLA	A	404	-	3/3/20/25	10/37/135/135	-
22	CLA	C	520	-	3/3/20/25	12/37/135/135	-
30	LMT	I	102	-	-	3/21/61/61	0/2/2/2
29	SQD	f	103	-	-	11/40/60/69	0/1/1/1
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
22	CLA	b	610	-	3/3/20/25	9/37/135/135	-
22	CLA	c	506	-	3/3/20/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	603	-	3/3/20/25	8/37/135/135	-
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	C	508	-	3/3/20/25	14/37/135/135	-
27	LMG	m	101	-	-	17/37/57/70	0/1/1/1
22	CLA	a	404	-	3/3/20/25	8/37/135/135	-
30	LMT	b	626	-	-	2/21/61/61	0/2/2/2
22	CLA	A	403	-	3/3/20/25	14/37/135/135	-
22	CLA	B	611	-	3/3/20/25	12/37/135/135	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
22	CLA	b	607	-	3/3/20/25	7/37/135/135	-
25	DGD	D	410	-	-	33/52/92/95	0/2/2/2
27	LMG	D	408	-	-	24/44/64/70	0/1/1/1
25	DGD	C	517	-	-	20/55/95/95	0/2/2/2
22	CLA	h	101	-	3/3/20/25	20/37/135/135	-
22	CLA	C	512	-	3/3/20/25	17/37/135/135	-
22	CLA	a	407	-	3/3/20/25	8/37/135/135	-
27	LMG	d	408	-	-	23/44/64/70	0/1/1/1
22	CLA	B	606	-	3/3/20/25	9/37/135/135	-
31	PHO	D	402	-	-	12/53/103/103	0/5/6/6
26	LHG	a	411	-	-	12/43/43/53	-
29	SQD	d	403	-	-	13/38/58/69	0/1/1/1
22	CLA	a	405	-	3/3/20/25	14/37/135/135	-
30	LMT	d	411	-	-	0/17/57/61	0/2/2/2
22	CLA	b	612	-	3/3/20/25	11/37/135/135	-
22	CLA	c	512	-	3/3/20/25	19/37/135/135	-
27	LMG	D	412	-	-	13/41/61/70	0/1/1/1
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
30	LMT	B	628	-	-	5/21/61/61	0/2/2/2
22	CLA	b	618	-	3/3/20/25	9/37/135/135	-

All (615) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	C4B-NB	7.85	1.42	1.35
22	c	508	CLA	C4B-NB	7.84	1.42	1.35
22	C	509	CLA	C4B-NB	7.79	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	601	CLA	C4B-NB	7.78	1.42	1.35
22	a	404	CLA	C4B-NB	7.77	1.42	1.35
22	b	605	CLA	C4B-NB	7.77	1.42	1.35
22	C	508	CLA	C4B-NB	7.76	1.42	1.35
22	b	619	CLA	C4B-NB	7.72	1.42	1.35
22	c	509	CLA	C4B-NB	7.71	1.42	1.35
22	C	505	CLA	C4B-NB	7.70	1.42	1.35
22	b	614	CLA	C4B-NB	7.70	1.42	1.35
22	B	610	CLA	C4B-NB	7.66	1.42	1.35
22	c	505	CLA	C4B-NB	7.65	1.42	1.35
22	B	615	CLA	C4B-NB	7.65	1.42	1.35
22	c	511	CLA	C4B-NB	7.65	1.42	1.35
22	C	507	CLA	C4B-NB	7.63	1.42	1.35
22	c	504	CLA	C4B-NB	7.63	1.42	1.35
22	b	612	CLA	C4B-NB	7.61	1.42	1.35
22	c	520	CLA	C4B-NB	7.61	1.42	1.35
22	B	614	CLA	C4B-NB	7.60	1.42	1.35
22	b	615	CLA	C4B-NB	7.60	1.42	1.35
22	c	503	CLA	C4B-NB	7.59	1.42	1.35
22	D	405	CLA	C4B-NB	7.59	1.42	1.35
22	d	406	CLA	C4B-NB	7.58	1.42	1.35
22	b	610	CLA	C4B-NB	7.58	1.42	1.35
22	a	405	CLA	C4B-NB	7.58	1.42	1.35
22	b	618	CLA	C4B-NB	7.58	1.42	1.35
22	B	611	CLA	C4B-NB	7.58	1.42	1.35
22	B	606	CLA	C4B-NB	7.57	1.42	1.35
22	B	608	CLA	C4B-NB	7.55	1.41	1.35
22	B	609	CLA	C4B-NB	7.55	1.41	1.35
22	c	510	CLA	C4B-NB	7.54	1.41	1.35
22	a	406	CLA	C4B-NB	7.53	1.41	1.35
22	d	405	CLA	C4B-NB	7.53	1.41	1.35
22	c	512	CLA	C4B-NB	7.52	1.41	1.35
22	C	511	CLA	C4B-NB	7.52	1.41	1.35
22	c	507	CLA	C4B-NB	7.52	1.41	1.35
22	H	101	CLA	C4B-NB	7.51	1.41	1.35
22	A	403	CLA	C4B-NB	7.51	1.41	1.35
22	B	604	CLA	C4B-NB	7.51	1.41	1.35
22	b	608	CLA	C4B-NB	7.51	1.41	1.35
22	A	405	CLA	C4B-NB	7.49	1.41	1.35
22	C	512	CLA	C4B-NB	7.49	1.41	1.35
22	D	406	CLA	C4B-NB	7.48	1.41	1.35
22	h	101	CLA	C4B-NB	7.47	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	C4B-NB	7.47	1.41	1.35
22	a	407	CLA	C4B-NB	7.46	1.41	1.35
22	b	611	CLA	C4B-NB	7.46	1.41	1.35
22	b	609	CLA	C4B-NB	7.46	1.41	1.35
22	C	502	CLA	C4B-NB	7.44	1.41	1.35
22	B	607	CLA	C4B-NB	7.42	1.41	1.35
22	b	616	CLA	C4B-NB	7.42	1.41	1.35
22	A	404	CLA	C4B-NB	7.42	1.41	1.35
22	C	503	CLA	C4B-NB	7.41	1.41	1.35
22	C	504	CLA	C4B-NB	7.41	1.41	1.35
22	B	605	CLA	C4B-NB	7.41	1.41	1.35
22	B	613	CLA	C4B-NB	7.40	1.41	1.35
22	C	520	CLA	C4B-NB	7.39	1.41	1.35
22	c	501	CLA	C4B-NB	7.38	1.41	1.35
22	b	617	CLA	C4B-NB	7.38	1.41	1.35
22	C	501	CLA	C4B-NB	7.37	1.41	1.35
22	b	613	CLA	C4B-NB	7.37	1.41	1.35
22	b	607	CLA	C4B-NB	7.36	1.41	1.35
22	c	506	CLA	C4B-NB	7.36	1.41	1.35
22	c	502	CLA	C4B-NB	7.35	1.41	1.35
22	B	612	CLA	C4B-NB	7.35	1.41	1.35
22	b	606	CLA	C4B-NB	7.34	1.41	1.35
22	C	506	CLA	C4B-NB	7.32	1.41	1.35
22	B	603	CLA	C4B-NB	7.31	1.41	1.35
22	B	602	CLA	C4B-NB	7.29	1.41	1.35
34	V	201	HEM	C3D-C2D	5.65	1.54	1.37
34	v	201	HEM	C3D-C2D	5.64	1.54	1.37
34	F	101	HEM	C3D-C2D	5.45	1.53	1.37
34	f	101	HEM	C3D-C2D	5.43	1.53	1.37
34	f	101	HEM	C3B-C2B	-4.85	1.33	1.40
34	F	101	HEM	C3B-C2B	-4.84	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.58	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.55	1.34	1.40
34	f	101	HEM	C3C-CAC	3.84	1.55	1.47
34	V	201	HEM	C3B-CAB	3.83	1.55	1.47
23	d	407	PL9	C7-C3	-3.83	1.47	1.51
34	v	201	HEM	C3B-CAB	3.80	1.55	1.47
34	F	101	HEM	C3C-CAC	3.80	1.55	1.47
34	v	201	HEM	C3B-C2B	-3.74	1.35	1.40
24	y	101	BCR	C1-C6	-3.74	1.48	1.53
34	v	201	HEM	C3C-CAC	3.74	1.55	1.47
34	V	201	HEM	C3B-C2B	-3.73	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3C-CAC	3.72	1.55	1.47
34	F	101	HEM	C3C-C2C	-3.71	1.35	1.40
24	H	102	BCR	C1-C6	-3.67	1.48	1.53
34	f	101	HEM	C3C-C2C	-3.66	1.35	1.40
22	b	614	CLA	CMB-C2B	-3.66	1.44	1.51
24	g	101	BCR	C1-C6	-3.65	1.48	1.53
24	F	102	BCR	C1-C6	-3.62	1.48	1.53
24	f	102	BCR	C1-C6	-3.57	1.48	1.53
24	x	101	BCR	C1-C6	-3.57	1.48	1.53
34	F	101	HEM	C3B-CAB	3.57	1.55	1.47
22	B	610	CLA	CMB-C2B	-3.57	1.44	1.51
34	f	101	HEM	C3B-CAB	3.53	1.55	1.47
23	D	407	PL9	C7-C3	-3.52	1.47	1.51
23	a	408	PL9	C7-C3	-3.46	1.47	1.51
31	D	402	PHO	C3B-C4B	3.39	1.50	1.43
31	d	402	PHO	C3B-C4B	3.37	1.50	1.43
24	B	616	BCR	C1-C6	-3.36	1.49	1.53
24	C	514	BCR	C1-C6	-3.35	1.49	1.53
24	c	514	BCR	C1-C6	-3.33	1.49	1.53
24	b	620	BCR	C1-C6	-3.31	1.49	1.53
22	B	608	CLA	CHC-C1C	3.29	1.43	1.35
22	B	613	CLA	CHC-C1C	3.28	1.43	1.35
31	D	401	PHO	C3B-C4B	3.28	1.50	1.43
24	b	621	BCR	C1-C6	-3.27	1.49	1.53
24	y	101	BCR	C30-C25	-3.26	1.49	1.53
24	b	622	BCR	C30-C25	-3.25	1.49	1.53
22	h	101	CLA	CHC-C1C	3.25	1.43	1.35
22	H	101	CLA	CHC-C1C	3.23	1.43	1.35
22	b	612	CLA	CHC-C1C	3.23	1.43	1.35
22	b	611	CLA	CHC-C1C	3.23	1.43	1.35
22	b	606	CLA	CHC-C1C	3.21	1.43	1.35
24	B	617	BCR	C1-C6	-3.21	1.49	1.53
22	b	617	CLA	CHC-C1C	3.20	1.43	1.35
24	J	102	BCR	C30-C25	-3.20	1.49	1.53
24	g	101	BCR	C30-C25	-3.20	1.49	1.53
24	C	513	BCR	C1-C6	-3.20	1.49	1.53
22	B	607	CLA	CHC-C1C	3.19	1.43	1.35
31	d	401	PHO	C3B-C4B	3.19	1.49	1.43
22	a	404	CLA	CHC-C1C	3.19	1.43	1.35
22	d	406	CLA	CHC-C1C	3.19	1.43	1.35
22	c	502	CLA	CHC-C1C	3.19	1.43	1.35
24	j	102	BCR	C30-C25	-3.18	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	401	SQD	O48-C23	3.18	1.42	1.33
22	C	505	CLA	CHC-C1C	3.18	1.43	1.35
22	c	507	CLA	CHC-C1C	3.17	1.43	1.35
22	C	512	CLA	CHC-C1C	3.17	1.43	1.35
22	c	511	CLA	CHC-C1C	3.17	1.43	1.35
22	c	512	CLA	CHC-C1C	3.17	1.43	1.35
22	C	511	CLA	CHC-C1C	3.17	1.43	1.35
22	c	509	CLA	CHC-C1C	3.17	1.43	1.35
22	d	405	CLA	CHC-C1C	3.17	1.43	1.35
29	b	602	SQD	O48-C23	3.16	1.42	1.33
22	C	502	CLA	CHC-C1C	3.16	1.43	1.35
22	a	406	CLA	CHC-C1C	3.16	1.43	1.35
24	c	513	BCR	C1-C6	-3.16	1.49	1.53
22	c	504	CLA	CHC-C1C	3.16	1.43	1.35
22	C	509	CLA	CHC-C1C	3.16	1.43	1.35
22	c	505	CLA	CHC-C1C	3.16	1.43	1.35
22	D	405	CLA	CHC-C1C	3.15	1.43	1.35
22	a	407	CLA	CHC-C1C	3.15	1.43	1.35
22	B	609	CLA	CHC-C1C	3.15	1.43	1.35
29	d	403	SQD	O48-C23	3.15	1.42	1.33
22	B	603	CLA	CHC-C1C	3.15	1.43	1.35
22	b	616	CLA	CHC-C1C	3.15	1.43	1.35
29	f	103	SQD	O48-C23	3.15	1.42	1.33
24	B	618	BCR	C30-C25	-3.15	1.49	1.53
22	b	607	CLA	CHC-C1C	3.15	1.43	1.35
22	B	602	CLA	CHC-C1C	3.14	1.43	1.35
22	B	614	CLA	CHC-C1C	3.14	1.43	1.35
22	C	504	CLA	CHC-C1C	3.14	1.43	1.35
22	b	618	CLA	CHC-C1C	3.14	1.43	1.35
22	B	604	CLA	CHC-C1C	3.14	1.43	1.35
24	K	102	BCR	C30-C25	-3.14	1.49	1.53
22	c	508	CLA	CHC-C1C	3.14	1.43	1.35
22	C	508	CLA	CHC-C1C	3.14	1.43	1.35
29	F	103	SQD	O48-C23	3.14	1.42	1.33
22	c	510	CLA	CHC-C1C	3.13	1.43	1.35
22	A	404	CLA	CHC-C1C	3.13	1.43	1.35
22	C	520	CLA	CHC-C1C	3.13	1.43	1.35
22	b	613	CLA	CHC-C1C	3.12	1.43	1.35
22	A	403	CLA	CHC-C1C	3.12	1.43	1.35
29	A	413	SQD	O48-C23	3.12	1.42	1.33
29	B	622	SQD	O48-C23	3.12	1.42	1.33
22	B	605	CLA	CHC-C1C	3.12	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	F	102	BCR	C30-C25	-3.11	1.49	1.53
22	B	606	CLA	CHC-C1C	3.11	1.42	1.35
22	b	608	CLA	CHC-C1C	3.11	1.42	1.35
22	C	510	CLA	CHC-C1C	3.11	1.42	1.35
29	B	626	SQD	O48-C23	3.11	1.42	1.33
22	c	503	CLA	CHC-C1C	3.11	1.42	1.35
22	A	402	CLA	CHC-C1C	3.11	1.42	1.35
22	B	612	CLA	CHC-C1C	3.11	1.42	1.35
22	b	610	CLA	CHC-C1C	3.11	1.42	1.35
22	c	520	CLA	CHC-C1C	3.10	1.42	1.35
22	C	506	CLA	CHC-C1C	3.10	1.42	1.35
23	J	101	PL9	C7-C3	-3.10	1.48	1.51
29	a	415	SQD	O48-C23	3.09	1.42	1.33
22	B	601	CLA	CHC-C1C	3.09	1.42	1.35
22	b	609	CLA	CHC-C1C	3.09	1.42	1.35
22	b	605	CLA	CHC-C1C	3.09	1.42	1.35
24	c	521	BCR	C30-C25	-3.09	1.49	1.53
22	C	507	CLA	CHC-C1C	3.09	1.42	1.35
23	A	406	PL9	C7-C3	-3.09	1.48	1.51
22	c	506	CLA	CHC-C1C	3.08	1.42	1.35
22	b	615	CLA	CHC-C1C	3.08	1.42	1.35
24	A	407	BCR	C30-C25	-3.08	1.49	1.53
22	C	501	CLA	CHC-C1C	3.08	1.42	1.35
22	C	503	CLA	CHC-C1C	3.08	1.42	1.35
24	B	618	BCR	C1-C6	-3.07	1.49	1.53
22	D	406	CLA	CHC-C1C	3.07	1.42	1.35
22	b	619	CLA	CHC-C1C	3.07	1.42	1.35
22	A	405	CLA	CHC-C1C	3.07	1.42	1.35
22	B	611	CLA	CHC-C1C	3.07	1.42	1.35
24	a	409	BCR	C30-C25	-3.06	1.49	1.53
24	f	102	BCR	C30-C25	-3.06	1.49	1.53
24	B	619	BCR	C30-C25	-3.06	1.49	1.53
22	B	615	CLA	CHC-C1C	3.06	1.42	1.35
29	A	412	SQD	O48-C23	3.05	1.42	1.33
24	b	623	BCR	C1-C6	-3.05	1.49	1.53
24	B	616	BCR	C30-C25	-3.05	1.49	1.53
22	c	501	CLA	CHC-C1C	3.04	1.42	1.35
24	b	620	BCR	C30-C25	-3.04	1.49	1.53
22	a	405	CLA	CHC-C1C	3.04	1.42	1.35
24	b	623	BCR	C30-C25	-3.03	1.49	1.53
24	B	619	BCR	C1-C6	-3.03	1.49	1.53
24	b	622	BCR	C1-C6	-3.03	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	BCR	C1-C6	-3.02	1.49	1.53
24	a	409	BCR	C1-C6	-3.02	1.49	1.53
31	D	402	PHO	CHC-C1C	3.00	1.44	1.38
31	d	402	PHO	CHC-C1C	2.99	1.44	1.38
23	j	101	PL9	C7-C3	-2.99	1.48	1.51
24	C	514	BCR	C30-C25	-2.98	1.49	1.53
24	K	102	BCR	C1-C6	-2.97	1.49	1.53
25	b	601	DGD	C1E-C2E	2.95	1.61	1.52
24	C	513	BCR	C30-C25	-2.94	1.49	1.53
24	c	514	BCR	C30-C25	-2.94	1.49	1.53
29	d	403	SQD	O47-C7	2.94	1.42	1.34
29	B	622	SQD	O47-C7	2.91	1.42	1.34
31	D	401	PHO	CHC-C1C	2.90	1.44	1.38
29	a	415	SQD	O47-C7	2.90	1.42	1.34
29	a	401	SQD	O47-C7	2.90	1.42	1.34
24	x	101	BCR	C30-C25	-2.89	1.49	1.53
29	A	413	SQD	O47-C7	2.89	1.42	1.34
29	A	412	SQD	O47-C7	2.88	1.42	1.34
24	c	521	BCR	C1-C6	-2.87	1.49	1.53
25	B	625	DGD	C1E-C2E	2.87	1.60	1.52
29	F	103	SQD	O47-C7	2.86	1.42	1.34
31	d	401	PHO	CHC-C1C	2.86	1.44	1.38
22	B	610	CLA	CHC-C1C	2.85	1.42	1.35
22	b	614	CLA	CHC-C1C	2.85	1.42	1.35
24	H	102	BCR	C30-C25	-2.85	1.49	1.53
29	b	602	SQD	O47-C7	2.83	1.42	1.34
29	B	626	SQD	O47-C7	2.82	1.42	1.34
29	f	103	SQD	O47-C7	2.81	1.42	1.34
22	c	512	CLA	C1D-C2D	2.78	1.48	1.42
24	J	102	BCR	C1-C6	-2.77	1.50	1.53
24	j	102	BCR	C1-C6	-2.77	1.50	1.53
24	c	513	BCR	C30-C25	-2.76	1.50	1.53
22	C	512	CLA	C1D-C2D	2.75	1.48	1.42
22	b	610	CLA	C1D-C2D	2.75	1.48	1.42
31	d	402	PHO	C4C-NC	2.75	1.42	1.36
22	B	609	CLA	C1D-C2D	2.74	1.48	1.42
22	c	508	CLA	C1D-C2D	2.74	1.48	1.42
22	c	520	CLA	C1D-C2D	2.74	1.48	1.42
22	C	501	CLA	C1D-C2D	2.74	1.48	1.42
23	a	408	PL9	C3-C4	-2.73	1.45	1.49
22	b	613	CLA	C1D-C2D	2.72	1.48	1.42
22	a	404	CLA	C1D-C2D	2.72	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C1D-C2D	2.72	1.48	1.42
22	a	406	CLA	C1D-C2D	2.72	1.48	1.42
22	a	405	CLA	C1D-C2D	2.72	1.48	1.42
22	c	501	CLA	C1D-C2D	2.72	1.48	1.42
22	A	403	CLA	C1D-C2D	2.71	1.48	1.42
31	D	402	PHO	C4C-NC	2.71	1.42	1.36
24	b	621	BCR	C30-C25	-2.71	1.50	1.53
22	d	406	CLA	C1D-C2D	2.71	1.48	1.42
22	D	406	CLA	C1D-C2D	2.70	1.48	1.42
22	B	604	CLA	C1D-C2D	2.70	1.48	1.42
24	B	617	BCR	C30-C25	-2.70	1.50	1.53
31	D	402	PHO	C1A-NA	2.69	1.42	1.37
22	C	509	CLA	C1D-C2D	2.69	1.48	1.42
22	C	505	CLA	C1D-C2D	2.69	1.48	1.42
22	B	614	CLA	C1D-C2D	2.69	1.48	1.42
22	C	520	CLA	C1D-C2D	2.69	1.48	1.42
31	D	401	PHO	C4C-NC	2.69	1.42	1.36
31	d	401	PHO	C4C-NC	2.69	1.42	1.36
31	d	401	PHO	C1A-NA	2.69	1.42	1.37
22	b	618	CLA	C1D-C2D	2.69	1.48	1.42
22	A	404	CLA	C1D-C2D	2.68	1.48	1.42
22	b	609	CLA	C1D-C2D	2.68	1.48	1.42
23	D	407	PL9	C3-C4	-2.68	1.45	1.49
22	A	402	CLA	C1D-C2D	2.68	1.48	1.42
22	c	510	CLA	C1D-C2D	2.68	1.48	1.42
22	b	616	CLA	C1D-C2D	2.68	1.48	1.42
22	b	605	CLA	C1D-C2D	2.68	1.48	1.42
22	C	507	CLA	C1D-C2D	2.67	1.48	1.42
22	A	405	CLA	C1D-C2D	2.67	1.48	1.42
22	B	615	CLA	C1D-C2D	2.67	1.48	1.42
22	c	503	CLA	C1D-C2D	2.67	1.48	1.42
22	b	619	CLA	C1D-C2D	2.67	1.48	1.42
22	c	505	CLA	C1D-C2D	2.67	1.48	1.42
22	b	608	CLA	C1D-C2D	2.66	1.48	1.42
22	C	508	CLA	C1D-C2D	2.66	1.48	1.42
22	B	613	CLA	C1D-C2D	2.66	1.48	1.42
22	B	601	CLA	C1D-C2D	2.66	1.48	1.42
22	b	606	CLA	C1D-C2D	2.65	1.48	1.42
22	C	503	CLA	C1D-C2D	2.65	1.48	1.42
22	B	612	CLA	C1D-C2D	2.65	1.48	1.42
22	B	605	CLA	C1D-C2D	2.65	1.48	1.42
22	B	610	CLA	C1D-C2D	2.65	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	401	PHO	C1A-NA	2.64	1.42	1.37
22	c	506	CLA	C1D-C2D	2.64	1.48	1.42
22	C	510	CLA	C1D-C2D	2.64	1.48	1.42
23	d	407	PL9	C3-C4	-2.64	1.45	1.49
22	H	101	CLA	C1D-C2D	2.63	1.48	1.42
30	d	411	LMT	O3'-C3'	-2.63	1.36	1.43
31	d	402	PHO	C1A-NA	2.63	1.42	1.37
22	a	407	CLA	C1D-C2D	2.63	1.48	1.42
30	b	627	LMT	O3'-C3'	-2.63	1.36	1.43
22	c	509	CLA	C1D-C2D	2.63	1.48	1.42
22	C	502	CLA	C1D-C2D	2.62	1.48	1.42
22	C	506	CLA	C1D-C2D	2.61	1.48	1.42
30	D	411	LMT	O3'-C3'	-2.61	1.36	1.43
30	M	102	LMT	O3'-C3'	-2.60	1.36	1.43
30	I	102	LMT	O3'-C3'	-2.60	1.36	1.43
22	B	608	CLA	C1D-C2D	2.60	1.48	1.42
22	b	617	CLA	C1D-C2D	2.60	1.48	1.42
22	B	607	CLA	C1D-C2D	2.60	1.48	1.42
22	b	611	CLA	C1D-C2D	2.60	1.48	1.42
22	h	101	CLA	C1D-C2D	2.60	1.48	1.42
30	M	103	LMT	O3'-C3'	-2.60	1.36	1.43
22	b	614	CLA	C1D-C2D	2.60	1.48	1.42
22	C	507	CLA	CMB-C2B	-2.60	1.46	1.51
22	B	602	CLA	C1D-C2D	2.60	1.48	1.42
22	c	507	CLA	C1D-C2D	2.59	1.48	1.42
22	c	507	CLA	CMB-C2B	-2.59	1.46	1.51
30	b	626	LMT	O3'-C3'	-2.58	1.36	1.43
22	C	511	CLA	C1D-C2D	2.58	1.48	1.42
22	b	607	CLA	C1D-C2D	2.57	1.48	1.42
22	c	511	CLA	C1D-C2D	2.57	1.48	1.42
22	b	612	CLA	C1D-C2D	2.57	1.48	1.42
30	b	603	LMT	O3'-C3'	-2.57	1.36	1.43
30	b	604	LMT	O3'-C3'	-2.56	1.36	1.43
22	c	502	CLA	C1D-C2D	2.56	1.48	1.42
30	B	627	LMT	O3'-C3'	-2.56	1.37	1.43
22	d	405	CLA	C1D-C2D	2.56	1.48	1.42
30	B	624	LMT	O3'-C3'	-2.55	1.37	1.43
23	A	406	PL9	C3-C4	-2.55	1.45	1.49
30	i	102	LMT	O3'-C3'	-2.54	1.37	1.43
30	B	623	LMT	O3'-C3'	-2.53	1.37	1.43
25	C	515	DGD	O2G-C2G	-2.50	1.40	1.46
22	B	603	CLA	C1D-C2D	2.50	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.48	1.46	1.51
30	B	628	LMT	O3'-C3'	-2.48	1.37	1.43
22	c	509	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.47	1.46	1.51
22	b	615	CLA	C1D-C2D	2.47	1.48	1.42
22	b	611	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	504	CLA	C1D-C2D	2.47	1.48	1.42
22	A	403	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.45	1.46	1.51
22	D	405	CLA	C1D-C2D	2.45	1.48	1.42
22	A	404	CLA	CMB-C2B	-2.45	1.46	1.51
31	d	402	PHO	CHD-C1D	2.44	1.43	1.38
22	A	405	CLA	CMB-C2B	-2.44	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.44	1.46	1.51
22	a	407	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	611	CLA	C1D-C2D	2.44	1.48	1.42
22	c	501	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.44	1.46	1.51
25	B	625	DGD	C4D-C5D	2.44	1.58	1.53
22	d	405	CLA	CMB-C2B	-2.44	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.44	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.42	1.46	1.51
31	D	402	PHO	CHD-C1D	2.42	1.43	1.38
22	b	610	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.41	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.41	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.41	1.46	1.51
31	d	402	PHO	C4C-C3C	2.41	1.49	1.45
22	B	615	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	504	CLA	C1D-C2D	2.40	1.48	1.42
22	c	520	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.40	1.46	1.51
22	D	406	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	d	406	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.38	1.46	1.51
31	D	401	PHO	C4C-C3C	2.38	1.49	1.45
22	b	619	CLA	CMB-C2B	-2.37	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.37	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.37	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.36	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.36	1.46	1.51
31	D	401	PHO	C1C-NC	-2.36	1.33	1.38
30	I	102	LMT	O2'-C2'	-2.36	1.37	1.43
31	D	402	PHO	C4C-C3C	2.35	1.49	1.45
31	d	402	PHO	C1C-NC	-2.35	1.33	1.38
22	B	611	CLA	CMD-C2D	-2.35	1.46	1.51
31	d	401	PHO	C4C-C3C	2.35	1.49	1.45
31	D	402	PHO	C1C-NC	-2.34	1.33	1.38
22	c	511	CLA	CMB-C2B	-2.34	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.34	1.46	1.51
30	I	102	LMT	O2B-C2B	-2.34	1.37	1.43
22	b	606	CLA	CMB-C2B	-2.34	1.46	1.51
31	d	401	PHO	C1C-NC	-2.34	1.33	1.38
22	b	615	CLA	CMB-C2B	-2.33	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	102	LMT	O2'-C2'	-2.32	1.37	1.43
30	i	102	LMT	O2B-C2B	-2.32	1.37	1.43
30	b	626	LMT	O2'-C2'	-2.32	1.37	1.43
22	B	613	CLA	CMB-C2B	-2.32	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.31	1.46	1.51
22	b	615	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	614	CLA	C3B-C2B	-2.28	1.37	1.40
31	D	401	PHO	CHD-C1D	2.28	1.43	1.38
30	M	103	LMT	O2'-C2'	-2.28	1.37	1.43
30	B	623	LMT	O2'-C2'	-2.27	1.37	1.43
30	M	103	LMT	O3B-C3B	-2.27	1.37	1.43
30	b	627	LMT	O2'-C2'	-2.27	1.37	1.43
31	d	401	PHO	CHD-C1D	2.26	1.43	1.38
30	B	627	LMT	O2'-C2'	-2.26	1.37	1.43
30	B	628	LMT	O3B-C3B	-2.26	1.37	1.43
30	M	102	LMT	O3B-C3B	-2.25	1.37	1.43
30	b	627	LMT	O3B-C3B	-2.25	1.37	1.43
30	M	103	LMT	O2B-C2B	-2.25	1.37	1.43
30	M	102	LMT	O2'-C2'	-2.25	1.37	1.43
23	a	408	PL9	C53-C6	-2.25	1.46	1.50
30	b	603	LMT	O2B-C2B	-2.25	1.37	1.43
30	D	411	LMT	O3B-C3B	-2.24	1.37	1.43
30	b	603	LMT	O3B-C3B	-2.24	1.37	1.43
22	c	504	CLA	CMD-C2D	-2.24	1.46	1.51
27	B	621	LMG	C4-C5	2.24	1.57	1.53
30	B	623	LMT	O3B-C3B	-2.24	1.37	1.43
30	M	102	LMT	O2B-C2B	-2.24	1.37	1.43
30	b	626	LMT	O2B-C2B	-2.23	1.37	1.43
30	b	604	LMT	O3B-C3B	-2.23	1.37	1.43
30	B	624	LMT	O3B-C3B	-2.23	1.37	1.43
30	I	102	LMT	O3B-C3B	-2.22	1.37	1.43
22	C	504	CLA	CMD-C2D	-2.22	1.46	1.51
22	B	610	CLA	C3B-C2B	-2.22	1.37	1.40
30	D	411	LMT	O2'-C2'	-2.22	1.37	1.43
30	B	627	LMT	O2B-C2B	-2.22	1.37	1.43
30	d	411	LMT	O3B-C3B	-2.21	1.37	1.43
29	b	602	SQD	O2-C2	-2.21	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.21	1.41	1.46
22	c	509	CLA	CMD-C2D	-2.21	1.46	1.51
30	b	603	LMT	O2'-C2'	-2.21	1.37	1.43
30	b	604	LMT	O2B-C2B	-2.20	1.37	1.43
30	d	411	LMT	O2'-C2'	-2.20	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	405	CLA	CMD-C2D	-2.20	1.46	1.51
30	D	411	LMT	O2B-C2B	-2.20	1.37	1.43
30	b	626	LMT	O3B-C3B	-2.20	1.37	1.43
30	B	624	LMT	O2'-C2'	-2.20	1.37	1.43
30	i	102	LMT	O3B-C3B	-2.20	1.37	1.43
23	A	406	PL9	C53-C6	-2.20	1.46	1.50
30	B	627	LMT	O3B-C3B	-2.19	1.37	1.43
30	B	628	LMT	O2'-C2'	-2.19	1.37	1.43
30	B	628	LMT	O2B-C2B	-2.19	1.37	1.43
29	B	626	SQD	O2-C2	-2.19	1.37	1.43
30	B	623	LMT	O2B-C2B	-2.18	1.37	1.43
30	d	411	LMT	O2B-C2B	-2.18	1.37	1.43
25	C	515	DGD	O1G-C1G	-2.17	1.40	1.45
22	C	509	CLA	CMD-C2D	-2.17	1.46	1.51
24	g	101	BCR	C33-C5	-2.17	1.47	1.50
22	b	611	CLA	CMD-C2D	-2.17	1.46	1.51
27	b	625	LMG	C4-C5	2.17	1.57	1.53
22	B	603	CLA	CMD-C2D	-2.16	1.46	1.51
30	b	604	LMT	O2'-C2'	-2.16	1.37	1.43
25	c	516	DGD	O2G-C2G	-2.16	1.41	1.46
25	B	625	DGD	C3G-C2G	2.15	1.57	1.50
23	D	407	PL9	C6-C1	-2.15	1.44	1.48
22	A	402	CLA	CMD-C2D	-2.15	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.15	1.46	1.51
26	a	411	LHG	O7-C5	-2.14	1.41	1.46
31	D	401	PHO	C4B-NB	2.14	1.41	1.36
31	D	402	PHO	C4B-NB	2.14	1.41	1.36
31	d	402	PHO	C4B-NB	2.14	1.41	1.36
22	A	404	CLA	CMD-C2D	-2.13	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.13	1.46	1.51
22	a	404	CLA	CMD-C2D	-2.13	1.46	1.51
25	C	516	DGD	O2G-C2G	-2.13	1.41	1.46
31	d	401	PHO	C4B-NB	2.12	1.41	1.36
25	b	601	DGD	C3G-C2G	2.12	1.57	1.50
29	A	413	SQD	O3-C3	-2.12	1.38	1.43
22	b	607	CLA	CMD-C2D	-2.12	1.46	1.51
25	d	410	DGD	C1D-C2D	2.12	1.58	1.52
25	b	601	DGD	C4D-C5D	2.12	1.57	1.53
22	b	619	CLA	CMD-C2D	-2.11	1.46	1.51
23	J	101	PL9	C3-C4	-2.11	1.46	1.49
30	b	627	LMT	O2B-C2B	-2.11	1.38	1.43
22	B	615	CLA	CMD-C2D	-2.11	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	B	624	LMT	O2B-C2B	-2.11	1.38	1.43
27	D	412	LMG	O7-C8	-2.11	1.41	1.46
22	d	405	CLA	CMD-C2D	-2.11	1.46	1.51
22	a	405	CLA	CMD-C2D	-2.10	1.46	1.51
25	B	620	DGD	O2G-C2G	-2.10	1.41	1.46
22	A	403	CLA	CMD-C2D	-2.10	1.46	1.51
22	B	602	CLA	CMD-C2D	-2.10	1.46	1.51
34	v	201	HEM	CAA-C2A	2.10	1.55	1.52
29	a	401	SQD	O3-C3	-2.10	1.38	1.43
30	M	103	LMT	O4'-C4B	-2.10	1.38	1.43
24	y	101	BCR	C33-C5	-2.09	1.47	1.50
22	C	508	CLA	CMD-C2D	-2.09	1.46	1.51
22	B	604	CLA	CMD-C2D	-2.09	1.46	1.51
22	H	101	CLA	CMD-C2D	-2.09	1.46	1.51
22	b	608	CLA	CMD-C2D	-2.09	1.46	1.51
27	d	412	LMG	O7-C8	-2.09	1.41	1.46
29	f	103	SQD	O3-C3	-2.08	1.38	1.43
29	A	412	SQD	O2-C2	-2.08	1.38	1.43
22	C	502	CLA	CMD-C2D	-2.08	1.46	1.51
30	M	102	LMT	O1'-C1'	-2.08	1.36	1.40
25	b	601	DGD	C1G-C2G	2.08	1.57	1.50
22	C	505	CLA	CMD-C2D	-2.08	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.08	1.46	1.51
23	j	101	PL9	C3-C4	-2.08	1.46	1.49
22	h	101	CLA	CMD-C2D	-2.08	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.07	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.07	1.46	1.51
29	a	415	SQD	O2-C2	-2.07	1.38	1.43
22	C	507	CLA	CMD-C2D	-2.07	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.07	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.07	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.07	1.46	1.51
29	b	602	SQD	O3-C3	-2.07	1.38	1.43
22	b	606	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.06	1.46	1.51
22	C	503	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.06	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.06	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.06	1.46	1.51
22	c	507	CLA	CMD-C2D	-2.06	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	CMD-C2D	-2.06	1.46	1.51
29	f	103	SQD	O2-C2	-2.06	1.38	1.43
30	B	628	LMT	O4'-C4B	-2.06	1.38	1.43
22	b	616	CLA	CMD-C2D	-2.06	1.46	1.51
22	c	503	CLA	CMD-C2D	-2.06	1.46	1.51
25	a	410	DGD	O1G-C1G	-2.06	1.40	1.45
29	F	103	SQD	O3-C3	-2.06	1.38	1.43
22	B	613	CLA	CMD-C2D	-2.06	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.06	1.46	1.51
27	D	408	LMG	O7-C8	-2.06	1.41	1.46
22	c	505	CLA	CMD-C2D	-2.06	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	618	CLA	CMD-C2D	-2.05	1.46	1.51
22	c	511	CLA	CMD-C2D	-2.05	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.05	1.46	1.51
30	M	102	LMT	O4'-C4B	-2.05	1.38	1.43
29	B	626	SQD	O3-C3	-2.05	1.38	1.43
29	d	403	SQD	O2-C2	-2.05	1.38	1.43
22	B	605	CLA	CMD-C2D	-2.04	1.46	1.51
31	D	402	PHO	C1B-C2B	2.04	1.50	1.45
23	A	406	PL9	C6-C1	-2.04	1.44	1.48
29	F	103	SQD	O2-C2	-2.04	1.38	1.43
30	d	411	LMT	O4'-C4B	-2.04	1.38	1.43
25	b	624	DGD	O2G-C2G	-2.04	1.41	1.46
22	a	407	CLA	CMD-C2D	-2.04	1.46	1.51
25	C	517	DGD	C1G-C2G	2.04	1.57	1.50
22	c	510	CLA	CMD-C2D	-2.04	1.46	1.51
22	d	406	CLA	CMD-C2D	-2.04	1.46	1.51
22	c	506	CLA	CMD-C2D	-2.04	1.46	1.51
29	d	403	SQD	O3-C3	-2.03	1.38	1.43
22	B	612	CLA	CMD-C2D	-2.03	1.46	1.51
22	b	619	CLA	CMC-C2C	-2.03	1.46	1.50
26	c	519	LHG	P-O6	2.03	1.67	1.59
30	b	603	LMT	O4'-C4B	-2.03	1.38	1.43
22	c	501	CLA	CMD-C2D	-2.03	1.46	1.51
29	B	622	SQD	O3-C3	-2.03	1.38	1.43
30	B	623	LMT	O4'-C4B	-2.03	1.38	1.43
29	B	622	SQD	O2-C2	-2.03	1.38	1.43
22	C	506	CLA	CMD-C2D	-2.03	1.46	1.51
25	c	517	DGD	C1G-C2G	2.03	1.56	1.50
22	b	613	CLA	CMD-C2D	-2.03	1.46	1.51
27	M	101	LMG	C4-C5	2.03	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	CMD-C2D	-2.03	1.46	1.51
27	A	414	LMG	C4-C5	2.02	1.57	1.53
27	a	412	LMG	C7-C8	2.02	1.56	1.50
30	B	627	LMT	O4'-C4B	-2.02	1.38	1.43
22	D	406	CLA	CMD-C2D	-2.02	1.46	1.51
30	D	411	LMT	O4'-C4B	-2.02	1.38	1.43
27	M	101	LMG	C7-C8	2.02	1.56	1.50
29	a	415	SQD	O3-C3	-2.02	1.38	1.43
26	C	519	LHG	O7-C5	-2.02	1.41	1.46
27	a	402	LMG	C4-C5	2.02	1.57	1.53
24	C	514	BCR	C38-C26	-2.02	1.47	1.50
30	I	102	LMT	O4'-C4B	-2.02	1.38	1.43
30	b	627	LMT	O4'-C4B	-2.02	1.38	1.43
22	B	615	CLA	CMC-C2C	-2.02	1.46	1.50
30	b	604	LMT	O4'-C4B	-2.02	1.38	1.43
31	D	402	PHO	CMC-C2C	-2.01	1.46	1.50
22	B	610	CLA	CMD-C2D	-2.01	1.46	1.51
29	A	413	SQD	O2-C2	-2.01	1.38	1.43
29	A	412	SQD	O3-C3	-2.01	1.38	1.43
22	c	512	CLA	CMD-C2D	-2.00	1.46	1.51
26	A	409	LHG	O7-C5	-2.00	1.41	1.46
22	C	501	CLA	CMD-C2D	-2.00	1.46	1.51
29	B	626	SQD	O4-C4	-2.00	1.38	1.43
27	m	101	LMG	C7-C8	2.00	1.56	1.50

All (1203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.32	110.00	106.71
22	B	611	CLA	C4A-NA-C1A	7.30	109.99	106.71
22	c	504	CLA	C4A-NA-C1A	7.22	109.95	106.71
22	B	603	CLA	C4A-NA-C1A	7.19	109.94	106.71
22	b	615	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	b	609	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	C	510	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	b	607	CLA	C4A-NA-C1A	6.99	109.85	106.71
22	C	501	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	A	403	CLA	C4A-NA-C1A	6.89	109.80	106.71
22	c	503	CLA	C4A-NA-C1A	6.87	109.80	106.71
22	a	405	CLA	C4A-NA-C1A	6.83	109.78	106.71
22	b	616	CLA	C4A-NA-C1A	6.83	109.78	106.71
22	C	520	CLA	C4A-NA-C1A	6.82	109.77	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	C4A-NA-C1A	6.82	109.77	106.71
22	B	605	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	b	618	CLA	C4A-NA-C1A	6.78	109.75	106.71
22	C	511	CLA	C4A-NA-C1A	6.76	109.75	106.71
22	b	608	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	606	CLA	C4A-NA-C1A	6.72	109.73	106.71
22	c	520	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	A	405	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	c	511	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	C	512	CLA	C4A-NA-C1A	6.67	109.70	106.71
22	B	615	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	B	614	CLA	C4A-NA-C1A	6.65	109.70	106.71
22	B	612	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	C	506	CLA	C4A-NA-C1A	6.63	109.69	106.71
22	c	506	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	b	617	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	C	505	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	a	406	CLA	C4A-NA-C1A	6.58	109.67	106.71
22	c	510	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	B	604	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	C	507	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	C	503	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	c	505	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	a	407	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	b	619	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	h	101	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	B	613	CLA	C4A-NA-C1A	6.47	109.62	106.71
22	B	607	CLA	C4A-NA-C1A	6.47	109.62	106.71
22	H	101	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	B	608	CLA	C4A-NA-C1A	6.46	109.61	106.71
22	B	609	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	b	610	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	A	404	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	c	507	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	c	508	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	c	502	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	c	512	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	B	602	CLA	C4A-NA-C1A	6.36	109.57	106.71
22	D	405	CLA	C4A-NA-C1A	6.36	109.56	106.71
22	d	406	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	b	611	CLA	C4A-NA-C1A	6.29	109.53	106.71
22	C	508	CLA	C4A-NA-C1A	6.26	109.52	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	C4A-NA-C1A	6.24	109.51	106.71
22	A	402	CLA	C4A-NA-C1A	6.21	109.50	106.71
22	C	509	CLA	C4A-NA-C1A	6.20	109.49	106.71
22	c	509	CLA	C4A-NA-C1A	6.19	109.49	106.71
22	D	406	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	b	613	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	B	601	CLA	C4A-NA-C1A	6.16	109.47	106.71
22	d	405	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	b	605	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	b	612	CLA	C4A-NA-C1A	6.09	109.45	106.71
22	a	404	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	b	606	CLA	C4A-NA-C1A	6.04	109.42	106.71
23	j	101	PL9	C7-C3-C4	5.69	121.50	116.88
29	a	415	SQD	O6-C1-C2	5.65	117.13	108.30
23	J	101	PL9	C7-C3-C4	5.59	121.42	116.88
22	b	614	CLA	C4A-NA-C1A	5.52	109.19	106.71
29	A	412	SQD	O6-C1-C2	5.51	116.91	108.30
23	A	406	PL9	C7-C3-C4	5.44	121.30	116.88
22	B	610	CLA	C4A-NA-C1A	5.42	109.14	106.71
29	b	602	SQD	O6-C1-C2	5.41	116.74	108.30
29	B	626	SQD	O6-C1-C2	5.27	116.53	108.30
23	d	407	PL9	C7-C3-C4	5.27	121.16	116.88
23	D	407	PL9	C7-C3-C4	5.22	121.12	116.88
23	a	408	PL9	C7-C3-C4	5.18	121.08	116.88
22	B	610	CLA	CMB-C2B-C1B	-5.16	120.54	128.46
22	b	614	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
29	A	412	SQD	O9-S-C6	5.03	112.92	106.94
29	a	415	SQD	O9-S-C6	4.94	112.81	106.94
25	A	408	DGD	O3G-C3G-C2G	-4.84	99.22	110.90
25	a	410	DGD	O3G-C3G-C2G	-4.74	99.46	110.90
29	d	403	SQD	O5-C5-C4	4.54	117.94	109.69
25	C	517	DGD	O3G-C3G-C2G	-4.46	100.13	110.90
29	B	622	SQD	O5-C5-C4	4.46	117.79	109.69
25	c	517	DGD	O3G-C3G-C2G	-4.26	100.61	110.90
29	f	103	SQD	O7-S-C6	4.25	111.99	106.94
22	c	507	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
29	F	103	SQD	O7-S-C6	4.22	111.95	106.94
26	c	519	LHG	O4-P-O5	4.21	133.05	112.24
26	C	519	LHG	O4-P-O5	4.21	133.04	112.24
26	a	411	LHG	O4-P-O5	4.20	133.03	112.24
26	A	409	LHG	O4-P-O5	4.18	132.89	112.24
29	d	403	SQD	O6-C1-C2	4.17	114.81	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	622	SQD	O6-C1-C2	4.16	114.79	108.30
22	C	507	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
22	b	616	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
29	a	401	SQD	O7-S-C6	4.10	111.81	106.94
22	B	612	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
29	A	413	SQD	O7-S-C6	4.07	111.78	106.94
29	b	602	SQD	O9-S-C6	4.05	111.76	106.94
29	B	626	SQD	O9-S-C6	4.05	111.75	106.94
24	J	102	BCR	C11-C10-C9	-3.93	121.71	127.31
29	A	413	SQD	O5-C5-C4	3.92	116.81	109.69
22	b	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
29	b	602	SQD	O7-S-C6	3.89	111.56	106.94
29	B	626	SQD	O5-C5-C4	3.87	116.72	109.69
27	D	409	LMG	C1-C2-C3	-3.86	101.95	110.00
29	a	401	SQD	O5-C5-C4	3.86	116.70	109.69
27	d	409	LMG	C1-C2-C3	-3.84	102.01	110.00
29	F	103	SQD	O9-S-O7	-3.82	100.74	113.95
29	b	602	SQD	O5-C5-C4	3.81	116.61	109.69
29	f	103	SQD	O9-S-O7	-3.80	100.78	113.95
22	B	607	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
29	A	412	SQD	O7-S-C6	3.78	111.44	106.94
24	C	513	BCR	C2-C1-C6	3.78	116.29	110.48
29	B	622	SQD	O7-S-C6	3.77	111.42	106.94
29	A	412	SQD	O9-S-O7	-3.77	100.90	113.95
29	a	415	SQD	O9-S-O7	-3.76	100.93	113.95
23	j	101	PL9	C7-C3-C2	-3.76	118.36	123.30
29	d	403	SQD	O9-S-O7	-3.75	100.97	113.95
25	c	516	DGD	O5D-C6D-C5D	-3.75	102.11	109.05
24	c	513	BCR	C2-C1-C6	3.75	116.25	110.48
29	B	626	SQD	O7-S-C6	3.74	111.39	106.94
24	j	102	BCR	C11-C10-C9	-3.74	121.97	127.31
22	c	510	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
29	a	415	SQD	O47-C7-C8	3.73	119.53	111.50
29	B	622	SQD	O9-S-O7	-3.72	101.06	113.95
29	a	401	SQD	O9-S-O7	-3.72	101.07	113.95
29	B	626	SQD	O9-S-O7	-3.72	101.08	113.95
29	d	403	SQD	O9-S-C6	3.72	111.36	106.94
23	J	101	PL9	C7-C3-C2	-3.71	118.42	123.30
29	a	415	SQD	O7-S-C6	3.71	111.35	106.94
29	b	602	SQD	O9-S-O7	-3.71	101.12	113.95
22	b	615	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
29	A	413	SQD	O9-S-O7	-3.70	101.13	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	415	SQD	O5-C5-C4	3.70	116.41	109.69
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	B	602	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	c	512	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	J	102	BCR	C2-C1-C6	3.67	116.13	110.48
22	C	505	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
24	j	102	BCR	C2-C1-C6	3.66	116.12	110.48
22	B	613	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
22	B	611	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
29	f	103	SQD	O5-C5-C4	3.66	116.33	109.69
22	b	613	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
29	A	412	SQD	O47-C7-C8	3.64	119.33	111.50
22	c	503	CLA	CMB-C2B-C1B	-3.64	122.88	128.46
22	A	405	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	C	510	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	c	506	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
29	F	103	SQD	O5-C5-C4	3.62	116.27	109.69
23	d	407	PL9	C7-C3-C2	-3.61	118.55	123.30
29	A	412	SQD	O5-C5-C4	3.60	116.23	109.69
22	a	404	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
25	d	410	DGD	O6D-C1D-O3G	-3.59	101.46	109.97
22	C	512	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
29	b	602	SQD	O47-C7-C8	3.59	119.24	111.50
29	B	626	SQD	O47-C7-C8	3.59	119.24	111.50
25	C	516	DGD	O5D-C6D-C5D	-3.59	102.40	109.05
22	c	511	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	a	407	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
29	B	622	SQD	O9-S-C6	3.58	111.19	106.94
22	C	502	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
25	D	410	DGD	O6D-C1D-O3G	-3.57	101.51	109.97
22	A	402	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
29	d	403	SQD	O7-S-C6	3.56	111.17	106.94
22	c	502	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
25	C	516	DGD	O3G-C3G-C2G	-3.53	102.37	110.90
22	D	405	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	c	516	DGD	O3G-C3G-C2G	-3.53	102.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	407	PL9	C7-C3-C2	-3.53	118.66	123.30
23	A	406	PL9	C7-C3-C2	-3.53	118.66	123.30
22	D	406	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	B	614	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
29	a	401	SQD	C44-O6-C1	3.50	120.57	113.74
22	C	509	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
22	b	605	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
22	c	520	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
22	a	405	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	F	103	SQD	O8-S-C6	3.47	111.27	105.74
22	c	509	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
29	d	403	SQD	O47-C7-C8	3.46	118.96	111.50
29	B	622	SQD	O47-C7-C8	3.46	118.96	111.50
22	B	601	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	B	605	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
22	C	520	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
23	a	408	PL9	C7-C3-C2	-3.43	118.78	123.30
29	f	103	SQD	O9-S-C6	3.43	111.02	106.94
22	b	618	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	d	406	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	B	612	CLA	CMB-C2B-C3B	3.43	131.09	124.68
29	F	103	SQD	O47-C7-C8	3.42	118.88	111.50
22	A	403	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	b	616	CLA	CMB-C2B-C3B	3.42	131.07	124.68
22	b	607	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
29	a	401	SQD	O9-S-C6	3.40	110.98	106.94
22	C	508	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
22	A	404	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
29	A	413	SQD	O9-S-C6	3.38	110.96	106.94
22	b	608	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
22	c	507	CLA	CMB-C2B-C3B	3.37	130.99	124.68
22	H	101	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
25	B	620	DGD	O3G-C3G-C2G	-3.36	102.78	110.90
29	f	103	SQD	O8-S-C6	3.35	111.08	105.74
29	f	103	SQD	O47-C7-C8	3.34	118.71	111.50
29	A	413	SQD	O47-C7-C8	3.34	118.70	111.50
22	h	101	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	b	610	CLA	CMB-C2B-C1B	-3.34	123.33	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
29	F	103	SQD	O9-S-C6	3.32	110.89	106.94
25	C	515	DGD	O3G-C3G-C2G	-3.32	102.89	110.90
29	F	103	SQD	O6-C1-C2	3.32	113.48	108.30
22	B	615	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.30	102.93	110.90
22	b	619	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
22	a	406	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
25	b	624	DGD	O3G-C3G-C2G	-3.28	102.98	110.90
24	A	407	BCR	C2-C1-C6	3.28	115.53	110.48
29	d	403	SQD	O8-S-C6	3.28	110.96	105.74
22	b	611	CLA	CMB-C2B-C3B	3.24	130.73	124.68
22	B	605	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
22	C	507	CLA	CMB-C2B-C3B	3.22	130.70	124.68
24	b	622	BCR	C24-C23-C22	-3.21	121.38	126.23
24	j	102	BCR	C24-C23-C22	-3.21	121.38	126.23
29	a	401	SQD	O47-C7-C8	3.21	118.42	111.50
22	B	606	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
22	B	603	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	b	609	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	610	CLA	CMB-C2B-C3B	3.19	130.65	124.68
22	B	602	CLA	CMB-C2B-C3B	3.19	130.65	124.68
22	b	606	CLA	CMB-C2B-C3B	3.18	130.63	124.68
22	b	612	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
22	B	608	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
29	A	413	SQD	C44-O6-C1	3.17	119.94	113.74
22	B	613	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
24	J	102	BCR	C24-C23-C22	-3.17	121.44	126.23
25	d	410	DGD	O3G-C3G-C2G	-3.16	103.28	110.90
24	a	409	BCR	C2-C1-C6	3.16	115.34	110.48
22	B	607	CLA	CMB-C2B-C3B	3.16	130.59	124.68
22	C	506	CLA	CMB-C2B-C3B	3.15	130.57	124.68
22	c	506	CLA	CMB-C2B-C3B	3.14	130.56	124.68
29	B	626	SQD	C3-C4-C5	3.14	115.85	110.24
22	B	613	CLA	CMB-C2B-C3B	3.14	130.55	124.68
29	B	622	SQD	O8-S-C6	3.14	110.74	105.74
25	b	624	DGD	O6D-C1D-O3G	-3.14	102.54	109.97
22	c	503	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
24	B	617	BCR	C15-C16-C17	-3.13	117.07	123.47
25	B	620	DGD	O6D-C1D-O3G	-3.12	102.58	109.97
22	b	617	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
29	f	103	SQD	O6-C1-C2	3.12	113.17	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	618	BCR	C2-C1-C6	3.12	115.28	110.48
22	b	606	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
22	c	510	CLA	CMB-C2B-C3B	3.11	130.50	124.68
30	B	628	LMT	C1'-O5'-C5'	-3.11	107.59	113.69
29	b	602	SQD	C3-C4-C5	3.11	115.78	110.24
24	J	102	BCR	C3-C4-C5	-3.10	108.53	114.08
25	c	516	DGD	O6D-C1D-O3G	-3.10	102.62	109.97
22	C	505	CLA	CMB-C2B-C3B	3.09	130.47	124.68
25	D	410	DGD	O3G-C3G-C2G	-3.09	103.44	110.90
22	b	617	CLA	CMB-C2B-C3B	3.09	130.46	124.68
22	c	507	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
22	a	407	CLA	CMB-C2B-C3B	3.08	130.44	124.68
22	b	614	CLA	CMB-C2B-C3B	3.08	130.44	124.68
22	b	615	CLA	CMB-C2B-C3B	3.07	130.43	124.68
22	b	607	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
22	C	505	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
24	b	622	BCR	C2-C1-C6	3.06	115.20	110.48
22	c	512	CLA	CMB-C2B-C3B	3.06	130.41	124.68
22	C	503	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
24	b	621	BCR	C15-C16-C17	-3.06	117.21	123.47
22	c	504	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	b	613	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	B	608	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	b	610	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	C	510	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	C	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
25	A	408	DGD	O6D-C1D-O3G	-3.05	102.75	109.97
22	C	502	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	j	102	BCR	C3-C4-C5	-3.05	108.63	114.08
22	c	505	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	j	102	BCR	C7-C8-C9	-3.05	121.63	126.23
22	c	504	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
22	B	606	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	C	516	DGD	O6D-C1D-O3G	-3.04	102.79	109.97
30	b	604	LMT	C1'-O5'-C5'	-3.03	107.73	113.69
22	C	504	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	b	605	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	A	405	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	C	503	CLA	CMB-C2B-C3B	3.03	130.34	124.68
22	B	611	CLA	CMB-C2B-C3B	3.02	130.34	124.68
24	J	102	BCR	C7-C8-C9	-3.02	121.67	126.23
24	B	617	BCR	C33-C5-C6	-3.02	121.14	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	621	BCR	C33-C5-C6	-3.01	121.15	124.53
22	C	512	CLA	CMB-C2B-C3B	3.01	130.30	124.68
22	c	511	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	c	503	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	B	609	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	D	405	CLA	CMB-C2B-C3B	2.99	130.26	124.68
22	b	611	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	b	608	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
22	D	406	CLA	CMB-C2B-C3B	2.97	130.24	124.68
22	c	502	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	C	502	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	B	602	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	C	511	CLA	CMB-C2B-C3B	2.96	130.21	124.68
22	B	604	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
29	d	403	SQD	C3-C4-C5	2.95	115.51	110.24
22	b	612	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	a	406	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	c	505	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
22	C	507	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
25	B	625	DGD	O5D-C1E-C2E	2.94	112.90	108.30
27	d	408	LMG	O6-C1-O1	-2.94	103.00	109.97
29	a	401	SQD	O8-S-C6	2.94	110.43	105.74
24	F	102	BCR	C33-C5-C6	-2.94	121.22	124.53
22	C	506	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	H	102	BCR	C33-C5-C6	-2.94	121.23	124.53
29	B	626	SQD	O8-S-C6	2.94	110.42	105.74
22	a	404	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
25	c	515	DGD	O6D-C1D-O3G	-2.93	103.04	109.97
24	c	521	BCR	C2-C1-C6	2.93	114.99	110.48
24	J	102	BCR	C27-C26-C25	2.93	126.98	122.73
22	B	604	CLA	CMB-C2B-C3B	2.93	130.15	124.68
22	d	405	CLA	CMB-C2B-C3B	2.92	130.15	124.68
22	B	607	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	a	410	DGD	O6D-C1D-O3G	-2.92	103.06	109.97
22	c	520	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
22	C	501	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
22	c	511	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
22	c	501	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
22	C	510	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	d	406	CLA	CMB-C2B-C3B	2.91	130.12	124.68
22	c	501	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
22	d	406	CLA	O2D-CGD-O1D	-2.91	118.15	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
22	c	506	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
24	x	101	BCR	C33-C5-C6	-2.90	121.27	124.53
24	f	102	BCR	C33-C5-C6	-2.90	121.27	124.53
22	B	605	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	A	402	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	c	512	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	A	403	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	c	510	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
25	c	517	DGD	CDB-CCB-CBB	-2.90	99.70	114.42
25	C	517	DGD	CDB-CCB-CBB	-2.90	99.70	114.42
22	b	608	CLA	CMB-C2B-C3B	2.90	130.10	124.68
22	b	613	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	J	102	BCR	C35-C13-C14	-2.89	118.87	122.92
22	B	601	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
30	B	624	LMT	C3'-C4'-C5'	-2.88	104.31	110.93
22	H	101	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
29	A	412	SQD	C3-C4-C5	2.88	115.38	110.24
25	C	515	DGD	O6D-C1D-O3G	-2.88	103.16	109.97
22	B	614	CLA	CMB-C2B-C3B	2.87	130.05	124.68
25	c	517	DGD	C1D-C2D-C3D	-2.87	104.01	110.00
22	B	609	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	A	413	SQD	O8-S-C6	2.87	110.31	105.74
22	B	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	d	407	PL9	C40-C39-C41	2.86	120.08	115.27
22	b	618	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	j	102	BCR	C27-C26-C25	2.86	126.88	122.73
22	c	502	CLA	O2D-CGD-O1D	-2.86	118.26	123.84
22	b	618	CLA	CMB-C2B-C3B	2.85	130.02	124.68
30	I	102	LMT	O1'-C1'-C2'	2.85	112.76	108.30
22	b	607	CLA	CMB-C2B-C3B	2.85	130.01	124.68
29	b	602	SQD	O8-S-C6	2.85	110.28	105.74
22	B	614	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
25	c	516	DGD	CDB-CCB-CBB	-2.85	99.97	114.42
24	B	619	BCR	C2-C1-C6	2.85	114.86	110.48
24	b	623	BCR	C2-C1-C6	2.84	114.86	110.48
22	C	520	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
22	C	520	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	H	101	CLA	CMB-C2B-C3B	2.84	129.99	124.68
29	a	415	SQD	C3-C4-C5	2.83	115.30	110.24
29	B	622	SQD	C3-C4-C5	2.83	115.29	110.24
22	D	406	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	CMB-C2B-C3B	2.83	129.97	124.68
25	C	517	DGD	O5D-C6D-C5D	-2.82	103.82	109.05
22	C	509	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	h	101	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	d	405	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	B	625	DGD	C1D-C2D-C3D	-2.82	104.12	110.00
25	C	516	DGD	CDB-CCB-CBB	-2.82	100.10	114.42
25	c	517	DGD	O5D-C6D-C5D	-2.82	103.83	109.05
22	C	501	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
22	C	509	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	A	404	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
31	D	402	PHO	O2D-CGD-O1D	-2.81	118.34	123.84
25	C	517	DGD	C1D-C2D-C3D	-2.81	104.14	110.00
22	A	403	CLA	CMB-C2B-C3B	2.81	129.94	124.68
24	f	102	BCR	C29-C30-C25	2.81	114.80	110.48
27	D	408	LMG	O6-C1-O1	-2.81	103.33	109.97
22	a	405	CLA	CMB-C2B-C3B	2.81	129.93	124.68
22	b	609	CLA	CMB-C2B-C3B	2.81	129.93	124.68
30	i	102	LMT	O1'-C1'-C2'	2.80	112.68	108.30
22	c	520	CLA	CMB-C2B-C3B	2.80	129.92	124.68
30	b	627	LMT	C3'-C4'-C5'	-2.80	104.50	110.93
22	c	509	CLA	CMB-C2B-C3B	2.80	129.92	124.68
25	b	601	DGD	O5D-C1E-C2E	2.80	112.67	108.30
22	A	404	CLA	CMB-C2B-C3B	2.79	129.91	124.68
23	D	407	PL9	C40-C39-C41	2.79	119.97	115.27
24	K	102	BCR	C15-C16-C17	-2.79	117.75	123.47
24	c	521	BCR	C15-C16-C17	-2.79	117.76	123.47
22	B	603	CLA	CMB-C2B-C3B	2.79	129.89	124.68
24	j	102	BCR	C35-C13-C14	-2.79	119.02	122.92
22	b	614	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
22	h	101	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
25	D	410	DGD	CDB-CCB-CBB	-2.78	100.31	114.42
25	b	601	DGD	O3G-C3G-C2G	-2.78	104.20	110.90
22	b	605	CLA	CMB-C2B-C3B	2.77	129.87	124.68
24	b	621	BCR	C15-C14-C13	-2.77	123.36	127.31
29	d	403	SQD	C44-O6-C1	2.77	119.15	113.74
22	C	512	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	y	101	BCR	C27-C26-C25	2.77	126.75	122.73
24	C	514	BCR	C15-C16-C17	-2.77	117.81	123.47
24	K	102	BCR	C2-C1-C6	2.77	114.74	110.48
25	d	410	DGD	CDB-CCB-CBB	-2.76	100.39	114.42
26	A	409	LHG	O8-C23-C24	2.76	120.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	CMD-C2D-C3D	2.76	129.84	124.68
22	B	610	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
22	b	612	CLA	CMB-C2B-C3B	2.76	129.83	124.68
22	C	511	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
25	b	601	DGD	C3G-C2G-C1G	-2.75	105.27	111.79
25	b	601	DGD	C1D-C2D-C3D	-2.75	104.26	110.00
22	b	614	CLA	CMD-C2D-C3D	2.75	129.83	124.68
22	a	404	CLA	CMB-C2B-C3B	2.75	129.83	124.68
22	c	509	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	a	415	SQD	O8-S-C6	2.75	110.12	105.74
22	a	405	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
23	d	407	PL9	C7-C8-C9	-2.74	122.22	126.79
24	B	619	BCR	C3-C4-C5	-2.74	109.18	114.08
22	B	608	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	j	102	BCR	C15-C14-C13	-2.74	123.40	127.31
22	C	504	CLA	CMD-C2D-C3D	2.74	129.81	124.68
22	C	511	CLA	CMD-C2D-C3D	2.74	129.81	124.68
23	A	406	PL9	C22-C23-C24	-2.74	121.07	127.66
31	D	401	PHO	O2D-CGD-O1D	-2.74	118.49	123.84
23	J	101	PL9	C7-C8-C9	-2.73	122.25	126.79
22	B	601	CLA	CMB-C2B-C3B	2.73	129.78	124.68
29	f	103	SQD	C44-O6-C1	2.73	119.07	113.74
22	a	406	CLA	CMB-C2B-C3B	2.73	129.78	124.68
24	g	101	BCR	C27-C26-C25	2.73	126.69	122.73
24	b	623	BCR	C3-C4-C5	-2.73	109.21	114.08
26	a	411	LHG	O8-C23-C24	2.73	120.46	111.91
22	B	606	CLA	CMB-C2B-C3B	2.73	129.78	124.68
22	C	508	CLA	CMB-C2B-C3B	2.72	129.78	124.68
22	A	402	CLA	CMB-C2B-C3B	2.72	129.76	124.68
31	d	401	PHO	O2D-CGD-O1D	-2.72	118.53	123.84
24	B	617	BCR	C28-C27-C26	-2.71	109.23	114.08
24	c	513	BCR	C11-C10-C9	-2.71	123.44	127.31
23	a	408	PL9	C22-C23-C24	-2.71	121.13	127.66
24	B	618	BCR	C24-C23-C22	-2.71	122.14	126.23
23	j	101	PL9	C7-C8-C9	-2.71	122.28	126.79
29	A	412	SQD	O8-S-C6	2.71	110.06	105.74
22	a	407	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
25	B	625	DGD	O3G-C3G-C2G	-2.70	104.37	110.90
25	B	625	DGD	C3G-C2G-C1G	-2.70	105.39	111.79
22	c	508	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	B	618	BCR	C29-C30-C25	2.70	114.64	110.48
24	F	102	BCR	C29-C30-C25	2.70	114.64	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	b	621	BCR	C28-C27-C26	-2.69	109.27	114.08
24	J	102	BCR	C15-C14-C13	-2.69	123.47	127.31
27	C	518	LMG	O6-C1-O1	-2.69	103.61	109.97
22	B	603	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	B	615	CLA	CMB-C2B-C3B	2.69	129.71	124.68
22	b	619	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	b	619	CLA	CMB-C2B-C3B	2.68	129.70	124.68
22	A	405	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
24	y	101	BCR	C38-C26-C25	-2.68	121.52	124.53
29	B	622	SQD	C44-O6-C1	2.68	118.97	113.74
24	y	101	BCR	C7-C8-C9	-2.68	122.19	126.23
22	C	504	CLA	CMB-C2B-C3B	2.68	129.69	124.68
23	D	407	PL9	C7-C8-C9	-2.67	122.34	126.79
22	B	611	CLA	CMD-C2D-C3D	2.67	129.68	124.68
27	i	101	LMG	O6-C1-O1	-2.67	103.65	109.97
22	b	615	CLA	CMD-C2D-C3D	2.67	129.67	124.68
29	b	602	SQD	C4-C3-C2	2.66	115.47	110.82
24	g	101	BCR	C38-C26-C25	-2.66	121.54	124.53
25	A	408	DGD	O5D-C6D-C5D	-2.66	104.12	109.05
24	c	514	BCR	C11-C10-C9	-2.66	123.51	127.31
22	a	405	CLA	CHB-C4A-NA	2.66	128.19	124.51
22	B	610	CLA	CMD-C2D-C3D	2.66	129.65	124.68
22	c	508	CLA	O2D-CGD-O1D	-2.66	118.65	123.84
22	b	607	CLA	CHB-C4A-NA	2.66	128.18	124.51
23	D	407	PL9	C22-C23-C24	-2.65	121.27	127.66
22	c	502	CLA	CMD-C2D-C3D	2.65	129.64	124.68
22	D	405	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
34	f	101	HEM	CBD-CAD-C3D	-2.65	107.60	112.48
27	I	101	LMG	O6-C1-O1	-2.65	103.71	109.97
31	d	402	PHO	O2D-CGD-O1D	-2.64	118.68	123.84
24	B	618	BCR	C11-C10-C9	-2.63	123.55	127.31
24	C	513	BCR	C15-C16-C17	-2.63	118.08	123.47
23	a	408	PL9	C7-C8-C9	-2.63	122.41	126.79
22	b	608	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	C	506	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	b	620	BCR	C33-C5-C6	-2.62	121.58	124.53
22	C	510	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	C	505	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	c	514	BCR	C28-C27-C26	-2.62	109.41	114.08
22	d	405	CLA	CMD-C2D-C3D	2.61	129.57	124.68
24	B	616	BCR	C33-C5-C6	-2.61	121.59	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	520	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	c	504	CLA	CMB-C2B-C3B	2.61	129.57	124.68
27	c	518	LMG	O6-C1-O1	-2.61	103.79	109.97
24	g	101	BCR	C7-C8-C9	-2.61	122.29	126.23
22	c	506	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	b	622	BCR	C29-C30-C25	2.61	114.49	110.48
22	B	615	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
22	C	504	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	b	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	a	407	CLA	CMD-C2D-C3D	2.61	129.55	124.68
22	c	504	CLA	CMD-C2D-C3D	2.60	129.55	124.68
22	c	507	CLA	CMD-C2D-C3D	2.60	129.54	124.68
30	M	102	LMT	C1'-O5'-C5'	-2.60	108.59	113.69
26	C	519	LHG	O8-C23-C24	2.59	120.04	111.91
23	a	408	PL9	C41-C39-C40	2.59	120.33	114.60
22	B	603	CLA	C1-C2-C3	-2.59	121.56	126.04
22	b	607	CLA	C1-C2-C3	-2.59	121.56	126.04
22	D	405	CLA	CMD-C2D-C3D	2.59	129.52	124.68
24	c	514	BCR	C15-C16-C17	-2.59	118.17	123.47
25	C	517	DGD	C1D-O6D-C5D	-2.59	108.61	113.69
26	c	519	LHG	O8-C23-C24	2.59	120.03	111.91
24	C	514	BCR	C28-C27-C26	-2.59	109.46	114.08
24	B	618	BCR	C15-C16-C17	-2.59	118.17	123.47
24	B	618	BCR	C15-C14-C13	-2.59	123.62	127.31
22	B	608	CLA	CMD-C2D-C3D	2.58	129.51	124.68
25	c	517	DGD	C1D-O6D-C5D	-2.58	108.62	113.69
24	C	513	BCR	C24-C23-C22	-2.58	122.34	126.23
23	J	101	PL9	C22-C23-C24	-2.58	121.45	127.66
31	D	402	PHO	CBD-CHA-C4D	-2.58	105.64	108.54
22	c	511	CLA	CHB-C4A-NA	2.58	128.07	124.51
27	a	402	LMG	O6-C1-O1	-2.57	103.88	109.97
31	D	401	PHO	CBD-CHA-C4D	-2.57	105.64	108.54
24	g	101	BCR	C33-C5-C6	-2.57	121.64	124.53
22	c	520	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	a	406	CLA	CHB-C4A-NA	2.57	128.07	124.51
22	b	617	CLA	CMD-C2D-C3D	2.57	129.49	124.68
22	b	615	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
30	B	623	LMT	C1'-O5'-C5'	-2.57	108.65	113.69
31	d	401	PHO	CBD-CHA-C4D	-2.56	105.65	108.54
22	B	605	CLA	CHB-C4A-NA	2.56	128.06	124.51
29	B	626	SQD	C4-C3-C2	2.56	115.30	110.82
23	d	407	PL9	C22-C23-C24	-2.56	121.49	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	CMD-C2D-C3D	2.56	129.46	124.68
27	M	101	LMG	C1-C2-C3	-2.56	104.67	110.00
24	C	514	BCR	C11-C10-C9	-2.56	123.66	127.31
22	C	512	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	612	CLA	CMD-C2D-C3D	2.55	129.46	124.68
24	J	102	BCR	C38-C26-C25	-2.55	121.66	124.53
22	c	505	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	508	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	C	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	B	608	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	C	511	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	D	410	DGD	CFB-CEB-CDB	-2.55	101.50	114.42
31	d	402	PHO	CBD-CHA-C4D	-2.54	105.67	108.54
23	j	101	PL9	C22-C23-C24	-2.54	121.54	127.66
34	F	101	HEM	C1D-C2D-C3D	-2.54	105.23	107.00
22	B	611	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	b	615	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	b	618	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	c	521	BCR	C15-C14-C13	-2.53	123.69	127.31
24	B	617	BCR	C15-C14-C13	-2.53	123.70	127.31
24	C	514	BCR	C15-C14-C13	-2.53	123.70	127.31
24	b	622	BCR	C11-C10-C9	-2.53	123.70	127.31
22	c	504	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	b	611	CLA	CMD-C2D-C3D	2.53	129.41	124.68
22	B	607	CLA	CMD-C2D-C3D	2.52	129.40	124.68
23	A	406	PL9	C7-C8-C9	-2.52	122.59	126.79
22	a	407	CLA	CHB-C4A-NA	2.52	128.00	124.51
24	b	622	BCR	C15-C16-C17	-2.52	118.31	123.47
24	C	513	BCR	C15-C14-C13	-2.52	123.71	127.31
24	B	619	BCR	C7-C8-C9	-2.52	122.42	126.23
24	j	102	BCR	C15-C16-C17	-2.52	118.31	123.47
22	B	604	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	C	508	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
22	C	506	CLA	CMD-C2D-C3D	2.52	129.39	124.68
22	c	510	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	h	101	CLA	CMD-C2D-C3D	2.51	129.38	124.68
34	f	101	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
22	B	601	CLA	CMD-C2D-C3D	2.51	129.37	124.68
29	F	103	SQD	C44-O6-C1	2.51	118.64	113.74
22	B	602	CLA	CMD-C2D-C3D	2.51	129.37	124.68
22	c	501	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	A	406	PL9	C41-C39-C40	2.51	120.14	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	BCR	C15-C16-C17	-2.51	118.34	123.47
24	j	102	BCR	C38-C26-C25	-2.51	121.72	124.53
24	y	101	BCR	C33-C5-C6	-2.51	121.72	124.53
24	C	514	BCR	C29-C30-C25	2.50	114.34	110.48
22	B	603	CLA	CMD-C2D-C3D	2.50	129.36	124.68
22	A	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	d	410	DGD	CFB-CEB-CDB	-2.50	101.72	114.42
27	A	414	LMG	O6-C1-O1	-2.50	104.05	109.97
22	a	407	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
22	B	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	512	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	a	410	DGD	O5D-C6D-C5D	-2.50	104.42	109.05
22	D	406	CLA	CMD-C2D-C3D	2.50	129.35	124.68
27	B	621	LMG	C1-C2-C3	-2.50	104.79	110.00
22	B	609	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	B	612	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	501	CLA	CMB-C2B-C3B	2.49	129.35	124.68
22	b	605	CLA	CMD-C2D-C3D	2.49	129.34	124.68
27	d	412	LMG	C38-C37-C36	-2.49	101.77	114.42
22	B	611	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
22	B	606	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	C	508	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	505	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
24	b	623	BCR	C7-C8-C9	-2.49	122.47	126.23
22	b	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	d	409	LMG	C38-C37-C36	-2.49	101.81	114.42
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
22	b	616	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	c	514	BCR	C29-C30-C25	2.48	114.30	110.48
30	b	626	LMT	C1'-O5'-C5'	-2.48	108.82	113.69
27	D	412	LMG	C38-C37-C36	-2.48	101.83	114.42
25	a	410	DGD	CBB-CAB-C9B	-2.48	101.83	114.42
22	B	607	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	C	514	BCR	C33-C5-C6	-2.48	121.74	124.53
22	d	406	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	M	103	LMT	C1'-O5'-C5'	-2.47	108.83	113.69
27	A	410	LMG	C40-C39-C38	-2.47	101.86	114.42
22	B	613	CLA	CMD-C2D-C3D	2.47	129.31	124.68
22	a	404	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	a	408	PL9	C20-C19-C21	2.47	119.42	115.27
22	d	406	CLA	CMD-C2D-C3D	2.47	129.30	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	DGD	CBB-CAB-C9B	-2.47	101.89	114.42
22	C	501	CLA	CMD-C2D-C3D	2.47	129.29	124.68
22	A	405	CLA	CMD-C2D-C3D	2.47	129.29	124.68
22	b	606	CLA	CMD-C2D-C3D	2.46	129.28	124.68
30	M	102	LMT	C3'-C4'-C5'	-2.46	105.28	110.93
24	c	514	BCR	C33-C5-C6	-2.46	121.77	124.53
24	K	102	BCR	C24-C23-C22	-2.46	122.52	126.23
24	c	521	BCR	C27-C26-C25	2.46	126.30	122.73
22	C	504	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	b	613	CLA	CMD-C2D-C3D	2.46	129.27	124.68
22	b	610	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
25	d	410	DGD	C3G-C2G-C1G	-2.45	105.99	111.79
31	d	402	PHO	O1D-CGD-CBD	2.45	129.50	124.48
24	y	101	BCR	C1-C6-C5	-2.45	119.16	122.61
22	A	402	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	c	519	LHG	C11-C10-C9	-2.45	101.99	114.42
22	D	406	CLA	CHB-C4A-NA	2.45	127.90	124.51
31	D	402	PHO	O1D-CGD-CBD	2.45	129.49	124.48
24	c	513	BCR	C15-C14-C13	-2.45	123.82	127.31
22	B	613	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	b	617	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	C	503	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	c	502	CLA	CHB-C4A-NA	2.45	127.89	124.51
24	K	102	BCR	C27-C26-C25	2.44	126.28	122.73
22	A	405	CLA	CHB-C4A-NA	2.44	127.89	124.51
22	c	506	CLA	CMD-C2D-C3D	2.44	129.24	124.68
22	h	101	CLA	CHB-C4A-NA	2.43	127.88	124.51
24	b	623	BCR	C11-C10-C9	-2.43	123.84	127.31
24	b	622	BCR	C15-C14-C13	-2.43	123.84	127.31
30	M	103	LMT	C3'-C4'-C5'	-2.43	105.35	110.93
22	c	505	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
24	K	102	BCR	C15-C14-C13	-2.43	123.84	127.31
30	D	411	LMT	C1'-O5'-C5'	-2.43	108.92	113.69
27	D	409	LMG	C38-C37-C36	-2.43	102.10	114.42
27	d	408	LMG	C38-C37-C36	-2.43	102.10	114.42
25	B	620	DGD	CBB-CAB-C9B	-2.43	102.10	114.42
22	b	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	c	501	CLA	CMD-C2D-C3D	2.43	129.22	124.68
22	B	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	D	407	PL9	C20-C19-C21	2.43	119.35	115.27
22	B	612	CLA	CMD-C2D-C3D	2.42	129.22	124.68
22	A	403	CLA	C1B-CHB-C4A	-2.42	125.31	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	624	DGD	CBB-CAB-C9B	-2.42	102.13	114.42
22	a	405	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	J	101	PL9	C20-C19-C21	2.42	119.34	115.27
22	b	606	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
26	C	519	LHG	C11-C10-C9	-2.42	102.14	114.42
22	c	507	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	a	412	LMG	C40-C39-C38	-2.42	102.15	114.42
24	b	621	BCR	C35-C13-C14	-2.41	119.54	122.92
24	b	620	BCR	C11-C10-C9	-2.41	123.86	127.31
27	C	521	LMG	C40-C39-C38	-2.41	102.19	114.42
22	B	608	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
25	C	517	DGD	CFB-CEB-CDB	-2.41	102.19	114.42
24	b	620	BCR	C2-C1-C6	2.41	114.19	110.48
25	c	516	DGD	O6E-C1E-O5D	-2.41	104.27	109.97
22	H	101	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	b	607	CLA	CMD-C2D-C3D	2.41	129.18	124.68
22	C	507	CLA	CMD-C2D-C3D	2.41	129.18	124.68
22	C	503	CLA	CMD-C2D-C3D	2.41	129.18	124.68
23	d	407	PL9	C20-C19-C21	2.41	119.32	115.27
25	c	517	DGD	CFB-CEB-CDB	-2.41	102.21	114.42
31	d	401	PHO	O1D-CGD-CBD	2.41	129.41	124.48
22	b	608	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
22	c	505	CLA	CMD-C2D-C3D	2.40	129.18	124.68
22	d	406	CLA	C1-C2-C3	-2.40	121.89	126.04
22	b	618	CLA	CMD-C2D-C3D	2.40	129.17	124.68
22	b	612	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	C	510	CLA	CMD-C2D-C3D	2.40	129.17	124.68
22	C	502	CLA	CHB-C4A-NA	2.40	127.83	124.51
22	b	612	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
29	A	412	SQD	O48-C23-C24	2.40	119.44	111.91
25	C	516	DGD	O6E-C1E-O5D	-2.40	104.29	109.97
22	C	511	CLA	O2A-CGA-O1A	-2.40	117.55	123.59
24	A	407	BCR	C27-C26-C25	2.40	126.21	122.73
22	c	509	CLA	CHB-C4A-NA	2.40	127.82	124.51
22	A	404	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	C	501	CLA	CMB-C2B-C3B	2.39	129.16	124.68
27	c	522	LMG	C40-C39-C38	-2.39	102.28	114.42
22	B	602	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
24	c	513	BCR	C7-C8-C9	-2.39	122.62	126.23
24	B	616	BCR	C11-C10-C9	-2.39	123.90	127.31
22	b	606	CLA	CHB-C4A-NA	2.39	127.82	124.51
27	E	101	LMG	O6-C1-O1	-2.39	104.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	E	101	LMG	C1-C2-C3	-2.39	105.02	110.00
22	H	101	CLA	CMD-C2D-C3D	2.39	129.15	124.68
24	b	621	BCR	C29-C30-C25	2.39	114.16	110.48
22	A	405	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
24	B	617	BCR	C29-C30-C25	2.39	114.15	110.48
22	a	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	c	516	DGD	CFB-CEB-CDB	-2.39	102.32	114.42
22	C	509	CLA	CHB-C4A-NA	2.38	127.81	124.51
22	C	507	CLA	CHB-C4A-NA	2.38	127.81	124.51
27	b	625	LMG	C1-C2-C3	-2.38	105.03	110.00
22	b	613	CLA	CHB-C4A-NA	2.38	127.81	124.51
27	c	522	LMG	O6-C1-O1	-2.38	104.33	109.97
22	a	406	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	D	408	LMG	C38-C37-C36	-2.38	102.34	114.42
34	f	101	HEM	CAA-CBA-CGA	-2.38	108.68	112.67
31	D	401	PHO	O1D-CGD-CBD	2.38	129.35	124.48
29	a	415	SQD	C4-C3-C2	2.38	114.97	110.82
24	b	623	BCR	C27-C26-C25	2.38	126.18	122.73
24	g	101	BCR	C1-C6-C5	-2.37	119.27	122.61
24	a	409	BCR	C27-C26-C25	2.37	126.18	122.73
24	c	514	BCR	C15-C14-C13	-2.37	123.92	127.31
23	D	407	PL9	C27-C28-C29	-2.37	121.95	127.66
22	A	402	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	C	506	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	c	507	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	b	603	LMT	C1'-O5'-C5'	-2.37	109.04	113.69
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	b	611	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
22	C	520	CLA	CMD-C2D-C3D	2.37	129.11	124.68
22	B	614	CLA	CMD-C2D-C3D	2.37	129.11	124.68
27	B	621	LMG	O6-C1-O1	-2.37	104.37	109.97
24	B	619	BCR	C27-C26-C25	2.37	126.17	122.73
27	A	410	LMG	C38-C37-C36	-2.37	102.42	114.42
22	C	520	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
29	B	622	SQD	O48-C23-C24	2.36	119.33	111.91
22	C	512	CLA	CMD-C2D-C3D	2.36	129.10	124.68
22	H	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	h	101	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
34	v	201	HEM	C1D-C2D-C3D	-2.36	105.36	107.00
22	B	615	CLA	CHB-C4A-NA	2.36	127.77	124.51
34	V	201	HEM	C1D-C2D-C3D	-2.36	105.36	107.00
22	b	614	CLA	C1-C2-C3	-2.35	121.97	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	401	SQD	O48-C23-C24	2.35	119.30	111.91
25	c	515	DGD	C3G-C2G-C1G	-2.35	106.22	111.79
27	A	410	LMG	O3-C3-C2	-2.35	104.91	110.35
27	C	518	LMG	C38-C37-C36	-2.35	102.49	114.42
25	c	516	DGD	C3G-C2G-C1G	-2.35	106.23	111.79
30	d	411	LMT	C3'-C4'-C5'	-2.35	105.54	110.93
24	a	409	BCR	C15-C16-C17	-2.35	118.67	123.47
22	b	616	CLA	CMD-C2D-C3D	2.34	129.06	124.68
22	d	406	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	B	603	CLA	O1D-CGD-CBD	2.34	129.28	124.48
22	B	613	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
25	C	515	DGD	C3G-C2G-C1G	-2.34	106.25	111.79
22	B	604	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	c	506	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	B	627	LMT	C1'-O5'-C5'	-2.34	109.10	113.69
27	C	521	LMG	O6-C1-O1	-2.34	104.44	109.97
22	B	605	CLA	CMD-C2D-C3D	2.34	129.05	124.68
27	B	621	LMG	C40-C39-C38	-2.33	102.58	114.42
27	c	518	LMG	C38-C37-C36	-2.33	102.58	114.42
24	B	619	BCR	C11-C10-C9	-2.33	123.98	127.31
25	C	516	DGD	CFB-CEB-CDB	-2.33	102.58	114.42
22	C	505	CLA	CMD-C2D-C3D	2.33	129.04	124.68
25	C	516	DGD	C3G-C2G-C1G	-2.33	106.27	111.79
22	b	605	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	a	408	PL9	C27-C28-C29	-2.33	122.05	127.66
27	e	101	LMG	O6-C1-O1	-2.33	104.45	109.97
22	B	610	CLA	C1-C2-C3	-2.33	122.01	126.04
22	B	609	CLA	CMD-C2D-C3D	2.33	129.04	124.68
24	F	102	BCR	C11-C10-C9	-2.33	123.99	127.31
22	c	510	CLA	CMD-C2D-C3D	2.33	129.03	124.68
23	A	406	PL9	C27-C28-C29	-2.33	122.06	127.66
22	c	504	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	c	512	CLA	CMD-C2D-C3D	2.32	129.03	124.68
29	a	401	SQD	C1-O5-C5	2.32	118.25	113.69
24	B	616	BCR	C2-C1-C6	2.32	114.05	110.48
23	d	407	PL9	C27-C28-C29	-2.32	122.07	127.66
22	c	503	CLA	CMD-C2D-C3D	2.32	129.02	124.68
25	d	410	DGD	C3D-C4D-C5D	-2.32	106.10	110.24
22	b	619	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	j	101	PL9	C20-C19-C21	2.32	119.17	115.27
30	i	102	LMT	C1'-O5'-C5'	-2.32	109.14	113.69
25	D	410	DGD	C3G-C2G-C1G	-2.32	106.31	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	C1-C2-C3	-2.31	122.04	126.04
27	a	412	LMG	C38-C37-C36	-2.31	102.68	114.42
22	D	405	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	c	520	CLA	CMD-C2D-C3D	2.31	129.00	124.68
29	a	415	SQD	O48-C23-C24	2.31	119.16	111.91
24	c	513	BCR	C24-C23-C22	-2.31	122.74	126.23
22	B	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
24	C	513	BCR	C11-C10-C9	-2.31	124.01	127.31
27	b	625	LMG	C40-C39-C38	-2.31	102.70	114.42
27	e	101	LMG	C1-C2-C3	-2.31	105.19	110.00
24	J	102	BCR	C15-C16-C17	-2.31	118.74	123.47
24	K	102	BCR	C11-C10-C9	-2.31	124.02	127.31
24	j	102	BCR	C29-C30-C25	2.31	114.03	110.48
22	B	605	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
24	J	102	BCR	C20-C21-C22	-2.31	124.02	127.31
22	c	511	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
22	D	406	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	b	605	CLA	CHB-C4A-NA	2.30	127.69	124.51
24	C	513	BCR	C3-C4-C5	-2.30	109.97	114.08
24	j	102	BCR	C20-C21-C22	-2.30	124.03	127.31
22	b	608	CLA	CMD-C2D-C3D	2.30	128.98	124.68
22	B	615	CLA	CMD-C2D-C3D	2.30	128.98	124.68
22	B	606	CLA	CMD-C2D-C3D	2.30	128.97	124.68
22	b	619	CLA	CMD-C2D-C3D	2.30	128.97	124.68
22	B	603	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
34	F	101	HEM	CBD-CAD-C3D	-2.29	108.25	112.48
27	a	412	LMG	O3-C3-C2	-2.29	105.05	110.35
22	B	607	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
27	d	412	LMG	O6-C1-O1	-2.29	104.55	109.97
27	D	409	LMG	O6-C1-C2	-2.29	105.50	110.35
27	b	625	LMG	O6-C1-O1	-2.29	104.56	109.97
24	A	407	BCR	C15-C16-C17	-2.29	118.79	123.47
27	C	521	LMG	C38-C37-C36	-2.29	102.82	114.42
24	f	102	BCR	C11-C10-C9	-2.29	124.05	127.31
22	B	601	CLA	CHB-C4A-NA	2.29	127.67	124.51
34	F	101	HEM	CAA-CBA-CGA	-2.28	108.84	112.67
30	D	411	LMT	C3'-C4'-C5'	-2.28	105.69	110.93
24	B	616	BCR	C15-C16-C17	-2.28	118.80	123.47
23	D	407	PL9	C37-C38-C39	-2.28	122.17	127.66
22	c	509	CLA	CMD-C2D-C3D	2.28	128.95	124.68
25	b	601	DGD	O6D-C1D-O3G	-2.28	104.58	109.97
22	c	502	CLA	C1B-CHB-C4A	-2.28	125.60	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	411	LMT	C1'-O5'-C5'	-2.28	109.22	113.69
29	d	403	SQD	O48-C23-C24	2.28	119.05	111.91
24	B	616	BCR	C15-C14-C13	-2.27	124.07	127.31
22	b	617	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
24	c	521	BCR	C11-C10-C9	-2.27	124.07	127.31
27	D	412	LMG	O3-C3-C2	-2.27	105.11	110.35
27	b	625	LMG	C38-C37-C36	-2.27	102.91	114.42
25	c	515	DGD	O5D-C6D-C5D	-2.27	104.85	109.05
29	A	412	SQD	C4-C3-C2	2.27	114.78	110.82
22	b	613	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
24	b	620	BCR	C15-C14-C13	-2.27	124.08	127.31
22	C	508	CLA	CMD-C2D-C3D	2.26	128.91	124.68
24	J	102	BCR	C29-C30-C25	2.26	113.97	110.48
27	A	410	LMG	C1-C2-C3	-2.26	105.28	110.00
22	c	520	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
29	B	626	SQD	O48-C23-C24	2.26	119.00	111.91
22	C	502	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	d	407	PL9	C37-C38-C39	-2.26	122.22	127.66
24	F	102	BCR	C15-C16-C17	-2.26	118.85	123.47
24	c	513	BCR	C3-C4-C5	-2.26	110.04	114.08
22	c	512	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
24	B	617	BCR	C35-C13-C14	-2.26	119.76	122.92
22	b	616	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
22	a	404	CLA	CMD-C2D-C3D	2.26	128.90	124.68
22	c	509	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
25	B	620	DGD	C1D-C2D-C3D	-2.25	105.30	110.00
22	C	509	CLA	CMD-C2D-C3D	2.25	128.89	124.68
29	A	413	SQD	O48-C23-C24	2.25	118.96	111.91
23	A	406	PL9	C20-C19-C21	2.25	119.05	115.27
22	B	609	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	C	512	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
24	B	616	BCR	C27-C26-C25	2.25	125.99	122.73
24	a	409	BCR	C33-C5-C6	-2.24	122.01	124.53
22	B	604	CLA	CMD-C2D-C3D	2.24	128.88	124.68
22	C	509	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
27	c	522	LMG	C38-C37-C36	-2.24	103.04	114.42
27	D	412	LMG	O6-C1-O1	-2.24	104.66	109.97
22	b	609	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
22	b	607	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
27	m	101	LMG	C1-C2-C3	-2.24	105.33	110.00
24	B	617	BCR	C11-C10-C9	-2.24	124.12	127.31
22	b	607	CLA	O1D-CGD-CBD	2.24	129.06	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	508	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
27	B	621	LMG	C38-C37-C36	-2.23	103.08	114.42
22	A	404	CLA	CMD-C2D-C3D	2.23	128.85	124.68
24	A	407	BCR	C15-C14-C13	-2.23	124.12	127.31
27	D	412	LMG	C1-C2-C3	-2.23	105.36	110.00
23	D	407	PL9	C32-C33-C34	-2.23	122.30	127.66
22	b	609	CLA	CMD-C2D-C3D	2.23	128.84	124.68
22	B	610	CLA	C1D-CHD-C4C	2.23	125.50	122.56
22	b	610	CLA	CMD-C2D-C3D	2.23	128.84	124.68
24	b	620	BCR	C27-C26-C25	2.23	125.96	122.73
22	c	510	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
25	b	624	DGD	C1D-C2D-C3D	-2.22	105.36	110.00
24	K	102	BCR	C33-C5-C6	-2.22	122.03	124.53
22	B	609	CLA	C1D-CHD-C4C	2.22	125.49	122.56
25	C	516	DGD	O3D-C3D-C4D	-2.22	105.21	110.35
25	c	516	DGD	O3D-C3D-C4D	-2.22	105.21	110.35
22	A	402	CLA	CMD-C2D-C3D	2.22	128.83	124.68
24	a	409	BCR	C15-C14-C13	-2.22	124.14	127.31
30	I	102	LMT	C1'-O5'-C5'	-2.22	109.33	113.69
24	f	102	BCR	C15-C16-C17	-2.22	118.93	123.47
27	i	101	LMG	O1-C7-C8	-2.22	105.55	110.90
22	C	510	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
22	b	614	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
22	C	507	CLA	C1-C2-C3	-2.22	122.21	126.04
24	c	513	BCR	C27-C26-C25	2.22	125.95	122.73
25	A	408	DGD	C3G-C2G-C1G	-2.21	106.55	111.79
24	C	513	BCR	C27-C26-C25	2.21	125.94	122.73
34	v	201	HEM	CMB-C2B-C3B	2.21	128.81	124.68
22	B	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	b	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
31	D	402	PHO	C1B-NB-C4B	2.21	110.67	106.51
22	C	511	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
24	A	407	BCR	C33-C5-C6	-2.21	122.05	124.53
25	a	410	DGD	CAB-C9B-C8B	-2.21	103.22	114.42
27	d	408	LMG	O3-C3-C2	-2.21	105.25	110.35
27	m	101	LMG	O2-C2-C1	-2.20	104.70	110.05
22	C	501	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
22	C	507	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
25	C	516	DGD	C3D-C4D-C5D	-2.20	106.32	110.24
22	c	508	CLA	CMD-C2D-C3D	2.20	128.79	124.68
29	b	602	SQD	O48-C23-C24	2.20	118.80	111.91
25	a	410	DGD	C3G-C2G-C1G	-2.20	106.59	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
27	d	412	LMG	C1-C2-C3	-2.19	105.42	110.00
29	F	103	SQD	C3-C4-C5	2.19	114.15	110.24
22	a	406	CLA	CMD-C2D-C3D	2.19	128.78	124.68
25	c	516	DGD	CBB-CAB-C9B	-2.19	103.29	114.42
22	c	506	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	a	411	LHG	C27-C26-C25	-2.19	103.29	114.42
29	f	103	SQD	C3-C4-C5	2.19	114.15	110.24
24	H	102	BCR	C16-C15-C14	-2.19	118.98	123.47
24	g	101	BCR	C15-C16-C17	-2.19	118.99	123.47
25	D	410	DGD	C3D-C4D-C5D	-2.19	106.33	110.24
27	a	412	LMG	C1-C2-C3	-2.19	105.44	110.00
34	V	201	HEM	CMB-C2B-C3B	2.19	128.77	124.68
22	C	503	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
25	A	408	DGD	CAB-C9B-C8B	-2.19	103.33	114.42
25	C	516	DGD	CBB-CAB-C9B	-2.19	103.33	114.42
24	c	521	BCR	C24-C23-C22	-2.18	122.94	126.23
25	a	410	DGD	C1D-C2D-C3D	-2.18	105.45	110.00
25	C	515	DGD	C1D-C2D-C3D	-2.18	105.45	110.00
22	b	618	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
22	c	511	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
25	C	517	DGD	CBB-CAB-C9B	-2.18	103.35	114.42
24	f	102	BCR	C27-C26-C25	2.18	125.90	122.73
25	B	625	DGD	O6D-C1D-O3G	-2.18	104.81	109.97
27	D	408	LMG	O3-C3-C2	-2.18	105.31	110.35
24	b	622	BCR	C7-C8-C9	-2.18	122.94	126.23
27	d	409	LMG	O6-C1-O1	-2.18	104.82	109.97
27	b	625	LMG	O3-C3-C2	-2.18	105.31	110.35
27	a	402	LMG	O3-C3-C2	-2.18	105.31	110.35
25	B	620	DGD	C3G-C2G-C1G	-2.18	106.64	111.79
29	B	622	SQD	C4-C3-C2	2.18	114.62	110.82
27	B	621	LMG	O3-C3-C2	-2.18	105.32	110.35
24	g	101	BCR	C3-C2-C1	-2.18	106.82	114.60
22	C	507	CLA	C1D-CHD-C4C	2.18	125.43	122.56
25	b	601	DGD	CBB-CAB-C9B	-2.17	103.38	114.42
27	D	409	LMG	O6-C1-O1	-2.17	104.83	109.97
27	I	101	LMG	O3-C3-C2	-2.17	105.33	110.35
24	x	101	BCR	C29-C30-C25	2.17	113.83	110.48
22	B	611	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	b	618	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
27	c	518	LMG	O7-C10-O9	-2.17	118.45	123.70
22	A	403	CLA	CMD-C2D-C3D	2.17	128.74	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	O1-C4-C3	-2.17	118.33	120.72
24	F	102	BCR	C27-C26-C25	2.17	125.88	122.73
29	F	103	SQD	O48-C23-C24	2.17	118.71	111.91
27	d	412	LMG	O3-C3-C2	-2.17	105.34	110.35
24	b	621	BCR	C11-C10-C9	-2.17	124.22	127.31
27	m	101	LMG	C1-O6-C5	-2.17	109.44	113.69
30	B	624	LMT	C1'-O5'-C5'	-2.16	109.44	113.69
22	c	508	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
27	D	408	LMG	O2-C2-C1	-2.16	104.79	110.05
22	d	405	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
25	C	516	DGD	CAB-C9B-C8B	-2.16	103.45	114.42
31	d	401	PHO	C1B-NB-C4B	2.16	110.58	106.51
22	b	619	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
27	I	101	LMG	O7-C10-O9	-2.16	118.48	123.70
24	b	621	BCR	C7-C8-C9	-2.16	122.97	126.23
27	a	402	LMG	O1-C7-C8	-2.16	105.69	110.90
29	d	403	SQD	C4-C3-C2	2.16	114.59	110.82
24	b	623	BCR	C24-C23-C22	-2.15	122.98	126.23
25	C	515	DGD	O5D-C6D-C5D	-2.15	105.06	109.05
31	D	401	PHO	C1B-NB-C4B	2.15	110.57	106.51
24	c	521	BCR	C33-C5-C6	-2.15	122.11	124.53
23	j	101	PL9	O2-C1-C6	2.15	124.32	120.59
27	C	521	LMG	O2-C2-C1	-2.15	104.81	110.05
22	B	610	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
22	B	601	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	b	623	BCR	C38-C26-C25	-2.15	122.11	124.53
22	B	603	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	C	513	BCR	C7-C8-C9	-2.15	122.99	126.23
25	B	625	DGD	CBB-CAB-C9B	-2.15	103.51	114.42
23	d	407	PL9	C32-C33-C34	-2.15	122.48	127.66
25	C	517	DGD	C3G-O3G-C1D	2.15	117.94	113.74
24	C	514	BCR	C38-C26-C25	-2.15	122.11	124.53
22	B	614	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
25	c	517	DGD	CBB-CAB-C9B	-2.15	103.52	114.42
24	y	101	BCR	C15-C16-C17	-2.15	119.08	123.47
23	a	408	PL9	O2-C1-C6	2.15	124.31	120.59
27	i	101	LMG	O2-C2-C1	-2.15	104.83	110.05
26	A	409	LHG	C27-C26-C25	-2.14	103.54	114.42
24	F	102	BCR	C7-C8-C9	-2.14	123.00	126.23
25	B	620	DGD	C4E-C3E-C2E	-2.14	107.08	110.82
23	D	407	PL9	O1-C4-C3	-2.14	118.36	120.72
22	B	605	CLA	O1D-CGD-CBD	2.14	128.86	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	407	PL9	O2-C1-C2	-2.14	116.88	121.78
25	b	624	DGD	C3G-C2G-C1G	-2.14	106.73	111.79
25	b	601	DGD	CAB-C9B-C8B	-2.14	103.58	114.42
24	B	619	BCR	C38-C26-C25	-2.14	122.13	124.53
23	j	101	PL9	O2-C1-C2	-2.14	116.89	121.78
24	b	623	BCR	C33-C5-C6	-2.13	122.13	124.53
27	C	518	LMG	O7-C10-O9	-2.13	118.54	123.70
27	c	522	LMG	O3-C3-C2	-2.13	105.42	110.35
27	I	101	LMG	O2-C2-C1	-2.13	104.87	110.05
31	d	402	PHO	C1B-NB-C4B	2.13	110.53	106.51
27	C	521	LMG	O3-C3-C2	-2.13	105.42	110.35
27	i	101	LMG	O3-C3-C2	-2.13	105.42	110.35
22	c	503	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
23	J	101	PL9	O2-C1-C6	2.13	124.28	120.59
22	d	405	CLA	O1D-CGD-CBD	2.13	128.84	124.48
24	B	617	BCR	C7-C8-C9	-2.13	123.02	126.23
22	b	610	CLA	C1D-CHD-C4C	2.13	125.37	122.56
22	c	507	CLA	O2D-CGD-CBD	2.13	115.05	111.27
24	B	618	BCR	C7-C8-C9	-2.13	123.02	126.23
25	d	410	DGD	C5B-C4B-C3B	-2.12	103.64	114.42
22	B	614	CLA	C1D-CHD-C4C	2.12	125.36	122.56
24	y	101	BCR	C3-C2-C1	-2.12	107.01	114.60
25	c	515	DGD	C1D-C2D-C3D	-2.12	105.57	110.00
27	a	412	LMG	O7-C10-O9	-2.12	118.57	123.70
27	e	101	LMG	O1-C7-C8	-2.12	105.77	110.90
22	B	606	CLA	C1-C2-C3	-2.12	122.37	126.04
27	e	101	LMG	O3-C3-C2	-2.12	105.44	110.35
27	A	410	LMG	O7-C10-O9	-2.12	118.57	123.70
22	c	520	CLA	C1D-CHD-C4C	2.12	125.36	122.56
25	c	517	DGD	CAB-C9B-C8B	-2.12	103.66	114.42
22	c	507	CLA	C1-C2-C3	-2.12	122.37	126.04
27	d	408	LMG	O2-C2-C1	-2.12	104.89	110.05
24	C	514	BCR	C24-C23-C22	-2.12	123.03	126.23
22	d	405	CLA	CHB-C4A-NA	2.12	127.44	124.51
22	c	509	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
27	A	414	LMG	O3-C3-C2	-2.12	105.45	110.35
23	d	407	PL9	O2-C1-C6	2.12	124.26	120.59
22	B	602	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	B	625	DGD	CAB-C9B-C8B	-2.12	103.68	114.42
23	A	406	PL9	O2-C1-C6	2.12	124.25	120.59
22	D	405	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
22	C	509	CLA	C1D-CHD-C4C	2.11	125.35	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	518	LMG	O3-C3-C2	-2.11	105.46	110.35
30	b	627	LMT	C1'-O5'-C5'	-2.11	109.54	113.69
22	b	607	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
22	C	502	CLA	C1-C2-C3	-2.11	122.39	126.04
23	J	101	PL9	O2-C1-C2	-2.11	116.94	121.78
24	B	619	BCR	C24-C23-C22	-2.11	123.05	126.23
26	C	519	LHG	C27-C26-C25	-2.11	103.73	114.42
22	D	406	CLA	C1-C2-C3	-2.11	122.40	126.04
22	b	615	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
24	c	514	BCR	C24-C23-C22	-2.10	123.06	126.23
27	A	414	LMG	O7-C10-O9	-2.10	118.62	123.70
25	D	410	DGD	C5B-C4B-C3B	-2.10	103.75	114.42
27	E	101	LMG	O1-C7-C8	-2.10	105.83	110.90
22	C	506	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	H	102	BCR	C29-C30-C25	2.10	113.71	110.48
22	D	405	CLA	CHB-C4A-NA	2.10	127.41	124.51
24	b	622	BCR	C33-C5-C6	-2.10	122.17	124.53
22	B	611	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
22	c	512	CLA	C1D-CHD-C4C	2.10	125.32	122.56
25	C	517	DGD	CAB-C9B-C8B	-2.09	103.79	114.42
22	B	612	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
25	c	516	DGD	C3D-C4D-C5D	-2.09	106.51	110.24
23	D	407	PL9	O2-C1-C2	-2.09	116.99	121.78
25	c	516	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
31	D	402	PHO	CMB-C2B-C1B	-2.09	121.85	125.06
27	A	414	LMG	O1-C7-C8	-2.09	105.86	110.90
24	B	619	BCR	C33-C5-C6	-2.09	122.18	124.53
23	A	406	PL9	O2-C1-C2	-2.09	117.00	121.78
27	C	518	LMG	O3-C3-C2	-2.09	105.53	110.35
22	C	501	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
24	c	514	BCR	C38-C26-C25	-2.09	122.19	124.53
27	c	522	LMG	O2-C2-C1	-2.09	104.98	110.05
23	a	408	PL9	O2-C1-C2	-2.09	117.00	121.78
26	c	519	LHG	C27-C26-C25	-2.08	103.84	114.42
27	d	409	LMG	O6-C1-C2	-2.08	105.94	110.35
25	C	515	DGD	C5B-C4B-C3B	-2.08	103.85	114.42
22	c	504	CLA	O1D-CGD-CBD	2.08	128.75	124.48
25	c	517	DGD	C3G-O3G-C1D	2.08	117.81	113.74
25	c	515	DGD	C5B-C4B-C3B	-2.08	103.87	114.42
23	d	407	PL9	C31-C32-C33	-2.08	105.05	111.88
25	A	408	DGD	C1D-C2D-C3D	-2.08	105.67	110.00
27	i	101	LMG	O7-C10-O9	-2.08	118.68	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	C1D-CHD-C4C	2.08	125.30	122.56
24	b	622	BCR	C27-C26-C25	2.08	125.75	122.73
22	b	616	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	a	405	CLA	CMD-C2D-C3D	2.07	128.56	124.68
27	E	101	LMG	O3-C3-C2	-2.07	105.56	110.35
22	b	605	CLA	C4D-C3D-CAD	-2.07	107.31	108.47
22	B	606	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	B	614	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
22	b	610	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
27	M	101	LMG	O3-C3-C2	-2.07	105.57	110.35
27	b	625	LMG	O2-C2-C1	-2.07	105.03	110.05
23	d	407	PL9	C36-C34-C33	-2.07	116.94	121.12
22	C	520	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	a	409	BCR	C24-C23-C22	-2.07	123.11	126.23
22	B	610	CLA	C4D-C3D-CAD	-2.07	107.32	108.47
22	c	508	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
31	d	402	PHO	CMB-C2B-C1B	-2.06	121.88	125.06
22	b	614	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
22	c	520	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
22	c	503	CLA	O2D-CGD-CBD	2.06	114.93	111.27
27	i	101	LMG	O1-C1-C2	-2.06	105.08	108.30
25	D	410	DGD	CAB-C9B-C8B	-2.06	103.96	114.42
22	C	508	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
29	f	103	SQD	O48-C23-C24	2.06	118.37	111.91
22	C	512	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	A	407	BCR	C38-C26-C25	-2.06	122.22	124.53
22	b	609	CLA	O1D-CGD-CBD	2.06	128.69	124.48
25	D	410	DGD	CBB-CAB-C9B	-2.06	103.98	114.42
27	M	101	LMG	O2-C2-C1	-2.06	105.05	110.05
22	a	405	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
23	D	407	PL9	O2-C1-C6	2.06	124.15	120.59
29	A	413	SQD	C1-O5-C5	2.05	117.72	113.69
22	a	406	CLA	C1D-CHD-C4C	2.05	125.27	122.56
25	d	410	DGD	CAB-C9B-C8B	-2.05	104.00	114.42
22	c	501	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
31	d	401	PHO	C2B-C1B-NB	-2.05	106.70	109.79
25	b	624	DGD	CAB-C9B-C8B	-2.05	104.02	114.42
25	d	410	DGD	CBB-CAB-C9B	-2.05	104.03	114.42
24	C	514	BCR	C7-C8-C9	-2.05	123.14	126.23
27	D	412	LMG	O7-C10-O9	-2.05	118.75	123.70
22	b	606	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
27	m	101	LMG	O3-C3-C2	-2.05	105.62	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C7-C8-C9	-2.04	123.15	126.23
22	b	618	CLA	C1D-CHD-C4C	2.04	125.25	122.56
24	a	409	BCR	C38-C26-C25	-2.04	122.24	124.53
25	c	517	DGD	C5B-C4B-C3B	-2.04	104.08	114.42
25	C	517	DGD	C5B-C4B-C3B	-2.04	104.08	114.42
24	b	620	BCR	C15-C16-C17	-2.04	119.30	123.47
23	a	408	PL9	O1-C4-C3	-2.04	118.48	120.72
25	B	620	DGD	C5B-C4B-C3B	-2.04	104.09	114.42
24	b	622	BCR	C20-C21-C22	-2.03	124.41	127.31
22	c	512	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
27	M	101	LMG	C1-O6-C5	-2.03	109.70	113.69
24	x	101	BCR	C16-C15-C14	-2.03	119.31	123.47
22	b	606	CLA	C1D-CHD-C4C	2.03	125.24	122.56
24	B	618	BCR	C33-C5-C6	-2.03	122.25	124.53
25	C	516	DGD	C5B-C4B-C3B	-2.03	104.12	114.42
22	b	610	CLA	C1-C2-C3	-2.03	122.53	126.04
27	d	412	LMG	O7-C10-O9	-2.03	118.80	123.70
22	B	609	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
24	b	621	BCR	C24-C23-C22	-2.03	123.17	126.23
22	C	504	CLA	O1D-CGD-CBD	2.03	128.63	124.48
25	A	408	DGD	C5B-C4B-C3B	-2.03	104.14	114.42
22	d	405	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
22	b	612	CLA	C1-C2-C3	-2.03	122.54	126.04
24	c	513	BCR	C8-C7-C6	-2.03	121.51	127.20
27	B	621	LMG	O7-C10-O9	-2.03	118.81	123.70
22	d	406	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
27	C	518	LMG	O2-C2-C1	-2.02	105.13	110.05
25	a	410	DGD	C5B-C4B-C3B	-2.02	104.15	114.42
27	c	518	LMG	O2-C2-C1	-2.02	105.13	110.05
22	c	508	CLA	C1D-CHD-C4C	2.02	125.23	122.56
34	F	101	HEM	CMC-C2C-C3C	2.02	128.46	124.68
22	c	511	CLA	C1D-CHD-C4C	2.02	125.23	122.56
25	B	620	DGD	CAB-C9B-C8B	-2.02	104.16	114.42
22	B	607	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	B	606	CLA	C1D-CHD-C4C	2.02	125.22	122.56
22	b	605	CLA	C1-C2-C3	-2.02	122.55	126.04
24	H	102	BCR	C7-C8-C9	-2.02	123.19	126.23
24	b	623	BCR	C15-C16-C17	-2.02	119.35	123.47
22	C	505	CLA	C1D-CHD-C4C	2.01	125.22	122.56
22	B	602	CLA	C1D-CHD-C4C	2.01	125.22	122.56
24	A	407	BCR	C11-C10-C9	-2.01	124.44	127.31
23	D	407	PL9	C12-C13-C14	-2.01	122.81	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	513	BCR	C8-C7-C6	-2.01	121.55	127.20
31	d	401	PHO	O2A-CGA-O1A	-2.01	118.52	123.59
25	b	624	DGD	C5B-C4B-C3B	-2.01	104.22	114.42
22	D	406	CLA	C1D-CHD-C4C	2.01	125.21	122.56
27	b	625	LMG	O7-C10-O9	-2.01	118.85	123.70
31	D	401	PHO	O2A-CGA-O1A	-2.01	118.53	123.59
22	A	403	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
22	C	502	CLA	C1D-CHD-C4C	2.00	125.20	122.56
24	B	616	BCR	C7-C8-C9	-2.00	123.21	126.23
29	a	401	SQD	C4-C3-C2	2.00	114.32	110.82
31	D	402	PHO	C2B-C1B-NB	-2.00	106.77	109.79
27	a	412	LMG	O2-C2-C1	-2.00	105.18	110.05
27	D	408	LMG	O1-C7-C8	-2.00	106.07	110.90

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	604	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	604	CLA	ND
22	B	604	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	D	406	CLA	NC
22	D	406	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	405	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	d	406	CLA	NC
22	d	406	CLA	ND
22	d	406	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	504	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	619	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	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	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	h	101	CLA	NC
22	h	101	CLA	ND
22	h	101	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	a	407	CLA	NC
22	a	407	CLA	ND

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Mol	Chain	Res	Type	Atom
22	a	407	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA

All (2133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	D	407	PL9	C27-C28-C29-C31
23	D	407	PL9	C34-C36-C37-C38
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
29	b	602	SQD	O5-C5-C6-S
24	J	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C21-C22-C23-C24
26	C	519	LHG	C4-O6-P-O4
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
27	d	412	LMG	O9-C10-O7-C8
27	d	412	LMG	C11-C10-O7-C8
34	V	201	HEM	C2D-C3D-CAD-CBD
34	V	201	HEM	C4D-C3D-CAD-CBD
29	a	415	SQD	C2-C1-O6-C44
29	a	415	SQD	C5-C6-S-O7
29	a	415	SQD	C5-C6-S-O8
29	a	415	SQD	C5-C6-S-O9
22	b	606	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
27	c	522	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	O6-C1-O1-C7
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	613	CLA	CAD-CBD-CGD-O2D
29	A	413	SQD	C24-C23-O48-C46
22	B	604	CLA	CBD-CGD-O2D-CED
24	b	620	BCR	C1-C6-C7-C8
24	F	102	BCR	C1-C6-C7-C8
24	F	102	BCR	C7-C8-C9-C10
22	B	601	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	CBD-CGD-O2D-CED
25	c	516	DGD	O1B-C1B-O2G-C2G
25	c	516	DGD	C2D-C1D-O3G-C3G
25	c	516	DGD	O6D-C1D-O3G-C3G
24	j	102	BCR	C1-C6-C7-C8
24	j	102	BCR	C21-C22-C23-C24
24	B	617	BCR	C21-C22-C23-C24
24	B	617	BCR	C23-C24-C25-C26
25	B	625	DGD	O1B-C1B-O2G-C2G
25	B	625	DGD	O2G-C2G-C3G-O3G
25	B	625	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	O6E-C1E-O5D-C6D
25	a	410	DGD	C2D-C1D-O3G-C3G
24	c	513	BCR	C1-C6-C7-C8
24	c	513	BCR	C6-C7-C8-C9
25	c	517	DGD	C2D-C1D-O3G-C3G
25	c	517	DGD	O6D-C1D-O3G-C3G
26	c	519	LHG	C4-O6-P-O4
27	b	625	LMG	C11-C10-O7-C8
34	v	201	HEM	C2D-C3D-CAD-CBD
25	d	410	DGD	O6D-C1D-O3G-C3G
29	a	401	SQD	C24-C23-O48-C46
25	b	624	DGD	C2E-C1E-O5D-C6D
29	B	626	SQD	O5-C5-C6-S
22	B	609	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	CBD-CGD-O2D-CED
27	e	101	LMG	C2-C1-O1-C7
27	e	101	LMG	O6-C1-O1-C7
27	e	101	LMG	C7-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C2-C3-C5-C6
22	d	405	CLA	C4-C3-C5-C6
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C2-C3-C5-C6
22	B	602	CLA	C4-C3-C5-C6
27	c	518	LMG	C2-C1-O1-C7
27	c	518	LMG	O6-C1-O1-C7
27	c	518	LMG	O9-C10-O7-C8
27	c	518	LMG	C11-C10-O7-C8
25	D	410	DGD	O6D-C1D-O3G-C3G
23	d	407	PL9	C27-C28-C29-C31
23	d	407	PL9	C34-C36-C37-C38
24	x	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C21-C22-C23-C24
24	x	101	BCR	C37-C22-C23-C24
27	d	409	LMG	C2-C1-O1-C7
27	d	409	LMG	O6-C1-O1-C7
22	C	511	CLA	C1A-C2A-CAA-CBA
22	b	608	CLA	CBD-CGD-O2D-CED
27	M	101	LMG	O9-C10-O7-C8
22	A	402	CLA	CBD-CGD-O2D-CED
27	C	521	LMG	C2-C1-O1-C7
27	C	521	LMG	O6-C1-O1-C7
23	A	406	PL9	C7-C8-C9-C10
23	A	406	PL9	C7-C8-C9-C11
23	A	406	PL9	C12-C13-C14-C15
23	A	406	PL9	C12-C13-C14-C16
23	A	406	PL9	C17-C18-C19-C21
23	A	406	PL9	C22-C23-C24-C25
23	A	406	PL9	C24-C26-C27-C28
23	A	406	PL9	C27-C28-C29-C30
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C30-C29-C31-C32
23	A	406	PL9	C37-C38-C39-C40
23	A	406	PL9	C37-C38-C39-C41
23	j	101	PL9	C12-C13-C14-C16
23	j	101	PL9	C22-C23-C24-C25
23	j	101	PL9	C22-C23-C24-C26
22	b	609	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C3A-C2A-CAA-CBA
22	H	101	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	H	101	CLA	C2-C3-C5-C6
22	H	101	CLA	C4-C3-C5-C6
22	H	101	CLA	C6-C7-C8-C9
24	c	521	BCR	C7-C8-C9-C10
24	c	521	BCR	C7-C8-C9-C34
27	E	101	LMG	C2-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7
22	B	605	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C3A-C2A-CAA-CBA
25	C	515	DGD	C2B-C1B-O2G-C2G
25	C	515	DGD	O1B-C1B-O2G-C2G
25	C	515	DGD	C2E-C1E-O5D-C6D
22	b	617	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O2D
26	A	409	LHG	C1-C2-C3-O3
25	c	515	DGD	C2B-C1B-O2G-C2G
25	c	515	DGD	O1B-C1B-O2G-C2G
25	c	515	DGD	C2E-C1E-O5D-C6D
25	B	620	DGD	C2E-C1E-O5D-C6D
22	B	612	CLA	CBD-CGD-O2D-CED
25	b	601	DGD	O1B-C1B-O2G-C2G
25	b	601	DGD	O2G-C2G-C3G-O3G
25	b	601	DGD	C2E-C1E-O5D-C6D
25	b	601	DGD	O6E-C1E-O5D-C6D
24	b	621	BCR	C21-C22-C23-C24
24	b	621	BCR	C23-C24-C25-C26
22	b	611	CLA	C1A-C2A-CAA-CBA
25	A	408	DGD	C2D-C1D-O3G-C3G
27	B	621	LMG	C11-C10-O7-C8
22	b	613	CLA	CBD-CGD-O2D-CED
22	c	504	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	CBD-CGD-O2D-CED
24	f	102	BCR	C1-C6-C7-C8
24	f	102	BCR	C7-C8-C9-C10
22	B	615	CLA	CBD-CGD-O2D-CED
27	C	518	LMG	C2-C1-O1-C7
27	C	518	LMG	O6-C1-O1-C7
27	C	518	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
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	c	510	CLA	CBD-CGD-O2D-CED
27	D	409	LMG	C2-C1-O1-C7
27	D	409	LMG	O6-C1-O1-C7
24	y	101	BCR	C7-C8-C9-C10
24	C	513	BCR	C1-C6-C7-C8
24	C	513	BCR	C6-C7-C8-C9
23	a	408	PL9	C7-C8-C9-C11
23	a	408	PL9	C12-C13-C14-C15
23	a	408	PL9	C12-C13-C14-C16
23	a	408	PL9	C17-C18-C19-C21
23	a	408	PL9	C22-C23-C24-C25
23	a	408	PL9	C24-C26-C27-C28
23	a	408	PL9	C27-C28-C29-C30
23	a	408	PL9	C27-C28-C29-C31
23	a	408	PL9	C30-C29-C31-C32
23	a	408	PL9	C37-C38-C39-C41
22	c	511	CLA	C1A-C2A-CAA-CBA
22	B	607	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C1A-C2A-CAA-CBA
22	D	405	CLA	C2-C3-C5-C6
22	D	405	CLA	C4-C3-C5-C6
22	b	619	CLA	CBD-CGD-O2D-CED
24	B	616	BCR	C1-C6-C7-C8
23	J	101	PL9	C12-C13-C14-C16
23	J	101	PL9	C22-C23-C24-C25
23	J	101	PL9	C22-C23-C24-C26
24	g	101	BCR	C7-C8-C9-C10
25	C	517	DGD	C2D-C1D-O3G-C3G
25	C	517	DGD	O6D-C1D-O3G-C3G
29	B	622	SQD	C2-C1-O6-C44
29	B	622	SQD	O5-C1-O6-C44
29	B	622	SQD	O49-C7-O47-C45
29	B	622	SQD	C8-C7-O47-C45
24	H	102	BCR	C7-C8-C9-C34
24	H	102	BCR	C21-C22-C23-C24
24	H	102	BCR	C37-C22-C23-C24
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	CBD-CGD-O2D-CED
25	C	516	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
25	C	516	DGD	O1B-C1B-O2G-C2G
25	C	516	DGD	C2D-C1D-O3G-C3G
25	C	516	DGD	O6D-C1D-O3G-C3G
27	m	101	LMG	O9-C10-O7-C8
22	a	404	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CBD-CGD-O2D-CED
29	A	412	SQD	C2-C1-O6-C44
29	A	412	SQD	C5-C6-S-O7
29	A	412	SQD	C5-C6-S-O8
29	A	412	SQD	C5-C6-S-O9
27	D	408	LMG	O1-C7-C8-O7
27	D	408	LMG	C11-C10-O7-C8
27	D	408	LMG	O10-C28-O8-C9
22	h	101	CLA	C1A-C2A-CAA-CBA
22	h	101	CLA	C2-C3-C5-C6
22	h	101	CLA	C4-C3-C5-C6
22	h	101	CLA	C6-C7-C8-C9
27	d	408	LMG	O1-C7-C8-O7
27	d	408	LMG	C11-C10-O7-C8
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C2A-CAA-CBA-CGA
26	a	411	LHG	C1-C2-C3-O3
29	d	403	SQD	C2-C1-O6-C44
29	d	403	SQD	O5-C1-O6-C44
29	d	403	SQD	O49-C7-O47-C45
29	d	403	SQD	C8-C7-O47-C45
22	a	405	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
27	D	412	LMG	O9-C10-O7-C8
27	D	412	LMG	C11-C10-O7-C8
22	C	504	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	C	503	CLA	O1D-CGD-O2D-CED
22	b	619	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	c	520	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	C	520	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
29	A	413	SQD	O10-C23-O48-C46
29	a	401	SQD	O10-C23-O48-C46
27	E	101	LMG	O10-C28-O8-C9
30	b	604	LMT	C3'-C4'-O1B-C1B
30	B	628	LMT	C3'-C4'-O1B-C1B
22	C	510	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	C8-C9-O8-C28
22	b	605	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
27	a	412	LMG	C29-C28-O8-C9
29	F	103	SQD	C24-C23-O48-C46
27	d	409	LMG	C29-C28-O8-C9
29	f	103	SQD	C24-C23-O48-C46
23	a	408	PL9	C37-C38-C39-C40
31	d	402	PHO	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
31	D	402	PHO	CBD-CGD-O2D-CED
27	a	412	LMG	O10-C28-O8-C9
29	F	103	SQD	O10-C23-O48-C46
27	A	410	LMG	O10-C28-O8-C9
27	e	101	LMG	O10-C28-O8-C9
27	c	518	LMG	O10-C28-O8-C9
27	d	409	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	D	409	LMG	O10-C28-O8-C9
29	f	103	SQD	O10-C23-O48-C46
27	d	408	LMG	O10-C28-O8-C9
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
30	b	603	LMT	C3'-C4'-O1B-C1B
30	B	627	LMT	C3'-C4'-O1B-C1B
22	B	607	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	C	520	CLA	O1D-CGD-O2D-CED
27	b	625	LMG	O9-C10-O7-C8
25	d	410	DGD	O1B-C1B-O2G-C2G
25	D	410	DGD	O1B-C1B-O2G-C2G
27	I	101	LMG	O9-C10-O7-C8
27	i	101	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
27	A	414	LMG	O9-C10-O7-C8
27	a	402	LMG	O9-C10-O7-C8
27	D	408	LMG	O9-C10-O7-C8
27	d	408	LMG	O9-C10-O7-C8
27	c	518	LMG	C8-C9-O8-C28
22	b	616	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
22	b	611	CLA	C3-C5-C6-C7
22	a	406	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	B	607	CLA	C3-C5-C6-C7
22	A	404	CLA	C3-C5-C6-C7
27	A	410	LMG	C29-C28-O8-C9
27	c	518	LMG	C29-C28-O8-C9
27	C	518	LMG	C29-C28-O8-C9
27	D	409	LMG	C29-C28-O8-C9
27	I	101	LMG	O6-C5-C6-O5
27	i	101	LMG	O6-C5-C6-O5
25	c	516	DGD	C2B-C1B-O2G-C2G
25	B	625	DGD	C2B-C1B-O2G-C2G
27	M	101	LMG	C11-C10-O7-C8
25	b	601	DGD	C2B-C1B-O2G-C2G
27	m	101	LMG	C11-C10-O7-C8
23	J	101	PL9	C27-C28-C29-C31
22	c	505	CLA	O1D-CGD-O2D-CED
25	A	408	DGD	O6E-C5E-C6E-O5E
22	B	604	CLA	C4-C3-C5-C6
22	b	608	CLA	C4-C3-C5-C6
22	b	611	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	609	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
30	i	102	LMT	C3'-C4'-O1B-C1B
30	I	102	LMT	C3'-C4'-O1B-C1B
31	d	401	PHO	C3-C5-C6-C7
27	c	522	LMG	C29-C28-O8-C9
25	d	410	DGD	C2A-C1A-O1G-C1G
25	D	410	DGD	C2A-C1A-O1G-C1G
27	C	521	LMG	C29-C28-O8-C9
27	D	408	LMG	C29-C28-O8-C9
27	d	408	LMG	C29-C28-O8-C9
25	a	410	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	O6E-C5E-C6E-O5E
25	B	620	DGD	O6E-C5E-C6E-O5E
22	c	508	CLA	O1D-CGD-O2D-CED
22	C	507	CLA	O1D-CGD-O2D-CED
25	b	624	DGD	C4D-C5D-C6D-O5D
25	B	620	DGD	C4D-C5D-C6D-O5D
23	j	101	PL9	C27-C28-C29-C31

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C17-C18-C19-C20
23	j	101	PL9	C7-C8-C9-C10
23	a	408	PL9	C7-C8-C9-C10
23	a	408	PL9	C17-C18-C19-C20
23	J	101	PL9	C7-C8-C9-C10
22	C	505	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
23	A	406	PL9	C22-C23-C24-C26
23	j	101	PL9	C7-C8-C9-C11
23	a	408	PL9	C22-C23-C24-C26
23	J	101	PL9	C7-C8-C9-C11
25	c	516	DGD	C4E-C5E-C6E-O5E
25	C	516	DGD	C4E-C5E-C6E-O5E
25	d	410	DGD	O1A-C1A-O1G-C1G
25	D	410	DGD	O1A-C1A-O1G-C1G
22	c	520	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
27	D	408	LMG	O6-C5-C6-O5
27	d	408	LMG	O6-C5-C6-O5
22	b	615	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
26	A	409	LHG	O2-C2-C3-O3
26	a	411	LHG	O2-C2-C3-O3
31	D	401	PHO	C3-C5-C6-C7
22	C	508	CLA	C3-C5-C6-C7
27	e	101	LMG	C29-C28-O8-C9
27	E	101	LMG	C29-C28-O8-C9
22	B	615	CLA	CBA-CGA-O2A-C1
27	c	522	LMG	O10-C28-O8-C9
27	C	521	LMG	O10-C28-O8-C9
22	C	501	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
29	F	103	SQD	C8-C7-O47-C45
25	D	410	DGD	C2B-C1B-O2G-C2G
27	d	409	LMG	C11-C10-O7-C8
27	A	414	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	D	409	LMG	C11-C10-O7-C8
29	f	103	SQD	C8-C7-O47-C45
27	a	402	LMG	C11-C10-O7-C8
22	C	509	CLA	CBD-CGD-O2D-CED
25	b	624	DGD	C4E-C5E-C6E-O5E
27	i	101	LMG	C4-C5-C6-O5
25	C	515	DGD	O6E-C5E-C6E-O5E
27	I	101	LMG	C4-C5-C6-O5
22	b	617	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7
25	c	515	DGD	O6E-C5E-C6E-O5E
27	e	101	LMG	O9-C10-O7-C8
25	A	408	DGD	C4E-C5E-C6E-O5E
27	C	518	LMG	O6-C5-C6-O5
25	C	516	DGD	O6E-C5E-C6E-O5E
31	d	401	PHO	C4-C3-C5-C6
31	D	401	PHO	C4-C3-C5-C6
31	d	401	PHO	C2-C3-C5-C6
31	D	401	PHO	C2-C3-C5-C6
22	B	601	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
25	c	516	DGD	O6E-C5E-C6E-O5E
27	c	518	LMG	O6-C5-C6-O5
25	B	620	DGD	C4E-C5E-C6E-O5E
25	b	624	DGD	O6E-C1E-O5D-C6D
25	C	515	DGD	O6E-C1E-O5D-C6D
25	c	515	DGD	O6E-C1E-O5D-C6D
25	B	620	DGD	O6E-C1E-O5D-C6D
27	A	414	LMG	O6-C1-O1-C7
27	a	402	LMG	O6-C1-O1-C7
31	d	401	PHO	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
25	C	515	DGD	C4E-C5E-C6E-O5E
22	B	606	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1A-CGA-O2A-C1
25	d	410	DGD	C2B-C1B-O2G-C2G
27	i	101	LMG	C11-C10-O7-C8
25	a	410	DGD	C4E-C5E-C6E-O5E
25	c	515	DGD	C4E-C5E-C6E-O5E
27	C	518	LMG	C4-C5-C6-O5
31	d	401	PHO	O1A-CGA-O2A-C1
22	h	101	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	d	402	PHO	O1D-CGD-O2D-CED
31	D	401	PHO	CBA-CGA-O2A-C1
22	b	619	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
27	d	408	LMG	C4-C5-C6-O5
27	C	518	LMG	C10-C11-C12-C13
27	c	522	LMG	O6-C5-C6-O5
27	c	518	LMG	C4-C5-C6-O5
27	c	522	LMG	C4-C5-C6-O5
22	b	615	CLA	C5-C6-C7-C8
22	B	615	CLA	C5-C6-C7-C8
22	B	608	CLA	C13-C15-C16-C17
22	A	404	CLA	C10-C11-C12-C13
22	C	508	CLA	C5-C6-C7-C8
22	B	611	CLA	C5-C6-C7-C8
22	b	612	CLA	C13-C15-C16-C17
22	H	101	CLA	C3-C5-C6-C7
25	d	410	DGD	C2D-C1D-O3G-C3G
25	D	410	DGD	C2D-C1D-O3G-C3G
25	c	516	DGD	O2G-C2G-C3G-O3G
25	C	516	DGD	O2G-C2G-C3G-O3G
27	m	101	LMG	O1-C7-C8-O7
31	D	401	PHO	O1A-CGA-O2A-C1
22	B	604	CLA	C2-C3-C5-C6
22	b	608	CLA	C2-C3-C5-C6
22	C	510	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	b	613	CLA	C14-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C9
22	B	607	CLA	C6-C7-C8-C9
22	C	508	CLA	C6-C7-C8-C9
22	B	605	CLA	O1D-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	C13-C15-C16-C17
22	b	613	CLA	C2A-CAA-CBA-CGA
24	J	102	BCR	C37-C22-C23-C24
24	j	102	BCR	C37-C22-C23-C24
24	B	617	BCR	C37-C22-C23-C24
24	b	621	BCR	C37-C22-C23-C24
24	f	102	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	y	101	BCR	C7-C8-C9-C34
24	g	101	BCR	C7-C8-C9-C34
24	B	617	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C10
22	b	609	CLA	O1D-CGD-O2D-CED
27	E	101	LMG	O9-C10-O7-C8
27	c	522	LMG	C11-C10-O7-C8
27	I	101	LMG	C11-C10-O7-C8
25	d	410	DGD	C1B-C2B-C3B-C4B
29	b	602	SQD	O10-C23-O48-C46
22	b	619	CLA	O1A-CGA-O2A-C1
31	d	402	PHO	C15-C16-C17-C18
22	c	508	CLA	C5-C6-C7-C8
22	b	613	CLA	C8-C10-C11-C12
22	D	405	CLA	C15-C16-C17-C18
22	b	619	CLA	C10-C11-C12-C13
22	b	610	CLA	C15-C16-C17-C18
22	c	511	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	CBA-CGA-O2A-C1
22	a	406	CLA	C10-C11-C12-C13
22	D	405	CLA	C13-C15-C16-C17
22	b	619	CLA	C5-C6-C7-C8
22	C	520	CLA	C13-C15-C16-C17
22	C	520	CLA	C15-C16-C17-C18
22	B	606	CLA	C15-C16-C17-C18
25	D	410	DGD	C1B-C2B-C3B-C4B
27	C	521	LMG	C10-C11-C12-C13
27	B	621	LMG	C10-C11-C12-C13
27	A	414	LMG	C28-C29-C30-C31
22	C	501	CLA	C8-C10-C11-C12
22	c	520	CLA	C15-C16-C17-C18
22	c	505	CLA	C5-C6-C7-C8
22	c	505	CLA	C13-C15-C16-C17
22	B	609	CLA	C8-C10-C11-C12
22	d	405	CLA	C13-C15-C16-C17
22	d	405	CLA	C15-C16-C17-C18
22	c	503	CLA	C10-C11-C12-C13
22	C	505	CLA	C15-C16-C17-C18
22	B	615	CLA	C10-C11-C12-C13
22	C	503	CLA	C10-C11-C12-C13
22	B	603	CLA	C13-C15-C16-C17
22	B	611	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C13-C15-C16-C17
31	D	402	PHO	C15-C16-C17-C18
23	D	407	PL9	C27-C28-C29-C30
27	d	412	LMG	C10-C11-C12-C13
27	c	522	LMG	C10-C11-C12-C13
27	b	625	LMG	C10-C11-C12-C13
27	c	518	LMG	C10-C11-C12-C13
27	c	518	LMG	C28-C29-C30-C31
25	c	515	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C28-C29-C30-C31
27	D	412	LMG	C10-C11-C12-C13
22	c	501	CLA	C15-C16-C17-C18
22	c	520	CLA	C13-C15-C16-C17
22	C	509	CLA	C15-C16-C17-C18
22	c	509	CLA	C15-C16-C17-C18
22	c	507	CLA	C15-C16-C17-C18
22	B	606	CLA	C13-C15-C16-C17
22	C	511	CLA	O1D-CGD-O2D-CED
31	D	402	PHO	O1D-CGD-O2D-CED
25	C	517	DGD	O1B-C1B-O2G-C2G
27	D	408	LMG	C4-C5-C6-O5
22	C	501	CLA	C15-C16-C17-C18
22	B	601	CLA	C13-C15-C16-C17
22	b	605	CLA	C13-C15-C16-C17
22	C	507	CLA	C10-C11-C12-C13
22	b	610	CLA	C13-C15-C16-C17
22	c	506	CLA	C5-C6-C7-C8
25	C	515	DGD	C1B-C2B-C3B-C4B
22	C	505	CLA	C13-C15-C16-C17
22	c	504	CLA	C10-C11-C12-C13
22	c	507	CLA	C10-C11-C12-C13
22	C	512	CLA	C15-C16-C17-C18
22	c	505	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C10-C8-C7
22	c	510	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	A	402	CLA	C3-C5-C6-C7
29	B	626	SQD	O10-C23-O48-C46
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	C10-C11-C12-C13
22	c	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C15-C16-C17-C18
22	B	607	CLA	C15-C16-C17-C18
22	A	404	CLA	C15-C16-C17-C18
22	A	403	CLA	C15-C16-C17-C18
22	C	512	CLA	O1A-CGA-O2A-C1
29	a	415	SQD	O5-C1-O6-C44
27	I	101	LMG	O6-C1-O1-C7
27	i	101	LMG	O6-C1-O1-C7
29	A	412	SQD	O5-C1-O6-C44
23	D	407	PL9	C29-C31-C32-C33
23	d	407	PL9	C29-C31-C32-C33
27	a	402	LMG	C28-C29-C30-C31
22	B	607	CLA	O1D-CGD-O2D-CED
25	c	517	DGD	O1B-C1B-O2G-C2G
27	d	409	LMG	O9-C10-O7-C8
22	a	404	CLA	C3-C5-C6-C7
22	c	501	CLA	C8-C10-C11-C12
22	C	506	CLA	C5-C6-C7-C8
22	b	611	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	c	510	CLA	C5-C6-C7-C8
22	C	507	CLA	C15-C16-C17-C18
22	a	405	CLA	C15-C16-C17-C18
22	b	608	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
25	b	624	DGD	C1B-C2B-C3B-C4B
22	C	510	CLA	C5-C6-C7-C8
22	b	611	CLA	C5-C6-C7-C8
22	B	615	CLA	C13-C15-C16-C17
22	b	619	CLA	C13-C15-C16-C17
22	b	618	CLA	C13-C15-C16-C17
22	c	511	CLA	O1A-CGA-O2A-C1
27	C	521	LMG	C11-C10-O7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	504	CLA	C10-C11-C12-C13
22	B	612	CLA	C5-C6-C7-C8
22	a	406	CLA	C15-C16-C17-C18
22	B	607	CLA	C5-C6-C7-C8
22	c	512	CLA	C15-C16-C17-C18
26	C	519	LHG	C3-O3-P-O6
26	C	519	LHG	C4-O6-P-O3
26	c	519	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
26	c	519	LHG	C4-O6-P-O3
29	a	415	SQD	C7-C8-C9-C10
22	C	511	CLA	CBA-CGA-O2A-C1
27	i	101	LMG	C29-C28-O8-C9
22	C	505	CLA	C5-C6-C7-C8
27	c	522	LMG	O9-C10-O7-C8
27	D	409	LMG	O9-C10-O7-C8
22	c	520	CLA	C10-C11-C12-C13
22	C	520	CLA	C10-C11-C12-C13
22	b	609	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C2A-CAA-CBA-CGA
27	d	412	LMG	O6-C5-C6-O5
29	b	602	SQD	C24-C23-O48-C46
22	B	604	CLA	CBA-CGA-O2A-C1
30	b	604	LMT	O1'-C1-C2-C3
27	C	518	LMG	C29-C30-C31-C32
30	I	102	LMT	C6-C7-C8-C9
25	C	516	DGD	C2A-C3A-C4A-C5A
22	b	619	CLA	C3-C5-C6-C7
29	b	602	SQD	C11-C10-C9-C8
30	i	102	LMT	C6-C7-C8-C9
25	a	410	DGD	C8B-C9B-CAB-CBB
29	F	103	SQD	C12-C13-C14-C15
27	b	625	LMG	C31-C32-C33-C34
25	b	624	DGD	C3B-C4B-C5B-C6B
27	A	410	LMG	C34-C35-C36-C37
25	c	515	DGD	C3B-C4B-C5B-C6B
27	B	621	LMG	C31-C32-C33-C34
27	A	414	LMG	C30-C31-C32-C33
27	I	101	LMG	C29-C28-O8-C9
27	c	522	LMG	C12-C13-C14-C15
25	B	625	DGD	C5B-C6B-C7B-C8B
25	d	410	DGD	C5B-C6B-C7B-C8B
25	d	410	DGD	CEB-CFB-CGB-CHB
25	D	410	DGD	C4B-C5B-C6B-C7B
25	D	410	DGD	C5B-C6B-C7B-C8B
25	D	410	DGD	CEB-CFB-CGB-CHB
27	I	101	LMG	C14-C15-C16-C17
27	i	101	LMG	C12-C13-C14-C15
25	B	620	DGD	C6B-C7B-C8B-C9B
25	b	601	DGD	C5B-C6B-C7B-C8B
25	b	601	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C9-C8-O7-C10
22	b	611	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	O1D-CGD-O2D-CED
29	F	103	SQD	O49-C7-O47-C45
27	C	521	LMG	O9-C10-O7-C8
22	C	501	CLA	C10-C11-C12-C13
22	b	616	CLA	C5-C6-C7-C8
25	B	620	DGD	C1B-C2B-C3B-C4B
27	a	412	LMG	C34-C35-C36-C37
25	d	410	DGD	C4B-C5B-C6B-C7B
25	d	410	DGD	CCB-CDB-CEB-CFB
25	b	624	DGD	C6B-C7B-C8B-C9B
29	B	626	SQD	C9-C10-C11-C12
27	c	518	LMG	C29-C30-C31-C32
25	D	410	DGD	CCB-CDB-CEB-CFB
27	I	101	LMG	C12-C13-C14-C15
27	C	521	LMG	C12-C13-C14-C15
27	i	101	LMG	C16-C17-C18-C19
25	C	515	DGD	C3B-C4B-C5B-C6B
25	A	408	DGD	C8B-C9B-CAB-CBB
29	f	103	SQD	C12-C13-C14-C15
25	c	516	DGD	C2A-C3A-C4A-C5A
25	c	516	DGD	C4A-C5A-C6A-C7A
25	B	625	DGD	C9B-CAB-CBB-CCB
27	A	410	LMG	C33-C34-C35-C36
25	B	620	DGD	C3B-C4B-C5B-C6B
27	a	402	LMG	C30-C31-C32-C33
25	b	624	DGD	C7A-C8A-C9A-CAA
29	B	626	SQD	C11-C10-C9-C8
27	d	409	LMG	C14-C15-C16-C17
25	c	515	DGD	C3A-C4A-C5A-C6A
27	a	402	LMG	C32-C33-C34-C35
29	A	412	SQD	C14-C15-C16-C17
22	c	509	CLA	C3-C5-C6-C7
25	C	515	DGD	C1A-C2A-C3A-C4A
24	j	102	BCR	C20-C21-C22-C23
25	d	410	DGD	C2E-C1E-O5D-C6D
25	D	410	DGD	C2E-C1E-O5D-C6D
24	x	101	BCR	C11-C10-C9-C8
27	I	101	LMG	C2-C1-O1-C7
27	i	101	LMG	C2-C1-O1-C7
24	H	102	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
27	a	412	LMG	C33-C34-C35-C36
29	b	602	SQD	C9-C10-C11-C12
29	a	415	SQD	C14-C15-C16-C17
25	d	410	DGD	C7B-C8B-C9B-CAB
25	C	515	DGD	C3A-C4A-C5A-C6A
25	B	620	DGD	C7A-C8A-C9A-CAA
27	D	408	LMG	C18-C19-C20-C21
22	B	604	CLA	O1A-CGA-O2A-C1
27	a	402	LMG	O6-C5-C6-O5
22	c	509	CLA	C4-C3-C5-C6
25	D	410	DGD	C7B-C8B-C9B-CAB
27	i	101	LMG	C14-C15-C16-C17
27	A	414	LMG	C18-C19-C20-C21
27	D	409	LMG	C14-C15-C16-C17
25	C	517	DGD	CBA-CCA-CDA-CEA
27	a	402	LMG	C18-C19-C20-C21
23	A	406	PL9	C33-C34-C36-C37
22	H	101	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
22	b	615	CLA	O1D-CGD-O2D-CED
29	a	415	SQD	C27-C28-C29-C30
27	A	410	LMG	C31-C32-C33-C34
27	d	409	LMG	C19-C20-C21-C22
25	C	515	DGD	C2B-C3B-C4B-C5B
27	A	414	LMG	C32-C33-C34-C35
27	D	409	LMG	C19-C20-C21-C22
25	C	517	DGD	C9B-CAB-CBB-CCB
29	A	412	SQD	C27-C28-C29-C30
27	D	408	LMG	C31-C32-C33-C34
27	d	408	LMG	C18-C19-C20-C21
22	c	520	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2A-CAA-CBA-CGA
22	b	608	CLA	O1A-CGA-O2A-C1
24	B	617	BCR	C7-C8-C9-C34
24	b	621	BCR	C7-C8-C9-C34
27	a	412	LMG	C31-C32-C33-C34
25	a	410	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
29	F	103	SQD	C11-C12-C13-C14
27	I	101	LMG	C16-C17-C18-C19
27	A	414	LMG	C15-C16-C17-C18
29	f	103	SQD	C11-C12-C13-C14
27	d	408	LMG	C31-C32-C33-C34
22	B	615	CLA	C3-C5-C6-C7
29	f	103	SQD	O49-C7-O47-C45
25	c	517	DGD	C9B-CAB-CBB-CCB
25	c	517	DGD	CAB-CBB-CCB-CDB
25	c	515	DGD	C2B-C3B-C4B-C5B
25	c	517	DGD	C1A-C2A-C3A-C4A
27	D	408	LMG	C28-C29-C30-C31
27	c	518	LMG	C12-C13-C14-C15
27	d	409	LMG	C15-C16-C17-C18
25	C	515	DGD	C4A-C5A-C6A-C7A
25	b	601	DGD	C4A-C5A-C6A-C7A
25	A	408	DGD	C5B-C6B-C7B-C8B
25	D	410	DGD	O6E-C1E-O5D-C6D
27	D	408	LMG	O6-C1-O1-C7
27	d	408	LMG	O6-C1-O1-C7
22	H	101	CLA	C5-C6-C7-C8
27	I	101	LMG	C13-C14-C15-C16
25	c	515	DGD	C4A-C5A-C6A-C7A
25	C	517	DGD	CAB-CBB-CCB-CDB
22	B	611	CLA	O1D-CGD-O2D-CED
27	a	412	LMG	C14-C15-C16-C17
25	B	625	DGD	C4A-C5A-C6A-C7A
27	i	101	LMG	C13-C14-C15-C16
25	C	516	DGD	C4A-C5A-C6A-C7A
27	m	101	LMG	C29-C30-C31-C32
26	a	411	LHG	C25-C26-C27-C28
30	B	628	LMT	C7-C8-C9-C10
25	B	625	DGD	C1A-C2A-C3A-C4A
27	d	408	LMG	C28-C29-C30-C31
22	c	503	CLA	C5-C6-C7-C8
22	C	503	CLA	C5-C6-C7-C8
22	C	511	CLA	O1A-CGA-O2A-C1
22	c	520	CLA	CBA-CGA-O2A-C1
29	B	626	SQD	C24-C23-O48-C46
25	c	517	DGD	CBA-CCA-CDA-CEA
25	d	410	DGD	C5A-C6A-C7A-C8A
27	D	409	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	b	619	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	h	101	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	a	405	CLA	C3A-C2A-CAA-CBA
25	b	624	DGD	C5B-C6B-C7B-C8B
27	A	410	LMG	C30-C31-C32-C33
27	d	409	LMG	C32-C33-C34-C35
30	b	604	LMT	C7-C8-C9-C10
27	a	412	LMG	C30-C31-C32-C33
27	A	410	LMG	C14-C15-C16-C17
25	D	410	DGD	C5A-C6A-C7A-C8A
27	D	409	LMG	C15-C16-C17-C18
27	a	402	LMG	C15-C16-C17-C18
27	D	408	LMG	C30-C31-C32-C33
27	M	101	LMG	O6-C5-C6-O5
30	B	623	LMT	C1-C2-C3-C4
25	B	625	DGD	C2B-C3B-C4B-C5B
27	C	518	LMG	C12-C13-C14-C15
30	B	628	LMT	O1'-C1-C2-C3
25	B	620	DGD	O6D-C5D-C6D-O5D
27	E	101	LMG	C28-C29-C30-C31
30	b	626	LMT	C1-C2-C3-C4
27	D	412	LMG	C17-C18-C19-C20
22	C	509	CLA	C4-C3-C5-C6
29	b	602	SQD	C8-C7-O47-C45
29	B	626	SQD	C8-C7-O47-C45
27	e	101	LMG	C15-C16-C17-C18
25	B	620	DGD	C5B-C6B-C7B-C8B
27	d	408	LMG	C36-C37-C38-C39
25	b	624	DGD	C4B-C5B-C6B-C7B
27	E	101	LMG	C15-C16-C17-C18
29	B	622	SQD	C9-C10-C11-C12
25	c	515	DGD	C1A-C2A-C3A-C4A
29	A	412	SQD	C7-C8-C9-C10
25	b	624	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
22	a	407	CLA	C10-C11-C12-C13
25	c	516	DGD	CAB-CBB-CCB-CDB
26	A	409	LHG	C25-C26-C27-C28
27	d	408	LMG	C30-C31-C32-C33
27	m	101	LMG	C29-C28-O8-C9
27	C	521	LMG	C4-C5-C6-O5
29	d	403	SQD	C9-C10-C11-C12
25	C	516	DGD	CAB-CBB-CCB-CDB
26	A	409	LHG	O9-C7-O7-C5
22	c	508	CLA	C2-C1-O2A-CGA
27	c	518	LMG	C34-C35-C36-C37
25	D	410	DGD	C3A-C4A-C5A-C6A
27	M	101	LMG	C29-C30-C31-C32
25	b	601	DGD	C2B-C3B-C4B-C5B
27	C	518	LMG	C34-C35-C36-C37
27	A	414	LMG	C31-C32-C33-C34
22	B	612	CLA	C16-C17-C18-C19
24	b	623	BCR	C23-C24-C25-C30
24	J	102	BCR	C5-C6-C7-C8
24	b	620	BCR	C5-C6-C7-C8
24	F	102	BCR	C5-C6-C7-C8
24	j	102	BCR	C5-C6-C7-C8
24	B	617	BCR	C23-C24-C25-C30
24	c	513	BCR	C5-C6-C7-C8
24	c	514	BCR	C23-C24-C25-C26
24	c	514	BCR	C23-C24-C25-C30
24	x	101	BCR	C1-C6-C7-C8
24	x	101	BCR	C5-C6-C7-C8
24	b	621	BCR	C23-C24-C25-C30
24	f	102	BCR	C5-C6-C7-C8
24	y	101	BCR	C23-C24-C25-C26
24	y	101	BCR	C23-C24-C25-C30
24	C	513	BCR	C5-C6-C7-C8
24	C	514	BCR	C23-C24-C25-C26
24	C	514	BCR	C23-C24-C25-C30
24	B	616	BCR	C5-C6-C7-C8
24	g	101	BCR	C23-C24-C25-C26
24	g	101	BCR	C23-C24-C25-C30
24	H	102	BCR	C1-C6-C7-C8
24	H	102	BCR	C5-C6-C7-C8
26	c	519	LHG	C24-C25-C26-C27
25	C	515	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
26	C	519	LHG	C24-C23-O8-C6
22	C	520	CLA	CBA-CGA-O2A-C1
22	C	511	CLA	C13-C15-C16-C17
22	H	101	CLA	C13-C15-C16-C17
22	B	603	CLA	C8-C10-C11-C12
22	b	607	CLA	C8-C10-C11-C12
22	h	101	CLA	C5-C6-C7-C8
22	h	101	CLA	C13-C15-C16-C17
25	c	517	DGD	C2B-C1B-O2G-C2G
29	F	103	SQD	C10-C11-C12-C13
27	D	412	LMG	O6-C5-C6-O5
25	a	410	DGD	C1B-C2B-C3B-C4B
25	C	517	DGD	C1A-C2A-C3A-C4A
25	D	410	DGD	C2A-C3A-C4A-C5A
25	D	410	DGD	C6B-C7B-C8B-C9B
29	b	602	SQD	C11-C12-C13-C14
26	C	519	LHG	C24-C25-C26-C27
25	d	410	DGD	C2A-C3A-C4A-C5A
25	d	410	DGD	CAB-CBB-CCB-CDB
30	b	627	LMT	C2B-C1B-O1B-C4'
22	c	512	CLA	C4-C3-C5-C6
22	C	510	CLA	C11-C10-C8-C7
31	d	402	PHO	C11-C10-C8-C7
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C12-C13-C15
22	C	509	CLA	C2-C3-C5-C6
23	a	408	PL9	C33-C34-C36-C37
22	a	406	CLA	C6-C7-C8-C10
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C11-C10-C8-C7
22	D	405	CLA	C12-C13-C15-C16
22	A	404	CLA	C6-C7-C8-C10
22	C	512	CLA	C2-C3-C5-C6
22	C	512	CLA	C12-C13-C15-C16
31	D	402	PHO	C11-C10-C8-C7
22	c	512	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C12-C13-C15-C16
22	c	502	CLA	C3-C5-C6-C7
22	a	405	CLA	C3-C5-C6-C7
22	c	520	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	C4B-C5B-C6B-C7B
27	D	412	LMG	C31-C32-C33-C34
22	b	605	CLA	C16-C17-C18-C20
27	m	101	LMG	O6-C5-C6-O5
30	B	624	LMT	C2B-C1B-O1B-C4'
26	a	411	LHG	O9-C7-O7-C5
25	c	516	DGD	C1A-C2A-C3A-C4A
27	e	101	LMG	C28-C29-C30-C31
25	A	408	DGD	C1B-C2B-C3B-C4B
22	c	508	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
22	b	614	CLA	CBA-CGA-O2A-C1
25	d	410	DGD	C3A-C4A-C5A-C6A
25	D	410	DGD	CAB-CBB-CCB-CDB
26	a	411	LHG	C30-C31-C32-C33
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C10-C11-C12-C13
22	c	512	CLA	C13-C15-C16-C17
27	A	410	LMG	C15-C16-C17-C18
23	D	407	PL9	C47-C48-C49-C51
23	d	407	PL9	C47-C48-C49-C51
27	d	412	LMG	C34-C35-C36-C37
26	A	409	LHG	C30-C31-C32-C33
25	b	601	DGD	C1A-C2A-C3A-C4A
27	C	521	LMG	O6-C5-C6-O5
22	C	512	CLA	C13-C15-C16-C17
29	B	626	SQD	C12-C13-C14-C15
27	c	518	LMG	C36-C37-C38-C39
29	f	103	SQD	C10-C11-C12-C13
27	D	408	LMG	C36-C37-C38-C39
27	d	412	LMG	C31-C32-C33-C34
29	B	626	SQD	C11-C12-C13-C14
25	C	515	DGD	C4B-C5B-C6B-C7B
25	c	515	DGD	C2A-C3A-C4A-C5A
27	A	414	LMG	C17-C18-C19-C20
26	c	519	LHG	C24-C23-O8-C6
22	b	616	CLA	C16-C17-C18-C19
25	d	410	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
22	c	505	CLA	C10-C11-C12-C13
22	A	405	CLA	C10-C11-C12-C13
22	d	406	CLA	C15-C16-C17-C18
29	b	602	SQD	C12-C13-C14-C15
27	D	412	LMG	C34-C35-C36-C37
25	C	516	DGD	C1A-C2A-C3A-C4A
27	e	101	LMG	C11-C10-O7-C8
27	E	101	LMG	C11-C10-O7-C8
26	A	409	LHG	C8-C7-O7-C5
25	C	517	DGD	C2B-C1B-O2G-C2G
26	a	411	LHG	C8-C7-O7-C5
22	D	406	CLA	C15-C16-C17-C18
22	c	506	CLA	CBD-CGD-O2D-CED
27	a	412	LMG	C15-C16-C17-C18
25	A	408	DGD	C3B-C4B-C5B-C6B
27	a	402	LMG	C31-C32-C33-C34
30	B	623	LMT	O1'-C1-C2-C3
27	C	518	LMG	C36-C37-C38-C39
27	D	408	LMG	C2-C1-O1-C7
29	a	415	SQD	O47-C45-C46-O48
29	A	413	SQD	O6-C44-C45-O47
29	a	401	SQD	O6-C44-C45-O47
27	A	410	LMG	O1-C7-C8-O7
27	I	101	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7
27	i	101	LMG	O1-C7-C8-O7
29	A	412	SQD	O47-C45-C46-O48
27	A	414	LMG	O6-C5-C6-O5
27	d	412	LMG	C17-C18-C19-C20
27	B	621	LMG	C34-C35-C36-C37
27	D	409	LMG	C13-C14-C15-C16
27	D	408	LMG	C15-C16-C17-C18
22	C	509	CLA	O1D-CGD-O2D-CED
27	c	522	LMG	C16-C17-C18-C19
25	d	410	DGD	C6B-C7B-C8B-C9B
27	C	521	LMG	C16-C17-C18-C19
22	b	605	CLA	C10-C11-C12-C13
23	j	101	PL9	C15-C14-C16-C17
22	C	512	CLA	C4-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
25	C	517	DGD	C3B-C4B-C5B-C6B
22	C	510	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
31	d	402	PHO	C11-C10-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	b	605	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C12-C13-C14
22	d	405	CLA	C14-C13-C15-C16
22	B	602	CLA	C11-C12-C13-C14
22	A	402	CLA	C11-C12-C13-C14
22	c	503	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	C	506	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C12-C13-C14
22	c	510	CLA	C11-C10-C8-C9
22	a	406	CLA	C6-C7-C8-C9
22	A	404	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
31	D	402	PHO	C11-C10-C8-C9
22	a	405	CLA	C6-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	C	509	CLA	C3-C5-C6-C7
22	C	501	CLA	C2A-CAA-CBA-CGA
22	C	520	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
27	e	101	LMG	O6-C5-C6-O5
22	C	520	CLA	O1A-CGA-O2A-C1
22	C	501	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C1A-C2A-CAA-CBA
22	b	619	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C20
22	B	603	CLA	C15-C16-C17-C18
25	a	410	DGD	C3B-C4B-C5B-C6B
25	A	408	DGD	C4B-C5B-C6B-C7B
27	D	408	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	a	411	LHG	C23-C24-C25-C26
22	C	502	CLA	C3-C5-C6-C7
25	c	515	DGD	C4B-C5B-C6B-C7B
22	c	511	CLA	C13-C15-C16-C17
27	b	625	LMG	C13-C14-C15-C16
27	d	409	LMG	C13-C14-C15-C16
27	B	621	LMG	C13-C14-C15-C16
25	a	410	DGD	C4B-C5B-C6B-C7B
25	D	410	DGD	CAA-CBA-CCA-CDA
27	d	408	LMG	C17-C18-C19-C20
22	b	616	CLA	C16-C17-C18-C20
25	c	517	DGD	C3B-C4B-C5B-C6B
27	i	101	LMG	C18-C19-C20-C21
25	d	410	DGD	C8B-C9B-CAB-CBB
27	e	101	LMG	C18-C19-C20-C21
29	A	412	SQD	C17-C18-C19-C20
27	d	408	LMG	C32-C33-C34-C35
22	B	601	CLA	C10-C11-C12-C13
27	I	101	LMG	C18-C19-C20-C21
30	b	626	LMT	O1'-C1-C2-C3
22	c	508	CLA	O1A-CGA-O2A-C1
26	c	519	LHG	C25-C26-C27-C28
27	b	625	LMG	C34-C35-C36-C37
22	B	609	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20
27	E	101	LMG	O6-C5-C6-O5
22	A	403	CLA	C3-C5-C6-C7
29	b	602	SQD	C44-C45-C46-O48
27	c	522	LMG	C7-C8-C9-O8
25	c	516	DGD	C1G-C2G-C3G-O3G
25	a	410	DGD	C1G-C2G-C3G-O3G
25	c	517	DGD	O1G-C1G-C2G-C3G
27	b	625	LMG	C7-C8-C9-O8
27	d	409	LMG	O1-C7-C8-C9
27	I	101	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	C	521	LMG	C7-C8-C9-O8
27	i	101	LMG	O1-C7-C8-C9
25	A	408	DGD	C1G-C2G-C3G-O3G
27	B	621	LMG	C7-C8-C9-O8
27	D	409	LMG	O1-C7-C8-C9
25	C	517	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C7-C8-C9-O8
27	D	408	LMG	O1-C7-C8-C9
27	d	408	LMG	O1-C7-C8-C9
29	a	401	SQD	C10-C11-C12-C13
25	B	625	DGD	O6D-C5D-C6D-O5D
27	d	409	LMG	C8-C7-O1-C1
27	D	409	LMG	C8-C7-O1-C1
29	B	622	SQD	C45-C44-O6-C1
29	d	403	SQD	C45-C44-O6-C1
29	a	415	SQD	C17-C18-C19-C20
27	a	402	LMG	C17-C18-C19-C20
22	b	608	CLA	C15-C16-C17-C18
25	d	410	DGD	CDB-CEB-CFB-CGB
26	c	519	LHG	C11-C10-C9-C8
25	D	410	DGD	C8B-C9B-CAB-CBB
27	D	408	LMG	C32-C33-C34-C35
22	C	504	CLA	CBA-CGA-O2A-C1
22	C	506	CLA	CBD-CGD-O2D-CED
29	A	412	SQD	C10-C11-C12-C13
22	b	614	CLA	O1A-CGA-O2A-C1
22	C	504	CLA	C4-C3-C5-C6
26	A	409	LHG	C23-C24-C25-C26
22	B	613	CLA	C16-C17-C18-C20
22	B	601	CLA	C16-C17-C18-C20
22	d	406	CLA	CBA-CGA-O2A-C1
22	c	504	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	C5A-C6A-C7A-C8A
25	D	410	DGD	CDB-CEB-CFB-CGB
22	C	502	CLA	C13-C15-C16-C17
22	A	405	CLA	C5-C6-C7-C8
22	c	503	CLA	C8-C10-C11-C12
22	C	503	CLA	C8-C10-C11-C12
22	b	607	CLA	C15-C16-C17-C18
30	i	102	LMT	C5'-C4'-O1B-C1B
30	I	102	LMT	C5'-C4'-O1B-C1B
25	d	410	DGD	C1G-C2G-O2G-C1B
27	c	518	LMG	C9-C8-O7-C10
25	D	410	DGD	C1G-C2G-O2G-C1B
27	E	101	LMG	C7-C8-O7-C10
22	c	509	CLA	O1D-CGD-O2D-CED
31	d	401	PHO	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	C2-C1-O2A-CGA
22	C	508	CLA	C2-C1-O2A-CGA
30	B	624	LMT	O5B-C1B-O1B-C4'
29	A	413	SQD	C10-C11-C12-C13
22	a	407	CLA	C13-C15-C16-C17
22	C	510	CLA	CBA-CGA-O2A-C1
22	D	406	CLA	CBA-CGA-O2A-C1
27	d	409	LMG	C28-C29-C30-C31
25	D	410	DGD	CBA-CCA-CDA-CEA
27	d	408	LMG	C19-C20-C21-C22
22	c	502	CLA	C13-C15-C16-C17
22	a	407	CLA	C5-C6-C7-C8
26	C	519	LHG	C11-C10-C9-C8
27	i	101	LMG	O10-C28-O8-C9
27	i	101	LMG	C17-C18-C19-C20
22	B	615	CLA	C15-C16-C17-C18
27	d	408	LMG	C2-C1-O1-C7
27	a	412	LMG	O1-C7-C8-O7
25	c	517	DGD	O1G-C1G-C2G-O2G
25	C	515	DGD	O2G-C2G-C3G-O3G
25	C	517	DGD	O1G-C1G-C2G-O2G
25	d	410	DGD	CBA-CCA-CDA-CEA
27	c	522	LMG	C17-C18-C19-C20
30	b	627	LMT	O5B-C1B-O1B-C4'
22	c	504	CLA	C4-C3-C5-C6
27	d	408	LMG	C15-C16-C17-C18
22	b	616	CLA	C11-C10-C8-C7
22	b	606	CLA	C11-C12-C13-C15
31	d	402	PHO	C12-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C7
22	C	502	CLA	C11-C12-C13-C15
22	B	609	CLA	C11-C12-C13-C15
22	C	504	CLA	C6-C7-C8-C10
22	d	405	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C7
22	H	101	CLA	C6-C7-C8-C10
22	B	605	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C12-C13-C15
22	c	504	CLA	C2-C3-C5-C6
22	c	504	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10
22	c	510	CLA	C12-C13-C15-C16
22	B	607	CLA	C6-C7-C8-C10
22	b	619	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	h	101	CLA	C6-C7-C8-C10
31	D	402	PHO	C12-C13-C15-C16
22	b	618	CLA	C11-C10-C8-C7
22	b	618	CLA	C12-C13-C15-C16
27	E	101	LMG	O7-C10-C11-C12
22	C	511	CLA	C3-C5-C6-C7
27	C	521	LMG	C17-C18-C19-C20
22	C	510	CLA	C14-C13-C15-C16
22	c	505	CLA	C14-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C9
22	b	606	CLA	C11-C12-C13-C14
31	d	402	PHO	C14-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16
22	C	504	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C9
22	c	502	CLA	C11-C12-C13-C14
22	c	502	CLA	C14-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	504	CLA	C14-C13-C15-C16
22	c	510	CLA	C14-C13-C15-C16
22	B	608	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	D	405	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C9
22	A	403	CLA	C6-C7-C8-C9
31	D	402	PHO	C14-C13-C15-C16
22	b	618	CLA	C11-C10-C8-C9
22	b	618	CLA	C14-C13-C15-C16
22	C	508	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	C15-C16-C17-C18
25	c	517	DGD	CFA-CGA-CHA-CIA
27	E	101	LMG	C17-C18-C19-C20
23	J	101	PL9	C27-C28-C29-C30
25	d	410	DGD	C4E-C5E-C6E-O5E
24	F	102	BCR	C37-C22-C23-C24
22	B	609	CLA	C16-C17-C18-C19
22	C	511	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20
26	C	519	LHG	C25-C26-C27-C28
25	c	516	DGD	O6D-C5D-C6D-O5D
25	C	516	DGD	O6D-C5D-C6D-O5D
27	A	410	LMG	C11-C10-O7-C8
27	I	101	LMG	C31-C32-C33-C34
27	E	101	LMG	C19-C20-C21-C22
27	A	414	LMG	C11-C12-C13-C14
27	D	412	LMG	C38-C39-C40-C41
27	d	412	LMG	C38-C39-C40-C41
22	C	504	CLA	C15-C16-C17-C18
22	b	617	CLA	C5-C6-C7-C8
29	a	415	SQD	C31-C32-C33-C34
27	e	101	LMG	C19-C20-C21-C22
27	d	409	LMG	C29-C30-C31-C32
27	d	408	LMG	C13-C14-C15-C16
27	A	410	LMG	C8-C9-O8-C28
23	D	407	PL9	C24-C26-C27-C28
27	I	101	LMG	C17-C18-C19-C20
27	C	521	LMG	C34-C35-C36-C37
22	C	504	CLA	O1A-CGA-O2A-C1
25	b	601	DGD	O6D-C5D-C6D-O5D
23	D	407	PL9	C15-C14-C16-C17
23	d	407	PL9	C35-C34-C36-C37
22	C	504	CLA	C2-C3-C5-C6
27	E	101	LMG	C18-C19-C20-C21
22	b	617	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
27	i	101	LMG	C31-C32-C33-C34
25	C	517	DGD	CDB-CEB-CFB-CGB
27	D	408	LMG	C19-C20-C21-C22
22	B	613	CLA	C5-C6-C7-C8
22	c	504	CLA	C15-C16-C17-C18
22	B	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	a	412	LMG	C11-C10-O7-C8
22	b	613	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
27	D	409	LMG	C28-C29-C30-C31
27	b	625	LMG	C17-C18-C19-C20
27	B	621	LMG	C17-C18-C19-C20
27	a	402	LMG	C11-C12-C13-C14
31	D	401	PHO	CBD-CGD-O2D-CED
22	d	406	CLA	O1A-CGA-O2A-C1
22	A	402	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
22	b	608	CLA	C10-C11-C12-C13
27	D	412	LMG	C19-C20-C21-C22
30	B	628	LMT	C2-C3-C4-C5
23	j	101	PL9	C27-C28-C29-C30
25	c	516	DGD	C4D-C5D-C6D-O5D
25	C	516	DGD	C4D-C5D-C6D-O5D
27	c	522	LMG	C34-C35-C36-C37
27	e	101	LMG	C17-C18-C19-C20
22	B	613	CLA	C16-C17-C18-C19
29	a	415	SQD	C10-C11-C12-C13
27	D	409	LMG	C29-C30-C31-C32
22	b	617	CLA	C15-C16-C17-C18
22	b	619	CLA	C15-C16-C17-C18
27	a	412	LMG	O1-C7-C8-C9
29	A	413	SQD	O6-C44-C45-C46
25	B	625	DGD	C1G-C2G-C3G-O3G
25	d	410	DGD	C1G-C2G-C3G-O3G
29	a	401	SQD	O6-C44-C45-C46
29	B	626	SQD	C44-C45-C46-O48
27	A	410	LMG	O1-C7-C8-C9
27	c	518	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
25	C	516	DGD	C1G-C2G-C3G-O3G
27	m	101	LMG	O1-C7-C8-C9
29	A	412	SQD	C44-C45-C46-O48
25	D	410	DGD	C3B-C4B-C5B-C6B
25	D	410	DGD	C1A-C2A-C3A-C4A
23	D	407	PL9	C32-C33-C34-C36
22	B	610	CLA	O1A-CGA-O2A-C1
25	C	516	DGD	C3A-C4A-C5A-C6A
23	D	407	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
23	d	407	PL9	C15-C14-C16-C17
22	B	601	CLA	C16-C17-C18-C19
25	d	410	DGD	C3B-C4B-C5B-C6B
22	b	619	CLA	C8-C10-C11-C12
27	a	412	LMG	C4-C5-C6-O5
22	D	406	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	C2A-CAA-CBA-CGA
29	A	412	SQD	C31-C32-C33-C34
23	d	407	PL9	C27-C28-C29-C30
22	c	504	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	C5-C6-C7-C8
27	d	412	LMG	C19-C20-C21-C22
22	C	510	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	C3-C5-C6-C7
29	b	602	SQD	O47-C45-C46-O48
27	c	522	LMG	O7-C8-C9-O8
27	c	518	LMG	O1-C7-C8-O7
27	M	101	LMG	O7-C8-C9-O8
27	C	521	LMG	O7-C8-C9-O8
25	c	515	DGD	O2G-C2G-C3G-O3G
27	B	621	LMG	O7-C8-C9-O8
27	C	518	LMG	O1-C7-C8-O7
27	m	101	LMG	O7-C8-C9-O8
29	d	403	SQD	O6-C44-C45-O47
22	B	613	CLA	C15-C16-C17-C18
25	c	516	DGD	C3A-C4A-C5A-C6A
22	C	511	CLA	C16-C17-C18-C19
29	f	103	SQD	C29-C30-C31-C32
22	c	501	CLA	C13-C15-C16-C17
29	b	602	SQD	C10-C11-C12-C13
25	C	517	DGD	CFA-CGA-CHA-CIA
22	b	613	CLA	C2-C1-O2A-CGA
31	D	401	PHO	C2-C1-O2A-CGA
22	a	405	CLA	C2-C1-O2A-CGA
31	d	401	PHO	C6-C7-C8-C9
22	C	511	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
22	B	605	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	c	511	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	D	405	CLA	C6-C7-C8-C9
22	a	404	CLA	C11-C12-C13-C14
26	a	411	LHG	C2-C3-O3-P
26	C	519	LHG	O10-C23-O8-C6
27	A	410	LMG	C4-C5-C6-O5
22	b	613	CLA	C16-C17-C18-C19
24	b	623	BCR	C1-C6-C7-C8
24	b	623	BCR	C5-C6-C7-C8
24	b	623	BCR	C23-C24-C25-C26
24	K	102	BCR	C23-C24-C25-C26
24	K	102	BCR	C23-C24-C25-C30
24	c	513	BCR	C23-C24-C25-C30
24	c	514	BCR	C5-C6-C7-C8
24	B	619	BCR	C1-C6-C7-C8
24	B	619	BCR	C5-C6-C7-C8
24	B	619	BCR	C23-C24-C25-C26
24	B	619	BCR	C23-C24-C25-C30
24	a	409	BCR	C1-C6-C7-C8
24	a	409	BCR	C5-C6-C7-C8
24	a	409	BCR	C23-C24-C25-C26
24	a	409	BCR	C23-C24-C25-C30
24	C	513	BCR	C23-C24-C25-C30
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C5-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	A	407	BCR	C23-C24-C25-C30
22	A	405	CLA	C13-C15-C16-C17
27	m	101	LMG	C30-C31-C32-C33
27	e	101	LMG	O7-C10-C11-C12
24	J	102	BCR	C7-C8-C9-C10
24	c	514	BCR	C7-C8-C9-C10
24	H	102	BCR	C7-C8-C9-C10
22	c	508	CLA	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
29	b	602	SQD	C17-C18-C19-C20
22	B	609	CLA	C10-C11-C12-C13
29	a	415	SQD	C15-C16-C17-C18
25	c	516	DGD	C4B-C5B-C6B-C7B
25	b	601	DGD	C5A-C6A-C7A-C8A
29	A	412	SQD	C15-C16-C17-C18
31	D	402	PHO	C10-C11-C12-C13
22	C	501	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C12-C13-C15
22	c	501	CLA	C11-C12-C13-C15
22	c	505	CLA	C12-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	504	CLA	C12-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C10
22	C	511	CLA	C11-C12-C13-C15
22	C	511	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C12-C13-C15-C16
22	H	101	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C7
22	c	504	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C7
22	B	610	CLA	C11-C10-C8-C7
22	c	511	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	b	619	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	A	403	CLA	C12-C13-C15-C16
22	a	405	CLA	C12-C13-C15-C16
22	b	612	CLA	C12-C13-C15-C16
22	c	506	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	C10-C11-C12-C13
22	C	511	CLA	C5-C6-C7-C8
22	B	613	CLA	C2A-CAA-CBA-CGA
29	B	626	SQD	C10-C11-C12-C13
24	b	621	BCR	C20-C21-C22-C37
22	b	617	CLA	C16-C17-C18-C19
22	B	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	c	517	DGD	CDB-CEB-CFB-CGB
27	A	410	LMG	C20-C21-C22-C23
27	c	518	LMG	C13-C14-C15-C16
27	d	408	LMG	C20-C21-C22-C23
22	B	604	CLA	C15-C16-C17-C18
22	b	608	CLA	C5-C6-C7-C8
22	c	511	CLA	C5-C6-C7-C8
22	B	611	CLA	C10-C11-C12-C13
31	d	401	PHO	C2B-C3B-CAB-CBB
31	d	401	PHO	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
31	D	401	PHO	CAD-CBD-CGD-O2D
22	C	507	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D
25	D	410	DGD	C2B-C3B-C4B-C5B
27	C	518	LMG	C13-C14-C15-C16
27	b	625	LMG	C28-C29-C30-C31
30	B	627	LMT	C5'-C4'-O1B-C1B
25	C	516	DGD	C4B-C5B-C6B-C7B
23	A	406	PL9	C35-C34-C36-C37
27	A	410	LMG	O6-C1-O1-C7
31	D	401	PHO	C5-C6-C7-C8
30	b	603	LMT	C5'-C4'-O1B-C1B
29	a	415	SQD	C44-C45-C46-O48
25	D	410	DGD	C1G-C2G-C3G-O3G
27	M	101	LMG	O1-C7-C8-C9
26	A	409	LHG	C2-C3-O3-P
25	b	601	DGD	C1G-C2G-C3G-O3G
31	d	401	PHO	CBD-CGD-O2D-CED
27	I	101	LMG	O10-C28-O8-C9
26	c	519	LHG	O6-C4-C5-O7
22	b	615	CLA	C10-C11-C12-C13
22	b	613	CLA	C10-C11-C12-C13
27	d	409	LMG	C31-C32-C33-C34
25	d	410	DGD	CAA-CBA-CCA-CDA
25	d	410	DGD	C2B-C3B-C4B-C5B
27	D	408	LMG	C16-C17-C18-C19
26	C	519	LHG	O2-C2-C3-O3
29	b	602	SQD	O49-C7-O47-C45
22	c	505	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	A	404	CLA	CHA-CBD-CGD-O1D
22	b	612	CLA	CHA-CBD-CGD-O1D
25	d	410	DGD	C1A-C2A-C3A-C4A
26	c	519	LHG	O10-C23-O8-C6
22	b	613	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	O1A-CGA-O2A-C1
24	J	102	BCR	C20-C21-C22-C23
25	a	410	DGD	O2G-C2G-C3G-O3G
29	B	622	SQD	O6-C44-C45-O47
27	d	409	LMG	C36-C37-C38-C39
22	b	613	CLA	C5-C6-C7-C8
25	D	410	DGD	C4A-C5A-C6A-C7A
23	A	406	PL9	C4-C3-C7-C8
23	a	408	PL9	C4-C3-C7-C8
29	F	103	SQD	C29-C30-C31-C32
29	B	626	SQD	C17-C18-C19-C20
29	B	626	SQD	O49-C7-O47-C45
22	B	608	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	C	506	CLA	O1D-CGD-O2D-CED
29	B	622	SQD	C5-C6-S-O8
29	d	403	SQD	C5-C6-S-O8
29	A	413	SQD	C9-C10-C11-C12
31	d	401	PHO	C5-C6-C7-C8
22	b	607	CLA	CBA-CGA-O2A-C1
24	j	102	BCR	C7-C8-C9-C10
22	A	402	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
29	A	413	SQD	C32-C33-C34-C35
25	b	624	DGD	C5A-C6A-C7A-C8A
27	C	521	LMG	C35-C36-C37-C38
23	d	407	PL9	C20-C19-C21-C22
23	a	408	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
27	a	412	LMG	C20-C21-C22-C23
27	D	409	LMG	C31-C32-C33-C34
22	B	603	CLA	O1A-CGA-O2A-C1
26	C	519	LHG	C3-O3-P-O5
26	C	519	LHG	C4-O6-P-O5
26	c	519	LHG	C3-O3-P-O5
26	c	519	LHG	C4-O6-P-O5
22	A	405	CLA	C16-C17-C18-C19
31	d	402	PHO	C10-C11-C12-C13
22	B	614	CLA	CBA-CGA-O2A-C1
26	C	519	LHG	O6-C4-C5-C6
26	c	519	LHG	O6-C4-C5-C6
29	a	401	SQD	C9-C10-C11-C12
22	b	616	CLA	C13-C15-C16-C17
22	C	506	CLA	C3-C5-C6-C7
31	D	401	PHO	O1D-CGD-O2D-CED
27	c	522	LMG	C35-C36-C37-C38
25	c	515	DGD	C5A-C6A-C7A-C8A
22	a	407	CLA	C16-C17-C18-C19
22	c	505	CLA	CAD-CBD-CGD-O1D
29	a	401	SQD	C5-C6-S-O9
22	c	503	CLA	CAD-CBD-CGD-O1D
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
29	B	622	SQD	O5-C5-C6-S
22	A	404	CLA	C5-C6-C7-C8
29	f	103	SQD	C24-C25-C26-C27
25	B	620	DGD	C5A-C6A-C7A-C8A
26	c	519	LHG	C7-C8-C9-C10
27	D	408	LMG	C20-C21-C22-C23
27	A	410	LMG	C29-C30-C31-C32
29	B	622	SQD	C10-C11-C12-C13
22	A	403	CLA	C4-C3-C5-C6
27	a	412	LMG	C10-C11-C12-C13
26	C	519	LHG	O6-C4-C5-O7
22	c	520	CLA	C6-C7-C8-C10
22	c	505	CLA	C11-C12-C13-C15
31	d	402	PHO	C6-C7-C8-C10
22	B	609	CLA	C12-C13-C15-C16
22	D	406	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
22	A	405	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	d	406	CLA	C11-C10-C8-C7
22	b	611	CLA	C6-C7-C8-C10
22	b	611	CLA	C11-C12-C13-C15
22	b	613	CLA	C11-C12-C13-C15
22	b	613	CLA	C12-C13-C15-C16
22	C	509	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C12-C13-C15
22	c	509	CLA	C6-C7-C8-C10
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	h	101	CLA	C11-C10-C8-C7
27	a	412	LMG	C16-C17-C18-C19
29	d	403	SQD	C10-C11-C12-C13
25	d	410	DGD	C4A-C5A-C6A-C7A
22	B	609	CLA	C5-C6-C7-C8
34	v	201	HEM	C4D-C3D-CAD-CBD
27	A	410	LMG	O6-C5-C6-O5
29	d	403	SQD	O6-C44-C45-C46
27	b	625	LMG	O7-C8-C9-O8
25	d	410	DGD	O2G-C2G-C3G-O3G
29	B	626	SQD	O47-C45-C46-O48
25	D	410	DGD	O2G-C2G-C3G-O3G
25	A	408	DGD	O2G-C2G-C3G-O3G
27	D	409	LMG	O1-C7-C8-O7
29	a	401	SQD	C32-C33-C34-C35
30	b	604	LMT	C2-C3-C4-C5
27	A	410	LMG	C10-C11-C12-C13
27	a	412	LMG	C8-C7-O1-C1
27	A	410	LMG	C8-C7-O1-C1
22	C	507	CLA	C5-C6-C7-C8
22	c	507	CLA	C5-C6-C7-C8
22	c	506	CLA	C3-C5-C6-C7
27	E	101	LMG	C31-C32-C33-C34
22	b	607	CLA	O1A-CGA-O2A-C1
22	b	615	CLA	C4-C3-C5-C6
22	B	611	CLA	C4-C3-C5-C6
27	a	412	LMG	O6-C5-C6-O5
27	B	621	LMG	C12-C13-C14-C15
22	A	403	CLA	C5-C6-C7-C8
22	C	501	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C9
22	d	405	CLA	C6-C7-C8-C9
22	C	511	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C9
22	B	612	CLA	C11-C12-C13-C14
31	D	401	PHO	C6-C7-C8-C9
22	B	615	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	c	511	CLA	C14-C13-C15-C16
22	B	608	CLA	C11-C12-C13-C14
22	b	619	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
22	A	403	CLA	C14-C13-C15-C16
22	a	405	CLA	C14-C13-C15-C16
22	b	618	CLA	C6-C7-C8-C9
25	C	515	DGD	C5A-C6A-C7A-C8A
23	d	407	PL9	C24-C26-C27-C28
22	B	614	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
22	c	508	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	C2A-CAA-CBA-CGA
29	a	415	SQD	C11-C10-C9-C8
27	c	518	LMG	C32-C33-C34-C35
24	f	102	BCR	C7-C8-C9-C34
31	d	402	PHO	C13-C15-C16-C17
27	A	410	LMG	C16-C17-C18-C19
27	A	414	LMG	C16-C17-C18-C19
27	B	621	LMG	C28-C29-C30-C31
24	C	514	BCR	C7-C8-C9-C10
25	b	624	DGD	CCA-CDA-CEA-CFA
25	c	516	DGD	C6A-C7A-C8A-C9A
22	C	504	CLA	C8-C10-C11-C12
27	c	522	LMG	C30-C31-C32-C33
25	c	516	DGD	C7B-C8B-C9B-CAB
27	A	410	LMG	C38-C39-C40-C41
30	b	603	LMT	C4'-C5'-C6'-O6'
29	A	412	SQD	C11-C10-C9-C8
22	b	617	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C10-C11-C12-C13
27	C	518	LMG	C32-C33-C34-C35
27	a	402	LMG	C16-C17-C18-C19
27	D	408	LMG	C13-C14-C15-C16
25	B	620	DGD	CAB-CBB-CCB-CDB
22	a	406	CLA	C5-C6-C7-C8
25	c	517	DGD	C3G-C2G-O2G-C1B
26	A	409	LHG	C6-C5-O7-C7
25	C	517	DGD	C3G-C2G-O2G-C1B
26	a	411	LHG	C6-C5-O7-C7
22	b	617	CLA	C2A-CAA-CBA-CGA
22	b	616	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C2-C1-O2A-CGA
22	B	612	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
22	C	511	CLA	CAA-CBA-CGA-O2A
31	d	401	PHO	O1D-CGD-O2D-CED
25	d	410	DGD	O6E-C5E-C6E-O5E
22	b	609	CLA	C13-C15-C16-C17
23	J	101	PL9	C15-C14-C16-C17
24	K	102	BCR	C1-C6-C7-C8
24	c	513	BCR	C23-C24-C25-C26
24	c	514	BCR	C1-C6-C7-C8
24	c	521	BCR	C23-C24-C25-C30
24	C	513	BCR	C23-C24-C25-C26
24	C	514	BCR	C1-C6-C7-C8
23	D	407	PL9	C13-C14-C16-C17
23	d	407	PL9	C13-C14-C16-C17
27	a	412	LMG	C11-C12-C13-C14
27	b	625	LMG	C15-C16-C17-C18
25	d	410	DGD	CBB-CCB-CDB-CEB
22	c	510	CLA	C3-C5-C6-C7
25	c	515	DGD	O6D-C1D-O3G-C3G
27	A	414	LMG	C12-C13-C14-C15
25	C	516	DGD	C7B-C8B-C9B-CAB
27	d	409	LMG	O1-C7-C8-O7
25	D	410	DGD	CBB-CCB-CDB-CEB
26	A	409	LHG	C3-O3-P-O6
26	a	411	LHG	C3-O3-P-O6
27	b	625	LMG	C12-C13-C14-C15
22	b	616	CLA	C8-C10-C11-C12
29	a	401	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C16-C17-C18-C20
22	a	407	CLA	C16-C17-C18-C20
25	C	515	DGD	C5B-C6B-C7B-C8B
27	e	101	LMG	O1-C7-C8-C9
29	B	622	SQD	O6-C44-C45-C46
29	A	413	SQD	C12-C13-C14-C15
22	H	101	CLA	C11-C10-C8-C7
22	H	101	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C7
22	D	405	CLA	C11-C10-C8-C7
22	C	520	CLA	C6-C7-C8-C10
31	D	402	PHO	C6-C7-C8-C10
27	C	521	LMG	C32-C33-C34-C35
27	d	412	LMG	C16-C17-C18-C19
25	b	624	DGD	C4A-C5A-C6A-C7A
22	c	505	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	C	505	CLA	C11-C12-C13-C14
22	b	611	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	B	615	CLA	C14-C13-C15-C16
22	B	607	CLA	C11-C12-C13-C14
22	b	619	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
27	e	101	LMG	C31-C32-C33-C34
22	b	609	CLA	CBA-CGA-O2A-C1
27	a	412	LMG	C35-C36-C37-C38
25	c	517	DGD	C8B-C9B-CAB-CBB
26	C	519	LHG	C7-C8-C9-C10
22	B	609	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	O2-C2-C3-O3
27	D	409	LMG	C36-C37-C38-C39
22	c	511	CLA	CAA-CBA-CGA-O2A
24	x	101	BCR	C7-C8-C9-C10
26	C	519	LHG	C1-C2-C3-O3
26	c	519	LHG	C1-C2-C3-O3
23	d	407	PL9	C32-C33-C34-C36
25	c	515	DGD	C5B-C6B-C7B-C8B
22	B	605	CLA	CBA-CGA-O2A-C1
22	h	101	CLA	CBA-CGA-O2A-C1
25	b	624	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
27	c	522	LMG	C32-C33-C34-C35
22	b	616	CLA	C10-C11-C12-C13
31	D	402	PHO	C13-C15-C16-C17
27	a	412	LMG	C29-C30-C31-C32
25	B	625	DGD	O6D-C1D-O3G-C3G
25	a	410	DGD	O6E-C1E-O5D-C6D
27	M	101	LMG	O6-C1-O1-C7
22	c	504	CLA	C8-C10-C11-C12
22	b	609	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	O10-C28-O8-C9
29	a	401	SQD	C26-C27-C28-C29
24	j	102	BCR	C18-C19-C20-C21
23	D	407	PL9	C20-C19-C21-C22
22	B	610	CLA	C4-C3-C5-C6
22	a	405	CLA	C4-C3-C5-C6
27	a	412	LMG	C8-C9-O8-C28
25	C	517	DGD	C8B-C9B-CAB-CBB
22	A	402	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
22	A	403	CLA	C2-C1-O2A-CGA
30	B	624	LMT	C6-C7-C8-C9
27	M	101	LMG	C16-C17-C18-C19
22	b	617	CLA	C4C-C3C-CAC-CBC
22	B	602	CLA	C15-C16-C17-C18
27	a	402	LMG	C12-C13-C14-C15
22	b	618	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C31-C32-C33-C34
22	D	405	CLA	C3A-C2A-CAA-CBA
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
22	B	602	CLA	C16-C17-C18-C19
25	d	410	DGD	C8A-C9A-CAA-CBA
27	D	408	LMG	C29-C30-C31-C32
27	A	410	LMG	C17-C18-C19-C20
29	f	103	SQD	C14-C15-C16-C17
27	e	101	LMG	C30-C31-C32-C33
27	B	621	LMG	C15-C16-C17-C18
25	b	624	DGD	CAB-CBB-CCB-CDB
25	B	620	DGD	CCA-CDA-CEA-CFA
31	d	402	PHO	C6-C7-C8-C9
22	B	614	CLA	C6-C7-C8-C9
22	d	406	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C6-C7-C8-C9
22	b	612	CLA	C11-C12-C13-C14
22	b	606	CLA	C16-C17-C18-C19
25	B	625	DGD	C2A-C3A-C4A-C5A
29	F	103	SQD	C24-C25-C26-C27
22	B	605	CLA	C13-C15-C16-C17
27	A	410	LMG	C35-C36-C37-C38
27	D	409	LMG	C18-C19-C20-C21
27	a	412	LMG	C38-C39-C40-C41
27	d	412	LMG	O1-C7-C8-C9
27	d	408	LMG	C16-C17-C18-C19
22	d	406	CLA	C2A-CAA-CBA-CGA
22	c	510	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	O1A-CGA-O2A-C1
22	h	101	CLA	O1A-CGA-O2A-C1
27	a	412	LMG	O6-C1-O1-C7
25	c	516	DGD	O6E-C1E-O5D-C6D
25	C	515	DGD	O6D-C1D-O3G-C3G
25	b	601	DGD	O6D-C1D-O3G-C3G
25	C	516	DGD	O6E-C1E-O5D-C6D
27	m	101	LMG	O6-C1-O1-C7
29	F	103	SQD	C9-C10-C11-C12
25	b	601	DGD	C2A-C3A-C4A-C5A
24	F	102	BCR	C21-C22-C23-C24
27	m	101	LMG	C31-C32-C33-C34
27	M	101	LMG	C9-C8-O7-C10
26	A	409	LHG	C4-C5-O7-C7
27	m	101	LMG	C9-C8-O7-C10
22	d	405	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	c	505	CLA	C6-C7-C8-C10
22	B	601	CLA	C12-C13-C15-C16
22	b	605	CLA	C12-C13-C15-C16
22	d	405	CLA	C11-C10-C8-C7
22	c	508	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C12-C13-C15
22	a	407	CLA	C11-C10-C8-C7
27	C	521	LMG	C30-C31-C32-C33
22	B	612	CLA	C8-C10-C11-C12
27	D	408	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	a	410	DGD	C2A-C3A-C4A-C5A
27	A	410	LMG	C11-C12-C13-C14
29	f	103	SQD	C9-C10-C11-C12
22	b	608	CLA	C8-C10-C11-C12
22	B	612	CLA	C13-C15-C16-C17
27	D	412	LMG	C16-C17-C18-C19
29	a	415	SQD	C12-C13-C14-C15
22	b	606	CLA	C15-C16-C17-C18
22	B	604	CLA	C8-C10-C11-C12
22	B	607	CLA	C13-C15-C16-C17
22	b	614	CLA	C4-C3-C5-C6
22	c	509	CLA	C13-C15-C16-C17
25	C	517	DGD	C4A-C5A-C6A-C7A
27	d	408	LMG	C29-C30-C31-C32
25	c	517	DGD	CBB-CCB-CDB-CEB
22	c	509	CLA	C16-C17-C18-C19
23	D	407	PL9	C40-C39-C41-C42
25	B	620	DGD	C7B-C8B-C9B-CAB
30	b	604	LMT	C6-C7-C8-C9
22	b	618	CLA	O1A-CGA-O2A-C1
30	B	624	LMT	O5'-C5'-C6'-O6'
22	b	615	CLA	C6-C7-C8-C9
22	c	503	CLA	C6-C7-C8-C9
22	C	503	CLA	C6-C7-C8-C9
22	A	403	CLA	C11-C10-C8-C9
22	h	101	CLA	C11-C12-C13-C14
25	A	408	DGD	C2A-C3A-C4A-C5A
27	D	412	LMG	C36-C37-C38-C39
22	D	406	CLA	C2A-CAA-CBA-CGA
22	b	609	CLA	C16-C17-C18-C20
24	K	102	BCR	C5-C6-C7-C8
24	F	102	BCR	C23-C24-C25-C30
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
24	b	622	BCR	C1-C6-C7-C8
24	b	622	BCR	C23-C24-C25-C30
24	c	521	BCR	C1-C6-C7-C8
24	c	521	BCR	C23-C24-C25-C26
24	b	621	BCR	C1-C6-C7-C8
24	b	621	BCR	C5-C6-C7-C8
24	f	102	BCR	C23-C24-C25-C30
24	B	618	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C23-C24-C25-C30
24	C	514	BCR	C5-C6-C7-C8
24	g	101	BCR	C1-C6-C7-C8
24	g	101	BCR	C5-C6-C7-C8
25	C	515	DGD	C1G-C2G-C3G-O3G
27	D	412	LMG	C32-C33-C34-C35
22	b	615	CLA	C2-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
22	B	611	CLA	C2-C3-C5-C6
25	C	516	DGD	C6A-C7A-C8A-C9A
27	d	412	LMG	C8-C7-O1-C1
25	B	625	DGD	C2G-C3G-O3G-C1D
25	b	601	DGD	C2G-C3G-O3G-C1D
22	C	502	CLA	CBA-CGA-O2A-C1
22	B	605	CLA	C16-C17-C18-C20
22	C	510	CLA	C4-C3-C5-C6
22	b	615	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
22	c	503	CLA	C6-C7-C8-C10
22	C	503	CLA	C6-C7-C8-C10
22	B	608	CLA	C11-C12-C13-C15
22	B	611	CLA	C6-C7-C8-C10
22	b	612	CLA	C11-C12-C13-C15
27	B	621	LMG	C35-C36-C37-C38
27	M	101	LMG	C30-C31-C32-C33
22	C	509	CLA	C13-C15-C16-C17
25	C	516	DGD	C2E-C1E-O5D-C6D
25	B	625	DGD	CAB-CBB-CCB-CDB
22	C	502	CLA	O1A-CGA-O2A-C1
27	A	410	LMG	O7-C10-C11-C12
22	B	612	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	C2A-CAA-CBA-CGA
22	H	101	CLA	CBA-CGA-O2A-C1
27	a	412	LMG	O7-C10-C11-C12
23	d	407	PL9	C40-C39-C41-C42
22	c	510	CLA	C4-C3-C5-C6
22	b	611	CLA	C13-C15-C16-C17
27	M	101	LMG	O10-C28-O8-C9
22	b	614	CLA	C2-C3-C5-C6
22	A	403	CLA	C2-C3-C5-C6
29	A	412	SQD	C16-C17-C18-C19
26	C	519	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	CAA-CBA-CGA-O2A
27	E	101	LMG	C30-C31-C32-C33
22	c	520	CLA	C6-C7-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	d	405	CLA	C11-C10-C8-C9
22	A	405	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C12-C13-C14
22	D	405	CLA	C11-C10-C8-C9
22	C	520	CLA	C6-C7-C8-C9
22	h	101	CLA	C11-C10-C8-C9
22	a	407	CLA	C11-C10-C8-C9
22	a	405	CLA	C11-C10-C8-C9
27	m	101	LMG	C16-C17-C18-C19
22	c	520	CLA	C3A-C2A-CAA-CBA
22	C	520	CLA	C3A-C2A-CAA-CBA
25	b	601	DGD	C4E-C5E-C6E-O5E
29	a	415	SQD	C16-C17-C18-C19
22	H	101	CLA	O1A-CGA-O2A-C1
26	c	519	LHG	O7-C7-C8-C9
22	C	506	CLA	CAA-CBA-CGA-O2A
22	B	611	CLA	CAA-CBA-CGA-O2A
22	C	501	CLA	CAD-CBD-CGD-O2D
22	c	501	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	b	608	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	CAD-CBD-CGD-O2D
26	a	411	LHG	C4-C5-O7-C7
25	D	410	DGD	C4E-C5E-C6E-O5E
22	c	511	CLA	C2-C1-O2A-CGA
22	d	405	CLA	CAA-CBA-CGA-O2A
22	C	501	CLA	C13-C15-C16-C17
22	C	501	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
27	A	414	LMG	O7-C10-C11-C12
25	C	517	DGD	O1G-C1A-C2A-C3A
24	f	102	BCR	C21-C22-C23-C24
29	F	103	SQD	C14-C15-C16-C17
25	d	410	DGD	C9B-CAB-CBB-CCB
27	c	518	LMG	C7-C8-C9-O8
27	I	101	LMG	C7-C8-C9-O8
25	c	515	DGD	C1G-C2G-C3G-O3G
27	C	518	LMG	C7-C8-C9-O8
27	c	522	LMG	O8-C28-C29-C30
27	d	412	LMG	C11-C12-C13-C14
27	E	101	LMG	C33-C34-C35-C36
31	d	402	PHO	O2A-C1-C2-C3
22	C	511	CLA	O2A-C1-C2-C3
22	B	615	CLA	O2A-C1-C2-C3
22	c	511	CLA	O2A-C1-C2-C3
22	b	619	CLA	O2A-C1-C2-C3
31	D	402	PHO	O2A-C1-C2-C3
31	d	401	PHO	C4B-C3B-CAB-CBB
31	D	401	PHO	C4B-C3B-CAB-CBB
27	b	625	LMG	C29-C28-O8-C9
22	b	606	CLA	C2A-CAA-CBA-CGA
25	c	517	DGD	O1G-C1A-C2A-C3A
22	b	606	CLA	C16-C17-C18-C20
22	c	509	CLA	C16-C17-C18-C20
30	B	623	LMT	C4-C5-C6-C7
29	A	412	SQD	C12-C13-C14-C15
22	c	508	CLA	CHA-CBD-CGD-O1D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	H	101	CLA	CHA-CBD-CGD-O1D
22	H	101	CLA	CHA-CBD-CGD-O2D
31	D	401	PHO	CHA-CBD-CGD-O2D
22	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	A	404	CLA	CHA-CBD-CGD-O2D
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	h	101	CLA	CHA-CBD-CGD-O1D
22	h	101	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CHA-CBD-CGD-O1D
22	c	512	CLA	CHA-CBD-CGD-O2D
29	a	401	SQD	O47-C7-C8-C9
22	c	506	CLA	CAA-CBA-CGA-O2A
27	a	402	LMG	O7-C10-C11-C12
25	b	601	DGD	CAB-CBB-CCB-CDB
22	C	502	CLA	C16-C17-C18-C20
29	A	413	SQD	O47-C7-C8-C9
27	C	521	LMG	O8-C28-C29-C30
27	b	625	LMG	O1-C7-C8-O7
27	e	101	LMG	O1-C7-C8-O7
27	B	621	LMG	O1-C7-C8-O7
27	c	518	LMG	C17-C18-C19-C20
22	c	501	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	CAA-CBA-CGA-O2A
30	B	627	LMT	C4'-C5'-C6'-O6'
22	b	609	CLA	C15-C16-C17-C18
27	d	412	LMG	C36-C37-C38-C39
29	B	622	SQD	O47-C7-C8-C9
22	A	405	CLA	C4-C3-C5-C6
22	a	407	CLA	C4-C3-C5-C6
22	b	609	CLA	C6-C7-C8-C10
22	c	510	CLA	C2-C3-C5-C6
22	c	507	CLA	C11-C12-C13-C15
22	c	506	CLA	C11-C12-C13-C15
22	h	101	CLA	C11-C12-C13-C15
22	C	501	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C19
29	a	401	SQD	C17-C18-C19-C20
25	A	408	DGD	O6E-C1E-O5D-C6D
22	c	509	CLA	CAA-CBA-CGA-O2A
22	B	601	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C10-C8-C9
22	D	406	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C12-C13-C14
22	B	611	CLA	C6-C7-C8-C9
31	D	402	PHO	C6-C7-C8-C9
22	b	618	CLA	C11-C12-C13-C14
25	a	410	DGD	O1A-C1A-O1G-C1G
26	c	519	LHG	C11-C12-C13-C14
22	D	405	CLA	CAA-CBA-CGA-O2A
29	d	403	SQD	O47-C7-C8-C9
22	A	404	CLA	O1A-CGA-O2A-C1
22	A	404	CLA	CBA-CGA-O2A-C1
24	b	623	BCR	C7-C8-C9-C34
22	b	616	CLA	CAA-CBA-CGA-O1A
29	B	622	SQD	O49-C7-C8-C9
22	B	605	CLA	C16-C17-C18-C19
26	A	409	LHG	C24-C25-C26-C27
22	B	601	CLA	C1A-C2A-CAA-CBA
22	C	520	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
29	d	403	SQD	O49-C7-C8-C9
25	a	410	DGD	C4A-C5A-C6A-C7A
22	B	603	CLA	C4C-C3C-CAC-CBC
27	B	621	LMG	C29-C28-O8-C9
27	E	101	LMG	O1-C7-C8-C9
22	B	602	CLA	C2A-CAA-CBA-CGA
22	h	101	CLA	C2A-CAA-CBA-CGA
27	e	101	LMG	C14-C15-C16-C17
27	C	521	LMG	O10-C28-C29-C30
22	B	612	CLA	CAA-CBA-CGA-O1A
22	c	509	CLA	CAA-CBA-CGA-O1A
29	A	413	SQD	C26-C27-C28-C29
27	D	409	LMG	O7-C10-C11-C12
25	C	517	DGD	O2G-C1B-C2B-C3B
27	d	412	LMG	O9-C10-C11-C12
22	b	615	CLA	CAA-CBA-CGA-O1A
22	C	506	CLA	CAA-CBA-CGA-O1A
22	c	506	CLA	CAA-CBA-CGA-O1A
22	B	611	CLA	CAA-CBA-CGA-O1A
22	a	405	CLA	C2-C3-C5-C6
25	c	516	DGD	C2E-C1E-O5D-C6D
25	a	410	DGD	C2E-C1E-O5D-C6D
25	A	408	DGD	C2E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
25	c	517	DGD	C5B-C6B-C7B-C8B
26	A	409	LHG	C3-O3-P-O5
26	a	411	LHG	C3-O3-P-O5
22	B	613	CLA	C4C-C3C-CAC-CBC
22	d	405	CLA	CAA-CBA-CGA-O1A
22	C	509	CLA	CAA-CBA-CGA-O1A
27	D	412	LMG	O9-C10-C11-C12
22	B	601	CLA	CAA-CBA-CGA-O2A
22	h	101	CLA	CAA-CBA-CGA-O2A
24	b	622	BCR	C23-C24-C25-C26
24	c	521	BCR	C5-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C26
22	B	613	CLA	C2C-C3C-CAC-CBC
22	b	606	CLA	C8-C10-C11-C12
22	c	501	CLA	CAA-CBA-CGA-O1A
27	c	522	LMG	O10-C28-C29-C30
29	A	413	SQD	O49-C7-C8-C9
29	A	413	SQD	C17-C18-C19-C20
25	B	620	DGD	C4A-C5A-C6A-C7A
25	c	517	DGD	C4A-C5A-C6A-C7A
22	C	501	CLA	C16-C17-C18-C19
22	c	502	CLA	C16-C17-C18-C20
22	B	610	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C20
29	a	401	SQD	C23-C24-C25-C26
22	C	501	CLA	CAA-CBA-CGA-O1A
29	a	401	SQD	O49-C7-C8-C9
25	C	517	DGD	C4B-C5B-C6B-C7B
27	D	409	LMG	C34-C35-C36-C37
29	A	413	SQD	C5-C6-S-O9
27	M	101	LMG	C7-C8-O7-C10
22	B	608	CLA	CAD-CBD-CGD-O1D
22	c	509	CLA	CAD-CBD-CGD-O1D
29	d	403	SQD	O5-C5-C6-S
22	b	612	CLA	CAD-CBD-CGD-O1D
27	a	402	LMG	O9-C10-C11-C12
22	B	604	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
22	b	609	CLA	C6-C7-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
22	B	601	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	c	517	DGD	O2G-C1B-C2B-C3B
22	B	609	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
27	M	101	LMG	O8-C28-C29-C30
25	B	620	DGD	O2G-C1B-C2B-C3B
25	D	410	DGD	C8A-C9A-CAA-CBA
25	b	601	DGD	C8B-C9B-CAB-CBB
25	C	517	DGD	CBB-CCB-CDB-CEB
29	A	412	SQD	C9-C10-C11-C12
29	a	415	SQD	C32-C33-C34-C35
27	m	101	LMG	C17-C18-C19-C20
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	605	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	CAA-CBA-CGA-O2A
26	C	519	LHG	C11-C12-C13-C14
27	M	101	LMG	C17-C18-C19-C20
30	B	628	LMT	C6-C7-C8-C9
22	b	606	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C10-C8-C7
23	A	406	PL9	C28-C29-C31-C32
22	C	506	CLA	C11-C12-C13-C15
22	b	619	CLA	C11-C12-C13-C15
22	h	101	CLA	C12-C13-C15-C16
22	c	512	CLA	C11-C12-C13-C15
27	a	412	LMG	O9-C10-C11-C12
27	A	410	LMG	O9-C10-C11-C12
22	c	504	CLA	CAA-CBA-CGA-O2A
22	B	613	CLA	CAA-CBA-CGA-O1A
22	D	405	CLA	CAA-CBA-CGA-O1A
29	A	412	SQD	O49-C7-C8-C9
27	a	412	LMG	C13-C14-C15-C16
25	b	624	DGD	O2G-C1B-C2B-C3B
27	d	409	LMG	O7-C10-C11-C12
27	m	101	LMG	O8-C28-C29-C30
22	D	406	CLA	C8-C10-C11-C12
29	B	626	SQD	C15-C16-C17-C18
27	d	409	LMG	C34-C35-C36-C37
22	B	609	CLA	CAA-CBA-CGA-O1A
22	C	504	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	b	617	CLA	CAA-CBA-CGA-O1A
22	c	504	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	CBA-CGA-O2A-C1
30	b	627	LMT	O5'-C5'-C6'-O6'
29	b	602	SQD	O47-C7-C8-C9
22	B	602	CLA	C8-C10-C11-C12
29	a	415	SQD	O49-C7-C8-C9
22	H	101	CLA	C2A-CAA-CBA-CGA
22	c	502	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	CAA-CBA-CGA-O1A
27	E	101	LMG	C14-C15-C16-C17

There are no ring outliers.

79 monomers are involved in 296 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	D	407	PL9	12	0
22	C	501	CLA	7	0
24	K	102	BCR	3	0
24	J	102	BCR	1	0
26	C	519	LHG	2	0
22	C	510	CLA	10	0
34	V	201	HEM	3	0
22	B	613	CLA	4	0
29	A	413	SQD	3	0
22	B	604	CLA	7	0
24	F	102	BCR	4	0
22	B	601	CLA	1	0
24	B	617	BCR	2	0
25	B	625	DGD	2	0
29	F	103	SQD	3	0
29	B	626	SQD	1	0
22	B	609	CLA	3	0
22	C	504	CLA	4	0
27	A	410	LMG	2	0
22	B	602	CLA	11	0
29	A	412	SQD	3	0
22	D	406	CLA	3	0
22	C	511	CLA	2	0
27	I	101	LMG	1	0
22	A	405	CLA	9	0
24	B	619	BCR	1	0

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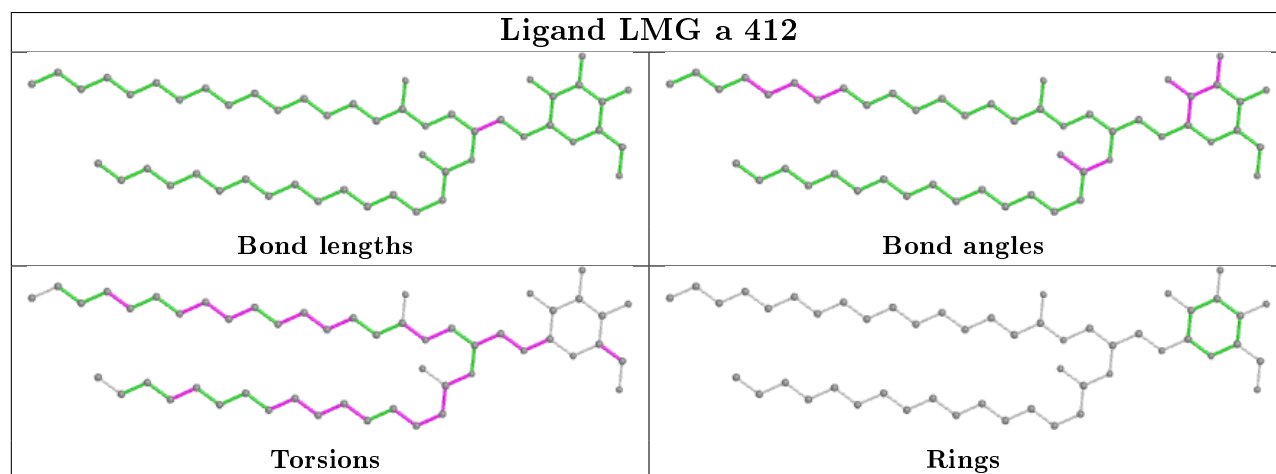
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	M	101	LMG	2	0
22	A	402	CLA	10	0
23	A	406	PL9	4	0
22	H	101	CLA	9	0
27	E	101	LMG	1	0
22	B	605	CLA	7	0
25	C	515	DGD	3	0
34	F	101	HEM	4	0
22	C	506	CLA	6	0
26	A	409	LHG	3	0
25	B	620	DGD	2	0
22	B	612	CLA	10	0
22	C	505	CLA	2	0
27	B	621	LMG	3	0
31	D	401	PHO	10	0
25	A	408	DGD	1	0
22	B	615	CLA	6	0
27	A	414	LMG	1	0
22	B	610	CLA	6	0
24	B	618	BCR	4	0
27	C	518	LMG	4	0
30	B	623	LMT	2	0
22	C	509	CLA	6	0
27	D	409	LMG	6	0
27	D	412	LMG	1	0
22	B	608	CLA	13	0
22	B	607	CLA	9	0
22	C	507	CLA	4	0
30	B	627	LMT	2	0
22	D	405	CLA	8	0
24	C	514	BCR	7	0
24	B	616	BCR	4	0
22	C	503	CLA	5	0
29	B	622	SQD	3	0
22	A	404	CLA	15	0
22	C	520	CLA	4	0
30	I	102	LMT	1	0
24	H	102	BCR	2	0
22	B	603	CLA	3	0
25	C	516	DGD	3	0
22	C	508	CLA	2	0
22	A	403	CLA	13	0

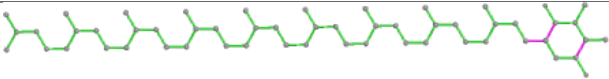
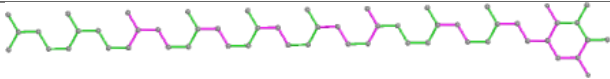
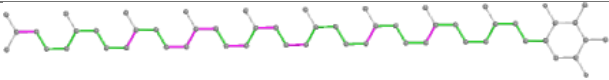
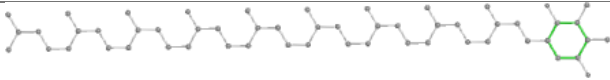
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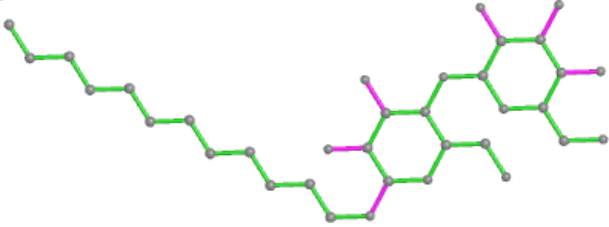
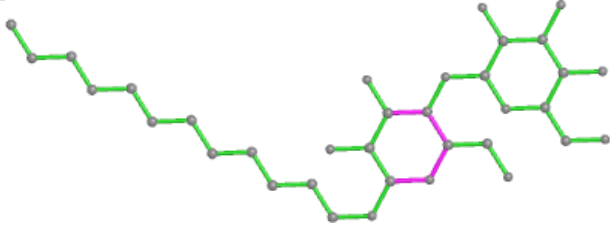
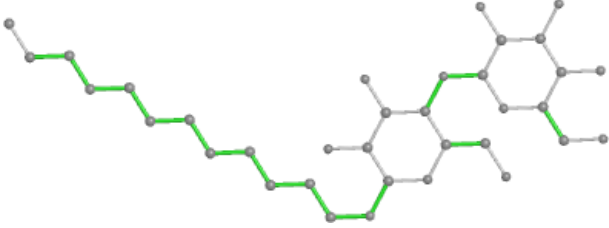
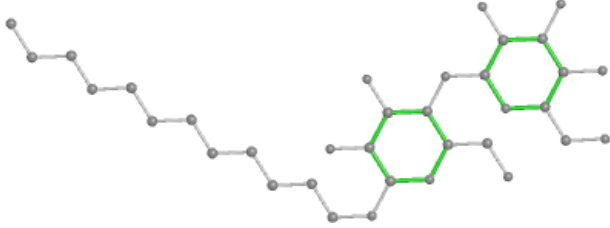
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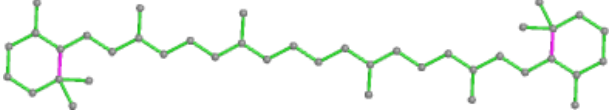
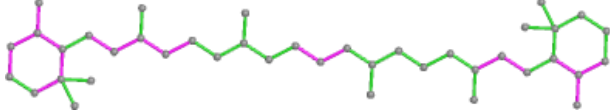
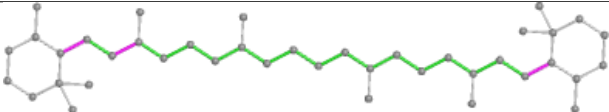
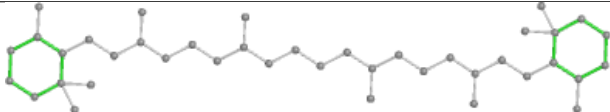
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	611	CLA	11	0
25	D	410	DGD	2	0
27	D	408	LMG	4	0
25	C	517	DGD	5	0
22	C	512	CLA	3	0
22	B	606	CLA	16	0
31	D	402	PHO	5	0
22	B	614	CLA	2	0
24	C	513	BCR	7	0
24	A	407	BCR	3	0
30	B	628	LMT	2	0

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.

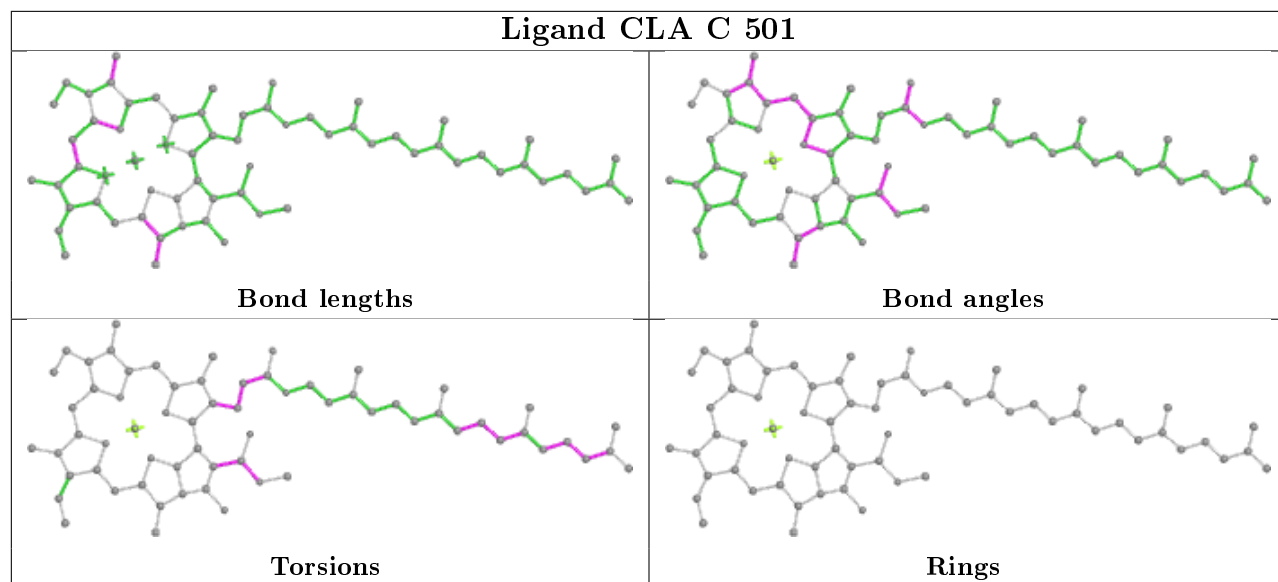


Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

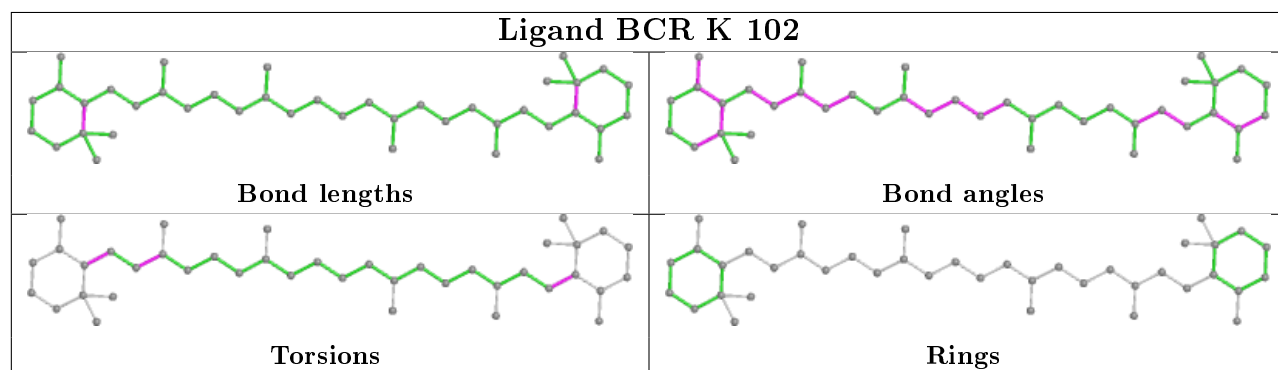
Ligand LMT M 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

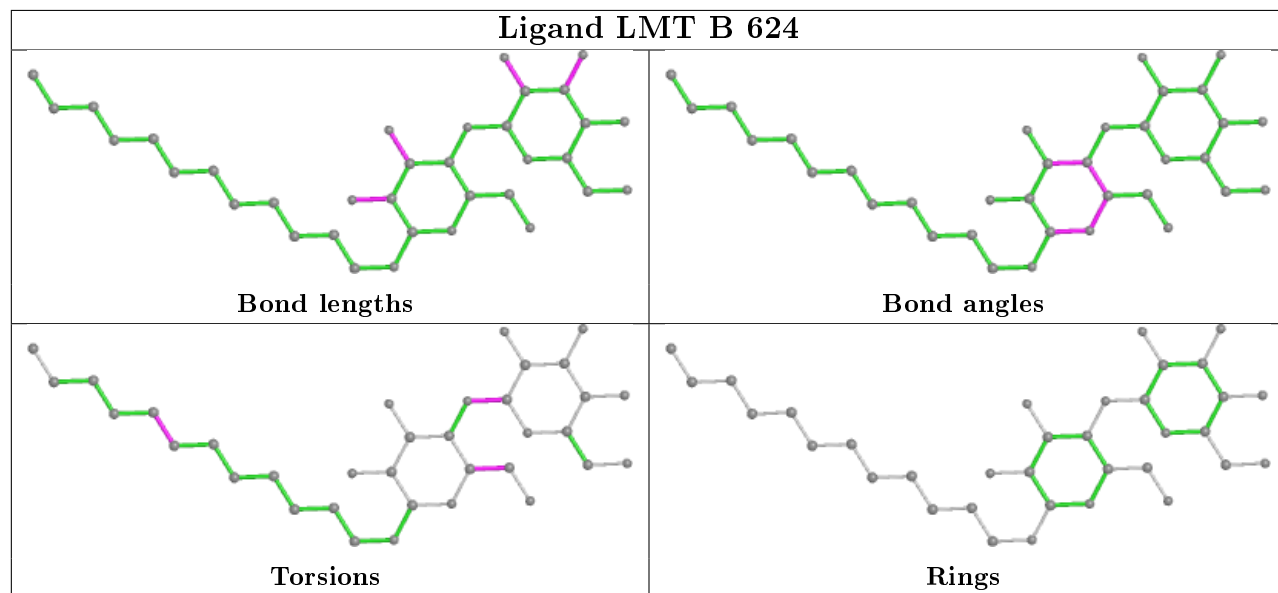
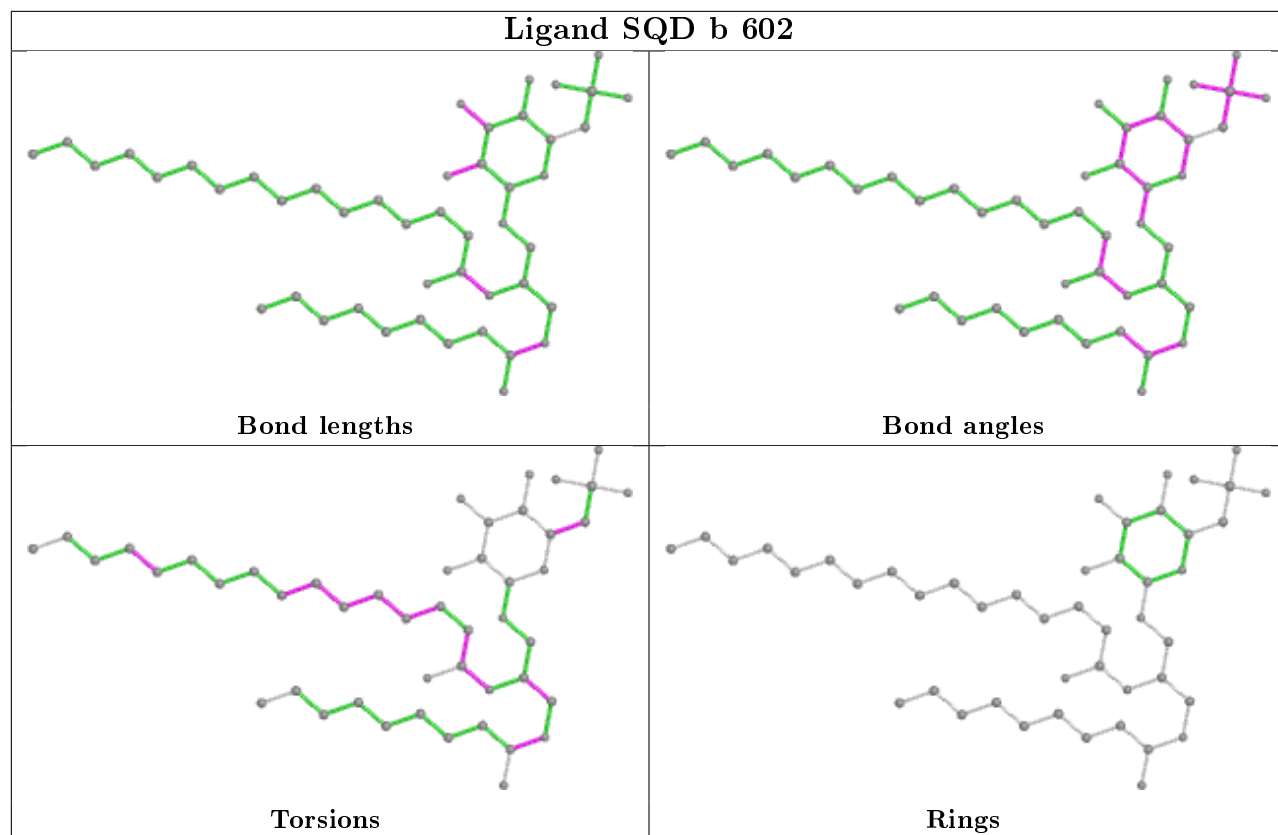
Ligand BCR b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

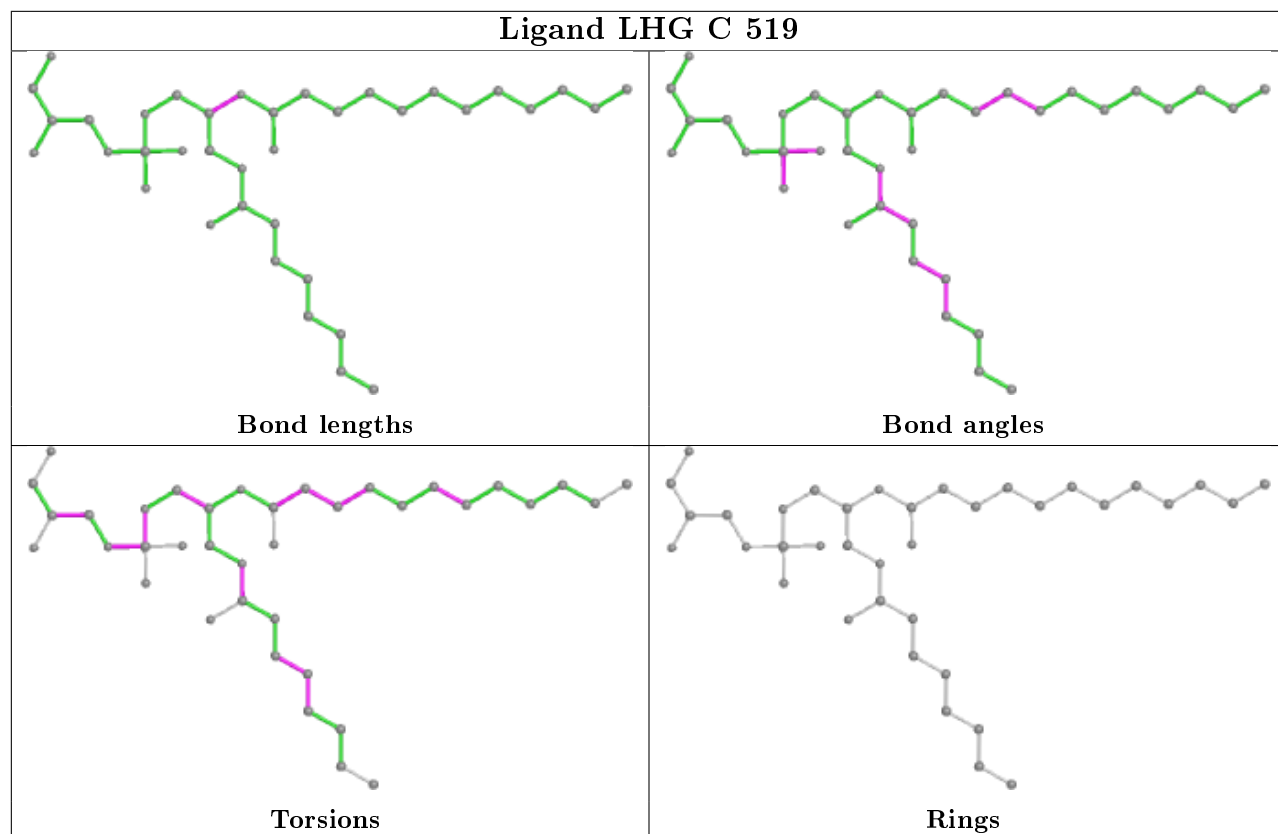
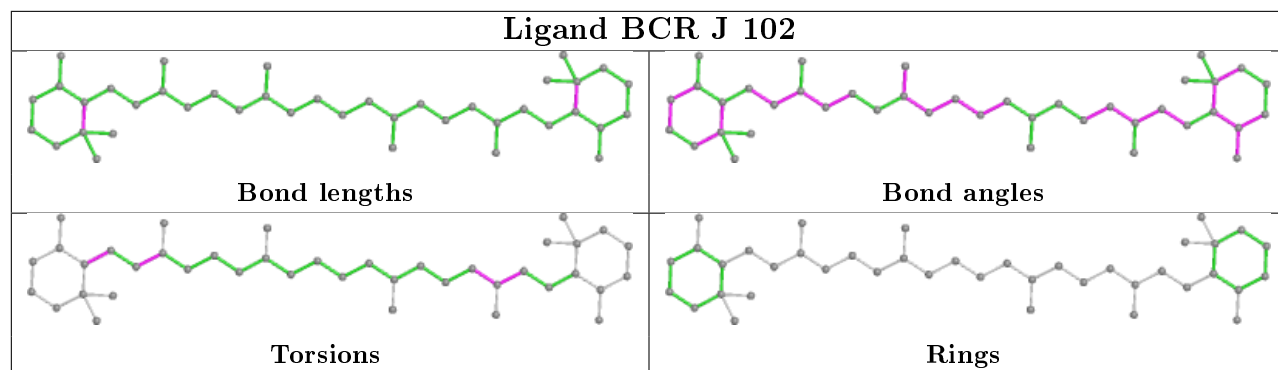
## Ligand CLA C 501

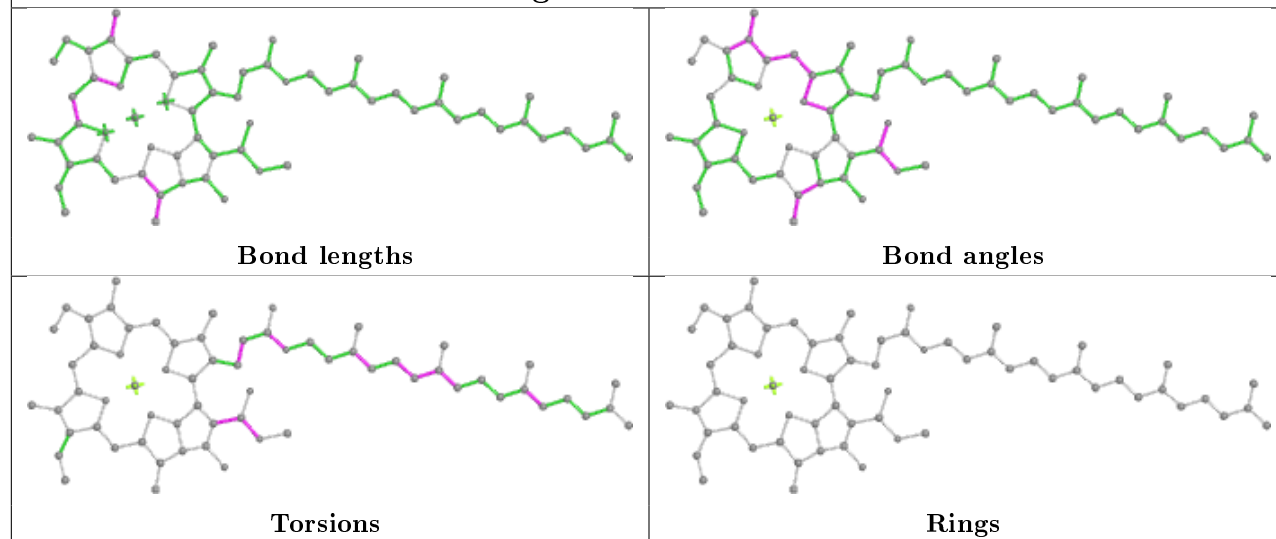
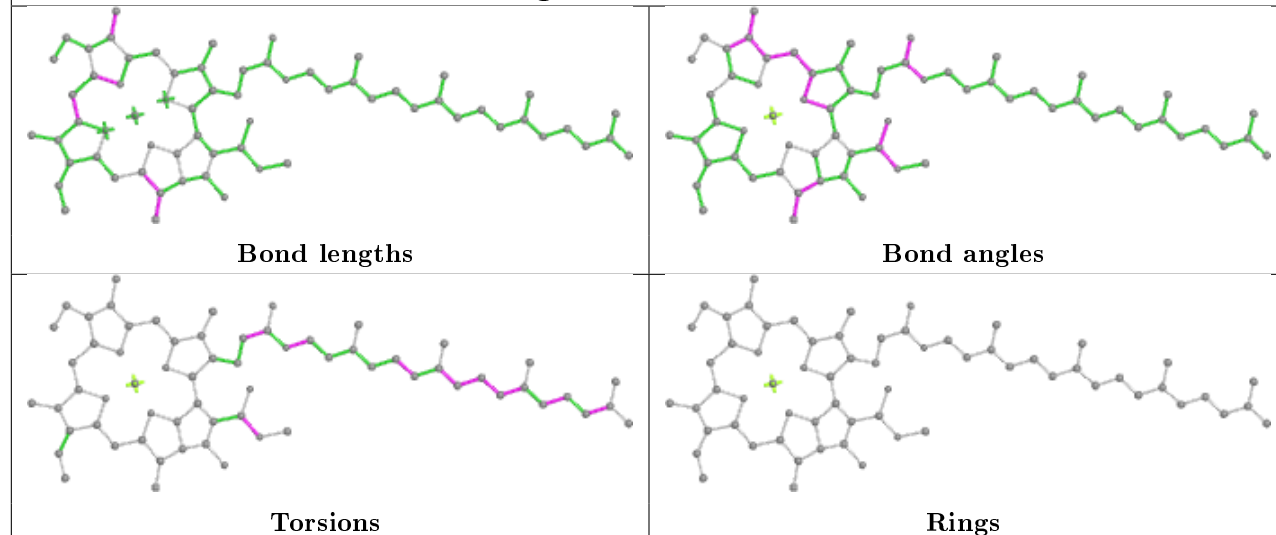
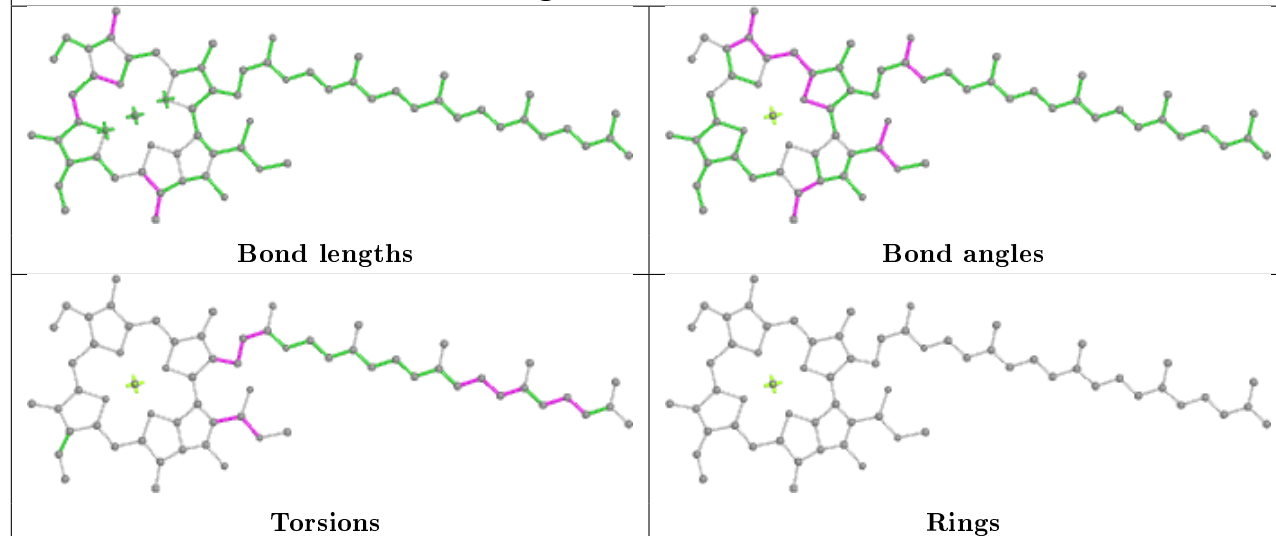


## Ligand BCR K 102



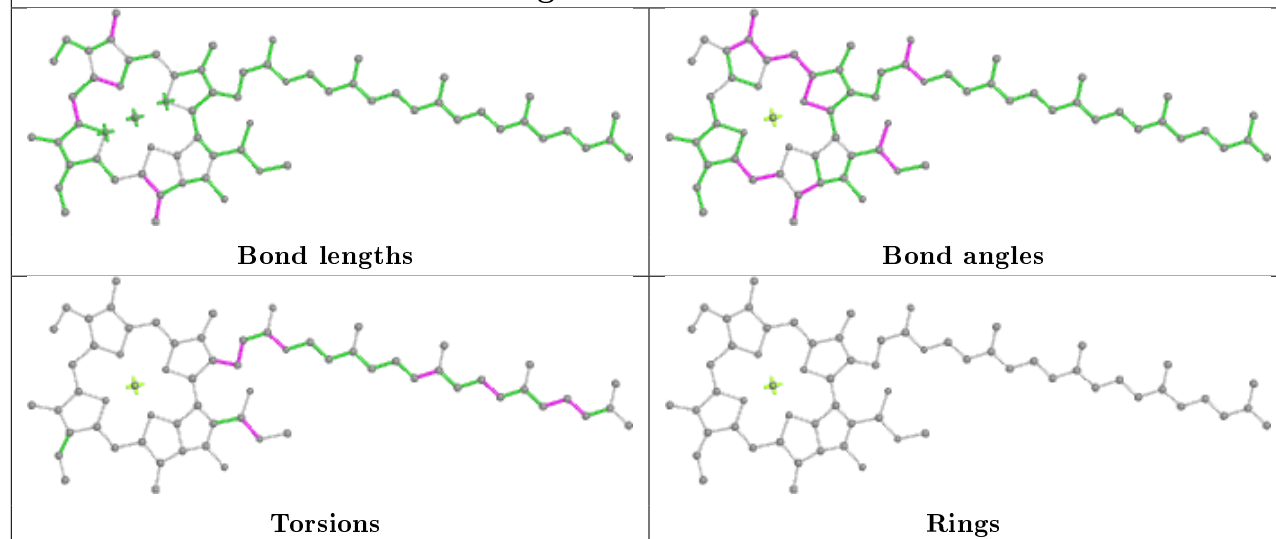




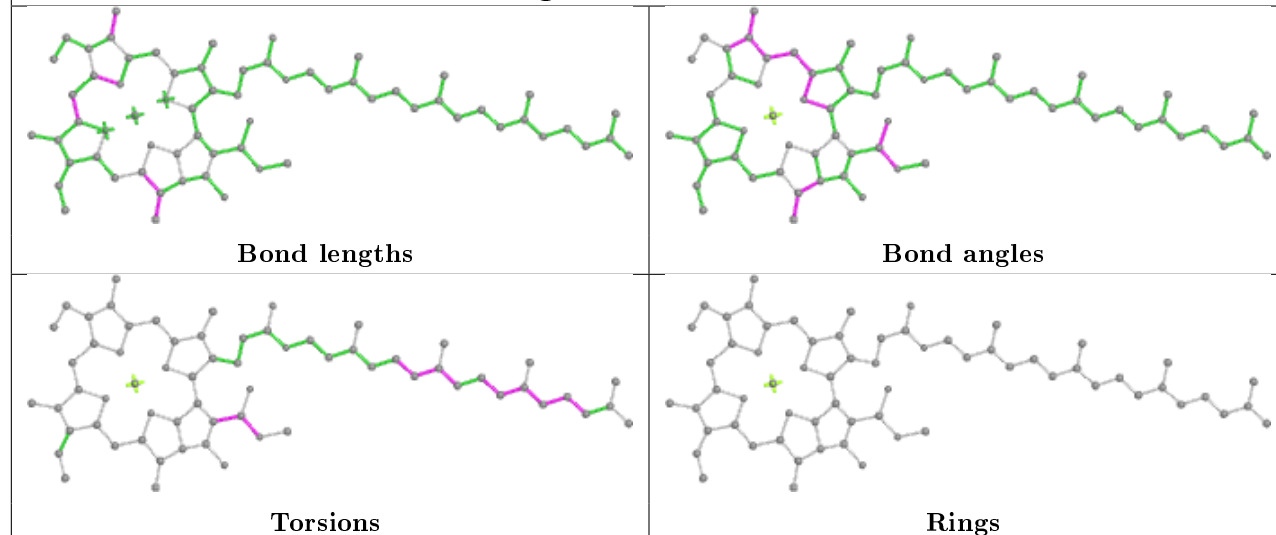
**Ligand CLA C 510****Ligand CLA b 616****Ligand CLA c 501**



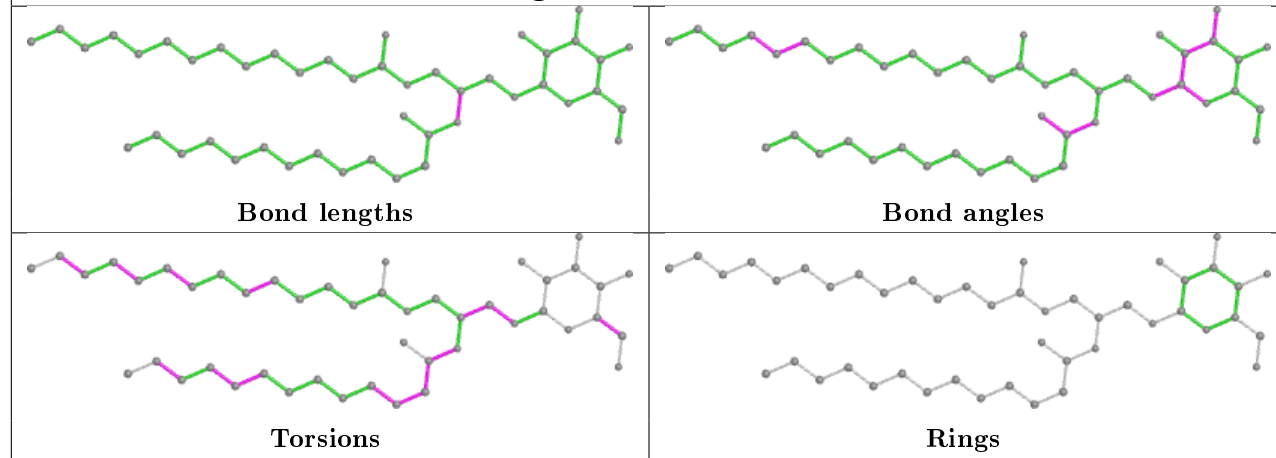
## Ligand CLA c 520

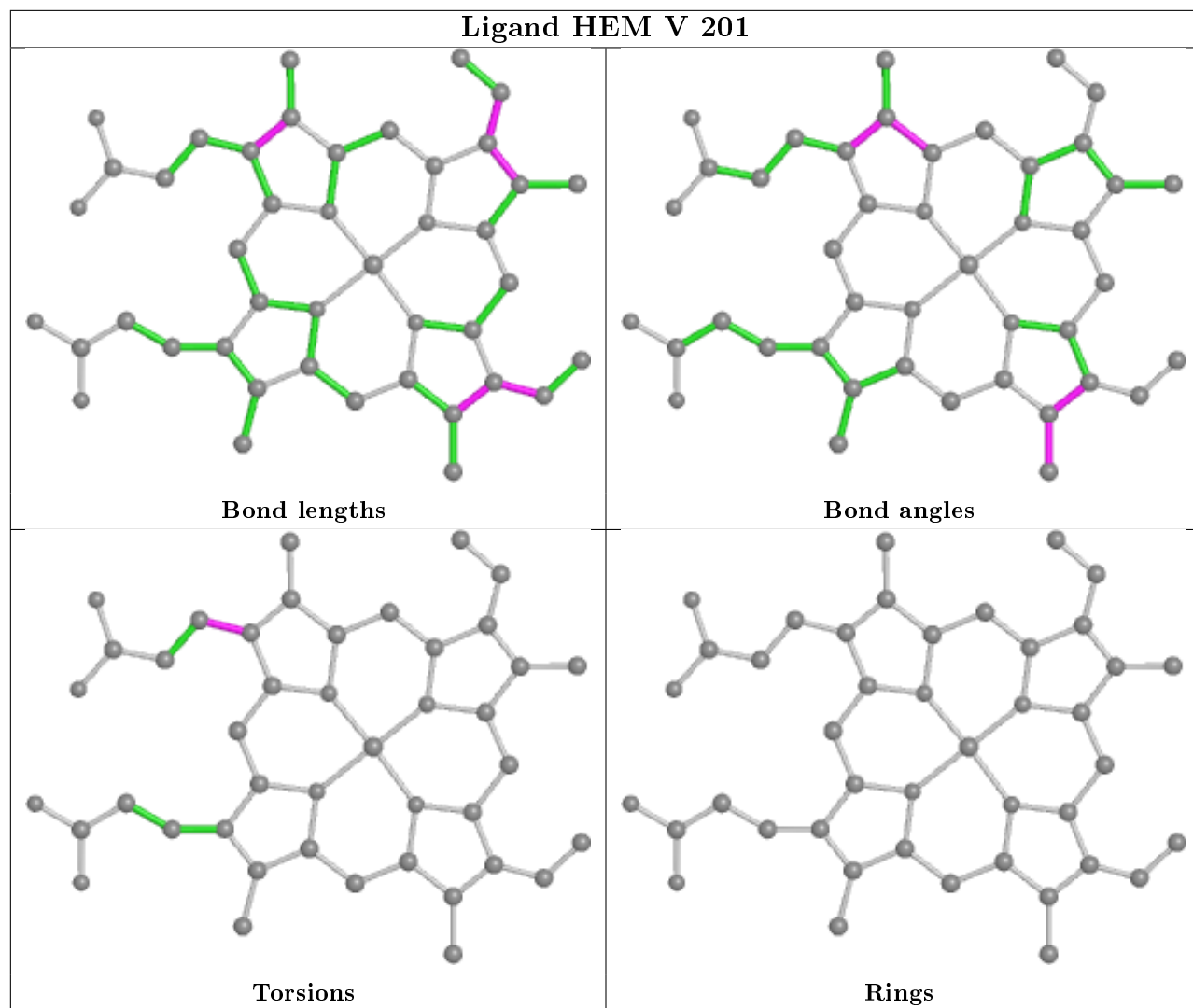


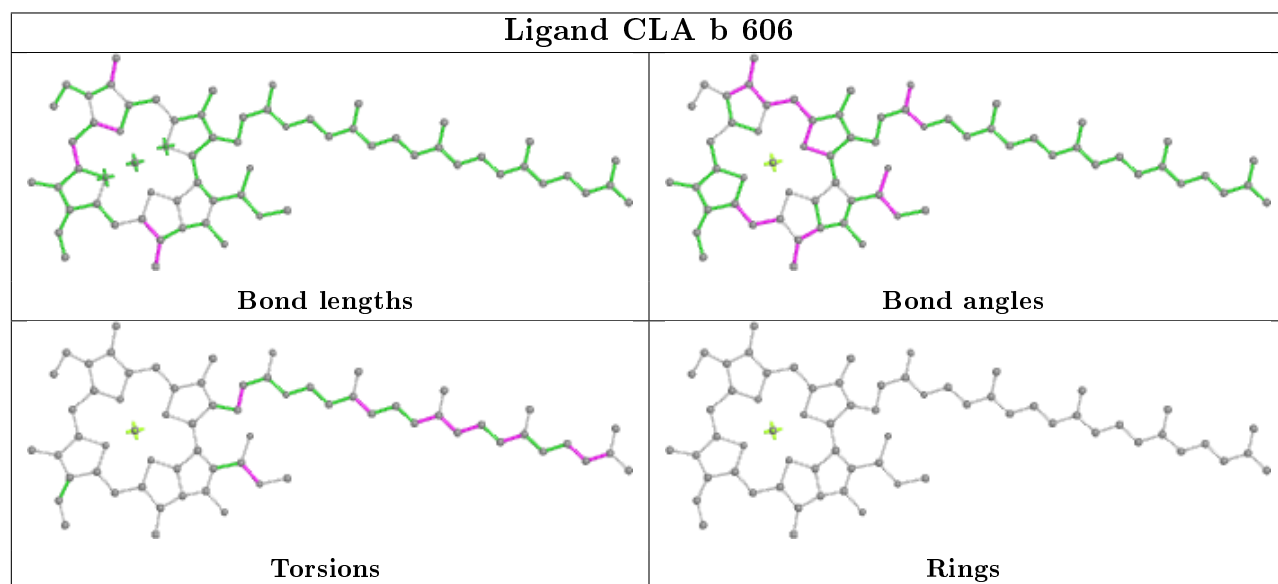
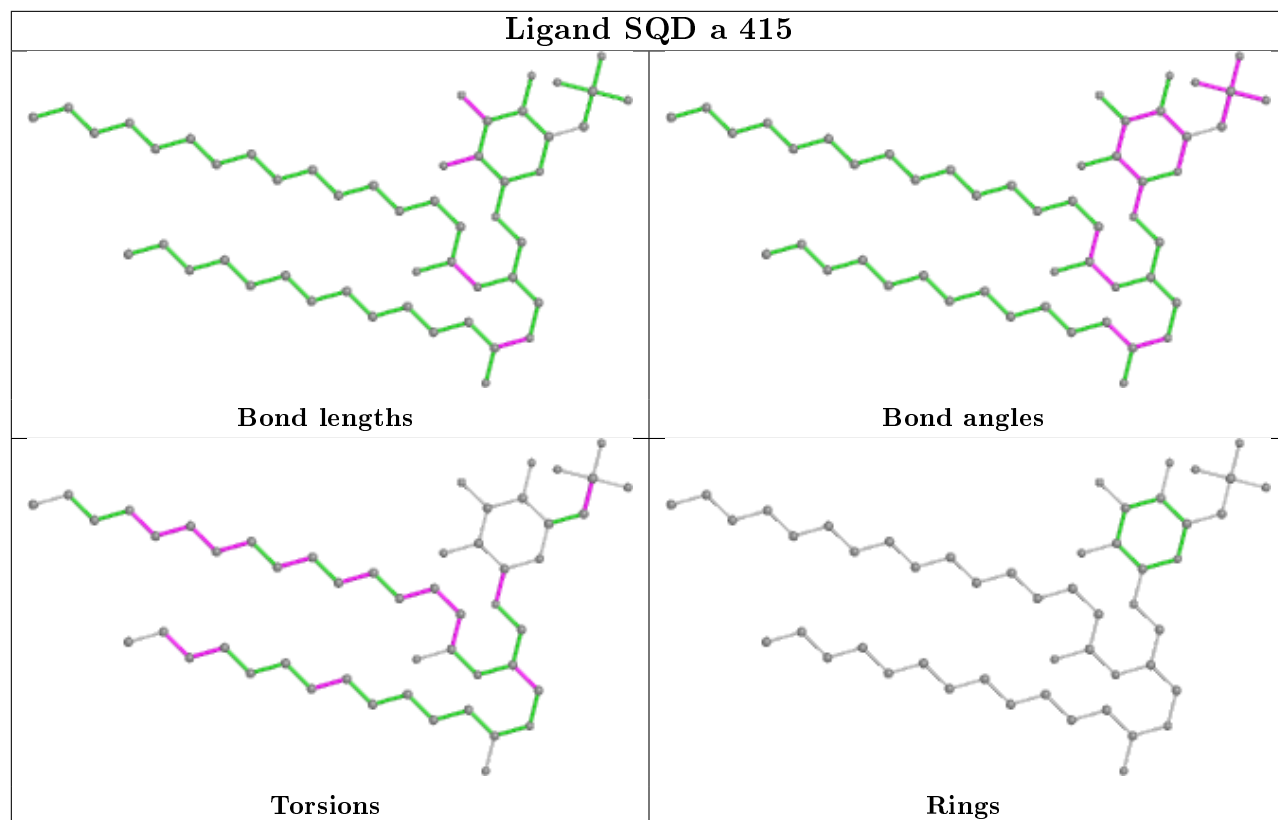
## Ligand CLA c 505

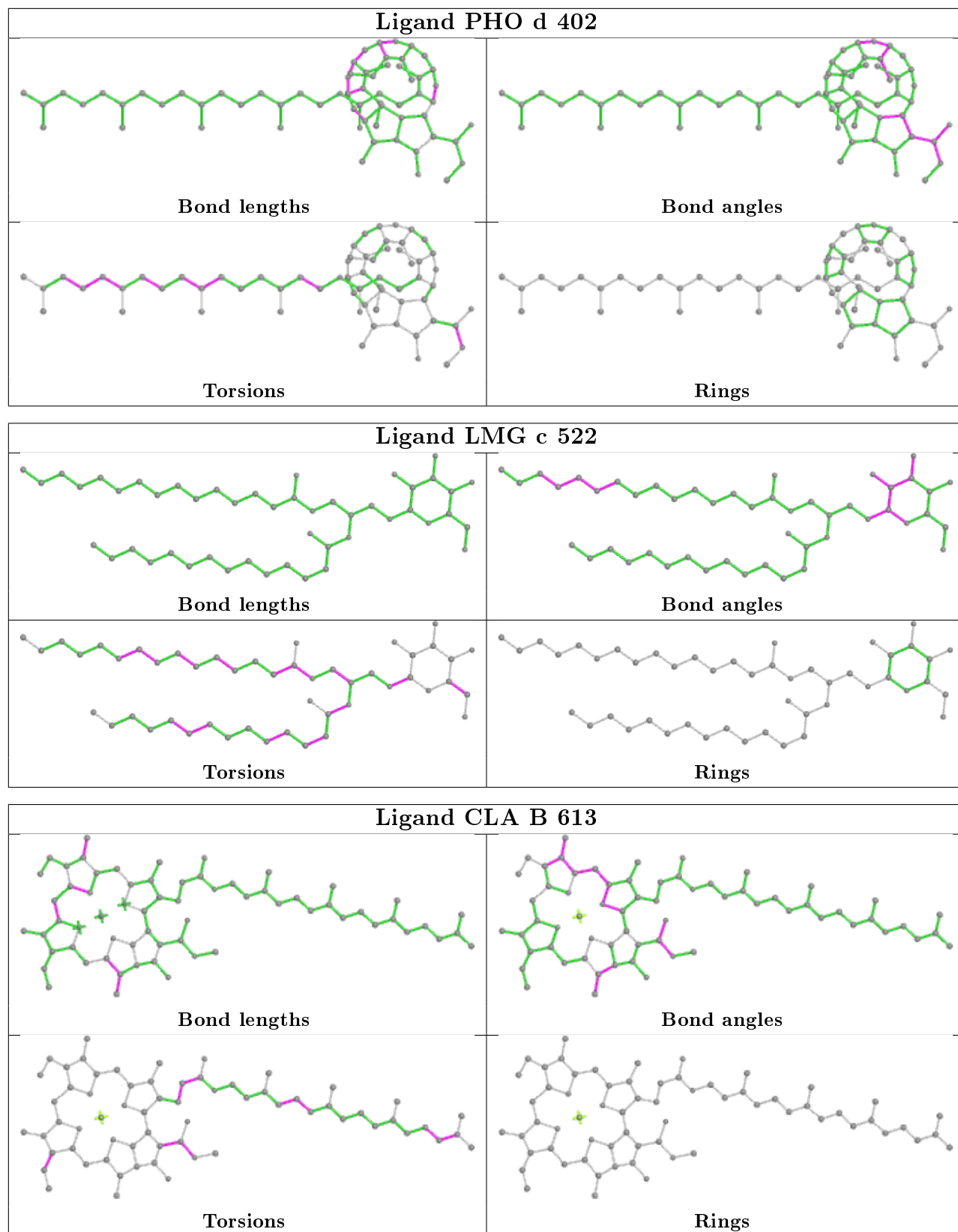


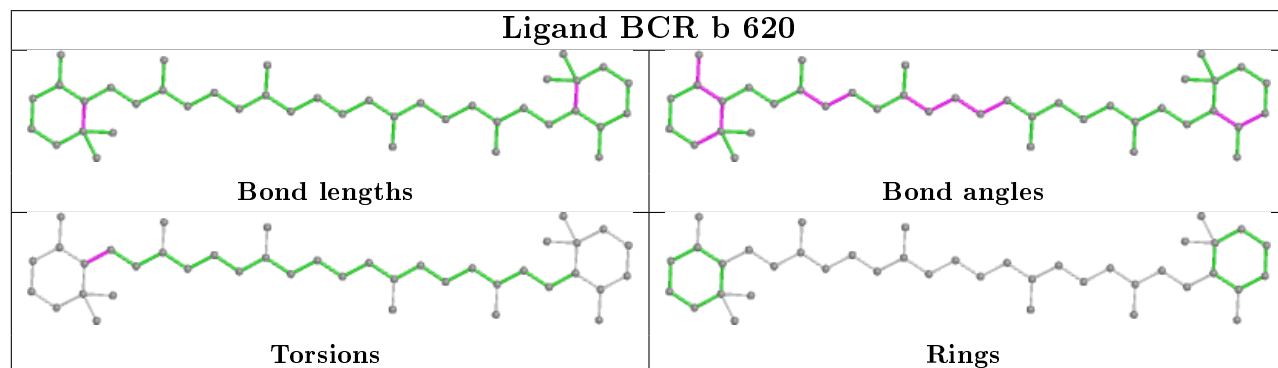
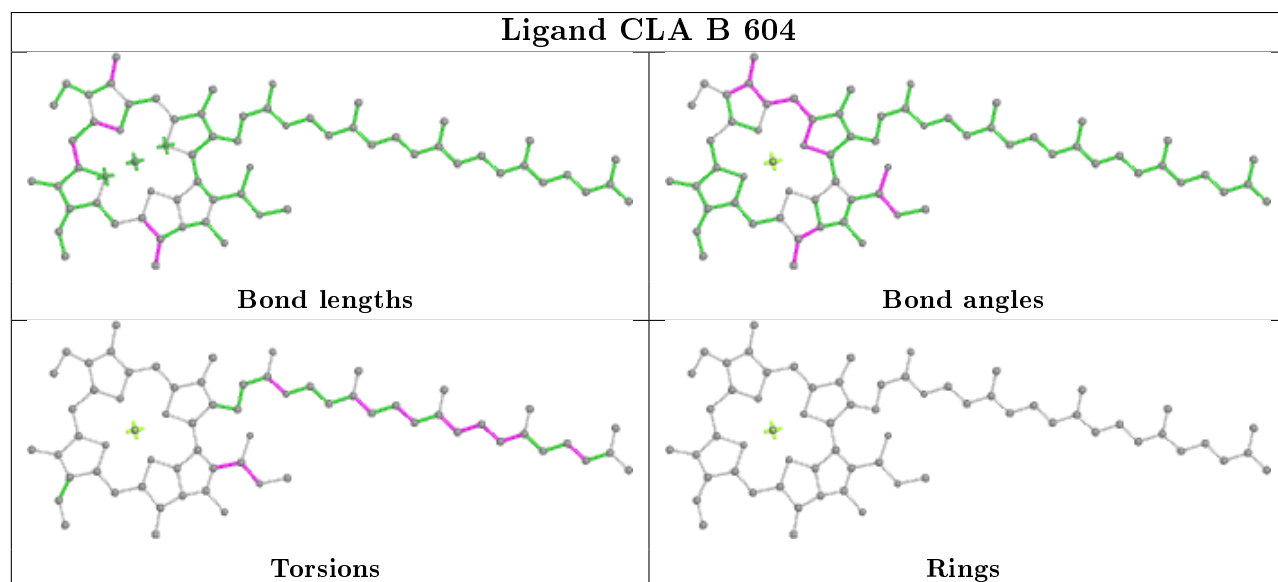
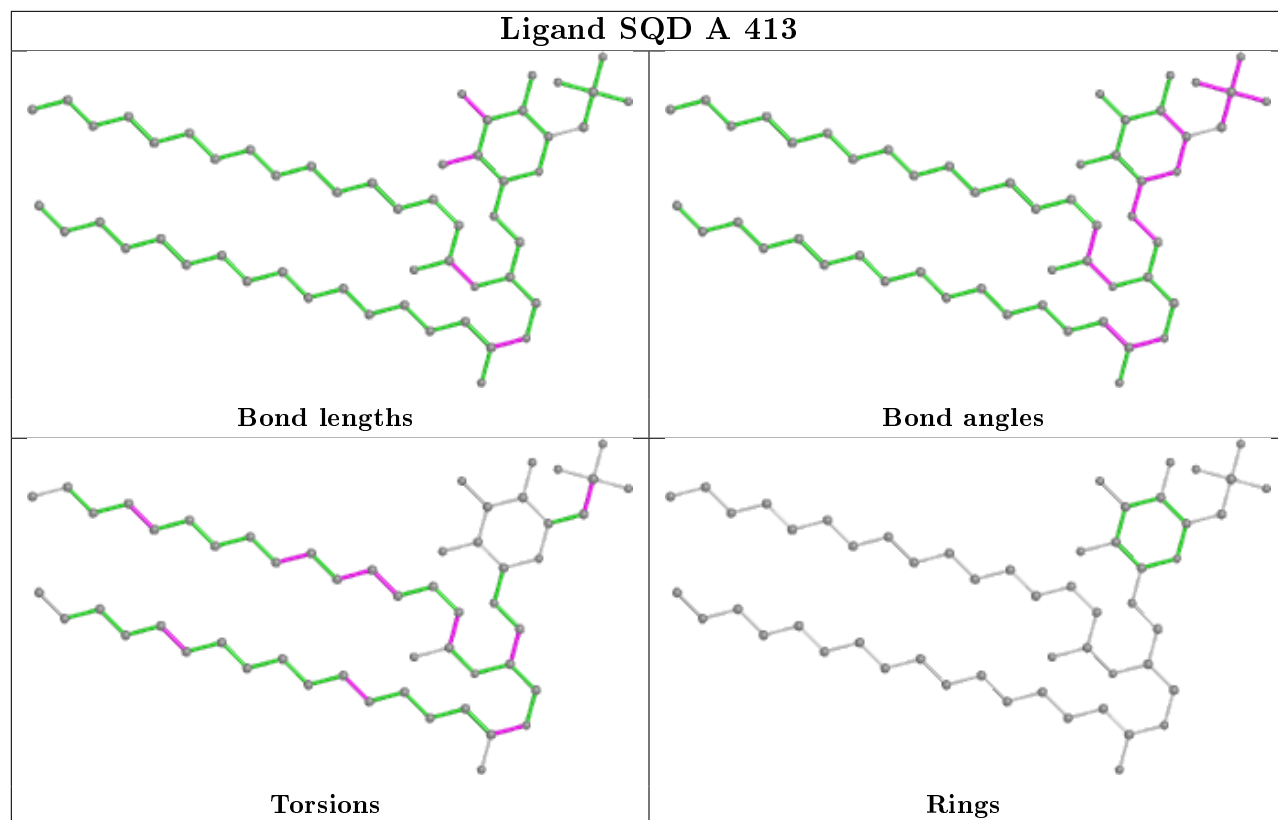
## Ligand LMG d 412

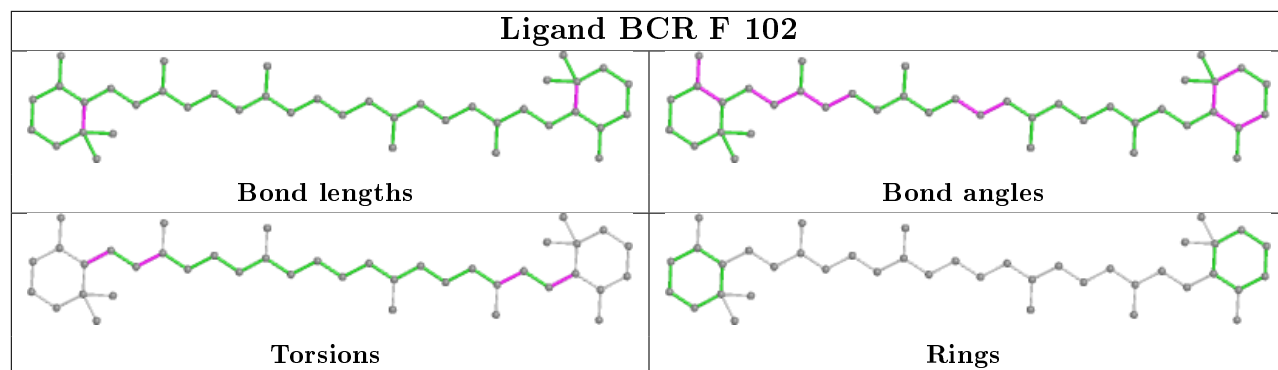
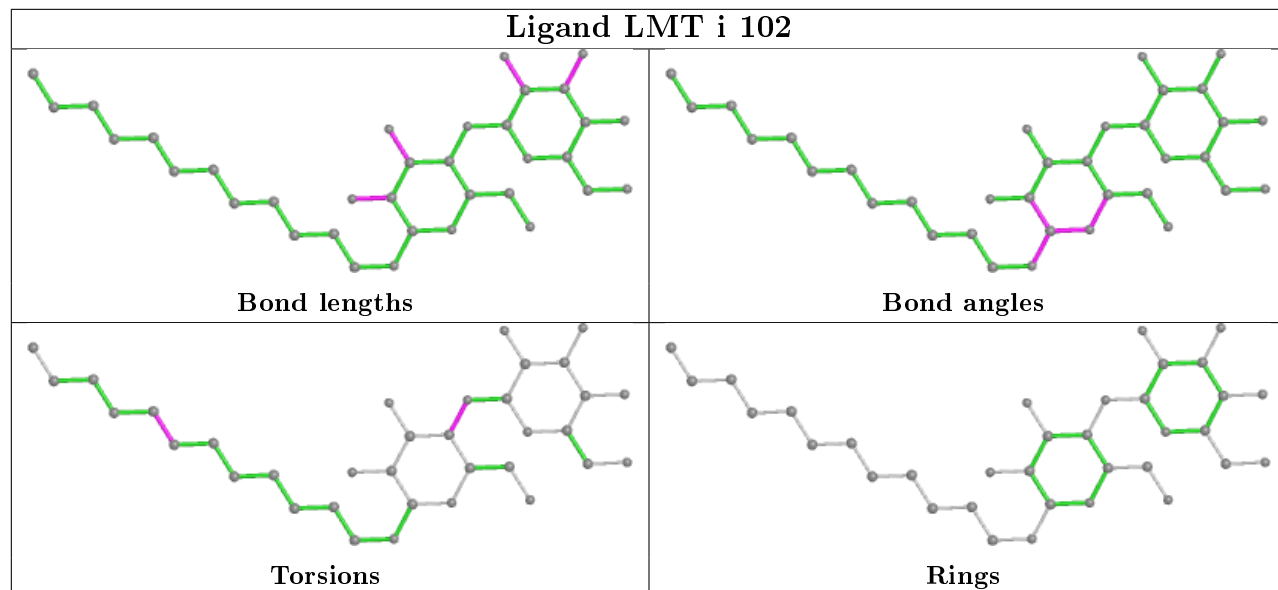
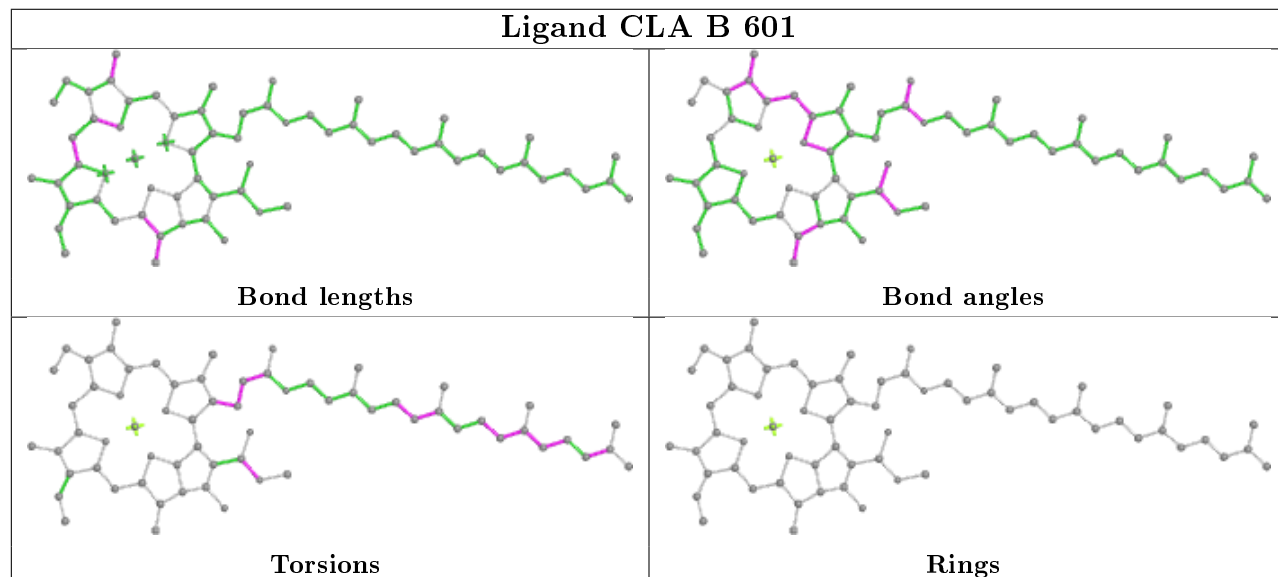




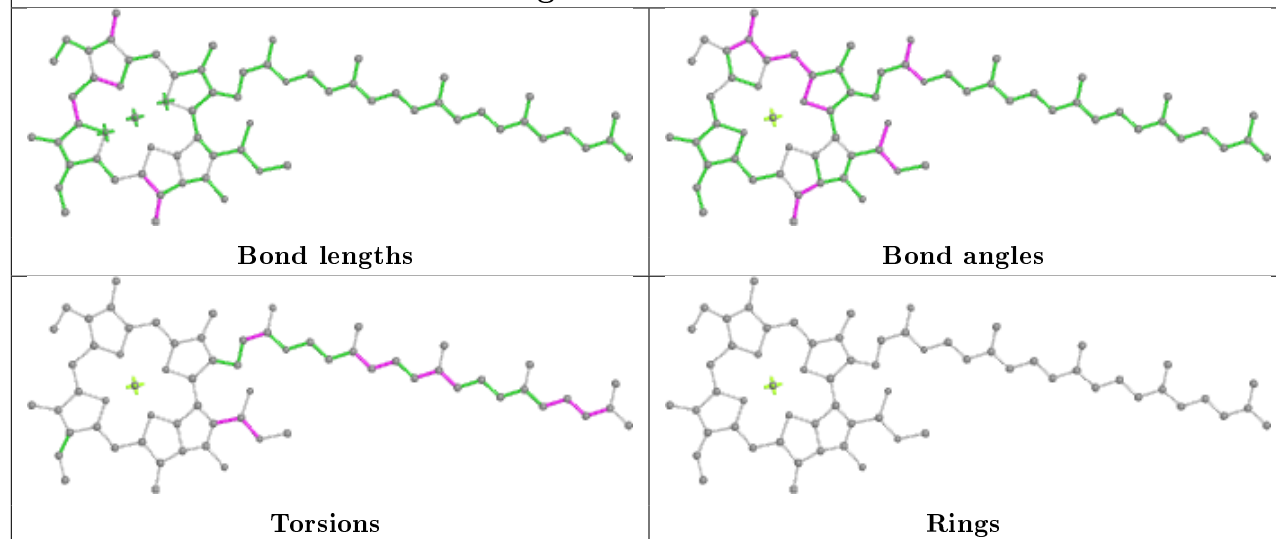




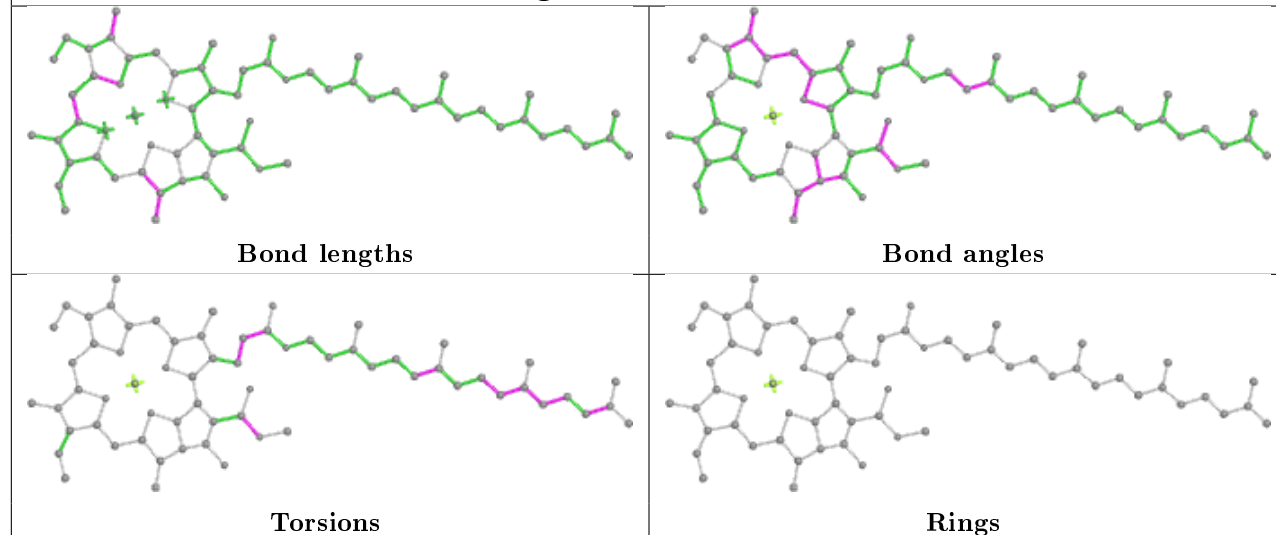


**Ligand BCR F 102****Ligand LMT i 102****Ligand CLA B 601**

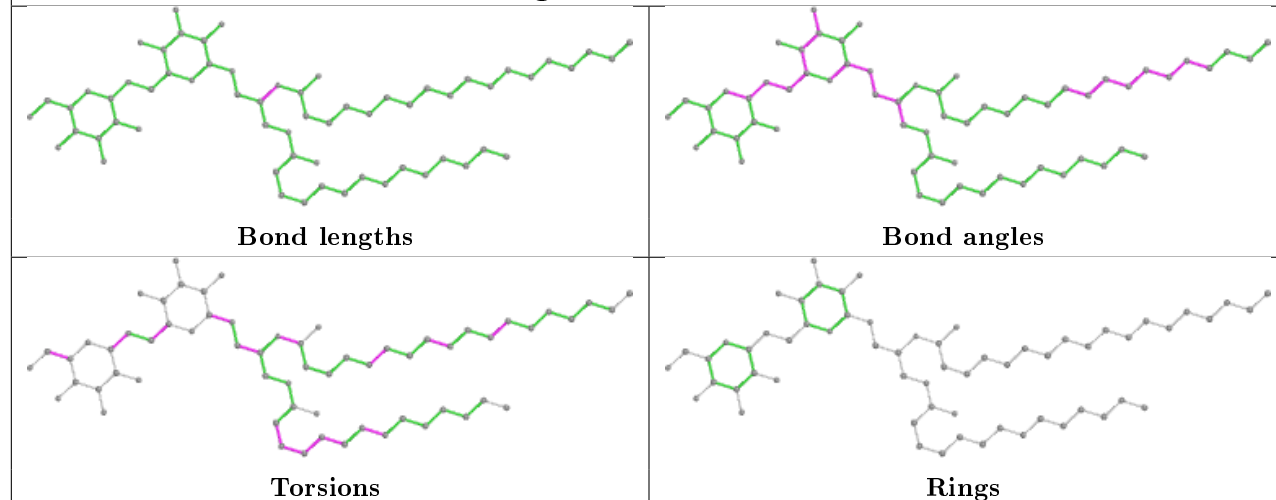
## Ligand CLA c 509

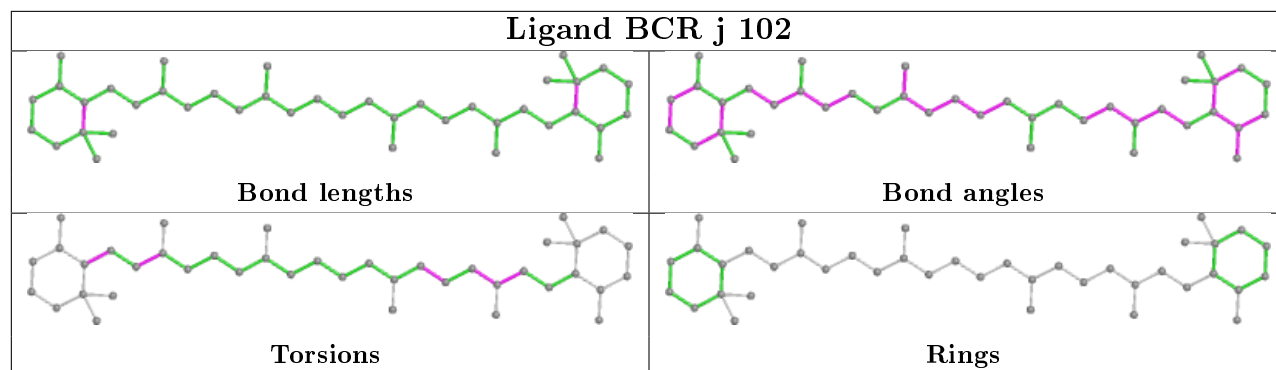
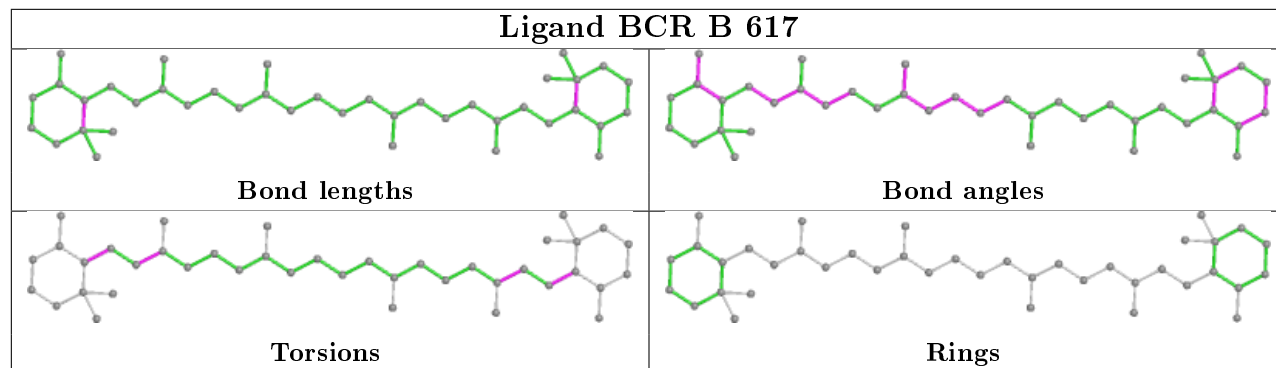
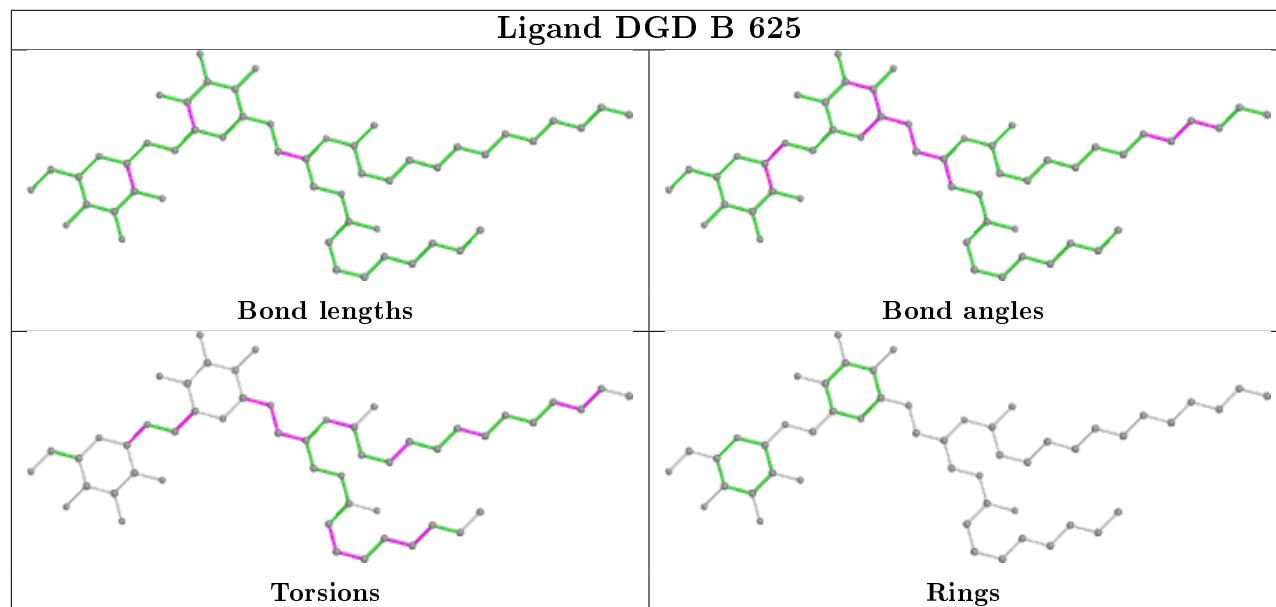


## Ligand CLA b 605

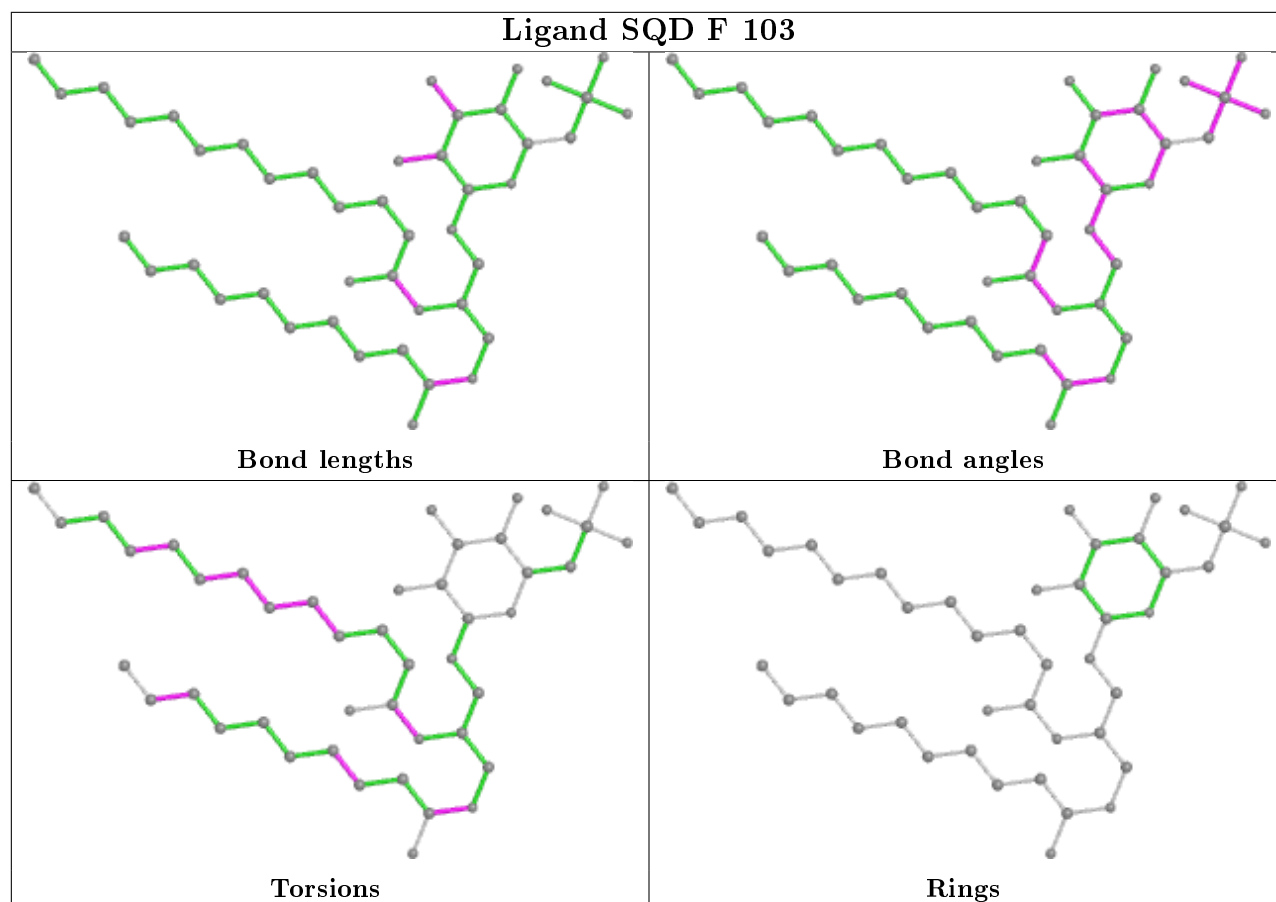
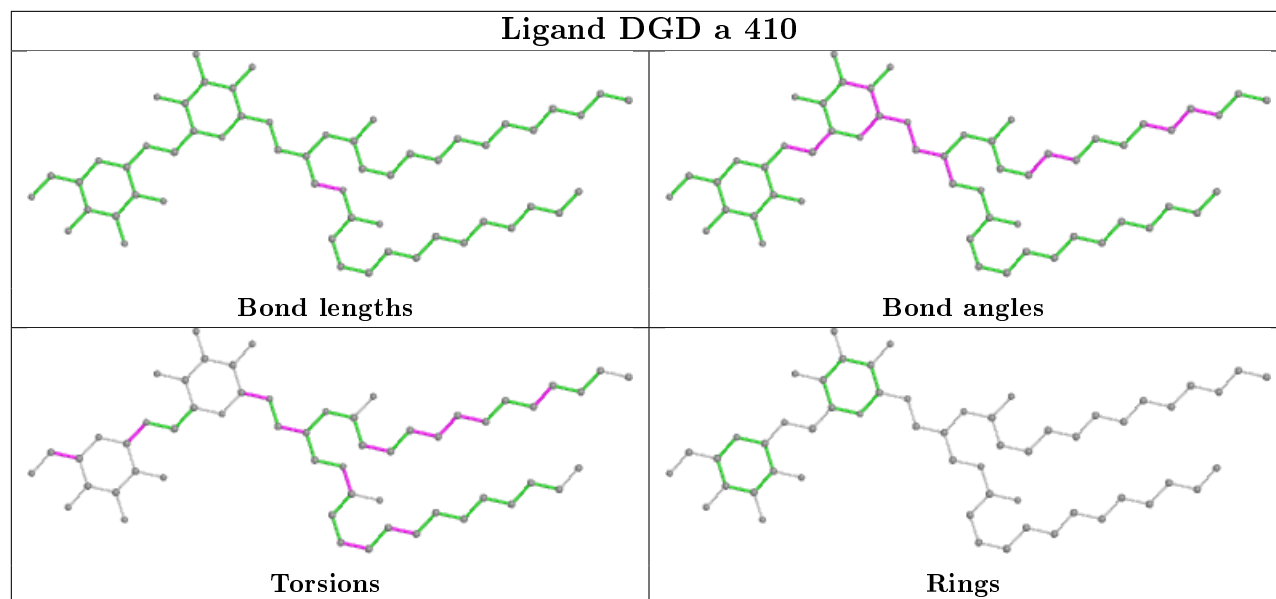


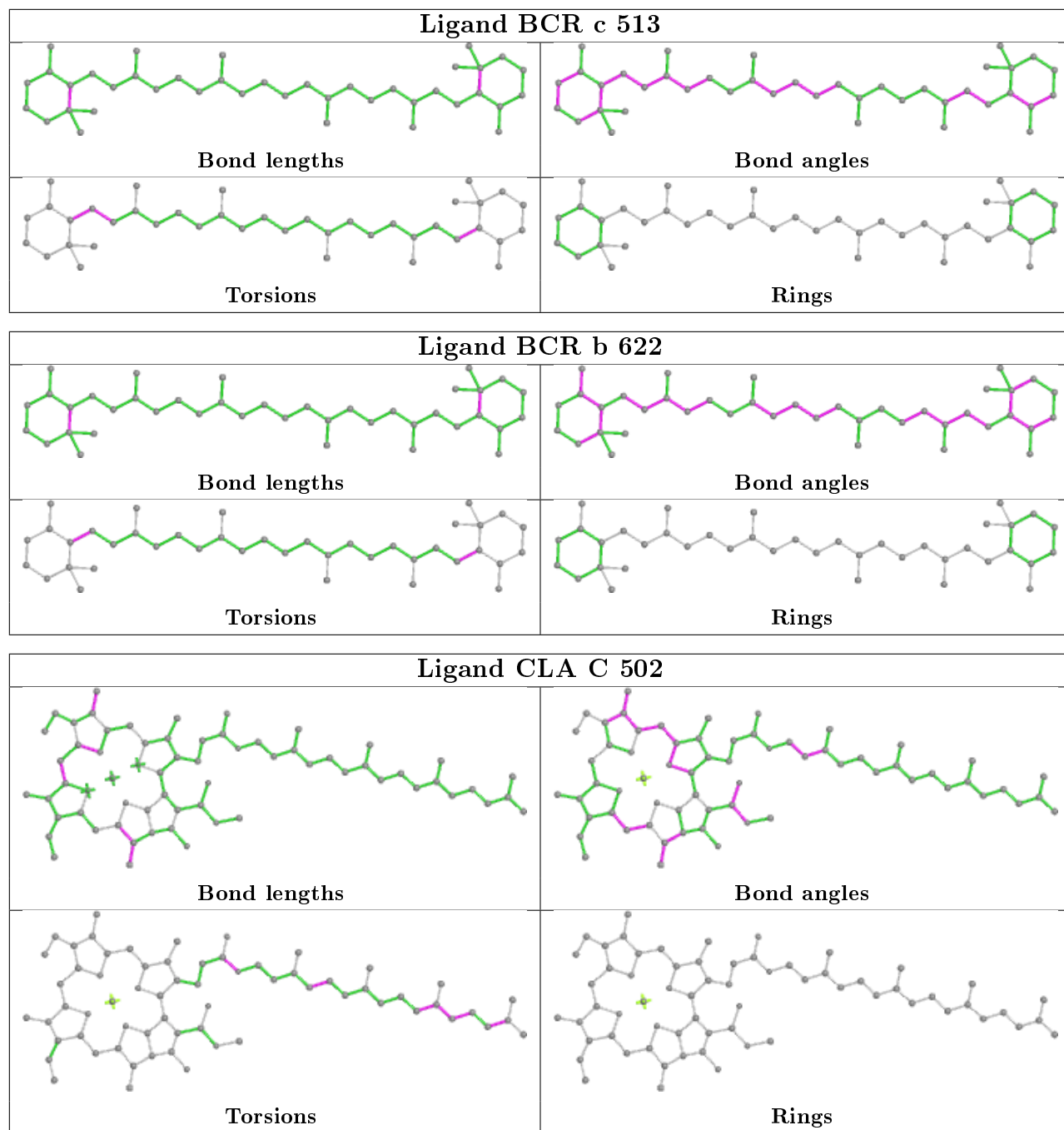
## Ligand DGD c 516



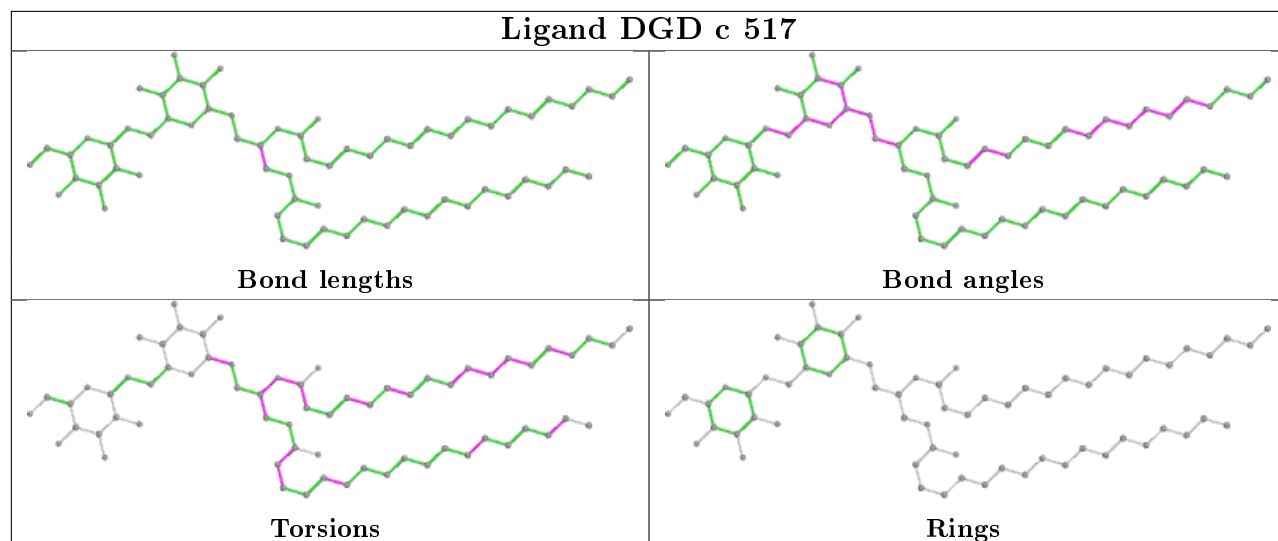
**Ligand BCR j 102****Ligand BCR B 617****Ligand DGD B 625**



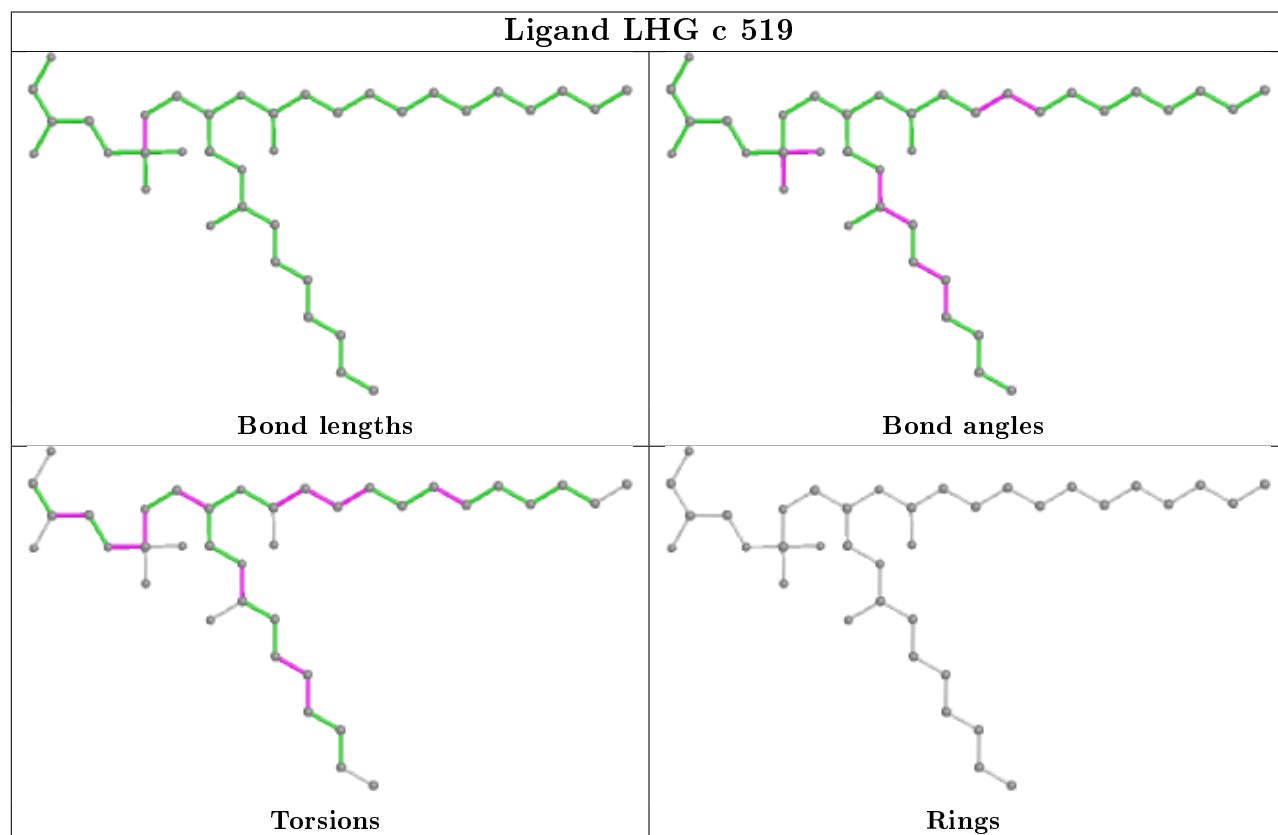


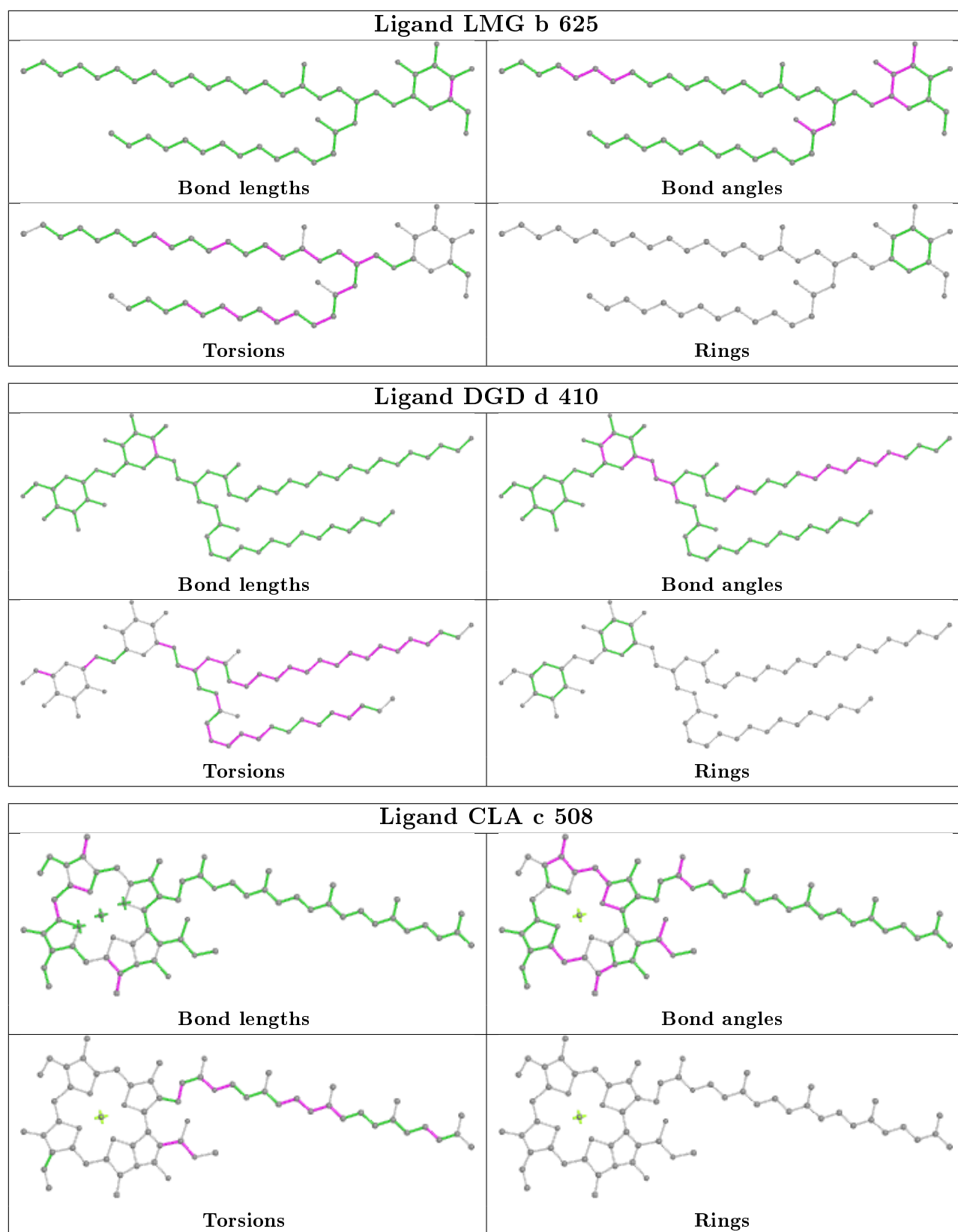


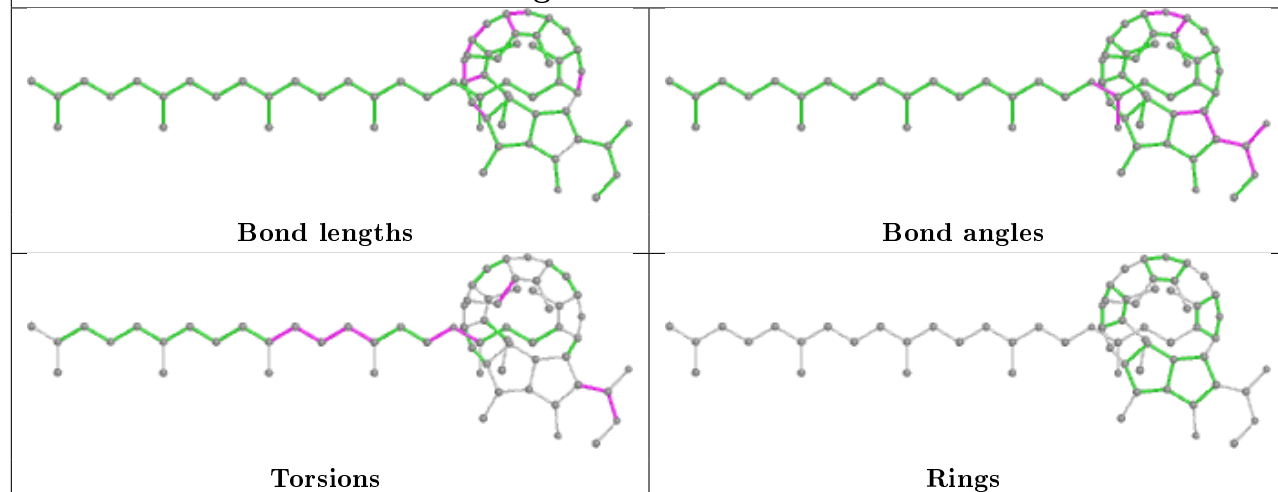
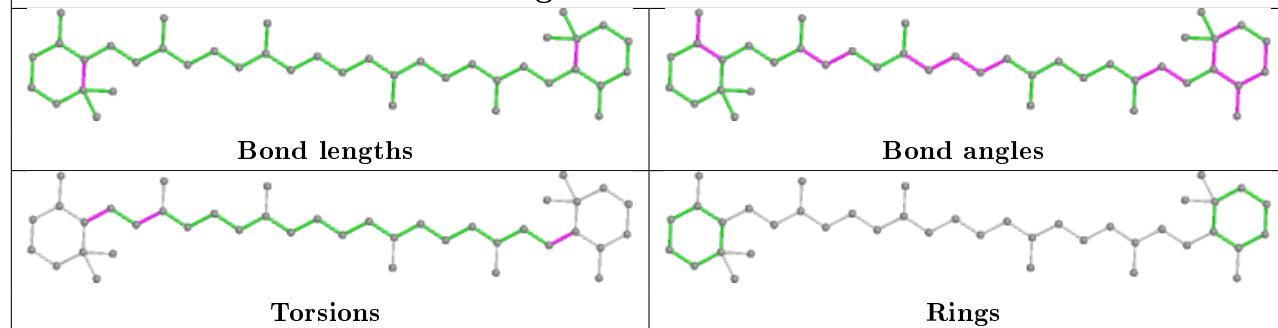
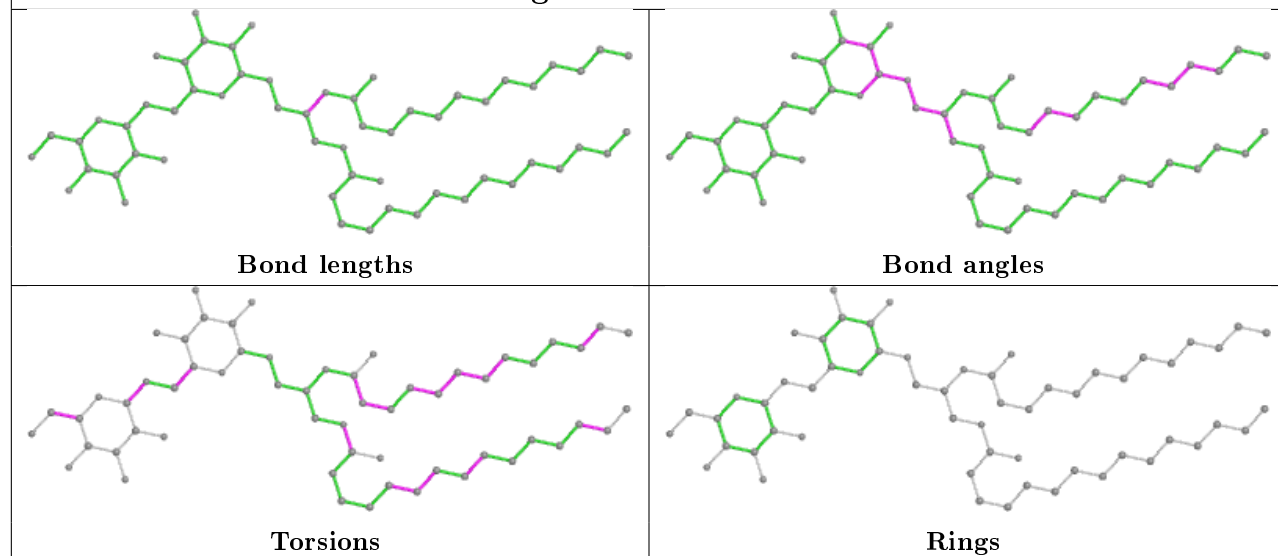
## Ligand DGD c 517

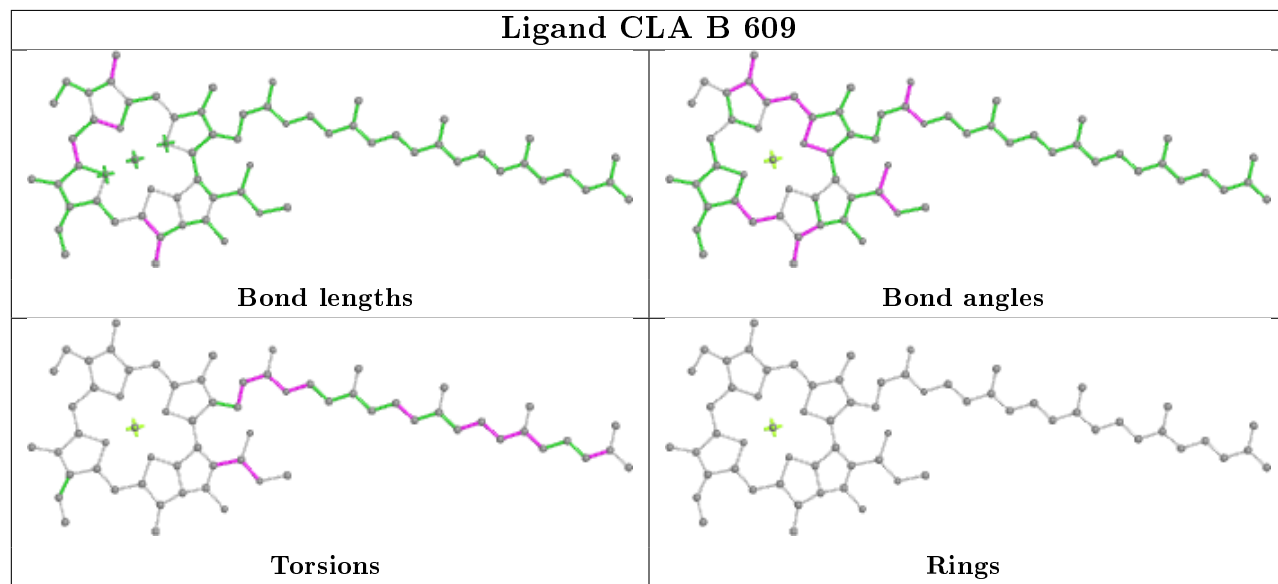
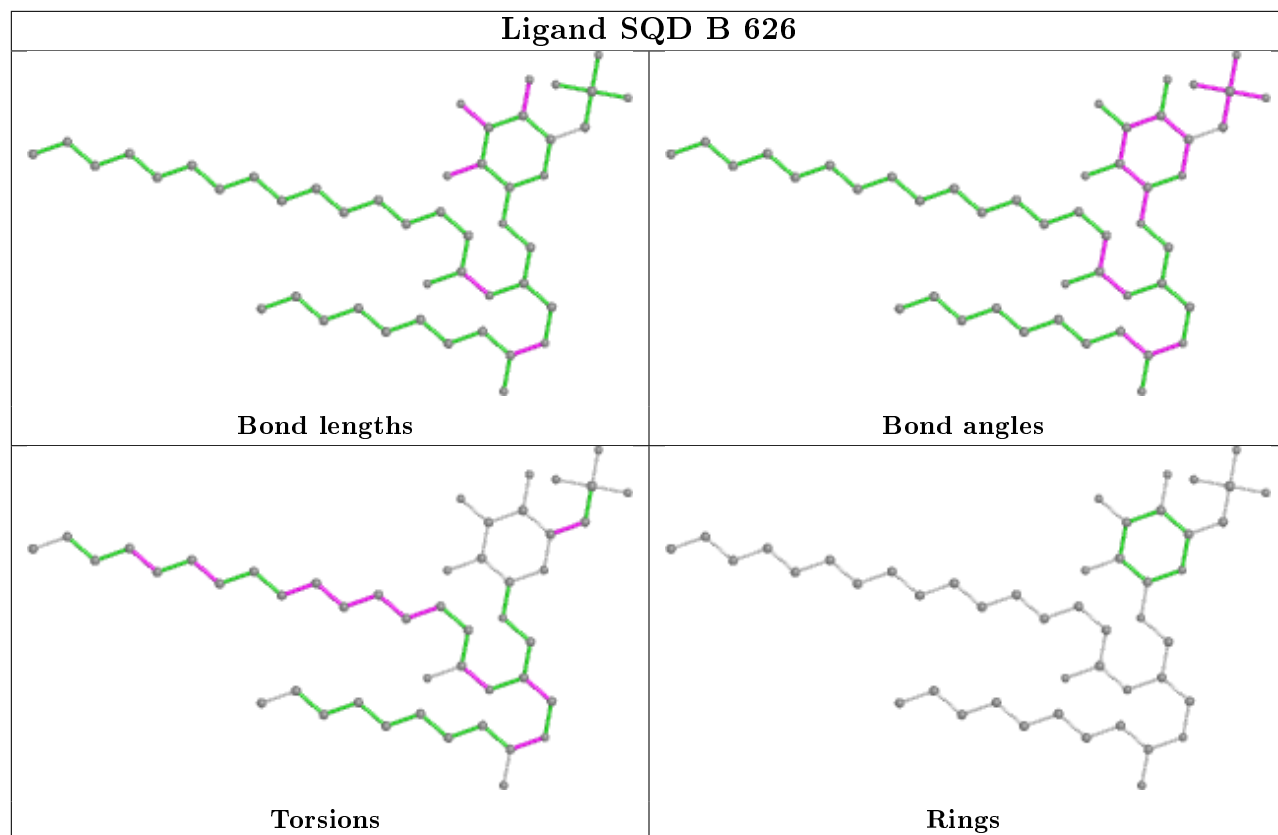


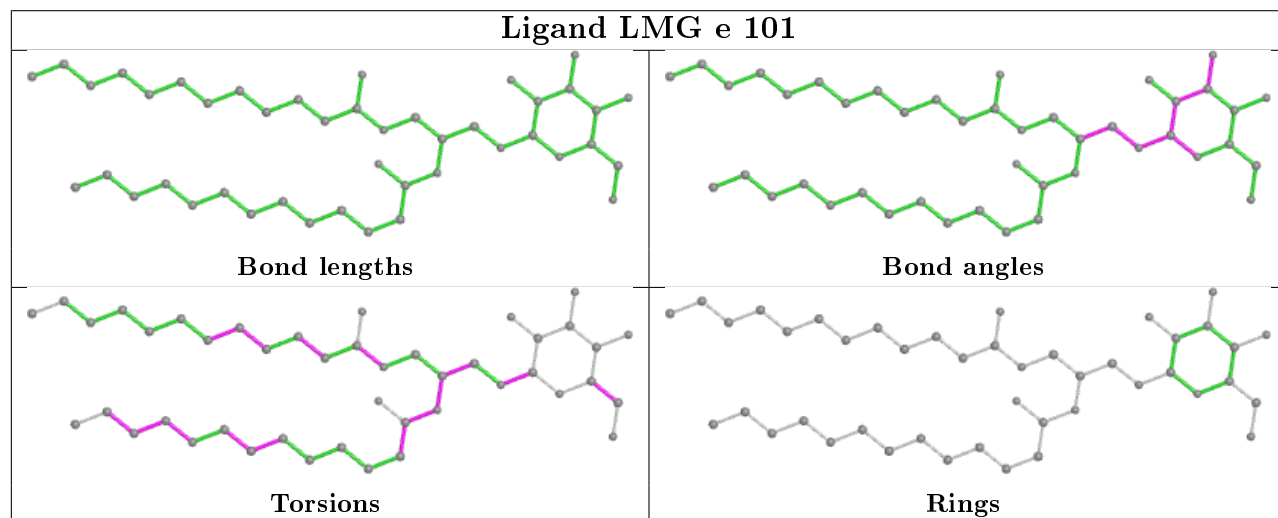
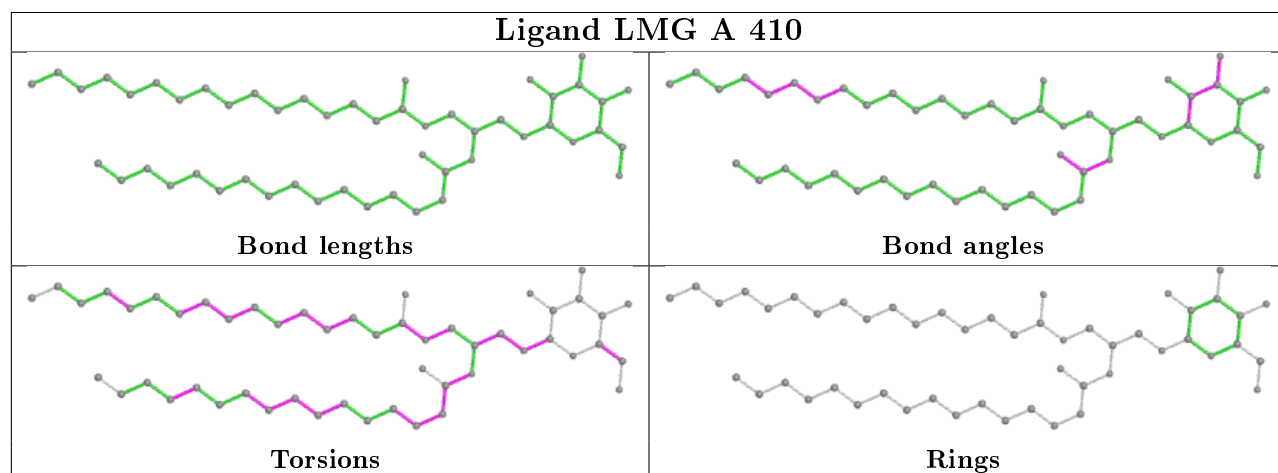
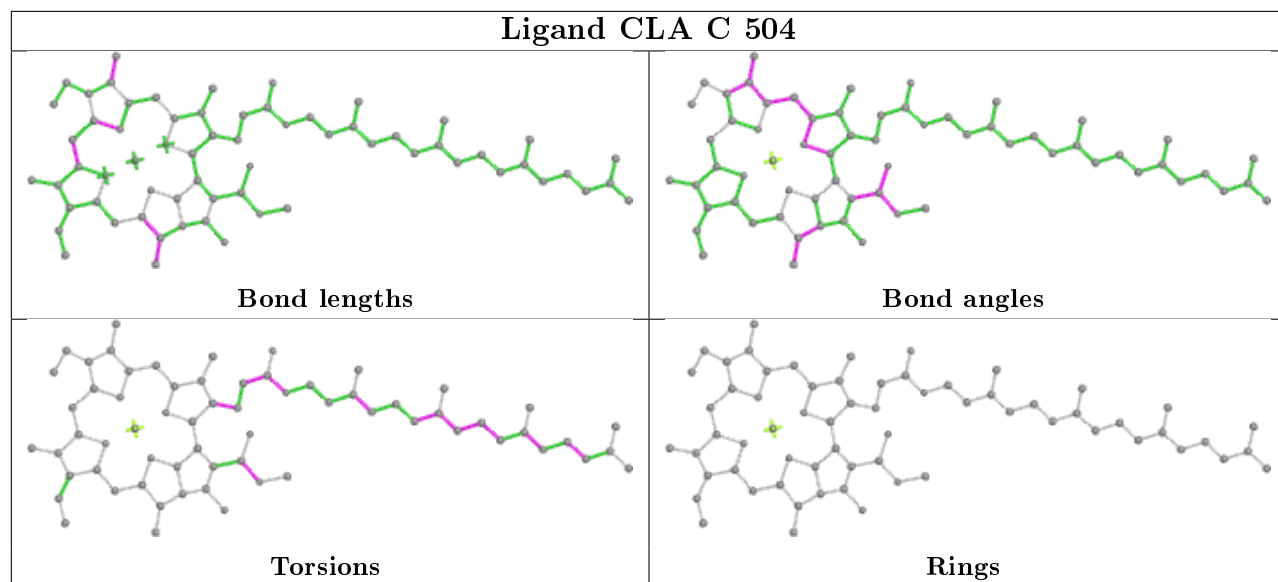
## Ligand LHG c 519



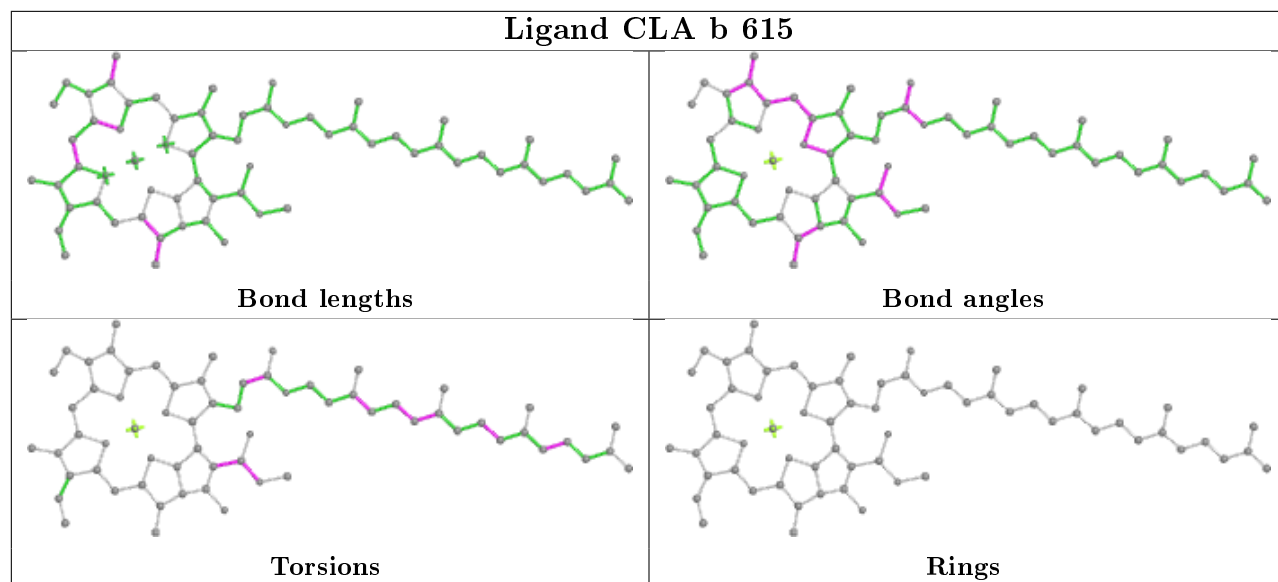


**Ligand PHO d 401****Ligand BCR c 514****Ligand DGD b 624**

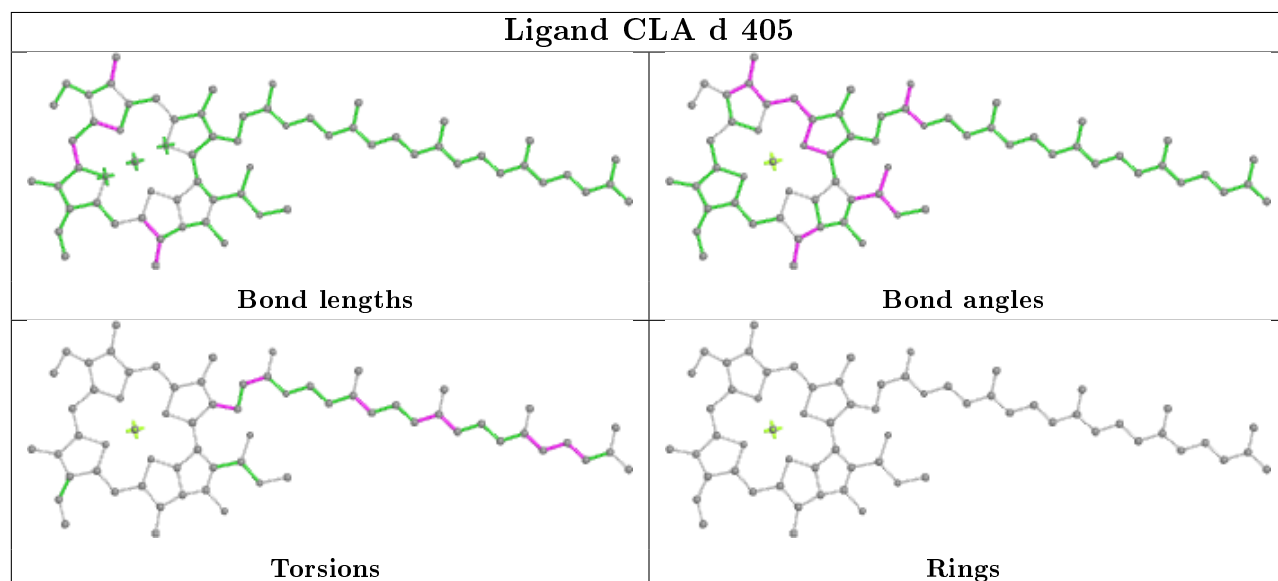




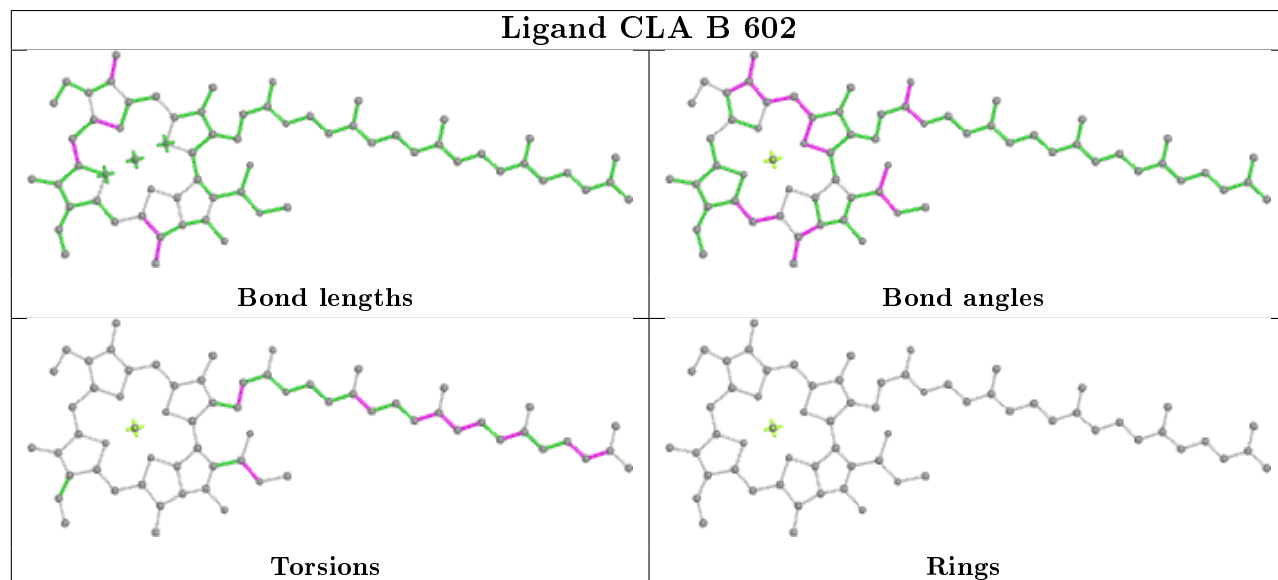
## Ligand CLA b 615



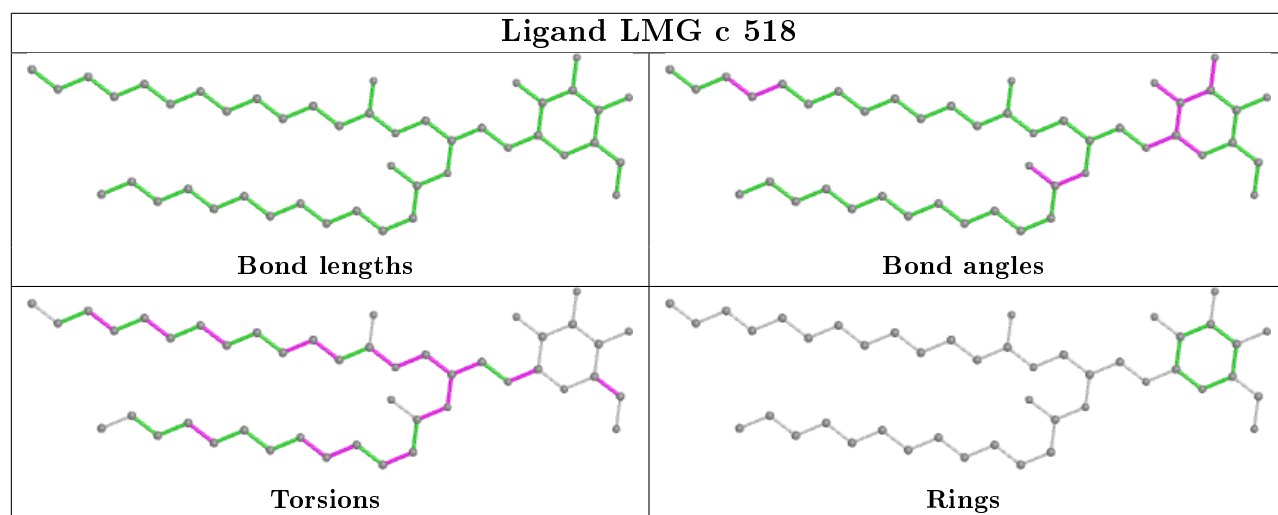
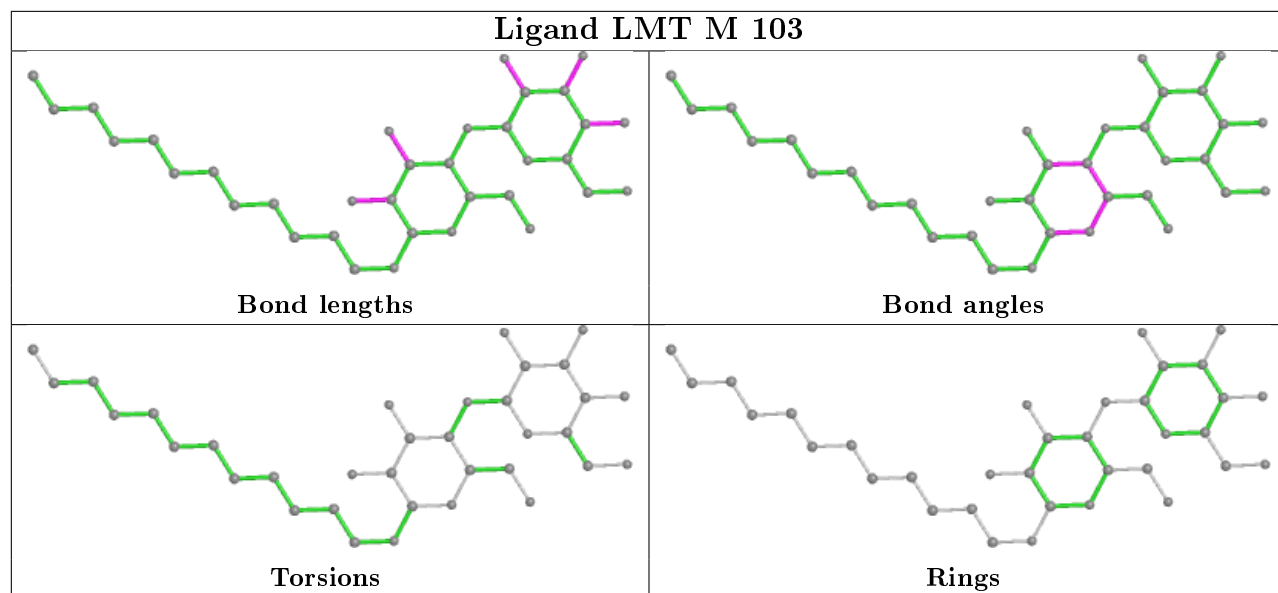
## Ligand CLA d 405

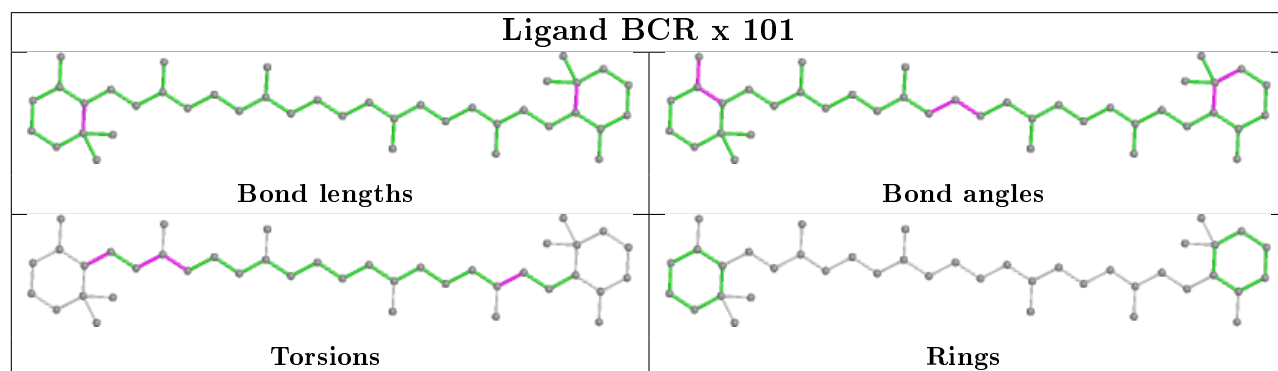
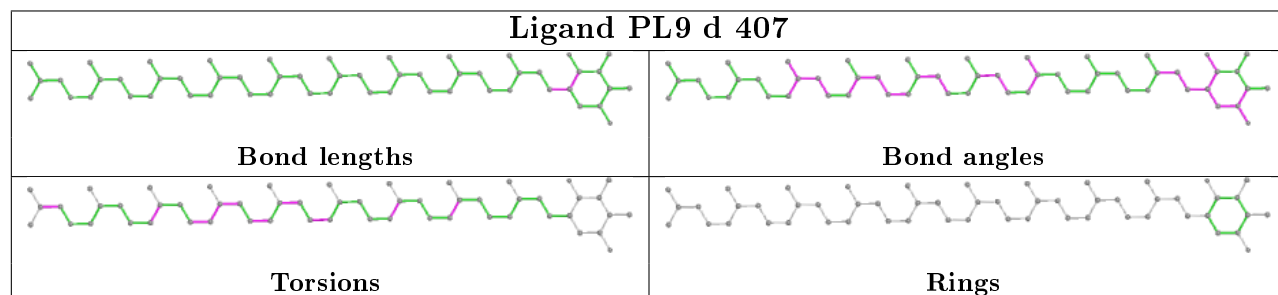
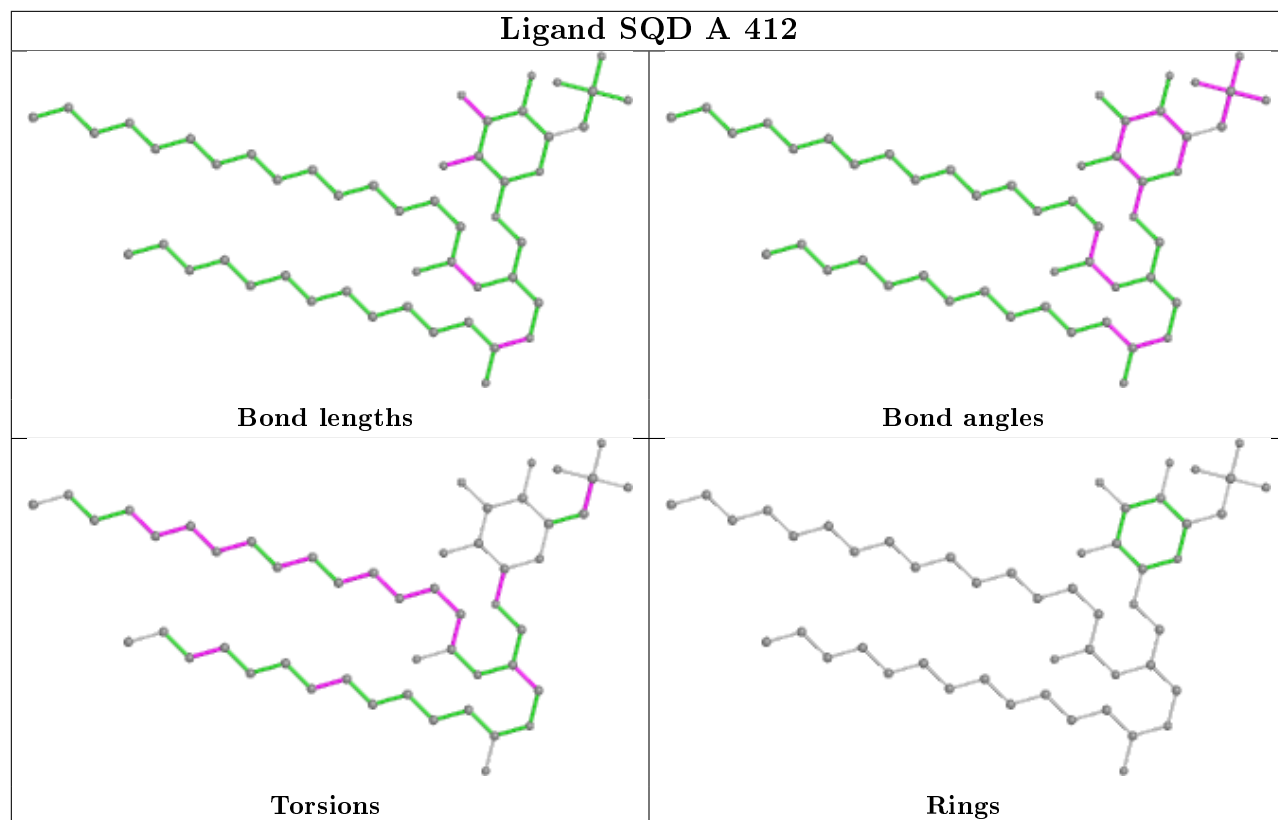


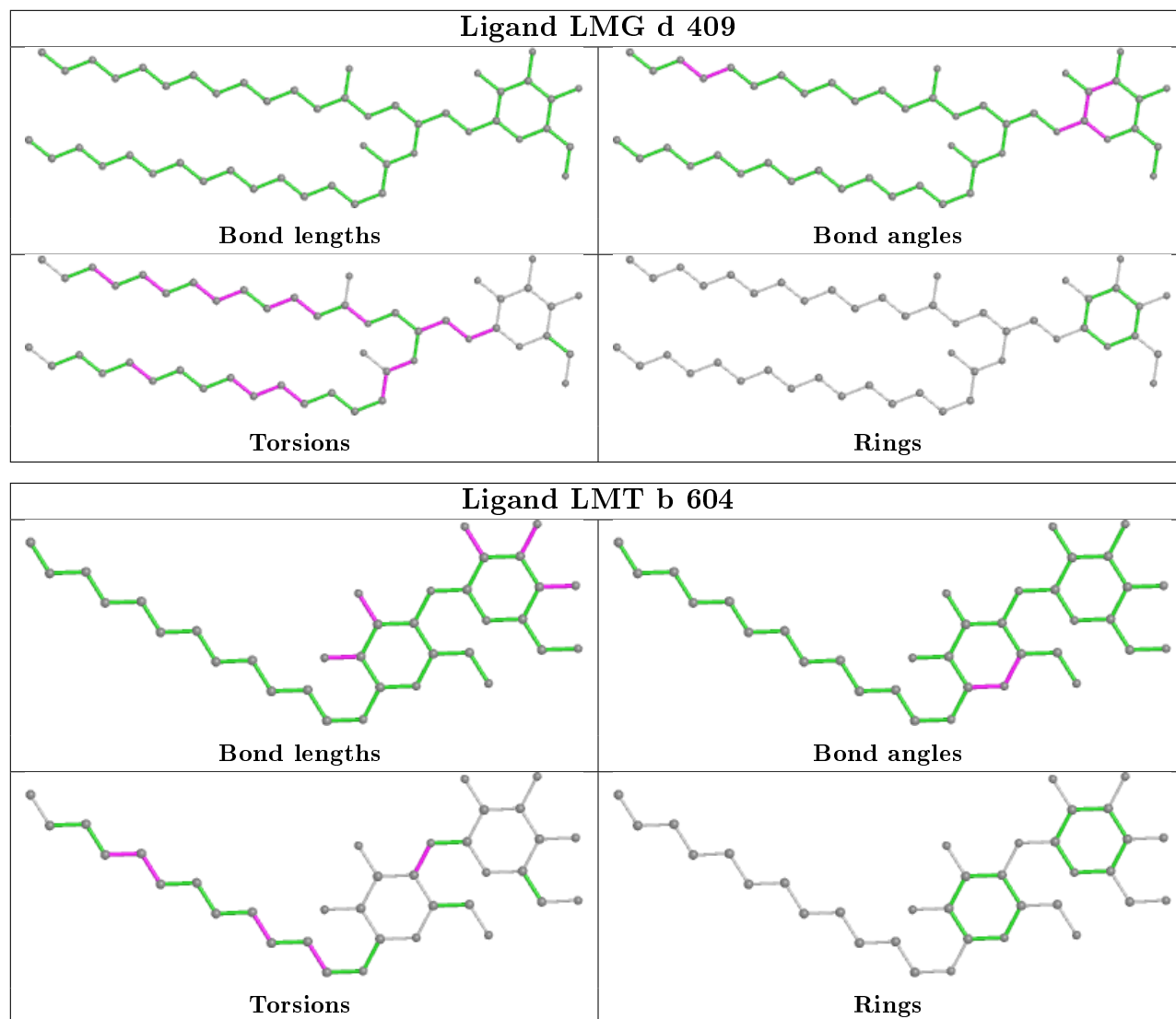
## Ligand CLA B 602



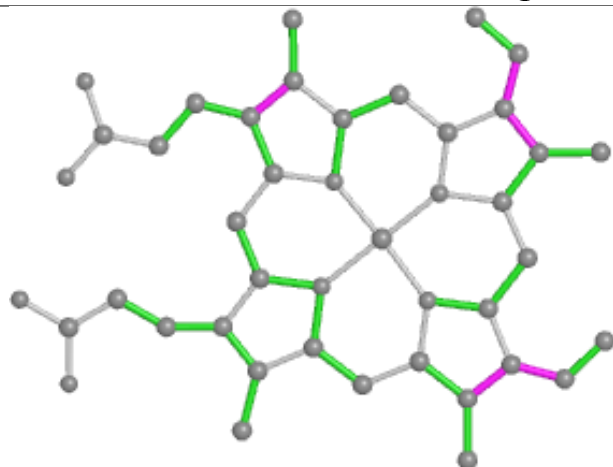




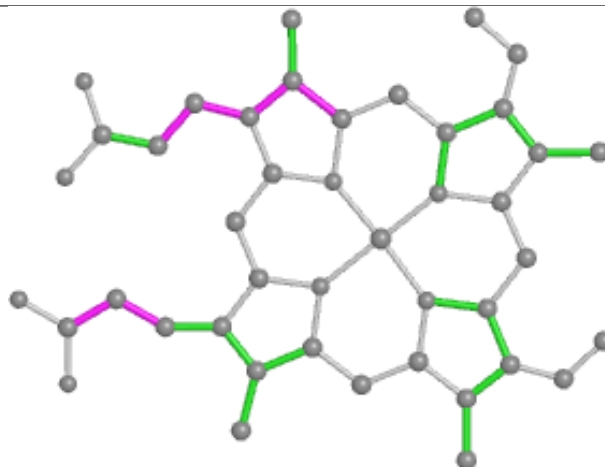




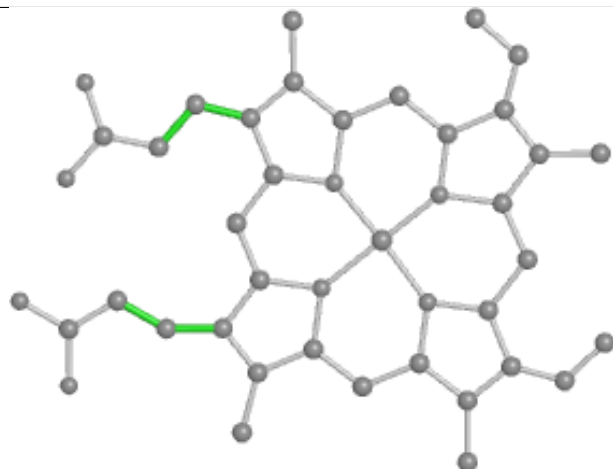
## Ligand HEM f 101



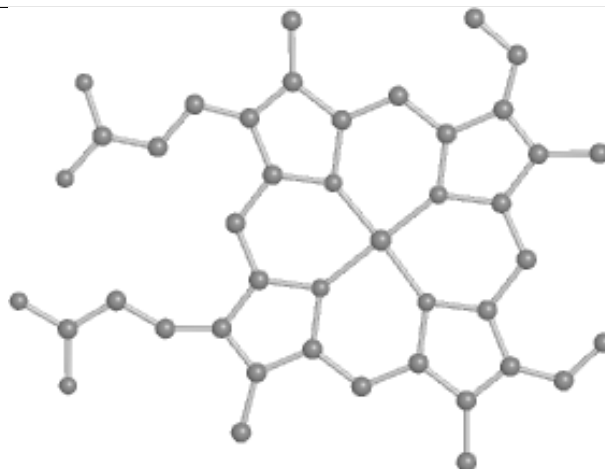
Bond lengths



Bond angles

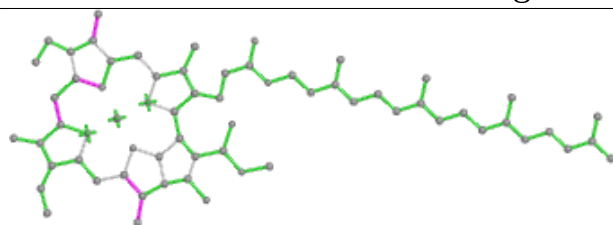


Torsions

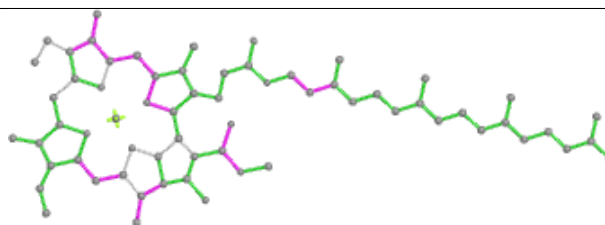


Rings

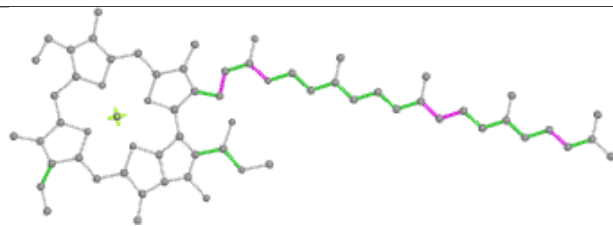
## Ligand CLA D 406



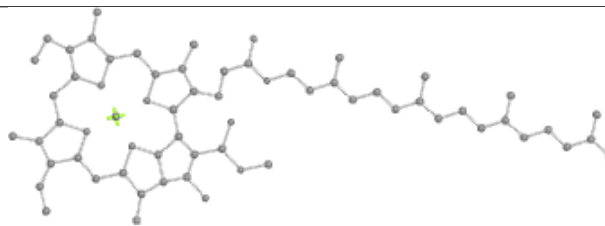
Bond lengths



Bond angles

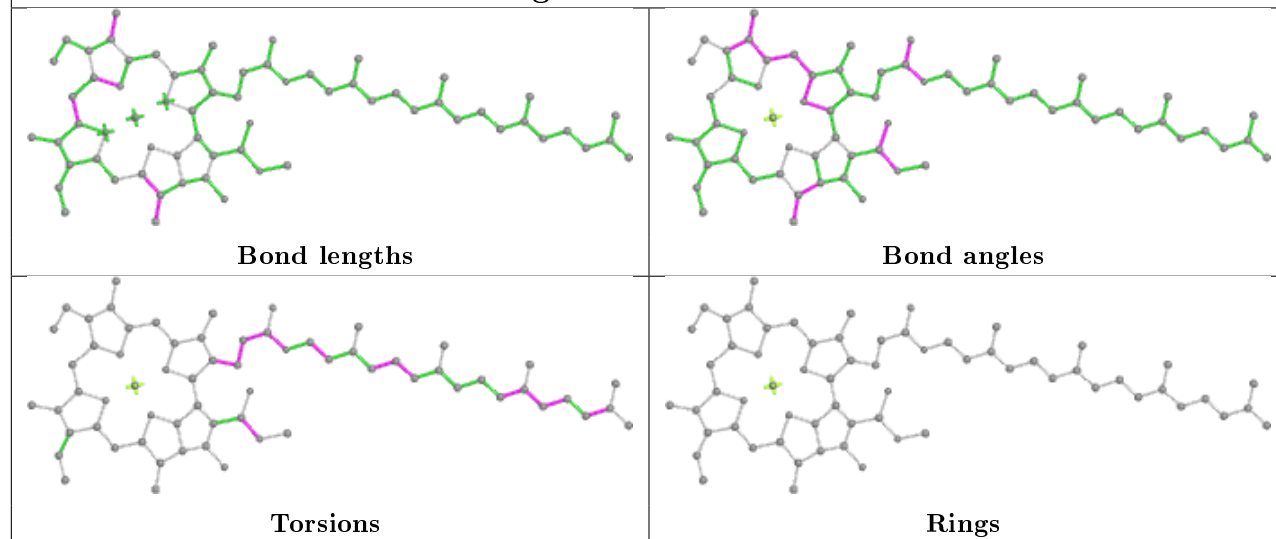


Torsions

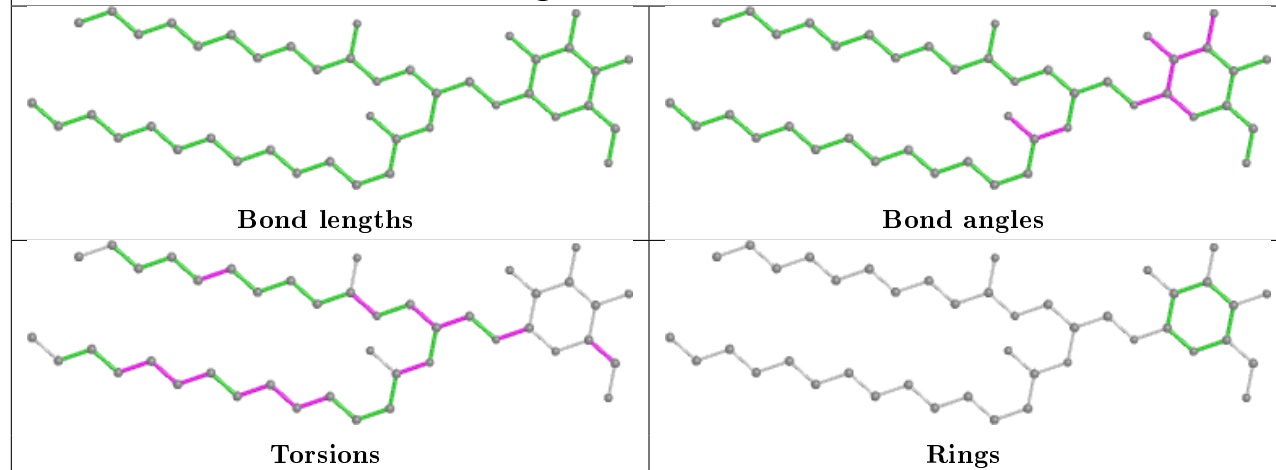


Rings

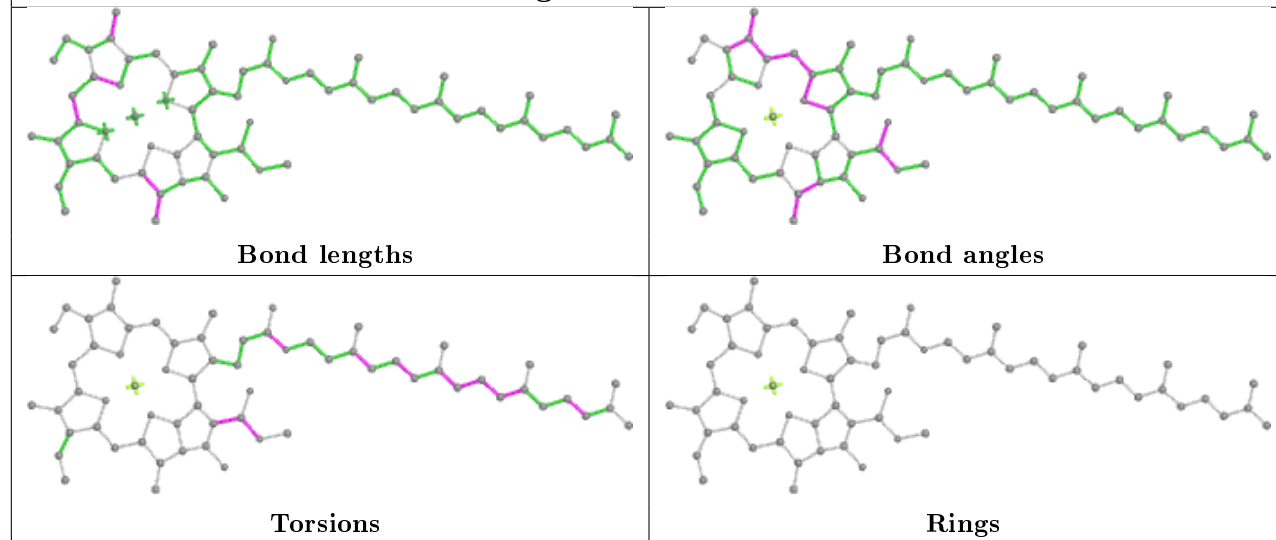
## Ligand CLA C 511

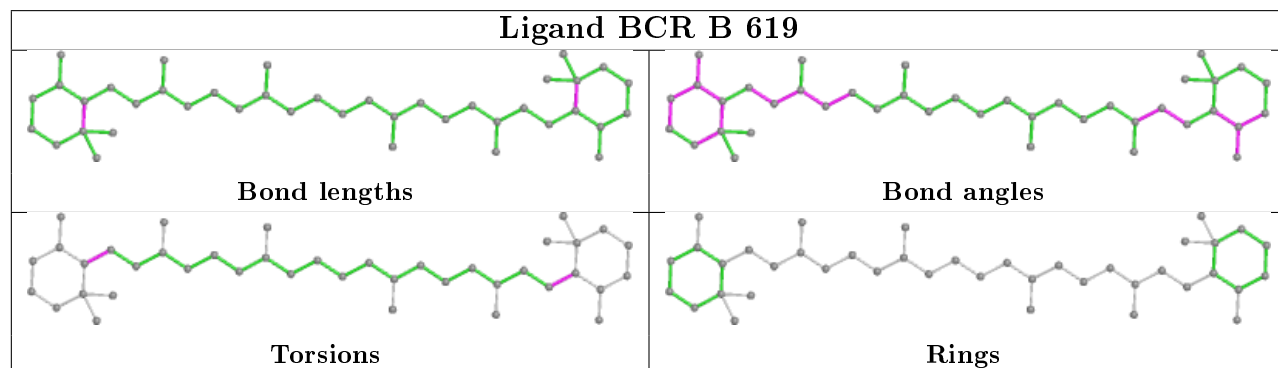
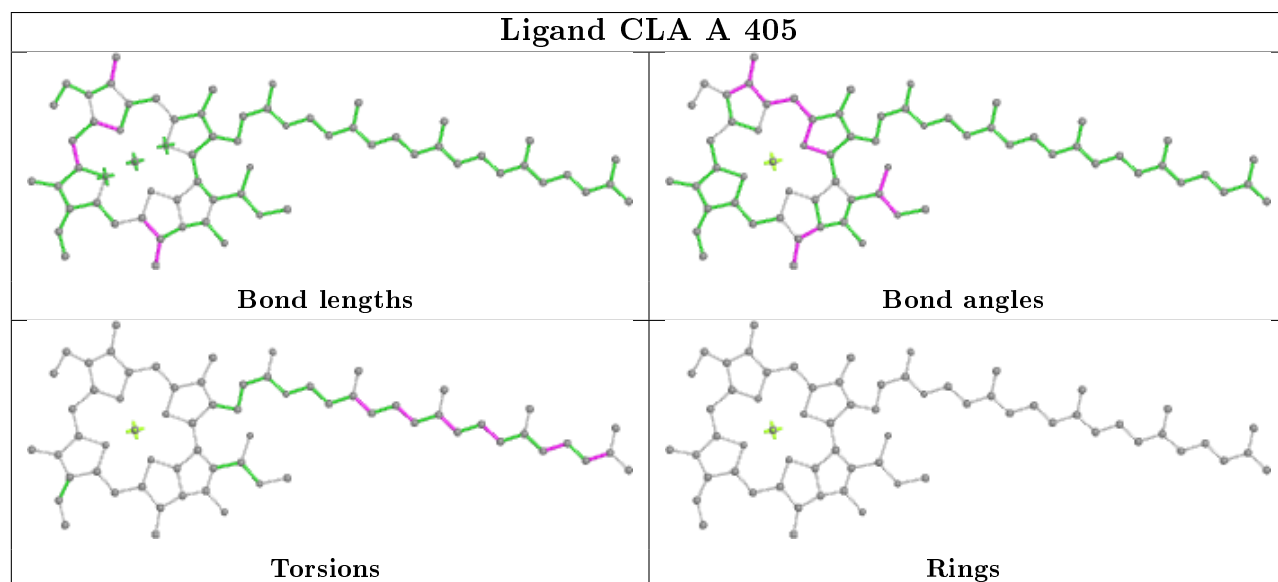
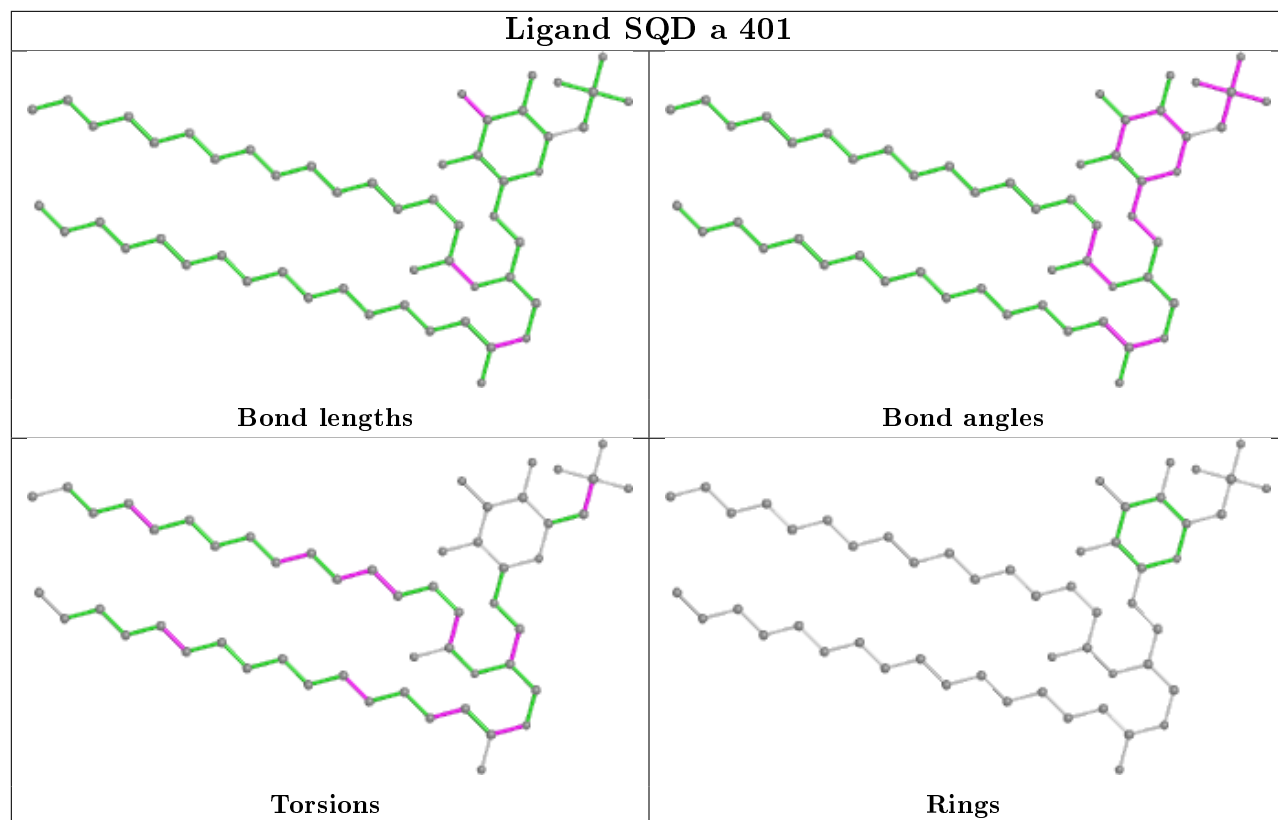


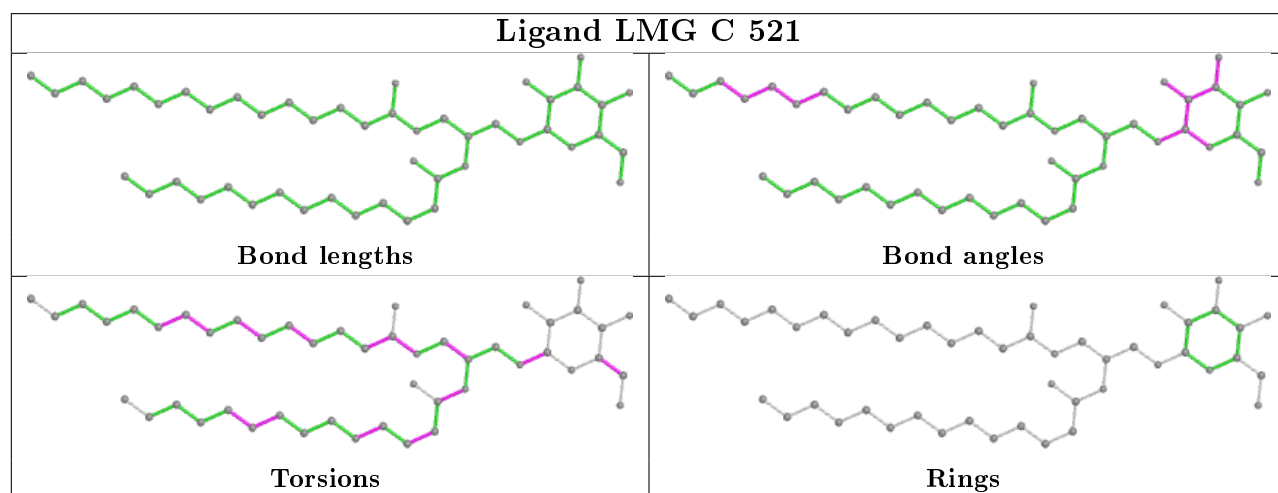
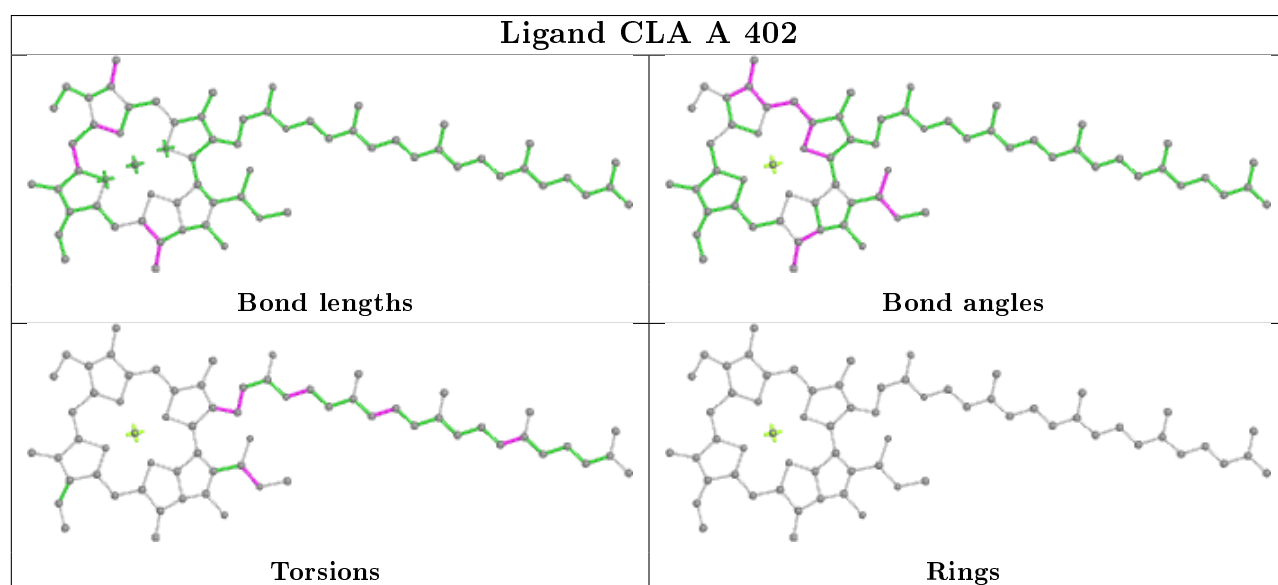
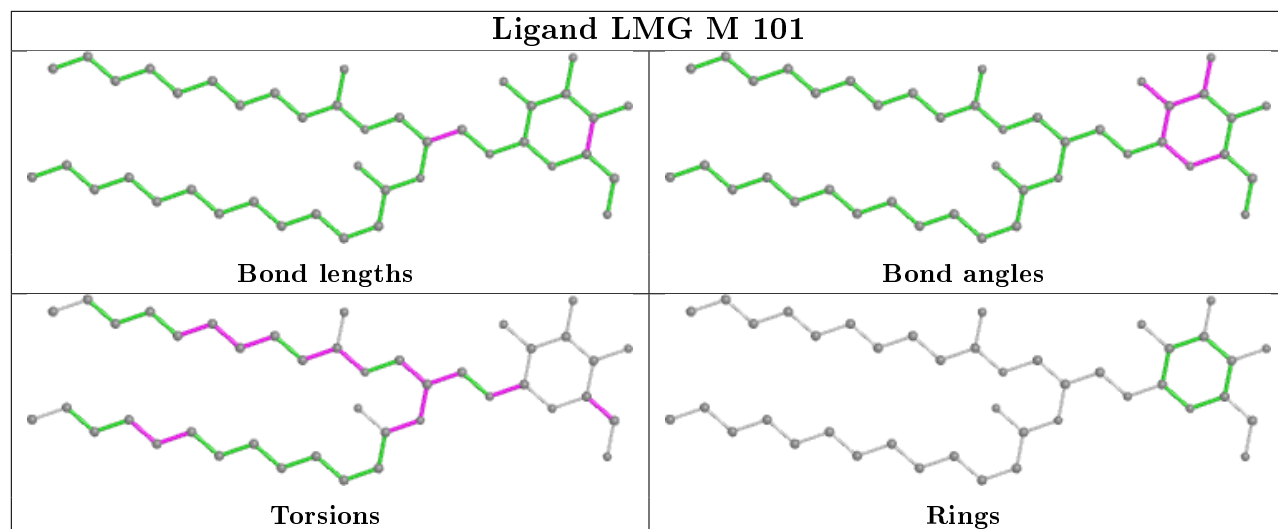
## Ligand LMG I 101



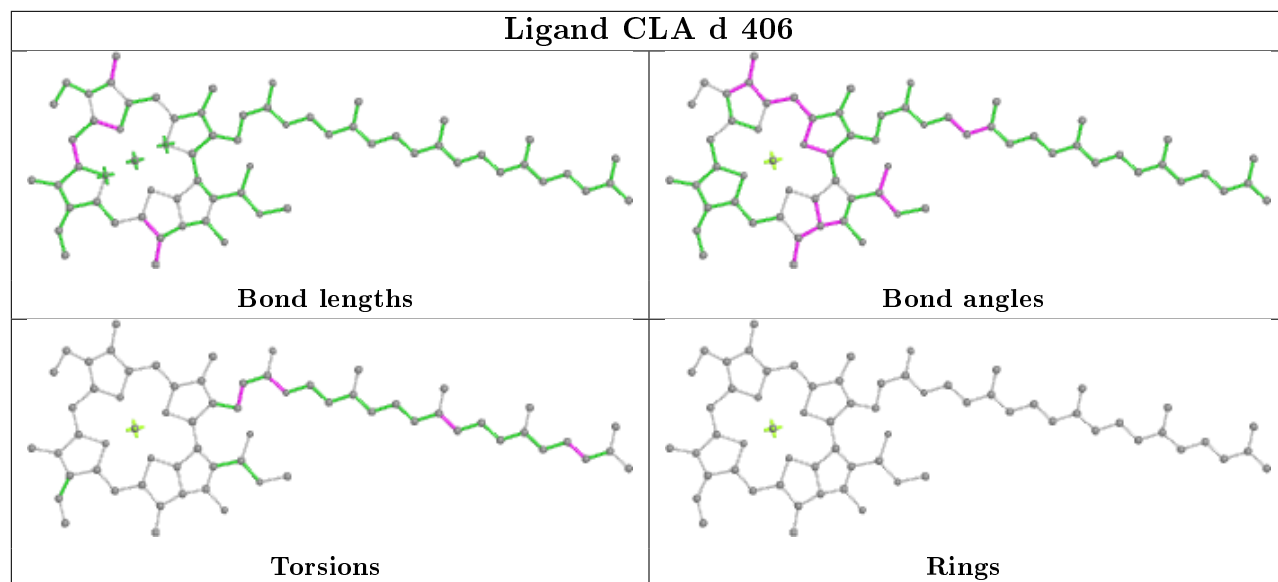
## Ligand CLA b 608



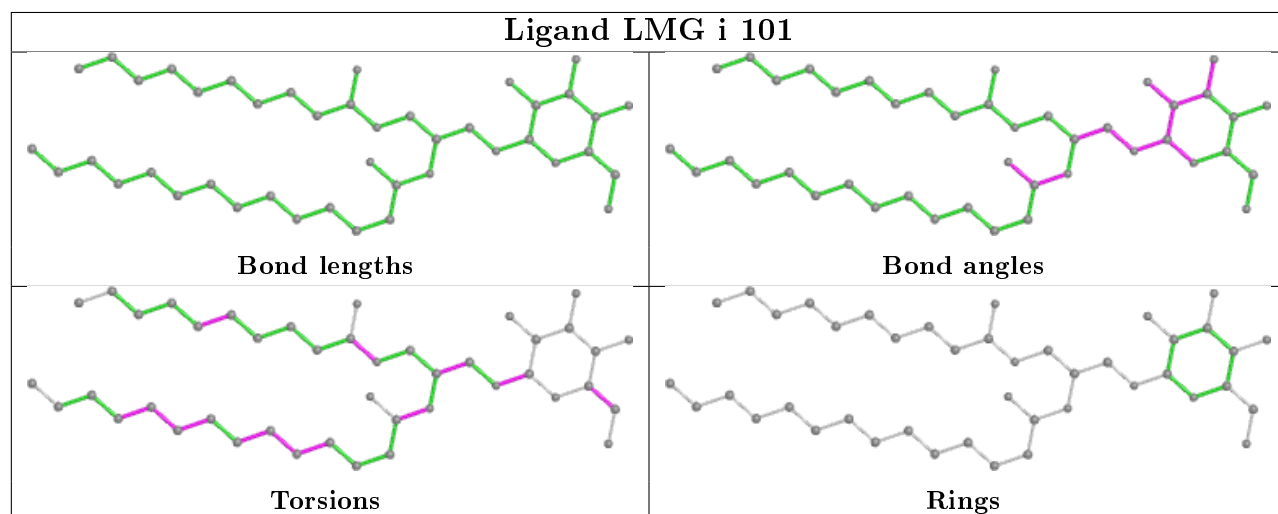




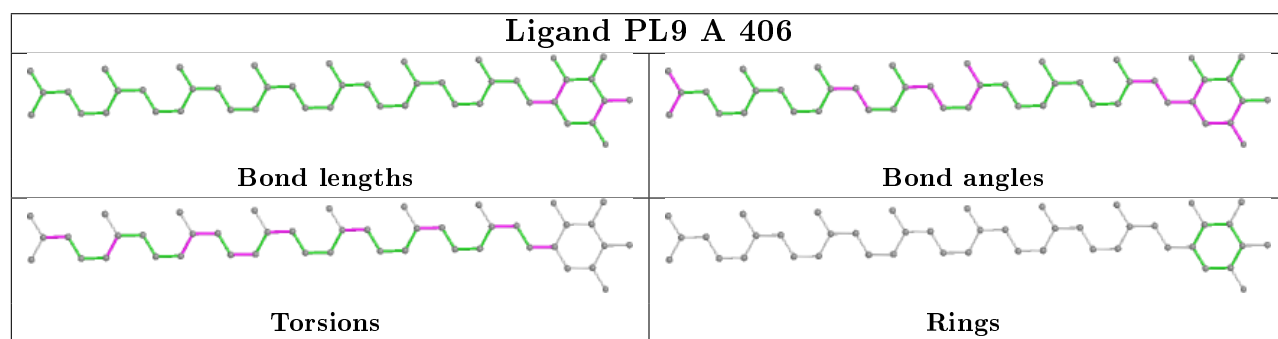
## Ligand CLA d 406



## Ligand LMG i 101

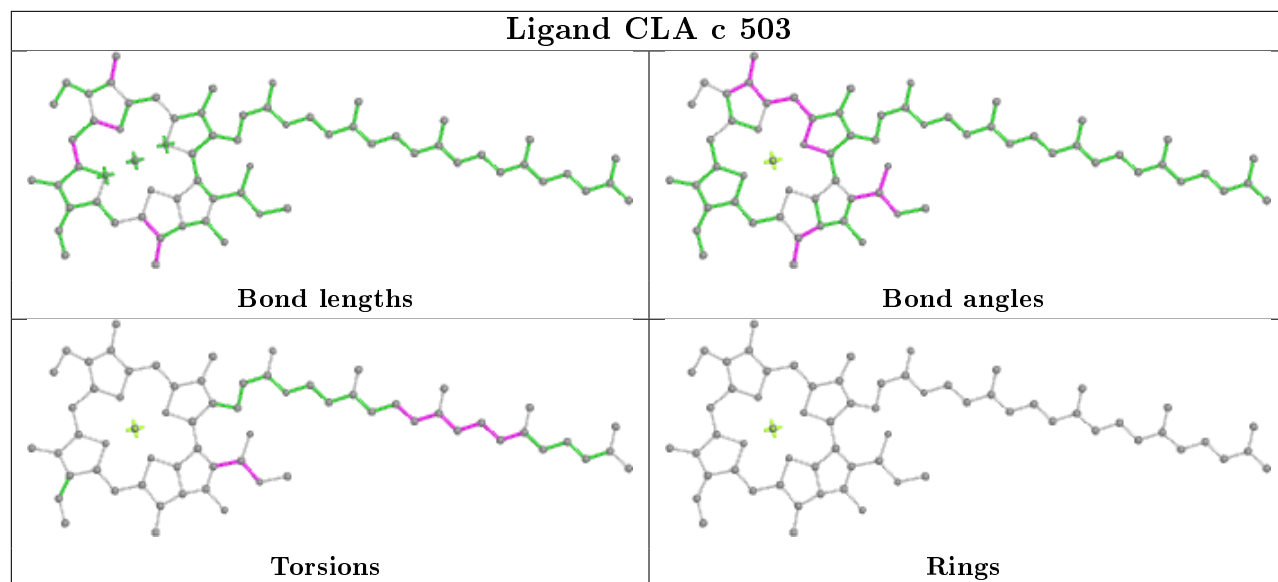


## Ligand PL9 A 406

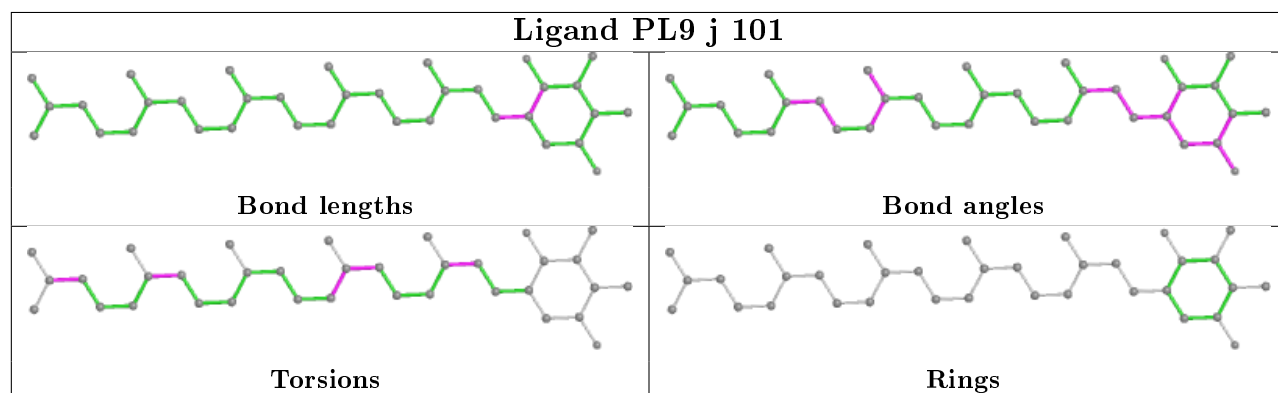




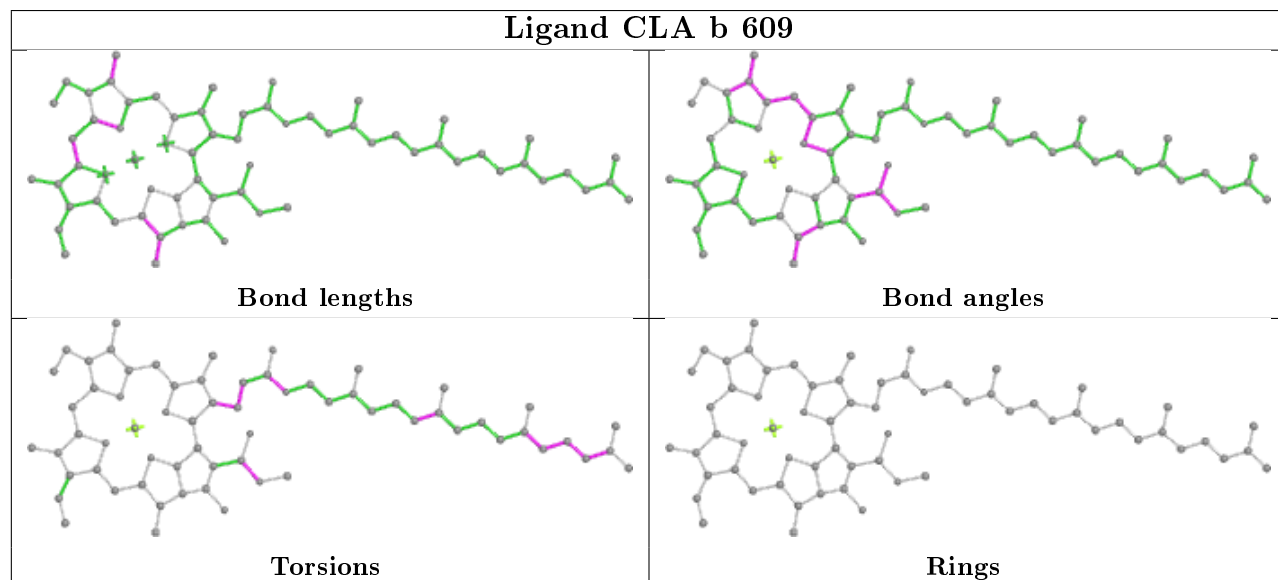
## Ligand CLA c 503



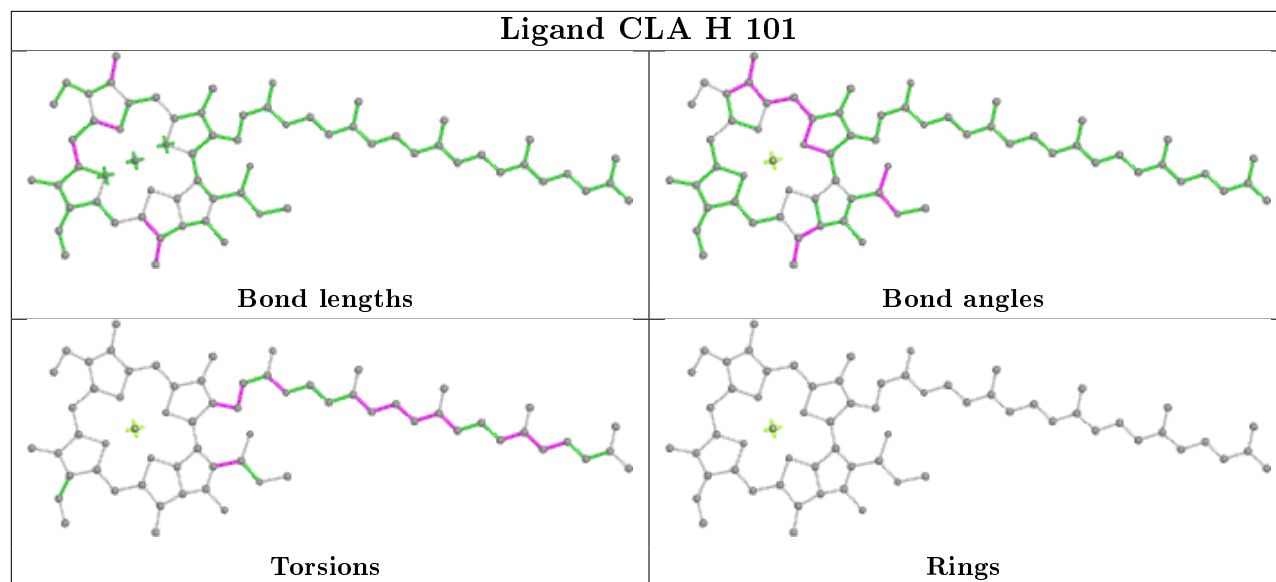
## Ligand PL9 j 101



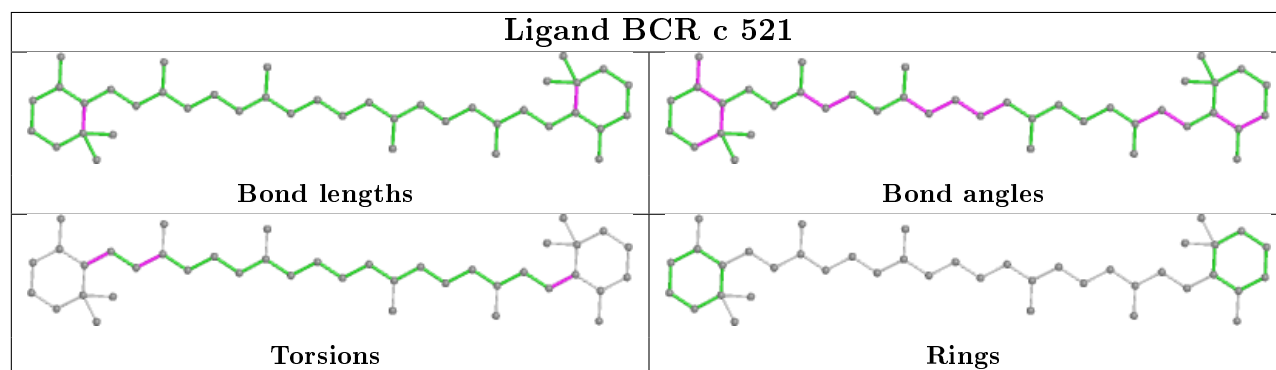
## Ligand CLA b 609



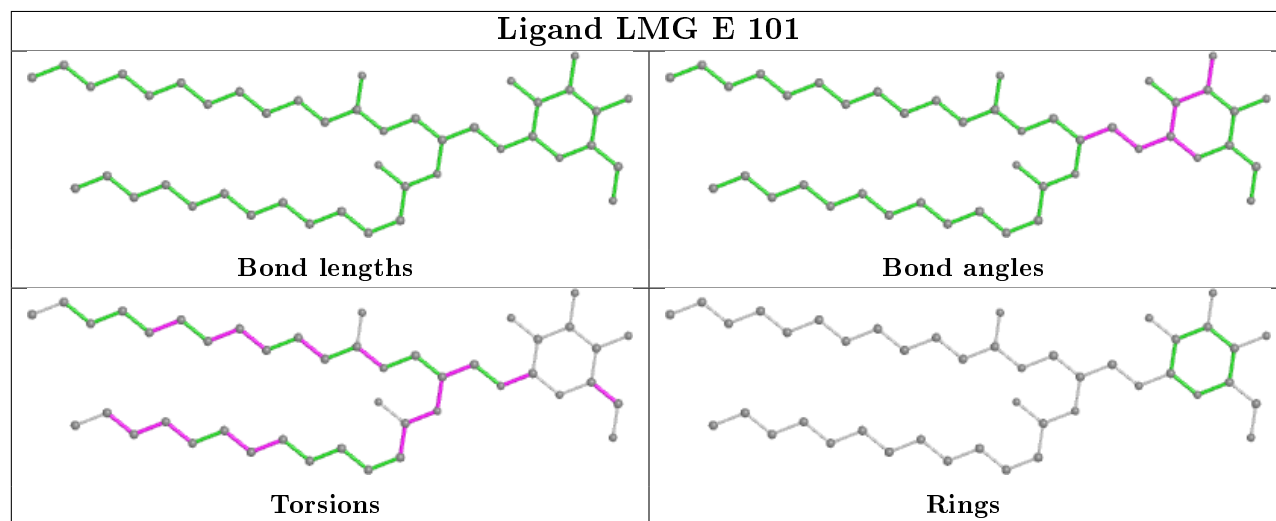
## Ligand CLA H 101



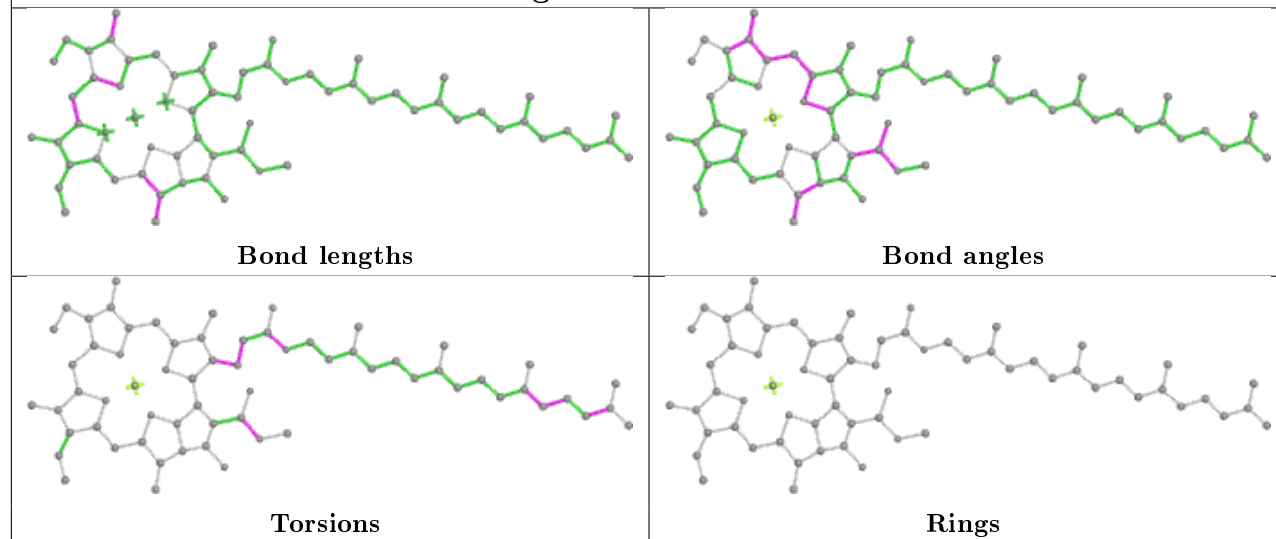
## Ligand BCR c 521



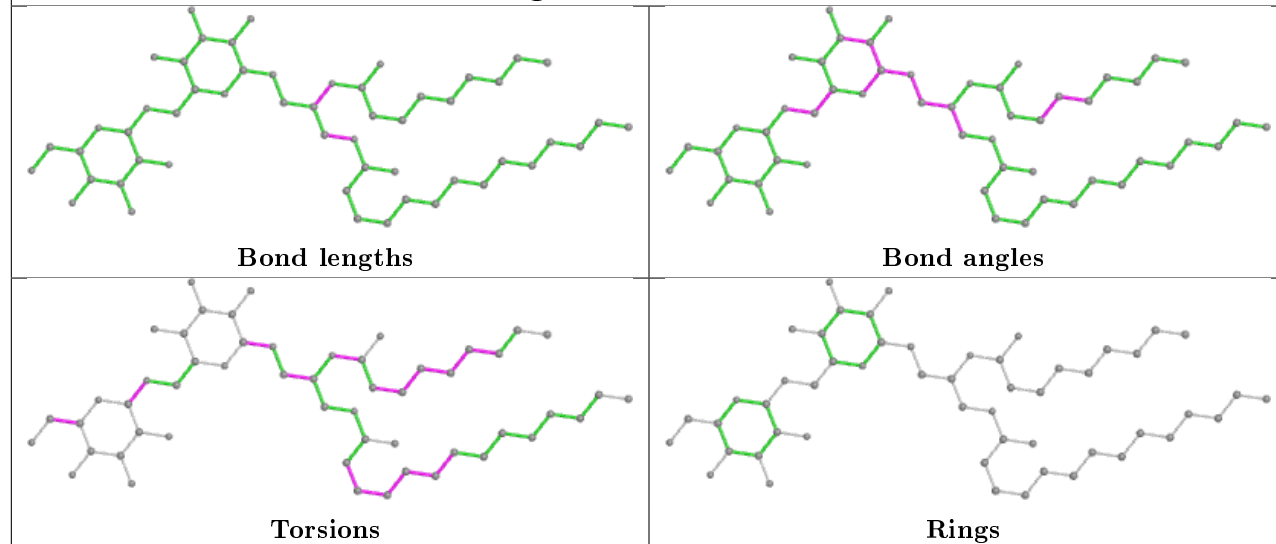
## Ligand LMG E 101

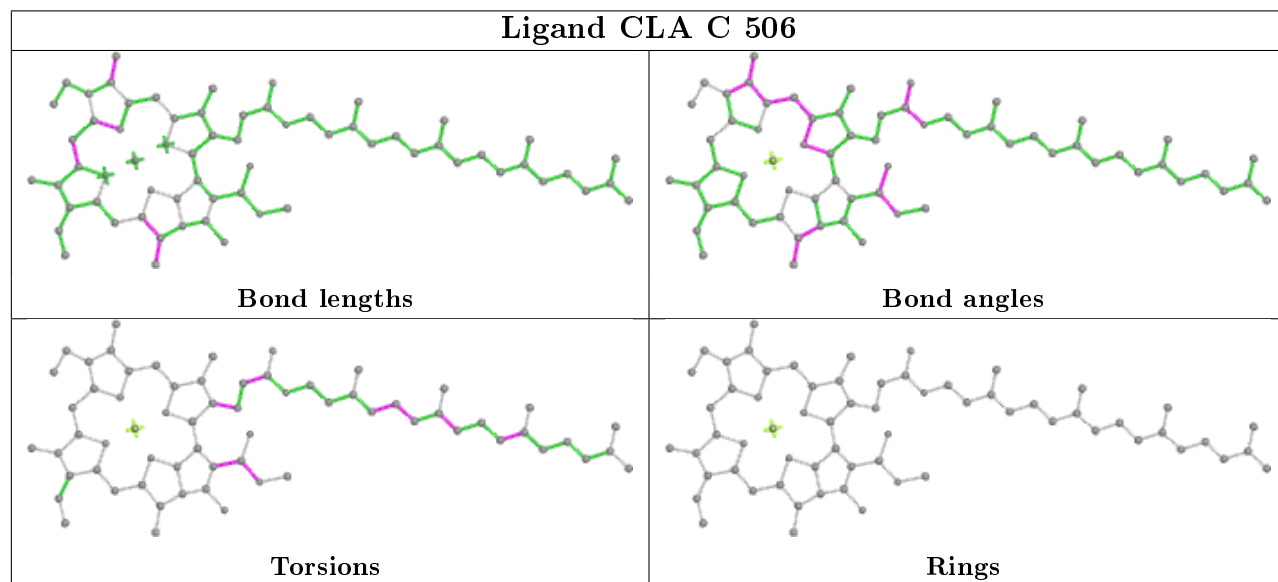
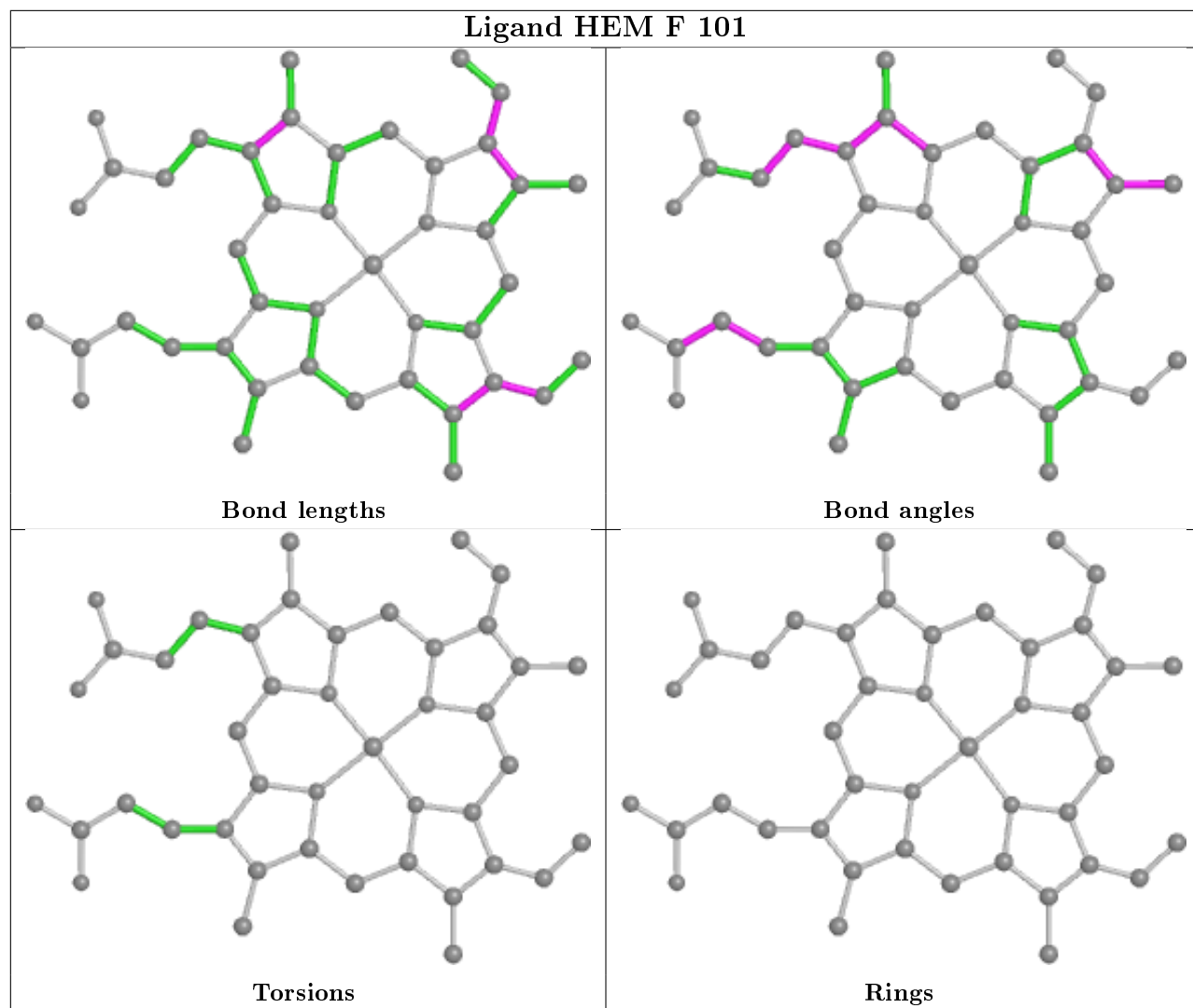


## Ligand CLA B 605

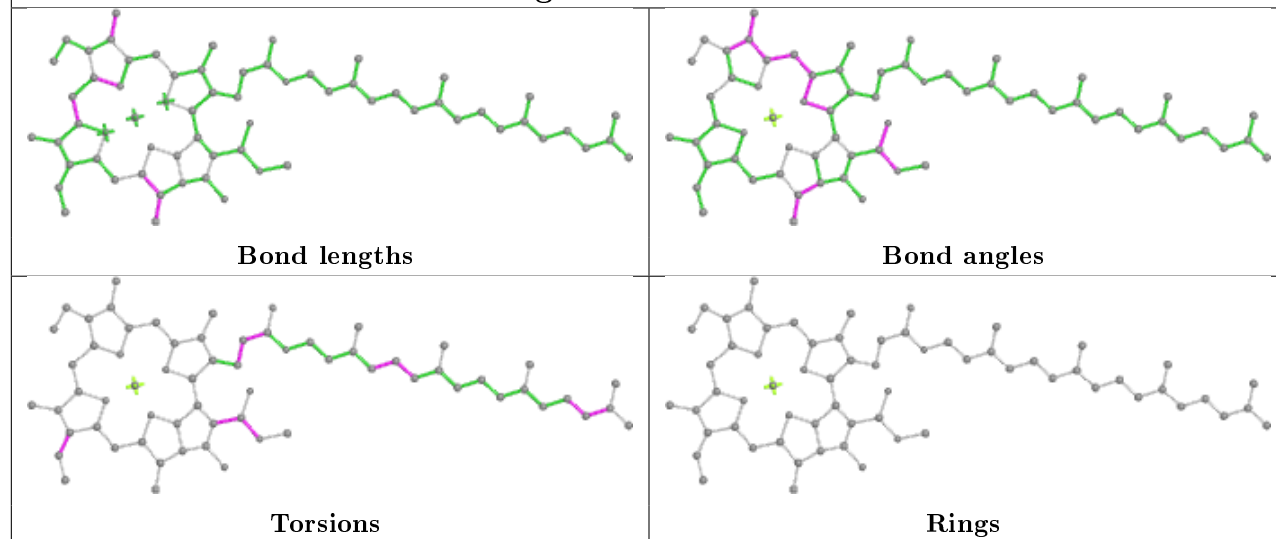


## Ligand DGD C 515

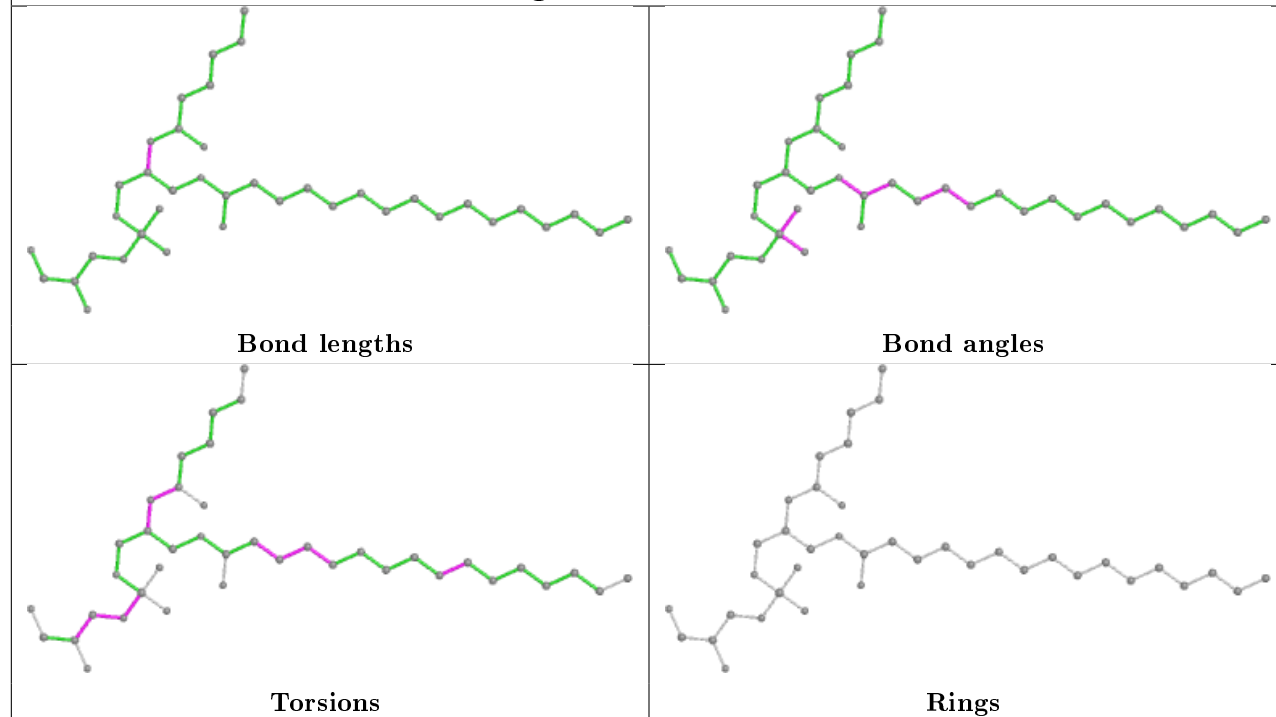


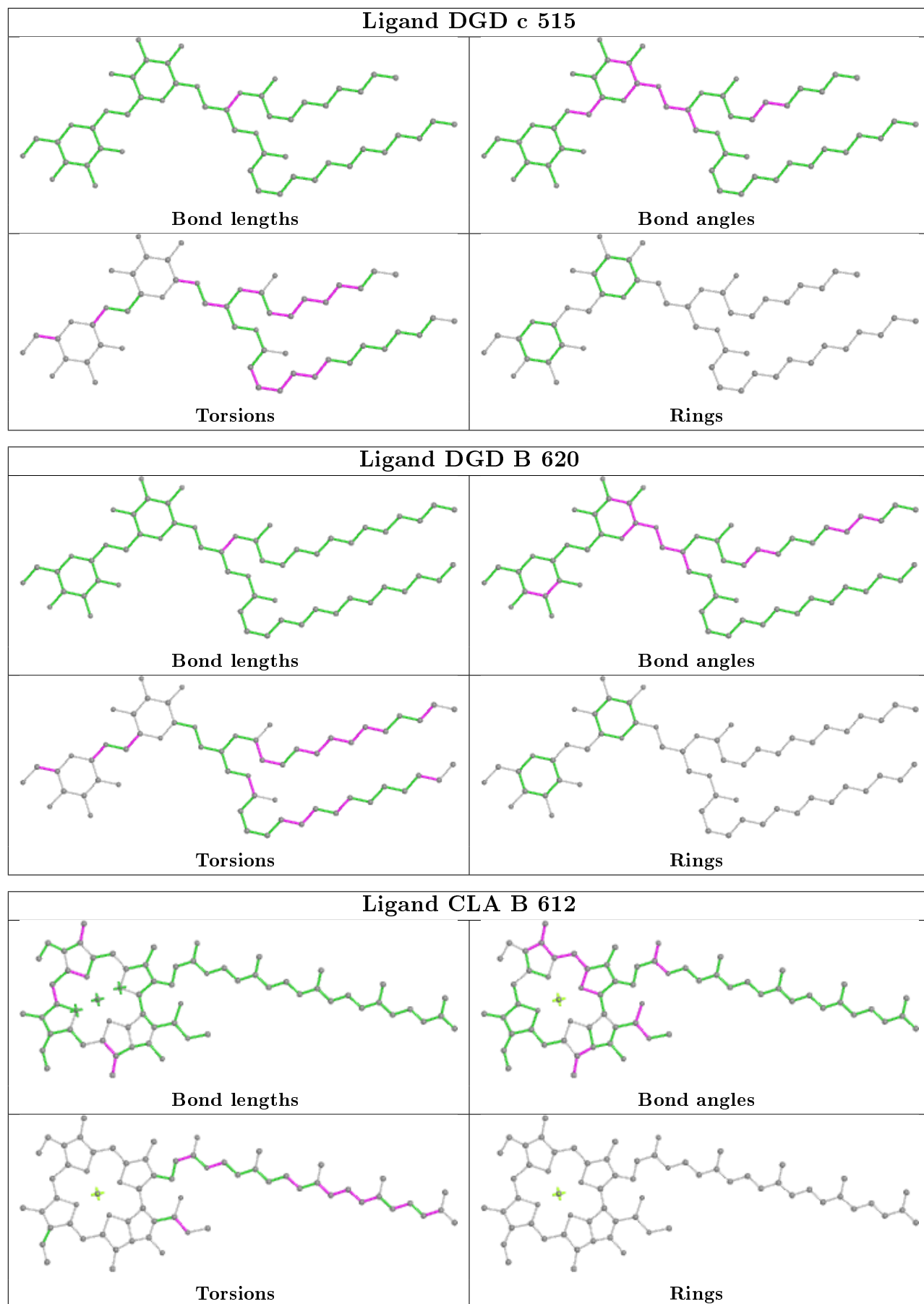


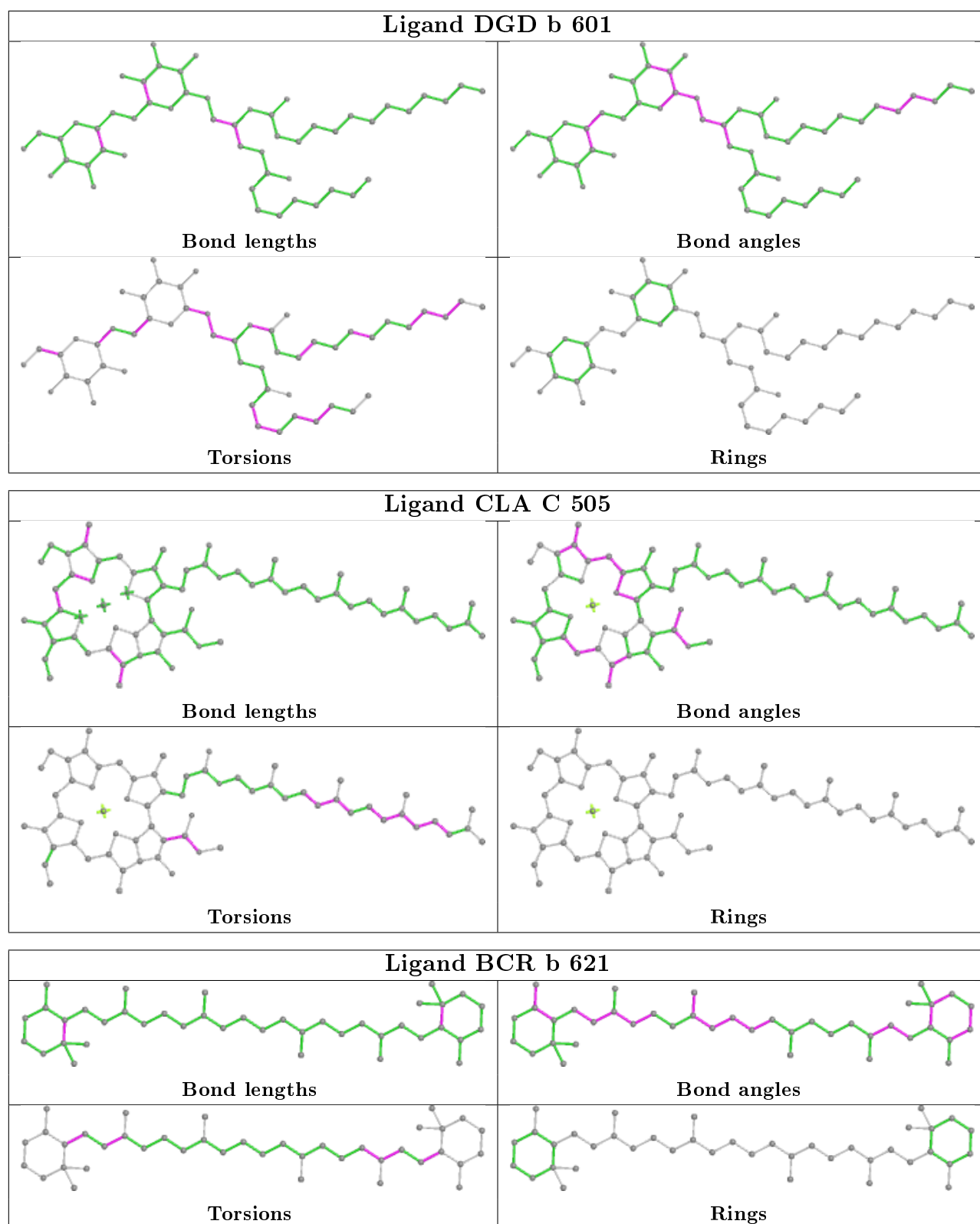
## Ligand CLA b 617



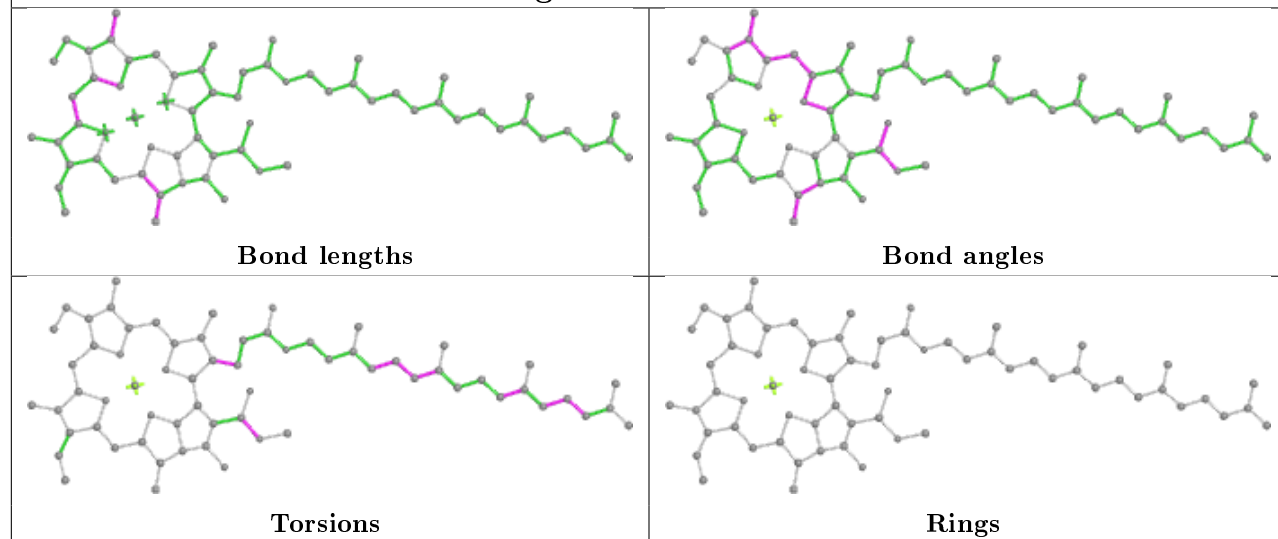
## Ligand LHG A 409



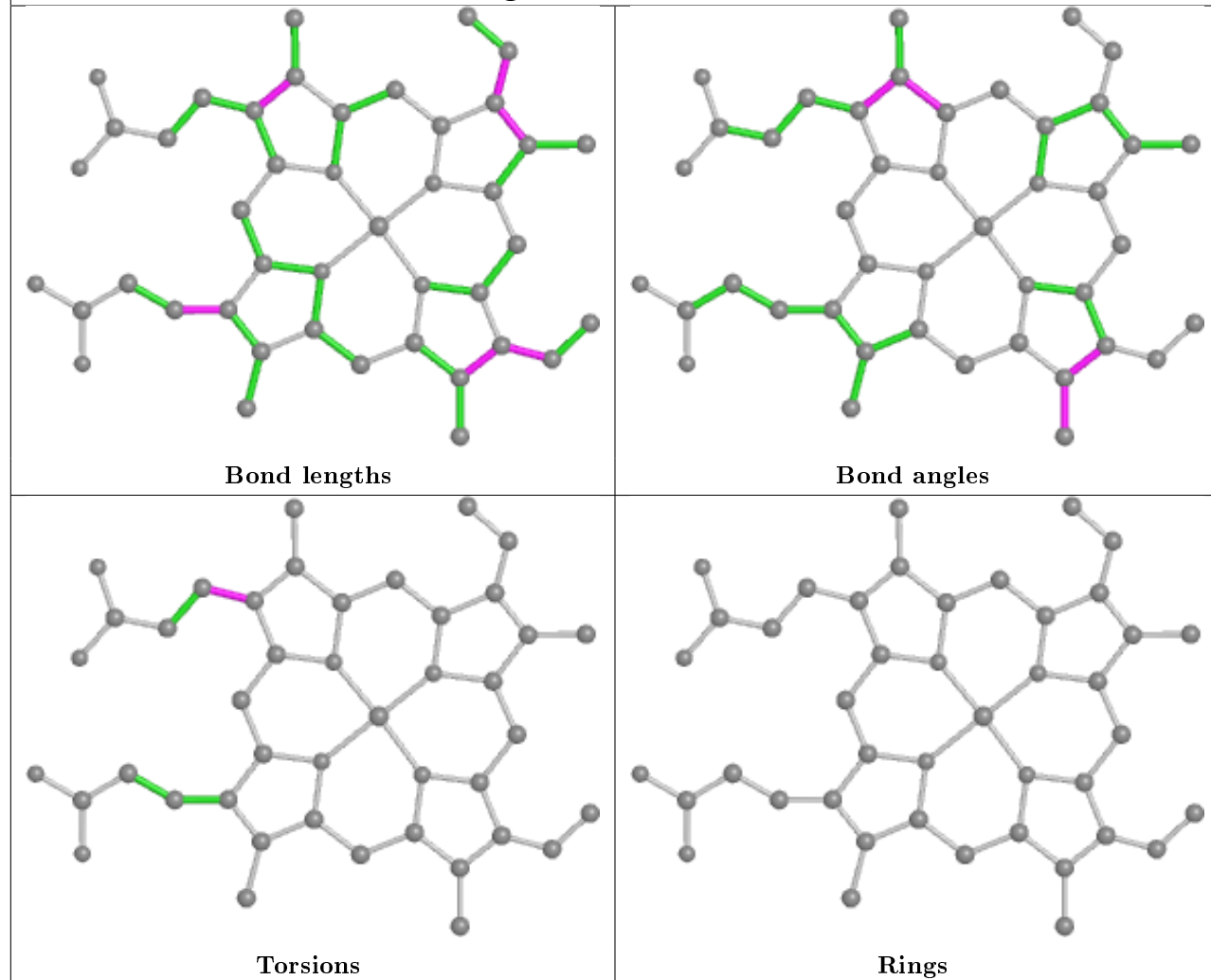




## Ligand CLA b 611

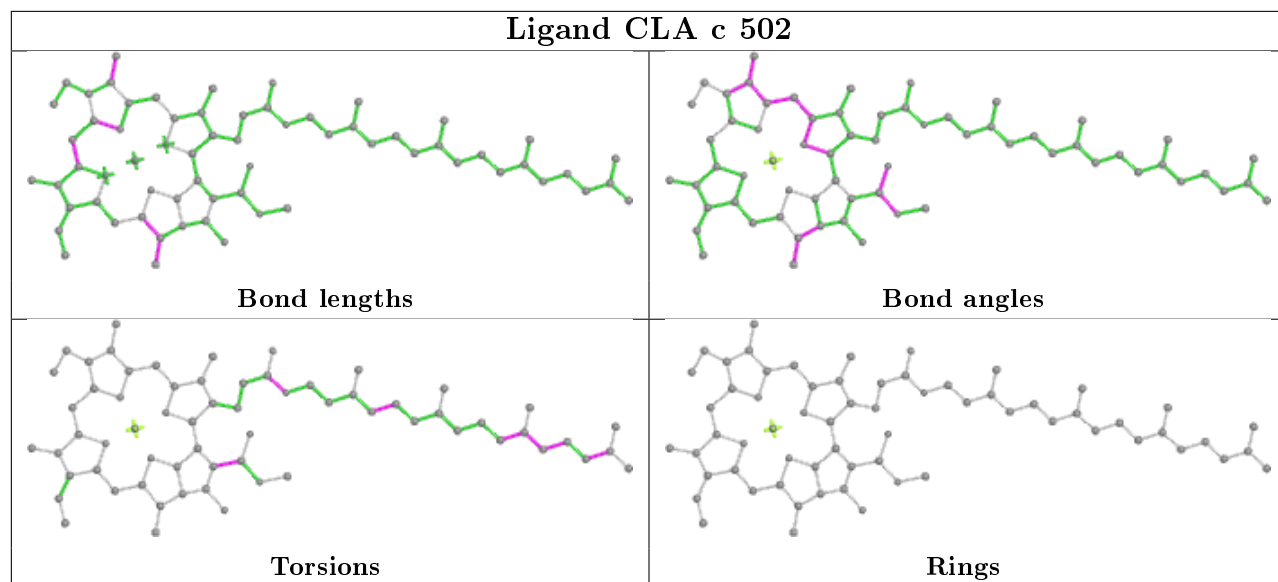


## Ligand HEM v 201

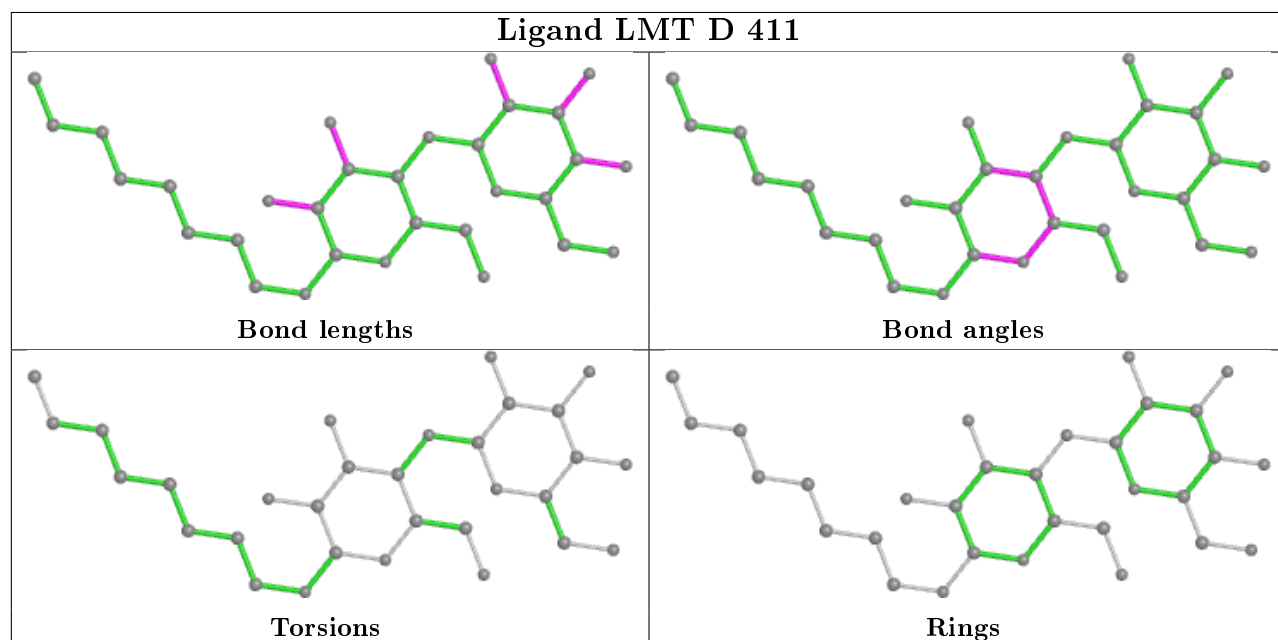




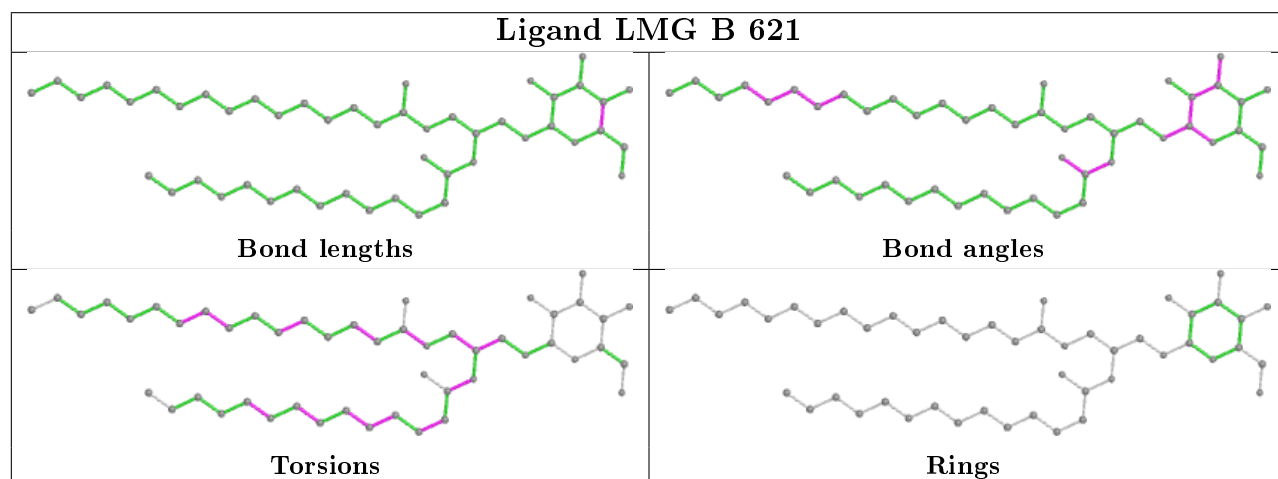
## Ligand CLA c 502

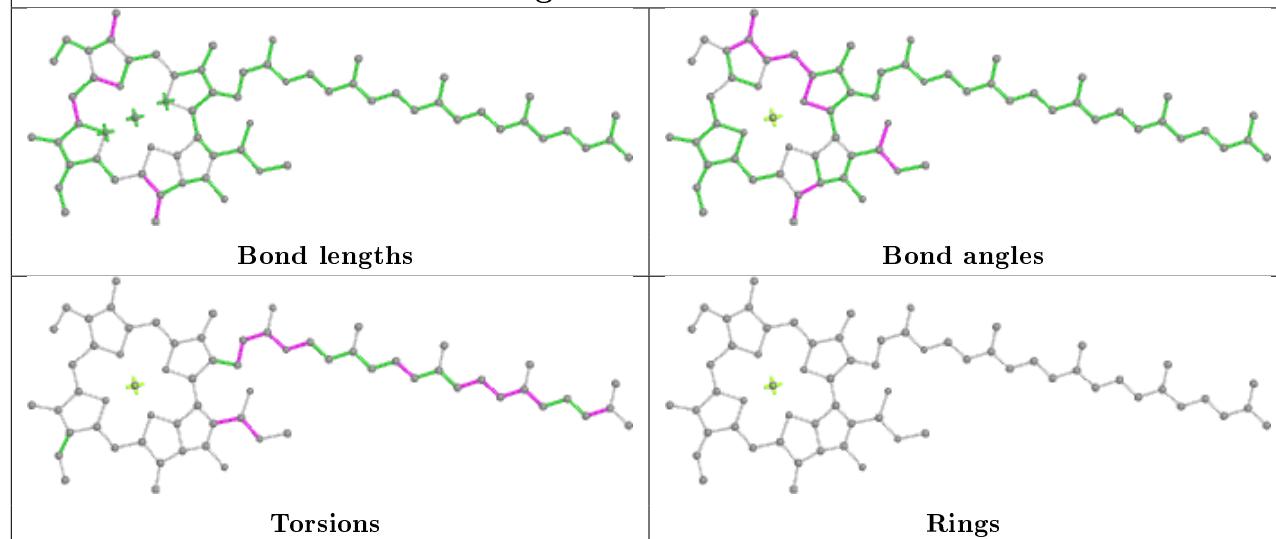
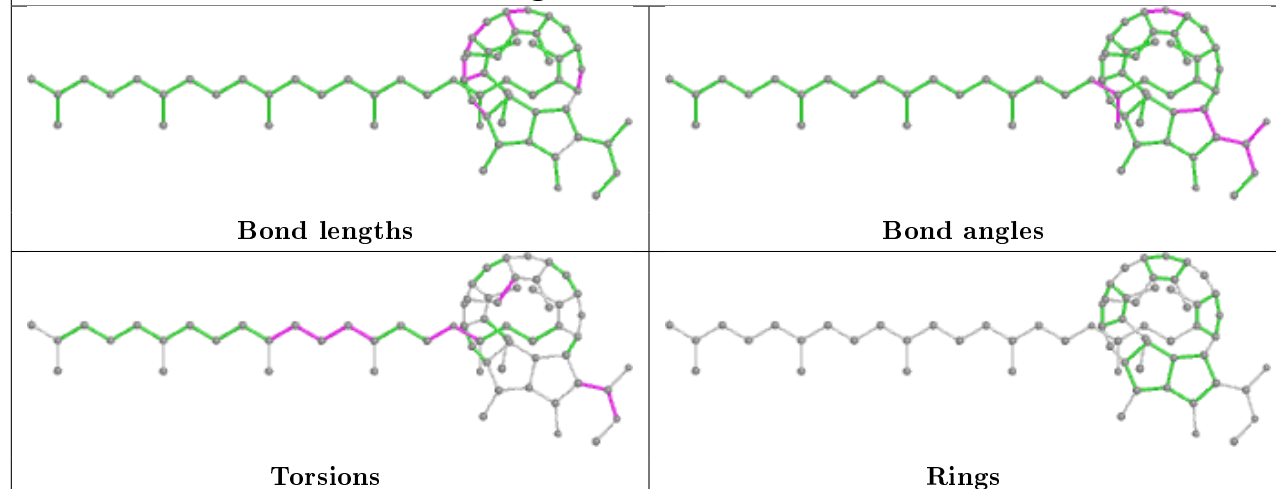
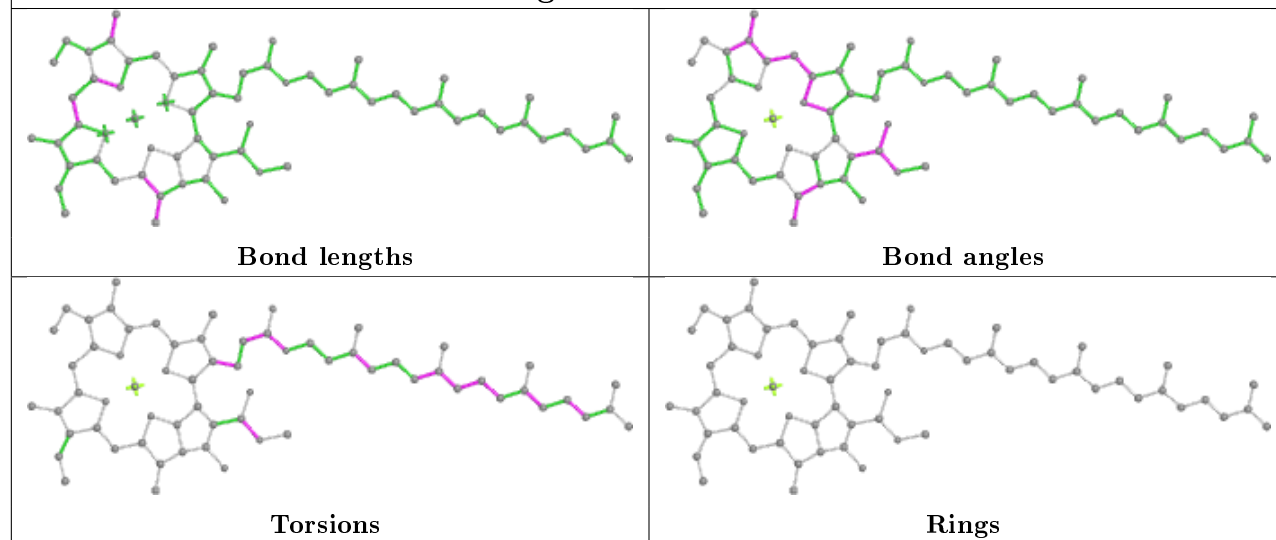


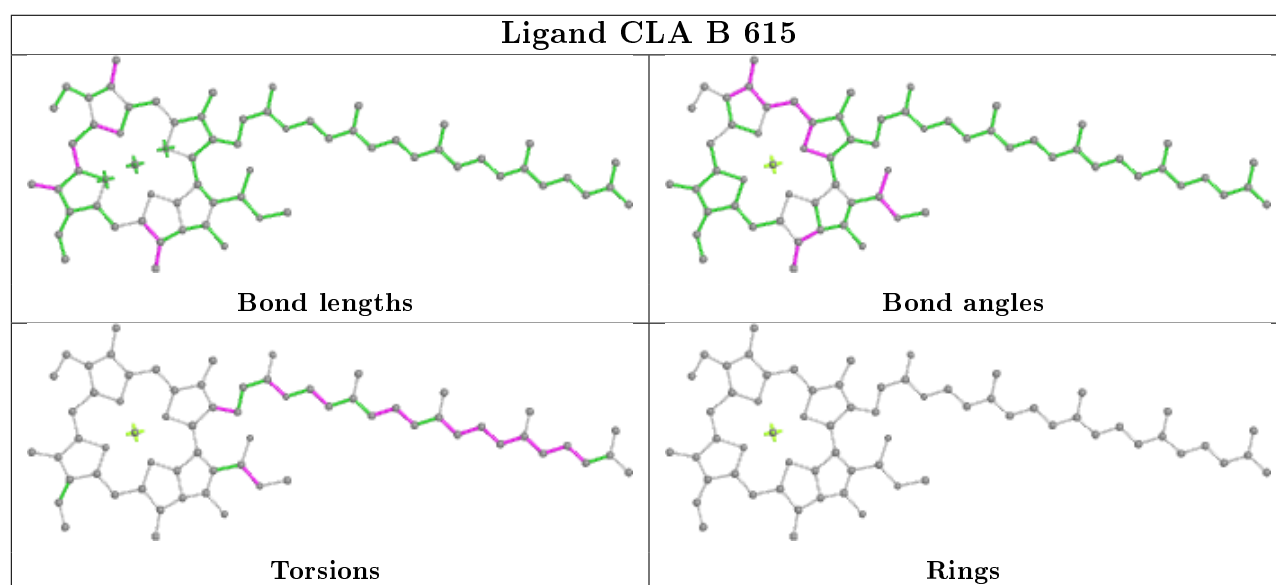
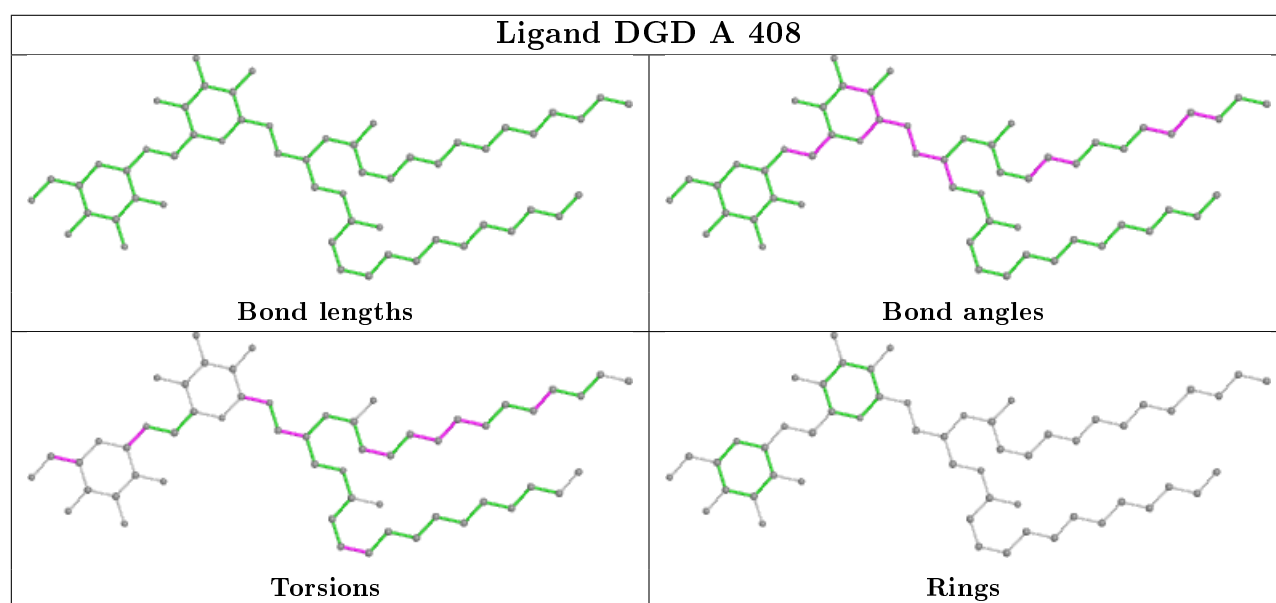
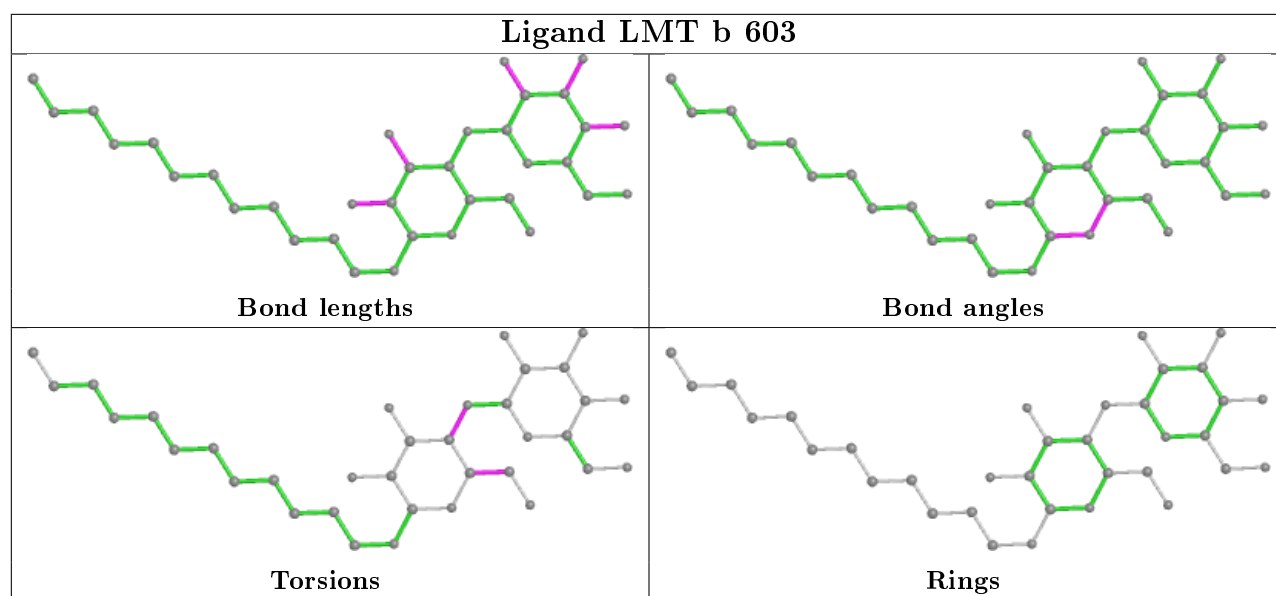
## Ligand LMT D 411

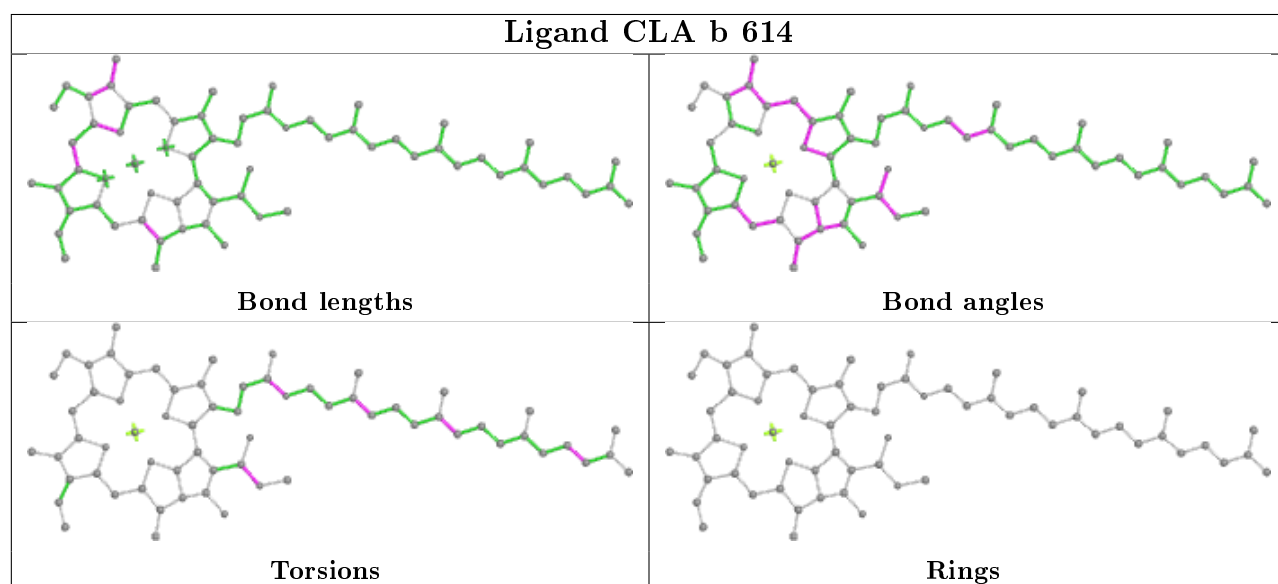
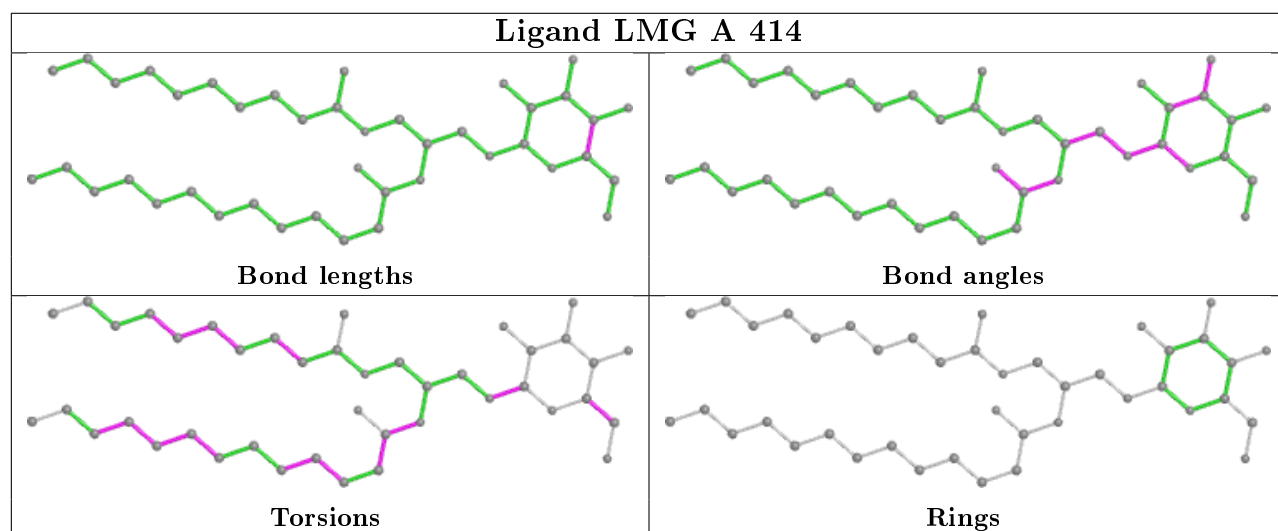
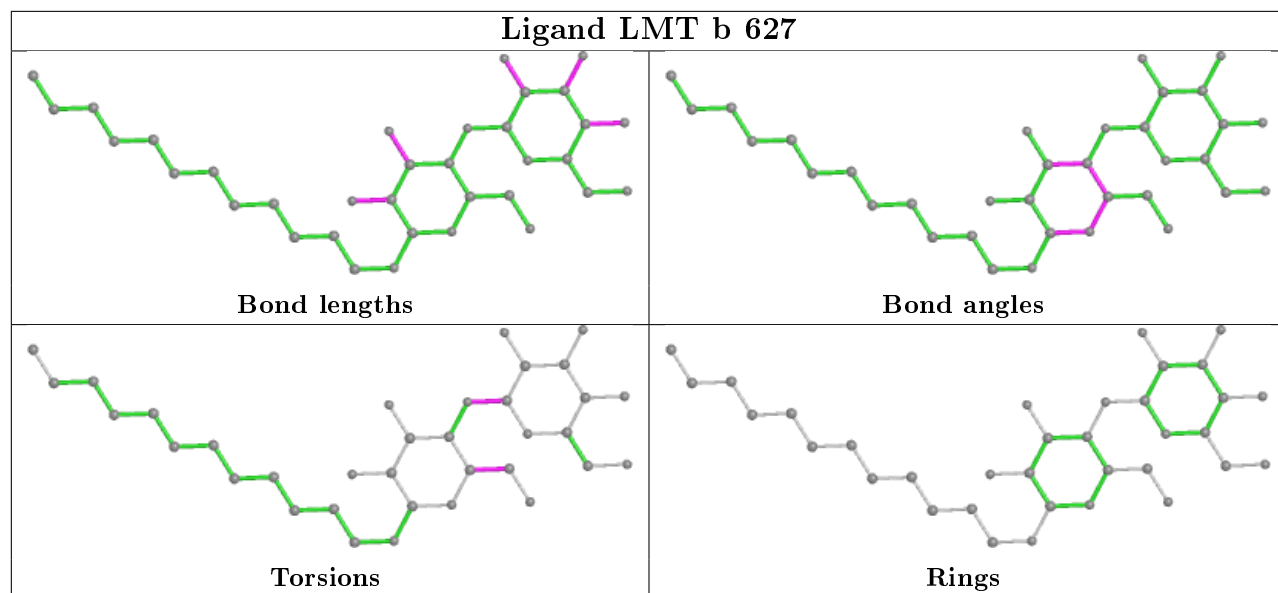


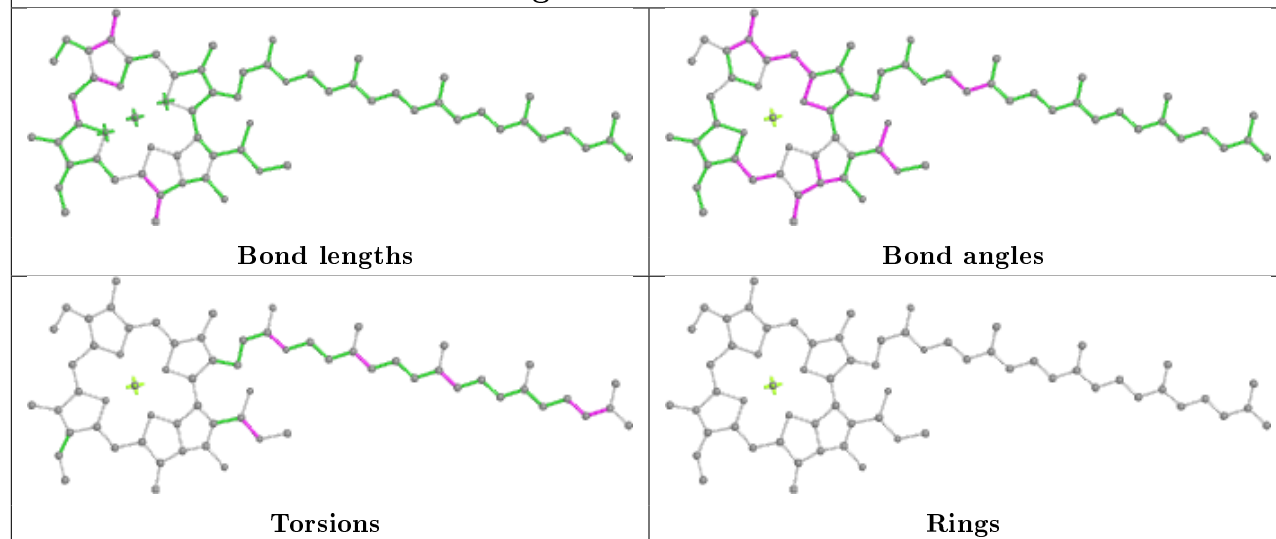
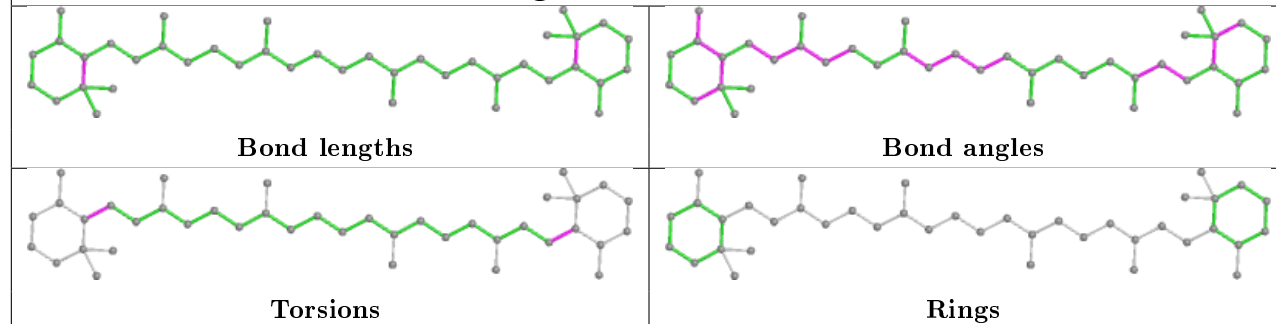
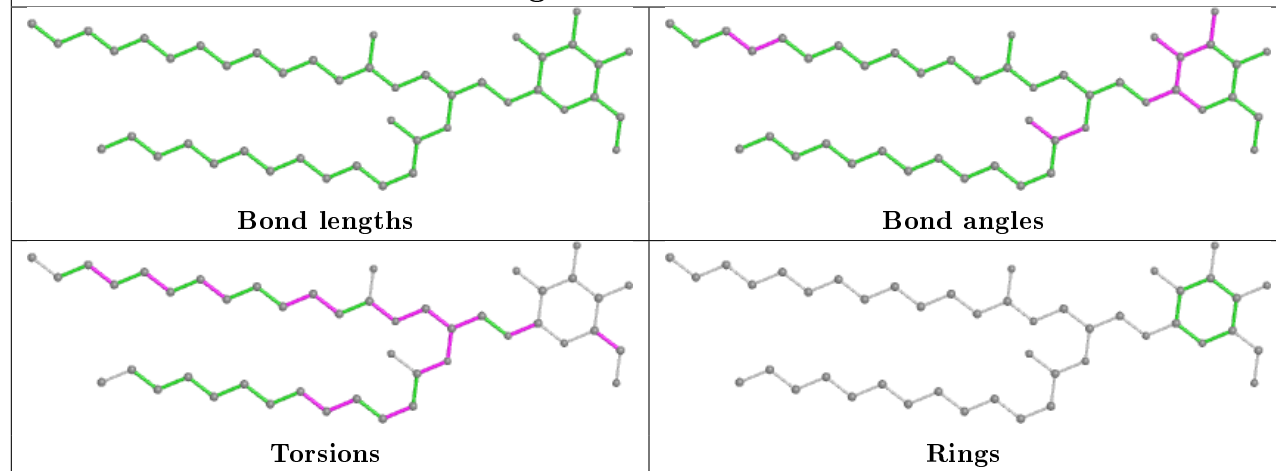
## Ligand LMG B 621

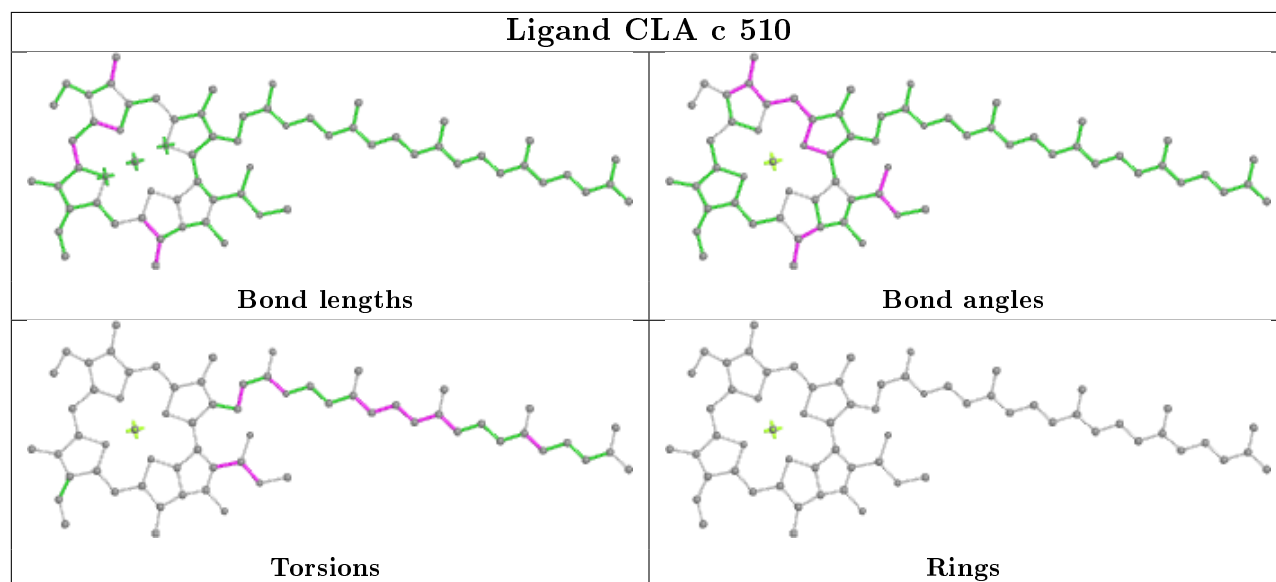
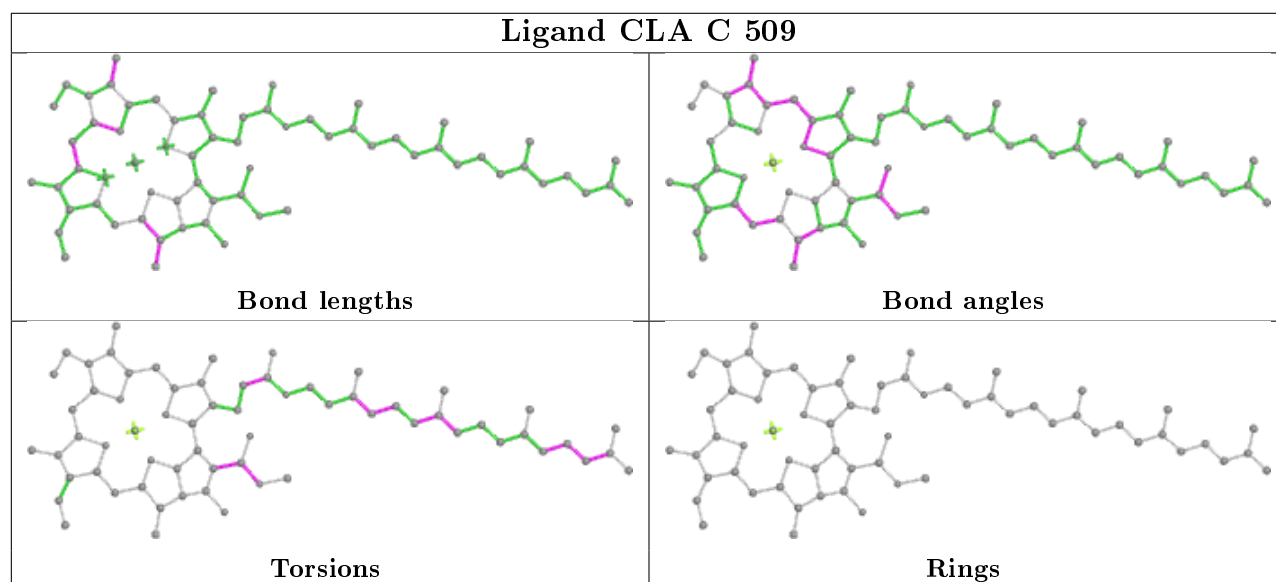
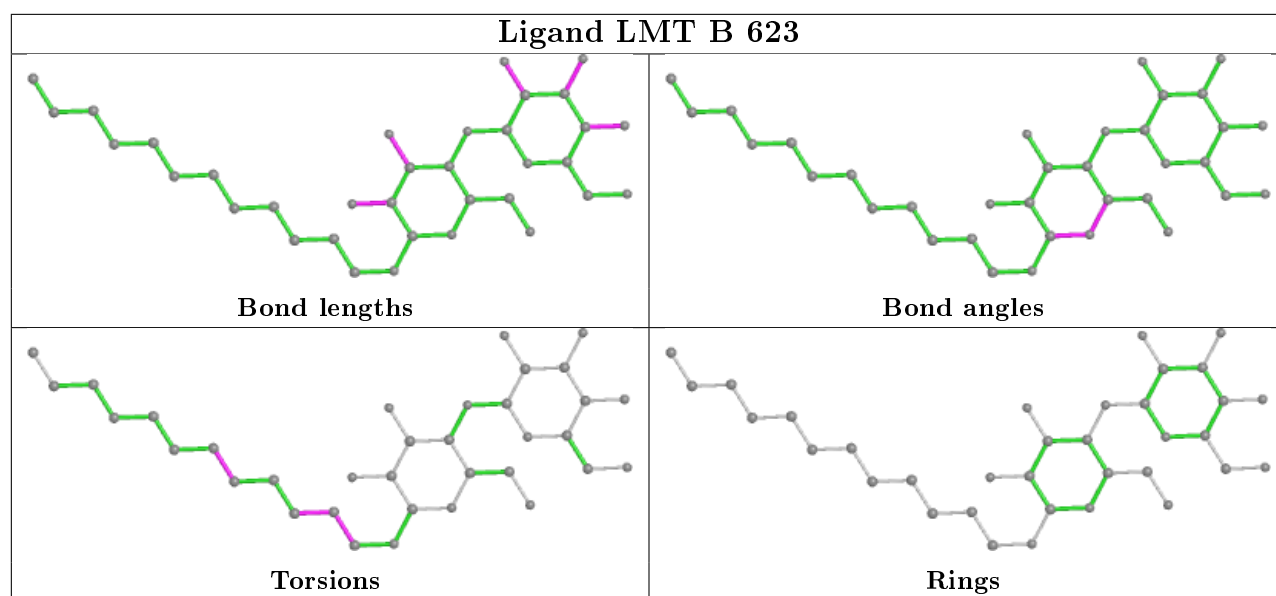


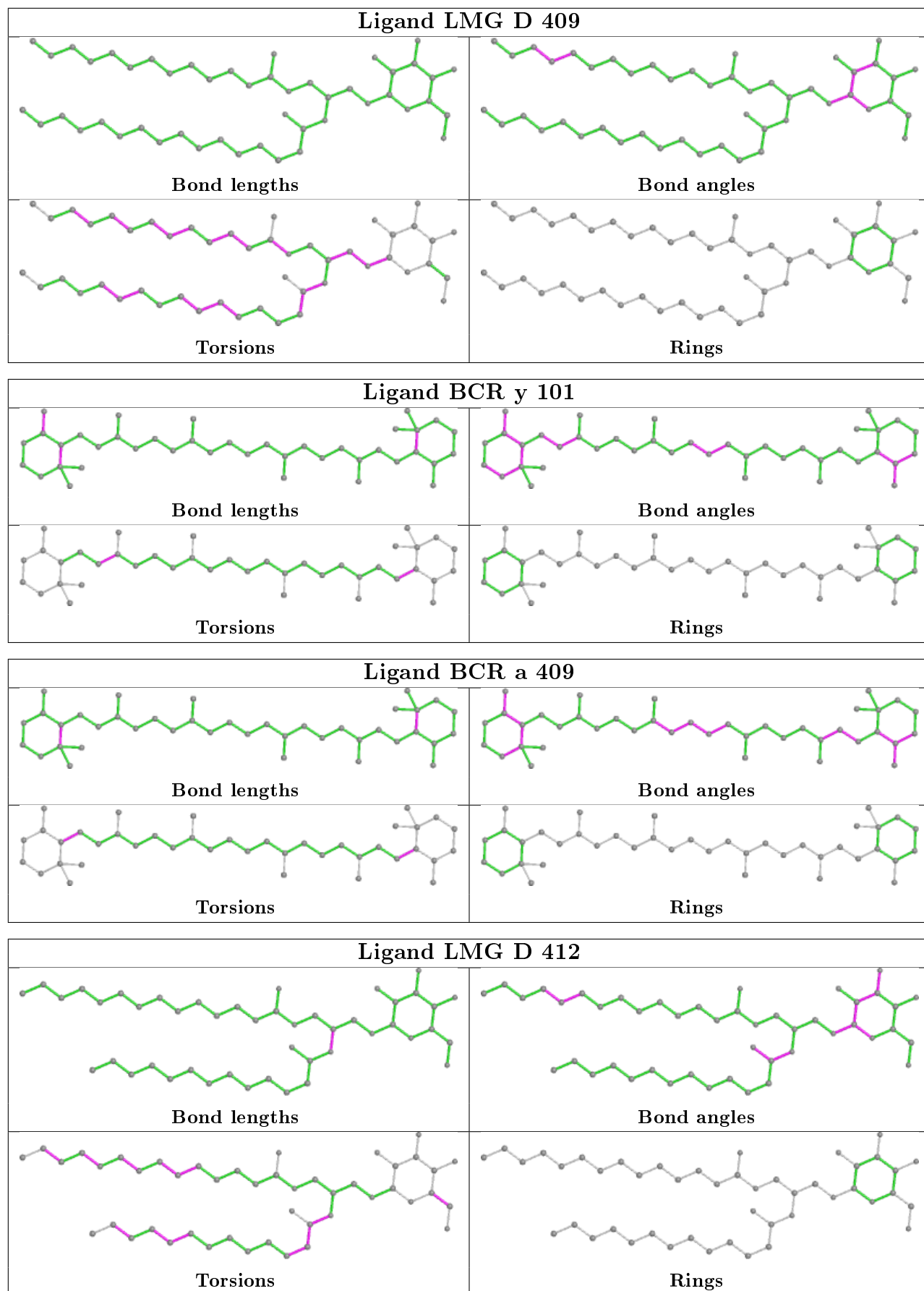
**Ligand CLA b 613****Ligand PHO D 401****Ligand CLA c 504**

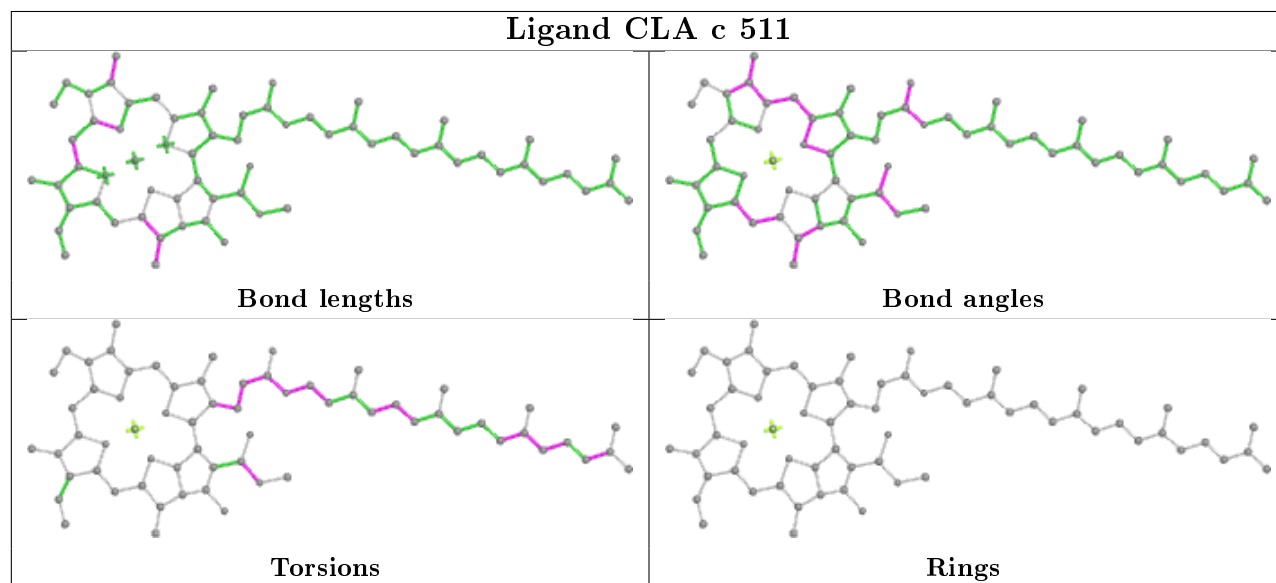
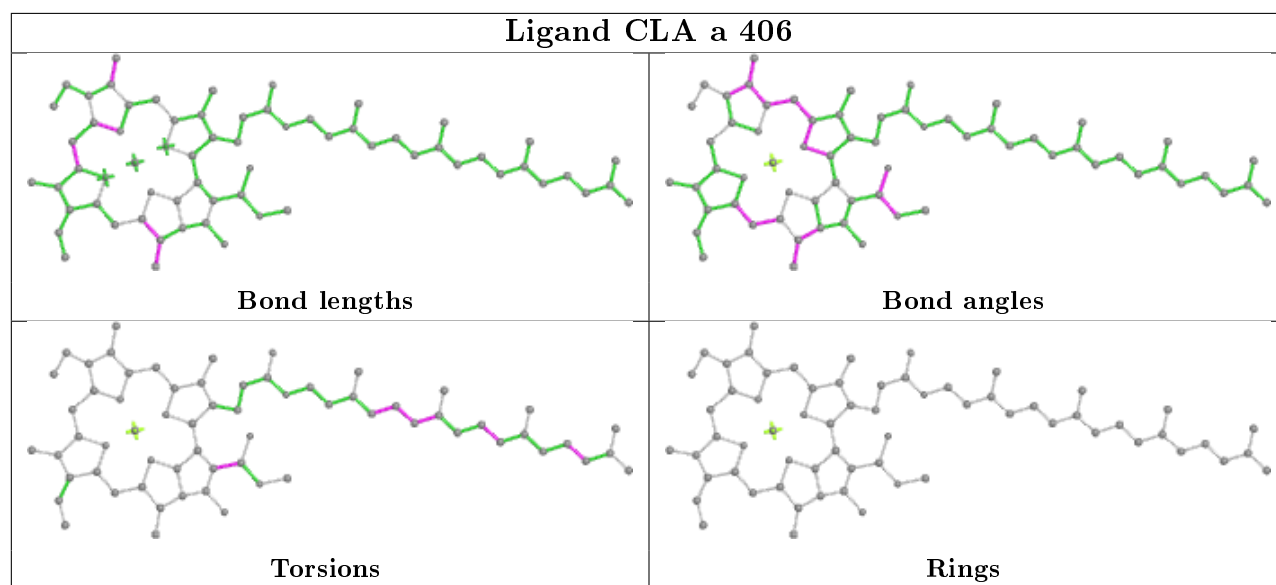
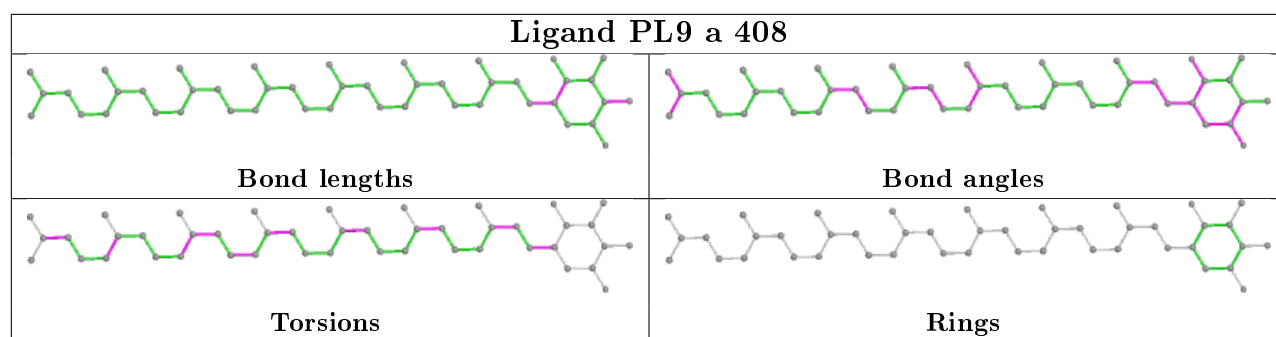




**Ligand CLA B 610****Ligand BCR B 618****Ligand LMG C 518**

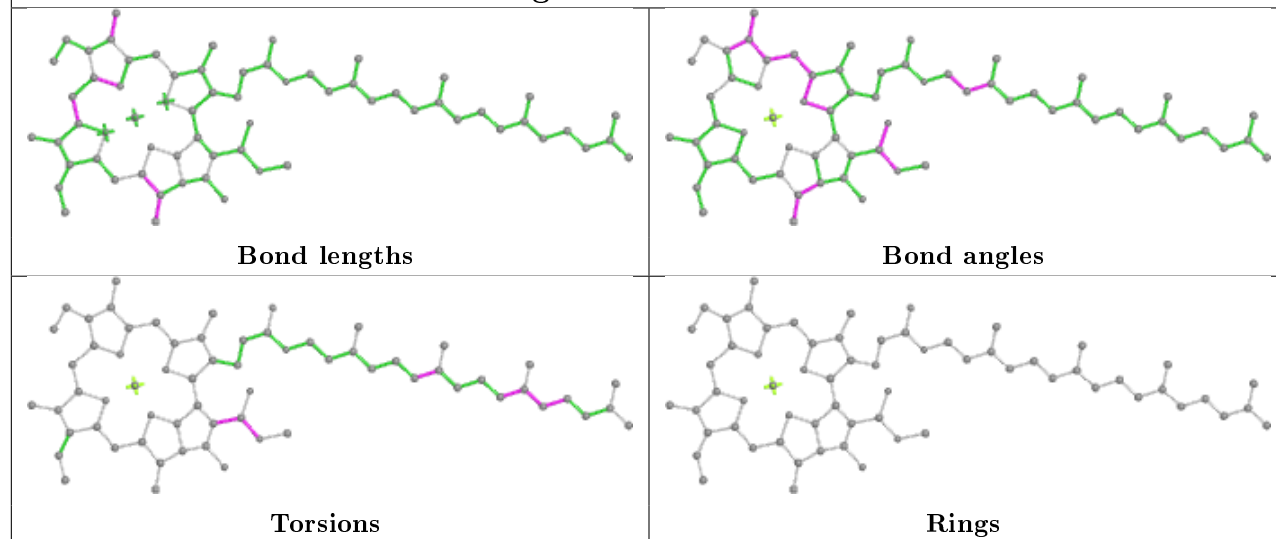




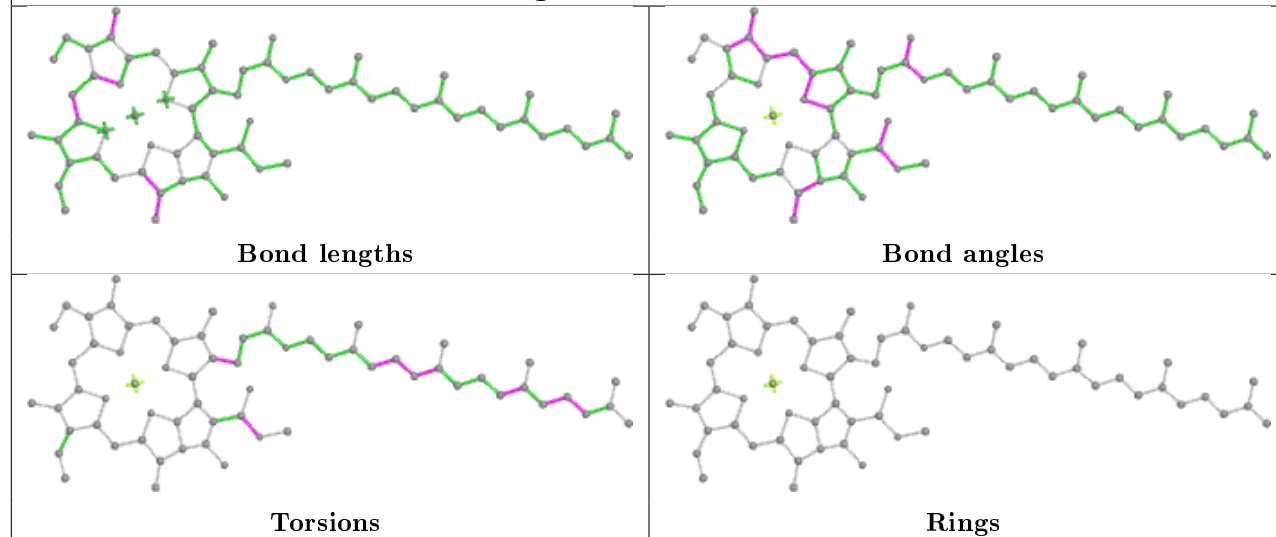




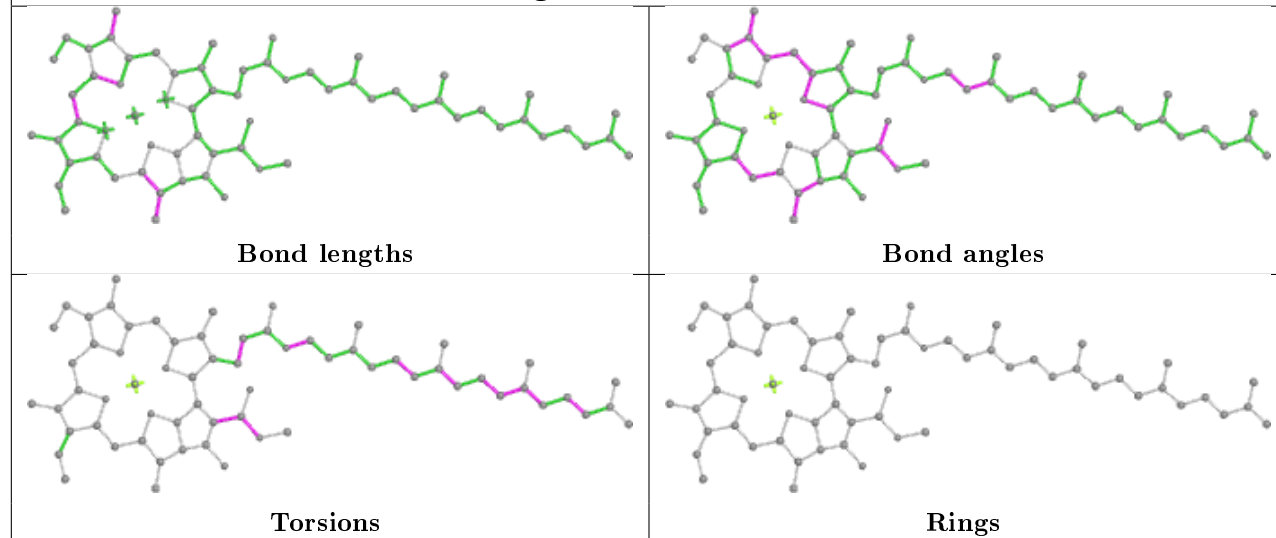
## Ligand CLA B 608

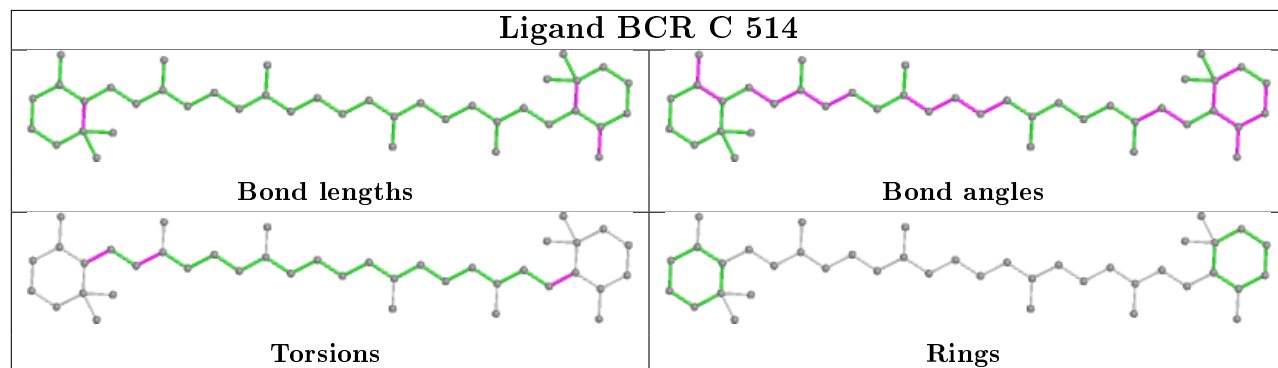
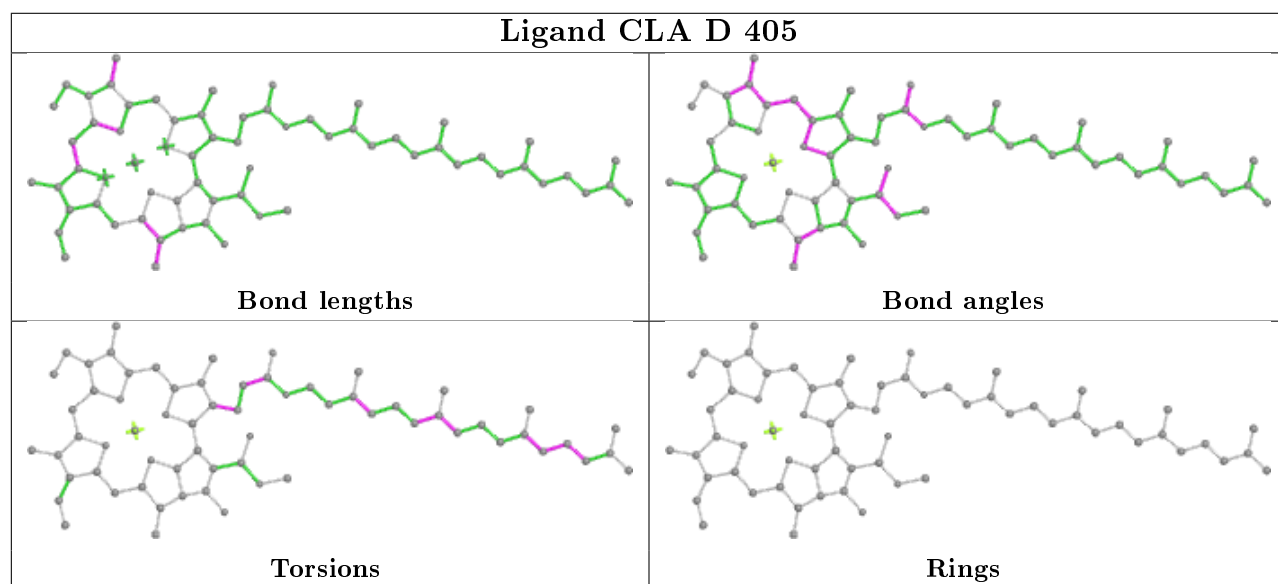
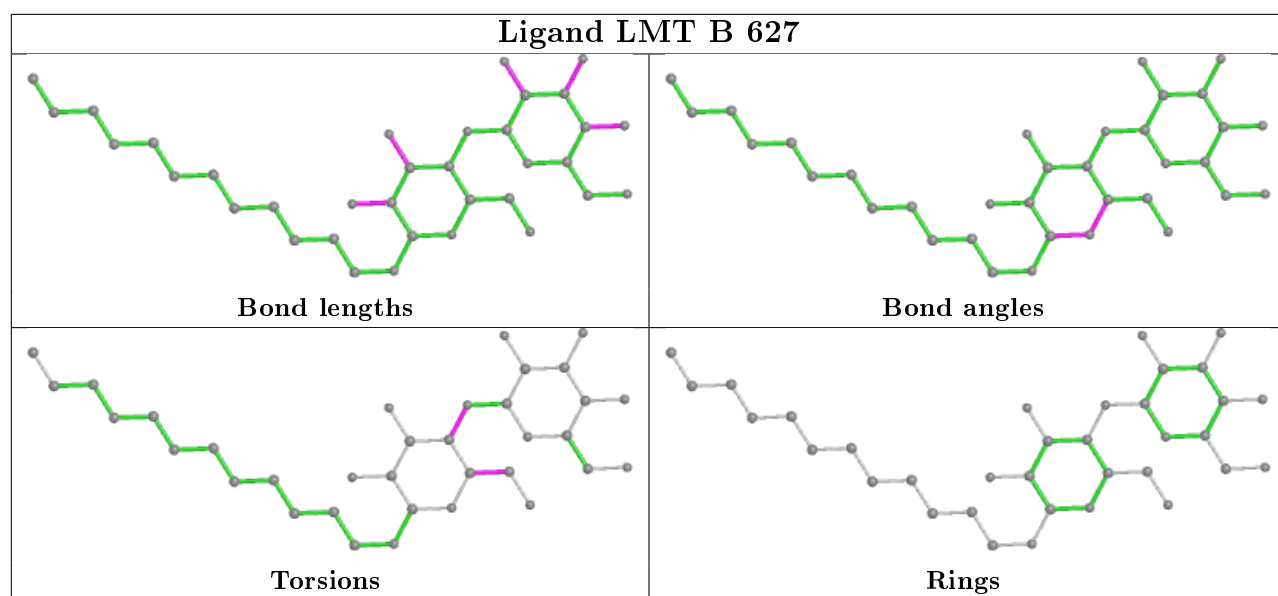


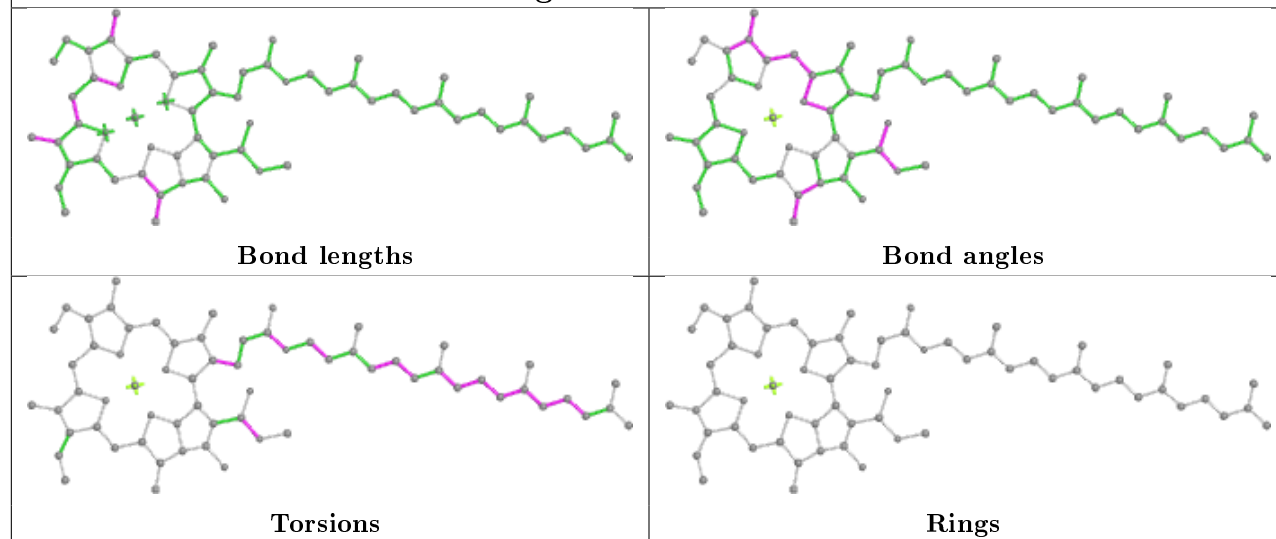
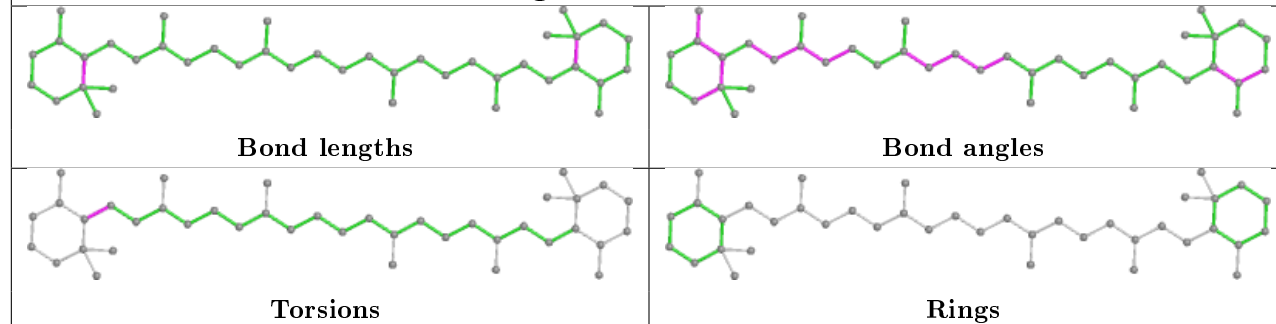
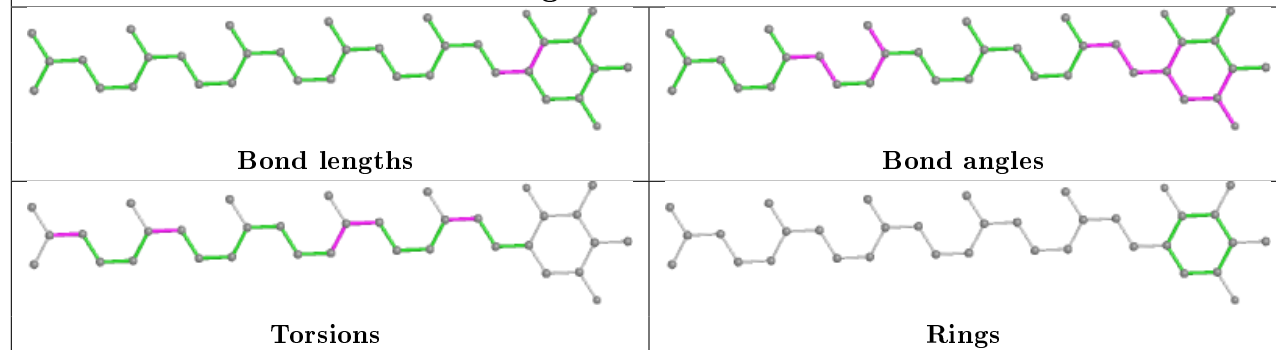
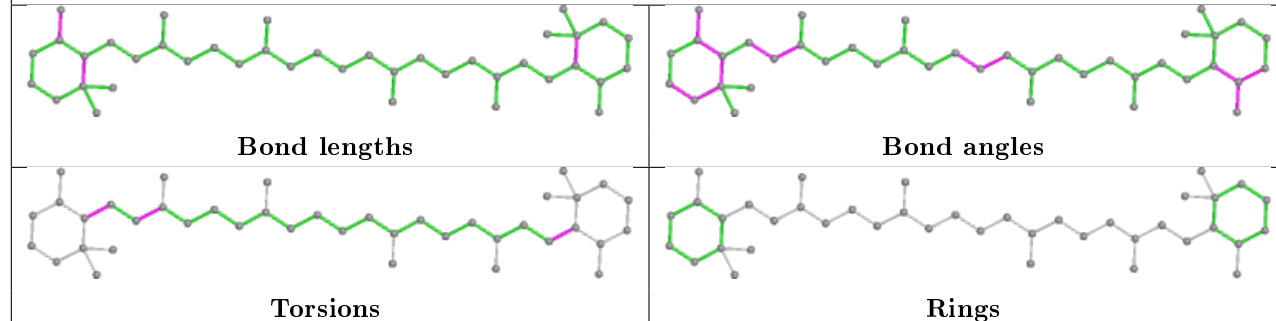
## Ligand CLA B 607



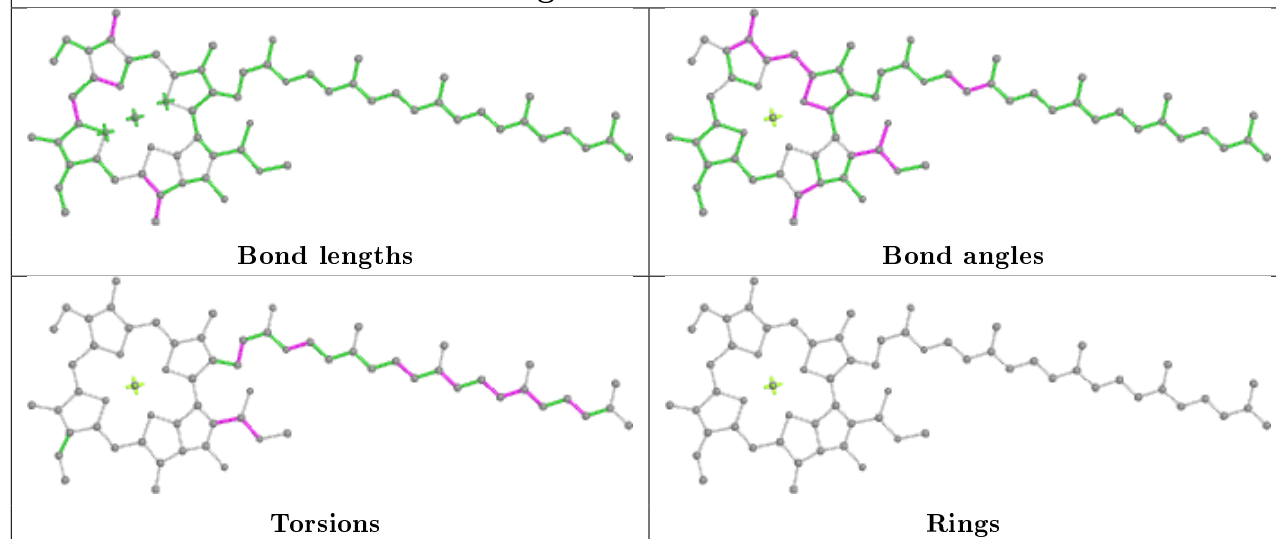
## Ligand CLA C 507



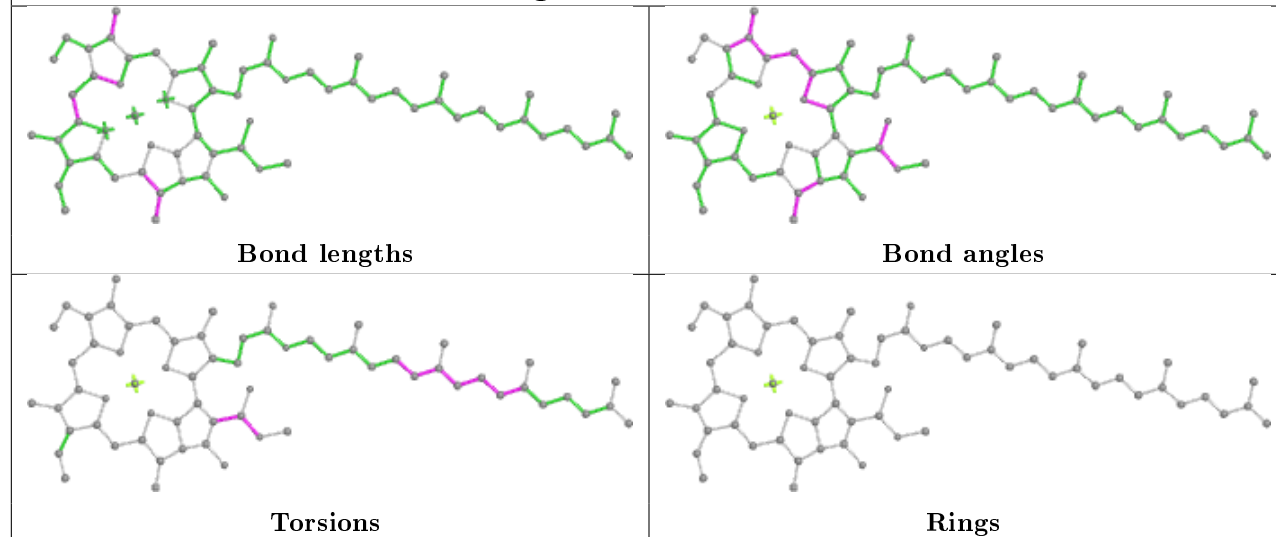


**Ligand CLA b 619****Ligand BCR B 616****Ligand PL9 J 101****Ligand BCR g 101**

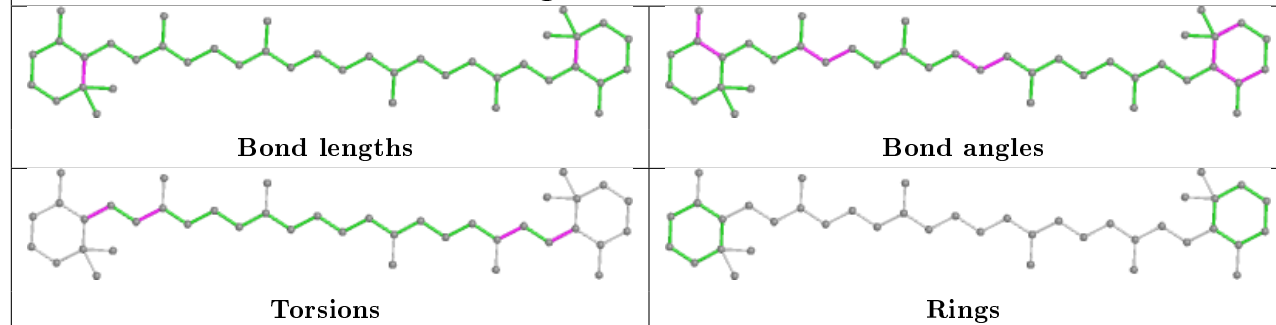
## Ligand CLA c 507



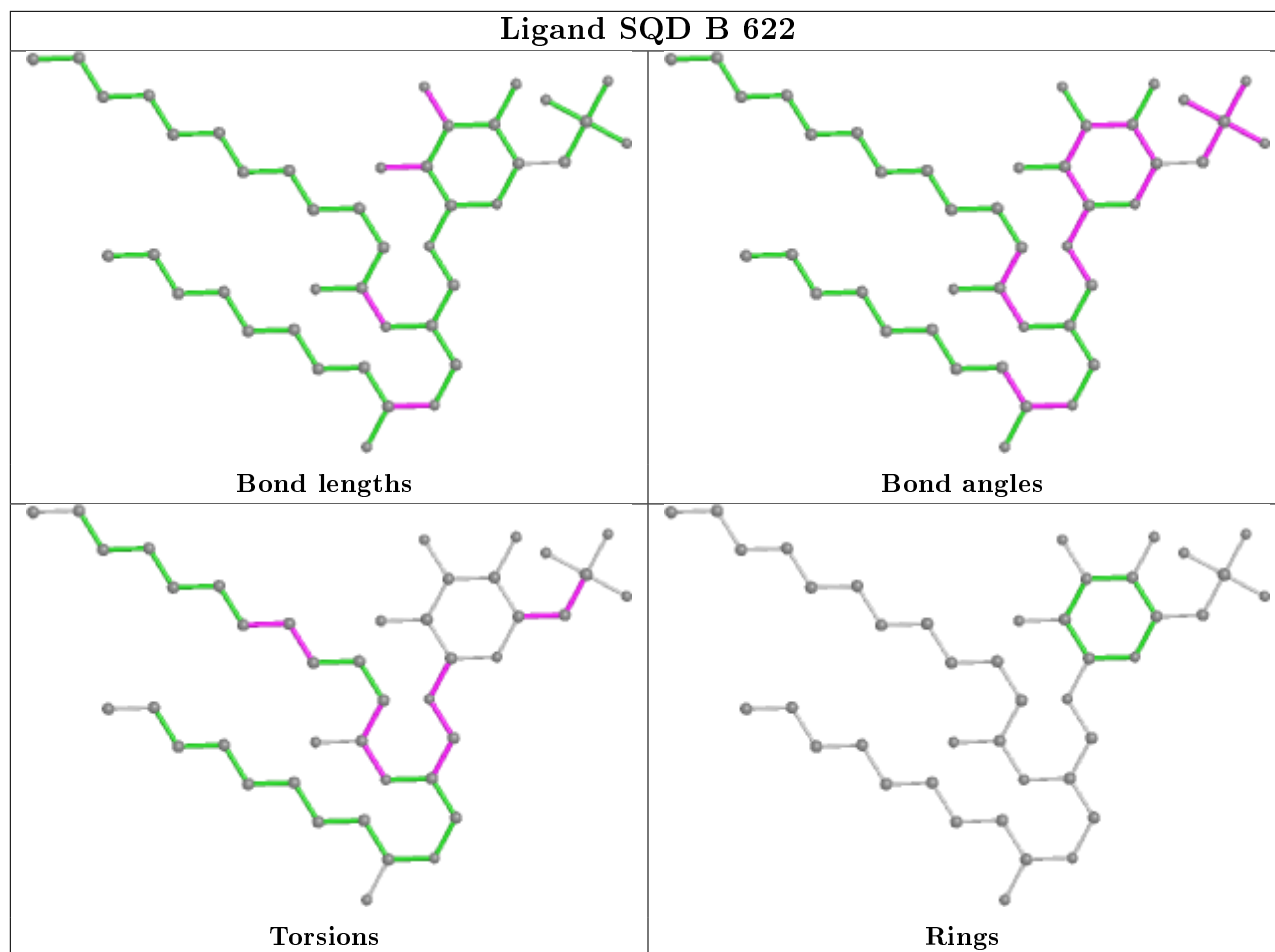
## Ligand CLA C 503



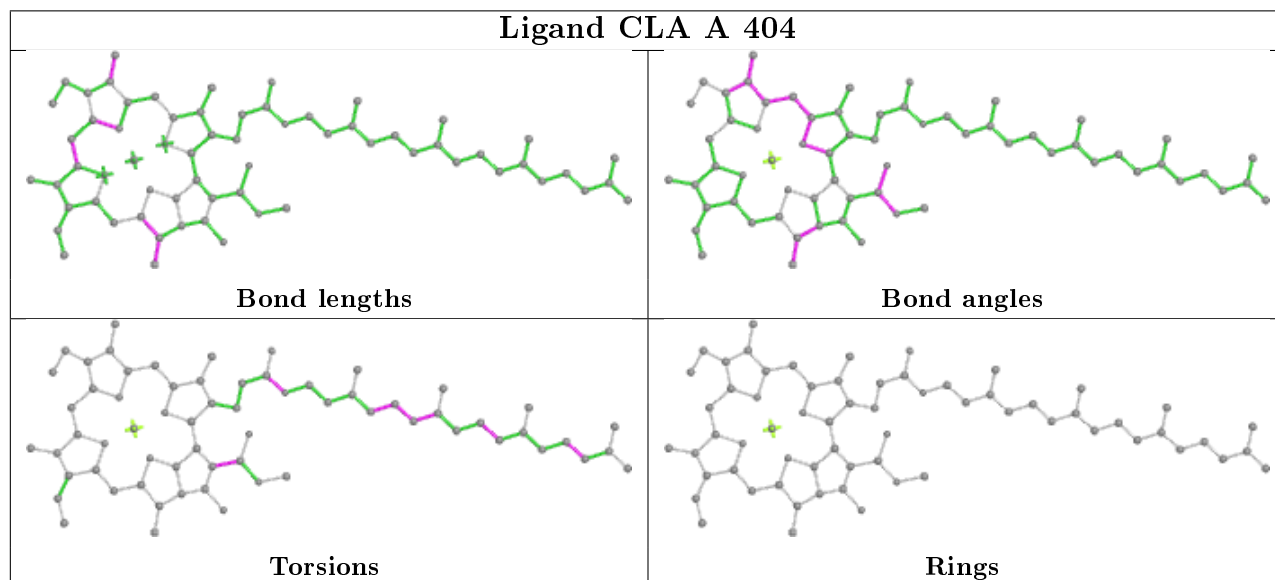
## Ligand BCR f 102

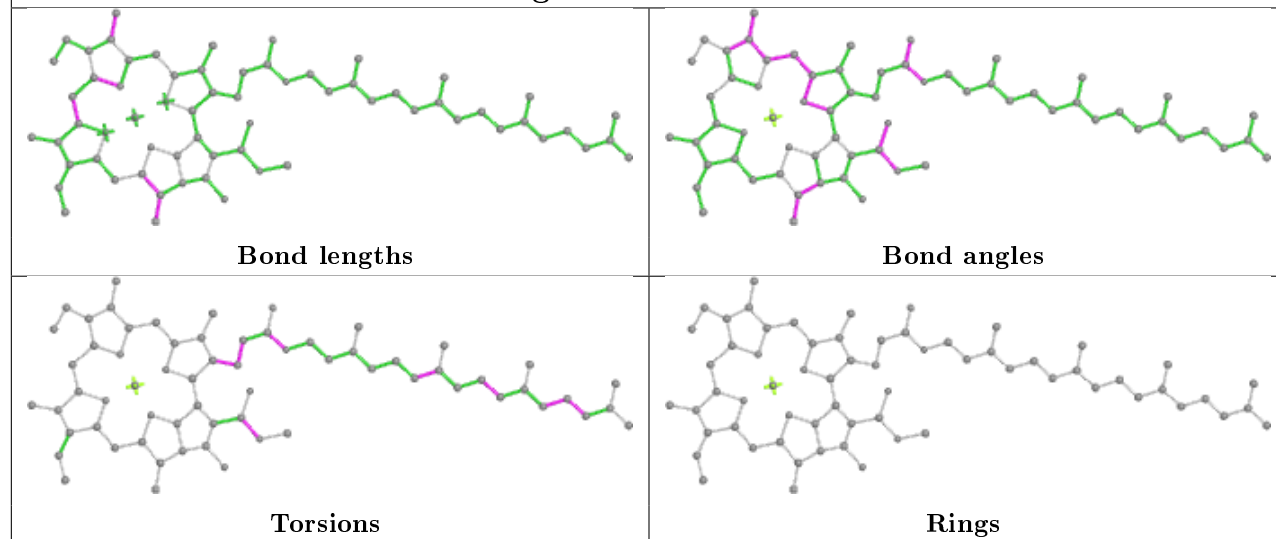
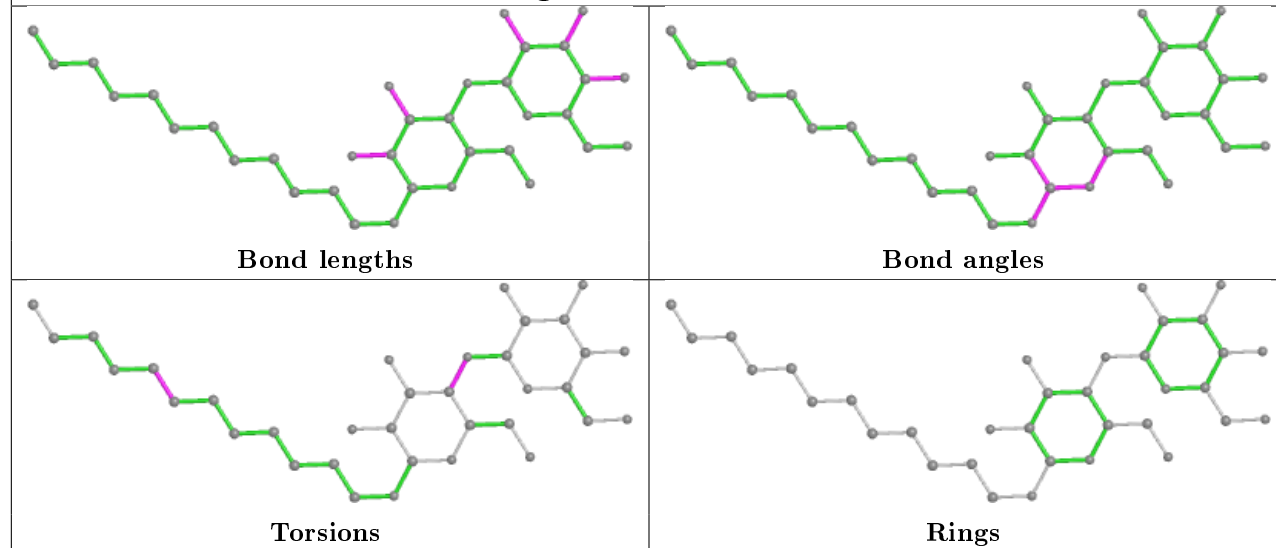


## Ligand SQD B 622

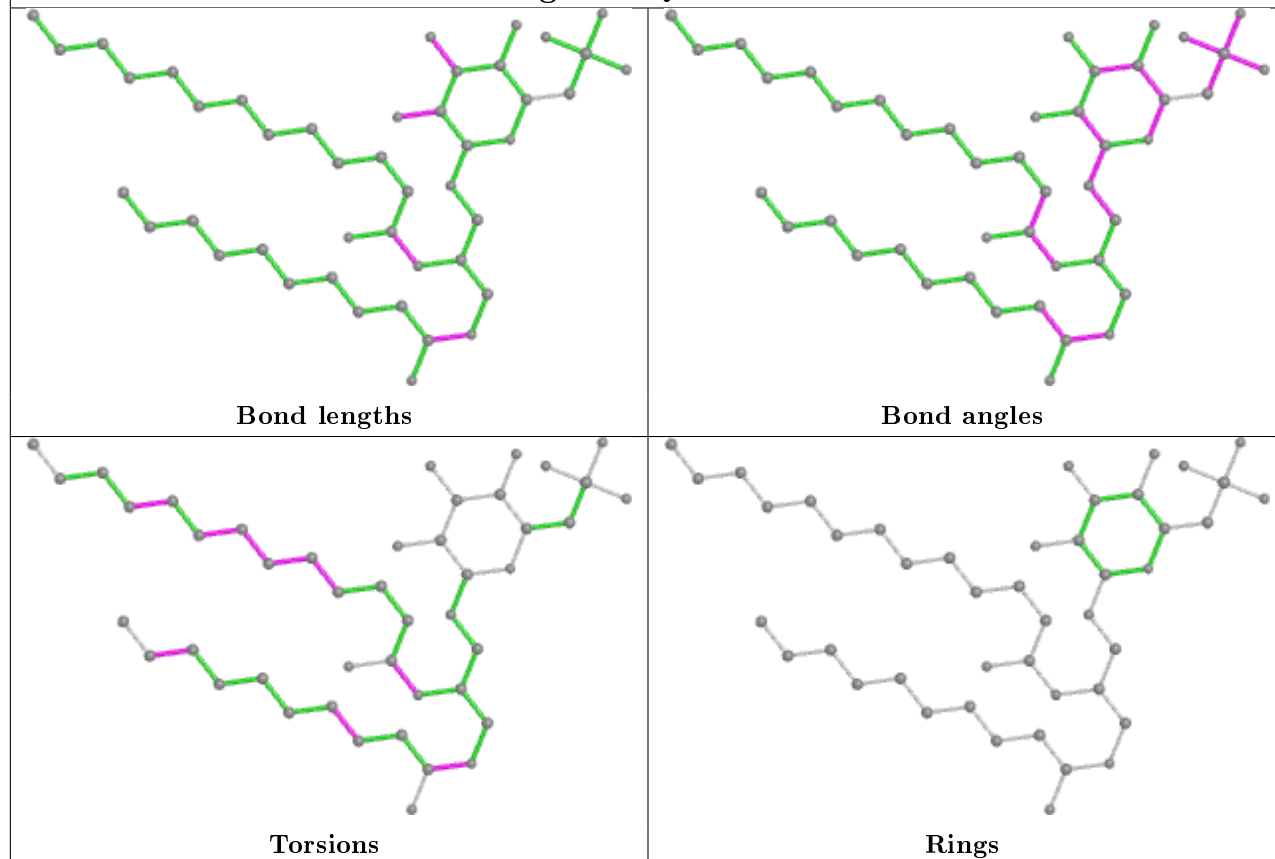


## Ligand CLA A 404

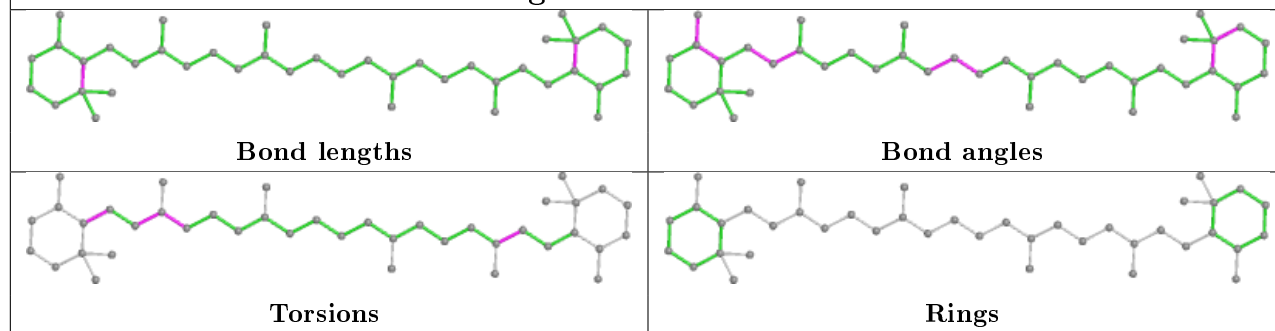


**Ligand CLA C 520****Ligand LMT I 102**

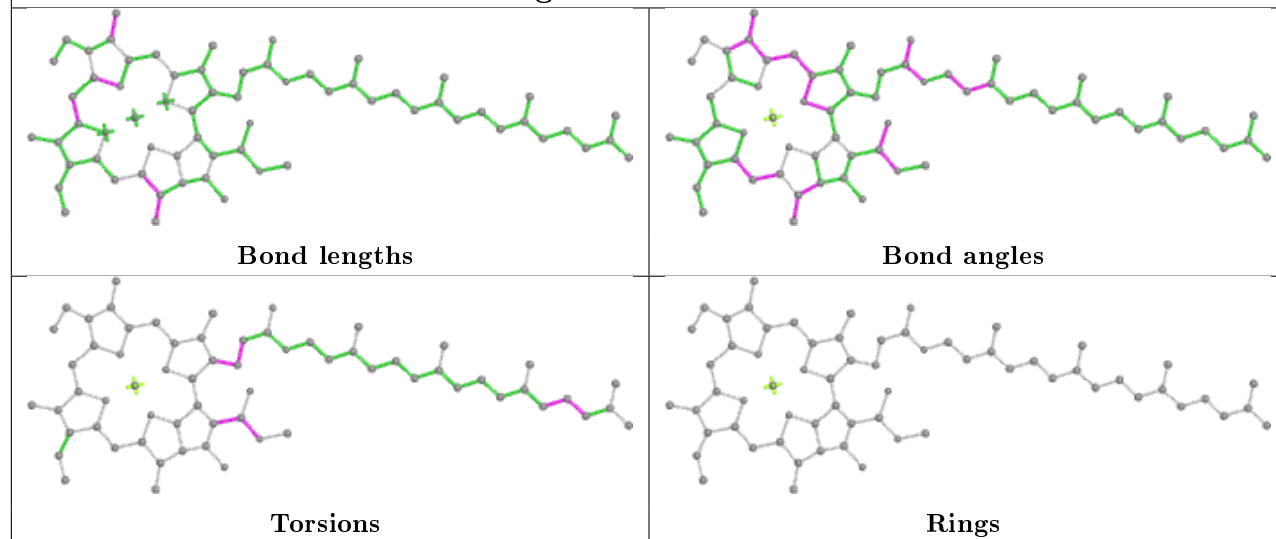
## Ligand SQD f 103



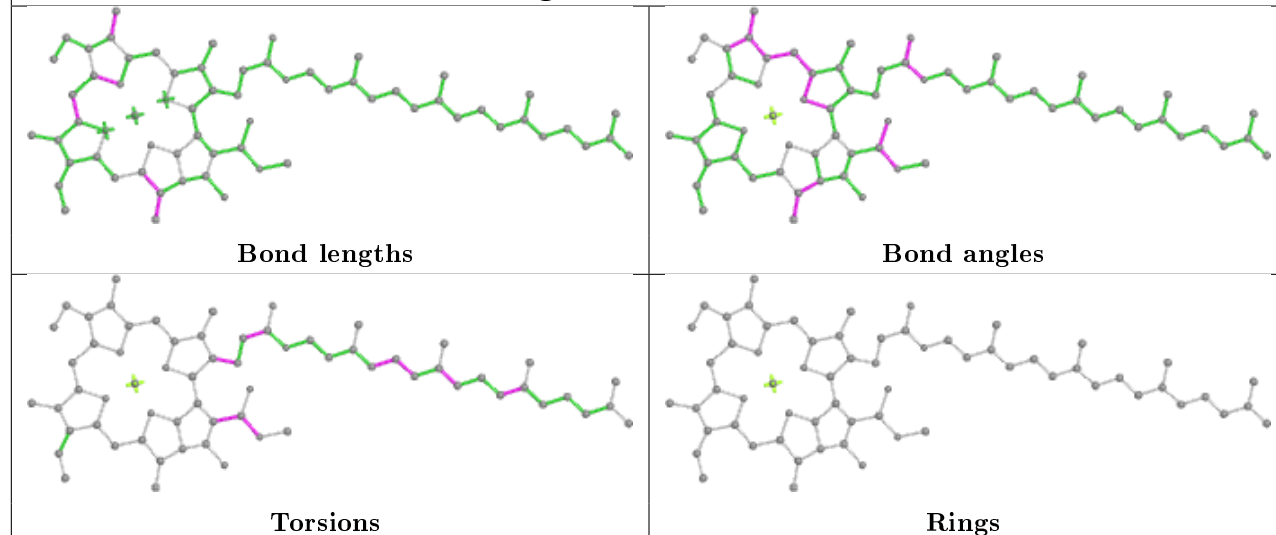
## Ligand BCR H 102



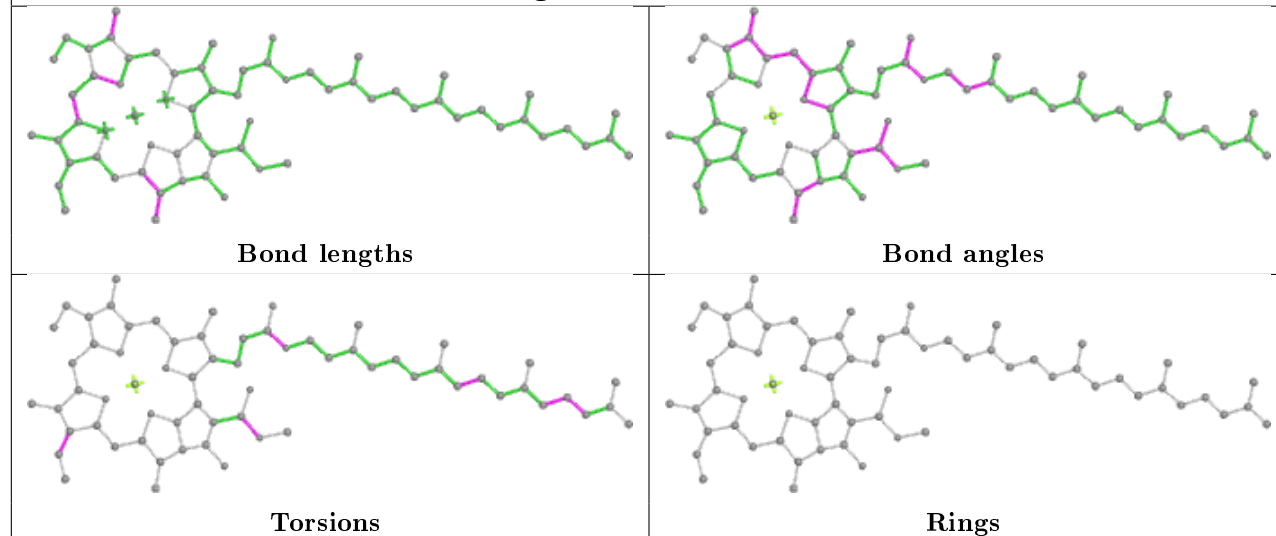
## Ligand CLA b 610



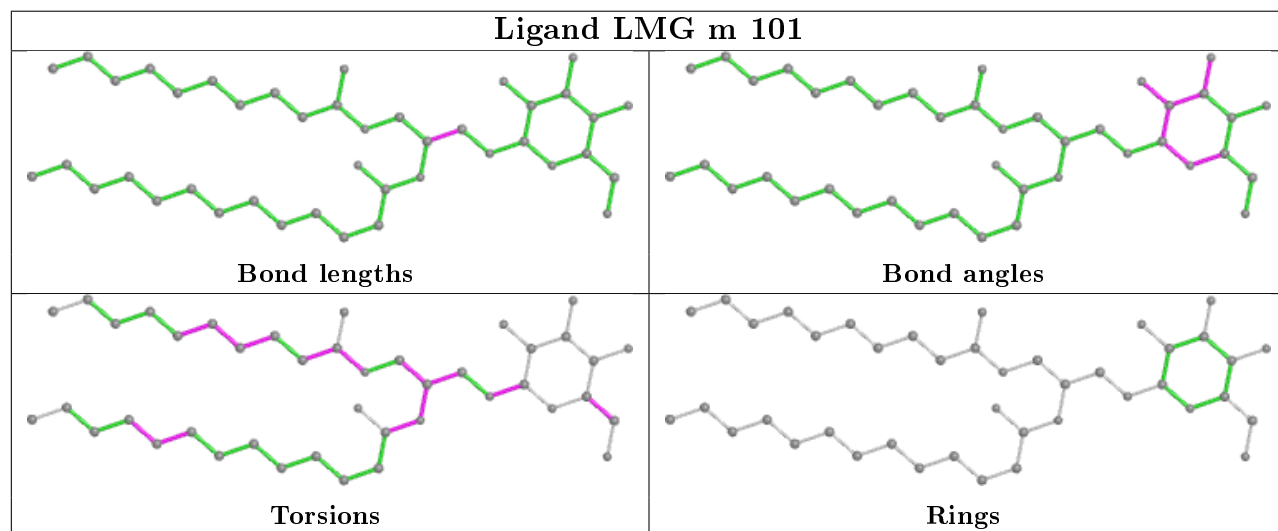
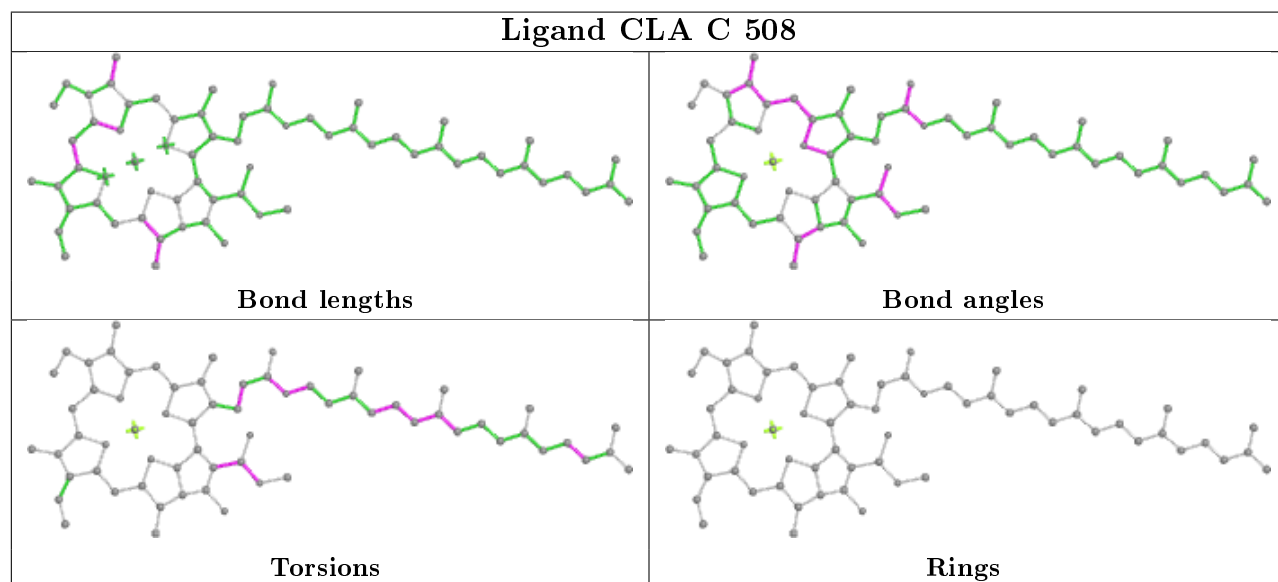
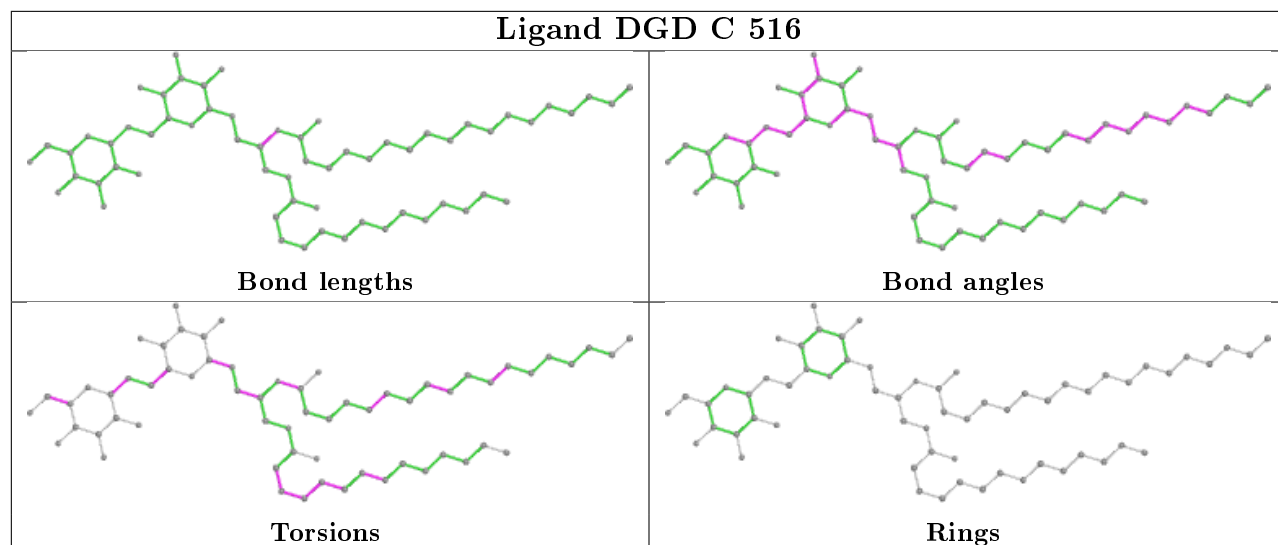
## Ligand CLA c 506



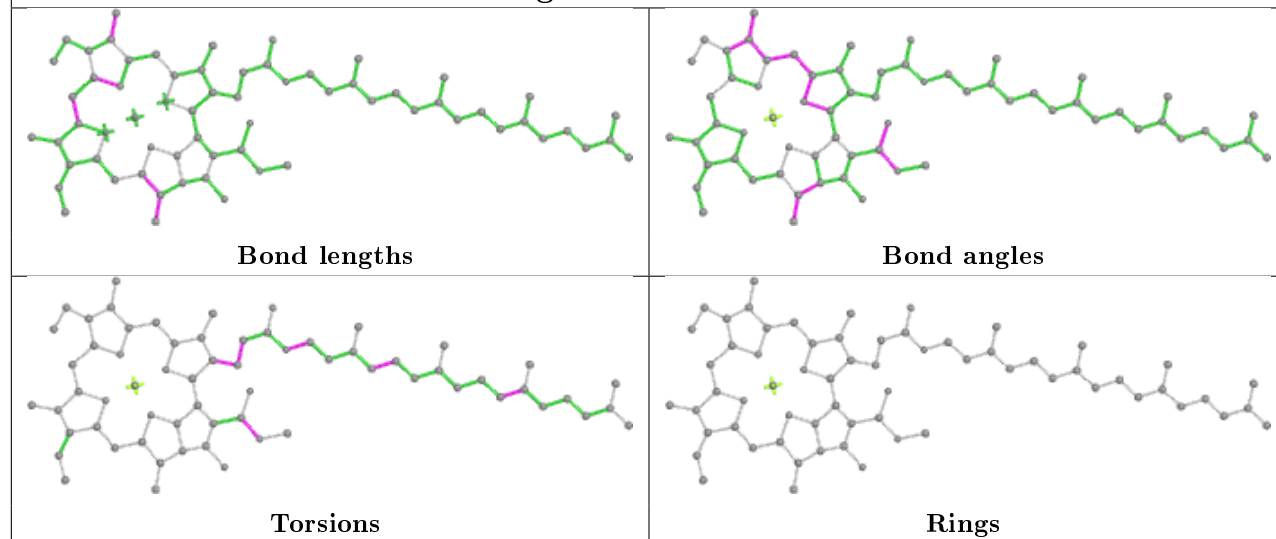
## Ligand CLA B 603



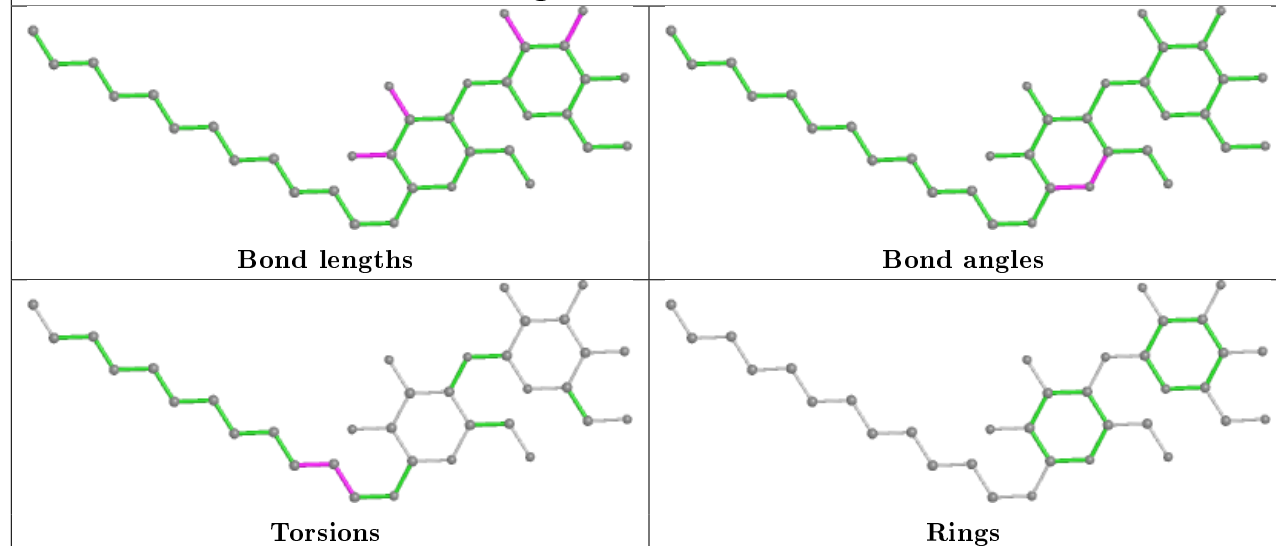




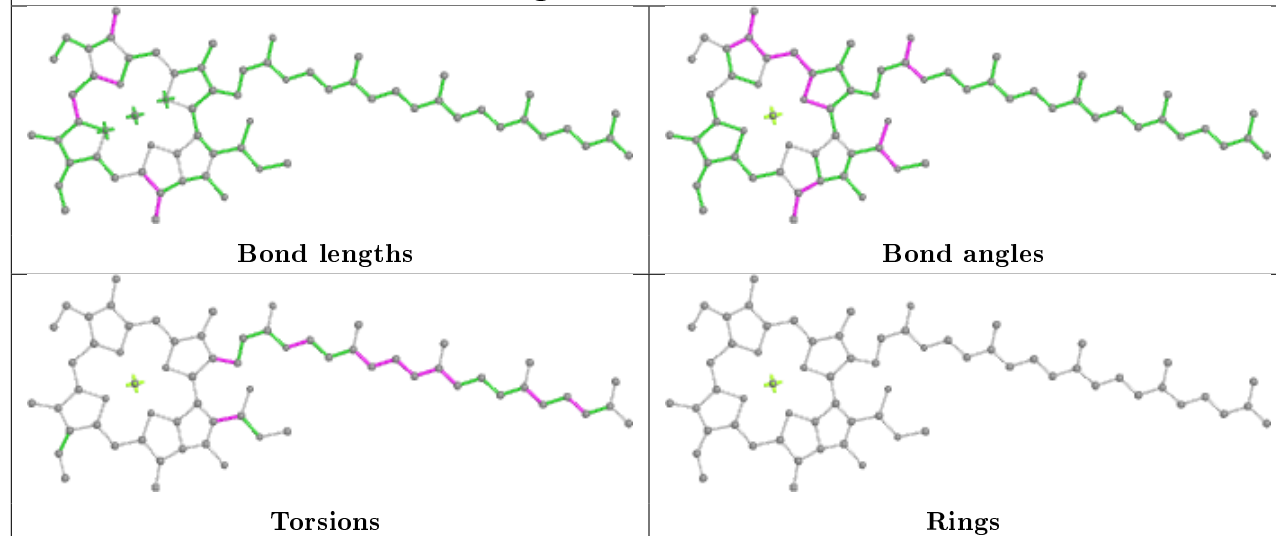
## Ligand CLA a 404



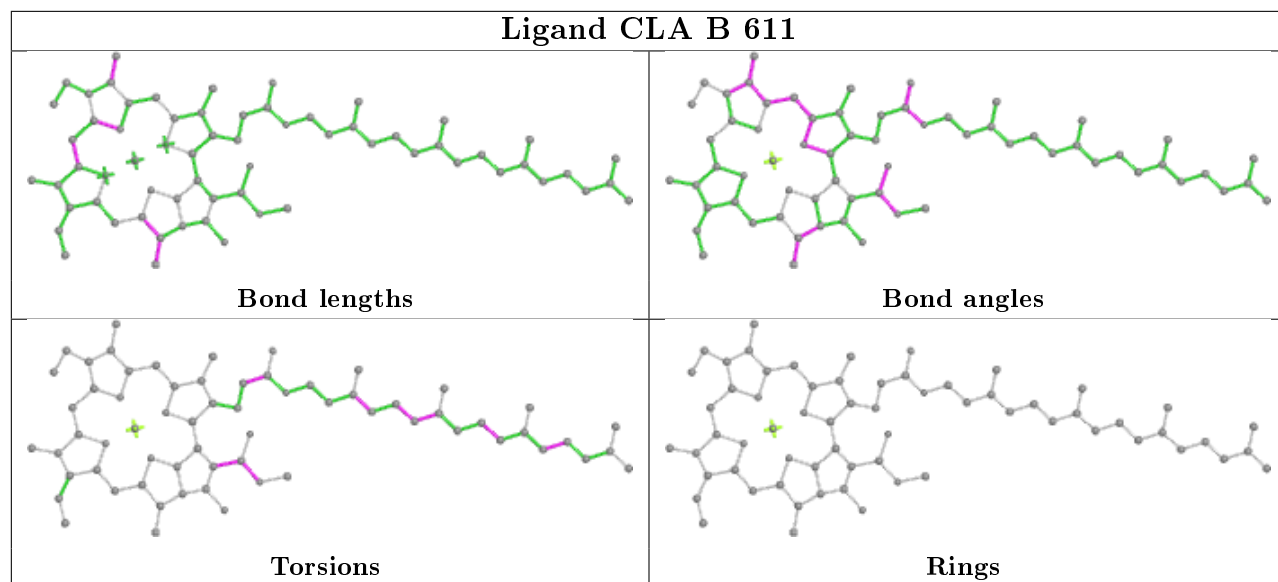
## Ligand LMT b 626



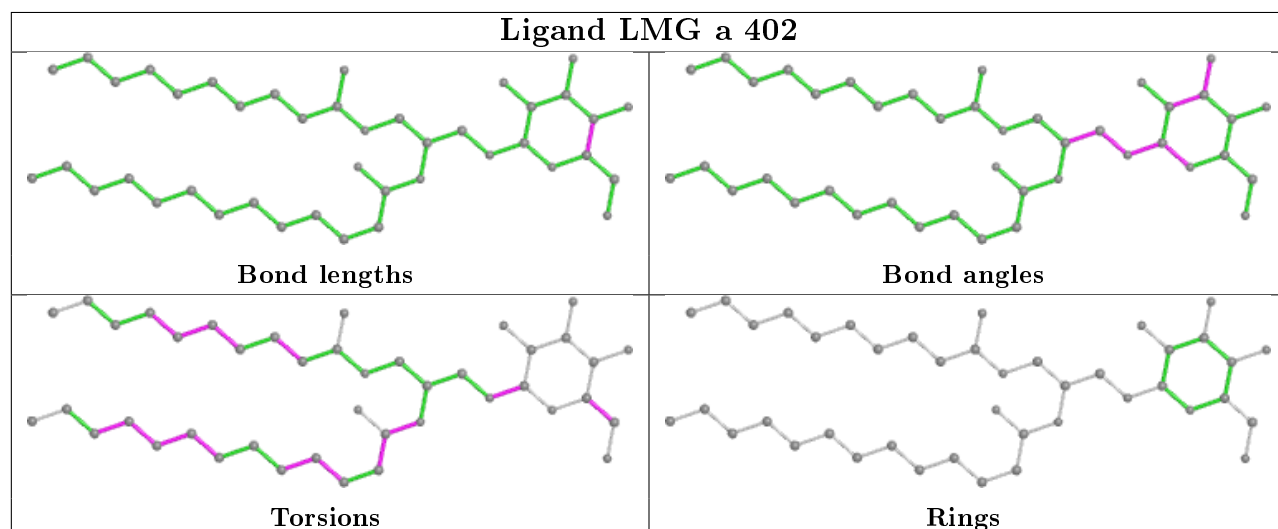
## Ligand CLA A 403



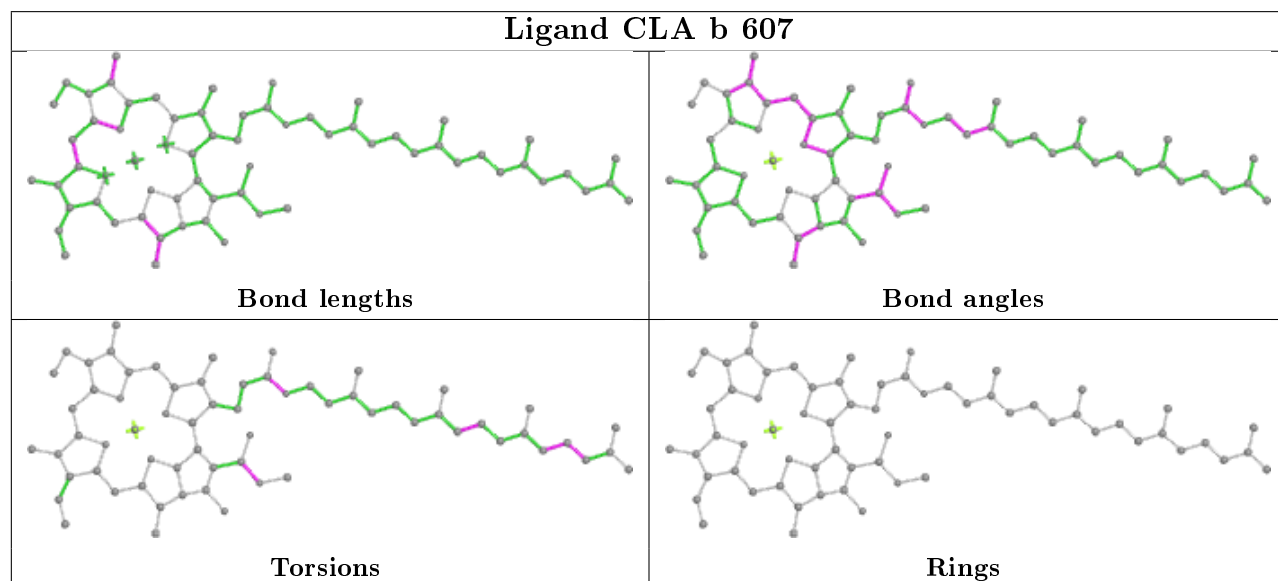
## Ligand CLA B 611

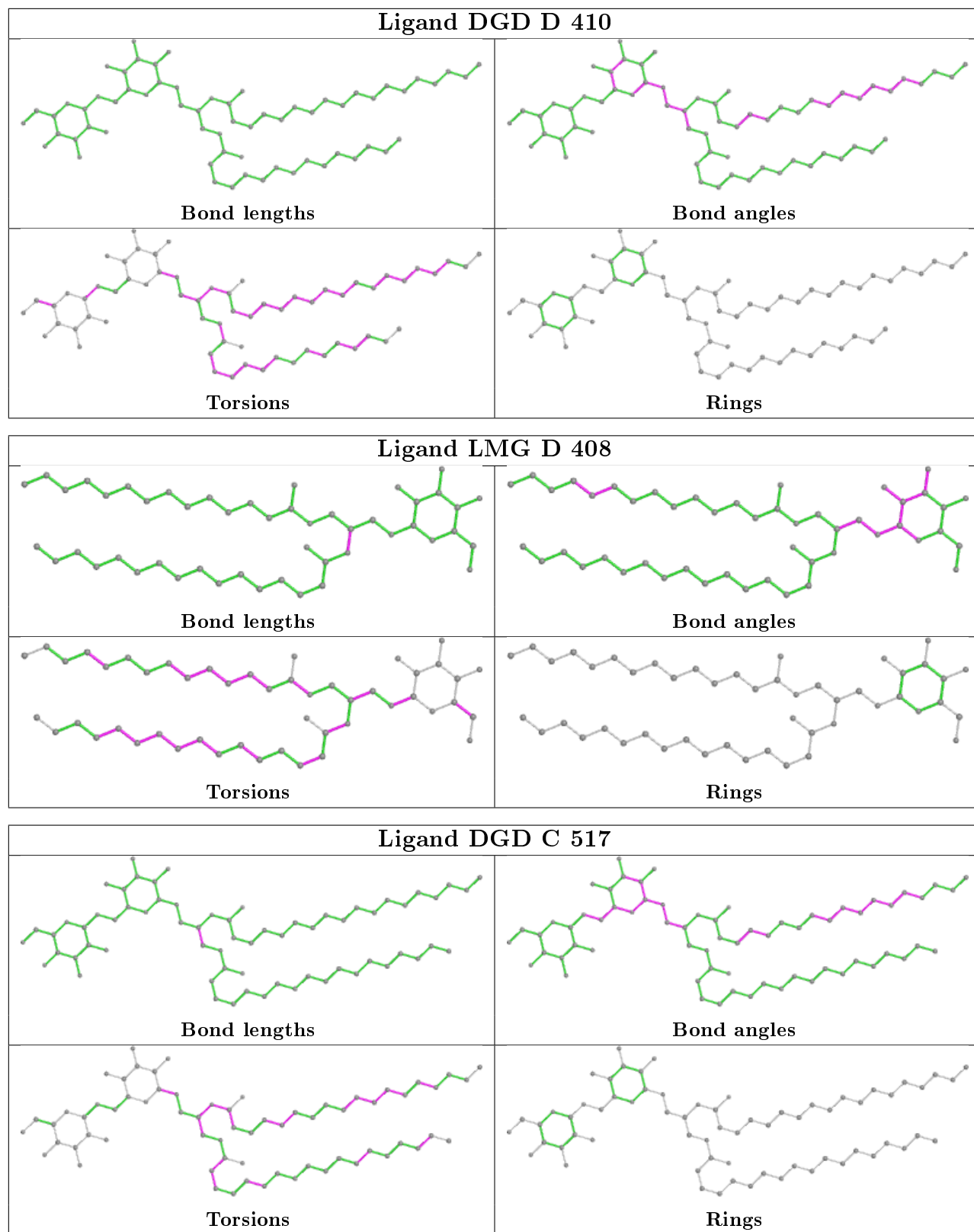


## Ligand LMG a 402

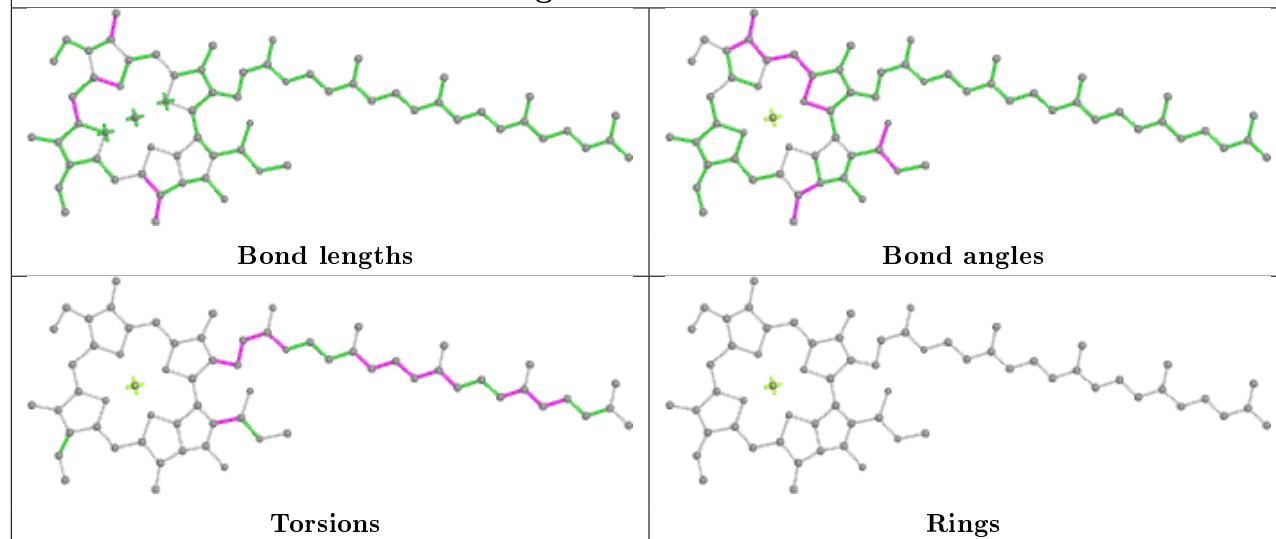


## Ligand CLA b 607

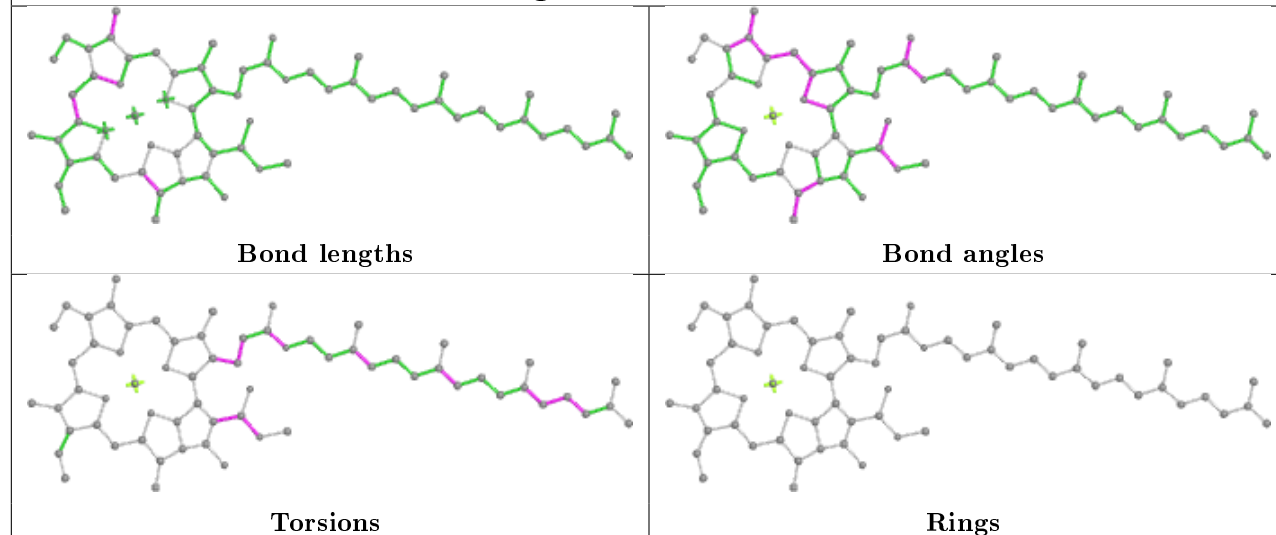




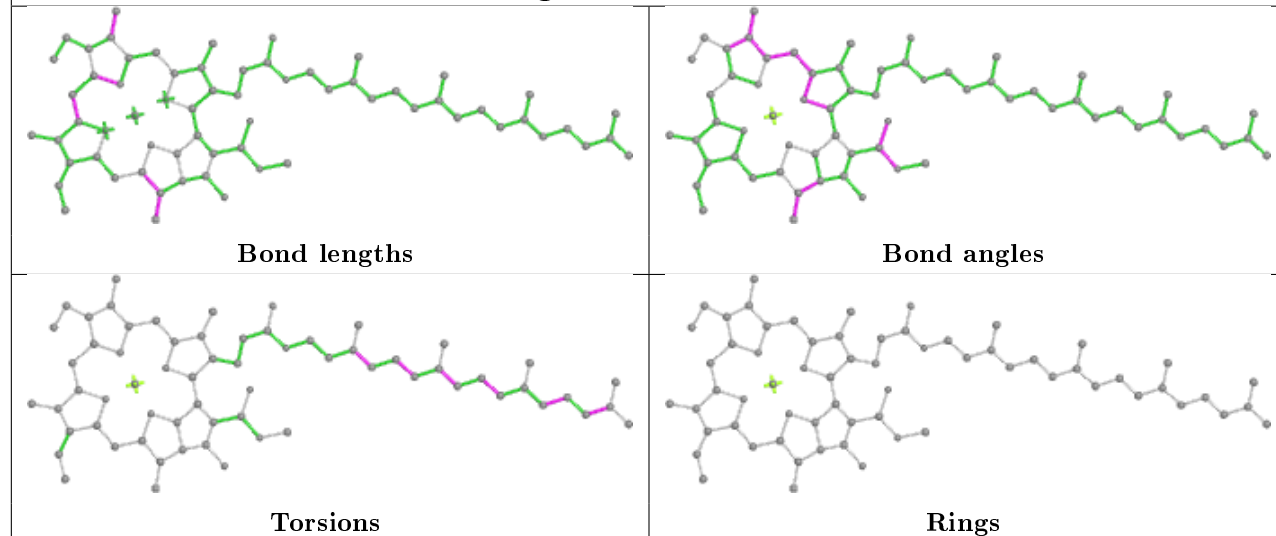
## Ligand CLA h 101

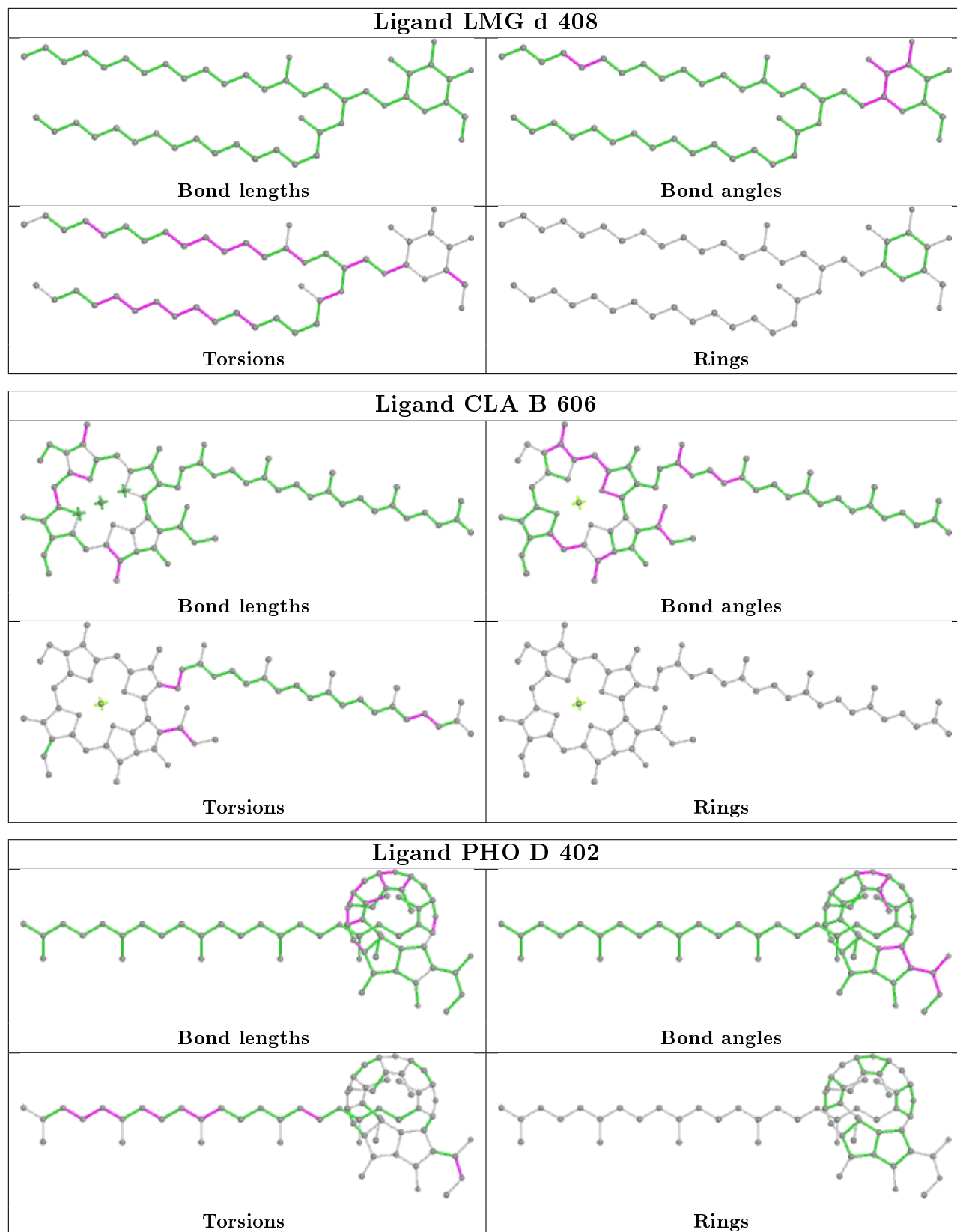


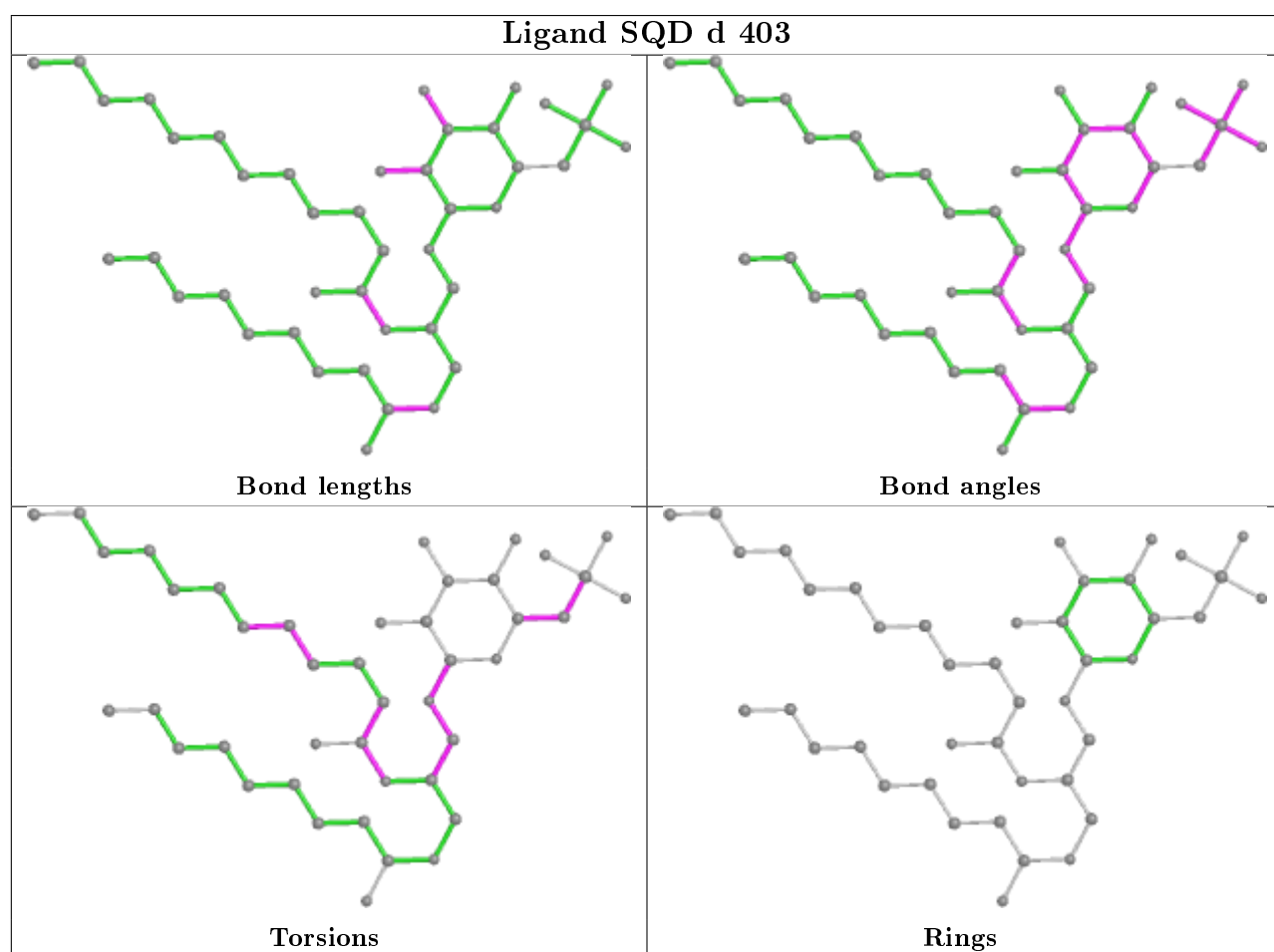
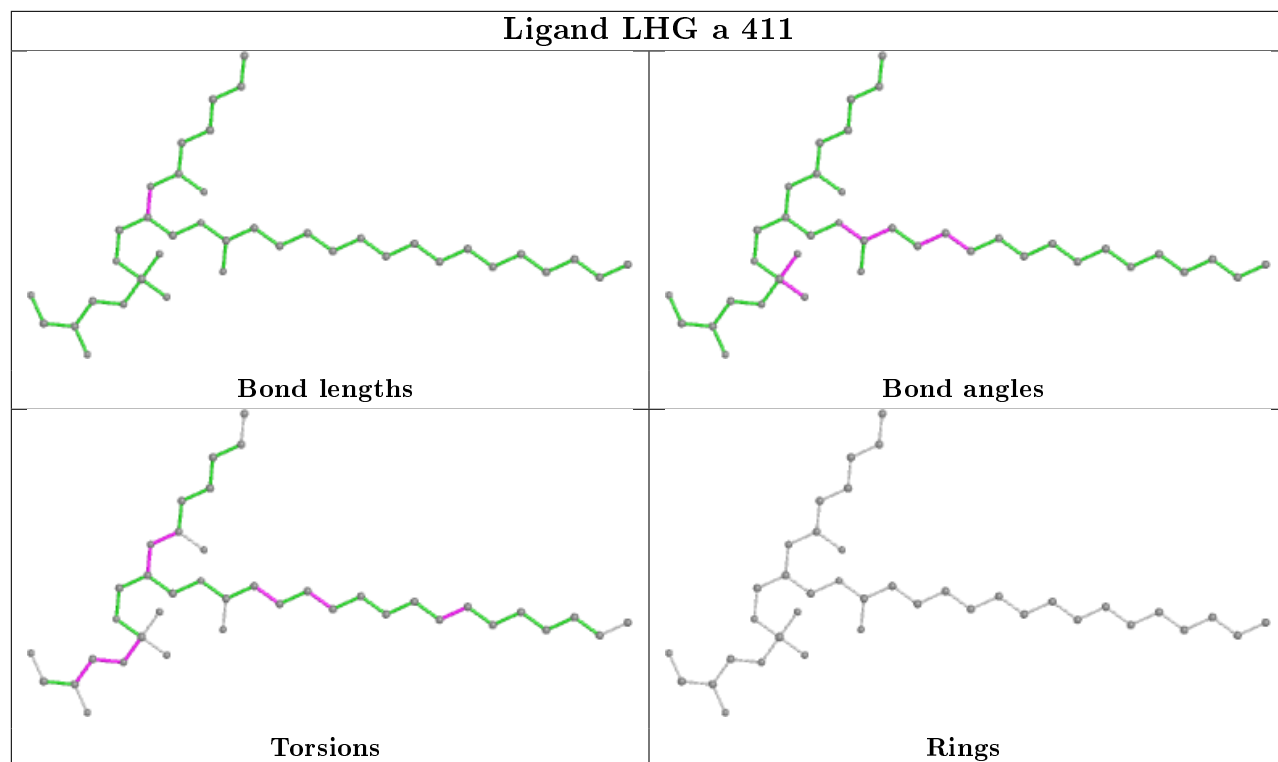
## Ligand CLA C 512



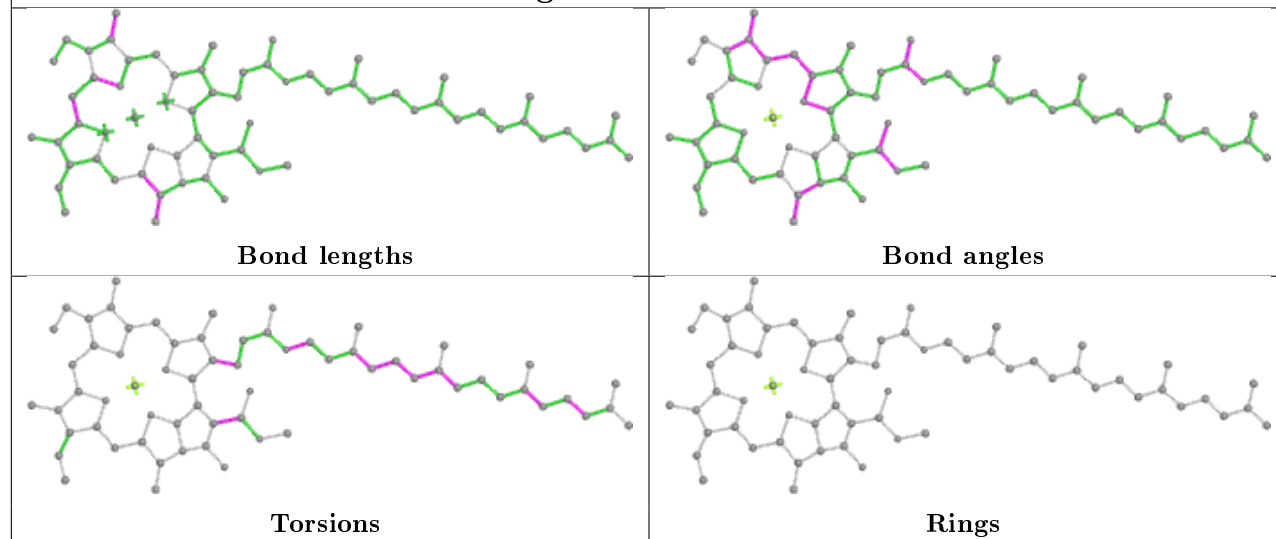
## Ligand CLA a 407



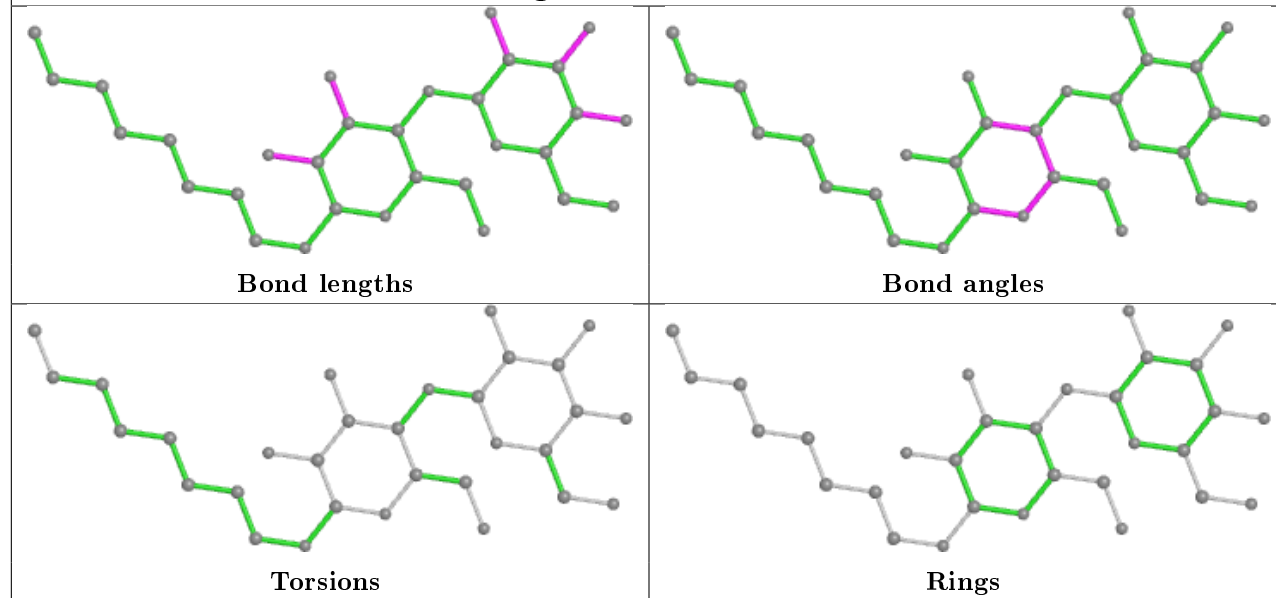




## Ligand CLA a 405

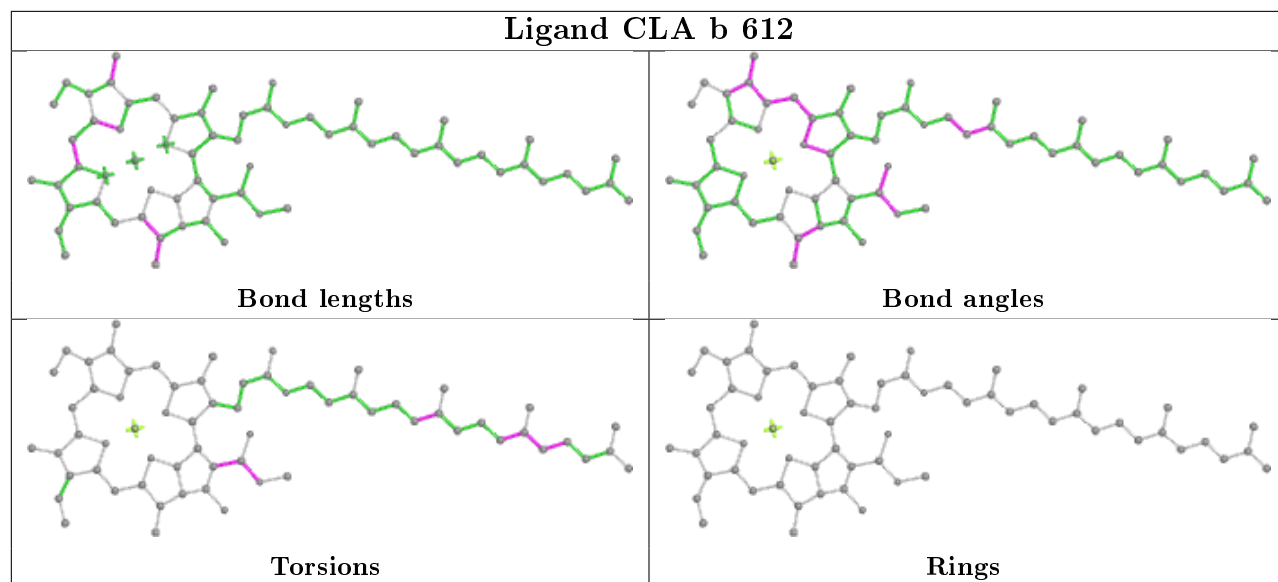


## Ligand LMT d 411

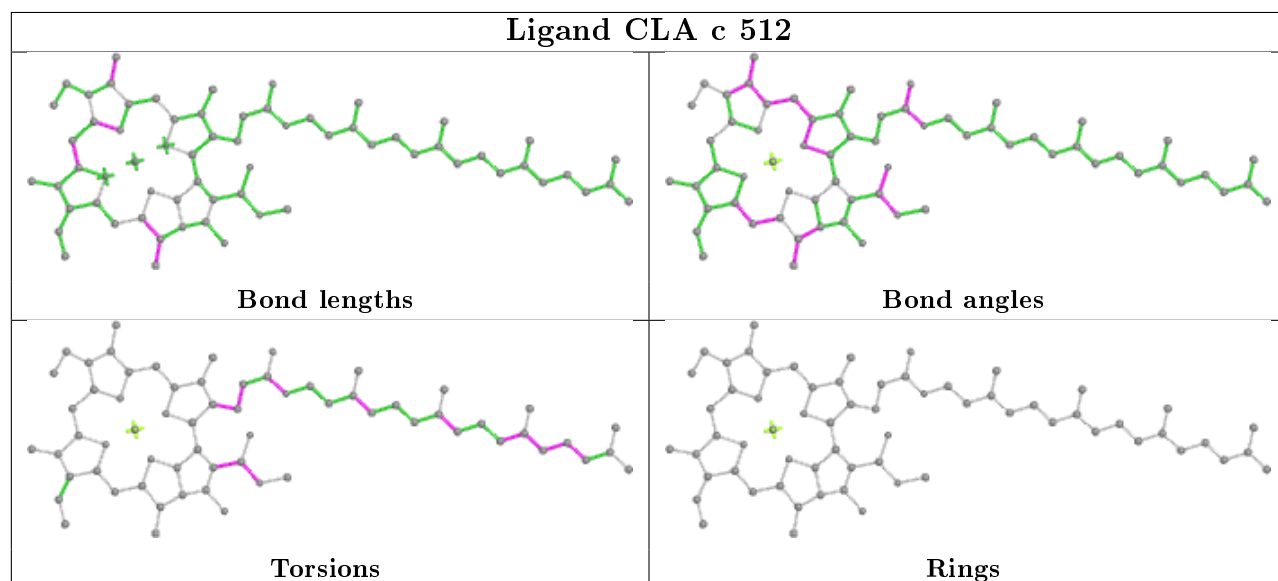




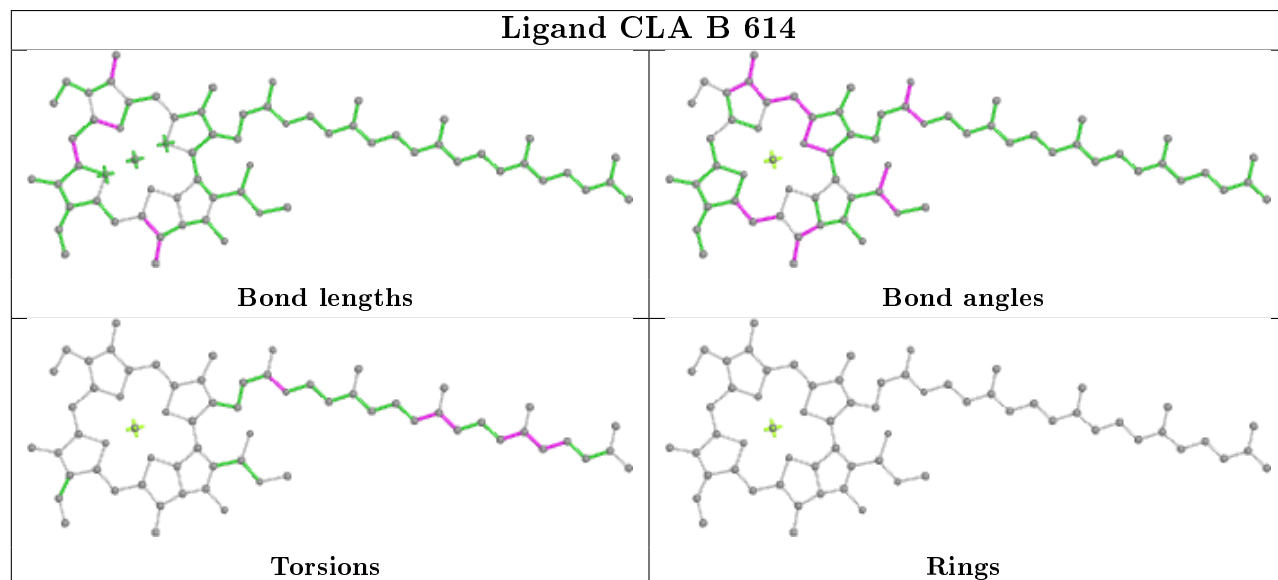
## Ligand CLA b 612

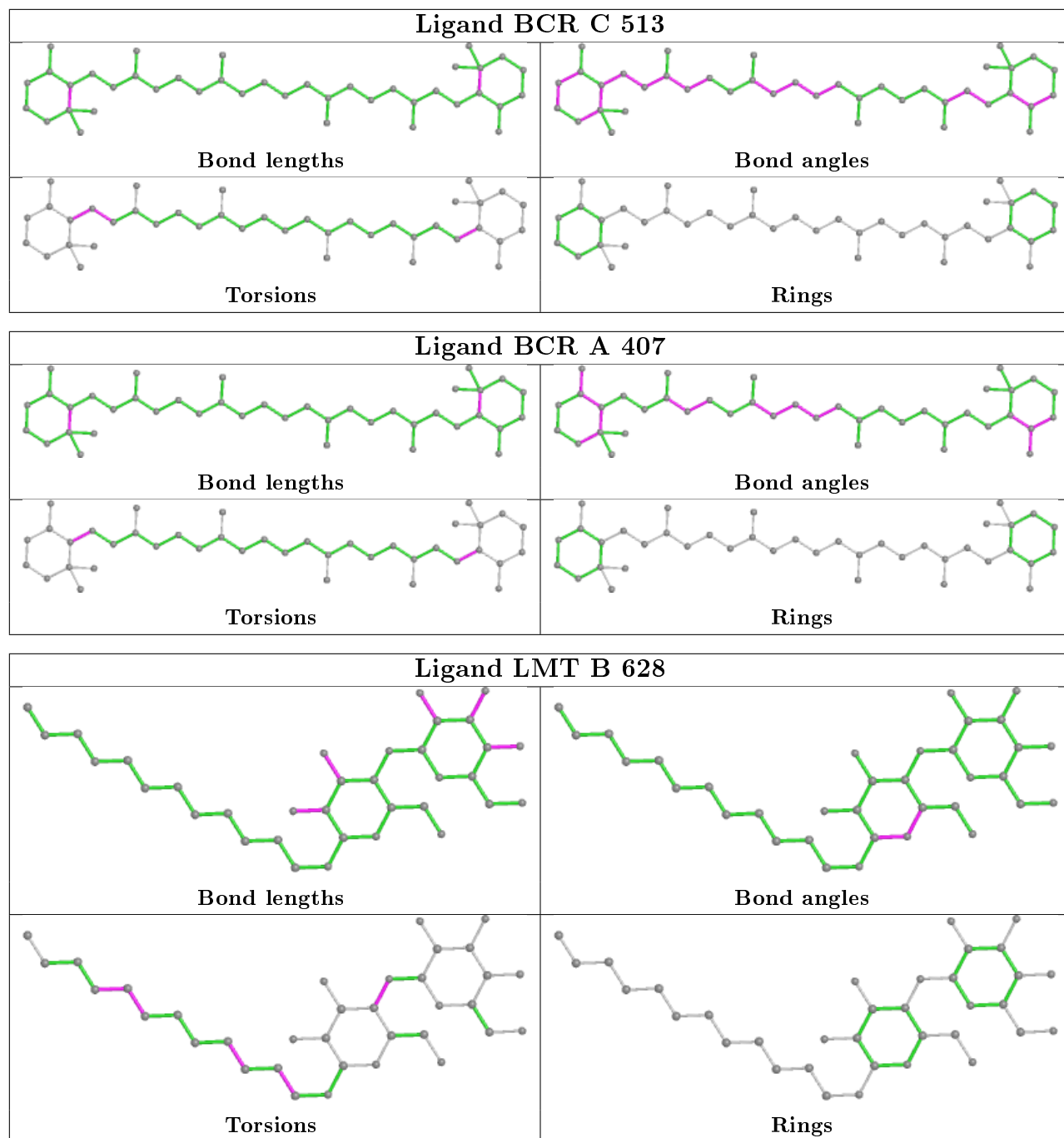


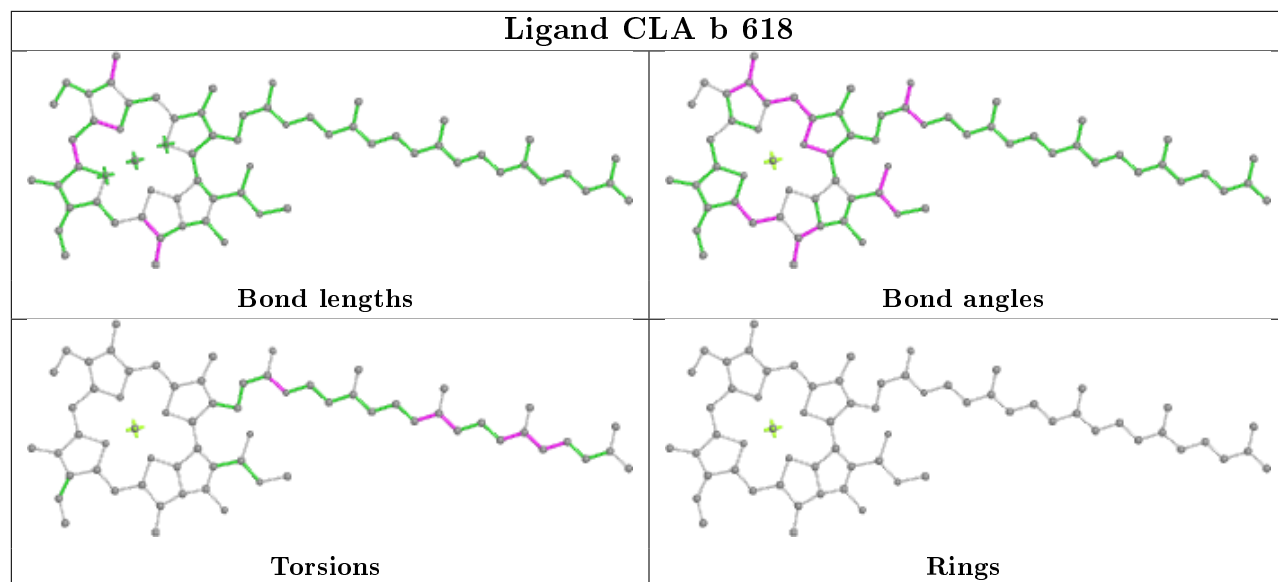
## Ligand CLA c 512



## Ligand CLA B 614







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/344 (97%)	0.43	28 (8%) 11 10	178, 179, 180, 181	0
1	a	335/344 (97%)	0.38	27 (8%) 12 11	178, 179, 180, 181	0
2	B	490/510 (96%)	0.21	22 (4%) 33 28	178, 179, 180, 181	0
2	b	490/510 (96%)	0.32	28 (5%) 23 20	178, 179, 180, 181	0
3	C	447/461 (96%)	0.27	28 (6%) 20 16	178, 179, 180, 181	0
3	c	447/461 (96%)	0.10	17 (3%) 40 33	178, 180, 180, 181	0
4	D	340/352 (96%)	0.18	11 (3%) 47 38	177, 179, 180, 181	0
4	d	340/352 (96%)	0.16	6 (1%) 68 60	177, 179, 180, 181	0
5	E	82/84 (97%)	0.09	2 (2%) 59 49	178, 180, 180, 181	0
5	e	82/84 (97%)	-0.02	4 (4%) 29 26	178, 180, 181, 181	0
6	F	35/45 (77%)	-0.18	1 (2%) 51 41	179, 179, 180, 180	0
6	f	35/45 (77%)	-0.46	0 100 100	179, 180, 181, 181	0
7	H	65/66 (98%)	0.39	9 (13%) 2 4	179, 180, 180, 181	0
7	h	65/66 (98%)	0.47	8 (12%) 4 5	179, 180, 181, 181	0
8	I	35/38 (92%)	0.43	2 (5%) 23 20	178, 179, 180, 181	0
8	i	35/38 (92%)	-0.01	0 100 100	179, 179, 181, 181	0
9	J	34/40 (85%)	-0.00	1 (2%) 51 41	178, 179, 180, 180	0
9	j	34/40 (85%)	-0.42	0 100 100	179, 180, 181, 181	0
10	K	37/46 (80%)	-0.08	0 100 100	179, 180, 180, 180	0
10	k	37/46 (80%)	0.48	3 (8%) 12 11	179, 180, 181, 181	0
11	L	37/37 (100%)	0.48	1 (2%) 54 45	178, 179, 180, 181	0
11	l	37/37 (100%)	0.12	0 100 100	178, 179, 180, 181	0
12	M	34/36 (94%)	0.28	2 (5%) 22 19	178, 179, 180, 181	0
12	m	34/36 (94%)	0.05	1 (2%) 51 41	178, 179, 180, 181	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.56	19 (7%) 13 12	177, 179, 180, 181	0
13	o	243/272 (89%)	0.57	20 (8%) 11 11	177, 179, 181, 181	0
14	T	32/32 (100%)	0.17	2 (6%) 20 16	178, 179, 181, 181	0
14	t	32/32 (100%)	0.36	4 (12%) 3 5	178, 179, 180, 181	0
15	U	97/134 (72%)	0.56	7 (7%) 15 13	178, 179, 180, 181	0
15	u	97/134 (72%)	0.73	11 (11%) 5 6	178, 179, 180, 181	0
16	V	137/163 (84%)	0.12	3 (2%) 62 53	178, 179, 180, 181	0
16	v	137/163 (84%)	0.47	8 (5%) 23 20	178, 180, 181, 181	0
17	g	28/46 (60%)	0.39	2 (7%) 16 13	179, 180, 181, 182	0
17	y	28/46 (60%)	0.14	0 100 100	178, 180, 181, 181	0
18	X	37/41 (90%)	0.50	3 (8%) 12 11	179, 179, 181, 181	0
18	x	37/41 (90%)	0.82	5 (13%) 3 4	179, 180, 180, 181	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.32	0 100 100	179, 180, 181, 181	0
20	z	62/62 (100%)	0.89	4 (6%) 18 15	179, 180, 181, 181	0
All	All	5214/5674 (91%)	0.29	289 (5%) 25 22	177, 179, 180, 182	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	84	LYS	7.4
15	U	38	GLU	6.3
13	o	169	LYS	6.0
3	C	148	GLY	5.5
7	H	66	GLY	5.4
1	A	10	SER	5.3
5	e	82	GLN	4.8
3	C	149	TYR	4.7
3	c	201	ASN	4.5
1	A	299	GLY	4.4
18	x	11	THR	4.3
16	v	132	ASN	4.2
5	E	84	LYS	4.2
2	b	490	GLN	4.2
3	c	372	PRO	4.1
3	c	202	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	69	LEU	4.1
13	O	90	GLU	4.0
1	A	179	THR	4.0
13	O	84	ASN	3.9
13	o	31	LEU	3.9
4	D	24	ARG	3.9
4	d	295	SER	3.9
1	A	11	ALA	3.8
13	o	168	PHE	3.8
1	a	137	LEU	3.8
1	a	224	ILE	3.7
3	C	147	PHE	3.7
3	C	140	LEU	3.7
3	C	141	GLU	3.7
15	U	39	LEU	3.7
17	g	27	MET	3.6
3	C	184	GLY	3.6
1	a	175	GLY	3.6
4	d	13	GLY	3.6
1	a	19	ASN	3.6
3	c	200	THR	3.6
1	a	190	HIS	3.4
2	B	411	PHE	3.4
13	O	91	PHE	3.4
1	A	175	GLY	3.4
4	D	190	ASN	3.4
3	C	143	TYR	3.4
3	c	260	ALA	3.4
13	o	124	GLU	3.3
14	t	31	LYS	3.3
2	b	218	LEU	3.3
9	J	7	ARG	3.3
2	B	83	GLU	3.3
1	a	165	GLN	3.2
2	B	295	GLY	3.2
15	u	53	GLU	3.2
4	D	174	GLY	3.2
3	C	183	GLY	3.2
1	A	195	HIS	3.1
14	t	30	THR	3.1
1	A	177	SER	3.1
1	A	138	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
3	C	266	TRP	3.1
1	A	12	ASN	3.1
13	o	154	SER	3.1
2	b	338	GLN	3.1
1	A	198	HIS	3.0
3	C	139	THR	3.0
1	A	294	ALA	3.0
1	a	179	THR	3.0
1	a	187	GLN	3.0
2	B	378	LYS	3.0
7	H	6	TRP	3.0
2	B	84	THR	3.0
20	z	1	MET	3.0
1	a	178	GLY	3.0
20	z	4	LEU	3.0
1	a	138	GLY	3.0
1	a	239	PHE	3.0
13	o	32	THR	3.0
13	O	50	ASP	2.9
3	C	142	GLU	2.9
2	b	302	TRP	2.9
3	C	473	ASP	2.9
3	c	203	THR	2.9
14	T	28	ARG	2.9
1	a	299	GLY	2.9
2	b	339	ALA	2.9
3	C	464	GLU	2.9
2	b	229	LEU	2.9
3	C	144	SER	2.8
3	C	212	TYR	2.8
14	t	32	LYS	2.8
10	k	14	ALA	2.8
2	B	183	PRO	2.8
15	u	58	ASN	2.8
7	h	66	GLY	2.8
4	d	191	TRP	2.8
2	b	301	ALA	2.8
15	U	40	VAL	2.8
18	x	12	ILE	2.8
13	O	170	GLY	2.8
13	O	243	SER	2.8
13	o	35	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	137	LEU	2.7
1	a	183	MET	2.7
1	A	80	GLY	2.7
7	H	56	ASP	2.7
3	c	403	SER	2.7
3	C	145	SER	2.7
1	a	298	ASN	2.7
1	a	282	GLY	2.7
2	b	303	SER	2.7
1	A	298	ASN	2.7
3	C	137	PRO	2.7
1	A	178	GLY	2.6
13	O	223	ILE	2.6
15	u	52	GLY	2.6
1	A	293	MET	2.6
16	v	133	LEU	2.6
15	U	121	LEU	2.6
14	t	29	ILE	2.6
15	u	72	TYR	2.6
2	B	161	LEU	2.6
2	b	133	LEU	2.6
18	X	42	GLN	2.6
2	B	294	SER	2.6
3	c	402	GLY	2.6
1	a	325	ASN	2.6
18	x	16	LEU	2.5
1	A	165	GLN	2.5
2	B	410	THR	2.5
3	C	136	GLY	2.5
2	b	340	TRP	2.5
13	o	153	ALA	2.5
2	B	165	GLY	2.5
1	A	15	GLU	2.5
3	C	332	GLN	2.5
3	C	135	ARG	2.5
18	x	47	GLN	2.5
2	b	482	ILE	2.5
1	a	177	SER	2.5
7	H	5	THR	2.5
1	A	196	PRO	2.5
2	b	412	THR	2.5
13	O	46	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
13	o	213	VAL	2.5
4	d	197	HIS	2.5
1	A	191	ASN	2.5
2	b	119	ASP	2.5
2	B	164	PRO	2.5
13	O	58	ILE	2.4
3	C	258	GLY	2.4
15	u	107	GLU	2.4
2	b	398	THR	2.4
15	u	131	GLY	2.4
13	O	195	ASP	2.4
1	A	183	MET	2.4
3	C	261	ARG	2.4
8	I	30	ARG	2.4
18	x	42	GLN	2.4
15	U	69	ARG	2.4
2	B	185	TRP	2.4
2	b	379	ALA	2.4
3	c	209	ILE	2.4
7	h	26	GLY	2.4
17	g	30	ILE	2.4
3	c	373	ASN	2.4
15	u	51	TYR	2.4
1	a	225	ARG	2.4
2	B	379	ALA	2.4
2	B	293	ALA	2.4
13	o	167	ASP	2.4
4	d	194	ASN	2.4
16	v	47	LEU	2.4
12	m	1	MET	2.4
10	k	43	VAL	2.3
15	u	65	PHE	2.3
1	A	262	TYR	2.3
2	b	397	VAL	2.3
7	h	14	LEU	2.3
13	O	225	LEU	2.3
4	D	171	PRO	2.3
4	d	241	GLU	2.3
13	o	215	ARG	2.3
16	v	131	ARG	2.3
13	o	229	LYS	2.3
3	c	211	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
13	O	169	LYS	2.3
2	B	326	ARG	2.3
15	u	57	LEU	2.3
2	b	298	LEU	2.3
2	b	402	TYR	2.3
13	o	269	ILE	2.3
15	U	42	VAL	2.3
5	E	17	VAL	2.3
3	c	411	ALA	2.3
4	D	197	HIS	2.3
16	V	94	ASN	2.3
2	B	412	THR	2.3
2	B	129	GLY	2.3
7	h	18	TYR	2.3
16	v	138	LEU	2.3
12	M	5	GLN	2.3
2	B	127	ARG	2.3
1	A	19	ASN	2.3
13	o	62	GLN	2.3
10	k	17	ILE	2.3
2	b	485	GLU	2.3
1	A	169	SER	2.3
1	a	198	HIS	2.3
7	h	56	ASP	2.3
7	h	3	ARG	2.3
7	H	62	TRP	2.2
7	H	63	LYS	2.2
18	X	45	LYS	2.2
1	a	199	GLN	2.2
4	D	176	ALA	2.2
7	H	8	GLY	2.2
16	v	51	GLN	2.2
1	A	181	ASN	2.2
7	h	2	ALA	2.2
2	b	420	TYR	2.2
13	o	63	THR	2.2
15	u	54	LYS	2.2
2	B	8	VAL	2.2
6	F	11	VAL	2.2
13	O	269	ILE	2.2
8	I	34	ARG	2.2
1	A	192	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
13	O	268	SER	2.2
3	c	371	GLY	2.2
3	C	27	ASP	2.2
4	D	194	ASN	2.2
3	c	180	MET	2.2
7	h	4	ARG	2.2
15	u	47	LEU	2.2
2	b	219	VAL	2.2
7	H	9	ASP	2.2
4	D	170	ALA	2.2
2	b	487	SER	2.2
1	a	139	MET	2.2
11	L	33	SER	2.2
15	U	65	PHE	2.2
4	D	199	MET	2.2
2	b	217	ILE	2.2
16	V	47	LEU	2.2
13	o	224	SER	2.2
3	c	207	ARG	2.1
16	v	142	ALA	2.1
1	a	301	ASN	2.1
2	b	411	PHE	2.1
13	o	125	ASP	2.1
13	O	79	LYS	2.1
1	a	191	ASN	2.1
3	C	465	PRO	2.1
5	e	57	ALA	2.1
12	M	2	GLU	2.1
13	o	123	GLU	2.1
1	A	342	ASP	2.1
14	T	27	PRO	2.1
16	v	145	ILE	2.1
4	D	172	SER	2.1
1	a	181	ASN	2.1
1	a	201	GLY	2.1
13	o	64	TYR	2.1
2	B	474	LEU	2.1
3	C	146	PHE	2.1
2	b	337	ALA	2.1
3	C	262	ARG	2.1
13	O	51	THR	2.1
2	b	431	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
13	O	68	ARG	2.1
13	o	237	ILE	2.1
3	C	257	PHE	2.1
1	a	172	MET	2.1
5	e	83	LEU	2.0
3	C	402	GLY	2.0
3	c	389	GLU	2.0
13	O	262	GLN	2.0
1	a	286	THR	2.0
13	O	113	VAL	2.0
2	b	120	LEU	2.0
4	D	295	SER	2.0
2	B	120	LEU	2.0
16	V	43	LYS	2.0
7	H	27	THR	2.0
1	A	190	HIS	2.0
18	X	13	THR	2.0
2	b	370	LEU	2.0
20	z	5	PHE	2.0
20	z	17	PHE	2.0
3	c	259	TRP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	PL9	J	101	35/55	0.24	0.59	177,180,181,181	0
30	LMT	i	102	35/35	0.48	1.16	178,181,183,183	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	LMT	I	102	35/35	0.49	1.04	178,180,182,183	0
30	LMT	d	411	31/35	0.49	0.78	178,181,182,183	0
23	PL9	j	101	35/55	0.52	0.35	179,180,181,181	0
24	BCR	J	102	40/40	0.52	0.37	178,180,181,181	0
22	CLA	c	502	65/65	0.55	0.64	178,179,180,181	0
27	LMG	I	101	43/55	0.56	1.04	178,180,181,182	0
23	PL9	d	407	55/55	0.57	0.42	177,179,180,181	0
30	LMT	B	628	35/35	0.58	0.50	177,180,182,183	0
35	CA	O	301	1/1	0.60	0.43	182,182,182,182	0
22	CLA	B	601	65/65	0.60	0.91	177,180,181,182	0
24	BCR	g	101	40/40	0.60	0.91	178,179,180,180	0
22	CLA	b	605	65/65	0.60	1.12	179,180,182,183	0
27	LMG	E	101	44/55	0.60	0.64	176,179,181,182	0
24	BCR	F	102	40/40	0.60	0.54	177,179,180,180	0
25	DGD	d	410	63/66	0.61	0.87	178,180,183,183	0
27	LMG	A	414	42/55	0.61	0.53	177,179,182,182	0
30	LMT	B	627	35/35	0.63	0.65	178,180,182,182	0
27	LMG	a	402	42/55	0.63	0.50	177,180,181,182	0
30	LMT	b	626	35/35	0.64	0.67	178,180,182,183	0
27	LMG	C	518	45/55	0.65	1.11	178,179,180,181	0
30	LMT	D	411	31/35	0.65	0.90	179,180,182,182	0
24	BCR	a	409	40/40	0.66	0.71	177,178,180,180	0
24	BCR	H	102	40/40	0.66	1.04	178,180,181,182	0
30	LMT	b	603	35/35	0.66	0.52	178,179,181,182	0
35	CA	K	101	1/1	0.67	0.53	184,184,184,184	0
22	CLA	C	502	65/65	0.67	0.55	178,179,180,180	0
29	SQD	d	403	43/54	0.67	0.83	178,180,182,186	0
27	LMG	M	101	42/55	0.67	0.55	178,180,181,182	0
22	CLA	b	619	65/65	0.67	0.76	177,179,180,181	0
24	BCR	B	617	40/40	0.68	0.49	177,179,180,180	0
30	LMT	B	623	35/35	0.68	0.86	177,181,182,183	0
24	BCR	B	616	40/40	0.68	0.47	176,178,180,180	0
30	LMT	b	627	35/35	0.69	1.06	178,180,182,182	0
24	BCR	j	102	40/40	0.70	0.29	179,180,182,183	0
23	PL9	D	407	55/55	0.70	0.41	177,178,179,180	0
25	DGD	A	408	56/66	0.70	0.44	178,179,181,182	0
25	DGD	b	624	58/66	0.70	0.44	177,178,180,180	0
30	LMT	b	604	35/35	0.71	0.56	177,179,181,182	0
25	DGD	b	601	52/66	0.71	0.56	178,180,181,182	0
23	PL9	A	406	45/55	0.71	0.41	177,179,180,180	0
25	DGD	a	410	56/66	0.71	0.42	178,180,181,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
24	BCR	B	619	40/40	0.72	0.85	178,179,180,180	0
24	BCR	b	623	40/40	0.72	0.76	177,178,180,180	0
24	BCR	c	514	40/40	0.72	0.77	177,179,180,180	0
24	BCR	K	102	40/40	0.72	0.89	178,180,181,182	0
31	PHO	d	401	64/64	0.73	0.43	178,179,180,180	0
26	LHG	c	519	37/49	0.73	0.32	178,180,183,187	0
24	BCR	x	101	40/40	0.73	0.85	178,179,180,181	0
24	BCR	b	622	40/40	0.74	0.37	176,178,179,179	0
29	SQD	B	626	47/54	0.74	0.53	175,179,181,183	0
25	DGD	D	410	63/66	0.74	0.88	178,181,182,183	0
22	CLA	B	613	65/65	0.74	0.43	177,179,180,180	0
30	LMT	M	102	35/35	0.74	0.36	178,179,181,182	0
27	LMG	c	518	45/55	0.75	1.03	178,180,181,181	0
25	DGD	B	625	52/66	0.75	0.58	177,180,182,182	0
27	LMG	C	521	48/55	0.75	0.33	177,179,180,181	0
27	LMG	i	101	43/55	0.75	0.85	177,180,182,184	0
22	CLA	c	512	65/65	0.75	0.81	178,180,181,182	0
24	BCR	c	513	40/40	0.75	0.88	178,179,180,180	0
22	CLA	a	407	65/65	0.76	0.73	178,179,180,181	0
27	LMG	e	101	44/55	0.76	0.38	177,179,181,181	0
22	CLA	a	404	65/65	0.76	0.60	177,178,180,180	0
25	DGD	C	517	66/66	0.76	0.38	177,179,180,181	0
24	BCR	A	407	40/40	0.76	0.52	177,179,180,180	0
35	CA	o	301	1/1	0.76	0.58	184,184,184,184	0
24	BCR	y	101	40/40	0.77	0.99	177,179,180,180	0
27	LMG	D	408	49/55	0.77	0.34	177,178,180,180	0
27	LMG	a	412	51/55	0.77	0.36	177,179,180,180	0
26	LHG	C	519	37/49	0.77	0.35	176,180,184,188	0
24	BCR	f	102	40/40	0.78	0.34	177,179,181,181	0
22	CLA	C	510	65/65	0.78	0.52	177,179,180,181	0
31	PHO	D	402	64/64	0.78	0.37	177,179,180,181	0
27	LMG	m	101	42/55	0.78	0.42	175,179,181,181	0
22	CLA	A	405	65/65	0.79	0.72	177,179,180,181	0
30	LMT	M	103	35/35	0.79	0.48	177,179,180,180	0
29	SQD	a	415	51/54	0.79	0.30	178,179,181,182	0
25	DGD	c	517	66/66	0.79	0.31	177,179,181,181	0
24	BCR	b	621	40/40	0.79	0.38	178,178,179,179	0
22	CLA	c	505	65/65	0.79	0.55	177,179,180,181	0
22	CLA	C	512	65/65	0.79	0.90	177,180,181,182	0
32	CL	D	403	1/1	0.80	0.28	180,180,180,180	0
22	CLA	C	505	65/65	0.80	0.50	177,179,180,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	LMG	D	412	46/55	0.80	0.32	178,179,180,181	0
30	LMT	B	624	35/35	0.80	0.51	178,180,182,183	0
29	SQD	b	602	47/54	0.80	0.41	176,179,182,185	0
24	BCR	C	514	40/40	0.81	0.74	178,179,180,181	0
22	CLA	B	615	65/65	0.81	0.74	176,179,180,181	0
22	CLA	B	603	65/65	0.81	0.50	176,179,180,180	0
27	LMG	A	410	51/55	0.81	0.33	177,178,180,181	0
22	CLA	a	405	65/65	0.81	0.59	174,178,179,180	0
29	SQD	F	103	45/54	0.81	0.65	178,180,182,182	0
23	PL9	a	408	45/55	0.81	0.31	176,179,180,180	0
22	CLA	c	510	65/65	0.81	0.53	178,179,181,181	0
29	SQD	A	412	51/54	0.81	0.30	178,179,180,181	0
22	CLA	A	404	65/65	0.81	0.38	176,178,180,181	0
22	CLA	b	618	65/65	0.81	0.65	177,179,180,180	0
22	CLA	c	503	65/65	0.82	0.58	177,179,180,181	0
22	CLA	C	507	65/65	0.82	0.37	178,179,180,181	0
22	CLA	h	101	65/65	0.83	0.49	176,179,180,181	0
22	CLA	b	617	65/65	0.83	0.41	178,179,180,182	0
25	DGD	c	515	53/66	0.83	0.41	176,179,181,182	0
25	DGD	B	620	58/66	0.83	0.34	176,179,181,182	0
22	CLA	d	406	65/65	0.83	0.59	177,179,180,181	0
22	CLA	C	506	65/65	0.83	0.71	177,179,180,180	0
27	LMG	c	522	48/55	0.84	0.28	178,180,180,181	0
22	CLA	B	614	65/65	0.84	0.65	177,179,180,181	0
22	CLA	C	508	65/65	0.84	0.87	177,179,180,180	0
29	SQD	a	401	54/54	0.84	0.62	178,180,181,183	0
22	CLA	C	509	65/65	0.84	0.37	177,179,180,180	0
22	CLA	a	406	65/65	0.84	0.32	177,179,180,181	0
22	CLA	b	612	65/65	0.84	0.63	176,179,181,181	0
22	CLA	B	608	65/65	0.84	0.59	177,179,180,180	0
22	CLA	b	607	65/65	0.84	0.41	177,179,180,181	0
27	LMG	d	409	48/55	0.84	0.29	177,179,180,180	0
22	CLA	C	520	65/65	0.84	0.33	178,179,180,181	0
24	BCR	b	620	40/40	0.84	0.36	177,179,179,180	0
22	CLA	b	613	65/65	0.85	0.74	178,179,180,181	0
25	DGD	C	515	53/66	0.85	0.32	177,178,179,180	0
24	BCR	c	521	40/40	0.85	1.27	178,179,181,181	0
22	CLA	b	609	65/65	0.85	0.65	178,179,180,181	0
22	CLA	B	606	65/65	0.85	0.36	177,179,180,180	0
26	LHG	A	409	39/49	0.85	0.30	178,179,181,181	0
26	LHG	a	411	39/49	0.85	0.26	177,179,180,181	0
29	SQD	B	622	43/54	0.85	0.43	177,180,182,185	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	DGD	C	516	62/66	0.86	0.25	177,179,180,181	0
22	CLA	c	501	65/65	0.86	0.49	177,179,180,181	0
24	BCR	B	618	40/40	0.86	0.32	177,178,179,179	0
31	PHO	d	402	64/64	0.86	0.25	178,179,180,181	0
22	CLA	C	503	65/65	0.86	0.40	177,179,180,180	0
27	LMG	b	625	49/55	0.86	0.28	178,179,180,180	0
22	CLA	c	509	65/65	0.86	0.33	177,179,180,180	0
22	CLA	C	501	65/65	0.86	0.47	178,179,180,180	0
22	CLA	c	508	65/65	0.86	0.44	177,179,180,181	0
29	SQD	f	103	45/54	0.86	0.60	177,179,181,182	0
22	CLA	b	611	65/65	0.86	0.36	177,179,180,180	0
22	CLA	H	101	65/65	0.86	0.32	177,179,180,181	0
22	CLA	B	605	65/65	0.87	0.71	178,179,180,180	0
27	LMG	D	409	48/55	0.87	0.28	175,178,180,181	0
22	CLA	b	615	65/65	0.87	0.38	177,179,180,180	0
29	SQD	A	413	54/54	0.87	0.38	178,180,182,184	0
21	FE2	a	403	1/1	0.87	0.07	182,182,182,182	0
31	PHO	D	401	64/64	0.87	0.36	177,179,180,180	0
22	CLA	B	610	65/65	0.87	0.38	177,179,180,180	0
22	CLA	c	511	65/65	0.87	0.68	178,180,181,182	0
22	CLA	C	504	65/65	0.87	0.39	177,179,180,180	0
22	CLA	d	405	65/65	0.88	0.44	177,178,179,180	0
22	CLA	c	506	65/65	0.88	0.57	178,179,180,181	0
35	CA	k	101	1/1	0.88	0.26	180,180,180,180	0
22	CLA	b	608	65/65	0.88	0.50	178,179,180,181	0
22	CLA	b	606	65/65	0.88	0.60	177,179,180,181	0
22	CLA	B	604	65/65	0.88	0.68	177,179,180,180	0
24	BCR	C	513	40/40	0.88	0.75	177,179,180,180	0
22	CLA	b	610	65/65	0.89	0.28	177,179,180,180	0
22	CLA	B	609	65/65	0.89	0.49	178,179,180,181	0
25	DGD	c	516	62/66	0.89	0.25	178,179,180,181	0
22	CLA	B	607	65/65	0.89	0.38	178,179,180,181	0
34	HEM	f	101	43/43	0.89	0.35	178,180,180,181	0
22	CLA	D	406	65/65	0.89	0.70	177,179,180,181	0
22	CLA	c	504	65/65	0.89	0.30	177,179,180,180	0
22	CLA	D	405	65/65	0.90	0.38	177,179,180,180	0
27	LMG	B	621	49/55	0.90	0.27	177,179,180,180	0
22	CLA	c	520	65/65	0.90	0.30	177,179,180,181	0
22	CLA	C	511	65/65	0.90	0.86	178,179,180,181	0
33	BCT	D	404	4/4	0.90	0.29	178,179,179,179	0
34	HEM	v	201	43/43	0.90	0.54	177,179,180,180	0
22	CLA	c	507	65/65	0.90	0.27	177,179,180,181	0

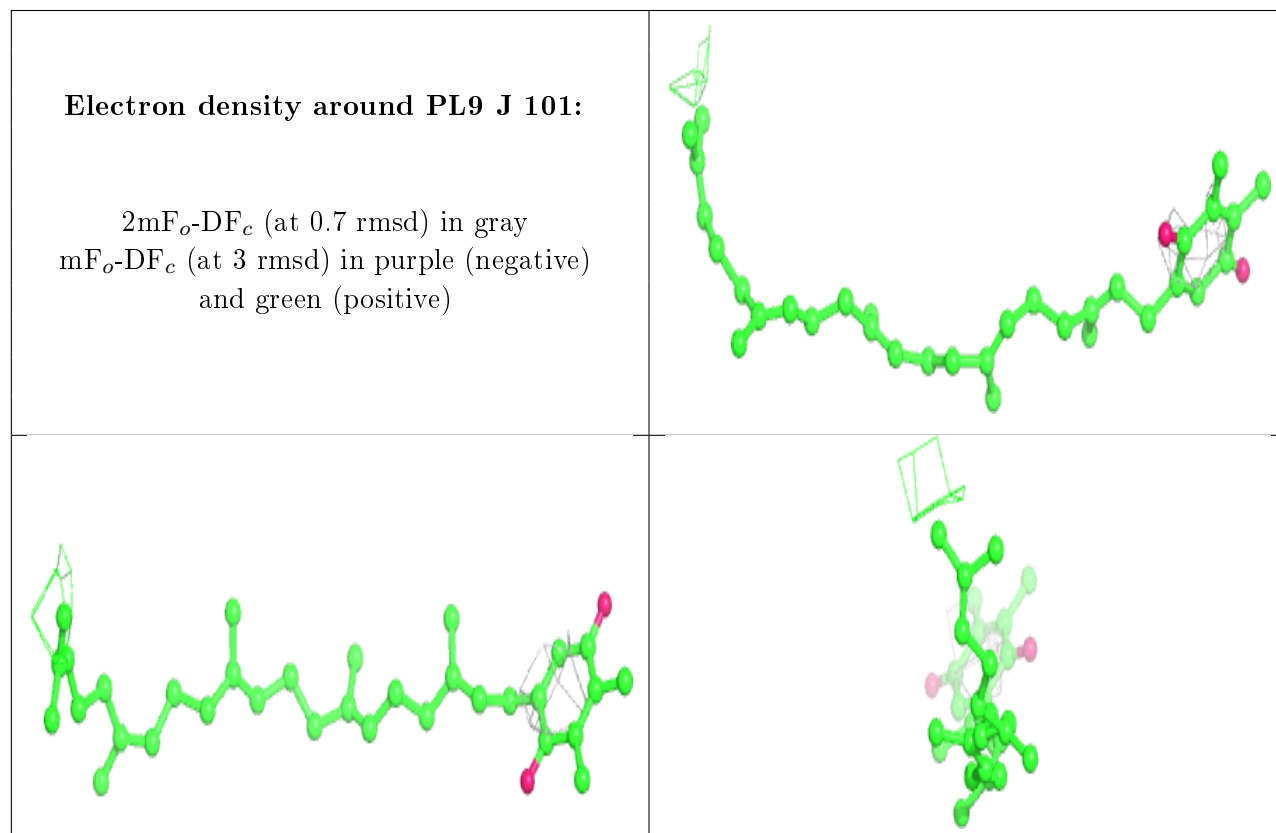
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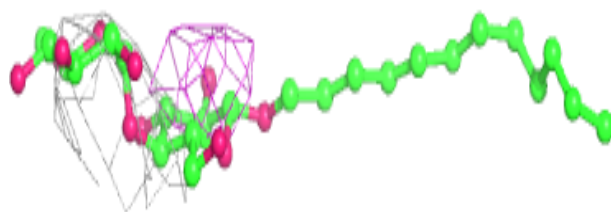
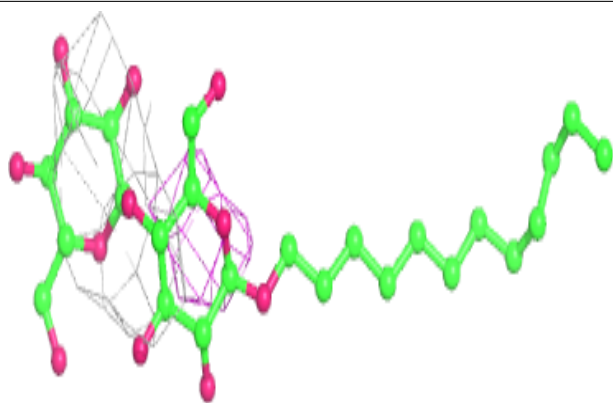
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	HEM	V	201	43/43	0.91	0.39	176,178,180,180	0
27	LMG	d	412	46/55	0.91	0.24	177,178,180,180	0
22	CLA	b	614	65/65	0.91	0.28	178,179,180,180	0
21	FE2	A	401	1/1	0.91	0.19	176,176,176,176	0
22	CLA	A	402	65/65	0.92	0.42	178,179,180,181	0
28	OEX	A	411	10/10	0.92	0.42	172,175,178,178	0
22	CLA	B	612	65/65	0.92	0.27	176,178,180,181	0
22	CLA	B	602	65/65	0.92	0.47	176,178,180,180	0
22	CLA	A	403	65/65	0.92	0.52	177,179,179,180	0
22	CLA	B	611	65/65	0.93	0.38	177,179,180,180	0
34	HEM	F	101	43/43	0.94	0.43	178,180,181,182	0
33	BCT	d	404	4/4	0.94	0.18	178,180,180,180	0
32	CL	a	413	1/1	0.94	0.57	177,177,177,177	0
22	CLA	b	616	65/65	0.94	0.29	177,179,180,180	0
27	LMG	d	408	49/55	0.94	0.19	178,179,180,180	0
28	OEX	a	414	10/10	0.94	0.41	174,177,179,182	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.

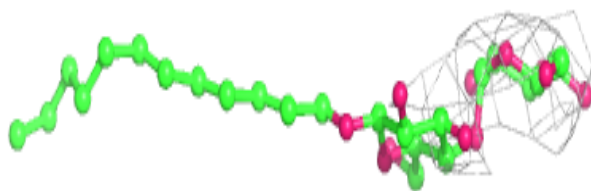
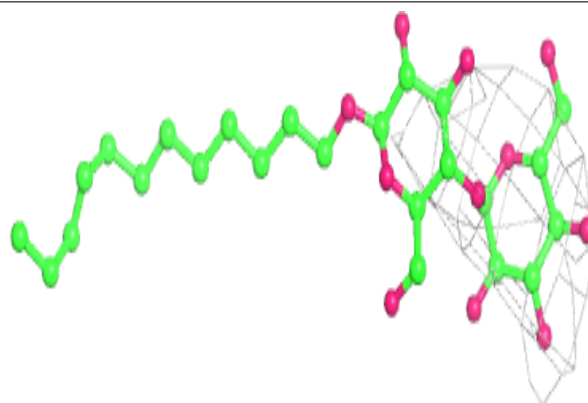


**Electron density around LMT i 102:**

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

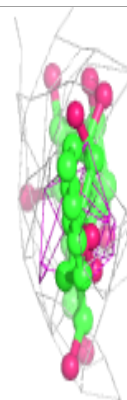
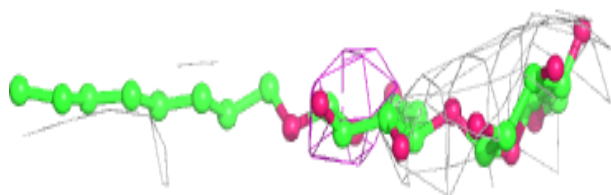
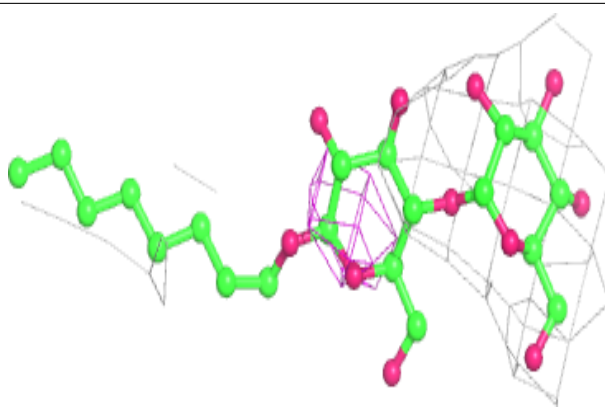
**Electron density around LMT I 102:**

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

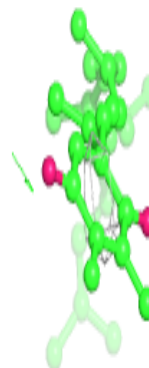
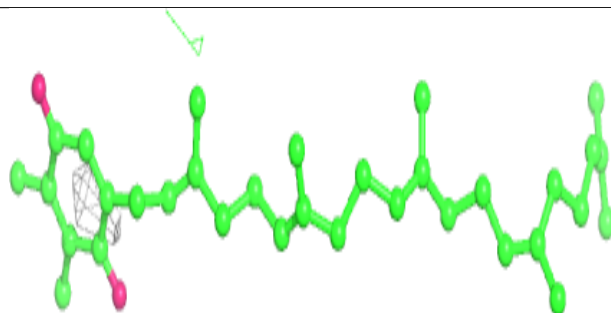
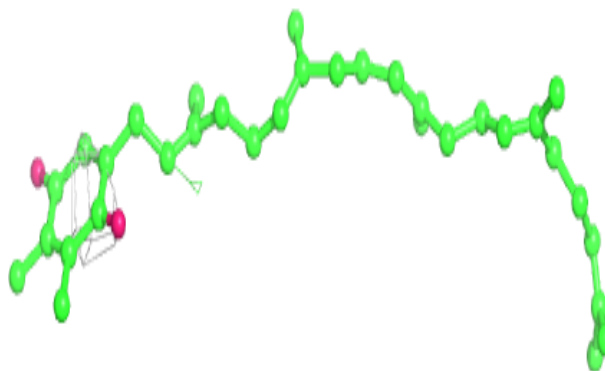


**Electron density around LMT d 411:**

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

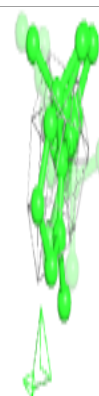
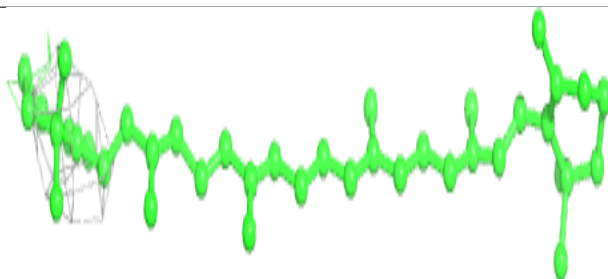
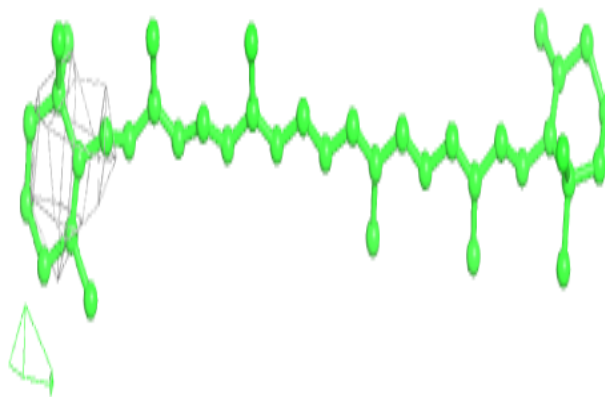
**Electron density around PL9 j 101:**

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

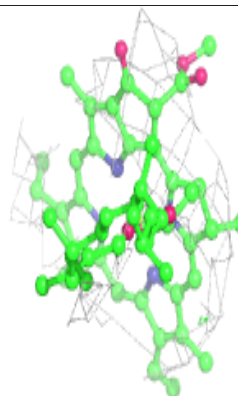
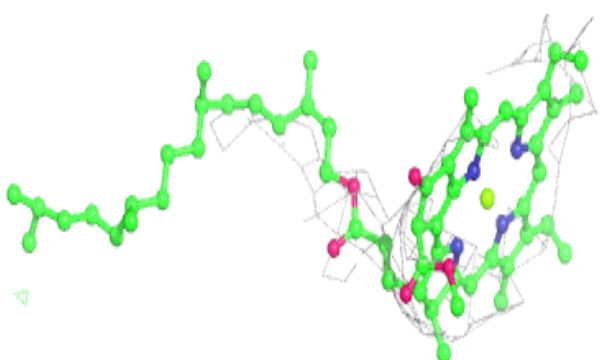
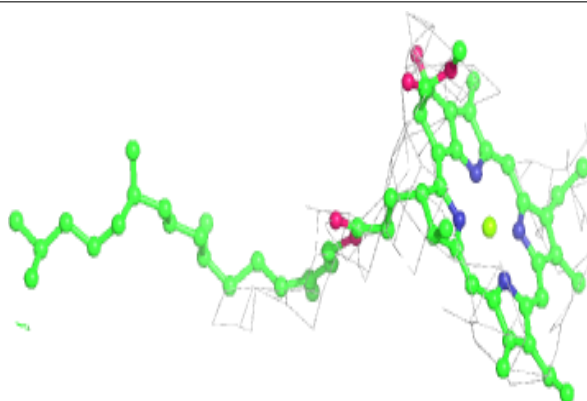


**Electron density around BCR J 102:**

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

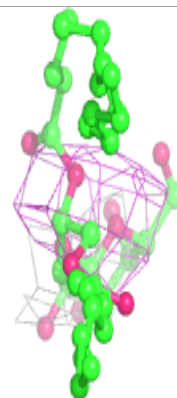
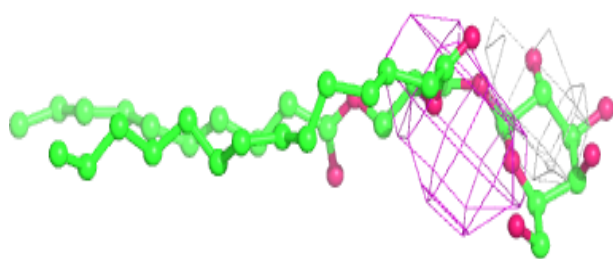
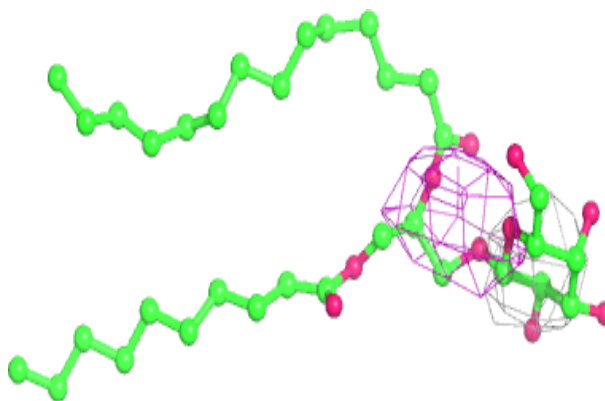
**Electron density around CLA c 502:**

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

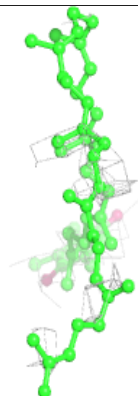
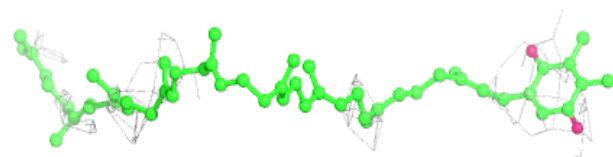
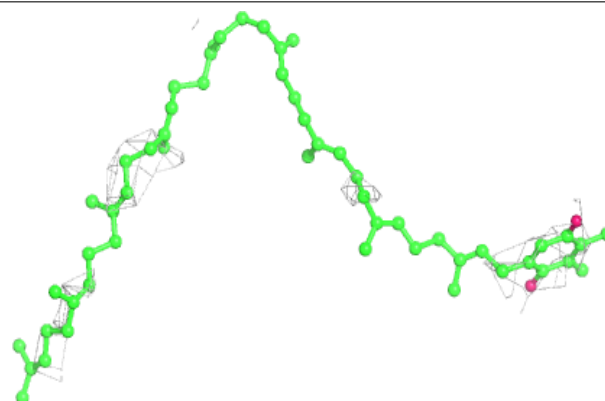


**Electron density around LMG I 101:**

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

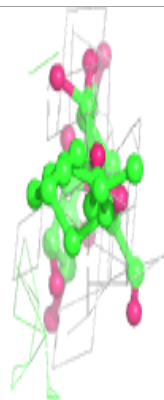
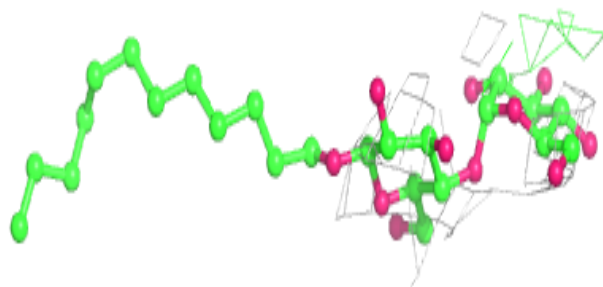
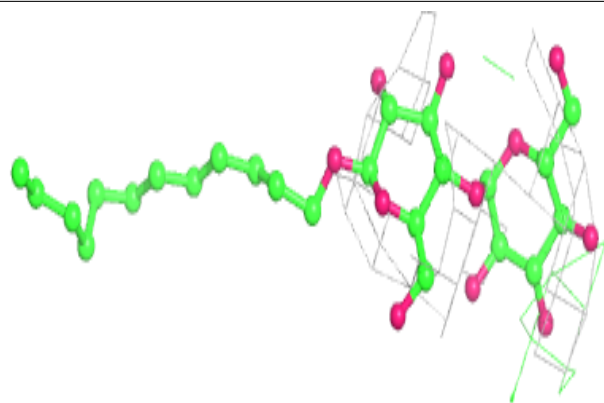
**Electron density around PL9 d 407:**

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



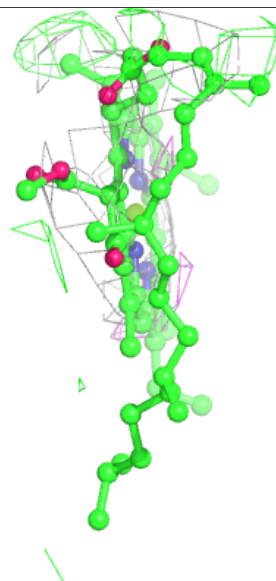
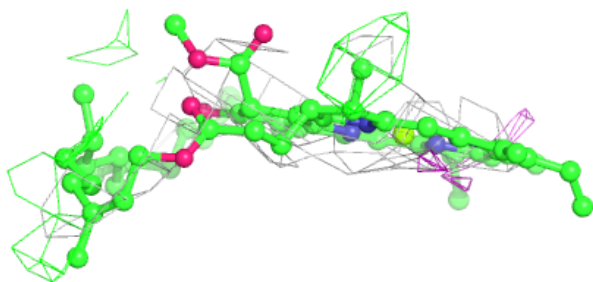
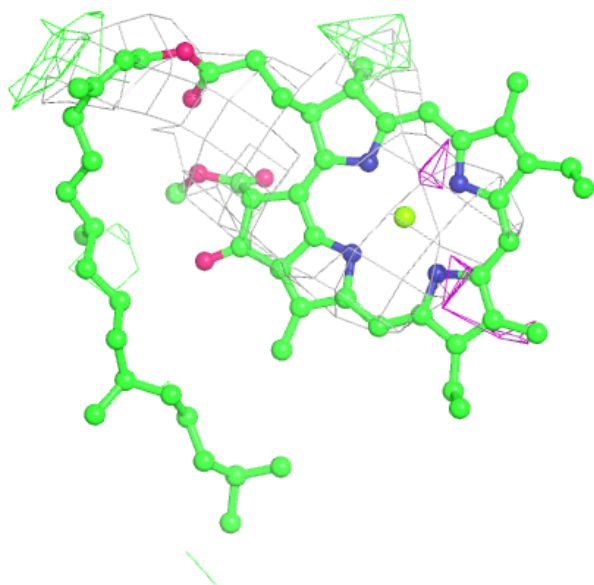
**Electron density around LMT B 628:**

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



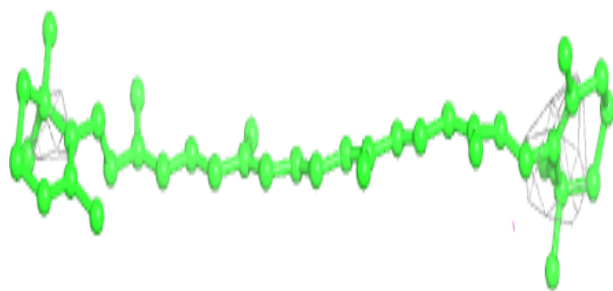
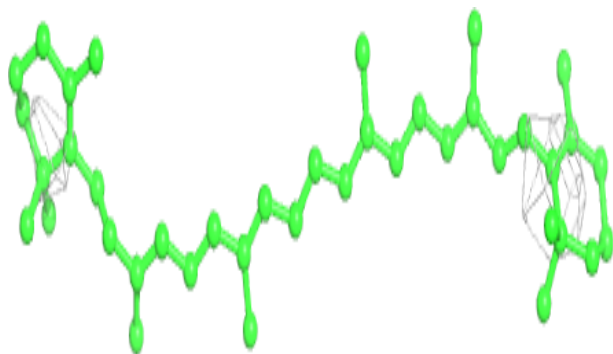
**Electron density around CLA B 601:**

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



**Electron density around BCR g 101:**

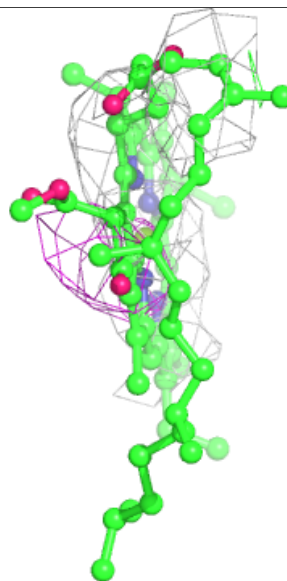
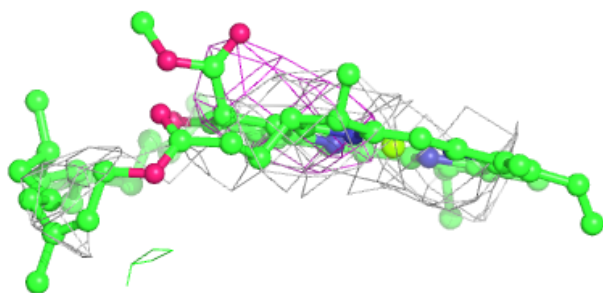
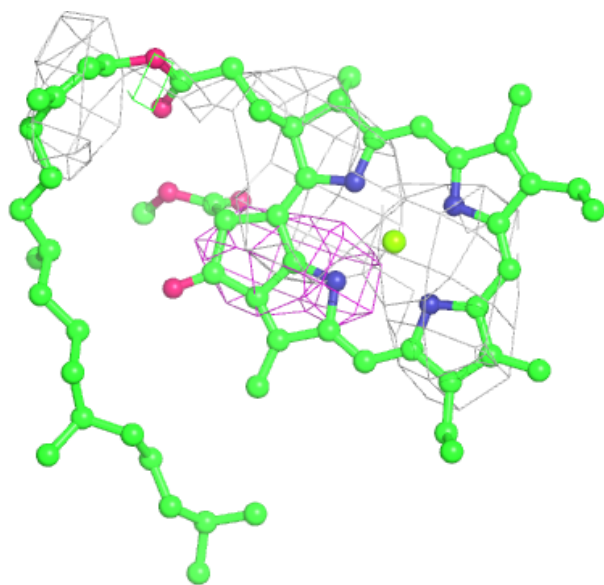
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





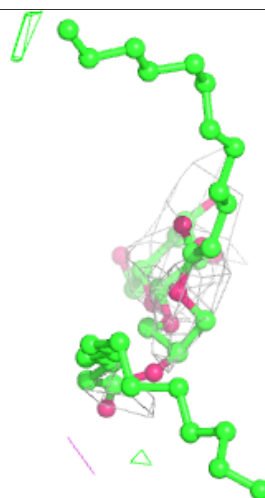
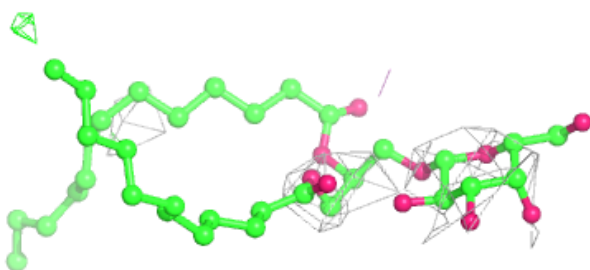
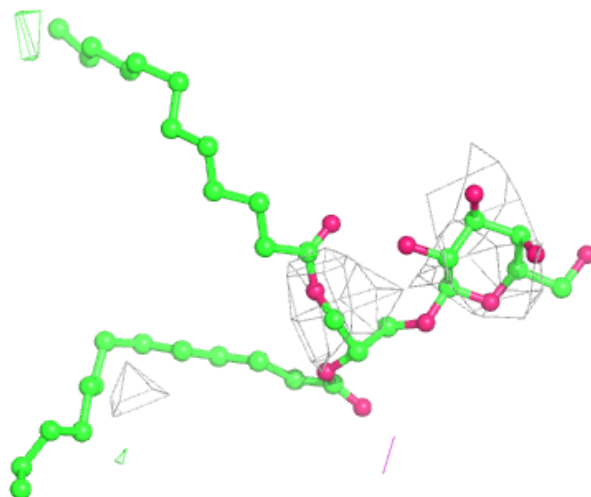
**Electron density around CLA b 605:**

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



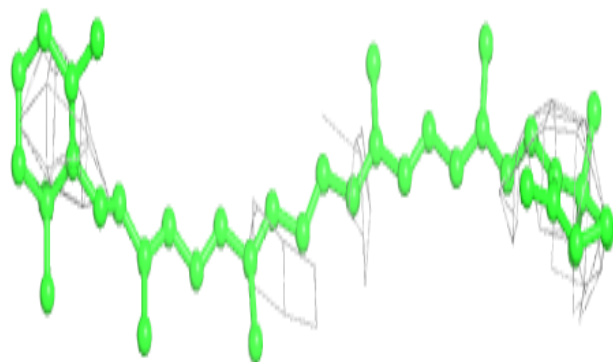
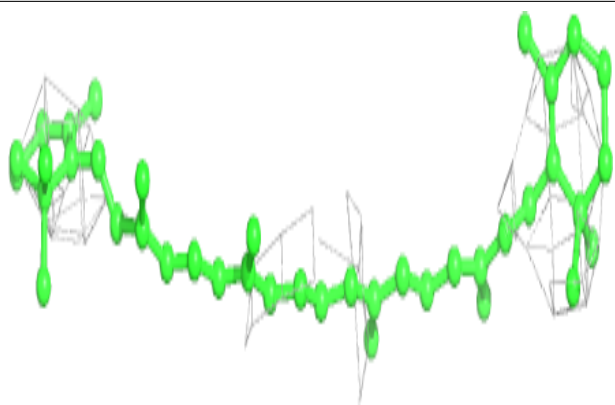
**Electron density around LMG E 101:**

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

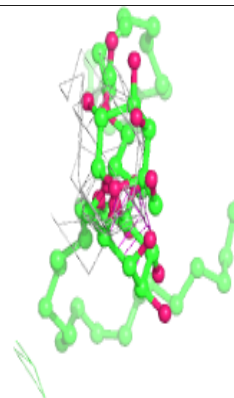
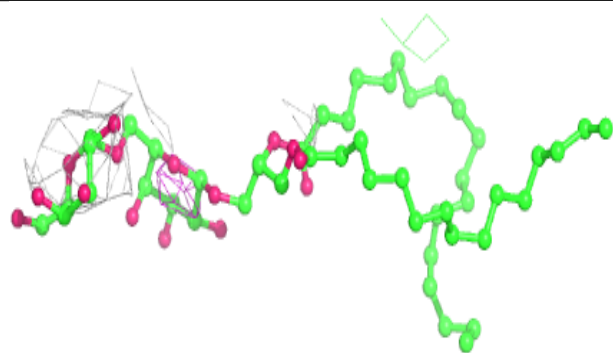
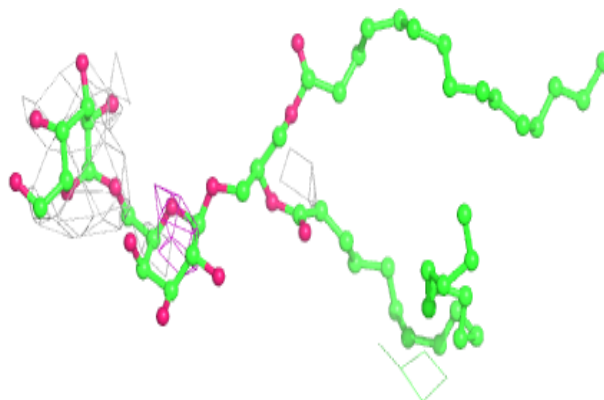


**Electron density around BCR F 102:**

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

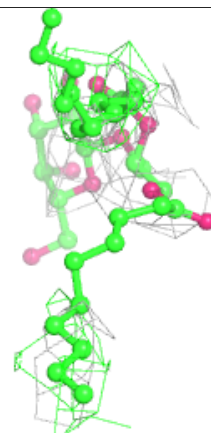
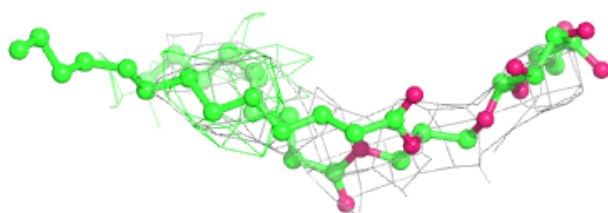
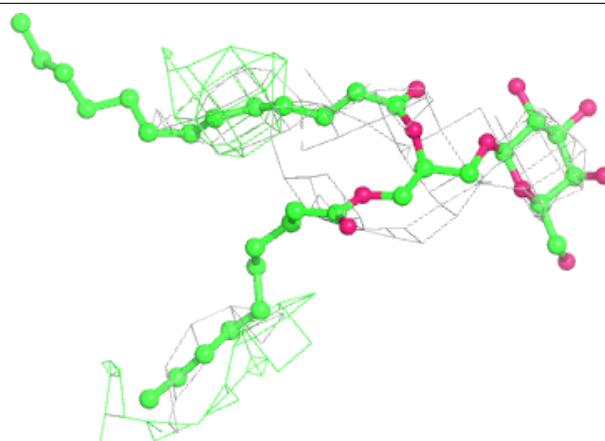
**Electron density around DGD d 410:**

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

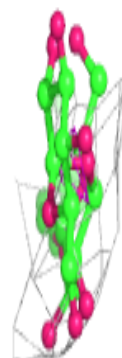
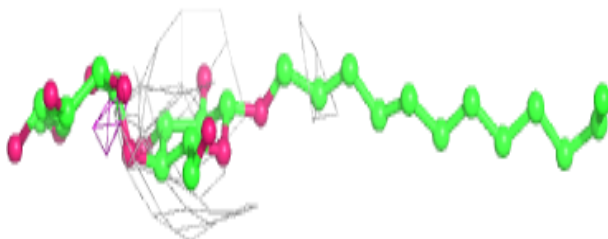
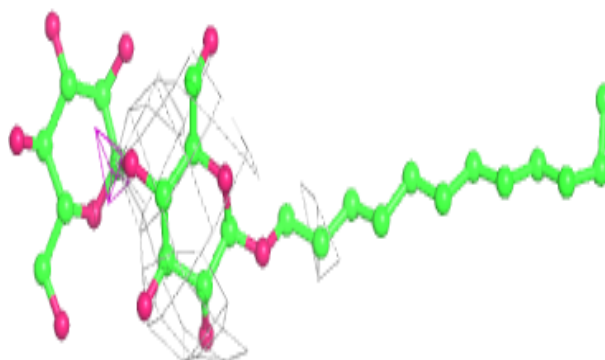


**Electron density around LMG A 414:**

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

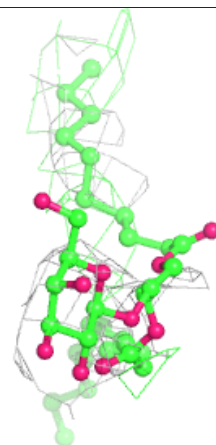
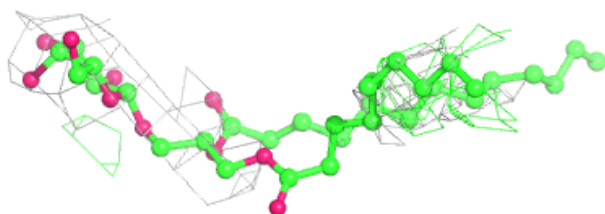
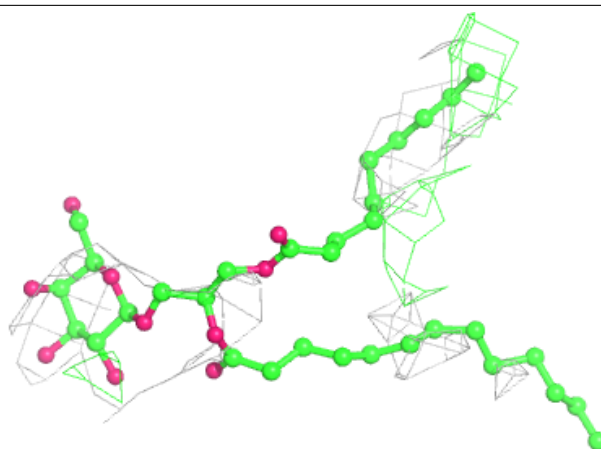
**Electron density around LMT B 627:**

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

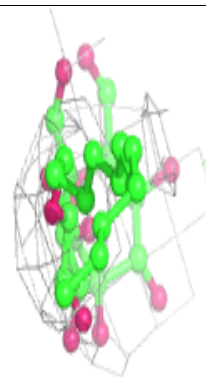
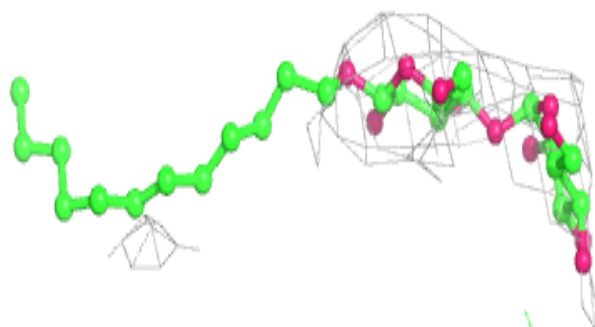
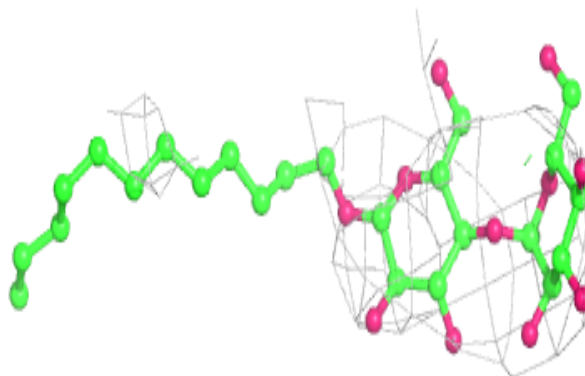


**Electron density around LMG a 402:**

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

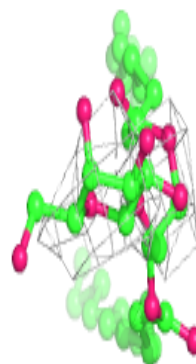
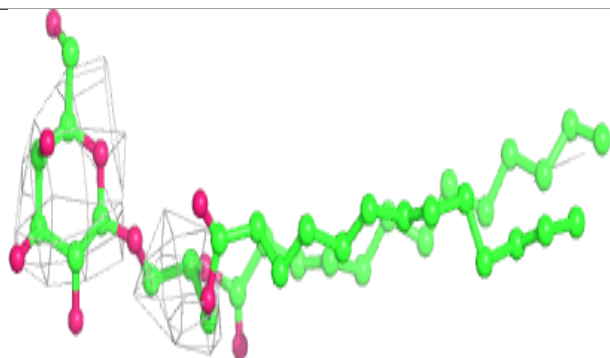
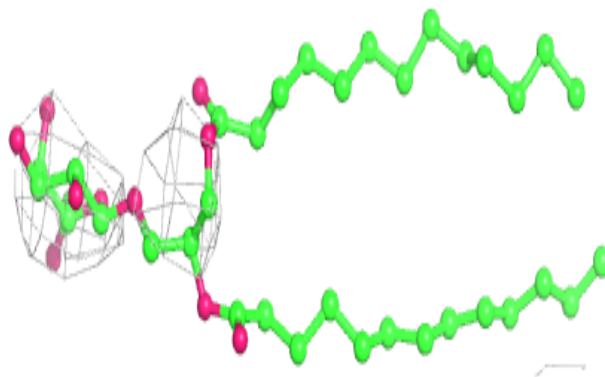
**Electron density around LMT b 626:**

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

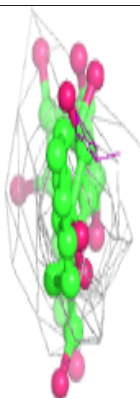
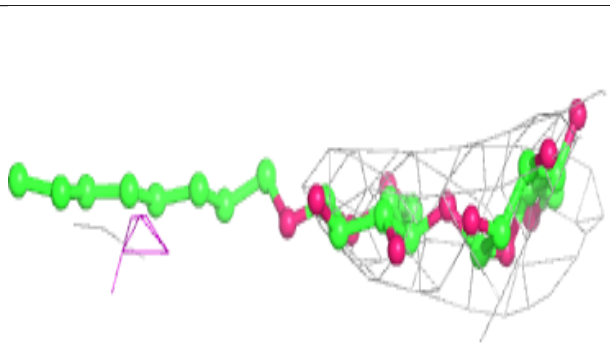
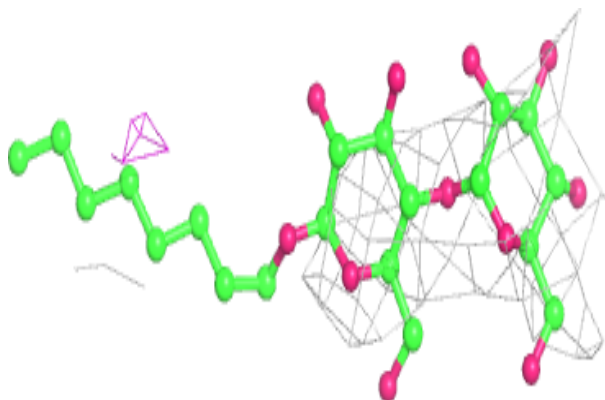


**Electron density around LMG C 518:**

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

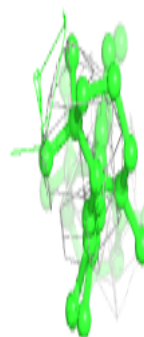
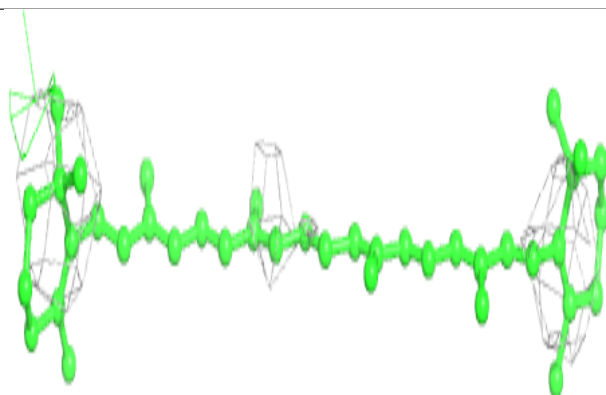
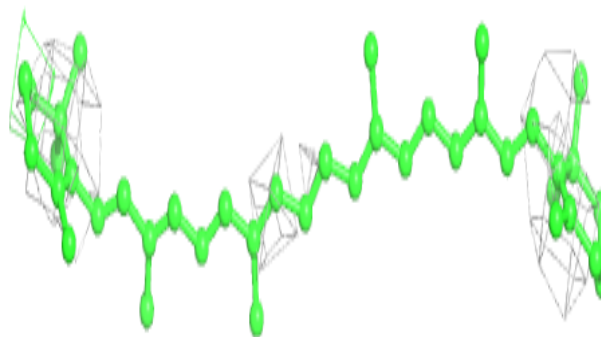
**Electron density around LMT D 411:**

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

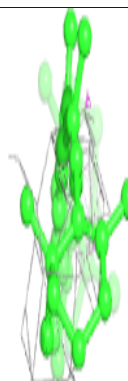
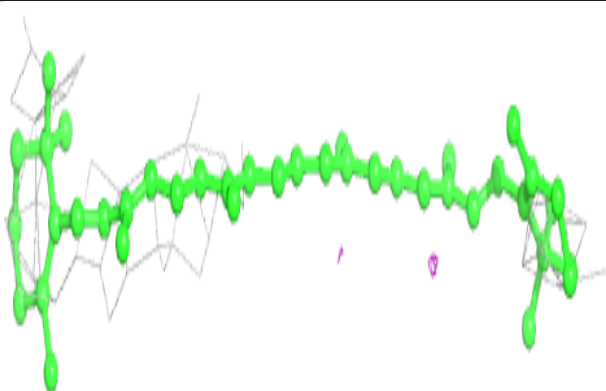
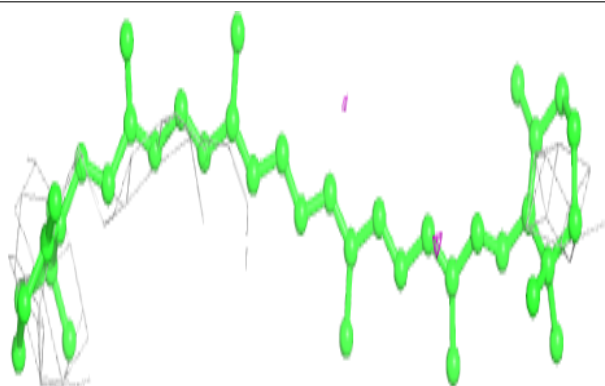


**Electron density around BCR a 409:**

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

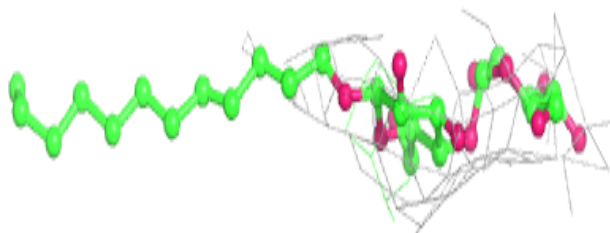
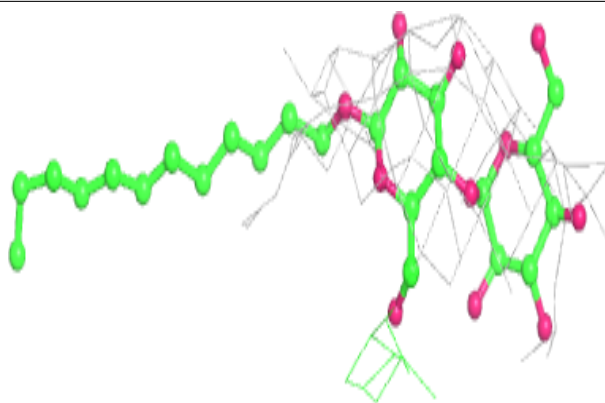
**Electron density around BCR H 102:**

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

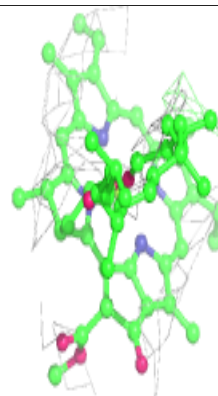
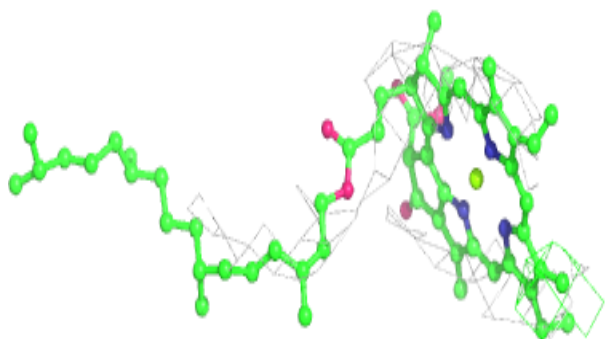
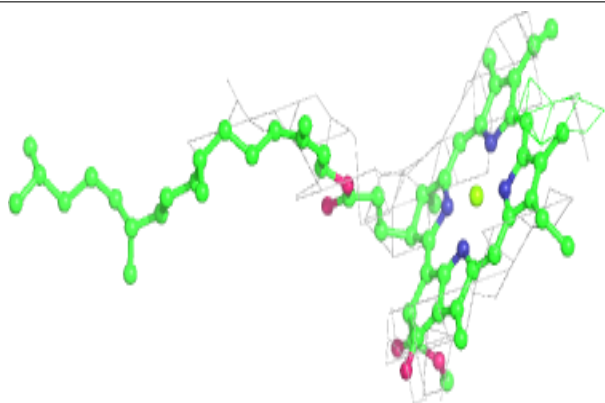


**Electron density around LMT b 603:**

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

**Electron density around CLA C 502:**

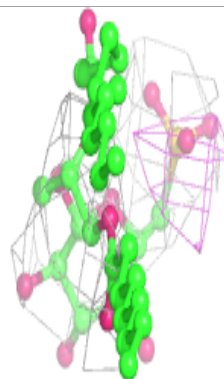
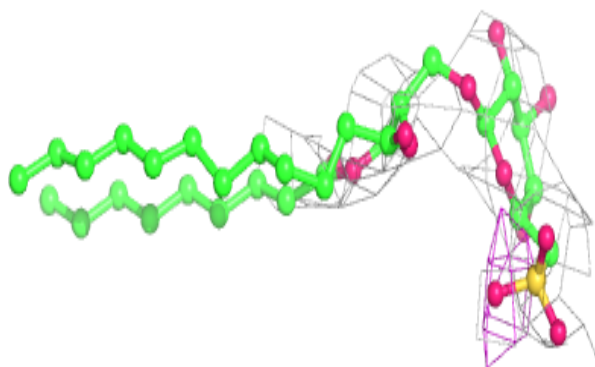
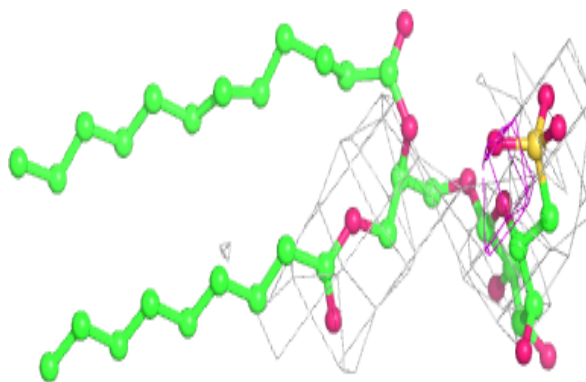
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



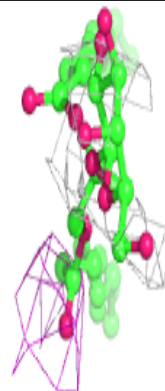
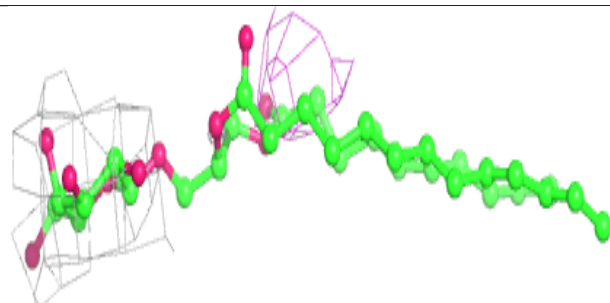
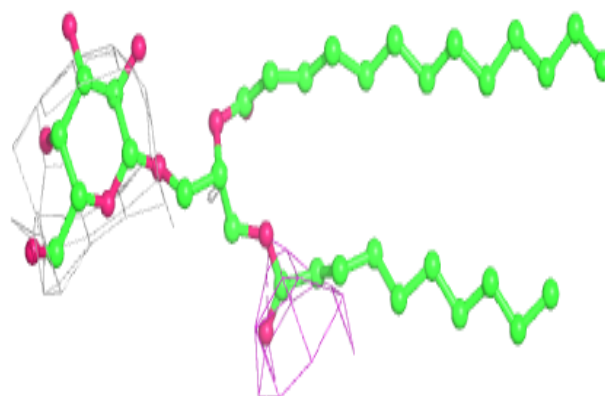


**Electron density around SQD d 403:**

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

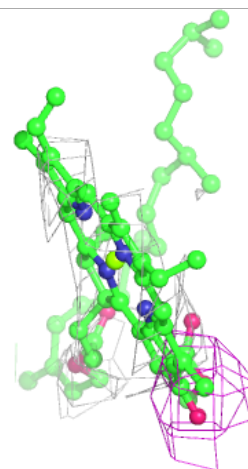
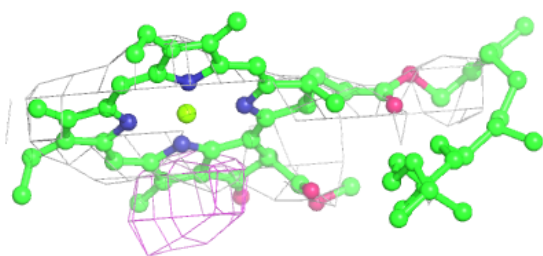
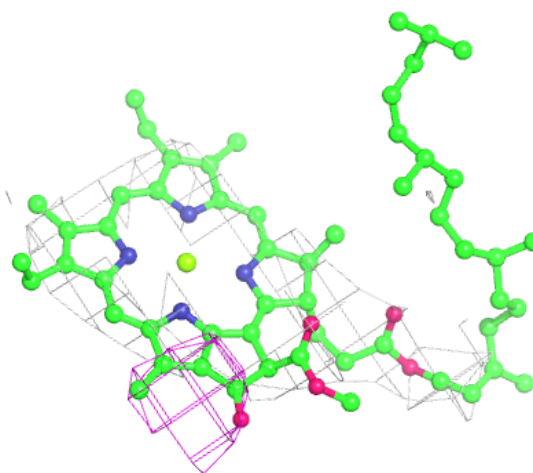
**Electron density around LMG M 101:**

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



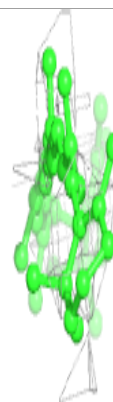
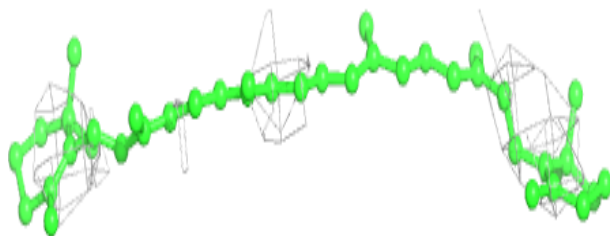
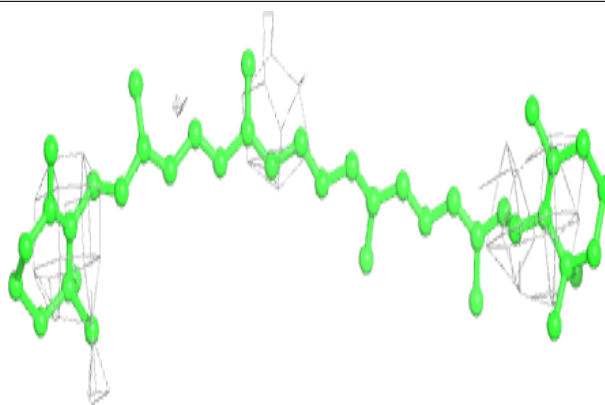
**Electron density around CLA b 619:**

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

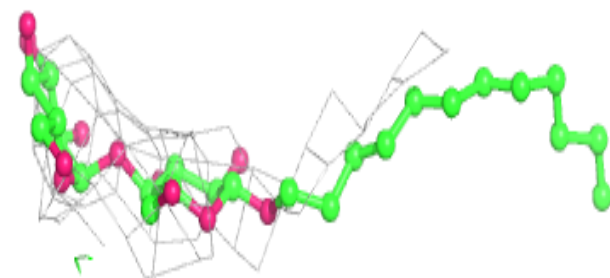
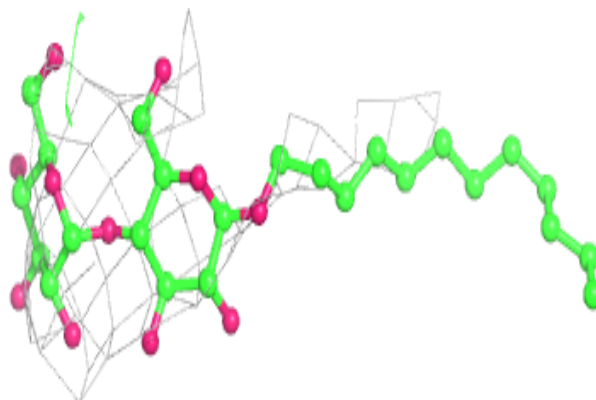


**Electron density around BCR B 617:**

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

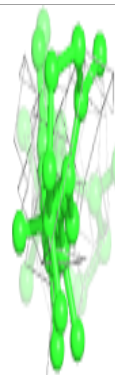
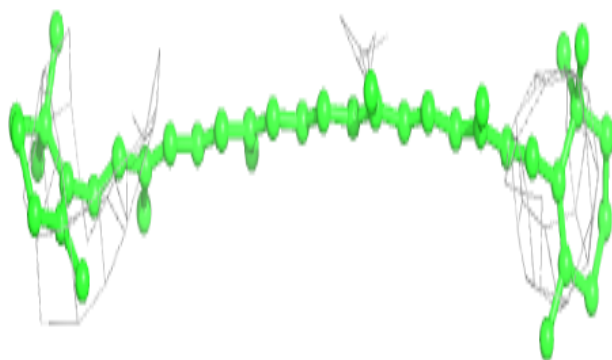
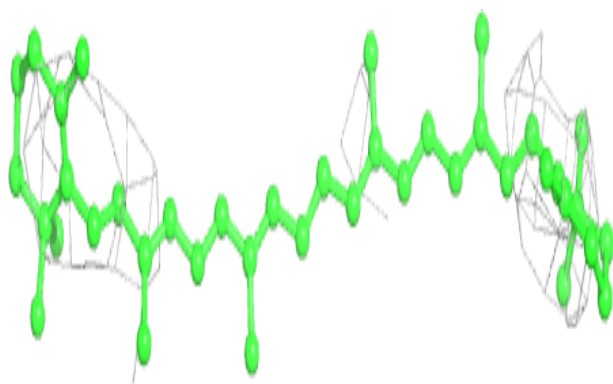
**Electron density around LMT B 623:**

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

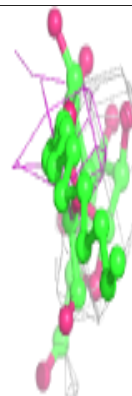
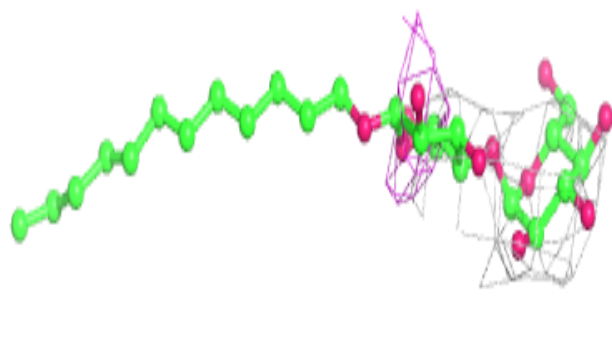
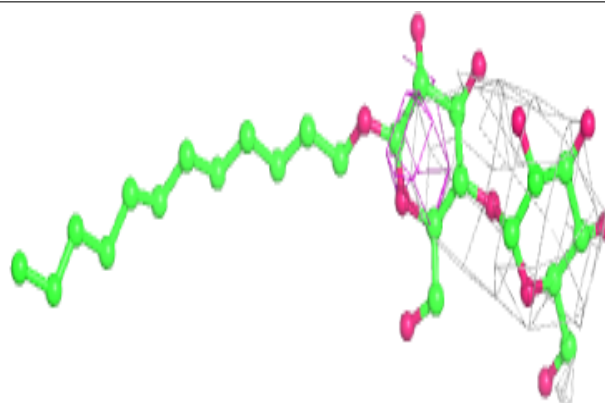


**Electron density around BCR B 616:**

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

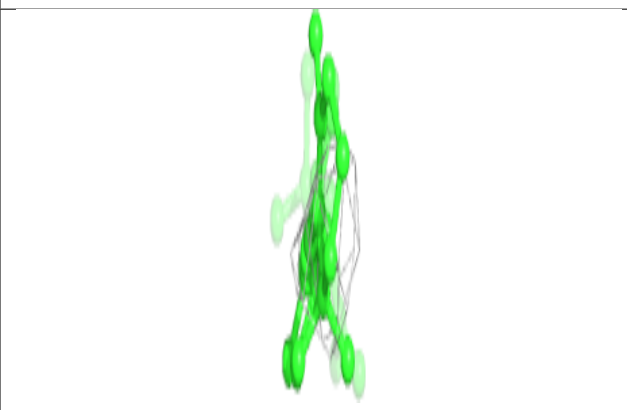
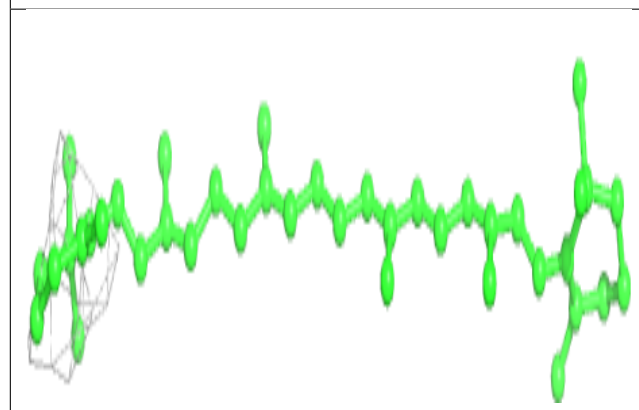
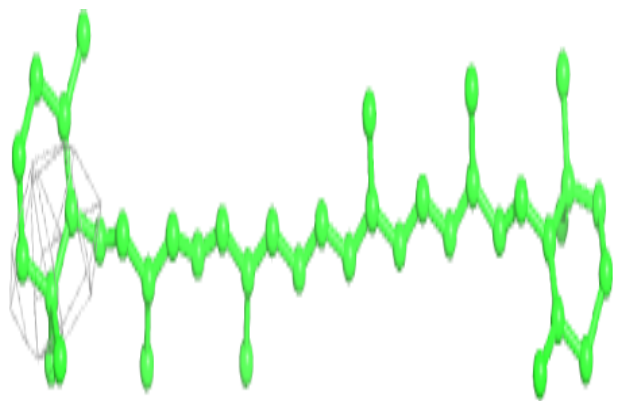
**Electron density around LMT b 627:**

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

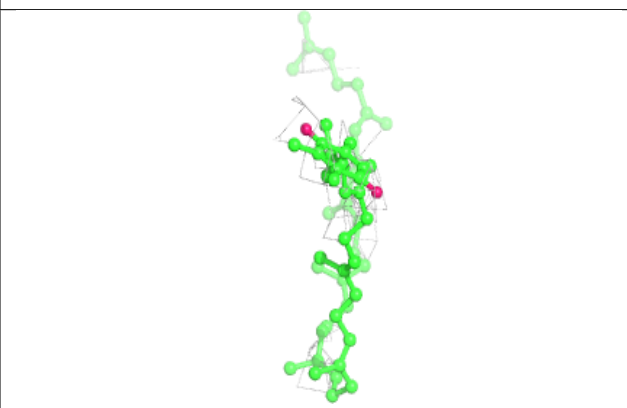
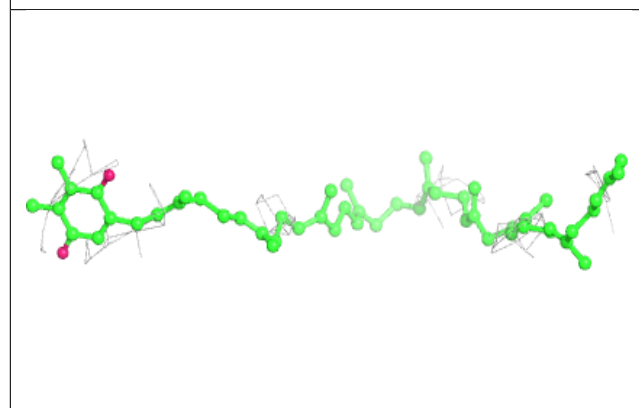
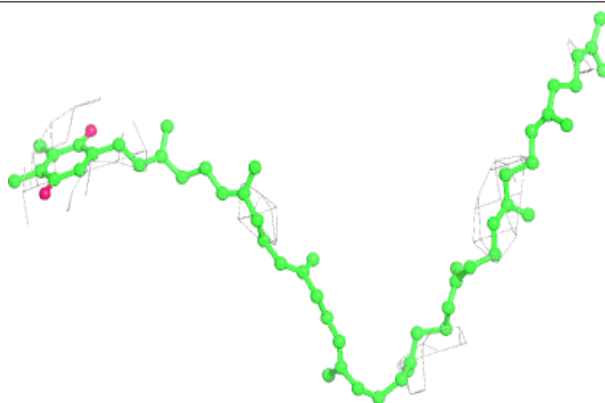


**Electron density around BCR j 102:**

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

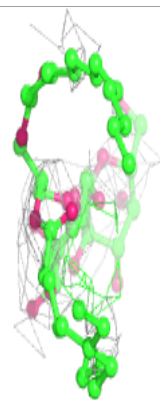
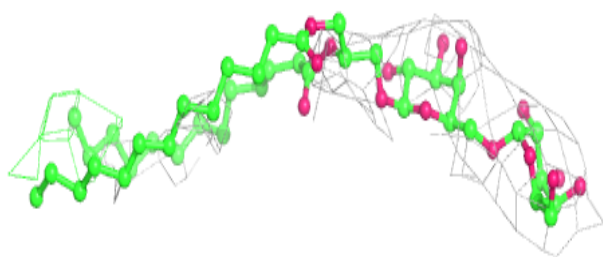
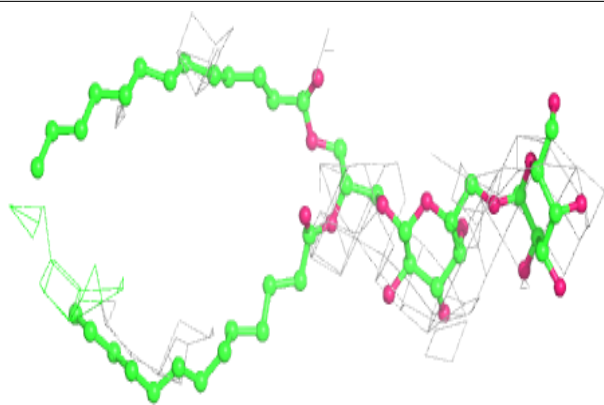
**Electron density around PL9 D 407:**

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

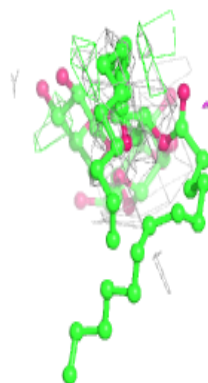
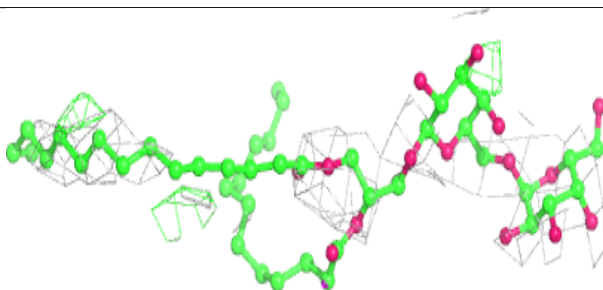
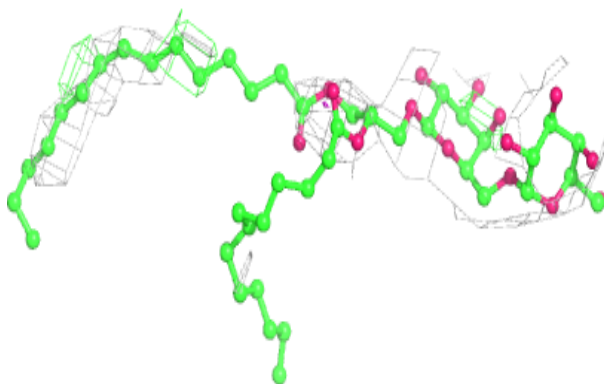


**Electron density around DGD A 408:**

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

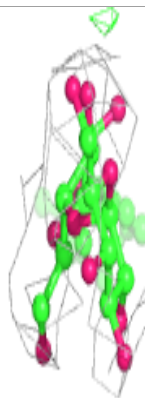
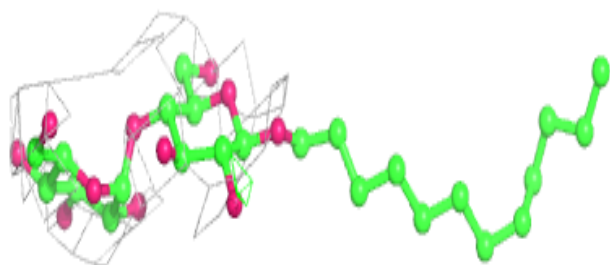
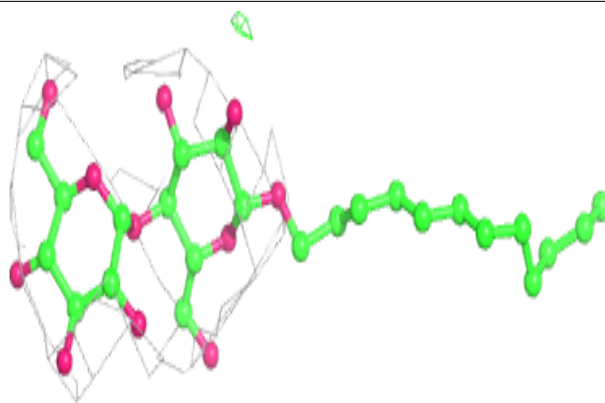
**Electron density around DGD b 624:**

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

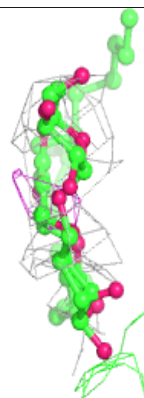
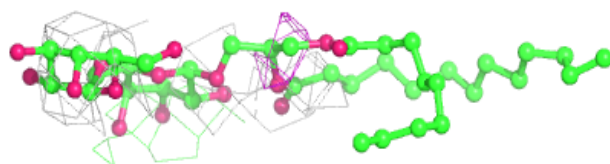
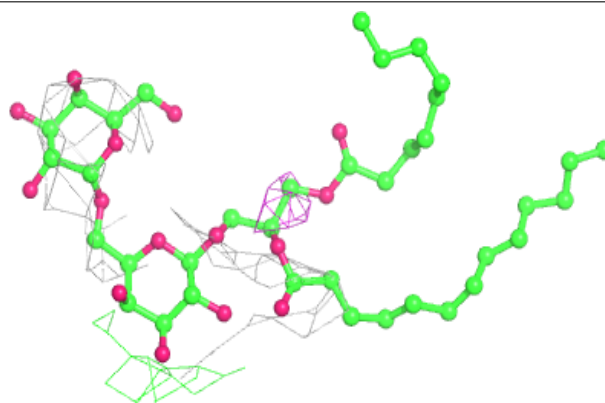


**Electron density around LMT b 604:**

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

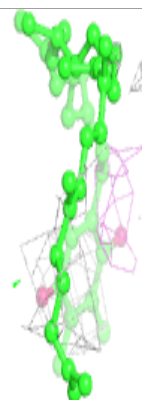
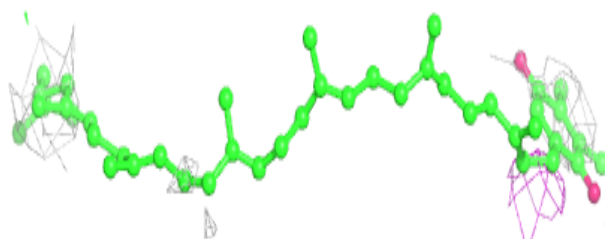
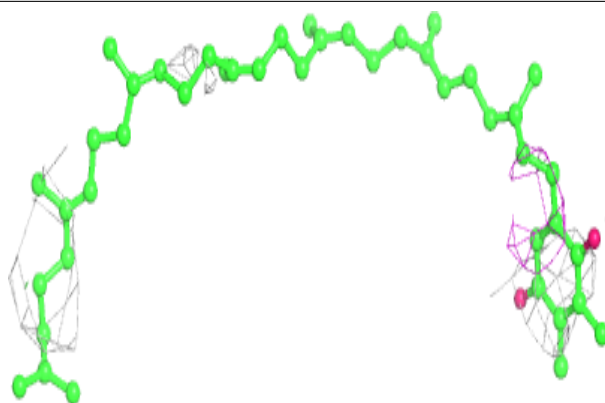
**Electron density around DGD b 601:**

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

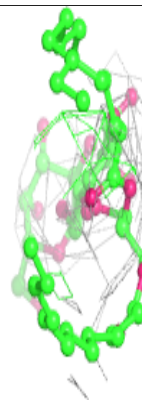
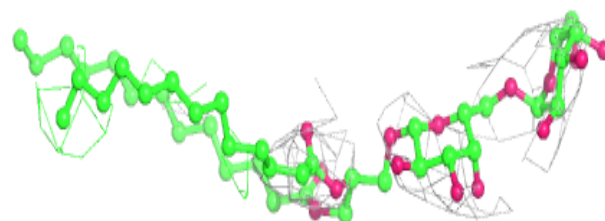
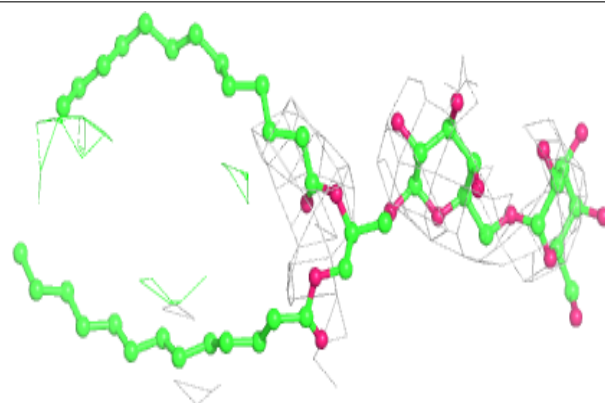


**Electron density around PL9 A 406:**

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

**Electron density around DGD a 410:**

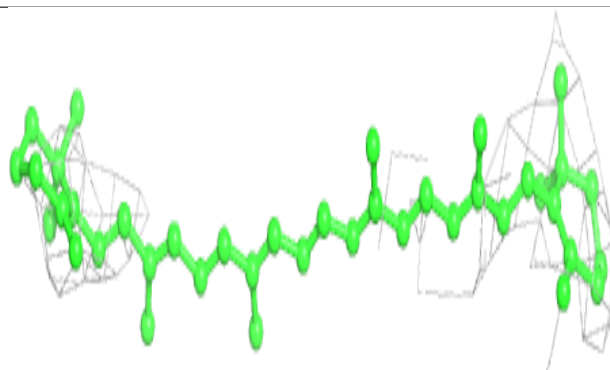
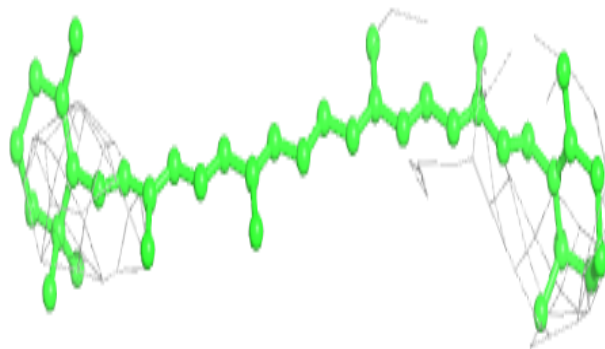
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



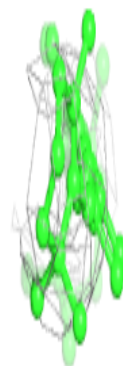
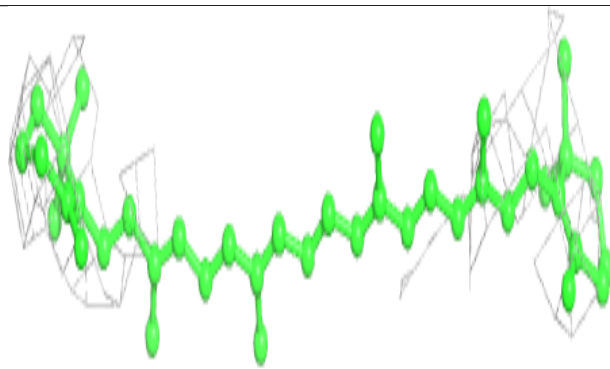
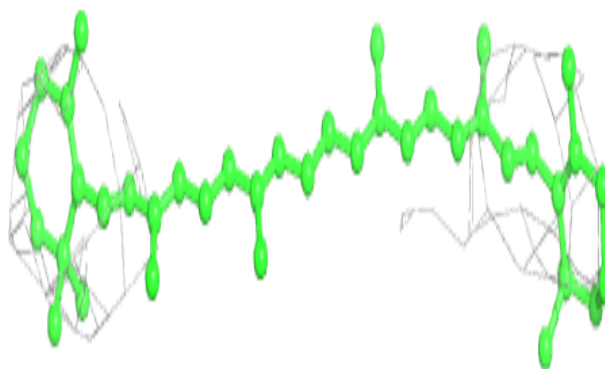


**Electron density around BCR B 619:**

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

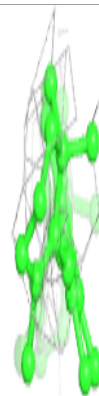
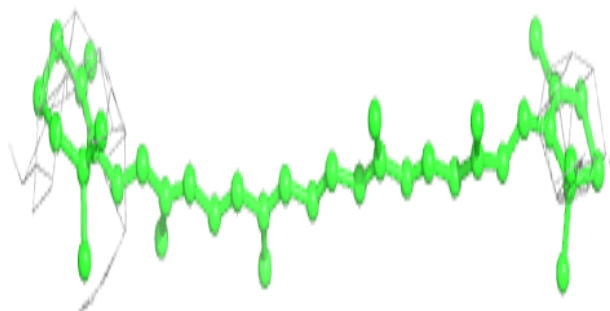
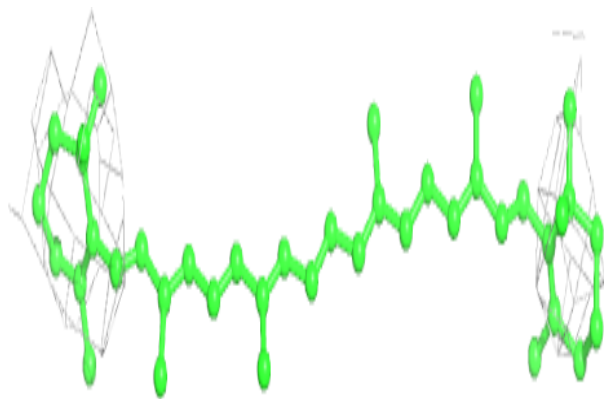
**Electron density around BCR b 623:**

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

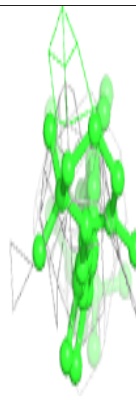
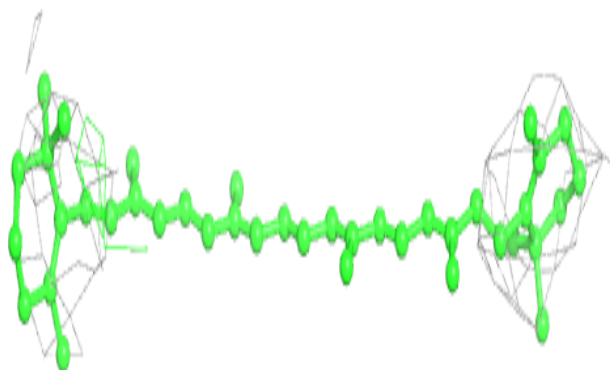
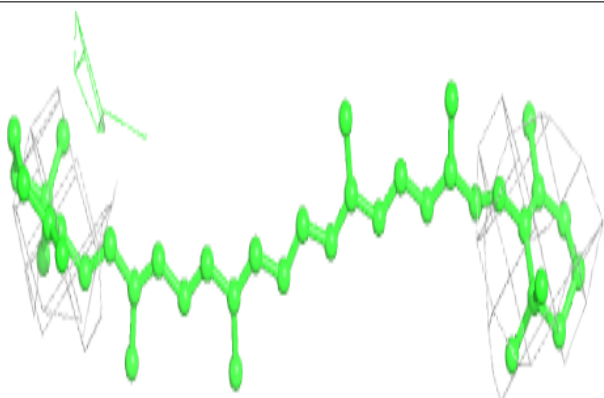


**Electron density around BCR c 514:**

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

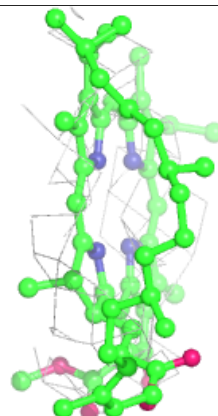
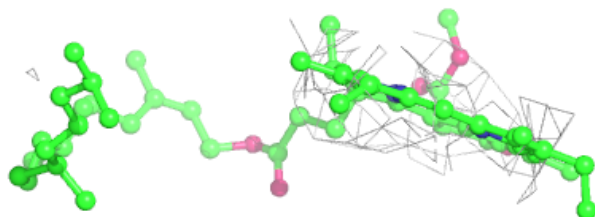
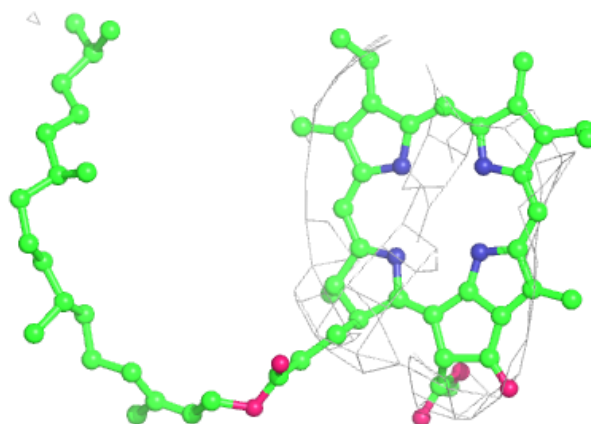
**Electron density around BCR K 102:**

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

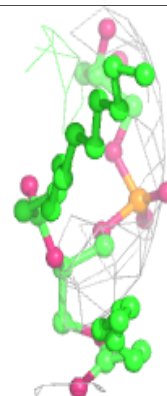
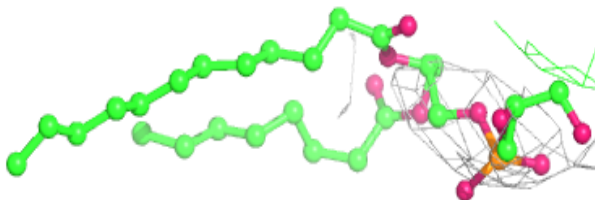
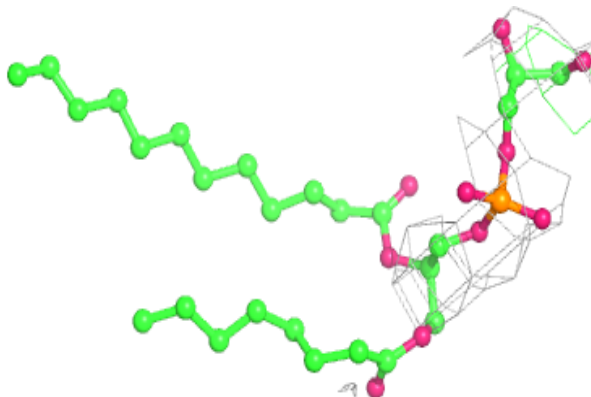


**Electron density around PHO d 401:**

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

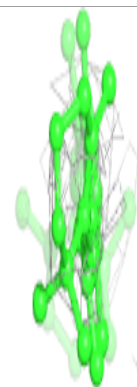
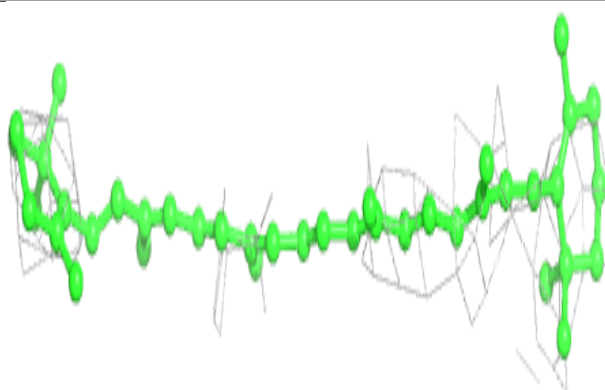
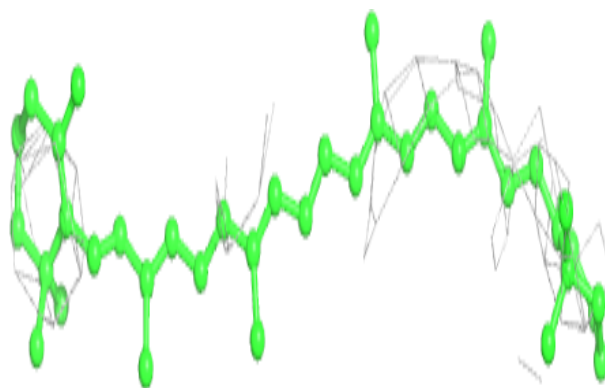
**Electron density around LHG c 519:**

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

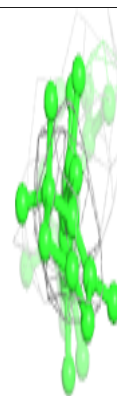
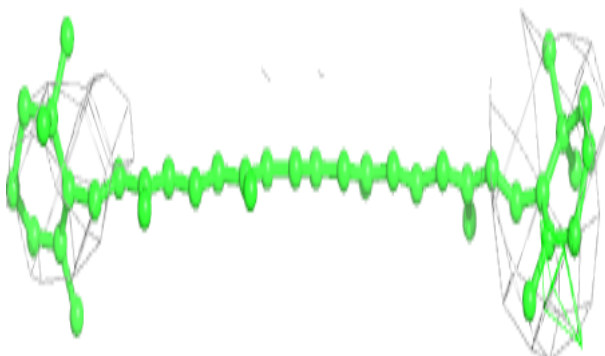
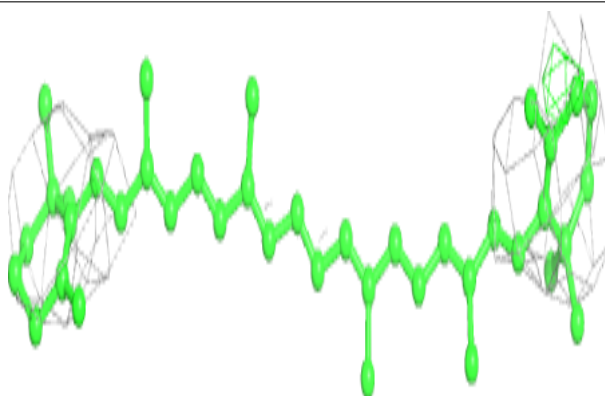


**Electron density around BCR x 101:**

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

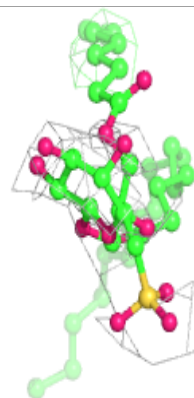
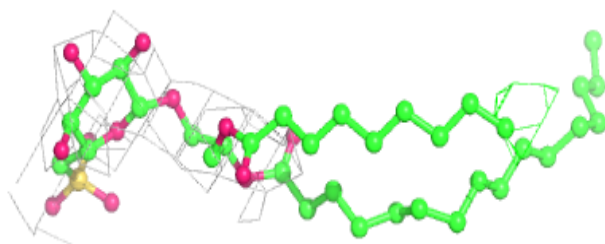
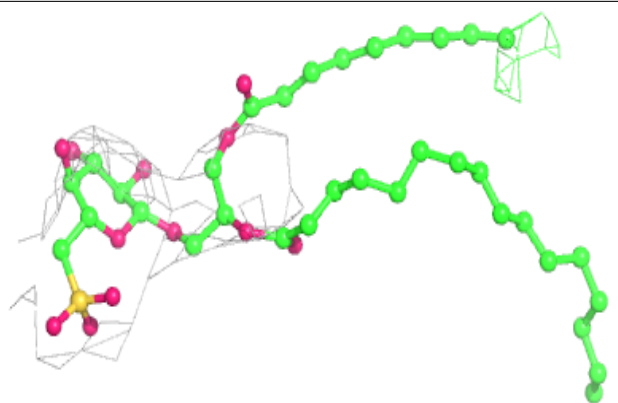
**Electron density around BCR b 622:**

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

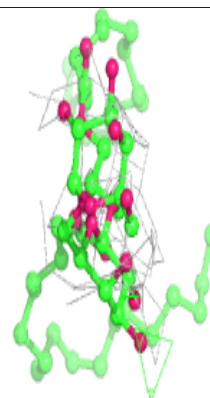
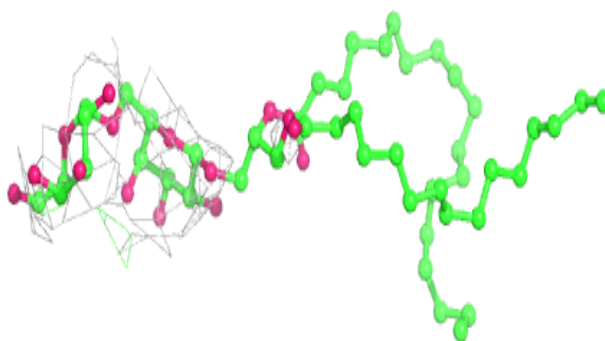
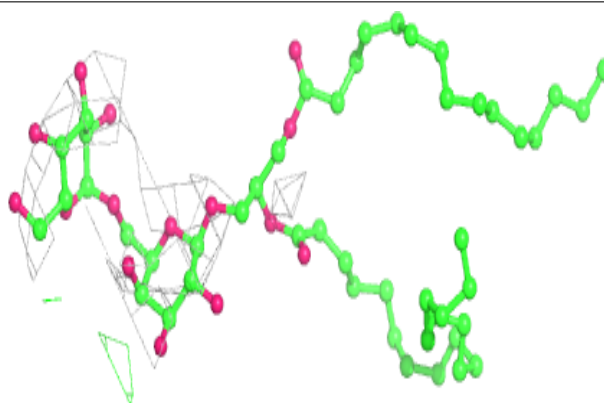


**Electron density around SQD B 626:**

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

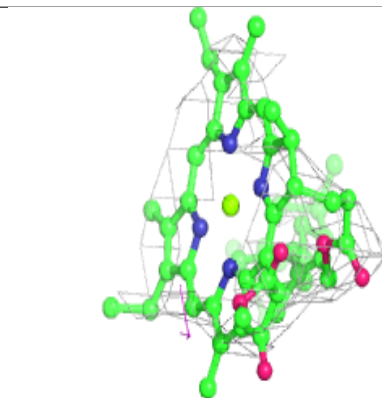
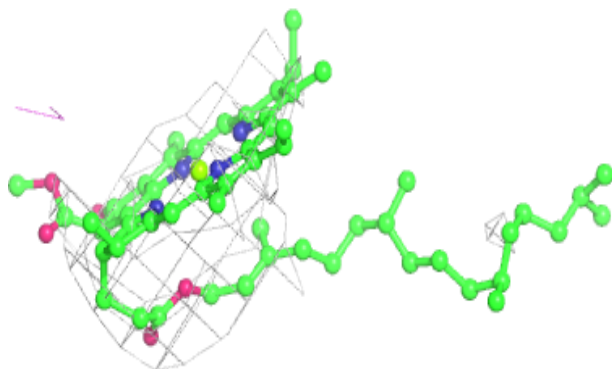
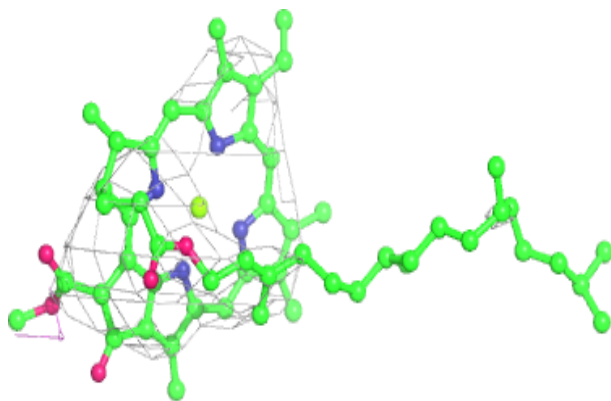
**Electron density around DGD D 410:**

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

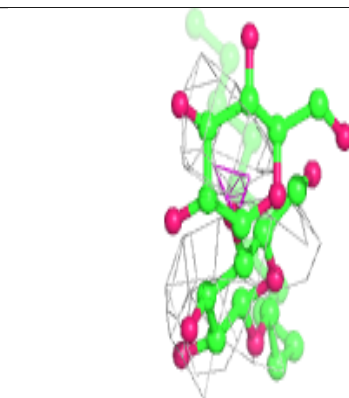
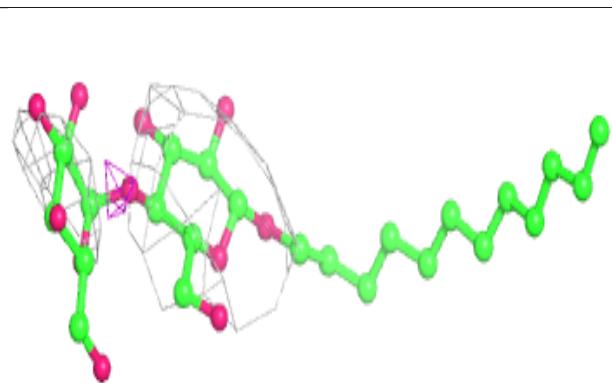
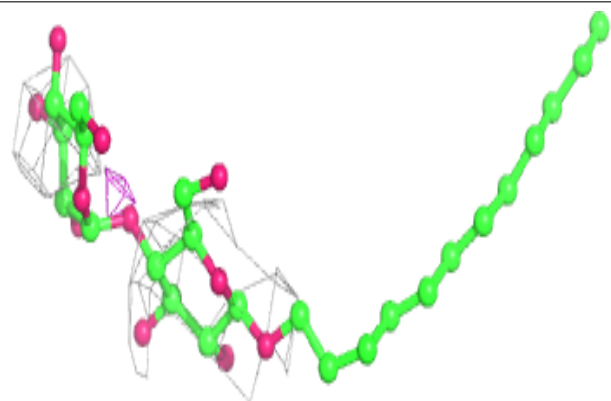


**Electron density around CLA B 613:**

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

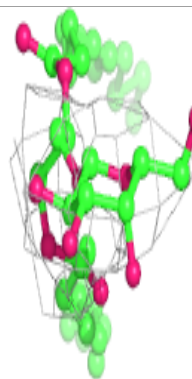
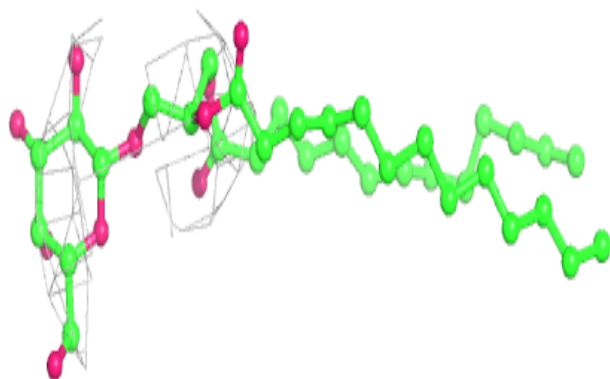
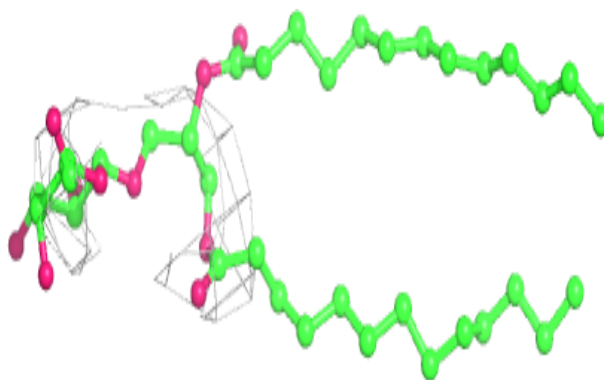
**Electron density around LMT M 102:**

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

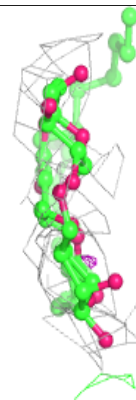
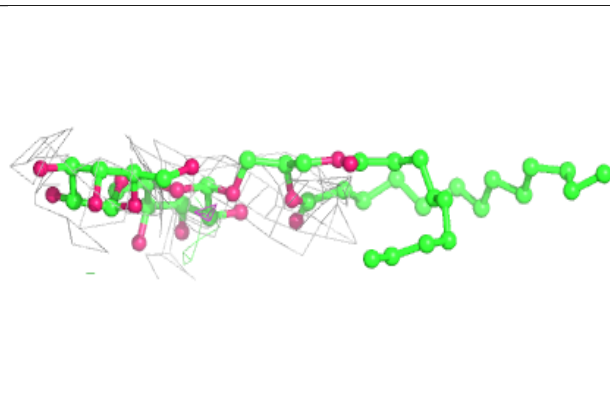
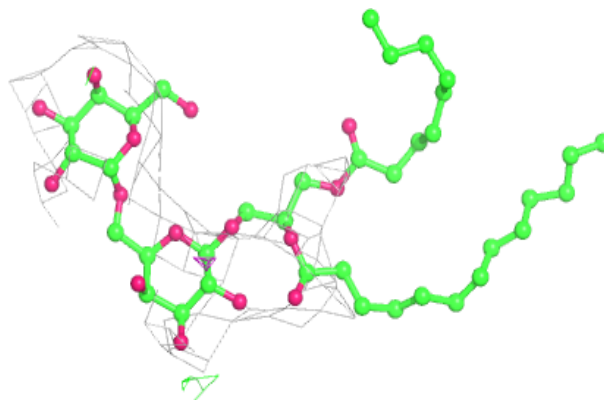


**Electron density around LMG c 518:**

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

**Electron density around DGD B 625:**

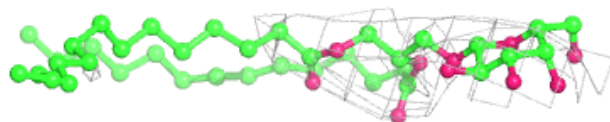
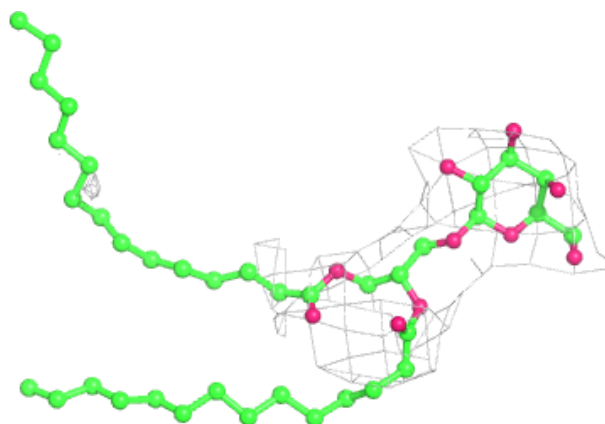
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



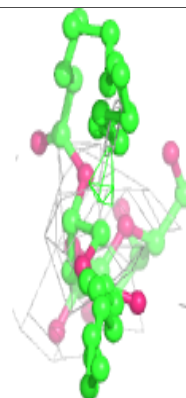
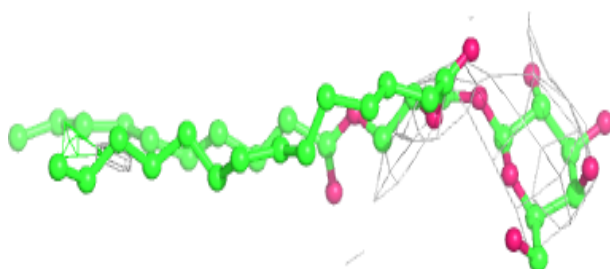
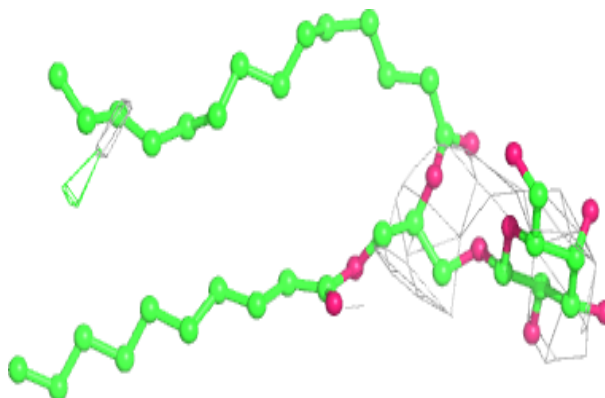


**Electron density around LMG C 521:**

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

**Electron density around LMG i 101:**

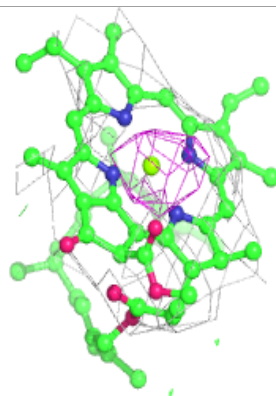
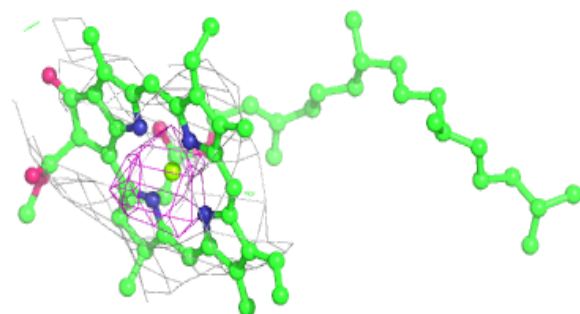
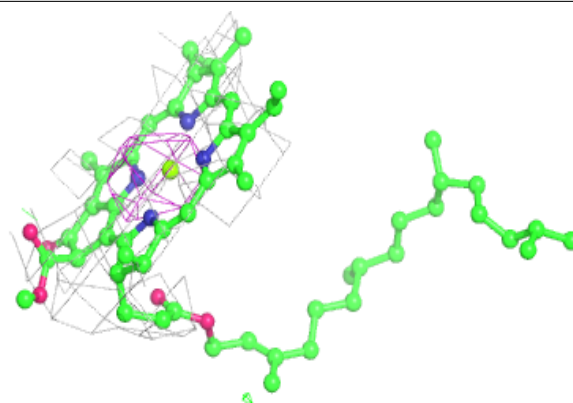
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



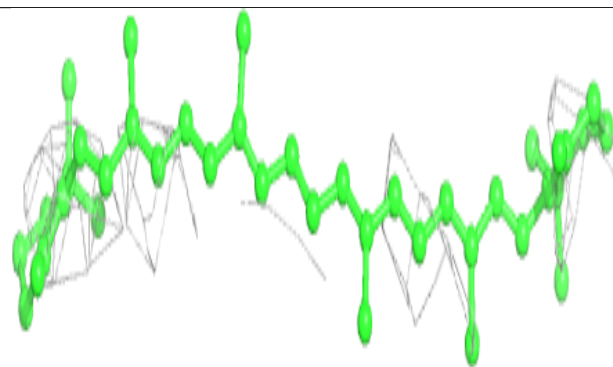
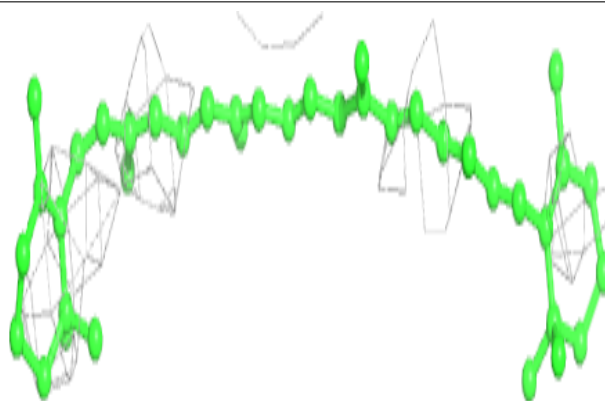


**Electron density around CLA c 512:**

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

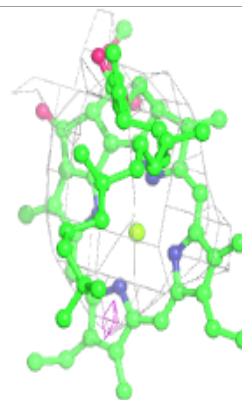
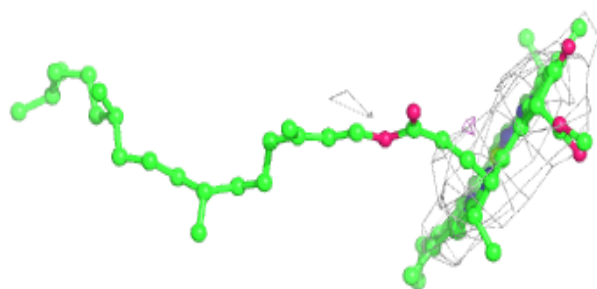
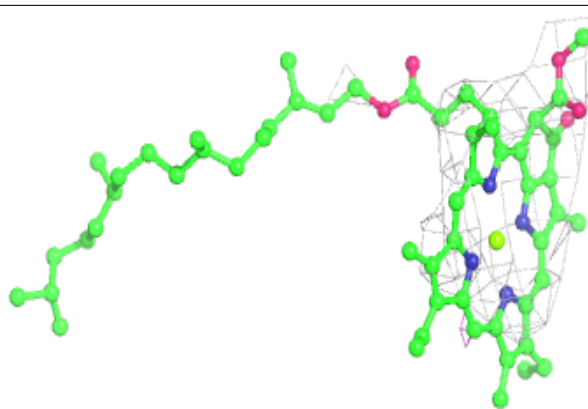
**Electron density around BCR c 513:**

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



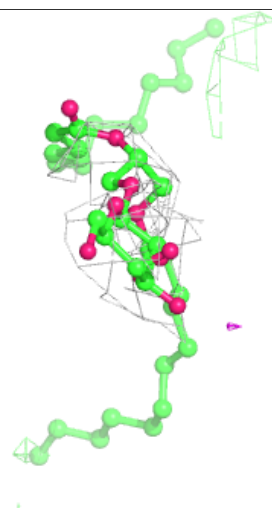
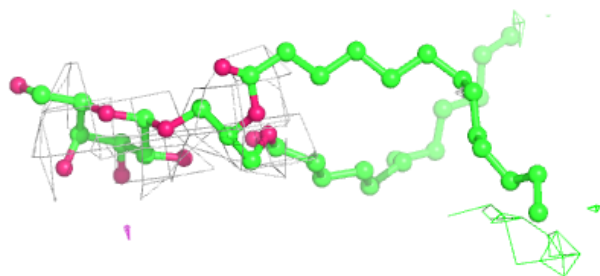
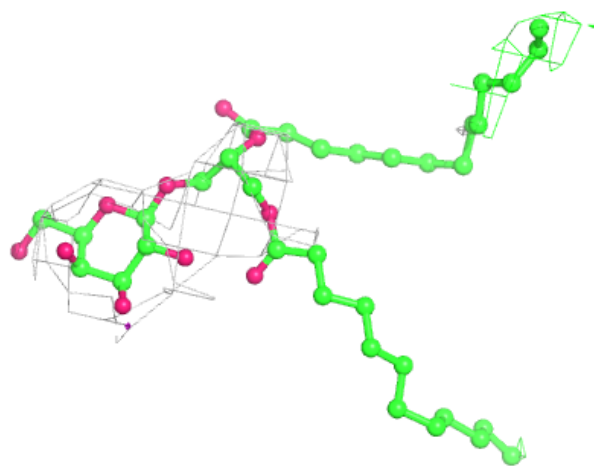
**Electron density around CLA a 407:**

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



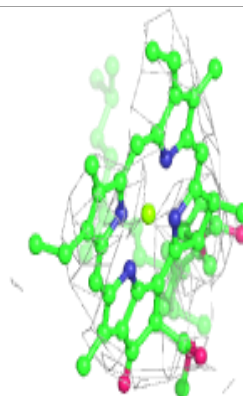
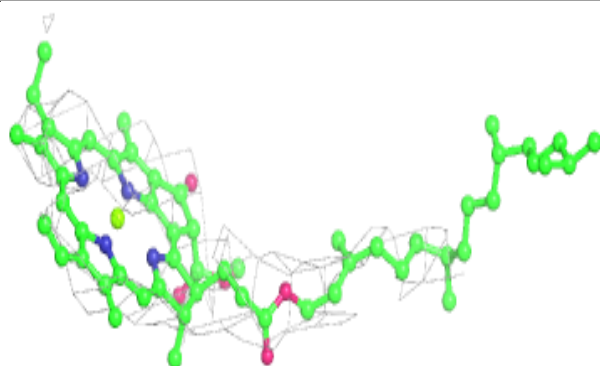
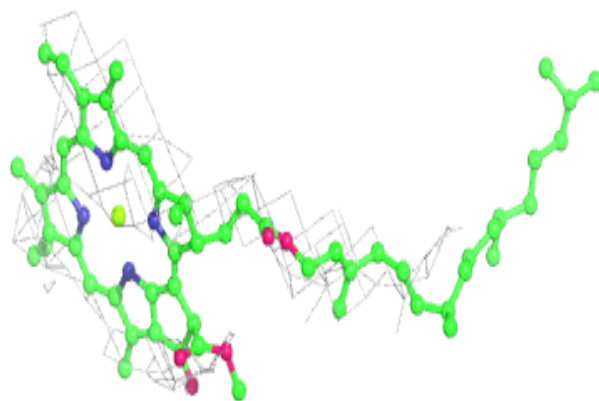
**Electron density around LMG e 101:**

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

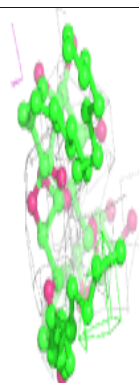
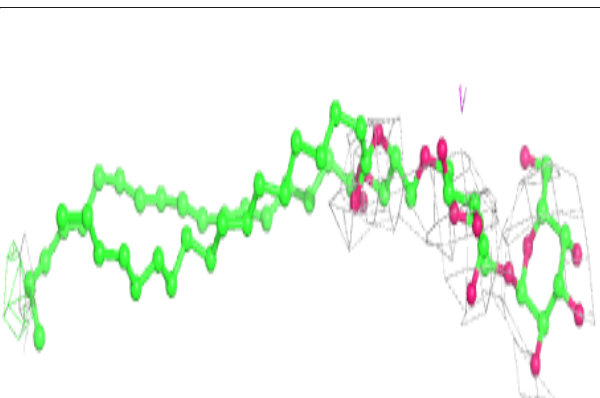
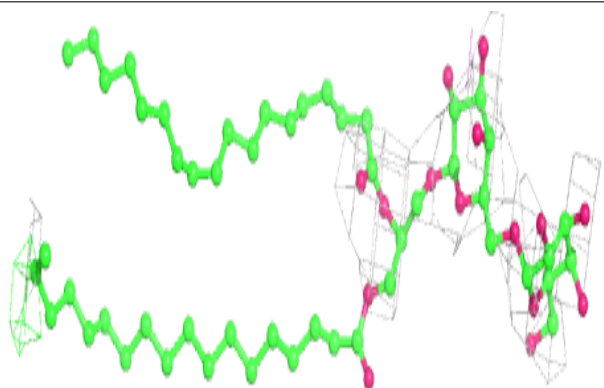


**Electron density around CLA a 404:**

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

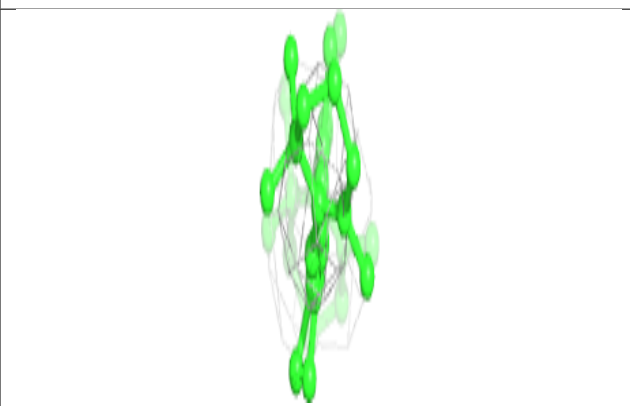
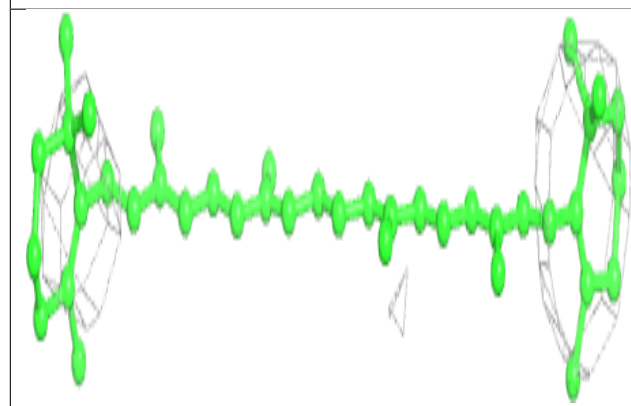
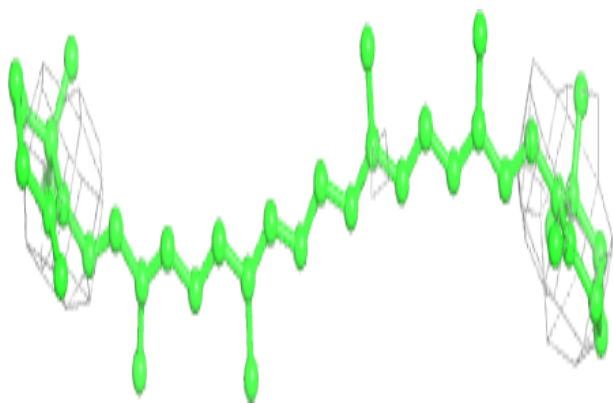
**Electron density around DGD C 517:**

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

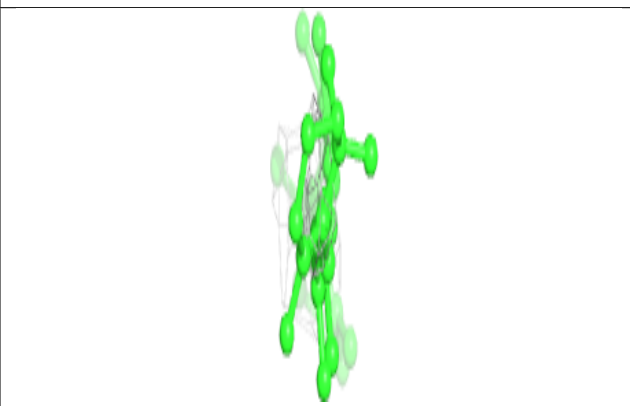
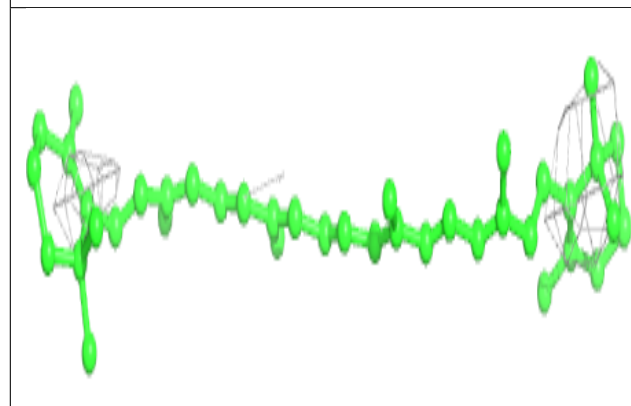
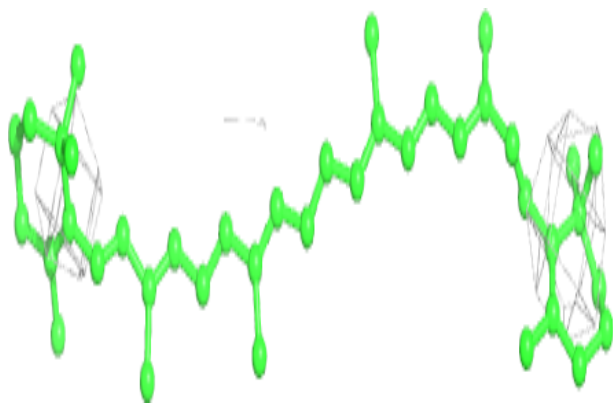


**Electron density around BCR A 407:**

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

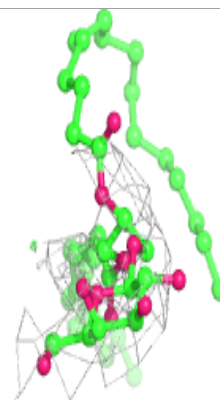
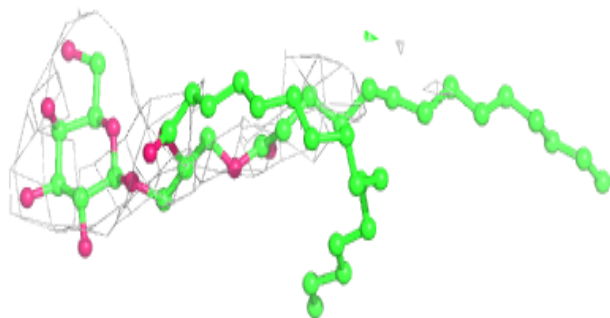
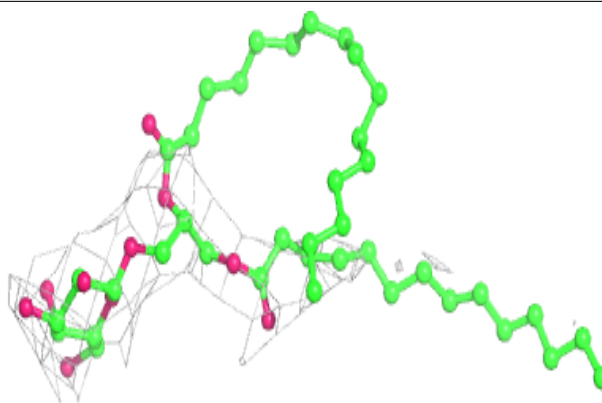
**Electron density around BCR y 101:**

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



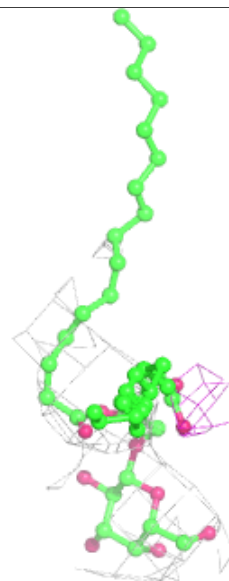
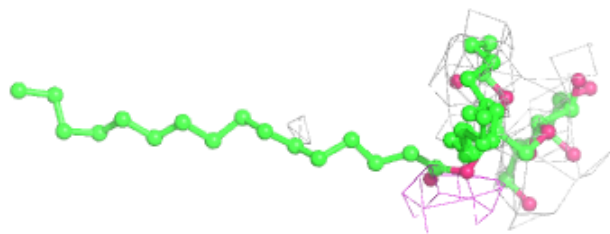
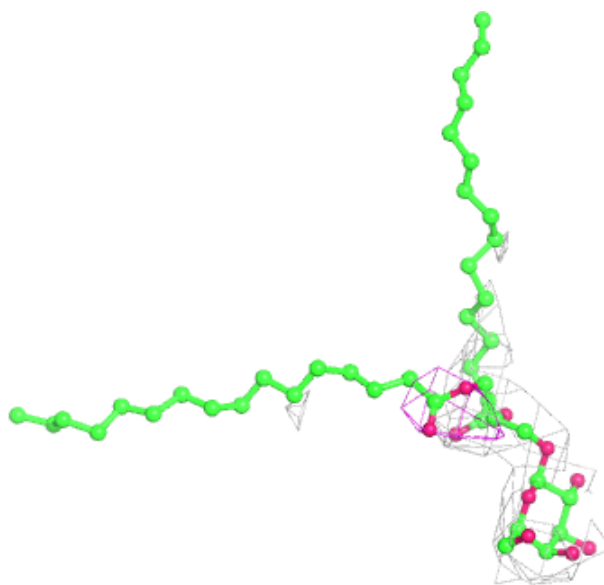
**Electron density around LMG D 408:**

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



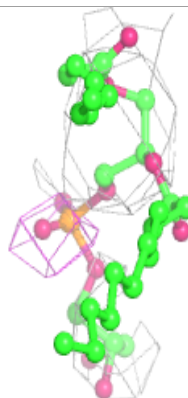
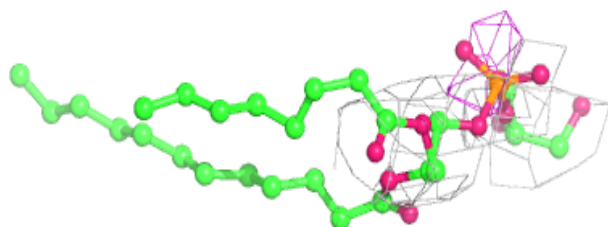
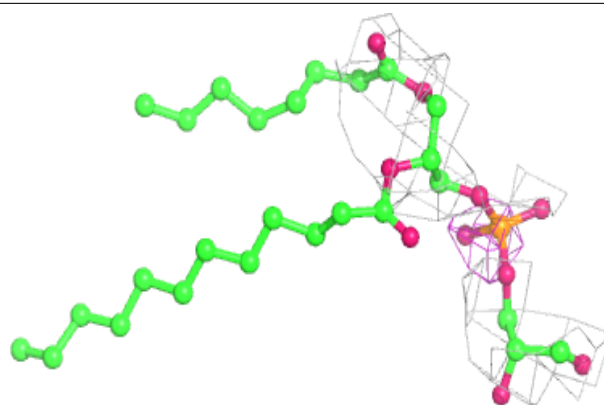
**Electron density around LMG a 412:**

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

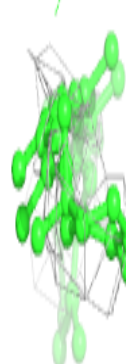
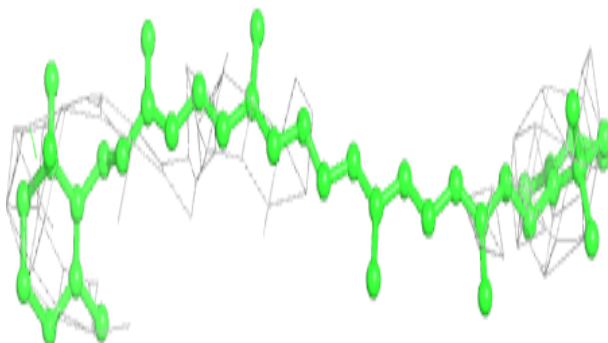
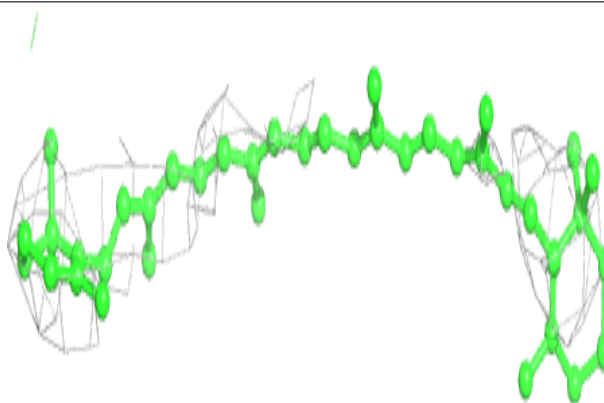


**Electron density around LHG C 519:**

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

**Electron density around BCR f 102:**

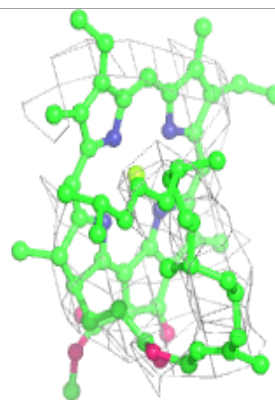
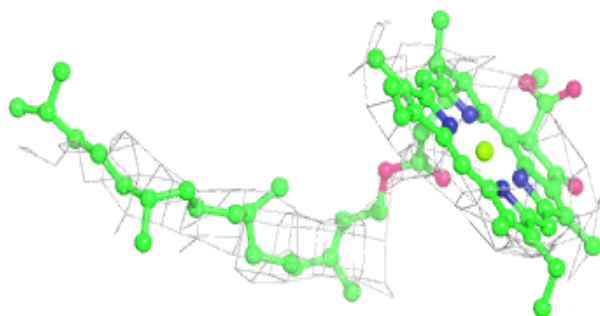
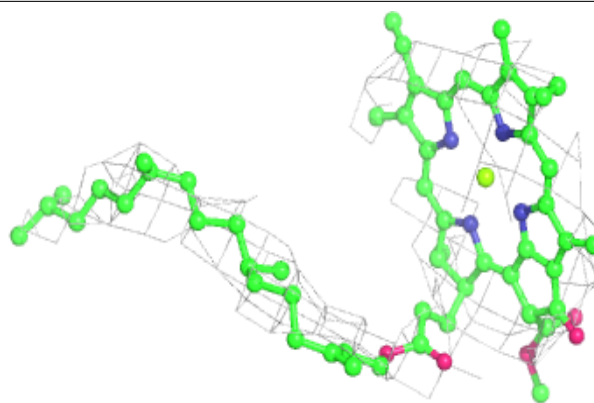
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





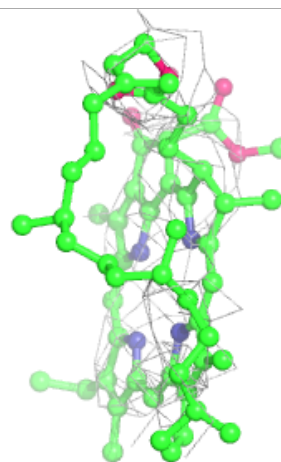
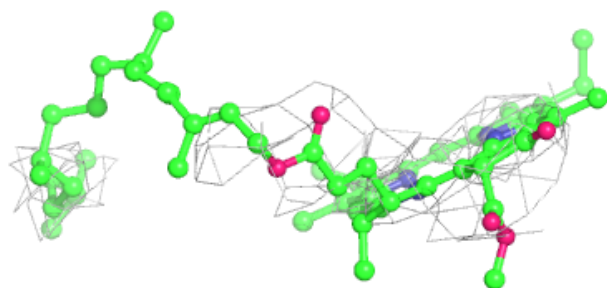
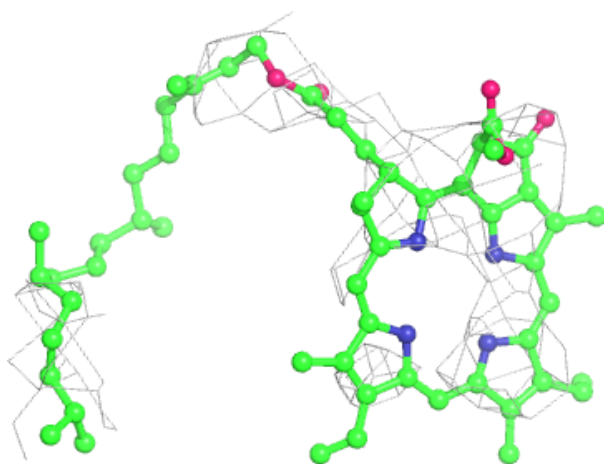
**Electron density around CLA C 510:**

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



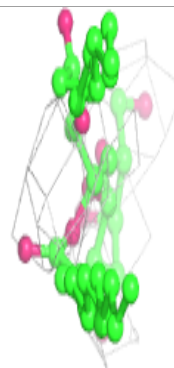
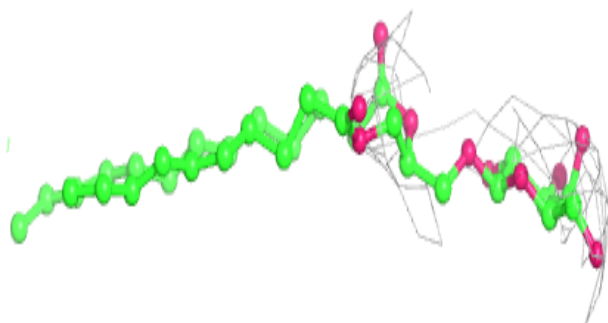
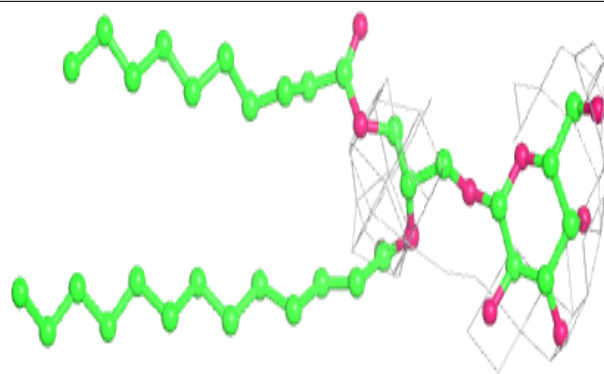
**Electron density around PHO D 402:**

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

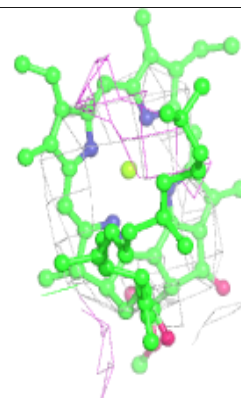
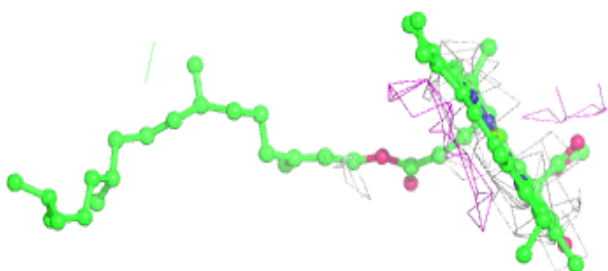
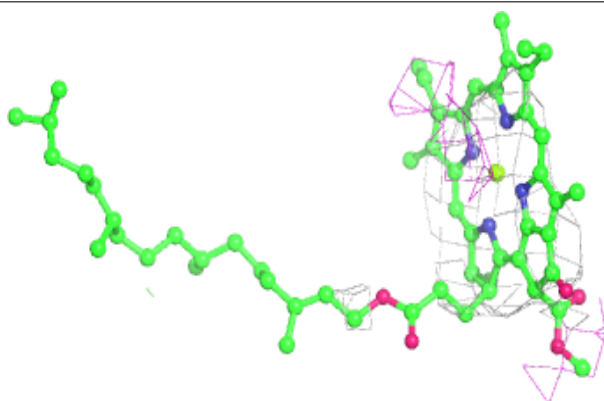


**Electron density around LMG m 101:**

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

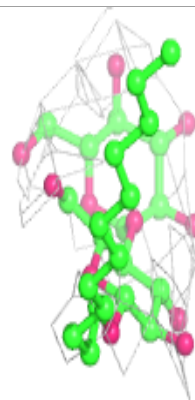
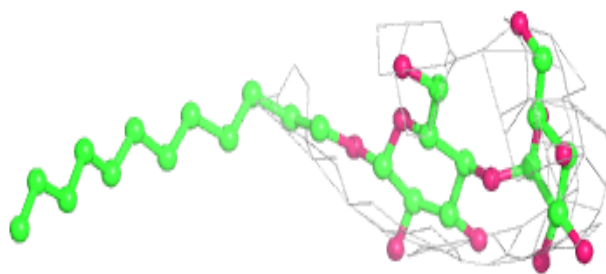
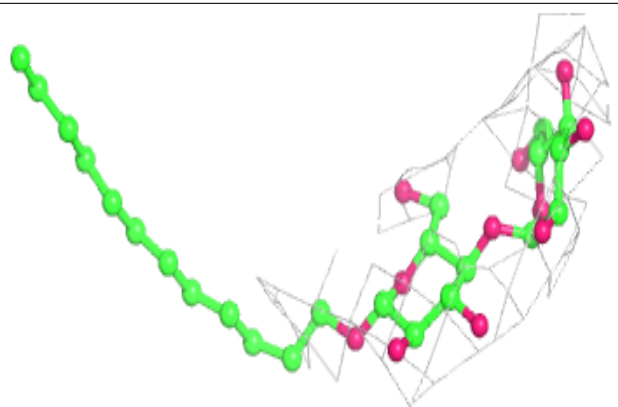
**Electron density around CLA A 405:**

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

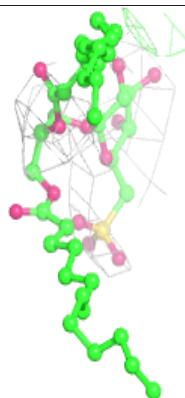
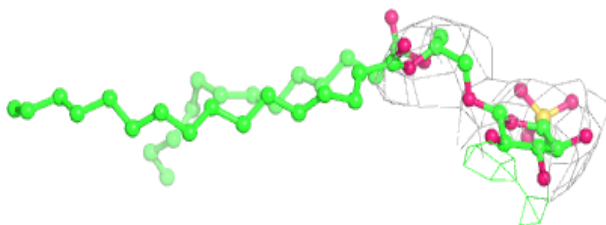
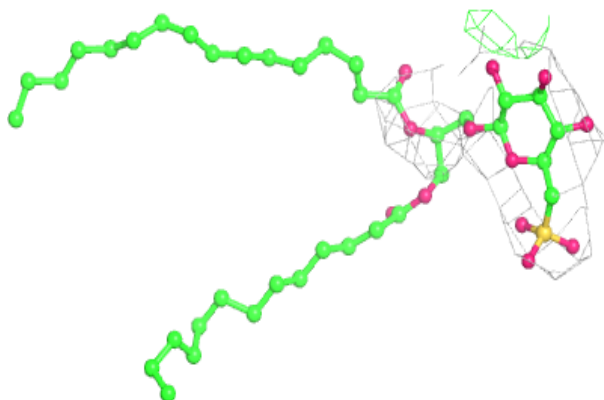


**Electron density around LMT M 103:**

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

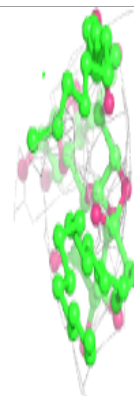
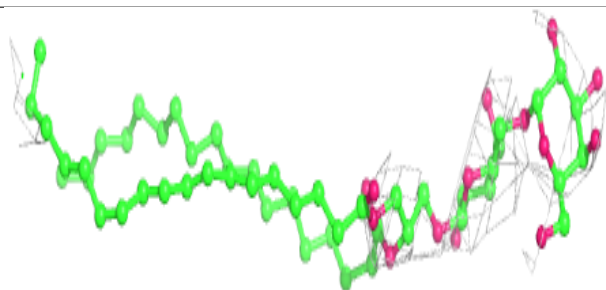
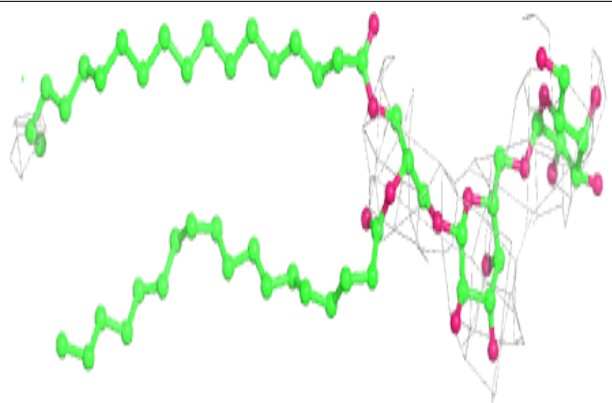
**Electron density around SQD a 415:**

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

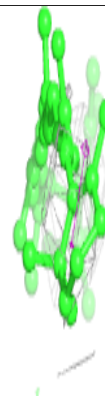
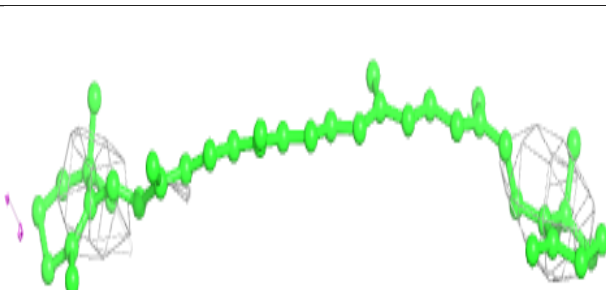
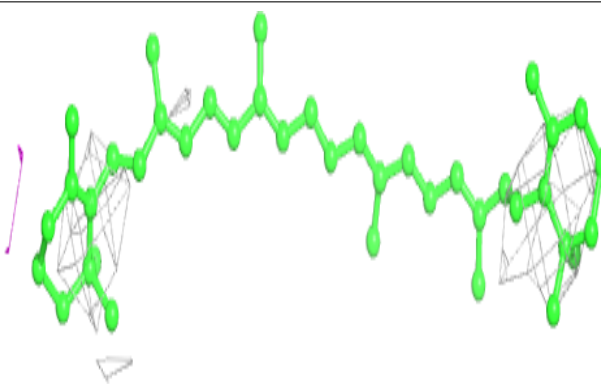


**Electron density around DGD c 517:**

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

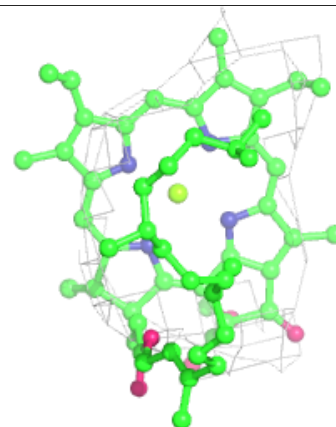
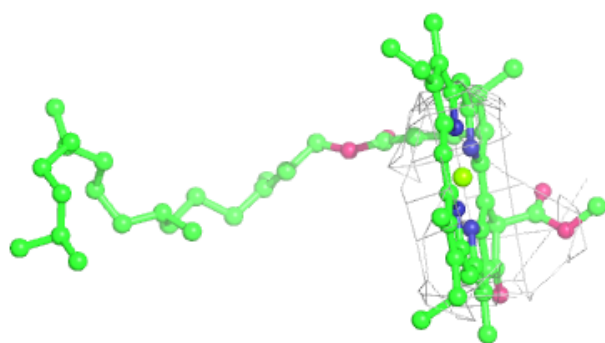
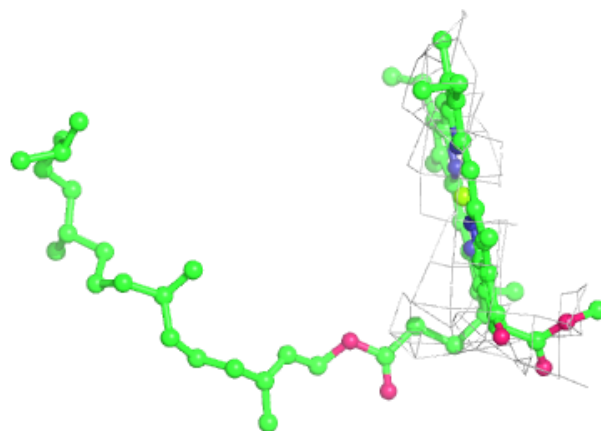
**Electron density around BCR b 621:**

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

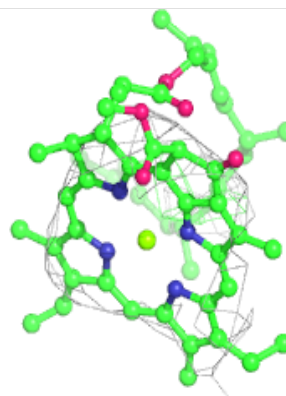
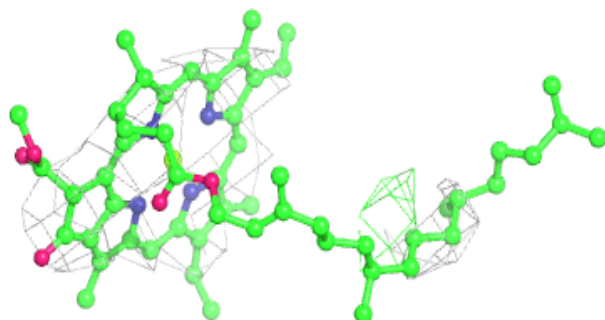
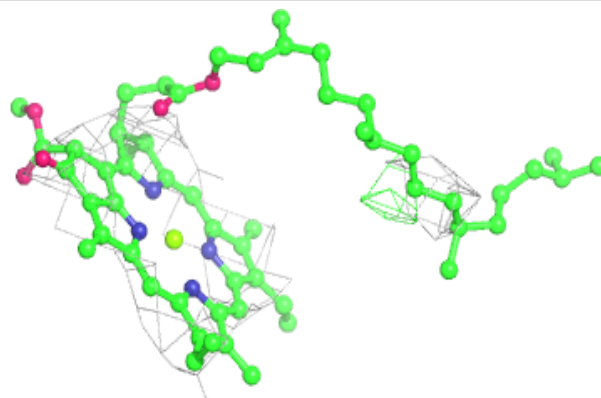


**Electron density around CLA c 505:**

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

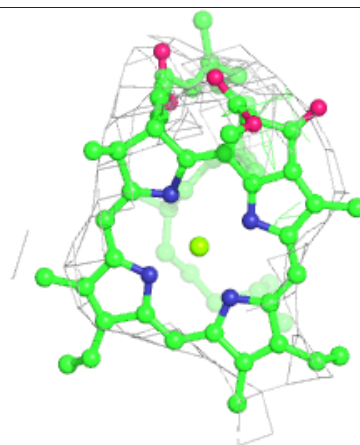
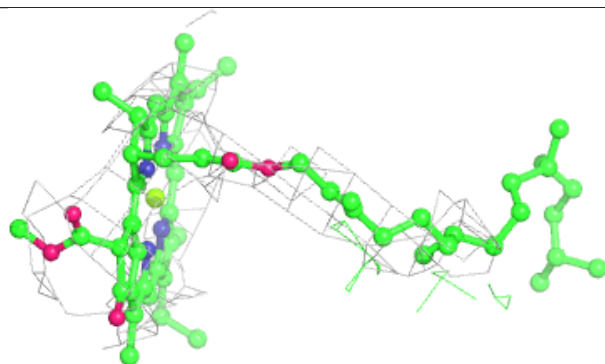
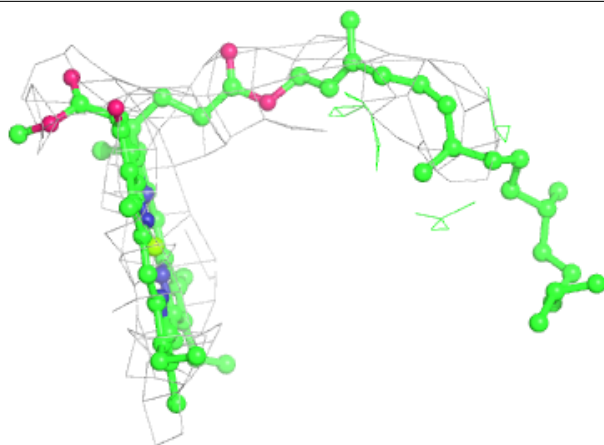
**Electron density around CLA C 512:**

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

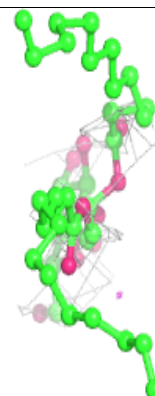
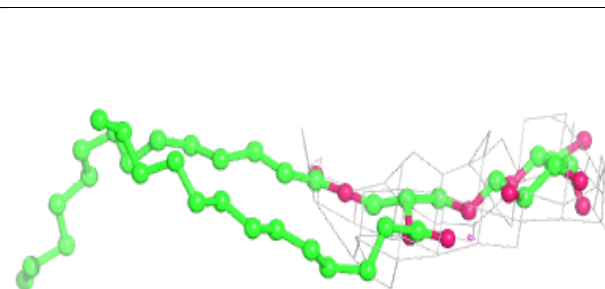
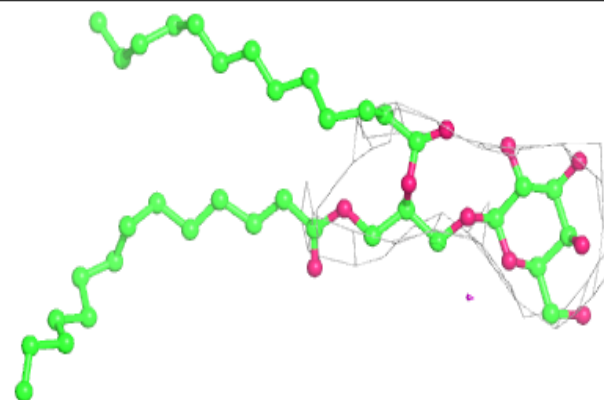


**Electron density around CLA C 505:**

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

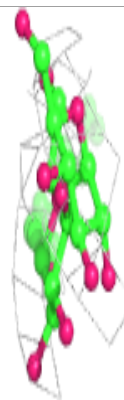
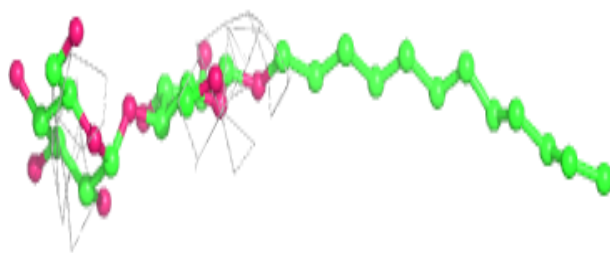
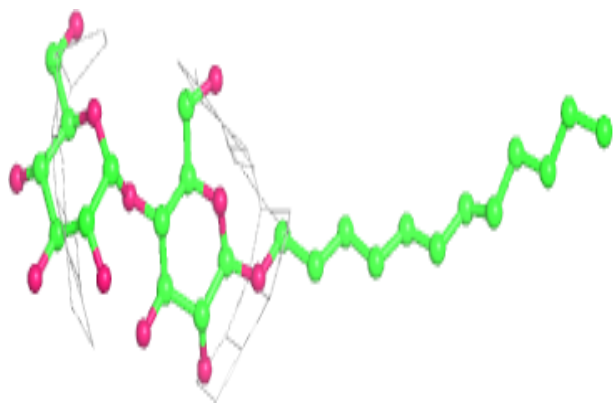
**Electron density around LMG D 412:**

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

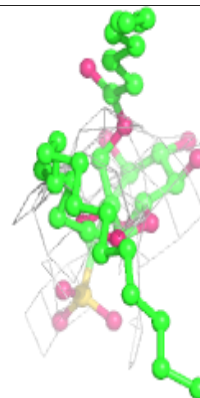
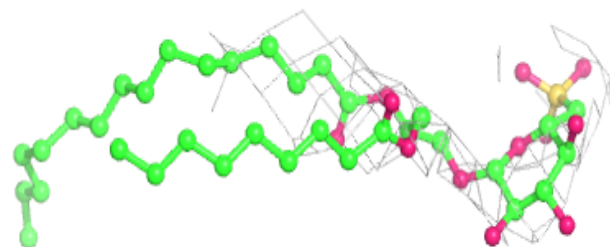
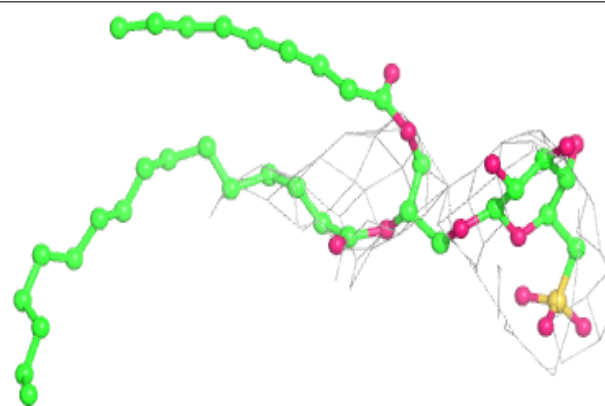


**Electron density around LMT B 624:**

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

**Electron density around SQD b 602:**

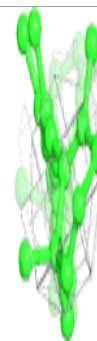
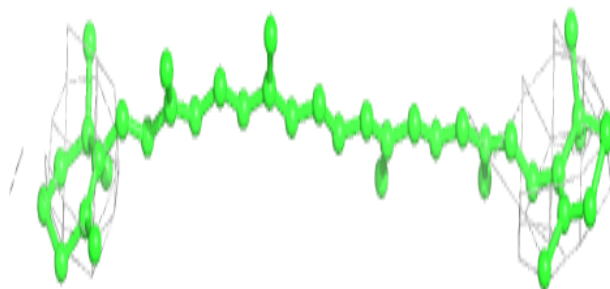
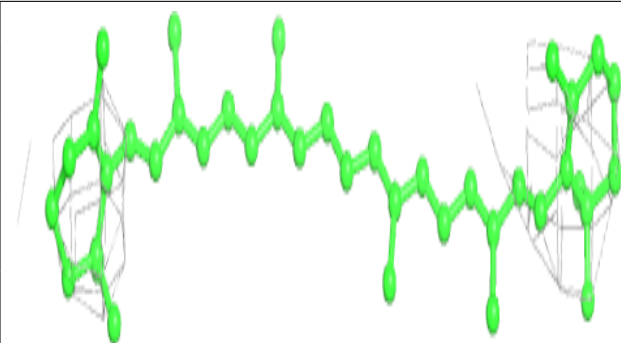
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



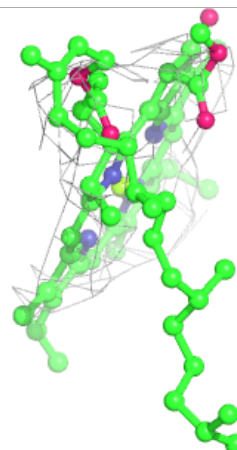
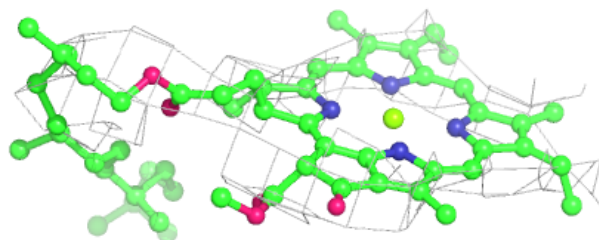
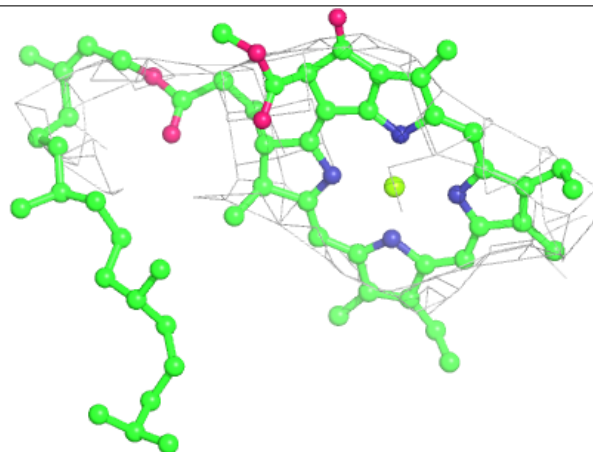


**Electron density around BCR C 514:**

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

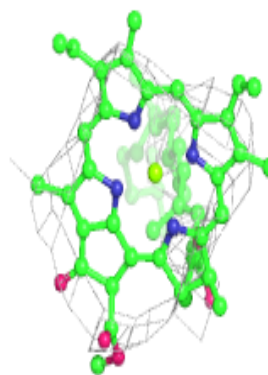
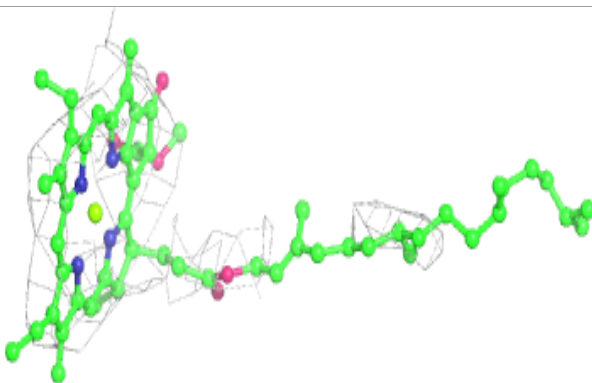
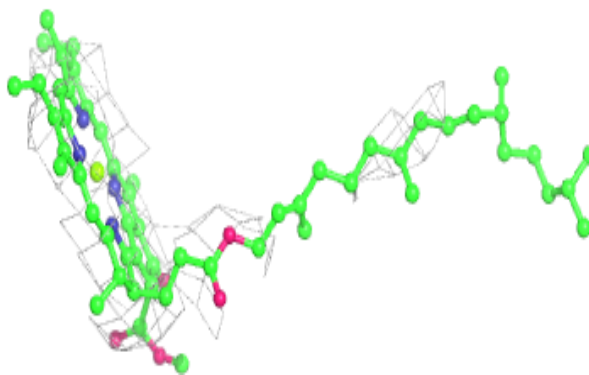
**Electron density around CLA B 615:**

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



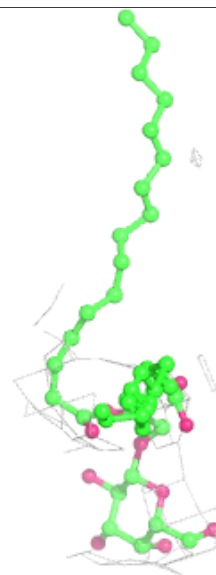
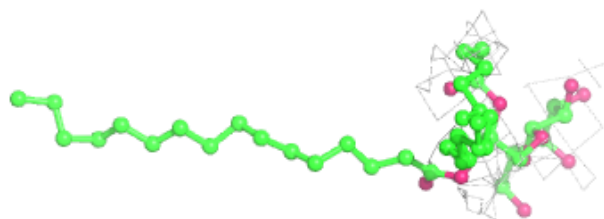
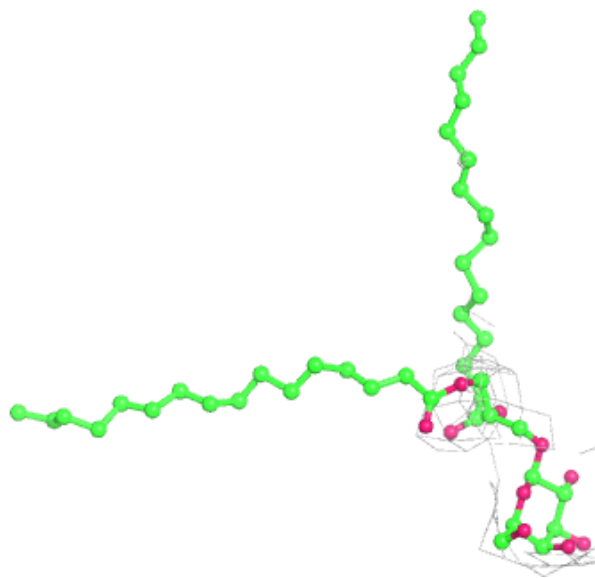
**Electron density around CLA B 603:**

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



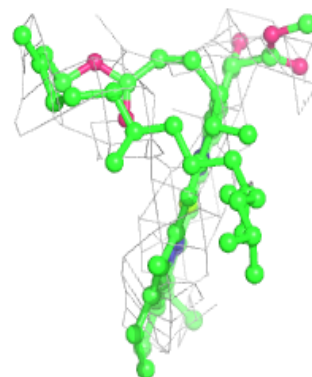
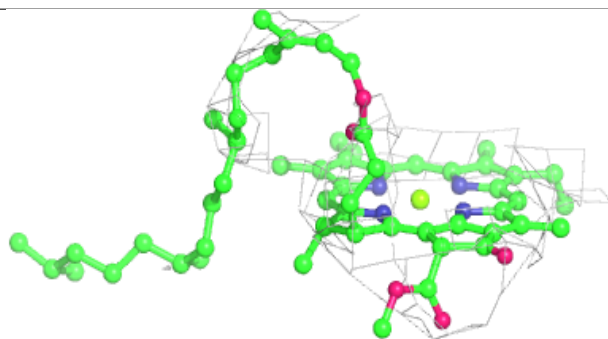
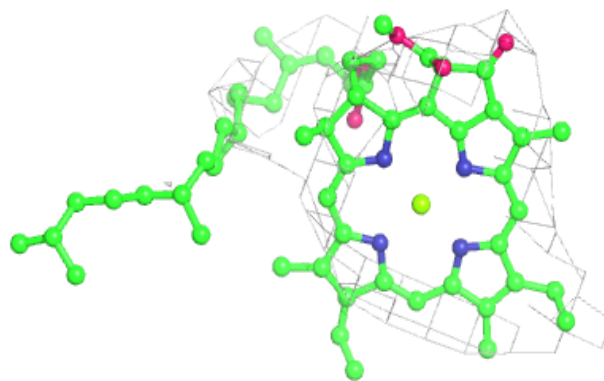
**Electron density around LMG A 410:**

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

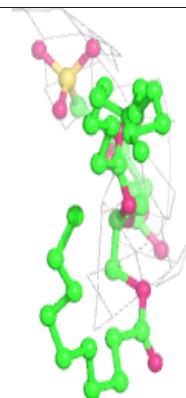
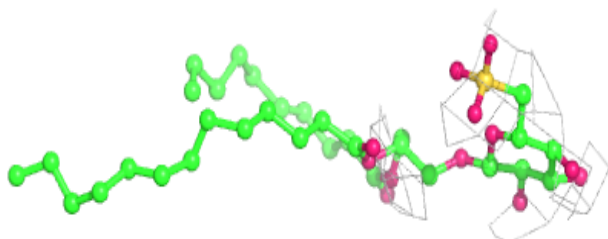
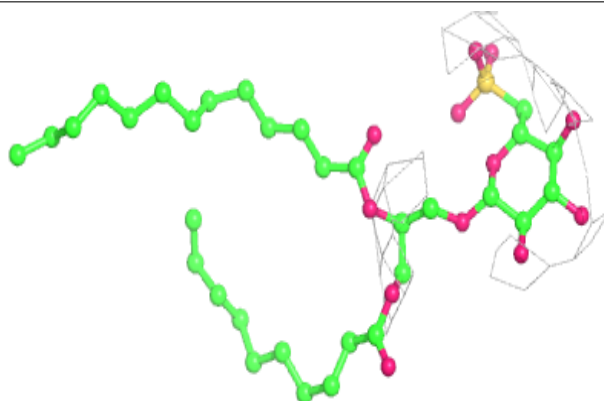


**Electron density around CLA a 405:**

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

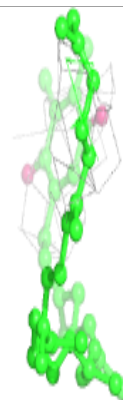
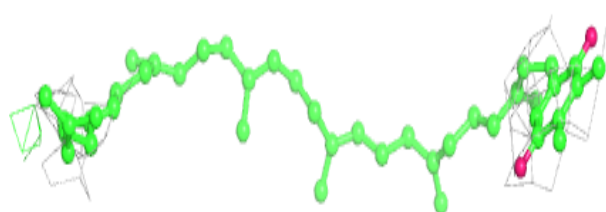
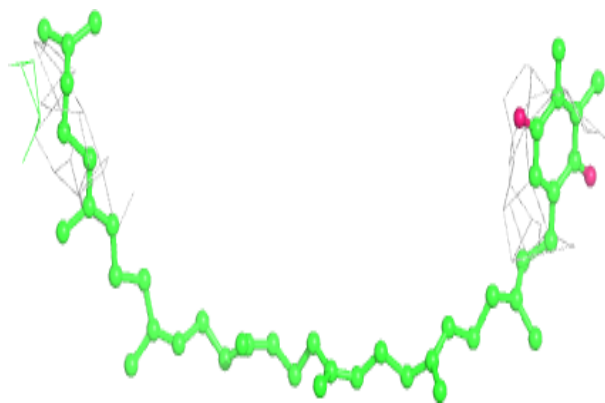
**Electron density around SQD F 103:**

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

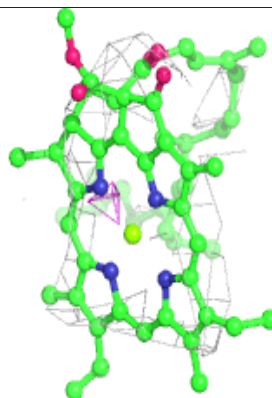
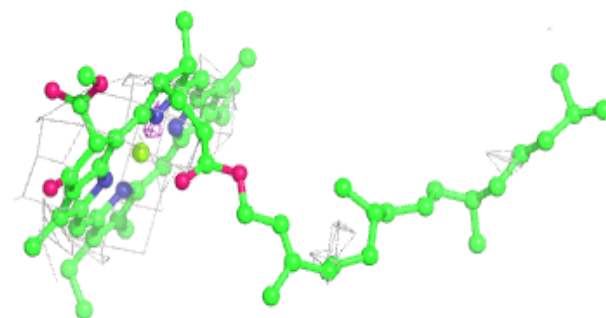
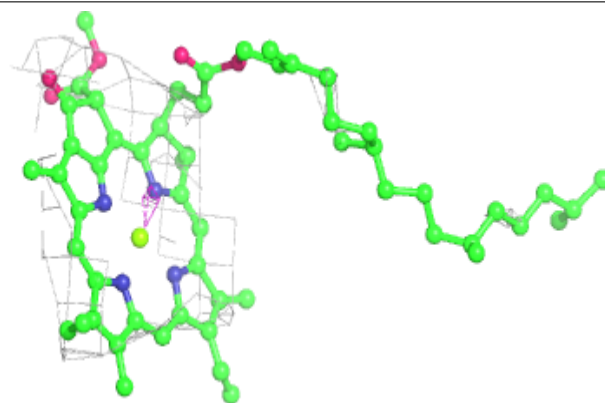


**Electron density around PL9 a 408:**

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

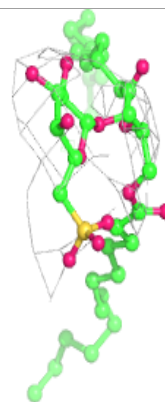
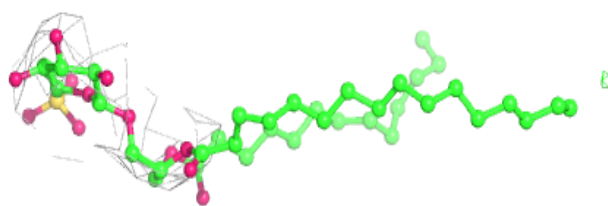
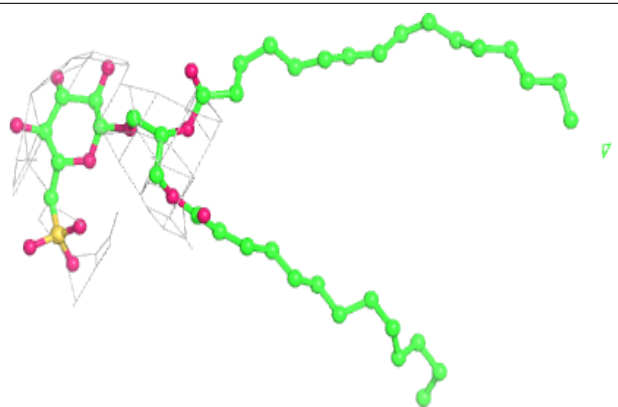
**Electron density around CLA c 510:**

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

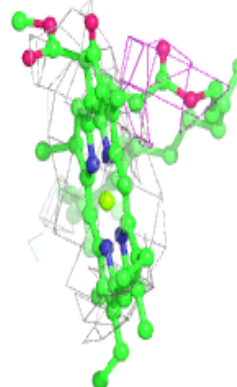
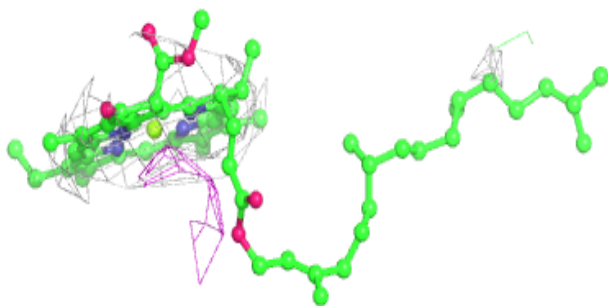
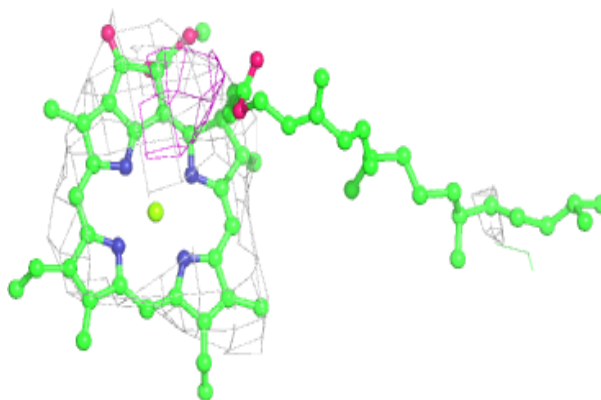


**Electron density around SQD A 412:**

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

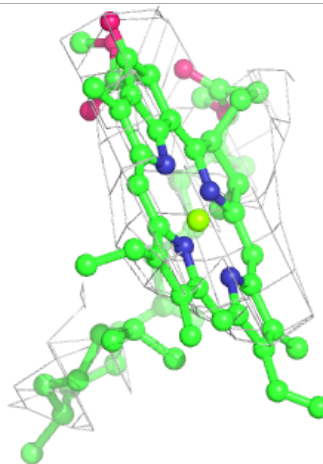
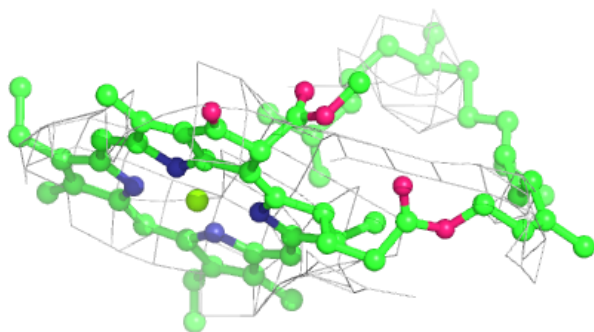
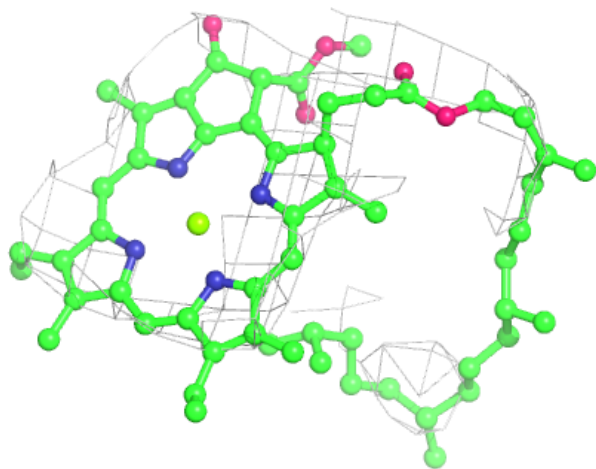
**Electron density around CLA A 404:**

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



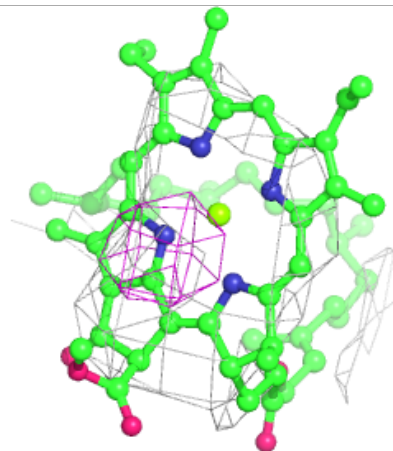
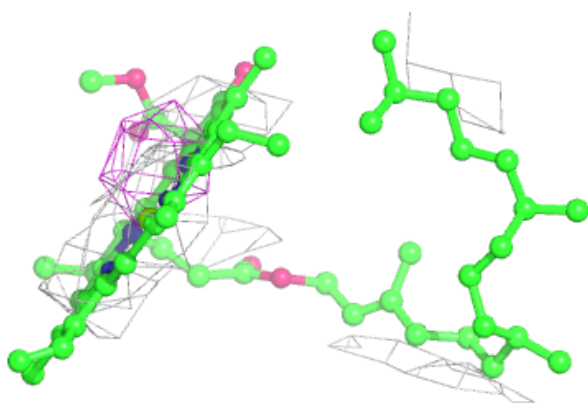
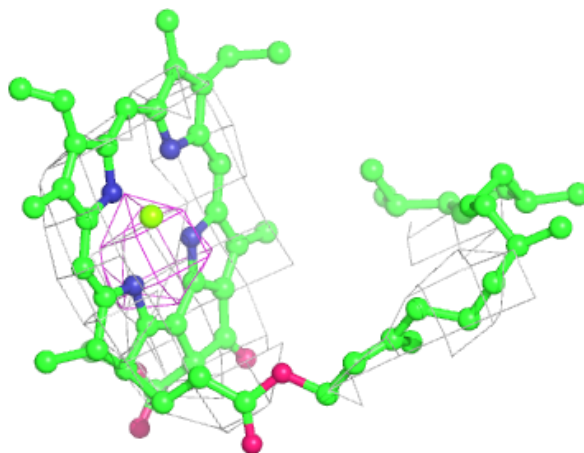
**Electron density around CLA b 618:**

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



**Electron density around CLA c 503:**

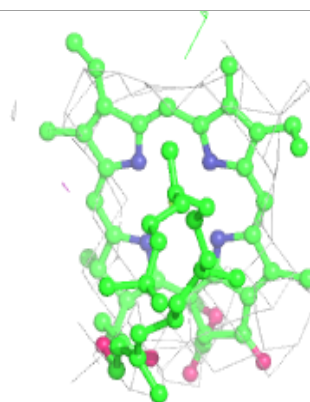
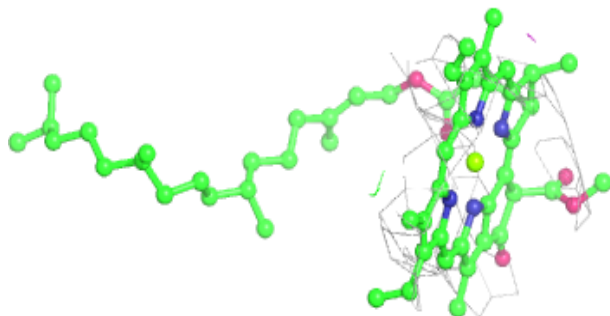
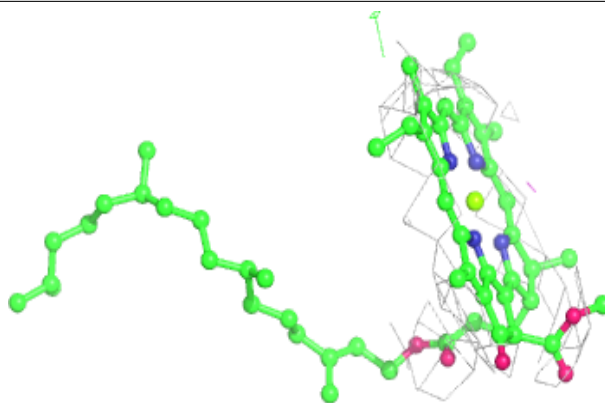
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



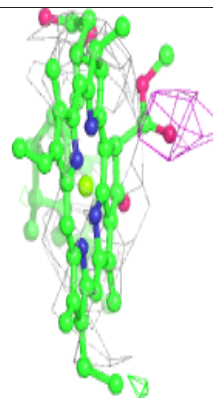
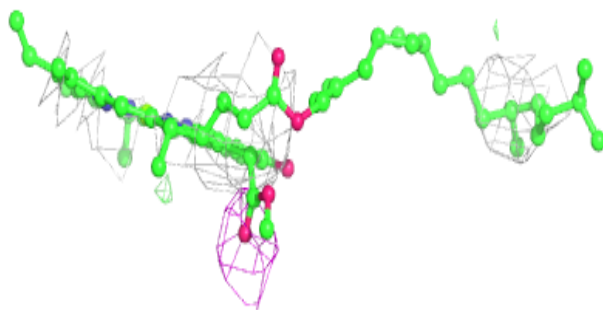
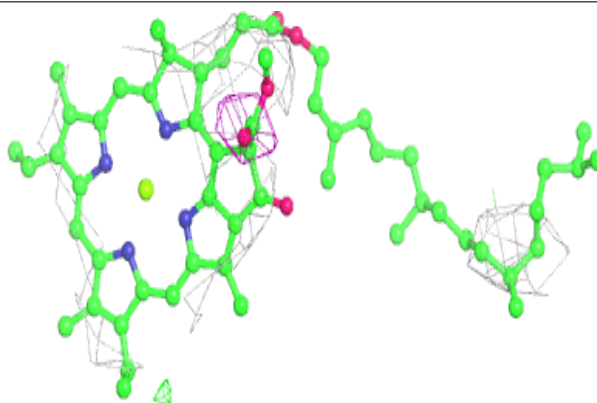


**Electron density around CLA C 507:**

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

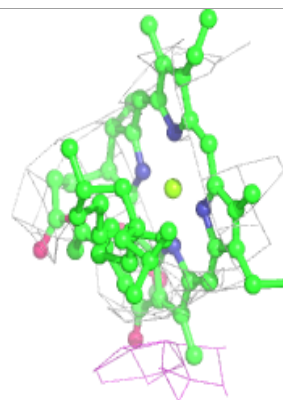
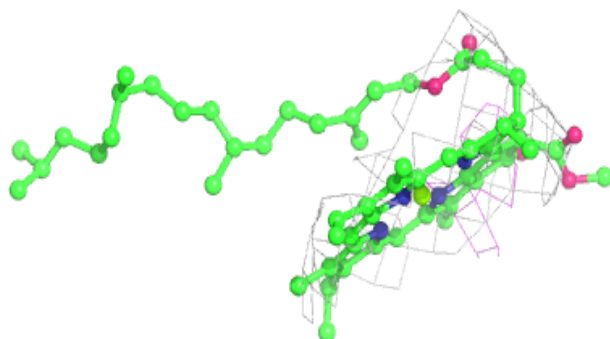
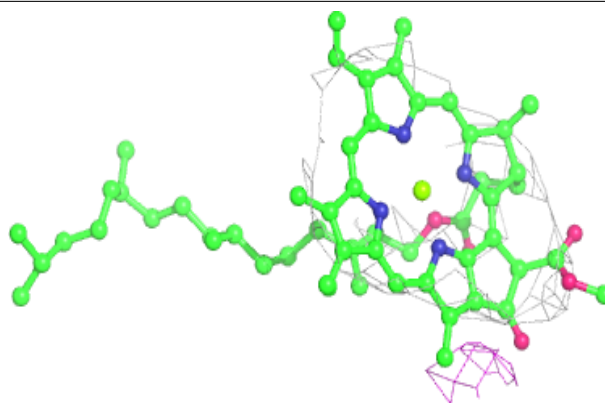
**Electron density around CLA h 101:**

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

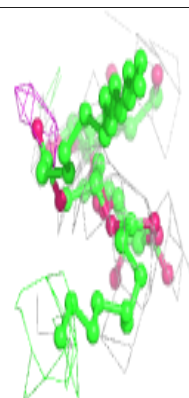
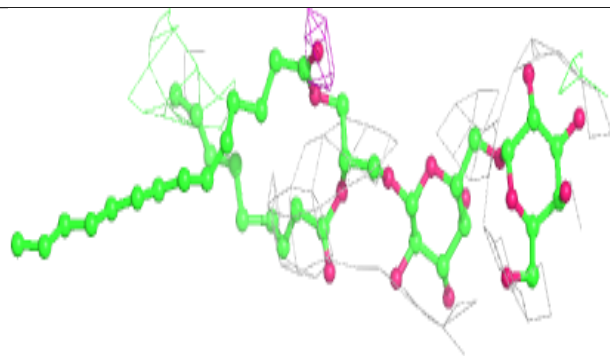
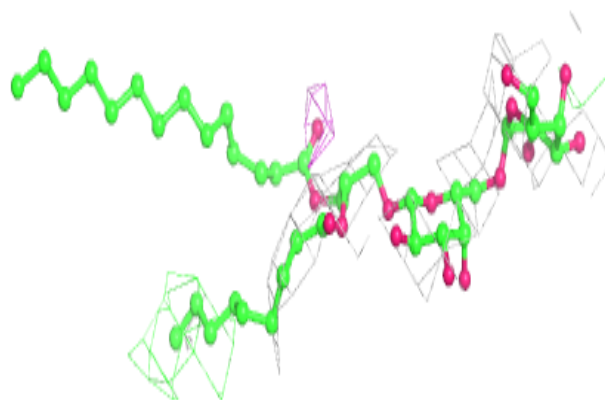


**Electron density around CLA b 617:**

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

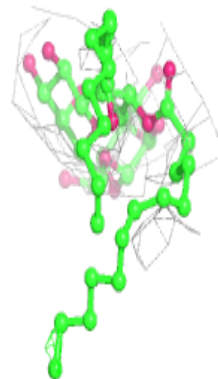
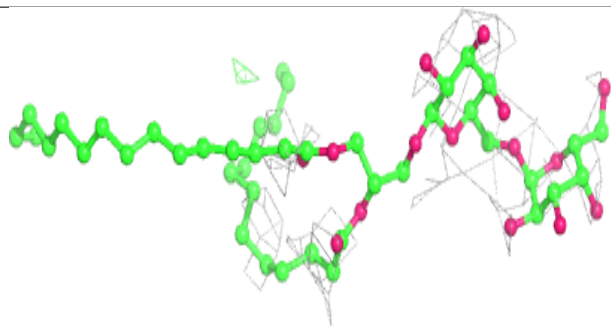
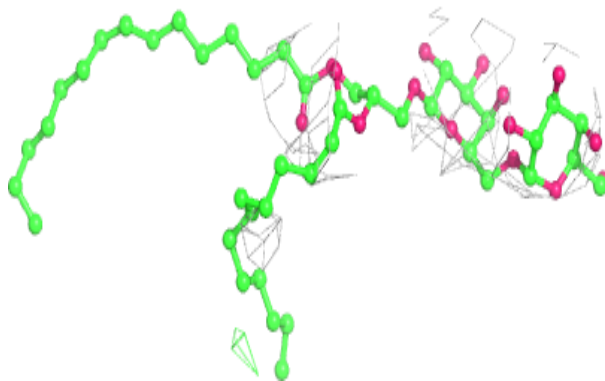
**Electron density around DGD c 515:**

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

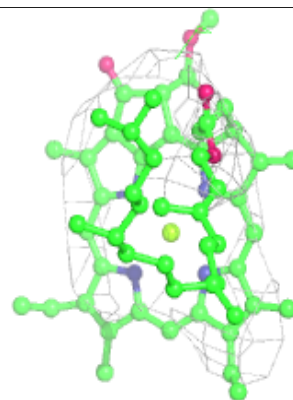
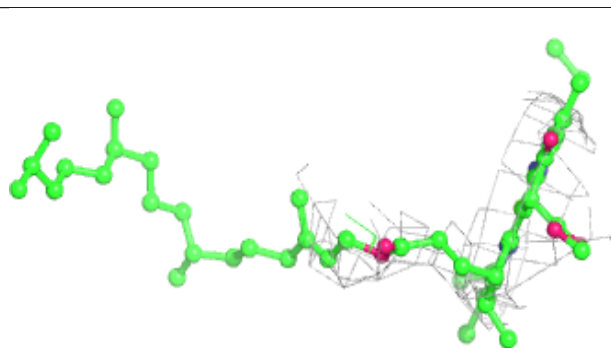
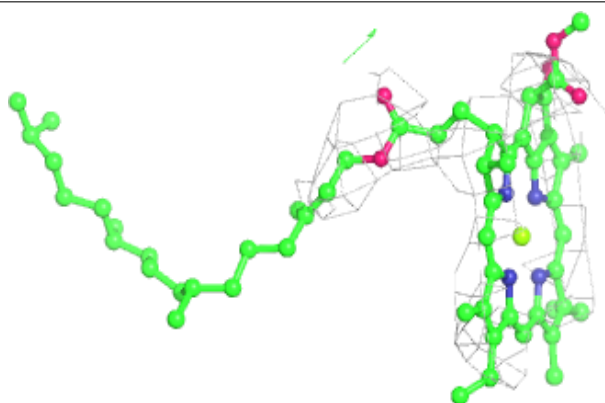


**Electron density around DGD B 620:**

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

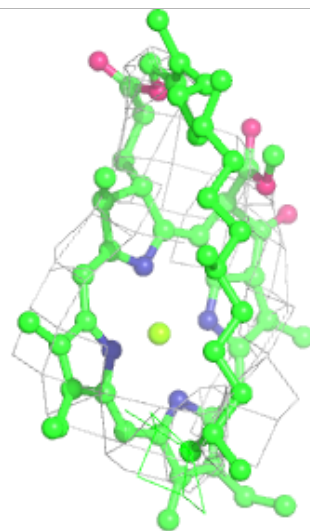
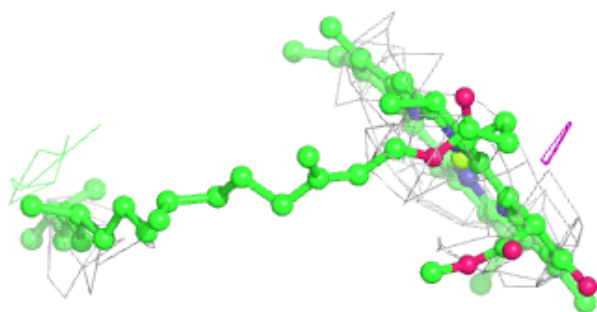
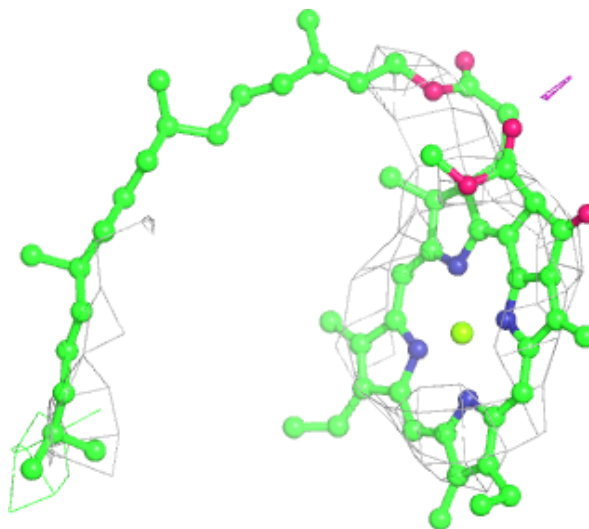
**Electron density around CLA d 406:**

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



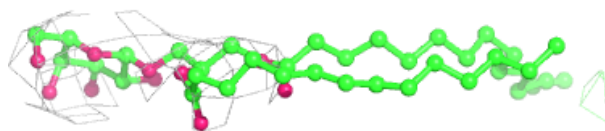
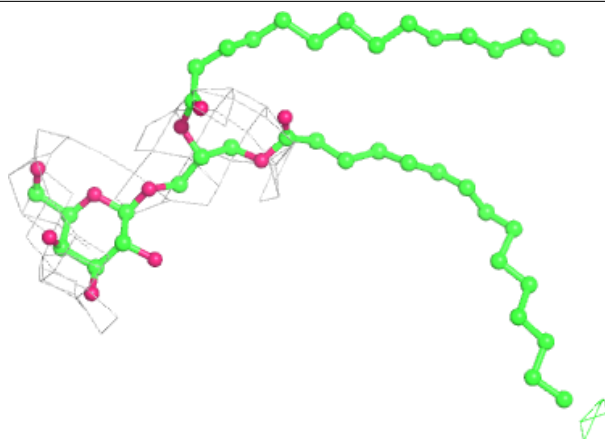
**Electron density around CLA C 506:**

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



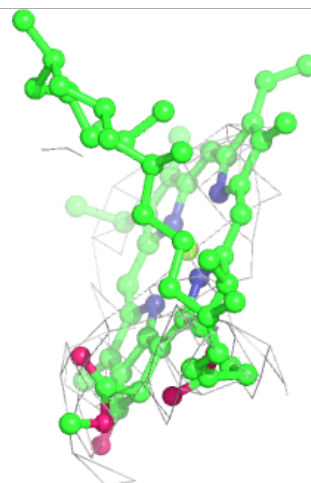
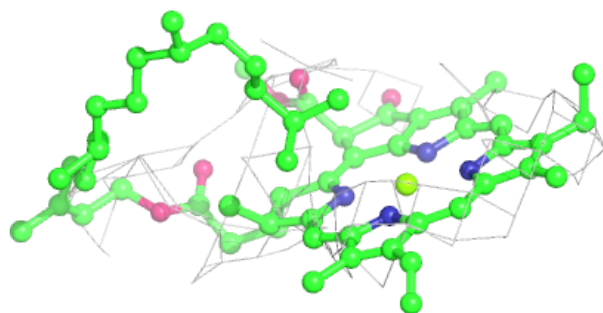
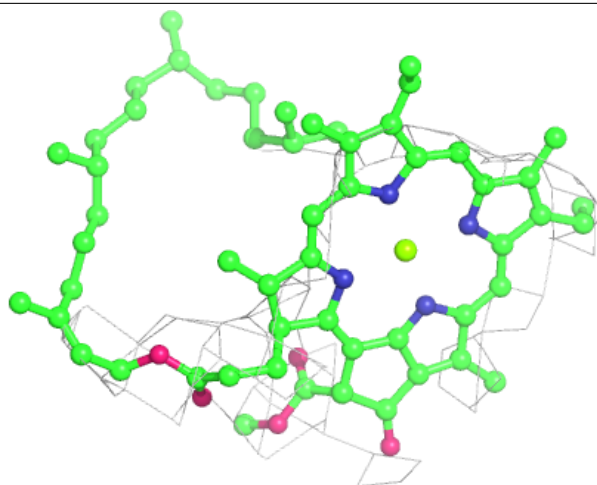
**Electron density around LMG c 522:**

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



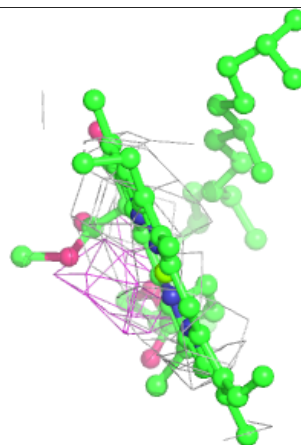
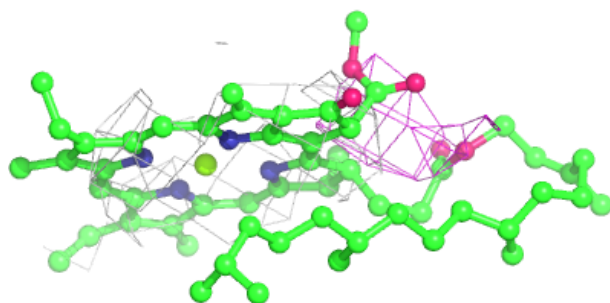
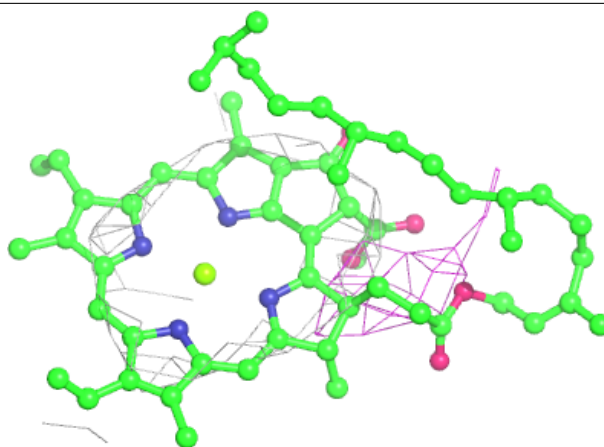
**Electron density around CLA B 614:**

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



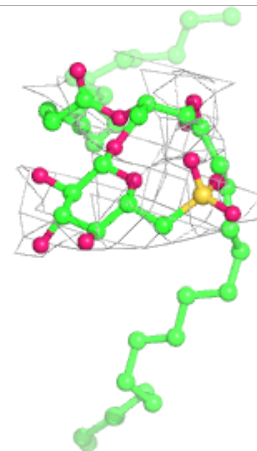
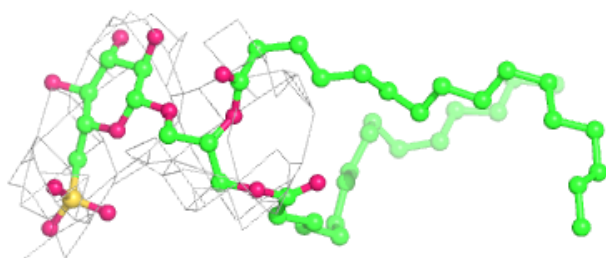
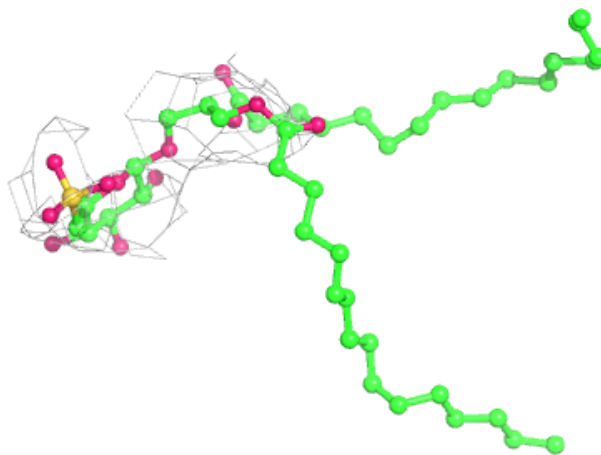
**Electron density around CLA C 508:**

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



**Electron density around SQD a 401:**

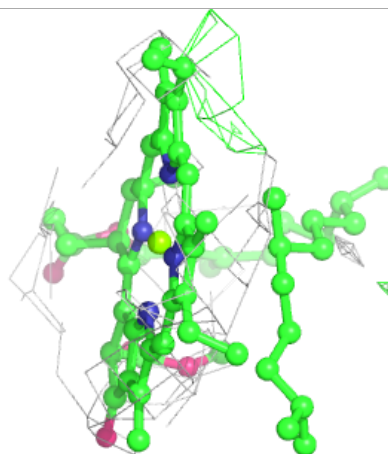
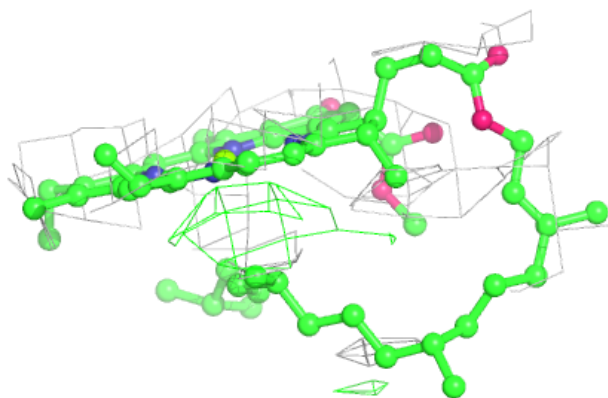
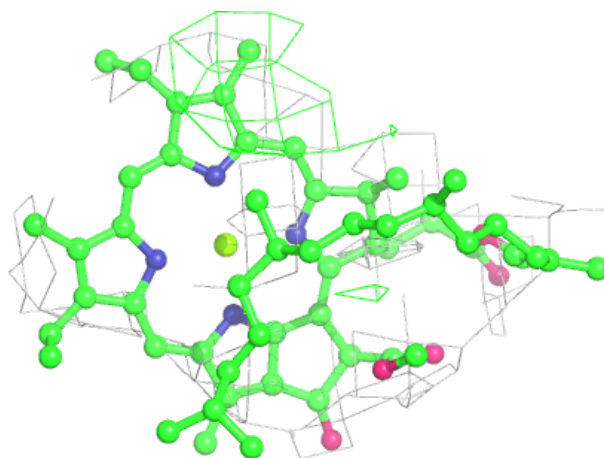
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





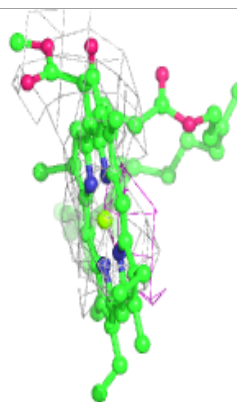
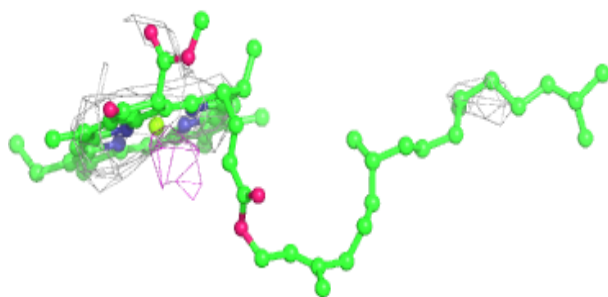
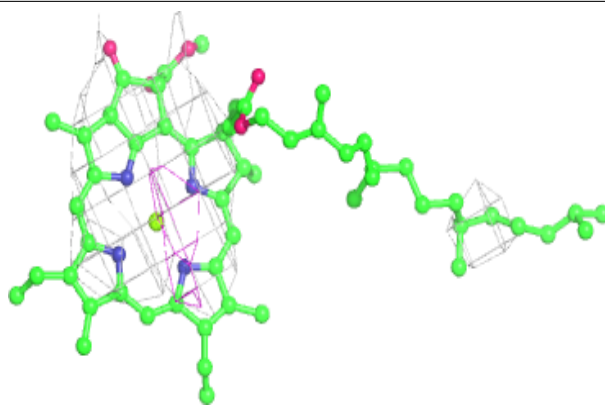
**Electron density around CLA C 509:**

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

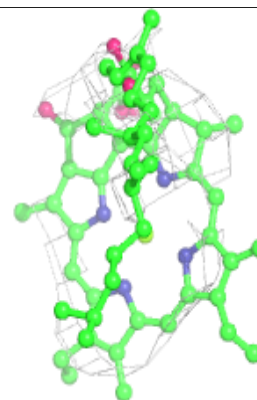
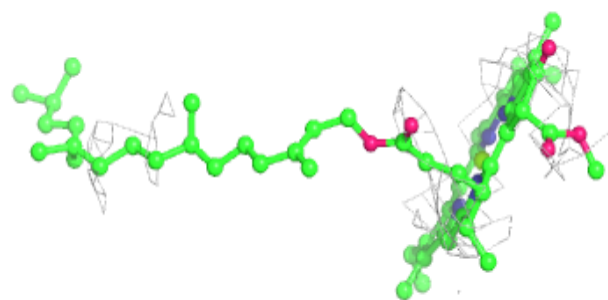
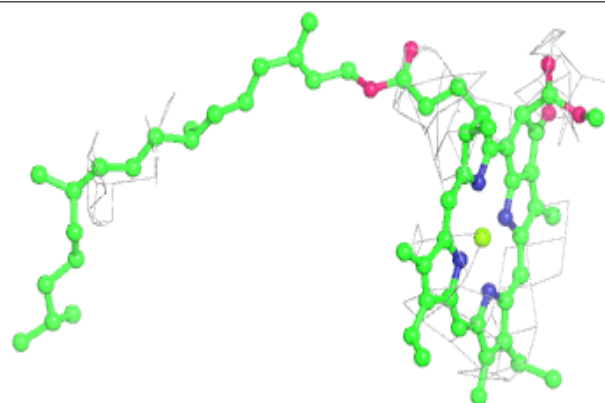


**Electron density around CLA a 406:**

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

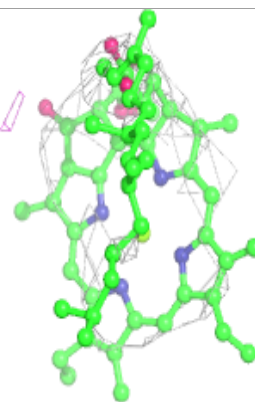
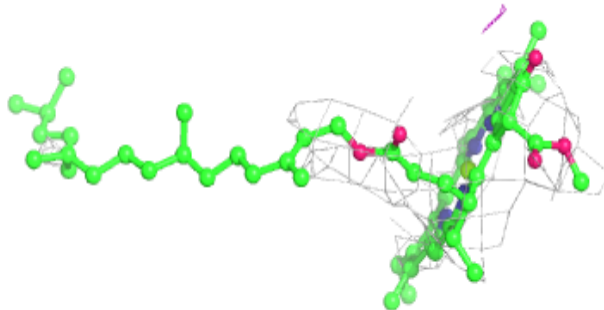
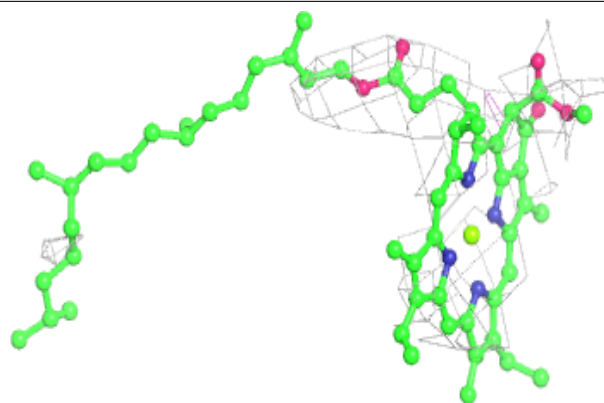
**Electron density around CLA b 612:**

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

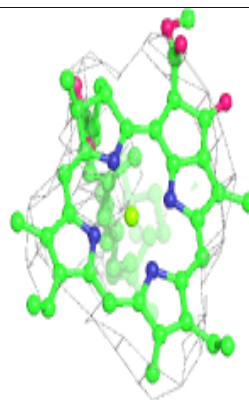
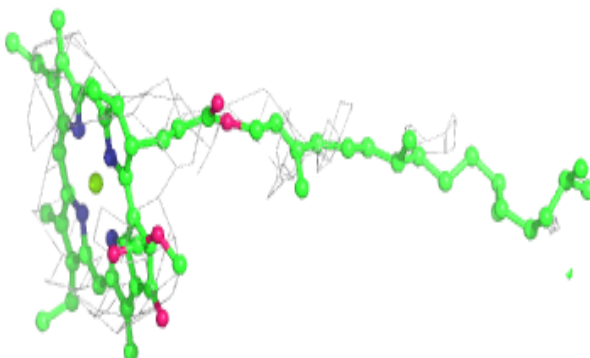
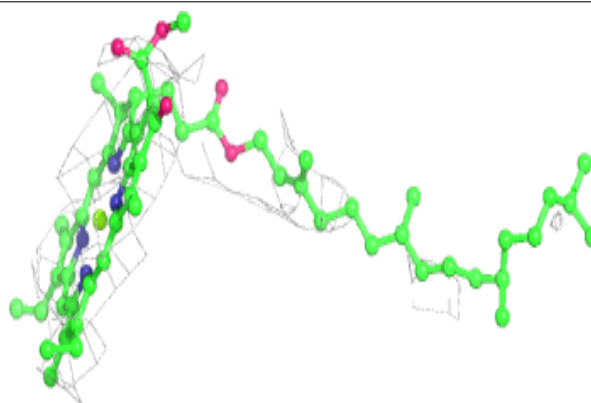


**Electron density around CLA B 608:**

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

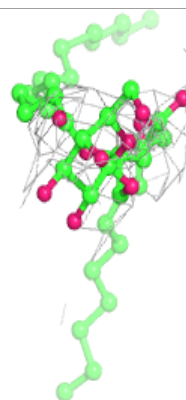
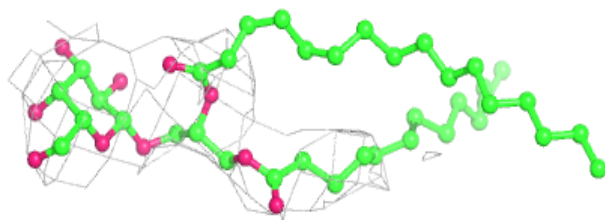
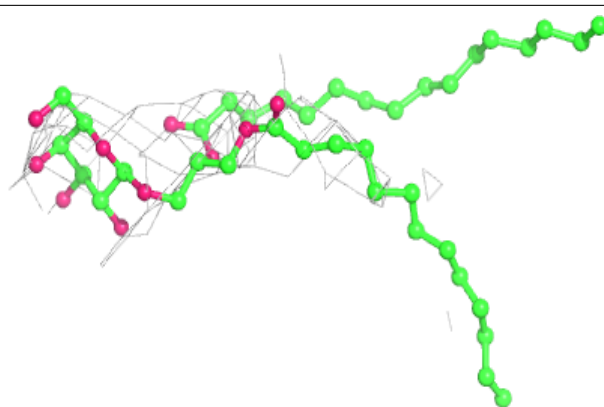
**Electron density around CLA b 607:**

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

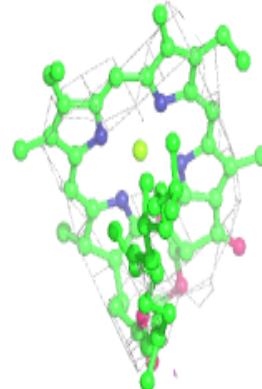
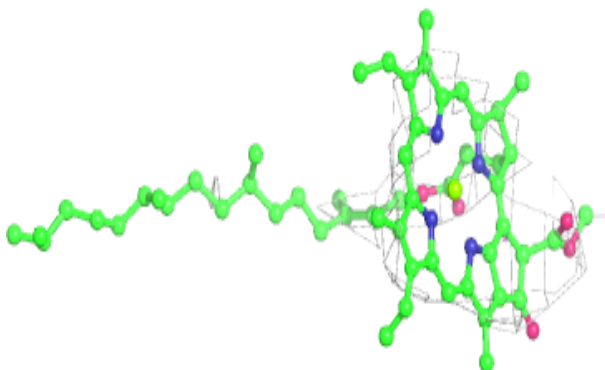
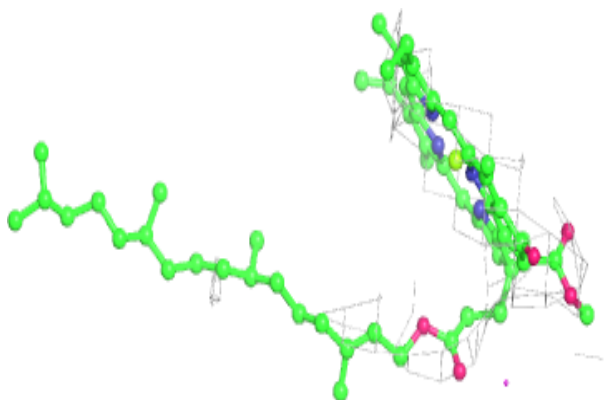


**Electron density around LMG d 409:**

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

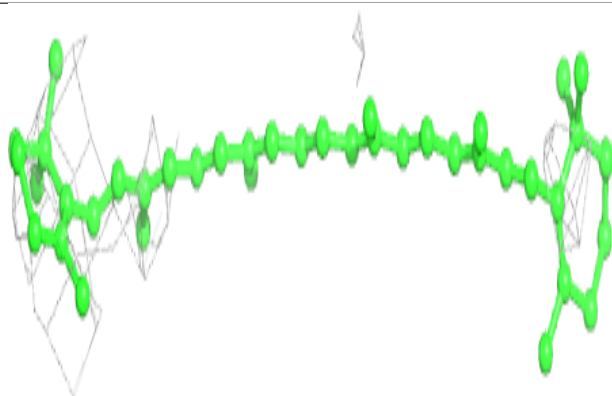
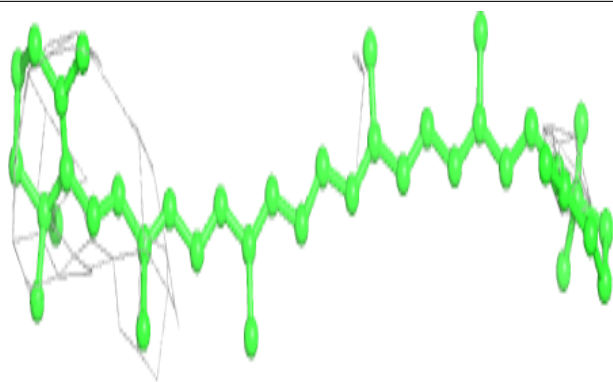
**Electron density around CLA C 520:**

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

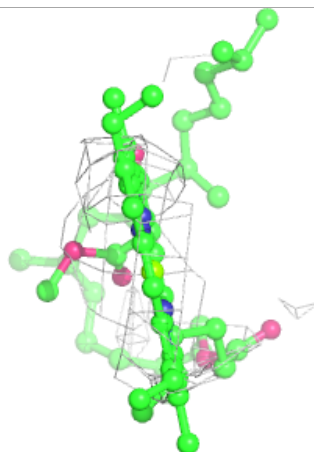
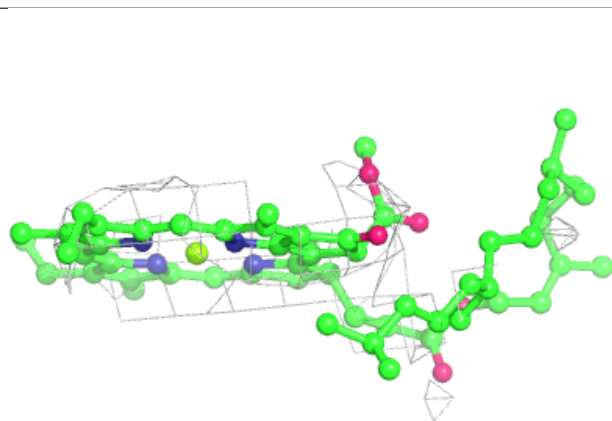
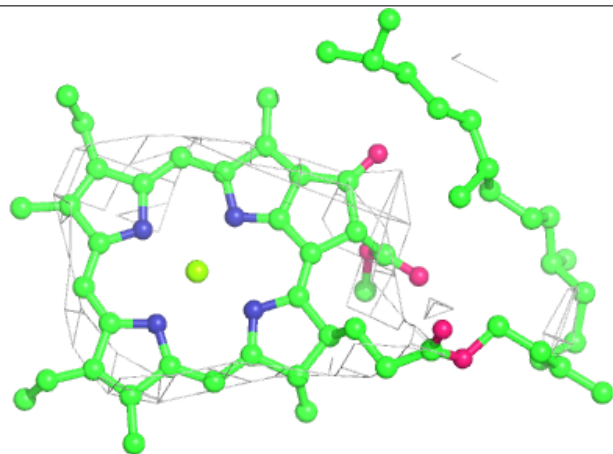


**Electron density around BCR b 620:**

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

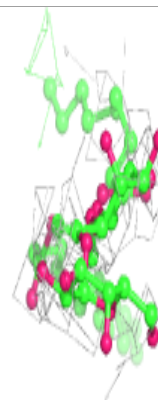
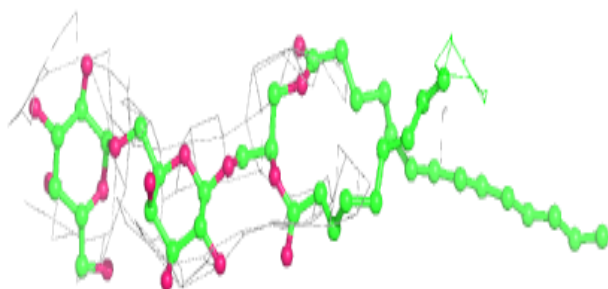
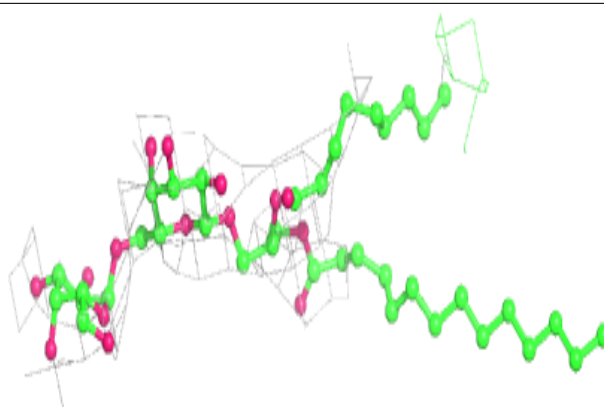
**Electron density around CLA b 613:**

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

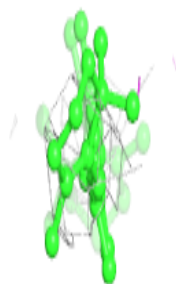
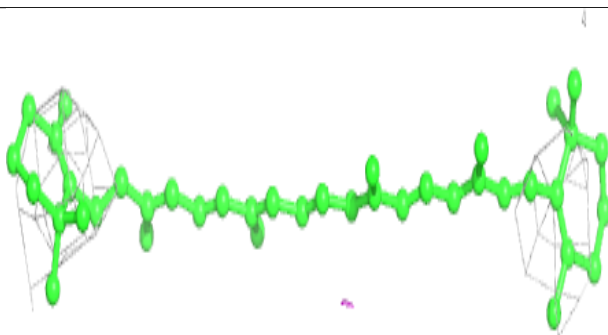
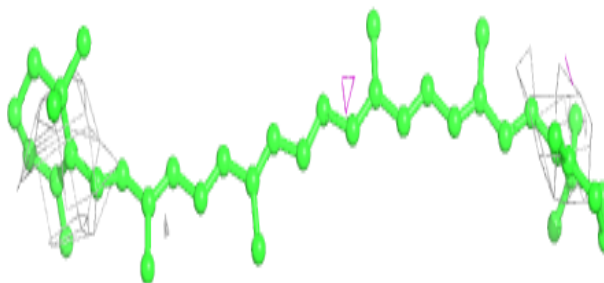


**Electron density around DGD C 515:**

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

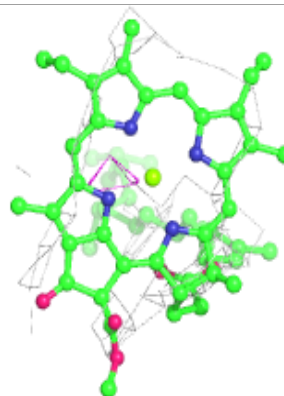
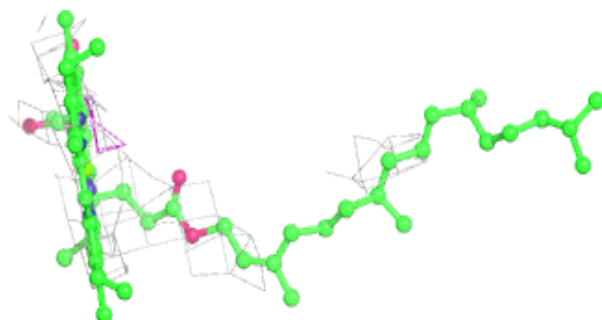
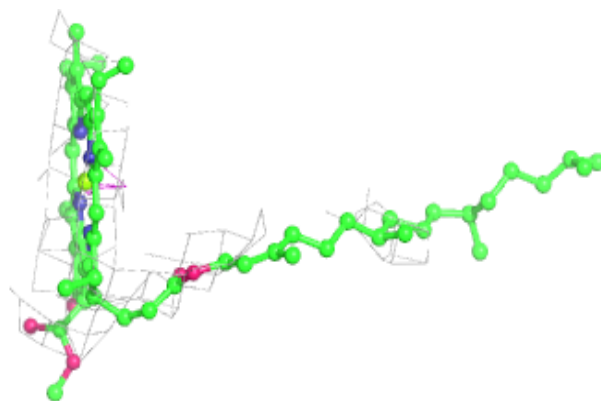
**Electron density around BCR c 521:**

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

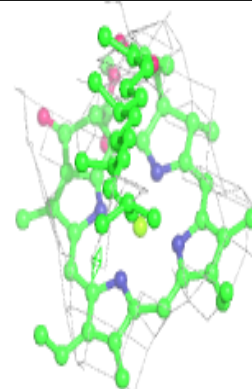
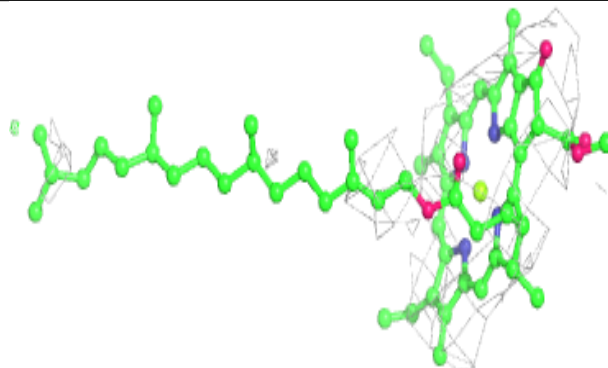
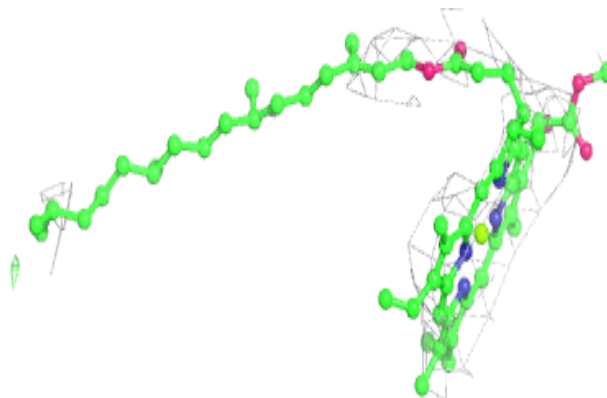


**Electron density around CLA b 609:**

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

**Electron density around CLA B 606:**

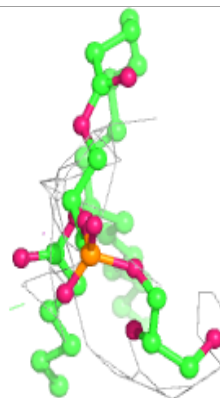
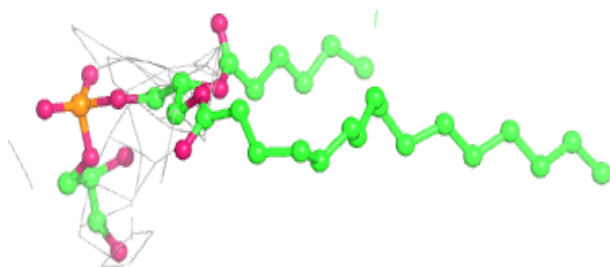
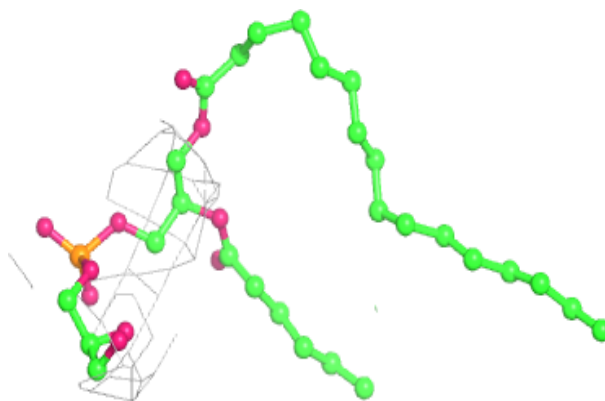
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



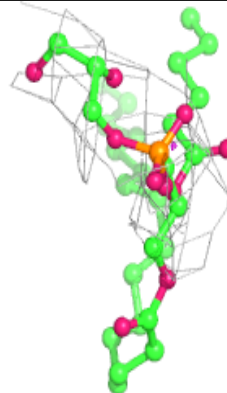
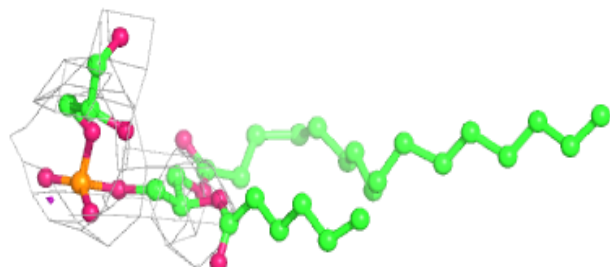
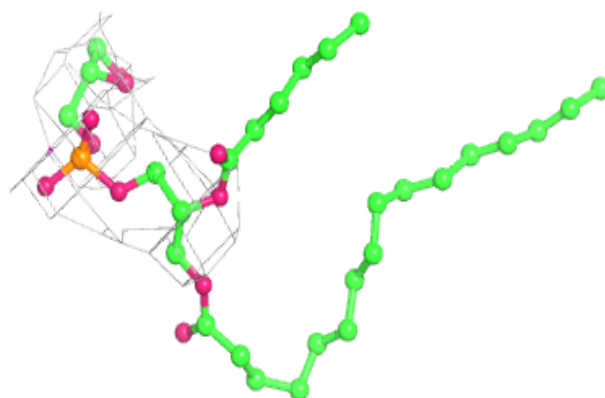


**Electron density around LHG A 409:**

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

**Electron density around LHG a 411:**

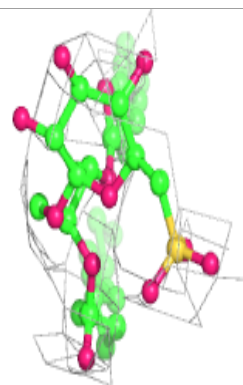
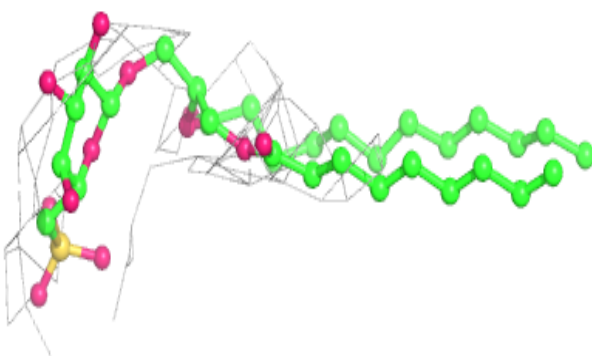
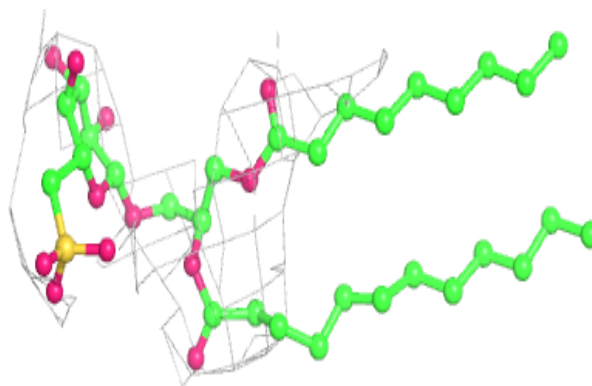
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



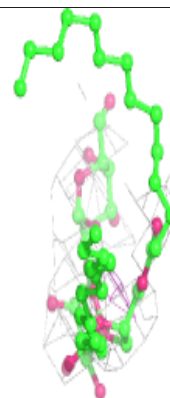
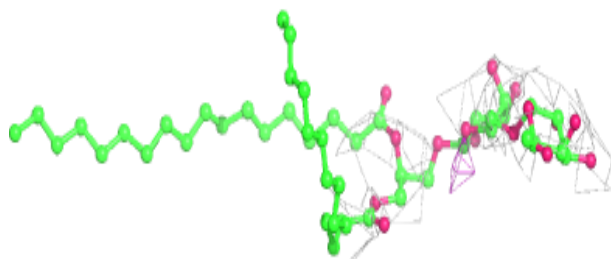
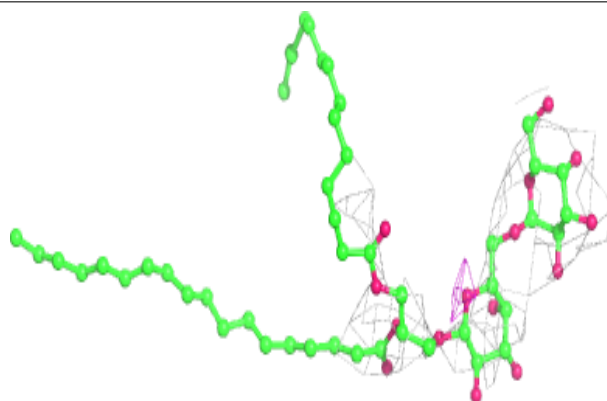


**Electron density around SQD B 622:**

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

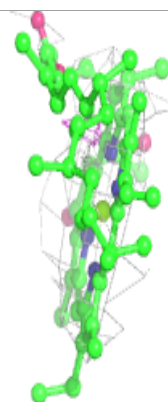
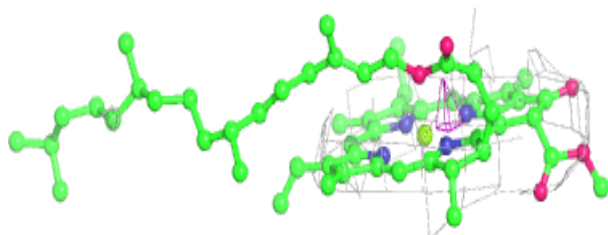
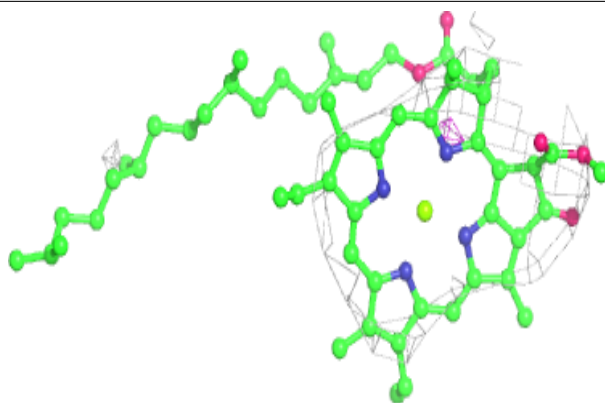
**Electron density around DGD C 516:**

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

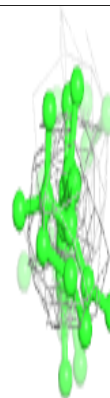
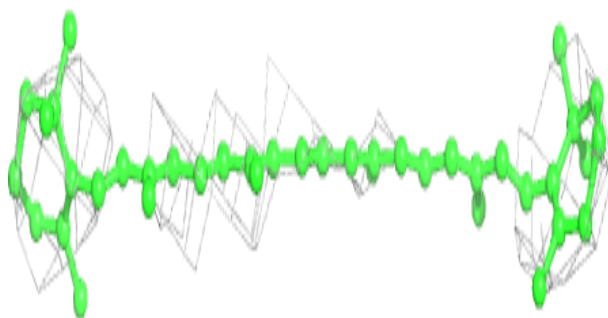
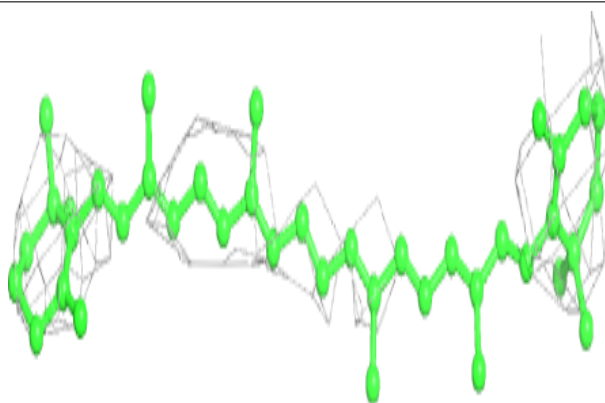


**Electron density around CLA c 501:**

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

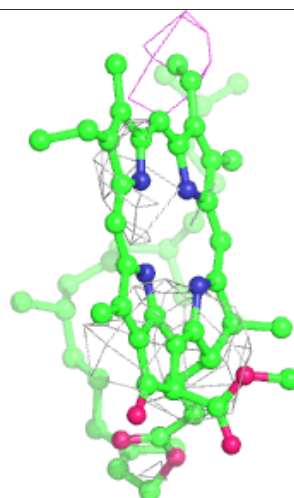
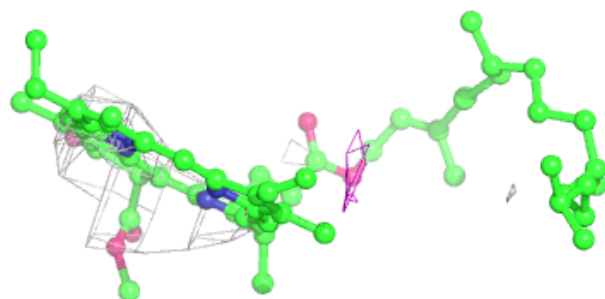
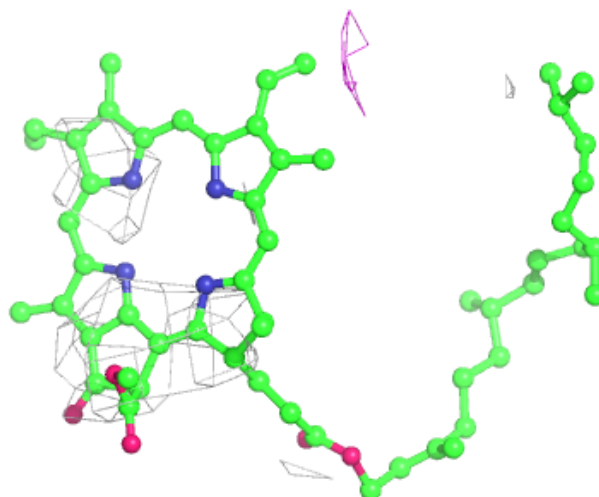
**Electron density around BCR B 618:**

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



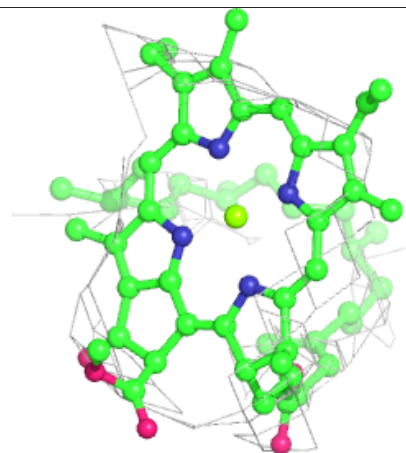
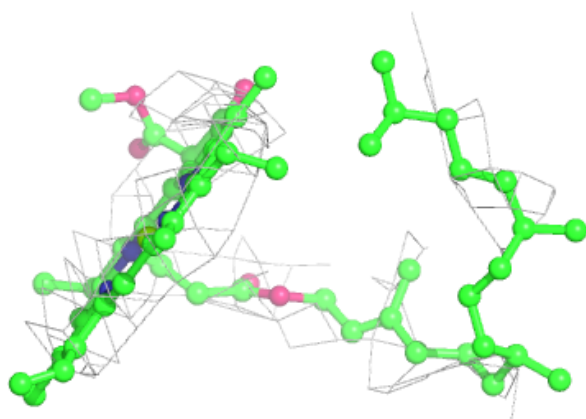
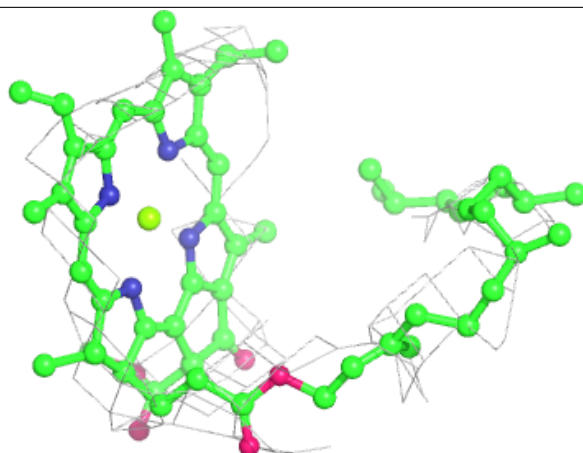
**Electron density around PHO d 402:**

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

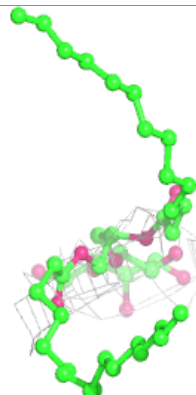
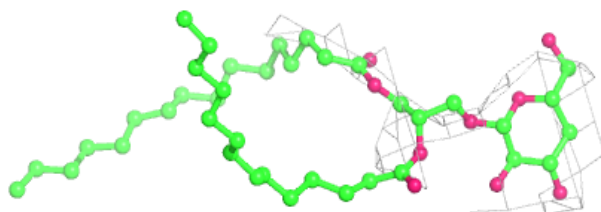
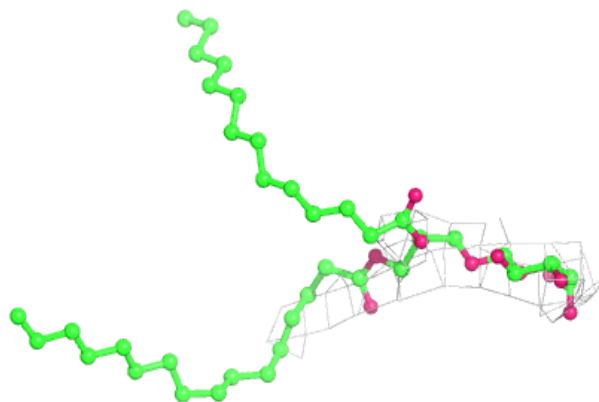


**Electron density around CLA C 503:**

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

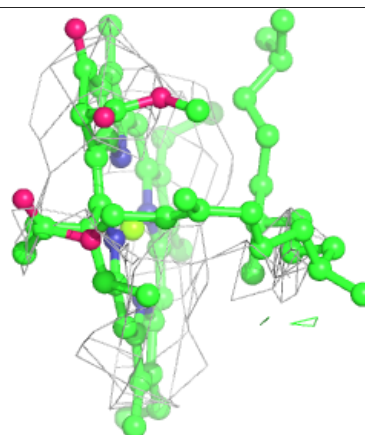
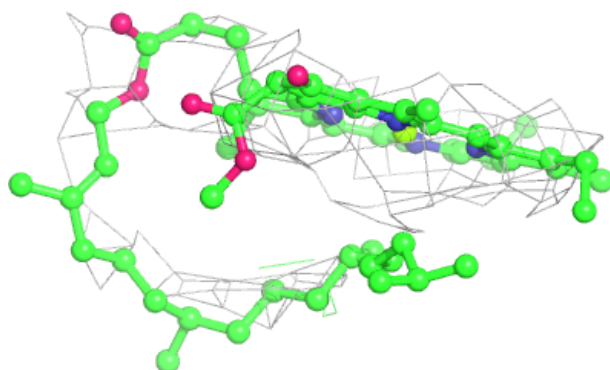
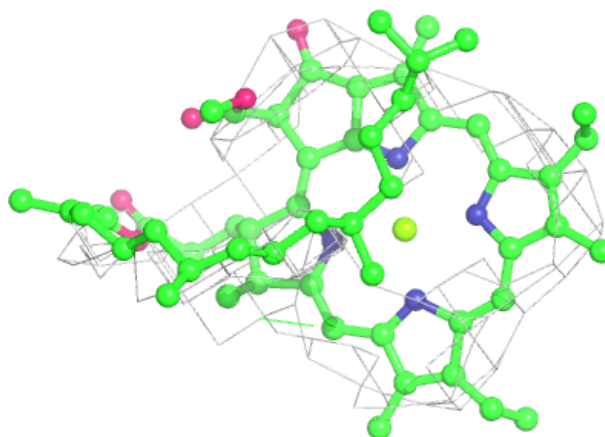
**Electron density around LMG b 625:**

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

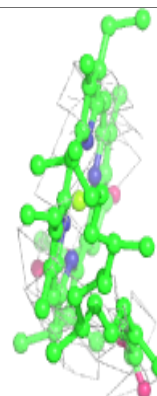
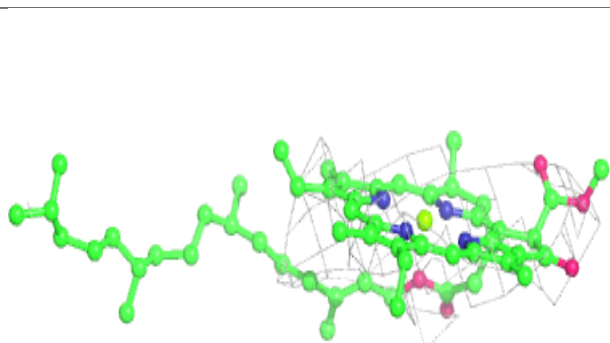
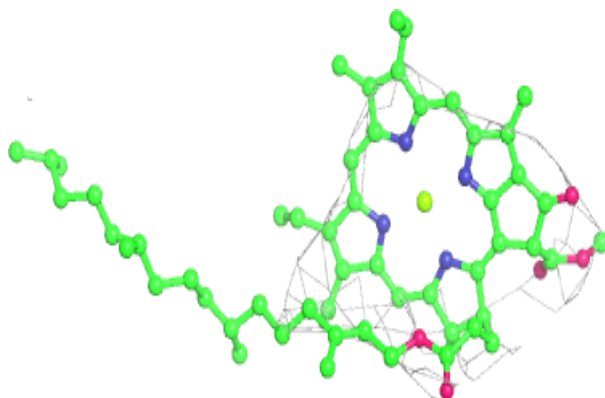


**Electron density around CLA c 509:**

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

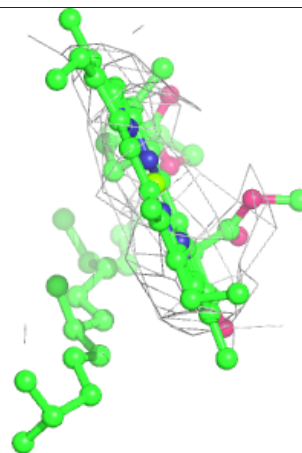
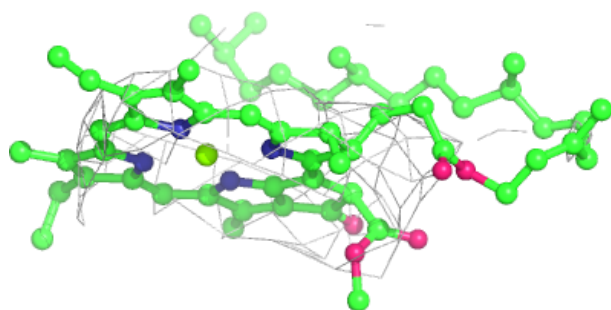
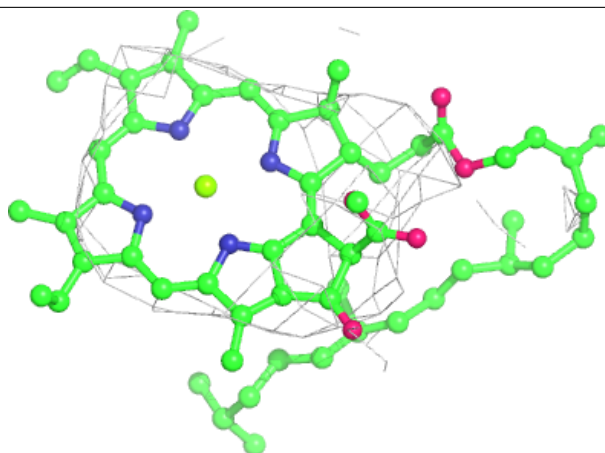
**Electron density around CLA C 501:**

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

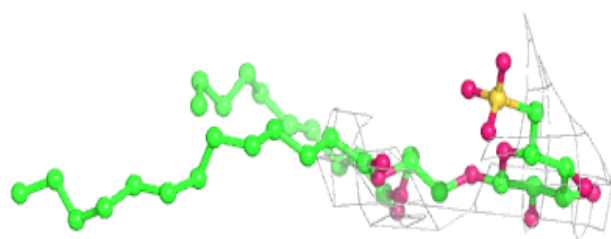
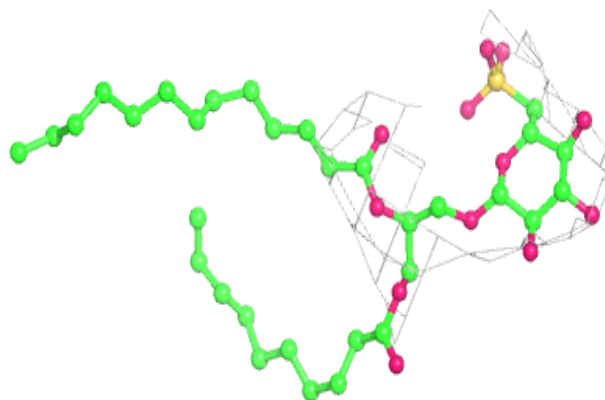


**Electron density around CLA c 508:**

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

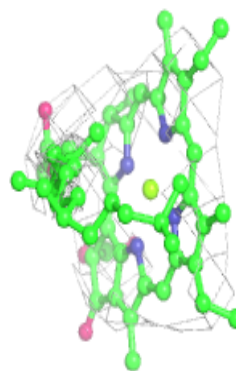
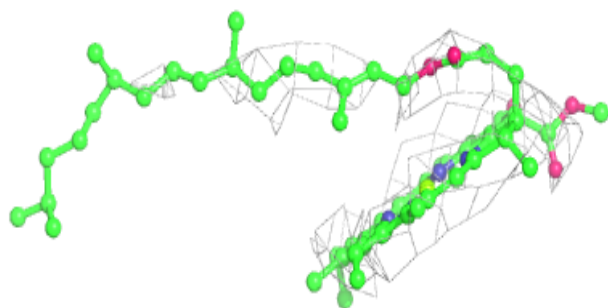
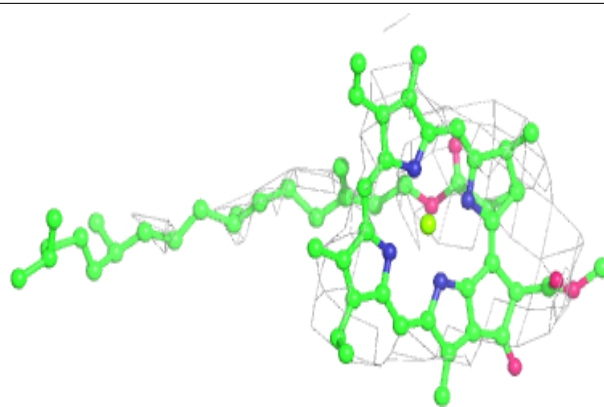
**Electron density around SQD f 103:**

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

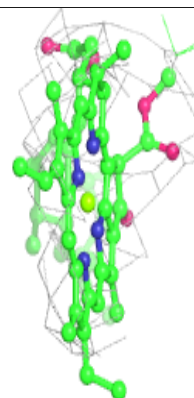
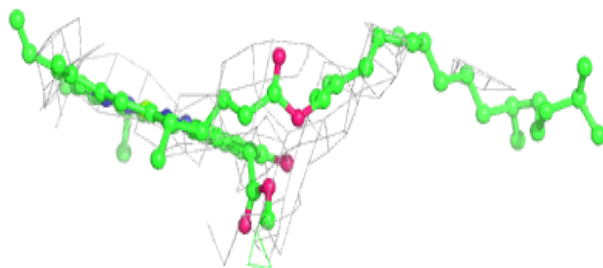
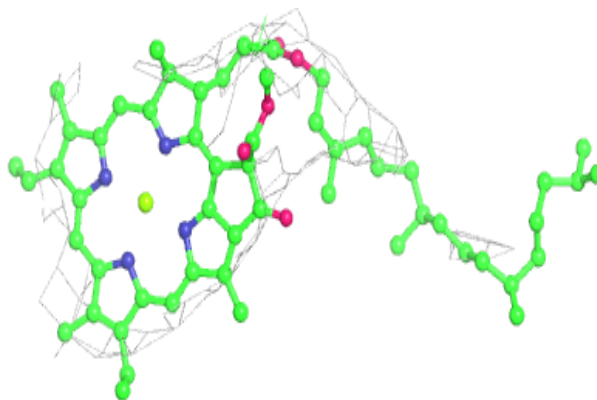


**Electron density around CLA b 611:**

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

**Electron density around CLA H 101:**

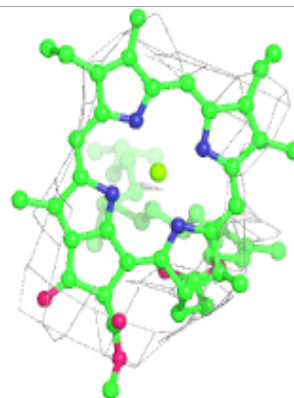
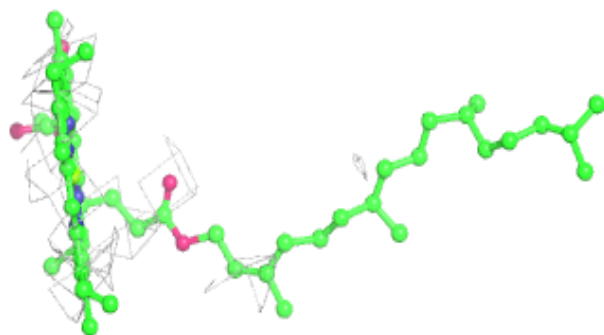
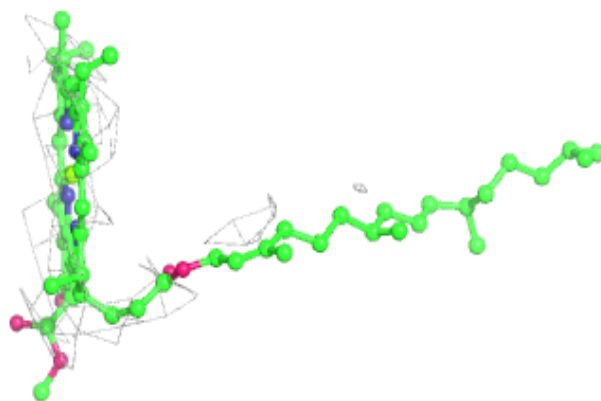
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



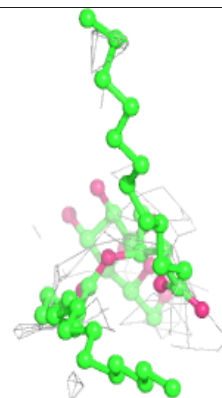
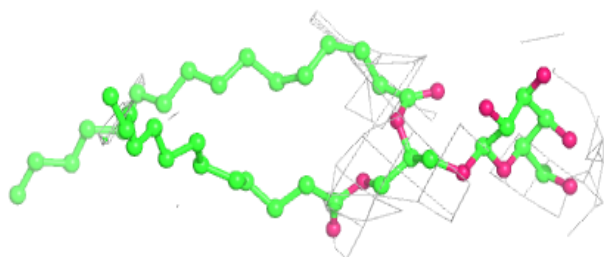
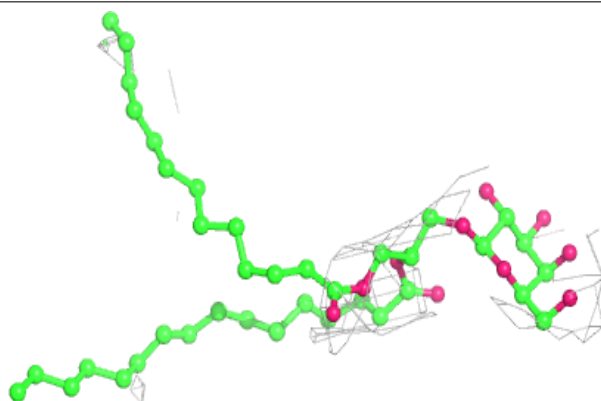


**Electron density around CLA B 605:**

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

**Electron density around LMG D 409:**

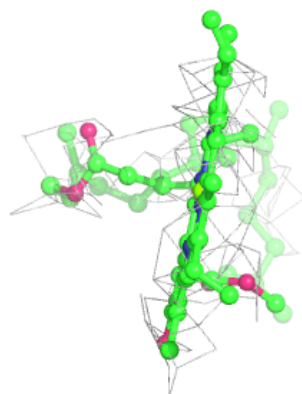
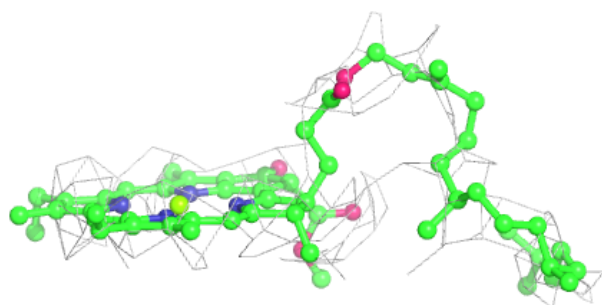
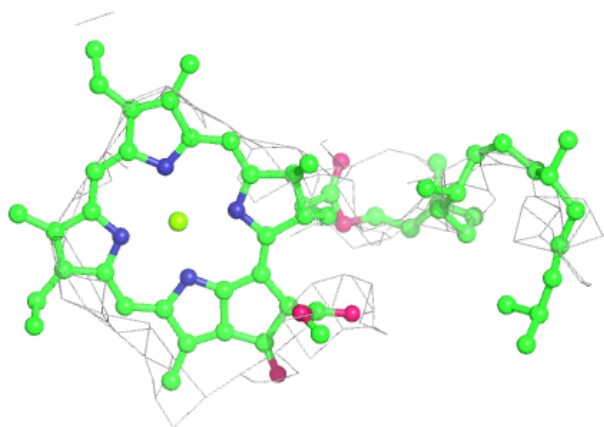
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





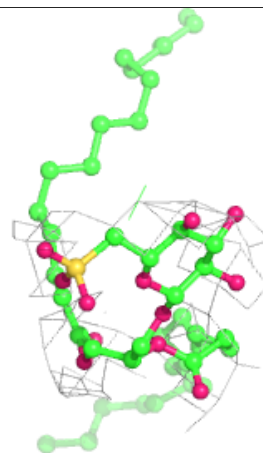
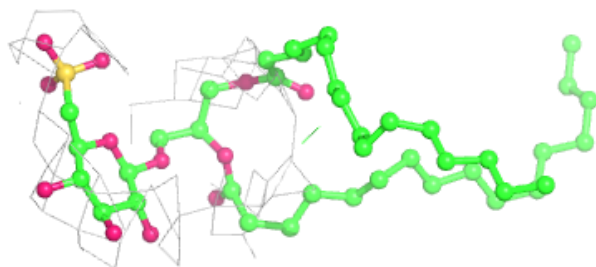
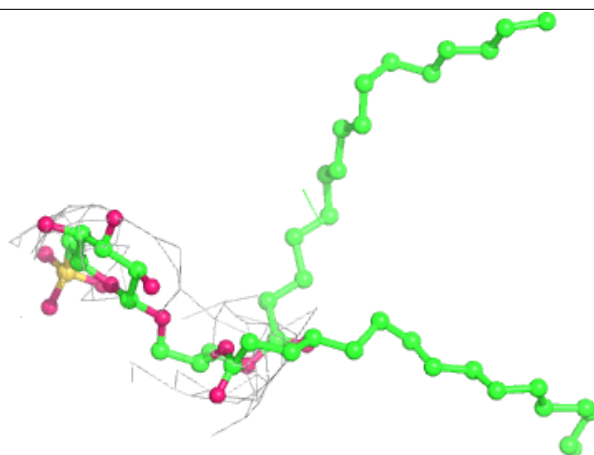
**Electron density around CLA b 615:**

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



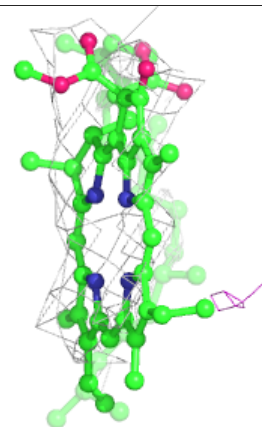
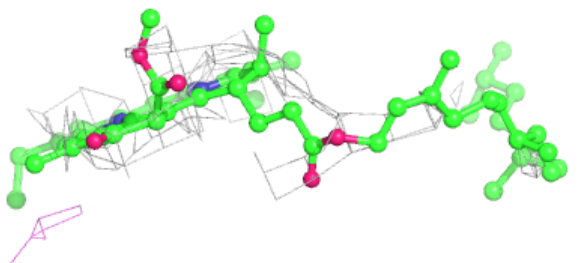
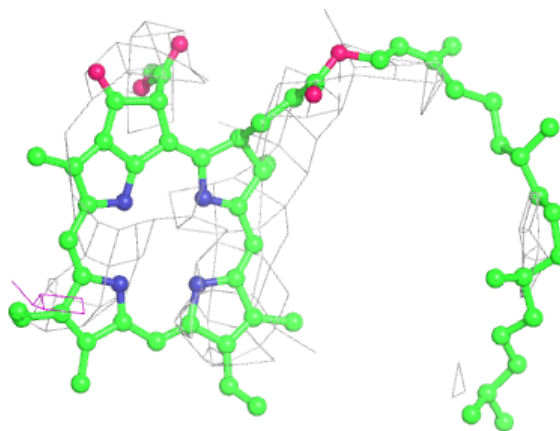
**Electron density around SQD A 413:**

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



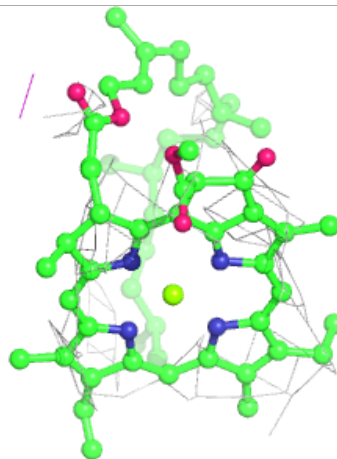
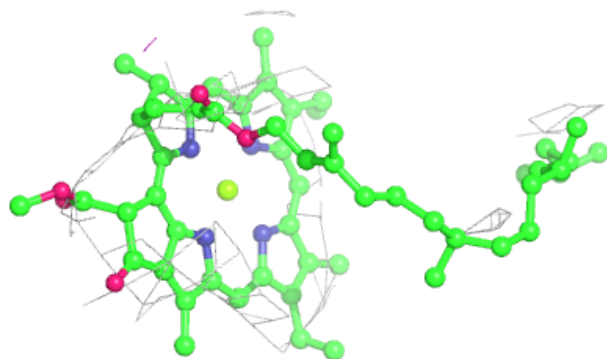
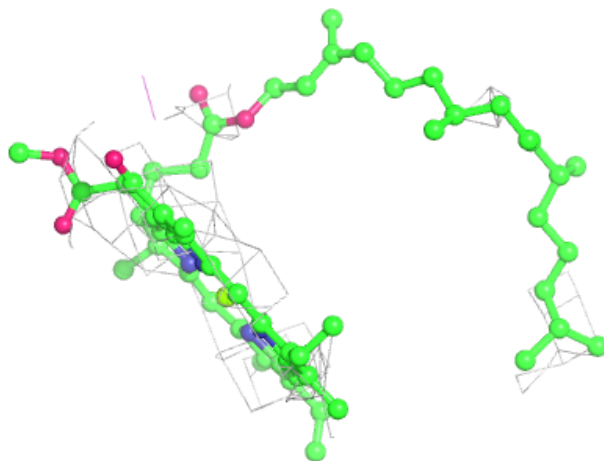
**Electron density around PHO D 401:**

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



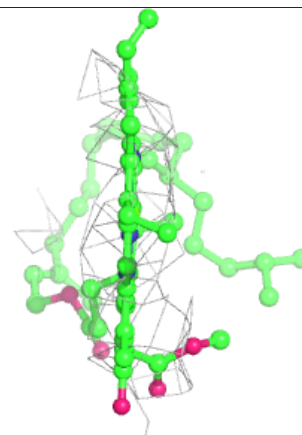
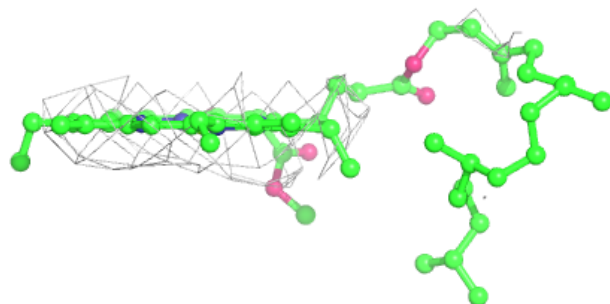
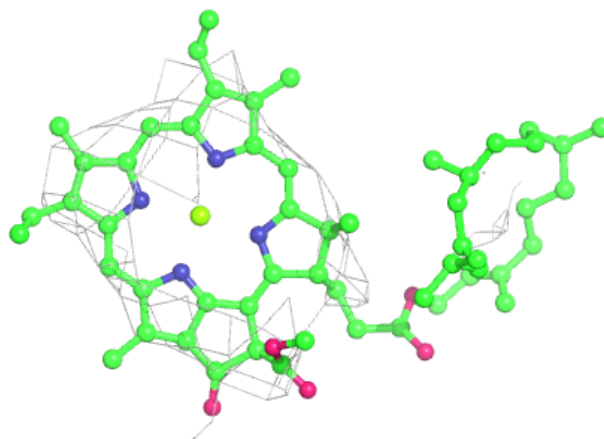
**Electron density around CLA B 610:**

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

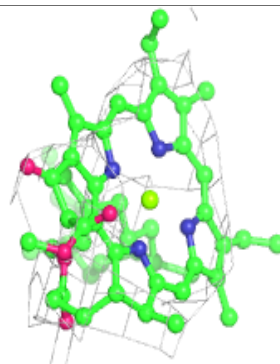
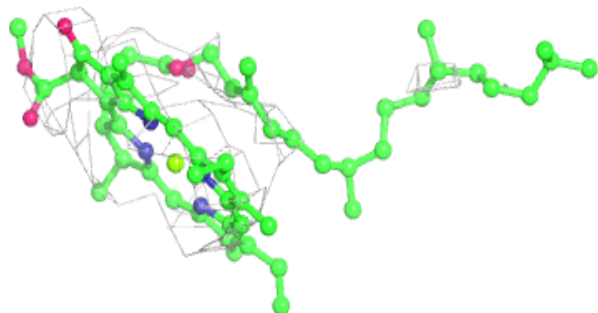
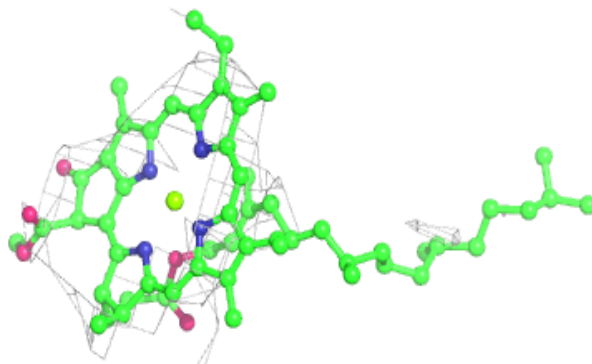


**Electron density around CLA c 511:**

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

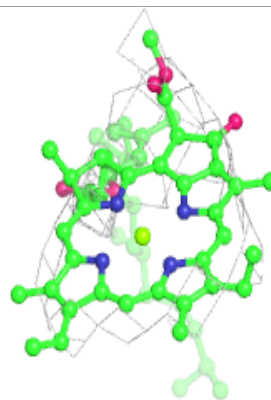
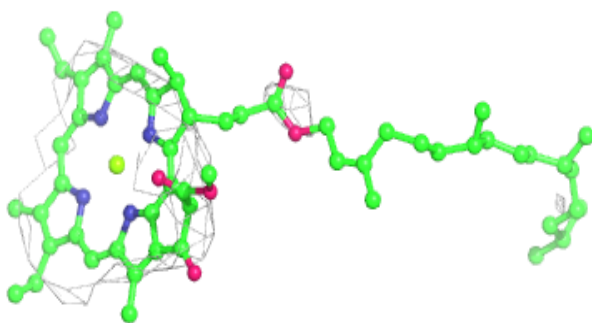
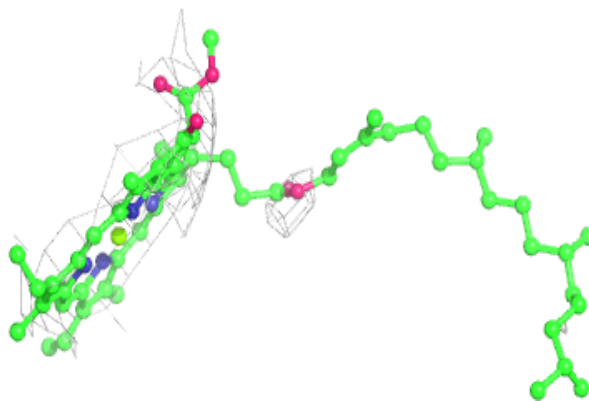
**Electron density around CLA C 504:**

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



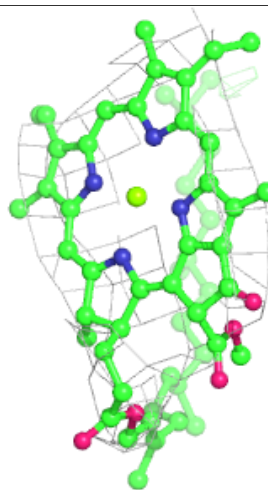
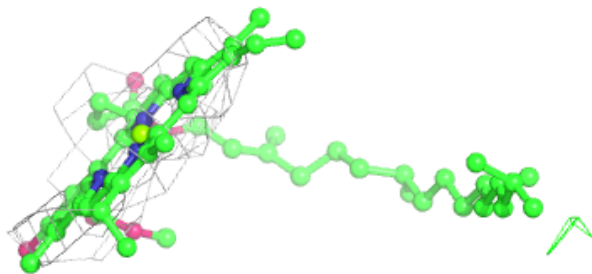
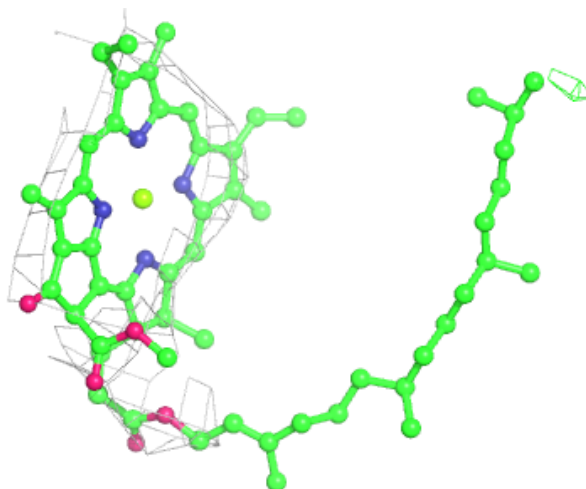
**Electron density around CLA d 405:**

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



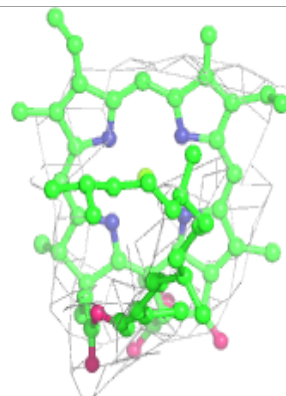
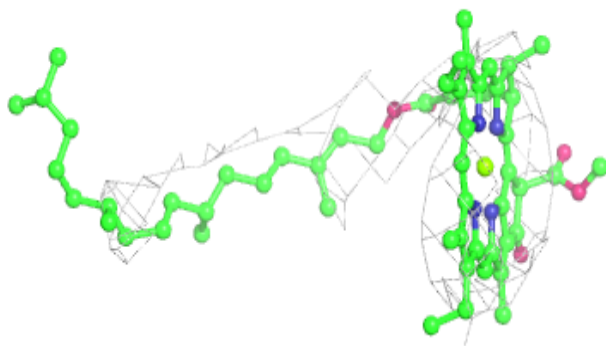
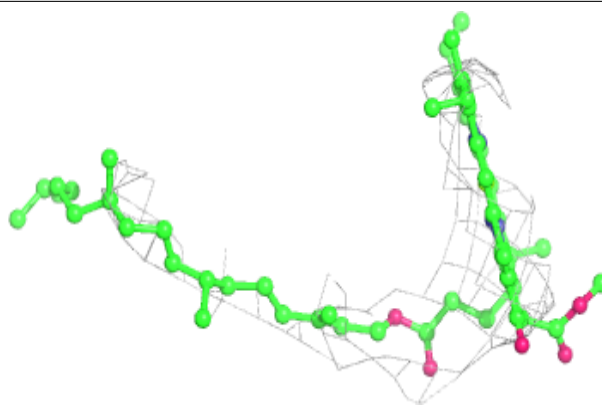
**Electron density around CLA c 506:**

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

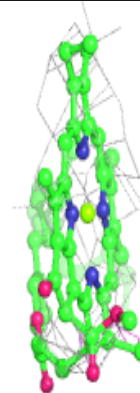
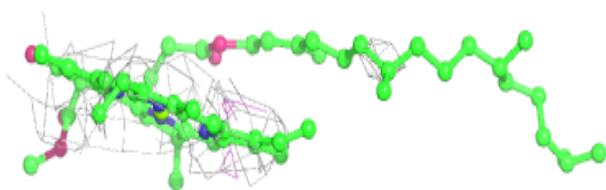
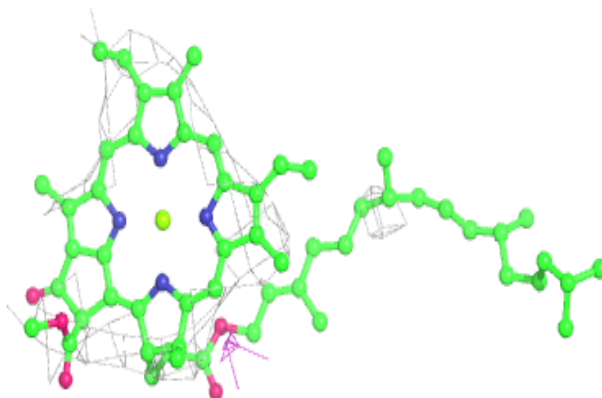


**Electron density around CLA b 608:**

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

**Electron density around CLA b 606:**

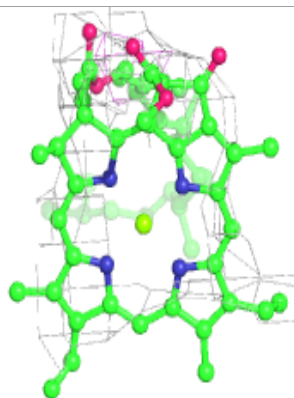
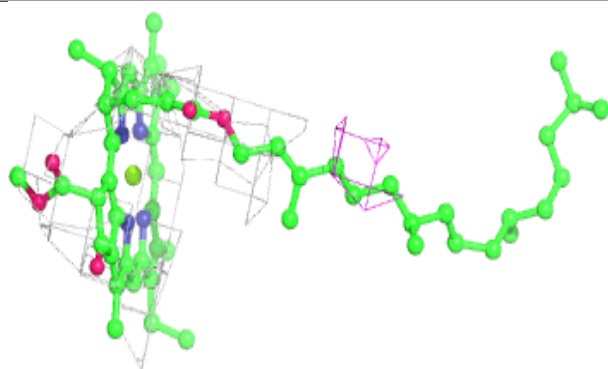
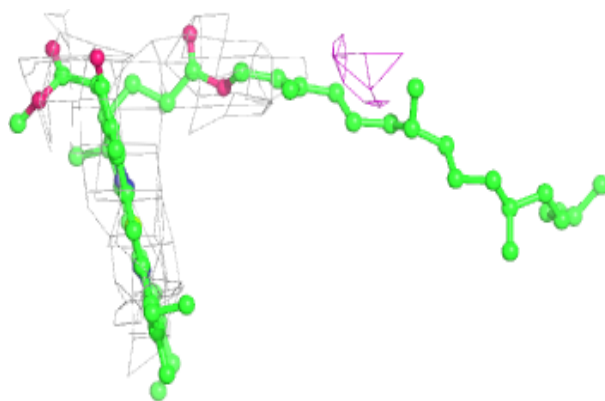
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



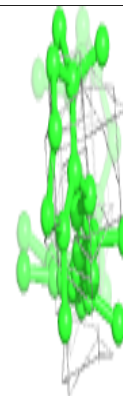
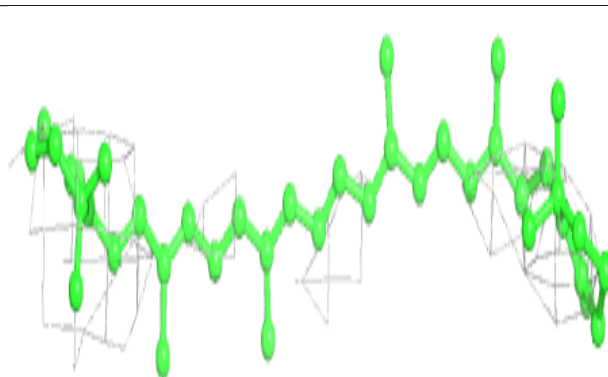
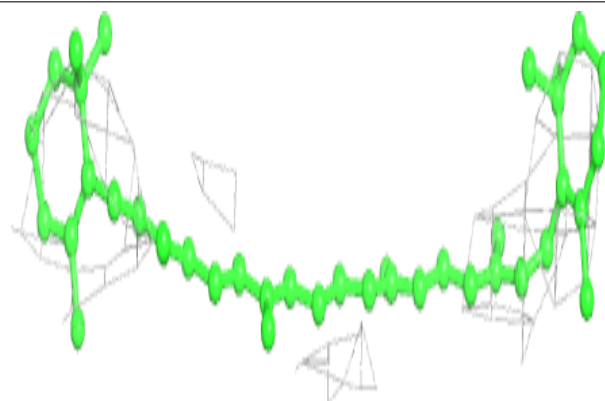


**Electron density around CLA B 604:**

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

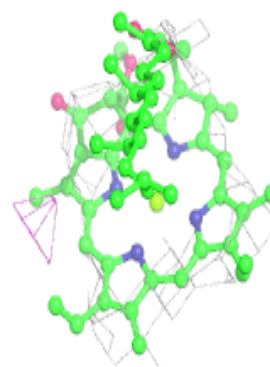
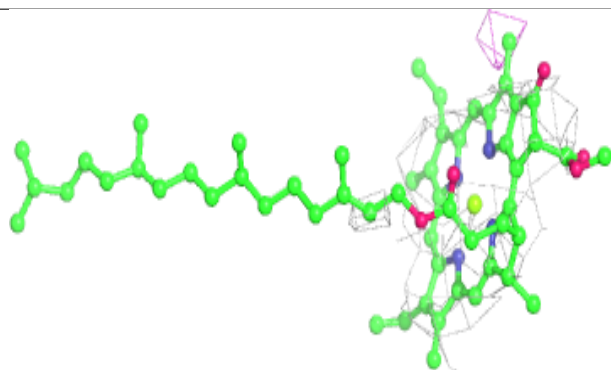
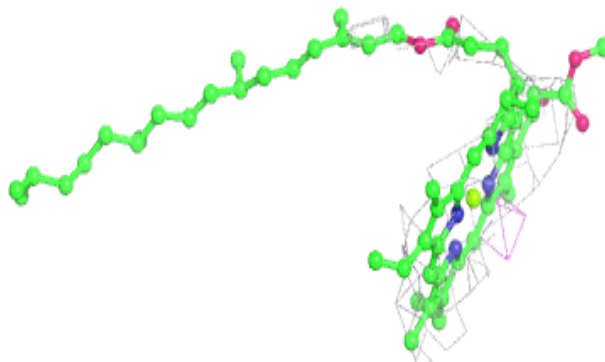
**Electron density around BCR C 513:**

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



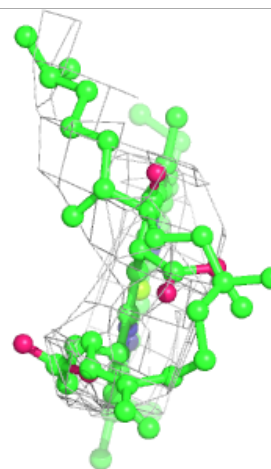
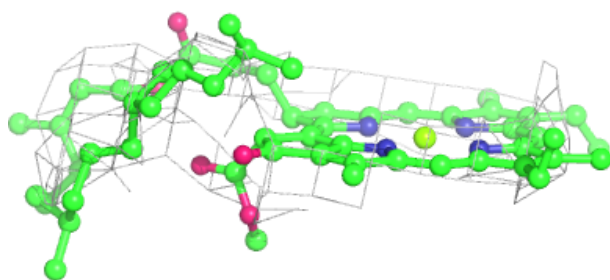
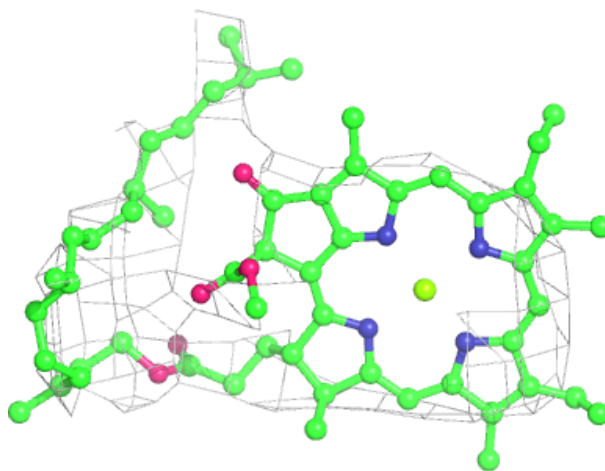
**Electron density around CLA b 610:**

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



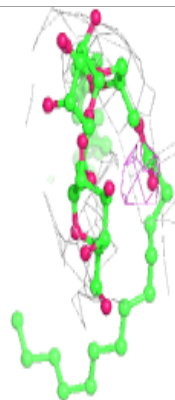
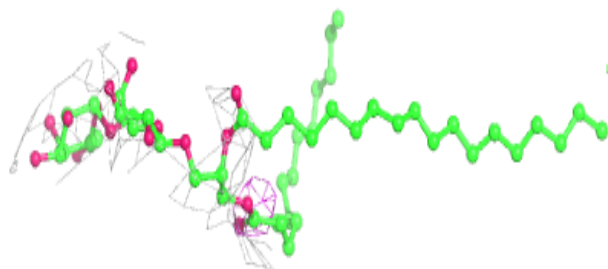
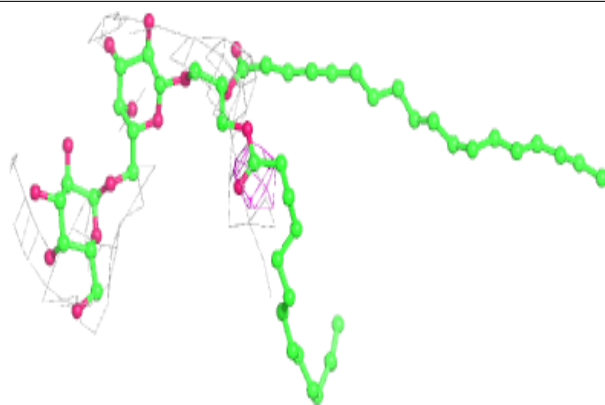
**Electron density around CLA B 609:**

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

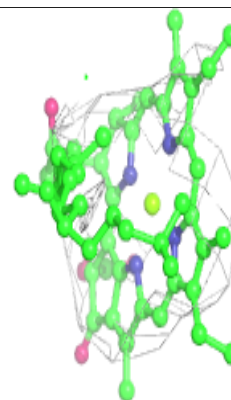
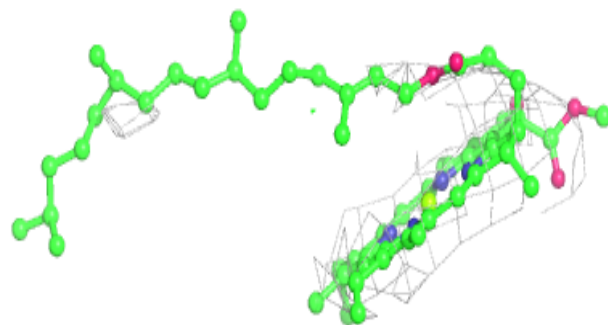
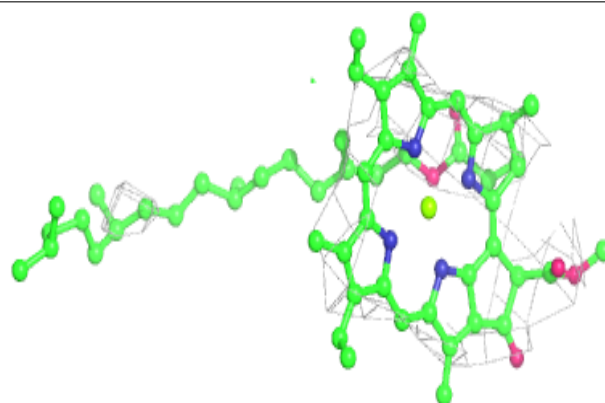


**Electron density around DGD c 516:**

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

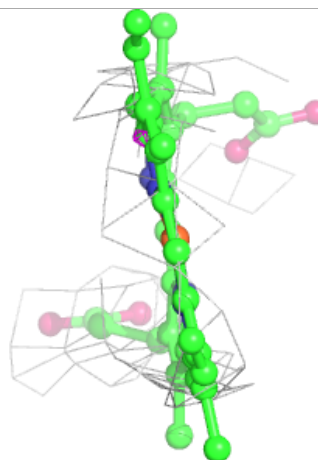
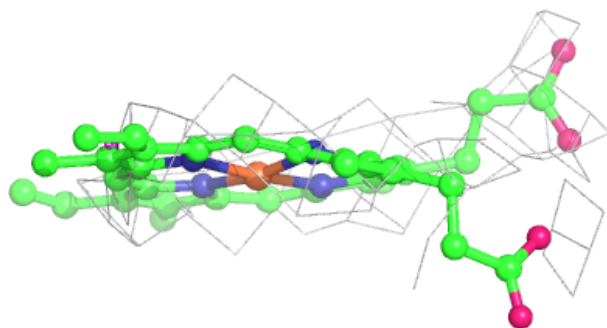
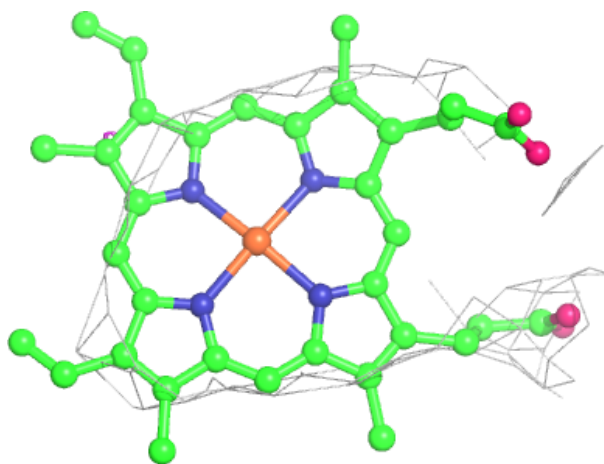
**Electron density around CLA B 607:**

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



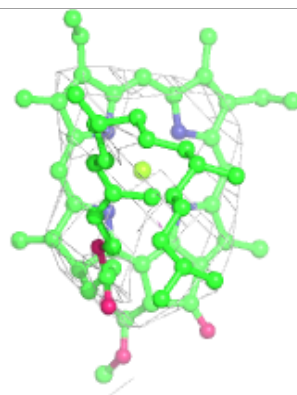
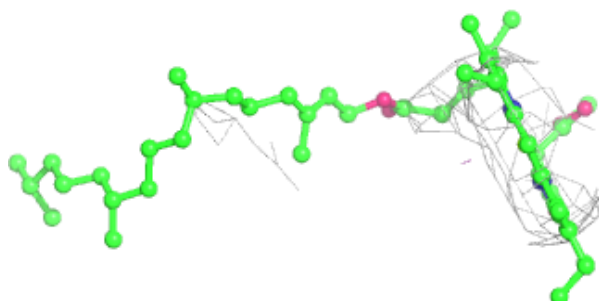
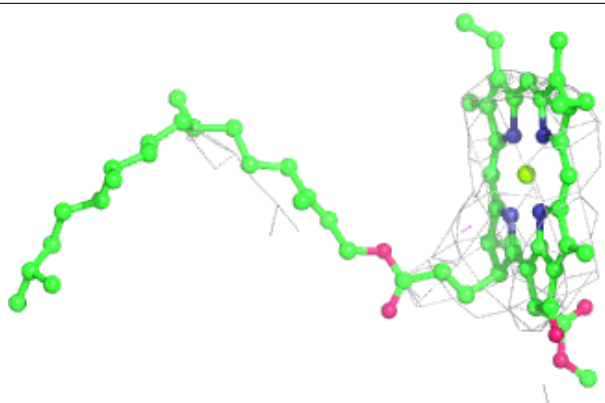
**Electron density around HEM f 101:**

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

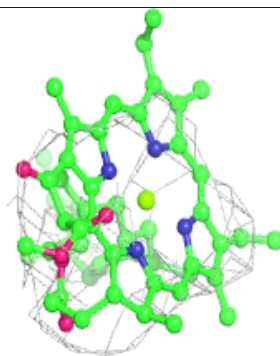
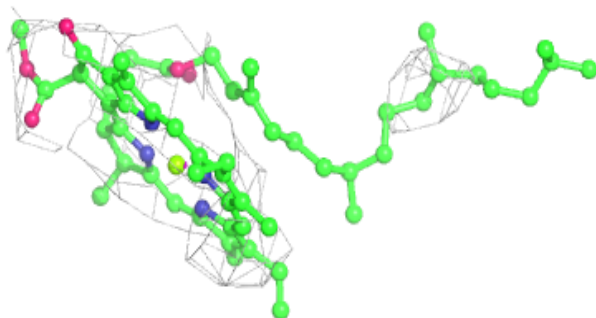
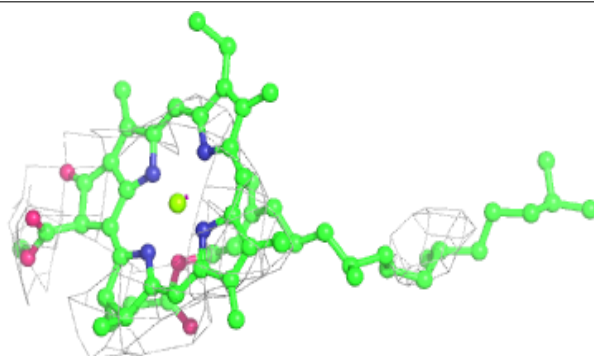


**Electron density around CLA D 406:**

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

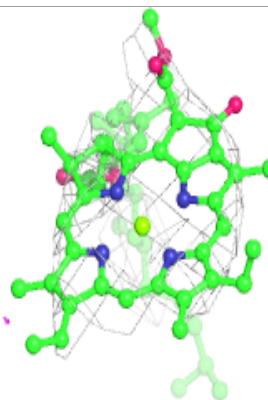
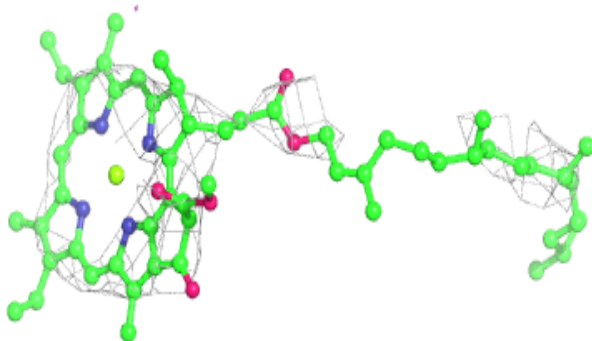
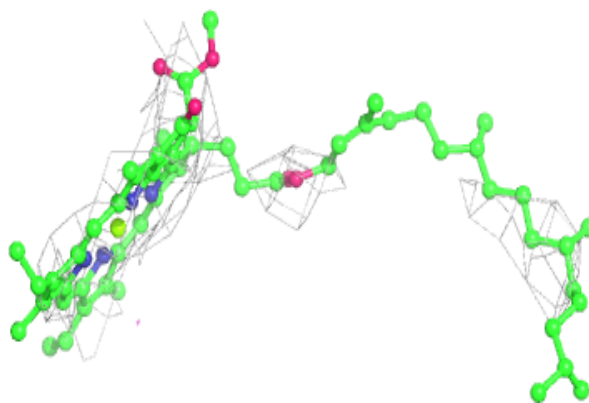
**Electron density around CLA c 504:**

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

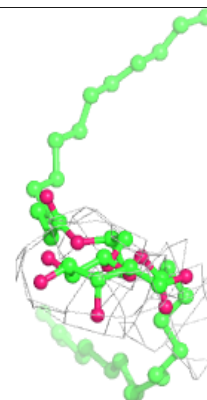
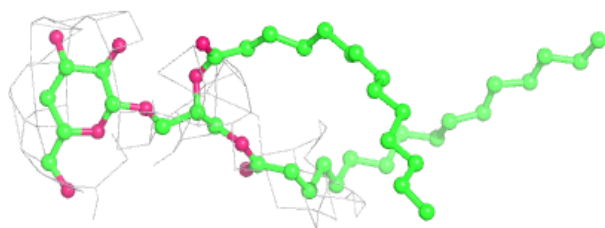
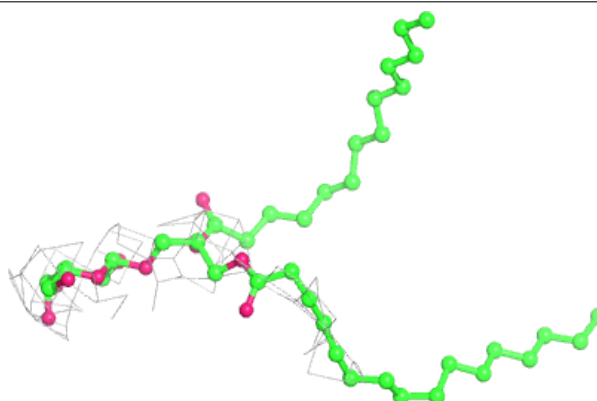


**Electron density around CLA D 405:**

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

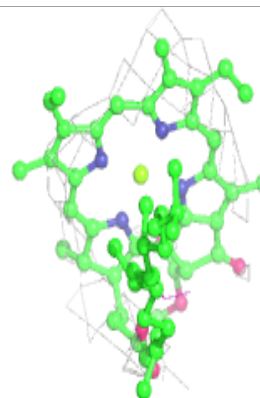
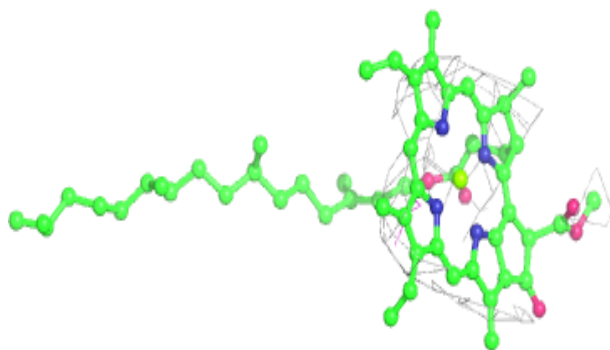
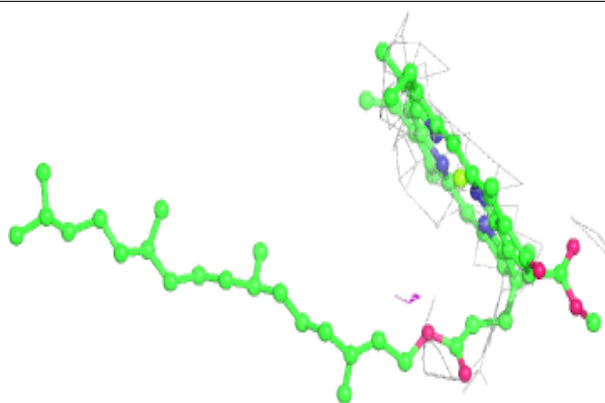
**Electron density around LMG B 621:**

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

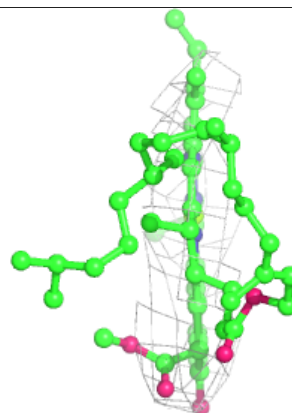
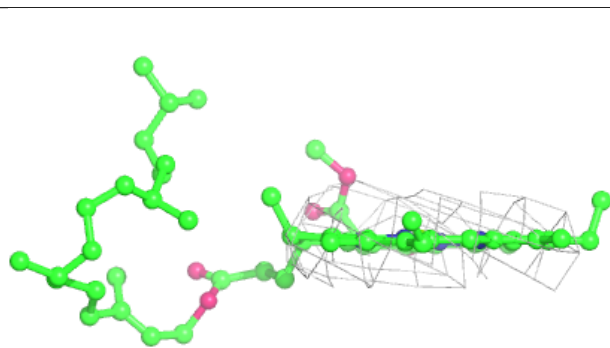
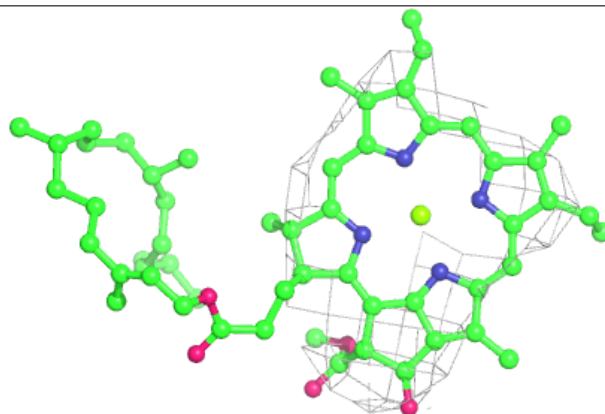


**Electron density around CLA c 520:**

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

**Electron density around CLA C 511:**

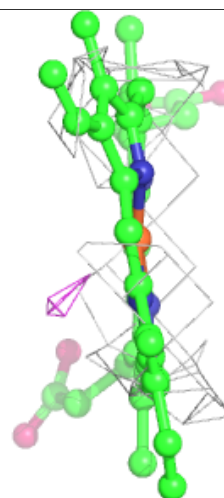
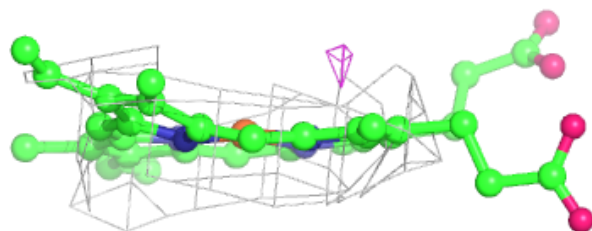
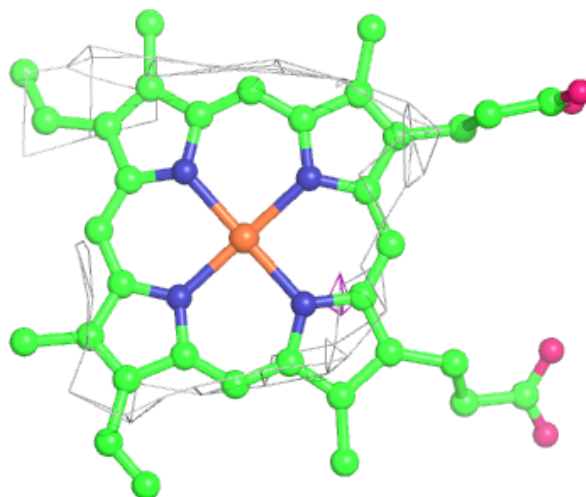
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





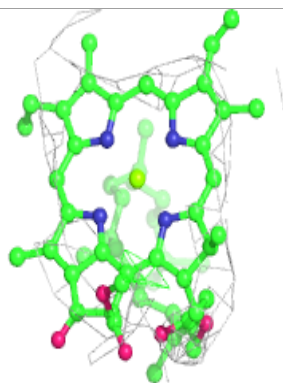
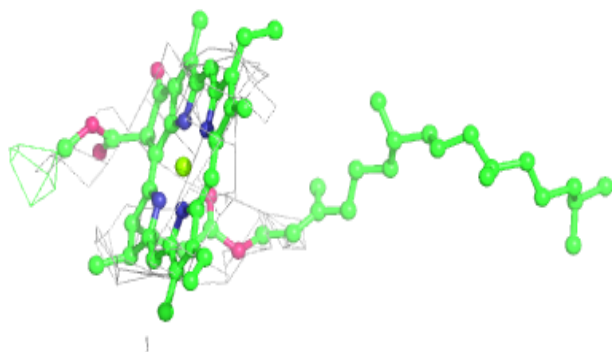
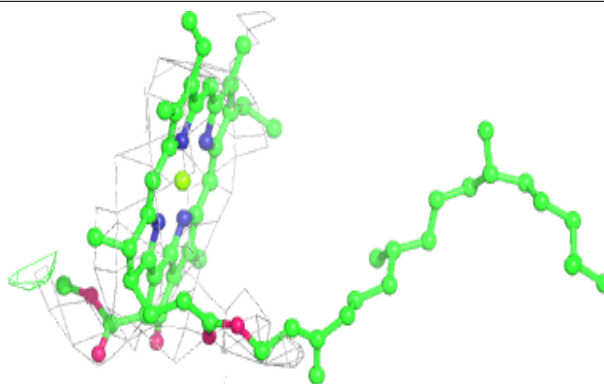
**Electron density around HEM v 201:**

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



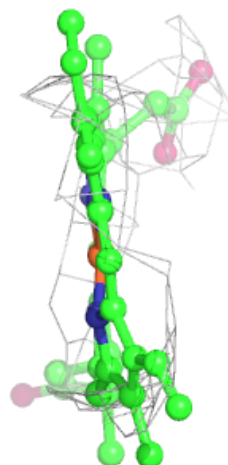
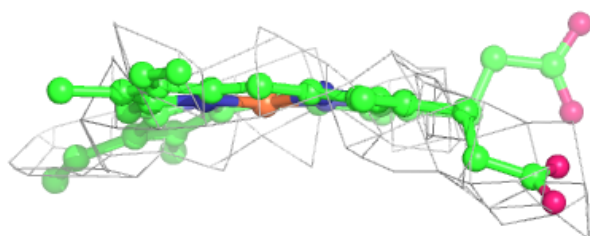
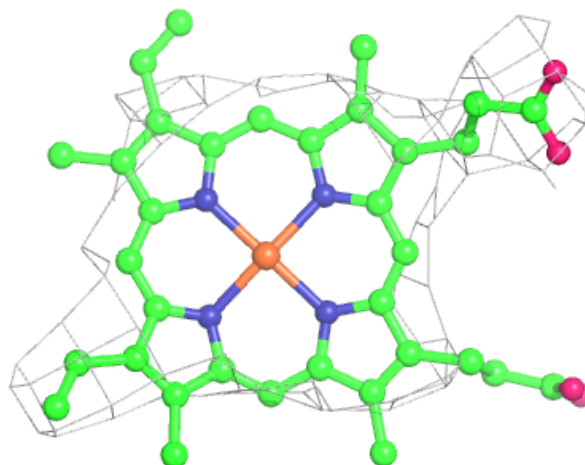
**Electron density around CLA c 507:**

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



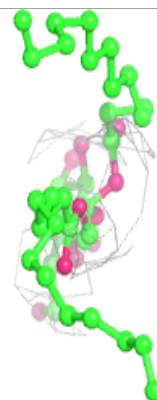
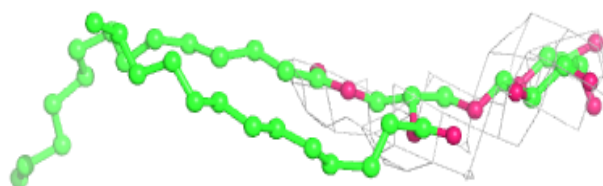
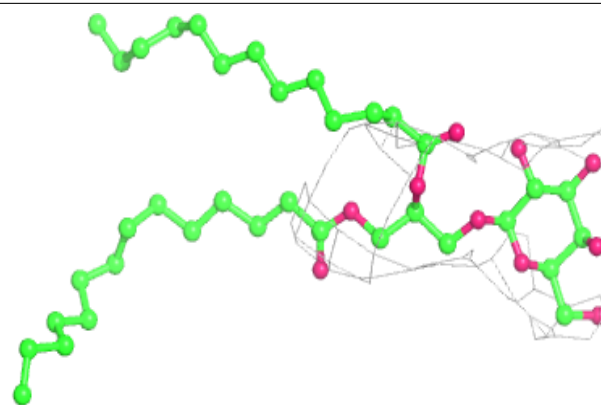
**Electron density around HEM V 201:**

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

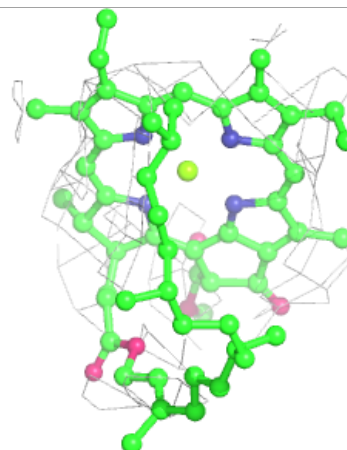
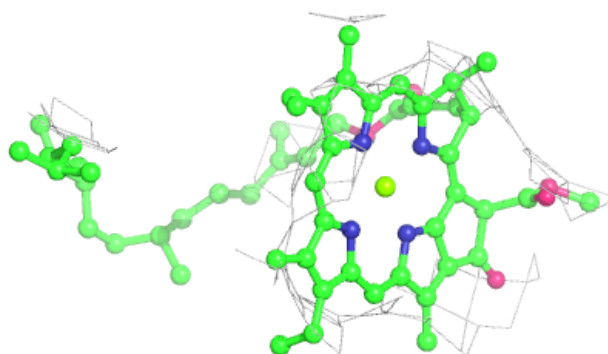
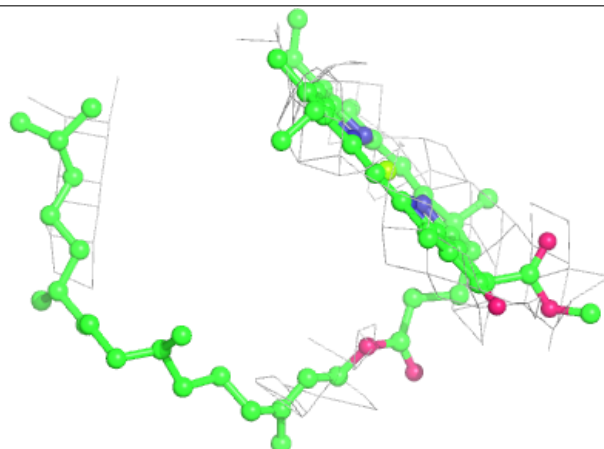


**Electron density around LMG d 412:**

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

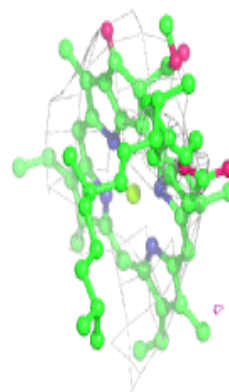
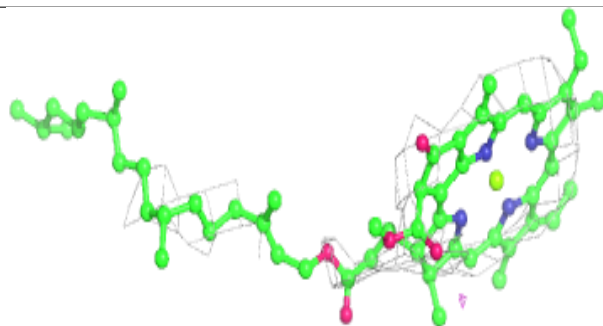
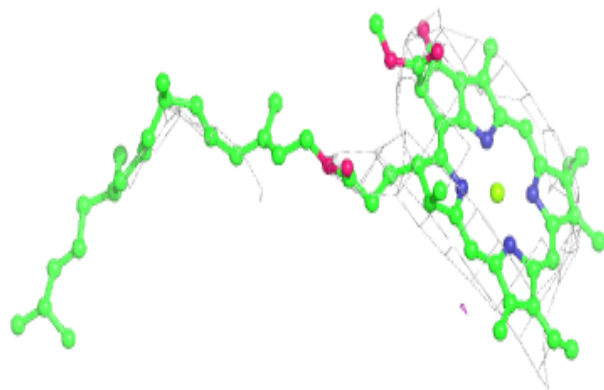
**Electron density around CLA b 614:**

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



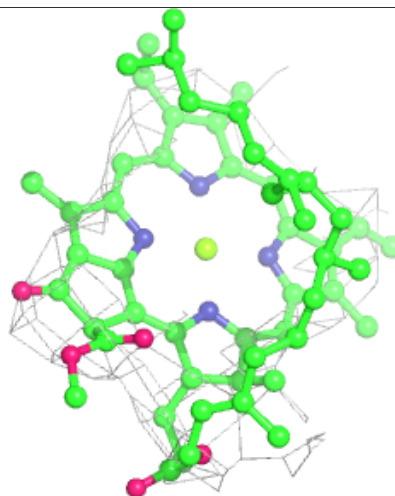
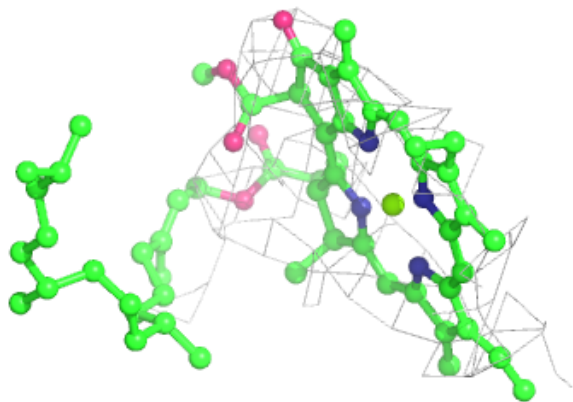
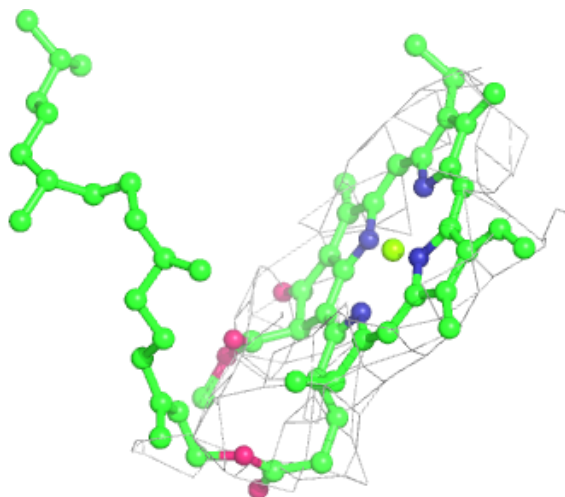
**Electron density around CLA A 402:**

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



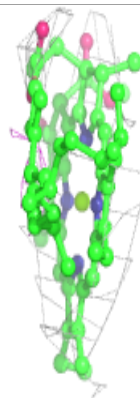
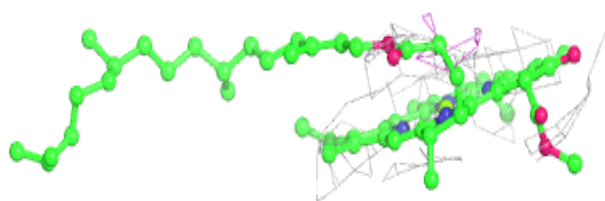
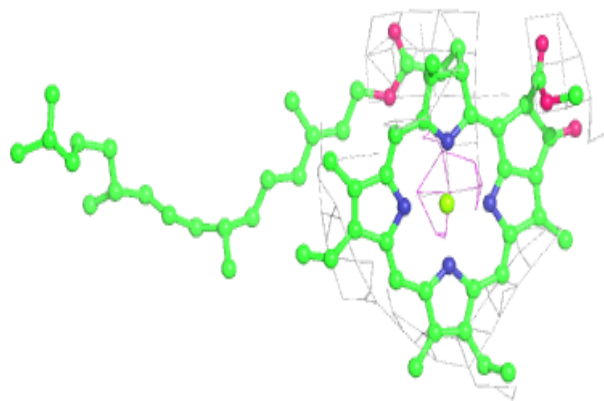
**Electron density around CLA B 612:**

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

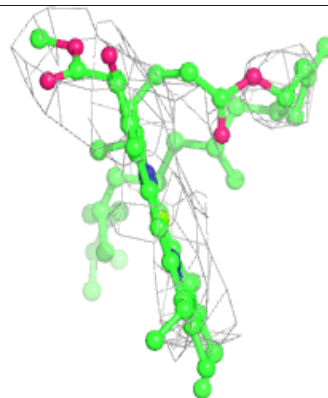
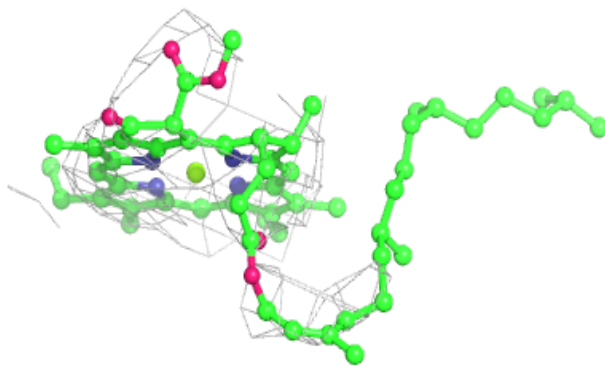
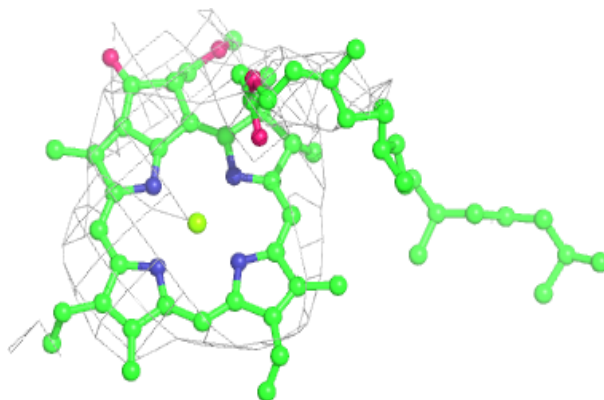


**Electron density around CLA B 602:**

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

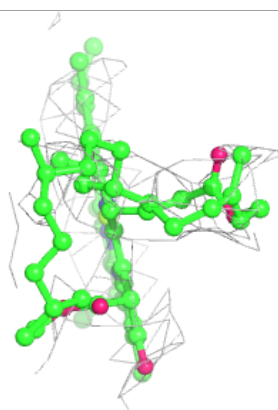
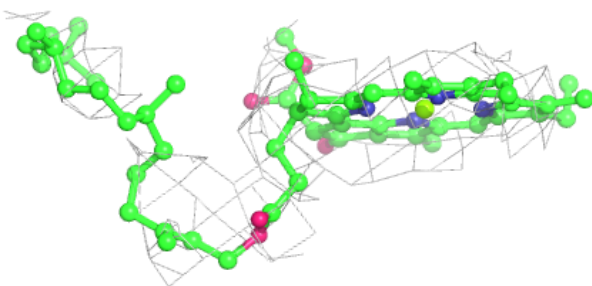
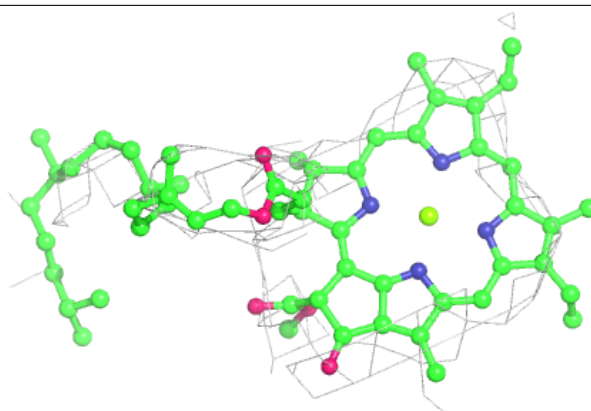
**Electron density around CLA A 403:**

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

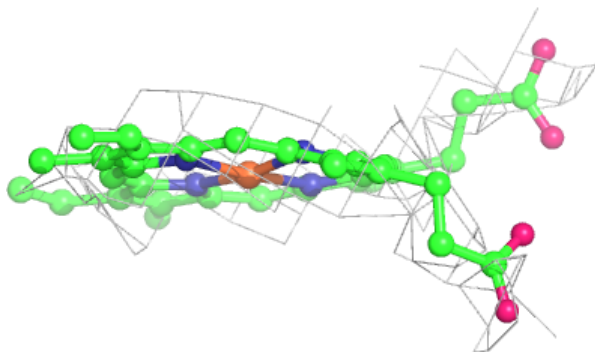
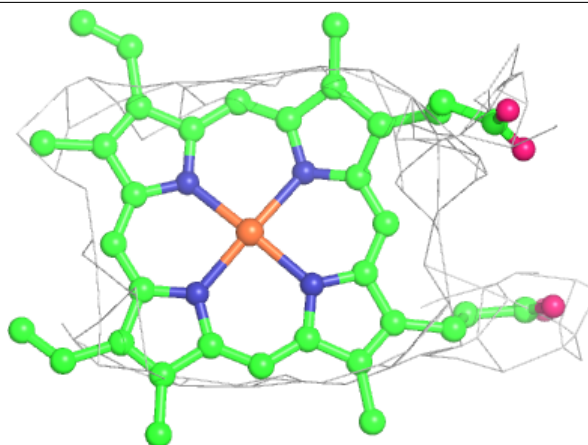


**Electron density around CLA B 611:**

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

**Electron density around HEM F 101:**

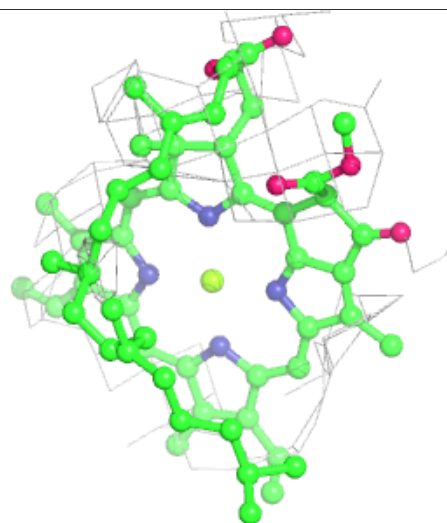
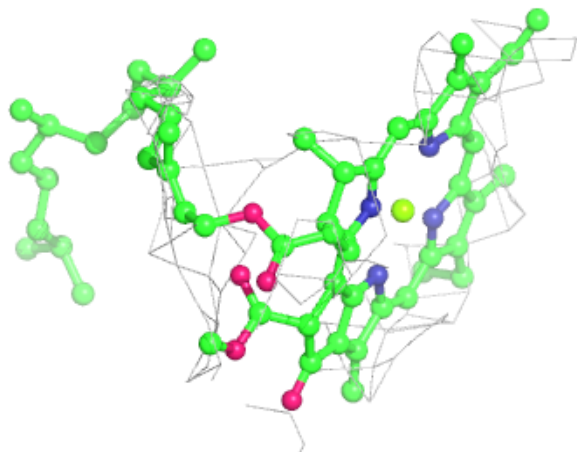
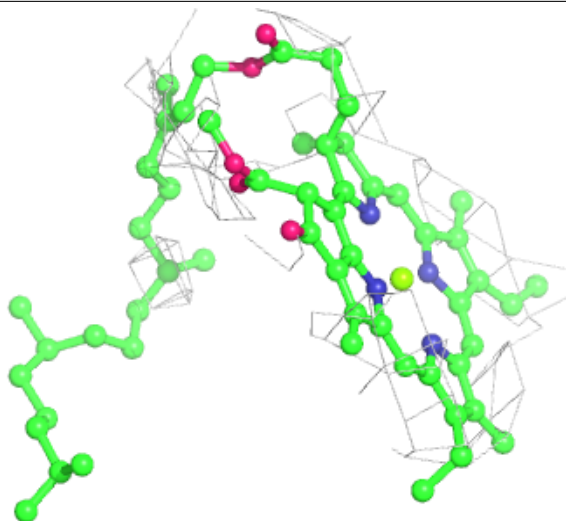
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

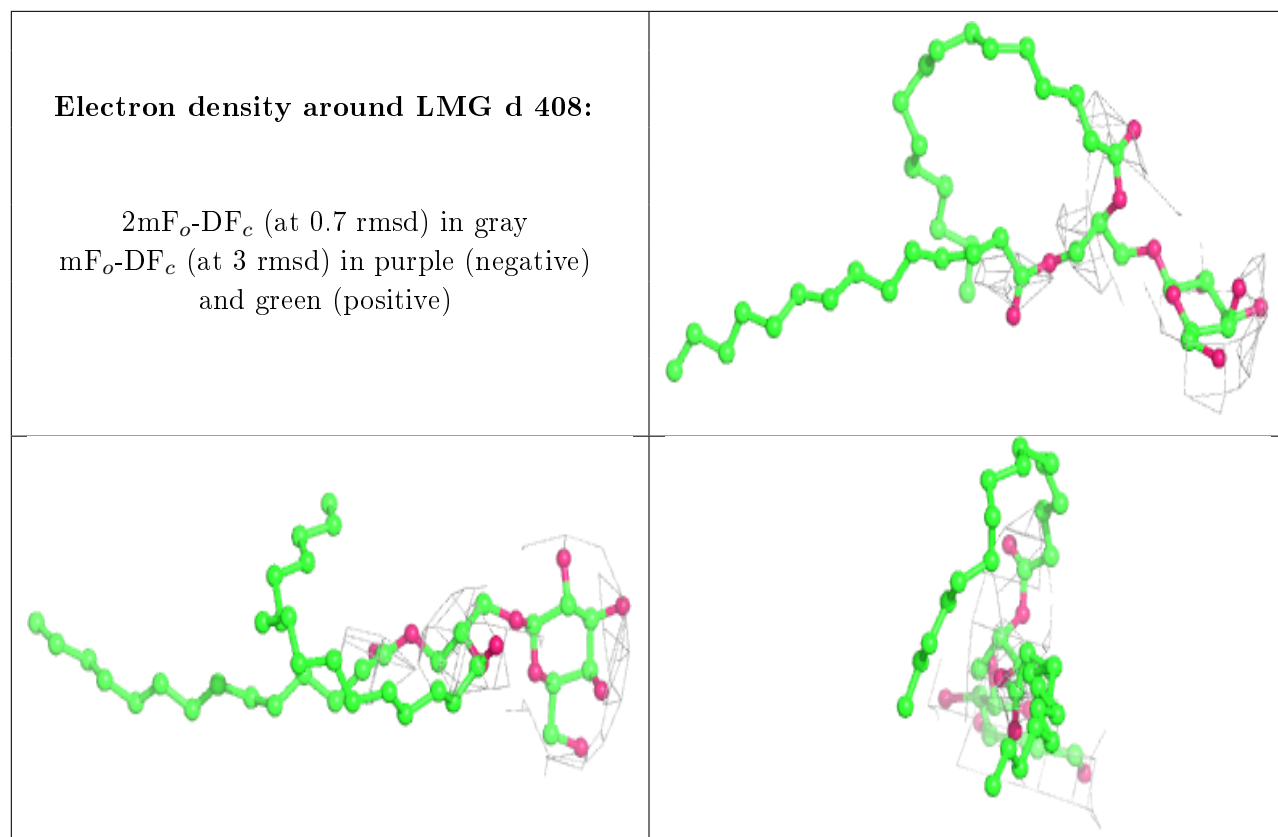




**Electron density around CLA b 616:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.