



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:21 pm BST

PDB ID : 4TNJ  
Title : RT XFEL structure of Photosystem II 500 ms after the 2nd illumination (2F) at 4.5 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 : 4.50 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)

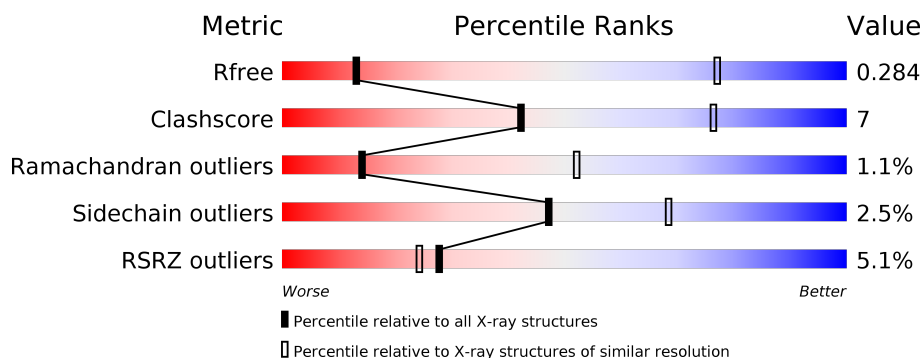
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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	1055 (5.20-3.80)
Clashscore	141614	1123 (5.20-3.80)
Ramachandran outliers	138981	1069 (5.20-3.80)
Sidechain outliers	138945	1050 (5.20-3.80)
RSRZ outliers	127900	1101 (5.30-3.70)

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	<div> <div>8%</div> <div>70%</div> <div>26%</div> <div>• •</div> </div>
1	a	344	<div> <div>8%</div> <div>95%</div> <div>• •</div> </div>
2	B	510	<div> <div>6%</div> <div>77%</div> <div>19%</div> <div>• •</div> </div>

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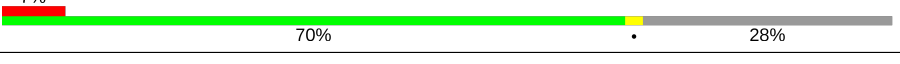
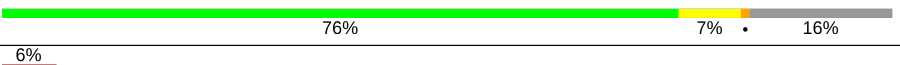

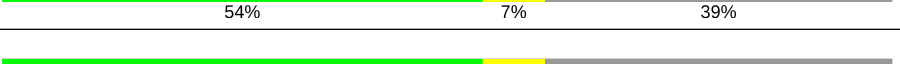
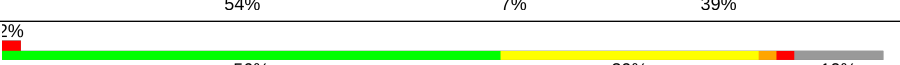
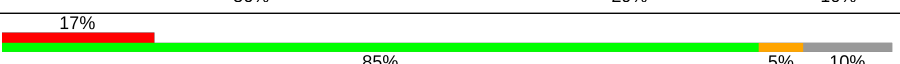
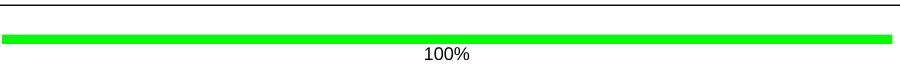
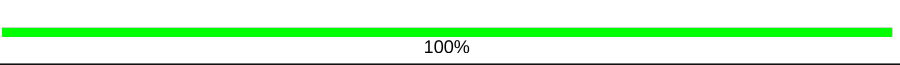

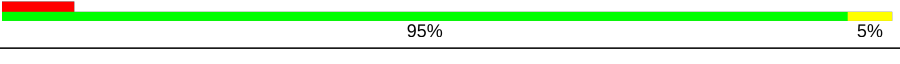

Ideal geometry (proteins) : Engh & Huber (2001)  
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
 Validation Pipeline (wwPDB-VP) : 2.11

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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	-	-	-
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	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	520	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	D	406	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	404	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	406	X	-	-	-
22	CLA	a	408	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	-	-	-

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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	404	X	-	-	-
22	CLA	d	405	X	-	-	-
22	CLA	h	101	X	-	-	X
23	PL9	A	406	-	-	-	X
23	PL9	J	101	-	-	-	X
24	BCR	A	407	-	-	-	X
24	BCR	B	616	-	-	-	X
24	BCR	B	617	-	-	-	X
24	BCR	B	619	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	521	-	-	-	X
24	BCR	D	411	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	J	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	f	102	-	-	-	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	409	-	-	-	X
25	DGD	a	411	-	-	-	X
25	DGD	b	601	-	-	-	X
25	DGD	b	624	-	-	-	X
25	DGD	d	408	-	-	-	X
26	LHG	C	519	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	I	101	-	-	-	X
27	LMG	M	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	a	402	-	-	-	X
27	LMG	a	413	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	m	101	-	-	-	X
28	CL	A	411	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	102	-	-	-	X
30	SQD	d	402	-	-	-	X
31	LMT	B	622	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	627	-	-	-	X
31	LMT	B	628	-	-	-	X
31	LMT	D	410	-	-	-	X
31	LMT	I	102	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	M	103	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	626	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	409	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	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				

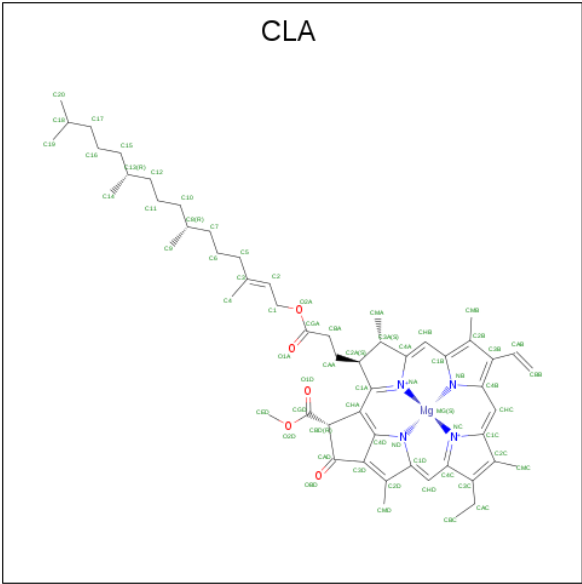
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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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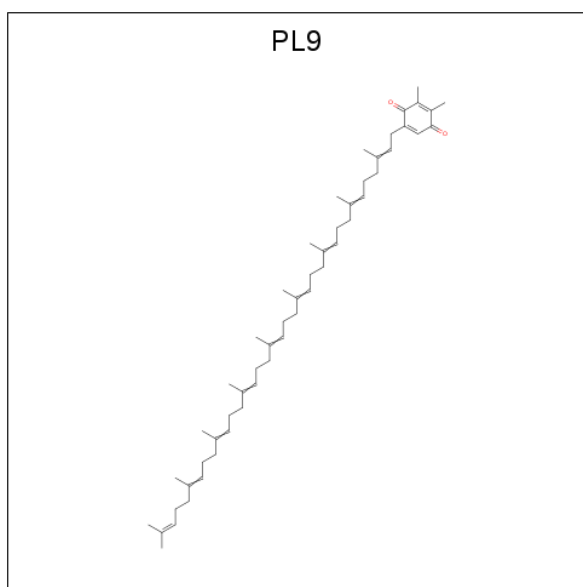
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 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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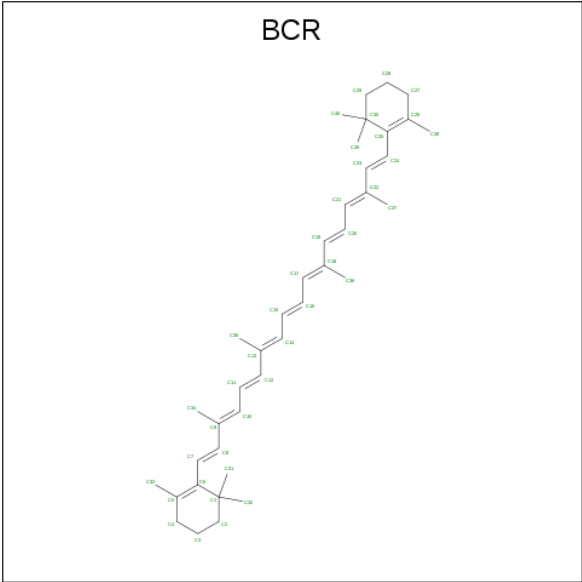
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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>).



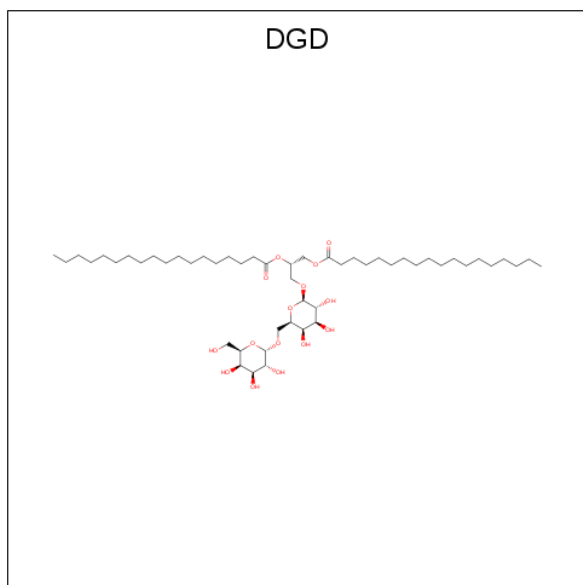
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total 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:  $C_{51}H_{96}O_{15}$ ).



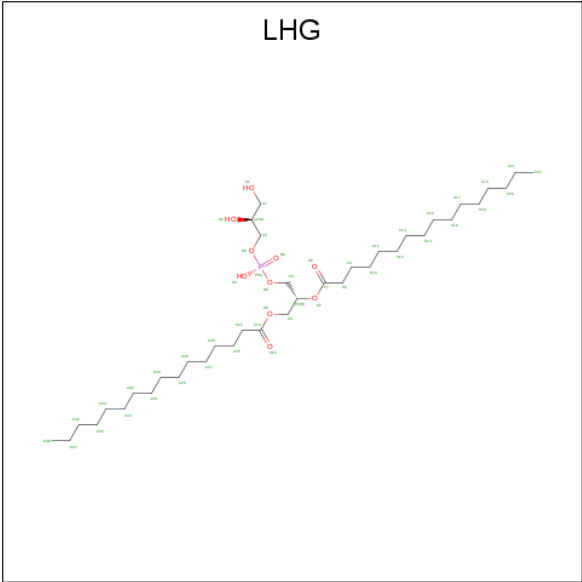
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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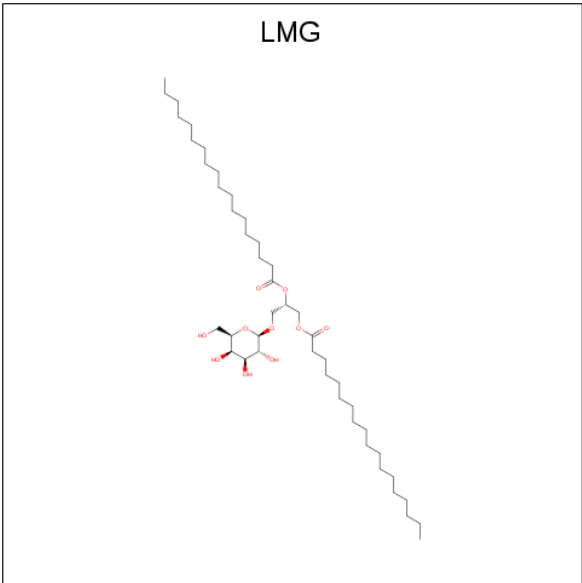
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total	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<sub>38</sub>H<sub>75</sub>O<sub>10</sub>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>).



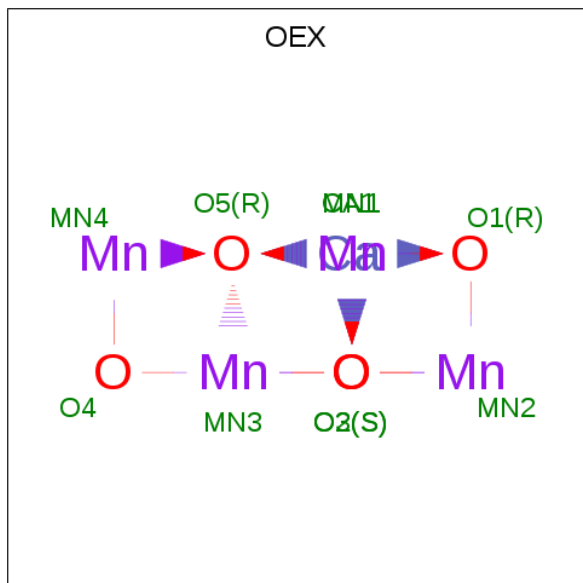


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	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	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
			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 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

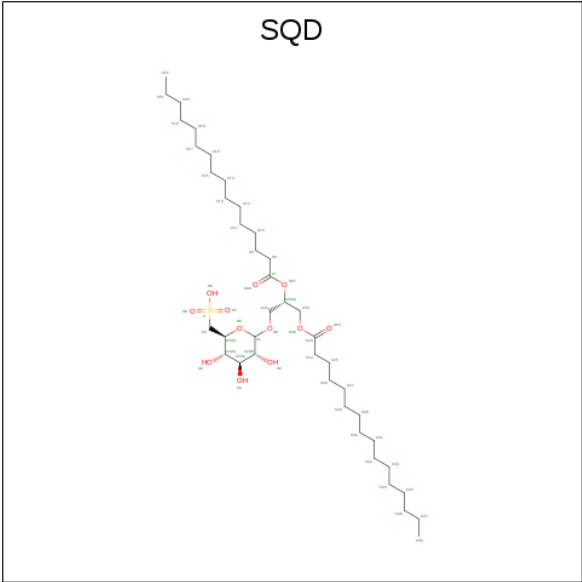
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



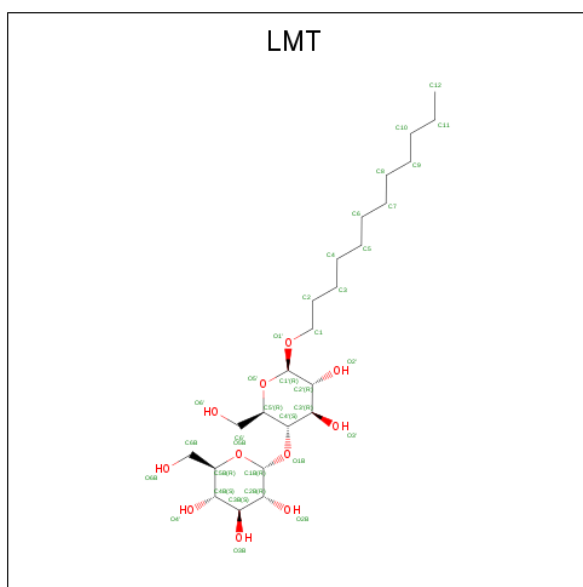
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $\text{C}_{41}\text{H}_{78}\text{O}_{12}\text{S}$ ).



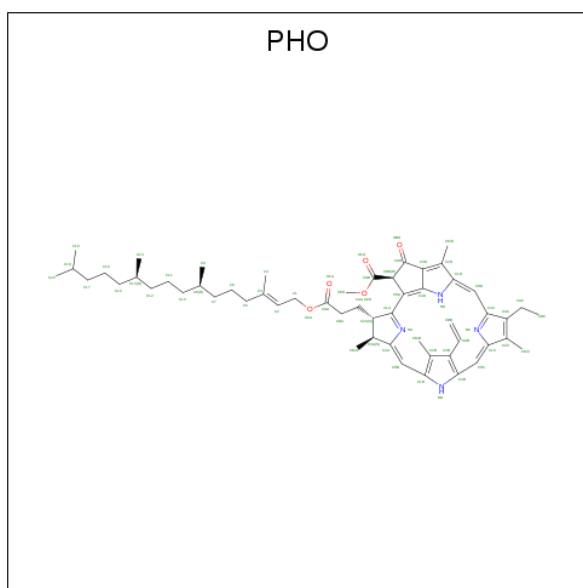
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	D	1	Total	C	O	S	0	0
			43	30	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



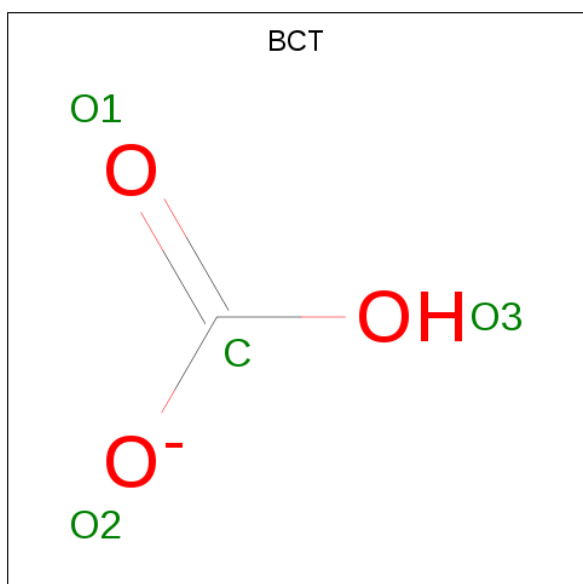
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	D	1	Total 31	C 20	O 11	0	0
31	I	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	b	1	Total 35	C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

- Molecule 32 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



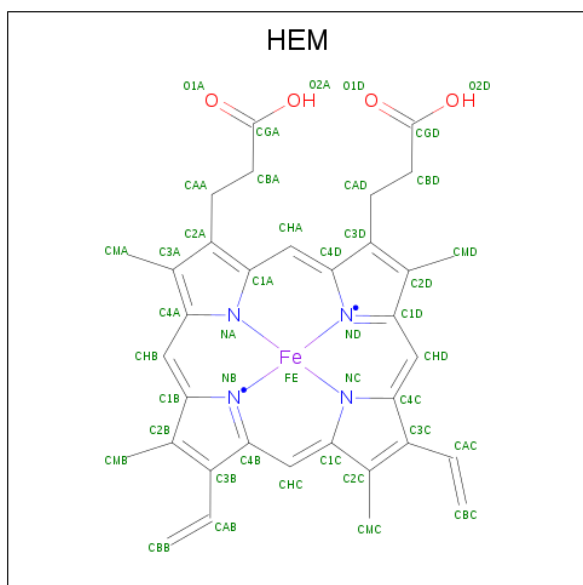
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula:  $CHO_3$ ).



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

- 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 43 34 1 4 4	0	0
34	V	1	Total C Fe N O 43 34 1 4 4	0	0
34	f	1	Total C Fe N O 43 34 1 4 4	0	0
34	v	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

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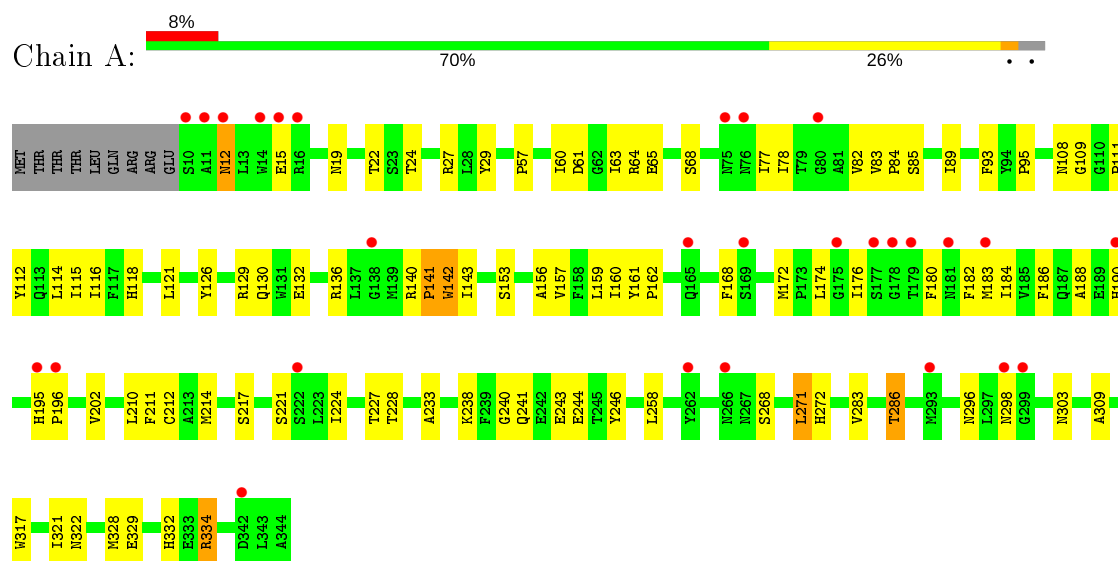
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	k	1	Total	Ca	0	0
			1	1		

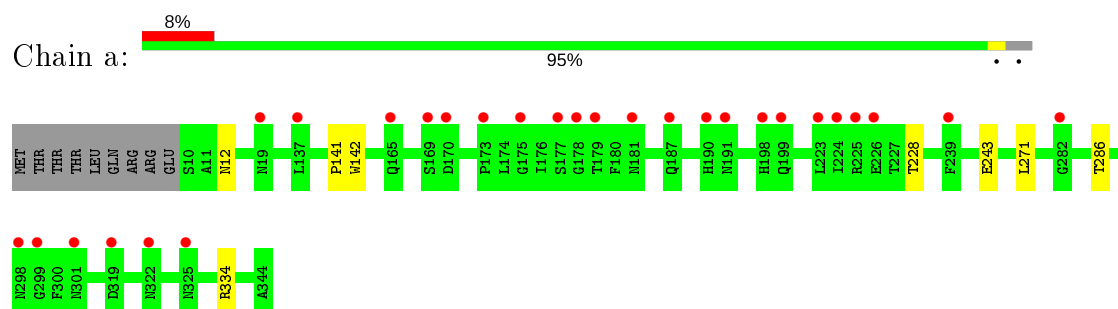
### 3 Residue-property plots [i](#)

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.

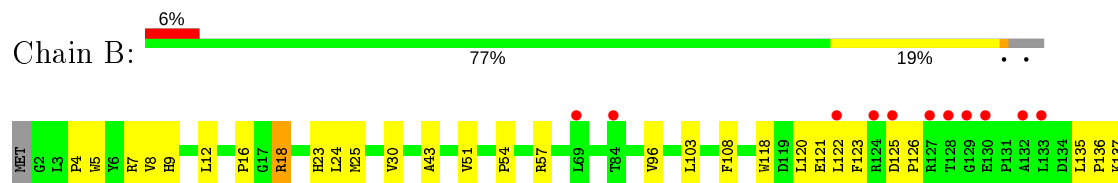
#### • Molecule 1: Photosystem Q(B) protein 1



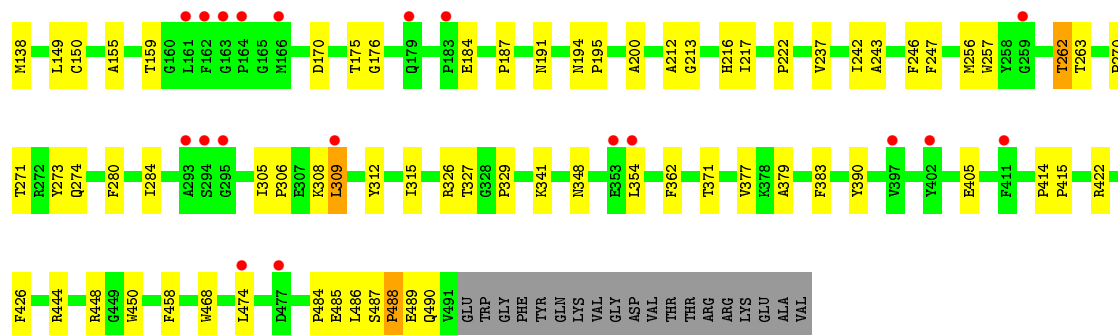
#### • Molecule 1: Photosystem Q(B) protein 1



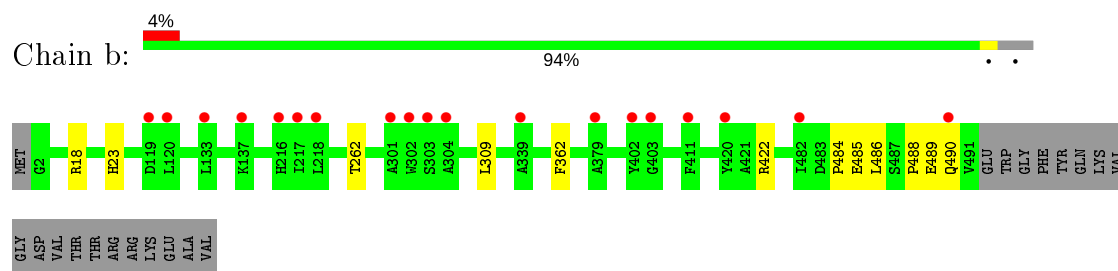
#### • Molecule 2: Photosystem II core light harvesting protein



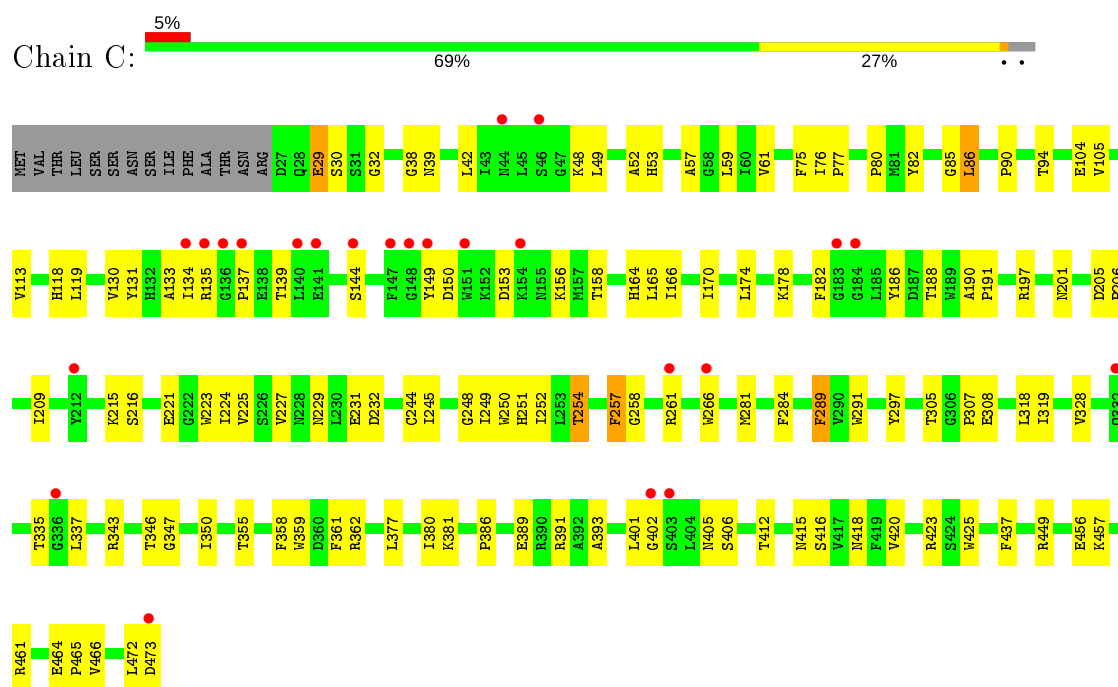




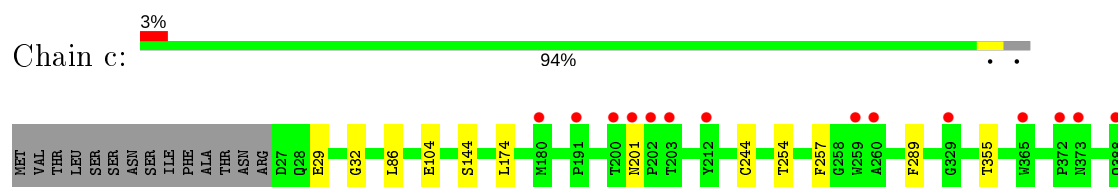
• Molecule 2: Photosystem II core light harvesting protein

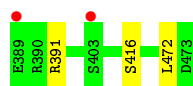


• Molecule 3: Photosystem II CP43 protein

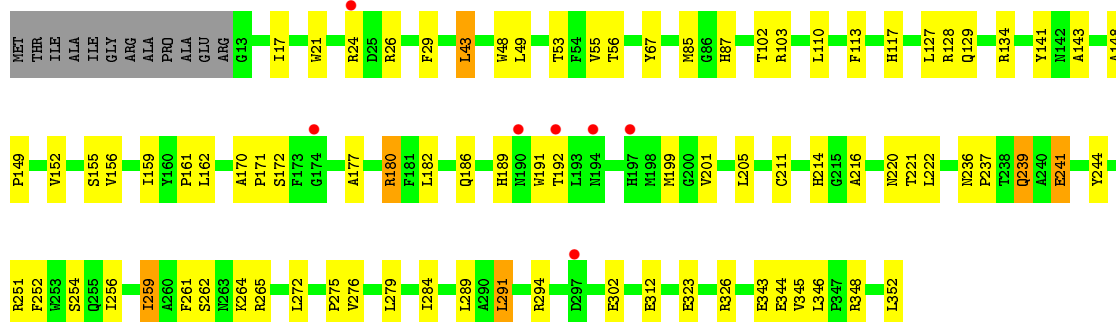
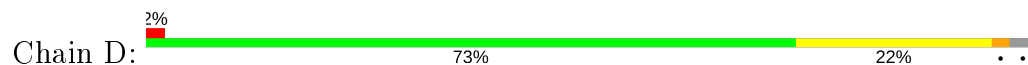


• Molecule 3: Photosystem II CP43 protein

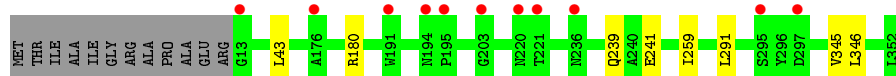




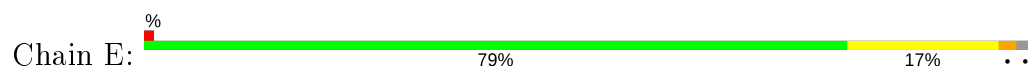
- Molecule 4: Photosystem II D2 protein



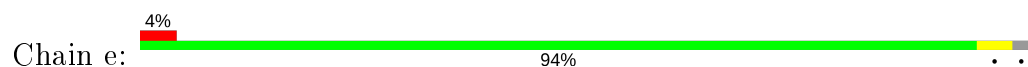
- Molecule 4: Photosystem II D2 protein



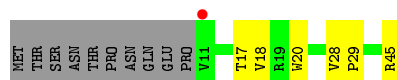
- Molecule 5: Cytochrome b559 subunit alpha




- Molecule 5: Cytochrome b559 subunit alpha

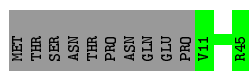


- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta

Chain f:  78% 22%




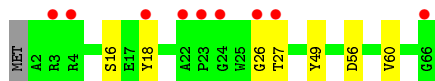
- Molecule 7: Photosystem II reaction center protein H

Chain H:  11% 70% 27% ..



- Molecule 7: Photosystem II reaction center protein H

Chain h:  14% 88% 11% .




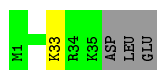
- Molecule 8: Photosystem II reaction center protein I

Chain I:  76% 16% 8%



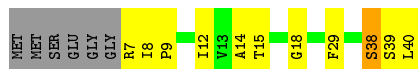
- Molecule 8: Photosystem II reaction center protein I

Chain i:  89% . 8%




- Molecule 9: Photosystem II reaction center protein J

Chain J:  58% 25% . 15%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  80% 5% 15%




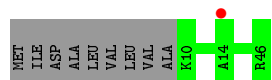
- Molecule 10: Photosystem II reaction center protein K

Chain K:  57% 24% 20%




- Molecule 10: Photosystem II reaction center protein K

Chain k:  2% 80% 20%



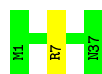
- Molecule 11: Photosystem II reaction center protein L

Chain L:  3% 81% 19%




- Molecule 11: Photosystem II reaction center protein L

Chain l:  97% 3%



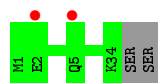
- Molecule 12: Photosystem II reaction center protein M

Chain M:  3% 78% 17% 6%



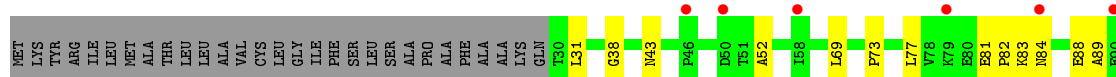
- Molecule 12: Photosystem II reaction center protein M

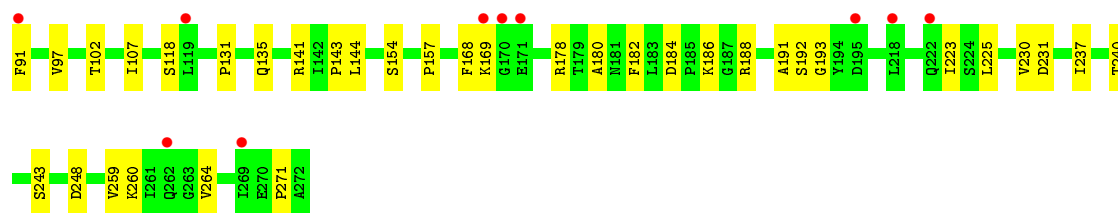
Chain m:  6% 94% 6%



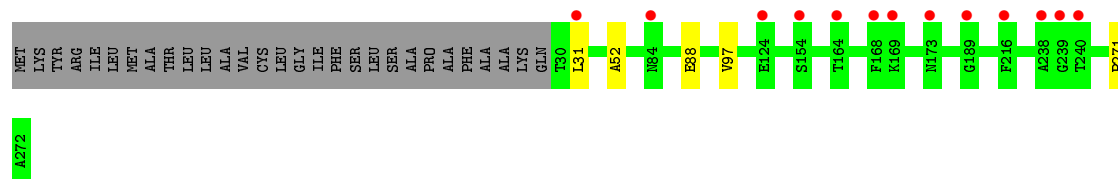
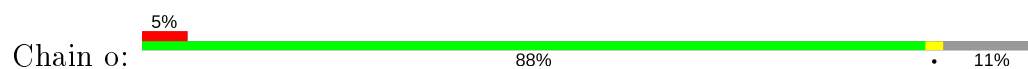
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  6% 72% 18% 11%

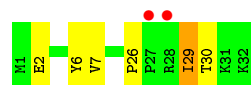
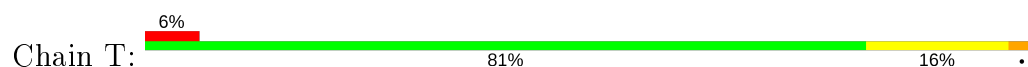




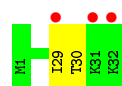
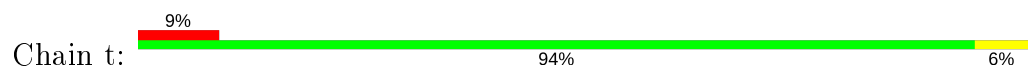
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



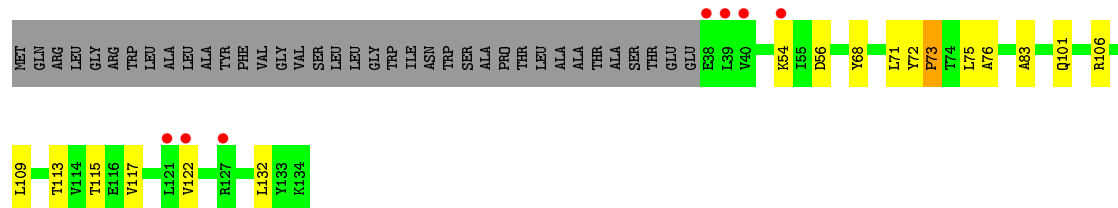
- Molecule 14: Photosystem II reaction center protein T



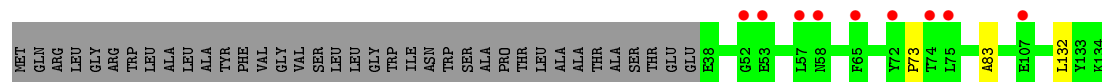
- Molecule 14: Photosystem II reaction center protein T




- Molecule 15: Photosystem II 12 kDa extrinsic protein

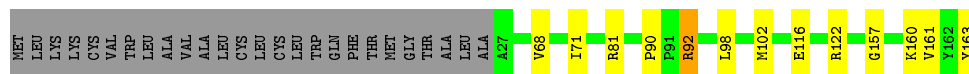


- Molecule 15: Photosystem II 12 kDa extrinsic protein




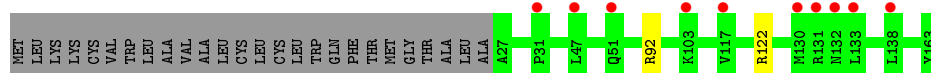
- Molecule 16: Cytochrome c-550

Chain V:  76% 7% 16%



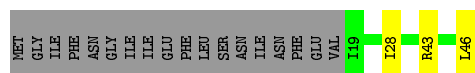
- Molecule 16: Cytochrome c-550

Chain v:  6% 83% 16%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  54% 7% 39%



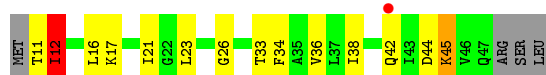
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain g:  2% 54% 7% 39%




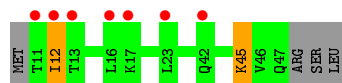
- Molecule 18: Photosystem II reaction center X protein

Chain X:  2% 56% 29% 10%



- Molecule 18: Photosystem II reaction center X protein

Chain x:  17% 85% 5% 10%



- Molecule 19: Photosystem II reaction center protein Y

Chain Y:  100%


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.

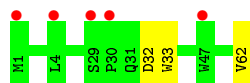
- Molecule 20: Photosystem II reaction center protein Z

Chain Z:  2% 84% 13%



- Molecule 20: Photosystem II reaction center protein Z

Chain z:  8% 95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.30Å 228.71Å 307.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.97 – 4.50 72.97 – 4.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (72.97-4.50) 96.8 (72.97-4.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 4.46Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, $R_{free}$	0.276 , 0.284 0.277 , 0.284	Depositor DCC
$R_{free}$ test set	2668 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	153.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 115.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.16$	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> )	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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	0.23	0/3556	0.41	0/4842
3	c	0.23	0/3556	0.41	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.43	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	0.46	0/709
7	h	0.23	0/520	0.45	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.25	0/293	0.43	0/395
9	J	0.22	0/255	0.40	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.26	0/303	0.48	0/416
10	k	0.26	0/303	0.49	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	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.25	0/284	0.40	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.44	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.26	0/273	0.44	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.25	0/490	0.44	0/669
All	All	0.23	0/41950	0.42	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	79	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	87	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	71	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	18	0
7	h	507	0	521	0	0
8	I	286	0	308	4	0
8	i	286	0	308	0	0
9	J	249	0	262	8	0
9	j	249	0	262	0	0
10	K	293	0	305	9	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	6	0
11	l	304	0	316	0	0
12	M	267	0	289	6	0
12	m	267	0	289	0	0
13	O	1845	0	1801	29	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	13	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	92	0
22	C	845	0	936	49	0
22	D	130	0	144	14	0
22	H	65	0	72	11	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	3	0
23	D	55	0	80	8	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	2	0
24	B	160	0	224	11	0
24	C	120	0	168	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	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	12	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	98	0	136	6	0
27	C	93	0	126	7	0
27	D	94	0	128	7	0
27	E	44	0	58	1	0
27	I	43	0	56	1	0
27	M	42	0	54	1	0
27	a	93	0	126	0	0
27	b	98	0	136	0	0
27	c	93	0	126	0	0
27	d	94	0	128	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	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	47	0	61	3	0
30	D	43	0	50	3	0
30	F	45	0	54	2	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	140	0	184	6	0
31	D	31	0	35	0	0
31	I	35	0	46	1	0
31	M	70	0	92	0	0
31	b	140	0	184	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	16	0
32	a	64	0	74	0	0
32	d	64	0	74	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	51374	586	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 (586) 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	1.56	0.87
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.60	0.82
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.61	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.50	0.80
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.77
34:V:201:HEM:HHD	34:V:201:HEM:HBC2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.71	0.72
22:B:605:CLA:H72	24:B:619:BCR:H311	1.71	0.72
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.74	0.71
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.71	0.71
4:D:199:MET:HG2	23:D:407:PL9:H322	1.73	0.71
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.73	0.71
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.73	0.71
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.56	0.70
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.74	0.70
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.74	0.69
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.74	0.69
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.69
22:C:506:CLA:H112	24:C:514:BCR:H362	1.75	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.67
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.75	0.67
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.76	0.67
4:D:29:PHE:O	4:D:128:ARG:NH2	2.29	0.67
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.30	0.67
4:D:236:ASN:ND2	4:D:239:GLN:O	2.29	0.67
3:C:250:TRP:O	3:C:254:THR:OG1	2.11	0.67
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.77	0.67
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.67
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.77	0.67
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.92	0.66
3:C:291:TRP:O	3:C:305:THR:OG1	2.13	0.66
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.77	0.65
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.77	0.65
4:D:259:ILE:HG12	27:D:408:LMG:H292	1.78	0.65
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.69	0.65
22:B:607:CLA:HBA2	30:D:403:SQD:H101	1.79	0.65
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.78	0.65
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
12:M:31:SER:HA	27:M:101:LMG:HC1	1.83	0.65
2:B:271:THR:HG22	2:B:273:TYR:H	1.64	0.64
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.79	0.64
1:A:174:LEU:HD22	32:D:401:PHO:H151	1.80	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.79	0.64
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.80	0.64
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.81	0.64
30:D:403:SQD:H171	30:D:403:SQD:H301	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.89	0.63
22:A:404:CLA:H142	22:D:405:CLA:H151	1.80	0.63
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.58	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	1.80	0.63
1:A:329:GLU:O	1:A:332:HIS:ND1	2.35	0.62
3:C:406:SER:O	3:C:418:ASN:ND2	2.33	0.62
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
3:C:297:TYR:O	3:C:423:ARG:NH2	2.32	0.62
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.82	0.62
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.83	0.62
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.65	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.33	0.61
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.90	0.61
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.90	0.61
2:B:327:THR:HG21	27:B:621:LMG:H111	1.83	0.60
4:D:186:GLN:HB2	22:D:405:CLA:HBC1	1.82	0.60
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.60
22:A:404:CLA:H71	22:A:405:CLA:HAB	47.01	0.60
3:C:49:LEU:O	3:C:53:HIS:ND1	2.34	0.60
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.41	0.59
4:D:216:ALA:O	4:D:220:ASN:ND2	2.34	0.59
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.85	0.59
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.68	0.59
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.55	0.59
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.88	0.59
30:A:413:SQD:H172	26:C:519:LHG:H172	1.85	0.59
22:A:403:CLA:H203	32:D:401:PHO:H71	1.84	0.59
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.22	0.59
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.84	0.59
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.85	0.59
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.84	0.58
13:O:83:LYS:HG2	13:O:84:ASN:H	1.68	0.58
22:B:611:CLA:H151	22:B:612:CLA:H203	19.93	0.58
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.69	0.58
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.84	0.58
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.88	0.58
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.86	0.58
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.85	0.58
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.33	0.58
12:M:25:LEU:O	12:M:28:GLN:HG3	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:H122	32:D:401:PHO:H3A	32.55	0.58
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.85	0.58
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.91	0.58
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.89	0.57
4:D:192:THR:HG23	22:D:405:CLA:HBC2	1.86	0.57
1:A:64:ARG:O	13:O:178:ARG:NH2	2.39	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.90	0.57
4:D:24:ARG:NH2	18:X:44:ASP:O	2.37	0.57
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.89	0.57
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.57
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.33	0.57
27:D:408:LMG:O6	11:L:15:THR:HG21	2.05	0.57
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.87	0.57
5:E:84:LYS:HB2	5:E:84:LYS:HZ2	1.70	0.57
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.36	0.56
2:B:256:MET:O	2:B:448:ARG:NH1	2.34	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.23	0.56
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.95	0.56
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
22:B:607:CLA:H151	22:B:608:CLA:H203	1.88	0.56
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.87	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.90	0.56
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.87	0.56
3:C:118:HIS:CE1	27:C:518:LMG:H192	2.41	0.56
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.56
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.35	0.55
32:D:402:PHO:H151	22:D:405:CLA:H172	1.88	0.55
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.55
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.87	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.55
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.63	0.55
22:D:406:CLA:H43	18:X:23:LEU:HA	1.89	0.55
22:A:404:CLA:H93	22:D:405:CLA:H152	1.89	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.90	0.55
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.89	0.55
27:D:408:LMG:HO4	27:D:408:LMG:HO5	1.52	0.55
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.89	0.55
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.55
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.89	0.55
22:B:606:CLA:C2D	22:B:608:CLA:H2	40.01	0.55
22:A:405:CLA:H203	32:D:401:PHO:H71	33.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.54
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.54
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.22	0.54
1:A:268:SER:O	1:A:272:HIS:ND1	2.37	0.54
2:B:262:THR:HG22	2:B:263:THR:HG23	1.89	0.54
24:A:407:BCR:H321	30:A:414:SQD:H321	1.90	0.54
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.40	0.54
27:A:410:LMG:H231	23:D:407:PL9:H352	1.90	0.54
22:D:405:CLA:H42	18:X:26:GLY:HA3	26.54	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.96	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
30:B:626:SQD:H1	30:B:626:SQD:H462	1.89	0.54
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.80	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.54
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.34	0.54
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.47	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.92	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.43	0.54
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.90	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.73	0.53
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.16	0.53
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.26	0.53
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.46	0.53
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.53
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.89	0.53
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.98	0.53
2:B:122:LEU:O	7:H:15:ASN:ND2	2.38	0.53
22:A:402:CLA:H122	32:D:401:PHO:H3A	1.90	0.53
24:A:407:BCR:H342	30:A:414:SQD:H311	1.91	0.53
1:A:85:SER:HA	1:A:109:GLY:HA3	1.95	0.53
1:A:29:TYR:O	1:A:129:ARG:NH1	2.52	0.53
30:A:413:SQD:H311	22:C:507:CLA:H71	1.91	0.53
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.39	0.53
22:D:406:CLA:H42	18:X:26:GLY:HA3	1.91	0.53
4:D:214:HIS:ND1	23:D:407:PL9:O2	2.29	0.53
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.92	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.52
26:C:519:LHG:H271	26:C:519:LHG:H101	1.89	0.52
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.34	0.52
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.90	0.52
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.25	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.92	0.52
2:B:474:LEU:O	4:D:134:ARG:NH1	2.48	0.52
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.91	0.52
3:C:85:GLY:N	25:C:516:DGD:HE4	2.25	0.52
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.91	0.52
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.92	0.52
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.92	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.76	0.52
22:B:605:CLA:OBD	31:B:622:LMT:O6'	2.21	0.51
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.51
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.86	0.51
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.75	0.51
1:A:211:PHE:HA	1:A:214:MET:HB2	1.91	0.51
30:A:413:SQD:H223	25:C:517:DGD:HAE1	1.91	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.13	0.51
1:A:132:GLU:O	1:A:136:ARG:HG2	2.10	0.51
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.51
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.44	0.51
13:O:73:PRO:HG2	13:O:102:THR:HB	1.92	0.51
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.03	0.51
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.93	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.82	0.50
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.93	0.50
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.44	0.50
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.93	0.50
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.94	0.50
22:A:403:CLA:HED1	23:D:407:PL9:H372	1.93	0.50
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.93	0.50
24:D:411:BCR:H383	27:D:412:LMG:H171	1.92	0.50
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.50
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.47	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.50
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.93	0.50
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.98	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:403:CLA:HMA2	23:D:407:PL9:H411	1.94	0.50
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.56	0.50
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.96	0.50
2:B:271:THR:HB	2:B:274:GLN:HG3	1.94	0.49
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.94	0.49
22:A:404:CLA:H161	23:A:406:PL9:H253	1.93	0.49
5:E:15:THR:HG23	9:J:8:ILE:O	2.13	0.49
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.28	0.49
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.92	0.49
27:A:415:LMG:H112	2:B:43:ALA:HA	42.24	0.49
22:C:501:CLA:H193	22:C:506:CLA:H111	2.04	0.49
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.94	0.49
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.93	0.49
30:D:403:SQD:H241	30:D:403:SQD:H111	1.95	0.49
15:U:54:LYS:HD2	15:U:113:THR:HG23	1.97	0.49
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.94	0.49
22:B:611:CLA:H51	22:B:612:CLA:H101	18.04	0.49
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.94	0.49
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.95	0.49
22:B:612:CLA:H51	27:B:624:LMG:H231	1.95	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.12	0.49
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.95	0.48
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.94	0.48
13:O:154:SER:N	13:O:169:LYS:O	2.45	0.48
4:D:221:THR:HG23	4:D:244:TYR:HB2	1.98	0.48
4:D:261:PHE:HB2	23:D:407:PL9:H522	1.95	0.48
13:O:118:SER:HB3	13:O:157:PRO:HA	2.00	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.71	0.48
2:B:135:LEU:HA	2:B:138:MET:HE3	2.04	0.48
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.95	0.48
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.95	0.48
31:B:627:LMT:H62	8:I:4:LEU:HD22	82.13	0.48
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.48
2:B:256:MET:HA	2:B:263:THR:HG21	1.95	0.48
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.43	0.48
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.82	0.48
1:A:210:LEU:HG	32:D:402:PHO:NC	2.29	0.48
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.99	0.48
22:A:405:CLA:H162	22:A:405:CLA:H141	1.69	0.48
2:B:222:PRO:HG3	7:H:27:THR:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.48
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.02	0.48
1:A:190:HIS:O	1:A:298:ASN:HB3	2.15	0.48
3:C:130:VAL:O	3:C:134:ILE:HG12	2.18	0.48
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.02	0.48
1:A:258:LEU:O	4:D:128:ARG:NH1	2.47	0.48
2:B:383:PHE:N	4:D:344:GLU:O	2.34	0.48
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.29	0.48
2:B:327:THR:HG22	22:B:606:CLA:H12	1.96	0.48
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.96	0.48
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.96	0.48
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.96	0.48
22:D:405:CLA:H43	18:X:23:LEU:HA	28.38	0.47
22:B:611:CLA:H171	22:B:612:CLA:HBB2	1.95	0.47
31:B:628:LMT:H122	14:T:7:VAL:HG12	34.49	0.47
4:D:279:LEU:HG	32:D:402:PHO:HBC3	1.96	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.78	0.47
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.78	0.47
22:B:615:CLA:H72	22:B:615:CLA:H12	1.96	0.47
4:D:85:MET:HA	5:E:69:ARG:HB3	2.04	0.47
1:A:78:ILE:O	1:A:176:ILE:HB	2.15	0.47
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.97	0.47
22:B:614:CLA:H172	22:B:614:CLA:H111	1.97	0.47
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.45	0.47
22:B:606:CLA:H2	22:B:608:CLA:H93	34.07	0.47
22:B:612:CLA:H171	27:B:624:LMG:H401	1.97	0.47
32:D:401:PHO:H41	32:D:401:PHO:H62	1.46	0.47
22:B:611:CLA:H18	22:B:612:CLA:H192	22.23	0.47
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.97	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	2.00	0.47
1:A:298:ASN:ND2	3:C:402:GLY:O	2.48	0.47
24:B:619:BCR:H361	24:B:619:BCR:H20C	1.77	0.47
30:F:102:SQD:H162	18:X:33:THR:HA	1.96	0.47
27:I:101:LMG:H181	31:I:102:LMT:H42	2.02	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.47
25:B:625:DGD:HD1	31:B:627:LMT:H32	1.97	0.47
22:C:506:CLA:H62	22:C:506:CLA:H92	1.73	0.47
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.47
1:A:224:ILE:O	4:D:265:ARG:NH2	2.52	0.46
2:B:170:ASP:OD1	2:B:175:THR:N	2.51	0.46
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:518:LMG:H292	27:C:518:LMG:H111	1.96	0.46
1:A:121:LEU:HD13	25:A:408:DGD:HB92	1.97	0.46
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.46
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.46
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.81	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.98	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.96	0.46
2:B:371:THR:HG22	2:B:377:VAL:HA	1.97	0.46
22:B:613:CLA:H51	24:B:616:BCR:H372	1.97	0.46
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.60	0.46
22:C:512:CLA:HAB	24:C:521:BCR:H24C	2.03	0.46
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.96	0.46
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.47	0.46
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.98	0.46
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.98	0.46
3:C:158:THR:O	3:C:251:HIS:HB3	2.15	0.46
27:D:408:LMG:H111	11:L:19:LEU:HD21	1.97	0.46
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.97	0.46
2:B:327:THR:HG22	22:B:610:CLA:H12	26.92	0.46
22:A:405:CLA:H62	22:A:405:CLA:H41	3.95	0.46
3:C:113:VAL:HG11	27:C:518:LMG:H132	2.02	0.46
22:C:503:CLA:H201	22:C:503:CLA:HMD2	2.02	0.46
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.46
1:A:114:LEU:O	1:A:118:HIS:ND1	2.45	0.45
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.55	0.45
25:B:620:DGD:HAW2	22:H:101:CLA:H152	1.99	0.45
22:C:510:CLA:H61	22:C:510:CLA:H93	1.82	0.45
4:D:348:ARG:NH2	4:D:352:LEU:O	2.39	0.45
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.65	0.45
22:H:101:CLA:H162	22:H:101:CLA:H122	1.51	0.45
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.04	0.45
24:B:616:BCR:H361	24:B:616:BCR:H20C	1.76	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.45
22:C:508:CLA:H11	22:C:508:CLA:H51	1.81	0.45
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.74	0.45
22:C:504:CLA:H11	24:C:514:BCR:H312	2.02	0.45
1:A:202:VAL:HB	22:A:404:CLA:HMB3	12.99	0.45
4:D:48:TRP:CE2	32:D:402:PHO:H161	2.52	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.15	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)
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.45
22:A:402:CLA:H51	32:D:401:PHO:C3B	2.47	0.45
27:B:621:LMG:H421	4:D:284:ILE:HD13	1.99	0.45
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.45
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.01	0.45
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.99	0.45
24:C:514:BCR:H361	24:C:514:BCR:H20C	1.84	0.45
7:H:46:LEU:HD13	22:H:101:CLA:H72	2.00	0.45
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.80	0.45
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.45
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.04	0.45
24:B:618:BCR:H20C	24:B:618:BCR:H361	1.82	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.17	0.45
3:C:224:ILE:O	3:C:227:VAL:HG23	2.17	0.45
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.01	0.45
8:I:29:ALA:HA	8:I:35:LYS:HB2	2.03	0.45
30:A:414:SQD:H332	22:B:609:CLA:H203	66.13	0.44
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.52	0.44
4:D:102:THR:OG1	25:D:409:DGD:HD62	2.17	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.17	0.44
2:B:213:GLY:O	2:B:217:ILE:HG13	2.17	0.44
22:B:611:CLA:H162	22:B:611:CLA:H122	1.76	0.44
22:B:605:CLA:H18	22:B:615:CLA:H121	1.99	0.44
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.44
5:E:60:GLN:HG2	5:E:62:SER:H	1.86	0.44
22:H:101:CLA:H62	22:H:101:CLA:H41	1.56	0.44
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.70	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	1.99	0.44
22:B:604:CLA:H62	22:B:604:CLA:H41	1.80	0.44
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.06	0.44
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.19	0.44
22:C:512:CLA:HBA2	22:C:512:CLA:H3A	1.72	0.44
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.53	0.44
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.50	0.44
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.20	0.44
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.00	0.44
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.00	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	2.00	0.44
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.89	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.52	0.44
22:C:512:CLA:HAB	24:C:521:BCR:H371	2.02	0.44
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.53	0.44
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.48	0.44
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.86	0.44
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.84	0.44
2:B:468:TRP:HH2	27:B:624:LMG:HO2	1.62	0.44
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.19	0.44
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.99	0.44
24:C:513:BCR:H343	24:C:513:BCR:H311	2.03	0.44
7:H:35:MET:HB2	7:H:35:MET:HE3	1.86	0.44
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.77	0.44
1:A:141:PRO:HB2	1:A:142:TRP:H	1.66	0.44
26:A:409:LHG:H382	22:C:509:CLA:H93	2.00	0.44
22:B:607:CLA:H51	22:B:608:CLA:H101	1.99	0.44
3:C:245:ILE:O	3:C:249:ILE:HG12	2.19	0.44
4:D:262:SER:N	27:D:408:LMG:O3	2.46	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.44
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.05	0.44
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.03	0.43
22:B:605:CLA:HBA2	22:B:605:CLA:H3A	1.27	0.43
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.79	0.43
24:B:616:BCR:H383	30:B:626:SQD:H111	1.99	0.43
3:C:456:GLU:N	3:C:456:GLU:OE1	2.51	0.43
22:C:520:CLA:H112	22:C:520:CLA:H142	1.76	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.53	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.65	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.18	0.43
27:D:408:LMG:O9	27:D:408:LMG:HC1	2.18	0.43
13:O:240:THR:HA	13:O:264:VAL:HA	1.99	0.43
25:B:620:DGD:HA71	22:H:101:CLA:H193	2.01	0.43
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.04	0.43
2:B:329:PRO:HB3	22:B:606:CLA:HED1	2.01	0.43
22:B:613:CLA:H12	22:B:613:CLA:H51	4.48	0.43
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.43
3:C:456:GLU:HG2	3:C:457:LYS:HG3	2.03	0.43
32:D:401:PHO:H13	32:D:401:PHO:H102	1.82	0.43
7:H:12:ARG:HD3	7:H:12:ARG:O	2.18	0.43
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:403:CLA:H51	22:A:403:CLA:H11	1.81	0.43
22:B:607:CLA:H18	22:B:608:CLA:H192	2.01	0.43
2:B:108:PHE:HB2	30:B:626:SQD:H223	2.00	0.43
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
15:U:106:ARG:HA	15:U:109:LEU:HG	1.99	0.43
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.01	0.43
1:A:240:GLY:HA3	14:T:29:ILE:HG22	2.00	0.43
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.83	0.43
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.79	0.43
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.54	0.43
22:B:606:CLA:H41	22:B:606:CLA:H61	2.86	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.78	0.43
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.04	0.43
4:D:252:PHE:O	4:D:256:ILE:HG22	2.21	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.93	0.43
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.00	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.43
24:C:521:BCR:H361	24:C:521:BCR:H20C	1.81	0.43
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.43
22:B:613:CLA:H91	22:B:613:CLA:H112	1.85	0.43
31:B:628:LMT:H1B	31:B:628:LMT:H3'	1.53	0.43
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.01	0.43
24:C:521:BCR:H371	24:C:521:BCR:H24C	1.82	0.43
32:D:402:PHO:CHB	22:D:405:CLA:H101	2.49	0.43
15:U:72:TYR:O	15:U:76:ALA:HB3	2.18	0.43
22:A:405:CLA:H11	22:A:405:CLA:H51	4.35	0.42
22:C:501:CLA:H162	22:C:501:CLA:H141	1.78	0.42
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.42
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.01	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.51	0.42
16:V:98:LEU:O	16:V:102:MET:HG3	2.24	0.42
22:A:403:CLA:H202	22:A:403:CLA:H162	1.76	0.42
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.02	0.42
27:C:522:LMG:H322	10:K:27:VAL:HG23	2.08	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.04	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.02	0.42
1:A:182:PHE:O	1:A:186:PHE:HB2	2.20	0.42
22:D:405:CLA:H62	22:D:405:CLA:H92	1.80	0.42
22:A:404:CLA:H143	22:A:404:CLA:H161	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.85	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.79	0.42
2:B:25:MET:HG2	24:B:616:BCR:H23C	2.00	0.42
22:B:605:CLA:C3D	31:B:622:LMT:H11	2.50	0.42
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.01	0.42
3:C:402:GLY:HA3	3:C:420:VAL:HG22	2.01	0.42
22:C:511:CLA:H61	22:C:511:CLA:H13	2.01	0.42
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.03	0.42
32:D:401:PHO:H202	32:D:401:PHO:H162	1.86	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.00	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.65	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.85	0.42
22:C:520:CLA:O2D	27:C:522:LMG:O2	2.40	0.42
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.19	0.42
22:A:405:CLA:H162	22:A:405:CLA:H202	3.78	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.92	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.94	0.42
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.02	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.42
25:D:409:DGD:O5E	25:D:409:DGD:O4E	2.25	0.42
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.20	0.42
1:A:238:LYS:O	1:A:241:GLN:HG3	2.20	0.42
22:A:404:CLA:H151	32:D:401:PHO:H72	40.46	0.42
22:B:615:CLA:H162	22:B:615:CLA:H122	5.17	0.42
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.02	0.42
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.84	0.42
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.42
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.56	0.42
2:B:212:ALA:O	2:B:216:HIS:ND1	2.51	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.74	0.42
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.88	0.42
4:D:155:SER:HA	4:D:159:ILE:HB	2.07	0.42
22:A:403:CLA:HAA1	23:D:407:PL9:H362	2.01	0.42
27:C:522:LMG:H112	24:J:102:BCR:H373	2.01	0.42
11:L:4:ASN:OD1	11:L:6:ASN:ND2	2.52	0.42
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.42
16:V:90:PRO:O	16:V:92:ARG:HD3	2.19	0.42
18:X:12:ILE:HA	18:X:16:LEU:HD12	2.06	0.42
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.02	0.42
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.42
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.02	0.41
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.95	0.41
24:D:411:BCR:H361	24:D:411:BCR:H20C	1.81	0.41
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.41
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.06	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.20	0.41
1:A:303:ASN:O	3:C:415:ASN:ND2	2.41	0.41
24:B:618:BCR:H11C	24:B:618:BCR:H341	1.87	0.41
18:X:17:LYS:O	18:X:21:ILE:HG13	2.20	0.41
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.02	0.41
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.60	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
6:F:45:ARG:NH2	9:J:40:LEU:O	2.53	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.57	0.41
3:C:248:GLY:O	3:C:252:ILE:HG12	2.21	0.41
24:C:521:BCR:H15C	24:C:521:BCR:H351	1.84	0.41
24:D:411:BCR:H11C	24:D:411:BCR:H341	1.94	0.41
1:A:24:THR:O	4:D:251:ARG:NH2	2.44	0.41
1:A:61:ASP:HB2	1:A:63:ILE:HG12	2.09	0.41
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.56	0.41
22:A:403:CLA:H42	23:D:407:PL9:H162	2.02	0.41
22:B:602:CLA:H162	22:B:602:CLA:H192	1.77	0.41
3:C:119:LEU:HG	24:C:513:BCR:H10C	2.18	0.41
13:O:192:SER:OG	13:O:193:GLY:N	2.53	0.41
22:A:403:CLA:H41	22:A:403:CLA:H62	1.78	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.95	0.41
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.35	0.41
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.50	0.41
18:X:34:PHE:O	18:X:38:ILE:HG12	2.21	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.41
22:B:604:CLA:H141	22:B:604:CLA:H161	1.90	0.41
22:B:606:CLA:H92	22:B:606:CLA:HBB2	11.33	0.41
3:C:420:VAL:H	25:C:516:DGD:HE62	1.85	0.41
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.78	0.41
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.09	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.04	0.41
1:A:22:THR:HG21	8:I:30:ARG:HD3	2.08	0.41
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:402:CLA:CBB	22:A:402:CLA:HHC	2.50	0.41
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.02	0.41
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.98	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.31	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41
20:Z:32:ASP:CG	20:Z:33:TRP:H	2.27	0.41
22:A:404:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
22:B:602:CLA:H161	22:B:602:CLA:H141	1.82	0.41
22:B:602:CLA:H61	22:B:602:CLA:H41	1.67	0.41
3:C:257:PHE:HB3	3:C:258:GLY:H	1.63	0.41
22:C:508:CLA:H92	22:C:508:CLA:H62	1.72	0.41
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.41
3:C:261:ARG:HA	3:C:266:TRP:HZ2	1.86	0.40
3:C:377:LEU:O	3:C:381:LYS:HB2	2.21	0.40
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.90	0.40
3:C:57:ALA:O	3:C:61:VAL:HG23	2.20	0.40
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.58	0.40
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.07	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	2.51	0.40
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.03	0.40
22:D:405:CLA:HBA1	22:D:405:CLA:H3A	1.86	0.40
1:A:317:TRP:O	1:A:321:ILE:HG13	2.22	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
22:B:604:CLA:H162	22:B:604:CLA:H202	1.88	0.40
4:D:49:LEU:O	4:D:53:THR:HG23	2.22	0.40
22:H:101:CLA:H62	22:H:101:CLA:H93	1.88	0.40
7:H:12:ARG:N	7:H:13:PRO:HD2	2.37	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:140:ARG:HH22	26:A:409:LHG:P	2.44	0.40
1:A:141:PRO:O	1:A:143:ILE:N	2.53	0.40
1:A:180:PHE:O	1:A:184:ILE:HG13	2.24	0.40
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.03	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.89	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.21	0.40
22:C:508:CLA:H142	22:C:508:CLA:H112	1.84	0.40
4:D:201:VAL:O	4:D:205:LEU:HB2	2.22	0.40
22:B:607:CLA:H172	22:D:406:CLA:H3A	2.03	0.40
7:H:46:LEU:HB2	22:H:101:CLA:H61	2.03	0.40
1:A:176:ILE:HD12	22:A:405:CLA:HED3	23.91	0.40
22:A:404:CLA:H51	32:D:401:PHO:C3B	21.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:HAB	22:D:405:CLA:H72	2.04	0.40
2:B:137:LYS:HB2	2:B:137:LYS:HE3	1.96	0.40
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.05	0.40
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.03	0.40
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.04	0.40
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	450 (92%)	34 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	405 (91%)	36 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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	39
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	39
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	3	27
17	y	26/46 (56%)	20 (77%)	5 (19%)	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%)	4673 (91%)	410 (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

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Mol	Chain	Res	Type
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
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	12	ILE
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
7	h	26	GLY
9	j	38	SER
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
4	D	239	GLN
13	O	88	GLU
13	O	271	PRO
2	b	489	GLU
4	d	239	GLN
13	o	88	GLU
1	A	142	TRP
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
1	a	334	ARG
3	c	32	GLY
5	e	82	GLN
13	o	271	PRO
1	A	334	ARG
3	C	144	SER
7	H	16	SER
15	U	73	PRO

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Mol	Chain	Res	Type
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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%)	268 (98%)	7 (2%)	47	68
4	d	275/283 (97%)	268 (98%)	7 (2%)	47	68
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	63
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	63
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	55
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	61
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	61
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84
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%)	4140 (98%)	104 (2%)	47	68

All (104) 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

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Mol	Chain	Res	Type
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
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	345	VAL
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

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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
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	345	VAL
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

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
29	OEX	a	414	1,3	0,15,15	0.00	-	-		
27	LMG	m	101	-	42,42,55	0.85	0	50,50,63	1.24	4 (8%)
31	LMT	B	627	-	36,36,36	1.13	5 (13%)	47,47,47	0.95	1 (2%)
27	LMG	d	407	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	8 (14%)
25	DGD	c	517	-	67,67,67	0.88	0	81,81,81	1.40	10 (12%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	53,56,65	1.64	10 (18%)
22	CLA	b	605	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	7 (10%)
30	SQD	f	103	-	44,45,54	1.04	4 (9%)	53,56,65	1.63	11 (20%)
25	DGD	c	516	-	63,63,67	0.92	1 (1%)	77,77,81	1.45	12 (15%)
22	CLA	A	404	-	59,73,73	1.41	5 (8%)	67,113,113	1.44	7 (10%)
22	CLA	c	510	3	59,73,73	1.42	5 (8%)	67,113,113	1.50	7 (10%)
22	CLA	C	511	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	b	610	-	59,73,73	1.44	5 (8%)	67,113,113	1.44	9 (13%)
27	LMG	A	415	-	42,42,55	0.83	0	50,50,63	1.25	4 (8%)
22	CLA	D	406	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	8 (11%)
22	CLA	B	615	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	7 (10%)
22	CLA	d	404	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
27	LMG	a	413	-	51,51,55	0.74	1 (1%)	59,59,63	1.34	7 (11%)
27	LMG	d	410	-	46,46,55	0.80	1 (2%)	54,54,63	1.31	4 (7%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	6 (10%)
31	LMT	D	410	-	32,32,36	1.18	5 (15%)	43,43,47	1.00	2 (4%)
22	CLA	B	614	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	9 (13%)
22	CLA	c	520	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)
27	LMG	E	101	-	44,44,55	0.75	0	52,52,63	1.30	4 (7%)
27	LMG	A	410	-	51,51,55	0.74	0	59,59,63	1.36	5 (8%)
27	LMG	M	101	-	42,42,55	0.86	0	50,50,63	1.24	4 (8%)
29	OEX	A	412	1,3	0,15,15	0.00	-	-		
30	SQD	a	401	-	53,54,54	0.96	4 (7%)	62,65,65	1.56	9 (14%)
33	BCT	D	404	21	0,3,3	0.00	-	0,3,3	0.00	-
27	LMG	b	625	-	49,49,55	0.78	1 (2%)	57,57,63	1.31	6 (10%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	51,54,65	1.79	10 (19%)
22	CLA	b	606	-	59,73,73	1.40	5 (8%)	67,113,113	1.46	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	LMT	b	604	-	36,36,36	1.14	5 (13%)	47,47,47	1.02	1 (2%)
31	LMT	b	603	-	36,36,36	1.13	5 (13%)	47,47,47	0.94	1 (2%)
24	BCR	x	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.17	2 (3%)
23	PL9	j	101	-	35,35,55	1.00	1 (2%)	44,45,69	1.56	7 (15%)
24	BCR	f	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	5 (8%)
23	PL9	D	407	-	55,55,55	1.03	3 (5%)	68,69,69	1.52	13 (19%)
22	CLA	b	607	-	59,73,73	1.41	5 (8%)	67,113,113	1.52	10 (14%)
31	LMT	I	102	-	36,36,36	1.11	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	c	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	8 (11%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	9 (16%)
22	CLA	c	512	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	9 (13%)
31	LMT	M	103	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	2 (4%)
34	HEM	F	101	5,6	27,50,50	2.17	5 (18%)	17,82,82	1.44	3 (17%)
25	DGD	A	408	-	57,57,67	0.93	0	71,71,81	1.41	7 (9%)
22	CLA	D	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.43	8 (11%)
25	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.28	6 (8%)
31	LMT	b	627	-	36,36,36	1.10	5 (13%)	47,47,47	0.99	2 (4%)
22	CLA	B	608	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	8 (11%)
25	DGD	C	515	-	54,54,67	0.98	2 (3%)	68,68,81	1.27	6 (8%)
22	CLA	C	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	8 (11%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
22	CLA	b	619	-	59,73,73	1.44	6 (10%)	67,113,113	1.43	7 (10%)
24	BCR	a	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.23	7 (12%)
24	BCR	y	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
34	HEM	V	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.45	2 (11%)
22	CLA	b	612	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	8 (11%)
30	SQD	B	626	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
22	CLA	c	509	-	59,73,73	1.44	5 (8%)	67,113,113	1.41	8 (11%)
22	CLA	a	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.50	8 (11%)
24	BCR	D	411	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	b	617	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	7 (10%)
22	CLA	C	507	-	59,73,73	1.43	5 (8%)	67,113,113	1.51	9 (13%)
22	CLA	B	611	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)
22	CLA	C	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.41	7 (10%)
22	CLA	C	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	D	412	-	46,46,55	0.79	1 (2%)	54,54,63	1.31	4 (7%)
24	BCR	c	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
24	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.57	12 (21%)
24	BCR	g	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
22	CLA	b	618	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
23	PL9	A	406	-	45,45,55	0.98	4 (8%)	56,57,69	1.56	10 (17%)
22	CLA	c	503	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	8 (11%)
24	BCR	c	513	-	41,41,41	1.11	2 (4%)	56,56,56	1.35	10 (17%)
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	55,58,65	1.79	10 (18%)
25	DGD	d	408	-	64,64,67	0.92	2 (3%)	78,78,81	1.34	9 (11%)
22	CLA	b	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
27	LMG	e	101	-	44,44,55	0.75	0	52,52,63	1.30	5 (9%)
24	BCR	c	521	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
22	CLA	A	403	-	59,73,73	1.42	5 (8%)	67,113,113	1.50	8 (11%)
27	LMG	I	101	-	43,43,55	0.80	0	51,51,63	1.26	4 (7%)
22	CLA	c	504	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	8 (11%)
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	1.44	8 (11%)
26	LHG	C	519	-	36,36,48	0.71	0	39,42,54	1.25	4 (10%)
25	DGD	D	409	-	64,64,67	0.91	0	78,78,81	1.33	9 (11%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	59,62,65	1.74	10 (16%)
22	CLA	A	402	-	59,73,73	1.44	5 (8%)	67,113,113	1.44	7 (10%)
34	HEM	v	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.42	2 (11%)
32	PHO	a	407	-	67,69,69	1.26	8 (11%)	85,99,99	1.00	5 (5%)
26	LHG	a	412	-	38,38,48	0.68	1 (2%)	41,44,54	1.19	3 (7%)
27	LMG	B	624	-	49,49,55	0.76	0	57,57,63	1.32	5 (8%)
22	CLA	a	408	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	b	615	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)
24	BCR	b	623	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	8 (14%)
24	BCR	B	617	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	B	607	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
30	SQD	D	403	-	42,43,54	1.04	3 (7%)	51,54,65	1.78	10 (19%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
24	BCR	C	513	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
22	CLA	a	406	-	59,73,73	1.42	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
31	LMT	i	102	-	36,36,36	1.11	5 (13%)	47,47,47	0.98	2 (4%)
25	DGD	C	517	-	67,67,67	0.88	1 (1%)	81,81,81	1.41	10 (12%)
22	CLA	C	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	8 (11%)
22	CLA	B	605	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	8 (11%)
25	DGD	b	601	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
22	CLA	d	405	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	8 (11%)
25	DGD	C	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	12 (15%)
22	CLA	b	616	-	59,73,73	1.40	5 (8%)	67,113,113	1.51	9 (13%)
23	PL9	a	409	-	45,45,55	1.02	3 (6%)	56,57,69	1.55	10 (17%)
31	LMT	d	409	-	32,32,36	1.18	5 (15%)	43,43,47	0.98	2 (4%)
22	CLA	B	603	-	59,73,73	1.41	5 (8%)	67,113,113	1.54	10 (14%)
24	BCR	C	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	C	503	-	59,73,73	1.41	5 (8%)	67,113,113	1.49	7 (10%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
32	PHO	D	402	-	67,69,69	1.27	10 (14%)	85,99,99	1.01	5 (5%)
31	LMT	b	626	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
30	SQD	A	414	-	53,54,54	0.96	5 (9%)	62,65,65	1.57	9 (14%)
22	CLA	C	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	8 (11%)
25	DGD	B	620	-	59,59,67	0.90	1 (1%)	73,73,81	1.34	8 (10%)
22	CLA	B	612	-	59,73,73	1.40	5 (8%)	67,113,113	1.50	8 (11%)
31	LMT	B	622	-	36,36,36	1.12	5 (13%)	47,47,47	0.96	1 (2%)
23	PL9	d	406	-	55,55,55	1.02	2 (3%)	68,69,69	1.53	14 (20%)
22	CLA	c	507	-	59,73,73	1.43	5 (8%)	67,113,113	1.53	10 (14%)
24	BCR	B	616	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	8 (14%)
22	CLA	c	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	8 (11%)
22	CLA	c	502	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	8 (11%)
31	LMT	M	102	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	C	520	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	9 (13%)
22	CLA	C	504	-	59,73,73	1.42	5 (8%)	67,113,113	1.52	8 (11%)
34	HEM	f	101	5,6	27,50,50	2.16	5 (18%)	17,82,82	1.46	3 (17%)
22	CLA	c	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.44	8 (11%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	601	-	59,73,73	1.45	5 (8%)	67,113,113	1.47	8 (11%)
26	LHG	A	409	-	38,38,48	0.69	0	41,44,54	1.18	3 (7%)
22	CLA	b	608	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	CLA	C	510	3	59,73,73	1.42	5 (8%)	67,113,113	1.53	7 (10%)
22	CLA	B	606	-	59,73,73	1.44	5 (8%)	67,113,113	1.45	10 (14%)
27	LMG	a	402	-	42,42,55	0.84	0	50,50,63	1.25	3 (6%)
22	CLA	B	602	-	59,73,73	1.40	5 (8%)	67,113,113	1.47	9 (13%)
23	PL9	J	101	-	35,35,55	1.02	1 (2%)	44,45,69	1.56	7 (15%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.27	6 (11%)
32	PHO	D	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.01	5 (5%)
24	BCR	H	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	3 (5%)
22	CLA	C	509	-	59,73,73	1.45	5 (8%)	67,113,113	1.41	8 (11%)
22	CLA	A	405	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	7 (10%)
22	CLA	B	609	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	8 (11%)
25	DGD	a	411	-	57,57,67	0.94	1 (1%)	71,71,81	1.39	7 (9%)
24	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
22	CLA	h	101	-	59,73,73	1.43	5 (8%)	67,113,113	1.45	7 (10%)
25	DGD	B	625	-	53,53,67	1.06	3 (5%)	67,67,81	1.32	7 (10%)
26	LHG	c	519	-	36,36,48	0.73	2 (5%)	39,42,54	1.26	4 (10%)
24	BCR	b	621	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	7 (12%)
22	CLA	b	614	-	59,73,73	1.48	5 (8%)	67,113,113	1.50	9 (13%)
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.33	6 (8%)
27	LMG	b	628	-	49,49,55	0.76	0	57,57,63	1.31	4 (7%)
24	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.58	12 (21%)
22	CLA	a	404	-	59,73,73	1.45	5 (8%)	67,113,113	1.44	8 (11%)
31	LMT	B	623	-	36,36,36	1.10	5 (13%)	47,47,47	1.00	2 (4%)
22	CLA	b	613	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	9 (13%)
24	BCR	b	620	-	41,41,41	1.12	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	B	610	-	59,73,73	1.47	5 (8%)	67,113,113	1.50	10 (14%)
22	CLA	c	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
24	BCR	C	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	9 (16%)
22	CLA	c	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.50	7 (10%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
22	CLA	B	604	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	7 (10%)
32	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.03	6 (7%)
30	SQD	A	413	-	50,51,54	0.97	4 (8%)	59,62,65	1.72	10 (16%)
22	CLA	B	613	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	7 (10%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	LMG	C	522	-	48,48,55	0.77	0	56,56,63	1.31	5 (8%)
31	LMT	B	628	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	1 (2%)
22	CLA	C	512	-	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	m	101	-	-	17/37/57/70	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
27	LMG	d	407	-	-	20/43/63/70	0/1/1/1
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
25	DGD	c	517	-	-	21/55/95/95	0/2/2/2
22	CLA	B	614	-	3/3/20/25	10/37/135/135	-
22	CLA	b	605	-	3/3/20/25	14/37/135/135	-
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2
22	CLA	A	404	-	3/3/20/25	10/37/135/135	-
22	CLA	c	510	3	3/3/20/25	17/37/135/135	-
22	CLA	C	511	-	3/3/20/25	19/37/135/135	-
22	CLA	b	610	-	3/3/20/25	9/37/135/135	-
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
22	CLA	D	406	-	2/2/20/25	6/37/135/135	-
22	CLA	B	615	-	3/3/20/25	18/37/135/135	-
22	CLA	d	404	-	3/3/20/25	12/37/135/135	-
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
27	LMG	d	410	-	-	15/41/61/70	0/1/1/1
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
31	LMT	D	410	-	-	0/17/57/61	0/2/2/2
30	SQD	F	102	-	-	10/40/60/69	0/1/1/1
22	CLA	c	520	-	3/3/20/25	10/37/135/135	-
27	LMG	E	101	-	-	18/39/59/70	0/1/1/1
27	LMG	A	410	-	-	26/46/66/70	0/1/1/1
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	401	-	-	13/49/69/69	0/1/1/1
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1
30	SQD	d	402	-	-	13/38/58/69	0/1/1/1
22	CLA	b	606	-	3/3/20/25	13/37/135/135	-
31	LMT	b	604	-	-	4/21/61/61	0/2/2/2
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	BCR	c	513	-	-	6/29/63/63	0/2/2/2
24	BCR	f	102	-	-	7/29/63/63	0/2/2/2
23	PL9	D	407	-	-	12/53/73/73	0/1/1/1
22	CLA	b	607	-	3/3/20/25	7/37/135/135	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
22	CLA	c	506	-	3/3/20/25	13/37/135/135	-
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	c	512	-	3/3/20/25	21/37/135/135	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
22	CLA	B	611	-	3/3/20/25	13/37/135/135	-
25	DGD	A	408	-	-	15/45/85/95	0/2/2/2
22	CLA	D	405	-	3/3/20/25	14/37/135/135	-
25	DGD	c	515	-	-	20/42/82/95	0/2/2/2
24	BCR	J	102	-	-	6/29/63/63	0/2/2/2
31	LMT	b	627	-	-	2/21/61/61	0/2/2/2
22	CLA	B	608	-	3/3/20/25	11/37/135/135	-
24	BCR	D	411	-	-	6/29/63/63	0/2/2/2
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
27	LMG	c	518	-	-	21/40/60/70	0/1/1/1
22	CLA	b	619	-	3/3/20/25	19/37/135/135	-
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2
31	LMT	B	622	-	-	3/21/61/61	0/2/2/2
22	CLA	C	520	-	3/3/20/25	12/37/135/135	-
34	HEM	V	201	16	-	2/6/54/54	-
22	CLA	b	612	-	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	B	626	-	-	13/42/62/69	0/1/1/1
22	CLA	c	509	-	3/3/20/25	16/37/135/135	-
22	CLA	a	405	-	3/3/20/25	14/37/135/135	-
22	CLA	b	618	-	3/3/20/25	9/37/135/135	-
22	CLA	b	617	-	3/3/20/25	15/37/135/135	-
22	CLA	C	507	-	3/3/20/25	15/37/135/135	-
22	CLA	C	508	-	3/3/20/25	16/37/135/135	-
22	CLA	C	502	-	3/3/20/25	9/37/135/135	-
27	LMG	D	412	-	-	14/41/61/70	0/1/1/1
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
23	PL9	A	406	-	-	17/41/61/73	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
30	SQD	b	602	-	-	15/42/62/69	0/1/1/1
25	DGD	d	408	-	-	35/52/92/95	0/2/2/2
22	CLA	b	611	-	3/3/20/25	12/37/135/135	-
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
22	CLA	A	403	-	3/3/20/25	14/37/135/135	-
27	LMG	I	101	-	-	17/38/58/70	0/1/1/1
22	CLA	c	504	-	3/3/20/25	19/37/135/135	-
22	CLA	b	609	-	3/3/20/25	15/37/135/135	-
22	CLA	H	101	-	3/3/20/25	19/37/135/135	-
26	LHG	C	519	-	-	16/41/41/53	-
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
30	SQD	a	415	-	-	18/46/66/69	0/1/1/1
22	CLA	A	402	-	3/3/20/25	8/37/135/135	-
34	HEM	v	201	16	-	2/6/54/54	-
32	PHO	a	407	-	-	12/53/103/103	0/5/6/6
26	LHG	a	412	-	-	12/43/43/53	-
27	LMG	B	624	-	-	24/44/64/70	0/1/1/1
22	CLA	a	408	-	3/3/20/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	615	-	3/3/20/25	13/37/135/135	-
24	BCR	b	623	-	-	4/29/63/63	0/2/2/2
24	BCR	B	617	-	-	9/29/63/63	0/2/2/2
22	CLA	B	607	-	3/3/20/25	12/37/135/135	-
30	SQD	D	403	-	-	13/38/58/69	0/1/1/1
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	a	406	-	3/3/20/25	9/37/135/135	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
25	DGD	C	517	-	-	22/55/95/95	0/2/2/2
22	CLA	C	505	-	3/3/20/25	17/37/135/135	-
22	CLA	B	605	-	3/3/20/25	12/37/135/135	-
25	DGD	b	601	-	-	18/41/81/95	0/2/2/2
22	CLA	d	405	-	3/3/20/25	6/37/135/135	-
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	b	616	-	3/3/20/25	15/37/135/135	-
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
31	LMT	d	409	-	-	0/17/57/61	0/2/2/2
22	CLA	B	603	-	3/3/20/25	7/37/135/135	-
22	CLA	c	511	-	3/3/20/25	19/37/135/135	-
22	CLA	C	503	-	3/3/20/25	15/37/135/135	-
27	LMG	C	518	-	-	21/40/60/70	0/1/1/1
32	PHO	D	402	-	-	12/53/103/103	0/5/6/6
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
30	SQD	A	414	-	-	11/49/69/69	0/1/1/1
22	CLA	C	501	-	3/3/20/25	15/37/135/135	-
25	DGD	B	620	-	-	19/47/87/95	0/2/2/2
22	CLA	B	612	-	3/3/20/25	15/37/135/135	-
22	CLA	C	504	-	3/3/20/25	19/37/135/135	-
23	PL9	d	406	-	-	11/53/73/73	0/1/1/1
22	CLA	c	507	-	3/3/20/25	14/37/135/135	-
22	CLA	C	506	-	3/3/20/25	13/37/135/135	-
22	CLA	c	508	-	3/3/20/25	15/37/135/135	-
22	CLA	c	502	-	3/3/20/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
24	BCR	C	521	-	-	6/29/63/63	0/2/2/2
34	HEM	f	101	5,6	-	0/6/54/54	-
22	CLA	c	501	-	3/3/20/25	13/37/135/135	-
22	CLA	B	601	-	3/3/20/25	16/37/135/135	-
26	LHG	A	409	-	-	14/43/43/53	-
22	CLA	b	608	-	3/3/20/25	15/37/135/135	-
22	CLA	C	510	3	3/3/20/25	15/37/135/135	-
27	LMG	C	522	-	-	20/43/63/70	0/1/1/1
22	CLA	B	606	-	3/3/20/25	9/37/135/135	-
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
22	CLA	B	602	-	3/3/20/25	15/37/135/135	-
23	PL9	J	101	-	-	8/29/49/73	0/1/1/1
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
32	PHO	D	401	-	-	13/53/103/103	0/5/6/6
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	509	-	3/3/20/25	16/37/135/135	-
22	CLA	A	405	-	3/3/20/25	8/37/135/135	-
22	CLA	B	609	-	3/3/20/25	18/37/135/135	-
25	DGD	a	411	-	-	14/45/85/95	0/2/2/2
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
25	DGD	B	625	-	-	17/41/81/95	0/2/2/2
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	b	621	-	-	9/29/63/63	0/2/2/2
22	CLA	b	614	-	3/3/20/25	9/37/135/135	-
27	LMG	a	413	-	-	25/46/66/70	0/1/1/1
27	LMG	b	628	-	-	24/44/64/70	0/1/1/1
34	HEM	F	101	5,6	-	0/6/54/54	-
22	CLA	a	404	-	3/3/20/25	8/37/135/135	-
31	LMT	B	623	-	-	4/21/61/61	0/2/2/2
22	CLA	b	613	-	3/3/20/25	18/37/135/135	-
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
22	CLA	B	610	-	3/3/20/25	10/37/135/135	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	c	505	-	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	B	621	-	-	16/44/64/70	0/1/1/1
22	CLA	B	604	-	3/3/20/25	14/37/135/135	-
32	PHO	d	401	-	-	14/53/103/103	0/5/6/6
30	SQD	A	413	-	-	20/46/66/69	0/1/1/1
22	CLA	B	613	-	3/3/20/25	16/37/135/135	-
27	LMG	D	408	-	-	21/43/63/70	0/1/1/1
22	CLA	h	101	-	3/3/20/25	19/37/135/135	-
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
22	CLA	C	512	-	3/3/20/25	17/37/135/135	-

All (606) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	C4B-NB	7.79	1.42	1.35
22	B	601	CLA	C4B-NB	7.74	1.42	1.35
22	a	404	CLA	C4B-NB	7.74	1.42	1.35
22	b	605	CLA	C4B-NB	7.74	1.42	1.35
22	c	508	CLA	C4B-NB	7.72	1.42	1.35
22	c	509	CLA	C4B-NB	7.70	1.42	1.35
22	C	509	CLA	C4B-NB	7.69	1.42	1.35
22	b	614	CLA	C4B-NB	7.69	1.42	1.35
22	b	619	CLA	C4B-NB	7.68	1.42	1.35
22	C	508	CLA	C4B-NB	7.68	1.42	1.35
22	C	505	CLA	C4B-NB	7.65	1.42	1.35
22	c	511	CLA	C4B-NB	7.65	1.42	1.35
22	B	610	CLA	C4B-NB	7.63	1.42	1.35
22	a	405	CLA	C4B-NB	7.62	1.42	1.35
22	B	615	CLA	C4B-NB	7.62	1.42	1.35
22	c	505	CLA	C4B-NB	7.62	1.42	1.35
22	c	520	CLA	C4B-NB	7.61	1.42	1.35
22	c	504	CLA	C4B-NB	7.60	1.42	1.35
22	c	512	CLA	C4B-NB	7.60	1.42	1.35
22	b	612	CLA	C4B-NB	7.60	1.42	1.35
22	d	405	CLA	C4B-NB	7.60	1.42	1.35
22	d	404	CLA	C4B-NB	7.60	1.42	1.35
22	b	610	CLA	C4B-NB	7.59	1.42	1.35
22	C	507	CLA	C4B-NB	7.59	1.42	1.35
22	b	618	CLA	C4B-NB	7.57	1.42	1.35
22	B	606	CLA	C4B-NB	7.57	1.42	1.35
22	D	406	CLA	C4B-NB	7.56	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	C4B-NB	7.56	1.42	1.35
22	c	503	CLA	C4B-NB	7.56	1.42	1.35
22	C	512	CLA	C4B-NB	7.56	1.42	1.35
22	H	101	CLA	C4B-NB	7.55	1.41	1.35
22	c	507	CLA	C4B-NB	7.54	1.41	1.35
22	B	604	CLA	C4B-NB	7.54	1.41	1.35
22	C	511	CLA	C4B-NB	7.53	1.41	1.35
22	B	614	CLA	C4B-NB	7.53	1.41	1.35
22	C	510	CLA	C4B-NB	7.53	1.41	1.35
22	c	510	CLA	C4B-NB	7.53	1.41	1.35
22	A	403	CLA	C4B-NB	7.53	1.41	1.35
22	a	408	CLA	C4B-NB	7.52	1.41	1.35
22	B	607	CLA	C4B-NB	7.50	1.41	1.35
22	C	503	CLA	C4B-NB	7.49	1.41	1.35
22	a	406	CLA	C4B-NB	7.49	1.41	1.35
22	b	608	CLA	C4B-NB	7.48	1.41	1.35
22	h	101	CLA	C4B-NB	7.48	1.41	1.35
22	B	609	CLA	C4B-NB	7.48	1.41	1.35
22	b	615	CLA	C4B-NB	7.47	1.41	1.35
22	A	405	CLA	C4B-NB	7.47	1.41	1.35
22	D	405	CLA	C4B-NB	7.47	1.41	1.35
22	b	611	CLA	C4B-NB	7.45	1.41	1.35
22	b	613	CLA	C4B-NB	7.45	1.41	1.35
22	C	520	CLA	C4B-NB	7.45	1.41	1.35
22	b	617	CLA	C4B-NB	7.43	1.41	1.35
22	C	501	CLA	C4B-NB	7.43	1.41	1.35
22	b	616	CLA	C4B-NB	7.42	1.41	1.35
22	B	611	CLA	C4B-NB	7.41	1.41	1.35
22	C	502	CLA	C4B-NB	7.41	1.41	1.35
22	b	609	CLA	C4B-NB	7.41	1.41	1.35
22	B	605	CLA	C4B-NB	7.40	1.41	1.35
22	C	504	CLA	C4B-NB	7.39	1.41	1.35
22	c	501	CLA	C4B-NB	7.39	1.41	1.35
22	B	612	CLA	C4B-NB	7.39	1.41	1.35
22	b	607	CLA	C4B-NB	7.38	1.41	1.35
22	c	506	CLA	C4B-NB	7.38	1.41	1.35
22	c	502	CLA	C4B-NB	7.37	1.41	1.35
22	C	506	CLA	C4B-NB	7.37	1.41	1.35
22	A	404	CLA	C4B-NB	7.36	1.41	1.35
22	B	613	CLA	C4B-NB	7.34	1.41	1.35
22	B	603	CLA	C4B-NB	7.33	1.41	1.35
22	B	602	CLA	C4B-NB	7.33	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	C4B-NB	7.30	1.41	1.35
34	v	201	HEM	C3D-C2D	5.64	1.54	1.37
34	V	201	HEM	C3D-C2D	5.64	1.54	1.37
34	F	101	HEM	C3D-C2D	5.46	1.53	1.37
34	f	101	HEM	C3D-C2D	5.42	1.53	1.37
34	f	101	HEM	C3B-C2B	-4.86	1.33	1.40
34	F	101	HEM	C3B-C2B	-4.86	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.58	1.34	1.40
34	V	201	HEM	C3C-C2C	-4.54	1.34	1.40
34	f	101	HEM	C3C-CAC	3.85	1.55	1.47
34	V	201	HEM	C3B-CAB	3.80	1.55	1.47
34	F	101	HEM	C3C-CAC	3.79	1.55	1.47
34	v	201	HEM	C3B-CAB	3.78	1.55	1.47
34	V	201	HEM	C3C-CAC	3.75	1.55	1.47
34	v	201	HEM	C3B-C2B	-3.74	1.35	1.40
34	V	201	HEM	C3B-C2B	-3.74	1.35	1.40
34	F	101	HEM	C3C-C2C	-3.74	1.35	1.40
34	v	201	HEM	C3C-CAC	3.72	1.55	1.47
34	f	101	HEM	C3C-C2C	-3.68	1.35	1.40
23	d	406	PL9	C7-C3	-3.66	1.47	1.51
24	H	102	BCR	C1-C6	-3.61	1.48	1.53
24	y	101	BCR	C1-C6	-3.60	1.48	1.53
34	F	101	HEM	C3B-CAB	3.56	1.55	1.47
24	D	411	BCR	C1-C6	-3.55	1.48	1.53
24	g	101	BCR	C1-C6	-3.52	1.48	1.53
34	f	101	HEM	C3B-CAB	3.51	1.55	1.47
24	f	102	BCR	C1-C6	-3.51	1.48	1.53
24	x	101	BCR	C1-C6	-3.49	1.49	1.53
22	b	614	CLA	CMB-C2B	-3.48	1.44	1.51
23	D	407	PL9	C7-C3	-3.41	1.47	1.51
32	D	402	PHO	C3B-C4B	3.40	1.50	1.43
22	B	610	CLA	CMB-C2B	-3.40	1.44	1.51
24	C	513	BCR	C1-C6	-3.36	1.49	1.53
32	a	407	PHO	C3B-C4B	3.36	1.50	1.43
23	J	101	PL9	C7-C3	-3.33	1.47	1.51
24	B	616	BCR	C1-C6	-3.33	1.49	1.53
24	b	620	BCR	C1-C6	-3.33	1.49	1.53
32	D	401	PHO	C3B-C4B	3.30	1.50	1.43
24	C	514	BCR	C1-C6	-3.29	1.49	1.53
24	c	513	BCR	C1-C6	-3.28	1.49	1.53
24	c	514	BCR	C1-C6	-3.27	1.49	1.53
22	B	613	CLA	CHC-C1C	3.27	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	101	CLA	CHC-C1C	3.25	1.43	1.35
23	a	409	PL9	C7-C3	-3.25	1.48	1.51
22	B	608	CLA	CHC-C1C	3.24	1.43	1.35
22	b	612	CLA	CHC-C1C	3.22	1.43	1.35
22	H	101	CLA	CHC-C1C	3.22	1.43	1.35
32	d	401	PHO	C3B-C4B	3.22	1.49	1.43
24	b	622	BCR	C30-C25	-3.22	1.49	1.53
23	j	101	PL9	C7-C3	-3.22	1.48	1.51
22	B	607	CLA	CHC-C1C	3.20	1.43	1.35
22	b	611	CLA	CHC-C1C	3.20	1.43	1.35
22	a	404	CLA	CHC-C1C	3.20	1.43	1.35
22	c	502	CLA	CHC-C1C	3.20	1.43	1.35
22	d	405	CLA	CHC-C1C	3.20	1.43	1.35
22	C	512	CLA	CHC-C1C	3.19	1.43	1.35
22	D	405	CLA	CHC-C1C	3.19	1.43	1.35
22	b	606	CLA	CHC-C1C	3.19	1.43	1.35
22	c	512	CLA	CHC-C1C	3.19	1.43	1.35
22	c	507	CLA	CHC-C1C	3.18	1.43	1.35
24	y	101	BCR	C30-C25	-3.18	1.49	1.53
22	d	404	CLA	CHC-C1C	3.18	1.43	1.35
22	b	617	CLA	CHC-C1C	3.17	1.43	1.35
30	A	414	SQD	O48-C23	3.17	1.42	1.33
30	a	401	SQD	O48-C23	3.17	1.42	1.33
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	C	505	CLA	CHC-C1C	3.17	1.43	1.35
22	c	509	CLA	CHC-C1C	3.17	1.43	1.35
30	d	402	SQD	O48-C23	3.17	1.42	1.33
22	C	504	CLA	CHC-C1C	3.16	1.43	1.35
22	b	616	CLA	CHC-C1C	3.16	1.43	1.35
22	C	511	CLA	CHC-C1C	3.16	1.43	1.35
24	b	621	BCR	C1-C6	-3.15	1.49	1.53
22	B	609	CLA	CHC-C1C	3.15	1.43	1.35
22	c	505	CLA	CHC-C1C	3.15	1.43	1.35
22	B	602	CLA	CHC-C1C	3.15	1.43	1.35
22	a	406	CLA	CHC-C1C	3.15	1.43	1.35
22	C	510	CLA	CHC-C1C	3.15	1.43	1.35
24	g	101	BCR	C30-C25	-3.15	1.49	1.53
22	B	614	CLA	CHC-C1C	3.15	1.43	1.35
30	b	602	SQD	O48-C23	3.15	1.42	1.33
22	A	402	CLA	CHC-C1C	3.14	1.43	1.35
22	b	618	CLA	CHC-C1C	3.14	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	CHC-C1C	3.14	1.43	1.35
22	a	408	CLA	CHC-C1C	3.14	1.43	1.35
22	c	510	CLA	CHC-C1C	3.14	1.43	1.35
22	B	605	CLA	CHC-C1C	3.14	1.43	1.35
22	C	506	CLA	CHC-C1C	3.14	1.43	1.35
22	c	504	CLA	CHC-C1C	3.14	1.43	1.35
22	b	613	CLA	CHC-C1C	3.14	1.43	1.35
22	B	604	CLA	CHC-C1C	3.14	1.43	1.35
22	C	502	CLA	CHC-C1C	3.13	1.43	1.35
22	b	607	CLA	CHC-C1C	3.13	1.43	1.35
22	b	608	CLA	CHC-C1C	3.13	1.43	1.35
30	f	103	SQD	O48-C23	3.13	1.42	1.33
24	B	618	BCR	C30-C25	-3.13	1.49	1.53
22	A	404	CLA	CHC-C1C	3.13	1.43	1.35
30	B	626	SQD	O48-C23	3.13	1.42	1.33
22	c	503	CLA	CHC-C1C	3.13	1.43	1.35
22	B	603	CLA	CHC-C1C	3.13	1.43	1.35
22	B	612	CLA	CHC-C1C	3.13	1.43	1.35
22	c	508	CLA	CHC-C1C	3.12	1.43	1.35
30	a	415	SQD	O48-C23	3.12	1.42	1.33
24	B	619	BCR	C30-C25	-3.12	1.49	1.53
30	D	403	SQD	O48-C23	3.12	1.42	1.33
22	D	406	CLA	CHC-C1C	3.11	1.42	1.35
22	c	520	CLA	CHC-C1C	3.11	1.42	1.35
22	B	606	CLA	CHC-C1C	3.11	1.42	1.35
22	A	403	CLA	CHC-C1C	3.11	1.42	1.35
22	B	601	CLA	CHC-C1C	3.11	1.42	1.35
30	F	102	SQD	O48-C23	3.10	1.42	1.33
22	C	520	CLA	CHC-C1C	3.10	1.42	1.35
24	C	521	BCR	C30-C25	-3.10	1.49	1.53
22	C	507	CLA	CHC-C1C	3.10	1.42	1.35
24	b	623	BCR	C30-C25	-3.10	1.49	1.53
22	b	609	CLA	CHC-C1C	3.10	1.42	1.35
24	a	410	BCR	C1-C6	-3.10	1.49	1.53
22	C	501	CLA	CHC-C1C	3.10	1.42	1.35
30	A	413	SQD	O48-C23	3.10	1.42	1.33
24	b	620	BCR	C30-C25	-3.10	1.49	1.53
22	b	619	CLA	CHC-C1C	3.10	1.42	1.35
22	C	503	CLA	CHC-C1C	3.09	1.42	1.35
22	c	506	CLA	CHC-C1C	3.09	1.42	1.35
24	B	617	BCR	C1-C6	-3.09	1.49	1.53
22	b	610	CLA	CHC-C1C	3.09	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	CHC-C1C	3.08	1.42	1.35
22	b	615	CLA	CHC-C1C	3.08	1.42	1.35
24	c	521	BCR	C30-C25	-3.08	1.49	1.53
24	a	410	BCR	C30-C25	-3.07	1.49	1.53
22	b	605	CLA	CHC-C1C	3.07	1.42	1.35
32	D	402	PHO	CHC-C1C	3.07	1.44	1.38
24	A	407	BCR	C30-C25	-3.07	1.49	1.53
24	B	616	BCR	C30-C25	-3.07	1.49	1.53
24	b	623	BCR	C1-C6	-3.06	1.49	1.53
24	D	411	BCR	C30-C25	-3.06	1.49	1.53
22	c	501	CLA	CHC-C1C	3.05	1.42	1.35
22	B	611	CLA	CHC-C1C	3.05	1.42	1.35
22	a	405	CLA	CHC-C1C	3.05	1.42	1.35
22	A	405	CLA	CHC-C1C	3.05	1.42	1.35
24	B	618	BCR	C1-C6	-3.04	1.49	1.53
24	f	102	BCR	C30-C25	-3.04	1.49	1.53
24	b	622	BCR	C1-C6	-3.03	1.49	1.53
24	B	619	BCR	C1-C6	-3.03	1.49	1.53
24	A	407	BCR	C1-C6	-3.03	1.49	1.53
24	J	102	BCR	C30-C25	-3.00	1.49	1.53
24	j	102	BCR	C30-C25	-2.99	1.49	1.53
32	a	407	PHO	CHC-C1C	2.99	1.44	1.38
24	x	101	BCR	C30-C25	-2.98	1.49	1.53
23	A	406	PL9	C7-C3	-2.98	1.48	1.51
24	C	513	BCR	C30-C25	-2.97	1.49	1.53
24	j	102	BCR	C1-C6	-2.96	1.49	1.53
24	J	102	BCR	C1-C6	-2.95	1.49	1.53
30	A	414	SQD	O47-C7	2.93	1.42	1.34
32	D	401	PHO	CHC-C1C	2.93	1.44	1.38
24	c	514	BCR	C30-C25	-2.93	1.49	1.53
24	C	514	BCR	C30-C25	-2.93	1.49	1.53
24	C	521	BCR	C1-C6	-2.93	1.49	1.53
30	D	403	SQD	O47-C7	2.92	1.42	1.34
25	b	601	DGD	C1E-C2E	2.92	1.60	1.52
30	d	402	SQD	O47-C7	2.91	1.42	1.34
24	H	102	BCR	C30-C25	-2.90	1.49	1.53
30	F	102	SQD	O47-C7	2.90	1.42	1.34
32	d	401	PHO	CHC-C1C	2.90	1.44	1.38
22	B	610	CLA	CHC-C1C	2.90	1.42	1.35
30	a	401	SQD	O47-C7	2.90	1.42	1.34
30	a	415	SQD	O47-C7	2.89	1.42	1.34
30	A	413	SQD	O47-C7	2.89	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	521	BCR	C1-C6	-2.87	1.49	1.53
30	b	602	SQD	O47-C7	2.84	1.42	1.34
25	B	625	DGD	C1E-C2E	2.84	1.60	1.52
30	B	626	SQD	O47-C7	2.83	1.42	1.34
30	f	103	SQD	O47-C7	2.83	1.42	1.34
22	b	614	CLA	CHC-C1C	2.83	1.42	1.35
22	c	512	CLA	C1D-C2D	2.76	1.48	1.42
24	c	513	BCR	C30-C25	-2.76	1.50	1.53
22	C	512	CLA	C1D-C2D	2.76	1.48	1.42
22	b	610	CLA	C1D-C2D	2.75	1.48	1.42
24	B	617	BCR	C30-C25	-2.75	1.50	1.53
22	b	613	CLA	C1D-C2D	2.75	1.48	1.42
32	a	407	PHO	C4C-NC	2.74	1.42	1.36
22	a	405	CLA	C1D-C2D	2.74	1.48	1.42
24	b	621	BCR	C30-C25	-2.73	1.50	1.53
22	c	520	CLA	C1D-C2D	2.73	1.48	1.42
22	B	609	CLA	C1D-C2D	2.73	1.48	1.42
32	D	402	PHO	C4C-NC	2.73	1.42	1.36
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	C	520	CLA	C1D-C2D	2.72	1.48	1.42
23	a	409	PL9	C3-C4	-2.72	1.45	1.49
22	A	403	CLA	C1D-C2D	2.71	1.48	1.42
22	c	508	CLA	C1D-C2D	2.71	1.48	1.42
22	a	404	CLA	C1D-C2D	2.71	1.48	1.42
22	b	605	CLA	C1D-C2D	2.71	1.48	1.42
22	C	501	CLA	C1D-C2D	2.71	1.48	1.42
32	d	401	PHO	C1A-NA	2.70	1.42	1.37
22	c	501	CLA	C1D-C2D	2.70	1.48	1.42
22	c	510	CLA	C1D-C2D	2.70	1.48	1.42
32	d	401	PHO	C4C-NC	2.70	1.42	1.36
22	b	616	CLA	C1D-C2D	2.69	1.48	1.42
22	B	604	CLA	C1D-C2D	2.69	1.48	1.42
22	A	404	CLA	C1D-C2D	2.68	1.48	1.42
32	D	401	PHO	C4C-NC	2.68	1.42	1.36
22	b	619	CLA	C1D-C2D	2.68	1.48	1.42
22	b	609	CLA	C1D-C2D	2.68	1.48	1.42
32	D	402	PHO	C1A-NA	2.68	1.42	1.37
22	D	406	CLA	C1D-C2D	2.68	1.48	1.42
22	B	612	CLA	C1D-C2D	2.67	1.48	1.42
22	C	507	CLA	C1D-C2D	2.67	1.48	1.42
22	B	615	CLA	C1D-C2D	2.67	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	C1D-C2D	2.67	1.48	1.42
22	B	613	CLA	C1D-C2D	2.67	1.48	1.42
22	H	101	CLA	C1D-C2D	2.67	1.48	1.42
22	b	618	CLA	C1D-C2D	2.67	1.48	1.42
22	C	505	CLA	C1D-C2D	2.67	1.48	1.42
22	B	601	CLA	C1D-C2D	2.67	1.48	1.42
22	C	509	CLA	C1D-C2D	2.66	1.48	1.42
22	C	508	CLA	C1D-C2D	2.66	1.48	1.42
22	C	510	CLA	C1D-C2D	2.66	1.48	1.42
22	c	505	CLA	C1D-C2D	2.65	1.48	1.42
22	b	608	CLA	C1D-C2D	2.65	1.48	1.42
22	c	506	CLA	C1D-C2D	2.65	1.48	1.42
22	b	617	CLA	C1D-C2D	2.65	1.48	1.42
22	B	610	CLA	C1D-C2D	2.65	1.48	1.42
22	B	614	CLA	C1D-C2D	2.65	1.48	1.42
22	A	402	CLA	C1D-C2D	2.65	1.48	1.42
22	h	101	CLA	C1D-C2D	2.65	1.48	1.42
32	D	401	PHO	C1A-NA	2.64	1.42	1.37
22	C	503	CLA	C1D-C2D	2.64	1.48	1.42
22	b	606	CLA	C1D-C2D	2.64	1.48	1.42
22	B	605	CLA	C1D-C2D	2.64	1.48	1.42
32	a	407	PHO	C1A-NA	2.64	1.42	1.37
22	C	506	CLA	C1D-C2D	2.64	1.48	1.42
22	c	503	CLA	C1D-C2D	2.63	1.48	1.42
22	b	611	CLA	C1D-C2D	2.63	1.48	1.42
22	C	502	CLA	C1D-C2D	2.62	1.48	1.42
22	A	405	CLA	C1D-C2D	2.62	1.48	1.42
22	c	507	CLA	C1D-C2D	2.62	1.48	1.42
22	c	509	CLA	C1D-C2D	2.62	1.48	1.42
22	B	602	CLA	C1D-C2D	2.60	1.48	1.42
22	b	612	CLA	C1D-C2D	2.60	1.48	1.42
22	B	608	CLA	C1D-C2D	2.59	1.48	1.42
22	b	614	CLA	C1D-C2D	2.59	1.48	1.42
31	b	627	LMT	O3'-C3'	-2.59	1.36	1.43
22	d	404	CLA	C1D-C2D	2.58	1.48	1.42
22	c	507	CLA	CMB-C2B	-2.58	1.46	1.51
22	C	507	CLA	CMB-C2B	-2.58	1.46	1.51
22	b	607	CLA	C1D-C2D	2.58	1.48	1.42
22	B	607	CLA	C1D-C2D	2.58	1.48	1.42
22	C	511	CLA	C1D-C2D	2.58	1.48	1.42
31	M	102	LMT	O3'-C3'	-2.58	1.36	1.43
22	c	511	CLA	C1D-C2D	2.57	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	408	CLA	C1D-C2D	2.57	1.48	1.42
31	B	623	LMT	O3'-C3'	-2.57	1.36	1.43
22	c	502	CLA	C1D-C2D	2.57	1.48	1.42
31	D	410	LMT	O3'-C3'	-2.56	1.36	1.43
22	D	405	CLA	C1D-C2D	2.56	1.48	1.42
31	d	409	LMT	O3'-C3'	-2.56	1.37	1.43
23	D	407	PL9	C3-C4	-2.54	1.45	1.49
31	M	103	LMT	O3'-C3'	-2.53	1.37	1.43
22	B	603	CLA	C1D-C2D	2.53	1.48	1.42
25	C	515	DGD	O2G-C2G	-2.52	1.40	1.46
31	b	603	LMT	O3'-C3'	-2.52	1.37	1.43
23	d	406	PL9	C3-C4	-2.51	1.45	1.49
31	I	102	LMT	O3'-C3'	-2.51	1.37	1.43
23	A	406	PL9	C3-C4	-2.51	1.45	1.49
22	b	615	CLA	C1D-C2D	2.50	1.48	1.42
31	b	626	LMT	O3'-C3'	-2.50	1.37	1.43
22	c	504	CLA	C1D-C2D	2.49	1.48	1.42
31	B	622	LMT	O3'-C3'	-2.49	1.37	1.43
22	B	611	CLA	C1D-C2D	2.48	1.48	1.42
22	a	404	CLA	CMB-C2B	-2.48	1.46	1.51
31	B	627	LMT	O3'-C3'	-2.48	1.37	1.43
31	b	604	LMT	O3'-C3'	-2.48	1.37	1.43
31	i	102	LMT	O3'-C3'	-2.47	1.37	1.43
22	A	403	CLA	CMB-C2B	-2.47	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.46	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	607	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	505	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	A	402	CLA	CMB-C2B	-2.45	1.46	1.51
32	a	407	PHO	CHD-C1D	2.45	1.43	1.38
22	A	404	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.44	1.46	1.51
32	a	407	PHO	C4C-C3C	2.44	1.49	1.45
22	C	509	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	601	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.43	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.43	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	C1D-C2D	2.42	1.48	1.42
22	B	605	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.42	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.42	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.42	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.41	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.41	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.41	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.41	1.46	1.51
31	B	628	LMT	O3'-C3'	-2.41	1.37	1.43
22	b	609	CLA	CMB-C2B	-2.40	1.46	1.51
22	a	408	CLA	CMB-C2B	-2.40	1.46	1.51
31	I	102	LMT	O2'-C2'	-2.40	1.37	1.43
22	A	405	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.39	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.38	1.46	1.51
32	D	402	PHO	CHD-C1D	2.38	1.43	1.38
22	B	602	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.38	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.38	1.46	1.51
32	d	401	PHO	C4C-C3C	2.38	1.49	1.45
22	c	503	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.38	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	CMB-C2B	-2.37	1.46	1.51
22	C	511	CLA	CMB-C2B	-2.37	1.46	1.51
32	D	401	PHO	C1C-NC	-2.37	1.33	1.38
22	D	406	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	625	DGD	C4D-C5D	2.37	1.58	1.53
22	B	612	CLA	CMB-C2B	-2.36	1.46	1.51
31	i	102	LMT	O2'-C2'	-2.36	1.37	1.43
22	b	616	CLA	CMB-C2B	-2.36	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.36	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.36	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.36	1.46	1.51
31	M	102	LMT	O3B-C3B	-2.35	1.37	1.43
32	a	407	PHO	C1C-NC	-2.35	1.33	1.38
22	c	511	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.35	1.46	1.51
32	D	402	PHO	C4C-C3C	2.34	1.49	1.45
22	B	611	CLA	CMD-C2D	-2.34	1.46	1.51
32	D	402	PHO	C1C-NC	-2.34	1.33	1.38
32	D	401	PHO	C4C-C3C	2.33	1.49	1.45
31	B	628	LMT	O3B-C3B	-2.33	1.37	1.43
32	d	401	PHO	C1C-NC	-2.32	1.33	1.38
31	b	604	LMT	O3B-C3B	-2.31	1.37	1.43
22	b	615	CLA	CMD-C2D	-2.31	1.46	1.51
31	b	627	LMT	O3B-C3B	-2.31	1.37	1.43
30	b	602	SQD	O2-C2	-2.30	1.37	1.43
31	I	102	LMT	O2B-C2B	-2.30	1.37	1.43
31	M	103	LMT	O3B-C3B	-2.29	1.37	1.43
31	B	627	LMT	O2'-C2'	-2.29	1.37	1.43
31	b	603	LMT	O3B-C3B	-2.29	1.37	1.43
32	d	401	PHO	CHD-C1D	2.28	1.43	1.38
31	B	622	LMT	O3B-C3B	-2.28	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.28	1.40	1.46
30	B	626	SQD	O2-C2	-2.28	1.37	1.43
31	B	623	LMT	O3B-C3B	-2.28	1.37	1.43
31	I	102	LMT	O3B-C3B	-2.27	1.37	1.43
31	i	102	LMT	O2B-C2B	-2.26	1.37	1.43
31	D	410	LMT	O3B-C3B	-2.26	1.37	1.43
31	d	409	LMT	O3B-C3B	-2.26	1.37	1.43
31	b	603	LMT	O2'-C2'	-2.25	1.37	1.43
22	c	504	CLA	CMD-C2D	-2.25	1.46	1.51
31	M	102	LMT	O2'-C2'	-2.25	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	401	PHO	CHD-C1D	2.24	1.43	1.38
22	b	614	CLA	C3B-C2B	-2.24	1.37	1.40
31	b	626	LMT	O3B-C3B	-2.24	1.37	1.43
27	b	625	LMG	C4-C5	2.24	1.57	1.53
31	M	103	LMT	O2'-C2'	-2.24	1.37	1.43
31	i	102	LMT	O3B-C3B	-2.23	1.37	1.43
25	b	601	DGD	C4D-C5D	2.23	1.57	1.53
31	B	627	LMT	O3B-C3B	-2.23	1.37	1.43
22	c	509	CLA	CMD-C2D	-2.22	1.46	1.51
31	b	626	LMT	O2'-C2'	-2.22	1.37	1.43
31	b	604	LMT	O2'-C2'	-2.22	1.37	1.43
31	B	622	LMT	O2'-C2'	-2.21	1.37	1.43
22	C	504	CLA	CMD-C2D	-2.21	1.46	1.51
23	a	409	PL9	C53-C6	-2.20	1.46	1.50
31	b	627	LMT	O2'-C2'	-2.20	1.37	1.43
25	C	516	DGD	O2G-C2G	-2.20	1.41	1.46
31	B	628	LMT	O2'-C2'	-2.20	1.37	1.43
31	b	603	LMT	O2B-C2B	-2.20	1.37	1.43
31	B	627	LMT	O2B-C2B	-2.20	1.37	1.43
22	C	509	CLA	CMD-C2D	-2.19	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.19	1.46	1.51
23	D	407	PL9	C6-C1	-2.19	1.44	1.48
25	B	625	DGD	C3G-C2G	2.19	1.57	1.50
31	M	102	LMT	O2B-C2B	-2.18	1.37	1.43
23	A	406	PL9	C53-C6	-2.18	1.46	1.50
31	M	103	LMT	O2B-C2B	-2.17	1.37	1.43
22	b	611	CLA	CMD-C2D	-2.17	1.46	1.51
22	B	610	CLA	C3B-C2B	-2.16	1.37	1.40
22	B	603	CLA	CMD-C2D	-2.16	1.46	1.51
31	B	623	LMT	O2'-C2'	-2.16	1.37	1.43
22	A	402	CLA	CMD-C2D	-2.16	1.46	1.51
25	b	601	DGD	C3G-C2G	2.15	1.57	1.50
27	D	412	LMG	O7-C8	-2.15	1.41	1.46
22	a	404	CLA	CMD-C2D	-2.15	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.14	1.46	1.51
31	b	626	LMT	O2B-C2B	-2.14	1.37	1.43
31	M	102	LMT	O4'-C4B	-2.14	1.37	1.43
30	d	402	SQD	O2-C2	-2.14	1.37	1.43
30	b	602	SQD	O3-C3	-2.14	1.37	1.43
27	B	621	LMG	C4-C5	2.13	1.57	1.53
31	D	410	LMT	O2B-C2B	-2.13	1.38	1.43
30	B	626	SQD	O3-C3	-2.13	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	409	LMT	O2'-C2'	-2.13	1.38	1.43
31	B	628	LMT	O4'-C4B	-2.13	1.38	1.43
30	f	103	SQD	O2-C2	-2.13	1.38	1.43
32	D	401	PHO	C4B-NB	2.13	1.41	1.36
32	a	407	PHO	C4B-NB	2.13	1.41	1.36
31	B	628	LMT	O2B-C2B	-2.13	1.38	1.43
22	B	604	CLA	CMD-C2D	-2.12	1.46	1.51
26	a	412	LHG	O7-C5	-2.12	1.41	1.46
31	D	410	LMT	O2'-C2'	-2.12	1.38	1.43
32	d	401	PHO	C4B-NB	2.12	1.41	1.36
31	b	603	LMT	O4'-C4B	-2.12	1.38	1.43
25	c	516	DGD	O2G-C2G	-2.12	1.41	1.46
32	D	402	PHO	C4B-NB	2.12	1.41	1.36
22	A	404	CLA	CMD-C2D	-2.12	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.12	1.46	1.51
30	D	403	SQD	O2-C2	-2.11	1.38	1.43
22	b	608	CLA	CMD-C2D	-2.11	1.46	1.51
30	F	102	SQD	O2-C2	-2.11	1.38	1.43
26	c	519	LHG	P-O6	2.11	1.67	1.59
31	B	622	LMT	O2B-C2B	-2.11	1.38	1.43
30	A	413	SQD	O2-C2	-2.11	1.38	1.43
22	a	406	CLA	CMD-C2D	-2.11	1.46	1.51
31	d	409	LMT	O2B-C2B	-2.11	1.38	1.43
22	c	503	CLA	CMD-C2D	-2.11	1.46	1.51
22	A	405	CLA	CMD-C2D	-2.11	1.46	1.51
31	M	103	LMT	O4'-C4B	-2.11	1.38	1.43
22	B	602	CLA	CMD-C2D	-2.10	1.46	1.51
25	d	408	DGD	C1D-C2D	2.10	1.58	1.52
31	b	604	LMT	O2B-C2B	-2.10	1.38	1.43
22	A	403	CLA	CMD-C2D	-2.10	1.46	1.51
27	d	410	LMG	O7-C8	-2.10	1.41	1.46
22	C	503	CLA	CMD-C2D	-2.10	1.46	1.51
31	d	409	LMT	O4'-C4B	-2.10	1.38	1.43
25	b	624	DGD	O2G-C2G	-2.10	1.41	1.46
22	b	619	CLA	CMD-C2D	-2.09	1.46	1.51
30	a	401	SQD	O3-C3	-2.09	1.38	1.43
30	A	414	SQD	O3-C3	-2.09	1.38	1.43
31	b	604	LMT	O4'-C4B	-2.09	1.38	1.43
22	a	405	CLA	CMD-C2D	-2.09	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.09	1.46	1.51
22	C	507	CLA	CMD-C2D	-2.09	1.46	1.51
30	a	415	SQD	O2-C2	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	408	CLA	CMD-C2D	-2.09	1.46	1.51
22	c	507	CLA	CMD-C2D	-2.08	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.08	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.08	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.08	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.08	1.46	1.51
22	C	502	CLA	CMD-C2D	-2.08	1.46	1.51
25	B	620	DGD	O2G-C2G	-2.07	1.41	1.46
30	A	414	SQD	O2-C2	-2.07	1.38	1.43
22	H	101	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.07	1.46	1.51
34	v	201	HEM	CAA-C2A	2.07	1.55	1.52
22	c	520	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.07	1.46	1.51
22	C	511	CLA	CMD-C2D	-2.07	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.07	1.46	1.51
31	B	627	LMT	O4'-C4B	-2.07	1.38	1.43
31	I	102	LMT	O4'-C4B	-2.07	1.38	1.43
22	B	605	CLA	CMD-C2D	-2.07	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.07	1.46	1.51
22	c	511	CLA	CMD-C2D	-2.07	1.46	1.51
30	f	103	SQD	O3-C3	-2.07	1.38	1.43
22	B	606	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	606	CLA	CMD-C2D	-2.06	1.46	1.51
30	a	401	SQD	O2-C2	-2.06	1.38	1.43
22	B	601	CLA	CMD-C2D	-2.06	1.46	1.51
22	c	501	CLA	CMD-C2D	-2.06	1.46	1.51
22	D	405	CLA	CMD-C2D	-2.06	1.46	1.51
31	B	623	LMT	O2B-C2B	-2.06	1.38	1.43
22	B	614	CLA	CMD-C2D	-2.06	1.46	1.51
22	C	520	CLA	CMD-C2D	-2.06	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.06	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	618	CLA	CMD-C2D	-2.05	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.05	1.46	1.51
22	c	512	CLA	CMD-C2D	-2.05	1.46	1.51
31	D	410	LMT	O4'-C4B	-2.05	1.38	1.43
22	D	406	CLA	CMD-C2D	-2.05	1.46	1.51
31	B	622	LMT	O4'-C4B	-2.05	1.38	1.43
25	C	515	DGD	O1G-C1G	-2.05	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	CMD-C2D	-2.05	1.46	1.51
22	h	101	CLA	CMD-C2D	-2.05	1.46	1.51
31	b	626	LMT	O4'-C4B	-2.05	1.38	1.43
22	c	506	CLA	CMD-C2D	-2.05	1.46	1.51
22	C	506	CLA	CMD-C2D	-2.05	1.46	1.51
22	d	404	CLA	CMD-C2D	-2.05	1.46	1.51
22	d	405	CLA	CMD-C2D	-2.05	1.46	1.51
23	A	406	PL9	C6-C1	-2.04	1.44	1.48
22	C	501	CLA	CMD-C2D	-2.04	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.04	1.46	1.51
30	F	102	SQD	O3-C3	-2.04	1.38	1.43
22	C	512	CLA	CMD-C2D	-2.04	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.03	1.46	1.51
22	C	510	CLA	CMD-C2D	-2.03	1.46	1.51
31	b	627	LMT	O2B-C2B	-2.03	1.38	1.43
31	i	102	LMT	O4'-C4B	-2.02	1.38	1.43
31	b	627	LMT	O4'-C4B	-2.02	1.38	1.43
31	B	623	LMT	O4'-C4B	-2.02	1.38	1.43
34	V	201	HEM	CAA-C2A	2.01	1.55	1.52
24	C	514	BCR	C38-C26	-2.01	1.47	1.50
32	D	402	PHO	C1B-C2B	2.01	1.50	1.45
25	C	517	DGD	C1G-C2G	2.01	1.56	1.50
25	d	408	DGD	O1G-C1G	-2.01	1.40	1.45
30	a	415	SQD	O3-C3	-2.01	1.38	1.43
32	D	402	PHO	CMC-C2C	-2.01	1.46	1.50
26	c	519	LHG	O7-C5	-2.01	1.41	1.46
30	A	413	SQD	O3-C3	-2.01	1.38	1.43
27	a	413	LMG	C7-C8	2.00	1.56	1.50
24	c	514	BCR	C38-C26	-2.00	1.47	1.50
22	b	619	CLA	CMC-C2C	-2.00	1.46	1.50
25	a	411	DGD	O1G-C1G	-2.00	1.40	1.45
30	A	414	SQD	O4-C4	-2.00	1.38	1.43
30	F	102	SQD	O4-C4	-2.00	1.38	1.43

All (1197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.20	109.94	106.71
22	c	504	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	C	510	CLA	C4A-NA-C1A	7.11	109.90	106.71
22	B	603	CLA	C4A-NA-C1A	7.06	109.88	106.71
22	B	611	CLA	C4A-NA-C1A	7.06	109.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C4A-NA-C1A	7.02	109.86	106.71
22	b	615	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	b	607	CLA	C4A-NA-C1A	6.98	109.84	106.71
22	a	405	CLA	C4A-NA-C1A	6.96	109.83	106.71
22	A	403	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	c	520	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	C	501	CLA	C4A-NA-C1A	6.79	109.76	106.71
22	c	503	CLA	C4A-NA-C1A	6.78	109.76	106.71
22	C	503	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	c	510	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	b	616	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	C	520	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	b	618	CLA	C4A-NA-C1A	6.73	109.73	106.71
22	B	605	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	c	501	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	c	511	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	B	615	CLA	C4A-NA-C1A	6.69	109.71	106.71
22	C	512	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	c	512	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	C	506	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	C	511	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	B	614	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	B	604	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	b	619	CLA	C4A-NA-C1A	6.58	109.66	106.71
22	B	606	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	B	612	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	c	506	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	b	608	CLA	C4A-NA-C1A	6.56	109.66	106.71
22	C	505	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	a	406	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	d	404	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	A	405	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	B	609	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	b	617	CLA	C4A-NA-C1A	6.47	109.61	106.71
22	B	607	CLA	C4A-NA-C1A	6.45	109.61	106.71
22	D	405	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	c	505	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	a	408	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	c	508	CLA	C4A-NA-C1A	6.43	109.60	106.71
22	h	101	CLA	C4A-NA-C1A	6.43	109.59	106.71
22	B	602	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	C	507	CLA	C4A-NA-C1A	6.42	109.59	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	c	507	CLA	C4A-NA-C1A	6.39	109.58	106.71
22	b	610	CLA	C4A-NA-C1A	6.33	109.55	106.71
22	b	611	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	C	502	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	d	405	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	C	508	CLA	C4A-NA-C1A	6.31	109.55	106.71
22	c	502	CLA	C4A-NA-C1A	6.30	109.54	106.71
22	B	601	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	B	608	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	H	101	CLA	C4A-NA-C1A	6.25	109.52	106.71
22	D	406	CLA	C4A-NA-C1A	6.25	109.51	106.71
22	A	404	CLA	C4A-NA-C1A	6.18	109.48	106.71
22	b	605	CLA	C4A-NA-C1A	6.16	109.47	106.71
22	b	606	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	b	613	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	C	509	CLA	C4A-NA-C1A	6.11	109.45	106.71
22	a	404	CLA	C4A-NA-C1A	6.08	109.44	106.71
22	A	402	CLA	C4A-NA-C1A	6.07	109.44	106.71
22	c	509	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	b	612	CLA	C4A-NA-C1A	6.02	109.41	106.71
23	j	101	PL9	C7-C3-C4	5.66	121.48	116.88
23	J	101	PL9	C7-C3-C4	5.58	121.41	116.88
30	b	602	SQD	O6-C1-C2	5.56	116.99	108.30
30	A	413	SQD	O9-S-C6	5.40	113.36	106.94
23	A	406	PL9	C7-C3-C4	5.38	121.25	116.88
30	B	626	SQD	O6-C1-C2	5.37	116.68	108.30
22	b	614	CLA	C4A-NA-C1A	5.36	109.11	106.71
22	B	610	CLA	C4A-NA-C1A	5.34	109.11	106.71
23	d	406	PL9	C7-C3-C4	5.31	121.19	116.88
23	D	407	PL9	C7-C3-C4	5.24	121.14	116.88
30	a	415	SQD	O6-C1-C2	5.22	116.45	108.30
30	a	415	SQD	O9-S-C6	5.17	113.08	106.94
23	a	409	PL9	C7-C3-C4	5.14	121.06	116.88
30	A	413	SQD	O6-C1-C2	4.91	115.97	108.30
25	A	408	DGD	O3G-C3G-C2G	-4.64	99.69	110.90
25	a	411	DGD	O3G-C3G-C2G	-4.64	99.70	110.90
22	B	610	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
30	D	403	SQD	O6-C1-C2	4.47	115.28	108.30
22	b	614	CLA	CMB-C2B-C1B	-4.44	121.63	128.46
30	A	414	SQD	O7-S-C6	4.44	112.21	106.94
30	d	402	SQD	O6-C1-C2	4.43	115.22	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	602	SQD	O7-S-C6	4.42	112.20	106.94
25	C	517	DGD	O3G-C3G-C2G	-4.37	100.36	110.90
30	a	401	SQD	O7-S-C6	4.34	112.09	106.94
30	d	402	SQD	O5-C5-C4	4.33	117.55	109.69
30	f	103	SQD	O7-S-C6	4.31	112.06	106.94
30	D	403	SQD	O5-C5-C4	4.25	117.40	109.69
30	B	626	SQD	O7-S-C6	4.23	111.96	106.94
26	a	412	LHG	O4-P-O5	4.18	132.92	112.24
22	C	507	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
22	c	507	CLA	CMB-C2B-C1B	-4.16	122.06	128.46
26	C	519	LHG	O4-P-O5	4.16	132.83	112.24
26	c	519	LHG	O4-P-O5	4.16	132.82	112.24
26	A	409	LHG	O4-P-O5	4.16	132.80	112.24
30	b	602	SQD	O9-S-C6	4.14	111.86	106.94
22	B	612	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
30	B	626	SQD	O9-S-C6	4.11	111.82	106.94
30	F	102	SQD	O7-S-C6	4.11	111.82	106.94
25	c	517	DGD	O3G-C3G-C2G	-4.10	101.01	110.90
22	b	616	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
30	d	402	SQD	O9-S-C6	4.07	111.78	106.94
30	D	403	SQD	O9-S-C6	4.02	111.72	106.94
30	b	602	SQD	O5-C5-C4	4.02	116.99	109.69
30	B	626	SQD	O5-C5-C4	4.02	116.99	109.69
30	A	414	SQD	O5-C5-C4	3.97	116.91	109.69
30	A	413	SQD	O47-C7-C8	3.94	119.99	111.50
30	a	415	SQD	O47-C7-C8	3.92	119.94	111.50
27	d	407	LMG	C1-C2-C3	-3.88	101.92	110.00
22	b	611	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
22	B	607	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
27	D	408	LMG	C1-C2-C3	-3.83	102.02	110.00
25	c	516	DGD	O5D-C6D-C5D	-3.82	101.98	109.05
30	D	403	SQD	O7-S-C6	3.82	111.47	106.94
30	D	403	SQD	O9-S-O7	-3.79	100.83	113.95
30	d	402	SQD	O9-S-O7	-3.79	100.84	113.95
30	f	103	SQD	O9-S-O7	-3.78	100.86	113.95
30	F	102	SQD	O9-S-O7	-3.77	100.89	113.95
24	C	513	BCR	C2-C1-C6	3.77	116.28	110.48
30	a	401	SQD	O5-C5-C4	3.75	116.50	109.69
30	A	413	SQD	O9-S-O7	-3.75	100.98	113.95
24	c	513	BCR	C2-C1-C6	3.73	116.23	110.48
30	a	415	SQD	O9-S-O7	-3.73	101.04	113.95
23	j	101	PL9	C7-C3-C2	-3.73	118.40	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
30	b	602	SQD	O9-S-O7	-3.72	101.07	113.95
30	a	401	SQD	O9-S-C6	3.72	111.36	106.94
30	B	626	SQD	O9-S-O7	-3.72	101.09	113.95
22	B	602	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
30	a	415	SQD	O5-C5-C4	3.70	116.42	109.69
23	J	101	PL9	C7-C3-C2	-3.70	118.44	123.30
30	a	401	SQD	O9-S-O7	-3.70	101.16	113.95
30	a	415	SQD	O7-S-C6	3.70	111.33	106.94
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	B	609	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	B	613	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
22	b	606	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	b	615	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	d	408	DGD	O6D-C1D-O3G	-3.67	101.28	109.97
22	B	611	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
30	A	414	SQD	O9-S-O7	-3.66	101.27	113.95
30	B	626	SQD	O47-C7-C8	3.66	119.39	111.50
30	A	413	SQD	O7-S-C6	3.66	111.29	106.94
30	F	102	SQD	O8-S-C6	3.66	111.57	105.74
30	b	602	SQD	O47-C7-C8	3.65	119.37	111.50
22	C	512	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
30	f	103	SQD	O8-S-C6	3.65	111.55	105.74
22	C	506	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
22	A	402	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
25	D	409	DGD	O6D-C1D-O3G	-3.63	101.37	109.97
22	c	506	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	A	405	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	c	512	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
22	C	505	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
22	c	502	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
30	f	103	SQD	O5-C5-C4	3.61	116.25	109.69
22	a	408	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
30	d	402	SQD	O7-S-C6	3.61	111.23	106.94
25	c	516	DGD	O3G-C3G-C2G	-3.60	102.22	110.90
24	J	102	BCR	C11-C10-C9	-3.60	122.18	127.31
25	C	516	DGD	O3G-C3G-C2G	-3.59	102.23	110.90
22	C	510	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
30	F	102	SQD	O5-C5-C4	3.58	116.20	109.69
22	b	613	CLA	CMB-C2B-C1B	-3.58	122.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	503	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
23	d	406	PL9	C7-C3-C2	-3.57	118.61	123.30
22	a	404	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
30	A	413	SQD	O5-C5-C4	3.55	116.14	109.69
25	C	516	DGD	O5D-C6D-C5D	-3.55	102.48	109.05
22	C	502	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	c	511	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
24	J	102	BCR	C3-C4-C5	-3.51	107.82	114.08
22	b	605	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
23	D	407	PL9	C7-C3-C2	-3.49	118.71	123.30
22	B	601	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	A	406	PL9	C7-C3-C2	-3.48	118.73	123.30
22	C	520	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
30	A	414	SQD	O47-C7-C8	3.47	118.98	111.50
22	B	614	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
30	A	414	SQD	O9-S-C6	3.46	111.06	106.94
22	B	612	CLA	CMB-C2B-C3B	3.46	131.15	124.68
22	c	520	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
22	b	618	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	A	403	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	A	404	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
24	j	102	BCR	C3-C4-C5	-3.43	107.94	114.08
22	D	406	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.42	102.64	110.90
22	B	603	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
25	C	515	DGD	O3G-C3G-C2G	-3.42	102.65	110.90
22	a	405	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
22	B	605	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
30	D	403	SQD	O47-C7-C8	3.41	118.84	111.50
24	j	102	BCR	C24-C23-C22	-3.40	121.09	126.23
22	b	616	CLA	CMB-C2B-C3B	3.40	131.04	124.68
30	a	401	SQD	C44-O6-C1	3.40	120.38	113.74
22	b	607	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
24	j	102	BCR	C11-C10-C9	-3.39	122.48	127.31
30	F	102	SQD	O6-C1-C2	3.38	113.57	108.30
22	b	608	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
22	b	609	CLA	CMB-C2B-C1B	-3.37	123.28	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	F	102	SQD	O47-C7-C8	3.37	118.77	111.50
23	a	409	PL9	C7-C3-C2	-3.36	118.88	123.30
30	d	402	SQD	C3-C4-C5	3.35	116.22	110.24
25	B	620	DGD	O3G-C3G-C2G	-3.35	102.82	110.90
22	d	404	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	h	101	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
22	c	508	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
30	f	103	SQD	O47-C7-C8	3.34	118.69	111.50
22	H	101	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
22	D	405	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	C	508	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	c	507	CLA	CMB-C2B-C3B	3.33	130.90	124.68
22	b	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
30	d	402	SQD	O47-C7-C8	3.31	118.63	111.50
22	a	406	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
30	d	402	SQD	O8-S-C6	3.28	110.97	105.74
30	a	401	SQD	O47-C7-C8	3.27	118.56	111.50
22	C	507	CLA	CMB-C2B-C3B	3.27	130.79	124.68
24	A	407	BCR	C2-C1-C6	3.27	115.51	110.48
22	b	619	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
24	J	102	BCR	C2-C1-C6	3.26	115.50	110.48
24	j	102	BCR	C2-C1-C6	3.26	115.50	110.48
22	B	603	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	b	624	DGD	O3G-C3G-C2G	-3.24	103.07	110.90
22	c	503	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
22	b	611	CLA	CMB-C2B-C3B	3.24	130.75	124.68
22	B	606	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
22	B	608	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
22	b	606	CLA	CMB-C2B-C3B	3.22	130.71	124.68
22	b	612	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	d	408	DGD	O3G-C3G-C2G	-3.21	103.16	110.90
30	A	414	SQD	C44-O6-C1	3.20	120.00	113.74
24	J	102	BCR	C24-C23-C22	-3.20	121.39	126.23
22	b	606	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
22	B	607	CLA	CMB-C2B-C3B	3.20	130.66	124.68
22	b	609	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	613	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	c	507	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
22	B	602	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	b	624	DGD	O6D-C1D-O3G	-3.17	102.46	109.97
22	B	605	CLA	O2D-CGD-O1D	-3.17	117.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	403	SQD	O8-S-C6	3.17	110.79	105.74
30	a	415	SQD	C3-C4-C5	3.17	115.89	110.24
22	b	617	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
22	C	506	CLA	CMB-C2B-C3B	3.15	130.58	124.68
22	B	613	CLA	CMB-C2B-C3B	3.15	130.57	124.68
25	c	516	DGD	O6D-C1D-O3G	-3.14	102.53	109.97
30	D	403	SQD	C3-C4-C5	3.14	115.84	110.24
22	c	506	CLA	CMB-C2B-C3B	3.14	130.55	124.68
24	a	410	BCR	C2-C1-C6	3.12	115.29	110.48
22	c	510	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	C	502	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
30	F	102	SQD	O9-S-C6	3.11	110.64	106.94
22	a	408	CLA	CMB-C2B-C3B	3.11	130.50	124.68
25	D	409	DGD	O3G-C3G-C2G	-3.11	103.40	110.90
31	B	628	LMT	C1'-O5'-C5'	-3.11	107.59	113.69
30	f	103	SQD	O6-C1-C2	3.11	113.15	108.30
22	b	617	CLA	CMB-C2B-C3B	3.11	130.49	124.68
25	B	620	DGD	O6D-C1D-O3G	-3.10	102.64	109.97
22	C	504	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
22	C	503	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	B	618	BCR	C2-C1-C6	3.09	115.24	110.48
22	C	512	CLA	CMB-C2B-C3B	3.09	130.46	124.68
30	A	413	SQD	C3-C4-C5	3.09	115.75	110.24
22	A	405	CLA	CMB-C2B-C3B	3.08	130.44	124.68
22	B	604	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
25	A	408	DGD	O6D-C1D-O3G	-3.07	102.70	109.97
22	B	610	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	C	505	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	b	607	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
22	C	504	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
22	b	610	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	c	505	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	b	622	BCR	C2-C1-C6	3.05	115.18	110.48
22	c	504	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	B	609	CLA	CMB-C2B-C3B	3.05	130.39	124.68
22	c	504	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
24	b	621	BCR	C15-C14-C13	-3.05	122.96	127.31
22	c	502	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	c	512	CLA	CMB-C2B-C3B	3.04	130.37	124.68
24	J	102	BCR	C7-C8-C9	-3.04	121.64	126.23
22	b	615	CLA	CMB-C2B-C3B	3.04	130.37	124.68
22	C	503	CLA	CMB-C2B-C3B	3.04	130.37	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	CMB-C2B-C3B	3.04	130.36	124.68
25	c	517	DGD	C1D-C2D-C3D	-3.03	103.68	110.00
22	c	502	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
24	g	101	BCR	C33-C5-C6	-3.03	121.13	124.53
22	B	606	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
22	B	611	CLA	CMB-C2B-C3B	3.02	130.34	124.68
22	C	505	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	B	608	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	C	516	DGD	O6D-C1D-O3G	-3.01	102.84	109.97
22	C	507	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
22	b	612	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
22	c	503	CLA	CMB-C2B-C3B	3.01	130.30	124.68
22	b	605	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
24	b	622	BCR	C24-C23-C22	-3.00	121.71	126.23
22	c	505	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
22	b	613	CLA	CMB-C2B-C3B	2.99	130.28	124.68
22	B	602	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
24	j	102	BCR	C7-C8-C9	-2.98	121.73	126.23
24	B	617	BCR	C15-C16-C17	-2.98	117.37	123.47
22	b	611	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	b	604	LMT	C1'-O5'-C5'	-2.97	107.85	113.69
25	c	515	DGD	O6D-C1D-O3G	-2.97	102.94	109.97
24	y	101	BCR	C33-C5-C6	-2.96	121.20	124.53
25	B	625	DGD	O5D-C1E-C2E	2.96	112.93	108.30
22	b	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	C	511	CLA	CMB-C2B-C3B	2.96	130.22	124.68
25	C	517	DGD	C1D-C2D-C3D	-2.96	103.83	110.00
24	j	102	BCR	C15-C14-C13	-2.96	123.09	127.31
24	B	619	BCR	C2-C1-C6	2.95	115.03	110.48
22	C	510	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	H	101	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
22	C	502	CLA	CMB-C2B-C3B	2.95	130.19	124.68
24	f	102	BCR	C29-C30-C25	2.94	115.01	110.48
22	a	406	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	a	404	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
25	B	625	DGD	C1D-C2D-C3D	-2.94	103.88	110.00
24	H	102	BCR	C33-C5-C6	-2.94	121.23	124.53
22	c	511	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
22	d	405	CLA	CMB-C2B-C3B	2.93	130.17	124.68
22	c	511	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	b	623	BCR	C2-C1-C6	2.93	114.99	110.48
25	b	601	DGD	C1D-C2D-C3D	-2.92	103.91	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
22	b	608	CLA	CMB-C2B-C3B	2.92	130.13	124.68
22	B	601	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	D	406	CLA	CMB-C2B-C3B	2.91	130.13	124.68
22	B	607	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	b	613	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	515	DGD	O6D-C1D-O3G	-2.91	103.08	109.97
30	B	626	SQD	C3-C4-C5	2.91	115.43	110.24
25	a	411	DGD	O6D-C1D-O3G	-2.91	103.08	109.97
22	c	506	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	B	604	CLA	CMB-C2B-C3B	2.90	130.11	124.68
22	A	403	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	B	612	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	D	406	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
22	c	520	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
22	c	512	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
24	b	621	BCR	C15-C16-C17	-2.89	117.54	123.47
22	A	402	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	b	616	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
22	b	614	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	C	501	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
27	b	628	LMG	O6-C1-O1	-2.89	103.14	109.97
24	c	521	BCR	C2-C1-C6	2.89	114.92	110.48
22	D	405	CLA	CMB-C2B-C3B	2.88	130.06	124.68
30	b	602	SQD	C3-C4-C5	2.88	115.37	110.24
22	d	404	CLA	CMB-C2B-C3B	2.87	130.06	124.68
22	b	618	CLA	CMB-C2B-C3B	2.87	130.06	124.68
24	x	101	BCR	C33-C5-C6	-2.87	121.30	124.53
22	B	614	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
22	B	605	CLA	CMB-C2B-C3B	2.87	130.05	124.68
22	c	510	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
25	b	601	DGD	O5D-C1E-C2E	2.87	112.78	108.30
22	C	520	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
22	B	614	CLA	CMB-C2B-C3B	2.86	130.03	124.68
22	A	404	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
25	C	517	DGD	CDB-CCB-CBB	-2.86	99.90	114.42
22	B	603	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	c	517	DGD	CDB-CCB-CBB	-2.86	99.92	114.42
24	D	411	BCR	C33-C5-C6	-2.86	121.32	124.53
22	A	404	CLA	CMB-C2B-C3B	2.86	130.02	124.68
24	B	617	BCR	C15-C14-C13	-2.85	123.24	127.31
22	C	520	CLA	CMB-C2B-C3B	2.85	130.01	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	405	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	f	103	SQD	C44-O6-C1	2.84	119.29	113.74
24	D	411	BCR	C29-C30-C25	2.84	114.86	110.48
22	C	511	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
31	B	623	LMT	C3'-C4'-C5'	-2.84	104.42	110.93
22	d	404	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	c	501	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	b	609	CLA	CMB-C2B-C3B	2.84	129.98	124.68
22	c	501	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
31	i	102	LMT	O1'-C1'-C2'	2.83	112.73	108.30
27	B	624	LMG	O6-C1-O1	-2.83	103.26	109.97
22	h	101	CLA	CMB-C2B-C3B	2.83	129.98	124.68
25	c	516	DGD	CDB-CCB-CBB	-2.83	100.05	114.42
22	C	501	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
22	b	607	CLA	CMB-C2B-C3B	2.82	129.96	124.68
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
25	b	601	DGD	O3G-C3G-C2G	-2.82	104.09	110.90
24	f	102	BCR	C33-C5-C6	-2.82	121.36	124.53
24	J	102	BCR	C15-C14-C13	-2.82	123.29	127.31
23	J	101	PL9	C7-C8-C9	-2.82	122.10	126.79
22	A	403	CLA	CMB-C2B-C3B	2.82	129.95	124.68
30	f	103	SQD	O9-S-C6	2.82	110.29	106.94
22	b	610	CLA	CMB-C2B-C3B	2.82	129.94	124.68
22	b	618	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
24	B	617	BCR	C33-C5-C6	-2.81	121.37	124.53
22	B	609	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	C	509	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	D	405	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
22	a	408	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
32	D	402	PHO	O2D-CGD-O1D	-2.81	118.34	123.84
22	h	101	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
25	C	516	DGD	CDB-CCB-CBB	-2.81	100.18	114.42
23	d	406	PL9	C40-C39-C41	2.80	119.98	115.27
25	C	517	DGD	O5D-C6D-C5D	-2.80	103.87	109.05
22	c	520	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	A	402	CLA	CMB-C2B-C3B	2.80	129.91	124.68
22	b	612	CLA	CMB-C2B-C3B	2.79	129.91	124.68
22	C	512	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	b	620	BCR	C33-C5-C6	-2.79	121.40	124.53
22	b	605	CLA	CMB-C2B-C3B	2.78	129.88	124.68
30	d	402	SQD	C44-O6-C1	2.78	119.17	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	102	BCR	C27-C26-C25	2.78	126.76	122.73
24	y	101	BCR	C7-C8-C9	-2.77	122.04	126.23
22	b	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	I	102	LMT	O1'-C1'-C2'	2.77	112.63	108.30
22	b	614	CLA	CMD-C2D-C3D	2.77	129.86	124.68
22	B	608	CLA	CMB-C2B-C3B	2.77	129.86	124.68
26	a	412	LHG	O8-C23-C24	2.77	120.60	111.91
23	d	406	PL9	C7-C8-C9	-2.77	122.18	126.79
24	B	616	BCR	C33-C5-C6	-2.77	121.42	124.53
22	B	601	CLA	CMB-C2B-C3B	2.77	129.85	124.68
22	a	405	CLA	CMB-C2B-C3B	2.77	129.85	124.68
24	C	521	BCR	C2-C1-C6	2.77	114.74	110.48
31	b	627	LMT	C3'-C4'-C5'	-2.76	104.59	110.93
22	c	509	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
22	B	606	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	a	405	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
24	B	618	BCR	C29-C30-C25	2.75	114.72	110.48
22	c	508	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	D	407	PL9	C22-C23-C24	-2.75	121.03	127.66
23	D	407	PL9	C7-C8-C9	-2.75	122.22	126.79
22	A	405	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
25	B	625	DGD	O3G-C3G-C2G	-2.74	104.28	110.90
24	b	621	BCR	C33-C5-C6	-2.74	121.45	124.53
23	j	101	PL9	C7-C8-C9	-2.74	122.23	126.79
26	A	409	LHG	O8-C23-C24	2.74	120.51	111.91
22	a	406	CLA	CMB-C2B-C3B	2.74	129.80	124.68
24	y	101	BCR	C27-C26-C25	2.73	126.70	122.73
24	C	514	BCR	C15-C16-C17	-2.73	117.88	123.47
24	b	622	BCR	C29-C30-C25	2.73	114.69	110.48
22	C	508	CLA	CMB-C2B-C3B	2.73	129.79	124.68
25	b	601	DGD	C3G-C2G-C1G	-2.73	105.33	111.79
22	a	404	CLA	CMB-C2B-C3B	2.73	129.78	124.68
24	b	621	BCR	C28-C27-C26	-2.73	109.21	114.08
22	b	609	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	A	403	CLA	CHB-C4A-NA	2.72	128.28	124.51
32	D	401	PHO	O2D-CGD-O1D	-2.72	118.52	123.84
25	D	409	DGD	CDB-CCB-CBB	-2.72	100.62	114.42
24	c	521	BCR	C15-C16-C17	-2.72	117.91	123.47
22	C	509	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
25	c	517	DGD	C1D-O6D-C5D	-2.71	108.36	113.69
24	y	101	BCR	C38-C26-C25	-2.71	121.48	124.53
30	D	403	SQD	C44-O6-C1	2.71	119.03	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	CMD-C2D-C3D	2.71	129.75	124.68
25	C	517	DGD	C1D-O6D-C5D	-2.71	108.37	113.69
22	b	619	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
22	a	405	CLA	CHB-C4A-NA	2.71	128.25	124.51
32	d	401	PHO	O2D-CGD-O1D	-2.71	118.55	123.84
23	D	407	PL9	C40-C39-C41	2.70	119.82	115.27
22	C	511	CLA	CMD-C2D-C3D	2.70	129.74	124.68
22	B	615	CLA	CMB-C2B-C3B	2.70	129.73	124.68
25	d	408	DGD	CDB-CCB-CBB	-2.70	100.71	114.42
23	A	406	PL9	C22-C23-C24	-2.70	121.17	127.66
22	C	504	CLA	CMB-C2B-C3B	2.70	129.72	124.68
24	B	617	BCR	C28-C27-C26	-2.69	109.27	114.08
24	g	101	BCR	C27-C26-C25	2.69	126.64	122.73
25	c	517	DGD	O5D-C6D-C5D	-2.69	104.06	109.05
32	a	407	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
27	C	518	LMG	O6-C1-O1	-2.69	103.60	109.97
22	B	610	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	B	625	DGD	C3G-C2G-C1G	-2.69	105.43	111.79
22	B	610	CLA	CMD-C2D-C3D	2.69	129.71	124.68
24	c	514	BCR	C28-C27-C26	-2.69	109.28	114.08
24	g	101	BCR	C38-C26-C25	-2.68	121.51	124.53
24	B	618	BCR	C24-C23-C22	-2.67	122.19	126.23
22	C	504	CLA	CMD-C2D-C3D	2.67	129.68	124.68
23	a	409	PL9	C22-C23-C24	-2.67	121.23	127.66
24	c	514	BCR	C11-C10-C9	-2.67	123.50	127.31
24	j	102	BCR	C27-C26-C25	2.67	126.61	122.73
27	c	518	LMG	O6-C1-O1	-2.67	103.66	109.97
24	C	514	BCR	C28-C27-C26	-2.67	109.32	114.08
22	C	510	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	d	406	PL9	C22-C23-C24	-2.66	121.25	127.66
22	B	611	CLA	CMD-C2D-C3D	2.66	129.65	124.68
24	g	101	BCR	C7-C8-C9	-2.65	122.22	126.23
24	C	521	BCR	C15-C16-C17	-2.65	118.04	123.47
27	E	101	LMG	C1-C2-C3	-2.65	104.47	110.00
22	b	619	CLA	CMB-C2B-C3B	2.65	129.64	124.68
22	C	506	CLA	CHB-C4A-NA	2.65	128.17	124.51
27	I	101	LMG	O6-C1-O1	-2.65	103.71	109.97
22	c	504	CLA	CMB-C2B-C3B	2.64	129.62	124.68
22	d	404	CLA	CMD-C2D-C3D	2.64	129.62	124.68
24	b	623	BCR	C7-C8-C9	-2.64	122.25	126.23
22	c	502	CLA	CMD-C2D-C3D	2.63	129.60	124.68
22	B	603	CLA	CHB-C4A-NA	2.63	128.15	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	b	622	BCR	C11-C10-C9	-2.63	123.56	127.31
22	a	408	CLA	CMD-C2D-C3D	2.63	129.59	124.68
22	B	605	CLA	CHB-C4A-NA	2.63	128.14	124.51
24	B	618	BCR	C11-C10-C9	-2.62	123.56	127.31
27	i	101	LMG	O6-C1-O1	-2.62	103.76	109.97
24	j	102	BCR	C33-C5-C6	-2.62	121.59	124.53
23	J	101	PL9	C22-C23-C24	-2.62	121.35	127.66
22	D	405	CLA	CMD-C2D-C3D	2.61	129.57	124.68
22	b	608	CLA	CHB-C4A-NA	2.61	128.12	124.51
30	B	626	SQD	C4-C3-C2	2.61	115.38	110.82
22	b	615	CLA	CMD-C2D-C3D	2.61	129.56	124.68
22	B	603	CLA	C1-C2-C3	-2.61	121.54	126.04
22	c	520	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	J	102	BCR	C33-C5-C6	-2.60	121.61	124.53
22	C	512	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	b	607	CLA	CHB-C4A-NA	2.60	128.11	124.51
30	B	626	SQD	O8-S-C6	2.60	109.88	105.74
23	j	101	PL9	C22-C23-C24	-2.60	121.41	127.66
22	b	607	CLA	C1-C2-C3	-2.60	121.55	126.04
26	c	519	LHG	O8-C23-C24	2.60	120.05	111.91
22	a	406	CLA	CHB-C4A-NA	2.60	128.10	124.51
34	F	101	HEM	C1D-C2D-C3D	-2.59	105.19	107.00
30	b	602	SQD	C4-C3-C2	2.59	115.35	110.82
24	c	514	BCR	C15-C16-C17	-2.59	118.17	123.47
30	a	401	SQD	O8-S-C6	2.59	109.87	105.74
26	C	519	LHG	O8-C23-C24	2.59	120.04	111.91
24	j	102	BCR	C15-C16-C17	-2.59	118.17	123.47
22	C	505	CLA	CHB-C4A-NA	2.59	128.09	124.51
32	D	402	PHO	CBD-CHA-C4D	-2.59	105.62	108.54
22	C	520	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	a	409	PL9	C7-C8-C9	-2.58	122.49	126.79
22	c	512	CLA	CHB-C4A-NA	2.58	128.08	124.51
22	B	608	CLA	CMD-C2D-C3D	2.58	129.50	124.68
24	C	513	BCR	C24-C23-C22	-2.58	122.34	126.23
34	f	101	HEM	CBD-CAD-C3D	-2.58	107.73	112.48
22	c	507	CLA	CMD-C2D-C3D	2.57	129.49	124.68
31	M	102	LMT	C1'-O5'-C5'	-2.57	108.64	113.69
24	c	513	BCR	C7-C8-C9	-2.57	122.35	126.23
22	B	615	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	J	102	BCR	C35-C13-C14	-2.57	119.33	122.92
30	a	415	SQD	O8-S-C6	2.57	109.83	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	CMD-C2D-C3D	2.57	129.48	124.68
22	C	504	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	C	513	BCR	C15-C16-C17	-2.56	118.22	123.47
31	b	626	LMT	C1'-O5'-C5'	-2.56	108.67	113.69
24	c	514	BCR	C15-C14-C13	-2.56	123.66	127.31
22	c	508	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
32	D	401	PHO	CBD-CHA-C4D	-2.55	105.66	108.54
22	b	612	CLA	CMD-C2D-C3D	2.55	129.46	124.68
22	C	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	c	510	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	A	408	DGD	O5D-C6D-C5D	-2.55	104.33	109.05
24	B	618	BCR	C15-C14-C13	-2.55	123.68	127.31
22	b	618	CLA	CHB-C4A-NA	2.54	128.03	124.51
24	B	619	BCR	C7-C8-C9	-2.54	122.40	126.23
22	b	615	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
22	C	503	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	d	408	DGD	C3D-C4D-C5D	-2.54	105.72	110.24
22	c	511	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	B	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
27	b	625	LMG	C1-C2-C3	-2.53	104.72	110.00
31	B	622	LMT	C1'-O5'-C5'	-2.53	108.72	113.69
22	c	505	CLA	CHB-C4A-NA	2.53	128.01	124.51
32	a	407	PHO	CBD-CHA-C4D	-2.53	105.69	108.54
22	c	508	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	504	CLA	CMD-C2D-C3D	2.52	129.40	124.68
24	C	514	BCR	C29-C30-C25	2.52	114.37	110.48
25	c	516	DGD	O6E-C1E-O5D	-2.52	104.00	109.97
24	c	514	BCR	C29-C30-C25	2.52	114.36	110.48
25	d	408	DGD	C3G-C2G-C1G	-2.52	105.83	111.79
34	f	101	HEM	C1D-C2D-C3D	-2.52	105.24	107.00
32	d	401	PHO	CBD-CHA-C4D	-2.51	105.71	108.54
25	D	409	DGD	CFB-CEB-CDB	-2.51	101.67	114.42
22	c	503	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	b	615	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	B	607	CLA	CMD-C2D-C3D	2.51	129.37	124.68
22	d	405	CLA	CMD-C2D-C3D	2.51	129.37	124.68
27	M	101	LMG	C1-C2-C3	-2.51	104.77	110.00
22	b	611	CLA	CMD-C2D-C3D	2.51	129.37	124.68
22	B	601	CLA	CMD-C2D-C3D	2.51	129.37	124.68
24	C	514	BCR	C33-C5-C6	-2.51	121.72	124.53
24	c	513	BCR	C11-C10-C9	-2.50	123.74	127.31
24	C	513	BCR	C15-C14-C13	-2.50	123.74	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	BCR	C3-C4-C5	-2.50	109.61	114.08
22	B	614	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	505	CLA	CMD-C2D-C3D	2.50	129.36	124.68
27	B	621	LMG	C1-C2-C3	-2.50	104.79	110.00
24	c	521	BCR	C15-C14-C13	-2.50	123.74	127.31
22	a	404	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	C	514	BCR	C15-C14-C13	-2.49	123.75	127.31
22	d	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
22	A	405	CLA	CMD-C2D-C3D	2.49	129.34	124.68
22	c	501	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	511	CLA	CHB-C4A-NA	2.49	127.95	124.51
30	b	602	SQD	O8-S-C6	2.49	109.70	105.74
24	a	410	BCR	C33-C5-C6	-2.49	121.73	124.53
22	c	504	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	C	521	BCR	C15-C14-C13	-2.48	123.76	127.31
27	d	410	LMG	C38-C37-C36	-2.48	101.83	114.42
22	B	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	b	622	BCR	C15-C14-C13	-2.48	123.77	127.31
22	A	404	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	A	413	SQD	O8-S-C6	2.48	109.69	105.74
27	D	412	LMG	C38-C37-C36	-2.48	101.85	114.42
22	h	101	CLA	CMD-C2D-C3D	2.48	129.31	124.68
22	B	606	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
22	D	406	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	b	617	CLA	CMD-C2D-C3D	2.47	129.30	124.68
22	B	607	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	b	616	CLA	CHB-C4A-NA	2.47	127.93	124.51
22	D	406	CLA	CMD-C2D-C3D	2.47	129.30	124.68
27	d	407	LMG	C38-C37-C36	-2.47	101.88	114.42
25	d	408	DGD	CFB-CEB-CDB	-2.47	101.88	114.42
23	a	409	PL9	C41-C39-C40	2.47	120.06	114.60
24	B	619	BCR	C3-C4-C5	-2.47	109.67	114.08
23	A	406	PL9	C7-C8-C9	-2.47	122.68	126.79
24	c	514	BCR	C33-C5-C6	-2.47	121.76	124.53
22	b	611	CLA	CHB-C4A-NA	2.47	127.92	124.51
22	B	611	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
22	h	101	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	B	608	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	A	408	DGD	CBB-CAB-C9B	-2.46	101.94	114.42
22	C	508	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
30	A	414	SQD	O8-S-C6	2.46	109.66	105.74
22	b	606	CLA	CMD-C2D-C3D	2.46	129.28	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	B	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
30	F	102	SQD	C3-C4-C5	2.46	114.62	110.24
27	A	410	LMG	C40-C39-C38	-2.46	101.96	114.42
22	b	613	CLA	CMD-C2D-C3D	2.46	129.27	124.68
24	c	513	BCR	C15-C14-C13	-2.46	123.81	127.31
22	C	507	CLA	CMD-C2D-C3D	2.45	129.27	124.68
24	C	513	BCR	C8-C7-C6	-2.45	120.31	127.20
22	c	501	CLA	CMB-C2B-C3B	2.45	129.27	124.68
22	a	408	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	602	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	b	605	CLA	CMD-C2D-C3D	2.45	129.26	124.68
22	C	508	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	602	CLA	CMD-C2D-C3D	2.45	129.26	124.68
22	C	506	CLA	CMD-C2D-C3D	2.45	129.26	124.68
31	M	102	LMT	C3'-C4'-C5'	-2.45	105.32	110.93
24	j	102	BCR	C35-C13-C14	-2.45	119.50	122.92
27	a	402	LMG	O6-C1-O1	-2.45	104.18	109.97
31	D	410	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
24	y	101	BCR	C1-C6-C5	-2.44	119.17	122.61
25	a	411	DGD	CBB-CAB-C9B	-2.44	102.02	114.42
24	B	618	BCR	C15-C16-C17	-2.44	118.47	123.47
22	B	614	CLA	CMD-C2D-C3D	2.44	129.25	124.68
22	B	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
27	D	408	LMG	O6-C1-C2	-2.44	105.18	110.35
22	b	606	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
22	A	402	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	D	403	SQD	O48-C23-C24	2.44	119.56	111.91
32	D	402	PHO	O1D-CGD-CBD	2.44	129.47	124.48
22	a	408	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
22	B	611	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	B	619	BCR	C27-C26-C25	2.43	126.27	122.73
22	b	610	CLA	CHB-C4A-NA	2.43	127.88	124.51
22	c	507	CLA	CHB-C4A-NA	2.43	127.88	124.51
30	a	401	SQD	C1-O5-C5	2.43	118.46	113.69
24	c	513	BCR	C8-C7-C6	-2.43	120.37	127.20
24	B	616	BCR	C11-C10-C9	-2.43	123.84	127.31
22	b	606	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	a	405	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	C	501	CLA	CMD-C2D-C3D	2.43	129.22	124.68
24	c	521	BCR	C27-C26-C25	2.43	126.26	122.73
22	c	501	CLA	CMD-C2D-C3D	2.43	129.22	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	CHB-C4A-NA	2.43	127.87	124.51
27	D	408	LMG	C38-C37-C36	-2.42	102.12	114.42
22	C	505	CLA	CMD-C2D-C3D	2.42	129.21	124.68
22	b	610	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	C	502	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	A	403	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	B	603	CLA	CMD-C2D-C3D	2.42	129.21	124.68
24	A	407	BCR	C33-C5-C6	-2.42	121.81	124.53
22	C	505	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	C	501	CLA	CMB-C2B-C3B	2.42	129.20	124.68
22	a	406	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
24	c	513	BCR	C15-C16-C17	-2.42	118.52	123.47
24	C	514	BCR	C11-C10-C9	-2.42	123.86	127.31
27	C	522	LMG	C40-C39-C38	-2.42	102.15	114.42
27	A	410	LMG	C1-C2-C3	-2.42	104.96	110.00
22	B	613	CLA	CMD-C2D-C3D	2.42	129.20	124.68
27	c	522	LMG	C40-C39-C38	-2.41	102.17	114.42
26	c	519	LHG	C11-C10-C9	-2.41	102.17	114.42
22	b	618	CLA	CMD-C2D-C3D	2.41	129.19	124.68
22	B	615	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	C	504	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
31	b	603	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
22	A	404	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
22	b	617	CLA	CHB-C4A-NA	2.41	127.84	124.51
22	B	613	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	c	516	DGD	C3G-C2G-C1G	-2.41	106.09	111.79
32	a	407	PHO	O1D-CGD-CBD	2.41	129.41	124.48
32	d	401	PHO	O1D-CGD-CBD	2.41	129.41	124.48
22	c	506	CLA	CMD-C2D-C3D	2.41	129.19	124.68
30	F	102	SQD	C44-O6-C1	2.41	118.44	113.74
24	C	521	BCR	C27-C26-C25	2.41	126.23	122.73
23	a	409	PL9	C20-C19-C21	2.41	119.32	115.27
25	a	411	DGD	O5D-C6D-C5D	-2.41	104.60	109.05
24	b	621	BCR	C29-C30-C25	2.40	114.18	110.48
22	B	612	CLA	CMD-C2D-C3D	2.40	129.18	124.68
27	a	413	LMG	C40-C39-C38	-2.40	102.22	114.42
25	B	620	DGD	CBB-CAB-C9B	-2.40	102.22	114.42
25	C	516	DGD	O6E-C1E-O5D	-2.40	104.28	109.97
24	B	617	BCR	C29-C30-C25	2.40	114.18	110.48
31	M	103	LMT	C1'-O5'-C5'	-2.40	108.97	113.69
27	B	624	LMG	C38-C37-C36	-2.40	102.23	114.42
24	b	623	BCR	C27-C26-C25	2.40	126.22	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	PL9	C41-C39-C40	2.40	119.90	114.60
22	C	503	CLA	CMD-C2D-C3D	2.40	129.16	124.68
22	A	402	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
25	b	624	DGD	CBB-CAB-C9B	-2.40	102.26	114.42
22	A	405	CLA	CHB-C4A-NA	2.40	127.83	124.51
27	e	101	LMG	O6-C1-O1	-2.40	104.30	109.97
24	c	513	BCR	C3-C4-C5	-2.40	109.80	114.08
22	B	605	CLA	CMD-C2D-C3D	2.40	129.16	124.68
31	M	103	LMT	C3'-C4'-C5'	-2.39	105.44	110.93
24	C	513	BCR	C3-C4-C5	-2.39	109.81	114.08
22	b	619	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	a	404	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
25	C	517	DGD	CFB-CEB-CDB	-2.39	102.30	114.42
22	C	511	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
25	c	516	DGD	CFB-CEB-CDB	-2.39	102.31	114.42
22	b	612	CLA	CHB-C4A-NA	2.39	127.81	124.51
27	A	415	LMG	O6-C1-O1	-2.39	104.33	109.97
22	B	608	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
34	v	201	HEM	C1D-C2D-C3D	-2.38	105.34	107.00
27	b	628	LMG	C38-C37-C36	-2.38	102.33	114.42
25	c	517	DGD	CFB-CEB-CDB	-2.38	102.33	114.42
27	e	101	LMG	C1-C2-C3	-2.38	105.04	110.00
23	d	406	PL9	C20-C19-C21	2.38	119.28	115.27
24	A	407	BCR	C27-C26-C25	2.38	126.19	122.73
27	c	522	LMG	O6-C1-O1	-2.38	104.34	109.97
24	b	622	BCR	C15-C16-C17	-2.38	118.60	123.47
23	a	409	PL9	C27-C28-C29	-2.38	121.93	127.66
34	V	201	HEM	C1D-C2D-C3D	-2.38	105.34	107.00
30	d	402	SQD	O48-C23-C24	2.38	119.37	111.91
22	C	506	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	b	612	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
22	c	511	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
25	B	620	DGD	C1D-C2D-C3D	-2.37	105.06	110.00
22	b	608	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
30	a	401	SQD	O48-C23-C24	2.37	119.35	111.91
22	B	601	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
24	b	620	BCR	C11-C10-C9	-2.37	123.93	127.31
25	c	515	DGD	C3G-C2G-C1G	-2.37	106.19	111.79
30	A	414	SQD	C1-O5-C5	2.37	118.33	113.69
22	b	611	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	C	509	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	H	101	CLA	CMD-C2D-C3D	2.36	129.10	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	102	BCR	C29-C30-C25	2.36	114.12	110.48
22	c	503	CLA	CMD-C2D-C3D	2.36	129.10	124.68
24	J	102	BCR	C29-C30-C25	2.36	114.12	110.48
22	c	506	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
24	C	521	BCR	C24-C23-C22	-2.36	122.67	126.23
22	C	510	CLA	CMD-C2D-C3D	2.36	129.09	124.68
22	C	507	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	D	407	PL9	C27-C28-C29	-2.36	121.98	127.66
31	B	627	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
22	h	101	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
24	g	101	BCR	C1-C6-C5	-2.36	119.29	122.61
31	i	102	LMT	C1'-O5'-C5'	-2.36	109.06	113.69
22	B	602	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
27	a	413	LMG	C1-C2-C3	-2.36	105.09	110.00
22	A	405	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
27	C	522	LMG	O6-C1-O1	-2.35	104.40	109.97
26	C	519	LHG	C11-C10-C9	-2.35	102.47	114.42
22	c	509	CLA	CHB-C4A-NA	2.35	127.77	124.51
24	a	410	BCR	C27-C26-C25	2.35	126.15	122.73
22	b	613	CLA	CHB-C4A-NA	2.35	127.76	124.51
31	d	409	LMT	C3'-C4'-C5'	-2.35	105.54	110.93
22	b	607	CLA	CMD-C2D-C3D	2.35	129.07	124.68
22	c	507	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	A	410	LMG	O3-C3-C2	-2.35	104.92	110.35
24	b	620	BCR	C2-C1-C6	2.35	114.10	110.48
23	J	101	PL9	C20-C19-C21	2.35	119.22	115.27
22	d	405	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
27	A	410	LMG	C38-C37-C36	-2.35	102.52	114.42
34	f	101	HEM	CAA-CBA-CGA	-2.34	108.74	112.67
22	b	616	CLA	CMD-C2D-C3D	2.34	129.06	124.68
25	C	516	DGD	C3D-C4D-C5D	-2.34	106.06	110.24
24	b	623	BCR	C11-C10-C9	-2.34	123.97	127.31
22	B	605	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	612	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	C	520	CLA	CMD-C2D-C3D	2.34	129.06	124.68
25	D	409	DGD	C3G-C2G-C1G	-2.34	106.26	111.79
22	H	101	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	C	515	DGD	C3G-C2G-C1G	-2.34	106.26	111.79
32	D	401	PHO	O1D-CGD-CBD	2.33	129.26	124.48
22	B	615	CLA	CMD-C2D-C3D	2.33	129.04	124.68
22	C	520	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
22	b	614	CLA	C4D-C3D-CAD	-2.33	107.17	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	407	PL9	C20-C19-C21	2.33	119.19	115.27
22	C	512	CLA	CMD-C2D-C3D	2.33	129.04	124.68
22	B	603	CLA	O1D-CGD-CBD	2.33	129.25	124.48
24	C	521	BCR	C33-C5-C6	-2.33	121.92	124.53
25	C	516	DGD	CFB-CEB-CDB	-2.33	102.61	114.42
22	H	101	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
25	C	516	DGD	C3G-C2G-C1G	-2.32	106.29	111.79
22	c	512	CLA	CMD-C2D-C3D	2.32	129.02	124.68
30	A	414	SQD	O48-C23-C24	2.32	119.19	111.91
30	a	415	SQD	O48-C23-C24	2.32	119.19	111.91
22	c	520	CLA	CMD-C2D-C3D	2.32	129.02	124.68
22	B	601	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	B	616	BCR	C2-C1-C6	2.32	114.05	110.48
22	B	609	CLA	CMD-C2D-C3D	2.32	129.01	124.68
27	D	412	LMG	C1-C2-C3	-2.31	105.17	110.00
24	c	513	BCR	C24-C23-C22	-2.31	122.74	126.23
27	C	518	LMG	C38-C37-C36	-2.31	102.68	114.42
25	b	601	DGD	O6D-C1D-O3G	-2.31	104.50	109.97
27	m	101	LMG	C1-C2-C3	-2.31	105.18	110.00
23	A	406	PL9	C20-C19-C21	2.31	119.16	115.27
22	b	608	CLA	CMD-C2D-C3D	2.31	129.00	124.68
25	D	409	DGD	C3D-C4D-C5D	-2.31	106.12	110.24
24	B	616	BCR	C15-C14-C13	-2.31	124.01	127.31
25	c	515	DGD	O5D-C6D-C5D	-2.31	104.77	109.05
22	b	614	CLA	C1-C2-C3	-2.31	122.05	126.04
27	b	625	LMG	C40-C39-C38	-2.31	102.70	114.42
27	a	413	LMG	C38-C37-C36	-2.31	102.72	114.42
27	B	621	LMG	C40-C39-C38	-2.31	102.72	114.42
22	B	608	CLA	C1-C2-C3	-2.30	122.06	126.04
22	d	405	CLA	C1-C2-C3	-2.30	122.06	126.04
22	b	605	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	A	402	CLA	CMD-C2D-C3D	2.30	128.99	124.68
31	d	409	LMT	C1'-O5'-C5'	-2.30	109.17	113.69
27	E	101	LMG	O6-C1-O1	-2.30	104.53	109.97
22	b	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	B	621	LMG	O6-C1-O1	-2.30	104.53	109.97
22	B	613	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	J	102	BCR	C15-C16-C17	-2.30	118.77	123.47
23	A	406	PL9	C27-C28-C29	-2.30	122.12	127.66
25	C	515	DGD	C1D-C2D-C3D	-2.30	105.21	110.00
24	C	521	BCR	C11-C10-C9	-2.30	124.03	127.31
27	c	518	LMG	C38-C37-C36	-2.30	102.77	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	CMD-C2D-C3D	2.30	128.97	124.68
24	B	619	BCR	C38-C26-C25	-2.29	121.95	124.53
27	d	410	LMG	O6-C1-O1	-2.29	104.54	109.97
27	m	101	LMG	O2-C2-C1	-2.29	104.47	110.05
25	c	516	DGD	C3D-C4D-C5D	-2.29	106.15	110.24
23	D	407	PL9	C37-C38-C39	-2.29	122.14	127.66
22	D	406	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	B	604	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
30	A	413	SQD	O48-C23-C24	2.29	119.09	111.91
22	B	609	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	D	407	PL9	C32-C33-C34	-2.29	122.15	127.66
23	d	406	PL9	C37-C38-C39	-2.29	122.15	127.66
24	B	616	BCR	C27-C26-C25	2.29	126.05	122.73
22	B	610	CLA	C4D-C3D-CAD	-2.29	107.19	108.47
23	d	406	PL9	C27-C28-C29	-2.29	122.16	127.66
24	b	623	BCR	C38-C26-C25	-2.29	121.96	124.53
27	b	625	LMG	C38-C37-C36	-2.28	102.83	114.42
22	b	619	CLA	CMD-C2D-C3D	2.28	128.95	124.68
22	A	404	CLA	CMD-C2D-C3D	2.28	128.95	124.68
22	B	607	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
22	c	520	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	c	512	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	b	609	CLA	CMD-C2D-C3D	2.28	128.94	124.68
22	c	509	CLA	CMD-C2D-C3D	2.28	128.94	124.68
22	c	507	CLA	O2D-CGD-CBD	2.28	115.31	111.27
25	b	624	DGD	C1D-C2D-C3D	-2.28	105.26	110.00
22	c	502	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
22	C	508	CLA	CMD-C2D-C3D	2.27	128.93	124.68
22	C	512	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	c	509	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	B	615	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
22	B	610	CLA	C1-C2-C3	-2.27	122.12	126.04
24	c	521	BCR	C33-C5-C6	-2.27	121.98	124.53
25	C	515	DGD	O5D-C6D-C5D	-2.27	104.85	109.05
22	C	509	CLA	CMD-C2D-C3D	2.27	128.92	124.68
22	c	510	CLA	CMD-C2D-C3D	2.27	128.92	124.68
31	D	410	LMT	C3'-C4'-C5'	-2.27	105.73	110.93
25	a	411	DGD	C1D-C2D-C3D	-2.26	105.28	110.00
22	b	616	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
27	B	624	LMG	O2-C2-C1	-2.26	104.55	110.05
27	c	522	LMG	C38-C37-C36	-2.26	102.95	114.42
27	d	407	LMG	O6-C1-C2	-2.26	105.56	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	BCR	C24-C23-C22	-2.26	122.82	126.23
22	b	605	CLA	CHB-C4A-NA	2.26	127.63	124.51
23	d	406	PL9	C32-C33-C34	-2.26	122.23	127.66
27	D	412	LMG	O3-C3-C2	-2.25	105.14	110.35
34	v	201	HEM	CMB-C2B-C3B	2.25	128.89	124.68
27	i	101	LMG	O2-C2-C1	-2.25	104.58	110.05
24	b	620	BCR	C27-C26-C25	2.25	126.00	122.73
22	a	404	CLA	CMD-C2D-C3D	2.25	128.88	124.68
27	C	522	LMG	C38-C37-C36	-2.25	103.02	114.42
22	c	504	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
24	b	622	BCR	C7-C8-C9	-2.24	122.84	126.23
25	A	408	DGD	C3G-C2G-C1G	-2.24	106.48	111.79
22	C	507	CLA	C1-C2-C3	-2.24	122.16	126.04
27	D	412	LMG	O6-C1-O1	-2.24	104.66	109.97
22	a	406	CLA	CMD-C2D-C3D	2.24	128.87	124.68
25	B	620	DGD	C3G-C2G-C1G	-2.24	106.49	111.79
30	f	103	SQD	C3-C4-C5	2.24	114.23	110.24
22	C	509	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
30	a	415	SQD	C4-C3-C2	2.24	114.73	110.82
22	b	613	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
31	I	102	LMT	C1'-O5'-C5'	-2.24	109.30	113.69
23	d	406	PL9	O1-C4-C3	-2.24	118.26	120.72
27	b	628	LMG	O3-C3-C2	-2.24	105.18	110.35
27	a	402	LMG	O1-C7-C8	-2.23	105.51	110.90
24	b	620	BCR	C15-C14-C13	-2.23	124.12	127.31
23	j	101	PL9	C20-C19-C21	2.23	119.03	115.27
27	B	621	LMG	C38-C37-C36	-2.23	103.09	114.42
22	B	603	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
22	c	508	CLA	CMD-C2D-C3D	2.23	128.85	124.68
27	C	522	LMG	O2-C2-C1	-2.23	104.63	110.05
22	c	503	CLA	O2D-CGD-CBD	2.22	115.22	111.27
27	B	624	LMG	O3-C3-C2	-2.22	105.21	110.35
24	B	618	BCR	C7-C8-C9	-2.22	122.88	126.23
34	F	101	HEM	CAA-CBA-CGA	-2.22	108.94	112.67
24	g	101	BCR	C3-C2-C1	-2.22	106.66	114.60
24	a	410	BCR	C38-C26-C25	-2.22	122.03	124.53
22	b	618	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
34	F	101	HEM	CBD-CAD-C3D	-2.22	108.39	112.48
22	C	501	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
24	A	407	BCR	C15-C14-C13	-2.22	124.14	127.31
22	C	511	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	B	609	CLA	C1D-CHD-C4C	2.22	125.48	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	625	LMG	O6-C1-O1	-2.22	104.72	109.97
25	B	625	DGD	O6D-C1D-O3G	-2.21	104.73	109.97
27	d	410	LMG	O3-C3-C2	-2.21	105.23	110.35
22	b	617	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
27	d	410	LMG	C1-C2-C3	-2.21	105.39	110.00
22	C	502	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	D	411	BCR	C11-C10-C9	-2.21	124.16	127.31
22	B	604	CLA	CMD-C2D-C3D	2.21	128.81	124.68
30	B	626	SQD	O48-C23-C24	2.21	118.84	111.91
24	a	410	BCR	C15-C16-C17	-2.21	118.95	123.47
27	e	101	LMG	O1-C7-C8	-2.21	105.58	110.90
27	a	413	LMG	O3-C3-C2	-2.21	105.25	110.35
24	C	513	BCR	C27-C26-C25	2.20	125.93	122.73
22	b	610	CLA	CMD-C2D-C3D	2.20	128.80	124.68
27	c	522	LMG	O2-C2-C1	-2.20	104.69	110.05
22	B	610	CLA	C1D-CHD-C4C	2.20	125.47	122.56
24	f	102	BCR	C15-C16-C17	-2.20	118.96	123.47
22	d	404	CLA	CHB-C4A-NA	2.20	127.56	124.51
22	C	507	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
32	D	402	PHO	C1B-NB-C4B	2.20	110.66	106.51
31	B	623	LMT	C1'-O5'-C5'	-2.20	109.37	113.69
23	d	406	PL9	O2-C1-C2	-2.20	116.74	121.78
25	c	516	DGD	CBB-CAB-C9B	-2.20	103.26	114.42
27	m	101	LMG	C1-O6-C5	-2.20	109.37	113.69
22	c	510	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
27	b	628	LMG	O2-C2-C1	-2.20	104.71	110.05
24	c	513	BCR	C27-C26-C25	2.20	125.92	122.73
22	D	405	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	C	514	BCR	C38-C26-C25	-2.20	122.06	124.53
25	a	411	DGD	C3G-C2G-C1G	-2.20	106.59	111.79
23	j	101	PL9	O2-C1-C2	-2.20	116.75	121.78
24	A	407	BCR	C38-C26-C25	-2.20	122.06	124.53
25	C	516	DGD	CBB-CAB-C9B	-2.20	103.28	114.42
22	C	510	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
22	b	610	CLA	C1D-CHD-C4C	2.19	125.45	122.56
24	A	407	BCR	C15-C16-C17	-2.19	118.98	123.47
22	b	607	CLA	O1D-CGD-CBD	2.19	128.97	124.48
25	c	517	DGD	C3G-O3G-C1D	2.19	118.02	113.74
27	I	101	LMG	O2-C2-C1	-2.19	104.72	110.05
22	B	614	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	b	615	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
22	C	508	CLA	C1B-CHB-C4A	-2.19	125.78	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	101	BCR	C3-C2-C1	-2.19	106.78	114.60
22	d	404	CLA	O1D-CGD-CBD	2.19	128.96	124.48
27	A	415	LMG	O1-C7-C8	-2.19	105.62	110.90
22	D	405	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
27	M	101	LMG	O2-C2-C1	-2.18	104.74	110.05
22	A	403	CLA	CMD-C2D-C3D	2.18	128.76	124.68
24	c	521	BCR	C24-C23-C22	-2.18	122.94	126.23
24	c	514	BCR	C38-C26-C25	-2.18	122.08	124.53
24	c	521	BCR	C11-C10-C9	-2.18	124.20	127.31
22	b	619	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
27	D	408	LMG	O6-C1-O1	-2.18	104.82	109.97
23	D	407	PL9	O1-C4-C3	-2.18	118.32	120.72
34	V	201	HEM	CMB-C2B-C3B	2.18	128.75	124.68
22	C	507	CLA	C1D-CHD-C4C	2.18	125.43	122.56
22	C	503	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
22	c	501	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	d	404	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
22	b	607	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
32	d	401	PHO	C1B-NB-C4B	2.17	110.60	106.51
23	J	101	PL9	O2-C1-C2	-2.17	116.81	121.78
22	c	508	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
22	B	603	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
22	D	405	CLA	O1D-CGD-CBD	2.17	128.92	124.48
22	B	605	CLA	O1D-CGD-CBD	2.17	128.92	124.48
32	D	401	PHO	C1B-NB-C4B	2.17	110.59	106.51
25	C	517	DGD	CBB-CAB-C9B	-2.17	103.43	114.42
27	c	518	LMG	O7-C10-O9	-2.16	118.47	123.70
24	C	514	BCR	C24-C23-C22	-2.16	122.97	126.23
24	f	102	BCR	C11-C10-C9	-2.16	124.22	127.31
22	b	618	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	x	101	BCR	C29-C30-C25	2.16	113.81	110.48
25	c	516	DGD	O3D-C3D-C4D	-2.16	105.35	110.35
27	C	522	LMG	O3-C3-C2	-2.16	105.36	110.35
25	a	411	DGD	CAB-C9B-C8B	-2.16	103.46	114.42
25	c	515	DGD	C1D-C2D-C3D	-2.16	105.50	110.00
25	b	601	DGD	CBB-CAB-C9B	-2.16	103.48	114.42
22	c	502	CLA	C1-C2-C3	-2.15	122.32	126.04
25	C	516	DGD	O3D-C3D-C4D	-2.15	105.37	110.35
22	c	507	CLA	C1-C2-C3	-2.15	122.32	126.04
25	A	408	DGD	CAB-C9B-C8B	-2.15	103.49	114.42
27	a	402	LMG	O3-C3-C2	-2.15	105.37	110.35
27	B	621	LMG	O3-C3-C2	-2.15	105.38	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	503	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
22	B	611	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
24	D	411	BCR	C7-C8-C9	-2.15	122.99	126.23
23	j	101	PL9	O2-C1-C6	2.15	124.31	120.59
24	g	101	BCR	C15-C16-C17	-2.15	119.07	123.47
22	B	602	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
24	B	619	BCR	C24-C23-C22	-2.15	122.99	126.23
26	a	412	LHG	C27-C26-C25	-2.15	103.53	114.42
23	d	406	PL9	C36-C34-C33	-2.15	116.78	121.12
27	i	101	LMG	O1-C7-C8	-2.15	105.72	110.90
27	I	101	LMG	O3-C3-C2	-2.14	105.39	110.35
25	B	625	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
30	b	602	SQD	O48-C23-C24	2.14	118.64	111.91
25	c	517	DGD	CBB-CAB-C9B	-2.14	103.54	114.42
25	C	516	DGD	CAB-C9B-C8B	-2.14	103.55	114.42
22	c	506	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
30	f	103	SQD	C1-O5-C5	2.14	117.89	113.69
27	i	101	LMG	O3-C3-C2	-2.14	105.40	110.35
22	B	611	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
22	c	511	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
27	C	518	LMG	O3-C3-C2	-2.14	105.41	110.35
23	a	409	PL9	O1-C4-C3	-2.14	118.37	120.72
27	c	522	LMG	O3-C3-C2	-2.14	105.41	110.35
22	D	406	CLA	C1-C2-C3	-2.14	122.35	126.04
24	H	102	BCR	C16-C15-C14	-2.13	119.10	123.47
22	c	509	CLA	O2A-CGA-O1A	-2.13	118.20	123.59
23	J	101	PL9	O2-C1-C6	2.13	124.28	120.59
27	b	625	LMG	O3-C3-C2	-2.13	105.42	110.35
25	b	624	DGD	C3G-C2G-C1G	-2.13	106.75	111.79
24	b	622	BCR	C33-C5-C6	-2.13	122.14	124.53
22	b	614	CLA	C1D-CHD-C4C	2.13	125.37	122.56
24	C	513	BCR	C7-C8-C9	-2.13	123.02	126.23
27	C	518	LMG	O7-C10-O9	-2.13	118.56	123.70
32	a	407	PHO	C1B-NB-C4B	2.13	110.52	106.51
24	D	411	BCR	C15-C16-C17	-2.12	119.12	123.47
22	b	615	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
22	c	512	CLA	C1D-CHD-C4C	2.12	125.36	122.56
24	a	410	BCR	C24-C23-C22	-2.12	123.03	126.23
27	C	518	LMG	O2-C2-C1	-2.12	104.90	110.05
24	B	616	BCR	C15-C16-C17	-2.12	119.14	123.47
31	b	627	LMT	C1'-O5'-C5'	-2.12	109.53	113.69
24	a	410	BCR	C15-C14-C13	-2.12	124.29	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
25	b	601	DGD	CAB-C9B-C8B	-2.11	103.69	114.42
27	e	101	LMG	O3-C3-C2	-2.11	105.46	110.35
25	C	517	DGD	CAB-C9B-C8B	-2.11	103.70	114.42
25	C	517	DGD	C3G-O3G-C1D	2.11	117.86	113.74
22	B	614	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
27	c	518	LMG	O3-C3-C2	-2.11	105.47	110.35
22	C	502	CLA	C1-C2-C3	-2.11	122.39	126.04
24	b	623	BCR	C15-C14-C13	-2.11	124.30	127.31
24	y	101	BCR	C15-C16-C17	-2.11	119.15	123.47
27	d	407	LMG	O6-C1-O1	-2.11	104.98	109.97
24	B	619	BCR	C11-C10-C9	-2.11	124.30	127.31
24	c	514	BCR	C24-C23-C22	-2.11	123.05	126.23
27	M	101	LMG	O3-C3-C2	-2.11	105.48	110.35
22	b	613	CLA	C1D-CHD-C4C	2.10	125.33	122.56
24	H	102	BCR	C29-C30-C25	2.10	113.72	110.48
30	A	413	SQD	C4-C3-C2	2.10	114.49	110.82
24	f	102	BCR	C27-C26-C25	2.10	125.78	122.73
22	b	614	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
23	D	407	PL9	O2-C1-C2	-2.10	116.97	121.78
27	c	518	LMG	O2-C2-C1	-2.10	104.94	110.05
22	b	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	A	415	LMG	O3-C3-C2	-2.10	105.50	110.35
24	b	621	BCR	C35-C13-C14	-2.10	119.98	122.92
22	c	520	CLA	C1D-CHD-C4C	2.10	125.33	122.56
22	C	506	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	I	101	LMG	O7-C10-O9	-2.09	118.64	123.70
25	B	625	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
30	F	102	SQD	O48-C23-C24	2.09	118.47	111.91
22	B	601	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
23	a	409	PL9	O2-C1-C6	2.09	124.21	120.59
24	j	102	BCR	C20-C21-C22	-2.09	124.33	127.31
25	A	408	DGD	C1D-C2D-C3D	-2.09	105.65	110.00
27	A	415	LMG	O7-C10-O9	-2.09	118.66	123.70
27	B	621	LMG	O2-C2-C1	-2.09	104.98	110.05
25	c	517	DGD	CAB-C9B-C8B	-2.08	103.84	114.42
22	b	616	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	d	406	PL9	O2-C1-C6	2.08	124.20	120.59
27	b	625	LMG	O2-C2-C1	-2.08	104.99	110.05
32	a	407	PHO	CMB-C2B-C1B	-2.08	121.86	125.06
26	A	409	LHG	C27-C26-C25	-2.08	103.86	114.42
25	b	624	DGD	CAB-C9B-C8B	-2.08	103.86	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	i	101	LMG	O1-C1-C2	-2.08	105.05	108.30
32	D	402	PHO	CMB-C2B-C1B	-2.08	121.86	125.06
25	d	408	DGD	C5B-C4B-C3B	-2.08	103.86	114.42
22	C	501	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
32	D	401	PHO	O2A-CGA-O1A	-2.08	118.34	123.59
24	C	514	BCR	C7-C8-C9	-2.08	123.09	126.23
22	b	607	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	C	516	DGD	C1D-C2D-C3D	-2.07	105.67	110.00
22	C	504	CLA	O1D-CGD-CBD	2.07	128.73	124.48
25	B	620	DGD	C4E-C3E-C2E	-2.07	107.20	110.82
22	B	606	CLA	C1-C2-C3	-2.07	122.46	126.04
25	c	516	DGD	CAB-C9B-C8B	-2.07	103.91	114.42
23	d	406	PL9	C31-C32-C33	-2.07	105.07	111.88
24	B	616	BCR	C38-C26-C25	-2.07	122.20	124.53
22	B	606	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
24	B	618	BCR	C33-C5-C6	-2.07	122.20	124.53
27	E	101	LMG	O1-C7-C8	-2.07	105.91	110.90
27	M	101	LMG	C1-O6-C5	-2.07	109.63	113.69
22	C	520	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
27	E	101	LMG	O3-C3-C2	-2.07	105.57	110.35
22	B	612	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
27	m	101	LMG	O3-C3-C2	-2.06	105.58	110.35
22	c	512	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	A	406	PL9	O2-C1-C2	-2.06	117.06	121.78
23	a	409	PL9	O2-C1-C2	-2.06	117.06	121.78
25	D	409	DGD	CAB-C9B-C8B	-2.06	103.96	114.42
27	B	624	LMG	O1-C1-C2	-2.06	105.08	108.30
24	g	101	BCR	C15-C14-C13	-2.06	124.37	127.31
25	D	409	DGD	C5B-C4B-C3B	-2.06	103.96	114.42
24	C	513	BCR	C11-C10-C9	-2.06	124.37	127.31
24	D	411	BCR	C27-C26-C25	2.06	125.72	122.73
22	b	606	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	c	508	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
22	c	504	CLA	O1D-CGD-CBD	2.06	128.69	124.48
22	B	614	CLA	C1D-CHD-C4C	2.06	125.27	122.56
22	C	512	CLA	C1D-CHD-C4C	2.06	125.27	122.56
22	a	405	CLA	CMD-C2D-C3D	2.05	128.52	124.68
24	C	521	BCR	C38-C26-C25	-2.05	122.22	124.53
22	C	509	CLA	C1D-CHD-C4C	2.05	125.27	122.56
24	b	622	BCR	C27-C26-C25	2.05	125.71	122.73
25	c	516	DGD	C1D-O6D-C5D	-2.05	109.67	113.69
22	b	606	CLA	O2D-CGD-CBD	2.05	114.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	PL9	O2-C1-C6	2.05	124.14	120.59
22	B	607	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	c	501	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
24	b	620	BCR	C15-C16-C17	-2.04	119.28	123.47
24	C	513	BCR	C38-C26-C25	-2.04	122.23	124.53
22	a	405	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	c	511	CLA	C1D-CHD-C4C	2.04	125.25	122.56
22	H	101	CLA	C1-C2-C3	-2.04	122.52	126.04
22	b	616	CLA	C1D-CHD-C4C	2.04	125.25	122.56
22	C	512	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
25	d	408	DGD	CAB-C9B-C8B	-2.04	104.08	114.42
24	b	621	BCR	C24-C23-C22	-2.04	123.16	126.23
22	b	613	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
24	B	616	BCR	C7-C8-C9	-2.04	123.16	126.23
25	C	517	DGD	C5B-C4B-C3B	-2.04	104.09	114.42
23	A	406	PL9	O1-C4-C3	-2.03	118.48	120.72
27	a	413	LMG	O2-C2-C1	-2.03	105.10	110.05
30	f	103	SQD	O48-C23-C24	2.03	118.29	111.91
22	B	610	CLA	CHB-C4A-NA	2.03	127.32	124.51
22	B	602	CLA	C1D-CHD-C4C	2.03	125.24	122.56
23	D	407	PL9	C12-C13-C14	-2.03	122.77	127.66
27	a	413	LMG	O7-C10-O9	-2.03	118.79	123.70
22	b	609	CLA	O1D-CGD-CBD	2.03	128.64	124.48
22	C	520	CLA	C1D-CHD-C4C	2.03	125.24	122.56
27	A	410	LMG	O7-C10-O9	-2.03	118.80	123.70
22	A	403	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	c	520	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	a	406	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	a	404	CLA	C1-C2-C3	-2.03	122.54	126.04
25	d	408	DGD	CBB-CAB-C9B	-2.03	104.14	114.42
32	d	401	PHO	O2A-CGA-O1A	-2.03	118.48	123.59
23	D	407	PL9	O2-C1-C6	2.02	124.10	120.59
32	d	401	PHO	C2B-C1B-NB	-2.02	106.74	109.79
27	e	101	LMG	O7-C10-O9	-2.02	118.81	123.70
25	c	517	DGD	C5B-C4B-C3B	-2.02	104.15	114.42
26	C	519	LHG	C27-C26-C25	-2.02	104.16	114.42
27	i	101	LMG	O7-C10-O9	-2.02	118.82	123.70
24	J	102	BCR	C34-C9-C10	-2.02	120.09	122.92
22	B	606	CLA	C1D-CHD-C4C	2.02	125.23	122.56
25	C	515	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
27	a	413	LMG	O1-C1-C2	-2.02	105.15	108.30
25	D	409	DGD	CBB-CAB-C9B	-2.02	104.18	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	DGD	C5B-C4B-C3B	-2.02	104.19	114.42
24	B	617	BCR	C38-C26-C25	-2.02	122.26	124.53
24	C	521	BCR	C7-C8-C9	-2.01	123.19	126.23
22	b	612	CLA	C1-C2-C3	-2.01	122.56	126.04
25	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.42
26	c	519	LHG	C27-C26-C25	-2.01	104.21	114.42
24	B	617	BCR	C24-C23-C22	-2.01	123.20	126.23
24	D	411	BCR	C24-C23-C22	-2.01	123.20	126.23
24	c	513	BCR	C38-C26-C25	-2.01	122.27	124.53
22	C	505	CLA	C1D-CHD-C4C	2.01	125.21	122.56
25	B	620	DGD	C5B-C4B-C3B	-2.01	104.24	114.42
27	C	518	LMG	O1-C7-C8	-2.01	106.06	110.90
22	b	618	CLA	C1D-CHD-C4C	2.01	125.20	122.56
22	c	507	CLA	C1D-CHD-C4C	2.01	125.20	122.56
22	a	406	CLA	C1D-CHD-C4C	2.00	125.20	122.56
27	c	518	LMG	O1-C7-C8	-2.00	106.07	110.90

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	D	406	CLA	NC
22	D	406	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	d	404	CLA	NC
22	d	404	CLA	ND

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Mol	Chain	Res	Type	Atom
22	d	404	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	509	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND

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Mol	Chain	Res	Type	Atom
22	A	402	CLA	NA
22	a	408	CLA	NC
22	a	408	CLA	ND
22	a	408	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	504	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND

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Mol	Chain	Res	Type	Atom
22	a	404	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	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

All (2136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	m	101	LMG	O9-C10-O7-C8
27	e	101	LMG	C2-C1-O1-C7
27	e	101	LMG	O6-C1-O1-C7
27	d	407	LMG	C2-C1-O1-C7
27	d	407	LMG	O6-C1-O1-C7
25	c	517	DGD	C2D-C1D-O3G-C3G
25	c	517	DGD	O6D-C1D-O3G-C3G
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
22	A	404	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	CBD-CGD-O2D-CED
22	d	404	CLA	C2-C3-C5-C6
22	d	404	CLA	C4-C3-C5-C6
25	b	624	DGD	C2E-C1E-O5D-C6D
27	d	410	LMG	O9-C10-O7-C8
27	d	410	LMG	C11-C10-O7-C8
27	E	101	LMG	C2-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7
27	M	101	LMG	O9-C10-O7-C8
30	a	401	SQD	C24-C23-O48-C46
27	b	625	LMG	C11-C10-O7-C8
30	d	402	SQD	C2-C1-O6-C44
30	d	402	SQD	O5-C1-O6-C44
30	d	402	SQD	O49-C7-O47-C45
30	d	402	SQD	C8-C7-O47-C45
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6
24	y	101	BCR	C7-C8-C9-C10
24	x	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C21-C22-C23-C24
24	x	101	BCR	C37-C22-C23-C24
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	f	102	BCR	C1-C6-C7-C8
24	f	102	BCR	C7-C8-C9-C10
24	f	102	BCR	C37-C22-C23-C24
23	D	407	PL9	C27-C28-C29-C31
23	D	407	PL9	C34-C36-C37-C38
22	b	607	CLA	CBD-CGD-O2D-CED
25	A	408	DGD	C2D-C1D-O3G-C3G
22	D	405	CLA	C2-C3-C5-C6
22	D	405	CLA	C4-C3-C5-C6
25	c	515	DGD	C2B-C1B-O2G-C2G
25	c	515	DGD	O1B-C1B-O2G-C2G
25	c	515	DGD	C2E-C1E-O5D-C6D
24	D	411	BCR	C1-C6-C7-C8
24	D	411	BCR	C7-C8-C9-C10
25	C	515	DGD	C2B-C1B-O2G-C2G
25	C	515	DGD	O1B-C1B-O2G-C2G
25	C	515	DGD	C2E-C1E-O5D-C6D
27	c	518	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
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	b	619	CLA	C3A-C2A-CAA-CBA
22	b	619	CLA	CBD-CGD-O2D-CED
34	V	201	HEM	C2D-C3D-CAD-CBD
34	V	201	HEM	C4D-C3D-CAD-CBD
30	B	626	SQD	O5-C5-C6-S
22	a	405	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
22	b	617	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O2D
27	D	412	LMG	O9-C10-O7-C8
27	D	412	LMG	C11-C10-O7-C8
24	j	102	BCR	C1-C6-C7-C8
24	j	102	BCR	C21-C22-C23-C24
24	g	101	BCR	C7-C8-C9-C10
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-C20
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-C41
24	c	513	BCR	C6-C7-C8-C9
30	b	602	SQD	O5-C5-C6-S
25	d	408	DGD	O6D-C1D-O3G-C3G
22	b	611	CLA	C1A-C2A-CAA-CBA
23	d	406	PL9	C27-C28-C29-C31
23	d	406	PL9	C34-C36-C37-C38
24	c	521	BCR	C7-C8-C9-C10
24	c	521	BCR	C7-C8-C9-C34
22	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	403	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	A	403	CLA	CHA-CBD-CGD-O2D
22	c	504	CLA	C1A-C2A-CAA-CBA
22	c	504	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C3A-C2A-CAA-CBA
22	B	604	CLA	CBD-CGD-O2D-CED
22	H	101	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C3A-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
26	C	519	LHG	C4-O6-P-O4
25	D	409	DGD	O1B-C1B-O2G-C2G
25	D	409	DGD	O6D-C1D-O3G-C3G
30	a	415	SQD	C2-C1-O6-C44
30	a	415	SQD	C5-C6-S-O7
30	a	415	SQD	C5-C6-S-O8
30	a	415	SQD	C5-C6-S-O9
22	A	402	CLA	CBD-CGD-O2D-CED
34	v	201	HEM	C2D-C3D-CAD-CBD
34	v	201	HEM	C4D-C3D-CAD-CBD
26	a	412	LHG	C1-C2-C3-O3
27	B	624	LMG	O1-C7-C8-O7
27	B	624	LMG	C11-C10-O7-C8
27	B	624	LMG	O10-C28-O8-C9
24	b	623	BCR	C23-C24-C25-C30
24	B	617	BCR	C21-C22-C23-C24
24	B	617	BCR	C37-C22-C23-C24
24	B	617	BCR	C23-C24-C25-C26
22	B	607	CLA	C1A-C2A-CAA-CBA
30	D	403	SQD	C2-C1-O6-C44
30	D	403	SQD	O5-C1-O6-C44
30	D	403	SQD	O49-C7-O47-C45
30	D	403	SQD	C8-C7-O47-C45
27	c	522	LMG	C2-C1-O1-C7
27	c	522	LMG	O6-C1-O1-C7
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
22	B	605	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C3A-C2A-CAA-CBA
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
25	C	516	DGD	O1B-C1B-O2G-C2G
25	C	516	DGD	C2D-C1D-O3G-C3G
25	C	516	DGD	O6D-C1D-O3G-C3G
22	b	616	CLA	CBD-CGD-O2D-CED
23	a	409	PL9	C7-C8-C9-C11
23	a	409	PL9	C12-C13-C14-C15
23	a	409	PL9	C12-C13-C14-C16
23	a	409	PL9	C17-C18-C19-C21
23	a	409	PL9	C22-C23-C24-C25
23	a	409	PL9	C24-C26-C27-C28
23	a	409	PL9	C27-C28-C29-C30
23	a	409	PL9	C27-C28-C29-C31
23	a	409	PL9	C30-C29-C31-C32
23	a	409	PL9	C37-C38-C39-C41
22	B	603	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	C1A-C2A-CAA-CBA
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
30	A	414	SQD	C24-C23-O48-C46
25	B	620	DGD	C2E-C1E-O5D-C6D
22	B	612	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	C	522	LMG	C2-C1-O1-C7
27	C	522	LMG	O6-C1-O1-C7
24	B	616	BCR	C1-C6-C7-C8
22	B	601	CLA	CBD-CGD-O2D-CED
26	A	409	LHG	C1-C2-C3-O3
22	b	608	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	C6-C7-C8-C9
22	B	606	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C2-C3-C5-C6
22	B	602	CLA	C4-C3-C5-C6
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	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	609	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	CBD-CGD-O2D-CED
25	a	411	DGD	C2D-C1D-O3G-C3G
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
26	c	519	LHG	C3-O3-P-O6
26	c	519	LHG	C4-O6-P-O4
24	b	621	BCR	C21-C22-C23-C24
24	b	621	BCR	C23-C24-C25-C26
27	b	628	LMG	O1-C7-C8-O7
27	b	628	LMG	C11-C10-O7-C8
24	J	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C21-C22-C23-C24
24	J	102	BCR	C37-C22-C23-C24
22	a	404	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
27	B	621	LMG	C11-C10-O7-C8
24	C	521	BCR	C7-C8-C9-C34
30	A	413	SQD	C2-C1-O6-C44
30	A	413	SQD	C5-C6-S-O7
30	A	413	SQD	C5-C6-S-O8
30	A	413	SQD	C5-C6-S-O9
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
27	D	408	LMG	C2-C1-O1-C7
27	D	408	LMG	O6-C1-O1-C7
22	h	101	CLA	C1A-C2A-CAA-CBA
22	h	101	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	h	101	CLA	C4-C3-C5-C6
22	h	101	CLA	C6-C7-C8-C9
24	b	620	BCR	C1-C6-C7-C8
22	b	607	CLA	O1D-CGD-O2D-CED
22	b	619	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	O1D-CGD-O2D-CED
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	c	520	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	C	520	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
27	e	101	LMG	O10-C28-O8-C9
27	E	101	LMG	O10-C28-O8-C9
30	a	401	SQD	O10-C23-O48-C46
30	A	414	SQD	O10-C23-O48-C46
31	b	604	LMT	C3'-C4'-O1B-C1B
31	B	628	LMT	C3'-C4'-O1B-C1B
22	b	605	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	C8-C9-O8-C28

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
27	d	407	LMG	C29-C28-O8-C9
30	F	102	SQD	C24-C23-O48-C46
30	f	103	SQD	C24-C23-O48-C46
27	a	413	LMG	C29-C28-O8-C9
23	A	406	PL9	C37-C38-C39-C40
23	a	409	PL9	C37-C38-C39-C40
22	b	609	CLA	CBD-CGD-O2D-CED
32	a	407	PHO	CBD-CGD-O2D-CED
22	B	605	CLA	CBD-CGD-O2D-CED
27	d	407	LMG	O10-C28-O8-C9
30	F	102	SQD	O10-C23-O48-C46
30	f	103	SQD	O10-C23-O48-C46
27	A	410	LMG	O10-C28-O8-C9
27	c	518	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	a	413	LMG	O10-C28-O8-C9
27	b	628	LMG	O10-C28-O8-C9
27	D	408	LMG	O10-C28-O8-C9
22	B	604	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
32	D	402	PHO	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
27	A	415	LMG	O9-C10-O7-C8
27	b	625	LMG	O9-C10-O7-C8
25	d	408	DGD	O1B-C1B-O2G-C2G
27	I	101	LMG	O9-C10-O7-C8
27	B	624	LMG	O9-C10-O7-C8
27	a	402	LMG	O9-C10-O7-C8
27	i	101	LMG	O9-C10-O7-C8
27	b	628	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
31	b	603	LMT	C3'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
31	B	627	LMT	C3'-C4'-O1B-C1B
27	c	518	LMG	C8-C9-O8-C28
22	A	404	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
22	b	611	CLA	C3-C5-C6-C7
22	B	607	CLA	C3-C5-C6-C7
22	a	406	CLA	C3-C5-C6-C7
32	d	401	PHO	C3-C5-C6-C7
22	B	613	CLA	C3-C5-C6-C7
27	A	410	LMG	C29-C28-O8-C9
27	c	518	LMG	C29-C28-O8-C9
27	c	522	LMG	C29-C28-O8-C9
27	C	518	LMG	C29-C28-O8-C9
27	D	408	LMG	C29-C28-O8-C9
27	I	101	LMG	O6-C5-C6-O5
27	m	101	LMG	C11-C10-O7-C8
30	F	102	SQD	C8-C7-O47-C45
25	c	516	DGD	C2B-C1B-O2G-C2G
27	M	101	LMG	C11-C10-O7-C8
25	b	601	DGD	C2B-C1B-O2G-C2G
25	C	516	DGD	C2B-C1B-O2G-C2G
27	a	402	LMG	C11-C10-O7-C8
25	B	625	DGD	C2B-C1B-O2G-C2G
23	j	101	PL9	C27-C28-C29-C31
23	J	101	PL9	C27-C28-C29-C31
22	c	520	CLA	O1D-CGD-O2D-CED
22	b	606	CLA	O1D-CGD-O2D-CED
22	C	520	CLA	O1D-CGD-O2D-CED
22	c	505	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
25	A	408	DGD	O6E-C5E-C6E-O5E
27	i	101	LMG	O6-C5-C6-O5
25	b	624	DGD	C4D-C5D-C6D-O5D
25	b	624	DGD	O6E-C5E-C6E-O5E
25	B	620	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	511	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
22	C	507	CLA	O1D-CGD-O2D-CED
31	i	102	LMT	C3'-C4'-O1B-C1B
25	d	408	DGD	C2A-C1A-O1G-C1G
25	D	409	DGD	C2A-C1A-O1G-C1G
27	B	624	LMG	C29-C28-O8-C9
27	C	522	LMG	C29-C28-O8-C9
27	b	628	LMG	C29-C28-O8-C9
31	I	102	LMT	C3'-C4'-O1B-C1B
22	C	508	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
25	B	620	DGD	C4D-C5D-C6D-O5D
23	j	101	PL9	C7-C8-C9-C10
23	a	409	PL9	C17-C18-C19-C20
23	J	101	PL9	C7-C8-C9-C10
22	c	512	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
27	e	101	LMG	O9-C10-O7-C8
23	j	101	PL9	C7-C8-C9-C11
23	A	406	PL9	C22-C23-C24-C26
23	a	409	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	408	DGD	O1A-C1A-O1G-C1G
25	D	409	DGD	O1A-C1A-O1G-C1G
27	C	522	LMG	O10-C28-O8-C9
22	b	614	CLA	O1D-CGD-O2D-CED
25	a	411	DGD	O6E-C5E-C6E-O5E
27	b	628	LMG	O6-C5-C6-O5
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	615	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
26	a	412	LHG	O2-C2-C3-O3
26	A	409	LHG	O2-C2-C3-O3
22	C	508	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	H	101	CLA	C3-C5-C6-C7
32	D	401	PHO	C3-C5-C6-C7
27	e	101	LMG	C29-C28-O8-C9
27	E	101	LMG	C29-C28-O8-C9
27	I	101	LMG	C4-C5-C6-O5
22	b	617	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
27	d	407	LMG	C11-C10-O7-C8
30	f	103	SQD	C8-C7-O47-C45
27	A	415	LMG	C11-C10-O7-C8
25	D	409	DGD	C2B-C1B-O2G-C2G
27	D	408	LMG	C11-C10-O7-C8
25	c	515	DGD	O6E-C5E-C6E-O5E
25	C	515	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	C4E-C5E-C6E-O5E
27	i	101	LMG	C4-C5-C6-O5
27	B	624	LMG	O6-C5-C6-O5
22	c	508	CLA	C3-C5-C6-C7
22	B	615	CLA	CBA-CGA-O2A-C1
25	c	516	DGD	O6E-C5E-C6E-O5E
25	C	516	DGD	O6E-C5E-C6E-O5E
27	c	522	LMG	O10-C28-O8-C9
27	C	518	LMG	O6-C5-C6-O5
32	D	401	PHO	C4-C3-C5-C6
32	d	401	PHO	C4-C3-C5-C6
25	A	408	DGD	C4E-C5E-C6E-O5E
32	D	401	PHO	C2-C3-C5-C6
32	d	401	PHO	C2-C3-C5-C6
22	b	605	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	O1D-CGD-O2D-CED
27	c	518	LMG	O6-C5-C6-O5
25	B	620	DGD	C4E-C5E-C6E-O5E
27	A	415	LMG	O6-C1-O1-C7
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	402	LMG	O6-C1-O1-C7
32	d	401	PHO	CBA-CGA-O2A-C1
25	c	515	DGD	C4E-C5E-C6E-O5E
25	C	515	DGD	C4E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	O1A-CGA-O2A-C1
25	d	408	DGD	C2B-C1B-O2G-C2G
27	i	101	LMG	C11-C10-O7-C8
23	a	409	PL9	C7-C8-C9-C10
22	c	509	CLA	CBD-CGD-O2D-CED
27	d	407	LMG	O9-C10-O7-C8
27	E	101	LMG	O9-C10-O7-C8
32	d	401	PHO	O1A-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
22	b	619	CLA	CBA-CGA-O2A-C1
32	D	401	PHO	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
27	c	518	LMG	C4-C5-C6-O5
27	C	518	LMG	C4-C5-C6-O5
22	B	605	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	C15-C16-C17-C18
22	B	611	CLA	C5-C6-C7-C8
22	B	606	CLA	C15-C16-C17-C18
25	a	411	DGD	C4E-C5E-C6E-O5E
22	B	615	CLA	C5-C6-C7-C8
27	C	518	LMG	C10-C11-C12-C13
25	d	408	DGD	C2D-C1D-O3G-C3G
25	D	409	DGD	C2D-C1D-O3G-C3G
27	m	101	LMG	O1-C7-C8-O7
25	c	516	DGD	O2G-C2G-C3G-O3G
25	C	516	DGD	O2G-C2G-C3G-O3G
30	b	602	SQD	O10-C23-O48-C46
32	D	401	PHO	O1A-CGA-O2A-C1
27	b	628	LMG	C4-C5-C6-O5
22	b	608	CLA	C2-C3-C5-C6
22	c	510	CLA	C6-C7-C8-C9
22	a	405	CLA	C6-C7-C8-C9
22	C	508	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	B	607	CLA	C6-C7-C8-C9
22	c	508	CLA	C6-C7-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	A	404	CLA	C10-C11-C12-C13
22	b	619	CLA	C5-C6-C7-C8
32	a	407	PHO	C15-C16-C17-C18
22	b	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	C13-C15-C16-C17
22	b	613	CLA	C2A-CAA-CBA-CGA
24	y	101	BCR	C7-C8-C9-C34
24	D	411	BCR	C37-C22-C23-C24
24	j	102	BCR	C37-C22-C23-C24
24	g	101	BCR	C7-C8-C9-C34
24	b	621	BCR	C37-C22-C23-C24
24	B	617	BCR	C7-C8-C9-C10
24	b	621	BCR	C7-C8-C9-C10
27	I	101	LMG	C11-C10-O7-C8
27	A	415	LMG	C28-C29-C30-C31
27	b	625	LMG	C10-C11-C12-C13
25	d	408	DGD	C1B-C2B-C3B-C4B
27	B	621	LMG	C10-C11-C12-C13
22	b	619	CLA	O1A-CGA-O2A-C1
22	B	611	CLA	C13-C15-C16-C17
22	c	503	CLA	C10-C11-C12-C13
22	b	609	CLA	O1D-CGD-O2D-CED
32	a	407	PHO	O1D-CGD-O2D-CED
27	c	522	LMG	O6-C5-C6-O5
22	h	101	CLA	C3-C5-C6-C7
22	c	520	CLA	C13-C15-C16-C17
22	c	520	CLA	C15-C16-C17-C18
22	b	619	CLA	C10-C11-C12-C13
22	C	520	CLA	C15-C16-C17-C18
22	a	406	CLA	C10-C11-C12-C13
22	B	603	CLA	C13-C15-C16-C17
32	D	402	PHO	C15-C16-C17-C18
22	B	609	CLA	C8-C10-C11-C12
22	B	615	CLA	C10-C11-C12-C13
22	d	404	CLA	C13-C15-C16-C17
22	d	404	CLA	C15-C16-C17-C18
22	b	607	CLA	C13-C15-C16-C17
22	D	405	CLA	C13-C15-C16-C17
22	D	405	CLA	C15-C16-C17-C18
22	B	608	CLA	C13-C15-C16-C17
22	C	520	CLA	C13-C15-C16-C17
22	b	612	CLA	C13-C15-C16-C17
22	C	507	CLA	C10-C11-C12-C13
22	C	508	CLA	C5-C6-C7-C8
22	c	504	CLA	C10-C11-C12-C13
22	C	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	503	CLA	C10-C11-C12-C13
22	C	501	CLA	C15-C16-C17-C18
22	C	504	CLA	C10-C11-C12-C13
22	c	507	CLA	C10-C11-C12-C13
22	c	508	CLA	C5-C6-C7-C8
22	b	613	CLA	C8-C10-C11-C12
22	c	505	CLA	C5-C6-C7-C8
22	c	505	CLA	C15-C16-C17-C18
23	D	407	PL9	C27-C28-C29-C30
27	d	410	LMG	C10-C11-C12-C13
25	C	515	DGD	C1B-C2B-C3B-C4B
27	c	518	LMG	C28-C29-C30-C31
27	D	412	LMG	C10-C11-C12-C13
25	D	409	DGD	C1B-C2B-C3B-C4B
27	C	518	LMG	C28-C29-C30-C31
22	b	610	CLA	C13-C15-C16-C17
22	c	509	CLA	C15-C16-C17-C18
22	C	505	CLA	C13-C15-C16-C17
22	C	501	CLA	C8-C10-C11-C12
22	C	509	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	c	505	CLA	C13-C15-C16-C17
27	c	522	LMG	C4-C5-C6-O5
22	b	605	CLA	C13-C15-C16-C17
22	c	510	CLA	C5-C6-C7-C8
22	c	501	CLA	C15-C16-C17-C18
22	B	601	CLA	C13-C15-C16-C17
22	B	606	CLA	C13-C15-C16-C17
25	c	515	DGD	C1B-C2B-C3B-C4B
27	c	518	LMG	C10-C11-C12-C13
27	c	522	LMG	C10-C11-C12-C13
27	C	522	LMG	C10-C11-C12-C13
27	c	522	LMG	C11-C10-O7-C8
22	c	506	CLA	C5-C6-C7-C8
22	b	611	CLA	C15-C16-C17-C18
22	C	512	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	C	506	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	A	402	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	O1A-CGA-O2A-C1
22	b	609	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C2A-CAA-CBA-CGA
22	B	607	CLA	O1D-CGD-O2D-CED
22	c	511	CLA	O1D-CGD-O2D-CED
32	D	402	PHO	O1D-CGD-O2D-CED
22	a	405	CLA	C15-C16-C17-C18
22	C	507	CLA	C15-C16-C17-C18
22	A	403	CLA	C15-C16-C17-C18
22	B	612	CLA	C5-C6-C7-C8
22	c	507	CLA	C15-C16-C17-C18
22	c	501	CLA	C10-C11-C12-C13
22	C	512	CLA	C15-C16-C17-C18
27	I	101	LMG	O6-C1-O1-C7
30	a	415	SQD	O5-C1-O6-C44
27	i	101	LMG	O6-C1-O1-C7
30	A	413	SQD	O5-C1-O6-C44
22	A	404	CLA	C15-C16-C17-C18
23	D	407	PL9	C29-C31-C32-C33
23	d	406	PL9	C29-C31-C32-C33
25	b	624	DGD	C1B-C2B-C3B-C4B
24	j	102	BCR	C18-C19-C20-C21
27	D	408	LMG	O9-C10-O7-C8
22	a	404	CLA	C3-C5-C6-C7
22	c	512	CLA	C15-C16-C17-C18
22	C	506	CLA	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
22	a	406	CLA	C15-C16-C17-C18
22	c	501	CLA	C8-C10-C11-C12
22	B	610	CLA	C15-C16-C17-C18
22	B	604	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
30	B	626	SQD	O10-C23-O48-C46
22	B	607	CLA	C5-C6-C7-C8
22	C	510	CLA	C5-C6-C7-C8
22	C	511	CLA	O1D-CGD-O2D-CED
27	C	522	LMG	C11-C10-O7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
26	C	519	LHG	C3-O3-P-O6
26	C	519	LHG	C4-O6-P-O3
26	c	519	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
27	a	402	LMG	C28-C29-C30-C31
27	I	101	LMG	C29-C28-O8-C9
22	b	619	CLA	C13-C15-C16-C17
25	C	515	DGD	C1A-C2A-C3A-C4A
30	a	415	SQD	C7-C8-C9-C10
25	c	517	DGD	O1B-C1B-O2G-C2G
27	c	522	LMG	O9-C10-O7-C8
25	C	517	DGD	O1B-C1B-O2G-C2G
22	B	604	CLA	C2-C3-C5-C6
22	c	520	CLA	C10-C11-C12-C13
22	b	618	CLA	C13-C15-C16-C17
22	C	501	CLA	C10-C11-C12-C13
22	C	511	CLA	CBA-CGA-O2A-C1
22	c	520	CLA	CBA-CGA-O2A-C1
30	b	602	SQD	C24-C23-O48-C46
22	c	511	CLA	CBA-CGA-O2A-C1
22	b	608	CLA	CBA-CGA-O2A-C1
31	b	604	LMT	O1'-C1-C2-C3
25	b	601	DGD	C5B-C6B-C7B-C8B
22	B	615	CLA	C13-C15-C16-C17
22	C	520	CLA	C10-C11-C12-C13
22	b	611	CLA	C5-C6-C7-C8
22	b	619	CLA	C3-C5-C6-C7
25	b	624	DGD	C3B-C4B-C5B-C6B
27	A	410	LMG	C34-C35-C36-C37
27	b	625	LMG	C31-C32-C33-C34
31	I	102	LMT	C6-C7-C8-C9
25	c	515	DGD	C3B-C4B-C5B-C6B
30	b	602	SQD	C11-C10-C9-C8
27	I	101	LMG	C14-C15-C16-C17
25	D	409	DGD	C4B-C5B-C6B-C7B
25	D	409	DGD	C5B-C6B-C7B-C8B
31	i	102	LMT	C6-C7-C8-C9
25	C	516	DGD	C2A-C3A-C4A-C5A
25	B	620	DGD	C3B-C4B-C5B-C6B
27	i	101	LMG	C12-C13-C14-C15
22	b	611	CLA	O1D-CGD-O2D-CED
30	F	102	SQD	C12-C13-C14-C15
30	f	103	SQD	C12-C13-C14-C15
27	A	415	LMG	C30-C31-C32-C33
25	b	624	DGD	C6B-C7B-C8B-C9B
27	c	518	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	I	101	LMG	C12-C13-C14-C15
25	D	409	DGD	CEB-CFB-CGB-CHB
25	b	601	DGD	C9B-CAB-CBB-CCB
27	C	518	LMG	C29-C30-C31-C32
25	a	411	DGD	C8B-C9B-CAB-CBB
25	B	625	DGD	C5B-C6B-C7B-C8B
27	B	621	LMG	C31-C32-C33-C34
27	e	101	LMG	C7-C8-O7-C10
27	C	518	LMG	C9-C8-O7-C10
30	F	102	SQD	O49-C7-O47-C45
27	C	522	LMG	O9-C10-O7-C8
25	c	516	DGD	C2A-C3A-C4A-C5A
25	A	408	DGD	C8B-C9B-CAB-CBB
25	C	515	DGD	C3B-C4B-C5B-C6B
30	B	626	SQD	C9-C10-C11-C12
25	d	408	DGD	C5B-C6B-C7B-C8B
25	d	408	DGD	CCB-CDB-CEB-CFB
25	d	408	DGD	CEB-CFB-CGB-CHB
27	c	522	LMG	C12-C13-C14-C15
27	C	522	LMG	C12-C13-C14-C15
27	i	101	LMG	C16-C17-C18-C19
27	C	522	LMG	O6-C5-C6-O5
27	d	407	LMG	C14-C15-C16-C17
25	c	516	DGD	C4A-C5A-C6A-C7A
25	d	408	DGD	C4B-C5B-C6B-C7B
25	D	409	DGD	CCB-CDB-CEB-CFB
25	B	620	DGD	C7A-C8A-C9A-CAA
27	a	402	LMG	C32-C33-C34-C35
25	B	625	DGD	C9B-CAB-CBB-CCB
27	a	413	LMG	C34-C35-C36-C37
30	A	413	SQD	C14-C15-C16-C17
22	b	616	CLA	C5-C6-C7-C8
27	A	415	LMG	C18-C19-C20-C21
25	c	515	DGD	C3A-C4A-C5A-C6A
30	a	415	SQD	C14-C15-C16-C17
25	B	620	DGD	C6B-C7B-C8B-C9B
27	a	402	LMG	C30-C31-C32-C33
31	B	628	LMT	O1'-C1-C2-C3
27	d	410	LMG	O6-C5-C6-O5
22	c	512	CLA	O1D-CGD-O2D-CED
24	x	101	BCR	C11-C10-C9-C8
24	j	102	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
25	d	408	DGD	C2E-C1E-O5D-C6D
27	I	101	LMG	C2-C1-O1-C7
25	D	409	DGD	C2E-C1E-O5D-C6D
27	i	101	LMG	C2-C1-O1-C7
24	H	102	BCR	C11-C10-C9-C8
27	B	624	LMG	C4-C5-C6-O5
27	A	415	LMG	C15-C16-C17-C18
25	b	624	DGD	C7A-C8A-C9A-CAA
27	A	410	LMG	C33-C34-C35-C36
25	C	515	DGD	C3A-C4A-C5A-C6A
22	b	608	CLA	O1A-CGA-O2A-C1
22	B	611	CLA	O1D-CGD-O2D-CED
22	c	509	CLA	C4-C3-C5-C6
27	A	410	LMG	C31-C32-C33-C34
30	B	626	SQD	C11-C10-C9-C8
30	b	602	SQD	C9-C10-C11-C12
25	d	408	DGD	C7B-C8B-C9B-CAB
25	D	409	DGD	C7B-C8B-C9B-CAB
27	B	624	LMG	C18-C19-C20-C21
27	a	402	LMG	C18-C19-C20-C21
27	a	413	LMG	C31-C32-C33-C34
27	a	413	LMG	C33-C34-C35-C36
27	D	408	LMG	C14-C15-C16-C17
27	D	408	LMG	C19-C20-C21-C22
22	b	605	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C10-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C10-C8-C9
22	A	403	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C10-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	a	404	CLA	C11-C12-C13-C14
22	C	512	CLA	C14-C13-C15-C16
25	B	620	DGD	C1B-C2B-C3B-C4B
27	d	407	LMG	C19-C20-C21-C22
30	F	102	SQD	C11-C12-C13-C14
27	A	415	LMG	C32-C33-C34-C35
27	I	101	LMG	C16-C17-C18-C19
30	a	415	SQD	C27-C28-C29-C30
27	B	624	LMG	C31-C32-C33-C34
27	i	101	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
27	b	628	LMG	C31-C32-C33-C34
27	D	412	LMG	O6-C5-C6-O5
22	c	520	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2A-CAA-CBA-CGA
27	C	522	LMG	C4-C5-C6-O5
24	B	617	BCR	C7-C8-C9-C34
24	b	621	BCR	C7-C8-C9-C34
25	c	517	DGD	C9B-CAB-CBB-CCB
30	f	103	SQD	C11-C12-C13-C14
25	C	515	DGD	C4A-C5A-C6A-C7A
25	C	515	DGD	C2B-C3B-C4B-C5B
25	C	517	DGD	CBA-CCA-CDA-CEA
25	C	517	DGD	C9B-CAB-CBB-CCB
24	C	521	BCR	C7-C8-C9-C10
30	b	602	SQD	C8-C7-O47-C45
25	a	411	DGD	C5B-C6B-C7B-C8B
27	b	628	LMG	C18-C19-C20-C21
30	A	413	SQD	C27-C28-C29-C30
27	E	101	LMG	C28-C29-C30-C31
27	B	624	LMG	C28-C29-C30-C31
22	b	615	CLA	O1D-CGD-O2D-CED
27	m	101	LMG	C29-C30-C31-C32
25	c	517	DGD	CAB-CBB-CCB-CDB
25	c	515	DGD	C4A-C5A-C6A-C7A
25	c	515	DGD	C2B-C3B-C4B-C5B
25	D	409	DGD	C5A-C6A-C7A-C8A
25	C	517	DGD	CAB-CBB-CCB-CDB
25	b	601	DGD	C4A-C5A-C6A-C7A
25	B	625	DGD	C4A-C5A-C6A-C7A
27	M	101	LMG	O6-C5-C6-O5
27	a	402	LMG	O6-C5-C6-O5
25	D	409	DGD	O6E-C1E-O5D-C6D
27	B	624	LMG	O6-C1-O1-C7
27	b	628	LMG	O6-C1-O1-C7
22	c	503	CLA	C5-C6-C7-C8
25	A	408	DGD	C5B-C6B-C7B-C8B
27	i	101	LMG	C13-C14-C15-C16
27	A	410	LMG	C14-C15-C16-C17
27	I	101	LMG	C13-C14-C15-C16
25	C	516	DGD	C4A-C5A-C6A-C7A
31	B	628	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	c	517	DGD	C1A-C2A-C3A-C4A
25	B	625	DGD	C1A-C2A-C3A-C4A
27	b	628	LMG	C28-C29-C30-C31
22	H	101	CLA	C5-C6-C7-C8
22	C	503	CLA	C5-C6-C7-C8
22	B	604	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	O1A-CGA-O2A-C1
27	d	407	LMG	C32-C33-C34-C35
25	d	408	DGD	C5A-C6A-C7A-C8A
27	a	413	LMG	C14-C15-C16-C17
27	m	101	LMG	C29-C28-O8-C9
30	B	626	SQD	C24-C23-O48-C46
27	i	101	LMG	C29-C28-O8-C9
25	b	624	DGD	O6D-C5D-C6D-O5D
22	C	511	CLA	C3A-C2A-CAA-CBA
22	B	615	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	C	506	CLA	C3A-C2A-CAA-CBA
22	a	405	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	h	101	CLA	C3A-C2A-CAA-CBA
31	B	622	LMT	C1-C2-C3-C4
25	c	517	DGD	CBA-CCA-CDA-CEA
25	b	624	DGD	C5B-C6B-C7B-C8B
31	b	604	LMT	C7-C8-C9-C10
27	c	518	LMG	C12-C13-C14-C15
22	C	511	CLA	O1A-CGA-O2A-C1
27	E	101	LMG	C15-C16-C17-C18
27	A	410	LMG	C30-C31-C32-C33
26	a	412	LHG	C25-C26-C27-C28
27	a	413	LMG	C30-C31-C32-C33
27	D	408	LMG	C32-C33-C34-C35
27	d	407	LMG	C15-C16-C17-C18
27	C	518	LMG	C12-C13-C14-C15
27	a	402	LMG	C15-C16-C17-C18
27	D	408	LMG	C15-C16-C17-C18
25	B	620	DGD	O6D-C5D-C6D-O5D
22	C	509	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C34-C35-C36-C37
25	B	625	DGD	C2B-C3B-C4B-C5B
22	c	512	CLA	C4-C3-C5-C6
22	C	509	CLA	C4-C3-C5-C6
22	C	520	CLA	CBA-CGA-O2A-C1
23	A	406	PL9	C33-C34-C36-C37
23	a	409	PL9	C33-C34-C36-C37
22	C	509	CLA	C2-C3-C5-C6
25	c	516	DGD	CAB-CBB-CCB-CDB
27	e	101	LMG	C15-C16-C17-C18
25	b	624	DGD	C4B-C5B-C6B-C7B
27	M	101	LMG	C29-C30-C31-C32
30	d	402	SQD	C9-C10-C11-C12
30	D	403	SQD	C9-C10-C11-C12
25	B	620	DGD	C5B-C6B-C7B-C8B
31	b	626	LMT	C1-C2-C3-C4
27	A	415	LMG	C31-C32-C33-C34
27	B	624	LMG	C30-C31-C32-C33
27	b	628	LMG	C30-C31-C32-C33
27	b	628	LMG	C36-C37-C38-C39
22	c	520	CLA	O1A-CGA-O2A-C1
25	c	515	DGD	C1A-C2A-C3A-C4A
25	C	515	DGD	C2A-C3A-C4A-C5A
27	c	518	LMG	C34-C35-C36-C37
30	f	103	SQD	O49-C7-O47-C45
26	A	409	LHG	O9-C7-O7-C5
22	C	508	CLA	C2-C1-O2A-CGA
22	c	508	CLA	C2-C1-O2A-CGA
27	A	410	LMG	C15-C16-C17-C18
25	b	601	DGD	C2B-C3B-C4B-C5B
22	H	101	CLA	C13-C15-C16-C17
30	b	602	SQD	C11-C12-C13-C14
26	C	519	LHG	C24-C25-C26-C27
25	B	620	DGD	C4B-C5B-C6B-C7B
31	b	627	LMT	C2B-C1B-O1B-C4'
26	a	412	LHG	C23-C24-C25-C26
25	C	516	DGD	C1A-C2A-C3A-C4A
22	c	506	CLA	CBD-CGD-O2D-CED
24	y	101	BCR	C23-C24-C25-C26
24	y	101	BCR	C23-C24-C25-C30
24	x	101	BCR	C1-C6-C7-C8
24	x	101	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	f	102	BCR	C5-C6-C7-C8
24	D	411	BCR	C5-C6-C7-C8
24	c	514	BCR	C23-C24-C25-C26
24	c	514	BCR	C23-C24-C25-C30
24	j	102	BCR	C5-C6-C7-C8
24	g	101	BCR	C23-C24-C25-C26
24	g	101	BCR	C23-C24-C25-C30
24	c	513	BCR	C1-C6-C7-C8
24	c	513	BCR	C5-C6-C7-C8
24	b	623	BCR	C23-C24-C25-C26
24	B	617	BCR	C23-C24-C25-C30
24	C	513	BCR	C5-C6-C7-C8
24	B	616	BCR	C5-C6-C7-C8
24	H	102	BCR	C1-C6-C7-C8
24	H	102	BCR	C5-C6-C7-C8
24	b	621	BCR	C23-C24-C25-C30
24	J	102	BCR	C5-C6-C7-C8
24	C	514	BCR	C23-C24-C25-C26
24	C	514	BCR	C23-C24-C25-C30
24	b	620	BCR	C5-C6-C7-C8
25	A	408	DGD	C3B-C4B-C5B-C6B
26	c	519	LHG	C24-C25-C26-C27
22	b	607	CLA	C8-C10-C11-C12
22	h	101	CLA	C5-C6-C7-C8
25	c	517	DGD	C2B-C1B-O2G-C2G
30	B	626	SQD	C8-C7-O47-C45
30	F	102	SQD	C10-C11-C12-C13
30	f	103	SQD	C10-C11-C12-C13
27	D	412	LMG	C17-C18-C19-C20
25	C	516	DGD	CAB-CBB-CCB-CDB
22	C	506	CLA	CBD-CGD-O2D-CED
27	e	101	LMG	C28-C29-C30-C31
25	b	601	DGD	C1A-C2A-C3A-C4A
30	A	413	SQD	C7-C8-C9-C10
26	A	409	LHG	C25-C26-C27-C28
23	d	406	PL9	C47-C48-C49-C51
22	C	505	CLA	C10-C11-C12-C13
22	B	603	CLA	C8-C10-C11-C12
27	A	415	LMG	C17-C18-C19-C20
25	D	409	DGD	CAB-CBB-CCB-CDB
27	a	402	LMG	C31-C32-C33-C34
23	j	101	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C4-C3-C5-C6
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	A	404	CLA	C6-C7-C8-C10
22	b	606	CLA	C11-C12-C13-C15
22	c	512	CLA	C2-C3-C5-C6
22	c	512	CLA	C11-C10-C8-C7
22	c	512	CLA	C12-C13-C15-C16
22	c	509	CLA	C2-C3-C5-C6
22	c	509	CLA	C11-C10-C8-C7
32	a	407	PHO	C11-C10-C8-C7
22	C	505	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C12-C13-C15
32	D	402	PHO	C11-C10-C8-C7
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C10-C8-C7
22	C	512	CLA	C2-C3-C5-C6
22	C	512	CLA	C12-C13-C15-C16
22	c	509	CLA	C3-C5-C6-C7
22	c	502	CLA	C3-C5-C6-C7
25	D	409	DGD	C6B-C7B-C8B-C9B
22	C	511	CLA	C13-C15-C16-C17
22	h	101	CLA	C13-C15-C16-C17
22	C	512	CLA	C13-C15-C16-C17
22	b	605	CLA	C16-C17-C18-C20
31	B	623	LMT	C2B-C1B-O1B-C4'
26	a	412	LHG	O9-C7-O7-C5
25	c	516	DGD	C1A-C2A-C3A-C4A
25	C	517	DGD	C1A-C2A-C3A-C4A
22	D	406	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
26	C	519	LHG	C24-C23-O8-C6
22	d	405	CLA	CBA-CGA-O2A-C1
22	b	614	CLA	CBA-CGA-O2A-C1
25	C	515	DGD	C4B-C5B-C6B-C7B
22	c	501	CLA	C2A-CAA-CBA-CGA
22	B	601	CLA	C10-C11-C12-C13
25	d	408	DGD	C2A-C3A-C4A-C5A
25	d	408	DGD	CAB-CBB-CCB-CDB
25	D	409	DGD	C2A-C3A-C4A-C5A
22	C	520	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	c	518	LMG	C36-C37-C38-C39
30	B	626	SQD	C12-C13-C14-C15
22	D	406	CLA	C15-C16-C17-C18
22	c	505	CLA	C10-C11-C12-C13
30	B	626	SQD	C11-C12-C13-C14
25	D	409	DGD	C3A-C4A-C5A-C6A
27	D	408	LMG	C13-C14-C15-C16
22	C	509	CLA	C3-C5-C6-C7
25	c	515	DGD	C2A-C3A-C4A-C5A
31	B	622	LMT	O1'-C1-C2-C3
25	d	408	DGD	C3A-C4A-C5A-C6A
26	a	412	LHG	C30-C31-C32-C33
27	B	624	LMG	C36-C37-C38-C39
27	C	518	LMG	C36-C37-C38-C39
22	b	616	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C19
25	d	408	DGD	O6E-C1E-O5D-C6D
22	b	605	CLA	C10-C11-C12-C13
22	a	408	CLA	C10-C11-C12-C13
27	d	410	LMG	C17-C18-C19-C20
27	b	625	LMG	C13-C14-C15-C16
27	D	412	LMG	C31-C32-C33-C34
27	e	101	LMG	C11-C10-O7-C8
27	E	101	LMG	C11-C10-O7-C8
26	a	412	LHG	C8-C7-O7-C5
25	C	517	DGD	C2B-C1B-O2G-C2G
26	A	409	LHG	C8-C7-O7-C5
27	D	412	LMG	C34-C35-C36-C37
26	A	409	LHG	C30-C31-C32-C33
22	c	511	CLA	C13-C15-C16-C17
23	D	407	PL9	C47-C48-C49-C51
30	b	602	SQD	C12-C13-C14-C15
27	C	522	LMG	C16-C17-C18-C19
27	a	413	LMG	C15-C16-C17-C18
22	a	405	CLA	C3-C5-C6-C7
27	d	410	LMG	C31-C32-C33-C34
27	A	410	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7
30	a	401	SQD	O6-C44-C45-O47
27	I	101	LMG	O1-C7-C8-O7
30	a	415	SQD	O47-C45-C46-O48
30	A	414	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
27	i	101	LMG	O1-C7-C8-O7
30	A	413	SQD	O47-C45-C46-O48
27	m	101	LMG	O6-C5-C6-O5
27	e	101	LMG	O6-C5-C6-O5
27	d	410	LMG	C34-C35-C36-C37
27	B	624	LMG	C17-C18-C19-C20
25	a	411	DGD	C3B-C4B-C5B-C6B
22	c	512	CLA	C13-C15-C16-C17
22	A	405	CLA	C10-C11-C12-C13
23	d	406	PL9	C35-C34-C36-C37
22	C	504	CLA	C2-C3-C5-C6
22	b	605	CLA	C6-C7-C8-C9
22	A	404	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C10-C8-C9
22	d	404	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	A	402	CLA	C11-C12-C13-C14
32	a	407	PHO	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
32	D	402	PHO	C11-C10-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	C	509	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
27	B	624	LMG	C15-C16-C17-C18
22	C	520	CLA	C2A-CAA-CBA-CGA
22	C	501	CLA	C2A-CAA-CBA-CGA
22	C	512	CLA	C2A-CAA-CBA-CGA
25	c	515	DGD	C4B-C5B-C6B-C7B
22	d	405	CLA	C15-C16-C17-C18
25	c	517	DGD	C3B-C4B-C5B-C6B
25	A	408	DGD	C4B-C5B-C6B-C7B
22	B	615	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	D	405	CLA	C1A-C2A-CAA-CBA
22	C	506	CLA	C1A-C2A-CAA-CBA
22	b	619	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
22	B	612	CLA	C16-C17-C18-C20
25	C	517	DGD	C3B-C4B-C5B-C6B
27	a	413	LMG	C4-C5-C6-O5
22	a	408	CLA	C13-C15-C16-C17
25	d	408	DGD	C6B-C7B-C8B-C9B
27	E	101	LMG	O6-C5-C6-O5
22	C	502	CLA	C3-C5-C6-C7
25	A	408	DGD	C1B-C2B-C3B-C4B
25	a	411	DGD	C1B-C2B-C3B-C4B
27	b	625	LMG	C34-C35-C36-C37
27	B	621	LMG	C34-C35-C36-C37
27	c	522	LMG	C16-C17-C18-C19
27	B	621	LMG	C13-C14-C15-C16
27	d	407	LMG	C13-C14-C15-C16
30	a	401	SQD	C10-C11-C12-C13
22	C	504	CLA	CBA-CGA-O2A-C1
27	B	624	LMG	C32-C33-C34-C35
31	b	626	LMT	O1'-C1-C2-C3
27	b	628	LMG	C17-C18-C19-C20
22	b	614	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	C8B-C9B-CAB-CBB
26	c	519	LHG	C25-C26-C27-C28
27	b	628	LMG	C32-C33-C34-C35
30	A	413	SQD	C17-C18-C19-C20
22	C	503	CLA	C8-C10-C11-C12
22	c	502	CLA	C13-C15-C16-C17
22	c	511	CLA	C16-C17-C18-C20
22	B	613	CLA	C16-C17-C18-C20
22	c	509	CLA	O1D-CGD-O2D-CED
22	A	403	CLA	C3-C5-C6-C7
27	m	101	LMG	C7-C8-C9-O8
27	e	101	LMG	C18-C19-C20-C21
27	d	407	LMG	O1-C7-C8-C9
25	c	517	DGD	O1G-C1G-C2G-C3G
27	M	101	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
27	b	625	LMG	C7-C8-C9-O8
25	A	408	DGD	C1G-C2G-C3G-O3G
30	B	626	SQD	C44-C45-C46-O48
30	b	602	SQD	C44-C45-C46-O48
25	d	408	DGD	C8B-C9B-CAB-CBB
27	I	101	LMG	O1-C7-C8-C9
27	I	101	LMG	C18-C19-C20-C21
27	B	624	LMG	O1-C7-C8-C9
27	c	522	LMG	C7-C8-C9-O8
25	C	517	DGD	O1G-C1G-C2G-C3G
30	A	414	SQD	O6-C44-C45-C46
27	C	522	LMG	C7-C8-C9-O8
27	i	101	LMG	O1-C7-C8-C9
27	a	413	LMG	O1-C7-C8-C9
27	b	628	LMG	O1-C7-C8-C9
27	B	621	LMG	C7-C8-C9-O8
27	D	408	LMG	O1-C7-C8-C9
22	c	508	CLA	CBA-CGA-O2A-C1
30	a	415	SQD	C17-C18-C19-C20
27	i	101	LMG	C31-C32-C33-C34
25	a	411	DGD	C4B-C5B-C6B-C7B
27	d	407	LMG	C8-C7-O1-C1
27	A	410	LMG	C8-C7-O1-C1
30	d	402	SQD	C45-C44-O6-C1
30	D	403	SQD	C45-C44-O6-C1
27	D	408	LMG	C8-C7-O1-C1
27	E	101	LMG	C17-C18-C19-C20
27	i	101	LMG	C18-C19-C20-C21
22	A	405	CLA	C5-C6-C7-C8
27	c	522	LMG	C17-C18-C19-C20
27	E	101	LMG	O7-C10-C11-C12
27	d	407	LMG	C28-C29-C30-C31
26	A	409	LHG	C23-C24-C25-C26
25	D	409	DGD	CDB-CEB-CFB-CGB
27	A	415	LMG	C11-C12-C13-C14
25	d	408	DGD	CDB-CEB-CFB-CGB
32	d	401	PHO	CBD-CGD-O2D-CED
31	I	102	LMT	C5'-C4'-O1B-C1B
22	b	607	CLA	C15-C16-C17-C18
22	D	406	CLA	O1A-CGA-O2A-C1
27	A	410	LMG	C11-C10-O7-C8
22	c	503	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	b	621	BCR	C20-C21-C22-C37
22	c	504	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	d	405	CLA	O1A-CGA-O2A-C1
22	c	504	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	C24-C23-O8-C6
26	c	519	LHG	C11-C10-C9-C8
31	i	102	LMT	C5'-C4'-O1B-C1B
30	A	413	SQD	C10-C11-C12-C13
27	E	101	LMG	C7-C8-O7-C10
27	c	518	LMG	C9-C8-O7-C10
25	d	408	DGD	C1G-C2G-O2G-C1B
25	D	409	DGD	C1G-C2G-O2G-C1B
31	B	623	LMT	O5B-C1B-O1B-C4'
22	a	408	CLA	C5-C6-C7-C8
22	b	613	CLA	C2-C1-O2A-CGA
26	C	519	LHG	C11-C10-C9-C8
30	A	414	SQD	C10-C11-C12-C13
27	A	415	LMG	O6-C5-C6-O5
25	D	409	DGD	CBA-CCA-CDA-CEA
27	a	402	LMG	C17-C18-C19-C20
27	A	410	LMG	C4-C5-C6-O5
31	b	627	LMT	O5B-C1B-O1B-C4'
27	B	624	LMG	C2-C1-O1-C7
27	b	628	LMG	C2-C1-O1-C7
24	J	102	BCR	C20-C21-C22-C23
27	A	410	LMG	C8-C9-O8-C28
27	m	101	LMG	O7-C8-C9-O8
25	c	517	DGD	O1G-C1G-C2G-O2G
25	C	515	DGD	O2G-C2G-C3G-O3G
27	a	413	LMG	O1-C7-C8-O7
25	d	408	DGD	CBA-CCA-CDA-CEA
25	c	516	DGD	O6D-C5D-C6D-O5D
25	B	625	DGD	O6D-C5D-C6D-O5D
22	B	603	CLA	C15-C16-C17-C18
22	C	504	CLA	C15-C16-C17-C18
22	c	508	CLA	O1A-CGA-O2A-C1
27	i	101	LMG	C17-C18-C19-C20
23	D	407	PL9	C15-C14-C16-C17
27	C	522	LMG	C34-C35-C36-C37
22	c	510	CLA	C6-C7-C8-C10
22	c	510	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C11-C10-C8-C7
22	d	404	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C7
22	D	405	CLA	C12-C13-C15-C16
22	b	619	CLA	C12-C13-C15-C16
22	b	618	CLA	C11-C10-C8-C7
22	b	618	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	502	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C12-C13-C15
22	c	504	CLA	C2-C3-C5-C6
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C12-C13-C15-C16
22	H	101	CLA	C11-C12-C13-C15
32	a	407	PHO	C12-C13-C15-C16
22	B	607	CLA	C6-C7-C8-C10
22	a	406	CLA	C6-C7-C8-C10
22	B	605	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C10-C8-C7
32	D	402	PHO	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	c	502	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C12-C13-C15
22	C	509	CLA	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	B	610	CLA	C11-C10-C8-C7
22	h	101	CLA	C6-C7-C8-C10
27	b	628	LMG	C15-C16-C17-C18
22	c	510	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C10-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C9
22	D	405	CLA	C14-C13-C15-C16
22	B	608	CLA	C6-C7-C8-C9
22	b	618	CLA	C11-C10-C8-C9
22	b	618	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	502	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C6-C7-C8-C9
22	c	504	CLA	C14-C13-C15-C16
32	a	407	PHO	C14-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C12-C13-C14
32	D	402	PHO	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	C	504	CLA	C6-C7-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C9
22	c	502	CLA	C11-C12-C13-C14
22	c	502	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C9
22	c	505	CLA	C14-C13-C15-C16
25	D	409	DGD	CAA-CBA-CCA-CDA
22	C	508	CLA	CBA-CGA-O2A-C1
22	B	610	CLA	CBA-CGA-O2A-C1
22	B	615	CLA	C15-C16-C17-C18
22	c	501	CLA	C13-C15-C16-C17
25	c	517	DGD	CFA-CGA-CHA-CIA
27	E	101	LMG	C19-C20-C21-C22
22	C	504	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C20
25	D	409	DGD	C1A-C2A-C3A-C4A
25	C	516	DGD	O6D-C5D-C6D-O5D
22	A	405	CLA	C13-C15-C16-C17
22	B	613	CLA	C15-C16-C17-C18
27	a	413	LMG	C11-C10-O7-C8
27	d	410	LMG	C38-C39-C40-C41
27	D	412	LMG	C38-C39-C40-C41
27	a	402	LMG	C11-C12-C13-C14
22	C	510	CLA	CBA-CGA-O2A-C1
27	e	101	LMG	C19-C20-C21-C22
22	b	617	CLA	C5-C6-C7-C8
22	C	502	CLA	C13-C15-C16-C17
27	B	624	LMG	C19-C20-C21-C22
22	C	511	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C19
22	B	609	CLA	C16-C17-C18-C20
22	b	613	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	B	613	CLA	C16-C17-C18-C19
22	B	604	CLA	C5-C6-C7-C8
23	D	407	PL9	C24-C26-C27-C28
27	E	101	LMG	C18-C19-C20-C21
27	C	522	LMG	C17-C18-C19-C20
22	c	504	CLA	C15-C16-C17-C18
27	B	621	LMG	C17-C18-C19-C20
25	b	601	DGD	O6D-C5D-C6D-O5D
23	D	407	PL9	C35-C34-C36-C37
23	A	406	PL9	C35-C34-C36-C37
23	J	101	PL9	C27-C28-C29-C30
27	b	625	LMG	C17-C18-C19-C20
27	b	628	LMG	C19-C20-C21-C22
25	c	516	DGD	C4D-C5D-C6D-O5D
22	b	617	CLA	C16-C17-C18-C20
27	I	101	LMG	C31-C32-C33-C34
22	b	619	CLA	C8-C10-C11-C12
22	b	617	CLA	C15-C16-C17-C18
22	c	510	CLA	CBA-CGA-O2A-C1
22	b	613	CLA	CBA-CGA-O2A-C1
27	D	408	LMG	C28-C29-C30-C31
27	b	628	LMG	C13-C14-C15-C16
22	A	402	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
22	B	604	CLA	C15-C16-C17-C18
25	c	516	DGD	C3A-C4A-C5A-C6A
25	D	409	DGD	C3B-C4B-C5B-C6B
25	C	516	DGD	C4D-C5D-C6D-O5D
25	C	517	DGD	CFA-CGA-CHA-CIA
25	d	408	DGD	CAA-CBA-CCA-CDA
25	B	625	DGD	C5A-C6A-C7A-C8A
22	C	508	CLA	C15-C16-C17-C18
27	m	101	LMG	O1-C7-C8-C9
25	c	516	DGD	C1G-C2G-C3G-O3G
27	A	410	LMG	O1-C7-C8-C9
27	M	101	LMG	O1-C7-C8-C9
30	a	401	SQD	O6-C44-C45-C46
27	c	518	LMG	O1-C7-C8-C9
25	d	408	DGD	C1G-C2G-C3G-O3G
25	D	409	DGD	C1G-C2G-C3G-O3G
25	C	516	DGD	C1G-C2G-C3G-O3G
27	C	518	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	a	411	DGD	C1G-C2G-C3G-O3G
25	B	625	DGD	C1G-C2G-C3G-O3G
30	a	415	SQD	C31-C32-C33-C34
30	A	414	SQD	C9-C10-C11-C12
27	I	101	LMG	O10-C28-O8-C9
27	m	101	LMG	C30-C31-C32-C33
30	a	415	SQD	C10-C11-C12-C13
27	a	413	LMG	O6-C5-C6-O5
23	j	101	PL9	C27-C28-C29-C30
27	D	412	LMG	C19-C20-C21-C22
22	c	511	CLA	C3-C5-C6-C7
27	I	101	LMG	C17-C18-C19-C20
30	A	413	SQD	C31-C32-C33-C34
23	d	406	PL9	C15-C14-C16-C17
27	e	101	LMG	C17-C18-C19-C20
26	C	519	LHG	C25-C26-C27-C28
27	D	408	LMG	C29-C30-C31-C32
22	b	608	CLA	C10-C11-C12-C13
22	B	613	CLA	C5-C6-C7-C8
26	c	519	LHG	O10-C23-O8-C6
22	c	512	CLA	C2A-CAA-CBA-CGA
25	d	408	DGD	C3B-C4B-C5B-C6B
23	d	406	PL9	C27-C28-C29-C30
22	c	504	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C16-C17-C18-C19
22	C	508	CLA	O1A-CGA-O2A-C1
26	C	519	LHG	O10-C23-O8-C6
25	c	516	DGD	C4B-C5B-C6B-C7B
27	c	522	LMG	C34-C35-C36-C37
27	M	101	LMG	O7-C8-C9-O8
30	d	402	SQD	O6-C44-C45-O47
25	c	515	DGD	O2G-C2G-C3G-O3G
27	c	518	LMG	O1-C7-C8-O7
30	b	602	SQD	O47-C45-C46-O48
30	D	403	SQD	O6-C44-C45-O47
27	c	522	LMG	O7-C8-C9-O8
25	C	517	DGD	O1G-C1G-C2G-O2G
27	C	518	LMG	O1-C7-C8-O7
27	C	522	LMG	O7-C8-C9-O8
22	c	506	CLA	O1D-CGD-O2D-CED
30	f	103	SQD	C29-C30-C31-C32
22	B	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	d	410	LMG	C19-C20-C21-C22
30	b	602	SQD	O49-C7-O47-C45
22	a	405	CLA	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
32	D	401	PHO	C2-C1-O2A-CGA
22	B	609	CLA	C2-C1-O2A-CGA
31	B	628	LMT	C2-C3-C4-C5
22	b	608	CLA	C15-C16-C17-C18
22	D	405	CLA	C6-C7-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	B	605	CLA	C14-C13-C15-C16
22	c	511	CLA	C11-C12-C13-C14
22	C	504	CLA	C11-C10-C8-C9
32	d	401	PHO	C6-C7-C8-C9
25	D	409	DGD	C2B-C3B-C4B-C5B
25	C	517	DGD	CDB-CEB-CFB-CGB
25	b	601	DGD	C5A-C6A-C7A-C8A
27	A	410	LMG	O6-C5-C6-O5
22	b	619	CLA	C15-C16-C17-C18
22	a	405	CLA	C5-C6-C7-C8
22	b	608	CLA	C5-C6-C7-C8
22	b	613	CLA	C5-C6-C7-C8
26	A	409	LHG	C2-C3-O3-P
22	B	610	CLA	O1A-CGA-O2A-C1
27	c	518	LMG	C13-C14-C15-C16
25	C	516	DGD	C3A-C4A-C5A-C6A
22	B	609	CLA	C16-C17-C18-C19
22	b	613	CLA	C16-C17-C18-C19
22	C	511	CLA	C3-C5-C6-C7
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	A	407	BCR	C23-C24-C25-C30
24	a	410	BCR	C1-C6-C7-C8
24	a	410	BCR	C5-C6-C7-C8
24	a	410	BCR	C23-C24-C25-C26
24	a	410	BCR	C23-C24-C25-C30
24	c	513	BCR	C23-C24-C25-C26
24	c	513	BCR	C23-C24-C25-C30
24	b	623	BCR	C1-C6-C7-C8
24	b	623	BCR	C5-C6-C7-C8
24	C	513	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	C	513	BCR	C23-C24-C25-C30
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	C	521	BCR	C23-C24-C25-C26
24	C	521	BCR	C23-C24-C25-C30
25	d	408	DGD	C4E-C5E-C6E-O5E
22	C	506	CLA	O1D-CGD-O2D-CED
24	c	514	BCR	C7-C8-C9-C10
24	J	102	BCR	C7-C8-C9-C10
22	c	511	CLA	C5-C6-C7-C8
22	B	609	CLA	C10-C11-C12-C13
25	d	408	DGD	C1A-C2A-C3A-C4A
27	b	625	LMG	C28-C29-C30-C31
32	D	402	PHO	C10-C11-C12-C13
27	B	624	LMG	C20-C21-C22-C23
25	b	624	DGD	C5A-C6A-C7A-C8A
22	C	511	CLA	C5-C6-C7-C8
27	d	407	LMG	C29-C30-C31-C32
22	C	511	CLA	C11-C12-C13-C15
22	C	511	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	B	614	CLA	C12-C13-C15-C16
22	b	606	CLA	C6-C7-C8-C10
22	B	608	CLA	C12-C13-C15-C16
22	b	619	CLA	C11-C10-C8-C7
22	a	405	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
22	C	508	CLA	C6-C7-C8-C10
22	C	502	CLA	C12-C13-C15-C16
22	b	611	CLA	C6-C7-C8-C10
22	A	403	CLA	C12-C13-C15-C16
22	b	609	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	H	101	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	b	616	CLA	C11-C12-C13-C15
22	c	511	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
22	C	501	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C11-C12-C13-C15
22	C	504	CLA	C6-C7-C8-C10
22	C	504	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C10
22	B	609	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C10-C8-C7
22	c	505	CLA	C12-C13-C15-C16
31	B	627	LMT	C5'-C4'-O1B-C1B
22	C	511	CLA	C16-C17-C18-C19
30	b	602	SQD	C10-C11-C12-C13
27	d	407	LMG	C36-C37-C38-C39
22	b	615	CLA	C10-C11-C12-C13
22	C	510	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C2A-CAA-CBA-CGA
31	b	603	LMT	C4'-C5'-C6'-O6'
31	b	603	LMT	C5'-C4'-O1B-C1B
30	B	626	SQD	C10-C11-C12-C13
24	B	617	BCR	C20-C21-C22-C37
30	B	626	SQD	C17-C18-C19-C20
25	C	516	DGD	C4B-C5B-C6B-C7B
22	B	611	CLA	C10-C11-C12-C13
27	A	410	LMG	C20-C21-C22-C23
30	a	415	SQD	C15-C16-C17-C18
30	A	413	SQD	C15-C16-C17-C18
22	A	404	CLA	C5-C6-C7-C8
22	c	506	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CAD-CBD-CGD-O2D
32	D	401	PHO	CAD-CBD-CGD-O2D
32	d	401	PHO	C2B-C3B-CAB-CBB
32	d	401	PHO	CAD-CBD-CGD-O2D
22	b	617	CLA	C16-C17-C18-C19
27	C	518	LMG	C13-C14-C15-C16
27	A	410	LMG	O6-C1-O1-C7
30	a	415	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
26	a	412	LHG	C2-C3-O3-P
25	b	601	DGD	C1G-C2G-C3G-O3G
30	A	413	SQD	C44-C45-C46-O48
32	D	401	PHO	CBD-CGD-O2D-CED
27	b	628	LMG	C20-C21-C22-C23
22	C	507	CLA	C5-C6-C7-C8
32	D	401	PHO	C5-C6-C7-C8
22	b	613	CLA	C10-C11-C12-C13
25	c	517	DGD	CDB-CEB-CFB-CGB
30	B	626	SQD	O49-C7-O47-C45
22	A	404	CLA	CHA-CBD-CGD-O2D
22	B	611	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	b	612	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	503	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	c	505	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O2D
27	e	101	LMG	O7-C10-C11-C12
22	c	510	CLA	O1A-CGA-O2A-C1
27	i	101	LMG	O10-C28-O8-C9
25	d	408	DGD	C2B-C3B-C4B-C5B
30	F	102	SQD	C29-C30-C31-C32
30	A	414	SQD	C32-C33-C34-C35
27	b	625	LMG	O7-C8-C9-O8
30	B	626	SQD	O47-C45-C46-O48
25	a	411	DGD	O2G-C2G-C3G-O3G
27	B	621	LMG	O7-C8-C9-O8
22	B	603	CLA	CBA-CGA-O2A-C1
27	c	522	LMG	C35-C36-C37-C38
22	b	613	CLA	O1A-CGA-O2A-C1
27	B	621	LMG	C28-C29-C30-C31
23	A	406	PL9	C4-C3-C7-C8
23	a	409	PL9	C4-C3-C7-C8
27	A	410	LMG	C29-C30-C31-C32
22	c	508	CLA	C15-C16-C17-C18
22	B	608	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	b	618	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	C	501	CLA	C11-C12-C13-C14
25	d	408	DGD	C4A-C5A-C6A-C7A
30	d	402	SQD	C5-C6-S-O8
30	D	403	SQD	C5-C6-S-O8
32	d	401	PHO	O1D-CGD-O2D-CED
25	D	409	DGD	C4A-C5A-C6A-C7A
22	B	605	CLA	CBA-CGA-O2A-C1
24	f	102	BCR	C7-C8-C9-C34
24	j	102	BCR	C7-C8-C9-C10
24	H	102	BCR	C7-C8-C9-C10
24	C	514	BCR	C7-C8-C9-C10
22	A	402	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
32	d	401	PHO	C5-C6-C7-C8
22	b	607	CLA	CBA-CGA-O2A-C1
26	c	519	LHG	O2-C2-C3-O3
30	D	403	SQD	C10-C11-C12-C13
27	C	522	LMG	C35-C36-C37-C38
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	403	CLA	C5-C6-C7-C8
22	B	604	CLA	C10-C11-C12-C13
27	B	624	LMG	C16-C17-C18-C19
25	D	409	DGD	C4E-C5E-C6E-O5E
22	c	506	CLA	C3-C5-C6-C7
27	c	518	LMG	C32-C33-C34-C35
27	D	408	LMG	C31-C32-C33-C34
27	a	413	LMG	C20-C21-C22-C23
30	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
22	c	505	CLA	CAD-CBD-CGD-O1D
27	a	413	LMG	C10-C11-C12-C13
32	a	407	PHO	C10-C11-C12-C13
25	c	515	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
27	d	407	LMG	C31-C32-C33-C34
26	c	519	LHG	C7-C8-C9-C10
22	B	614	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	C8-C10-C11-C12
23	a	409	PL9	C35-C34-C36-C37
23	D	407	PL9	C32-C33-C34-C36
22	D	406	CLA	C11-C10-C8-C7
22	c	520	CLA	C6-C7-C8-C10
22	b	612	CLA	C12-C13-C15-C16
22	c	509	CLA	C6-C7-C8-C10
22	b	611	CLA	C11-C12-C13-C15
22	H	101	CLA	C11-C10-C8-C7
26	C	519	LHG	O6-C4-C5-O7
32	a	407	PHO	C6-C7-C8-C10
22	B	607	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C12-C13-C15
22	d	405	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
22	A	405	CLA	C11-C10-C8-C7
22	B	609	CLA	C12-C13-C15-C16
26	c	519	LHG	O6-C4-C5-O7
22	b	613	CLA	C11-C12-C13-C15
22	b	613	CLA	C12-C13-C15-C16
22	c	505	CLA	C11-C12-C13-C15
22	h	101	CLA	C11-C10-C8-C7
22	C	512	CLA	C3A-C2A-CAA-CBA
27	a	413	LMG	C16-C17-C18-C19
31	b	604	LMT	C2-C3-C4-C5
22	A	405	CLA	C16-C17-C18-C19
27	e	101	LMG	O1-C7-C8-C9
30	d	402	SQD	O6-C44-C45-C46
30	D	403	SQD	O6-C44-C45-C46
25	A	408	DGD	O2G-C2G-C3G-O3G
25	d	408	DGD	O2G-C2G-C3G-O3G
25	D	409	DGD	O2G-C2G-C3G-O3G
25	B	620	DGD	CAB-CBB-CCB-CDB
22	B	605	CLA	O1A-CGA-O2A-C1
22	B	603	CLA	O1A-CGA-O2A-C1
25	b	624	DGD	CCA-CDA-CEA-CFA
27	a	413	LMG	C8-C7-O1-C1
22	a	408	CLA	C16-C17-C18-C19
22	C	506	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
30	a	401	SQD	C9-C10-C11-C12
27	b	625	LMG	C12-C13-C14-C15
27	m	101	LMG	O10-C28-O8-C9
22	b	607	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
22	b	615	CLA	C4-C3-C5-C6
32	a	407	PHO	C13-C15-C16-C17
32	D	402	PHO	C13-C15-C16-C17
22	B	609	CLA	C5-C6-C7-C8
22	C	511	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C10-C8-C9
22	d	404	CLA	C6-C7-C8-C9
22	b	619	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C12-C13-C14
22	a	405	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
22	A	403	CLA	C14-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C14
22	c	507	CLA	C14-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
32	D	401	PHO	C6-C7-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	B	609	CLA	C11-C12-C13-C14
22	b	614	CLA	C11-C10-C8-C9
23	d	406	PL9	C24-C26-C27-C28
27	B	624	LMG	C10-C11-C12-C13
22	C	508	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
27	B	621	LMG	C12-C13-C14-C15
24	c	513	BCR	C11-C12-C13-C35
22	b	609	CLA	C13-C15-C16-C17
22	h	101	CLA	CBA-CGA-O2A-C1
30	d	402	SQD	C10-C11-C12-C13
27	b	628	LMG	C16-C17-C18-C19
22	B	611	CLA	C4-C3-C5-C6
22	C	511	CLA	CAA-CBA-CGA-O2A
30	f	103	SQD	C24-C25-C26-C27
30	a	401	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C32-C33-C34-C35
27	a	402	LMG	C16-C17-C18-C19
23	d	406	PL9	C13-C14-C16-C17
25	c	517	DGD	C8B-C9B-CAB-CBB
25	c	516	DGD	C6A-C7A-C8A-C9A
27	E	101	LMG	C31-C32-C33-C34
32	D	401	PHO	O1D-CGD-O2D-CED
30	a	415	SQD	C11-C10-C9-C8
22	c	510	CLA	C3-C5-C6-C7
22	c	511	CLA	CAA-CBA-CGA-O2A
25	b	624	DGD	CAB-CBB-CCB-CDB
27	a	413	LMG	C29-C30-C31-C32
27	m	101	LMG	C9-C8-O7-C10
25	c	517	DGD	C3G-C2G-O2G-C1B
26	a	412	LHG	C6-C5-O7-C7
25	C	517	DGD	C3G-C2G-O2G-C1B
26	A	409	LHG	C6-C5-O7-C7
26	C	519	LHG	O6-C4-C5-C6
26	c	519	LHG	O6-C4-C5-C6
22	b	617	CLA	C2A-CAA-CBA-CGA
22	B	614	CLA	O1A-CGA-O2A-C1
22	A	403	CLA	C2-C1-O2A-CGA
22	b	616	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
32	d	401	PHO	C2-C1-O2A-CGA
27	A	410	LMG	C10-C11-C12-C13
30	b	602	SQD	C17-C18-C19-C20
27	M	101	LMG	O10-C28-O8-C9
22	a	406	CLA	C5-C6-C7-C8
27	A	410	LMG	C38-C39-C40-C41
25	C	515	DGD	C5A-C6A-C7A-C8A
22	h	101	CLA	O1A-CGA-O2A-C1
23	D	407	PL9	C20-C19-C21-C22
23	d	406	PL9	C20-C19-C21-C22
27	B	624	LMG	C13-C14-C15-C16
24	A	407	BCR	C5-C6-C7-C8
24	c	514	BCR	C1-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	g	101	BCR	C5-C6-C7-C8
24	c	521	BCR	C1-C6-C7-C8
24	c	521	BCR	C23-C24-C25-C26
24	c	521	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	B	617	BCR	C1-C6-C7-C8
24	C	514	BCR	C1-C6-C7-C8
24	C	514	BCR	C5-C6-C7-C8
24	C	521	BCR	C1-C6-C7-C8
24	C	521	BCR	C5-C6-C7-C8
22	b	616	CLA	C10-C11-C12-C13
27	D	412	LMG	C16-C17-C18-C19
30	A	413	SQD	C11-C10-C9-C8
25	c	515	DGD	O6D-C1D-O3G-C3G
22	d	405	CLA	C2A-CAA-CBA-CGA
27	d	407	LMG	O1-C7-C8-O7
27	D	408	LMG	O1-C7-C8-O7
26	a	412	LHG	C3-O3-P-O6
26	A	409	LHG	C3-O3-P-O6
22	b	606	CLA	C16-C17-C18-C19
27	m	101	LMG	C31-C32-C33-C34
27	M	101	LMG	C31-C32-C33-C34
25	C	517	DGD	C8B-C9B-CAB-CBB
22	B	612	CLA	C10-C11-C12-C13
22	c	504	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	c	508	CLA	C6-C7-C8-C10
22	B	615	CLA	C14-C13-C15-C16
22	b	619	CLA	C14-C13-C15-C16
22	c	509	CLA	C6-C7-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	b	611	CLA	C11-C12-C13-C14
32	a	407	PHO	C6-C7-C8-C9
22	B	607	CLA	C11-C12-C13-C14
22	C	505	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C12-C13-C14
22	B	610	CLA	C11-C10-C8-C9
22	c	505	CLA	C11-C12-C13-C14
30	a	401	SQD	C12-C13-C14-C15
25	c	515	DGD	C5B-C6B-C7B-C8B
27	c	522	LMG	C32-C33-C34-C35
25	B	620	DGD	C5A-C6A-C7A-C8A
27	A	415	LMG	C12-C13-C14-C15
27	A	415	LMG	C16-C17-C18-C19
27	C	522	LMG	C32-C33-C34-C35
22	c	504	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C16-C17-C18-C20
22	B	609	CLA	CBA-CGA-O2A-C1
22	b	617	CLA	C2C-C3C-CAC-CBC
22	b	608	CLA	C8-C10-C11-C12
27	b	625	LMG	C15-C16-C17-C18
26	c	519	LHG	C1-C2-C3-O3
23	d	406	PL9	C32-C33-C34-C36
27	d	410	LMG	C16-C17-C18-C19
27	c	522	LMG	C30-C31-C32-C33
27	a	413	LMG	C35-C36-C37-C38
27	A	410	LMG	C16-C17-C18-C19
25	C	515	DGD	C5B-C6B-C7B-C8B
27	a	413	LMG	C11-C12-C13-C14
22	b	616	CLA	C8-C10-C11-C12
25	A	408	DGD	O6E-C1E-O5D-C6D
25	b	601	DGD	O6D-C1D-O3G-C3G
25	C	516	DGD	O6E-C1E-O5D-C6D
25	b	624	DGD	O1A-C1A-O1G-C1G
22	b	616	CLA	C13-C15-C16-C17
25	C	516	DGD	C7B-C8B-C9B-CAB
22	b	609	CLA	C16-C17-C18-C20
22	a	408	CLA	C16-C17-C18-C20
23	D	407	PL9	C40-C39-C41-C42
22	A	403	CLA	C4-C3-C5-C6
23	J	101	PL9	C15-C14-C16-C17
27	M	101	LMG	C30-C31-C32-C33
23	D	407	PL9	C13-C14-C16-C17
26	C	519	LHG	O2-C2-C3-O3
27	M	101	LMG	C16-C17-C18-C19
22	A	402	CLA	C2-C1-O2A-CGA
27	B	624	LMG	C29-C30-C31-C32
27	B	621	LMG	C15-C16-C17-C18
22	c	512	CLA	C3A-C2A-CAA-CBA
22	b	606	CLA	C15-C16-C17-C18
22	B	602	CLA	C16-C17-C18-C19
27	e	101	LMG	C31-C32-C33-C34
22	B	610	CLA	C4-C3-C5-C6
27	D	408	LMG	C18-C19-C20-C21
22	D	406	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	B	614	CLA	C6-C7-C8-C9
22	c	520	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C11-C12-C13-C14
22	d	405	CLA	C11-C10-C8-C9
22	h	101	CLA	C11-C12-C13-C14
22	B	605	CLA	C13-C15-C16-C17
25	c	516	DGD	C7B-C8B-C9B-CAB
30	A	414	SQD	C12-C13-C14-C15
27	D	408	LMG	C36-C37-C38-C39
22	B	602	CLA	C15-C16-C17-C18
27	d	410	LMG	O1-C7-C8-C9
25	d	408	DGD	CBB-CCB-CDB-CEB
27	m	101	LMG	O6-C1-O1-C7
25	c	516	DGD	O6E-C1E-O5D-C6D
27	M	101	LMG	O6-C1-O1-C7
25	C	515	DGD	O6D-C1D-O3G-C3G
25	a	411	DGD	O6E-C1E-O5D-C6D
25	B	625	DGD	O6D-C1D-O3G-C3G
30	F	102	SQD	C9-C10-C11-C12
30	a	415	SQD	C12-C13-C14-C15
27	A	410	LMG	C35-C36-C37-C38
27	C	522	LMG	C30-C31-C32-C33
27	M	101	LMG	C9-C8-O7-C10
22	a	405	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	d	404	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	b	605	CLA	C12-C13-C15-C16
22	D	405	CLA	C11-C10-C8-C7
22	B	608	CLA	C11-C12-C13-C15
22	C	520	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C12-C13-C15
22	b	609	CLA	C6-C7-C8-C10
22	H	101	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10
27	a	413	LMG	C38-C39-C40-C41
22	B	609	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	CBB-CCB-CDB-CEB
22	B	604	CLA	C8-C10-C11-C12
22	B	612	CLA	C13-C15-C16-C17
30	F	102	SQD	C24-C25-C26-C27
25	b	601	DGD	C2A-C3A-C4A-C5A
27	A	410	LMG	C17-C18-C19-C20
27	b	625	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	b	624	DGD	C4A-C5A-C6A-C7A
22	c	509	CLA	C16-C17-C18-C19
22	B	612	CLA	C8-C10-C11-C12
30	a	401	SQD	C26-C27-C28-C29
27	a	413	LMG	C8-C9-O8-C28
30	f	103	SQD	C9-C10-C11-C12
27	b	628	LMG	C29-C30-C31-C32
31	B	623	LMT	C6-C7-C8-C9
30	A	413	SQD	C12-C13-C14-C15
27	e	101	LMG	C30-C31-C32-C33
27	a	402	LMG	C12-C13-C14-C15
27	e	101	LMG	C14-C15-C16-C17
22	b	609	CLA	C15-C16-C17-C18
22	C	503	CLA	C15-C16-C17-C18
22	C	501	CLA	C13-C15-C16-C17
25	B	620	DGD	CCA-CDA-CEA-CFA
22	b	617	CLA	C4C-C3C-CAC-CBC
22	B	612	CLA	C2-C1-O2A-CGA
22	B	611	CLA	C2-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
25	B	620	DGD	C7B-C8B-C9B-CAB
22	c	503	CLA	C6-C7-C8-C9
22	A	403	CLA	C11-C10-C8-C9
22	C	503	CLA	C6-C7-C8-C9
25	d	408	DGD	O6E-C5E-C6E-O5E
27	A	410	LMG	C11-C12-C13-C14
25	c	517	DGD	CBB-CCB-CDB-CEB
26	A	409	LHG	C27-C28-C29-C30
22	c	510	CLA	C2A-CAA-CBA-CGA
22	D	406	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C16-C17-C18-C20
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C30
24	f	102	BCR	C23-C24-C25-C30
24	b	622	BCR	C1-C6-C7-C8
24	b	622	BCR	C23-C24-C25-C30
24	D	411	BCR	C23-C24-C25-C30
24	g	101	BCR	C1-C6-C7-C8
24	c	521	BCR	C5-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
24	b	621	BCR	C1-C6-C7-C8
25	a	411	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
30	f	103	SQD	C14-C15-C16-C17
24	x	101	BCR	C7-C8-C9-C10
24	f	102	BCR	C21-C22-C23-C24
22	B	607	CLA	C13-C15-C16-C17
22	b	615	CLA	C2-C3-C5-C6
27	d	410	LMG	C8-C7-O1-C1
25	b	601	DGD	C2G-C3G-O3G-C1D
25	B	625	DGD	C2G-C3G-O3G-C1D
27	m	101	LMG	C17-C18-C19-C20
25	A	408	DGD	C2A-C3A-C4A-C5A
22	b	609	CLA	C16-C17-C18-C19
22	c	509	CLA	C13-C15-C16-C17
22	b	618	CLA	CBA-CGA-O2A-C1
22	b	609	CLA	CBA-CGA-O2A-C1
27	D	408	LMG	C34-C35-C36-C37
22	C	510	CLA	C4-C3-C5-C6
31	B	622	LMT	C4-C5-C6-C7
22	b	612	CLA	C11-C12-C13-C15
22	b	615	CLA	C6-C7-C8-C10
22	C	503	CLA	C6-C7-C8-C10
32	D	402	PHO	C6-C7-C8-C10
22	b	614	CLA	C2-C3-C5-C6
22	h	101	CLA	C11-C12-C13-C15
25	c	516	DGD	C2E-C1E-O5D-C6D
25	C	516	DGD	C2E-C1E-O5D-C6D
22	C	509	CLA	C16-C17-C18-C19
27	e	101	LMG	O1-C7-C8-O7
27	b	625	LMG	O1-C7-C8-O7
22	c	507	CLA	C5-C6-C7-C8
26	C	519	LHG	O7-C7-C8-C9
22	b	616	CLA	CAA-CBA-CGA-O2A
27	a	413	LMG	O7-C10-C11-C12
22	b	618	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C2C-C3C-CAC-CBC
22	b	606	CLA	C16-C17-C18-C20
27	B	621	LMG	C29-C28-O8-C9
22	B	612	CLA	CAA-CBA-CGA-O2A
26	c	519	LHG	O7-C7-C8-C9
22	c	510	CLA	C4-C3-C5-C6
25	D	409	DGD	C8A-C9A-CAA-CBA
30	a	415	SQD	C16-C17-C18-C19
25	B	625	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
22	b	609	CLA	O1A-CGA-O2A-C1
22	c	502	CLA	C16-C17-C18-C20
25	b	601	DGD	C4E-C5E-C6E-O5E
22	b	605	CLA	C14-C13-C15-C16
22	a	405	CLA	C11-C10-C8-C9
22	C	507	CLA	C11-C12-C13-C14
22	b	609	CLA	C6-C7-C8-C9
22	H	101	CLA	C11-C10-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	c	508	CLA	C11-C10-C8-C9
22	A	405	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	h	101	CLA	C11-C10-C8-C9
22	D	405	CLA	C3A-C2A-CAA-CBA
22	C	520	CLA	C3A-C2A-CAA-CBA
22	d	404	CLA	CAA-CBA-CGA-O2A
22	B	611	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
26	a	412	LHG	C4-C5-O7-C7
22	b	615	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	CAD-CBD-CGD-O2D
22	c	501	CLA	CAD-CBD-CGD-O2D
22	B	601	CLA	CAD-CBD-CGD-O2D
26	A	409	LHG	C4-C5-O7-C7
22	b	608	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	C16-C17-C18-C20
27	A	410	LMG	O7-C10-C11-C12
22	B	611	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	O1G-C1A-C2A-C3A
27	C	522	LMG	O8-C28-C29-C30
27	a	402	LMG	O7-C10-C11-C12
27	E	101	LMG	C33-C34-C35-C36
30	A	413	SQD	C16-C17-C18-C19
22	c	510	CLA	C2-C3-C5-C6
25	c	517	DGD	O1G-C1A-C2A-C3A
24	D	411	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C16-C17-C18-C19
27	E	101	LMG	O1-C7-C8-C9
25	c	515	DGD	C1G-C2G-C3G-O3G
25	C	515	DGD	C1G-C2G-C3G-O3G
27	c	518	LMG	C7-C8-C9-O8
27	A	415	LMG	O7-C10-C11-C12
27	d	410	LMG	C11-C12-C13-C14
27	D	412	LMG	C36-C37-C38-C39
27	E	101	LMG	C30-C31-C32-C33
22	C	511	CLA	O2A-C1-C2-C3
22	B	615	CLA	O2A-C1-C2-C3
22	b	619	CLA	O2A-C1-C2-C3
32	a	407	PHO	O2A-C1-C2-C3
22	c	511	CLA	O2A-C1-C2-C3
32	D	402	PHO	O2A-C1-C2-C3
27	B	621	LMG	C35-C36-C37-C38
32	D	401	PHO	C4B-C3B-CAB-CBB
32	d	401	PHO	C4B-C3B-CAB-CBB
25	B	625	DGD	CAB-CBB-CCB-CDB
27	c	522	LMG	O8-C28-C29-C30
22	c	512	CLA	C16-C17-C18-C20
22	b	610	CLA	CHA-CBD-CGD-O1D
22	b	610	CLA	CHA-CBD-CGD-O2D
22	c	512	CLA	CHA-CBD-CGD-O1D
22	c	512	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O2D
22	C	507	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	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
32	d	401	PHO	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
22	C	512	CLA	CHA-CBD-CGD-O2D
25	C	517	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C13-C15-C16-C17
27	M	101	LMG	C17-C18-C19-C20
22	B	613	CLA	C4C-C3C-CAC-CBC
25	A	408	DGD	C2E-C1E-O5D-C6D
25	a	411	DGD	C2E-C1E-O5D-C6D
26	C	519	LHG	C11-C12-C13-C14
22	C	501	CLA	C16-C17-C18-C20
30	a	401	SQD	O47-C7-C8-C9
30	A	414	SQD	O47-C7-C8-C9
27	d	410	LMG	O1-C7-C8-O7
27	B	621	LMG	O1-C7-C8-O7
26	C	519	LHG	C7-C8-C9-C10
25	C	517	DGD	CBB-CCB-CDB-CEB
22	c	501	CLA	CAA-CBA-CGA-O2A
26	c	519	LHG	C11-C12-C13-C14
32	D	401	PHO	C13-C15-C16-C17
22	H	101	CLA	CBA-CGA-O2A-C1
27	b	628	LMG	C10-C11-C12-C13
30	A	413	SQD	C8-C7-O47-C45
22	D	405	CLA	CAA-CBA-CGA-O2A
22	C	501	CLA	CAA-CBA-CGA-O2A
30	f	103	SQD	C15-C16-C17-C18
25	c	517	DGD	C4A-C5A-C6A-C7A
22	c	512	CLA	C11-C12-C13-C15
22	B	611	CLA	C6-C7-C8-C10
22	C	506	CLA	C11-C12-C13-C15
22	c	503	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C12-C13-C15
22	a	408	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C12-C13-C15
22	B	601	CLA	C12-C13-C15-C16
22	b	608	CLA	C11-C12-C13-C15
22	b	611	CLA	C13-C15-C16-C17
30	d	402	SQD	O47-C7-C8-C9
22	c	509	CLA	CAA-CBA-CGA-O2A
22	B	614	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C12-C13-C14
22	B	611	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	C	520	CLA	C6-C7-C8-C9
22	b	618	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C12-C13-C14
22	B	601	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C10-C8-C9
30	D	403	SQD	O49-C7-C8-C9
25	C	517	DGD	C4B-C5B-C6B-C7B
22	C	502	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	CAA-CBA-CGA-O2A
22	B	605	CLA	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C20
22	H	101	CLA	O1A-CGA-O2A-C1
22	b	606	CLA	C2A-CAA-CBA-CGA
22	H	101	CLA	C2A-CAA-CBA-CGA
22	C	510	CLA	C2A-CAA-CBA-CGA
22	C	506	CLA	CAA-CBA-CGA-O2A
22	C	509	CLA	CAA-CBA-CGA-O2A
25	c	517	DGD	C4B-C5B-C6B-C7B
22	c	502	CLA	CBA-CGA-O2A-C1
22	C	501	CLA	C16-C17-C18-C19
22	C	509	CLA	CAA-CBA-CGA-O1A
22	A	404	CLA	CBA-CGA-O2A-C1
25	B	620	DGD	C4A-C5A-C6A-C7A
22	c	512	CLA	C1A-C2A-CAA-CBA
22	C	520	CLA	C1A-C2A-CAA-CBA
22	B	601	CLA	C1A-C2A-CAA-CBA
25	a	411	DGD	C4A-C5A-C6A-C7A
22	c	509	CLA	CAA-CBA-CGA-O1A
22	b	616	CLA	CAA-CBA-CGA-O1A
30	A	414	SQD	O49-C7-C8-C9
25	C	517	DGD	O2G-C1B-C2B-C3B
22	C	511	CLA	C2-C1-O2A-CGA
22	c	511	CLA	C2-C1-O2A-CGA
31	B	623	LMT	O5'-C5'-C6'-O6'
30	d	402	SQD	O49-C7-C8-C9
27	c	522	LMG	O10-C28-C29-C30
25	d	408	DGD	C8A-C9A-CAA-CBA
27	a	413	LMG	C17-C18-C19-C20
27	C	518	LMG	C7-C8-C9-O8
27	i	101	LMG	C7-C8-C9-O8
22	B	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	d	410	LMG	O9-C10-C11-C12
22	B	611	CLA	CAA-CBA-CGA-O1A
22	b	615	CLA	CAA-CBA-CGA-O1A
22	d	404	CLA	CAA-CBA-CGA-O1A
22	c	501	CLA	CAA-CBA-CGA-O1A
25	A	408	DGD	O6D-C5D-C6D-O5D
22	A	404	CLA	O1A-CGA-O2A-C1
22	C	502	CLA	O1A-CGA-O2A-C1
25	c	515	DGD	C2D-C1D-O3G-C3G
22	B	602	CLA	C8-C10-C11-C12
26	a	412	LHG	C3-O3-P-O5
26	A	409	LHG	C3-O3-P-O5
25	d	408	DGD	C9B-CAB-CBB-CCB
22	c	506	CLA	CAA-CBA-CGA-O1A
22	D	405	CLA	CAA-CBA-CGA-O1A
27	D	412	LMG	O9-C10-C11-C12
22	C	501	CLA	CAA-CBA-CGA-O1A
22	B	612	CLA	CAA-CBA-CGA-O1A
27	D	408	LMG	O7-C10-C11-C12
22	h	101	CLA	CAA-CBA-CGA-O2A
24	B	618	BCR	C23-C24-C25-C26
24	b	622	BCR	C23-C24-C25-C26
24	b	621	BCR	C5-C6-C7-C8
27	d	407	LMG	C34-C35-C36-C37
27	D	412	LMG	C32-C33-C34-C35
22	c	508	CLA	C8-C10-C11-C12
22	C	506	CLA	CAA-CBA-CGA-O1A
22	c	502	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	C16-C17-C18-C19
25	D	409	DGD	O6E-C5E-C6E-O5E
30	a	401	SQD	O49-C7-C8-C9
22	a	408	CLA	C4-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
22	B	610	CLA	C16-C17-C18-C19
27	M	101	LMG	C7-C8-O7-C10
30	d	402	SQD	O5-C5-C6-S
22	B	608	CLA	CAD-CBD-CGD-O1D
22	b	612	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
30	D	403	SQD	O5-C5-C6-S
22	a	406	CLA	CAD-CBD-CGD-O1D
30	A	414	SQD	C5-C6-S-O9

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	CAD-CBD-CGD-O1D
25	A	408	DGD	C4D-C5D-C6D-O5D
22	d	404	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	a	408	CLA	C11-C10-C8-C9
32	D	402	PHO	C6-C7-C8-C9
25	C	517	DGD	CEA-CFA-CGA-CHA
25	C	516	DGD	C6A-C7A-C8A-C9A
26	A	409	LHG	C24-C25-C26-C27
22	D	405	CLA	C3-C5-C6-C7
22	b	615	CLA	C3-C5-C6-C7
27	m	101	LMG	O8-C28-C29-C30
25	c	517	DGD	O2G-C1B-C2B-C3B
22	b	605	CLA	CAA-CBA-CGA-O2A
30	D	403	SQD	O47-C7-C8-C9
30	A	413	SQD	C9-C10-C11-C12
22	b	617	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	CAA-CBA-CGA-O2A
22	B	613	CLA	CAA-CBA-CGA-O2A
30	b	602	SQD	C15-C16-C17-C18
27	a	413	LMG	O9-C10-C11-C12
22	C	508	CLA	C8-C10-C11-C12
22	d	404	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	b	619	CLA	C11-C12-C13-C15
22	a	405	CLA	C2-C3-C5-C6
22	A	403	CLA	C2-C3-C5-C6
22	B	602	CLA	C11-C10-C8-C7
22	h	101	CLA	C12-C13-C15-C16
27	A	410	LMG	O9-C10-C11-C12
27	a	402	LMG	O9-C10-C11-C12
27	M	101	LMG	O8-C28-C29-C30
22	c	504	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	CAA-CBA-CGA-O2A
25	b	601	DGD	CAB-CBB-CCB-CDB
22	c	502	CLA	C16-C17-C18-C19
27	d	407	LMG	O7-C10-C11-C12
25	b	624	DGD	O2G-C1B-C2B-C3B
25	B	620	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
27	B	621	LMG	O6-C1-O1-C7
22	B	609	CLA	C13-C15-C16-C17
27	C	522	LMG	O10-C28-C29-C30
25	c	517	DGD	C5B-C6B-C7B-C8B
30	a	401	SQD	C25-C26-C27-C28
31	B	627	LMT	C4'-C5'-C6'-O6'
30	b	602	SQD	O47-C7-C8-C9
22	B	601	CLA	CAA-CBA-CGA-O2A
25	C	517	DGD	O1A-C1A-C2A-C3A
22	C	508	CLA	C10-C11-C12-C13
30	a	415	SQD	C24-C25-C26-C27
22	c	504	CLA	CAA-CBA-CGA-O1A
22	C	504	CLA	CAA-CBA-CGA-O1A
22	b	613	CLA	CAA-CBA-CGA-O1A
30	A	413	SQD	O49-C7-C8-C9
22	B	613	CLA	CAA-CBA-CGA-O1A
27	D	412	LMG	C12-C13-C14-C15

There are no ring outliers.

80 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	627	LMT	2	0
24	B	618	BCR	3	0
30	F	102	SQD	2	0
22	A	404	CLA	16	0
22	C	511	CLA	1	0
27	A	415	LMG	1	0
22	D	406	CLA	3	0
22	B	615	CLA	6	0
24	A	407	BCR	2	0
22	B	614	CLA	2	0
27	E	101	LMG	1	0
27	A	410	LMG	2	0
27	M	101	LMG	1	0
23	D	407	PL9	8	0
31	I	102	LMT	1	0
34	F	101	HEM	4	0
25	A	408	DGD	1	0
22	D	405	CLA	11	0
22	B	608	CLA	14	0
25	C	515	DGD	3	0

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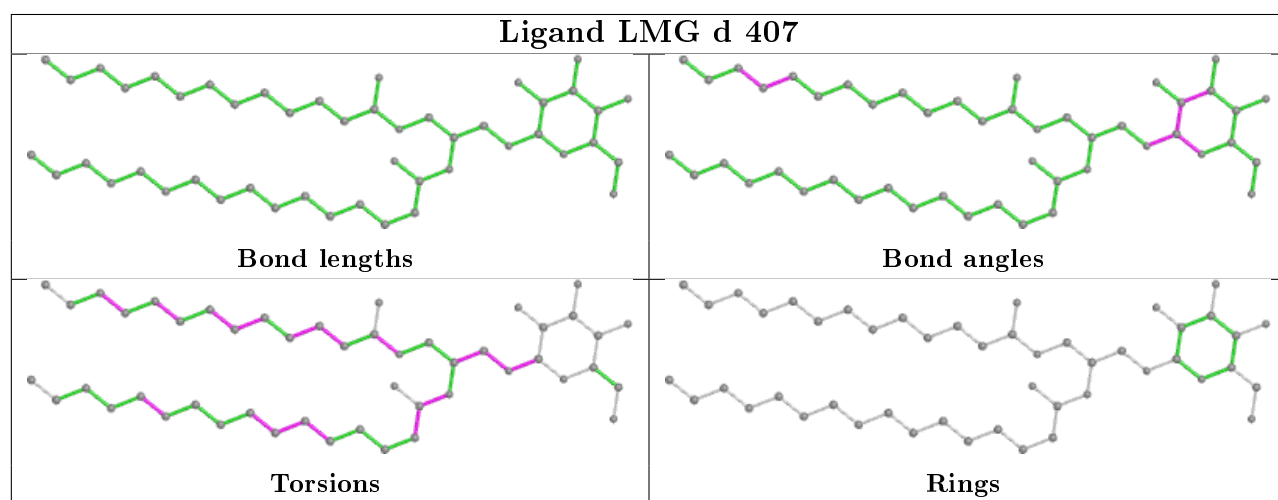
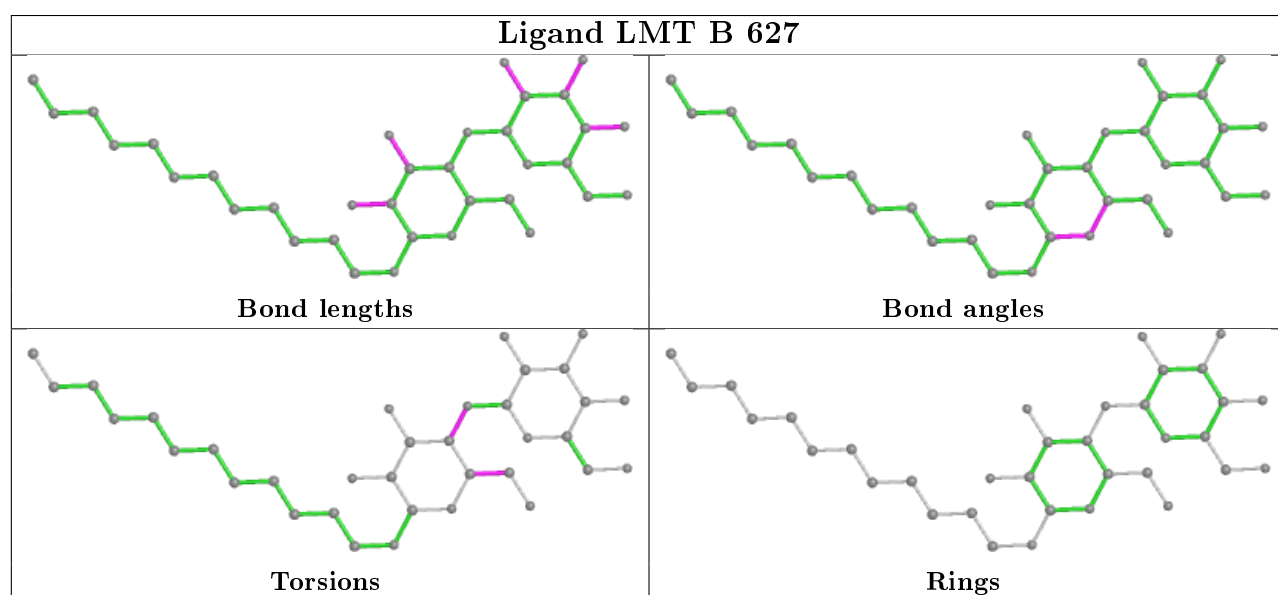
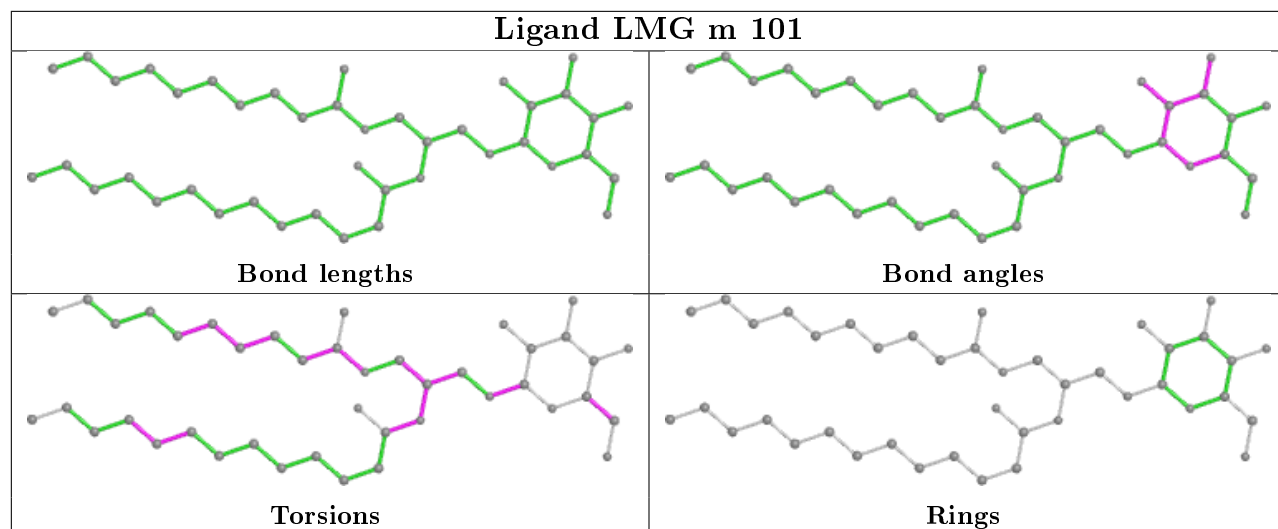
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	506	CLA	6	0
34	V	201	HEM	3	0
30	B	626	SQD	3	0
24	D	411	BCR	3	0
22	C	507	CLA	4	0
22	B	611	CLA	10	0
22	C	508	CLA	4	0
27	D	412	LMG	1	0
23	A	406	PL9	3	0
22	A	403	CLA	12	0
27	I	101	LMG	1	0
22	H	101	CLA	11	0
26	C	519	LHG	2	0
25	D	409	DGD	2	0
22	A	402	CLA	11	0
27	B	624	LMG	3	0
24	B	617	BCR	1	0
22	B	607	CLA	10	0
30	D	403	SQD	3	0
24	C	513	BCR	8	0
25	C	517	DGD	5	0
22	C	505	CLA	2	0
22	B	605	CLA	6	0
25	C	516	DGD	4	0
22	B	603	CLA	3	0
24	C	521	BCR	5	0
22	C	503	CLA	5	0
27	C	518	LMG	4	0
32	D	402	PHO	5	0
30	A	414	SQD	3	0
22	C	501	CLA	6	0
25	B	620	DGD	2	0
22	B	612	CLA	10	0
31	B	622	LMT	2	0
24	B	616	BCR	6	0
22	C	520	CLA	5	0
22	C	504	CLA	4	0
22	B	601	CLA	1	0
26	A	409	LHG	3	0
22	C	510	CLA	10	0
22	B	606	CLA	16	0
22	B	602	CLA	11	0

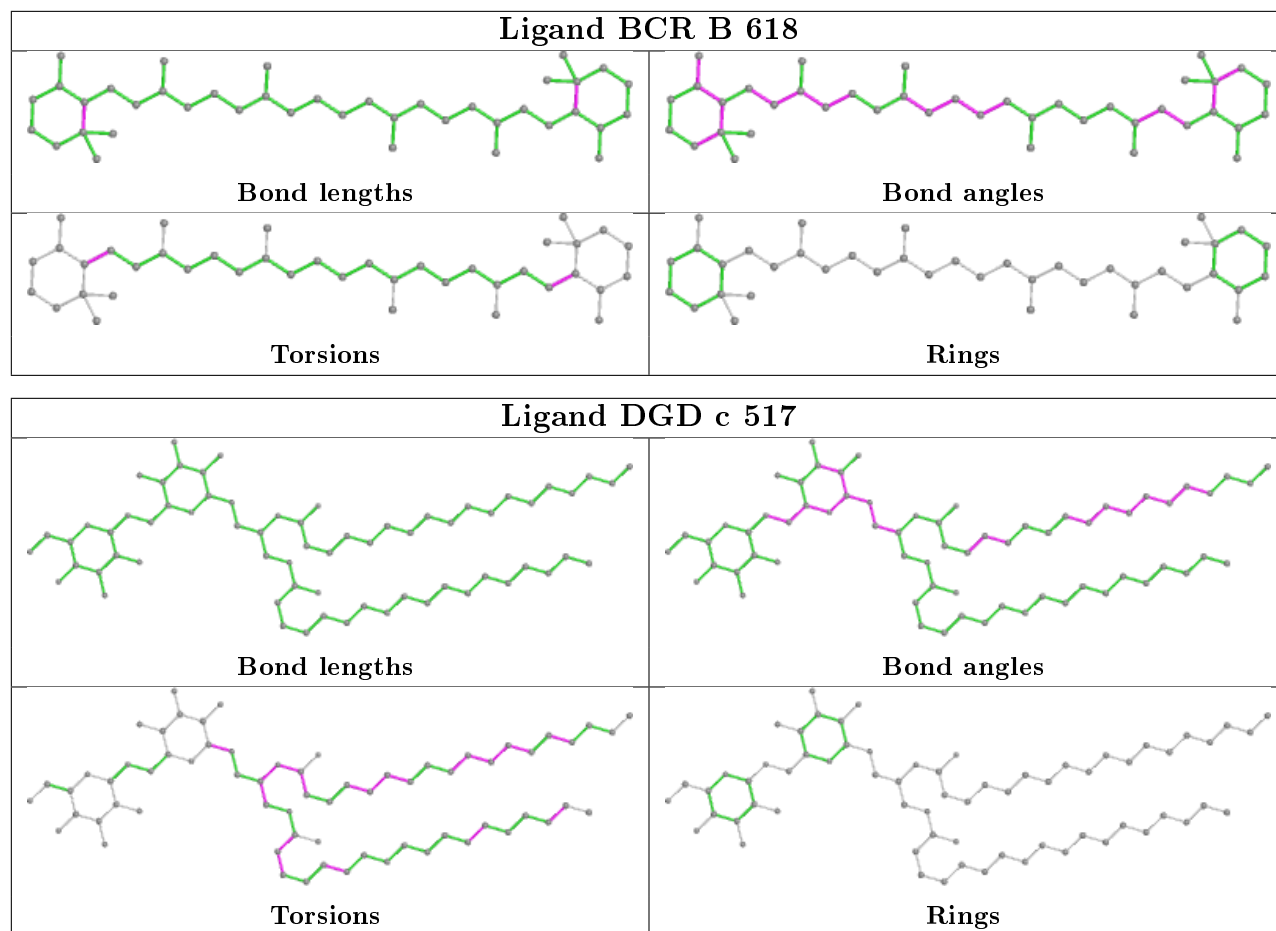
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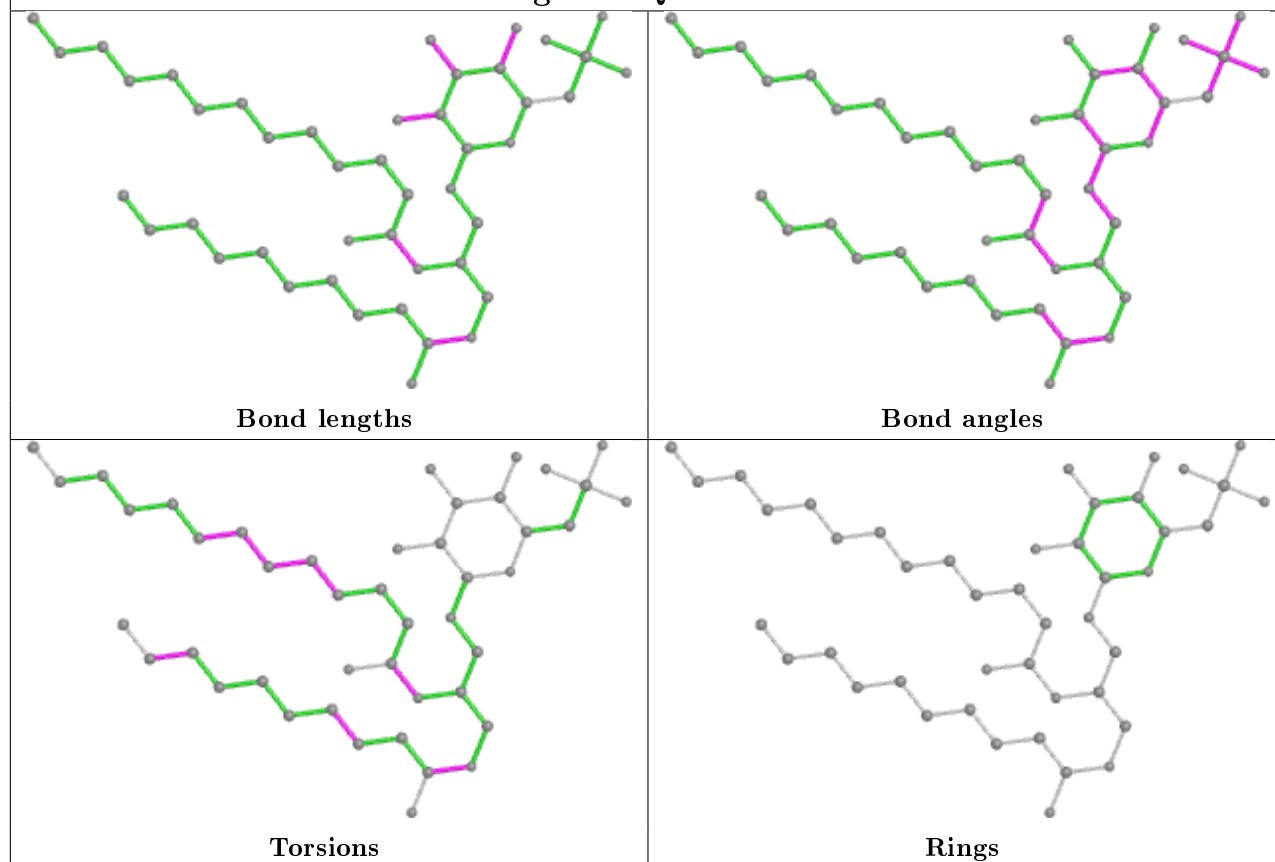
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	401	PHO	11	0
24	H	102	BCR	1	0
22	C	509	CLA	6	0
22	A	405	CLA	8	0
22	B	609	CLA	3	0
24	B	619	BCR	2	0
25	B	625	DGD	2	0
24	J	102	BCR	2	0
22	B	610	CLA	6	0
24	C	514	BCR	7	0
27	B	621	LMG	3	0
22	B	604	CLA	10	0
30	A	413	SQD	3	0
22	B	613	CLA	4	0
27	D	408	LMG	6	0
27	C	522	LMG	3	0
31	B	628	LMT	2	0
22	C	512	CLA	3	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.

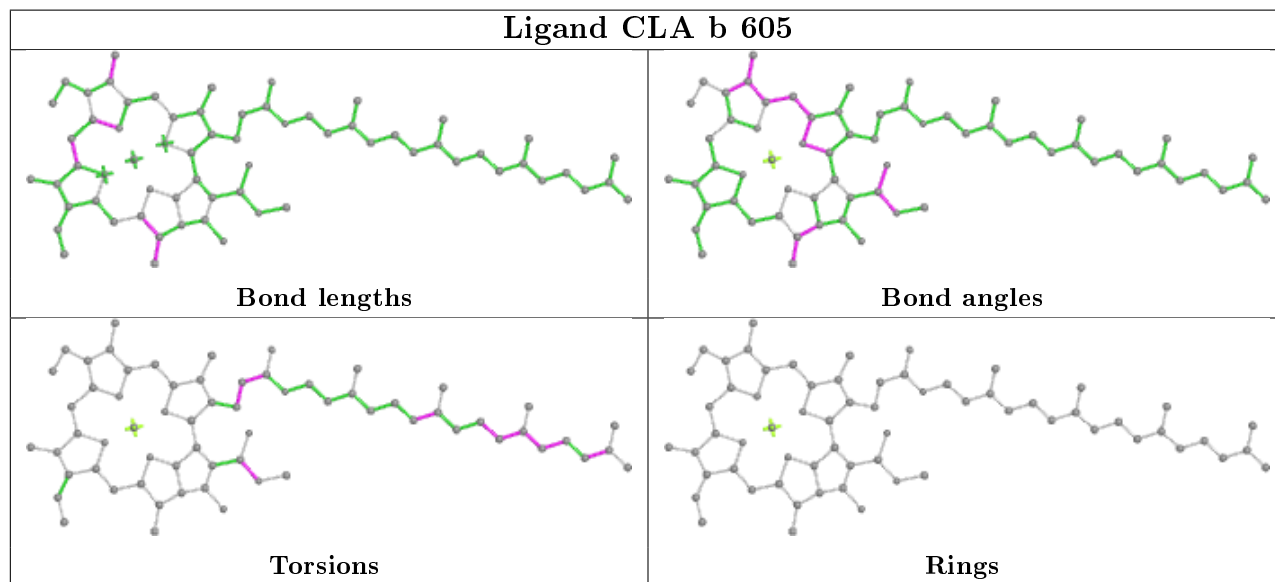




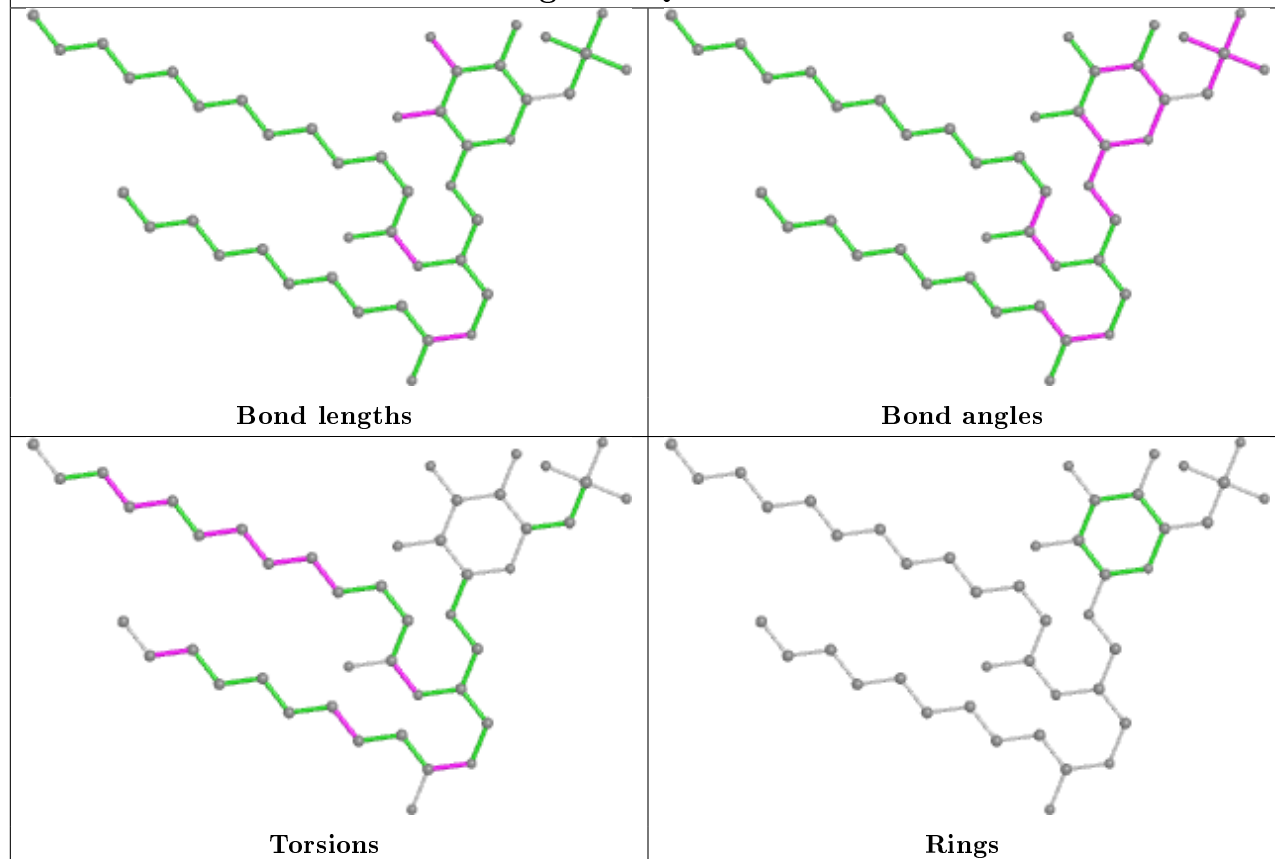
## Ligand SQD F 102



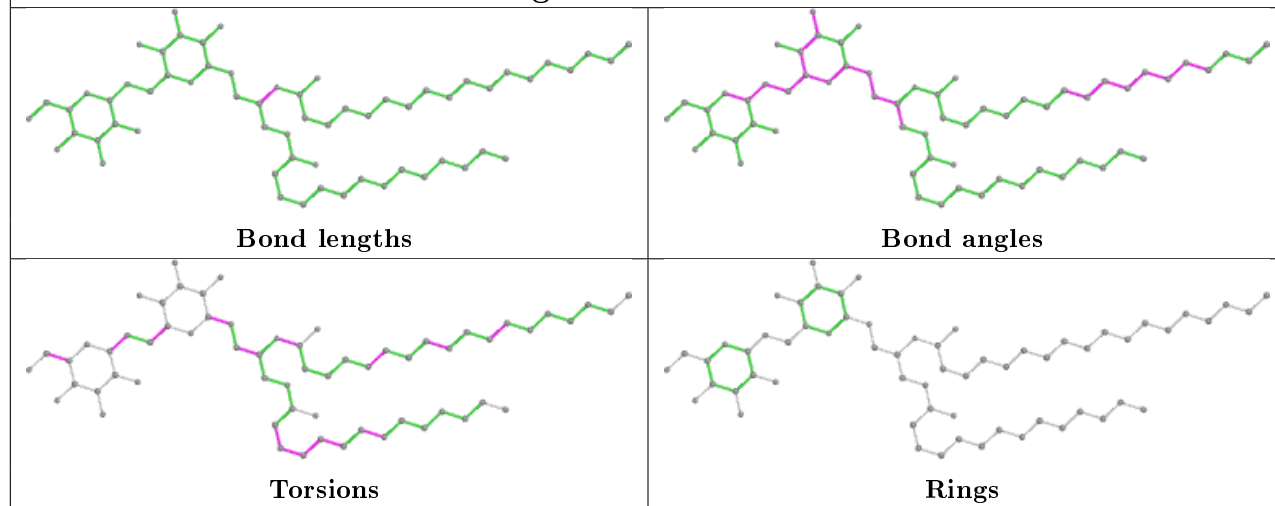
## Ligand CLA b 605



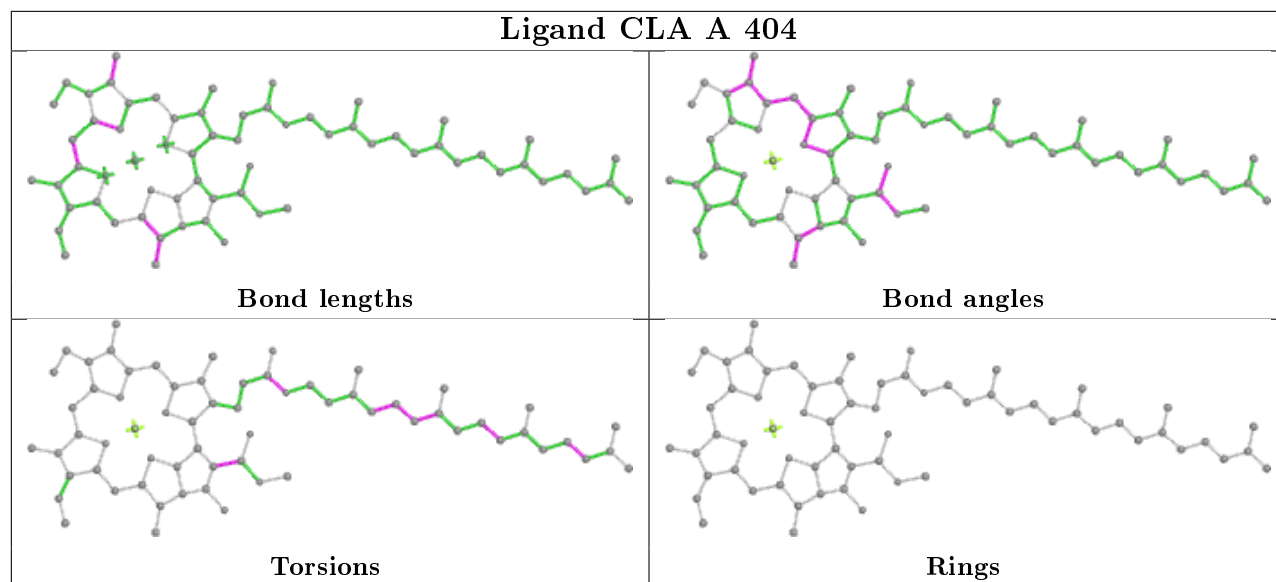
## Ligand SQD f 103



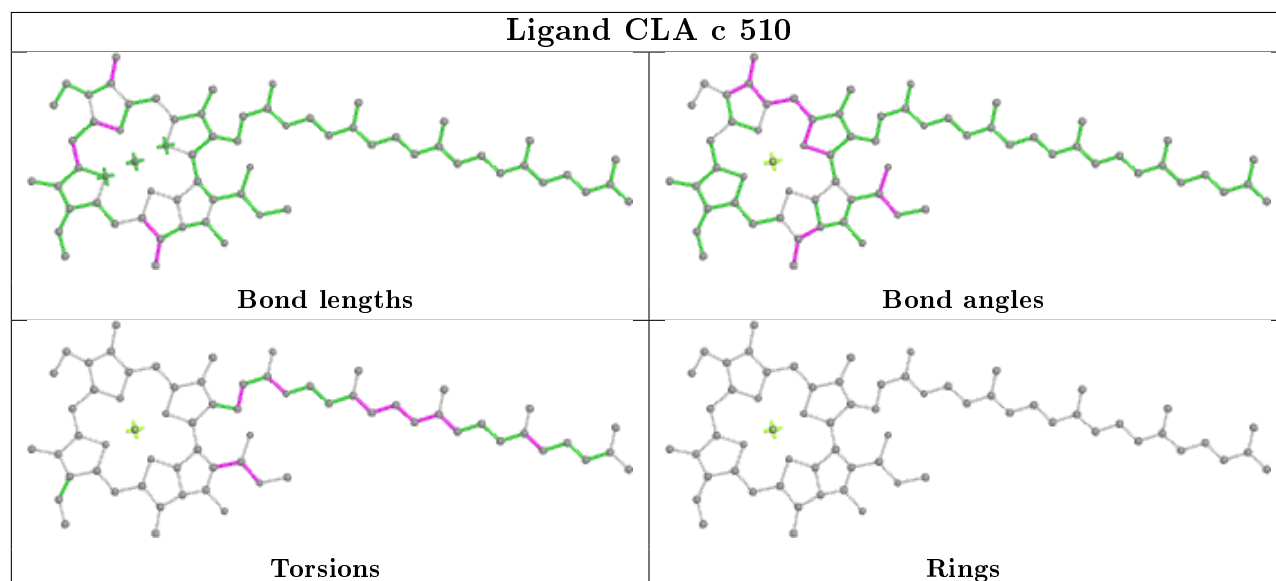
## Ligand DGD c 516



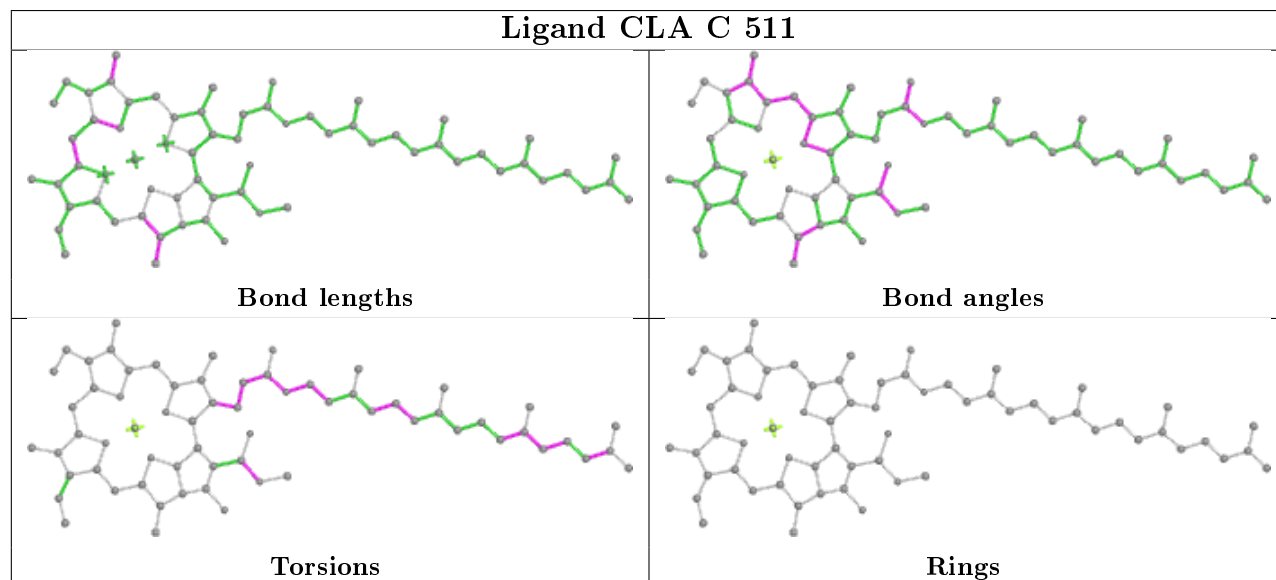
## Ligand CLA A 404



## Ligand CLA c 510

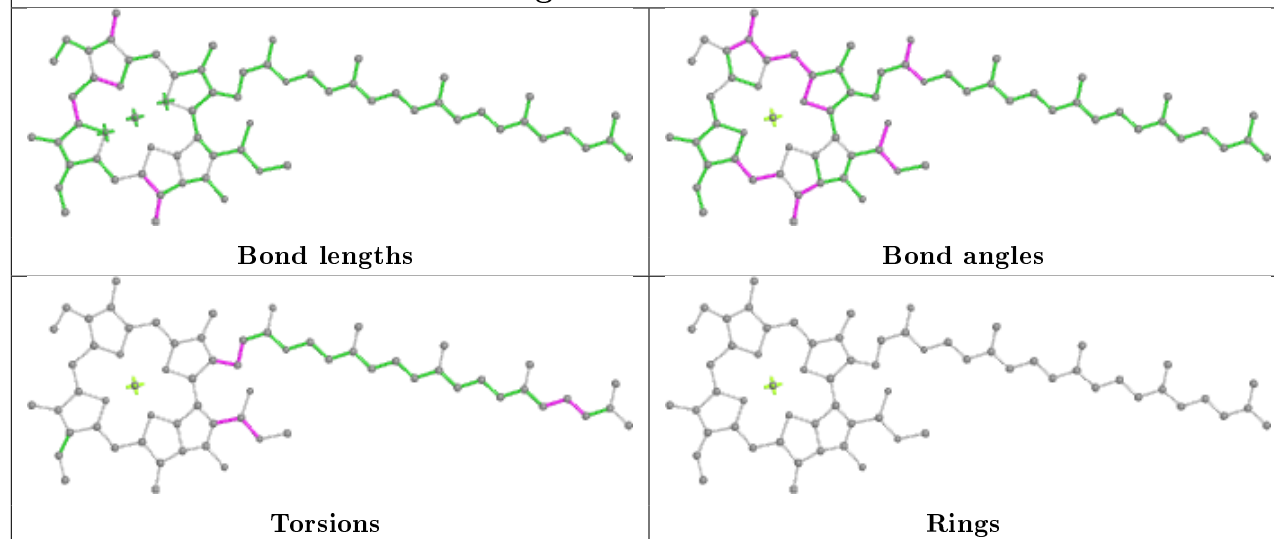


## Ligand CLA C 511

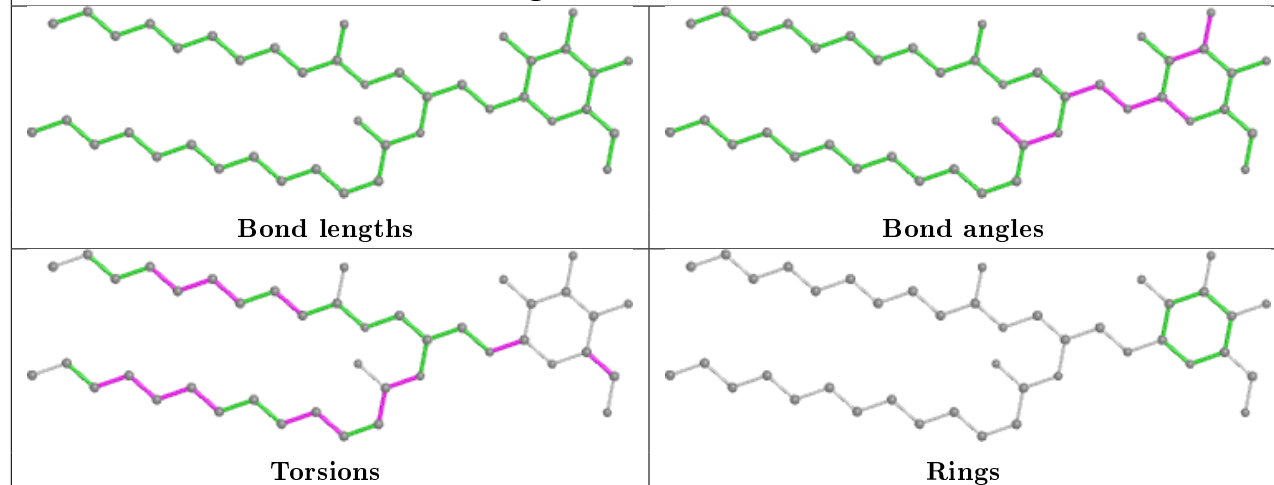




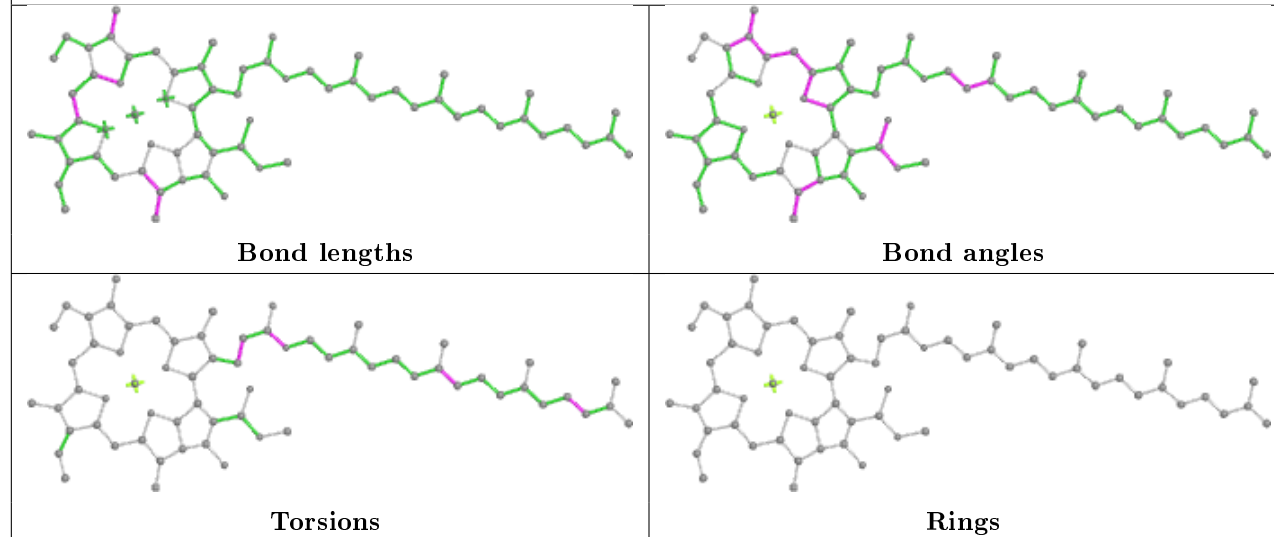
## Ligand CLA b 610



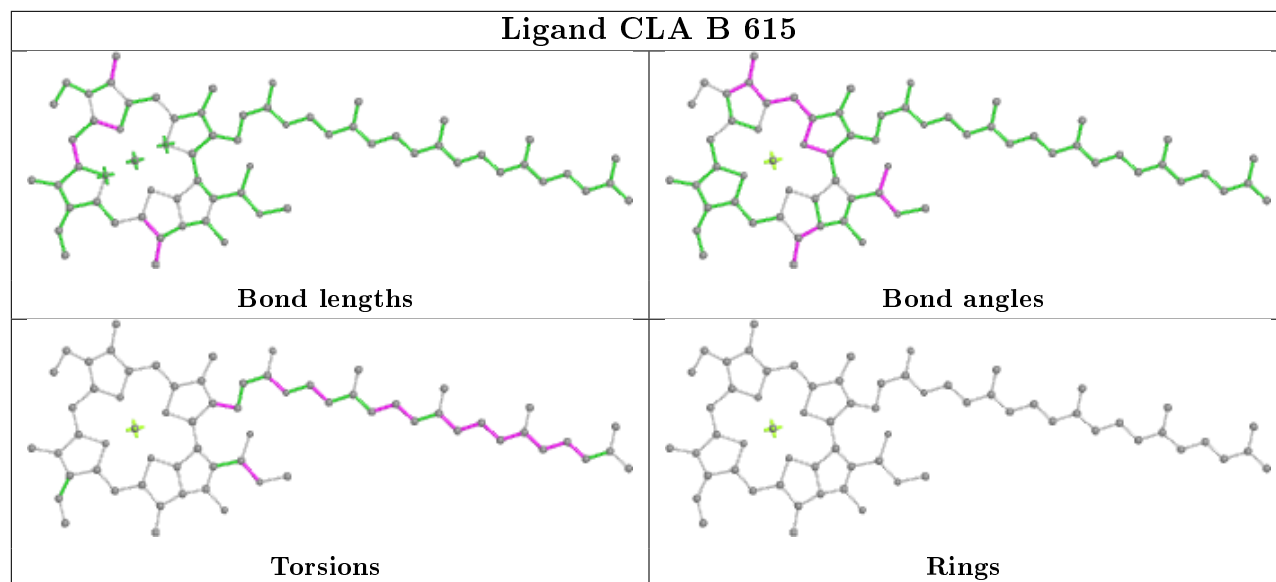
## Ligand LMG A 415



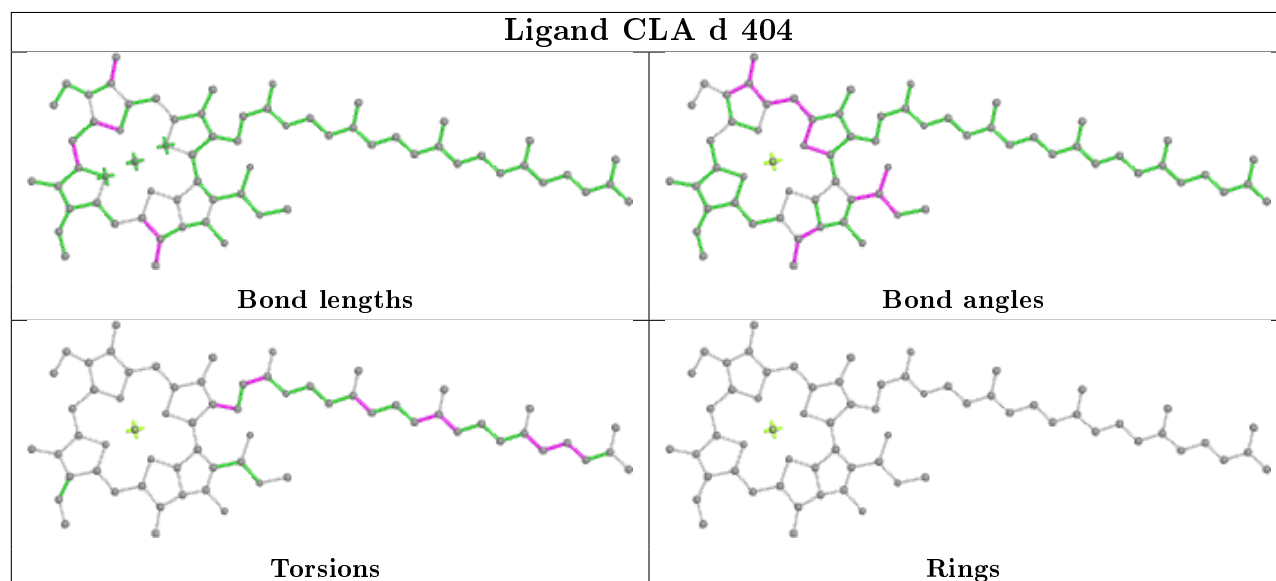
## Ligand CLA D 406



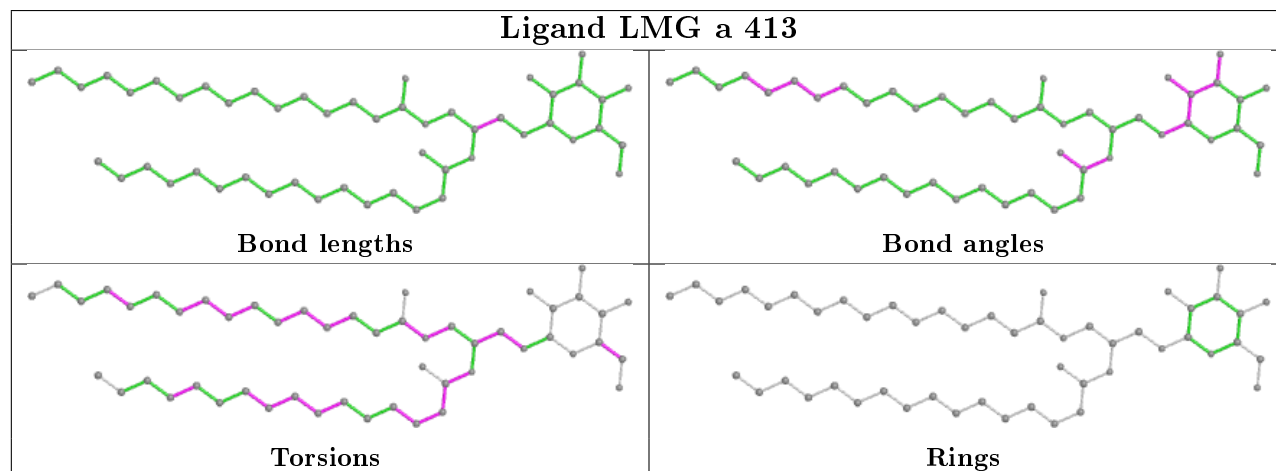
## Ligand CLA B 615

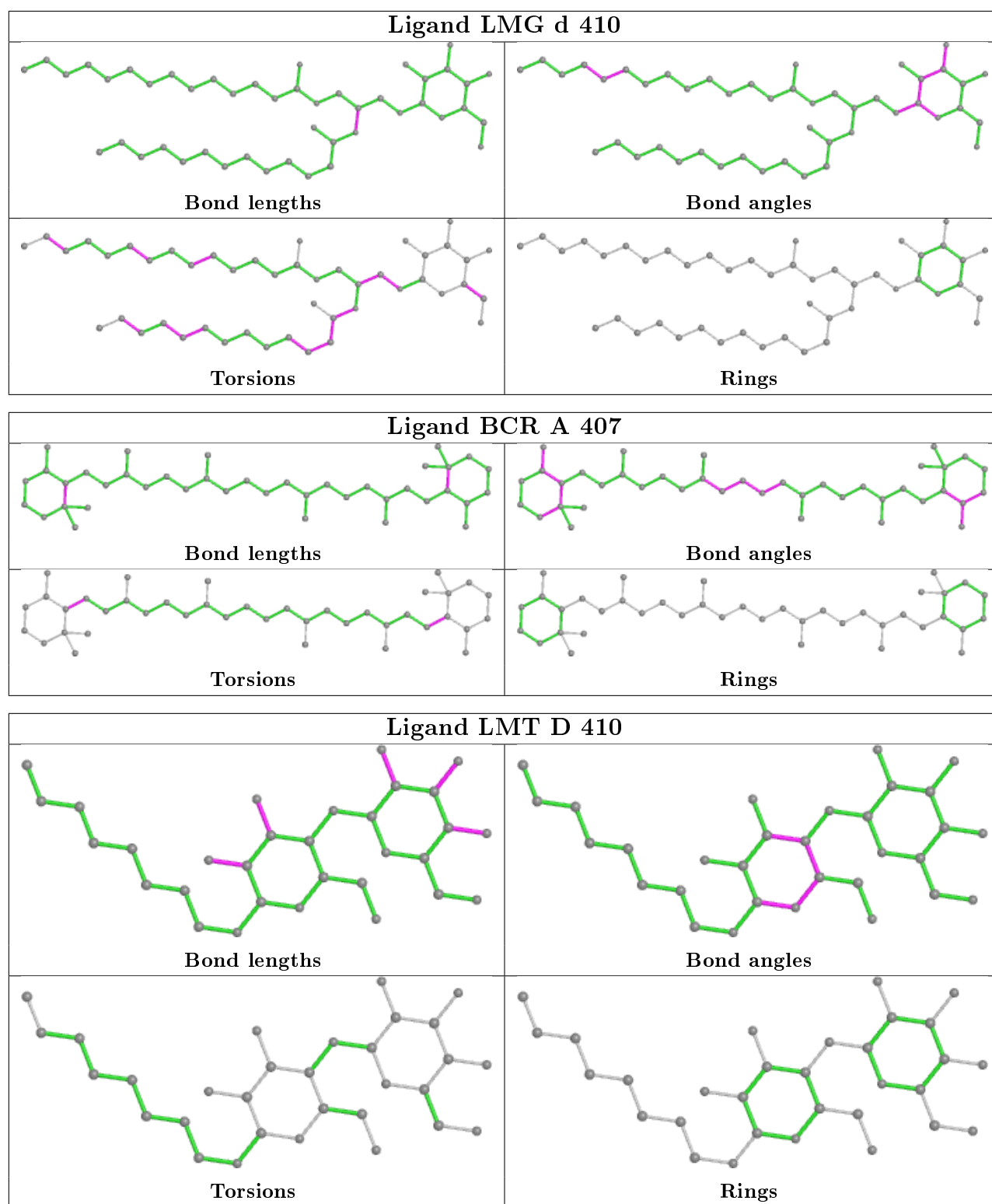


## Ligand CLA d 404

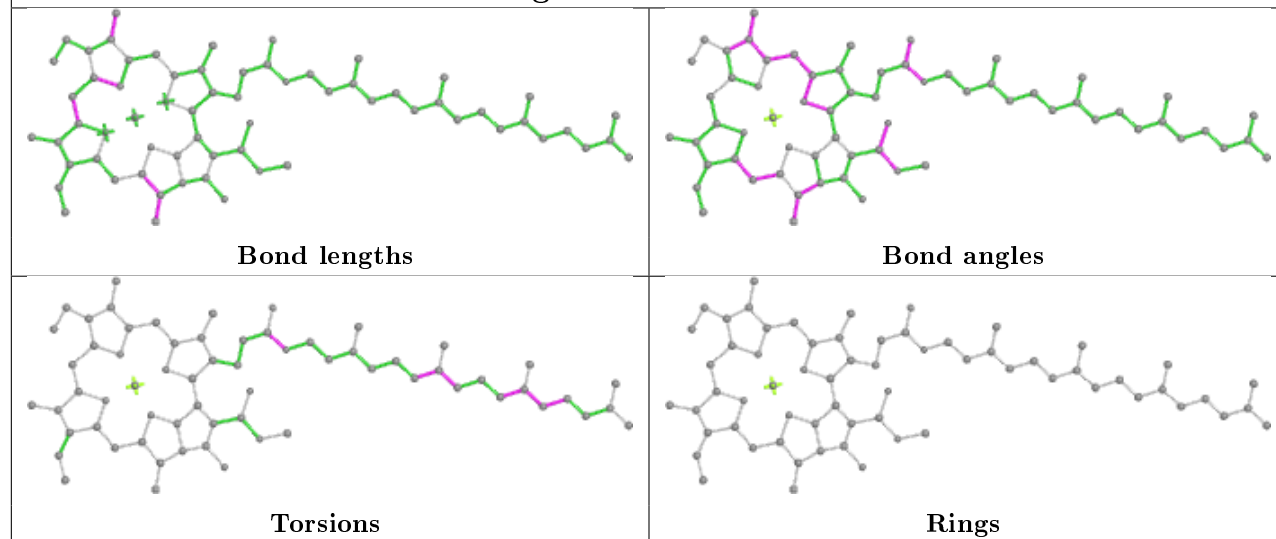


## Ligand LMG a 413

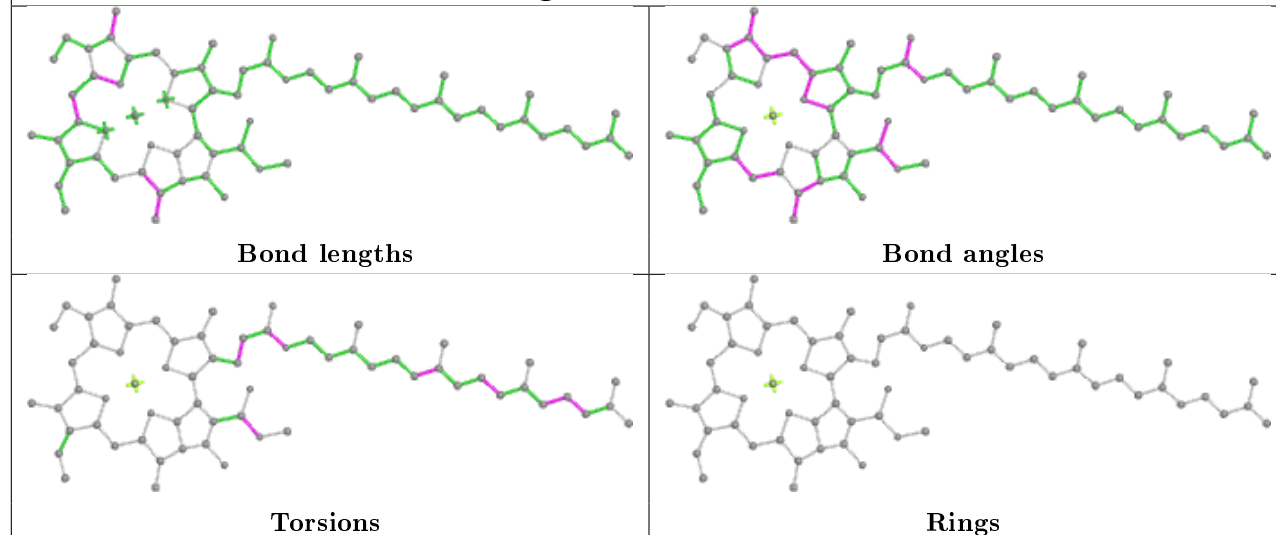




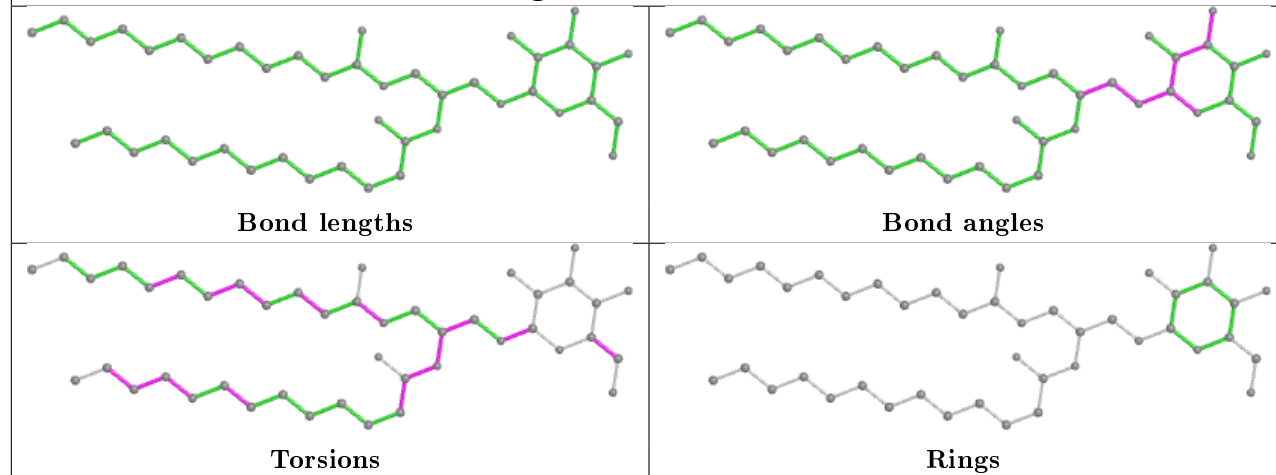
## Ligand CLA B 614

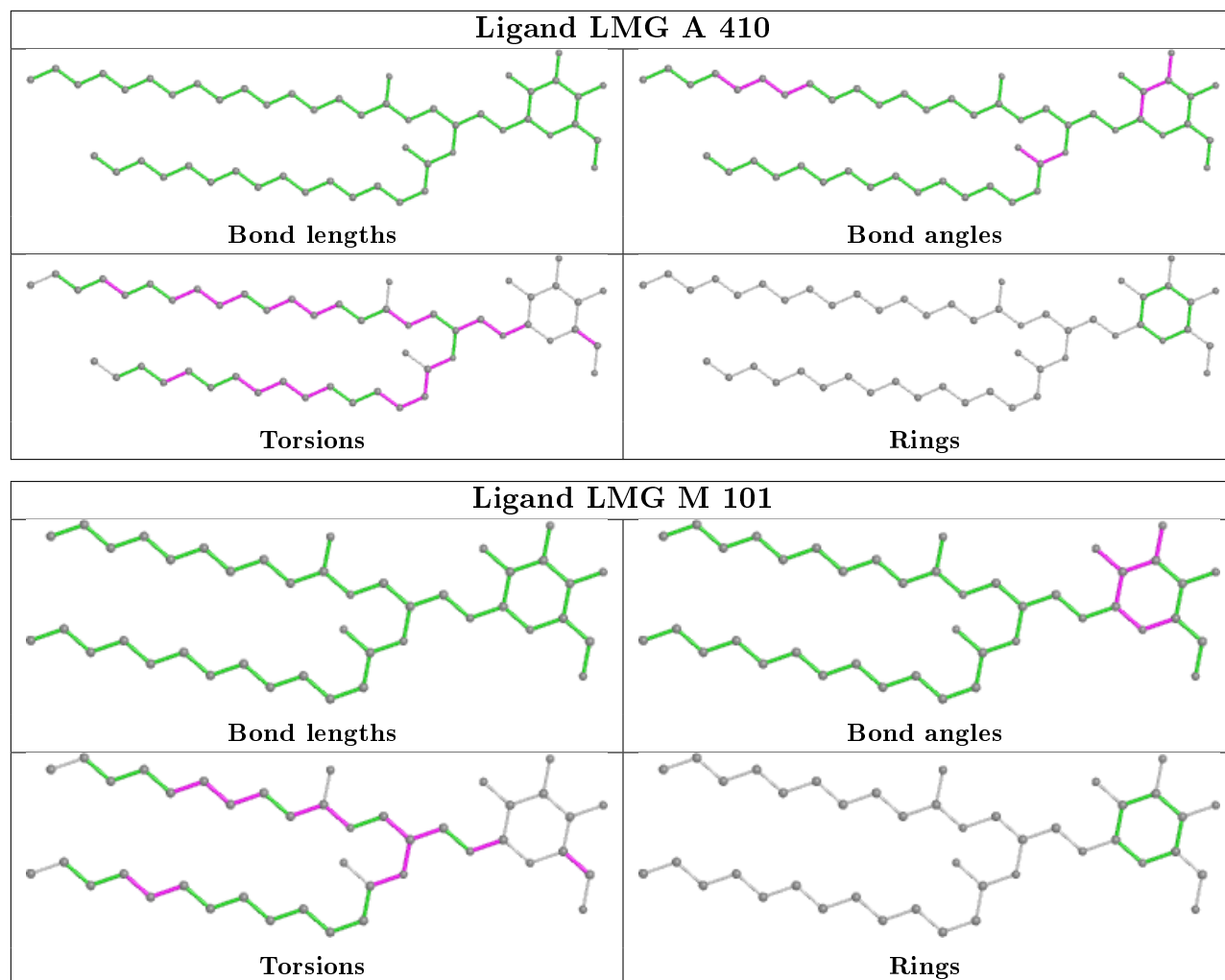


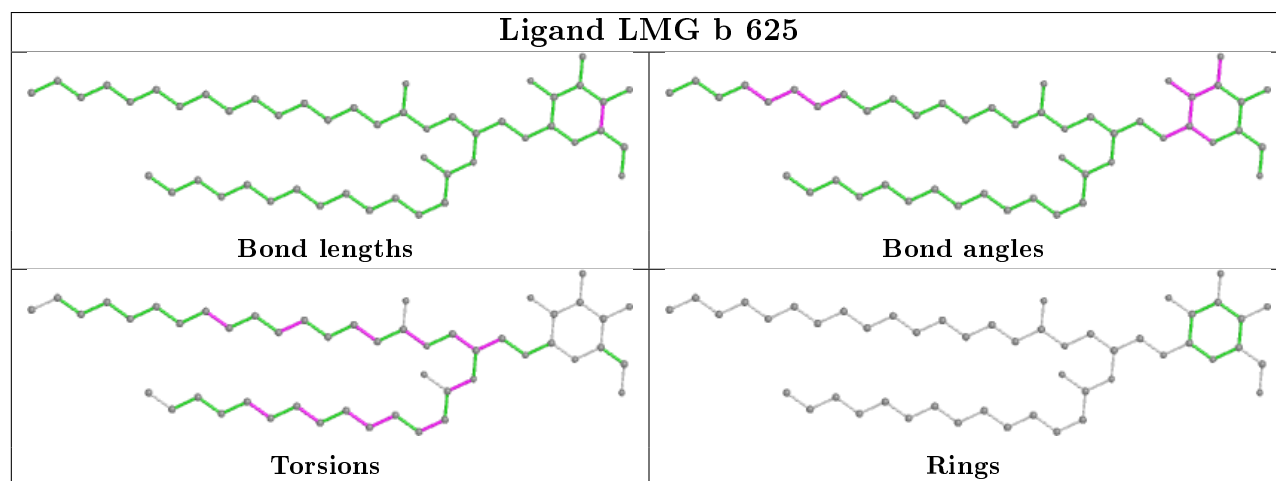
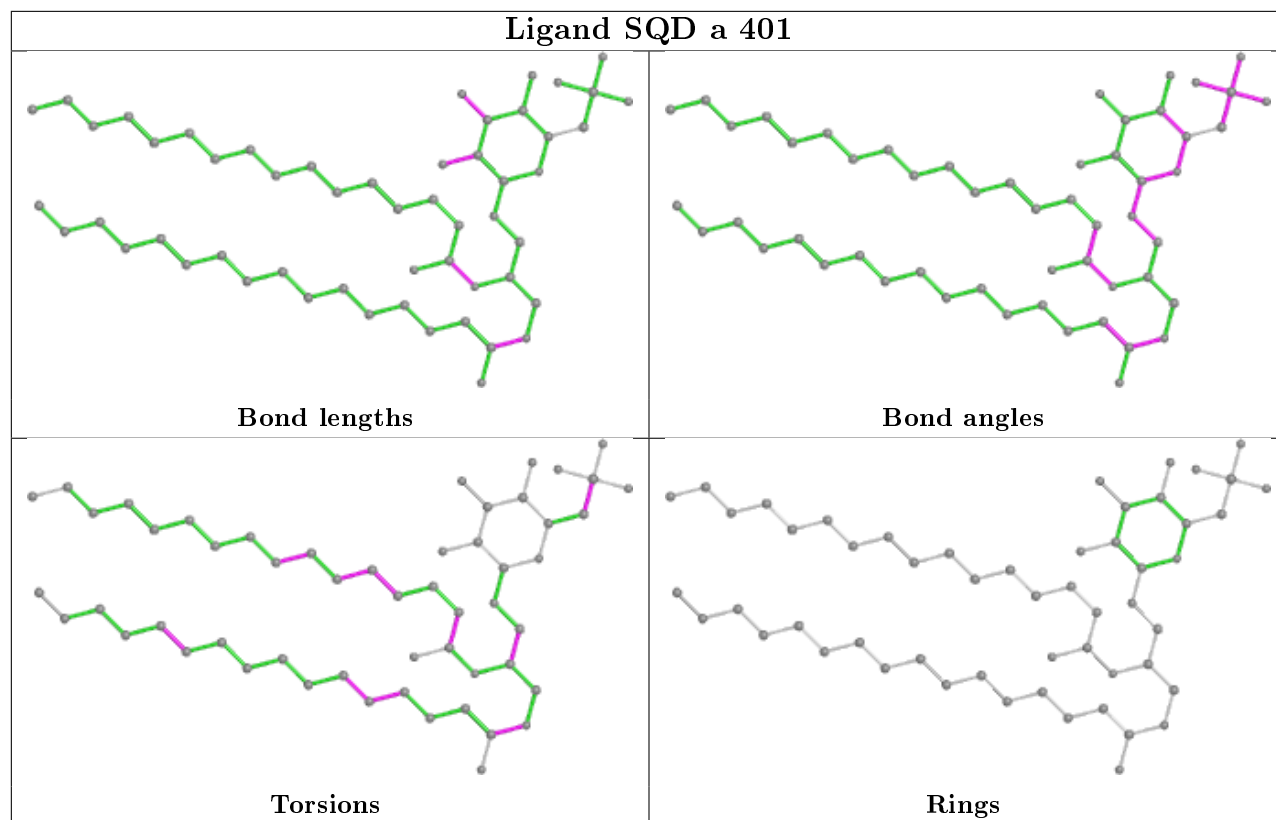
## Ligand CLA c 520

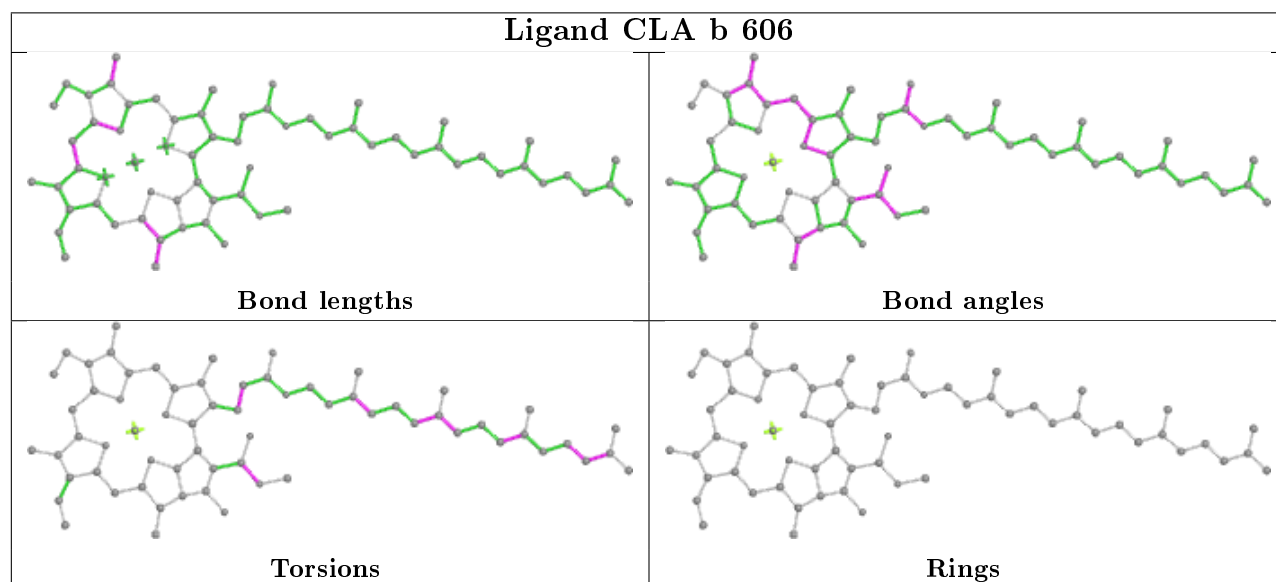
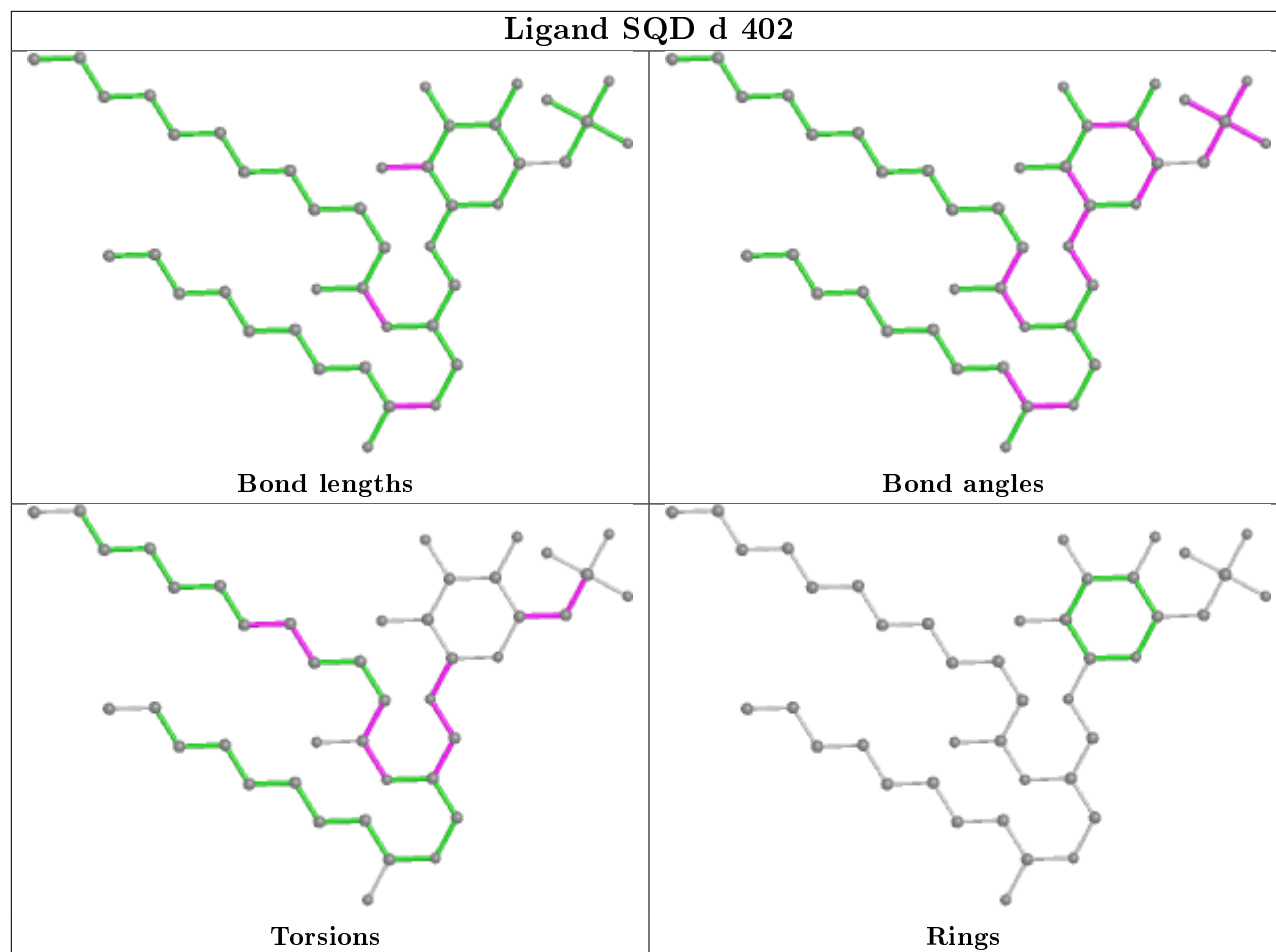


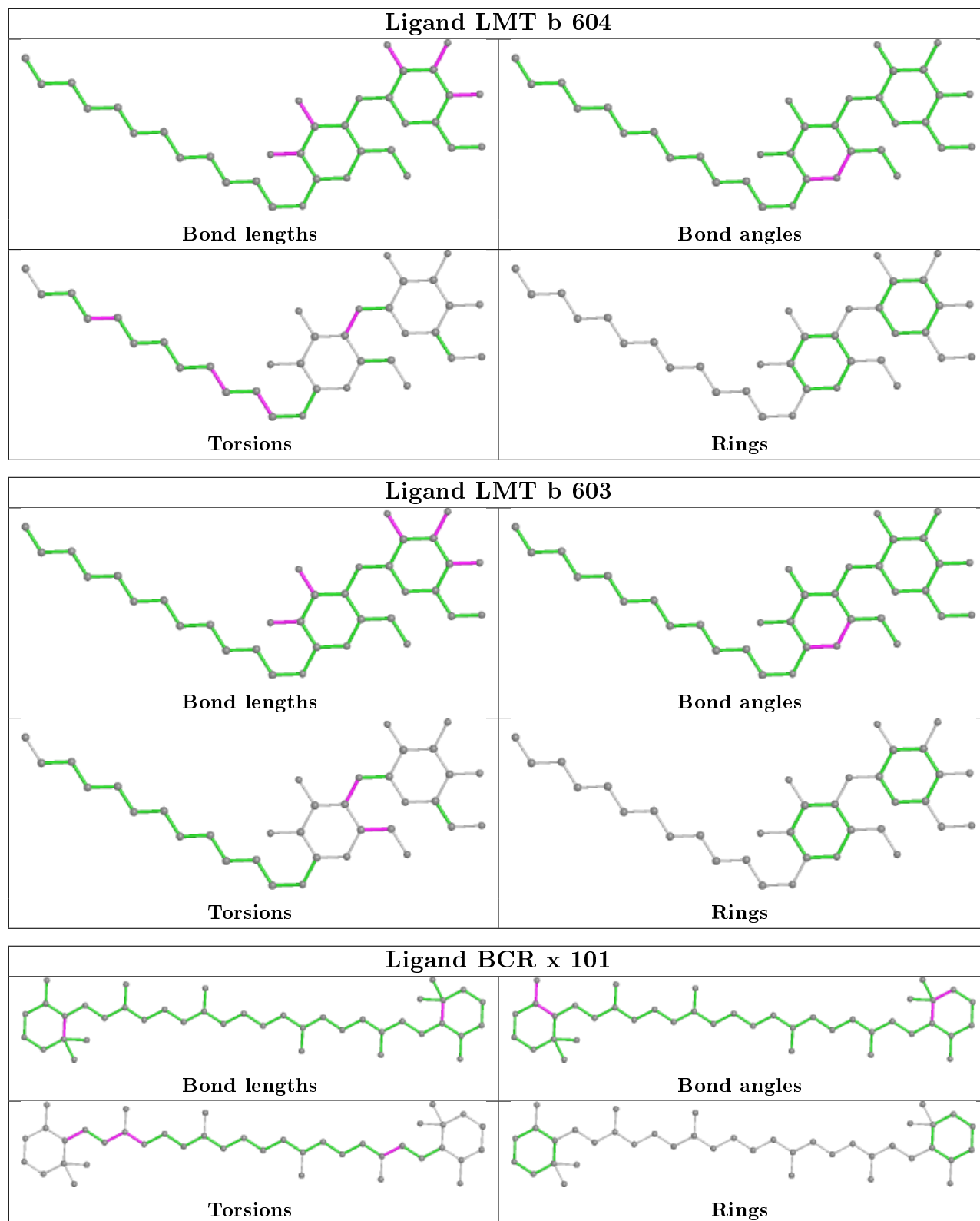
## Ligand LMG E 101



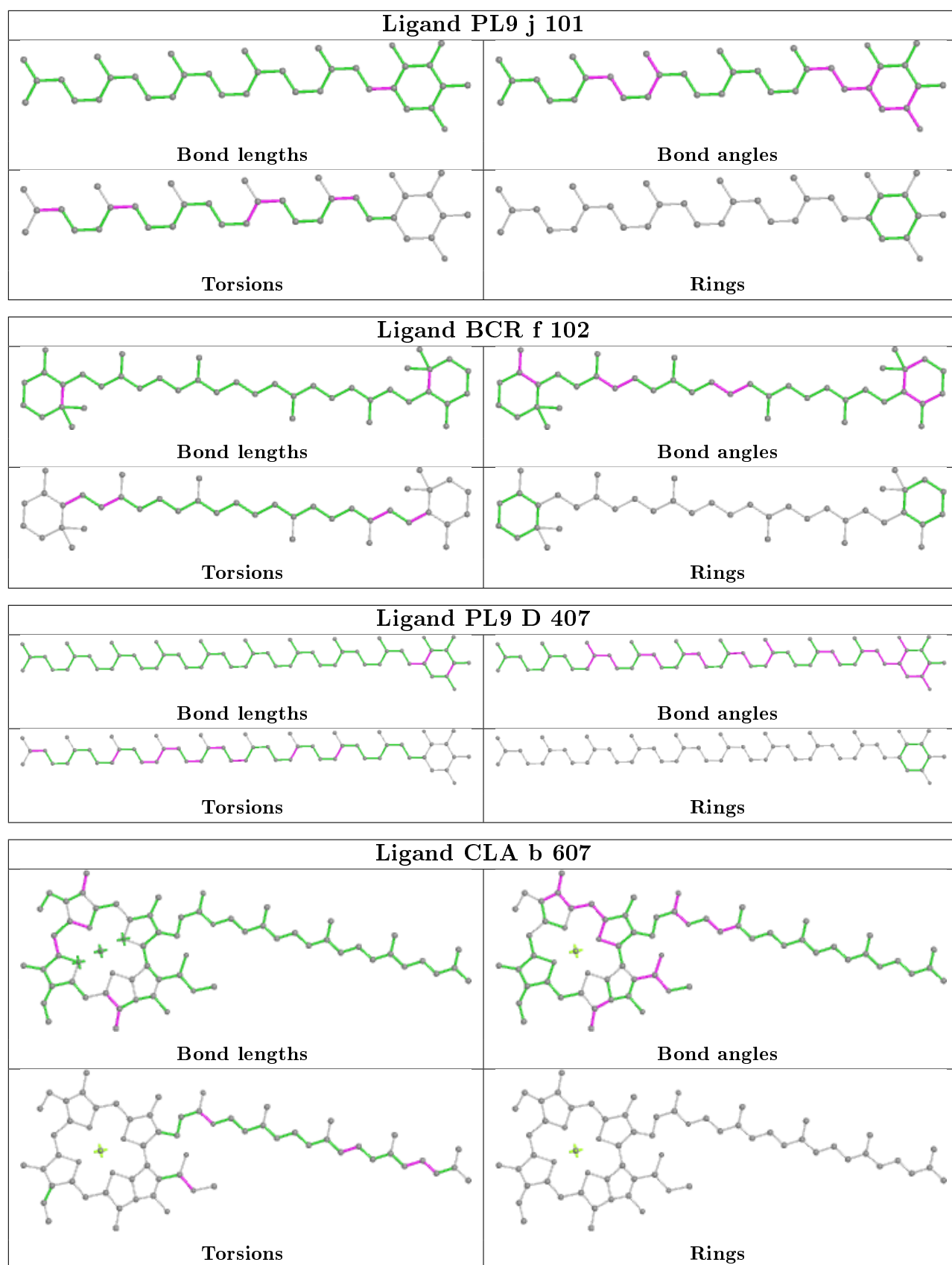


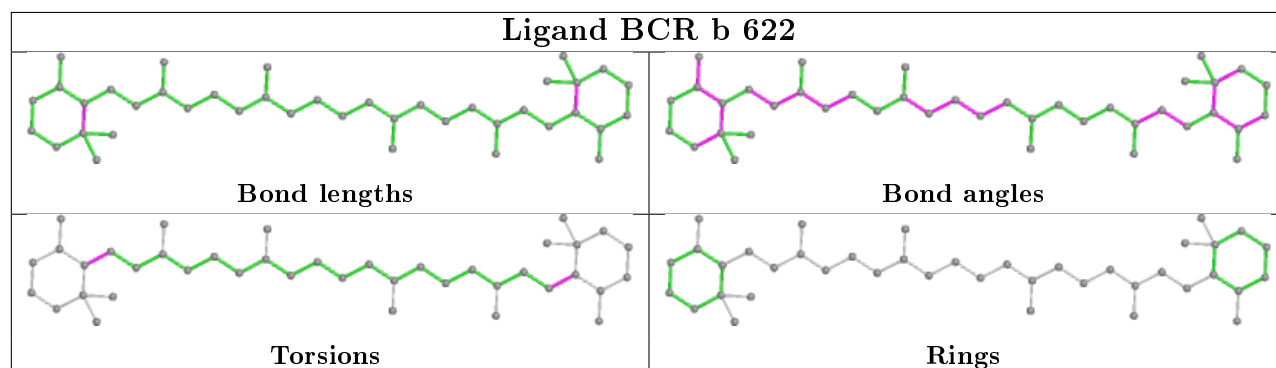
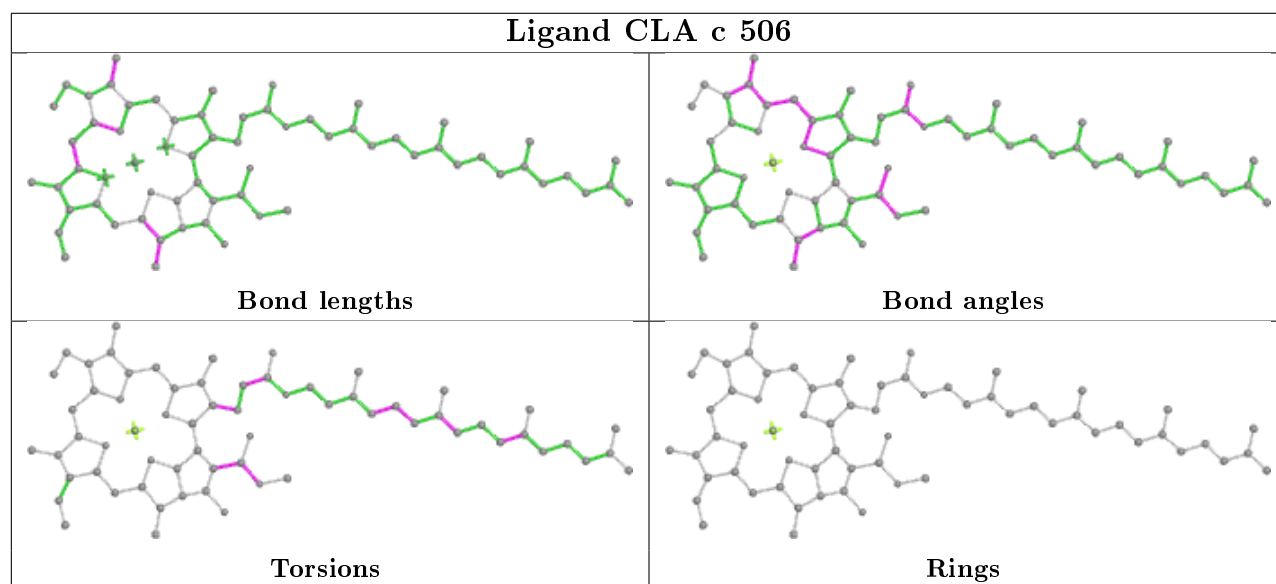
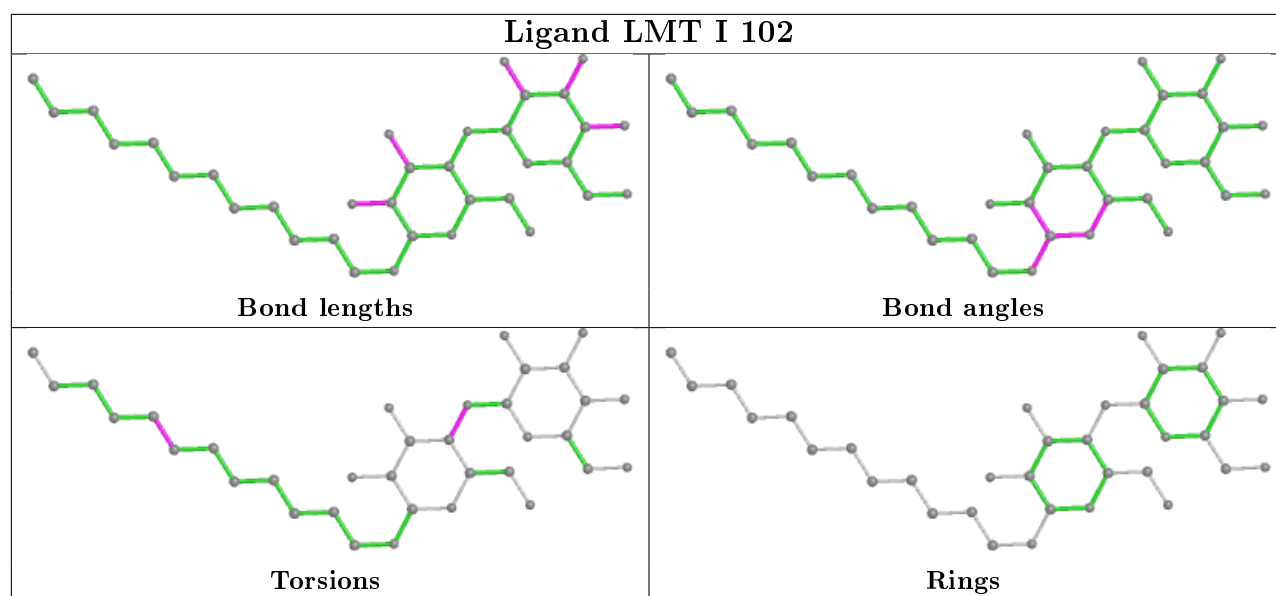


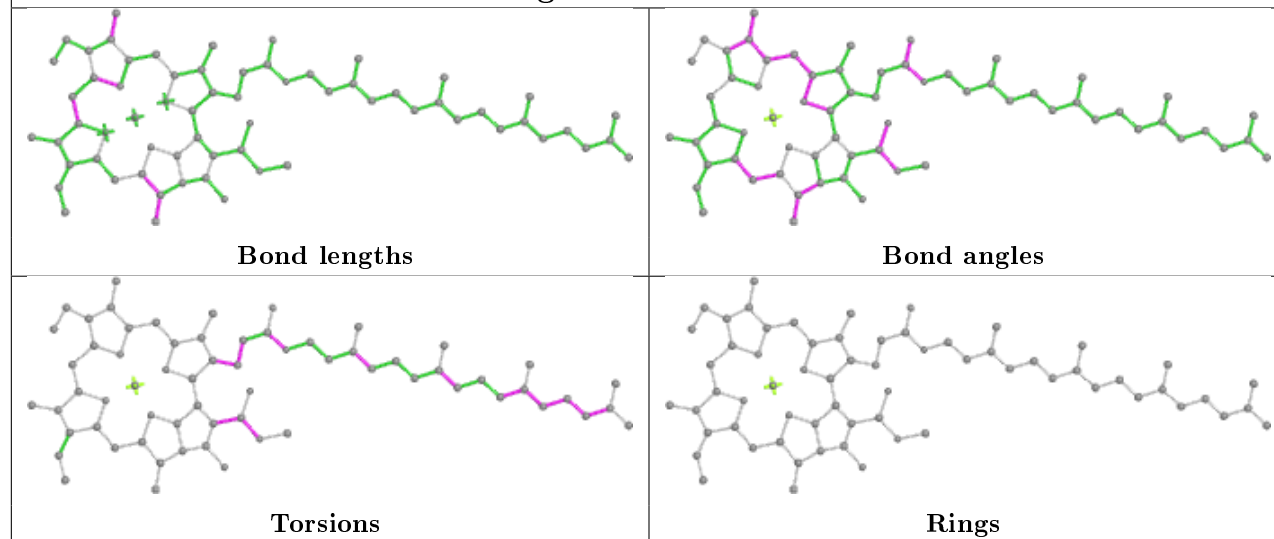
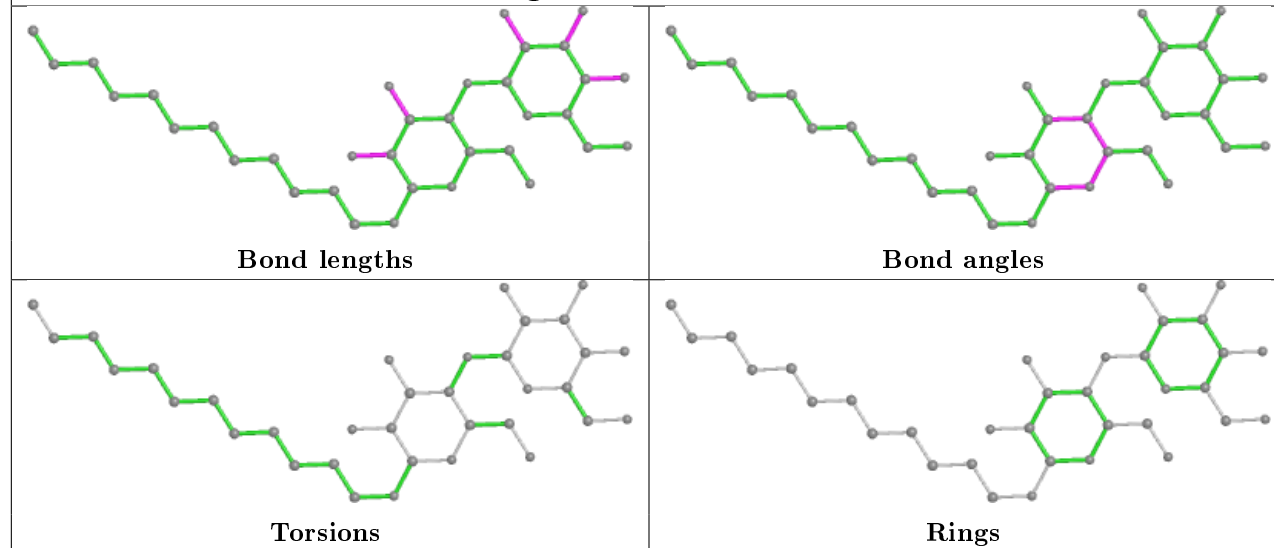


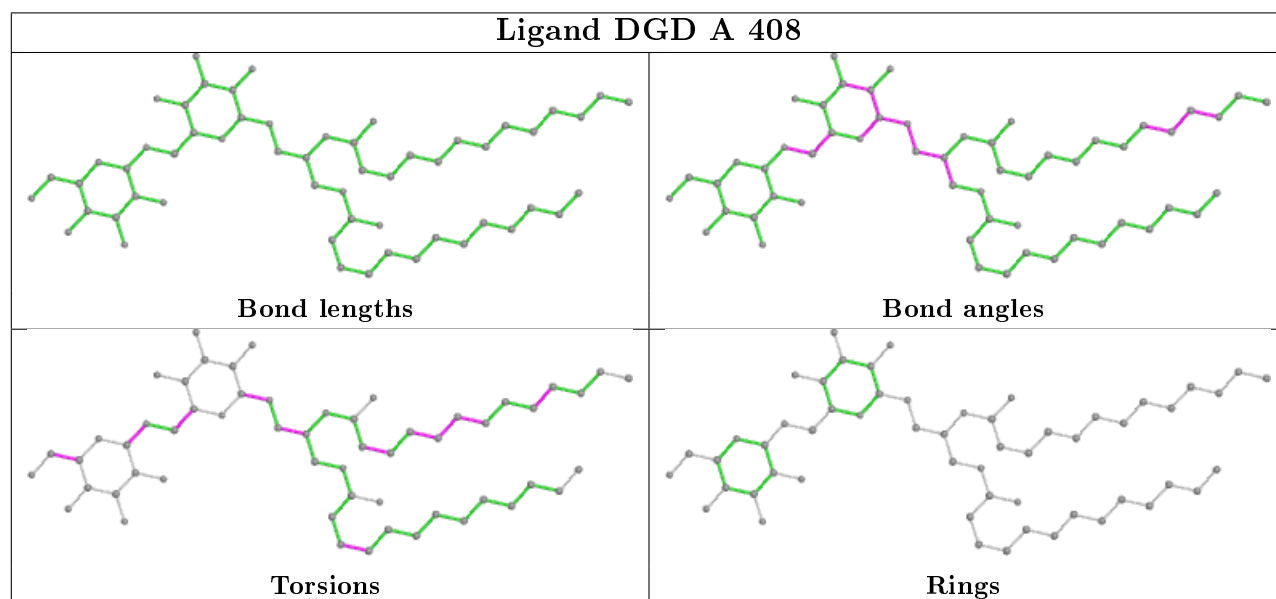
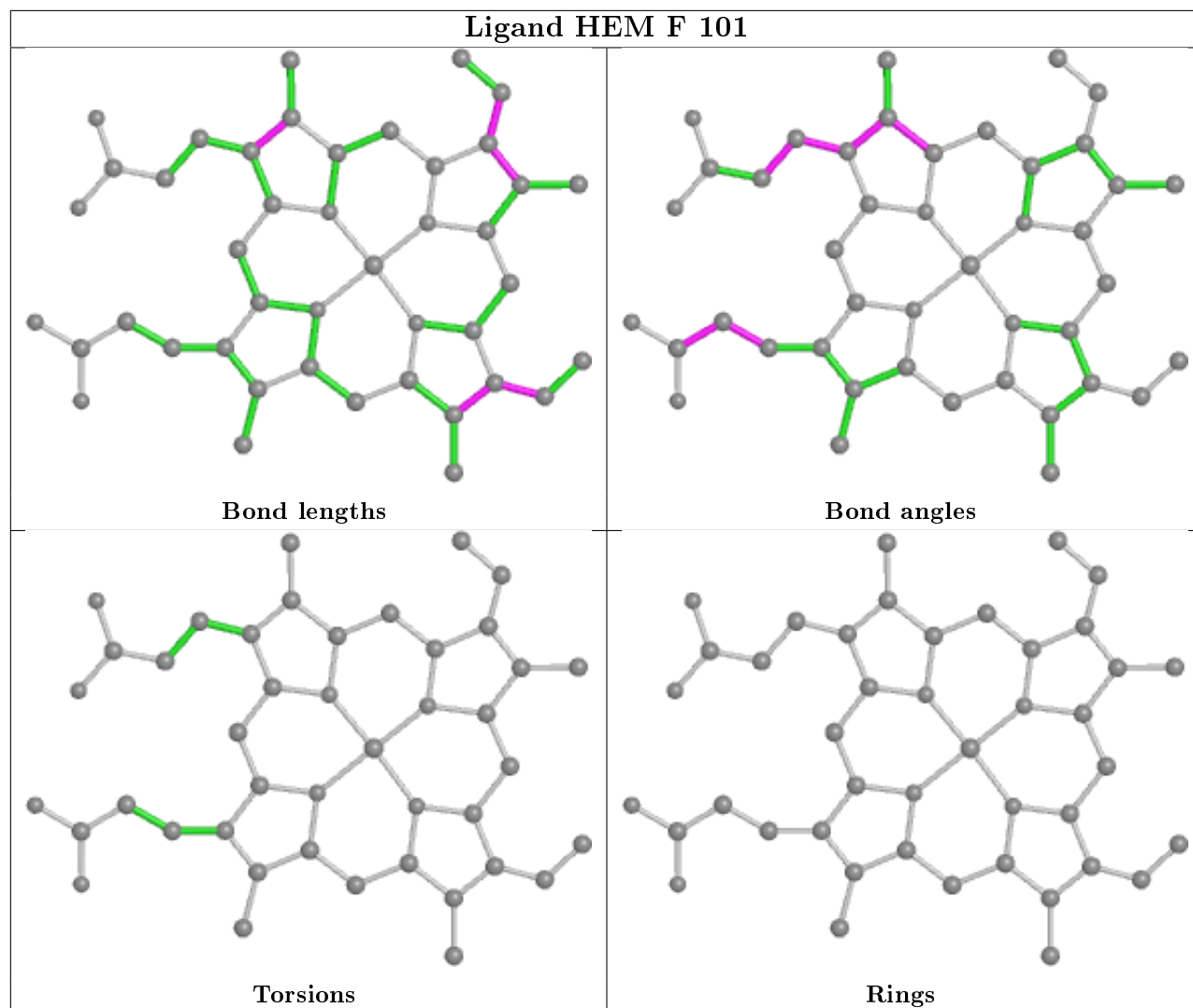




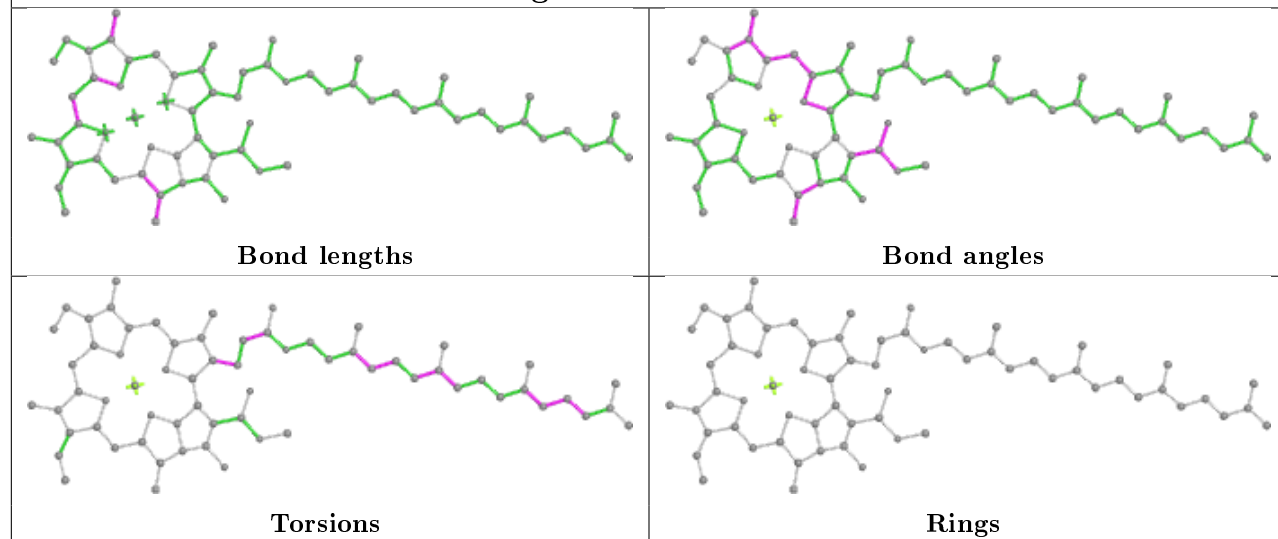




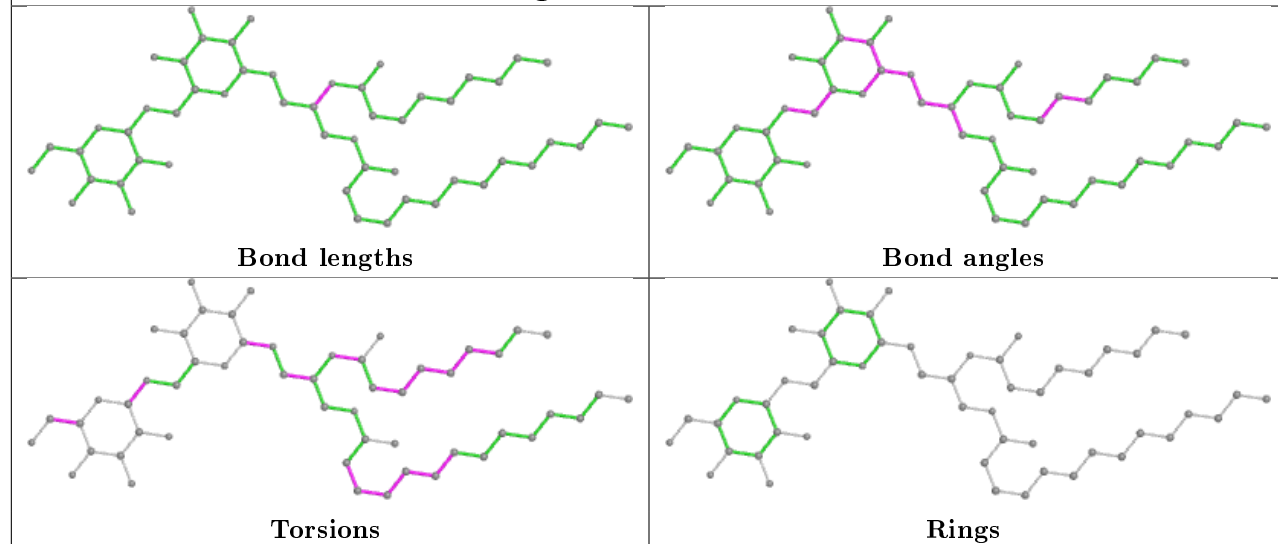
**Ligand CLA c 512****Ligand LMT M 103**



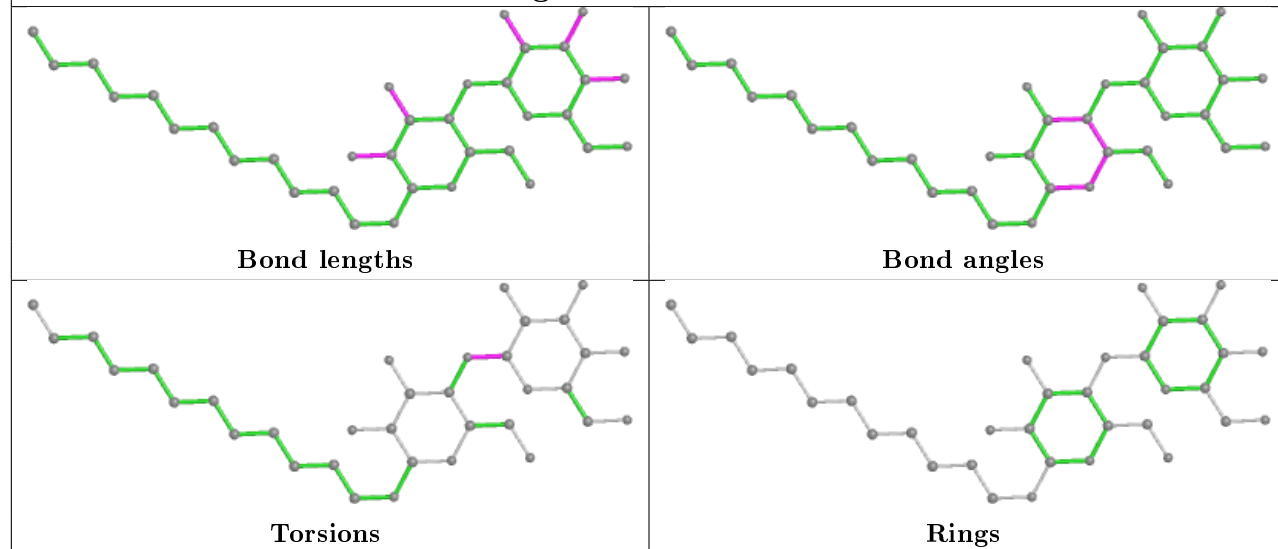
## Ligand CLA D 405



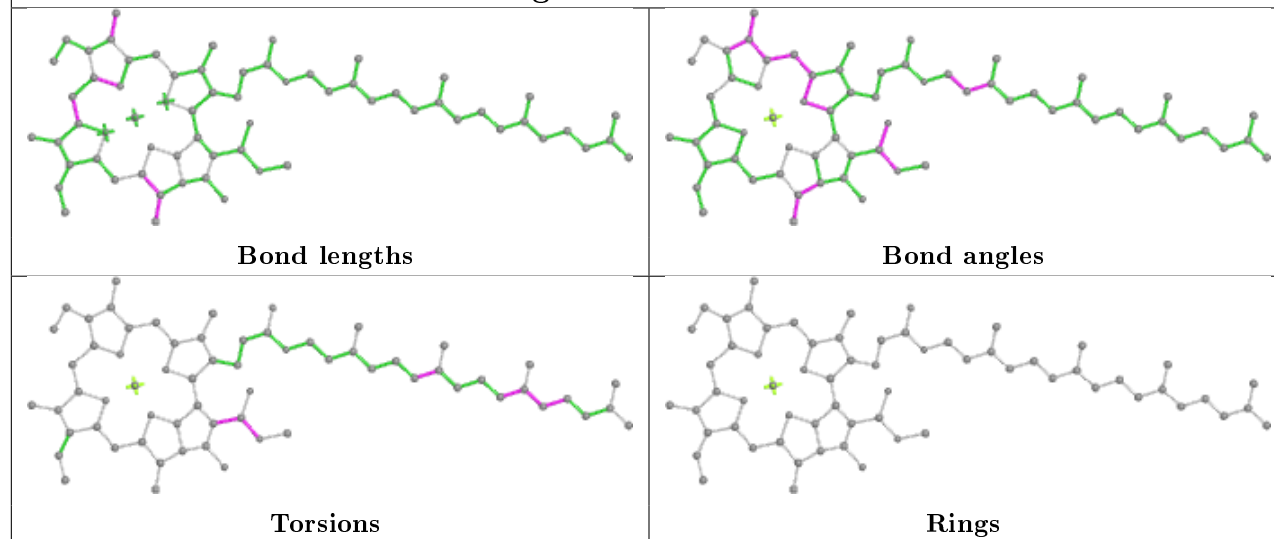
## Ligand DGD c 515



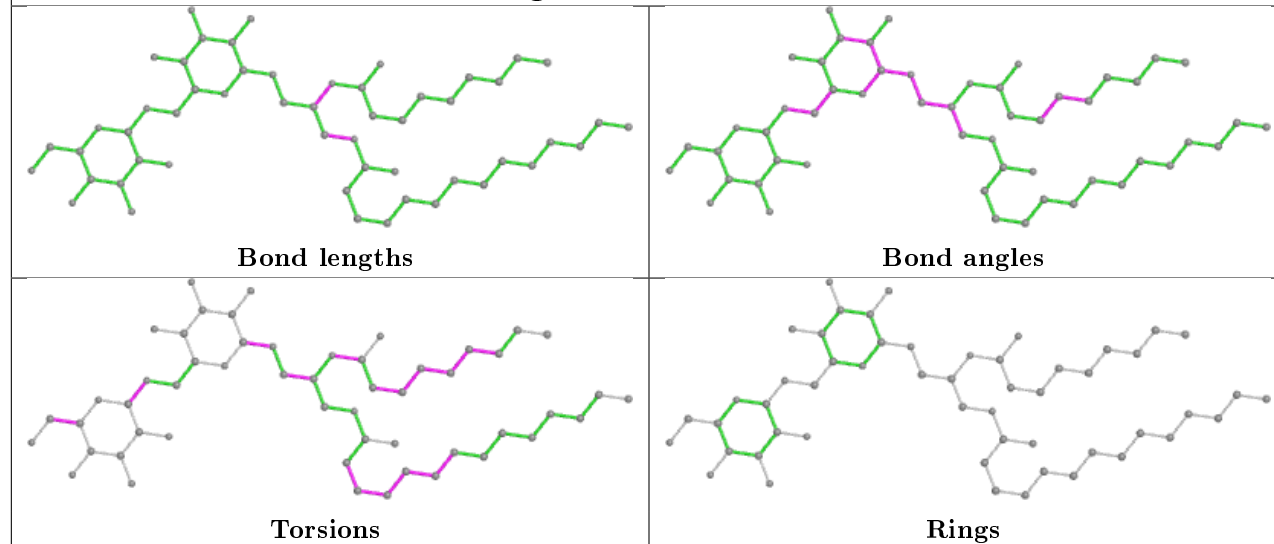
## Ligand LMT b 627



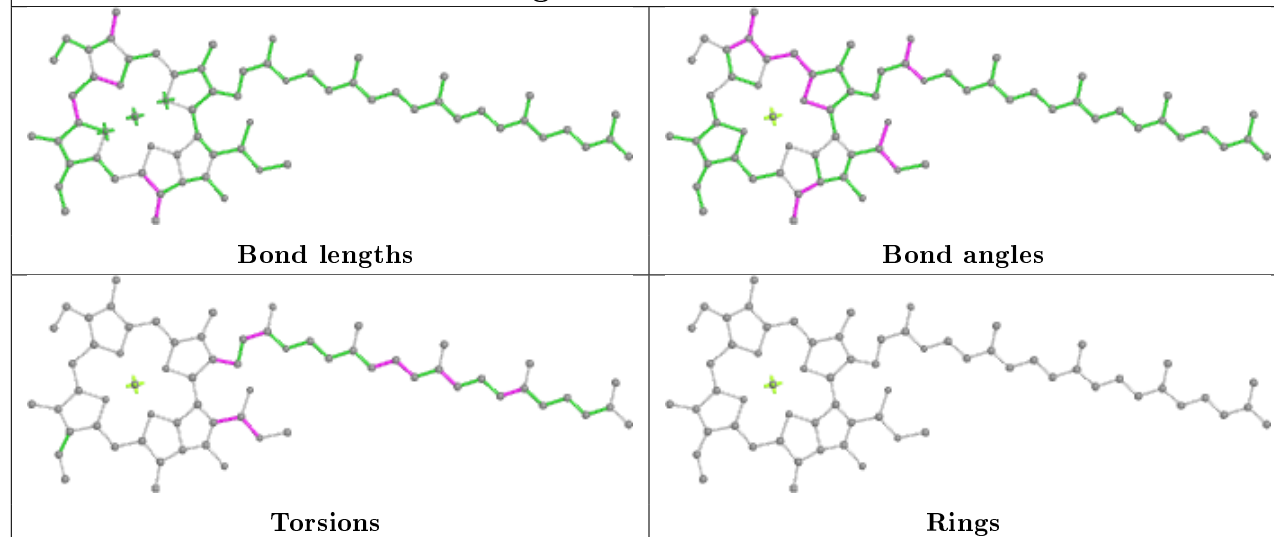
## Ligand CLA B 608

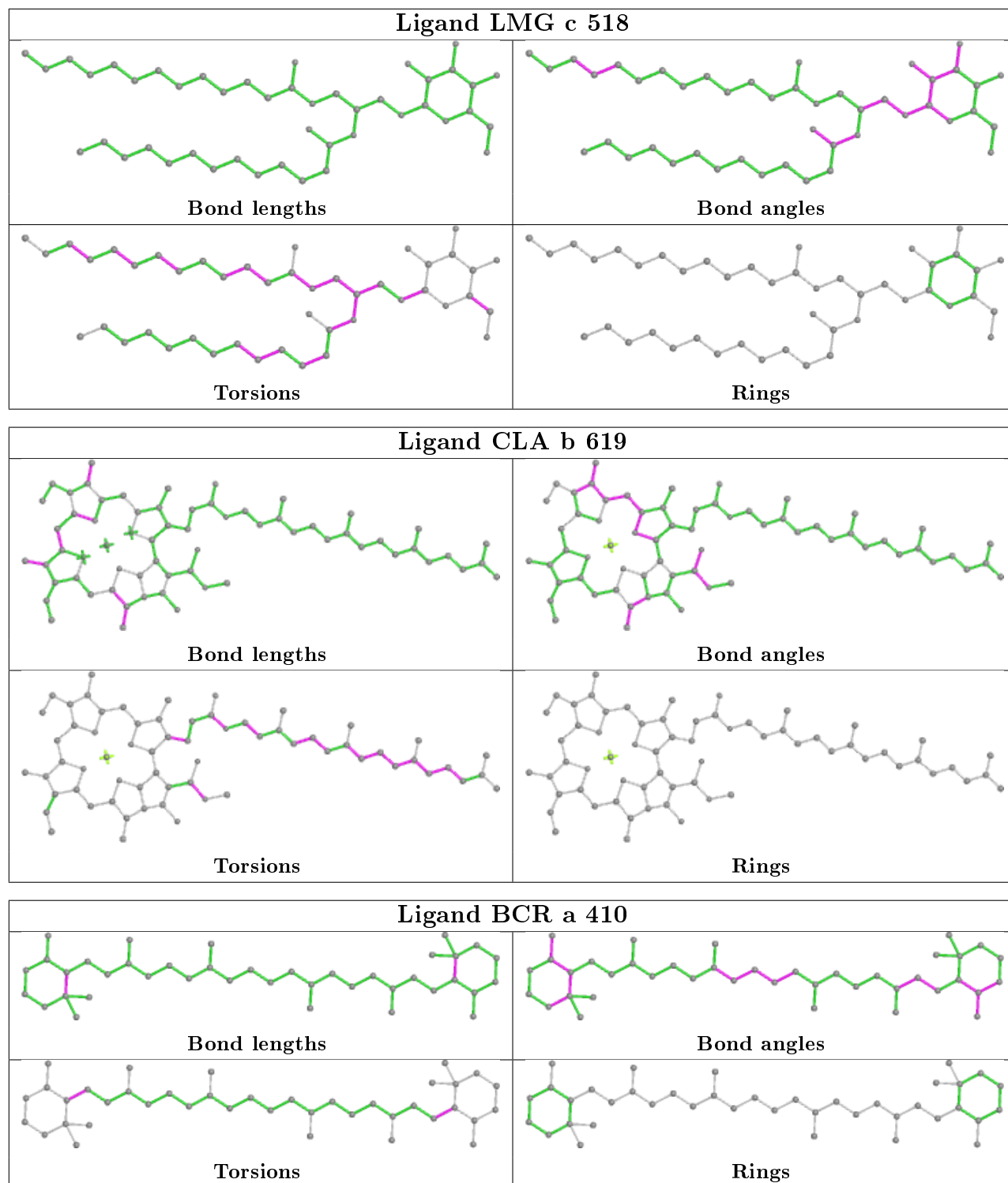


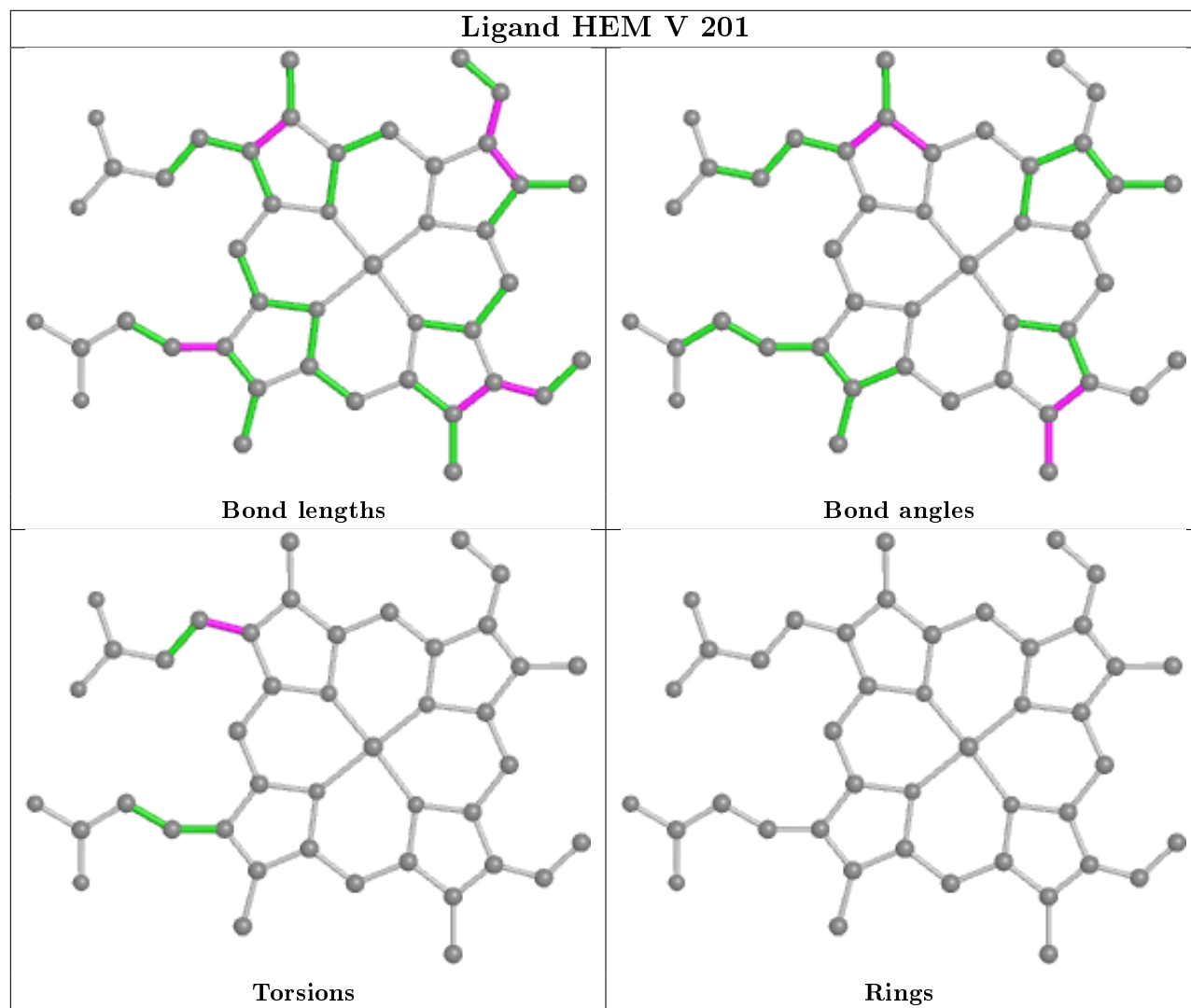
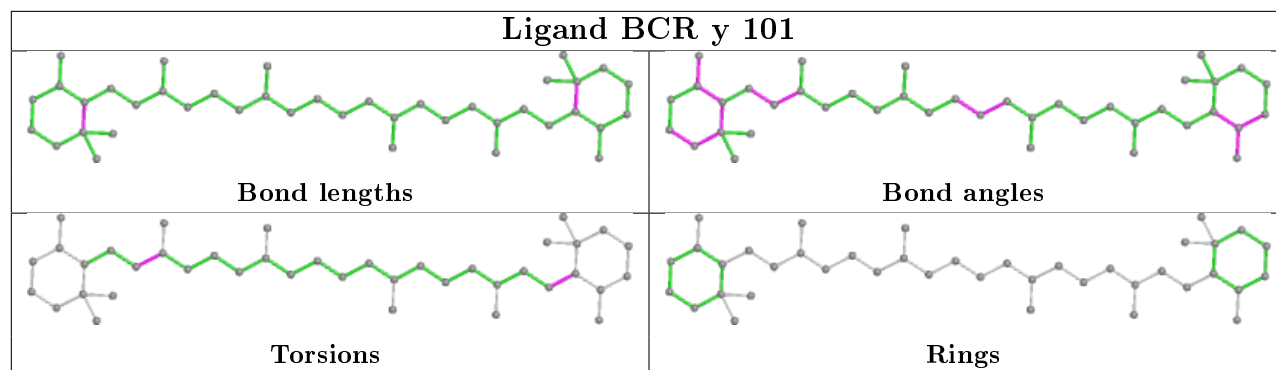
## Ligand DGD C 515



## Ligand CLA C 506

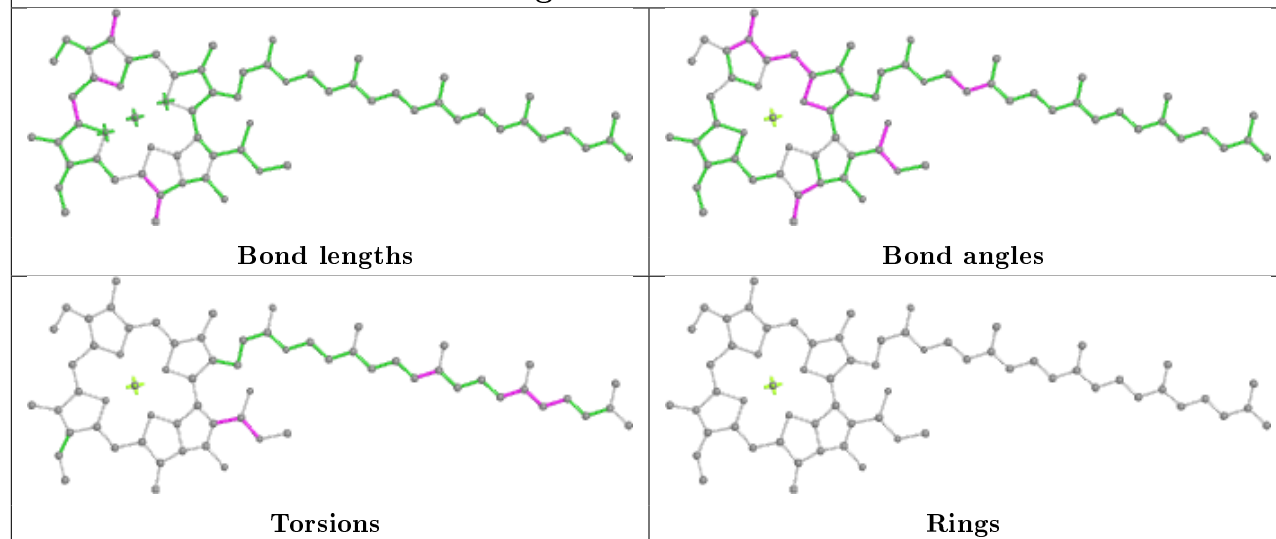




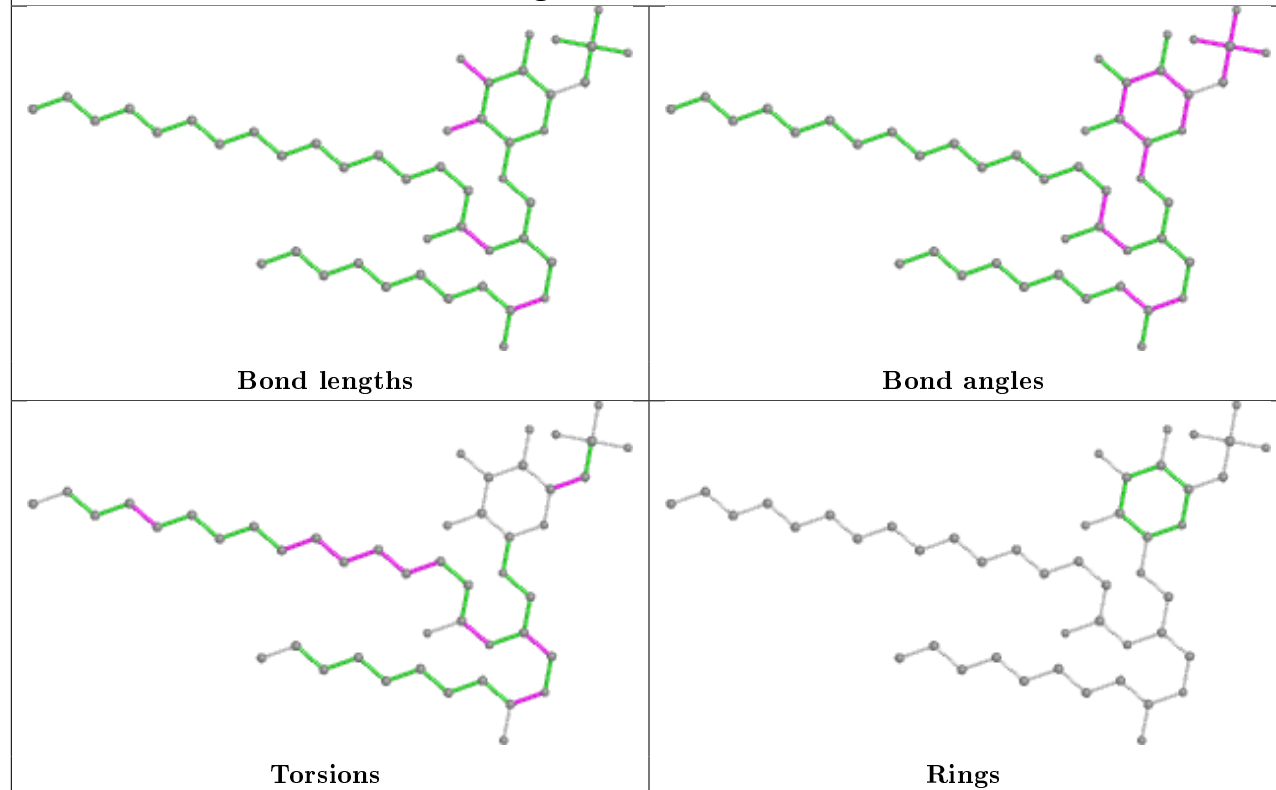




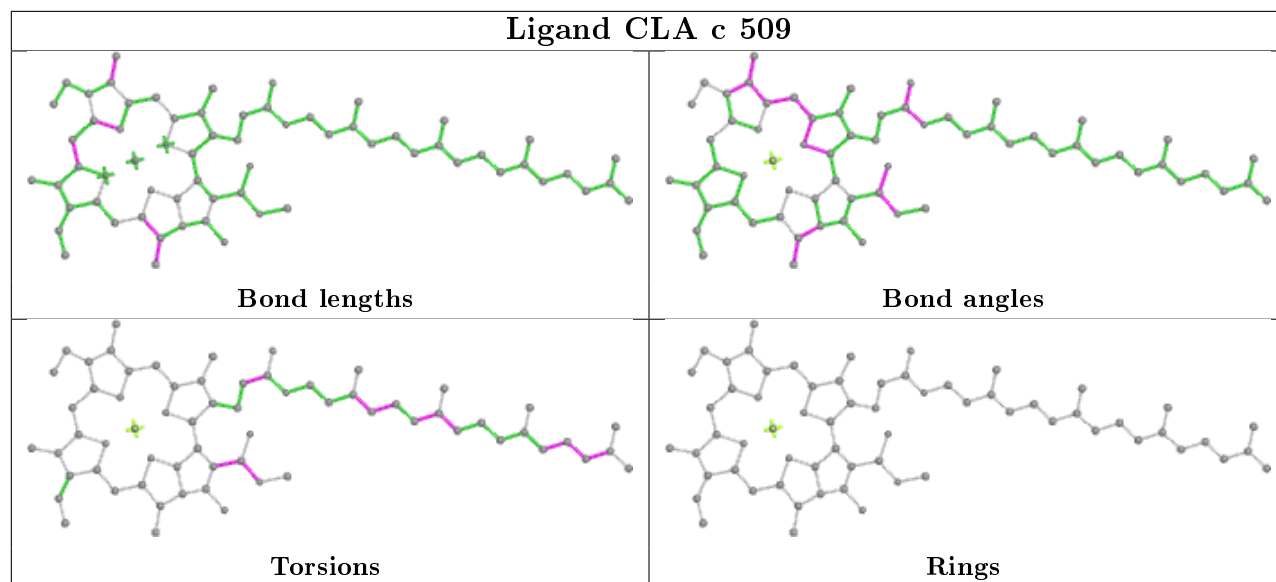
## Ligand CLA b 612



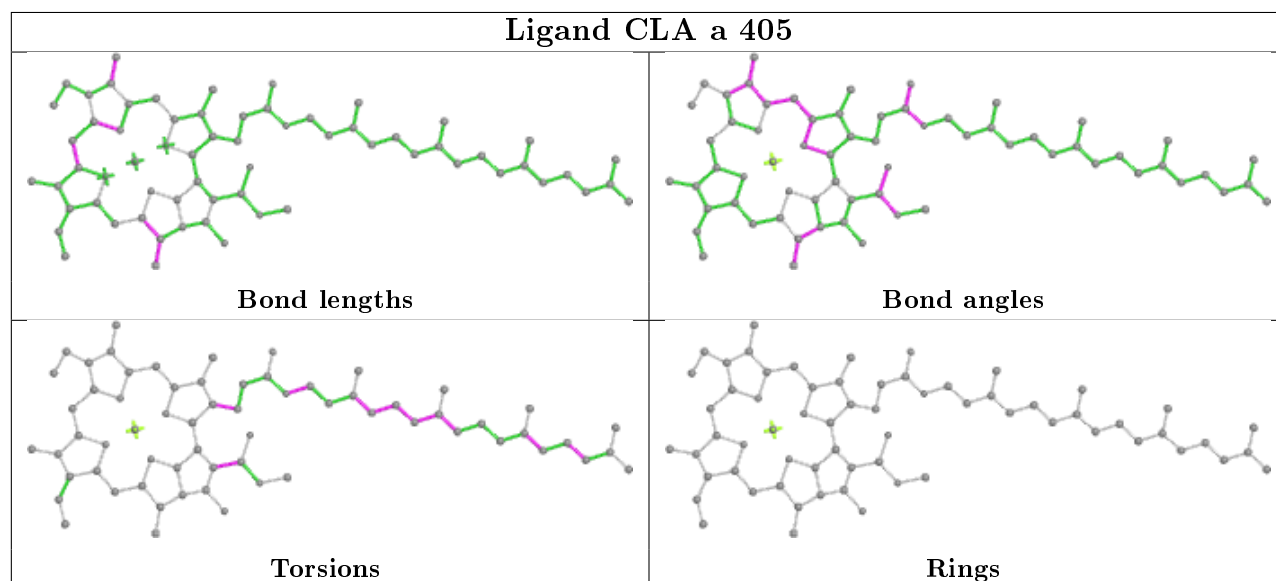
## Ligand SQD B 626



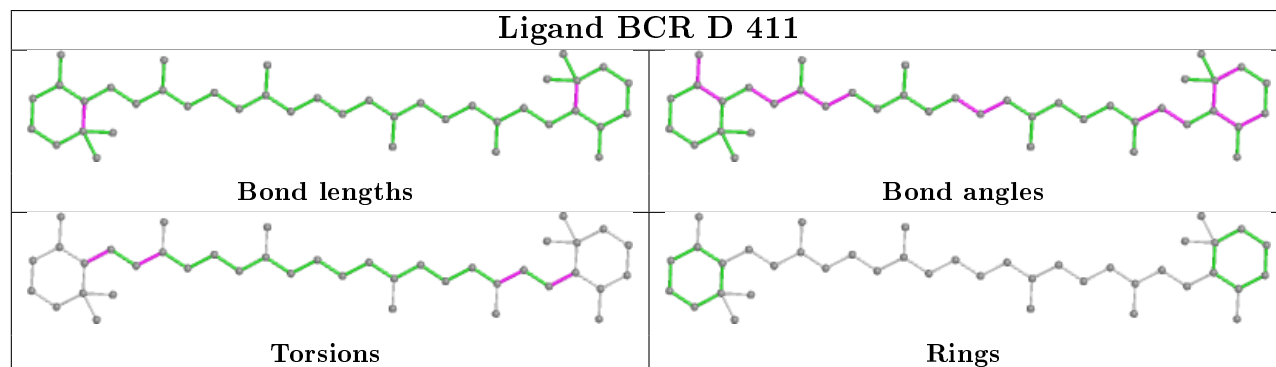
## Ligand CLA c 509



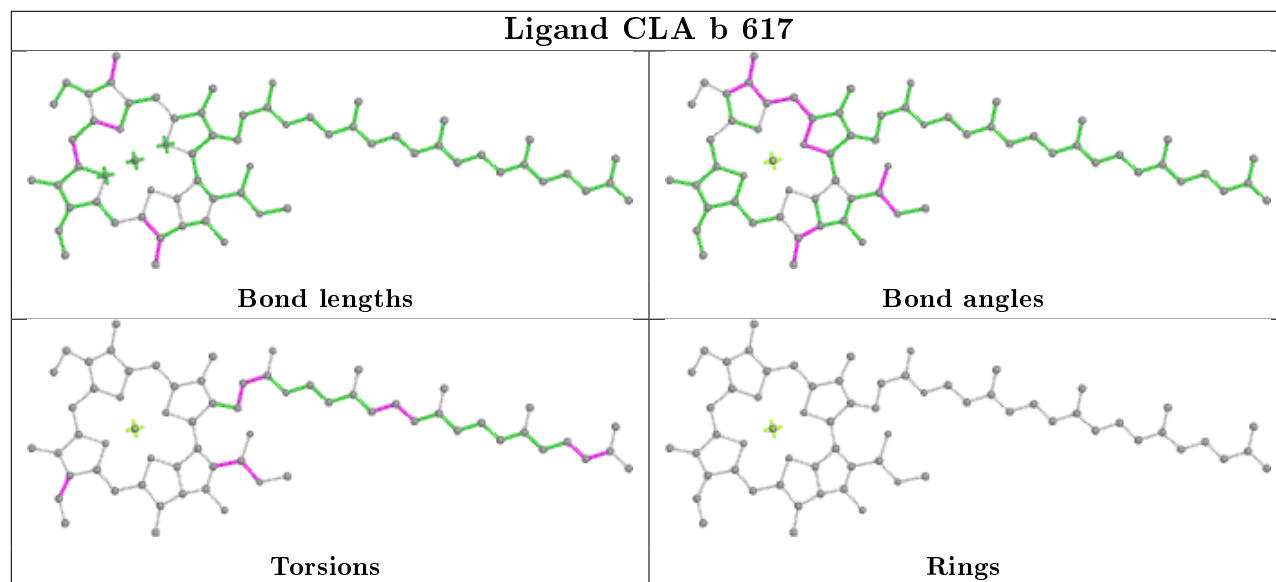
## Ligand CLA a 405



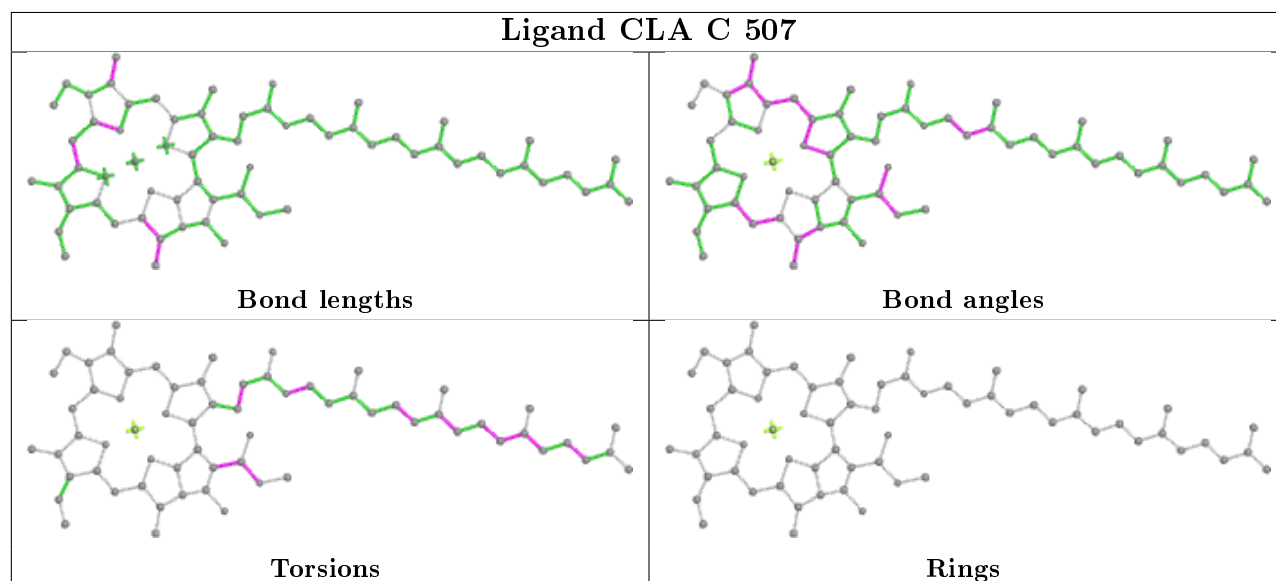
## Ligand BCR D 411



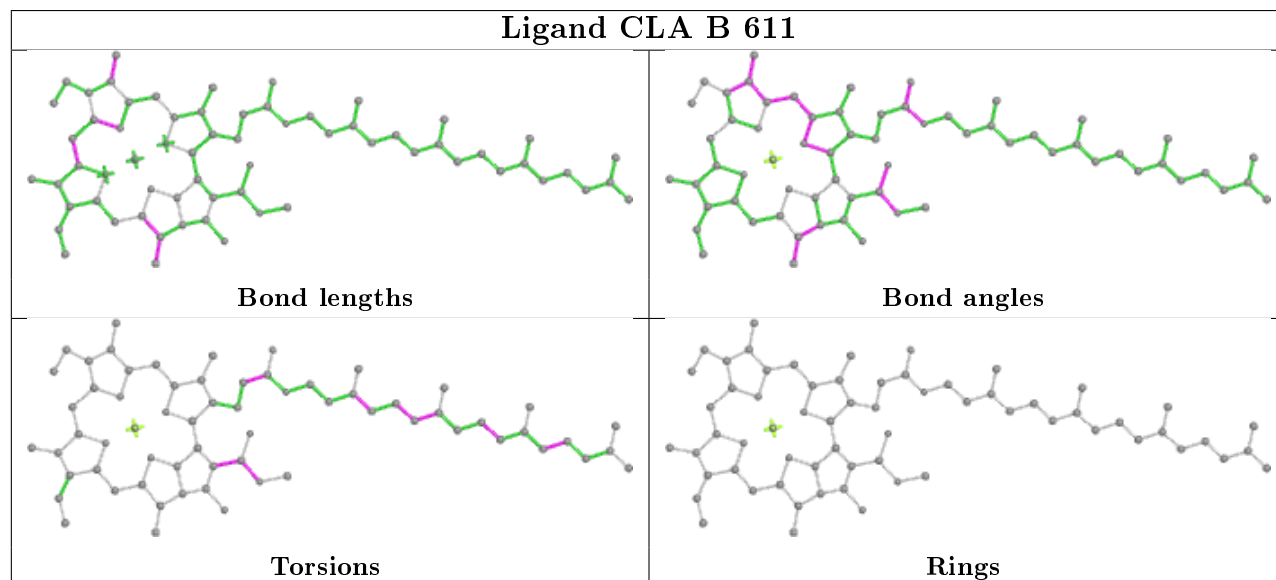
## Ligand CLA b 617



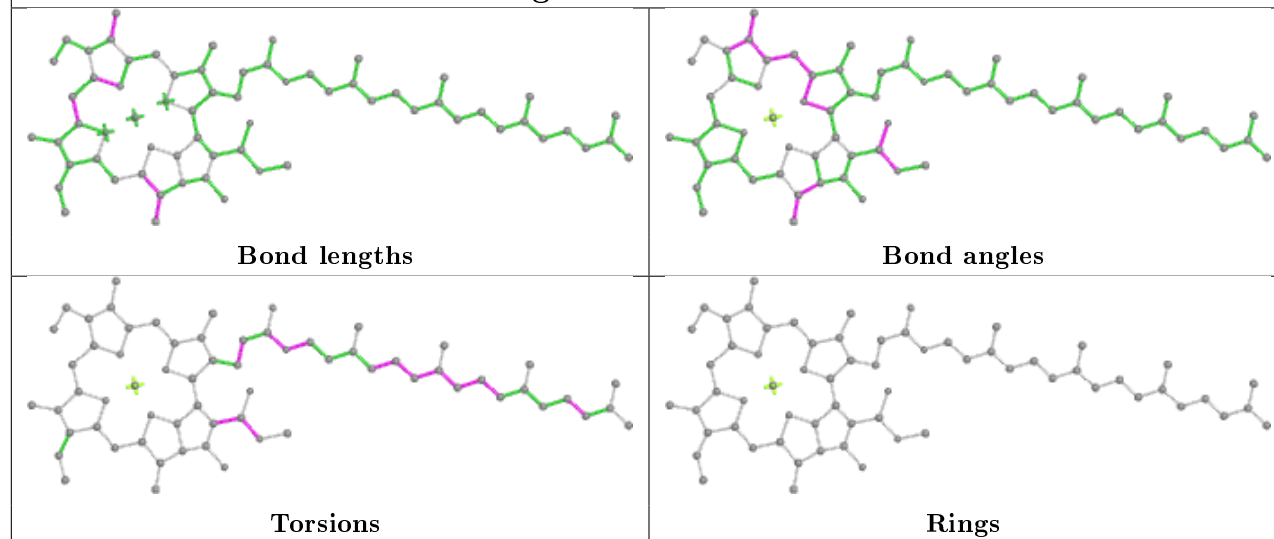
## Ligand CLA C 507



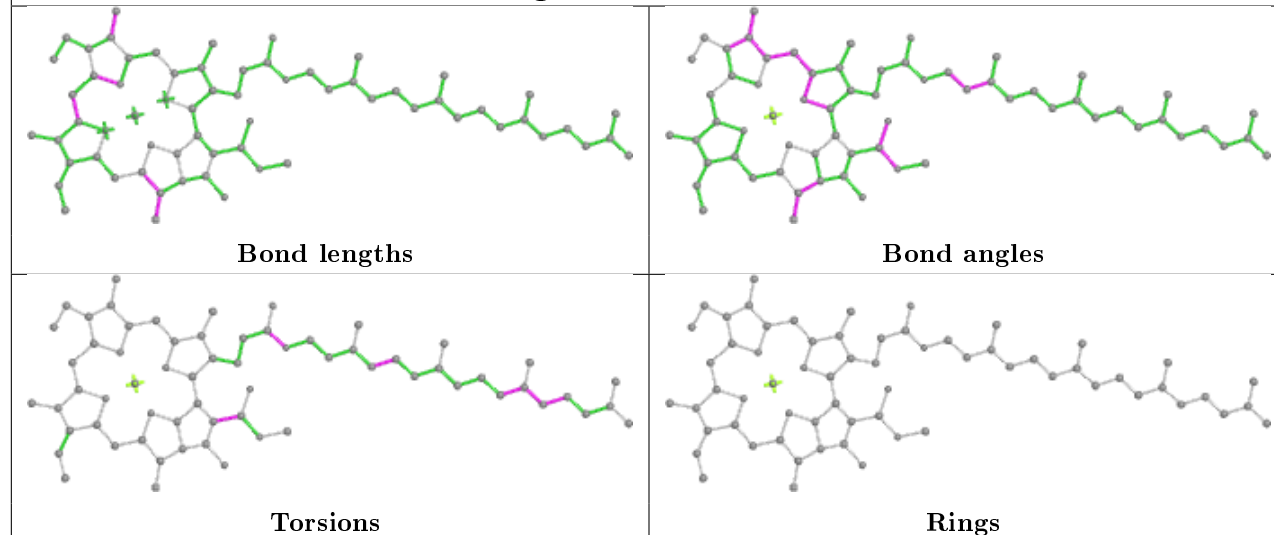
## Ligand CLA B 611



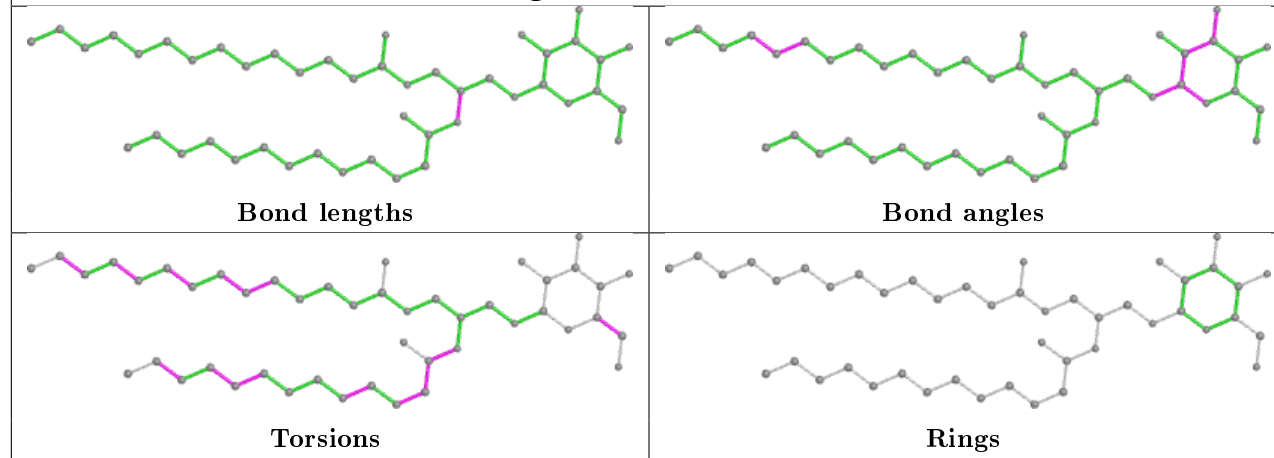
## Ligand CLA C 508



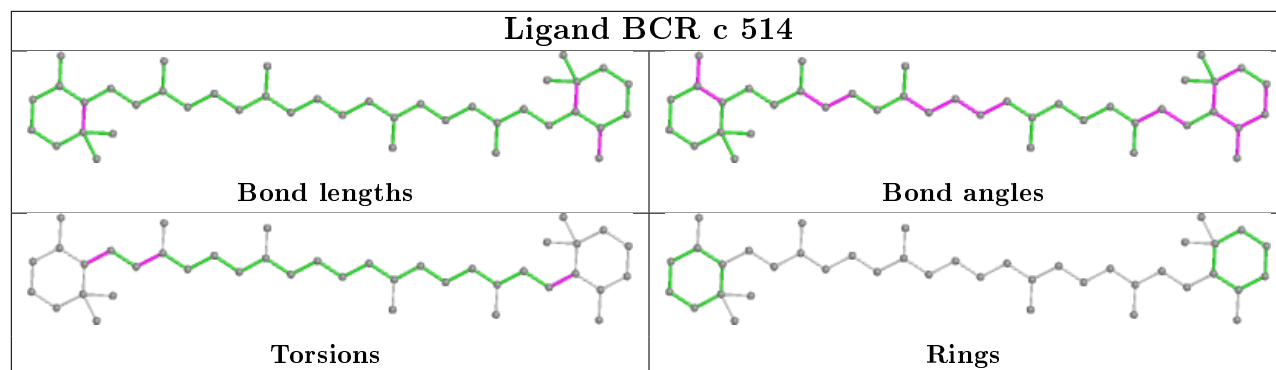
## Ligand CLA C 502



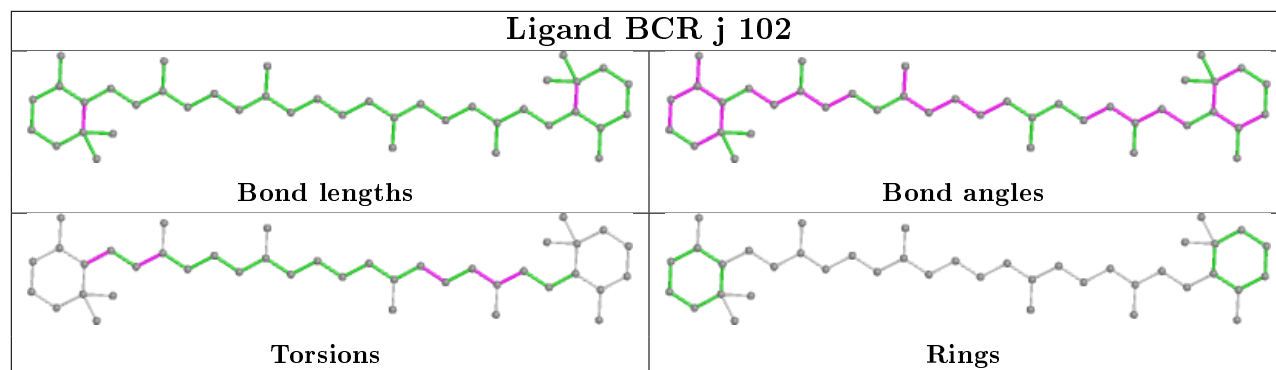
## Ligand LMG D 412



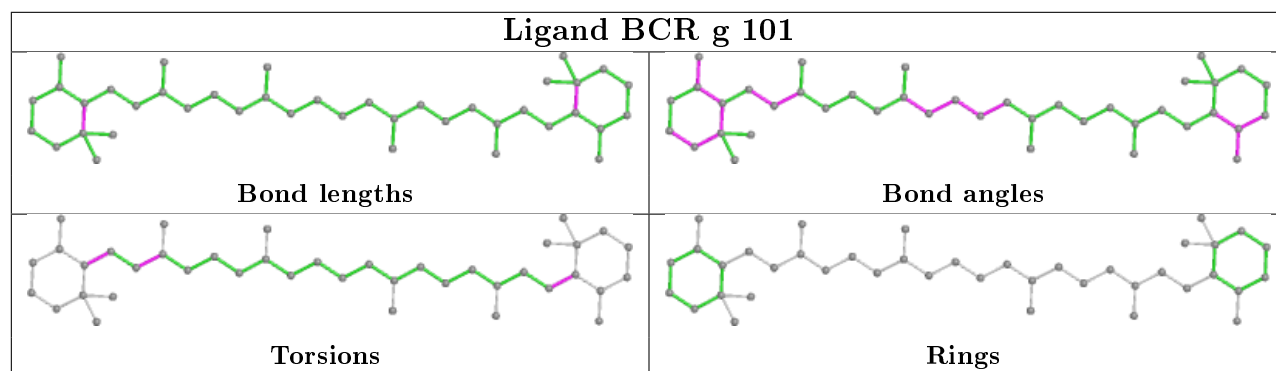
## Ligand BCR c 514



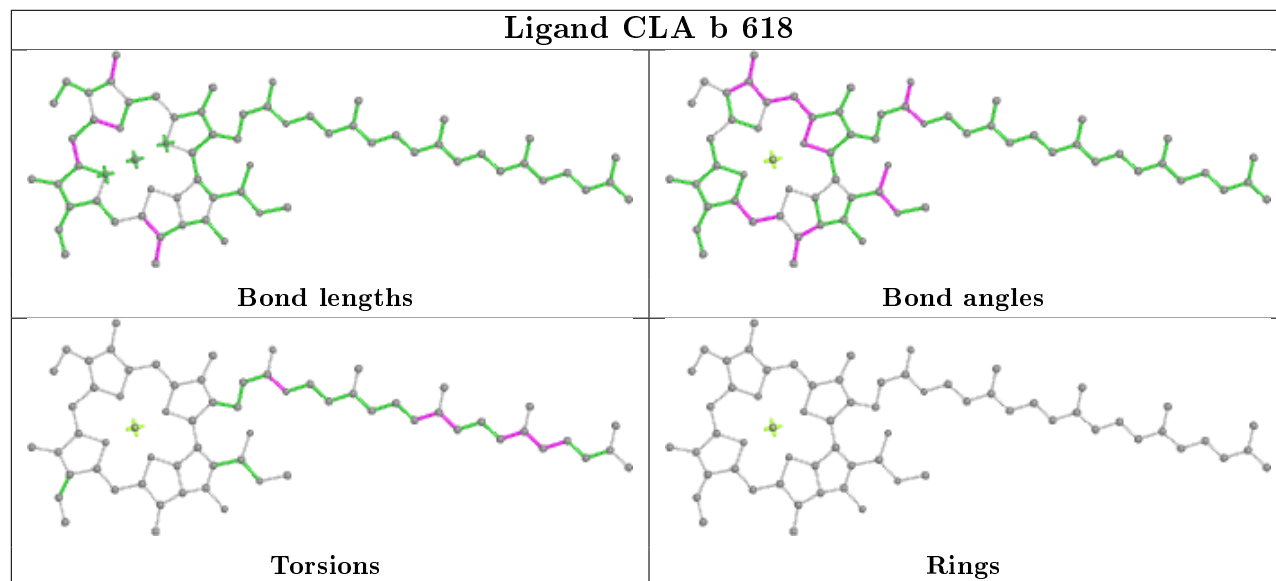
## Ligand BCR j 102

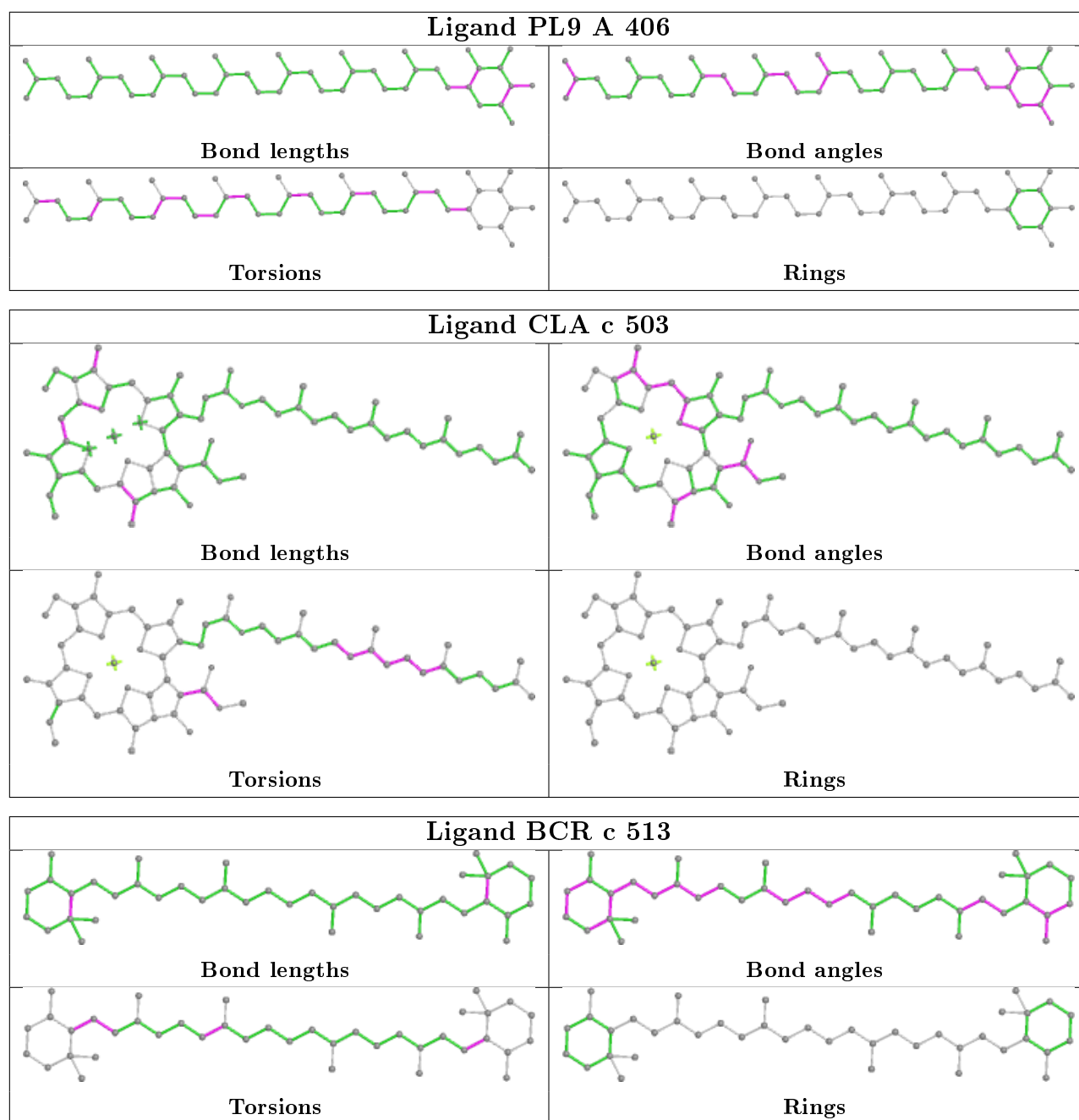


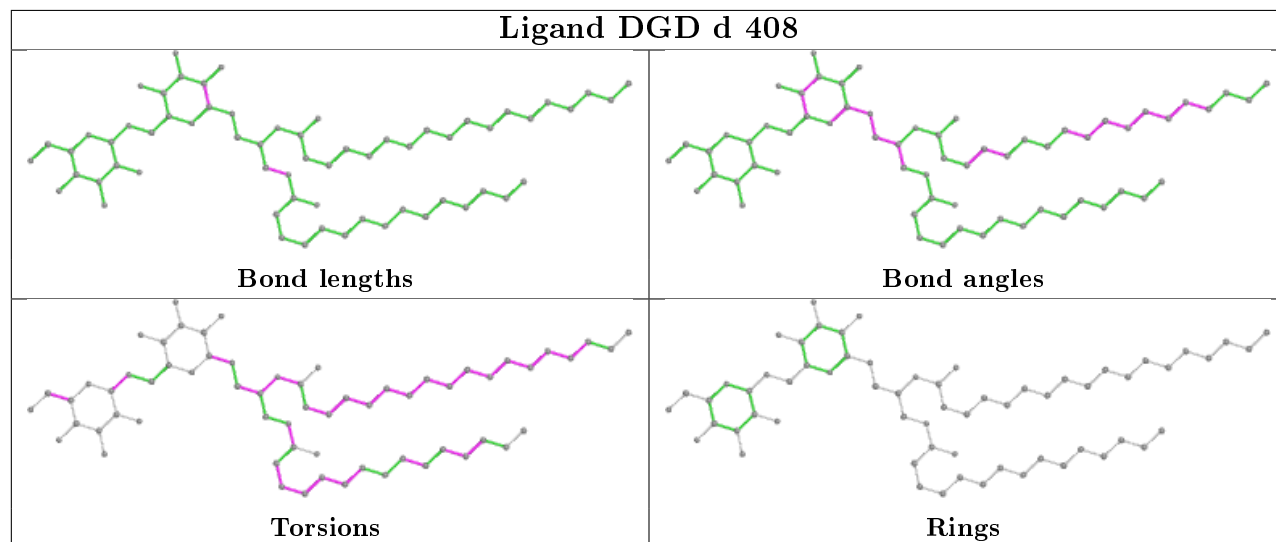
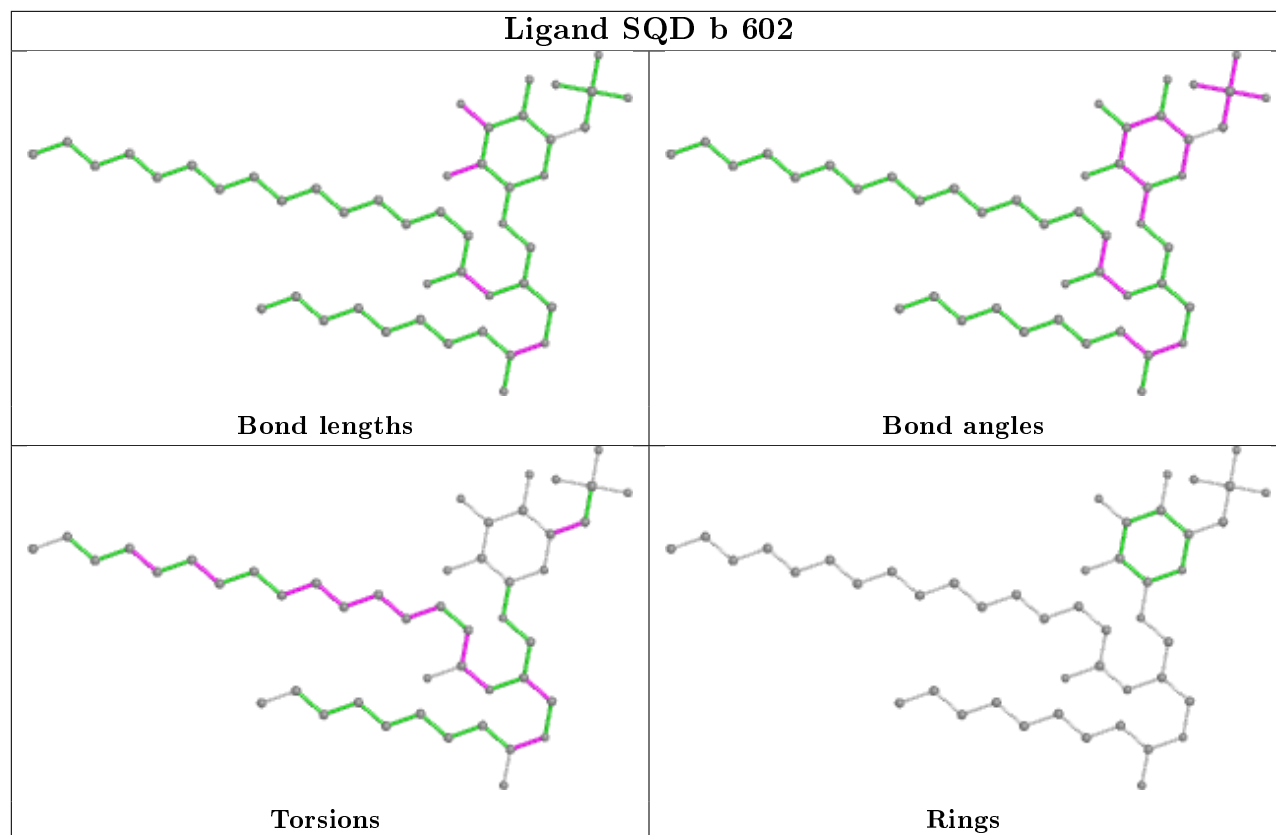
## Ligand BCR g 101



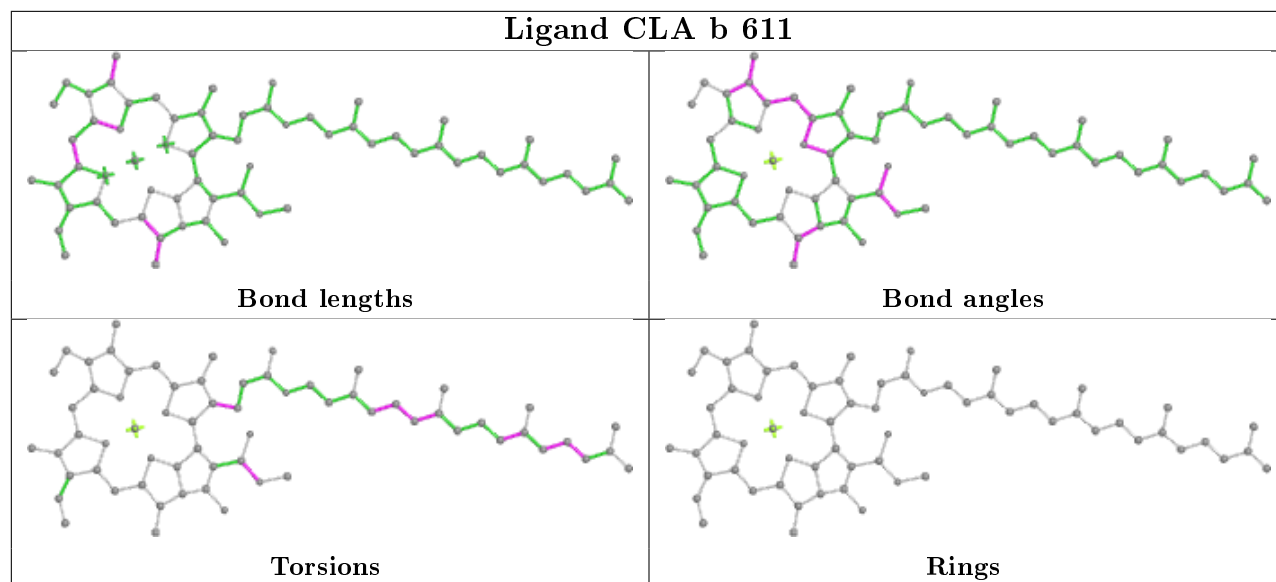
## Ligand CLA b 618



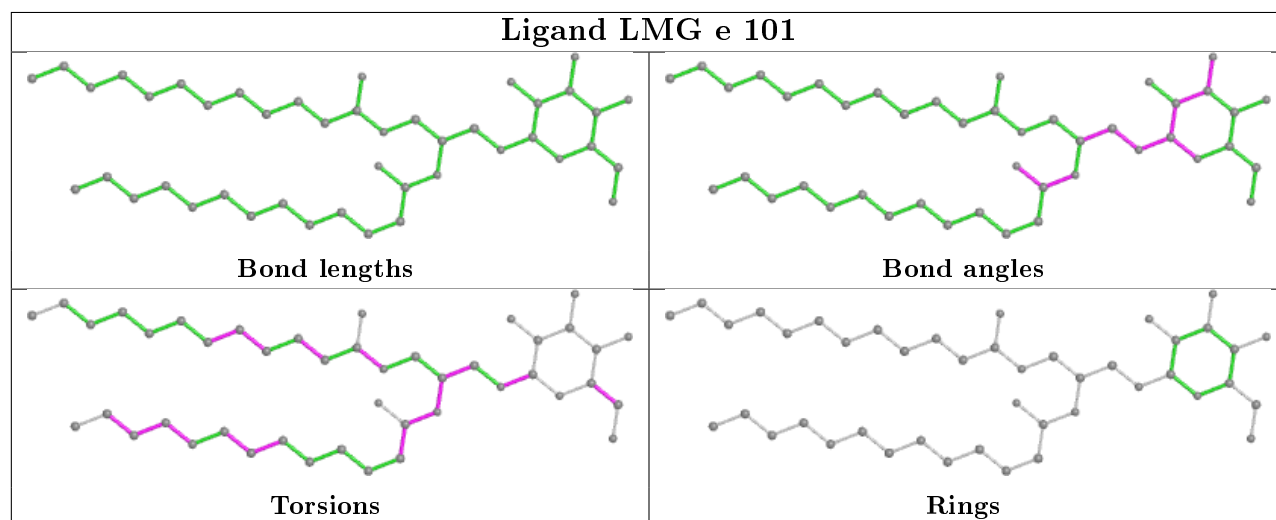




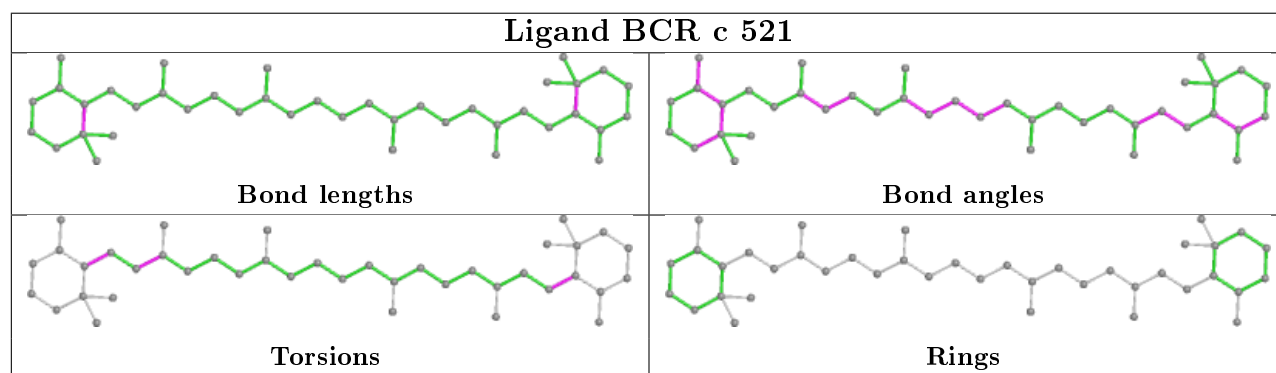
## Ligand CLA b 611



## Ligand LMG e 101

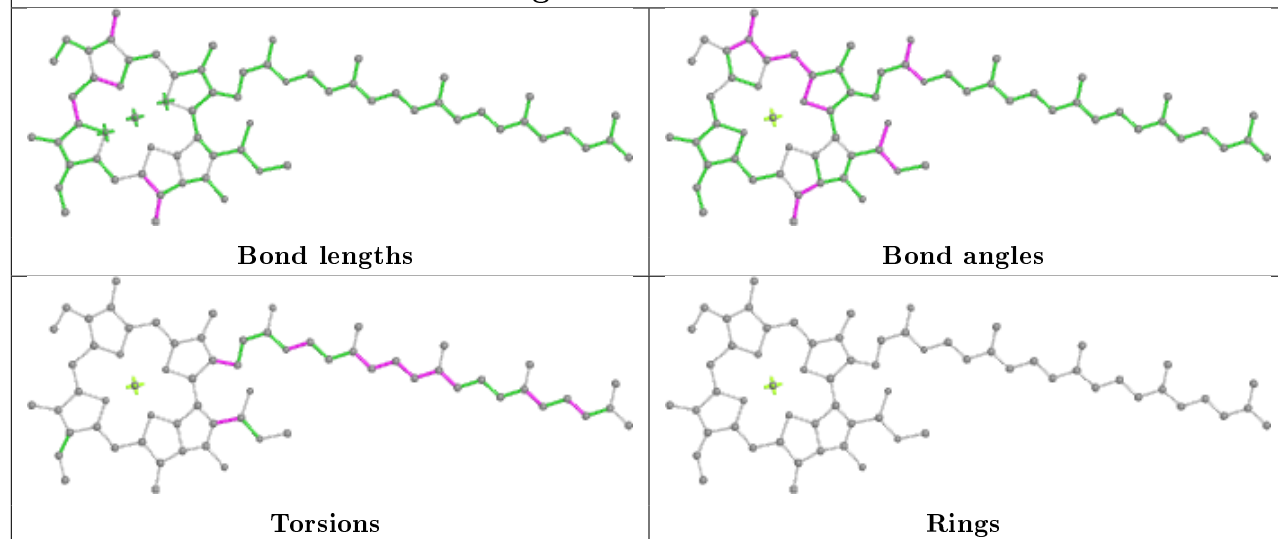


## Ligand BCR c 521

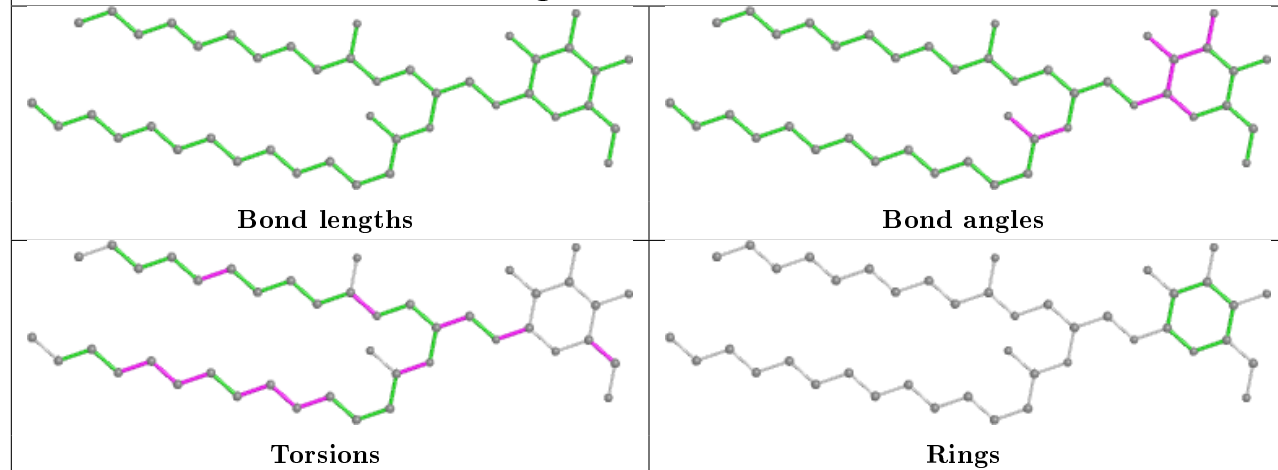




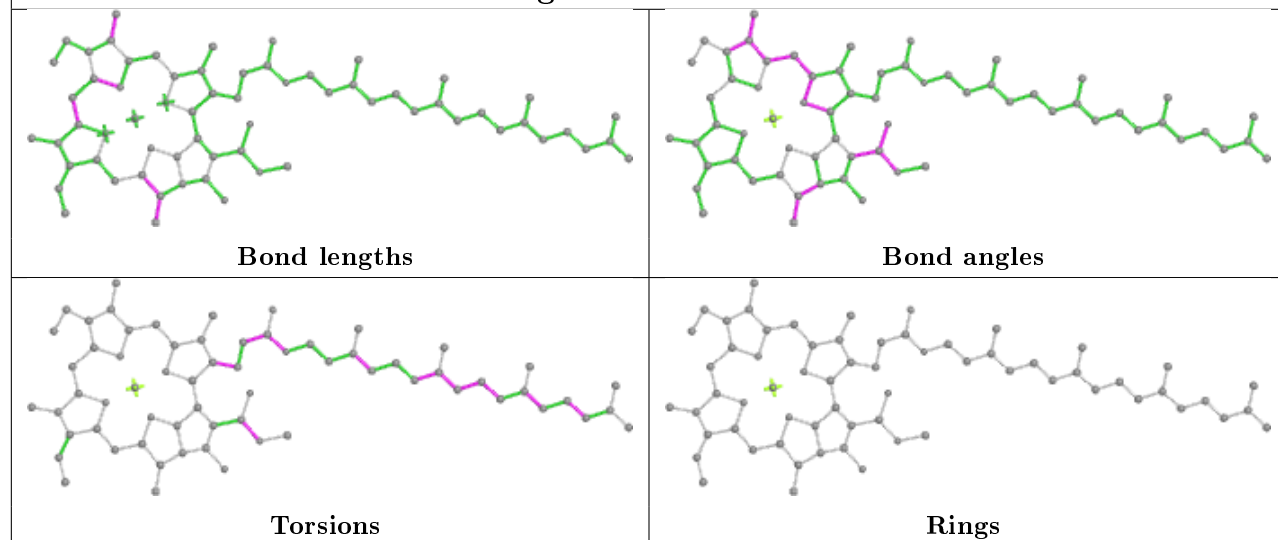
## Ligand CLA A 403



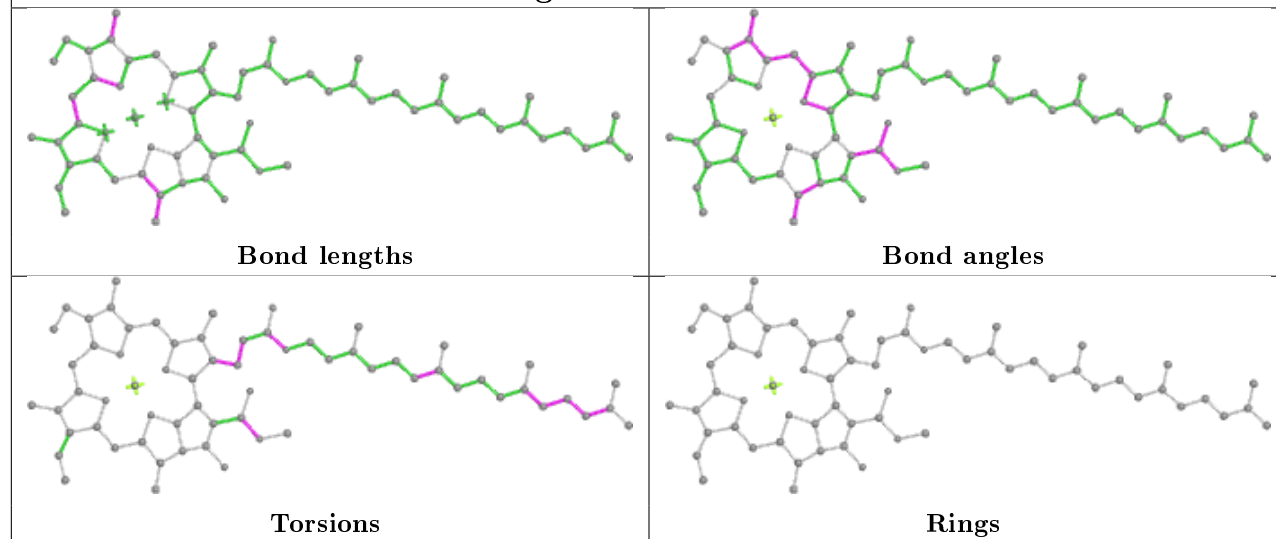
## Ligand LMG I 101



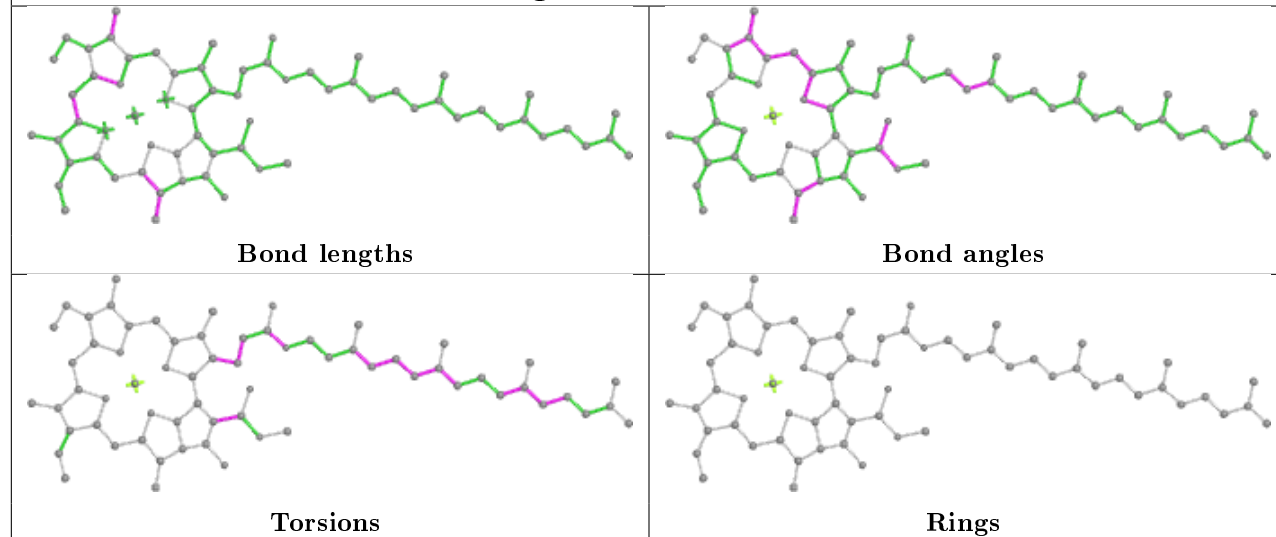
## Ligand CLA c 504

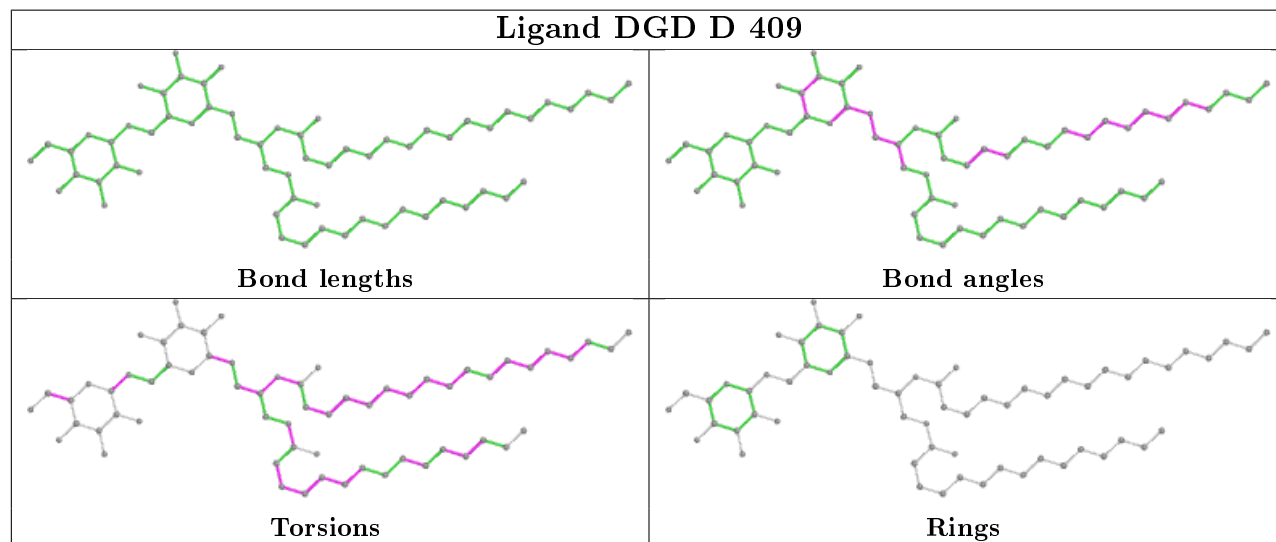
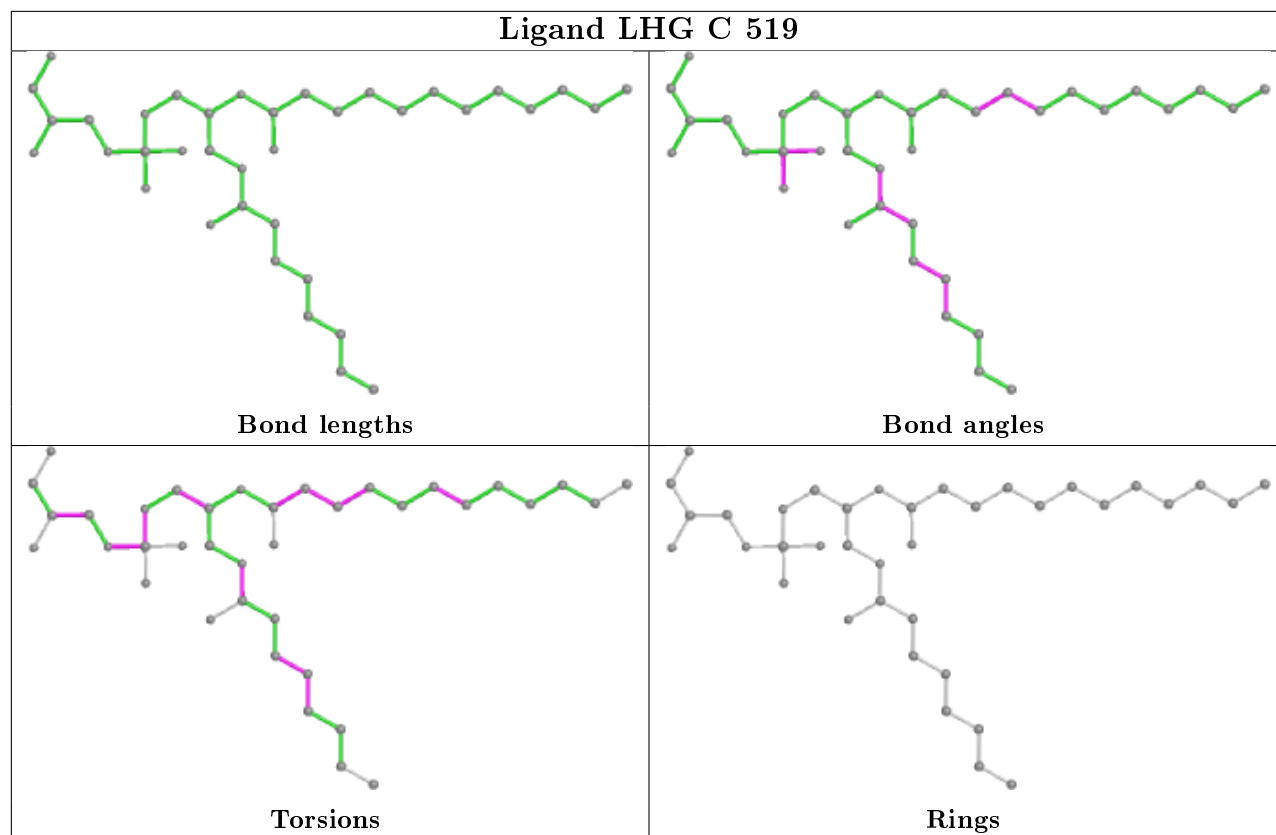


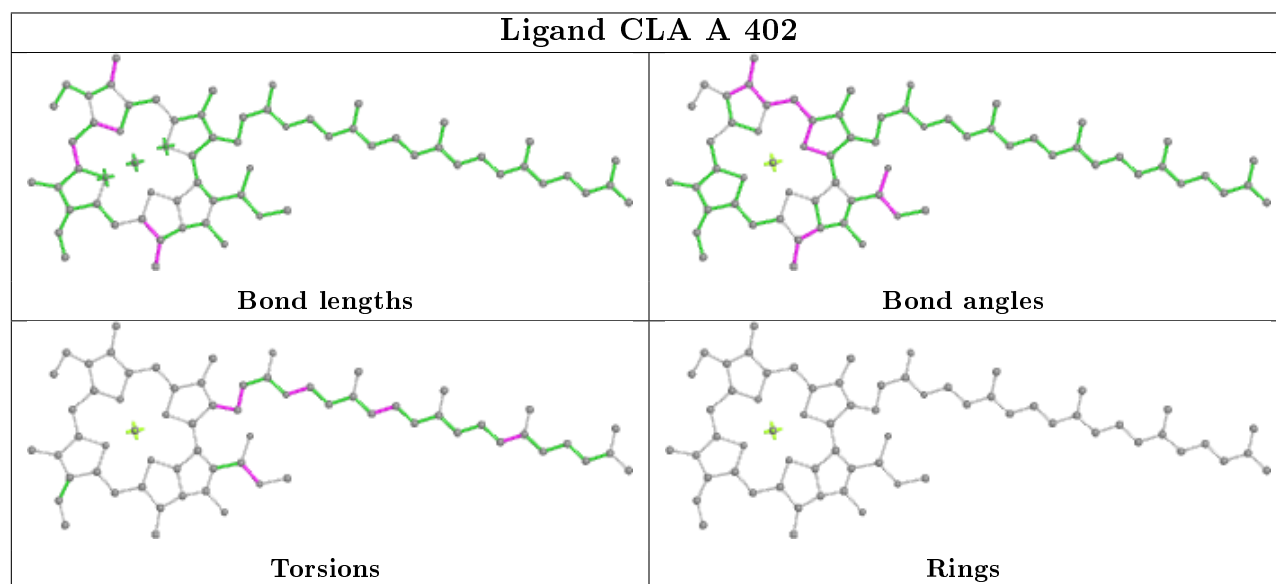
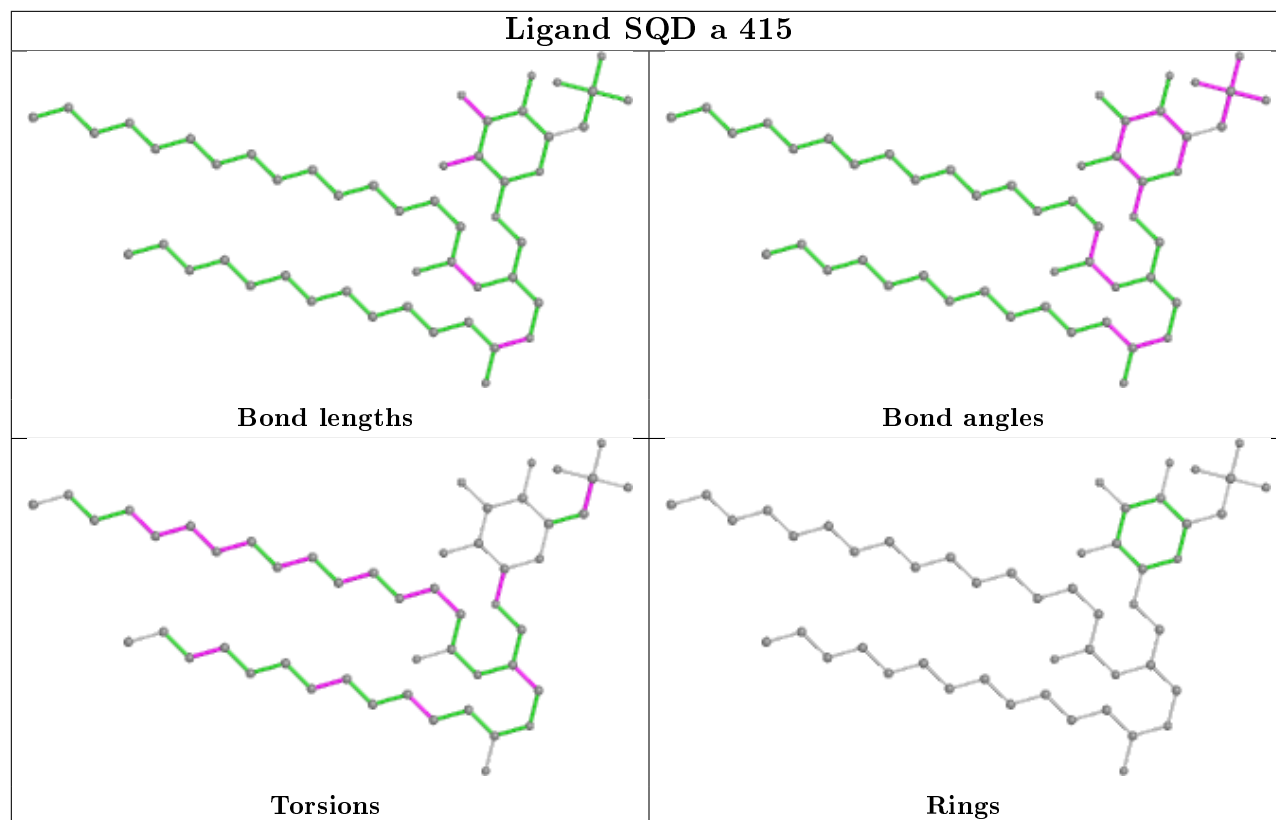
## Ligand CLA b 609

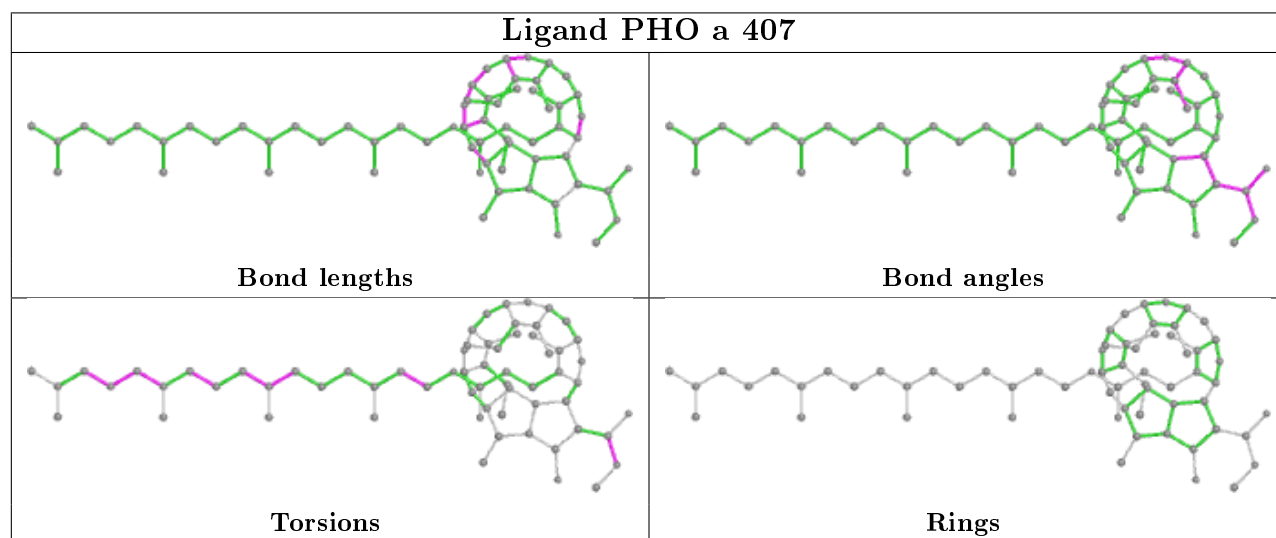
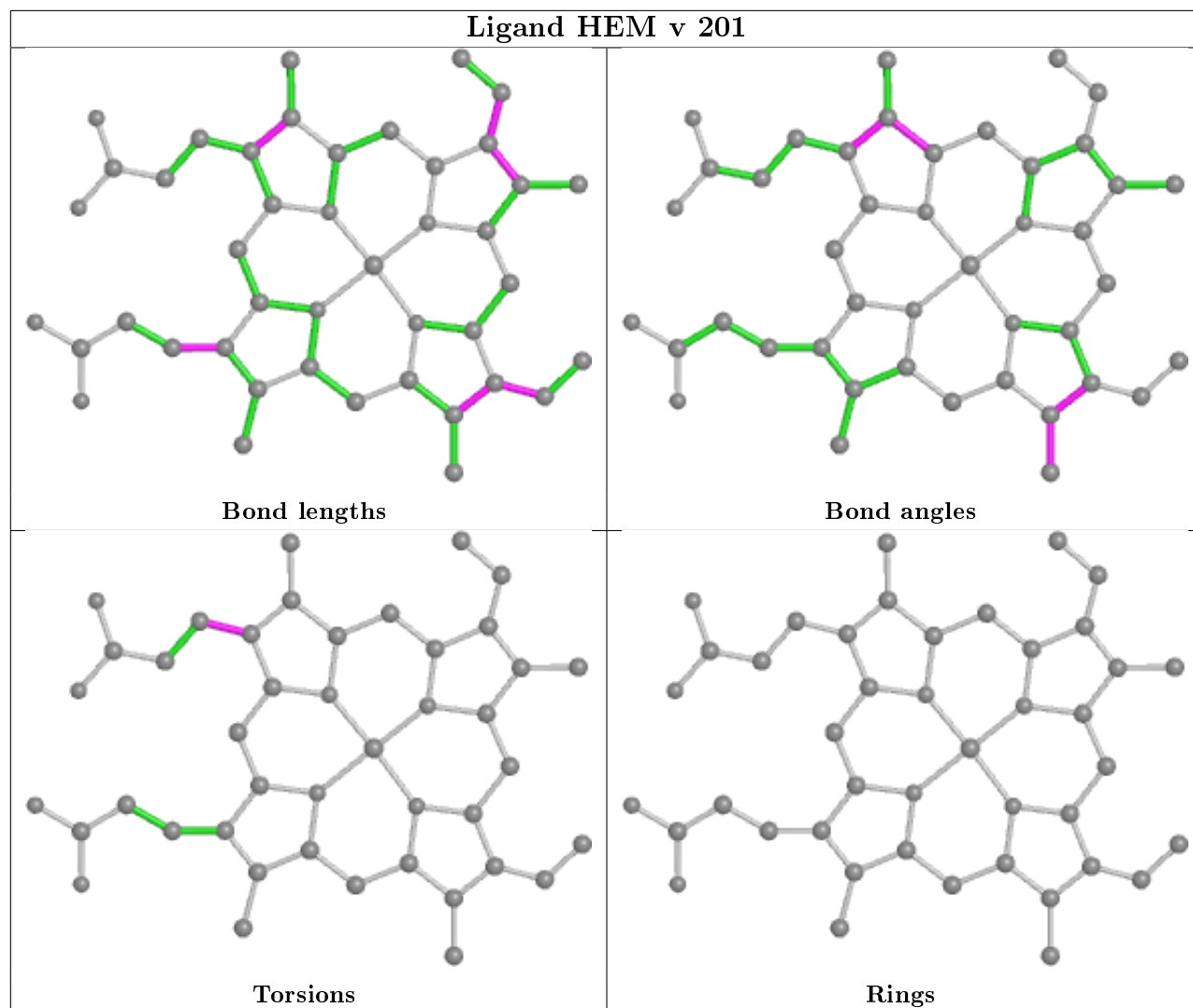


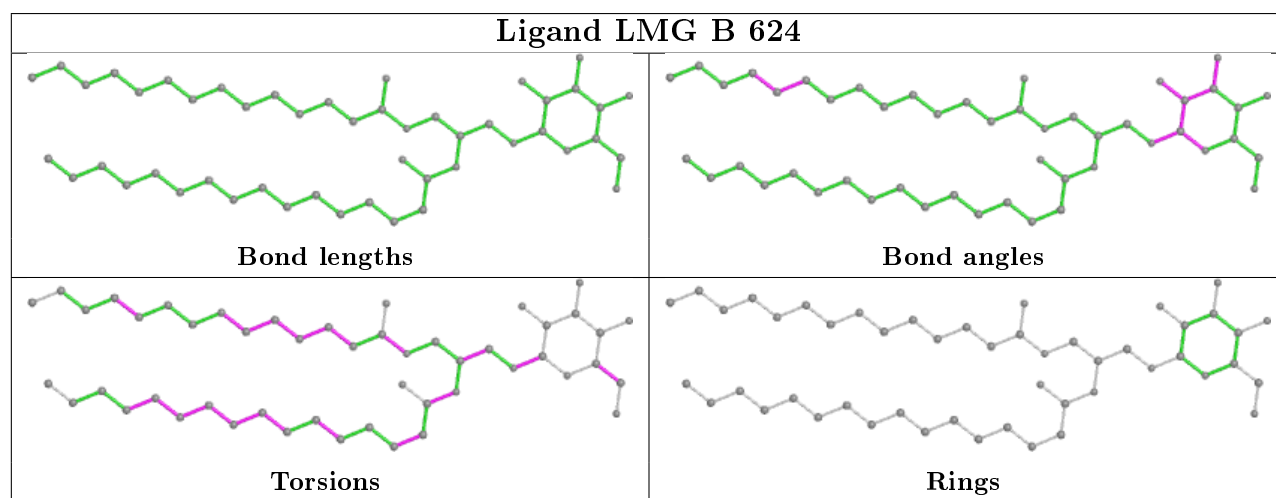
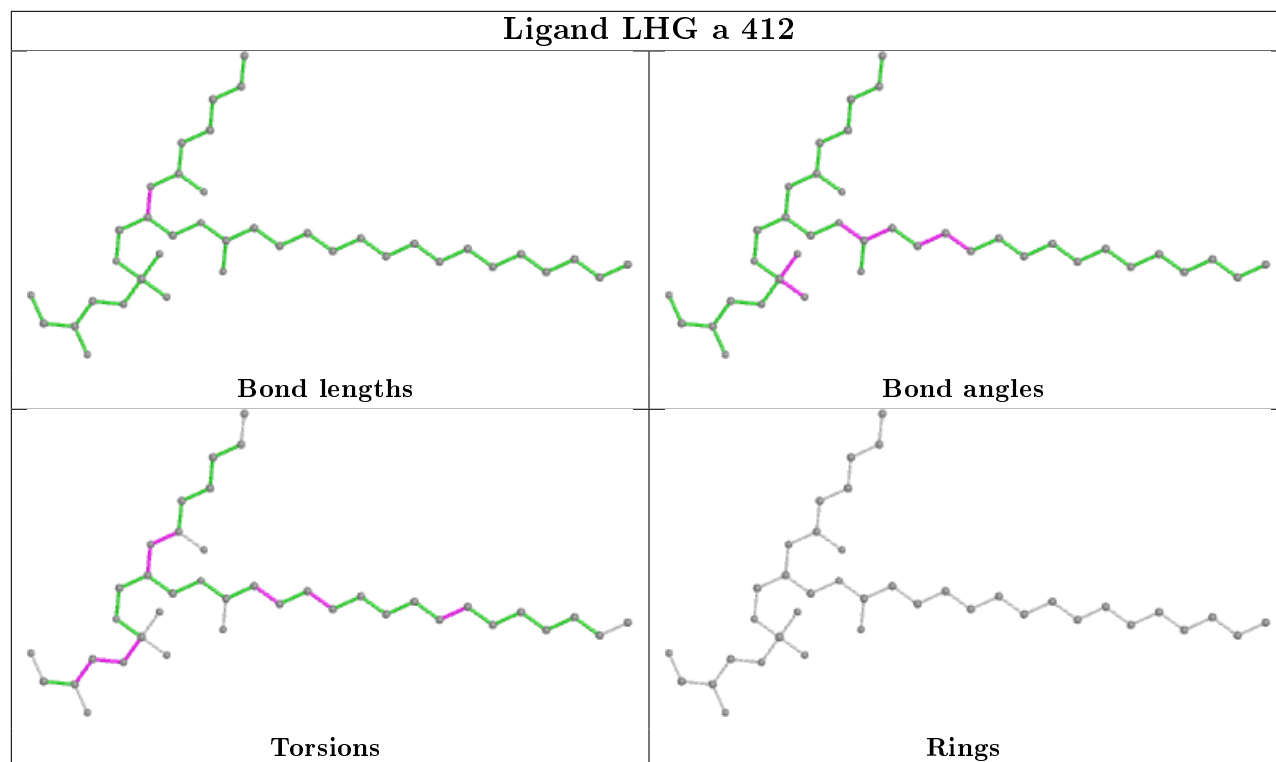
## Ligand CLA H 101



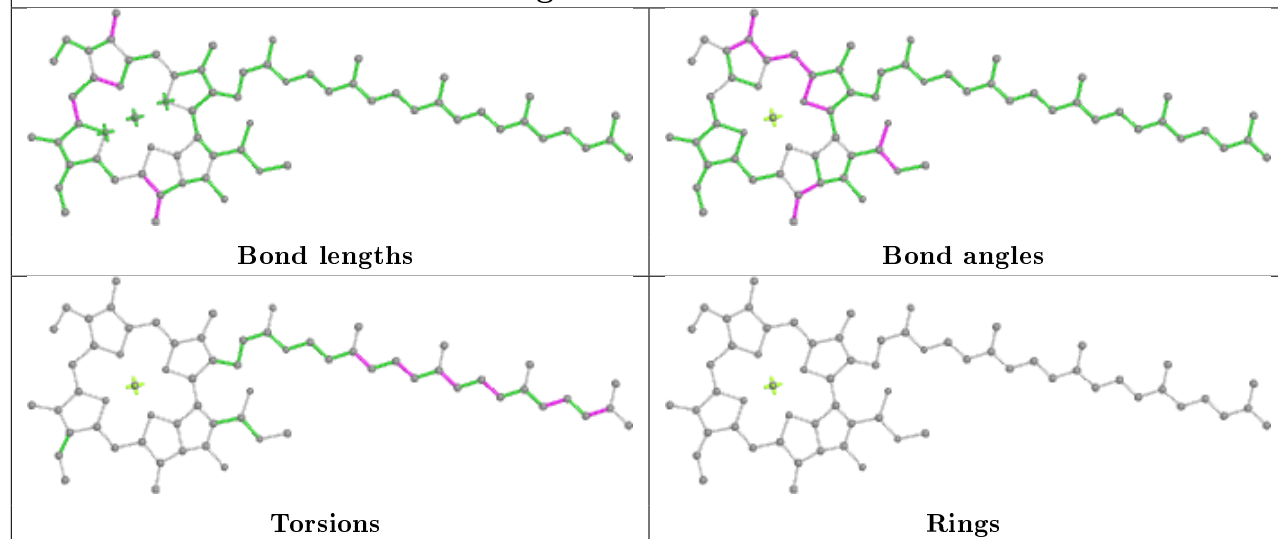




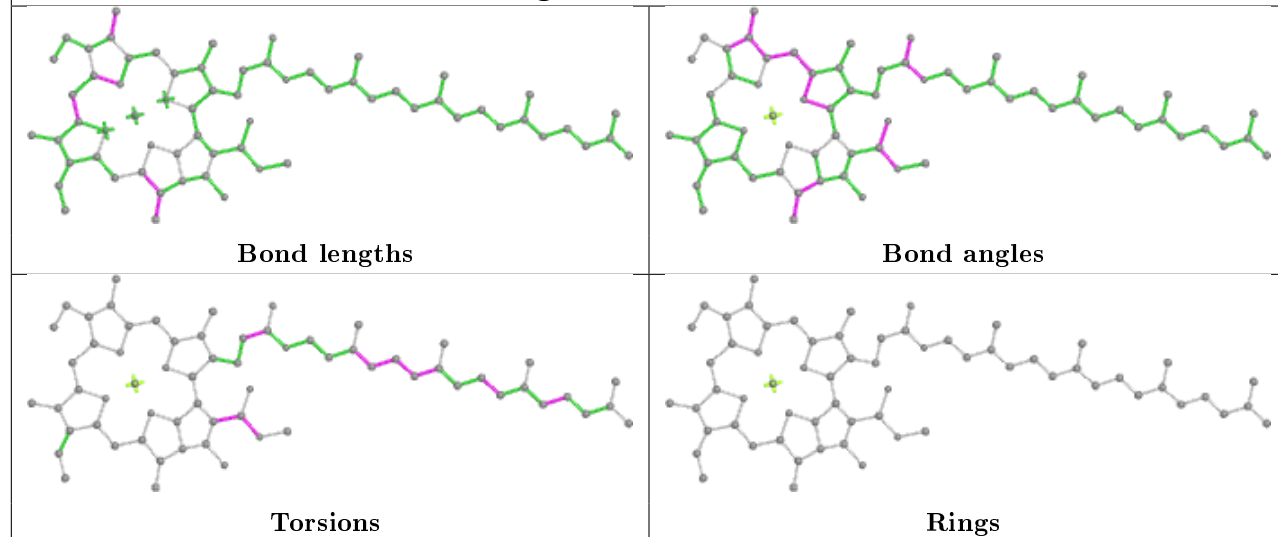




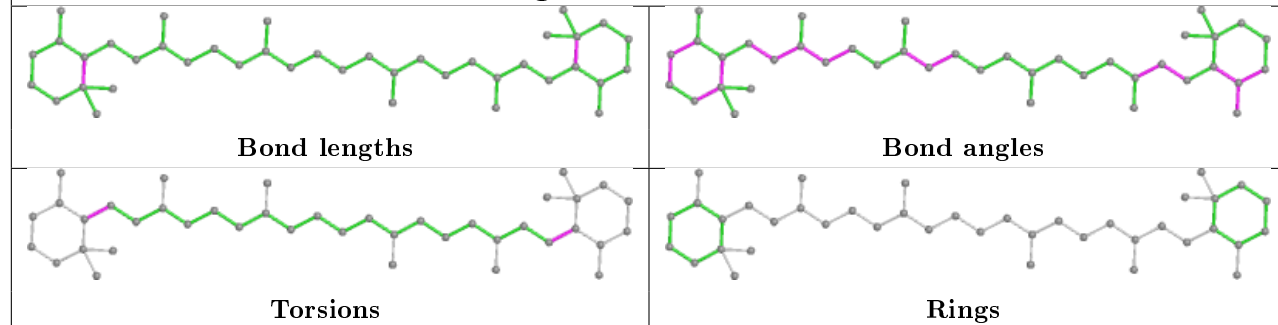
## Ligand CLA a 408

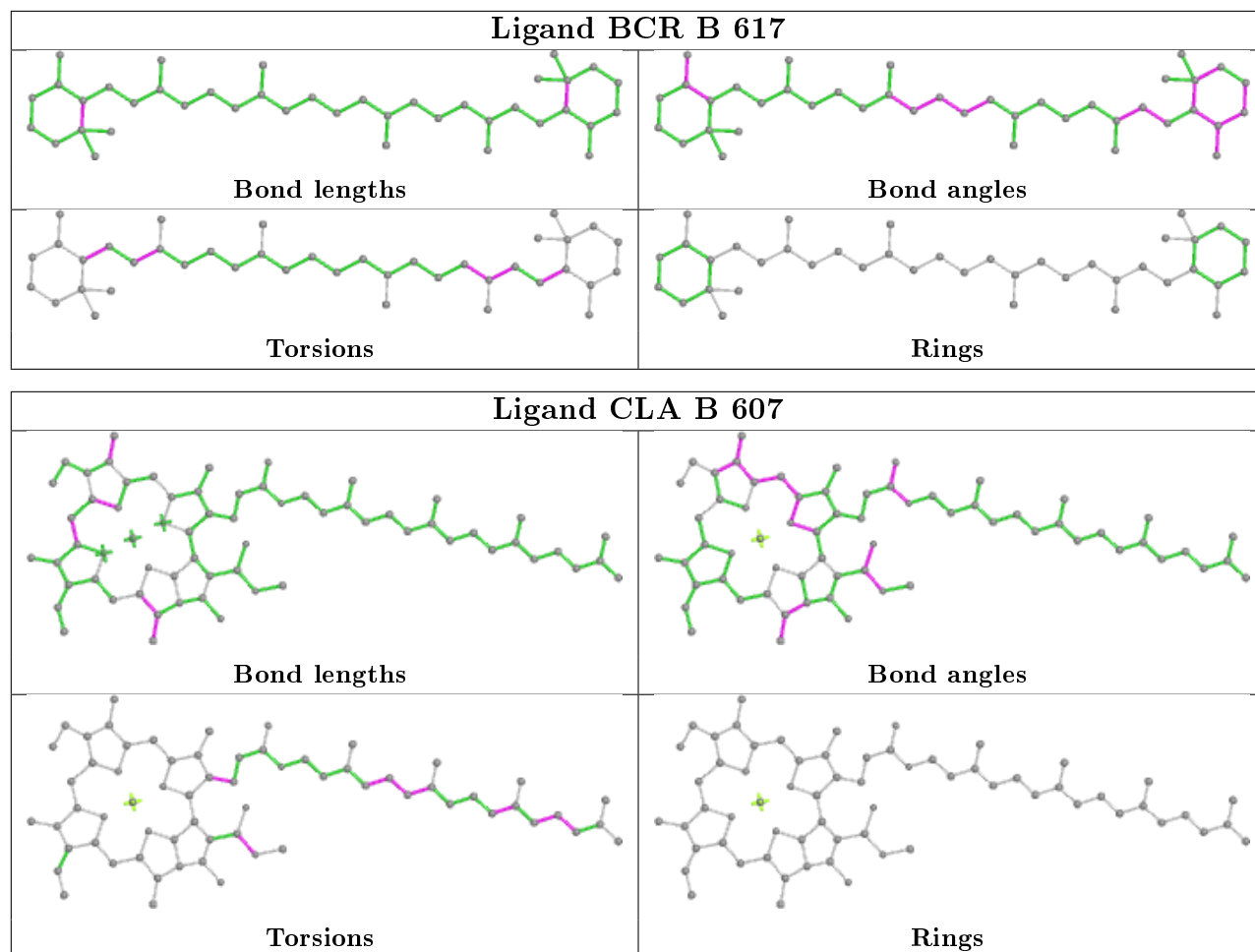


## Ligand CLA b 615

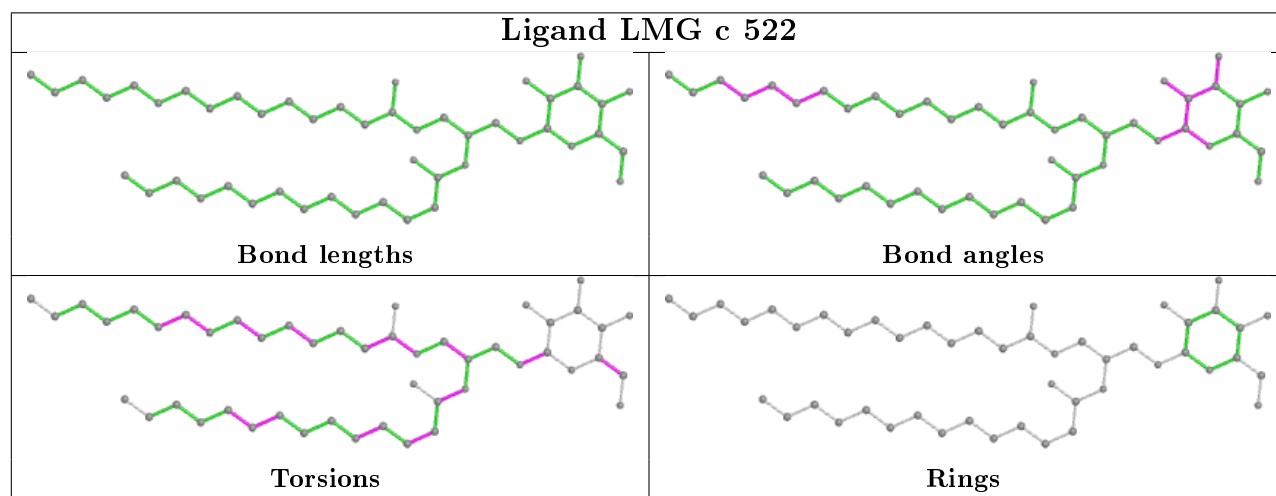
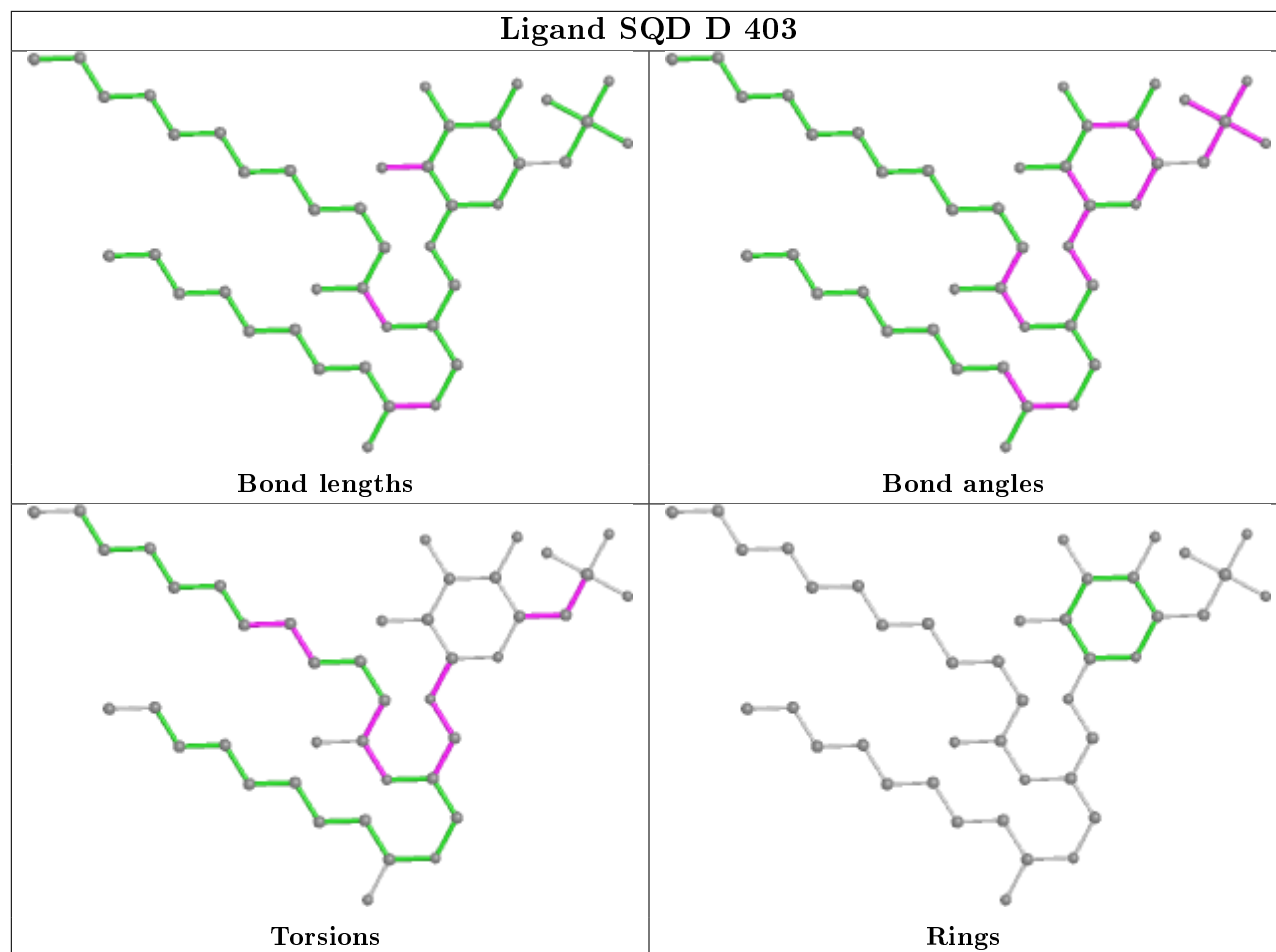


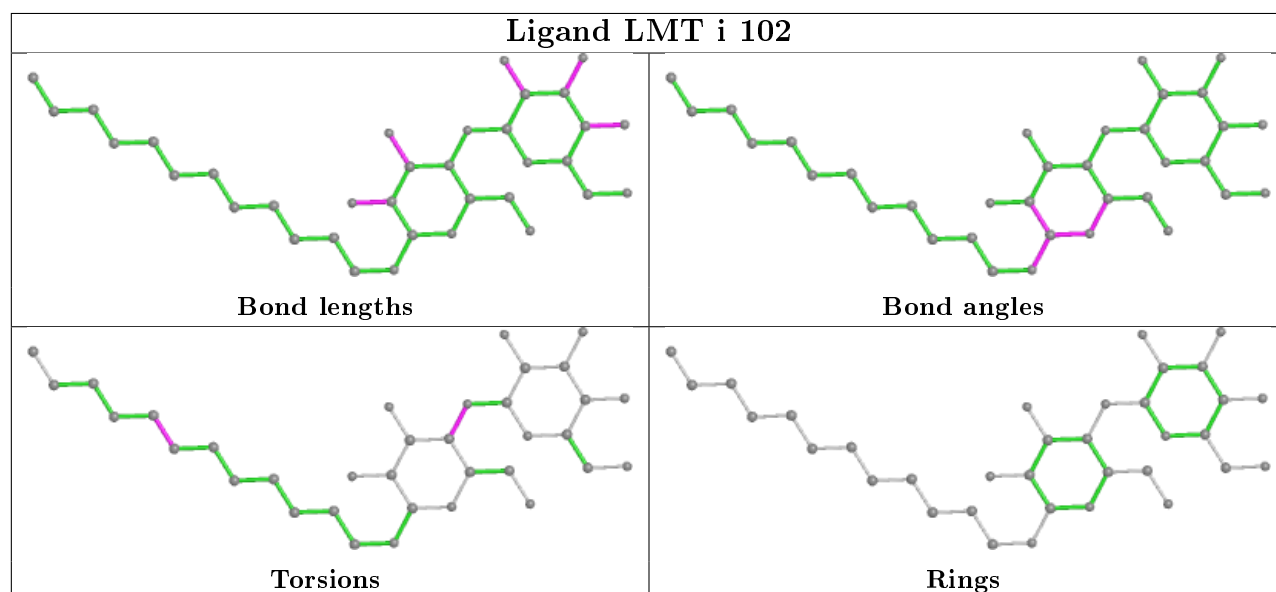
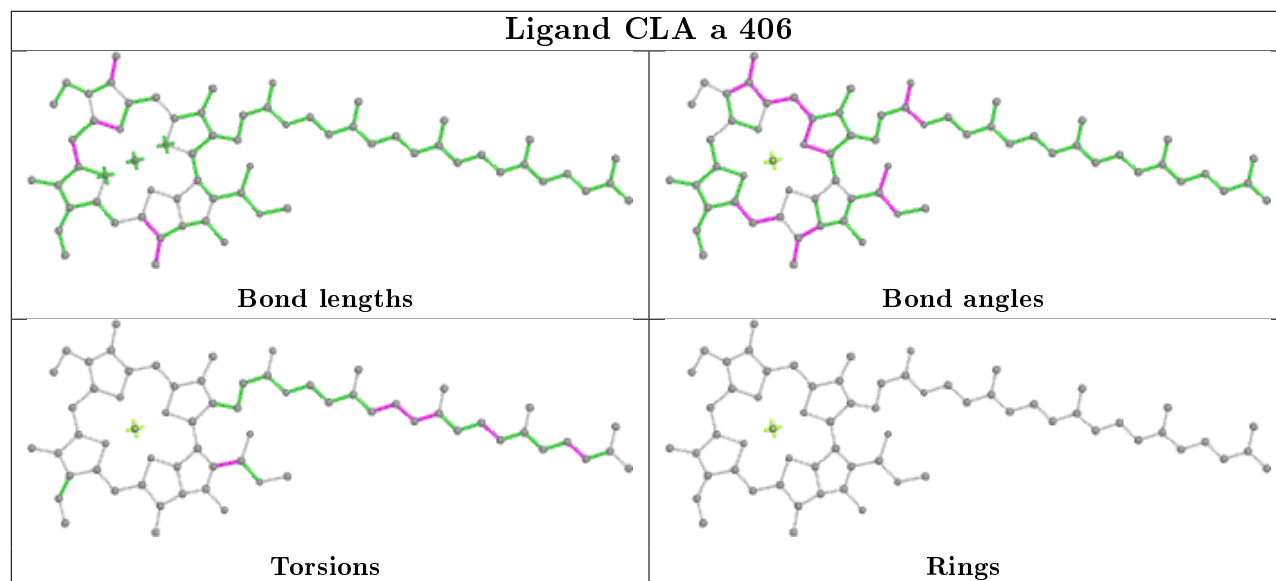
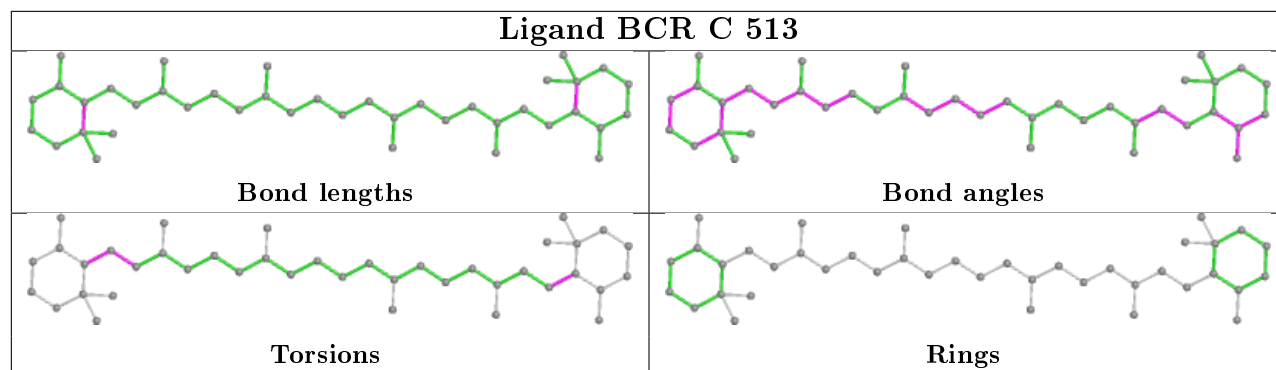
## Ligand BCR b 623

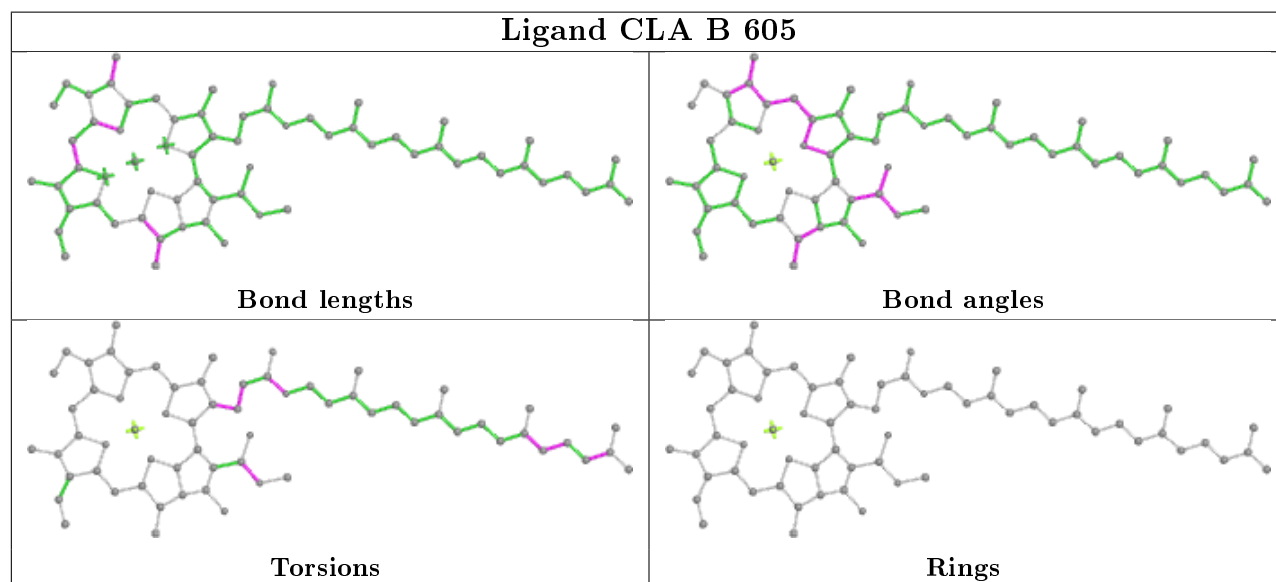
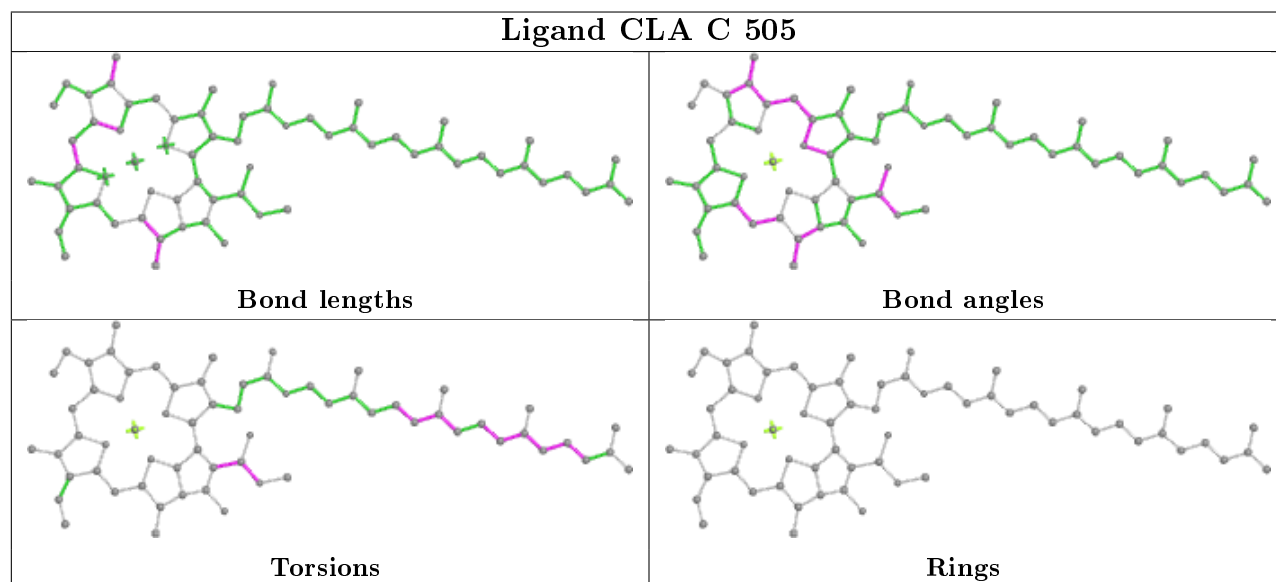
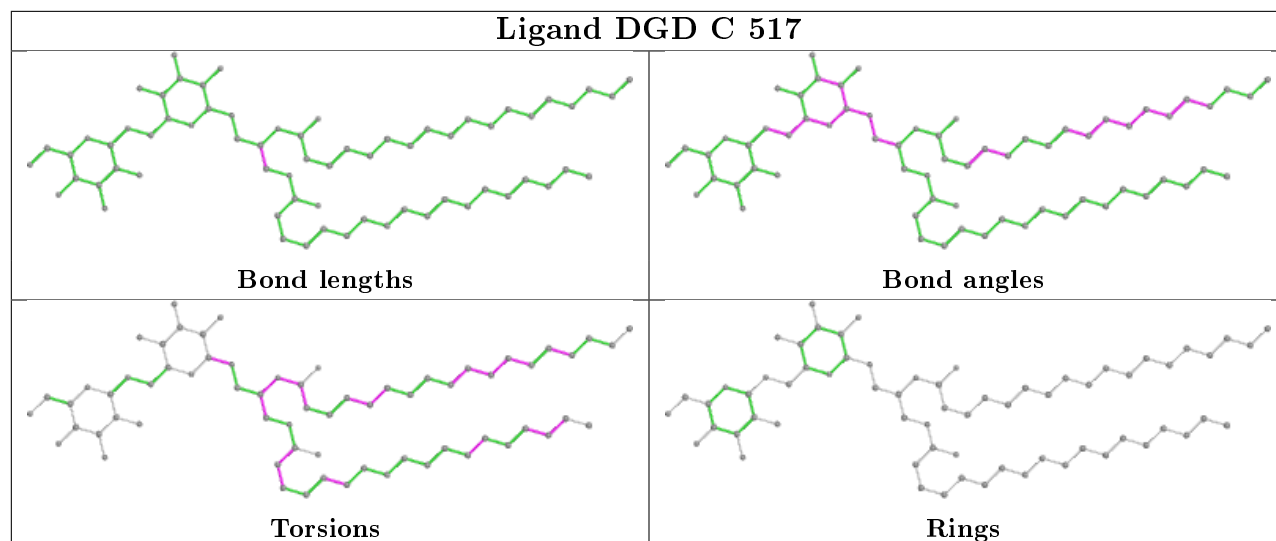


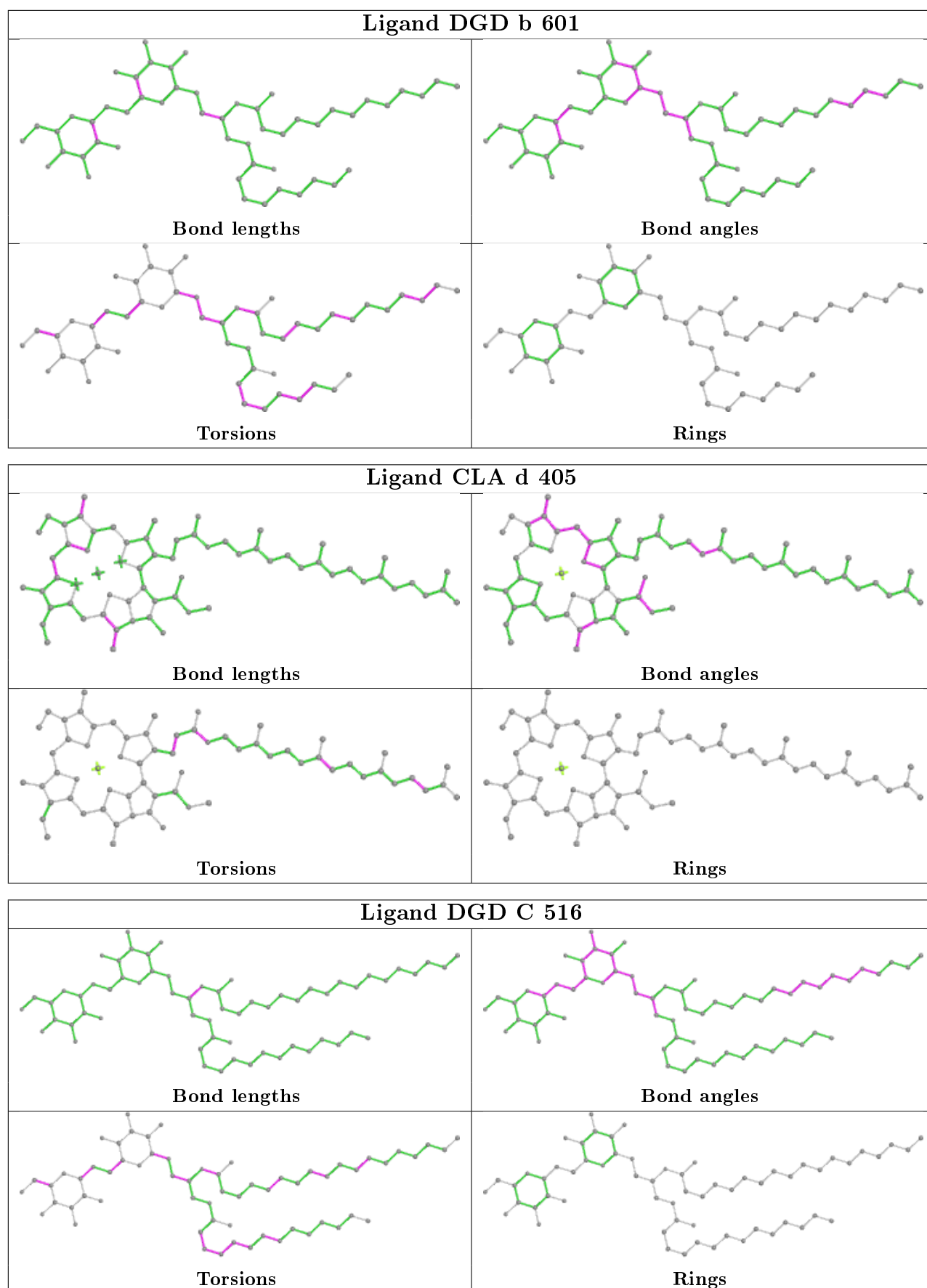




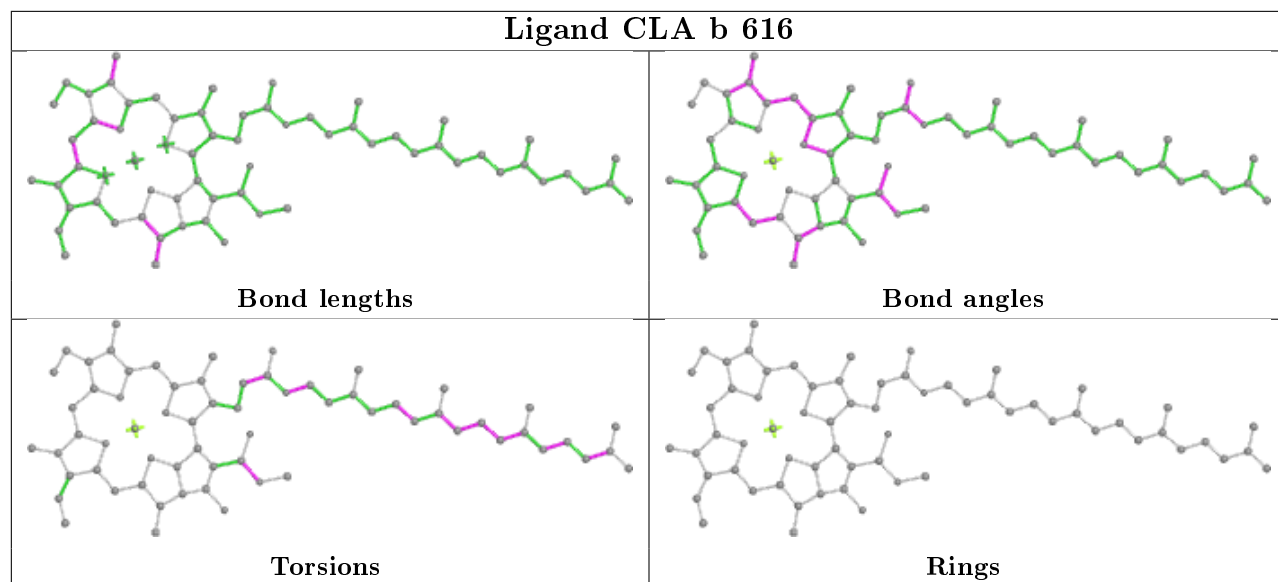




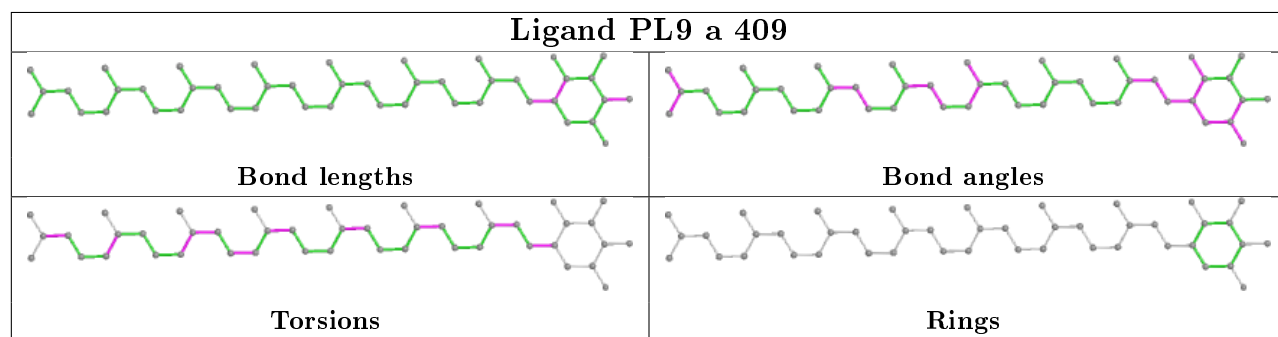




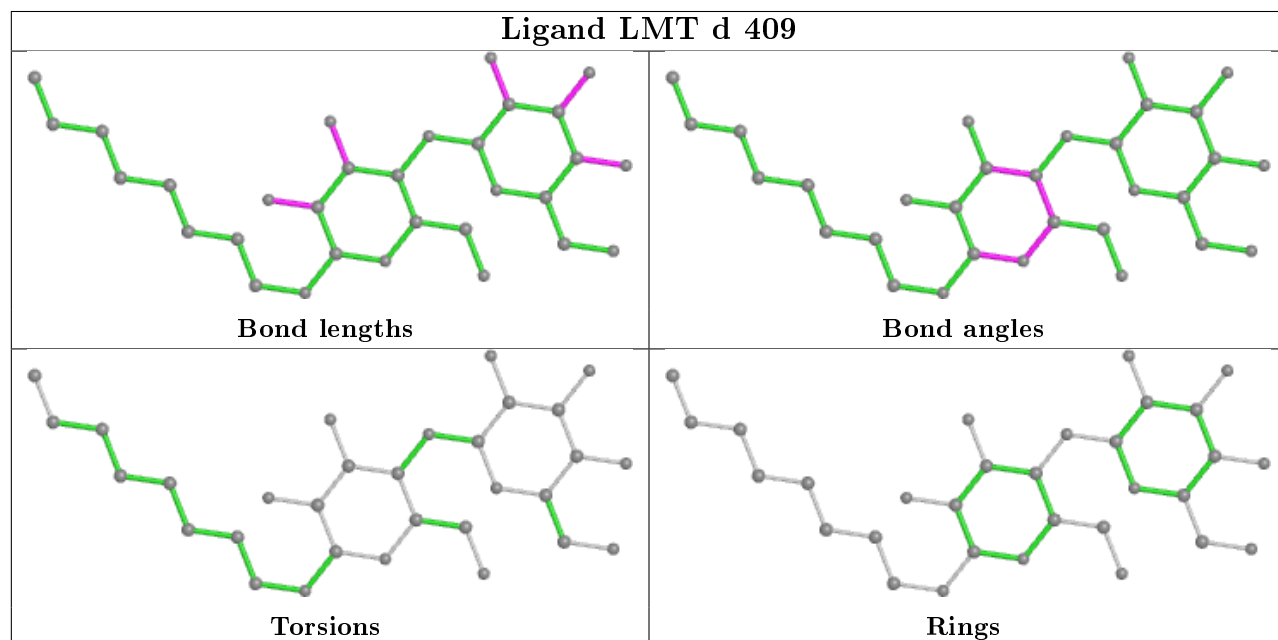
## Ligand CLA b 616

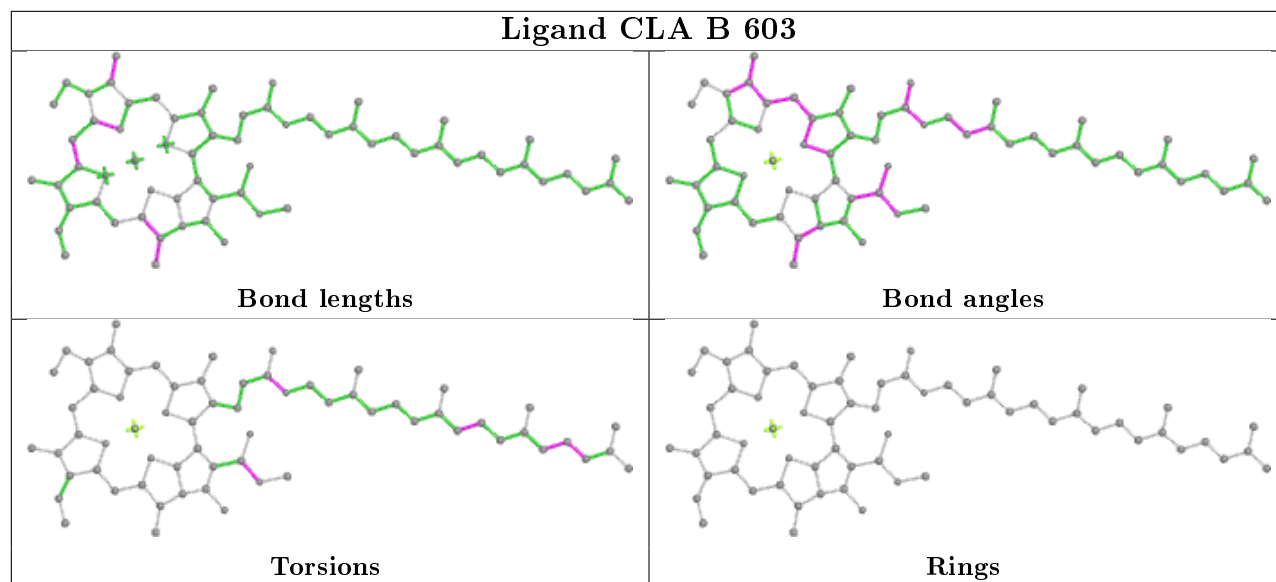
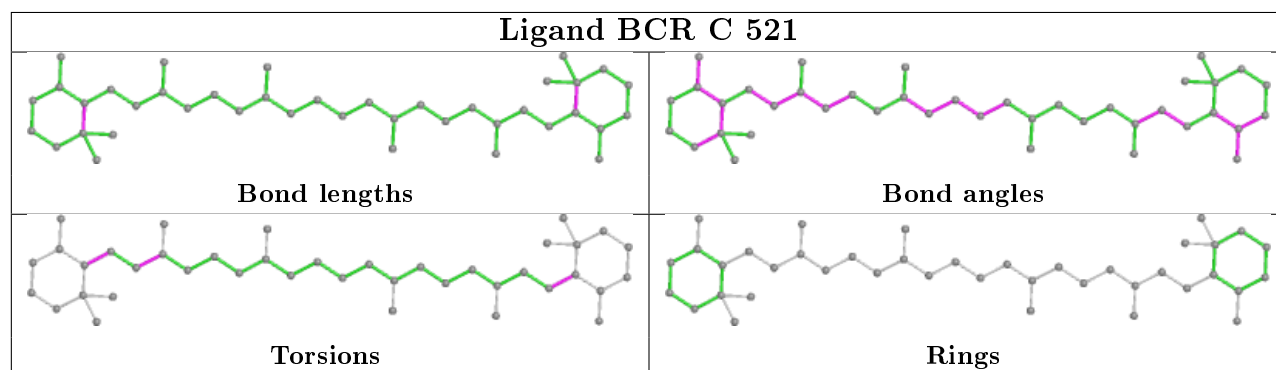
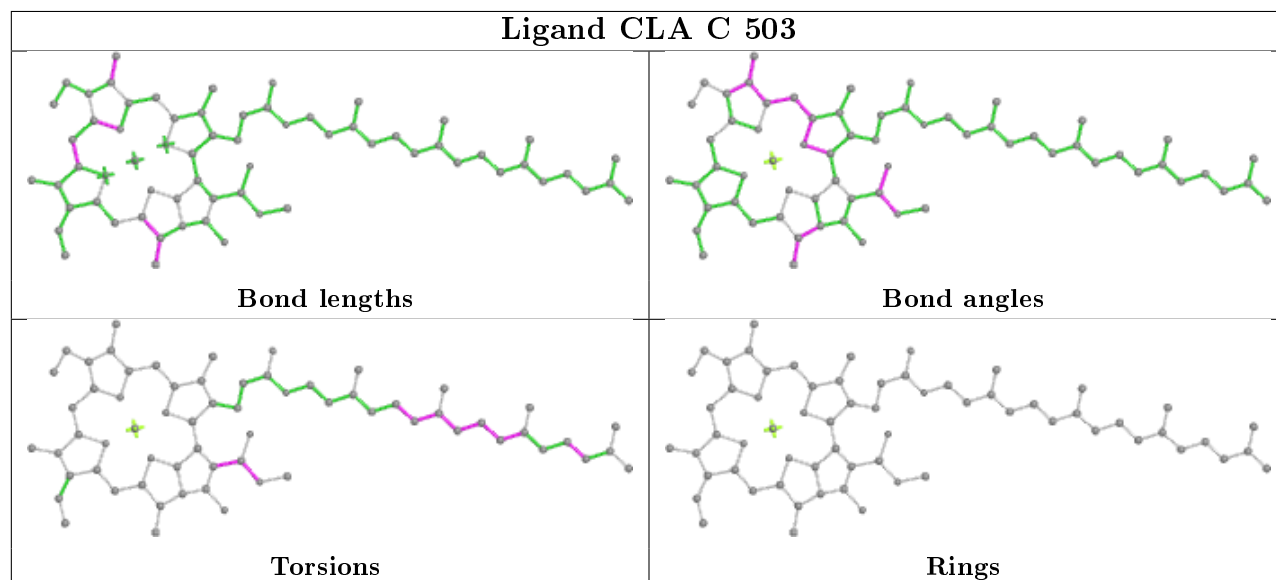


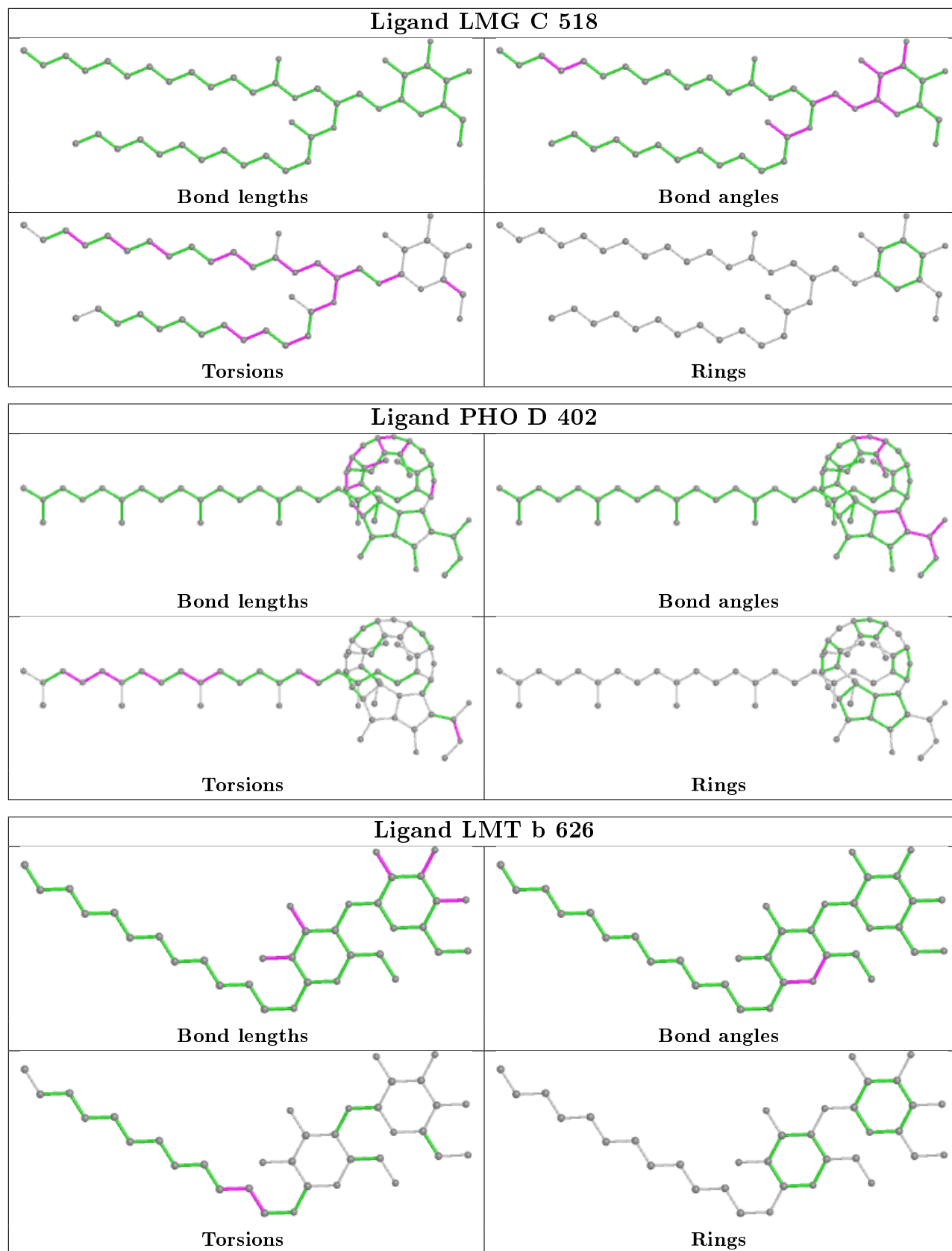
## Ligand PL9 a 409

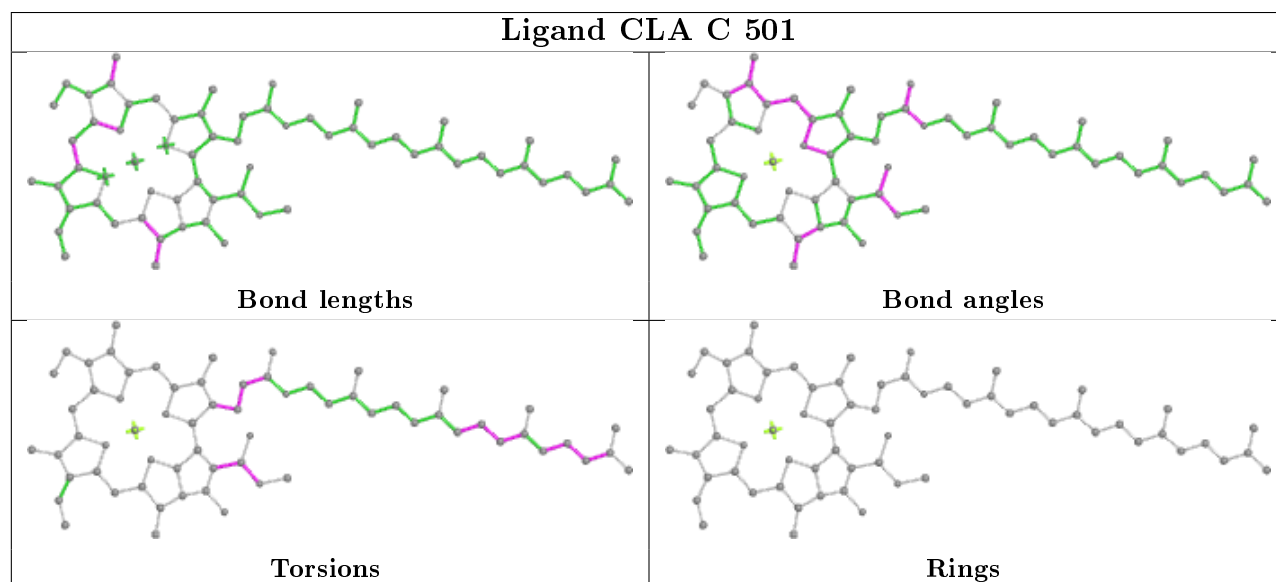
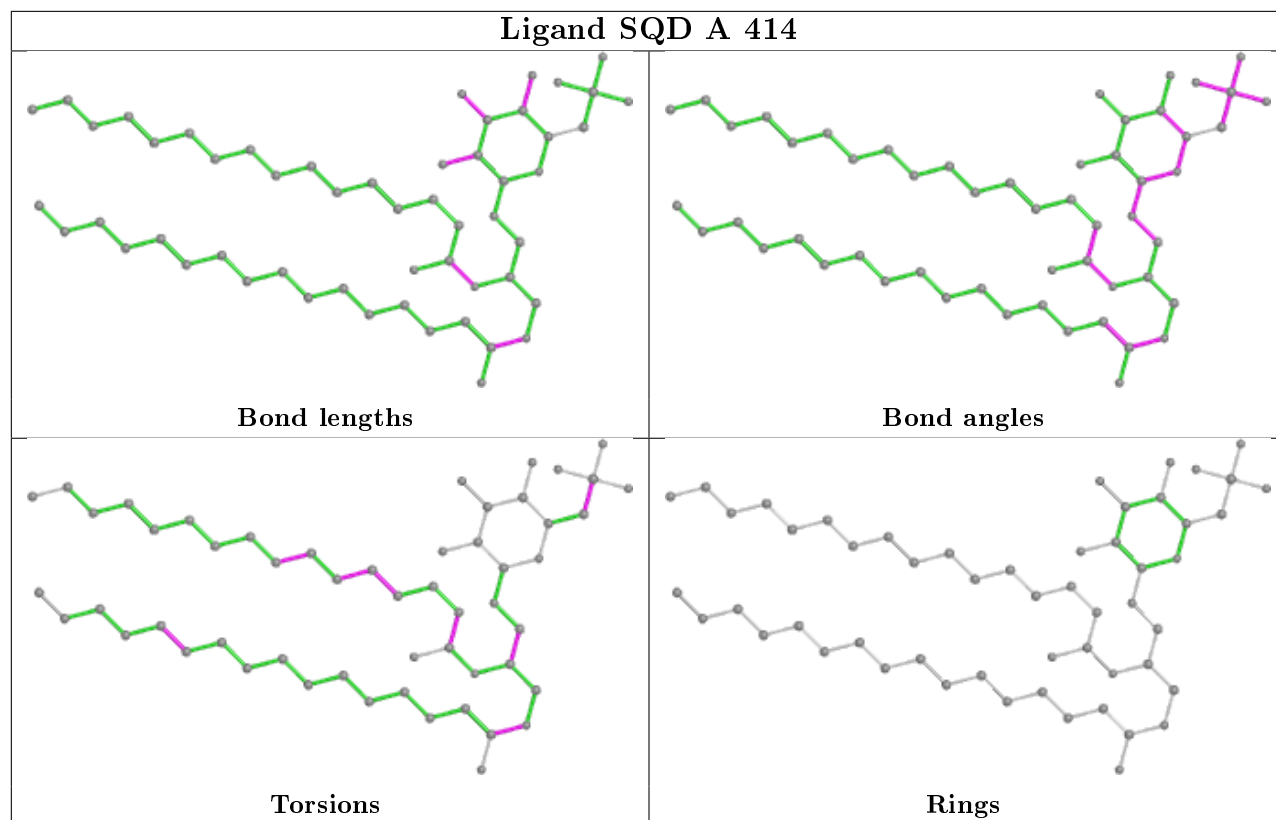


## Ligand LMT d 409

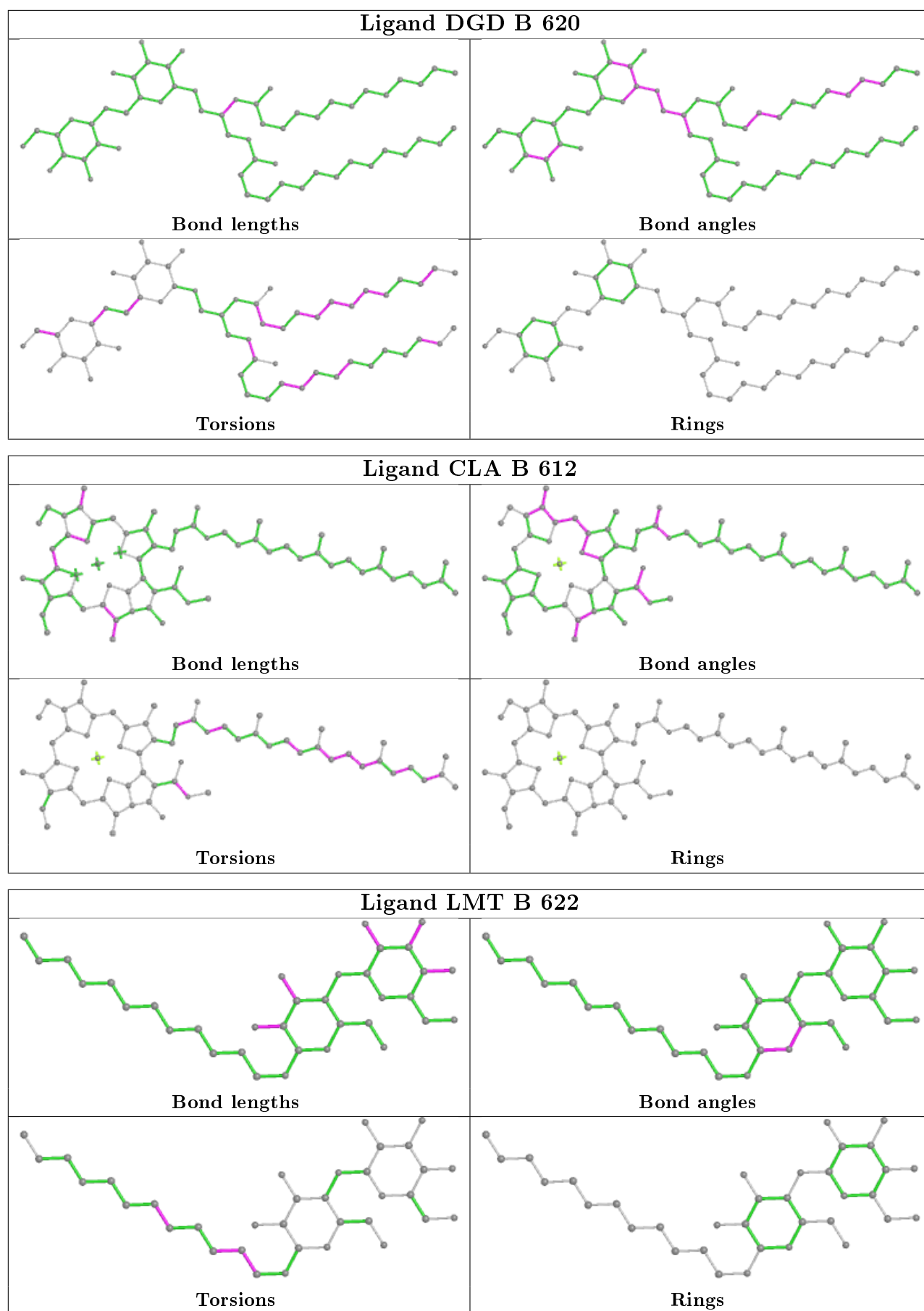


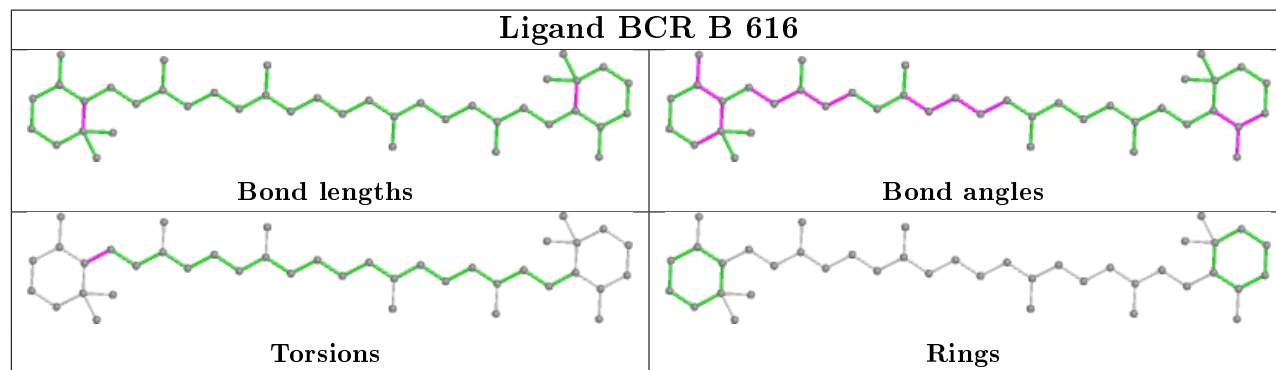
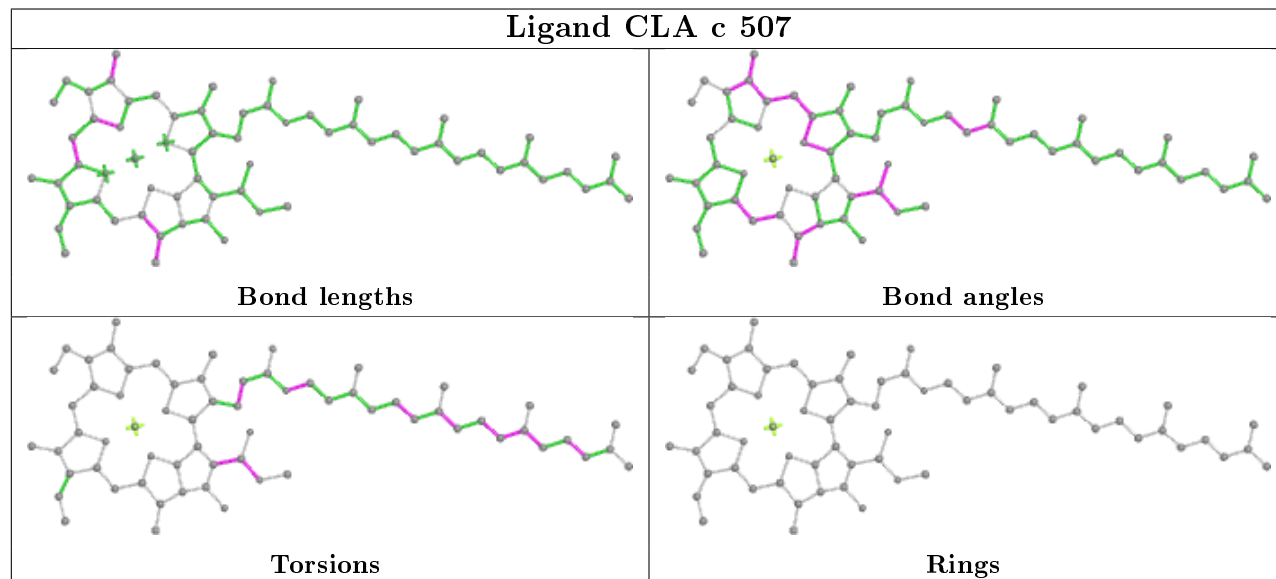
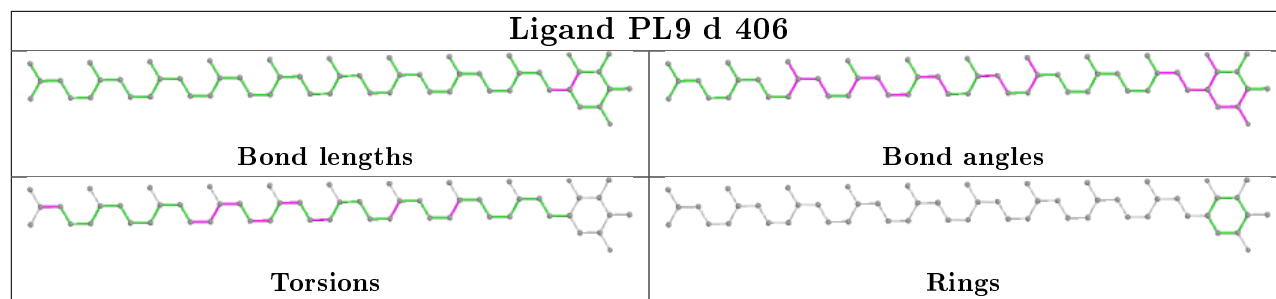
**Ligand CLA B 603****Ligand BCR C 521****Ligand CLA C 503**



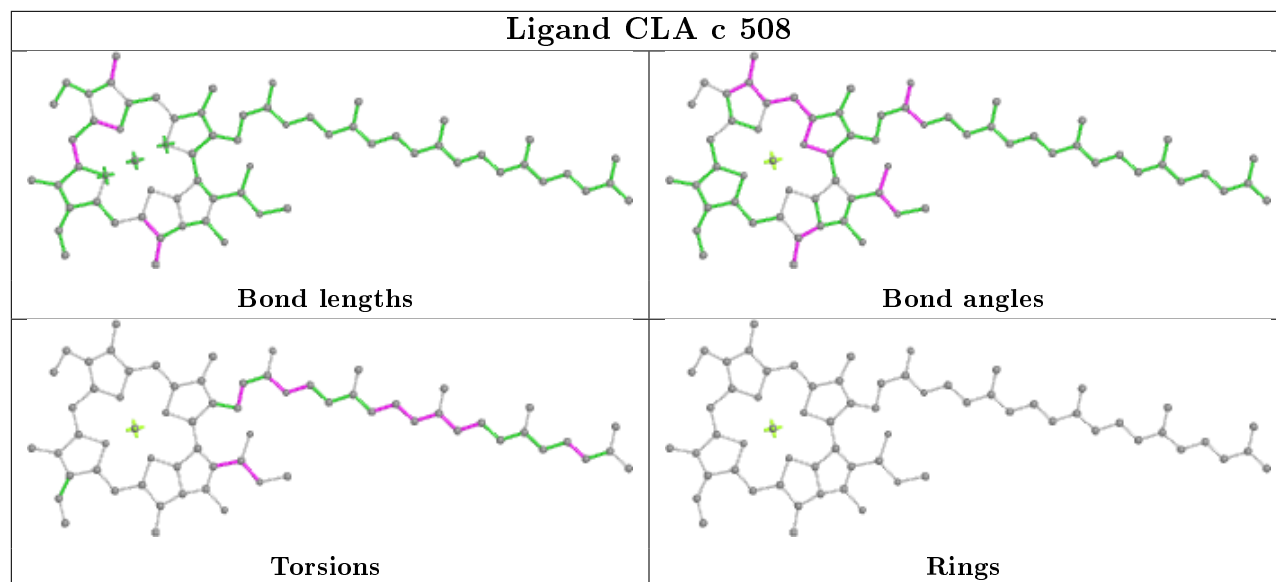




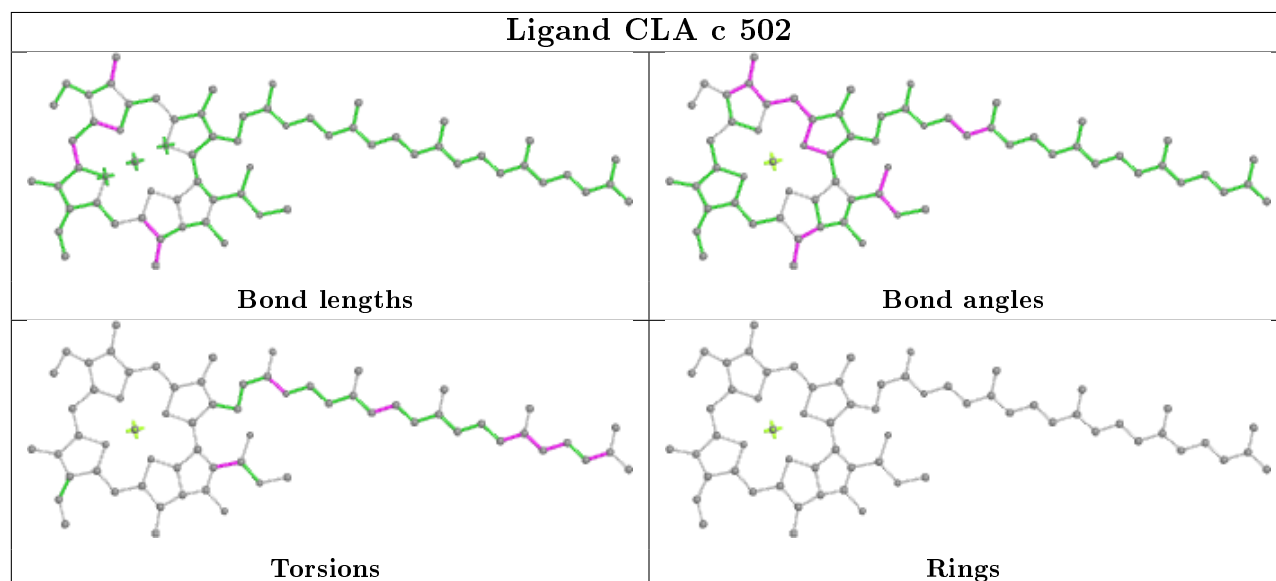




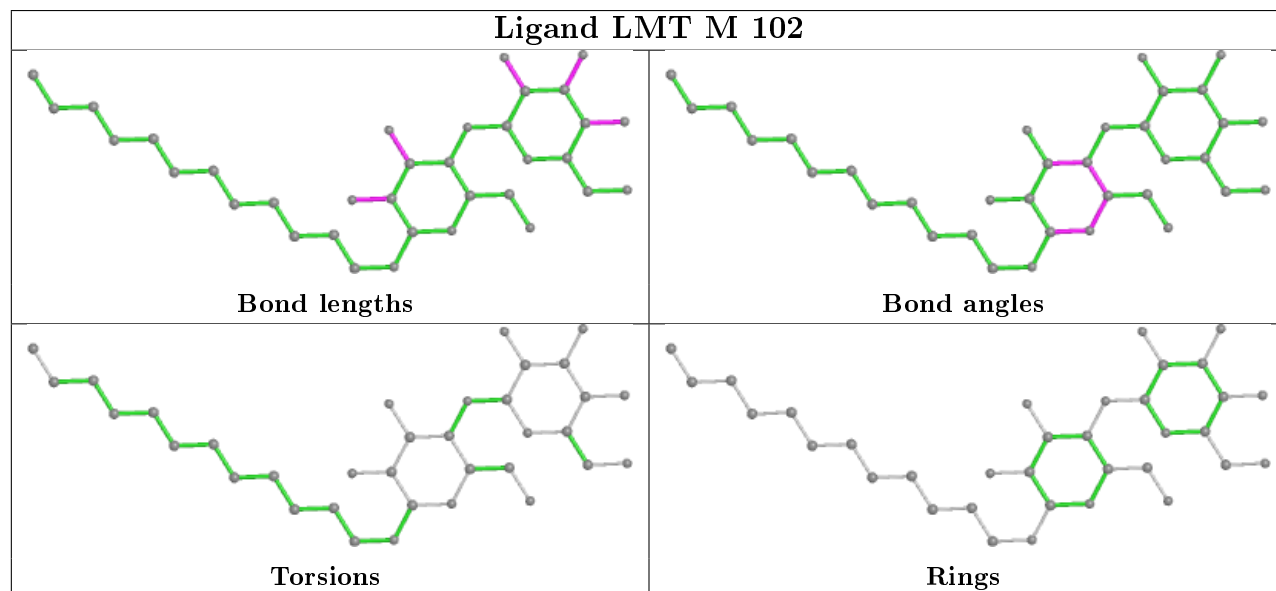
## Ligand CLA c 508

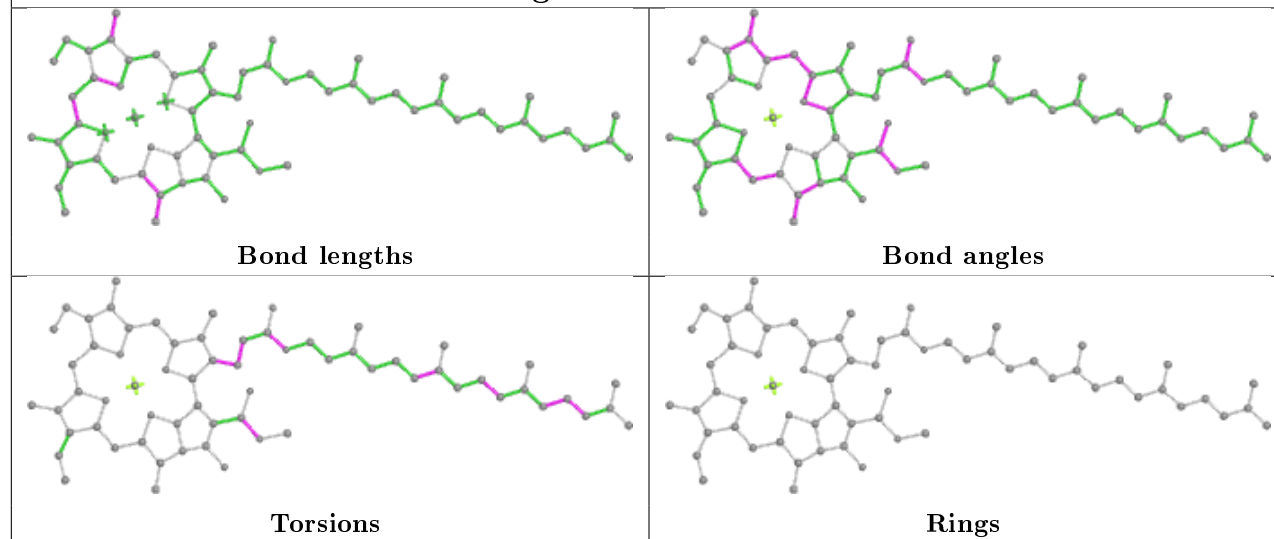
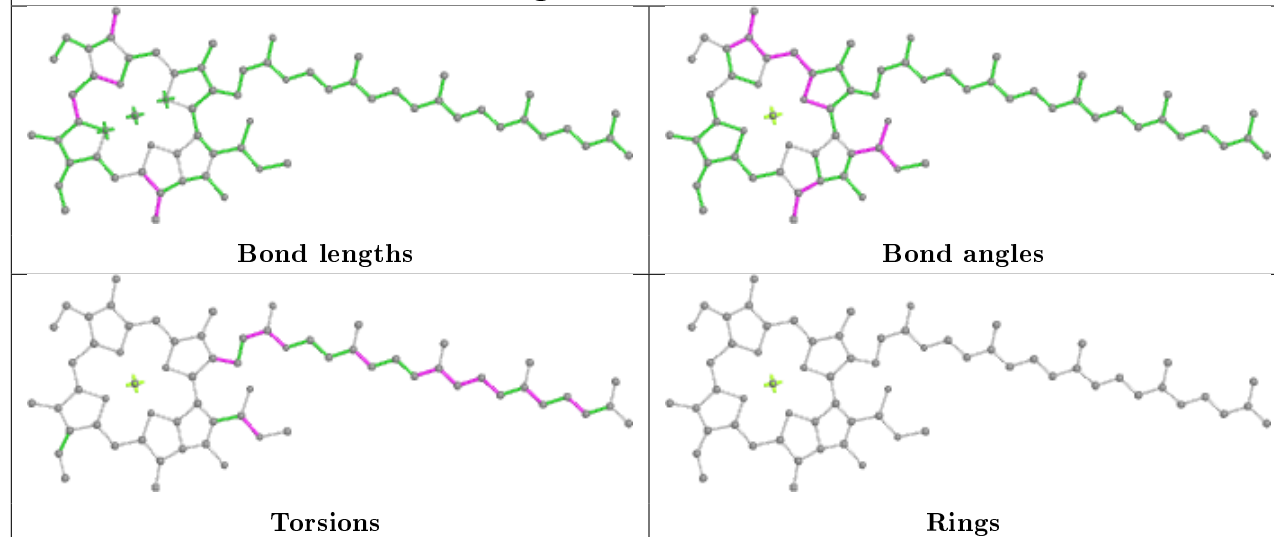


## Ligand CLA c 502

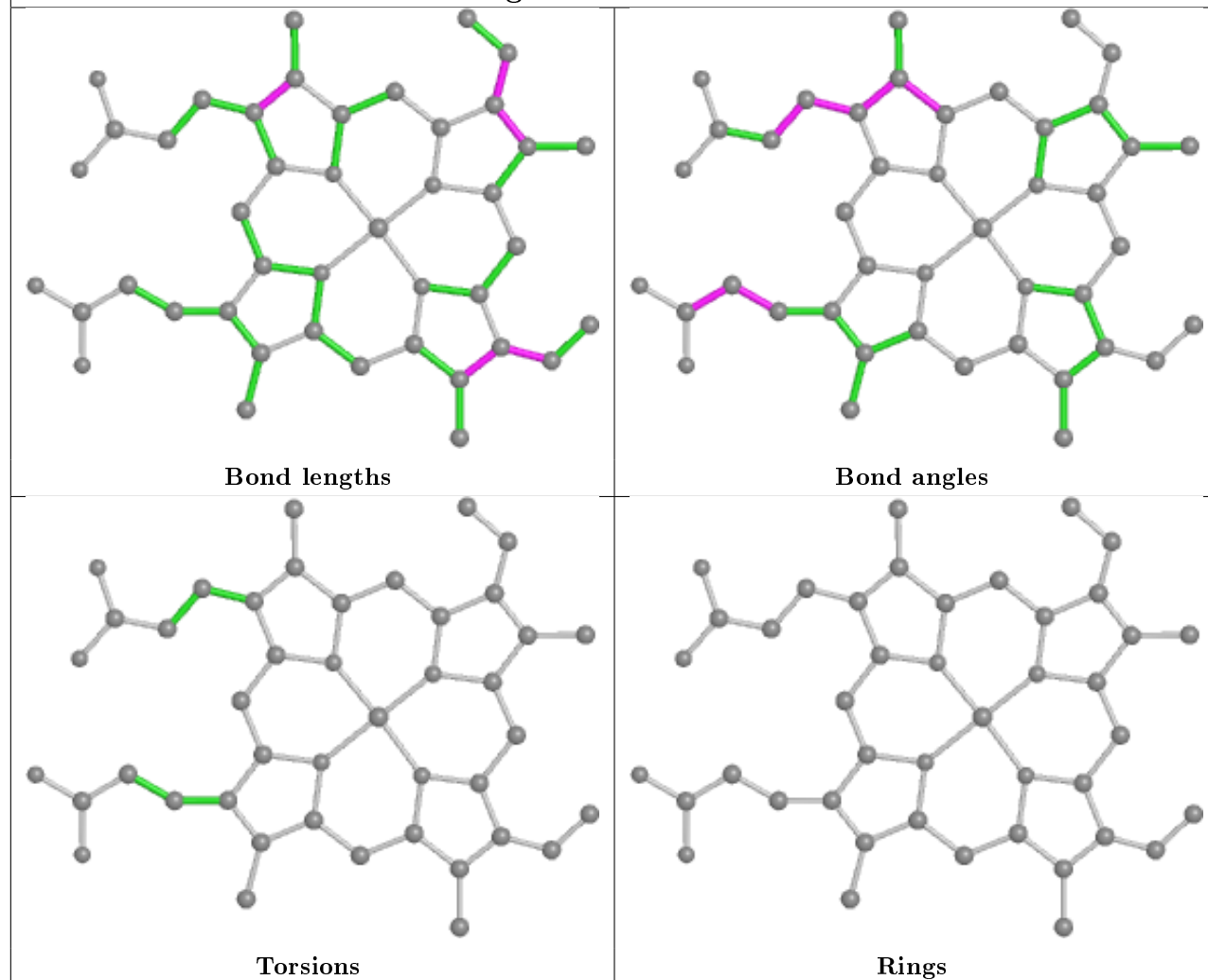


## Ligand LMT M 102

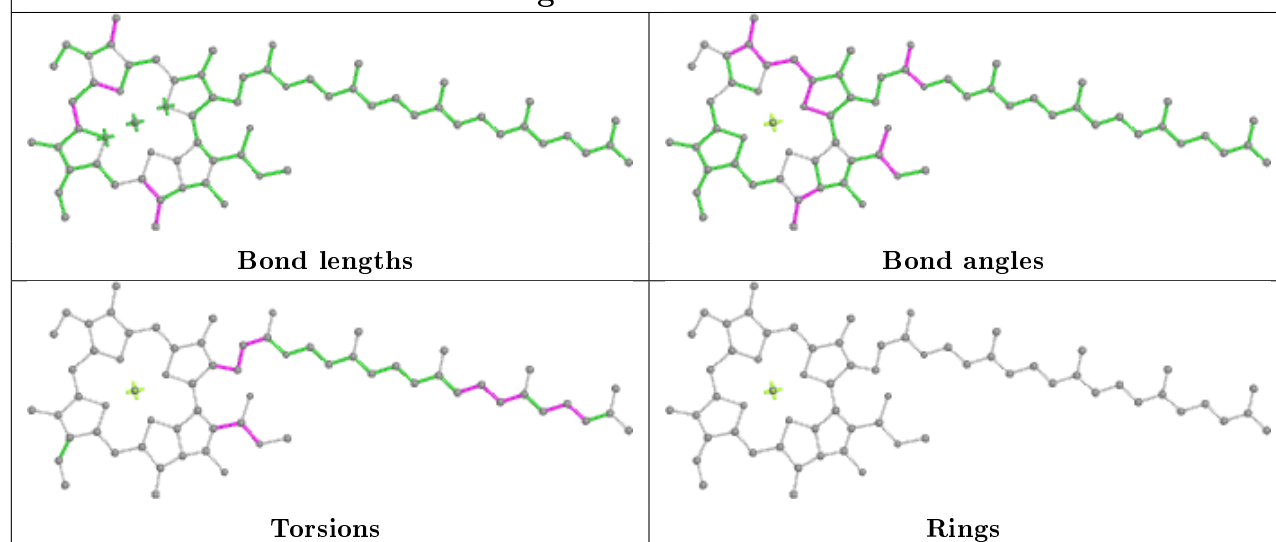


**Ligand CLA C 520****Ligand CLA C 504**

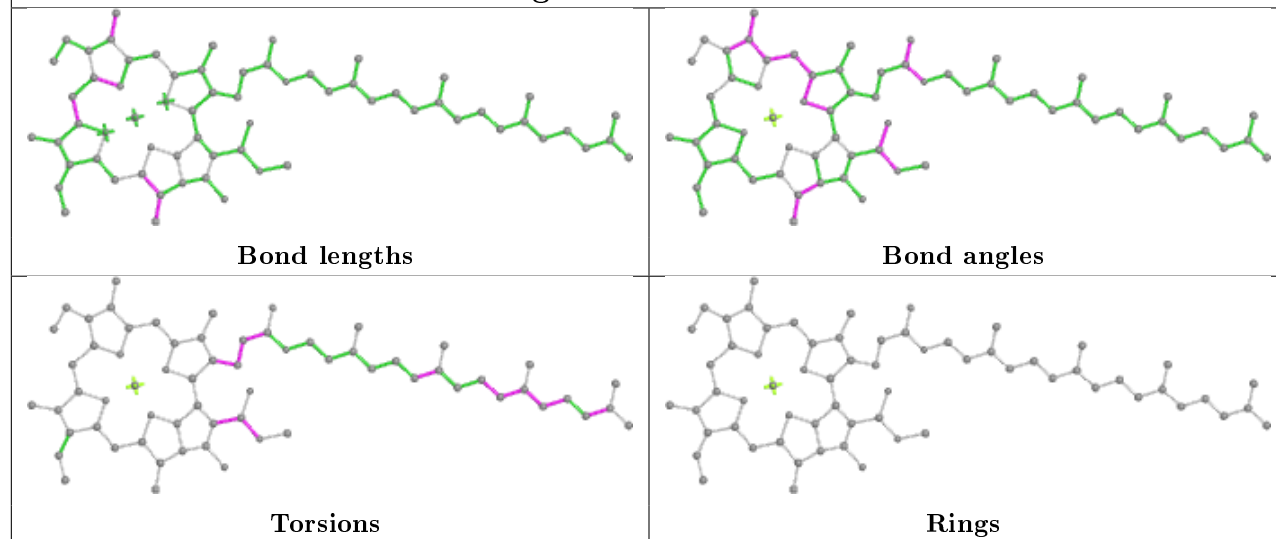
## Ligand HEM f 101



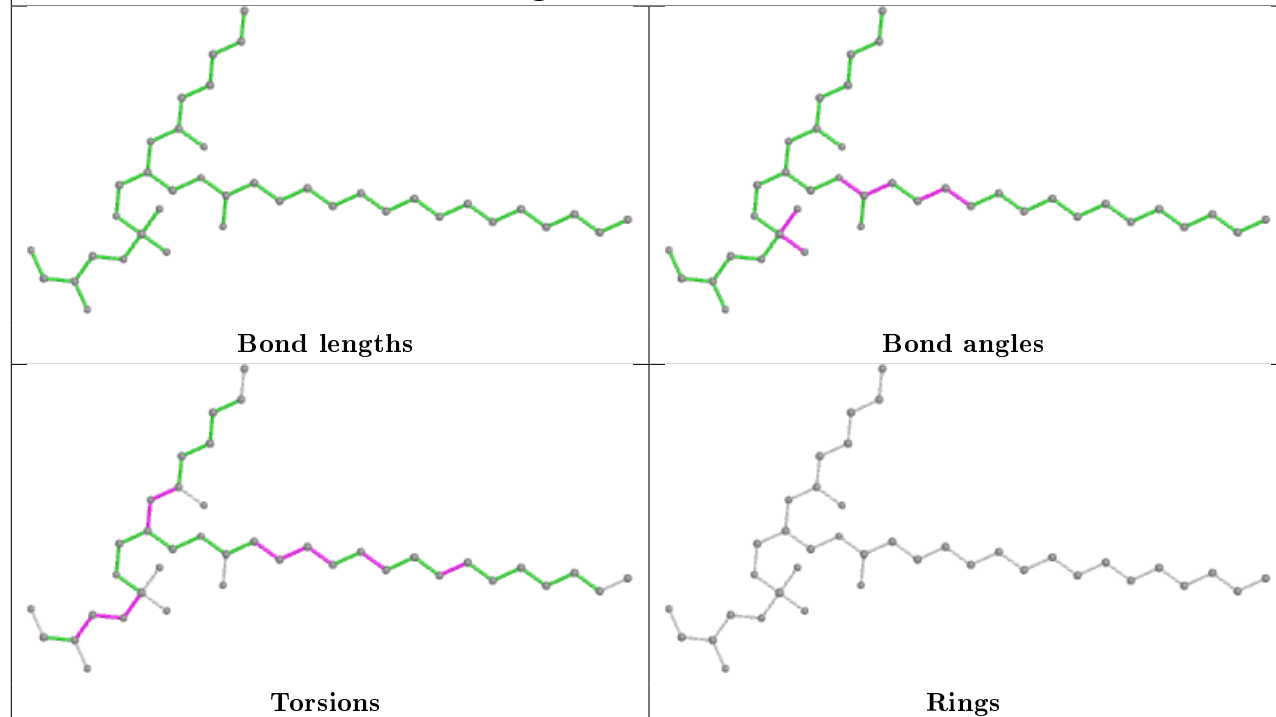
## Ligand CLA c 501



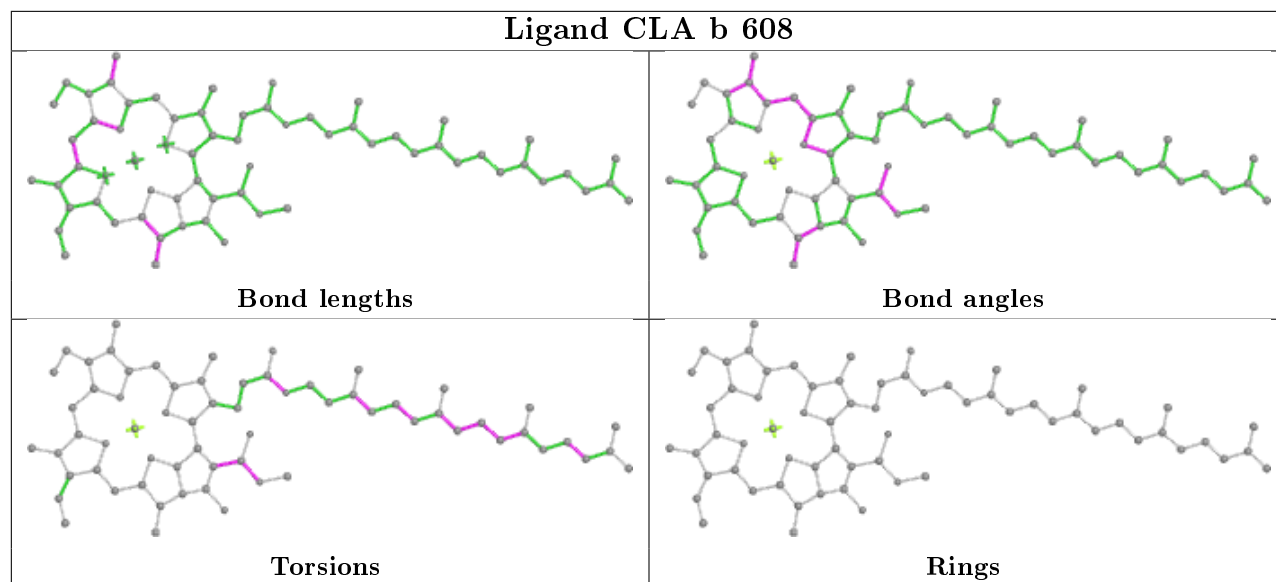
## Ligand CLA B 601



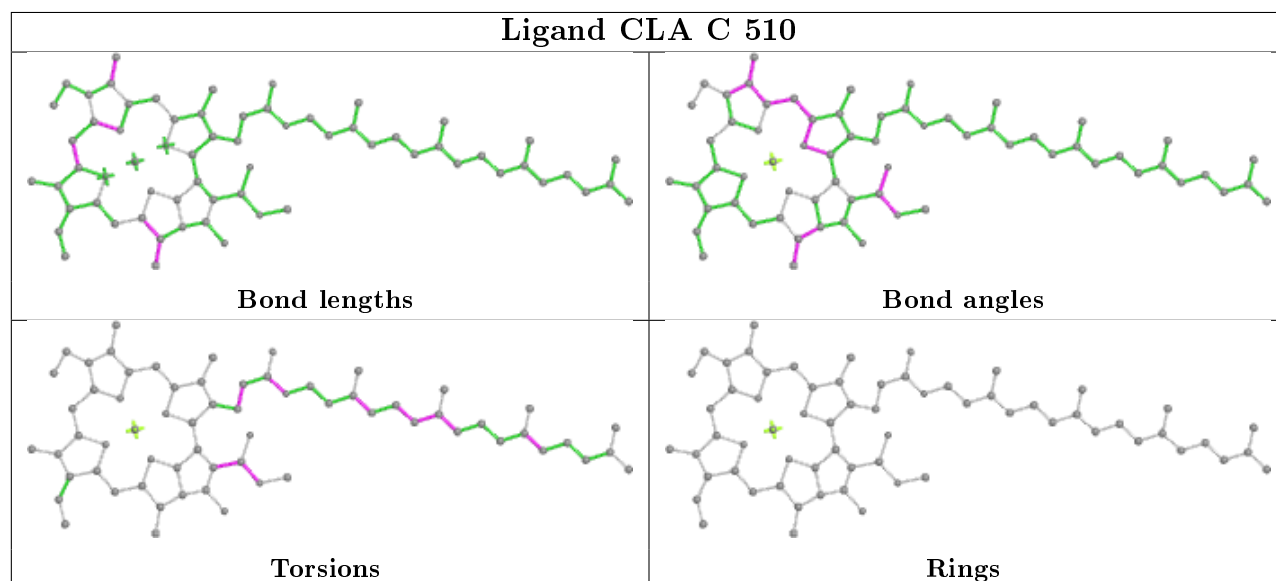
## Ligand LHG A 409



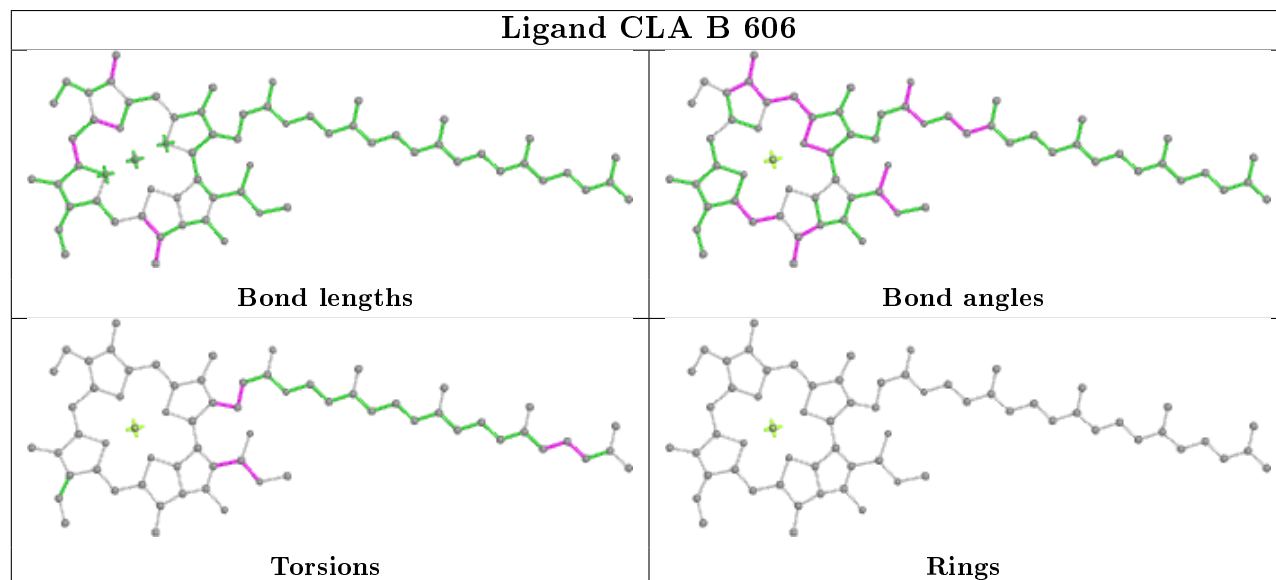
## Ligand CLA b 608

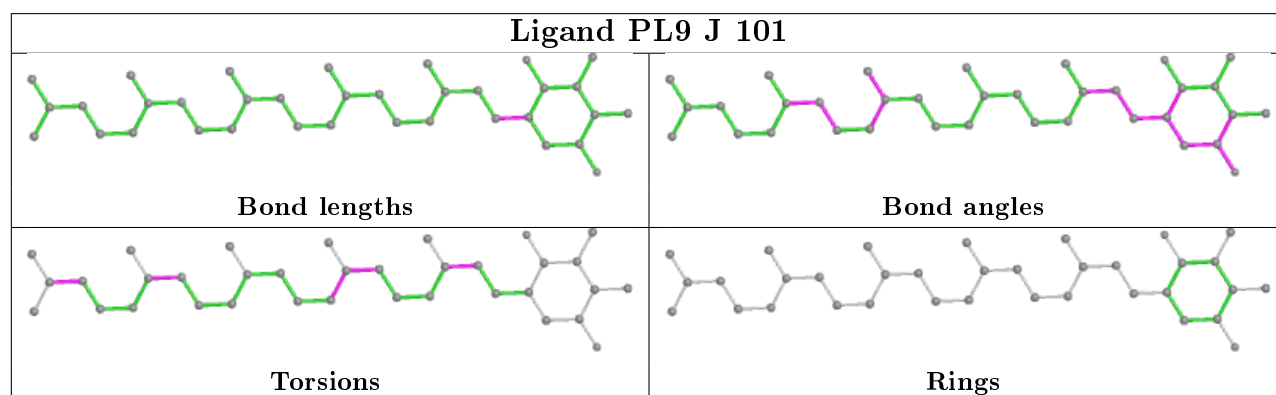
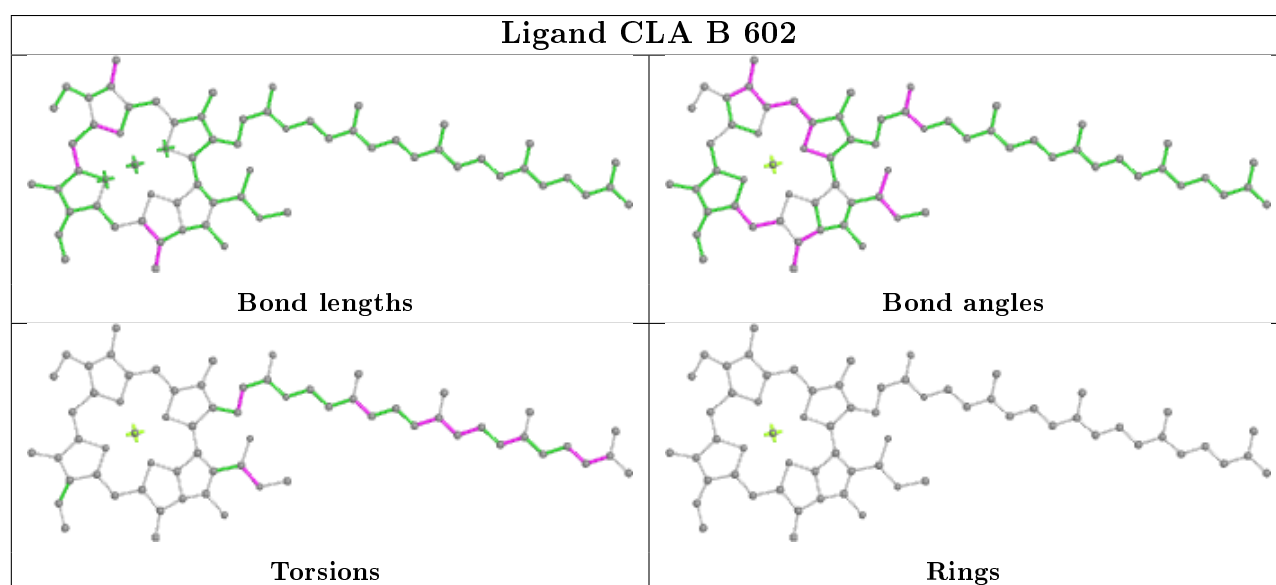
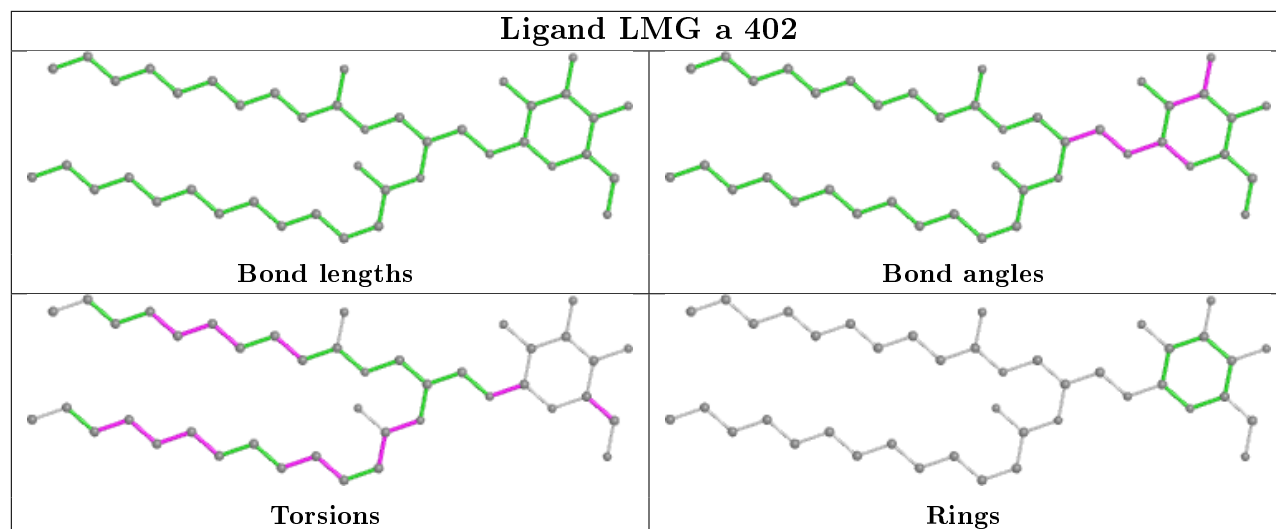


## Ligand CLA C 510

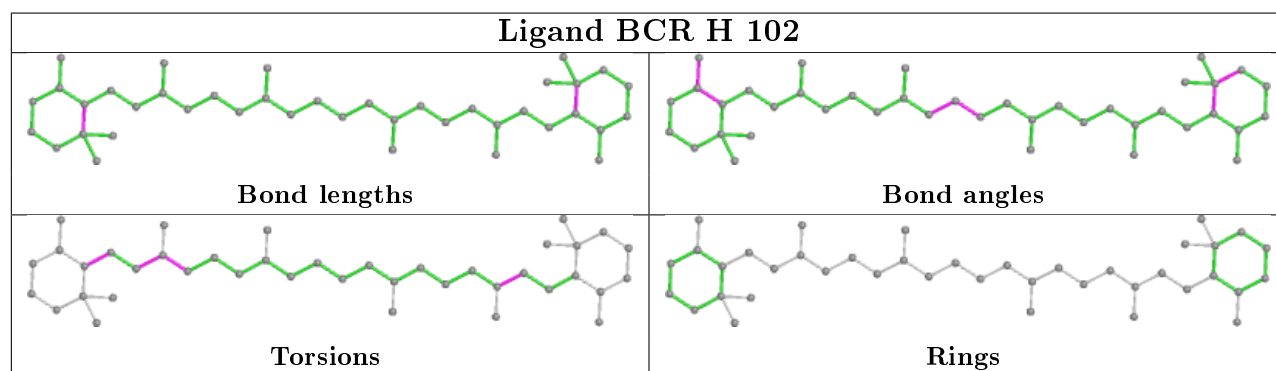
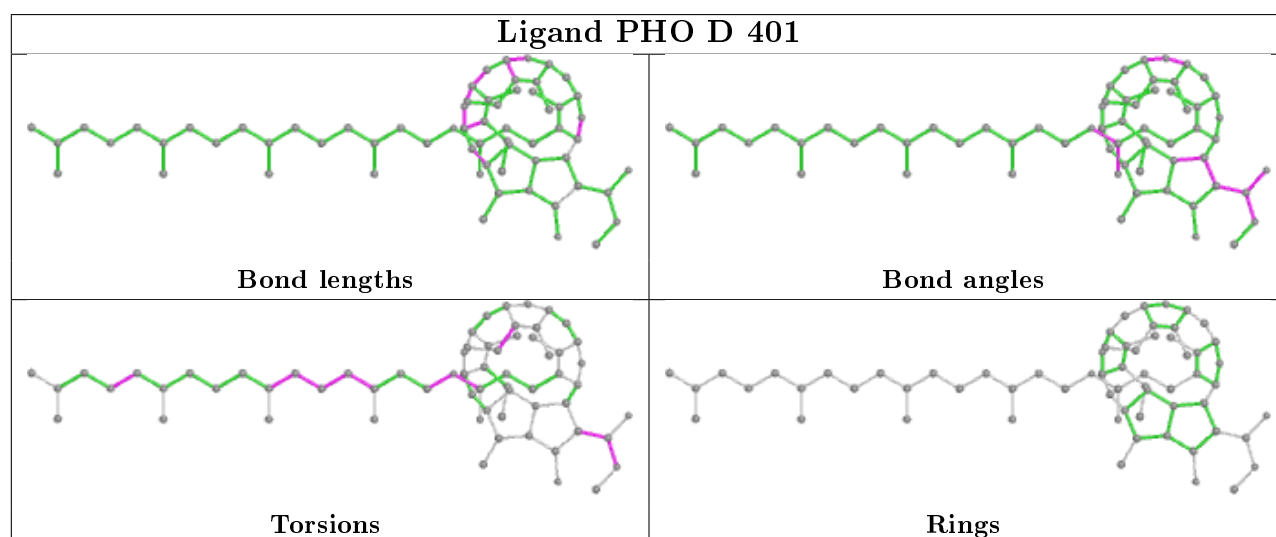
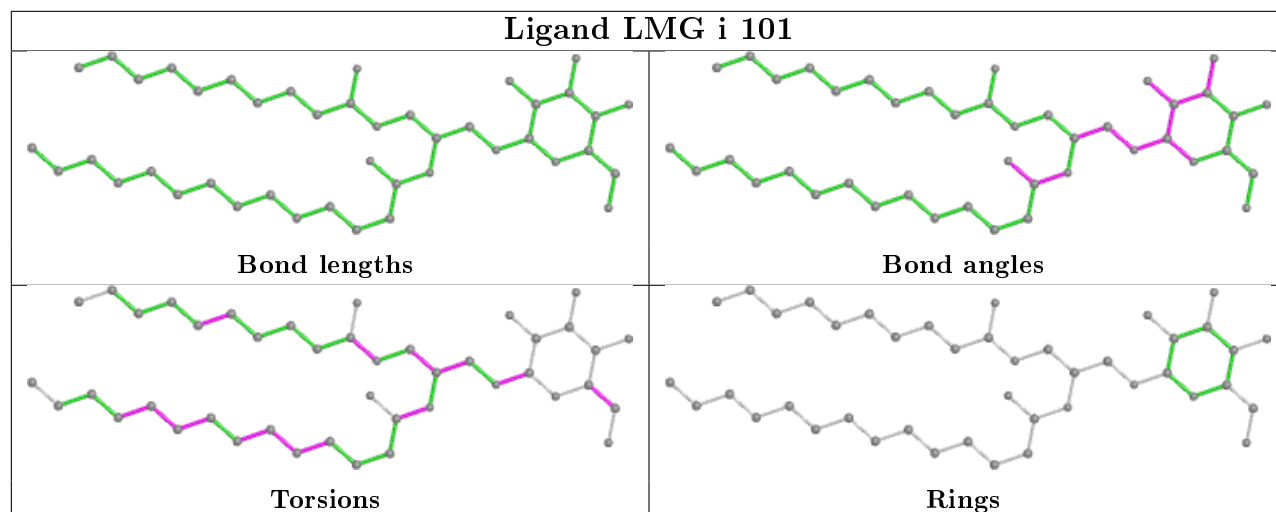


## Ligand CLA B 606

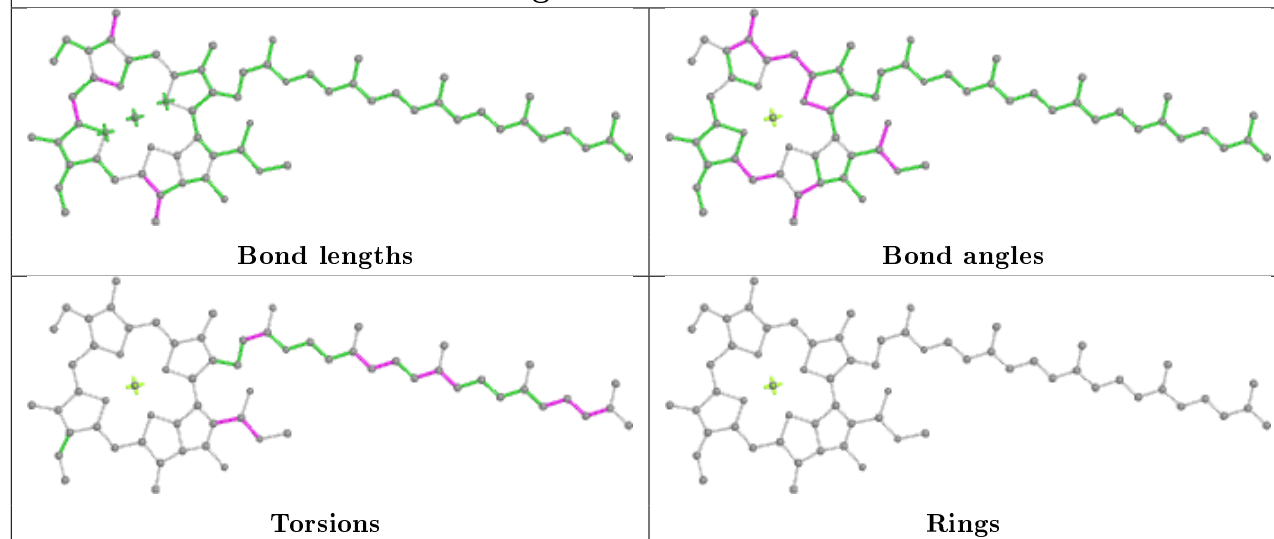




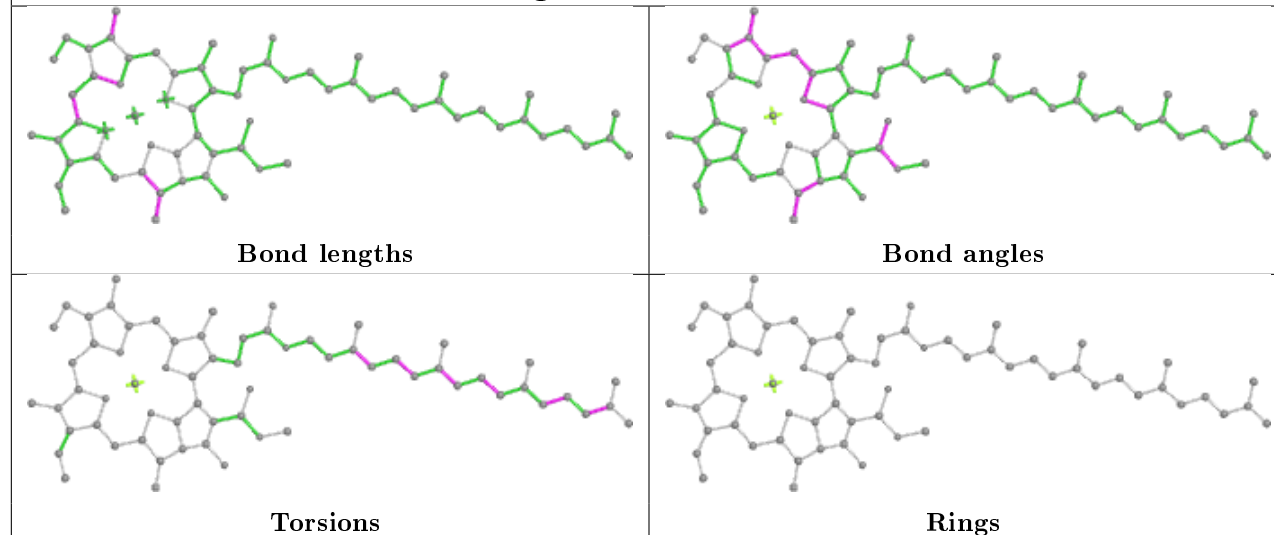




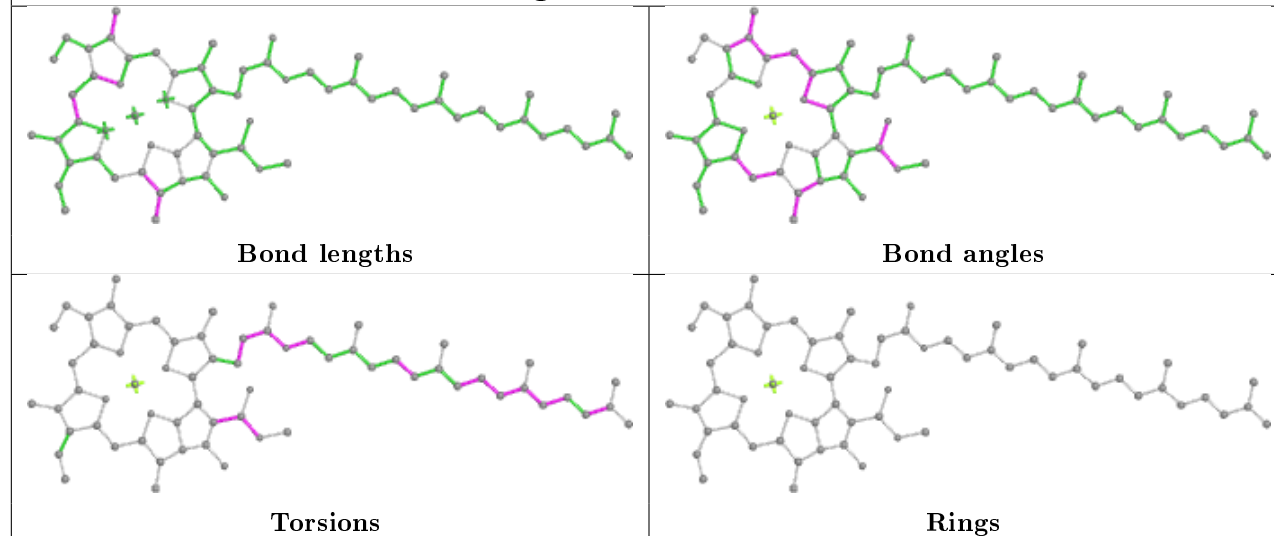
## Ligand CLA C 509

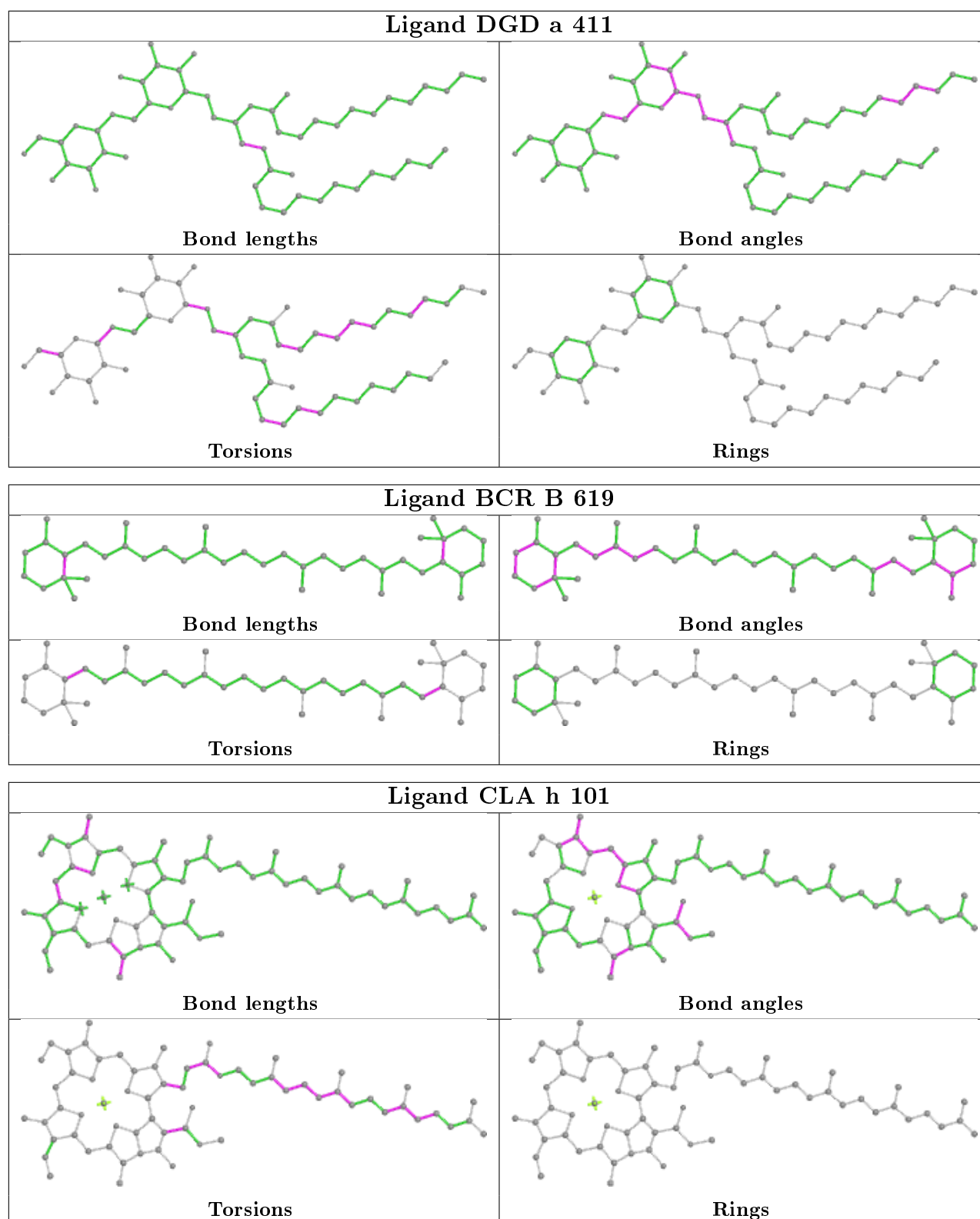


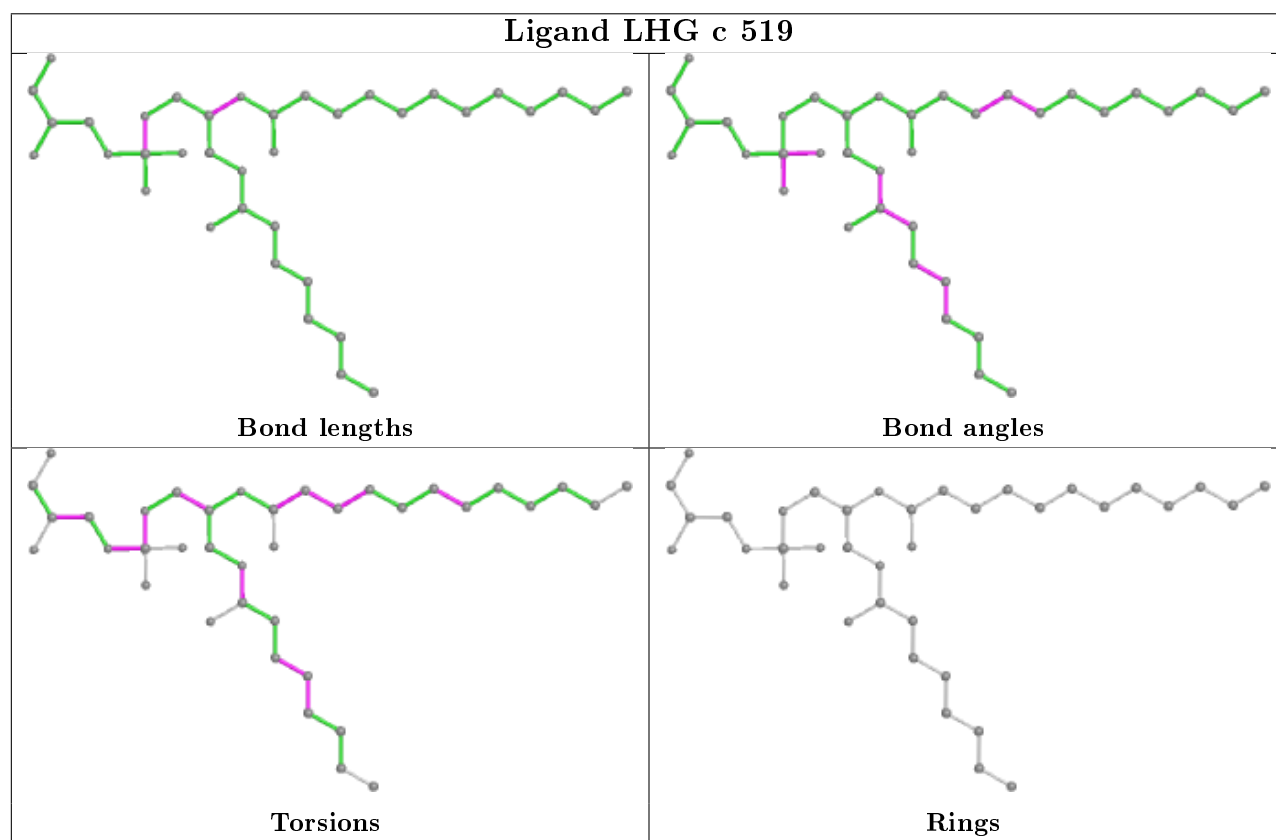
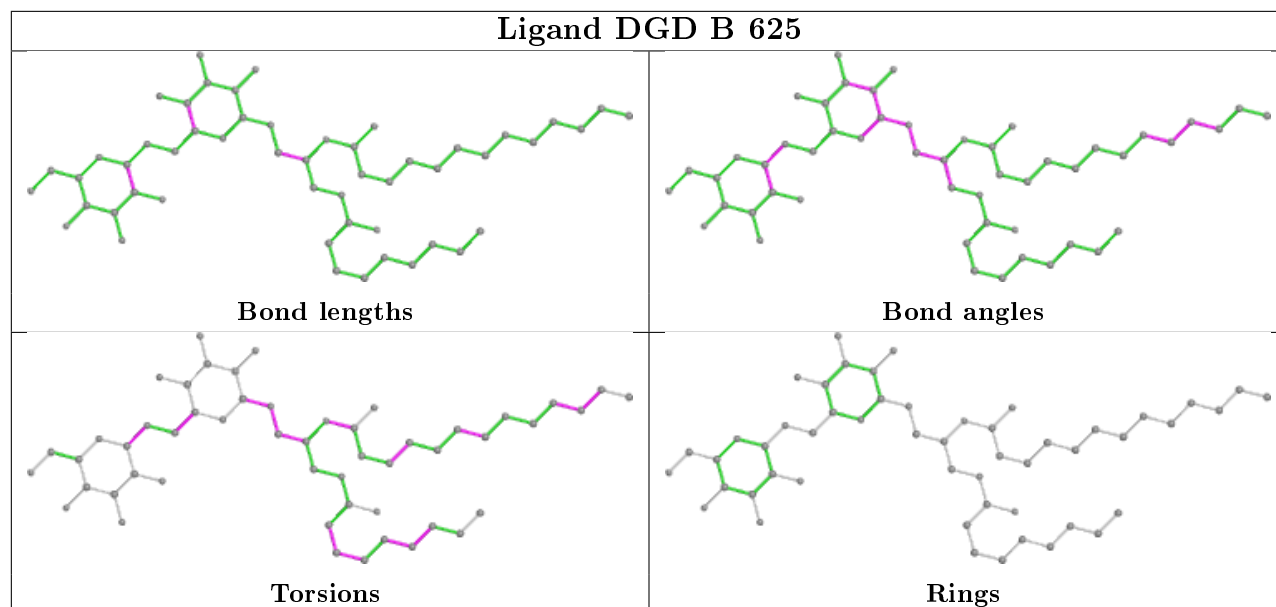
## Ligand CLA A 405

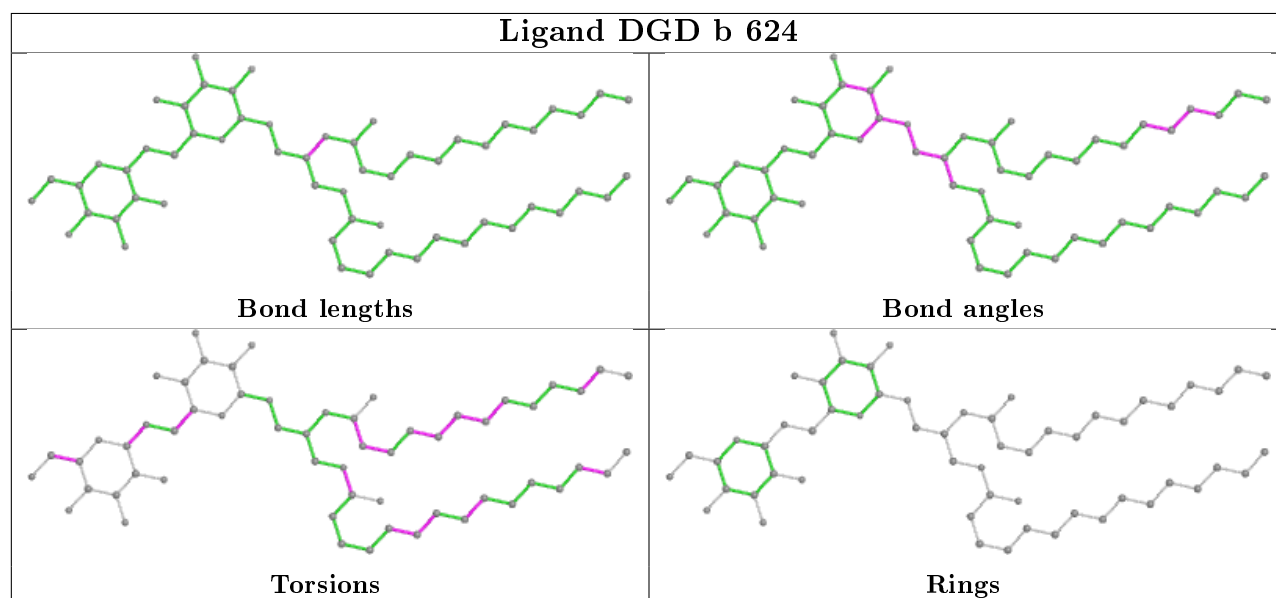
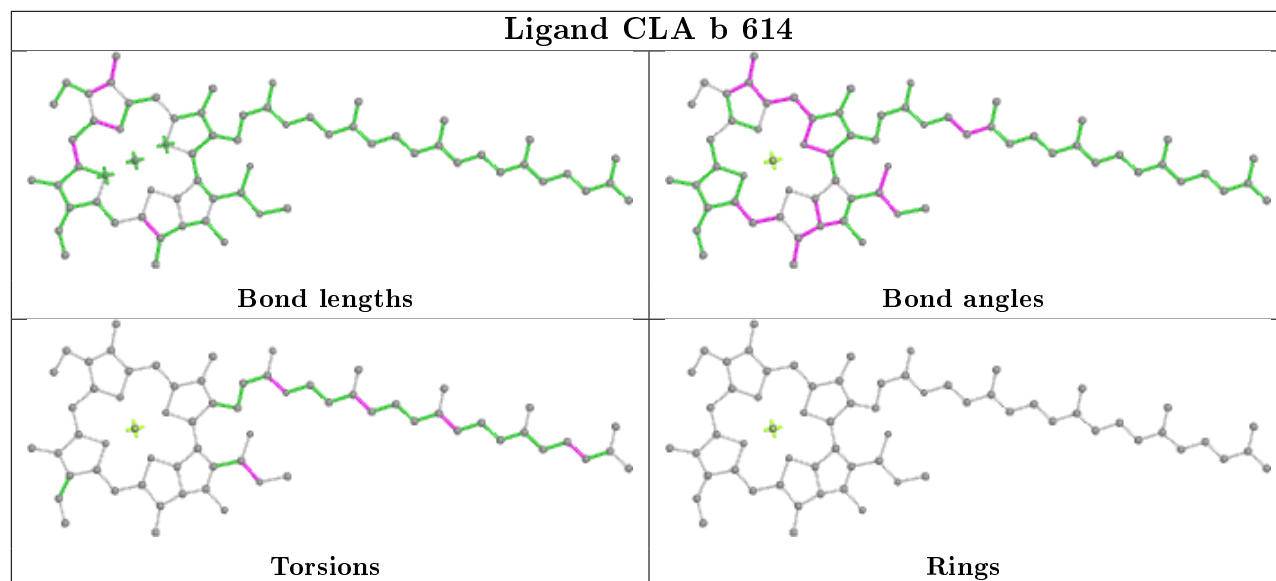
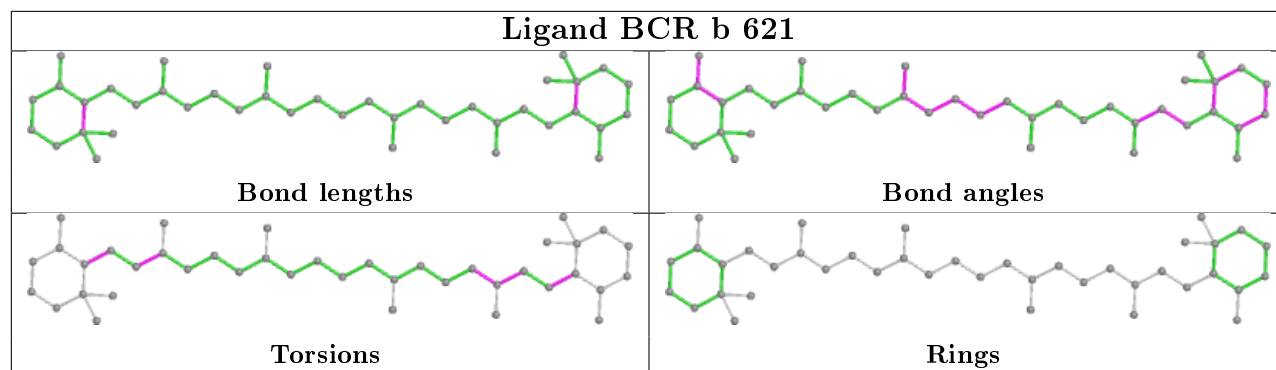


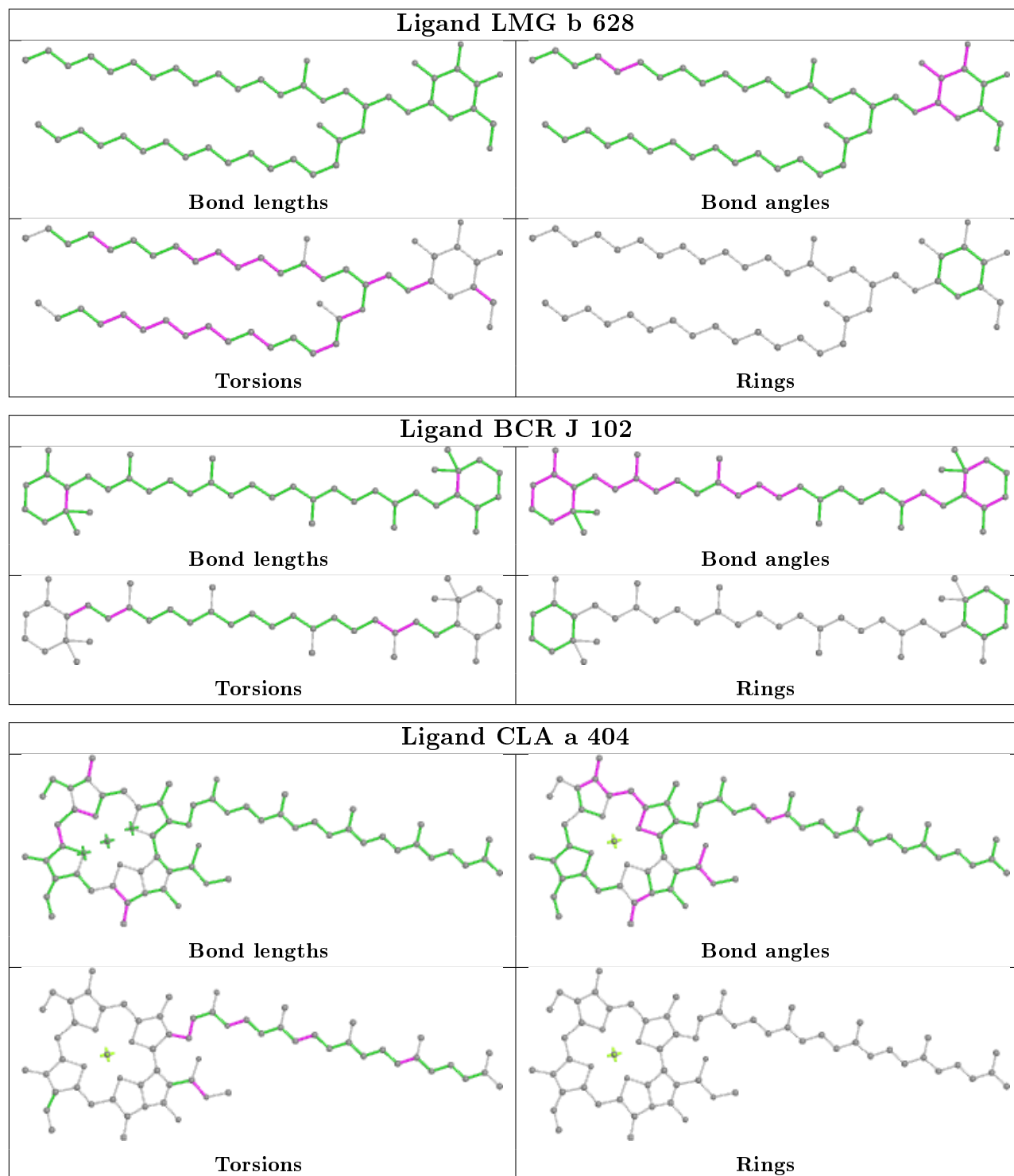
## Ligand CLA B 609

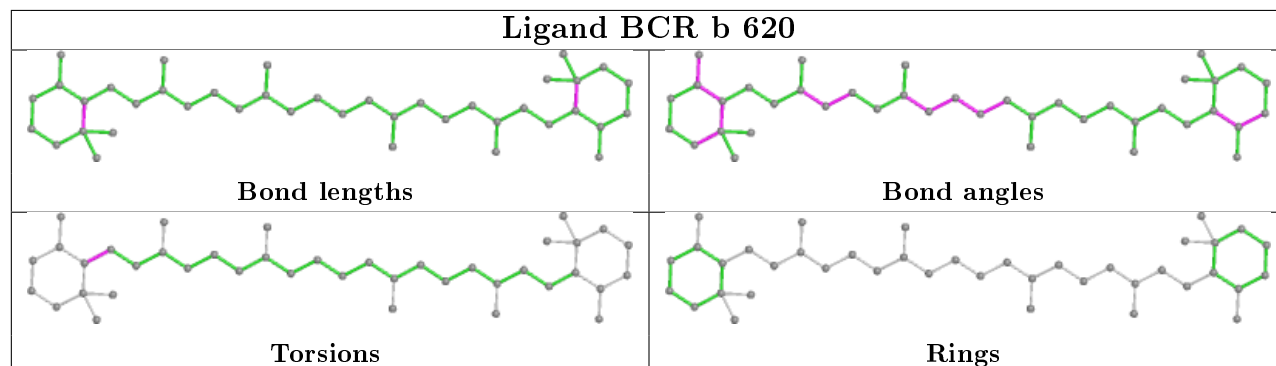
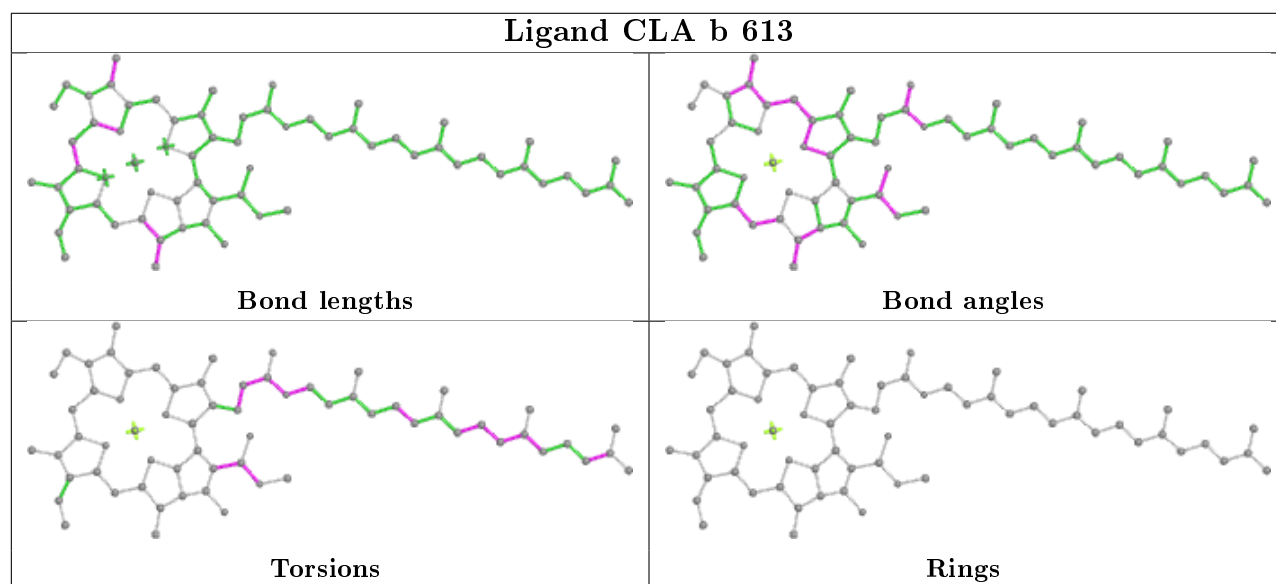
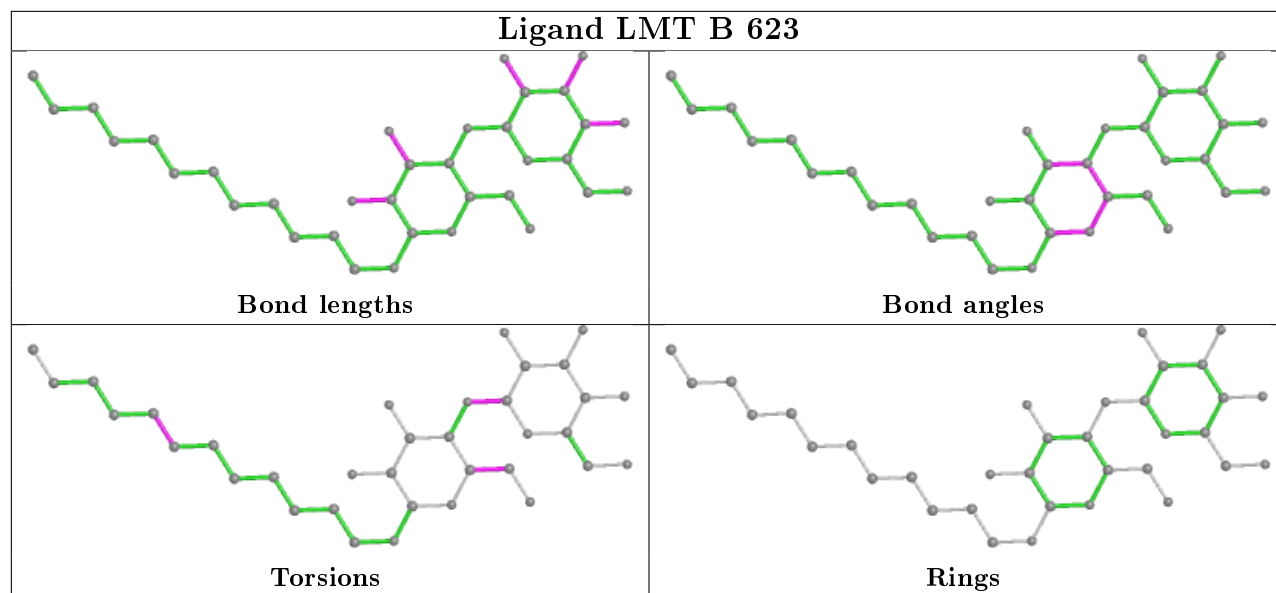




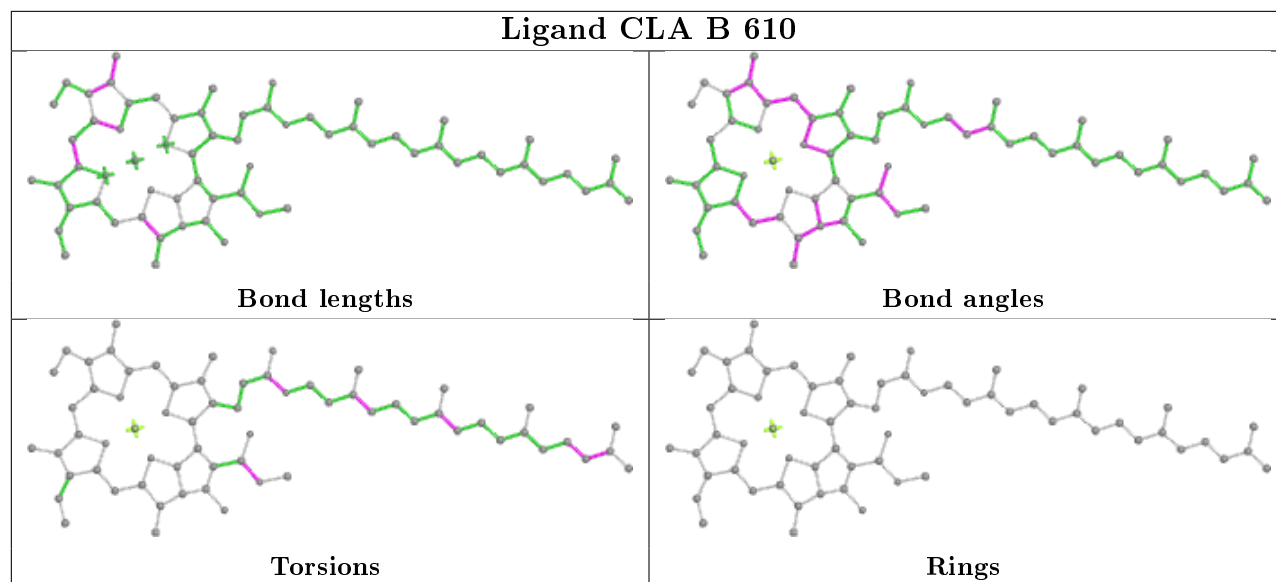




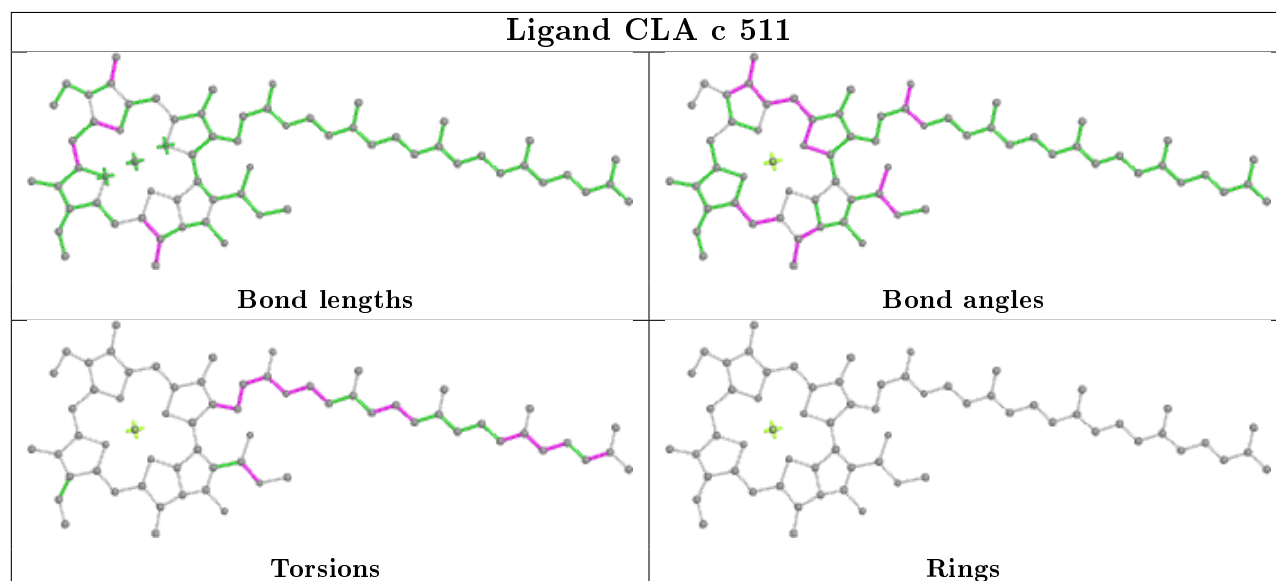




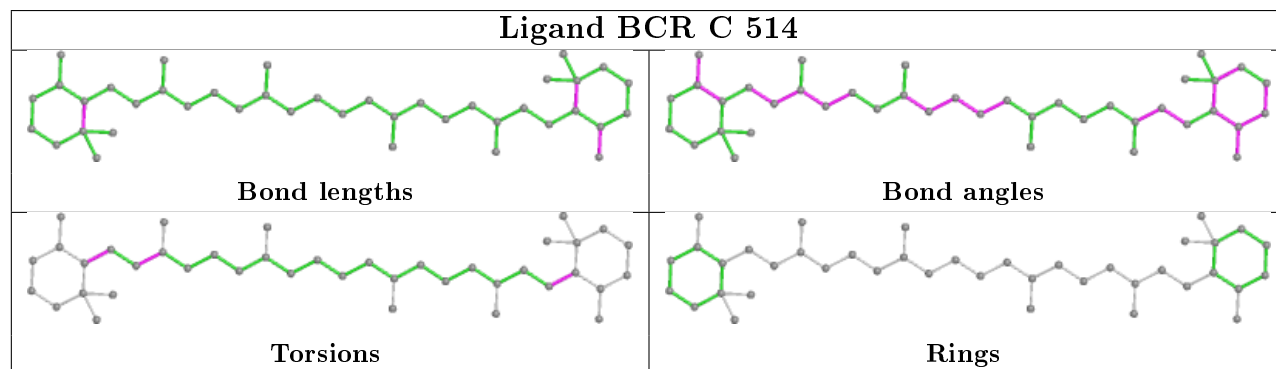
## Ligand CLA B 610



## Ligand CLA c 511

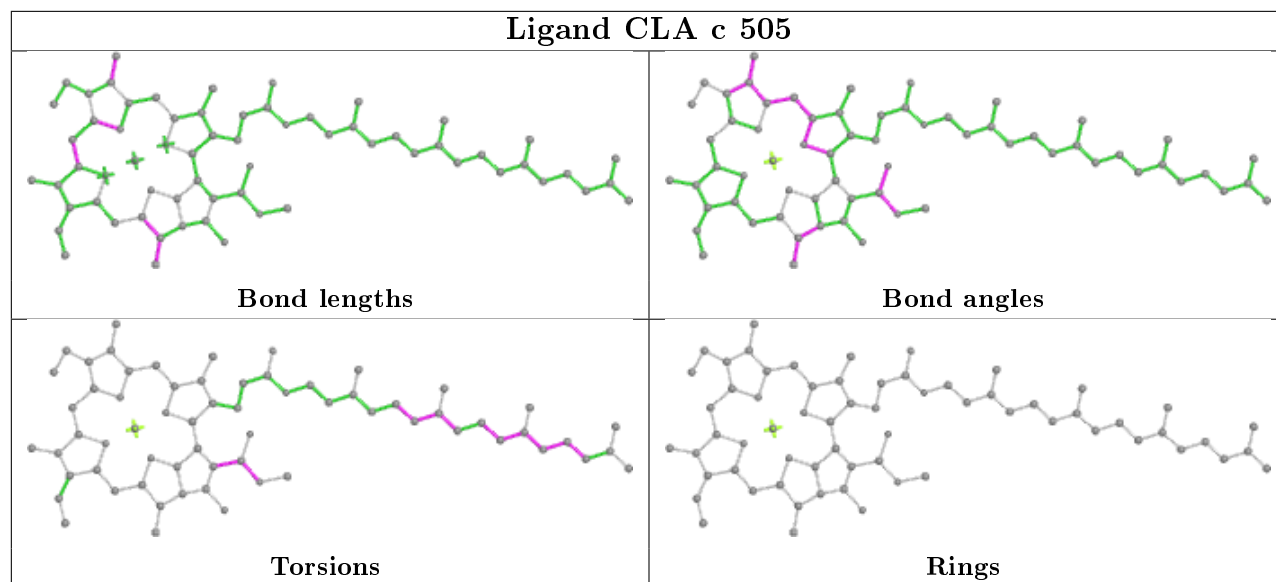


## Ligand BCR C 514

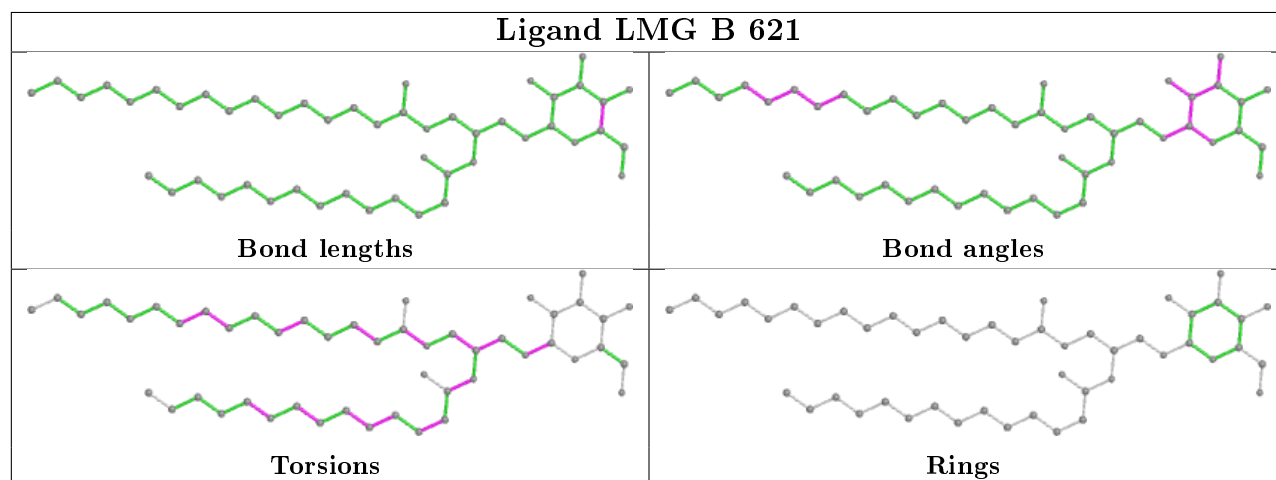




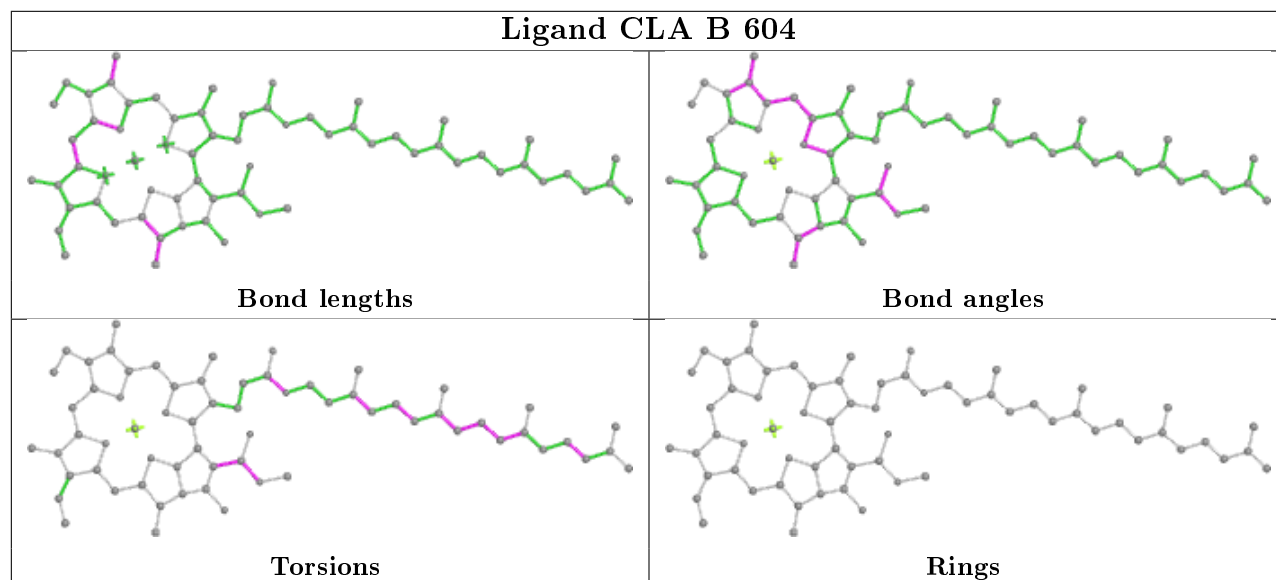
## Ligand CLA c 505

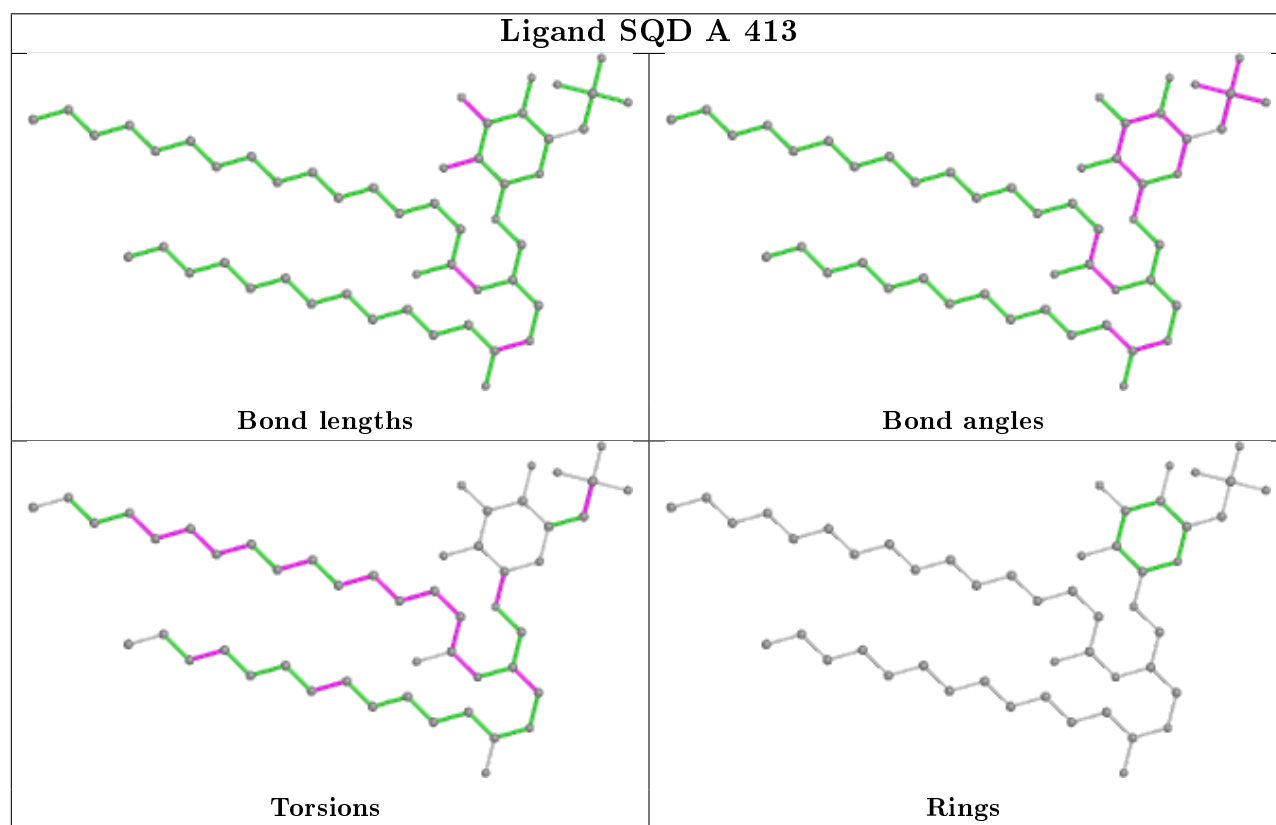
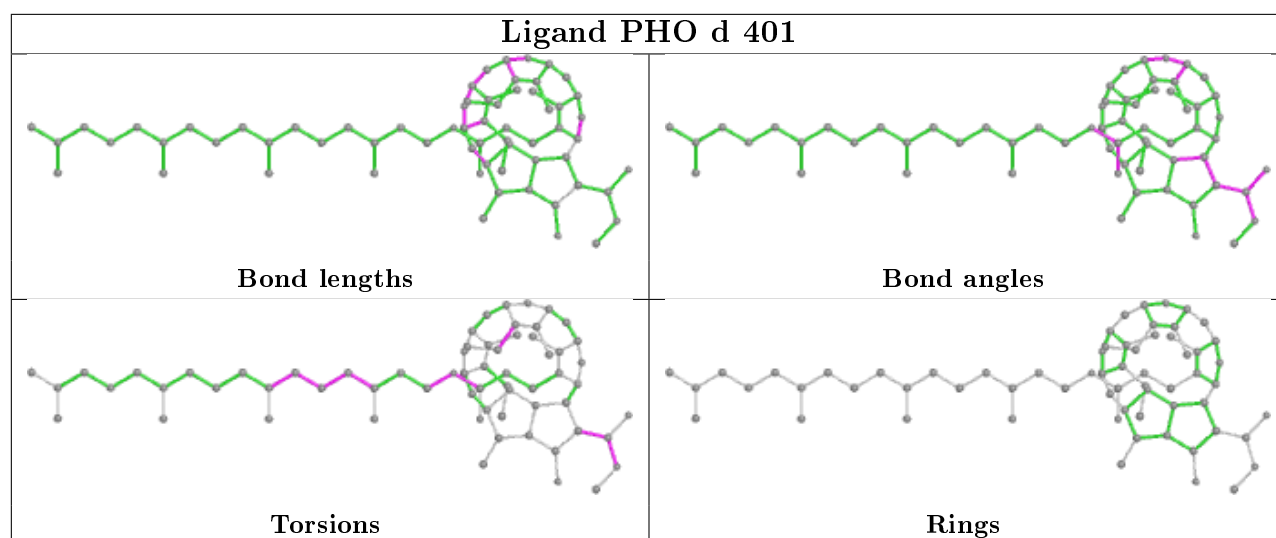


## Ligand LMG B 621

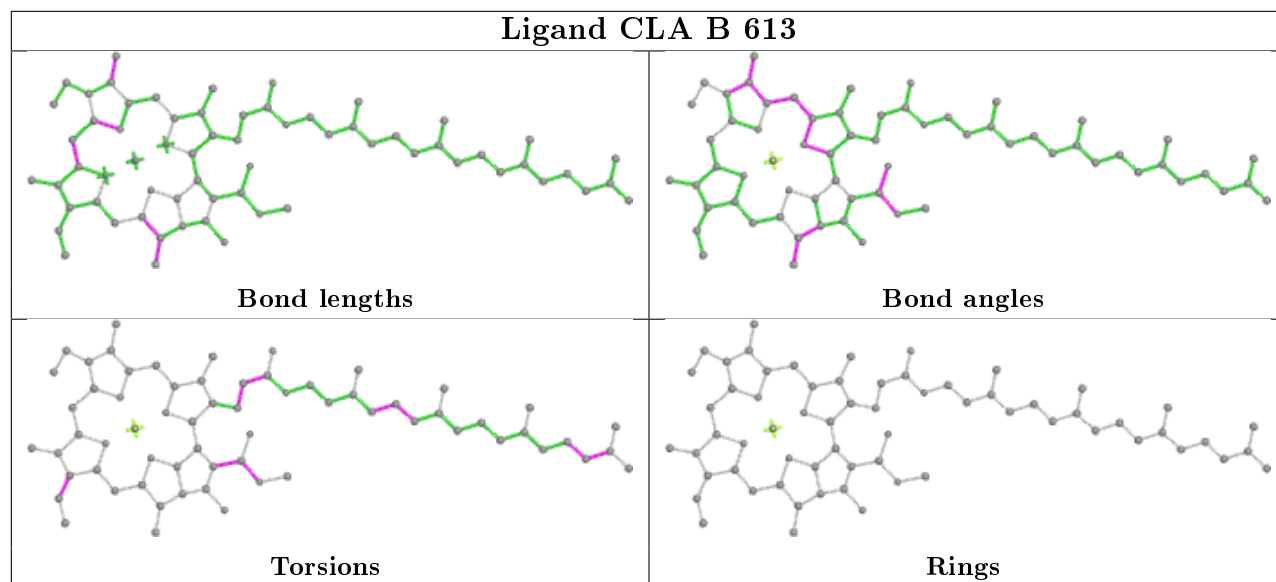


## Ligand CLA B 604

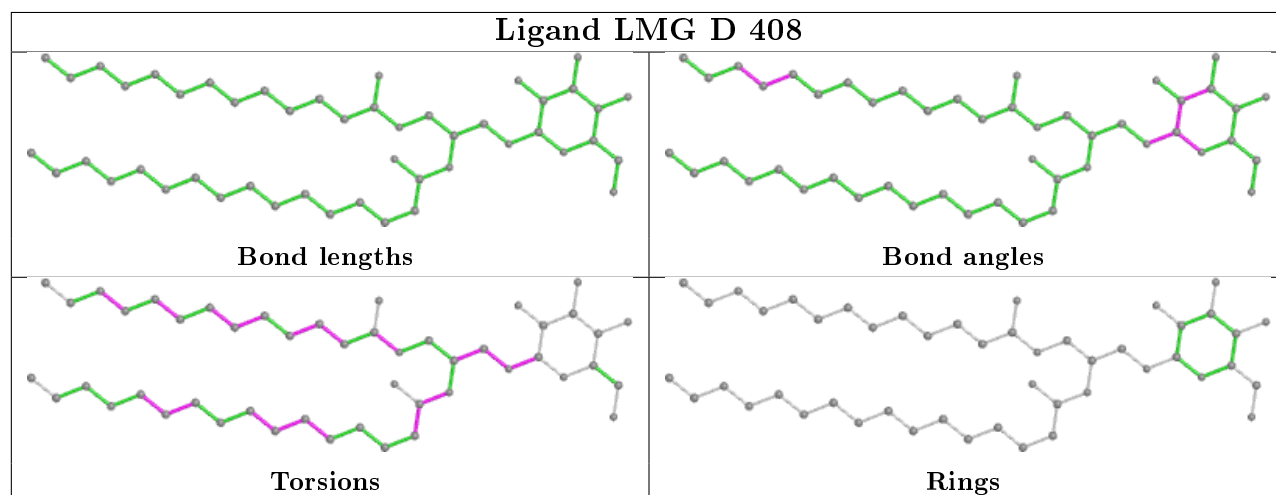




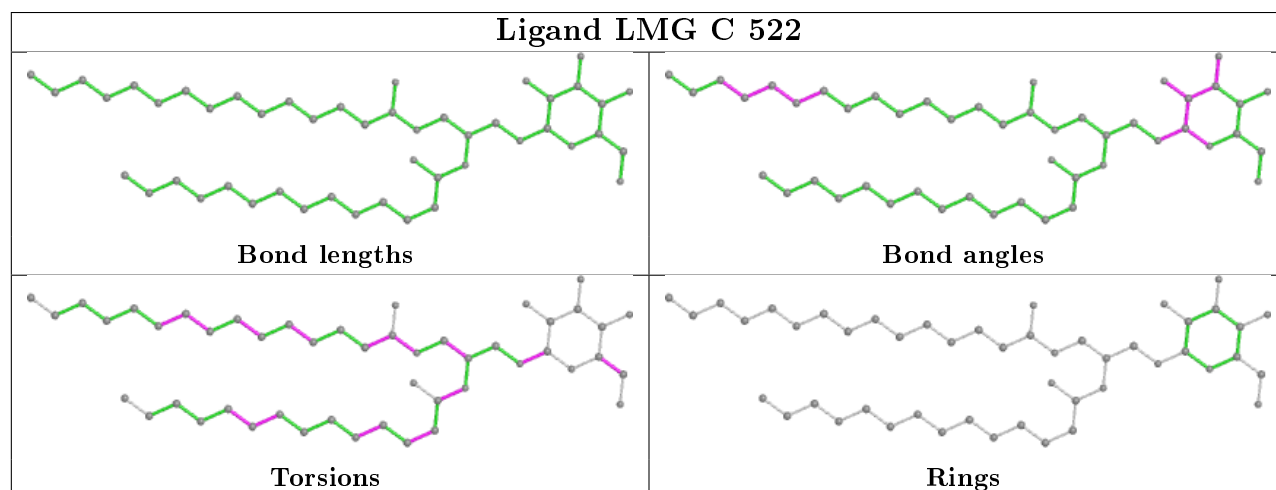
## Ligand CLA B 613

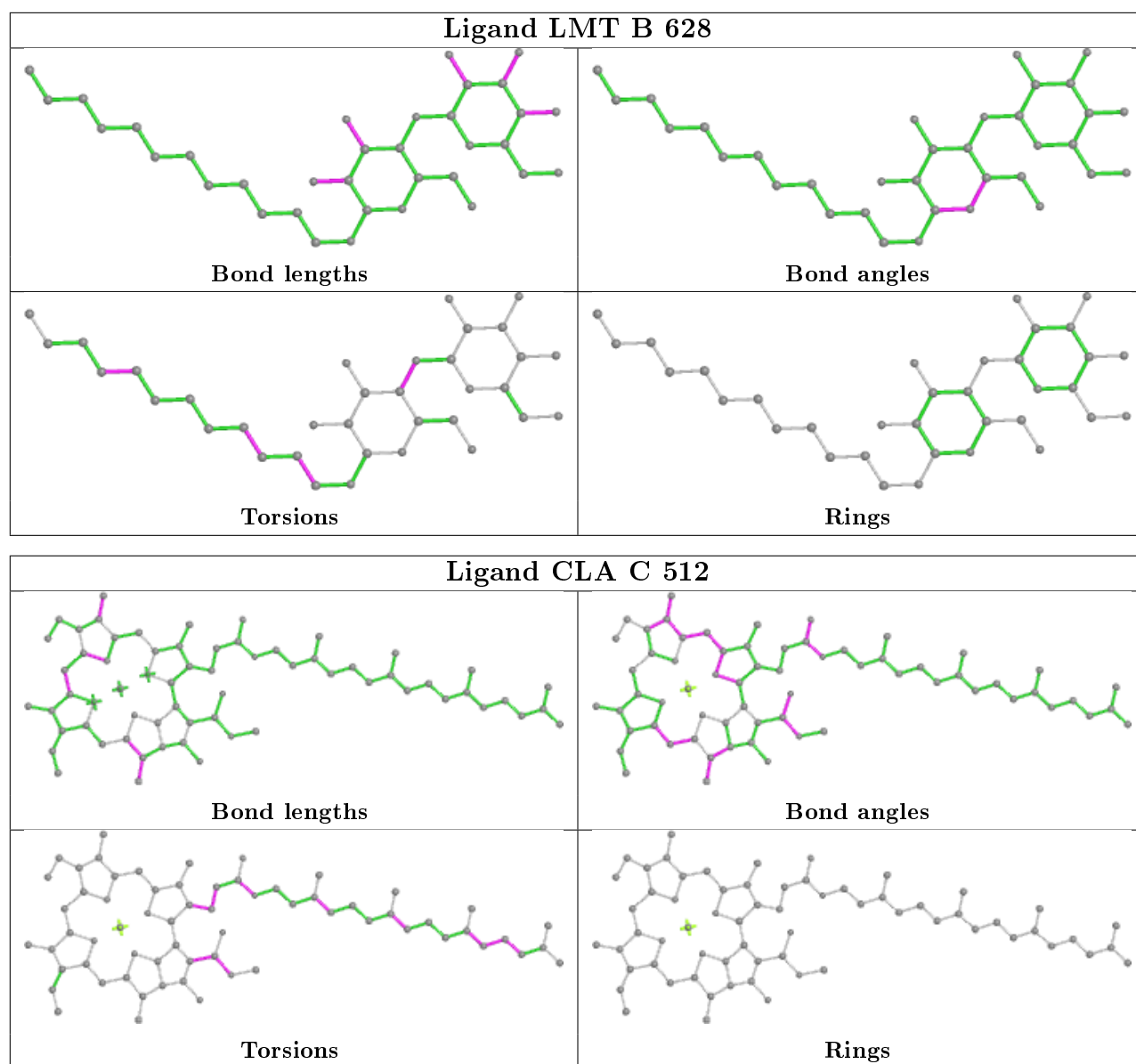


## Ligand LMG D 408



## Ligand LMG C 522





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	172, 174, 175, 176	0
1	a	335/344 (97%)	0.45	28 (8%) 11 10	172, 174, 175, 176	0
2	B	490/510 (96%)	0.22	30 (6%) 21 17	172, 174, 175, 176	0
2	b	490/510 (96%)	0.27	19 (3%) 39 31	172, 174, 175, 176	0
3	C	447/461 (96%)	0.25	24 (5%) 25 22	172, 174, 175, 176	0
3	c	447/461 (96%)	0.13	16 (3%) 42 35	173, 174, 175, 176	0
4	D	340/352 (96%)	0.17	7 (2%) 63 54	171, 174, 175, 176	0
4	d	340/352 (96%)	0.17	11 (3%) 47 38	172, 174, 175, 175	0
5	E	82/84 (97%)	-0.07	1 (1%) 79 70	172, 174, 175, 175	0
5	e	82/84 (97%)	0.03	3 (3%) 41 33	173, 174, 175, 177	0
6	F	35/45 (77%)	-0.14	1 (2%) 51 41	173, 174, 175, 175	0
6	f	35/45 (77%)	-0.45	0 100 100	174, 174, 175, 176	0
7	H	65/66 (98%)	0.42	7 (10%) 5 6	173, 174, 175, 176	0
7	h	65/66 (98%)	0.71	9 (13%) 2 3	173, 174, 175, 176	0
8	I	35/38 (92%)	0.24	0 100 100	173, 174, 175, 176	0
8	i	35/38 (92%)	-0.12	0 100 100	173, 174, 175, 176	0
9	J	34/40 (85%)	-0.11	0 100 100	173, 174, 175, 175	0
9	j	34/40 (85%)	-0.43	0 100 100	173, 174, 175, 175	0
10	K	37/46 (80%)	-0.31	0 100 100	173, 174, 175, 175	0
10	k	37/46 (80%)	0.15	1 (2%) 54 45	174, 174, 175, 176	0
11	L	37/37 (100%)	0.35	1 (2%) 54 45	172, 174, 175, 175	0
11	l	37/37 (100%)	0.16	0 100 100	173, 174, 175, 176	0
12	M	34/36 (94%)	0.21	1 (2%) 51 41	172, 174, 174, 176	0
12	m	34/36 (94%)	0.11	2 (5%) 22 19	173, 173, 174, 175	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/272 (89%)	0.47	16 (6%) 18 15	172, 174, 175, 176	0
13	o	243/272 (89%)	0.47	13 (5%) 26 23	172, 174, 175, 176	0
14	T	32/32 (100%)	0.27	2 (6%) 20 16	173, 174, 176, 176	0
14	t	32/32 (100%)	0.34	3 (9%) 8 8	173, 174, 175, 176	0
15	U	97/134 (72%)	0.46	7 (7%) 15 13	172, 174, 174, 175	0
15	u	97/134 (72%)	0.63	9 (9%) 8 8	173, 174, 175, 175	0
16	V	137/163 (84%)	0.05	0 100 100	172, 174, 175, 175	0
16	v	137/163 (84%)	0.49	10 (7%) 15 12	173, 174, 175, 176	0
17	g	28/46 (60%)	0.32	1 (3%) 42 35	174, 175, 176, 176	0
17	y	28/46 (60%)	-0.06	0 100 100	173, 174, 176, 176	0
18	X	37/41 (90%)	0.31	1 (2%) 54 45	173, 174, 175, 176	0
18	x	37/41 (90%)	0.84	7 (18%) 1 2	173, 175, 175, 175	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.26	1 (1%) 72 62	173, 174, 175, 176	0
20	z	62/62 (100%)	0.88	5 (8%) 12 11	173, 175, 176, 176	0
All	All	5214/5674 (91%)	0.27	264 (5%) 28 24	171, 174, 175, 177	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	11	THR	5.6
1	a	224	ILE	5.2
5	e	84	LYS	5.0
15	U	38	GLU	4.9
3	C	135	ARG	4.6
13	O	90	GLU	4.3
5	E	84	LYS	4.3
3	C	332	GLN	4.3
14	t	31	LYS	4.3
1	a	191	ASN	4.3
1	a	165	GLN	4.2
4	d	295	SER	4.1
7	h	66	GLY	4.1
7	h	23	PRO	3.9
1	A	299	GLY	3.9
1	A	175	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	b	217	ILE	3.8
3	c	200	THR	3.8
14	t	32	LYS	3.7
7	H	56	ASP	3.7
18	x	42	GLN	3.7
13	o	169	LYS	3.7
15	U	39	LEU	3.7
1	a	225	ARG	3.7
20	z	1	MET	3.7
7	h	26	GLY	3.6
18	x	12	ILE	3.6
15	u	53	GLU	3.6
10	k	14	ALA	3.5
1	A	190	HIS	3.5
2	B	69	LEU	3.5
3	C	184	GLY	3.5
1	A	293	MET	3.5
5	e	82	GLN	3.4
3	C	136	GLY	3.4
15	u	58	ASN	3.4
2	B	295	GLY	3.3
2	B	162	PHE	3.3
1	a	175	GLY	3.3
3	C	137	PRO	3.3
14	T	28	ARG	3.3
7	H	66	GLY	3.3
3	C	147	PHE	3.3
1	a	282	GLY	3.2
1	A	177	SER	3.2
3	c	201	ASN	3.2
7	H	5	THR	3.2
7	h	4	ARG	3.2
3	C	402	GLY	3.2
3	C	140	LEU	3.1
4	D	190	ASN	3.1
16	v	51	GLN	3.1
1	a	223	LEU	3.1
2	B	309	LEU	3.1
2	b	411	PHE	3.1
1	A	15	GLU	3.1
1	a	226	GLU	3.1
2	B	179	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	379	ALA	3.0
7	H	63	LYS	3.0
1	A	266	ASN	3.0
3	c	202	PRO	3.0
3	c	372	PRO	3.0
14	T	27	PRO	3.0
1	a	325	ASN	3.0
16	v	47	LEU	3.0
1	a	178	GLY	3.0
7	h	24	GLY	3.0
15	u	74	THR	3.0
2	b	303	SER	3.0
1	a	190	HIS	3.0
1	A	179	THR	3.0
18	X	42	GLN	2.9
2	B	259	GLY	2.9
2	B	474	LEU	2.9
1	A	298	ASN	2.9
7	H	64	ALA	2.9
13	o	124	GLU	2.9
15	U	40	VAL	2.9
15	u	107	GLU	2.9
1	A	138	GLY	2.8
3	C	149	TYR	2.8
2	B	164	PRO	2.8
3	c	403	SER	2.8
13	O	170	GLY	2.8
13	o	31	LEU	2.8
2	b	301	ALA	2.8
1	a	299	GLY	2.8
16	v	131	ARG	2.8
18	x	17	LYS	2.8
13	O	222	GLN	2.8
7	h	3	ARG	2.8
1	A	196	PRO	2.8
2	b	482	ILE	2.8
13	o	240	THR	2.8
2	b	218	LEU	2.8
4	D	24	ARG	2.7
1	A	195	HIS	2.7
1	A	181	ASN	2.7
4	d	221	THR	2.7

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Mol	Chain	Res	Type	RSRZ
15	u	65	PHE	2.7
13	O	262	GLN	2.7
2	B	132	ALA	2.7
1	a	181	ASN	2.7
3	C	44	ASN	2.7
13	O	218	LEU	2.6
16	v	133	LEU	2.6
1	a	239	PHE	2.6
2	B	294	SER	2.6
12	m	5	GLN	2.6
13	O	79	LYS	2.6
13	O	46	PRO	2.6
3	c	329	GLY	2.6
3	C	266	TRP	2.6
15	u	57	LEU	2.6
2	B	477	ASP	2.6
4	D	174	GLY	2.6
1	a	19	ASN	2.5
3	C	183	GLY	2.5
15	u	72	TYR	2.5
3	C	151	TRP	2.5
1	a	198	HIS	2.5
3	C	473	ASP	2.5
13	O	269	ILE	2.5
13	o	154	SER	2.5
3	c	260	ALA	2.5
2	B	127	ARG	2.5
4	d	236	ASN	2.5
2	b	119	ASP	2.5
2	b	120	LEU	2.5
13	O	84	ASN	2.5
1	a	187	GLN	2.5
1	A	10	SER	2.5
13	o	173	ASN	2.4
13	O	195	ASP	2.4
6	F	11	VAL	2.4
13	o	189	GLY	2.4
2	b	490	GLN	2.4
20	z	4	LEU	2.4
2	B	129	GLY	2.4
16	v	138	LEU	2.4
2	B	161	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
11	L	33	SER	2.4
2	B	402	TYR	2.4
18	x	16	LEU	2.4
2	B	84	THR	2.4
7	h	18	TYR	2.4
1	A	14	TRP	2.4
2	b	402	TYR	2.4
20	z	47	TRP	2.4
15	u	75	LEU	2.4
1	a	319	ASP	2.4
4	d	195	PRO	2.4
13	o	84	ASN	2.4
13	o	168	PHE	2.3
13	O	58	ILE	2.3
15	u	52	GLY	2.3
16	v	130	MET	2.3
2	B	128	THR	2.3
1	a	170	ASP	2.3
1	A	178	GLY	2.3
3	c	203	THR	2.3
1	A	222	SER	2.3
2	B	293	ALA	2.3
13	O	169	LYS	2.3
13	O	91	PHE	2.3
1	a	137	LEU	2.3
12	M	2	GLU	2.3
7	h	27	THR	2.3
1	a	199	GLN	2.3
2	B	397	VAL	2.3
3	c	259	TRP	2.3
1	A	165	GLN	2.3
3	C	148	GLY	2.3
4	d	194	ASN	2.3
2	b	302	TRP	2.3
5	e	8	ARG	2.3
16	v	31	PRO	2.3
12	m	2	GLU	2.3
4	d	203	GLY	2.3
1	A	80	GLY	2.3
2	b	133	LEU	2.2
13	o	239	GLY	2.2
17	g	27	MET	2.2

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Mol	Chain	Res	Type	RSRZ
15	U	127	ARG	2.2
3	C	46	SER	2.2
20	Z	62	VAL	2.2
3	c	180	MET	2.2
15	U	121	LEU	2.2
4	d	176	ALA	2.2
3	C	144	SER	2.2
1	A	169	SER	2.2
4	d	13	GLY	2.2
2	B	130	GLU	2.2
13	O	119	LEU	2.2
3	C	154	LYS	2.2
1	A	262	TYR	2.2
16	v	103	LYS	2.2
13	o	238	ALA	2.2
2	b	216	HIS	2.2
3	c	373	ASN	2.2
2	B	122	LEU	2.2
1	a	298	ASN	2.2
1	a	301	ASN	2.2
1	a	177	SER	2.2
1	A	16	ARG	2.2
7	H	62	TRP	2.2
7	H	55	LEU	2.2
3	C	134	ILE	2.2
3	c	191	PRO	2.2
3	c	388	GLN	2.2
4	d	220	ASN	2.2
3	C	261	ARG	2.2
20	z	30	PRO	2.1
1	a	169	SER	2.1
3	C	336	GLY	2.1
15	U	122	VAL	2.1
4	D	297	ASP	2.1
3	c	365	TRP	2.1
2	B	411	PHE	2.1
2	b	420	TYR	2.1
2	B	124	ARG	2.1
13	O	171	GLU	2.1
2	B	354	LEU	2.1
3	C	403	SER	2.1
2	B	125	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	75	ASN	2.1
3	C	141	GLU	2.1
1	a	179	THR	2.1
18	x	13	THR	2.1
1	A	183	MET	2.1
2	b	339	ALA	2.1
3	c	212	TYR	2.1
4	D	194	ASN	2.1
16	v	117	VAL	2.1
1	A	76	ASN	2.1
4	d	297	ASP	2.1
4	D	192	THR	2.1
16	v	132	ASN	2.1
20	z	29	SER	2.1
13	o	216	PHE	2.1
1	a	173	PRO	2.1
1	a	322	ASN	2.1
18	x	23	LEU	2.1
2	B	183	PRO	2.1
15	U	54	LYS	2.1
3	C	212	TYR	2.0
2	B	163	GLY	2.0
13	O	50	ASP	2.0
2	B	166	MET	2.0
7	h	22	ALA	2.0
4	D	197	HIS	2.0
14	t	29	ILE	2.0
13	o	164	THR	2.0
1	A	11	ALA	2.0
3	c	389	GLU	2.0
2	B	133	LEU	2.0
2	b	403	GLY	2.0
4	d	191	TRP	2.0
2	b	137	LYS	2.0
2	b	304	ALA	2.0
1	A	12	ASN	2.0
1	A	342	ASP	2.0
2	B	353	GLU	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(Å <sup>2</sup> )	Q<0.9
35	CA	o	301	1/1	0.32	0.68	180,180,180,180	0
31	LMT	I	102	35/35	0.40	0.94	173,175,176,178	0
23	PL9	J	101	35/55	0.43	0.54	172,175,176,176	0
23	PL9	j	101	35/55	0.49	0.37	173,175,175,176	0
24	BCR	J	102	40/40	0.50	0.44	172,174,176,177	0
31	LMT	i	102	35/35	0.52	1.29	173,175,176,177	0
31	LMT	d	409	31/35	0.53	0.66	172,175,177,177	0
35	CA	O	301	1/1	0.53	0.38	177,177,177,177	0
31	LMT	b	627	35/35	0.54	1.22	173,175,177,177	0
31	LMT	b	626	35/35	0.59	0.69	172,175,176,177	0
22	CLA	b	605	65/65	0.61	1.14	172,175,176,176	0
27	LMG	A	415	42/55	0.62	0.53	171,174,176,177	0
22	CLA	B	601	65/65	0.62	0.85	172,175,176,177	0
27	LMG	C	518	45/55	0.62	1.09	171,174,175,175	0
27	LMG	E	101	44/55	0.63	0.56	170,174,176,177	0
24	BCR	f	102	40/40	0.63	0.47	171,173,175,175	0
24	BCR	j	102	40/40	0.63	0.34	173,175,177,178	0
24	BCR	g	101	40/40	0.64	0.78	173,174,175,175	0
31	LMT	D	410	31/35	0.64	0.93	174,175,176,176	0
22	CLA	b	619	65/65	0.65	0.77	172,174,175,175	0
27	LMG	a	402	42/55	0.65	0.49	171,174,176,176	0
26	LHG	C	519	37/49	0.65	0.48	172,174,179,183	0
27	LMG	I	101	43/55	0.66	1.04	172,174,177,177	0
25	DGD	d	408	63/66	0.66	0.77	172,175,177,178	0
31	LMT	B	628	35/35	0.66	0.46	172,174,177,178	0
22	CLA	c	502	65/65	0.66	0.54	173,174,175,175	0
24	BCR	c	514	40/40	0.67	0.71	172,173,175,175	0
24	BCR	D	411	40/40	0.67	0.44	171,173,174,175	0
31	LMT	B	622	35/35	0.67	0.88	171,175,177,177	0
23	PL9	D	407	55/55	0.68	0.39	171,173,174,175	0
23	PL9	d	406	55/55	0.68	0.39	172,173,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	PL9	A	406	45/55	0.69	0.43	172,174,175,175	0
24	BCR	H	102	40/40	0.69	0.94	173,174,175,176	0
27	LMG	a	413	51/55	0.69	0.42	172,173,175,176	0
25	DGD	D	409	63/66	0.70	0.81	172,174,176,178	0
31	LMT	b	604	35/35	0.70	0.47	172,174,176,176	0
22	CLA	C	502	65/65	0.70	0.53	173,174,174,175	0
27	LMG	c	518	45/55	0.71	1.01	172,174,176,176	0
24	BCR	x	101	40/40	0.71	0.86	173,174,175,175	0
25	DGD	A	408	56/66	0.71	0.45	172,174,175,176	0
25	DGD	b	601	52/66	0.72	0.47	172,174,176,177	0
32	PHO	d	401	64/64	0.72	0.42	172,173,174,174	0
24	BCR	B	616	40/40	0.72	0.43	172,173,174,175	0
27	LMG	C	522	48/55	0.73	0.36	172,174,174,175	0
27	LMG	M	101	42/55	0.73	0.53	173,174,176,176	0
25	DGD	a	411	56/66	0.73	0.44	173,174,175,176	0
30	SQD	A	413	51/54	0.73	0.37	172,174,175,176	0
24	BCR	a	410	40/40	0.73	0.68	172,173,174,175	0
22	CLA	a	408	65/65	0.74	0.82	173,174,175,175	0
27	LMG	i	101	43/55	0.74	0.80	172,174,177,178	0
26	LHG	c	519	37/49	0.74	0.35	172,174,178,181	0
30	SQD	d	402	43/54	0.75	0.83	172,174,176,178	0
24	BCR	B	617	40/40	0.75	0.44	172,173,174,174	0
27	LMG	e	101	44/55	0.75	0.39	171,174,175,176	0
23	PL9	a	409	45/55	0.76	0.38	171,173,174,175	0
31	LMT	B	627	35/35	0.76	0.55	172,175,177,177	0
28	CL	A	411	1/1	0.76	0.42	172,172,172,172	0
31	LMT	M	103	35/35	0.76	0.47	172,173,175,176	0
25	DGD	B	625	52/66	0.76	0.56	172,175,177,177	0
22	CLA	B	613	65/65	0.76	0.46	172,174,174,175	0
25	DGD	b	624	58/66	0.76	0.40	171,173,174,175	0
22	CLA	C	507	65/65	0.77	0.40	173,174,175,177	0
31	LMT	M	102	35/35	0.77	0.46	172,174,175,175	0
35	CA	k	101	1/1	0.77	0.20	172,172,172,172	0
25	DGD	C	517	66/66	0.77	0.34	172,173,174,175	0
22	CLA	C	506	65/65	0.77	0.73	172,174,175,175	0
24	BCR	y	101	40/40	0.77	1.00	173,173,174,175	0
27	LMG	B	624	49/55	0.78	0.31	171,173,174,175	0
27	LMG	D	412	46/55	0.78	0.40	172,174,175,175	0
24	BCR	C	514	40/40	0.78	0.83	172,173,175,175	0
22	CLA	c	512	65/65	0.78	0.68	172,174,176,176	0
27	LMG	m	101	42/55	0.78	0.45	170,174,175,175	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
27	LMG	b	625	49/55	0.78	0.34	172,174,175,175	0
22	CLA	h	101	65/65	0.78	0.53	171,174,175,175	0
24	BCR	b	622	40/40	0.78	0.36	171,172,173,173	0
24	BCR	A	407	40/40	0.79	0.48	171,173,174,174	0
32	PHO	D	402	64/64	0.79	0.37	171,173,175,175	0
24	BCR	C	521	40/40	0.79	0.82	172,174,175,176	0
22	CLA	C	505	65/65	0.79	0.45	172,174,175,176	0
27	LMG	A	410	51/55	0.79	0.35	171,173,174,175	0
30	SQD	F	102	45/54	0.79	0.69	172,175,177,178	0
30	SQD	B	626	47/54	0.79	0.46	170,174,176,178	0
31	LMT	B	623	35/35	0.79	0.50	173,174,177,177	0
25	DGD	c	517	66/66	0.80	0.35	172,173,175,176	0
24	BCR	b	623	40/40	0.80	0.76	171,173,174,174	0
24	BCR	B	619	40/40	0.80	0.83	172,173,174,175	0
30	SQD	b	602	47/54	0.80	0.38	171,174,176,178	0
27	LMG	c	522	48/55	0.81	0.29	172,174,175,176	0
31	LMT	b	603	35/35	0.81	0.44	172,174,175,176	0
22	CLA	B	603	65/65	0.81	0.49	171,173,175,175	0
22	CLA	b	609	65/65	0.81	0.55	172,174,175,175	0
35	CA	K	101	1/1	0.81	0.35	177,177,177,177	0
22	CLA	b	613	65/65	0.81	0.67	172,174,175,175	0
24	BCR	c	521	40/40	0.81	1.26	172,174,175,175	0
22	CLA	b	618	65/65	0.82	0.66	172,174,175,175	0
22	CLA	c	503	65/65	0.82	0.57	172,174,175,175	0
22	CLA	b	617	65/65	0.82	0.45	173,173,175,176	0
22	CLA	C	520	65/65	0.82	0.33	172,174,175,176	0
30	SQD	D	403	43/54	0.82	0.41	172,174,177,180	0
22	CLA	b	607	65/65	0.82	0.43	172,173,175,176	0
25	DGD	C	515	53/66	0.83	0.36	172,173,174,174	0
24	BCR	c	513	40/40	0.83	0.87	172,173,175,175	0
26	LHG	a	412	39/49	0.83	0.28	171,174,176,177	0
24	BCR	B	618	40/40	0.83	0.32	171,172,174,174	0
22	CLA	A	405	65/65	0.83	0.62	172,174,175,176	0
22	CLA	C	510	65/65	0.83	0.46	172,173,175,175	0
22	CLA	C	512	65/65	0.83	0.88	172,174,176,177	0
22	CLA	a	405	65/65	0.83	0.58	170,172,174,175	0
25	DGD	C	516	62/66	0.84	0.29	171,174,175,176	0
22	CLA	B	610	65/65	0.84	0.34	172,174,174,175	0
30	SQD	f	103	45/54	0.84	0.52	172,174,176,178	0
25	DGD	B	620	58/66	0.84	0.33	171,173,175,176	0
22	CLA	C	504	65/65	0.84	0.41	171,173,175,175	0
22	CLA	d	404	65/65	0.84	0.45	172,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	SQD	a	401	54/54	0.84	0.58	172,174,176,178	0
22	CLA	c	508	65/65	0.84	0.56	172,174,175,175	0
32	PHO	D	401	64/64	0.84	0.40	171,173,174,175	0
22	CLA	b	612	65/65	0.84	0.66	171,174,175,176	0
22	CLA	a	406	65/65	0.85	0.36	172,174,175,176	0
22	CLA	B	607	65/65	0.85	0.42	172,174,174,175	0
22	CLA	c	505	65/65	0.85	0.45	172,174,175,175	0
22	CLA	c	501	65/65	0.85	0.45	172,174,175,175	0
24	BCR	b	621	40/40	0.85	0.33	171,173,174,174	0
30	SQD	a	415	51/54	0.85	0.29	173,174,175,176	0
26	LHG	A	409	39/49	0.85	0.28	172,173,175,176	0
22	CLA	C	509	65/65	0.85	0.34	173,173,174,174	0
22	CLA	b	606	65/65	0.85	0.61	172,173,174,174	0
30	SQD	A	414	54/54	0.85	0.40	171,174,176,179	0
22	CLA	d	405	65/65	0.86	0.45	172,174,175,175	0
27	LMG	d	407	48/55	0.86	0.28	171,173,175,175	0
22	CLA	B	615	65/65	0.86	0.66	172,174,175,175	0
32	PHO	a	407	64/64	0.86	0.26	173,174,175,175	0
24	BCR	C	513	40/40	0.86	0.77	172,173,174,174	0
22	CLA	B	609	65/65	0.86	0.53	172,174,175,175	0
22	CLA	C	503	65/65	0.86	0.41	172,174,175,176	0
21	FE2	a	403	1/1	0.86	0.18	175,175,175,175	0
22	CLA	c	510	65/65	0.86	0.53	173,174,175,176	0
22	CLA	c	506	65/65	0.86	0.55	173,174,175,175	0
22	CLA	H	101	65/65	0.86	0.35	172,174,175,175	0
22	CLA	B	605	65/65	0.86	0.72	172,173,175,176	0
25	DGD	c	515	53/66	0.86	0.36	171,174,175,177	0
22	CLA	C	508	65/65	0.87	0.86	172,174,175,175	0
22	CLA	c	509	65/65	0.87	0.32	172,173,175,175	0
22	CLA	D	406	65/65	0.87	0.64	172,174,175,176	0
22	CLA	c	520	65/65	0.87	0.36	173,174,174,175	0
22	CLA	B	604	65/65	0.87	0.67	172,173,175,175	0
27	LMG	D	408	48/55	0.87	0.28	170,173,175,175	0
25	DGD	c	516	62/66	0.87	0.30	172,174,175,175	0
22	CLA	A	404	65/65	0.87	0.47	170,173,174,175	0
22	CLA	C	501	65/65	0.87	0.40	172,174,174,175	0
22	CLA	b	608	65/65	0.88	0.51	172,173,175,176	0
22	CLA	a	404	65/65	0.88	0.54	172,173,174,176	0
34	HEM	V	201	43/43	0.88	0.45	172,173,175,175	0
27	LMG	B	621	49/55	0.88	0.26	172,173,174,174	0
22	CLA	b	614	65/65	0.88	0.30	172,173,174,175	0
22	CLA	B	606	65/65	0.88	0.34	172,173,174,175	0

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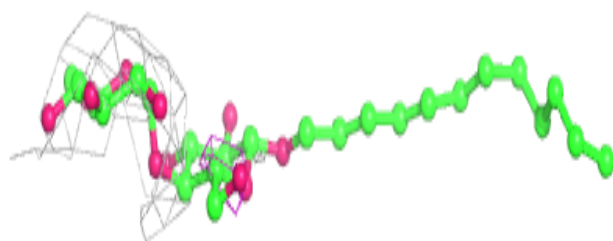
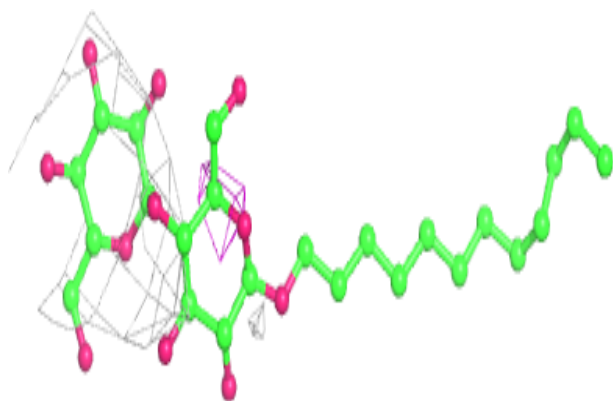
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	CLA	D	405	65/65	0.89	0.36	172,173,174,175	0
22	CLA	B	614	65/65	0.89	0.62	172,174,175,175	0
22	CLA	c	504	65/65	0.89	0.33	172,174,175,175	0
22	CLA	c	511	65/65	0.89	0.62	172,174,175,176	0
22	CLA	C	511	65/65	0.90	0.92	172,174,175,175	0
22	CLA	A	402	65/65	0.90	0.42	172,173,174,175	0
22	CLA	B	612	65/65	0.90	0.28	171,173,175,175	0
34	HEM	v	201	43/43	0.90	0.55	171,174,175,175	0
24	BCR	b	620	40/40	0.90	0.32	172,173,174,175	0
22	CLA	B	608	65/65	0.90	0.50	172,174,175,175	0
22	CLA	b	610	65/65	0.90	0.33	172,173,175,175	0
27	LMG	d	410	46/55	0.91	0.23	172,173,175,175	0
34	HEM	F	101	43/43	0.91	0.48	173,174,175,176	0
33	BCT	d	403	4/4	0.91	0.92	174,174,175,176	0
28	CL	a	416	1/1	0.91	0.33	173,173,173,173	0
22	CLA	c	507	65/65	0.91	0.24	172,174,175,176	0
21	FE2	A	401	1/1	0.92	0.18	170,170,170,170	0
22	CLA	b	615	65/65	0.92	0.40	172,173,174,175	0
22	CLA	b	611	65/65	0.92	0.31	172,174,175,175	0
22	CLA	B	611	65/65	0.92	0.36	171,173,174,174	0
22	CLA	B	602	65/65	0.92	0.52	171,173,174,175	0
27	LMG	b	628	49/55	0.93	0.23	172,174,175,175	0
22	CLA	A	403	65/65	0.93	0.54	171,173,174,175	0
34	HEM	f	101	43/43	0.93	0.34	173,174,175,175	0
29	OEX	A	412	10/10	0.93	0.42	165,169,172,173	0
22	CLA	b	616	65/65	0.95	0.29	171,173,174,175	0
33	BCT	D	404	4/4	0.95	0.25	173,174,174,174	0
29	OEX	a	414	10/10	0.96	0.45	168,171,173,177	0

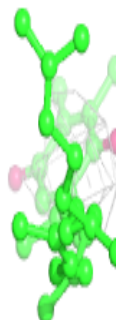
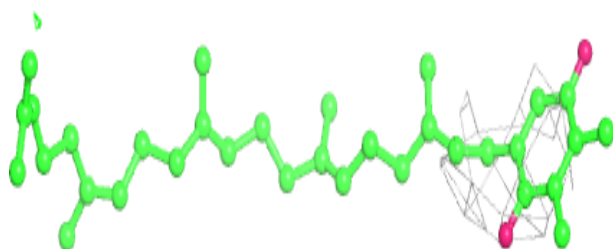
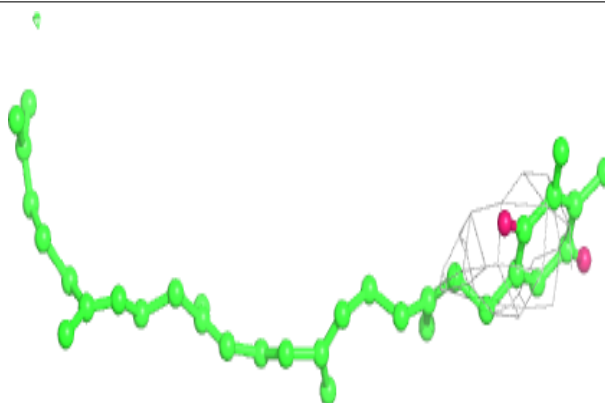
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

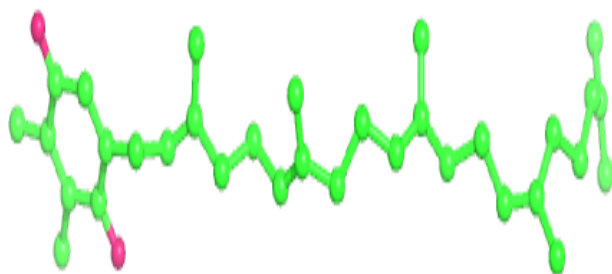
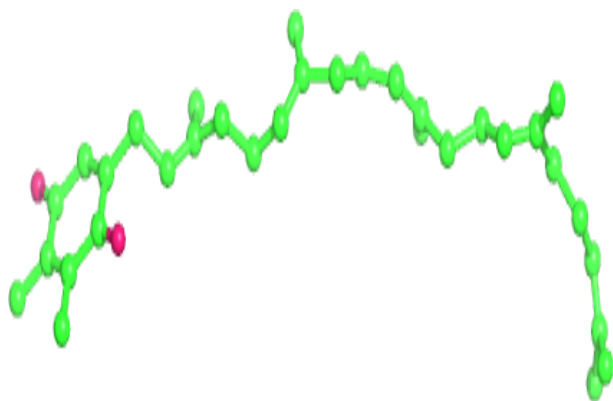
**Electron density around PL9 J 101:**

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

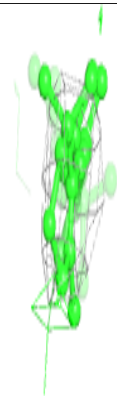
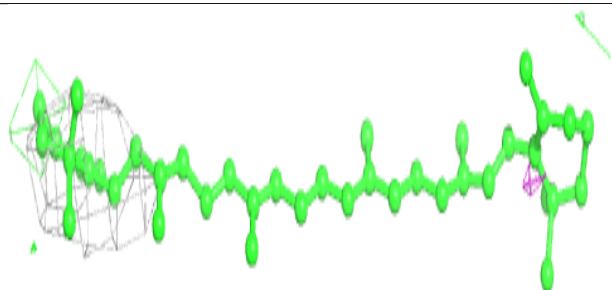
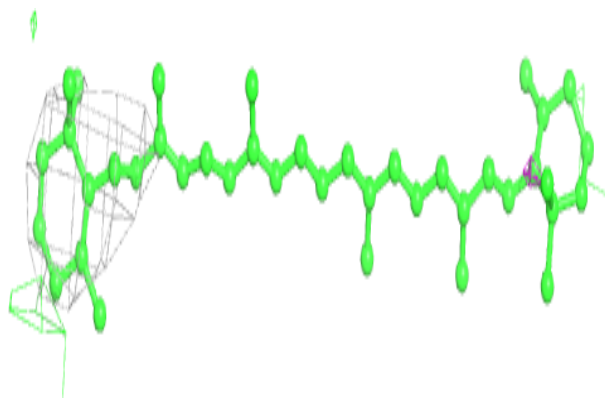


**Electron density around PL9 j 101:**

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

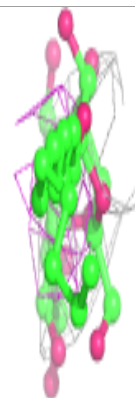
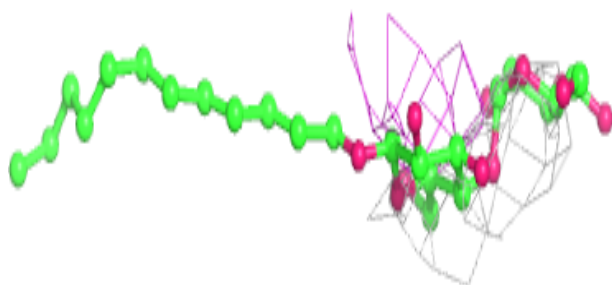
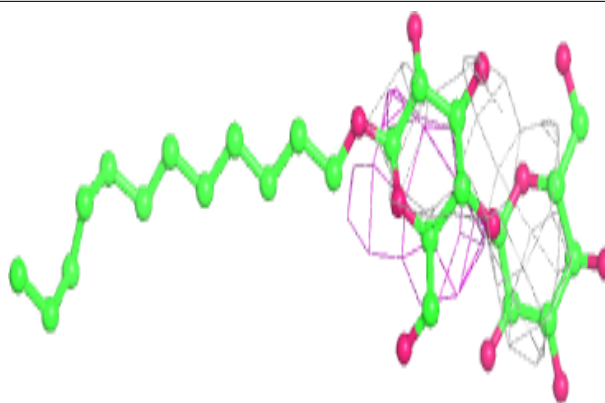
**Electron density around BCR J 102:**

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

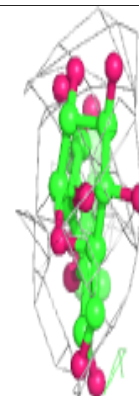
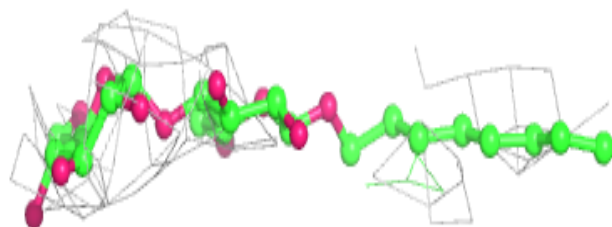
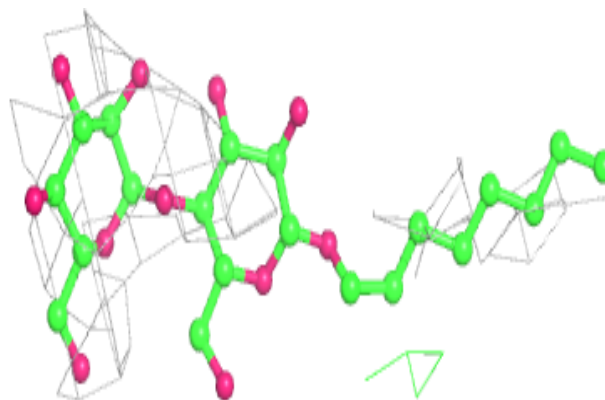


**Electron density around LMT i 102:**

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

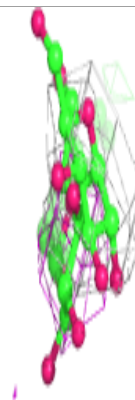
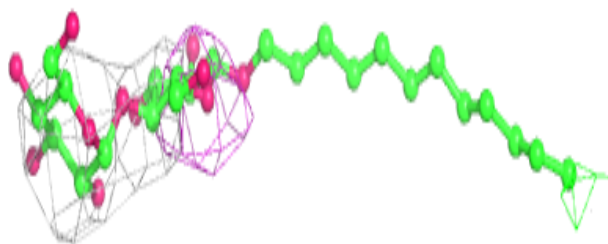
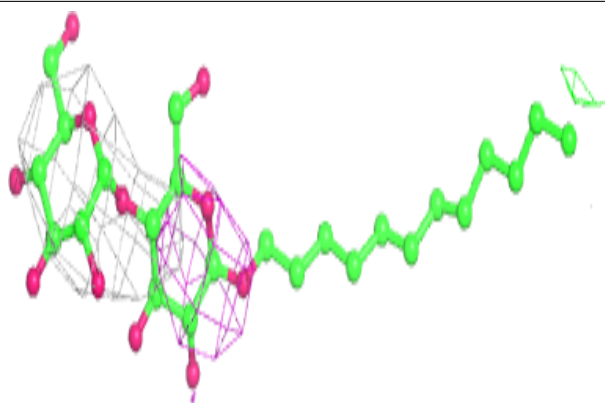
**Electron density around LMT d 409:**

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

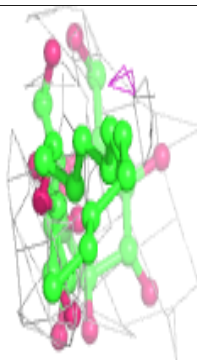
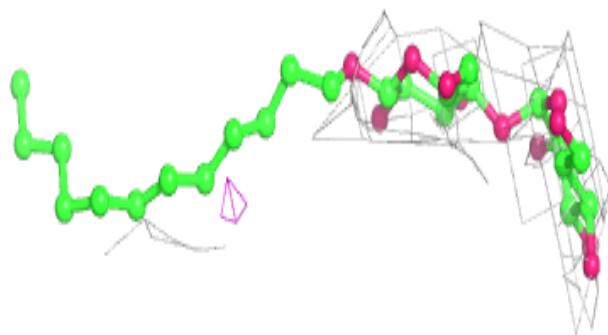
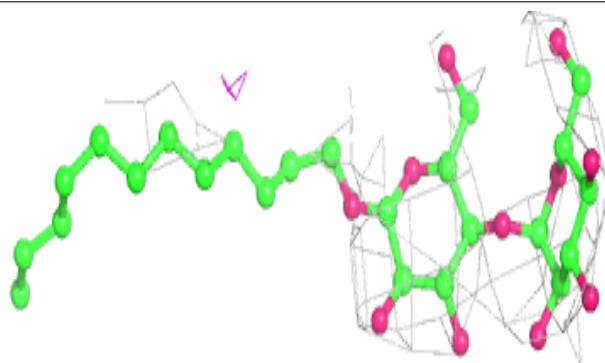


**Electron density around LMT b 627:**

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

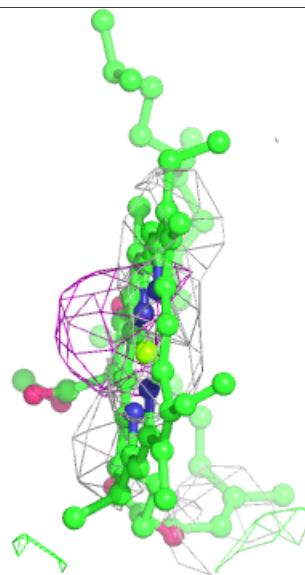
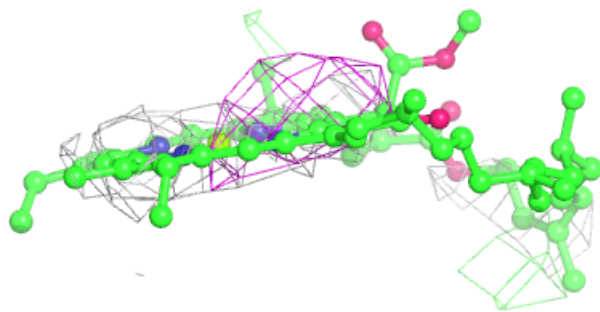
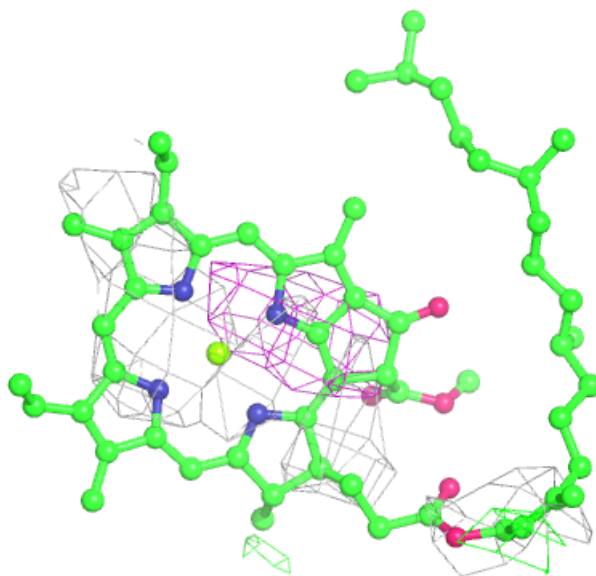
**Electron density around LMT b 626:**

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



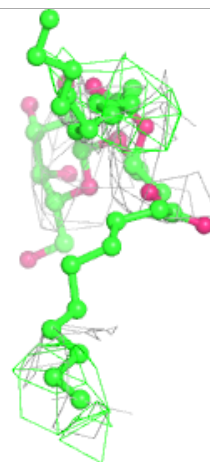
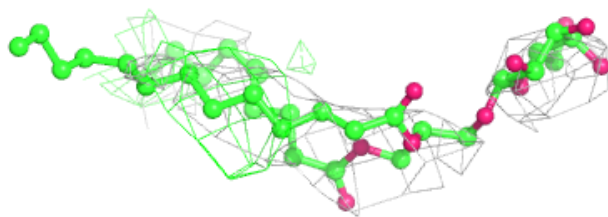
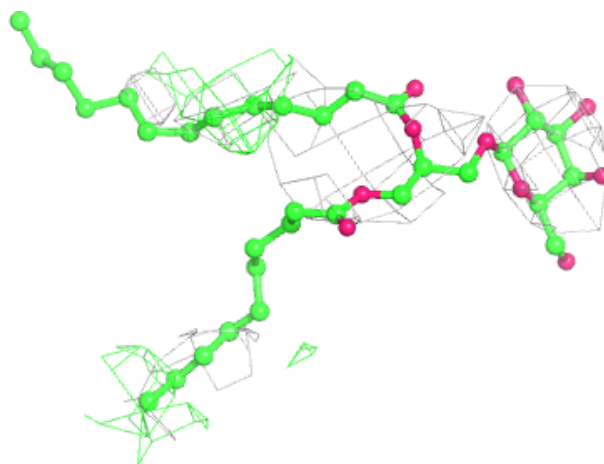
**Electron density around CLA b 605:**

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



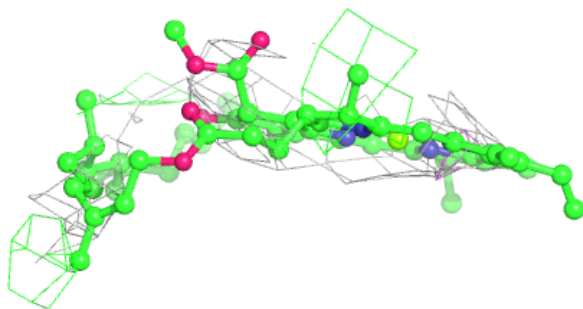
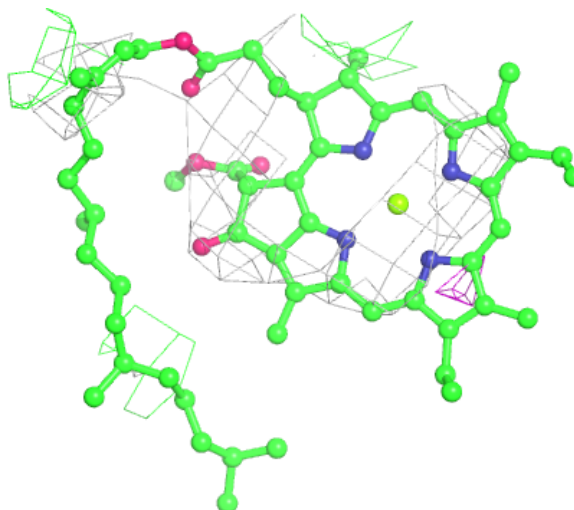
**Electron density around LMG A 415:**

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



**Electron density around CLA B 601:**

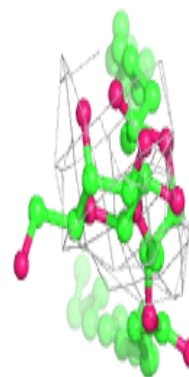
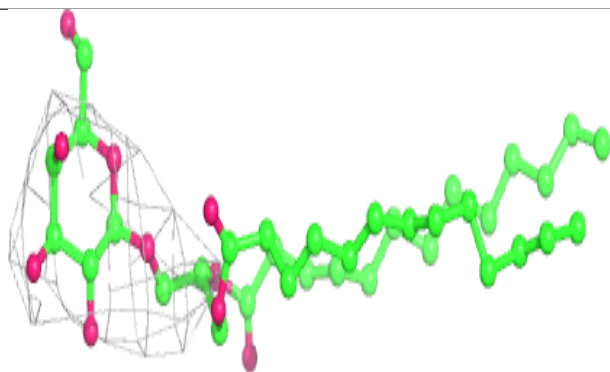
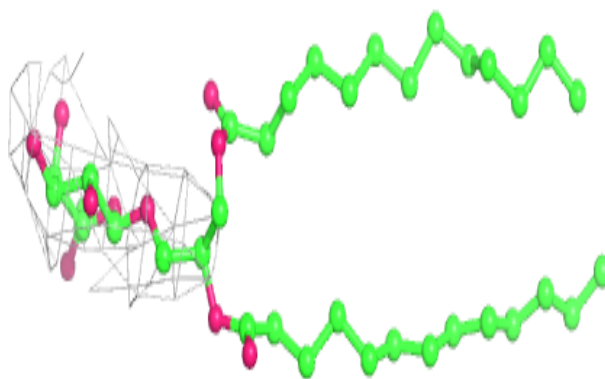
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





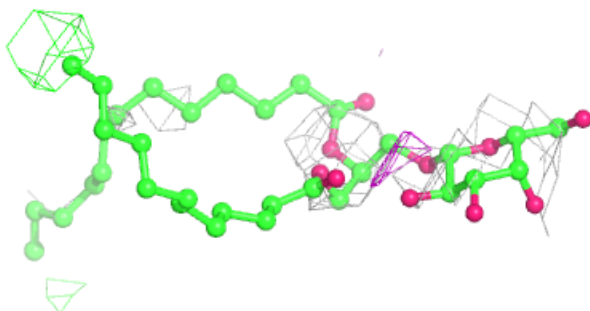
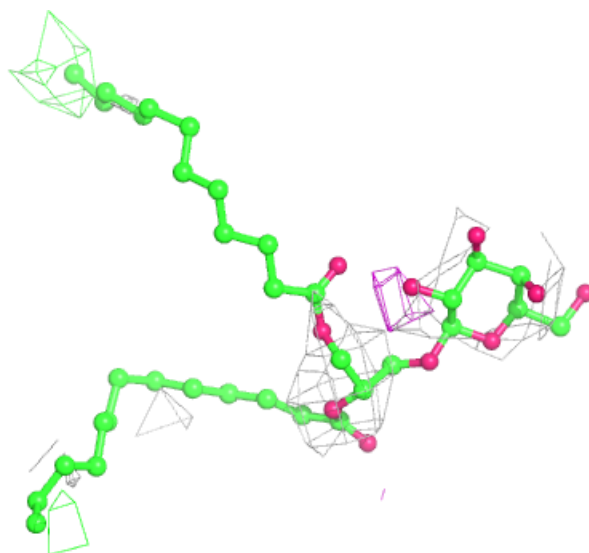
**Electron density around LMG C 518:**

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



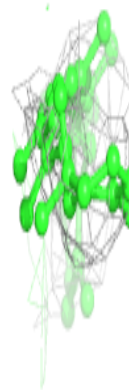
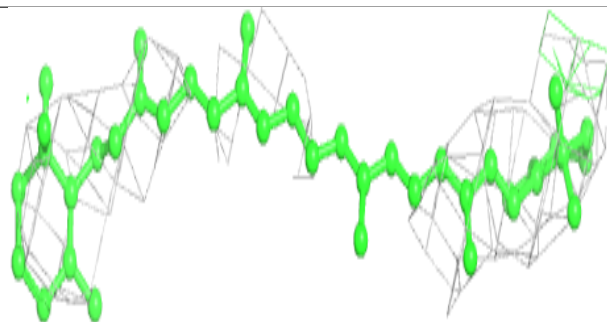
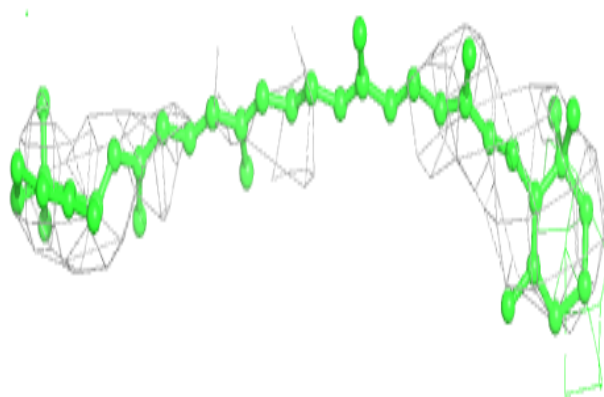
**Electron density around LMG E 101:**

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

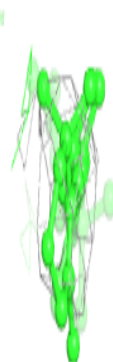
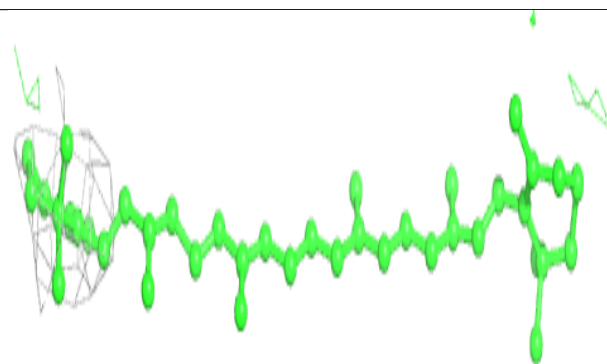
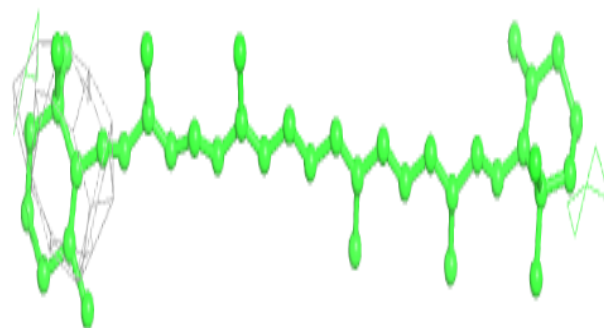


**Electron density around BCR f 102:**

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

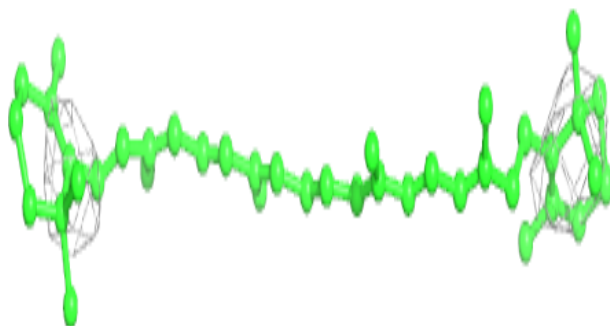
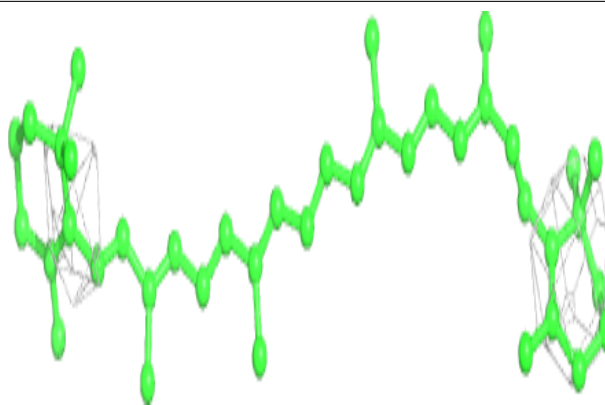
**Electron density around BCR j 102:**

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

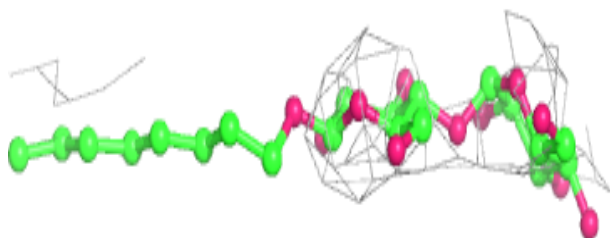
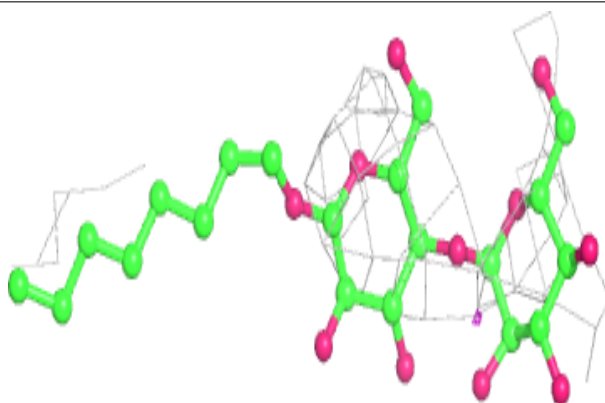


**Electron density around BCR g 101:**

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

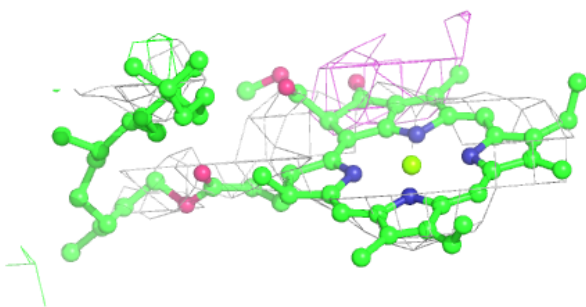
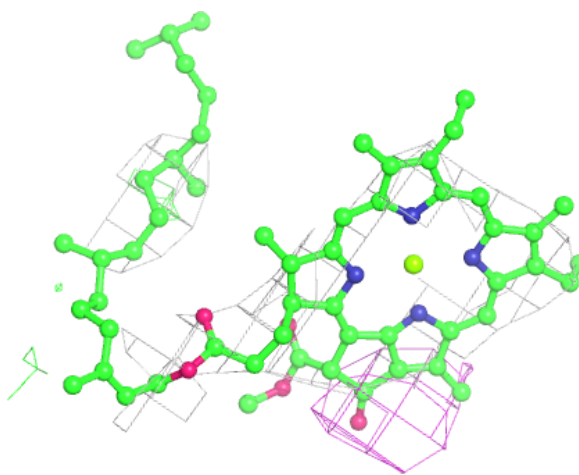
**Electron density around LMT D 410:**

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



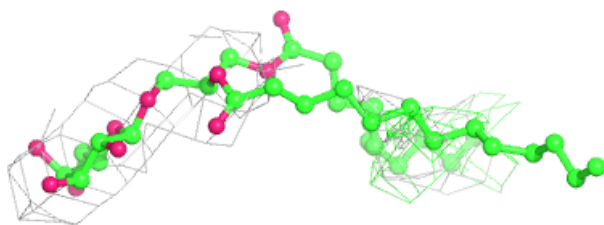
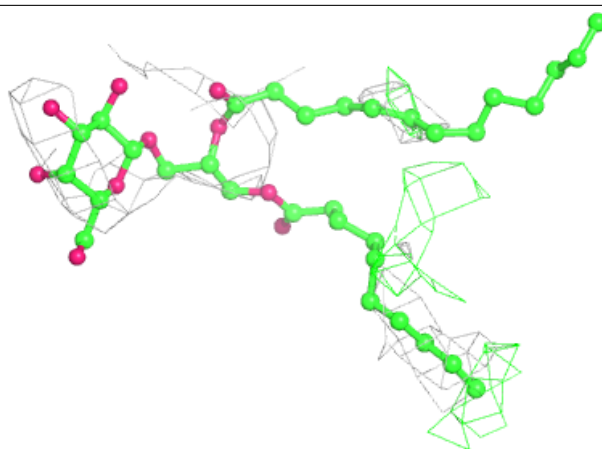
**Electron density around CLA b 619:**

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

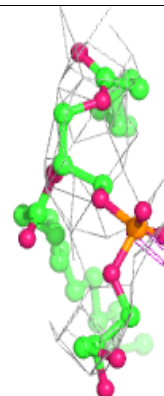
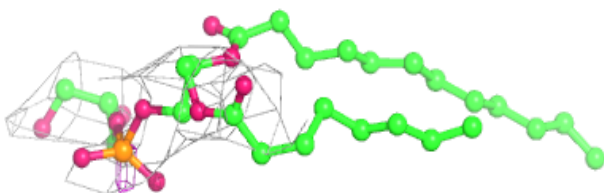
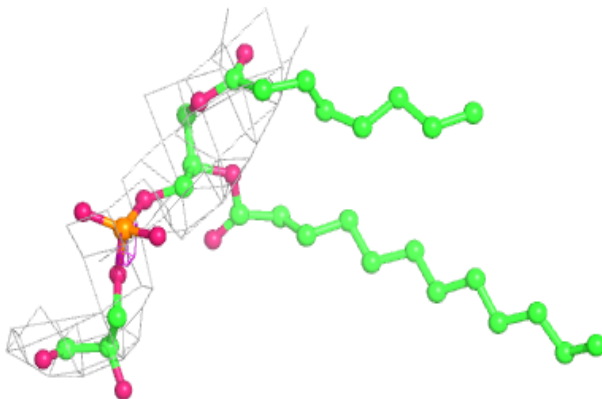


**Electron density around LMG a 402:**

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

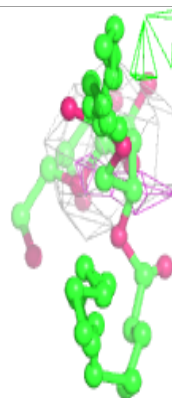
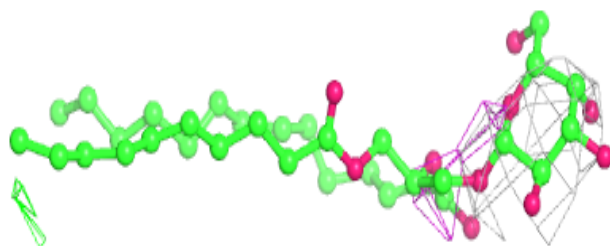
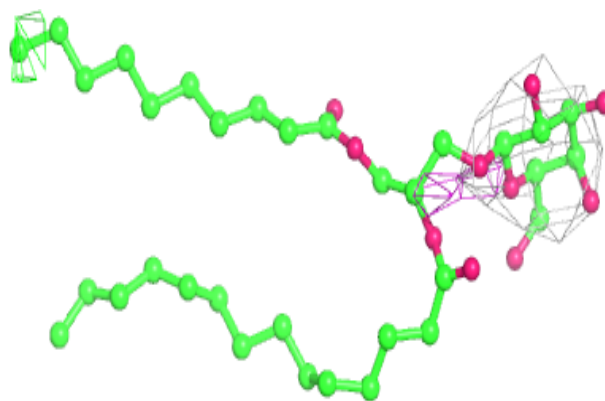
**Electron density around LHG C 519:**

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

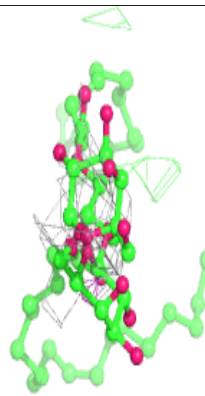
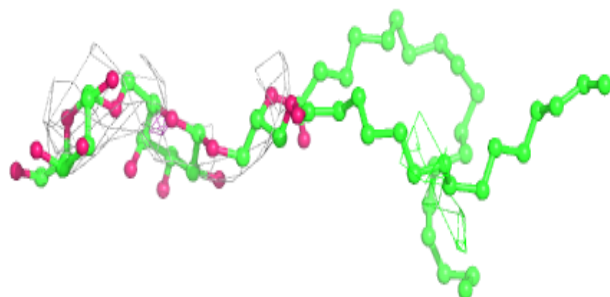
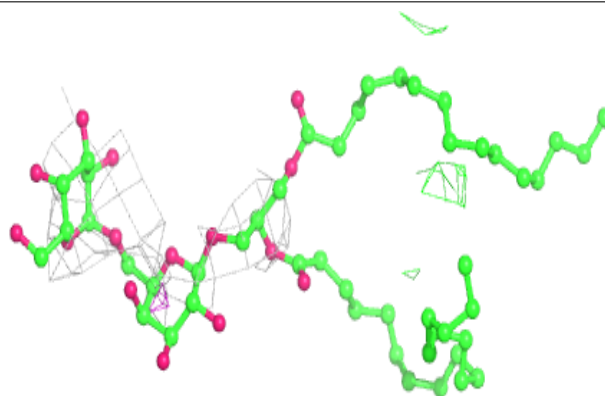


**Electron density around LMG I 101:**

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

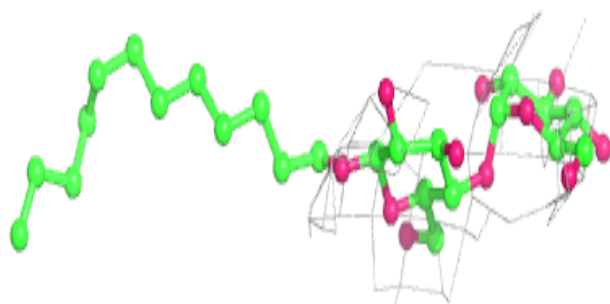
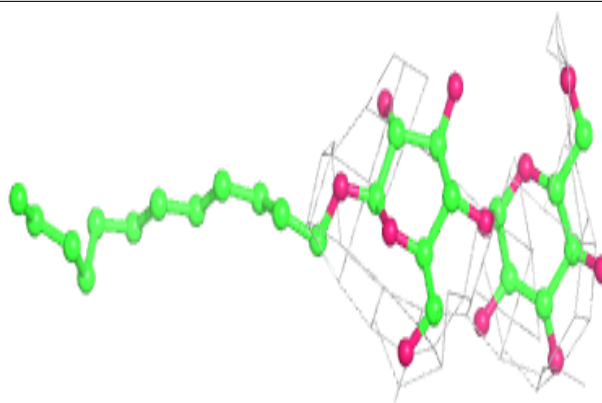
**Electron density around DGD d 408:**

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

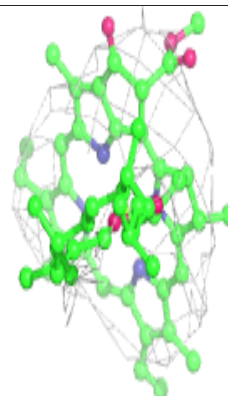
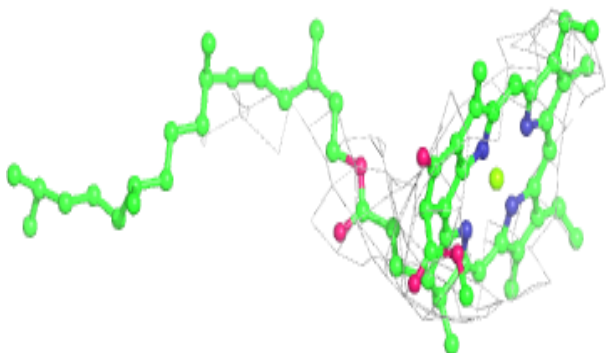
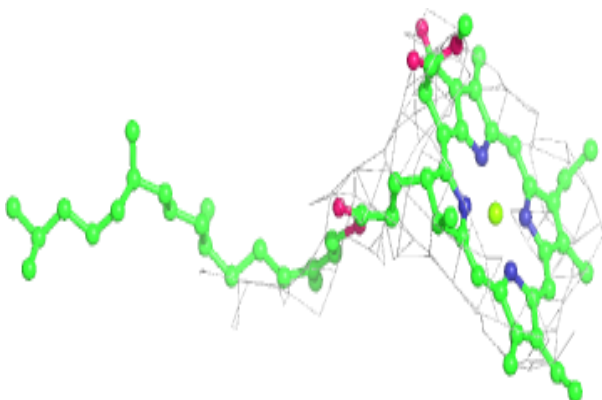


**Electron density around LMT B 628:**

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

**Electron density around CLA c 502:**

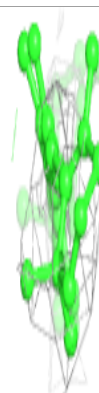
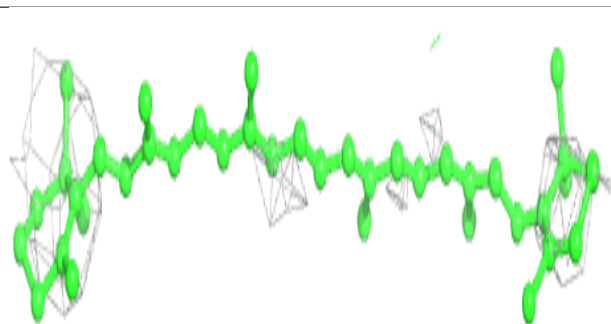
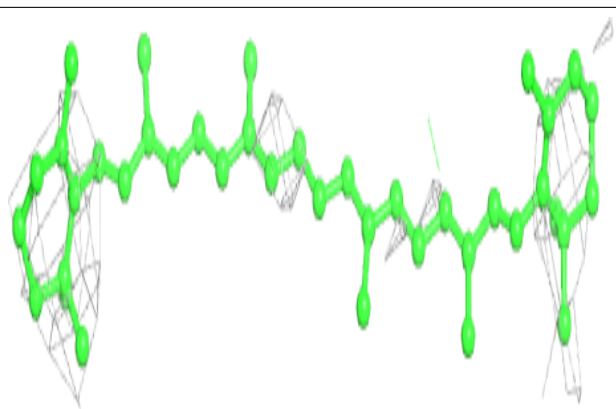
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



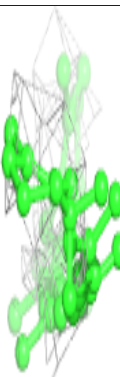
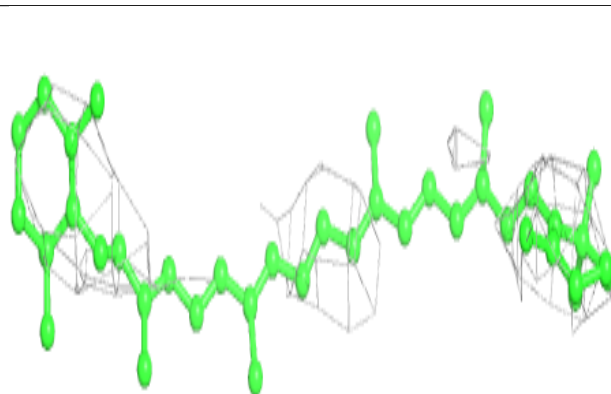
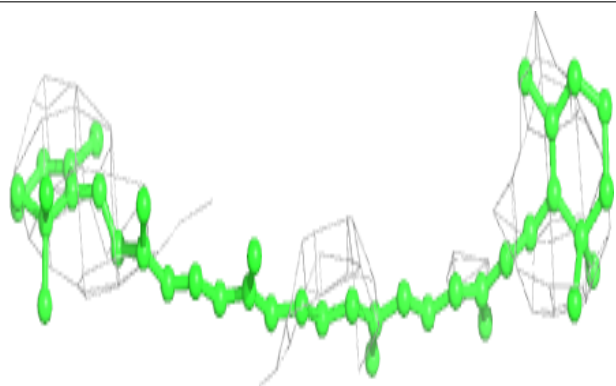


**Electron density around BCR c 514:**

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

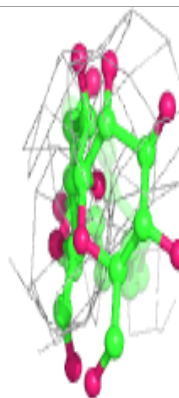
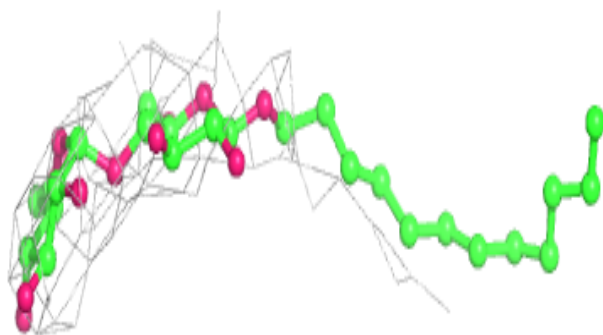
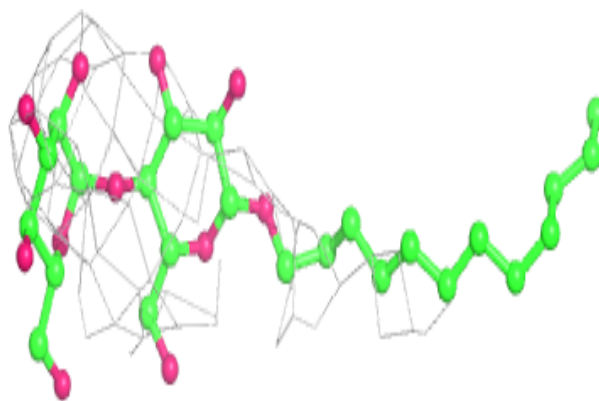
**Electron density around BCR D 411:**

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

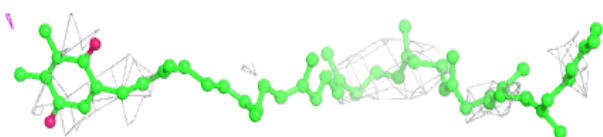
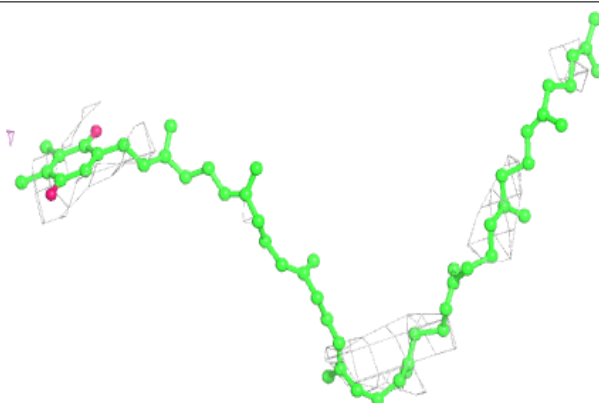


**Electron density around LMT B 622:**

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

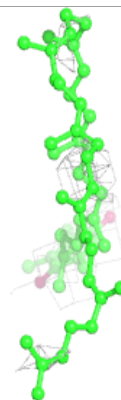
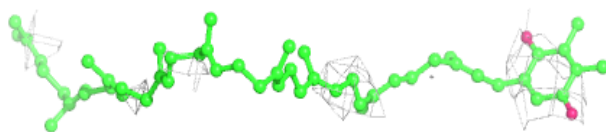
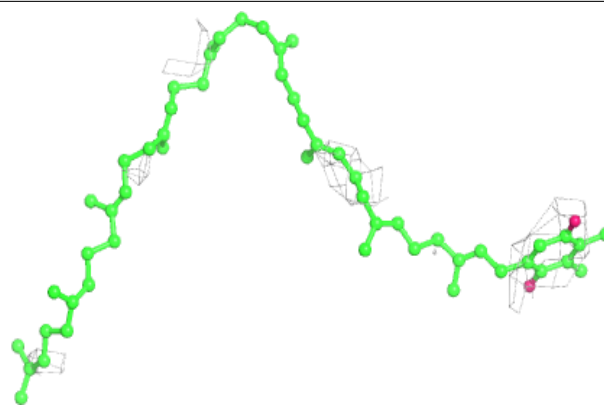
**Electron density around PL9 D 407:**

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

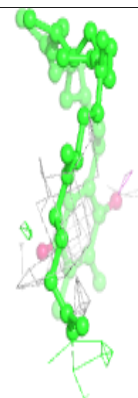
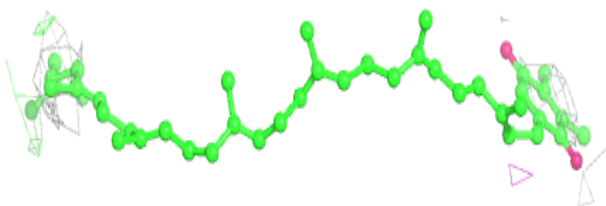
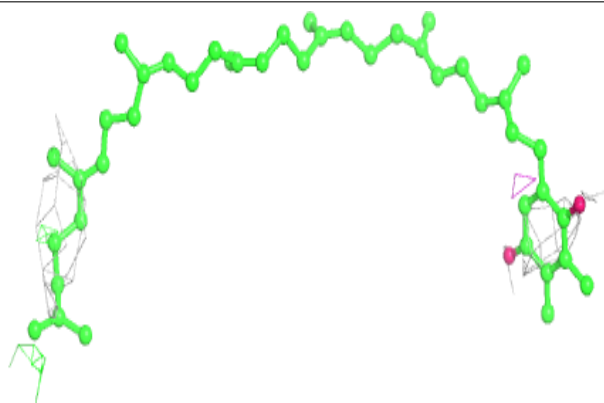


**Electron density around PL9 d 406:**

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

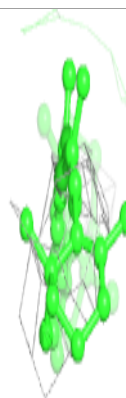
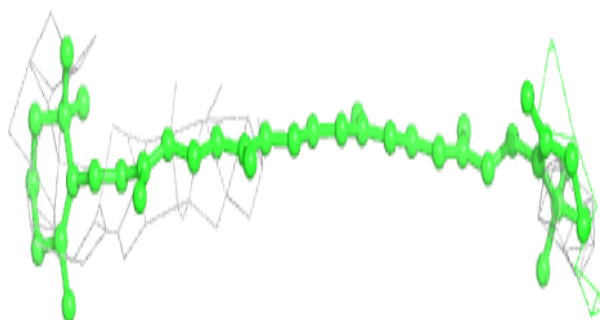
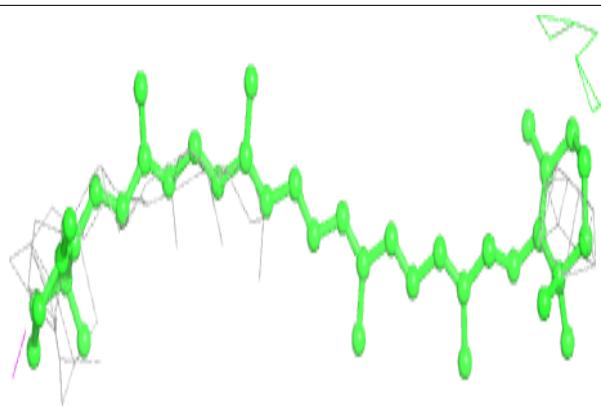
**Electron density around PL9 A 406:**

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



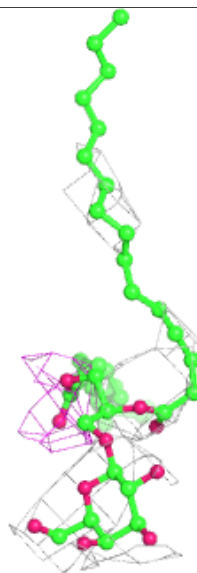
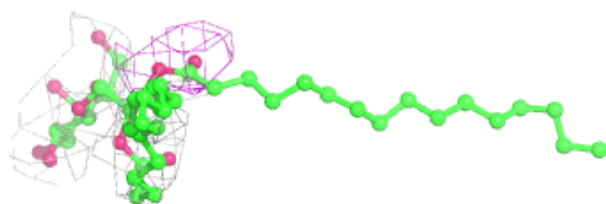
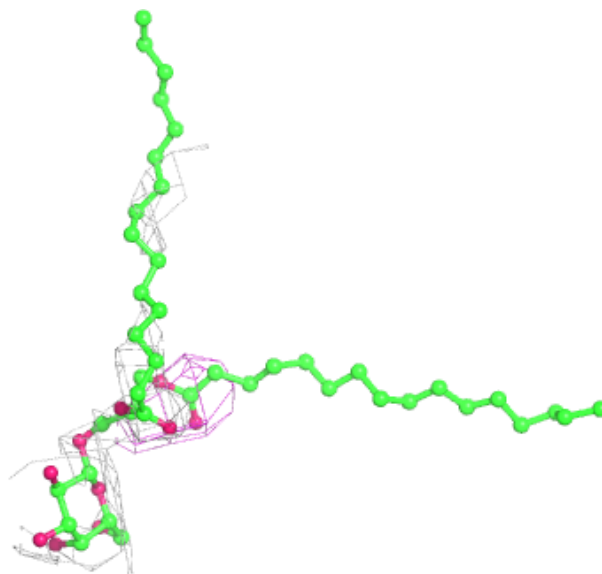
**Electron density around BCR H 102:**

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



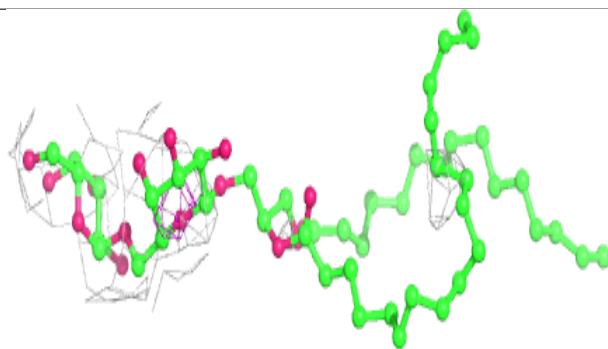
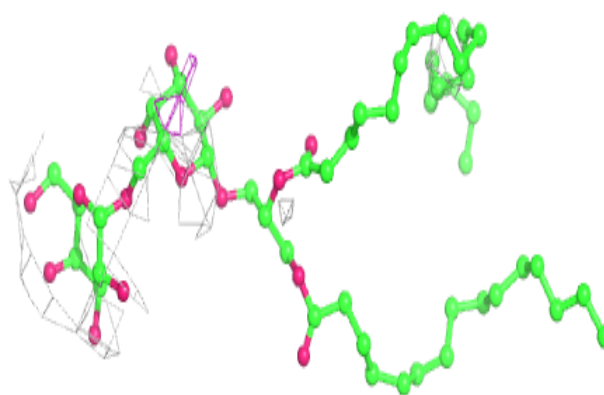
**Electron density around LMG a 413:**

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

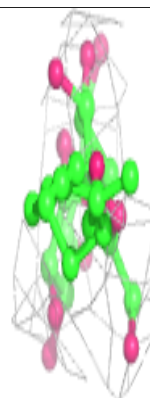
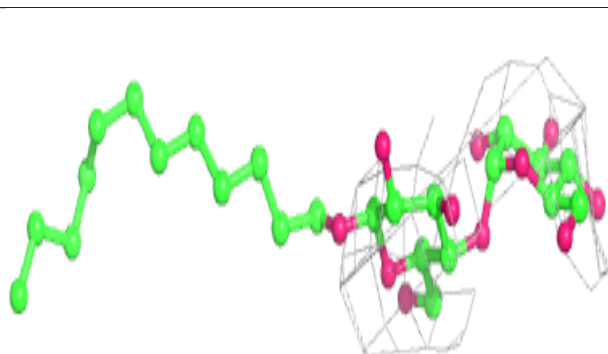
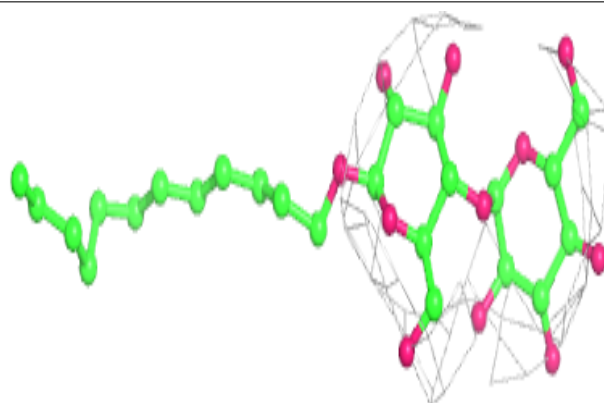


**Electron density around DGD D 409:**

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

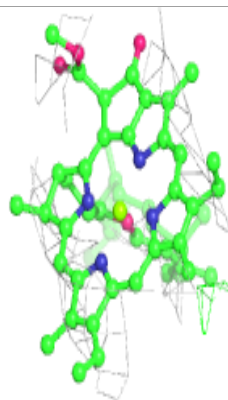
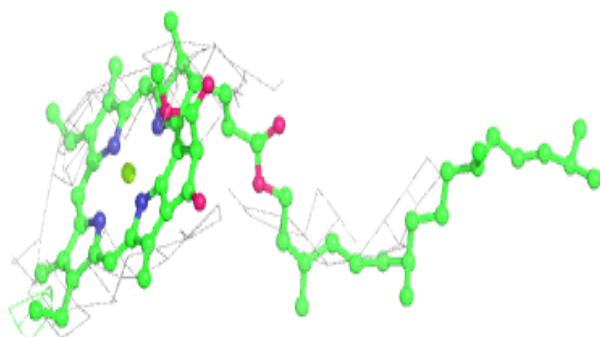
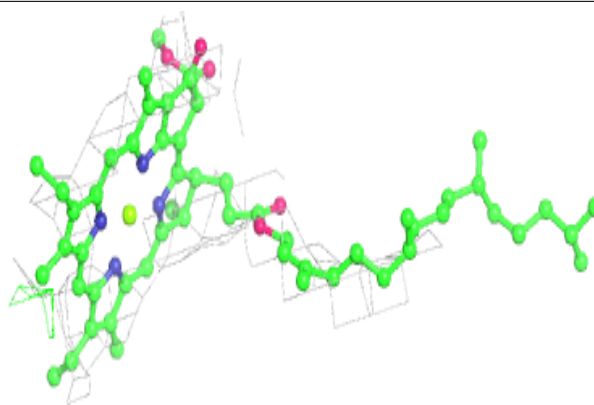
**Electron density around LMT b 604:**

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

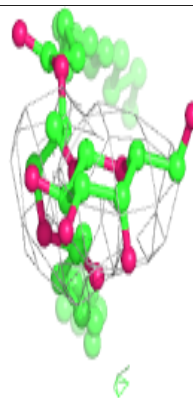
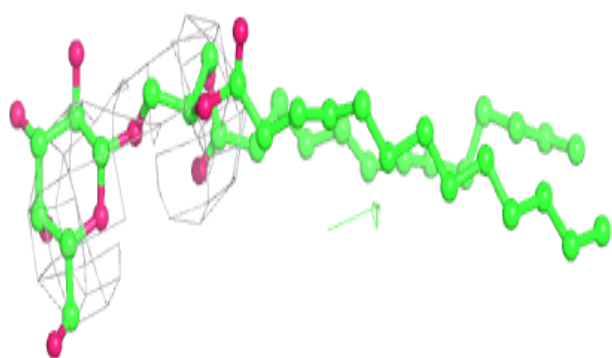
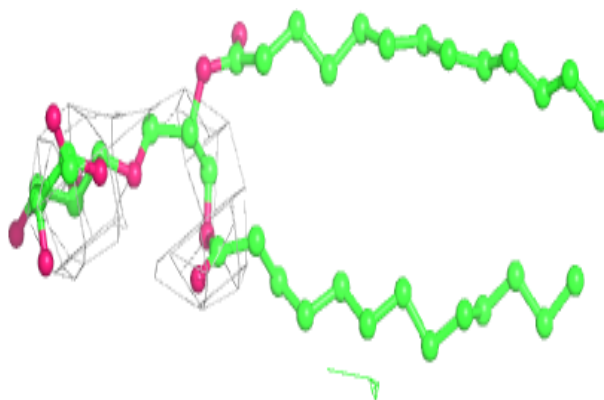


**Electron density around CLA C 502:**

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

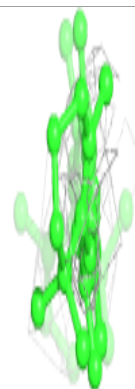
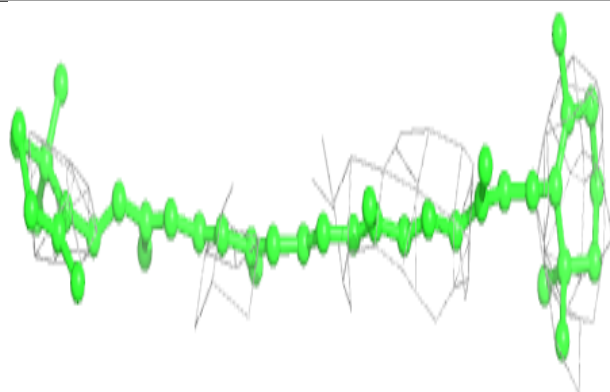
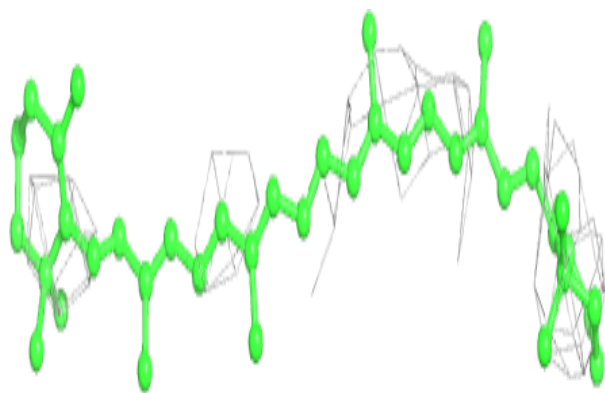
**Electron density around LMG c 518:**

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

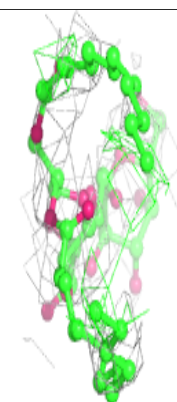
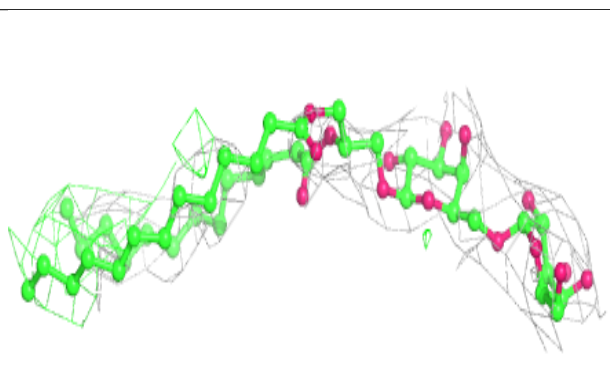
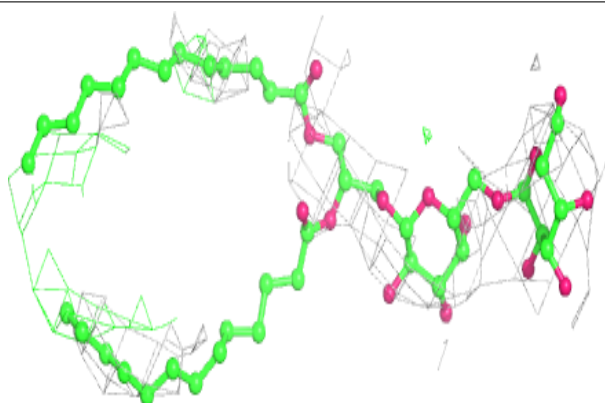


**Electron density around BCR x 101:**

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

**Electron density around DGD A 408:**

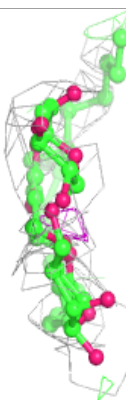
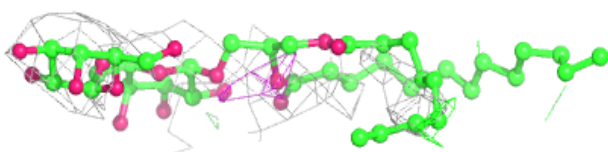
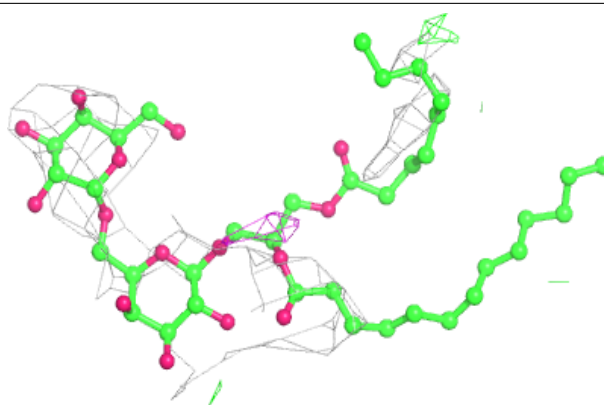
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



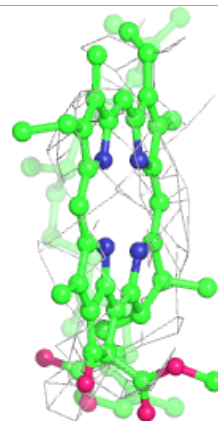
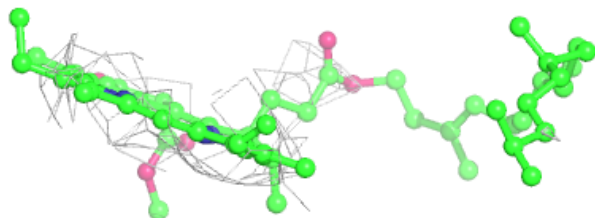
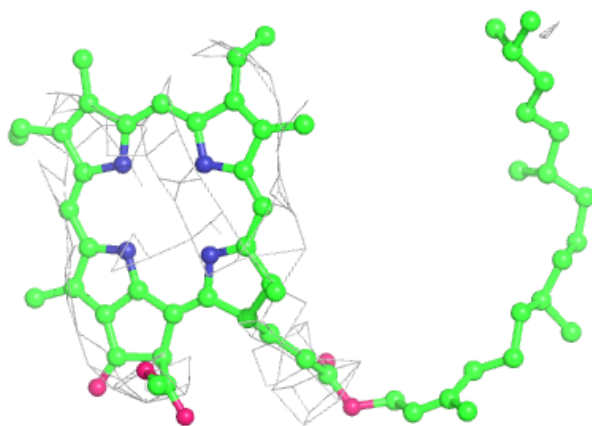


**Electron density around DGD b 601:**

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

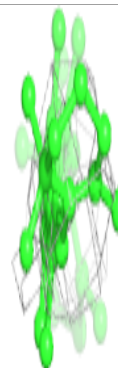
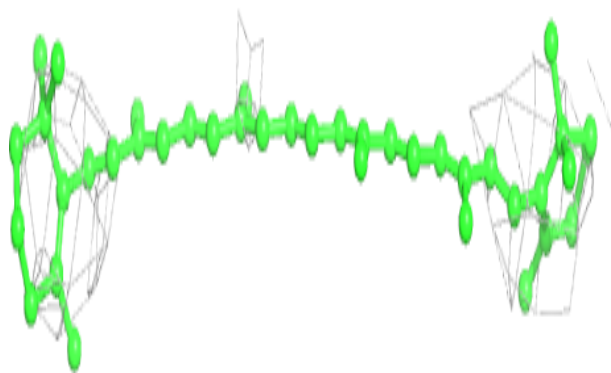
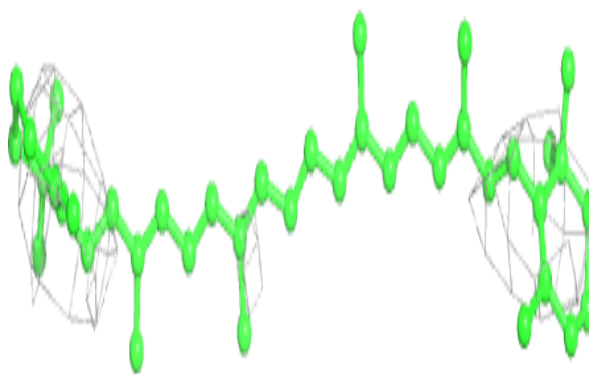
**Electron density around PHO d 401:**

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

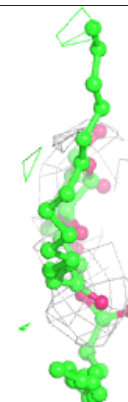
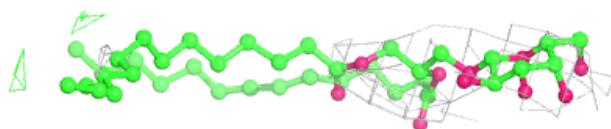
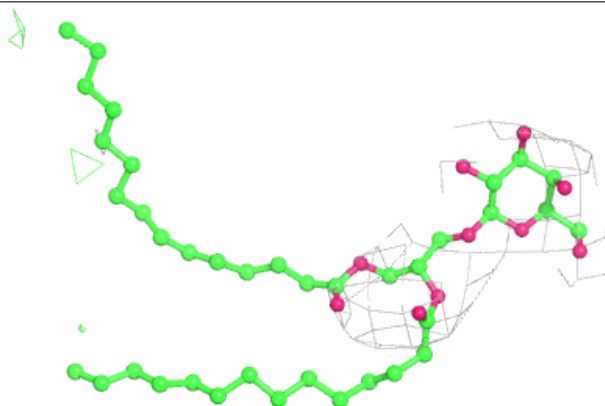


**Electron density around BCR B 616:**

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

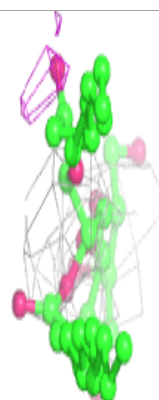
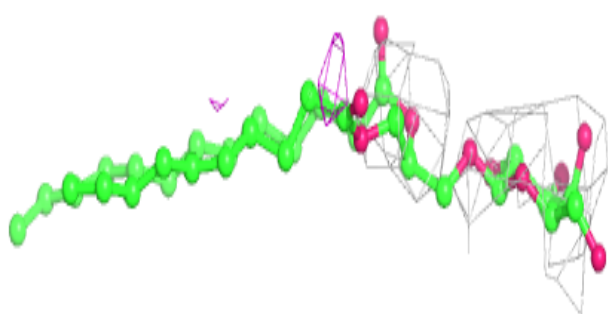
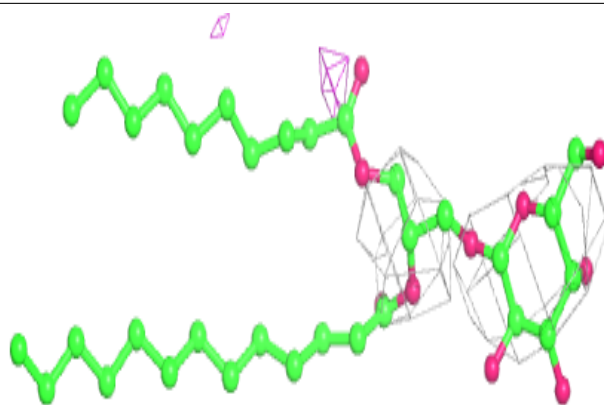
**Electron density around LMG C 522:**

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

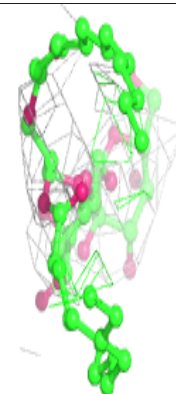
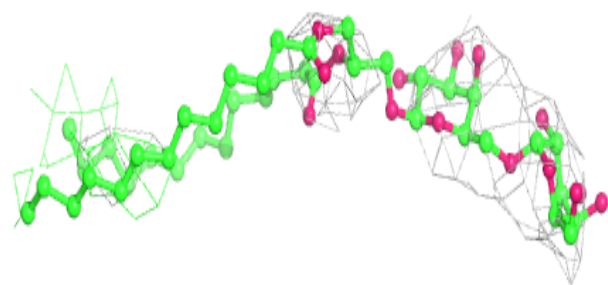
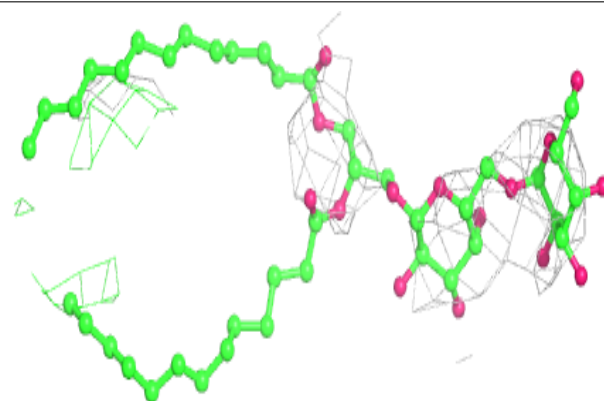


**Electron density around LMG M 101:**

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

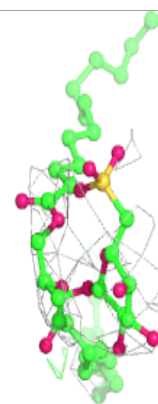
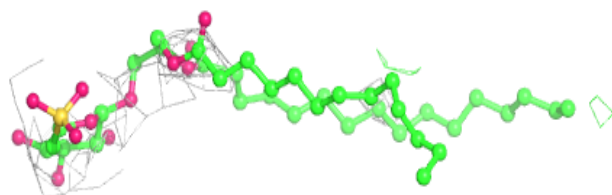
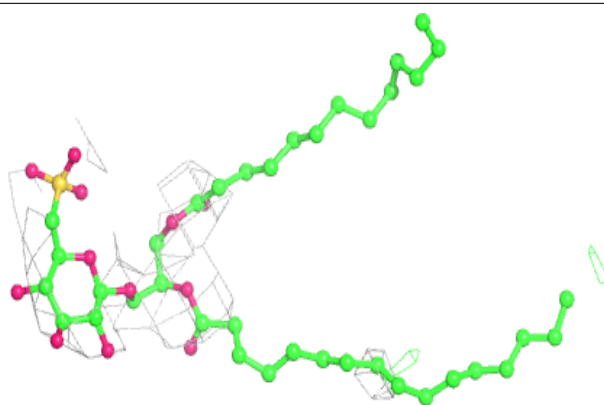
**Electron density around DGD a 411:**

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

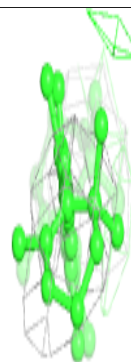
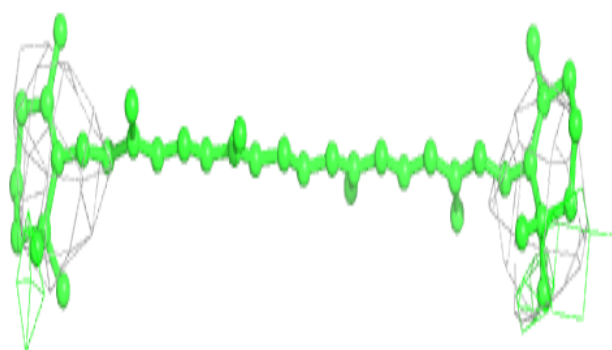
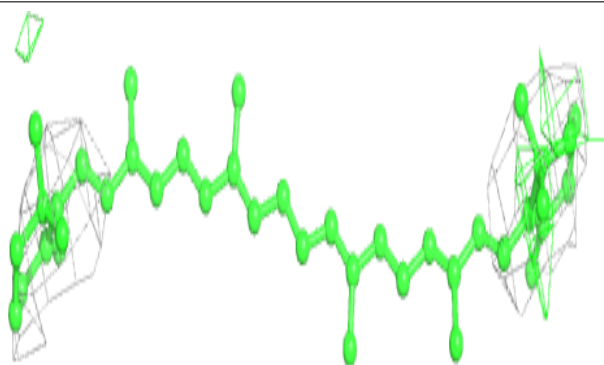


**Electron density around SQD A 413:**

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

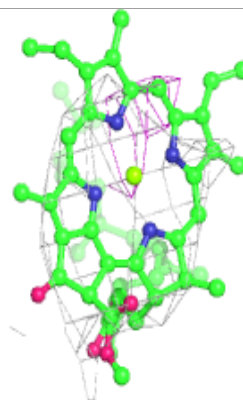
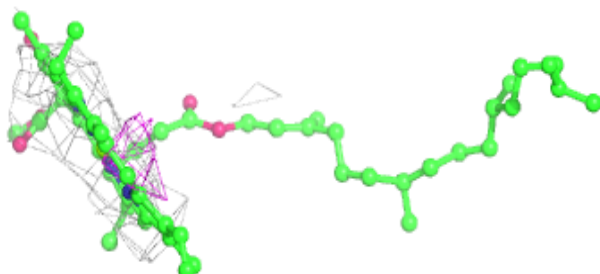
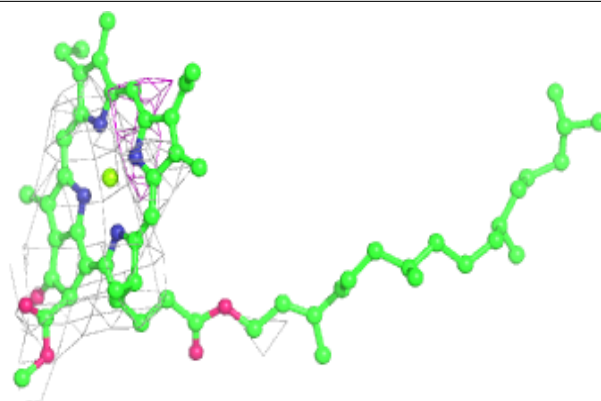
**Electron density around BCR a 410:**

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

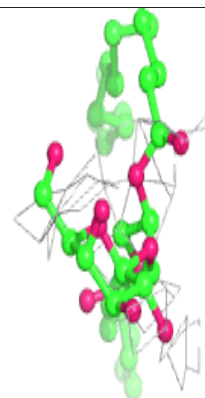
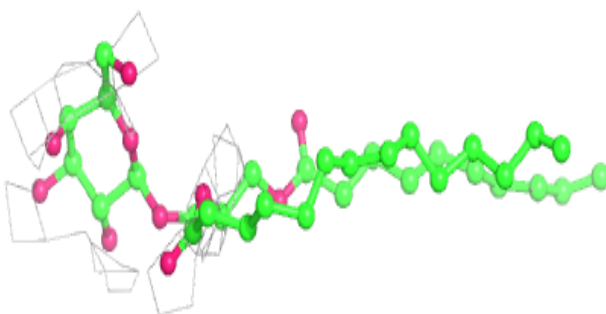
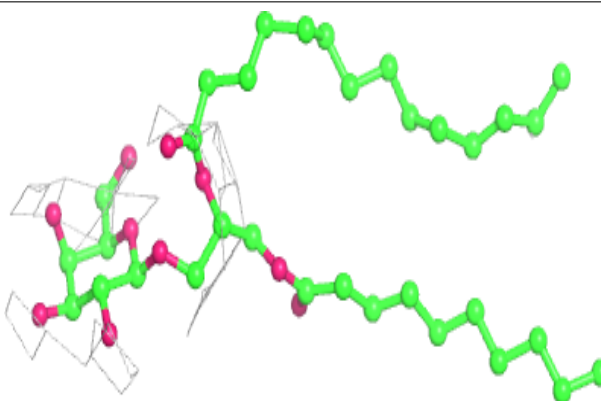


**Electron density around CLA a 408:**

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

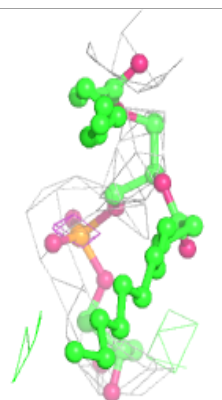
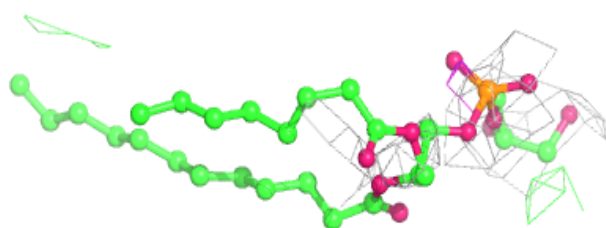
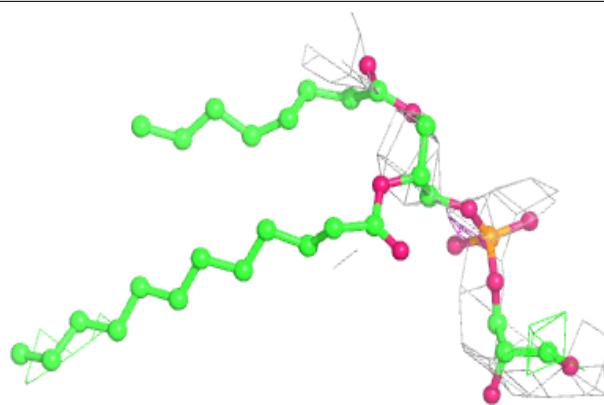
**Electron density around LMG i 101:**

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

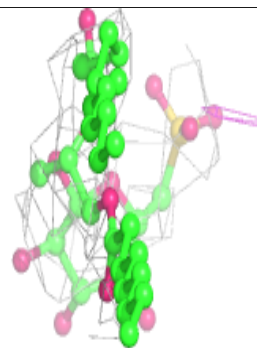
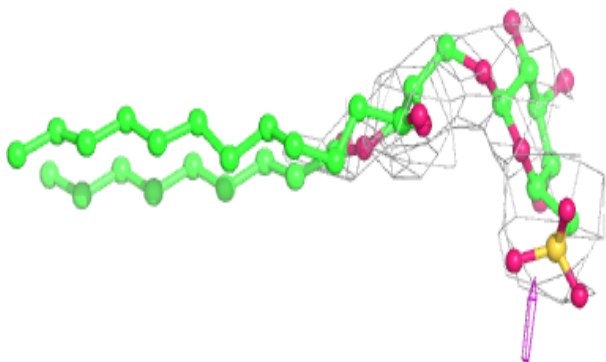
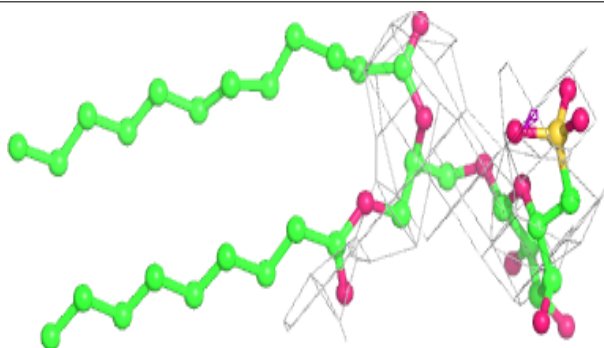


**Electron density around LHG c 519:**

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

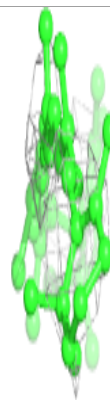
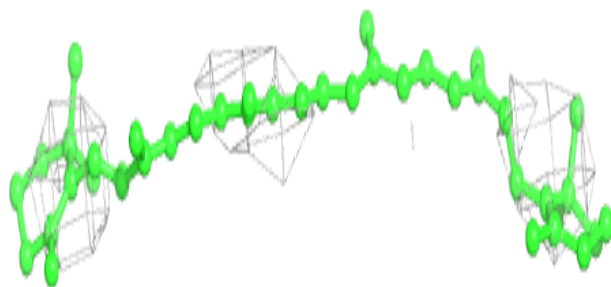
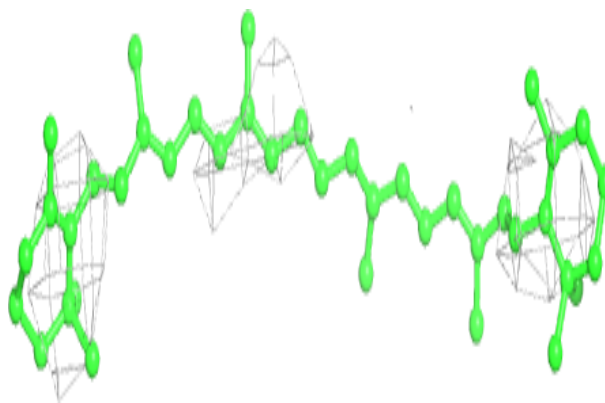
**Electron density around SQD d 402:**

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



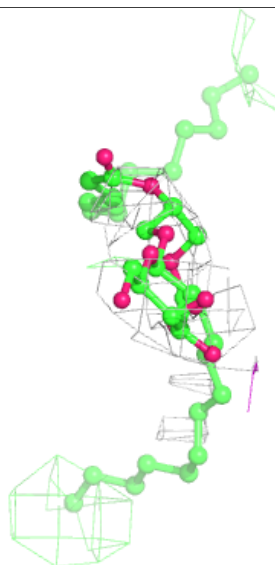
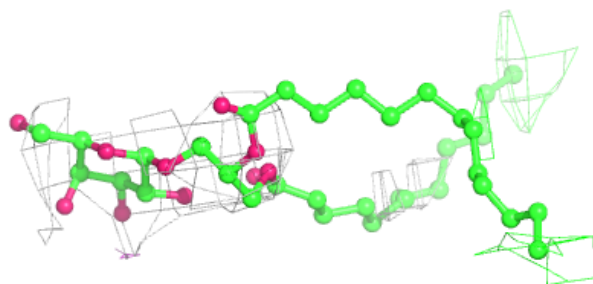
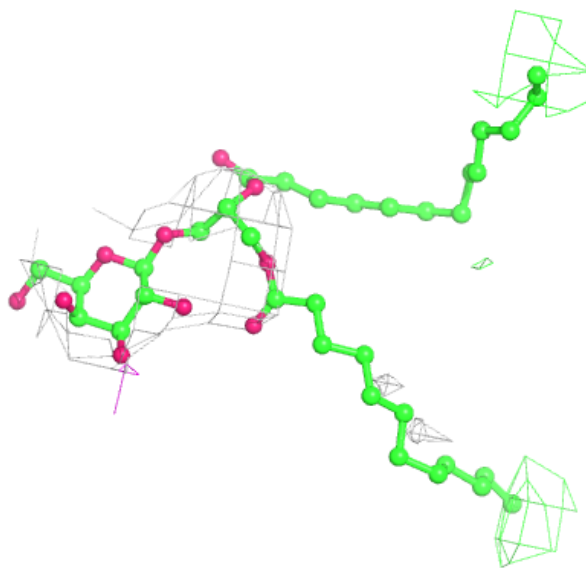
**Electron density around BCR B 617:**

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



**Electron density around LMG e 101:**

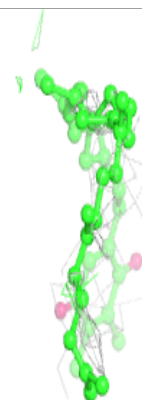
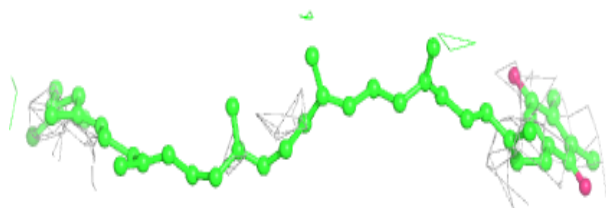
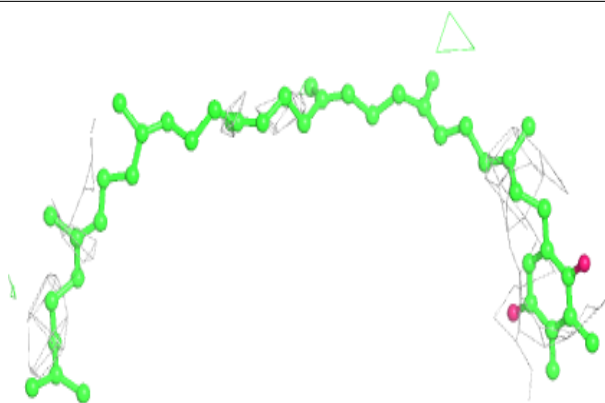
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



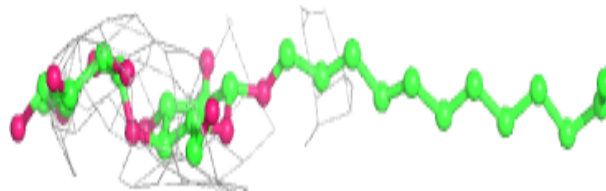
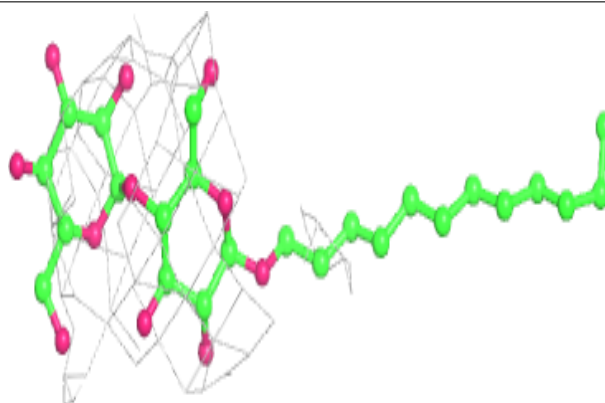


**Electron density around PL9 a 409:**

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

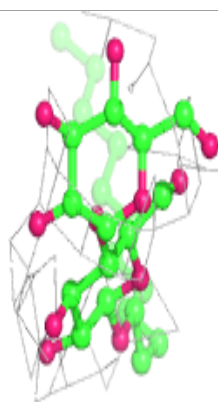
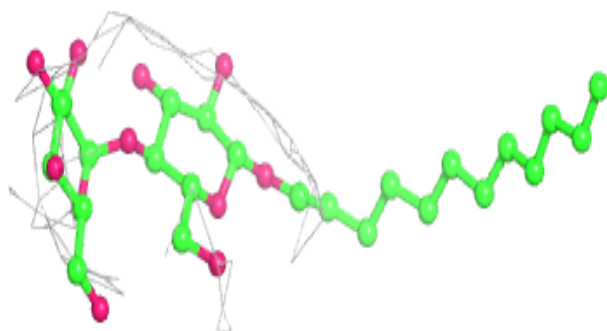
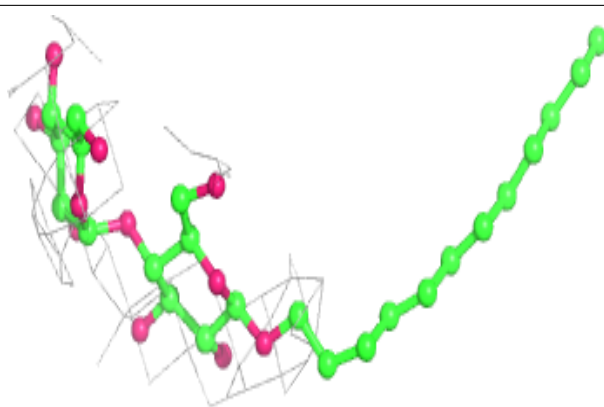
**Electron density around LMT B 627:**

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

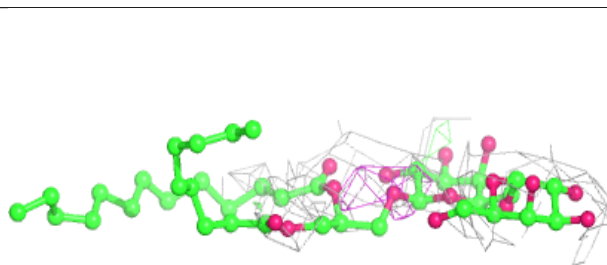
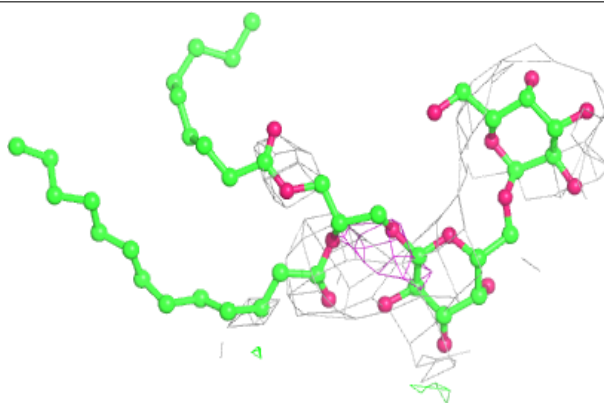


**Electron density around LMT M 103:**

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

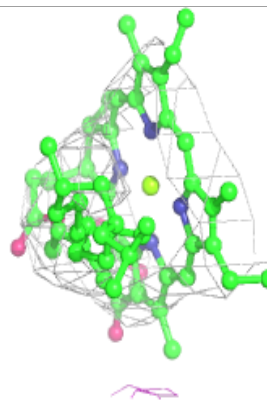
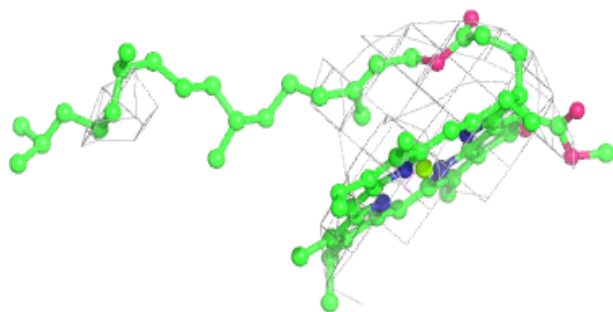
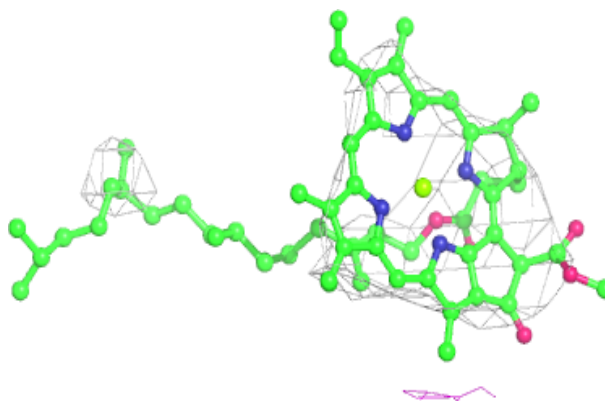
**Electron density around DGD B 625:**

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

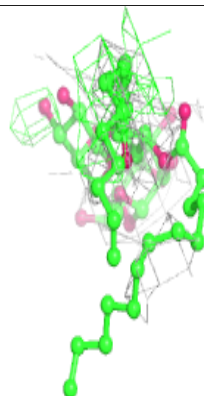
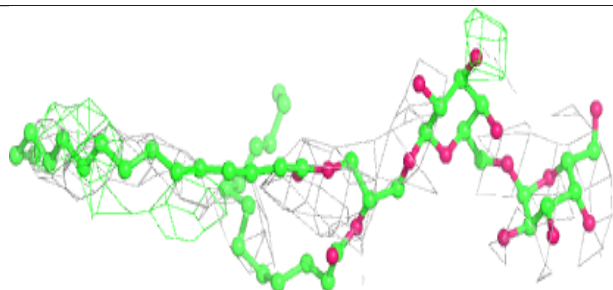
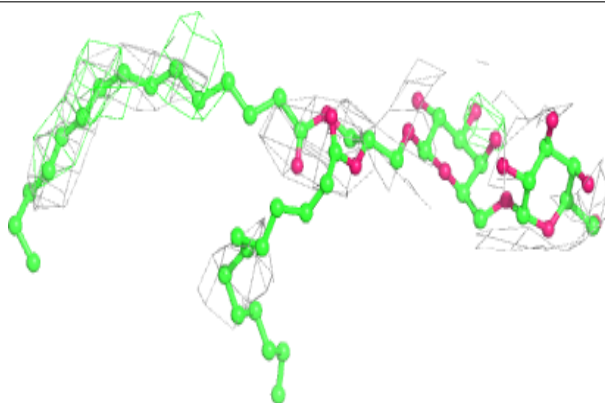


**Electron density around CLA B 613:**

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

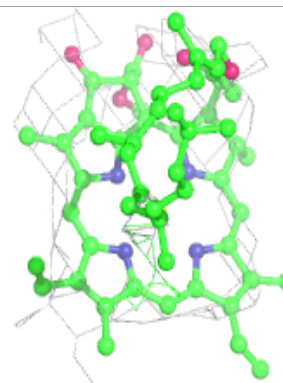
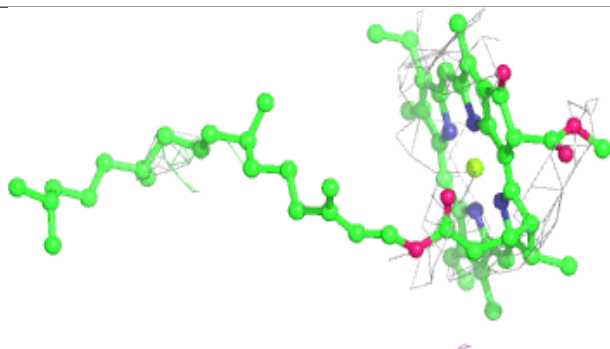
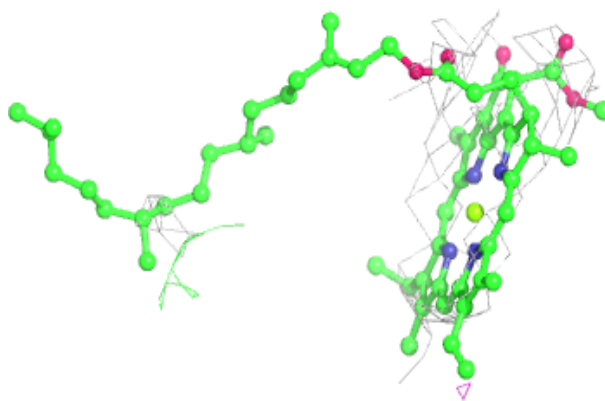
**Electron density around DGD b 624:**

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

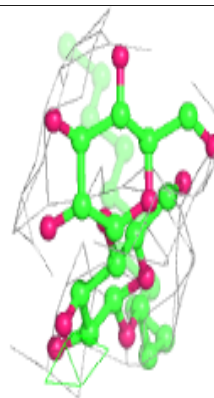
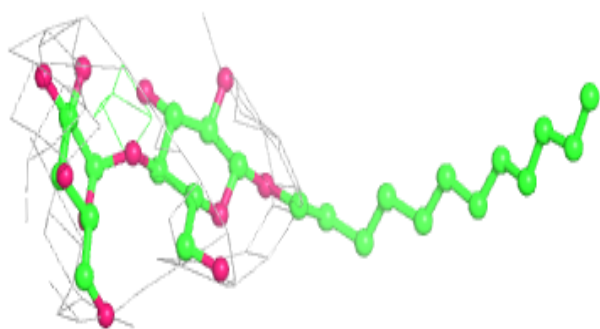
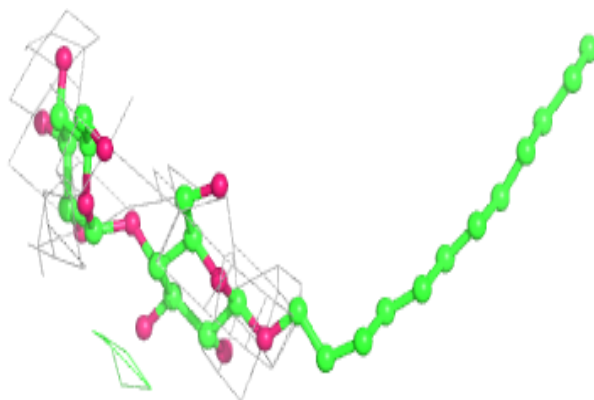


**Electron density around CLA C 507:**

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

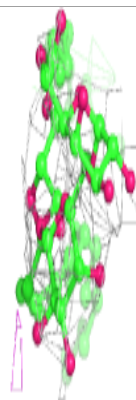
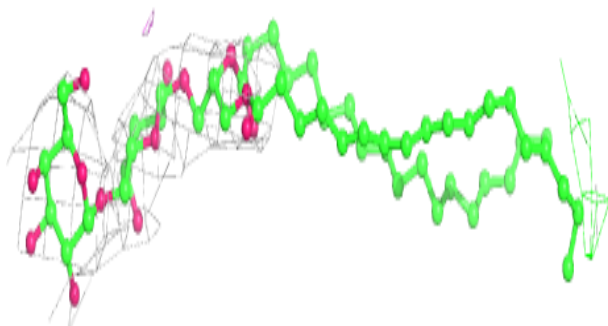
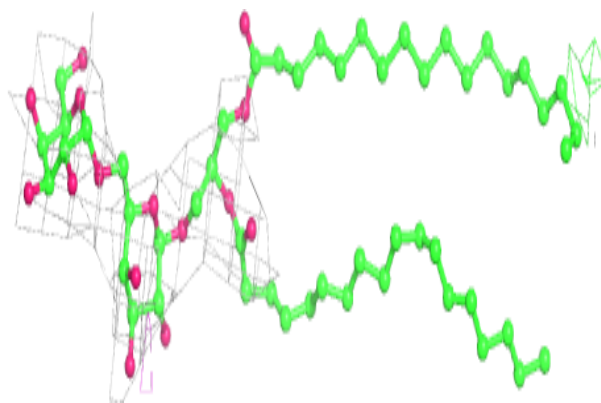
**Electron density around LMT M 102:**

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



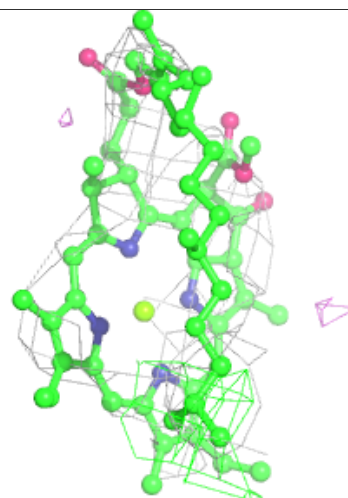
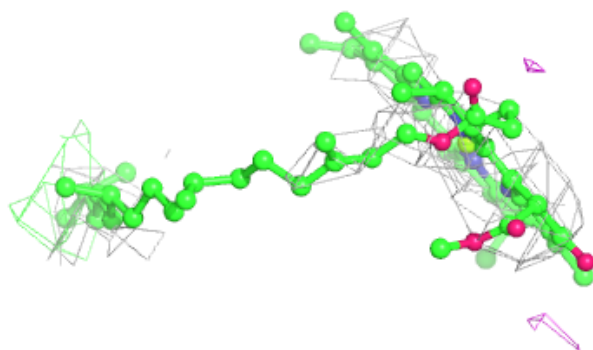
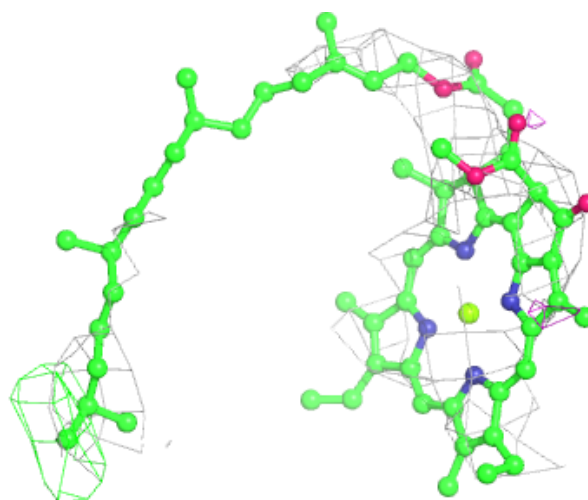
**Electron density around DGD C 517:**

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



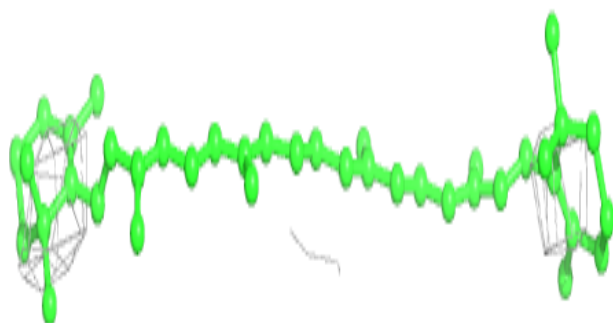
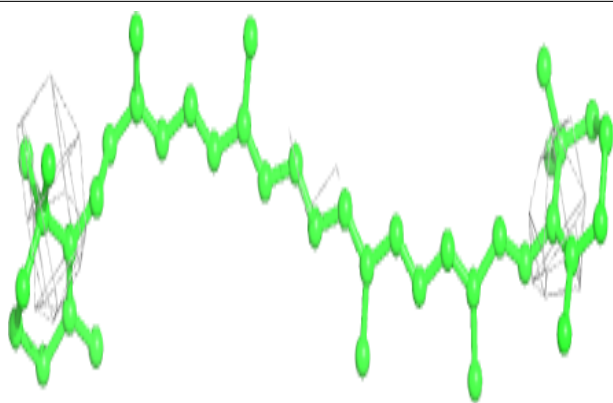
**Electron density around CLA C 506:**

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

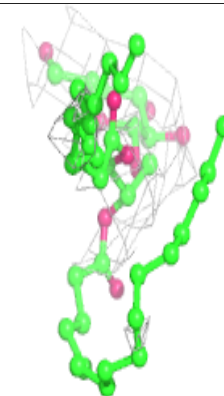
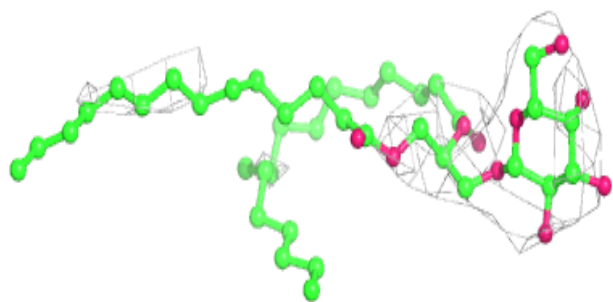
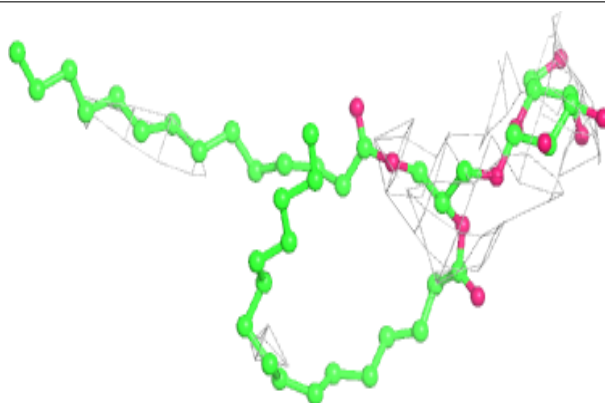


**Electron density around BCR y 101:**

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

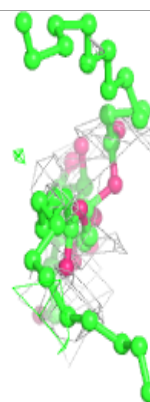
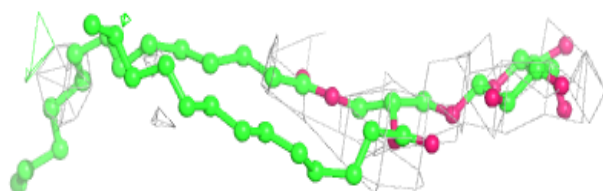
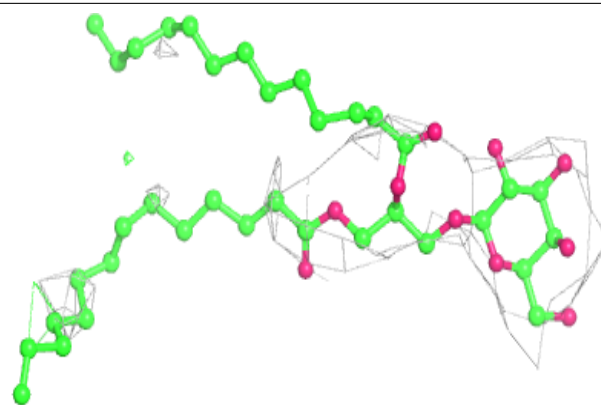
**Electron density around LMG B 624:**

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

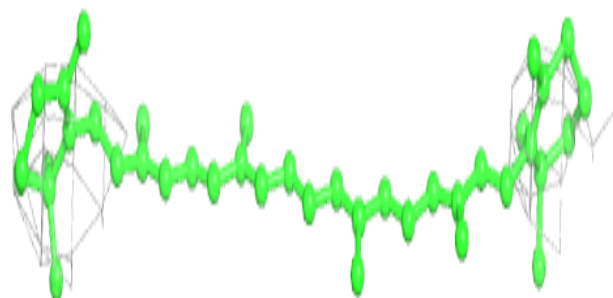
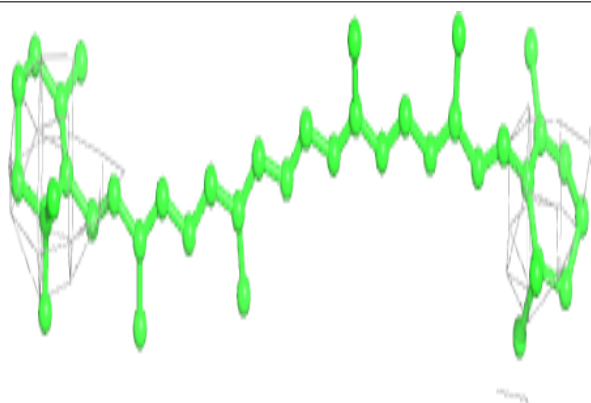


**Electron density around LMG D 412:**

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

**Electron density around BCR C 514:**

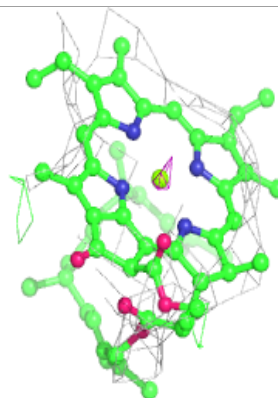
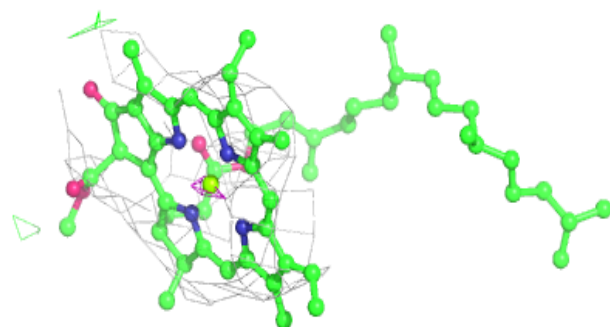
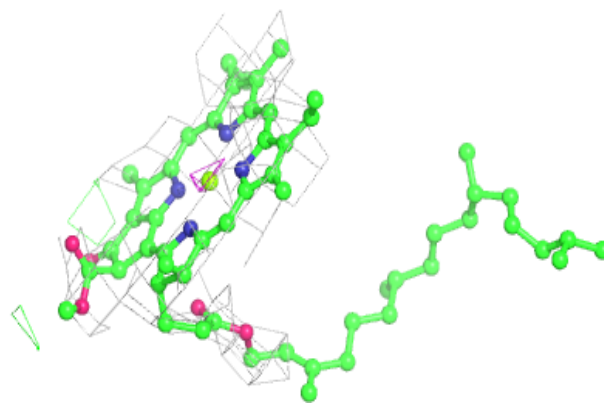
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



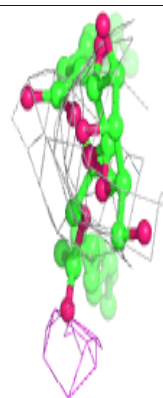
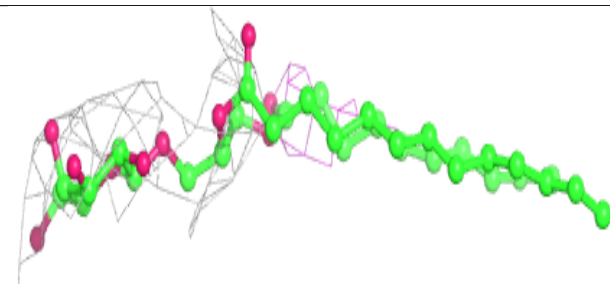
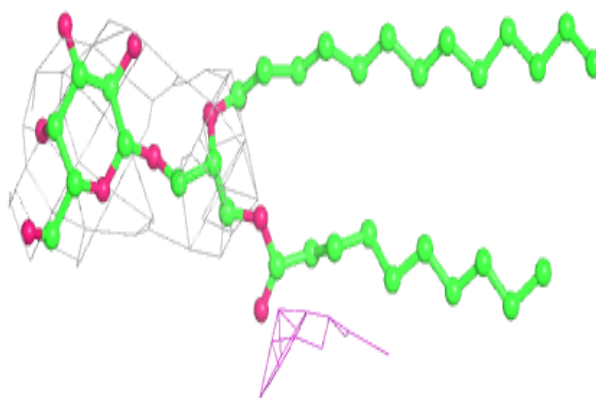


**Electron density around CLA c 512:**

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

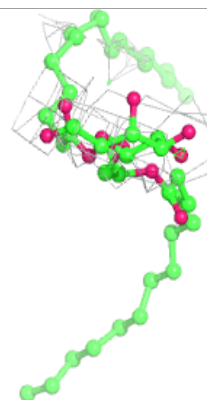
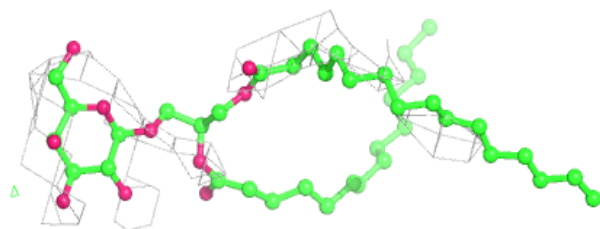
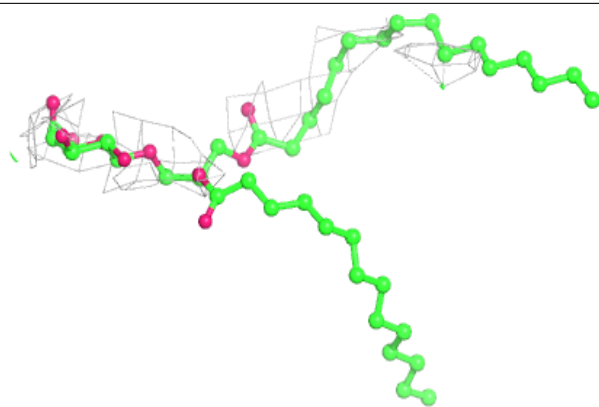
**Electron density around LMG m 101:**

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

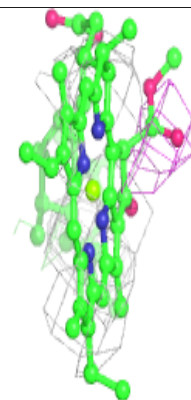
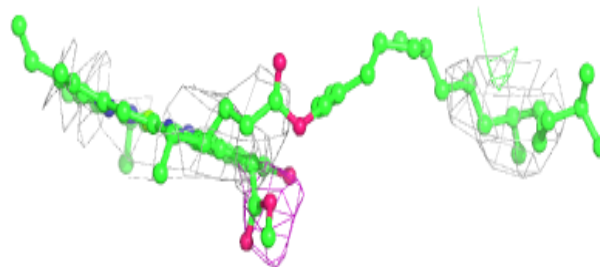
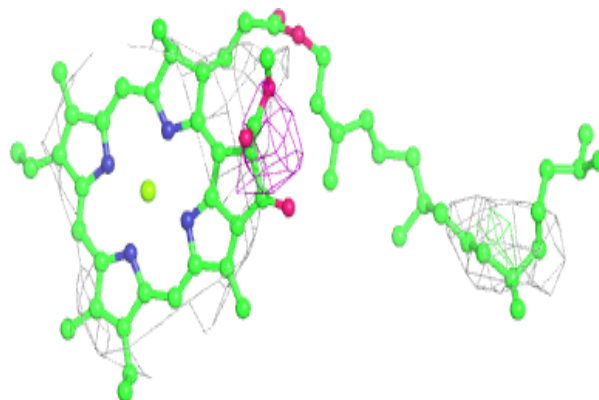


**Electron density around LMG b 625:**

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

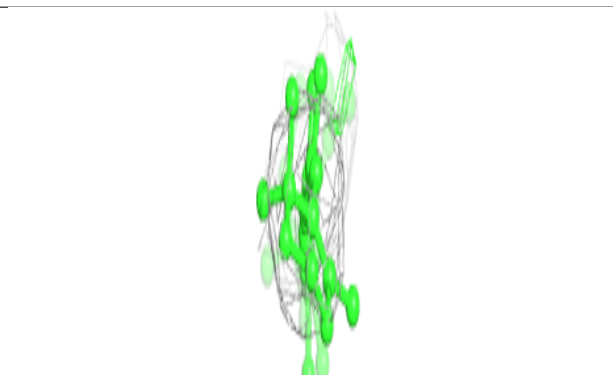
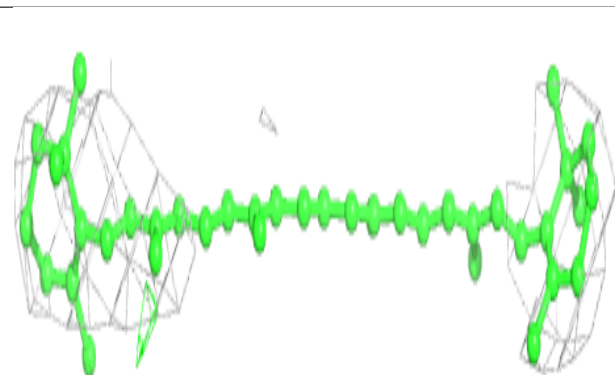
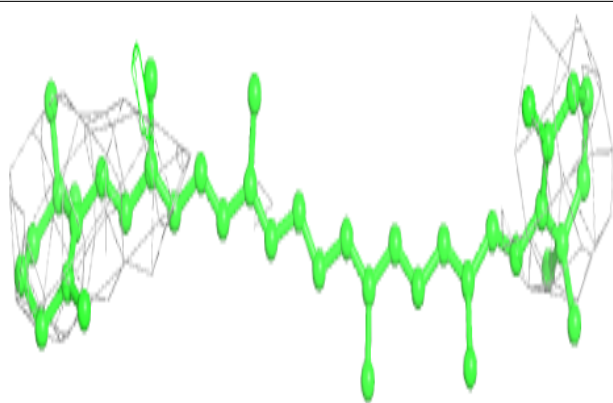
**Electron density around CLA h 101:**

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

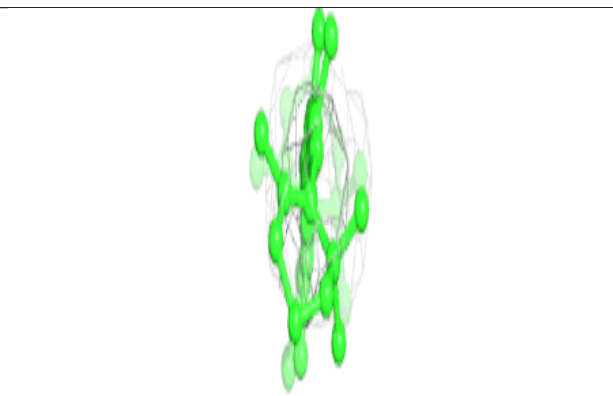
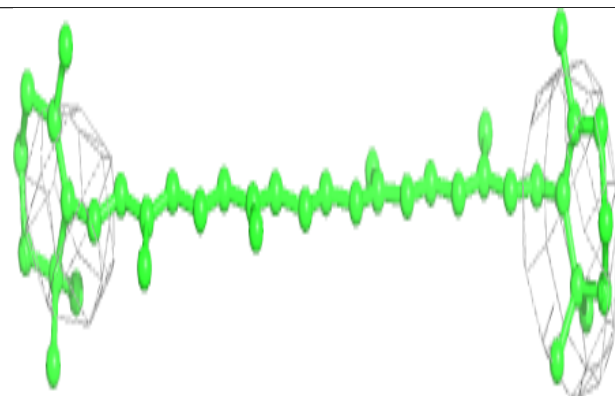
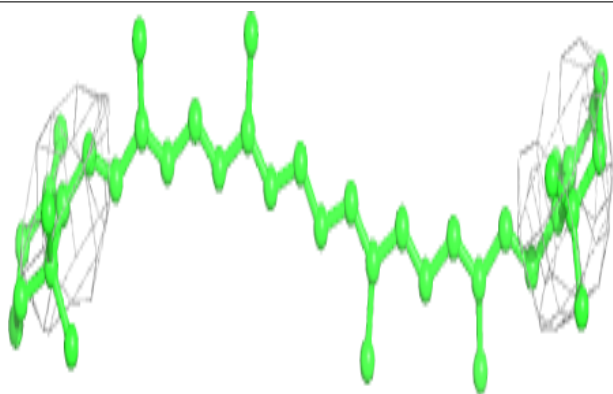


**Electron density around BCR b 622:**

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

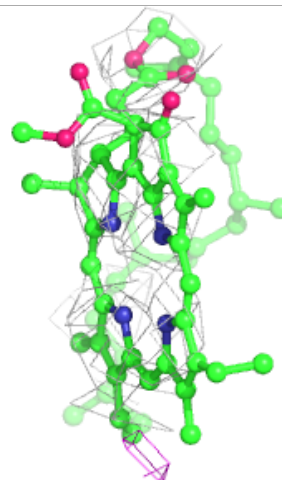
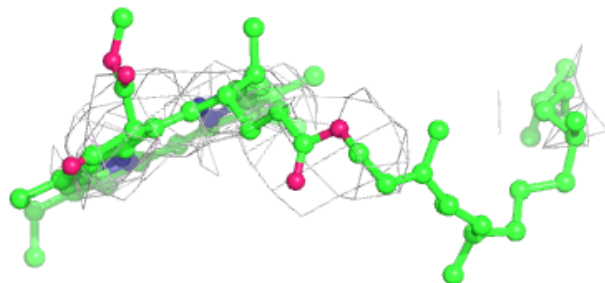
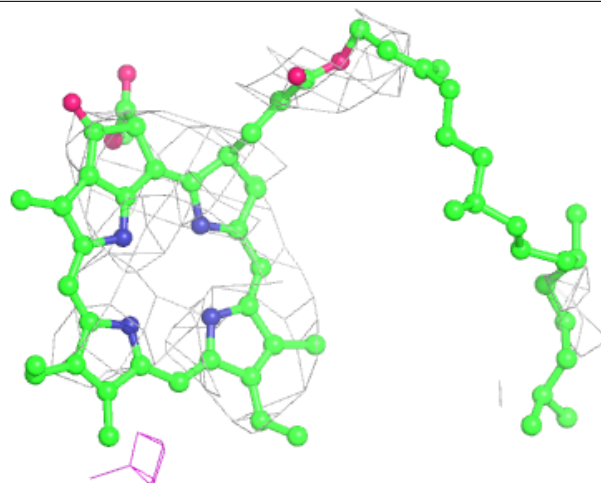
**Electron density around BCR A 407:**

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



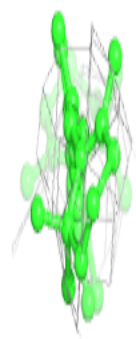
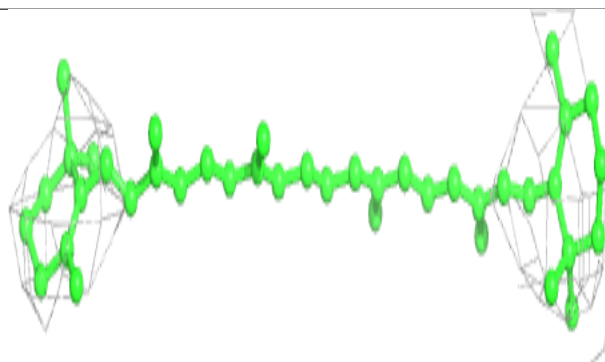
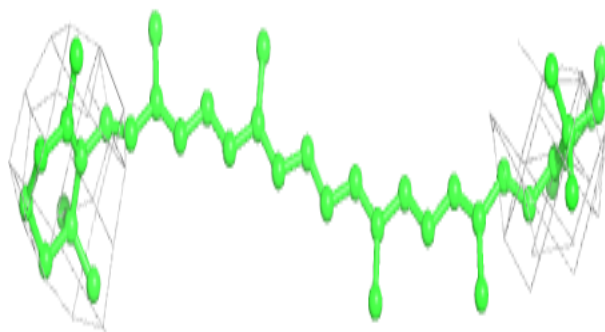
**Electron density around PHO D 402:**

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

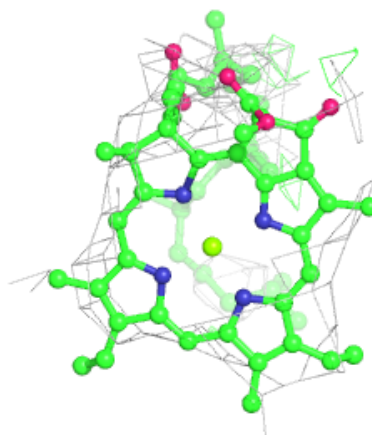
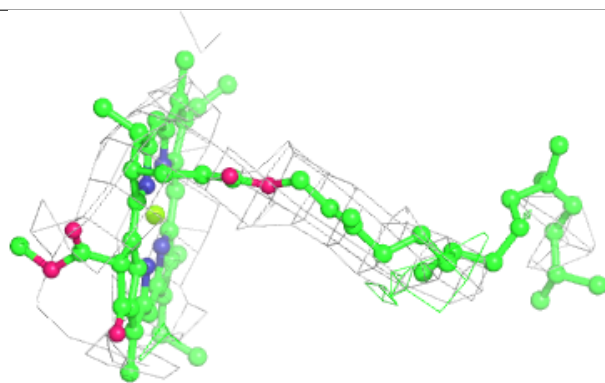
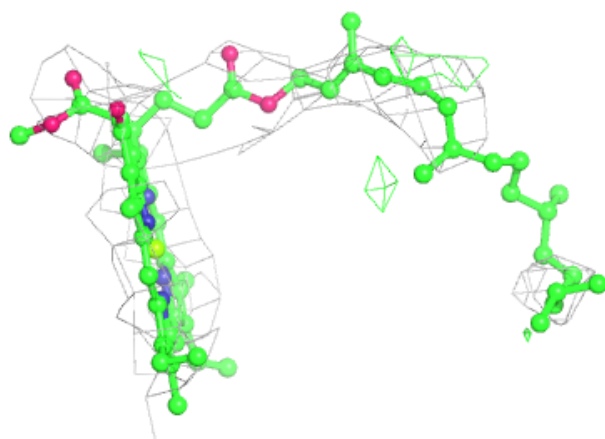


**Electron density around BCR C 521:**

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

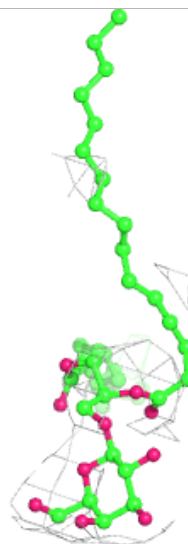
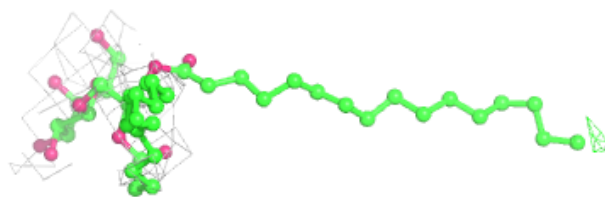
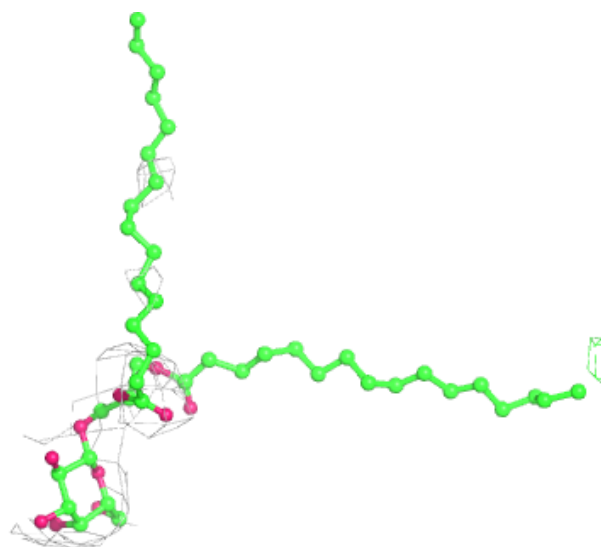
**Electron density around CLA C 505:**

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



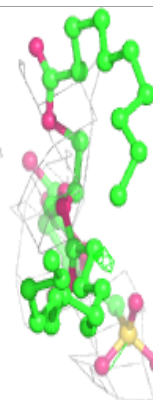
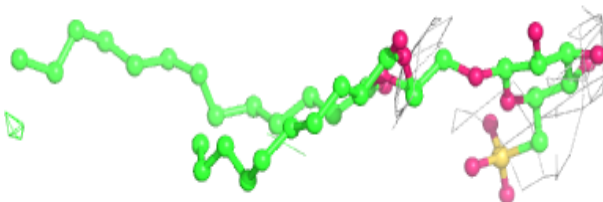
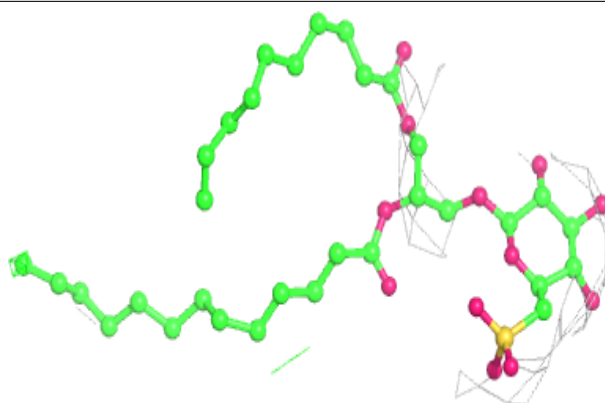
**Electron density around LMG A 410:**

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

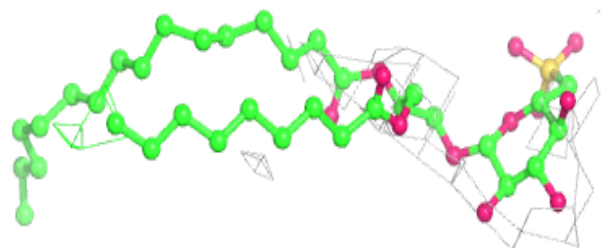
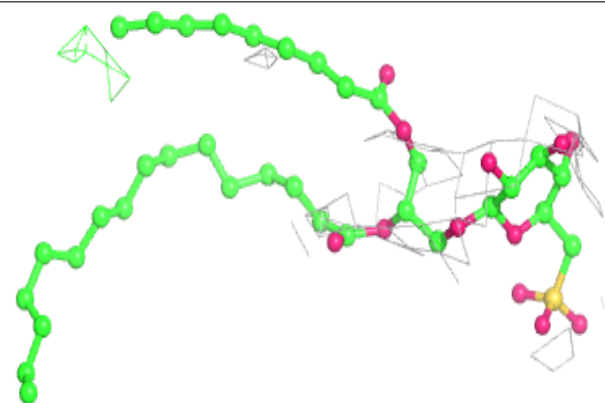


**Electron density around SQD F 102:**

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

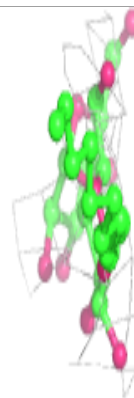
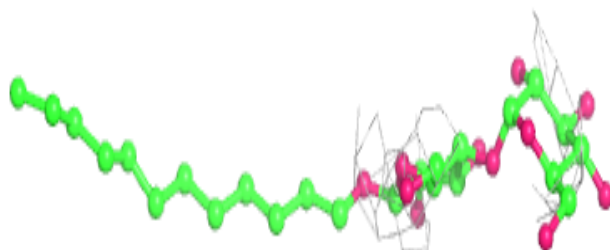
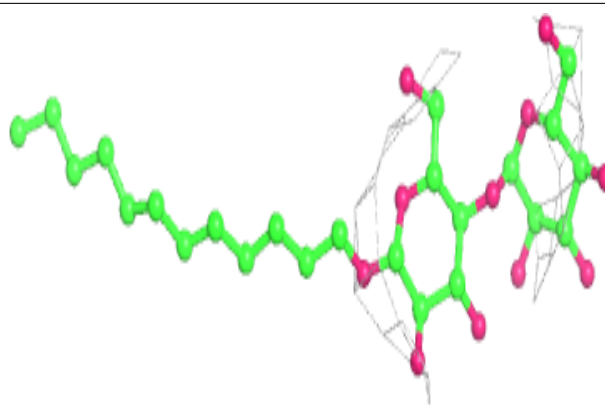
**Electron density around SQD B 626:**

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

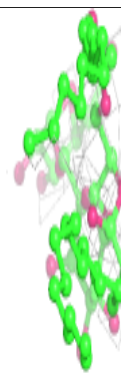
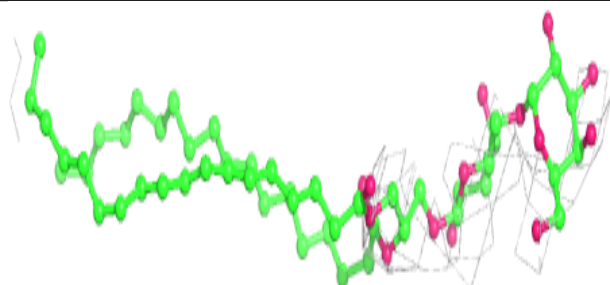
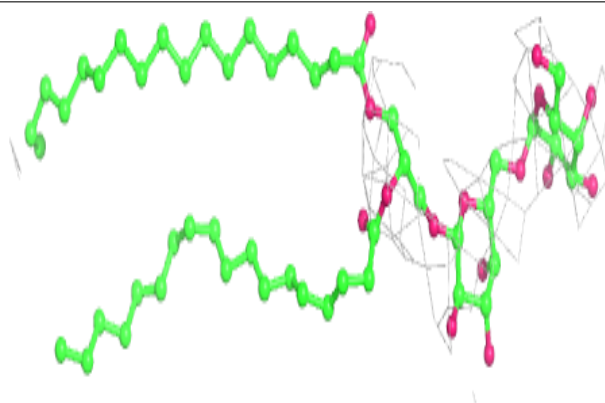


**Electron density around LMT B 623:**

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

**Electron density around DGD c 517:**

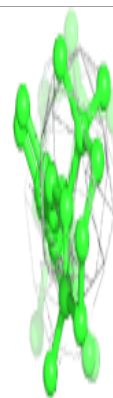
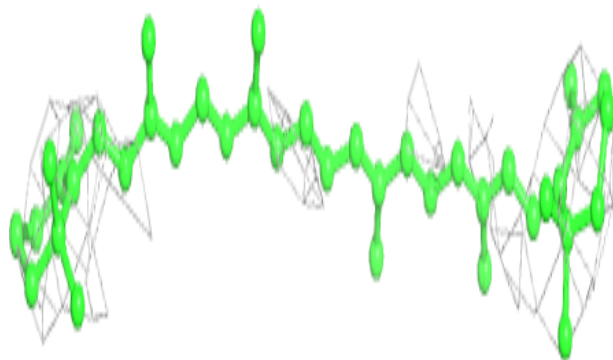
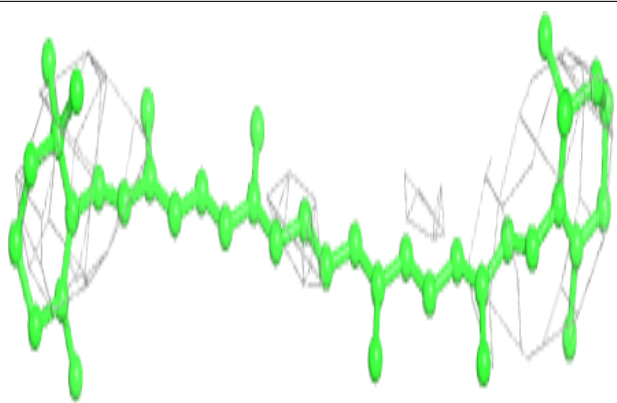
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



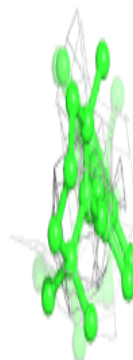
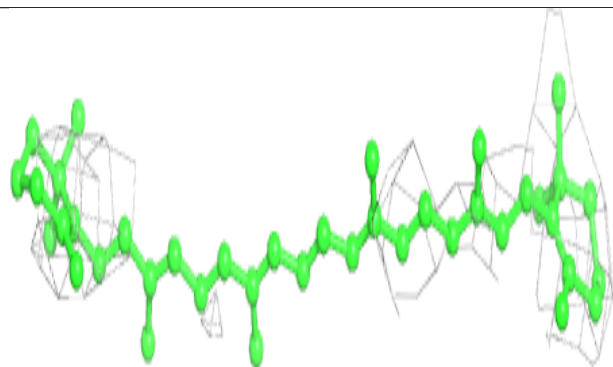
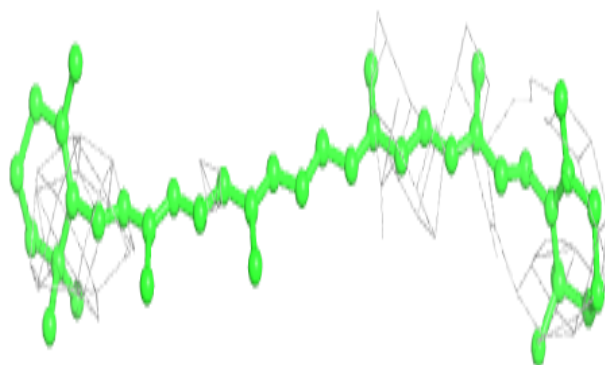


**Electron density around BCR b 623:**

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

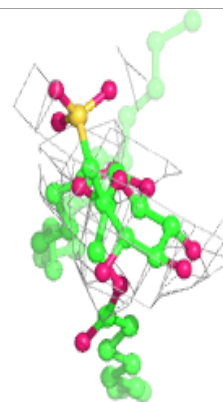
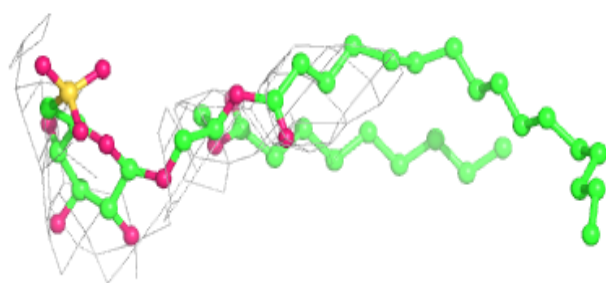
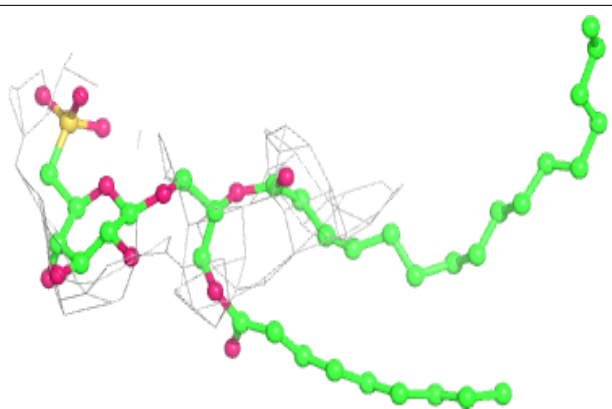
**Electron density around BCR B 619:**

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

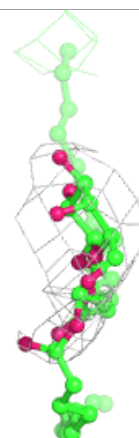
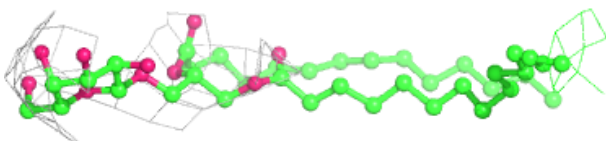
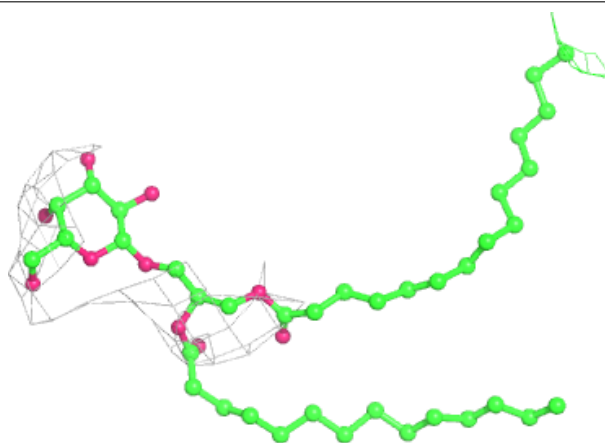


**Electron density around SQD b 602:**

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

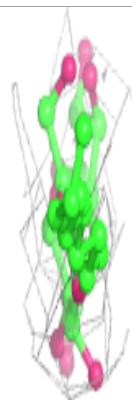
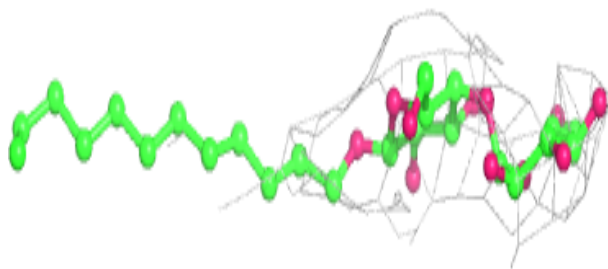
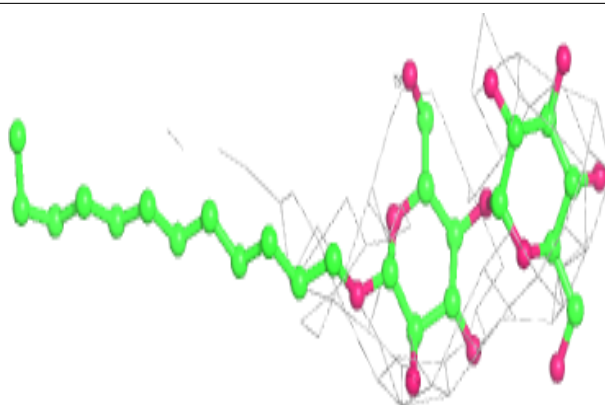
**Electron density around LMG c 522:**

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

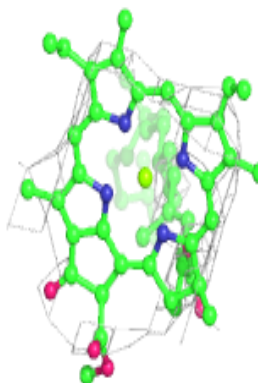
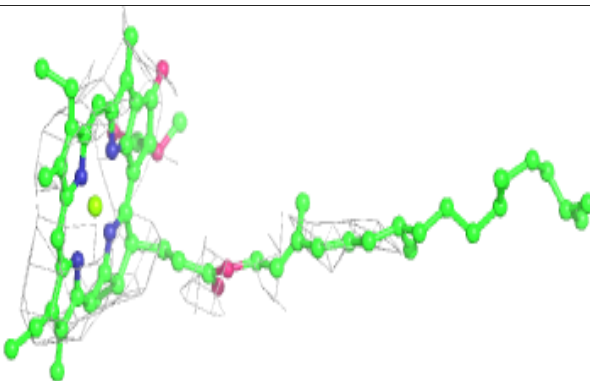
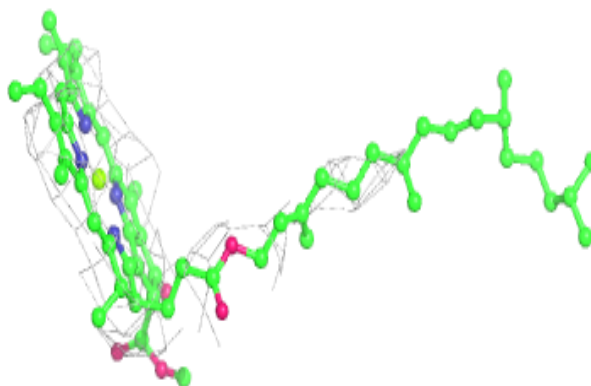


**Electron density around LMT b 603:**

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

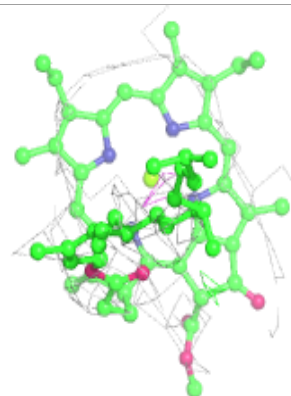
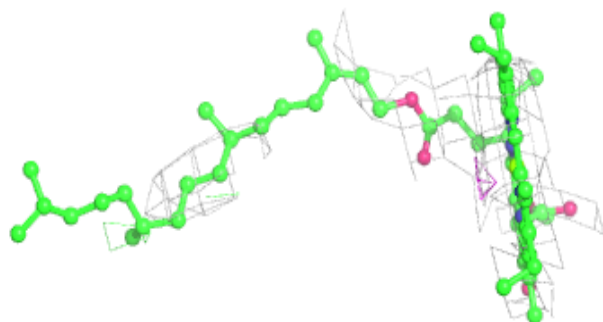
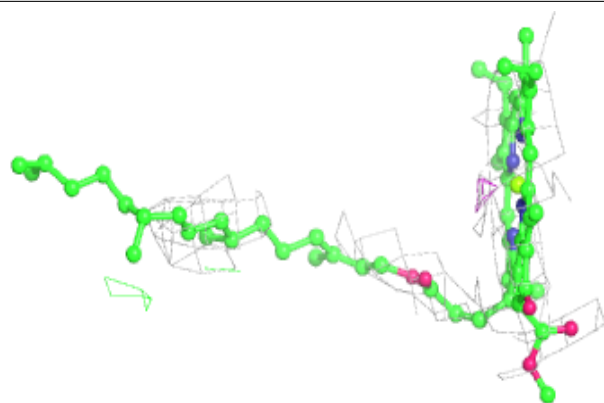
**Electron density around CLA B 603:**

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

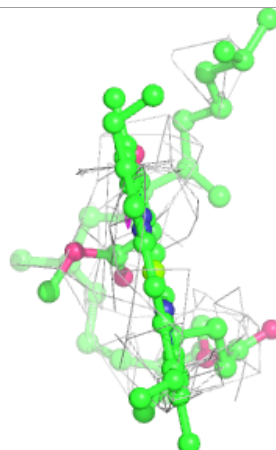
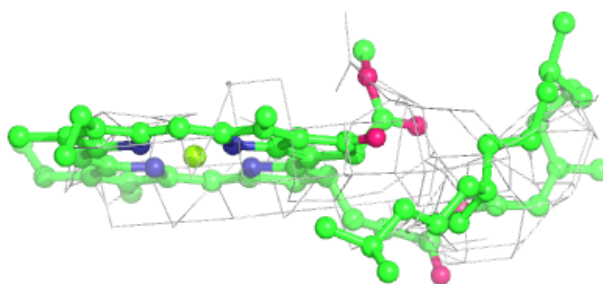
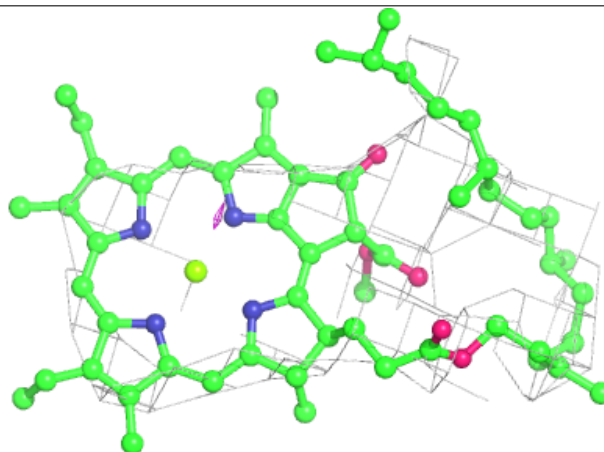


**Electron density around CLA b 609:**

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

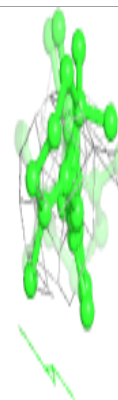
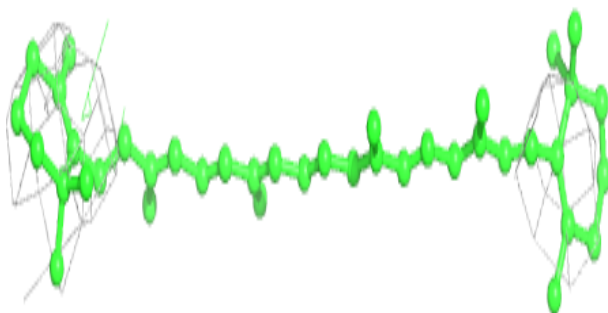
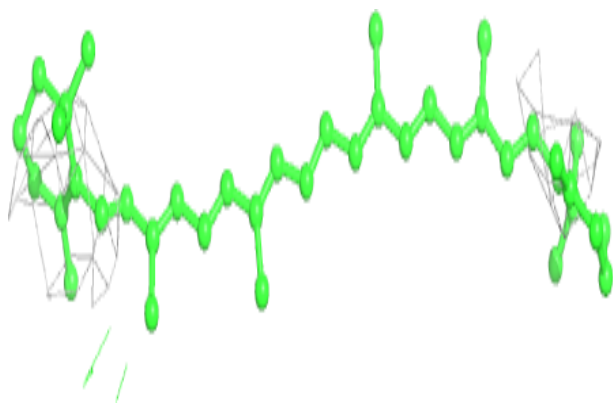
**Electron density around CLA b 613:**

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



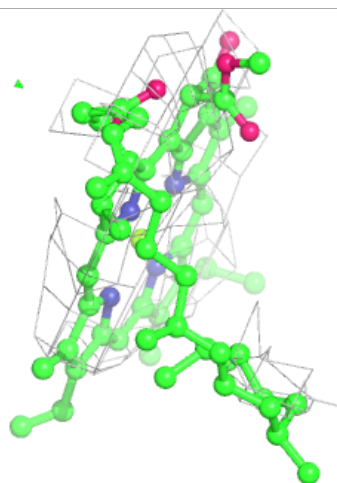
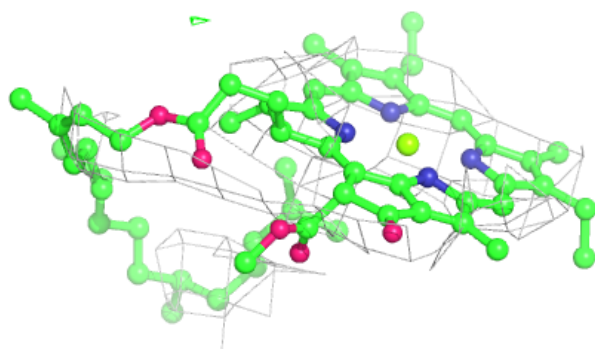
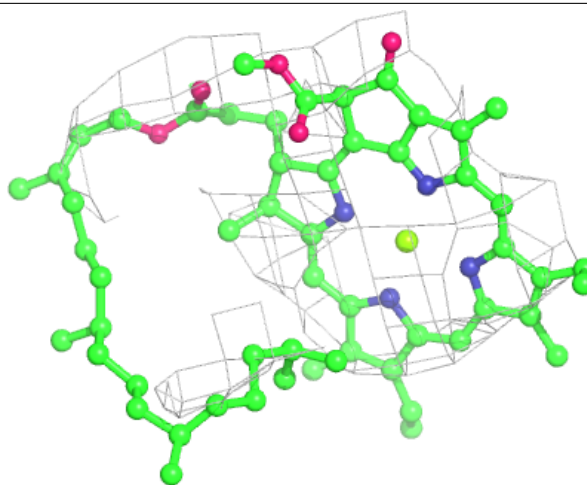
**Electron density around BCR c 521:**

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



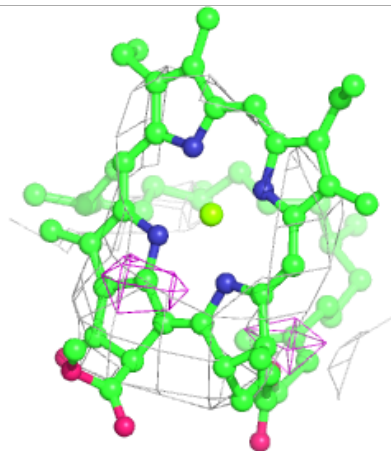
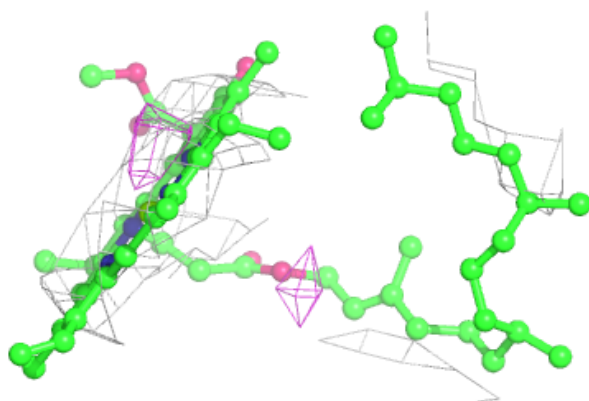
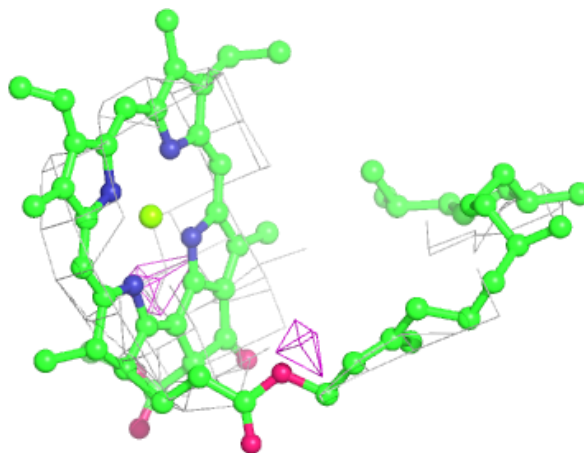
**Electron density around CLA b 618:**

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



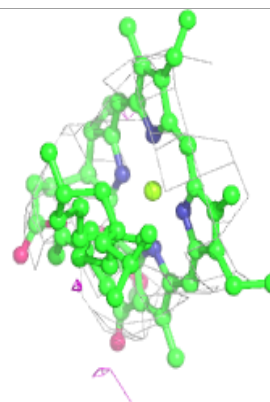
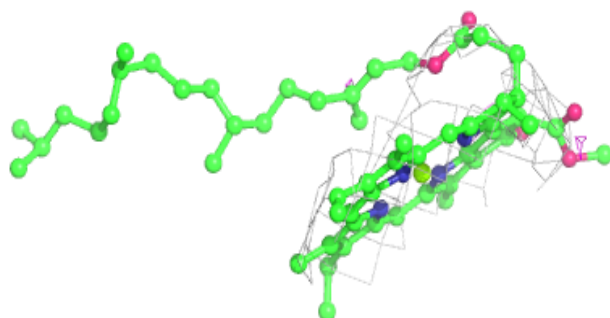
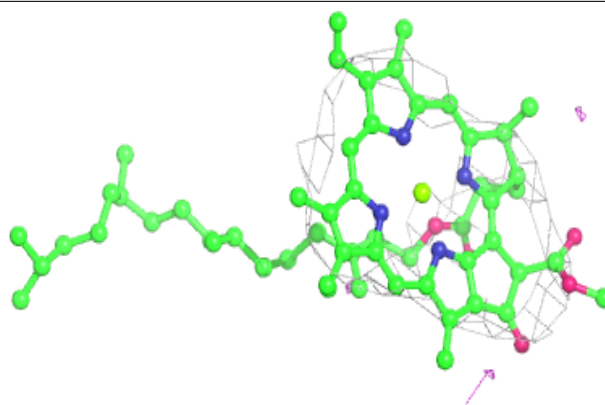
**Electron density around CLA c 503:**

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

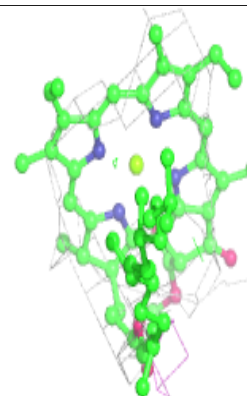
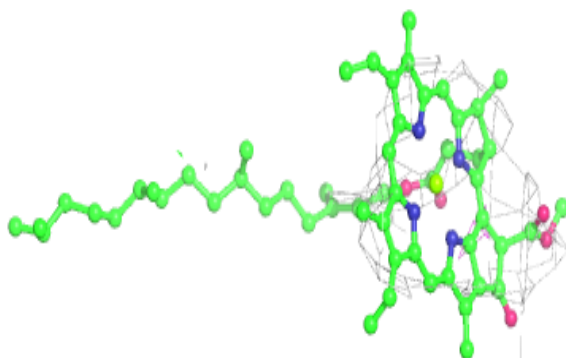
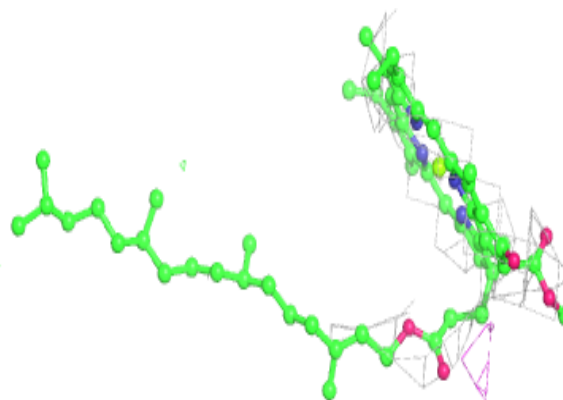


**Electron density around CLA b 617:**

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

**Electron density around CLA C 520:**

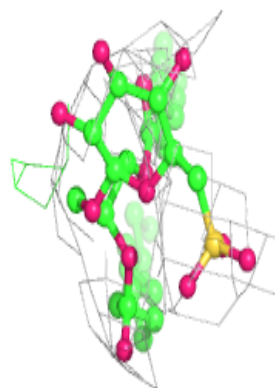
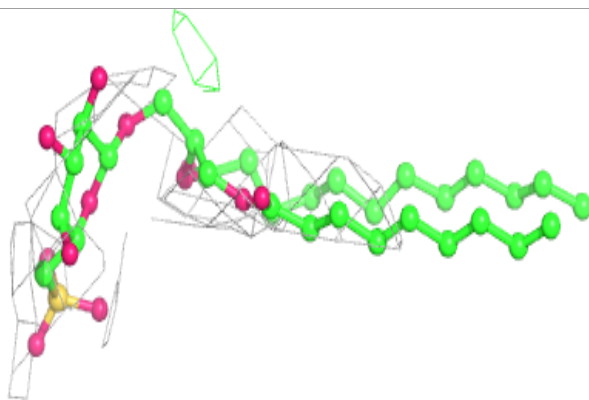
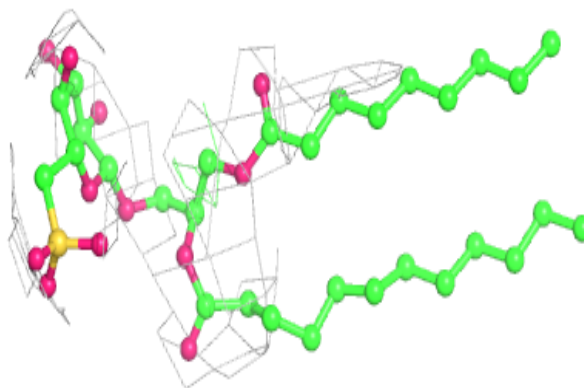
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



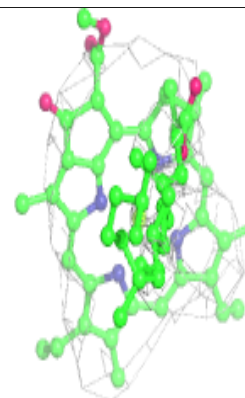
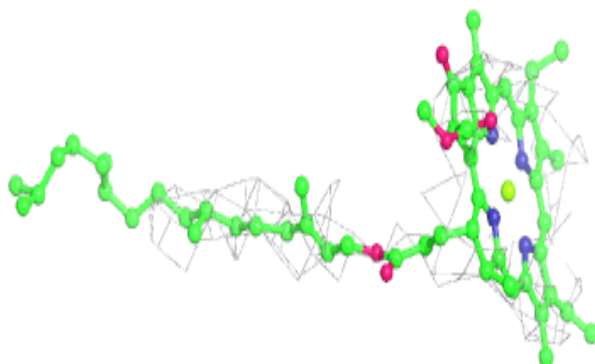
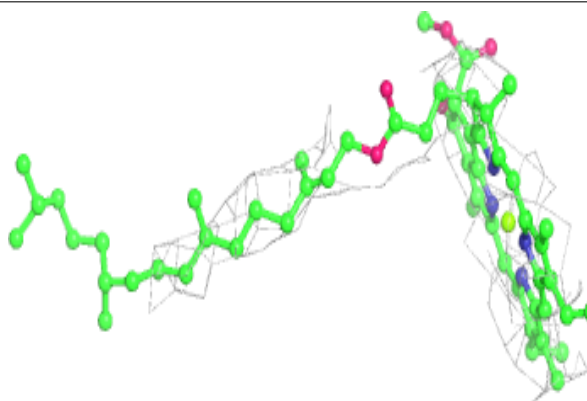


**Electron density around SQD D 403:**

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

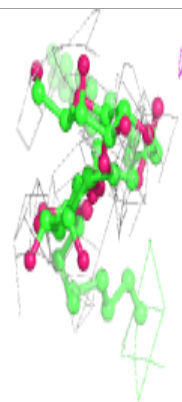
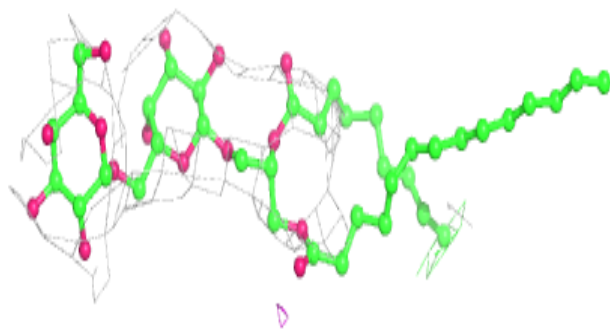
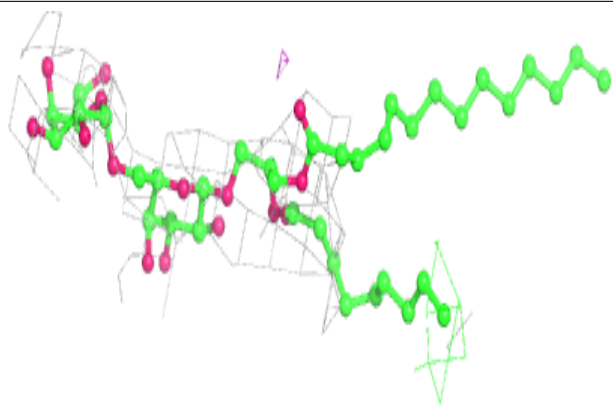
**Electron density around CLA b 607:**

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

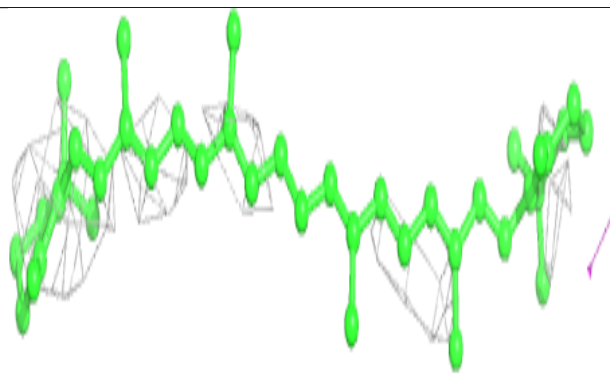
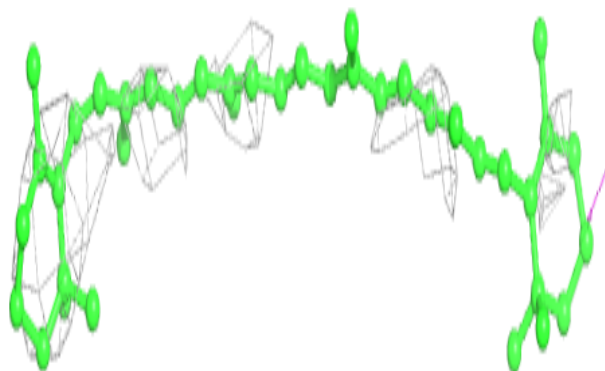


**Electron density around DGD C 515:**

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

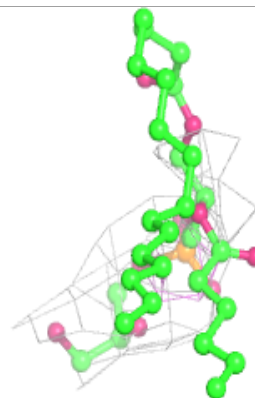
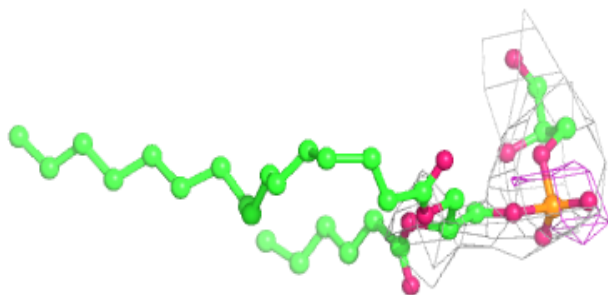
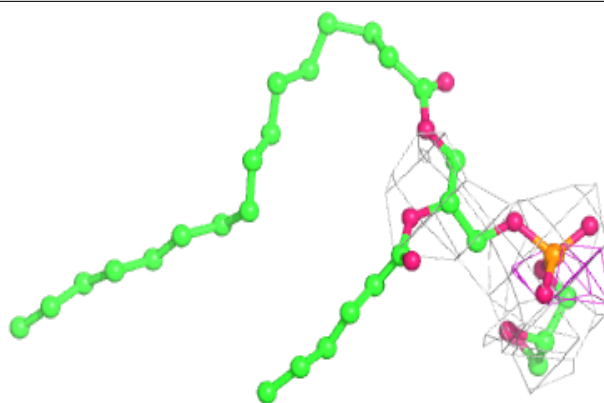
**Electron density around BCR c 513:**

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

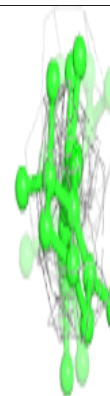
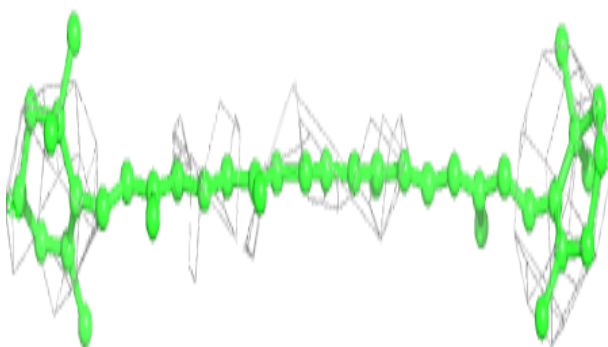
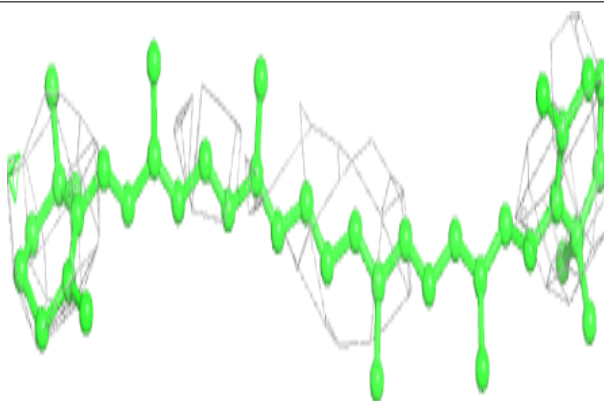


**Electron density around LHG a 412:**

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

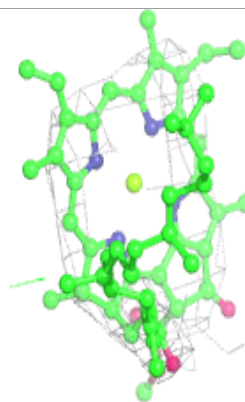
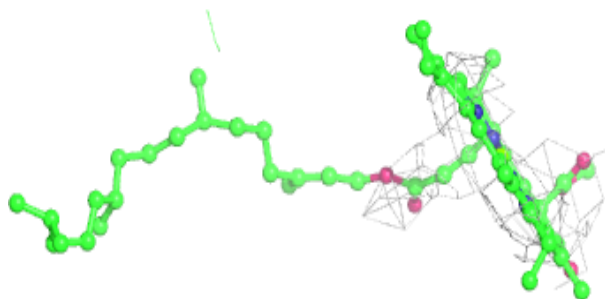
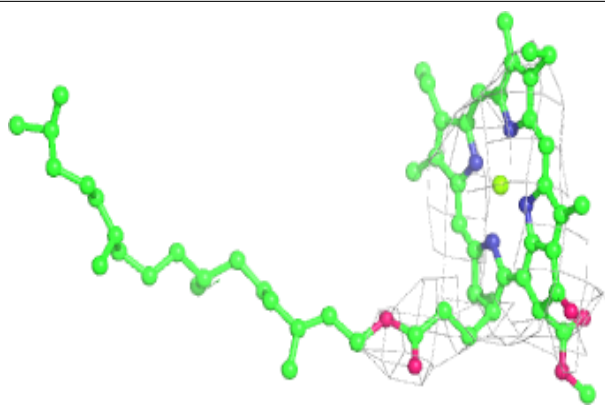
**Electron density around BCR B 618:**

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

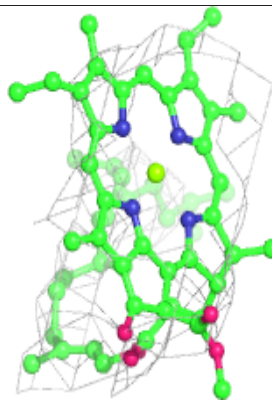
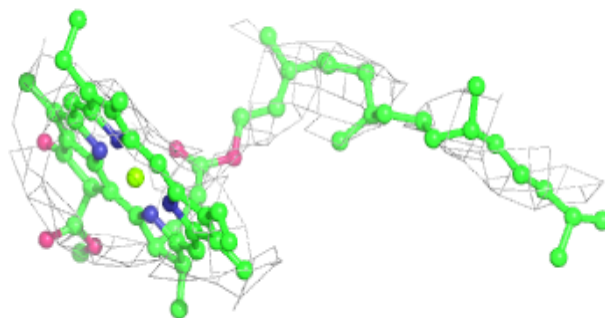
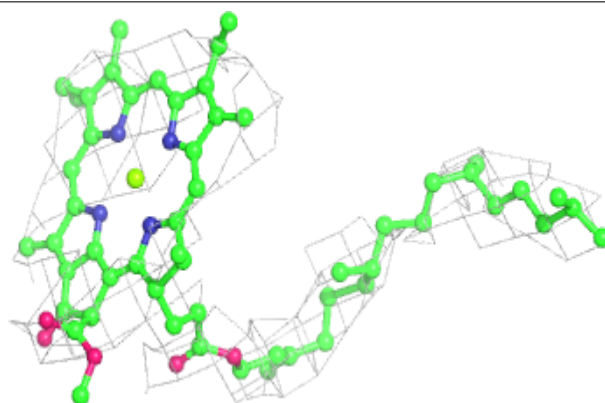


**Electron density around CLA A 405:**

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

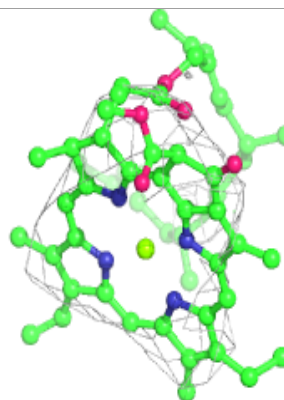
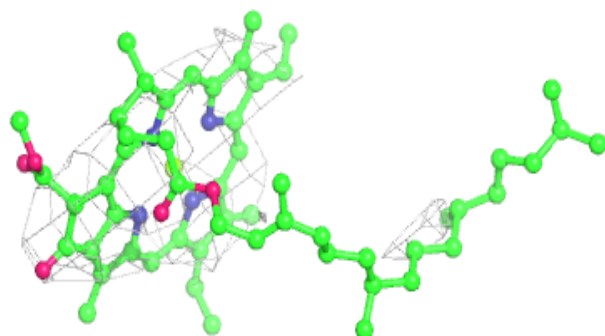
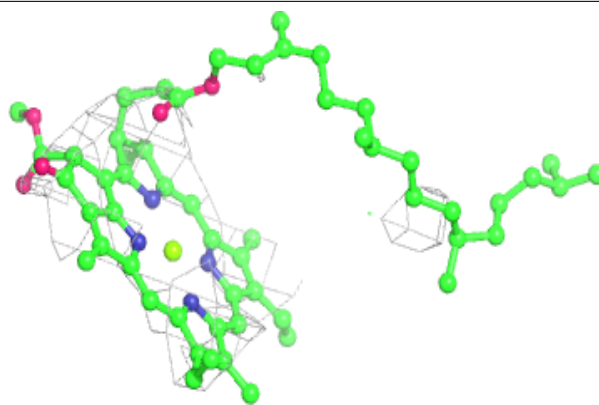
**Electron density around CLA C 510:**

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

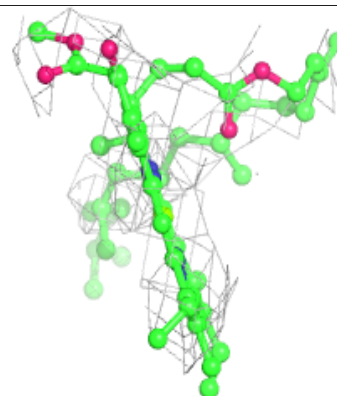
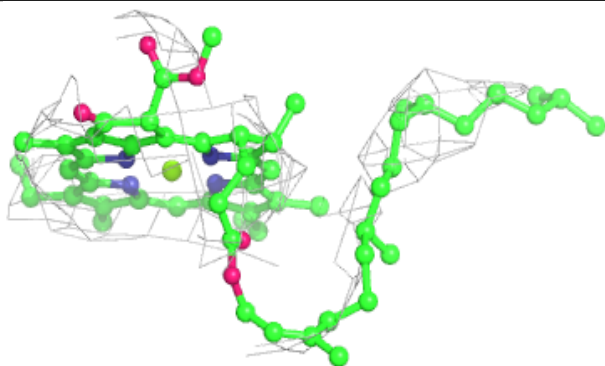
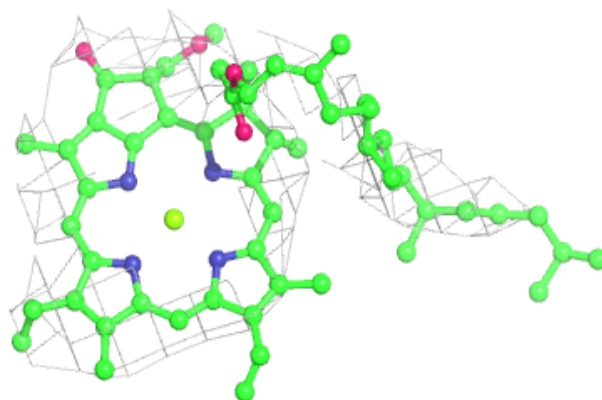


**Electron density around CLA C 512:**

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

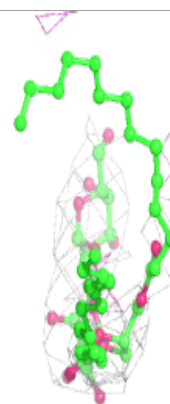
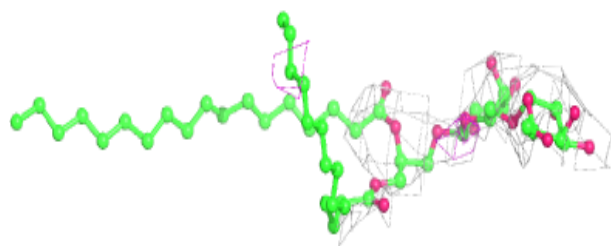
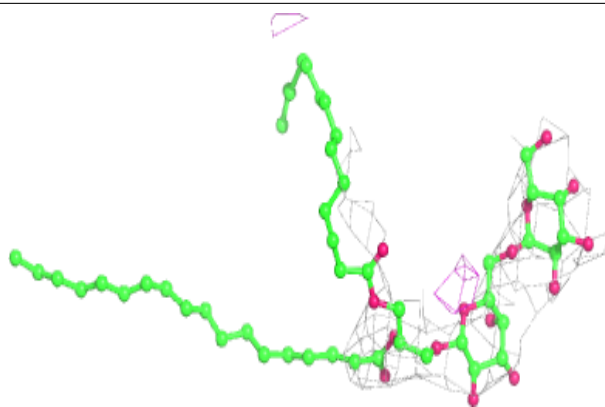
**Electron density around CLA a 405:**

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



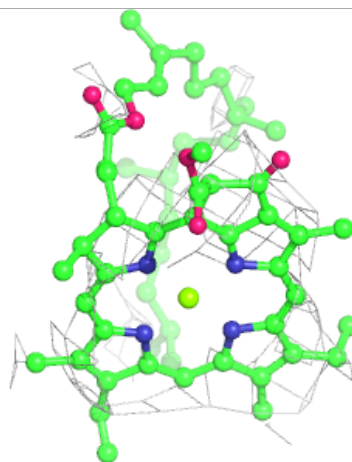
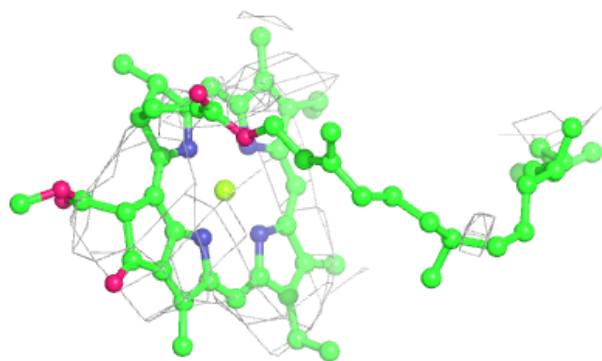
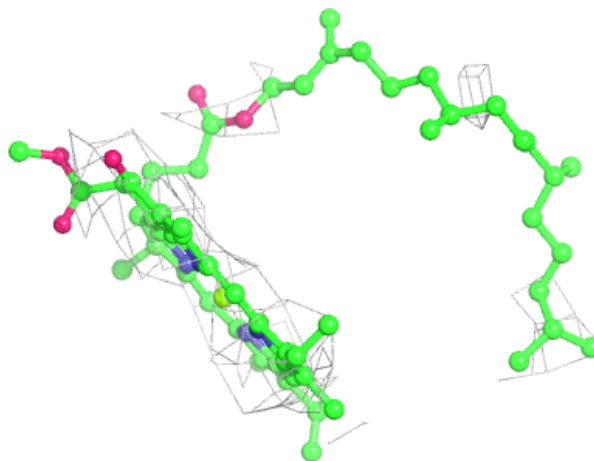
**Electron density around DGD C 516:**

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



**Electron density around CLA B 610:**

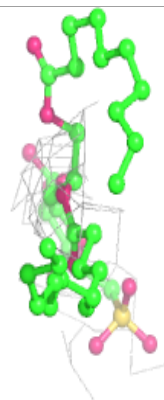
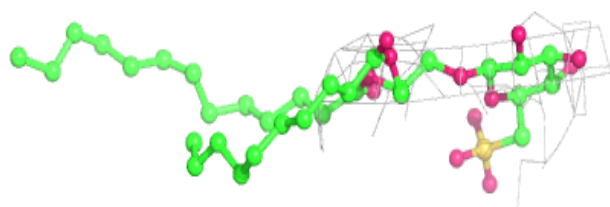
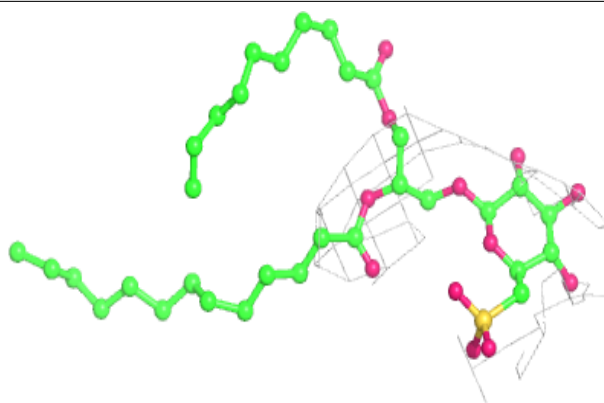
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



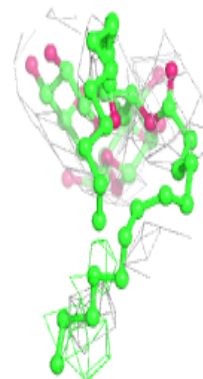
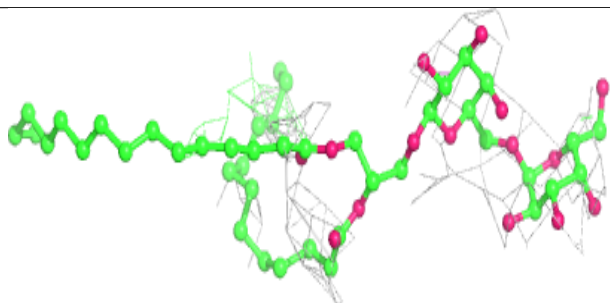
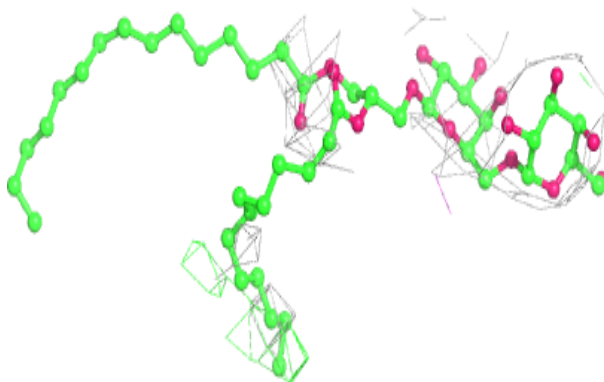


**Electron density around SQD f 103:**

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

**Electron density around DGD B 620:**

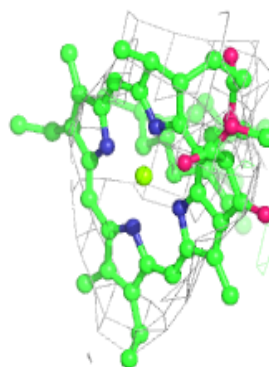
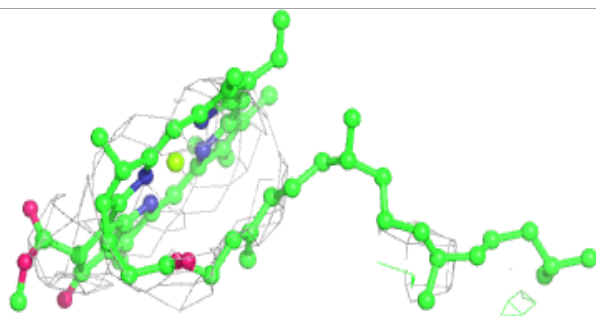
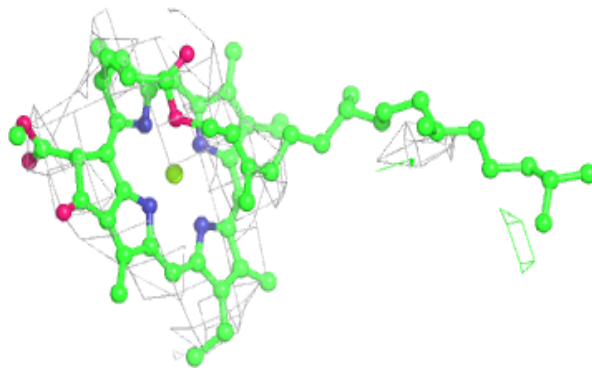
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



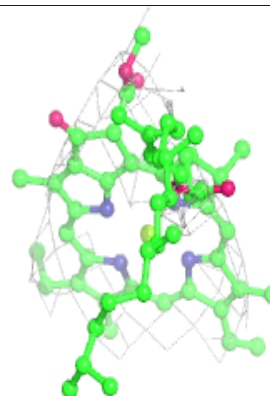
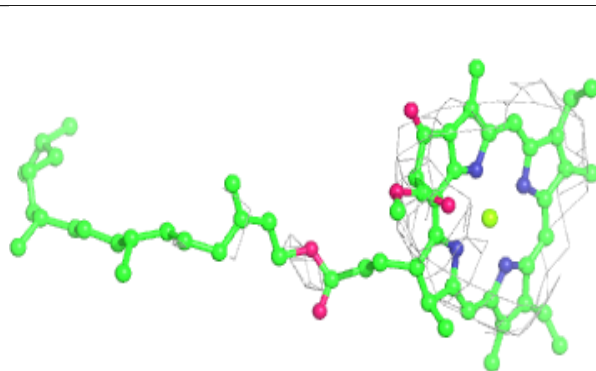
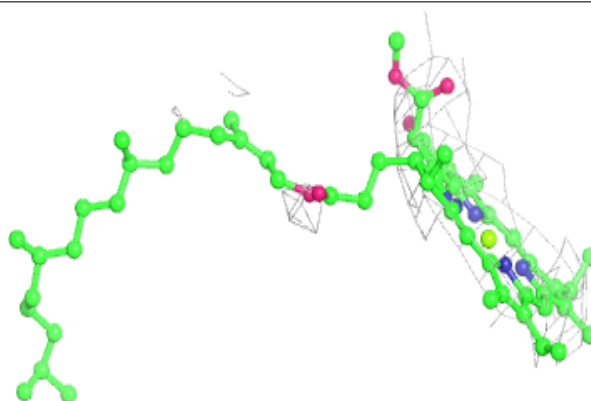


**Electron density around CLA C 504:**

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

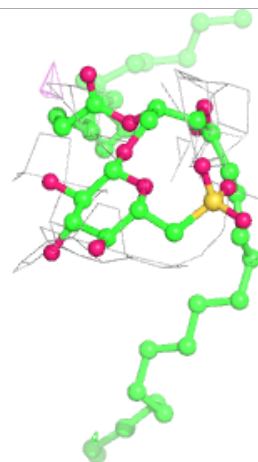
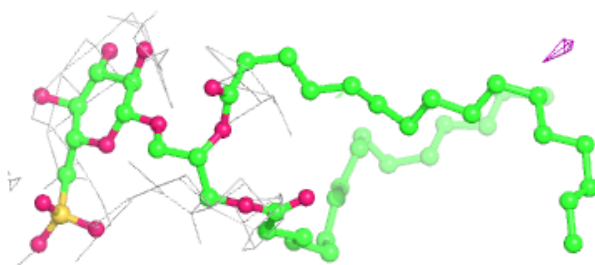
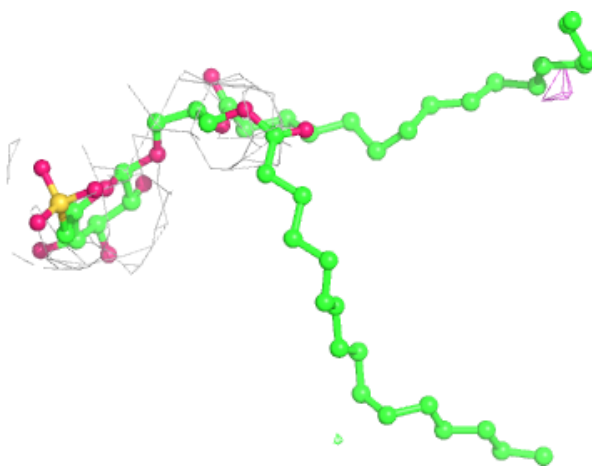
**Electron density around CLA d 404:**

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



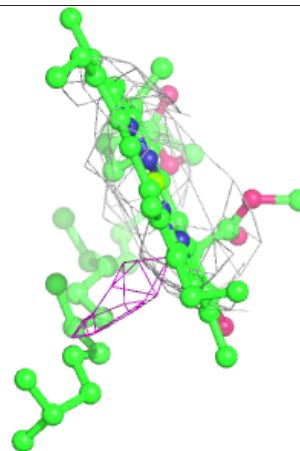
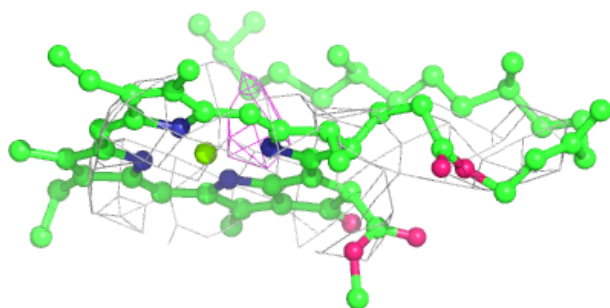
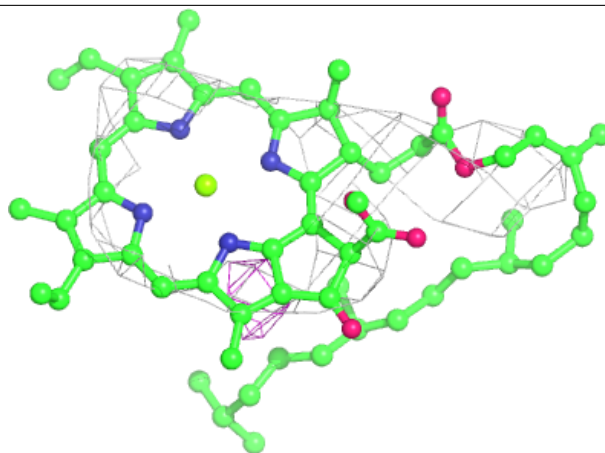
**Electron density around SQD a 401:**

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



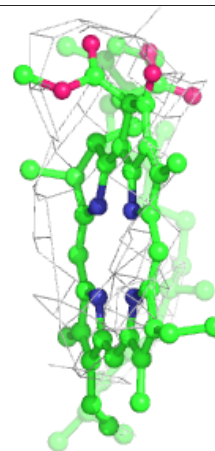
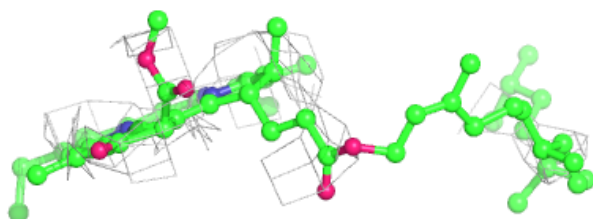
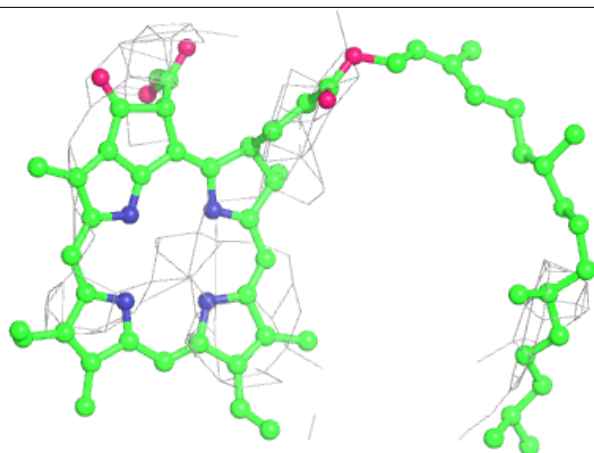
**Electron density around CLA c 508:**

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

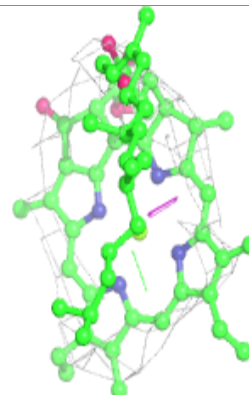
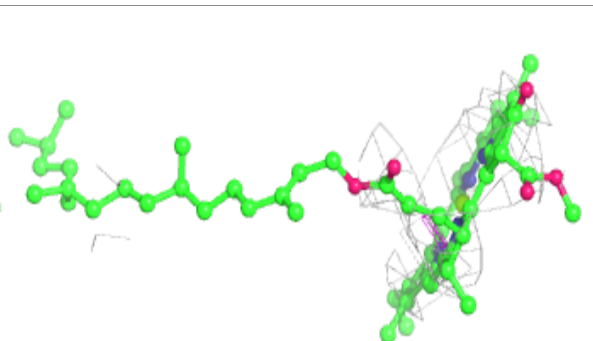
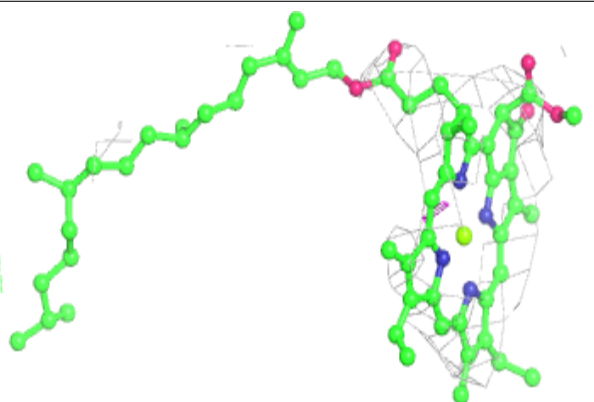


**Electron density around PHO D 401:**

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

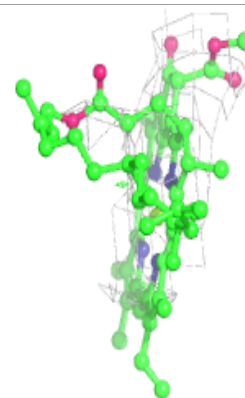
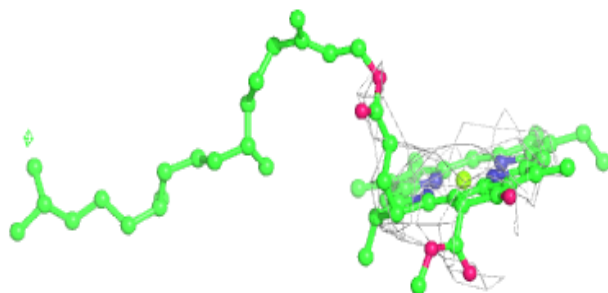
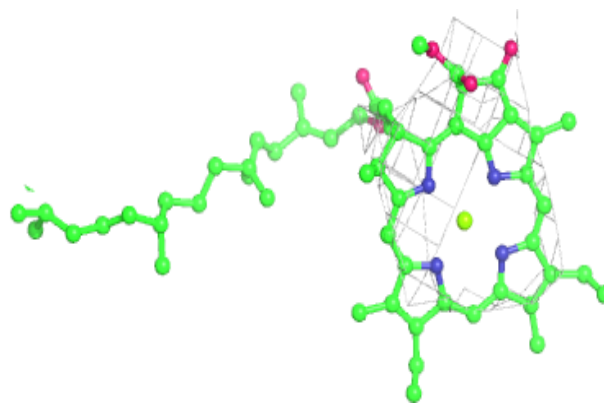
**Electron density around CLA b 612:**

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

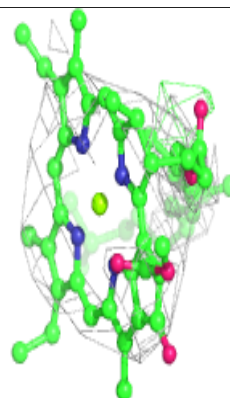
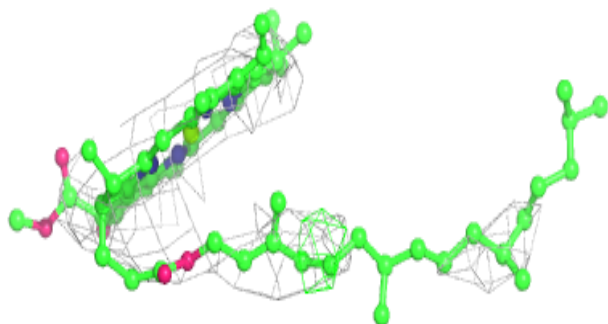
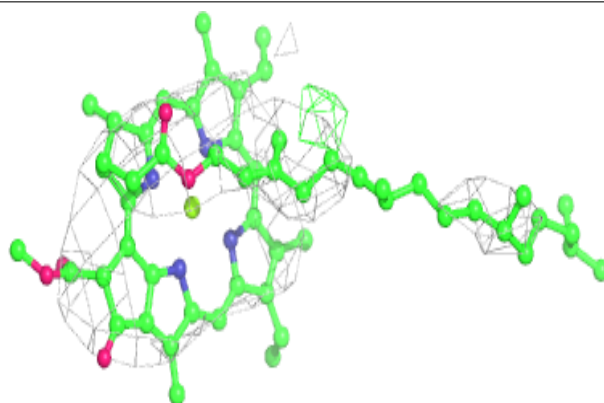


**Electron density around CLA a 406:**

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

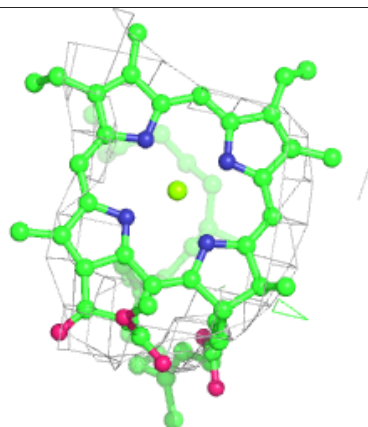
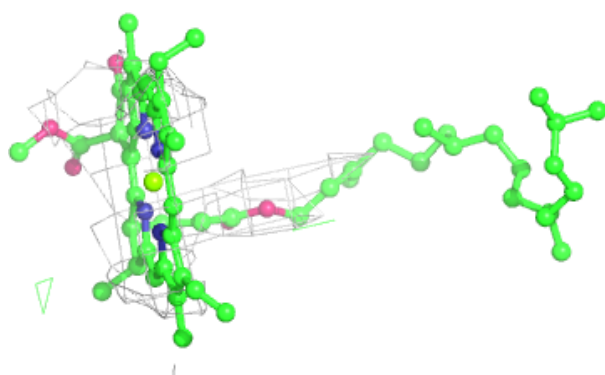
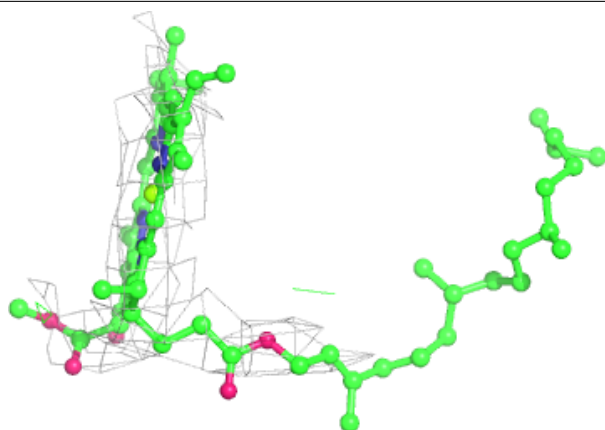
**Electron density around CLA B 607:**

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

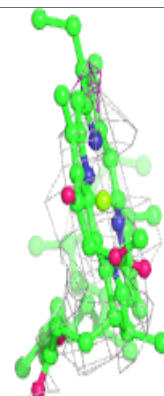
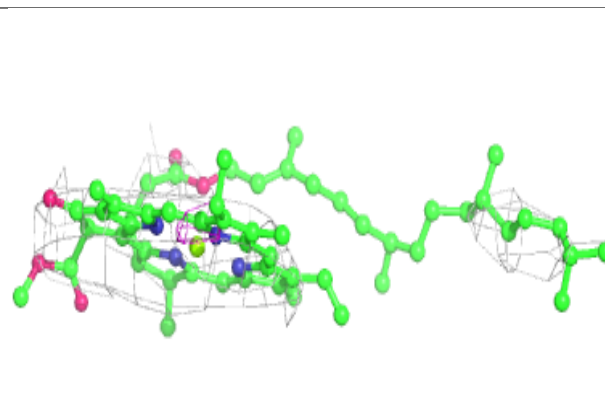
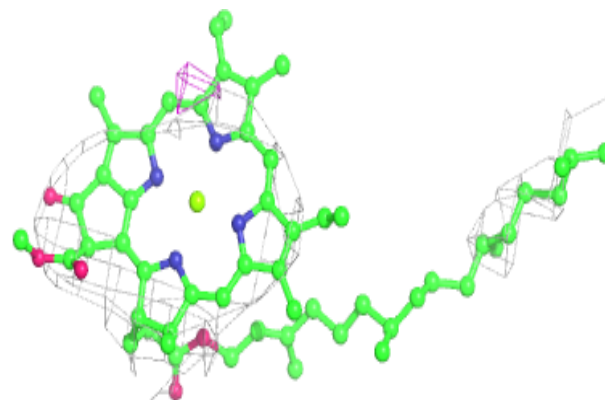


**Electron density around CLA c 505:**

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

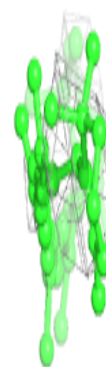
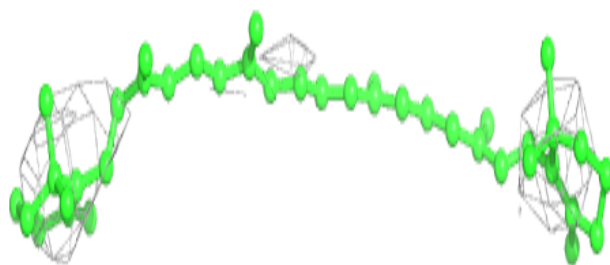
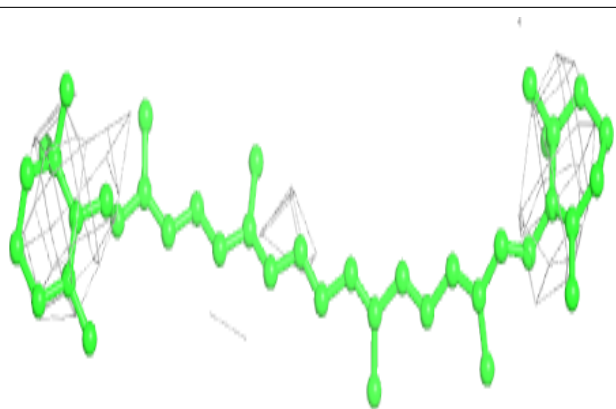
**Electron density around CLA c 501:**

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

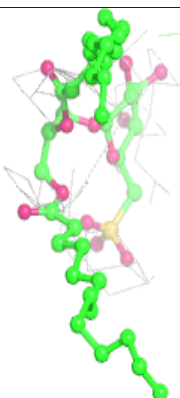
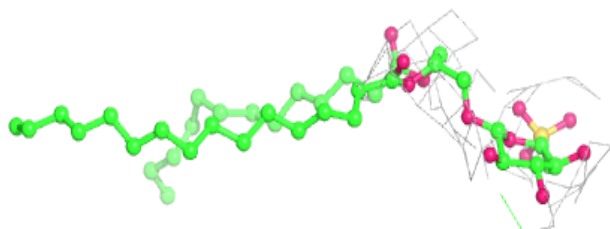
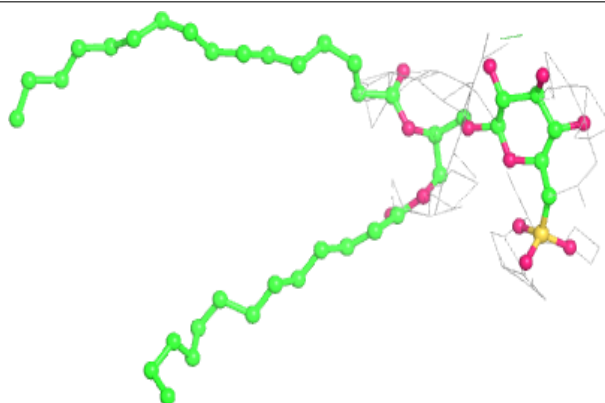


**Electron density around BCR b 621:**

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

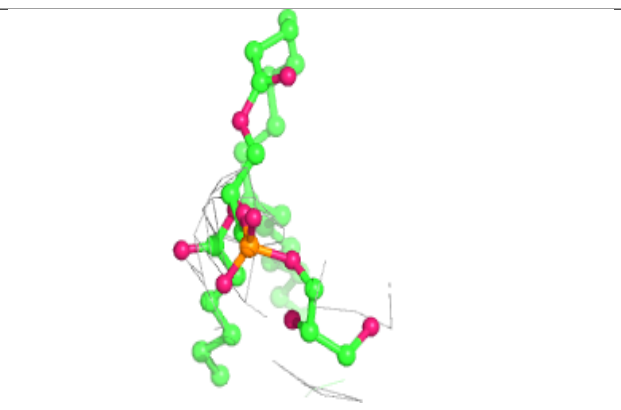
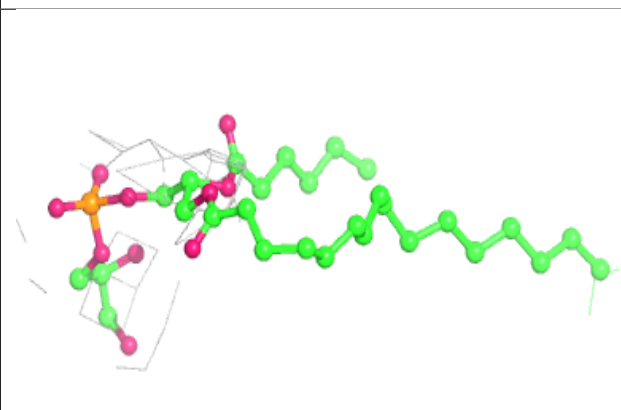
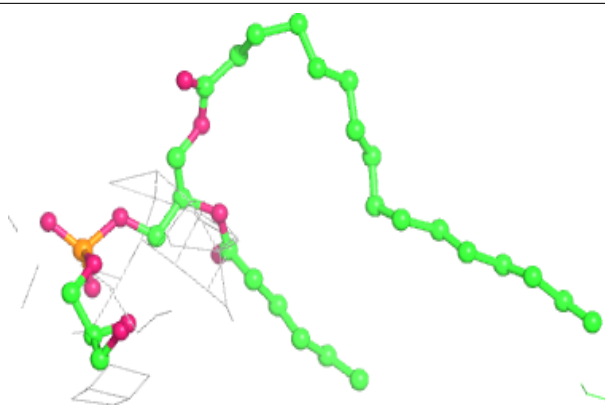
**Electron density around SQD a 415:**

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



**Electron density around LHG A 409:**

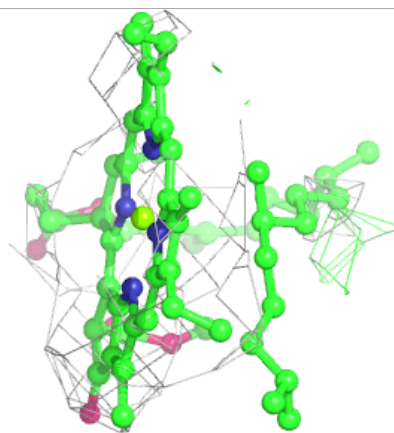
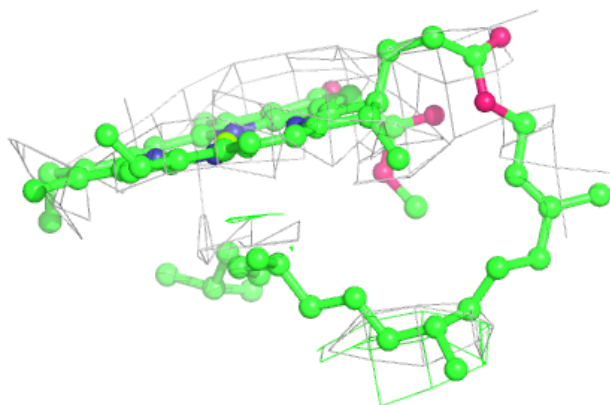
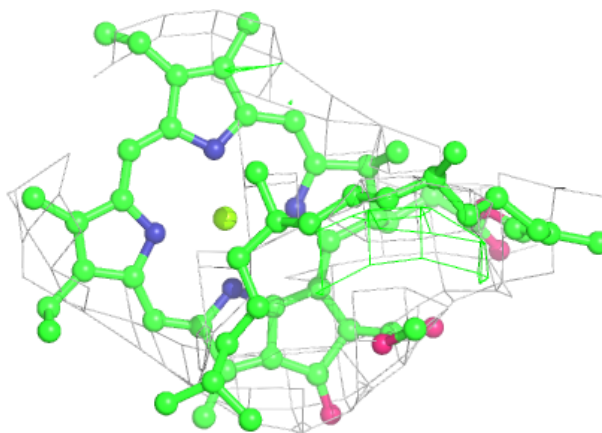
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





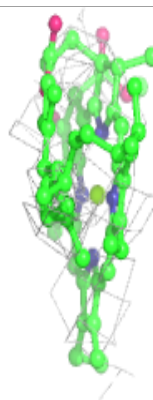
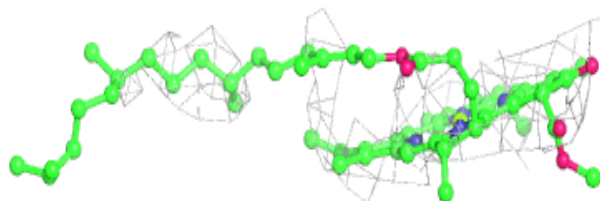
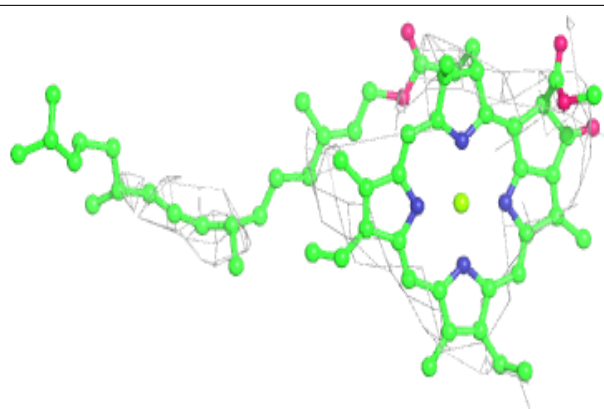
**Electron density around CLA C 509:**

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

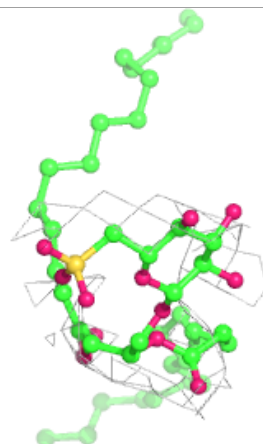
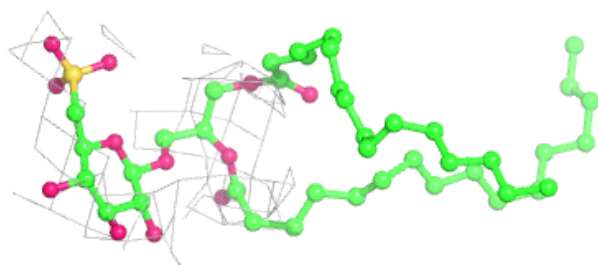
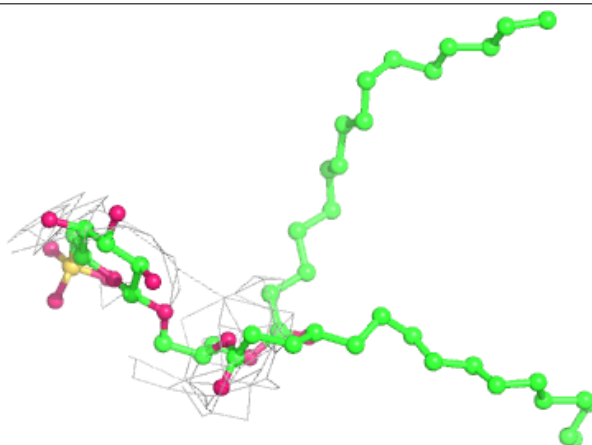


**Electron density around CLA b 606:**

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

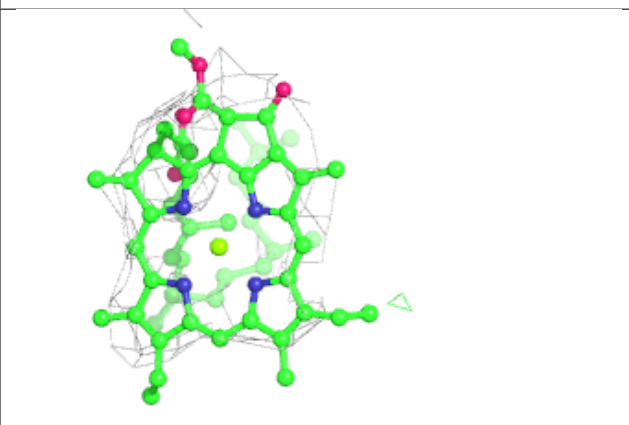
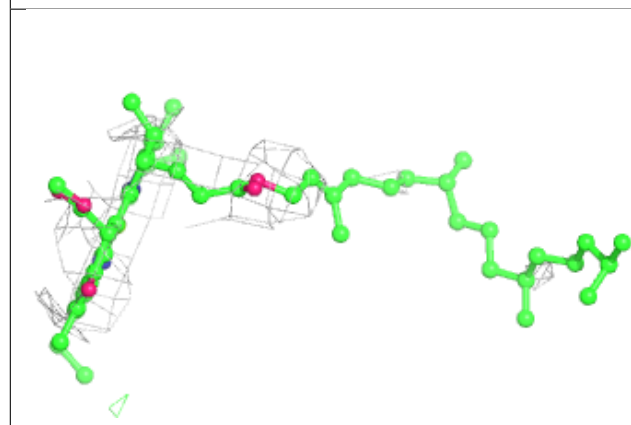
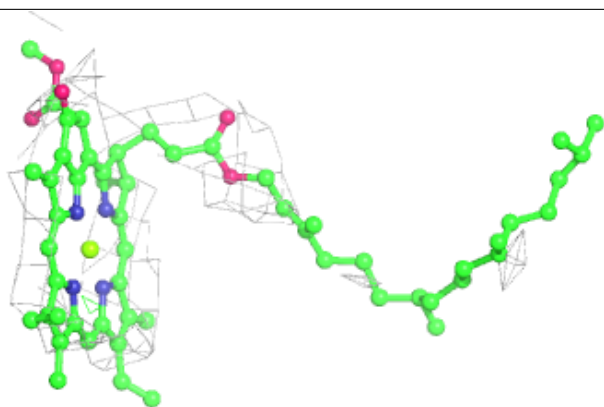
**Electron density around SQD A 414:**

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

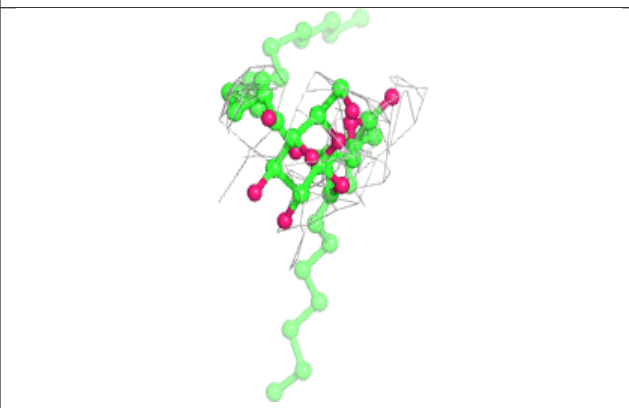
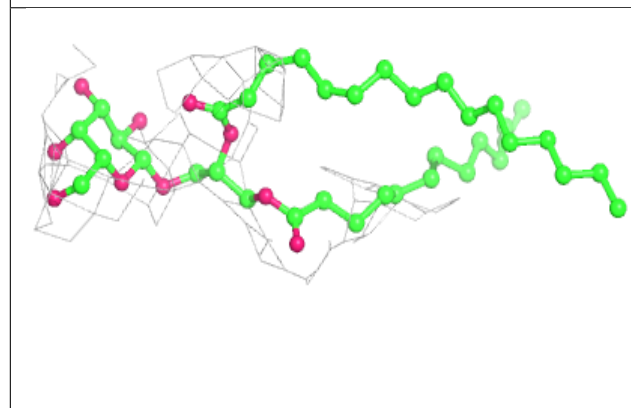
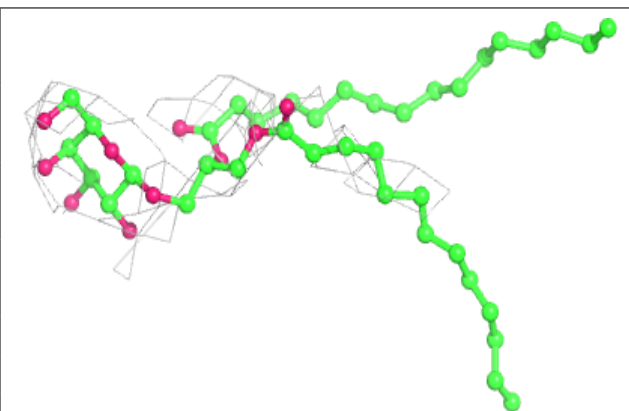


**Electron density around CLA d 405:**

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

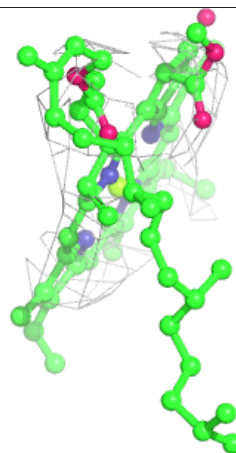
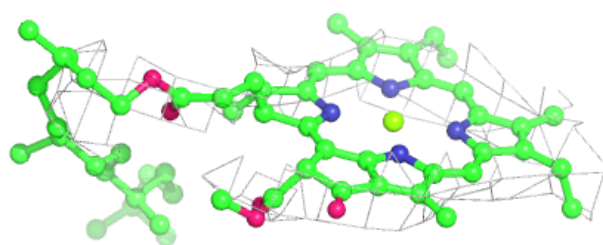
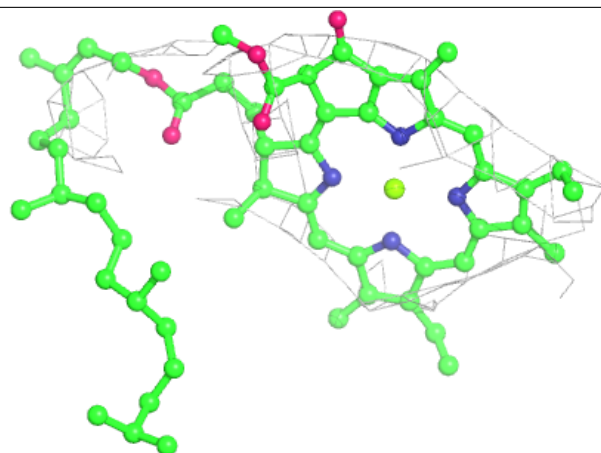
**Electron density around LMG d 407:**

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



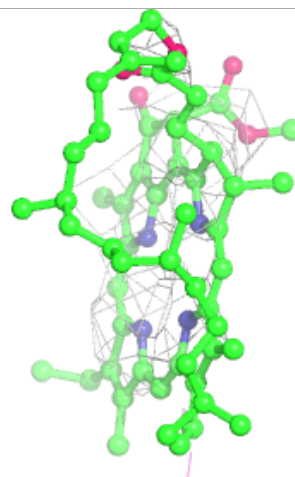
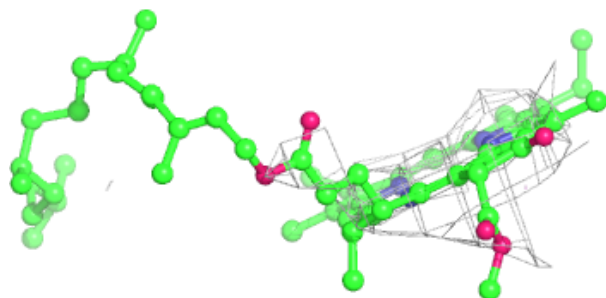
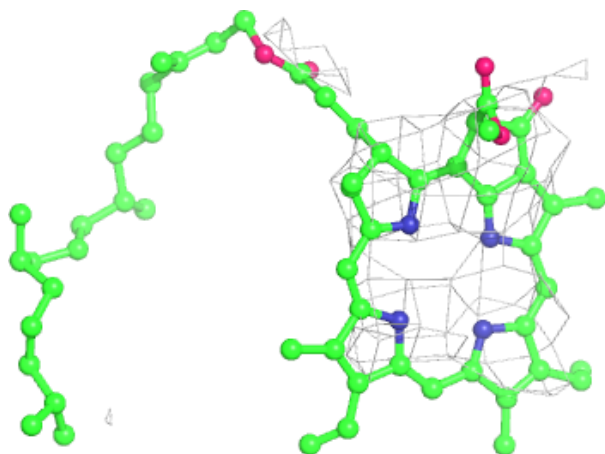
**Electron density around CLA B 615:**

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



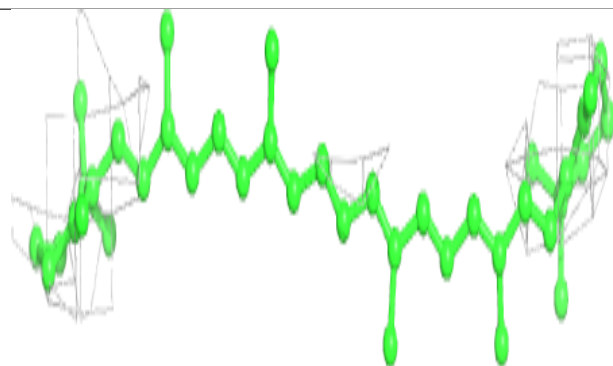
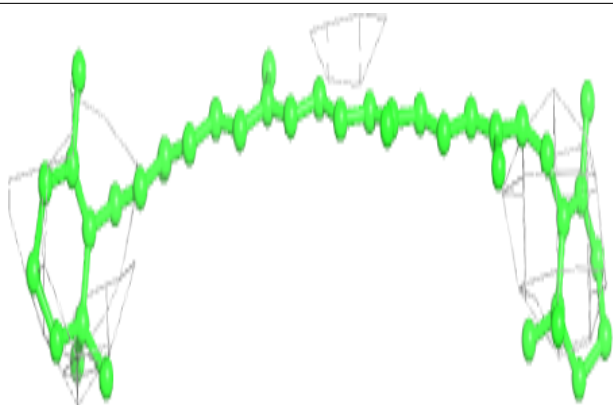
**Electron density around PHO a 407:**

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



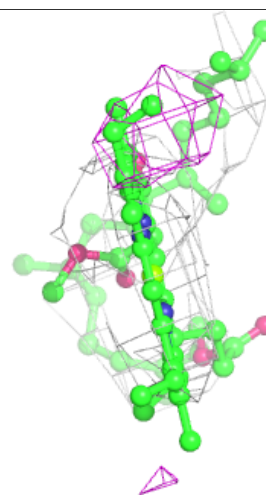
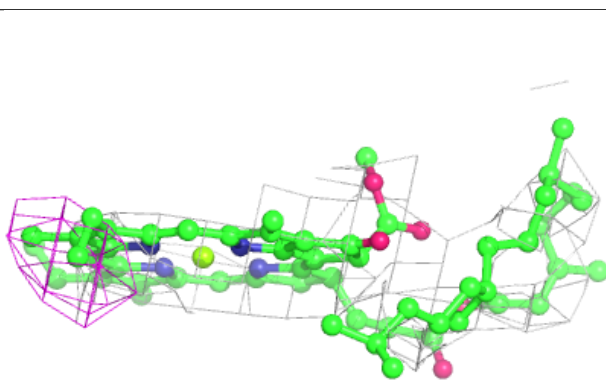
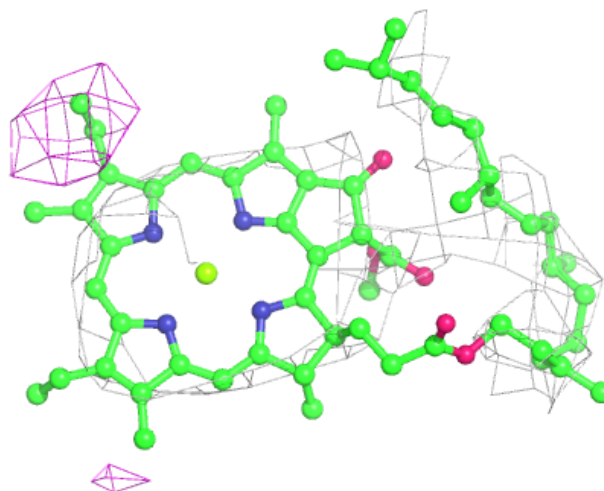
**Electron density around BCR C 513:**

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



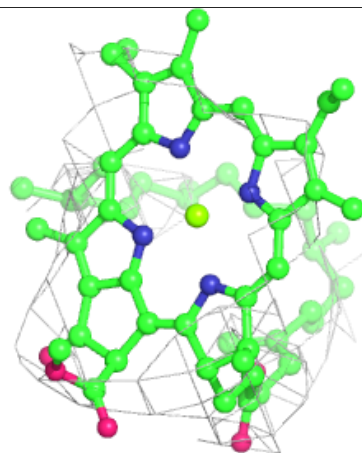
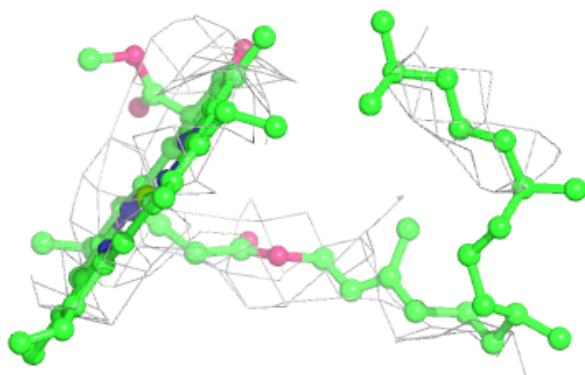
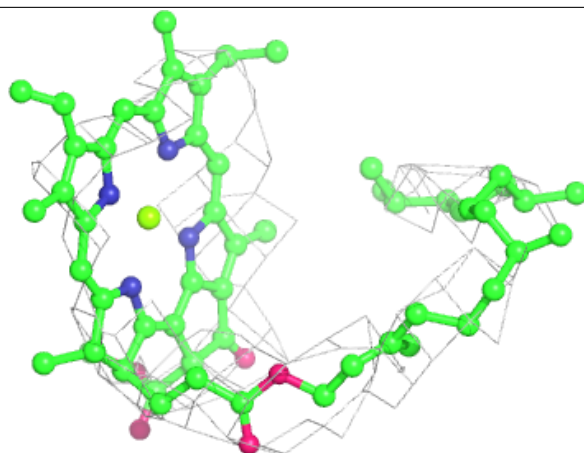
**Electron density around CLA B 609:**

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

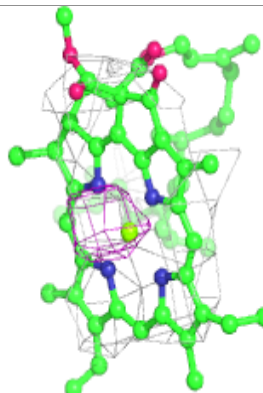
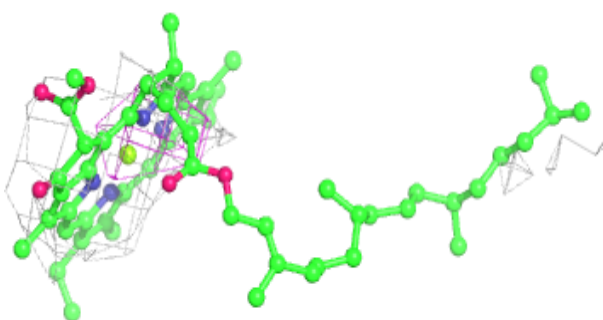
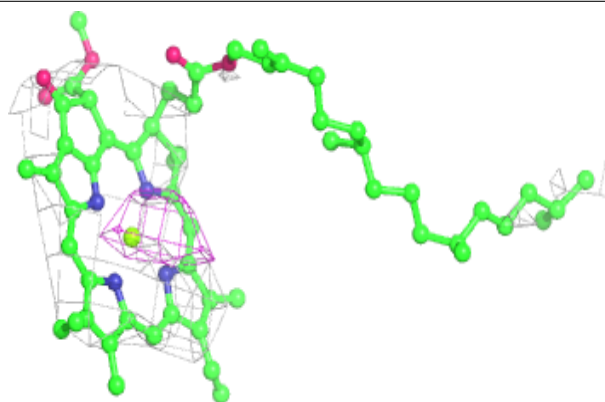


**Electron density around CLA C 503:**

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

**Electron density around CLA c 510:**

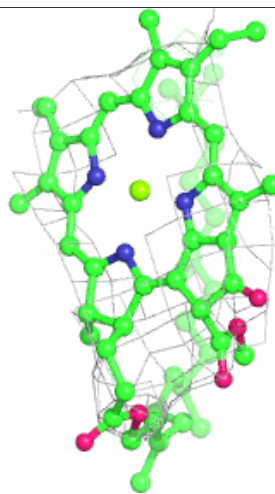
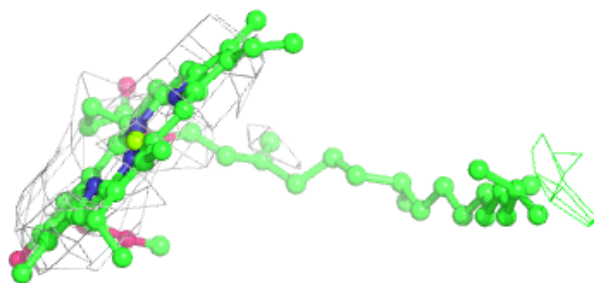
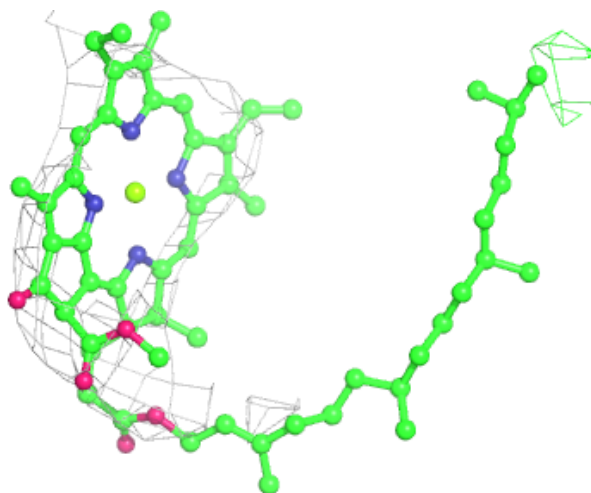
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





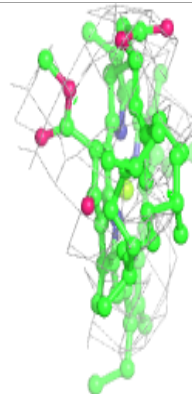
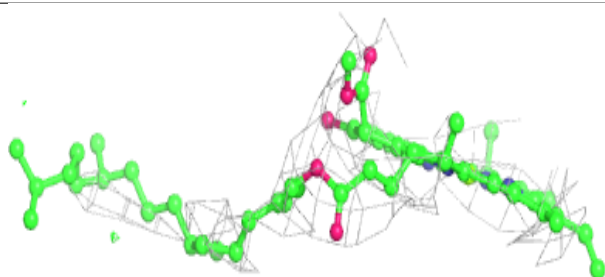
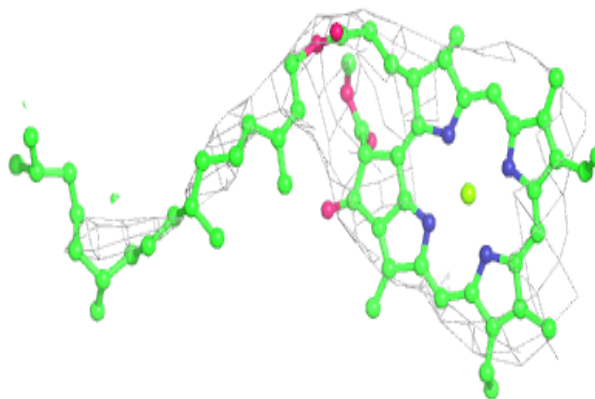
**Electron density around CLA c 506:**

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

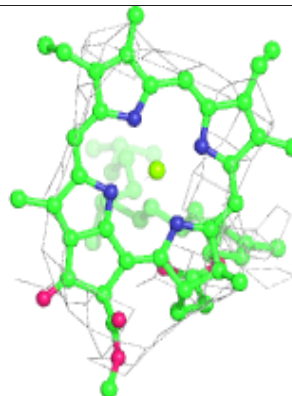
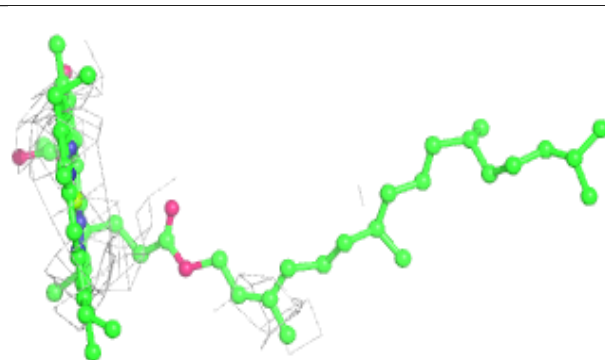
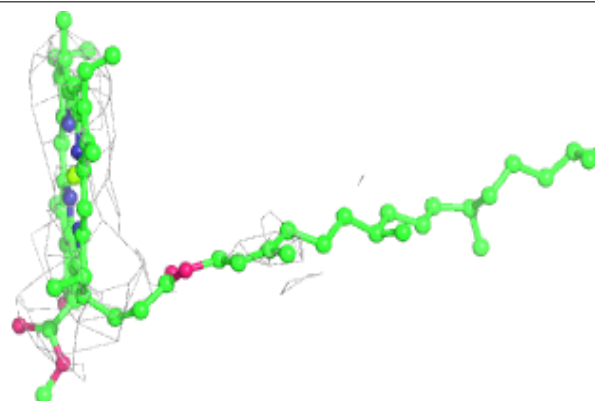


**Electron density around CLA H 101:**

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

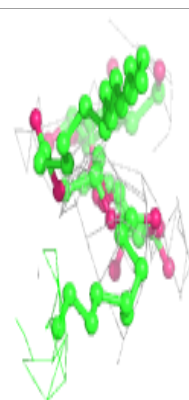
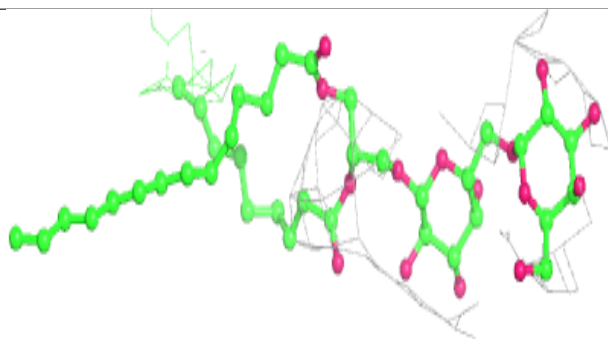
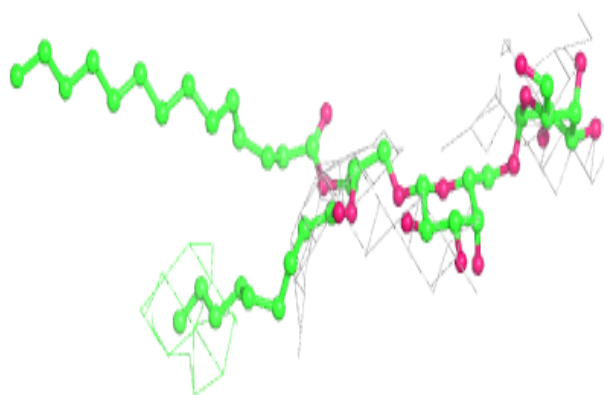
**Electron density around CLA B 605:**

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

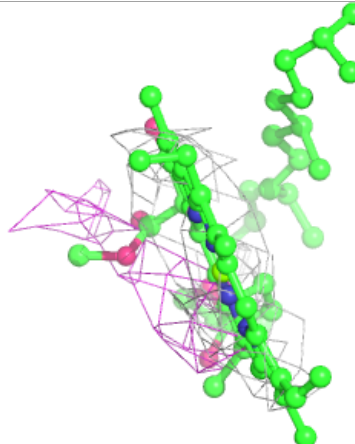
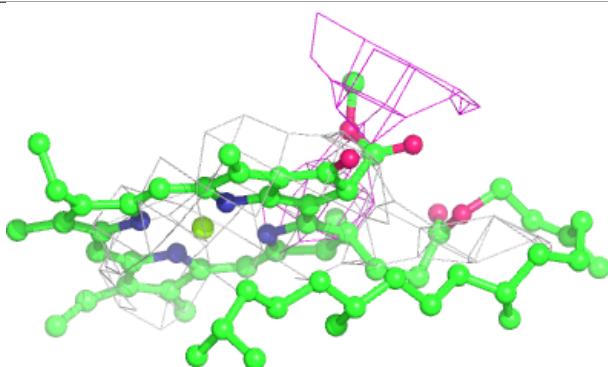
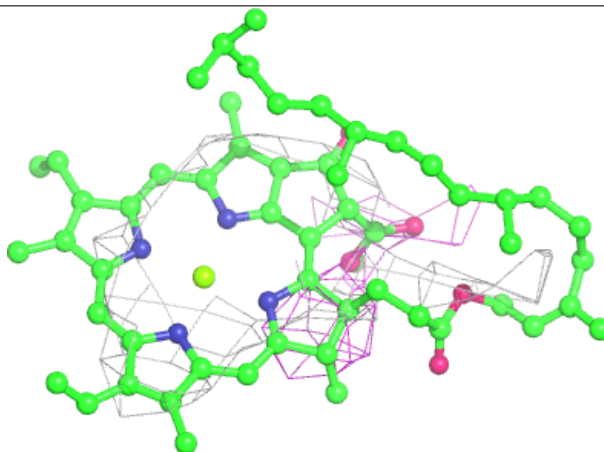


**Electron density around DGD c 515:**

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

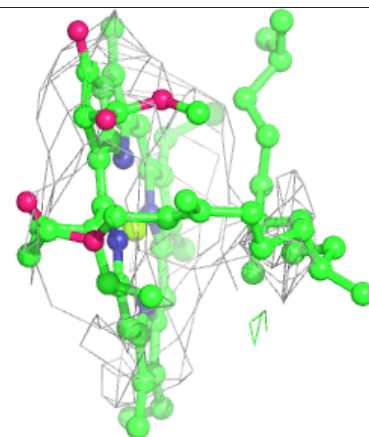
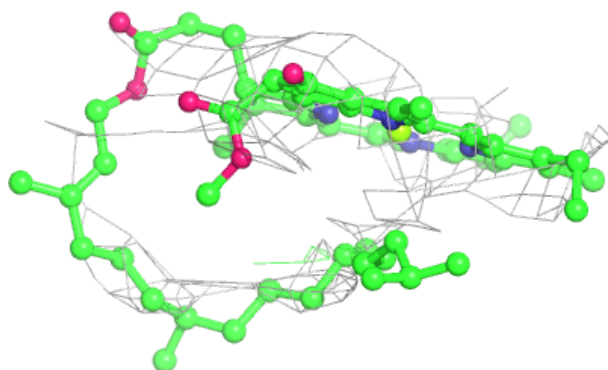
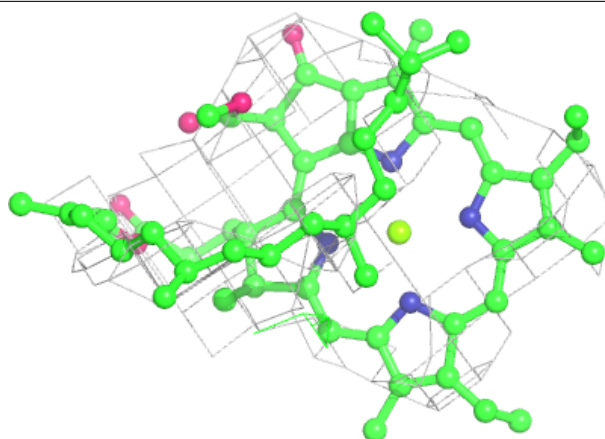
**Electron density around CLA C 508:**

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

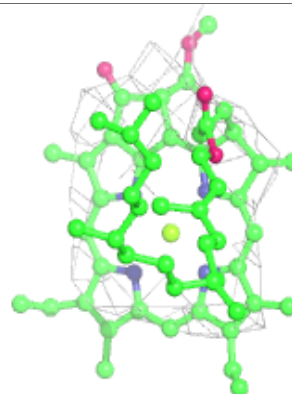
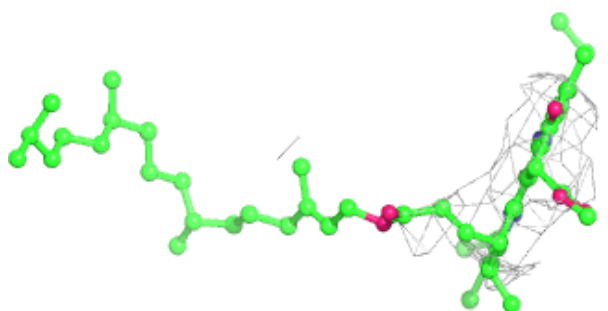
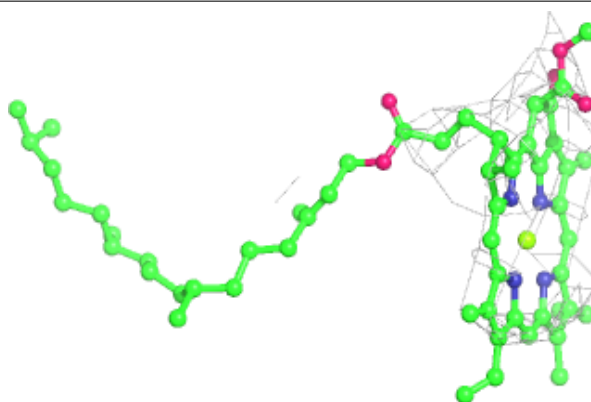


**Electron density around CLA c 509:**

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

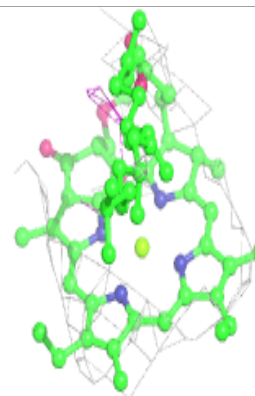
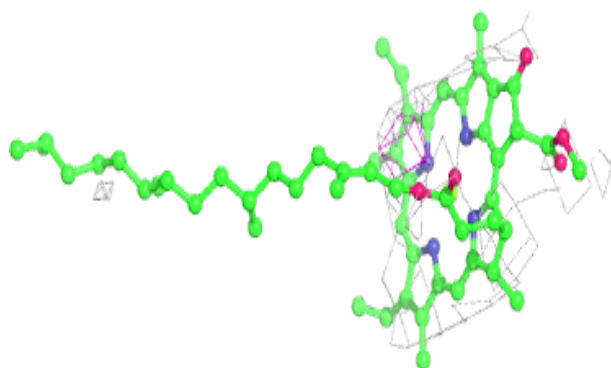
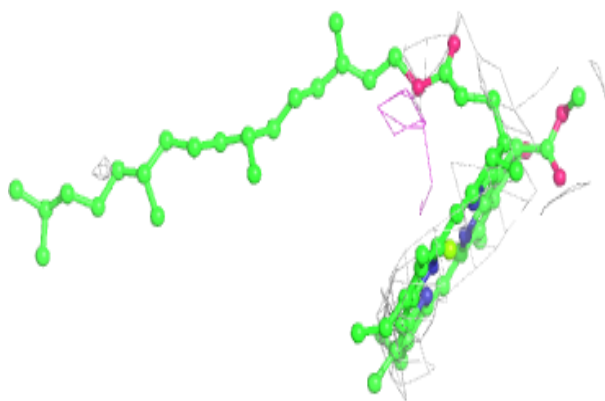
**Electron density around CLA D 406:**

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

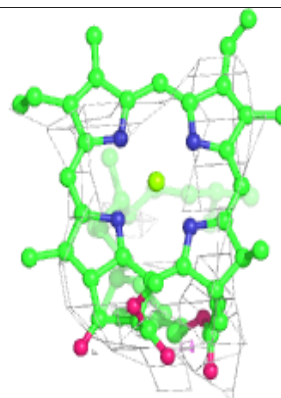
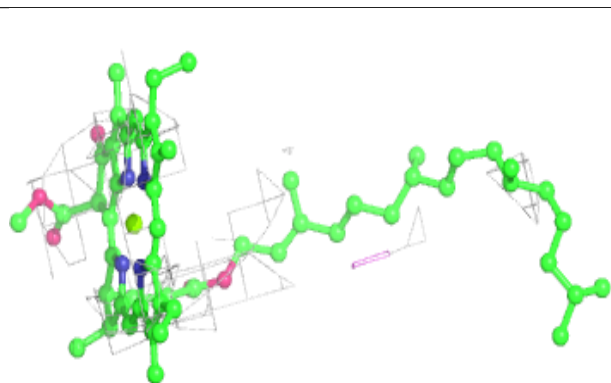
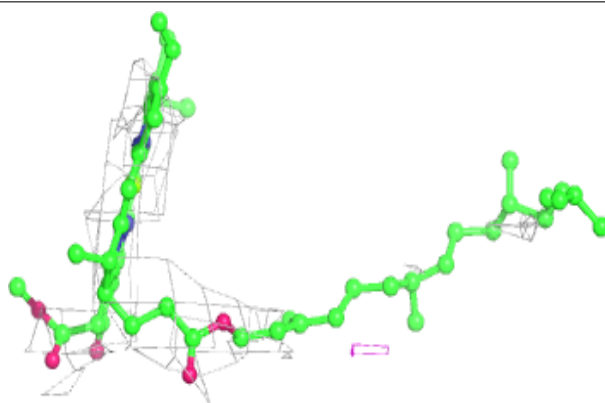


**Electron density around CLA c 520:**

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

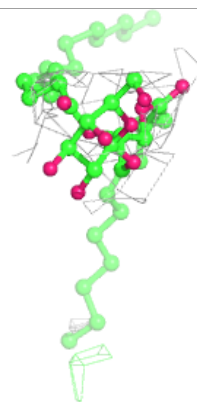
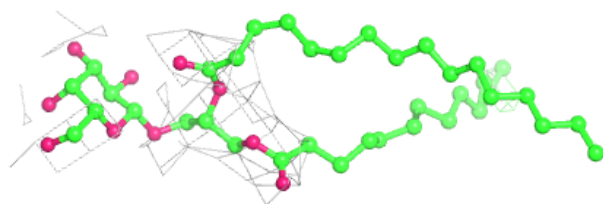
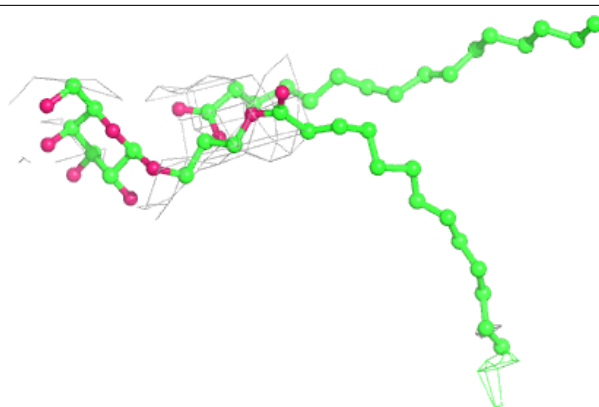
**Electron density around CLA B 604:**

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

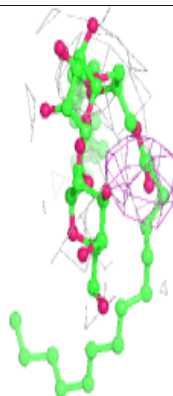
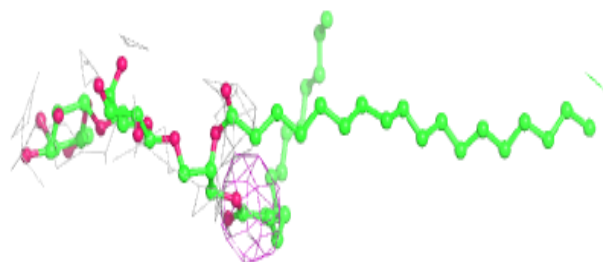
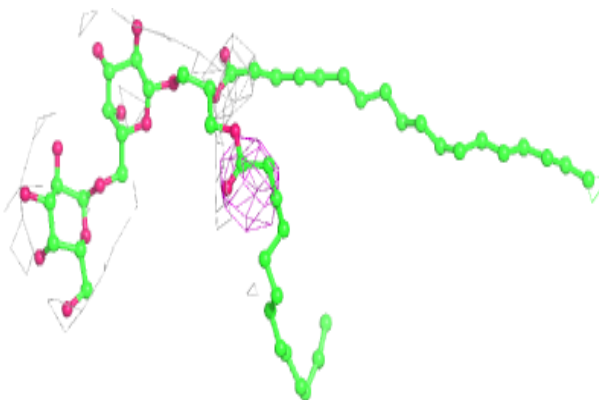


**Electron density around LMG D 408:**

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

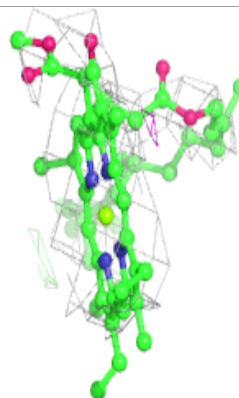
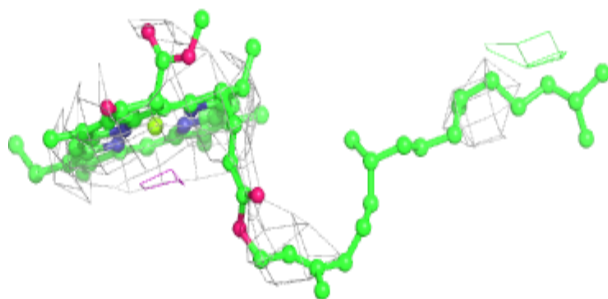
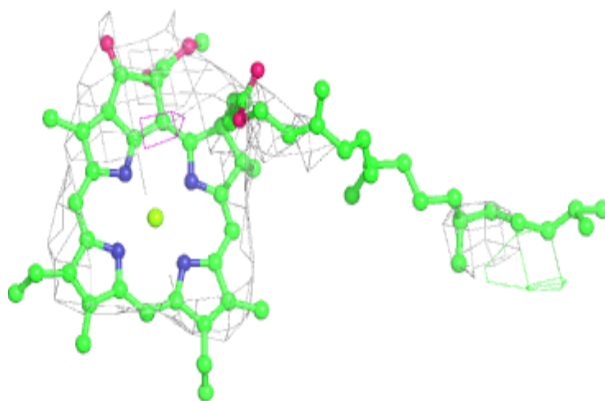
**Electron density around DGD c 516:**

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

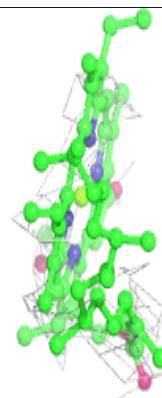
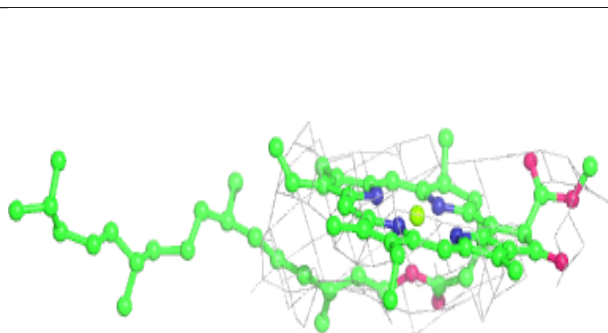
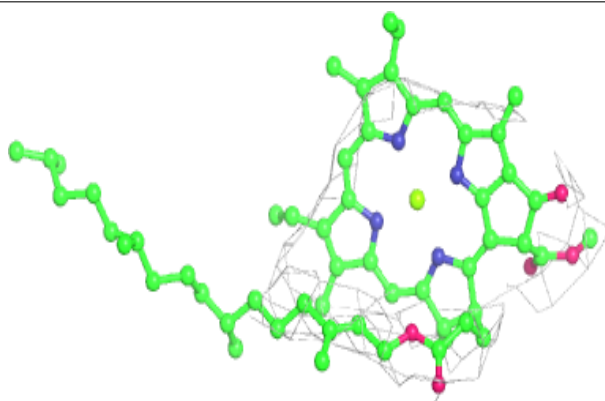


**Electron density around CLA A 404:**

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

**Electron density around CLA C 501:**

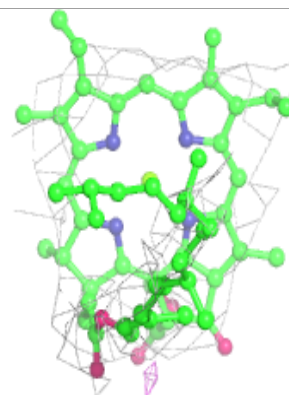
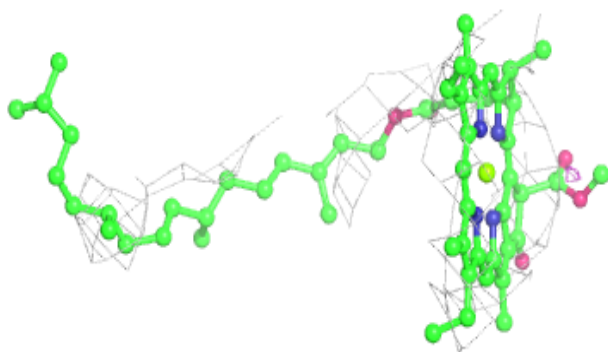
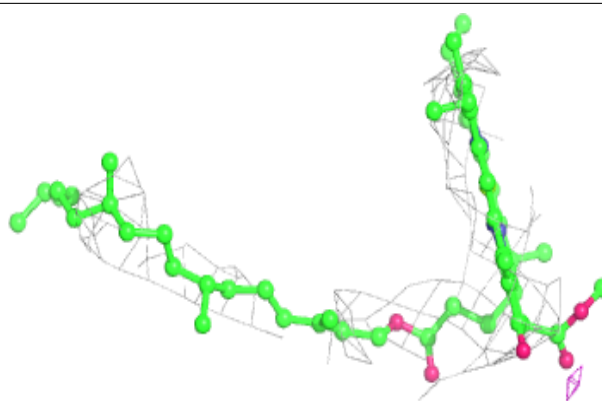
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



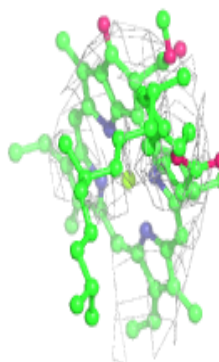
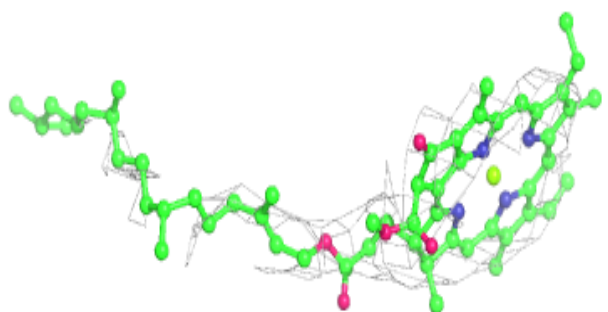
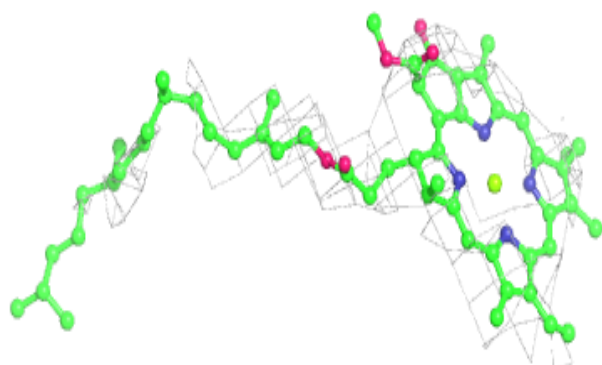


**Electron density around CLA b 608:**

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

**Electron density around CLA a 404:**

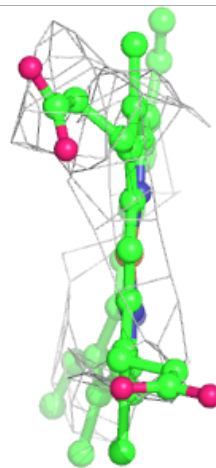
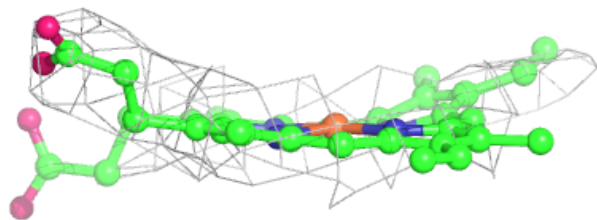
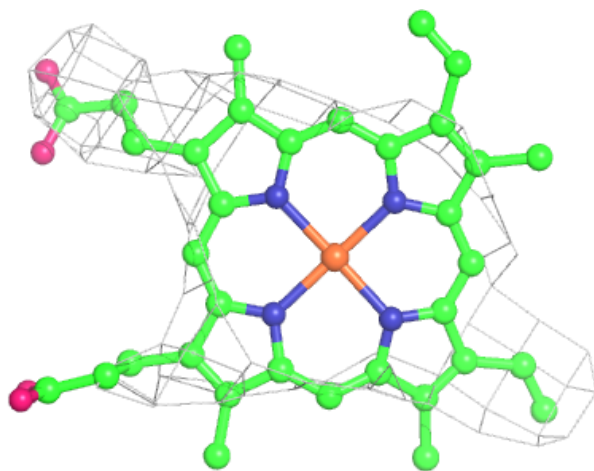
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





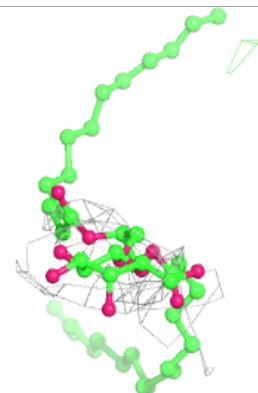
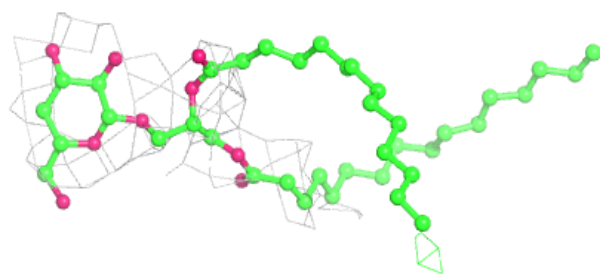
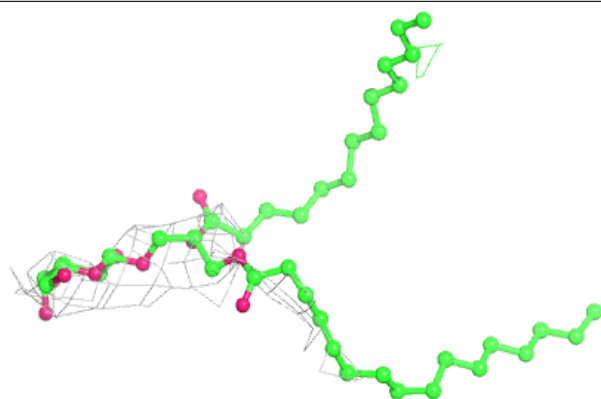
**Electron density around HEM V 201:**

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



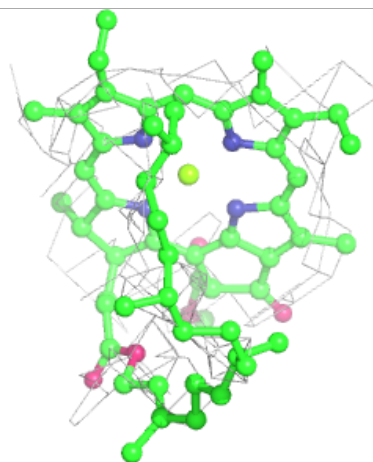
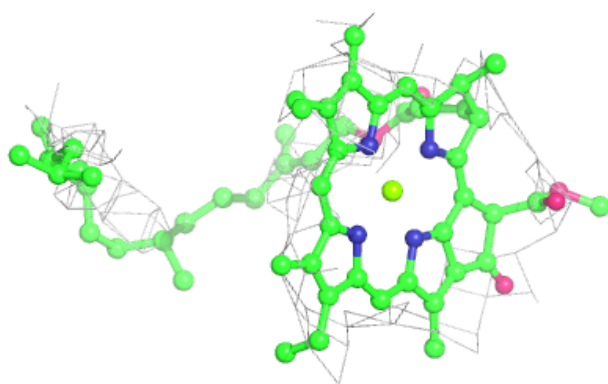
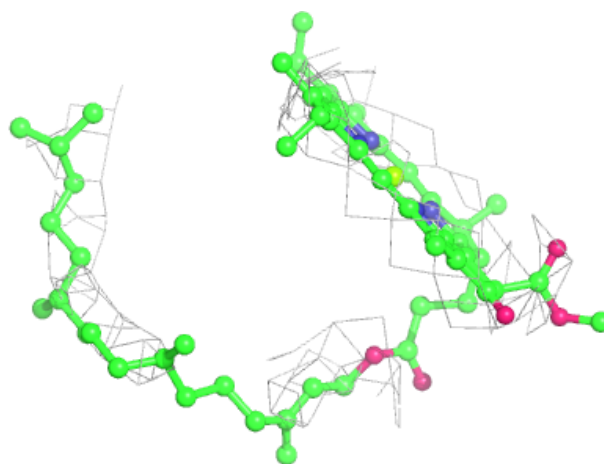
**Electron density around LMG B 621:**

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



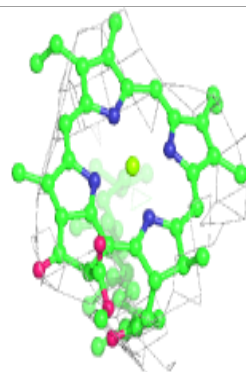
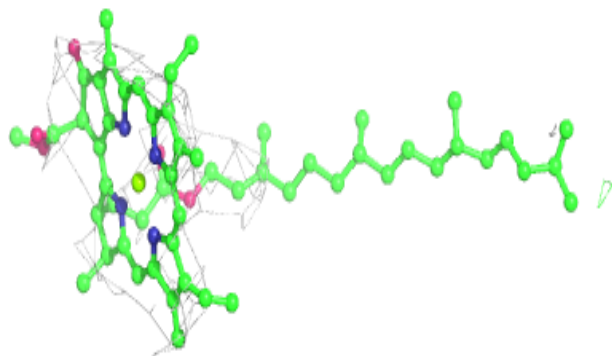
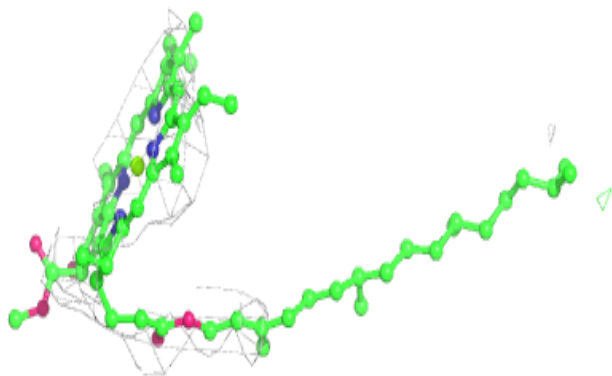
**Electron density around CLA b 614:**

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

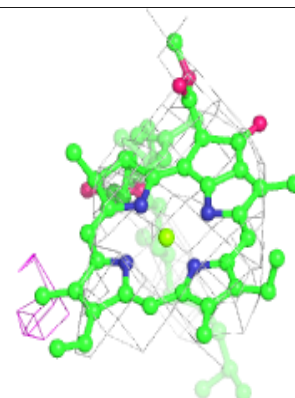
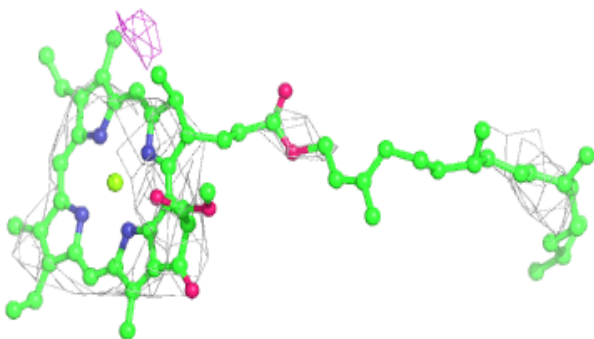
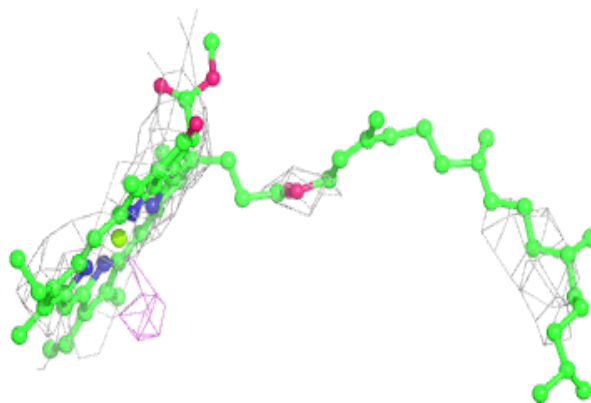


**Electron density around CLA B 606:**

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

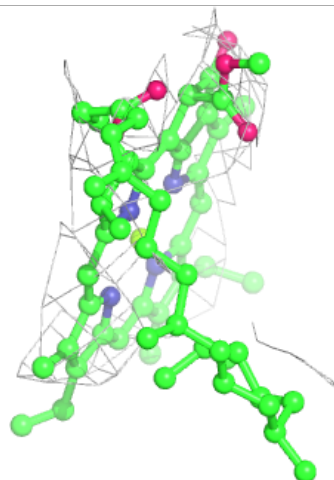
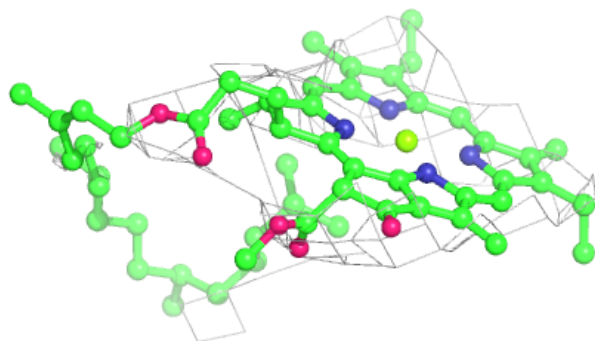
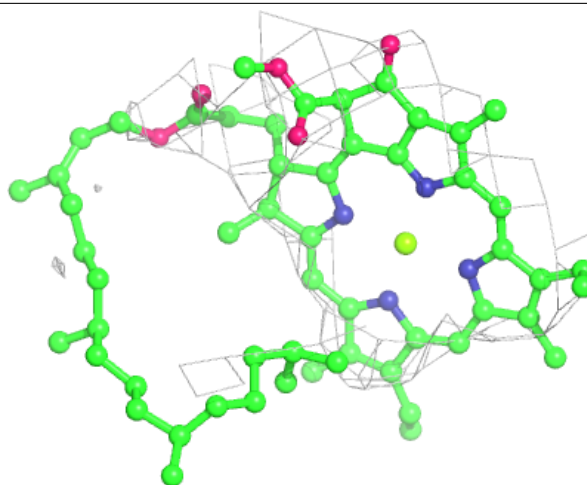
**Electron density around CLA D 405:**

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



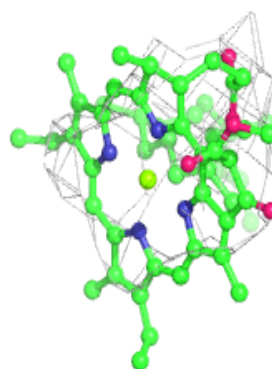
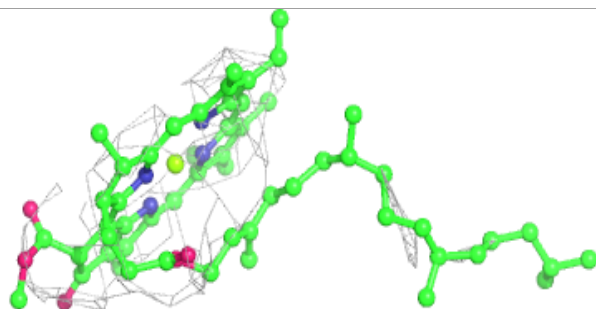
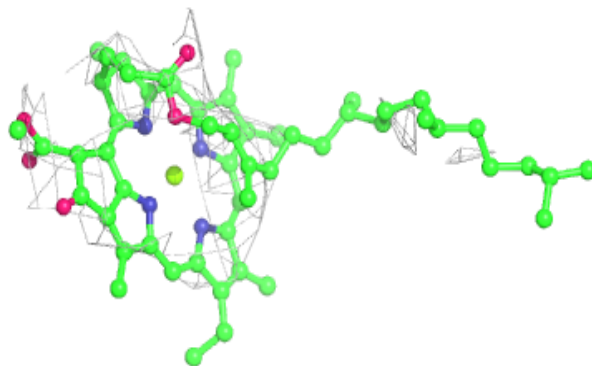
**Electron density around CLA B 614:**

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

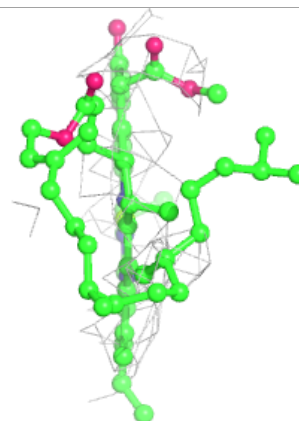
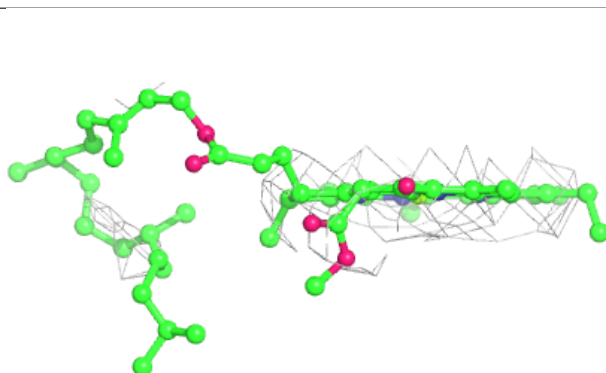
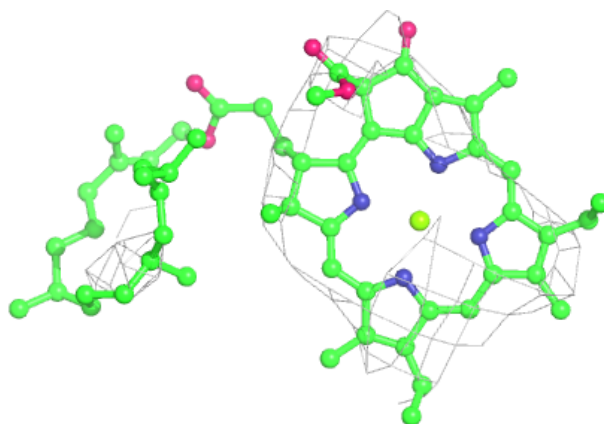


**Electron density around CLA c 504:**

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

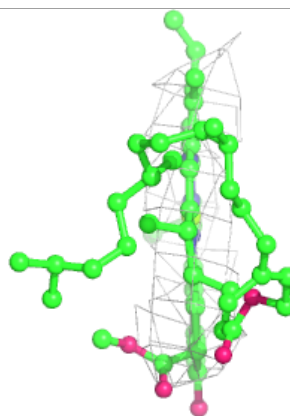
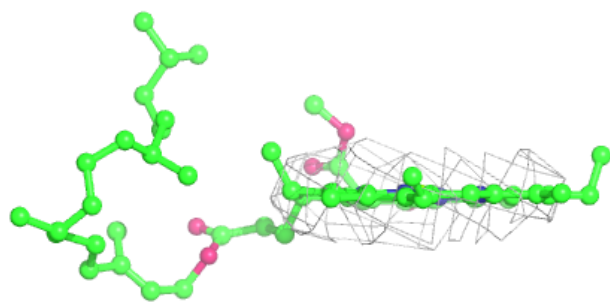
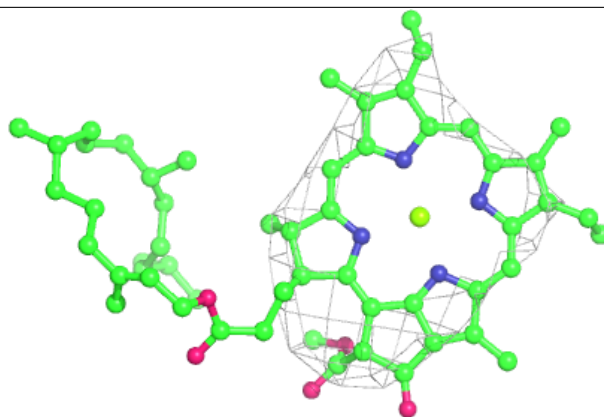
**Electron density around CLA c 511:**

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

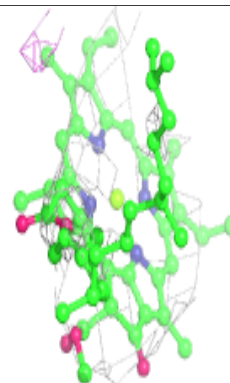
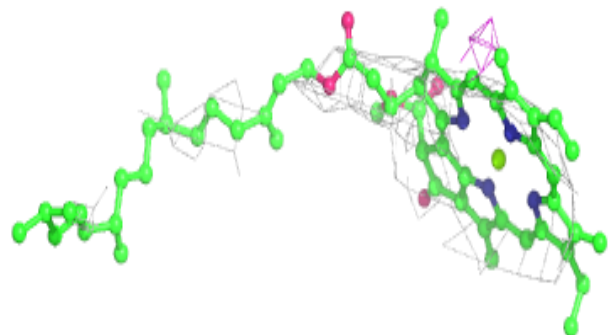
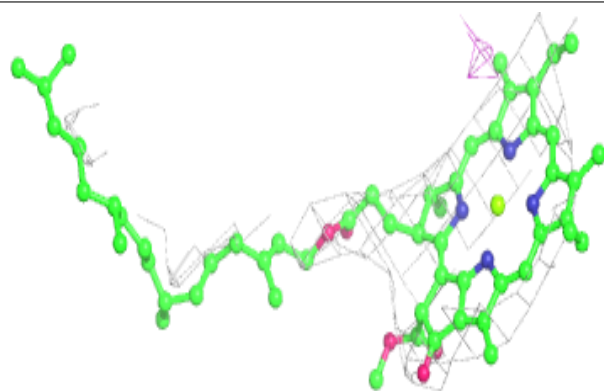


**Electron density around CLA C 511:**

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

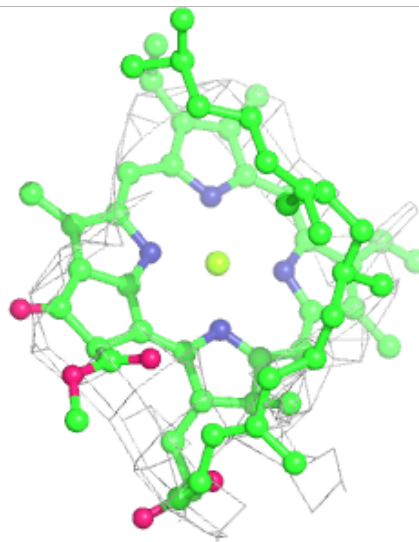
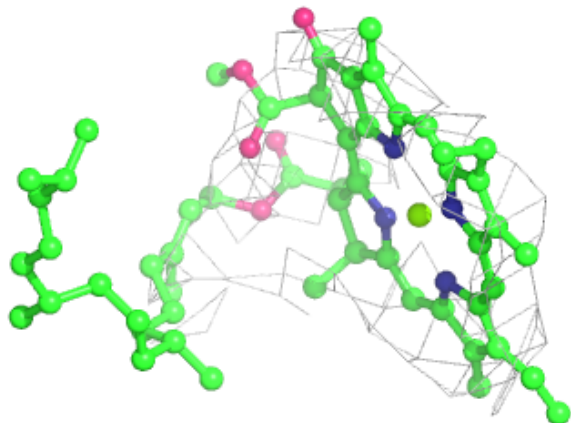
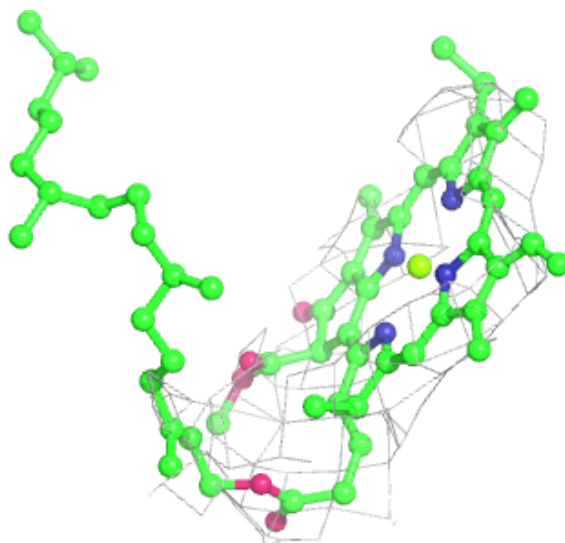
**Electron density around CLA A 402:**

$2mF_o-DF_c$  (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:**

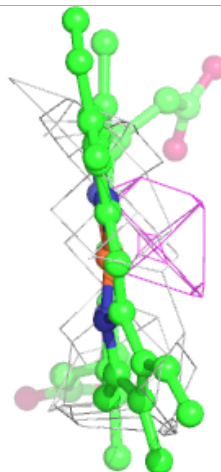
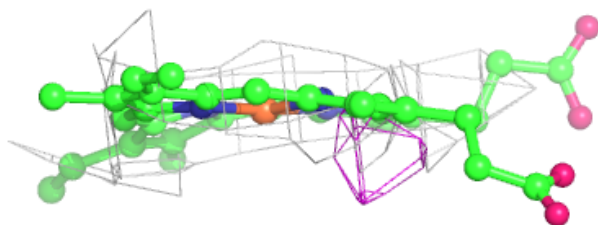
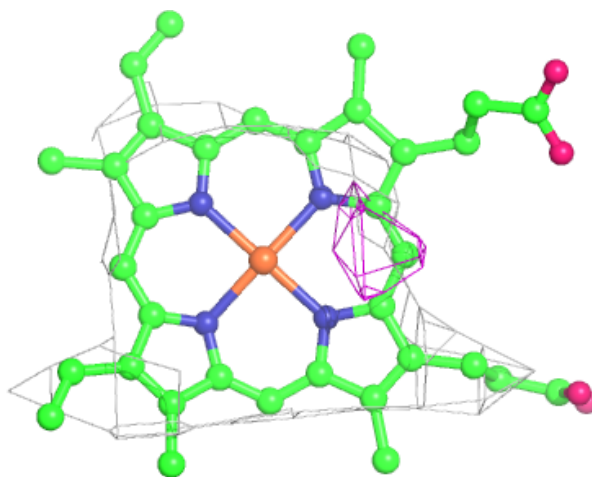
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





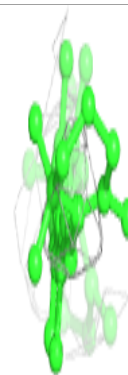
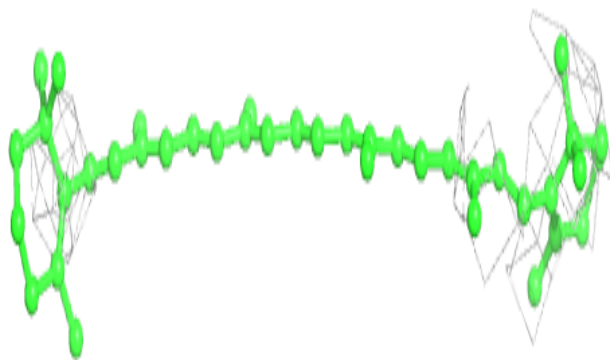
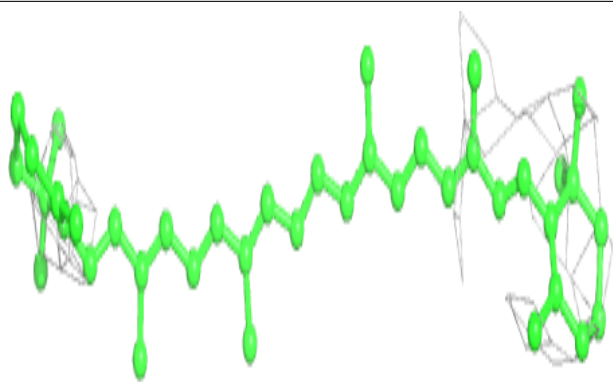
**Electron density around HEM v 201:**

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

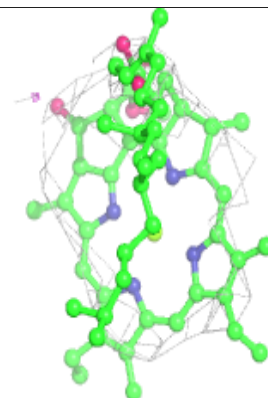
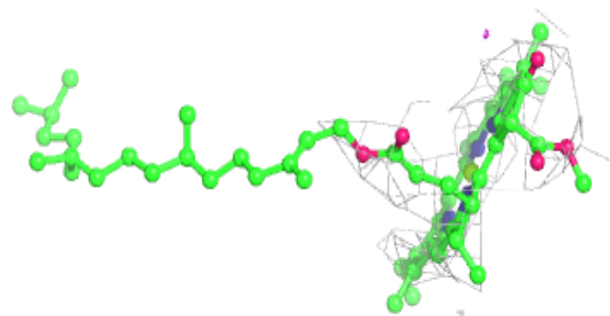
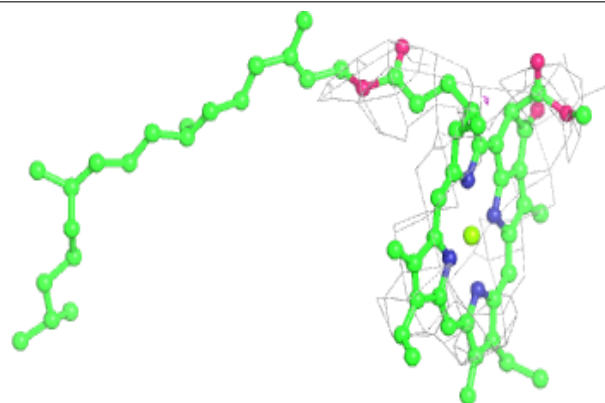


**Electron density around BCR b 620:**

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

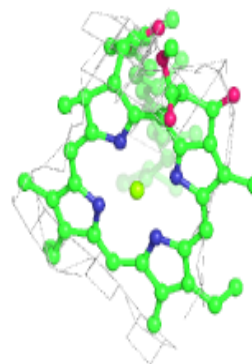
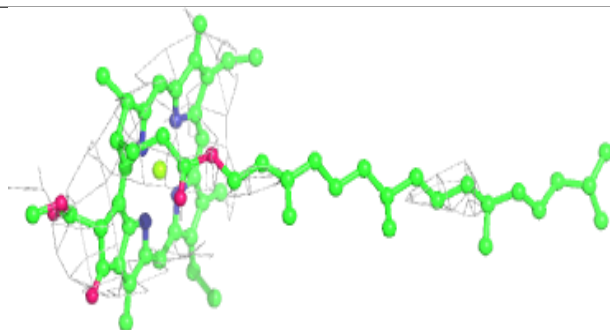
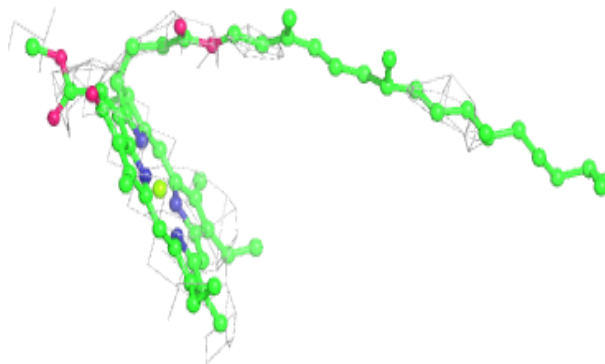
**Electron density around CLA B 608:**

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

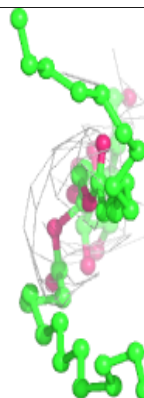
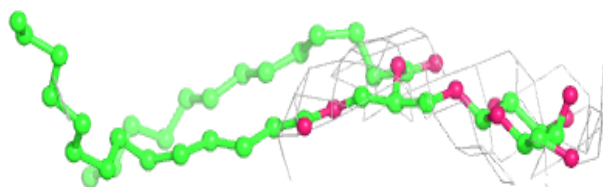
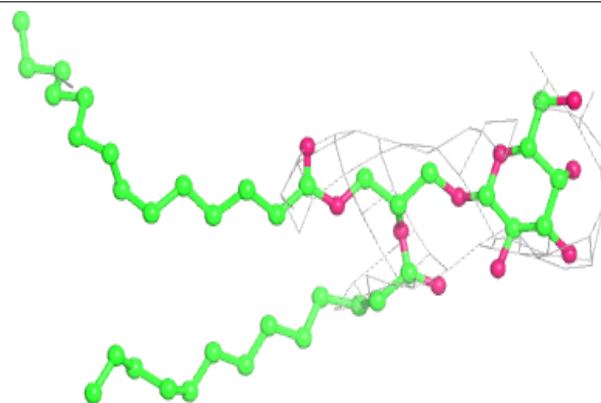


**Electron density around CLA b 610:**

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

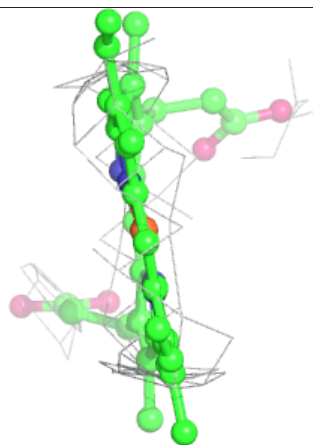
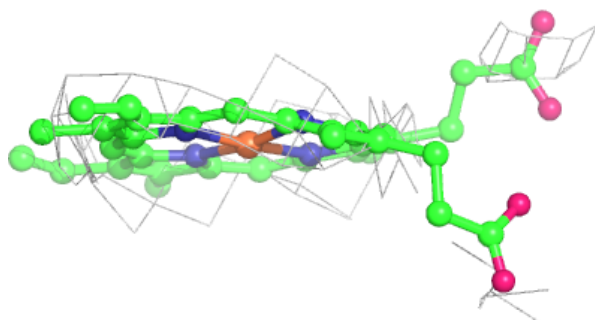
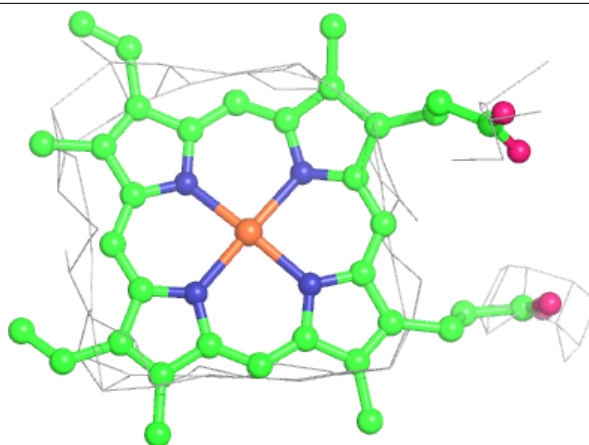
**Electron density around LMG d 410:**

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

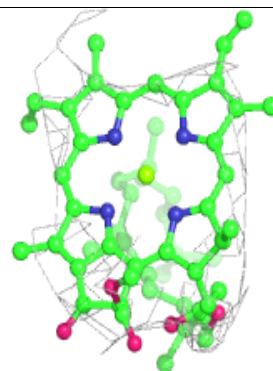
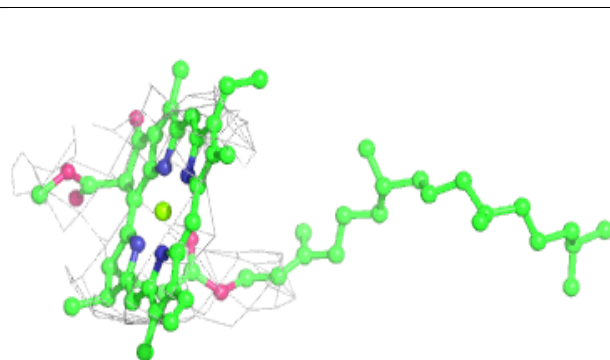
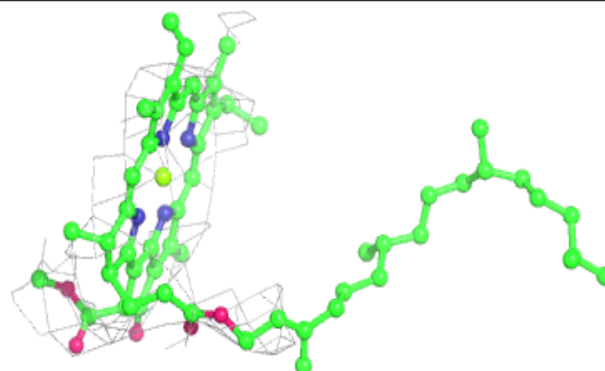


**Electron density around HEM F 101:**

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

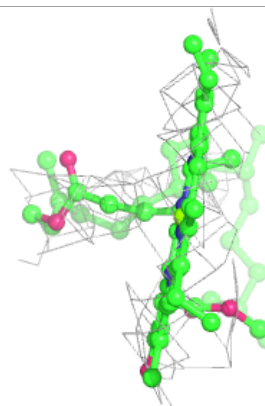
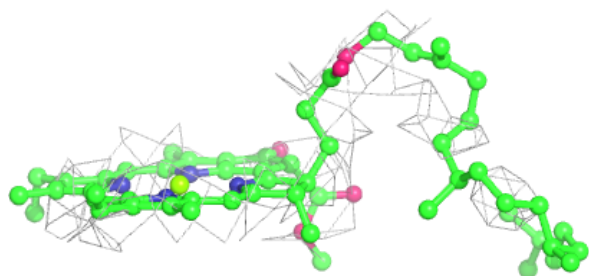
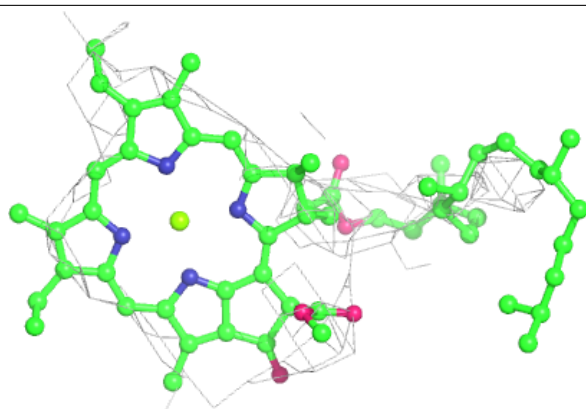
**Electron density around CLA c 507:**

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

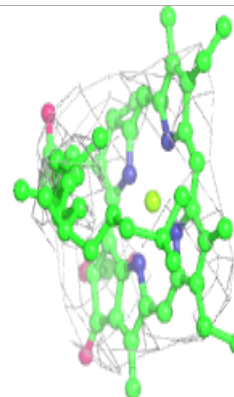
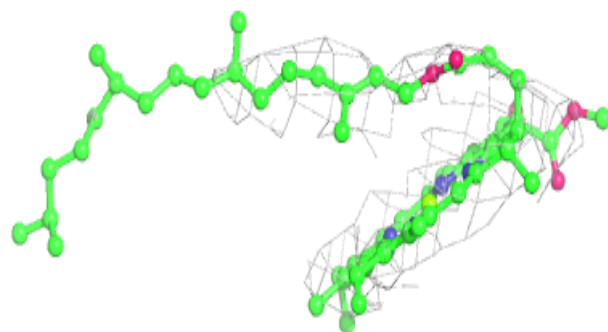
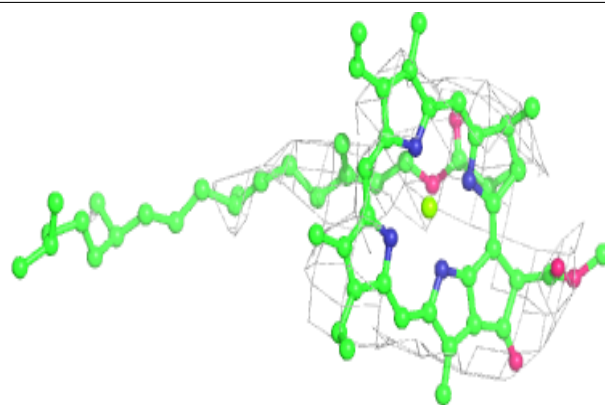


**Electron density around CLA b 615:**

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

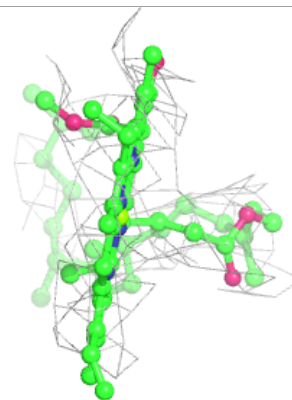
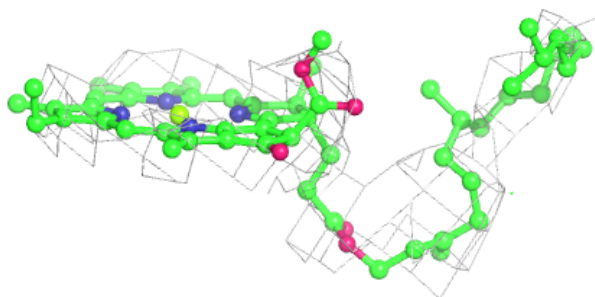
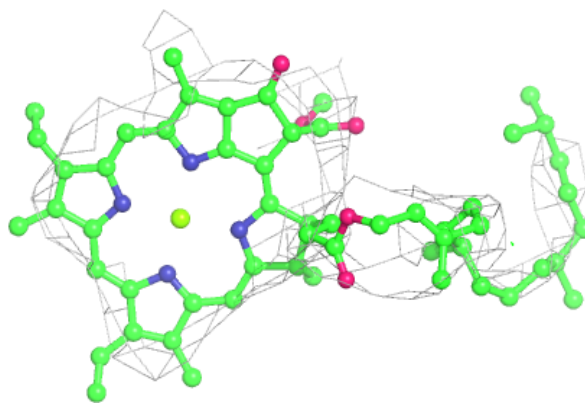
**Electron density around CLA b 611:**

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

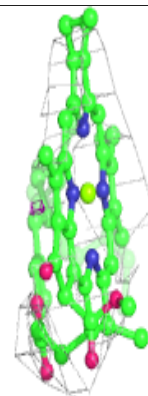
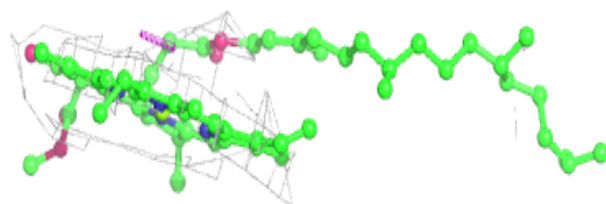
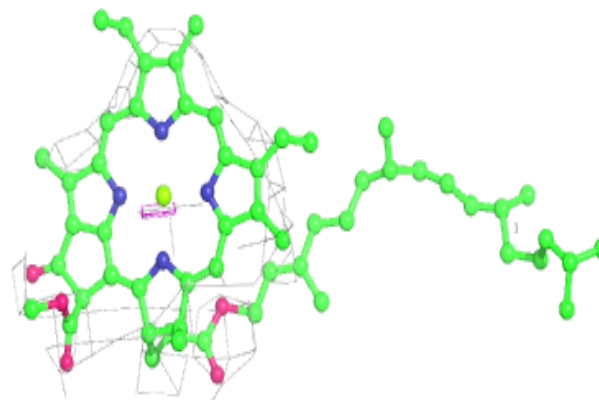


**Electron density around CLA B 611:**

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

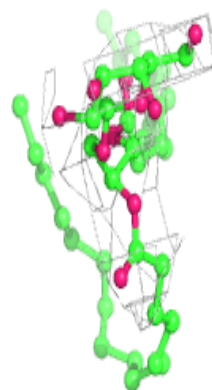
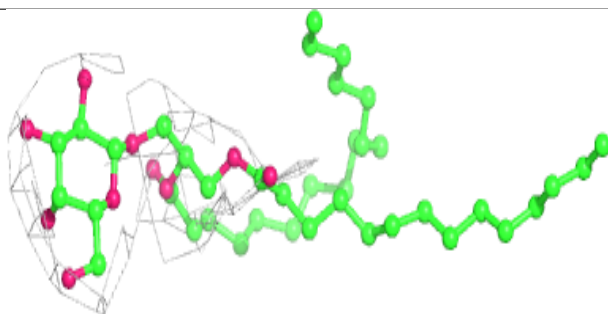
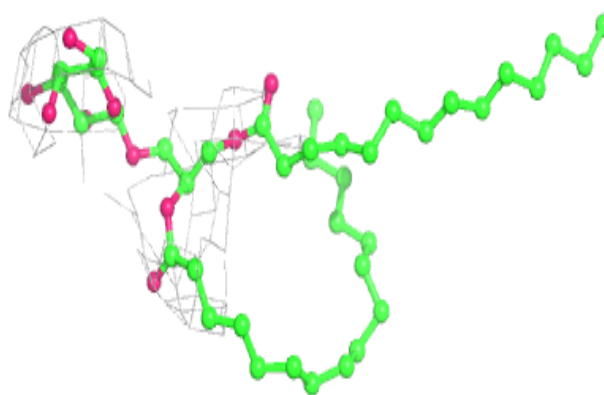
**Electron density around CLA B 602:**

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

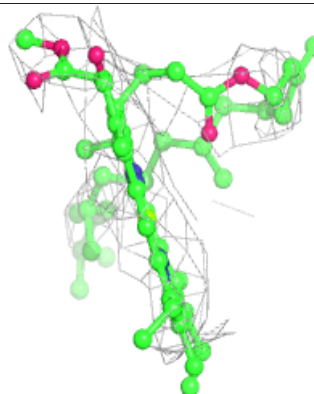
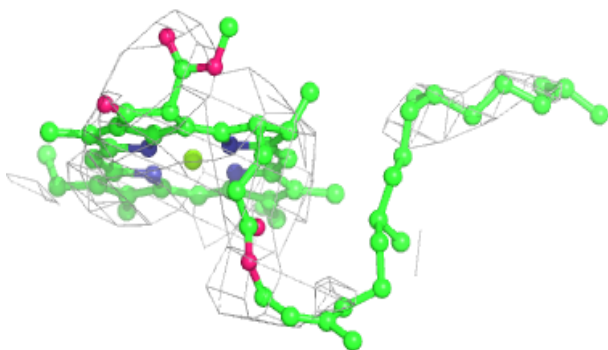
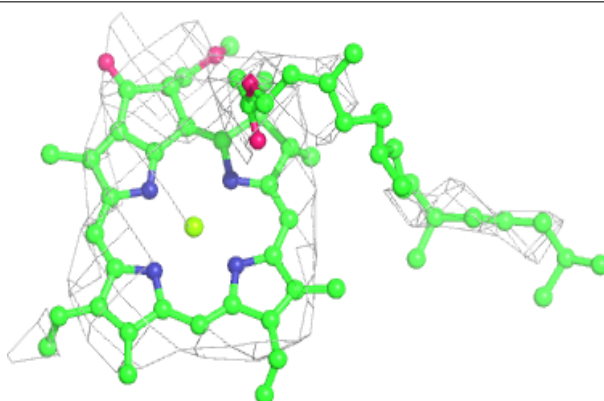


**Electron density around LMG b 628:**

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

**Electron density around CLA A 403:**

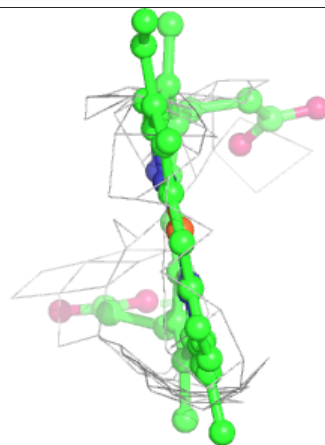
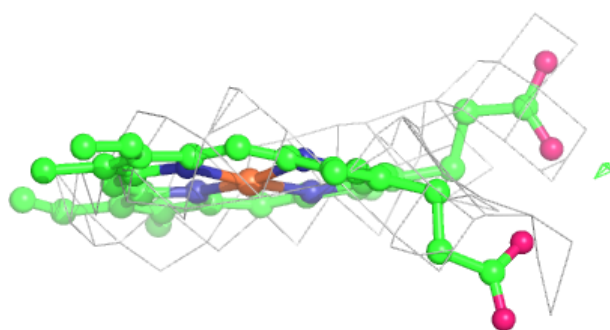
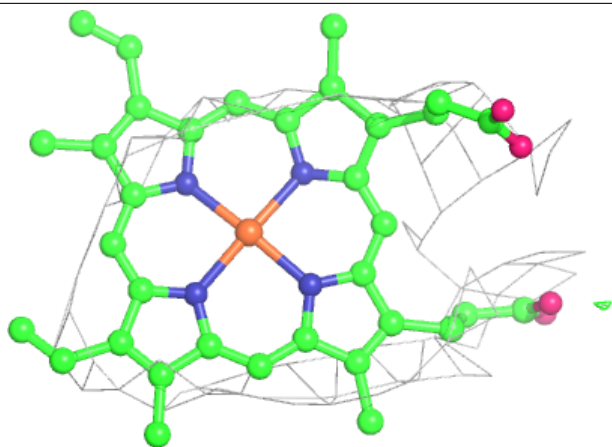
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM f 101:**

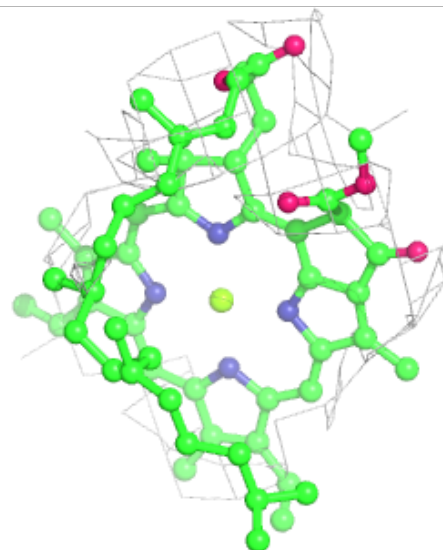
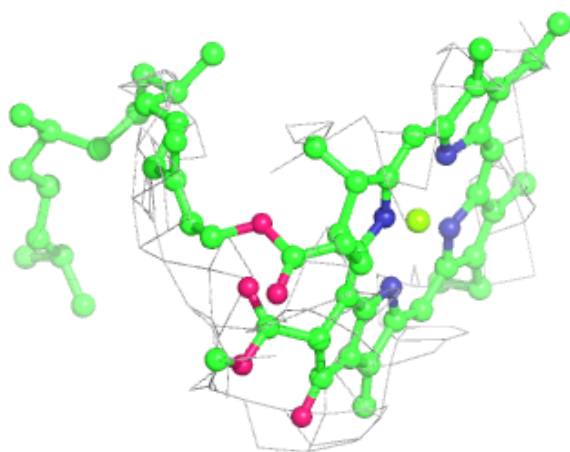
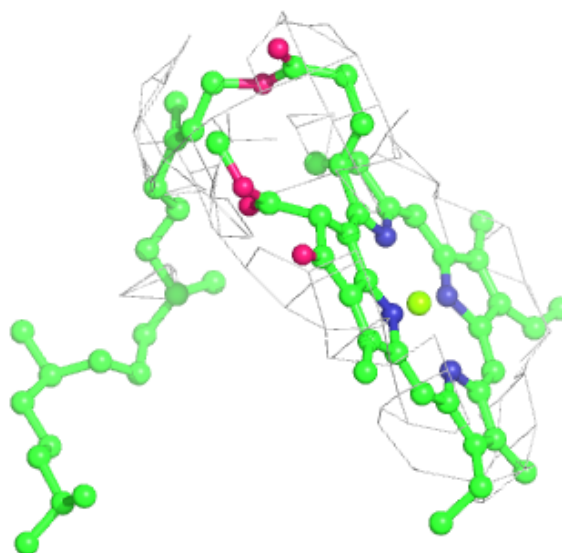
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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.