



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:42 am BST

PDB ID : 4TNH
Title : RT XFEL structure of Photosystem II in the dark state at 4.9 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 : 4.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)
Ideal geometry (proteins)	:	Engh & Huber (2001)

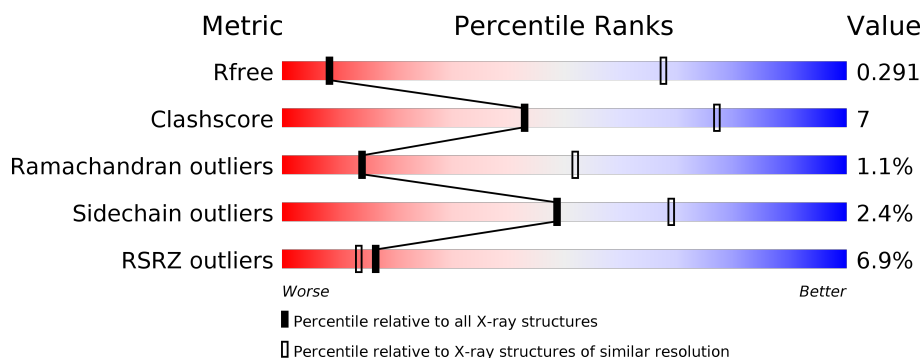
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.90 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	1134 (6.00-3.80)
Clashscore	141614	1209 (6.00-3.80)
Ramachandran outliers	138981	1140 (6.00-3.80)
Sidechain outliers	138945	1117 (6.00-3.80)
RSRZ outliers	127900	1005 (6.00-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>8%</div> <div>69%</div> <div>27%</div> <div>• •</div> </div>
1	a	344	<div> <div>9%</div> <div>95%</div> <div>• •</div> </div>
2	B	510	<div> <div>7%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
2	b	510	<div> <div>7%</div> <div>94%</div> <div>• •</div> </div>

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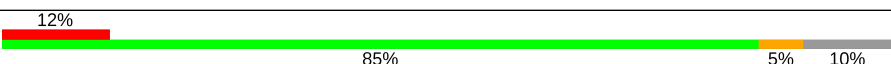
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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Mol	Chain	Length	Quality of chain
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	
15	U	134	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	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
22	CLA	B	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	X
22	CLA	C	520	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	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	-	-	X
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	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	-	-	X
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	d	405	X	-	-	-
22	CLA	h	101	X	-	-	-
23	PL9	A	406	-	-	-	X
23	PL9	D	406	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	d	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	F	102	-	-	-	X
24	BCR	H	102	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	a	410	-	-	-	X
24	BCR	b	623	-	-	-	X
24	BCR	c	513	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	521	-	-	-	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	b	601	-	-	-	X
25	DGD	d	409	-	-	-	X
27	LMG	A	415	-	-	-	X
27	LMG	C	518	-	-	-	X
27	LMG	D	411	-	-	-	X
27	LMG	E	101	-	-	-	X
27	LMG	I	101	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	M	101	-	-	-	X
27	LMG	a	402	-	-	-	X
27	LMG	c	518	-	-	-	X
27	LMG	d	408	-	-	-	X
27	LMG	e	101	-	-	-	X
27	LMG	i	101	-	-	-	X
27	LMG	l	101	-	-	-	X
27	LMG	m	101	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	F	103	-	-	-	X
30	SQD	d	402	-	-	-	X
31	LMT	B	623	-	-	-	X
31	LMT	B	624	-	-	-	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	603	-	-	-	X
31	LMT	b	604	-	-	-	X
31	LMT	b	626	-	-	-	X
31	LMT	b	627	-	-	-	X
31	LMT	d	410	-	-	-	X
31	LMT	i	102	-	-	-	X
32	PHO	d	401	-	-	-	X
33	BCT	d	403	-	-	-	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				

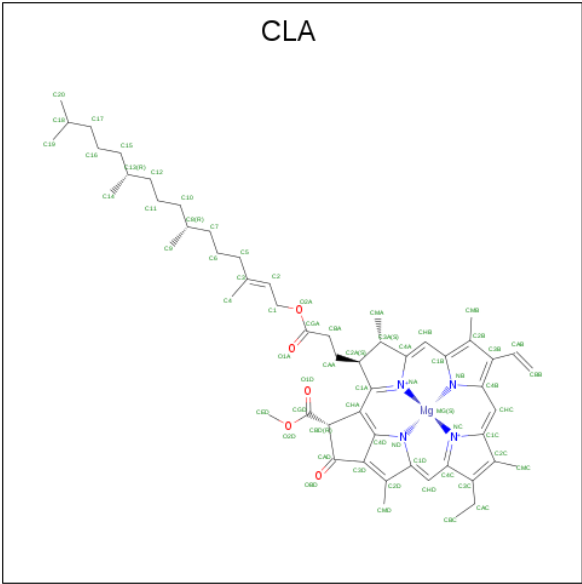
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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: C₅₅H₇₂MgN₄O₅).



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

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

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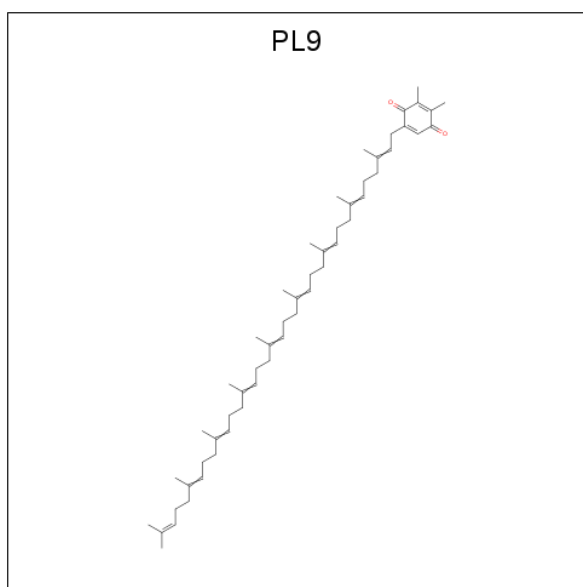
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 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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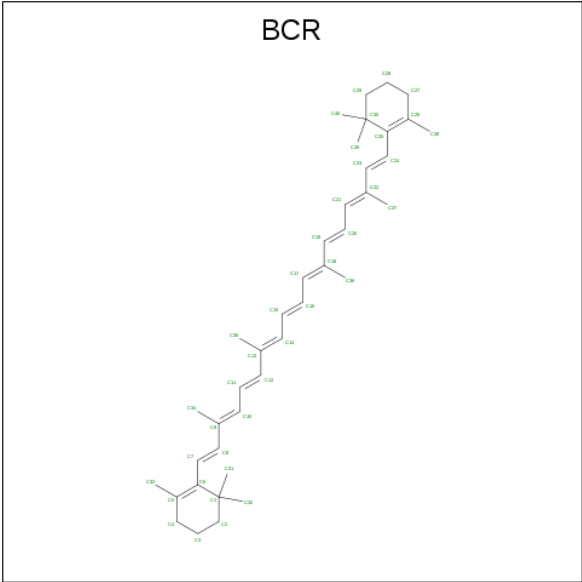
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: C₅₃H₈₀O₂).



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: $C_{40}H_{56}$).



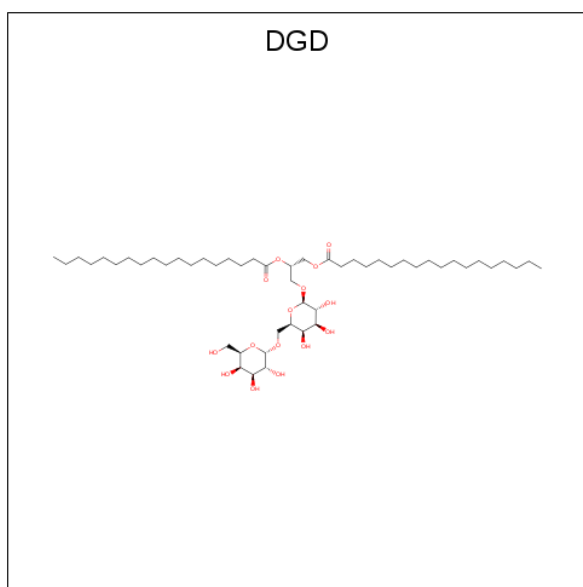
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	F	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	J	1	Total C 40 40	0	0
24	K	1	Total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

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

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



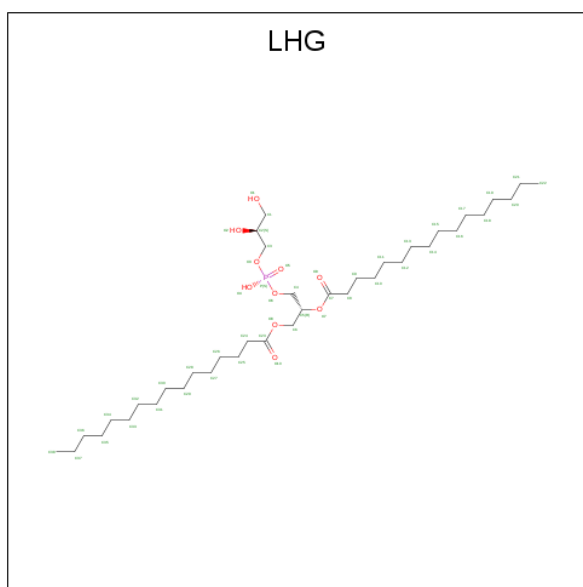
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 56 41 15	0	0

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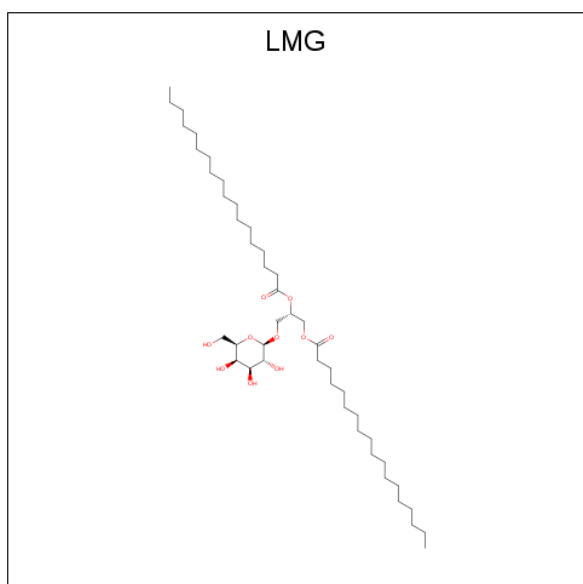
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			58	43	15		
25	B	1	Total	C	O	0	0
			52	37	15		
25	C	1	Total	C	O	0	0
			53	38	15		
25	C	1	Total	C	O	0	0
			62	47	15		
25	C	1	Total	C	O	0	0
			66	51	15		
25	D	1	Total	C	O	0	0
			63	48	15		
25	a	1	Total	C	O	0	0
			56	41	15		
25	b	1	Total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

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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: $C_{45}H_{86}O_{10}$).

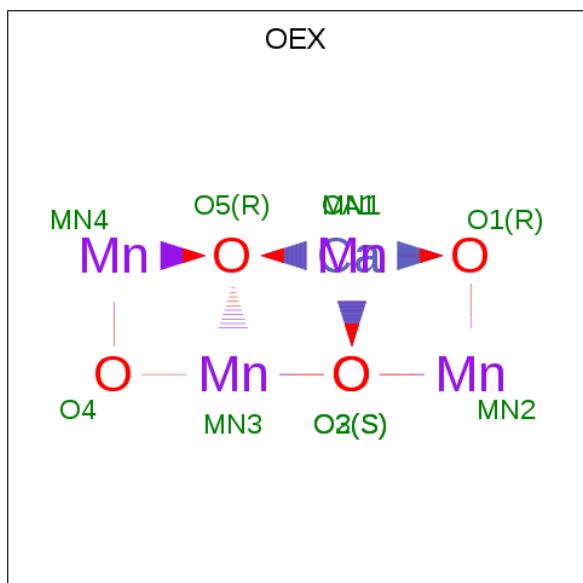


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	A	1	Total	C	O	0	0
			42	32	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			49	39	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total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

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

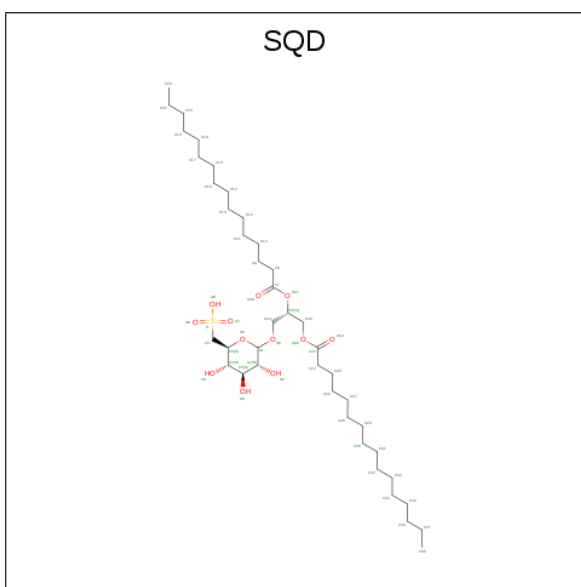
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



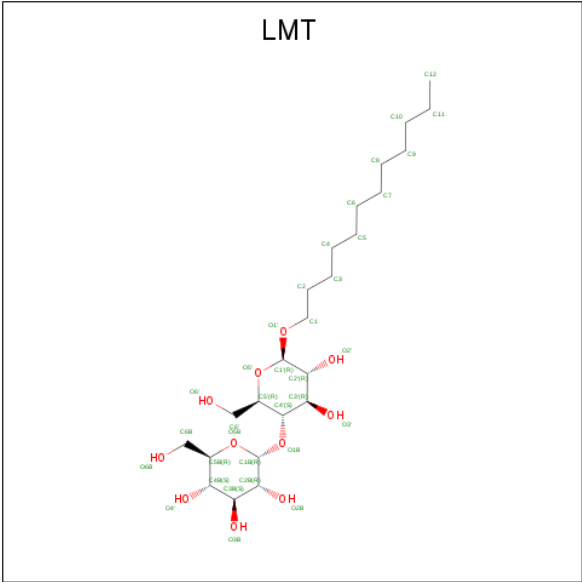
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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



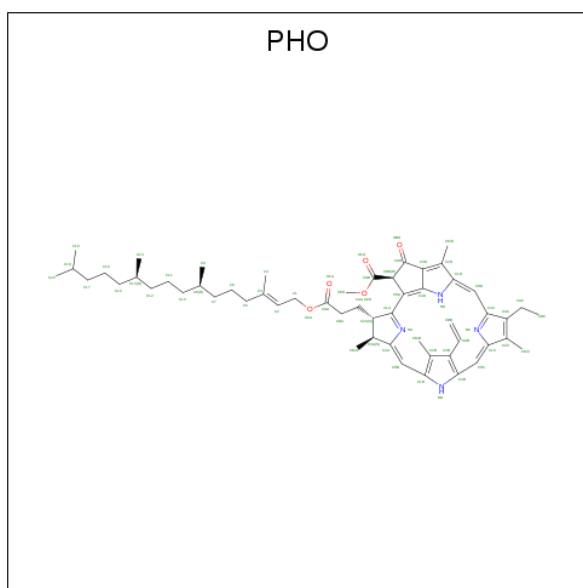
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			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-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



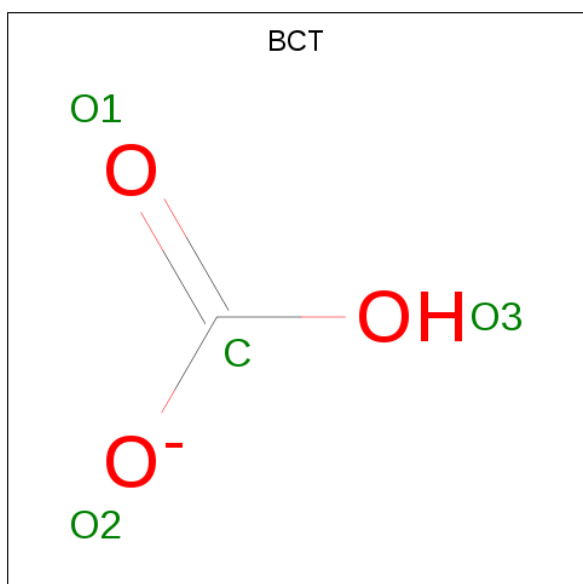
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	D	1	Total	C	O	0	0
			31	20	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total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

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



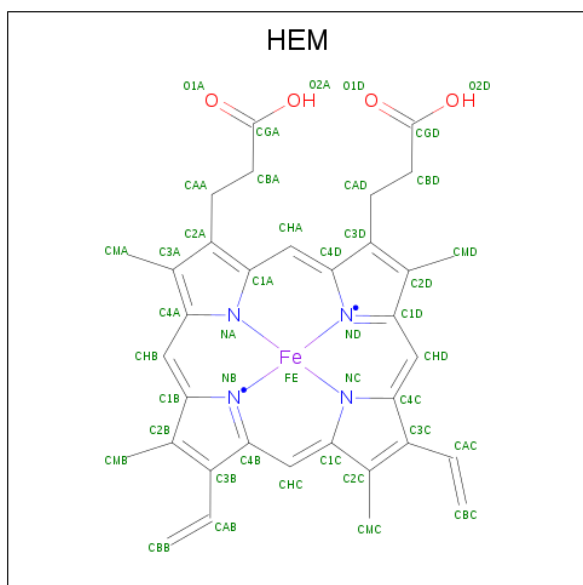
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	D	1	Total	C	N	O	0	0
			64	55	4	5		
32	a	1	Total	C	N	O	0	0
			64	55	4	5		
32	d	1	Total	C	N	O	0	0
			64	55	4	5		

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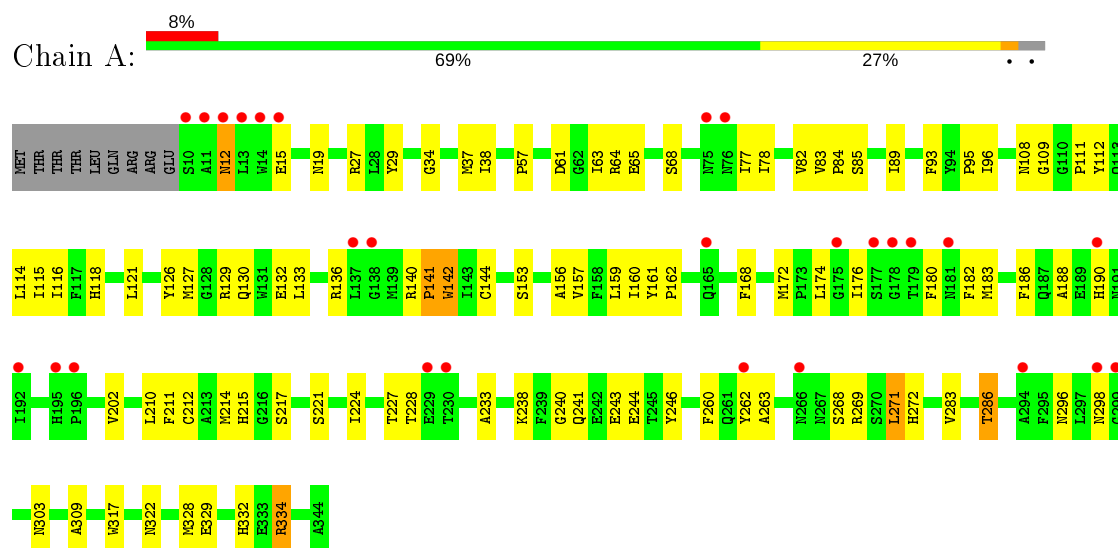
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	k	1	Total	Ca	0	0
			1	1		

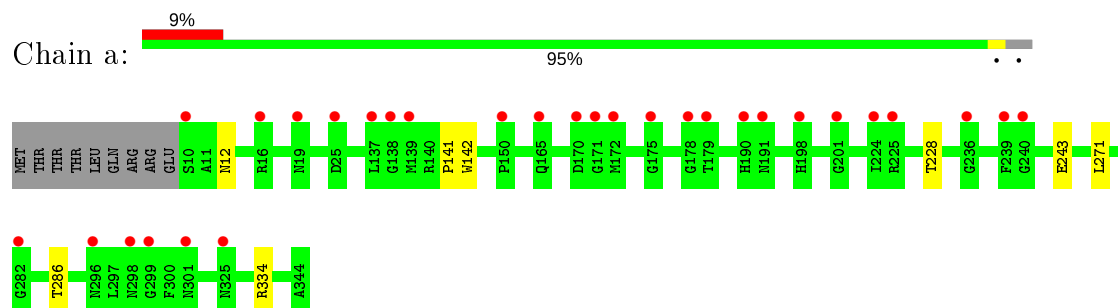
3 Residue-property plots [i](#)

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.

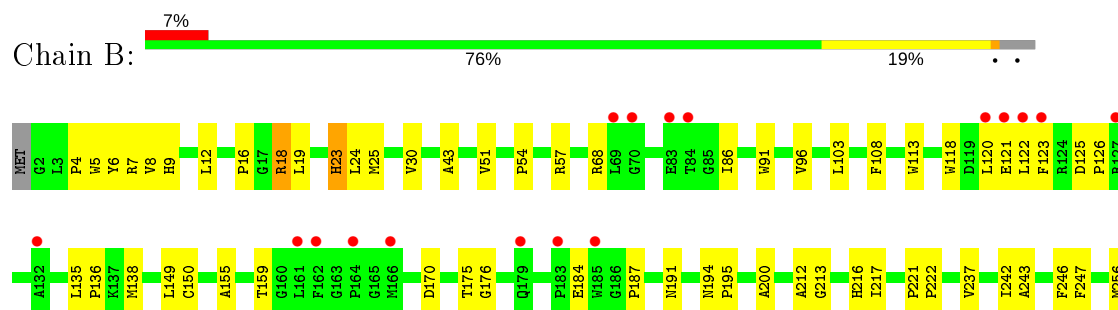
• Molecule 1: Photosystem Q(B) protein 1

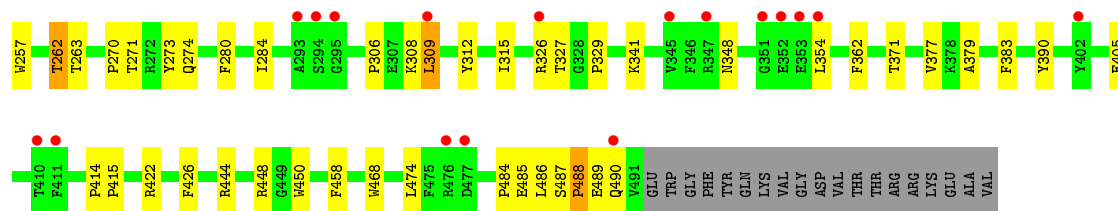


• Molecule 1: Photosystem Q(B) protein 1

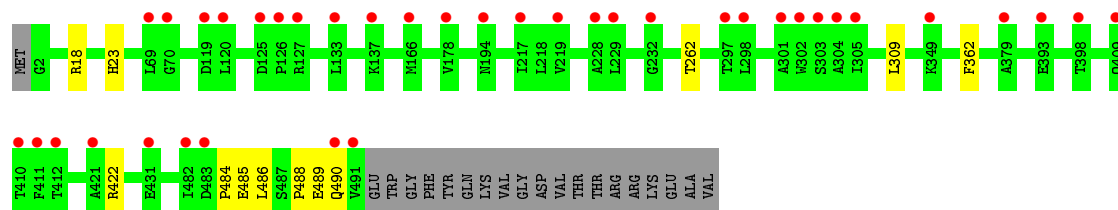
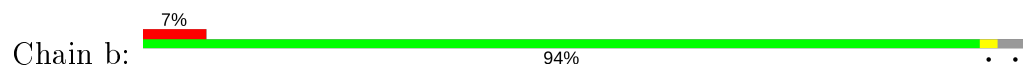


• Molecule 2: Photosystem II core light harvesting protein

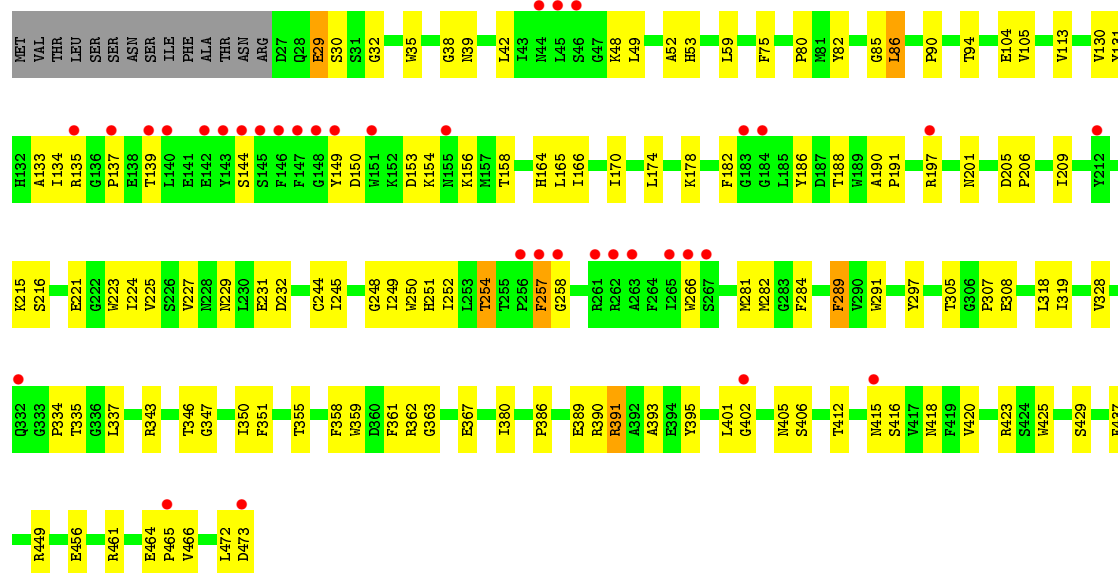




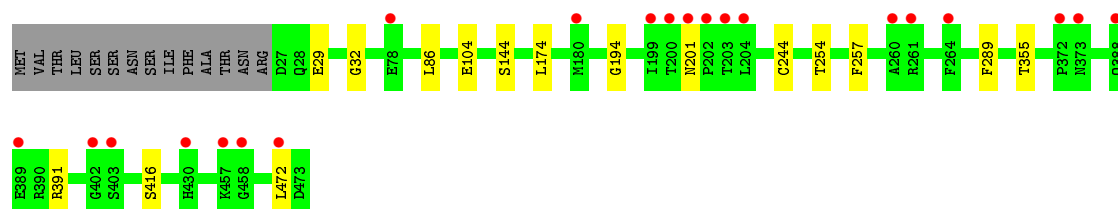
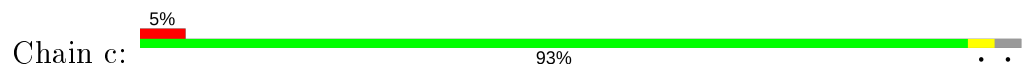
• Molecule 2: Photosystem II core light harvesting protein



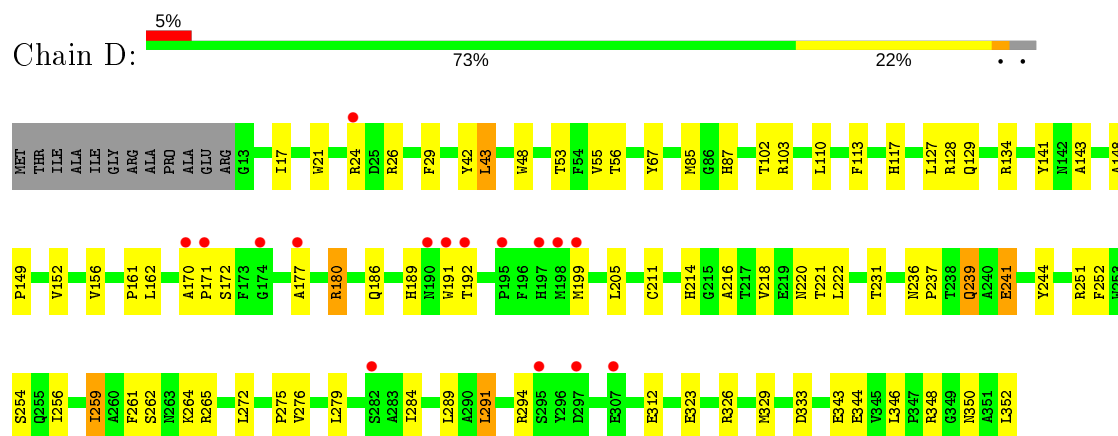
• Molecule 3: Photosystem II CP43 protein



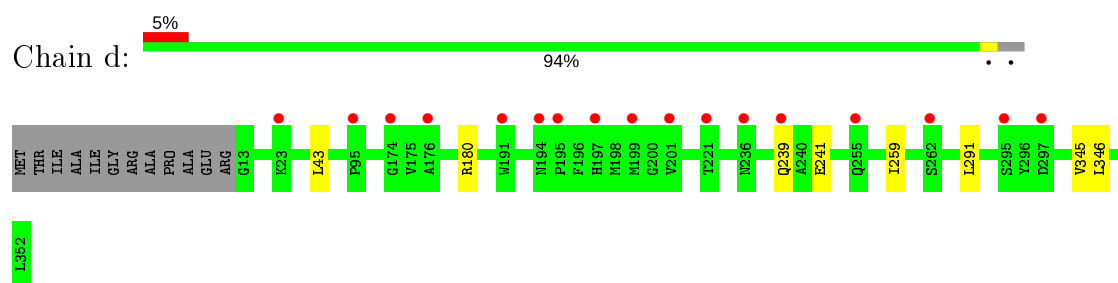
• Molecule 3: Photosystem II CP43 protein



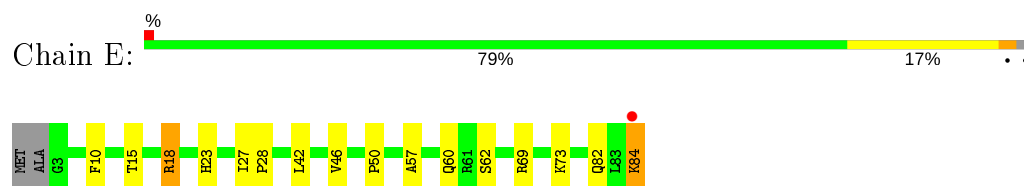
- Molecule 4: Photosystem II D2 protein



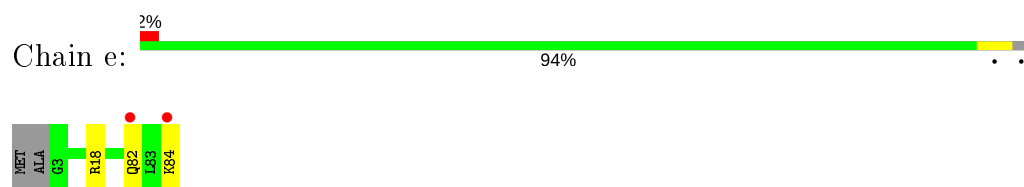
- Molecule 4: Photosystem II D2 protein



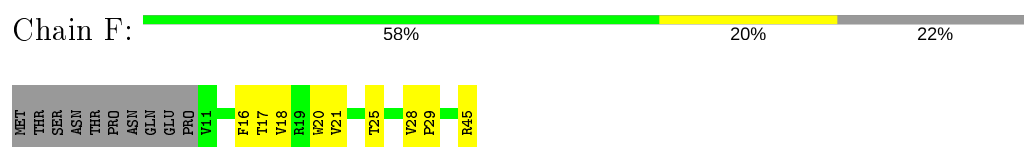
- Molecule 5: Cytochrome b559 subunit alpha



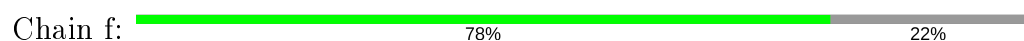
- Molecule 5: Cytochrome b559 subunit alpha

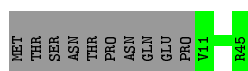


- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta

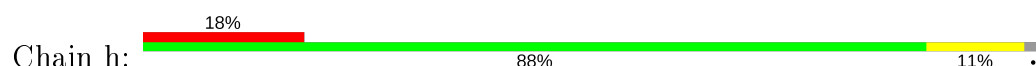




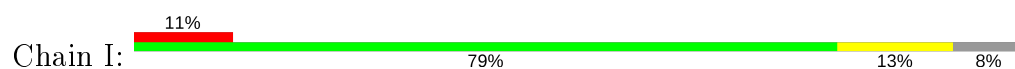
- Molecule 7: Photosystem II reaction center protein H



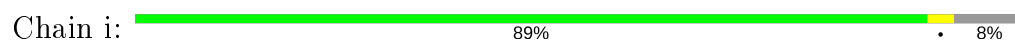
- Molecule 7: Photosystem II reaction center protein H



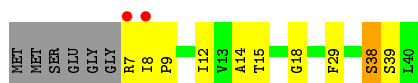
- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J

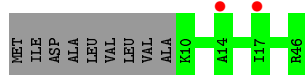
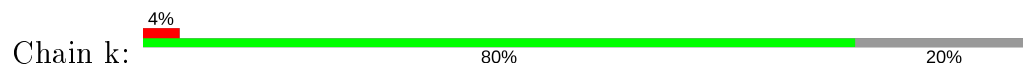


- Molecule 10: Photosystem II reaction center protein K

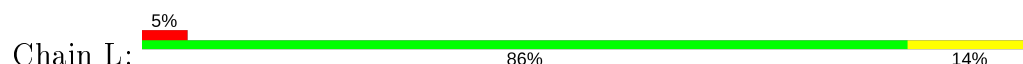




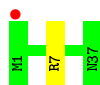
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



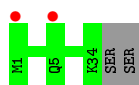
- Molecule 11: Photosystem II reaction center protein L



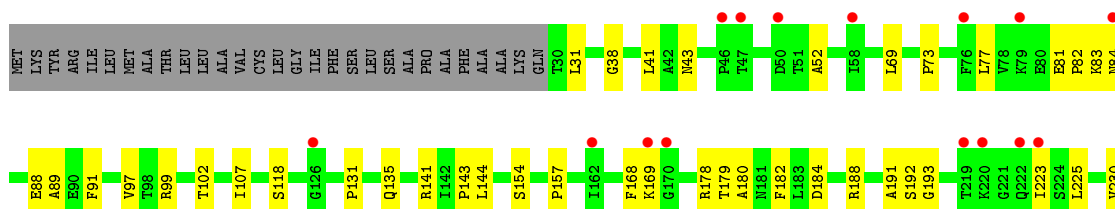
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

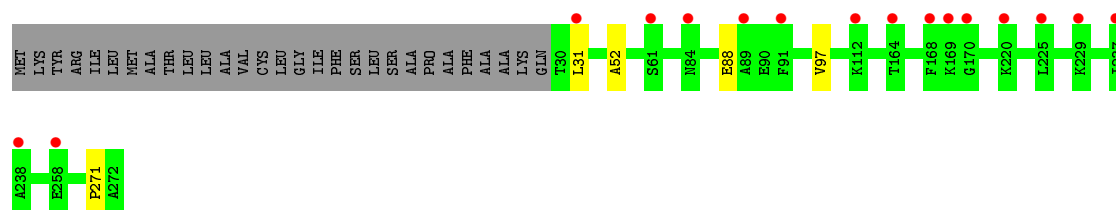
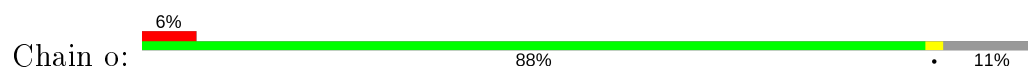


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

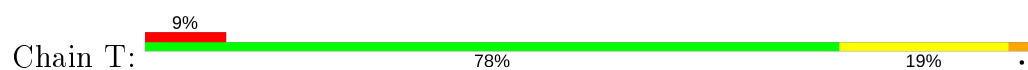




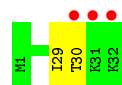
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



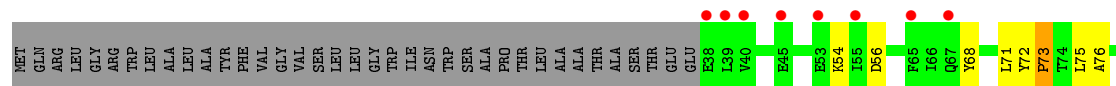
- Molecule 14: Photosystem II reaction center protein T



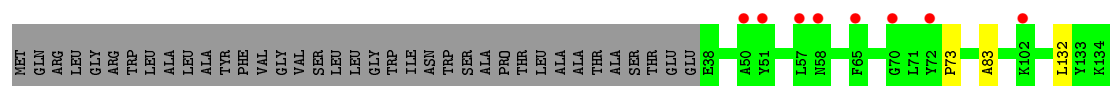
- Molecule 14: Photosystem II reaction center protein T



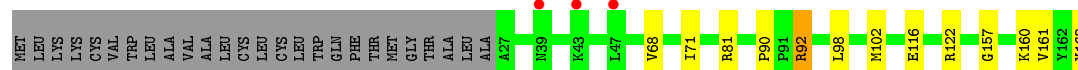
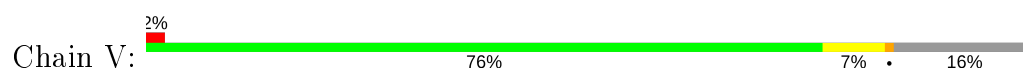
- Molecule 15: Photosystem II 12 kDa extrinsic protein



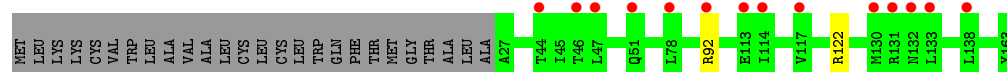
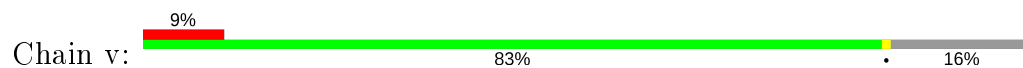
- Molecule 15: Photosystem II 12 kDa extrinsic protein



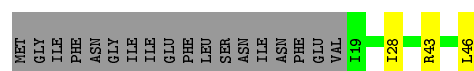
- Molecule 16: Cytochrome c-550



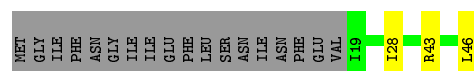
- Molecule 16: Cytochrome c-550



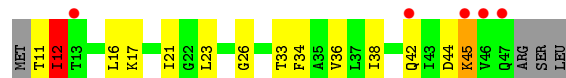
- Molecule 17: Photosystem II reaction center protein Ycf12



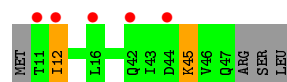
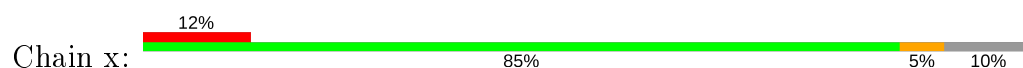
- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Y



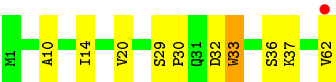
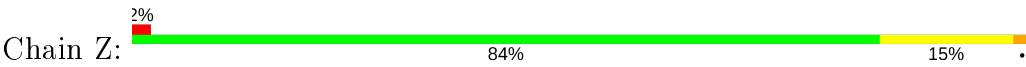
There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

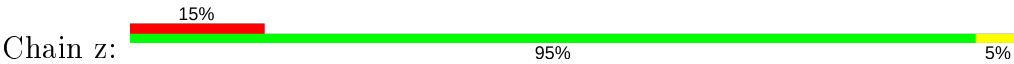


There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.88Å 229.03Å 307.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.93 – 4.90 72.93 – 4.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (72.93-4.90) 97.8 (72.93-4.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.281 , 0.292 0.283 , 0.291	Depositor DCC
R_{free} test set	2096 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	173.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 153.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å ²)	206.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, 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	0.46	0/709
8	I	0.24	0/293	0.42	0/395
8	i	0.24	0/293	0.42	0/395
9	J	0.21	0/255	0.40	0/346
9	j	0.21	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	0.23	0/270	0.43	0/367
13	O	0.22	0/1876	0.43	0/2548
13	o	0.22	0/1876	0.43	0/2548
14	T	0.24	0/284	0.40	0/381
14	t	0.24	0/284	0.40	0/381
15	U	0.22	0/785	0.43	0/1064
15	u	0.22	0/785	0.43	0/1064
16	V	0.21	0/1081	0.41	0/1468
16	v	0.21	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.21	0/202	0.46	0/272
17	y	0.22	0/202	0.45	0/272
18	X	0.26	0/273	0.43	0/370
18	x	0.26	0/273	0.44	0/370
20	Z	0.24	0/490	0.44	0/669
20	z	0.24	0/490	0.44	0/669
All	All	0.23	0/41950	0.41	0/57100

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2628	0	2524	85	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	89	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	88	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	12	0
5	e	666	0	651	0	0
6	F	282	0	291	7	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	3	0
8	i	286	0	308	0	0
9	J	249	0	262	7	0
9	j	249	0	262	0	0
10	K	293	0	305	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	5	0
11	l	304	0	316	0	0
12	M	267	0	289	8	0
12	m	267	0	289	0	0
13	O	1845	0	1801	31	0
13	o	1845	0	1801	0	0
14	T	275	0	288	6	0
14	t	275	0	288	0	0
15	U	774	0	773	8	0
15	u	774	0	773	0	0
16	V	1060	0	1068	7	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	6	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	46	0
22	B	975	0	1080	97	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	5	0
23	D	55	0	80	12	0
23	J	35	0	45	0	0
23	a	45	0	61	0	0
23	d	55	0	80	0	0
23	j	35	0	45	0	0
24	A	40	0	56	2	0
24	B	160	0	224	12	0
24	C	80	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	40	0	56	3	0
24	H	40	0	56	1	0
24	J	40	0	56	2	0
24	K	40	0	56	3	0
24	a	40	0	56	0	0
24	b	160	0	224	0	0
24	c	120	0	168	0	0
24	f	40	0	56	0	0
24	g	40	0	56	0	0
24	j	40	0	56	0	0
24	x	40	0	56	0	0
24	y	40	0	56	0	0
25	A	56	0	70	1	0
25	B	110	0	136	4	0
25	C	181	0	245	12	0
25	D	63	0	87	1	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	3	0
26	a	39	0	51	0	0
26	c	37	0	44	0	0
27	A	93	0	126	3	0
27	B	49	0	68	3	0
27	C	93	0	126	3	0
27	D	143	0	196	11	0
27	E	44	0	58	2	0
27	I	43	0	56	1	0
27	M	42	0	54	2	0
27	a	42	0	54	0	0
27	b	49	0	68	0	0
27	c	93	0	126	0	0
27	d	143	0	196	0	0
27	e	44	0	58	0	0
27	i	43	0	56	0	0
27	l	51	0	72	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	a	10	0	0	0	0
30	A	105	0	147	8	0
30	B	90	0	111	5	0
30	F	45	0	54	3	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	183	0	0
31	d	31	0	35	0	0
31	i	35	0	46	0	0
32	D	128	0	148	13	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	51373	595	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 (595) 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	0.86
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.82
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.81
3:C:362:ARG:H	25:C:515:DGD:HE4	1.53	0.80
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:V:201:HEM:HHH	34:V:201:HEM:HBC2	1.66	0.78
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.71	0.74
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.71	0.73
22:B:605:CLA:H72	24:B:619:BCR:H311	1.71	0.73
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.55	0.72
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.76	0.71
4:D:199:MET:HG2	23:D:406:PL9:H322	1.75	0.71
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.73	0.71
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.73	0.70
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.72	0.70
4:D:29:PHE:O	4:D:128:ARG:NH2	2.25	0.69
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.69
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.74	0.69
22:C:506:CLA:H112	24:C:514:BCR:H362	1.75	0.69
4:D:259:ILE:HG12	27:D:408:LMG:H292	1.76	0.68
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.76	0.68
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.76	0.68
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.30	0.68
25:C:517:DGD:HAF2	22:C:520:CLA:H202	1.76	0.68
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.76	0.67
1:A:15:GLU:O	1:A:19:ASN:ND2	2.26	0.67
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.77	0.67
4:D:21:TRP:O	4:D:26:ARG:NH2	2.26	0.67
4:D:236:ASN:ND2	4:D:239:GLN:O	2.31	0.66
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.81	0.66
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.66	0.66
3:C:48:LYS:NZ	3:C:133:ALA:O	2.28	0.65
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.65
1:A:174:LEU:HD22	32:D:401:PHO:H151	1.79	0.65
27:D:408:LMG:HO4	27:D:408:LMG:HO5	1.54	0.64
30:B:622:SQD:H171	30:B:622:SQD:H301	1.80	0.64
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.78	0.64
3:C:291:TRP:O	3:C:305:THR:OG1	2.15	0.64
22:B:606:CLA:HBB1	27:B:621:LMG:H341	1.80	0.64
2:B:271:THR:HG22	2:B:273:TYR:H	1.64	0.64
12:M:31:SER:HA	27:M:101:LMG:HC1	1.82	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.82	0.63
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.79	0.63
3:C:250:TRP:O	3:C:254:THR:OG1	2.12	0.63
22:B:611:CLA:H42	4:D:127:LEU:HD11	29.91	0.63
22:A:404:CLA:H142	22:D:404:CLA:H151	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:607:CLA:HBA2	30:B:622:SQD:H101	1.81	0.63
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.64	0.62
22:A:404:CLA:HHC	22:A:404:CLA:HBB1	3.75	0.62
6:F:17:THR:HG23	6:F:20:TRP:H	1.64	0.62
1:A:183:MET:HA	22:A:404:CLA:HMD2	12.62	0.62
1:A:183:MET:HB3	22:A:404:CLA:HBC2	14.90	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
3:C:49:LEU:O	3:C:53:HIS:ND1	2.32	0.62
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.86	0.62
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.81	0.62
4:D:24:ARG:NH2	18:X:44:ASP:O	2.33	0.61
4:D:186:GLN:HB2	22:D:404:CLA:HBC1	1.81	0.61
2:B:149:LEU:HG	22:B:606:CLA:HBC1	27.92	0.61
22:B:612:CLA:HMD1	7:H:27:THR:HB	39.61	0.61
30:A:413:SQD:H172	26:C:519:LHG:H172	1.83	0.60
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.82	0.60
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.82	0.60
3:C:406:SER:O	3:C:418:ASN:ND2	2.35	0.60
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.83	0.60
22:B:606:CLA:H193	7:H:42:LEU:HD12	33.87	0.60
4:D:216:ALA:O	4:D:220:ASN:ND2	2.33	0.60
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.83	0.60
1:A:329:GLU:O	1:A:332:HIS:ND1	2.37	0.60
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.84	0.60
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.83	0.60
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.35	0.60
22:A:404:CLA:H122	32:D:401:PHO:H3A	32.53	0.59
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.74	0.59
4:D:192:THR:HG23	22:D:404:CLA:HBC2	1.85	0.59
22:A:404:CLA:H71	22:A:405:CLA:HAB	47.00	0.59
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.59
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.83	0.58
22:B:605:CLA:OBD	31:B:623:LMT:O6'	2.20	0.58
2:B:121:GLU:O	7:H:12:ARG:NH2	2.36	0.58
2:B:262:THR:OG1	22:B:606:CLA:O1D	22.19	0.58
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.86	0.58
22:B:606:CLA:C2D	22:B:608:CLA:H2	39.98	0.58
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.93	0.58
1:A:217:SER:HA	4:D:272:LEU:HD12	1.90	0.58
32:D:402:PHO:H151	22:D:404:CLA:H172	1.85	0.58
22:H:101:CLA:HBD	22:H:101:CLA:H2	1.89	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:O	1:A:129:ARG:NH1	2.55	0.58
24:B:617:BCR:H19C	24:B:618:BCR:H363	1.85	0.58
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.24	0.58
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.34	0.57
3:C:284:PHE:HB3	25:C:515:DGD:HA51	1.93	0.57
22:B:611:CLA:H151	22:B:612:CLA:H203	19.90	0.57
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.85	0.57
22:A:403:CLA:H203	32:D:401:PHO:H71	1.85	0.57
13:O:83:LYS:HG2	13:O:84:ASN:H	1.69	0.57
22:C:501:CLA:HMB3	24:C:514:BCR:H403	1.87	0.57
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.57
1:A:84:PRO:HA	1:A:112:TYR:CG	2.39	0.57
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.85	0.57
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.86	0.57
2:B:12:LEU:HB2	22:B:615:CLA:HMC2	13.40	0.57
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.90	0.57
2:B:487:SER:N	2:B:488:PRO:HD2	2.21	0.56
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.87	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.70	0.56
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.30	0.56
26:C:519:LHG:H101	26:C:519:LHG:H271	1.86	0.56
4:D:214:HIS:ND1	23:D:406:PL9:O2	2.26	0.56
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.88	0.56
1:A:224:ILE:O	4:D:265:ARG:NH2	2.46	0.56
27:D:408:LMG:O6	11:L:15:THR:HG21	2.05	0.56
1:A:140:ARG:NH2	26:A:409:LHG:O5	2.34	0.56
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.56
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.88	0.56
2:B:327:THR:HG21	27:B:621:LMG:H111	1.87	0.56
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.24	0.56
2:B:262:THR:HG22	2:B:263:THR:HG23	1.87	0.56
2:B:256:MET:O	2:B:448:ARG:NH1	2.34	0.55
22:B:607:CLA:HBD	22:B:608:CLA:H43	4.12	0.55
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.36	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.88	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.55
1:A:85:SER:HA	1:A:109:GLY:HA3	1.94	0.55
30:B:626:SQD:H1	30:B:626:SQD:H462	1.88	0.55
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.38	0.55
2:B:474:LEU:O	4:D:134:ARG:NH1	2.47	0.55
25:C:517:DGD:HA22	9:J:29:PHE:HE1	1.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:404:CLA:H93	22:D:404:CLA:H152	1.89	0.55
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.94	0.55
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.88	0.55
22:B:606:CLA:C3D	22:B:608:CLA:H2	40.21	0.55
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.91	0.55
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.42	0.55
1:A:64:ARG:O	13:O:178:ARG:NH2	2.40	0.55
24:A:407:BCR:H321	30:A:414:SQD:H321	1.89	0.54
2:B:184:GLU:H	2:B:200:ALA:HB2	1.72	0.54
2:B:458:PHE:HB3	22:B:607:CLA:HBC2	12.95	0.54
22:C:510:CLA:HMB2	24:C:513:BCR:H382	1.88	0.54
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.90	0.54
22:A:405:CLA:H203	32:D:401:PHO:H71	33.20	0.54
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.54
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.42	0.54
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.90	0.54
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.89	0.54
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.07	0.54
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.93	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.90	0.54
1:A:268:SER:O	1:A:272:HIS:ND1	2.38	0.54
2:B:271:THR:HB	2:B:274:GLN:HG3	1.90	0.54
27:A:410:LMG:O5	11:L:13:ASN:ND2	2.39	0.54
22:D:405:CLA:H42	18:X:26:GLY:HA3	1.90	0.54
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.44	0.53
22:D:405:CLA:H43	18:X:23:LEU:HA	1.90	0.53
5:E:10:PHE:N	27:E:101:LMG:O3	2.40	0.53
24:A:407:BCR:H342	30:A:414:SQD:H311	1.90	0.53
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.91	0.53
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.89	0.53
2:B:150:CYS:HB2	22:B:606:CLA:HMC3	24.94	0.53
22:A:405:CLA:HED1	23:D:406:PL9:H372	28.92	0.53
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.91	0.53
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.61	0.53
13:O:73:PRO:HG2	13:O:102:THR:HB	1.91	0.53
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.91	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.91	0.53
22:A:402:CLA:H122	32:D:401:PHO:H3A	1.90	0.53
22:B:603:CLA:HBD	22:B:604:CLA:H43	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:403:CLA:HED1	23:D:406:PL9:H372	1.90	0.53
22:A:403:CLA:HMA2	23:D:406:PL9:H411	1.90	0.53
22:B:607:CLA:H151	22:B:608:CLA:H203	1.91	0.53
27:A:410:LMG:H231	23:D:406:PL9:H352	1.91	0.52
31:B:627:LMT:H62	8:I:4:LEU:HD22	82.16	0.52
22:B:608:CLA:H202	22:B:612:CLA:HBB2	21.91	0.52
2:B:103:LEU:HD21	22:B:608:CLA:HMC3	26.61	0.52
25:B:625:DGD:O2D	25:B:625:DGD:O1B	2.27	0.52
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.75	0.52
3:C:209:ILE:HG23	24:C:514:BCR:H382	1.94	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.42	0.52
3:C:85:GLY:N	25:C:516:DGD:HE4	2.24	0.52
30:A:413:SQD:H311	22:C:507:CLA:H71	1.92	0.52
2:B:212:ALA:HB2	22:B:612:CLA:HMC3	27.30	0.52
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.91	0.52
22:C:507:CLA:H172	25:C:516:DGD:HBW2	1.95	0.52
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.73	0.52
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	2.06	0.52
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.49	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.93	0.51
27:A:415:LMG:H112	2:B:43:ALA:HA	42.20	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.51
3:C:405:ASN:HB2	25:C:517:DGD:HG31	1.98	0.51
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.41	0.51
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.51
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.91	0.51
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.92	0.51
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.96	0.51
4:D:275:PRO:O	4:D:279:LEU:HD23	2.14	0.51
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.92	0.50
22:B:611:CLA:H51	22:B:612:CLA:H101	17.99	0.50
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.92	0.50
22:B:612:CLA:H51	27:D:407:LMG:H231	1.93	0.50
1:A:132:GLU:O	1:A:136:ARG:HG2	2.12	0.50
1:A:210:LEU:HG	32:D:402:PHO:NC	2.27	0.50
22:C:504:CLA:HBD	22:C:504:CLA:HBA1	1.93	0.50
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.93	0.50
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.96	0.50
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.50
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.95	0.50
13:O:168:PHE:HB2	13:O:225:LEU:HB2	1.95	0.50
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.97	0.50
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.92	0.50
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.42	0.50
1:A:153:SER:HB3	22:A:404:CLA:HED1	19.23	0.50
1:A:211:PHE:HA	1:A:214:MET:HB2	1.93	0.50
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.76	0.50
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.94	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.49
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.76	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.47	0.49
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.02	0.49
13:O:118:SER:HB3	13:O:157:PRO:HA	1.98	0.49
2:B:155:ALA:O	2:B:159:THR:OG1	2.20	0.49
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.49
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.96	0.49
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.95	0.49
2:B:327:THR:HG22	22:B:610:CLA:H12	26.95	0.49
3:C:158:THR:O	3:C:251:HIS:HB3	2.13	0.49
30:A:413:SQD:H223	25:C:517:DGD:HAE1	1.93	0.49
27:D:411:LMG:H171	24:F:102:BCR:H383	1.96	0.49
2:B:150:CYS:HA	22:B:606:CLA:HBC2	29.85	0.49
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.28	0.49
3:C:166:ILE:O	3:C:170:ILE:HG13	2.17	0.49
22:A:405:CLA:HBA1	22:A:405:CLA:CHA	3.72	0.49
3:C:361:PHE:HD1	25:C:515:DGD:HE61	1.80	0.49
30:F:103:SQD:H162	18:X:33:THR:HA	1.94	0.49
1:A:190:HIS:O	1:A:298:ASN:HB3	2.14	0.49
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.95	0.49
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.95	0.49
1:A:244:GLU:HG3	1:A:246:TYR:H	1.78	0.48
2:B:5:TRP:HZ3	22:B:614:CLA:H51	29.14	0.48
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.96	0.48
27:D:408:LMG:H111	11:L:19:LEU:HD21	1.99	0.48
1:A:78:ILE:O	1:A:176:ILE:HB	2.13	0.48
25:C:517:DGD:HA22	9:J:29:PHE:CE1	2.53	0.48
22:B:610:CLA:H193	11:L:27:LEU:HD11	15.76	0.48
5:E:15:THR:HG23	9:J:8:ILE:O	2.14	0.48
22:A:405:CLA:H42	23:D:406:PL9:H162	36.94	0.48
26:A:409:LHG:H382	22:C:509:CLA:H93	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.95	0.48
4:D:102:THR:OG1	25:D:409:DGD:HD62	2.18	0.48
22:A:404:CLA:H161	23:A:406:PL9:H253	1.94	0.48
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.94	0.48
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.98	0.48
22:A:404:CLA:HAB	22:D:404:CLA:H72	1.96	0.48
2:B:212:ALA:O	2:B:216:HIS:ND1	2.47	0.48
32:D:401:PHO:H41	32:D:401:PHO:H62	1.45	0.48
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
9:J:14:ALA:O	9:J:18:GLY:N	2.45	0.47
13:O:240:THR:HA	13:O:264:VAL:HA	1.98	0.47
1:A:271:LEU:HD11	23:A:406:PL9:C4	2.44	0.47
2:B:256:MET:HA	2:B:263:THR:HG21	1.96	0.47
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.79	0.47
22:B:613:CLA:H51	24:B:616:BCR:H372	1.96	0.47
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.78	0.47
4:D:279:LEU:HG	32:D:402:PHO:HBC3	1.96	0.47
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.45	0.47
4:D:85:MET:HA	5:E:69:ARG:HB3	1.98	0.47
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.01	0.47
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.96	0.47
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.96	0.47
22:D:404:CLA:H61	22:D:404:CLA:H41	1.64	0.47
4:D:262:SER:N	27:D:408:LMG:O3	2.44	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.00	0.47
22:B:614:CLA:H172	22:B:614:CLA:H111	1.97	0.47
18:X:12:ILE:HG12	18:X:16:LEU:HD12	2.01	0.47
1:A:156:ALA:HA	1:A:160:ILE:HB	2.01	0.47
7:H:46:LEU:HD13	22:H:101:CLA:H72	1.98	0.47
1:A:202:VAL:HB	22:A:404:CLA:HMB3	13.00	0.47
2:B:222:PRO:HG3	7:H:27:THR:H	1.80	0.47
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.79	0.47
3:C:425:TRP:CE2	22:C:520:CLA:HBA1	2.50	0.47
9:J:38:SER:OG	9:J:39:SER:N	2.47	0.47
13:O:154:SER:N	13:O:169:LYS:O	2.46	0.47
13:O:230:VAL:HG12	13:O:231:ASP:H	1.79	0.47
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.98	0.46
2:B:450:TRP:NE1	22:B:610:CLA:HBA1	29.99	0.46
22:B:605:CLA:H18	22:B:615:CLA:H121	1.97	0.46
24:B:616:BCR:H361	24:B:616:BCR:H20C	1.75	0.46
1:A:176:ILE:HD12	22:A:403:CLA:HED3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:405:CLA:H162	22:A:405:CLA:H141	1.70	0.46
1:A:215:HIS:ND1	23:A:406:PL9:O1	2.48	0.46
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.97	0.46
24:C:513:BCR:H343	24:C:513:BCR:H311	2.00	0.46
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.09	0.46
30:A:414:SQD:HO8	2:B:113:TRP:HE1	62.74	0.46
22:B:604:CLA:H62	22:B:604:CLA:H41	1.79	0.46
25:B:625:DGD:HD1	31:B:627:LMT:H32	1.97	0.46
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.46
4:D:48:TRP:CE2	32:D:402:PHO:H161	2.51	0.46
25:B:620:DGD:HAW2	22:H:101:CLA:H152	1.98	0.46
4:D:348:ARG:NH2	4:D:352:LEU:O	2.35	0.46
27:C:518:LMG:H292	27:C:518:LMG:H111	1.96	0.46
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.64	0.46
1:A:114:LEU:O	1:A:118:HIS:ND1	2.45	0.46
2:B:18:ARG:HD3	2:B:118:TRP:HB3	2.00	0.46
31:B:628:LMT:H122	14:T:7:VAL:HG12	34.43	0.46
3:C:224:ILE:O	3:C:227:VAL:HG23	2.16	0.46
22:H:101:CLA:H62	22:H:101:CLA:H41	1.57	0.46
22:A:402:CLA:HBA1	22:A:402:CLA:H3A	1.53	0.46
22:B:606:CLA:H2	22:B:608:CLA:H93	34.04	0.46
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.99	0.46
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.98	0.46
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.46
22:A:403:CLA:H42	23:D:406:PL9:H162	1.96	0.46
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	1.98	0.46
22:B:607:CLA:H51	22:B:608:CLA:H101	1.97	0.46
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.51	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.98	0.46
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.56	0.46
24:B:618:BCR:H20C	24:B:618:BCR:H361	1.82	0.46
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.45
22:A:404:CLA:HBA1	22:A:404:CLA:H3A	2.33	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.17	0.45
22:H:101:CLA:H162	22:H:101:CLA:H122	1.51	0.45
27:I:101:LMG:H181	31:I:102:LMT:H42	2.06	0.45
2:B:213:GLY:O	2:B:217:ILE:HG13	2.15	0.45
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.05	0.45
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.52	0.45
22:C:510:CLA:H61	22:C:510:CLA:H93	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.98	0.45
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.85	0.45
22:B:611:CLA:H162	22:B:611:CLA:H122	1.75	0.45
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.98	0.45
27:D:408:LMG:O9	27:D:408:LMG:HC1	2.20	0.45
2:B:329:PRO:HB3	22:B:606:CLA:HED1	1.99	0.45
22:B:607:CLA:H18	22:B:608:CLA:H192	1.99	0.45
22:B:608:CLA:H62	22:B:608:CLA:H41	4.36	0.45
2:B:247:PHE:HB2	22:B:611:CLA:HBC1	19.53	0.45
3:C:318:LEU:HD21	3:C:380:ILE:HG23	1.99	0.45
22:C:510:CLA:H121	24:C:513:BCR:H21C	2.03	0.45
25:B:620:DGD:HA71	22:H:101:CLA:H193	1.99	0.45
1:A:202:VAL:HB	22:A:402:CLA:HMB3	1.99	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.72	0.45
3:C:113:VAL:HG11	27:C:518:LMG:H132	1.99	0.45
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.99	0.45
2:B:150:CYS:HA	22:B:602:CLA:HBC2	2.00	0.44
2:B:96:VAL:HG22	22:B:609:CLA:HBA1	23.21	0.44
24:C:513:BCR:H24C	24:C:513:BCR:H371	1.79	0.44
4:D:56:THR:HG21	5:E:50:PRO:HD3	1.99	0.44
30:F:103:SQD:H131	18:X:36:VAL:HG11	2.00	0.44
15:U:106:ARG:HA	15:U:109:LEU:HG	1.98	0.44
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.21	0.44
1:A:238:LYS:O	1:A:241:GLN:HG3	2.17	0.44
2:B:327:THR:HG22	22:B:606:CLA:H12	1.99	0.44
3:C:245:ILE:O	3:C:249:ILE:HG12	2.19	0.44
22:C:503:CLA:HMB3	27:C:518:LMG:H181	2.06	0.44
22:C:506:CLA:H62	22:C:506:CLA:H92	1.75	0.44
2:B:383:PHE:N	4:D:344:GLU:O	2.36	0.44
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.01	0.44
20:Z:33:TRP:CD1	20:Z:33:TRP:O	2.70	0.44
22:A:402:CLA:H51	32:D:401:PHO:C3B	2.48	0.44
22:C:501:CLA:H193	22:C:506:CLA:H111	2.10	0.44
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.00	0.44
22:B:606:CLA:H41	22:B:606:CLA:H61	2.90	0.44
3:C:29:GLU:HB2	3:C:30:SER:H	1.65	0.44
22:C:508:CLA:H11	22:C:508:CLA:H51	1.82	0.44
32:D:401:PHO:H13	32:D:401:PHO:H102	1.82	0.44
24:H:102:BCR:H361	24:H:102:BCR:H20C	1.78	0.44
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.79	0.44
22:B:602:CLA:H162	22:B:602:CLA:H192	1.76	0.44
22:B:613:CLA:H91	22:B:613:CLA:H112	1.82	0.44
24:C:514:BCR:H361	24:C:514:BCR:H20C	1.84	0.44
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.02	0.44
22:A:405:CLA:HMA2	23:D:406:PL9:H411	24.67	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.44
3:C:343:ARG:NH1	3:C:347:GLY:O	2.50	0.44
25:C:516:DGD:HA91	25:C:516:DGD:HAW2	1.75	0.44
1:A:303:ASN:O	3:C:415:ASN:ND2	2.40	0.44
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.03	0.44
22:A:403:CLA:H51	22:A:403:CLA:H11	1.82	0.44
22:B:612:CLA:H171	27:D:407:LMG:H401	2.00	0.44
24:B:616:BCR:H341	24:B:616:BCR:H11C	1.90	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.20	0.43
22:B:603:CLA:HMD2	22:B:611:CLA:H193	2.00	0.43
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.53	0.43
16:V:68:VAL:O	16:V:71:ILE:HG12	2.19	0.43
2:B:170:ASP:OD1	2:B:175:THR:N	2.51	0.43
24:C:514:BCR:H351	24:C:514:BCR:H15C	1.83	0.43
13:O:192:SER:OG	13:O:193:GLY:N	2.51	0.43
3:C:90:PRO:O	3:C:94:THR:HG23	2.19	0.43
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
22:C:501:CLA:C1D	22:C:503:CLA:H2	2.49	0.43
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.02	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.53	0.43
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.43
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.43
7:H:35:MET:HB2	7:H:35:MET:HE3	1.85	0.43
15:U:72:TYR:O	15:U:76:ALA:HB3	2.20	0.43
22:B:611:CLA:H18	22:B:612:CLA:H192	22.19	0.43
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.00	0.43
24:C:513:BCR:H20C	24:C:513:BCR:H361	1.77	0.43
22:B:605:CLA:H3A	22:B:605:CLA:HBA2	1.25	0.43
30:A:414:SQD:H332	22:B:609:CLA:H203	66.19	0.43
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.75	0.43
24:C:513:BCR:H15C	24:C:513:BCR:H351	1.90	0.43
22:D:404:CLA:HBA1	22:D:404:CLA:H3A	1.84	0.43
22:C:512:CLA:HAB	24:K:102:BCR:H371	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:405:CLA:H11	22:A:405:CLA:H51	4.35	0.43
2:B:30:VAL:HG12	22:B:608:CLA:HHD	31.17	0.43
3:C:456:GLU:N	3:C:456:GLU:OE1	2.51	0.43
16:V:90:PRO:O	16:V:92:ARG:HD3	2.18	0.43
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.01	0.43
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.03	0.43
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.01	0.43
4:D:261:PHE:HB2	23:D:406:PL9:H522	2.01	0.43
24:J:102:BCR:H351	24:J:102:BCR:H15C	1.76	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.70	0.43
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.02	0.43
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.54	0.43
22:B:615:CLA:H162	22:B:615:CLA:H122	5.18	0.43
2:B:86:ILE:H	2:B:86:ILE:HG13	1.75	0.43
22:C:504:CLA:H11	24:C:514:BCR:H312	2.04	0.43
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.01	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.43
24:J:102:BCR:H11C	24:J:102:BCR:H341	1.80	0.43
22:B:615:CLA:H72	22:B:615:CLA:H12	2.01	0.42
22:C:501:CLA:H162	22:C:501:CLA:H141	1.79	0.42
1:A:176:ILE:HD12	22:A:405:CLA:HED3	23.97	0.42
1:A:38:ILE:HD13	30:A:414:SQD:H121	2.01	0.42
22:A:404:CLA:H143	22:A:404:CLA:H161	1.85	0.42
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.54	0.42
22:B:613:CLA:H152	22:B:613:CLA:H112	1.85	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.23	0.42
3:C:464:GLU:HA	3:C:465:PRO:HD2	1.78	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.42
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.00	0.42
22:B:611:CLA:HBA1	22:B:611:CLA:CHA	3.78	0.42
31:B:628:LMT:H3'	31:B:628:LMT:H1B	1.53	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.42
3:C:248:GLY:O	3:C:252:ILE:HG12	2.20	0.42
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.19	0.42
27:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
23:D:406:PL9:H421	23:D:406:PL9:H401	1.85	0.42
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.06	0.42
22:A:402:CLA:H102	22:A:402:CLA:H62	1.88	0.42
1:A:271:LEU:HD21	23:A:406:PL9:HC71	2.01	0.42
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:614:CLA:H52	22:B:614:CLA:H12	1.85	0.42
30:B:622:SQD:H111	30:B:622:SQD:H241	2.02	0.42
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.62	0.42
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.55	0.42
1:A:61:ASP:HB2	1:A:63:ILE:HG12	2.08	0.42
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.02	0.42
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.91	0.42
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.06	0.42
24:B:616:BCR:H333	12:M:13:LEU:HD12	2.02	0.42
20:Z:10:ALA:O	20:Z:14:ILE:HG13	2.20	0.42
1:A:34:GLY:HA2	1:A:37:MET:HB3	2.13	0.42
22:C:503:CLA:HMD2	22:C:503:CLA:H201	2.02	0.42
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.01	0.42
1:A:262:TYR:HB3	27:E:101:LMG:H112	2.09	0.42
7:H:12:ARG:HD3	7:H:12:ARG:O	2.20	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.92	0.42
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.42
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.83	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.42
18:X:34:PHE:O	18:X:38:ILE:HG12	2.20	0.42
1:A:153:SER:HB2	22:A:404:CLA:H43	19.21	0.42
1:A:238:LYS:HD2	14:T:32:LYS:HB3	2.03	0.42
22:A:403:CLA:H202	22:A:403:CLA:H162	1.75	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.42
3:C:282:MET:HG2	22:C:501:CLA:H61	2.07	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.95	0.42
22:D:404:CLA:H62	22:D:404:CLA:H92	1.81	0.42
2:B:6:TYR:OH	27:D:407:LMG:HC5	2.23	0.42
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.02	0.42
1:A:180:PHE:HA	1:A:183:MET:HE2	2.09	0.42
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.01	0.42
3:C:466:VAL:HG13	4:D:251:ARG:HD2	2.05	0.42
22:C:520:CLA:H161	22:C:520:CLA:H141	1.87	0.42
4:D:113:PHE:O	4:D:117:HIS:HB2	2.20	0.42
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.02	0.42
22:B:609:CLA:HBA2	22:B:609:CLA:H3A	2.64	0.42
24:B:616:BCR:H351	24:B:616:BCR:H15C	1.86	0.42
22:C:505:CLA:H202	22:C:505:CLA:H161	1.86	0.42
22:C:512:CLA:HAB	24:K:102:BCR:H24C	2.02	0.42
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.57	0.42
1:A:127:MET:HG3	1:A:144:CYS:HB2	2.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:HB2	1:A:142:TRP:H	1.68	0.41
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.85	0.41
24:C:513:BCR:H391	10:K:36:ALA:HB2	2.05	0.41
4:D:252:PHE:O	4:D:256:ILE:HG22	2.23	0.41
22:B:604:CLA:H202	22:B:604:CLA:H162	1.86	0.41
22:B:611:CLA:H161	22:B:611:CLA:H143	4.41	0.41
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.84	0.41
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.03	0.41
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.88	0.41
22:D:405:CLA:H41	22:D:405:CLA:H61	1.87	0.41
1:A:140:ARG:HH22	26:A:409:LHG:P	2.43	0.41
1:A:298:ASN:ND2	3:C:402:GLY:O	2.55	0.41
2:B:135:LEU:HD23	2:B:138:MET:HE3	2.03	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
22:B:606:CLA:HBC3	24:B:618:BCR:HC8	2.01	0.41
22:B:608:CLA:H141	22:B:608:CLA:H161	4.19	0.41
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.02	0.41
22:C:511:CLA:H61	22:C:511:CLA:H13	2.02	0.41
22:C:520:CLA:H112	22:C:520:CLA:H142	1.76	0.41
1:A:27:ARG:NH1	4:D:254:SER:O	2.52	0.41
5:E:42:LEU:O	5:E:46:VAL:HG23	2.22	0.41
16:V:98:LEU:O	16:V:102:MET:HG3	2.21	0.41
1:A:182:PHE:O	1:A:186:PHE:HB2	2.22	0.41
22:A:405:CLA:H202	22:A:405:CLA:H162	3.74	0.41
2:B:108:PHE:HB2	30:B:626:SQD:H223	2.02	0.41
2:B:68:ARG:HH22	22:B:603:CLA:HED1	1.85	0.41
3:C:429:SER:HB3	25:C:516:DGD:HA81	2.02	0.41
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.03	0.41
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.60	0.41
1:A:121:LEU:HD13	25:A:408:DGD:HB92	2.03	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.93	0.41
22:B:602:CLA:H61	22:B:602:CLA:H41	1.66	0.41
22:B:607:CLA:H161	22:B:607:CLA:H202	4.72	0.41
24:C:514:BCR:H11C	24:C:514:BCR:H341	1.89	0.41
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.41
1:A:240:GLY:HA3	14:T:29:ILE:HG22	2.02	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.03	0.41
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.89	0.41
4:D:350:ASN:O	4:D:352:LEU:N	2.49	0.41
13:O:77:LEU:HB2	13:O:260:LYS:HB3	2.03	0.41
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:19:SER:O	12:M:23:ILE:HG13	2.22	0.41
1:A:96:ILE:HD12	22:A:405:CLA:HMD1	2.02	0.41
22:C:508:CLA:H142	22:C:508:CLA:H112	1.84	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.85	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.29	0.41
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.35	0.41
7:H:12:ARG:N	7:H:13:PRO:HD2	2.36	0.41
1:A:269:ARG:NH1	4:D:231:THR:HB	2.43	0.41
1:A:283:VAL:O	1:A:286:THR:HG22	2.21	0.41
22:B:605:CLA:C3D	31:B:623:LMT:H11	2.51	0.41
3:C:386:PRO:O	3:C:390:ARG:HG2	2.26	0.41
12:M:31:SER:HA	27:M:101:LMG:HC5	2.09	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.43	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.98	0.41
2:B:19:LEU:O	2:B:23:HIS:ND1	2.53	0.41
2:B:25:MET:HG2	24:B:616:BCR:H23C	2.02	0.41
3:C:281:MET:HE3	22:C:504:CLA:HAC2	2.03	0.41
6:F:16:PHE:HB3	30:F:103:SQD:H241	2.07	0.41
3:C:425:TRP:CZ2	22:C:520:CLA:HBA1	2.57	0.41
32:D:402:PHO:CHB	22:D:404:CLA:H101	2.51	0.41
24:F:102:BCR:H11C	24:F:102:BCR:H341	1.94	0.41
2:B:191:ASN:HB2	7:H:58:VAL:HG23	2.05	0.41
10:K:24:VAL:O	10:K:27:VAL:HG12	2.21	0.41
3:C:334:PRO:HA	13:O:179:THR:OG1	2.21	0.41
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.51	0.40
22:B:606:CLA:H62	22:B:606:CLA:H41	1.90	0.40
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.50	0.40
22:B:613:CLA:H12	22:B:613:CLA:H51	4.47	0.40
3:C:257:PHE:HB3	3:C:258:GLY:H	1.63	0.40
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.95	0.40
7:H:46:LEU:HB2	22:H:101:CLA:H61	2.06	0.40
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.58	0.40
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.81	0.40
24:F:102:BCR:H361	24:F:102:BCR:H20C	1.81	0.40
6:F:21:VAL:O	6:F:25:THR:HG23	2.22	0.40
22:B:602:CLA:HBB	22:H:101:CLA:O1D	2.21	0.40
1:A:112:TYR:O	1:A:116:ILE:HG12	2.21	0.40
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.40
22:A:403:CLA:HMA1	22:A:403:CLA:H122	2.02	0.40
22:A:403:CLA:HAA1	23:D:406:PL9:H362	2.03	0.40
22:A:405:CLA:H122	22:A:405:CLA:HMA1	15.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.98	0.40
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.40	0.40
2:B:468:TRP:HH2	27:D:407:LMG:HO2	1.66	0.40
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.60	0.40
22:A:402:CLA:H202	22:A:403:CLA:H93	2.03	0.40
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.04	0.40
2:B:91:TRP:CH2	22:B:605:CLA:H12	2.56	0.40
2:B:242:ILE:HG12	22:B:614:CLA:HBB1	23.30	0.40
3:C:35:TRP:CZ2	26:C:519:LHG:H261	2.56	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.22	0.40
4:D:329:MET:HG2	4:D:333:ASP:HB2	2.04	0.40
22:B:607:CLA:H172	22:D:405:CLA:H3A	2.03	0.40
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.56	0.40
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.05	0.40
4:D:294:ARG:HG2	4:D:294:ARG:H	1.64	0.40
23:A:406:PL9:H301	4:D:42:TYR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	312 (94%)	17 (5%)	4 (1%)	13	50
1	a	333/344 (97%)	310 (93%)	19 (6%)	4 (1%)	13	50
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	19	60
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	25	65
3	C	445/461 (96%)	406 (91%)	35 (8%)	4 (1%)	17	56
3	c	445/461 (96%)	405 (91%)	35 (8%)	5 (1%)	14	52
4	D	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	338/352 (96%)	314 (93%)	23 (7%)	1 (0%)	41	76
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	48
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	12	48
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	23
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100	100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	4	30
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	29
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	29
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	38
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	7	38
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
16	v	135/163 (83%)	123 (91%)	12 (9%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	26
17	y	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	3	26
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5138/5618 (92%)	4678 (91%)	404 (8%)	56 (1%)	14	52

All (56) 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
13	O	52	ALA
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
9	J	38	SER
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
9	j	38	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
4	D	239	GLN
7	H	26	GLY
13	O	88	GLU
2	b	489	GLU
4	d	239	GLN
7	h	26	GLY
13	o	88	GLU
1	A	142	TRP
1	A	334	ARG

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Mol	Chain	Res	Type
2	B	489	GLU
3	C	32	GLY
5	E	82	GLN
13	O	271	PRO
1	a	334	ARG
3	c	32	GLY
5	e	82	GLN
13	o	271	PRO
7	H	16	SER
15	U	73	PRO
1	a	142	TRP
3	c	144	SER
7	h	16	SER
15	u	73	PRO
3	C	144	SER
15	U	83	ALA
15	u	83	ALA
2	B	176	GLY
3	c	194	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	61
3	c	347/362 (96%)	336 (97%)	11 (3%)	39	61
4	D	275/283 (97%)	269 (98%)	6 (2%)	52	71
4	d	275/283 (97%)	268 (98%)	7 (2%)	47	68
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	39
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	39
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	i	32/35 (91%)	31 (97%)	1 (3%)	40	62
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	54
9	j	24/28 (86%)	23 (96%)	1 (4%)	30	54
10	K	30/37 (81%)	30 (100%)	0	100	100
10	k	30/37 (81%)	30 (100%)	0	100	100
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	64
11	l	35/35 (100%)	34 (97%)	1 (3%)	42	64
12	M	31/33 (94%)	31 (100%)	0	100	100
12	m	31/33 (94%)	31 (100%)	0	100	100
13	O	202/228 (89%)	200 (99%)	2 (1%)	76	86
13	o	202/228 (89%)	200 (99%)	2 (1%)	76	86
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	t	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/112 (75%)	83 (99%)	1 (1%)	71	84
15	u	84/112 (75%)	83 (99%)	1 (1%)	71	84
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	42
18	x	30/34 (88%)	28 (93%)	2 (7%)	16	42
20	Z	52/52 (100%)	50 (96%)	2 (4%)	33	57
20	z	52/52 (100%)	50 (96%)	2 (4%)	33	57
All	All	4244/4594 (92%)	4141 (98%)	103 (2%)	49	69

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU

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Mol	Chain	Res	Type
16	V	92	ARG
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
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

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Mol	Chain	Res	Type
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	132	LEU
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

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

Mol	Chain	Res	Type
1	A	241	GLN
4	D	117	HIS
4	d	117	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
32	PHO	a	407	-	67,69,69	1.26	8 (11%)	85,99,99	1.00	5 (5%)
22	CLA	c	505	-	59,73,73	1.44	5 (8%)	67,113,113	1.51	7 (10%)
22	CLA	a	408	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	7 (10%)
34	HEM	f	101	5,6	27,50,50	2.16	5 (18%)	17,82,82	1.46	3 (17%)
24	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	8 (14%)
31	LMT	D	410	-	32,32,36	1.20	5 (15%)	43,43,47	0.99	2 (4%)
27	LMG	C	521	-	48,48,55	0.77	0	56,56,63	1.30	6 (10%)
22	CLA	C	510	3	59,73,73	1.41	5 (8%)	67,113,113	1.51	8 (11%)
23	PL9	D	406	-	55,55,55	1.06	3 (5%)	68,69,69	1.51	12 (17%)
26	LHG	C	519	-	36,36,48	0.70	0	39,42,54	1.26	4 (10%)
22	CLA	B	601	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	8 (11%)
22	CLA	b	610	-	59,73,73	1.43	5 (8%)	67,113,113	1.43	9 (13%)
27	LMG	c	518	-	45,45,55	0.77	0	53,53,63	1.28	6 (11%)
30	SQD	a	401	-	53,54,54	0.95	4 (7%)	62,65,65	1.55	9 (14%)
27	LMG	E	101	-	44,44,55	0.76	0	52,52,63	1.28	4 (7%)
27	LMG	l	101	-	51,51,55	0.76	1 (1%)	59,59,63	1.34	6 (10%)
22	CLA	c	510	3	59,73,73	1.43	5 (8%)	67,113,113	1.48	7 (10%)
25	DGD	c	516	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	11 (14%)
22	CLA	c	506	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	8 (11%)
25	DGD	c	515	-	54,54,67	0.96	1 (1%)	68,68,81	1.27	6 (8%)
22	CLA	C	502	-	59,73,73	1.41	5 (8%)	67,113,113	1.47	9 (13%)
22	CLA	a	405	-	59,73,73	1.42	5 (8%)	67,113,113	1.49	8 (11%)
25	DGD	A	408	-	57,57,67	0.92	0	71,71,81	1.41	8 (11%)
25	DGD	C	517	-	67,67,67	0.89	2 (2%)	81,81,81	1.40	10 (12%)
25	DGD	D	409	-	64,64,67	0.92	0	78,78,81	1.33	9 (11%)
24	BCR	g	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.29	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HEM	V	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.43	2 (11%)
32	PHO	d	401	-	67,69,69	1.24	8 (11%)	85,99,99	1.01	5 (5%)
31	LMT	b	604	-	36,36,36	1.15	5 (13%)	47,47,47	1.03	1 (2%)
22	CLA	C	503	-	59,73,73	1.41	5 (8%)	67,113,113	1.51	8 (11%)
31	LMT	B	623	-	36,36,36	1.13	5 (13%)	47,47,47	0.97	1 (2%)
22	CLA	c	509	-	59,73,73	1.45	5 (8%)	67,113,113	1.42	9 (13%)
22	CLA	c	502	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	7 (10%)
23	PL9	A	406	-	45,45,55	1.00	3 (6%)	56,57,69	1.57	10 (17%)
32	PHO	D	402	-	67,69,69	1.26	8 (11%)	85,99,99	1.01	5 (5%)
24	BCR	c	521	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	8 (14%)
22	CLA	h	101	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
22	CLA	b	609	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	8 (11%)
32	PHO	D	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.01	5 (5%)
22	CLA	b	613	-	59,73,73	1.41	5 (8%)	67,113,113	1.44	9 (13%)
31	LMT	i	102	-	36,36,36	1.11	4 (11%)	47,47,47	1.00	2 (4%)
22	CLA	A	404	-	59,73,73	1.41	5 (8%)	67,113,113	1.45	7 (10%)
27	LMG	i	101	-	43,43,55	0.82	0	51,51,63	1.26	5 (9%)
31	LMT	b	627	-	36,36,36	1.11	4 (11%)	47,47,47	1.00	2 (4%)
22	CLA	B	615	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	9 (13%)
22	CLA	b	619	-	59,73,73	1.43	6 (10%)	67,113,113	1.42	8 (11%)
22	CLA	b	612	-	59,73,73	1.44	5 (8%)	67,113,113	1.43	7 (10%)
24	BCR	b	621	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	8 (14%)
22	CLA	B	609	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	8 (11%)
22	CLA	A	402	-	59,73,73	1.45	5 (8%)	67,113,113	1.42	8 (11%)
31	LMT	b	603	-	36,36,36	1.14	5 (13%)	47,47,47	0.95	1 (2%)
22	CLA	C	509	-	59,73,73	1.44	5 (8%)	67,113,113	1.42	9 (13%)
31	LMT	B	628	-	36,36,36	1.15	5 (13%)	47,47,47	1.04	1 (2%)
29	OEX	A	412	1,3	0,15,15	0.00	-	-	-	-
22	CLA	C	506	-	59,73,73	1.40	5 (8%)	67,113,113	1.49	8 (11%)
30	SQD	f	103	-	44,45,54	1.03	4 (9%)	53,56,65	1.65	10 (18%)
24	BCR	f	102	-	41,41,41	1.13	2 (4%)	56,56,56	1.22	5 (8%)
22	CLA	a	406	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	8 (11%)
22	CLA	c	512	-	59,73,73	1.44	5 (8%)	67,113,113	1.48	9 (13%)
23	PL9	d	406	-	55,55,55	1.05	2 (3%)	68,69,69	1.53	14 (20%)
26	LHG	c	519	-	36,36,48	0.73	1 (2%)	39,42,54	1.25	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.58	13 (23%)
24	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	8 (14%)
24	BCR	C	514	-	41,41,41	1.11	3 (7%)	56,56,56	1.29	8 (14%)
22	CLA	b	607	-	59,73,73	1.42	5 (8%)	67,113,113	1.52	10 (14%)
31	LMT	I	102	-	36,36,36	1.12	5 (13%)	47,47,47	1.02	2 (4%)
27	LMG	D	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
27	LMG	e	101	-	44,44,55	0.76	0	52,52,63	1.29	4 (7%)
31	LMT	M	102	-	36,36,36	1.16	6 (16%)	47,47,47	0.99	2 (4%)
23	PL9	J	101	-	35,35,55	1.04	2 (5%)	44,45,69	1.57	7 (15%)
27	LMG	A	410	-	51,51,55	0.75	0	59,59,63	1.36	7 (11%)
24	BCR	y	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.27	7 (12%)
22	CLA	B	608	-	59,73,73	1.45	5 (8%)	67,113,113	1.45	8 (11%)
27	LMG	I	101	-	43,43,55	0.81	0	51,51,63	1.26	4 (7%)
31	LMT	B	627	-	36,36,36	1.14	5 (13%)	47,47,47	0.96	1 (2%)
27	LMG	m	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
33	BCT	d	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	b	615	-	59,73,73	1.40	5 (8%)	67,113,113	1.51	8 (11%)
27	LMG	c	522	-	48,48,55	0.77	0	56,56,63	1.29	5 (8%)
24	BCR	B	618	-	41,41,41	1.11	2 (4%)	56,56,56	1.38	8 (14%)
31	LMT	d	410	-	32,32,36	1.19	5 (15%)	43,43,47	0.99	2 (4%)
24	BCR	b	623	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	9 (16%)
22	CLA	c	511	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	9 (13%)
34	HEM	F	101	5,6	27,50,50	2.16	5 (18%)	17,82,82	1.45	4 (23%)
30	SQD	A	413	-	50,51,54	0.96	3 (6%)	59,62,65	1.75	10 (16%)
22	CLA	B	605	-	59,73,73	1.40	5 (8%)	67,113,113	1.48	8 (11%)
27	LMG	b	625	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	7 (12%)
22	CLA	c	504	-	59,73,73	1.43	5 (8%)	67,113,113	1.52	8 (11%)
27	LMG	A	415	-	42,42,55	0.83	0	50,50,63	1.25	4 (8%)
22	CLA	A	403	-	59,73,73	1.42	5 (8%)	67,113,113	1.50	8 (11%)
25	DGD	B	625	-	53,53,67	1.07	3 (5%)	67,67,81	1.30	7 (10%)
22	CLA	a	404	-	59,73,73	1.45	5 (8%)	67,113,113	1.44	8 (11%)
31	LMT	B	624	-	36,36,36	1.12	4 (11%)	47,47,47	1.00	2 (4%)
30	SQD	d	402	-	42,43,54	1.05	3 (7%)	51,54,65	1.77	11 (21%)
22	CLA	B	612	-	59,73,73	1.39	5 (8%)	67,113,113	1.49	8 (11%)
31	LMT	M	103	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	DGD	b	624	-	59,59,67	0.91	1 (1%)	73,73,81	1.34	6 (8%)
26	LHG	a	412	-	38,38,48	0.69	1 (2%)	41,44,54	1.20	3 (7%)
22	CLA	b	616	-	59,73,73	1.40	5 (8%)	67,113,113	1.50	9 (13%)
30	SQD	A	414	-	53,54,54	0.96	4 (7%)	62,65,65	1.56	9 (14%)
34	HEM	v	201	16	27,50,50	2.19	6 (22%)	17,82,82	1.40	2 (11%)
23	PL9	a	409	-	45,45,55	1.07	3 (6%)	56,57,69	1.57	10 (17%)
24	BCR	H	102	-	41,41,41	1.13	2 (4%)	56,56,56	1.21	4 (7%)
22	CLA	B	610	-	59,73,73	1.48	5 (8%)	67,113,113	1.55	9 (13%)
30	SQD	F	103	-	44,45,54	1.03	4 (9%)	53,56,65	1.65	10 (18%)
24	BCR	C	513	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
22	CLA	b	605	-	59,73,73	1.46	5 (8%)	67,113,113	1.47	8 (11%)
27	LMG	d	407	-	49,49,55	0.77	0	57,57,63	1.30	4 (7%)
22	CLA	B	607	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	8 (11%)
30	SQD	B	626	-	46,47,54	1.02	4 (8%)	55,58,65	1.77	10 (18%)
25	DGD	a	411	-	57,57,67	0.92	1 (1%)	71,71,81	1.40	7 (9%)
30	SQD	a	415	-	50,51,54	0.96	4 (8%)	59,62,65	1.75	10 (16%)
24	BCR	x	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.19	4 (7%)
22	CLA	b	617	-	59,73,73	1.41	5 (8%)	67,113,113	1.48	7 (10%)
24	BCR	c	513	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	9 (16%)
25	DGD	C	516	-	63,63,67	0.91	2 (3%)	77,77,81	1.44	12 (15%)
22	CLA	C	520	-	59,73,73	1.41	5 (8%)	67,113,113	1.46	8 (11%)
24	BCR	c	514	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
24	BCR	b	620	-	41,41,41	1.11	2 (4%)	56,56,56	1.21	5 (8%)
22	CLA	c	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.43	8 (11%)
22	CLA	C	505	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	7 (10%)
27	LMG	D	407	-	49,49,55	0.76	0	57,57,63	1.31	4 (7%)
25	DGD	b	601	-	53,53,67	1.05	3 (5%)	67,67,81	1.32	7 (10%)
27	LMG	C	518	-	45,45,55	0.77	0	53,53,63	1.29	6 (11%)
30	SQD	b	602	-	46,47,54	1.01	4 (8%)	55,58,65	1.77	10 (18%)
27	LMG	a	402	-	42,42,55	0.83	0	50,50,63	1.25	3 (6%)
22	CLA	c	507	-	59,73,73	1.42	5 (8%)	67,113,113	1.53	9 (13%)
22	CLA	d	405	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	9 (13%)
22	CLA	c	520	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	9 (13%)
22	CLA	B	606	-	59,73,73	1.43	5 (8%)	67,113,113	1.44	10 (14%)
22	CLA	B	614	-	59,73,73	1.43	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
22	CLA	b	618	-	59,73,73	1.43	5 (8%)	67,113,113	1.48	9 (13%)
22	CLA	B	603	-	59,73,73	1.41	5 (8%)	67,113,113	1.54	10 (14%)
22	CLA	c	501	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	8 (11%)
27	LMG	D	411	-	46,46,55	0.76	1 (2%)	54,54,63	1.30	5 (9%)
22	CLA	H	101	-	59,73,73	1.43	5 (8%)	67,113,113	1.46	8 (11%)
24	BCR	B	617	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	9 (16%)
22	CLA	B	613	-	59,73,73	1.40	5 (8%)	67,113,113	1.48	8 (11%)
22	CLA	B	602	-	59,73,73	1.40	5 (8%)	67,113,113	1.46	8 (11%)
31	LMT	b	626	-	36,36,36	1.13	5 (13%)	47,47,47	0.96	1 (2%)
24	BCR	j	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.57	13 (23%)
27	LMG	B	621	-	49,49,55	0.77	1 (2%)	57,57,63	1.32	6 (10%)
27	LMG	d	411	-	46,46,55	0.78	1 (2%)	54,54,63	1.30	5 (9%)
22	CLA	A	405	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
24	BCR	A	407	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	7 (12%)
25	DGD	c	517	-	67,67,67	0.88	0	81,81,81	1.40	10 (12%)
25	DGD	d	409	-	64,64,67	0.93	1 (1%)	78,78,81	1.34	9 (11%)
23	PL9	j	101	-	35,35,55	1.00	2 (5%)	44,45,69	1.58	7 (15%)
22	CLA	b	608	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	7 (10%)
26	LHG	A	409	-	38,38,48	0.69	1 (2%)	41,44,54	1.19	3 (7%)
22	CLA	b	611	-	59,73,73	1.42	5 (8%)	67,113,113	1.45	7 (10%)
33	BCT	D	403	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	604	-	59,73,73	1.43	5 (8%)	67,113,113	1.47	7 (10%)
22	CLA	D	404	-	59,73,73	1.42	5 (8%)	67,113,113	1.43	8 (11%)
22	CLA	b	606	-	59,73,73	1.41	5 (8%)	67,113,113	1.45	9 (13%)
24	BCR	F	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
24	BCR	a	410	-	41,41,41	1.10	2 (4%)	56,56,56	1.21	7 (12%)
22	CLA	C	508	-	59,73,73	1.44	5 (8%)	67,113,113	1.43	8 (11%)
22	CLA	C	507	-	59,73,73	1.42	5 (8%)	67,113,113	1.53	9 (13%)
27	LMG	d	408	-	48,48,55	0.76	0	56,56,63	1.37	4 (7%)
29	OEX	a	414	1,3	0,15,15	0.00	-	-	-	-
22	CLA	D	405	-	59,73,73	1.42	5 (8%)	67,113,113	1.46	8 (11%)
24	BCR	B	616	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
30	SQD	B	622	-	42,43,54	1.05	3 (7%)	51,54,65	1.76	11 (21%)
22	CLA	C	511	-	59,73,73	1.42	5 (8%)	67,113,113	1.48	8 (11%)
25	DGD	C	515	-	54,54,67	0.97	2 (3%)	68,68,81	1.26	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	611	-	59,73,73	1.41	5 (8%)	67,113,113	1.50	9 (13%)
22	CLA	b	614	-	59,73,73	1.48	5 (8%)	67,113,113	1.55	9 (13%)
22	CLA	d	404	-	59,73,73	1.43	5 (8%)	67,113,113	1.43	9 (13%)
27	LMG	M	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.22	4 (8%)
22	CLA	C	504	-	59,73,73	1.42	5 (8%)	67,113,113	1.53	8 (11%)
22	CLA	C	501	-	59,73,73	1.42	4 (6%)	67,113,113	1.45	8 (11%)
22	CLA	C	512	-	59,73,73	1.42	5 (8%)	67,113,113	1.47	9 (13%)
24	BCR	b	622	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	10 (17%)
22	CLA	c	503	-	59,73,73	1.43	5 (8%)	67,113,113	1.49	8 (11%)
25	DGD	B	620	-	59,59,67	0.92	1 (1%)	73,73,81	1.33	8 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	505	-	3/3/20/25	17/37/135/135	-
32	PHO	a	407	-	-	12/53/103/103	0/5/6/6
22	CLA	c	505	-	3/3/20/25	17/37/135/135	-
22	CLA	a	408	-	3/3/20/25	8/37/135/135	-
34	HEM	f	101	5,6	-	0/6/54/54	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
31	LMT	D	410	-	-	2/17/57/61	0/2/2/2
27	LMG	C	521	-	-	20/43/63/70	0/1/1/1
22	CLA	C	510	3	3/3/20/25	17/37/135/135	-
23	PL9	D	406	-	-	12/53/73/73	0/1/1/1
26	LHG	C	519	-	-	16/41/41/53	-
22	CLA	B	601	-	3/3/20/25	14/37/135/135	-
22	CLA	b	610	-	3/3/20/25	8/37/135/135	-
27	LMG	c	518	-	-	22/40/60/70	0/1/1/1
30	SQD	a	401	-	-	14/49/69/69	0/1/1/1
27	LMG	E	101	-	-	17/39/59/70	0/1/1/1
27	LMG	l	101	-	-	25/46/66/70	0/1/1/1
22	CLA	b	605	-	3/3/20/25	15/37/135/135	-
25	DGD	c	516	-	-	20/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	506	-	3/3/20/25	13/37/135/135	-
25	DGD	c	515	-	-	19/42/82/95	0/2/2/2
22	CLA	C	502	-	3/3/20/25	11/37/135/135	-
22	CLA	a	405	-	3/3/20/25	14/37/135/135	-
25	DGD	A	408	-	-	14/45/85/95	0/2/2/2
25	DGD	C	517	-	-	20/55/95/95	0/2/2/2
25	DGD	D	409	-	-	34/52/92/95	0/2/2/2
24	BCR	g	101	-	-	6/29/63/63	0/2/2/2
34	HEM	V	201	16	-	2/6/54/54	-
32	PHO	d	401	-	-	14/53/103/103	0/5/6/6
31	LMT	b	604	-	-	5/21/61/61	0/2/2/2
22	CLA	C	503	-	3/3/20/25	15/37/135/135	-
31	LMT	B	623	-	-	3/21/61/61	0/2/2/2
22	CLA	c	509	-	3/3/20/25	16/37/135/135	-
22	CLA	c	502	-	3/3/20/25	11/37/135/135	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
32	PHO	D	402	-	-	12/53/103/103	0/5/6/6
24	BCR	c	521	-	-	6/29/63/63	0/2/2/2
22	CLA	h	101	-	3/3/20/25	19/37/135/135	-
22	CLA	b	609	-	3/3/20/25	14/37/135/135	-
32	PHO	D	401	-	-	13/53/103/103	0/5/6/6
22	CLA	b	613	-	3/3/20/25	18/37/135/135	-
31	LMT	i	102	-	-	3/21/61/61	0/2/2/2
22	CLA	A	404	-	3/3/20/25	8/37/135/135	-
27	LMG	i	101	-	-	18/38/58/70	0/1/1/1
31	LMT	b	627	-	-	3/21/61/61	0/2/2/2
22	CLA	B	615	-	3/3/20/25	18/37/135/135	-
22	CLA	b	619	-	3/3/20/25	19/37/135/135	-
22	CLA	b	612	-	3/3/20/25	11/37/135/135	-
24	BCR	b	621	-	-	8/29/63/63	0/2/2/2
22	CLA	B	609	-	3/3/20/25	18/37/135/135	-
22	CLA	A	402	-	3/3/20/25	8/37/135/135	-
31	LMT	b	603	-	-	3/21/61/61	0/2/2/2
24	BCR	B	619	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	B	628	-	-	4/21/61/61	0/2/2/2
22	CLA	C	506	-	3/3/20/25	13/37/135/135	-
30	SQD	f	103	-	-	12/40/60/69	0/1/1/1
24	BCR	f	102	-	-	6/29/63/63	0/2/2/2
22	CLA	a	406	-	3/3/20/25	8/37/135/135	-
22	CLA	c	512	-	3/3/20/25	18/37/135/135	-
23	PL9	d	406	-	-	12/53/73/73	0/1/1/1
26	LHG	c	519	-	-	17/41/41/53	-
24	BCR	J	102	-	-	7/29/63/63	0/2/2/2
22	CLA	C	509	-	3/3/20/25	16/37/135/135	-
24	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	b	607	-	3/3/20/25	7/37/135/135	-
22	CLA	B	604	-	3/3/20/25	14/37/135/135	-
31	LMT	I	102	-	-	3/21/61/61	0/2/2/2
27	LMG	D	408	-	-	22/43/63/70	0/1/1/1
27	LMG	e	101	-	-	19/39/59/70	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
23	PL9	J	101	-	-	9/29/49/73	0/1/1/1
27	LMG	A	410	-	-	28/46/66/70	0/1/1/1
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
22	CLA	B	608	-	3/3/20/25	11/37/135/135	-
27	LMG	I	101	-	-	18/38/58/70	0/1/1/1
31	LMT	B	627	-	-	3/21/61/61	0/2/2/2
27	LMG	m	101	-	-	16/37/57/70	0/1/1/1
22	CLA	b	615	-	3/3/20/25	12/37/135/135	-
27	LMG	c	522	-	-	20/43/63/70	0/1/1/1
27	LMG	d	411	-	-	15/41/61/70	0/1/1/1
22	CLA	B	602	-	3/3/20/25	14/37/135/135	-
31	LMT	d	410	-	-	0/17/57/61	0/2/2/2
24	BCR	b	623	-	-	5/29/63/63	0/2/2/2
22	CLA	c	511	-	3/3/20/25	19/37/135/135	-
34	HEM	F	101	5,6	-	0/6/54/54	-
30	SQD	A	413	-	-	19/46/66/69	0/1/1/1
22	CLA	C	507	-	3/3/20/25	14/37/135/135	-
27	LMG	b	625	-	-	14/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	504	-	3/3/20/25	19/37/135/135	-
27	LMG	A	415	-	-	15/37/57/70	0/1/1/1
22	CLA	A	403	-	3/3/20/25	14/37/135/135	-
25	DGD	B	625	-	-	19/41/81/95	0/2/2/2
22	CLA	a	404	-	3/3/20/25	8/37/135/135	-
31	LMT	B	624	-	-	3/21/61/61	0/2/2/2
30	SQD	d	402	-	-	14/38/58/69	0/1/1/1
22	CLA	B	612	-	3/3/20/25	15/37/135/135	-
31	LMT	M	103	-	-	0/21/61/61	0/2/2/2
25	DGD	b	624	-	-	18/47/87/95	0/2/2/2
26	LHG	a	412	-	-	12/43/43/53	-
22	CLA	b	616	-	3/3/20/25	15/37/135/135	-
30	SQD	A	414	-	-	12/49/69/69	0/1/1/1
34	HEM	v	201	16	-	2/6/54/54	-
23	PL9	a	409	-	-	17/41/61/73	0/1/1/1
24	BCR	H	102	-	-	7/29/63/63	0/2/2/2
22	CLA	B	610	-	3/3/20/25	9/37/135/135	-
30	SQD	F	103	-	-	12/40/60/69	0/1/1/1
24	BCR	C	513	-	-	5/29/63/63	0/2/2/2
22	CLA	c	510	3	3/3/20/25	17/37/135/135	-
22	CLA	c	520	-	3/3/20/25	10/37/135/135	-
27	LMG	d	407	-	-	24/44/64/70	0/1/1/1
30	SQD	B	626	-	-	14/42/62/69	0/1/1/1
25	DGD	a	411	-	-	13/45/85/95	0/2/2/2
30	SQD	a	415	-	-	19/46/66/69	0/1/1/1
24	BCR	x	101	-	-	7/29/63/63	0/2/2/2
24	BCR	c	513	-	-	5/29/63/63	0/2/2/2
25	DGD	C	516	-	-	20/51/91/95	0/2/2/2
22	CLA	C	520	-	3/3/20/25	12/37/135/135	-
24	BCR	c	514	-	-	5/29/63/63	0/2/2/2
24	BCR	b	620	-	-	2/29/63/63	0/2/2/2
22	CLA	c	508	-	3/3/20/25	14/37/135/135	-
22	CLA	B	607	-	3/3/20/25	12/37/135/135	-
27	LMG	D	407	-	-	24/44/64/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	b	601	-	-	19/41/81/95	0/2/2/2
27	LMG	C	518	-	-	22/40/60/70	0/1/1/1
30	SQD	b	602	-	-	13/42/62/69	0/1/1/1
27	LMG	a	402	-	-	16/37/57/70	0/1/1/1
22	CLA	c	507	-	3/3/20/25	14/37/135/135	-
22	CLA	d	405	-	2/2/20/25	6/37/135/135	-
22	CLA	b	617	-	3/3/20/25	16/37/135/135	-
22	CLA	B	606	-	3/3/20/25	8/37/135/135	-
22	CLA	B	614	-	3/3/20/25	10/37/135/135	-
22	CLA	b	618	-	3/3/20/25	10/37/135/135	-
22	CLA	C	501	-	3/3/20/25	14/37/135/135	-
22	CLA	c	501	-	3/3/20/25	13/37/135/135	-
27	LMG	D	411	-	-	15/41/61/70	0/1/1/1
22	CLA	H	101	-	3/3/20/25	18/37/135/135	-
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
22	CLA	B	613	-	3/3/20/25	16/37/135/135	-
24	BCR	B	618	-	-	3/29/63/63	0/2/2/2
31	LMT	b	626	-	-	2/21/61/61	0/2/2/2
24	BCR	j	102	-	-	7/29/63/63	0/2/2/2
27	LMG	B	621	-	-	14/44/64/70	0/1/1/1
22	CLA	C	512	-	3/3/20/25	19/37/135/135	-
22	CLA	A	405	-	3/3/20/25	8/37/135/135	-
24	BCR	A	407	-	-	4/29/63/63	0/2/2/2
25	DGD	c	517	-	-	20/55/95/95	0/2/2/2
25	DGD	d	409	-	-	34/52/92/95	0/2/2/2
23	PL9	j	101	-	-	8/29/49/73	0/1/1/1
22	CLA	b	608	-	3/3/20/25	15/37/135/135	-
26	LHG	A	409	-	-	12/43/43/53	-
22	CLA	b	611	-	3/3/20/25	12/37/135/135	-
22	CLA	D	404	-	3/3/20/25	13/37/135/135	-
22	CLA	C	508	-	3/3/20/25	16/37/135/135	-
22	CLA	b	606	-	3/3/20/25	14/37/135/135	-
24	BCR	F	102	-	-	6/29/63/63	0/2/2/2
24	BCR	a	410	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	-	3/3/20/25	12/37/135/135	-
27	LMG	d	408	-	-	20/43/63/70	0/1/1/1
22	CLA	D	405	-	3/3/20/25	6/37/135/135	-
24	BCR	B	616	-	-	2/29/63/63	0/2/2/2
30	SQD	B	622	-	-	14/38/58/69	0/1/1/1
22	CLA	C	511	-	3/3/20/25	19/37/135/135	-
25	DGD	C	515	-	-	19/42/82/95	0/2/2/2
22	CLA	B	611	-	3/3/20/25	12/37/135/135	-
22	CLA	b	614	-	3/3/20/25	9/37/135/135	-
22	CLA	d	404	-	3/3/20/25	12/37/135/135	-
27	LMG	M	101	-	-	18/37/57/70	0/1/1/1
22	CLA	C	504	-	3/3/20/25	19/37/135/135	-
22	CLA	B	603	-	3/3/20/25	8/37/135/135	-
24	BCR	b	622	-	-	3/29/63/63	0/2/2/2
22	CLA	c	503	-	3/3/20/25	15/37/135/135	-
25	DGD	B	620	-	-	18/47/87/95	0/2/2/2

All (603) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	402	CLA	C4B-NB	7.82	1.42	1.35
22	b	605	CLA	C4B-NB	7.82	1.42	1.35
22	c	509	CLA	C4B-NB	7.81	1.42	1.35
22	a	404	CLA	C4B-NB	7.80	1.42	1.35
22	c	508	CLA	C4B-NB	7.72	1.42	1.35
22	C	508	CLA	C4B-NB	7.71	1.42	1.35
22	c	512	CLA	C4B-NB	7.69	1.42	1.35
22	B	601	CLA	C4B-NB	7.68	1.42	1.35
22	c	505	CLA	C4B-NB	7.67	1.42	1.35
22	B	610	CLA	C4B-NB	7.67	1.42	1.35
22	B	615	CLA	C4B-NB	7.66	1.42	1.35
22	C	509	CLA	C4B-NB	7.66	1.42	1.35
22	c	511	CLA	C4B-NB	7.66	1.42	1.35
22	c	503	CLA	C4B-NB	7.64	1.42	1.35
22	b	619	CLA	C4B-NB	7.63	1.42	1.35
22	C	505	CLA	C4B-NB	7.63	1.42	1.35
22	B	608	CLA	C4B-NB	7.62	1.42	1.35
22	c	504	CLA	C4B-NB	7.61	1.42	1.35
22	b	612	CLA	C4B-NB	7.61	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	C4B-NB	7.61	1.42	1.35
22	b	618	CLA	C4B-NB	7.60	1.42	1.35
22	B	604	CLA	C4B-NB	7.59	1.42	1.35
22	d	405	CLA	C4B-NB	7.58	1.42	1.35
22	B	614	CLA	C4B-NB	7.58	1.42	1.35
22	c	520	CLA	C4B-NB	7.58	1.42	1.35
22	A	405	CLA	C4B-NB	7.57	1.42	1.35
22	c	510	CLA	C4B-NB	7.57	1.42	1.35
22	C	507	CLA	C4B-NB	7.55	1.41	1.35
22	B	611	CLA	C4B-NB	7.55	1.41	1.35
22	b	610	CLA	C4B-NB	7.54	1.41	1.35
22	a	405	CLA	C4B-NB	7.54	1.41	1.35
22	H	101	CLA	C4B-NB	7.52	1.41	1.35
22	a	406	CLA	C4B-NB	7.52	1.41	1.35
22	C	511	CLA	C4B-NB	7.52	1.41	1.35
22	A	403	CLA	C4B-NB	7.51	1.41	1.35
22	c	507	CLA	C4B-NB	7.51	1.41	1.35
22	B	609	CLA	C4B-NB	7.50	1.41	1.35
22	a	408	CLA	C4B-NB	7.50	1.41	1.35
22	B	606	CLA	C4B-NB	7.50	1.41	1.35
22	b	611	CLA	C4B-NB	7.50	1.41	1.35
22	D	405	CLA	C4B-NB	7.50	1.41	1.35
22	b	615	CLA	C4B-NB	7.49	1.41	1.35
22	b	609	CLA	C4B-NB	7.48	1.41	1.35
22	b	607	CLA	C4B-NB	7.48	1.41	1.35
22	C	504	CLA	C4B-NB	7.48	1.41	1.35
22	C	512	CLA	C4B-NB	7.46	1.41	1.35
22	d	404	CLA	C4B-NB	7.45	1.41	1.35
22	h	101	CLA	C4B-NB	7.44	1.41	1.35
22	C	510	CLA	C4B-NB	7.44	1.41	1.35
22	b	608	CLA	C4B-NB	7.44	1.41	1.35
22	c	502	CLA	C4B-NB	7.44	1.41	1.35
22	C	520	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	7.41	1.41	1.35
22	D	404	CLA	C4B-NB	7.41	1.41	1.35
22	b	617	CLA	C4B-NB	7.40	1.41	1.35
22	B	605	CLA	C4B-NB	7.39	1.41	1.35
22	b	606	CLA	C4B-NB	7.39	1.41	1.35
22	C	501	CLA	C4B-NB	7.39	1.41	1.35
22	B	603	CLA	C4B-NB	7.38	1.41	1.35
22	b	613	CLA	C4B-NB	7.38	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C4B-NB	7.38	1.41	1.35
22	C	503	CLA	C4B-NB	7.38	1.41	1.35
22	A	404	CLA	C4B-NB	7.37	1.41	1.35
22	B	612	CLA	C4B-NB	7.37	1.41	1.35
22	C	502	CLA	C4B-NB	7.37	1.41	1.35
22	c	506	CLA	C4B-NB	7.36	1.41	1.35
22	B	613	CLA	C4B-NB	7.35	1.41	1.35
22	C	506	CLA	C4B-NB	7.32	1.41	1.35
22	B	602	CLA	C4B-NB	7.28	1.41	1.35
34	v	201	HEM	C3D-C2D	5.64	1.54	1.37
34	V	201	HEM	C3D-C2D	5.62	1.54	1.37
34	f	101	HEM	C3D-C2D	5.45	1.53	1.37
34	F	101	HEM	C3D-C2D	5.45	1.53	1.37
34	F	101	HEM	C3B-C2B	-4.86	1.33	1.40
34	f	101	HEM	C3B-C2B	-4.82	1.33	1.40
34	V	201	HEM	C3C-C2C	-4.57	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	C3B-C2B	-3.77	1.35	1.40
34	v	201	HEM	C3B-C2B	-3.76	1.35	1.40
24	g	101	BCR	C1-C6	-3.75	1.48	1.53
34	v	201	HEM	C3C-CAC	3.75	1.55	1.47
34	V	201	HEM	C3C-CAC	3.73	1.55	1.47
34	F	101	HEM	C3C-C2C	-3.71	1.35	1.40
24	y	101	BCR	C1-C6	-3.70	1.48	1.53
22	b	614	CLA	CMB-C2B	-3.67	1.44	1.51
23	d	406	PL9	C7-C3	-3.65	1.47	1.51
34	f	101	HEM	C3C-C2C	-3.65	1.35	1.40
24	H	102	BCR	C1-C6	-3.63	1.48	1.53
24	x	101	BCR	C1-C6	-3.62	1.48	1.53
22	B	610	CLA	CMB-C2B	-3.60	1.44	1.51
24	F	102	BCR	C1-C6	-3.59	1.48	1.53
24	f	102	BCR	C1-C6	-3.57	1.48	1.53
34	F	101	HEM	C3B-CAB	3.53	1.55	1.47
23	a	409	PL9	C7-C3	-3.52	1.47	1.51
34	f	101	HEM	C3B-CAB	3.52	1.55	1.47
23	D	406	PL9	C7-C3	-3.43	1.47	1.51
32	a	407	PHO	C3B-C4B	3.39	1.50	1.43
32	D	402	PHO	C3B-C4B	3.38	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	BCR	C1-C6	-3.35	1.49	1.53
24	c	514	BCR	C1-C6	-3.34	1.49	1.53
24	b	620	BCR	C1-C6	-3.33	1.49	1.53
24	B	616	BCR	C1-C6	-3.32	1.49	1.53
22	b	612	CLA	CHC-C1C	3.28	1.43	1.35
22	B	608	CLA	CHC-C1C	3.26	1.43	1.35
23	J	101	PL9	C7-C3	-3.25	1.48	1.51
22	B	613	CLA	CHC-C1C	3.25	1.43	1.35
32	d	401	PHO	C3B-C4B	3.25	1.50	1.43
24	g	101	BCR	C30-C25	-3.24	1.49	1.53
22	b	611	CLA	CHC-C1C	3.24	1.43	1.35
32	D	401	PHO	C3B-C4B	3.24	1.50	1.43
24	y	101	BCR	C30-C25	-3.23	1.49	1.53
24	J	102	BCR	C30-C25	-3.23	1.49	1.53
22	H	101	CLA	CHC-C1C	3.23	1.43	1.35
24	j	102	BCR	C30-C25	-3.22	1.49	1.53
22	b	617	CLA	CHC-C1C	3.22	1.43	1.35
22	c	502	CLA	CHC-C1C	3.22	1.43	1.35
22	c	512	CLA	CHC-C1C	3.21	1.43	1.35
22	h	101	CLA	CHC-C1C	3.21	1.43	1.35
24	b	622	BCR	C30-C25	-3.21	1.49	1.53
22	b	606	CLA	CHC-C1C	3.20	1.43	1.35
24	b	621	BCR	C1-C6	-3.19	1.49	1.53
24	C	513	BCR	C1-C6	-3.19	1.49	1.53
22	C	511	CLA	CHC-C1C	3.19	1.43	1.35
24	B	617	BCR	C1-C6	-3.19	1.49	1.53
22	a	404	CLA	CHC-C1C	3.18	1.43	1.35
22	c	505	CLA	CHC-C1C	3.18	1.43	1.35
24	F	102	BCR	C30-C25	-3.18	1.49	1.53
22	c	511	CLA	CHC-C1C	3.18	1.43	1.35
22	B	607	CLA	CHC-C1C	3.17	1.43	1.35
23	A	406	PL9	C7-C3	-3.17	1.48	1.51
22	c	509	CLA	CHC-C1C	3.16	1.43	1.35
24	c	513	BCR	C1-C6	-3.16	1.49	1.53
22	d	404	CLA	CHC-C1C	3.16	1.43	1.35
24	B	618	BCR	C30-C25	-3.16	1.49	1.53
30	B	626	SQD	O48-C23	3.16	1.42	1.33
22	C	512	CLA	CHC-C1C	3.16	1.43	1.35
22	b	618	CLA	CHC-C1C	3.16	1.43	1.35
30	b	602	SQD	O48-C23	3.16	1.42	1.33
22	B	603	CLA	CHC-C1C	3.15	1.43	1.35
22	B	602	CLA	CHC-C1C	3.15	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	CHC-C1C	3.15	1.43	1.35
22	c	507	CLA	CHC-C1C	3.15	1.43	1.35
22	a	408	CLA	CHC-C1C	3.15	1.43	1.35
22	d	405	CLA	CHC-C1C	3.15	1.43	1.35
24	K	102	BCR	C30-C25	-3.15	1.49	1.53
22	D	404	CLA	CHC-C1C	3.15	1.43	1.35
30	a	401	SQD	O48-C23	3.15	1.42	1.33
22	b	616	CLA	CHC-C1C	3.15	1.43	1.35
22	a	406	CLA	CHC-C1C	3.14	1.43	1.35
22	c	508	CLA	CHC-C1C	3.14	1.43	1.35
23	j	101	PL9	C7-C3	-3.14	1.48	1.51
22	C	505	CLA	CHC-C1C	3.14	1.43	1.35
30	A	414	SQD	O48-C23	3.14	1.42	1.33
30	d	402	SQD	O48-C23	3.14	1.42	1.33
22	C	520	CLA	CHC-C1C	3.14	1.43	1.35
22	c	503	CLA	CHC-C1C	3.14	1.43	1.35
22	b	607	CLA	CHC-C1C	3.14	1.43	1.35
22	C	508	CLA	CHC-C1C	3.14	1.43	1.35
22	B	614	CLA	CHC-C1C	3.14	1.43	1.35
24	b	623	BCR	C30-C25	-3.14	1.49	1.53
30	B	622	SQD	O48-C23	3.13	1.42	1.33
22	A	404	CLA	CHC-C1C	3.13	1.43	1.35
22	C	509	CLA	CHC-C1C	3.13	1.43	1.35
24	B	619	BCR	C30-C25	-3.13	1.49	1.53
22	c	504	CLA	CHC-C1C	3.13	1.43	1.35
30	f	103	SQD	O48-C23	3.12	1.42	1.33
22	c	510	CLA	CHC-C1C	3.12	1.43	1.35
22	C	504	CLA	CHC-C1C	3.12	1.43	1.35
22	C	503	CLA	CHC-C1C	3.12	1.43	1.35
22	B	606	CLA	CHC-C1C	3.12	1.43	1.35
30	F	103	SQD	O48-C23	3.12	1.42	1.33
24	f	102	BCR	C30-C25	-3.12	1.49	1.53
22	C	510	CLA	CHC-C1C	3.11	1.42	1.35
22	A	403	CLA	CHC-C1C	3.11	1.42	1.35
22	b	608	CLA	CHC-C1C	3.11	1.42	1.35
22	b	605	CLA	CHC-C1C	3.11	1.42	1.35
22	C	502	CLA	CHC-C1C	3.11	1.42	1.35
22	b	613	CLA	CHC-C1C	3.11	1.42	1.35
22	B	612	CLA	CHC-C1C	3.11	1.42	1.35
22	B	604	CLA	CHC-C1C	3.11	1.42	1.35
22	C	506	CLA	CHC-C1C	3.10	1.42	1.35
24	c	521	BCR	C30-C25	-3.10	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	CHC-C1C	3.10	1.42	1.35
22	c	506	CLA	CHC-C1C	3.10	1.42	1.35
24	a	410	BCR	C30-C25	-3.09	1.49	1.53
22	B	601	CLA	CHC-C1C	3.09	1.42	1.35
22	c	520	CLA	CHC-C1C	3.09	1.42	1.35
22	c	501	CLA	CHC-C1C	3.09	1.42	1.35
30	a	415	SQD	O48-C23	3.08	1.42	1.33
24	B	618	BCR	C1-C6	-3.08	1.49	1.53
24	A	407	BCR	C30-C25	-3.08	1.49	1.53
22	B	605	CLA	CHC-C1C	3.08	1.42	1.35
22	D	405	CLA	CHC-C1C	3.08	1.42	1.35
24	B	619	BCR	C1-C6	-3.08	1.49	1.53
24	b	623	BCR	C1-C6	-3.08	1.49	1.53
22	A	402	CLA	CHC-C1C	3.08	1.42	1.35
22	b	615	CLA	CHC-C1C	3.08	1.42	1.35
24	b	620	BCR	C30-C25	-3.08	1.49	1.53
22	b	610	CLA	CHC-C1C	3.07	1.42	1.35
22	A	405	CLA	CHC-C1C	3.07	1.42	1.35
22	C	501	CLA	CHC-C1C	3.07	1.42	1.35
24	b	622	BCR	C1-C6	-3.07	1.49	1.53
22	C	507	CLA	CHC-C1C	3.06	1.42	1.35
22	b	619	CLA	CHC-C1C	3.06	1.42	1.35
24	a	410	BCR	C1-C6	-3.06	1.49	1.53
30	A	413	SQD	O48-C23	3.05	1.42	1.33
22	B	611	CLA	CHC-C1C	3.05	1.42	1.35
24	B	616	BCR	C30-C25	-3.04	1.49	1.53
22	B	615	CLA	CHC-C1C	3.03	1.42	1.35
22	a	405	CLA	CHC-C1C	3.02	1.42	1.35
24	A	407	BCR	C1-C6	-3.02	1.49	1.53
32	D	402	PHO	CHC-C1C	3.00	1.44	1.38
32	a	407	PHO	CHC-C1C	3.00	1.44	1.38
24	K	102	BCR	C1-C6	-3.00	1.49	1.53
24	H	102	BCR	C30-C25	-2.98	1.49	1.53
24	C	513	BCR	C30-C25	-2.98	1.49	1.53
24	C	514	BCR	C30-C25	-2.97	1.49	1.53
24	x	101	BCR	C30-C25	-2.96	1.49	1.53
25	b	601	DGD	C1E-C2E	2.96	1.61	1.52
24	c	521	BCR	C1-C6	-2.94	1.49	1.53
30	A	414	SQD	O47-C7	2.93	1.42	1.34
24	c	514	BCR	C30-C25	-2.93	1.49	1.53
30	d	402	SQD	O47-C7	2.92	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)
30	a	401	SQD	O47-C7	2.89	1.42	1.34
30	F	103	SQD	O47-C7	2.88	1.42	1.34
30	B	622	SQD	O47-C7	2.87	1.42	1.34
32	d	401	PHO	CHC-C1C	2.86	1.44	1.38
25	B	625	DGD	C1E-C2E	2.86	1.60	1.52
30	a	415	SQD	O47-C7	2.86	1.42	1.34
32	D	401	PHO	CHC-C1C	2.85	1.44	1.38
30	B	626	SQD	O47-C7	2.85	1.42	1.34
30	b	602	SQD	O47-C7	2.85	1.42	1.34
30	f	103	SQD	O47-C7	2.82	1.42	1.34
24	c	513	BCR	C30-C25	-2.81	1.49	1.53
22	B	610	CLA	CHC-C1C	2.80	1.42	1.35
22	c	512	CLA	C1D-C2D	2.79	1.48	1.42
22	b	614	CLA	CHC-C1C	2.78	1.42	1.35
24	J	102	BCR	C1-C6	-2.77	1.50	1.53
23	D	406	PL9	C3-C4	-2.77	1.45	1.49
22	b	610	CLA	C1D-C2D	2.76	1.48	1.42
24	j	102	BCR	C1-C6	-2.76	1.50	1.53
24	b	621	BCR	C30-C25	-2.76	1.50	1.53
22	c	520	CLA	C1D-C2D	2.75	1.48	1.42
24	B	617	BCR	C30-C25	-2.75	1.50	1.53
32	a	407	PHO	C4C-NC	2.74	1.42	1.36
22	a	405	CLA	C1D-C2D	2.74	1.48	1.42
23	a	409	PL9	C3-C4	-2.74	1.45	1.49
22	B	609	CLA	C1D-C2D	2.74	1.48	1.42
22	c	501	CLA	C1D-C2D	2.74	1.48	1.42
22	A	403	CLA	C1D-C2D	2.74	1.48	1.42
22	C	501	CLA	C1D-C2D	2.74	1.48	1.42
22	b	613	CLA	C1D-C2D	2.74	1.48	1.42
22	b	608	CLA	C1D-C2D	2.73	1.48	1.42
22	C	512	CLA	C1D-C2D	2.73	1.48	1.42
32	D	402	PHO	C4C-NC	2.73	1.42	1.36
22	a	404	CLA	C1D-C2D	2.72	1.48	1.42
22	B	604	CLA	C1D-C2D	2.71	1.48	1.42
22	c	505	CLA	C1D-C2D	2.71	1.48	1.42
22	B	615	CLA	C1D-C2D	2.71	1.48	1.42
22	B	606	CLA	C1D-C2D	2.70	1.48	1.42
22	c	510	CLA	C1D-C2D	2.70	1.48	1.42
22	C	510	CLA	C1D-C2D	2.70	1.48	1.42
22	b	618	CLA	C1D-C2D	2.70	1.48	1.42
32	d	401	PHO	C4C-NC	2.69	1.42	1.36
22	b	605	CLA	C1D-C2D	2.69	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	508	CLA	C1D-C2D	2.69	1.48	1.42
22	b	609	CLA	C1D-C2D	2.69	1.48	1.42
22	A	402	CLA	C1D-C2D	2.69	1.48	1.42
22	D	405	CLA	C1D-C2D	2.68	1.48	1.42
22	A	404	CLA	C1D-C2D	2.68	1.48	1.42
22	C	520	CLA	C1D-C2D	2.68	1.48	1.42
22	c	506	CLA	C1D-C2D	2.67	1.48	1.42
22	b	619	CLA	C1D-C2D	2.67	1.48	1.42
22	c	503	CLA	C1D-C2D	2.67	1.48	1.42
22	a	406	CLA	C1D-C2D	2.67	1.48	1.42
22	b	606	CLA	C1D-C2D	2.67	1.48	1.42
32	D	401	PHO	C4C-NC	2.67	1.42	1.36
22	B	613	CLA	C1D-C2D	2.66	1.48	1.42
22	B	605	CLA	C1D-C2D	2.66	1.48	1.42
22	b	616	CLA	C1D-C2D	2.66	1.48	1.42
22	C	509	CLA	C1D-C2D	2.66	1.48	1.42
22	H	101	CLA	C1D-C2D	2.65	1.48	1.42
32	d	401	PHO	C1A-NA	2.65	1.42	1.37
22	C	505	CLA	C1D-C2D	2.65	1.48	1.42
32	D	401	PHO	C1A-NA	2.65	1.42	1.37
22	C	507	CLA	C1D-C2D	2.65	1.48	1.42
22	d	405	CLA	C1D-C2D	2.65	1.48	1.42
22	B	614	CLA	C1D-C2D	2.65	1.48	1.42
32	a	407	PHO	C1A-NA	2.65	1.42	1.37
22	B	612	CLA	C1D-C2D	2.65	1.48	1.42
22	b	617	CLA	C1D-C2D	2.65	1.48	1.42
22	B	601	CLA	C1D-C2D	2.64	1.48	1.42
22	A	405	CLA	C1D-C2D	2.64	1.48	1.42
32	D	402	PHO	C1A-NA	2.64	1.42	1.37
22	C	508	CLA	C1D-C2D	2.63	1.48	1.42
22	c	507	CLA	C1D-C2D	2.63	1.48	1.42
22	c	509	CLA	C1D-C2D	2.62	1.48	1.42
22	C	506	CLA	C1D-C2D	2.62	1.48	1.42
31	d	410	LMT	O3'-C3'	-2.62	1.36	1.43
22	B	608	CLA	C1D-C2D	2.61	1.48	1.42
22	a	408	CLA	C1D-C2D	2.61	1.48	1.42
22	C	503	CLA	C1D-C2D	2.61	1.48	1.42
31	b	627	LMT	O3'-C3'	-2.61	1.36	1.43
23	d	406	PL9	C3-C4	-2.61	1.45	1.49
31	D	410	LMT	O3'-C3'	-2.60	1.36	1.43
22	B	607	CLA	C1D-C2D	2.60	1.48	1.42
22	C	507	CLA	CMB-C2B	-2.60	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	C1D-C2D	2.60	1.48	1.42
31	M	102	LMT	O3'-C3'	-2.60	1.36	1.43
31	B	624	LMT	O3'-C3'	-2.59	1.36	1.43
22	h	101	CLA	C1D-C2D	2.59	1.48	1.42
22	B	610	CLA	C1D-C2D	2.59	1.48	1.42
22	b	614	CLA	C1D-C2D	2.59	1.48	1.42
31	M	103	LMT	O3'-C3'	-2.58	1.36	1.43
22	b	612	CLA	C1D-C2D	2.57	1.48	1.42
22	C	511	CLA	C1D-C2D	2.57	1.48	1.42
31	b	603	LMT	O3'-C3'	-2.57	1.36	1.43
22	B	602	CLA	C1D-C2D	2.57	1.48	1.42
22	C	502	CLA	C1D-C2D	2.57	1.48	1.42
22	c	511	CLA	C1D-C2D	2.57	1.48	1.42
22	b	611	CLA	C1D-C2D	2.57	1.48	1.42
22	c	507	CLA	CMB-C2B	-2.57	1.46	1.51
31	b	626	LMT	O3'-C3'	-2.56	1.36	1.43
31	i	102	LMT	O3'-C3'	-2.56	1.36	1.43
31	I	102	LMT	O3'-C3'	-2.56	1.36	1.43
22	d	404	CLA	C1D-C2D	2.54	1.48	1.42
22	c	502	CLA	C1D-C2D	2.54	1.48	1.42
31	B	627	LMT	O3'-C3'	-2.54	1.37	1.43
31	B	623	LMT	O3'-C3'	-2.53	1.37	1.43
22	B	603	CLA	C1D-C2D	2.52	1.48	1.42
31	b	604	LMT	O3'-C3'	-2.51	1.37	1.43
22	D	404	CLA	C1D-C2D	2.51	1.48	1.42
23	A	406	PL9	C3-C4	-2.50	1.45	1.49
22	a	404	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	615	CLA	C1D-C2D	2.47	1.48	1.42
22	c	509	CLA	CMB-C2B	-2.47	1.46	1.51
22	A	403	CLA	CMB-C2B	-2.46	1.46	1.51
31	B	628	LMT	O3'-C3'	-2.46	1.37	1.43
22	c	504	CLA	C1D-C2D	2.46	1.48	1.42
22	B	611	CLA	C1D-C2D	2.46	1.48	1.42
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	B	601	CLA	CMB-C2B	-2.45	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.45	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.44	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.44	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.44	1.46	1.51
25	C	515	DGD	O2G-C2G	-2.44	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	607	CLA	CMB-C2B	-2.44	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	520	CLA	CMB-C2B	-2.43	1.46	1.51
22	d	404	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.43	1.46	1.51
22	C	520	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	625	DGD	C4D-C5D	2.42	1.58	1.53
22	a	408	CLA	CMB-C2B	-2.42	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.42	1.46	1.51
22	D	404	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.41	1.46	1.51
22	A	405	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	504	CLA	C1D-C2D	2.41	1.48	1.42
22	b	616	CLA	CMB-C2B	-2.40	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	608	CLA	CMB-C2B	-2.40	1.46	1.51
32	a	407	PHO	CHD-C1D	2.40	1.43	1.38
22	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.39	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.39	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.39	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.39	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.39	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.39	1.46	1.51
22	h	101	CLA	CMB-C2B	-2.39	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CMB-C2B	-2.38	1.46	1.51
22	c	504	CLA	CMB-C2B	-2.38	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.38	1.46	1.51
22	D	405	CLA	CMB-C2B	-2.38	1.46	1.51
32	D	401	PHO	C1C-NC	-2.38	1.33	1.38
22	C	506	CLA	CMB-C2B	-2.38	1.46	1.51
32	D	402	PHO	CHD-C1D	2.38	1.43	1.38
22	b	617	CLA	CMB-C2B	-2.38	1.46	1.51
32	a	407	PHO	C4C-C3C	2.38	1.49	1.45
22	C	511	CLA	CMB-C2B	-2.38	1.46	1.51
32	D	401	PHO	C4C-C3C	2.37	1.49	1.45
31	I	102	LMT	O2B-C2B	-2.37	1.37	1.43
22	B	611	CLA	CMD-C2D	-2.37	1.45	1.51
22	B	611	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.37	1.46	1.51
22	b	615	CLA	CMB-C2B	-2.37	1.46	1.51
32	a	407	PHO	C1C-NC	-2.36	1.33	1.38
32	d	401	PHO	C1C-NC	-2.36	1.33	1.38
31	I	102	LMT	O2'-C2'	-2.36	1.37	1.43
22	b	612	CLA	CMB-C2B	-2.36	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.35	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.35	1.46	1.51
32	D	402	PHO	C4C-C3C	2.34	1.49	1.45
32	D	402	PHO	C1C-NC	-2.34	1.33	1.38
31	i	102	LMT	O2B-C2B	-2.33	1.37	1.43
22	b	606	CLA	CMB-C2B	-2.33	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.32	1.46	1.51
22	b	615	CLA	CMD-C2D	-2.32	1.46	1.51
31	i	102	LMT	O2'-C2'	-2.31	1.37	1.43
31	M	103	LMT	O3B-C3B	-2.30	1.37	1.43
31	b	604	LMT	O3B-C3B	-2.29	1.37	1.43
32	D	401	PHO	CHD-C1D	2.29	1.43	1.38
31	b	626	LMT	O2'-C2'	-2.29	1.37	1.43
31	I	102	LMT	O3B-C3B	-2.28	1.37	1.43
31	b	627	LMT	O3B-C3B	-2.28	1.37	1.43
25	c	515	DGD	O2G-C2G	-2.28	1.40	1.46
31	B	628	LMT	O3B-C3B	-2.28	1.37	1.43
31	b	603	LMT	O3B-C3B	-2.27	1.37	1.43
22	b	614	CLA	C3B-C2B	-2.27	1.37	1.40
31	B	627	LMT	O2B-C2B	-2.27	1.37	1.43
31	B	623	LMT	O2'-C2'	-2.27	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	103	LMT	O2'-C2'	-2.26	1.37	1.43
31	D	410	LMT	O3B-C3B	-2.26	1.37	1.43
32	d	401	PHO	C4C-C3C	2.26	1.49	1.45
31	M	102	LMT	O3B-C3B	-2.26	1.37	1.43
31	B	628	LMT	O2'-C2'	-2.26	1.37	1.43
31	B	624	LMT	O3B-C3B	-2.26	1.37	1.43
31	b	603	LMT	O2'-C2'	-2.26	1.37	1.43
23	a	409	PL9	C53-C6	-2.25	1.46	1.50
31	M	102	LMT	O2'-C2'	-2.25	1.37	1.43
31	b	603	LMT	O2B-C2B	-2.25	1.37	1.43
31	i	102	LMT	O3B-C3B	-2.25	1.37	1.43
31	B	627	LMT	O2'-C2'	-2.25	1.37	1.43
22	c	504	CLA	CMD-C2D	-2.25	1.46	1.51
31	B	628	LMT	O2B-C2B	-2.24	1.37	1.43
31	d	410	LMT	O3B-C3B	-2.24	1.37	1.43
31	B	623	LMT	O3B-C3B	-2.24	1.37	1.43
31	B	627	LMT	O3B-C3B	-2.23	1.37	1.43
31	M	103	LMT	O2B-C2B	-2.23	1.37	1.43
22	B	610	CLA	C3B-C2B	-2.23	1.37	1.40
31	B	624	LMT	O2'-C2'	-2.23	1.37	1.43
31	b	626	LMT	O3B-C3B	-2.22	1.37	1.43
22	C	504	CLA	CMD-C2D	-2.22	1.46	1.51
27	b	625	LMG	C4-C5	2.21	1.57	1.53
31	D	410	LMT	O2B-C2B	-2.21	1.37	1.43
22	c	509	CLA	CMD-C2D	-2.21	1.46	1.51
31	M	102	LMT	O2B-C2B	-2.21	1.37	1.43
27	B	621	LMG	C4-C5	2.21	1.57	1.53
25	d	409	DGD	C1D-C2D	2.21	1.58	1.52
31	b	604	LMT	O2'-C2'	-2.21	1.37	1.43
31	D	410	LMT	O2'-C2'	-2.21	1.37	1.43
31	b	626	LMT	O2B-C2B	-2.21	1.37	1.43
25	B	625	DGD	C3G-C2G	2.20	1.57	1.50
27	M	101	LMG	C4-C5	2.20	1.57	1.53
31	d	410	LMT	O2B-C2B	-2.20	1.37	1.43
30	B	626	SQD	O2-C2	-2.19	1.37	1.43
30	b	602	SQD	O2-C2	-2.19	1.37	1.43
22	b	611	CLA	CMD-C2D	-2.19	1.46	1.51
31	b	627	LMT	O2'-C2'	-2.19	1.37	1.43
31	b	604	LMT	O2B-C2B	-2.19	1.37	1.43
26	a	412	LHG	O7-C5	-2.18	1.41	1.46
27	D	411	LMG	O7-C8	-2.18	1.41	1.46
23	D	406	PL9	C6-C1	-2.17	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	601	DGD	C4D-C5D	2.17	1.57	1.53
22	C	509	CLA	CMD-C2D	-2.17	1.46	1.51
26	c	519	LHG	P-O6	2.17	1.68	1.59
31	B	623	LMT	O2B-C2B	-2.17	1.37	1.43
22	B	603	CLA	CMD-C2D	-2.16	1.46	1.51
31	d	410	LMT	O2'-C2'	-2.16	1.37	1.43
22	A	402	CLA	CMD-C2D	-2.16	1.46	1.51
25	c	516	DGD	O2G-C2G	-2.15	1.41	1.46
22	B	607	CLA	CMD-C2D	-2.15	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.15	1.46	1.51
34	V	201	HEM	CAA-C2A	2.14	1.55	1.52
32	D	401	PHO	C4B-NB	2.14	1.41	1.36
32	d	401	PHO	CHD-C1D	2.13	1.42	1.38
22	a	404	CLA	CMD-C2D	-2.13	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.13	1.46	1.51
32	D	402	PHO	C4B-NB	2.12	1.41	1.36
22	A	404	CLA	CMD-C2D	-2.12	1.46	1.51
30	a	401	SQD	O3-C3	-2.11	1.38	1.43
27	m	101	LMG	C4-C5	2.11	1.57	1.53
22	B	615	CLA	CMD-C2D	-2.11	1.46	1.51
32	a	407	PHO	C4B-NB	2.11	1.41	1.36
30	A	414	SQD	O3-C3	-2.11	1.38	1.43
25	C	516	DGD	O2G-C2G	-2.11	1.41	1.46
25	C	515	DGD	O1G-C1G	-2.10	1.40	1.45
22	b	619	CLA	CMD-C2D	-2.10	1.46	1.51
22	C	502	CLA	CMD-C2D	-2.10	1.46	1.51
31	B	627	LMT	O4'-C4B	-2.10	1.38	1.43
22	C	508	CLA	CMD-C2D	-2.10	1.46	1.51
22	B	602	CLA	CMD-C2D	-2.10	1.46	1.51
23	A	406	PL9	C53-C6	-2.09	1.46	1.50
31	B	624	LMT	O2B-C2B	-2.09	1.38	1.43
31	M	102	LMT	O1'-C1'	-2.09	1.36	1.40
22	A	403	CLA	CMD-C2D	-2.09	1.46	1.51
30	B	622	SQD	O2-C2	-2.09	1.38	1.43
22	a	405	CLA	CMD-C2D	-2.09	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.09	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.08	1.46	1.51
32	d	401	PHO	C4B-NB	2.08	1.41	1.36
24	g	101	BCR	C33-C5	-2.08	1.47	1.50
22	D	404	CLA	CMD-C2D	-2.08	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.08	1.46	1.51
31	B	628	LMT	O4'-C4B	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	517	DGD	C1G-C2G	2.08	1.57	1.50
31	M	102	LMT	O4'-C4B	-2.08	1.38	1.43
22	B	604	CLA	CMD-C2D	-2.08	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.08	1.46	1.51
31	M	103	LMT	O4'-C4B	-2.08	1.38	1.43
27	l	101	LMG	C7-C8	2.07	1.57	1.50
22	A	405	CLA	CMD-C2D	-2.07	1.46	1.51
31	I	102	LMT	O4'-C4B	-2.07	1.38	1.43
22	h	101	CLA	CMD-C2D	-2.07	1.46	1.51
31	b	627	LMT	O2B-C2B	-2.07	1.38	1.43
22	B	614	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.07	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.07	1.46	1.51
30	a	415	SQD	O2-C2	-2.07	1.38	1.43
31	d	410	LMT	O4'-C4B	-2.07	1.38	1.43
22	B	601	CLA	CMD-C2D	-2.07	1.46	1.51
31	D	410	LMT	O4'-C4B	-2.07	1.38	1.43
22	c	502	CLA	CMD-C2D	-2.07	1.46	1.51
30	A	413	SQD	O2-C2	-2.07	1.38	1.43
22	H	101	CLA	CMD-C2D	-2.06	1.46	1.51
31	b	604	LMT	O4'-C4B	-2.06	1.38	1.43
30	f	103	SQD	O3-C3	-2.06	1.38	1.43
22	c	511	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.06	1.46	1.51
31	b	603	LMT	O4'-C4B	-2.06	1.38	1.43
22	C	520	CLA	CMD-C2D	-2.06	1.46	1.51
22	B	605	CLA	CMD-C2D	-2.06	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.06	1.46	1.51
24	y	101	BCR	C33-C5	-2.06	1.47	1.50
22	B	609	CLA	CMD-C2D	-2.06	1.46	1.51
22	c	503	CLA	CMD-C2D	-2.06	1.46	1.51
22	C	507	CLA	CMD-C2D	-2.06	1.46	1.51
22	d	404	CLA	CMD-C2D	-2.06	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.05	1.46	1.51
34	v	201	HEM	CAA-C2A	2.05	1.55	1.52
30	d	402	SQD	O2-C2	-2.05	1.38	1.43
25	b	601	DGD	C3G-C2G	2.05	1.57	1.50
25	B	620	DGD	O2G-C2G	-2.05	1.41	1.46
23	J	101	PL9	C3-C4	-2.05	1.46	1.49
22	a	408	CLA	CMD-C2D	-2.05	1.46	1.51
22	c	507	CLA	CMD-C2D	-2.05	1.46	1.51
22	b	608	CLA	CMD-C2D	-2.04	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CMD-C2D	-2.04	1.46	1.51
30	F	103	SQD	O3-C3	-2.04	1.38	1.43
25	C	516	DGD	C1E-C2E	2.04	1.58	1.52
22	C	511	CLA	CMD-C2D	-2.04	1.46	1.51
26	A	409	LHG	O7-C5	-2.04	1.41	1.46
22	b	618	CLA	CMD-C2D	-2.04	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.04	1.46	1.51
31	b	626	LMT	O4'-C4B	-2.04	1.38	1.43
25	a	411	DGD	O1G-C1G	-2.04	1.40	1.45
22	B	612	CLA	CMD-C2D	-2.04	1.46	1.51
30	b	602	SQD	O3-C3	-2.04	1.38	1.43
22	C	503	CLA	CMD-C2D	-2.04	1.46	1.51
22	C	506	CLA	CMD-C2D	-2.04	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.04	1.46	1.51
22	c	510	CLA	CMD-C2D	-2.04	1.46	1.51
30	f	103	SQD	O2-C2	-2.03	1.38	1.43
22	d	405	CLA	CMD-C2D	-2.03	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.03	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.03	1.46	1.51
30	B	626	SQD	O3-C3	-2.03	1.38	1.43
22	c	512	CLA	CMD-C2D	-2.03	1.46	1.51
30	a	415	SQD	O3-C3	-2.03	1.38	1.43
27	d	411	LMG	O7-C8	-2.03	1.41	1.46
22	D	405	CLA	CMD-C2D	-2.03	1.46	1.51
25	b	624	DGD	O2G-C2G	-2.03	1.41	1.46
22	c	506	CLA	CMD-C2D	-2.03	1.46	1.51
31	B	623	LMT	O4'-C4B	-2.02	1.38	1.43
22	b	613	CLA	CMD-C2D	-2.02	1.46	1.51
30	A	414	SQD	O2-C2	-2.01	1.38	1.43
22	b	619	CLA	CMC-C2C	-2.01	1.46	1.50
22	c	501	CLA	CMD-C2D	-2.01	1.46	1.51
23	j	101	PL9	C3-C4	-2.01	1.46	1.49
30	a	401	SQD	O2-C2	-2.01	1.38	1.43
30	F	103	SQD	O2-C2	-2.01	1.38	1.43
24	C	514	BCR	C38-C26	-2.01	1.47	1.50
22	C	510	CLA	CMD-C2D	-2.01	1.46	1.51
22	C	512	CLA	CMD-C2D	-2.00	1.46	1.51
25	C	517	DGD	C3G-C2G	2.00	1.56	1.50

All (1211) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	7.31	109.99	106.71
22	B	611	CLA	C4A-NA-C1A	7.26	109.97	106.71
22	c	504	CLA	C4A-NA-C1A	7.25	109.97	106.71
22	b	615	CLA	C4A-NA-C1A	7.17	109.93	106.71
22	B	603	CLA	C4A-NA-C1A	7.12	109.91	106.71
22	b	607	CLA	C4A-NA-C1A	7.08	109.89	106.71
22	b	609	CLA	C4A-NA-C1A	6.97	109.84	106.71
22	C	510	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	A	403	CLA	C4A-NA-C1A	6.95	109.83	106.71
22	C	503	CLA	C4A-NA-C1A	6.94	109.83	106.71
22	B	605	CLA	C4A-NA-C1A	6.90	109.81	106.71
22	b	618	CLA	C4A-NA-C1A	6.85	109.79	106.71
22	c	503	CLA	C4A-NA-C1A	6.84	109.78	106.71
22	C	501	CLA	C4A-NA-C1A	6.80	109.76	106.71
22	C	520	CLA	C4A-NA-C1A	6.77	109.75	106.71
22	c	511	CLA	C4A-NA-C1A	6.76	109.74	106.71
22	a	405	CLA	C4A-NA-C1A	6.76	109.74	106.71
22	C	511	CLA	C4A-NA-C1A	6.75	109.74	106.71
22	B	615	CLA	C4A-NA-C1A	6.74	109.74	106.71
22	c	520	CLA	C4A-NA-C1A	6.71	109.72	106.71
22	c	501	CLA	C4A-NA-C1A	6.70	109.72	106.71
22	B	604	CLA	C4A-NA-C1A	6.67	109.70	106.71
22	b	616	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	a	408	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	c	506	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	c	512	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	b	608	CLA	C4A-NA-C1A	6.62	109.68	106.71
22	C	506	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	B	614	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	C	507	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	b	617	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	B	607	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	c	505	CLA	C4A-NA-C1A	6.57	109.66	106.71
22	H	101	CLA	C4A-NA-C1A	6.55	109.65	106.71
22	c	510	CLA	C4A-NA-C1A	6.51	109.63	106.71
22	B	612	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	C	512	CLA	C4A-NA-C1A	6.49	109.62	106.71
22	B	609	CLA	C4A-NA-C1A	6.48	109.62	106.71
22	b	619	CLA	C4A-NA-C1A	6.47	109.62	106.71
22	c	507	CLA	C4A-NA-C1A	6.44	109.60	106.71
22	A	405	CLA	C4A-NA-C1A	6.44	109.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	h	101	CLA	C4A-NA-C1A	6.42	109.59	106.71
22	B	602	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	d	404	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	B	606	CLA	C4A-NA-C1A	6.40	109.58	106.71
22	B	613	CLA	C4A-NA-C1A	6.38	109.58	106.71
22	a	406	CLA	C4A-NA-C1A	6.38	109.57	106.71
22	C	508	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	C	505	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	B	608	CLA	C4A-NA-C1A	6.34	109.56	106.71
22	c	508	CLA	C4A-NA-C1A	6.32	109.55	106.71
22	b	610	CLA	C4A-NA-C1A	6.28	109.53	106.71
22	b	611	CLA	C4A-NA-C1A	6.27	109.52	106.71
22	B	601	CLA	C4A-NA-C1A	6.26	109.52	106.71
22	d	405	CLA	C4A-NA-C1A	6.23	109.51	106.71
22	c	502	CLA	C4A-NA-C1A	6.22	109.50	106.71
22	b	612	CLA	C4A-NA-C1A	6.21	109.50	106.71
22	b	605	CLA	C4A-NA-C1A	6.21	109.50	106.71
22	c	509	CLA	C4A-NA-C1A	6.17	109.48	106.71
22	A	404	CLA	C4A-NA-C1A	6.16	109.47	106.71
22	b	606	CLA	C4A-NA-C1A	6.16	109.47	106.71
22	D	404	CLA	C4A-NA-C1A	6.15	109.47	106.71
22	a	404	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	D	405	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	C	509	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	C	502	CLA	C4A-NA-C1A	6.04	109.42	106.71
22	A	402	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	b	613	CLA	C4A-NA-C1A	6.01	109.41	106.71
23	j	101	PL9	C7-C3-C4	5.69	121.50	116.88
23	J	101	PL9	C7-C3-C4	5.66	121.48	116.88
30	a	415	SQD	O6-C1-C2	5.64	117.11	108.30
30	A	413	SQD	O6-C1-C2	5.54	116.95	108.30
30	b	602	SQD	O6-C1-C2	5.48	116.86	108.30
23	A	406	PL9	C7-C3-C4	5.44	121.30	116.88
30	B	626	SQD	O6-C1-C2	5.43	116.78	108.30
22	b	614	CLA	C4A-NA-C1A	5.40	109.14	106.71
23	d	406	PL9	C7-C3-C4	5.28	121.17	116.88
22	b	614	CLA	CMB-C2B-C1B	-5.25	120.40	128.46
30	A	413	SQD	O9-S-C6	5.22	113.15	106.94
22	B	610	CLA	C4A-NA-C1A	5.19	109.04	106.71
23	a	409	PL9	C7-C3-C4	5.19	121.09	116.88
30	a	415	SQD	O9-S-C6	5.18	113.10	106.94
22	B	610	CLA	CMB-C2B-C1B	-5.18	120.51	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	PL9	C7-C3-C4	5.16	121.07	116.88
25	a	411	DGD	O3G-C3G-C2G	-4.71	99.54	110.90
25	A	408	DGD	O3G-C3G-C2G	-4.66	99.65	110.90
30	B	622	SQD	O5-C5-C4	4.46	117.79	109.69
30	d	402	SQD	O5-C5-C4	4.40	117.68	109.69
30	d	402	SQD	O6-C1-C2	4.32	115.05	108.30
30	f	103	SQD	O7-S-C6	4.30	112.05	106.94
25	C	517	DGD	O3G-C3G-C2G	-4.27	100.60	110.90
30	B	622	SQD	O6-C1-C2	4.27	114.96	108.30
30	a	401	SQD	O7-S-C6	4.23	111.97	106.94
22	c	507	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
26	C	519	LHG	O4-P-O5	4.19	132.97	112.24
30	F	103	SQD	O7-S-C6	4.19	111.92	106.94
26	a	412	LHG	O4-P-O5	4.18	132.92	112.24
22	C	507	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
26	c	519	LHG	O4-P-O5	4.17	132.88	112.24
26	A	409	LHG	O4-P-O5	4.17	132.87	112.24
30	B	626	SQD	O9-S-C6	4.16	111.88	106.94
25	c	517	DGD	O3G-C3G-C2G	-4.11	100.97	110.90
22	b	616	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
22	B	612	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
30	A	414	SQD	O7-S-C6	4.10	111.81	106.94
30	b	602	SQD	O7-S-C6	4.01	111.70	106.94
30	b	602	SQD	O9-S-C6	3.98	111.67	106.94
30	A	414	SQD	O5-C5-C4	3.94	116.84	109.69
24	J	102	BCR	C11-C10-C9	-3.92	121.71	127.31
30	b	602	SQD	O5-C5-C4	3.90	116.78	109.69
22	b	611	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
27	d	408	LMG	C1-C2-C3	-3.86	101.95	110.00
30	B	626	SQD	O5-C5-C4	3.86	116.71	109.69
30	B	622	SQD	O7-S-C6	3.86	111.52	106.94
27	D	408	LMG	C1-C2-C3	-3.85	101.97	110.00
30	F	103	SQD	O9-S-O7	-3.85	100.64	113.95
30	f	103	SQD	O9-S-O7	-3.84	100.64	113.95
24	C	513	BCR	C2-C1-C6	3.84	116.39	110.48
30	A	413	SQD	O47-C7-C8	3.83	119.75	111.50
24	c	513	BCR	C2-C1-C6	3.81	116.35	110.48
30	d	402	SQD	O9-S-O7	-3.80	100.81	113.95
30	A	413	SQD	O7-S-C6	3.79	111.44	106.94
30	a	401	SQD	O5-C5-C4	3.79	116.57	109.69
24	j	102	BCR	C11-C10-C9	-3.79	121.91	127.31
30	A	413	SQD	O9-S-O7	-3.78	100.85	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	j	101	PL9	C7-C3-C2	-3.77	118.34	123.30
23	J	101	PL9	C7-C3-C2	-3.77	118.35	123.30
30	a	415	SQD	O9-S-O7	-3.76	100.93	113.95
30	B	626	SQD	O7-S-C6	3.76	111.40	106.94
30	B	622	SQD	O9-S-O7	-3.75	100.96	113.95
25	c	516	DGD	O5D-C6D-C5D	-3.75	102.11	109.05
30	d	402	SQD	O7-S-C6	3.74	111.38	106.94
30	a	401	SQD	O9-S-O7	-3.73	101.03	113.95
30	f	103	SQD	O5-C5-C4	3.73	116.47	109.69
22	c	510	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
22	B	607	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
30	a	415	SQD	O47-C7-C8	3.71	119.51	111.50
22	b	615	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
22	B	613	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
30	a	415	SQD	O5-C5-C4	3.71	116.43	109.69
30	B	626	SQD	O9-S-O7	-3.71	101.12	113.95
22	b	613	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
30	a	415	SQD	O7-S-C6	3.70	111.34	106.94
30	b	602	SQD	O9-S-O7	-3.70	101.16	113.95
22	b	617	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
22	C	503	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
25	C	516	DGD	O5D-C6D-C5D	-3.69	102.22	109.05
22	C	505	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
22	B	602	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	d	409	DGD	O6D-C1D-O3G	-3.66	101.31	109.97
22	B	611	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
30	A	414	SQD	O9-S-O7	-3.66	101.29	113.95
22	c	512	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
25	c	516	DGD	O3G-C3G-C2G	-3.66	102.08	110.90
30	d	402	SQD	O9-S-C6	3.65	111.28	106.94
30	B	622	SQD	O9-S-C6	3.64	111.26	106.94
22	C	512	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
22	C	506	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
25	C	516	DGD	O3G-C3G-C2G	-3.63	102.14	110.90
22	B	609	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
22	b	606	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	502	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
25	D	409	DGD	O6D-C1D-O3G	-3.62	101.41	109.97
30	b	602	SQD	O47-C7-C8	3.61	119.29	111.50
30	F	103	SQD	O5-C5-C4	3.61	116.25	109.69
30	B	626	SQD	O47-C7-C8	3.60	119.27	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
22	c	505	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
23	d	406	PL9	C7-C3-C2	-3.59	118.58	123.30
22	A	405	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
22	C	510	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
22	B	601	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
30	A	413	SQD	O5-C5-C4	3.57	116.19	109.69
30	a	401	SQD	O9-S-C6	3.57	111.18	106.94
30	F	103	SQD	O8-S-C6	3.56	111.42	105.74
22	a	404	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
23	A	406	PL9	C7-C3-C2	-3.55	118.63	123.30
22	c	502	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	c	511	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
22	c	509	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	C	511	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
22	a	408	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
22	A	402	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
22	a	405	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	C	509	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
22	B	604	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
24	j	102	BCR	C2-C1-C6	3.49	115.86	110.48
30	a	401	SQD	C44-O6-C1	3.48	120.54	113.74
30	A	414	SQD	O47-C7-C8	3.47	118.98	111.50
24	J	102	BCR	C2-C1-C6	3.47	115.82	110.48
22	b	608	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	B	614	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	c	520	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	D	404	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
22	b	605	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	B	605	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
23	a	409	PL9	C7-C3-C2	-3.46	118.76	123.30
22	D	405	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
23	D	406	PL9	C7-C3-C2	-3.45	118.76	123.30
22	C	520	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
30	F	103	SQD	O6-C1-C2	3.44	113.68	108.30
30	A	414	SQD	O9-S-C6	3.43	111.02	106.94
22	B	612	CLA	CMB-C2B-C3B	3.43	131.10	124.68
30	F	103	SQD	O47-C7-C8	3.43	118.89	111.50
22	d	404	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	b	618	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	d	405	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
30	f	103	SQD	O8-S-C6	3.43	111.20	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	A	404	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
22	C	508	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
30	d	402	SQD	O47-C7-C8	3.39	118.80	111.50
22	A	403	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
22	c	507	CLA	CMB-C2B-C3B	3.38	131.00	124.68
22	b	616	CLA	CMB-C2B-C3B	3.38	131.00	124.68
30	B	622	SQD	O47-C7-C8	3.37	118.77	111.50
22	B	603	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
25	b	624	DGD	O3G-C3G-C2G	-3.37	102.77	110.90
30	f	103	SQD	O9-S-C6	3.36	110.93	106.94
22	h	101	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	H	101	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	b	610	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
22	b	607	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
25	c	515	DGD	O3G-C3G-C2G	-3.35	102.81	110.90
25	C	515	DGD	O3G-C3G-C2G	-3.35	102.82	110.90
22	b	609	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	a	406	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
30	d	402	SQD	O8-S-C6	3.30	111.00	105.74
30	f	103	SQD	O47-C7-C8	3.30	118.60	111.50
22	B	606	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
22	c	503	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
30	A	414	SQD	C44-O6-C1	3.28	120.15	113.74
22	b	614	CLA	CMB-C2B-C3B	3.28	130.82	124.68
24	A	407	BCR	C2-C1-C6	3.28	115.53	110.48
30	F	103	SQD	O9-S-C6	3.28	110.83	106.94
25	B	620	DGD	O3G-C3G-C2G	-3.27	103.01	110.90
22	C	507	CLA	CMB-C2B-C3B	3.27	130.79	124.68
24	B	617	BCR	C15-C16-C17	-3.26	116.79	123.47
22	b	619	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
22	B	613	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
22	B	610	CLA	CMB-C2B-C3B	3.25	130.76	124.68
22	b	611	CLA	CMB-C2B-C3B	3.24	130.74	124.68
30	a	401	SQD	O47-C7-C8	3.24	118.47	111.50
22	B	608	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
30	f	103	SQD	O6-C1-C2	3.23	113.34	108.30
22	B	603	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
24	a	410	BCR	C2-C1-C6	3.21	115.42	110.48
22	B	605	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
22	B	613	CLA	CMB-C2B-C3B	3.20	130.67	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	409	DGD	O3G-C3G-C2G	-3.19	103.20	110.90
22	C	503	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
25	b	624	DGD	O6D-C1D-O3G	-3.18	102.44	109.97
30	B	622	SQD	O8-S-C6	3.18	110.80	105.74
22	C	506	CLA	CMB-C2B-C3B	3.18	130.62	124.68
22	b	606	CLA	CMB-C2B-C3B	3.17	130.61	124.68
24	J	102	BCR	C3-C4-C5	-3.17	108.42	114.08
22	b	617	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	B	620	DGD	O6D-C1D-O3G	-3.16	102.49	109.97
22	b	612	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
22	B	602	CLA	CMB-C2B-C3B	3.15	130.58	124.68
25	d	409	DGD	O3G-C3G-C2G	-3.15	103.31	110.90
24	J	102	BCR	C24-C23-C22	-3.15	121.48	126.23
22	b	606	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
30	B	626	SQD	C3-C4-C5	3.14	115.84	110.24
24	j	102	BCR	C3-C4-C5	-3.14	108.47	114.08
30	b	602	SQD	C3-C4-C5	3.14	115.83	110.24
22	b	609	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
30	d	402	SQD	C3-C4-C5	3.13	115.83	110.24
22	C	503	CLA	CMB-C2B-C3B	3.13	130.53	124.68
22	B	607	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	c	506	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	c	507	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	B	608	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	b	617	CLA	CMB-C2B-C3B	3.11	130.50	124.68
31	B	628	LMT	C1'-O5'-C5'	-3.11	107.59	113.69
25	c	516	DGD	O6D-C1D-O3G	-3.10	102.62	109.97
22	b	615	CLA	CMB-C2B-C3B	3.10	130.48	124.68
22	c	510	CLA	CMB-C2B-C3B	3.10	130.47	124.68
25	C	516	DGD	O6D-C1D-O3G	-3.10	102.64	109.97
22	b	613	CLA	CMB-C2B-C3B	3.10	130.47	124.68
22	c	504	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	b	621	BCR	C15-C16-C17	-3.09	117.14	123.47
24	B	617	BCR	C33-C5-C6	-3.09	121.06	124.53
24	j	102	BCR	C24-C23-C22	-3.09	121.57	126.23
22	C	505	CLA	CMB-C2B-C3B	3.08	130.45	124.68
22	C	504	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
24	b	622	BCR	C24-C23-C22	-3.07	121.59	126.23
22	C	512	CLA	CMB-C2B-C3B	3.07	130.42	124.68
24	B	618	BCR	C2-C1-C6	3.06	115.20	110.48
22	c	505	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	b	607	CLA	O2D-CGD-O1D	-3.06	117.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	c	512	CLA	CMB-C2B-C3B	3.05	130.38	124.68
22	a	408	CLA	CMB-C2B-C3B	3.04	130.36	124.68
22	C	504	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
22	c	505	CLA	CMB-C2B-C3B	3.03	130.35	124.68
22	C	510	CLA	CMB-C2B-C3B	3.03	130.35	124.68
22	b	612	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
22	C	505	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
30	B	622	SQD	C3-C4-C5	3.03	115.64	110.24
22	C	502	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	B	609	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	B	606	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	B	604	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
22	c	503	CLA	CMB-C2B-C3B	3.01	130.32	124.68
22	B	611	CLA	CMB-C2B-C3B	3.01	130.31	124.68
22	c	504	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
24	b	621	BCR	C33-C5-C6	-3.01	121.15	124.53
31	b	604	LMT	C1'-O5'-C5'	-3.01	107.79	113.69
22	c	502	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
22	a	404	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
22	b	610	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
24	b	622	BCR	C2-C1-C6	2.99	115.09	110.48
25	A	408	DGD	O6D-C1D-O3G	-2.99	102.89	109.97
22	A	405	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	D	404	CLA	CMB-C2B-C3B	2.99	130.27	124.68
22	b	605	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
22	a	406	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	a	411	DGD	O6D-C1D-O3G	-2.98	102.92	109.97
22	c	502	CLA	CMB-C2B-C3B	2.97	130.24	124.68
30	A	413	SQD	C3-C4-C5	2.97	115.54	110.24
22	b	613	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	b	611	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
22	C	511	CLA	CMB-C2B-C3B	2.97	130.23	124.68
22	c	511	CLA	CMB-C2B-C3B	2.96	130.22	124.68
22	b	608	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
22	B	602	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	x	101	BCR	C33-C5-C6	-2.96	121.21	124.53
22	c	512	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
22	A	402	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
22	b	608	CLA	CMB-C2B-C3B	2.95	130.19	124.68
22	d	405	CLA	CMB-C2B-C3B	2.95	130.19	124.68
30	B	626	SQD	O8-S-C6	2.94	110.43	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	f	102	BCR	C33-C5-C6	-2.94	121.22	124.53
22	B	609	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
24	F	102	BCR	C33-C5-C6	-2.94	121.23	124.53
22	C	506	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	C	507	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
22	c	510	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
27	D	407	LMG	O6-C1-O1	-2.93	103.03	109.97
22	D	405	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	j	102	BCR	C7-C8-C9	-2.93	121.81	126.23
22	d	404	CLA	CMB-C2B-C3B	2.92	130.15	124.68
30	a	415	SQD	C3-C4-C5	2.92	115.45	110.24
27	d	407	LMG	O6-C1-O1	-2.92	103.05	109.97
22	c	520	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
22	B	605	CLA	CMB-C2B-C3B	2.92	130.15	124.68
25	C	515	DGD	O6D-C1D-O3G	-2.92	103.06	109.97
22	A	403	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
22	C	501	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
25	C	517	DGD	CDB-CCB-CBB	-2.91	99.64	114.42
24	H	102	BCR	C33-C5-C6	-2.91	121.26	124.53
25	c	517	DGD	CDB-CCB-CBB	-2.90	99.68	114.42
25	c	515	DGD	O6D-C1D-O3G	-2.90	103.10	109.97
24	J	102	BCR	C35-C13-C14	-2.90	118.86	122.92
22	c	511	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
22	B	604	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	c	517	DGD	C1D-C2D-C3D	-2.90	103.95	110.00
22	h	101	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
24	J	102	BCR	C7-C8-C9	-2.89	121.86	126.23
22	B	612	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
24	c	521	BCR	C2-C1-C6	2.89	114.93	110.48
24	b	623	BCR	C2-C1-C6	2.89	114.93	110.48
22	H	101	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
22	d	405	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
23	j	101	PL9	C7-C8-C9	-2.88	121.99	126.79
22	B	607	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	D	404	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
22	c	506	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	b	616	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	C	512	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
22	A	404	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
31	B	624	LMT	C3'-C4'-C5'	-2.87	104.34	110.93
22	C	510	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
25	B	625	DGD	O5D-C1E-C2E	2.87	112.78	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
31	I	102	LMT	O1'-C1'-C2'	2.87	112.78	108.30
23	d	406	PL9	C40-C39-C41	2.87	120.09	115.27
22	b	618	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	b	601	DGD	C1D-C2D-C3D	-2.87	104.03	110.00
24	j	102	BCR	C35-C13-C14	-2.87	118.91	122.92
24	C	514	BCR	C15-C16-C17	-2.87	117.60	123.47
22	B	601	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	h	101	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	C	520	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
24	B	619	BCR	C2-C1-C6	2.85	114.88	110.48
26	a	412	LHG	O8-C23-C24	2.85	120.86	111.91
22	c	501	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	c	516	DGD	CDB-CCB-CBB	-2.85	99.95	114.42
22	B	601	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
22	B	614	CLA	CMB-C2B-C3B	2.85	130.01	124.68
24	c	521	BCR	C15-C16-C17	-2.85	117.64	123.47
22	D	405	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
22	d	404	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	J	101	PL9	C7-C8-C9	-2.84	122.06	126.79
25	b	601	DGD	O3G-C3G-C2G	-2.84	104.05	110.90
22	a	405	CLA	CMB-C2B-C3B	2.84	129.99	124.68
22	C	520	CLA	CMB-C2B-C3B	2.83	129.98	124.68
22	c	509	CLA	CMB-C2B-C3B	2.83	129.98	124.68
25	C	516	DGD	CDB-CCB-CBB	-2.83	100.04	114.42
30	d	402	SQD	C44-O6-C1	2.83	119.27	113.74
22	b	610	CLA	CMB-C2B-C3B	2.83	129.98	124.68
24	J	102	BCR	C27-C26-C25	2.83	126.84	122.73
22	A	404	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	C	509	CLA	CMB-C2B-C3B	2.83	129.97	124.68
24	f	102	BCR	C29-C30-C25	2.83	114.83	110.48
22	b	609	CLA	CMB-C2B-C3B	2.82	129.96	124.68
22	H	101	CLA	CMB-C2B-C3B	2.82	129.96	124.68
24	B	618	BCR	C11-C10-C9	-2.82	123.29	127.31
24	B	618	BCR	C24-C23-C22	-2.82	121.98	126.23
22	B	610	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
30	A	414	SQD	O8-S-C6	2.82	110.23	105.74
32	D	402	PHO	O2D-CGD-O1D	-2.82	118.33	123.84
22	B	606	CLA	CMB-C2B-C3B	2.82	129.94	124.68
22	a	408	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
31	i	102	LMT	O1'-C1'-C2'	2.81	112.69	108.30
22	b	618	CLA	O2D-CGD-O1D	-2.81	118.35	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
25	b	601	DGD	O5D-C1E-C2E	2.81	112.68	108.30
24	b	623	BCR	C3-C4-C5	-2.80	109.08	114.08
24	j	102	BCR	C27-C26-C25	2.80	126.79	122.73
23	D	406	PL9	C40-C39-C41	2.80	119.98	115.27
24	F	102	BCR	C29-C30-C25	2.80	114.79	110.48
26	A	409	LHG	O8-C23-C24	2.80	120.68	111.91
25	c	517	DGD	O5D-C6D-C5D	-2.80	103.87	109.05
24	B	619	BCR	C3-C4-C5	-2.80	109.08	114.08
23	d	406	PL9	C7-C8-C9	-2.79	122.14	126.79
22	A	403	CLA	CMB-C2B-C3B	2.79	129.91	124.68
22	b	614	CLA	CMD-C2D-C3D	2.79	129.90	124.68
22	a	406	CLA	CMB-C2B-C3B	2.79	129.90	124.68
22	B	603	CLA	CMB-C2B-C3B	2.79	129.90	124.68
30	B	622	SQD	C44-O6-C1	2.79	119.19	113.74
24	b	621	BCR	C15-C14-C13	-2.79	123.33	127.31
30	a	401	SQD	O8-S-C6	2.79	110.18	105.74
22	c	520	CLA	CMB-C2B-C3B	2.79	129.89	124.68
22	B	608	CLA	CMB-C2B-C3B	2.78	129.88	124.68
22	c	508	CLA	CMB-C2B-C3B	2.78	129.87	124.68
22	B	610	CLA	CMD-C2D-C3D	2.77	129.87	124.68
22	B	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
24	K	102	BCR	C2-C1-C6	2.77	114.75	110.48
25	b	601	DGD	C3G-C2G-C1G	-2.77	105.23	111.79
30	b	602	SQD	C4-C3-C2	2.77	115.66	110.82
22	b	607	CLA	CMB-C2B-C3B	2.77	129.86	124.68
22	C	504	CLA	CMD-C2D-C3D	2.77	129.86	124.68
25	D	409	DGD	CDB-CCB-CBB	-2.77	100.38	114.42
22	C	511	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
27	C	518	LMG	O6-C1-O1	-2.76	103.44	109.97
23	A	406	PL9	C22-C23-C24	-2.76	121.02	127.66
32	d	401	PHO	O2D-CGD-O1D	-2.76	118.45	123.84
30	b	602	SQD	O8-S-C6	2.76	110.13	105.74
25	d	409	DGD	CDB-CCB-CBB	-2.76	100.43	114.42
22	b	612	CLA	CMB-C2B-C3B	2.76	129.84	124.68
22	a	405	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
22	A	405	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
24	y	101	BCR	C27-C26-C25	2.75	126.72	122.73
22	C	508	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	C	517	DGD	O5D-C6D-C5D	-2.75	103.97	109.05
22	c	511	CLA	CMD-C2D-C3D	2.75	129.82	124.68
22	b	605	CLA	CMB-C2B-C3B	2.74	129.81	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	BCR	C11-C10-C9	-2.74	123.39	127.31
31	b	627	LMT	C3'-C4'-C5'	-2.74	104.64	110.93
22	C	509	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
25	B	625	DGD	O3G-C3G-C2G	-2.74	104.30	110.90
22	C	511	CLA	CMD-C2D-C3D	2.73	129.78	124.68
24	g	101	BCR	C27-C26-C25	2.73	126.69	122.73
24	g	101	BCR	C33-C5-C6	-2.73	121.46	124.53
24	B	617	BCR	C28-C27-C26	-2.73	109.20	114.08
22	A	403	CLA	CHB-C4A-NA	2.72	128.28	124.51
24	K	102	BCR	C15-C16-C17	-2.72	117.90	123.47
23	a	409	PL9	C22-C23-C24	-2.72	121.11	127.66
30	f	103	SQD	C44-O6-C1	2.72	119.05	113.74
24	J	102	BCR	C15-C14-C13	-2.72	123.43	127.31
25	C	517	DGD	C1D-C2D-C3D	-2.72	104.33	110.00
22	a	404	CLA	CMB-C2B-C3B	2.72	129.76	124.68
24	j	102	BCR	C15-C14-C13	-2.72	123.44	127.31
24	g	101	BCR	C7-C8-C9	-2.71	122.14	126.23
24	B	617	BCR	C15-C14-C13	-2.71	123.44	127.31
24	y	101	BCR	C38-C26-C25	-2.71	121.49	124.53
24	g	101	BCR	C38-C26-C25	-2.70	121.49	124.53
24	b	621	BCR	C28-C27-C26	-2.70	109.25	114.08
22	b	614	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
32	D	401	PHO	O2D-CGD-O1D	-2.70	118.56	123.84
27	i	101	LMG	O6-C1-O1	-2.70	103.59	109.97
22	c	509	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	B	615	CLA	CMB-C2B-C3B	2.69	129.72	124.68
24	y	101	BCR	C7-C8-C9	-2.69	122.17	126.23
27	I	101	LMG	O6-C1-O1	-2.69	103.60	109.97
27	c	518	LMG	O6-C1-O1	-2.69	103.61	109.97
22	A	402	CLA	CMB-C2B-C3B	2.69	129.71	124.68
23	D	406	PL9	C7-C8-C9	-2.68	122.33	126.79
24	b	620	BCR	C33-C5-C6	-2.68	121.52	124.53
22	D	404	CLA	CMD-C2D-C3D	2.68	129.69	124.68
25	B	625	DGD	C1D-C2D-C3D	-2.67	104.42	110.00
23	D	406	PL9	C22-C23-C24	-2.67	121.22	127.66
30	A	413	SQD	O8-S-C6	2.67	110.00	105.74
24	B	616	BCR	C33-C5-C6	-2.67	121.53	124.53
32	a	407	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
22	b	607	CLA	CHB-C4A-NA	2.67	128.20	124.51
22	c	502	CLA	CMD-C2D-C3D	2.67	129.67	124.68
22	b	619	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	C	506	CLA	CHB-C4A-NA	2.66	128.19	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	A	408	DGD	O5D-C6D-C5D	-2.65	104.14	109.05
31	M	102	LMT	C1'-O5'-C5'	-2.65	108.48	113.69
22	d	404	CLA	CMD-C2D-C3D	2.65	129.64	124.68
22	C	510	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	c	514	BCR	C15-C16-C17	-2.65	118.05	123.47
22	c	504	CLA	CMD-C2D-C3D	2.65	129.63	124.68
22	C	504	CLA	CMB-C2B-C3B	2.64	129.61	124.68
25	c	517	DGD	C1D-O6D-C5D	-2.64	108.51	113.69
24	c	514	BCR	C28-C27-C26	-2.63	109.38	114.08
22	b	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
22	b	608	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	B	618	BCR	C29-C30-C25	2.63	114.53	110.48
22	a	405	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	b	622	BCR	C29-C30-C25	2.63	114.52	110.48
22	B	605	CLA	CHB-C4A-NA	2.63	128.14	124.51
24	B	618	BCR	C15-C16-C17	-2.62	118.10	123.47
24	y	101	BCR	C33-C5-C6	-2.62	121.58	124.53
22	c	506	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	d	406	PL9	C22-C23-C24	-2.62	121.36	127.66
22	b	615	CLA	CMD-C2D-C3D	2.62	129.57	124.68
30	B	626	SQD	C4-C3-C2	2.61	115.39	110.82
30	F	103	SQD	C44-O6-C1	2.61	118.83	113.74
24	b	622	BCR	C15-C16-C17	-2.61	118.13	123.47
24	b	622	BCR	C11-C10-C9	-2.61	123.59	127.31
22	c	511	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	C	503	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	c	513	BCR	C7-C8-C9	-2.60	122.31	126.23
22	c	508	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
22	b	618	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	b	619	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
22	C	520	CLA	CHB-C4A-NA	2.59	128.10	124.51
24	B	618	BCR	C15-C14-C13	-2.59	123.61	127.31
23	a	409	PL9	C41-C39-C40	2.59	120.33	114.60
24	C	513	BCR	C24-C23-C22	-2.59	122.32	126.23
22	C	511	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	a	408	CLA	CMD-C2D-C3D	2.59	129.52	124.68
22	b	607	CLA	C1-C2-C3	-2.59	121.57	126.04
23	a	409	PL9	C7-C8-C9	-2.58	122.49	126.79
22	B	611	CLA	CMD-C2D-C3D	2.58	129.51	124.68
22	c	505	CLA	CHB-C4A-NA	2.58	128.09	124.51
22	c	507	CLA	CMD-C2D-C3D	2.58	129.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	CMD-C2D-C3D	2.58	129.51	124.68
22	c	504	CLA	CMB-C2B-C3B	2.58	129.51	124.68
26	c	519	LHG	O8-C23-C24	2.58	120.00	111.91
22	b	615	CLA	CHB-C4A-NA	2.57	128.07	124.51
25	B	625	DGD	C3G-C2G-C1G	-2.57	105.70	111.79
22	B	615	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
24	C	514	BCR	C28-C27-C26	-2.57	109.48	114.08
22	c	512	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	C	514	BCR	C15-C14-C13	-2.56	123.65	127.31
22	B	608	CLA	CMD-C2D-C3D	2.56	129.47	124.68
31	B	623	LMT	C1'-O5'-C5'	-2.56	108.67	113.69
24	C	513	BCR	C15-C16-C17	-2.56	118.23	123.47
25	D	409	DGD	CFB-CEB-CDB	-2.56	101.44	114.42
22	c	501	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	b	612	CLA	CMD-C2D-C3D	2.55	129.46	124.68
24	C	514	BCR	C29-C30-C25	2.55	114.41	110.48
22	B	608	CLA	CHB-C4A-NA	2.55	128.04	124.51
32	a	407	PHO	CBD-CHA-C4D	-2.55	105.67	108.54
22	B	606	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	J	101	PL9	C22-C23-C24	-2.54	121.53	127.66
22	C	504	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	a	408	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	c	508	CLA	CHB-C4A-NA	2.54	128.03	124.51
22	C	512	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	C	501	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	B	609	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	a	409	PL9	C20-C19-C21	2.53	119.53	115.27
25	d	409	DGD	CFB-CEB-CDB	-2.53	101.58	114.42
26	C	519	LHG	O8-C23-C24	2.53	119.84	111.91
24	c	514	BCR	C29-C30-C25	2.53	114.37	110.48
23	A	406	PL9	C41-C39-C40	2.53	120.18	114.60
30	a	415	SQD	O8-S-C6	2.53	109.77	105.74
22	d	405	CLA	CMD-C2D-C3D	2.52	129.40	124.68
22	B	604	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	c	520	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	B	602	CLA	CMD-C2D-C3D	2.52	129.40	124.68
22	A	405	CLA	CMD-C2D-C3D	2.52	129.40	124.68
25	C	517	DGD	C1D-O6D-C5D	-2.52	108.74	113.69
22	c	504	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	C	508	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	a	404	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	j	101	PL9	C22-C23-C24	-2.51	121.61	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	CMD-C2D-C3D	2.51	129.38	124.68
22	b	617	CLA	CMD-C2D-C3D	2.51	129.37	124.68
24	c	514	BCR	C33-C5-C6	-2.51	121.71	124.53
24	b	622	BCR	C15-C14-C13	-2.50	123.73	127.31
24	c	513	BCR	C24-C23-C22	-2.50	122.45	126.23
32	d	401	PHO	CBD-CHA-C4D	-2.50	105.72	108.54
22	D	405	CLA	CMD-C2D-C3D	2.50	129.36	124.68
22	C	505	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	c	503	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	D	411	LMG	C38-C37-C36	-2.50	101.72	114.42
24	c	513	BCR	C15-C16-C17	-2.50	118.35	123.47
22	B	601	CLA	CMD-C2D-C3D	2.50	129.36	124.68
24	C	514	BCR	C33-C5-C6	-2.50	121.72	124.53
22	B	607	CLA	CHB-C4A-NA	2.50	127.97	124.51
31	M	103	LMT	C1'-O5'-C5'	-2.50	108.79	113.69
27	d	411	LMG	C38-C37-C36	-2.49	101.77	114.42
22	b	615	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
27	A	415	LMG	O6-C1-O1	-2.49	104.07	109.97
27	E	101	LMG	C1-C2-C3	-2.49	104.81	110.00
22	B	607	CLA	CMD-C2D-C3D	2.49	129.34	124.68
27	a	402	LMG	O6-C1-O1	-2.49	104.08	109.97
22	b	617	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	B	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	b	625	LMG	C1-C2-C3	-2.49	104.81	110.00
22	a	406	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	b	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
24	b	623	BCR	C7-C8-C9	-2.49	122.48	126.23
22	B	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
22	d	405	CLA	CHB-C4A-NA	2.48	127.95	124.51
24	C	513	BCR	C15-C14-C13	-2.48	123.77	127.31
22	c	501	CLA	CMB-C2B-C3B	2.48	129.32	124.68
22	C	507	CLA	CMD-C2D-C3D	2.48	129.32	124.68
24	c	513	BCR	C15-C14-C13	-2.48	123.77	127.31
24	b	621	BCR	C35-C13-C14	-2.48	119.45	122.92
25	A	408	DGD	CBB-CAB-C9B	-2.48	101.83	114.42
27	d	408	LMG	C38-C37-C36	-2.48	101.83	114.42
22	C	505	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
32	D	401	PHO	CBD-CHA-C4D	-2.48	105.75	108.54
23	A	406	PL9	C7-C8-C9	-2.48	122.67	126.79
22	B	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	c	514	BCR	C15-C14-C13	-2.48	123.78	127.31
27	B	621	LMG	C1-C2-C3	-2.48	104.84	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
24	J	102	BCR	C15-C16-C17	-2.47	118.41	123.47
22	B	612	CLA	CHB-C4A-NA	2.47	127.93	124.51
34	F	101	HEM	C1D-C2D-C3D	-2.47	105.28	107.00
22	h	101	CLA	CMD-C2D-C3D	2.47	129.30	124.68
25	a	411	DGD	O5D-C6D-C5D	-2.47	104.47	109.05
25	d	409	DGD	C3G-C2G-C1G	-2.47	105.94	111.79
22	C	508	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
24	A	407	BCR	C15-C14-C13	-2.47	123.79	127.31
25	C	516	DGD	O6E-C1E-O5D	-2.47	104.14	109.97
22	b	610	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
22	C	501	CLA	CMD-C2D-C3D	2.46	129.28	124.68
22	C	506	CLA	CMD-C2D-C3D	2.46	129.28	124.68
25	a	411	DGD	CBB-CAB-C9B	-2.46	101.94	114.42
34	f	101	HEM	C1D-C2D-C3D	-2.46	105.28	107.00
22	a	408	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
22	C	503	CLA	CMD-C2D-C3D	2.46	129.28	124.68
24	C	514	BCR	C11-C10-C9	-2.46	123.80	127.31
22	b	611	CLA	CHB-C4A-NA	2.46	127.91	124.51
24	j	102	BCR	C38-C26-C25	-2.46	121.77	124.53
27	A	410	LMG	C40-C39-C38	-2.46	101.96	114.42
22	B	612	CLA	CMD-C2D-C3D	2.45	129.27	124.68
27	l	101	LMG	C40-C39-C38	-2.45	101.96	114.42
22	D	405	CLA	CHB-C4A-NA	2.45	127.91	124.51
25	B	620	DGD	CBB-CAB-C9B	-2.45	101.97	114.42
22	h	101	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	c	505	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
22	b	605	CLA	CMD-C2D-C3D	2.45	129.26	124.68
34	f	101	HEM	CBD-CAD-C3D	-2.45	107.96	112.48
25	b	624	DGD	CBB-CAB-C9B	-2.45	101.99	114.42
22	B	613	CLA	CMD-C2D-C3D	2.45	129.26	124.68
24	j	102	BCR	C15-C16-C17	-2.45	118.46	123.47
22	c	510	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	404	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	c	507	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	A	403	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
24	y	101	BCR	C1-C6-C5	-2.45	119.17	122.61
22	c	502	CLA	CHB-C4A-NA	2.45	127.89	124.51
22	b	613	CLA	CMD-C2D-C3D	2.45	129.25	124.68
31	d	410	LMT	C3'-C4'-C5'	-2.45	105.32	110.93
22	b	612	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
31	M	103	LMT	C3'-C4'-C5'	-2.44	105.32	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	521	BCR	C27-C26-C25	2.44	126.28	122.73
24	K	102	BCR	C27-C26-C25	2.44	126.28	122.73
22	B	606	CLA	CHB-C4A-NA	2.44	127.89	124.51
31	b	626	LMT	C1'-O5'-C5'	-2.44	108.90	113.69
22	B	603	CLA	CMD-C2D-C3D	2.44	129.24	124.68
25	C	517	DGD	CFB-CEB-CDB	-2.44	102.05	114.42
22	c	501	CLA	CMD-C2D-C3D	2.44	129.24	124.68
27	D	408	LMG	C38-C37-C36	-2.44	102.06	114.42
32	D	402	PHO	CBD-CHA-C4D	-2.44	105.80	108.54
25	c	516	DGD	O6E-C1E-O5D	-2.43	104.21	109.97
27	D	407	LMG	C38-C37-C36	-2.43	102.07	114.42
24	b	623	BCR	C11-C10-C9	-2.43	123.84	127.31
24	J	102	BCR	C38-C26-C25	-2.43	121.80	124.53
32	a	407	PHO	O1D-CGD-CBD	2.43	129.46	124.48
22	b	606	CLA	CMD-C2D-C3D	2.43	129.22	124.68
24	c	521	BCR	C15-C14-C13	-2.43	123.84	127.31
32	D	402	PHO	O1D-CGD-CBD	2.43	129.45	124.48
24	b	623	BCR	C27-C26-C25	2.43	126.25	122.73
22	a	405	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
26	C	519	LHG	C11-C10-C9	-2.42	102.13	114.42
22	B	601	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
22	C	511	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
22	B	602	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	b	616	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	H	101	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	c	511	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
22	B	615	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	B	614	CLA	CMD-C2D-C3D	2.42	129.20	124.68
22	b	610	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	C	507	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	a	406	CLA	C1B-CHB-C4A	-2.41	125.33	130.12
22	C	504	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
27	d	407	LMG	C38-C37-C36	-2.41	102.17	114.42
31	D	410	LMT	C3'-C4'-C5'	-2.41	105.40	110.93
22	A	404	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	c	522	LMG	C40-C39-C38	-2.40	102.22	114.42
24	b	621	BCR	C29-C30-C25	2.40	114.18	110.48
22	A	402	CLA	CHB-C4A-NA	2.40	127.84	124.51
24	C	513	BCR	C7-C8-C9	-2.40	122.60	126.23
22	b	611	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	c	517	DGD	CFB-CEB-CDB	-2.40	102.23	114.42
22	C	512	CLA	CMD-C2D-C3D	2.40	129.17	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	DGD	C3G-C2G-C1G	-2.40	106.11	111.79
22	d	405	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
26	c	519	LHG	C11-C10-C9	-2.40	102.25	114.42
22	H	101	CLA	CMD-C2D-C3D	2.40	129.16	124.68
23	D	406	PL9	C27-C28-C29	-2.40	121.89	127.66
22	B	603	CLA	C1-C2-C3	-2.40	121.90	126.04
22	c	506	CLA	CMD-C2D-C3D	2.40	129.16	124.68
24	g	101	BCR	C1-C6-C5	-2.40	119.24	122.61
22	c	507	CLA	C1B-CHB-C4A	-2.39	125.37	130.12
22	C	501	CLA	CMB-C2B-C3B	2.39	129.16	124.68
24	K	102	BCR	C11-C10-C9	-2.39	123.89	127.31
22	b	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	c	516	DGD	CFB-CEB-CDB	-2.39	102.29	114.42
24	c	513	BCR	C11-C10-C9	-2.39	123.90	127.31
22	C	505	CLA	CMD-C2D-C3D	2.39	129.15	124.68
25	c	515	DGD	C3G-C2G-C1G	-2.39	106.14	111.79
22	C	506	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
22	b	606	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
34	V	201	HEM	C1D-C2D-C3D	-2.39	105.34	107.00
34	F	101	HEM	CAA-CBA-CGA	-2.39	108.67	112.67
22	b	608	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
24	b	620	BCR	C2-C1-C6	2.39	114.15	110.48
22	b	606	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	A	407	BCR	C15-C16-C17	-2.38	118.59	123.47
24	B	616	BCR	C2-C1-C6	2.38	114.15	110.48
30	a	415	SQD	O48-C23-C24	2.38	119.38	111.91
27	C	521	LMG	C40-C39-C38	-2.38	102.33	114.42
22	B	602	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
22	B	611	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
22	C	520	CLA	CMD-C2D-C3D	2.38	129.13	124.68
22	h	101	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
27	c	522	LMG	O6-C1-O1	-2.38	104.34	109.97
22	A	405	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	B	619	BCR	C27-C26-C25	2.37	126.18	122.73
24	B	619	BCR	C7-C8-C9	-2.37	122.65	126.23
24	B	617	BCR	C29-C30-C25	2.37	114.13	110.48
22	B	613	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
31	M	102	LMT	C3'-C4'-C5'	-2.37	105.50	110.93
30	A	413	SQD	O48-C23-C24	2.37	119.34	111.91
22	b	618	CLA	CMD-C2D-C3D	2.37	129.11	124.68
22	c	503	CLA	CMD-C2D-C3D	2.37	129.11	124.68
25	C	515	DGD	C3G-C2G-C1G	-2.37	106.19	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	406	PL9	C20-C19-C21	2.37	119.25	115.27
22	c	505	CLA	CMD-C2D-C3D	2.37	129.11	124.68
31	D	410	LMT	C1'-O5'-C5'	-2.37	109.05	113.69
25	C	516	DGD	C3G-C2G-C1G	-2.37	106.19	111.79
30	a	401	SQD	C1-O5-C5	2.36	118.33	113.69
32	d	401	PHO	O1D-CGD-CBD	2.36	129.32	124.48
22	a	404	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	A	405	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
27	M	101	LMG	C1-C2-C3	-2.36	105.08	110.00
27	C	518	LMG	C38-C37-C36	-2.36	102.45	114.42
24	b	620	BCR	C11-C10-C9	-2.36	123.95	127.31
24	A	407	BCR	C27-C26-C25	2.36	126.15	122.73
24	a	410	BCR	C27-C26-C25	2.36	126.15	122.73
22	c	509	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	e	101	LMG	O6-C1-O1	-2.35	104.40	109.97
22	B	610	CLA	C1-C2-C3	-2.35	121.97	126.04
22	b	616	CLA	CMD-C2D-C3D	2.35	129.08	124.68
22	b	619	CLA	CHB-C4A-NA	2.35	127.76	124.51
27	D	411	LMG	C1-C2-C3	-2.35	105.10	110.00
22	C	502	CLA	CHB-C4A-NA	2.35	127.76	124.51
27	A	410	LMG	C38-C37-C36	-2.35	102.50	114.42
27	A	410	LMG	O3-C3-C2	-2.35	104.92	110.35
23	d	406	PL9	C20-C19-C21	2.35	119.22	115.27
27	D	408	LMG	O6-C1-C2	-2.35	105.38	110.35
27	b	625	LMG	C40-C39-C38	-2.35	102.51	114.42
22	c	506	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
25	D	409	DGD	C3G-C2G-C1G	-2.35	106.24	111.79
27	B	621	LMG	O6-C1-O1	-2.35	104.42	109.97
24	y	101	BCR	C3-C2-C1	-2.35	106.22	114.60
22	A	402	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	C	520	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
22	B	601	CLA	CHB-C4A-NA	2.34	127.75	124.51
25	C	516	DGD	CFB-CEB-CDB	-2.34	102.54	114.42
32	D	401	PHO	O1D-CGD-CBD	2.34	129.27	124.48
22	H	101	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
30	a	401	SQD	O48-C23-C24	2.34	119.24	111.91
27	l	101	LMG	C38-C37-C36	-2.34	102.56	114.42
24	K	102	BCR	C15-C14-C13	-2.33	123.98	127.31
30	B	622	SQD	O48-C23-C24	2.33	119.23	111.91
22	B	604	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	d	402	SQD	O48-C23-C24	2.33	119.23	111.91
31	B	627	LMT	C1'-O5'-C5'	-2.33	109.11	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	BCR	C33-C5-C6	-2.33	121.91	124.53
27	m	101	LMG	C1-C2-C3	-2.33	105.15	110.00
34	f	101	HEM	CAA-CBA-CGA	-2.33	108.77	112.67
23	J	101	PL9	C20-C19-C21	2.33	119.19	115.27
22	B	612	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
23	a	409	PL9	C27-C28-C29	-2.33	122.06	127.66
22	C	509	CLA	CMD-C2D-C3D	2.32	129.03	124.68
22	B	603	CLA	O1D-CGD-CBD	2.32	129.24	124.48
24	B	617	BCR	C35-C13-C14	-2.32	119.67	122.92
23	A	406	PL9	C20-C19-C21	2.32	119.17	115.27
22	D	404	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
24	g	101	BCR	C3-C2-C1	-2.32	106.31	114.60
27	c	518	LMG	C38-C37-C36	-2.32	102.66	114.42
22	D	405	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
22	c	520	CLA	CMD-C2D-C3D	2.31	129.01	124.68
27	B	621	LMG	C40-C39-C38	-2.31	102.68	114.42
22	b	607	CLA	CMD-C2D-C3D	2.31	129.00	124.68
22	a	406	CLA	CMD-C2D-C3D	2.31	129.00	124.68
22	B	605	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
22	c	502	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
31	b	603	LMT	C1'-O5'-C5'	-2.31	109.16	113.69
22	B	606	CLA	CMD-C2D-C3D	2.31	128.99	124.68
22	C	508	CLA	CMD-C2D-C3D	2.31	128.99	124.68
24	B	616	BCR	C27-C26-C25	2.31	126.08	122.73
23	d	406	PL9	C27-C28-C29	-2.31	122.11	127.66
22	b	613	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
22	C	512	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
22	C	509	CLA	CHB-C4A-NA	2.30	127.70	124.51
24	g	101	BCR	C15-C16-C17	-2.30	118.75	123.47
24	F	102	BCR	C11-C10-C9	-2.30	124.02	127.31
22	B	607	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	B	609	CLA	CMD-C2D-C3D	2.30	128.99	124.68
22	b	614	CLA	C1-C2-C3	-2.30	122.06	126.04
22	C	510	CLA	CMD-C2D-C3D	2.30	128.98	124.68
24	a	410	BCR	C15-C16-C17	-2.30	118.77	123.47
23	A	406	PL9	C27-C28-C29	-2.30	122.13	127.66
22	c	512	CLA	CMD-C2D-C3D	2.30	128.98	124.68
24	B	616	BCR	C11-C10-C9	-2.29	124.03	127.31
22	A	404	CLA	CMD-C2D-C3D	2.29	128.97	124.68
22	c	508	CLA	CMD-C2D-C3D	2.29	128.97	124.68
22	c	510	CLA	CMD-C2D-C3D	2.29	128.97	124.68
30	A	414	SQD	O48-C23-C24	2.29	119.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	i	102	LMT	C1'-O5'-C5'	-2.29	109.20	113.69
24	b	620	BCR	C27-C26-C25	2.29	126.05	122.73
22	b	619	CLA	CMD-C2D-C3D	2.28	128.95	124.68
23	D	406	PL9	C37-C38-C39	-2.28	122.16	127.66
27	e	101	LMG	C1-C2-C3	-2.28	105.24	110.00
30	b	602	SQD	O48-C23-C24	2.28	119.07	111.91
27	E	101	LMG	O6-C1-O1	-2.28	104.57	109.97
22	c	504	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
24	K	102	BCR	C24-C23-C22	-2.28	122.79	126.23
27	C	521	LMG	O6-C1-O1	-2.28	104.58	109.97
27	A	410	LMG	C1-C2-C3	-2.28	105.25	110.00
22	B	605	CLA	CMD-C2D-C3D	2.28	128.94	124.68
24	C	513	BCR	C3-C4-C5	-2.28	110.01	114.08
22	b	609	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
24	b	621	BCR	C11-C10-C9	-2.28	124.06	127.31
25	d	409	DGD	C3D-C4D-C5D	-2.28	106.18	110.24
22	b	615	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
27	d	411	LMG	O6-C1-O1	-2.28	104.58	109.97
25	a	411	DGD	C3G-C2G-C1G	-2.28	106.41	111.79
23	j	101	PL9	C20-C19-C21	2.27	119.10	115.27
25	A	408	DGD	C3G-C2G-C1G	-2.27	106.41	111.79
22	B	609	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	b	617	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
27	b	625	LMG	C38-C37-C36	-2.27	102.89	114.42
22	D	404	CLA	O1D-CGD-CBD	2.27	129.13	124.48
30	B	626	SQD	O48-C23-C24	2.27	119.03	111.91
24	f	102	BCR	C15-C16-C17	-2.27	118.82	123.47
30	A	414	SQD	C1-O5-C5	2.27	118.14	113.69
22	b	605	CLA	CHB-C4A-NA	2.27	127.65	124.51
24	B	618	BCR	C7-C8-C9	-2.27	122.81	126.23
22	C	508	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	b	605	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
27	C	521	LMG	C38-C37-C36	-2.27	102.92	114.42
22	B	604	CLA	CMD-C2D-C3D	2.27	128.92	124.68
22	B	603	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
24	K	102	BCR	C33-C5-C6	-2.27	121.98	124.53
24	B	616	BCR	C15-C14-C13	-2.27	124.08	127.31
27	d	411	LMG	C1-C2-C3	-2.26	105.28	110.00
24	A	407	BCR	C33-C5-C6	-2.26	121.99	124.53
23	d	406	PL9	C37-C38-C39	-2.26	122.21	127.66
22	C	503	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
24	c	513	BCR	C3-C4-C5	-2.26	110.04	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	l	101	LMG	C1-C2-C3	-2.26	105.28	110.00
25	b	601	DGD	O6D-C1D-O3G	-2.26	104.62	109.97
22	C	502	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
22	B	615	CLA	CMD-C2D-C3D	2.26	128.91	124.68
25	b	624	DGD	C1D-C2D-C3D	-2.26	105.29	110.00
27	D	411	LMG	O3-C3-C2	-2.26	105.13	110.35
22	c	501	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
24	b	620	BCR	C15-C14-C13	-2.26	124.09	127.31
25	c	516	DGD	O3D-C3D-C4D	-2.25	105.14	110.35
27	c	522	LMG	C38-C37-C36	-2.25	102.99	114.42
24	y	101	BCR	C15-C16-C17	-2.25	118.86	123.47
30	f	103	SQD	C3-C4-C5	2.25	114.25	110.24
24	B	619	BCR	C11-C10-C9	-2.25	124.10	127.31
22	c	512	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
24	F	102	BCR	C15-C16-C17	-2.25	118.86	123.47
22	c	509	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	c	508	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	b	608	CLA	CMD-C2D-C3D	2.25	128.88	124.68
31	d	410	LMT	C1'-O5'-C5'	-2.25	109.28	113.69
22	b	616	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
22	C	507	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
27	A	415	LMG	O1-C7-C8	-2.24	105.48	110.90
22	c	509	CLA	CMD-C2D-C3D	2.24	128.87	124.68
24	B	619	BCR	C38-C26-C25	-2.24	122.01	124.53
34	v	201	HEM	C1D-C2D-C3D	-2.24	105.44	107.00
24	b	623	BCR	C38-C26-C25	-2.24	122.02	124.53
25	C	517	DGD	C3G-O3G-C1D	2.24	118.11	113.74
27	B	621	LMG	C38-C37-C36	-2.24	103.07	114.42
24	C	513	BCR	C11-C10-C9	-2.24	124.12	127.31
34	v	201	HEM	CMB-C2B-C3B	2.24	128.86	124.68
22	b	607	CLA	O1D-CGD-CBD	2.24	129.06	124.48
34	F	101	HEM	CBD-CAD-C3D	-2.23	108.36	112.48
22	C	510	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
24	c	521	BCR	C33-C5-C6	-2.23	122.02	124.53
23	D	406	PL9	C32-C33-C34	-2.23	122.28	127.66
24	B	619	BCR	C24-C23-C22	-2.23	122.86	126.23
30	d	402	SQD	C4-C3-C2	2.23	114.72	110.82
22	B	609	CLA	C1D-CHD-C4C	2.23	125.50	122.56
24	x	101	BCR	C29-C30-C25	2.23	113.91	110.48
22	c	520	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	C	511	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
25	B	625	DGD	O6D-C1D-O3G	-2.23	104.70	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	521	BCR	C11-C10-C9	-2.23	124.13	127.31
30	a	415	SQD	C4-C3-C2	2.22	114.70	110.82
22	C	501	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	C	509	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	B	605	CLA	O1D-CGD-CBD	2.22	129.02	124.48
22	D	404	CLA	CHB-C4A-NA	2.22	127.58	124.51
27	m	101	LMG	O2-C2-C1	-2.22	104.66	110.05
27	m	101	LMG	C1-O6-C5	-2.22	109.34	113.69
22	a	404	CLA	CMD-C2D-C3D	2.22	128.82	124.68
24	c	521	BCR	C24-C23-C22	-2.22	122.89	126.23
22	d	404	CLA	O1D-CGD-CBD	2.22	129.02	124.48
24	c	513	BCR	C8-C7-C6	-2.22	120.98	127.20
22	d	404	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	D	406	PL9	O1-C4-C3	-2.21	118.28	120.72
27	b	625	LMG	O6-C1-O1	-2.21	104.73	109.97
23	d	406	PL9	C32-C33-C34	-2.21	122.33	127.66
25	C	515	DGD	C1D-C2D-C3D	-2.21	105.39	110.00
22	d	404	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	f	102	BCR	C11-C10-C9	-2.21	124.16	127.31
22	b	610	CLA	CMD-C2D-C3D	2.21	128.81	124.68
22	b	607	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	j	102	BCR	C20-C21-C22	-2.21	124.16	127.31
25	C	516	DGD	CBB-CAB-C9B	-2.20	103.24	114.42
24	a	410	BCR	C15-C14-C13	-2.20	124.17	127.31
22	b	610	CLA	C1D-CHD-C4C	2.20	125.46	122.56
27	d	407	LMG	O3-C3-C2	-2.20	105.27	110.35
22	A	402	CLA	CMD-C2D-C3D	2.20	128.79	124.68
27	D	407	LMG	O3-C3-C2	-2.20	105.27	110.35
27	e	101	LMG	O3-C3-C2	-2.19	105.28	110.35
24	J	102	BCR	C20-C21-C22	-2.19	124.18	127.31
24	c	513	BCR	C27-C26-C25	2.19	125.92	122.73
22	b	618	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
25	c	516	DGD	C3D-C4D-C5D	-2.19	106.33	110.24
25	A	408	DGD	CAB-C9B-C8B	-2.19	103.30	114.42
22	c	503	CLA	O2D-CGD-CBD	2.19	115.16	111.27
25	B	620	DGD	C4E-C3E-C2E	-2.19	107.00	110.82
25	c	515	DGD	O5D-C6D-C5D	-2.19	105.00	109.05
25	c	516	DGD	CBB-CAB-C9B	-2.19	103.33	114.42
27	D	408	LMG	O6-C1-O1	-2.18	104.80	109.97
27	b	625	LMG	O3-C3-C2	-2.18	105.30	110.35
30	F	103	SQD	C3-C4-C5	2.18	114.13	110.24
22	b	615	CLA	O2A-CGA-O1A	-2.18	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	102	BCR	C29-C30-C25	2.18	113.84	110.48
25	C	516	DGD	C3D-C4D-C5D	-2.18	106.35	110.24
22	B	614	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
25	a	411	DGD	CAB-C9B-C8B	-2.18	103.35	114.42
24	J	102	BCR	C29-C30-C25	2.18	113.84	110.48
25	B	620	DGD	C3G-C2G-C1G	-2.18	106.63	111.79
27	I	101	LMG	O3-C3-C2	-2.18	105.31	110.35
24	C	513	BCR	C8-C7-C6	-2.18	121.08	127.20
27	c	518	LMG	O7-C10-O9	-2.18	118.44	123.70
23	j	101	PL9	O2-C1-C2	-2.18	116.79	121.78
31	B	624	LMT	C1'-O5'-C5'	-2.18	109.42	113.69
25	a	411	DGD	C1D-C2D-C3D	-2.18	105.46	110.00
27	d	411	LMG	O3-C3-C2	-2.18	105.32	110.35
30	A	413	SQD	C4-C3-C2	2.17	114.62	110.82
22	A	403	CLA	CMD-C2D-C3D	2.17	128.75	124.68
24	C	514	BCR	C38-C26-C25	-2.17	122.09	124.53
31	I	102	LMT	C1'-O5'-C5'	-2.17	109.42	113.69
27	d	408	LMG	O6-C1-O1	-2.17	104.83	109.97
27	a	402	LMG	O1-C7-C8	-2.17	105.66	110.90
22	B	615	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
27	B	621	LMG	O3-C3-C2	-2.17	105.33	110.35
22	B	608	CLA	C1-C2-C3	-2.17	122.29	126.04
27	A	410	LMG	O7-C10-O9	-2.17	118.46	123.70
24	f	102	BCR	C27-C26-C25	2.17	125.88	122.73
23	d	406	PL9	O1-C4-C3	-2.17	118.33	120.72
27	C	518	LMG	O3-C3-C2	-2.17	105.34	110.35
22	b	614	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
25	C	516	DGD	O3D-C3D-C4D	-2.17	105.34	110.35
23	d	406	PL9	O2-C1-C2	-2.17	116.82	121.78
23	j	101	PL9	O2-C1-C6	2.17	124.34	120.59
22	c	511	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
25	C	517	DGD	CBB-CAB-C9B	-2.17	103.43	114.42
25	b	601	DGD	CBB-CAB-C9B	-2.17	103.43	114.42
27	l	101	LMG	O3-C3-C2	-2.16	105.34	110.35
25	b	624	DGD	C3G-C2G-C1G	-2.16	106.67	111.79
22	c	507	CLA	O2D-CGD-CBD	2.16	115.11	111.27
22	B	610	CLA	C4D-C3D-CAD	-2.16	107.26	108.47
24	b	622	BCR	C7-C8-C9	-2.16	122.97	126.23
27	c	522	LMG	O2-C2-C1	-2.16	104.79	110.05
27	D	411	LMG	O6-C1-O1	-2.16	104.85	109.97
22	c	520	CLA	C1D-CHD-C4C	2.16	125.41	122.56
26	a	412	LHG	C27-C26-C25	-2.16	103.46	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	C1D-CHD-C4C	2.16	125.41	122.56
24	B	617	BCR	C11-C10-C9	-2.16	124.23	127.31
25	B	625	DGD	CBB-CAB-C9B	-2.16	103.46	114.42
27	C	518	LMG	O7-C10-O9	-2.16	118.49	123.70
34	V	201	HEM	CMB-C2B-C3B	2.16	128.71	124.68
25	c	517	DGD	CBB-CAB-C9B	-2.16	103.48	114.42
22	b	619	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
22	C	507	CLA	C1-C2-C3	-2.15	122.32	126.04
24	H	102	BCR	C29-C30-C25	2.15	113.80	110.48
24	C	513	BCR	C27-C26-C25	2.15	125.86	122.73
24	b	623	BCR	C24-C23-C22	-2.15	122.98	126.23
27	D	407	LMG	O2-C2-C1	-2.15	104.82	110.05
26	A	409	LHG	C27-C26-C25	-2.15	103.51	114.42
22	B	611	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
23	J	101	PL9	O2-C1-C2	-2.15	116.86	121.78
22	c	510	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
32	D	402	PHO	C1B-NB-C4B	2.14	110.55	106.51
22	B	610	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
22	b	618	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
27	a	402	LMG	O3-C3-C2	-2.14	105.40	110.35
25	C	516	DGD	CAB-C9B-C8B	-2.14	103.56	114.42
22	B	603	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
25	d	409	DGD	C5B-C4B-C3B	-2.14	103.57	114.42
24	H	102	BCR	C16-C15-C14	-2.14	119.09	123.47
25	D	409	DGD	C3D-C4D-C5D	-2.14	106.43	110.24
27	d	408	LMG	O6-C1-C2	-2.14	105.83	110.35
22	b	609	CLA	O1D-CGD-CBD	2.14	128.85	124.48
24	K	102	BCR	C7-C8-C9	-2.13	123.01	126.23
24	b	621	BCR	C7-C8-C9	-2.13	123.01	126.23
27	i	101	LMG	O2-C2-C1	-2.13	104.86	110.05
24	c	514	BCR	C38-C26-C25	-2.13	122.14	124.53
22	c	512	CLA	C1D-CHD-C4C	2.13	125.37	122.56
25	b	601	DGD	CAB-C9B-C8B	-2.13	103.61	114.42
24	A	407	BCR	C24-C23-C22	-2.13	123.02	126.23
24	b	622	BCR	C33-C5-C6	-2.13	122.14	124.53
23	a	409	PL9	O2-C1-C6	2.13	124.28	120.59
25	c	515	DGD	C1D-C2D-C3D	-2.13	105.56	110.00
27	M	101	LMG	O2-C2-C1	-2.13	104.88	110.05
25	B	625	DGD	CAB-C9B-C8B	-2.13	103.62	114.42
22	C	506	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
27	c	518	LMG	O3-C3-C2	-2.13	105.43	110.35
27	c	522	LMG	O3-C3-C2	-2.13	105.43	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	PL9	O2-C1-C6	2.13	124.27	120.59
27	l	101	LMG	O7-C10-O9	-2.13	118.56	123.70
27	d	407	LMG	O2-C2-C1	-2.13	104.88	110.05
23	J	101	PL9	O2-C1-C6	2.13	124.27	120.59
22	b	609	CLA	CMD-C2D-C3D	2.12	128.65	124.68
31	b	627	LMT	C1'-O5'-C5'	-2.12	109.52	113.69
24	J	102	BCR	C33-C5-C6	-2.12	122.14	124.53
24	A	407	BCR	C38-C26-C25	-2.12	122.15	124.53
24	g	101	BCR	C24-C23-C22	-2.12	123.03	126.23
32	D	401	PHO	C1B-NB-C4B	2.12	110.51	106.51
27	b	625	LMG	O2-C2-C1	-2.12	104.90	110.05
27	I	101	LMG	O2-C2-C1	-2.12	104.90	110.05
32	a	407	PHO	CMB-C2B-C1B	-2.12	121.80	125.06
32	a	407	PHO	C1B-NB-C4B	2.12	110.50	106.51
27	I	101	LMG	O7-C10-O9	-2.12	118.58	123.70
23	A	406	PL9	O2-C1-C2	-2.12	116.93	121.78
27	i	101	LMG	O3-C3-C2	-2.12	105.46	110.35
27	E	101	LMG	O3-C3-C2	-2.12	105.46	110.35
24	B	616	BCR	C15-C16-C17	-2.11	119.14	123.47
23	d	406	PL9	O2-C1-C6	2.11	124.25	120.59
30	B	622	SQD	C4-C3-C2	2.11	114.51	110.82
22	b	614	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
24	C	514	BCR	C24-C23-C22	-2.11	123.04	126.23
22	c	509	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
22	c	507	CLA	C1-C2-C3	-2.11	122.39	126.04
27	A	415	LMG	O3-C3-C2	-2.11	105.47	110.35
23	D	406	PL9	O2-C1-C2	-2.11	116.95	121.78
22	c	504	CLA	O1D-CGD-CBD	2.11	128.79	124.48
32	D	402	PHO	CMB-C2B-C1B	-2.11	121.82	125.06
25	B	620	DGD	C1D-C2D-C3D	-2.11	105.61	110.00
27	C	521	LMG	O3-C3-C2	-2.10	105.48	110.35
22	c	506	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
30	f	103	SQD	O48-C23-C24	2.10	118.51	111.91
24	b	622	BCR	C20-C21-C22	-2.10	124.31	127.31
25	c	517	DGD	CAB-C9B-C8B	-2.10	103.75	114.42
22	C	512	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
22	C	503	CLA	O2D-CGD-CBD	2.10	115.00	111.27
22	D	405	CLA	C1-C2-C3	-2.10	122.41	126.04
22	B	614	CLA	C1D-CHD-C4C	2.10	125.33	122.56
32	d	401	PHO	C1B-NB-C4B	2.10	110.47	106.51
27	i	101	LMG	O1-C7-C8	-2.10	105.83	110.90
32	d	401	PHO	C1-C2-C3	-2.10	122.41	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	618	CLA	C1D-CHD-C4C	2.10	125.33	122.56
24	F	102	BCR	C27-C26-C25	2.10	125.78	122.73
22	C	504	CLA	O1D-CGD-CBD	2.10	128.78	124.48
27	C	521	LMG	O2-C2-C1	-2.10	104.95	110.05
22	c	512	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
24	a	410	BCR	C24-C23-C22	-2.09	123.07	126.23
25	C	515	DGD	O5D-C6D-C5D	-2.09	105.18	109.05
22	B	611	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
24	F	102	BCR	C7-C8-C9	-2.09	123.08	126.23
22	B	602	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	D	409	DGD	C5B-C4B-C3B	-2.09	103.81	114.42
22	C	507	CLA	C1D-CHD-C4C	2.09	125.31	122.56
23	a	409	PL9	O2-C1-C2	-2.09	117.00	121.78
22	B	601	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
25	D	409	DGD	CAB-C9B-C8B	-2.09	103.83	114.42
26	C	519	LHG	C27-C26-C25	-2.09	103.84	114.42
27	c	518	LMG	O2-C2-C1	-2.09	104.98	110.05
25	C	517	DGD	CAB-C9B-C8B	-2.08	103.85	114.42
25	c	517	DGD	C3G-O3G-C1D	2.08	117.81	113.74
26	c	519	LHG	C27-C26-C25	-2.08	103.85	114.42
22	c	508	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
24	a	410	BCR	C38-C26-C25	-2.08	122.19	124.53
25	c	516	DGD	CAB-C9B-C8B	-2.08	103.87	114.42
22	c	503	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
22	c	501	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
22	b	606	CLA	C1D-CHD-C4C	2.08	125.30	122.56
24	j	102	BCR	C33-C5-C6	-2.07	122.20	124.53
27	A	415	LMG	O7-C10-O9	-2.07	118.69	123.70
27	c	518	LMG	O1-C7-C8	-2.07	105.89	110.90
24	B	618	BCR	C33-C5-C6	-2.07	122.20	124.53
22	B	615	CLA	OBD-CAD-CBD	-2.07	122.94	125.89
22	a	405	CLA	CMD-C2D-C3D	2.07	128.55	124.68
27	m	101	LMG	O3-C3-C2	-2.07	105.56	110.35
27	d	411	LMG	O7-C10-O9	-2.07	118.70	123.70
24	x	101	BCR	C15-C16-C17	-2.07	119.24	123.47
22	B	612	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
23	a	409	PL9	O1-C4-C3	-2.06	118.45	120.72
24	B	619	BCR	C33-C5-C6	-2.06	122.21	124.53
24	b	623	BCR	C33-C5-C6	-2.06	122.21	124.53
25	d	409	DGD	CAB-C9B-C8B	-2.06	103.95	114.42
22	B	606	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
22	B	614	CLA	O2A-CGA-O1A	-2.06	118.39	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	C1D-CHD-C4C	2.06	125.28	122.56
22	b	616	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	c	514	BCR	C24-C23-C22	-2.06	123.13	126.23
22	C	509	CLA	C1D-CHD-C4C	2.06	125.27	122.56
22	b	614	CLA	C1D-CHD-C4C	2.06	125.27	122.56
25	D	409	DGD	CBB-CAB-C9B	-2.06	103.98	114.42
27	M	101	LMG	O3-C3-C2	-2.06	105.59	110.35
22	C	501	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	c	521	BCR	C7-C8-C9	-2.06	123.13	126.23
24	H	102	BCR	C15-C16-C17	-2.06	119.26	123.47
25	C	515	DGD	C5B-C4B-C3B	-2.05	104.00	114.42
24	b	623	BCR	C15-C16-C17	-2.05	119.27	123.47
25	A	408	DGD	C5B-C4B-C3B	-2.05	104.00	114.42
24	B	617	BCR	C24-C23-C22	-2.05	123.13	126.23
22	C	508	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	d	409	DGD	CBB-CAB-C9B	-2.05	104.00	114.42
22	B	615	CLA	C1D-CHD-C4C	2.05	125.27	122.56
25	A	408	DGD	C1D-C2D-C3D	-2.05	105.73	110.00
27	D	411	LMG	O7-C10-O9	-2.05	118.75	123.70
22	b	610	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
22	b	605	CLA	C1-C2-C3	-2.05	122.50	126.04
24	b	622	BCR	C27-C26-C25	2.05	125.70	122.73
22	d	405	CLA	C4D-C3D-CAD	-2.05	107.33	108.47
22	C	520	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
22	b	606	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
23	D	406	PL9	O2-C1-C6	2.04	124.13	120.59
25	c	515	DGD	C5B-C4B-C3B	-2.04	104.05	114.42
25	b	624	DGD	CAB-C9B-C8B	-2.04	104.06	114.42
22	B	606	CLA	C1-C2-C3	-2.04	122.51	126.04
23	d	406	PL9	C36-C34-C33	-2.04	116.99	121.12
27	e	101	LMG	O1-C7-C8	-2.04	105.97	110.90
23	d	406	PL9	C31-C32-C33	-2.04	105.18	111.88
30	F	103	SQD	O48-C23-C24	2.04	118.31	111.91
22	C	502	CLA	C1-C2-C3	-2.04	122.52	126.04
27	B	621	LMG	O2-C2-C1	-2.04	105.10	110.05
22	b	613	CLA	C1D-CHD-C4C	2.03	125.24	122.56
22	c	520	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
27	C	518	LMG	O2-C2-C1	-2.03	105.11	110.05
32	D	401	PHO	O2A-CGA-O1A	-2.03	118.47	123.59
22	B	607	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	c	511	CLA	C1D-CHD-C4C	2.03	125.24	122.56
22	b	607	CLA	O2A-CGA-O1A	-2.03	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	DGD	C5B-C4B-C3B	-2.03	104.14	114.42
22	a	406	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
27	b	625	LMG	O7-C10-O9	-2.02	118.81	123.70
22	C	509	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
25	C	517	DGD	C5B-C4B-C3B	-2.02	104.16	114.42
25	B	620	DGD	C5B-C4B-C3B	-2.02	104.17	114.42
27	l	101	LMG	O2-C2-C1	-2.02	105.14	110.05
27	M	101	LMG	C1-O6-C5	-2.02	109.72	113.69
22	b	619	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	a	405	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
22	A	403	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
27	C	518	LMG	O1-C7-C8	-2.01	106.04	110.90
25	B	620	DGD	CAB-C9B-C8B	-2.01	104.21	114.42
27	A	410	LMG	O2-C2-C1	-2.01	105.16	110.05
22	A	402	CLA	O1D-CGD-CBD	2.01	128.60	124.48
22	C	502	CLA	C1D-CHD-C4C	2.01	125.21	122.56
24	x	101	BCR	C16-C15-C14	-2.01	119.36	123.47
22	C	510	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
22	d	404	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
27	i	101	LMG	O7-C10-O9	-2.01	118.85	123.70
22	B	606	CLA	C1D-CHD-C4C	2.01	125.21	122.56
25	c	517	DGD	C5B-C4B-C3B	-2.01	104.25	114.42
22	b	613	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
27	E	101	LMG	O1-C7-C8	-2.00	106.06	110.90
34	F	101	HEM	CMC-C2C-C3C	2.00	128.43	124.68
27	C	521	LMG	C1-C2-C3	-2.00	105.82	110.00
24	B	617	BCR	C7-C8-C9	-2.00	123.21	126.23
22	B	613	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
22	d	405	CLA	C1-C2-C3	-2.00	122.58	126.04
22	c	509	CLA	C1D-CHD-C4C	2.00	125.20	122.56
22	B	611	CLA	C1D-CHD-C4C	2.00	125.20	122.56
22	a	404	CLA	O1D-CGD-CBD	2.00	128.58	124.48
23	A	406	PL9	O1-C4-C3	-2.00	118.52	120.72
22	C	512	CLA	C1D-CHD-C4C	2.00	125.20	122.56
22	H	101	CLA	C1-C2-C3	-2.00	122.58	126.04
27	A	410	LMG	O1-C1-C2	-2.00	105.18	108.30

All (209) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	505	CLA	NC
22	C	505	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	505	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	a	408	CLA	NC
22	a	408	CLA	ND
22	a	408	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	h	101	CLA	NC
22	h	101	CLA	ND

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Mol	Chain	Res	Type	Atom
22	h	101	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	608	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	C	520	CLA	NC
22	C	520	CLA	ND
22	C	520	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	607	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	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	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA

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Mol	Chain	Res	Type	Atom
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	ND
22	D	404	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	d	404	CLA	NC
22	d	404	CLA	ND
22	d	404	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA

All (2133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	K	102	BCR	C7-C8-C9-C10
24	K	102	BCR	C7-C8-C9-C34
27	C	521	LMG	C2-C1-O1-C7
27	C	521	LMG	O6-C1-O1-C7
22	C	510	CLA	CHA-CBD-CGD-O1D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	C6-C7-C8-C9
23	D	406	PL9	C27-C28-C29-C31
23	D	406	PL9	C34-C36-C37-C38
26	C	519	LHG	C4-O6-P-O4
22	B	601	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	C1A-C2A-CAA-CBA
22	b	610	CLA	C3A-C2A-CAA-CBA
22	b	610	CLA	C2A-CAA-CBA-CGA
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
27	c	518	LMG	O10-C28-O8-C9
30	a	401	SQD	C24-C23-O48-C46
27	E	101	LMG	C2-C1-O1-C7
27	E	101	LMG	O6-C1-O1-C7
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CBD-CGD-O2D-CED
25	c	516	DGD	O1B-C1B-O2G-C2G
25	c	516	DGD	O2G-C2G-C3G-O3G
25	c	516	DGD	C2D-C1D-O3G-C3G
25	c	516	DGD	O6D-C1D-O3G-C3G
25	c	515	DGD	C2B-C1B-O2G-C2G
25	c	515	DGD	O1B-C1B-O2G-C2G
25	c	515	DGD	C2E-C1E-O5D-C6D
22	a	405	CLA	C1A-C2A-CAA-CBA
22	a	405	CLA	C3A-C2A-CAA-CBA
22	a	405	CLA	CHA-CBD-CGD-O1D
22	a	405	CLA	CHA-CBD-CGD-O2D
25	C	517	DGD	C2D-C1D-O3G-C3G
25	C	517	DGD	O6D-C1D-O3G-C3G
25	D	409	DGD	O6D-C1D-O3G-C3G
24	g	101	BCR	C7-C8-C9-C10
34	V	201	HEM	C2D-C3D-CAD-CBD
34	V	201	HEM	C4D-C3D-CAD-CBD
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	C9-C8-O7-C10
27	C	518	LMG	O9-C10-O7-C8
27	C	518	LMG	C11-C10-O7-C8
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	521	BCR	C7-C8-C9-C34
22	h	101	CLA	C1A-C2A-CAA-CBA
22	h	101	CLA	C2-C3-C5-C6
22	h	101	CLA	C4-C3-C5-C6
22	h	101	CLA	C6-C7-C8-C9
22	b	609	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C3A-C2A-CAA-CBA
27	D	408	LMG	C2-C1-O1-C7
27	D	408	LMG	O6-C1-O1-C7
22	A	404	CLA	CHA-CBD-CGD-O1D
22	B	615	CLA	CBD-CGD-O2D-CED
22	b	619	CLA	C3A-C2A-CAA-CBA
22	b	619	CLA	CBD-CGD-O2D-CED
24	b	621	BCR	C21-C22-C23-C24
24	b	621	BCR	C23-C24-C25-C26
22	B	609	CLA	CBD-CGD-O2D-CED
22	A	402	CLA	CBD-CGD-O2D-CED
27	d	411	LMG	O9-C10-O7-C8
27	d	411	LMG	C11-C10-O7-C8
22	B	604	CLA	CBD-CGD-O2D-CED
24	f	102	BCR	C1-C6-C7-C8
24	f	102	BCR	C7-C8-C9-C10
23	d	406	PL9	C27-C28-C29-C31
23	d	406	PL9	C34-C36-C37-C38
26	c	519	LHG	C3-O3-P-O6
26	c	519	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
24	J	102	BCR	C1-C6-C7-C8
24	J	102	BCR	C21-C22-C23-C24
22	b	607	CLA	CBD-CGD-O2D-CED
27	e	101	LMG	C2-C1-O1-C7
27	e	101	LMG	O6-C1-O1-C7
27	e	101	LMG	C7-C8-O7-C10
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	y	101	BCR	C7-C8-C9-C10
27	m	101	LMG	O9-C10-O7-C8
27	c	522	LMG	C2-C1-O1-C7
27	c	522	LMG	O6-C1-O1-C7
24	b	623	BCR	C23-C24-C25-C30
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	605	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C3A-C2A-CAA-CBA
27	b	625	LMG	C11-C10-O7-C8
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	A	403	CLA	C1A-C2A-CAA-CBA
22	A	403	CLA	C3A-C2A-CAA-CBA
22	A	403	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
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
22	a	404	CLA	CBD-CGD-O2D-CED
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	612	CLA	CBD-CGD-O2D-CED
25	A	408	DGD	C2D-C1D-O3G-C3G
25	b	624	DGD	C2E-C1E-O5D-C6D
26	a	412	LHG	C1-C2-C3-O3
22	b	616	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	A	414	SQD	C24-C23-O48-C46
34	v	201	HEM	C2D-C3D-CAD-CBD
23	a	409	PL9	C7-C8-C9-C10
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-C20
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
24	H	102	BCR	C7-C8-C9-C34
24	H	102	BCR	C21-C22-C23-C24
24	H	102	BCR	C37-C22-C23-C24
24	C	513	BCR	C1-C6-C7-C8
24	C	513	BCR	C6-C7-C8-C9
22	b	605	CLA	CBD-CGD-O2D-CED
27	d	407	LMG	O1-C7-C8-O7
27	d	407	LMG	C11-C10-O7-C8
30	B	626	SQD	O5-C5-C6-S
25	a	411	DGD	C2D-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
24	x	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C21-C22-C23-C24
22	b	617	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	b	617	CLA	CAD-CBD-CGD-O1D
22	b	617	CLA	CAD-CBD-CGD-O2D
24	c	513	BCR	C6-C7-C8-C9
25	C	516	DGD	O1B-C1B-O2G-C2G
25	C	516	DGD	C2D-C1D-O3G-C3G
25	C	516	DGD	O6D-C1D-O3G-C3G
24	b	620	BCR	C1-C6-C7-C8
22	B	607	CLA	C1A-C2A-CAA-CBA
27	D	407	LMG	O1-C7-C8-O7
27	D	407	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
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
30	b	602	SQD	O5-C5-C6-S
22	B	606	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C3A-C2A-CAA-CBA
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	CBD-CGD-O2D-CED
27	D	411	LMG	O9-C10-O7-C8
27	D	411	LMG	C11-C10-O7-C8
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
24	B	617	BCR	C21-C22-C23-C24
24	B	617	BCR	C23-C24-C25-C26
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
22	B	602	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C2-C3-C5-C6
22	B	602	CLA	C4-C3-C5-C6
24	j	102	BCR	C1-C6-C7-C8
24	j	102	BCR	C21-C22-C23-C24
27	B	621	LMG	C11-C10-O7-C8
25	c	517	DGD	C2D-C1D-O3G-C3G
25	c	517	DGD	O6D-C1D-O3G-C3G
25	d	409	DGD	O6D-C1D-O3G-C3G
23	j	101	PL9	C12-C13-C14-C16
23	j	101	PL9	C22-C23-C24-C25
23	j	101	PL9	C22-C23-C24-C26
22	b	608	CLA	CBD-CGD-O2D-CED
22	b	608	CLA	C4-C3-C5-C6
26	A	409	LHG	C1-C2-C3-O3
22	b	611	CLA	C1A-C2A-CAA-CBA
22	D	404	CLA	C2-C3-C5-C6
22	D	404	CLA	C4-C3-C5-C6
22	b	606	CLA	C2-C3-C5-C6
22	b	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	F	102	BCR	C1-C6-C7-C8
24	F	102	BCR	C7-C8-C9-C10
27	d	408	LMG	C2-C1-O1-C7
27	d	408	LMG	O6-C1-O1-C7
24	B	616	BCR	C1-C6-C7-C8
30	B	622	SQD	C2-C1-O6-C44
30	B	622	SQD	O5-C1-O6-C44
30	B	622	SQD	O49-C7-O47-C45
30	B	622	SQD	C8-C7-O47-C45
22	C	511	CLA	C1A-C2A-CAA-CBA
25	C	515	DGD	C2B-C1B-O2G-C2G
25	C	515	DGD	O1B-C1B-O2G-C2G
25	C	515	DGD	C2E-C1E-O5D-C6D
22	d	404	CLA	C2-C3-C5-C6
22	d	404	CLA	C4-C3-C5-C6
27	M	101	LMG	O9-C10-O7-C8
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	CBD-CGD-O2D-CED
25	B	620	DGD	C2E-C1E-O5D-C6D
22	C	503	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
22	c	504	CLA	O1D-CGD-O2D-CED
22	a	404	CLA	O1D-CGD-O2D-CED
22	C	504	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	O1D-CGD-O2D-CED
22	b	619	CLA	O1D-CGD-O2D-CED
22	A	402	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	O1D-CGD-O2D-CED
22	C	505	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	CBD-CGD-O2D-CED
22	C	510	CLA	CBD-CGD-O2D-CED
22	b	610	CLA	CBD-CGD-O2D-CED
22	C	503	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
22	b	612	CLA	CBD-CGD-O2D-CED
22	B	608	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	b	617	CLA	CBD-CGD-O2D-CED
22	C	520	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	520	CLA	CBD-CGD-O2D-CED
22	c	501	CLA	CBD-CGD-O2D-CED
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	508	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	CBD-CGD-O2D-CED
22	C	507	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
30	a	401	SQD	O10-C23-O48-C46
27	E	101	LMG	O10-C28-O8-C9
30	A	414	SQD	O10-C23-O48-C46
31	b	604	LMT	C3'-C4'-O1B-C1B
31	B	628	LMT	C3'-C4'-O1B-C1B
25	b	624	DGD	C4D-C5D-C6D-O5D
22	C	510	CLA	O1D-CGD-O2D-CED
22	B	601	CLA	O1D-CGD-O2D-CED
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	O1D-CGD-O2D-CED
27	l	101	LMG	C29-C28-O8-C9
30	f	103	SQD	C24-C23-O48-C46
30	F	103	SQD	C24-C23-O48-C46
23	A	406	PL9	C37-C38-C39-C40
23	a	409	PL9	C37-C38-C39-C40
32	a	407	PHO	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	CBD-CGD-O2D-CED
22	B	606	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
27	l	101	LMG	O10-C28-O8-C9
27	C	518	LMG	O10-C28-O8-C9
27	D	408	LMG	O10-C28-O8-C9
30	f	103	SQD	O10-C23-O48-C46
27	e	101	LMG	O10-C28-O8-C9
27	A	410	LMG	O10-C28-O8-C9
30	F	103	SQD	O10-C23-O48-C46
27	d	407	LMG	O10-C28-O8-C9
27	D	407	LMG	O10-C28-O8-C9
27	d	408	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	616	CLA	O1D-CGD-O2D-CED
31	B	627	LMT	C3'-C4'-O1B-C1B
32	D	402	PHO	CBD-CGD-O2D-CED
22	B	607	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
25	D	409	DGD	O1B-C1B-O2G-C2G
27	i	101	LMG	O9-C10-O7-C8
27	I	101	LMG	O9-C10-O7-C8
27	b	625	LMG	O9-C10-O7-C8
27	A	415	LMG	O9-C10-O7-C8
27	d	407	LMG	O9-C10-O7-C8
27	D	407	LMG	O9-C10-O7-C8
27	a	402	LMG	O9-C10-O7-C8
27	B	621	LMG	O9-C10-O7-C8
25	d	409	DGD	O1B-C1B-O2G-C2G
31	b	603	LMT	C3'-C4'-O1B-C1B
22	A	404	CLA	C3-C5-C6-C7
22	a	406	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
22	B	607	CLA	C3-C5-C6-C7
22	B	613	CLA	C3-C5-C6-C7
22	b	611	CLA	C3-C5-C6-C7
27	c	518	LMG	C29-C28-O8-C9
27	C	518	LMG	C29-C28-O8-C9
27	D	408	LMG	C29-C28-O8-C9
27	A	410	LMG	C29-C28-O8-C9
27	d	408	LMG	C29-C28-O8-C9
25	c	516	DGD	C2B-C1B-O2G-C2G
27	m	101	LMG	C11-C10-O7-C8
25	B	625	DGD	C2B-C1B-O2G-C2G
25	C	516	DGD	C2B-C1B-O2G-C2G
25	b	601	DGD	C2B-C1B-O2G-C2G
27	M	101	LMG	C11-C10-O7-C8
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	507	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	i	101	LMG	O6-C5-C6-O5
27	I	101	LMG	O6-C5-C6-O5
22	B	604	CLA	C4-C3-C5-C6
22	b	608	CLA	C2-C3-C5-C6
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	609	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	C2A-CAA-CBA-CGA
22	b	605	CLA	C2A-CAA-CBA-CGA
22	c	507	CLA	C2A-CAA-CBA-CGA
22	C	507	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2A-CAA-CBA-CGA
31	i	102	LMT	C3'-C4'-O1B-C1B
32	d	401	PHO	C3-C5-C6-C7
27	C	521	LMG	C29-C28-O8-C9
25	D	409	DGD	C2A-C1A-O1G-C1G
27	c	522	LMG	C29-C28-O8-C9
27	d	407	LMG	C29-C28-O8-C9
27	D	407	LMG	C29-C28-O8-C9
25	A	408	DGD	O6E-C5E-C6E-O5E
25	b	624	DGD	O6E-C5E-C6E-O5E
25	B	620	DGD	O6E-C5E-C6E-O5E
31	I	102	LMT	C3'-C4'-O1B-C1B
22	c	505	CLA	O1D-CGD-O2D-CED
25	B	620	DGD	C4D-C5D-C6D-O5D
23	J	101	PL9	C7-C8-C9-C10
23	j	101	PL9	C7-C8-C9-C10
22	b	610	CLA	O1D-CGD-O2D-CED
22	b	612	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
22	c	520	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	O1D-CGD-O2D-CED
22	C	501	CLA	O1D-CGD-O2D-CED
25	a	411	DGD	O6E-C5E-C6E-O5E
27	e	101	LMG	O9-C10-O7-C8
23	A	406	PL9	C22-C23-C24-C26
23	J	101	PL9	C7-C8-C9-C11
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	409	DGD	O1A-C1A-O1G-C1G
25	d	409	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	C8-C9-O8-C28
27	d	407	LMG	O6-C5-C6-O5
27	I	101	LMG	C4-C5-C6-O5
22	b	615	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED
26	a	412	LHG	O2-C2-C3-O3
26	A	409	LHG	O2-C2-C3-O3
32	D	401	PHO	C3-C5-C6-C7
22	C	508	CLA	C3-C5-C6-C7
27	E	101	LMG	C29-C28-O8-C9
27	e	101	LMG	C29-C28-O8-C9
25	d	409	DGD	C2A-C1A-O1G-C1G
27	C	521	LMG	O10-C28-O8-C9
27	c	522	LMG	O10-C28-O8-C9
25	c	515	DGD	O6E-C5E-C6E-O5E
27	D	407	LMG	O6-C5-C6-O5
27	i	101	LMG	C4-C5-C6-O5
22	C	505	CLA	O1D-CGD-O2D-CED
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	O1D-CGD-O2D-CED
25	D	409	DGD	C2B-C1B-O2G-C2G
27	D	408	LMG	C11-C10-O7-C8
30	f	103	SQD	C8-C7-O47-C45
27	A	415	LMG	C11-C10-O7-C8
30	F	103	SQD	C8-C7-O47-C45
27	a	402	LMG	C11-C10-O7-C8
25	d	409	DGD	C2B-C1B-O2G-C2G
27	d	408	LMG	C11-C10-O7-C8
22	b	611	CLA	CBD-CGD-O2D-CED
25	b	624	DGD	C4E-C5E-C6E-O5E
27	c	518	LMG	C8-C9-O8-C28
25	C	515	DGD	O6E-C5E-C6E-O5E
25	B	620	DGD	C4E-C5E-C6E-O5E
22	C	509	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	C3-C5-C6-C7
32	D	401	PHO	CBA-CGA-O2A-C1
22	B	608	CLA	O1D-CGD-O2D-CED
27	D	408	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	c	518	LMG	O6-C5-C6-O5
25	C	516	DGD	O6E-C5E-C6E-O5E
32	d	401	PHO	C4-C3-C5-C6
32	D	401	PHO	C4-C3-C5-C6
32	d	401	PHO	C2-C3-C5-C6
32	D	401	PHO	C2-C3-C5-C6
22	B	601	CLA	C2A-CAA-CBA-CGA
25	c	516	DGD	O6E-C5E-C6E-O5E
27	C	518	LMG	O6-C5-C6-O5
25	c	515	DGD	O6E-C1E-O5D-C6D
27	A	415	LMG	O6-C1-O1-C7
25	b	624	DGD	O6E-C1E-O5D-C6D
27	a	402	LMG	O6-C1-O1-C7
25	C	515	DGD	O6E-C1E-O5D-C6D
25	B	620	DGD	O6E-C1E-O5D-C6D
32	d	401	PHO	CBA-CGA-O2A-C1
22	B	615	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	CBA-CGA-O2A-C1
25	c	515	DGD	C4E-C5E-C6E-O5E
22	B	606	CLA	O1D-CGD-O2D-CED
32	D	401	PHO	O1A-CGA-O2A-C1
27	i	101	LMG	C11-C10-O7-C8
25	A	408	DGD	C4E-C5E-C6E-O5E
25	C	515	DGD	C4E-C5E-C6E-O5E
27	d	407	LMG	C4-C5-C6-O5
25	a	411	DGD	C4E-C5E-C6E-O5E
32	d	401	PHO	O1A-CGA-O2A-C1
22	B	615	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	O1D-CGD-O2D-CED
22	b	619	CLA	CBA-CGA-O2A-C1
22	c	512	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	C4-C5-C6-O5
22	B	615	CLA	C5-C6-C7-C8
27	c	518	LMG	C4-C5-C6-O5
22	b	619	CLA	C5-C6-C7-C8
22	b	612	CLA	C13-C15-C16-C17
22	B	608	CLA	C13-C15-C16-C17
22	b	615	CLA	C5-C6-C7-C8
22	B	606	CLA	C15-C16-C17-C18
22	C	508	CLA	C5-C6-C7-C8
22	B	611	CLA	C5-C6-C7-C8
27	C	518	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	D	409	DGD	C2D-C1D-O3G-C3G
25	d	409	DGD	C2D-C1D-O3G-C3G
25	C	516	DGD	O2G-C2G-C3G-O3G
30	b	602	SQD	O10-C23-O48-C46
22	B	604	CLA	C2-C3-C5-C6
22	c	510	CLA	C6-C7-C8-C9
22	b	613	CLA	C14-C13-C15-C16
22	B	609	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	B	607	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	C	508	CLA	C6-C7-C8-C9
22	b	609	CLA	O1D-CGD-O2D-CED
24	g	101	BCR	C7-C8-C9-C34
24	b	621	BCR	C37-C22-C23-C24
24	J	102	BCR	C37-C22-C23-C24
24	y	101	BCR	C7-C8-C9-C34
24	x	101	BCR	C37-C22-C23-C24
24	j	102	BCR	C37-C22-C23-C24
24	F	102	BCR	C37-C22-C23-C24
24	b	621	BCR	C7-C8-C9-C10
24	B	617	BCR	C7-C8-C9-C10
27	c	522	LMG	O6-C5-C6-O5
27	E	101	LMG	O9-C10-O7-C8
27	d	408	LMG	O9-C10-O7-C8
27	C	521	LMG	C11-C10-O7-C8
27	I	101	LMG	C11-C10-O7-C8
27	c	522	LMG	C11-C10-O7-C8
27	A	415	LMG	C28-C29-C30-C31
22	b	619	CLA	O1A-CGA-O2A-C1
22	c	505	CLA	C5-C6-C7-C8
22	b	610	CLA	C15-C16-C17-C18
22	b	619	CLA	C10-C11-C12-C13
22	h	101	CLA	C3-C5-C6-C7
22	H	101	CLA	C3-C5-C6-C7
22	C	505	CLA	C15-C16-C17-C18
32	a	407	PHO	C15-C16-C17-C18
22	b	610	CLA	C13-C15-C16-C17
22	c	509	CLA	C15-C16-C17-C18
32	D	402	PHO	C15-C16-C17-C18
22	b	613	CLA	C8-C10-C11-C12
22	B	609	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	504	CLA	C10-C11-C12-C13
22	c	507	CLA	C10-C11-C12-C13
22	B	603	CLA	C13-C15-C16-C17
22	c	501	CLA	C15-C16-C17-C18
22	d	404	CLA	C13-C15-C16-C17
27	C	518	LMG	C28-C29-C30-C31
25	d	409	DGD	C1B-C2B-C3B-C4B
32	a	407	PHO	O1D-CGD-O2D-CED
22	C	503	CLA	C10-C11-C12-C13
22	A	404	CLA	C10-C11-C12-C13
22	B	615	CLA	C10-C11-C12-C13
22	b	607	CLA	C13-C15-C16-C17
22	b	615	CLA	C13-C15-C16-C17
22	C	520	CLA	C13-C15-C16-C17
22	c	508	CLA	C5-C6-C7-C8
22	c	520	CLA	C13-C15-C16-C17
22	c	520	CLA	C15-C16-C17-C18
22	D	404	CLA	C13-C15-C16-C17
22	D	404	CLA	C15-C16-C17-C18
22	B	611	CLA	C13-C15-C16-C17
22	d	404	CLA	C15-C16-C17-C18
22	c	503	CLA	C10-C11-C12-C13
27	c	518	LMG	C10-C11-C12-C13
27	c	518	LMG	C28-C29-C30-C31
25	c	515	DGD	C1B-C2B-C3B-C4B
25	D	409	DGD	C1B-C2B-C3B-C4B
27	d	411	LMG	C10-C11-C12-C13
27	b	625	LMG	C10-C11-C12-C13
27	a	402	LMG	C28-C29-C30-C31
27	D	411	LMG	C10-C11-C12-C13
27	B	621	LMG	C10-C11-C12-C13
25	C	515	DGD	C1B-C2B-C3B-C4B
22	B	601	CLA	C13-C15-C16-C17
22	C	509	CLA	C15-C16-C17-C18
22	c	507	CLA	C15-C16-C17-C18
22	B	606	CLA	C13-C15-C16-C17
22	B	604	CLA	CBA-CGA-O2A-C1
22	C	512	CLA	O1D-CGD-O2D-CED
27	D	407	LMG	C4-C5-C6-O5
22	C	505	CLA	C13-C15-C16-C17
22	b	605	CLA	C13-C15-C16-C17
22	C	520	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	C	521	LMG	C10-C11-C12-C13
27	c	522	LMG	C10-C11-C12-C13
22	c	509	CLA	CBD-CGD-O2D-CED
22	c	505	CLA	C13-C15-C16-C17
22	C	501	CLA	C8-C10-C11-C12
22	C	501	CLA	C15-C16-C17-C18
22	c	505	CLA	C11-C10-C8-C7
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	A	402	CLA	C3-C5-C6-C7
22	a	404	CLA	C3-C5-C6-C7
22	b	609	CLA	C2A-CAA-CBA-CGA
22	b	613	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C2A-CAA-CBA-CGA
22	c	511	CLA	O1D-CGD-O2D-CED
22	B	607	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
22	c	506	CLA	C5-C6-C7-C8
22	a	405	CLA	C15-C16-C17-C18
22	A	404	CLA	C15-C16-C17-C18
22	a	406	CLA	C15-C16-C17-C18
22	A	403	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	c	501	CLA	C10-C11-C12-C13
22	C	507	CLA	C10-C11-C12-C13
22	C	507	CLA	C15-C16-C17-C18
22	b	614	CLA	C15-C16-C17-C18
22	C	504	CLA	C10-C11-C12-C13
22	c	512	CLA	O1A-CGA-O2A-C1
27	c	522	LMG	C4-C5-C6-O5
27	i	101	LMG	O6-C1-O1-C7
27	I	101	LMG	O6-C1-O1-C7
30	A	413	SQD	O5-C1-O6-C44
30	a	415	SQD	O5-C1-O6-C44
22	C	506	CLA	C5-C6-C7-C8
23	D	406	PL9	C29-C31-C32-C33
23	d	406	PL9	C29-C31-C32-C33
27	C	521	LMG	O6-C5-C6-O5
25	C	517	DGD	O1B-C1B-O2G-C2G
27	c	522	LMG	O9-C10-O7-C8
22	c	505	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	C5-C6-C7-C8
22	a	406	CLA	C10-C11-C12-C13
22	c	512	CLA	C15-C16-C17-C18
22	c	501	CLA	C8-C10-C11-C12
22	b	611	CLA	C15-C16-C17-C18
27	i	101	LMG	C29-C28-O8-C9
30	B	626	SQD	O10-C23-O48-C46
22	C	512	CLA	O1A-CGA-O2A-C1
25	b	624	DGD	C1B-C2B-C3B-C4B
22	C	510	CLA	C5-C6-C7-C8
22	b	619	CLA	C13-C15-C16-C17
22	B	607	CLA	C5-C6-C7-C8
22	b	618	CLA	C13-C15-C16-C17
22	C	512	CLA	C15-C16-C17-C18
22	b	611	CLA	C5-C6-C7-C8
32	D	402	PHO	O1D-CGD-O2D-CED
27	C	521	LMG	C4-C5-C6-O5
22	B	612	CLA	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
22	c	520	CLA	C10-C11-C12-C13
22	B	614	CLA	C13-C15-C16-C17
26	C	519	LHG	C3-O3-P-O6
26	C	519	LHG	C4-O6-P-O3
26	c	519	LHG	C4-O6-P-O3
30	a	415	SQD	C7-C8-C9-C10
30	b	602	SQD	C24-C23-O48-C46
22	b	608	CLA	CBA-CGA-O2A-C1
22	C	511	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C5-C6-C7-C8
22	c	512	CLA	O1D-CGD-O2D-CED
27	D	411	LMG	O6-C5-C6-O5
25	c	517	DGD	O1B-C1B-O2G-C2G
23	j	101	PL9	C15-C14-C16-C17
22	b	616	CLA	C5-C6-C7-C8
22	C	501	CLA	C10-C11-C12-C13
22	c	511	CLA	CBA-CGA-O2A-C1
30	B	626	SQD	C24-C23-O48-C46
22	c	520	CLA	CBA-CGA-O2A-C1
22	C	520	CLA	C10-C11-C12-C13
25	B	620	DGD	C1B-C2B-C3B-C4B
25	D	409	DGD	CCB-CDB-CEB-CFB
25	B	625	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
25	b	624	DGD	C3B-C4B-C5B-C6B
22	H	101	CLA	C5-C6-C7-C8
27	c	518	LMG	C29-C30-C31-C32
27	C	518	LMG	C29-C30-C31-C32
27	i	101	LMG	C12-C13-C14-C15
30	f	103	SQD	C12-C13-C14-C15
31	I	102	LMT	C6-C7-C8-C9
27	I	101	LMG	C12-C13-C14-C15
27	I	101	LMG	C14-C15-C16-C17
27	b	625	LMG	C31-C32-C33-C34
27	A	415	LMG	C30-C31-C32-C33
25	C	516	DGD	C2A-C3A-C4A-C5A
25	b	601	DGD	C5B-C6B-C7B-C8B
25	b	601	DGD	C9B-CAB-CBB-CCB
27	a	402	LMG	C30-C31-C32-C33
27	B	621	LMG	C31-C32-C33-C34
25	d	409	DGD	CCB-CDB-CEB-CFB
22	b	616	CLA	C16-C17-C18-C19
25	c	515	DGD	C3B-C4B-C5B-C6B
25	D	409	DGD	C4B-C5B-C6B-C7B
25	D	409	DGD	C5B-C6B-C7B-C8B
31	i	102	LMT	C6-C7-C8-C9
27	c	522	LMG	C12-C13-C14-C15
25	B	625	DGD	C9B-CAB-CBB-CCB
25	A	408	DGD	C8B-C9B-CAB-CBB
30	F	103	SQD	C12-C13-C14-C15
25	d	409	DGD	C4B-C5B-C6B-C7B
25	d	409	DGD	C5B-C6B-C7B-C8B
25	B	620	DGD	C7A-C8A-C9A-CAA
25	B	620	DGD	C3B-C4B-C5B-C6B
27	c	518	LMG	C9-C8-O7-C10
27	M	101	LMG	O6-C5-C6-O5
27	C	521	LMG	O9-C10-O7-C8
30	f	103	SQD	O49-C7-O47-C45
30	F	103	SQD	O49-C7-O47-C45
27	l	101	LMG	C34-C35-C36-C37
25	D	409	DGD	CEB-CFB-CGB-CHB
27	A	410	LMG	C34-C35-C36-C37
25	d	409	DGD	CEB-CFB-CGB-CHB
25	B	620	DGD	C6B-C7B-C8B-C9B
27	l	101	LMG	C33-C34-C35-C36
25	c	516	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
25	c	516	DGD	C4A-C5A-C6A-C7A
27	A	410	LMG	C33-C34-C35-C36
25	b	624	DGD	C6B-C7B-C8B-C9B
30	B	626	SQD	C9-C10-C11-C12
25	C	515	DGD	C3B-C4B-C5B-C6B
25	b	624	DGD	O6D-C5D-C6D-O5D
27	C	521	LMG	C12-C13-C14-C15
27	i	101	LMG	C16-C17-C18-C19
30	A	413	SQD	C14-C15-C16-C17
25	a	411	DGD	C8B-C9B-CAB-CBB
30	a	415	SQD	C14-C15-C16-C17
25	C	515	DGD	C2B-C3B-C4B-C5B
25	C	515	DGD	C1A-C2A-C3A-C4A
25	D	409	DGD	C2E-C1E-O5D-C6D
27	i	101	LMG	C2-C1-O1-C7
24	J	102	BCR	C20-C21-C22-C23
27	I	101	LMG	C2-C1-O1-C7
24	H	102	BCR	C11-C10-C9-C8
24	x	101	BCR	C11-C10-C9-C8
24	j	102	BCR	C20-C21-C22-C23
25	d	409	DGD	C2E-C1E-O5D-C6D
25	c	515	DGD	C3A-C4A-C5A-C6A
25	D	409	DGD	C7B-C8B-C9B-CAB
27	D	408	LMG	C14-C15-C16-C17
31	B	628	LMT	O1'-C1-C2-C3
27	A	415	LMG	C15-C16-C17-C18
25	b	624	DGD	C7A-C8A-C9A-CAA
27	D	407	LMG	C18-C19-C20-C21
30	b	602	SQD	C11-C10-C9-C8
27	d	408	LMG	C14-C15-C16-C17
25	C	515	DGD	C3A-C4A-C5A-C6A
22	B	615	CLA	C13-C15-C16-C17
22	B	604	CLA	O1A-CGA-O2A-C1
23	D	406	PL9	C27-C28-C29-C30
22	C	509	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
27	i	101	LMG	C14-C15-C16-C17
27	A	415	LMG	C18-C19-C20-C21
27	d	407	LMG	C18-C19-C20-C21
30	b	602	SQD	C9-C10-C11-C12
27	a	402	LMG	C18-C19-C20-C21
27	a	402	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C2-C3-C5-C6
22	C	505	CLA	C11-C10-C8-C9
22	B	601	CLA	C11-C12-C13-C14
22	a	405	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C10-C8-C9
22	b	612	CLA	C6-C7-C8-C9
22	A	402	CLA	C11-C12-C13-C14
22	c	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C14
22	H	101	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
27	E	101	LMG	C28-C29-C30-C31
27	A	410	LMG	C31-C32-C33-C34
27	I	101	LMG	C16-C17-C18-C19
30	A	413	SQD	C27-C28-C29-C30
27	A	415	LMG	C32-C33-C34-C35
30	F	103	SQD	C11-C12-C13-C14
27	d	407	LMG	C31-C32-C33-C34
30	B	626	SQD	C11-C10-C9-C8
30	a	415	SQD	C27-C28-C29-C30
27	D	407	LMG	C31-C32-C33-C34
25	d	409	DGD	C7B-C8B-C9B-CAB
22	B	605	CLA	C2A-CAA-CBA-CGA
22	a	404	CLA	C2A-CAA-CBA-CGA
22	c	520	CLA	C2A-CAA-CBA-CGA
24	b	621	BCR	C7-C8-C9-C34
24	B	617	BCR	C7-C8-C9-C34
27	l	101	LMG	C31-C32-C33-C34
25	c	517	DGD	CAB-CBB-CCB-CDB
24	c	521	BCR	C7-C8-C9-C10
22	B	615	CLA	C3-C5-C6-C7
22	b	619	CLA	C3-C5-C6-C7
22	c	503	CLA	C5-C6-C7-C8
30	f	103	SQD	C11-C12-C13-C14
22	b	615	CLA	O1D-CGD-O2D-CED
27	l	101	LMG	C14-C15-C16-C17
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

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Mol	Chain	Res	Type	Atoms
25	C	517	DGD	CAB-CBB-CCB-CDB
27	D	408	LMG	C19-C20-C21-C22
27	I	101	LMG	C13-C14-C15-C16
27	m	101	LMG	C29-C30-C31-C32
25	A	408	DGD	C5B-C6B-C7B-C8B
25	a	411	DGD	C5B-C6B-C7B-C8B
25	c	517	DGD	C9B-CAB-CBB-CCB
27	d	408	LMG	C19-C20-C21-C22
25	C	515	DGD	C4A-C5A-C6A-C7A
27	d	411	LMG	O6-C5-C6-O5
25	D	409	DGD	O6E-C1E-O5D-C6D
27	d	407	LMG	O6-C1-O1-C7
27	D	407	LMG	O6-C1-O1-C7
22	h	101	CLA	C5-C6-C7-C8
22	A	405	CLA	C10-C11-C12-C13
22	B	611	CLA	O1D-CGD-O2D-CED
25	B	625	DGD	C4A-C5A-C6A-C7A
25	c	517	DGD	CBA-CCA-CDA-CEA
27	c	518	LMG	C12-C13-C14-C15
27	i	101	LMG	C13-C14-C15-C16
31	B	628	LMT	C7-C8-C9-C10
25	C	516	DGD	C4A-C5A-C6A-C7A
25	b	601	DGD	C4A-C5A-C6A-C7A
27	d	408	LMG	C32-C33-C34-C35
27	d	407	LMG	C28-C29-C30-C31
27	D	407	LMG	C28-C29-C30-C31
25	b	601	DGD	C1A-C2A-C3A-C4A
22	C	503	CLA	C5-C6-C7-C8
22	H	101	CLA	C13-C15-C16-C17
22	c	511	CLA	O1A-CGA-O2A-C1
22	b	608	CLA	O1A-CGA-O2A-C1
25	D	409	DGD	C3A-C4A-C5A-C6A
27	A	410	LMG	C14-C15-C16-C17
27	d	407	LMG	C30-C31-C32-C33
27	a	402	LMG	C15-C16-C17-C18
27	I	101	LMG	C29-C28-O8-C9
22	C	520	CLA	CBA-CGA-O2A-C1
27	d	407	LMG	C36-C37-C38-C39
26	A	409	LHG	C25-C26-C27-C28
22	C	506	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	h	101	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	B	615	CLA	C3A-C2A-CAA-CBA
22	c	511	CLA	C3A-C2A-CAA-CBA
22	B	607	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C3A-C2A-CAA-CBA
22	C	504	CLA	C3A-C2A-CAA-CBA
27	E	101	LMG	C15-C16-C17-C18
27	C	518	LMG	C12-C13-C14-C15
31	b	604	LMT	O1'-C1-C2-C3
31	b	604	LMT	C7-C8-C9-C10
27	A	410	LMG	C30-C31-C32-C33
27	D	407	LMG	C36-C37-C38-C39
27	l	101	LMG	C30-C31-C32-C33
26	a	412	LHG	C25-C26-C27-C28
25	d	409	DGD	C5A-C6A-C7A-C8A
31	b	627	LMT	C2B-C1B-O1B-C4'
31	B	623	LMT	C1-C2-C3-C4
27	D	408	LMG	C15-C16-C17-C18
27	D	408	LMG	C32-C33-C34-C35
25	b	624	DGD	C5B-C6B-C7B-C8B
25	C	515	DGD	C2A-C3A-C4A-C5A
25	B	620	DGD	O6D-C5D-C6D-O5D
27	e	101	LMG	C28-C29-C30-C31
30	A	413	SQD	C7-C8-C9-C10
26	a	412	LHG	C23-C24-C25-C26
25	c	517	DGD	C1A-C2A-C3A-C4A
31	b	626	LMT	C1-C2-C3-C4
30	B	622	SQD	C9-C10-C11-C12
22	c	509	CLA	C4-C3-C5-C6
22	c	509	CLA	C2-C3-C5-C6
30	B	626	SQD	C8-C7-O47-C45
30	b	602	SQD	C8-C7-O47-C45
27	c	518	LMG	C34-C35-C36-C37
25	D	409	DGD	C5A-C6A-C7A-C8A
22	b	607	CLA	C8-C10-C11-C12
27	d	408	LMG	C15-C16-C17-C18
27	M	101	LMG	C29-C30-C31-C32
25	a	411	DGD	C1B-C2B-C3B-C4B
22	B	612	CLA	C16-C17-C18-C19
27	e	101	LMG	C15-C16-C17-C18
25	B	620	DGD	C5B-C6B-C7B-C8B
22	B	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	C13-C15-C16-C17
25	c	516	DGD	CAB-CBB-CCB-CDB
30	d	402	SQD	C9-C10-C11-C12
27	D	407	LMG	C30-C31-C32-C33
22	d	405	CLA	CBA-CGA-O2A-C1
27	l	101	LMG	C4-C5-C6-O5
25	C	516	DGD	CAB-CBB-CCB-CDB
25	b	601	DGD	C2B-C3B-C4B-C5B
22	c	520	CLA	O1A-CGA-O2A-C1
22	C	511	CLA	O1A-CGA-O2A-C1
25	c	515	DGD	C1A-C2A-C3A-C4A
25	C	517	DGD	C1A-C2A-C3A-C4A
25	B	625	DGD	C1A-C2A-C3A-C4A
27	A	415	LMG	C31-C32-C33-C34
25	b	624	DGD	C4B-C5B-C6B-C7B
22	c	508	CLA	C2-C1-O2A-CGA
22	C	508	CLA	C2-C1-O2A-CGA
27	C	518	LMG	C34-C35-C36-C37
27	D	411	LMG	C17-C18-C19-C20
25	A	408	DGD	C1B-C2B-C3B-C4B
24	g	101	BCR	C23-C24-C25-C26
24	g	101	BCR	C23-C24-C25-C30
24	b	621	BCR	C23-C24-C25-C30
24	f	102	BCR	C5-C6-C7-C8
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	y	101	BCR	C23-C24-C25-C26
24	y	101	BCR	C23-C24-C25-C30
24	b	623	BCR	C23-C24-C25-C26
22	A	403	CLA	C3-C5-C6-C7
24	H	102	BCR	C1-C6-C7-C8
24	H	102	BCR	C5-C6-C7-C8
24	C	513	BCR	C5-C6-C7-C8
24	x	101	BCR	C1-C6-C7-C8
24	x	101	BCR	C5-C6-C7-C8
24	c	513	BCR	C1-C6-C7-C8
24	c	513	BCR	C5-C6-C7-C8
24	c	514	BCR	C23-C24-C25-C26
24	c	514	BCR	C23-C24-C25-C30
24	b	620	BCR	C5-C6-C7-C8
24	B	617	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	j	102	BCR	C5-C6-C7-C8
24	F	102	BCR	C5-C6-C7-C8
24	B	616	BCR	C5-C6-C7-C8
27	c	518	LMG	C36-C37-C38-C39
27	A	410	LMG	C15-C16-C17-C18
26	C	519	LHG	C24-C23-O8-C6
31	B	624	LMT	C2B-C1B-O1B-C4'
25	c	517	DGD	C2B-C1B-O2G-C2G
31	b	626	LMT	O1'-C1-C2-C3
25	d	409	DGD	C3A-C4A-C5A-C6A
23	d	406	PL9	C47-C48-C49-C51
26	C	519	LHG	C24-C25-C26-C27
25	D	409	DGD	C2A-C3A-C4A-C5A
22	C	505	CLA	C11-C10-C8-C7
32	a	407	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	502	CLA	C11-C12-C13-C15
22	c	509	CLA	C11-C10-C8-C7
32	D	402	PHO	C11-C10-C8-C7
22	A	404	CLA	C6-C7-C8-C10
22	C	509	CLA	C2-C3-C5-C6
22	c	512	CLA	C11-C10-C8-C7
22	c	512	CLA	C12-C13-C15-C16
22	b	605	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C12-C13-C15
22	C	512	CLA	C2-C3-C5-C6
22	C	512	CLA	C11-C10-C8-C7
22	D	404	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C15
22	c	503	CLA	C11-C12-C13-C15
22	C	520	CLA	O1A-CGA-O2A-C1
25	c	515	DGD	C2A-C3A-C4A-C5A
22	h	101	CLA	C13-C15-C16-C17
22	d	405	CLA	C15-C16-C17-C18
26	a	412	LHG	O9-C7-O7-C5
25	C	516	DGD	C1A-C2A-C3A-C4A
27	m	101	LMG	C29-C28-O8-C9
27	D	408	LMG	C13-C14-C15-C16
25	B	625	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
30	b	602	SQD	C11-C12-C13-C14
25	B	620	DGD	C4B-C5B-C6B-C7B
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	505	CLA	C10-C11-C12-C13
22	C	512	CLA	C13-C15-C16-C17
25	D	409	DGD	C6B-C7B-C8B-C9B
30	b	602	SQD	C12-C13-C14-C15
25	d	409	DGD	C2A-C3A-C4A-C5A
25	d	409	DGD	CAB-CBB-CCB-CDB
26	c	519	LHG	C24-C25-C26-C27
30	F	103	SQD	C10-C11-C12-C13
25	c	516	DGD	C1A-C2A-C3A-C4A
22	b	611	CLA	O1D-CGD-O2D-CED
25	D	409	DGD	CAB-CBB-CCB-CDB
27	d	411	LMG	C17-C18-C19-C20
25	A	408	DGD	C3B-C4B-C5B-C6B
30	B	626	SQD	C11-C12-C13-C14
27	D	411	LMG	C34-C35-C36-C37
27	B	621	LMG	C34-C35-C36-C37
25	d	409	DGD	C6B-C7B-C8B-C9B
23	d	406	PL9	C27-C28-C29-C30
22	C	502	CLA	C3-C5-C6-C7
30	B	626	SQD	C12-C13-C14-C15
22	B	601	CLA	C16-C17-C18-C20
25	d	409	DGD	O6E-C1E-O5D-C6D
22	a	408	CLA	C10-C11-C12-C13
22	D	405	CLA	C15-C16-C17-C18
27	d	411	LMG	C31-C32-C33-C34
27	a	402	LMG	C31-C32-C33-C34
27	E	101	LMG	C11-C10-O7-C8
25	C	517	DGD	C2B-C1B-O2G-C2G
27	e	101	LMG	C11-C10-O7-C8
26	a	412	LHG	C8-C7-O7-C5
26	A	409	LHG	C8-C7-O7-C5
27	d	411	LMG	C34-C35-C36-C37
25	C	515	DGD	C4B-C5B-C6B-C7B
22	c	511	CLA	C13-C15-C16-C17
22	C	506	CLA	CBD-CGD-O2D-CED
22	c	506	CLA	CBD-CGD-O2D-CED
27	B	621	LMG	C13-C14-C15-C16
26	A	409	LHG	C30-C31-C32-C33
26	A	409	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
27	d	407	LMG	C2-C1-O1-C7
22	c	505	CLA	C10-C11-C12-C13
30	a	401	SQD	O6-C44-C45-O47
27	i	101	LMG	O1-C7-C8-O7
27	I	101	LMG	O1-C7-C8-O7
27	m	101	LMG	O1-C7-C8-O7
30	A	413	SQD	O47-C45-C46-O48
30	A	414	SQD	O6-C44-C45-O47
30	a	415	SQD	O47-C45-C46-O48
27	M	101	LMG	O1-C7-C8-O7
27	l	101	LMG	C15-C16-C17-C18
27	C	518	LMG	C36-C37-C38-C39
31	B	623	LMT	O1'-C1-C2-C3
27	A	415	LMG	C17-C18-C19-C20
26	a	412	LHG	C30-C31-C32-C33
27	D	411	LMG	C31-C32-C33-C34
27	d	408	LMG	C13-C14-C15-C16
22	d	405	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	C13-C15-C16-C17
23	A	406	PL9	C33-C34-C36-C37
23	a	409	PL9	C33-C34-C36-C37
32	a	407	PHO	C11-C10-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C10-C8-C9
22	B	601	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
32	D	402	PHO	C11-C10-C8-C9
22	A	404	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	b	605	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	b	606	CLA	C11-C12-C13-C14
22	d	404	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C10-C8-C9
23	D	406	PL9	C47-C48-C49-C51
27	m	101	LMG	O6-C5-C6-O5
27	c	522	LMG	C16-C17-C18-C19
22	c	509	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	O1D-CGD-O2D-CED
22	C	520	CLA	C2A-CAA-CBA-CGA
22	C	501	CLA	C2A-CAA-CBA-CGA
27	D	407	LMG	C17-C18-C19-C20
24	B	617	BCR	C37-C22-C23-C24
27	C	521	LMG	C16-C17-C18-C19
22	C	506	CLA	C1A-C2A-CAA-CBA
27	E	101	LMG	O6-C5-C6-O5
27	l	101	LMG	O6-C5-C6-O5
22	c	506	CLA	C1A-C2A-CAA-CBA
22	B	615	CLA	C1A-C2A-CAA-CBA
22	b	619	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
22	c	501	CLA	C1A-C2A-CAA-CBA
22	C	501	CLA	C1A-C2A-CAA-CBA
22	B	612	CLA	C16-C17-C18-C20
22	b	616	CLA	C16-C17-C18-C20
25	c	515	DGD	C4B-C5B-C6B-C7B
25	A	408	DGD	C4B-C5B-C6B-C7B
27	e	101	LMG	O6-C5-C6-O5
32	D	401	PHO	CBD-CGD-O2D-CED
22	c	502	CLA	C3-C5-C6-C7
22	C	509	CLA	C3-C5-C6-C7
25	a	411	DGD	C4B-C5B-C6B-C7B
22	a	408	CLA	C13-C15-C16-C17
22	b	605	CLA	C10-C11-C12-C13
30	f	103	SQD	C10-C11-C12-C13
25	a	411	DGD	C3B-C4B-C5B-C6B
25	c	517	DGD	C3B-C4B-C5B-C6B
25	C	517	DGD	C3B-C4B-C5B-C6B
27	D	407	LMG	C32-C33-C34-C35
22	B	603	CLA	C15-C16-C17-C18
30	a	415	SQD	C17-C18-C19-C20
27	b	625	LMG	C28-C29-C30-C31
25	D	409	DGD	C8B-C9B-CAB-CBB
27	d	407	LMG	C17-C18-C19-C20
25	d	409	DGD	C8B-C9B-CAB-CBB
22	C	512	CLA	C4-C3-C5-C6
27	I	101	LMG	C18-C19-C20-C21
22	A	405	CLA	C5-C6-C7-C8
30	A	413	SQD	C17-C18-C19-C20
27	a	402	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	a	401	SQD	C10-C11-C12-C13
30	A	414	SQD	C10-C11-C12-C13
22	b	605	CLA	C16-C17-C18-C20
22	a	405	CLA	C3-C5-C6-C7
27	C	521	LMG	C7-C8-C9-O8
25	C	517	DGD	O1G-C1G-C2G-C3G
27	D	408	LMG	O1-C7-C8-C9
27	i	101	LMG	O1-C7-C8-C9
27	I	101	LMG	O1-C7-C8-C9
27	m	101	LMG	C7-C8-C9-O8
27	c	522	LMG	C7-C8-C9-O8
27	b	625	LMG	C7-C8-C9-O8
27	b	625	LMG	C13-C14-C15-C16
25	A	408	DGD	C1G-C2G-C3G-O3G
27	d	407	LMG	O1-C7-C8-C9
30	B	626	SQD	C44-C45-C46-O48
27	D	407	LMG	O1-C7-C8-C9
30	b	602	SQD	C44-C45-C46-O48
27	B	621	LMG	C7-C8-C9-O8
25	c	517	DGD	O1G-C1G-C2G-C3G
27	d	408	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
31	B	624	LMT	O5B-C1B-O1B-C4'
27	D	407	LMG	C15-C16-C17-C18
25	B	625	DGD	O6D-C5D-C6D-O5D
27	D	408	LMG	C8-C7-O1-C1
30	d	402	SQD	C45-C44-O6-C1
27	d	408	LMG	C8-C7-O1-C1
30	B	622	SQD	C45-C44-O6-C1
22	b	608	CLA	C15-C16-C17-C18
27	i	101	LMG	C18-C19-C20-C21
27	A	415	LMG	C11-C12-C13-C14
27	d	408	LMG	C28-C29-C30-C31
27	b	625	LMG	C34-C35-C36-C37
25	d	409	DGD	CDB-CEB-CFB-CGB
22	B	615	CLA	C15-C16-C17-C18
26	C	519	LHG	C11-C10-C9-C8
30	A	413	SQD	C10-C11-C12-C13
31	I	102	LMT	C5'-C4'-O1B-C1B
27	d	407	LMG	C32-C33-C34-C35
22	a	408	CLA	C5-C6-C7-C8
22	b	607	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	D	409	DGD	CAA-CBA-CCA-CDA
26	c	519	LHG	C11-C10-C9-C8
22	c	503	CLA	C8-C10-C11-C12
23	D	406	PL9	C15-C14-C16-C17
22	c	504	CLA	C4-C3-C5-C6
23	a	409	PL9	C35-C34-C36-C37
22	C	504	CLA	C4-C3-C5-C6
25	D	409	DGD	CBA-CCA-CDA-CEA
25	d	409	DGD	CBA-CCA-CDA-CEA
26	c	519	LHG	C24-C23-O8-C6
22	B	610	CLA	CBA-CGA-O2A-C1
22	c	508	CLA	CBA-CGA-O2A-C1
22	b	614	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	C5A-C6A-C7A-C8A
22	C	503	CLA	C8-C10-C11-C12
25	D	409	DGD	CDB-CEB-CFB-CGB
27	E	101	LMG	C7-C8-O7-C10
25	D	409	DGD	C1G-C2G-O2G-C1B
25	d	409	DGD	C1G-C2G-O2G-C1B
22	c	502	CLA	C13-C15-C16-C17
32	d	401	PHO	C2-C1-O2A-CGA
27	A	415	LMG	O6-C5-C6-O5
27	a	402	LMG	O6-C5-C6-O5
27	C	521	LMG	C17-C18-C19-C20
26	c	519	LHG	C25-C26-C27-C28
22	c	504	CLA	CBA-CGA-O2A-C1
22	C	508	CLA	CBA-CGA-O2A-C1
22	D	405	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
22	B	601	CLA	C16-C17-C18-C19
22	b	605	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
31	i	102	LMT	C5'-C4'-O1B-C1B
27	i	101	LMG	C17-C18-C19-C20
22	B	601	CLA	C10-C11-C12-C13
31	b	627	LMT	O5B-C1B-O1B-C4'
26	c	519	LHG	O2-C2-C3-O3
26	c	519	LHG	O10-C23-O8-C6
27	e	101	LMG	C18-C19-C20-C21
27	D	407	LMG	C2-C1-O1-C7
27	I	101	LMG	C31-C32-C33-C34
27	E	101	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	c	518	LMG	O1-C7-C8-O7
27	l	101	LMG	O1-C7-C8-O7
25	C	517	DGD	O1G-C1G-C2G-O2G
27	C	518	LMG	O1-C7-C8-O7
27	A	410	LMG	O1-C7-C8-O7
25	c	517	DGD	O1G-C1G-C2G-O2G
25	C	515	DGD	O2G-C2G-C3G-O3G
22	c	509	CLA	O1D-CGD-O2D-CED
27	E	101	LMG	C17-C18-C19-C20
25	c	516	DGD	O6D-C5D-C6D-O5D
25	C	516	DGD	O6D-C5D-C6D-O5D
27	D	407	LMG	C19-C20-C21-C22
23	d	406	PL9	C15-C14-C16-C17
32	a	407	PHO	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
22	C	503	CLA	C11-C10-C8-C7
22	C	503	CLA	C11-C12-C13-C15
22	c	502	CLA	C11-C12-C13-C15
32	D	402	PHO	C12-C13-C15-C16
22	h	101	CLA	C6-C7-C8-C10
22	b	619	CLA	C12-C13-C15-C16
22	B	609	CLA	C11-C12-C13-C15
22	C	509	CLA	C6-C7-C8-C10
22	a	406	CLA	C6-C7-C8-C10
22	B	605	CLA	C12-C13-C15-C16
22	c	504	CLA	C2-C3-C5-C6
22	B	612	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C10-C8-C7
22	B	607	CLA	C6-C7-C8-C10
22	B	614	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
22	b	618	CLA	C11-C10-C8-C7
22	b	618	CLA	C12-C13-C15-C16
22	H	101	CLA	C6-C7-C8-C10
22	H	101	CLA	C11-C12-C13-C15
22	C	512	CLA	C12-C13-C15-C16
22	b	611	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	b	606	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C10-C8-C7
22	d	404	CLA	C12-C13-C15-C16
22	C	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	c	503	CLA	C11-C10-C8-C7
22	c	508	CLA	O1A-CGA-O2A-C1
27	d	407	LMG	C19-C20-C21-C22
32	a	407	PHO	C14-C13-C15-C16
22	c	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C14-C13-C15-C16
22	c	510	CLA	C14-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C14
22	C	502	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C12-C13-C14
22	c	502	CLA	C11-C12-C13-C14
22	c	502	CLA	C14-C13-C15-C16
32	D	402	PHO	C14-C13-C15-C16
22	b	609	CLA	C14-C13-C15-C16
22	a	406	CLA	C6-C7-C8-C9
22	B	608	CLA	C6-C7-C8-C9
22	c	504	CLA	C6-C7-C8-C9
22	c	504	CLA	C11-C10-C8-C9
22	c	504	CLA	C14-C13-C15-C16
22	A	403	CLA	C6-C7-C8-C9
22	a	404	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C10-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	b	618	CLA	C14-C13-C15-C16
22	B	602	CLA	C6-C7-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	511	CLA	C11-C12-C13-C14
22	C	504	CLA	C6-C7-C8-C9
22	C	504	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C14
27	d	407	LMG	C15-C16-C17-C18
22	b	613	CLA	CBA-CGA-O2A-C1
22	C	504	CLA	CBA-CGA-O2A-C1
22	b	619	CLA	C15-C16-C17-C18
22	B	613	CLA	C15-C16-C17-C18
22	A	405	CLA	C13-C15-C16-C17
22	C	512	CLA	C2A-CAA-CBA-CGA
27	E	101	LMG	C19-C20-C21-C22
22	b	613	CLA	C16-C17-C18-C20
22	c	511	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	C	511	CLA	C16-C17-C18-C20
27	d	411	LMG	C38-C39-C40-C41
27	C	521	LMG	C34-C35-C36-C37
27	e	101	LMG	C19-C20-C21-C22
27	D	408	LMG	C28-C29-C30-C31
22	C	502	CLA	C13-C15-C16-C17
23	J	101	PL9	C27-C28-C29-C30
27	c	522	LMG	C17-C18-C19-C20
30	b	602	SQD	C17-C18-C19-C20
27	D	411	LMG	C38-C39-C40-C41
25	c	517	DGD	CFA-CGA-CHA-CIA
27	a	402	LMG	C11-C12-C13-C14
27	A	410	LMG	C4-C5-C6-O5
22	c	504	CLA	C15-C16-C17-C18
22	C	511	CLA	C3-C5-C6-C7
30	a	415	SQD	C10-C11-C12-C13
24	j	102	BCR	C18-C19-C20-C21
22	b	617	CLA	C5-C6-C7-C8
22	b	617	CLA	C15-C16-C17-C18
22	C	504	CLA	C15-C16-C17-C18
25	c	516	DGD	C3A-C4A-C5A-C6A
27	c	522	LMG	C34-C35-C36-C37
23	D	406	PL9	C35-C34-C36-C37
23	d	406	PL9	C35-C34-C36-C37
25	d	409	DGD	C3B-C4B-C5B-C6B
22	c	508	CLA	C15-C16-C17-C18
27	d	407	LMG	C13-C14-C15-C16
25	c	516	DGD	C4D-C5D-C6D-O5D
25	C	516	DGD	C4D-C5D-C6D-O5D
22	B	609	CLA	C16-C17-C18-C20
22	b	617	CLA	C16-C17-C18-C20
30	a	415	SQD	C31-C32-C33-C34
22	B	615	CLA	C8-C10-C11-C12
27	l	101	LMG	C11-C10-O7-C8
31	B	628	LMT	C2-C3-C4-C5
22	A	402	CLA	C3A-C2A-CAA-CBA
22	a	404	CLA	C3A-C2A-CAA-CBA
23	j	101	PL9	C27-C28-C29-C30
25	C	517	DGD	CDB-CEB-CFB-CGB
27	B	621	LMG	C17-C18-C19-C20
27	E	101	LMG	C18-C19-C20-C21
27	i	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	I	101	LMG	C17-C18-C19-C20
27	b	625	LMG	C29-C28-O8-C9
22	B	604	CLA	C5-C6-C7-C8
27	c	518	LMG	O1-C7-C8-C9
30	a	401	SQD	O6-C44-C45-C46
27	l	101	LMG	O1-C7-C8-C9
25	c	516	DGD	C1G-C2G-C3G-O3G
25	D	409	DGD	C1G-C2G-C3G-O3G
27	C	518	LMG	O1-C7-C8-C9
27	A	410	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
30	A	413	SQD	C44-C45-C46-O48
25	B	625	DGD	C1G-C2G-C3G-O3G
30	A	414	SQD	O6-C44-C45-C46
25	a	411	DGD	C1G-C2G-C3G-O3G
25	C	516	DGD	C1G-C2G-C3G-O3G
25	d	409	DGD	C1G-C2G-C3G-O3G
27	D	411	LMG	C19-C20-C21-C22
25	d	409	DGD	C1A-C2A-C3A-C4A
26	A	409	LHG	C23-C24-C25-C26
22	b	614	CLA	O1A-CGA-O2A-C1
27	D	408	LMG	C29-C30-C31-C32
22	b	608	CLA	C10-C11-C12-C13
22	c	511	CLA	C3-C5-C6-C7
25	D	409	DGD	C3B-C4B-C5B-C6B
22	b	619	CLA	C8-C10-C11-C12
23	A	406	PL9	C35-C34-C36-C37
23	d	406	PL9	C20-C19-C21-C22
25	C	517	DGD	CFA-CGA-CHA-CIA
25	b	601	DGD	O6D-C5D-C6D-O5D
22	B	613	CLA	C5-C6-C7-C8
22	D	405	CLA	O1A-CGA-O2A-C1
30	A	413	SQD	C31-C32-C33-C34
22	C	510	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	CBA-CGA-O2A-C1
27	d	411	LMG	C19-C20-C21-C22
27	b	625	LMG	C17-C18-C19-C20
27	i	101	LMG	O10-C28-O8-C9
22	B	610	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	C16-C17-C18-C19
26	C	519	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	C	518	LMG	C13-C14-C15-C16
27	e	101	LMG	C17-C18-C19-C20
22	c	504	CLA	O1A-CGA-O2A-C1
30	B	626	SQD	C17-C18-C19-C20
25	d	409	DGD	CAA-CBA-CCA-CDA
25	C	516	DGD	C3A-C4A-C5A-C6A
27	d	408	LMG	C29-C30-C31-C32
27	C	521	LMG	O7-C8-C9-O8
25	c	515	DGD	O2G-C2G-C3G-O3G
27	m	101	LMG	O7-C8-C9-O8
27	c	522	LMG	O7-C8-C9-O8
30	b	602	SQD	O47-C45-C46-O48
30	B	622	SQD	O6-C44-C45-O47
22	b	613	CLA	C16-C17-C18-C19
22	B	609	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
22	a	405	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C2-C1-O2A-CGA
32	D	401	PHO	C2-C1-O2A-CGA
22	C	507	CLA	C2-C1-O2A-CGA
30	A	413	SQD	C15-C16-C17-C18
22	C	505	CLA	C14-C13-C15-C16
32	d	401	PHO	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	B	605	CLA	C14-C13-C15-C16
22	b	618	CLA	C11-C10-C8-C9
22	D	404	CLA	C6-C7-C8-C9
22	b	606	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
30	F	103	SQD	C29-C30-C31-C32
32	d	401	PHO	CBD-CGD-O2D-CED
25	c	516	DGD	C4B-C5B-C6B-C7B
22	B	609	CLA	C10-C11-C12-C13
22	B	604	CLA	C15-C16-C17-C18
22	C	508	CLA	C15-C16-C17-C18
22	b	613	CLA	O1A-CGA-O2A-C1
27	I	101	LMG	O10-C28-O8-C9
25	C	516	DGD	C4B-C5B-C6B-C7B
30	b	602	SQD	C10-C11-C12-C13
22	B	613	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C16-C17-C18-C19
24	B	619	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	B	619	BCR	C5-C6-C7-C8
24	B	619	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
24	C	513	BCR	C23-C24-C25-C30
24	c	513	BCR	C23-C24-C25-C26
24	c	513	BCR	C23-C24-C25-C30
24	A	407	BCR	C1-C6-C7-C8
24	A	407	BCR	C5-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C26
24	a	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
31	b	603	LMT	C5'-C4'-O1B-C1B
27	d	408	LMG	C36-C37-C38-C39
24	J	102	BCR	C7-C8-C9-C10
24	c	514	BCR	C7-C8-C9-C10
22	C	511	CLA	C5-C6-C7-C8
30	b	602	SQD	O49-C7-O47-C45
27	A	410	LMG	C11-C10-O7-C8
30	a	415	SQD	C15-C16-C17-C18
22	C	504	CLA	O1A-CGA-O2A-C1
27	c	518	LMG	C13-C14-C15-C16
30	f	103	SQD	C29-C30-C31-C32
30	A	414	SQD	C32-C33-C34-C35
22	C	506	CLA	O1D-CGD-O2D-CED
25	c	517	DGD	CDB-CEB-CFB-CGB
22	C	505	CLA	C12-C13-C15-C16
22	c	505	CLA	C12-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	a	405	CLA	C12-C13-C15-C16
22	c	502	CLA	C12-C13-C15-C16
22	b	609	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	b	619	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
22	c	504	CLA	C6-C7-C8-C10
22	c	504	CLA	C11-C10-C8-C7
22	c	504	CLA	C12-C13-C15-C16
22	A	403	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C15
22	b	616	CLA	C11-C12-C13-C15
22	B	610	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C10-C8-C7
22	c	507	CLA	C12-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C15
22	H	101	CLA	C11-C10-C8-C7
22	B	602	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	C	507	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C15
22	C	511	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C7
22	C	504	CLA	C6-C7-C8-C10
22	C	504	CLA	C12-C13-C15-C16
22	C	501	CLA	C11-C12-C13-C15
27	D	407	LMG	C13-C14-C15-C16
22	c	501	CLA	C13-C15-C16-C17
25	d	409	DGD	C2B-C3B-C4B-C5B
27	e	101	LMG	O7-C10-C11-C12
27	A	410	LMG	C20-C21-C22-C23
31	B	627	LMT	C5'-C4'-O1B-C1B
25	b	601	DGD	C5A-C6A-C7A-C8A
22	b	608	CLA	C5-C6-C7-C8
27	B	621	LMG	C28-C29-C30-C31
27	A	410	LMG	C8-C9-O8-C28
27	D	407	LMG	C20-C21-C22-C23
25	b	601	DGD	C4E-C5E-C6E-O5E
27	m	101	LMG	C30-C31-C32-C33
22	a	405	CLA	C5-C6-C7-C8
22	C	506	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
32	d	401	PHO	CAD-CBD-CGD-O2D
32	D	401	PHO	CAD-CBD-CGD-O2D
22	C	507	CLA	CAD-CBD-CGD-O2D
25	C	515	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
22	b	613	CLA	C10-C11-C12-C13
22	c	511	CLA	C5-C6-C7-C8
22	c	507	CLA	C5-C6-C7-C8
25	d	409	DGD	C4A-C5A-C6A-C7A
23	D	406	PL9	C20-C19-C21-C22
22	b	617	CLA	C16-C17-C18-C19
32	d	401	PHO	C5-C6-C7-C8
22	B	604	CLA	C10-C11-C12-C13
27	d	407	LMG	C20-C21-C22-C23
26	a	412	LHG	C2-C3-O3-P
30	a	415	SQD	C44-C45-C46-O48
25	b	601	DGD	C1G-C2G-C3G-O3G
27	M	101	LMG	O1-C7-C8-C9
22	C	510	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	O1A-CGA-O2A-C1
22	b	615	CLA	C10-C11-C12-C13
22	c	506	CLA	O1D-CGD-O2D-CED
22	a	406	CLA	C5-C6-C7-C8
26	c	519	LHG	C1-C2-C3-O3
30	B	626	SQD	O49-C7-O47-C45
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	505	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	A	404	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O1D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
32	D	401	PHO	O1D-CGD-O2D-CED
25	D	409	DGD	C4E-C5E-C6E-O5E
26	C	519	LHG	O10-C23-O8-C6
31	b	604	LMT	C2-C3-C4-C5
30	d	402	SQD	O6-C44-C45-O47
25	A	408	DGD	O2G-C2G-C3G-O3G
30	B	626	SQD	O47-C45-C46-O48
27	B	621	LMG	O7-C8-C9-O8
27	M	101	LMG	O7-C8-C9-O8
22	A	404	CLA	C5-C6-C7-C8
27	C	521	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C4-C3-C7-C8
23	a	409	PL9	C4-C3-C7-C8
22	h	101	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	B	608	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
27	l	101	LMG	C20-C21-C22-C23
25	D	409	DGD	C1A-C2A-C3A-C4A
30	d	402	SQD	C5-C6-S-O8
30	B	622	SQD	C5-C6-S-O8
27	A	410	LMG	O6-C5-C6-O5
27	C	518	LMG	C32-C33-C34-C35
30	B	626	SQD	C10-C11-C12-C13
22	B	603	CLA	CBA-CGA-O2A-C1
24	b	623	BCR	C7-C8-C9-C34
24	C	514	BCR	C7-C8-C9-C10
24	x	101	BCR	C7-C8-C9-C10
30	A	414	SQD	C9-C10-C11-C12
22	A	402	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
22	D	404	CLA	C1A-C2A-CAA-CBA
32	D	401	PHO	C5-C6-C7-C8
25	b	624	DGD	C5A-C6A-C7A-C8A
25	c	515	DGD	C5B-C6B-C7B-C8B
22	c	506	CLA	C3-C5-C6-C7
26	A	409	LHG	C2-C3-O3-P
25	D	409	DGD	C2B-C3B-C4B-C5B
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
27	A	410	LMG	O6-C1-O1-C7
22	B	614	CLA	CBA-CGA-O2A-C1
26	C	519	LHG	O6-C4-C5-C6
32	D	402	PHO	C10-C11-C12-C13
25	c	515	DGD	C5A-C6A-C7A-C8A
30	d	402	SQD	C10-C11-C12-C13
22	C	505	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	b	612	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	CAD-CBD-CGD-O1D
30	d	402	SQD	O5-C5-C6-S
22	c	503	CLA	CAD-CBD-CGD-O1D
27	A	410	LMG	C38-C39-C40-C41
22	B	611	CLA	C10-C11-C12-C13
30	a	401	SQD	C32-C33-C34-C35
26	c	519	LHG	C7-C8-C9-C10
22	b	618	CLA	CBA-CGA-O2A-C1
23	J	101	PL9	C15-C14-C16-C17
22	C	505	CLA	C11-C12-C13-C15
32	a	407	PHO	C6-C7-C8-C10
22	c	505	CLA	C11-C12-C13-C15
26	C	519	LHG	O6-C4-C5-O7
22	c	509	CLA	C6-C7-C8-C10
22	h	101	CLA	C11-C10-C8-C7
22	b	613	CLA	C11-C12-C13-C15
22	b	613	CLA	C12-C13-C15-C16
22	b	612	CLA	C12-C13-C15-C16
22	B	609	CLA	C12-C13-C15-C16
26	c	519	LHG	O6-C4-C5-O7
22	B	608	CLA	C12-C13-C15-C16
22	C	520	CLA	C6-C7-C8-C10
22	c	508	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	d	405	CLA	C11-C10-C8-C7
22	c	520	CLA	C6-C7-C8-C10
22	A	405	CLA	C11-C10-C8-C7
22	b	611	CLA	C11-C12-C13-C15
22	C	508	CLA	C6-C7-C8-C10
22	D	405	CLA	C11-C10-C8-C7
25	D	409	DGD	C4A-C5A-C6A-C7A
27	A	415	LMG	C12-C13-C14-C15
27	b	625	LMG	C12-C13-C14-C15
22	b	609	CLA	C13-C15-C16-C17
27	d	408	LMG	C31-C32-C33-C34
25	B	620	DGD	C5A-C6A-C7A-C8A
22	B	609	CLA	C5-C6-C7-C8
22	A	403	CLA	C5-C6-C7-C8
22	c	512	CLA	C2A-CAA-CBA-CGA
27	e	101	LMG	O1-C7-C8-C9
34	v	201	HEM	C4D-C3D-CAD-CBD
30	B	622	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
25	D	409	DGD	O2G-C2G-C3G-O3G
25	a	411	DGD	O2G-C2G-C3G-O3G
25	d	409	DGD	O2G-C2G-C3G-O3G
25	c	516	DGD	C6A-C7A-C8A-C9A
25	B	625	DGD	C4E-C5E-C6E-O5E
27	D	408	LMG	C31-C32-C33-C34
30	a	415	SQD	C11-C10-C9-C8
27	l	101	LMG	C8-C7-O1-C1
27	A	410	LMG	C8-C7-O1-C1
22	c	504	CLA	C8-C10-C11-C12
27	c	522	LMG	C35-C36-C37-C38
22	B	603	CLA	O1A-CGA-O2A-C1
32	a	407	PHO	C10-C11-C12-C13
27	l	101	LMG	C16-C17-C18-C19
23	d	406	PL9	C13-C14-C16-C17
27	A	410	LMG	C29-C30-C31-C32
22	a	405	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C10-C8-C9
22	b	619	CLA	C11-C10-C8-C9
22	C	509	CLA	C6-C7-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	B	608	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	A	403	CLA	C14-C13-C15-C16
22	b	616	CLA	C11-C12-C13-C14
22	B	610	CLA	C11-C10-C8-C9
22	B	607	CLA	C11-C12-C13-C14
22	B	614	CLA	C6-C7-C8-C9
22	c	501	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	C	507	CLA	C14-C13-C15-C16
22	C	511	CLA	C14-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C9
22	d	404	CLA	C6-C7-C8-C9
22	C	501	CLA	C11-C12-C13-C14
22	B	614	CLA	O1A-CGA-O2A-C1
25	B	620	DGD	O1A-C1A-O1G-C1G
27	l	101	LMG	C29-C30-C31-C32
30	a	401	SQD	C9-C10-C11-C12
27	c	518	LMG	C32-C33-C34-C35
24	B	619	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
32	D	402	PHO	C13-C15-C16-C17
24	j	102	BCR	C7-C8-C9-C10
22	C	511	CLA	CAA-CBA-CGA-O2A
32	a	407	PHO	C13-C15-C16-C17
22	b	613	CLA	C5-C6-C7-C8
27	B	621	LMG	C12-C13-C14-C15
25	d	409	DGD	C4E-C5E-C6E-O5E
22	b	618	CLA	O1A-CGA-O2A-C1
27	b	625	LMG	C15-C16-C17-C18
22	C	506	CLA	C3-C5-C6-C7
22	b	615	CLA	C4-C3-C5-C6
22	B	611	CLA	C4-C3-C5-C6
22	c	511	CLA	CAA-CBA-CGA-O2A
27	A	410	LMG	C35-C36-C37-C38
25	C	517	DGD	C3G-C2G-O2G-C1B
27	m	101	LMG	C9-C8-O7-C10
26	a	412	LHG	C6-C5-O7-C7
25	c	517	DGD	C3G-C2G-O2G-C1B
26	c	519	LHG	O6-C4-C5-C6
22	b	617	CLA	C2A-CAA-CBA-CGA
22	c	508	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	CBA-CGA-O2A-C1
22	b	613	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
27	l	101	LMG	C10-C11-C12-C13
32	d	401	PHO	O1D-CGD-O2D-CED
27	a	402	LMG	C16-C17-C18-C19
30	a	401	SQD	C12-C13-C14-C15
22	B	605	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	C16-C17-C18-C19
22	a	405	CLA	C4-C3-C5-C6
24	K	102	BCR	C1-C6-C7-C8
24	K	102	BCR	C23-C24-C25-C26
24	K	102	BCR	C23-C24-C25-C30
24	c	521	BCR	C1-C6-C7-C8
24	c	521	BCR	C23-C24-C25-C26
24	c	521	BCR	C23-C24-C25-C30
24	B	619	BCR	C23-C24-C25-C26
24	C	514	BCR	C1-C6-C7-C8
24	C	514	BCR	C5-C6-C7-C8
24	c	514	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	c	514	BCR	C5-C6-C7-C8
24	A	407	BCR	C23-C24-C25-C30
27	l	101	LMG	C11-C12-C13-C14
22	B	612	CLA	C10-C11-C12-C13
22	a	408	CLA	C16-C17-C18-C19
22	A	405	CLA	C16-C17-C18-C19
25	c	515	DGD	O6D-C1D-O3G-C3G
30	f	103	SQD	C24-C25-C26-C27
25	B	620	DGD	CAB-CBB-CCB-CDB
27	D	408	LMG	O1-C7-C8-O7
27	b	625	LMG	O7-C8-C9-O8
27	d	408	LMG	O1-C7-C8-O7
27	D	407	LMG	C16-C17-C18-C19
22	h	101	CLA	CBA-CGA-O2A-C1
22	B	609	CLA	CBA-CGA-O2A-C1
26	a	412	LHG	C3-O3-P-O6
26	A	409	LHG	C3-O3-P-O6
25	c	516	DGD	C7B-C8B-C9B-CAB
30	B	622	SQD	C10-C11-C12-C13
27	M	101	LMG	C31-C32-C33-C34
27	d	411	LMG	O1-C7-C8-C9
30	d	402	SQD	O6-C44-C45-C46
22	B	610	CLA	C4-C3-C5-C6
27	A	415	LMG	C16-C17-C18-C19
25	B	625	DGD	C2A-C3A-C4A-C5A
22	b	616	CLA	C10-C11-C12-C13
23	D	406	PL9	C13-C14-C16-C17
22	h	101	CLA	C11-C12-C13-C15
22	B	608	CLA	C11-C12-C13-C15
22	C	504	CLA	C11-C10-C8-C7
22	c	503	CLA	C6-C7-C8-C10
30	a	401	SQD	C26-C27-C28-C29
22	c	510	CLA	C3-C5-C6-C7
22	C	505	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	b	619	CLA	C14-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C14
22	B	609	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C11-C10-C8-C9
22	c	520	CLA	C6-C7-C8-C9
22	A	405	CLA	C11-C10-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	c	503	CLA	C6-C7-C8-C9
22	b	606	CLA	C16-C17-C18-C19
27	D	411	LMG	C16-C17-C18-C19
25	c	517	DGD	C8B-C9B-CAB-CBB
31	b	603	LMT	C4'-C5'-C6'-O6'
24	f	102	BCR	C7-C8-C9-C34
27	E	101	LMG	C31-C32-C33-C34
27	l	101	LMG	C35-C36-C37-C38
27	A	410	LMG	C11-C12-C13-C14
22	B	609	CLA	O1A-CGA-O2A-C1
30	F	103	SQD	C24-C25-C26-C27
31	b	627	LMT	O5'-C5'-C6'-O6'
27	c	522	LMG	C32-C33-C34-C35
25	b	624	DGD	CCA-CDA-CEA-CFA
22	b	607	CLA	CBA-CGA-O2A-C1
22	h	101	CLA	O1A-CGA-O2A-C1
27	e	101	LMG	C31-C32-C33-C34
27	c	522	LMG	C30-C31-C32-C33
27	m	101	LMG	O6-C1-O1-C7
25	a	411	DGD	O6E-C1E-O5D-C6D
25	C	516	DGD	O6E-C1E-O5D-C6D
25	b	601	DGD	O6D-C1D-O3G-C3G
23	D	406	PL9	C24-C26-C27-C28
23	d	406	PL9	C24-C26-C27-C28
22	B	602	CLA	C15-C16-C17-C18
27	A	410	LMG	C16-C17-C18-C19
27	d	407	LMG	C16-C17-C18-C19
24	J	102	BCR	C18-C19-C20-C21
27	A	410	LMG	C10-C11-C12-C13
22	b	609	CLA	C16-C17-C18-C20
32	d	401	PHO	C4B-C3B-CAB-CBB
22	A	403	CLA	C4-C3-C5-C6
22	b	607	CLA	O1A-CGA-O2A-C1
22	C	507	CLA	C5-C6-C7-C8
30	A	414	SQD	C12-C13-C14-C15
22	A	402	CLA	C2-C1-O2A-CGA
22	a	404	CLA	C2-C1-O2A-CGA
22	B	612	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	C2-C1-O2A-CGA
25	b	624	DGD	CAB-CBB-CCB-CDB
25	C	516	DGD	C7B-C8B-C9B-CAB
31	D	410	LMT	O5'-C5'-C6'-O6'
25	C	517	DGD	C4A-C5A-C6A-C7A
25	C	517	DGD	C8B-C9B-CAB-CBB
25	C	515	DGD	C5B-C6B-C7B-C8B
27	d	407	LMG	C29-C30-C31-C32
27	D	407	LMG	C29-C30-C31-C32
22	c	512	CLA	C3A-C2A-CAA-CBA
22	C	512	CLA	C3A-C2A-CAA-CBA
22	B	612	CLA	C13-C15-C16-C17
27	C	521	LMG	C30-C31-C32-C33
27	l	101	LMG	C8-C9-O8-C28
22	b	606	CLA	C15-C16-C17-C18
27	D	408	LMG	C18-C19-C20-C21
27	D	408	LMG	C36-C37-C38-C39
22	b	617	CLA	C2C-C3C-CAC-CBC
25	b	601	DGD	C2A-C3A-C4A-C5A
25	b	601	DGD	O6E-C5E-C6E-O5E
22	B	615	CLA	C11-C12-C13-C14
22	b	619	CLA	C11-C12-C13-C14
32	D	401	PHO	C6-C7-C8-C9
22	b	618	CLA	C6-C7-C8-C9
22	A	405	CLA	C16-C17-C18-C20
30	A	413	SQD	C16-C17-C18-C19
27	D	411	LMG	C36-C37-C38-C39
24	b	621	BCR	C20-C21-C22-C37
27	D	411	LMG	O1-C7-C8-C9
30	A	413	SQD	C11-C10-C9-C8
23	D	406	PL9	C32-C33-C34-C36
22	c	510	CLA	C2A-CAA-CBA-CGA
27	M	101	LMG	C30-C31-C32-C33
22	a	408	CLA	C16-C17-C18-C20
25	c	516	DGD	O6E-C1E-O5D-C6D
25	B	625	DGD	O6D-C1D-O3G-C3G
25	C	515	DGD	O6D-C1D-O3G-C3G
27	M	101	LMG	O6-C1-O1-C7
27	d	411	LMG	C16-C17-C18-C19
31	D	410	LMT	O5B-C5B-C6B-O6B
26	a	412	LHG	C4-C5-O7-C7
26	A	409	LHG	C6-C5-O7-C7

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C9-C8-O7-C10
22	c	503	CLA	C15-C16-C17-C18
22	b	614	CLA	C4-C3-C5-C6
22	c	512	CLA	C1A-C2A-CAA-CBA
22	C	505	CLA	C6-C7-C8-C10
22	c	505	CLA	C6-C7-C8-C10
22	a	408	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
32	D	402	PHO	C6-C7-C8-C10
22	C	509	CLA	C11-C10-C8-C7
22	b	605	CLA	C12-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C10
22	H	101	CLA	C12-C13-C15-C16
22	D	404	CLA	C11-C10-C8-C7
22	C	507	CLA	C11-C12-C13-C15
22	d	404	CLA	C11-C10-C8-C7
22	b	616	CLA	C8-C10-C11-C12
25	A	408	DGD	C2A-C3A-C4A-C5A
30	F	103	SQD	C9-C10-C11-C12
22	H	101	CLA	CBA-CGA-O2A-C1
22	B	607	CLA	C13-C15-C16-C17
22	C	504	CLA	C8-C10-C11-C12
30	a	415	SQD	C12-C13-C14-C15
25	d	409	DGD	CBB-CCB-CDB-CEB
27	D	407	LMG	C10-C11-C12-C13
22	B	605	CLA	C13-C15-C16-C17
27	B	621	LMG	C29-C28-O8-C9
25	D	409	DGD	CBB-CCB-CDB-CEB
27	a	402	LMG	C12-C13-C14-C15
22	c	509	CLA	C16-C17-C18-C19
27	l	101	LMG	C38-C39-C40-C41
27	m	101	LMG	C31-C32-C33-C34
22	B	604	CLA	C8-C10-C11-C12
27	m	101	LMG	C17-C18-C19-C20
22	B	612	CLA	C8-C10-C11-C12
27	D	408	LMG	C34-C35-C36-C37
27	B	621	LMG	C15-C16-C17-C18
25	d	409	DGD	C8A-C9A-CAA-CBA
30	a	401	SQD	C17-C18-C19-C20
31	B	624	LMT	C6-C7-C8-C9
22	A	403	CLA	C2-C1-O2A-CGA
22	b	615	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C2-C3-C5-C6
22	B	611	CLA	C2-C3-C5-C6
25	D	409	DGD	C8A-C9A-CAA-CBA
22	a	405	CLA	C11-C10-C8-C9
22	b	615	CLA	C6-C7-C8-C9
22	A	403	CLA	C11-C10-C8-C9
22	H	101	CLA	O1A-CGA-O2A-C1
25	B	625	DGD	CAB-CBB-CCB-CDB
22	d	405	CLA	C2A-CAA-CBA-CGA
22	D	405	CLA	C2A-CAA-CBA-CGA
22	C	501	CLA	C16-C17-C18-C20
25	B	620	DGD	C7B-C8B-C9B-CAB
24	K	102	BCR	C5-C6-C7-C8
24	g	101	BCR	C1-C6-C7-C8
24	c	521	BCR	C5-C6-C7-C8
24	b	621	BCR	C1-C6-C7-C8
24	f	102	BCR	C23-C24-C25-C30
24	B	618	BCR	C1-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C30
24	B	617	BCR	C1-C6-C7-C8
24	F	102	BCR	C23-C24-C25-C30
24	b	622	BCR	C1-C6-C7-C8
24	b	622	BCR	C23-C24-C25-C30
22	b	617	CLA	C4C-C3C-CAC-CBC
27	M	101	LMG	C16-C17-C18-C19
22	C	510	CLA	C4-C3-C5-C6
23	D	406	PL9	C40-C39-C41-C42
24	H	102	BCR	C7-C8-C9-C10
24	F	102	BCR	C21-C22-C23-C24
22	B	602	CLA	C16-C17-C18-C20
25	b	624	DGD	O1A-C1A-O1G-C1G
25	B	625	DGD	C2G-C3G-O3G-C1D
25	b	601	DGD	C2G-C3G-O3G-C1D
27	D	411	LMG	C8-C7-O1-C1
22	B	613	CLA	C2C-C3C-CAC-CBC
22	b	609	CLA	C16-C17-C18-C19
27	C	518	LMG	C17-C18-C19-C20
27	e	101	LMG	C30-C31-C32-C33
27	C	521	LMG	C32-C33-C34-C35
22	B	601	CLA	C12-C13-C15-C16
22	h	101	CLA	C12-C13-C15-C16
22	b	612	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
25	B	620	DGD	CCA-CDA-CEA-CFA
25	a	411	DGD	C2A-C3A-C4A-C5A
26	C	519	LHG	O7-C7-C8-C9
25	c	516	DGD	C2E-C1E-O5D-C6D
25	C	516	DGD	C2E-C1E-O5D-C6D
27	d	411	LMG	O1-C7-C8-O7
27	b	625	LMG	O1-C7-C8-O7
22	b	609	CLA	CBA-CGA-O2A-C1
27	d	411	LMG	C11-C12-C13-C14
26	c	519	LHG	O7-C7-C8-C9
22	d	404	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	C2A-CAA-CBA-CGA
25	c	517	DGD	CBB-CCB-CDB-CEB
22	c	502	CLA	CBA-CGA-O2A-C1
27	l	101	LMG	O7-C10-C11-C12
22	b	614	CLA	C2-C3-C5-C6
22	B	612	CLA	CAA-CBA-CGA-O2A
30	a	415	SQD	C16-C17-C18-C19
32	a	407	PHO	C6-C7-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	h	101	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	b	605	CLA	C14-C13-C15-C16
22	C	520	CLA	C6-C7-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C12-C13-C14
22	C	520	CLA	C3A-C2A-CAA-CBA
22	D	404	CLA	C3A-C2A-CAA-CBA
27	m	101	LMG	O10-C28-O8-C9
27	A	410	LMG	O7-C10-C11-C12
22	b	616	CLA	CAA-CBA-CGA-O2A
32	d	401	PHO	C2B-C3B-CAB-CBB
22	c	509	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	C	509	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
32	D	401	PHO	C2B-C3B-CAB-CBB
22	b	615	CLA	CAD-CBD-CGD-O2D
22	c	507	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	CAD-CBD-CGD-O2D
22	b	608	CLA	CAD-CBD-CGD-O2D
26	A	409	LHG	C4-C5-O7-C7
22	B	611	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	C16-C17-C18-C20
22	b	606	CLA	C16-C17-C18-C20
22	b	616	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
22	c	502	CLA	O1A-CGA-O2A-C1
23	d	406	PL9	C32-C33-C34-C36
22	C	506	CLA	CAA-CBA-CGA-O2A
22	b	615	CLA	CAA-CBA-CGA-O2A
22	c	510	CLA	C4-C3-C5-C6
30	B	622	SQD	C7-C8-C9-C10
27	C	521	LMG	O8-C28-C29-C30
25	C	517	DGD	O1G-C1A-C2A-C3A
22	c	501	CLA	CAA-CBA-CGA-O2A
22	b	609	CLA	O1A-CGA-O2A-C1
24	f	102	BCR	C21-C22-C23-C24
27	c	518	LMG	C7-C8-C9-O8
27	E	101	LMG	O1-C7-C8-C9
27	C	518	LMG	C7-C8-C9-O8
25	C	515	DGD	C1G-C2G-C3G-O3G
22	C	508	CLA	C10-C11-C12-C13
27	a	402	LMG	O7-C10-C11-C12
30	f	103	SQD	C9-C10-C11-C12
27	A	410	LMG	C17-C18-C19-C20
32	a	407	PHO	O2A-C1-C2-C3
32	D	402	PHO	O2A-C1-C2-C3
22	B	615	CLA	O2A-C1-C2-C3
22	b	619	CLA	O2A-C1-C2-C3
22	c	511	CLA	O2A-C1-C2-C3
22	C	511	CLA	O2A-C1-C2-C3
22	B	613	CLA	C4C-C3C-CAC-CBC
32	D	401	PHO	C4B-C3B-CAB-CBB
27	A	415	LMG	O7-C10-C11-C12
25	c	517	DGD	O1G-C1A-C2A-C3A
22	C	510	CLA	C3-C5-C6-C7
22	C	501	CLA	C16-C17-C18-C19
25	C	516	DGD	C6A-C7A-C8A-C9A
22	b	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
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	b	612	CLA	CHA-CBD-CGD-O2D
22	a	406	CLA	CHA-CBD-CGD-O1D
22	a	406	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	606	CLA	CHA-CBD-CGD-O2D
22	H	101	CLA	CHA-CBD-CGD-O1D
22	H	101	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O1D
22	C	512	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	C2-C3-C5-C6
27	E	101	LMG	C30-C31-C32-C33
25	D	409	DGD	O6E-C5E-C6E-O5E
22	C	509	CLA	C16-C17-C18-C19
22	C	509	CLA	CAA-CBA-CGA-O2A
30	A	414	SQD	O47-C7-C8-C9
26	C	519	LHG	C11-C12-C13-C14
27	e	101	LMG	O1-C7-C8-O7
27	B	621	LMG	O1-C7-C8-O7
30	a	401	SQD	C23-C24-C25-C26
30	d	402	SQD	C7-C8-C9-C10
30	A	413	SQD	C12-C13-C14-C15
30	a	401	SQD	O47-C7-C8-C9
27	c	522	LMG	O8-C28-C29-C30
22	C	501	CLA	CAA-CBA-CGA-O2A
22	c	508	CLA	C8-C10-C11-C12
22	C	502	CLA	CBA-CGA-O2A-C1
25	B	625	DGD	O6E-C5E-C6E-O5E
30	f	103	SQD	C14-C15-C16-C17
22	C	506	CLA	C11-C12-C13-C15
22	a	405	CLA	C2-C3-C5-C6
22	B	604	CLA	C11-C12-C13-C15
22	B	611	CLA	C6-C7-C8-C10
25	A	408	DGD	O6E-C1E-O5D-C6D
22	c	509	CLA	CAA-CBA-CGA-O2A
22	D	404	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C6-C7-C8-C9
22	a	408	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	B	601	CLA	C14-C13-C15-C16
22	C	503	CLA	C6-C7-C8-C9
32	D	402	PHO	C6-C7-C8-C9
22	b	609	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C12-C13-C14
22	B	614	CLA	C11-C12-C13-C14
22	b	618	CLA	C11-C12-C13-C14
22	H	101	CLA	C11-C10-C8-C9
22	B	602	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C10-C8-C9
22	B	611	CLA	C6-C7-C8-C9
22	d	404	CLA	C11-C10-C8-C9
26	C	519	LHG	C7-C8-C9-C10
22	c	506	CLA	CAA-CBA-CGA-O2A
27	A	410	LMG	C13-C14-C15-C16
25	d	409	DGD	C9B-CAB-CBB-CCB
25	b	601	DGD	CAB-CBB-CCB-CDB
30	a	415	SQD	C8-C7-O47-C45
25	C	517	DGD	C4B-C5B-C6B-C7B
22	B	611	CLA	CAA-CBA-CGA-O2A
30	A	414	SQD	C26-C27-C28-C29
22	B	605	CLA	C16-C17-C18-C20
25	c	517	DGD	C4A-C5A-C6A-C7A
22	A	405	CLA	C4-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6
22	c	509	CLA	CAA-CBA-CGA-O1A
22	C	509	CLA	C13-C15-C16-C17
22	b	608	CLA	C8-C10-C11-C12
22	C	520	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	d	404	CLA	C1A-C2A-CAA-CBA
27	d	411	LMG	O9-C10-C11-C12
30	B	622	SQD	O49-C7-C8-C9
22	C	503	CLA	C15-C16-C17-C18
22	C	502	CLA	O1A-CGA-O2A-C1
22	c	511	CLA	C2-C1-O2A-CGA
22	C	511	CLA	C2-C1-O2A-CGA
31	b	604	LMT	C6-C7-C8-C9
27	m	101	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	d	402	SQD	O49-C7-C8-C9
22	d	404	CLA	CAA-CBA-CGA-O1A
25	c	515	DGD	C1G-C2G-C3G-O3G
27	I	101	LMG	C7-C8-C9-O8
27	d	407	LMG	C7-C8-C9-O8
25	C	517	DGD	O2G-C1B-C2B-C3B
30	d	402	SQD	O47-C7-C8-C9
25	c	517	DGD	O2G-C1B-C2B-C3B
22	B	602	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA
25	C	517	DGD	CBB-CCB-CDB-CEB
27	d	408	LMG	C18-C19-C20-C21
26	C	519	LHG	O2-C2-C3-O3
22	b	615	CLA	CAA-CBA-CGA-O1A
22	B	612	CLA	CAA-CBA-CGA-O1A
22	b	616	CLA	CAA-CBA-CGA-O1A
27	D	411	LMG	O9-C10-C11-C12
25	b	624	DGD	C4A-C5A-C6A-C7A
27	D	408	LMG	O7-C10-C11-C12
30	B	622	SQD	O47-C7-C8-C9
22	C	506	CLA	CAA-CBA-CGA-O1A
27	c	522	LMG	O10-C28-C29-C30
30	A	414	SQD	O49-C7-C8-C9
22	B	611	CLA	CAA-CBA-CGA-O1A
25	A	408	DGD	C2E-C1E-O5D-C6D
25	a	411	DGD	C2E-C1E-O5D-C6D
30	f	103	SQD	C15-C16-C17-C18
27	D	411	LMG	C32-C33-C34-C35
26	a	412	LHG	C3-O3-P-O5
26	A	409	LHG	C3-O3-P-O5
22	c	502	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C20
22	c	506	CLA	CAA-CBA-CGA-O1A
22	D	404	CLA	CAA-CBA-CGA-O1A
22	C	501	CLA	CAA-CBA-CGA-O1A
26	c	519	LHG	C11-C12-C13-C14
24	g	101	BCR	C5-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C26
24	B	617	BCR	C5-C6-C7-C8
24	b	622	BCR	C23-C24-C25-C26
22	b	606	CLA	C8-C10-C11-C12
27	d	408	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C4C-C3C-CAC-CBC
22	C	502	CLA	C16-C17-C18-C20
22	c	509	CLA	C13-C15-C16-C17
25	b	624	DGD	O2G-C1B-C2B-C3B
30	a	401	SQD	O49-C7-C8-C9
22	c	501	CLA	CAA-CBA-CGA-O1A
22	a	408	CLA	C4-C3-C5-C6
31	B	623	LMT	C4-C5-C6-C7
22	A	403	CLA	C2-C3-C5-C6
22	B	605	CLA	C15-C16-C17-C18
30	a	401	SQD	C5-C6-S-O9
22	C	502	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
30	A	414	SQD	C5-C6-S-O9
30	B	626	SQD	C5-C6-S-O9
30	B	622	SQD	O5-C5-C6-S
27	M	101	LMG	C7-C8-O7-C10
27	M	101	LMG	O10-C28-O8-C9
27	l	101	LMG	O9-C10-C11-C12
27	a	402	LMG	O9-C10-C11-C12
30	A	413	SQD	C9-C10-C11-C12
30	F	103	SQD	C14-C15-C16-C17
27	M	101	LMG	O8-C28-C29-C30
22	c	506	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
22	h	101	CLA	CAA-CBA-CGA-O2A
22	b	613	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	CAA-CBA-CGA-O2A
22	c	504	CLA	CAA-CBA-CGA-O2A
22	b	605	CLA	CAA-CBA-CGA-O2A
22	b	617	CLA	CAA-CBA-CGA-O2A
30	F	103	SQD	C15-C16-C17-C18
27	i	101	LMG	O7-C10-C11-C12
27	A	410	LMG	O9-C10-C11-C12
23	d	406	PL9	C40-C39-C41-C42
22	c	502	CLA	C5-C6-C7-C8
22	C	503	CLA	C6-C7-C8-C10
22	b	609	CLA	C6-C7-C8-C10
22	b	619	CLA	C11-C12-C13-C15
22	c	512	CLA	C11-C12-C13-C15
22	c	507	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C11-C12-C13-C15
22	b	618	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	B	613	CLA	CAA-CBA-CGA-O1A
25	A	408	DGD	O6D-C5D-C6D-O5D
22	B	601	CLA	CAA-CBA-CGA-O2A
22	B	613	CLA	CAA-CBA-CGA-O2A
22	C	504	CLA	CAA-CBA-CGA-O2A
27	d	411	LMG	C12-C13-C14-C15
27	e	101	LMG	C14-C15-C16-C17
27	C	521	LMG	O10-C28-C29-C30
22	C	509	CLA	CAA-CBA-CGA-O1A
23	J	101	PL9	C2-C3-C7-C8
27	c	518	LMG	C17-C18-C19-C20
27	M	101	LMG	C17-C18-C19-C20
25	B	620	DGD	O2G-C1B-C2B-C3B
22	C	502	CLA	C5-C6-C7-C8
27	l	101	LMG	C17-C18-C19-C20
27	D	408	LMG	O9-C10-C11-C12
22	B	609	CLA	CAA-CBA-CGA-O1A
30	A	413	SQD	O49-C7-C8-C9
22	c	504	CLA	CAA-CBA-CGA-O1A
30	a	415	SQD	O49-C7-C8-C9
25	c	517	DGD	O1A-C1A-C2A-C3A
31	B	627	LMT	C4'-C5'-C6'-O6'
22	b	605	CLA	CAA-CBA-CGA-O1A
22	C	504	CLA	CAA-CBA-CGA-O1A
22	b	613	CLA	CAA-CBA-CGA-O1A
22	b	617	CLA	CAA-CBA-CGA-O1A
27	A	410	LMG	C39-C40-C41-C42

There are no ring outliers.

79 monomers are involved in 311 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	K	102	BCR	3	0
22	C	510	CLA	9	0
23	D	406	PL9	12	0
26	C	519	LHG	3	0
22	B	601	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	E	101	LMG	2	0
25	A	408	DGD	1	0
25	C	517	DGD	5	0
25	D	409	DGD	1	0
34	V	201	HEM	3	0
22	C	503	CLA	5	0
31	B	623	LMT	2	0
23	A	406	PL9	5	0
32	D	402	PHO	5	0
32	D	401	PHO	8	0
22	A	404	CLA	14	0
22	B	615	CLA	6	0
22	B	609	CLA	3	0
22	A	402	CLA	11	0
22	C	509	CLA	6	0
31	B	628	LMT	2	0
22	C	506	CLA	6	0
24	J	102	BCR	2	0
24	B	619	BCR	1	0
24	C	514	BCR	7	0
31	I	102	LMT	1	0
27	D	408	LMG	6	0
27	A	410	LMG	2	0
22	B	608	CLA	15	0
27	I	101	LMG	1	0
31	B	627	LMT	2	0
24	B	618	BCR	4	0
34	F	101	HEM	4	0
30	A	413	SQD	3	0
22	B	605	CLA	7	0
27	A	415	LMG	1	0
22	A	403	CLA	12	0
25	B	625	DGD	2	0
22	B	612	CLA	9	0
30	A	414	SQD	5	0
24	H	102	BCR	1	0
22	B	610	CLA	5	0
30	F	103	SQD	3	0
24	C	513	BCR	7	0
22	B	607	CLA	11	0
30	B	626	SQD	2	0
25	C	516	DGD	4	0

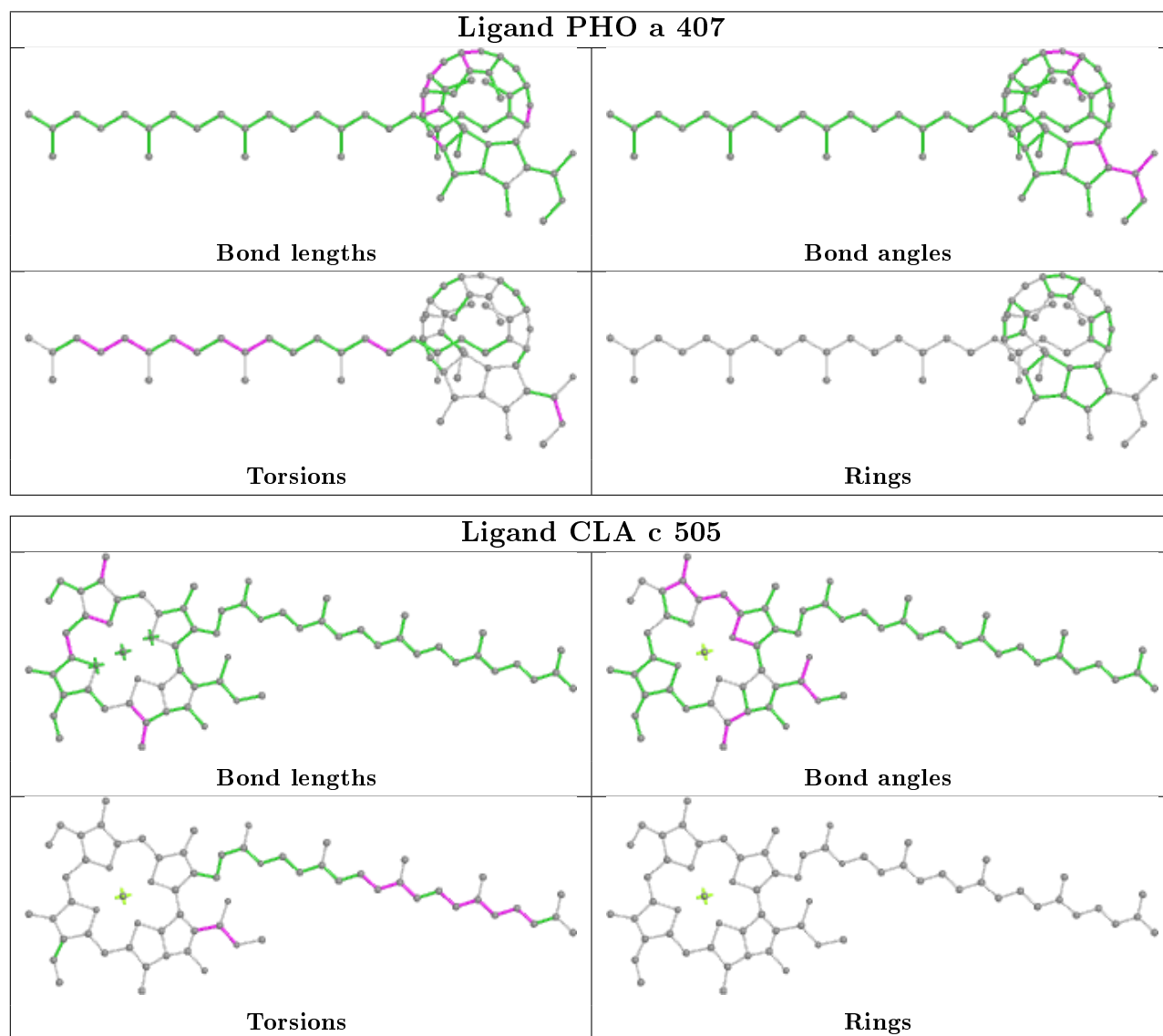
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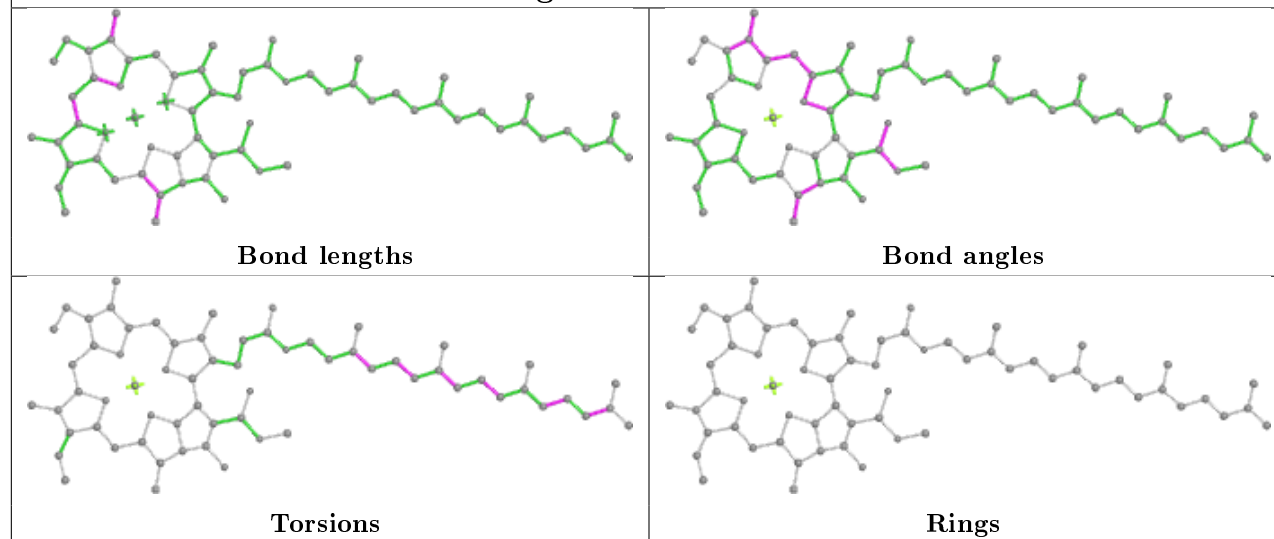
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	520	CLA	5	0
22	C	505	CLA	3	0
27	D	407	LMG	4	0
27	C	518	LMG	3	0
22	B	606	CLA	16	0
22	B	614	CLA	4	0
22	B	603	CLA	4	0
27	D	411	LMG	1	0
22	H	101	CLA	11	0
24	B	617	BCR	2	0
22	B	613	CLA	5	0
22	B	602	CLA	11	0
27	B	621	LMG	3	0
22	A	405	CLA	12	0
24	A	407	BCR	2	0
26	A	409	LHG	3	0
22	B	604	CLA	9	0
22	D	404	CLA	10	0
24	F	102	BCR	3	0
22	C	508	CLA	3	0
22	C	507	CLA	4	0
22	D	405	CLA	4	0
24	B	616	BCR	6	0
30	B	622	SQD	3	0
22	C	511	CLA	1	0
25	C	515	DGD	3	0
22	B	611	CLA	10	0
27	M	101	LMG	2	0
22	C	504	CLA	4	0
22	C	501	CLA	7	0
22	C	512	CLA	3	0
25	B	620	DGD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

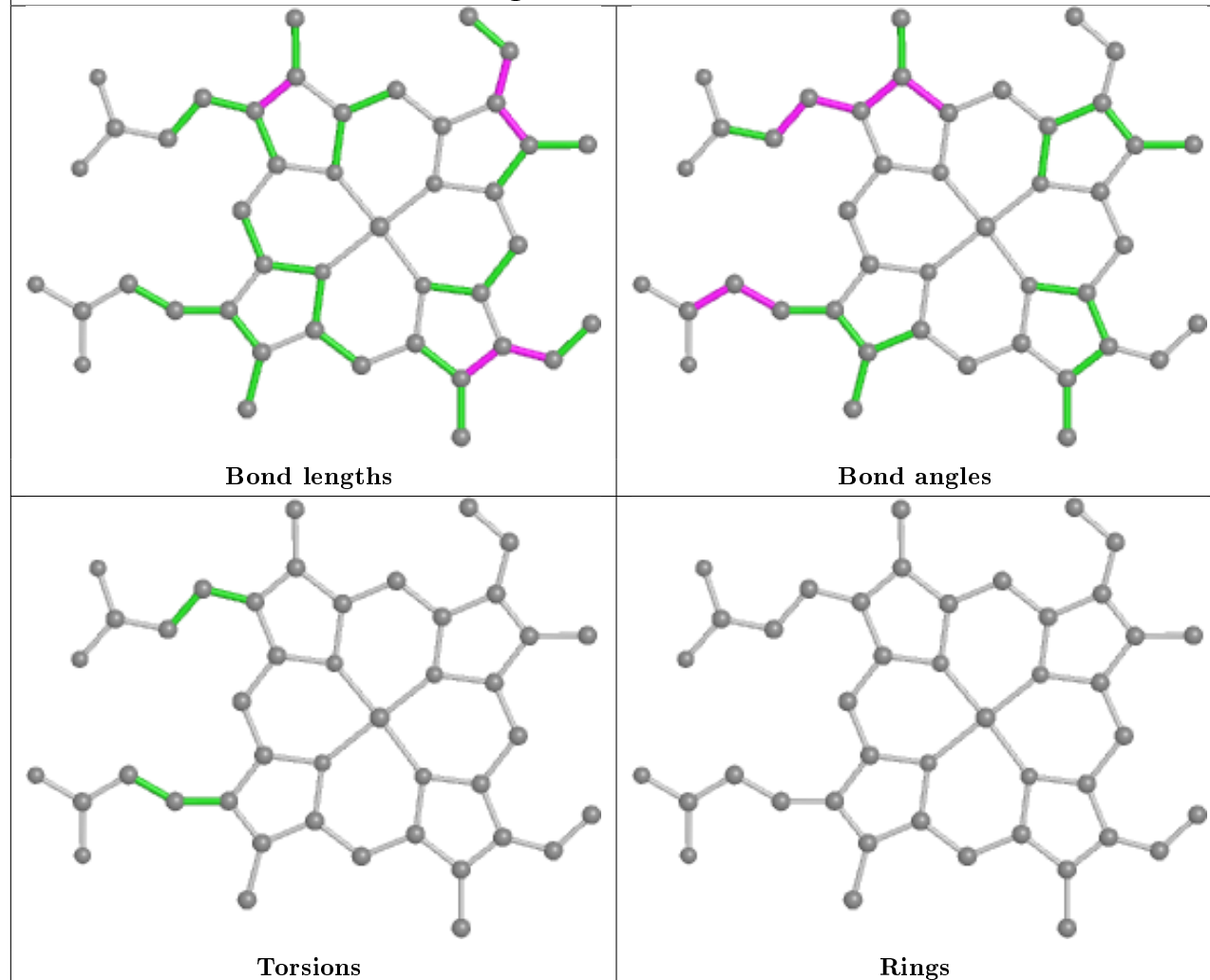
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

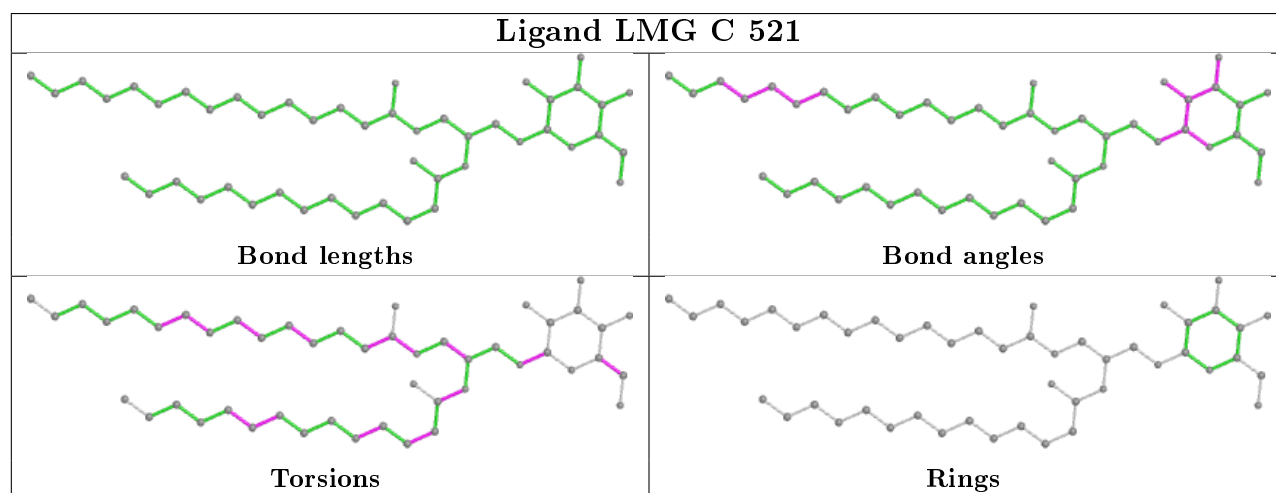
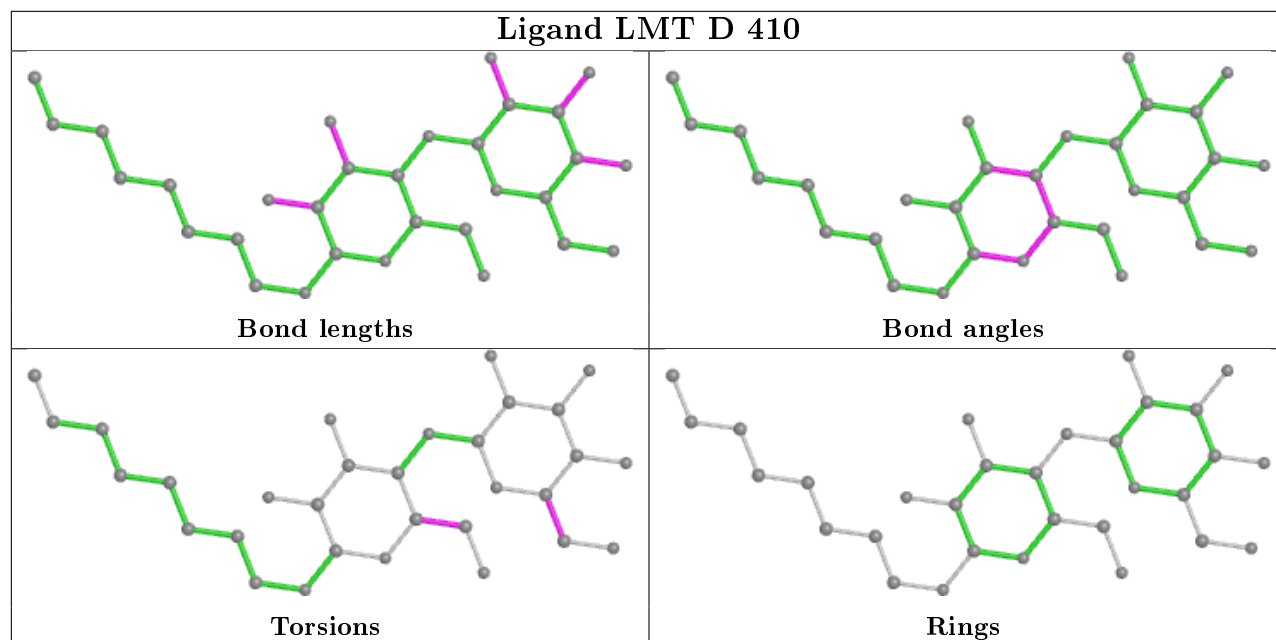
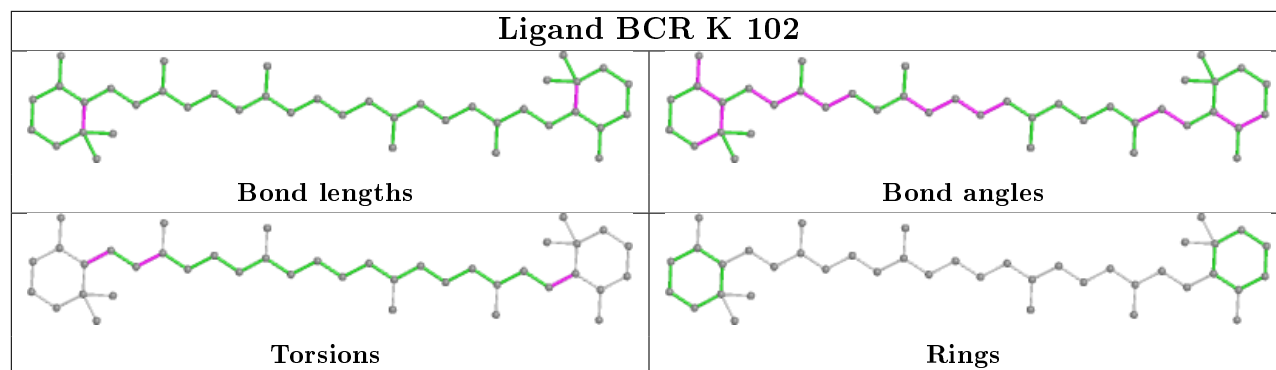


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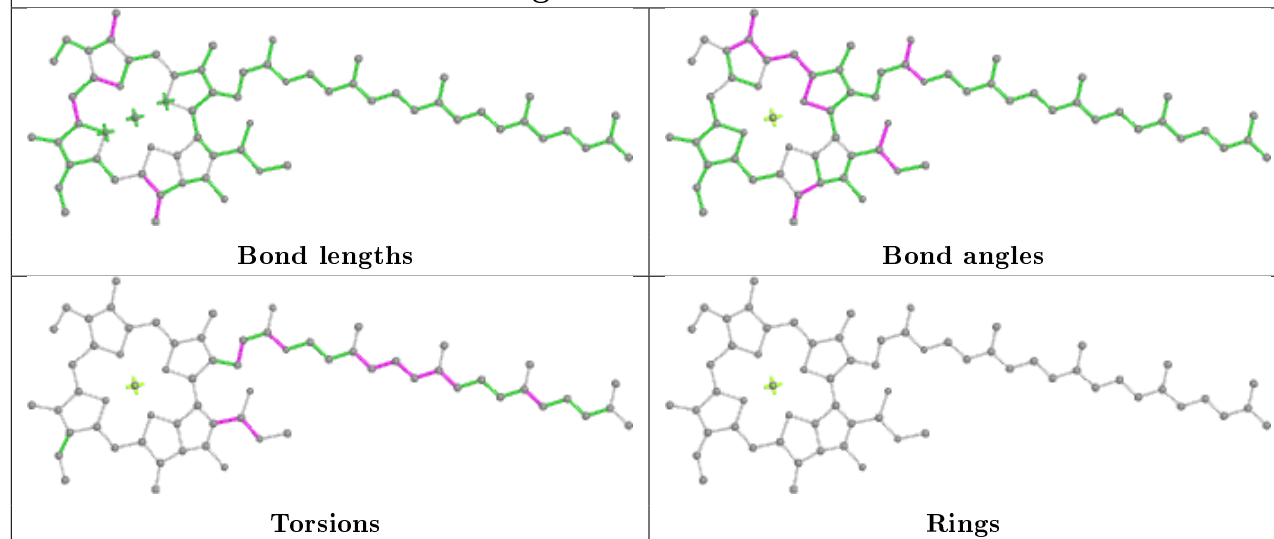


Ligand HEM f 101

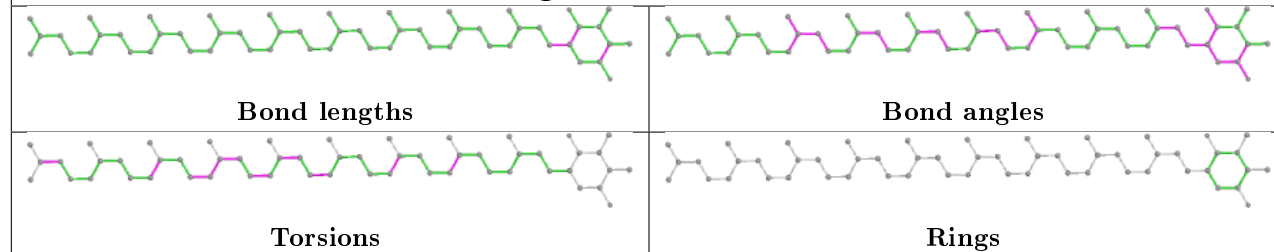




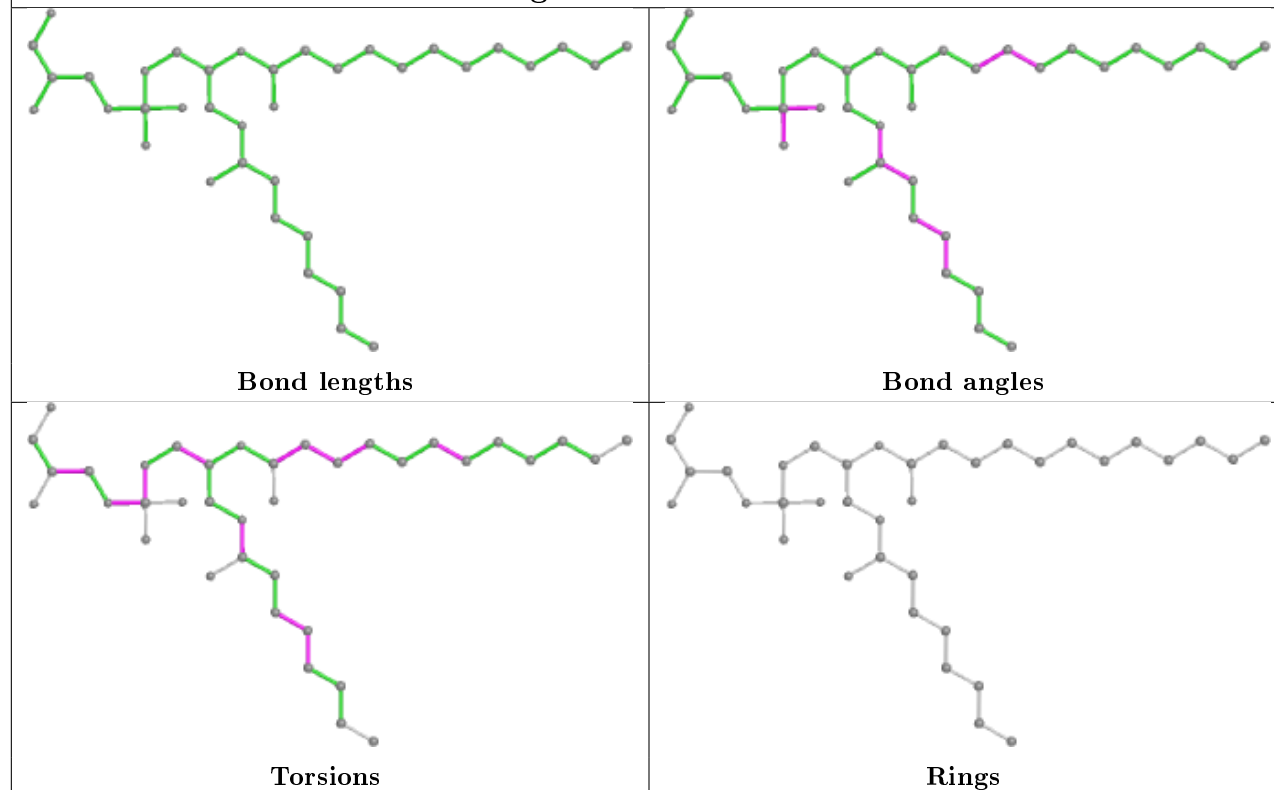
Ligand CLA C 510



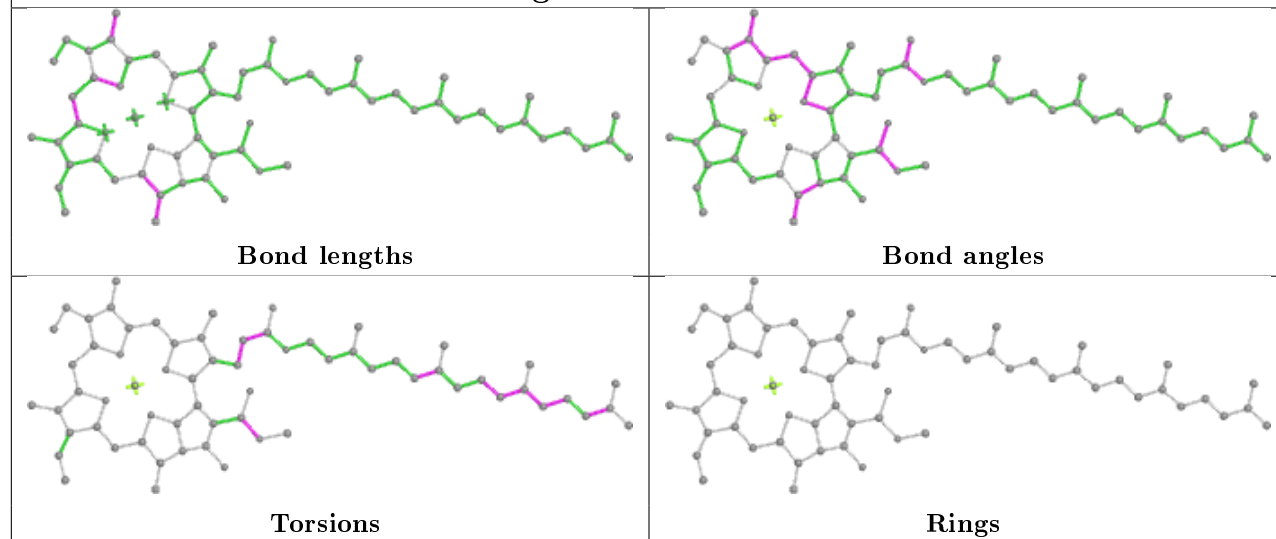
Ligand PL9 D 406



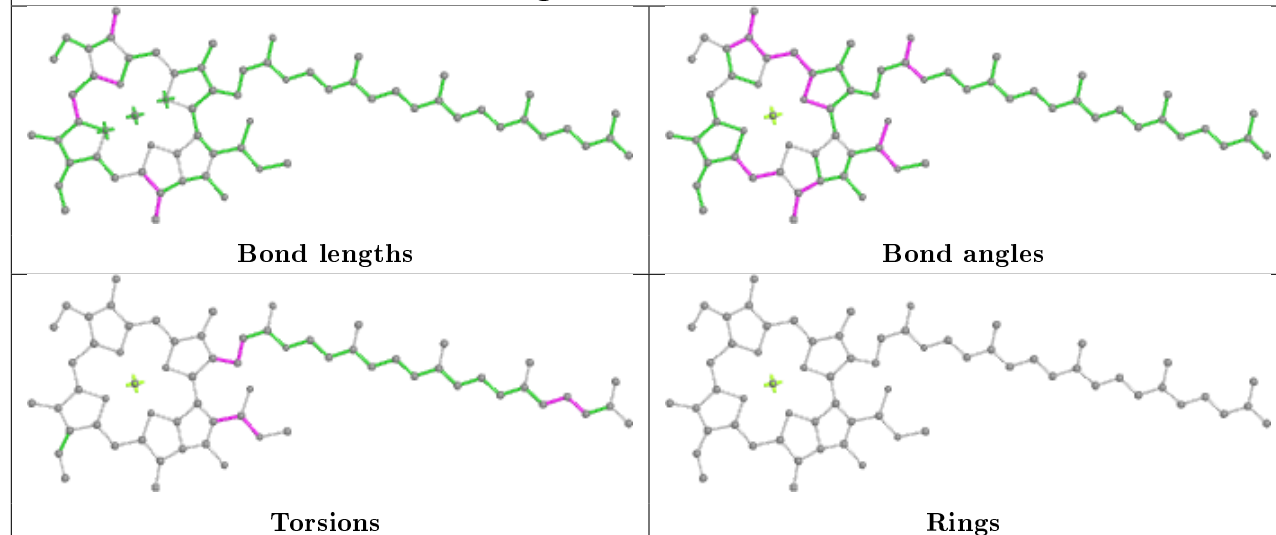
Ligand LHG C 519



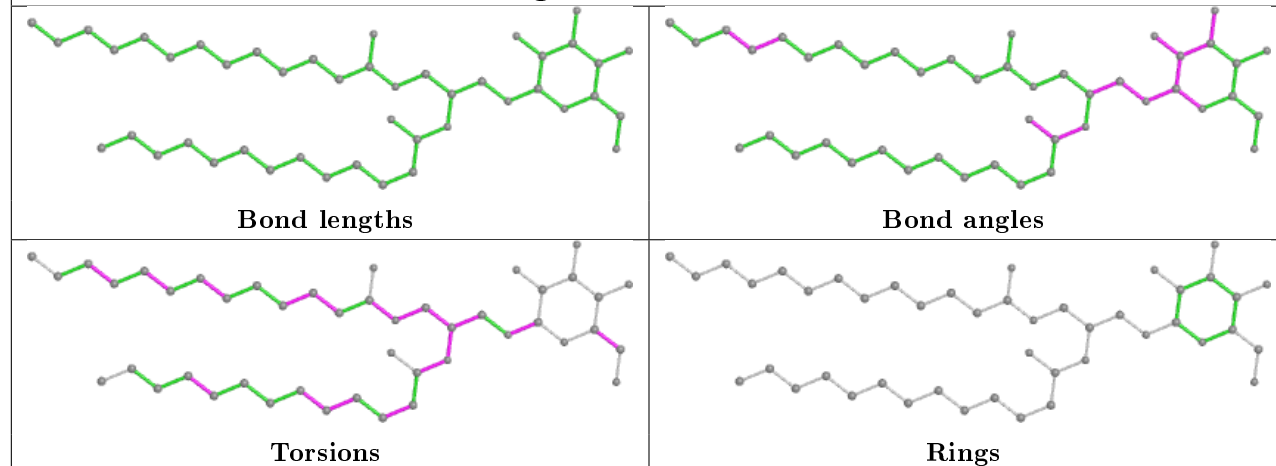
Ligand CLA B 601

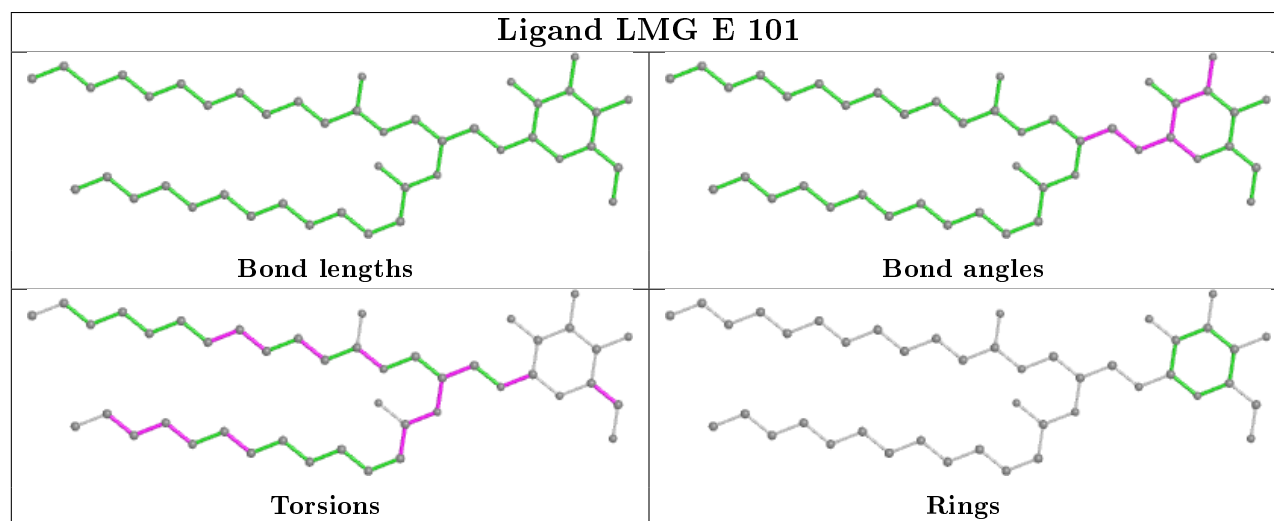
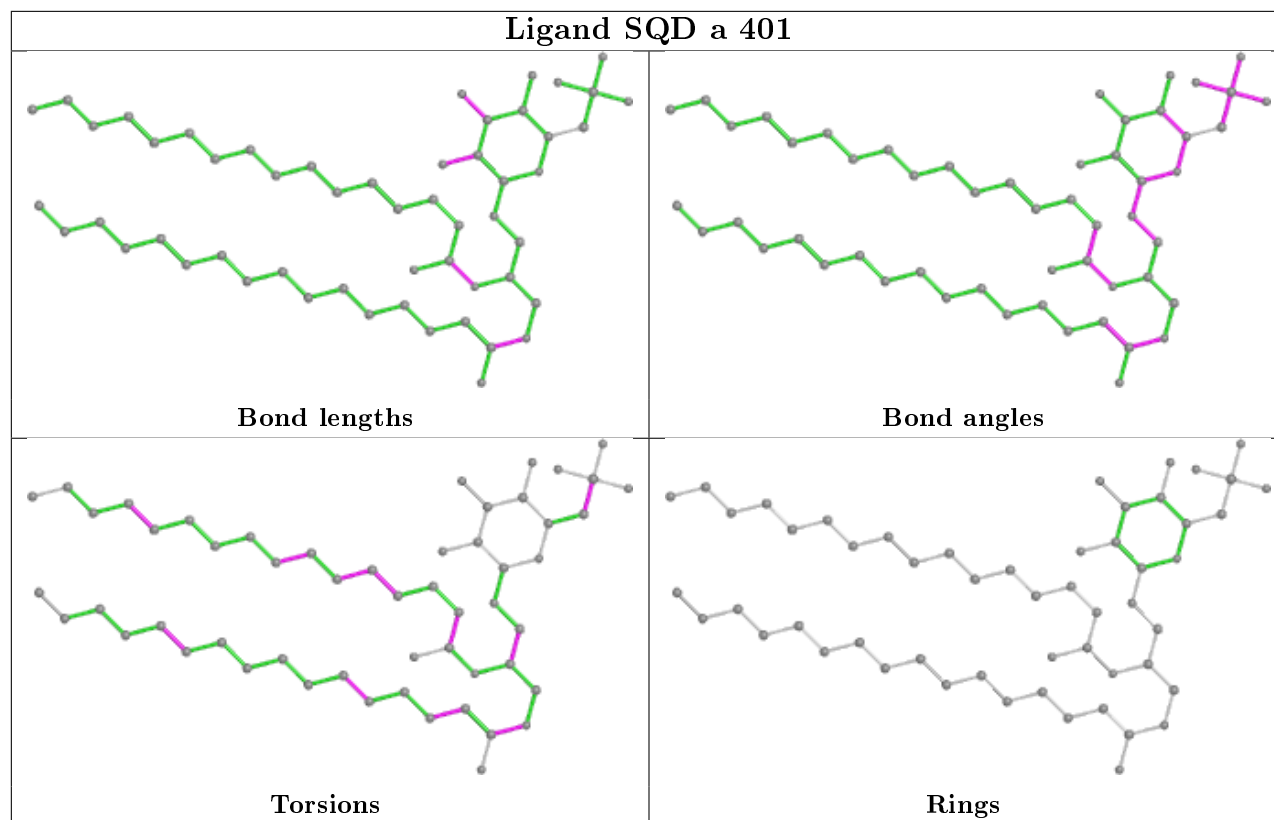


Ligand CLA b 610

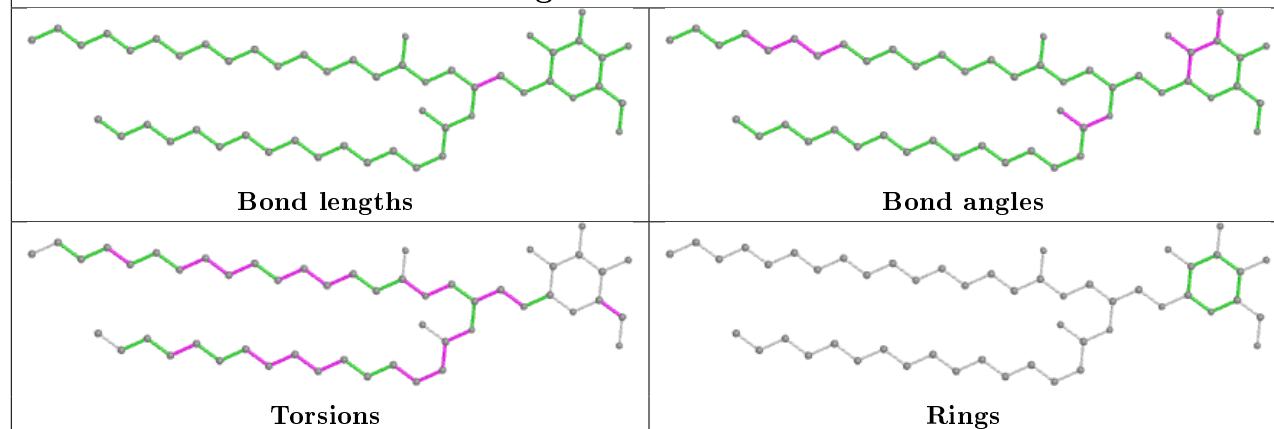


Ligand LMG c 518

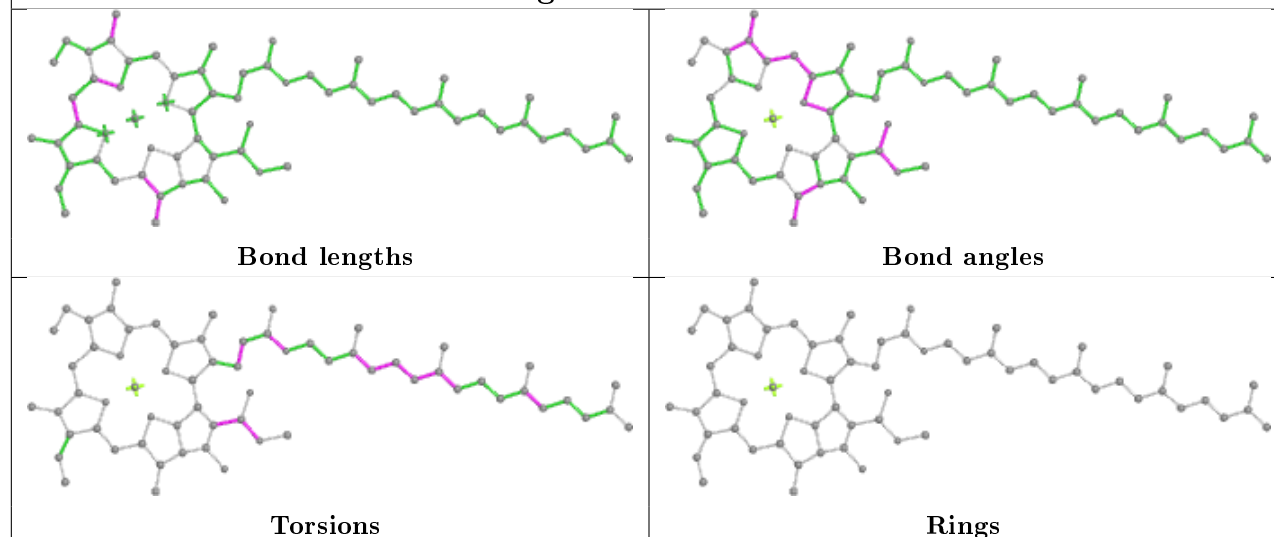




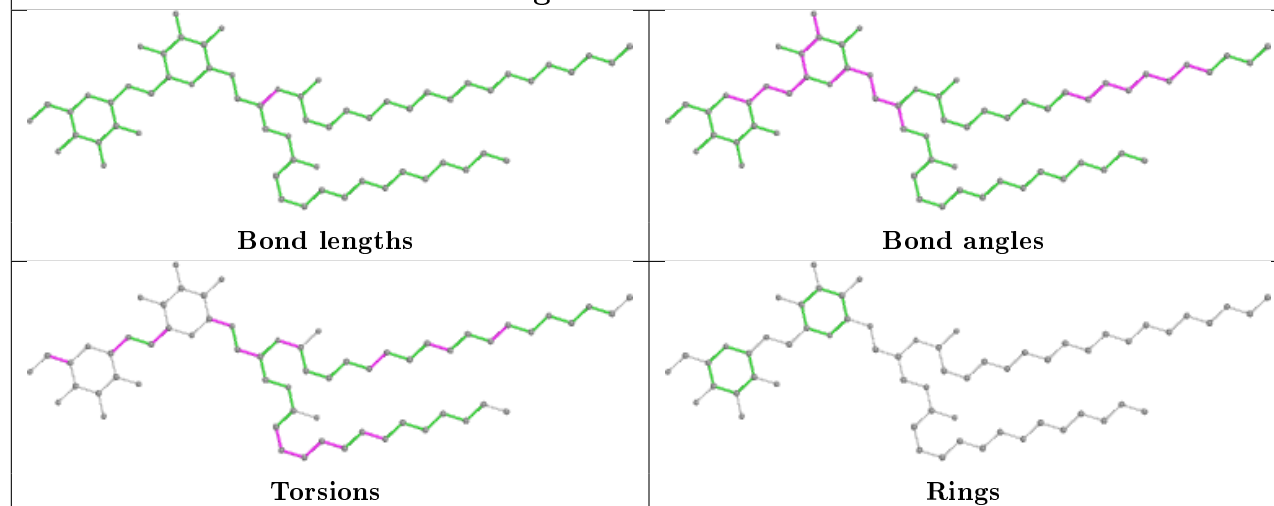
Ligand LMG l 101



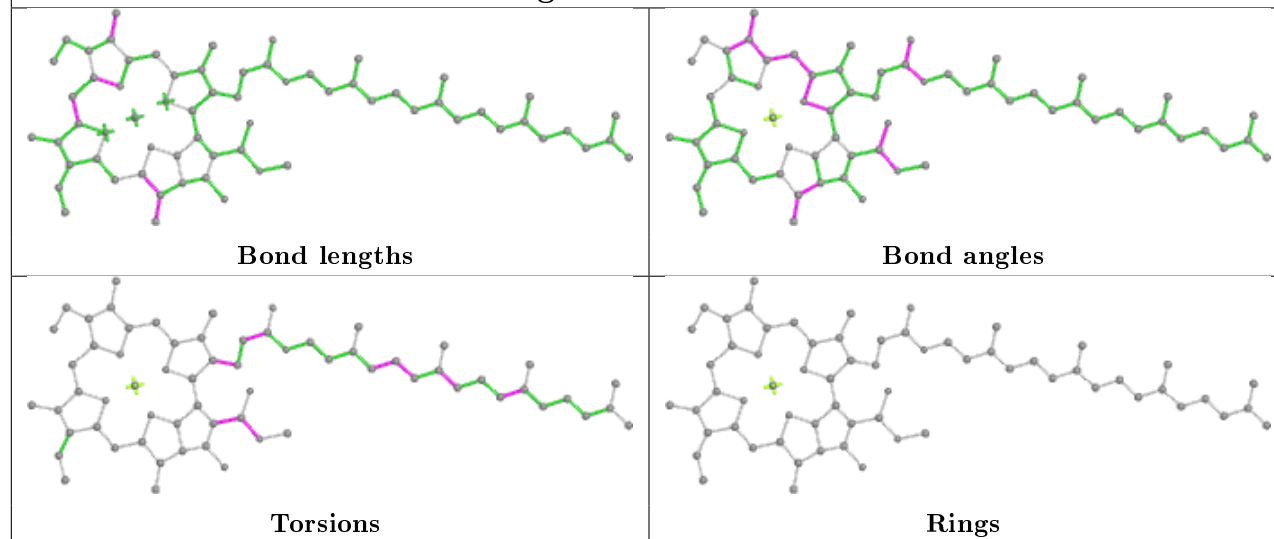
Ligand CLA c 510



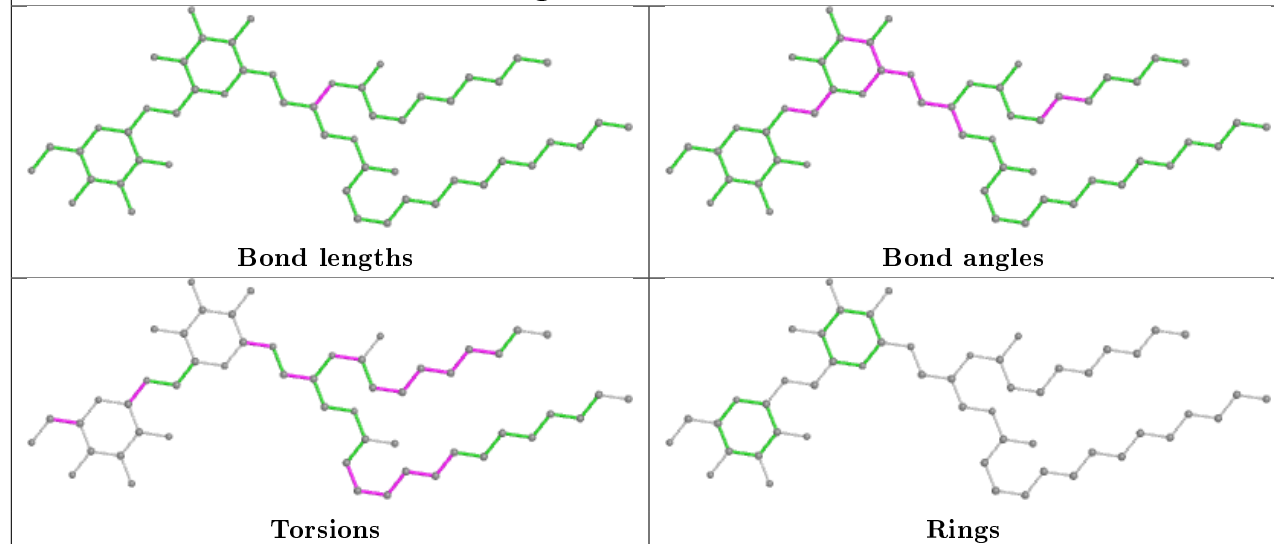
Ligand DGD c 516



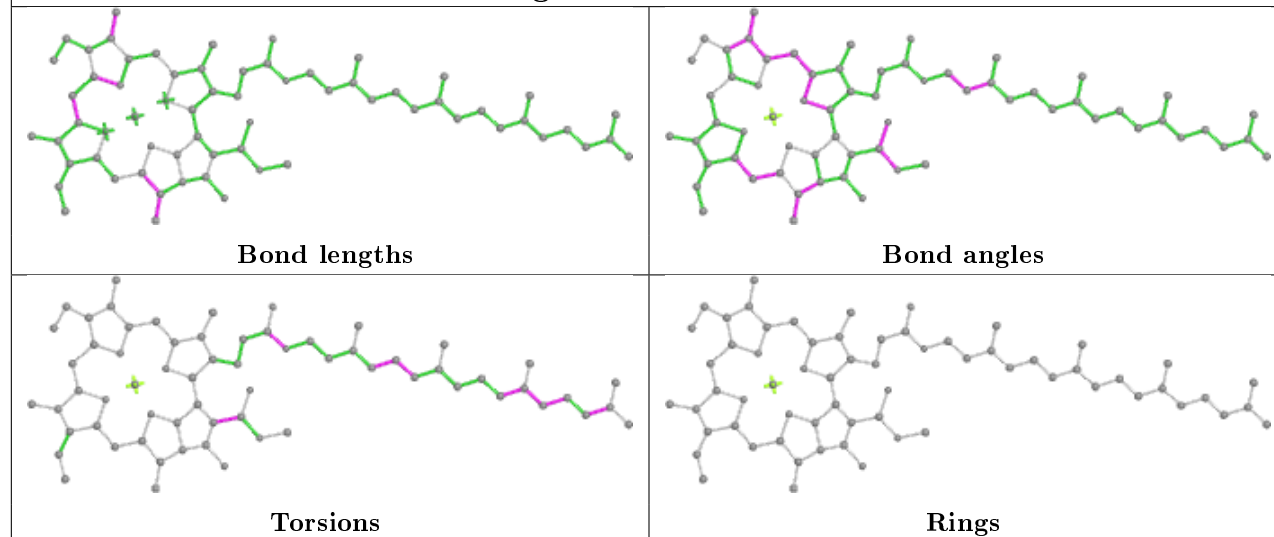
Ligand CLA c 506



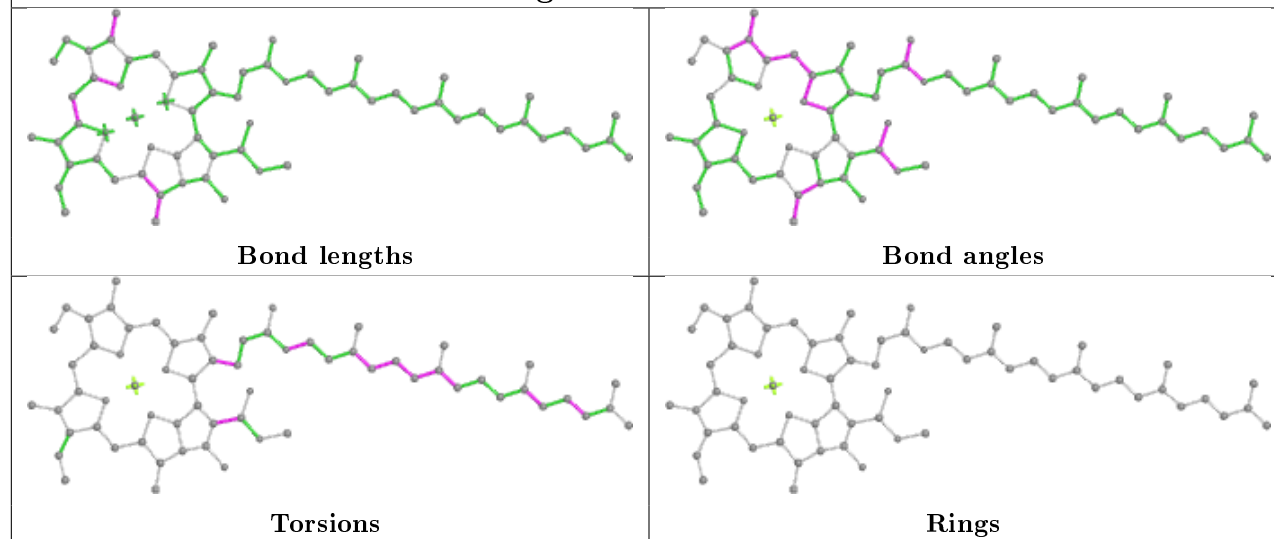
Ligand DGD c 515



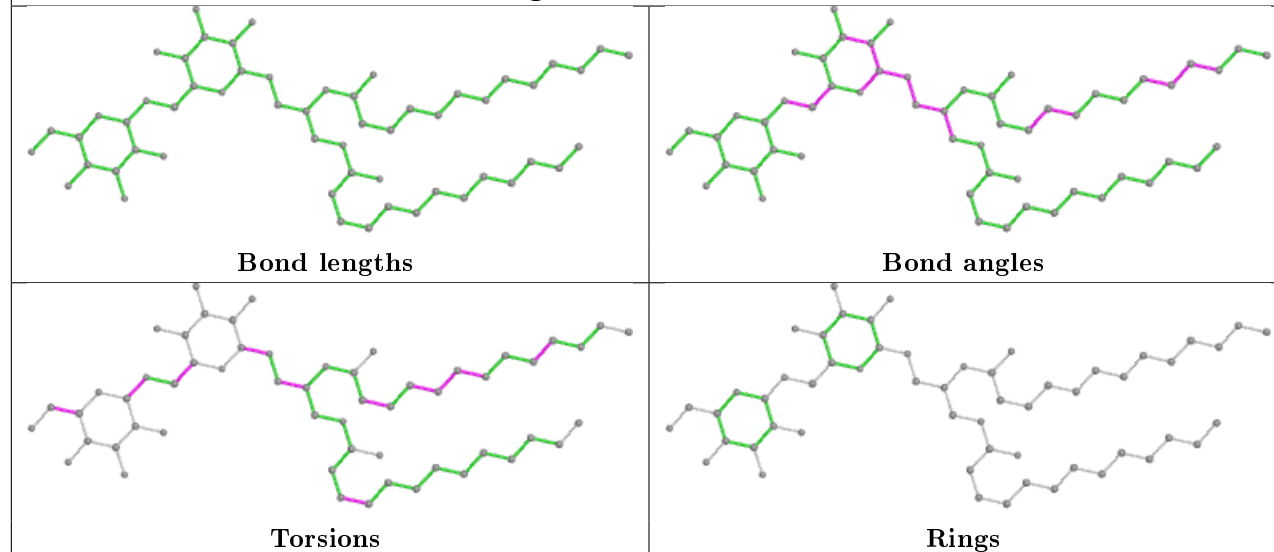
Ligand CLA C 502



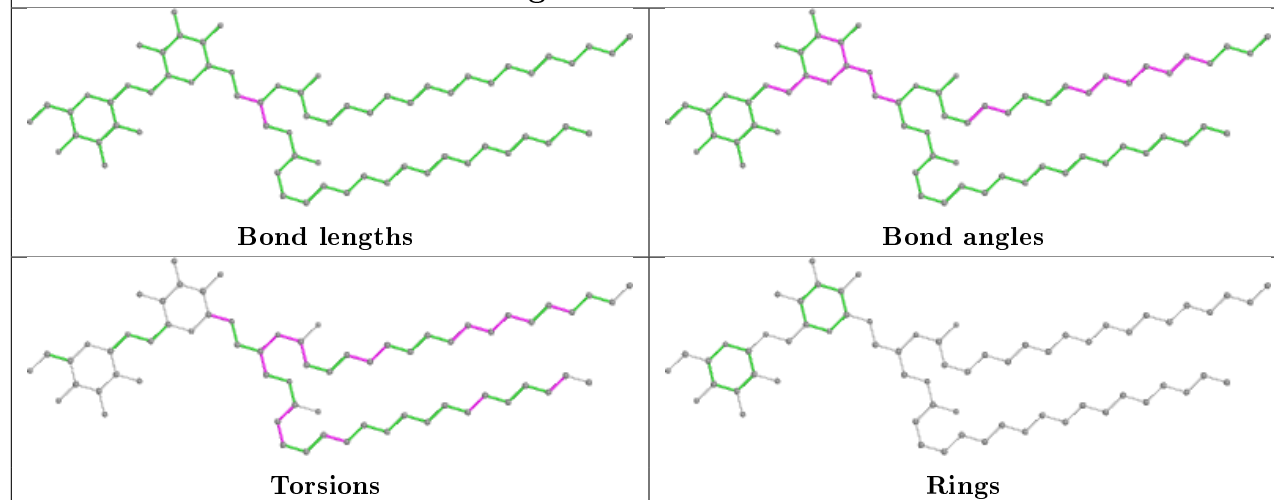
Ligand CLA a 405

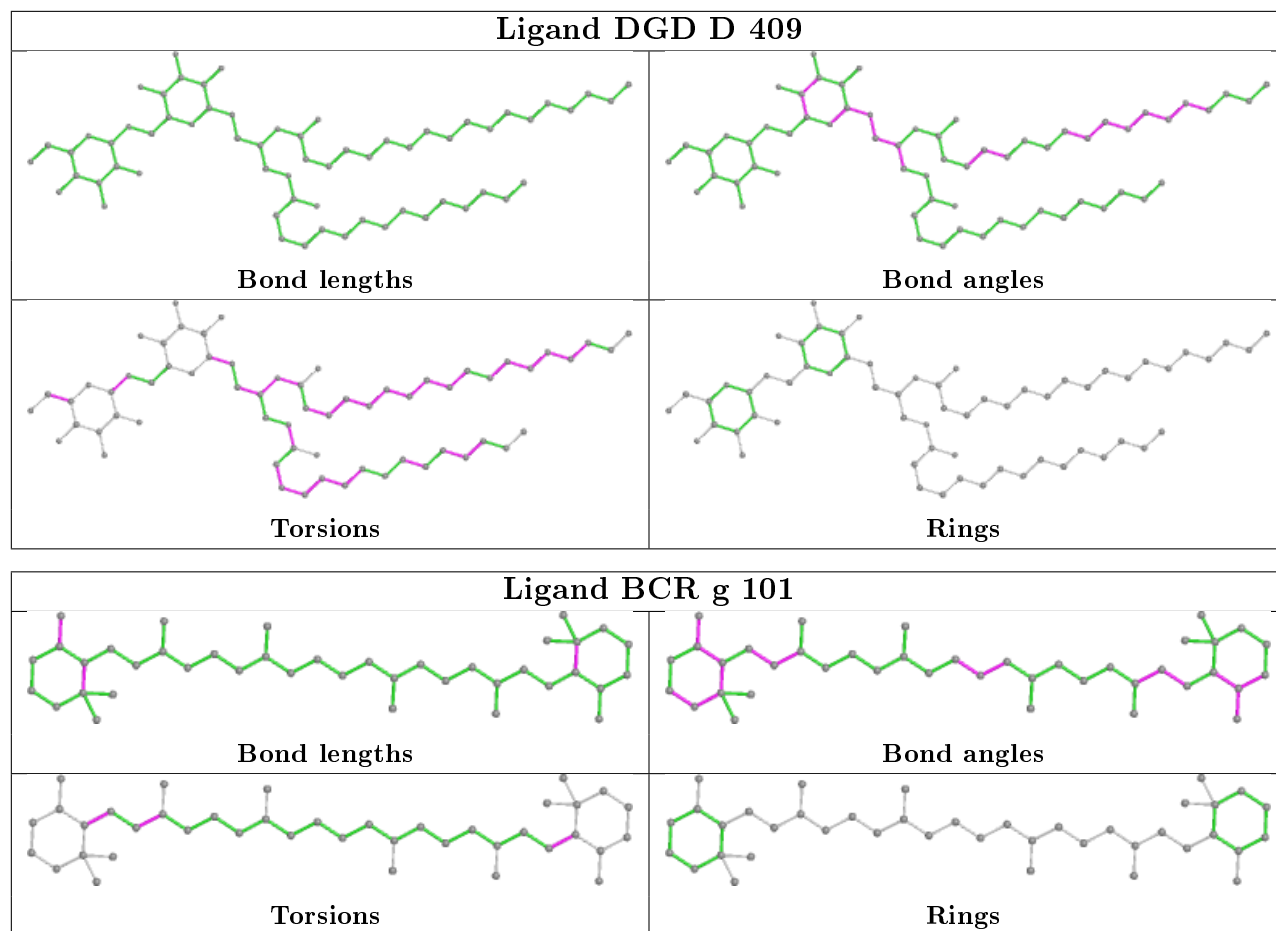


Ligand DGD A 408

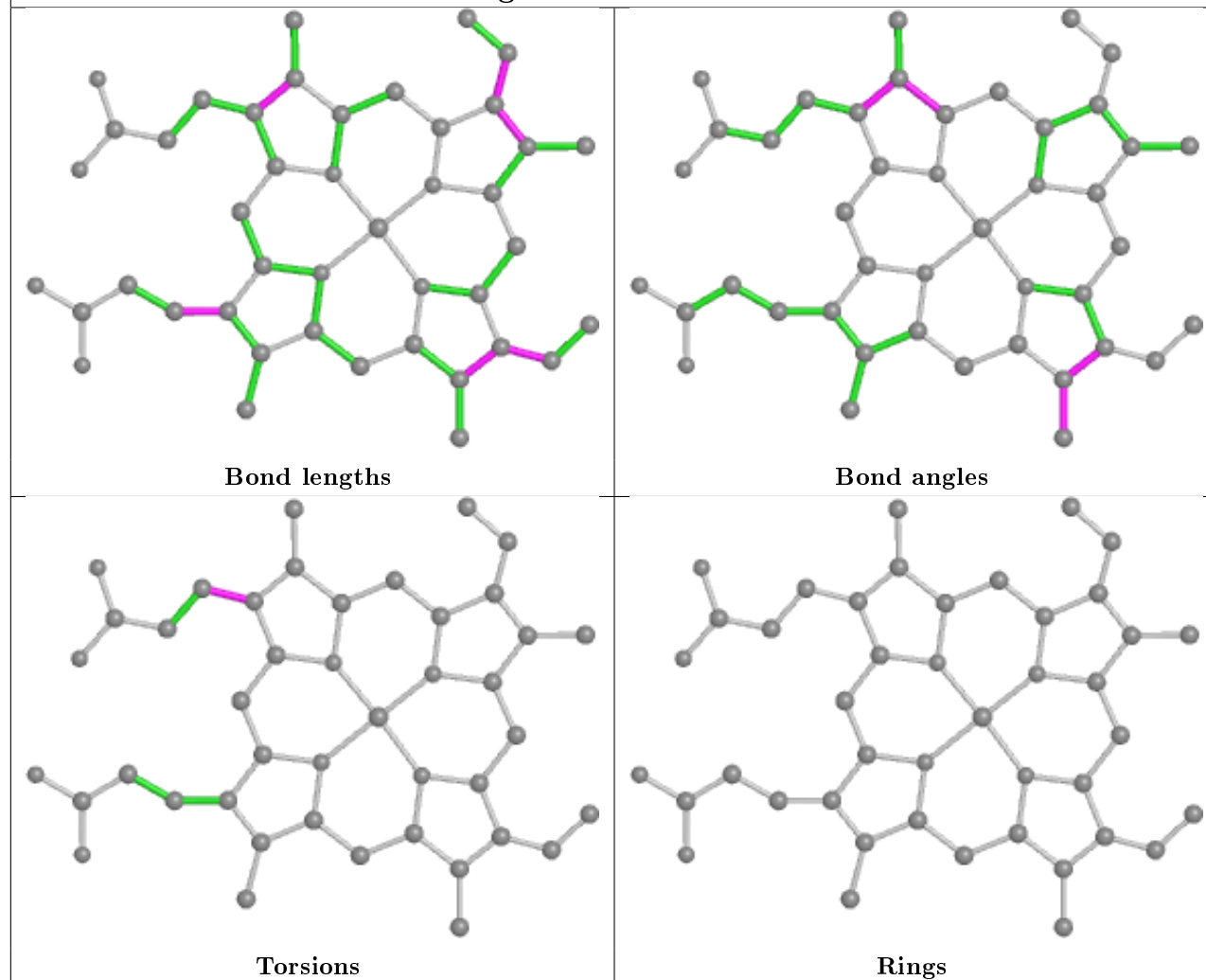


Ligand DGD C 517

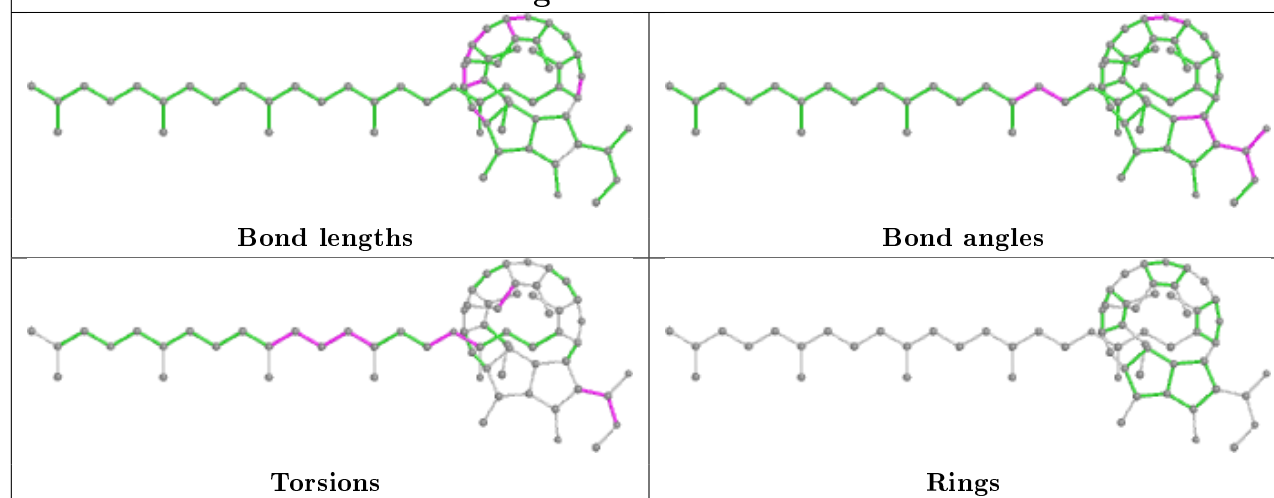


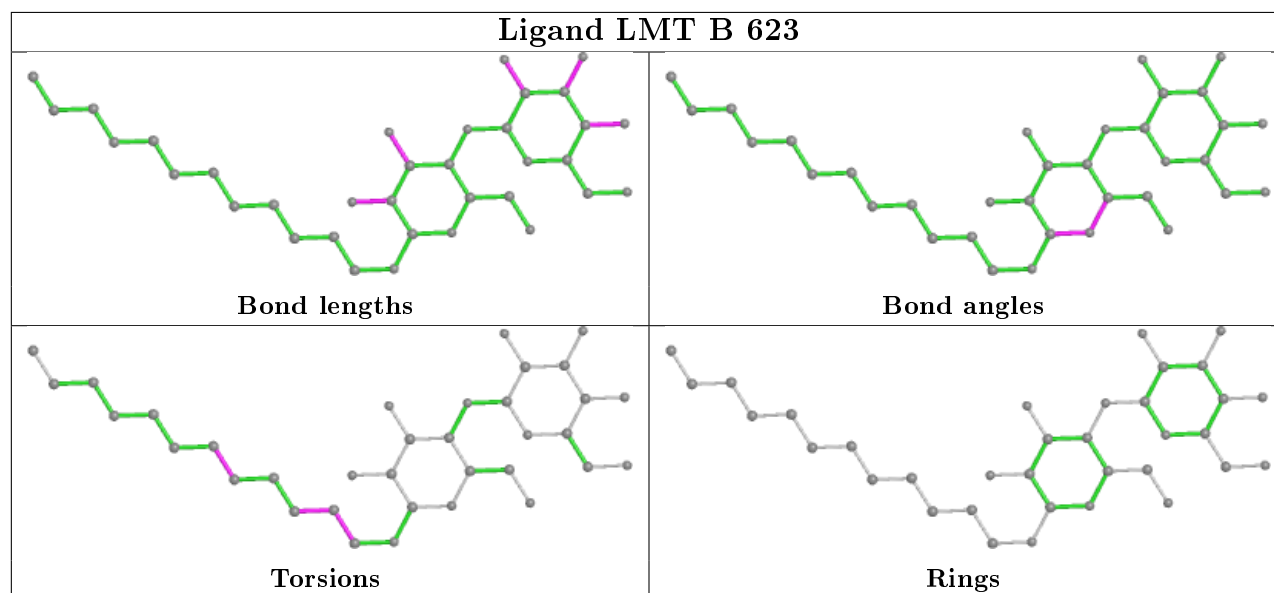
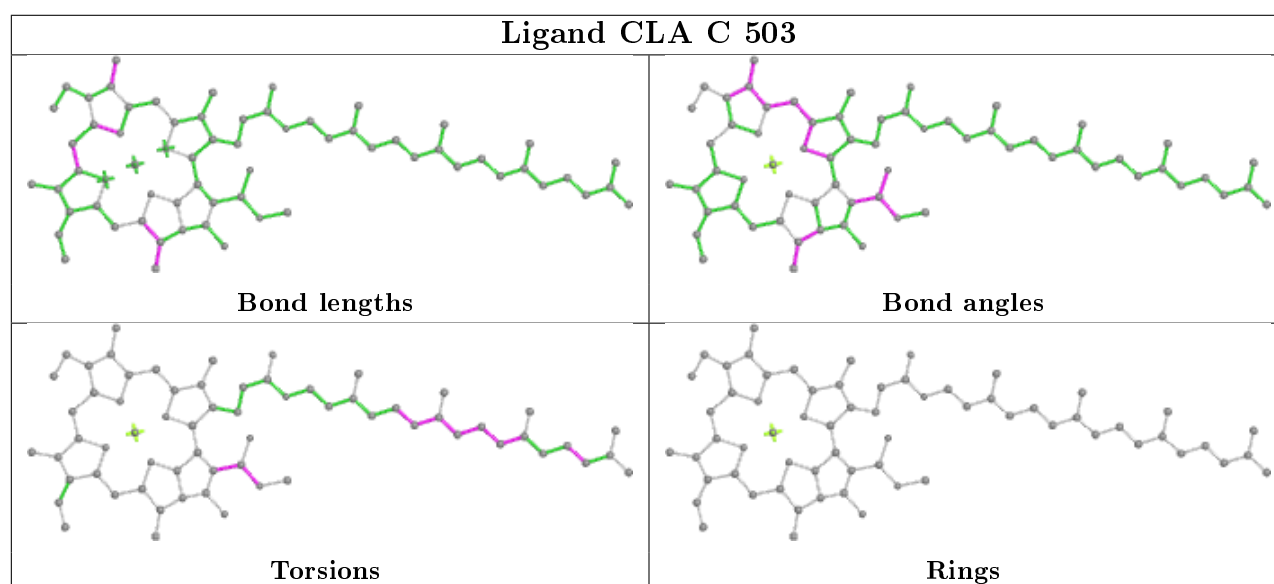
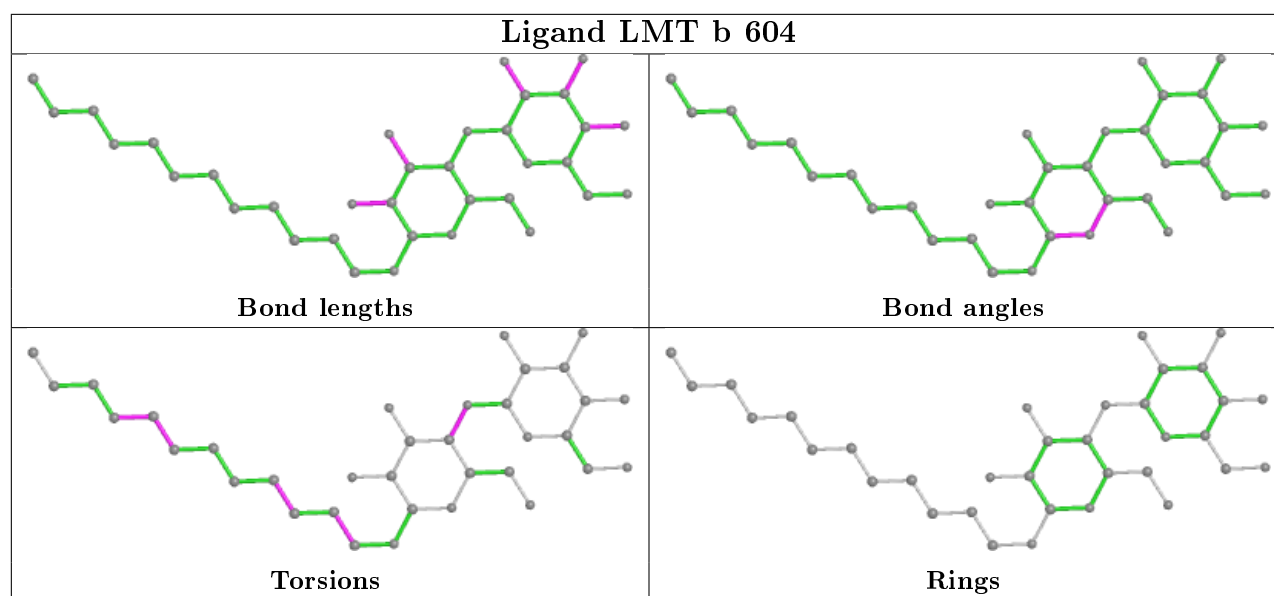


Ligand HEM V 201

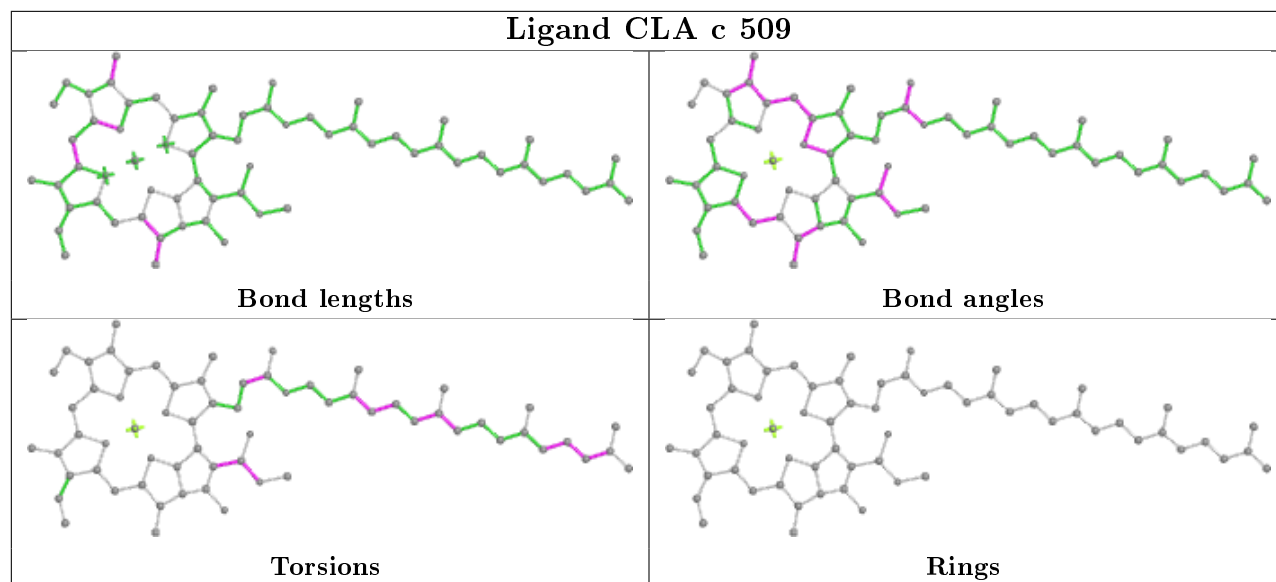


Ligand PHO d 401

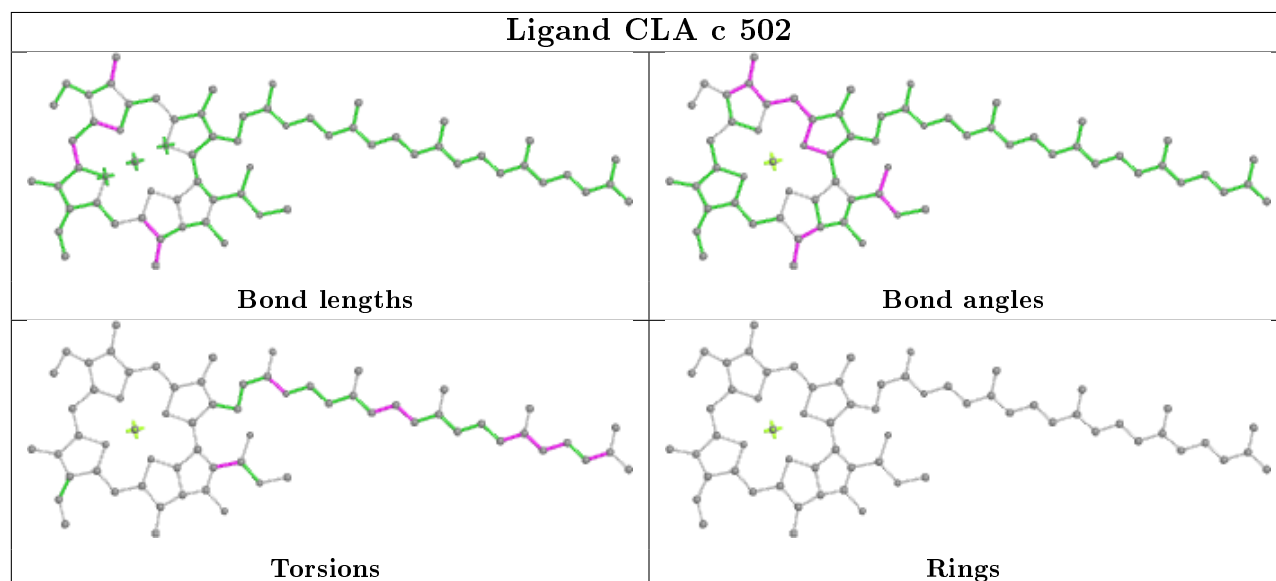




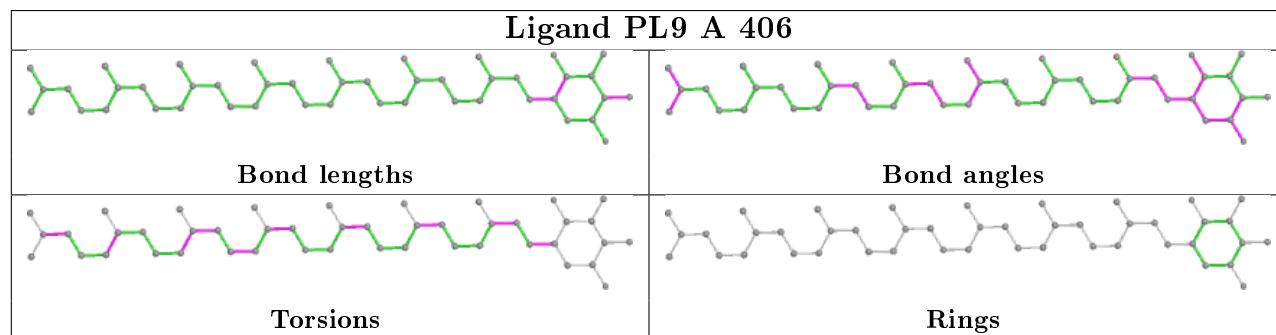
Ligand CLA c 509

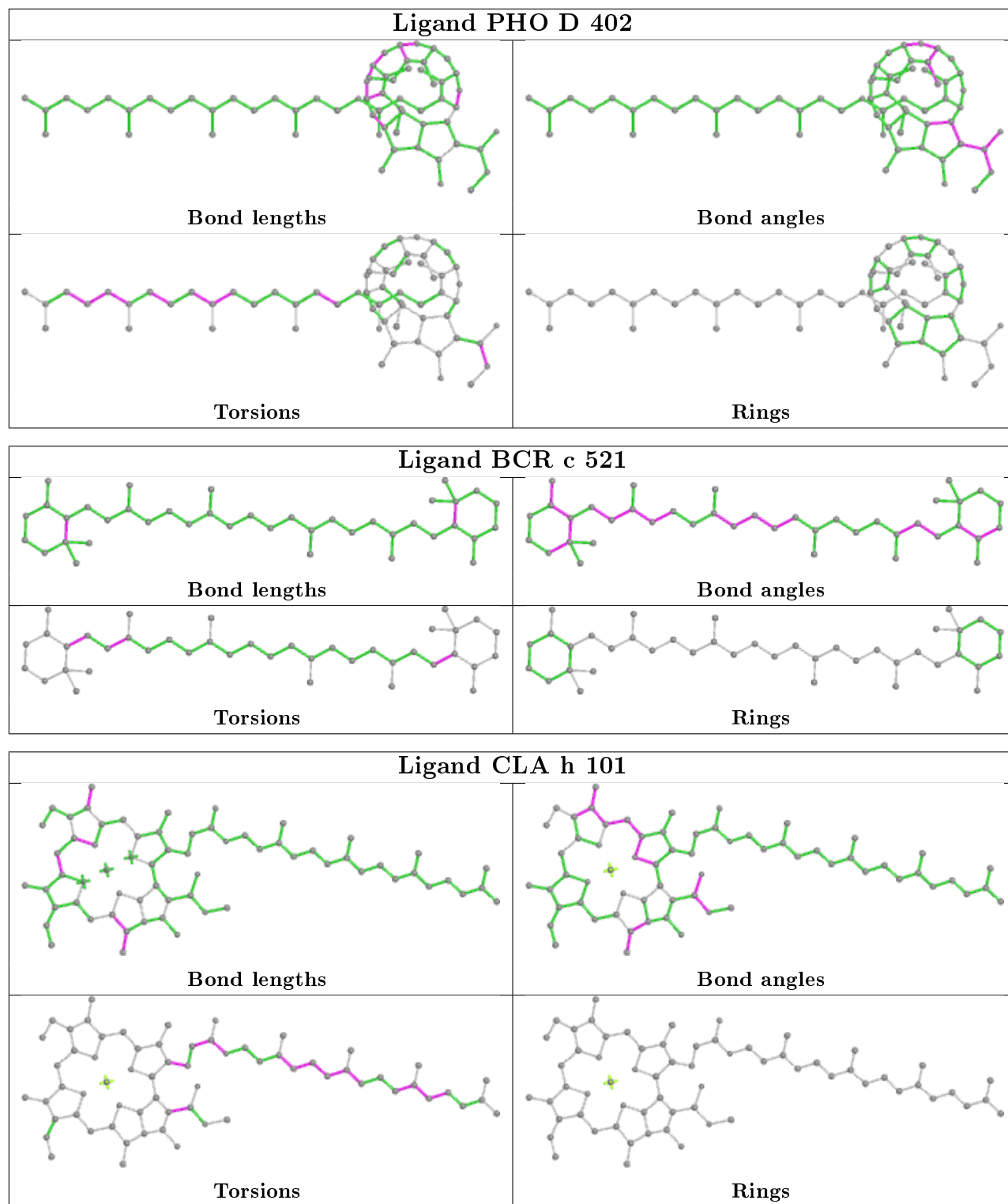


Ligand CLA c 502

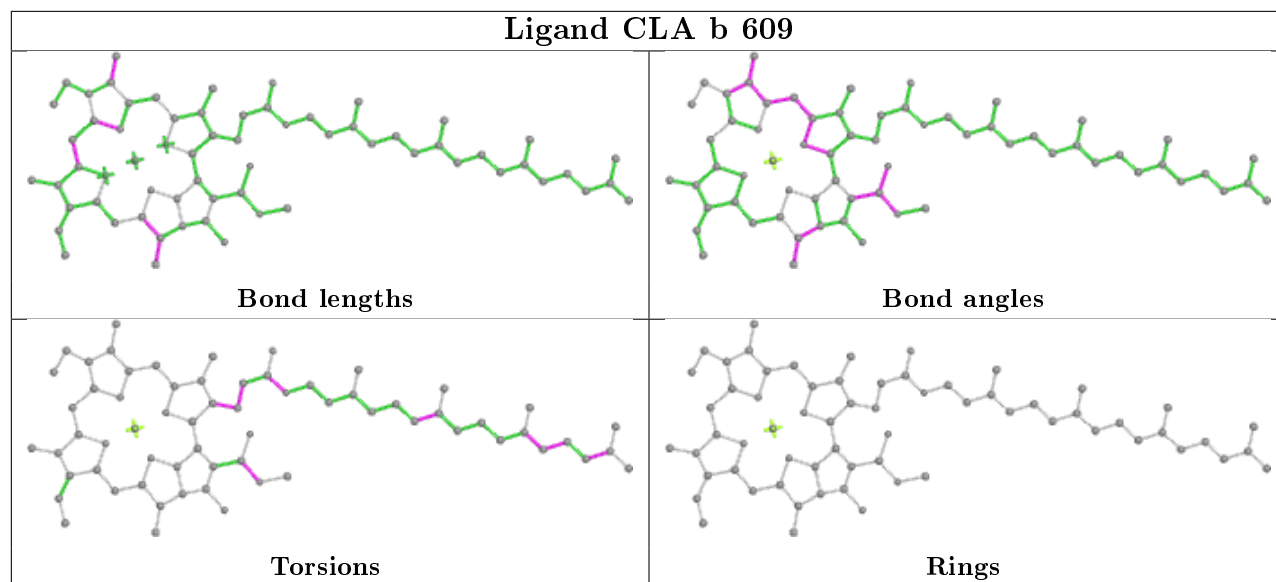


Ligand PL9 A 406

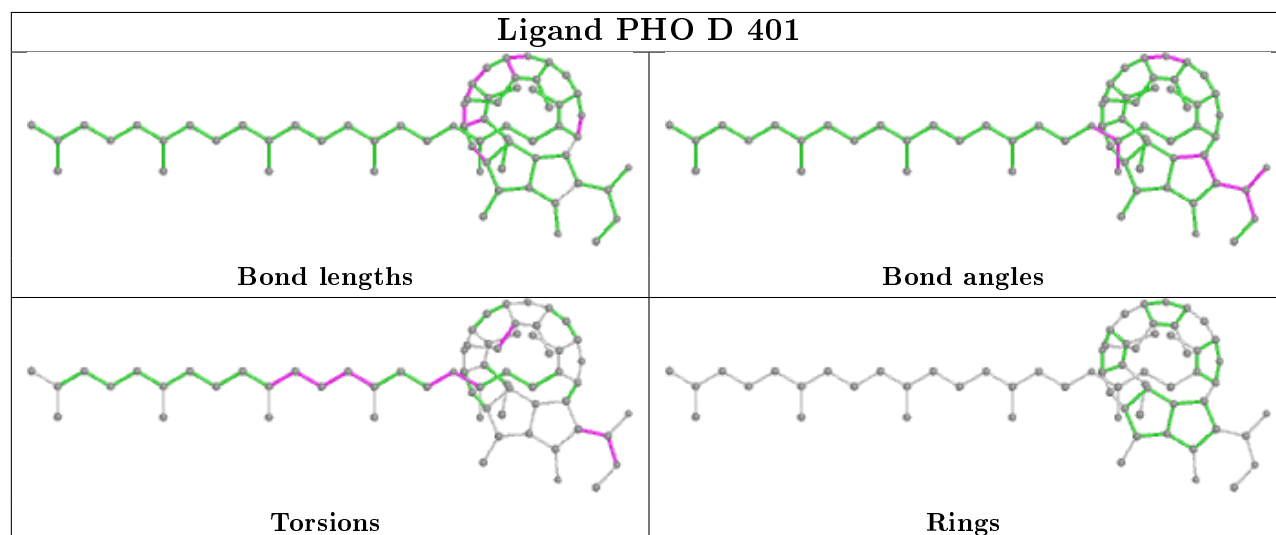




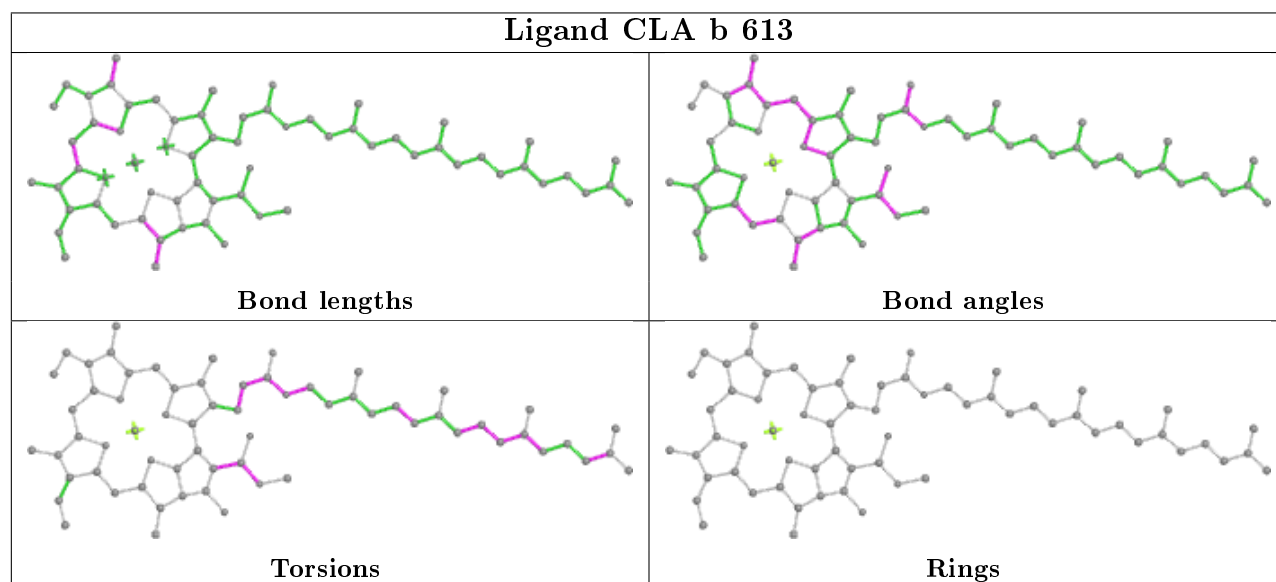
Ligand CLA b 609

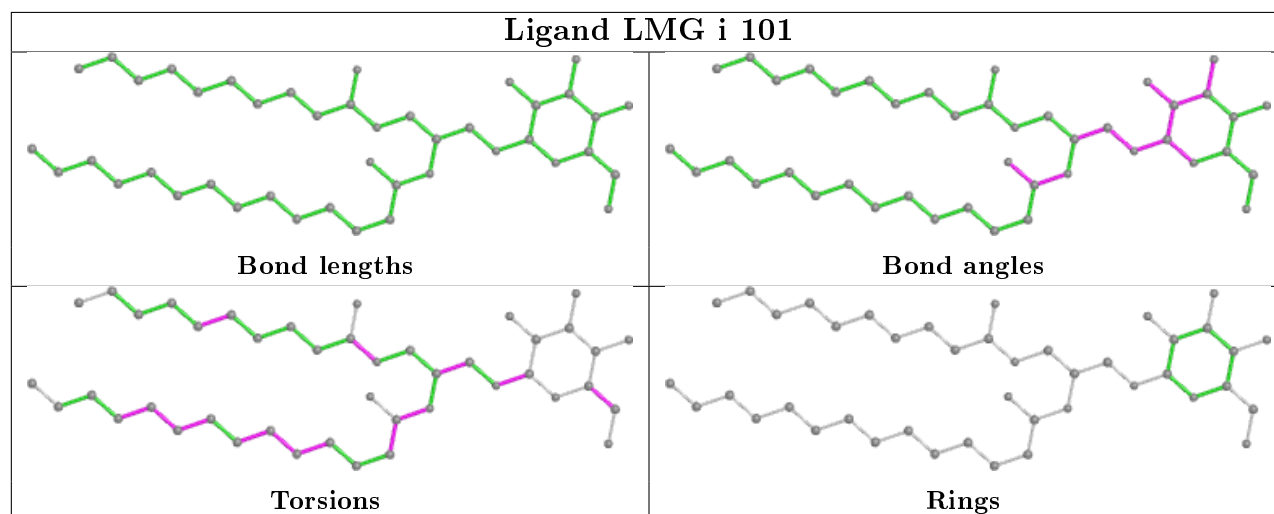
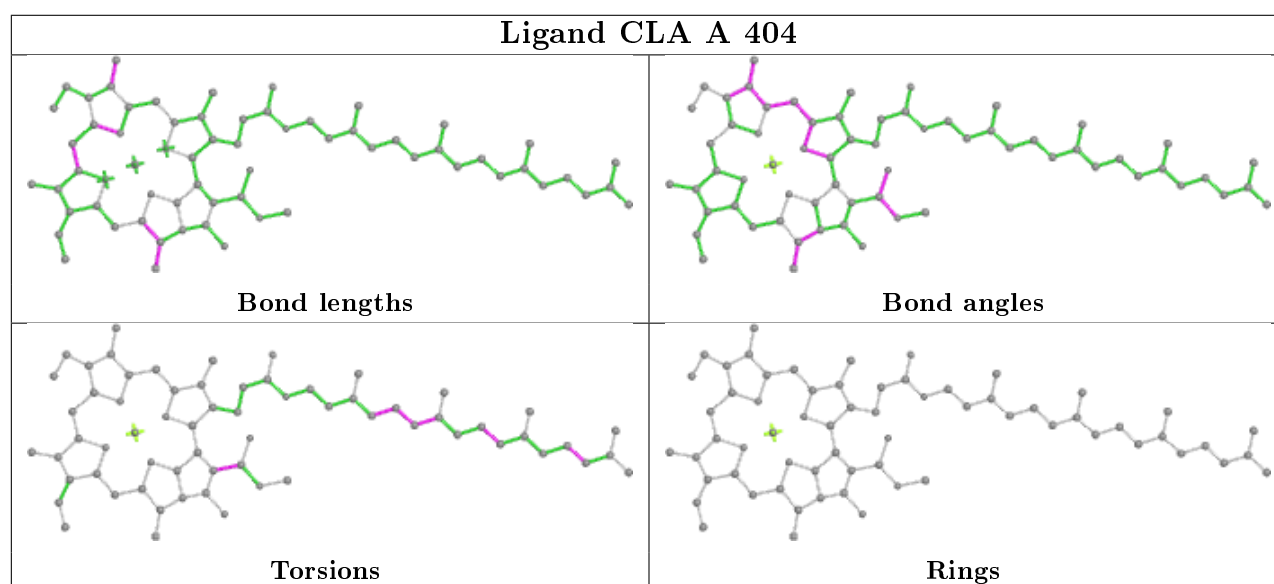
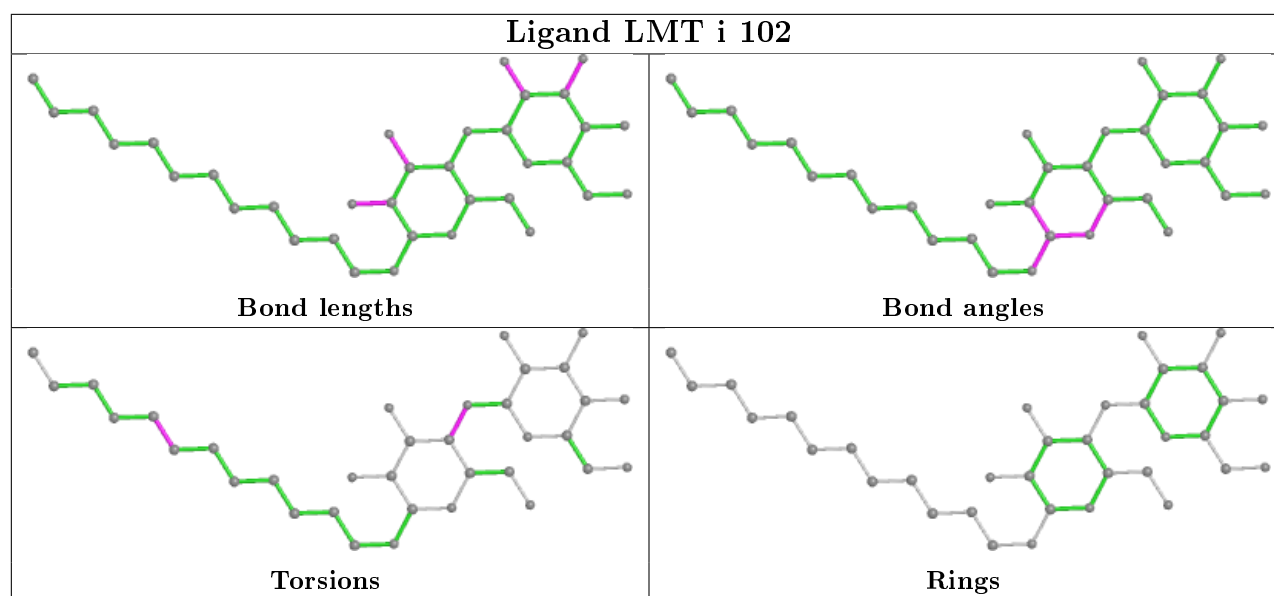


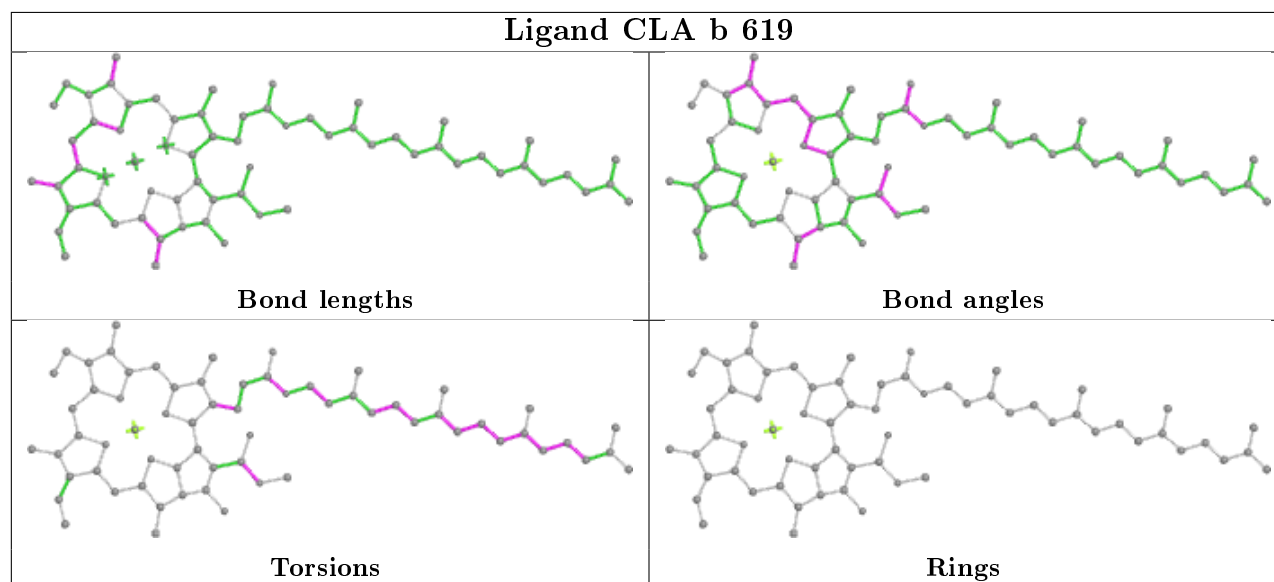
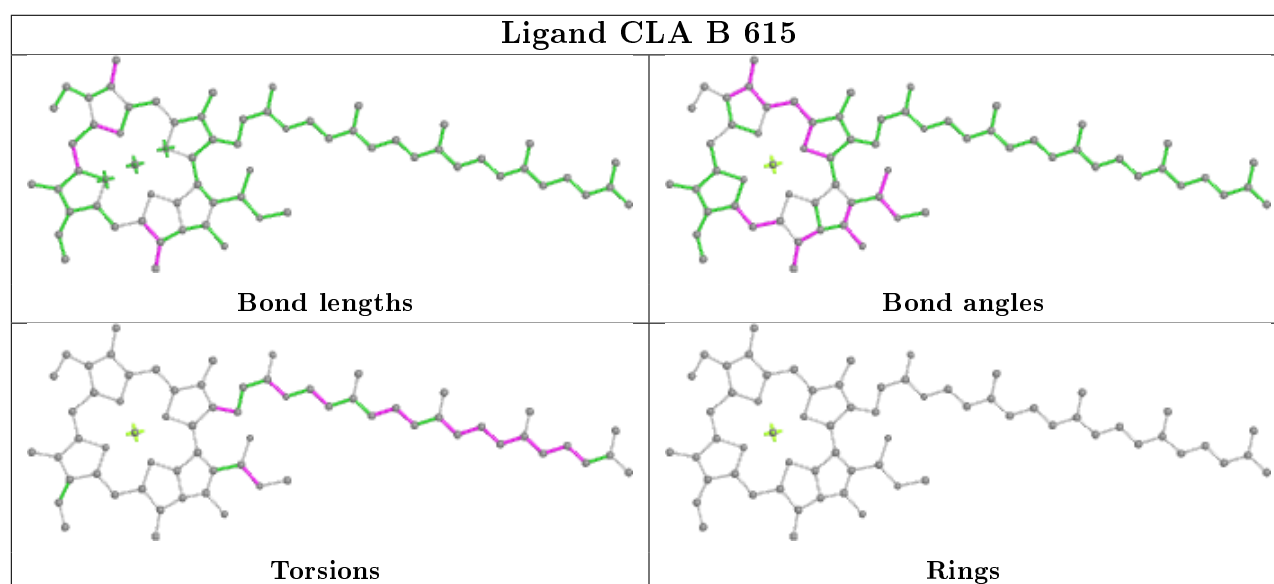
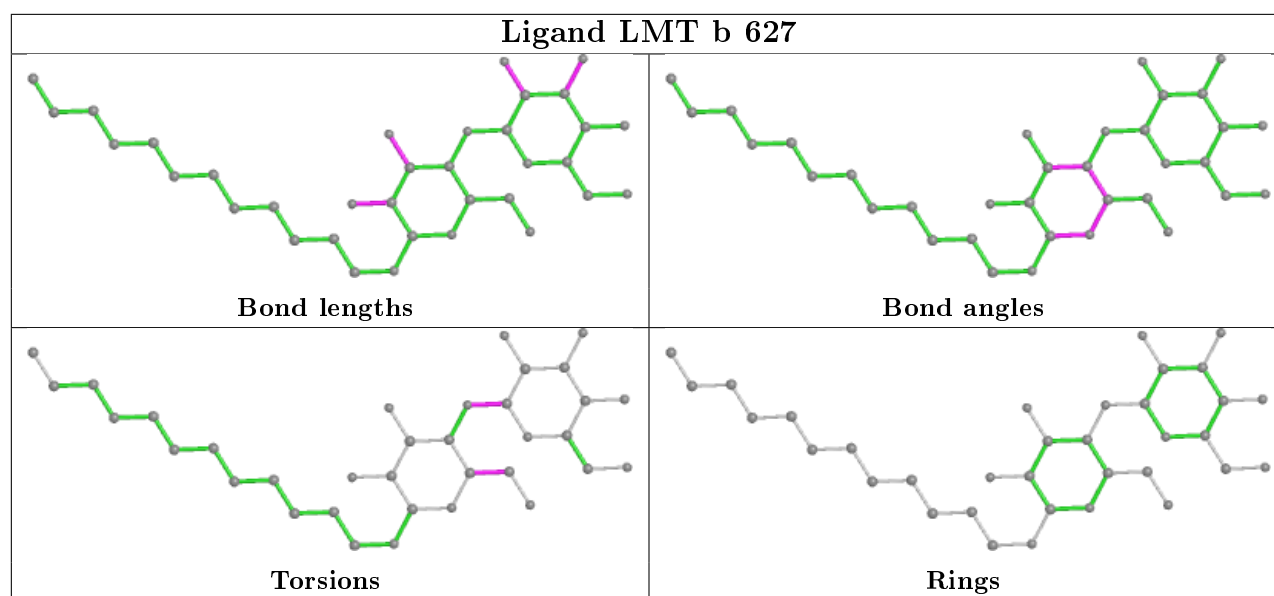
Ligand PHO D 401



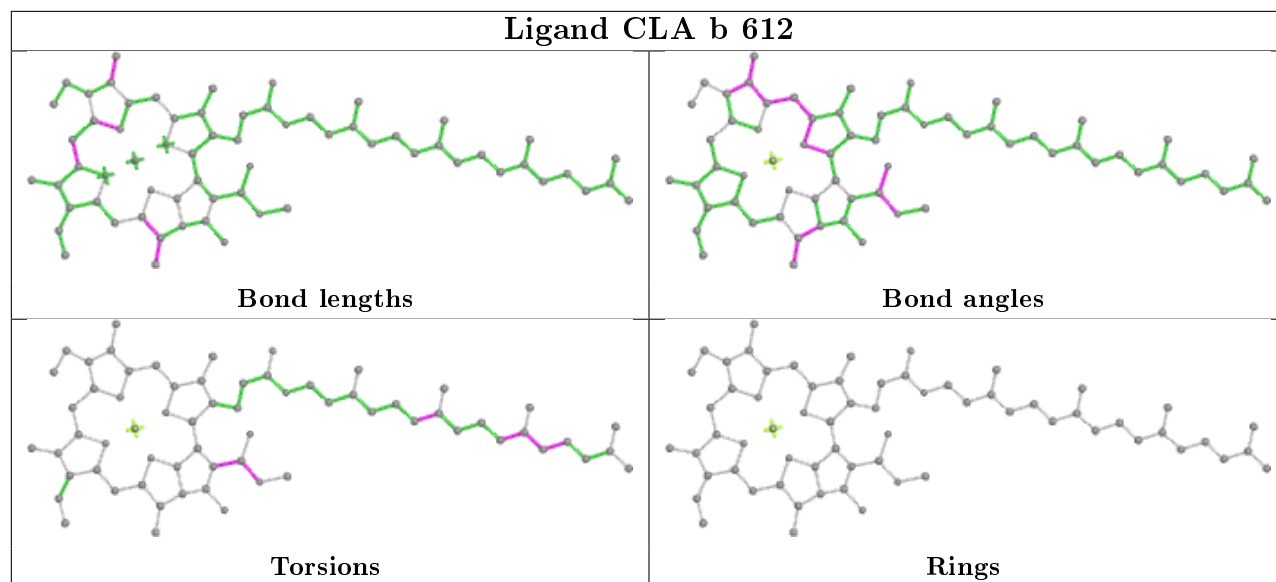
Ligand CLA b 613



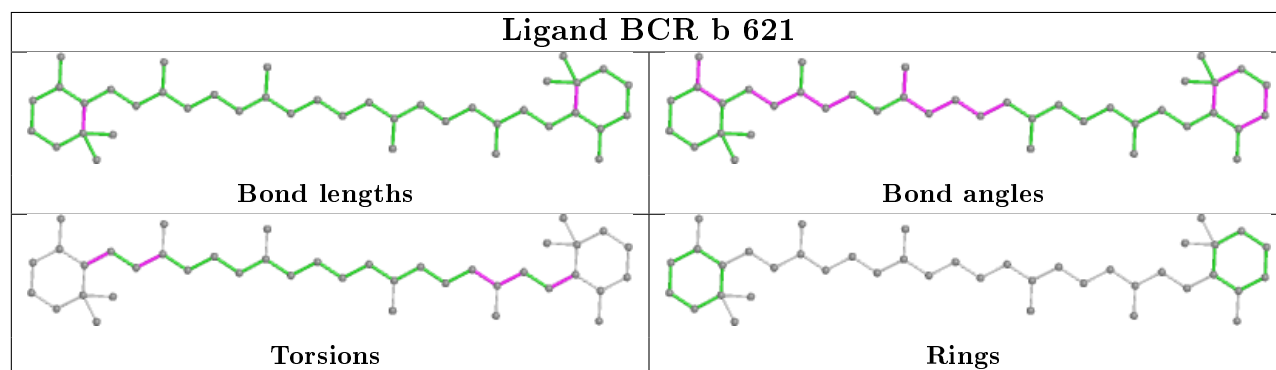




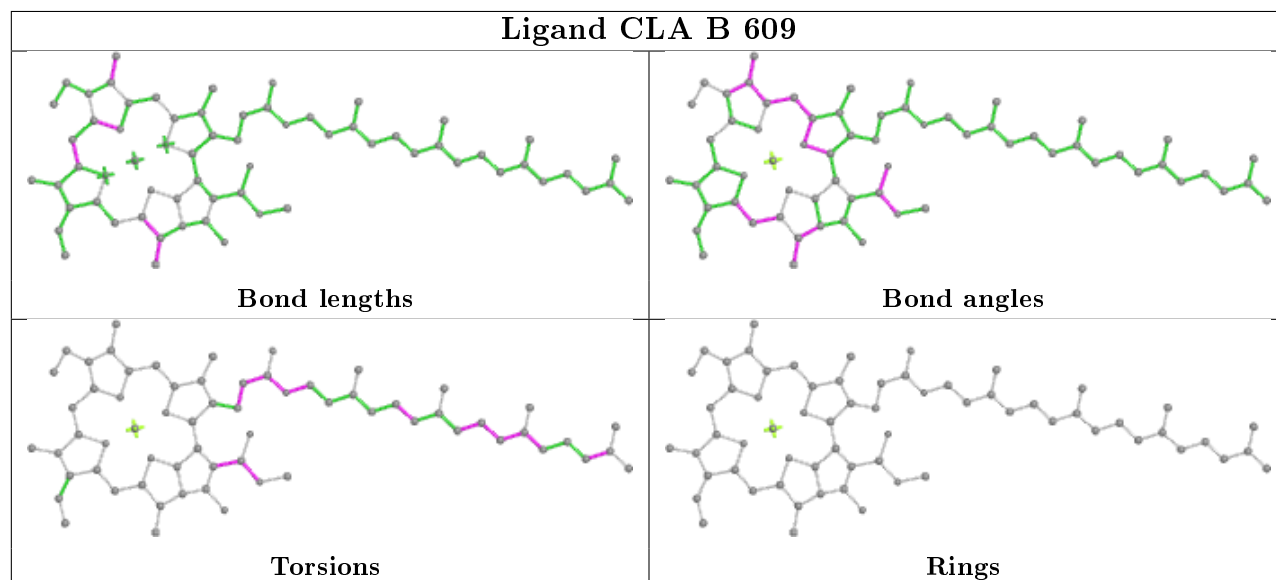
Ligand CLA b 612



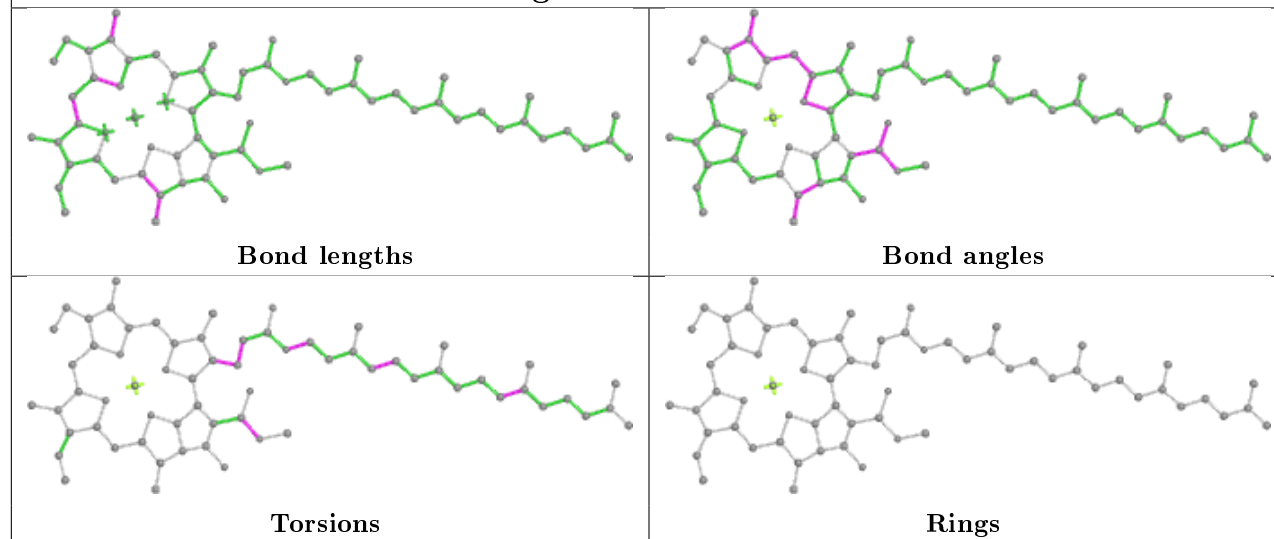
Ligand BCR b 621



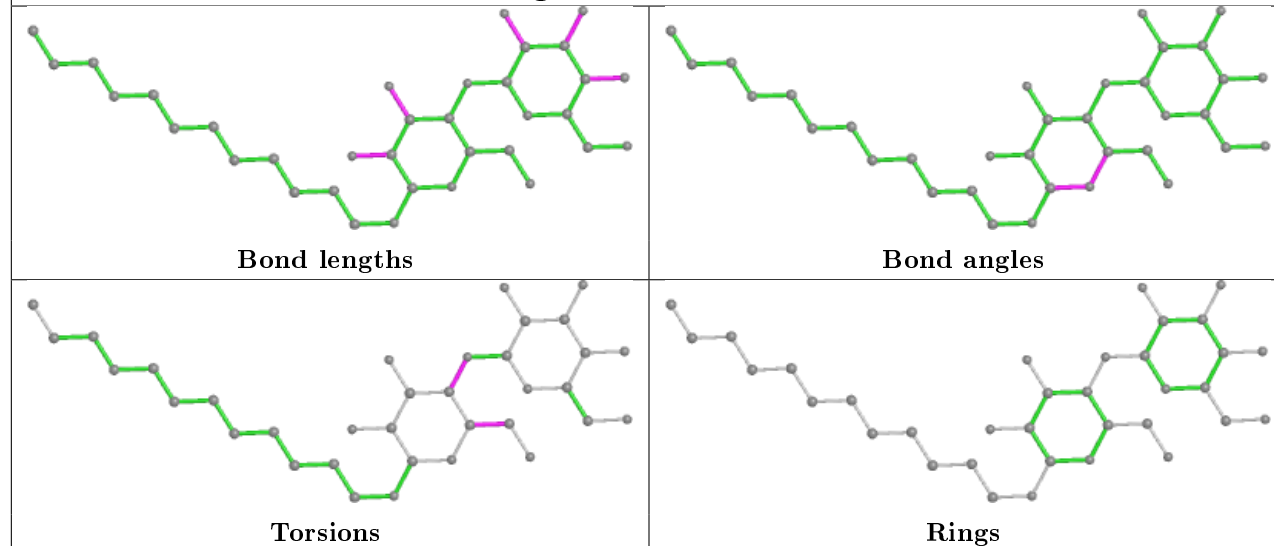
Ligand CLA B 609



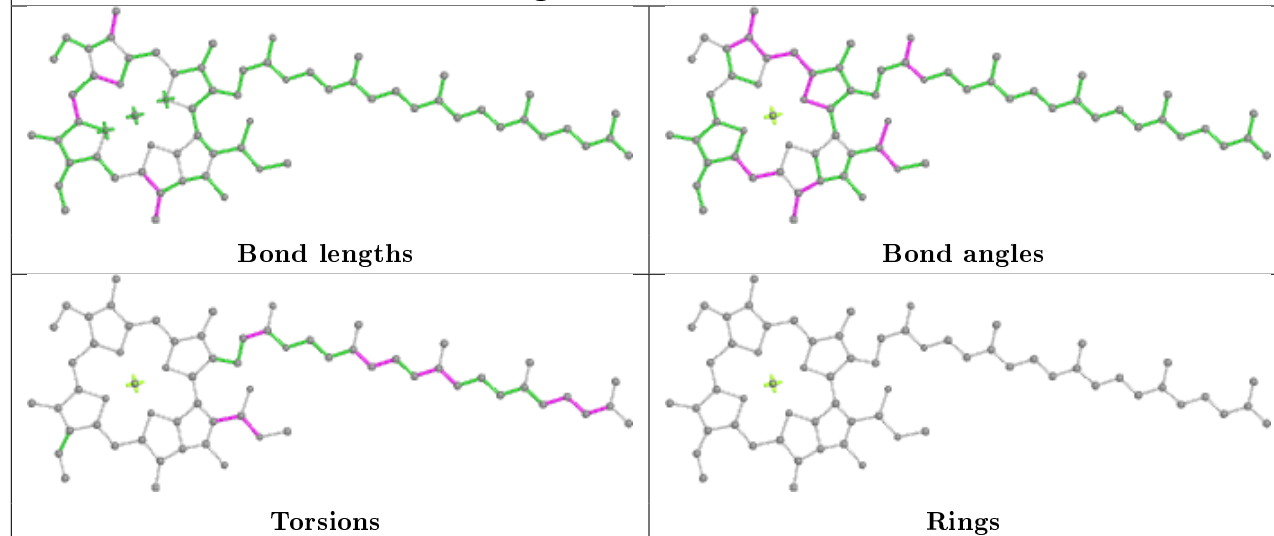
Ligand CLA A 402

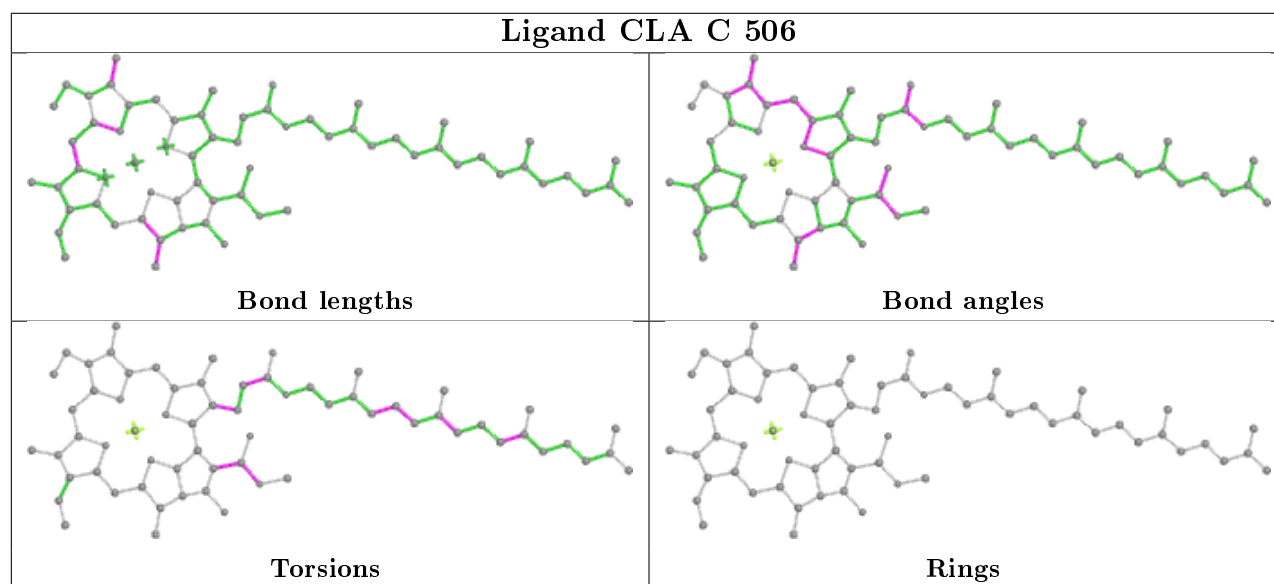
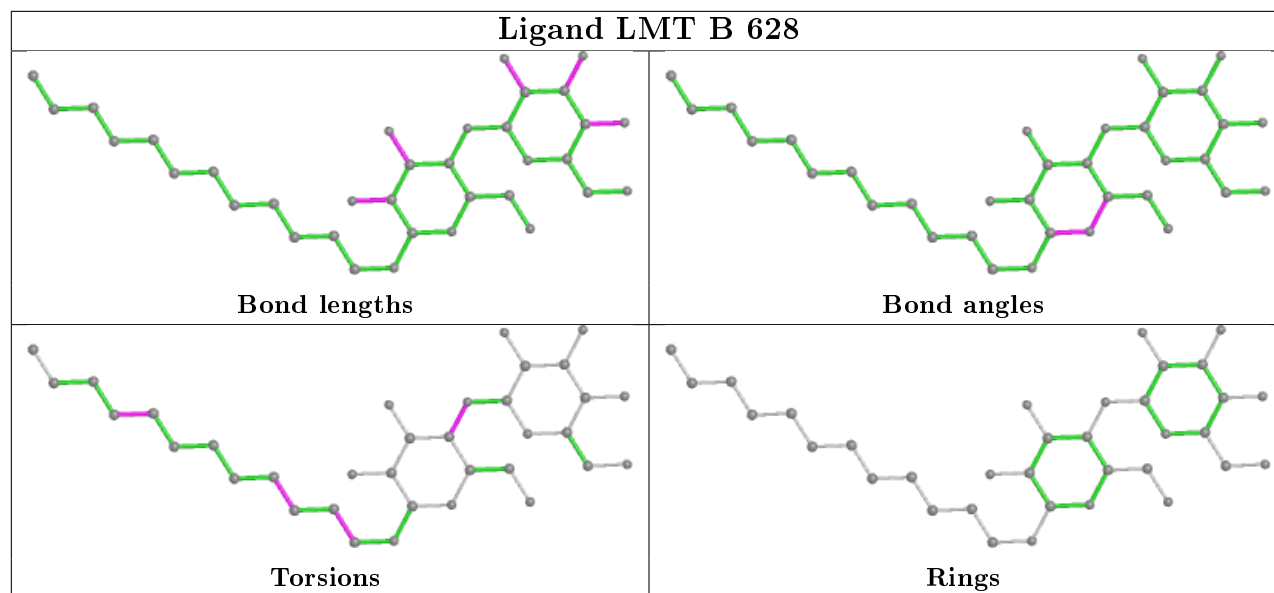


Ligand LMT b 603

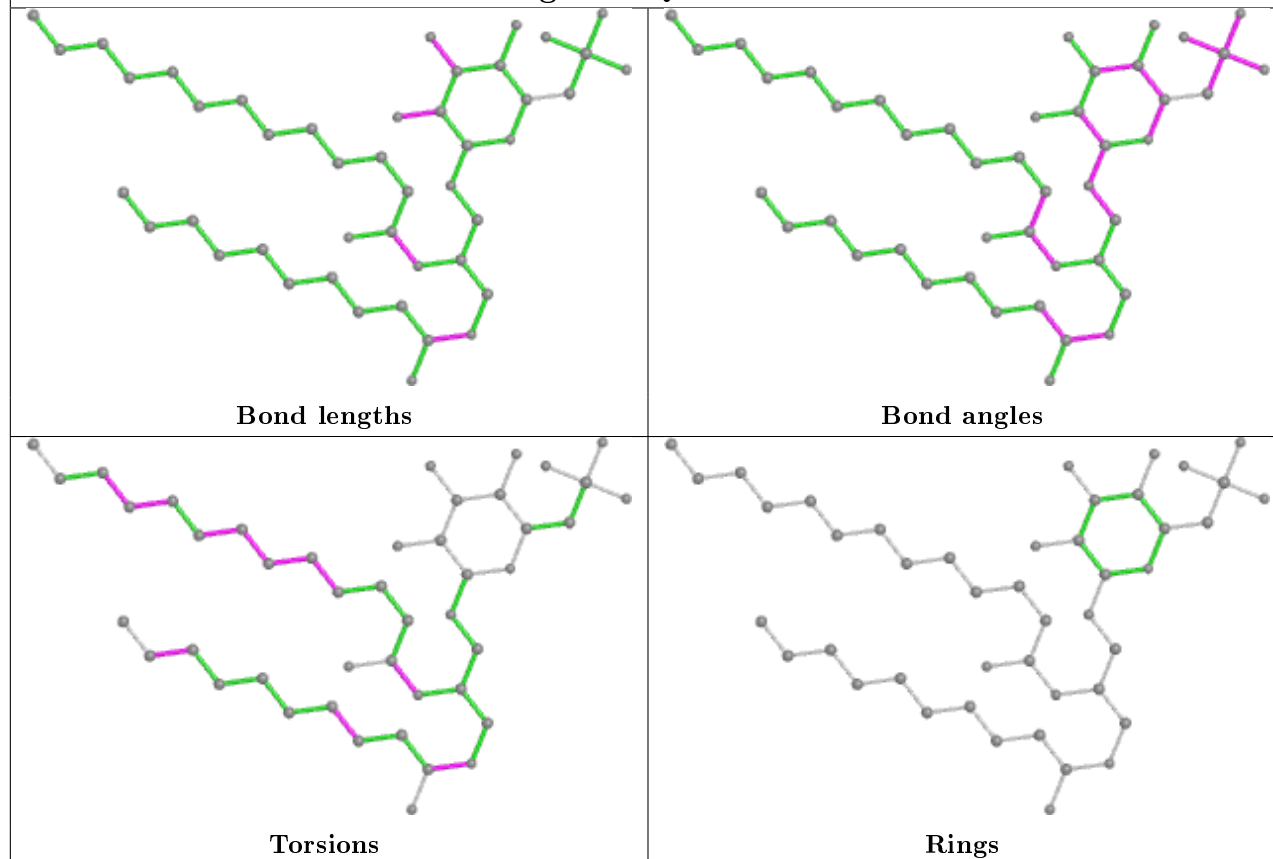


Ligand CLA C 509

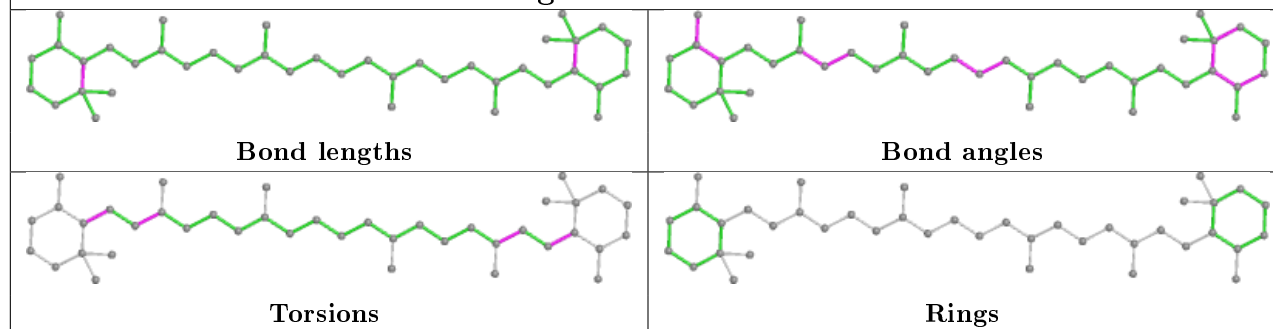




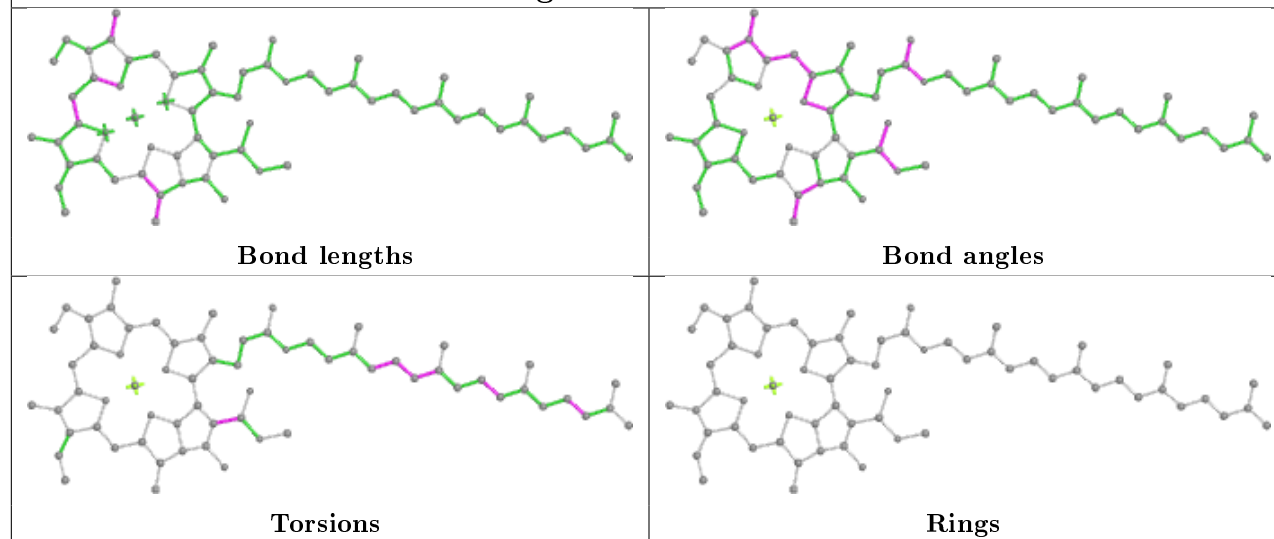
Ligand SQD f 103



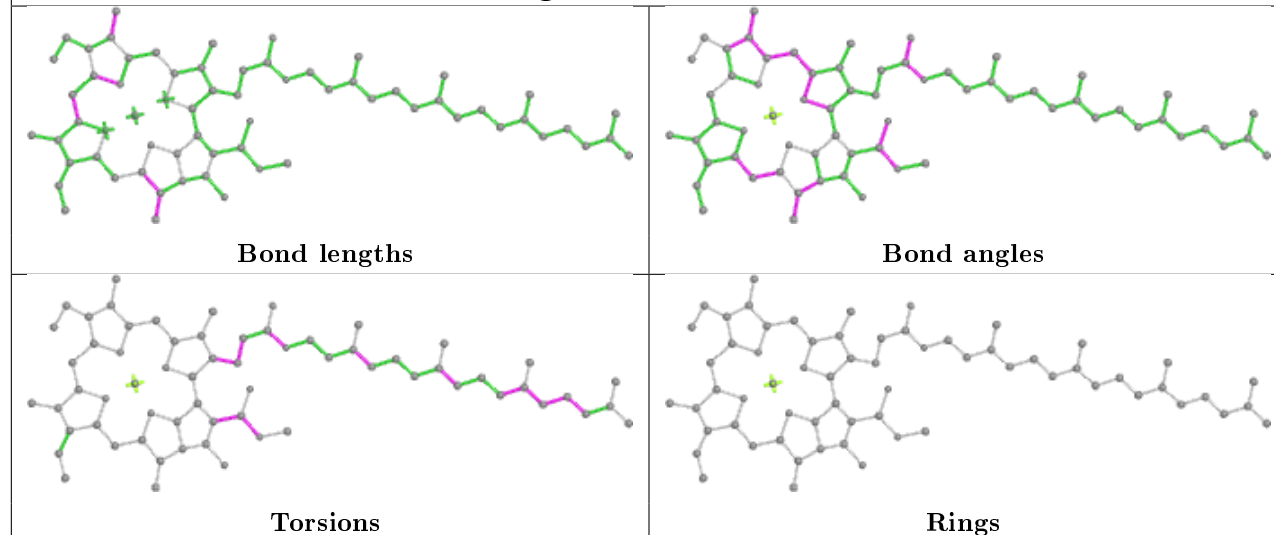
Ligand BCR f 102



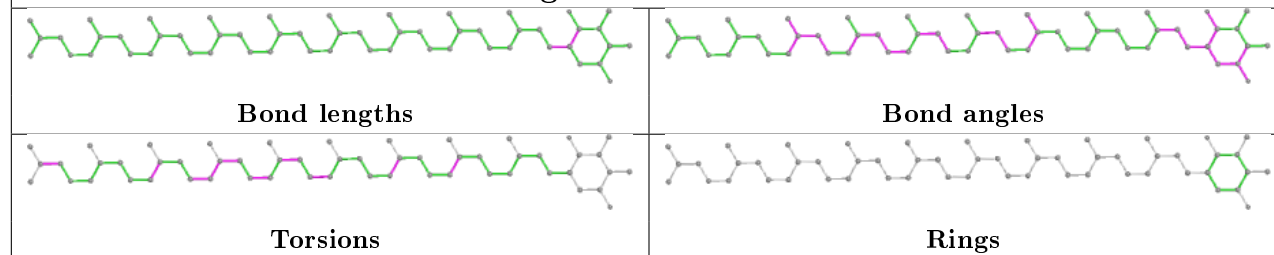
Ligand CLA a 406

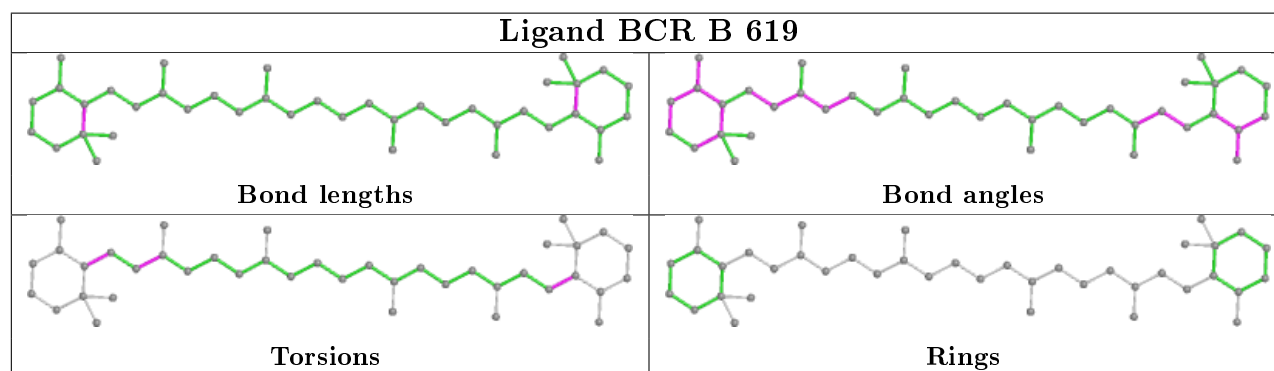
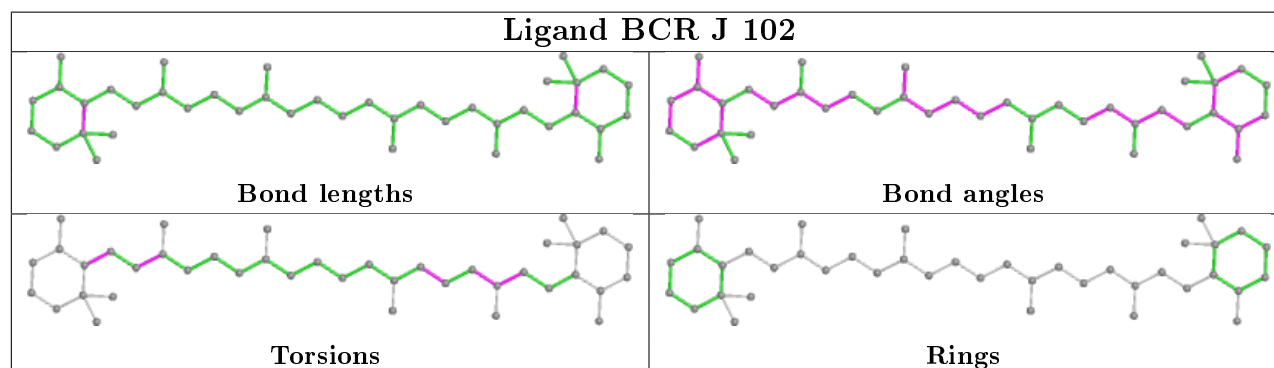
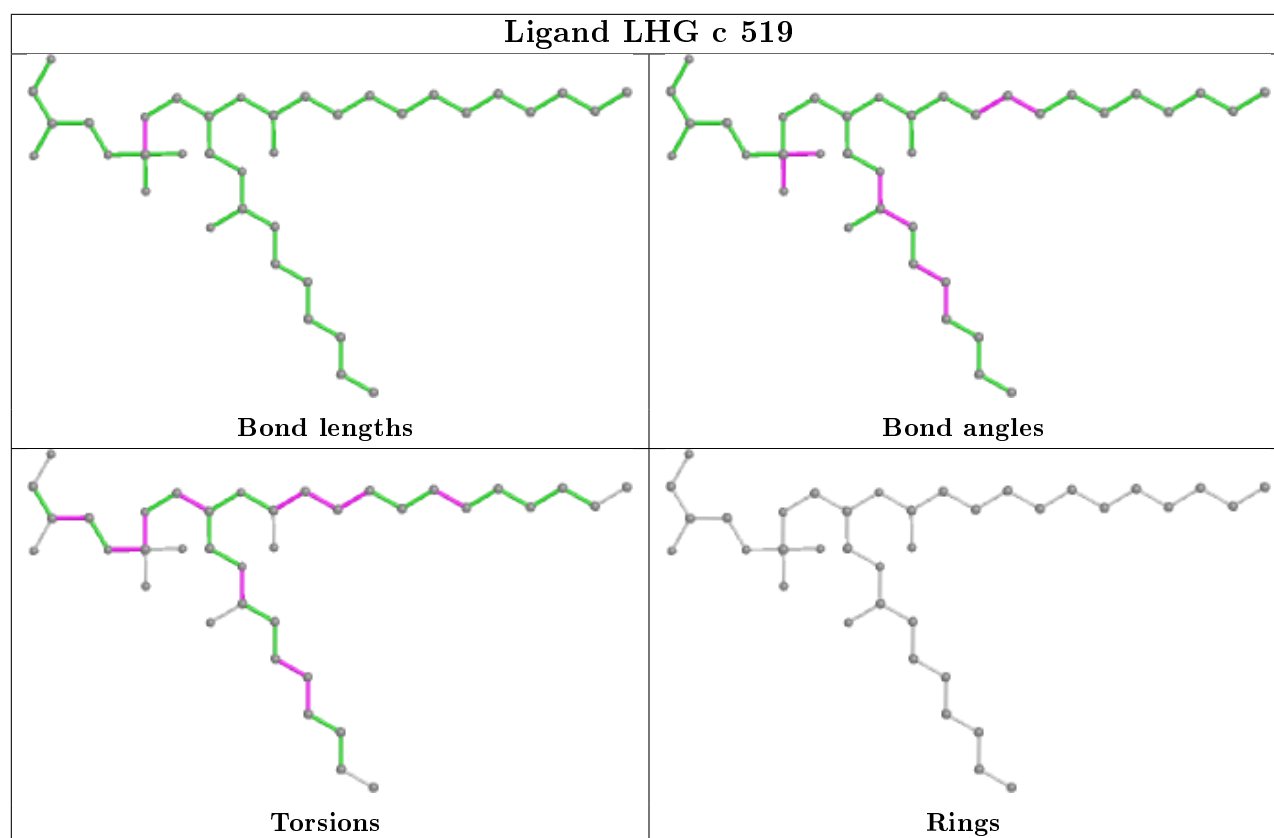


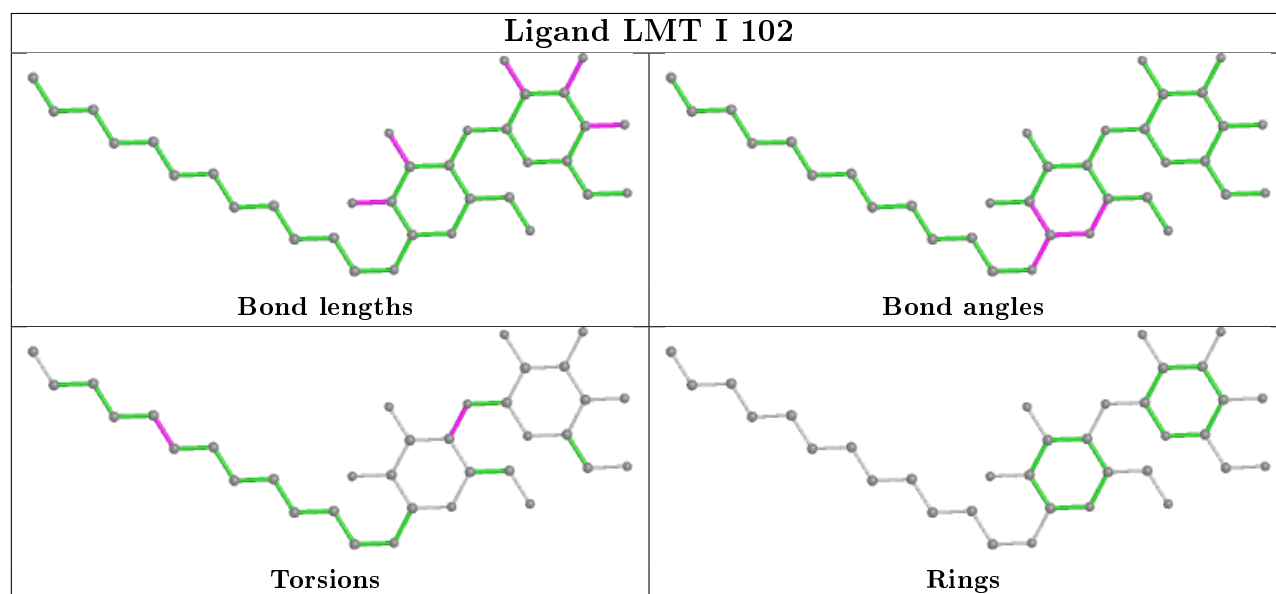
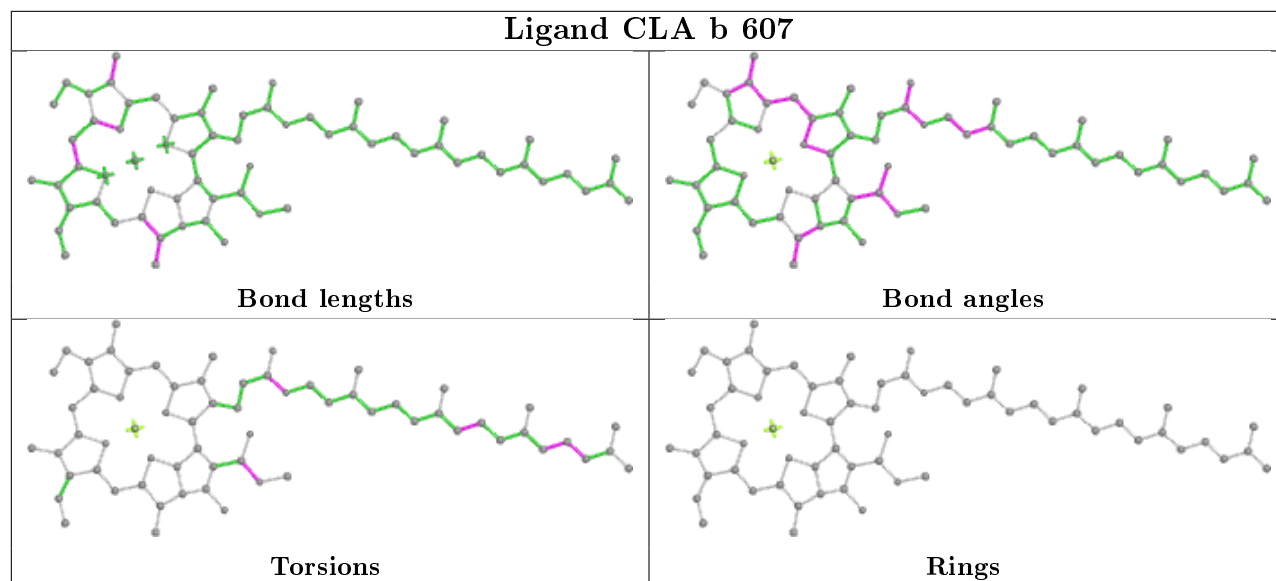
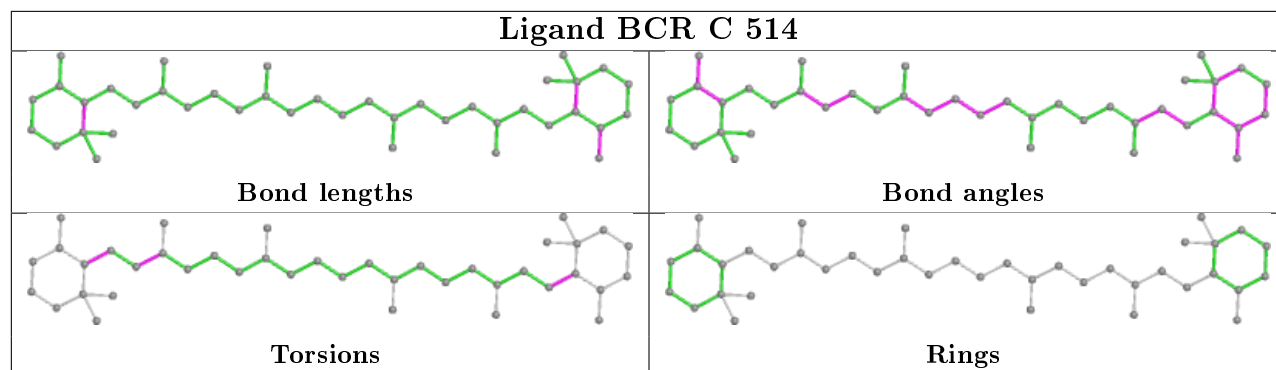
Ligand CLA c 512

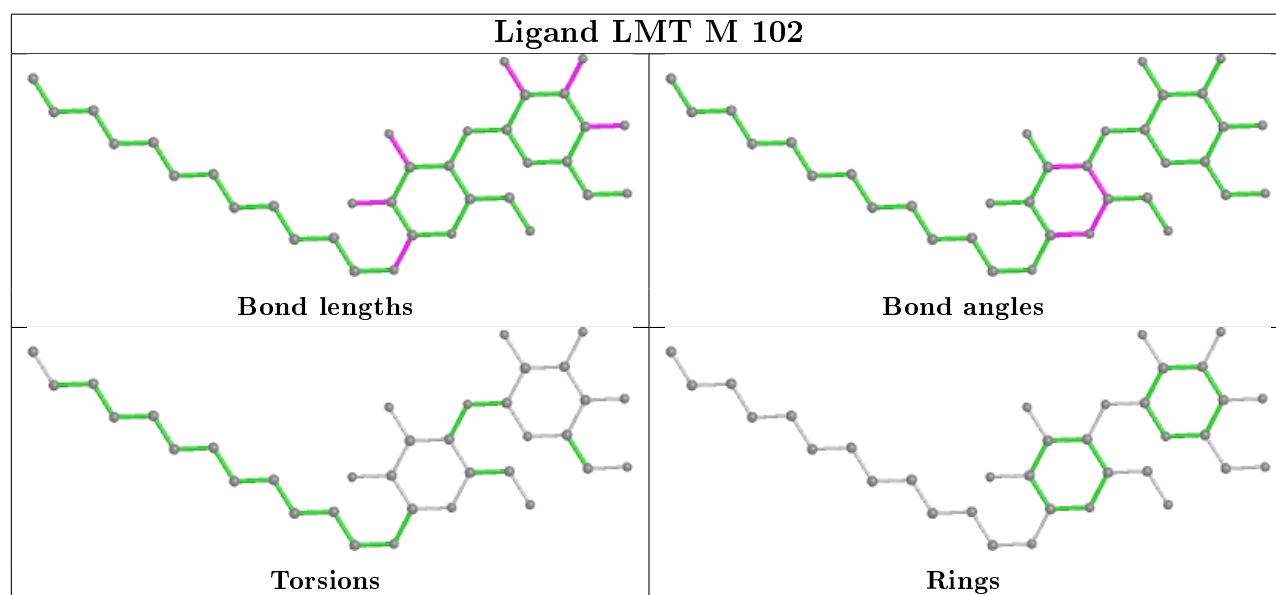
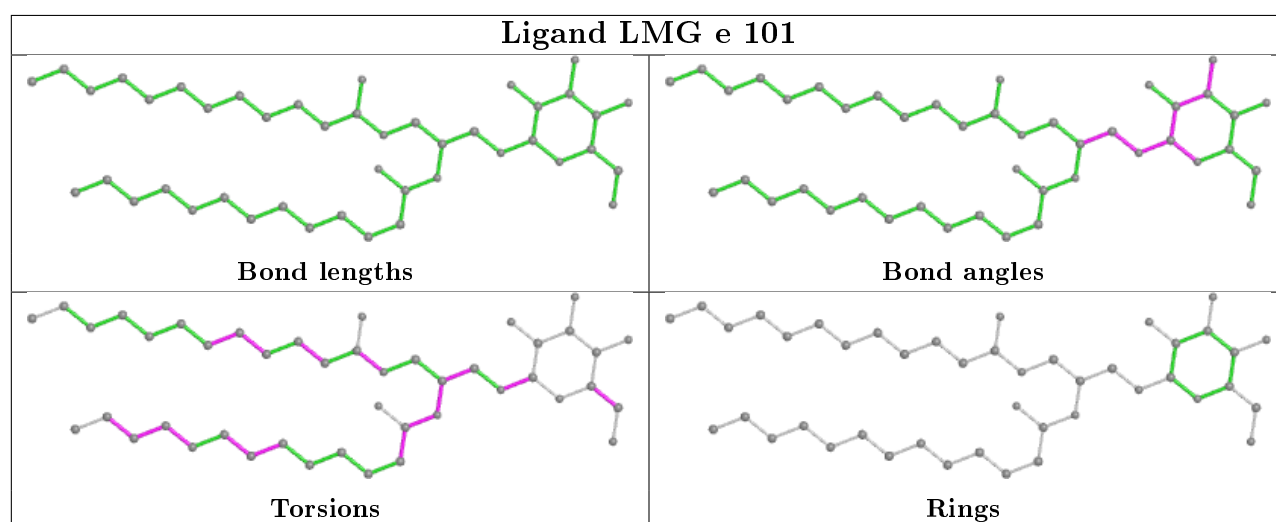
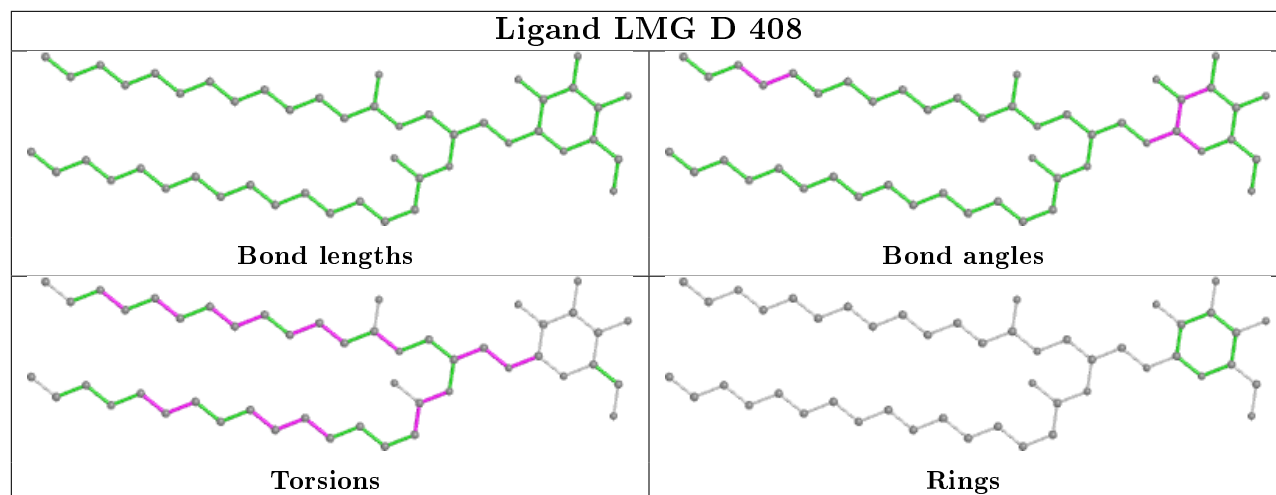


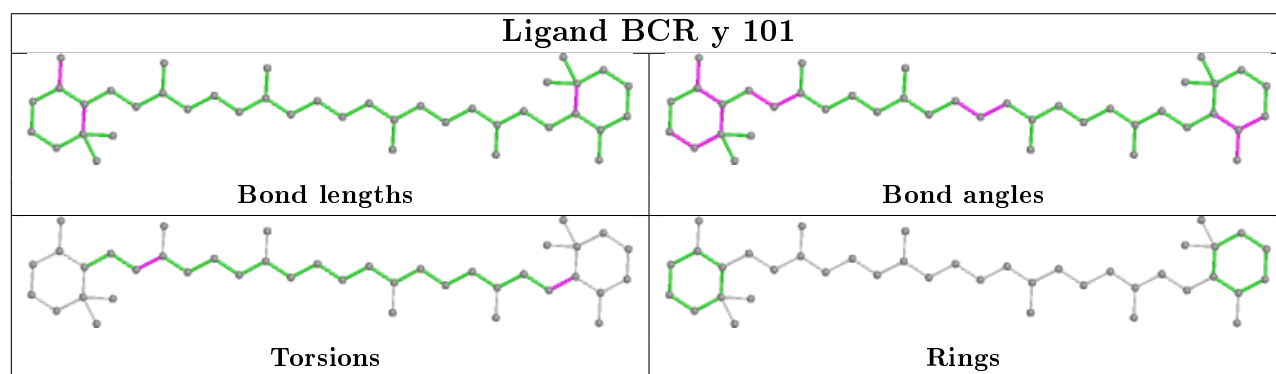
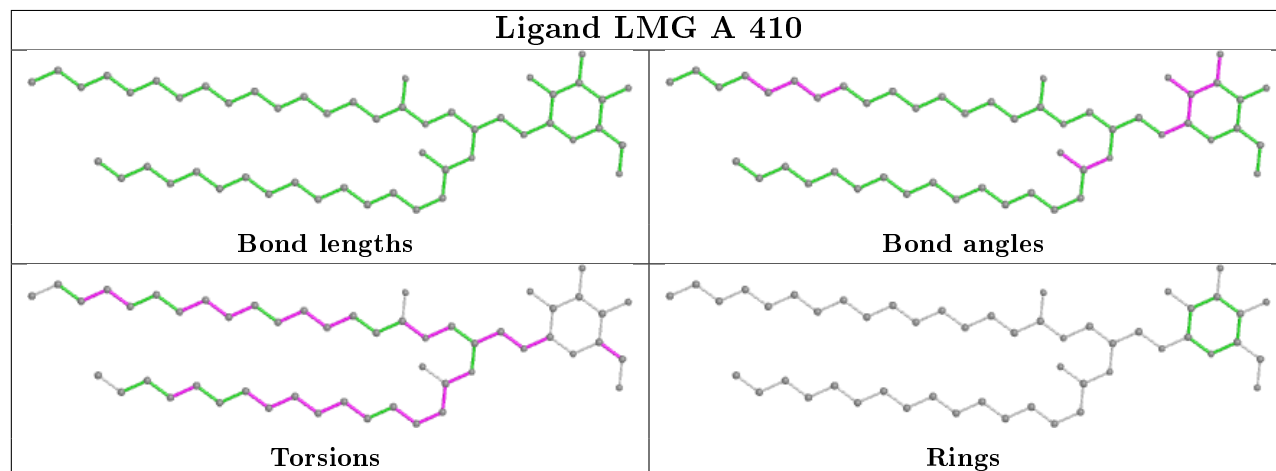
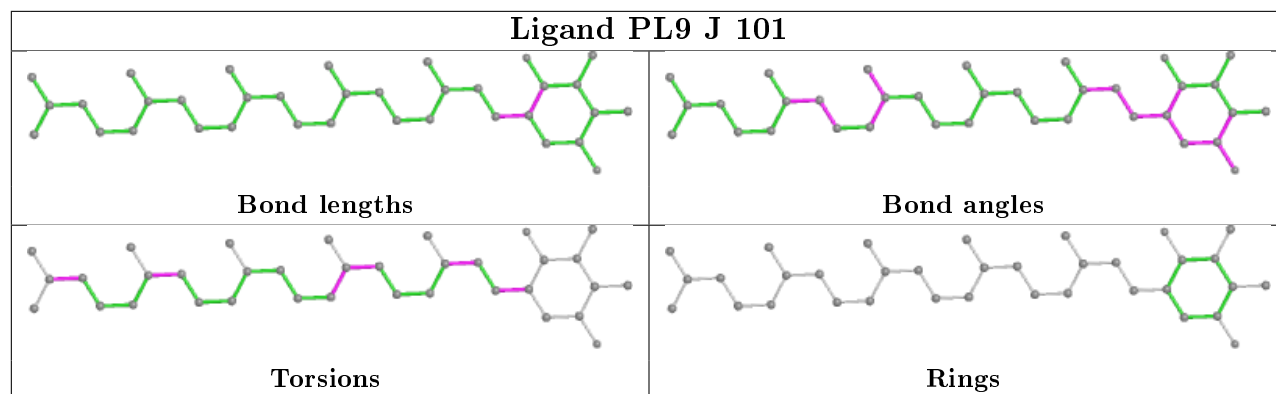
Ligand PL9 d 406

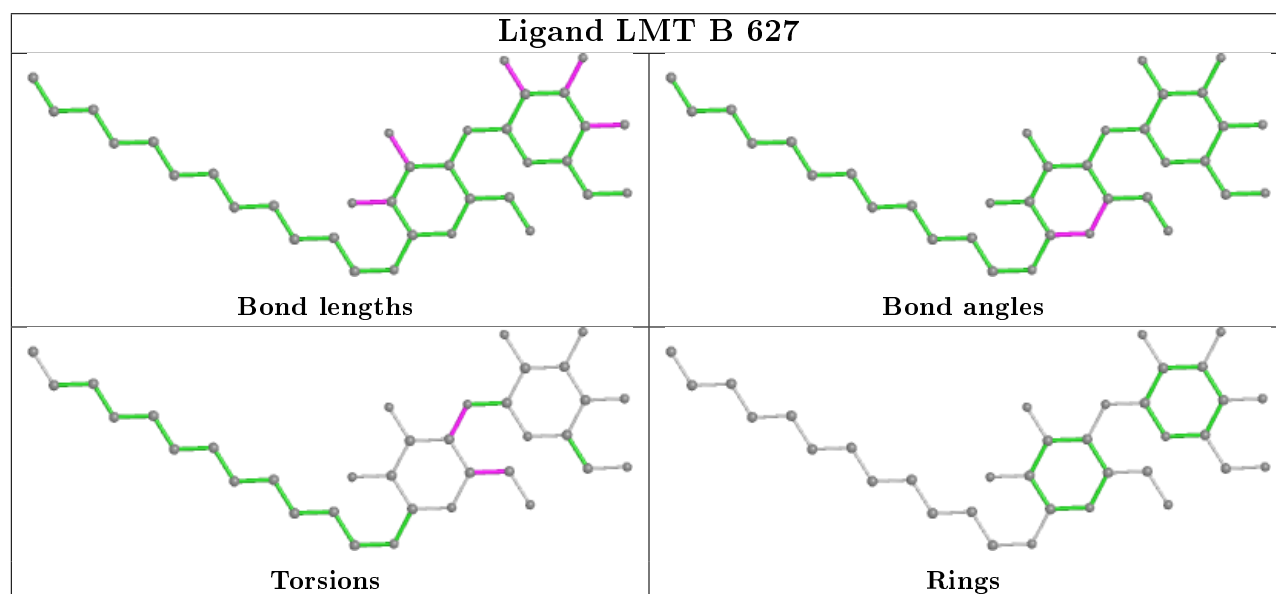
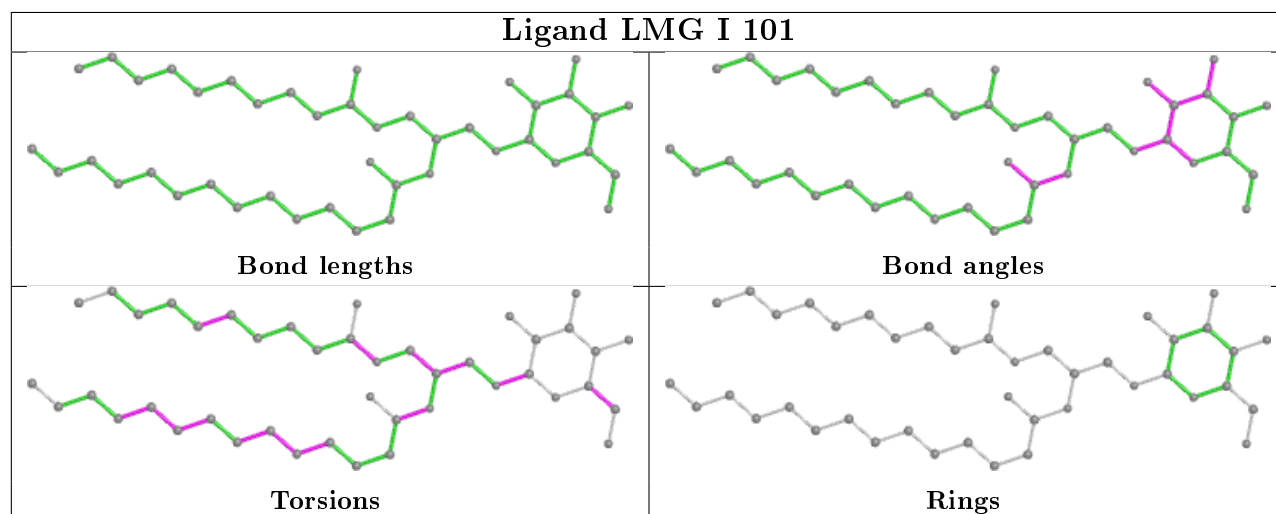
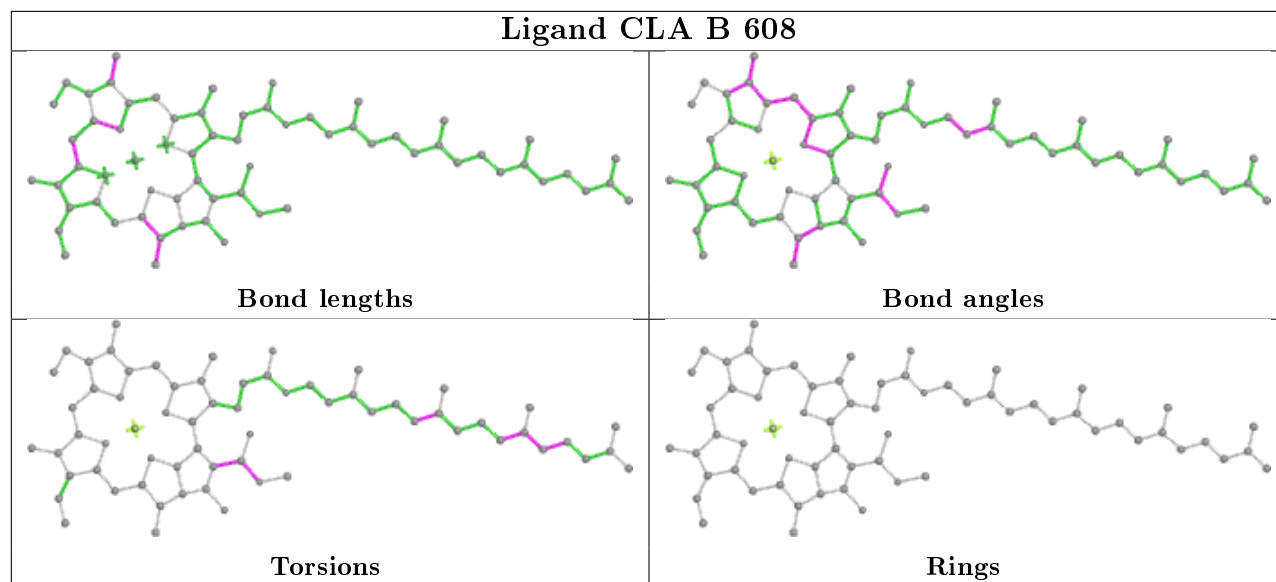


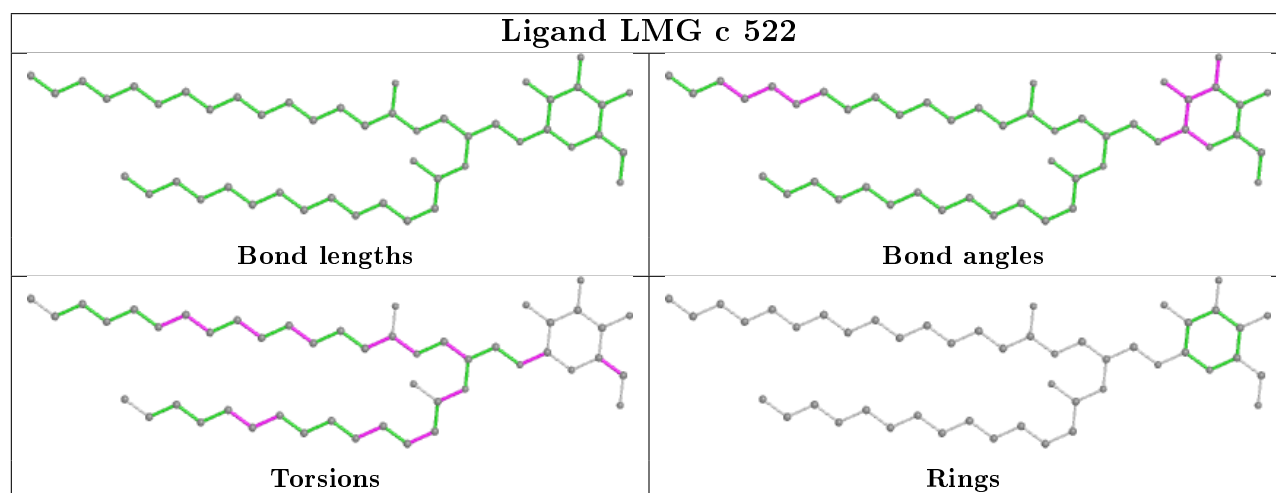
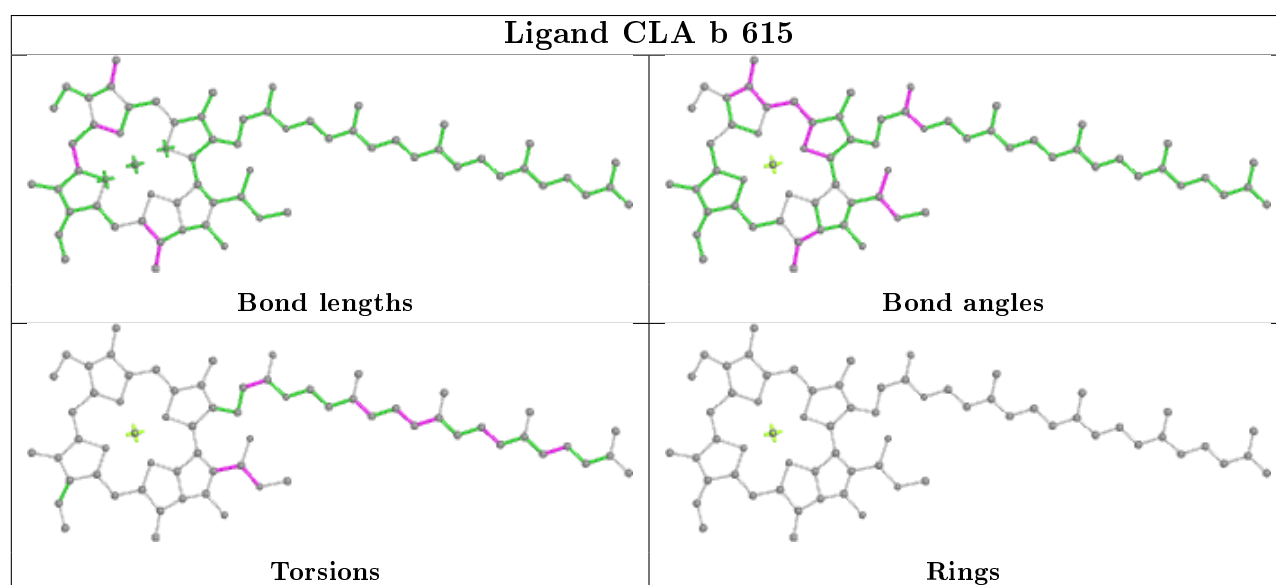
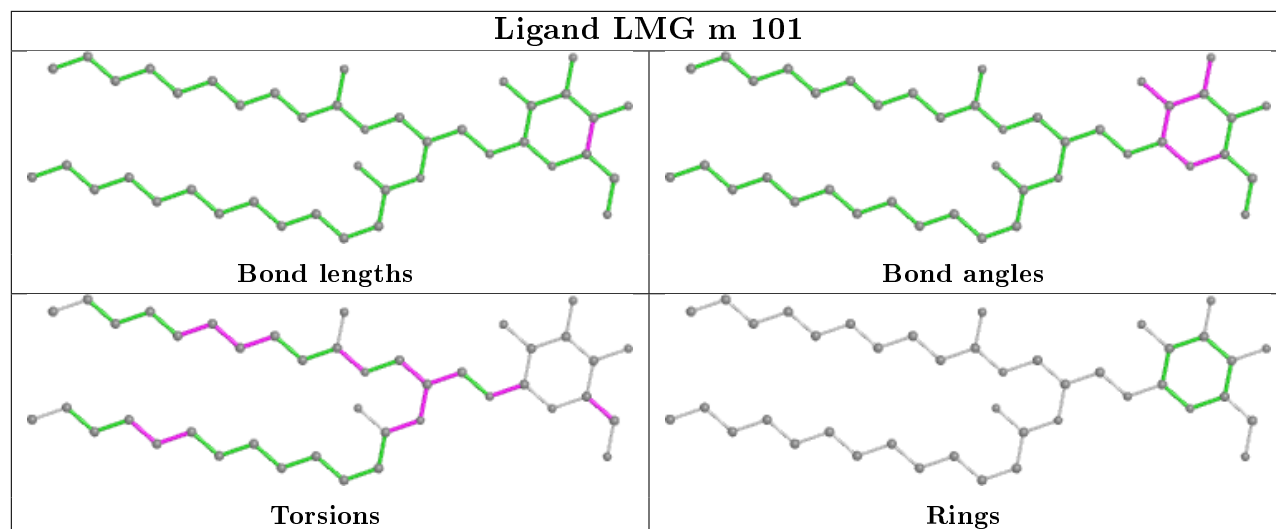




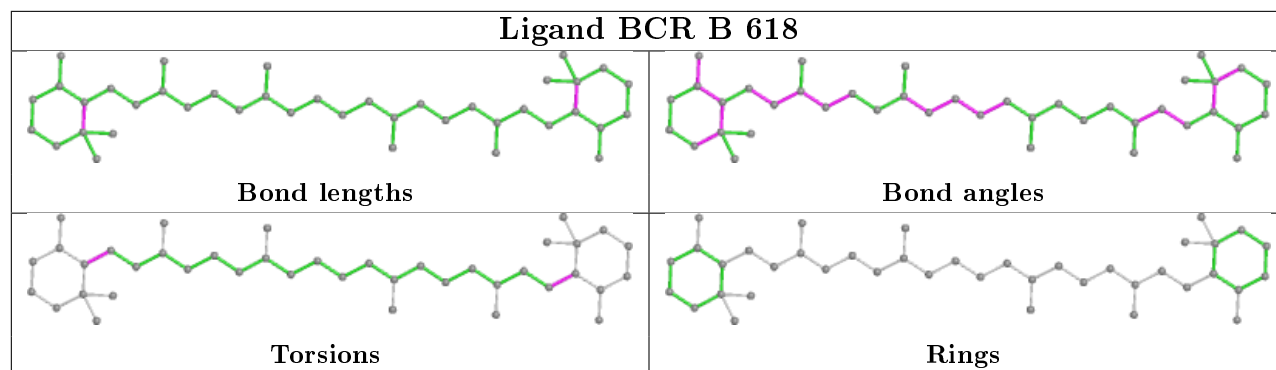




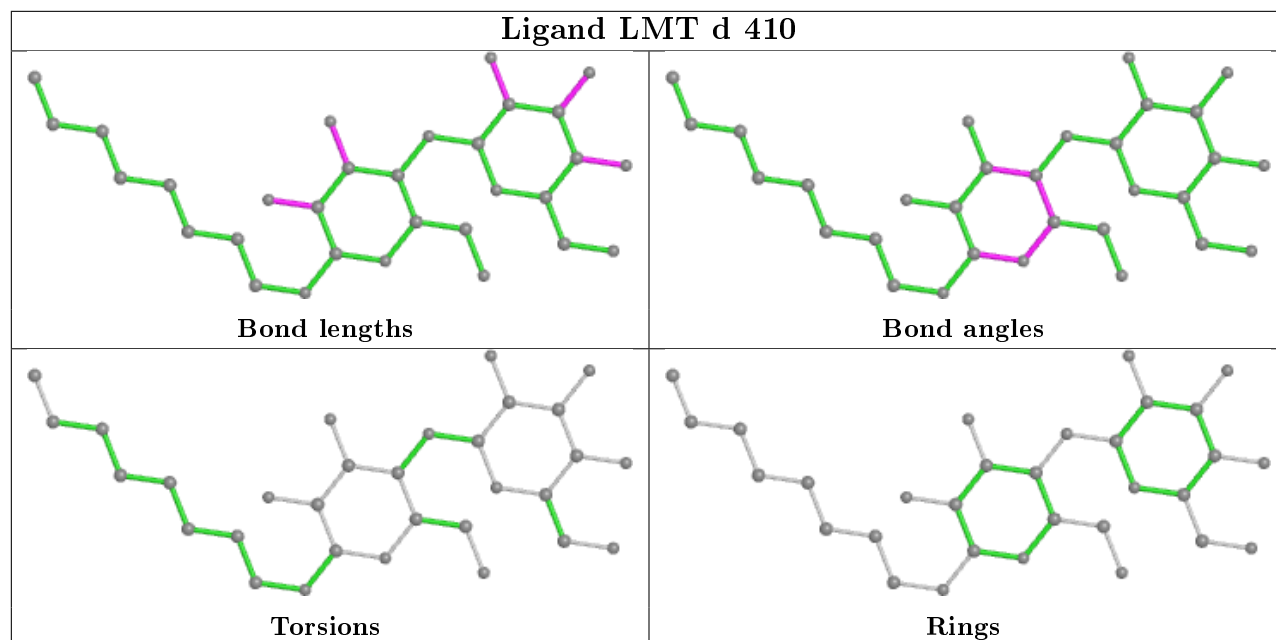




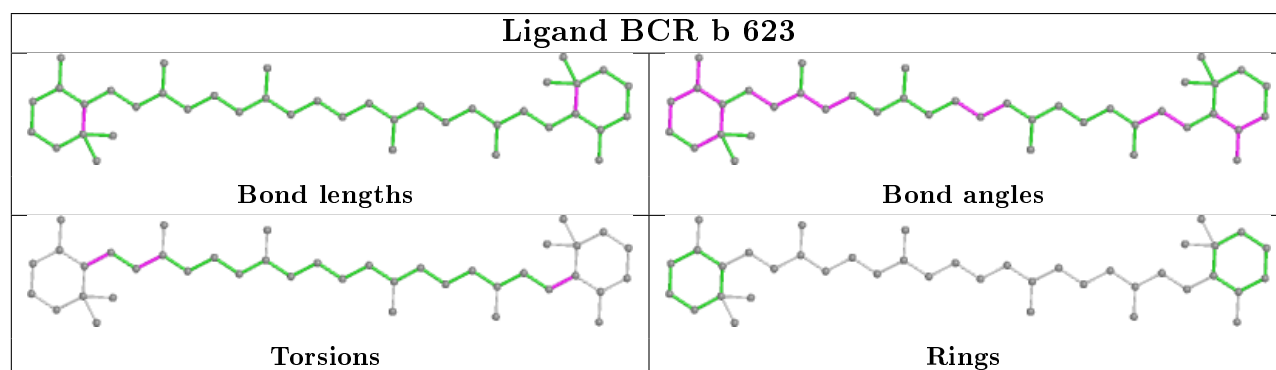
Ligand BCR B 618



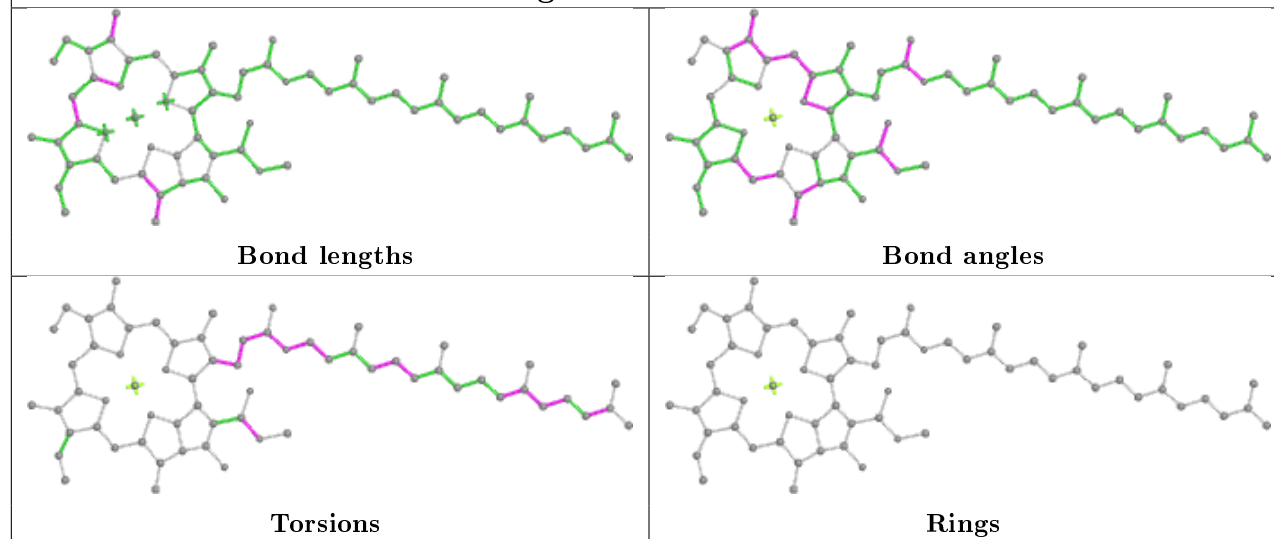
Ligand LMT d 410



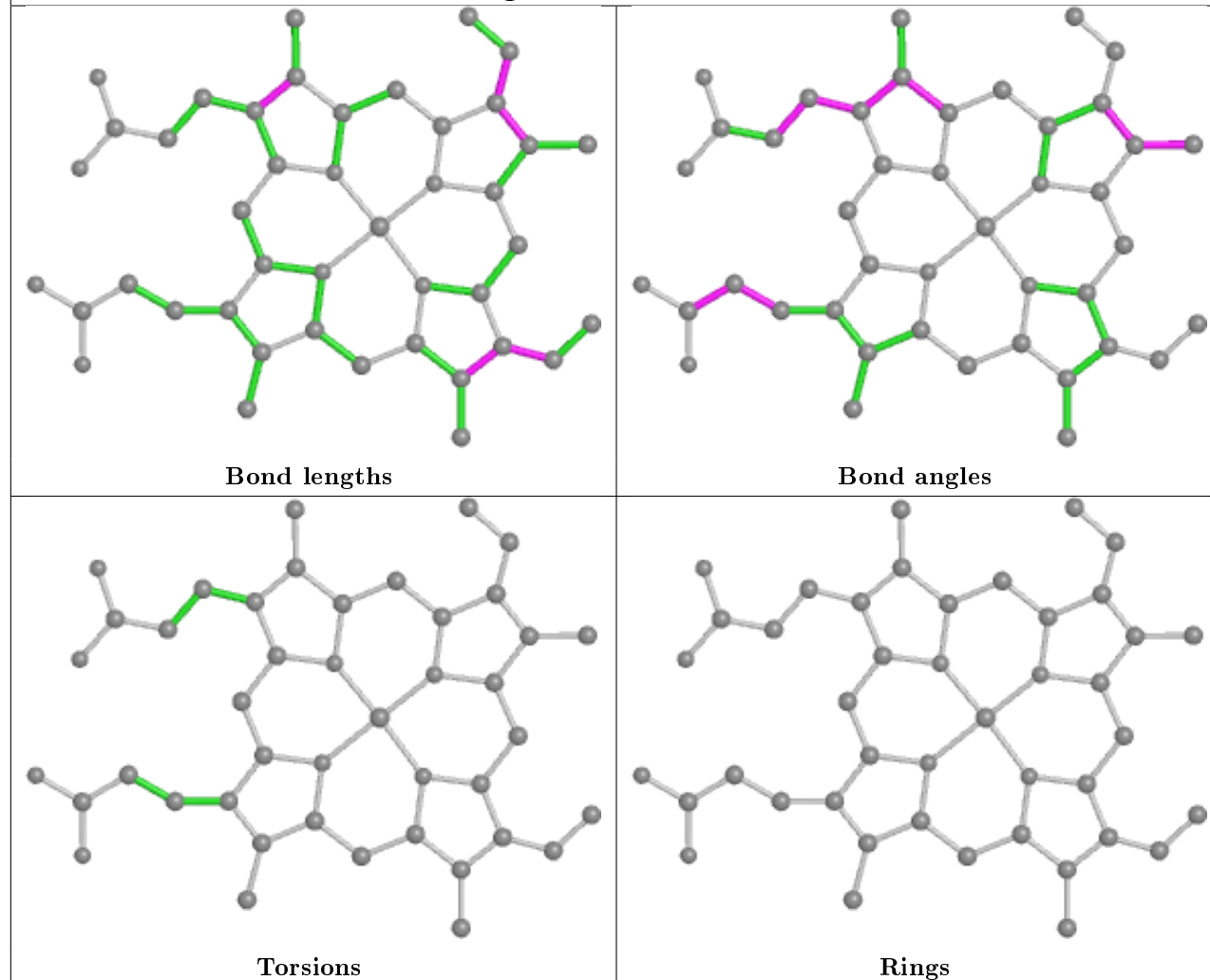
Ligand BCR b 623

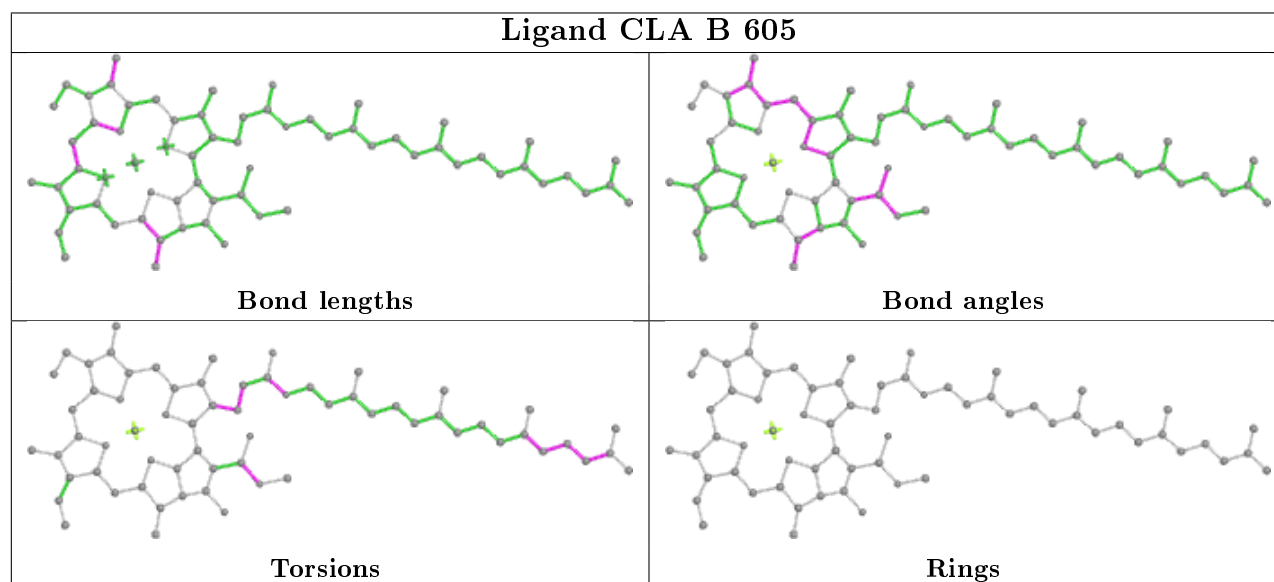
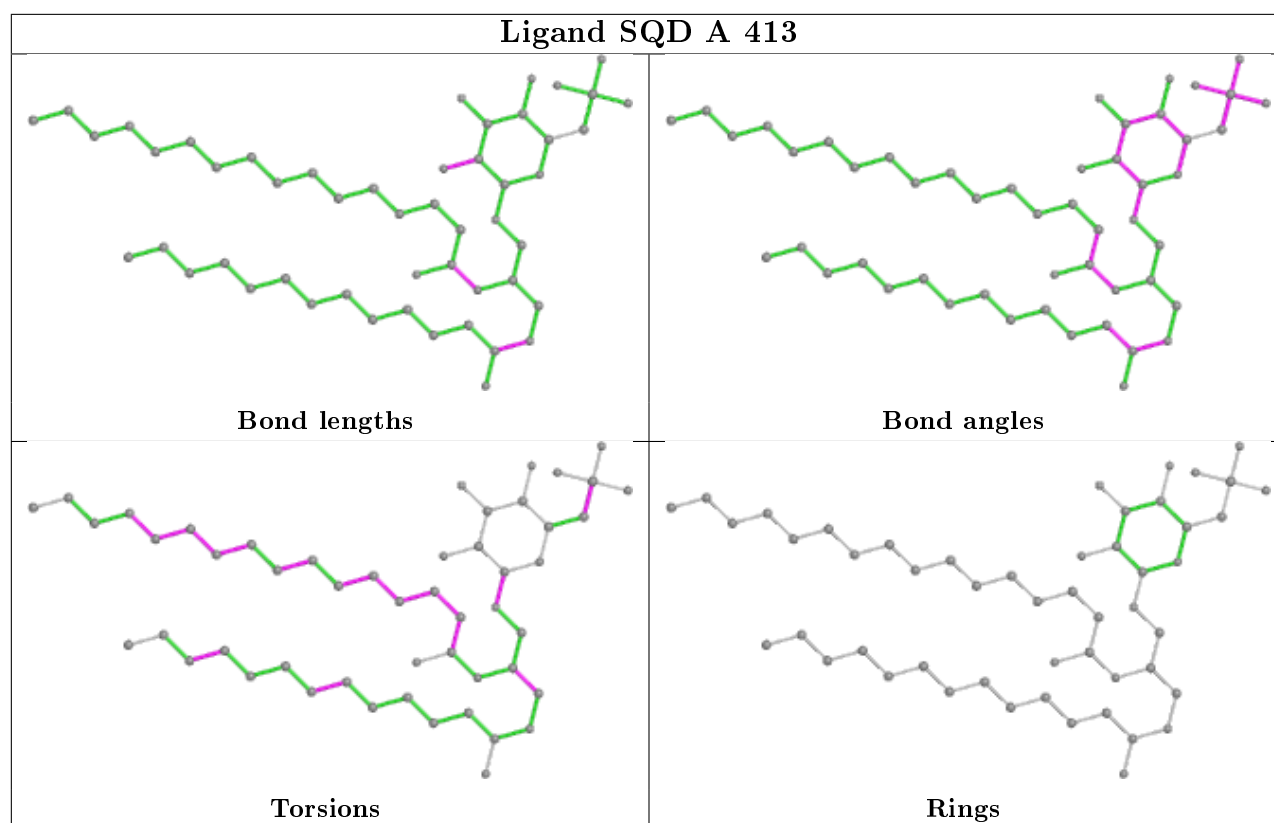


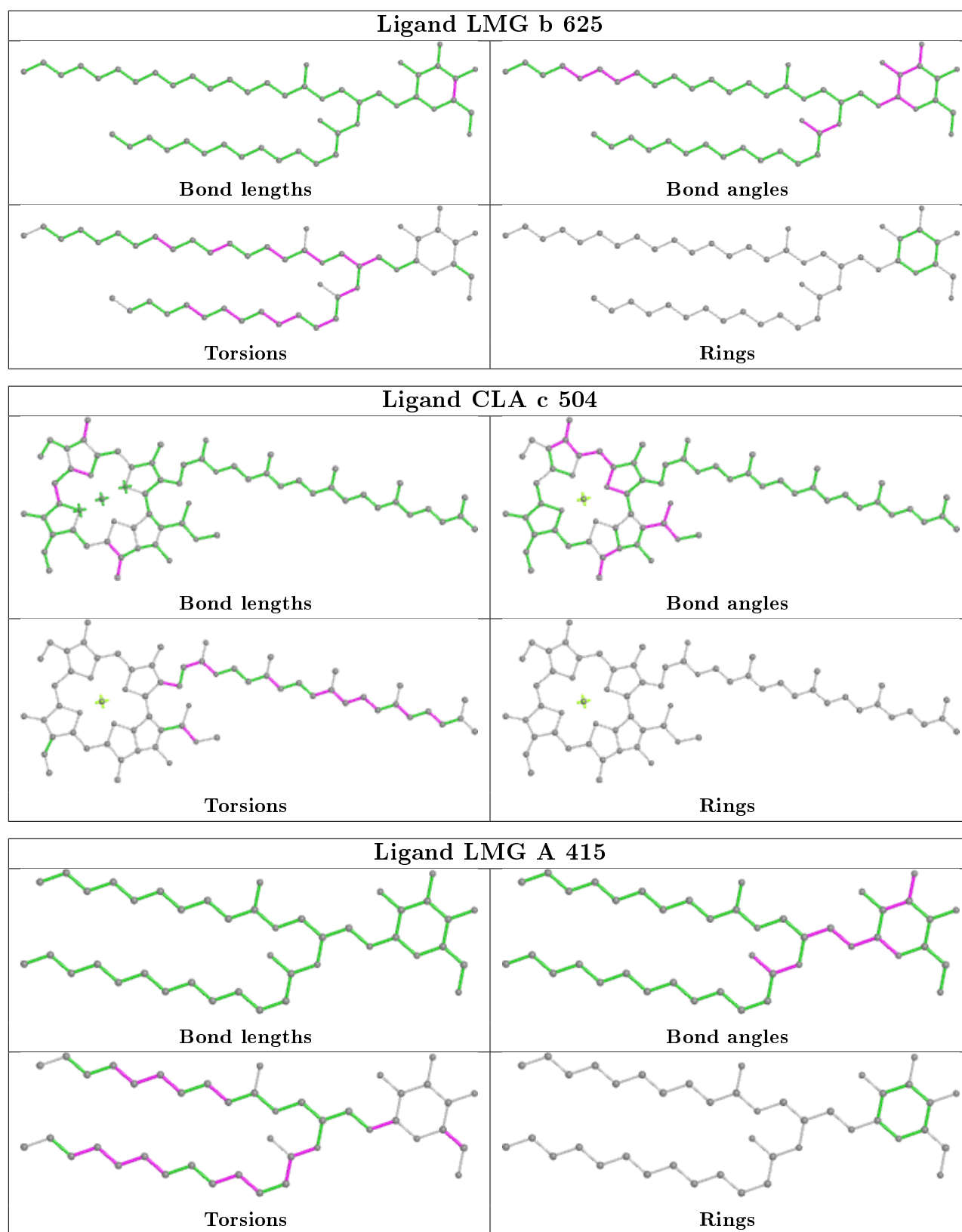
Ligand CLA c 511



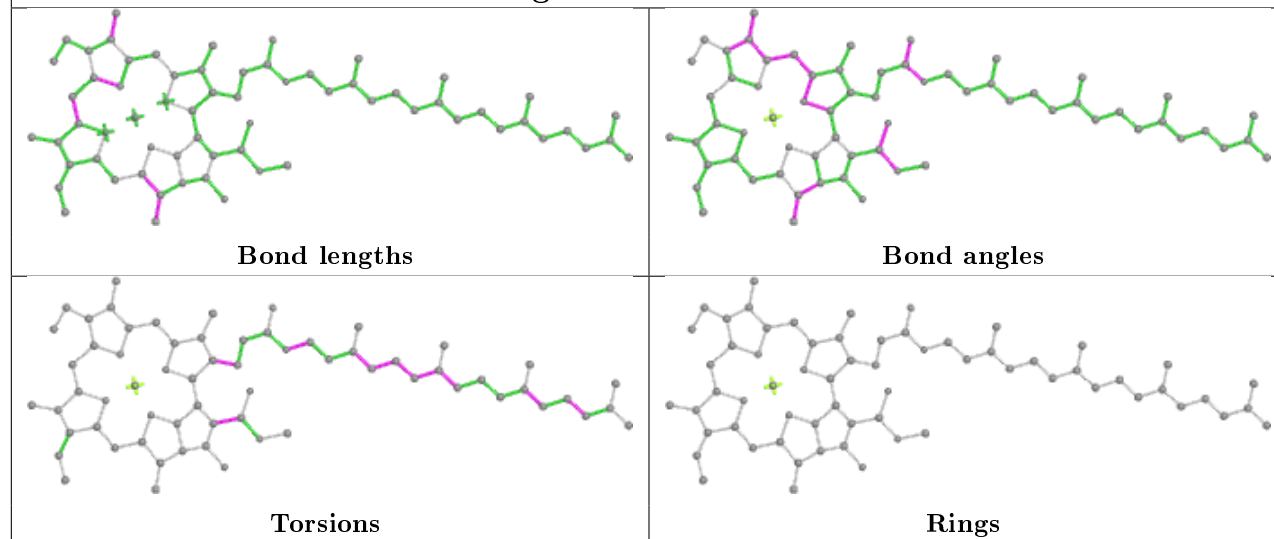
Ligand HEM F 101



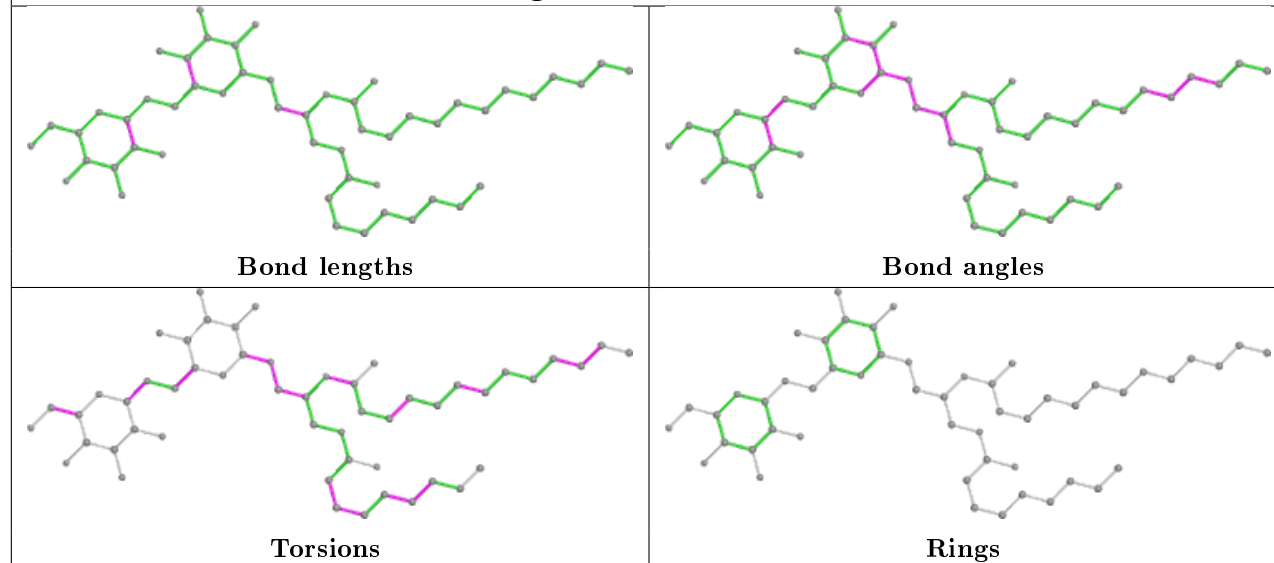




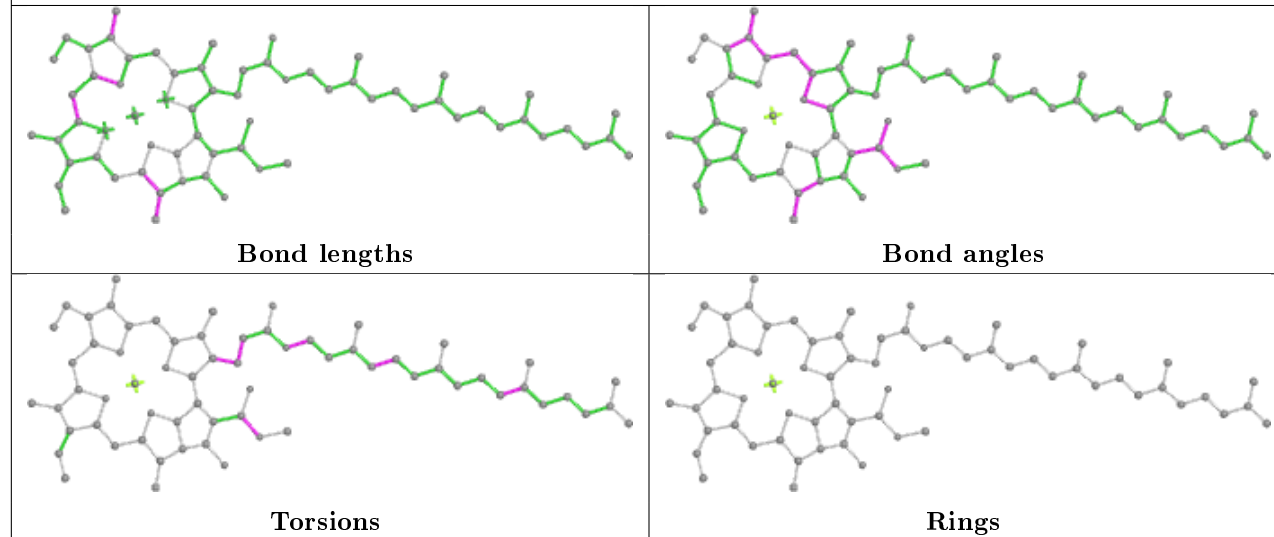
Ligand CLA A 403

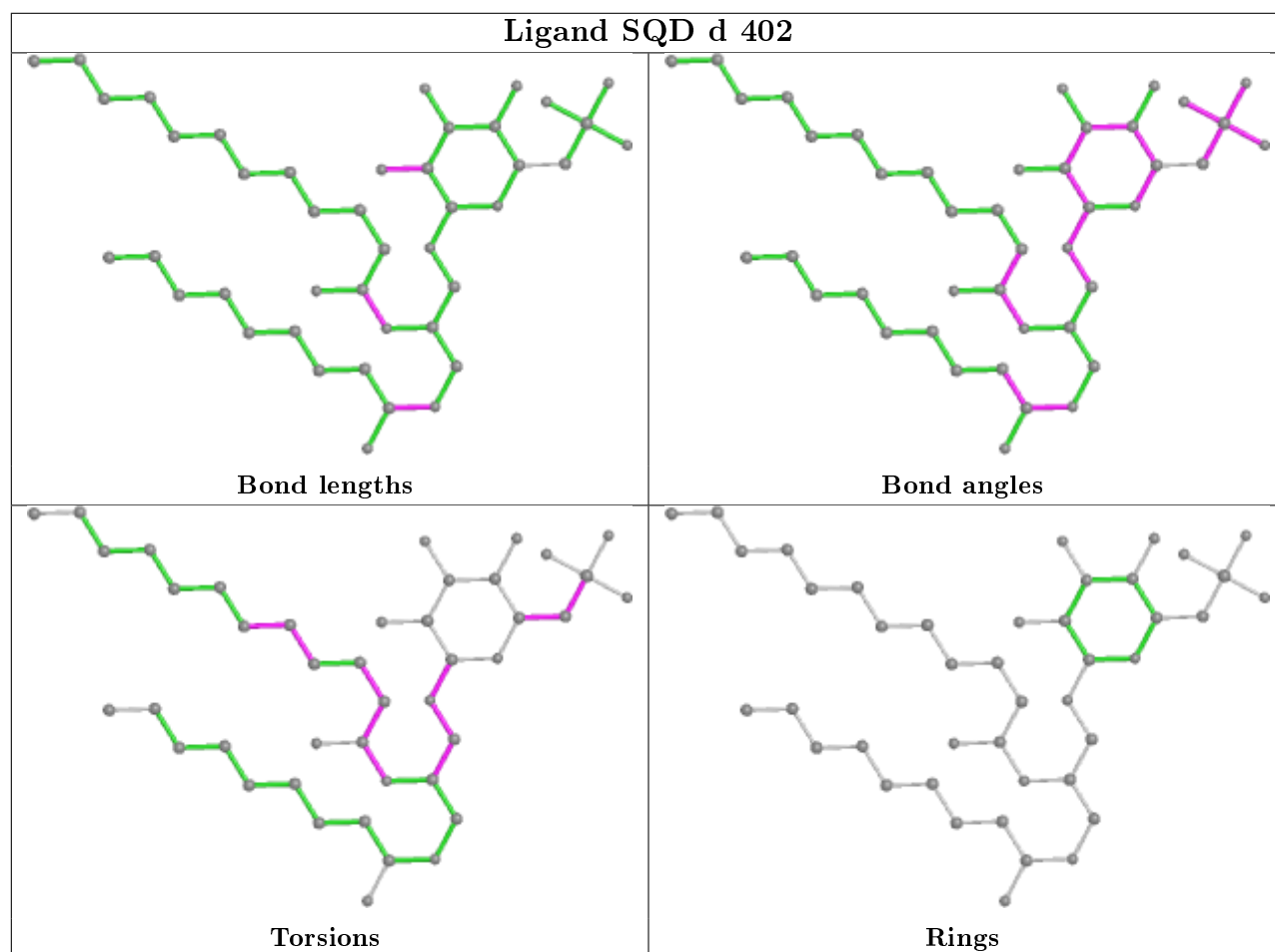
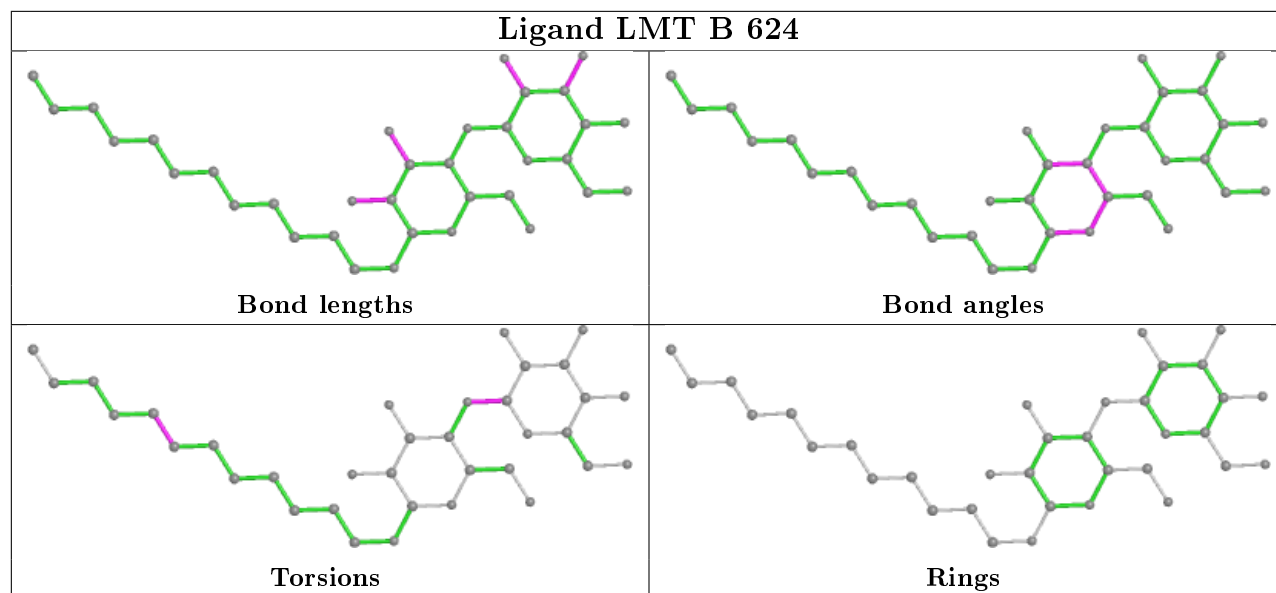


Ligand DGD B 625

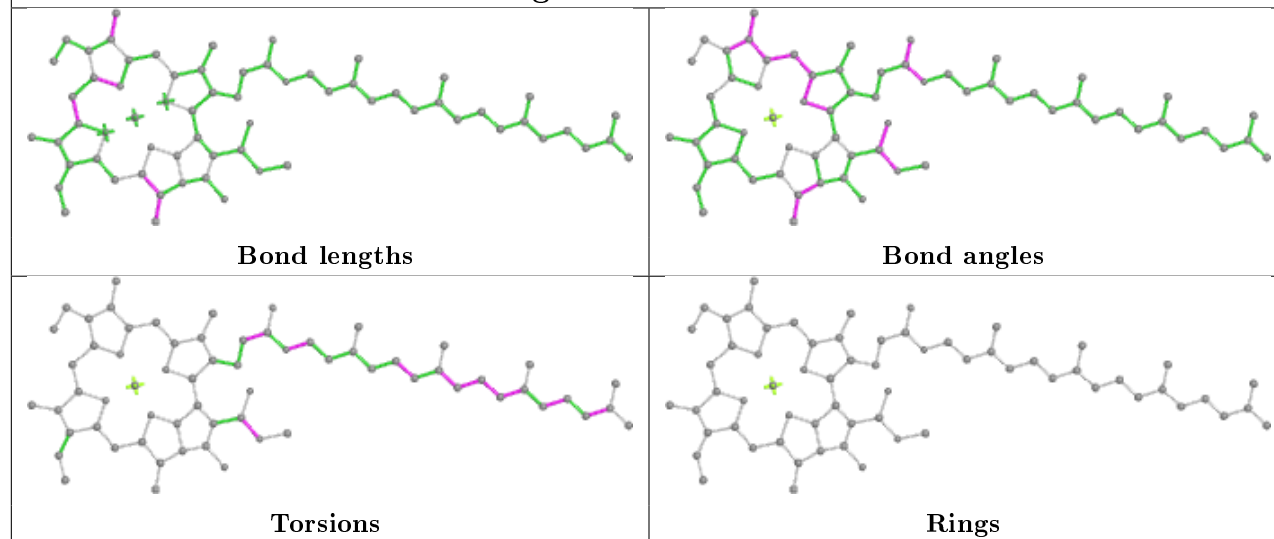


Ligand CLA a 404

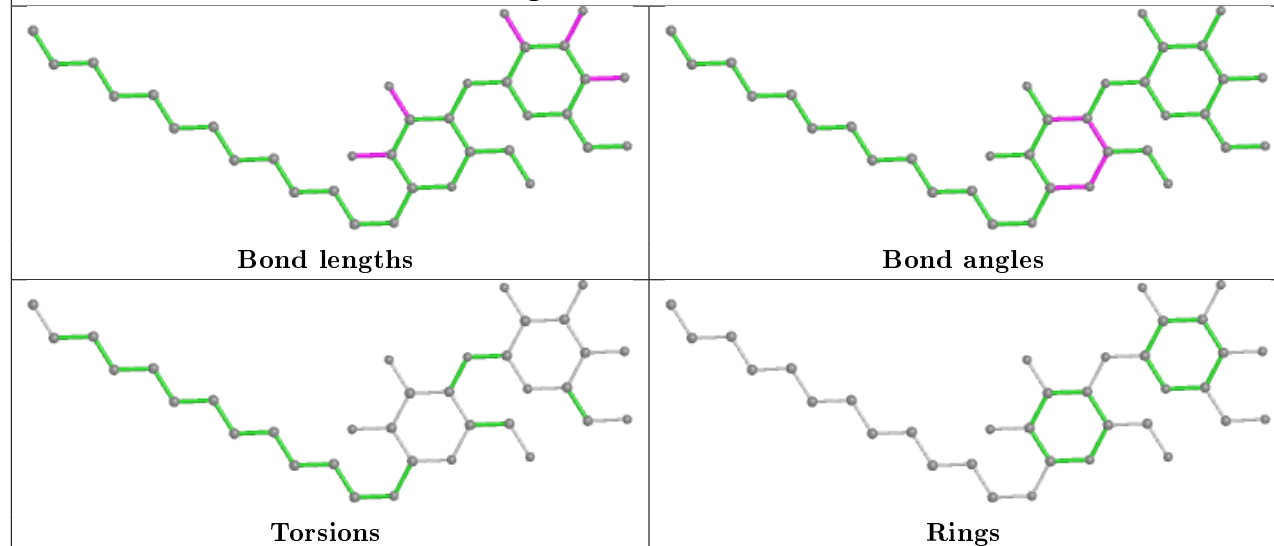




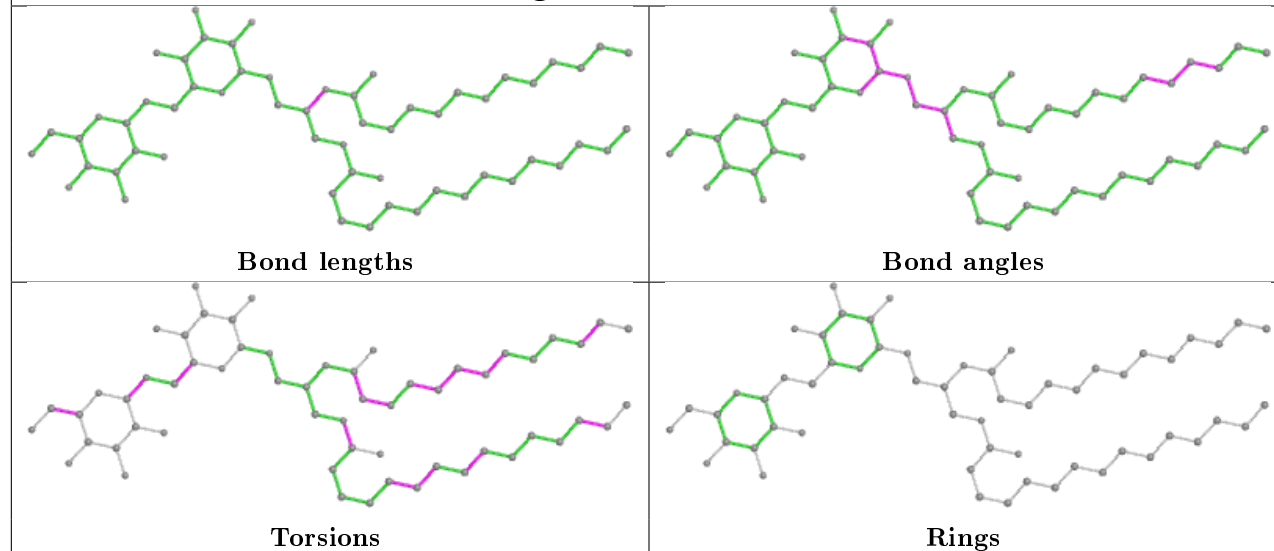
Ligand CLA B 612

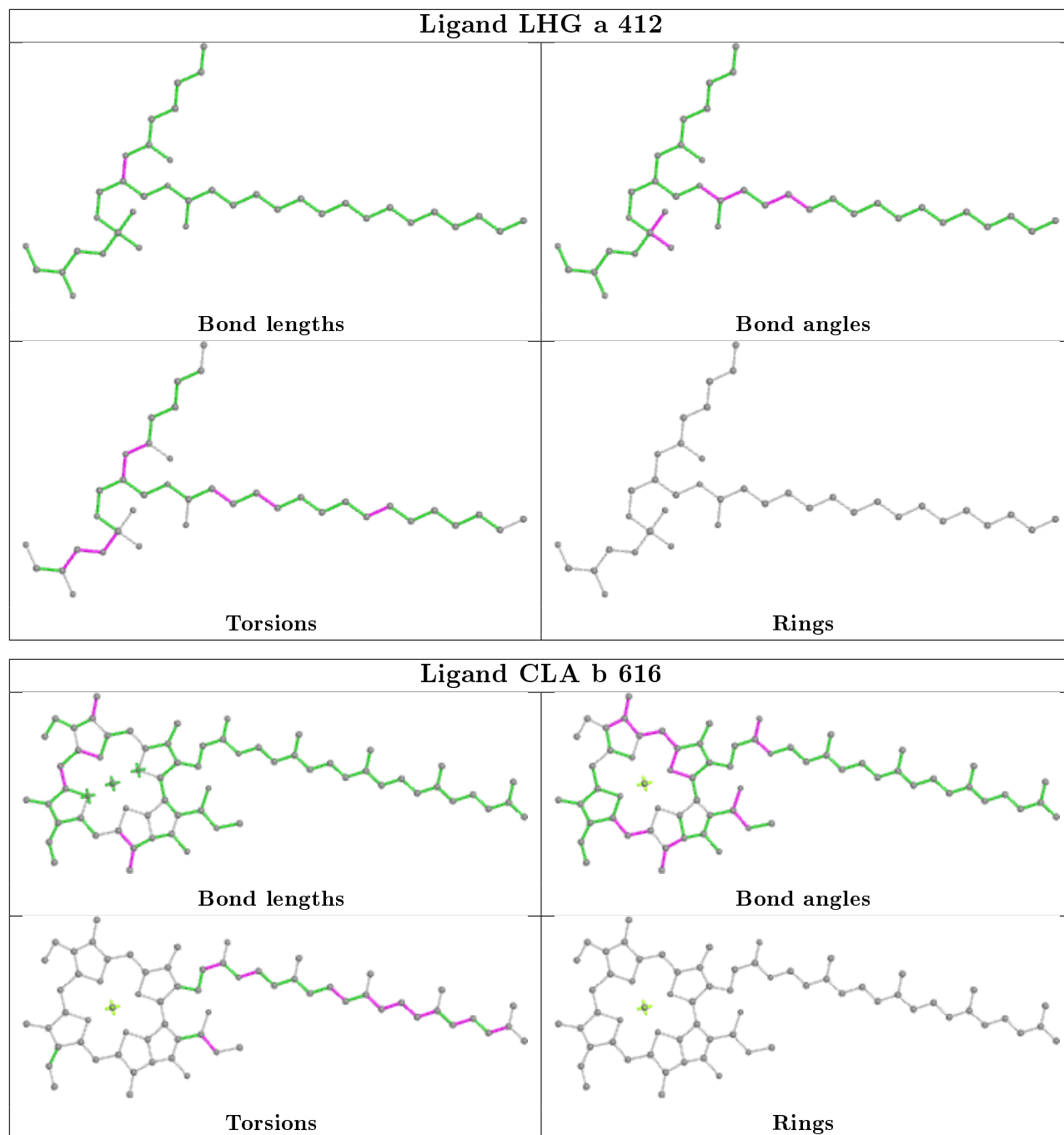


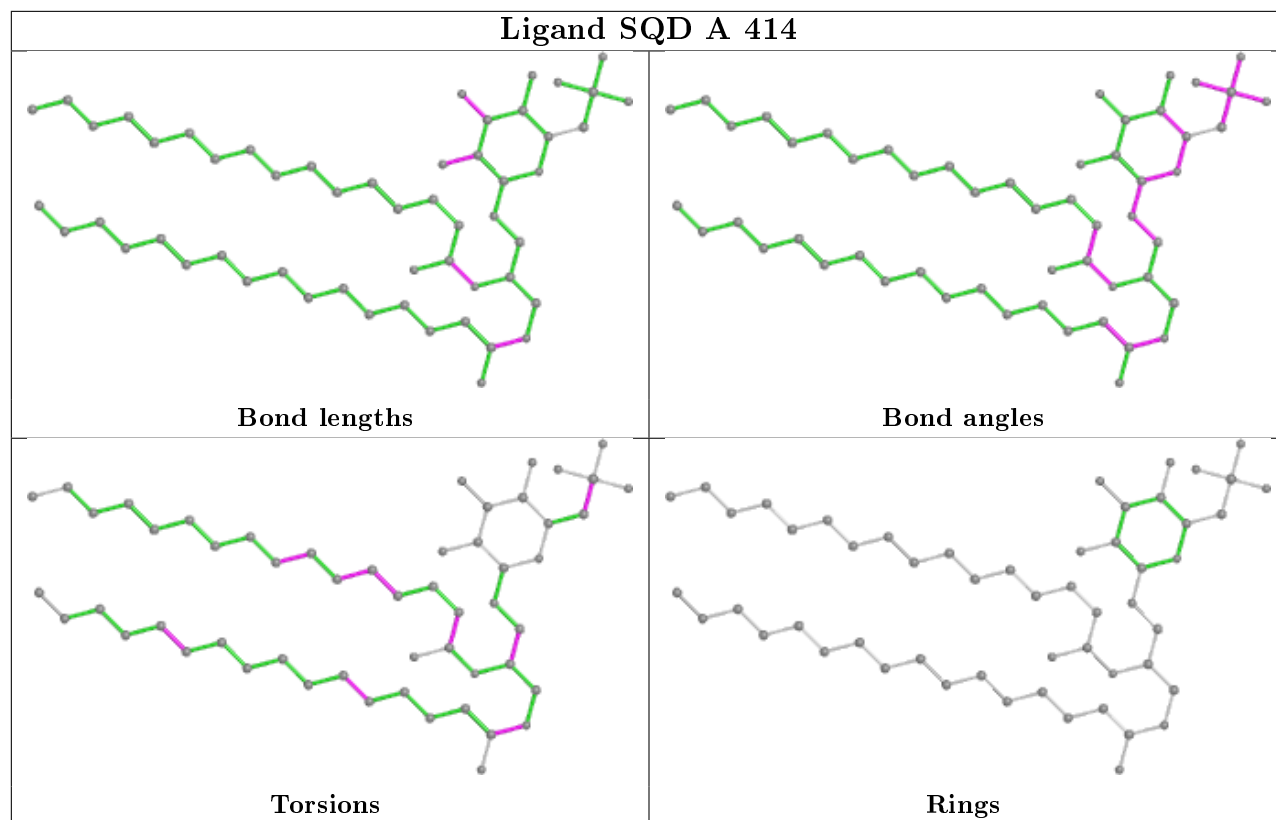
Ligand LMT M 103

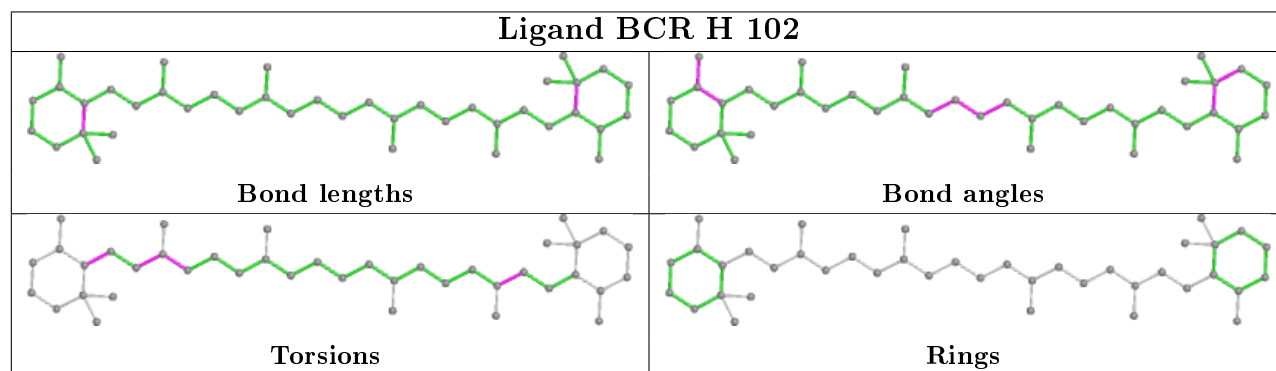
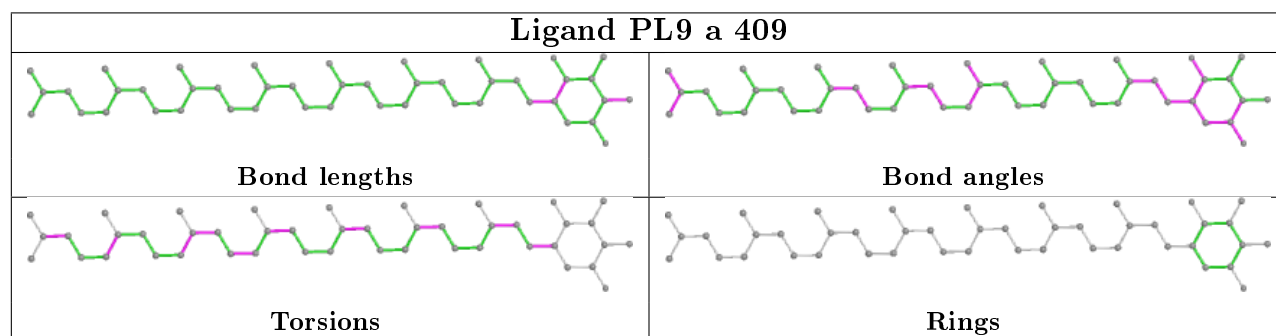
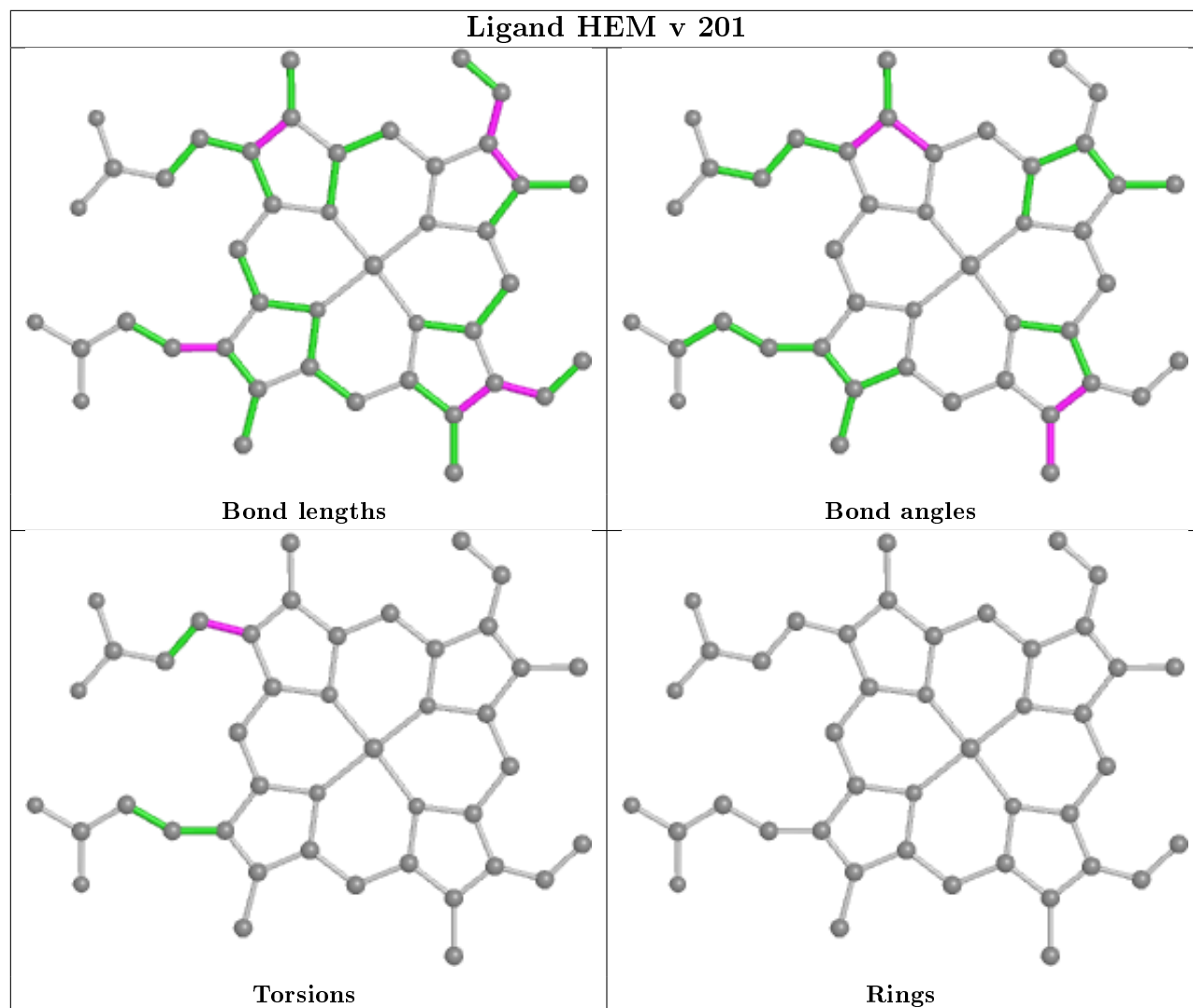


Ligand DGD b 624

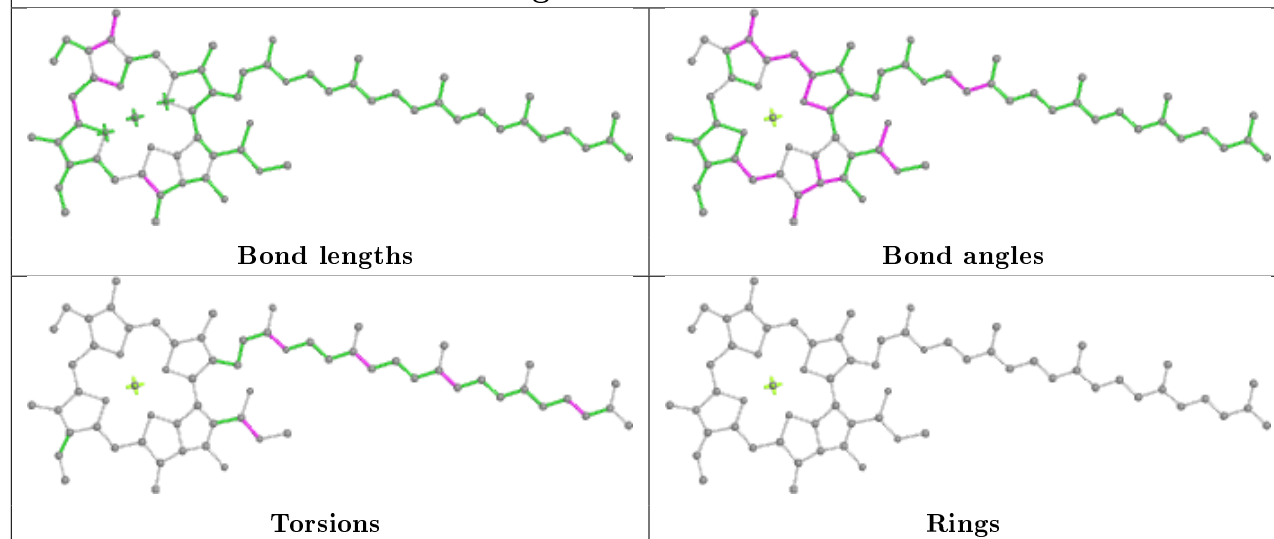




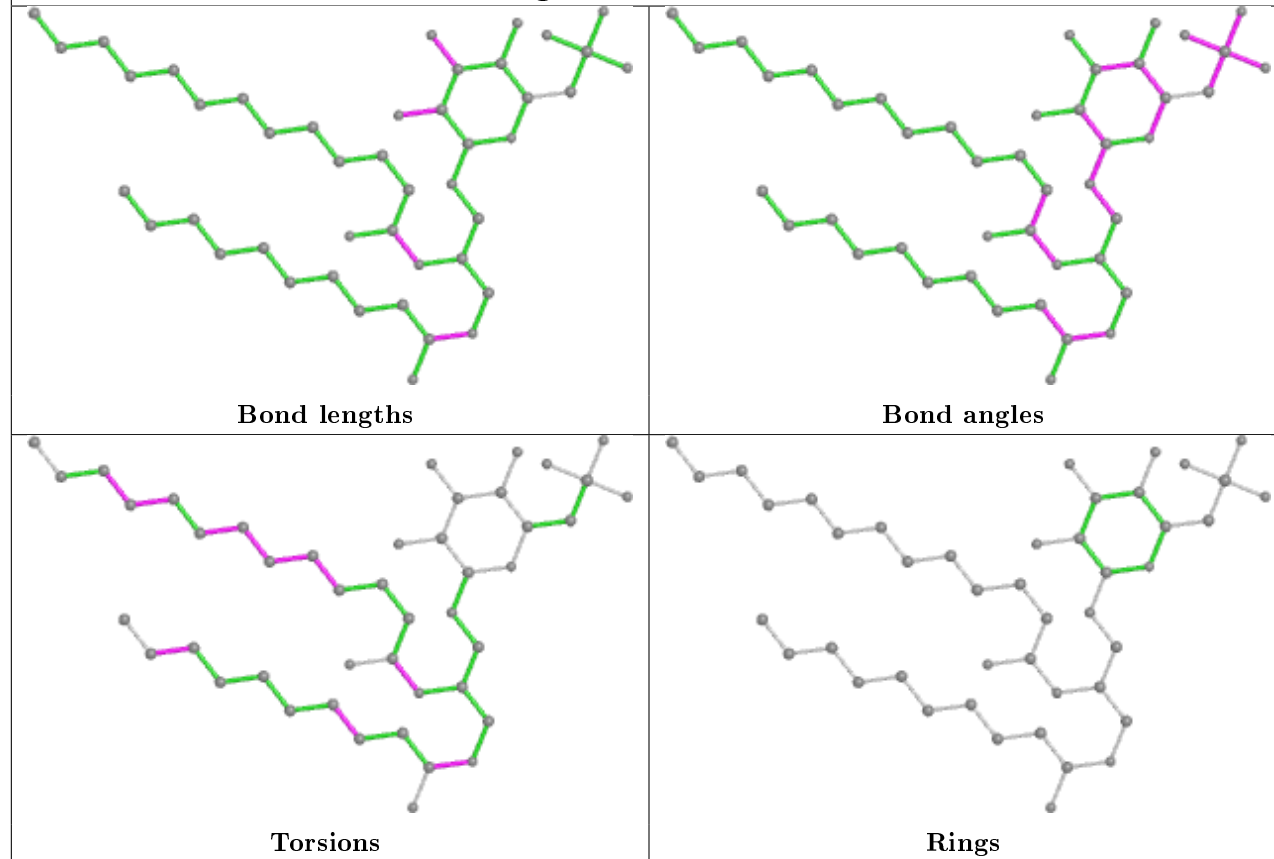


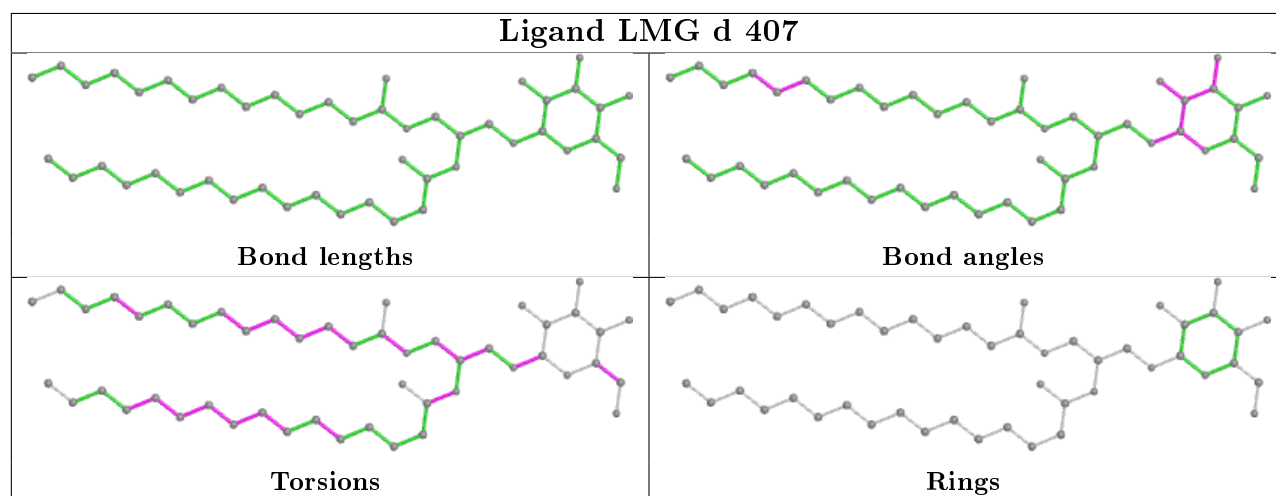
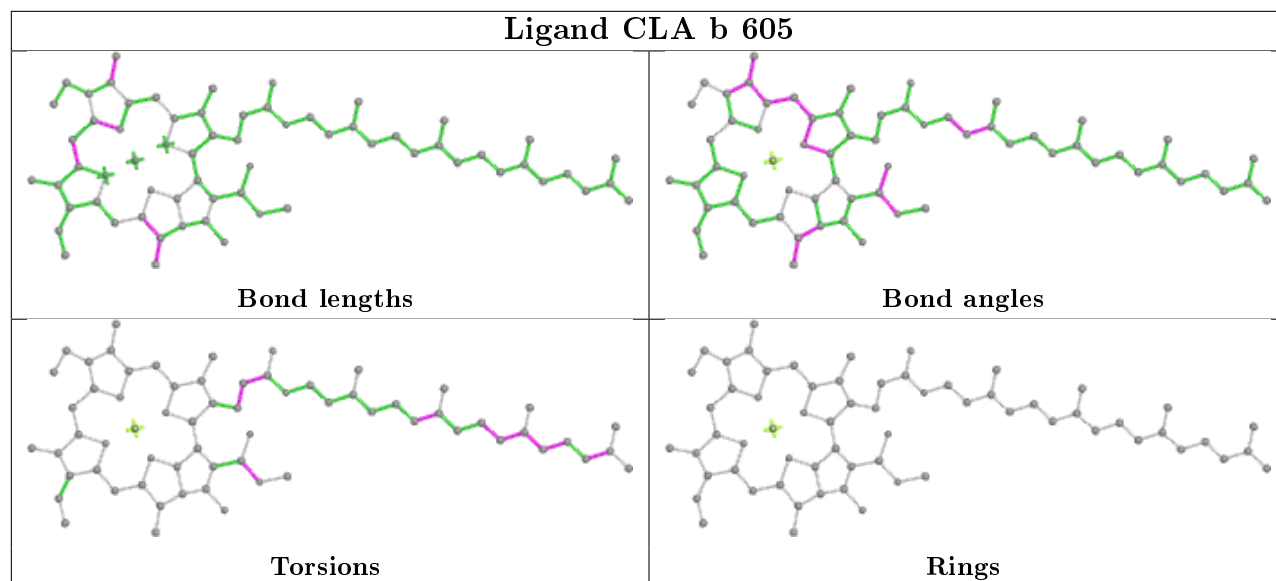
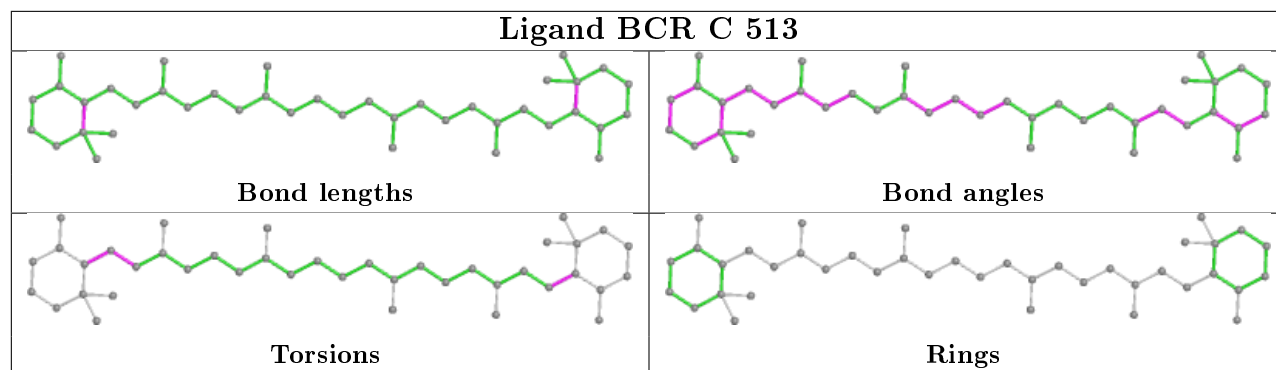


Ligand CLA B 610

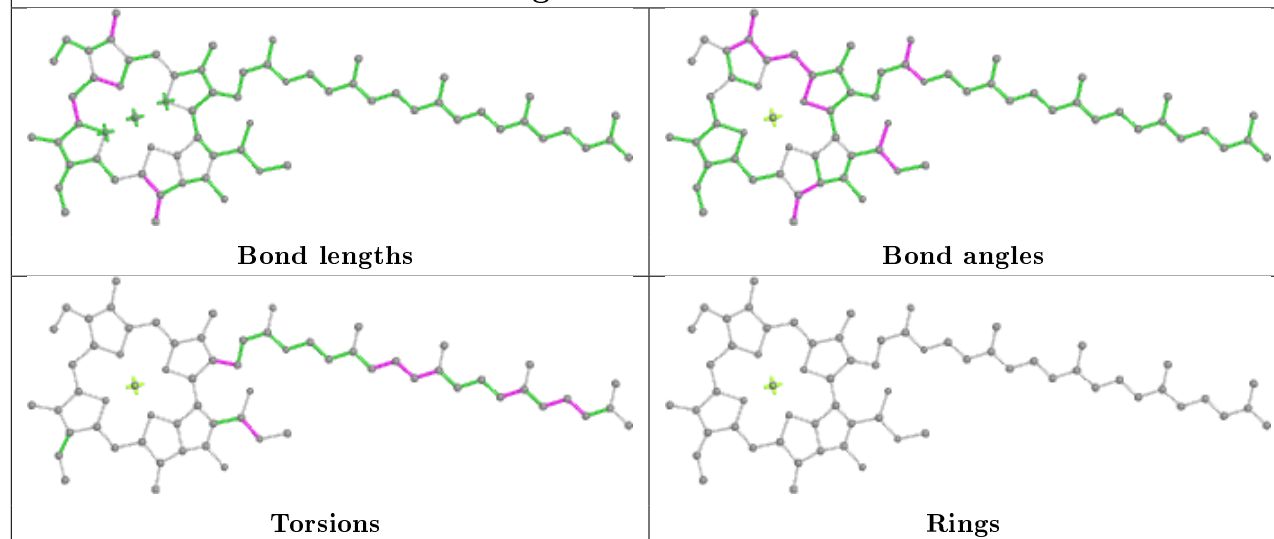


Ligand SQD F 103

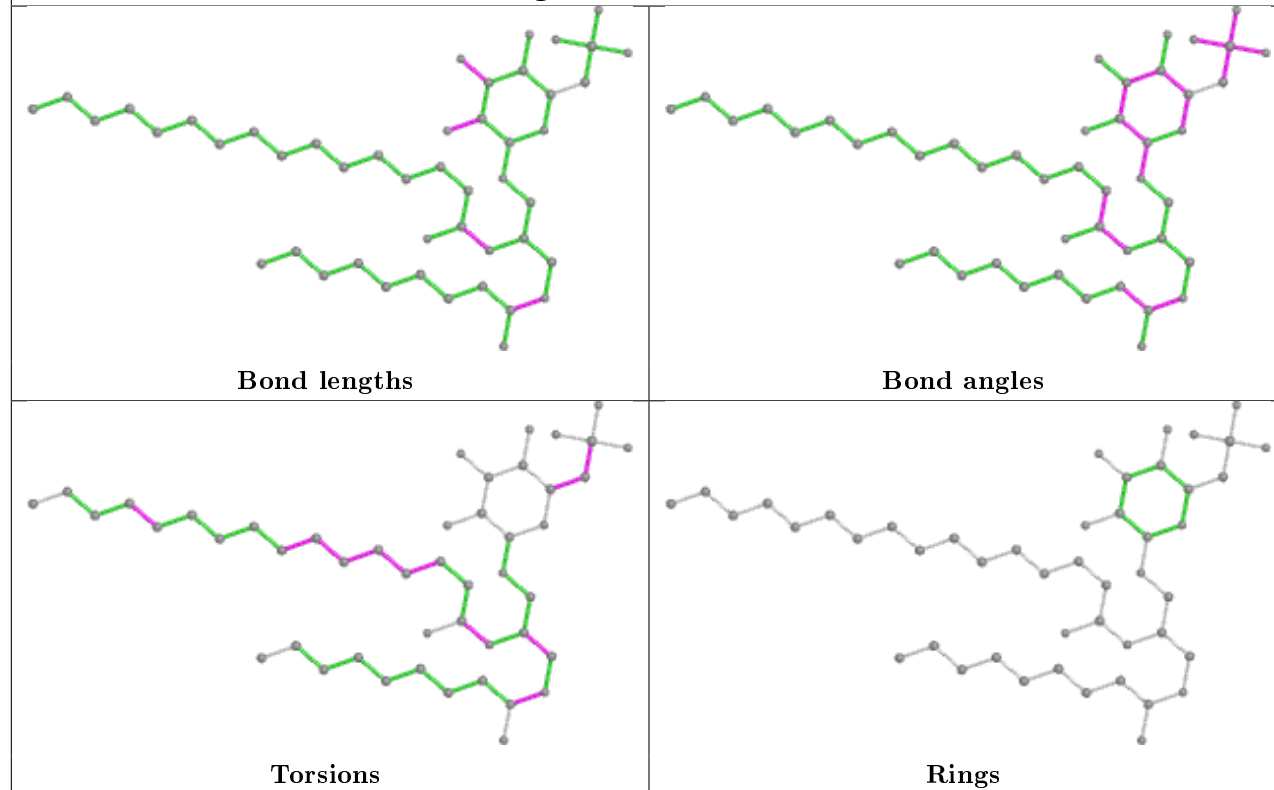




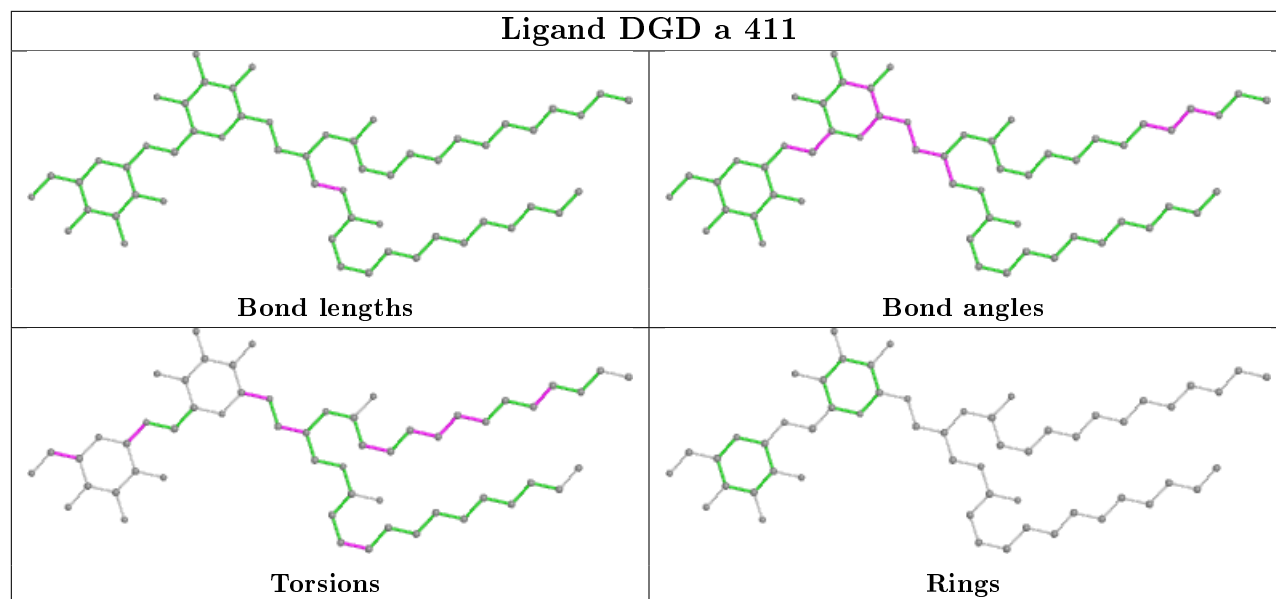
Ligand CLA B 607



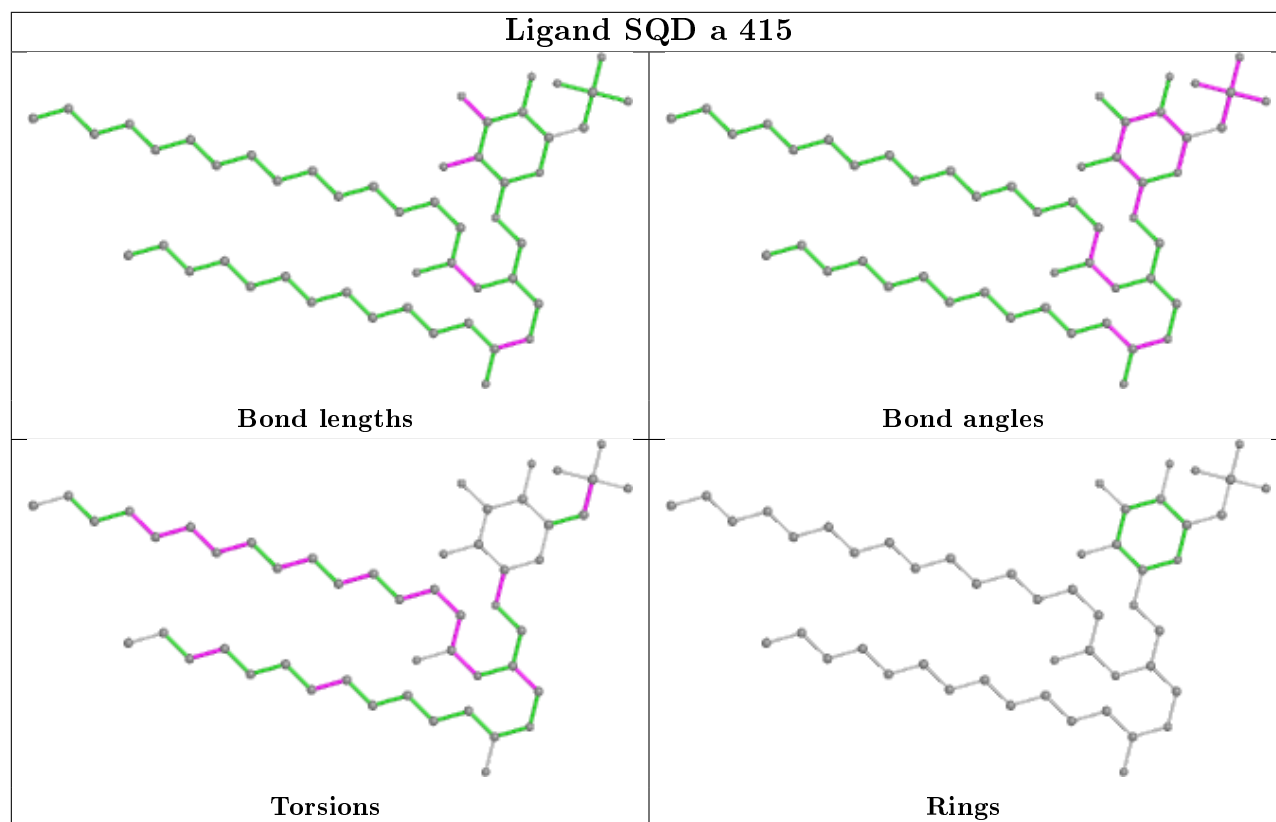
Ligand SQD B 626

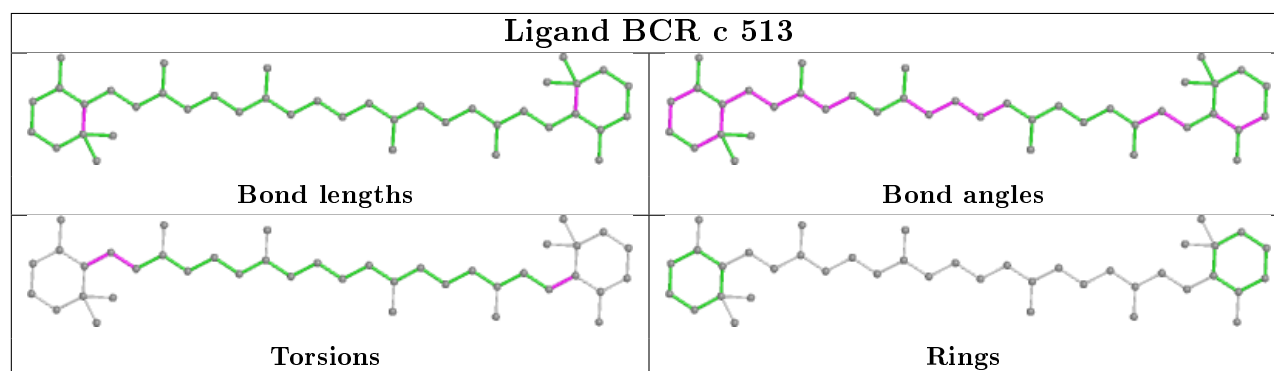
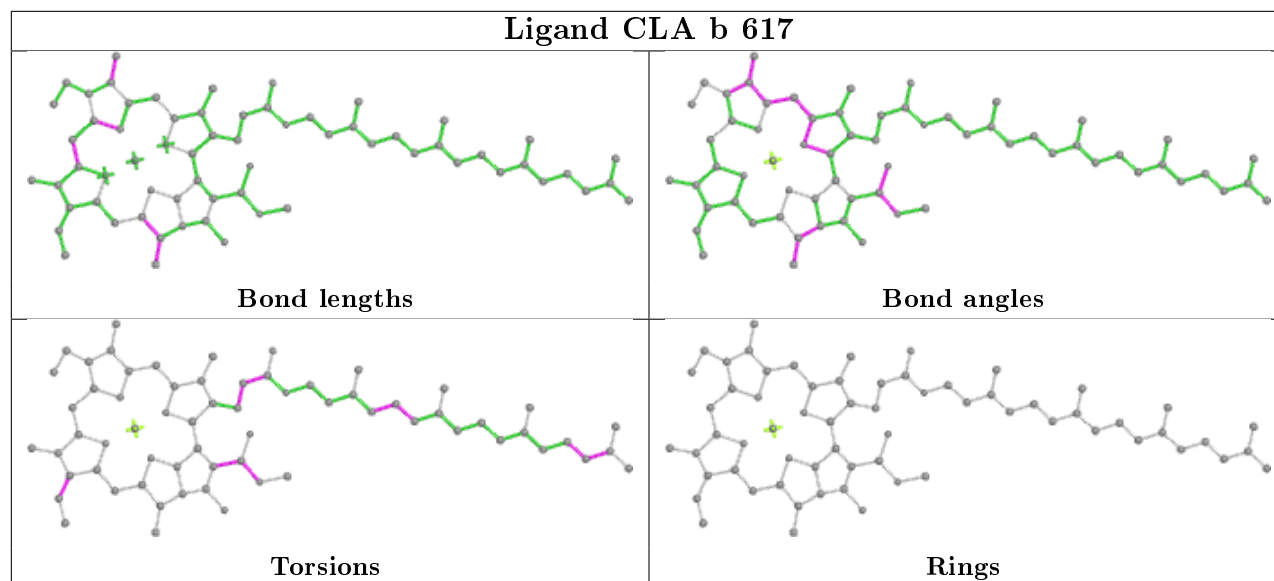
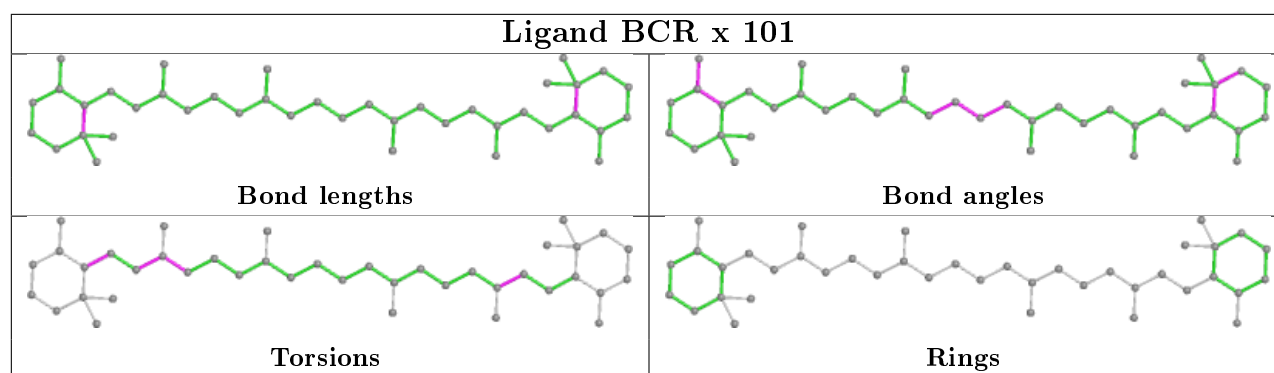


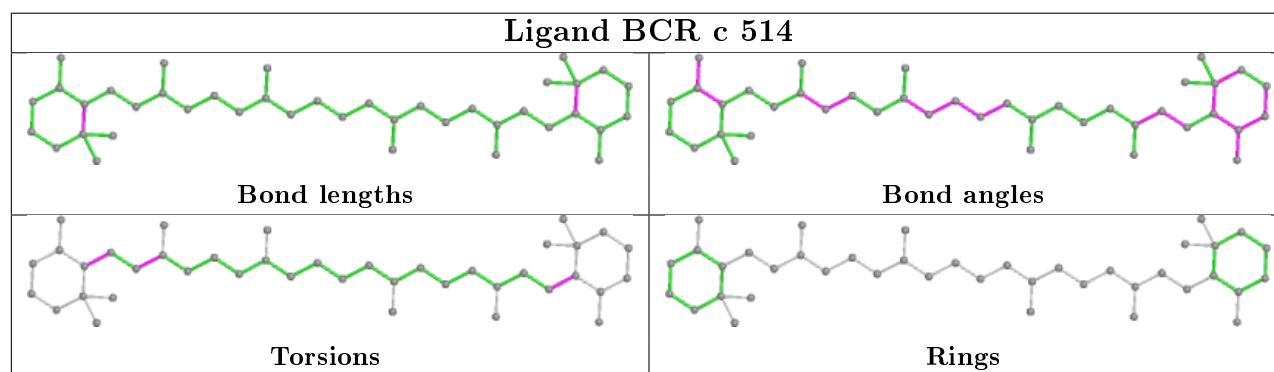
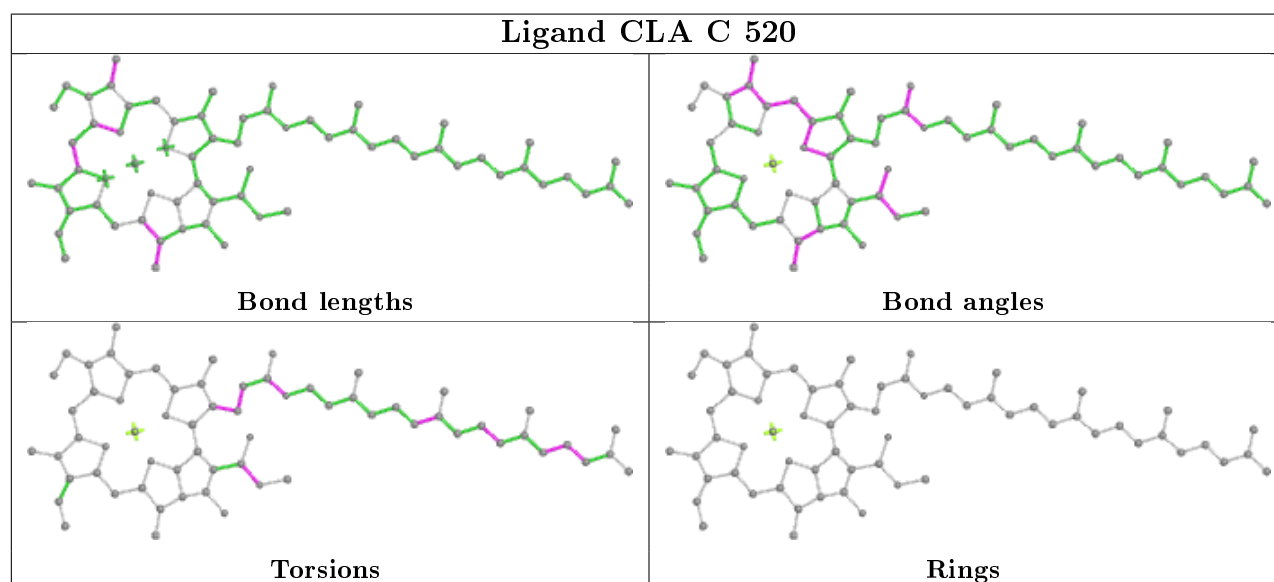
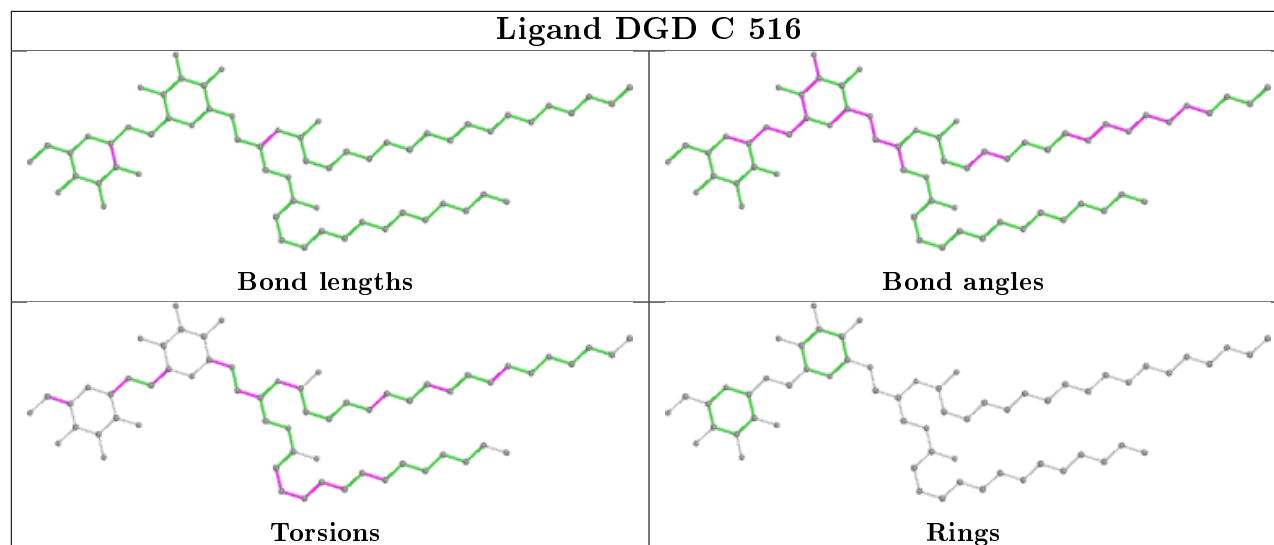
Ligand DGD a 411

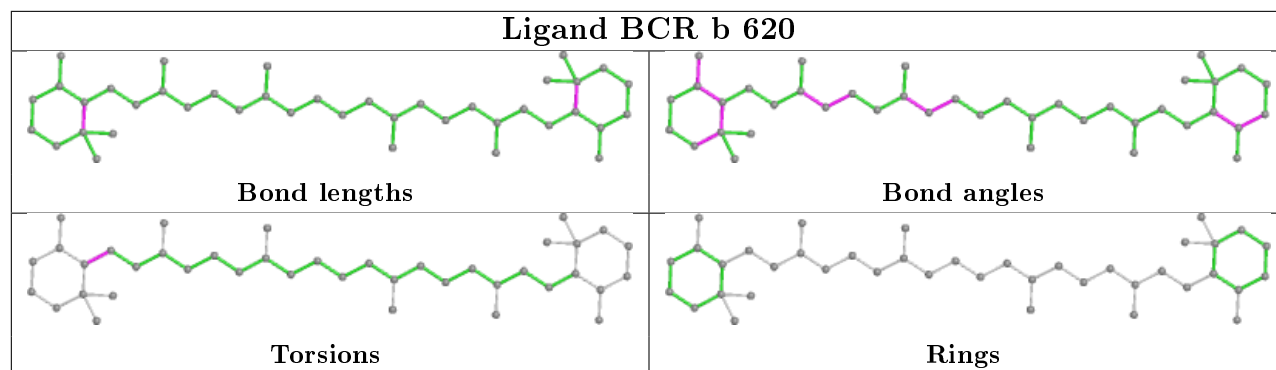
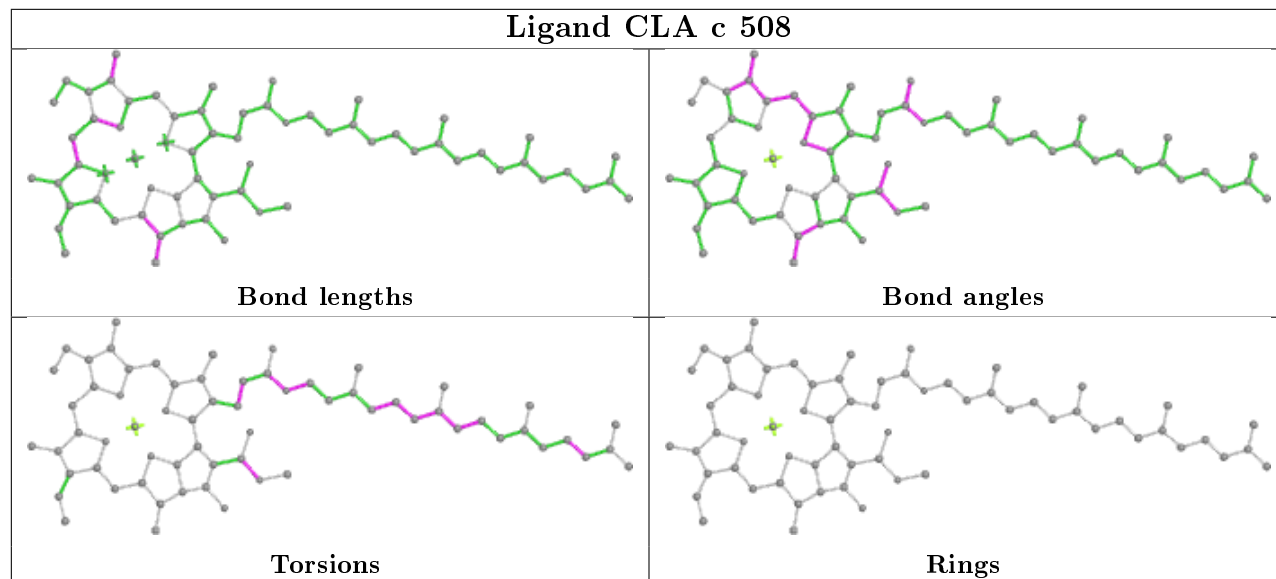
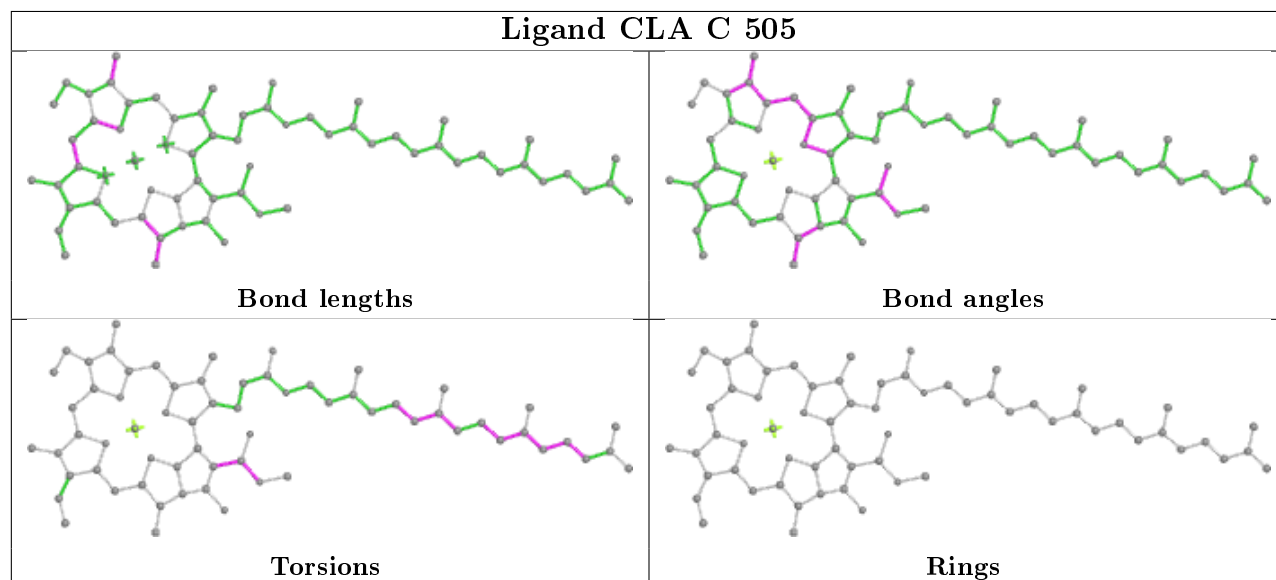


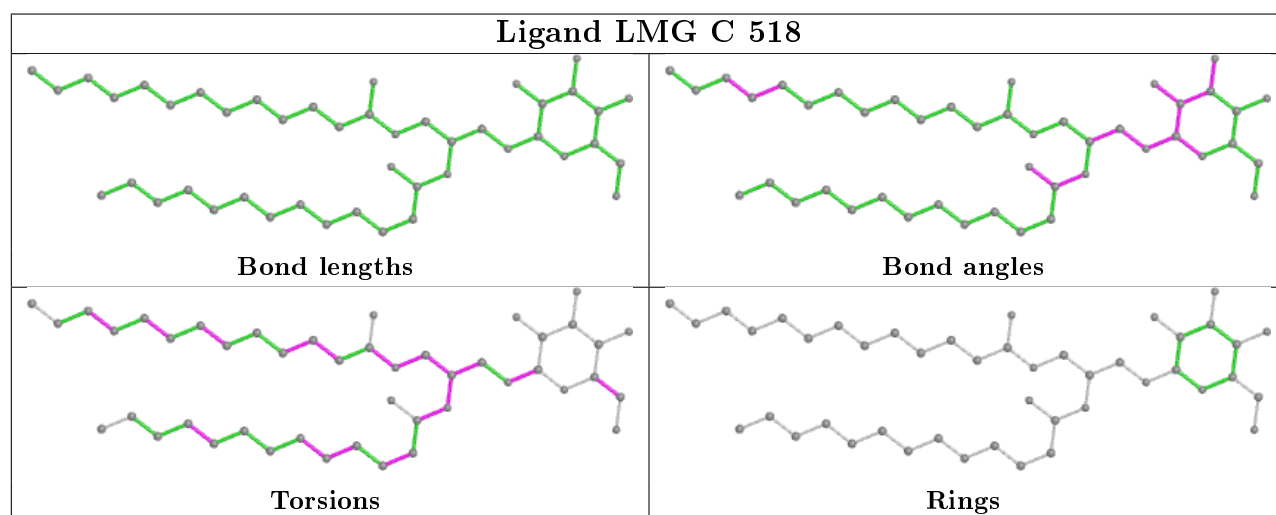
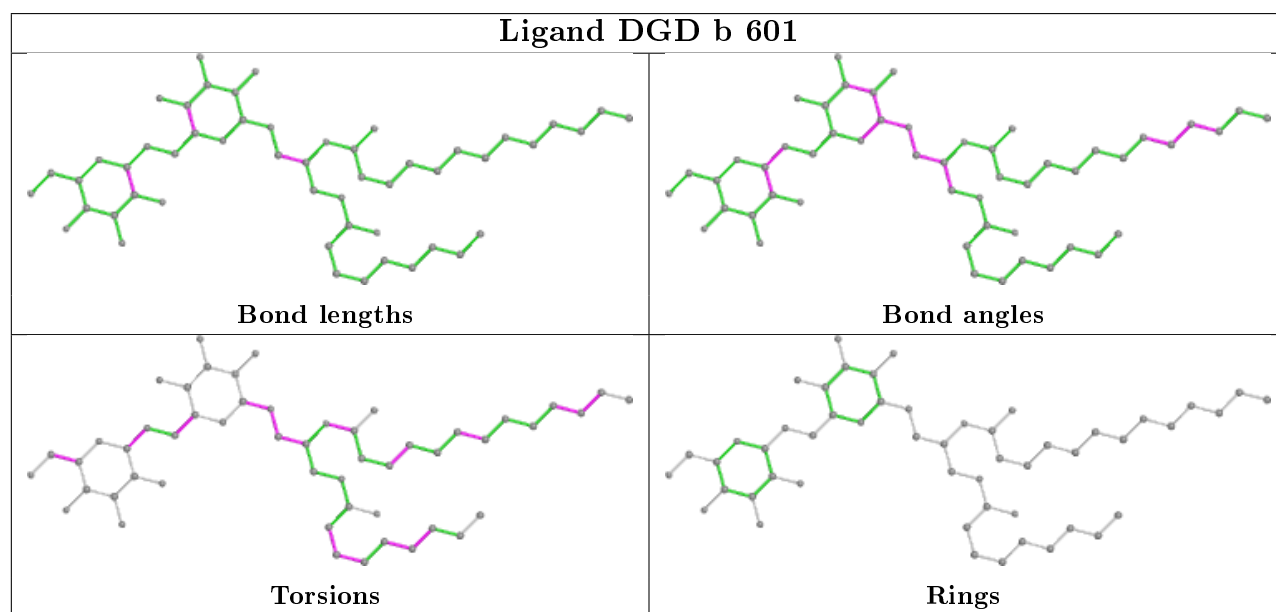
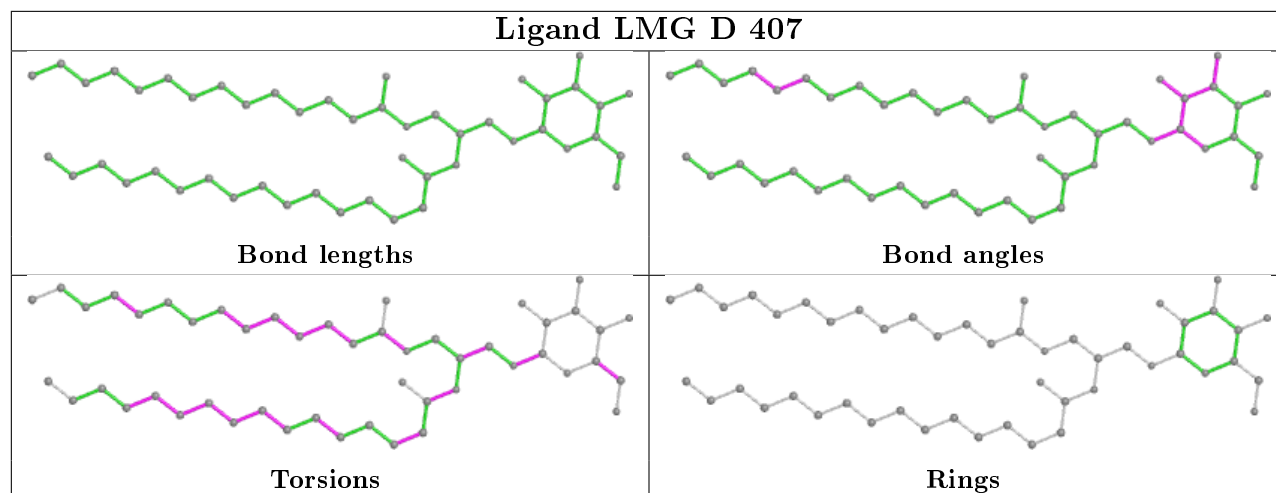
Ligand SQD a 415

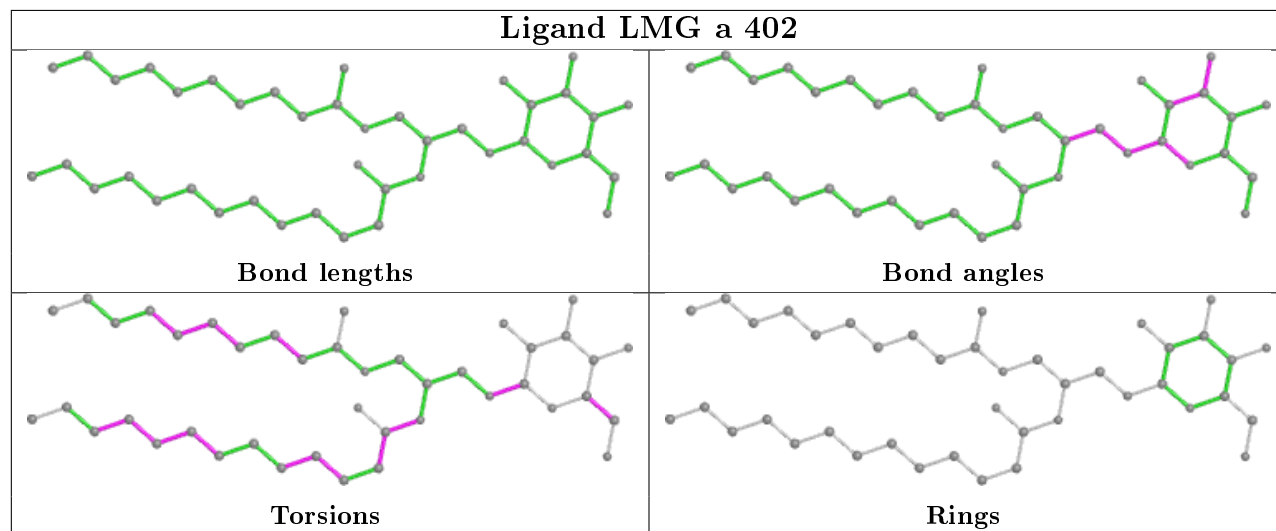
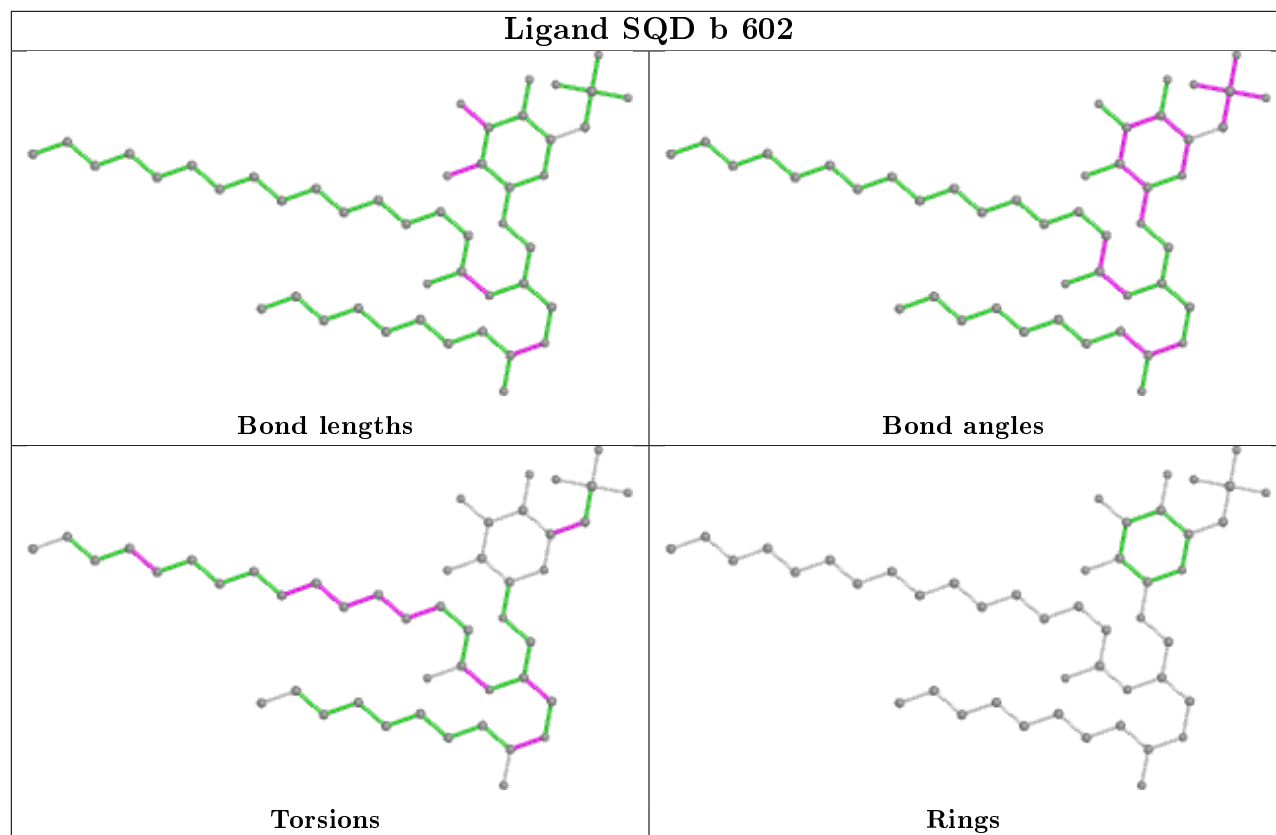




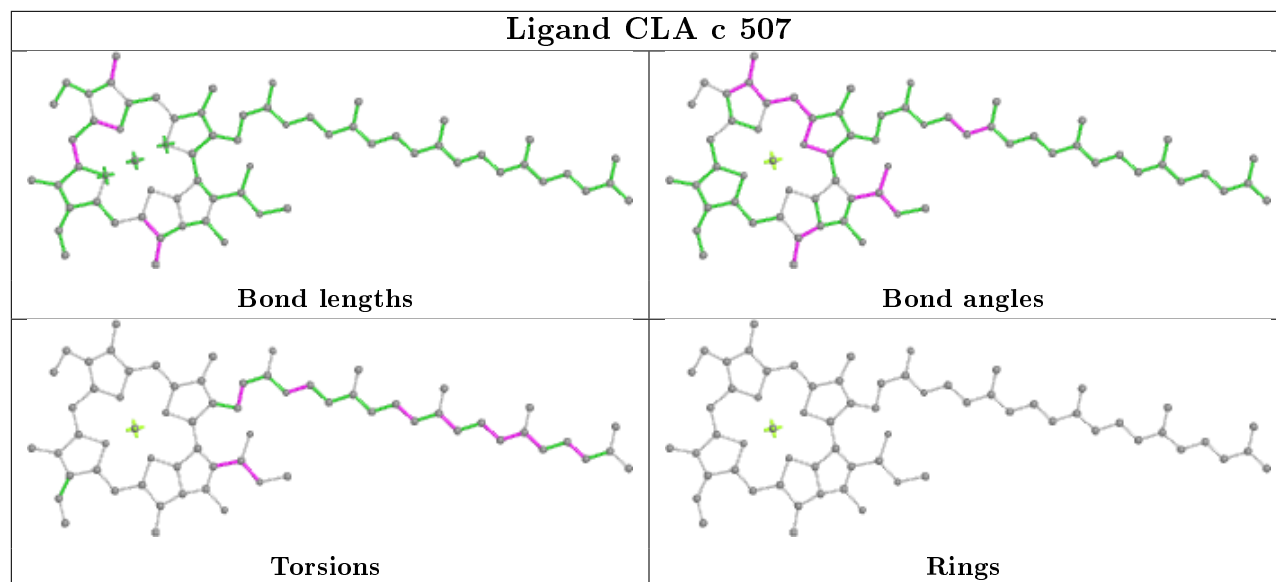


Ligand BCR b 620**Ligand CLA c 508****Ligand CLA C 505**

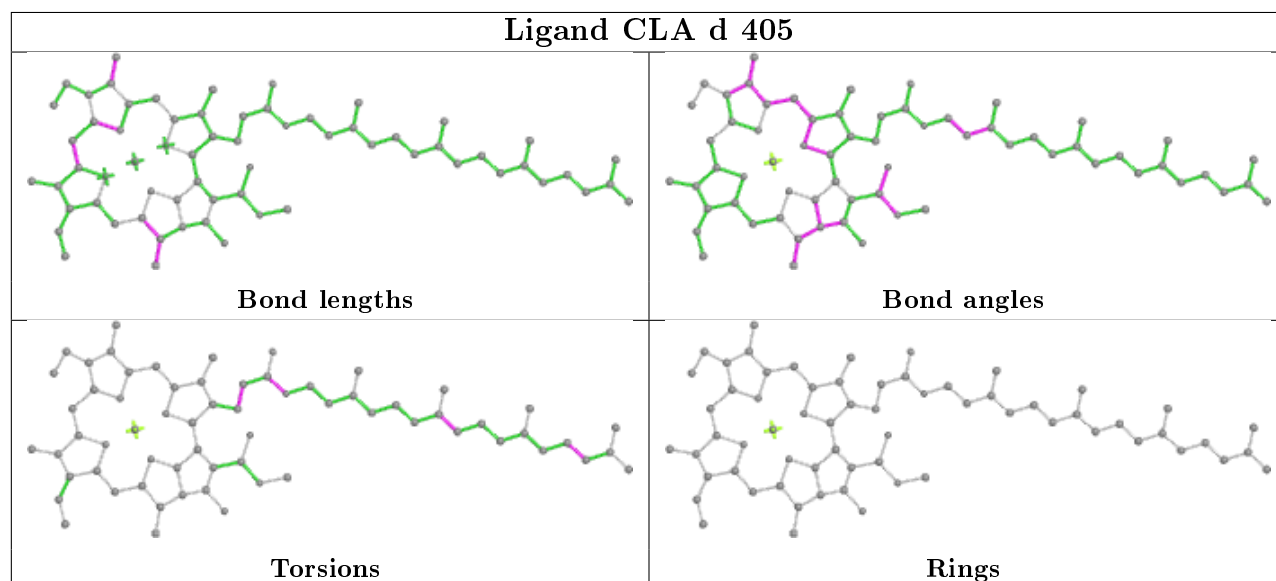




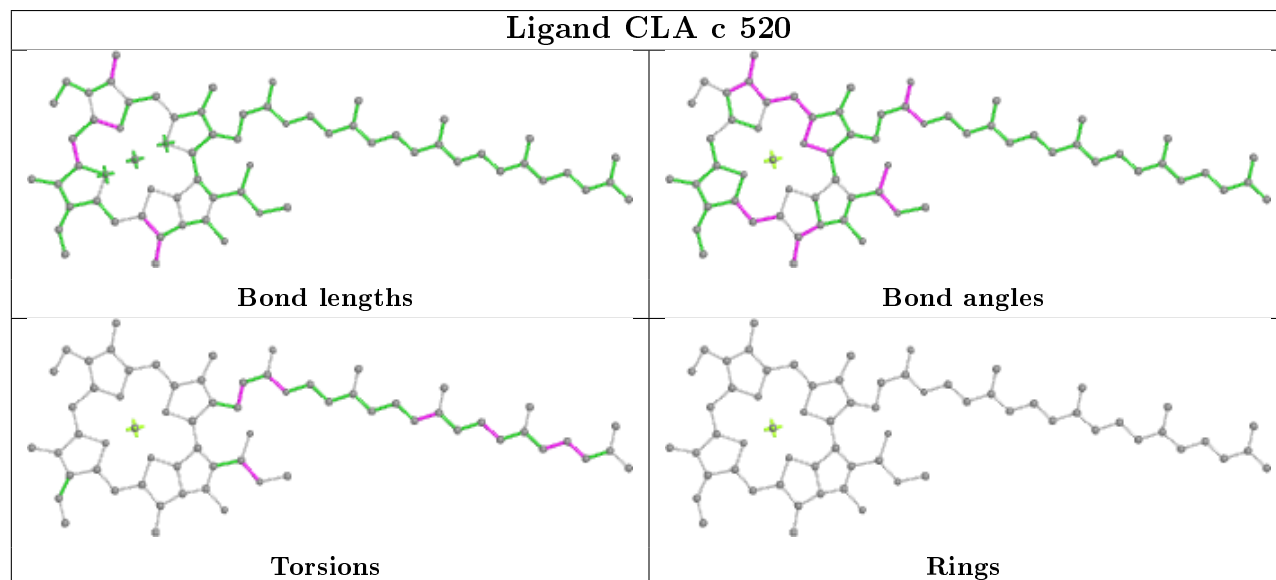
Ligand CLA c 507



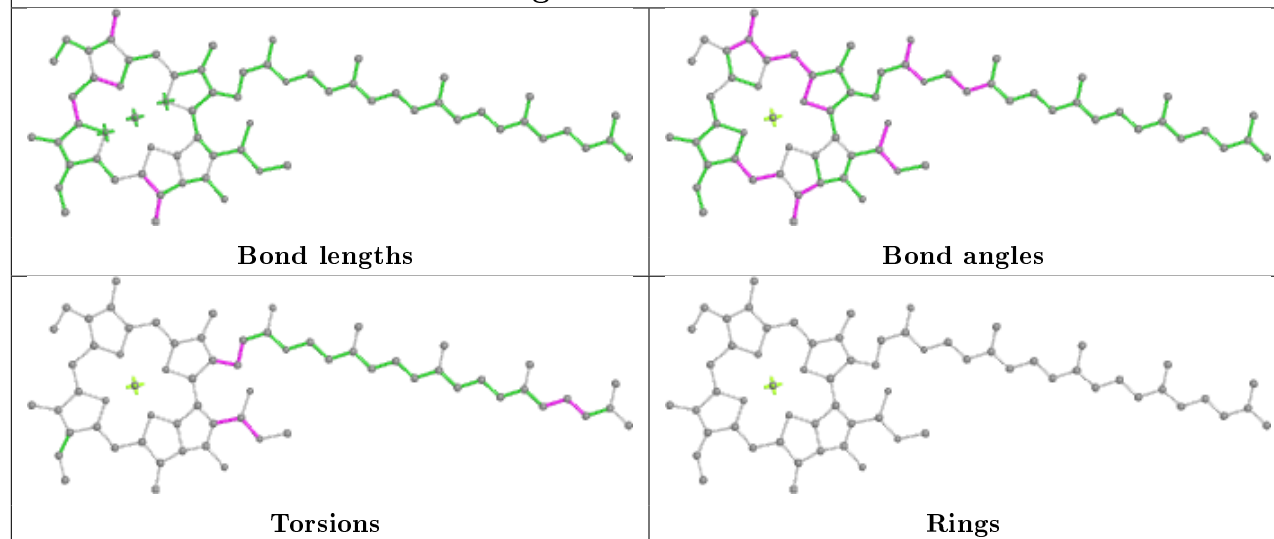
Ligand CLA d 405



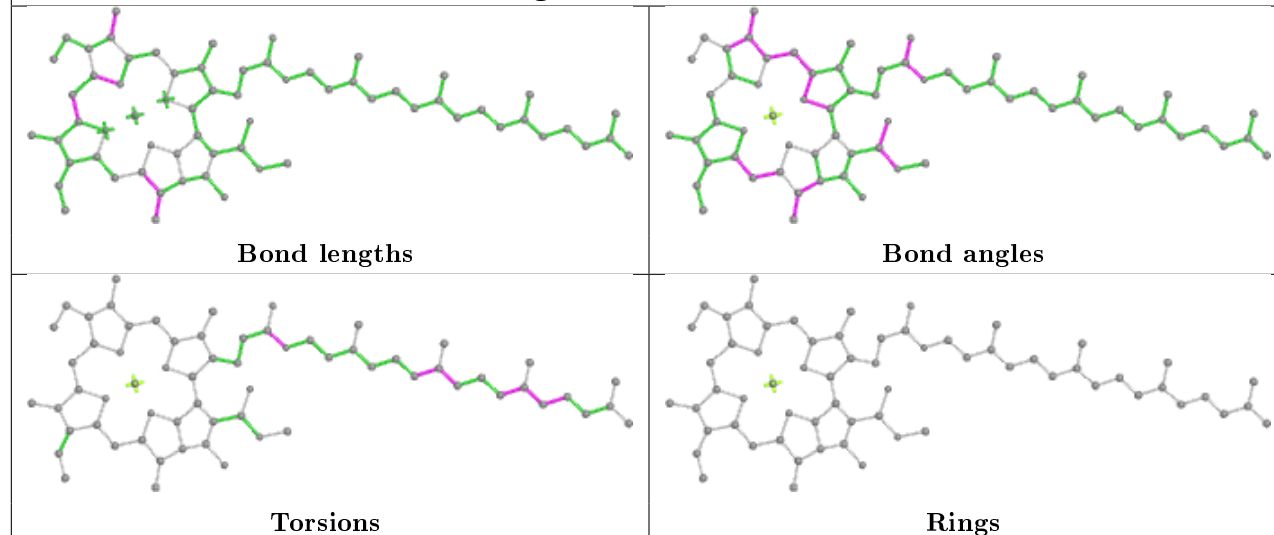
Ligand CLA c 520



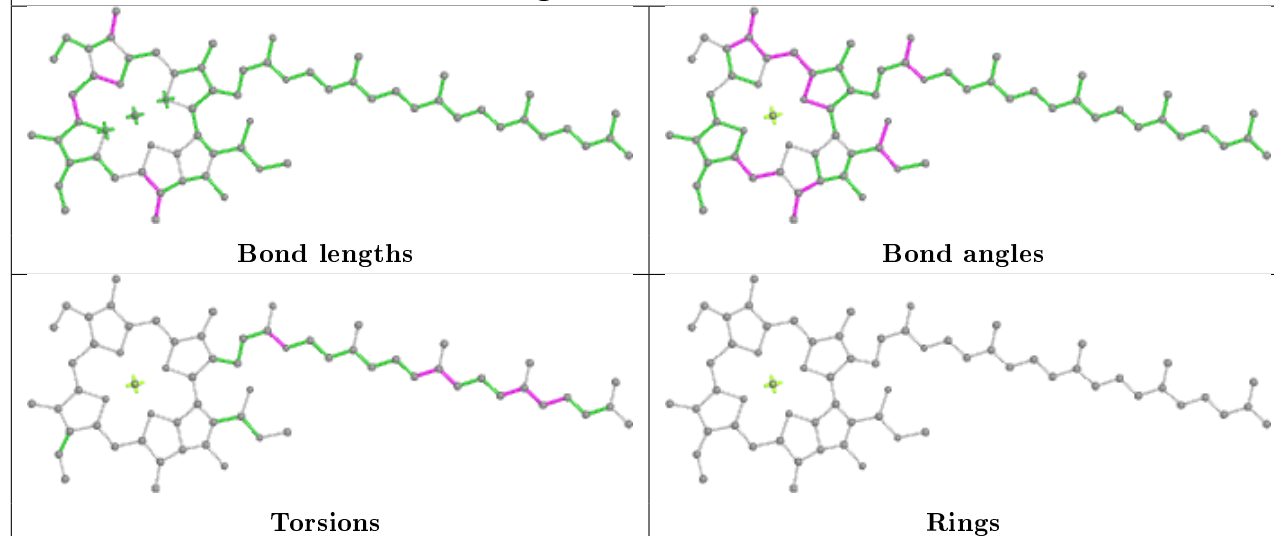
Ligand CLA B 606

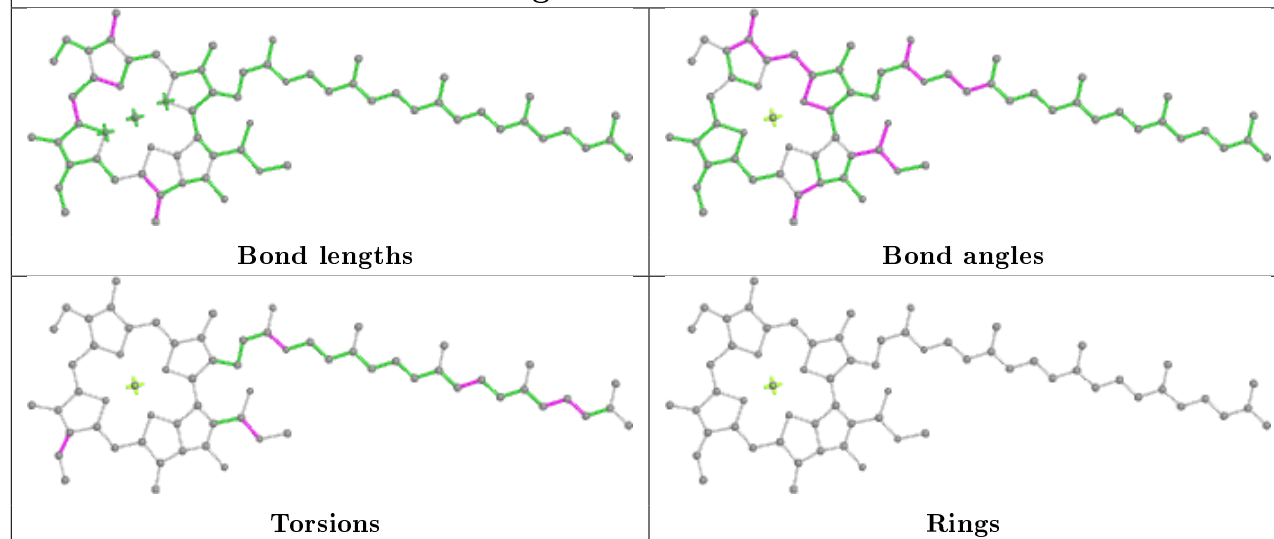
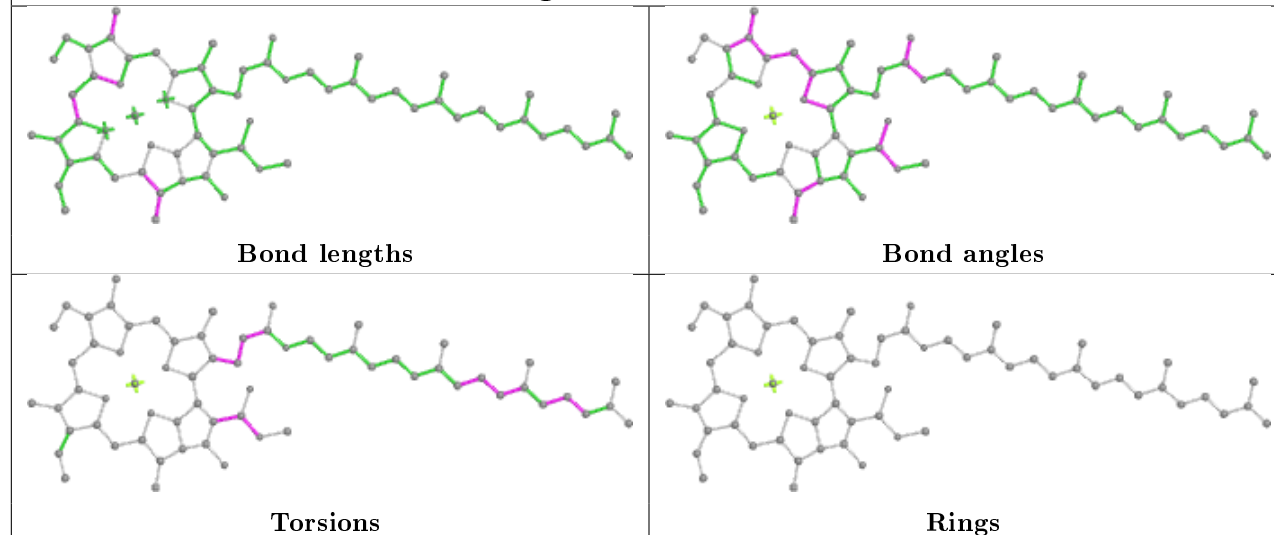
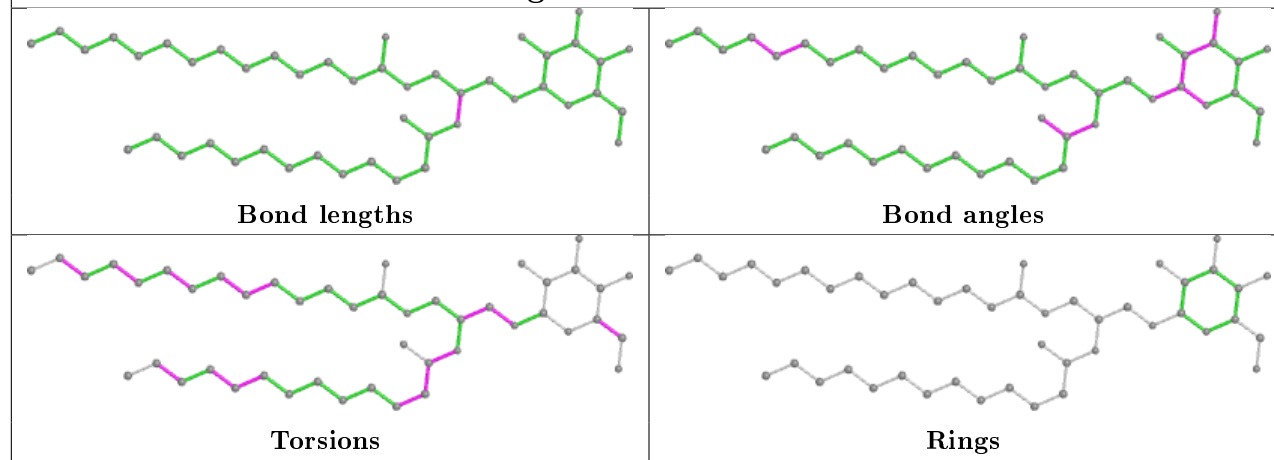


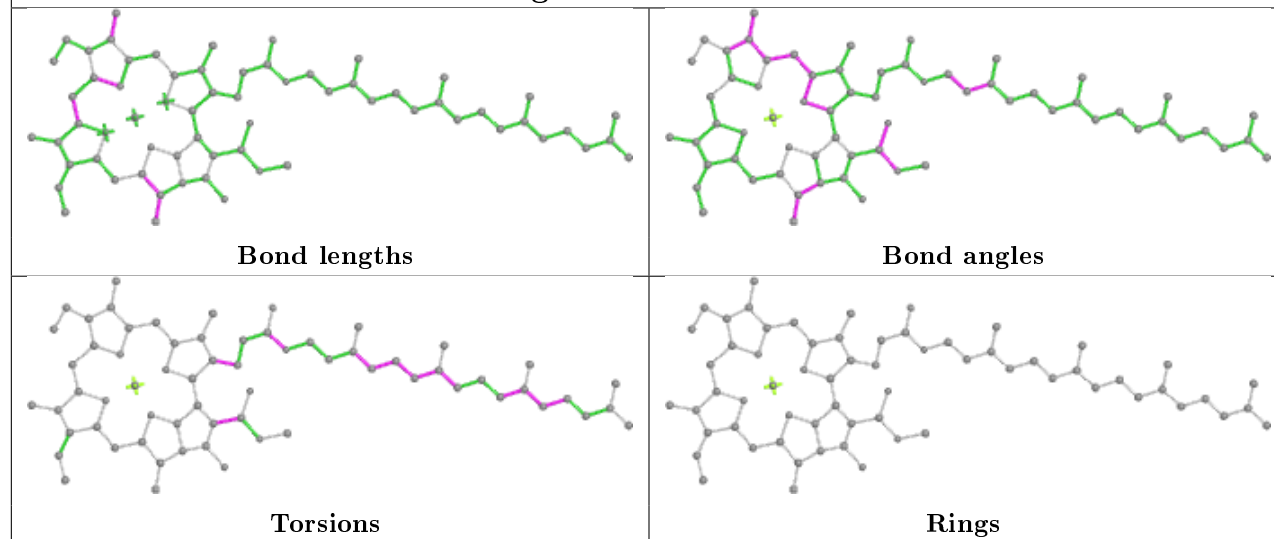
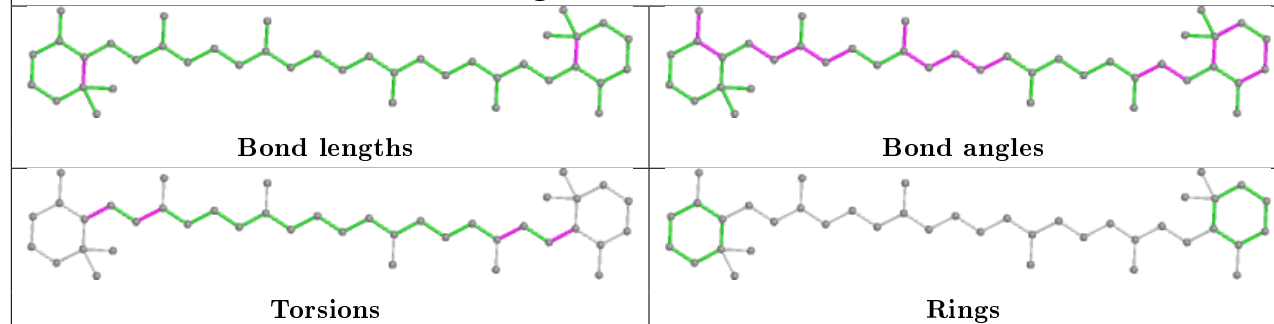
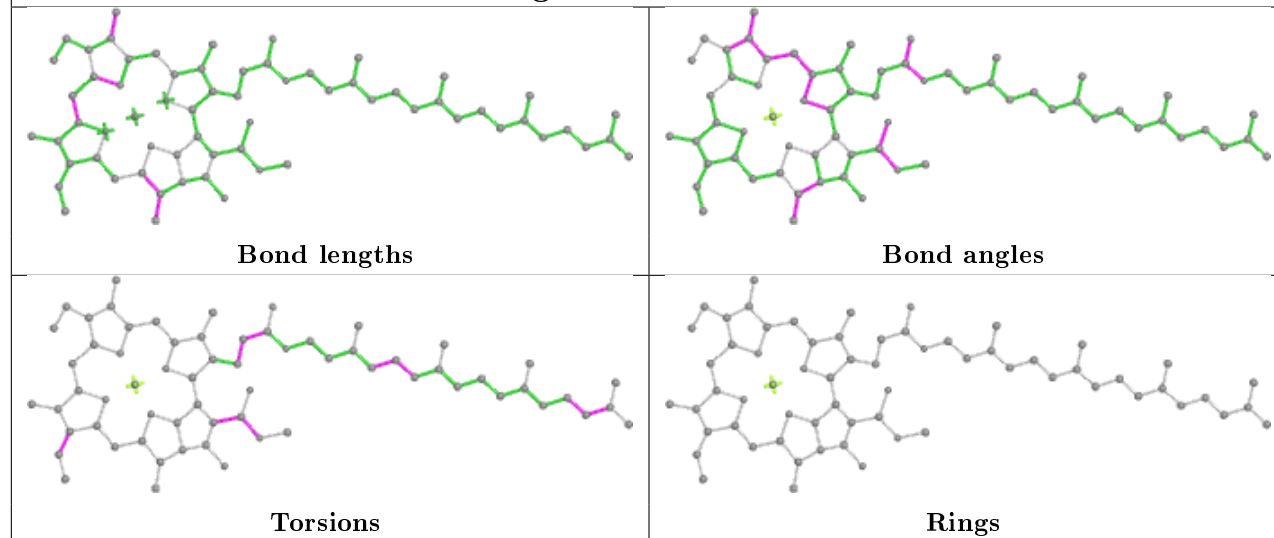
Ligand CLA B 614

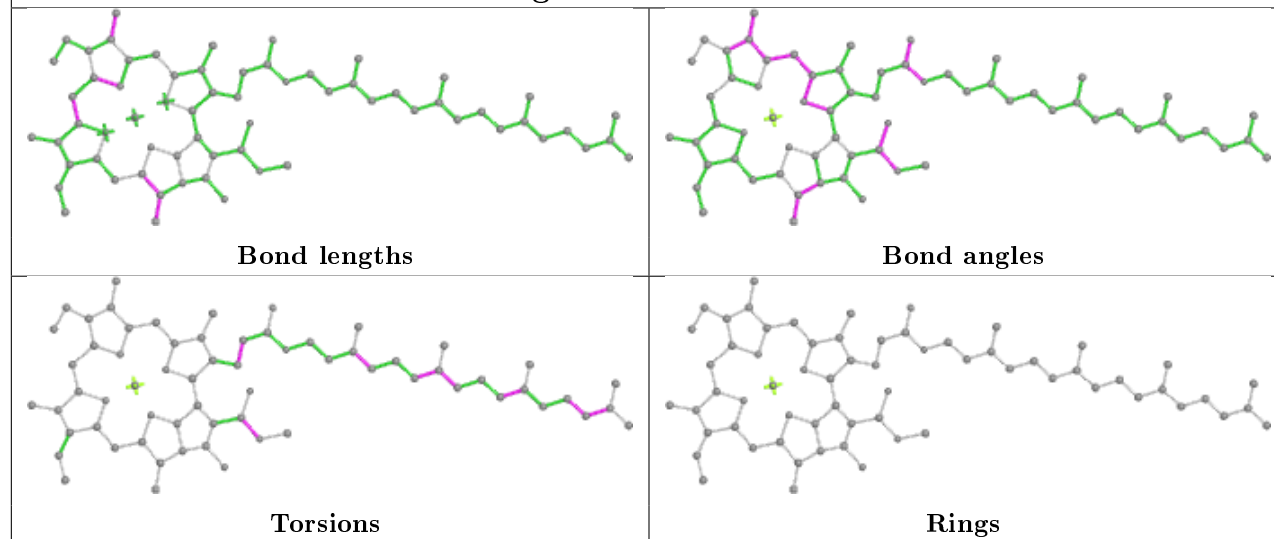
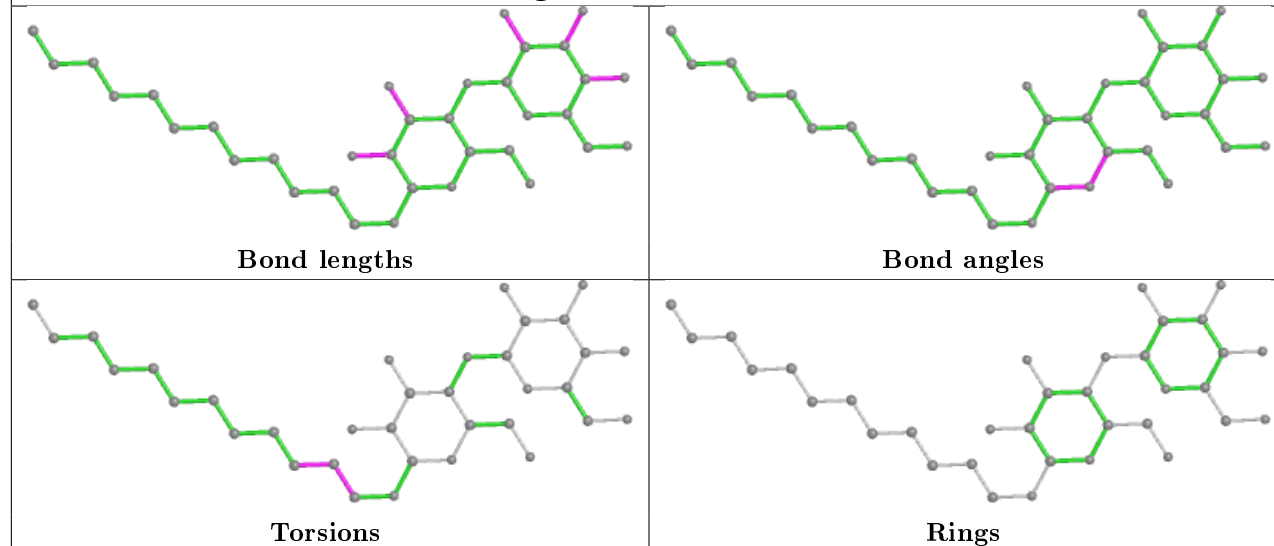
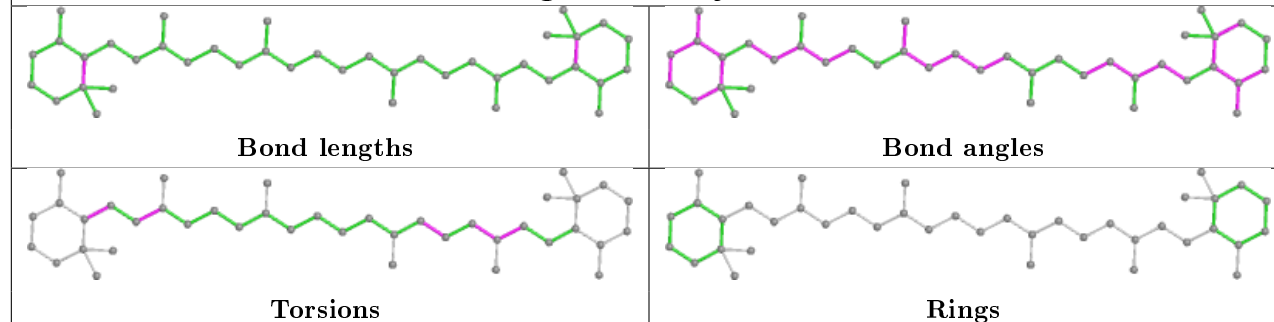


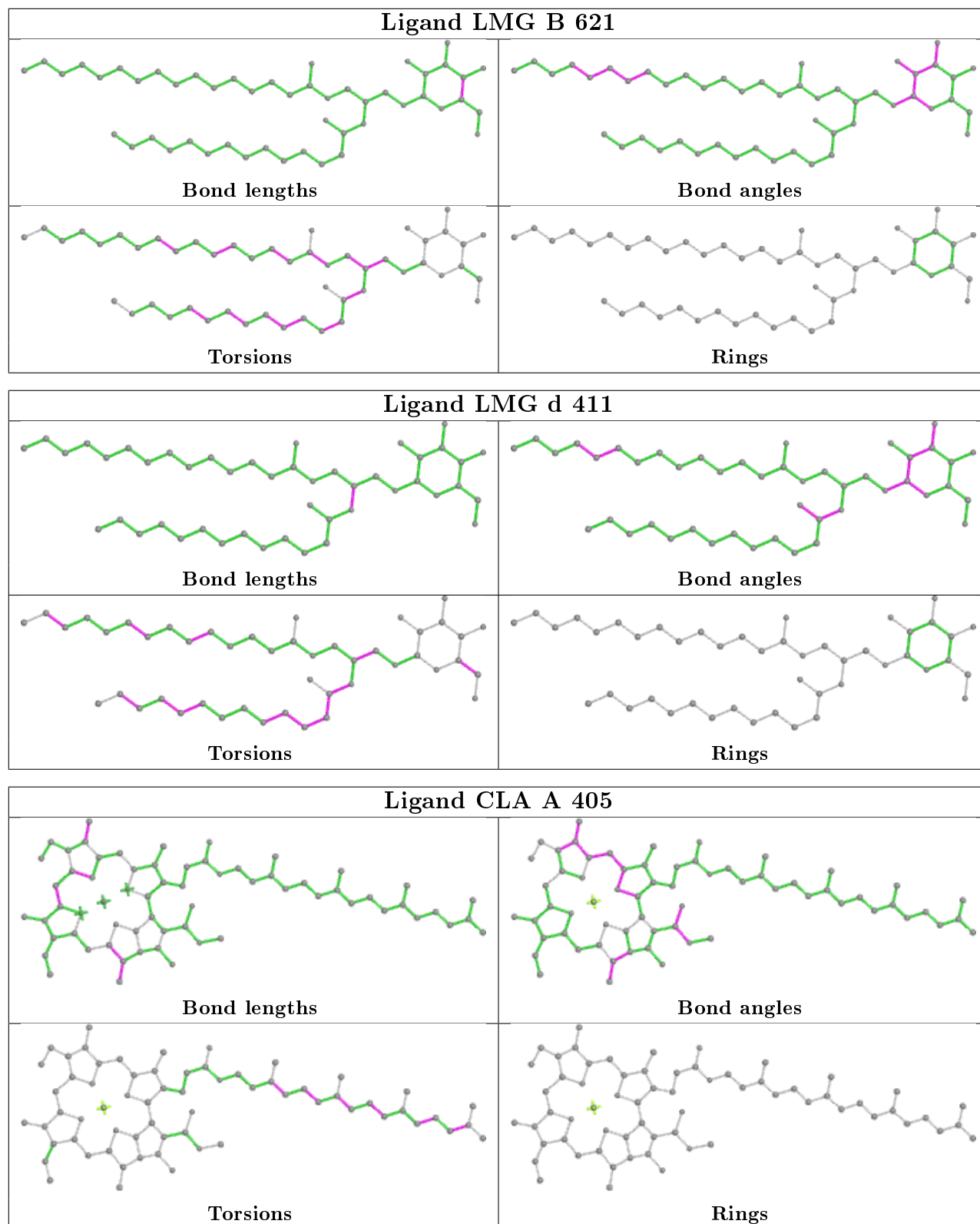
Ligand CLA b 618

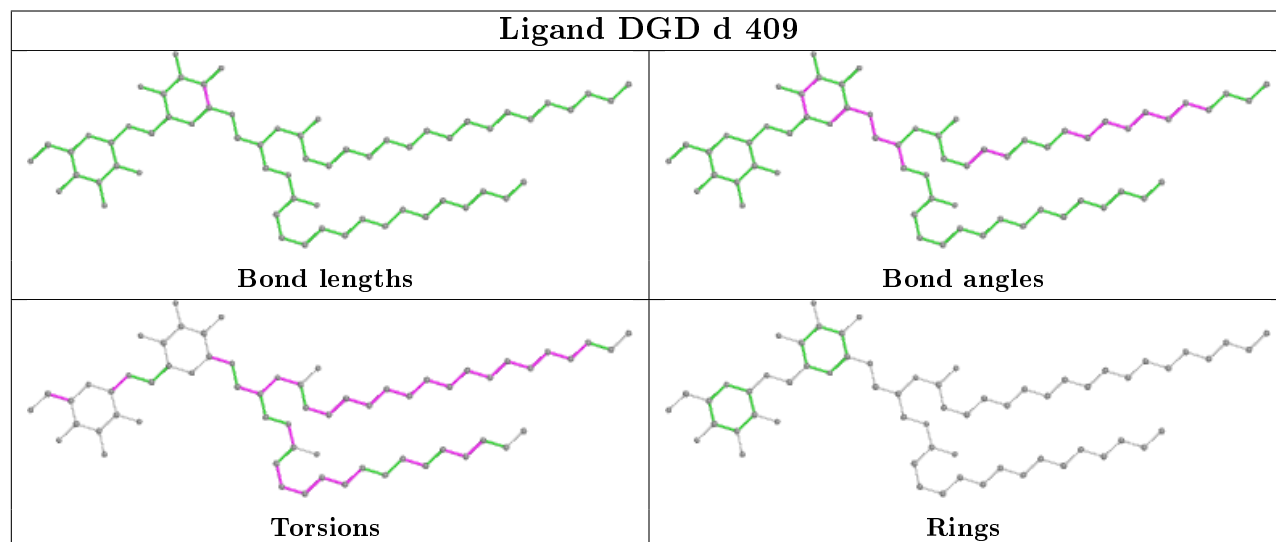
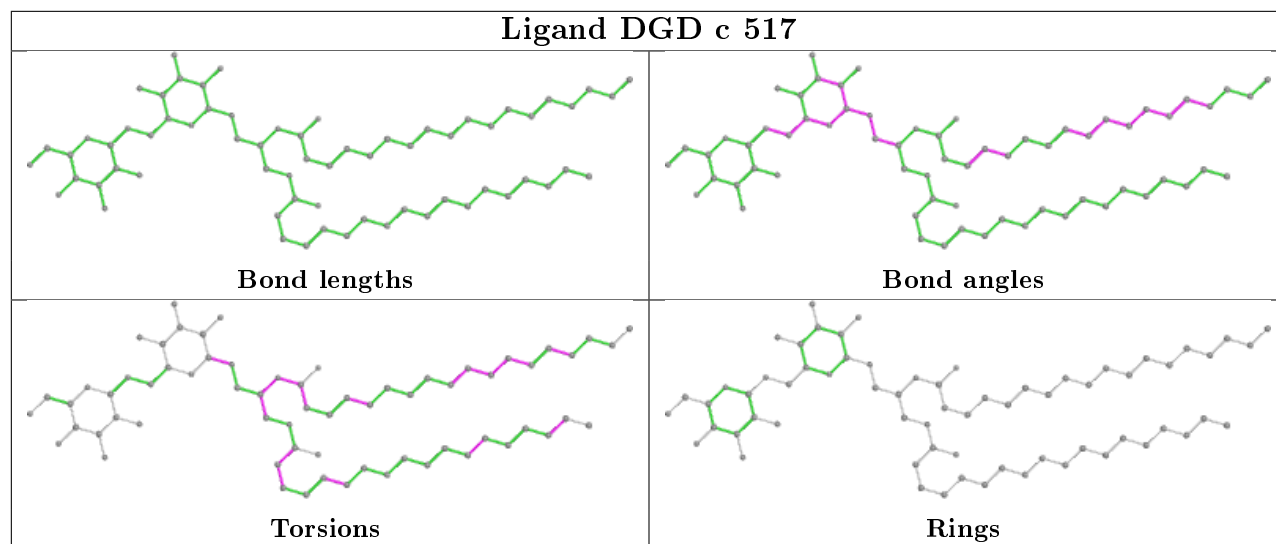
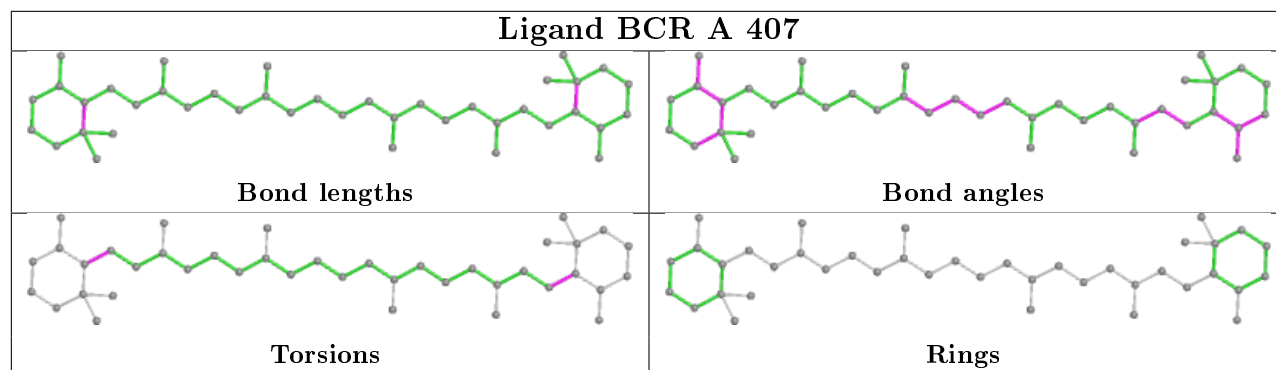


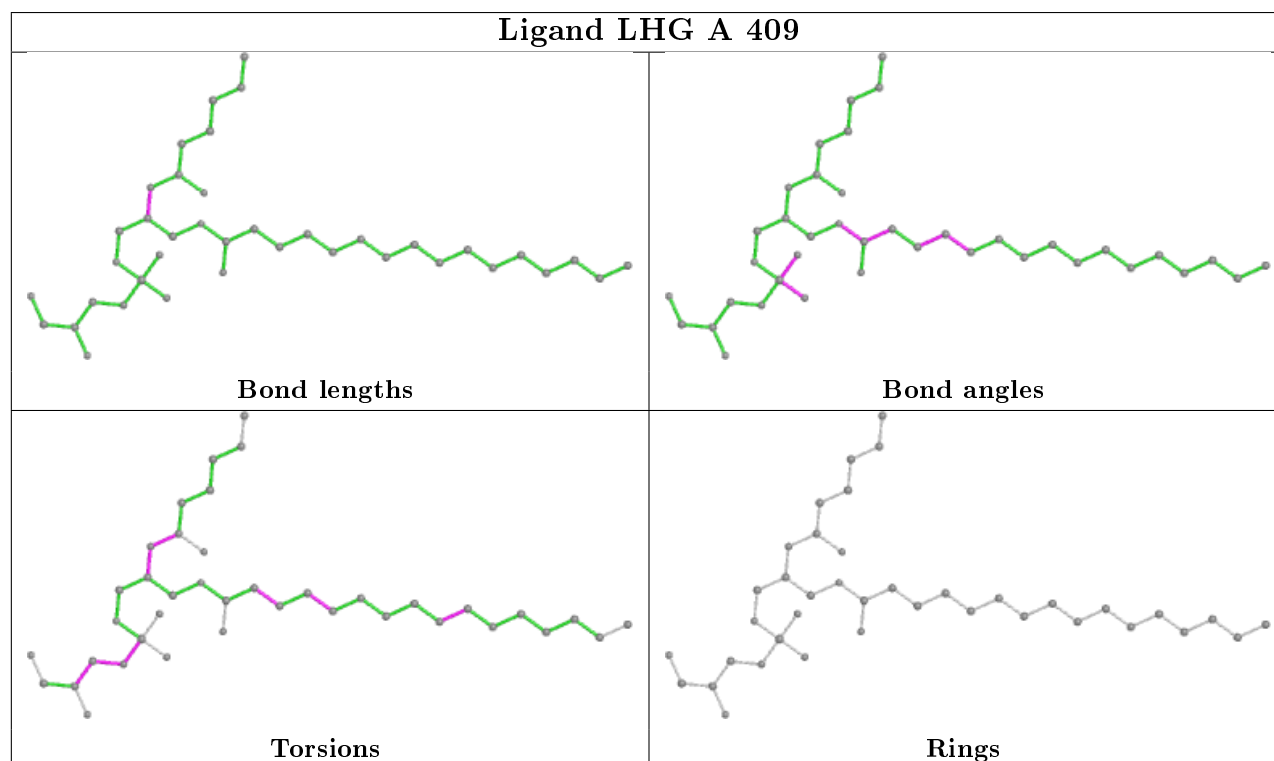
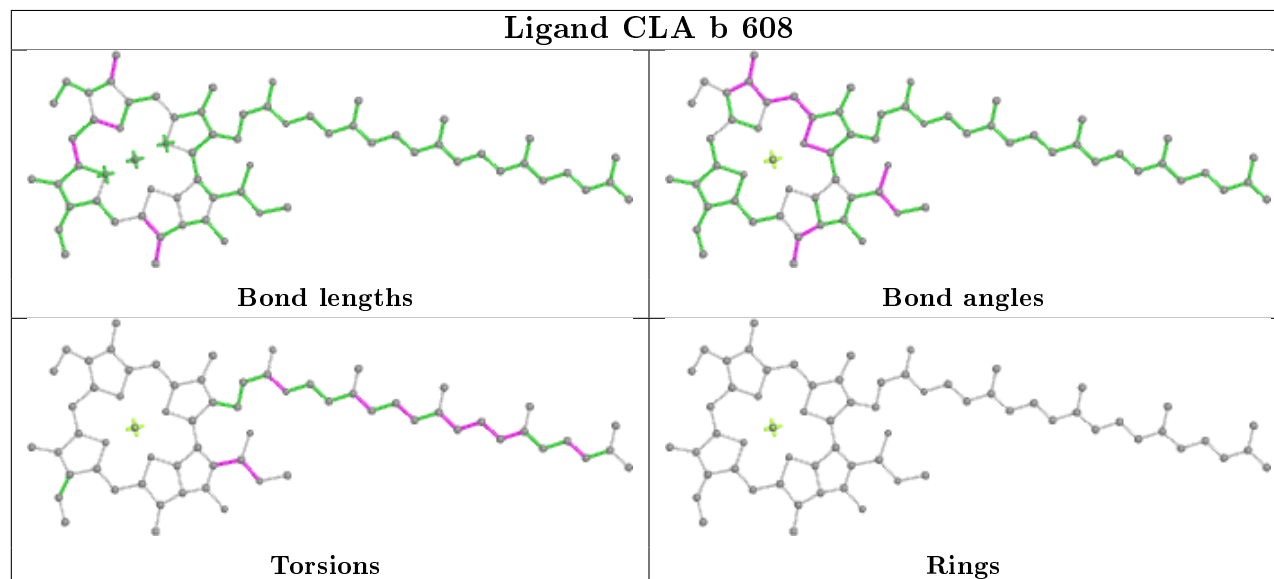
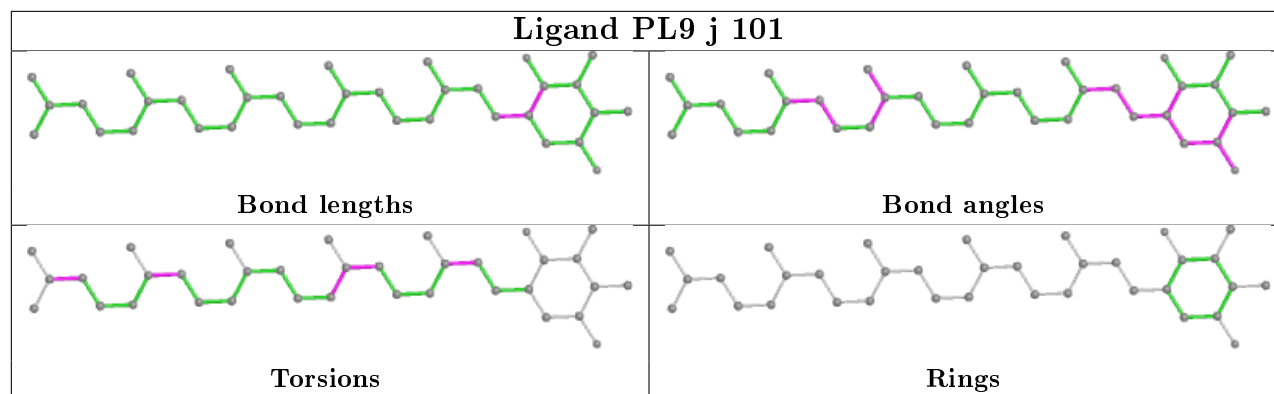
Ligand CLA B 603**Ligand CLA c 501****Ligand LMG D 411**

Ligand CLA H 101**Ligand BCR B 617****Ligand CLA B 613**

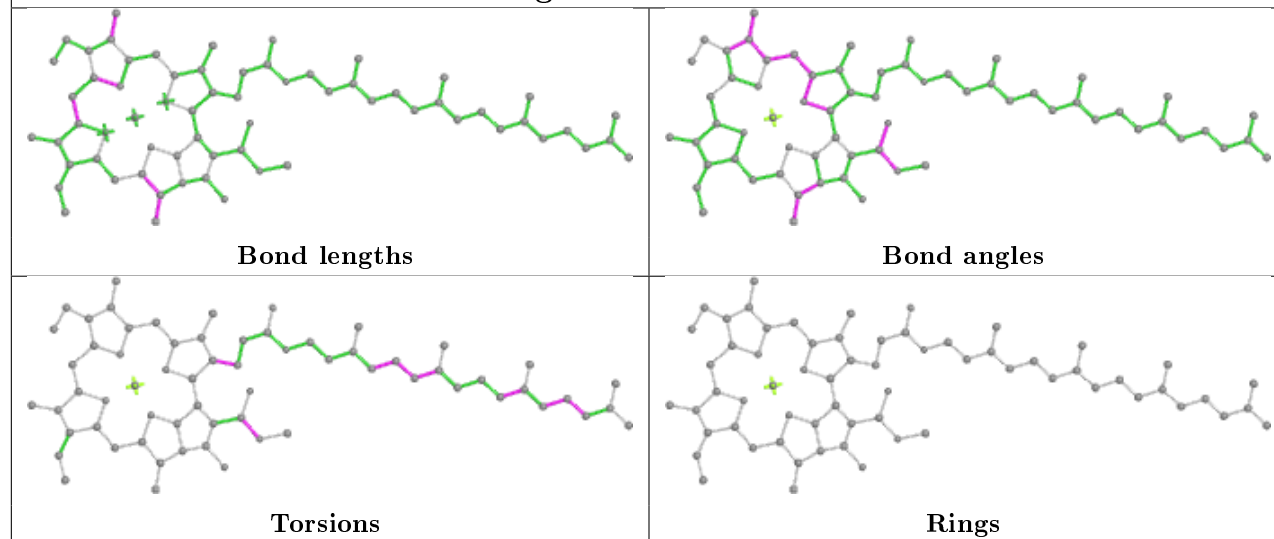
Ligand CLA B 602**Ligand LMT b 626****Ligand BCR j 102**



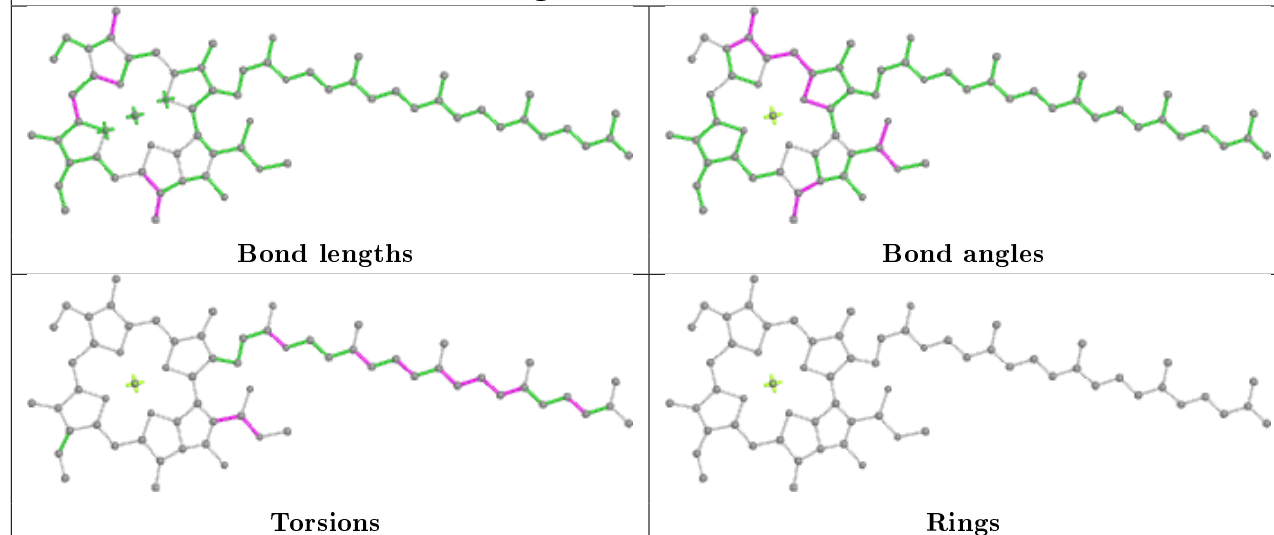




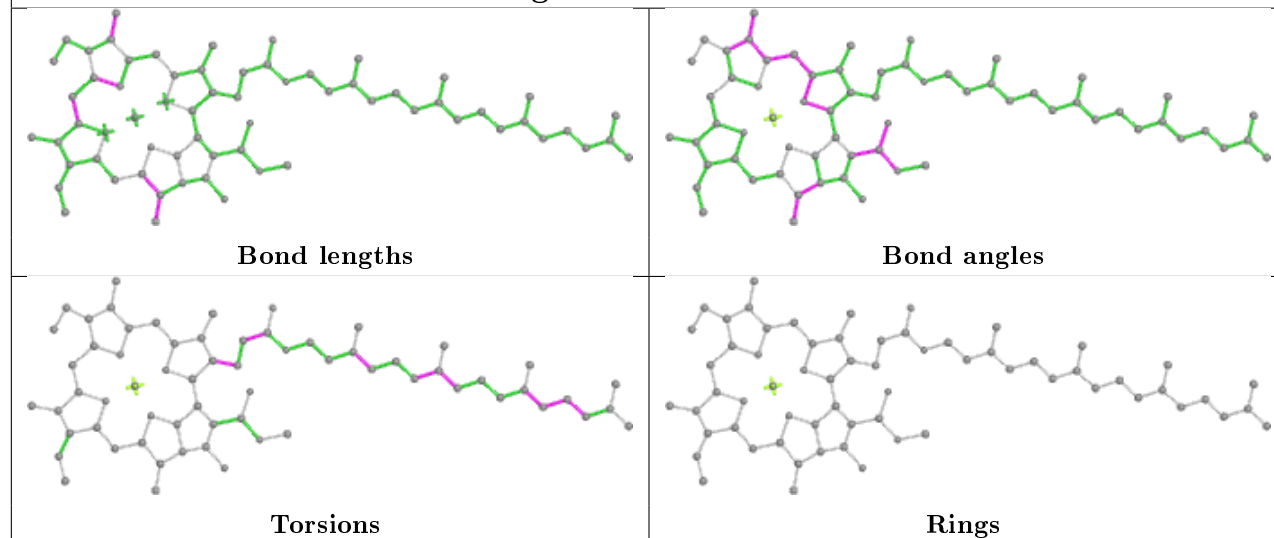
Ligand CLA b 611

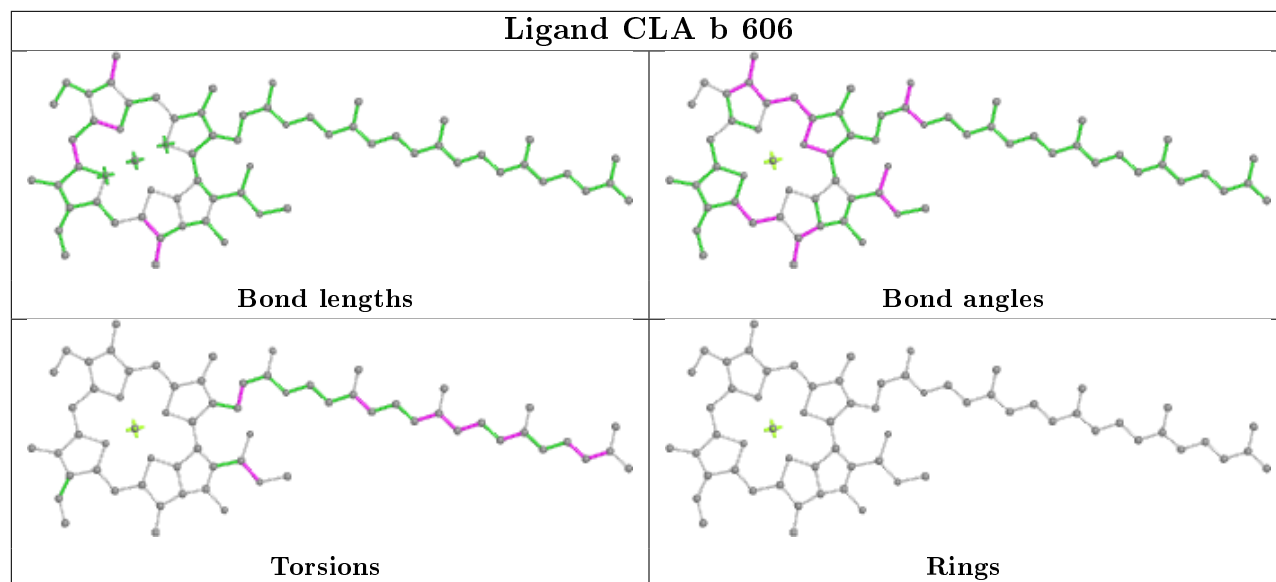
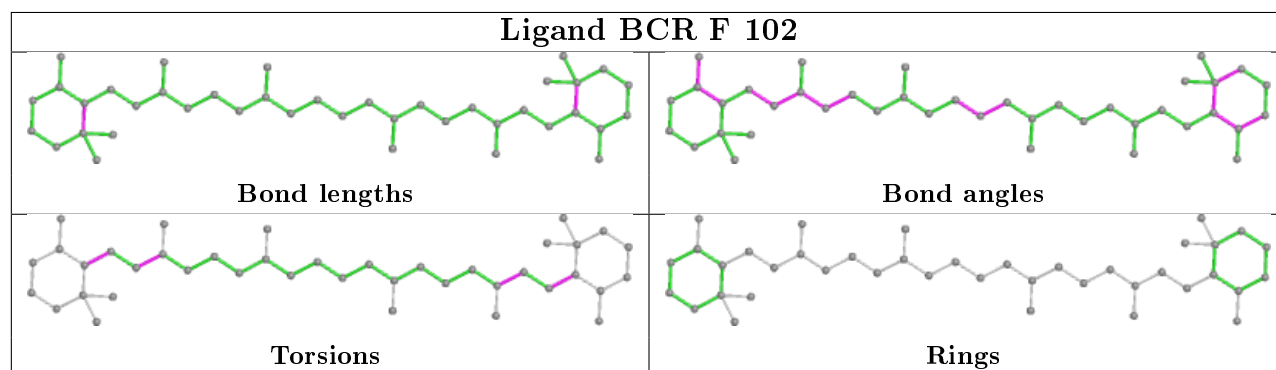
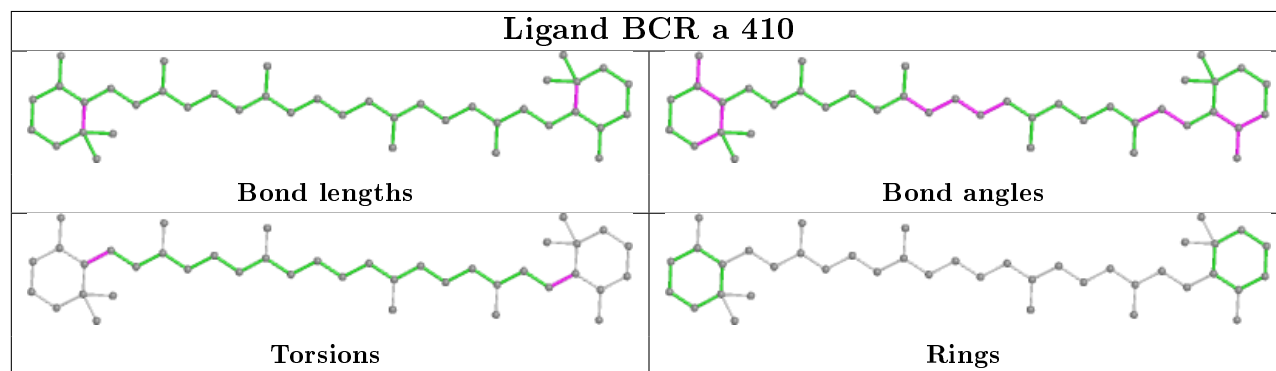


Ligand CLA B 604

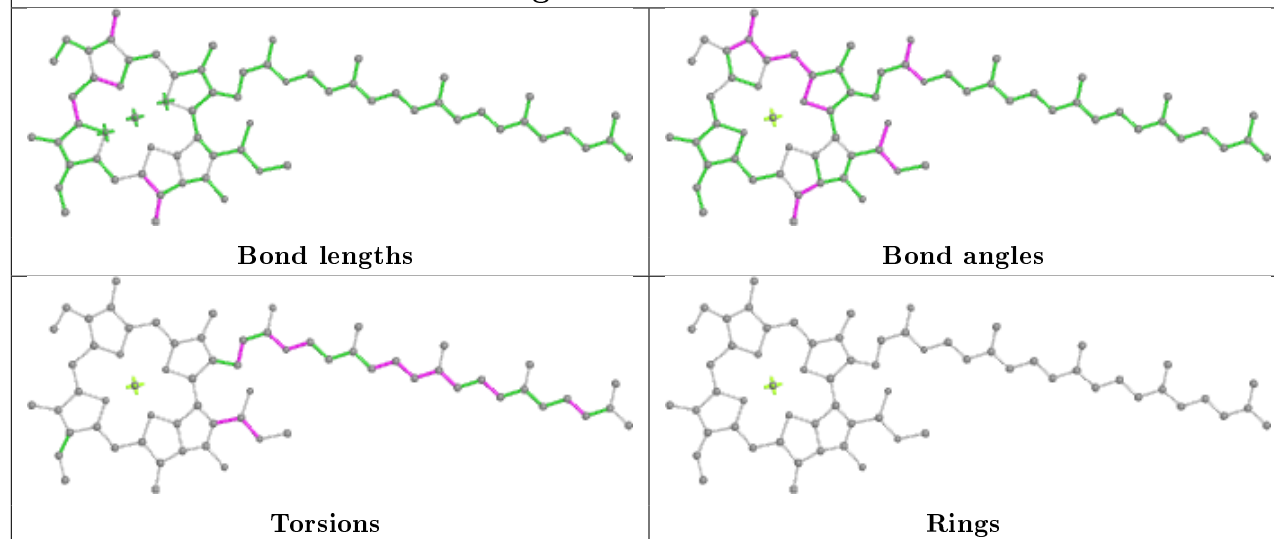


Ligand CLA D 404

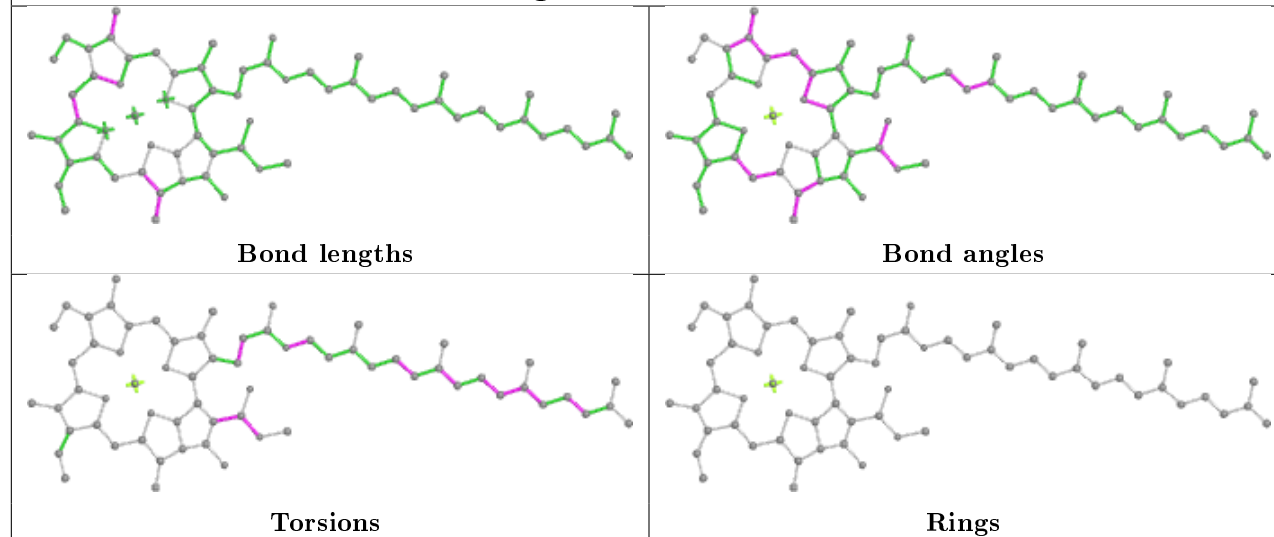


Ligand CLA b 606**Ligand BCR F 102****Ligand BCR a 410**

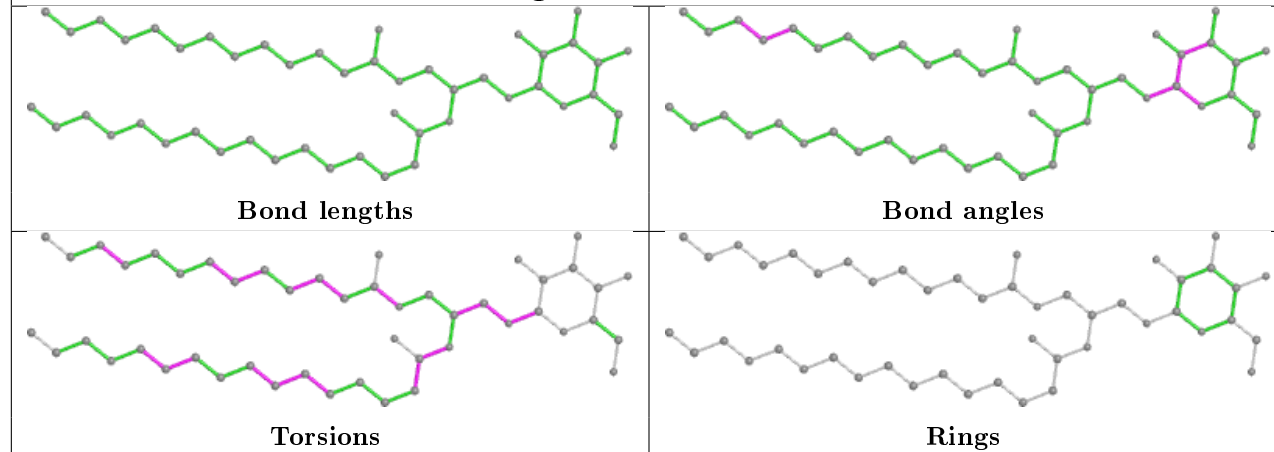
Ligand CLA C 508



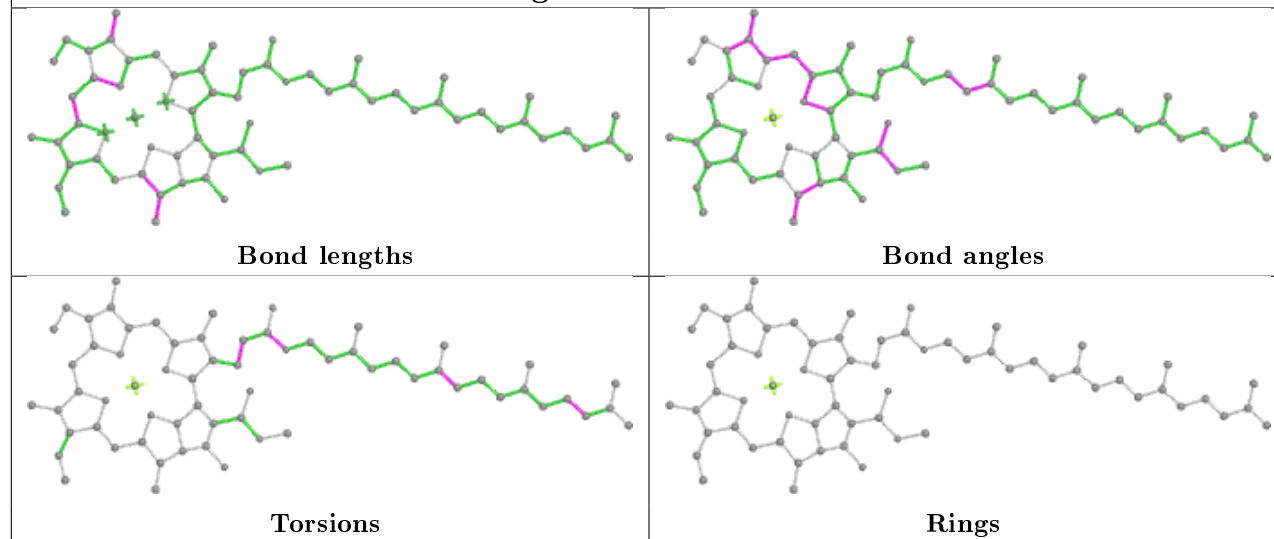
Ligand CLA C 507



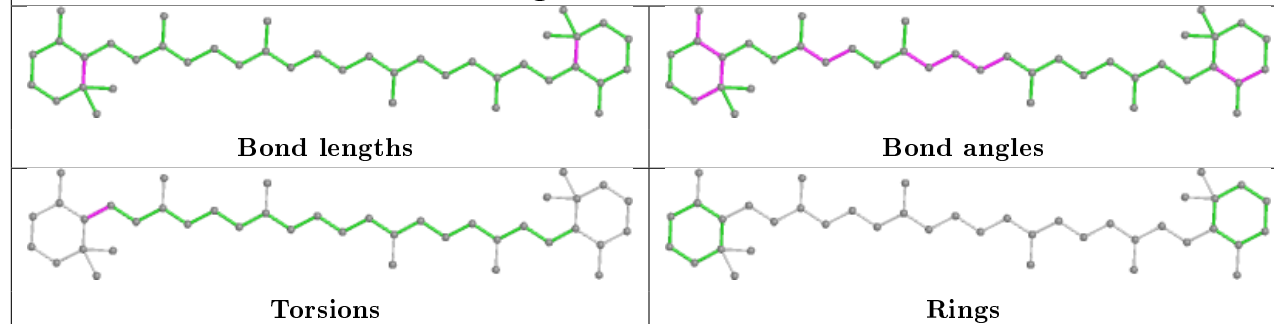
Ligand LMG d 408



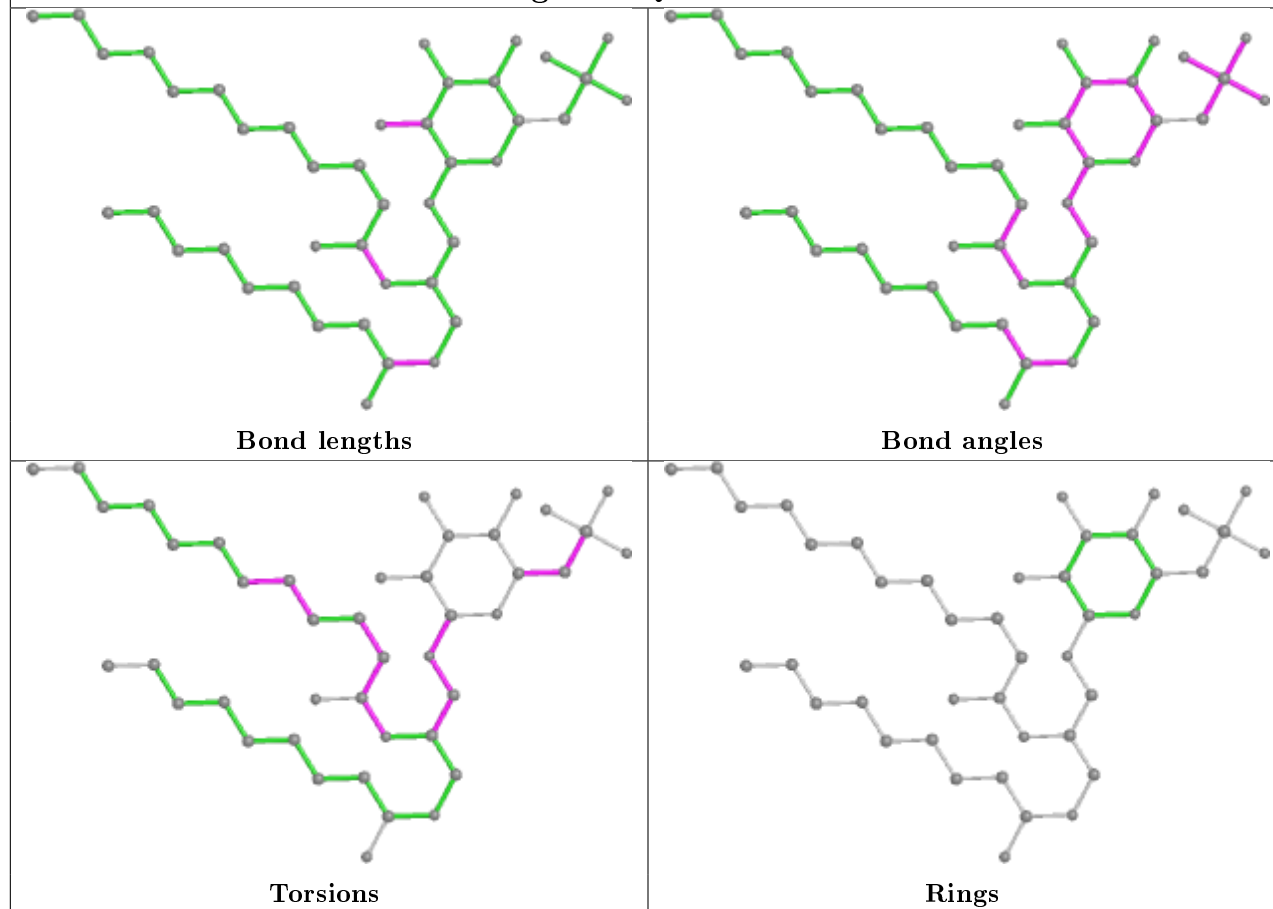
Ligand CLA D 405



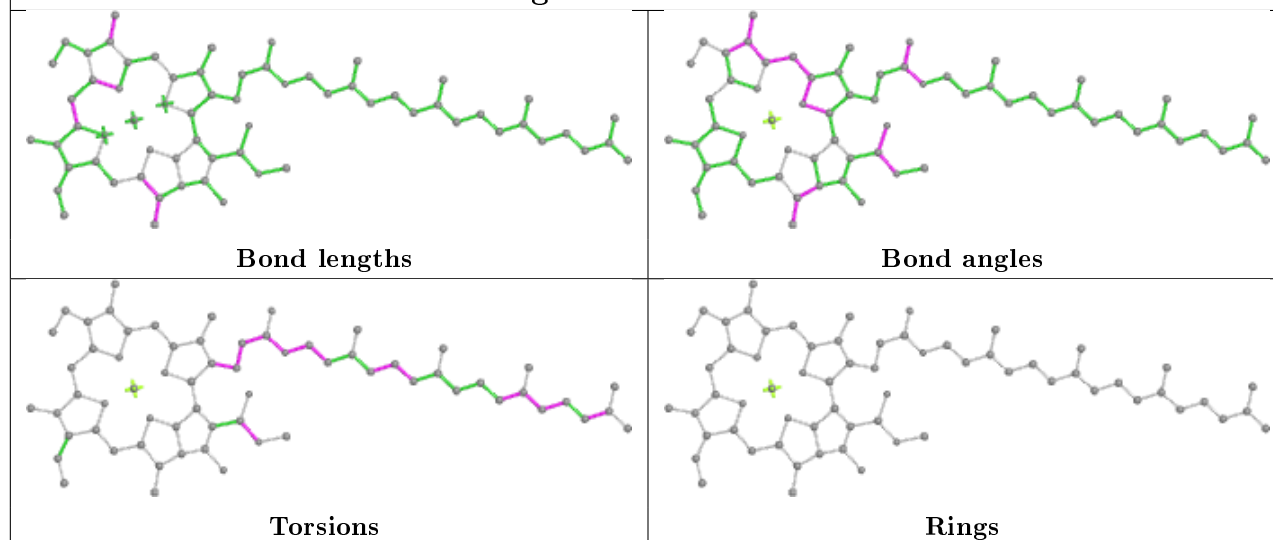
Ligand BCR B 616

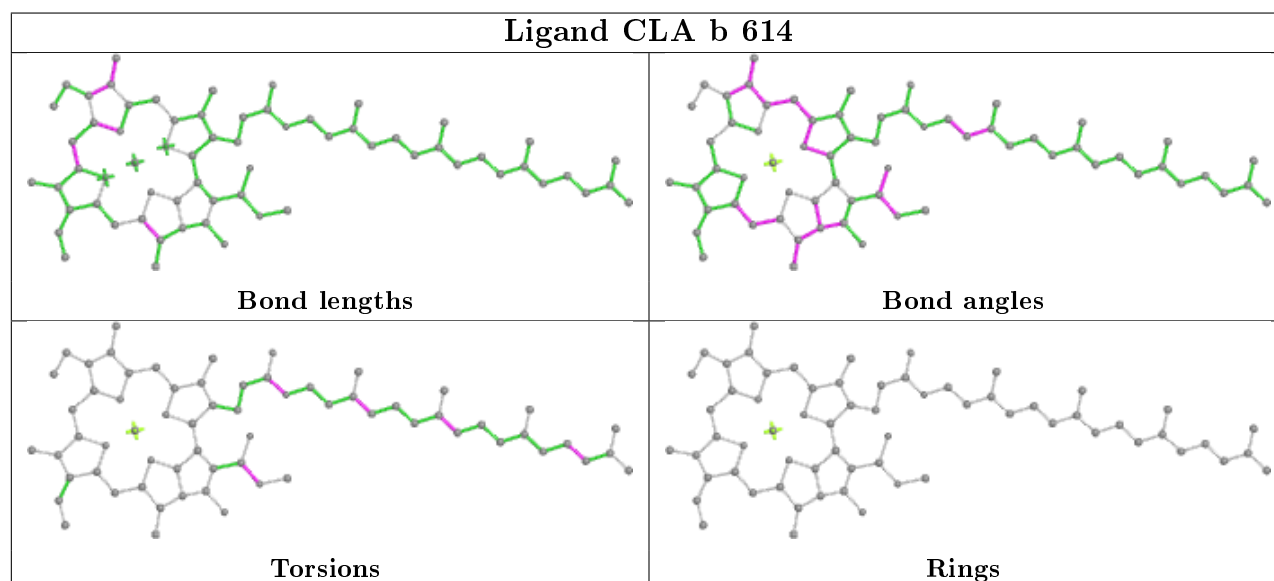
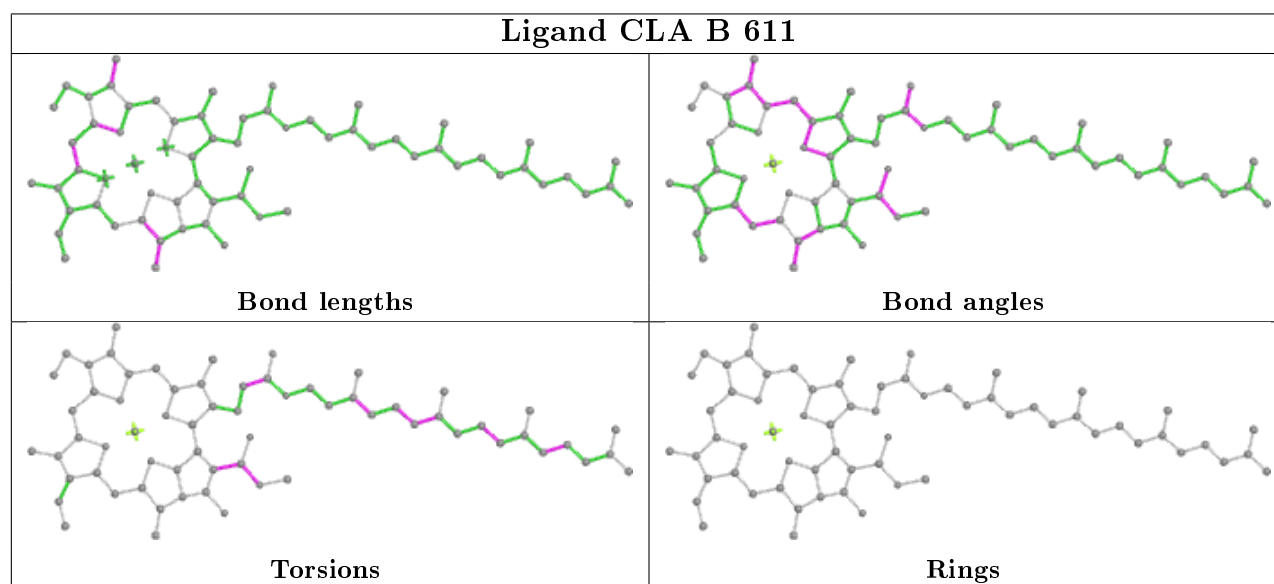
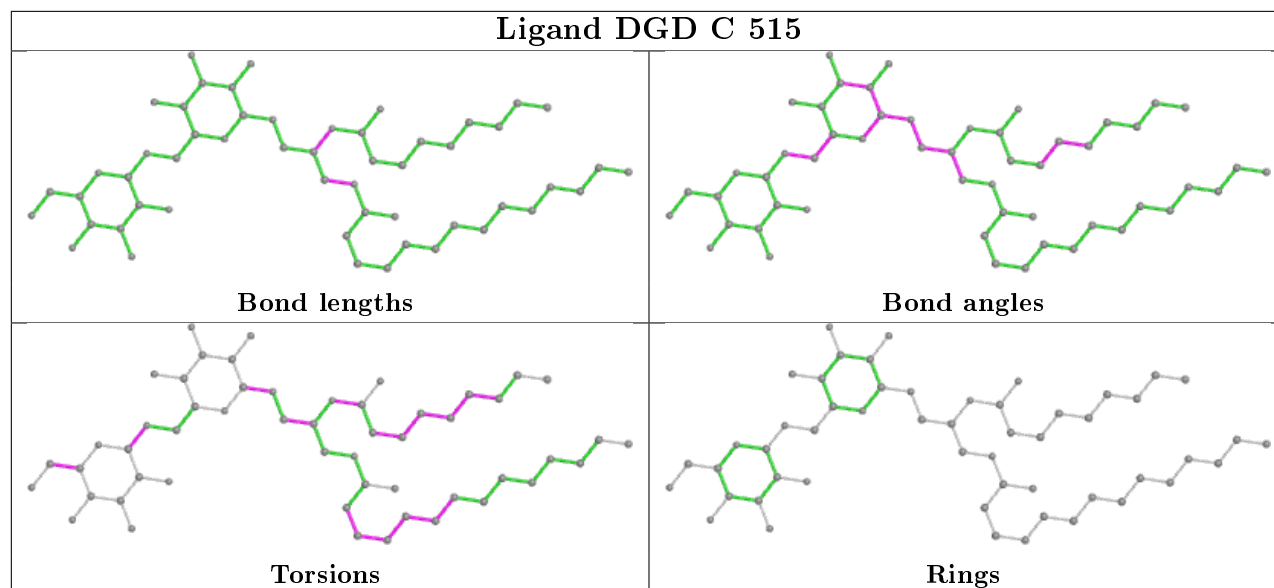


Ligand SQD B 622

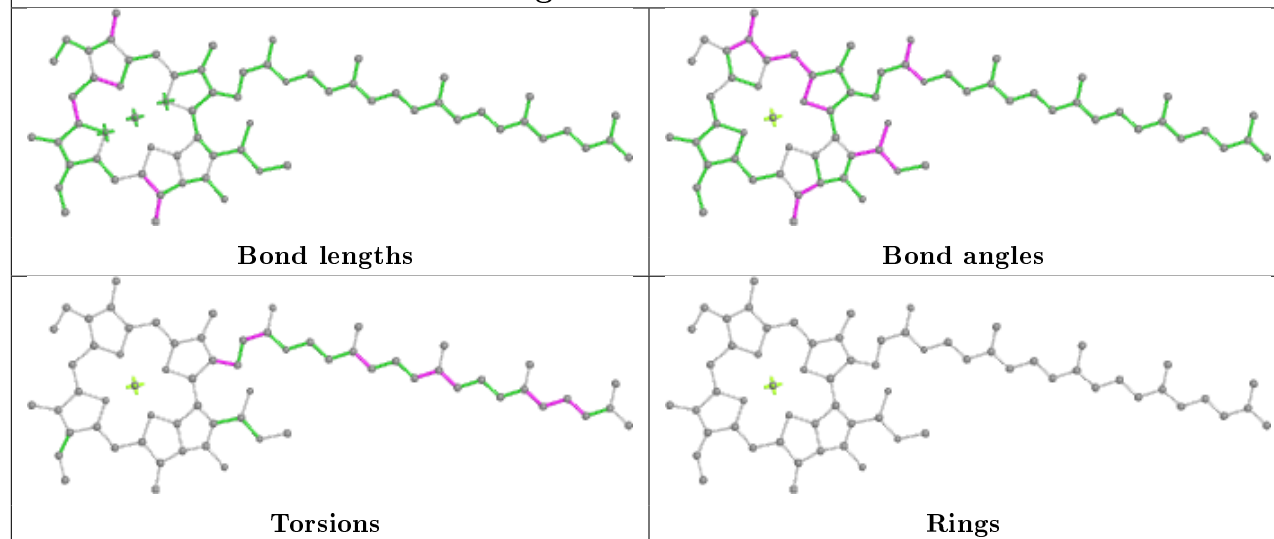


Ligand CLA C 511

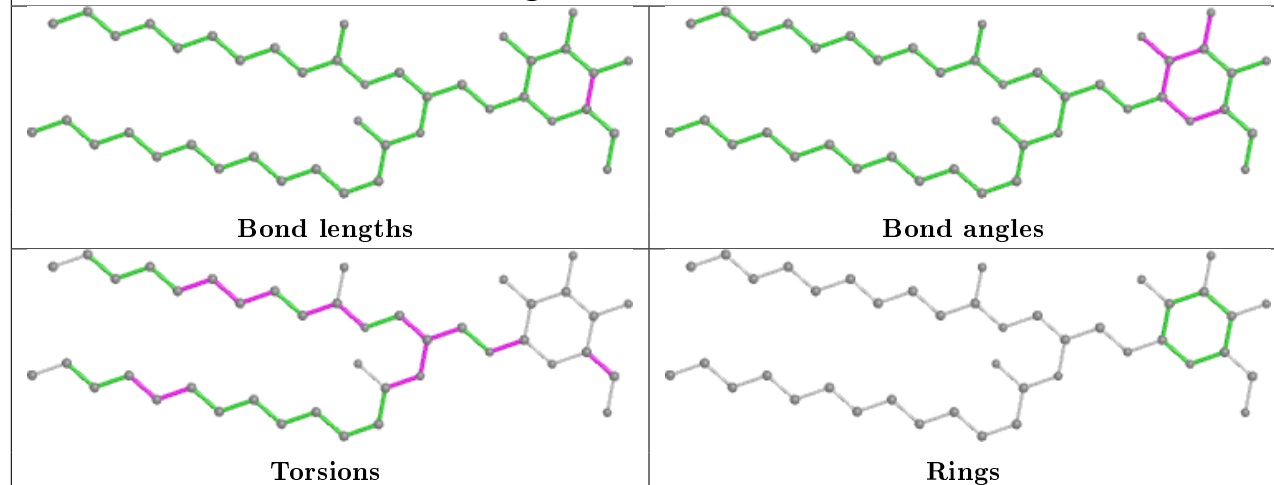




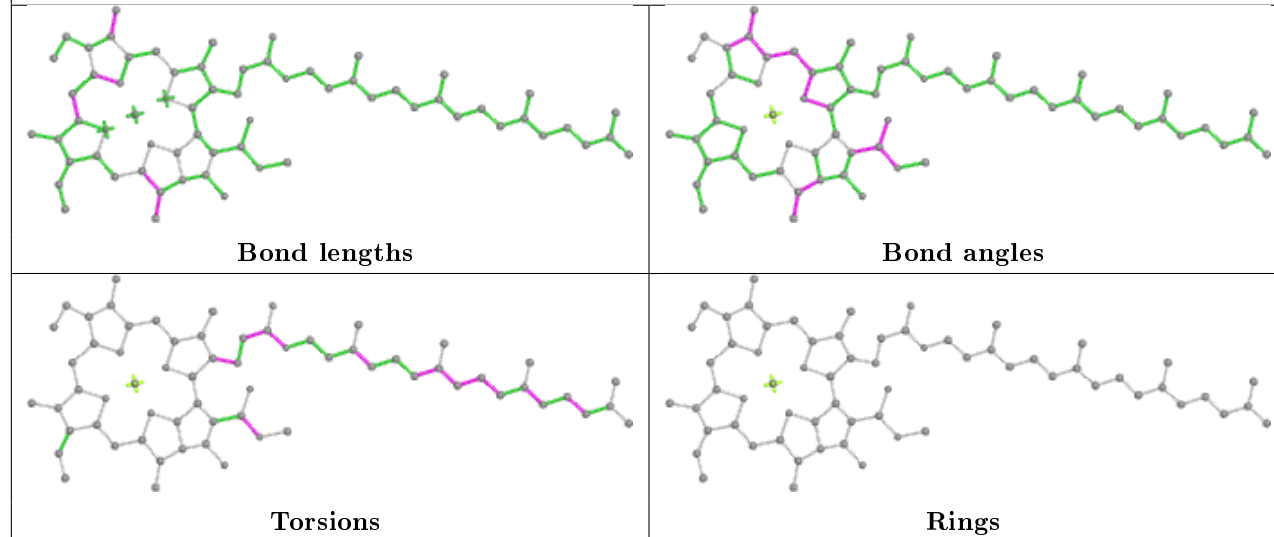
Ligand CLA d 404



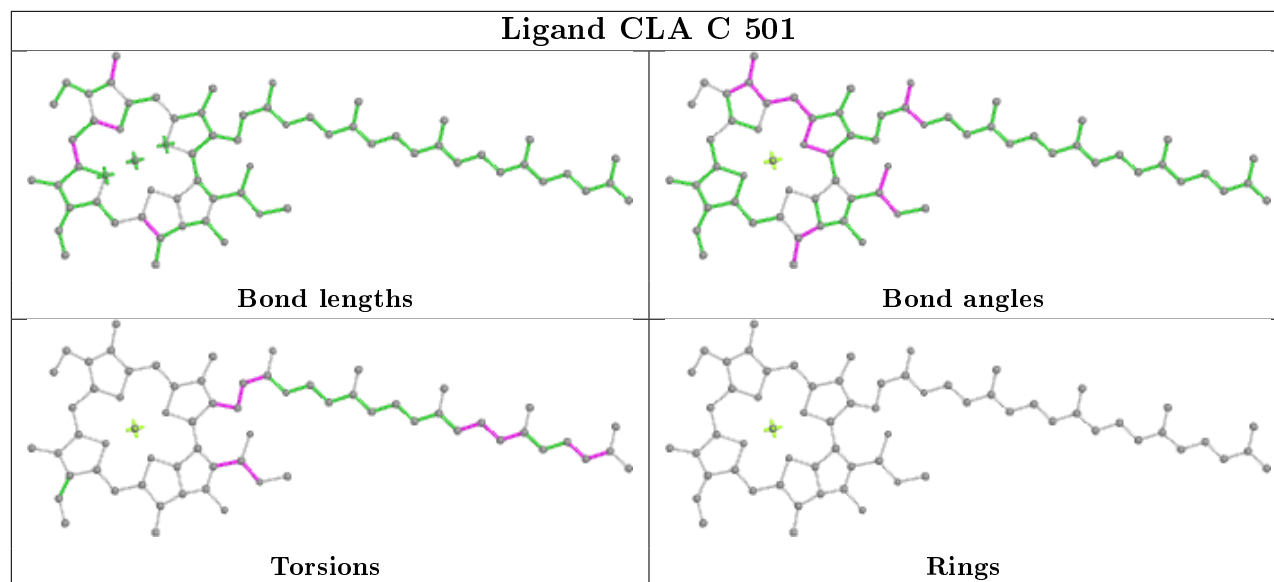
Ligand LMG M 101



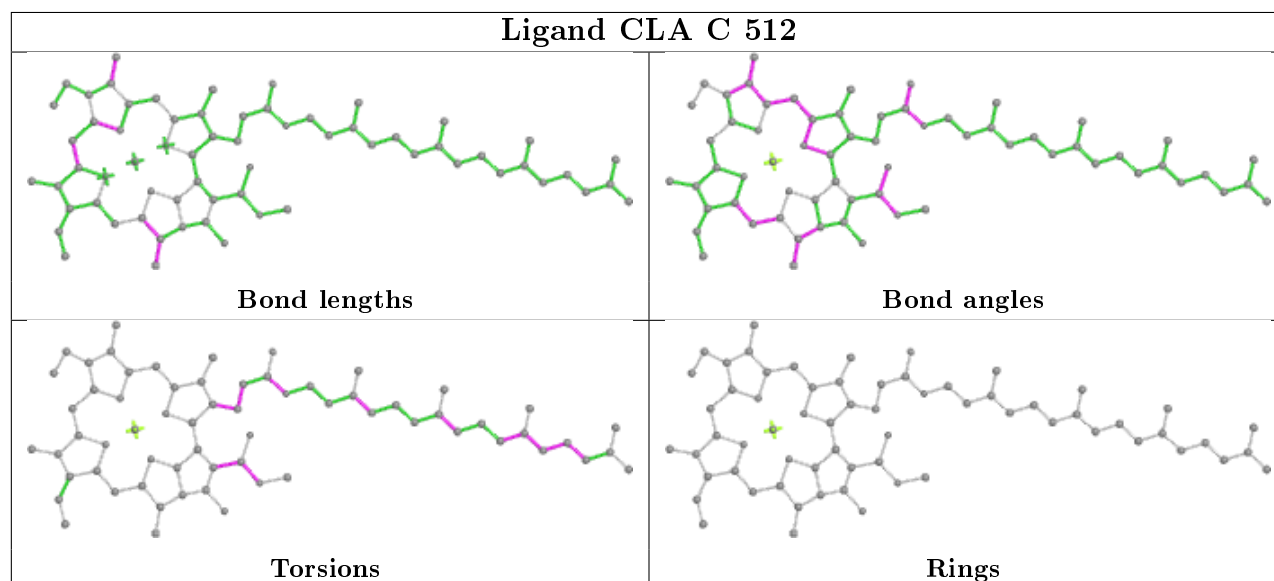
Ligand CLA C 504



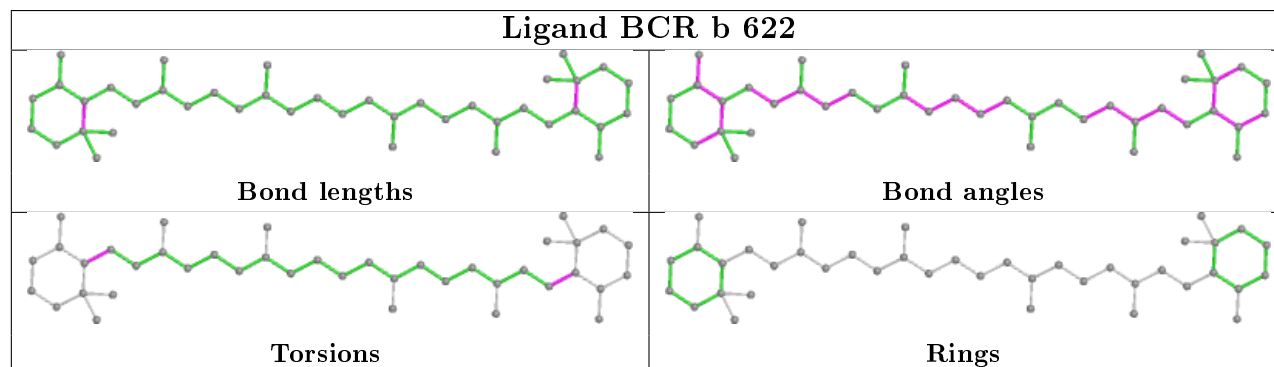
Ligand CLA C 501

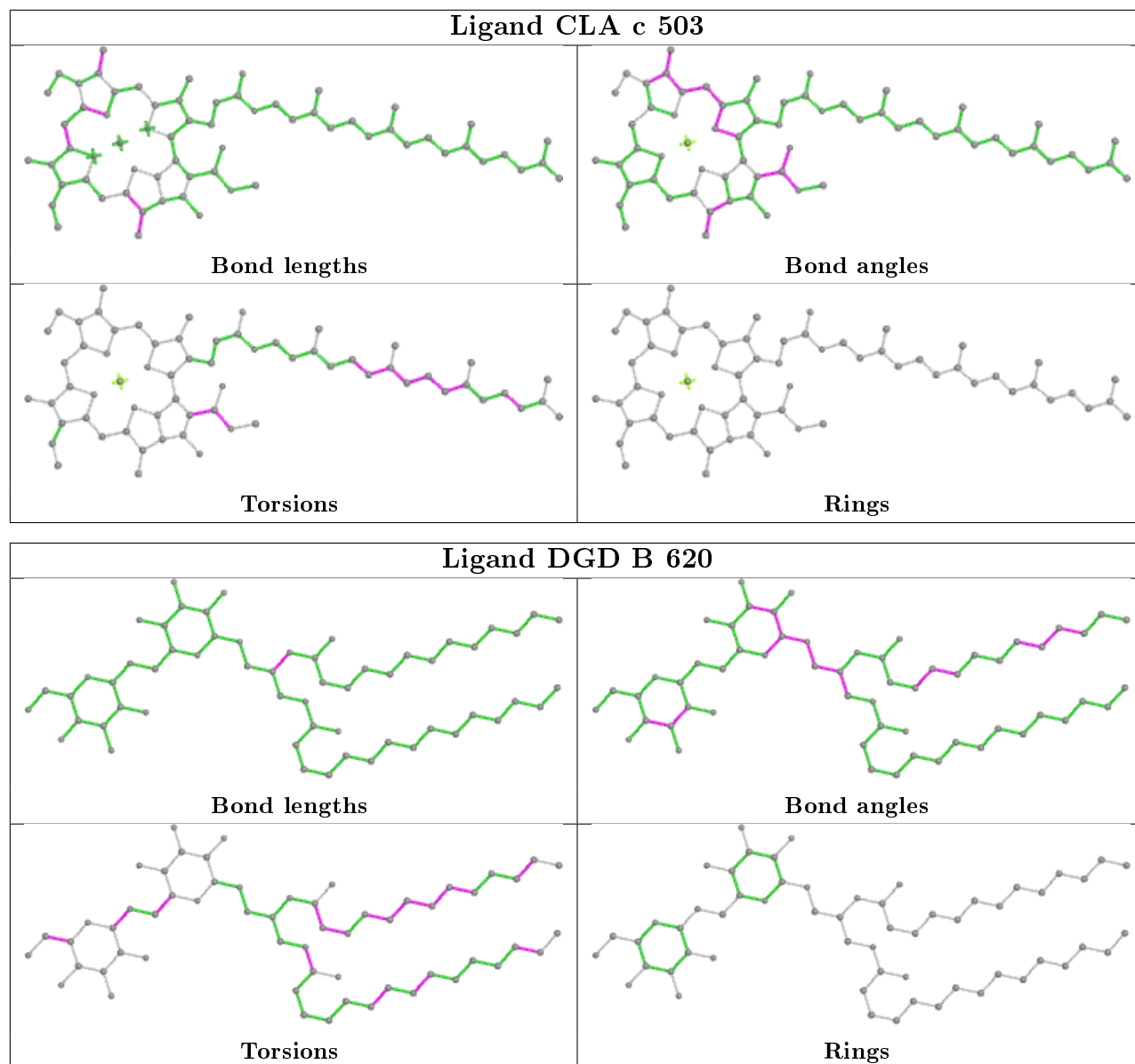


Ligand CLA C 512



Ligand BCR b 622





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	0.52	27 (8%) 12 11	205, 207, 208, 208	0
1	a	335/344 (97%)	0.54	30 (8%) 9 9	204, 207, 208, 209	0
2	B	490/510 (96%)	0.33	34 (6%) 16 13	205, 207, 208, 208	0
2	b	490/510 (96%)	0.42	38 (7%) 13 11	205, 207, 208, 209	0
3	C	447/461 (96%)	0.37	35 (7%) 13 11	205, 207, 208, 209	0
3	c	447/461 (96%)	0.20	21 (4%) 31 27	206, 207, 208, 209	0
4	D	340/352 (96%)	0.36	16 (4%) 31 27	204, 207, 208, 209	0
4	d	340/352 (96%)	0.34	17 (5%) 28 25	204, 207, 208, 208	0
5	E	82/84 (97%)	0.22	1 (1%) 79 70	205, 207, 208, 208	0
5	e	82/84 (97%)	0.10	2 (2%) 59 49	206, 207, 208, 208	0
6	F	35/45 (77%)	-0.02	0 100 100	206, 207, 208, 208	0
6	f	35/45 (77%)	-0.39	0 100 100	206, 207, 208, 208	0
7	H	65/66 (98%)	0.45	9 (13%) 2 4	206, 207, 208, 209	0
7	h	65/66 (98%)	0.77	12 (18%) 1 2	206, 207, 208, 208	0
8	I	35/38 (92%)	0.54	4 (11%) 5 6	206, 207, 208, 208	0
8	i	35/38 (92%)	-0.09	0 100 100	206, 207, 208, 208	0
9	J	34/40 (85%)	0.08	2 (5%) 22 19	205, 207, 207, 208	0
9	j	34/40 (85%)	-0.44	0 100 100	206, 207, 208, 209	0
10	K	37/46 (80%)	-0.11	0 100 100	206, 207, 208, 208	0
10	k	37/46 (80%)	0.32	2 (5%) 25 22	206, 207, 208, 209	0
11	L	37/37 (100%)	0.56	2 (5%) 25 22	205, 207, 208, 208	0
11	l	37/37 (100%)	0.21	1 (2%) 54 45	206, 207, 208, 209	0
12	M	34/36 (94%)	0.58	4 (11%) 4 6	205, 206, 207, 208	0
12	m	34/36 (94%)	0.27	2 (5%) 22 19	205, 207, 207, 208	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/272 (89%)	0.64	22 (9%) 9 8	205, 207, 208, 209	0
13	o	243/272 (89%)	0.62	16 (6%) 18 15	205, 207, 208, 209	0
14	T	32/32 (100%)	0.23	3 (9%) 8 8	206, 207, 208, 209	0
14	t	32/32 (100%)	0.49	3 (9%) 8 8	205, 206, 208, 208	0
15	U	97/134 (72%)	0.86	11 (11%) 5 6	205, 207, 208, 208	0
15	u	97/134 (72%)	0.67	8 (8%) 11 10	205, 207, 208, 208	0
16	V	137/163 (84%)	0.24	3 (2%) 62 52	205, 207, 208, 208	0
16	v	137/163 (84%)	0.70	14 (10%) 6 7	206, 207, 208, 208	0
17	g	28/46 (60%)	0.18	0 100 100	206, 207, 208, 209	0
17	y	28/46 (60%)	-0.04	0 100 100	206, 207, 208, 208	0
18	X	37/41 (90%)	0.71	5 (13%) 3 4	205, 207, 208, 209	0
18	x	37/41 (90%)	0.96	5 (13%) 3 4	206, 207, 208, 208	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.22	1 (1%) 72 62	205, 207, 208, 209	0
20	z	62/62 (100%)	0.84	9 (14%) 2 3	206, 207, 208, 209	0
All	All	5214/5674 (91%)	0.41	359 (6%) 16 13	204, 207, 208, 209	0

All (359) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	7.3
18	x	11	THR	6.7
13	o	169	LYS	6.3
5	e	84	LYS	5.2
18	x	42	GLN	5.2
1	a	239	PHE	5.1
3	C	149	TYR	5.1
7	H	64	ALA	5.0
15	U	38	GLU	4.8
1	A	138	GLY	4.7
4	D	24	ARG	4.6
15	U	39	LEU	4.5
5	e	82	GLN	4.5
1	a	299	GLY	4.5
18	x	12	ILE	4.4
1	A	299	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
4	d	295	SER	4.3
1	A	11	ALA	4.3
3	C	332	GLN	4.3
3	c	372	PRO	4.3
2	B	347	ARG	4.2
1	A	179	THR	4.2
3	C	147	PHE	4.2
13	O	84	ASN	4.1
3	c	202	PRO	4.0
14	t	31	LYS	4.0
3	C	212	TYR	3.9
3	C	148	GLY	3.8
2	b	482	ILE	3.8
1	A	177	SER	3.8
16	v	132	ASN	3.8
12	M	2	GLU	3.8
18	X	45	LYS	3.8
14	T	28	ARG	3.8
1	A	175	GLY	3.8
7	h	4	ARG	3.7
1	A	190	HIS	3.7
13	o	84	ASN	3.7
16	v	133	LEU	3.7
2	b	483	ASP	3.7
1	A	165	GLN	3.7
18	X	46	VAL	3.6
7	H	63	LYS	3.6
14	t	32	LYS	3.6
1	a	165	GLN	3.6
2	B	354	LEU	3.6
3	C	44	ASN	3.6
1	A	12	ASN	3.6
2	b	133	LEU	3.6
3	C	46	SER	3.6
16	v	47	LEU	3.6
18	X	42	GLN	3.5
2	b	127	ARG	3.5
2	b	490	GLN	3.5
2	B	309	LEU	3.5
3	c	201	ASN	3.4
15	U	40	VAL	3.4
15	u	50	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	b	229	LEU	3.4
3	c	200	THR	3.4
1	A	10	SER	3.4
1	A	14	TRP	3.4
2	B	353	GLU	3.4
7	h	66	GLY	3.3
2	b	228	ALA	3.3
2	B	183	PRO	3.3
13	O	234	THR	3.3
3	C	145	SER	3.3
1	a	191	ASN	3.2
3	C	266	TRP	3.2
2	b	302	TRP	3.2
4	d	95	PRO	3.2
16	v	130	MET	3.2
3	C	151	TRP	3.2
3	c	260	ALA	3.2
2	B	477	ASP	3.1
4	d	176	ALA	3.1
3	C	144	SER	3.1
13	o	168	PHE	3.1
1	a	190	HIS	3.1
3	c	457	LYS	3.1
13	O	262	GLN	3.1
2	B	411	PHE	3.1
12	M	4	ASN	3.1
8	I	25	SER	3.1
2	B	120	LEU	3.0
1	a	282	GLY	3.0
16	v	117	VAL	3.0
2	b	393	GLU	3.0
1	A	178	GLY	3.0
2	B	127	ARG	3.0
3	C	261	ARG	3.0
13	O	222	GLN	3.0
4	d	236	ASN	3.0
7	H	4	ARG	3.0
2	B	123	PHE	3.0
3	C	402	GLY	3.0
7	h	14	LEU	2.9
16	V	47	LEU	2.9
2	b	305	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	a	138	GLY	2.9
7	h	27	THR	2.9
13	o	220	LYS	2.9
18	X	47	GLN	2.9
16	v	113	GLU	2.9
1	a	16	ARG	2.9
4	d	195	PRO	2.9
1	A	13	LEU	2.9
12	M	5	GLN	2.9
2	b	70	GLY	2.9
13	O	47	THR	2.9
1	a	240	GLY	2.9
3	C	45	LEU	2.9
4	D	190	ASN	2.9
3	C	142	GLU	2.8
4	D	295	SER	2.8
1	a	178	GLY	2.8
1	a	325	ASN	2.8
1	a	171	GLY	2.8
4	d	262	SER	2.8
2	b	398	THR	2.8
3	C	265	ILE	2.8
1	a	175	GLY	2.8
2	B	293	ALA	2.8
3	C	139	THR	2.8
4	D	192	THR	2.8
1	a	201	GLY	2.8
2	b	431	GLU	2.8
2	B	84	THR	2.8
13	O	269	ILE	2.8
2	B	70	GLY	2.8
3	C	137	PRO	2.8
16	V	43	LYS	2.8
13	O	170	GLY	2.8
11	L	33	SER	2.8
1	A	294	ALA	2.8
2	b	217	ILE	2.8
1	a	225	ARG	2.8
2	b	125	ASP	2.8
13	o	89	ALA	2.8
13	o	238	ALA	2.7
1	A	262	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
3	c	78	GLU	2.7
2	B	121	GLU	2.7
3	C	140	LEU	2.7
3	c	199	ILE	2.7
13	O	50	ASP	2.7
14	t	30	THR	2.7
20	z	1	MET	2.7
1	a	10	SER	2.7
1	a	179	THR	2.7
2	B	164	PRO	2.7
2	b	120	LEU	2.7
13	O	79	LYS	2.7
15	u	72	TYR	2.7
3	c	180	MET	2.7
1	A	181	ASN	2.7
2	b	411	PHE	2.7
16	v	51	GLN	2.7
1	a	224	ILE	2.7
4	d	199	MET	2.7
2	B	351	GLY	2.6
7	H	2	ALA	2.6
4	D	297	ASP	2.6
1	a	19	ASN	2.6
13	O	223	ILE	2.6
2	B	122	LEU	2.6
10	k	14	ALA	2.6
1	a	301	ASN	2.6
1	A	15	GLU	2.6
1	A	137	LEU	2.6
16	v	46	THR	2.6
14	T	27	PRO	2.6
4	D	197	HIS	2.6
4	D	171	PRO	2.6
3	C	184	GLY	2.6
16	v	78	LEU	2.6
3	c	261	ARG	2.6
3	c	373	ASN	2.6
9	J	8	ILE	2.6
1	A	195	HIS	2.5
2	B	410	THR	2.5
13	o	31	LEU	2.5
2	B	162	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	c	388	GLN	2.5
4	d	255	GLN	2.5
13	O	220	LYS	2.5
16	v	44	THR	2.5
1	a	137	LEU	2.5
13	O	169	LYS	2.5
2	b	304	ALA	2.5
4	d	221	THR	2.5
13	O	126	GLY	2.5
7	H	27	THR	2.5
3	c	389	GLU	2.5
3	C	155	ASN	2.5
2	b	409	GLN	2.5
15	u	57	LEU	2.5
7	h	11	LEU	2.5
15	U	65	PHE	2.5
2	b	412	THR	2.5
1	a	170	ASP	2.5
7	H	65	LEU	2.5
15	u	51	TYR	2.5
1	a	198	HIS	2.5
13	O	46	PRO	2.5
20	z	29	SER	2.5
7	h	16	SER	2.4
13	O	235	GLY	2.4
2	B	294	SER	2.4
13	o	225	LEU	2.4
7	h	26	GLY	2.4
13	o	258	GLU	2.4
13	O	58	ILE	2.4
8	I	35	LYS	2.4
3	C	267	SER	2.4
15	U	55	ILE	2.4
7	H	6	TRP	2.4
4	d	197	HIS	2.4
18	X	13	THR	2.4
2	b	137	LYS	2.4
2	B	326	ARG	2.4
20	z	4	LEU	2.4
13	O	261	ILE	2.4
1	A	298	ASN	2.4
15	u	65	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	491	VAL	2.4
12	m	1	MET	2.4
2	B	295	GLY	2.4
4	D	199	MET	2.4
4	d	191	TRP	2.4
3	C	262	ARG	2.4
3	c	458	GLY	2.4
4	D	198	MET	2.4
1	a	139	MET	2.4
3	C	143	TYR	2.4
2	B	352	GLU	2.4
1	a	296	ASN	2.3
2	b	297	THR	2.3
3	c	264	PHE	2.3
2	b	219	VAL	2.3
4	d	201	VAL	2.3
4	D	170	ALA	2.3
13	O	219	THR	2.3
14	T	3	THR	2.3
20	z	60	PHE	2.3
7	H	3	ARG	2.3
7	h	23	PRO	2.3
15	U	122	VAL	2.3
2	B	83	GLU	2.3
1	a	298	ASN	2.3
2	B	402	TYR	2.3
15	U	117	VAL	2.3
13	o	229	LYS	2.3
15	u	102	LYS	2.3
15	U	45	GLU	2.3
2	B	185	TRP	2.3
3	C	135	ARG	2.3
13	o	91	PHE	2.3
9	J	7	ARG	2.3
11	l	1	MET	2.3
4	d	297	ASP	2.3
13	O	76	PHE	2.3
3	C	465	PRO	2.3
2	b	194	ASN	2.3
2	b	298	LEU	2.2
13	o	237	ILE	2.2
4	D	174	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
12	m	5	GLN	2.2
18	x	16	LEU	2.2
1	a	236	GLY	2.2
2	b	303	SER	2.2
2	b	178	VAL	2.2
4	d	239	GLN	2.2
3	C	473	ASP	2.2
2	b	379	ALA	2.2
20	z	2	THR	2.2
1	A	266	ASN	2.2
1	a	172	MET	2.2
2	B	166	MET	2.2
1	A	230	THR	2.2
2	B	69	LEU	2.2
3	c	203	THR	2.2
3	C	183	GLY	2.2
3	C	258	GLY	2.2
13	O	243	SER	2.2
1	A	196	PRO	2.2
1	a	150	PRO	2.2
4	D	307	GLU	2.2
10	k	17	ILE	2.2
7	h	18	TYR	2.2
2	b	126	PRO	2.2
3	C	263	ALA	2.2
1	A	76	ASN	2.2
20	z	7	LEU	2.2
20	z	3	ILE	2.2
3	C	256	PRO	2.2
4	d	23	LYS	2.2
16	V	39	ASN	2.2
3	c	402	GLY	2.2
3	C	197	ARG	2.2
4	D	195	PRO	2.2
16	v	92	ARG	2.2
15	u	58	ASN	2.2
7	H	62	TRP	2.2
3	C	146	PHE	2.1
8	I	34	ARG	2.1
16	v	131	ARG	2.1
12	M	34	LYS	2.1
13	o	170	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
20	z	6	GLN	2.1
2	b	349	LYS	2.1
16	v	114	ILE	2.1
2	b	421	ALA	2.1
3	c	472	LEU	2.1
7	h	5	THR	2.1
16	v	138	LEU	2.1
15	U	53	GLU	2.1
13	o	164	THR	2.1
1	a	25	ASP	2.1
2	b	410	THR	2.1
3	C	415	ASN	2.1
2	B	132	ALA	2.1
2	b	301	ALA	2.1
15	U	67	GLN	2.1
1	A	75	ASN	2.1
11	L	37	ASN	2.1
1	A	229	GLU	2.1
20	Z	62	VAL	2.1
13	o	112	LYS	2.1
1	A	192	ILE	2.1
8	I	3	THR	2.1
2	B	490	GLN	2.1
3	c	204	LEU	2.1
15	u	70	GLY	2.1
2	B	345	VAL	2.1
4	D	177	ALA	2.1
2	B	179	GLN	2.0
2	b	232	GLY	2.0
3	c	403	SER	2.0
2	b	69	LEU	2.0
13	O	162	ILE	2.0
7	h	53	LEU	2.0
13	O	242	GLU	2.0
3	C	257	PHE	2.0
3	c	430	HIS	2.0
18	x	44	ASP	2.0
15	U	121	LEU	2.0
4	D	282	SER	2.0
13	o	61	SER	2.0
20	z	44	SER	2.0
7	h	13	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	166	MET	2.0
4	D	191	TRP	2.0
2	B	476	ARG	2.0
4	d	174	GLY	2.0
2	b	119	ASP	2.0
2	B	161	LEU	2.0
4	d	194	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	PL9	J	101	35/55	0.24	0.59	204,207,208,209	0
23	PL9	j	101	35/55	0.26	0.53	205,208,209,209	0
31	LMT	i	102	35/35	0.29	1.67	206,208,209,210	0
27	LMG	E	101	44/55	0.37	0.77	204,207,209,210	0
31	LMT	I	102	35/35	0.39	0.88	205,207,209,210	0
35	CA	O	301	1/1	0.45	0.28	207,207,207,207	0
23	PL9	A	406	45/55	0.49	0.54	205,206,207,208	0
35	CA	K	101	1/1	0.51	0.37	210,210,210,210	0
24	BCR	J	102	40/40	0.52	0.38	205,207,208,209	0
22	CLA	b	605	65/65	0.52	1.06	205,208,209,209	0
35	CA	o	301	1/1	0.52	1.13	209,209,209,209	0
22	CLA	c	502	65/65	0.54	0.65	205,207,208,208	0
23	PL9	D	406	55/55	0.55	0.45	204,206,207,207	0
31	LMT	d	410	31/35	0.56	0.76	206,208,209,210	0
25	DGD	A	408	56/66	0.57	0.56	206,207,209,210	0
24	BCR	g	101	40/40	0.57	0.76	204,206,207,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LMG	a	402	42/55	0.57	0.47	204,207,209,209	0
35	CA	k	101	1/1	0.58	0.23	204,204,204,204	0
24	BCR	f	102	40/40	0.60	0.47	206,206,207,208	0
24	BCR	F	102	40/40	0.60	0.51	205,206,207,208	0
24	BCR	B	616	40/40	0.60	0.52	205,206,207,207	0
27	LMG	C	518	45/55	0.60	1.02	205,206,208,208	0
22	CLA	B	601	65/65	0.61	0.93	206,207,208,209	0
27	LMG	A	415	42/55	0.61	0.46	204,207,208,209	0
24	BCR	x	101	40/40	0.61	0.84	205,207,208,208	0
31	LMT	b	626	35/35	0.61	0.61	205,208,210,210	0
23	PL9	d	406	55/55	0.62	0.43	204,206,207,208	0
27	LMG	I	101	43/55	0.64	1.00	204,207,209,210	0
31	LMT	B	623	35/35	0.64	0.77	205,208,209,210	0
30	SQD	d	402	43/54	0.65	1.12	205,207,209,211	0
26	LHG	c	519	37/49	0.65	0.36	205,207,211,214	0
31	LMT	b	603	35/35	0.66	0.58	205,207,208,209	0
31	LMT	B	628	35/35	0.67	0.54	204,207,209,209	0
24	BCR	j	102	40/40	0.67	0.30	206,207,209,209	0
27	LMG	c	518	45/55	0.67	0.97	206,207,208,208	0
27	LMG	l	101	51/55	0.67	0.42	205,206,208,208	0
24	BCR	C	514	40/40	0.67	0.77	205,206,207,207	0
30	SQD	B	626	47/54	0.67	0.59	204,207,209,211	0
25	DGD	C	517	66/66	0.68	0.34	205,206,207,208	0
24	BCR	b	623	40/40	0.68	0.83	204,206,207,207	0
30	SQD	F	103	45/54	0.68	0.82	205,207,209,210	0
22	CLA	b	619	65/65	0.68	0.79	205,207,208,209	0
24	BCR	H	102	40/40	0.69	1.06	206,207,208,208	0
31	LMT	M	102	35/35	0.69	0.42	205,207,208,209	0
25	DGD	D	409	63/66	0.69	0.79	205,208,209,211	0
31	LMT	b	604	35/35	0.69	0.45	205,207,209,209	0
27	LMG	C	521	48/55	0.69	0.37	204,206,207,208	0
25	DGD	d	409	63/66	0.70	0.74	205,208,210,211	0
25	DGD	B	625	52/66	0.70	0.63	205,208,210,210	0
22	CLA	B	613	65/65	0.70	0.49	205,206,207,208	0
25	DGD	a	411	56/66	0.70	0.39	205,207,209,209	0
27	LMG	M	101	42/55	0.70	0.51	205,207,209,210	0
31	LMT	b	627	35/35	0.70	1.20	205,208,210,210	0
27	LMG	e	101	44/55	0.71	0.47	204,207,208,209	0
24	BCR	B	617	40/40	0.71	0.43	204,206,207,208	0
24	BCR	c	514	40/40	0.71	0.85	205,206,207,208	0
27	LMG	m	101	42/55	0.72	0.57	203,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PHO	d	401	64/64	0.72	0.42	204,206,207,207	0
27	LMG	d	408	48/55	0.72	0.41	204,206,207,208	0
26	LHG	C	519	37/49	0.72	0.38	204,207,210,212	0
23	PL9	a	409	45/55	0.72	0.37	204,206,207,208	0
31	LMT	D	410	31/35	0.72	0.81	206,208,208,209	0
22	CLA	c	512	65/65	0.73	0.75	205,207,208,208	0
22	CLA	b	613	65/65	0.73	0.83	205,207,208,209	0
24	BCR	B	619	40/40	0.73	1.02	205,206,207,207	0
32	PHO	D	402	64/64	0.74	0.36	205,206,207,208	0
22	CLA	C	505	65/65	0.74	0.60	205,206,207,208	0
30	SQD	A	413	51/54	0.74	0.35	205,207,208,208	0
24	BCR	y	101	40/40	0.74	0.81	205,206,207,207	0
22	CLA	c	510	65/65	0.74	0.57	206,207,208,209	0
22	CLA	C	502	65/65	0.74	0.51	205,206,207,208	0
22	CLA	C	512	65/65	0.75	0.94	205,207,208,209	0
27	LMG	i	101	43/55	0.75	0.84	205,207,209,209	0
22	CLA	C	506	65/65	0.75	0.83	204,207,207,208	0
22	CLA	a	408	65/65	0.75	0.80	205,206,207,209	0
31	LMT	B	627	35/35	0.76	0.56	205,207,209,209	0
27	LMG	D	407	49/55	0.76	0.30	205,206,207,208	0
24	BCR	b	621	40/40	0.77	0.34	204,206,207,207	0
30	SQD	b	602	47/54	0.77	0.38	205,207,209,212	0
22	CLA	b	617	65/65	0.77	0.42	205,206,208,209	0
24	BCR	a	410	40/40	0.77	0.70	205,206,207,207	0
24	BCR	c	513	40/40	0.77	0.96	204,206,207,208	0
31	LMT	B	624	35/35	0.77	0.56	205,207,210,210	0
27	LMG	D	411	46/55	0.77	0.40	205,206,207,208	0
25	DGD	c	517	66/66	0.77	0.30	204,206,207,208	0
22	CLA	c	503	65/65	0.77	0.62	205,207,208,208	0
22	CLA	A	405	65/65	0.78	0.67	204,206,208,208	0
24	BCR	A	407	40/40	0.78	0.53	205,206,207,208	0
25	DGD	b	601	52/66	0.78	0.46	204,207,208,209	0
30	SQD	B	622	43/54	0.78	0.45	205,207,209,212	0
22	CLA	C	520	65/65	0.78	0.34	205,207,208,209	0
31	LMT	M	103	35/35	0.78	0.42	205,206,208,210	0
33	BCT	d	403	4/4	0.78	0.96	207,207,207,208	0
27	LMG	A	410	51/55	0.79	0.33	204,206,207,208	0
21	FE2	a	403	1/1	0.79	0.27	211,211,211,211	0
27	LMG	c	522	48/55	0.79	0.30	205,206,207,208	0
22	CLA	c	508	65/65	0.79	0.53	205,207,208,208	0
24	BCR	c	521	40/40	0.79	1.36	205,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	K	102	40/40	0.79	0.90	204,207,208,209	0
22	CLA	a	405	65/65	0.80	0.63	202,206,207,208	0
22	CLA	a	406	65/65	0.80	0.38	205,207,208,209	0
27	LMG	b	625	49/55	0.80	0.28	205,206,207,208	0
30	SQD	a	415	51/54	0.80	0.31	205,206,208,208	0
22	CLA	B	603	65/65	0.80	0.52	204,206,207,208	0
22	CLA	c	505	65/65	0.81	0.60	204,206,208,208	0
32	PHO	a	407	64/64	0.81	0.29	205,207,207,208	0
22	CLA	C	504	65/65	0.81	0.41	205,206,207,207	0
24	BCR	b	622	40/40	0.81	0.31	204,206,207,207	0
26	LHG	a	412	39/49	0.81	0.28	205,207,208,210	0
22	CLA	c	504	65/65	0.81	0.36	205,207,208,208	0
22	CLA	H	101	65/65	0.82	0.41	205,206,207,208	0
22	CLA	d	405	65/65	0.82	0.54	204,206,207,208	0
25	DGD	C	516	62/66	0.82	0.28	204,206,208,208	0
22	CLA	d	404	65/65	0.82	0.41	204,206,207,207	0
28	CL	a	413	1/1	0.82	0.18	204,204,204,204	0
22	CLA	b	618	65/65	0.82	0.70	205,207,208,208	0
22	CLA	C	508	65/65	0.82	0.86	205,206,207,208	0
22	CLA	B	605	65/65	0.82	0.82	205,206,207,208	0
32	PHO	D	401	64/64	0.82	0.34	203,206,207,208	0
22	CLA	b	606	65/65	0.83	0.77	205,206,207,207	0
25	DGD	b	624	58/66	0.83	0.34	205,206,207,208	0
22	CLA	a	404	65/65	0.83	0.57	205,206,207,208	0
22	CLA	C	510	65/65	0.83	0.46	205,206,207,208	0
22	CLA	B	608	65/65	0.83	0.69	205,207,208,209	0
22	CLA	b	607	65/65	0.83	0.51	205,206,207,209	0
22	CLA	B	615	65/65	0.84	0.84	205,206,208,208	0
22	CLA	C	511	65/65	0.84	1.06	205,207,208,208	0
22	CLA	B	607	65/65	0.84	0.44	205,206,207,209	0
30	SQD	A	414	54/54	0.84	0.37	204,207,208,210	0
22	CLA	h	101	65/65	0.85	0.57	204,207,208,209	0
22	CLA	b	612	65/65	0.85	0.59	205,206,207,209	0
22	CLA	B	614	65/65	0.85	0.87	205,206,207,208	0
30	SQD	f	103	45/54	0.85	0.60	205,207,208,210	0
30	SQD	a	401	54/54	0.85	0.46	205,207,209,211	0
22	CLA	c	501	65/65	0.85	0.61	205,207,208,209	0
22	CLA	c	509	65/65	0.85	0.39	204,206,208,209	0
24	BCR	B	618	40/40	0.85	0.30	204,205,207,207	0
22	CLA	D	405	65/65	0.85	0.68	205,206,207,207	0
22	CLA	C	503	65/65	0.86	0.44	205,207,207,208	0
22	CLA	b	610	65/65	0.86	0.29	205,206,207,208	0

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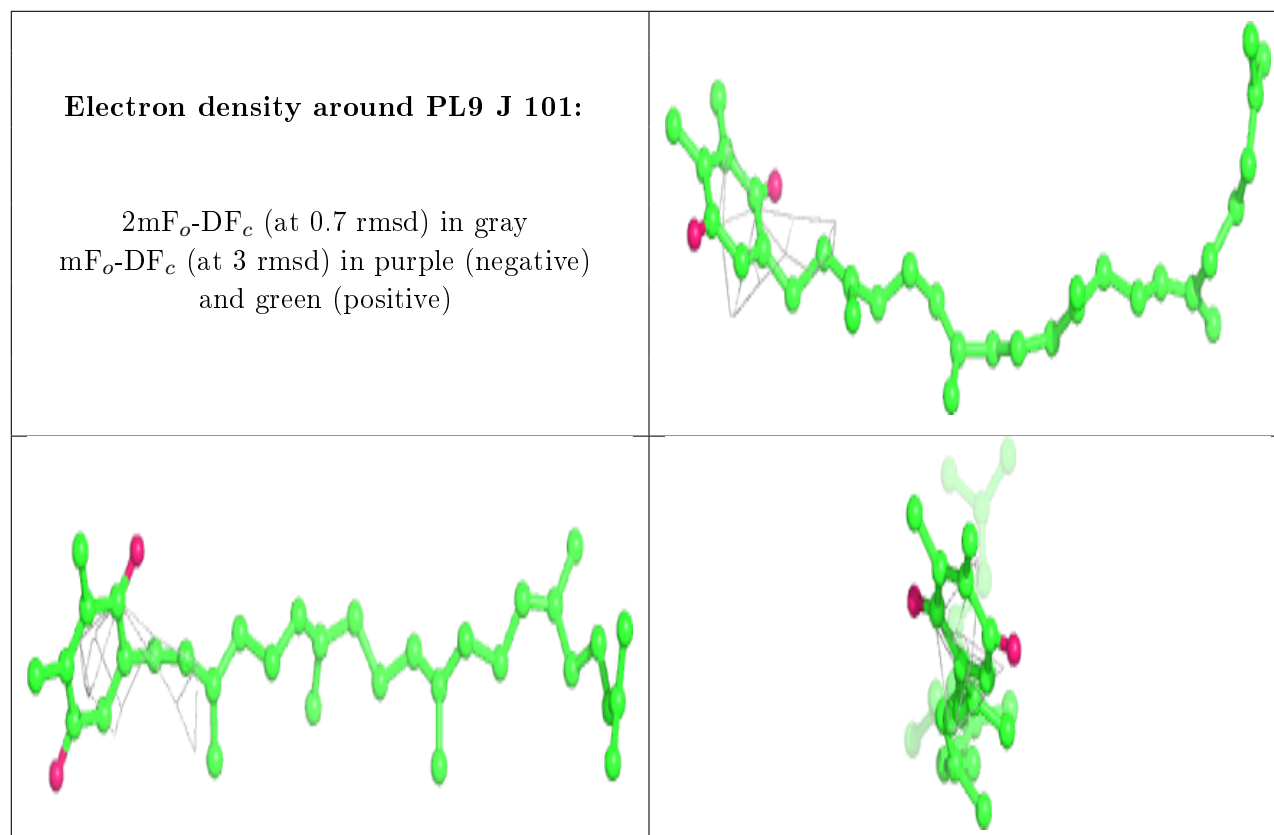
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	c	511	65/65	0.86	0.72	205,207,208,209	0
22	CLA	A	404	65/65	0.86	0.40	204,206,207,208	0
22	CLA	C	507	65/65	0.86	0.32	205,206,208,210	0
22	CLA	C	509	65/65	0.86	0.36	205,206,207,208	0
22	CLA	c	506	65/65	0.86	0.75	206,207,208,208	0
27	LMG	B	621	49/55	0.86	0.26	204,206,207,208	0
34	HEM	v	201	43/43	0.86	0.75	205,207,207,208	0
25	DGD	c	515	53/66	0.86	0.41	205,207,208,209	0
22	CLA	B	604	65/65	0.86	0.63	205,207,208,208	0
22	CLA	B	610	65/65	0.86	0.34	205,206,207,207	0
28	CL	A	411	1/1	0.86	0.25	207,207,207,207	0
22	CLA	b	609	65/65	0.86	0.64	205,207,208,209	0
22	CLA	b	608	65/65	0.86	0.60	205,206,207,208	0
22	CLA	b	611	65/65	0.86	0.43	205,206,207,208	0
25	DGD	B	620	58/66	0.86	0.30	203,206,208,209	0
34	HEM	V	201	43/43	0.87	0.52	203,206,207,208	0
25	DGD	C	515	53/66	0.87	0.28	204,206,207,208	0
22	CLA	B	609	65/65	0.87	0.62	205,206,208,208	0
25	DGD	c	516	62/66	0.88	0.26	205,207,208,209	0
22	CLA	A	403	65/65	0.88	0.62	204,206,207,207	0
22	CLA	b	615	65/65	0.88	0.35	205,206,207,208	0
27	LMG	d	411	46/55	0.88	0.29	204,206,207,208	0
22	CLA	B	611	65/65	0.88	0.43	204,206,207,208	0
22	CLA	c	507	65/65	0.88	0.33	205,207,208,208	0
27	LMG	D	408	48/55	0.89	0.25	202,206,208,208	0
34	HEM	F	101	43/43	0.89	0.61	205,207,208,209	0
22	CLA	c	520	65/65	0.89	0.29	205,207,207,208	0
26	LHG	A	409	39/49	0.89	0.26	205,206,208,209	0
24	BCR	C	513	40/40	0.89	0.82	205,206,207,208	0
22	CLA	B	606	65/65	0.89	0.31	205,206,207,208	0
22	CLA	A	402	65/65	0.89	0.47	205,206,207,208	0
21	FE2	A	401	1/1	0.89	0.17	206,206,206,206	0
22	CLA	B	612	65/65	0.90	0.28	204,206,207,207	0
22	CLA	D	404	65/65	0.90	0.39	203,206,207,208	0
22	CLA	b	614	65/65	0.90	0.31	205,206,207,208	0
22	CLA	C	501	65/65	0.90	0.44	205,206,207,208	0
24	BCR	b	620	40/40	0.91	0.30	205,206,207,208	0
27	LMG	d	407	49/55	0.92	0.23	205,206,207,207	0
22	CLA	B	602	65/65	0.92	0.47	204,206,208,209	0
33	BCT	D	403	4/4	0.93	0.44	206,206,206,206	0
34	HEM	f	101	43/43	0.93	0.32	206,207,207,208	0
22	CLA	b	616	65/65	0.94	0.33	204,206,208,209	0

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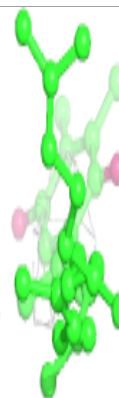
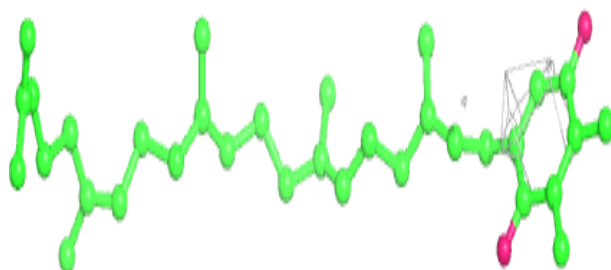
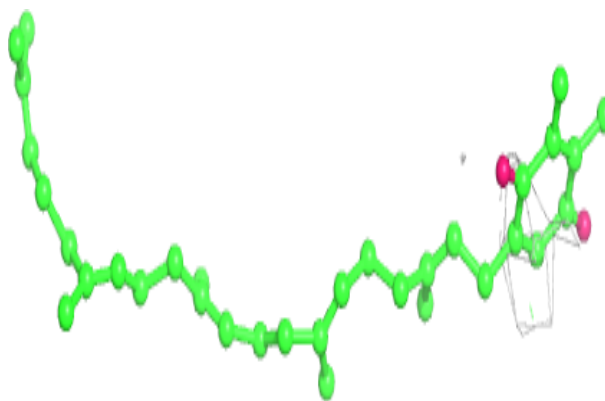
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	OEX	a	414	10/10	0.95	0.48	198,203,205,207	0
29	OEX	A	412	10/10	0.95	0.43	198,204,206,206	0

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.

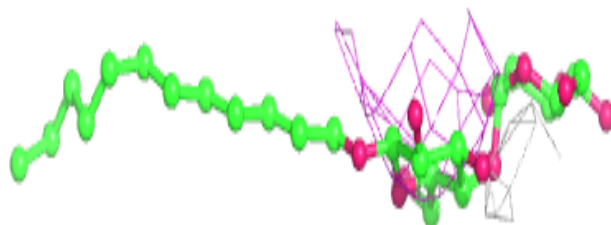
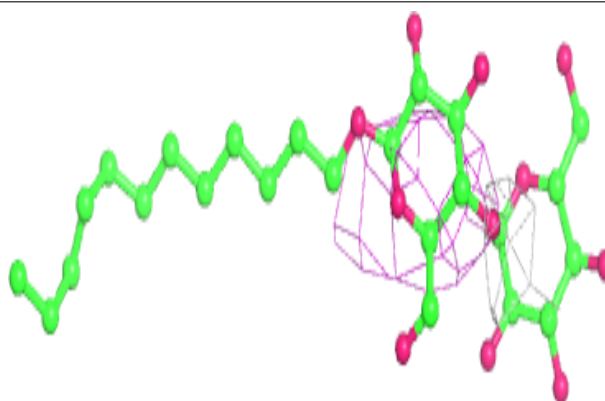


Electron density around PL9 j 101:

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

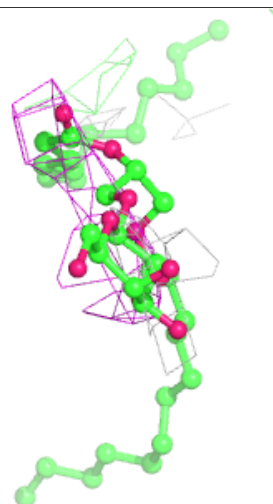
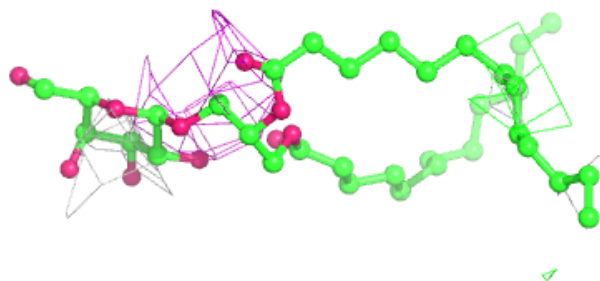
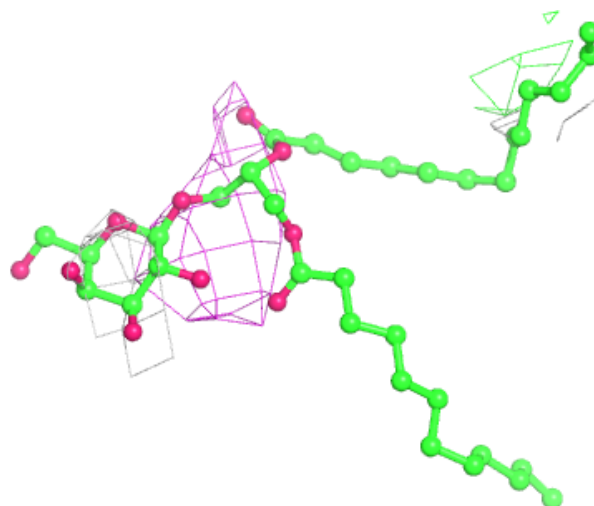
**Electron density around LMT i 102:**

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



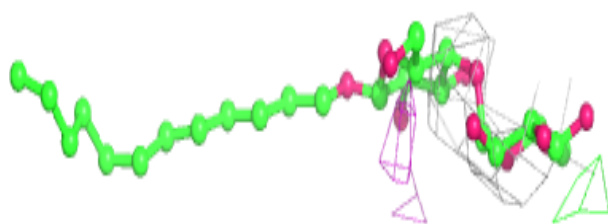
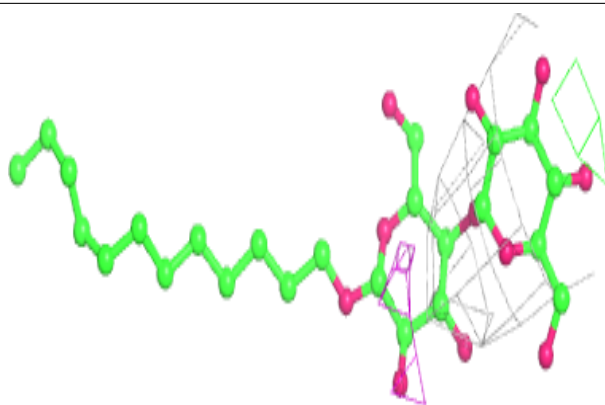
Electron density around LMG E 101:

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

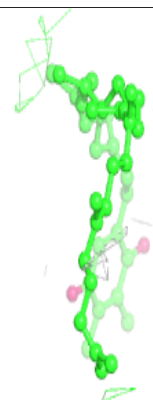
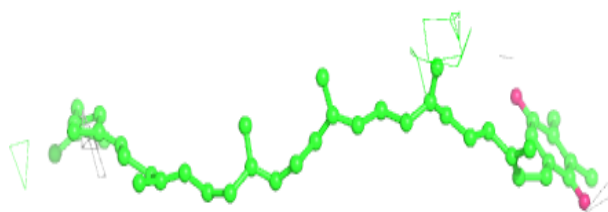
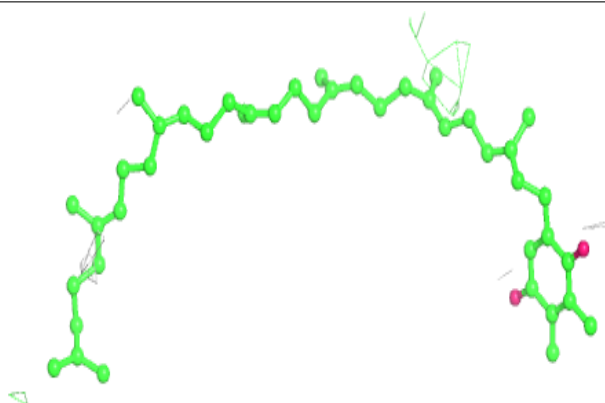


Electron density around LMT I 102:

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

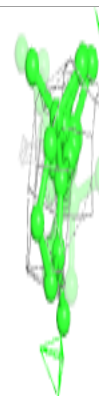
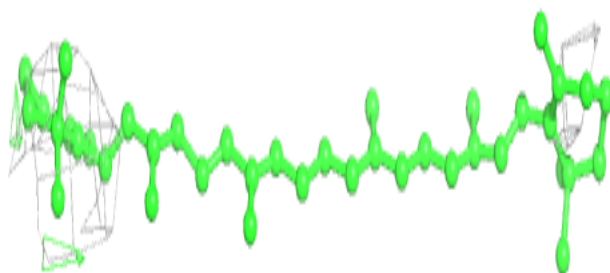
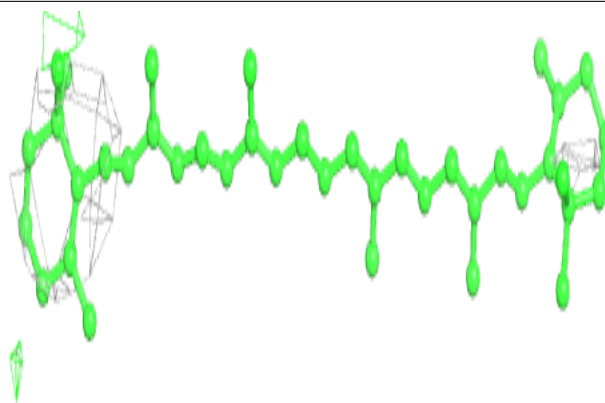
**Electron density around PL9 A 406:**

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



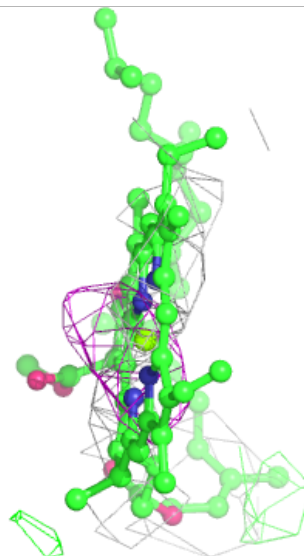
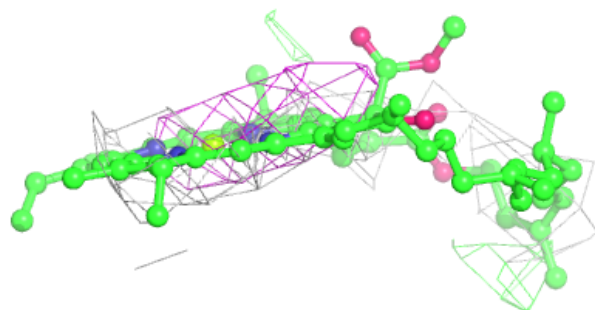
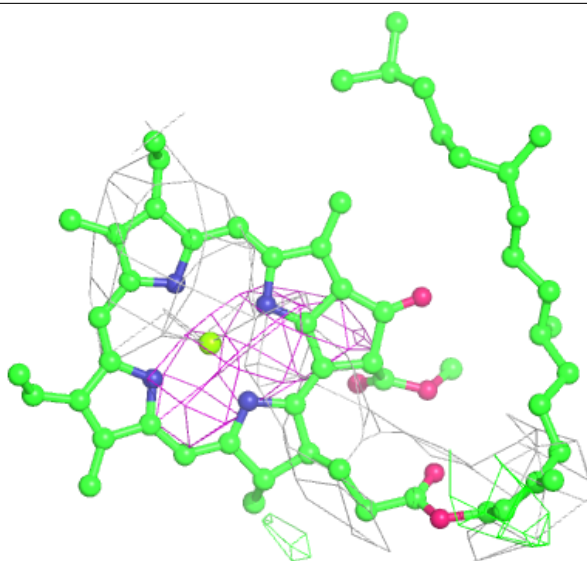
Electron density around BCR J 102:

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



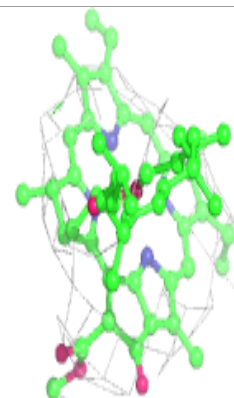
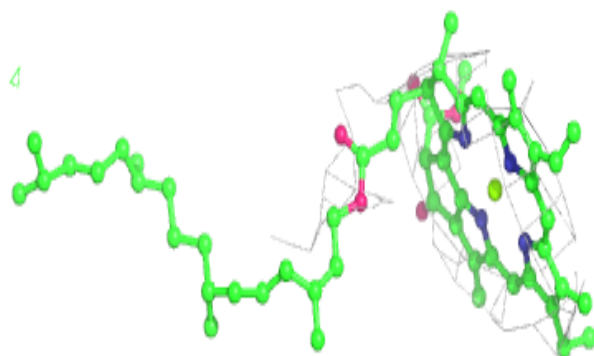
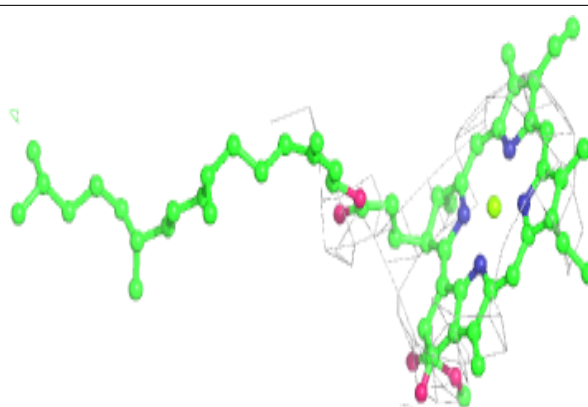
Electron density around CLA b 605:

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

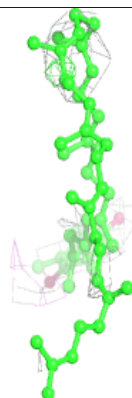
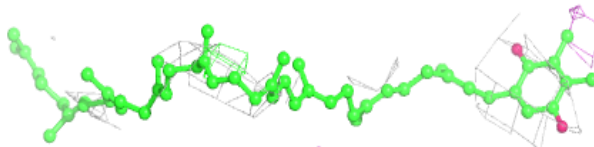
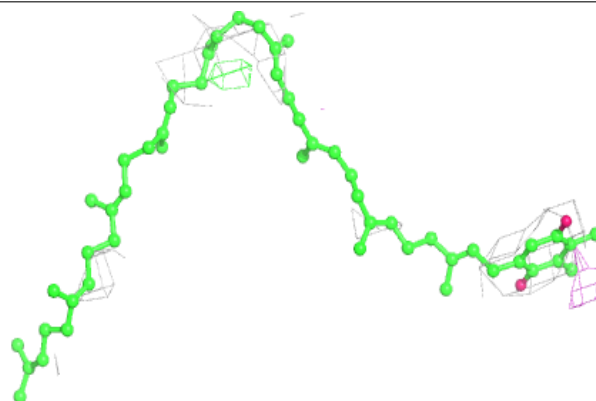


Electron density around CLA c 502:

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

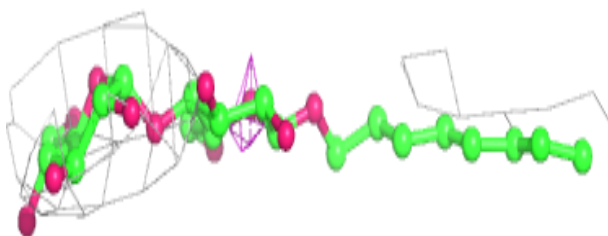
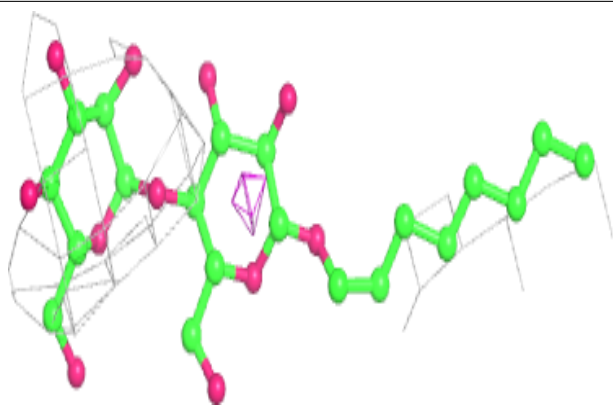
**Electron density around PL9 D 406:**

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

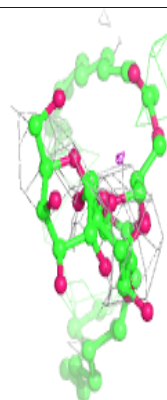
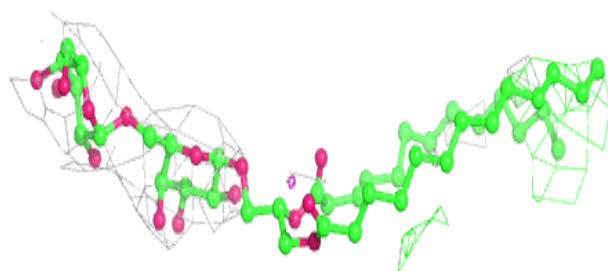
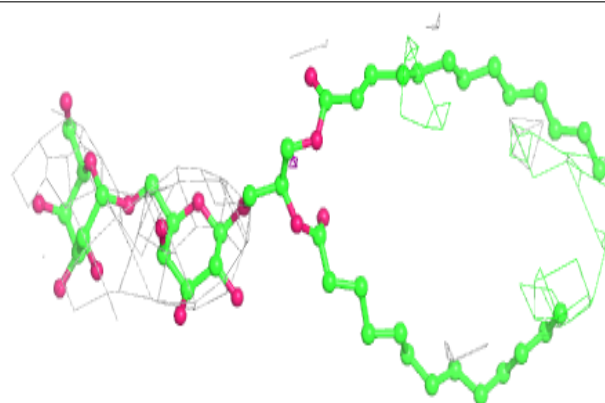


Electron density around LMT d 410:

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

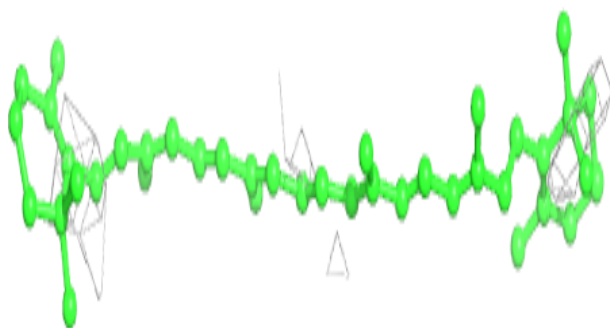
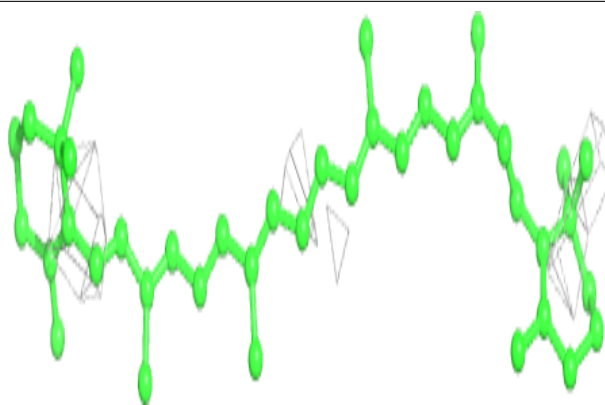
**Electron density around DGD A 408:**

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

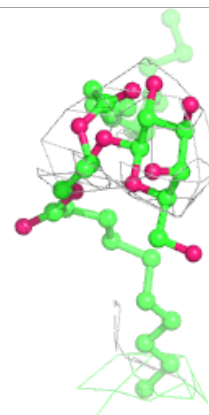
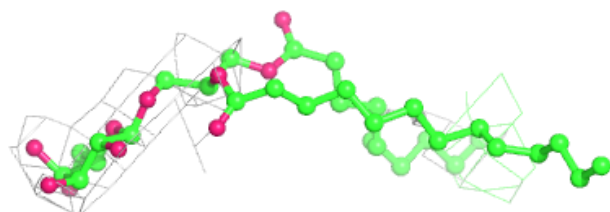
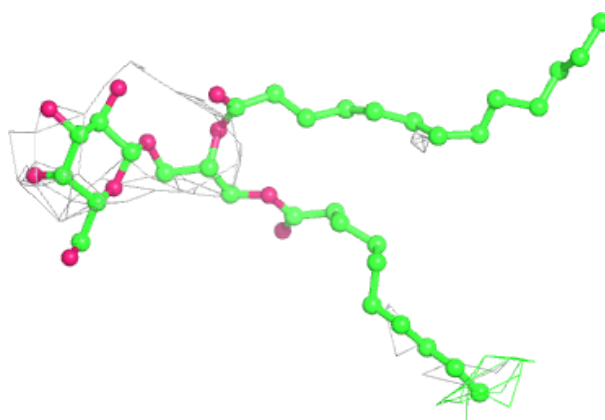


Electron density around BCR g 101:

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

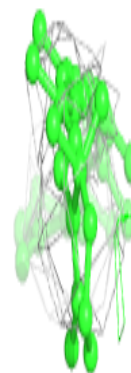
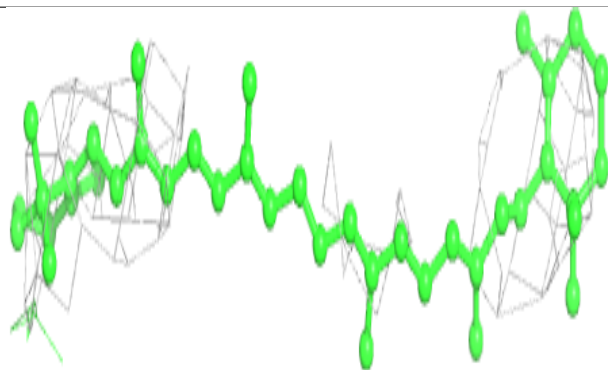
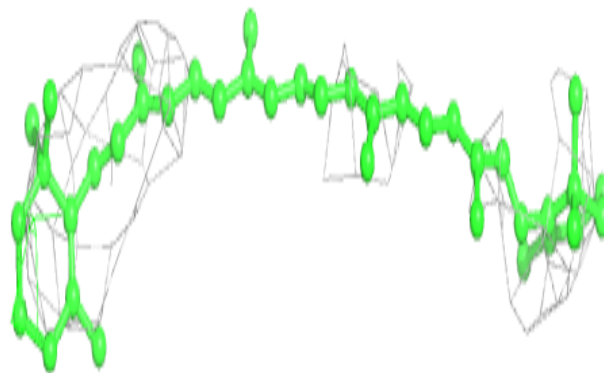
**Electron density around LMG a 402:**

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

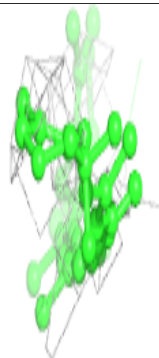
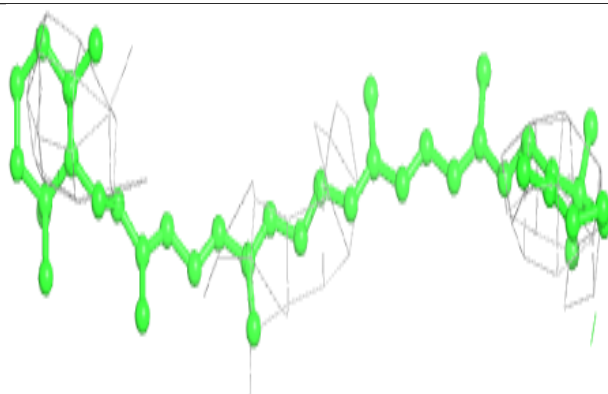
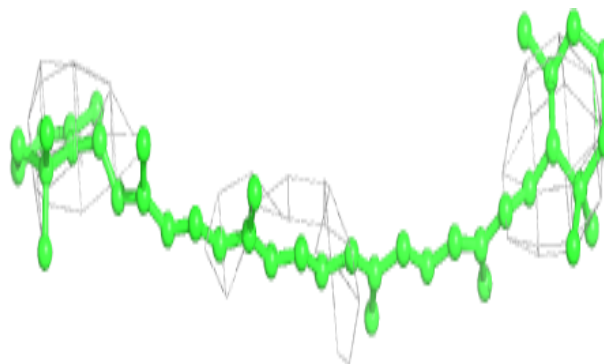


Electron density around BCR f 102:

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

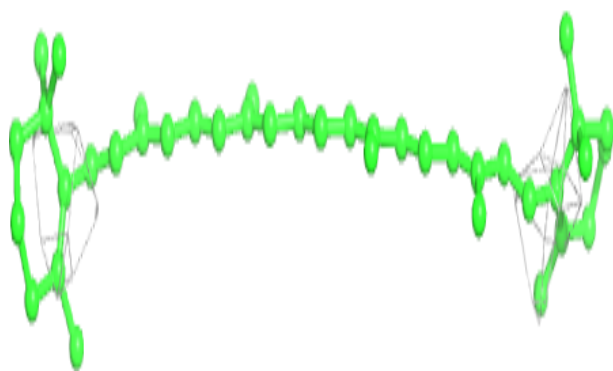
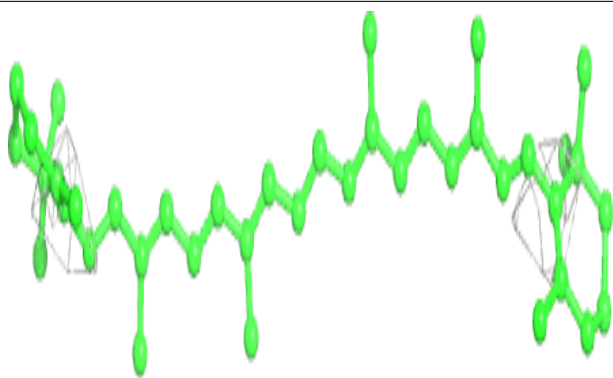
**Electron density around BCR F 102:**

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

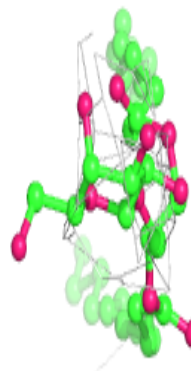
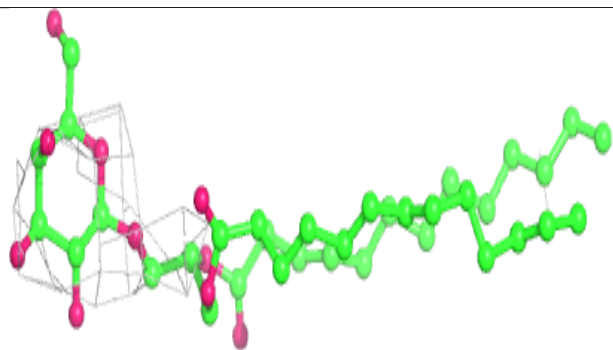
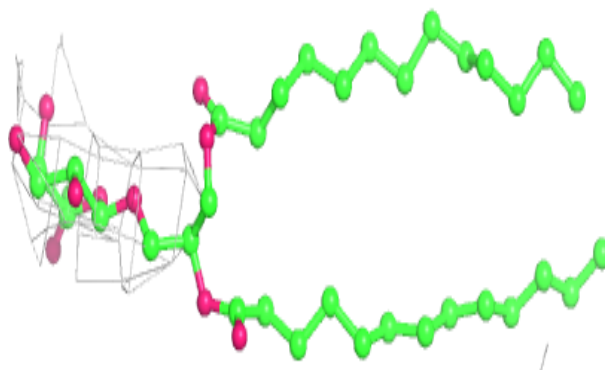


Electron density around BCR B 616:

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

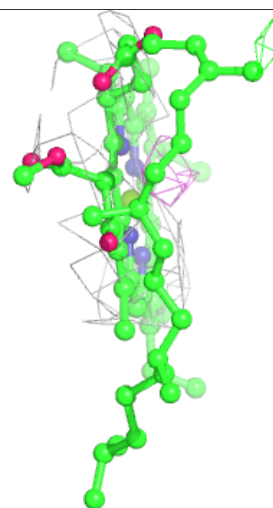
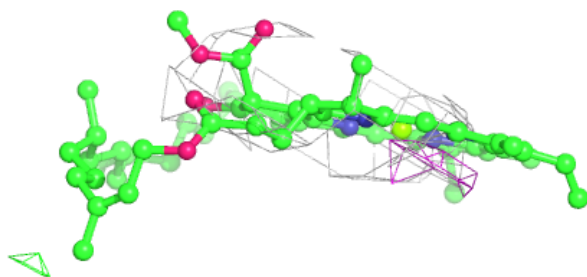
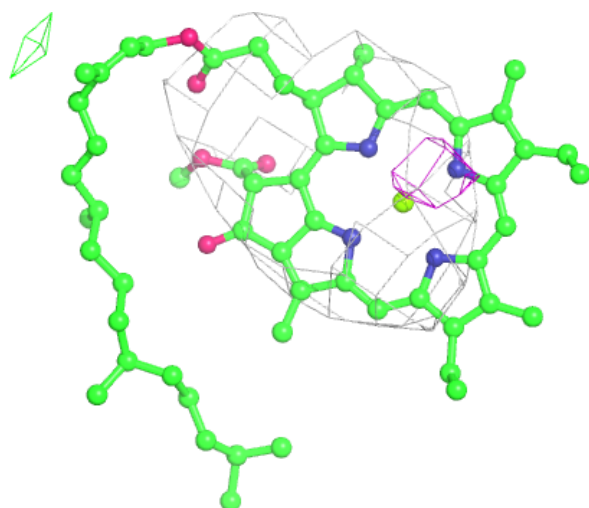
**Electron density around LMG C 518:**

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



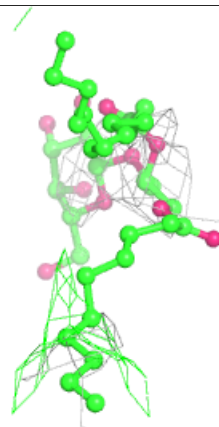
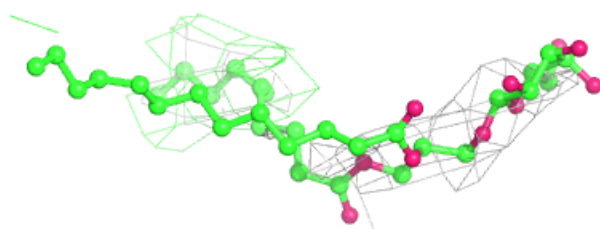
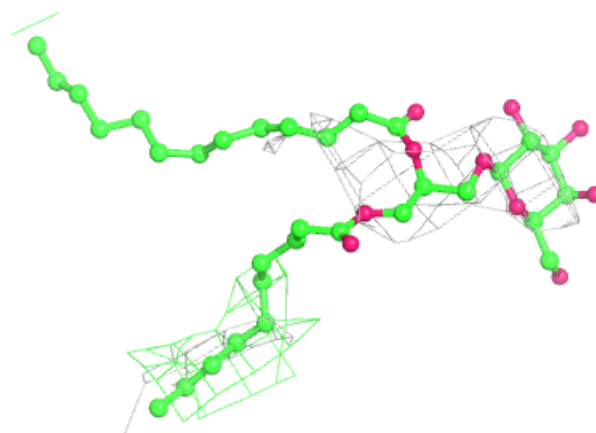
Electron density around CLA B 601:

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

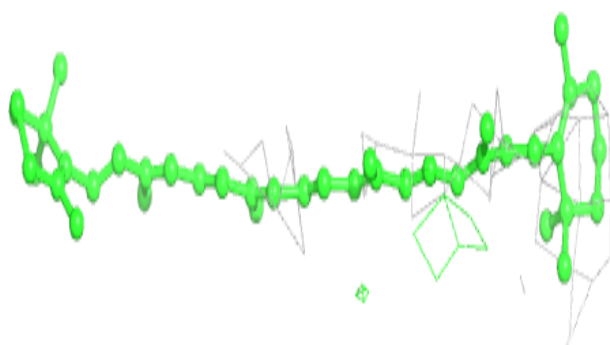
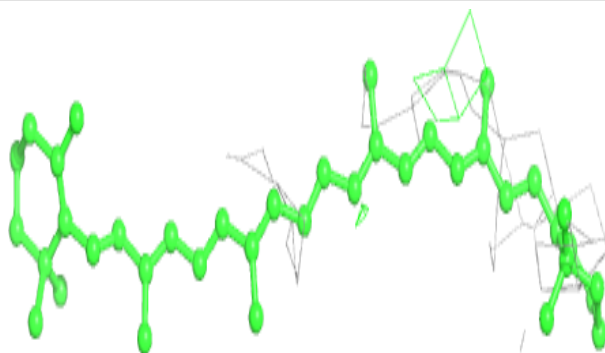


Electron density around LMG A 415:

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

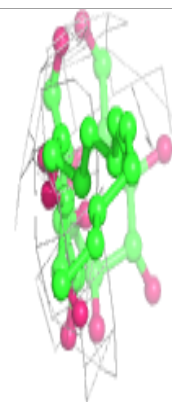
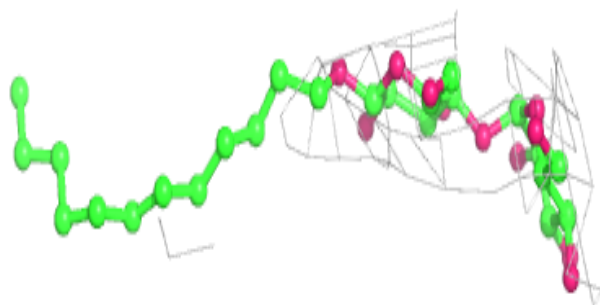
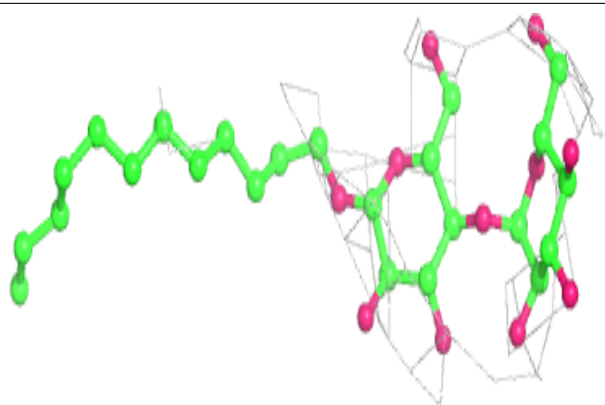
**Electron density around BCR x 101:**

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

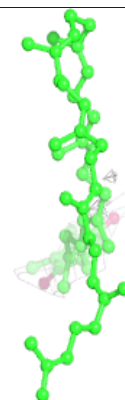
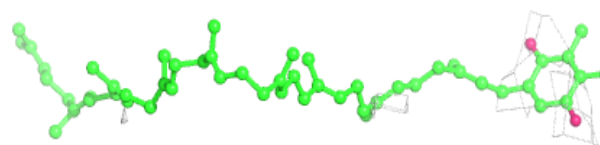
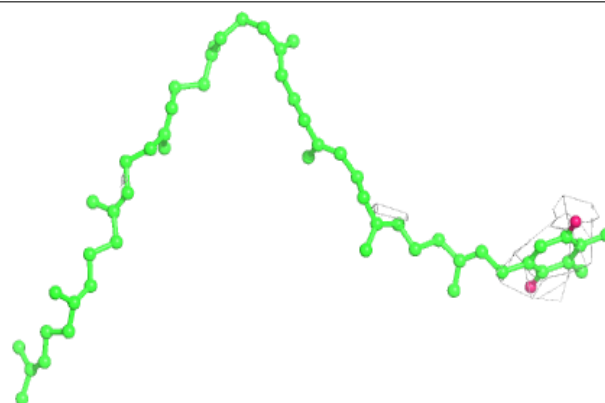


Electron density around LMT b 626:

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

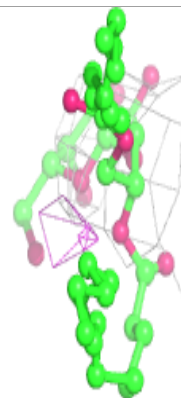
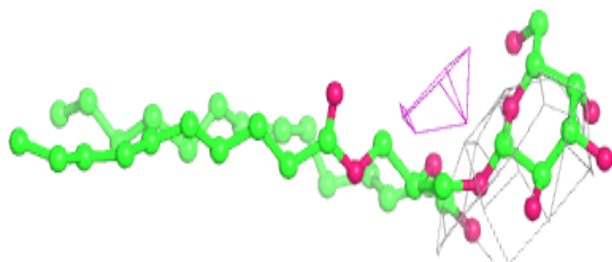
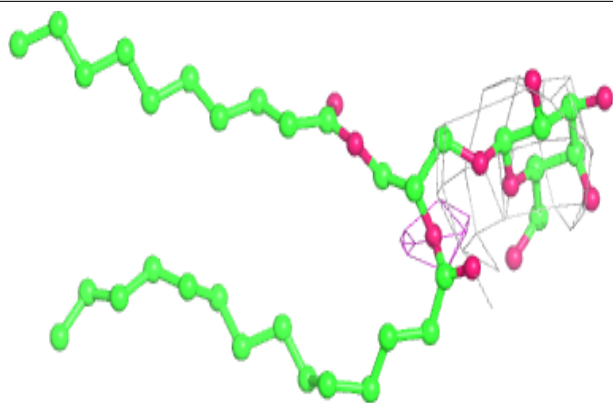
**Electron density around PL9 d 406:**

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

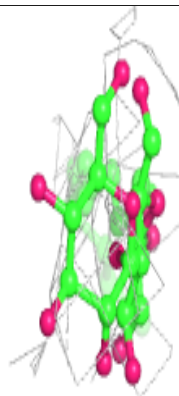
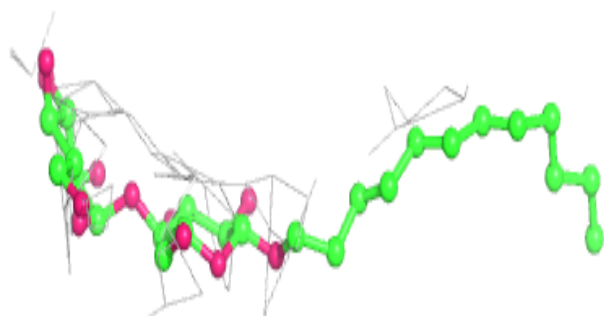
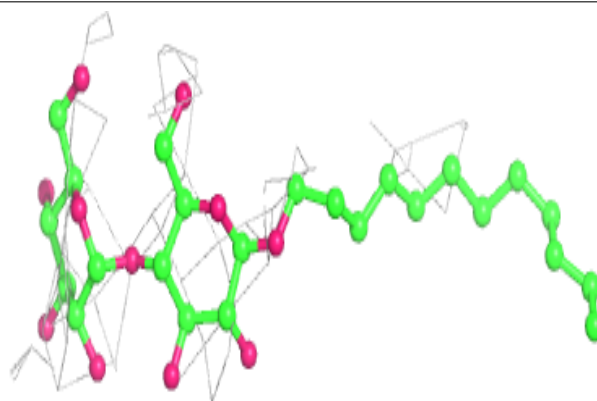


Electron density around LMG I 101:

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

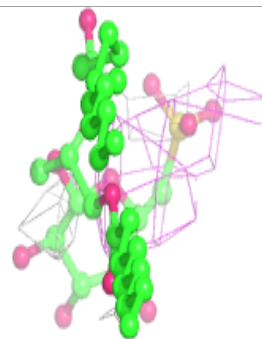
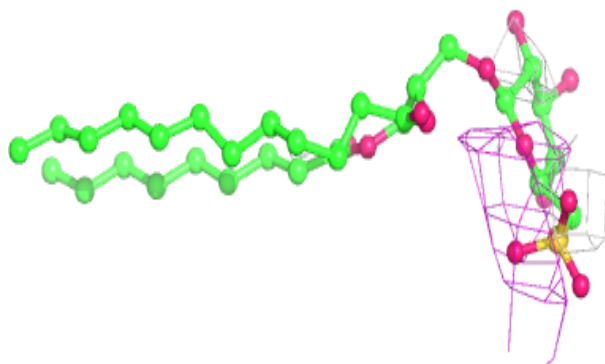
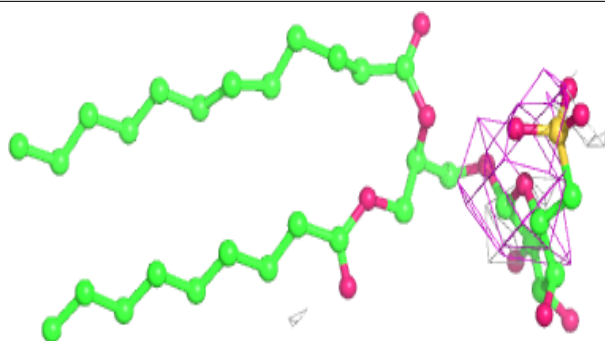
**Electron density around LMT B 623:**

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

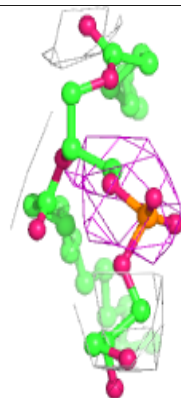
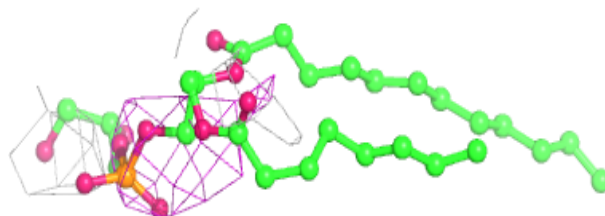
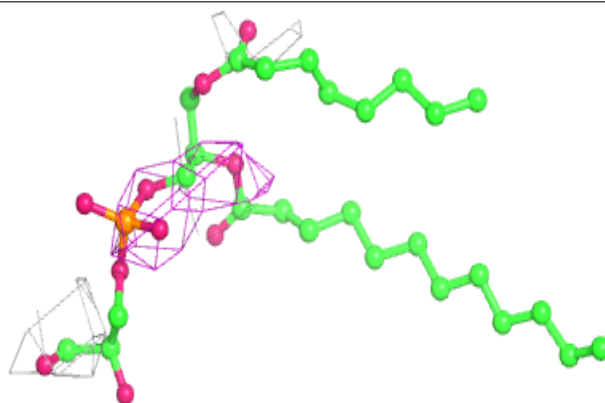


Electron density around SQD d 402:

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

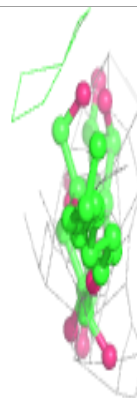
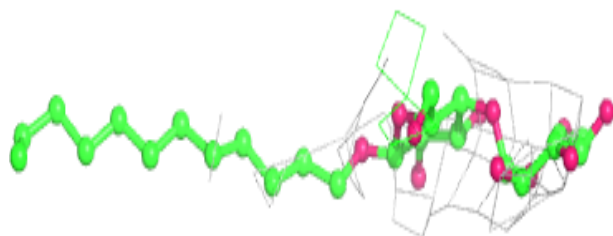
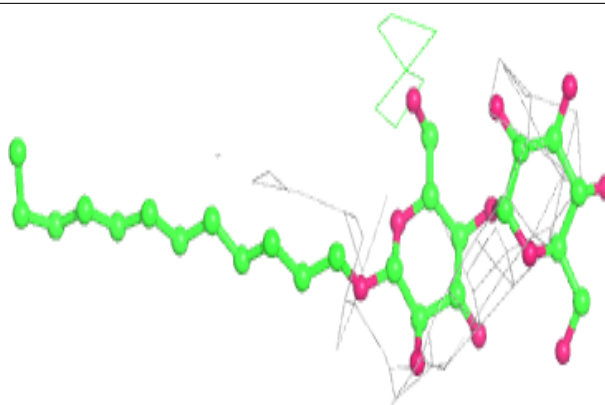
**Electron density around LHG c 519:**

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

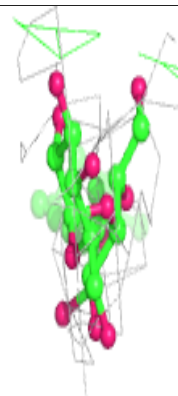
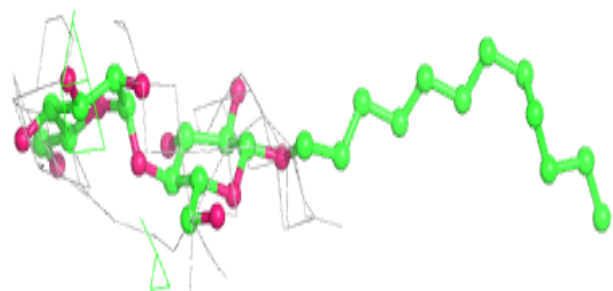
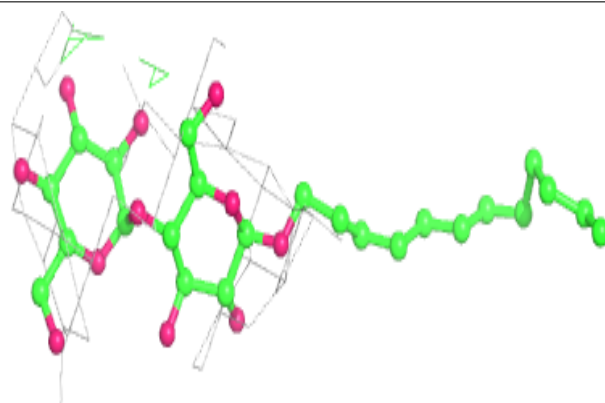


Electron density around LMT b 603:

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

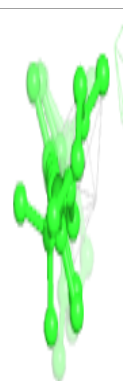
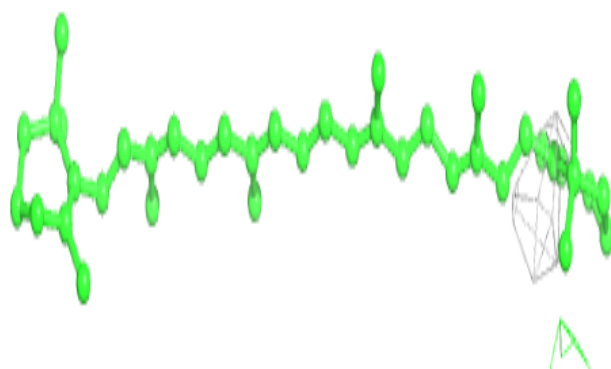
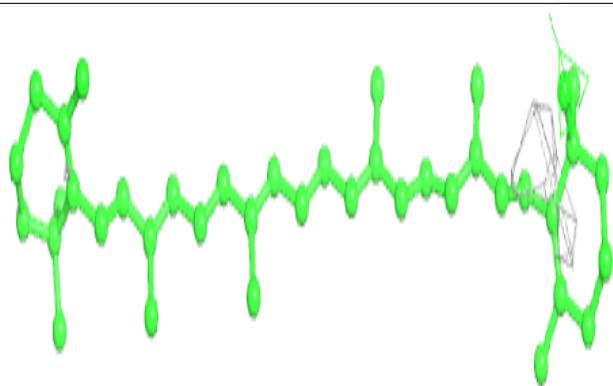
**Electron density around LMT B 628:**

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

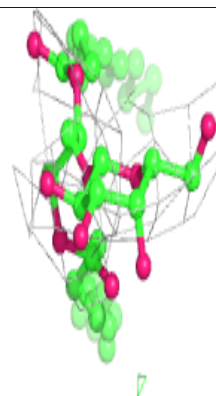
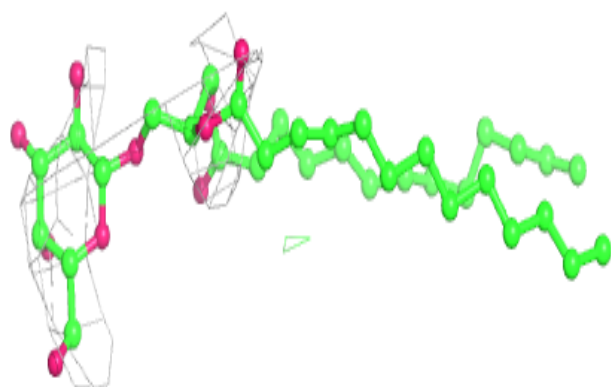
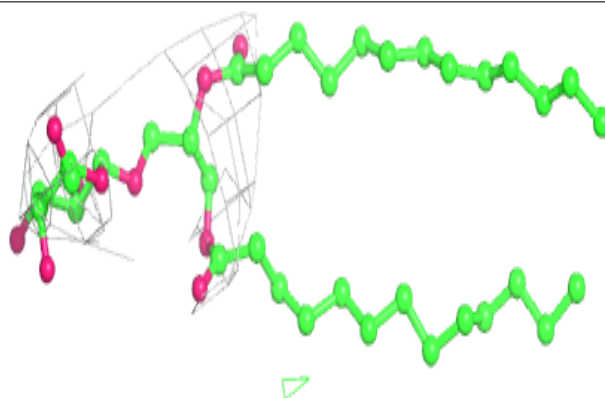


Electron density around BCR j 102:

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

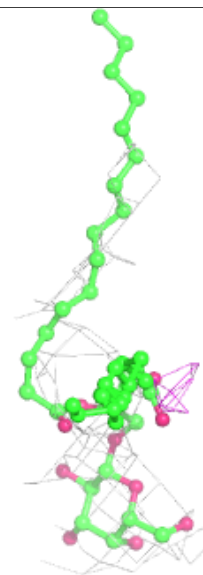
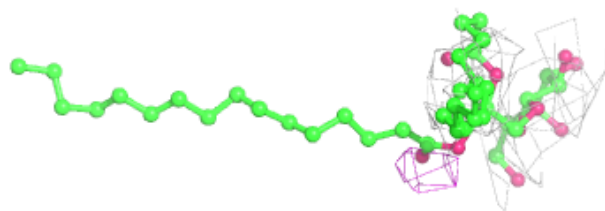
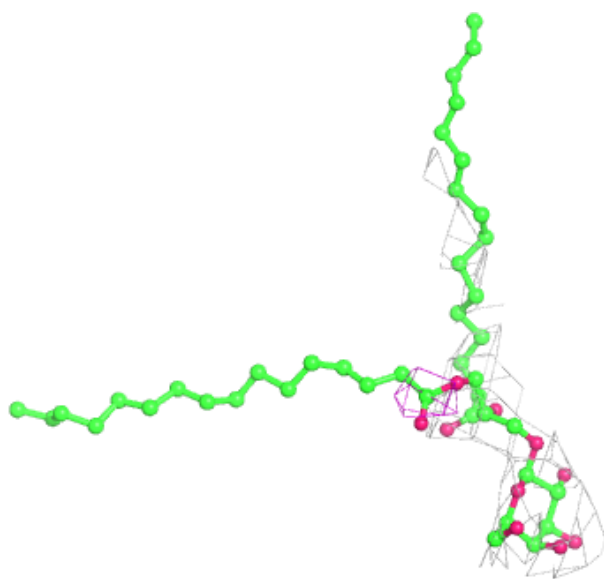
**Electron density around LMG c 518:**

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



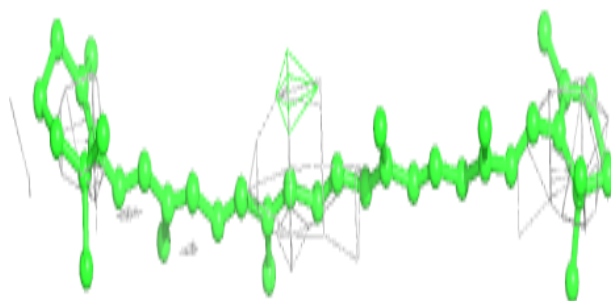
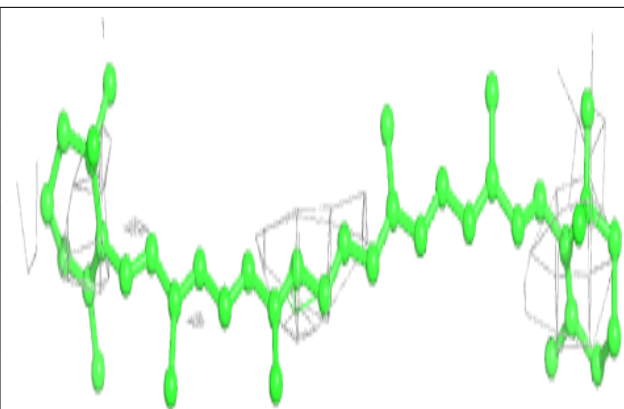
Electron density around LMG 1 101:

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

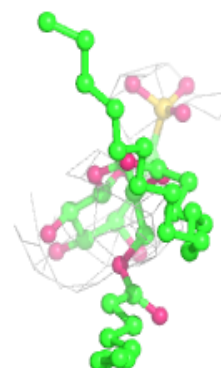
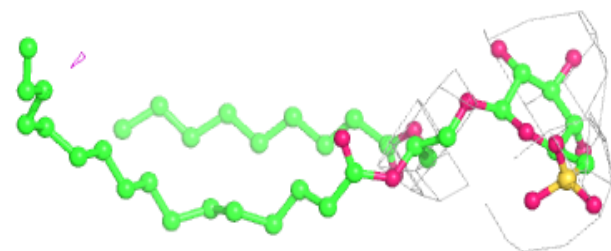
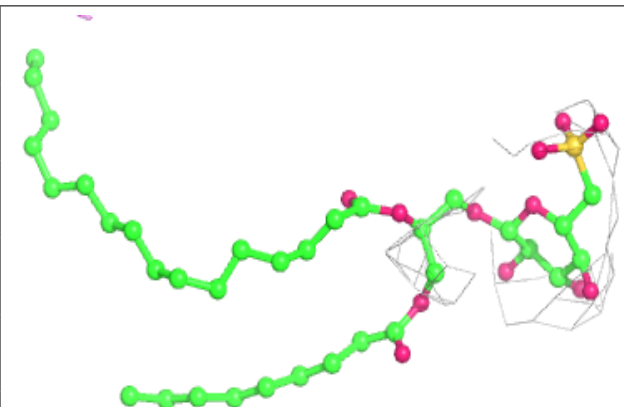


Electron density around BCR C 514:

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

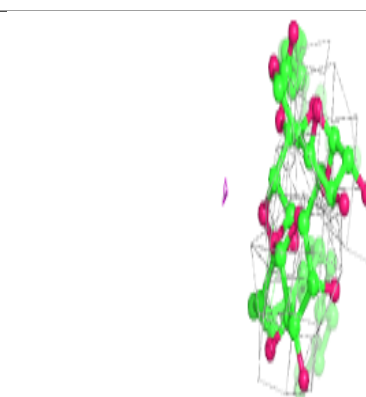
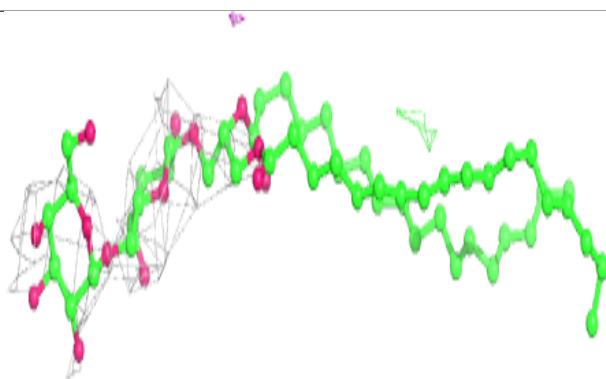
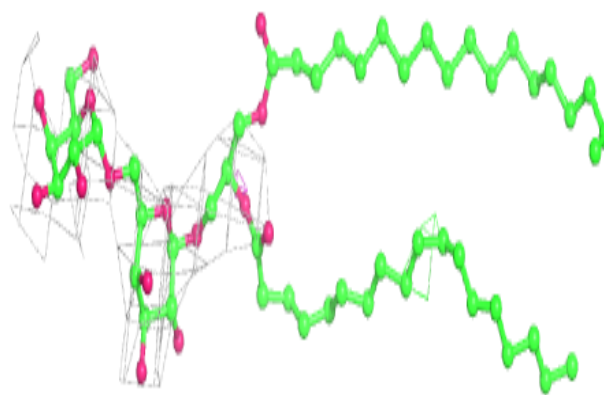
**Electron density around SQD B 626:**

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

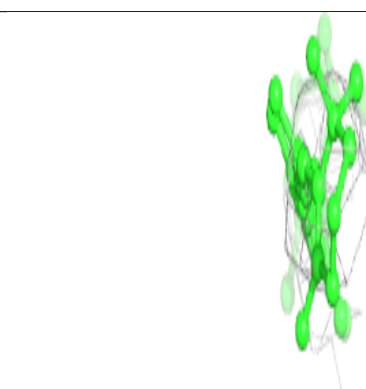
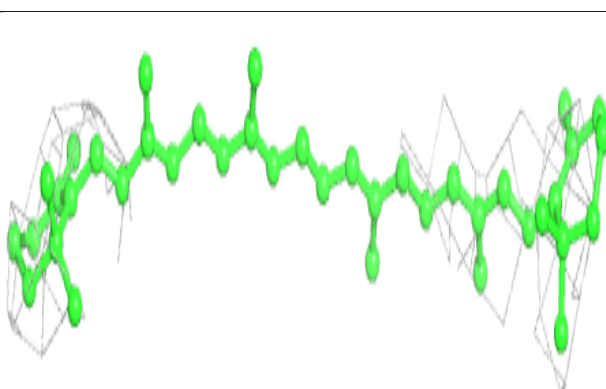
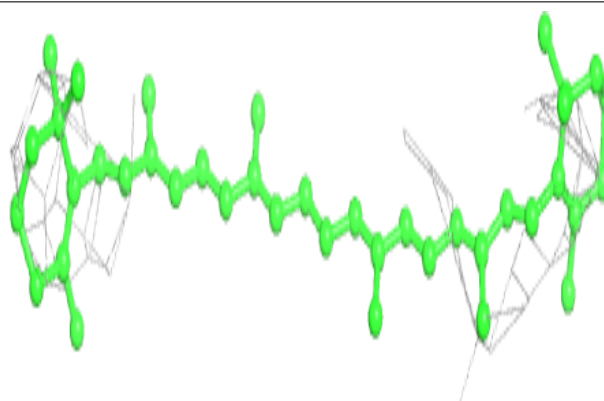


Electron density around DGD C 517:

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

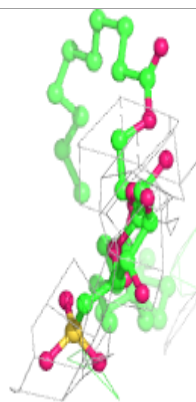
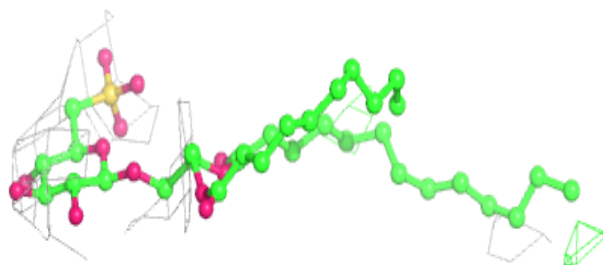
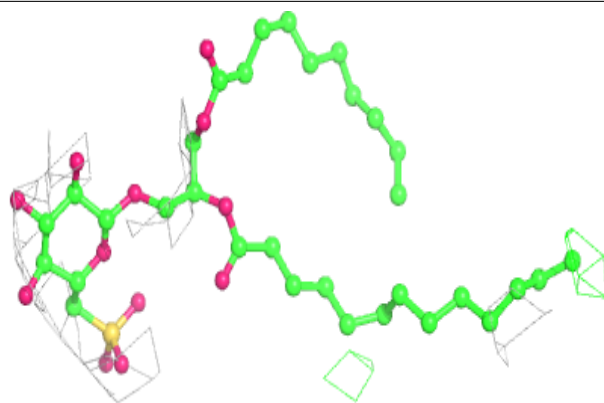
**Electron density around BCR b 623:**

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



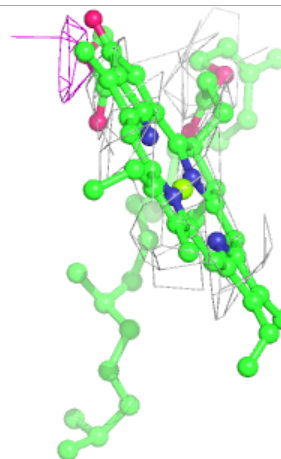
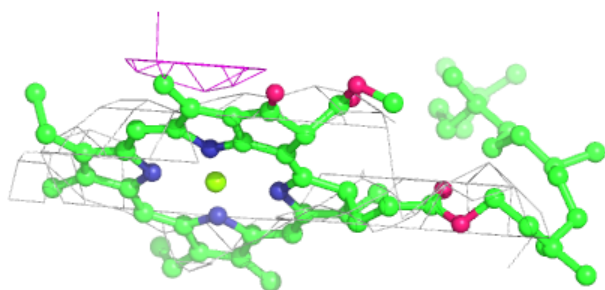
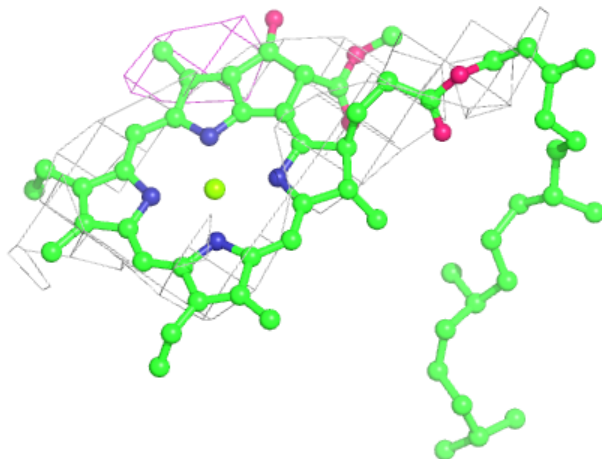
Electron density around SQD F 103:

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



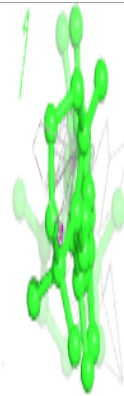
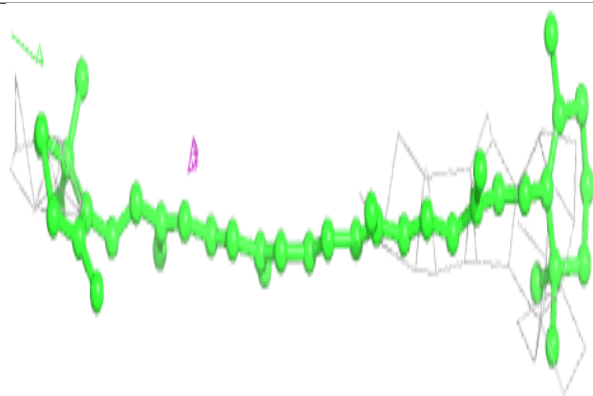
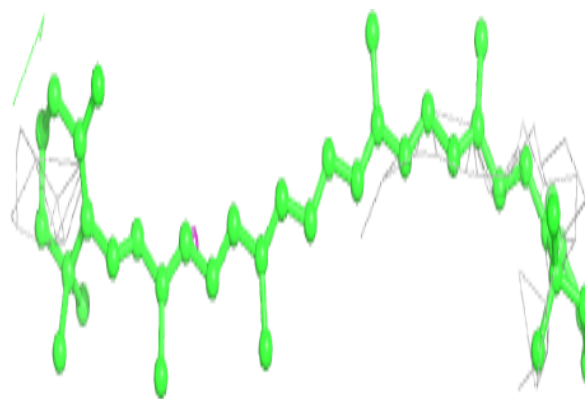
Electron density around CLA b 619:

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

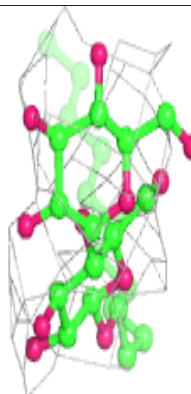
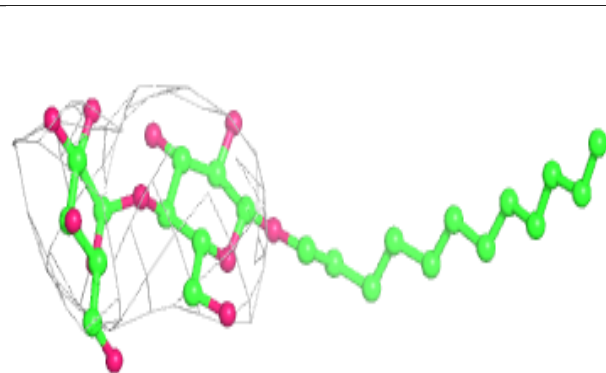
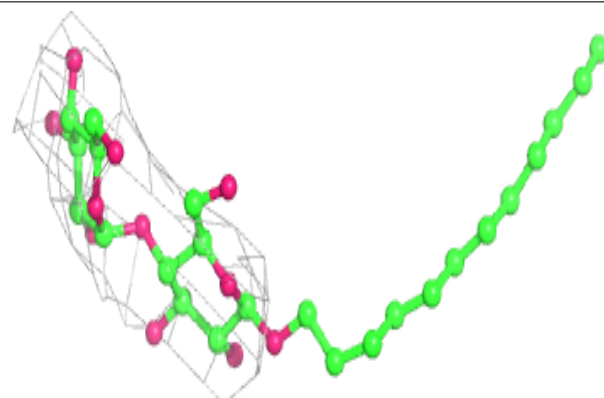


Electron density around BCR H 102:

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

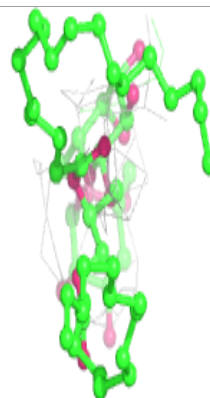
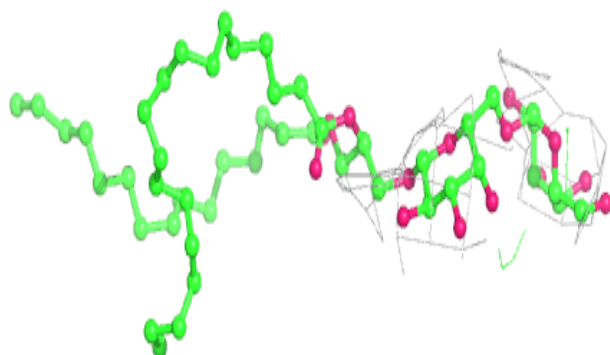
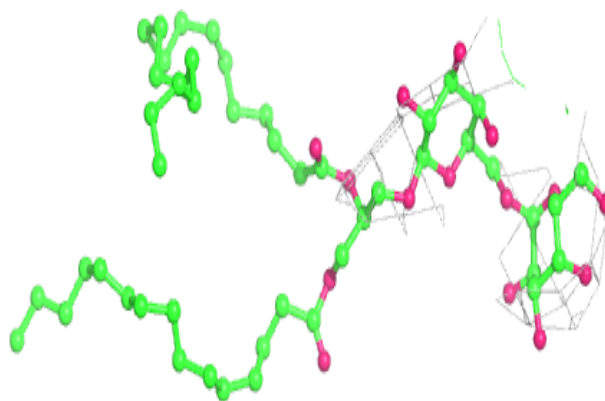
**Electron density around LMT M 102:**

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

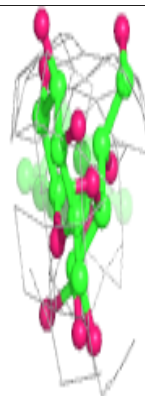
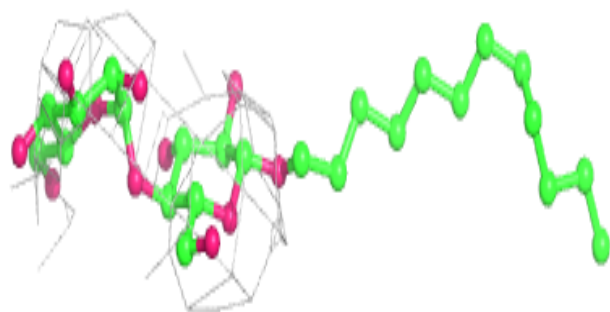
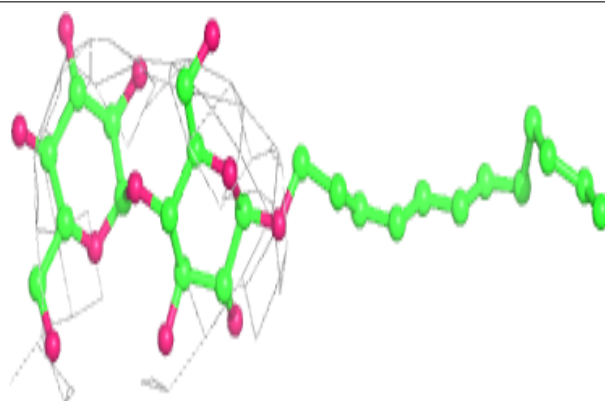


Electron density around DGD D 409:

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

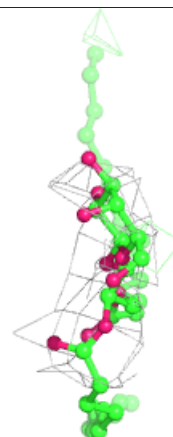
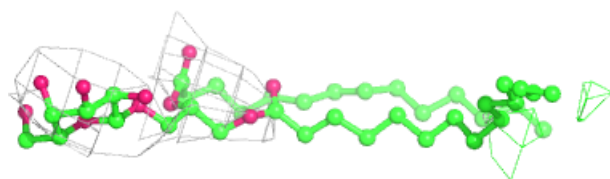
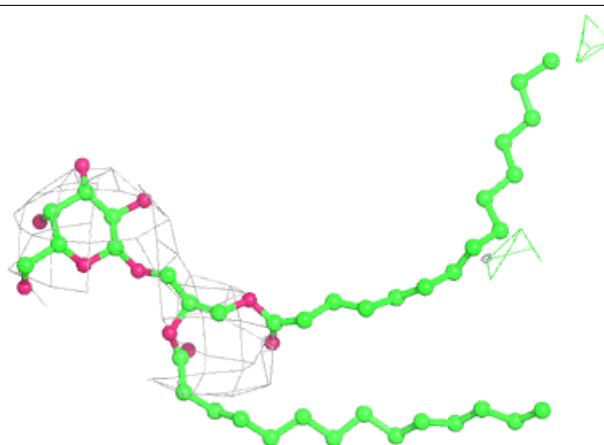
**Electron density around LMT b 604:**

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

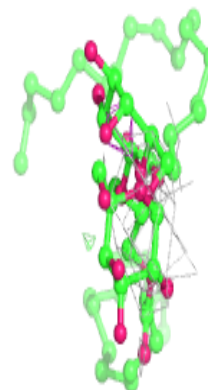
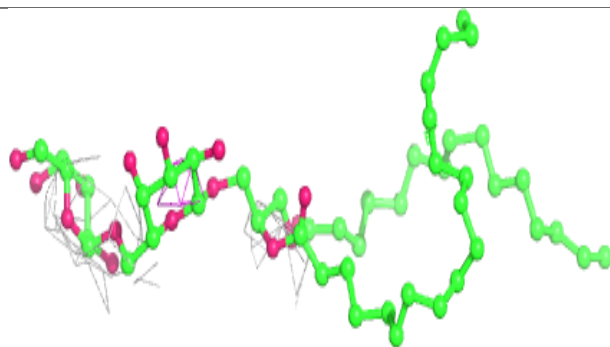
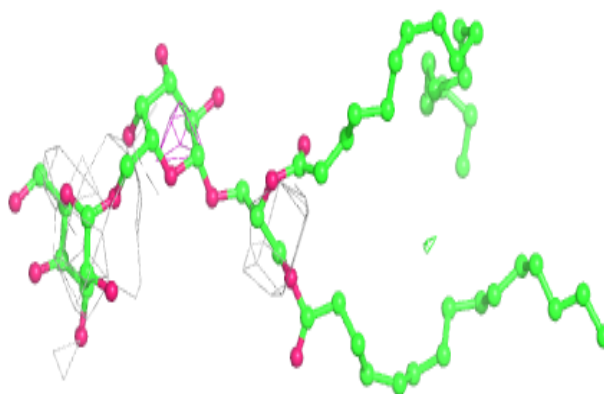


Electron density around LMG C 521:

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

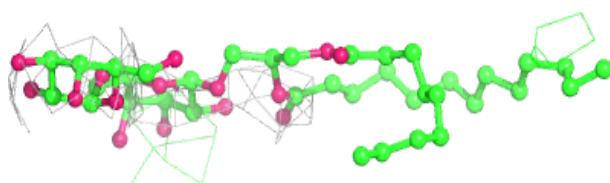
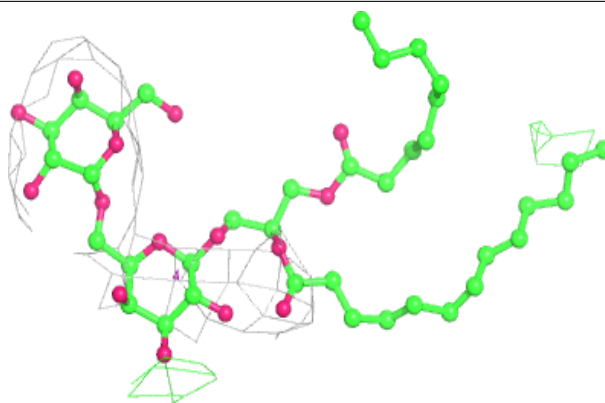
**Electron density around DGD d 409:**

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

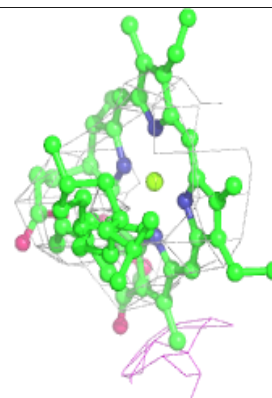
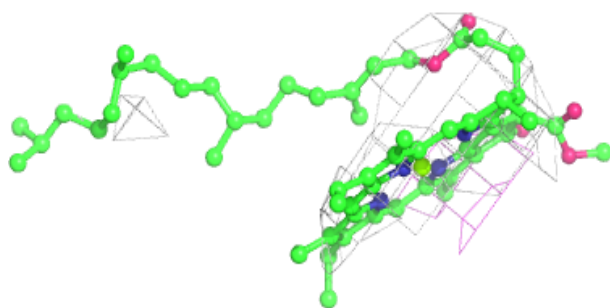
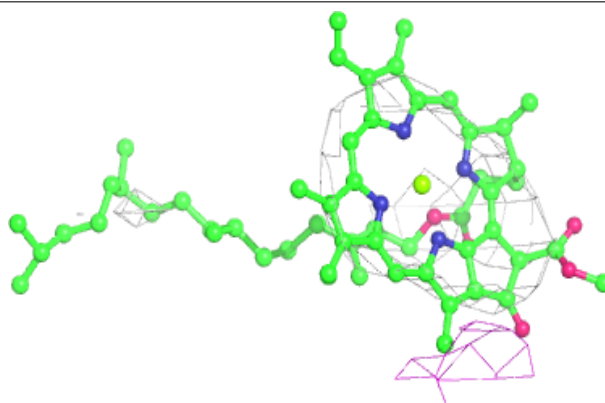


Electron density around DGD B 625:

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

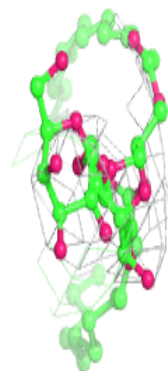
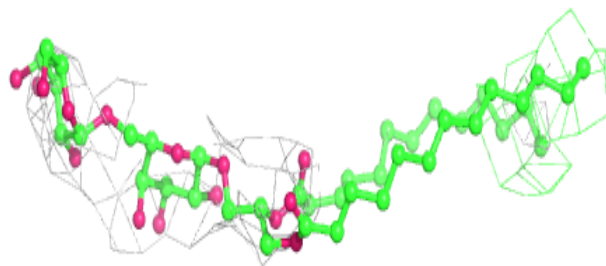
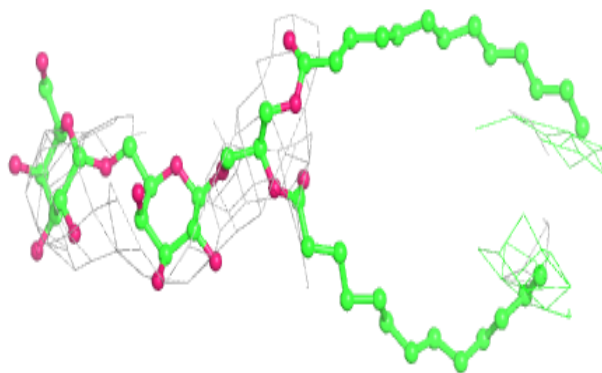
**Electron density around CLA B 613:**

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

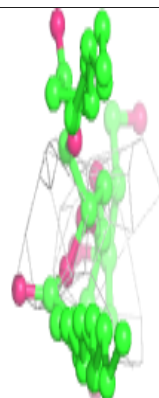
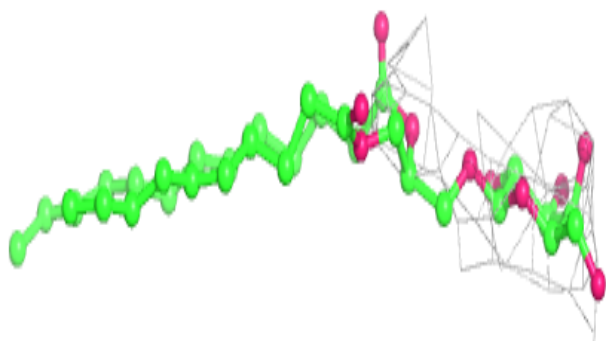
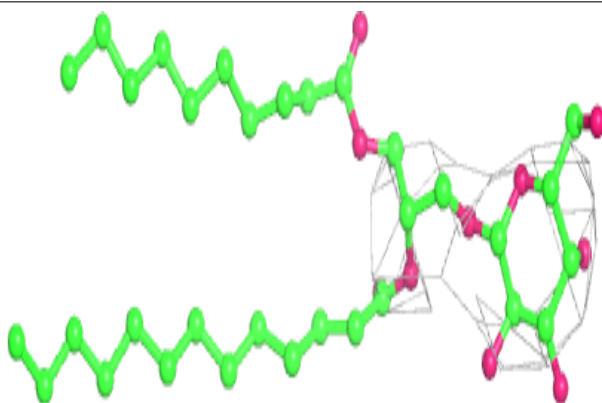


Electron density around DGD a 411:

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

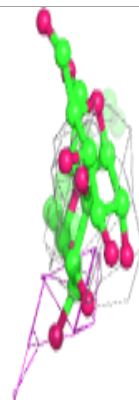
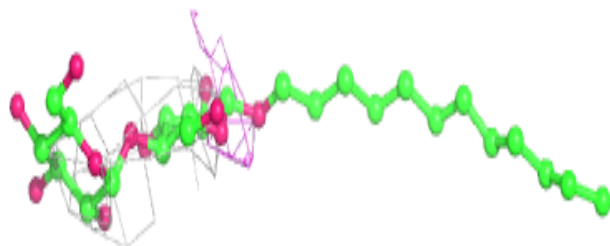
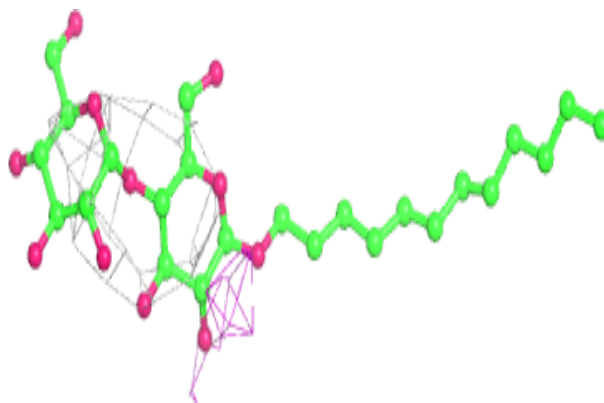
**Electron density around LMG M 101:**

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



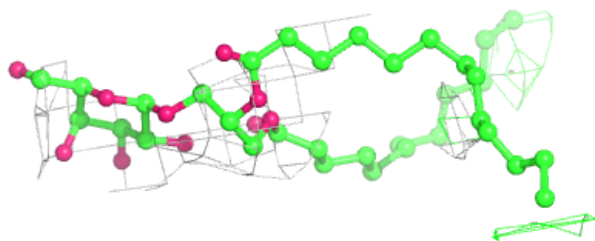
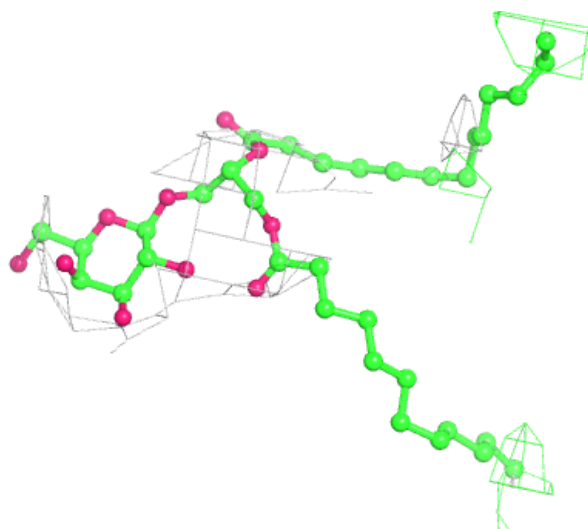
Electron density around LMT b 627:

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



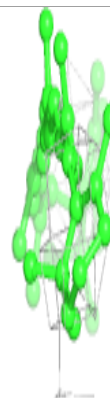
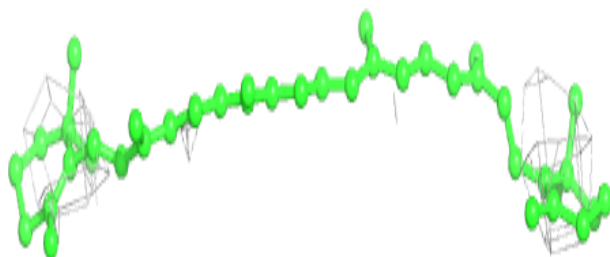
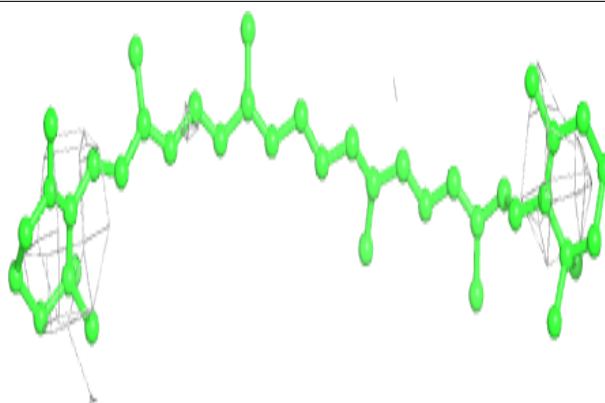
Electron density around LMG e 101:

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

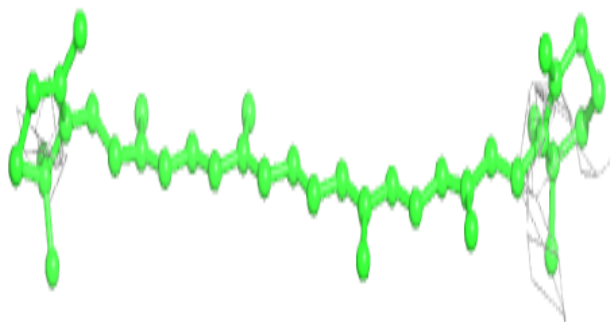
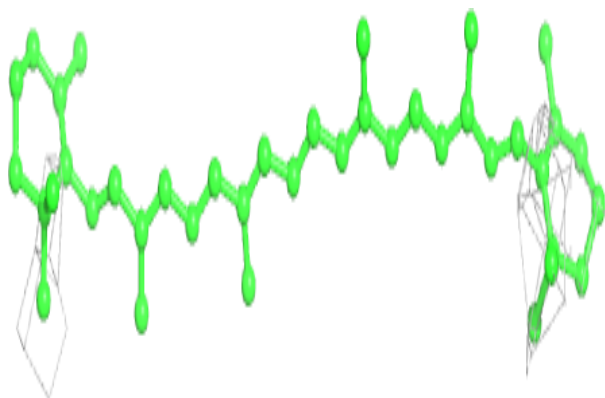


Electron density around BCR B 617:

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

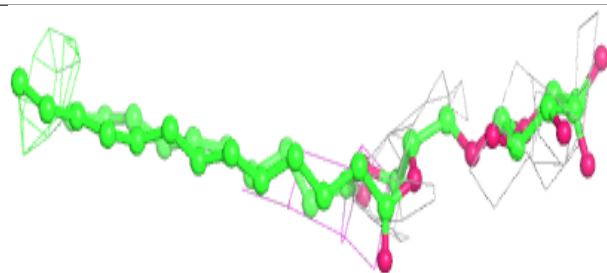
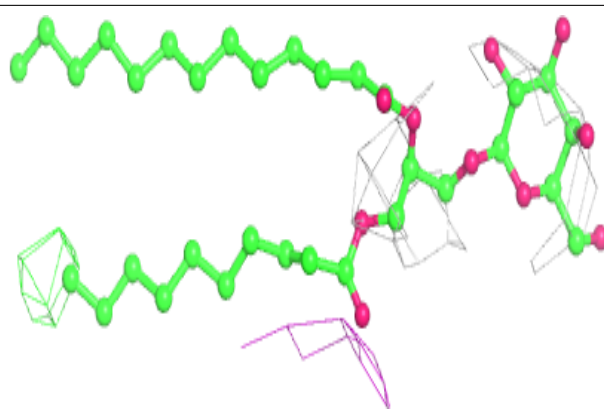
**Electron density around BCR c 514:**

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



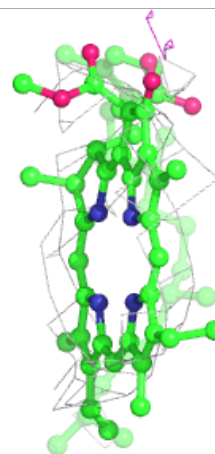
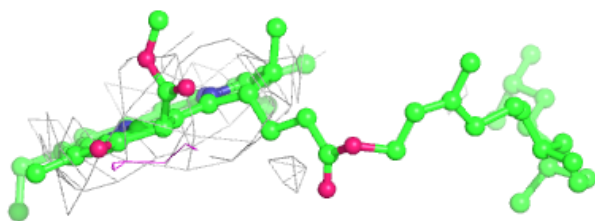
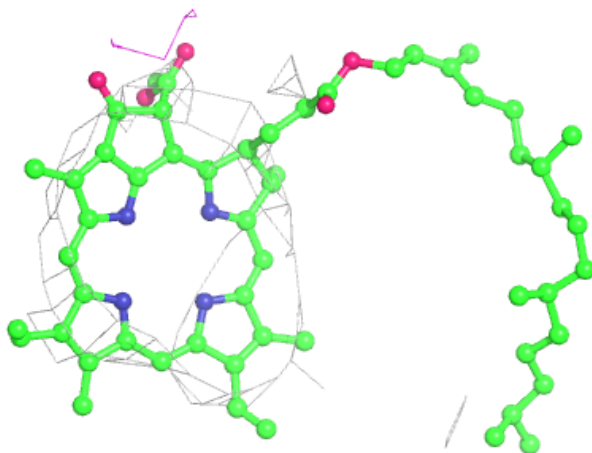
Electron density around LMG m 101:

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



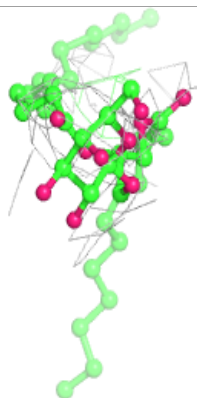
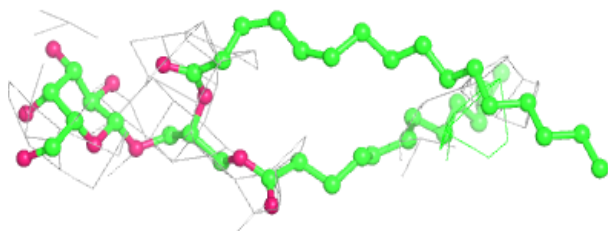
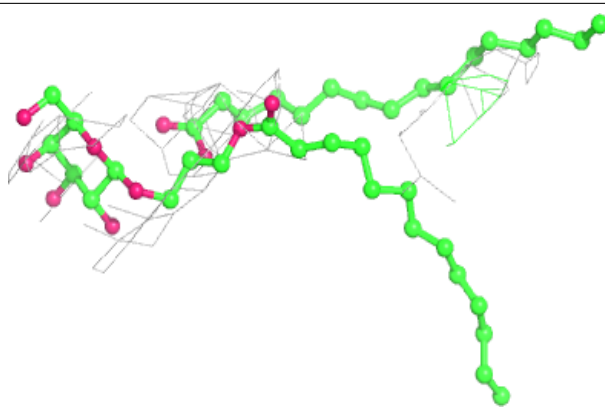
Electron density around PHO d 401:

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

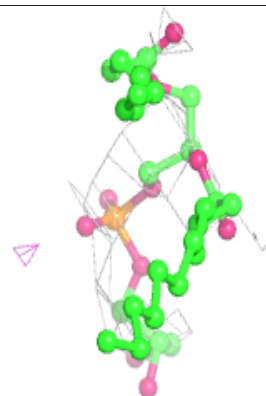
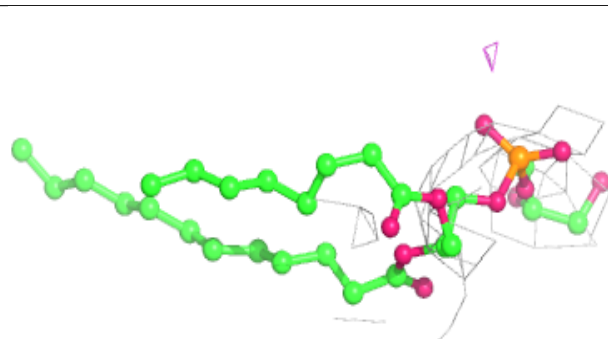
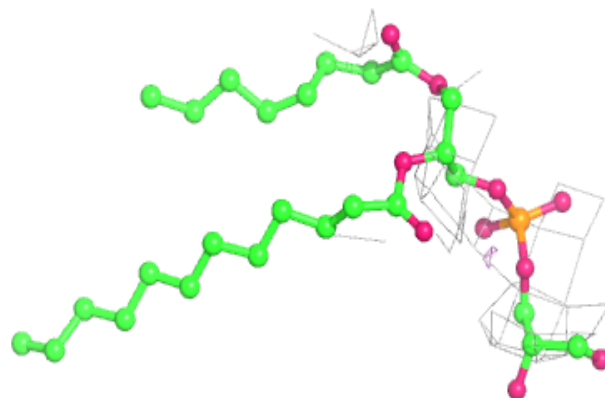


Electron density around LMG d 408:

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

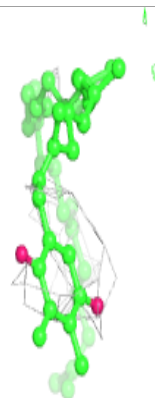
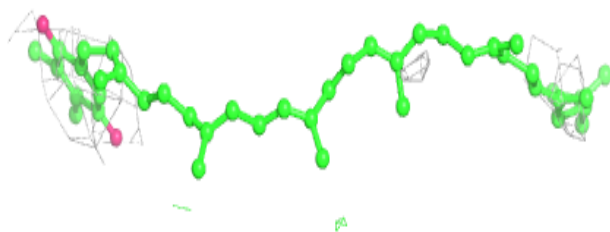
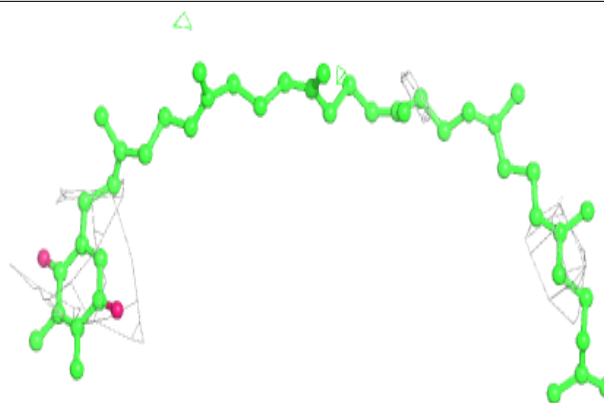
**Electron density around LHG C 519:**

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

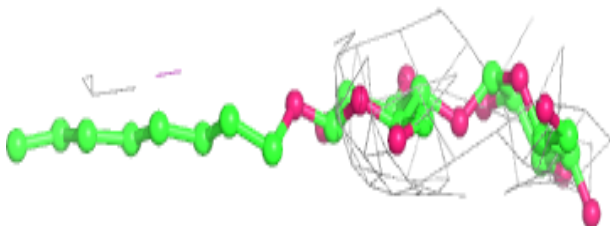
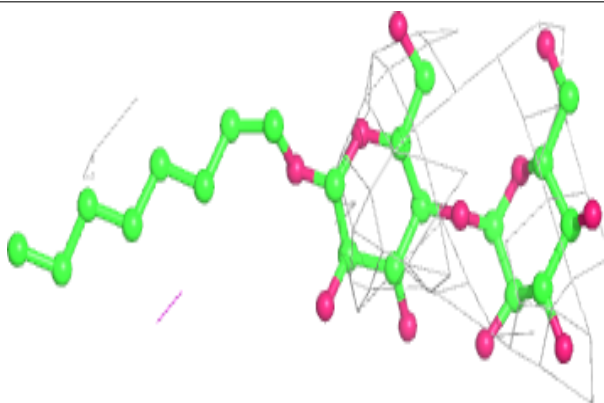


Electron density around PL9 a 409:

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

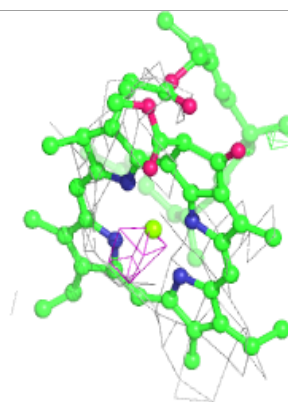
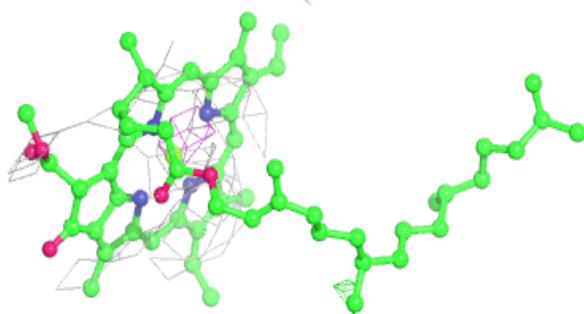
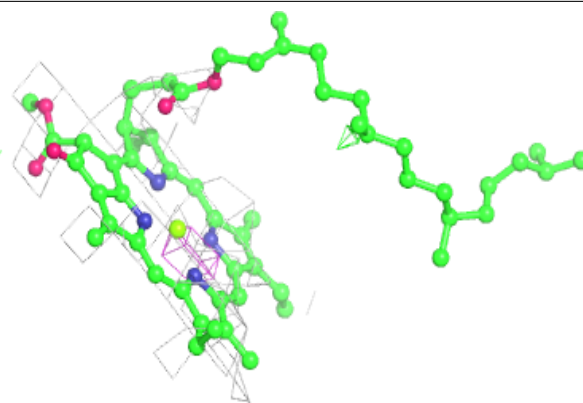
**Electron density around LMT D 410:**

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

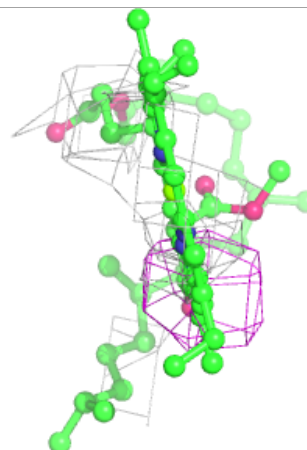
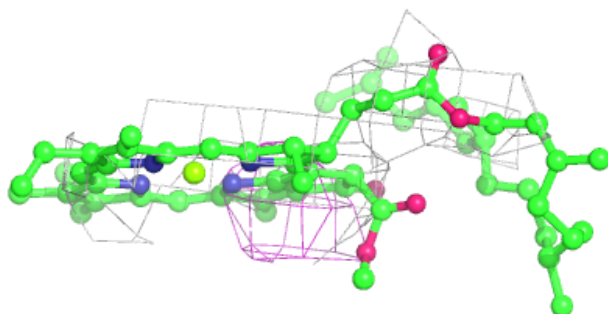
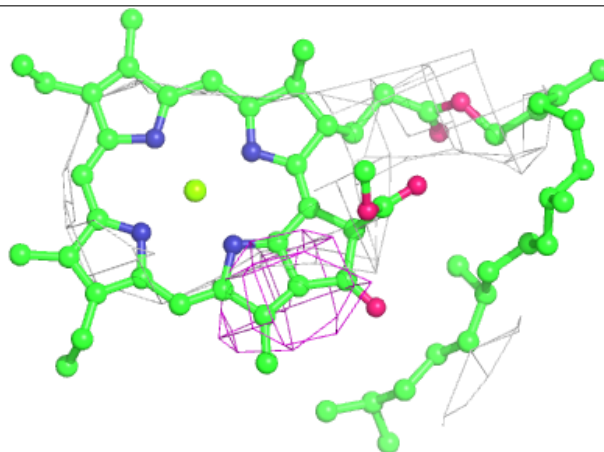


Electron density around CLA c 512:

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

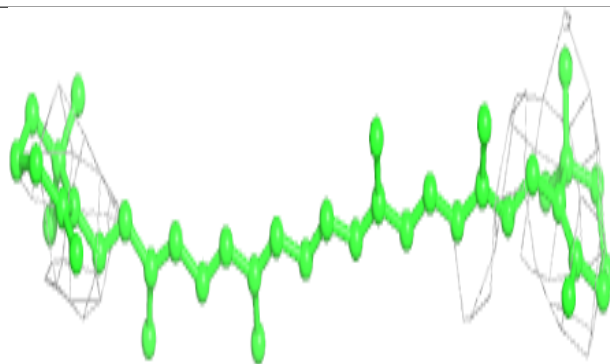
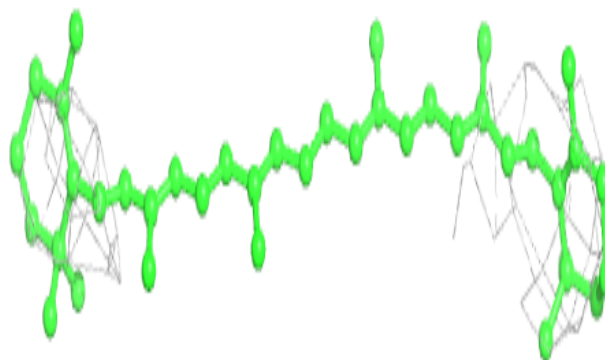
**Electron density around CLA b 613:**

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

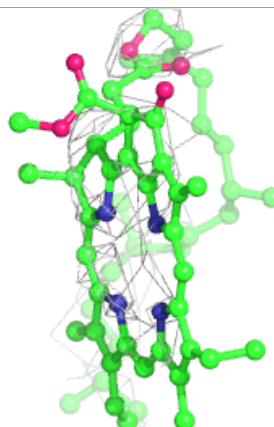
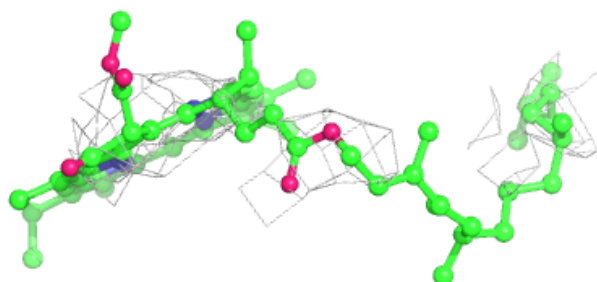
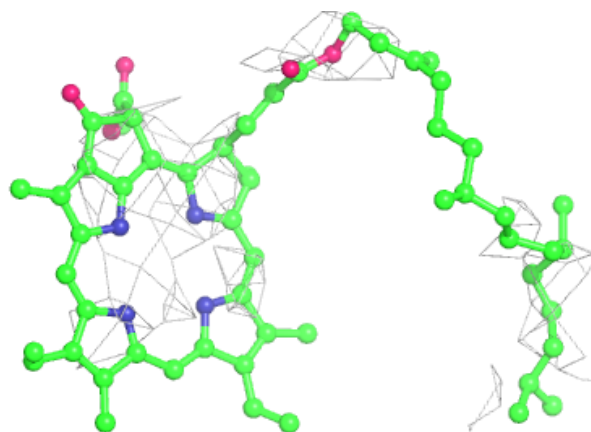


Electron density around BCR B 619:

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

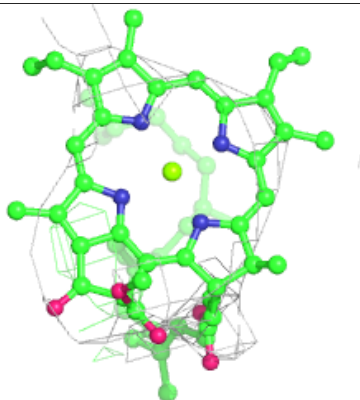
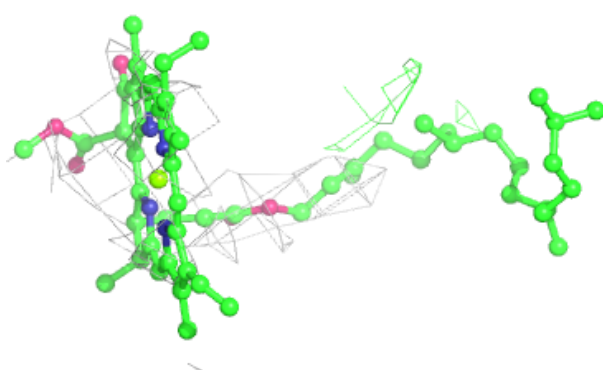
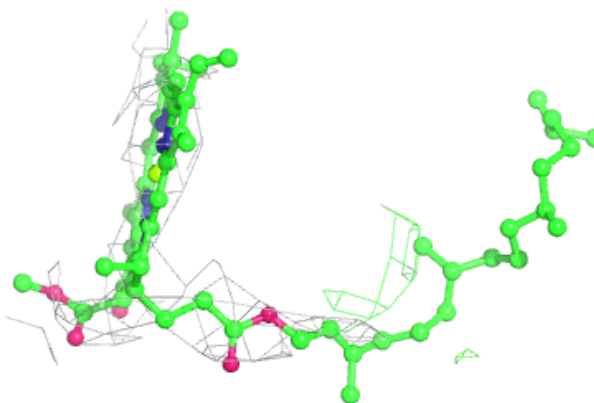
**Electron density around PHO D 402:**

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

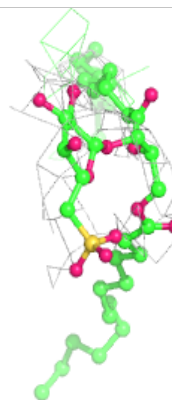
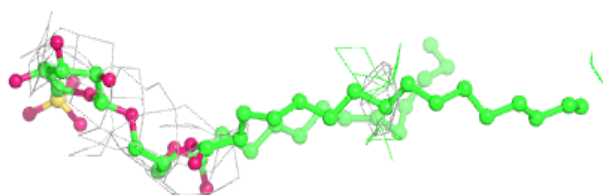
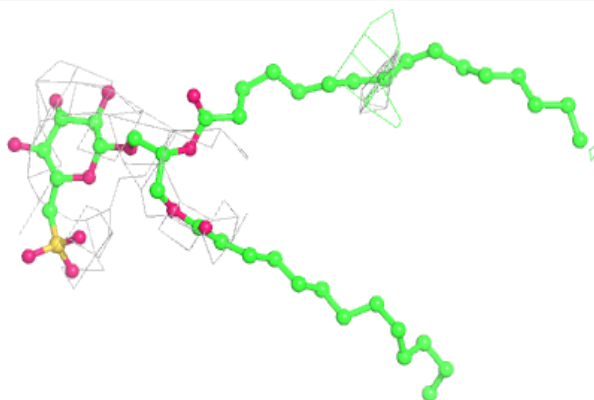


Electron density around CLA C 505:

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

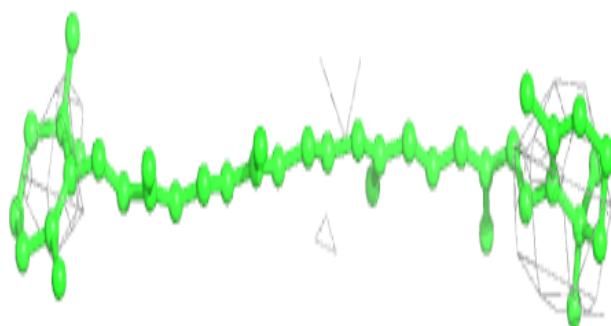
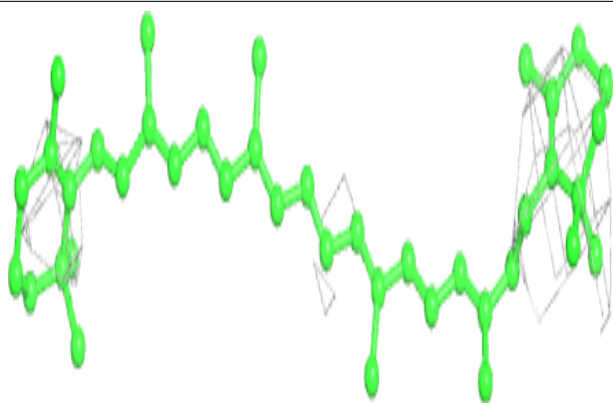
**Electron density around SQD A 413:**

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

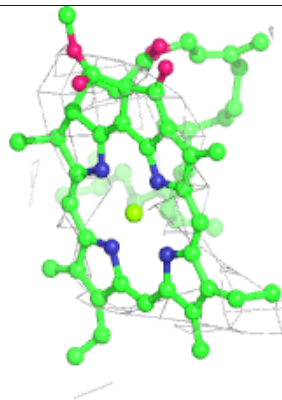
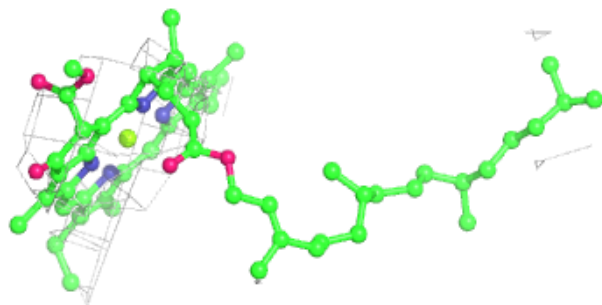
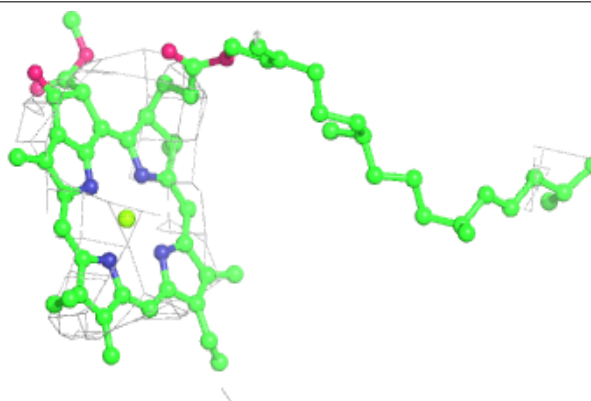


Electron density around BCR y 101:

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

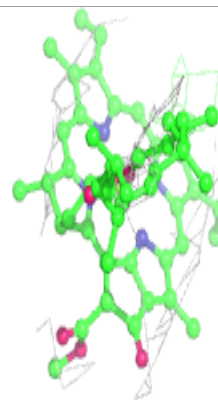
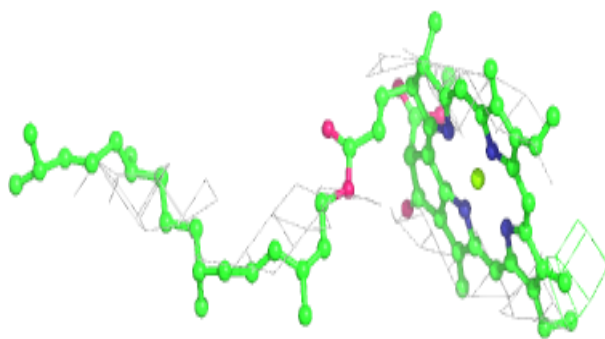
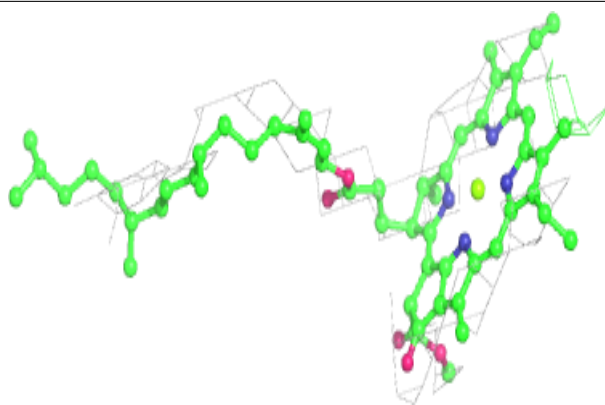
**Electron density around CLA c 510:**

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

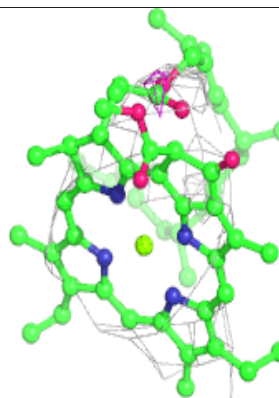
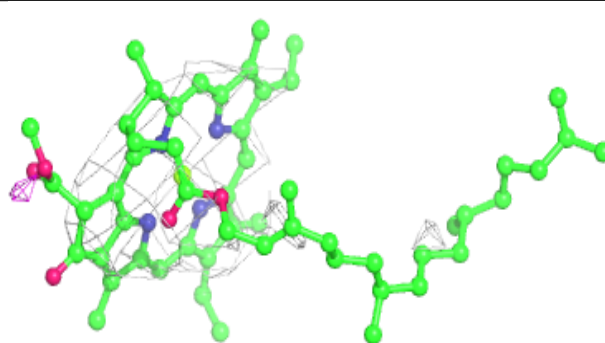
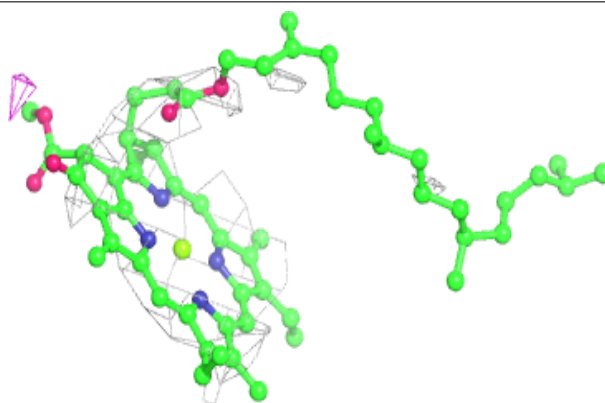


Electron density around CLA C 502:

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

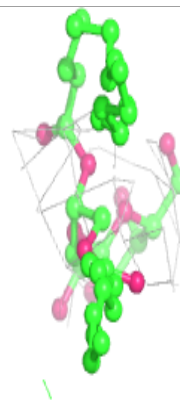
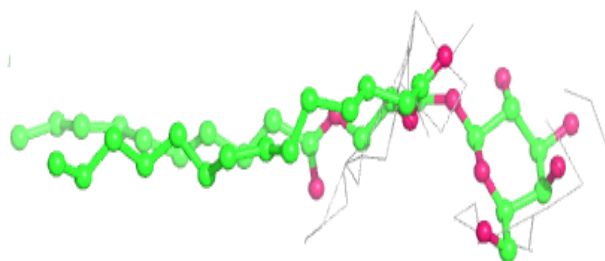
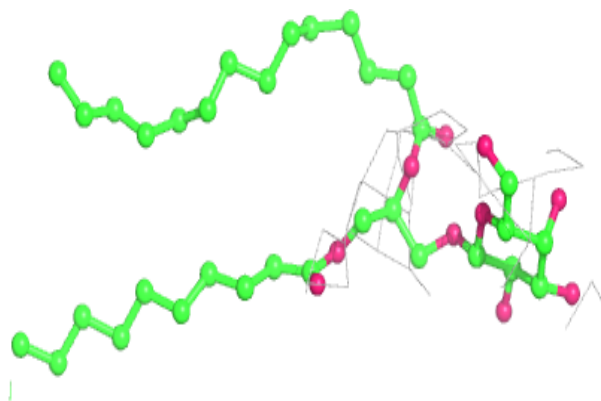
**Electron density around CLA C 512:**

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



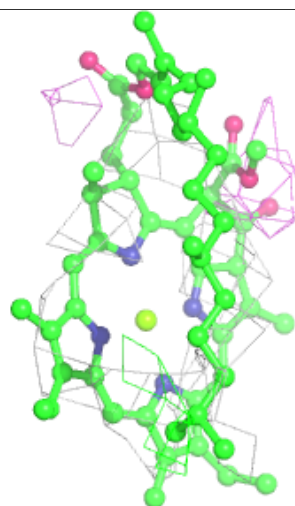
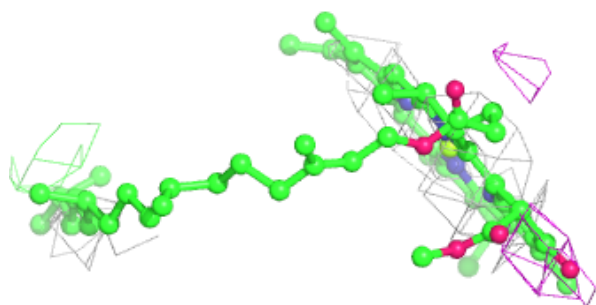
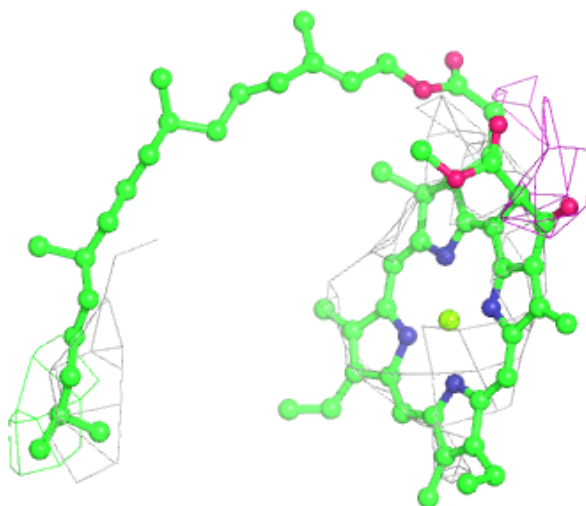
Electron density around LMG i 101:

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



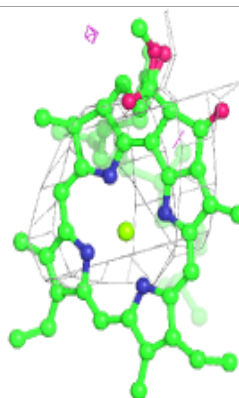
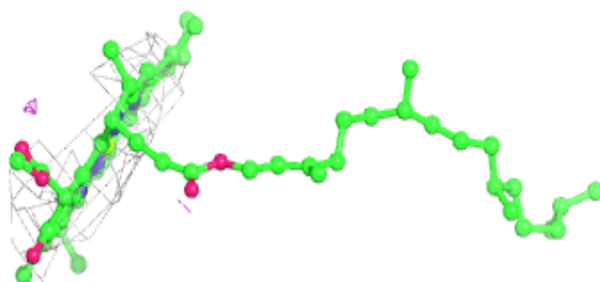
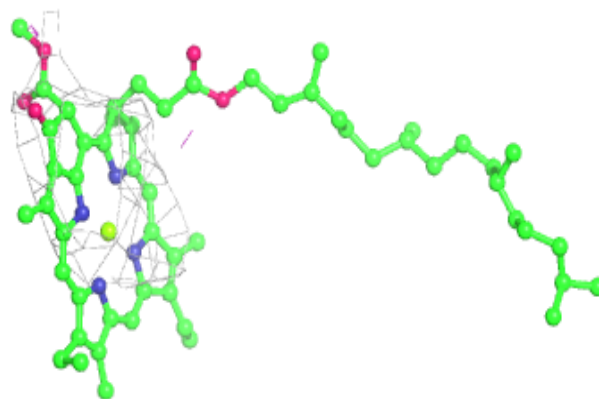
Electron density around CLA C 506:

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

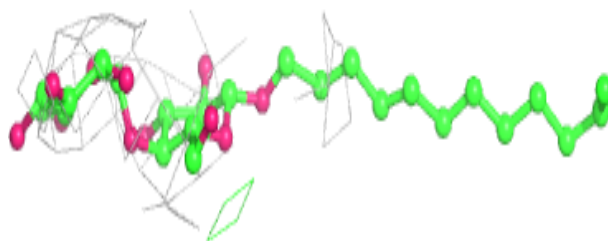
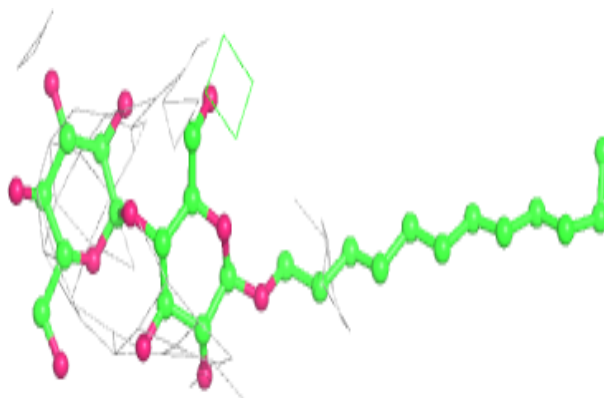


Electron density around CLA a 408:

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

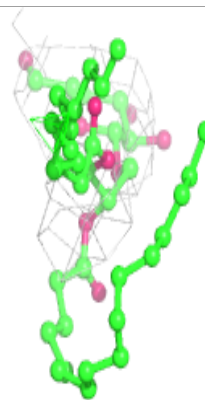
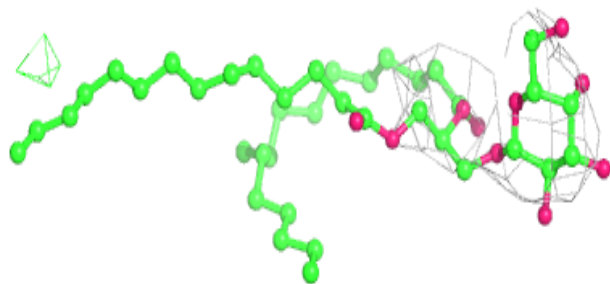
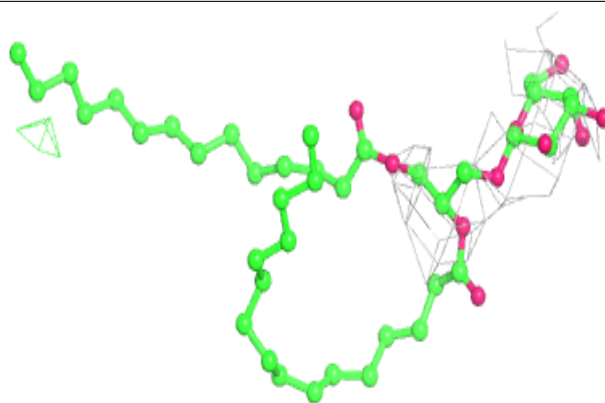
**Electron density around LMT B 627:**

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

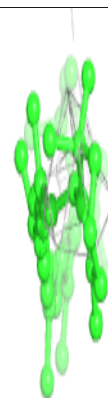
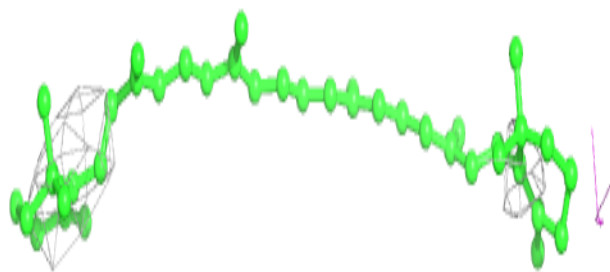
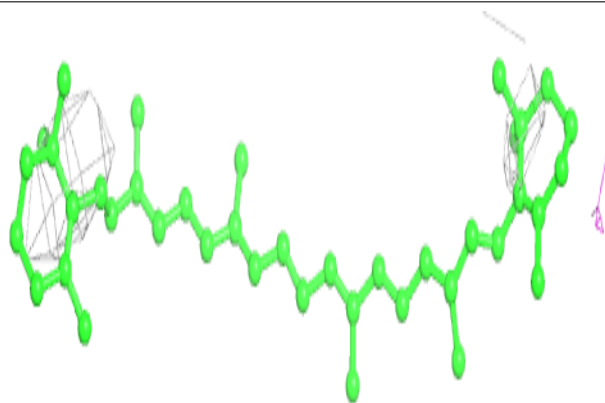


Electron density around LMG D 407:

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

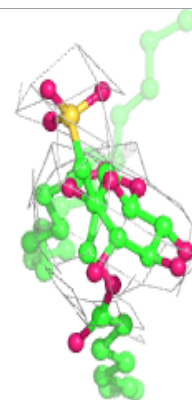
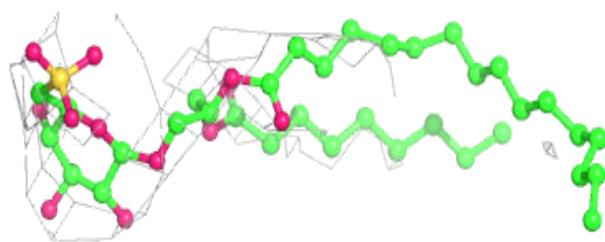
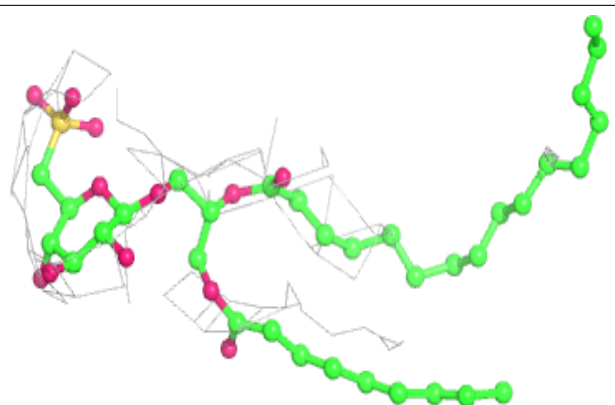
**Electron density around BCR b 621:**

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

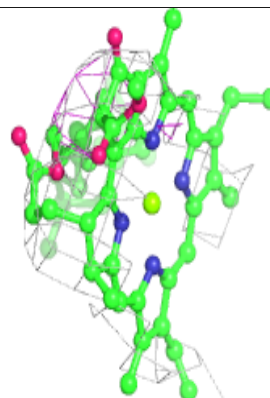
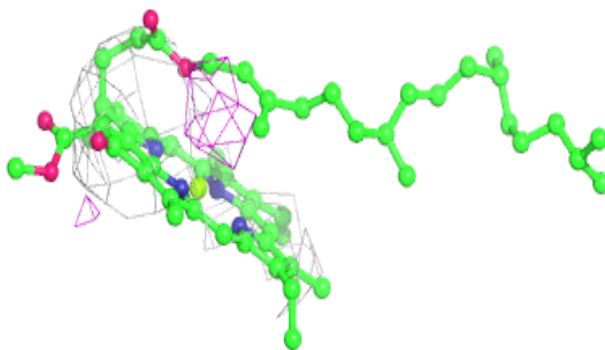
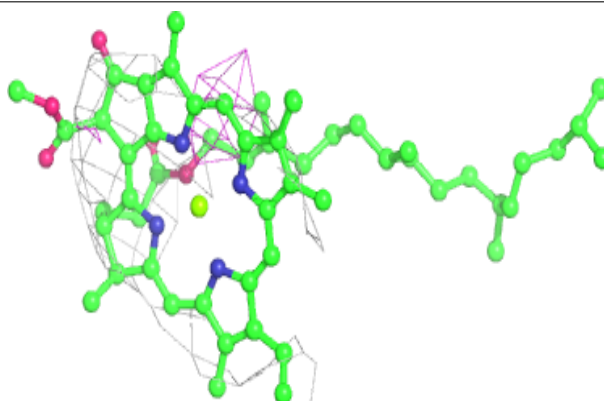


Electron density around SQD b 602:

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

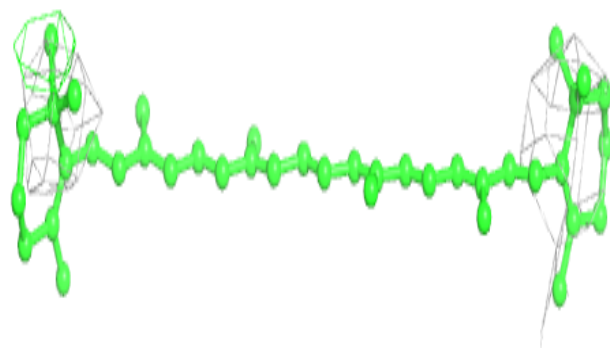
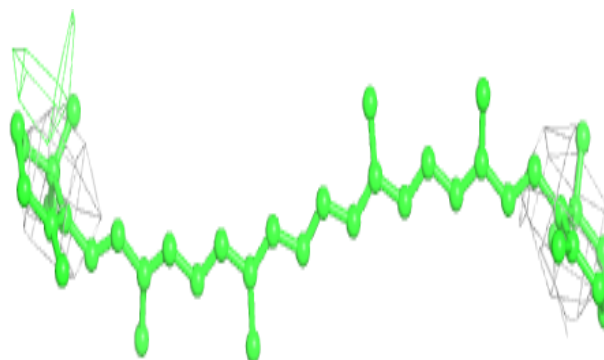
**Electron density around CLA b 617:**

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

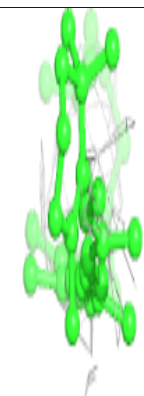
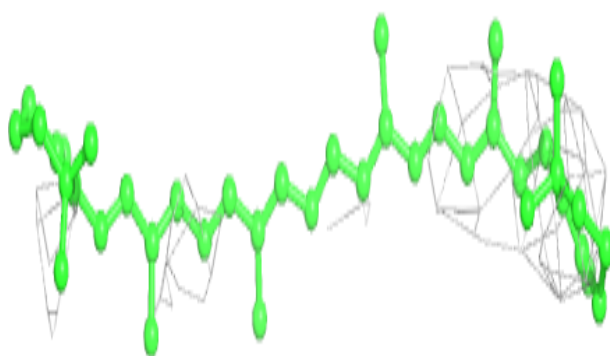
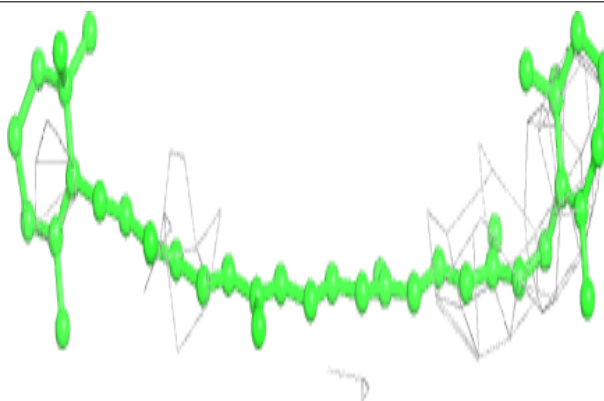


Electron density around BCR a 410:

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

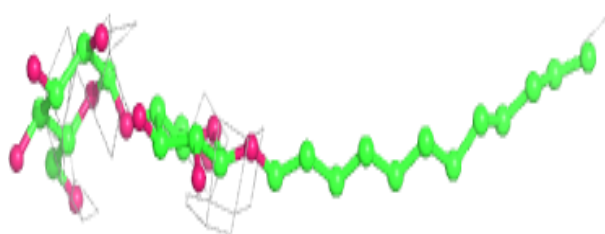
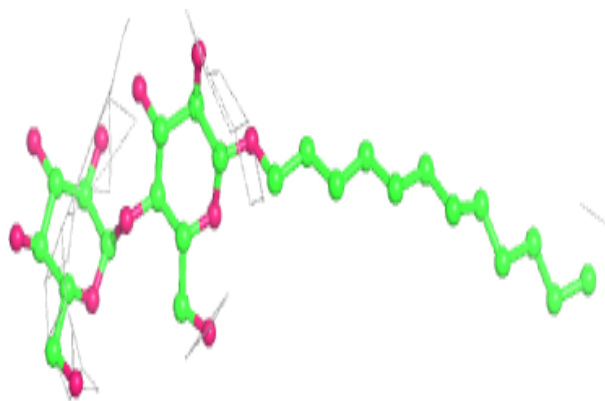
**Electron density around BCR c 513:**

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

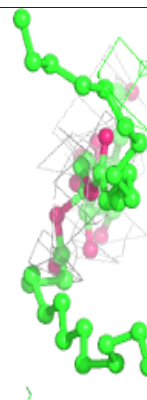
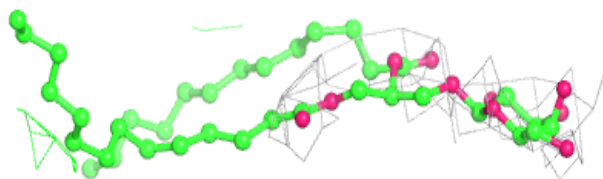
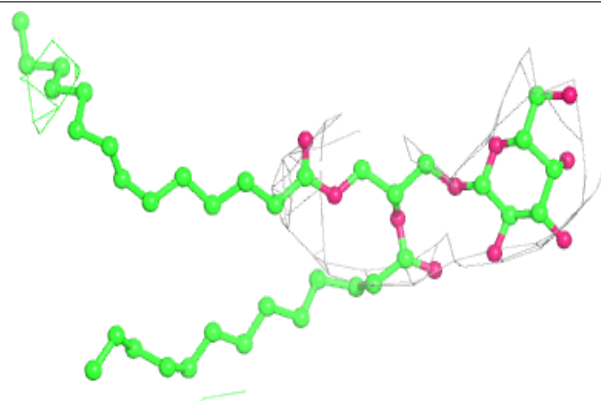


Electron density around LMT B 624:

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

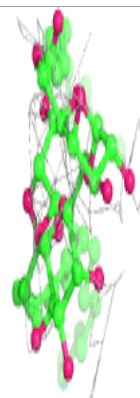
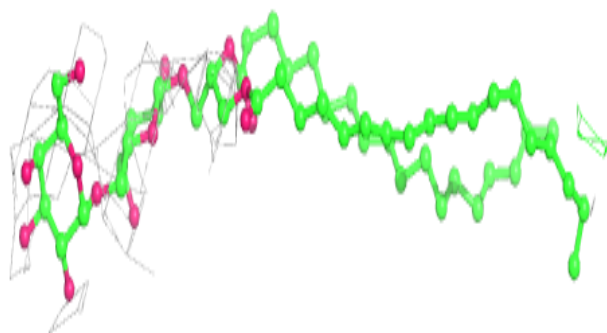
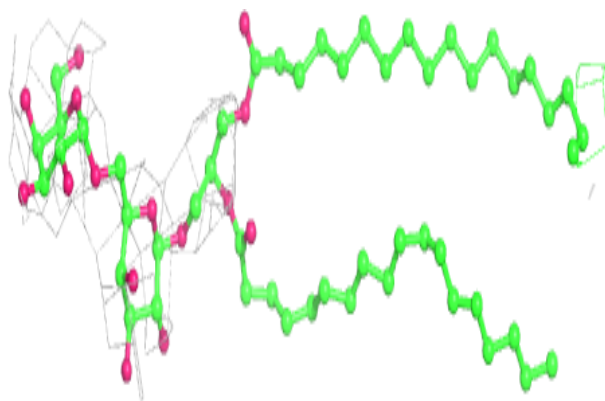
**Electron density around LMG D 411:**

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



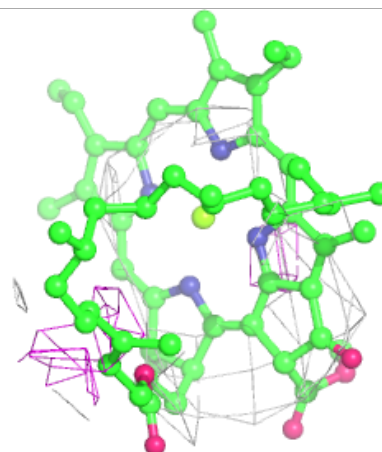
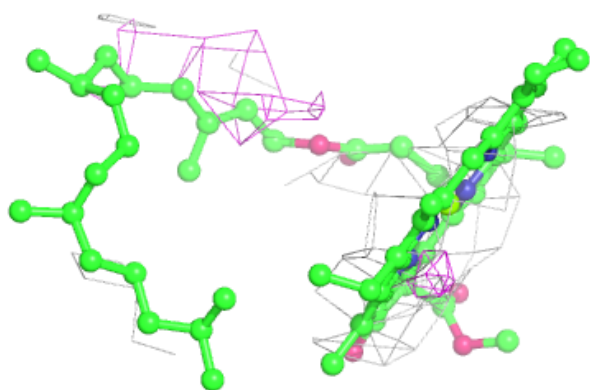
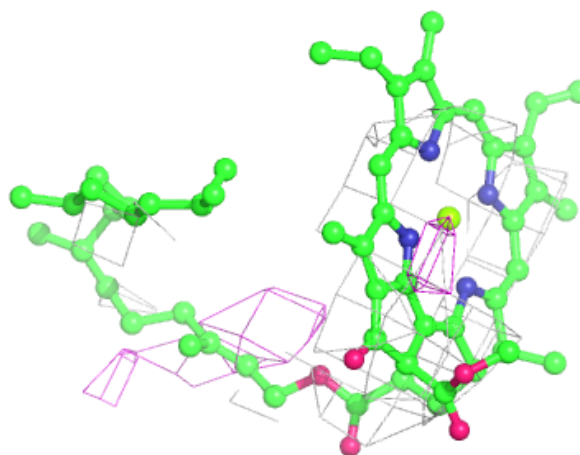
Electron density around DGD c 517:

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

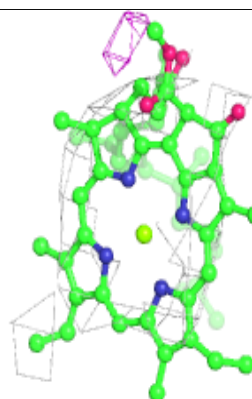
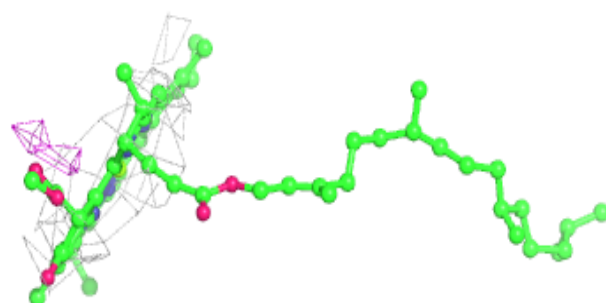
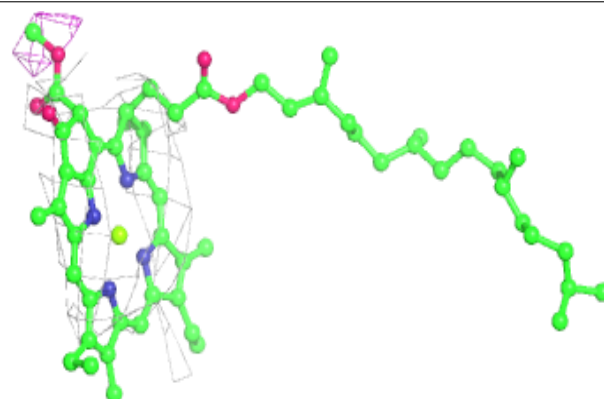


Electron density around CLA c 503:

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

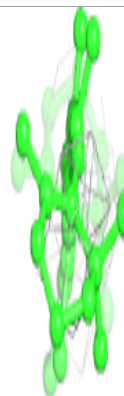
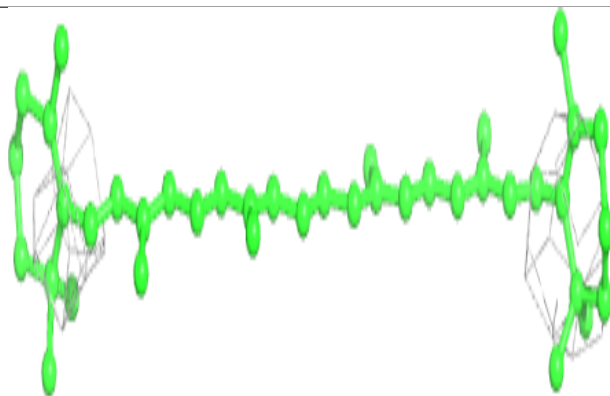
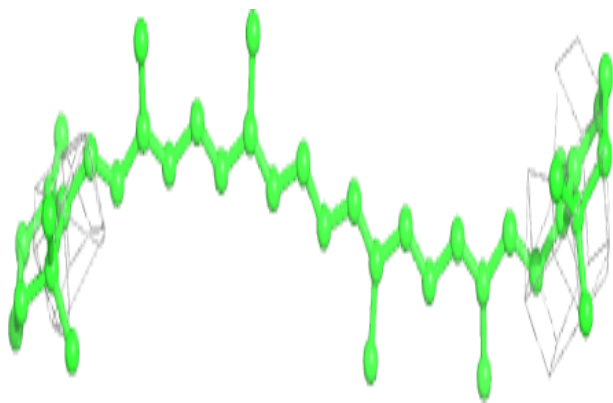
**Electron density around CLA A 405:**

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

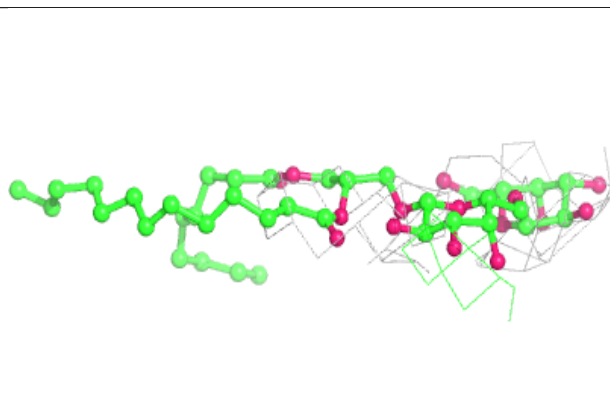
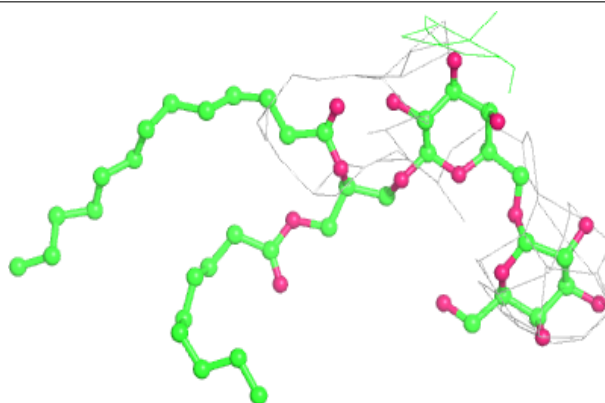


Electron density around BCR A 407:

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

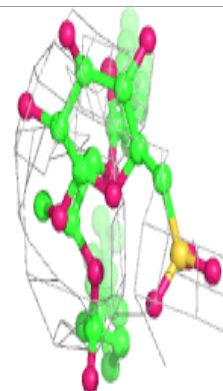
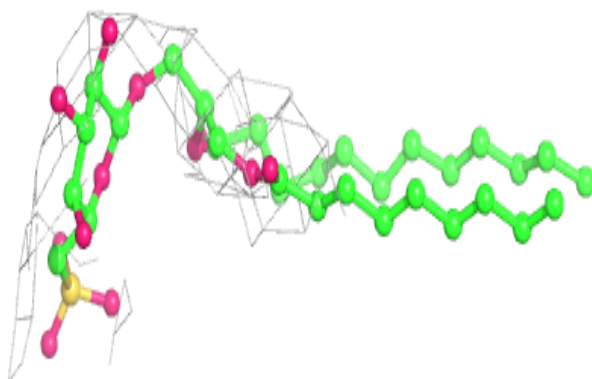
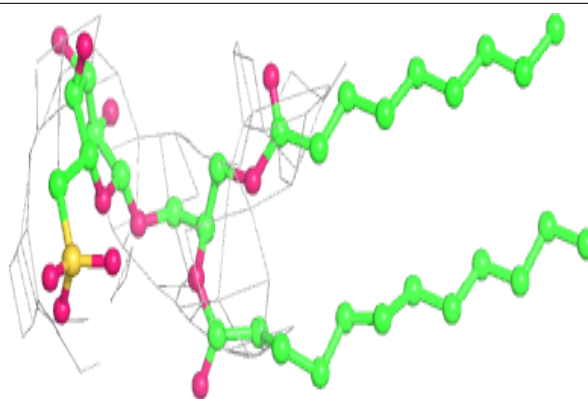
**Electron density around DGD b 601:**

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

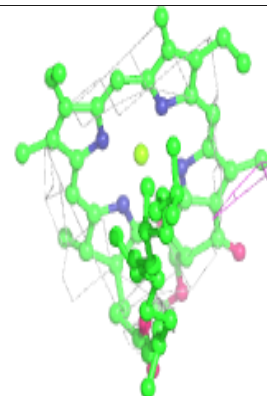
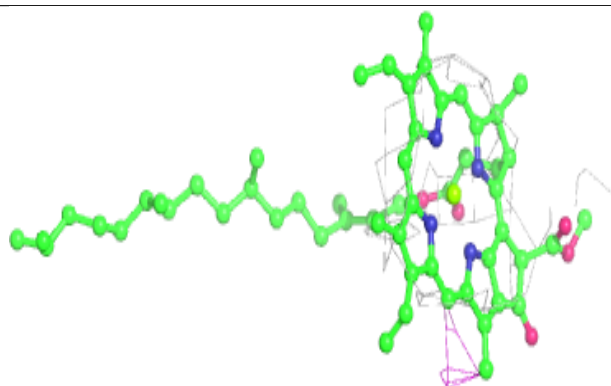
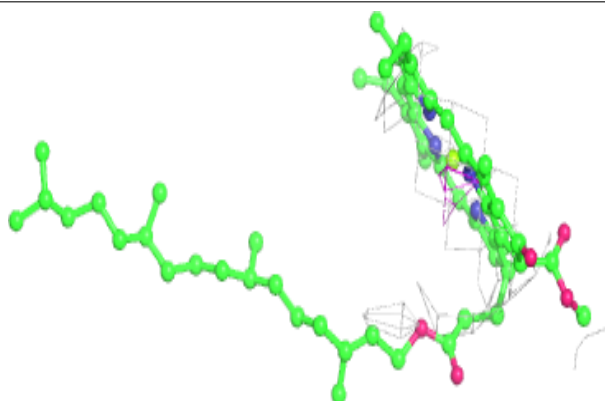


Electron density around SQD B 622:

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

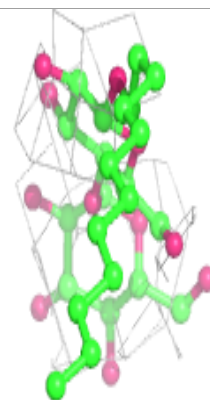
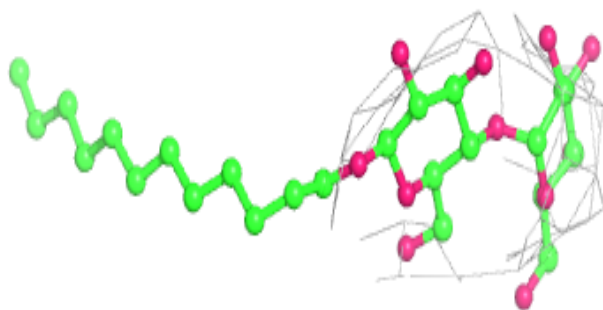
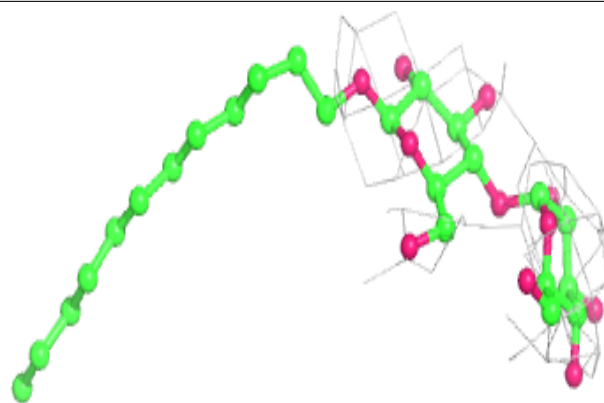
**Electron density around CLA C 520:**

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



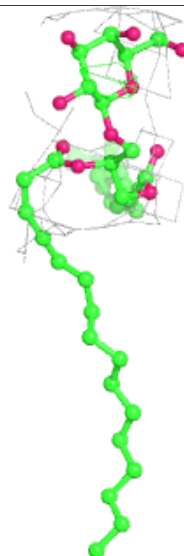
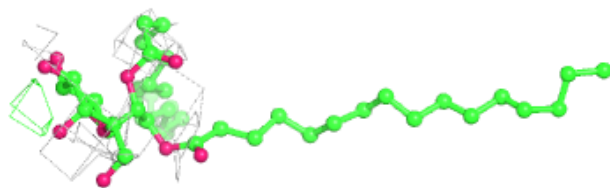
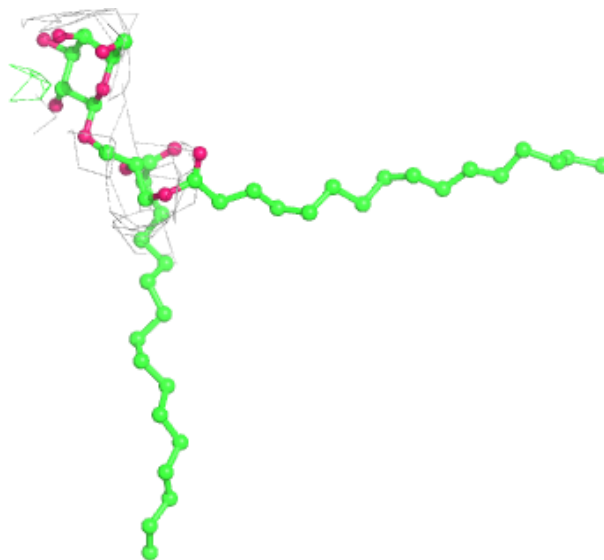
Electron density around LMT M 103:

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



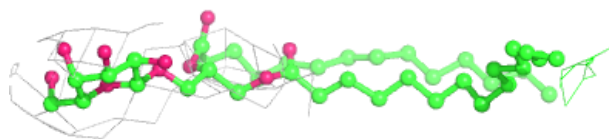
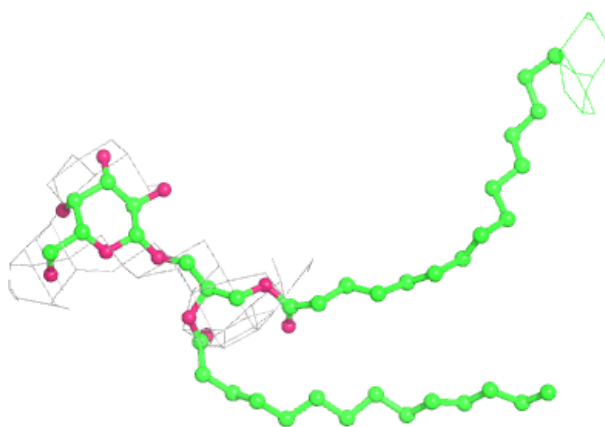
Electron density around LMG A 410:

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



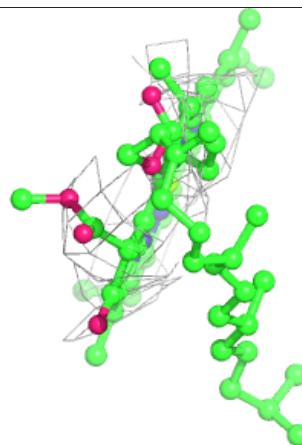
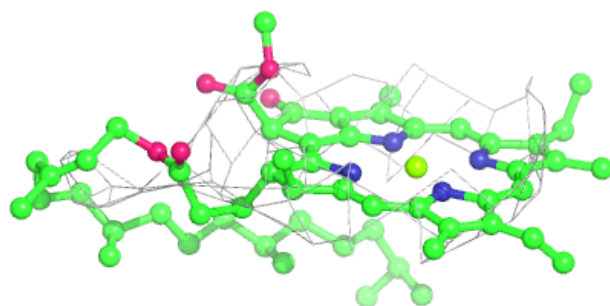
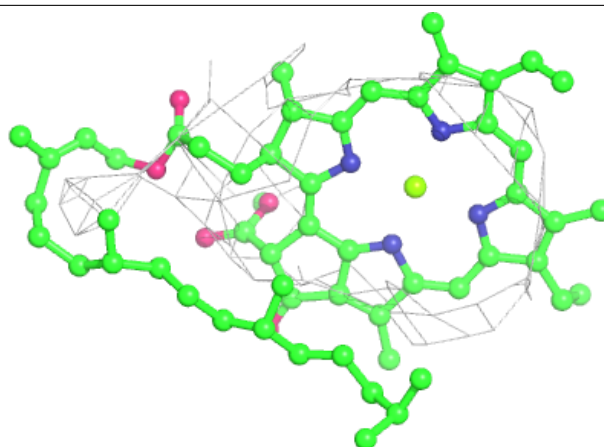
Electron density around LMG c 522:

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

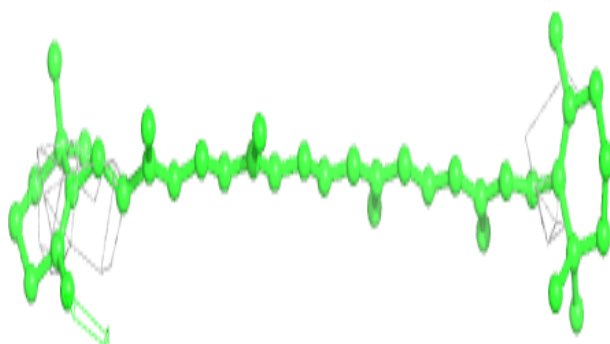
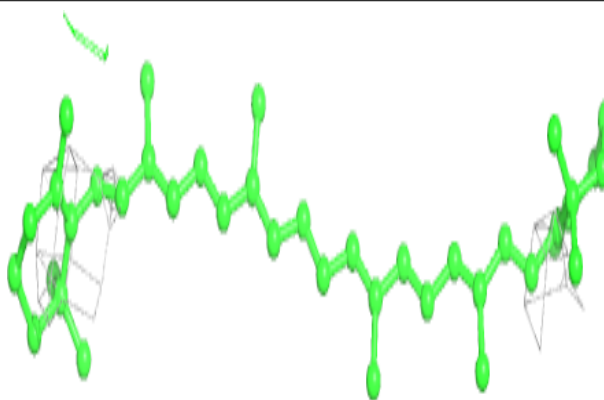


Electron density around CLA c 508:

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

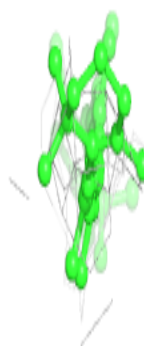
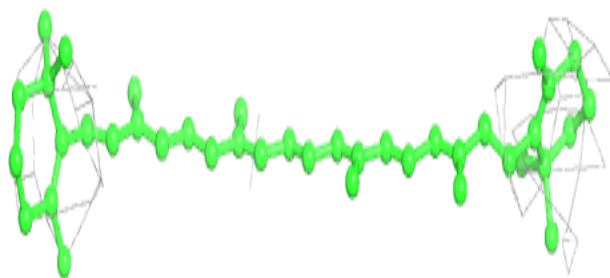
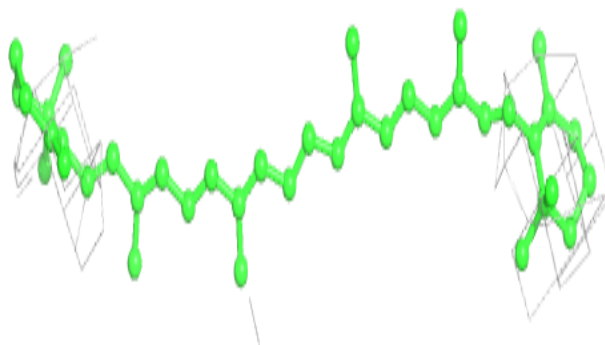
**Electron density around BCR c 521:**

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

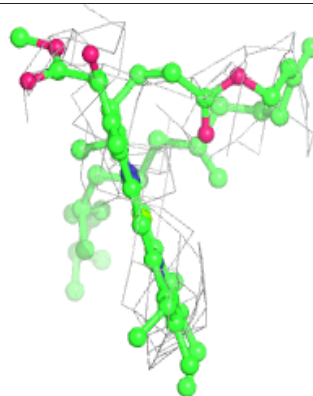
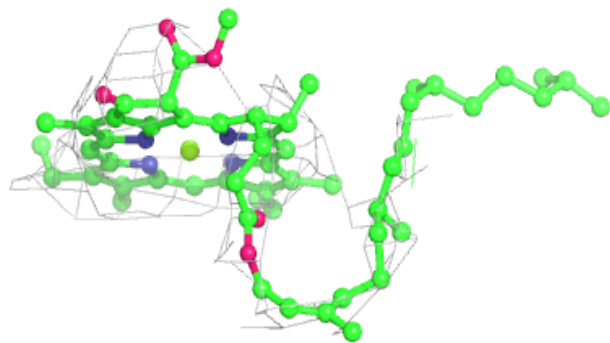
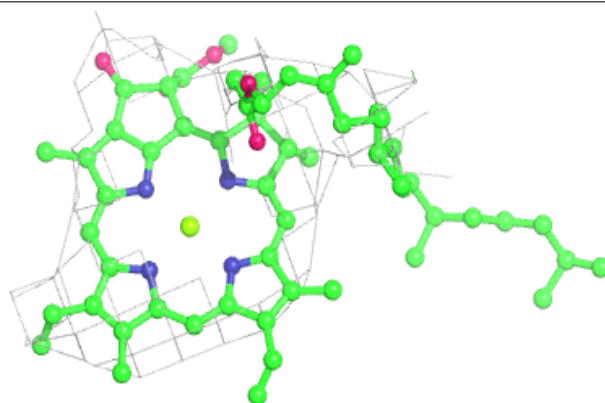


Electron density around BCR K 102:

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

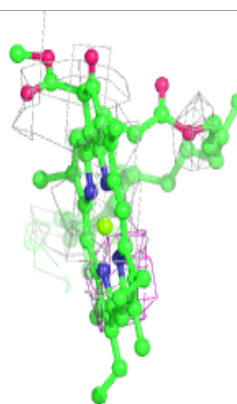
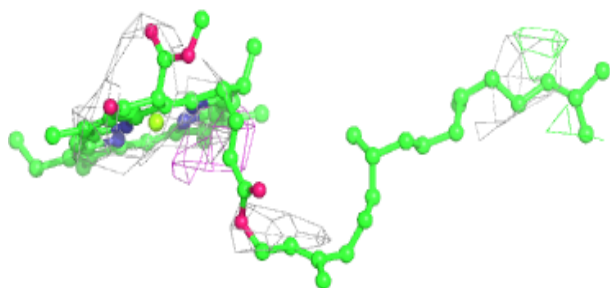
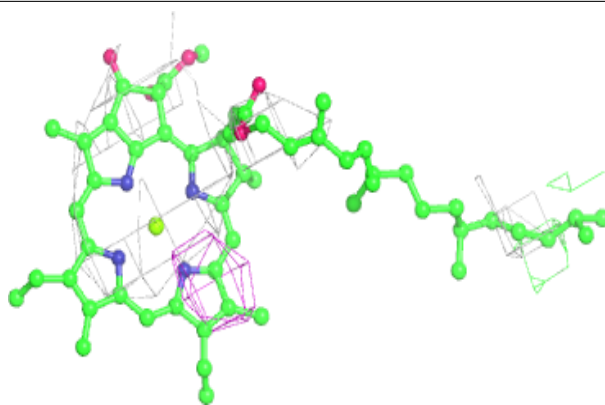
**Electron density around CLA a 405:**

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

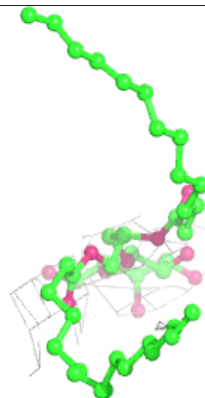
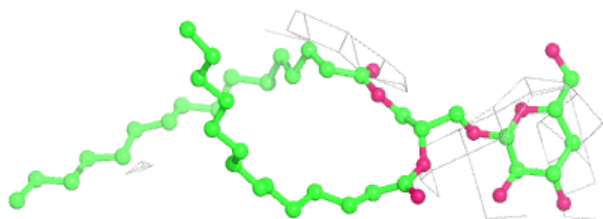
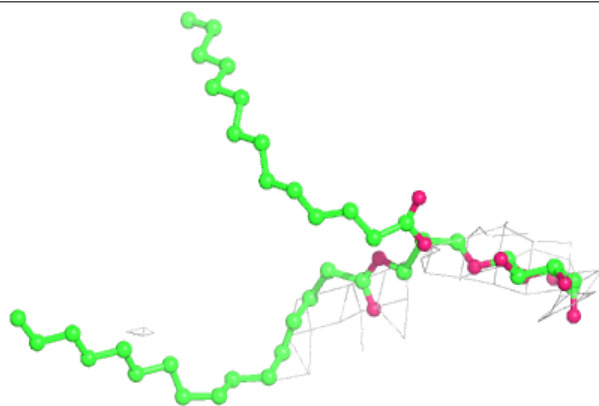


Electron density around CLA a 406:

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

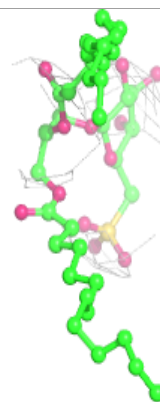
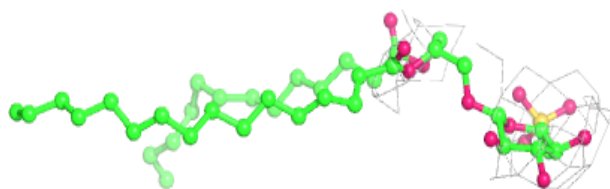
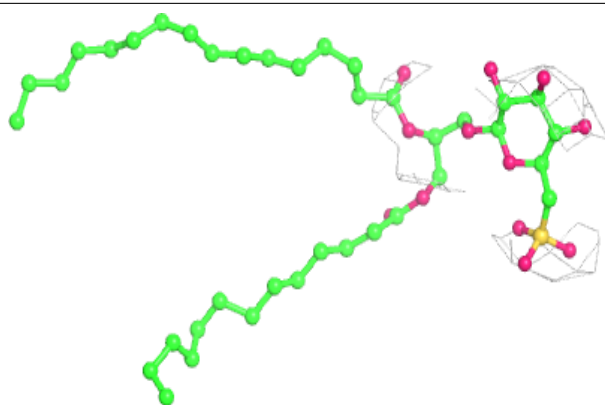
**Electron density around LMG b 625:**

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

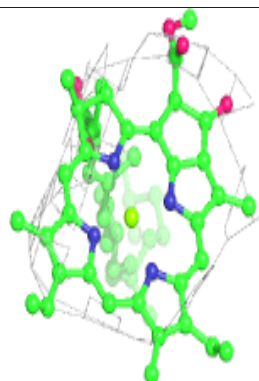
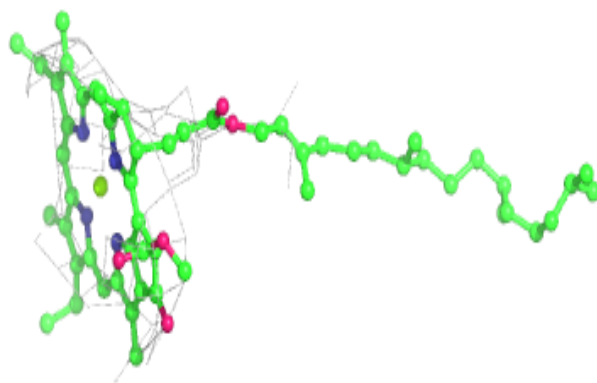
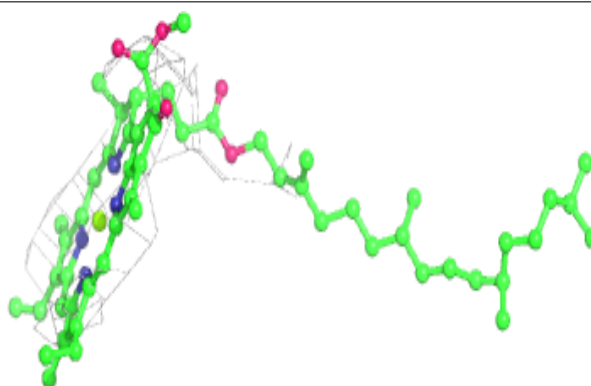


Electron density around SQD a 415:

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

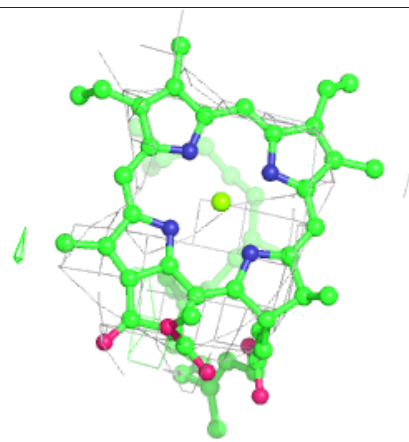
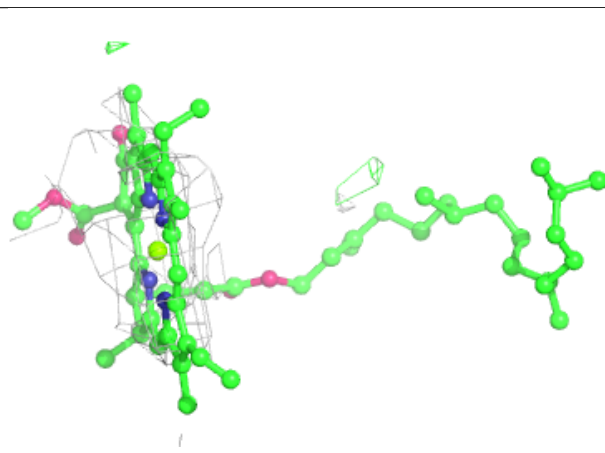
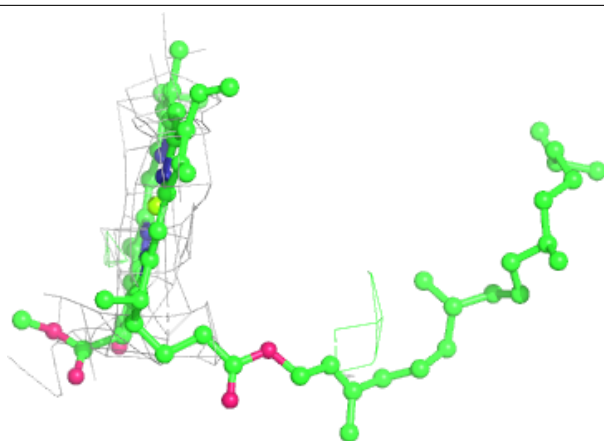
**Electron density around CLA B 603:**

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



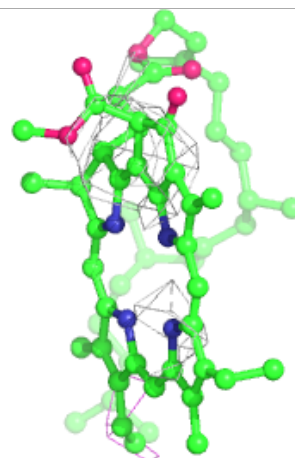
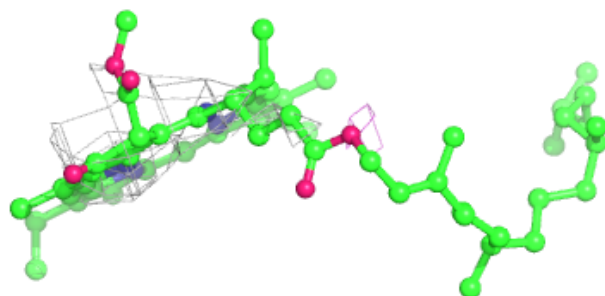
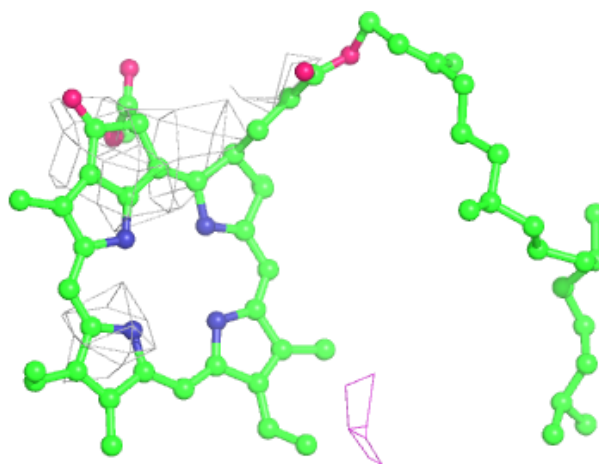
Electron density around CLA c 505:

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



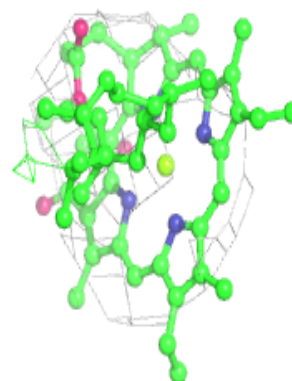
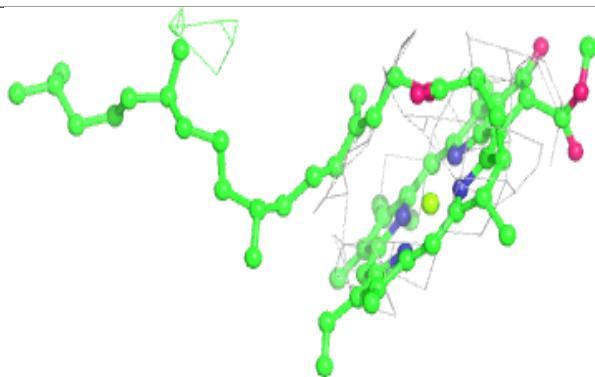
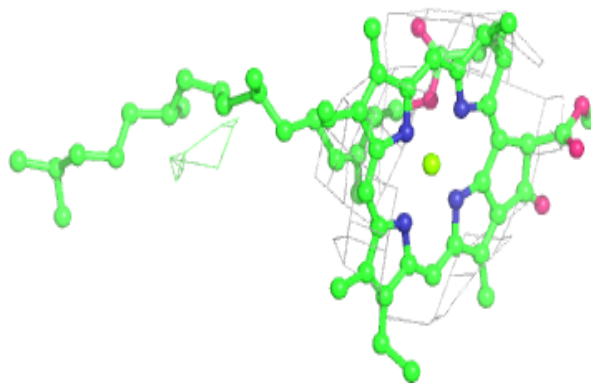
Electron density around PHO a 407:

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

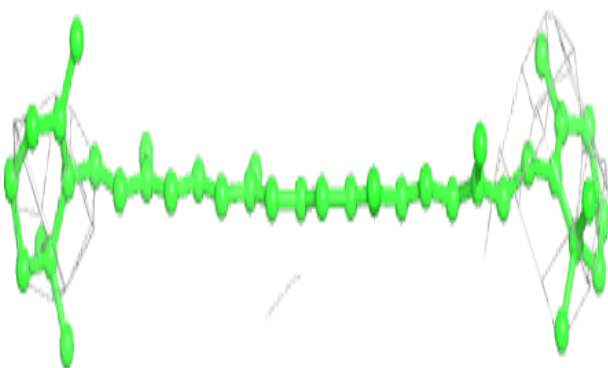
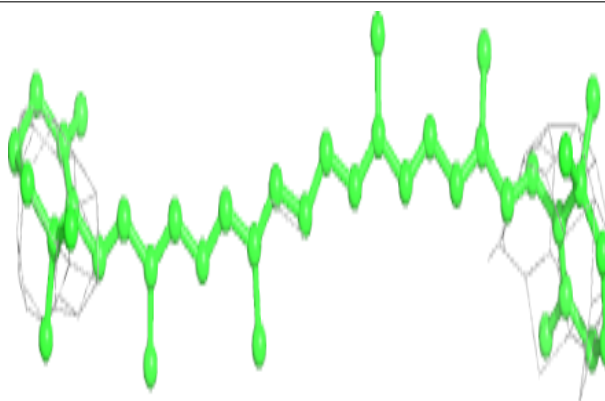


Electron density around CLA C 504:

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

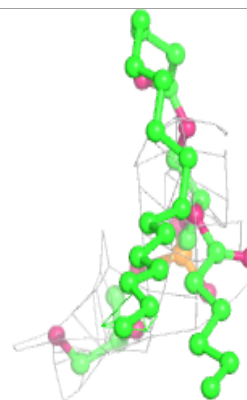
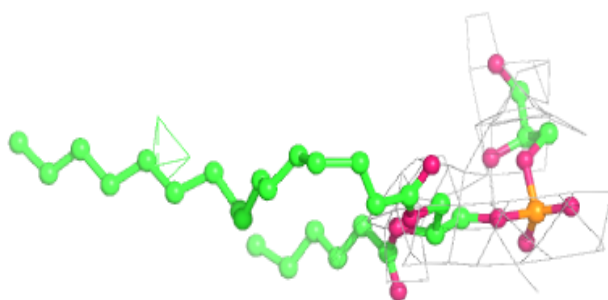
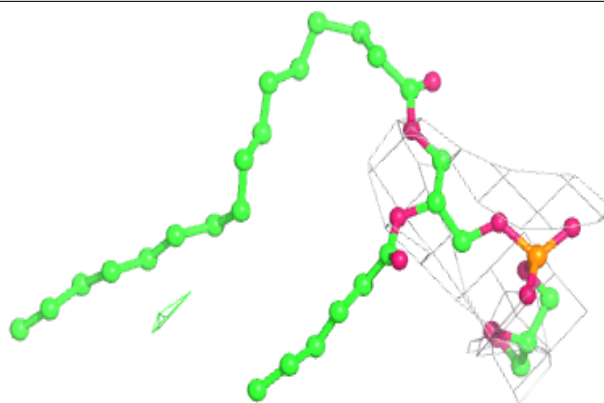
**Electron density around BCR b 622:**

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

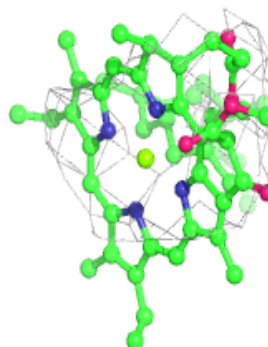
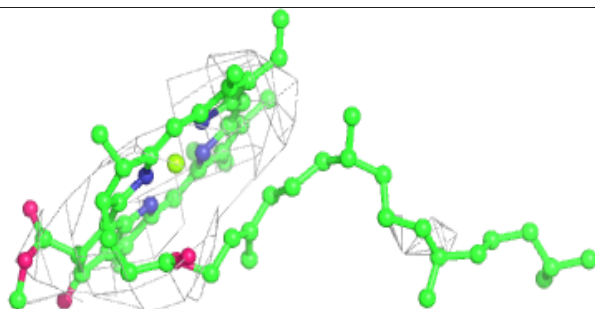
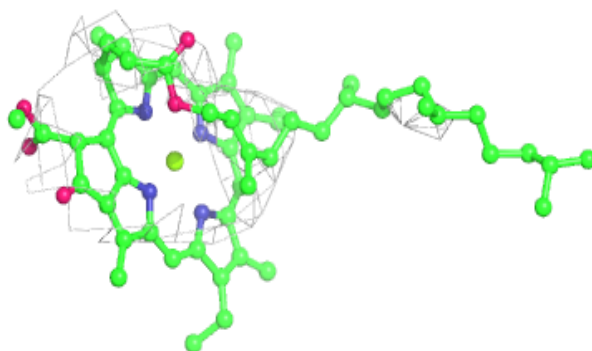


Electron density around LHG a 412:

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

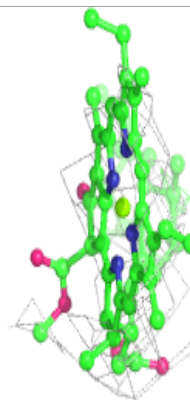
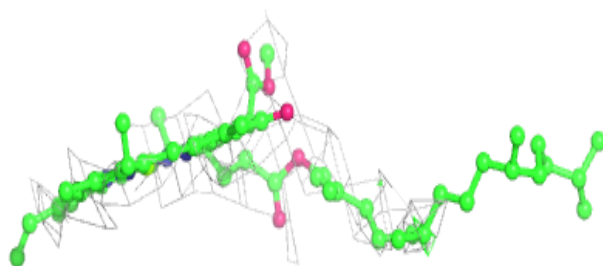
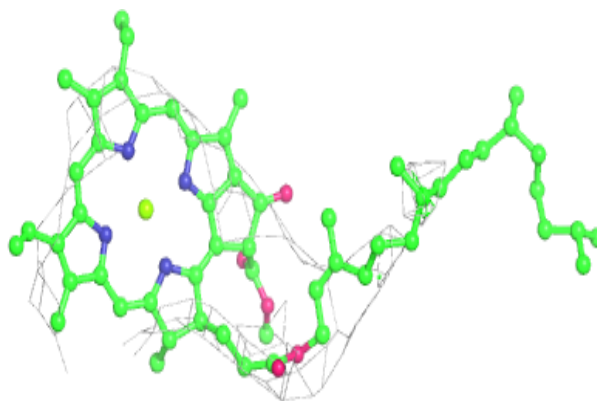
**Electron density around CLA c 504:**

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

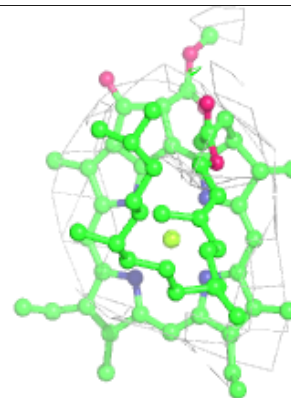
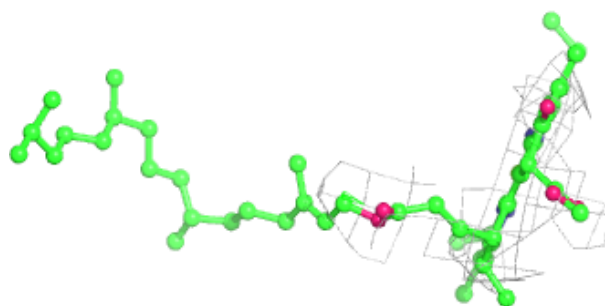


Electron density around CLA H 101:

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

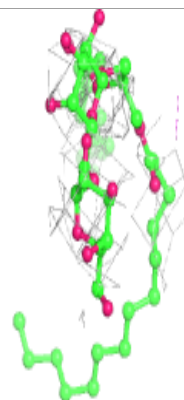
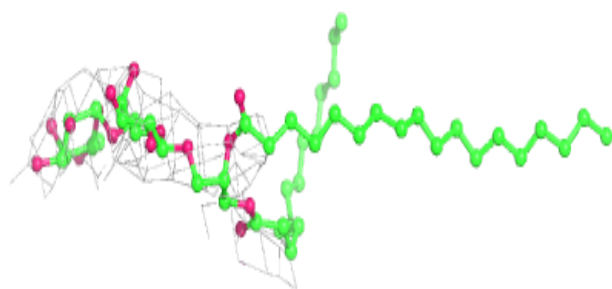
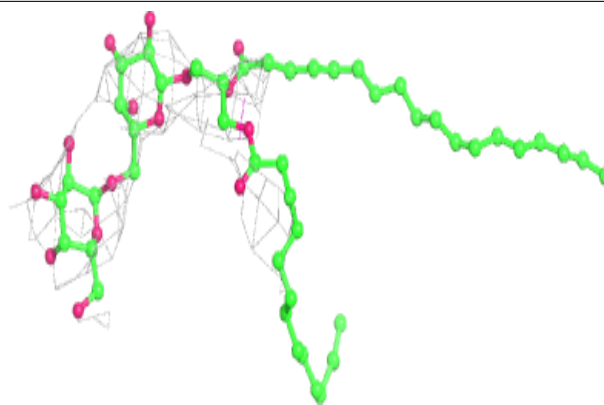
**Electron density around CLA d 405:**

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

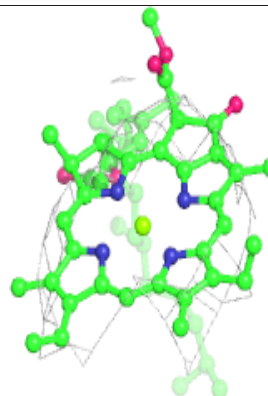
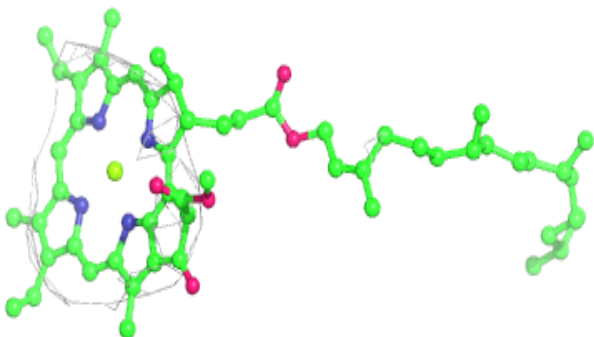
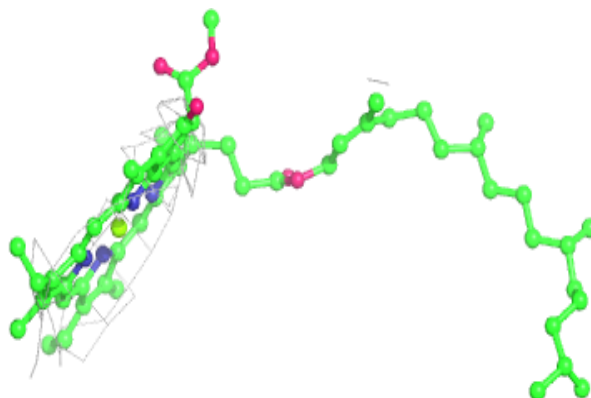


Electron density around DGD C 516:

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

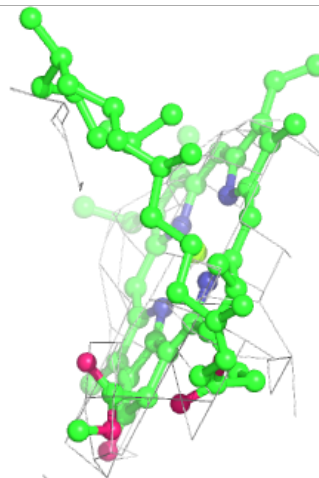
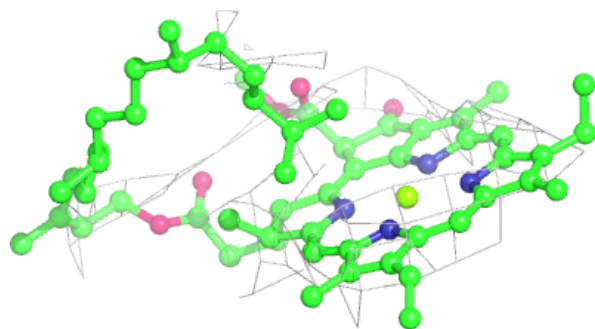
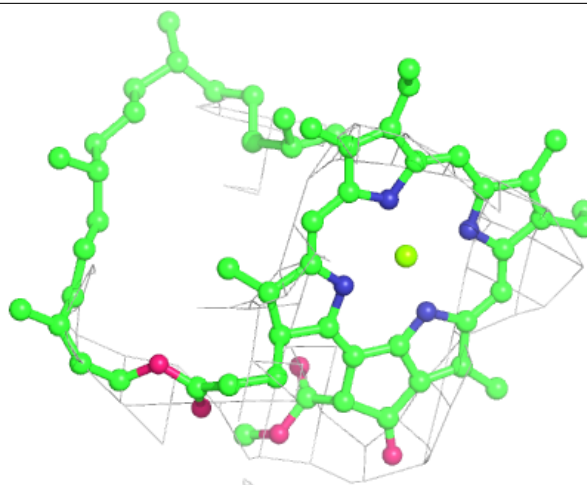
**Electron density around CLA d 404:**

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



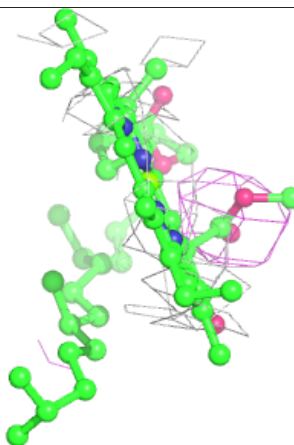
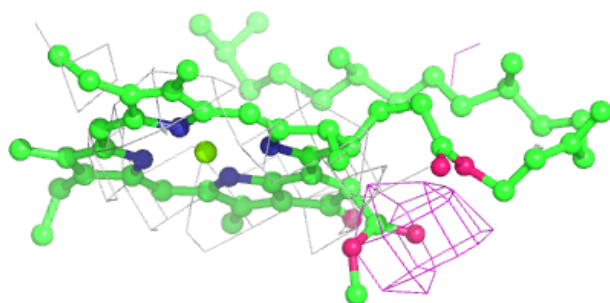
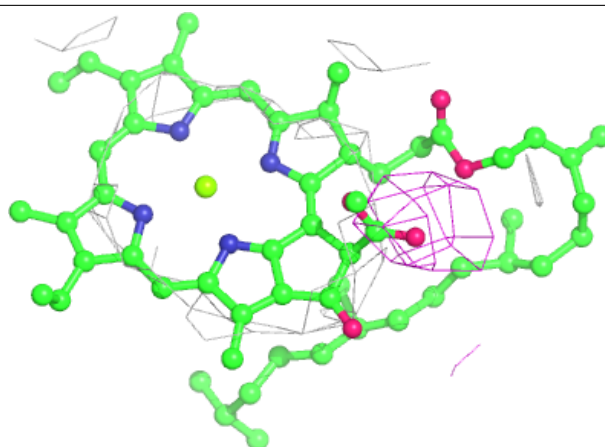
Electron density around CLA b 618:

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

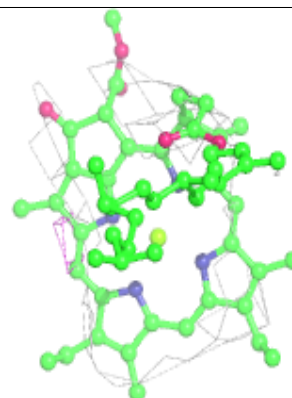
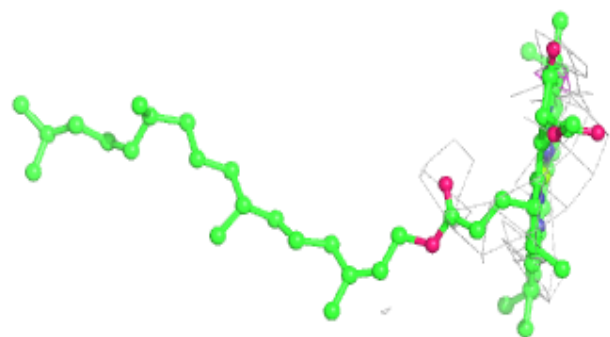
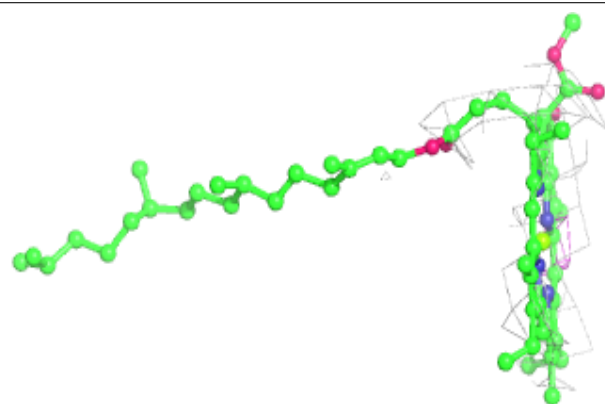


Electron density around CLA C 508:

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

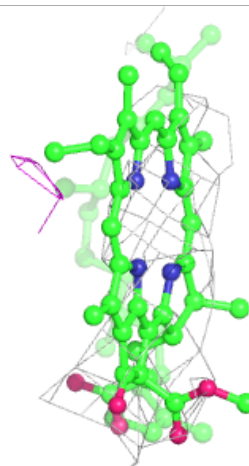
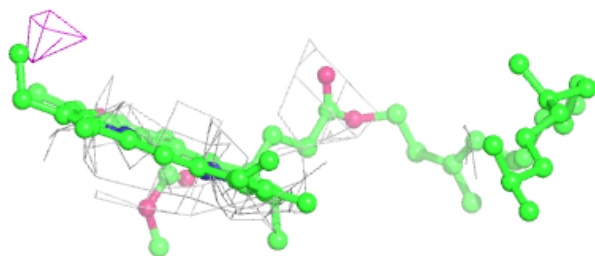
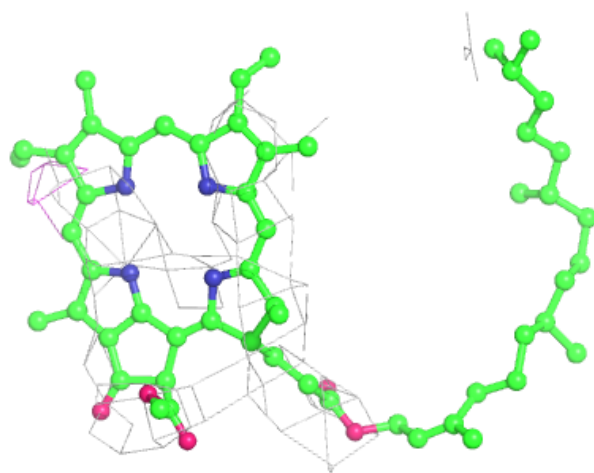
**Electron density around CLA B 605:**

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



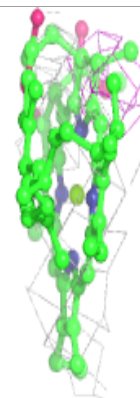
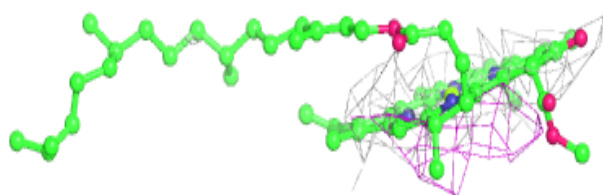
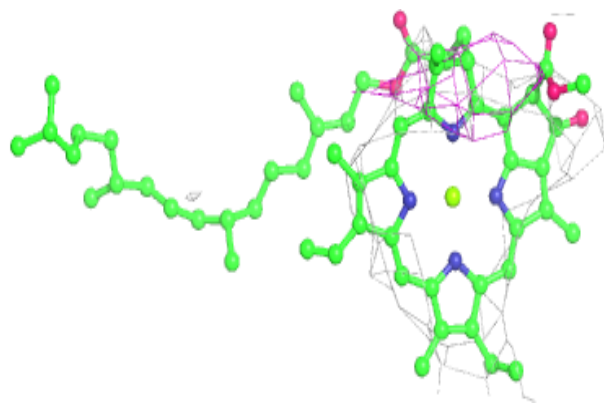
Electron density around PHO D 401:

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

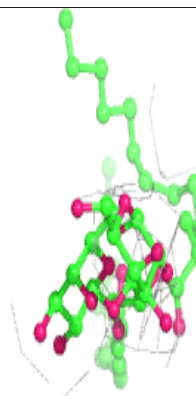
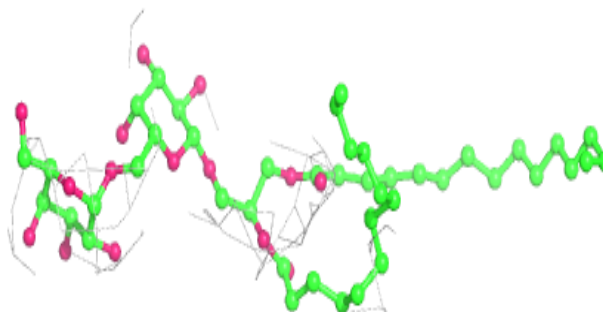
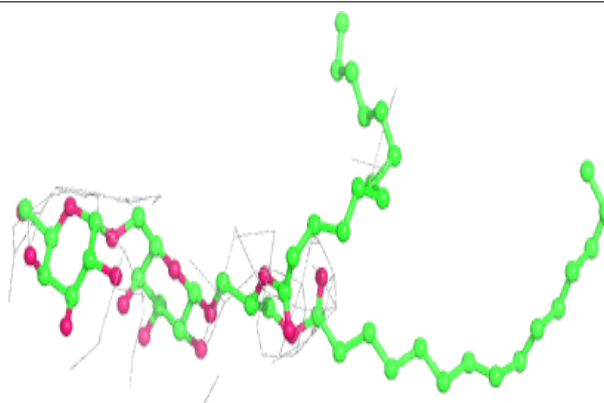


Electron density around CLA b 606:

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

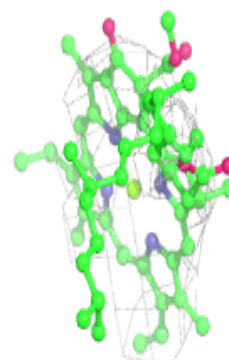
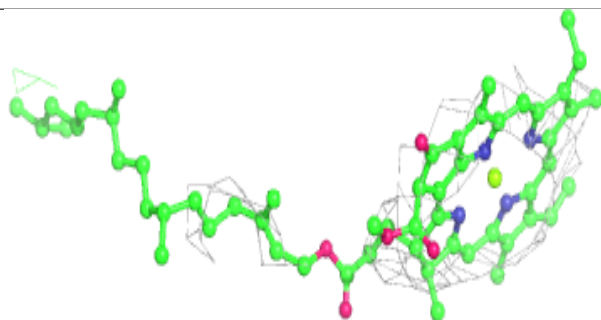
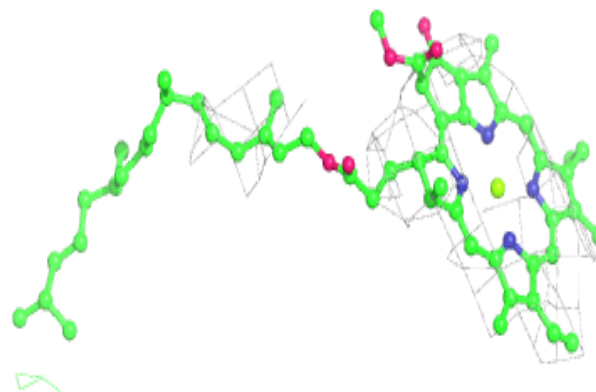
**Electron density around DGD b 624:**

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

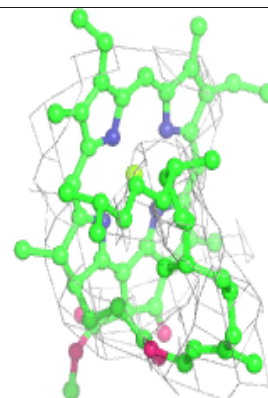
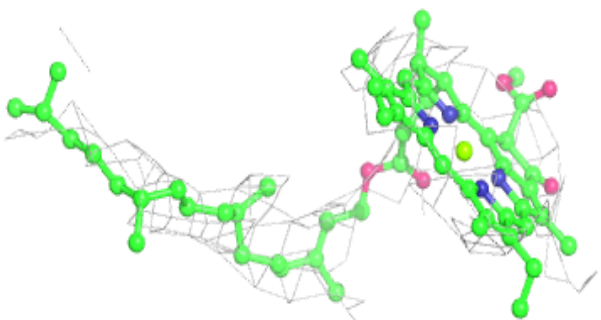
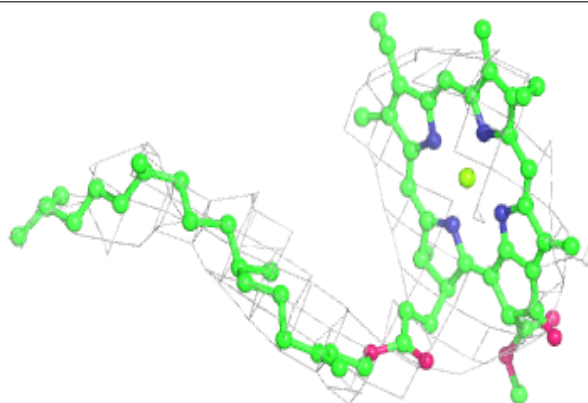


Electron density around CLA a 404:

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

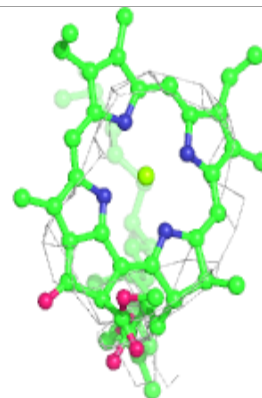
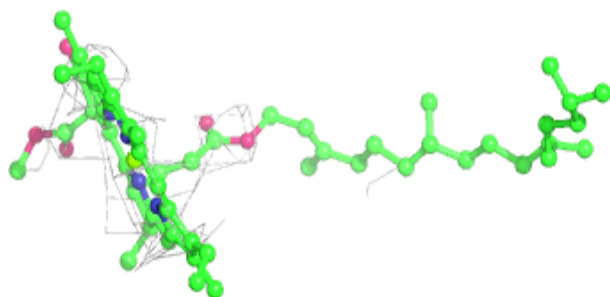
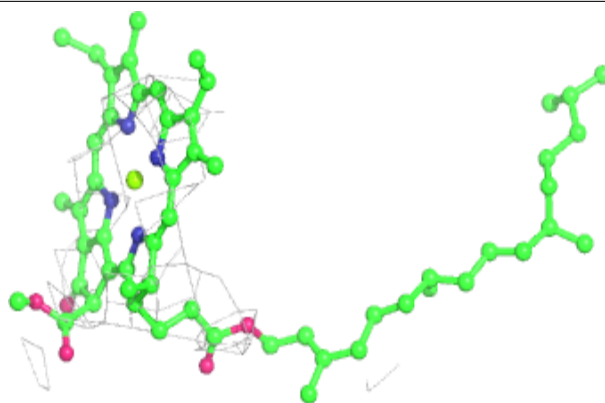
**Electron density around CLA C 510:**

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

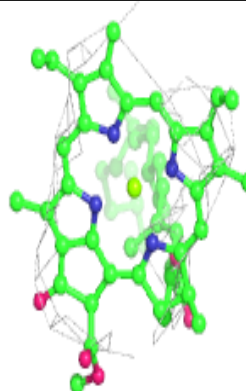
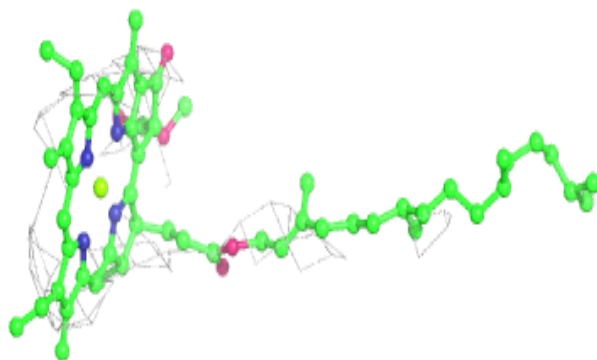
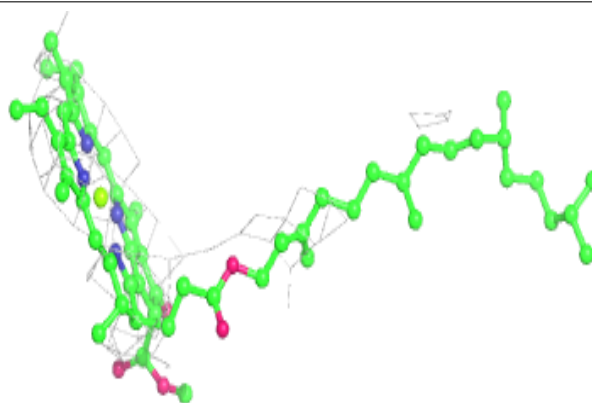


Electron density around CLA B 608:

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

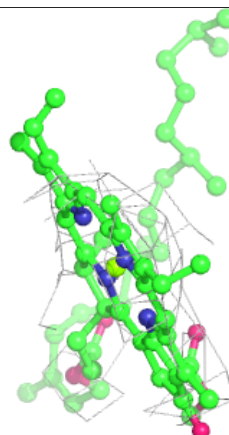
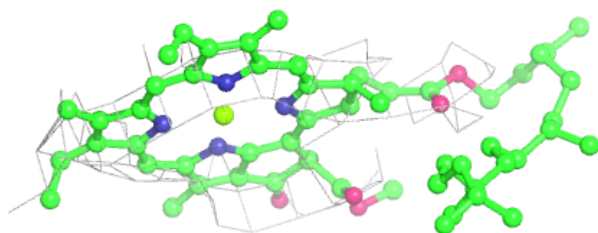
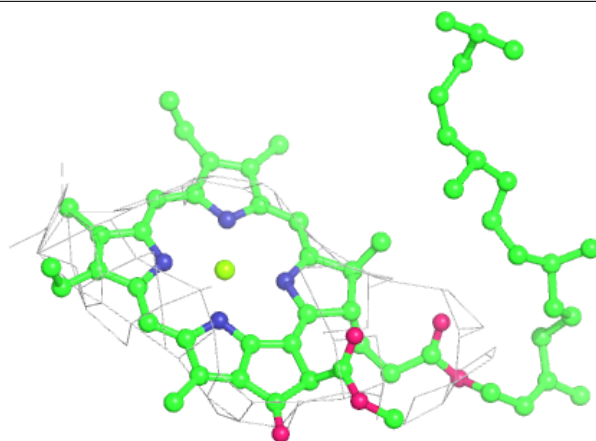
**Electron density around CLA b 607:**

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

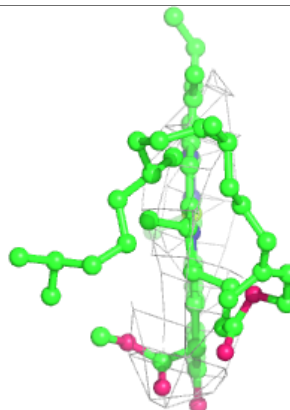
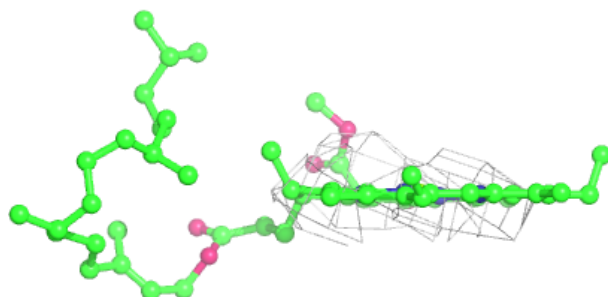
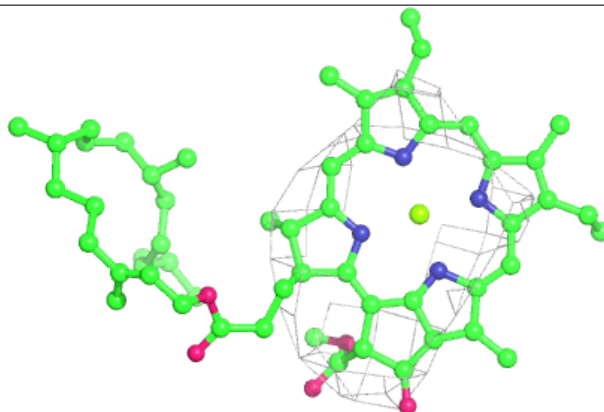


Electron density around CLA B 615:

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

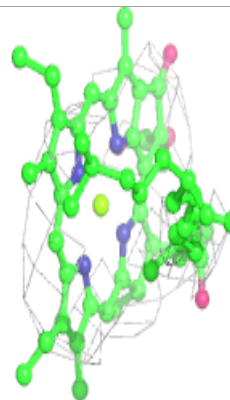
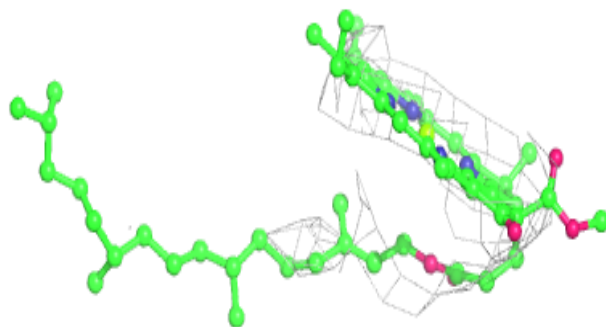
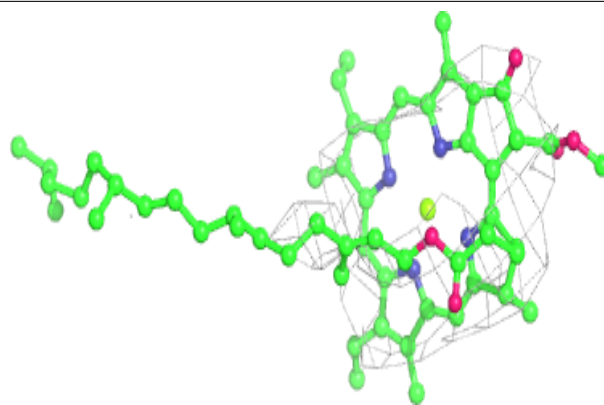
**Electron density around CLA C 511:**

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



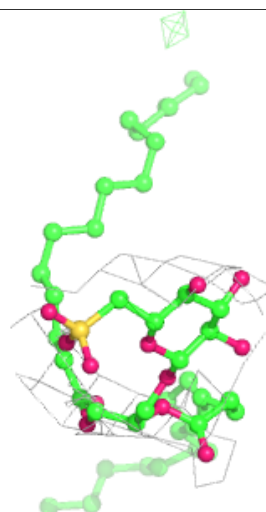
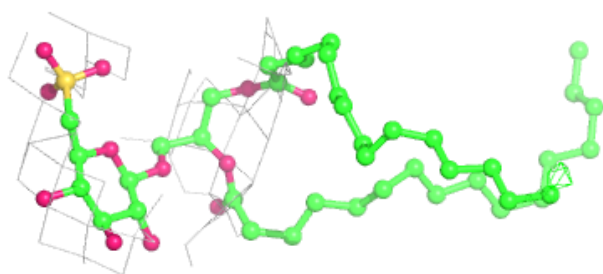
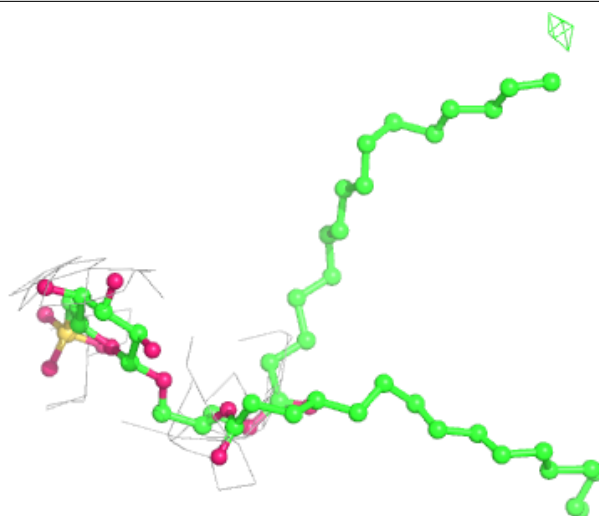
Electron density around CLA B 607:

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



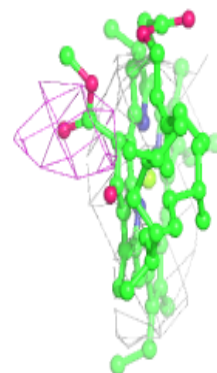
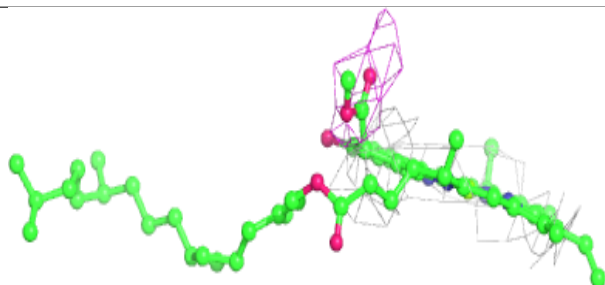
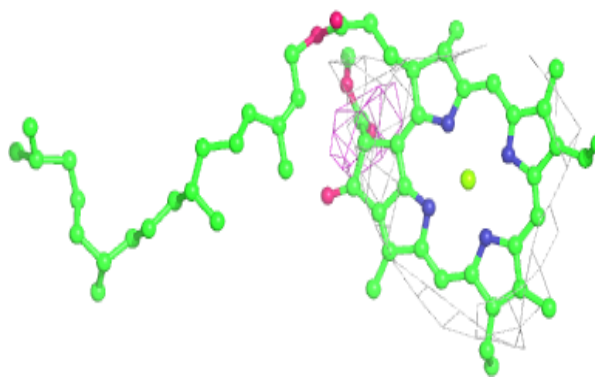
Electron density around SQD A 414:

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

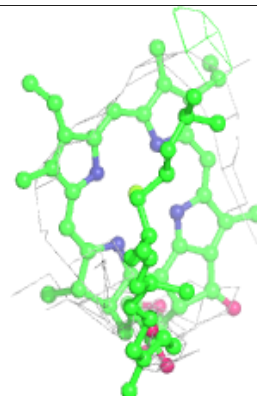
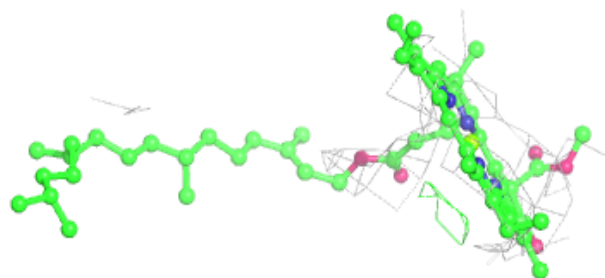
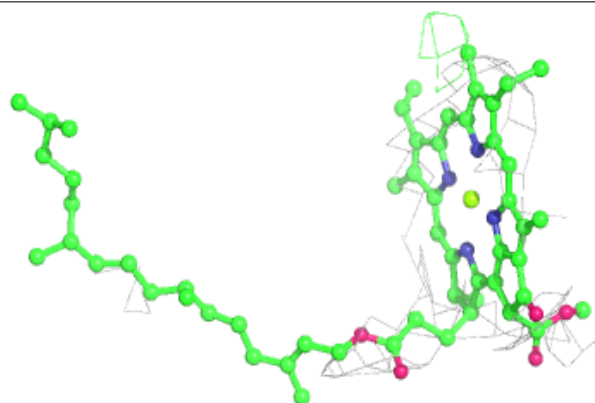


Electron density around CLA h 101:

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

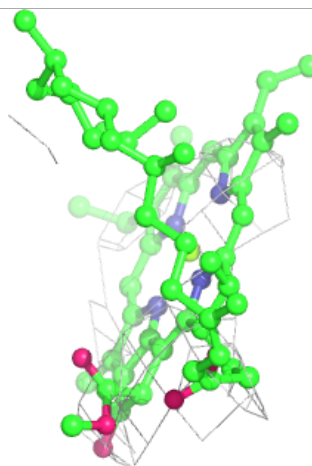
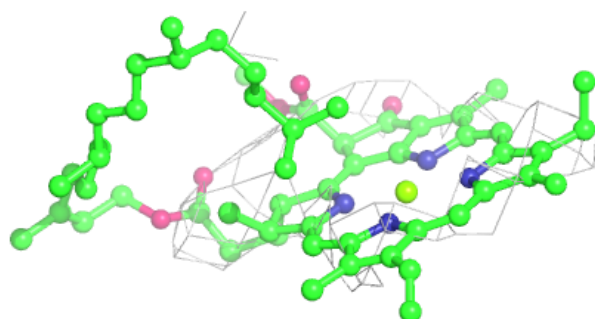
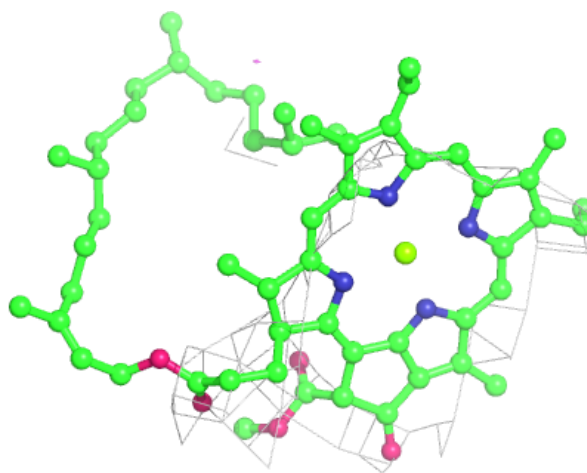
**Electron density around CLA b 612:**

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



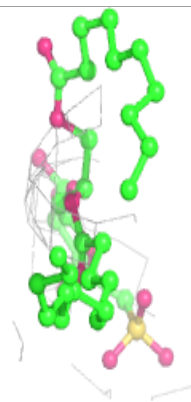
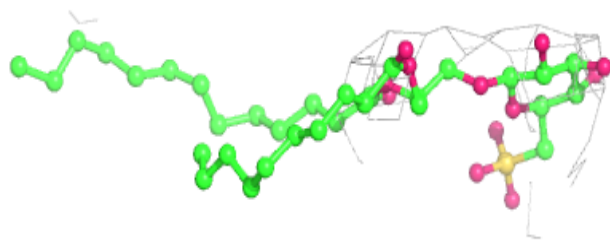
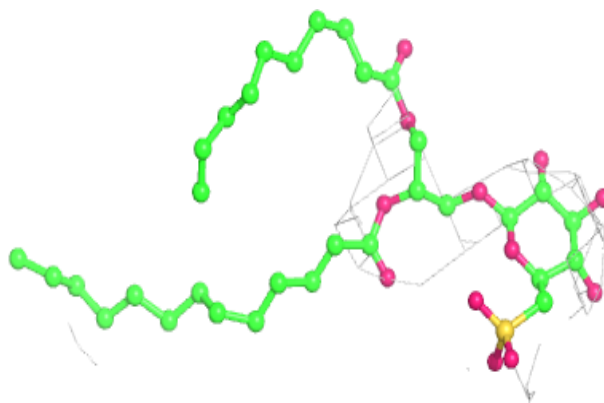
Electron density around CLA B 614:

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



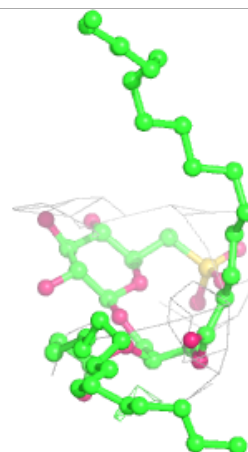
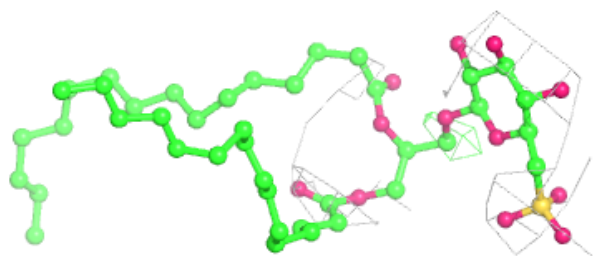
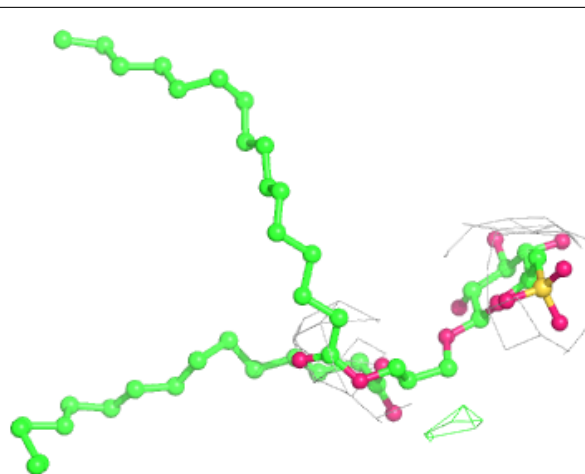
Electron density around SQD f 103:

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



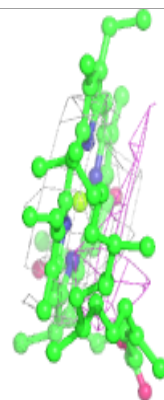
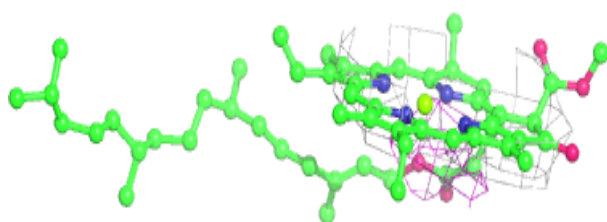
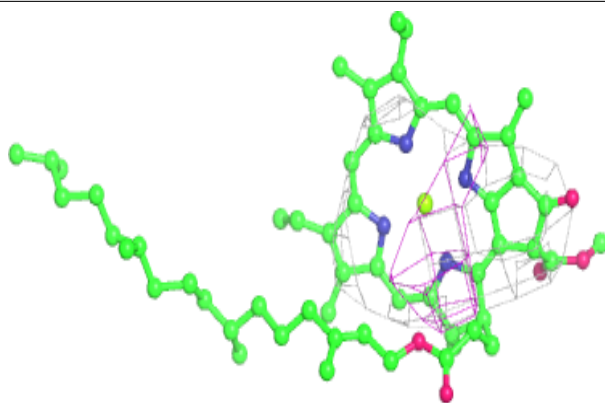
Electron density around SQD a 401:

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

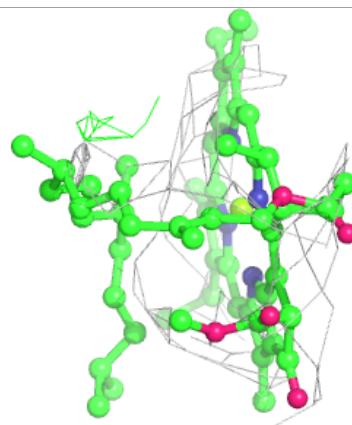
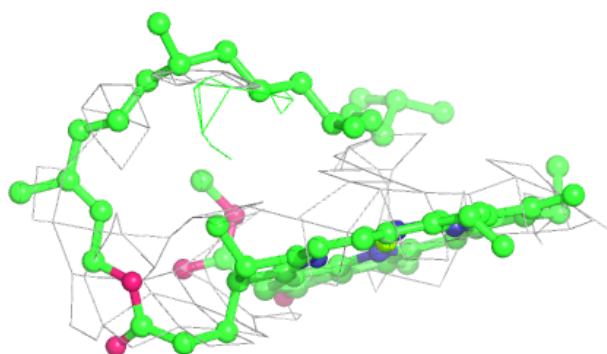
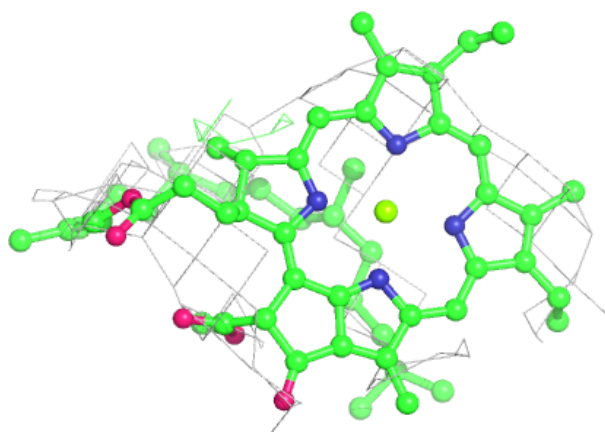


Electron density around CLA c 501:

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

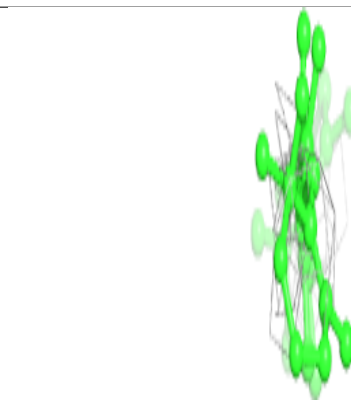
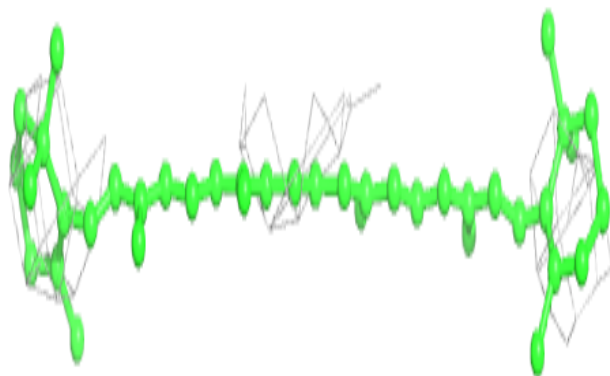
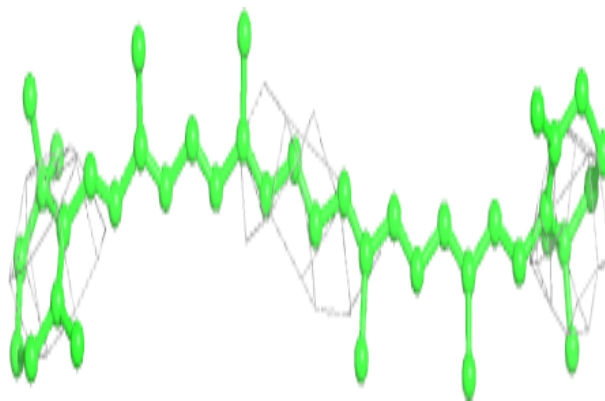
**Electron density around CLA c 509:**

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

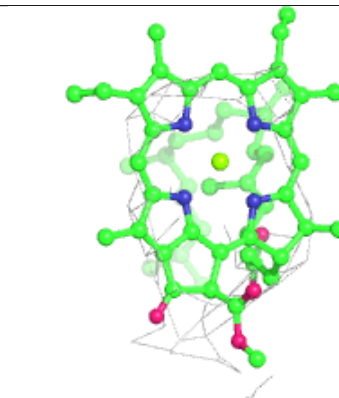
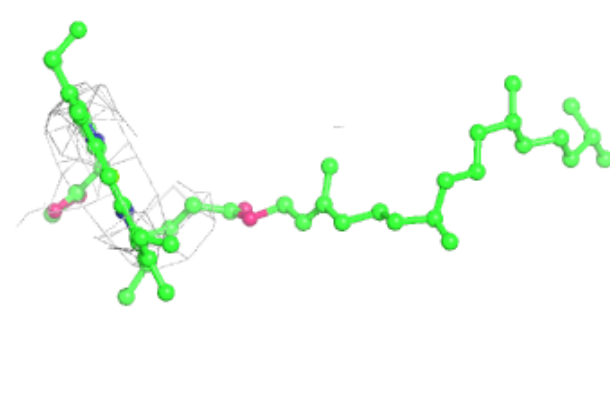
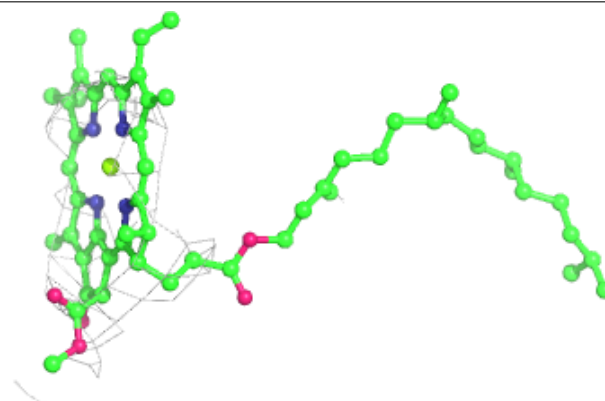


Electron density around BCR B 618:

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

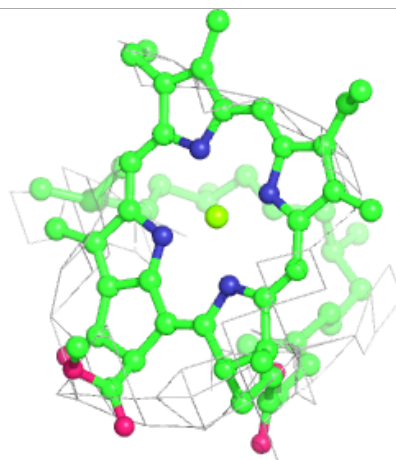
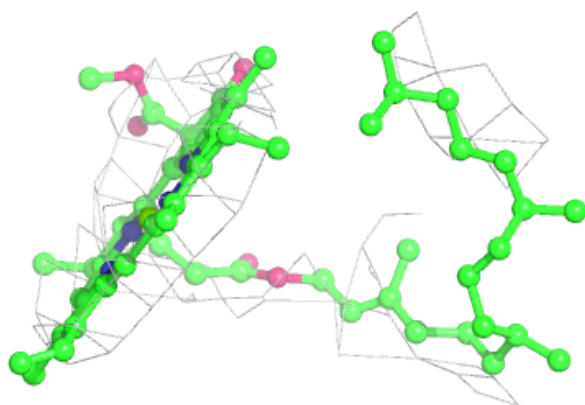
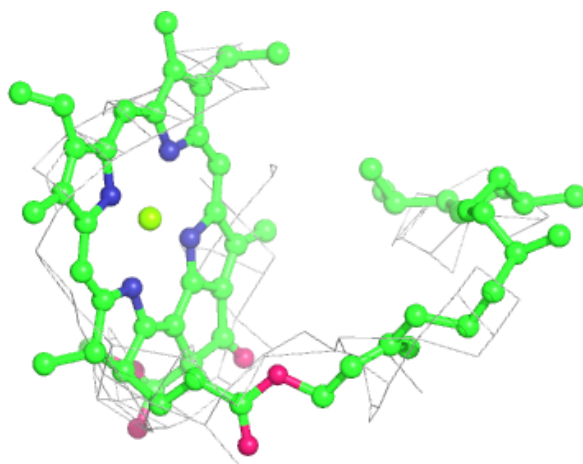
**Electron density around CLA D 405:**

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



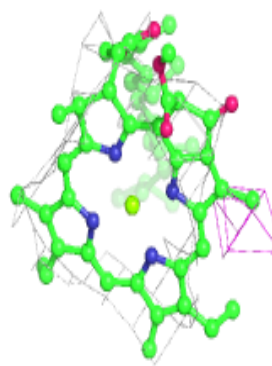
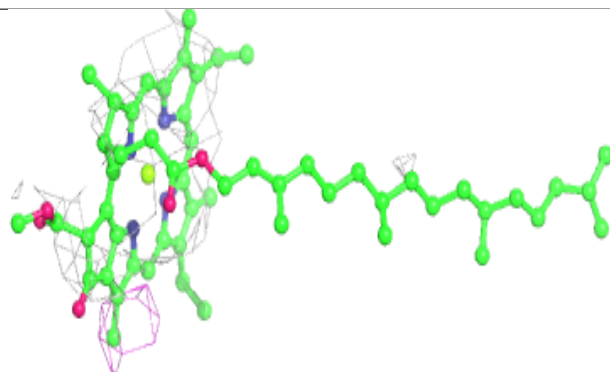
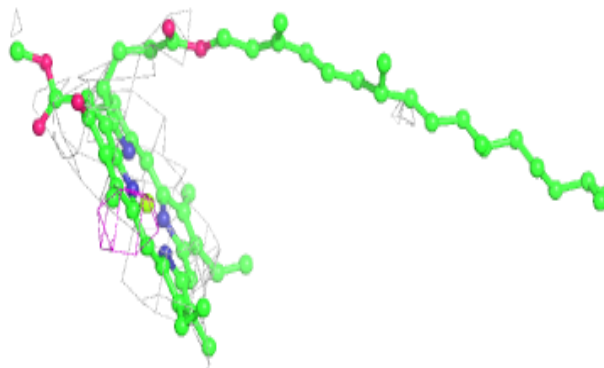
Electron density around CLA C 503:

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

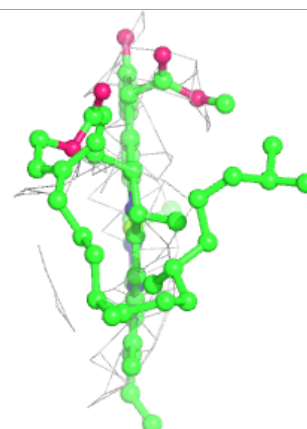
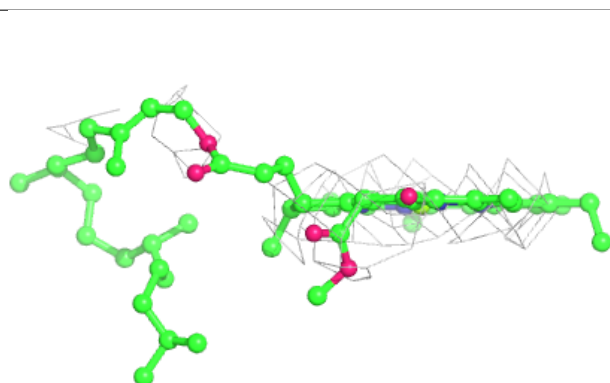
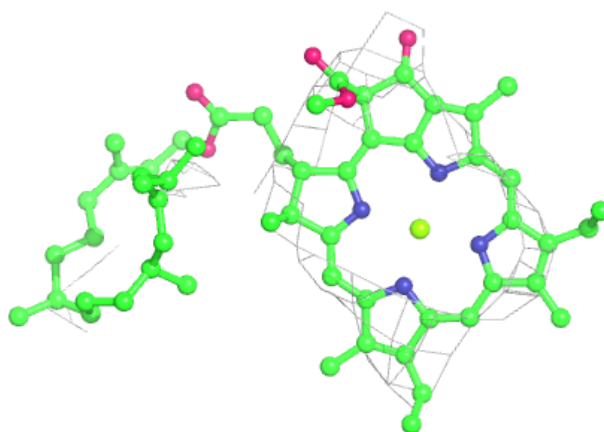


Electron density around CLA b 610:

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

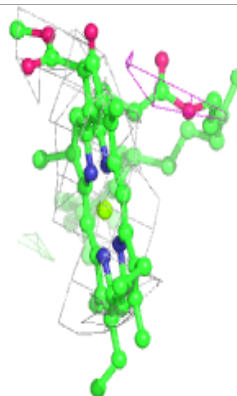
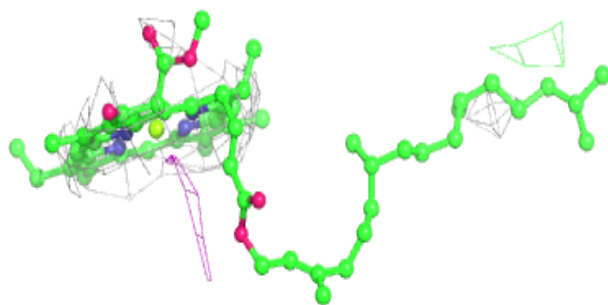
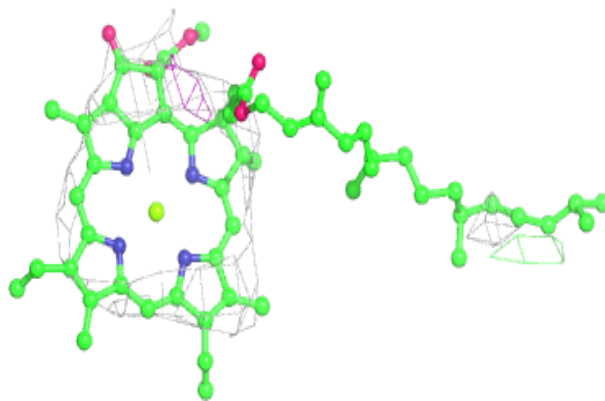
**Electron density around CLA c 511:**

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

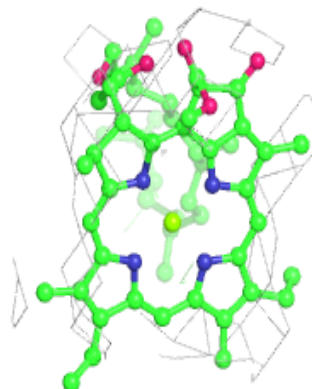
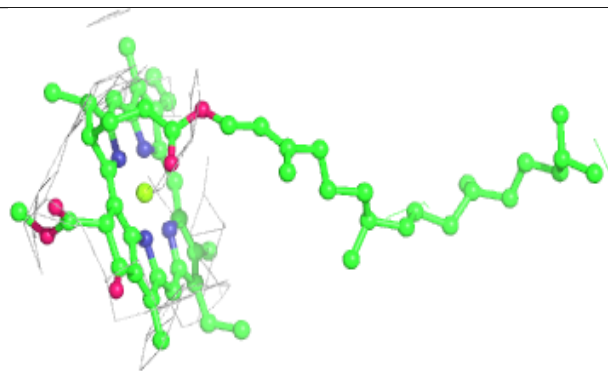
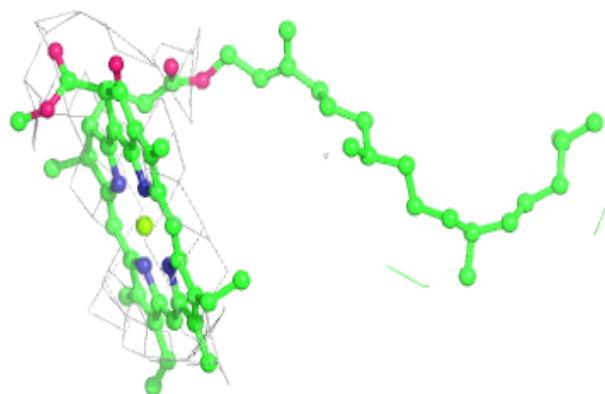


Electron density around CLA A 404:

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

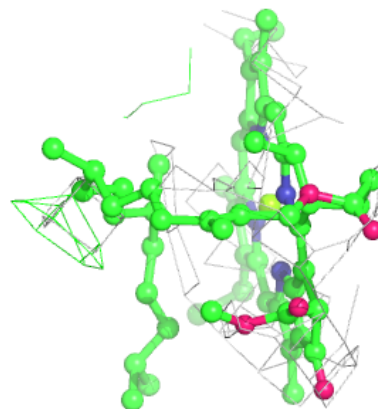
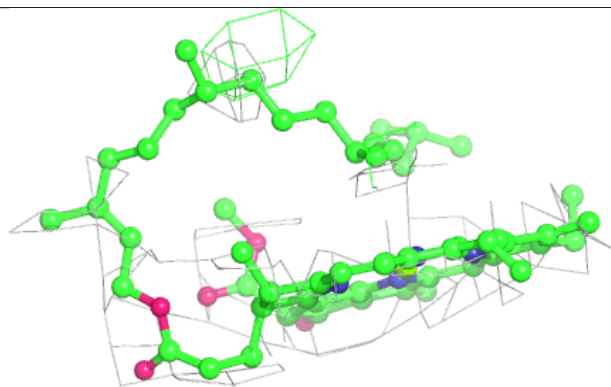
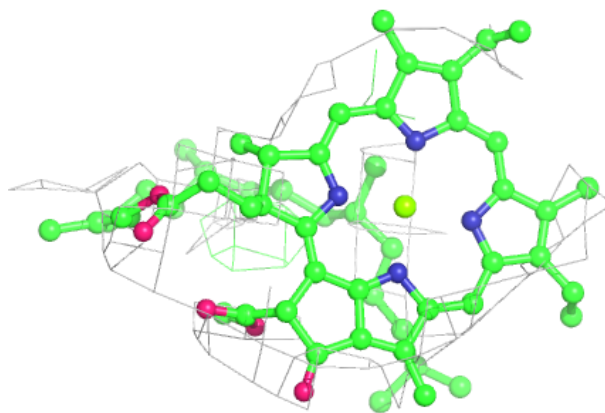
**Electron density around CLA C 507:**

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



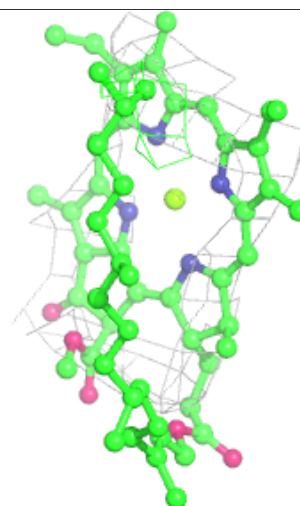
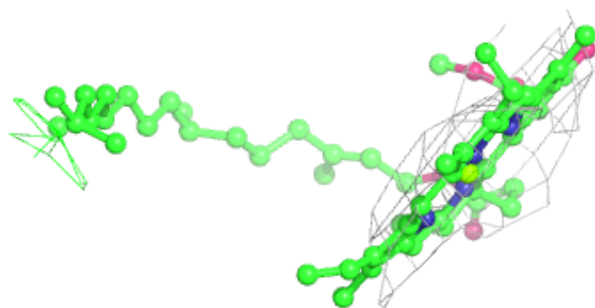
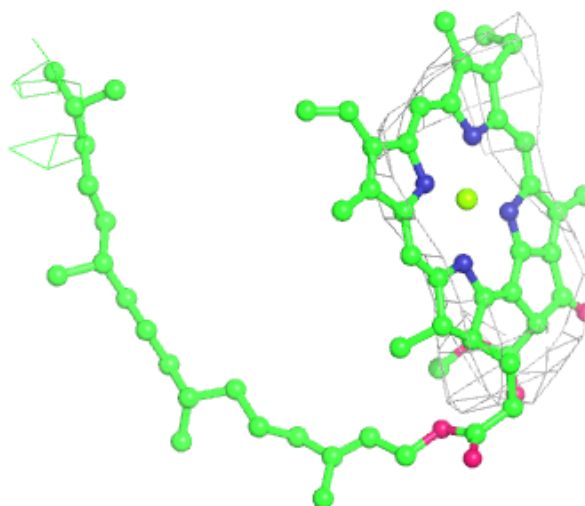
Electron density around CLA C 509:

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



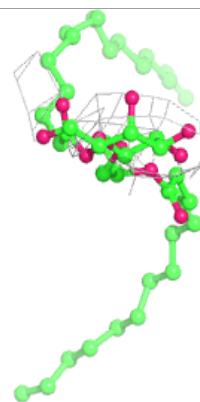
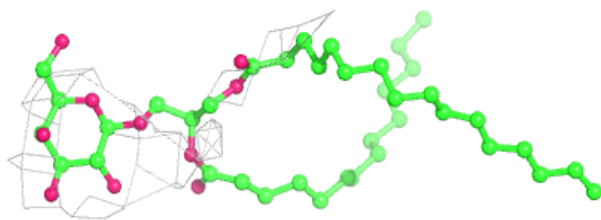
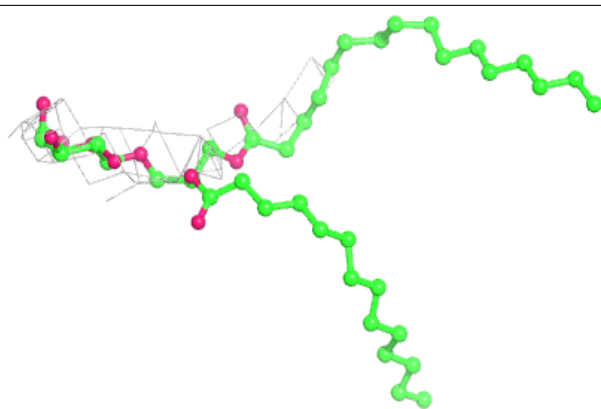
Electron density around CLA c 506:

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



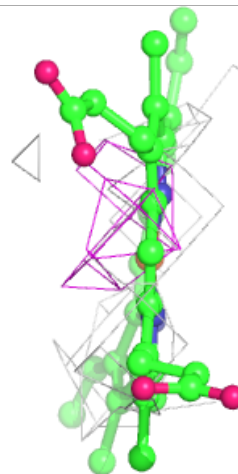
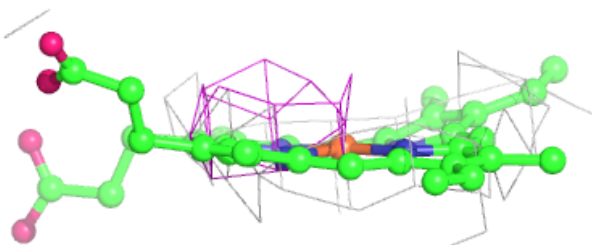
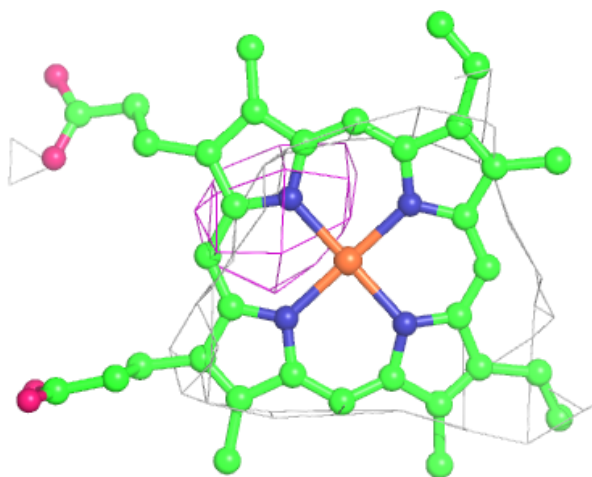
Electron density around LMG B 621:

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



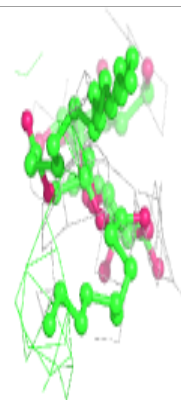
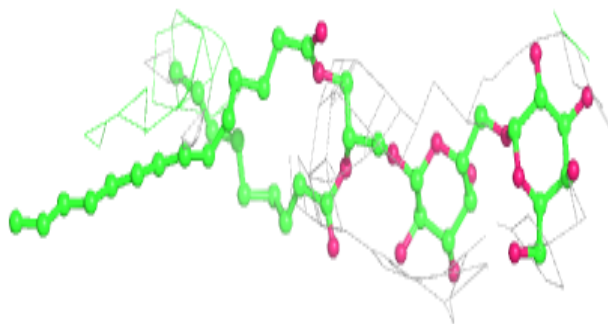
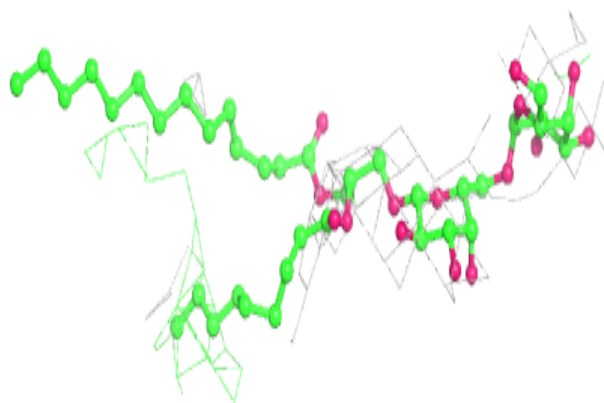
Electron density around HEM v 201:

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

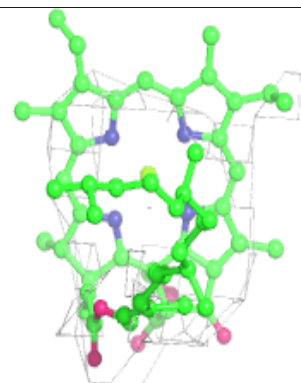
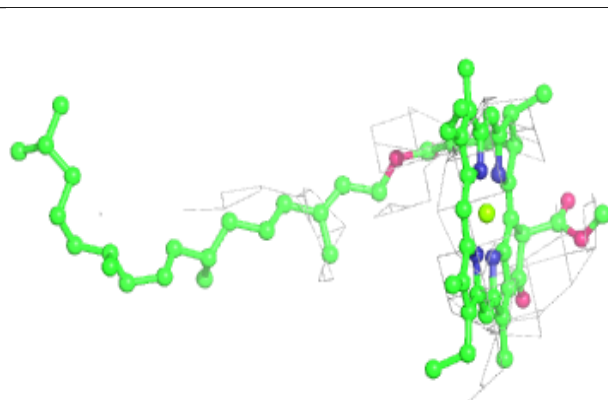
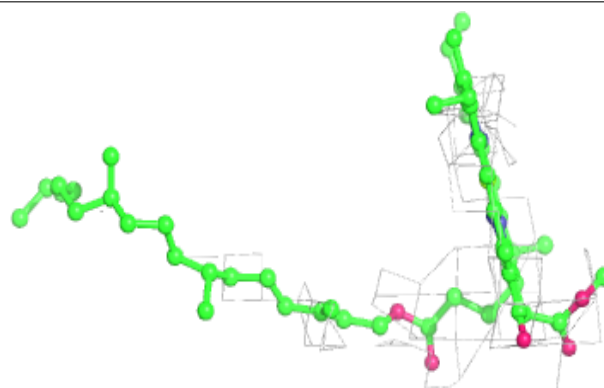


Electron density around DGD c 515:

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

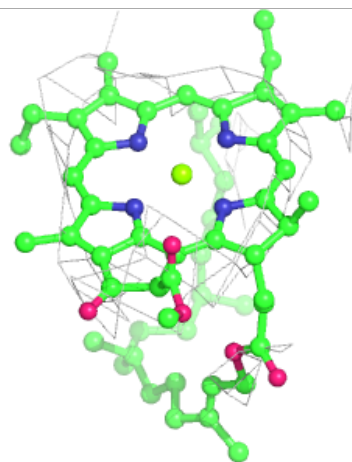
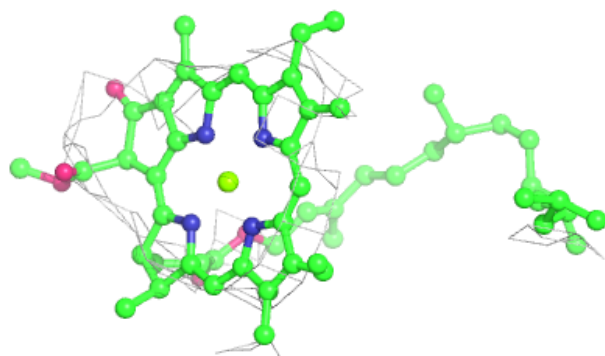
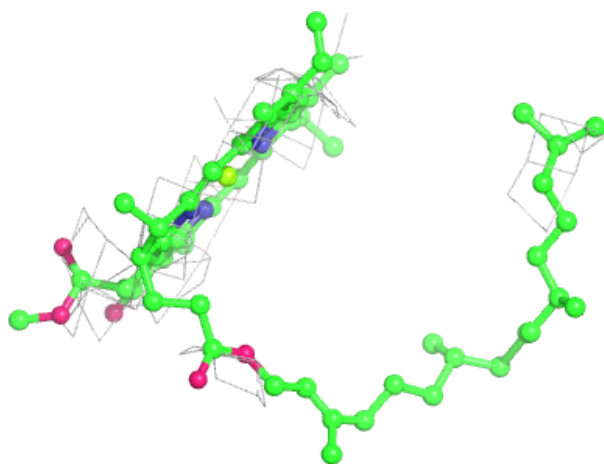
**Electron density around CLA B 604:**

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



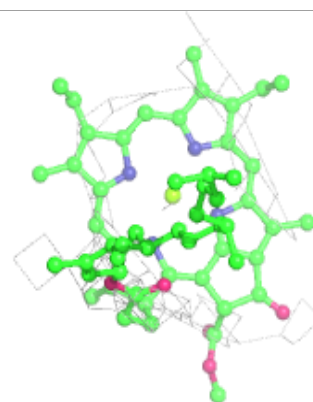
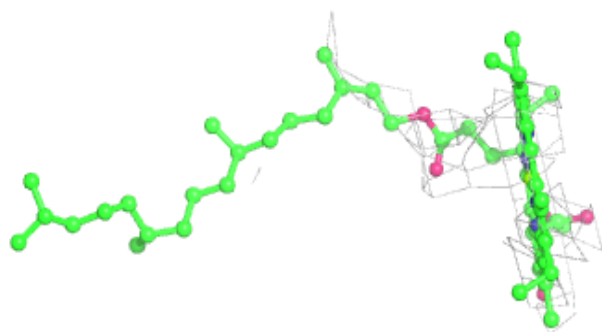
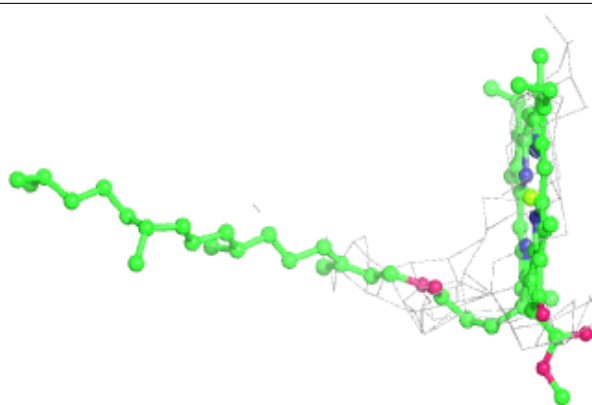
Electron density around CLA B 610:

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

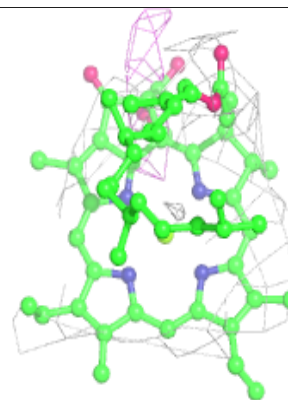
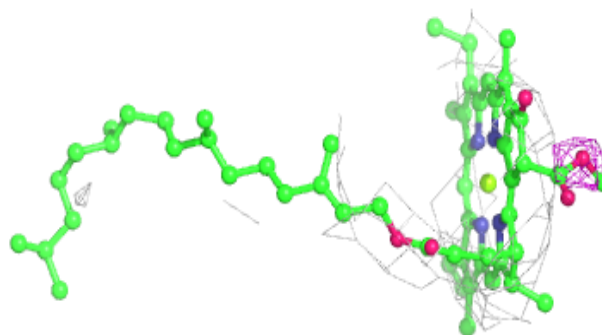
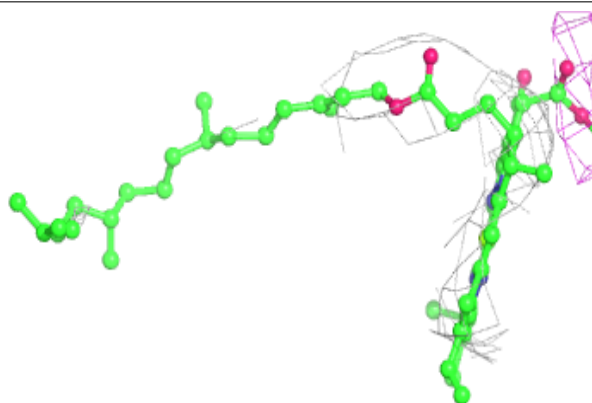


Electron density around CLA b 609:

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

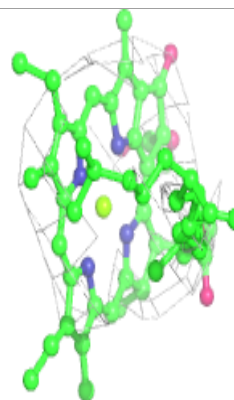
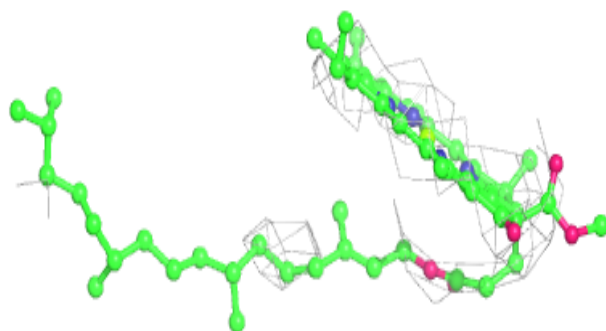
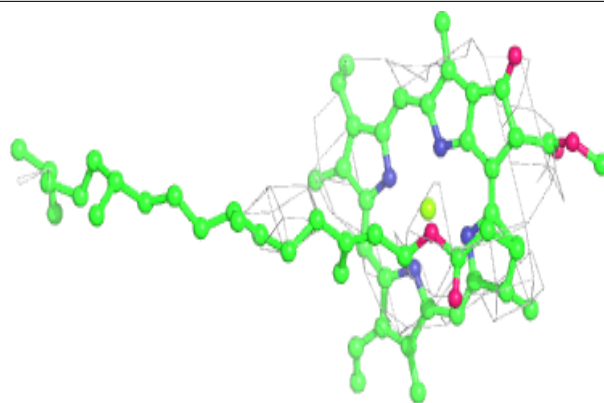
**Electron density around CLA b 608:**

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

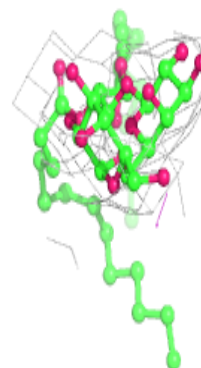
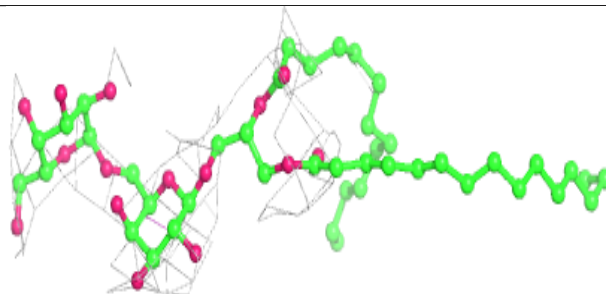
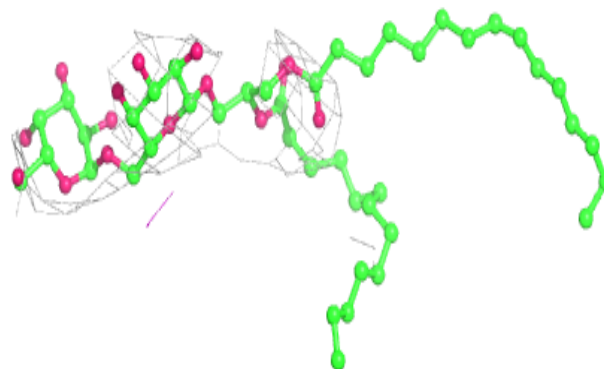


Electron density around CLA b 611:

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

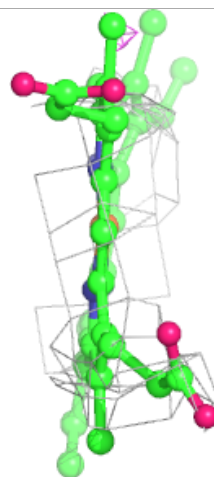
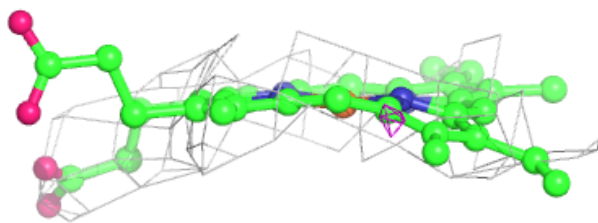
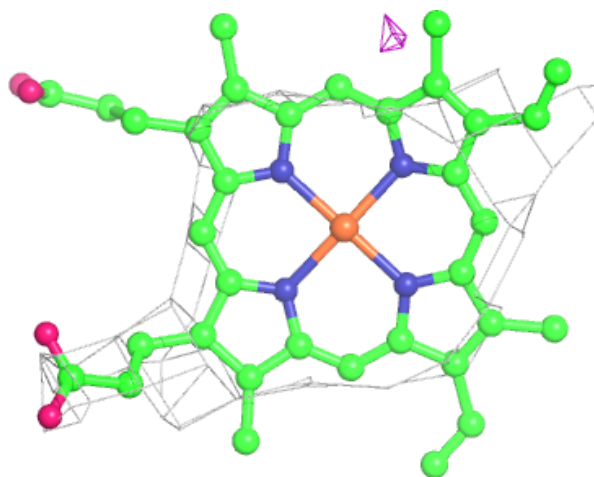
**Electron density around DGD B 620:**

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



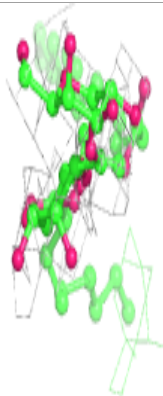
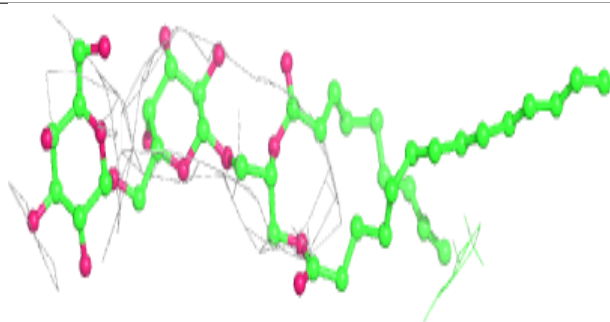
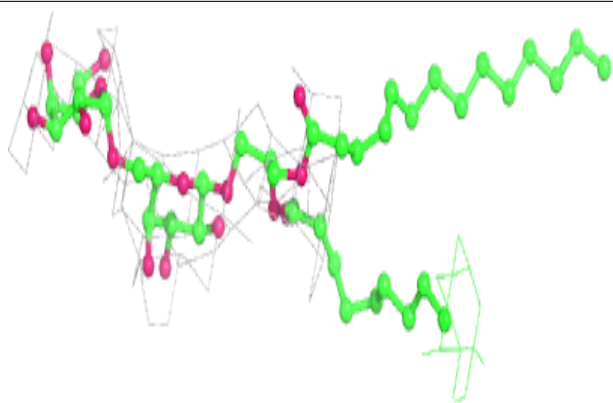
Electron density around HEM V 201:

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



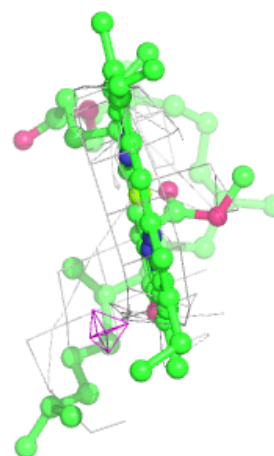
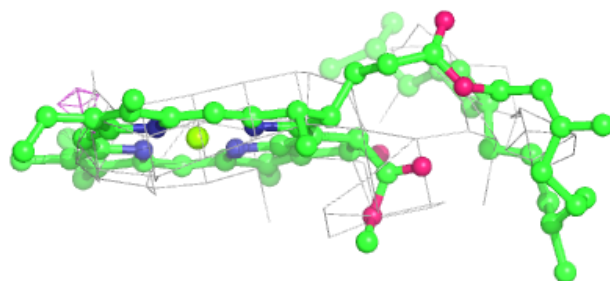
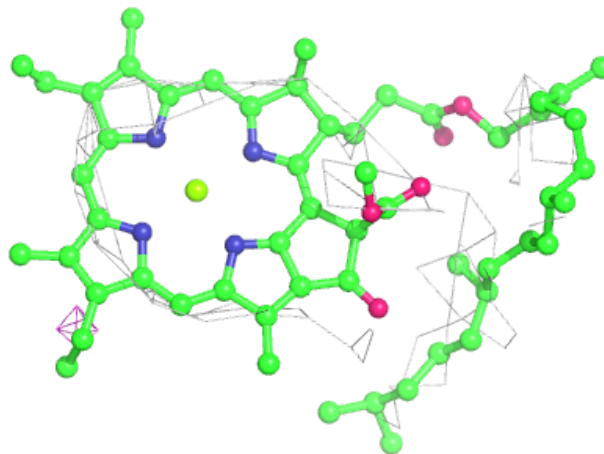
Electron density around DGD C 515:

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



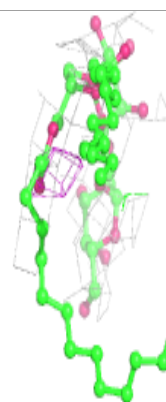
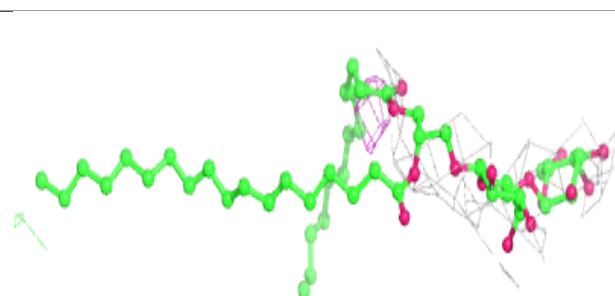
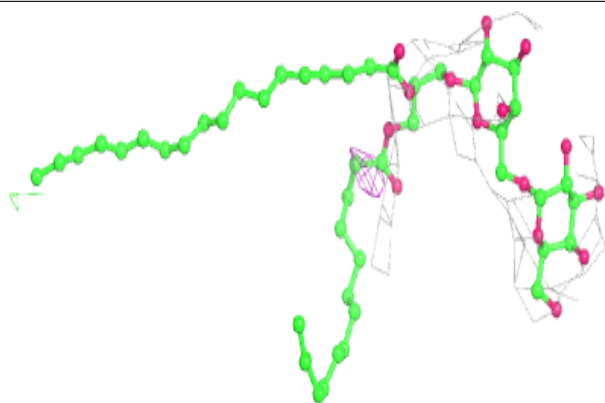
Electron density around CLA B 609:

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

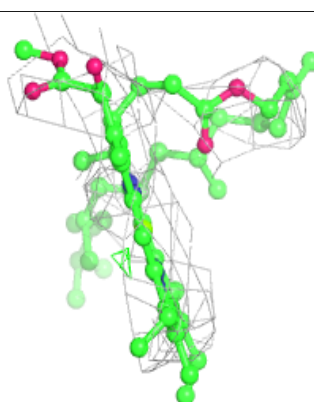
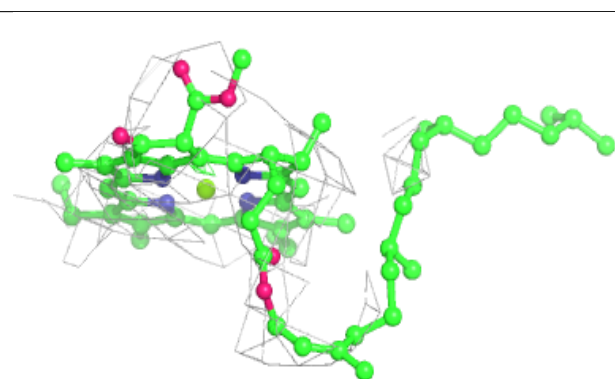
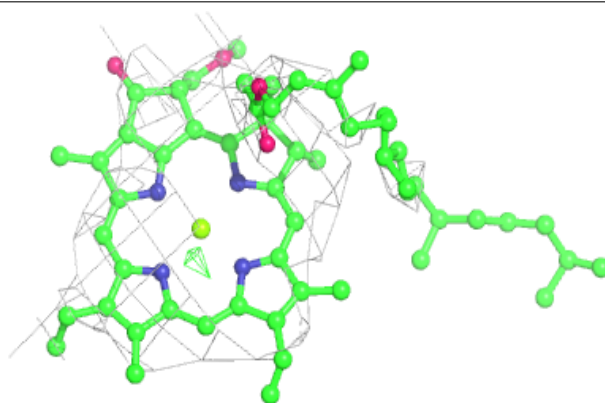


Electron density around DGD c 516:

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

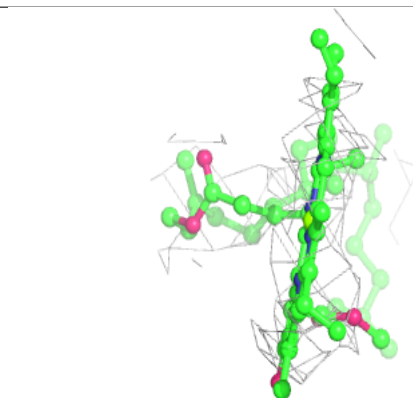
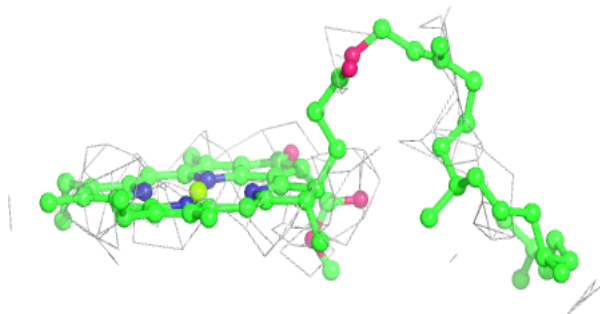
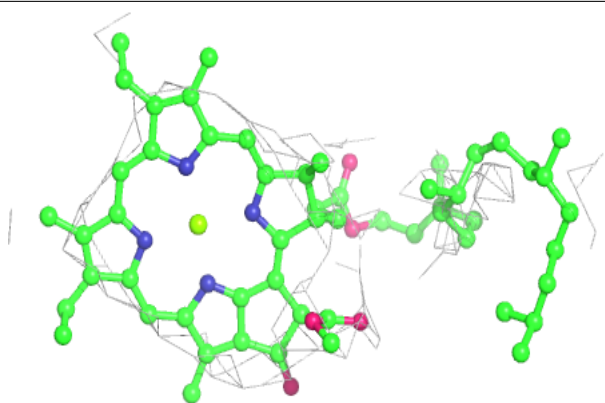
**Electron density around CLA A 403:**

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

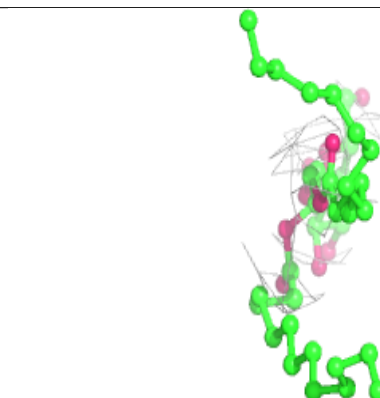
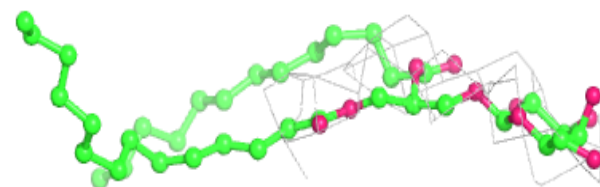
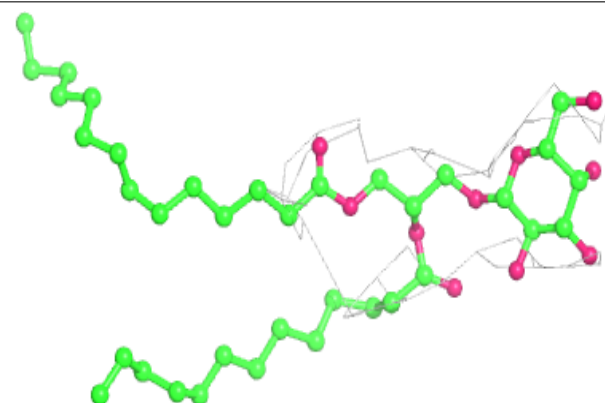


Electron density around CLA b 615:

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

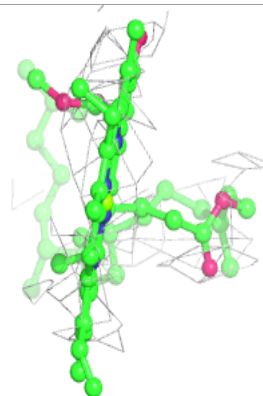
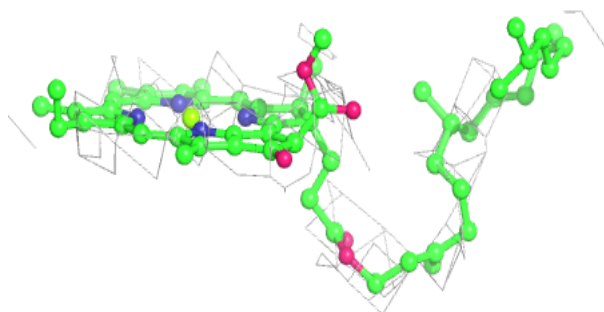
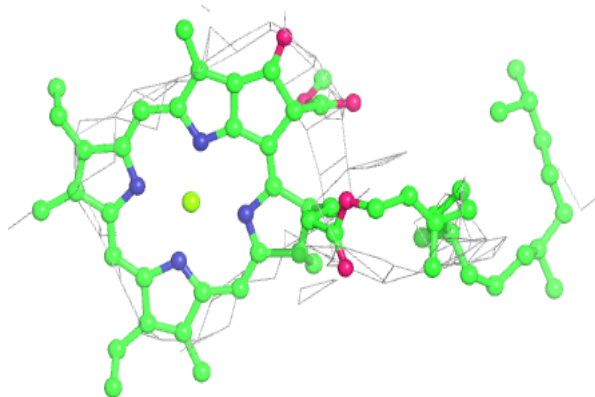
**Electron density around LMG d 411:**

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

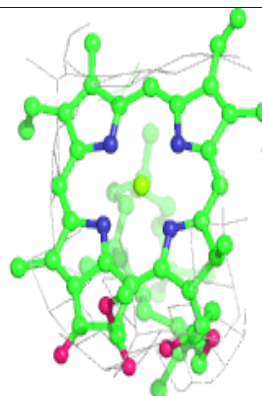
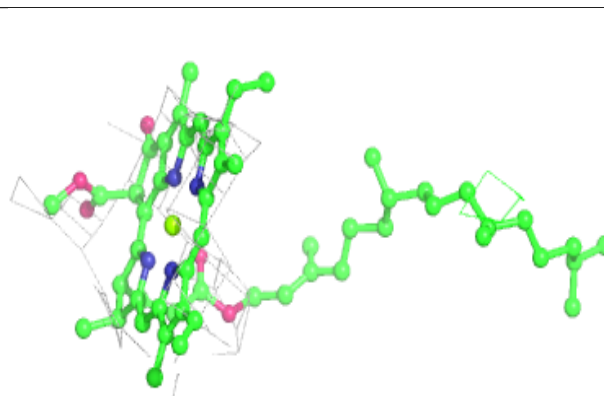
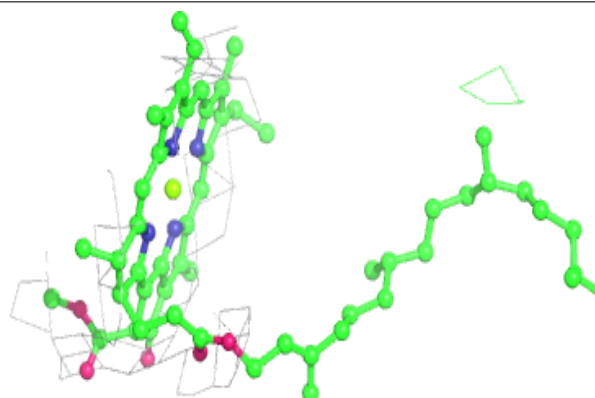


Electron density around CLA B 611:

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

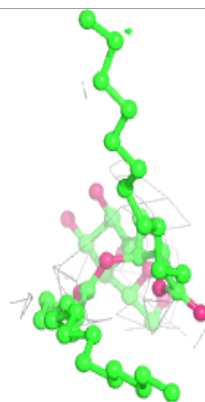
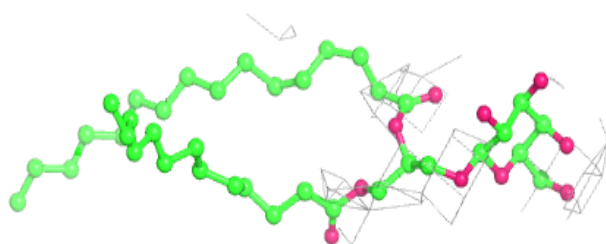
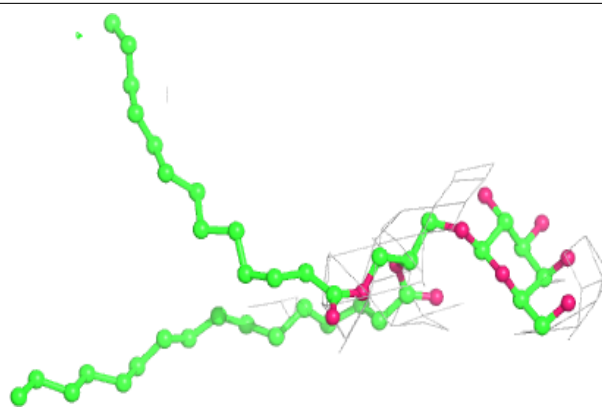
**Electron density around CLA c 507:**

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



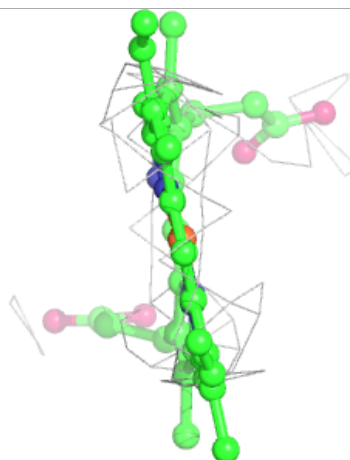
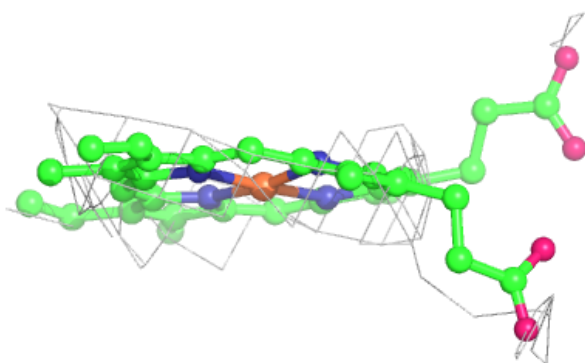
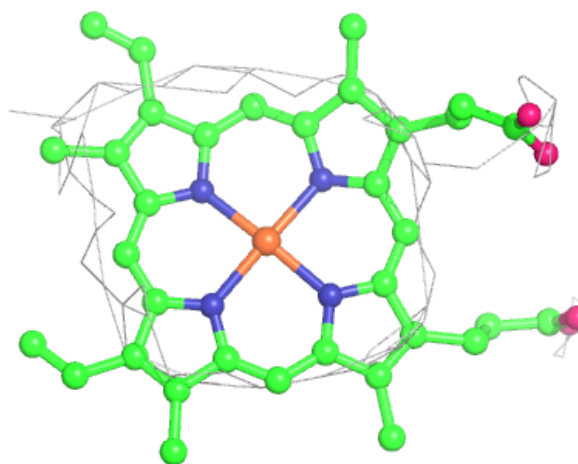
Electron density around LMG D 408:

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



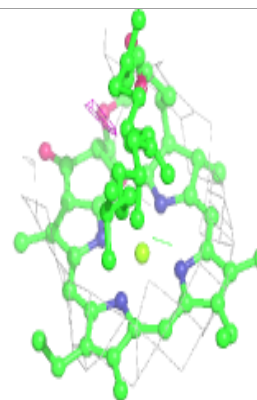
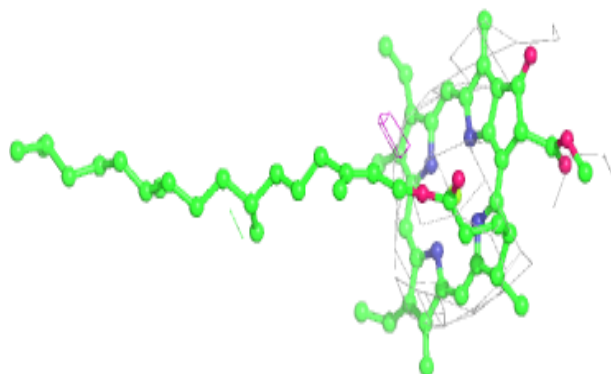
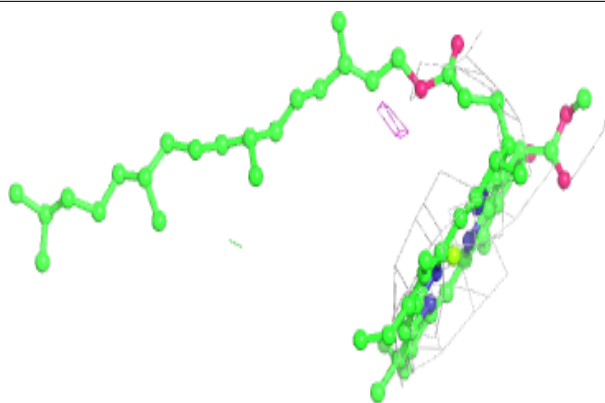
Electron density around HEM F 101:

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

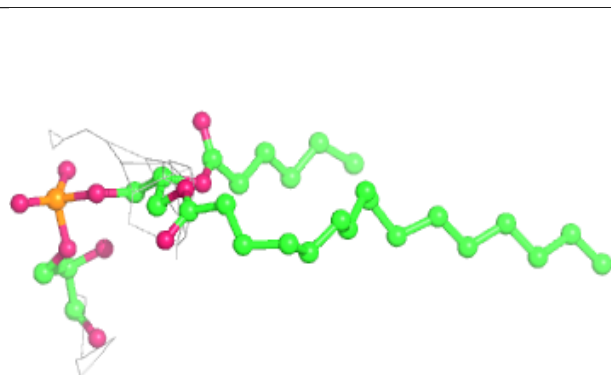
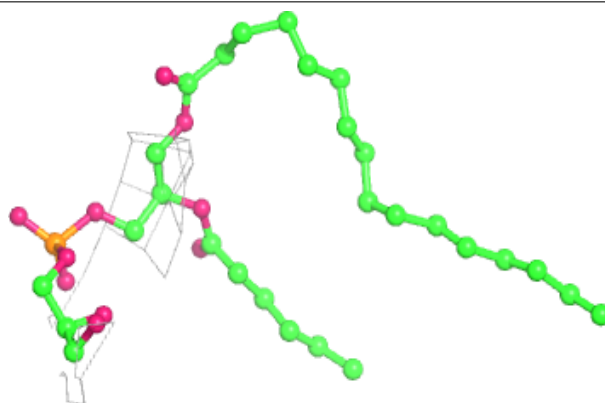


Electron density around CLA c 520:

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

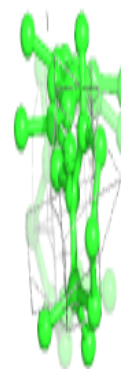
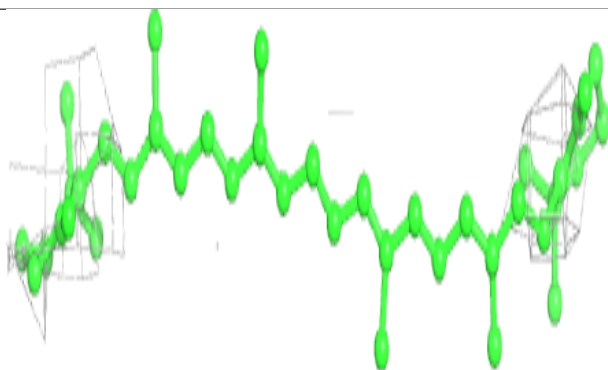
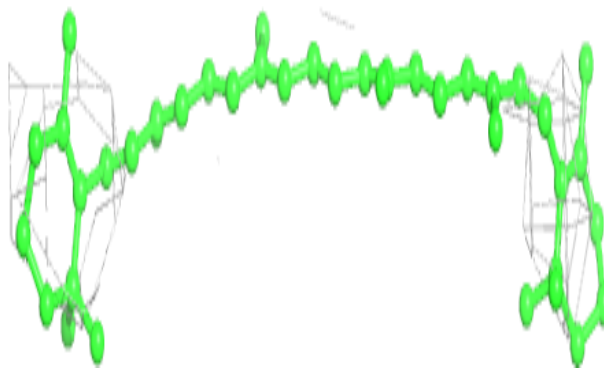
**Electron density around LHG A 409:**

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

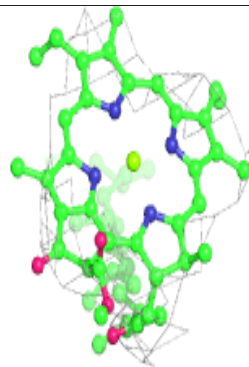
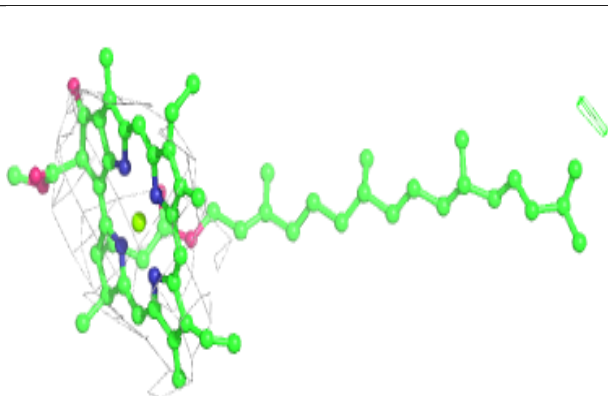
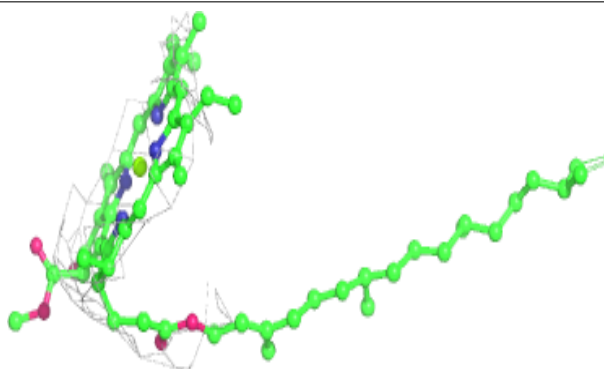


Electron density around BCR C 513:

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

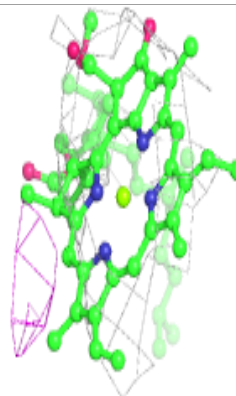
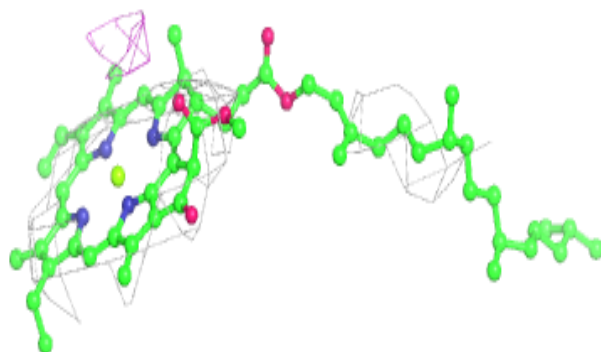
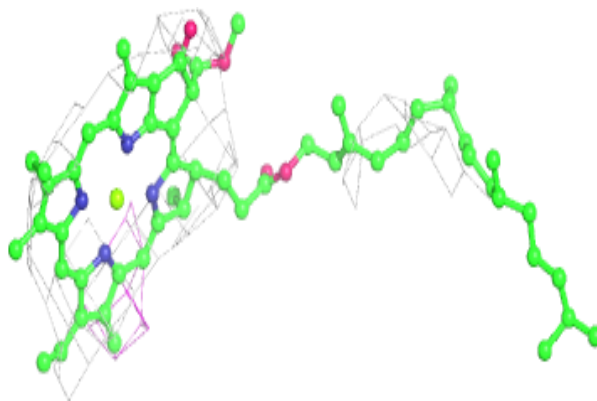
**Electron density around CLA B 606:**

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



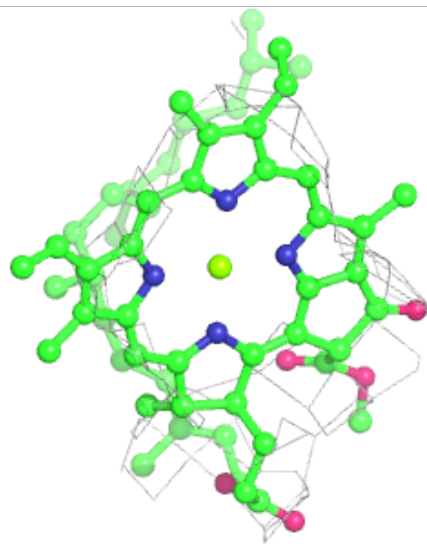
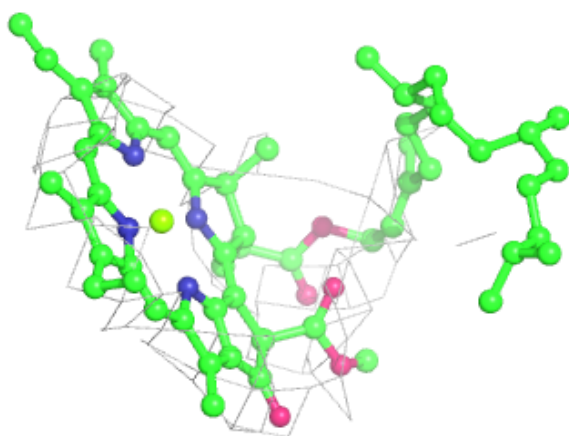
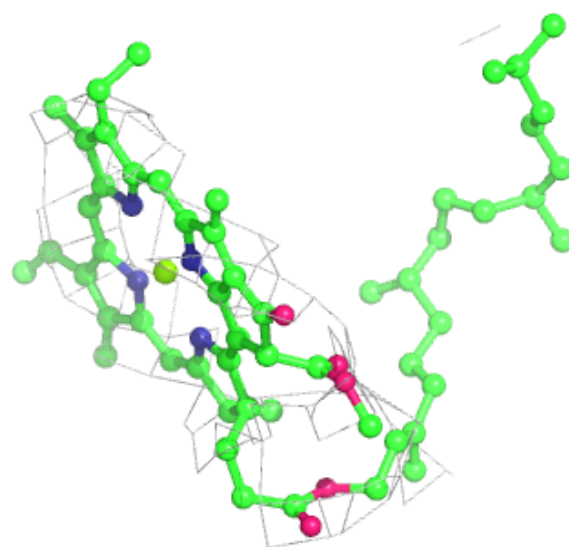
Electron density around CLA A 402:

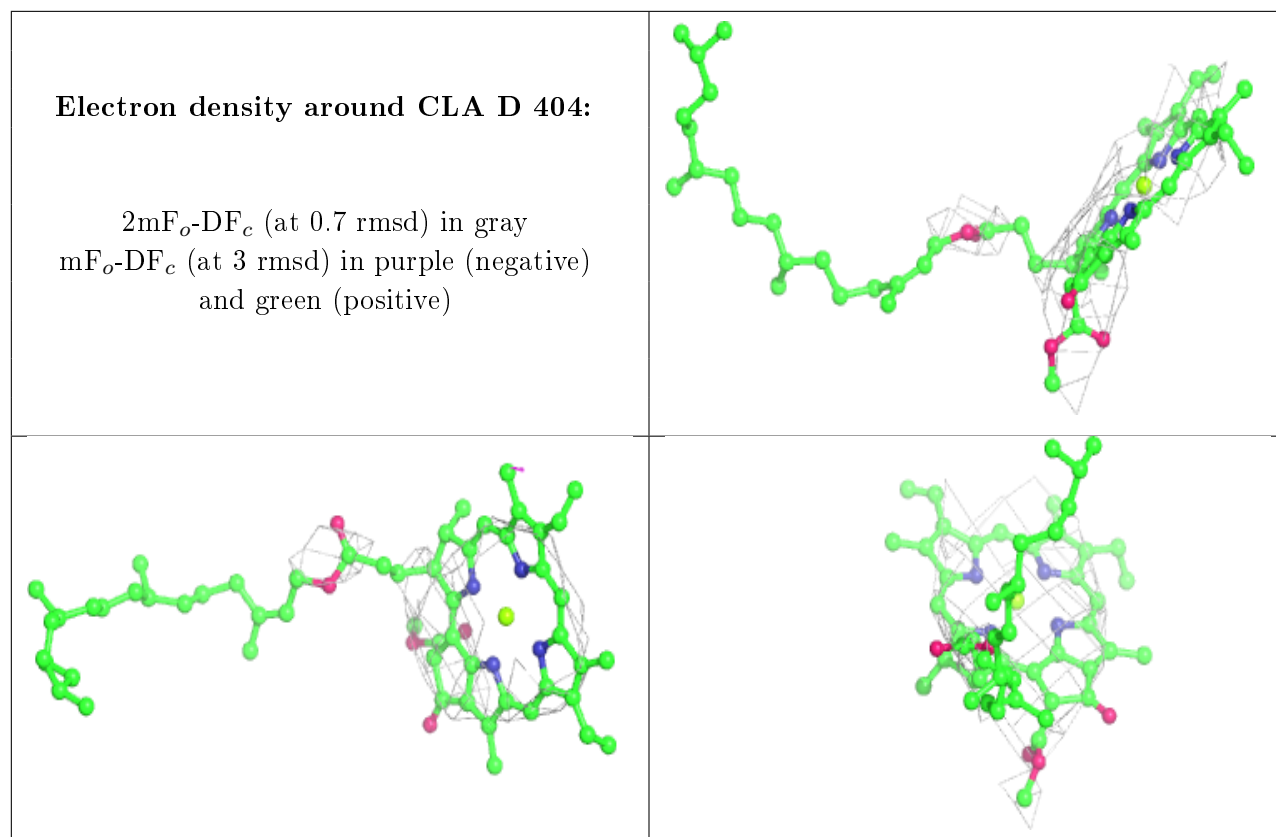
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA B 612:

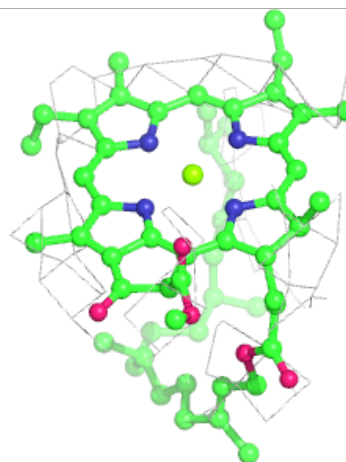
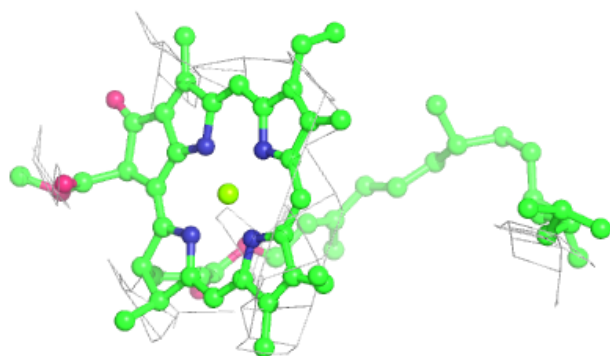
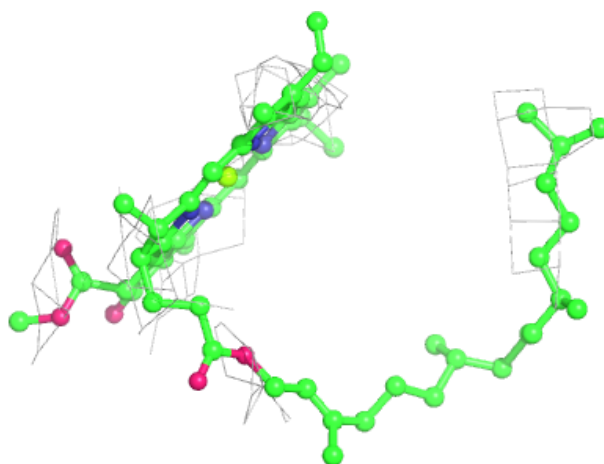
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





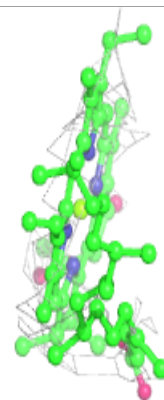
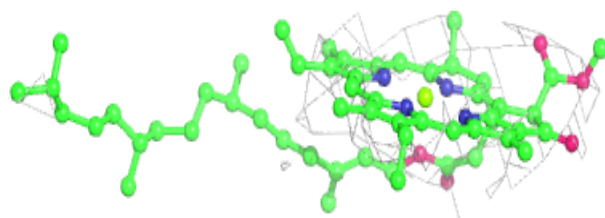
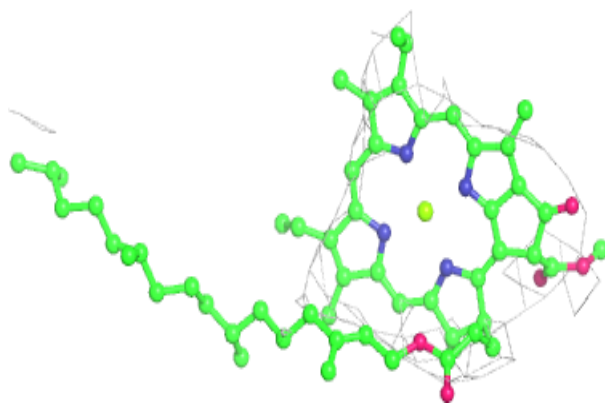
Electron density around CLA b 614:

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

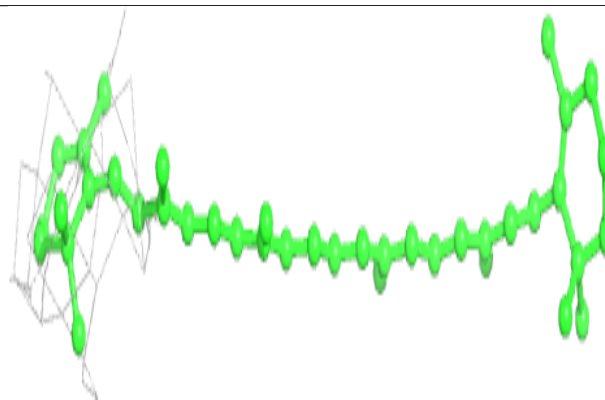
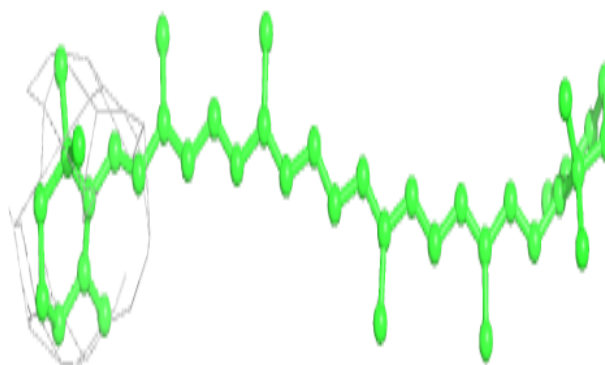


Electron density around CLA C 501:

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

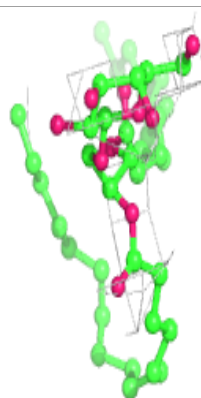
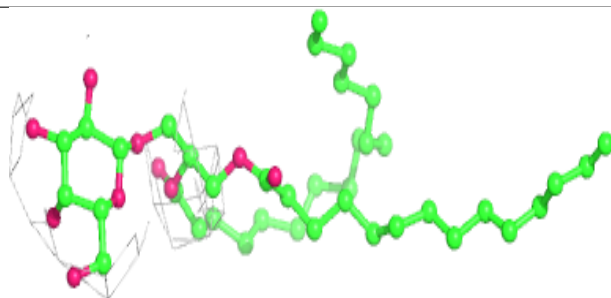
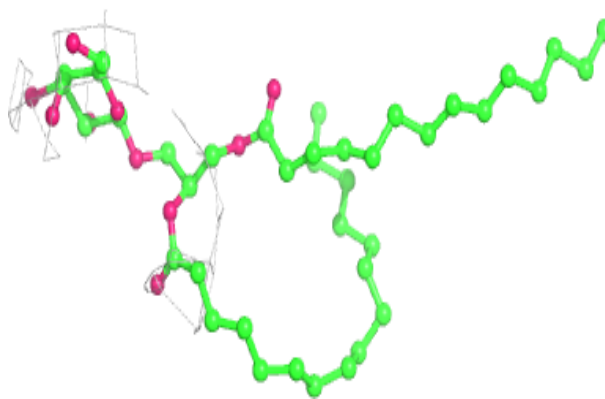
**Electron density around BCR b 620:**

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

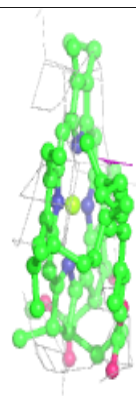
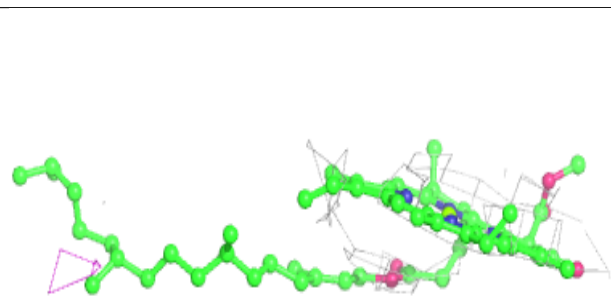
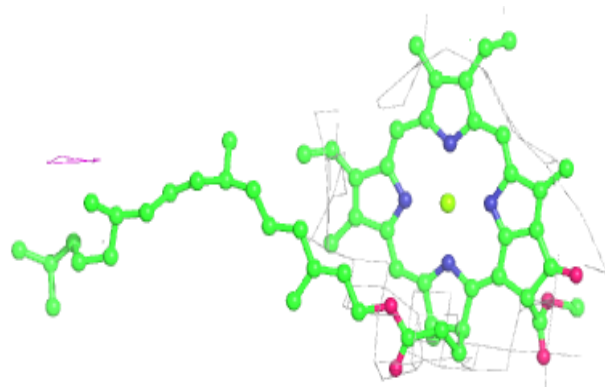


Electron density around LMG d 407:

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

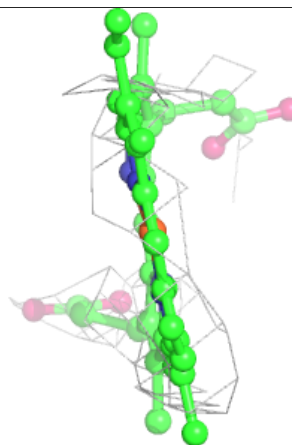
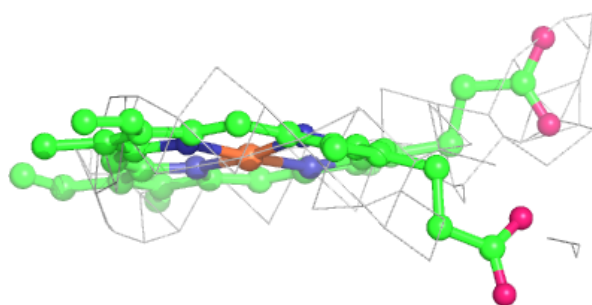
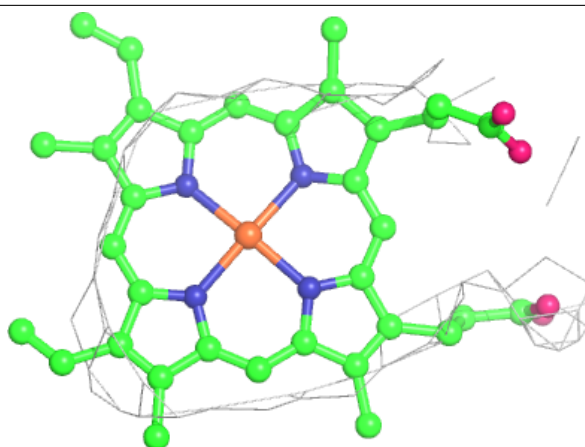
**Electron density around CLA B 602:**

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



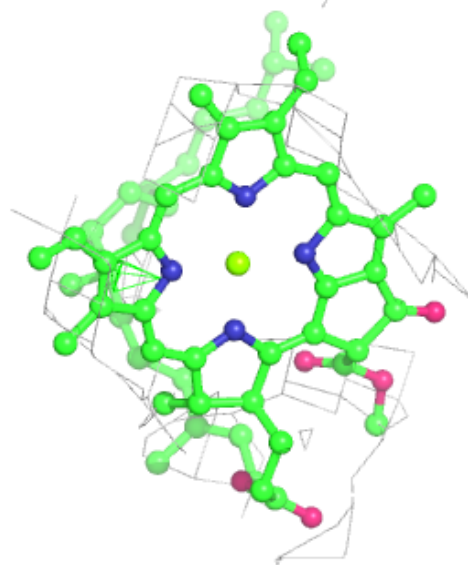
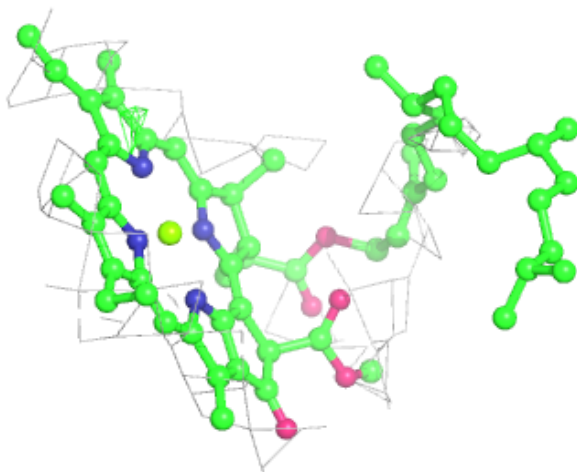
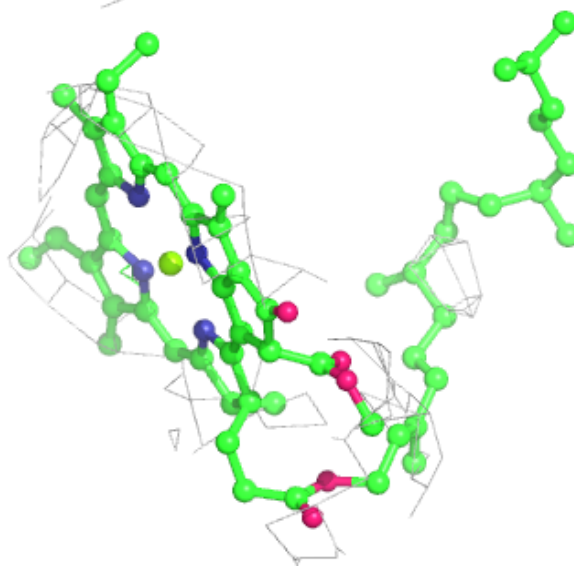
Electron density around HEM f 101:

$2mF_o - DF_c$ (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.