



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:02 PM BST

PDB ID : 4FBY
Title : fs X-ray diffraction of Photosystem II
Authors : Kern, J.; Alonso-Mori, R.; Hellmich, J.; Tran, R.; Hattne, J.; Laksmono, H.; Gloeckner, C.; Echols, N.; Sierra, R.G.; Sellberg, J.; Lassalle-Kaiser, B.; Gildea, R.J.; Glatzel, P.; Grosse-Kunstleve, R.W.; Latimer, M.J.; McQueen, T.A.; Difiore, D.; Fry, A.R.; Messerschmidt, M.M.; Miahnahri, A.; Schafer, D.W.; Seibert, M.M.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; White, W.E.; Adams, P.D.; Bogan, M.J.; Boutet, S.; Williams, G.J.; Messinger, J.; Sauter, N.K.; Zouni, A.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on : 2012-05-23
Resolution : 6.56 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](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

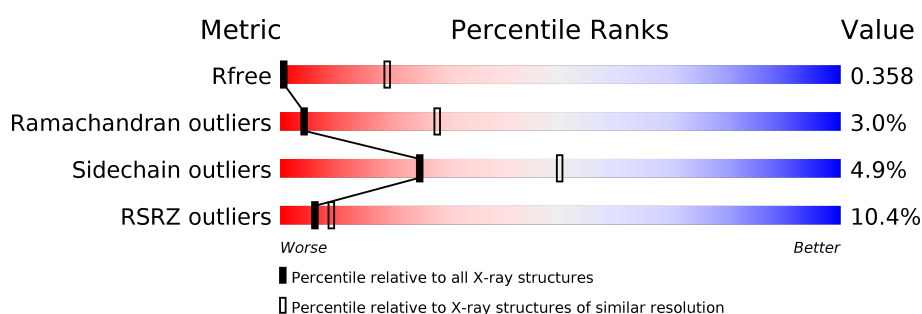
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.56 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	1000 (9.00-3.90)
Ramachandran outliers	138981	1012 (9.00-3.88)
Sidechain outliers	138945	1010 (9.00-3.84)
RSRZ outliers	127900	1002 (9.00-3.80)

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>93%</div> <div>5%</div> <div>.</div> </div>
1	G	344	<div> <div>6%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
2	B	510	<div> <div>11%</div> <div>91%</div> <div>.</div> <div>.</div> <div>.</div> </div>
2	N	510	<div> <div>13%</div> <div>91%</div> <div>.</div> <div>.</div> <div>.</div> </div>
3	C	461	<div> <div>5%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
3	P	461	<div> <div>15%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>
4	D	352	<div> <div>7%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	Q	352	
5	E	83	
5	R	83	
6	F	44	
6	S	44	
7	H	65	
7	W	65	
8	I	38	
8	a	38	
9	J	39	
9	b	39	
10	K	37	
10	c	37	
11	L	37	
11	d	37	
12	M	36	
12	e	36	
13	O	246	
13	f	246	
14	T	32	
14	g	32	
15	U	104	
15	h	104	
16	V	137	
16	i	137	

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Mol	Chain	Length	Quality of chain
17	m	46	
17	y	46	
18	X	40	
18	j	40	
19	Y	28	
19	k	28	
20	Z	62	
20	l	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
21	CLA	A	401	X	-	-	-
21	CLA	A	402	X	-	-	-
21	CLA	A	403	X	-	-	-
21	CLA	A	405	X	-	-	X
21	CLA	B	601	X	-	-	X
21	CLA	B	602	X	-	-	-
21	CLA	B	603	X	-	-	-
21	CLA	B	604	X	-	-	X
21	CLA	B	605	X	-	-	X
21	CLA	B	606	X	-	-	-
21	CLA	B	607	X	-	-	-
21	CLA	B	608	X	-	-	X
21	CLA	B	609	X	-	-	-
21	CLA	B	610	X	-	-	-
21	CLA	B	611	X	-	-	-
21	CLA	B	612	X	-	-	X
21	CLA	B	613	X	-	-	-
21	CLA	B	614	X	-	-	-
21	CLA	B	615	X	-	-	X
21	CLA	B	616	X	-	-	X
21	CLA	C	501	X	-	-	X
21	CLA	C	502	X	-	-	X
21	CLA	C	503	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	C	504	X	-	-	-
21	CLA	C	505	X	-	-	X
21	CLA	C	506	X	-	-	X
21	CLA	C	507	X	-	-	X
21	CLA	C	508	X	-	-	-
21	CLA	C	509	X	-	-	X
21	CLA	C	510	X	-	-	-
21	CLA	C	511	X	-	-	X
21	CLA	C	512	X	-	-	X
21	CLA	C	513	X	-	-	X
21	CLA	D	401	X	-	-	X
21	CLA	D	403	X	-	-	-
21	CLA	G	402	X	-	-	-
21	CLA	G	403	X	-	-	-
21	CLA	G	404	X	-	-	-
21	CLA	G	406	X	-	-	X
21	CLA	N	605	X	-	-	X
21	CLA	N	606	X	-	-	-
21	CLA	N	607	X	-	-	X
21	CLA	N	608	X	-	-	X
21	CLA	N	609	X	-	-	X
21	CLA	N	610	X	-	-	X
21	CLA	N	611	X	-	-	-
21	CLA	N	612	X	-	-	-
21	CLA	N	613	X	-	-	X
21	CLA	N	614	X	-	-	-
21	CLA	N	615	X	-	-	-
21	CLA	N	616	X	-	-	X
21	CLA	N	617	X	-	-	-
21	CLA	N	618	X	-	-	-
21	CLA	N	619	X	-	-	X
21	CLA	N	620	X	-	-	X
21	CLA	P	501	X	-	-	-
21	CLA	P	502	X	-	-	X
21	CLA	P	503	X	-	-	X
21	CLA	P	504	X	-	-	-
21	CLA	P	505	X	-	-	-
21	CLA	P	506	X	-	-	-
21	CLA	P	507	X	-	-	X
21	CLA	P	508	X	-	-	-
21	CLA	P	509	X	-	-	X
21	CLA	P	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	P	511	X	-	-	X
21	CLA	P	512	X	-	-	-
21	CLA	P	513	X	-	-	X
21	CLA	Q	402	X	-	-	X
21	CLA	Q	404	X	-	-	-
22	PHO	D	402	-	-	-	X
23	PL9	G	407	-	-	-	X
23	PL9	J	101	-	-	-	X
23	PL9	b	101	-	-	-	X
24	DGD	A	407	X	-	-	-
24	DGD	B	621	X	-	-	X
24	DGD	B	628	X	-	-	X
24	DGD	C	516	X	-	-	-
24	DGD	C	517	X	-	-	-
24	DGD	C	518	X	-	-	-
24	DGD	D	408	X	-	-	X
24	DGD	G	408	X	-	-	X
24	DGD	N	602	X	-	-	X
24	DGD	P	517	X	-	-	-
24	DGD	P	518	X	-	-	-
24	DGD	P	519	X	-	-	-
24	DGD	Q	409	X	-	-	X
24	DGD	W	102	X	-	-	-
25	LHG	A	411	-	-	-	X
25	LHG	G	412	-	-	-	X
26	SQD	A	414	-	-	-	X
26	SQD	B	624	-	-	-	X
26	SQD	B	627	-	-	-	X
26	SQD	F	101	-	-	-	X
26	SQD	N	601	-	-	-	X
26	SQD	Q	408	-	-	-	X
27	LMG	A	410	X	-	-	-
27	LMG	B	622	X	-	-	-
27	LMG	B	623	X	-	-	-
27	LMG	C	519	X	-	-	-
27	LMG	C	520	X	-	-	X
27	LMG	D	406	X	-	-	-
27	LMG	D	407	X	-	-	-
27	LMG	D	412	X	-	-	X
27	LMG	E	102	X	-	-	X
27	LMG	G	411	X	-	-	-
27	LMG	I	102	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	LMG	M	101	X	-	-	-
27	LMG	N	622	X	-	-	-
27	LMG	N	623	X	-	-	-
27	LMG	P	520	X	-	-	X
27	LMG	P	521	X	-	-	X
27	LMG	Q	401	X	-	-	X
27	LMG	Q	406	X	-	-	-
27	LMG	Q	407	X	-	-	-
27	LMG	R	102	X	-	-	X
27	LMG	a	102	X	-	-	X
27	LMG	e	102	X	-	-	-
30	BCR	B	620	-	-	-	X
30	BCR	C	514	-	-	-	X
30	BCR	C	515	-	-	-	X
30	BCR	D	405	-	-	-	X
30	BCR	H	101	-	-	-	X
30	BCR	I	101	-	-	-	X
30	BCR	J	102	-	-	-	X
30	BCR	K	101	-	-	-	X
30	BCR	P	514	-	-	-	X
30	BCR	P	516	-	-	-	X
30	BCR	T	103	-	-	-	X
30	BCR	W	101	-	-	-	X
30	BCR	a	101	-	-	-	X
30	BCR	b	102	-	-	-	X
30	BCR	c	101	-	-	-	X
31	LMT	B	625	-	-	-	X
31	LMT	B	626	-	-	-	X
31	LMT	B	629	-	-	-	X
31	LMT	B	630	-	-	-	X
31	LMT	D	409	-	-	-	X
31	LMT	I	103	-	-	-	X
31	LMT	M	102	-	-	-	X
31	LMT	N	603	-	-	-	X
31	LMT	N	604	-	-	-	X
31	LMT	N	624	-	-	-	X
31	LMT	N	625	-	-	-	X
31	LMT	Q	410	-	-	-	X
31	LMT	a	103	-	-	-	X
31	LMT	e	101	-	-	-	X
33	CL	D	411	-	-	-	X
35	CA	O	301	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CA	f	301	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50232 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	G	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	N	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	P	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	Q	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	R	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	S	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	W	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	a	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	b	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	c	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	d	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	e	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	f	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	g	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	h	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	i	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	m	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O		0	0	0
			270	182	41	47				
18	j	37	Total	C	N	O		0	0	0
			270	182	41	47				

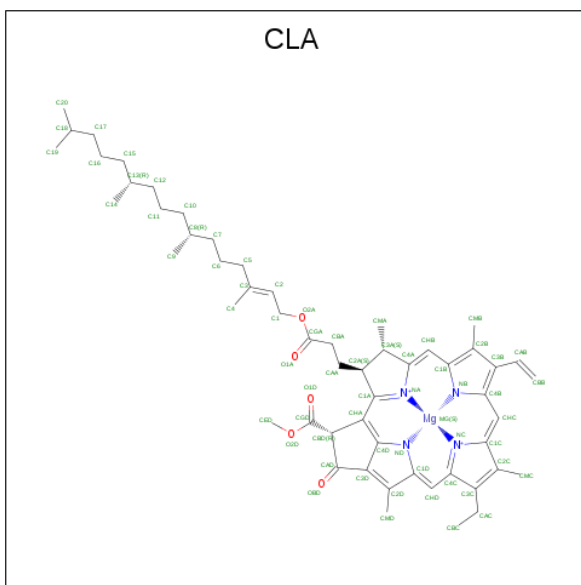
- Molecule 19 is a protein called Photosystem II reaction center protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O		0	0	0
			140	84	28	28				
19	k	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	l	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).

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

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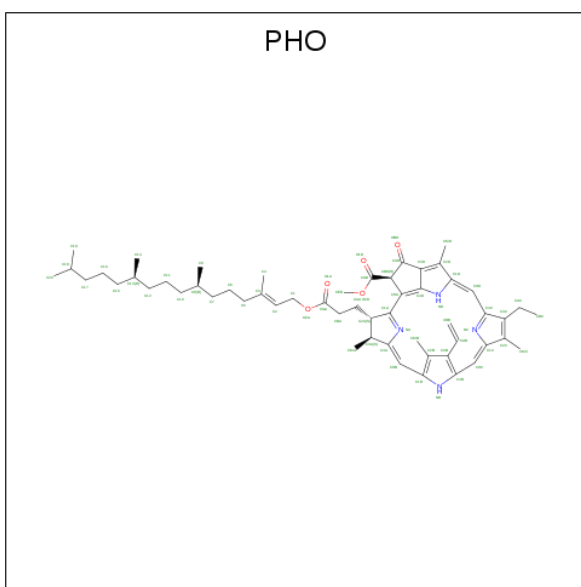
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	G	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	N	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	P	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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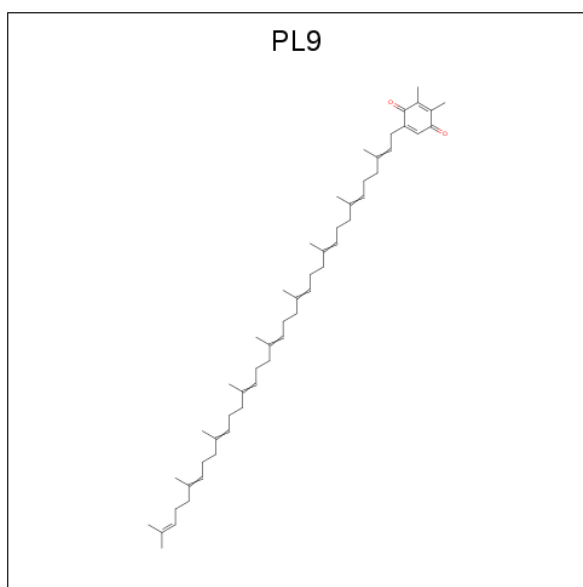
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	P	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	Q	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



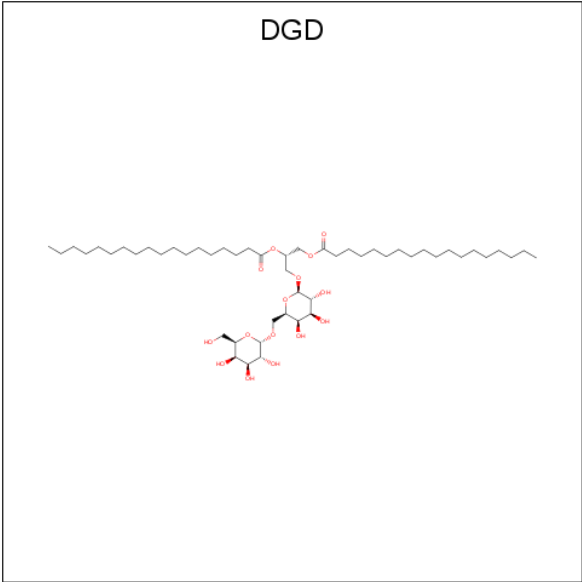
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			64	55	4	5		
22	D	1	Total	C	N	O	0	0
			64	55	4	5		
22	G	1	Total	C	N	O	0	0
			64	55	4	5		
22	Q	1	Total	C	N	O	0	0
			64	55	4	5		

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



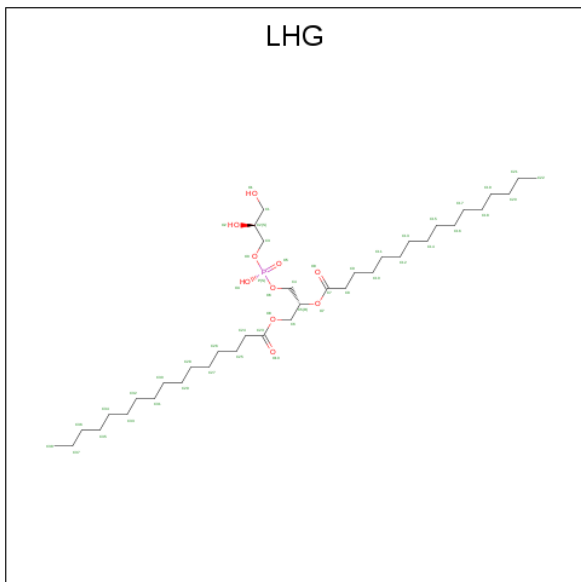
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			45	43	2		
23	D	1	Total	C	O	0	0
			55	53	2		
23	J	1	Total	C	O	0	0
			35	33	2		
23	G	1	Total	C	O	0	0
			45	43	2		
23	Q	1	Total	C	O	0	0
			55	53	2		
23	b	1	Total	C	O	0	0
			35	33	2		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



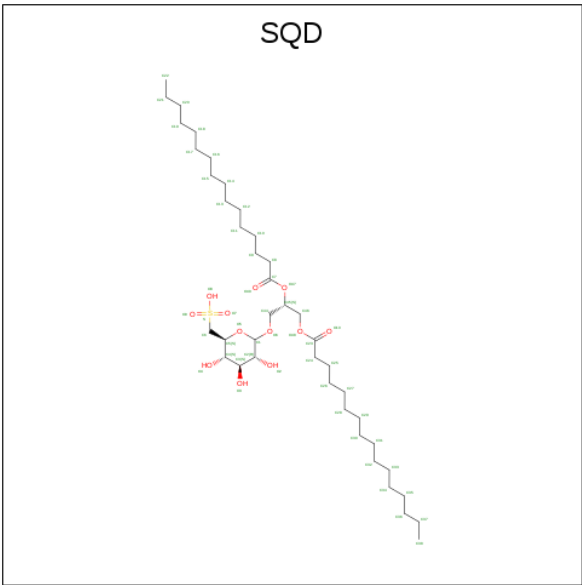
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total	C	O	0	0
			56	41	15		
24	B	1	Total	C	O	0	0
			58	43	15		
24	B	1	Total	C	O	0	0
			52	37	15		
24	C	1	Total	C	O	0	0
			53	38	15		
24	C	1	Total	C	O	0	0
			62	47	15		
24	C	1	Total	C	O	0	0
			66	51	15		
24	D	1	Total	C	O	0	0
			63	48	15		
24	G	1	Total	C	O	0	0
			56	41	15		
24	N	1	Total	C	O	0	0
			52	37	15		
24	P	1	Total	C	O	0	0
			53	38	15		
24	P	1	Total	C	O	0	0
			62	47	15		
24	P	1	Total	C	O	0	0
			66	51	15		
24	Q	1	Total	C	O	0	0
			63	48	15		
24	W	1	Total	C	O	0	0
			58	43	15		

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



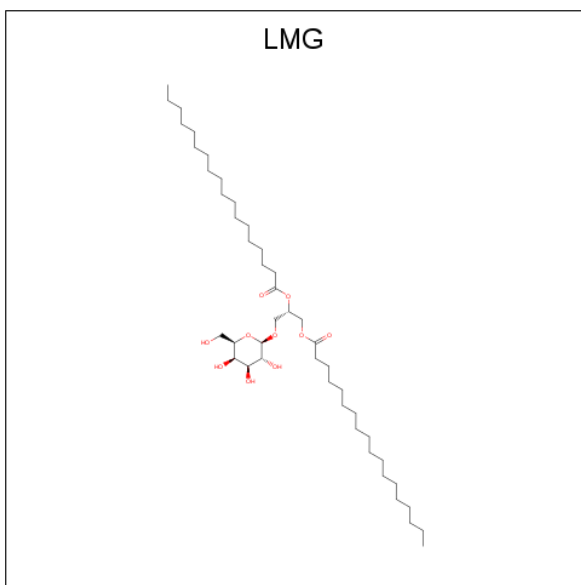
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	P	0	0
			39	28	10	1		
25	A	1	Total	C	O	P	0	0
			37	26	10	1		
25	G	1	Total	C	O	P	0	0
			39	28	10	1		
25	G	1	Total	C	O	P	0	0
			37	26	10	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			51	38	12	1		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			43	30	12	1		
26	B	1	Total	C	O	S	0	0
			47	34	12	1		
26	F	1	Total	C	O	S	0	0
			45	32	12	1		
26	G	1	Total	C	O	S	0	0
			54	41	12	1		
26	G	1	Total	C	O	S	0	0
			51	38	12	1		
26	N	1	Total	C	O	S	0	0
			47	34	12	1		
26	Q	1	Total	C	O	S	0	0
			43	30	12	1		
26	S	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



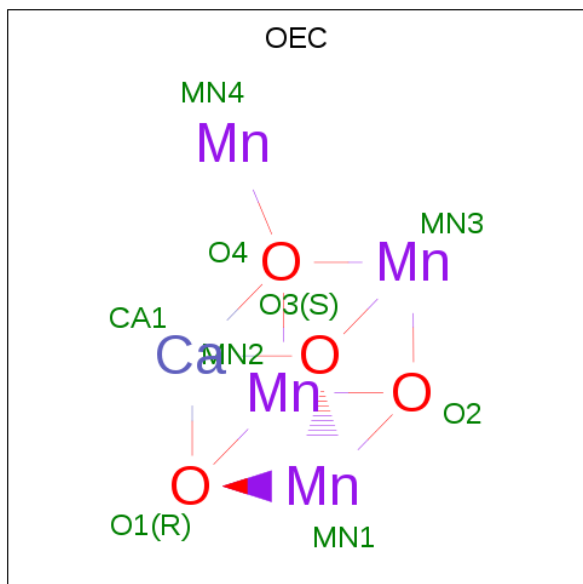
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			51	41	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	B	1	Total	C	O	0	0
			49	39	10		
27	C	1	Total	C	O	0	0
			48	38	10		
27	C	1	Total	C	O	0	0
			45	35	10		
27	D	1	Total	C	O	0	0
			46	36	10		
27	D	1	Total	C	O	0	0
			48	38	10		
27	D	1	Total	C	O	0	0
			42	32	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	G	1	Total	C	O	0	0
			51	41	10		
27	N	1	Total	C	O	0	0
			49	39	10		
27	N	1	Total	C	O	0	0
			49	39	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	P	1	Total	C	O	0	0
			48	38	10		
27	P	1	Total	C	O	0	0
			45	35	10		
27	Q	1	Total	C	O	0	0
			42	32	10		
27	Q	1	Total	C	O	0	0
			48	38	10		
27	Q	1	Total	C	O	0	0
			46	36	10		
27	R	1	Total	C	O	0	0
			44	34	10		
27	a	1	Total	C	O	0	0
			43	33	10		
27	e	1	Total	C	O	0	0
			42	32	10		

- Molecule 28 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).

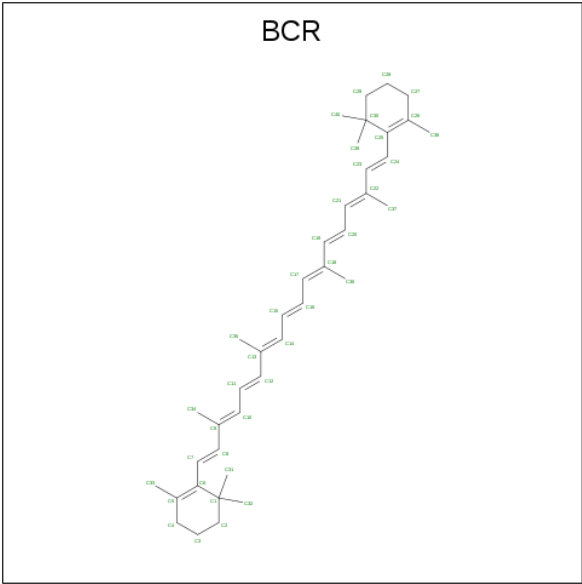


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	Ca	Mn	0	0
			5	1	4		
28	G	1	Total	Ca	Mn	0	0
			5	1	4		

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

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

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



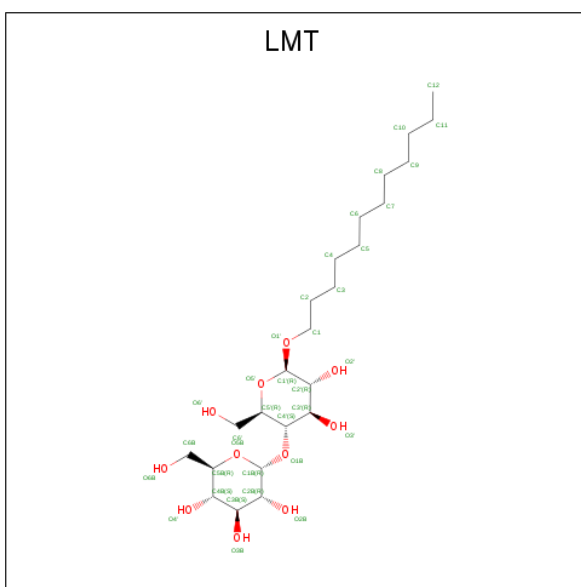
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	B	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	C	1	Total C 40 40	0	0
30	D	1	Total C 40 40	0	0
30	H	1	Total C 40 40	0	0
30	I	1	Total C 40 40	0	0
30	J	1	Total C 40 40	0	0

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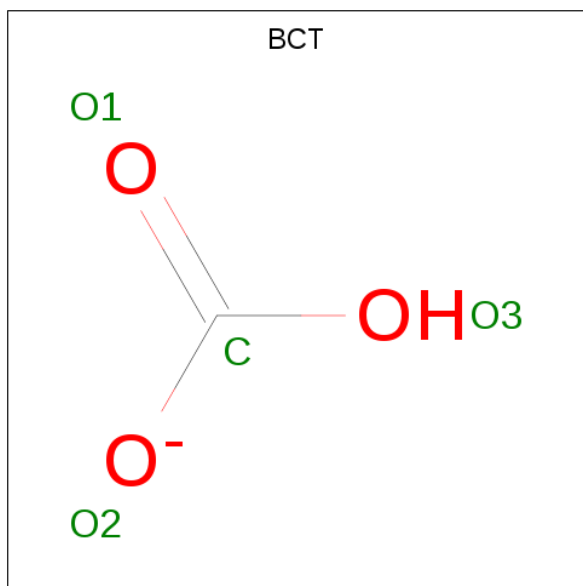
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	K	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	T	1	Total C 40 40	0	0
30	Z	1	Total C 40 40	0	0
30	N	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	P	1	Total C 40 40	0	0
30	S	1	Total C 40 40	0	0
30	W	1	Total C 40 40	0	0
30	a	1	Total C 40 40	0	0
30	b	1	Total C 40 40	0	0
30	c	1	Total C 40 40	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	B	1	Total 35	C 24	O 11	0	0
31	D	1	Total 31	C 20	O 11	0	0
31	I	1	Total 35	C 24	O 11	0	0
31	M	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	N	1	Total 35	C 24	O 11	0	0
31	Q	1	Total 31	C 20	O 11	0	0
31	a	1	Total 35	C 24	O 11	0	0
31	e	1	Total 35	C 24	O 11	0	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

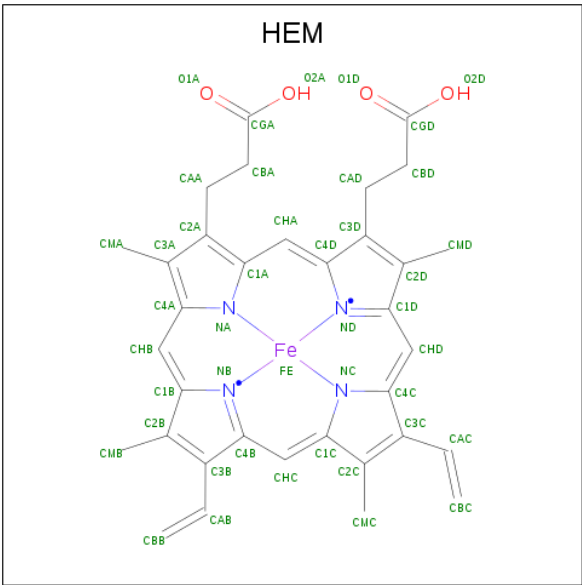


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	0
			4	1	3		
32	Q	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	G	1	Total	Cl	0	0
			1	1		
33	D	1	Total	Cl	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	R	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	i	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

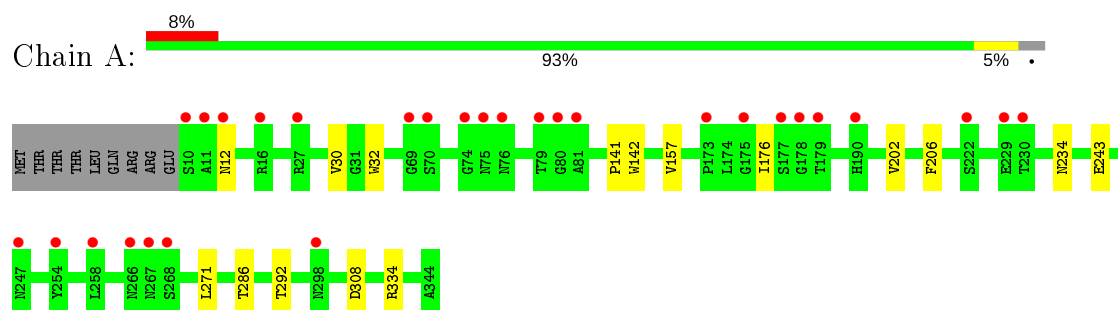
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

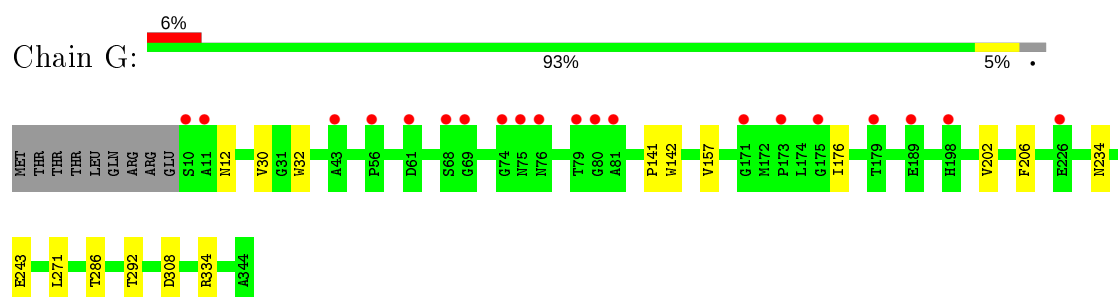
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

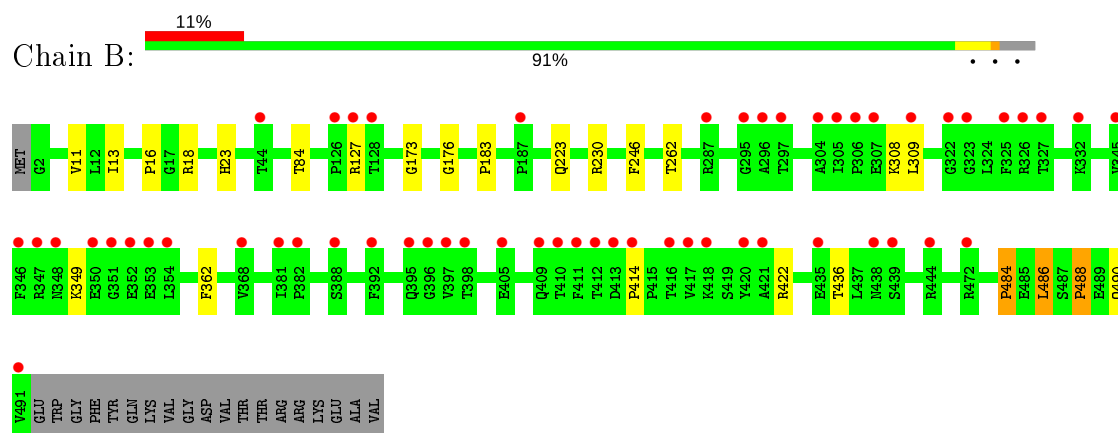
- Molecule 1: Photosystem Q(B) protein 1



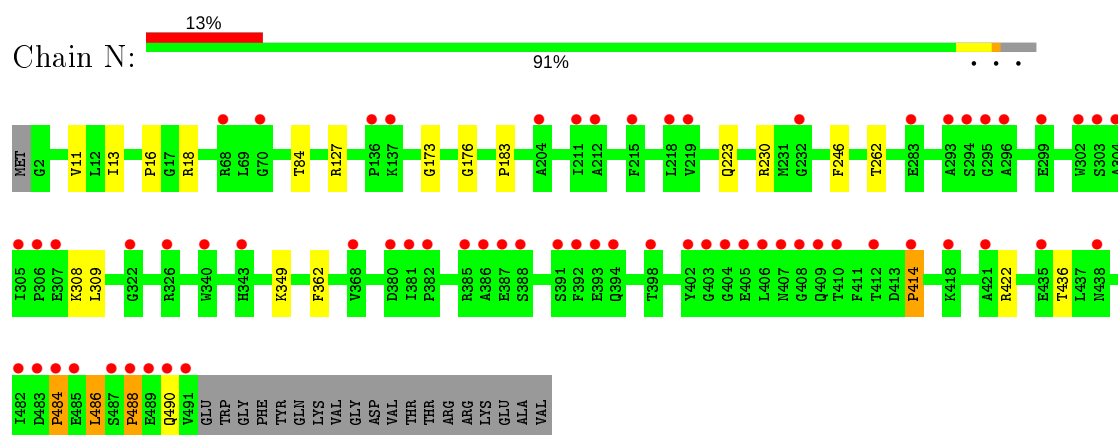
- Molecule 1: Photosystem Q(B) protein 1



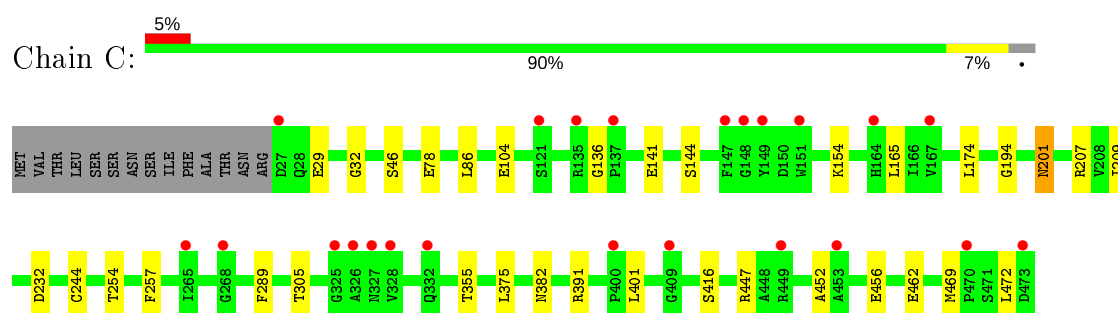
- Molecule 2: Photosystem II core light harvesting protein



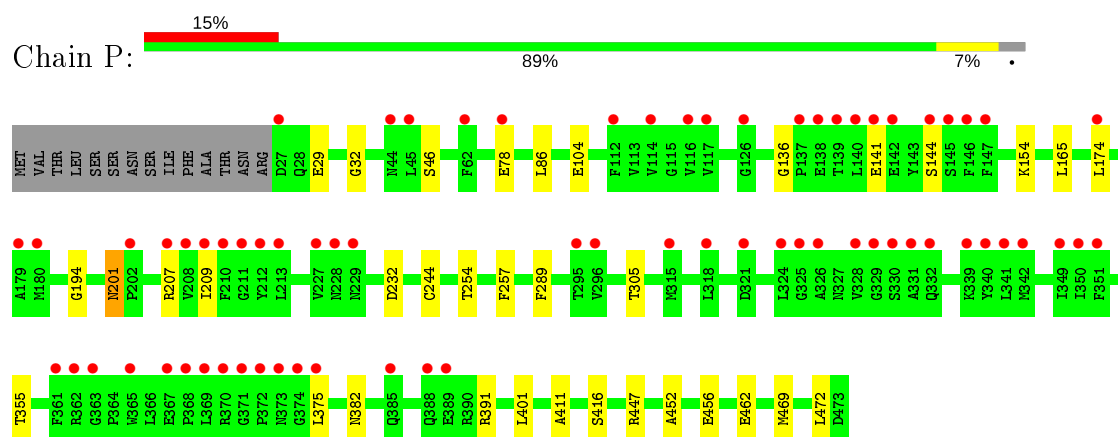
- Molecule 2: Photosystem II core light harvesting protein



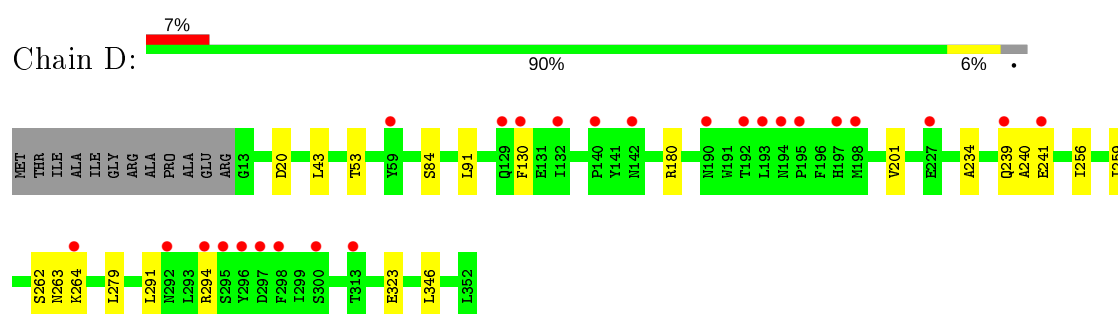
- Molecule 3: Photosystem II CP43 protein



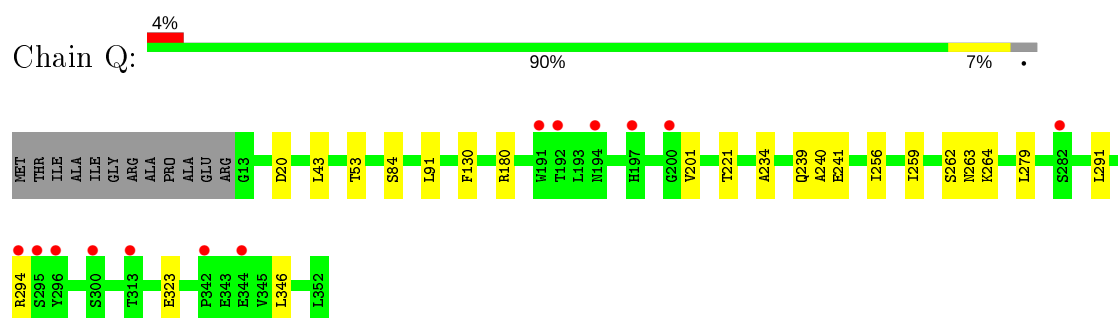
- Molecule 3: Photosystem II CP43 protein



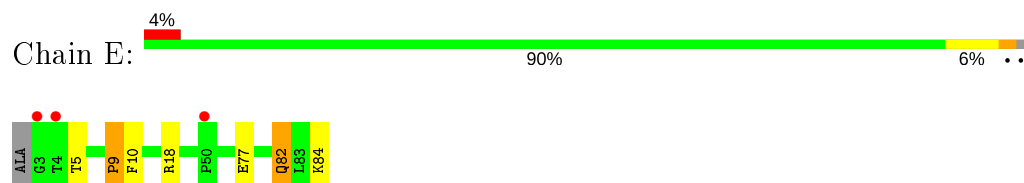
- Molecule 4: Photosystem II D2 protein



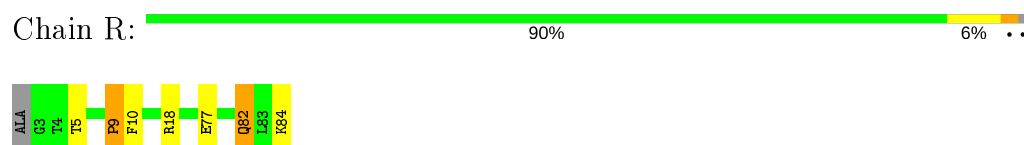
- Molecule 4: Photosystem II D2 protein



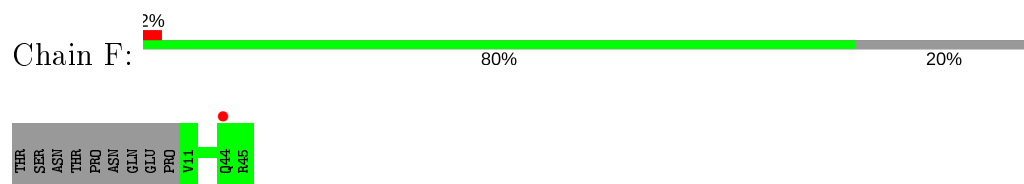
- Molecule 5: Cytochrome b559 subunit alpha



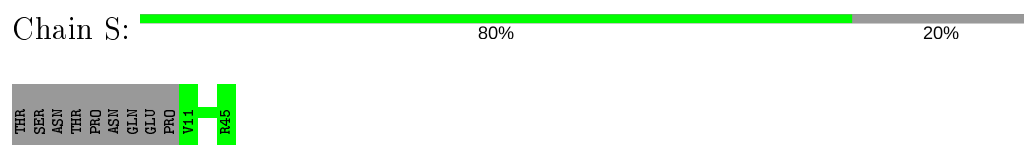
- Molecule 5: Cytochrome b559 subunit alpha



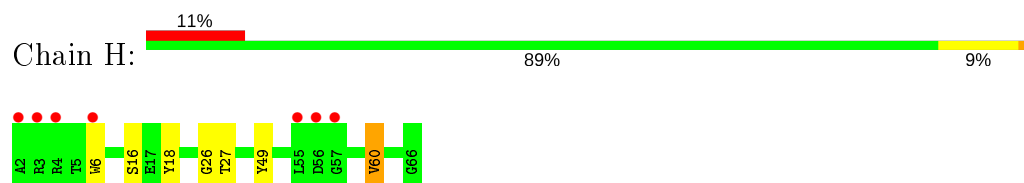
- Molecule 6: Cytochrome b559 subunit beta



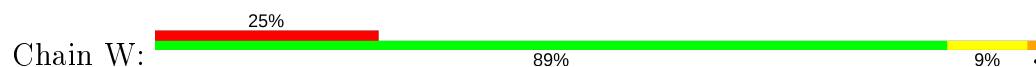
- Molecule 6: Cytochrome b559 subunit beta

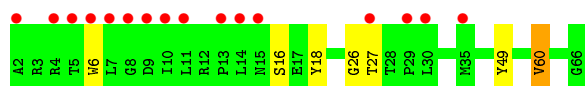


- Molecule 7: Photosystem II reaction center protein H

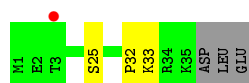
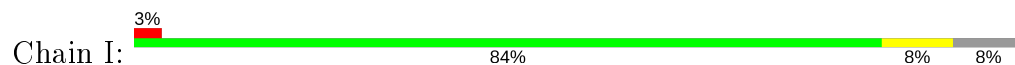


- Molecule 7: Photosystem II reaction center protein H

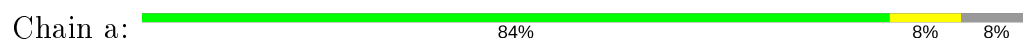




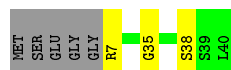
- Molecule 8: Photosystem II reaction center protein I



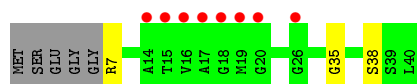
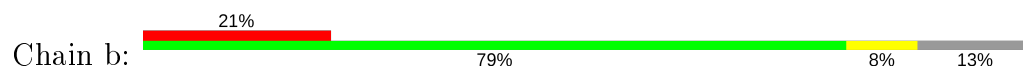
- Molecule 8: Photosystem II reaction center protein I



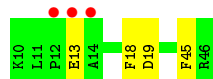
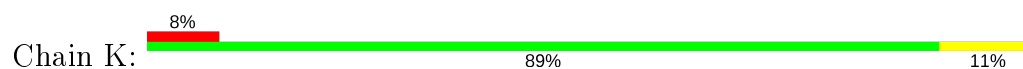
- Molecule 9: Photosystem II reaction center protein J



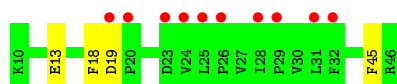
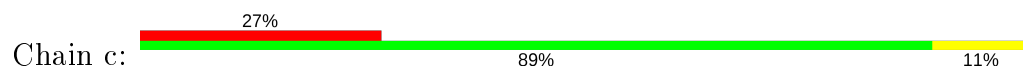
- Molecule 9: Photosystem II reaction center protein J



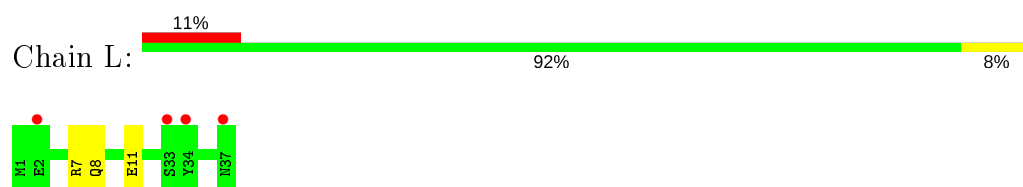
- Molecule 10: Photosystem II reaction center protein K



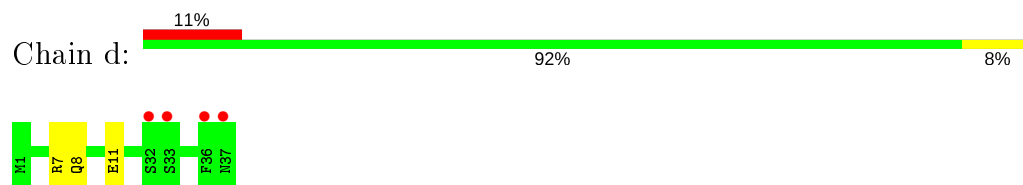
- Molecule 10: Photosystem II reaction center protein K



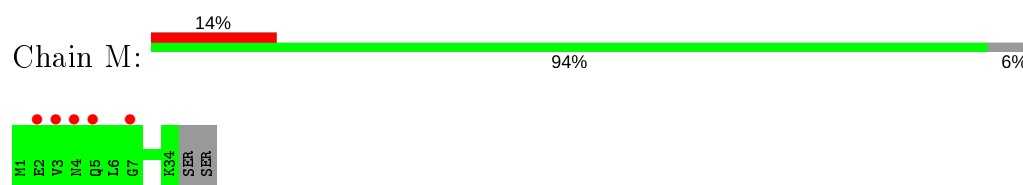
- Molecule 11: Photosystem II reaction center protein L



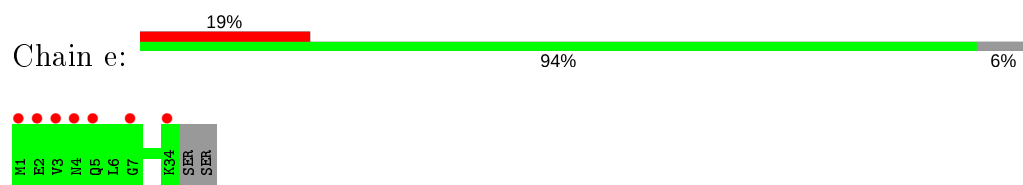
- Molecule 11: Photosystem II reaction center protein L



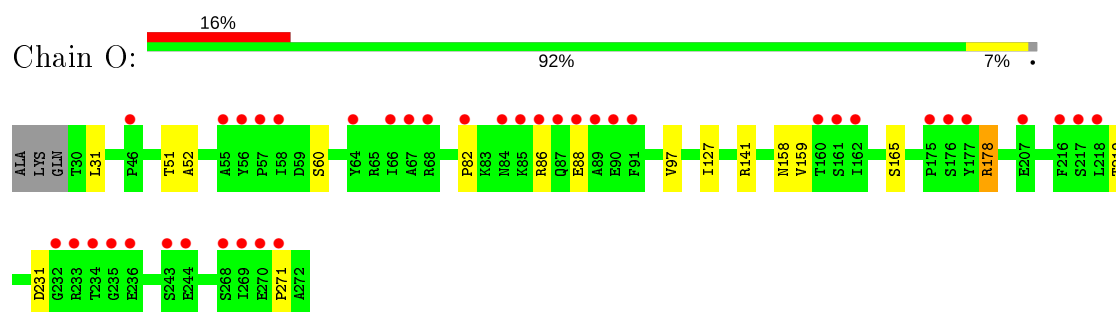
- Molecule 12: Photosystem II reaction center protein M



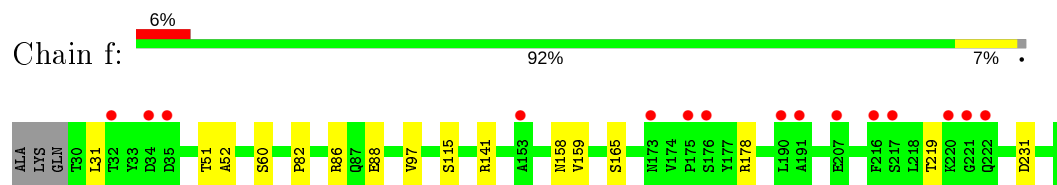
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

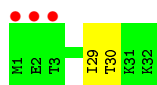
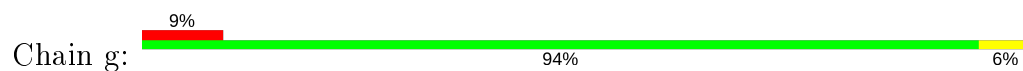


- Molecule 14: Photosystem II reaction center protein T

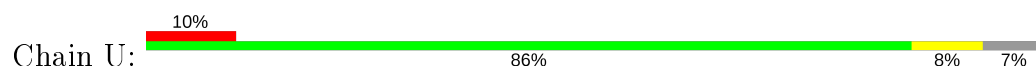




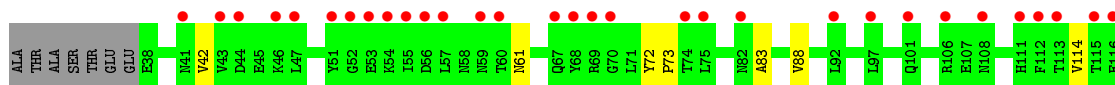
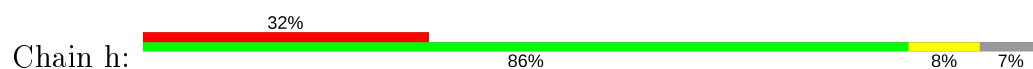
- Molecule 14: Photosystem II reaction center protein T



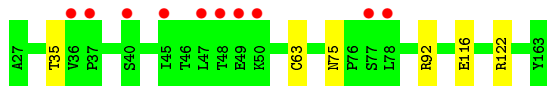
- Molecule 15: Photosystem II 12 kDa extrinsic protein



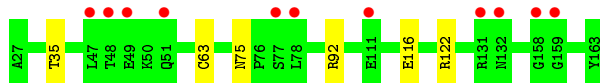
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

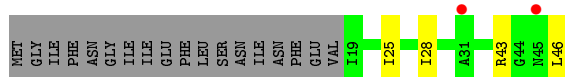


- Molecule 16: Cytochrome c-550

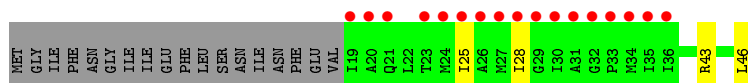


- Molecule 17: Photosystem II reaction center protein ycf12





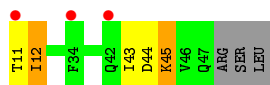
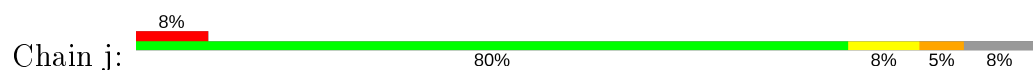
- Molecule 17: Photosystem II reaction center protein ycf12



- Molecule 18: Photosystem II reaction center protein X



- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Y



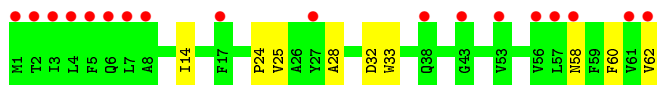
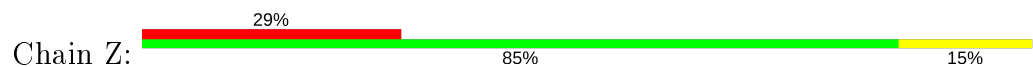
There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Y

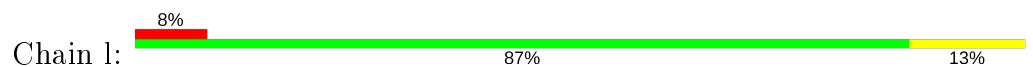


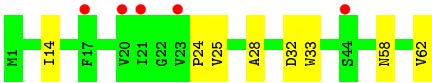
There are no outlier residues recorded for this chain.

- 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	130.78 Å 227.76 Å 308.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.89 – 6.56 85.88 – 6.56	Depositor EDS
% Data completeness (in resolution range)	97.8 (85.89-6.56) 97.8 (85.88-6.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.06 (at 6.72 Å)	Xtriage
Refinement program	PHENIX 1.7.3	Depositor
R, R_{free}	0.366 , 0.385 0.342 , 0.358	Depositor DCC
R_{free} test set	895 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	6.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 88.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2713	0.55	0/3700
1	G	0.26	0/2713	0.54	0/3700
2	B	0.26	0/3986	0.55	2/5433 (0.0%)
2	N	0.27	0/3986	0.56	2/5433 (0.0%)
3	C	0.25	0/3556	0.56	0/4842
3	P	0.25	0/3556	0.56	0/4842
4	D	0.26	0/2801	0.55	0/3818
4	Q	0.26	0/2801	0.54	0/3818
5	E	0.27	0/685	0.58	0/933
5	R	0.27	0/685	0.58	0/933
6	F	0.25	0/291	0.49	0/397
6	S	0.23	0/291	0.48	0/397
7	H	0.27	0/520	0.61	0/709
7	W	0.28	0/520	0.61	0/709
8	I	0.26	0/293	0.53	0/395
8	a	0.27	0/293	0.53	0/395
9	J	0.24	0/255	0.56	0/346
9	b	0.24	0/255	0.57	0/346
10	K	0.30	0/303	0.59	0/416
10	c	0.30	0/303	0.59	0/416
11	L	0.25	0/311	0.52	0/422
11	d	0.26	0/311	0.52	0/422
12	M	0.28	0/270	0.58	0/367
12	e	0.29	0/270	0.57	0/367
13	O	0.26	0/1876	0.60	1/2548 (0.0%)
13	f	0.26	0/1876	0.61	0/2548
14	T	0.27	0/284	0.53	0/381
14	g	0.27	0/284	0.53	0/381
15	U	0.27	0/785	0.61	0/1064
15	h	0.27	0/785	0.62	0/1064
16	V	0.24	0/1081	0.54	0/1468
16	i	0.24	0/1081	0.53	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	m	0.27	0/202	0.68	0/272
17	y	0.30	0/202	0.69	0/272
18	X	0.32	0/273	0.59	0/370
18	j	0.32	0/273	0.59	0/370
20	Z	0.28	0/490	0.62	0/669
20	l	0.28	0/490	0.62	0/669
All	All	0.26	0/41950	0.56	5/57100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	486	LEU	CA-CB-CG	7.03	131.46	115.30
2	N	486	LEU	CA-CB-CG	6.79	130.91	115.30
2	N	484	PRO	N-CA-C	5.16	125.51	112.10
2	B	484	PRO	N-CA-C	5.05	125.24	112.10
13	O	178	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	23	HIS	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	10	46
1	G	333/344 (97%)	297 (89%)	31 (9%)	5 (2%)	10	46
2	B	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	5	32
2	N	488/510 (96%)	422 (86%)	54 (11%)	12 (2%)	5	32
3	C	445/461 (96%)	375 (84%)	55 (12%)	15 (3%)	3	26
3	P	445/461 (96%)	376 (84%)	53 (12%)	16 (4%)	3	25
4	D	338/352 (96%)	292 (86%)	40 (12%)	6 (2%)	8	40
4	Q	338/352 (96%)	291 (86%)	41 (12%)	6 (2%)	8	40
5	E	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	3	24
5	R	80/83 (96%)	72 (90%)	5 (6%)	3 (4%)	3	24
6	F	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
6	S	33/44 (75%)	24 (73%)	9 (27%)	0	100	100
7	H	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	13
7	W	63/65 (97%)	48 (76%)	10 (16%)	5 (8%)	1	13
8	I	33/38 (87%)	24 (73%)	7 (21%)	2 (6%)	1	17
8	a	33/38 (87%)	25 (76%)	6 (18%)	2 (6%)	1	17
9	J	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	16
9	b	32/39 (82%)	26 (81%)	4 (12%)	2 (6%)	1	16
10	K	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	18
10	c	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	18
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	d	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	M	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	e	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
13	O	241/246 (98%)	203 (84%)	27 (11%)	11 (5%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	f	241/246 (98%)	203 (84%)	29 (12%)	9 (4%)	3	24
14	T	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	26
14	g	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	4	26
15	U	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	22
15	h	95/104 (91%)	81 (85%)	10 (10%)	4 (4%)	3	22
16	V	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	22	63
16	i	135/137 (98%)	113 (84%)	21 (16%)	1 (1%)	22	63
17	m	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	13
17	y	26/46 (56%)	15 (58%)	9 (35%)	2 (8%)	1	13
18	X	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	7
18	j	35/40 (88%)	27 (77%)	4 (11%)	4 (11%)	0	7
20	Z	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	2	20
20	l	60/62 (97%)	49 (82%)	8 (13%)	3 (5%)	2	20
All	All	5138/5426 (95%)	4357 (85%)	626 (12%)	155 (3%)	4	28

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	142	TRP
2	B	176	GLY
2	B	230	ARG
2	B	484	PRO
2	B	488	PRO
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	262	SER
7	H	18	TYR
8	I	25	SER
9	J	35	GLY
13	O	52	ALA
14	T	30	THR
15	U	72	TYR
15	U	83	ALA

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Mol	Chain	Res	Type
16	V	75	ASN
17	y	43	ARG
18	X	45	LYS
20	Z	32	ASP
1	G	12	ASN
1	G	142	TRP
2	N	176	GLY
2	N	230	ARG
2	N	484	PRO
2	N	488	PRO
3	P	144	SER
3	P	257	PHE
3	P	416	SER
3	P	452	ALA
4	Q	239	GLN
4	Q	240	ALA
4	Q	262	SER
7	W	18	TYR
8	a	25	SER
9	b	35	GLY
13	f	52	ALA
14	g	30	THR
15	h	72	TYR
15	h	83	ALA
16	i	75	ASN
17	m	43	ARG
18	j	45	LYS
20	l	32	ASP
1	A	141	PRO
2	B	349	LYS
3	C	46	SER
3	C	136	GLY
3	C	194	GLY
3	C	452	ALA
4	D	234	ALA
4	D	264	LYS
5	E	82	GLN
7	H	26	GLY
9	J	38	SER
13	O	231	ASP
15	U	73	PRO
1	G	141	PRO

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Mol	Chain	Res	Type
2	N	349	LYS
3	P	46	SER
3	P	136	GLY
3	P	194	GLY
4	Q	234	ALA
4	Q	264	LYS
5	R	82	GLN
7	W	26	GLY
9	b	38	SER
13	f	231	ASP
15	h	73	PRO
17	m	25	ILE
2	B	436	THR
3	C	32	GLY
3	C	141	GLU
3	C	209	ILE
3	C	375	LEU
3	C	456	GLU
4	D	263	ASN
5	E	9	PRO
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
13	O	158	ASN
13	O	165	SER
17	y	25	ILE
18	X	43	ILE
2	N	436	THR
3	P	32	GLY
3	P	141	GLU
3	P	209	ILE
3	P	375	LEU
3	P	456	GLU
4	Q	263	ASN
5	R	9	PRO
7	W	16	SER
10	c	13	GLU
10	c	45	PHE
13	f	158	ASN
13	f	165	SER
18	j	43	ILE
20	l	28	ALA

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Mol	Chain	Res	Type
2	B	127	ARG
2	B	183	PRO
2	B	414	PRO
13	O	60	SER
13	O	82	PRO
20	Z	24	PRO
20	Z	28	ALA
2	N	127	ARG
2	N	183	PRO
2	N	414	PRO
13	f	60	SER
13	f	82	PRO
20	l	24	PRO
1	A	334	ARG
2	B	13	ILE
2	B	173	GLY
3	C	154	LYS
3	C	462	GLU
5	E	10	PHE
7	H	6	TRP
13	O	51	THR
13	O	88	GLU
1	G	334	ARG
2	N	13	ILE
2	N	173	GLY
3	P	154	LYS
3	P	411	ALA
3	P	462	GLU
5	R	10	PHE
7	W	6	TRP
13	f	51	THR
13	f	88	GLU
15	U	42	VAL
18	X	12	ILE
18	X	44	ASP
18	j	12	ILE
18	j	44	ASP
15	h	42	VAL
8	I	32	PRO
8	a	32	PRO
1	A	176	ILE
2	B	16	PRO

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Mol	Chain	Res	Type
3	C	201	ASN
7	H	60	VAL
13	O	127	ILE
13	O	159	VAL
1	G	176	ILE
2	N	16	PRO
3	P	201	ASN
13	f	159	VAL
13	O	271	PRO
7	W	60	VAL

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%)	260 (96%)	11 (4%)	30	55
1	G	271/280 (97%)	260 (96%)	11 (4%)	30	55
2	B	390/407 (96%)	377 (97%)	13 (3%)	38	61
2	N	390/407 (96%)	376 (96%)	14 (4%)	35	59
3	C	347/362 (96%)	327 (94%)	20 (6%)	20	45
3	P	347/362 (96%)	327 (94%)	20 (6%)	20	45
4	D	275/283 (97%)	259 (94%)	16 (6%)	20	45
4	Q	275/283 (97%)	258 (94%)	17 (6%)	18	43
5	E	72/72 (100%)	66 (92%)	6 (8%)	11	34
5	R	72/72 (100%)	66 (92%)	6 (8%)	11	34
6	F	29/38 (76%)	29 (100%)	0	100	100
6	S	29/38 (76%)	29 (100%)	0	100	100
7	H	53/54 (98%)	50 (94%)	3 (6%)	20	45
7	W	53/54 (98%)	50 (94%)	3 (6%)	20	45
8	I	32/35 (91%)	31 (97%)	1 (3%)	40	62
8	a	32/35 (91%)	31 (97%)	1 (3%)	40	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	24/27 (89%)	23 (96%)	1 (4%)	30	54
9	b	24/27 (89%)	23 (96%)	1 (4%)	30	54
10	K	30/30 (100%)	28 (93%)	2 (7%)	16	41
10	c	30/30 (100%)	28 (93%)	2 (7%)	16	41
11	L	35/35 (100%)	32 (91%)	3 (9%)	10	32
11	d	35/35 (100%)	32 (91%)	3 (9%)	10	32
12	M	31/33 (94%)	31 (100%)	0	100	100
12	e	31/33 (94%)	31 (100%)	0	100	100
13	O	202/208 (97%)	196 (97%)	6 (3%)	41	63
13	f	202/208 (97%)	196 (97%)	6 (3%)	41	63
14	T	29/29 (100%)	28 (97%)	1 (3%)	37	60
14	g	29/29 (100%)	28 (97%)	1 (3%)	37	60
15	U	84/89 (94%)	80 (95%)	4 (5%)	25	51
15	h	84/89 (94%)	80 (95%)	4 (5%)	25	51
16	V	116/117 (99%)	111 (96%)	5 (4%)	29	53
16	i	116/117 (99%)	111 (96%)	5 (4%)	29	53
17	m	20/37 (54%)	18 (90%)	2 (10%)	7	26
17	y	20/37 (54%)	18 (90%)	2 (10%)	7	26
18	X	30/33 (91%)	27 (90%)	3 (10%)	7	26
18	j	30/33 (91%)	27 (90%)	3 (10%)	7	26
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	27
20	l	52/52 (100%)	47 (90%)	5 (10%)	8	27
All	All	4244/4442 (96%)	4038 (95%)	206 (5%)	25	50

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	32	TRP
1	A	157	VAL
1	A	202	VAL
1	A	206	PHE
1	A	234	ASN
1	A	243	GLU

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Mol	Chain	Res	Type
1	A	271	LEU
1	A	286	THR
1	A	292	THR
1	A	308	ASP
2	B	11	VAL
2	B	18	ARG
2	B	84	THR
2	B	223	GLN
2	B	246	PHE
2	B	262	THR
2	B	308	LYS
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	486	LEU
2	B	488	PRO
2	B	490	GLN
3	C	29	GLU
3	C	78	GLU
3	C	86	LEU
3	C	104	GLU
3	C	165	LEU
3	C	174	LEU
3	C	201	ASN
3	C	207	ARG
3	C	232	ASP
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	401	LEU
3	C	447	ARG
3	C	469	MET
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	53	THR
4	D	84	SER
4	D	91	LEU

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Mol	Chain	Res	Type
4	D	130	PHE
4	D	180	ARG
4	D	201	VAL
4	D	241	GLU
4	D	256	ILE
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	346	LEU
5	E	5	THR
5	E	9	PRO
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
10	K	18	PHE
10	K	19	ASP
11	L	7	ARG
11	L	8	GLN
11	L	11	GLU
13	O	31	LEU
13	O	86	ARG
13	O	97	VAL
13	O	141	ARG
13	O	178	ARG
13	O	219	THR
14	T	29	ILE
15	U	61	ASN
15	U	88	VAL
15	U	114	VAL
15	U	132	LEU
16	V	35	THR
16	V	63	CYS
16	V	92	ARG
16	V	116	GLU

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Mol	Chain	Res	Type
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
20	Z	14	ILE
20	Z	25	VAL
20	Z	33	TRP
20	Z	58	ASN
20	Z	62	VAL
1	G	30	VAL
1	G	32	TRP
1	G	157	VAL
1	G	202	VAL
1	G	206	PHE
1	G	234	ASN
1	G	243	GLU
1	G	271	LEU
1	G	286	THR
1	G	292	THR
1	G	308	ASP
2	N	11	VAL
2	N	18	ARG
2	N	84	THR
2	N	223	GLN
2	N	246	PHE
2	N	262	THR
2	N	308	LYS
2	N	309	LEU
2	N	362	PHE
2	N	414	PRO
2	N	422	ARG
2	N	486	LEU
2	N	488	PRO
2	N	490	GLN
3	P	29	GLU
3	P	78	GLU
3	P	86	LEU
3	P	104	GLU
3	P	165	LEU
3	P	174	LEU

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Mol	Chain	Res	Type
3	P	201	ASN
3	P	207	ARG
3	P	232	ASP
3	P	244	CYS
3	P	254	THR
3	P	289	PHE
3	P	305	THR
3	P	355	THR
3	P	382	ASN
3	P	391	ARG
3	P	401	LEU
3	P	447	ARG
3	P	469	MET
3	P	472	LEU
4	Q	20	ASP
4	Q	43	LEU
4	Q	53	THR
4	Q	84	SER
4	Q	91	LEU
4	Q	130	PHE
4	Q	180	ARG
4	Q	201	VAL
4	Q	221	THR
4	Q	241	GLU
4	Q	256	ILE
4	Q	259	ILE
4	Q	279	LEU
4	Q	291	LEU
4	Q	294	ARG
4	Q	323	GLU
4	Q	346	LEU
5	R	5	THR
5	R	9	PRO
5	R	18	ARG
5	R	77	GLU
5	R	82	GLN
5	R	84	LYS
7	W	27	THR
7	W	49	TYR
7	W	60	VAL
8	a	33	LYS
9	b	7	ARG

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Mol	Chain	Res	Type
10	c	18	PHE
10	c	19	ASP
11	d	7	ARG
11	d	8	GLN
11	d	11	GLU
13	f	31	LEU
13	f	86	ARG
13	f	97	VAL
13	f	141	ARG
13	f	178	ARG
13	f	219	THR
14	g	29	ILE
15	h	61	ASN
15	h	88	VAL
15	h	114	VAL
15	h	132	LEU
16	i	35	THR
16	i	63	CYS
16	i	92	ARG
16	i	116	GLU
16	i	122	ARG
17	m	28	ILE
17	m	46	LEU
18	j	11	THR
18	j	12	ILE
18	j	45	LYS
20	l	14	ILE
20	l	25	VAL
20	l	33	TRP
20	l	58	ASN
20	l	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	241	GLN
2	B	201	HIS
3	C	118	HIS
11	L	8	GLN
1	G	234	ASN
1	G	241	GLN

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Mol	Chain	Res	Type
2	N	201	HIS
4	Q	129	GLN
4	Q	250	ASN
11	d	8	GLN
13	f	135	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 182 ligands modelled in this entry, 6 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	$\# Z > 2$
24	DGD	B	628	-	53,53,67	1.02	3 (5%)	67,67,81	1.53	11 (16%)
21	CLA	B	615	-	59,73,73	1.40	12 (20%)	67,113,113	2.09	11 (16%)
21	CLA	Q	404	-	59,73,73	1.41	12 (20%)	67,113,113	2.08	9 (13%)
30	BCR	J	102	-	41,41,41	0.79	0	56,56,56	3.06	21 (37%)
31	LMT	B	625	-	36,36,36	0.41	0	47,47,47	0.70	0
27	LMG	I	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.31	5 (9%)
31	LMT	B	630	-	36,36,36	0.39	0	47,47,47	0.62	0
31	LMT	N	604	-	36,36,36	0.42	0	47,47,47	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	BCR	K	101	-	41,41,41	0.79	0	56,56,56	1.62	12 (21%)
21	CLA	P	512	-	59,73,73	1.41	12 (20%)	67,113,113	2.07	10 (14%)
24	DGD	A	407	-	57,57,67	0.99	4 (7%)	71,71,81	1.48	8 (11%)
22	PHO	D	402	-	67,69,69	2.15	18 (26%)	85,99,99	1.84	19 (22%)
24	DGD	B	621	-	59,59,67	0.95	3 (5%)	73,73,81	1.39	9 (12%)
27	LMG	D	412	-	42,42,55	1.04	2 (4%)	50,50,63	1.26	5 (10%)
27	LMG	D	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.34	7 (12%)
21	CLA	B	603	-	59,73,73	1.43	14 (23%)	67,113,113	2.07	10 (14%)
21	CLA	B	609	-	59,73,73	1.41	12 (20%)	67,113,113	2.04	8 (11%)
21	CLA	P	502	-	59,73,73	1.41	13 (22%)	67,113,113	2.06	9 (13%)
30	BCR	H	101	-	41,41,41	0.76	0	56,56,56	1.46	11 (19%)
27	LMG	G	411	-	51,51,55	0.96	2 (3%)	59,59,63	1.23	4 (6%)
21	CLA	C	506	-	59,73,73	1.42	14 (23%)	67,113,113	2.05	10 (14%)
23	PL9	b	101	-	35,35,55	1.18	5 (14%)	44,45,69	1.59	10 (22%)
21	CLA	C	503	-	59,73,73	1.40	12 (20%)	67,113,113	2.06	10 (14%)
30	BCR	Z	101	-	41,41,41	0.67	0	56,56,56	1.62	12 (21%)
27	LMG	N	622	-	49,49,55	0.93	2 (4%)	57,57,63	1.36	7 (12%)
21	CLA	N	605	-	59,73,73	1.38	14 (23%)	67,113,113	2.07	10 (14%)
28	OEC	G	413	1	0,0,13	0.00	-	-		
21	CLA	D	401	-	59,73,73	1.42	10 (16%)	67,113,113	2.04	11 (16%)
30	BCR	b	102	-	41,41,41	0.78	0	56,56,56	3.10	20 (35%)
21	CLA	G	404	-	59,73,73	1.39	13 (22%)	67,113,113	2.06	10 (14%)
21	CLA	B	611	-	59,73,73	1.41	14 (23%)	67,113,113	2.12	12 (17%)
26	SQD	B	627	-	46,47,54	1.28	5 (10%)	55,58,65	1.47	9 (16%)
31	LMT	M	102	-	36,36,36	0.41	0	47,47,47	0.69	1 (2%)
30	BCR	T	102	-	41,41,41	0.69	0	56,56,56	1.86	15 (26%)
28	OEC	A	412	1,3	0,0,13	0.00	-	-		
30	BCR	P	514	-	41,41,41	0.70	0	56,56,56	2.37	18 (32%)
21	CLA	N	614	-	59,73,73	1.41	13 (22%)	67,113,113	2.03	10 (14%)
34	HEM	R	101	5,6	27,50,50	2.14	5 (18%)	17,82,82	2.25	3 (17%)
23	PL9	D	404	-	55,55,55	1.24	8 (14%)	68,69,69	1.64	19 (27%)
26	SQD	F	101	-	44,45,54	1.30	4 (9%)	53,56,65	1.22	8 (15%)
27	LMG	R	102	-	44,44,55	1.00	2 (4%)	52,52,63	1.12	5 (9%)
30	BCR	c	101	-	41,41,41	0.78	0	56,56,56	1.57	11 (19%)
21	CLA	N	608	-	59,73,73	1.41	13 (22%)	67,113,113	2.07	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	P	511	3	59,73,73	1.40	12 (20%)	67,113,113	2.07	10 (14%)
21	CLA	N	609	-	59,73,73	1.40	13 (22%)	67,113,113	2.13	12 (17%)
22	PHO	Q	403	-	67,69,69	2.15	18 (26%)	85,99,99	1.82	19 (22%)
21	CLA	C	505	-	59,73,73	1.40	12 (20%)	67,113,113	2.12	10 (14%)
27	LMG	P	520	-	48,48,55	0.96	2 (4%)	56,56,63	1.29	6 (10%)
27	LMG	A	410	-	51,51,55	0.95	2 (3%)	59,59,63	1.26	4 (6%)
31	LMT	N	624	-	36,36,36	0.41	0	47,47,47	0.67	0
21	CLA	C	511	3	59,73,73	1.40	13 (22%)	67,113,113	2.11	10 (14%)
27	LMG	e	102	-	42,42,55	1.03	2 (4%)	50,50,63	1.32	6 (12%)
27	LMG	Q	401	-	42,42,55	1.04	2 (4%)	50,50,63	1.23	5 (10%)
21	CLA	P	510	-	59,73,73	1.41	13 (22%)	67,113,113	2.05	9 (13%)
21	CLA	A	405	-	59,73,73	1.40	13 (22%)	67,113,113	2.08	11 (16%)
21	CLA	B	607	-	59,73,73	1.42	12 (20%)	67,113,113	2.06	9 (13%)
34	HEM	V	201	16	27,50,50	2.15	5 (18%)	17,82,82	1.95	3 (17%)
21	CLA	N	610	-	59,73,73	1.42	12 (20%)	67,113,113	2.06	11 (16%)
24	DGD	P	517	-	54,54,67	0.99	3 (5%)	68,68,81	1.55	10 (14%)
27	LMG	P	521	-	45,45,55	1.03	2 (4%)	53,53,63	1.22	5 (9%)
21	CLA	P	501	-	59,73,73	1.41	12 (20%)	67,113,113	2.08	9 (13%)
21	CLA	C	501	-	59,73,73	1.41	12 (20%)	67,113,113	2.06	9 (13%)
30	BCR	B	619	-	41,41,41	0.74	0	56,56,56	1.52	10 (17%)
21	CLA	N	607	-	59,73,73	1.43	13 (22%)	67,113,113	2.04	12 (17%)
23	PL9	A	406	-	45,45,55	1.23	7 (15%)	56,57,69	1.71	18 (32%)
27	LMG	Q	407	-	48,48,55	0.96	2 (4%)	56,56,63	1.29	5 (8%)
30	BCR	B	620	-	41,41,41	0.71	0	56,56,56	1.61	10 (17%)
21	CLA	B	608	-	59,73,73	1.42	14 (23%)	67,113,113	2.03	8 (11%)
30	BCR	D	405	-	41,41,41	0.70	0	56,56,56	1.72	10 (17%)
30	BCR	B	617	-	41,41,41	0.71	0	56,56,56	1.60	11 (19%)
21	CLA	Q	402	-	59,73,73	1.41	10 (16%)	67,113,113	2.03	11 (16%)
21	CLA	C	512	-	59,73,73	1.40	12 (20%)	67,113,113	2.09	10 (14%)
30	BCR	N	621	-	41,41,41	0.73	0	56,56,56	1.55	13 (23%)
30	BCR	P	516	-	41,41,41	0.75	0	56,56,56	1.69	15 (26%)
26	SQD	B	624	-	42,43,54	1.34	5 (11%)	51,54,65	1.45	7 (13%)
31	LMT	D	409	-	32,32,36	0.47	0	43,43,47	0.65	1 (2%)
21	CLA	C	502	-	59,73,73	1.40	13 (22%)	67,113,113	2.05	7 (10%)
21	CLA	B	614	-	59,73,73	1.42	11 (18%)	67,113,113	2.03	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	e	101	-	36,36,36	0.41	0	47,47,47	0.65	1 (2%)
21	CLA	B	604	-	59,73,73	1.41	12 (20%)	67,113,113	2.05	11 (16%)
21	CLA	P	505	-	59,73,73	1.40	12 (20%)	67,113,113	2.11	8 (11%)
21	CLA	N	606	-	59,73,73	1.42	13 (22%)	67,113,113	2.08	10 (14%)
31	LMT	Q	410	-	32,32,36	0.47	0	43,43,47	0.64	1 (2%)
30	BCR	B	618	-	41,41,41	0.70	0	56,56,56	1.88	15 (26%)
24	DGD	P	519	-	67,67,67	0.90	4 (5%)	81,81,81	1.28	7 (8%)
21	CLA	P	503	-	59,73,73	1.40	11 (18%)	67,113,113	2.02	10 (14%)
27	LMG	D	407	-	48,48,55	0.95	2 (4%)	56,56,63	1.28	5 (8%)
26	SQD	Q	408	-	42,43,54	1.35	5 (11%)	51,54,65	1.45	6 (11%)
34	HEM	i	201	16	27,50,50	2.15	6 (22%)	17,82,82	1.94	5 (29%)
25	LHG	G	409	-	38,38,48	1.07	2 (5%)	41,44,54	0.95	2 (4%)
30	BCR	I	101	-	41,41,41	0.69	0	56,56,56	1.58	12 (21%)
24	DGD	G	408	-	57,57,67	0.98	4 (7%)	71,71,81	1.47	8 (11%)
21	CLA	G	403	-	59,73,73	1.40	13 (22%)	67,113,113	2.05	12 (17%)
25	LHG	G	412	-	36,36,48	1.09	2 (5%)	39,42,54	1.05	2 (5%)
21	CLA	D	403	-	59,73,73	1.40	12 (20%)	67,113,113	2.08	9 (13%)
21	CLA	B	612	-	59,73,73	1.42	14 (23%)	67,113,113	2.04	10 (14%)
21	CLA	A	401	-	59,73,73	1.42	13 (22%)	67,113,113	1.98	11 (16%)
27	LMG	Q	406	-	46,46,55	0.99	2 (4%)	54,54,63	1.30	4 (7%)
32	BCT	Q	411	29	0,3,3	0.00	-	0,3,3	0.00	-
21	CLA	A	403	-	59,73,73	1.41	13 (22%)	67,113,113	2.01	9 (13%)
21	CLA	N	615	-	59,73,73	1.41	14 (23%)	67,113,113	2.07	11 (16%)
31	LMT	N	625	-	36,36,36	0.42	0	47,47,47	0.66	1 (2%)
27	LMG	M	101	-	42,42,55	1.03	2 (4%)	50,50,63	1.30	6 (12%)
30	BCR	W	101	-	41,41,41	0.76	0	56,56,56	1.46	8 (14%)
23	PL9	J	101	-	35,35,55	1.18	5 (14%)	44,45,69	1.57	9 (20%)
27	LMG	B	622	-	49,49,55	0.94	2 (4%)	57,57,63	1.28	6 (10%)
21	CLA	P	506	-	59,73,73	1.42	14 (23%)	67,113,113	2.04	10 (14%)
24	DGD	Q	409	-	64,64,67	0.91	2 (3%)	78,78,81	1.33	9 (11%)
21	CLA	C	509	-	59,73,73	1.42	14 (23%)	67,113,113	1.99	10 (14%)
31	LMT	B	629	-	36,36,36	0.45	0	47,47,47	0.76	1 (2%)
24	DGD	W	102	-	59,59,67	0.95	3 (5%)	73,73,81	1.41	9 (12%)
21	CLA	G	406	-	59,73,73	1.39	13 (22%)	67,113,113	2.08	10 (14%)
21	CLA	C	507	-	59,73,73	1.39	13 (22%)	67,113,113	2.05	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	P	507	-	59,73,73	1.39	13 (22%)	67,113,113	2.03	8 (11%)
21	CLA	P	508	-	59,73,73	1.41	13 (22%)	67,113,113	2.12	11 (16%)
26	SQD	S	102	-	44,45,54	1.31	5 (11%)	53,56,65	1.22	7 (13%)
27	LMG	C	519	-	48,48,55	0.96	2 (4%)	56,56,63	1.29	6 (10%)
24	DGD	N	602	-	53,53,67	1.02	3 (5%)	67,67,81	1.53	9 (13%)
21	CLA	N	620	-	59,73,73	1.40	12 (20%)	67,113,113	2.09	10 (14%)
22	PHO	G	405	-	67,69,69	2.13	18 (26%)	85,99,99	1.94	23 (27%)
24	DGD	C	518	-	67,67,67	0.92	4 (5%)	81,81,81	1.33	8 (9%)
25	LHG	A	411	-	36,36,48	1.08	2 (5%)	39,42,54	1.08	2 (5%)
24	DGD	P	518	-	63,63,67	0.92	3 (4%)	77,77,81	1.51	13 (16%)
21	CLA	N	611	-	59,73,73	1.43	12 (20%)	67,113,113	2.03	8 (11%)
27	LMG	N	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.24	8 (14%)
23	PL9	G	407	-	45,45,55	1.23	7 (15%)	56,57,69	1.72	17 (30%)
21	CLA	N	613	-	59,73,73	1.40	12 (20%)	67,113,113	2.06	9 (13%)
24	DGD	C	516	-	54,54,67	0.98	3 (5%)	68,68,81	1.52	10 (14%)
21	CLA	P	504	-	59,73,73	1.42	13 (22%)	67,113,113	2.00	8 (11%)
30	BCR	S	101	-	41,41,41	0.71	0	56,56,56	1.74	11 (19%)
21	CLA	B	610	-	59,73,73	1.41	12 (20%)	67,113,113	2.07	10 (14%)
21	CLA	B	602	-	59,73,73	1.41	12 (20%)	67,113,113	2.03	12 (17%)
21	CLA	C	510	-	59,73,73	1.41	14 (23%)	67,113,113	2.02	9 (13%)
21	CLA	A	402	-	59,73,73	1.41	13 (22%)	67,113,113	2.08	11 (16%)
26	SQD	G	401	-	53,54,54	1.18	4 (7%)	62,65,65	1.06	4 (6%)
31	LMT	I	103	-	36,36,36	0.47	1 (2%)	47,47,47	0.70	1 (2%)
30	BCR	C	515	-	41,41,41	0.75	0	56,56,56	1.69	12 (21%)
27	LMG	B	623	-	49,49,55	0.95	2 (4%)	57,57,63	1.26	8 (14%)
21	CLA	B	601	-	59,73,73	1.39	13 (22%)	67,113,113	2.11	10 (14%)
23	PL9	Q	405	-	55,55,55	1.25	9 (16%)	68,69,69	1.66	19 (27%)
22	PHO	A	404	-	67,69,69	2.14	18 (26%)	85,99,99	1.92	21 (24%)
21	CLA	G	402	-	59,73,73	1.42	13 (22%)	67,113,113	2.04	10 (14%)
30	BCR	P	515	-	41,41,41	0.68	0	56,56,56	1.57	12 (21%)
27	LMG	E	102	-	44,44,55	1.02	2 (4%)	52,52,63	1.11	5 (9%)
24	DGD	C	517	-	63,63,67	0.92	3 (4%)	77,77,81	1.51	13 (16%)
30	BCR	C	514	-	41,41,41	0.72	0	56,56,56	2.34	18 (32%)
26	SQD	N	601	-	46,47,54	1.28	5 (10%)	55,58,65	1.54	10 (18%)
21	CLA	C	504	-	59,73,73	1.42	13 (22%)	67,113,113	2.03	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	N	617	-	59,73,73	1.43	14 (23%)	67,113,113	2.03	7 (10%)
21	CLA	N	616	-	59,73,73	1.44	13 (22%)	67,113,113	2.11	9 (13%)
30	BCR	T	103	-	41,41,41	0.69	0	56,56,56	1.63	11 (19%)
26	SQD	G	410	-	50,51,54	1.21	4 (8%)	59,62,65	1.46	9 (15%)
26	SQD	A	414	-	53,54,54	1.17	4 (7%)	62,65,65	1.08	4 (6%)
31	LMT	N	603	-	36,36,36	0.45	0	47,47,47	0.79	1 (2%)
27	LMG	C	520	-	45,45,55	1.04	2 (4%)	53,53,63	1.26	6 (11%)
21	CLA	P	513	-	59,73,73	1.42	13 (22%)	67,113,113	2.02	10 (14%)
21	CLA	B	606	-	59,73,73	1.40	12 (20%)	67,113,113	2.04	12 (17%)
31	LMT	a	103	-	36,36,36	0.46	0	47,47,47	0.69	1 (2%)
30	BCR	T	101	-	41,41,41	0.71	0	56,56,56	1.59	11 (19%)
21	CLA	P	509	-	59,73,73	1.41	14 (23%)	67,113,113	2.02	10 (14%)
24	DGD	D	408	-	64,64,67	0.91	2 (3%)	78,78,81	1.32	9 (11%)
25	LHG	A	408	-	38,38,48	1.07	2 (5%)	41,44,54	0.95	2 (4%)
26	SQD	A	409	-	50,51,54	1.21	4 (8%)	59,62,65	1.44	9 (15%)
21	CLA	B	605	-	59,73,73	1.41	13 (22%)	67,113,113	2.09	12 (17%)
31	LMT	B	626	-	36,36,36	0.44	0	47,47,47	0.66	1 (2%)
27	LMG	a	102	-	43,43,55	1.01	2 (4%)	51,51,63	1.33	6 (11%)
21	CLA	N	619	-	59,73,73	1.38	12 (20%)	67,113,113	2.11	11 (16%)
21	CLA	N	618	-	59,73,73	1.42	12 (20%)	67,113,113	2.01	10 (14%)
21	CLA	B	613	-	59,73,73	1.41	14 (23%)	67,113,113	2.03	8 (11%)
21	CLA	C	508	-	59,73,73	1.41	12 (20%)	67,113,113	2.09	13 (19%)
34	HEM	E	101	5,6	27,50,50	2.13	5 (18%)	17,82,82	2.06	4 (23%)
30	BCR	a	101	-	41,41,41	0.69	0	56,56,56	1.59	11 (19%)
21	CLA	C	513	-	59,73,73	1.41	13 (22%)	67,113,113	2.04	9 (13%)
21	CLA	B	616	-	59,73,73	1.40	13 (22%)	67,113,113	2.08	10 (14%)
32	BCT	D	410	29	0,3,3	0.00	-	0,3,3	0.00	-
21	CLA	N	612	-	59,73,73	1.42	13 (22%)	67,113,113	2.00	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DGD	B	628	-	3/3/13/13	22/41/81/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	615	-	3/3/20/25	9/37/135/135	-
21	CLA	Q	404	-	3/3/20/25	4/37/135/135	-
30	BCR	J	102	-	-	2/29/63/63	0/2/2/2
31	LMT	B	625	-	-	3/21/61/61	0/2/2/2
27	LMG	I	102	-	2/2/8/8	18/38/58/70	0/1/1/1
31	LMT	B	630	-	-	5/21/61/61	0/2/2/2
31	LMT	N	604	-	-	5/21/61/61	0/2/2/2
30	BCR	K	101	-	-	6/29/63/63	0/2/2/2
21	CLA	P	512	-	3/3/20/25	19/37/135/135	-
24	DGD	A	407	-	3/3/13/13	14/45/85/95	0/2/2/2
22	PHO	D	402	-	-	15/53/103/103	0/5/6/6
24	DGD	B	621	-	3/3/13/13	16/47/87/95	0/2/2/2
27	LMG	D	412	-	2/2/8/8	15/37/57/70	0/1/1/1
21	CLA	B	603	-	3/3/20/25	14/37/135/135	-
21	CLA	B	609	-	3/3/20/25	8/37/135/135	-
21	CLA	P	502	-	3/3/20/25	10/37/135/135	-
30	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	LMG	G	411	-	2/2/8/8	22/46/66/70	0/1/1/1
21	CLA	C	506	-	3/3/20/25	17/37/135/135	-
23	PL9	b	101	-	-	11/29/49/73	0/1/1/1
21	CLA	C	503	-	3/3/20/25	14/37/135/135	-
30	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
27	LMG	N	622	-	2/2/8/8	22/44/64/70	0/1/1/1
26	SQD	B	624	-	-	10/38/58/69	0/1/1/1
21	CLA	N	605	-	3/3/20/25	21/37/135/135	-
21	CLA	D	401	-	3/3/20/25	15/37/135/135	-
30	BCR	b	102	-	-	2/29/63/63	0/2/2/2
21	CLA	G	404	-	3/3/20/25	12/37/135/135	-
21	CLA	B	611	-	3/3/20/25	14/37/135/135	-
26	SQD	B	627	-	-	14/42/62/69	0/1/1/1
31	LMT	M	102	-	-	0/21/61/61	0/2/2/2
28	OEC	A	412	1,3	-	-	0/1/0/5
30	BCR	P	514	-	-	5/29/63/63	0/2/2/2
21	CLA	N	614	-	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	T	102	-	-	4/29/63/63	0/2/2/2
23	PL9	D	404	-	-	16/53/73/73	0/1/1/1
26	SQD	F	101	-	-	14/40/60/69	0/1/1/1
27	LMG	R	102	-	2/2/8/8	16/39/59/70	0/1/1/1
30	BCR	c	101	-	-	6/29/63/63	0/2/2/2
21	CLA	N	608	-	3/3/20/25	9/37/135/135	-
21	CLA	P	511	3	3/3/20/25	16/37/135/135	-
21	CLA	N	609	-	3/3/20/25	20/37/135/135	-
22	PHO	Q	403	-	-	15/53/103/103	0/5/6/6
21	CLA	C	505	-	3/3/20/25	19/37/135/135	-
27	LMG	P	520	-	2/2/8/8	20/43/63/70	0/1/1/1
27	LMG	A	410	-	2/2/8/8	22/46/66/70	0/1/1/1
34	HEM	R	101	5,6	-	1/6/54/54	-
31	LMT	N	624	-	-	3/21/61/61	0/2/2/2
21	CLA	C	511	3	3/3/20/25	17/37/135/135	-
27	LMG	e	102	-	2/2/8/8	12/37/57/70	0/1/1/1
27	LMG	Q	401	-	2/2/8/8	15/37/57/70	0/1/1/1
21	CLA	P	510	-	3/3/20/25	13/37/135/135	-
21	CLA	A	405	-	3/3/20/25	11/37/135/135	-
21	CLA	B	607	-	3/3/20/25	10/37/135/135	-
34	HEM	V	201	16	-	0/6/54/54	-
21	CLA	N	610	-	3/3/20/25	14/37/135/135	-
24	DGD	P	517	-	3/3/13/13	17/42/82/95	0/2/2/2
27	LMG	P	521	-	2/2/8/8	19/40/60/70	0/1/1/1
21	CLA	P	501	-	3/3/20/25	12/37/135/135	-
21	CLA	C	501	-	3/3/20/25	13/37/135/135	-
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
21	CLA	N	607	-	3/3/20/25	13/37/135/135	-
23	PL9	A	406	-	-	17/41/61/73	0/1/1/1
27	LMG	Q	407	-	2/2/8/8	18/43/63/70	0/1/1/1
30	BCR	B	620	-	-	4/29/63/63	0/2/2/2
21	CLA	B	608	-	3/3/20/25	17/37/135/135	-
30	BCR	D	405	-	-	8/29/63/63	0/2/2/2
30	BCR	B	617	-	-	2/29/63/63	0/2/2/2
21	CLA	Q	402	-	3/3/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	C	512	-	3/3/20/25	20/37/135/135	-
30	BCR	N	621	-	-	0/29/63/63	0/2/2/2
30	BCR	P	516	-	-	8/29/63/63	0/2/2/2
27	LMG	D	406	-	2/2/8/8	12/41/61/70	0/1/1/1
31	LMT	D	409	-	-	0/17/57/61	0/2/2/2
21	CLA	C	502	-	3/3/20/25	10/37/135/135	-
21	CLA	B	614	-	3/3/20/25	20/37/135/135	-
31	LMT	e	101	-	-	0/21/61/61	0/2/2/2
21	CLA	B	604	-	3/3/20/25	9/37/135/135	-
21	CLA	P	505	-	3/3/20/25	19/37/135/135	-
21	CLA	N	606	-	3/3/20/25	21/37/135/135	-
31	LMT	Q	410	-	-	0/17/57/61	0/2/2/2
30	BCR	B	618	-	-	4/29/63/63	0/2/2/2
24	DGD	P	519	-	3/3/13/13	20/55/95/95	0/2/2/2
21	CLA	P	503	-	3/3/20/25	14/37/135/135	-
27	LMG	D	407	-	2/2/8/8	20/43/63/70	0/1/1/1
26	SQD	Q	408	-	-	10/38/58/69	0/1/1/1
34	HEM	i	201	16	-	0/6/54/54	-
25	LHG	G	409	-	-	14/43/43/53	-
30	BCR	I	101	-	-	4/29/63/63	0/2/2/2
24	DGD	G	408	-	3/3/13/13	14/45/85/95	0/2/2/2
21	CLA	G	403	-	3/3/20/25	16/37/135/135	-
25	LHG	G	412	-	-	14/41/41/53	-
21	CLA	D	403	-	3/3/20/25	6/37/135/135	-
21	CLA	B	612	-	3/3/20/25	10/37/135/135	-
21	CLA	A	401	-	3/3/20/25	9/37/135/135	-
27	LMG	Q	406	-	2/2/8/8	14/41/61/70	0/1/1/1
21	CLA	A	403	-	3/3/20/25	13/37/135/135	-
21	CLA	N	615	-	3/3/20/25	13/37/135/135	-
31	LMT	N	625	-	-	2/21/61/61	0/2/2/2
27	LMG	M	101	-	2/2/8/8	14/37/57/70	0/1/1/1
30	BCR	W	101	-	-	2/29/63/63	0/2/2/2
23	PL9	J	101	-	-	11/29/49/73	0/1/1/1
27	LMG	B	622	-	2/2/8/8	23/44/64/70	0/1/1/1
21	CLA	P	506	-	3/3/20/25	17/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DGD	Q	409	-	3/3/13/13	32/52/92/95	0/2/2/2
21	CLA	C	509	-	3/3/20/25	10/37/135/135	-
31	LMT	B	629	-	-	3/21/61/61	0/2/2/2
24	DGD	W	102	-	3/3/13/13	16/47/87/95	0/2/2/2
21	CLA	G	406	-	3/3/20/25	11/37/135/135	-
21	CLA	C	507	-	3/3/20/25	15/37/135/135	-
21	CLA	P	507	-	3/3/20/25	12/37/135/135	-
21	CLA	P	508	-	3/3/20/25	11/37/135/135	-
26	SQD	S	102	-	-	13/40/60/69	0/1/1/1
27	LMG	C	519	-	2/2/8/8	20/43/63/70	0/1/1/1
24	DGD	N	602	-	3/3/13/13	22/41/81/95	0/2/2/2
21	CLA	N	620	-	3/3/20/25	19/37/135/135	-
22	PHO	G	405	-	-	12/53/103/103	0/5/6/6
24	DGD	C	518	-	3/3/13/13	21/55/95/95	0/2/2/2
25	LHG	A	411	-	-	12/41/41/53	-
24	DGD	P	518	-	3/3/13/13	19/51/91/95	0/2/2/2
21	CLA	N	611	-	3/3/20/25	10/37/135/135	-
27	LMG	N	623	-	2/2/8/8	17/44/64/70	0/1/1/1
23	PL9	G	407	-	-	18/41/61/73	0/1/1/1
21	CLA	N	613	-	3/3/20/25	7/37/135/135	-
24	DGD	C	516	-	3/3/13/13	18/42/82/95	0/2/2/2
21	CLA	P	504	-	3/3/20/25	10/37/135/135	-
30	BCR	S	101	-	-	7/29/63/63	0/2/2/2
21	CLA	B	610	-	3/3/20/25	17/37/135/135	-
21	CLA	B	602	-	3/3/20/25	19/37/135/135	-
21	CLA	C	510	-	3/3/20/25	17/37/135/135	-
21	CLA	A	402	-	3/3/20/25	17/37/135/135	-
26	SQD	G	401	-	-	16/49/69/69	0/1/1/1
31	LMT	I	103	-	-	4/21/61/61	0/2/2/2
30	BCR	C	515	-	-	8/29/63/63	0/2/2/2
27	LMG	B	623	-	2/2/8/8	15/44/64/70	0/1/1/1
21	CLA	B	601	-	3/3/20/25	18/37/135/135	-
23	PL9	Q	405	-	-	17/53/73/73	0/1/1/1
22	PHO	A	404	-	-	12/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	G	402	-	3/3/20/25	8/37/135/135	-
30	BCR	P	515	-	-	4/29/63/63	0/2/2/2
27	LMG	E	102	-	2/2/8/8	14/39/59/70	0/1/1/1
24	DGD	C	517	-	3/3/13/13	19/51/91/95	0/2/2/2
30	BCR	C	514	-	-	4/29/63/63	0/2/2/2
26	SQD	N	601	-	-	13/42/62/69	0/1/1/1
21	CLA	C	504	-	3/3/20/25	10/37/135/135	-
21	CLA	N	617	-	3/3/20/25	19/37/135/135	-
21	CLA	N	616	-	3/3/20/25	11/37/135/135	-
30	BCR	T	103	-	-	4/29/63/63	0/2/2/2
26	SQD	G	410	-	-	15/46/66/69	0/1/1/1
26	SQD	A	414	-	-	17/49/69/69	0/1/1/1
31	LMT	N	603	-	-	3/21/61/61	0/2/2/2
27	LMG	C	520	-	2/2/8/8	17/40/60/70	0/1/1/1
21	CLA	P	513	-	3/3/20/25	20/37/135/135	-
21	CLA	B	606	-	3/3/20/25	14/37/135/135	-
31	LMT	a	103	-	-	4/21/61/61	0/2/2/2
30	BCR	T	101	-	-	2/29/63/63	0/2/2/2
21	CLA	P	509	-	3/3/20/25	10/37/135/135	-
24	DGD	D	408	-	3/3/13/13	32/52/92/95	0/2/2/2
25	LHG	A	408	-	-	13/43/43/53	-
26	SQD	A	409	-	-	16/46/66/69	0/1/1/1
21	CLA	B	605	-	3/3/20/25	19/37/135/135	-
31	LMT	B	626	-	-	2/21/61/61	0/2/2/2
27	LMG	a	102	-	2/2/8/8	20/38/58/70	0/1/1/1
21	CLA	N	619	-	3/3/20/25	9/37/135/135	-
21	CLA	N	618	-	3/3/20/25	19/37/135/135	-
21	CLA	B	613	-	3/3/20/25	17/37/135/135	-
21	CLA	C	508	-	3/3/20/25	11/37/135/135	-
34	HEM	E	101	5,6	-	1/6/54/54	-
30	BCR	a	101	-	-	4/29/63/63	0/2/2/2
21	CLA	C	513	-	3/3/20/25	20/37/135/135	-
21	CLA	B	616	-	3/3/20/25	19/37/135/135	-
21	CLA	N	612	-	3/3/20/25	16/37/135/135	-

All (1165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	404	PHO	CHB-C1B	5.79	1.49	1.38
22	G	405	PHO	CHB-C1B	5.69	1.49	1.38
22	D	402	PHO	CHB-C1B	5.65	1.49	1.38
22	Q	403	PHO	CHB-C1B	5.64	1.49	1.38
34	i	201	HEM	C3D-C2D	5.46	1.53	1.37
34	V	201	HEM	C3D-C2D	5.45	1.53	1.37
34	E	101	HEM	C3D-C2D	5.39	1.53	1.37
22	Q	403	PHO	CHC-C1C	5.37	1.49	1.38
22	G	405	PHO	C3C-C2C	5.37	1.48	1.36
34	R	101	HEM	C3D-C2D	5.34	1.53	1.37
22	A	404	PHO	C3C-C2C	5.32	1.48	1.36
22	D	402	PHO	CHC-C1C	5.30	1.49	1.38
22	Q	403	PHO	C3C-C2C	5.29	1.48	1.36
22	A	404	PHO	CHC-C1C	5.26	1.48	1.38
22	D	402	PHO	C3C-C2C	5.26	1.47	1.36
22	G	405	PHO	CHC-C1C	5.18	1.48	1.38
22	D	402	PHO	O2D-CGD	5.17	1.45	1.33
22	Q	403	PHO	O2D-CGD	5.15	1.45	1.33
22	Q	403	PHO	C3B-C2B	5.14	1.47	1.37
22	D	402	PHO	C3B-C2B	5.07	1.47	1.37
22	G	405	PHO	C3B-C2B	5.06	1.47	1.37
22	A	404	PHO	C3B-C2B	5.06	1.47	1.37
34	R	101	HEM	C3B-C2B	-5.05	1.33	1.40
34	E	101	HEM	C3B-C2B	-5.05	1.33	1.40
22	D	402	PHO	CHD-C1D	5.01	1.48	1.38
22	G	405	PHO	O2D-CGD	4.98	1.45	1.33
22	G	405	PHO	CHD-C1D	4.89	1.48	1.38
22	A	404	PHO	CHD-C1D	4.89	1.48	1.38
22	Q	403	PHO	CHD-C1D	4.89	1.48	1.38
22	A	404	PHO	O2D-CGD	4.88	1.45	1.33
34	i	201	HEM	C3C-C2C	-4.68	1.33	1.40
34	V	201	HEM	C3C-C2C	-4.68	1.33	1.40
26	G	401	SQD	O8-S	4.53	1.63	1.47
26	G	410	SQD	O8-S	4.53	1.63	1.47
26	Q	408	SQD	O8-S	4.53	1.63	1.47
26	F	101	SQD	O8-S	4.52	1.63	1.47
26	B	624	SQD	O8-S	4.52	1.63	1.47
26	S	102	SQD	O8-S	4.49	1.63	1.47
26	A	414	SQD	O8-S	4.49	1.63	1.47
27	C	519	LMG	O8-C28	4.48	1.46	1.33
26	A	409	SQD	O8-S	4.48	1.63	1.47
27	P	521	LMG	O8-C28	4.47	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	520	LMG	O8-C28	4.47	1.46	1.33
26	B	627	SQD	O8-S	4.46	1.63	1.47
26	N	601	SQD	O8-S	4.44	1.63	1.47
24	Q	409	DGD	O2G-C1B	4.43	1.46	1.34
24	N	602	DGD	O1G-C1A	4.41	1.46	1.33
27	C	520	LMG	O7-C10	4.41	1.46	1.34
27	G	411	LMG	O7-C10	4.41	1.46	1.34
24	D	408	DGD	O2G-C1B	4.40	1.46	1.34
24	A	407	DGD	O2G-C1B	4.40	1.46	1.34
27	P	520	LMG	O8-C28	4.40	1.46	1.33
27	E	102	LMG	O7-C10	4.39	1.46	1.34
24	D	408	DGD	O1G-C1A	4.38	1.46	1.33
24	Q	409	DGD	O1G-C1A	4.38	1.46	1.33
27	A	410	LMG	O7-C10	4.36	1.46	1.34
24	C	517	DGD	O1G-C1A	4.36	1.46	1.33
24	B	628	DGD	O1G-C1A	4.35	1.46	1.33
24	P	518	DGD	O1G-C1A	4.35	1.46	1.33
27	P	521	LMG	O7-C10	4.34	1.46	1.34
26	A	409	SQD	O48-C23	4.34	1.46	1.33
24	W	102	DGD	O1G-C1A	4.34	1.46	1.33
26	Q	408	SQD	O48-C23	4.34	1.46	1.33
25	G	409	LHG	O8-C23	4.33	1.46	1.33
26	N	601	SQD	O48-C23	4.32	1.46	1.33
24	G	408	DGD	O2G-C1B	4.32	1.46	1.34
27	R	102	LMG	O7-C10	4.32	1.46	1.34
26	B	627	SQD	O48-C23	4.32	1.46	1.33
26	B	624	SQD	O48-C23	4.32	1.46	1.33
26	G	410	SQD	O48-C23	4.31	1.45	1.33
25	A	408	LHG	O8-C23	4.31	1.45	1.33
27	M	101	LMG	O7-C10	4.31	1.46	1.34
27	a	102	LMG	O8-C28	4.29	1.45	1.33
34	i	201	HEM	C3B-C2B	-4.29	1.34	1.40
24	C	518	DGD	O1G-C1A	4.28	1.45	1.33
27	E	102	LMG	O8-C28	4.28	1.45	1.33
27	I	102	LMG	O8-C28	4.27	1.45	1.33
27	N	623	LMG	O8-C28	4.27	1.45	1.33
27	Q	406	LMG	O8-C28	4.27	1.45	1.33
24	B	621	DGD	O1G-C1A	4.27	1.45	1.33
22	A	404	PHO	O2A-CGA	4.27	1.45	1.33
34	V	201	HEM	C3B-C2B	-4.27	1.34	1.40
26	A	414	SQD	O48-C23	4.27	1.45	1.33
24	C	518	DGD	O2G-C1B	4.27	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	623	LMG	O8-C28	4.26	1.45	1.33
27	A	410	LMG	O8-C28	4.26	1.45	1.33
26	G	401	SQD	O48-C23	4.25	1.45	1.33
25	G	412	LHG	O8-C23	4.24	1.45	1.33
27	e	102	LMG	O7-C10	4.24	1.46	1.34
27	G	411	LMG	O8-C28	4.24	1.45	1.33
24	B	628	DGD	O2G-C1B	4.24	1.46	1.34
27	D	406	LMG	O8-C28	4.24	1.45	1.33
24	P	519	DGD	O2G-C1B	4.24	1.46	1.34
24	N	602	DGD	O2G-C1B	4.24	1.46	1.34
27	Q	407	LMG	O8-C28	4.23	1.45	1.33
24	P	517	DGD	O2G-C1B	4.23	1.46	1.34
25	A	408	LHG	O7-C7	4.23	1.46	1.34
24	P	519	DGD	O1G-C1A	4.23	1.45	1.33
26	S	102	SQD	O47-C7	4.22	1.46	1.34
27	e	102	LMG	O8-C28	4.22	1.45	1.33
26	S	102	SQD	O48-C23	4.22	1.45	1.33
24	C	516	DGD	O1G-C1A	4.21	1.45	1.33
25	A	411	LHG	O8-C23	4.21	1.45	1.33
24	P	517	DGD	O1G-C1A	4.21	1.45	1.33
27	Q	401	LMG	O7-C10	4.21	1.46	1.34
27	D	407	LMG	O8-C28	4.20	1.45	1.33
27	D	412	LMG	O7-C10	4.19	1.46	1.34
27	Q	401	LMG	O8-C28	4.19	1.45	1.33
26	F	101	SQD	O48-C23	4.18	1.45	1.33
24	C	517	DGD	O2G-C1B	4.18	1.46	1.34
27	B	623	LMG	O7-C10	4.18	1.46	1.34
25	G	409	LHG	O7-C7	4.17	1.46	1.34
27	D	412	LMG	O8-C28	4.17	1.45	1.33
27	Q	406	LMG	O7-C10	4.17	1.46	1.34
27	N	623	LMG	O7-C10	4.16	1.46	1.34
25	G	412	LHG	O7-C7	4.16	1.46	1.34
22	D	402	PHO	O2A-CGA	4.16	1.45	1.33
22	G	405	PHO	O2A-CGA	4.16	1.45	1.33
24	G	408	DGD	O1G-C1A	4.16	1.45	1.33
24	A	407	DGD	O1G-C1A	4.15	1.45	1.33
27	R	102	LMG	O8-C28	4.15	1.45	1.33
27	M	101	LMG	O8-C28	4.15	1.45	1.33
26	A	414	SQD	O47-C7	4.15	1.46	1.34
24	C	516	DGD	O2G-C1B	4.14	1.46	1.34
27	D	406	LMG	O7-C10	4.14	1.46	1.34
26	Q	408	SQD	O47-C7	4.13	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	101	SQD	O47-C7	4.12	1.45	1.34
25	A	411	LHG	O7-C7	4.12	1.45	1.34
26	G	401	SQD	O47-C7	4.12	1.45	1.34
27	I	102	LMG	O7-C10	4.12	1.45	1.34
26	B	624	SQD	O47-C7	4.12	1.45	1.34
27	B	622	LMG	O8-C28	4.10	1.45	1.33
22	Q	403	PHO	O2A-CGA	4.10	1.45	1.33
27	B	622	LMG	O7-C10	4.09	1.45	1.34
24	P	518	DGD	O2G-C1B	4.09	1.45	1.34
27	a	102	LMG	O7-C10	4.09	1.45	1.34
24	B	621	DGD	O2G-C1B	4.09	1.45	1.34
27	N	622	LMG	O8-C28	4.08	1.45	1.33
27	N	622	LMG	O7-C10	4.07	1.45	1.34
27	Q	407	LMG	O7-C10	4.07	1.45	1.34
26	N	601	SQD	O47-C7	4.06	1.45	1.34
24	W	102	DGD	O2G-C1B	4.06	1.45	1.34
26	B	627	SQD	O47-C7	4.05	1.45	1.34
27	D	407	LMG	O7-C10	4.04	1.45	1.34
26	G	410	SQD	O47-C7	4.04	1.45	1.34
26	A	409	SQD	O47-C7	4.02	1.45	1.34
27	C	519	LMG	O7-C10	3.93	1.45	1.34
27	P	520	LMG	O7-C10	3.92	1.45	1.34
22	Q	403	PHO	C4A-NA	-3.84	1.26	1.35
22	D	402	PHO	C4A-NA	-3.83	1.26	1.35
21	N	616	CLA	C1C-C2C	3.82	1.52	1.44
21	C	505	CLA	C1C-C2C	3.81	1.51	1.44
22	A	404	PHO	C4A-NA	-3.81	1.26	1.35
21	B	609	CLA	C1C-C2C	3.81	1.51	1.44
22	G	405	PHO	C4A-NA	-3.79	1.26	1.35
21	Q	402	CLA	C1C-C2C	3.77	1.51	1.44
21	G	402	CLA	C1C-C2C	3.74	1.51	1.44
22	Q	403	PHO	CHC-C4B	3.74	1.49	1.40
34	R	101	HEM	C3C-C2C	-3.74	1.35	1.40
22	D	402	PHO	CHC-C4B	3.74	1.49	1.40
21	P	505	CLA	C1C-C2C	3.73	1.51	1.44
21	N	617	CLA	C1C-C2C	3.73	1.51	1.44
34	E	101	HEM	C3C-CAC	3.72	1.55	1.47
21	Q	404	CLA	C1C-C2C	3.70	1.51	1.44
21	B	610	CLA	C1C-C2C	3.70	1.51	1.44
21	P	511	CLA	C1C-C2C	3.70	1.51	1.44
21	D	401	CLA	C1C-C2C	3.69	1.51	1.44
21	C	513	CLA	C1C-C2C	3.68	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	603	CLA	C1C-C2C	3.68	1.51	1.44
21	N	606	CLA	C1C-C2C	3.67	1.51	1.44
21	P	506	CLA	C1C-C2C	3.67	1.51	1.44
21	P	513	CLA	C1C-C2C	3.67	1.51	1.44
22	A	404	PHO	CHC-C4B	3.67	1.49	1.40
21	N	607	CLA	C1C-C2C	3.67	1.51	1.44
34	R	101	HEM	C3C-CAC	3.67	1.55	1.47
21	B	602	CLA	C1C-C2C	3.66	1.51	1.44
21	N	613	CLA	C1C-C2C	3.66	1.51	1.44
21	N	610	CLA	C1C-C2C	3.65	1.51	1.44
21	B	612	CLA	C1C-C2C	3.65	1.51	1.44
34	V	201	HEM	C3C-CAC	3.65	1.55	1.47
21	C	512	CLA	C1C-C2C	3.64	1.51	1.44
21	N	614	CLA	C1C-C2C	3.64	1.51	1.44
21	P	508	CLA	C1C-C2C	3.64	1.51	1.44
22	G	405	PHO	CHC-C4B	3.63	1.48	1.40
21	B	608	CLA	C1C-C2C	3.63	1.51	1.44
21	N	618	CLA	C1C-C2C	3.63	1.51	1.44
21	C	508	CLA	C1C-C2C	3.62	1.51	1.44
21	B	606	CLA	C1C-C2C	3.62	1.51	1.44
21	P	503	CLA	C1C-C2C	3.61	1.51	1.44
21	D	403	CLA	C1C-C2C	3.61	1.51	1.44
21	C	510	CLA	C1C-C2C	3.61	1.51	1.44
21	P	512	CLA	C1C-C2C	3.61	1.51	1.44
34	E	101	HEM	C3C-C2C	-3.60	1.35	1.40
21	P	510	CLA	C1C-C2C	3.60	1.51	1.44
21	B	614	CLA	C1C-C2C	3.60	1.51	1.44
21	N	612	CLA	C1C-C2C	3.60	1.51	1.44
22	D	402	PHO	OBD-CAD	3.60	1.28	1.22
34	i	201	HEM	C3C-CAC	3.59	1.55	1.47
21	C	509	CLA	C1C-C2C	3.59	1.51	1.44
21	B	615	CLA	C1C-C2C	3.58	1.51	1.44
22	Q	403	PHO	OBD-CAD	3.58	1.28	1.22
21	C	503	CLA	C1C-C2C	3.58	1.51	1.44
22	D	402	PHO	CHD-C4C	3.58	1.48	1.40
21	B	613	CLA	C1C-C2C	3.58	1.51	1.44
21	N	609	CLA	C1C-C2C	3.57	1.51	1.44
22	G	405	PHO	OBD-CAD	3.57	1.28	1.22
21	C	511	CLA	C1C-C2C	3.57	1.51	1.44
21	P	501	CLA	C1C-C2C	3.57	1.51	1.44
21	P	509	CLA	C1C-C2C	3.56	1.51	1.44
21	B	611	CLA	C1C-C2C	3.55	1.51	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	604	CLA	C1C-C2C	3.55	1.51	1.44
21	A	401	CLA	C1C-C2C	3.55	1.51	1.44
22	G	405	PHO	CHD-C4C	3.55	1.48	1.40
21	A	405	CLA	C1C-C2C	3.55	1.51	1.44
22	A	404	PHO	CHD-C4C	3.55	1.48	1.40
21	N	611	CLA	C1C-C2C	3.54	1.51	1.44
21	C	507	CLA	C1C-C2C	3.54	1.51	1.44
21	N	619	CLA	C1C-C2C	3.53	1.51	1.44
21	C	501	CLA	C1C-C2C	3.53	1.51	1.44
22	Q	403	PHO	CHD-C4C	3.52	1.48	1.40
21	B	605	CLA	C1C-C2C	3.52	1.51	1.44
21	P	502	CLA	C1C-C2C	3.51	1.51	1.44
21	P	507	CLA	C1C-C2C	3.51	1.51	1.44
21	A	403	CLA	C1C-C2C	3.51	1.51	1.44
21	C	506	CLA	C1C-C2C	3.50	1.51	1.44
22	A	404	PHO	OBD-CAD	3.50	1.28	1.22
21	B	607	CLA	C1C-C2C	3.50	1.51	1.44
21	N	615	CLA	C1C-C2C	3.49	1.51	1.44
21	G	406	CLA	C1C-C2C	3.48	1.51	1.44
21	C	504	CLA	C1C-C2C	3.47	1.51	1.44
21	C	502	CLA	C1C-C2C	3.47	1.51	1.44
21	G	404	CLA	C1C-C2C	3.46	1.51	1.44
21	N	608	CLA	C1C-C2C	3.46	1.51	1.44
22	A	404	PHO	CHB-C4A	3.46	1.48	1.40
21	P	504	CLA	C1C-C2C	3.43	1.51	1.44
22	G	405	PHO	CHB-C4A	3.42	1.48	1.40
21	A	402	CLA	C4C-C3C	3.40	1.50	1.45
34	R	101	HEM	C3B-CAB	3.39	1.54	1.47
21	G	403	CLA	C4C-C3C	3.39	1.50	1.45
22	D	402	PHO	CHB-C4A	3.39	1.48	1.40
21	N	620	CLA	C1C-C2C	3.37	1.51	1.44
21	B	603	CLA	C2-C3	3.37	1.41	1.33
34	E	101	HEM	C3B-CAB	3.37	1.54	1.47
21	B	607	CLA	C2-C3	3.37	1.41	1.33
21	N	607	CLA	C2-C3	3.36	1.41	1.33
21	B	601	CLA	C4C-C3C	3.35	1.50	1.45
21	P	504	CLA	C2-C3	3.34	1.41	1.33
21	B	616	CLA	C1C-C2C	3.33	1.51	1.44
21	B	608	CLA	C2-C3	3.33	1.41	1.33
21	N	605	CLA	C4C-C3C	3.33	1.50	1.45
21	B	614	CLA	C4C-C3C	3.32	1.50	1.45
23	A	406	PL9	C33-C34	3.32	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	611	CLA	C2-C3	3.32	1.40	1.33
21	N	612	CLA	C2-C3	3.30	1.40	1.33
21	A	403	CLA	C4C-C3C	3.29	1.50	1.45
21	N	610	CLA	C4C-C3C	3.29	1.50	1.45
22	Q	403	PHO	CHB-C4A	3.29	1.48	1.40
23	G	407	PL9	C33-C34	3.28	1.40	1.33
21	A	402	CLA	C1C-C2C	3.28	1.50	1.44
21	G	404	CLA	C4C-C3C	3.27	1.50	1.45
23	Q	405	PL9	C38-C39	3.26	1.40	1.33
21	N	616	CLA	C2-C3	3.26	1.40	1.33
21	N	611	CLA	C4C-C3C	3.26	1.50	1.45
21	B	604	CLA	C2-C3	3.25	1.40	1.33
21	N	618	CLA	C4C-C3C	3.25	1.50	1.45
21	D	401	CLA	C2-C3	3.25	1.40	1.33
21	B	604	CLA	C4C-C3C	3.25	1.50	1.45
21	C	505	CLA	C4C-C3C	3.25	1.50	1.45
21	C	504	CLA	C2-C3	3.25	1.40	1.33
21	B	615	CLA	C4C-C3C	3.24	1.50	1.45
21	C	509	CLA	C4C-C3C	3.24	1.50	1.45
21	C	501	CLA	C4C-C3C	3.23	1.50	1.45
21	N	614	CLA	C4C-C3C	3.23	1.50	1.45
21	B	610	CLA	C4C-C3C	3.23	1.50	1.45
21	P	502	CLA	C2-C3	3.23	1.40	1.33
21	N	620	CLA	C2-C3	3.23	1.40	1.33
21	C	513	CLA	C2-C3	3.22	1.40	1.33
21	B	601	CLA	C1C-C2C	3.22	1.50	1.44
21	N	608	CLA	C4C-C3C	3.22	1.50	1.45
21	P	501	CLA	C4C-C3C	3.22	1.50	1.45
21	P	505	CLA	C4C-C3C	3.21	1.50	1.45
21	P	501	CLA	C2-C3	3.21	1.40	1.33
21	B	606	CLA	C4C-C3C	3.21	1.50	1.45
21	P	509	CLA	C2-C3	3.21	1.40	1.33
21	P	513	CLA	C4C-C3C	3.21	1.50	1.45
23	D	404	PL9	C38-C39	3.21	1.40	1.33
21	N	608	CLA	C2-C3	3.21	1.40	1.33
21	B	614	CLA	C2-C3	3.20	1.40	1.33
21	N	618	CLA	C2-C3	3.20	1.40	1.33
21	P	509	CLA	C4C-C3C	3.20	1.50	1.45
21	Q	402	CLA	C2-C3	3.19	1.40	1.33
21	G	402	CLA	C4C-C3C	3.19	1.50	1.45
21	Q	404	CLA	C2-C3	3.19	1.40	1.33
21	P	512	CLA	C2-C3	3.19	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	512	CLA	C2-C3	3.19	1.40	1.33
21	D	403	CLA	C2-C3	3.19	1.40	1.33
34	i	201	HEM	C3B-CAB	3.18	1.54	1.47
21	C	501	CLA	C2-C3	3.18	1.40	1.33
21	B	605	CLA	C2-C3	3.18	1.40	1.33
21	N	614	CLA	C2-C3	3.18	1.40	1.33
21	N	610	CLA	C2-C3	3.18	1.40	1.33
21	C	509	CLA	C2-C3	3.18	1.40	1.33
21	B	616	CLA	C2-C3	3.18	1.40	1.33
21	P	504	CLA	C4C-C3C	3.18	1.50	1.45
21	B	610	CLA	C2-C3	3.18	1.40	1.33
21	N	605	CLA	C2-C3	3.18	1.40	1.33
21	C	504	CLA	C4C-C3C	3.17	1.50	1.45
21	B	601	CLA	C2-C3	3.17	1.40	1.33
21	N	605	CLA	C1C-C2C	3.17	1.50	1.44
21	N	609	CLA	C2-C3	3.17	1.40	1.33
21	P	511	CLA	C2-C3	3.17	1.40	1.33
21	C	506	CLA	C2-C3	3.17	1.40	1.33
21	P	512	CLA	C4C-C3C	3.17	1.50	1.45
23	D	404	PL9	C33-C34	3.17	1.40	1.33
23	Q	405	PL9	C33-C34	3.16	1.40	1.33
21	C	503	CLA	C2-C3	3.16	1.40	1.33
21	N	606	CLA	C2-C3	3.15	1.40	1.33
21	P	503	CLA	C2-C3	3.15	1.40	1.33
21	B	609	CLA	C2-C3	3.15	1.40	1.33
21	C	502	CLA	C2-C3	3.15	1.40	1.33
21	B	612	CLA	C2-C3	3.15	1.40	1.33
21	A	403	CLA	C2-C3	3.15	1.40	1.33
21	A	405	CLA	C2-C3	3.15	1.40	1.33
21	P	506	CLA	C2-C3	3.14	1.40	1.33
21	P	511	CLA	C4C-C3C	3.14	1.50	1.45
21	P	513	CLA	C2-C3	3.14	1.40	1.33
21	B	602	CLA	C4C-C3C	3.14	1.50	1.45
21	C	508	CLA	C2-C3	3.14	1.40	1.33
21	A	402	CLA	C2-C3	3.13	1.40	1.33
21	B	607	CLA	C4C-C3C	3.13	1.50	1.45
21	G	403	CLA	C1C-C2C	3.13	1.50	1.44
21	D	401	CLA	C4C-C3C	3.12	1.50	1.45
21	A	401	CLA	C2-C3	3.12	1.40	1.33
21	N	620	CLA	C4C-C3C	3.12	1.50	1.45
21	B	611	CLA	C4C-C3C	3.12	1.50	1.45
21	Q	402	CLA	C4C-C3C	3.11	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	404	CLA	C4C-C3C	3.11	1.50	1.45
21	C	511	CLA	C4C-C3C	3.11	1.50	1.45
21	C	510	CLA	C2-C3	3.11	1.40	1.33
21	G	403	CLA	C2-C3	3.11	1.40	1.33
21	P	507	CLA	C4C-C3C	3.11	1.50	1.45
21	C	513	CLA	C4C-C3C	3.10	1.50	1.45
21	P	503	CLA	C4C-C3C	3.10	1.50	1.45
21	N	619	CLA	C4C-C3C	3.10	1.50	1.45
21	B	602	CLA	C2-C3	3.10	1.40	1.33
21	B	615	CLA	C2-C3	3.10	1.40	1.33
21	N	617	CLA	C4C-C3C	3.09	1.50	1.45
21	N	612	CLA	C4C-C3C	3.09	1.50	1.45
21	C	511	CLA	C2-C3	3.09	1.40	1.33
21	D	403	CLA	C4C-C3C	3.09	1.50	1.45
34	V	201	HEM	C3B-CAB	3.09	1.54	1.47
21	N	613	CLA	C2-C3	3.09	1.40	1.33
21	P	508	CLA	C2-C3	3.09	1.40	1.33
21	C	503	CLA	C4C-C3C	3.09	1.50	1.45
21	N	615	CLA	C4C-C3C	3.09	1.50	1.45
21	C	512	CLA	C4C-C3C	3.09	1.50	1.45
21	N	606	CLA	C4C-C3C	3.09	1.50	1.45
21	N	617	CLA	C2-C3	3.09	1.40	1.33
21	P	510	CLA	C4C-C3C	3.08	1.50	1.45
21	G	402	CLA	C2-C3	3.08	1.40	1.33
21	P	507	CLA	C2-C3	3.08	1.40	1.33
21	A	401	CLA	C4C-C3C	3.08	1.50	1.45
21	G	404	CLA	C2-C3	3.07	1.40	1.33
21	B	609	CLA	C4C-C3C	3.07	1.50	1.45
21	N	619	CLA	C2-C3	3.07	1.40	1.33
21	A	405	CLA	C4C-C3C	3.07	1.50	1.45
21	B	606	CLA	C2-C3	3.06	1.40	1.33
21	P	506	CLA	C4C-C3C	3.06	1.50	1.45
23	G	407	PL9	C38-C39	3.06	1.41	1.32
21	P	510	CLA	C2-C3	3.06	1.40	1.33
26	N	601	SQD	C6-S	-3.06	1.66	1.77
26	B	627	SQD	C6-S	-3.06	1.66	1.77
21	B	613	CLA	C4C-C3C	3.06	1.50	1.45
21	P	502	CLA	C4C-C3C	3.05	1.50	1.45
21	B	608	CLA	C4C-C3C	3.05	1.50	1.45
21	C	505	CLA	C2-C3	3.05	1.40	1.33
21	B	616	CLA	C4C-C3C	3.04	1.50	1.45
21	N	616	CLA	C4C-C3C	3.04	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	510	CLA	C4C-C3C	3.04	1.50	1.45
21	G	406	CLA	C2-C3	3.04	1.40	1.33
26	A	414	SQD	C6-S	-3.04	1.66	1.77
21	P	508	CLA	C4C-C3C	3.04	1.50	1.45
21	C	507	CLA	C2-C3	3.03	1.40	1.33
21	P	505	CLA	C2-C3	3.03	1.40	1.33
21	C	508	CLA	C4C-C3C	3.03	1.50	1.45
23	Q	405	PL9	C43-C44	3.03	1.40	1.33
21	C	507	CLA	C4C-C3C	3.02	1.50	1.45
21	C	506	CLA	C4C-C3C	3.02	1.50	1.45
21	B	613	CLA	C2-C3	3.02	1.40	1.33
21	G	406	CLA	C4C-C3C	3.02	1.50	1.45
21	N	615	CLA	C2-C3	3.01	1.40	1.33
21	N	607	CLA	C4C-C3C	3.01	1.50	1.45
23	A	406	PL9	C38-C39	3.01	1.41	1.32
21	B	605	CLA	C4C-C3C	3.01	1.50	1.45
21	B	603	CLA	C4C-C3C	2.99	1.50	1.45
23	D	404	PL9	C43-C44	2.99	1.40	1.33
21	B	611	CLA	C2-C3	2.99	1.40	1.33
26	Q	408	SQD	C6-S	-2.97	1.66	1.77
21	C	502	CLA	C4C-C3C	2.96	1.50	1.45
26	G	401	SQD	C6-S	-2.96	1.66	1.77
26	B	624	SQD	C6-S	-2.94	1.66	1.77
21	N	609	CLA	C4C-C3C	2.93	1.50	1.45
22	A	404	PHO	C3D-C4D	-2.93	1.34	1.43
21	B	612	CLA	C4C-C3C	2.91	1.50	1.45
26	A	409	SQD	C6-S	-2.90	1.66	1.77
21	N	613	CLA	C4C-C3C	2.90	1.50	1.45
26	G	410	SQD	C6-S	-2.90	1.66	1.77
22	D	402	PHO	C3D-C4D	-2.88	1.34	1.43
23	J	101	PL9	C23-C24	2.86	1.39	1.33
26	S	102	SQD	C6-S	-2.84	1.66	1.77
26	F	101	SQD	C6-S	-2.84	1.66	1.77
22	G	405	PHO	C3D-C4D	-2.84	1.34	1.43
22	Q	403	PHO	C3D-C4D	-2.84	1.34	1.43
22	Q	403	PHO	C3D-C2D	2.80	1.46	1.39
23	b	101	PL9	C23-C24	2.78	1.39	1.33
23	D	404	PL9	C23-C24	2.76	1.39	1.33
23	Q	405	PL9	C23-C24	2.75	1.39	1.33
23	b	101	PL9	C8-C9	2.75	1.39	1.33
23	b	101	PL9	C13-C14	2.75	1.39	1.33
21	D	401	CLA	C3B-CAB	2.74	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	J	101	PL9	C13-C14	2.72	1.39	1.33
21	Q	402	CLA	C3B-CAB	2.71	1.53	1.47
23	J	101	PL9	C8-C9	2.71	1.39	1.33
22	D	402	PHO	C3D-C2D	2.70	1.46	1.39
23	J	101	PL9	C18-C19	2.68	1.39	1.33
23	b	101	PL9	C18-C19	2.68	1.39	1.33
23	A	406	PL9	C23-C24	2.67	1.39	1.33
23	Q	405	PL9	C8-C9	2.67	1.39	1.33
23	Q	405	PL9	C13-C14	2.67	1.39	1.33
23	D	404	PL9	C13-C14	2.66	1.39	1.33
23	G	407	PL9	C23-C24	2.66	1.39	1.33
23	D	404	PL9	C18-C19	2.65	1.39	1.33
21	Q	402	CLA	O2D-CED	-2.64	1.39	1.45
21	D	401	CLA	O2D-CED	-2.63	1.39	1.45
23	D	404	PL9	C8-C9	2.63	1.39	1.33
22	G	405	PHO	C3D-C2D	2.63	1.46	1.39
21	N	618	CLA	C3B-CAB	2.62	1.53	1.47
21	C	503	CLA	C3B-CAB	2.62	1.53	1.47
22	Q	403	PHO	C3B-C4B	2.62	1.48	1.43
22	D	402	PHO	C3B-C4B	2.62	1.48	1.43
21	P	503	CLA	C3B-CAB	2.60	1.53	1.47
23	A	406	PL9	C13-C14	2.59	1.39	1.33
22	A	404	PHO	C3D-C2D	2.59	1.46	1.39
21	G	403	CLA	C3B-CAB	2.58	1.53	1.47
21	A	402	CLA	C3B-CAB	2.58	1.53	1.47
23	G	407	PL9	C13-C14	2.58	1.39	1.33
23	Q	405	PL9	C18-C19	2.56	1.39	1.33
23	G	407	PL9	C8-C9	2.56	1.39	1.33
21	B	615	CLA	C3B-CAB	2.55	1.53	1.47
21	N	610	CLA	C3B-CAB	2.55	1.53	1.47
23	A	406	PL9	C18-C19	2.54	1.39	1.33
21	B	602	CLA	C3B-CAB	2.54	1.53	1.47
21	B	614	CLA	C3B-CAB	2.54	1.53	1.47
23	G	407	PL9	C18-C19	2.53	1.39	1.33
21	P	508	CLA	C3B-CAB	2.53	1.53	1.47
21	N	606	CLA	C3B-CAB	2.53	1.53	1.47
23	A	406	PL9	C8-C9	2.53	1.39	1.33
21	P	504	CLA	O2D-CED	-2.53	1.39	1.45
21	B	601	CLA	C3B-CAB	2.52	1.53	1.47
21	A	401	CLA	C1A-CHA	-2.52	1.32	1.43
21	C	508	CLA	C3B-CAB	2.52	1.53	1.47
21	P	510	CLA	C3B-CAB	2.52	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	615	CLA	C3B-CAB	2.52	1.53	1.47
21	C	509	CLA	O2D-CED	-2.52	1.39	1.45
21	C	504	CLA	O2D-CED	-2.51	1.39	1.45
21	N	619	CLA	C3B-CAB	2.51	1.53	1.47
21	P	504	CLA	C3B-CAB	2.50	1.53	1.47
21	G	406	CLA	C3B-CAB	2.50	1.53	1.47
21	C	510	CLA	O2D-CED	-2.50	1.39	1.45
21	A	405	CLA	C3B-CAB	2.50	1.53	1.47
21	C	508	CLA	O2D-CED	-2.50	1.39	1.45
24	P	517	DGD	O5D-C1E	2.50	1.44	1.40
21	C	507	CLA	O2D-CED	-2.49	1.39	1.45
21	N	613	CLA	O2D-CED	-2.49	1.39	1.45
24	A	407	DGD	O5D-C1E	2.49	1.44	1.40
21	N	611	CLA	O2D-CED	-2.49	1.39	1.45
21	B	602	CLA	O2D-CED	-2.49	1.39	1.45
21	B	612	CLA	C3B-CAB	2.49	1.53	1.47
21	B	608	CLA	O2D-CED	-2.49	1.39	1.45
21	B	607	CLA	O2D-CED	-2.49	1.39	1.45
21	P	511	CLA	C3B-CAB	2.49	1.53	1.47
24	G	408	DGD	O5D-C1E	2.48	1.44	1.40
21	P	505	CLA	C3B-CAB	2.48	1.53	1.47
21	P	509	CLA	O2D-CED	-2.48	1.39	1.45
21	G	403	CLA	O2D-CED	-2.48	1.39	1.45
21	P	513	CLA	O2D-CED	-2.48	1.39	1.45
21	B	613	CLA	O2D-CED	-2.48	1.39	1.45
21	A	402	CLA	O2D-CED	-2.48	1.39	1.45
21	C	510	CLA	C3B-CAB	2.48	1.53	1.47
24	C	518	DGD	O5D-C1E	2.48	1.44	1.40
21	P	512	CLA	C3B-CAB	2.48	1.53	1.47
21	P	501	CLA	O2D-CED	-2.47	1.39	1.45
21	A	403	CLA	O2D-CED	-2.47	1.39	1.45
21	N	617	CLA	O2D-CED	-2.47	1.39	1.45
21	C	506	CLA	C3B-CAB	2.47	1.53	1.47
21	P	513	CLA	C3B-CAB	2.47	1.53	1.47
21	P	506	CLA	O2D-CED	-2.47	1.39	1.45
21	B	601	CLA	O2D-CED	-2.47	1.39	1.45
21	N	618	CLA	O2D-CED	-2.47	1.39	1.45
21	N	608	CLA	C3B-CAB	2.47	1.53	1.47
21	N	616	CLA	O2D-CED	-2.47	1.39	1.45
21	B	609	CLA	O2D-CED	-2.46	1.39	1.45
21	B	615	CLA	O2D-CED	-2.46	1.39	1.45
21	N	612	CLA	C3B-CAB	2.46	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	509	CLA	C3B-CAB	2.46	1.53	1.47
21	B	613	CLA	C3B-CAB	2.46	1.53	1.47
21	B	612	CLA	O2D-CED	-2.46	1.39	1.45
21	B	604	CLA	O2D-CED	-2.46	1.39	1.45
21	N	611	CLA	O2A-CGA	2.46	1.40	1.33
21	B	614	CLA	O2D-CED	-2.46	1.39	1.45
21	N	608	CLA	O2D-CED	-2.46	1.39	1.45
21	G	402	CLA	C1A-CHA	-2.46	1.32	1.43
21	C	511	CLA	C3B-CAB	2.46	1.52	1.47
21	P	511	CLA	O2D-CED	-2.46	1.39	1.45
21	P	507	CLA	O2D-CED	-2.46	1.39	1.45
21	P	506	CLA	C3B-CAB	2.45	1.52	1.47
21	C	506	CLA	O2D-CED	-2.45	1.39	1.45
21	C	512	CLA	O2D-CED	-2.45	1.39	1.45
21	D	403	CLA	C3B-CAB	2.45	1.52	1.47
21	C	502	CLA	O2D-CED	-2.45	1.39	1.45
21	Q	404	CLA	O2D-CED	-2.45	1.39	1.45
21	N	607	CLA	C3B-CAB	2.45	1.52	1.47
21	C	503	CLA	O2D-CED	-2.45	1.39	1.45
21	P	508	CLA	O2D-CED	-2.45	1.39	1.45
21	N	605	CLA	C3B-CAB	2.45	1.52	1.47
21	B	606	CLA	C3B-CAB	2.45	1.52	1.47
21	G	402	CLA	O2D-CED	-2.45	1.39	1.45
21	P	510	CLA	O2D-CED	-2.45	1.39	1.45
21	G	402	CLA	O2A-C1	-2.45	1.39	1.46
21	B	611	CLA	C3B-CAB	2.45	1.52	1.47
21	D	403	CLA	O2D-CED	-2.45	1.39	1.45
21	N	619	CLA	O2D-CED	-2.44	1.39	1.45
21	P	502	CLA	C3B-CAB	2.44	1.52	1.47
21	N	612	CLA	O2D-CED	-2.44	1.39	1.45
21	C	512	CLA	C3B-CAB	2.44	1.52	1.47
21	C	501	CLA	O2D-CED	-2.44	1.39	1.45
21	N	605	CLA	O2D-CED	-2.44	1.39	1.45
23	D	404	PL9	C28-C29	2.44	1.38	1.33
21	N	614	CLA	O2D-CED	-2.44	1.39	1.45
21	N	607	CLA	O2A-CGA	2.44	1.40	1.33
21	N	617	CLA	C3B-CAB	2.43	1.52	1.47
21	B	611	CLA	C3B-C2B	-2.43	1.37	1.40
21	C	511	CLA	O2D-CED	-2.43	1.39	1.45
21	Q	404	CLA	C3B-CAB	2.43	1.52	1.47
21	C	502	CLA	C3B-CAB	2.43	1.52	1.47
21	C	504	CLA	C3B-CAB	2.43	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	616	CLA	O2D-CED	-2.43	1.39	1.45
21	C	513	CLA	C3B-CAB	2.43	1.52	1.47
21	B	606	CLA	C1A-CHA	-2.43	1.33	1.43
21	P	503	CLA	O2D-CED	-2.43	1.39	1.45
21	N	615	CLA	O2D-CED	-2.43	1.39	1.45
21	G	406	CLA	O2D-CED	-2.42	1.39	1.45
21	N	607	CLA	O2D-CED	-2.42	1.39	1.45
21	N	613	CLA	C3B-CAB	2.42	1.52	1.47
21	B	604	CLA	C3B-CAB	2.42	1.52	1.47
23	Q	405	PL9	C28-C29	2.42	1.38	1.33
21	B	605	CLA	O2D-CED	-2.42	1.39	1.45
21	B	605	CLA	C3B-CAB	2.42	1.52	1.47
21	C	506	CLA	C3B-C2B	-2.42	1.37	1.40
21	P	512	CLA	O2D-CED	-2.42	1.39	1.45
21	P	505	CLA	O2D-CED	-2.42	1.39	1.45
21	B	607	CLA	C3B-CAB	2.42	1.52	1.47
21	B	611	CLA	O2D-CED	-2.42	1.39	1.45
21	D	401	CLA	C1A-CHA	-2.41	1.33	1.43
21	G	404	CLA	O2D-CED	-2.41	1.39	1.45
22	G	405	PHO	C3B-C4B	2.41	1.48	1.43
21	A	401	CLA	C3B-CAB	2.41	1.52	1.47
21	A	401	CLA	O2A-C1	-2.41	1.39	1.46
21	B	606	CLA	O2D-CED	-2.41	1.39	1.45
21	A	405	CLA	O2D-CED	-2.41	1.39	1.45
21	B	607	CLA	O2A-CGA	2.41	1.40	1.33
21	B	603	CLA	O2D-CED	-2.41	1.39	1.45
21	A	403	CLA	C3B-CAB	2.41	1.52	1.47
21	N	609	CLA	C3B-CAB	2.40	1.52	1.47
21	N	606	CLA	O2D-CED	-2.40	1.39	1.45
21	B	603	CLA	C5-C3	2.40	1.56	1.51
21	B	608	CLA	C3B-CAB	2.40	1.52	1.47
21	C	505	CLA	O2D-CED	-2.40	1.39	1.45
21	C	513	CLA	O2D-CED	-2.40	1.39	1.45
21	N	620	CLA	C3B-CAB	2.39	1.52	1.47
21	B	612	CLA	C1A-CHA	-2.39	1.33	1.43
21	P	504	CLA	C1A-CHA	-2.39	1.33	1.43
21	N	617	CLA	C3B-C2B	-2.39	1.37	1.40
21	N	611	CLA	C5-C3	2.39	1.56	1.51
21	C	509	CLA	C3B-CAB	2.39	1.52	1.47
21	B	610	CLA	O2D-CED	-2.39	1.39	1.45
21	P	504	CLA	O2A-CGA	2.39	1.40	1.33
21	B	609	CLA	C3B-CAB	2.39	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	402	CLA	C3B-CAB	2.39	1.52	1.47
21	G	403	CLA	C3B-C2B	-2.39	1.37	1.40
21	N	620	CLA	O2D-CED	-2.38	1.39	1.45
21	Q	402	CLA	C1A-CHA	-2.38	1.33	1.43
21	A	401	CLA	O2D-CED	-2.38	1.39	1.45
21	G	404	CLA	C3B-CAB	2.38	1.52	1.47
24	C	516	DGD	O5D-C1E	2.38	1.44	1.40
24	P	519	DGD	O5D-C1E	2.38	1.44	1.40
21	N	609	CLA	O2D-CED	-2.38	1.39	1.45
21	N	616	CLA	C1A-CHA	-2.38	1.33	1.43
21	P	502	CLA	O2D-CED	-2.38	1.39	1.45
21	B	607	CLA	C5-C3	2.38	1.56	1.51
21	C	505	CLA	C3B-CAB	2.37	1.52	1.47
21	C	501	CLA	C3B-CAB	2.37	1.52	1.47
21	A	402	CLA	C3B-C2B	-2.37	1.37	1.40
21	P	505	CLA	O2A-C1	-2.37	1.39	1.46
21	C	504	CLA	O2A-CGA	2.37	1.40	1.33
21	P	504	CLA	C5-C3	2.37	1.56	1.51
21	B	614	CLA	C5-C3	2.37	1.56	1.51
21	B	603	CLA	C3B-CAB	2.37	1.52	1.47
21	N	611	CLA	C3B-CAB	2.37	1.52	1.47
21	N	618	CLA	C5-C3	2.37	1.56	1.51
21	P	501	CLA	C3B-CAB	2.37	1.52	1.47
21	B	616	CLA	C3B-CAB	2.37	1.52	1.47
21	N	616	CLA	C3B-C2B	-2.36	1.37	1.40
21	C	504	CLA	C1A-CHA	-2.36	1.33	1.43
21	N	614	CLA	C3B-CAB	2.36	1.52	1.47
21	N	615	CLA	C3B-C2B	-2.36	1.37	1.40
21	B	613	CLA	C3B-C2B	-2.36	1.37	1.40
21	N	607	CLA	C5-C3	2.36	1.56	1.51
21	B	610	CLA	C3B-CAB	2.36	1.52	1.47
21	C	509	CLA	C1A-CHA	-2.36	1.33	1.43
22	A	404	PHO	C3B-C4B	2.36	1.48	1.43
21	B	608	CLA	C1A-CHA	-2.36	1.33	1.43
21	N	612	CLA	C1A-CHA	-2.36	1.33	1.43
21	N	615	CLA	O2A-C1	-2.36	1.39	1.46
21	N	610	CLA	O2D-CED	-2.35	1.39	1.45
21	P	513	CLA	C1A-CHA	-2.35	1.33	1.43
21	B	614	CLA	C1A-CHA	-2.35	1.33	1.43
21	C	510	CLA	C1A-CHA	-2.35	1.33	1.43
21	C	510	CLA	O2A-C1	-2.35	1.39	1.46
21	B	611	CLA	O2A-C1	-2.35	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	406	CLA	O2A-C1	-2.35	1.39	1.46
21	B	603	CLA	O2A-CGA	2.34	1.40	1.33
21	N	618	CLA	C1A-CHA	-2.34	1.33	1.43
21	C	505	CLA	O2A-C1	-2.34	1.39	1.46
21	N	620	CLA	C5-C3	2.34	1.56	1.51
21	G	403	CLA	C1A-CHA	-2.34	1.33	1.43
21	C	507	CLA	C3B-C2B	-2.34	1.37	1.40
21	N	607	CLA	C3B-C2B	-2.34	1.37	1.40
21	B	616	CLA	O2A-C1	-2.34	1.39	1.46
21	N	612	CLA	C5-C3	2.34	1.56	1.51
21	B	605	CLA	C1A-CHA	-2.34	1.33	1.43
21	D	401	CLA	C5-C3	2.33	1.56	1.51
21	A	403	CLA	C1A-CHA	-2.33	1.33	1.43
21	P	503	CLA	C1A-CHA	-2.33	1.33	1.43
21	N	617	CLA	O2A-C1	-2.33	1.39	1.46
21	N	616	CLA	C5-C3	2.33	1.56	1.51
21	P	510	CLA	C1A-CHA	-2.33	1.33	1.43
21	B	608	CLA	O2A-CGA	2.33	1.40	1.33
21	B	615	CLA	O2A-C1	-2.33	1.39	1.46
21	G	402	CLA	C3B-C2B	-2.33	1.37	1.40
21	P	505	CLA	C1A-CHA	-2.33	1.33	1.43
21	A	402	CLA	C1B-CHB	-2.33	1.34	1.41
21	N	612	CLA	O2A-CGA	2.32	1.40	1.33
21	B	613	CLA	O2A-C1	-2.32	1.39	1.46
21	N	619	CLA	O2A-C1	-2.32	1.39	1.46
21	C	513	CLA	C1A-CHA	-2.32	1.33	1.43
21	P	501	CLA	C5-C3	2.32	1.56	1.51
21	C	511	CLA	C3B-C2B	-2.32	1.37	1.40
21	N	614	CLA	C1A-CHA	-2.32	1.33	1.43
23	J	101	PL9	C28-C29	2.32	1.39	1.32
21	P	506	CLA	C1A-CHA	-2.32	1.33	1.43
21	B	614	CLA	O2A-CGA	2.32	1.40	1.33
21	C	502	CLA	C1A-CHA	-2.31	1.33	1.43
21	N	611	CLA	C1A-CHA	-2.31	1.33	1.43
21	P	501	CLA	C3B-C2B	-2.31	1.37	1.40
21	N	613	CLA	O2A-C1	-2.31	1.39	1.46
21	C	508	CLA	O2A-C1	-2.31	1.39	1.46
21	P	502	CLA	C5-C3	2.31	1.56	1.51
21	C	509	CLA	C3B-C2B	-2.31	1.37	1.40
21	C	503	CLA	C1A-CHA	-2.31	1.33	1.43
21	Q	404	CLA	O2A-CGA	2.31	1.40	1.33
21	B	606	CLA	O2A-C1	-2.31	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	603	CLA	C3B-C2B	-2.31	1.37	1.40
21	A	401	CLA	C3B-C2B	-2.31	1.37	1.40
21	P	508	CLA	O2A-C1	-2.31	1.39	1.46
21	N	608	CLA	C3B-C2B	-2.31	1.37	1.40
21	N	608	CLA	C1A-CHA	-2.31	1.33	1.43
21	N	618	CLA	O2A-CGA	2.31	1.40	1.33
21	P	502	CLA	C3B-C2B	-2.30	1.37	1.40
24	P	518	DGD	O5D-C1E	2.30	1.44	1.40
22	D	402	PHO	C1D-C2D	2.30	1.50	1.45
21	C	502	CLA	C5-C3	2.30	1.56	1.51
21	Q	404	CLA	C1A-CHA	-2.30	1.33	1.43
21	C	506	CLA	C1A-CHA	-2.30	1.33	1.43
21	N	614	CLA	O2A-C1	-2.30	1.39	1.46
21	P	510	CLA	O2A-C1	-2.30	1.39	1.46
21	B	607	CLA	C1A-CHA	-2.30	1.33	1.43
21	D	403	CLA	C1A-CHA	-2.30	1.33	1.43
21	C	510	CLA	C3B-C2B	-2.30	1.37	1.40
21	N	615	CLA	CMB-C2B	-2.30	1.46	1.51
21	N	615	CLA	C1A-CHA	-2.30	1.33	1.43
23	b	101	PL9	C28-C29	2.30	1.39	1.32
21	Q	402	CLA	C5-C3	2.30	1.56	1.51
21	P	506	CLA	C3B-C2B	-2.30	1.37	1.40
21	B	608	CLA	C5-C3	2.30	1.56	1.51
21	B	604	CLA	C1A-CHA	-2.29	1.33	1.43
21	C	511	CLA	O2A-C1	-2.29	1.39	1.46
21	N	609	CLA	C1A-CHA	-2.29	1.33	1.43
24	W	102	DGD	O5D-C1E	2.29	1.44	1.40
21	C	501	CLA	C5-C3	2.29	1.56	1.51
24	N	602	DGD	O5D-C1E	2.28	1.44	1.40
21	N	610	CLA	C5-C3	2.28	1.56	1.51
21	B	602	CLA	C1A-CHA	-2.28	1.33	1.43
21	C	512	CLA	O2A-CGA	2.28	1.40	1.33
21	D	401	CLA	O2A-CGA	2.28	1.40	1.33
21	P	512	CLA	C1A-CHA	-2.28	1.33	1.43
21	A	402	CLA	C1A-CHA	-2.28	1.33	1.43
21	B	613	CLA	C1A-CHA	-2.28	1.33	1.43
21	N	607	CLA	C1B-CHB	-2.28	1.34	1.41
21	C	508	CLA	C1A-CHA	-2.28	1.33	1.43
21	B	616	CLA	C5-C3	2.28	1.56	1.51
21	A	405	CLA	O2A-C1	-2.28	1.39	1.46
21	C	508	CLA	C5-C3	2.28	1.56	1.51
21	N	616	CLA	O2A-CGA	2.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	404	CLA	O2A-C1	-2.28	1.39	1.46
21	N	605	CLA	C1A-CHA	-2.28	1.33	1.43
21	P	509	CLA	C1A-CHA	-2.28	1.33	1.43
21	C	507	CLA	O2A-C1	-2.27	1.39	1.46
21	B	612	CLA	O2A-C1	-2.27	1.39	1.46
21	C	507	CLA	C1A-CHA	-2.27	1.33	1.43
21	P	512	CLA	O2A-CGA	2.27	1.40	1.33
21	P	512	CLA	C5-C3	2.27	1.56	1.51
21	P	513	CLA	O2A-C1	-2.27	1.39	1.46
21	N	610	CLA	C1A-CHA	-2.27	1.33	1.43
21	P	508	CLA	C1A-CHA	-2.27	1.33	1.43
21	N	613	CLA	C1A-CHA	-2.27	1.33	1.43
21	N	606	CLA	C1B-CHB	-2.27	1.34	1.41
21	P	509	CLA	O2A-C1	-2.27	1.39	1.46
21	B	609	CLA	O2A-C1	-2.27	1.39	1.46
21	P	507	CLA	O2A-C1	-2.27	1.39	1.46
24	B	628	DGD	O5D-C1E	2.27	1.44	1.40
21	B	610	CLA	C1A-CHA	-2.27	1.33	1.43
24	C	517	DGD	O5D-C1E	2.27	1.44	1.40
21	N	605	CLA	C5-C3	2.27	1.56	1.51
21	N	606	CLA	O2A-C1	-2.27	1.39	1.46
21	P	501	CLA	O2A-CGA	2.27	1.40	1.33
21	N	620	CLA	O2A-C1	-2.26	1.39	1.46
21	B	609	CLA	C1A-CHA	-2.26	1.33	1.43
21	C	501	CLA	O2A-CGA	2.26	1.39	1.33
21	P	502	CLA	C1A-CHA	-2.26	1.33	1.43
21	C	501	CLA	C3B-C2B	-2.26	1.37	1.40
21	B	602	CLA	O2A-C1	-2.26	1.39	1.46
21	B	615	CLA	C1A-CHA	-2.26	1.33	1.43
21	A	402	CLA	C5-C3	2.26	1.56	1.51
24	C	518	DGD	O3G-C1D	2.26	1.44	1.40
21	C	509	CLA	O2A-C1	-2.26	1.39	1.46
21	Q	404	CLA	C5-C3	2.26	1.56	1.51
21	P	509	CLA	C5-C3	2.26	1.56	1.51
21	P	502	CLA	O2D-CGD	2.26	1.38	1.33
21	B	601	CLA	O2A-C1	-2.26	1.39	1.46
21	A	403	CLA	O2A-C1	-2.26	1.39	1.46
21	P	506	CLA	O2A-C1	-2.26	1.39	1.46
21	B	612	CLA	C5-C3	2.26	1.56	1.51
21	B	601	CLA	C5-C3	2.26	1.56	1.51
21	D	403	CLA	C5-C3	2.26	1.56	1.51
21	B	604	CLA	C3B-C2B	-2.25	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	406	CLA	C1A-CHA	-2.25	1.33	1.43
21	N	612	CLA	C3B-C2B	-2.25	1.37	1.40
21	C	503	CLA	O2A-CGA	2.25	1.39	1.33
21	N	608	CLA	C5-C3	2.25	1.56	1.51
21	A	402	CLA	O2A-C1	-2.25	1.39	1.46
21	N	605	CLA	O2A-C1	-2.25	1.39	1.46
21	G	403	CLA	C1B-CHB	-2.25	1.34	1.41
21	B	610	CLA	O2A-C1	-2.25	1.39	1.46
21	B	605	CLA	O2A-CGA	2.25	1.39	1.33
21	A	403	CLA	C5-C3	2.25	1.56	1.51
21	A	401	CLA	C5-C3	2.25	1.56	1.51
21	N	610	CLA	O2A-C1	-2.25	1.39	1.46
21	B	605	CLA	O2A-C1	-2.25	1.39	1.46
21	A	405	CLA	C1A-CHA	-2.25	1.33	1.43
21	P	502	CLA	O2A-CGA	2.25	1.39	1.33
21	C	504	CLA	C5-C3	2.25	1.56	1.51
21	N	611	CLA	C3B-C2B	-2.24	1.37	1.40
21	A	405	CLA	C1B-CHB	-2.24	1.34	1.41
21	B	601	CLA	C1A-CHA	-2.24	1.33	1.43
21	G	403	CLA	O2A-C1	-2.24	1.39	1.46
21	Q	404	CLA	C3B-C2B	-2.24	1.37	1.40
21	P	513	CLA	C5-C3	2.24	1.55	1.51
21	G	404	CLA	C1A-CHA	-2.24	1.33	1.43
22	G	405	PHO	C1D-C2D	2.24	1.50	1.45
23	A	406	PL9	C28-C29	2.24	1.38	1.33
21	C	506	CLA	O2A-C1	-2.24	1.39	1.46
21	C	505	CLA	C1A-CHA	-2.24	1.33	1.43
21	N	616	CLA	C4B-NB	2.24	1.37	1.35
21	N	617	CLA	C1A-CHA	-2.24	1.33	1.43
21	N	609	CLA	O2A-CGA	2.24	1.39	1.33
21	C	511	CLA	C1A-CHA	-2.24	1.33	1.43
21	C	507	CLA	C1B-CHB	-2.23	1.34	1.41
21	B	604	CLA	C5-C3	2.23	1.55	1.51
21	P	510	CLA	C3B-C2B	-2.23	1.37	1.40
21	C	502	CLA	O2A-CGA	2.23	1.39	1.33
21	B	604	CLA	O2A-CGA	2.23	1.39	1.33
21	G	403	CLA	MG-NC	-2.23	2.01	2.06
21	B	616	CLA	C3B-C2B	-2.23	1.37	1.40
21	P	503	CLA	O2A-CGA	2.23	1.39	1.33
21	N	614	CLA	C5-C3	2.23	1.55	1.51
21	A	405	CLA	C5-C3	2.23	1.55	1.51
21	G	402	CLA	C5-C3	2.23	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	503	CLA	C5-C3	2.23	1.55	1.51
21	C	513	CLA	O2A-CGA	2.23	1.39	1.33
21	N	606	CLA	C3B-C2B	-2.23	1.37	1.40
21	N	610	CLA	C1B-CHB	-2.23	1.34	1.41
21	N	608	CLA	O2A-C1	-2.23	1.39	1.46
21	C	501	CLA	C1A-CHA	-2.23	1.33	1.43
21	B	611	CLA	CMB-C2B	-2.23	1.47	1.51
21	B	604	CLA	O2A-C1	-2.22	1.39	1.46
21	A	403	CLA	O2A-CGA	2.22	1.39	1.33
21	B	612	CLA	C3B-C2B	-2.22	1.37	1.40
21	D	403	CLA	O2A-C1	-2.22	1.39	1.46
21	A	401	CLA	O2D-CGD	2.22	1.38	1.33
23	G	407	PL9	C28-C29	2.22	1.38	1.33
21	B	615	CLA	C3B-C2B	-2.22	1.37	1.40
21	P	507	CLA	C3B-C2B	-2.22	1.37	1.40
21	C	513	CLA	C5-C3	2.22	1.55	1.51
21	D	403	CLA	O2A-CGA	2.22	1.39	1.33
21	N	609	CLA	O2D-CGD	2.22	1.38	1.33
21	P	511	CLA	O2A-C1	-2.22	1.39	1.46
21	B	603	CLA	C1B-CHB	-2.22	1.34	1.41
21	N	613	CLA	C5-C3	2.22	1.55	1.51
21	B	607	CLA	C1B-CHB	-2.22	1.34	1.41
21	A	402	CLA	MG-NC	-2.22	2.01	2.06
21	B	609	CLA	O2D-CGD	2.22	1.38	1.33
21	N	609	CLA	O2A-C1	-2.22	1.39	1.46
21	C	501	CLA	O2A-C1	-2.22	1.39	1.46
21	G	403	CLA	C5-C3	2.22	1.55	1.51
21	N	606	CLA	C1A-CHA	-2.22	1.33	1.43
21	P	509	CLA	C3B-C2B	-2.22	1.37	1.40
22	Q	403	PHO	C1D-C2D	2.22	1.50	1.45
21	B	607	CLA	C3B-C2B	-2.22	1.37	1.40
21	P	513	CLA	O2A-CGA	2.21	1.39	1.33
21	C	503	CLA	O2A-C1	-2.21	1.39	1.46
21	N	620	CLA	O2A-CGA	2.21	1.39	1.33
21	N	615	CLA	C5-C3	2.21	1.55	1.51
22	Q	403	PHO	C1A-NA	-2.21	1.33	1.37
21	B	615	CLA	C5-C3	2.21	1.55	1.51
21	N	609	CLA	C1B-CHB	-2.21	1.34	1.41
21	G	402	CLA	C1B-CHB	-2.21	1.34	1.41
21	C	512	CLA	C1A-CHA	-2.21	1.33	1.43
21	B	616	CLA	C1A-CHA	-2.21	1.33	1.43
21	N	608	CLA	O2A-CGA	2.21	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	611	CLA	C5-C3	2.21	1.55	1.51
21	N	606	CLA	O2A-CGA	2.21	1.39	1.33
21	B	602	CLA	O2A-CGA	2.21	1.39	1.33
21	B	605	CLA	MG-NC	-2.21	2.01	2.06
21	A	401	CLA	C1B-CHB	-2.21	1.34	1.41
21	B	610	CLA	C5-C3	2.21	1.55	1.51
21	P	503	CLA	O2A-C1	-2.21	1.39	1.46
21	P	508	CLA	C1B-CHB	-2.21	1.34	1.41
21	N	606	CLA	C5-C3	2.21	1.55	1.51
21	C	509	CLA	C5-C3	2.21	1.55	1.51
21	P	507	CLA	C1A-CHA	-2.20	1.34	1.43
21	C	513	CLA	O2A-C1	-2.20	1.40	1.46
21	N	620	CLA	C3B-C2B	-2.20	1.37	1.40
21	C	502	CLA	O2A-C1	-2.20	1.40	1.46
21	C	504	CLA	C3B-C2B	-2.20	1.37	1.40
21	N	615	CLA	MG-NC	-2.20	2.01	2.06
21	A	403	CLA	C1B-CHB	-2.20	1.34	1.41
21	G	406	CLA	C5-C3	2.20	1.55	1.51
21	C	509	CLA	O2A-CGA	2.20	1.39	1.33
21	P	507	CLA	C5-C3	2.20	1.55	1.51
21	B	603	CLA	C1A-CHA	-2.20	1.34	1.43
21	B	602	CLA	C1B-CHB	-2.20	1.34	1.41
21	N	606	CLA	O2D-CGD	2.20	1.38	1.33
21	C	512	CLA	C5-C3	2.20	1.55	1.51
21	B	609	CLA	O2A-CGA	2.20	1.39	1.33
21	P	507	CLA	C1B-CHB	-2.20	1.34	1.41
21	G	406	CLA	C1B-CHB	-2.19	1.34	1.41
21	B	602	CLA	C3B-C2B	-2.19	1.37	1.40
21	P	501	CLA	C1A-CHA	-2.19	1.34	1.43
21	B	609	CLA	C5-C3	2.19	1.55	1.51
21	P	511	CLA	C1A-CHA	-2.19	1.34	1.43
21	N	619	CLA	C1A-CHA	-2.19	1.34	1.43
21	G	404	CLA	O2A-CGA	2.19	1.39	1.33
21	B	605	CLA	O2D-CGD	2.19	1.38	1.33
21	Q	402	CLA	O2A-CGA	2.19	1.39	1.33
21	N	611	CLA	C1B-CHB	-2.19	1.34	1.41
21	C	503	CLA	C5-C3	2.19	1.55	1.51
21	B	610	CLA	O2A-CGA	2.19	1.39	1.33
21	N	607	CLA	C1A-CHA	-2.19	1.34	1.43
21	N	605	CLA	C3B-C2B	-2.19	1.37	1.40
21	N	617	CLA	C1B-CHB	-2.19	1.34	1.41
21	B	611	CLA	C1A-CHA	-2.19	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	506	CLA	O2D-CGD	2.19	1.38	1.33
21	A	403	CLA	C3B-C2B	-2.18	1.37	1.40
21	P	513	CLA	C3B-C2B	-2.18	1.37	1.40
22	A	404	PHO	C1D-C2D	2.18	1.50	1.45
21	P	502	CLA	O2A-C1	-2.18	1.40	1.46
21	N	609	CLA	MG-NC	-2.18	2.01	2.06
21	G	404	CLA	C5-C3	2.18	1.55	1.51
21	C	506	CLA	MG-NC	-2.18	2.01	2.06
21	A	402	CLA	O2A-CGA	2.18	1.39	1.33
21	N	617	CLA	O2D-CGD	2.18	1.38	1.33
21	N	612	CLA	C1B-CHB	-2.18	1.34	1.41
21	C	513	CLA	C3B-C2B	-2.18	1.37	1.40
24	B	621	DGD	O5D-C1E	2.18	1.43	1.40
21	A	401	CLA	MG-NC	-2.18	2.01	2.06
21	N	609	CLA	C5-C3	2.18	1.55	1.51
21	P	506	CLA	O2A-CGA	2.17	1.39	1.33
21	N	610	CLA	O2A-CGA	2.17	1.39	1.33
21	N	617	CLA	C5-C3	2.17	1.55	1.51
21	C	507	CLA	C3B-CAB	2.17	1.52	1.47
21	G	403	CLA	O2A-CGA	2.17	1.39	1.33
21	C	506	CLA	C1B-CHB	-2.17	1.35	1.41
21	C	504	CLA	O2A-C1	-2.17	1.40	1.46
21	C	508	CLA	O2A-CGA	2.17	1.39	1.33
21	C	505	CLA	C5-C3	2.17	1.55	1.51
22	A	404	PHO	C4C-C3C	2.17	1.49	1.45
21	C	508	CLA	C1B-CHB	-2.17	1.35	1.41
21	G	404	CLA	C3B-C2B	-2.17	1.37	1.40
21	P	506	CLA	C5-C3	2.17	1.55	1.51
21	Q	402	CLA	O2A-C1	-2.17	1.40	1.46
21	C	507	CLA	C5-C3	2.17	1.55	1.51
21	P	506	CLA	C1B-CHB	-2.17	1.35	1.41
21	N	613	CLA	O2D-CGD	2.17	1.38	1.33
21	D	403	CLA	C1B-CHB	-2.17	1.35	1.41
21	P	509	CLA	O2A-CGA	2.17	1.39	1.33
21	Q	404	CLA	O2A-C1	-2.17	1.40	1.46
21	N	609	CLA	C3B-C2B	-2.17	1.37	1.40
21	B	608	CLA	MG-NC	-2.16	2.01	2.06
21	C	506	CLA	O2D-CGD	2.16	1.38	1.33
21	C	502	CLA	C3B-C2B	-2.16	1.37	1.40
21	B	601	CLA	C3B-C2B	-2.16	1.37	1.40
21	B	608	CLA	C1B-CHB	-2.16	1.35	1.41
21	N	614	CLA	O2A-CGA	2.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	P	508	CLA	MG-NC	-2.16	2.01	2.06
21	B	613	CLA	C5-C3	2.16	1.55	1.51
21	N	613	CLA	O2A-CGA	2.16	1.39	1.33
21	N	620	CLA	C1A-CHA	-2.16	1.34	1.43
21	P	508	CLA	C5-C3	2.16	1.55	1.51
21	B	602	CLA	C5-C3	2.16	1.55	1.51
22	D	402	PHO	C1A-NA	-2.16	1.33	1.37
21	N	616	CLA	O2A-C1	-2.16	1.40	1.46
21	N	618	CLA	O2A-C1	-2.16	1.40	1.46
21	B	608	CLA	C3B-C2B	-2.16	1.37	1.40
26	Q	408	SQD	O6-C1	2.16	1.43	1.40
21	P	501	CLA	O2A-C1	-2.16	1.40	1.46
21	P	511	CLA	C5-C3	2.16	1.55	1.51
21	P	510	CLA	C5-C3	2.15	1.55	1.51
21	B	605	CLA	C5-C3	2.15	1.55	1.51
21	G	404	CLA	C1B-CHB	-2.15	1.35	1.41
21	A	405	CLA	MG-NC	-2.15	2.01	2.06
21	B	612	CLA	O2A-CGA	2.15	1.39	1.33
21	B	616	CLA	O2A-CGA	2.15	1.39	1.33
21	P	511	CLA	O2A-CGA	2.15	1.39	1.33
21	P	508	CLA	C3B-C2B	-2.15	1.37	1.40
21	G	406	CLA	MG-NC	-2.15	2.01	2.06
21	N	612	CLA	MG-NC	-2.15	2.01	2.06
21	P	507	CLA	C3B-CAB	2.15	1.52	1.47
21	N	620	CLA	C1B-CHB	-2.15	1.35	1.41
21	P	513	CLA	C1B-CHB	-2.15	1.35	1.41
21	B	606	CLA	C5-C3	2.15	1.55	1.51
21	B	601	CLA	O2A-CGA	2.15	1.39	1.33
21	C	513	CLA	C1B-CHB	-2.14	1.35	1.41
21	B	611	CLA	C1B-CHB	-2.14	1.35	1.41
21	B	606	CLA	C1B-CHB	-2.14	1.35	1.41
21	C	512	CLA	C1B-CHB	-2.14	1.35	1.41
21	P	508	CLA	O2A-CGA	2.14	1.39	1.33
21	C	511	CLA	C1B-CHB	-2.14	1.35	1.41
21	P	510	CLA	O2A-CGA	2.14	1.39	1.33
21	A	405	CLA	O2D-CGD	2.14	1.38	1.33
21	N	620	CLA	O2D-CGD	2.14	1.38	1.33
21	C	506	CLA	O2A-CGA	2.14	1.39	1.33
21	B	611	CLA	O2D-CGD	2.14	1.38	1.33
26	S	102	SQD	O6-C1	2.14	1.43	1.40
21	D	401	CLA	O2A-C1	-2.14	1.40	1.46
21	B	603	CLA	O2D-CGD	2.14	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	513	CLA	MG-NC	-2.14	2.01	2.06
21	B	614	CLA	C1B-CHB	-2.14	1.35	1.41
21	B	610	CLA	O2D-CGD	2.13	1.38	1.33
21	N	612	CLA	O2D-CGD	2.13	1.38	1.33
21	C	511	CLA	C5-C3	2.13	1.55	1.51
21	P	505	CLA	O2D-CGD	2.13	1.38	1.33
21	A	405	CLA	O2A-CGA	2.13	1.39	1.33
21	P	507	CLA	O2A-CGA	2.13	1.39	1.33
21	P	502	CLA	C1B-CHB	-2.13	1.35	1.41
21	P	504	CLA	C3B-C2B	-2.13	1.37	1.40
21	N	619	CLA	C5-C3	2.13	1.55	1.51
21	P	504	CLA	O2A-C1	-2.13	1.40	1.46
21	N	618	CLA	C1B-CHB	-2.13	1.35	1.41
21	N	616	CLA	CMB-C2B	-2.13	1.47	1.51
21	P	502	CLA	MG-NC	-2.13	2.01	2.06
21	C	506	CLA	C5-C3	2.13	1.55	1.51
21	C	505	CLA	C3B-C2B	-2.13	1.37	1.40
21	C	504	CLA	MG-NC	-2.13	2.01	2.06
21	P	513	CLA	O2D-CGD	2.13	1.38	1.33
21	C	513	CLA	O2D-CGD	2.12	1.38	1.33
21	B	605	CLA	C1B-CHB	-2.12	1.35	1.41
21	B	614	CLA	O2A-C1	-2.12	1.40	1.46
21	C	505	CLA	O2A-CGA	2.12	1.39	1.33
21	N	617	CLA	O2A-CGA	2.12	1.39	1.33
21	C	510	CLA	O2A-CGA	2.12	1.39	1.33
21	Q	404	CLA	C1B-CHB	-2.12	1.35	1.41
21	C	504	CLA	C1B-CHB	-2.12	1.35	1.41
21	P	509	CLA	C1B-CHB	-2.12	1.35	1.41
21	B	610	CLA	C1B-CHB	-2.12	1.35	1.41
21	C	505	CLA	O2D-CGD	2.12	1.38	1.33
21	G	402	CLA	O2D-CGD	2.12	1.38	1.33
21	P	504	CLA	MG-NC	-2.12	2.01	2.06
21	P	512	CLA	C1B-CHB	-2.12	1.35	1.41
21	C	507	CLA	MG-NC	-2.12	2.01	2.06
21	P	512	CLA	O2A-C1	-2.12	1.40	1.46
21	B	616	CLA	C1B-CHB	-2.12	1.35	1.41
21	P	505	CLA	C3B-C2B	-2.12	1.37	1.40
21	C	512	CLA	O2D-CGD	2.12	1.38	1.33
21	N	614	CLA	C1B-CHB	-2.12	1.35	1.41
21	B	608	CLA	O2A-C1	-2.11	1.40	1.46
21	C	507	CLA	O2A-CGA	2.11	1.39	1.33
21	P	503	CLA	O2D-CGD	2.11	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	508	CLA	C3B-C2B	-2.11	1.37	1.40
21	N	615	CLA	O2D-CGD	2.11	1.38	1.33
21	N	615	CLA	C1B-CHB	-2.11	1.35	1.41
21	G	404	CLA	O2D-CGD	2.11	1.38	1.33
21	C	510	CLA	C5-C3	2.11	1.55	1.51
21	C	502	CLA	C1B-CHB	-2.11	1.35	1.41
21	P	505	CLA	O2A-CGA	2.11	1.39	1.33
21	D	403	CLA	C3B-C2B	-2.11	1.37	1.40
21	C	502	CLA	MG-NC	-2.11	2.01	2.06
21	B	613	CLA	O2A-CGA	2.11	1.39	1.33
21	N	615	CLA	O2A-CGA	2.10	1.39	1.33
21	B	615	CLA	O2A-CGA	2.10	1.39	1.33
21	C	509	CLA	C1B-CHB	-2.10	1.35	1.41
21	C	501	CLA	O2D-CGD	2.10	1.38	1.33
21	N	605	CLA	O2A-CGA	2.10	1.39	1.33
21	N	605	CLA	O2D-CGD	2.10	1.38	1.33
21	B	607	CLA	O2A-C1	-2.10	1.40	1.46
21	C	512	CLA	O2A-C1	-2.10	1.40	1.46
21	N	614	CLA	O2D-CGD	2.10	1.38	1.33
21	N	616	CLA	C3B-CAB	2.10	1.52	1.47
21	B	611	CLA	MG-NC	-2.10	2.01	2.06
21	P	509	CLA	O2D-CGD	2.10	1.38	1.33
21	N	612	CLA	O2A-C1	-2.10	1.40	1.46
21	C	511	CLA	O2A-CGA	2.10	1.39	1.33
21	G	406	CLA	C3B-C2B	-2.10	1.37	1.40
21	C	508	CLA	MG-NC	-2.10	2.01	2.06
24	P	519	DGD	O3G-C1D	2.10	1.43	1.40
21	C	511	CLA	O2D-CGD	2.10	1.38	1.33
21	P	511	CLA	C1B-CHB	-2.09	1.35	1.41
21	N	608	CLA	C1B-CHB	-2.09	1.35	1.41
21	P	512	CLA	O2D-CGD	2.09	1.38	1.33
21	B	616	CLA	MG-NC	-2.09	2.01	2.06
21	N	614	CLA	C3B-C2B	-2.09	1.37	1.40
21	B	601	CLA	O2D-CGD	2.09	1.38	1.33
21	B	606	CLA	O2A-CGA	2.09	1.39	1.33
21	P	510	CLA	O2D-CGD	2.09	1.38	1.33
21	P	507	CLA	O2D-CGD	2.09	1.38	1.33
21	N	619	CLA	O2A-CGA	2.09	1.39	1.33
21	G	406	CLA	O2D-CGD	2.09	1.38	1.33
26	B	624	SQD	O6-C1	2.09	1.43	1.40
21	P	512	CLA	C3B-C2B	-2.09	1.37	1.40
21	P	504	CLA	C1B-CHB	-2.09	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	501	CLA	C1B-CHB	-2.09	1.35	1.41
21	B	616	CLA	O2D-CGD	2.09	1.38	1.33
21	P	505	CLA	C5-C3	2.08	1.55	1.51
21	C	511	CLA	MG-NC	-2.08	2.01	2.06
21	N	610	CLA	O2D-CGD	2.08	1.38	1.33
21	C	509	CLA	CMB-C2B	-2.08	1.47	1.51
21	G	402	CLA	MG-NC	-2.08	2.01	2.06
21	B	603	CLA	O2A-C1	-2.08	1.40	1.46
21	P	501	CLA	O2D-CGD	2.08	1.38	1.33
21	C	503	CLA	O2D-CGD	2.08	1.38	1.33
21	G	404	CLA	MG-NC	-2.08	2.01	2.06
21	P	511	CLA	C3B-C2B	-2.08	1.37	1.40
21	B	607	CLA	MG-NC	-2.08	2.01	2.06
21	N	607	CLA	O2D-CGD	2.08	1.38	1.33
21	B	605	CLA	C3B-C2B	-2.08	1.37	1.40
21	C	502	CLA	O2D-CGD	2.08	1.38	1.33
21	N	614	CLA	MG-NC	-2.08	2.01	2.06
22	A	404	PHO	C1A-NA	-2.08	1.33	1.37
21	A	401	CLA	O2A-CGA	2.08	1.39	1.33
21	B	611	CLA	O2A-CGA	2.07	1.39	1.33
21	B	610	CLA	C3B-C2B	-2.07	1.37	1.40
21	B	601	CLA	C1B-CHB	-2.07	1.35	1.41
21	B	613	CLA	O2D-CGD	2.07	1.38	1.33
21	P	513	CLA	MG-NC	-2.07	2.01	2.06
21	B	612	CLA	O2D-CGD	2.07	1.38	1.33
21	B	608	CLA	O2D-CGD	2.07	1.38	1.33
21	P	511	CLA	O2D-CGD	2.07	1.38	1.33
21	N	607	CLA	MG-NC	-2.07	2.01	2.06
21	B	609	CLA	C3B-C2B	-2.07	1.37	1.40
21	P	510	CLA	C1B-CHB	-2.07	1.35	1.41
21	N	611	CLA	O2A-C1	-2.07	1.40	1.46
21	C	509	CLA	O2D-CGD	2.07	1.38	1.33
21	P	505	CLA	C1B-CHB	-2.06	1.35	1.41
21	N	613	CLA	C3B-C2B	-2.06	1.37	1.40
21	N	619	CLA	MG-NC	-2.06	2.01	2.06
21	N	616	CLA	O2D-CGD	2.06	1.38	1.33
21	N	617	CLA	CMB-C2B	-2.06	1.47	1.51
21	B	606	CLA	O2D-CGD	2.06	1.38	1.33
21	D	403	CLA	MG-NC	-2.06	2.01	2.06
21	N	619	CLA	C1B-CHB	-2.06	1.35	1.41
21	C	512	CLA	C3B-C2B	-2.06	1.37	1.40
21	N	608	CLA	MG-NC	-2.05	2.01	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	619	CLA	C3B-C2B	-2.05	1.37	1.40
22	G	405	PHO	C4C-C3C	2.05	1.49	1.45
21	P	501	CLA	C1B-CHB	-2.05	1.35	1.41
21	G	406	CLA	O2A-CGA	2.05	1.39	1.33
21	B	601	CLA	MG-NC	-2.05	2.01	2.06
21	N	618	CLA	O2D-CGD	2.05	1.38	1.33
21	A	403	CLA	MG-NC	-2.05	2.01	2.06
21	B	609	CLA	C1B-CHB	-2.05	1.35	1.41
26	B	627	SQD	O6-C1	2.05	1.43	1.40
21	N	610	CLA	C3B-C2B	-2.05	1.37	1.40
21	C	506	CLA	CMB-C2B	-2.05	1.47	1.51
21	C	503	CLA	MG-NC	-2.05	2.01	2.06
21	C	510	CLA	O2D-CGD	2.05	1.38	1.33
21	A	403	CLA	O2D-CGD	2.05	1.38	1.33
21	P	508	CLA	O2D-CGD	2.05	1.38	1.33
21	P	503	CLA	C1B-CHB	-2.05	1.35	1.41
21	C	507	CLA	O2D-CGD	2.04	1.38	1.33
21	B	613	CLA	C1B-CHB	-2.04	1.35	1.41
21	B	615	CLA	C1B-CHB	-2.04	1.35	1.41
21	N	606	CLA	MG-NC	-2.04	2.01	2.06
21	B	613	CLA	MG-NC	-2.04	2.01	2.06
21	P	509	CLA	CMB-C2B	-2.04	1.47	1.51
21	N	605	CLA	MG-NC	-2.04	2.01	2.06
21	Q	402	CLA	C1B-CHB	-2.04	1.35	1.41
21	D	401	CLA	C1B-CHB	-2.04	1.35	1.41
21	B	612	CLA	CMB-C2B	-2.04	1.47	1.51
21	B	606	CLA	C3B-C2B	-2.04	1.37	1.40
21	A	405	CLA	C3B-C2B	-2.04	1.37	1.40
21	B	612	CLA	C1B-CHB	-2.04	1.35	1.41
34	i	201	HEM	CAA-C2A	2.04	1.55	1.52
21	B	613	CLA	CMB-C2B	-2.04	1.47	1.51
31	I	103	LMT	O1'-C1'	2.04	1.43	1.40
21	C	504	CLA	O2D-CGD	2.04	1.38	1.33
21	B	603	CLA	MG-NC	-2.03	2.01	2.06
21	G	402	CLA	O2A-CGA	2.03	1.39	1.33
21	P	510	CLA	MG-NC	-2.03	2.01	2.06
26	N	601	SQD	O6-C1	2.03	1.43	1.40
21	B	602	CLA	O2D-CGD	2.03	1.38	1.33
21	N	618	CLA	C3B-C2B	-2.03	1.37	1.40
21	N	611	CLA	MG-NC	-2.03	2.01	2.06
21	B	604	CLA	C1B-CHB	-2.03	1.35	1.41
21	C	510	CLA	CMB-C2B	-2.03	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	510	CLA	MG-NC	-2.03	2.01	2.06
21	N	605	CLA	CMB-C2B	-2.02	1.47	1.51
24	G	408	DGD	O3G-C1D	2.02	1.43	1.40
21	B	612	CLA	MG-NC	-2.02	2.01	2.06
22	G	405	PHO	C1A-NA	-2.02	1.33	1.37
21	N	605	CLA	C1B-CHB	-2.02	1.35	1.41
21	P	509	CLA	MG-NC	-2.02	2.01	2.06
21	P	506	CLA	CMB-C2B	-2.02	1.47	1.51
21	N	607	CLA	O2A-C1	-2.02	1.40	1.46
21	N	617	CLA	MG-NC	-2.02	2.01	2.06
21	Q	404	CLA	MG-NC	-2.02	2.01	2.06
21	P	506	CLA	MG-NC	-2.02	2.01	2.06
22	Q	403	PHO	C4C-C3C	2.02	1.48	1.45
21	C	510	CLA	C1B-CHB	-2.02	1.35	1.41
21	B	614	CLA	C3B-C2B	-2.02	1.37	1.40
21	P	507	CLA	MG-NC	-2.02	2.01	2.06
21	N	608	CLA	CMB-C2B	-2.02	1.47	1.51
21	B	615	CLA	O2D-CGD	2.01	1.38	1.33
21	G	403	CLA	CMB-C2B	-2.01	1.47	1.51
21	C	509	CLA	MG-NC	-2.01	2.01	2.06
23	Q	405	PL9	C48-C49	2.01	1.38	1.32
21	B	608	CLA	CMB-C2B	-2.01	1.47	1.51
22	D	402	PHO	C4C-C3C	2.01	1.48	1.45
21	N	613	CLA	C1B-CHB	-2.01	1.35	1.41
21	C	503	CLA	C1B-CHB	-2.01	1.35	1.41
21	C	505	CLA	C1B-CHB	-2.01	1.35	1.41
21	A	402	CLA	O2D-CGD	2.01	1.38	1.33
24	A	407	DGD	O3G-C1D	2.01	1.43	1.40
21	B	603	CLA	CMB-C2B	-2.00	1.47	1.51
21	P	504	CLA	O2D-CGD	2.00	1.38	1.33
21	B	604	CLA	CMB-C2B	-2.00	1.47	1.51

All (1536) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	102	BCR	C32-C1-C6	-13.47	88.45	110.30
30	J	102	BCR	C32-C1-C6	-13.40	88.56	110.30
21	C	505	CLA	C4A-NA-C1A	13.25	112.67	106.71
21	P	505	CLA	C4A-NA-C1A	13.10	112.60	106.71
21	B	611	CLA	C4A-NA-C1A	12.83	112.47	106.71
21	N	609	CLA	C4A-NA-C1A	12.82	112.47	106.71
21	P	501	CLA	C4A-NA-C1A	12.80	112.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	616	CLA	C4A-NA-C1A	12.62	112.38	106.71
21	C	511	CLA	C4A-NA-C1A	12.61	112.38	106.71
21	C	501	CLA	C4A-NA-C1A	12.57	112.36	106.71
21	B	608	CLA	C4A-NA-C1A	12.53	112.34	106.71
21	N	619	CLA	C4A-NA-C1A	12.50	112.33	106.71
21	B	605	CLA	C4A-NA-C1A	12.46	112.31	106.71
21	N	613	CLA	C4A-NA-C1A	12.45	112.30	106.71
21	B	610	CLA	C4A-NA-C1A	12.42	112.29	106.71
21	B	604	CLA	C4A-NA-C1A	12.41	112.28	106.71
21	N	608	CLA	C4A-NA-C1A	12.39	112.28	106.71
21	C	503	CLA	C4A-NA-C1A	12.38	112.27	106.71
21	C	504	CLA	C4A-NA-C1A	12.38	112.27	106.71
21	B	601	CLA	C4A-NA-C1A	12.36	112.26	106.71
21	P	502	CLA	C4A-NA-C1A	12.35	112.26	106.71
21	C	513	CLA	C4A-NA-C1A	12.35	112.26	106.71
21	C	508	CLA	C4A-NA-C1A	12.32	112.25	106.71
21	B	616	CLA	C4A-NA-C1A	12.32	112.24	106.71
21	B	615	CLA	C4A-NA-C1A	12.31	112.24	106.71
21	N	606	CLA	C4A-NA-C1A	12.31	112.24	106.71
21	B	603	CLA	C4A-NA-C1A	12.30	112.24	106.71
21	P	508	CLA	C4A-NA-C1A	12.30	112.23	106.71
21	N	617	CLA	C4A-NA-C1A	12.30	112.23	106.71
21	P	511	CLA	C4A-NA-C1A	12.29	112.23	106.71
21	D	401	CLA	C4A-NA-C1A	12.28	112.23	106.71
21	C	502	CLA	C4A-NA-C1A	12.28	112.23	106.71
21	B	609	CLA	C4A-NA-C1A	12.27	112.22	106.71
21	N	620	CLA	C4A-NA-C1A	12.26	112.22	106.71
21	P	504	CLA	C4A-NA-C1A	12.25	112.21	106.71
21	A	405	CLA	C4A-NA-C1A	12.24	112.21	106.71
21	G	406	CLA	C4A-NA-C1A	12.24	112.21	106.71
21	B	613	CLA	C4A-NA-C1A	12.22	112.20	106.71
21	C	507	CLA	C4A-NA-C1A	12.20	112.19	106.71
21	N	615	CLA	C4A-NA-C1A	12.18	112.18	106.71
21	B	607	CLA	C4A-NA-C1A	12.17	112.18	106.71
21	P	513	CLA	C4A-NA-C1A	12.16	112.17	106.71
21	N	612	CLA	C4A-NA-C1A	12.16	112.17	106.71
21	P	507	CLA	C4A-NA-C1A	12.12	112.15	106.71
21	A	402	CLA	C4A-NA-C1A	12.09	112.14	106.71
21	B	614	CLA	C4A-NA-C1A	12.08	112.14	106.71
21	Q	402	CLA	C4A-NA-C1A	12.06	112.13	106.71
21	D	403	CLA	C4A-NA-C1A	12.04	112.12	106.71
21	N	605	CLA	C4A-NA-C1A	12.03	112.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	404	CLA	C4A-NA-C1A	12.03	112.11	106.71
21	B	602	CLA	C4A-NA-C1A	12.01	112.11	106.71
21	N	614	CLA	C4A-NA-C1A	12.01	112.10	106.71
21	P	509	CLA	C4A-NA-C1A	11.98	112.09	106.71
21	P	510	CLA	C4A-NA-C1A	11.98	112.09	106.71
21	N	611	CLA	C4A-NA-C1A	11.96	112.08	106.71
21	N	610	CLA	C4A-NA-C1A	11.96	112.08	106.71
21	C	512	CLA	C4A-NA-C1A	11.94	112.08	106.71
21	P	503	CLA	C4A-NA-C1A	11.91	112.06	106.71
21	P	506	CLA	C4A-NA-C1A	11.89	112.05	106.71
21	G	404	CLA	C4A-NA-C1A	11.88	112.05	106.71
21	G	402	CLA	C4A-NA-C1A	11.88	112.05	106.71
21	N	607	CLA	C4A-NA-C1A	11.86	112.04	106.71
21	C	510	CLA	C4A-NA-C1A	11.86	112.04	106.71
21	P	512	CLA	C4A-NA-C1A	11.84	112.03	106.71
21	C	506	CLA	C4A-NA-C1A	11.82	112.02	106.71
21	G	403	CLA	C4A-NA-C1A	11.80	112.01	106.71
21	B	612	CLA	C4A-NA-C1A	11.80	112.01	106.71
21	C	509	CLA	C4A-NA-C1A	11.76	111.99	106.71
21	N	618	CLA	C4A-NA-C1A	11.70	111.97	106.71
21	B	606	CLA	C4A-NA-C1A	11.67	111.95	106.71
21	A	403	CLA	C4A-NA-C1A	11.64	111.94	106.71
21	A	401	CLA	C4A-NA-C1A	11.37	111.82	106.71
30	C	514	BCR	C7-C8-C9	9.40	140.43	126.23
22	A	404	PHO	CMD-C2D-C1D	9.25	139.31	125.06
30	P	514	BCR	C7-C8-C9	9.22	140.16	126.23
22	G	405	PHO	CMD-C2D-C1D	9.20	139.23	125.06
22	D	402	PHO	CMD-C2D-C1D	8.86	138.71	125.06
22	Q	403	PHO	CMD-C2D-C1D	8.66	138.40	125.06
30	b	102	BCR	C32-C1-C31	-8.52	82.38	108.53
30	J	102	BCR	C32-C1-C31	-8.51	82.42	108.53
30	T	102	BCR	C7-C8-C9	-6.85	115.89	126.23
30	B	618	BCR	C7-C8-C9	-6.78	115.99	126.23
34	R	101	HEM	CBD-CAD-C3D	-6.69	100.15	112.48
30	b	102	BCR	C31-C1-C6	6.62	121.04	110.30
30	J	102	BCR	C31-C1-C6	6.61	121.02	110.30
30	S	101	BCR	C7-C8-C9	-5.94	117.26	126.23
26	N	601	SQD	O9-S-C6	5.93	113.99	106.94
26	B	627	SQD	O9-S-C6	5.84	113.88	106.94
30	D	405	BCR	C7-C8-C9	-5.79	117.48	126.23
34	V	201	HEM	CBD-CAD-C3D	-5.71	101.96	112.48
34	i	201	HEM	CBD-CAD-C3D	-5.67	102.03	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	101	HEM	CBD-CAD-C3D	-5.59	102.19	112.48
21	A	402	CLA	O2D-CGD-CBD	5.49	121.03	111.27
21	G	403	CLA	O2D-CGD-CBD	5.42	120.90	111.27
21	N	619	CLA	O2D-CGD-CBD	5.26	120.61	111.27
21	D	403	CLA	O2D-CGD-CBD	5.24	120.58	111.27
30	J	102	BCR	C32-C1-C2	-5.23	87.99	108.91
30	b	102	BCR	C32-C1-C2	-5.22	88.04	108.91
21	B	615	CLA	O2D-CGD-CBD	5.22	120.54	111.27
21	Q	404	CLA	O2D-CGD-CBD	5.18	120.47	111.27
24	G	408	DGD	O6E-C5E-C4E	5.17	119.08	109.69
21	P	512	CLA	O2D-CGD-CBD	5.13	120.39	111.27
30	C	514	BCR	C8-C7-C6	5.11	141.57	127.20
30	P	514	BCR	C8-C7-C6	5.09	141.49	127.20
24	A	407	DGD	O6E-C5E-C4E	5.06	118.88	109.69
21	C	511	CLA	O2D-CGD-CBD	5.05	120.25	111.27
21	P	508	CLA	O2D-CGD-CBD	5.01	120.17	111.27
21	G	404	CLA	O2D-CGD-CBD	5.01	120.16	111.27
21	N	614	CLA	O2D-CGD-CBD	5.00	120.16	111.27
21	P	511	CLA	O2D-CGD-CBD	5.00	120.15	111.27
21	C	512	CLA	O2D-CGD-CBD	4.99	120.14	111.27
24	D	408	DGD	O6E-C5E-C4E	4.91	118.60	109.69
21	B	610	CLA	O2D-CGD-CBD	4.87	119.92	111.27
21	A	403	CLA	O2D-CGD-CBD	4.84	119.87	111.27
21	P	510	CLA	O2D-CGD-CBD	4.82	119.83	111.27
24	Q	409	DGD	O6E-C5E-C4E	4.81	118.43	109.69
27	e	102	LMG	O7-C10-C11	4.80	121.84	111.50
22	G	405	PHO	O2D-CGD-CBD	4.79	119.78	111.27
21	B	612	CLA	O2D-CGD-CBD	4.79	119.78	111.27
21	N	620	CLA	O2D-CGD-CBD	4.78	119.76	111.27
24	C	518	DGD	O6E-C5E-C4E	4.75	118.32	109.69
27	M	101	LMG	O7-C10-C11	4.74	121.73	111.50
21	N	616	CLA	O2D-CGD-CBD	4.74	119.70	111.27
23	b	101	PL9	C7-C3-C4	4.71	120.71	116.88
21	P	502	CLA	O2D-CGD-CBD	4.71	119.63	111.27
30	P	514	BCR	C33-C5-C6	-4.70	119.25	124.53
30	b	102	BCR	C15-C14-C13	-4.68	120.63	127.31
21	N	606	CLA	O2D-CGD-CBD	4.64	119.51	111.27
24	A	407	DGD	O2G-C1B-C2B	4.63	121.47	111.50
30	b	102	BCR	C24-C23-C22	-4.61	119.26	126.23
21	B	607	CLA	O2D-CGD-CBD	4.61	119.47	111.27
21	A	405	CLA	O2D-CGD-CBD	4.60	119.45	111.27
30	J	102	BCR	C15-C14-C13	-4.60	120.74	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	519	DGD	O6E-C5E-C4E	4.60	118.05	109.69
21	C	501	CLA	O2D-CGD-CBD	4.59	119.43	111.27
30	b	102	BCR	C20-C21-C22	-4.59	120.75	127.31
21	C	502	CLA	O2D-CGD-CBD	4.59	119.42	111.27
21	C	510	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	Q	405	PL9	C7-C3-C4	4.58	120.60	116.88
21	G	406	CLA	O2D-CGD-CBD	4.57	119.39	111.27
21	P	503	CLA	O2D-CGD-CBD	4.57	119.38	111.27
24	P	517	DGD	O6E-C5E-C4E	4.55	117.96	109.69
27	G	411	LMG	O7-C10-C11	4.55	121.30	111.50
27	A	410	LMG	O7-C10-C11	4.55	121.30	111.50
21	P	513	CLA	O2D-CGD-CBD	4.55	119.35	111.27
27	D	406	LMG	O7-C10-C11	4.53	121.27	111.50
21	G	402	CLA	O2D-CGD-CBD	4.52	119.31	111.27
21	C	507	CLA	O2D-CGD-CBD	4.51	119.28	111.27
21	C	513	CLA	O2D-CGD-CBD	4.50	119.27	111.27
24	C	516	DGD	O6D-C5D-C6D	4.47	115.69	106.67
24	C	518	DGD	O6D-C5D-C6D	4.47	115.68	106.67
21	P	507	CLA	O2D-CGD-CBD	4.46	119.20	111.27
26	Q	408	SQD	O6-C1-C2	4.46	115.27	108.30
27	Q	401	LMG	O7-C10-C11	4.46	121.11	111.50
21	C	503	CLA	O2D-CGD-CBD	4.46	119.19	111.27
30	J	102	BCR	C24-C23-C22	-4.45	119.51	126.23
27	D	412	LMG	O7-C10-C11	4.45	121.09	111.50
27	C	520	LMG	O7-C10-C11	4.45	121.09	111.50
23	J	101	PL9	C7-C3-C4	4.43	120.48	116.88
22	A	404	PHO	O2D-CGD-CBD	4.42	119.12	111.27
24	C	516	DGD	O6E-C5E-C4E	4.41	117.70	109.69
21	P	501	CLA	O2D-CGD-CBD	4.40	119.09	111.27
30	J	102	BCR	C20-C21-C22	-4.40	121.03	127.31
27	Q	406	LMG	O7-C10-C11	4.40	120.98	111.50
21	B	616	CLA	O2D-CGD-CBD	4.39	119.08	111.27
24	G	408	DGD	O2G-C1B-C2B	4.39	120.96	111.50
30	C	514	BCR	C33-C5-C6	-4.39	119.60	124.53
24	N	602	DGD	O2G-C1B-C2B	4.39	120.95	111.50
21	B	602	CLA	O2D-CGD-CBD	4.38	119.06	111.27
21	C	508	CLA	O2D-CGD-CBD	4.38	119.06	111.27
21	N	605	CLA	O2D-CGD-CBD	4.38	119.06	111.27
26	B	624	SQD	O6-C1-C2	4.37	115.13	108.30
24	W	102	DGD	O6E-C5E-C4E	4.37	117.63	109.69
21	P	509	CLA	O2D-CGD-CBD	4.37	119.03	111.27
24	C	517	DGD	C1E-O6E-C5E	4.36	122.25	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	628	DGD	O2G-C1B-C2B	4.36	120.90	111.50
21	C	509	CLA	O2D-CGD-CBD	4.35	118.99	111.27
21	C	504	CLA	O2D-CGD-CBD	4.34	118.98	111.27
21	P	504	CLA	O2D-CGD-CBD	4.33	118.97	111.27
24	P	519	DGD	O6D-C5D-C6D	4.33	115.40	106.67
21	N	611	CLA	O2D-CGD-CBD	4.33	118.96	111.27
24	P	518	DGD	C1E-O6E-C5E	4.33	122.18	113.69
21	B	608	CLA	O2D-CGD-CBD	4.32	118.95	111.27
27	P	521	LMG	O7-C10-C11	4.31	120.79	111.50
21	A	401	CLA	O2D-CGD-CBD	4.29	118.90	111.27
24	P	517	DGD	O6D-C5D-C6D	4.29	115.33	106.67
24	B	621	DGD	O6E-C5E-C4E	4.29	117.48	109.69
21	N	612	CLA	O2D-CGD-CBD	4.27	118.86	111.27
24	B	621	DGD	O6D-C5D-C6D	4.25	115.25	106.67
27	Q	407	LMG	O7-C10-C11	4.25	120.67	111.50
24	P	518	DGD	O6E-C5E-C4E	4.25	117.41	109.69
30	J	102	BCR	C2-C1-C6	4.23	116.99	110.48
23	G	407	PL9	C7-C3-C4	4.23	120.31	116.88
24	W	102	DGD	O6D-C5D-C6D	4.22	115.19	106.67
24	C	517	DGD	O6E-C5E-C4E	4.17	117.27	109.69
30	T	102	BCR	C28-C27-C26	-4.16	106.64	114.08
30	B	618	BCR	C28-C27-C26	-4.14	106.69	114.08
30	T	103	BCR	C24-C23-C22	-4.13	119.99	126.23
21	N	618	CLA	O2D-CGD-CBD	4.13	118.61	111.27
24	N	602	DGD	C1E-O6E-C5E	4.12	121.78	113.69
24	A	407	DGD	O6D-C5D-C6D	4.12	114.98	106.67
30	b	102	BCR	C2-C1-C6	4.12	116.82	110.48
21	B	606	CLA	O2D-CGD-CBD	4.12	118.58	111.27
27	D	407	LMG	O7-C10-C11	4.11	120.36	111.50
24	G	408	DGD	O6D-C5D-C6D	4.11	114.96	106.67
24	B	628	DGD	C1E-O6E-C5E	4.10	121.75	113.69
21	B	601	CLA	O2D-CGD-CBD	4.10	118.56	111.27
30	P	516	BCR	C7-C8-C9	-4.10	120.04	126.23
22	A	404	PHO	C3D-C2D-C1D	-4.09	99.91	105.87
21	C	506	CLA	O2D-CGD-CBD	4.09	118.54	111.27
22	G	405	PHO	C3D-C2D-C1D	-4.08	99.93	105.87
30	P	516	BCR	C28-C27-C26	-4.06	106.82	114.08
21	B	614	CLA	O2D-CGD-CBD	4.05	118.46	111.27
30	K	101	BCR	C38-C26-C25	-4.04	119.99	124.53
30	C	515	BCR	C28-C27-C26	-4.04	106.86	114.08
26	G	410	SQD	O9-S-C6	4.04	111.74	106.94
22	Q	403	PHO	C3D-C2D-C1D	-4.03	100.00	105.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	505	CLA	O2D-CGD-CBD	4.02	118.40	111.27
21	N	617	CLA	O2D-CGD-CBD	4.01	118.39	111.27
21	N	609	CLA	O2D-CGD-CBD	4.01	118.39	111.27
30	Z	101	BCR	C15-C14-C13	-4.00	121.60	127.31
21	C	505	CLA	O2D-CGD-CBD	4.00	118.37	111.27
23	A	406	PL9	C7-C3-C4	3.99	120.12	116.88
24	C	517	DGD	O2G-C1B-C2B	3.98	120.07	111.50
22	D	402	PHO	C3D-C2D-C1D	-3.98	100.08	105.87
30	W	101	BCR	C33-C5-C6	-3.97	120.07	124.53
27	Q	407	LMG	O6-C5-C6	3.96	116.28	106.44
27	D	407	LMG	O6-C5-C6	3.95	116.27	106.44
21	B	603	CLA	O2D-CGD-CBD	3.95	118.29	111.27
21	N	615	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	N	607	CLA	O2D-CGD-CBD	3.94	118.27	111.27
21	B	605	CLA	O2D-CGD-CBD	3.93	118.24	111.27
34	E	101	HEM	CBA-CAA-C2A	-3.89	105.31	112.49
30	c	101	BCR	C38-C26-C25	-3.89	120.16	124.53
26	G	410	SQD	O6-C1-C2	3.88	114.36	108.30
24	P	517	DGD	O2G-C1B-C2B	3.87	119.85	111.50
24	P	518	DGD	O2G-C1B-C2B	3.87	119.84	111.50
30	H	101	BCR	C33-C5-C6	-3.86	120.19	124.53
30	B	620	BCR	C24-C23-C22	-3.85	120.41	126.23
25	A	411	LHG	O7-C7-C8	3.85	119.79	111.50
23	D	404	PL9	C7-C3-C4	3.83	119.99	116.88
26	A	409	SQD	O8-S-C6	3.82	111.83	105.74
25	G	412	LHG	O7-C7-C8	3.82	119.73	111.50
24	W	102	DGD	O2G-C1B-C2B	3.81	119.71	111.50
23	G	407	PL9	C35-C34-C36	3.80	121.66	115.27
24	C	518	DGD	C1E-O6E-C5E	3.79	121.13	113.69
30	P	516	BCR	C38-C26-C25	-3.78	120.28	124.53
23	A	406	PL9	C25-C24-C26	3.78	121.63	115.27
21	B	609	CLA	O2D-CGD-CBD	3.78	117.99	111.27
26	S	102	SQD	O8-S-C6	3.77	111.75	105.74
24	C	516	DGD	O2G-C1B-C2B	3.76	119.61	111.50
26	Q	408	SQD	O47-C7-C8	3.75	119.59	111.50
27	N	622	LMG	O7-C10-C11	3.75	119.59	111.50
30	C	515	BCR	C38-C26-C25	-3.75	120.31	124.53
30	P	515	BCR	C15-C14-C13	-3.75	121.96	127.31
30	P	514	BCR	C1-C6-C7	3.75	126.39	115.78
21	P	506	CLA	O2D-CGD-CBD	3.74	117.91	111.27
23	A	406	PL9	C35-C34-C36	3.73	121.55	115.27
30	B	617	BCR	C7-C8-C9	-3.73	120.60	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	515	BCR	C7-C8-C9	-3.73	120.60	126.23
24	B	621	DGD	O2G-C1B-C2B	3.72	119.53	111.50
30	T	101	BCR	C33-C5-C6	-3.72	120.35	124.53
24	C	517	DGD	C3G-O3G-C1D	-3.72	106.47	113.74
26	G	410	SQD	O47-C7-C8	3.71	119.50	111.50
23	G	407	PL9	C25-C24-C26	3.71	121.51	115.27
24	P	518	DGD	C3G-O3G-C1D	-3.71	106.50	113.74
26	B	624	SQD	O47-C7-C8	3.71	119.49	111.50
22	D	402	PHO	O2D-CGD-CBD	3.70	117.85	111.27
26	A	409	SQD	O47-C7-C8	3.70	119.48	111.50
30	P	514	BCR	C7-C6-C5	-3.69	112.52	121.46
30	P	514	BCR	C15-C14-C13	-3.69	122.05	127.31
30	B	620	BCR	C3-C4-C5	-3.69	107.50	114.08
21	B	613	CLA	O2D-CGD-CBD	3.68	117.80	111.27
21	N	610	CLA	O2D-CGD-CBD	3.67	117.80	111.27
30	b	102	BCR	C7-C8-C9	-3.67	120.69	126.23
27	N	622	LMG	C7-O1-C1	-3.67	106.58	113.74
30	B	618	BCR	C3-C4-C5	-3.66	107.54	114.08
30	S	101	BCR	C28-C27-C26	-3.66	107.54	114.08
26	F	101	SQD	O8-S-C6	3.66	111.57	105.74
21	N	608	CLA	O2D-CGD-CBD	3.65	117.76	111.27
30	C	514	BCR	C1-C6-C7	3.65	126.11	115.78
21	N	613	CLA	O2D-CGD-CBD	3.64	117.75	111.27
30	C	514	BCR	C7-C6-C5	-3.64	112.64	121.46
26	A	409	SQD	O9-S-C6	3.64	111.27	106.94
24	N	602	DGD	O6D-C5D-C6D	3.64	114.02	106.67
24	B	628	DGD	O6D-C5D-C6D	3.63	113.99	106.67
30	c	101	BCR	C3-C4-C5	-3.63	107.60	114.08
26	N	601	SQD	O6-C1-C2	3.63	113.96	108.30
21	Q	402	CLA	O2D-CGD-CBD	3.61	117.69	111.27
27	B	623	LMG	O7-C10-C11	3.61	119.29	111.50
30	D	405	BCR	C28-C27-C26	-3.61	107.64	114.08
30	B	617	BCR	C33-C5-C6	-3.60	120.49	124.53
24	A	407	DGD	C1E-O6E-C5E	3.60	120.75	113.69
26	G	401	SQD	O47-C7-C8	3.59	119.24	111.50
30	T	103	BCR	C3-C4-C5	-3.57	107.71	114.08
22	Q	403	PHO	O2D-CGD-CBD	3.57	117.61	111.27
30	T	101	BCR	C7-C8-C9	-3.56	120.85	126.23
26	S	102	SQD	O47-C7-C8	3.56	119.17	111.50
26	A	414	SQD	O47-C7-C8	3.56	119.17	111.50
27	B	622	LMG	O7-C10-C11	3.56	119.17	111.50
21	D	401	CLA	O2D-CGD-CBD	3.55	117.58	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	T	102	BCR	C3-C4-C5	-3.54	107.75	114.08
24	P	519	DGD	O2G-C1B-C2B	3.54	119.13	111.50
30	C	514	BCR	C15-C14-C13	-3.54	122.26	127.31
24	P	517	DGD	C1E-O6E-C5E	3.54	120.63	113.69
24	C	518	DGD	O2G-C1B-C2B	3.52	119.09	111.50
21	B	611	CLA	O2D-CGD-CBD	3.52	117.52	111.27
24	Q	409	DGD	O2G-C1B-C2B	3.52	119.08	111.50
30	K	101	BCR	C3-C4-C5	-3.52	107.80	114.08
34	R	101	HEM	CBA-CAA-C2A	-3.51	106.00	112.49
27	N	623	LMG	O7-C10-C11	3.51	119.07	111.50
26	N	601	SQD	O47-C7-C8	3.51	119.07	111.50
21	B	604	CLA	O2D-CGD-CBD	3.50	117.49	111.27
24	G	408	DGD	C1E-O6E-C5E	3.49	120.55	113.69
24	N	602	DGD	O6E-C5E-C4E	3.49	116.03	109.69
25	A	408	LHG	O7-C7-C8	3.48	119.00	111.50
24	B	628	DGD	O5D-C6D-C5D	3.45	115.43	109.05
24	D	408	DGD	C3E-C4E-C5E	3.44	116.37	110.24
27	N	622	LMG	O6-C5-C6	3.44	114.98	106.44
23	b	101	PL9	C25-C24-C26	3.43	121.05	115.27
26	A	414	SQD	O9-S-C6	3.43	111.01	106.94
30	B	618	BCR	C38-C26-C25	-3.43	120.68	124.53
26	F	101	SQD	O47-C7-C8	3.41	118.86	111.50
24	W	102	DGD	C3E-C4E-C5E	3.41	116.31	110.24
27	a	102	LMG	O6-C1-O1	-3.40	101.91	109.97
26	B	627	SQD	O47-C7-C8	3.40	118.83	111.50
24	D	408	DGD	O2G-C1B-C2B	3.40	118.82	111.50
30	J	102	BCR	C7-C8-C9	-3.39	121.11	126.23
30	P	514	BCR	C34-C9-C8	3.39	123.41	118.08
23	J	101	PL9	C25-C24-C26	3.38	120.96	115.27
25	G	409	LHG	O7-C7-C8	3.38	118.78	111.50
26	A	409	SQD	O6-C1-C2	3.38	113.57	108.30
24	Q	409	DGD	C3E-C4E-C5E	3.38	116.26	110.24
30	T	102	BCR	C38-C26-C25	-3.37	120.75	124.53
30	P	514	BCR	C16-C17-C18	-3.36	122.51	127.31
27	C	520	LMG	O8-C28-C29	3.36	122.46	111.91
30	a	101	BCR	C38-C26-C25	-3.36	120.76	124.53
22	Q	403	PHO	C4C-C3C-C2C	-3.35	103.07	106.78
26	G	410	SQD	C44-O6-C1	-3.35	107.19	113.74
26	G	410	SQD	O8-S-C6	3.34	111.06	105.74
27	I	102	LMG	O6-C1-O1	-3.34	102.07	109.97
30	C	514	BCR	C3-C4-C5	-3.34	108.12	114.08
24	B	628	DGD	O6E-C5E-C4E	3.33	115.75	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	610	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
24	P	519	DGD	C1E-O6E-C5E	3.33	120.22	113.69
30	P	514	BCR	C3-C4-C5	-3.32	108.14	114.08
30	a	101	BCR	C33-C5-C6	-3.32	120.80	124.53
21	C	506	CLA	C4D-C3D-CAD	-3.32	106.62	108.47
21	N	616	CLA	C2A-C3A-C4A	3.32	107.23	101.87
27	P	520	LMG	O7-C10-C11	3.32	118.65	111.50
24	B	621	DGD	C3E-C4E-C5E	3.32	116.16	110.24
23	D	404	PL9	C25-C24-C26	3.32	120.85	115.27
26	G	401	SQD	O9-S-C6	3.31	110.88	106.94
21	C	512	CLA	O2A-CGA-CBA	3.31	122.30	111.91
27	a	102	LMG	O1-C1-C2	3.31	113.47	108.30
30	Z	101	BCR	C33-C5-C6	-3.30	120.82	124.53
24	D	408	DGD	O6D-C5D-C6D	3.30	113.33	106.67
27	C	519	LMG	O7-C10-C11	3.29	118.60	111.50
23	Q	405	PL9	C25-C24-C26	3.29	120.80	115.27
27	I	102	LMG	O7-C10-C11	3.28	118.58	111.50
21	N	610	CLA	O1D-CGD-CBD	-3.28	117.77	124.48
21	N	618	CLA	C4D-C3D-CAD	-3.28	106.64	108.47
27	D	406	LMG	O6-C5-C6	3.28	114.59	106.44
26	N	601	SQD	C1-C2-C3	-3.27	103.18	110.00
21	P	512	CLA	O2A-CGA-CBA	3.27	122.18	111.91
24	N	602	DGD	O5D-C6D-C5D	3.27	115.10	109.05
21	N	611	CLA	O1D-CGD-CBD	-3.26	117.82	124.48
30	T	103	BCR	C38-C26-C25	-3.26	120.87	124.53
30	J	102	BCR	C29-C30-C25	3.26	115.50	110.48
30	b	102	BCR	C29-C30-C25	3.26	115.50	110.48
30	B	620	BCR	C38-C26-C25	-3.26	120.87	124.53
21	N	613	CLA	C4D-C3D-CAD	-3.26	106.65	108.47
27	a	102	LMG	O7-C10-C11	3.26	118.52	111.50
21	P	506	CLA	C4D-C3D-CAD	-3.25	106.66	108.47
30	C	514	BCR	C34-C9-C8	3.25	123.19	118.08
22	A	404	PHO	C4C-C3C-C2C	-3.24	103.19	106.78
21	B	614	CLA	C4D-C3D-CAD	-3.24	106.66	108.47
30	Z	101	BCR	C24-C23-C22	-3.24	121.34	126.23
30	C	515	BCR	C33-C5-C6	-3.24	120.89	124.53
27	B	622	LMG	O6-C5-C6	3.23	114.48	106.44
23	D	404	PL9	C35-C34-C36	3.23	120.71	115.27
34	R	101	HEM	C1D-C2D-C3D	-3.22	104.75	107.00
27	I	102	LMG	O1-C1-C2	3.21	113.32	108.30
22	D	402	PHO	C4C-C3C-C2C	-3.21	103.23	106.78
30	P	515	BCR	C24-C23-C22	-3.21	121.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	I	101	BCR	C33-C5-C6	-3.20	120.93	124.53
21	D	401	CLA	C2A-C3A-C4A	3.20	107.04	101.87
30	N	621	BCR	C24-C23-C22	-3.20	121.41	126.23
24	N	602	DGD	C3E-C4E-C5E	3.19	115.93	110.24
30	S	101	BCR	C33-C5-C6	-3.19	120.94	124.53
22	G	405	PHO	C4C-C3C-C2C	-3.19	103.25	106.78
21	B	612	CLA	C2A-C3A-C4A	3.19	107.02	101.87
21	B	607	CLA	O1D-CGD-CBD	-3.19	117.96	124.48
30	I	101	BCR	C38-C26-C25	-3.18	120.95	124.53
26	B	627	SQD	O6-C1-C2	3.18	113.27	108.30
21	B	605	CLA	C2A-C3A-C4A	3.18	107.01	101.87
30	I	101	BCR	C3-C4-C5	-3.17	108.41	114.08
24	C	516	DGD	C3E-C4E-C5E	3.17	115.90	110.24
26	Q	408	SQD	O9-S-C6	3.16	110.69	106.94
21	D	403	CLA	C4D-C3D-CAD	-3.16	106.71	108.47
27	R	102	LMG	O6-C5-C6	3.15	114.27	106.44
27	M	101	LMG	C7-O1-C1	-3.15	107.59	113.74
21	B	609	CLA	C4D-C3D-CAD	-3.15	106.72	108.47
23	Q	405	PL9	C35-C34-C36	3.14	120.55	115.27
30	P	515	BCR	C33-C5-C6	-3.14	121.01	124.53
24	Q	409	DGD	C1E-O6E-C5E	3.13	119.83	113.69
22	A	404	PHO	C4A-NA-C1A	3.13	110.67	108.14
30	B	620	BCR	C2-C1-C6	3.13	115.29	110.48
24	Q	409	DGD	O6D-C5D-C6D	3.13	112.97	106.67
27	P	521	LMG	O8-C28-C29	3.12	121.71	111.91
27	Q	406	LMG	O6-C5-C6	3.12	114.20	106.44
21	N	607	CLA	C2A-C1A-CHA	3.12	129.31	123.86
27	B	622	LMG	C7-O1-C1	-3.11	107.66	113.74
26	A	409	SQD	C44-O6-C1	-3.11	107.66	113.74
21	B	603	CLA	C2A-C1A-CHA	3.11	129.30	123.86
21	G	402	CLA	C2A-C3A-C4A	3.10	106.88	101.87
21	B	612	CLA	C1-C2-C3	-3.10	120.68	126.04
22	A	404	PHO	CAC-C3C-C4C	3.10	128.60	125.22
21	Q	402	CLA	C2A-C3A-C4A	3.10	106.87	101.87
21	B	613	CLA	C1-C2-C3	-3.10	120.69	126.04
21	N	620	CLA	C2A-C3A-C4A	3.09	106.86	101.87
21	N	606	CLA	C4D-C3D-CAD	-3.09	106.75	108.47
21	A	401	CLA	C2A-C3A-C4A	3.09	106.85	101.87
21	N	609	CLA	C2A-C3A-C4A	3.08	106.85	101.87
24	P	517	DGD	C3E-C4E-C5E	3.08	115.74	110.24
27	C	519	LMG	O6-C5-C6	3.08	114.10	106.44
24	C	516	DGD	C1E-O6E-C5E	3.08	119.73	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	LMG	O6-C5-C6	3.08	114.09	106.44
21	C	511	CLA	C4D-C3D-CAD	-3.08	106.75	108.47
27	e	102	LMG	C7-O1-C1	-3.08	107.73	113.74
30	J	102	BCR	C35-C13-C14	-3.08	118.61	122.92
21	B	606	CLA	C2A-C3A-C4A	3.07	106.83	101.87
21	B	607	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
30	P	516	BCR	C33-C5-C6	-3.07	121.08	124.53
21	B	607	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
21	B	616	CLA	C2A-C1A-CHA	3.07	129.23	123.86
22	G	405	PHO	C4A-NA-C1A	3.07	110.62	108.14
21	N	620	CLA	C4D-C3D-CAD	-3.07	106.76	108.47
21	B	613	CLA	C2A-C3A-C4A	3.07	106.82	101.87
21	C	510	CLA	C2A-C3A-C4A	3.07	106.82	101.87
22	Q	403	PHO	C4A-NA-C1A	3.06	110.61	108.14
24	P	519	DGD	C3E-C4E-C5E	3.06	115.70	110.24
27	E	102	LMG	O6-C5-C6	3.06	114.04	106.44
30	N	621	BCR	C15-C14-C13	-3.06	122.95	127.31
30	b	102	BCR	C11-C10-C9	-3.05	122.95	127.31
21	B	615	CLA	C4D-C3D-CAD	-3.05	106.77	108.47
22	G	405	PHO	C2C-C1C-NC	3.05	114.40	109.79
21	B	604	CLA	O1D-CGD-CBD	-3.05	118.24	124.48
21	P	510	CLA	C2A-C3A-C4A	3.05	106.79	101.87
21	N	608	CLA	C2A-C3A-C4A	3.05	106.79	101.87
21	P	513	CLA	C2A-C3A-C4A	3.05	106.79	101.87
22	D	402	PHO	C4A-NA-C1A	3.05	110.60	108.14
30	C	514	BCR	C16-C17-C18	-3.05	122.96	127.31
30	K	101	BCR	C2-C1-C6	3.04	115.16	110.48
26	B	624	SQD	O9-S-C6	3.04	110.55	106.94
21	C	504	CLA	C2A-C3A-C4A	3.04	106.78	101.87
21	P	507	CLA	C2A-C1A-CHA	3.04	129.17	123.86
30	T	101	BCR	C15-C14-C13	-3.04	122.98	127.31
21	P	504	CLA	C2A-C3A-C4A	3.04	106.77	101.87
30	B	617	BCR	C15-C14-C13	-3.03	122.98	127.31
24	B	628	DGD	C3E-C4E-C5E	3.03	115.65	110.24
23	G	407	PL9	C22-C23-C24	-3.03	120.36	127.66
27	B	623	LMG	C7-O1-C1	-3.03	107.81	113.74
21	B	611	CLA	O1D-CGD-CBD	-3.03	118.28	124.48
23	D	404	PL9	C22-C23-C24	-3.03	120.36	127.66
21	N	615	CLA	C1-C2-C3	-3.03	120.80	126.04
26	B	624	SQD	C45-O47-C7	-3.03	110.34	117.79
21	B	609	CLA	C2A-C3A-C4A	3.03	106.76	101.87
21	B	611	CLA	C1-C2-C3	-3.03	120.81	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	604	CLA	C2A-C3A-C4A	3.02	106.75	101.87
21	C	513	CLA	C2A-C3A-C4A	3.02	106.75	101.87
21	N	608	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
21	N	620	CLA	C2A-C1A-CHA	3.02	129.14	123.86
27	N	623	LMG	C7-O1-C1	-3.02	107.85	113.74
30	B	618	BCR	C11-C10-C9	-3.02	123.01	127.31
27	C	519	LMG	O6-C1-O1	-3.01	102.84	109.97
23	Q	405	PL9	C22-C23-C24	-3.01	120.41	127.66
21	B	608	CLA	C2A-C3A-C4A	3.01	106.73	101.87
21	C	502	CLA	C4D-C3D-CAD	-3.01	106.79	108.47
30	I	101	BCR	C15-C14-C13	-3.01	123.02	127.31
23	A	406	PL9	C22-C23-C24	-3.00	120.43	127.66
21	N	615	CLA	C2A-C3A-C4A	3.00	106.72	101.87
22	A	404	PHO	O2A-CGA-CBA	3.00	121.33	111.91
22	A	404	PHO	C2C-C1C-NC	3.00	114.32	109.79
27	P	520	LMG	O6-C5-C6	3.00	113.90	106.44
22	Q	403	PHO	C4-C3-C5	3.00	120.32	115.27
21	P	505	CLA	C2A-C3A-C4A	3.00	106.71	101.87
21	P	512	CLA	C2A-C3A-C4A	3.00	106.71	101.87
30	T	103	BCR	C2-C1-C6	3.00	115.09	110.48
26	Q	408	SQD	C45-O47-C7	-2.99	110.42	117.79
30	D	405	BCR	C33-C5-C6	-2.99	121.17	124.53
21	B	615	CLA	C2A-C3A-C4A	2.99	106.70	101.87
21	C	509	CLA	C2A-C3A-C4A	2.99	106.70	101.87
30	B	619	BCR	C33-C5-C6	-2.99	121.17	124.53
21	D	403	CLA	C2A-C3A-C4A	2.99	106.70	101.87
30	b	102	BCR	C31-C1-C2	2.99	120.85	108.91
21	N	613	CLA	C2A-C3A-C4A	2.98	106.69	101.87
22	G	405	PHO	C2D-C1D-ND	2.98	114.29	109.79
21	C	507	CLA	C4D-C3D-CAD	-2.98	106.81	108.47
21	B	616	CLA	C2A-C3A-C4A	2.98	106.69	101.87
21	N	608	CLA	O1D-CGD-CBD	-2.98	118.39	124.48
30	P	515	BCR	C3-C4-C5	-2.98	108.76	114.08
22	Q	403	PHO	C2C-C1C-NC	2.97	114.28	109.79
22	A	404	PHO	CMD-C2D-C3D	-2.97	120.78	127.61
21	P	509	CLA	C2A-C3A-C4A	2.97	106.67	101.87
21	C	512	CLA	C2A-C3A-C4A	2.97	106.67	101.87
30	b	102	BCR	C28-C27-C26	-2.97	108.78	114.08
21	N	610	CLA	C2A-C3A-C4A	2.97	106.66	101.87
24	P	518	DGD	O1G-C1A-C2A	2.97	121.22	111.91
22	Q	403	PHO	CAC-C3C-C4C	2.97	128.46	125.22
21	Q	404	CLA	C4D-C3D-CAD	-2.97	106.81	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	102	DGD	C1E-O6E-C5E	2.97	119.51	113.69
24	C	518	DGD	C3E-C4E-C5E	2.97	115.53	110.24
30	S	101	BCR	C3-C4-C5	-2.96	108.78	114.08
21	Q	404	CLA	C2A-C3A-C4A	2.96	106.66	101.87
22	D	402	PHO	C2C-C1C-NC	2.96	114.26	109.79
21	C	503	CLA	C2A-C3A-C4A	2.96	106.65	101.87
24	G	408	DGD	C1D-O6D-C5D	2.96	119.50	113.69
30	J	102	BCR	C31-C1-C2	2.96	120.74	108.91
21	G	406	CLA	C4D-C3D-CAD	-2.96	106.82	108.47
21	C	507	CLA	C2A-C3A-C4A	2.96	106.64	101.87
24	P	517	DGD	C3G-O3G-C1D	-2.96	107.96	113.74
22	A	404	PHO	C2D-C1D-ND	2.96	114.25	109.79
21	N	612	CLA	C2A-C3A-C4A	2.95	106.64	101.87
21	P	512	CLA	C4D-C3D-CAD	-2.95	106.82	108.47
21	N	605	CLA	C2A-C3A-C4A	2.95	106.64	101.87
21	P	503	CLA	C2A-C3A-C4A	2.95	106.63	101.87
22	G	405	PHO	CMD-C2D-C3D	-2.95	120.83	127.61
21	N	613	CLA	C1-C2-C3	-2.95	120.94	126.04
22	G	405	PHO	O2A-CGA-CBA	2.95	121.16	111.91
21	C	512	CLA	C4D-C3D-CAD	-2.95	106.83	108.47
30	B	617	BCR	C38-C26-C25	-2.94	121.22	124.53
21	N	609	CLA	C4D-C3D-CAD	-2.94	106.83	108.47
21	C	507	CLA	C2A-C1A-CHA	2.94	129.01	123.86
21	P	511	CLA	C4D-C3D-CAD	-2.94	106.83	108.47
30	b	102	BCR	C35-C13-C14	-2.94	118.81	122.92
22	D	402	PHO	C4-C3-C5	2.94	120.21	115.27
21	B	606	CLA	O1D-CGD-CBD	-2.94	118.48	124.48
21	N	618	CLA	O1D-CGD-CBD	-2.93	118.48	124.48
34	E	101	HEM	C1D-C2D-C3D	-2.93	104.96	107.00
27	C	519	LMG	O8-C28-C29	2.93	121.11	111.91
22	Q	403	PHO	C2B-C1B-NB	2.93	114.21	109.79
21	A	403	CLA	C2A-C3A-C4A	2.93	106.60	101.87
21	C	512	CLA	C2A-C1A-CHA	2.93	128.98	123.86
21	N	617	CLA	C1-C2-C3	-2.93	120.98	126.04
27	P	520	LMG	O6-C1-O1	-2.93	103.04	109.97
21	B	601	CLA	C2A-C3A-C4A	2.93	106.60	101.87
21	B	601	CLA	C4D-C3D-CAD	-2.93	106.84	108.47
21	A	402	CLA	C2A-C1A-CHA	2.93	128.98	123.86
21	G	403	CLA	C2A-C1A-CHA	2.93	128.97	123.86
21	N	616	CLA	C1-C2-C3	-2.93	120.98	126.04
22	A	404	PHO	CMB-C2B-C1B	2.92	129.57	125.06
21	B	611	CLA	C2A-C3A-C4A	2.92	106.59	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	627	SQD	C1-C2-C3	-2.92	103.91	110.00
21	C	501	CLA	C2A-C3A-C4A	2.92	106.58	101.87
21	N	619	CLA	C2A-C3A-C4A	2.92	106.58	101.87
24	C	518	DGD	O1G-C1A-C2A	2.92	121.06	111.91
21	B	605	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
21	P	501	CLA	C2A-C3A-C4A	2.91	106.58	101.87
22	G	405	PHO	C4-C3-C5	2.91	120.17	115.27
21	P	501	CLA	C2A-C1A-CHA	2.91	128.95	123.86
21	C	502	CLA	C2A-C3A-C4A	2.91	106.57	101.87
30	N	621	BCR	C33-C5-C6	-2.91	121.26	124.53
24	C	517	DGD	O1G-C1A-C2A	2.91	121.04	111.91
21	P	509	CLA	C4D-C3D-CAD	-2.91	106.85	108.47
30	a	101	BCR	C24-C23-C22	-2.91	121.84	126.23
30	T	103	BCR	C7-C8-C9	-2.91	121.84	126.23
21	D	403	CLA	C2A-C1A-CHA	2.91	128.94	123.86
21	P	508	CLA	C1-C2-C3	-2.91	121.02	126.04
21	B	604	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
21	P	508	CLA	C2A-C3A-C4A	2.90	106.56	101.87
21	N	615	CLA	O1D-CGD-CBD	-2.90	118.54	124.48
30	a	101	BCR	C15-C14-C13	-2.90	123.17	127.31
21	N	619	CLA	C2A-C1A-CHA	2.90	128.93	123.86
30	B	618	BCR	C29-C30-C25	2.90	114.95	110.48
21	P	502	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
27	I	102	LMG	O6-C5-C6	2.90	113.64	106.44
30	B	619	BCR	C24-C23-C22	-2.90	121.86	126.23
21	N	617	CLA	C2A-C3A-C4A	2.89	106.54	101.87
22	Q	403	PHO	C2D-C1D-ND	2.89	114.16	109.79
21	P	512	CLA	C2A-C1A-CHA	2.89	128.92	123.86
21	P	506	CLA	C2A-C3A-C4A	2.89	106.54	101.87
22	D	402	PHO	CAC-C3C-C4C	2.89	128.37	125.22
30	J	102	BCR	C28-C27-C26	-2.89	108.92	114.08
24	P	517	DGD	O5D-C6D-C5D	2.89	114.39	109.05
21	C	505	CLA	C2A-C3A-C4A	2.89	106.54	101.87
21	P	507	CLA	C2A-C3A-C4A	2.89	106.53	101.87
21	N	605	CLA	C4D-C3D-CAD	-2.89	106.86	108.47
21	B	614	CLA	C2A-C3A-C4A	2.88	106.53	101.87
22	D	402	PHO	C2D-C1D-ND	2.88	114.14	109.79
21	P	502	CLA	C2A-C3A-C4A	2.88	106.53	101.87
21	Q	404	CLA	C2A-C1A-CHA	2.88	128.90	123.86
21	C	508	CLA	C2A-C3A-C4A	2.88	106.52	101.87
24	C	517	DGD	O6D-C5D-C6D	2.88	112.47	106.67
30	N	621	BCR	C3-C4-C5	-2.88	108.94	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	619	BCR	C7-C8-C9	-2.88	121.89	126.23
21	B	601	CLA	O2A-CGA-CBA	2.87	120.92	111.91
22	D	402	PHO	C2B-C1B-NB	2.87	114.12	109.79
21	P	507	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
27	N	623	LMG	C8-O7-C10	-2.87	110.73	117.79
30	Z	101	BCR	C3-C4-C5	-2.87	108.95	114.08
27	D	407	LMG	C8-O7-C10	-2.87	110.73	117.79
21	P	510	CLA	C1-C2-C3	-2.87	121.08	126.04
21	N	607	CLA	C4D-C3D-CAD	-2.87	106.87	108.47
21	P	511	CLA	C2A-C1A-CHA	2.87	128.87	123.86
21	C	506	CLA	C2A-C3A-C4A	2.87	106.50	101.87
21	N	614	CLA	C2A-C3A-C4A	2.86	106.50	101.87
21	N	605	CLA	O2A-CGA-CBA	2.86	120.89	111.91
22	G	405	PHO	C2B-C1B-NB	2.86	114.11	109.79
21	N	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
27	P	520	LMG	O8-C28-C29	2.86	120.88	111.91
30	N	621	BCR	C29-C30-C25	2.86	114.88	110.48
21	G	404	CLA	C2A-C3A-C4A	2.86	106.48	101.87
30	c	101	BCR	C10-C11-C12	-2.86	114.31	123.22
21	B	615	CLA	C2A-C1A-CHA	2.85	128.84	123.86
21	C	509	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
21	N	618	CLA	C2A-C3A-C4A	2.85	106.47	101.87
27	G	411	LMG	O6-C5-C6	2.85	113.52	106.44
21	B	606	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
24	P	519	DGD	O1G-C1A-C2A	2.85	120.85	111.91
21	C	501	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
21	N	613	CLA	C2A-C1A-CHA	2.85	128.84	123.86
30	P	514	BCR	C28-C27-C26	-2.85	108.99	114.08
21	C	511	CLA	C2A-C1A-CHA	2.85	128.84	123.86
21	N	614	CLA	C4D-C3D-CAD	-2.85	106.88	108.47
30	a	101	BCR	C3-C4-C5	-2.84	109.00	114.08
23	D	404	PL9	C37-C38-C39	-2.84	120.81	127.66
21	B	616	CLA	C4D-C3D-CAD	-2.84	106.88	108.47
27	B	623	LMG	C8-O7-C10	-2.84	110.79	117.79
21	G	406	CLA	C4-C3-C5	2.84	120.05	115.27
30	B	619	BCR	C15-C14-C13	-2.84	123.25	127.31
27	a	102	LMG	O6-C5-C6	2.84	113.50	106.44
21	N	606	CLA	C2A-C1A-CHA	2.84	128.82	123.86
21	N	611	CLA	C4D-C3D-CAD	-2.84	106.89	108.47
21	G	404	CLA	C2A-C1A-CHA	2.84	128.82	123.86
21	B	601	CLA	C2A-C1A-CHA	2.83	128.81	123.86
21	N	611	CLA	C2A-C1A-CHA	2.83	128.81	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	602	DGD	O1G-C1A-C2A	2.83	120.78	111.91
30	D	405	BCR	C3-C4-C5	-2.83	109.03	114.08
21	P	508	CLA	C4D-C3D-CAD	-2.82	106.89	108.47
30	H	101	BCR	C10-C11-C12	-2.82	114.41	123.22
30	C	514	BCR	C24-C23-C22	-2.82	121.97	126.23
22	G	405	PHO	C1C-C2C-C3C	-2.82	103.27	106.51
21	B	609	CLA	C2A-C1A-CHA	2.82	128.79	123.86
21	N	610	CLA	C4D-C3D-CAD	-2.82	106.90	108.47
21	C	501	CLA	C2A-C1A-CHA	2.82	128.79	123.86
24	P	518	DGD	O6D-C5D-C6D	2.82	112.35	106.67
21	G	403	CLA	C2A-C3A-C4A	2.82	106.42	101.87
21	N	611	CLA	C2A-C3A-C4A	2.81	106.42	101.87
22	G	405	PHO	CAC-C3C-C4C	2.81	128.29	125.22
24	A	407	DGD	C1D-O6D-C5D	2.81	119.21	113.69
21	B	616	CLA	O1D-CGD-CBD	-2.81	118.73	124.48
24	P	518	DGD	O5D-C6D-C5D	2.81	114.25	109.05
21	Q	404	CLA	O1D-CGD-CBD	-2.81	118.74	124.48
30	B	620	BCR	C15-C14-C13	-2.81	123.30	127.31
21	C	506	CLA	C2A-C1A-CHA	2.81	128.77	123.86
30	K	101	BCR	C10-C11-C12	-2.81	114.45	123.22
24	C	517	DGD	O5D-C6D-C5D	2.81	114.24	109.05
30	T	102	BCR	C29-C30-C25	2.80	114.80	110.48
21	B	603	CLA	C2A-C3A-C4A	2.80	106.40	101.87
21	B	612	CLA	C4D-C3D-CAD	-2.80	106.91	108.47
21	C	511	CLA	C2A-C3A-C4A	2.80	106.40	101.87
23	Q	405	PL9	C7-C3-C2	-2.80	119.61	123.30
31	N	603	LMT	O1B-C4'-C3'	2.80	114.73	107.28
26	A	409	SQD	C1-C2-C3	-2.80	104.16	110.00
30	T	103	BCR	C16-C17-C18	-2.80	123.32	127.31
27	Q	407	LMG	C8-O7-C10	-2.80	110.91	117.79
21	C	508	CLA	O1D-CGD-CBD	-2.80	118.77	124.48
21	C	510	CLA	C1-C2-C3	-2.79	121.21	126.04
21	N	610	CLA	C2A-C1A-CHA	2.79	128.74	123.86
23	J	101	PL9	C7-C3-C2	-2.79	119.63	123.30
21	N	616	CLA	O2A-CGA-CBA	2.79	120.67	111.91
23	G	407	PL9	C12-C13-C14	-2.79	120.95	127.66
21	N	607	CLA	C2A-C3A-C4A	2.79	106.37	101.87
23	Q	405	PL9	C37-C38-C39	-2.79	120.95	127.66
21	C	508	CLA	C1-C2-C3	-2.79	121.22	126.04
21	B	609	CLA	C1-C2-C3	-2.79	121.22	126.04
27	P	520	LMG	O1-C1-C2	2.78	112.65	108.30
26	G	401	SQD	O8-S-C6	2.78	110.18	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	405	CLA	C2A-C1A-CHA	2.78	128.73	123.86
22	D	402	PHO	CMD-C2D-C3D	-2.78	121.21	127.61
21	B	610	CLA	C4D-C3D-CAD	-2.78	106.92	108.47
21	B	601	CLA	O1D-CGD-CBD	-2.78	118.79	124.48
30	J	102	BCR	C11-C10-C9	-2.78	123.34	127.31
22	A	404	PHO	C2B-C1B-NB	2.78	113.99	109.79
30	W	101	BCR	C29-C30-C25	2.78	114.76	110.48
30	P	514	BCR	C24-C23-C22	-2.78	122.04	126.23
30	P	516	BCR	C3-C4-C5	-2.78	109.12	114.08
22	G	405	PHO	C4D-ND-C1D	-2.78	101.77	106.76
23	b	101	PL9	C7-C3-C2	-2.78	119.65	123.30
30	B	619	BCR	C29-C30-C25	2.78	114.75	110.48
21	B	603	CLA	O1D-CGD-CBD	-2.78	118.81	124.48
30	T	101	BCR	C28-C27-C26	-2.77	109.12	114.08
21	B	607	CLA	C2A-C3A-C4A	2.77	106.35	101.87
21	A	402	CLA	C2A-C3A-C4A	2.77	106.35	101.87
27	A	410	LMG	O8-C28-C29	2.77	120.61	111.91
21	N	617	CLA	C2A-C1A-CHA	2.77	128.71	123.86
21	P	506	CLA	C2A-C1A-CHA	2.77	128.70	123.86
22	A	404	PHO	C4D-ND-C1D	-2.77	101.78	106.76
21	P	511	CLA	C2A-C3A-C4A	2.77	106.34	101.87
30	C	515	BCR	C15-C14-C13	-2.77	123.36	127.31
21	B	610	CLA	C2A-C3A-C4A	2.77	106.34	101.87
30	B	620	BCR	C7-C8-C9	-2.77	122.06	126.23
21	Q	402	CLA	O2A-CGA-CBA	2.77	120.58	111.91
30	P	516	BCR	C15-C14-C13	-2.76	123.36	127.31
27	A	410	LMG	C8-O7-C10	-2.76	110.99	117.79
21	N	619	CLA	C4D-C3D-CAD	-2.76	106.93	108.47
22	G	405	PHO	CMB-C2B-C1B	2.76	129.32	125.06
23	A	406	PL9	C12-C13-C14	-2.76	121.01	127.66
30	T	101	BCR	C38-C26-C25	-2.76	121.43	124.53
22	D	402	PHO	C4D-ND-C1D	-2.76	101.80	106.76
30	C	514	BCR	C28-C27-C26	-2.76	109.15	114.08
30	T	103	BCR	C15-C14-C13	-2.76	123.37	127.31
22	Q	403	PHO	C3C-C4C-NC	2.76	114.56	110.28
30	D	405	BCR	C24-C23-C22	-2.76	122.07	126.23
24	D	408	DGD	C1E-O6E-C5E	2.76	119.10	113.69
30	W	101	BCR	C10-C11-C12	-2.76	114.62	123.22
21	N	605	CLA	C2A-C1A-CHA	2.75	128.67	123.86
21	B	602	CLA	C2A-C1A-CHA	2.75	128.67	123.86
27	N	622	LMG	C9-C8-C7	-2.75	105.28	111.79
22	A	404	PHO	C1C-C2C-C3C	-2.75	103.35	106.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	607	CLA	C2A-C1A-CHA	2.75	128.67	123.86
30	B	617	BCR	C16-C17-C18	-2.75	123.39	127.31
21	C	512	CLA	O1D-CGD-CBD	-2.75	118.86	124.48
21	N	618	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
30	S	101	BCR	C29-C30-C25	2.75	114.71	110.48
21	B	613	CLA	C2A-C1A-CHA	2.75	128.66	123.86
27	D	412	LMG	O6-C5-C6	2.74	113.26	106.44
22	D	402	PHO	C1C-C2C-C3C	-2.74	103.36	106.51
21	B	602	CLA	C2A-C3A-C4A	2.74	106.30	101.87
21	D	403	CLA	C1-C2-C3	-2.74	121.30	126.04
21	N	619	CLA	C1-C2-C3	-2.74	121.30	126.04
30	B	619	BCR	C3-C4-C5	-2.74	109.18	114.08
30	T	102	BCR	C11-C10-C9	-2.74	123.40	127.31
24	C	516	DGD	O1G-C1A-C2A	2.74	120.50	111.91
23	A	406	PL9	C20-C19-C21	2.74	119.88	115.27
26	G	410	SQD	C1-C2-C3	-2.74	104.30	110.00
21	P	505	CLA	C2A-C1A-CHA	2.74	128.64	123.86
24	B	621	DGD	C1E-O6E-C5E	2.74	119.06	113.69
21	B	606	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
24	W	102	DGD	O1G-C1A-C2A	2.73	120.48	111.91
21	G	406	CLA	C2A-C3A-C4A	2.73	106.28	101.87
21	G	406	CLA	C2A-C1A-CHA	2.73	128.63	123.86
24	C	516	DGD	O5D-C6D-C5D	2.73	114.09	109.05
21	N	606	CLA	C2A-C3A-C4A	2.73	106.27	101.87
27	Q	406	LMG	O8-C28-C29	2.72	120.46	111.91
24	P	517	DGD	O5D-C1E-C2E	2.72	112.56	108.30
21	B	606	CLA	C4-C3-C5	2.72	119.85	115.27
21	B	602	CLA	C4D-C3D-CAD	-2.72	106.95	108.47
22	D	402	PHO	CMB-C2B-C1B	2.72	129.25	125.06
21	D	401	CLA	O2A-CGA-CBA	2.72	120.44	111.91
24	P	517	DGD	O1G-C1A-C2A	2.72	120.44	111.91
21	C	509	CLA	C2A-C1A-CHA	2.72	128.61	123.86
21	P	509	CLA	C2A-C1A-CHA	2.72	128.61	123.86
21	B	603	CLA	C4D-C3D-CAD	-2.71	106.96	108.47
21	B	601	CLA	C1-C2-C3	-2.71	121.35	126.04
21	B	608	CLA	C2A-C1A-CHA	2.71	128.60	123.86
22	Q	403	PHO	C1C-C2C-C3C	-2.71	103.40	106.51
21	C	505	CLA	C2A-C1A-CHA	2.71	128.59	123.86
31	B	629	LMT	O1B-C4'-C3'	2.71	114.48	107.28
21	Q	404	CLA	C1-C2-C3	-2.71	121.36	126.04
27	B	623	LMG	O6-C1-O1	-2.71	103.56	109.97
21	N	610	CLA	C4-C3-C5	2.71	119.82	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	515	BCR	C29-C30-C25	2.70	114.64	110.48
21	A	401	CLA	O1D-CGD-CBD	-2.70	118.95	124.48
30	K	101	BCR	C15-C14-C13	-2.70	123.45	127.31
21	D	401	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
24	B	621	DGD	O1G-C1A-C2A	2.70	120.37	111.91
30	b	102	BCR	C37-C22-C21	-2.69	119.15	122.92
24	C	516	DGD	C3G-O3G-C1D	-2.69	108.48	113.74
21	N	607	CLA	O1D-CGD-CBD	-2.69	118.98	124.48
21	G	402	CLA	C1-C2-C3	-2.69	121.39	126.04
24	B	628	DGD	O1G-C1A-C2A	2.69	120.34	111.91
27	B	623	LMG	O1-C1-C2	2.69	112.50	108.30
21	C	508	CLA	C4D-C3D-CAD	-2.68	106.97	108.47
27	G	411	LMG	C8-O7-C10	-2.68	111.19	117.79
21	A	405	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
30	N	621	BCR	C7-C8-C9	-2.68	122.19	126.23
21	A	405	CLA	C2A-C3A-C4A	2.68	106.19	101.87
21	A	403	CLA	C2A-C1A-CHA	2.68	128.54	123.86
21	G	402	CLA	C4-C3-C5	2.68	119.77	115.27
21	A	401	CLA	C1-C2-C3	-2.68	121.42	126.04
27	N	622	LMG	C8-O7-C10	-2.67	111.21	117.79
30	J	102	BCR	C37-C22-C21	-2.67	119.18	122.92
26	A	414	SQD	O48-C23-C24	2.67	120.28	111.91
30	D	405	BCR	C29-C30-C25	2.67	114.59	110.48
21	N	605	CLA	C1-C2-C3	-2.66	121.44	126.04
22	Q	403	PHO	C4D-ND-C1D	-2.66	101.97	106.76
21	D	401	CLA	C2A-C1A-CHA	2.66	128.51	123.86
21	B	614	CLA	O1D-CGD-CBD	-2.66	119.04	124.48
24	G	408	DGD	O1G-C1A-C2A	2.66	120.26	111.91
27	N	623	LMG	O1-C1-C2	2.66	112.46	108.30
34	i	201	HEM	CAA-CBA-CGA	-2.66	108.21	112.67
21	P	510	CLA	C4-C3-C5	2.66	119.74	115.27
21	N	612	CLA	O2A-CGA-CBA	2.66	120.25	111.91
21	C	508	CLA	C2A-C1A-CHA	2.66	128.50	123.86
30	S	101	BCR	C38-C26-C25	-2.66	121.55	124.53
22	Q	403	PHO	CMB-C2B-C1B	2.65	129.15	125.06
30	B	618	BCR	C35-C13-C12	2.65	122.26	118.08
24	P	518	DGD	C3E-C4E-C5E	2.65	114.97	110.24
21	D	403	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
21	C	504	CLA	C4D-C3D-CAD	-2.65	106.99	108.47
21	G	403	CLA	C1-C2-C3	-2.65	121.46	126.04
27	D	406	LMG	O8-C28-C29	2.65	120.22	111.91
21	Q	402	CLA	CMB-C2B-C1B	-2.65	124.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	404	CLA	C4-C3-C5	2.64	119.72	115.27
23	J	101	PL9	C20-C19-C21	2.64	119.72	115.27
21	B	612	CLA	C2A-C1A-CHA	2.64	128.48	123.86
30	T	102	BCR	C2-C1-C6	2.64	114.55	110.48
21	Q	402	CLA	C2A-C1A-CHA	2.64	128.47	123.86
24	A	407	DGD	O1G-C1A-C2A	2.64	120.19	111.91
21	N	608	CLA	O2A-CGA-CBA	2.64	120.19	111.91
21	G	404	CLA	C4D-C3D-CAD	-2.64	107.00	108.47
21	B	614	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
21	C	510	CLA	C4-C3-C5	2.64	119.71	115.27
21	G	404	CLA	C1-C2-C3	-2.64	121.48	126.04
22	G	405	PHO	C3C-C4C-NC	2.64	114.36	110.28
30	D	405	BCR	C38-C26-C25	-2.63	121.57	124.53
30	C	514	BCR	C38-C26-C25	-2.63	121.58	124.53
21	B	610	CLA	C2A-C1A-CHA	2.63	128.46	123.86
22	D	402	PHO	C3C-C4C-NC	2.63	114.36	110.28
21	P	506	CLA	O2A-CGA-CBA	2.63	120.16	111.91
21	N	612	CLA	C2A-C1A-CHA	2.63	128.46	123.86
23	D	404	PL9	C7-C8-C9	-2.63	122.42	126.79
21	B	615	CLA	C1-C2-C3	-2.63	121.50	126.04
21	P	508	CLA	C2A-C1A-CHA	2.62	128.45	123.86
21	A	402	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
21	P	511	CLA	O2A-CGA-CBA	2.62	120.14	111.91
30	P	516	BCR	C29-C30-C25	2.62	114.52	110.48
30	H	101	BCR	C29-C30-C25	2.62	114.52	110.48
30	c	101	BCR	C2-C1-C6	2.62	114.52	110.48
21	P	501	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
22	Q	403	PHO	CMD-C2D-C3D	-2.62	121.59	127.61
21	B	604	CLA	O2A-CGA-CBA	2.62	120.12	111.91
27	B	622	LMG	C9-C8-C7	-2.61	105.60	111.79
26	Q	408	SQD	C1-C2-C3	-2.61	104.55	110.00
21	G	403	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
21	B	611	CLA	C2A-C1A-CHA	2.61	128.43	123.86
30	B	618	BCR	C21-C20-C19	-2.61	115.06	123.22
24	C	517	DGD	C3E-C4E-C5E	2.61	114.90	110.24
27	Q	401	LMG	O6-C5-C6	2.61	112.93	106.44
23	Q	405	PL9	C12-C13-C14	-2.61	121.37	127.66
30	B	618	BCR	C2-C1-C6	2.61	114.50	110.48
26	N	601	SQD	C3-C4-C5	2.61	114.89	110.24
22	D	402	PHO	O2A-CGA-CBA	2.61	120.08	111.91
21	B	606	CLA	C2A-C1A-CHA	2.60	128.41	123.86
30	T	101	BCR	C16-C17-C18	-2.60	123.60	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	PL9	C36-C34-C33	-2.60	115.86	121.12
30	C	515	BCR	C3-C4-C5	-2.60	109.44	114.08
21	A	405	CLA	C4-C3-C5	2.59	119.64	115.27
30	Z	101	BCR	C20-C21-C22	-2.59	123.61	127.31
23	G	407	PL9	C20-C19-C21	2.59	119.63	115.27
21	C	510	CLA	C4D-C3D-CAD	-2.59	107.03	108.47
21	P	502	CLA	C2A-C1A-CHA	2.59	128.39	123.86
30	N	621	BCR	C28-C27-C26	-2.59	109.46	114.08
30	P	515	BCR	C28-C27-C26	-2.59	109.46	114.08
21	B	604	CLA	C2A-C1A-CHA	2.59	128.38	123.86
22	A	404	PHO	C3C-C4C-NC	2.59	114.29	110.28
23	A	406	PL9	C30-C29-C31	2.58	119.62	115.27
30	T	102	BCR	C21-C20-C19	-2.58	115.15	123.22
30	c	101	BCR	C15-C14-C13	-2.58	123.62	127.31
21	B	612	CLA	O2A-CGA-CBA	2.58	120.01	111.91
21	A	402	CLA	C1-C2-C3	-2.58	121.58	126.04
23	Q	405	PL9	C36-C34-C33	-2.58	115.90	121.12
30	T	101	BCR	C3-C4-C5	-2.58	109.48	114.08
21	B	601	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
27	C	519	LMG	O1-C1-C2	2.58	112.32	108.30
21	N	608	CLA	C1-C2-C3	-2.58	121.59	126.04
21	Q	404	CLA	O2D-CGD-O1D	-2.57	118.80	123.84
21	C	511	CLA	C4-C3-C5	2.57	119.60	115.27
26	G	401	SQD	O48-C23-C24	2.57	119.99	111.91
21	D	403	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
27	G	411	LMG	O8-C28-C29	2.57	119.99	111.91
21	N	609	CLA	C2A-C1A-CHA	2.57	128.35	123.86
22	A	404	PHO	C4-C3-C5	2.57	119.59	115.27
21	B	614	CLA	C2A-C1A-CHA	2.57	128.35	123.86
21	A	403	CLA	C4-C3-C5	2.57	119.59	115.27
21	A	405	CLA	C4D-C3D-CAD	-2.57	107.04	108.47
21	G	402	CLA	C4D-C3D-CAD	-2.56	107.04	108.47
24	A	407	DGD	C3E-C4E-C5E	2.56	114.80	110.24
24	G	408	DGD	O5D-C6D-C5D	2.56	113.78	109.05
21	N	615	CLA	C4D-C3D-CAD	-2.56	107.04	108.47
21	A	401	CLA	C4-C3-C5	2.56	119.57	115.27
21	N	614	CLA	C2A-C1A-CHA	2.55	128.32	123.86
21	P	510	CLA	C2A-C1A-CHA	2.55	128.32	123.86
21	N	615	CLA	C2A-C1A-CHA	2.55	128.31	123.86
21	C	503	CLA	C2A-C1A-CHA	2.55	128.31	123.86
21	C	506	CLA	O2A-CGA-CBA	2.55	119.90	111.91
21	N	608	CLA	C2A-C1A-CHA	2.55	128.31	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	405	PL9	C7-C8-C9	-2.55	122.55	126.79
30	B	617	BCR	C28-C27-C26	-2.55	109.53	114.08
21	N	608	CLA	C4D-C3D-CAD	-2.54	107.05	108.47
21	C	504	CLA	C2A-C1A-CHA	2.54	128.31	123.86
21	P	511	CLA	C4-C3-C5	2.54	119.55	115.27
21	B	610	CLA	O1D-CGD-CBD	-2.54	119.28	124.48
24	A	407	DGD	O5D-C6D-C5D	2.54	113.75	109.05
24	G	408	DGD	C3E-C4E-C5E	2.54	114.77	110.24
27	P	520	LMG	C8-O7-C10	-2.54	111.54	117.79
30	I	101	BCR	C24-C23-C22	-2.54	122.40	126.23
24	B	628	DGD	C3D-C4D-C5D	2.54	114.77	110.24
31	Q	410	LMT	C1B-O1B-C4'	-2.54	111.68	117.96
21	N	616	CLA	C2A-C1A-CHA	2.54	128.29	123.86
30	B	620	BCR	C28-C27-C26	-2.53	109.55	114.08
21	P	503	CLA	C2A-C1A-CHA	2.53	128.29	123.86
24	N	602	DGD	O5D-C1E-C2E	2.53	112.26	108.30
21	B	608	CLA	O2A-CGA-CBA	2.53	119.86	111.91
23	G	407	PL9	C7-C3-C2	-2.53	119.97	123.30
21	N	619	CLA	O2A-CGA-CBA	2.53	119.85	111.91
24	B	628	DGD	O5D-C1E-C2E	2.53	112.25	108.30
21	B	611	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	Z	101	BCR	C28-C27-C26	-2.53	109.57	114.08
21	C	503	CLA	O1D-CGD-CBD	-2.53	119.32	124.48
21	C	502	CLA	C2A-C1A-CHA	2.52	128.27	123.86
27	C	519	LMG	C8-O7-C10	-2.52	111.58	117.79
21	B	609	CLA	CED-O2D-CGD	2.52	121.64	115.94
21	B	603	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
23	D	404	PL9	C12-C13-C14	-2.52	121.59	127.66
30	P	514	BCR	C35-C13-C14	-2.52	119.39	122.92
24	N	602	DGD	C3D-C4D-C5D	2.52	114.73	110.24
21	P	503	CLA	O1D-CGD-CBD	-2.52	119.33	124.48
21	N	616	CLA	C4D-C3D-CAD	-2.52	107.07	108.47
21	Q	402	CLA	C4-C3-C5	2.52	119.51	115.27
21	N	618	CLA	C2A-C1A-CHA	2.52	128.26	123.86
30	N	621	BCR	C38-C26-C25	-2.52	121.70	124.53
23	A	406	PL9	C15-C14-C16	2.51	119.50	115.27
22	Q	403	PHO	O2A-CGA-CBA	2.51	119.80	111.91
21	P	510	CLA	O2A-CGA-CBA	2.51	119.79	111.91
27	N	623	LMG	O6-C5-C6	2.51	112.68	106.44
21	G	406	CLA	C1-C2-C3	-2.51	121.70	126.04
21	N	605	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
21	N	607	CLA	O2A-CGA-CBA	2.51	119.78	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	617	BCR	C3-C4-C5	-2.51	109.60	114.08
21	P	510	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
21	C	513	CLA	O2A-CGA-CBA	2.51	119.77	111.91
30	B	619	BCR	C38-C26-C25	-2.51	121.71	124.53
30	B	620	BCR	C16-C17-C18	-2.50	123.74	127.31
21	B	604	CLA	C1-C2-C3	-2.50	121.72	126.04
27	B	622	LMG	C8-O7-C10	-2.50	111.63	117.79
21	N	620	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
26	B	624	SQD	C1-C2-C3	-2.50	104.79	110.00
21	N	611	CLA	O2A-CGA-CBA	2.50	119.75	111.91
21	C	506	CLA	C1-C2-C3	-2.49	121.73	126.04
26	N	601	SQD	C44-O6-C1	-2.49	108.87	113.74
22	A	404	PHO	CAA-C2A-C3A	-2.49	105.95	112.78
21	C	509	CLA	C1-C2-C3	-2.49	121.74	126.04
21	B	602	CLA	C1-C2-C3	-2.49	121.74	126.04
23	b	101	PL9	C20-C19-C21	2.49	119.46	115.27
21	N	620	CLA	O1D-CGD-CBD	-2.48	119.40	124.48
21	P	503	CLA	C4D-C3D-CAD	-2.48	107.08	108.47
27	Q	407	LMG	O8-C28-C29	2.48	119.70	111.91
21	N	609	CLA	C4-C3-C5	2.48	119.45	115.27
21	B	606	CLA	O2A-CGA-CBA	2.48	119.70	111.91
26	N	601	SQD	C1-O5-C5	-2.48	108.82	113.69
21	C	501	CLA	O2A-CGA-CBA	2.48	119.69	111.91
21	P	513	CLA	O2A-CGA-CBA	2.48	119.69	111.91
23	J	101	PL9	C12-C13-C14	-2.48	121.69	127.66
21	C	510	CLA	C2A-C1A-CHA	2.48	128.19	123.86
34	V	201	HEM	C1D-C2D-C3D	-2.48	105.27	107.00
21	N	607	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
23	b	101	PL9	C15-C14-C16	2.47	119.43	115.27
30	B	619	BCR	C2-C1-C6	2.47	114.28	110.48
21	G	406	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
24	C	518	DGD	O5D-C6D-C5D	2.47	113.62	109.05
30	I	101	BCR	C16-C17-C18	-2.47	123.79	127.31
21	B	605	CLA	C2A-C1A-CHA	2.47	128.17	123.86
21	B	613	CLA	C4D-C3D-CAD	-2.47	107.09	108.47
21	N	605	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
25	A	411	LHG	O8-C23-C24	2.46	119.62	111.91
21	A	403	CLA	C4D-C3D-CAD	-2.46	107.10	108.47
30	a	101	BCR	C20-C21-C22	-2.46	123.80	127.31
24	D	408	DGD	O1G-C1A-C2A	2.46	119.61	111.91
27	a	102	LMG	C7-O1-C1	-2.46	108.94	113.74
21	P	501	CLA	O2A-CGA-CBA	2.45	119.61	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	615	CLA	O2A-CGA-CBA	2.45	119.60	111.91
21	Q	404	CLA	O2A-CGA-CBA	2.45	119.60	111.91
23	D	404	PL9	C40-C39-C41	2.45	119.39	115.27
21	B	603	CLA	O2A-CGA-CBA	2.45	119.59	111.91
24	C	516	DGD	O5D-C1E-C2E	2.45	112.12	108.30
27	D	406	LMG	C8-O7-C10	-2.45	111.77	117.79
27	D	407	LMG	O8-C28-C29	2.45	119.58	111.91
21	N	618	CLA	C4-C3-C5	2.44	119.38	115.27
30	C	514	BCR	C35-C13-C14	-2.44	119.50	122.92
21	C	513	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
21	P	503	CLA	C1-C2-C3	-2.44	121.82	126.04
21	B	611	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
30	H	101	BCR	C3-C4-C5	-2.44	109.72	114.08
23	D	404	PL9	C42-C43-C44	-2.44	121.79	127.66
23	b	101	PL9	C12-C13-C14	-2.44	121.79	127.66
30	B	619	BCR	C28-C27-C26	-2.44	109.73	114.08
30	T	102	BCR	C35-C13-C12	2.43	121.91	118.08
24	P	518	DGD	C6E-C5E-C4E	-2.43	107.30	113.00
21	C	513	CLA	C2A-C1A-CHA	2.43	128.11	123.86
21	B	609	CLA	O2A-CGA-CBA	2.43	119.54	111.91
27	C	520	LMG	O1-C1-C2	2.43	112.10	108.30
21	C	505	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
25	G	412	LHG	O8-C23-C24	2.43	119.54	111.91
30	b	102	BCR	C33-C5-C6	-2.43	121.80	124.53
22	G	405	PHO	CAA-C2A-C3A	-2.43	106.14	112.78
21	P	504	CLA	C2A-C1A-CHA	2.43	128.10	123.86
26	B	627	SQD	C1-O5-C5	-2.42	108.93	113.69
30	B	617	BCR	C11-C10-C9	-2.42	123.85	127.31
21	N	617	CLA	O2A-CGA-CBA	2.42	119.51	111.91
31	D	409	LMT	C1B-O1B-C4'	-2.42	111.97	117.96
27	D	412	LMG	C8-O7-C10	-2.42	111.83	117.79
21	C	505	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
23	D	404	PL9	C32-C33-C34	-2.42	121.83	127.66
27	P	521	LMG	O6-C5-C6	2.42	112.45	106.44
21	P	506	CLA	C1-C2-C3	-2.42	121.86	126.04
21	D	403	CLA	O2A-CGA-CBA	2.42	119.49	111.91
23	D	404	PL9	C7-C3-C2	-2.42	120.12	123.30
21	D	401	CLA	C4-C3-C5	2.41	119.33	115.27
23	A	406	PL9	C7-C3-C2	-2.41	120.13	123.30
21	B	616	CLA	O2A-CGA-CBA	2.41	119.46	111.91
24	Q	409	DGD	O1G-C1A-C2A	2.41	119.46	111.91
21	C	501	CLA	C1-C2-C3	-2.41	121.88	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	101	PL9	C22-C23-C24	-2.40	121.87	127.66
27	C	520	LMG	O6-C5-C6	2.40	112.41	106.44
21	N	619	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
21	P	504	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
21	N	620	CLA	O2A-CGA-CBA	2.40	119.44	111.91
21	B	605	CLA	C1-C2-C3	-2.40	121.89	126.04
23	G	407	PL9	C30-C29-C31	2.40	119.31	115.27
23	Q	405	PL9	C42-C43-C44	-2.40	121.88	127.66
30	P	514	BCR	C38-C26-C25	-2.40	121.83	124.53
21	B	604	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
30	T	101	BCR	C24-C23-C22	-2.40	122.62	126.23
21	G	404	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
23	G	407	PL9	C15-C14-C16	2.39	119.30	115.27
23	Q	405	PL9	C20-C19-C21	2.39	119.30	115.27
23	J	101	PL9	C15-C14-C16	2.39	119.29	115.27
27	N	623	LMG	O6-C1-O1	-2.39	104.32	109.97
21	P	509	CLA	C1-C2-C3	-2.39	121.92	126.04
21	C	503	CLA	C4D-C3D-CAD	-2.39	107.14	108.47
21	N	618	CLA	O2A-CGA-CBA	2.38	119.38	111.91
21	C	503	CLA	C4-C3-C5	2.38	119.28	115.27
22	G	405	PHO	C1-C2-C3	-2.38	121.93	126.04
27	I	102	LMG	O8-C28-C29	2.38	119.37	111.91
21	B	602	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
21	B	614	CLA	O2A-CGA-CBA	2.38	119.36	111.91
23	D	404	PL9	C45-C44-C43	-2.38	117.58	123.68
21	N	610	CLA	O2A-CGA-CBA	2.37	119.36	111.91
23	Q	405	PL9	C32-C33-C34	-2.37	121.94	127.66
23	J	101	PL9	C22-C23-C24	-2.37	121.94	127.66
21	A	405	CLA	O2A-CGA-CBA	2.37	119.36	111.91
24	D	408	DGD	O5D-C1E-C2E	-2.37	104.60	108.30
26	B	627	SQD	O5-C1-O6	2.37	115.59	109.97
24	Q	409	DGD	C6E-C5E-C4E	-2.37	107.45	113.00
27	e	102	LMG	C8-O7-C10	-2.37	111.96	117.79
21	C	511	CLA	O2A-CGA-CBA	2.37	119.34	111.91
30	W	101	BCR	C16-C17-C18	-2.37	123.93	127.31
27	e	102	LMG	O6-C5-C6	2.37	112.32	106.44
21	G	406	CLA	O2A-CGA-CBA	2.37	119.33	111.91
21	G	402	CLA	O2A-CGA-CBA	2.37	119.33	111.91
21	B	616	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
21	N	613	CLA	CED-O2D-CGD	2.37	121.29	115.94
30	c	101	BCR	C29-C30-C25	2.37	114.12	110.48
21	C	509	CLA	O2A-CGA-CBA	2.36	119.33	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	M	102	LMT	C1B-O1B-C4'	-2.36	112.11	117.96
22	G	405	PHO	CHD-C1D-ND	-2.36	119.66	124.58
30	P	514	BCR	C35-C13-C12	2.36	121.80	118.08
21	P	501	CLA	C1-C2-C3	-2.36	121.96	126.04
21	G	402	CLA	C2A-C1A-CHA	2.36	127.98	123.86
21	N	609	CLA	C1-C2-C3	-2.36	121.97	126.04
21	A	403	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
22	D	402	PHO	CMC-C2C-C1C	2.36	128.69	125.06
21	C	508	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
21	B	613	CLA	O2A-CGA-CBA	2.35	119.30	111.91
30	P	515	BCR	C20-C21-C22	-2.35	123.95	127.31
30	B	618	BCR	C15-C16-C17	-2.35	118.66	123.47
21	B	603	CLA	C4-C3-C5	2.35	119.22	115.27
21	N	617	CLA	C4D-C3D-CAD	-2.35	107.16	108.47
21	P	503	CLA	C4-C3-C5	2.35	119.22	115.27
21	P	512	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
21	D	401	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
27	e	102	LMG	O8-C28-C29	2.35	119.27	111.91
21	N	609	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
30	J	102	BCR	C33-C5-C6	-2.34	121.90	124.53
30	I	101	BCR	C28-C27-C26	-2.34	109.89	114.08
30	T	103	BCR	C28-C27-C26	-2.34	109.89	114.08
21	N	606	CLA	C1-C2-C3	-2.34	121.99	126.04
22	A	404	PHO	CHD-C1D-ND	-2.34	119.71	124.58
23	J	101	PL9	C7-C8-C9	-2.34	122.90	126.79
30	J	102	BCR	C12-C13-C14	2.34	122.53	118.94
30	T	101	BCR	C11-C10-C9	-2.34	123.97	127.31
21	P	505	CLA	C1-C2-C3	-2.34	122.00	126.04
27	B	623	LMG	O6-C5-C6	2.34	112.24	106.44
21	Q	402	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
30	T	102	BCR	C38-C26-C27	2.33	118.10	113.62
30	S	101	BCR	C11-C10-C9	-2.33	123.98	127.31
21	P	513	CLA	C2A-C1A-CHA	2.33	127.94	123.86
22	D	402	PHO	CHD-C1D-ND	-2.33	119.72	124.58
27	M	101	LMG	C8-O7-C10	-2.33	112.05	117.79
30	K	101	BCR	C29-C30-C25	2.33	114.07	110.48
21	B	608	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
24	C	518	DGD	O6E-C1E-O5D	2.33	115.49	109.97
21	B	605	CLA	C4-C3-C5	2.33	119.19	115.27
30	N	621	BCR	C2-C1-C6	2.33	114.06	110.48
21	N	619	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
21	C	508	CLA	O2A-CGA-CBA	2.33	119.20	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	619	CLA	C4-C3-C5	2.32	119.18	115.27
21	C	506	CLA	C4-C3-C5	2.32	119.18	115.27
26	A	414	SQD	O8-S-C6	2.32	109.44	105.74
27	Q	406	LMG	C8-O7-C10	-2.32	112.08	117.79
21	P	508	CLA	O2A-CGA-CBA	2.32	119.19	111.91
30	S	101	BCR	C37-C22-C23	2.32	121.73	118.08
27	E	102	LMG	O8-C28-C29	2.32	119.19	111.91
26	A	409	SQD	O48-C23-C24	2.32	119.18	111.91
30	B	619	BCR	C16-C17-C18	-2.32	124.00	127.31
21	A	403	CLA	C1-C2-C3	-2.32	122.04	126.04
21	C	507	CLA	C4-C3-C5	2.32	119.17	115.27
26	S	102	SQD	O9-S-C6	2.32	109.69	106.94
27	B	623	LMG	O8-C28-C29	2.32	119.18	111.91
21	B	614	CLA	C4-C3-C5	2.31	119.16	115.27
26	B	624	SQD	O48-C23-C24	2.31	119.17	111.91
23	Q	405	PL9	C45-C44-C43	-2.31	117.75	123.68
26	B	627	SQD	C3-C4-C5	2.31	114.36	110.24
24	P	518	DGD	C3G-C2G-C1G	-2.31	106.33	111.79
21	N	615	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
23	D	404	PL9	C15-C14-C16	2.31	119.15	115.27
21	P	513	CLA	C4D-C3D-CAD	-2.31	107.18	108.47
21	P	505	CLA	O2A-CGA-CBA	2.31	119.15	111.91
21	C	512	CLA	C4-C3-C5	2.31	119.15	115.27
23	A	406	PL9	C7-C8-C9	-2.30	122.95	126.79
30	H	101	BCR	C28-C27-C26	-2.30	109.96	114.08
23	b	101	PL9	C7-C8-C9	-2.30	122.96	126.79
26	N	601	SQD	O5-C1-O6	2.30	115.43	109.97
21	P	513	CLA	C1-C2-C3	-2.30	122.06	126.04
23	G	407	PL9	C53-C6-C1	2.30	119.69	114.99
21	P	509	CLA	O2A-CGA-CBA	2.30	119.12	111.91
21	C	505	CLA	O2A-CGA-CBA	2.30	119.11	111.91
21	B	615	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
30	b	102	BCR	C12-C13-C14	2.29	122.46	118.94
21	C	511	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
30	Z	101	BCR	C10-C11-C12	-2.29	116.06	123.22
21	N	613	CLA	O2A-CGA-CBA	2.29	119.11	111.91
30	D	405	BCR	C11-C10-C9	-2.29	124.04	127.31
23	A	406	PL9	C11-C9-C8	-2.29	116.48	121.12
23	G	407	PL9	C17-C18-C19	-2.29	122.14	127.66
21	A	405	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
21	C	512	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	P	514	BCR	C34-C9-C10	-2.29	119.72	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	618	BCR	C4-C5-C6	-2.29	119.41	122.73
30	C	515	BCR	C2-C1-C6	2.29	114.00	110.48
27	N	623	LMG	O8-C28-C29	2.29	119.09	111.91
21	A	401	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
30	a	101	BCR	C28-C27-C26	-2.29	110.00	114.08
21	C	503	CLA	O2A-CGA-CBA	2.29	119.08	111.91
21	G	402	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
26	Q	408	SQD	O48-C23-C24	2.28	119.07	111.91
27	R	102	LMG	O8-C28-C29	2.28	119.07	111.91
21	C	510	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
21	C	502	CLA	O2A-CGA-CBA	2.28	119.06	111.91
21	A	401	CLA	O2A-CGA-CBA	2.28	119.06	111.91
21	N	614	CLA	O1D-CGD-CBD	-2.28	119.82	124.48
30	C	514	BCR	C34-C9-C10	-2.28	119.73	122.92
30	T	102	BCR	C4-C5-C6	-2.28	119.43	122.73
30	B	618	BCR	C38-C26-C27	2.27	117.98	113.62
21	C	513	CLA	O1D-CGD-CBD	-2.27	119.83	124.48
21	A	401	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
21	P	506	CLA	CED-O2D-CGD	2.27	121.07	115.94
22	G	405	PHO	O1D-CGD-CBD	-2.27	119.84	124.48
24	C	517	DGD	C6E-C5E-C4E	-2.27	107.69	113.00
21	C	503	CLA	C1-C2-C3	-2.27	122.12	126.04
21	B	605	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
23	A	406	PL9	C17-C18-C19	-2.27	122.20	127.66
21	P	511	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
23	A	406	PL9	C27-C28-C29	-2.27	122.20	127.66
21	B	605	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
30	B	618	BCR	C30-C25-C24	2.27	122.19	115.78
27	a	102	LMG	O8-C28-C29	2.26	119.02	111.91
21	N	609	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
23	Q	405	PL9	C17-C18-C19	-2.26	122.21	127.66
30	T	102	BCR	C36-C18-C19	2.26	121.64	118.08
30	a	101	BCR	C7-C8-C9	-2.26	122.82	126.23
27	C	520	LMG	O8-C28-O10	-2.26	117.89	123.59
30	B	617	BCR	C24-C23-C22	-2.26	122.82	126.23
26	A	409	SQD	O5-C5-C4	2.26	113.79	109.69
21	P	503	CLA	O2A-CGA-CBA	2.26	118.99	111.91
21	N	614	CLA	C4-C3-C5	2.26	119.06	115.27
21	C	503	CLA	O2D-CGD-O1D	-2.26	119.43	123.84
21	P	502	CLA	O2A-CGA-CBA	2.25	118.98	111.91
22	Q	403	PHO	CHD-C1D-ND	-2.25	119.89	124.58
30	D	405	BCR	C21-C20-C19	-2.25	116.19	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	610	CLA	O2D-CGD-O1D	-2.25	119.43	123.84
30	D	405	BCR	C37-C22-C23	2.25	121.63	118.08
21	C	510	CLA	O2A-CGA-CBA	2.25	118.98	111.91
30	C	515	BCR	C21-C20-C19	-2.25	116.19	123.22
23	Q	405	PL9	C40-C39-C41	2.25	119.06	115.27
21	N	606	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
21	C	504	CLA	C4-C3-C5	2.25	119.05	115.27
30	b	102	BCR	C36-C18-C17	-2.25	119.78	122.92
24	C	517	DGD	C3G-C2G-C1G	-2.25	106.48	111.79
21	N	612	CLA	C1-C2-C3	-2.25	122.16	126.04
21	B	607	CLA	O2A-CGA-CBA	2.24	118.95	111.91
21	A	401	CLA	C2A-C1A-CHA	2.24	127.78	123.86
30	Z	101	BCR	C11-C10-C9	-2.24	124.11	127.31
22	A	404	PHO	CMC-C2C-C1C	2.24	128.51	125.06
21	G	403	CLA	C4D-C3D-CAD	-2.24	107.22	108.47
23	G	407	PL9	C7-C8-C9	-2.24	123.06	126.79
21	P	513	CLA	O1D-CGD-CBD	-2.24	119.91	124.48
21	G	402	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
27	Q	401	LMG	O8-C28-C29	2.23	118.92	111.91
27	Q	401	LMG	C8-O7-C10	-2.23	112.29	117.79
27	M	101	LMG	O6-C5-C6	2.23	111.99	106.44
30	K	101	BCR	C15-C16-C17	-2.23	118.90	123.47
30	C	515	BCR	C30-C25-C24	2.23	122.09	115.78
23	G	407	PL9	C27-C28-C29	-2.23	122.29	127.66
31	e	101	LMT	C1B-O1B-C4'	-2.23	112.44	117.96
30	c	101	BCR	C1-C6-C5	-2.23	119.47	122.61
30	K	101	BCR	C1-C6-C5	-2.23	119.47	122.61
30	b	102	BCR	C23-C22-C21	2.23	122.36	118.94
24	B	621	DGD	C1E-C2E-C3E	-2.23	105.36	110.00
24	P	518	DGD	O6E-C1E-O5D	2.23	115.25	109.97
21	N	612	CLA	C4D-C3D-CAD	-2.23	107.23	108.47
30	C	514	BCR	C29-C30-C25	2.23	113.91	110.48
21	A	402	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	S	102	SQD	C3-C4-C5	2.23	114.21	110.24
30	H	101	BCR	C16-C17-C18	-2.23	124.13	127.31
30	P	515	BCR	C10-C11-C12	-2.22	116.28	123.22
21	Q	402	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
26	F	101	SQD	C3-C4-C5	2.22	114.20	110.24
30	S	101	BCR	C21-C20-C19	-2.22	116.28	123.22
21	A	405	CLA	C1-C2-C3	-2.22	122.20	126.04
21	P	512	CLA	C4-C3-C5	2.22	119.01	115.27
26	F	101	SQD	O9-S-C6	2.22	109.58	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	602	CLA	C4-C3-C5	2.22	119.00	115.27
21	P	503	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
21	G	406	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
27	P	521	LMG	O1-C1-C2	2.22	111.76	108.30
21	A	402	CLA	O2A-CGA-CBA	2.21	118.85	111.91
26	G	410	SQD	O48-C23-C24	2.21	118.84	111.91
30	P	515	BCR	C15-C16-C17	-2.21	118.95	123.47
30	P	516	BCR	C2-C1-C6	2.21	113.88	110.48
30	B	617	BCR	C20-C21-C22	-2.21	124.16	127.31
24	D	408	DGD	C6E-C5E-C4E	-2.21	107.84	113.00
21	C	509	CLA	C4-C3-C5	2.21	118.98	115.27
21	B	610	CLA	O2A-CGA-CBA	2.20	118.82	111.91
22	Q	403	PHO	CAA-C2A-C3A	-2.20	106.75	112.78
21	B	606	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
21	B	612	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
21	P	513	CLA	C1D-CHD-C4C	2.20	125.46	122.56
21	B	615	CLA	C4-C3-C5	2.20	118.97	115.27
30	P	515	BCR	C38-C26-C25	-2.20	122.06	124.53
23	Q	405	PL9	C15-C14-C16	2.20	118.97	115.27
23	G	407	PL9	C41-C39-C40	2.20	119.45	114.60
22	Q	403	PHO	CMC-C2C-C1C	2.20	128.44	125.06
30	P	515	BCR	C8-C7-C6	-2.20	121.04	127.20
21	N	606	CLA	CED-O2D-CGD	2.19	120.90	115.94
21	N	607	CLA	C1-O2A-CGA	2.19	122.20	116.44
30	N	621	BCR	C20-C21-C22	-2.19	124.18	127.31
27	D	412	LMG	O8-C28-C29	2.19	118.79	111.91
23	A	406	PL9	C53-C6-C1	2.19	119.47	114.99
26	F	101	SQD	O7-S-C6	2.19	109.55	106.94
21	N	615	CLA	CBA-CAA-C2A	-2.19	107.39	113.86
30	N	621	BCR	C16-C17-C18	-2.19	124.18	127.31
30	N	621	BCR	C35-C13-C14	-2.19	119.85	122.92
30	Z	101	BCR	C38-C26-C25	-2.19	122.07	124.53
30	K	101	BCR	C36-C18-C19	2.19	121.53	118.08
21	P	509	CLA	C4-C3-C5	2.19	118.95	115.27
21	C	506	CLA	CBA-CAA-C2A	-2.19	107.40	113.86
21	C	513	CLA	C1-C2-C3	-2.19	122.26	126.04
30	W	101	BCR	C28-C27-C26	-2.19	110.17	114.08
21	B	616	CLA	C1-C2-C3	-2.19	122.26	126.04
21	P	505	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
30	T	102	BCR	C30-C25-C24	2.19	121.96	115.78
21	B	606	CLA	C1-C2-C3	-2.18	122.26	126.04
24	C	517	DGD	O6E-C1E-O5D	2.18	115.14	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	410	SQD	C45-O47-C7	-2.18	112.42	117.79
23	Q	405	PL9	C51-C49-C50	2.18	119.42	114.60
21	B	615	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
24	C	517	DGD	C6D-C5D-C4D	2.18	116.65	112.09
21	N	614	CLA	O2A-CGA-CBA	2.18	118.75	111.91
21	G	403	CLA	O2A-CGA-CBA	2.18	118.75	111.91
21	D	401	CLA	C4D-C3D-CAD	-2.18	107.25	108.47
30	P	516	BCR	C16-C17-C18	-2.18	124.20	127.31
30	T	103	BCR	C20-C21-C22	-2.18	124.20	127.31
30	a	101	BCR	C16-C17-C18	-2.18	124.20	127.31
21	B	608	CLA	C1-C2-C3	-2.18	122.28	126.04
21	C	511	CLA	C1-C2-C3	-2.18	122.28	126.04
21	C	502	CLA	C1-C2-C3	-2.18	122.28	126.04
27	N	622	LMG	O6-C1-O1	-2.18	104.82	109.97
21	P	509	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
24	C	517	DGD	C1D-O6D-C5D	2.17	117.95	113.69
23	Q	405	PL9	C27-C28-C29	-2.17	122.44	127.66
23	G	407	PL9	C36-C34-C33	-2.17	116.73	121.12
34	V	201	HEM	CAA-CBA-CGA	-2.17	109.03	112.67
23	D	404	PL9	C20-C19-C21	2.17	118.92	115.27
30	W	101	BCR	C3-C4-C5	-2.16	110.21	114.08
21	N	610	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
26	B	624	SQD	O8-S-C6	2.16	109.19	105.74
30	Z	101	BCR	C16-C17-C18	-2.16	124.22	127.31
30	P	516	BCR	C35-C13-C14	-2.16	119.90	122.92
21	A	402	CLA	C4D-C3D-CAD	-2.16	107.27	108.47
30	H	101	BCR	C35-C13-C12	2.16	121.48	118.08
34	i	201	HEM	C1D-C2D-C3D	-2.16	105.50	107.00
23	A	406	PL9	C41-C39-C40	2.16	119.36	114.60
21	B	610	CLA	C4-C3-C5	2.16	118.90	115.27
21	N	612	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
21	N	616	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
21	B	608	CLA	CMB-C2B-C1B	-2.15	125.15	128.46
30	P	514	BCR	C21-C20-C19	-2.15	116.50	123.22
21	P	501	CLA	C4-C3-C5	2.15	118.89	115.27
21	P	508	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
30	S	101	BCR	C24-C23-C22	-2.15	122.98	126.23
30	P	514	BCR	C29-C30-C25	2.15	113.79	110.48
31	I	103	LMT	O1B-C4'-C3'	2.15	113.00	107.28
21	C	501	CLA	C4-C3-C5	2.15	118.88	115.27
27	E	102	LMG	O7-C10-C11	2.15	116.13	111.50
21	C	505	CLA	C1-C2-C3	-2.15	122.33	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	507	CLA	C5-C3-C2	-2.15	116.77	121.12
21	P	504	CLA	C1-O2A-CGA	2.15	122.08	116.44
21	C	507	CLA	C5-C3-C2	-2.15	116.77	121.12
21	B	604	CLA	C1D-CHD-C4C	2.15	125.39	122.56
23	D	404	PL9	C51-C49-C50	2.14	119.34	114.60
30	b	102	BCR	C39-C30-C25	-2.14	106.83	110.30
21	N	614	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
21	P	502	CLA	CED-O2D-CGD	2.14	120.78	115.94
21	G	403	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
30	T	103	BCR	C33-C5-C6	-2.14	122.13	124.53
24	P	517	DGD	O3D-C3D-C4D	-2.14	105.40	110.35
30	C	514	BCR	C35-C13-C12	2.14	121.45	118.08
30	I	101	BCR	C2-C1-C6	2.14	113.77	110.48
24	P	519	DGD	O6E-C1E-O5D	2.14	115.03	109.97
24	Q	409	DGD	O5D-C1E-C2E	-2.14	104.97	108.30
30	I	101	BCR	C7-C8-C9	-2.14	123.01	126.23
30	H	101	BCR	C21-C20-C19	-2.14	116.55	123.22
23	G	407	PL9	C11-C9-C8	-2.13	116.80	121.12
21	P	508	CLA	C4-C3-C5	2.13	118.86	115.27
21	N	615	CLA	C5-C3-C2	-2.13	116.80	121.12
25	G	409	LHG	O8-C23-C24	2.13	118.60	111.91
30	B	618	BCR	C36-C18-C19	2.13	121.44	118.08
21	P	507	CLA	C4-C3-C5	2.13	118.86	115.27
24	W	102	DGD	O6D-C5D-C4D	2.13	113.56	109.69
27	D	412	LMG	O7-C10-O9	-2.13	118.56	123.70
27	R	102	LMG	C9-C8-C7	-2.13	106.75	111.79
27	B	622	LMG	O6-C1-O1	-2.13	104.93	109.97
22	A	404	PHO	O1D-CGD-CBD	-2.13	120.13	124.48
22	G	405	PHO	C9-C8-C10	-2.13	103.59	111.29
22	D	402	PHO	CAA-C2A-C3A	-2.13	106.95	112.78
21	P	508	CLA	CMB-C2B-C1B	-2.13	125.20	128.46
21	N	609	CLA	CED-O2D-CGD	2.13	120.74	115.94
23	D	404	PL9	C27-C28-C29	-2.13	122.54	127.66
30	Z	101	BCR	C15-C16-C17	-2.13	119.12	123.47
21	N	605	CLA	CMC-C2C-C1C	-2.12	121.80	125.04
21	B	605	CLA	CED-O2D-CGD	2.12	120.74	115.94
23	A	406	PL9	C36-C34-C33	-2.12	116.82	121.12
21	C	505	CLA	C1D-CHD-C4C	2.12	125.36	122.56
21	C	506	CLA	CED-O2D-CGD	2.12	120.74	115.94
21	P	507	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
21	B	611	CLA	CBA-CAA-C2A	-2.12	107.60	113.86
30	N	621	BCR	C11-C10-C9	-2.12	124.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	102	LMG	C1-O6-C5	2.12	117.85	113.69
27	M	101	LMG	O7-C10-O9	-2.12	118.58	123.70
26	B	627	SQD	C44-O6-C1	-2.12	109.60	113.74
26	S	102	SQD	O6-C1-C2	2.12	111.61	108.30
30	J	102	BCR	C23-C22-C21	2.11	122.19	118.94
21	N	608	CLA	C4-C3-C5	2.11	118.83	115.27
30	c	101	BCR	C28-C27-C26	-2.11	110.30	114.08
24	P	518	DGD	C6D-C5D-C4D	2.11	116.50	112.09
27	Q	401	LMG	O7-C10-O9	-2.11	118.60	123.70
26	B	627	SQD	O48-C23-C24	2.11	118.53	111.91
30	Z	101	BCR	C8-C7-C6	-2.11	121.28	127.20
21	P	511	CLA	C1-C2-C3	-2.11	122.39	126.04
27	e	102	LMG	O7-C10-O9	-2.11	118.61	123.70
21	N	615	CLA	O2A-CGA-CBA	2.11	118.53	111.91
30	K	101	BCR	C24-C23-C22	-2.11	123.05	126.23
26	F	101	SQD	O6-C1-C2	2.11	111.59	108.30
25	A	408	LHG	O8-C23-C24	2.11	118.52	111.91
27	C	520	LMG	C7-O1-C1	-2.10	109.63	113.74
21	A	402	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
27	E	102	LMG	C1-O6-C5	2.10	117.81	113.69
21	P	508	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
27	M	101	LMG	O8-C28-C29	2.10	118.50	111.91
21	B	613	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
21	P	502	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
23	G	407	PL9	C10-C9-C11	2.10	118.80	115.27
30	B	620	BCR	C20-C21-C22	-2.10	124.31	127.31
21	N	616	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
21	N	620	CLA	CED-O2D-CGD	2.10	120.68	115.94
24	C	516	DGD	O3D-C3D-C4D	-2.10	105.50	110.35
30	W	101	BCR	C35-C13-C12	2.09	121.37	118.08
21	P	510	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
24	Q	409	DGD	O3G-C1D-C2D	2.09	111.57	108.30
21	B	611	CLA	C5-C3-C2	-2.09	116.89	121.12
21	C	509	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
23	b	101	PL9	C10-C9-C11	2.09	118.78	115.27
27	N	623	LMG	O2-C2-C3	-2.09	105.52	110.35
21	C	513	CLA	C1D-CHD-C4C	2.09	125.31	122.56
27	B	623	LMG	O2-C2-C3	-2.08	105.53	110.35
30	J	102	BCR	C39-C30-C25	-2.08	106.92	110.30
30	I	101	BCR	C20-C21-C22	-2.08	124.34	127.31
21	P	506	CLA	C4-C3-C5	2.08	118.77	115.27
34	i	201	HEM	CMB-C2B-C3B	2.08	128.57	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	508	CLA	CBA-CAA-C2A	-2.08	107.72	113.86
30	H	101	BCR	C24-C23-C22	-2.08	123.09	126.23
21	B	611	CLA	O2A-CGA-CBA	2.08	118.44	111.91
21	P	513	CLA	CED-O2D-CGD	2.08	120.64	115.94
30	P	515	BCR	C11-C10-C9	-2.08	124.34	127.31
21	B	602	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
30	B	618	BCR	C34-C9-C10	-2.08	120.01	122.92
26	A	409	SQD	C45-O47-C7	-2.08	112.68	117.79
21	G	403	CLA	C1D-CHD-C4C	2.08	125.30	122.56
27	N	622	LMG	O3-C3-C4	-2.08	105.55	110.35
21	B	605	CLA	C11-C10-C8	-2.08	109.21	115.92
21	N	607	CLA	C4-C3-C5	2.07	118.76	115.27
21	N	609	CLA	C11-C10-C8	-2.07	109.22	115.92
30	c	101	BCR	C36-C18-C19	2.07	121.34	118.08
24	W	102	DGD	C1D-O6D-C5D	2.07	117.75	113.69
26	S	102	SQD	O7-S-C6	2.07	109.40	106.94
27	Q	407	LMG	O7-C10-O9	-2.07	118.70	123.70
30	C	514	BCR	C21-C20-C19	-2.07	116.76	123.22
21	P	509	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
21	P	504	CLA	C4-C3-C5	2.07	118.75	115.27
30	c	101	BCR	C38-C26-C27	2.07	117.59	113.62
21	A	402	CLA	C1D-CHD-C4C	2.07	125.29	122.56
21	B	606	CLA	C1D-CHD-C4C	2.07	125.29	122.56
21	G	403	CLA	C4-C3-C5	2.07	118.75	115.27
21	P	501	CLA	C1D-CHD-C4C	2.07	125.28	122.56
30	P	516	BCR	C30-C25-C24	2.07	121.62	115.78
21	B	611	CLA	C1D-CHD-C4C	2.07	125.28	122.56
21	B	604	CLA	C4-C3-C5	2.07	118.75	115.27
30	H	101	BCR	C33-C5-C4	2.07	117.58	113.62
30	T	101	BCR	C29-C30-C25	2.06	113.66	110.48
21	N	618	CLA	C1D-CHD-C4C	2.06	125.28	122.56
21	N	607	CLA	C1D-CHD-C4C	2.06	125.28	122.56
21	Q	402	CLA	CED-O2D-CGD	2.06	120.60	115.94
21	N	609	CLA	O2A-CGA-CBA	2.06	118.38	111.91
24	B	628	DGD	O6D-C1D-O3G	-2.06	105.09	109.97
21	B	612	CLA	C4-C3-C5	2.06	118.73	115.27
30	K	101	BCR	C38-C26-C27	2.06	117.57	113.62
30	P	514	BCR	C33-C5-C4	2.06	117.57	113.62
30	C	515	BCR	C38-C26-C27	2.06	117.57	113.62
21	C	505	CLA	C5-C3-C2	-2.06	116.96	121.12
21	N	606	CLA	C4-C3-C5	2.06	118.73	115.27
21	N	610	CLA	C1D-CHD-C4C	2.05	125.27	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	601	SQD	C45-O47-C7	-2.05	112.73	117.79
30	T	103	BCR	C33-C5-C4	2.05	117.56	113.62
21	N	606	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
30	I	101	BCR	C21-C20-C19	-2.05	116.81	123.22
21	P	506	CLA	CBA-CAA-C2A	-2.05	107.80	113.86
31	N	625	LMT	O1B-C1B-C2B	2.05	113.42	108.10
26	N	601	SQD	O48-C23-C24	2.05	118.35	111.91
21	P	512	CLA	C1D-CHD-C4C	2.05	125.27	122.56
30	P	515	BCR	C36-C18-C19	2.05	121.31	118.08
31	a	103	LMT	O1B-C4'-C3'	2.05	112.74	107.28
30	K	101	BCR	C28-C27-C26	-2.05	110.42	114.08
21	B	602	CLA	O2A-CGA-CBA	2.05	118.34	111.91
21	B	602	CLA	C1D-CHD-C4C	2.05	125.26	122.56
27	P	521	LMG	O8-C28-O10	-2.05	118.42	123.59
30	c	101	BCR	C15-C16-C17	-2.05	119.28	123.47
30	P	516	BCR	C23-C24-C25	-2.05	121.45	127.20
30	B	620	BCR	C33-C5-C4	2.05	117.55	113.62
21	B	610	CLA	C1-C2-C3	-2.05	122.50	126.04
22	G	405	PHO	CMC-C2C-C1C	2.05	128.21	125.06
21	A	405	CLA	C11-C10-C8	-2.04	109.31	115.92
24	B	628	DGD	C2G-O2G-C1B	-2.04	112.76	117.79
30	P	516	BCR	C38-C26-C27	2.04	117.54	113.62
30	T	102	BCR	C34-C9-C10	-2.04	120.06	122.92
30	W	101	BCR	C21-C20-C19	-2.04	116.85	123.22
24	D	408	DGD	O3G-C1D-C2D	2.04	111.49	108.30
24	B	621	DGD	O4D-C4D-C3D	2.04	115.06	110.35
24	P	518	DGD	C1D-O6D-C5D	2.04	117.69	113.69
27	D	407	LMG	O7-C10-O9	-2.04	118.78	123.70
21	B	601	CLA	CMC-C2C-C1C	-2.04	121.94	125.04
21	C	501	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
23	A	406	PL9	C26-C24-C23	-2.04	117.00	121.12
27	D	406	LMG	O3-C3-C4	-2.04	105.64	110.35
27	D	406	LMG	O2-C2-C1	-2.04	105.10	110.05
21	B	614	CLA	C1D-CHD-C4C	2.04	125.25	122.56
21	B	616	CLA	CED-O2D-CGD	2.04	120.54	115.94
23	D	404	PL9	C17-C18-C19	-2.03	122.76	127.66
26	G	410	SQD	O5-C5-C4	2.03	113.39	109.69
21	D	401	CLA	CED-O2D-CGD	2.03	120.54	115.94
27	D	406	LMG	O7-C10-O9	-2.03	118.78	123.70
21	N	612	CLA	CED-O2D-CGD	2.03	120.54	115.94
23	A	406	PL9	C10-C9-C11	2.03	118.69	115.27
30	J	102	BCR	C1-C6-C5	-2.03	119.75	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	403	CLA	CBA-CAA-C2A	-2.03	107.86	113.86
30	T	101	BCR	C20-C21-C22	-2.03	124.41	127.31
23	D	404	PL9	C30-C29-C31	2.03	118.69	115.27
21	G	403	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
30	a	101	BCR	C36-C18-C19	2.03	121.28	118.08
21	B	605	CLA	O2A-CGA-CBA	2.03	118.28	111.91
21	B	602	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
21	C	509	CLA	C7-C6-C5	-2.03	107.85	113.36
21	P	504	CLA	O2A-CGA-CBA	2.03	118.27	111.91
30	J	102	BCR	C36-C18-C17	-2.03	120.08	122.92
21	N	614	CLA	C1-C2-C3	-2.03	122.54	126.04
21	N	619	CLA	C1D-CHD-C4C	2.03	125.23	122.56
21	C	508	CLA	C4-C3-C5	2.02	118.68	115.27
23	Q	405	PL9	C53-C6-C1	2.02	119.13	114.99
23	J	101	PL9	C10-C9-C11	2.02	118.67	115.27
23	b	101	PL9	C53-C6-C1	2.02	119.12	114.99
21	C	511	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
21	B	607	CLA	C4-C3-C5	2.02	118.67	115.27
22	A	404	PHO	C4-C3-C2	-2.02	118.49	123.68
21	B	615	CLA	C1D-CHD-C4C	2.02	125.22	122.56
21	P	512	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
30	B	617	BCR	C29-C30-C25	2.02	113.59	110.48
30	S	101	BCR	C15-C14-C13	-2.02	124.43	127.31
21	C	504	CLA	C1-O2A-CGA	2.02	121.74	116.44
30	P	516	BCR	C11-C10-C9	-2.02	124.43	127.31
21	A	401	CLA	C1D-CHD-C4C	2.02	125.22	122.56
21	G	404	CLA	O2A-CGA-CBA	2.02	118.23	111.91
34	E	101	HEM	C3B-C4B-NB	-2.02	106.60	109.21
21	D	401	CLA	C1D-CHD-C4C	2.02	125.22	122.56
26	S	102	SQD	O48-C23-C24	2.02	118.23	111.91
21	C	512	CLA	C1D-CHD-C4C	2.01	125.22	122.56
26	F	101	SQD	O8-S-O7	-2.01	106.36	111.27
21	N	620	CLA	C1-C2-C3	-2.01	122.56	126.04
21	N	607	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
21	N	613	CLA	C4-C3-C5	2.01	118.65	115.27
21	Q	402	CLA	CAA-C2A-C1A	2.01	118.56	111.97
21	P	511	CLA	C1D-CHD-C4C	2.01	125.21	122.56
30	I	101	BCR	C35-C13-C12	2.01	121.24	118.08
34	i	201	HEM	CMA-C3A-C4A	-2.01	125.38	128.46
22	G	405	PHO	C4-C3-C2	-2.01	118.52	123.68
24	W	102	DGD	C1E-C2E-C3E	-2.01	105.81	110.00
21	P	502	CLA	C1-C2-C3	-2.01	122.57	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	101	SQD	O48-C23-C24	2.01	118.21	111.91
30	a	101	BCR	C21-C20-C19	-2.01	116.95	123.22
21	B	612	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
27	R	102	LMG	O1-C7-C8	-2.01	106.06	110.90
30	C	514	BCR	C20-C21-C22	-2.01	124.45	127.31
21	C	508	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
21	B	603	CLA	C3A-C2A-C1A	2.00	104.34	101.34
30	C	515	BCR	C35-C13-C14	-2.00	120.11	122.92
21	P	505	CLA	C4-C3-C5	2.00	118.64	115.27
30	T	102	BCR	C15-C16-C17	-2.00	119.37	123.47
21	G	404	CLA	O2D-CGD-O1D	-2.00	119.92	123.84
31	B	626	LMT	O1B-C1B-C2B	2.00	113.29	108.10
27	E	102	LMG	C9-C8-C7	-2.00	107.05	111.79
30	H	101	BCR	C2-C1-C6	2.00	113.56	110.48
24	B	621	DGD	O6E-C5E-C6E	2.00	111.41	106.44
30	P	516	BCR	C21-C20-C19	-2.00	116.97	123.22
21	C	508	CLA	C1D-CHD-C4C	2.00	125.20	122.56

All (296) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	B	628	DGD	C2D
24	B	628	DGD	C5D
24	B	628	DGD	C5E
21	B	615	CLA	NC
21	B	615	CLA	ND
21	B	615	CLA	NA
21	Q	404	CLA	NC
21	Q	404	CLA	ND
21	Q	404	CLA	NA
27	I	102	LMG	C2
27	I	102	LMG	C5
21	P	512	CLA	NC
21	P	512	CLA	ND
21	P	512	CLA	NA
24	A	407	DGD	C2D
24	A	407	DGD	C5D
24	A	407	DGD	C5E
24	B	621	DGD	C2D
24	B	621	DGD	C5D
24	B	621	DGD	C5E
27	D	412	LMG	C2

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Mol	Chain	Res	Type	Atom
27	D	412	LMG	C5
21	B	603	CLA	NC
21	B	603	CLA	ND
21	B	603	CLA	NA
21	B	609	CLA	NC
21	B	609	CLA	ND
21	B	609	CLA	NA
21	P	502	CLA	NC
21	P	502	CLA	ND
21	P	502	CLA	NA
27	G	411	LMG	C2
27	G	411	LMG	C5
21	C	506	CLA	NC
21	C	506	CLA	ND
21	C	506	CLA	NA
21	C	503	CLA	NC
21	C	503	CLA	ND
21	C	503	CLA	NA
27	N	622	LMG	C2
27	N	622	LMG	C5
21	N	605	CLA	NC
21	N	605	CLA	ND
21	N	605	CLA	NA
21	D	401	CLA	NC
21	D	401	CLA	ND
21	D	401	CLA	NA
21	G	404	CLA	NC
21	G	404	CLA	ND
21	G	404	CLA	NA
21	B	611	CLA	NC
21	B	611	CLA	ND
21	B	611	CLA	NA
21	N	614	CLA	NC
21	N	614	CLA	ND
21	N	614	CLA	NA
27	R	102	LMG	C2
27	R	102	LMG	C5
21	N	608	CLA	NC
21	N	608	CLA	ND
21	N	608	CLA	NA
21	P	511	CLA	NC
21	P	511	CLA	ND

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Mol	Chain	Res	Type	Atom
21	P	511	CLA	NA
21	N	609	CLA	NC
21	N	609	CLA	ND
21	N	609	CLA	NA
21	C	505	CLA	NC
21	C	505	CLA	ND
21	C	505	CLA	NA
27	P	520	LMG	C2
27	P	520	LMG	C5
27	A	410	LMG	C2
27	A	410	LMG	C5
21	C	511	CLA	NC
21	C	511	CLA	ND
21	C	511	CLA	NA
27	e	102	LMG	C2
27	e	102	LMG	C5
27	Q	401	LMG	C2
27	Q	401	LMG	C5
21	P	510	CLA	NC
21	P	510	CLA	ND
21	P	510	CLA	NA
21	A	405	CLA	NC
21	A	405	CLA	ND
21	A	405	CLA	NA
21	B	607	CLA	NC
21	B	607	CLA	ND
21	B	607	CLA	NA
21	N	610	CLA	NC
21	N	610	CLA	ND
21	N	610	CLA	NA
24	P	517	DGD	C2D
24	P	517	DGD	C5D
24	P	517	DGD	C5E
27	D	406	LMG	C2
27	D	406	LMG	C5
21	P	501	CLA	NC
21	P	501	CLA	ND
21	P	501	CLA	NA
21	C	501	CLA	NC
21	C	501	CLA	ND
21	C	501	CLA	NA
21	C	507	CLA	NC

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Mol	Chain	Res	Type	Atom
21	C	507	CLA	ND
21	C	507	CLA	NA
21	N	607	CLA	NC
21	N	607	CLA	ND
21	N	607	CLA	NA
27	Q	407	LMG	C2
27	Q	407	LMG	C5
21	B	608	CLA	NC
21	B	608	CLA	ND
21	B	608	CLA	NA
21	Q	402	CLA	NC
21	Q	402	CLA	ND
21	Q	402	CLA	NA
21	C	512	CLA	NC
21	C	512	CLA	ND
21	C	512	CLA	NA
21	C	502	CLA	NC
21	C	502	CLA	ND
21	C	502	CLA	NA
21	B	614	CLA	NC
21	B	614	CLA	ND
21	B	614	CLA	NA
21	B	604	CLA	NC
21	B	604	CLA	ND
21	B	604	CLA	NA
21	P	505	CLA	NC
21	P	505	CLA	ND
21	P	505	CLA	NA
21	N	606	CLA	NC
21	N	606	CLA	ND
21	N	606	CLA	NA
24	P	519	DGD	C2D
24	P	519	DGD	C5D
24	P	519	DGD	C5E
21	P	503	CLA	NC
21	P	503	CLA	ND
21	P	503	CLA	NA
27	D	407	LMG	C2
27	D	407	LMG	C5
24	G	408	DGD	C2D
24	G	408	DGD	C5D
24	G	408	DGD	C5E

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Mol	Chain	Res	Type	Atom
21	G	403	CLA	NC
21	G	403	CLA	ND
21	G	403	CLA	NA
21	D	403	CLA	NC
21	D	403	CLA	ND
21	D	403	CLA	NA
21	B	612	CLA	NC
21	B	612	CLA	ND
21	B	612	CLA	NA
21	A	401	CLA	NC
21	A	401	CLA	ND
21	A	401	CLA	NA
27	Q	406	LMG	C2
27	Q	406	LMG	C5
21	A	403	CLA	NC
21	A	403	CLA	ND
21	A	403	CLA	NA
21	N	615	CLA	NC
21	N	615	CLA	ND
21	N	615	CLA	NA
27	M	101	LMG	C2
27	M	101	LMG	C5
27	B	622	LMG	C2
27	B	622	LMG	C5
21	P	506	CLA	NC
21	P	506	CLA	ND
21	P	506	CLA	NA
24	Q	409	DGD	C2D
24	Q	409	DGD	C5D
24	Q	409	DGD	C5E
21	C	509	CLA	NC
21	C	509	CLA	ND
21	C	509	CLA	NA
24	W	102	DGD	C2D
24	W	102	DGD	C5D
24	W	102	DGD	C5E
21	G	406	CLA	NC
21	G	406	CLA	ND
21	G	406	CLA	NA
21	P	507	CLA	NC
21	P	507	CLA	ND
21	P	507	CLA	NA

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Mol	Chain	Res	Type	Atom
21	P	508	CLA	NC
21	P	508	CLA	ND
21	P	508	CLA	NA
27	C	519	LMG	C2
27	C	519	LMG	C5
24	N	602	DGD	C2D
24	N	602	DGD	C5D
24	N	602	DGD	C5E
21	N	620	CLA	NC
21	N	620	CLA	ND
21	N	620	CLA	NA
24	C	518	DGD	C2D
24	C	518	DGD	C5D
24	C	518	DGD	C5E
24	P	518	DGD	C2D
24	P	518	DGD	C5D
24	P	518	DGD	C5E
21	N	611	CLA	NC
21	N	611	CLA	ND
21	N	611	CLA	NA
27	N	623	LMG	C2
27	N	623	LMG	C5
21	N	613	CLA	NC
21	N	613	CLA	ND
21	N	613	CLA	NA
24	C	516	DGD	C2D
24	C	516	DGD	C5D
24	C	516	DGD	C5E
21	P	504	CLA	NC
21	P	504	CLA	ND
21	P	504	CLA	NA
21	B	610	CLA	NC
21	B	610	CLA	ND
21	B	610	CLA	NA
21	B	602	CLA	NC
21	B	602	CLA	ND
21	B	602	CLA	NA
21	C	510	CLA	NC
21	C	510	CLA	ND
21	C	510	CLA	NA
21	A	402	CLA	NC
21	A	402	CLA	ND

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Mol	Chain	Res	Type	Atom
21	A	402	CLA	NA
27	B	623	LMG	C2
27	B	623	LMG	C5
21	B	601	CLA	NC
21	B	601	CLA	ND
21	B	601	CLA	NA
21	G	402	CLA	NC
21	G	402	CLA	ND
21	G	402	CLA	NA
27	P	521	LMG	C2
27	P	521	LMG	C5
27	E	102	LMG	C2
27	E	102	LMG	C5
24	C	517	DGD	C2D
24	C	517	DGD	C5D
24	C	517	DGD	C5E
21	C	504	CLA	NC
21	C	504	CLA	ND
21	C	504	CLA	NA
21	N	617	CLA	NC
21	N	617	CLA	ND
21	N	617	CLA	NA
21	N	616	CLA	NC
21	N	616	CLA	ND
21	N	616	CLA	NA
27	C	520	LMG	C2
27	C	520	LMG	C5
21	P	513	CLA	NC
21	P	513	CLA	ND
21	P	513	CLA	NA
21	B	606	CLA	NC
21	B	606	CLA	ND
21	B	606	CLA	NA
21	P	509	CLA	NC
21	P	509	CLA	ND
21	P	509	CLA	NA
24	D	408	DGD	C2D
24	D	408	DGD	C5D
24	D	408	DGD	C5E
21	B	605	CLA	NC
21	B	605	CLA	ND
21	B	605	CLA	NA

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Mol	Chain	Res	Type	Atom
27	a	102	LMG	C2
27	a	102	LMG	C5
21	N	619	CLA	NC
21	N	619	CLA	ND
21	N	619	CLA	NA
21	N	618	CLA	NC
21	N	618	CLA	ND
21	N	618	CLA	NA
21	B	613	CLA	NC
21	B	613	CLA	ND
21	B	613	CLA	NA
21	C	508	CLA	NC
21	C	508	CLA	ND
21	C	508	CLA	NA
21	C	513	CLA	NC
21	C	513	CLA	ND
21	C	513	CLA	NA
21	B	616	CLA	NC
21	B	616	CLA	ND
21	B	616	CLA	NA
21	N	612	CLA	NC
21	N	612	CLA	ND
21	N	612	CLA	NA

All (2119) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	628	DGD	O1B-C1B-O2G-C2G
24	B	628	DGD	O2G-C2G-C3G-O3G
24	B	628	DGD	C2D-C1D-O3G-C3G
24	B	628	DGD	O6D-C1D-O3G-C3G
24	B	628	DGD	C5D-C6D-O5D-C1E
24	B	628	DGD	C2E-C1E-O5D-C6D
21	B	615	CLA	C1-C2-C3-C4
21	B	615	CLA	C1-C2-C3-C5
30	K	101	BCR	C21-C22-C23-C24
30	K	101	BCR	C37-C22-C23-C24
24	A	407	DGD	C2D-C1D-O3G-C3G
24	A	407	DGD	O6D-C1D-O3G-C3G
24	A	407	DGD	C4D-C5D-C6D-O5D
24	B	621	DGD	C2E-C1E-O5D-C6D
24	B	621	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
21	B	603	CLA	C4-C3-C5-C6
21	P	502	CLA	C1-C2-C3-C4
21	P	502	CLA	C1-C2-C3-C5
21	C	506	CLA	C1-C2-C3-C4
23	b	101	PL9	C7-C8-C9-C10
23	b	101	PL9	C7-C8-C9-C11
23	b	101	PL9	C12-C13-C14-C15
23	b	101	PL9	C12-C13-C14-C16
23	b	101	PL9	C17-C18-C19-C21
23	b	101	PL9	C22-C23-C24-C25
23	b	101	PL9	C22-C23-C24-C26
23	b	101	PL9	C27-C28-C29-C31
27	N	622	LMG	C11-C10-O7-C8
27	N	622	LMG	O10-C28-O8-C9
21	N	605	CLA	C2A-CAA-CBA-CGA
21	N	605	CLA	CBD-CGD-O2D-CED
21	D	401	CLA	C1-C2-C3-C4
21	D	401	CLA	C1-C2-C3-C5
30	b	102	BCR	C7-C8-C9-C34
21	G	404	CLA	CHA-CBD-CGD-O1D
21	G	404	CLA	C1-C2-C3-C4
21	G	404	CLA	C1-C2-C3-C5
21	B	611	CLA	C1-C2-C3-C4
26	B	627	SQD	O5-C5-C6-S
30	P	514	BCR	C7-C8-C9-C10
30	P	514	BCR	C7-C8-C9-C34
30	P	514	BCR	C11-C12-C13-C14
30	P	514	BCR	C11-C12-C13-C35
21	N	614	CLA	C1-C2-C3-C4
21	N	614	CLA	C1-C2-C3-C5
23	D	404	PL9	C12-C13-C14-C15
23	D	404	PL9	C12-C13-C14-C16
23	D	404	PL9	C24-C26-C27-C28
23	D	404	PL9	C34-C36-C37-C38
23	D	404	PL9	C42-C43-C44-C46
27	R	102	LMG	C2-C1-O1-C7
27	R	102	LMG	O6-C1-O1-C7
30	c	101	BCR	C21-C22-C23-C24
30	c	101	BCR	C37-C22-C23-C24
21	N	608	CLA	CHA-CBD-CGD-O1D
21	N	608	CLA	CBD-CGD-O2D-CED
21	N	608	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	P	511	CLA	CHA-CBD-CGD-O1D
21	P	511	CLA	CHA-CBD-CGD-O2D
21	P	511	CLA	C1-C2-C3-C4
21	P	511	CLA	C1-C2-C3-C5
21	N	609	CLA	C1A-C2A-CAA-CBA
21	N	609	CLA	C1-C2-C3-C4
21	N	609	CLA	C1-C2-C3-C5
21	C	505	CLA	C1A-C2A-CAA-CBA
21	C	505	CLA	C3A-C2A-CAA-CBA
21	C	505	CLA	CBD-CGD-O2D-CED
21	C	505	CLA	C1-C2-C3-C4
21	C	505	CLA	C1-C2-C3-C5
27	P	520	LMG	C2-C1-O1-C7
27	P	520	LMG	O6-C1-O1-C7
34	R	101	HEM	C3D-CAD-CBD-CGD
21	C	511	CLA	CHA-CBD-CGD-O1D
21	C	511	CLA	CHA-CBD-CGD-O2D
21	C	511	CLA	C1-C2-C3-C4
21	C	511	CLA	C1-C2-C3-C5
27	e	102	LMG	O6-C1-O1-C7
27	e	102	LMG	O9-C10-O7-C8
21	P	510	CLA	C1-C2-C3-C4
21	P	510	CLA	C1-C2-C3-C5
21	B	607	CLA	C1A-C2A-CAA-CBA
21	B	607	CLA	C3A-C2A-CAA-CBA
21	N	610	CLA	C3A-C2A-CAA-CBA
21	N	610	CLA	CHA-CBD-CGD-O1D
21	N	610	CLA	C1-C2-C3-C4
21	N	610	CLA	C1-C2-C3-C5
24	P	517	DGD	C2D-C1D-O3G-C3G
24	P	517	DGD	O6D-C1D-O3G-C3G
27	D	406	LMG	C11-C10-O7-C8
26	Q	408	SQD	C2-C1-O6-C44
26	Q	408	SQD	O5-C1-O6-C44
26	Q	408	SQD	O49-C7-O47-C45
21	N	607	CLA	C4-C3-C5-C6
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	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C27-C28-C29-C31
23	A	406	PL9	C37-C38-C39-C41
27	Q	407	LMG	O6-C1-O1-C7
30	B	620	BCR	C37-C22-C23-C24
21	B	608	CLA	C1A-C2A-CAA-CBA
21	B	608	CLA	C1-C2-C3-C4
21	B	608	CLA	C2-C3-C5-C6
30	D	405	BCR	C1-C6-C7-C8
30	D	405	BCR	C7-C8-C9-C10
30	D	405	BCR	C7-C8-C9-C34
30	B	617	BCR	C1-C6-C7-C8
21	Q	402	CLA	C1-C2-C3-C4
21	Q	402	CLA	C1-C2-C3-C5
30	P	516	BCR	C7-C8-C9-C10
30	P	516	BCR	C7-C8-C9-C34
26	B	624	SQD	C2-C1-O6-C44
26	B	624	SQD	O5-C1-O6-C44
26	B	624	SQD	O49-C7-O47-C45
26	B	624	SQD	C8-C7-O47-C45
21	C	502	CLA	C1-C2-C3-C4
21	C	502	CLA	C1-C2-C3-C5
21	B	614	CLA	CAD-CBD-CGD-O2D
21	B	614	CLA	C1-C2-C3-C5
21	B	604	CLA	CHA-CBD-CGD-O1D
21	B	604	CLA	CBD-CGD-O2D-CED
21	B	604	CLA	C1-C2-C3-C4
21	P	505	CLA	C1A-C2A-CAA-CBA
21	P	505	CLA	C3A-C2A-CAA-CBA
21	P	505	CLA	CBD-CGD-O2D-CED
21	P	505	CLA	O1D-CGD-O2D-CED
21	P	505	CLA	C1-C2-C3-C4
21	P	505	CLA	C1-C2-C3-C5
21	N	606	CLA	CHA-CBD-CGD-O1D
21	N	606	CLA	C1-C2-C3-C4
21	N	606	CLA	C1-C2-C3-C5
21	N	606	CLA	C6-C7-C8-C9
24	P	519	DGD	O6D-C1D-O3G-C3G
27	D	407	LMG	O6-C1-O1-C7
25	G	409	LHG	C1-C2-C3-O3
24	G	408	DGD	C2D-C1D-O3G-C3G
24	G	408	DGD	O6D-C1D-O3G-C3G
24	G	408	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
21	G	403	CLA	C1A-C2A-CAA-CBA
21	G	403	CLA	CHA-CBD-CGD-O1D
21	G	403	CLA	CHA-CBD-CGD-O2D
21	G	403	CLA	C1-C2-C3-C4
21	G	403	CLA	C1-C2-C3-C5
21	G	403	CLA	C2-C3-C5-C6
21	B	612	CLA	C1-C2-C3-C4
21	A	401	CLA	C1A-C2A-CAA-CBA
21	A	401	CLA	C3A-C2A-CAA-CBA
21	A	401	CLA	CBD-CGD-O2D-CED
27	Q	406	LMG	C11-C10-O7-C8
21	A	403	CLA	C1-C2-C3-C4
21	A	403	CLA	C1-C2-C3-C5
21	N	615	CLA	C1-C2-C3-C4
27	M	101	LMG	O6-C1-O1-C7
27	M	101	LMG	O9-C10-O7-C8
23	J	101	PL9	C7-C8-C9-C10
23	J	101	PL9	C7-C8-C9-C11
23	J	101	PL9	C12-C13-C14-C15
23	J	101	PL9	C12-C13-C14-C16
23	J	101	PL9	C17-C18-C19-C21
23	J	101	PL9	C22-C23-C24-C25
23	J	101	PL9	C22-C23-C24-C26
23	J	101	PL9	C27-C28-C29-C31
27	B	622	LMG	C11-C10-O7-C8
21	P	506	CLA	C1-C2-C3-C4
21	P	506	CLA	C1-C2-C3-C5
24	Q	409	DGD	O6D-C1D-O3G-C3G
21	C	509	CLA	O2A-C1-C2-C3
21	C	509	CLA	C1-C2-C3-C4
21	C	509	CLA	C1-C2-C3-C5
24	W	102	DGD	C2E-C1E-O5D-C6D
24	W	102	DGD	O6E-C1E-O5D-C6D
23	Q	405	PL9	C12-C13-C14-C15
23	Q	405	PL9	C12-C13-C14-C16
23	Q	405	PL9	C27-C28-C29-C31
23	Q	405	PL9	C42-C43-C44-C46
21	P	508	CLA	CBD-CGD-O2D-CED
27	C	519	LMG	C2-C1-O1-C7
27	C	519	LMG	O6-C1-O1-C7
24	N	602	DGD	O1B-C1B-O2G-C2G
24	N	602	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
24	N	602	DGD	C2D-C1D-O3G-C3G
24	N	602	DGD	O6D-C1D-O3G-C3G
24	N	602	DGD	C5D-C6D-O5D-C1E
24	N	602	DGD	C2E-C1E-O5D-C6D
21	N	620	CLA	C1A-C2A-CAA-CBA
21	N	620	CLA	CBD-CGD-O2D-CED
21	N	620	CLA	C1-C2-C3-C4
21	N	620	CLA	C1-C2-C3-C5
22	G	405	PHO	C2B-C3B-CAB-CBB
22	G	405	PHO	C4B-C3B-CAB-CBB
24	C	518	DGD	O6D-C1D-O3G-C3G
24	P	518	DGD	C2B-C1B-O2G-C2G
24	P	518	DGD	C2D-C1D-O3G-C3G
24	P	518	DGD	O6D-C1D-O3G-C3G
24	P	518	DGD	C4D-C5D-C6D-O5D
21	N	611	CLA	C1A-C2A-CAA-CBA
21	N	611	CLA	C3A-C2A-CAA-CBA
21	N	611	CLA	CHA-CBD-CGD-O1D
27	N	623	LMG	C2-C1-O1-C7
27	N	623	LMG	O6-C1-O1-C7
27	N	623	LMG	C11-C10-O7-C8
23	G	407	PL9	C7-C8-C9-C11
23	G	407	PL9	C12-C13-C14-C15
23	G	407	PL9	C12-C13-C14-C16
23	G	407	PL9	C17-C18-C19-C21
23	G	407	PL9	C27-C28-C29-C30
23	G	407	PL9	C27-C28-C29-C31
23	G	407	PL9	C37-C38-C39-C41
24	C	516	DGD	C2D-C1D-O3G-C3G
24	C	516	DGD	O6D-C1D-O3G-C3G
30	S	101	BCR	C7-C8-C9-C10
30	S	101	BCR	C7-C8-C9-C34
21	B	610	CLA	C1-C2-C3-C4
21	B	610	CLA	C1-C2-C3-C5
21	B	602	CLA	C1A-C2A-CAA-CBA
21	B	602	CLA	CHA-CBD-CGD-O1D
21	B	602	CLA	C1-C2-C3-C4
21	B	602	CLA	C1-C2-C3-C5
21	B	602	CLA	C6-C7-C8-C9
21	C	510	CLA	C1-C2-C3-C4
21	C	510	CLA	C1-C2-C3-C5
21	A	402	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	A	402	CLA	CHA-CBD-CGD-O1D
21	A	402	CLA	CHA-CBD-CGD-O2D
21	A	402	CLA	C1-C2-C3-C4
21	A	402	CLA	C1-C2-C3-C5
21	A	402	CLA	C2-C3-C5-C6
26	G	401	SQD	C5-C6-S-O9
30	C	515	BCR	C7-C8-C9-C10
30	C	515	BCR	C7-C8-C9-C34
27	B	623	LMG	C2-C1-O1-C7
27	B	623	LMG	O6-C1-O1-C7
27	B	623	LMG	C11-C10-O7-C8
21	B	601	CLA	C2A-CAA-CBA-CGA
21	B	601	CLA	CBD-CGD-O2D-CED
22	A	404	PHO	C2B-C3B-CAB-CBB
22	A	404	PHO	C4-C3-C5-C6
21	G	402	CLA	C1A-C2A-CAA-CBA
21	G	402	CLA	C3A-C2A-CAA-CBA
21	G	402	CLA	CBD-CGD-O2D-CED
30	P	515	BCR	C7-C8-C9-C34
27	P	521	LMG	C2-C1-O1-C7
27	P	521	LMG	O6-C1-O1-C7
27	P	521	LMG	C11-C10-O7-C8
27	E	102	LMG	C2-C1-O1-C7
27	E	102	LMG	O6-C1-O1-C7
24	C	517	DGD	C2B-C1B-O2G-C2G
24	C	517	DGD	C2D-C1D-O3G-C3G
24	C	517	DGD	O6D-C1D-O3G-C3G
24	C	517	DGD	C4D-C5D-C6D-O5D
30	C	514	BCR	C7-C8-C9-C10
30	C	514	BCR	C7-C8-C9-C34
30	C	514	BCR	C11-C12-C13-C35
26	N	601	SQD	O5-C5-C6-S
21	C	504	CLA	CBD-CGD-O2D-CED
21	N	617	CLA	CBD-CGD-O2D-CED
21	N	617	CLA	C1-C2-C3-C4
21	N	616	CLA	C1-C2-C3-C4
30	T	103	BCR	C21-C22-C23-C24
30	T	103	BCR	C37-C22-C23-C24
26	G	410	SQD	C2-C1-O6-C44
26	G	410	SQD	O5-C1-O6-C44
26	G	410	SQD	C5-C6-S-O7
26	G	410	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
26	G	410	SQD	C5-C6-S-O9
26	A	414	SQD	C5-C6-S-O9
27	C	520	LMG	C2-C1-O1-C7
27	C	520	LMG	O6-C1-O1-C7
27	C	520	LMG	C11-C10-O7-C8
21	P	513	CLA	C1A-C2A-CAA-CBA
21	P	513	CLA	C1-C2-C3-C4
21	B	606	CLA	C3A-C2A-CAA-CBA
21	B	606	CLA	CHA-CBD-CGD-O1D
21	B	606	CLA	C1-C2-C3-C4
21	B	606	CLA	C1-C2-C3-C5
30	T	101	BCR	C1-C6-C7-C8
21	P	509	CLA	O2A-C1-C2-C3
21	P	509	CLA	C1-C2-C3-C4
21	P	509	CLA	C1-C2-C3-C5
24	D	408	DGD	O6D-C1D-O3G-C3G
25	A	408	LHG	C1-C2-C3-O3
26	A	409	SQD	C2-C1-O6-C44
26	A	409	SQD	O5-C1-O6-C44
26	A	409	SQD	C5-C6-S-O7
26	A	409	SQD	C5-C6-S-O8
26	A	409	SQD	C5-C6-S-O9
21	B	605	CLA	C1-C2-C3-C4
21	B	605	CLA	C1-C2-C3-C5
21	N	619	CLA	C1-C2-C3-C4
21	N	619	CLA	C1-C2-C3-C5
21	N	618	CLA	CAD-CBD-CGD-O2D
21	B	613	CLA	CBD-CGD-O2D-CED
21	B	613	CLA	C1-C2-C3-C4
21	C	508	CLA	CBD-CGD-O2D-CED
34	E	101	HEM	C3D-CAD-CBD-CGD
21	C	513	CLA	C1A-C2A-CAA-CBA
21	C	513	CLA	CHA-CBD-CGD-O1D
21	C	513	CLA	C1-C2-C3-C4
21	B	616	CLA	C1A-C2A-CAA-CBA
21	B	616	CLA	CBD-CGD-O2D-CED
21	B	616	CLA	O1D-CGD-O2D-CED
21	B	616	CLA	C1-C2-C3-C4
21	B	616	CLA	C1-C2-C3-C5
21	N	612	CLA	C1A-C2A-CAA-CBA
21	N	612	CLA	C1-C2-C3-C4
21	N	612	CLA	C1-C2-C3-C5

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Mol	Chain	Res	Type	Atoms
21	N	612	CLA	C2-C3-C5-C6
21	N	614	CLA	O1D-CGD-O2D-CED
21	P	511	CLA	O1D-CGD-O2D-CED
21	C	505	CLA	O1D-CGD-O2D-CED
21	A	401	CLA	O1D-CGD-O2D-CED
21	N	620	CLA	O1D-CGD-O2D-CED
21	B	610	CLA	O1D-CGD-O2D-CED
21	C	508	CLA	O1D-CGD-O2D-CED
31	B	629	LMT	C3'-C4'-O1B-C1B
21	N	609	CLA	O1D-CGD-O2D-CED
21	C	511	CLA	O1D-CGD-O2D-CED
21	G	402	CLA	O1D-CGD-O2D-CED
21	B	605	CLA	O1D-CGD-O2D-CED
21	P	512	CLA	CBD-CGD-O2D-CED
21	B	603	CLA	CBD-CGD-O2D-CED
21	C	506	CLA	CBD-CGD-O2D-CED
21	C	503	CLA	CBD-CGD-O2D-CED
21	N	614	CLA	CBD-CGD-O2D-CED
21	P	511	CLA	CBD-CGD-O2D-CED
21	N	609	CLA	CBD-CGD-O2D-CED
21	C	511	CLA	CBD-CGD-O2D-CED
21	B	607	CLA	CBD-CGD-O2D-CED
21	N	610	CLA	CBD-CGD-O2D-CED
21	P	501	CLA	CBD-CGD-O2D-CED
21	C	501	CLA	CBD-CGD-O2D-CED
21	C	507	CLA	CBD-CGD-O2D-CED
21	N	607	CLA	CBD-CGD-O2D-CED
21	C	512	CLA	CBD-CGD-O2D-CED
21	P	503	CLA	CBD-CGD-O2D-CED
21	P	507	CLA	CBD-CGD-O2D-CED
21	N	611	CLA	CBD-CGD-O2D-CED
21	P	504	CLA	CBD-CGD-O2D-CED
21	B	610	CLA	CBD-CGD-O2D-CED
21	B	606	CLA	CBD-CGD-O2D-CED
21	B	605	CLA	CBD-CGD-O2D-CED
27	A	410	LMG	O10-C28-O8-C9
27	B	622	LMG	O10-C28-O8-C9
26	G	401	SQD	O10-C23-O48-C46
26	A	414	SQD	O10-C23-O48-C46
31	N	603	LMT	C3'-C4'-O1B-C1B
21	C	503	CLA	O1D-CGD-O2D-CED
21	N	608	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	604	CLA	O1D-CGD-O2D-CED
21	P	503	CLA	O1D-CGD-O2D-CED
21	P	507	CLA	O1D-CGD-O2D-CED
27	P	521	LMG	C8-C9-O8-C28
27	C	520	LMG	C8-C9-O8-C28
21	P	504	CLA	O1D-CGD-O2D-CED
21	C	504	CLA	O1D-CGD-O2D-CED
27	A	410	LMG	C29-C28-O8-C9
26	G	401	SQD	C24-C23-O48-C46
26	A	414	SQD	C24-C23-O48-C46
23	A	406	PL9	C37-C38-C39-C40
23	G	407	PL9	C37-C38-C39-C40
21	B	614	CLA	CBD-CGD-O2D-CED
21	C	509	CLA	CBD-CGD-O2D-CED
21	C	510	CLA	CBD-CGD-O2D-CED
21	P	513	CLA	CBD-CGD-O2D-CED
21	P	509	CLA	CBD-CGD-O2D-CED
21	N	618	CLA	CBD-CGD-O2D-CED
27	G	411	LMG	O10-C28-O8-C9
26	F	101	SQD	O10-C23-O48-C46
27	D	407	LMG	O10-C28-O8-C9
26	S	102	SQD	O10-C23-O48-C46
27	P	521	LMG	O10-C28-O8-C9
27	C	520	LMG	O10-C28-O8-C9
21	C	512	CLA	O1D-CGD-O2D-CED
27	P	521	LMG	C4-C5-C6-O5
21	P	508	CLA	O1D-CGD-O2D-CED
21	P	506	CLA	CBD-CGD-O2D-CED
27	N	622	LMG	O9-C10-O7-C8
27	D	406	LMG	O9-C10-O7-C8
27	Q	406	LMG	O9-C10-O7-C8
27	B	622	LMG	O9-C10-O7-C8
24	Q	409	DGD	O1B-C1B-O2G-C2G
24	P	518	DGD	O1B-C1B-O2G-C2G
27	N	623	LMG	O9-C10-O7-C8
27	B	623	LMG	O9-C10-O7-C8
27	P	521	LMG	O9-C10-O7-C8
24	C	517	DGD	O1B-C1B-O2G-C2G
27	C	520	LMG	O9-C10-O7-C8
27	C	520	LMG	C4-C5-C6-O5
21	B	608	CLA	C3-C5-C6-C7
27	G	411	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
27	N	622	LMG	C29-C28-O8-C9
27	P	520	LMG	C29-C28-O8-C9
27	B	622	LMG	C29-C28-O8-C9
27	C	519	LMG	C29-C28-O8-C9
27	P	521	LMG	C29-C28-O8-C9
27	C	520	LMG	C29-C28-O8-C9
24	B	628	DGD	C2B-C1B-O2G-C2G
27	e	102	LMG	C11-C10-O7-C8
26	Q	408	SQD	C8-C7-O47-C45
27	M	101	LMG	C11-C10-O7-C8
24	Q	409	DGD	C2B-C1B-O2G-C2G
24	N	602	DGD	C2B-C1B-O2G-C2G
21	B	608	CLA	CBD-CGD-O2D-CED
21	C	513	CLA	CBD-CGD-O2D-CED
21	C	507	CLA	O1D-CGD-O2D-CED
27	C	520	LMG	O6-C5-C6-O5
21	N	614	CLA	C2-C3-C5-C6
21	B	610	CLA	C2-C3-C5-C6
22	A	404	PHO	C2-C3-C5-C6
21	P	510	CLA	CBD-CGD-O2D-CED
21	A	401	CLA	C2A-CAA-CBA-CGA
21	N	611	CLA	C2A-CAA-CBA-CGA
21	B	610	CLA	C2A-CAA-CBA-CGA
21	G	402	CLA	C2A-CAA-CBA-CGA
21	N	612	CLA	C3-C5-C6-C7
26	F	101	SQD	C24-C23-O48-C46
27	D	407	LMG	C29-C28-O8-C9
24	Q	409	DGD	C2A-C1A-O1G-C1G
26	S	102	SQD	C24-C23-O48-C46
27	E	102	LMG	C29-C28-O8-C9
21	C	501	CLA	O1D-CGD-O2D-CED
21	B	611	CLA	C1-C2-C3-C5
21	B	608	CLA	C1-C2-C3-C5
21	N	615	CLA	C1-C2-C3-C5
21	P	513	CLA	C1-C2-C3-C5
21	C	513	CLA	C1-C2-C3-C5
23	D	404	PL9	C27-C28-C29-C30
23	A	406	PL9	C22-C23-C24-C25
23	Q	405	PL9	C27-C28-C29-C30
23	G	407	PL9	C17-C18-C19-C20
23	G	407	PL9	C22-C23-C24-C25
21	P	512	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	N	605	CLA	O1D-CGD-O2D-CED
27	P	521	LMG	O6-C5-C6-O5
23	D	404	PL9	C27-C28-C29-C31
23	A	406	PL9	C22-C23-C24-C26
23	G	407	PL9	C22-C23-C24-C26
27	P	520	LMG	O10-C28-O8-C9
27	Q	407	LMG	O10-C28-O8-C9
27	A	410	LMG	C4-C5-C6-O5
31	B	630	LMT	C3'-C4'-O1B-C1B
22	D	402	PHO	CBD-CGD-O2D-CED
21	B	611	CLA	CBD-CGD-O2D-CED
22	Q	403	PHO	CBD-CGD-O2D-CED
21	N	615	CLA	CBD-CGD-O2D-CED
21	N	612	CLA	CBD-CGD-O2D-CED
25	G	409	LHG	O2-C2-C3-O3
25	A	408	LHG	O2-C2-C3-O3
21	P	512	CLA	C3-C5-C6-C7
21	C	512	CLA	C3-C5-C6-C7
27	I	102	LMG	C29-C28-O8-C9
27	R	102	LMG	C29-C28-O8-C9
24	D	408	DGD	C2A-C1A-O1G-C1G
31	N	604	LMT	C3'-C4'-O1B-C1B
31	a	103	LMT	C3'-C4'-O1B-C1B
27	C	519	LMG	O10-C28-O8-C9
27	C	519	LMG	O6-C5-C6-O5
27	C	519	LMG	C4-C5-C6-O5
21	C	513	CLA	O1D-CGD-O2D-CED
24	P	517	DGD	C2B-C1B-O2G-C2G
24	C	516	DGD	C2B-C1B-O2G-C2G
24	D	408	DGD	C2B-C1B-O2G-C2G
23	J	101	PL9	C27-C28-C29-C30
27	N	622	LMG	O6-C5-C6-O5
27	B	622	LMG	O6-C5-C6-O5
24	D	408	DGD	O6E-C5E-C6E-O5E
27	P	520	LMG	C4-C5-C6-O5
31	I	103	LMT	C3'-C4'-O1B-C1B
24	Q	409	DGD	O1A-C1A-O1G-C1G
27	A	410	LMG	O6-C5-C6-O5
27	D	407	LMG	O6-C5-C6-O5
27	G	411	LMG	C4-C5-C6-O5
27	Q	407	LMG	C29-C28-O8-C9
27	G	411	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
27	Q	407	LMG	O6-C5-C6-O5
24	Q	409	DGD	O6E-C5E-C6E-O5E
24	D	408	DGD	O1B-C1B-O2G-C2G
27	E	102	LMG	O10-C28-O8-C9
23	b	101	PL9	C27-C28-C29-C30
23	Q	405	PL9	C47-C48-C49-C50
23	Q	405	PL9	C47-C48-C49-C51
27	P	520	LMG	O6-C5-C6-O5
22	G	405	PHO	C4-C3-C5-C6
21	B	603	CLA	C2-C3-C5-C6
21	N	607	CLA	C2-C3-C5-C6
22	G	405	PHO	C2-C3-C5-C6
24	P	518	DGD	O6D-C5D-C6D-O5D
24	C	517	DGD	O6D-C5D-C6D-O5D
21	B	607	CLA	C2A-CAA-CBA-CGA
21	N	617	CLA	O1D-CGD-O2D-CED
24	D	408	DGD	O1A-C1A-O1G-C1G
23	D	404	PL9	C29-C31-C32-C33
23	Q	405	PL9	C29-C31-C32-C33
23	Q	405	PL9	C34-C36-C37-C38
21	P	501	CLA	O1D-CGD-O2D-CED
21	B	601	CLA	O1D-CGD-O2D-CED
21	P	513	CLA	O1D-CGD-O2D-CED
21	B	613	CLA	O1D-CGD-O2D-CED
27	Q	406	LMG	O6-C5-C6-O5
24	P	517	DGD	O1B-C1B-O2G-C2G
24	C	516	DGD	O1B-C1B-O2G-C2G
24	D	408	DGD	C4E-C5E-C6E-O5E
27	I	102	LMG	O10-C28-O8-C9
27	R	102	LMG	O10-C28-O8-C9
21	N	618	CLA	C3-C5-C6-C7
22	G	405	PHO	CBA-CGA-O2A-C1
22	A	404	PHO	CBA-CGA-O2A-C1
27	a	102	LMG	C29-C28-O8-C9
21	A	403	CLA	CBD-CGD-O2D-CED
27	C	519	LMG	C10-C11-C12-C13
21	B	608	CLA	C15-C16-C17-C18
27	D	406	LMG	O6-C5-C6-O5
26	F	101	SQD	C24-C25-C26-C27
26	S	102	SQD	C24-C25-C26-C27
21	G	404	CLA	CBD-CGD-O2D-CED
27	I	102	LMG	C4-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
27	Q	407	LMG	C4-C5-C6-O5
27	D	407	LMG	C4-C5-C6-O5
21	C	505	CLA	C10-C11-C12-C13
21	P	501	CLA	C15-C16-C17-C18
21	C	512	CLA	C13-C15-C16-C17
21	N	606	CLA	C5-C6-C7-C8
21	N	620	CLA	C13-C15-C16-C17
25	G	412	LHG	O2-C2-C3-O3
25	A	411	LHG	O2-C2-C3-O3
27	B	623	LMG	C10-C11-C12-C13
27	e	102	LMG	C2-C1-O1-C7
27	M	101	LMG	C2-C1-O1-C7
24	Q	409	DGD	C2D-C1D-O3G-C3G
24	D	408	DGD	C2D-C1D-O3G-C3G
26	G	410	SQD	O47-C45-C46-O48
22	A	404	PHO	O1A-CGA-O2A-C1
24	Q	409	DGD	C4E-C5E-C6E-O5E
21	B	613	CLA	C2-C3-C5-C6
21	N	614	CLA	C14-C13-C15-C16
21	P	511	CLA	C6-C7-C8-C9
21	C	511	CLA	C6-C7-C8-C9
21	B	608	CLA	C6-C7-C8-C9
21	G	403	CLA	C6-C7-C8-C9
21	B	610	CLA	C14-C13-C15-C16
21	A	402	CLA	C6-C7-C8-C9
21	N	612	CLA	C6-C7-C8-C9
21	D	401	CLA	O1D-CGD-O2D-CED
21	C	501	CLA	C15-C16-C17-C18
30	K	101	BCR	C7-C8-C9-C34
30	Z	101	BCR	C7-C8-C9-C34
30	c	101	BCR	C7-C8-C9-C34
30	D	405	BCR	C37-C22-C23-C24
30	P	516	BCR	C37-C22-C23-C24
30	C	515	BCR	C37-C22-C23-C24
30	K	101	BCR	C7-C8-C9-C10
30	c	101	BCR	C7-C8-C9-C10
26	F	101	SQD	C8-C7-O47-C45
27	Q	401	LMG	C11-C10-O7-C8
26	S	102	SQD	C8-C7-O47-C45
27	P	520	LMG	C10-C11-C12-C13
24	W	102	DGD	C1B-C2B-C3B-C4B
23	D	404	PL9	C47-C48-C49-C50

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Mol	Chain	Res	Type	Atoms
27	a	102	LMG	O10-C28-O8-C9
21	D	401	CLA	C13-C15-C16-C17
21	P	506	CLA	C5-C6-C7-C8
21	P	508	CLA	C15-C16-C17-C18
21	C	510	CLA	C15-C16-C17-C18
21	N	616	CLA	C13-C15-C16-C17
21	C	506	CLA	O1D-CGD-O2D-CED
21	B	614	CLA	C3-C5-C6-C7
21	P	512	CLA	C13-C15-C16-C17
22	D	402	PHO	C15-C16-C17-C18
21	C	506	CLA	C5-C6-C7-C8
21	C	503	CLA	C10-C11-C12-C13
21	N	608	CLA	C13-C15-C16-C17
21	P	510	CLA	C15-C16-C17-C18
21	Q	402	CLA	C13-C15-C16-C17
21	Q	402	CLA	C15-C16-C17-C18
21	N	606	CLA	C13-C15-C16-C17
21	N	615	CLA	C15-C16-C17-C18
21	B	602	CLA	C5-C6-C7-C8
21	C	504	CLA	C13-C15-C16-C17
21	B	613	CLA	C5-C6-C7-C8
27	D	407	LMG	C10-C11-C12-C13
24	Q	409	DGD	C1B-C2B-C3B-C4B
27	N	623	LMG	C10-C11-C12-C13
27	P	521	LMG	C28-C29-C30-C31
24	A	407	DGD	O6D-C5D-C6D-O5D
24	G	408	DGD	O6D-C5D-C6D-O5D
27	M	101	LMG	O6-C5-C6-O5
21	B	615	CLA	C13-C15-C16-C17
21	D	401	CLA	C15-C16-C17-C18
21	P	505	CLA	C10-C11-C12-C13
21	G	403	CLA	C15-C16-C17-C18
21	B	612	CLA	C13-C15-C16-C17
21	P	508	CLA	C10-C11-C12-C13
21	N	611	CLA	C15-C16-C17-C18
21	P	504	CLA	C13-C15-C16-C17
21	P	504	CLA	C15-C16-C17-C18
21	B	602	CLA	C13-C15-C16-C17
21	C	504	CLA	C15-C16-C17-C18
21	P	513	CLA	C15-C16-C17-C18
21	N	619	CLA	C13-C15-C16-C17
21	C	508	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
21	C	508	CLA	C15-C16-C17-C18
21	C	513	CLA	C15-C16-C17-C18
21	B	616	CLA	C5-C6-C7-C8
21	B	616	CLA	C13-C15-C16-C17
21	N	612	CLA	C15-C16-C17-C18
23	b	101	PL9	C17-C18-C19-C20
27	N	622	LMG	C10-C11-C12-C13
27	Q	407	LMG	C10-C11-C12-C13
24	G	408	DGD	C1B-C2B-C3B-C4B
27	B	622	LMG	C10-C11-C12-C13
24	C	516	DGD	C1A-C2A-C3A-C4A
24	C	516	DGD	C1B-C2B-C3B-C4B
27	C	520	LMG	C28-C29-C30-C31
24	D	408	DGD	C1B-C2B-C3B-C4B
21	N	605	CLA	C10-C11-C12-C13
22	Q	403	PHO	C15-C16-C17-C18
21	C	507	CLA	C5-C6-C7-C8
21	B	604	CLA	C13-C15-C16-C17
21	N	620	CLA	C5-C6-C7-C8
21	N	620	CLA	C10-C11-C12-C13
21	A	402	CLA	C15-C16-C17-C18
21	B	601	CLA	C10-C11-C12-C13
21	B	601	CLA	C13-C15-C16-C17
21	B	616	CLA	C10-C11-C12-C13
24	P	518	DGD	O6E-C5E-C6E-O5E
24	G	408	DGD	C4E-C5E-C6E-O5E
21	N	605	CLA	C13-C15-C16-C17
21	B	611	CLA	C15-C16-C17-C18
21	B	607	CLA	C13-C15-C16-C17
21	P	503	CLA	C10-C11-C12-C13
21	P	507	CLA	C5-C6-C7-C8
21	N	611	CLA	C13-C15-C16-C17
24	B	621	DGD	C1B-C2B-C3B-C4B
24	P	517	DGD	C1B-C2B-C3B-C4B
27	D	406	LMG	C10-C11-C12-C13
27	Q	406	LMG	C10-C11-C12-C13
24	N	602	DGD	C1A-C2A-C3A-C4A
24	A	407	DGD	C4E-C5E-C6E-O5E
27	D	412	LMG	C11-C10-O7-C8
21	B	607	CLA	C15-C16-C17-C18
21	P	502	CLA	C11-C12-C13-C15
21	C	505	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	C	511	CLA	C12-C13-C15-C16
21	C	502	CLA	C11-C12-C13-C15
21	P	505	CLA	C6-C7-C8-C10
21	P	505	CLA	C11-C10-C8-C7
21	N	606	CLA	C11-C12-C13-C15
21	B	602	CLA	C11-C12-C13-C15
21	P	513	CLA	C12-C13-C15-C16
22	G	405	PHO	O1A-CGA-O2A-C1
21	N	614	CLA	C2A-CAA-CBA-CGA
21	C	511	CLA	C2A-CAA-CBA-CGA
21	P	508	CLA	C2A-CAA-CBA-CGA
21	C	508	CLA	C2A-CAA-CBA-CGA
21	P	510	CLA	O1D-CGD-O2D-CED
21	B	602	CLA	O1D-CGD-O2D-CED
21	Q	404	CLA	C15-C16-C17-C18
21	P	501	CLA	C10-C11-C12-C13
21	B	614	CLA	C15-C16-C17-C18
21	B	604	CLA	C8-C10-C11-C12
21	D	403	CLA	C15-C16-C17-C18
21	C	509	CLA	C15-C16-C17-C18
21	B	610	CLA	C8-C10-C11-C12
21	N	617	CLA	C5-C6-C7-C8
21	B	605	CLA	C5-C6-C7-C8
21	N	618	CLA	C15-C16-C17-C18
21	B	613	CLA	C13-C15-C16-C17
24	B	628	DGD	O6E-C1E-O5D-C6D
21	C	506	CLA	C15-C16-C17-C18
21	G	404	CLA	C10-C11-C12-C13
21	N	614	CLA	C8-C10-C11-C12
21	N	609	CLA	C5-C6-C7-C8
21	C	501	CLA	C10-C11-C12-C13
21	A	403	CLA	C15-C16-C17-C18
21	P	509	CLA	C15-C16-C17-C18
21	C	513	CLA	C13-C15-C16-C17
23	Q	405	PL9	C24-C26-C27-C28
24	B	628	DGD	C1A-C2A-C3A-C4A
27	Q	401	LMG	O9-C10-O7-C8
21	C	506	CLA	C13-C15-C16-C17
21	N	608	CLA	C8-C10-C11-C12
21	A	405	CLA	C13-C15-C16-C17
21	P	501	CLA	C8-C10-C11-C12
21	C	501	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	P	506	CLA	C13-C15-C16-C17
21	N	613	CLA	C13-C15-C16-C17
21	P	504	CLA	C10-C11-C12-C13
21	C	504	CLA	C10-C11-C12-C13
21	P	513	CLA	C13-C15-C16-C17
21	B	616	CLA	C15-C16-C17-C18
21	P	511	CLA	C5-C6-C7-C8
21	P	503	CLA	C5-C6-C7-C8
21	A	403	CLA	C10-C11-C12-C13
21	G	406	CLA	C13-C15-C16-C17
21	N	616	CLA	C5-C6-C7-C8
21	N	618	CLA	C5-C6-C7-C8
21	N	612	CLA	C5-C6-C7-C8
21	B	608	CLA	O1D-CGD-O2D-CED
27	a	102	LMG	C11-C10-O7-C8
21	G	404	CLA	O1D-CGD-O2D-CED
21	B	609	CLA	C13-C15-C16-C17
21	B	608	CLA	C5-C6-C7-C8
21	B	614	CLA	C5-C6-C7-C8
21	B	612	CLA	C5-C6-C7-C8
21	P	506	CLA	C15-C16-C17-C18
21	G	406	CLA	C10-C11-C12-C13
21	N	617	CLA	C13-C15-C16-C17
25	G	409	LHG	C24-C23-O8-C6
25	A	408	LHG	C24-C23-O8-C6
21	G	406	CLA	C5-C6-C7-C8
27	B	622	LMG	C4-C5-C6-O5
24	B	621	DGD	O6D-C5D-C6D-O5D
24	P	517	DGD	C1A-C2A-C3A-C4A
25	G	412	LHG	C1-C2-C3-O3
25	A	411	LHG	C1-C2-C3-O3
27	D	412	LMG	O9-C10-O7-C8
26	F	101	SQD	O49-C7-O47-C45
26	S	102	SQD	O49-C7-O47-C45
27	a	102	LMG	O9-C10-O7-C8
23	G	407	PL9	C35-C34-C36-C37
21	C	512	CLA	C2A-CAA-CBA-CGA
21	P	513	CLA	C2A-CAA-CBA-CGA
21	C	513	CLA	C2A-CAA-CBA-CGA
23	D	404	PL9	C47-C48-C49-C51
25	G	412	LHG	C24-C23-O8-C6
24	W	102	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
21	C	503	CLA	C5-C6-C7-C8
21	G	404	CLA	C15-C16-C17-C18
24	B	621	DGD	C6B-C7B-C8B-C9B
25	A	411	LHG	C11-C10-C9-C8
24	D	408	DGD	CAB-CBB-CCB-CDB
27	I	102	LMG	C11-C10-O7-C8
21	B	604	CLA	C15-C16-C17-C18
27	e	102	LMG	O6-C5-C6-O5
24	C	516	DGD	O6D-C5D-C6D-O5D
27	I	102	LMG	C12-C13-C14-C15
24	A	407	DGD	C8B-C9B-CAB-CBB
27	G	411	LMG	C34-C35-C36-C37
27	Q	401	LMG	C18-C19-C20-C21
27	Q	401	LMG	C32-C33-C34-C35
27	Q	407	LMG	C15-C16-C17-C18
27	D	407	LMG	C15-C16-C17-C18
24	G	408	DGD	C8B-C9B-CAB-CBB
25	G	412	LHG	C25-C26-C27-C28
24	Q	409	DGD	CAB-CBB-CCB-CDB
24	C	516	DGD	C3A-C4A-C5A-C6A
27	a	102	LMG	C12-C13-C14-C15
24	P	517	DGD	C4E-C5E-C6E-O5E
21	N	606	CLA	O1D-CGD-O2D-CED
24	B	628	DGD	C9B-CAB-CBB-CCB
27	D	412	LMG	C11-C12-C13-C14
27	D	412	LMG	C18-C19-C20-C21
27	A	410	LMG	C34-C35-C36-C37
24	C	518	DGD	C3B-C4B-C5B-C6B
24	C	518	DGD	C9B-CAB-CBB-CCB
24	C	516	DGD	C3B-C4B-C5B-C6B
27	C	520	LMG	C29-C30-C31-C32
24	D	408	DGD	CDB-CEB-CFB-CGB
27	I	102	LMG	O9-C10-O7-C8
21	C	506	CLA	C10-C11-C12-C13
27	I	102	LMG	C14-C15-C16-C17
27	D	412	LMG	C32-C33-C34-C35
27	N	622	LMG	C31-C32-C33-C34
24	P	517	DGD	C3B-C4B-C5B-C6B
24	P	519	DGD	C9B-CAB-CBB-CCB
27	C	520	LMG	C12-C13-C14-C15
21	Q	402	CLA	O1D-CGD-O2D-CED
24	P	517	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
25	G	409	LHG	C30-C31-C32-C33
27	M	101	LMG	C29-C30-C31-C32
25	A	411	LHG	C25-C26-C27-C28
31	I	103	LMT	C6-C7-C8-C9
27	E	102	LMG	C15-C16-C17-C18
25	A	408	LHG	C30-C31-C32-C33
24	P	517	DGD	O6D-C5D-C6D-O5D
24	P	517	DGD	C3A-C4A-C5A-C6A
27	D	407	LMG	C19-C20-C21-C22
27	D	407	LMG	C36-C37-C38-C39
25	G	412	LHG	C24-C25-C26-C27
24	W	102	DGD	C7A-C8A-C9A-CAA
26	S	102	SQD	C27-C28-C29-C30
24	C	516	DGD	C4A-C5A-C6A-C7A
31	N	603	LMT	C2-C3-C4-C5
24	C	517	DGD	CAB-CBB-CCB-CDB
24	D	408	DGD	C1A-C2A-C3A-C4A
27	I	102	LMG	C2-C1-O1-C7
27	a	102	LMG	C2-C1-O1-C7
25	A	411	LHG	C24-C23-O8-C6
27	Q	407	LMG	C36-C37-C38-C39
25	G	409	LHG	C25-C26-C27-C28
24	Q	409	DGD	C3B-C4B-C5B-C6B
24	Q	409	DGD	CDB-CEB-CFB-CGB
24	W	102	DGD	C6B-C7B-C8B-C9B
25	A	411	LHG	C24-C25-C26-C27
27	P	521	LMG	C12-C13-C14-C15
27	P	521	LMG	C29-C30-C31-C32
24	D	408	DGD	C3B-C4B-C5B-C6B
21	C	511	CLA	C5-C6-C7-C8
21	A	405	CLA	C10-C11-C12-C13
21	C	509	CLA	O1D-CGD-O2D-CED
27	I	102	LMG	O6-C5-C6-O5
23	D	404	PL9	C22-C23-C24-C25
23	Q	405	PL9	C22-C23-C24-C25
23	G	407	PL9	C7-C8-C9-C10
21	N	613	CLA	C4-C3-C5-C6
27	R	102	LMG	C15-C16-C17-C18
27	e	102	LMG	C29-C30-C31-C32
24	P	517	DGD	C4B-C5B-C6B-C7B
27	Q	407	LMG	C19-C20-C21-C22
24	Q	409	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
24	W	102	DGD	C5B-C6B-C7B-C8B
31	a	103	LMT	C6-C7-C8-C9
24	D	408	DGD	C3A-C4A-C5A-C6A
25	A	408	LHG	C25-C26-C27-C28
21	B	603	CLA	C6-C7-C8-C9
21	P	502	CLA	C11-C12-C13-C14
21	C	506	CLA	C11-C10-C8-C9
21	C	503	CLA	C6-C7-C8-C9
21	N	605	CLA	C11-C12-C13-C14
21	N	607	CLA	C6-C7-C8-C9
21	P	505	CLA	C11-C10-C8-C9
21	P	503	CLA	C6-C7-C8-C9
21	P	506	CLA	C11-C10-C8-C9
21	B	601	CLA	C11-C12-C13-C14
24	A	407	DGD	C1B-C2B-C3B-C4B
24	B	621	DGD	C7A-C8A-C9A-CAA
24	B	621	DGD	C5B-C6B-C7B-C8B
27	Q	401	LMG	C11-C12-C13-C14
24	P	519	DGD	C3B-C4B-C5B-C6B
25	G	412	LHG	C11-C10-C9-C8
24	N	602	DGD	C9B-CAB-CBB-CCB
24	P	518	DGD	C2A-C3A-C4A-C5A
27	N	623	LMG	C15-C16-C17-C18
27	B	623	LMG	C13-C14-C15-C16
24	C	517	DGD	C2A-C3A-C4A-C5A
26	N	601	SQD	C11-C10-C9-C8
24	D	408	DGD	CEB-CFB-CGB-CHB
21	A	405	CLA	C5-C6-C7-C8
24	C	517	DGD	O6E-C5E-C6E-O5E
21	Q	404	CLA	C2A-CAA-CBA-CGA
21	P	512	CLA	C2A-CAA-CBA-CGA
21	P	511	CLA	C2A-CAA-CBA-CGA
21	D	403	CLA	C2A-CAA-CBA-CGA
21	P	504	CLA	C2A-CAA-CBA-CGA
21	C	504	CLA	C2A-CAA-CBA-CGA
30	T	102	BCR	C7-C8-C9-C34
30	B	618	BCR	C7-C8-C9-C34
27	Q	401	LMG	C30-C31-C32-C33
24	Q	409	DGD	C5A-C6A-C7A-C8A
27	a	102	LMG	C14-C15-C16-C17
25	G	412	LHG	O1-C1-C2-C3
25	A	411	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
30	T	102	BCR	C7-C8-C9-C10
30	D	405	BCR	C21-C22-C23-C24
30	B	618	BCR	C7-C8-C9-C10
30	C	514	BCR	C11-C12-C13-C14
21	N	607	CLA	C5-C6-C7-C8
21	P	506	CLA	C10-C11-C12-C13
25	G	409	LHG	C8-C7-O7-C5
27	I	102	LMG	C13-C14-C15-C16
27	D	412	LMG	C30-C31-C32-C33
27	D	412	LMG	C31-C32-C33-C34
27	B	622	LMG	C15-C16-C17-C18
24	P	518	DGD	C2B-C3B-C4B-C5B
24	C	516	DGD	C4B-C5B-C6B-C7B
24	Q	409	DGD	C1A-C2A-C3A-C4A
27	C	520	LMG	C10-C11-C12-C13
27	I	102	LMG	C16-C17-C18-C19
27	N	622	LMG	C15-C16-C17-C18
27	A	410	LMG	C14-C15-C16-C17
27	Q	401	LMG	C31-C32-C33-C34
24	Q	409	DGD	C7B-C8B-C9B-CAB
31	B	629	LMT	C7-C8-C9-C10
24	N	602	DGD	C8B-C9B-CAB-CBB
31	N	603	LMT	C7-C8-C9-C10
24	D	408	DGD	C7B-C8B-C9B-CAB
27	N	622	LMG	C4-C5-C6-O5
27	I	102	LMG	O6-C1-O1-C7
24	N	602	DGD	O6E-C1E-O5D-C6D
27	a	102	LMG	O6-C1-O1-C7
21	P	503	CLA	C8-C10-C11-C12
27	N	622	LMG	C36-C37-C38-C39
24	Q	409	DGD	C6B-C7B-C8B-C9B
24	D	408	DGD	C6B-C7B-C8B-C9B
21	N	607	CLA	O1D-CGD-O2D-CED
27	G	411	LMG	C14-C15-C16-C17
27	A	410	LMG	C29-C30-C31-C32
27	D	407	LMG	C32-C33-C34-C35
27	N	623	LMG	C31-C32-C33-C34
24	C	517	DGD	C4B-C5B-C6B-C7B
27	a	102	LMG	C13-C14-C15-C16
27	a	102	LMG	C16-C17-C18-C19
27	N	623	LMG	C13-C14-C15-C16
24	B	628	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
27	B	622	LMG	C36-C37-C38-C39
24	D	408	DGD	C5A-C6A-C7A-C8A
22	Q	403	PHO	O1D-CGD-O2D-CED
21	P	512	CLA	C3A-C2A-CAA-CBA
21	C	507	CLA	C3A-C2A-CAA-CBA
21	B	608	CLA	C3A-C2A-CAA-CBA
21	C	512	CLA	C3A-C2A-CAA-CBA
21	G	403	CLA	C3A-C2A-CAA-CBA
21	P	507	CLA	C3A-C2A-CAA-CBA
21	B	602	CLA	C3A-C2A-CAA-CBA
21	A	402	CLA	C3A-C2A-CAA-CBA
21	N	612	CLA	C3A-C2A-CAA-CBA
27	G	411	LMG	C29-C30-C31-C32
26	B	627	SQD	C11-C10-C9-C8
27	Q	407	LMG	C32-C33-C34-C35
24	Q	409	DGD	CEB-CFB-CGB-CHB
24	Q	409	DGD	CCB-CDB-CEB-CFB
24	D	408	DGD	CCB-CDB-CEB-CFB
27	A	410	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
31	N	624	LMT	C1-C2-C3-C4
25	G	409	LHG	O9-C7-O7-C5
27	B	622	LMG	C31-C32-C33-C34
24	Q	409	DGD	C2A-C3A-C4A-C5A
27	B	623	LMG	C31-C32-C33-C34
21	A	402	CLA	O2A-C1-C2-C3
31	B	625	LMT	C1-C2-C3-C4
27	B	623	LMG	C29-C28-O8-C9
21	B	604	CLA	C2-C3-C5-C6
27	Q	407	LMG	C11-C10-O7-C8
24	P	519	DGD	C2B-C1B-O2G-C2G
27	D	407	LMG	C11-C10-O7-C8
27	C	519	LMG	C11-C10-O7-C8
26	F	101	SQD	C27-C28-C29-C30
24	P	518	DGD	CAB-CBB-CCB-CDB
26	G	410	SQD	C17-C18-C19-C20
26	A	409	SQD	C15-C16-C17-C18
25	G	409	LHG	O10-C23-O8-C6
24	C	517	DGD	C2B-C3B-C4B-C5B
27	D	407	LMG	C13-C14-C15-C16
31	B	629	LMT	C2-C3-C4-C5
27	N	623	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
25	A	408	LHG	O10-C23-O8-C6
27	P	521	LMG	C10-C11-C12-C13
26	B	627	SQD	C11-C12-C13-C14
27	Q	407	LMG	O9-C10-O7-C8
27	D	407	LMG	O9-C10-O7-C8
27	C	519	LMG	O9-C10-O7-C8
24	P	519	DGD	C8B-C9B-CAB-CBB
27	B	623	LMG	C15-C16-C17-C18
27	E	102	LMG	C17-C18-C19-C20
24	D	408	DGD	C2A-C3A-C4A-C5A
21	N	608	CLA	C15-C16-C17-C18
21	P	505	CLA	C15-C16-C17-C18
27	G	411	LMG	C30-C31-C32-C33
27	B	622	LMG	C17-C18-C19-C20
24	C	516	DGD	C2A-C3A-C4A-C5A
30	K	101	BCR	C23-C24-C25-C26
30	K	101	BCR	C23-C24-C25-C30
30	H	101	BCR	C1-C6-C7-C8
30	H	101	BCR	C5-C6-C7-C8
30	Z	101	BCR	C1-C6-C7-C8
30	Z	101	BCR	C5-C6-C7-C8
30	T	102	BCR	C23-C24-C25-C26
30	T	102	BCR	C23-C24-C25-C30
30	c	101	BCR	C23-C24-C25-C26
30	c	101	BCR	C23-C24-C25-C30
30	D	405	BCR	C5-C6-C7-C8
30	B	617	BCR	C5-C6-C7-C8
30	P	516	BCR	C23-C24-C25-C26
30	P	516	BCR	C23-C24-C25-C30
30	B	618	BCR	C23-C24-C25-C26
30	B	618	BCR	C23-C24-C25-C30
30	W	101	BCR	C1-C6-C7-C8
30	W	101	BCR	C5-C6-C7-C8
30	S	101	BCR	C1-C6-C7-C8
30	S	101	BCR	C5-C6-C7-C8
30	C	515	BCR	C1-C6-C7-C8
30	C	515	BCR	C23-C24-C25-C26
30	C	515	BCR	C23-C24-C25-C30
30	P	515	BCR	C1-C6-C7-C8
30	P	515	BCR	C5-C6-C7-C8
30	T	101	BCR	C5-C6-C7-C8
27	B	622	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	P	509	CLA	O1D-CGD-O2D-CED
21	N	620	CLA	C15-C16-C17-C18
25	A	408	LHG	C8-C7-O7-C5
27	N	622	LMG	C17-C18-C19-C20
24	Q	409	DGD	C4B-C5B-C6B-C7B
25	G	412	LHG	O10-C23-O8-C6
24	D	408	DGD	C4B-C5B-C6B-C7B
21	B	609	CLA	C4-C3-C5-C6
21	B	603	CLA	C6-C7-C8-C10
21	B	603	CLA	C11-C12-C13-C15
21	C	506	CLA	C11-C10-C8-C7
21	C	503	CLA	C6-C7-C8-C10
21	C	503	CLA	C11-C12-C13-C15
21	N	605	CLA	C11-C12-C13-C15
21	P	511	CLA	C12-C13-C15-C16
22	Q	403	PHO	C11-C10-C8-C7
22	Q	403	PHO	C12-C13-C15-C16
21	C	505	CLA	C11-C10-C8-C7
21	N	607	CLA	C6-C7-C8-C10
21	N	607	CLA	C11-C12-C13-C15
21	N	606	CLA	C12-C13-C15-C16
21	P	503	CLA	C6-C7-C8-C10
21	P	503	CLA	C11-C12-C13-C15
21	P	506	CLA	C11-C10-C8-C7
21	P	507	CLA	C11-C10-C8-C7
21	B	601	CLA	C6-C7-C8-C10
21	B	601	CLA	C11-C12-C13-C15
21	C	513	CLA	C12-C13-C15-C16
25	A	411	LHG	O10-C23-O8-C6
24	W	102	DGD	C4B-C5B-C6B-C7B
26	B	627	SQD	O49-C7-O47-C45
27	P	520	LMG	O9-C10-O7-C8
24	P	519	DGD	O1B-C1B-O2G-C2G
26	N	601	SQD	O49-C7-O47-C45
25	A	408	LHG	O9-C7-O7-C5
27	D	412	LMG	C28-C29-C30-C31
27	B	622	LMG	C28-C29-C30-C31
27	E	102	LMG	C28-C29-C30-C31
27	A	410	LMG	C30-C31-C32-C33
27	Q	407	LMG	C14-C15-C16-C17
24	N	602	DGD	O6E-C5E-C6E-O5E
27	N	622	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	E	102	LMG	C18-C19-C20-C21
22	D	402	PHO	O1D-CGD-O2D-CED
21	A	403	CLA	O1D-CGD-O2D-CED
24	B	621	DGD	C4B-C5B-C6B-C7B
23	J	101	PL9	C17-C18-C19-C20
27	N	622	LMG	C18-C19-C20-C21
27	a	102	LMG	C4-C5-C6-O5
21	B	615	CLA	C5-C6-C7-C8
23	G	407	PL9	C24-C26-C27-C28
24	A	407	DGD	C5B-C6B-C7B-C8B
24	P	517	DGD	C2A-C3A-C4A-C5A
26	B	627	SQD	C8-C7-O47-C45
27	P	520	LMG	C11-C10-O7-C8
24	C	518	DGD	C2B-C1B-O2G-C2G
26	N	601	SQD	C8-C7-O47-C45
26	N	601	SQD	C11-C12-C13-C14
26	G	410	SQD	C15-C16-C17-C18
22	A	404	PHO	C4B-C3B-CAB-CBB
21	N	614	CLA	C10-C11-C12-C13
22	Q	403	PHO	C10-C11-C12-C13
31	N	625	LMT	C2B-C1B-O1B-C4'
21	B	612	CLA	CBD-CGD-O2D-CED
24	C	518	DGD	O1B-C1B-O2G-C2G
27	N	622	LMG	C28-C29-C30-C31
27	Q	401	LMG	C28-C29-C30-C31
27	B	622	LMG	C19-C20-C21-C22
27	Q	407	LMG	C2-C1-O1-C7
27	D	407	LMG	C2-C1-O1-C7
21	N	609	CLA	C15-C16-C17-C18
27	G	411	LMG	O1-C7-C8-O7
27	A	410	LMG	O1-C7-C8-O7
26	Q	408	SQD	O6-C44-C45-O47
26	B	624	SQD	O6-C44-C45-O47
24	P	518	DGD	O2G-C2G-C3G-O3G
24	C	517	DGD	O2G-C2G-C3G-O3G
26	A	409	SQD	O47-C45-C46-O48
27	D	407	LMG	C14-C15-C16-C17
27	B	622	LMG	C18-C19-C20-C21
27	N	622	LMG	C19-C20-C21-C22
27	R	102	LMG	C18-C19-C20-C21
24	G	408	DGD	C5B-C6B-C7B-C8B
27	D	412	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
21	P	505	CLA	C8-C10-C11-C12
21	B	610	CLA	C10-C11-C12-C13
21	N	619	CLA	C5-C6-C7-C8
23	D	404	PL9	C18-C19-C21-C22
21	N	617	CLA	C2-C3-C5-C6
23	G	407	PL9	C4-C3-C7-C8
22	D	402	PHO	C14-C13-C15-C16
21	B	603	CLA	C11-C12-C13-C14
21	C	503	CLA	C11-C10-C8-C9
21	C	503	CLA	C11-C12-C13-C14
21	N	605	CLA	C6-C7-C8-C9
21	P	511	CLA	C14-C13-C15-C16
22	Q	403	PHO	C14-C13-C15-C16
21	C	505	CLA	C6-C7-C8-C9
21	C	511	CLA	C14-C13-C15-C16
21	N	607	CLA	C11-C12-C13-C14
21	C	502	CLA	C11-C12-C13-C14
21	P	505	CLA	C6-C7-C8-C9
21	N	606	CLA	C11-C12-C13-C14
21	P	503	CLA	C11-C12-C13-C14
21	P	507	CLA	C11-C10-C8-C9
21	B	602	CLA	C11-C12-C13-C14
21	B	601	CLA	C6-C7-C8-C9
21	P	513	CLA	C11-C10-C8-C9
21	N	619	CLA	C14-C13-C15-C16
21	C	513	CLA	C11-C10-C8-C9
21	N	605	CLA	C2C-C3C-CAC-CBC
26	F	101	SQD	C11-C12-C13-C14
24	C	518	DGD	CAB-CBB-CCB-CDB
21	N	610	CLA	C2A-CAA-CBA-CGA
21	B	603	CLA	C5-C6-C7-C8
21	C	503	CLA	C8-C10-C11-C12
21	B	605	CLA	C15-C16-C17-C18
26	S	102	SQD	C15-C16-C17-C18
26	A	409	SQD	C27-C28-C29-C30
30	b	102	BCR	C7-C8-C9-C10
27	N	623	LMG	O10-C28-O8-C9
27	B	623	LMG	O10-C28-O8-C9
21	C	510	CLA	O1D-CGD-O2D-CED
21	P	512	CLA	C1A-C2A-CAA-CBA
21	D	401	CLA	C1A-C2A-CAA-CBA
21	N	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	C	507	CLA	C1A-C2A-CAA-CBA
21	C	512	CLA	C1A-C2A-CAA-CBA
21	P	507	CLA	C1A-C2A-CAA-CBA
21	B	606	CLA	C1A-C2A-CAA-CBA
21	Q	402	CLA	C5-C6-C7-C8
21	C	502	CLA	C13-C15-C16-C17
21	G	403	CLA	C5-C6-C7-C8
21	N	613	CLA	C5-C6-C7-C8
21	A	402	CLA	C5-C6-C7-C8
24	P	518	DGD	CCB-CDB-CEB-CFB
26	G	410	SQD	C27-C28-C29-C30
21	C	505	CLA	C8-C10-C11-C12
23	A	406	PL9	C7-C8-C9-C10
27	G	411	LMG	C31-C32-C33-C34
27	R	102	LMG	C17-C18-C19-C20
27	E	102	LMG	O6-C5-C6-O5
24	B	621	DGD	C3B-C4B-C5B-C6B
24	W	102	DGD	C3B-C4B-C5B-C6B
21	N	614	CLA	C13-C15-C16-C17
31	B	626	LMT	C2B-C1B-O1B-C4'
26	S	102	SQD	C11-C12-C13-C14
27	Q	401	LMG	O6-C5-C6-O5
22	D	402	PHO	C10-C11-C12-C13
21	B	610	CLA	C13-C15-C16-C17
24	A	407	DGD	C3B-C4B-C5B-C6B
24	P	517	DGD	C4D-C5D-C6D-O5D
24	C	516	DGD	C4D-C5D-C6D-O5D
24	B	621	DGD	O1G-C1G-C2G-C3G
27	P	520	LMG	C7-C8-C9-O8
27	e	102	LMG	C7-C8-C9-O8
24	W	102	DGD	O1G-C1G-C2G-C3G
27	C	519	LMG	C7-C8-C9-O8
24	P	518	DGD	C1G-C2G-C3G-O3G
24	C	517	DGD	C1G-C2G-C3G-O3G
26	G	410	SQD	C44-C45-C46-O48
21	P	502	CLA	C13-C15-C16-C17
21	N	610	CLA	C10-C11-C12-C13
24	B	621	DGD	CAB-CBB-CCB-CDB
26	Q	408	SQD	C45-C44-O6-C1
27	Q	407	LMG	C8-C7-O1-C1
26	B	624	SQD	C45-C44-O6-C1
27	D	407	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
27	Q	406	LMG	C31-C32-C33-C34
26	A	409	SQD	C17-C18-C19-C20
27	N	623	LMG	C12-C13-C14-C15
26	G	410	SQD	C7-C8-C9-C10
24	G	408	DGD	C7B-C8B-C9B-CAB
23	A	406	PL9	C24-C26-C27-C28
27	R	102	LMG	O6-C5-C6-O5
24	P	518	DGD	C4B-C5B-C6B-C7B
23	Q	405	PL9	C42-C43-C44-C45
24	W	102	DGD	CAB-CBB-CCB-CDB
24	C	517	DGD	C3A-C4A-C5A-C6A
24	C	517	DGD	CCB-CDB-CEB-CFB
21	B	612	CLA	C4-C3-C5-C6
21	N	615	CLA	C4-C3-C5-C6
21	N	616	CLA	C4-C3-C5-C6
24	B	628	DGD	C4A-C5A-C6A-C7A
24	C	518	DGD	C8B-C9B-CAB-CBB
21	P	501	CLA	C13-C15-C16-C17
21	N	607	CLA	C13-C15-C16-C17
27	D	406	LMG	C38-C39-C40-C41
24	P	518	DGD	C4A-C5A-C6A-C7A
26	N	601	SQD	C9-C10-C11-C12
24	Q	409	DGD	C1G-C2G-O2G-C1B
24	D	408	DGD	C1G-C2G-O2G-C1B
21	C	505	CLA	C15-C16-C17-C18
27	N	622	LMG	C30-C31-C32-C33
24	C	518	DGD	CDB-CEB-CFB-CGB
21	B	609	CLA	C5-C6-C7-C8
27	E	102	LMG	C19-C20-C21-C22
26	A	409	SQD	C7-C8-C9-C10
27	B	622	LMG	C30-C31-C32-C33
24	D	408	DGD	C7A-C8A-C9A-CAA
31	N	625	LMT	O5B-C1B-O1B-C4'
24	P	519	DGD	CFA-CGA-CHA-CIA
21	D	401	CLA	C5-C6-C7-C8
27	Q	406	LMG	C36-C37-C38-C39
21	B	601	CLA	C2C-C3C-CAC-CBC
24	P	519	DGD	O1G-C1G-C2G-O2G
26	G	401	SQD	O6-C44-C45-O47
26	A	414	SQD	O6-C44-C45-O47
21	C	506	CLA	C1-C2-C3-C5
26	S	102	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
21	B	606	CLA	C10-C11-C12-C13
27	I	102	LMG	C18-C19-C20-C21
31	B	626	LMT	O5B-C1B-O1B-C4'
21	B	611	CLA	C4-C3-C5-C6
23	Q	405	PL9	C35-C34-C36-C37
21	B	615	CLA	C12-C13-C15-C16
22	D	402	PHO	C11-C10-C8-C7
22	D	402	PHO	C12-C13-C15-C16
21	B	609	CLA	C12-C13-C15-C16
21	P	502	CLA	C12-C13-C15-C16
21	C	506	CLA	C11-C12-C13-C15
21	C	503	CLA	C11-C10-C8-C7
21	N	605	CLA	C6-C7-C8-C10
21	D	401	CLA	C12-C13-C15-C16
21	G	404	CLA	C6-C7-C8-C10
21	N	614	CLA	C12-C13-C15-C16
21	P	511	CLA	C11-C10-C8-C7
21	C	505	CLA	C12-C13-C15-C16
21	C	511	CLA	C11-C10-C8-C7
21	N	610	CLA	C12-C13-C15-C16
21	Q	402	CLA	C12-C13-C15-C16
21	C	502	CLA	C12-C13-C15-C16
21	P	503	CLA	C11-C10-C8-C7
21	G	403	CLA	C6-C7-C8-C10
21	N	615	CLA	C6-C7-C8-C10
21	G	406	CLA	C11-C10-C8-C7
21	P	508	CLA	C12-C13-C15-C16
21	P	504	CLA	C6-C7-C8-C10
21	B	610	CLA	C12-C13-C15-C16
21	B	602	CLA	C12-C13-C15-C16
21	C	510	CLA	C6-C7-C8-C10
21	C	504	CLA	C6-C7-C8-C10
21	N	617	CLA	C11-C10-C8-C7
21	P	513	CLA	C11-C10-C8-C7
21	B	606	CLA	C12-C13-C15-C16
21	N	619	CLA	C12-C13-C15-C16
21	B	613	CLA	C11-C10-C8-C7
21	C	513	CLA	C11-C10-C8-C7
21	B	615	CLA	C11-C10-C8-C9
21	B	615	CLA	C14-C13-C15-C16
22	D	402	PHO	C11-C10-C8-C9
21	B	609	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	P	502	CLA	C14-C13-C15-C16
21	D	401	CLA	C14-C13-C15-C16
21	G	404	CLA	C6-C7-C8-C9
21	P	511	CLA	C11-C10-C8-C9
22	Q	403	PHO	C11-C10-C8-C9
21	C	505	CLA	C14-C13-C15-C16
21	C	511	CLA	C11-C10-C8-C9
21	B	608	CLA	C11-C12-C13-C14
21	Q	402	CLA	C14-C13-C15-C16
21	C	502	CLA	C14-C13-C15-C16
21	P	505	CLA	C14-C13-C15-C16
21	P	503	CLA	C11-C10-C8-C9
21	N	613	CLA	C14-C13-C15-C16
21	B	602	CLA	C11-C10-C8-C9
21	N	617	CLA	C11-C10-C8-C9
21	P	513	CLA	C14-C13-C15-C16
21	B	613	CLA	C11-C10-C8-C9
21	C	508	CLA	C11-C10-C8-C9
21	C	513	CLA	C14-C13-C15-C16
27	D	412	LMG	C15-C16-C17-C18
27	R	102	LMG	C19-C20-C21-C22
27	Q	407	LMG	C13-C14-C15-C16
24	G	408	DGD	C7A-C8A-C9A-CAA
24	P	518	DGD	C3A-C4A-C5A-C6A
21	C	501	CLA	C13-C15-C16-C17
21	C	509	CLA	C10-C11-C12-C13
21	B	616	CLA	C2A-CAA-CBA-CGA
27	A	410	LMG	C19-C20-C21-C22
27	A	410	LMG	C31-C32-C33-C34
21	B	614	CLA	C2C-C3C-CAC-CBC
26	N	601	SQD	C12-C13-C14-C15
30	B	620	BCR	C21-C22-C23-C24
21	B	605	CLA	C10-C11-C12-C13
26	B	627	SQD	C9-C10-C11-C12
27	Q	406	LMG	C38-C39-C40-C41
27	N	623	LMG	C4-C5-C6-O5
26	B	627	SQD	C24-C23-O48-C46
26	N	601	SQD	C24-C23-O48-C46
24	B	628	DGD	C5B-C6B-C7B-C8B
24	C	518	DGD	CEA-CFA-CGA-CHA
27	B	623	LMG	C12-C13-C14-C15
27	M	101	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
21	N	620	CLA	C8-C10-C11-C12
21	B	603	CLA	O1D-CGD-O2D-CED
26	F	101	SQD	C15-C16-C17-C18
23	D	404	PL9	C35-C34-C36-C37
23	A	406	PL9	C35-C34-C36-C37
21	B	603	CLA	C13-C15-C16-C17
21	N	609	CLA	C10-C11-C12-C13
27	N	622	LMG	C32-C33-C34-C35
27	G	411	LMG	C19-C20-C21-C22
27	D	406	LMG	C36-C37-C38-C39
21	N	606	CLA	CBD-CGD-O2D-CED
21	N	609	CLA	C3A-C2A-CAA-CBA
21	P	504	CLA	C3A-C2A-CAA-CBA
21	P	513	CLA	C3A-C2A-CAA-CBA
21	C	513	CLA	C3A-C2A-CAA-CBA
21	B	616	CLA	C8-C10-C11-C12
27	D	406	LMG	C31-C32-C33-C34
24	C	518	DGD	CFA-CGA-CHA-CIA
27	Q	401	LMG	C12-C13-C14-C15
24	P	519	DGD	CEA-CFA-CGA-CHA
24	Q	409	DGD	C8B-C9B-CAB-CBB
22	A	404	PHO	C5-C6-C7-C8
24	P	519	DGD	CAB-CBB-CCB-CDB
26	G	401	SQD	C17-C18-C19-C20
26	G	410	SQD	C24-C25-C26-C27
27	G	411	LMG	O1-C7-C8-C9
26	Q	408	SQD	O6-C44-C45-C46
26	B	624	SQD	O6-C44-C45-C46
27	B	622	LMG	O1-C7-C8-C9
24	Q	409	DGD	C1G-C2G-C3G-O3G
24	N	602	DGD	C1G-C2G-C3G-O3G
27	N	623	LMG	C7-C8-C9-O8
27	B	623	LMG	C7-C8-C9-O8
26	A	409	SQD	C44-C45-C46-O48
27	A	410	LMG	C20-C21-C22-C23
31	I	103	LMT	C5'-C4'-O1B-C1B
24	D	408	DGD	CBA-CCA-CDA-CEA
24	A	407	DGD	C7A-C8A-C9A-CAA
24	B	621	DGD	C2A-C3A-C4A-C5A
24	N	602	DGD	C4A-C5A-C6A-C7A
24	B	628	DGD	O6E-C5E-C6E-O5E
31	a	103	LMT	C5'-C4'-O1B-C1B

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Mol	Chain	Res	Type	Atoms
21	N	613	CLA	C2-C3-C5-C6
24	W	102	DGD	C4D-C5D-C6D-O5D
31	N	604	LMT	C5'-C4'-O1B-C1B
24	G	408	DGD	C3B-C4B-C5B-C6B
24	Q	409	DGD	CBA-CCA-CDA-CEA
24	N	602	DGD	C2A-C3A-C4A-C5A
24	D	408	DGD	C8B-C9B-CAB-CBB
27	D	412	LMG	C12-C13-C14-C15
24	C	516	DGD	C4E-C5E-C6E-O5E
26	B	627	SQD	C10-C11-C12-C13
21	B	606	CLA	C2A-CAA-CBA-CGA
26	N	601	SQD	C10-C11-C12-C13
27	a	102	LMG	C18-C19-C20-C21
24	B	621	DGD	C4D-C5D-C6D-O5D
23	A	406	PL9	C32-C33-C34-C35
23	G	407	PL9	C32-C33-C34-C35
24	P	519	DGD	CDB-CEB-CFB-CGB
24	W	102	DGD	C2A-C3A-C4A-C5A
27	C	519	LMG	C34-C35-C36-C37
21	N	611	CLA	O1D-CGD-O2D-CED
21	N	609	CLA	C13-C15-C16-C17
22	G	405	PHO	C5-C6-C7-C8
31	B	630	LMT	C1-C2-C3-C4
26	N	601	SQD	O10-C23-O48-C46
26	F	101	SQD	C29-C30-C31-C32
27	B	622	LMG	O1-C7-C8-O7
27	C	519	LMG	O7-C8-C9-O8
24	C	518	DGD	O1G-C1G-C2G-O2G
21	P	512	CLA	CAA-CBA-CGA-O2A
24	Q	409	DGD	O6E-C1E-O5D-C6D
24	A	407	DGD	C7B-C8B-C9B-CAB
27	P	520	LMG	C34-C35-C36-C37
21	P	510	CLA	C2-C1-O2A-CGA
21	P	505	CLA	C2-C1-O2A-CGA
21	C	510	CLA	C2-C1-O2A-CGA
21	N	617	CLA	C2-C1-O2A-CGA
21	N	616	CLA	C2-C1-O2A-CGA
21	N	618	CLA	C2-C1-O2A-CGA
21	B	613	CLA	C2-C1-O2A-CGA
24	A	407	DGD	C4B-C5B-C6B-C7B
22	Q	403	PHO	C6-C7-C8-C9
21	C	505	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	N	610	CLA	C14-C13-C15-C16
21	N	606	CLA	C11-C10-C8-C9
21	A	403	CLA	C6-C7-C8-C9
21	P	508	CLA	C11-C10-C8-C9
21	B	606	CLA	C14-C13-C15-C16
21	N	619	CLA	C11-C10-C8-C9
27	A	410	LMG	C15-C16-C17-C18
21	P	509	CLA	C10-C11-C12-C13
21	C	513	CLA	C5-C6-C7-C8
30	P	516	BCR	C1-C6-C7-C8
30	P	516	BCR	C5-C6-C7-C8
30	I	101	BCR	C1-C6-C7-C8
30	I	101	BCR	C5-C6-C7-C8
30	I	101	BCR	C23-C24-C25-C26
30	I	101	BCR	C23-C24-C25-C30
30	C	515	BCR	C5-C6-C7-C8
30	a	101	BCR	C1-C6-C7-C8
30	a	101	BCR	C5-C6-C7-C8
30	a	101	BCR	C23-C24-C25-C26
30	a	101	BCR	C23-C24-C25-C30
21	P	510	CLA	C13-C15-C16-C17
21	P	508	CLA	C5-C6-C7-C8
24	B	628	DGD	C4B-C5B-C6B-C7B
27	G	411	LMG	C20-C21-C22-C23
26	B	627	SQD	C12-C13-C14-C15
24	G	408	DGD	C4B-C5B-C6B-C7B
26	B	627	SQD	O10-C23-O48-C46
30	P	515	BCR	C7-C8-C9-C10
21	P	503	CLA	C15-C16-C17-C18
25	G	412	LHG	C7-C8-C9-C10
21	C	510	CLA	C13-C15-C16-C17
26	F	101	SQD	C12-C13-C14-C15
21	C	512	CLA	CAA-CBA-CGA-O2A
24	N	602	DGD	C5B-C6B-C7B-C8B
21	B	615	CLA	C11-C10-C8-C7
21	P	512	CLA	C11-C12-C13-C15
21	P	512	CLA	C12-C13-C15-C16
21	C	506	CLA	C12-C13-C15-C16
21	N	609	CLA	C11-C10-C8-C7
21	C	511	CLA	C6-C7-C8-C10
21	C	507	CLA	C11-C10-C8-C7
21	B	608	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	C	512	CLA	C11-C12-C13-C15
21	P	505	CLA	C12-C13-C15-C16
21	N	606	CLA	C6-C7-C8-C10
21	N	606	CLA	C11-C10-C8-C7
21	A	403	CLA	C6-C7-C8-C10
21	P	506	CLA	C11-C12-C13-C15
21	P	506	CLA	C12-C13-C15-C16
21	P	508	CLA	C11-C10-C8-C7
21	N	620	CLA	C11-C10-C8-C7
21	N	613	CLA	C12-C13-C15-C16
21	B	602	CLA	C6-C7-C8-C10
21	B	602	CLA	C11-C10-C8-C7
21	A	402	CLA	C12-C13-C15-C16
21	N	617	CLA	C11-C12-C13-C15
21	B	605	CLA	C11-C10-C8-C7
21	B	613	CLA	C11-C12-C13-C15
21	C	508	CLA	C11-C10-C8-C7
21	B	616	CLA	C11-C10-C8-C7
21	N	612	CLA	C11-C12-C13-C15
27	Q	401	LMG	C15-C16-C17-C18
31	N	604	LMT	C1-C2-C3-C4
24	P	519	DGD	C1A-C2A-C3A-C4A
25	A	411	LHG	C7-C8-C9-C10
31	B	630	LMT	C5'-C4'-O1B-C1B
22	D	402	PHO	C13-C15-C16-C17
21	C	511	CLA	C10-C11-C12-C13
26	S	102	SQD	C10-C11-C12-C13
27	a	102	LMG	C10-C11-C12-C13
21	N	618	CLA	C1-C2-C3-C5
21	N	615	CLA	C8-C10-C11-C12
27	E	102	LMG	O7-C10-C11-C12
27	N	622	LMG	C16-C17-C18-C19
27	B	622	LMG	C16-C17-C18-C19
21	C	510	CLA	C5-C6-C7-C8
21	B	606	CLA	C15-C16-C17-C18
22	A	404	PHO	CBD-CGD-O2D-CED
24	B	628	DGD	C2A-C3A-C4A-C5A
27	N	622	LMG	C13-C14-C15-C16
22	D	402	PHO	C2B-C3B-CAB-CBB
27	R	102	LMG	C7-C8-O7-C10
22	Q	403	PHO	C2B-C3B-CAB-CBB
21	C	512	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	P	519	DGD	C3G-C2G-O2G-C1B
21	P	508	CLA	CAD-CBD-CGD-O2D
27	E	102	LMG	C7-C8-O7-C10
21	C	508	CLA	CAD-CBD-CGD-O2D
27	B	623	LMG	C4-C5-C6-O5
27	e	102	LMG	C30-C31-C32-C33
26	A	409	SQD	C24-C25-C26-C27
21	N	605	CLA	C4C-C3C-CAC-CBC
24	D	408	DGD	CBB-CCB-CDB-CEB
24	B	628	DGD	C1G-C2G-C3G-O3G
27	N	622	LMG	O1-C7-C8-C9
24	D	408	DGD	C1G-C2G-C3G-O3G
21	A	403	CLA	C5-C6-C7-C8
21	B	605	CLA	C13-C15-C16-C17
22	A	404	PHO	C3-C5-C6-C7
27	R	102	LMG	O7-C10-C11-C12
26	S	102	SQD	C12-C13-C14-C15
21	B	614	CLA	C2A-CAA-CBA-CGA
27	G	411	LMG	C15-C16-C17-C18
24	C	517	DGD	C4A-C5A-C6A-C7A
27	a	102	LMG	C19-C20-C21-C22
21	C	506	CLA	CHA-CBD-CGD-O1D
21	B	607	CLA	CHA-CBD-CGD-O1D
21	B	614	CLA	CHA-CBD-CGD-O1D
21	B	614	CLA	CHA-CBD-CGD-O2D
21	P	506	CLA	CHA-CBD-CGD-O1D
21	N	618	CLA	CHA-CBD-CGD-O1D
21	N	618	CLA	CHA-CBD-CGD-O2D
23	D	404	PL9	C22-C23-C24-C26
27	M	101	LMG	O10-C28-O8-C9
26	A	414	SQD	C10-C11-C12-C13
24	B	621	DGD	O1G-C1G-C2G-O2G
27	M	101	LMG	O7-C8-C9-O8
24	Q	409	DGD	O2G-C2G-C3G-O3G
24	W	102	DGD	O1G-C1G-C2G-O2G
27	N	623	LMG	O7-C8-C9-O8
27	B	623	LMG	O7-C8-C9-O8
27	P	521	LMG	O7-C8-C9-O8
24	D	408	DGD	O2G-C2G-C3G-O3G
21	B	606	CLA	O1D-CGD-O2D-CED
27	D	412	LMG	C13-C14-C15-C16
24	N	602	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
23	A	406	PL9	C4-C3-C7-C8
21	C	506	CLA	C14-C13-C15-C16
21	N	609	CLA	C11-C10-C8-C9
21	C	512	CLA	C14-C13-C15-C16
21	P	506	CLA	C14-C13-C15-C16
21	N	620	CLA	C11-C10-C8-C9
21	A	402	CLA	C14-C13-C15-C16
21	N	617	CLA	C11-C12-C13-C14
21	B	605	CLA	C11-C10-C8-C9
21	B	613	CLA	C11-C12-C13-C14
24	C	518	DGD	CBA-CCA-CDA-CEA
25	A	408	LHG	C9-C10-C11-C12
21	B	614	CLA	C4C-C3C-CAC-CBC
24	Q	409	DGD	C7A-C8A-C9A-CAA
26	G	401	SQD	C5-C6-S-O8
26	A	414	SQD	C5-C6-S-O8
27	C	520	LMG	C13-C14-C15-C16
21	N	620	CLA	C2A-CAA-CBA-CGA
30	J	102	BCR	C7-C8-C9-C34
30	S	101	BCR	C37-C22-C23-C24
30	Z	101	BCR	C7-C8-C9-C10
27	C	519	LMG	C16-C17-C18-C19
21	C	501	CLA	C1A-C2A-CAA-CBA
21	N	606	CLA	C1A-C2A-CAA-CBA
21	N	614	CLA	C5-C6-C7-C8
27	B	622	LMG	C32-C33-C34-C35
25	A	408	LHG	C2-C3-O3-P
21	N	608	CLA	C2-C3-C5-C6
23	G	407	PL9	C33-C34-C36-C37
27	P	520	LMG	C16-C17-C18-C19
27	P	521	LMG	C13-C14-C15-C16
26	G	410	SQD	C29-C30-C31-C32
26	A	414	SQD	C12-C13-C14-C15
21	N	618	CLA	C16-C17-C18-C20
26	G	401	SQD	C26-C27-C28-C29
24	D	408	DGD	O6E-C1E-O5D-C6D
27	B	622	LMG	C13-C14-C15-C16
21	B	607	CLA	O1D-CGD-O2D-CED
21	P	506	CLA	O1D-CGD-O2D-CED
21	B	608	CLA	C13-C15-C16-C17
21	C	508	CLA	C5-C6-C7-C8
21	P	512	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	P	512	CLA	C16-C17-C18-C20
27	Q	401	LMG	C13-C14-C15-C16
25	G	409	LHG	C9-C10-C11-C12
21	C	506	CLA	CAD-CBD-CGD-O1D
26	Q	408	SQD	O5-C5-C6-S
26	B	624	SQD	O5-C5-C6-S
21	B	614	CLA	CAD-CBD-CGD-O1D
21	P	506	CLA	CAD-CBD-CGD-O1D
21	N	618	CLA	CAD-CBD-CGD-O1D
27	I	102	LMG	C19-C20-C21-C22
27	M	101	LMG	C13-C14-C15-C16
26	G	410	SQD	C10-C11-C12-C13
21	G	404	CLA	C5-C6-C7-C8
27	M	101	LMG	C4-C5-C6-O5
27	I	102	LMG	C10-C11-C12-C13
24	C	518	DGD	C1A-C2A-C3A-C4A
27	D	406	LMG	C17-C18-C19-C20
21	B	601	CLA	C4C-C3C-CAC-CBC
21	C	512	CLA	C16-C17-C18-C20
21	N	615	CLA	C16-C17-C18-C19
21	Q	404	CLA	C11-C10-C8-C7
22	D	402	PHO	C6-C7-C8-C10
21	P	502	CLA	C11-C10-C8-C7
21	B	611	CLA	C6-C7-C8-C10
21	B	611	CLA	C11-C10-C8-C7
21	P	511	CLA	C6-C7-C8-C10
21	N	609	CLA	C11-C12-C13-C15
22	Q	403	PHO	C6-C7-C8-C10
21	P	510	CLA	C6-C7-C8-C10
21	A	405	CLA	C11-C10-C8-C7
21	P	501	CLA	C11-C12-C13-C15
21	C	501	CLA	C11-C12-C13-C15
21	B	608	CLA	C6-C7-C8-C10
21	C	512	CLA	C12-C13-C15-C16
21	C	502	CLA	C11-C10-C8-C7
21	G	403	CLA	C12-C13-C15-C16
21	D	403	CLA	C11-C10-C8-C7
21	N	615	CLA	C11-C10-C8-C7
21	N	620	CLA	C12-C13-C15-C16
21	A	402	CLA	C6-C7-C8-C10
21	C	504	CLA	C3A-C2A-CAA-CBA
21	P	513	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
21	N	619	CLA	C11-C10-C8-C7
21	C	508	CLA	C12-C13-C15-C16
21	C	513	CLA	C6-C7-C8-C10
21	B	616	CLA	C3A-C2A-CAA-CBA
21	N	612	CLA	C6-C7-C8-C10
26	A	409	SQD	C29-C30-C31-C32
24	B	621	DGD	C5A-C6A-C7A-C8A
21	P	511	CLA	C10-C11-C12-C13
21	N	610	CLA	C15-C16-C17-C18
22	G	405	PHO	CBD-CGD-O2D-CED
26	A	409	SQD	C10-C11-C12-C13
27	R	102	LMG	C28-C29-C30-C31
24	P	518	DGD	C1A-C2A-C3A-C4A
26	B	627	SQD	C44-C45-C46-O48
27	D	407	LMG	C11-C12-C13-C14
26	N	601	SQD	C44-C45-C46-O48
27	N	622	LMG	O1-C7-C8-O7
26	B	627	SQD	O47-C45-C46-O48
26	F	101	SQD	O47-C45-C46-O48
27	P	520	LMG	O7-C8-C9-O8
26	S	102	SQD	O47-C45-C46-O48
26	N	601	SQD	O47-C45-C46-O48
21	G	403	CLA	O2A-C1-C2-C3
27	Q	406	LMG	C4-C5-C6-O5
24	P	519	DGD	C4B-C5B-C6B-C7B
27	I	102	LMG	C29-C30-C31-C32
25	G	409	LHG	C2-C3-O3-P
26	G	401	SQD	C12-C13-C14-C15
21	C	511	CLA	O1A-CGA-O2A-C1
21	C	509	CLA	C5-C6-C7-C8
27	D	406	LMG	C34-C35-C36-C37
26	G	401	SQD	C10-C11-C12-C13
21	B	609	CLA	C2-C3-C5-C6
23	A	406	PL9	C33-C34-C36-C37
21	P	512	CLA	C11-C12-C13-C14
21	P	512	CLA	C14-C13-C15-C16
21	C	501	CLA	C11-C12-C13-C14
21	C	507	CLA	C11-C10-C8-C9
21	C	512	CLA	C11-C12-C13-C14
21	G	403	CLA	C14-C13-C15-C16
21	N	615	CLA	C6-C7-C8-C9
21	P	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	G	406	CLA	C11-C10-C8-C9
21	N	620	CLA	C11-C12-C13-C14
21	P	504	CLA	C6-C7-C8-C9
21	C	510	CLA	C6-C7-C8-C9
21	C	504	CLA	C6-C7-C8-C9
21	B	616	CLA	C11-C10-C8-C9
21	N	612	CLA	C11-C12-C13-C14
22	G	405	PHO	C3-C5-C6-C7
21	C	512	CLA	C16-C17-C18-C19
21	N	615	CLA	C16-C17-C18-C20
21	N	618	CLA	C16-C17-C18-C19
24	N	602	DGD	C5A-C6A-C7A-C8A
27	D	412	LMG	C10-C11-C12-C13
27	a	102	LMG	O6-C5-C6-O5
21	N	620	CLA	C3-C5-C6-C7
21	B	610	CLA	C5-C6-C7-C8
27	G	411	LMG	C35-C36-C37-C38
24	W	102	DGD	C7B-C8B-C9B-CAB
30	S	101	BCR	C21-C22-C23-C24
21	B	613	CLA	C8-C10-C11-C12
26	A	414	SQD	C7-C8-C9-C10
21	B	611	CLA	C16-C17-C18-C19
27	A	410	LMG	C38-C39-C40-C41
25	A	411	LHG	C11-C12-C13-C14
21	N	618	CLA	C2C-C3C-CAC-CBC
31	B	625	LMT	C4-C5-C6-C7
25	G	409	LHG	C4-C5-O7-C7
24	C	518	DGD	C3G-C2G-O2G-C1B
27	C	520	LMG	C7-C8-O7-C10
25	A	408	LHG	C4-C5-O7-C7
21	P	501	CLA	C2A-CAA-CBA-CGA
21	C	501	CLA	C2A-CAA-CBA-CGA
21	N	618	CLA	C2A-CAA-CBA-CGA
21	G	404	CLA	C2-C1-O2A-CGA
21	N	610	CLA	C2-C1-O2A-CGA
21	C	512	CLA	C2-C1-O2A-CGA
21	B	612	CLA	C2-C1-O2A-CGA
21	A	403	CLA	C2-C1-O2A-CGA
21	N	620	CLA	C2-C1-O2A-CGA
22	G	405	PHO	C2-C1-O2A-CGA
22	A	404	PHO	C2-C1-O2A-CGA
21	B	616	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
21	B	611	CLA	C16-C17-C18-C20
21	D	401	CLA	O1A-CGA-O2A-C1
21	C	503	CLA	C15-C16-C17-C18
24	B	621	DGD	C7B-C8B-C9B-CAB
24	W	102	DGD	C5A-C6A-C7A-C8A
21	N	617	CLA	C8-C10-C11-C12
27	Q	401	LMG	C10-C11-C12-C13
24	B	628	DGD	CAB-CBB-CCB-CDB
30	T	103	BCR	C23-C24-C25-C26
21	N	616	CLA	C2-C3-C5-C6
24	C	517	DGD	CBB-CCB-CDB-CEB
21	N	616	CLA	C8-C10-C11-C12
21	B	612	CLA	C8-C10-C11-C12
27	A	410	LMG	C11-C10-O7-C8
27	B	622	LMG	O6-C1-O1-C7
24	A	407	DGD	C2A-C3A-C4A-C5A
21	N	609	CLA	C2A-CAA-CBA-CGA
27	R	102	LMG	O7-C8-C9-O8
27	e	102	LMG	O7-C8-C9-O8
26	F	101	SQD	C10-C11-C12-C13
25	G	409	LHG	C3-O3-P-O6
25	G	412	LHG	C3-O3-P-O6
25	A	411	LHG	C3-O3-P-O6
25	A	408	LHG	C3-O3-P-O6
27	P	520	LMG	C30-C31-C32-C33
24	P	519	DGD	O1G-C1G-C2G-C3G
27	P	521	LMG	C7-C8-C9-O8
26	A	414	SQD	O6-C44-C45-C46
23	D	404	PL9	C15-C14-C16-C17
21	C	505	CLA	C4-C3-C5-C6
21	A	405	CLA	C11-C12-C13-C15
21	G	406	CLA	C11-C12-C13-C15
21	B	616	CLA	C12-C13-C15-C16
24	N	602	DGD	C3A-C4A-C5A-C6A
24	P	518	DGD	CBB-CCB-CDB-CEB
21	Q	404	CLA	C11-C10-C8-C9
22	D	402	PHO	C6-C7-C8-C9
21	C	506	CLA	C11-C12-C13-C14
21	B	611	CLA	C6-C7-C8-C9
21	P	510	CLA	C6-C7-C8-C9
21	A	405	CLA	C11-C10-C8-C9
21	P	501	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	D	403	CLA	C11-C10-C8-C9
21	N	615	CLA	C11-C10-C8-C9
21	P	508	CLA	C14-C13-C15-C16
21	P	513	CLA	C6-C7-C8-C9
21	C	508	CLA	C14-C13-C15-C16
21	C	513	CLA	C6-C7-C8-C9
27	I	102	LMG	C17-C18-C19-C20
27	C	519	LMG	C30-C31-C32-C33
21	P	509	CLA	C5-C6-C7-C8
26	A	414	SQD	C17-C18-C19-C20
27	a	102	LMG	C17-C18-C19-C20
21	N	610	CLA	C13-C15-C16-C17
24	Q	409	DGD	CBB-CCB-CDB-CEB
21	B	601	CLA	C16-C17-C18-C20
27	M	101	LMG	C30-C31-C32-C33
21	N	618	CLA	C13-C15-C16-C17
26	A	414	SQD	C26-C27-C28-C29
23	Q	405	PL9	C22-C23-C24-C26
21	B	601	CLA	C16-C17-C18-C19
21	B	616	CLA	CBA-CGA-O2A-C1
27	G	411	LMG	C16-C17-C18-C19
26	G	401	SQD	C23-C24-C25-C26
27	C	519	LMG	C32-C33-C34-C35
25	G	412	LHG	C11-C12-C13-C14
24	D	408	DGD	C2B-C3B-C4B-C5B
31	N	624	LMT	C4-C5-C6-C7
21	B	611	CLA	C8-C10-C11-C12
21	B	614	CLA	O1A-CGA-O2A-C1
24	N	602	DGD	CAB-CBB-CCB-CDB
27	A	410	LMG	O9-C10-O7-C8
26	N	601	SQD	C15-C16-C17-C18
21	C	505	CLA	C2-C1-O2A-CGA
21	B	614	CLA	C2-C1-O2A-CGA
24	G	408	DGD	C2A-C3A-C4A-C5A
27	B	622	LMG	C2-C1-O1-C7
24	C	516	DGD	O2G-C2G-C3G-O3G
27	E	102	LMG	O7-C8-C9-O8
24	C	517	DGD	C1A-C2A-C3A-C4A
24	P	519	DGD	CCB-CDB-CEB-CFB
27	a	102	LMG	C31-C32-C33-C34
21	N	620	CLA	C3A-C2A-CAA-CBA
21	B	605	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	C	516	DGD	C5A-C6A-C7A-C8A
26	A	409	SQD	C11-C10-C9-C8
21	N	618	CLA	C4C-C3C-CAC-CBC
27	G	411	LMG	C38-C39-C40-C41
24	Q	409	DGD	C2B-C3B-C4B-C5B
24	C	518	DGD	C4B-C5B-C6B-C7B
31	B	630	LMT	C4-C5-C6-C7
21	B	611	CLA	C11-C10-C8-C9
21	C	502	CLA	C11-C10-C8-C9
21	A	401	CLA	C11-C12-C13-C14
21	G	402	CLA	C11-C12-C13-C14
21	B	614	CLA	C16-C17-C18-C19
27	P	520	LMG	C32-C33-C34-C35
22	Q	403	PHO	C13-C15-C16-C17
27	D	412	LMG	C17-C18-C19-C20
21	A	405	CLA	C2A-CAA-CBA-CGA
21	G	406	CLA	C2A-CAA-CBA-CGA
21	B	605	CLA	C2A-CAA-CBA-CGA
31	N	604	LMT	C4-C5-C6-C7
24	D	408	DGD	CAA-CBA-CCA-CDA
21	N	608	CLA	O1A-CGA-O2A-C1
21	B	614	CLA	C16-C17-C18-C20
22	D	402	PHO	O2A-C1-C2-C3
27	N	622	LMG	O6-C1-O1-C7
27	D	412	LMG	C29-C30-C31-C32
27	G	411	LMG	C11-C12-C13-C14
24	P	519	DGD	CBA-CCA-CDA-CEA
27	a	102	LMG	C29-C30-C31-C32
21	B	616	CLA	C3-C5-C6-C7
21	P	501	CLA	C1A-C2A-CAA-CBA
21	Q	402	CLA	C1A-C2A-CAA-CBA
21	A	403	CLA	C1A-C2A-CAA-CBA
21	P	504	CLA	C1A-C2A-CAA-CBA
21	C	504	CLA	C1A-C2A-CAA-CBA
21	B	605	CLA	C1A-C2A-CAA-CBA
27	C	519	LMG	C20-C21-C22-C23
21	B	610	CLA	C16-C17-C18-C19
21	D	401	CLA	C11-C10-C8-C7
21	N	609	CLA	C6-C7-C8-C10
21	Q	402	CLA	C11-C10-C8-C7
21	B	605	CLA	C11-C12-C13-C15
21	N	612	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	C	509	CLA	O1A-CGA-O2A-C1
27	e	102	LMG	C13-C14-C15-C16
21	A	402	CLA	C3-C5-C6-C7
21	N	612	CLA	C13-C15-C16-C17
27	B	623	LMG	C34-C35-C36-C37
26	A	414	SQD	C25-C26-C27-C28
27	A	410	LMG	C35-C36-C37-C38
26	A	409	SQD	C31-C32-C33-C34
21	P	505	CLA	C4-C3-C5-C6
23	Q	405	PL9	C15-C14-C16-C17
31	B	630	LMT	O1'-C1-C2-C3
21	B	604	CLA	O1A-CGA-O2A-C1
21	B	605	CLA	O1A-CGA-O2A-C1
21	G	403	CLA	C3-C5-C6-C7
21	P	507	CLA	C3-C5-C6-C7
21	P	513	CLA	C5-C6-C7-C8
27	C	519	LMG	C12-C13-C14-C15
27	A	410	LMG	C16-C17-C18-C19
21	P	512	CLA	C2-C1-O2A-CGA
23	Q	405	PL9	C13-C14-C16-C17
21	N	614	CLA	C16-C17-C18-C19
21	N	617	CLA	C16-C17-C18-C20
21	Q	402	CLA	C6-C7-C8-C9
26	B	627	SQD	C17-C18-C19-C20
27	D	406	LMG	C4-C5-C6-O5
24	P	517	DGD	C5A-C6A-C7A-C8A
24	D	408	DGD	C5B-C6B-C7B-C8B
21	C	512	CLA	CAA-CBA-CGA-O1A
27	e	102	LMG	C29-C28-O8-C9
30	P	514	BCR	C23-C24-C25-C30
30	B	620	BCR	C23-C24-C25-C30
30	D	405	BCR	C23-C24-C25-C30
30	S	101	BCR	C23-C24-C25-C30
30	T	103	BCR	C23-C24-C25-C30
27	N	623	LMG	C34-C35-C36-C37
27	P	521	LMG	C36-C37-C38-C39
27	P	520	LMG	C17-C18-C19-C20
30	J	102	BCR	C7-C8-C9-C10
21	B	612	CLA	C2-C3-C5-C6
23	Q	405	PL9	C18-C19-C21-C22
21	C	505	CLA	C2C-C3C-CAC-CBC
24	A	407	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
24	G	408	DGD	C5D-C6D-O5D-C1E
24	C	517	DGD	C5D-C6D-O5D-C1E
27	P	520	LMG	C12-C13-C14-C15
27	Q	401	LMG	C17-C18-C19-C20
21	B	614	CLA	C13-C15-C16-C17
21	P	503	CLA	C2A-CAA-CBA-CGA
31	N	604	LMT	O1'-C1-C2-C3
21	C	512	CLA	C10-C11-C12-C13
21	N	605	CLA	C12-C13-C15-C16
23	D	404	PL9	C13-C14-C16-C17
21	C	510	CLA	C11-C10-C8-C7
21	N	616	CLA	C12-C13-C15-C16
25	G	412	LHG	O1-C1-C2-O2
21	B	607	CLA	C1-C2-C3-C4
21	B	614	CLA	C1-C2-C3-C4
21	N	611	CLA	C1-C2-C3-C4
21	N	618	CLA	C1-C2-C3-C4
21	A	401	CLA	C13-C15-C16-C17
21	C	507	CLA	CAA-CBA-CGA-O2A
27	D	407	LMG	O1-C7-C8-O7
24	B	628	DGD	O2G-C1B-C2B-C3B
27	P	520	LMG	O8-C28-C29-C30
26	Q	408	SQD	O47-C7-C8-C9
21	P	507	CLA	CAA-CBA-CGA-O2A
21	N	617	CLA	CAA-CBA-CGA-O2A
26	G	410	SQD	C31-C32-C33-C34
21	C	503	CLA	C2A-CAA-CBA-CGA
21	N	605	CLA	C15-C16-C17-C18
21	B	610	CLA	C16-C17-C18-C20
21	N	617	CLA	C16-C17-C18-C19
21	B	606	CLA	C13-C15-C16-C17
26	A	414	SQD	C23-C24-C25-C26
27	A	410	LMG	O7-C10-C11-C12
21	B	602	CLA	CAA-CBA-CGA-O2A
26	A	414	SQD	O47-C7-C8-C9
21	P	512	CLA	C4-C3-C5-C6
21	P	506	CLA	C4-C3-C5-C6
21	N	617	CLA	C10-C11-C12-C13
27	G	411	LMG	O7-C10-C11-C12
21	C	501	CLA	CAA-CBA-CGA-O2A
26	G	401	SQD	O47-C7-C8-C9
21	N	605	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
21	D	401	CLA	C6-C7-C8-C9
21	D	401	CLA	C11-C10-C8-C9
21	N	609	CLA	C11-C12-C13-C14
21	A	405	CLA	C11-C12-C13-C14
21	Q	402	CLA	C11-C10-C8-C9
21	N	606	CLA	C14-C13-C15-C16
21	G	406	CLA	C11-C12-C13-C14
21	N	620	CLA	C14-C13-C15-C16
21	B	602	CLA	C14-C13-C15-C16
21	C	510	CLA	C11-C10-C8-C9
21	B	605	CLA	C6-C7-C8-C9
21	B	605	CLA	C11-C12-C13-C14
21	B	616	CLA	C14-C13-C15-C16
25	G	409	LHG	C35-C36-C37-C38
21	N	606	CLA	C3A-C2A-CAA-CBA
21	N	609	CLA	O1A-CGA-O2A-C1
27	e	102	LMG	O10-C28-O8-C9
21	Q	402	CLA	O1A-CGA-O2A-C1
26	B	624	SQD	O47-C7-C8-C9
24	P	519	DGD	O2G-C1B-C2B-C3B
21	B	610	CLA	CAA-CBA-CGA-O2A
27	Q	406	LMG	C14-C15-C16-C17
21	P	512	CLA	CAD-CBD-CGD-O2D
22	D	402	PHO	CAD-CBD-CGD-O2D
21	B	603	CLA	CAD-CBD-CGD-O2D
21	P	502	CLA	CAD-CBD-CGD-O2D
22	Q	403	PHO	CAD-CBD-CGD-O2D
21	P	510	CLA	CAD-CBD-CGD-O2D
21	C	501	CLA	CAD-CBD-CGD-O2D
21	C	507	CLA	CAD-CBD-CGD-O2D
21	N	607	CLA	CAD-CBD-CGD-O2D
21	C	502	CLA	CAD-CBD-CGD-O2D
21	B	612	CLA	CAD-CBD-CGD-O2D
21	P	507	CLA	CAD-CBD-CGD-O2D
22	G	405	PHO	CAD-CBD-CGD-O2D
21	N	617	CLA	CAD-CBD-CGD-O2D
27	C	520	LMG	C9-C8-O7-C10
21	B	613	CLA	CAD-CBD-CGD-O2D
21	A	401	CLA	C16-C17-C18-C20
21	G	402	CLA	C16-C17-C18-C20
24	B	628	DGD	C3A-C4A-C5A-C6A
21	B	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	D	406	LMG	C14-C15-C16-C17
26	G	401	SQD	C32-C33-C34-C35
21	C	512	CLA	C4-C3-C5-C6
21	B	611	CLA	C2-C3-C5-C6
21	N	615	CLA	C2-C3-C5-C6
21	P	501	CLA	CAA-CBA-CGA-O2A
24	N	602	DGD	O2G-C1B-C2B-C3B
30	P	516	BCR	C21-C22-C23-C24
30	C	515	BCR	C21-C22-C23-C24
26	F	101	SQD	C44-C45-C46-O48
27	Q	407	LMG	O1-C7-C8-C9
27	D	407	LMG	O1-C7-C8-C9
26	S	102	SQD	C44-C45-C46-O48
26	G	401	SQD	O6-C44-C45-C46
27	C	520	LMG	C7-C8-C9-O8
26	A	414	SQD	C33-C34-C35-C36
21	P	512	CLA	CAA-CBA-CGA-O1A
21	P	501	CLA	CBA-CGA-O2A-C1
21	C	507	CLA	C3-C5-C6-C7
31	B	625	LMT	O1'-C1-C2-C3
31	a	103	LMT	C7-C8-C9-C10
21	B	615	CLA	O2A-C1-C2-C3
22	Q	403	PHO	O2A-C1-C2-C3
21	N	617	CLA	O2A-C1-C2-C3
21	N	619	CLA	O2A-C1-C2-C3
21	B	613	CLA	O2A-C1-C2-C3
22	D	402	PHO	C4B-C3B-CAB-CBB
22	Q	403	PHO	C4B-C3B-CAB-CBB
21	N	614	CLA	CAA-CBA-CGA-O2A
21	B	613	CLA	CAA-CBA-CGA-O2A
21	N	614	CLA	C16-C17-C18-C20
21	A	405	CLA	C16-C17-C18-C20
27	D	406	LMG	C13-C14-C15-C16
27	Q	406	LMG	C32-C33-C34-C35
22	A	404	PHO	O1D-CGD-O2D-CED
21	C	506	CLA	CHA-CBD-CGD-O2D
21	C	503	CLA	CHA-CBD-CGD-O2D
21	G	404	CLA	CHA-CBD-CGD-O2D
21	N	609	CLA	CHA-CBD-CGD-O2D
21	B	607	CLA	CHA-CBD-CGD-O2D
21	C	512	CLA	CHA-CBD-CGD-O1D
21	N	606	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	P	503	CLA	CHA-CBD-CGD-O2D
21	A	403	CLA	CHA-CBD-CGD-O1D
21	A	403	CLA	CHA-CBD-CGD-O2D
21	C	509	CLA	CHA-CBD-CGD-O1D
21	N	611	CLA	CHA-CBD-CGD-O2D
21	B	602	CLA	CHA-CBD-CGD-O2D
21	C	510	CLA	CHA-CBD-CGD-O1D
21	P	513	CLA	CHA-CBD-CGD-O1D
21	P	513	CLA	CHA-CBD-CGD-O2D
21	P	509	CLA	CHA-CBD-CGD-O1D
21	P	509	CLA	CHA-CBD-CGD-O2D
21	C	513	CLA	CHA-CBD-CGD-O2D
27	C	519	LMG	O8-C28-C29-C30
21	N	606	CLA	C3-C5-C6-C7
27	D	407	LMG	C29-C30-C31-C32
24	Q	409	DGD	C5B-C6B-C7B-C8B
27	Q	407	LMG	O1-C7-C8-O7
27	C	519	LMG	C17-C18-C19-C20
21	B	601	CLA	C15-C16-C17-C18
24	P	517	DGD	O2G-C1B-C2B-C3B
24	C	518	DGD	O2G-C1B-C2B-C3B
24	C	516	DGD	O2G-C1B-C2B-C3B
21	G	402	CLA	C13-C15-C16-C17
24	B	628	DGD	C5A-C6A-C7A-C8A
21	B	603	CLA	C11-C10-C8-C7
21	P	510	CLA	C11-C10-C8-C7
21	C	507	CLA	C12-C13-C15-C16
21	B	608	CLA	C11-C10-C8-C7
21	P	507	CLA	C11-C12-C13-C15
21	B	610	CLA	C11-C12-C13-C15
21	B	601	CLA	C12-C13-C15-C16
21	B	605	CLA	C6-C7-C8-C10
21	C	513	CLA	C11-C12-C13-C15
21	N	609	CLA	C16-C17-C18-C20
24	C	518	DGD	O1G-C1A-C2A-C3A
21	B	603	CLA	C11-C10-C8-C9
21	P	502	CLA	C11-C10-C8-C9
21	N	605	CLA	C14-C13-C15-C16
21	N	609	CLA	C6-C7-C8-C9
21	C	507	CLA	C14-C13-C15-C16
21	P	507	CLA	C11-C12-C13-C14
21	C	510	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	C	513	CLA	C11-C12-C13-C14
21	N	612	CLA	C11-C10-C8-C9
21	P	505	CLA	C2C-C3C-CAC-CBC
31	I	103	LMT	C7-C8-C9-C10
31	N	624	LMT	O1'-C1-C2-C3
27	N	623	LMG	C36-C37-C38-C39
21	P	512	CLA	C10-C11-C12-C13
21	D	401	CLA	CAA-CBA-CGA-O2A
21	N	616	CLA	CBD-CGD-O2D-CED
21	B	605	CLA	C16-C17-C18-C20
21	B	612	CLA	C3-C5-C6-C7
21	A	401	CLA	C3-C5-C6-C7
23	b	101	PL9	C21-C22-C23-C24
23	J	101	PL9	C21-C22-C23-C24
27	C	519	LMG	O10-C28-C29-C30
21	N	606	CLA	CAA-CBA-CGA-O2A
24	C	518	DGD	C4E-C5E-C6E-O5E
27	A	410	LMG	C11-C12-C13-C14
27	Q	406	LMG	C17-C18-C19-C20
24	N	602	DGD	O1B-C1B-C2B-C3B
21	N	607	CLA	C15-C16-C17-C18
21	N	614	CLA	C4-C3-C5-C6
21	B	601	CLA	C4-C3-C5-C6
21	D	401	CLA	CAA-CBA-CGA-O1A
27	A	410	LMG	O9-C10-C11-C12
21	C	501	CLA	CBA-CGA-O2A-C1
21	P	510	CLA	C5-C6-C7-C8
26	G	401	SQD	C33-C34-C35-C36
21	N	605	CLA	C1A-C2A-CAA-CBA
21	P	511	CLA	C1A-C2A-CAA-CBA
21	C	511	CLA	C1A-C2A-CAA-CBA
21	D	403	CLA	C1A-C2A-CAA-CBA
21	B	601	CLA	C1A-C2A-CAA-CBA
21	N	605	CLA	C16-C17-C18-C19
21	G	406	CLA	C16-C17-C18-C20
21	Q	402	CLA	CAA-CBA-CGA-O1A
21	G	403	CLA	CAA-CBA-CGA-O1A
21	N	617	CLA	CAA-CBA-CGA-O1A
21	N	618	CLA	CAA-CBA-CGA-O1A
21	Q	402	CLA	CAA-CBA-CGA-O2A
21	N	605	CLA	C2-C1-O2A-CGA
26	G	401	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
21	B	613	CLA	C10-C11-C12-C13
27	P	520	LMG	O10-C28-C29-C30
26	B	624	SQD	O49-C7-C8-C9
21	B	614	CLA	CAA-CBA-CGA-O1A
26	A	414	SQD	O49-C7-C8-C9
27	I	102	LMG	C31-C32-C33-C34
27	R	102	LMG	C7-C8-C9-O8
24	B	628	DGD	O1B-C1B-C2B-C3B
26	G	401	SQD	O49-C7-C8-C9
21	B	613	CLA	CAA-CBA-CGA-O1A
26	A	414	SQD	C32-C33-C34-C35
24	P	518	DGD	C6B-C7B-C8B-C9B
21	P	510	CLA	C4-C3-C5-C6
27	G	411	LMG	O9-C10-O7-C8
27	R	102	LMG	C30-C31-C32-C33
26	Q	408	SQD	O49-C7-C8-C9
21	C	507	CLA	O1A-CGA-O2A-C1
25	G	409	LHG	C3-O3-P-O5
25	A	411	LHG	C3-O3-P-O5
25	A	408	LHG	C3-O3-P-O5
22	G	405	PHO	O1D-CGD-O2D-CED
27	G	411	LMG	O9-C10-C11-C12
27	Q	401	LMG	C29-C30-C31-C32
30	B	620	BCR	C23-C24-C25-C26
30	D	405	BCR	C23-C24-C25-C26
21	B	603	CLA	C15-C16-C17-C18
24	P	519	DGD	O1B-C1B-C2B-C3B
24	C	516	DGD	O1B-C1B-C2B-C3B
24	P	517	DGD	O1B-C1B-C2B-C3B
27	E	102	LMG	O9-C10-C11-C12
24	Q	409	DGD	CAA-CBA-CCA-CDA
21	B	601	CLA	CAA-CBA-CGA-O2A
27	Q	406	LMG	C34-C35-C36-C37
25	G	412	LHG	C23-C24-C25-C26
27	R	102	LMG	O9-C10-C11-C12
21	N	605	CLA	C4-C3-C5-C6
21	A	402	CLA	CBA-CGA-O2A-C1
21	B	609	CLA	CAD-CBD-CGD-O1D
21	B	611	CLA	CAD-CBD-CGD-O1D
26	F	101	SQD	O5-C5-C6-S
21	C	510	CLA	CAD-CBD-CGD-O1D
27	P	521	LMG	C7-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
27	P	521	LMG	C9-C8-O7-C10
24	C	518	DGD	C1B-C2B-C3B-C4B
24	C	518	DGD	O1A-C1A-C2A-C3A
21	A	402	CLA	CAA-CBA-CGA-O1A
21	A	405	CLA	C6-C7-C8-C9
21	C	507	CLA	C11-C12-C13-C14
21	N	607	CLA	C11-C10-C8-C9
21	G	406	CLA	C6-C7-C8-C9
21	B	610	CLA	C11-C12-C13-C14
21	N	616	CLA	C11-C12-C13-C14
21	P	513	CLA	C11-C12-C13-C14
21	D	403	CLA	C8-C10-C11-C12
27	Q	406	LMG	C13-C14-C15-C16
21	C	505	CLA	CAA-CBA-CGA-O2A
21	P	505	CLA	CAA-CBA-CGA-O2A
27	M	101	LMG	O8-C28-C29-C30
21	N	618	CLA	CAA-CBA-CGA-O2A
22	A	404	PHO	C13-C15-C16-C17
27	P	520	LMG	C20-C21-C22-C23
27	N	623	LMG	C11-C12-C13-C14
21	B	614	CLA	CAA-CBA-CGA-O2A
24	C	518	DGD	O1B-C1B-C2B-C3B
27	a	102	LMG	C20-C21-C22-C23
21	N	605	CLA	C11-C10-C8-C7
21	N	614	CLA	C11-C12-C13-C15
21	A	405	CLA	C6-C7-C8-C10
21	C	507	CLA	C11-C12-C13-C15
21	G	406	CLA	C6-C7-C8-C10
21	C	510	CLA	C11-C12-C13-C15
21	P	513	CLA	C11-C12-C13-C15
21	N	610	CLA	C5-C6-C7-C8
21	B	602	CLA	C3-C5-C6-C7
26	B	627	SQD	C15-C16-C17-C18
21	C	510	CLA	C16-C17-C18-C20
21	N	605	CLA	CAA-CBA-CGA-O2A
25	G	412	LHG	O7-C7-C8-C9
27	Q	406	LMG	O6-C1-O1-C7
23	G	407	PL9	C19-C21-C22-C23
27	G	411	LMG	C11-C10-O7-C8
21	N	616	CLA	C3-C5-C6-C7
21	B	609	CLA	C15-C16-C17-C18
21	N	613	CLA	C15-C16-C17-C18

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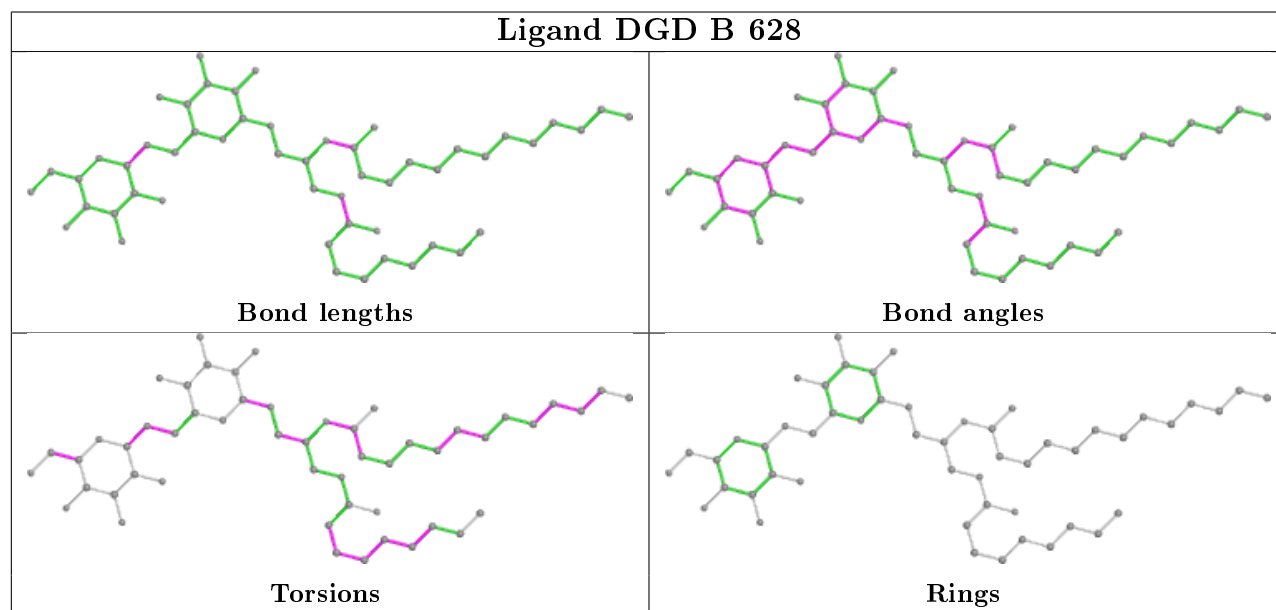
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Mol	Chain	Res	Type	Atoms
21	B	608	CLA	CAA-CBA-CGA-O1A
21	N	606	CLA	CAA-CBA-CGA-O1A
24	P	519	DGD	O1G-C1A-C2A-C3A
27	a	102	LMG	O7-C10-C11-C12

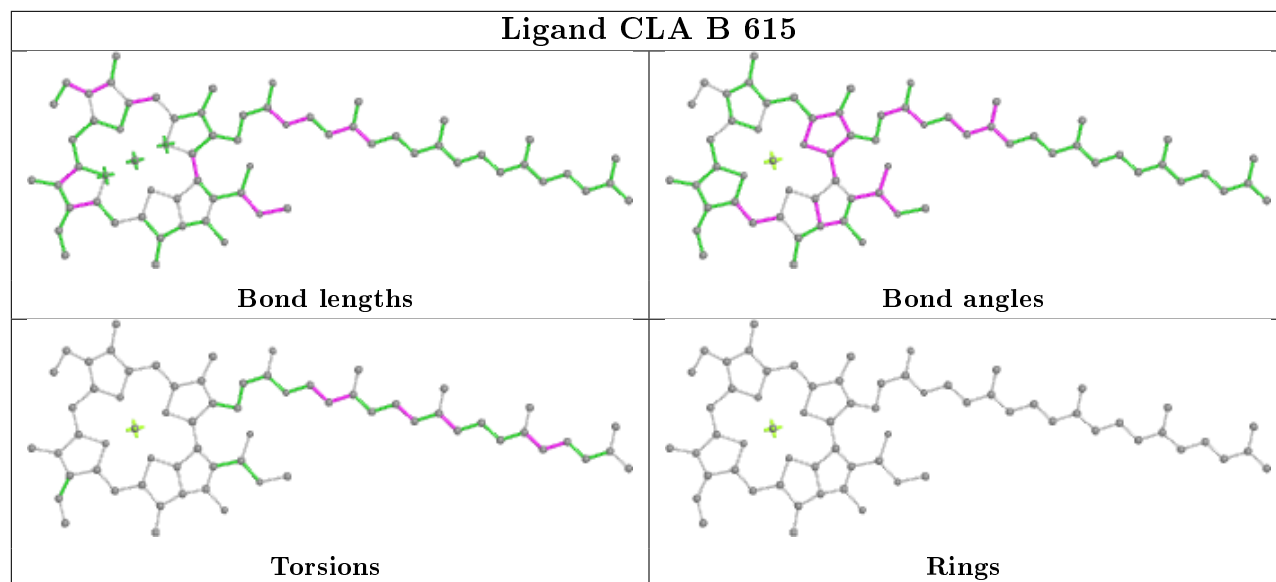
There are no ring outliers.

No monomer is involved in short contacts.

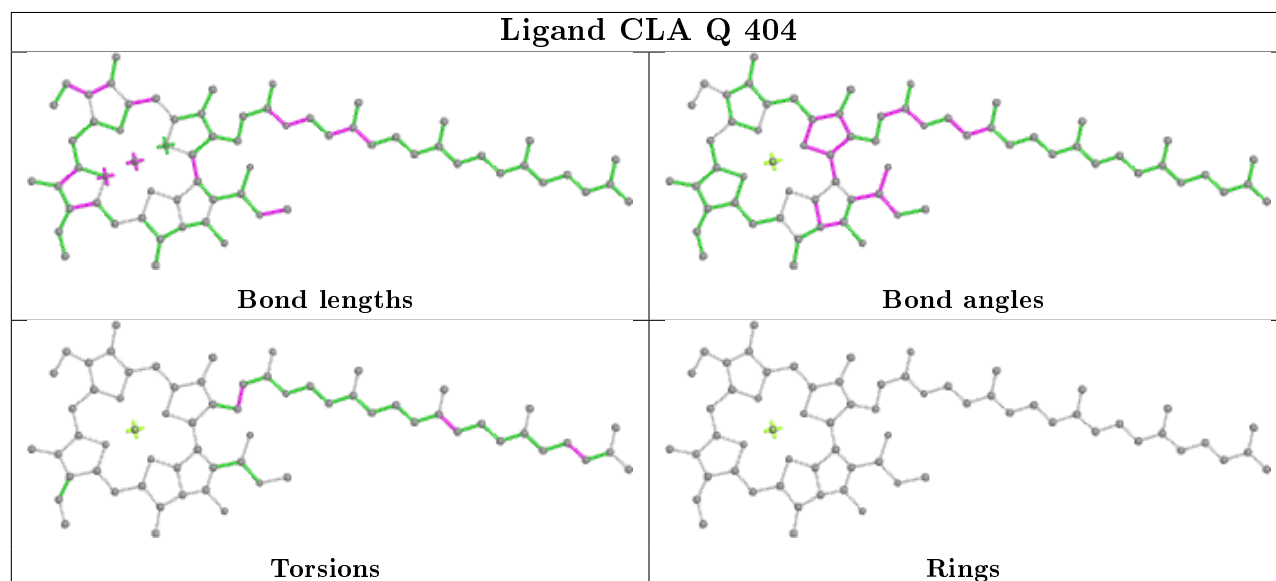
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



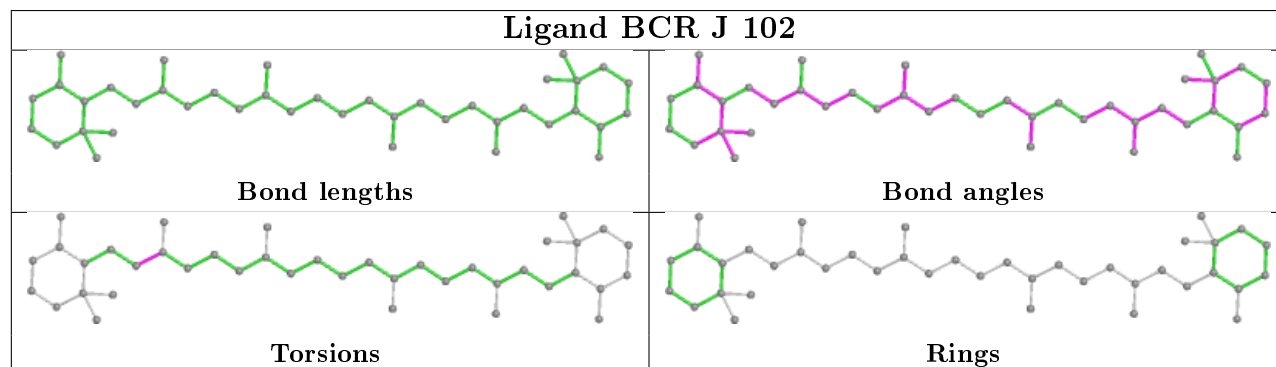
Ligand CLA B 615

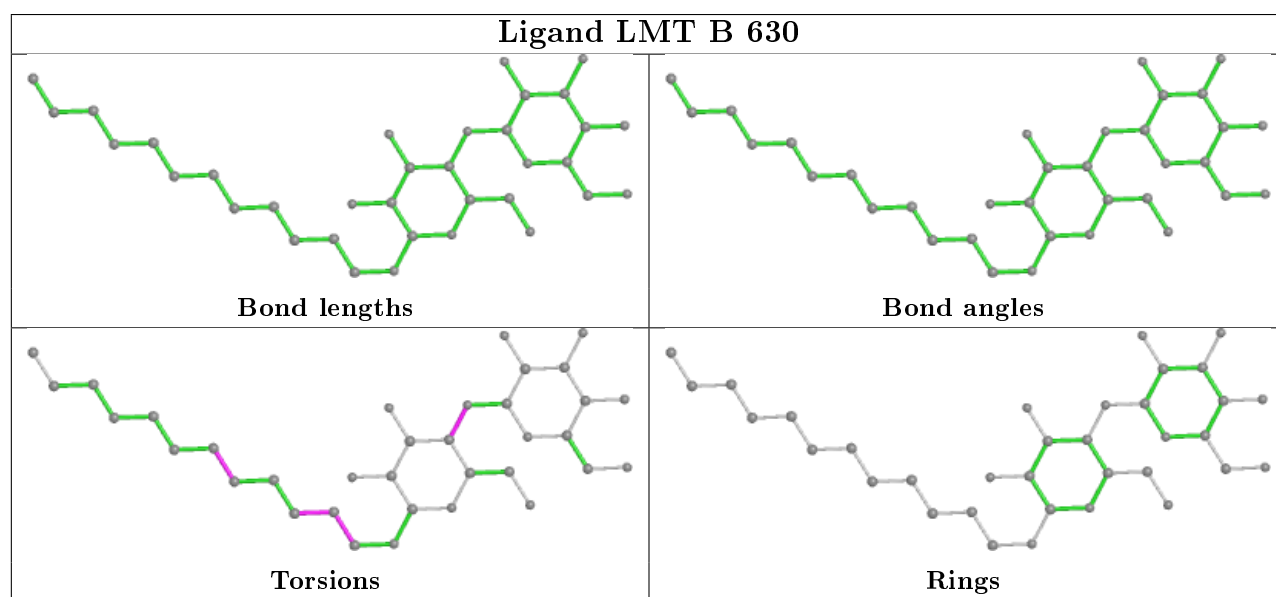
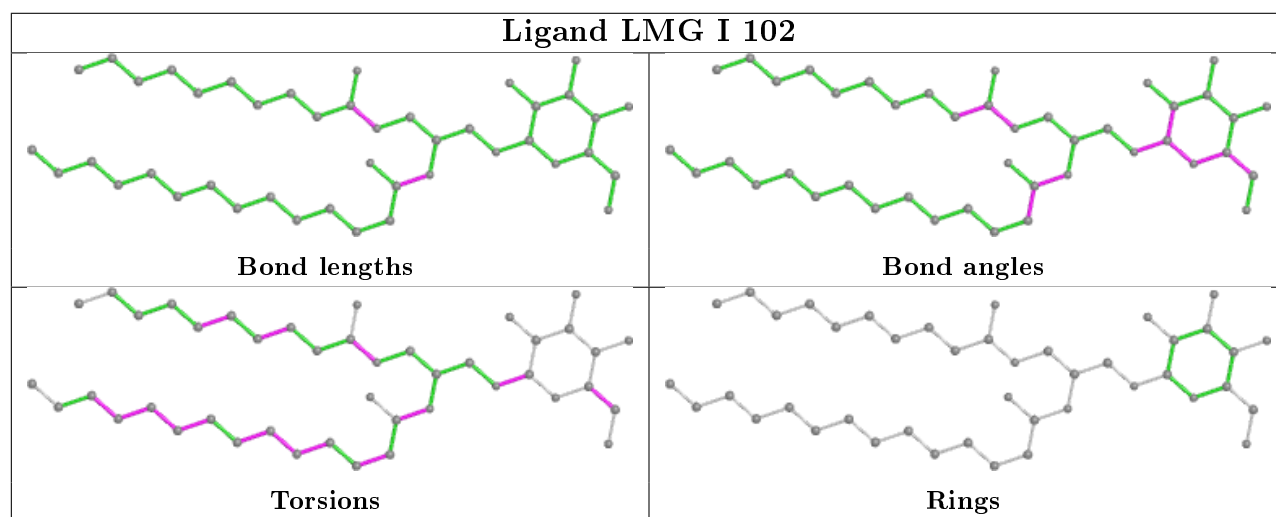
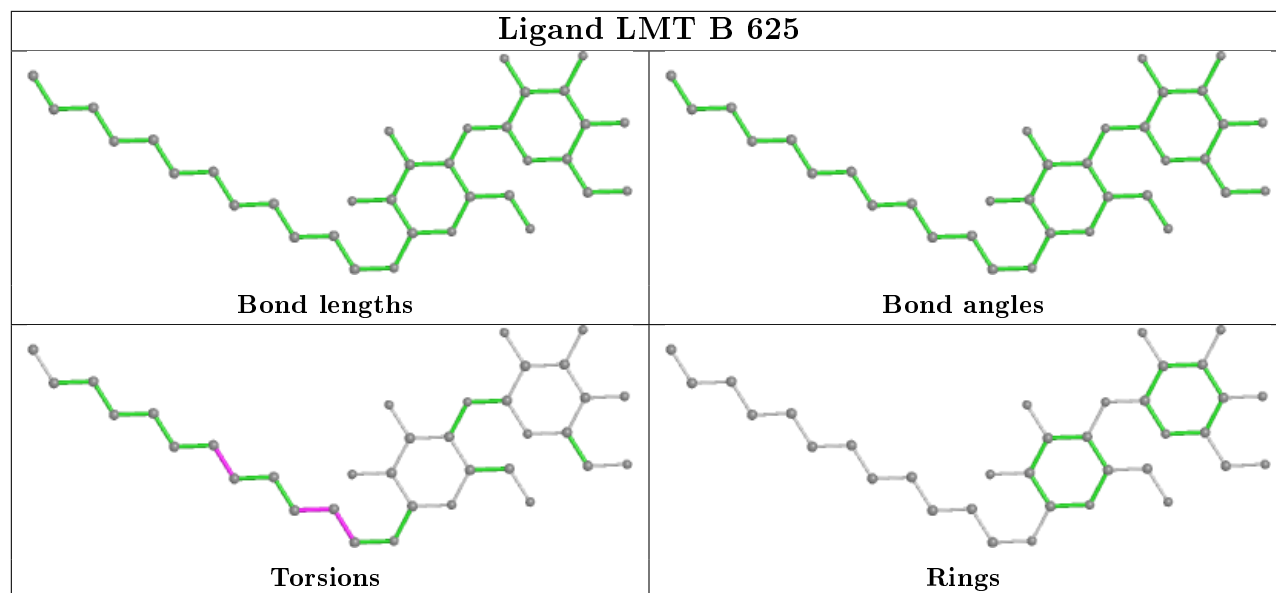


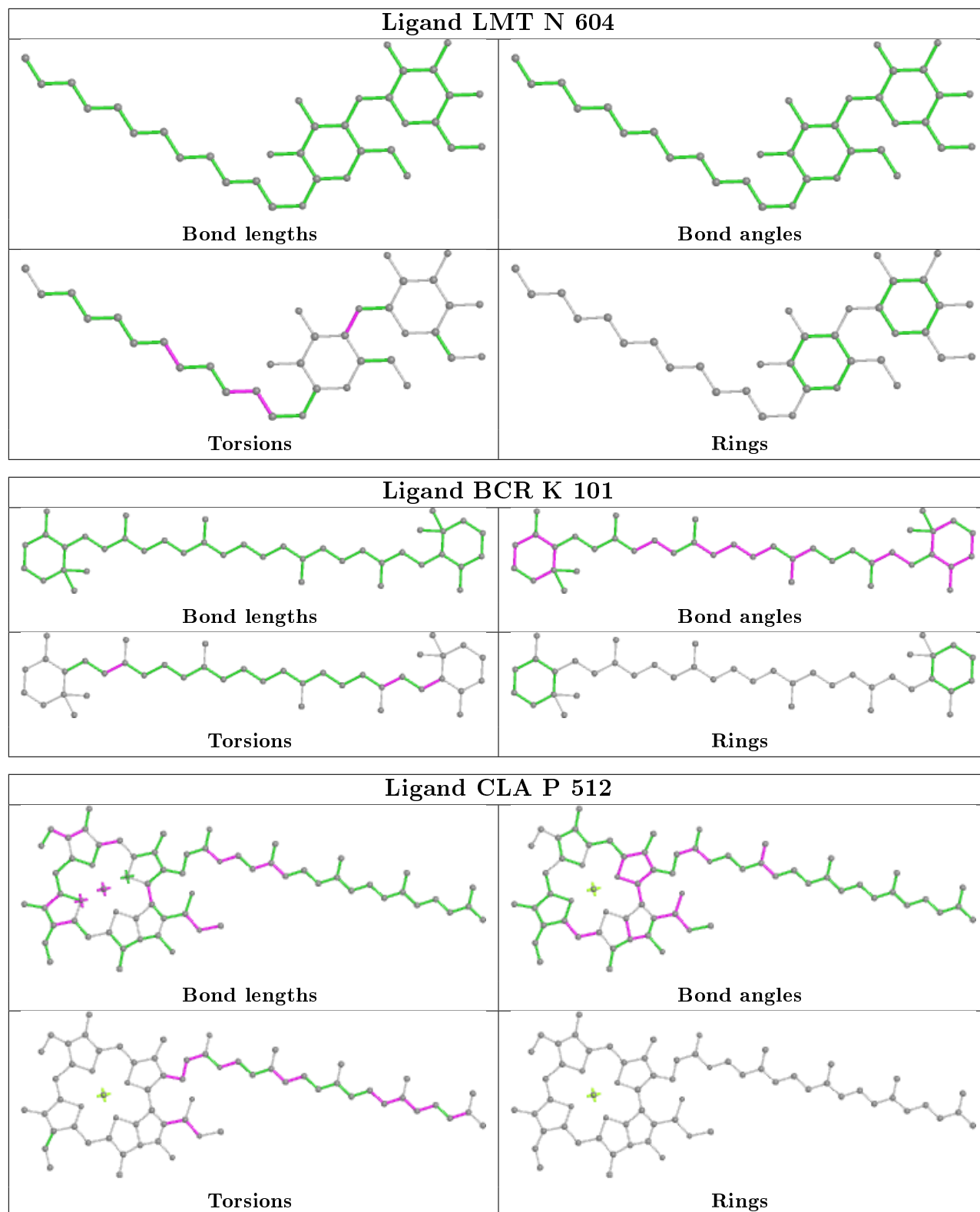
Ligand CLA Q 404

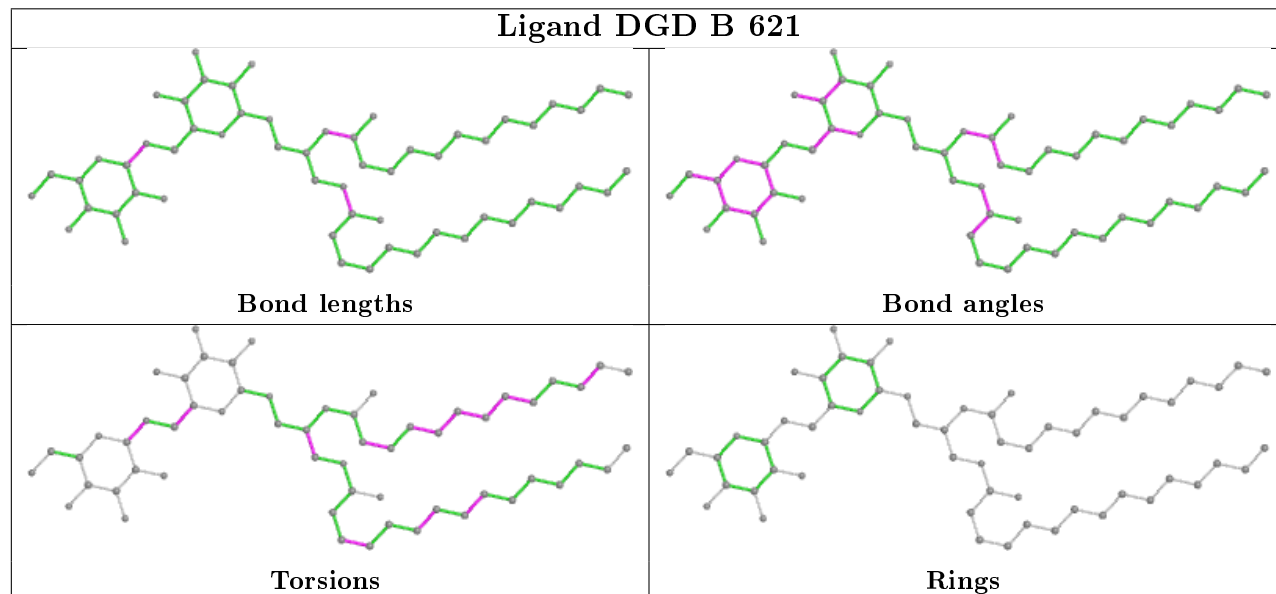
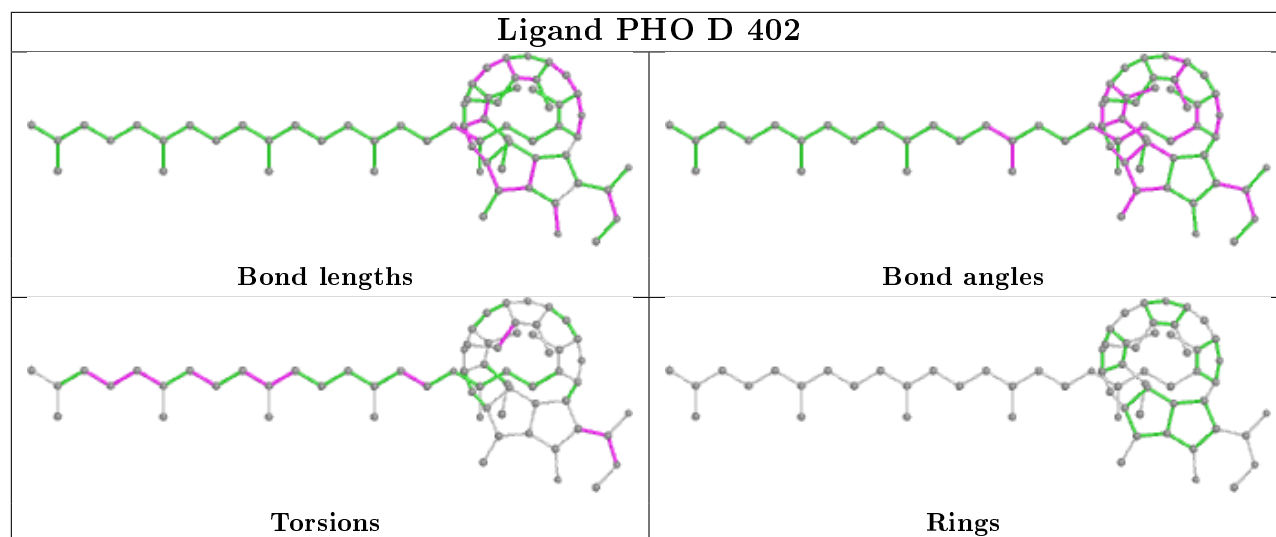
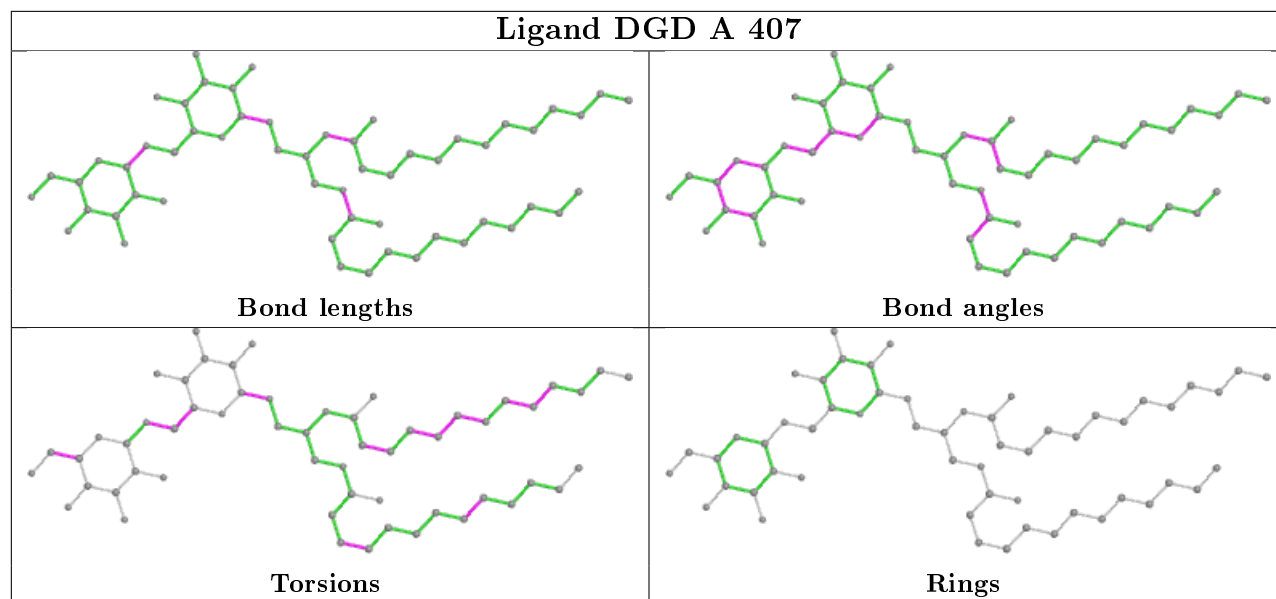


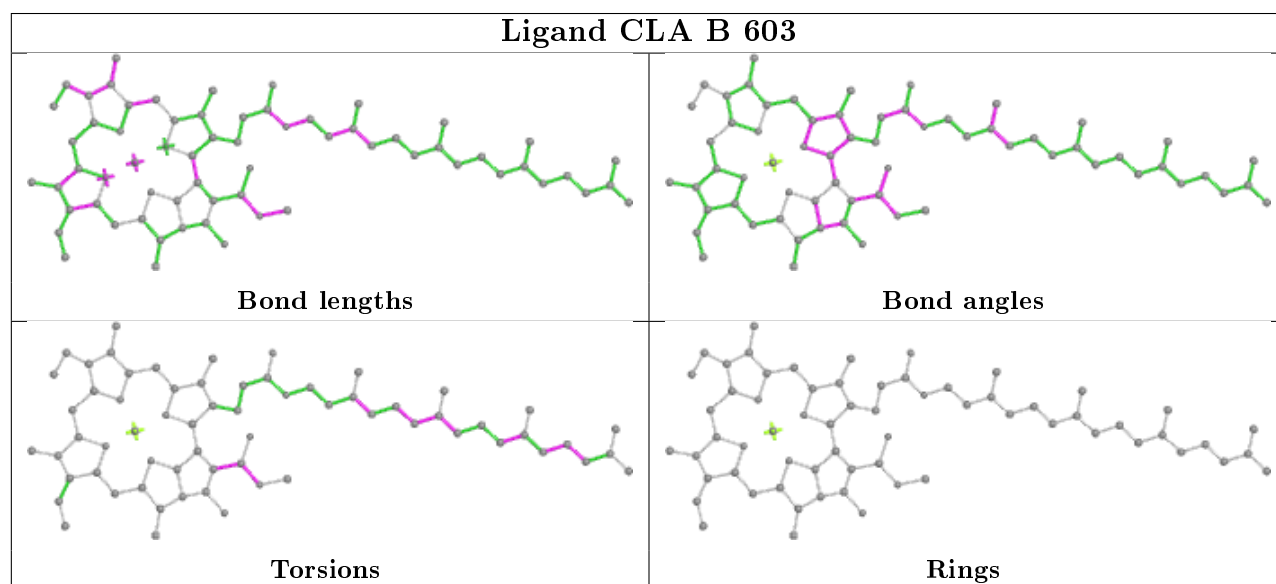
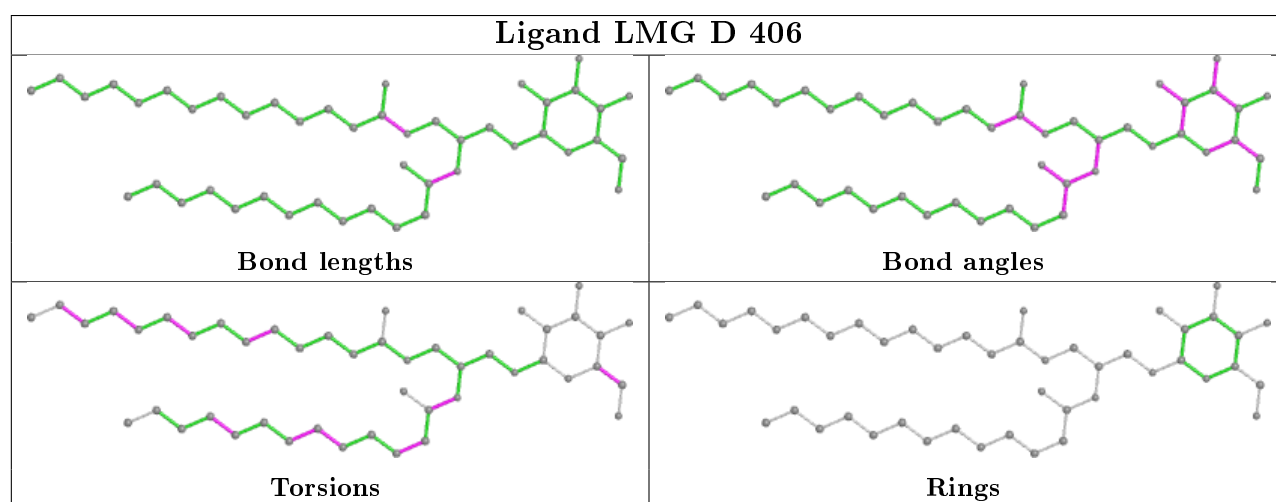
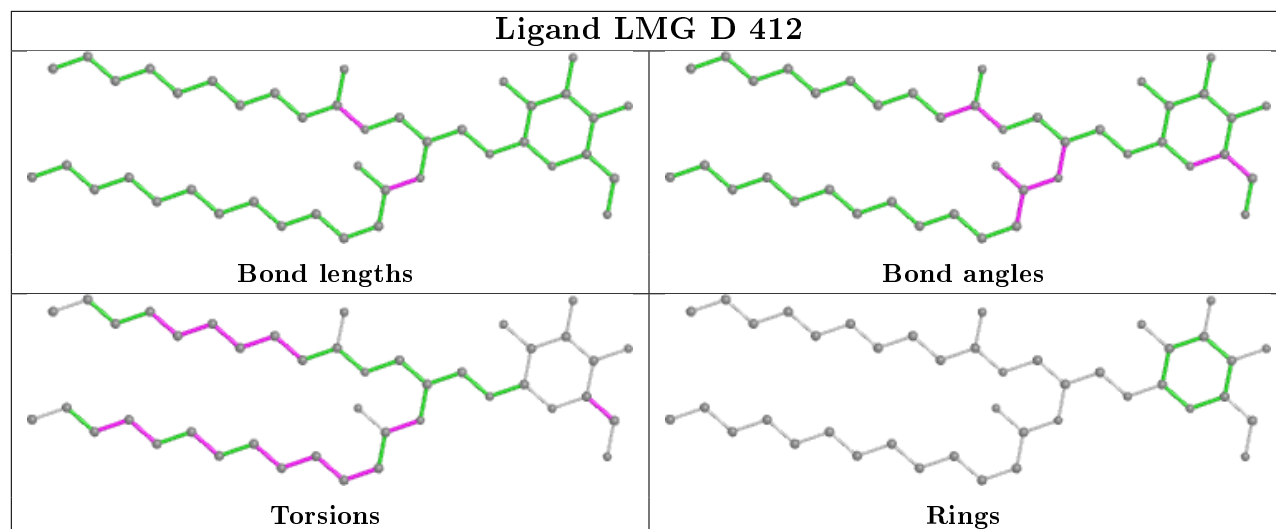
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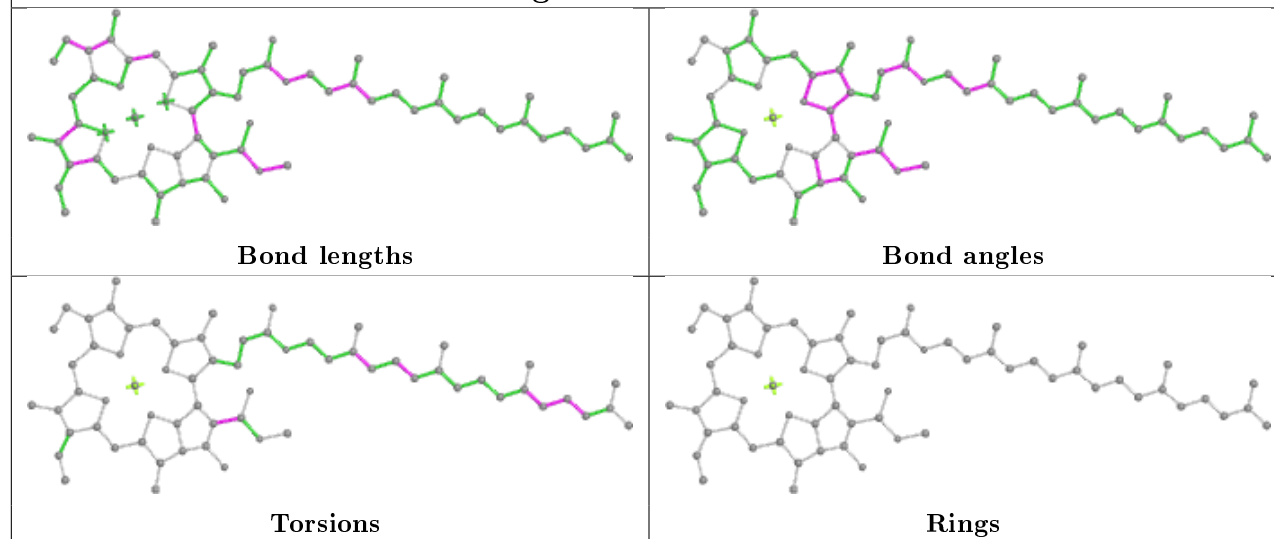
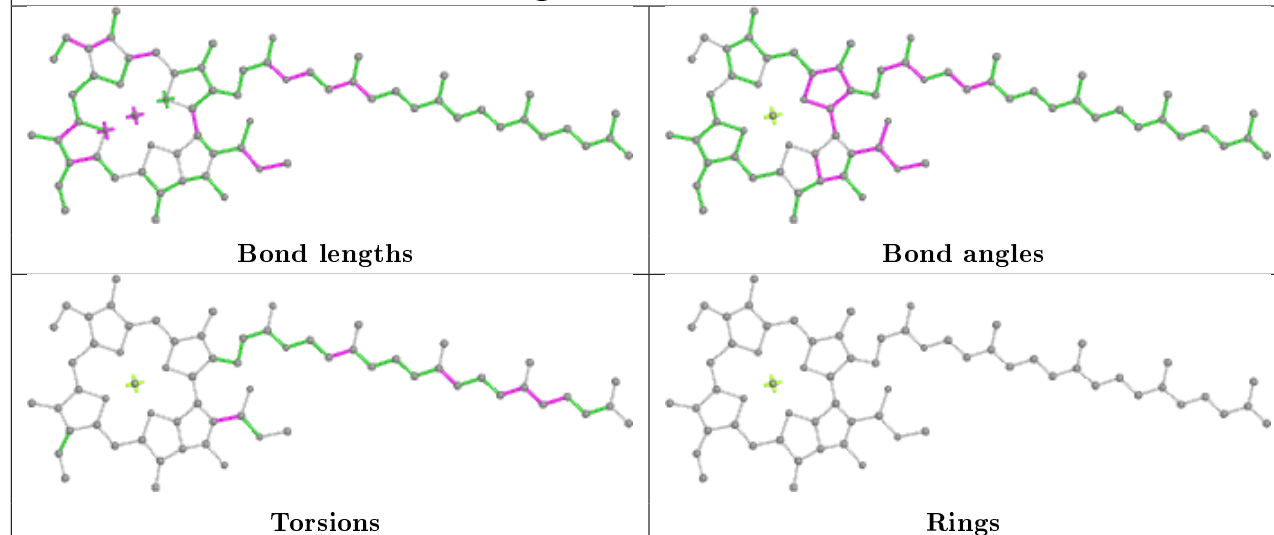
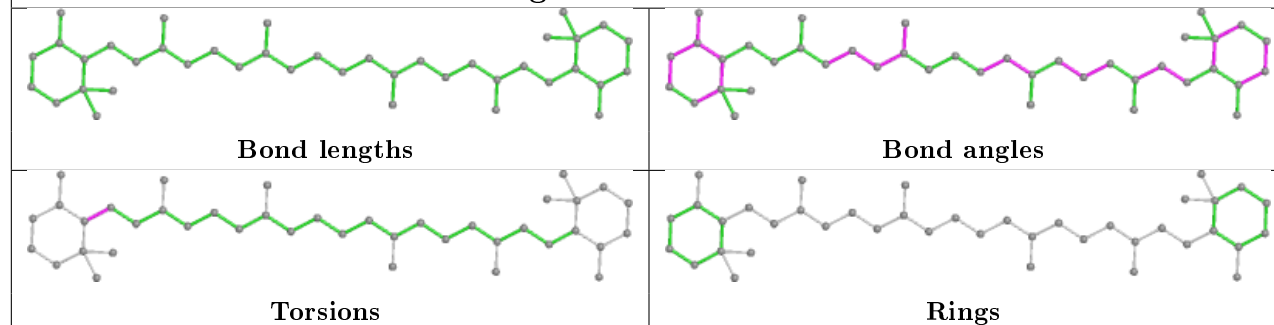


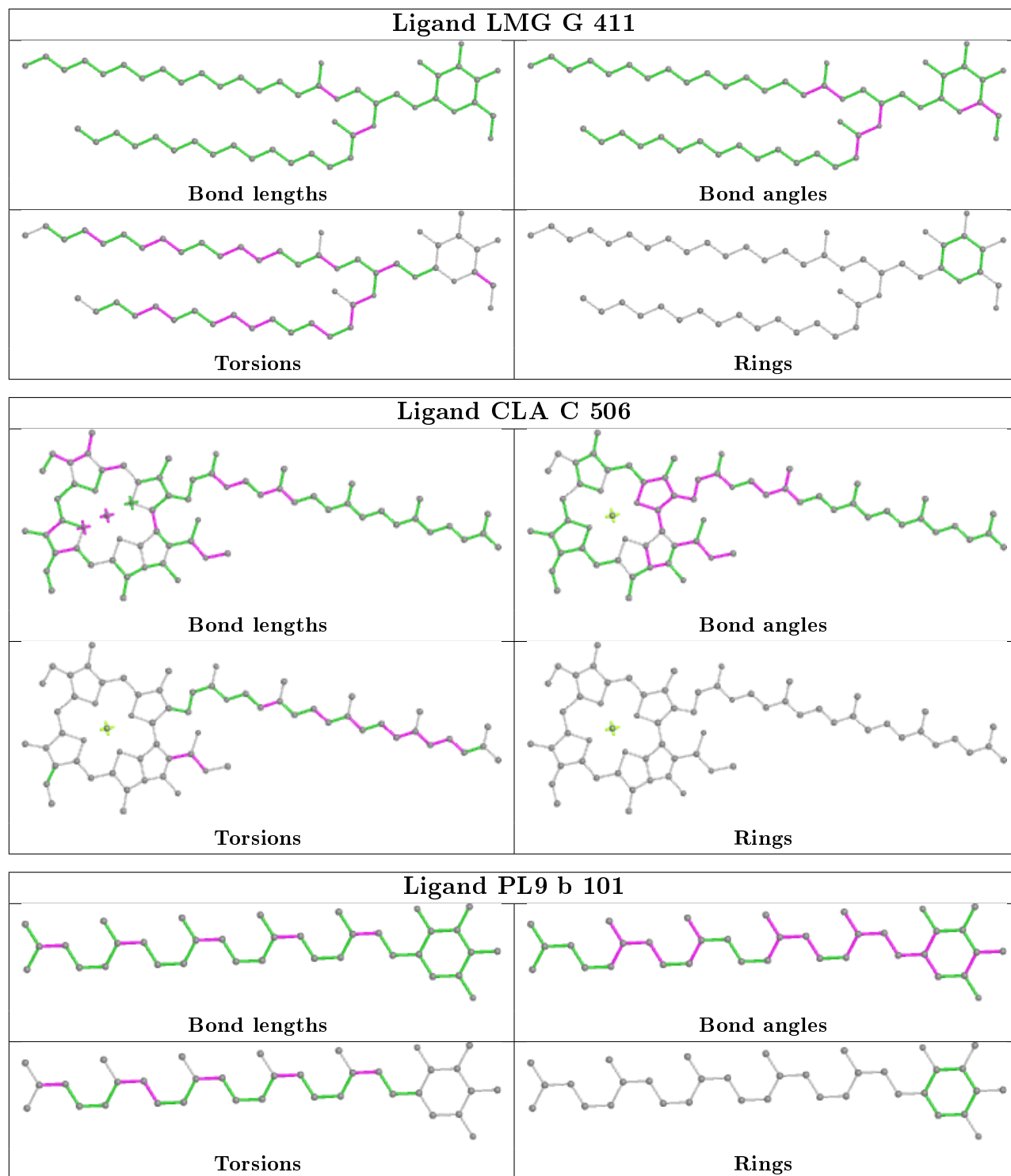


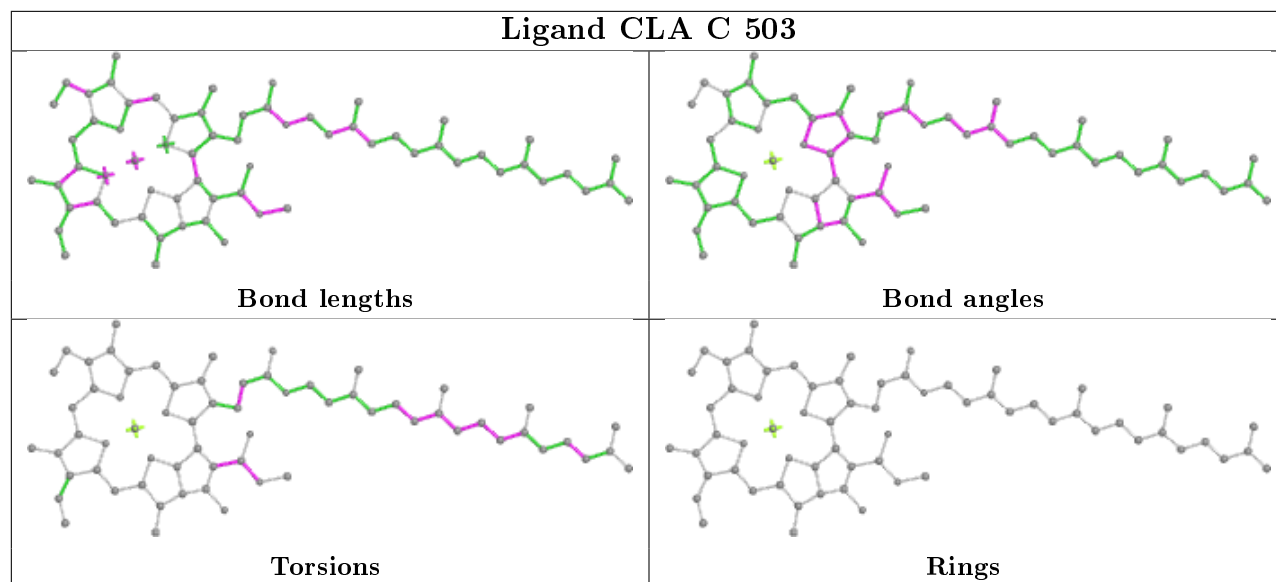
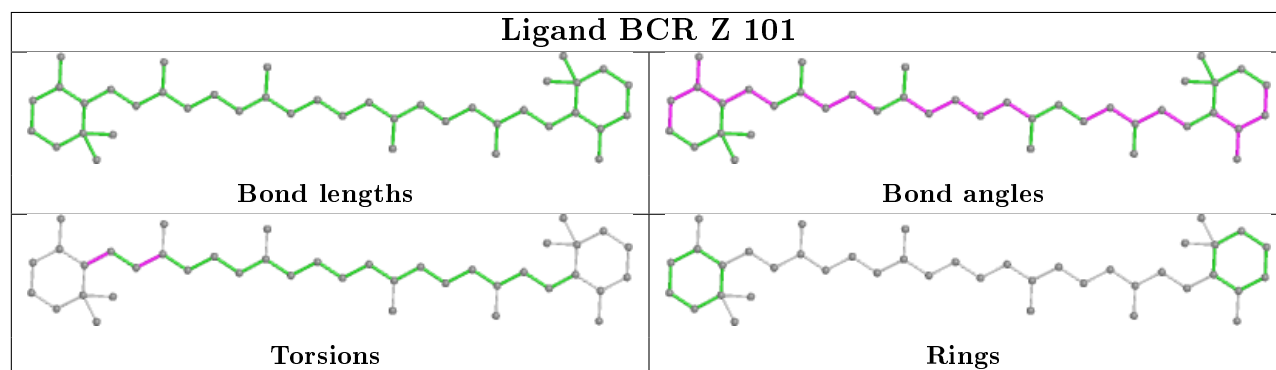
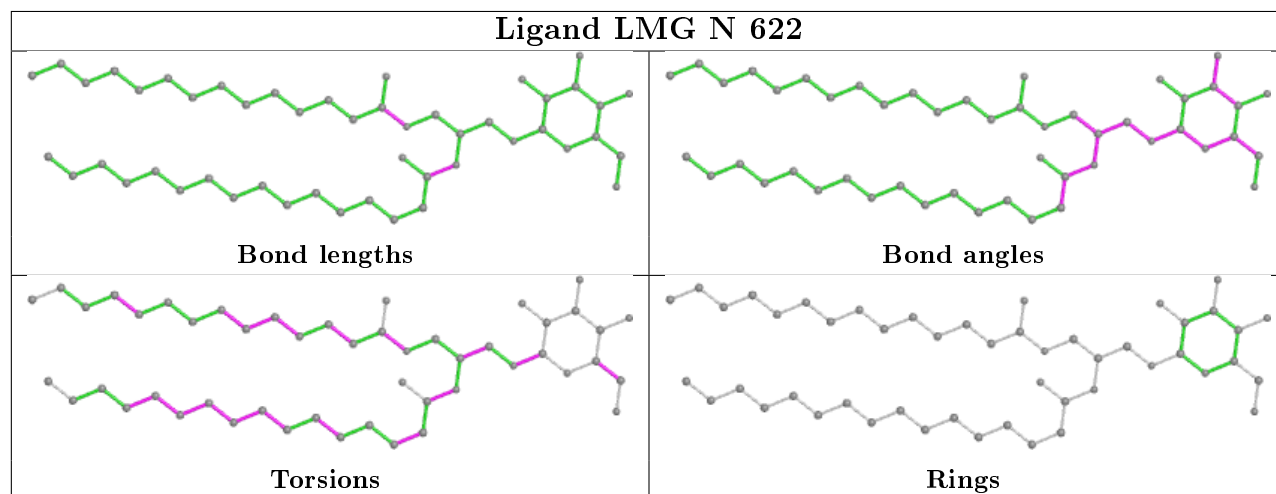


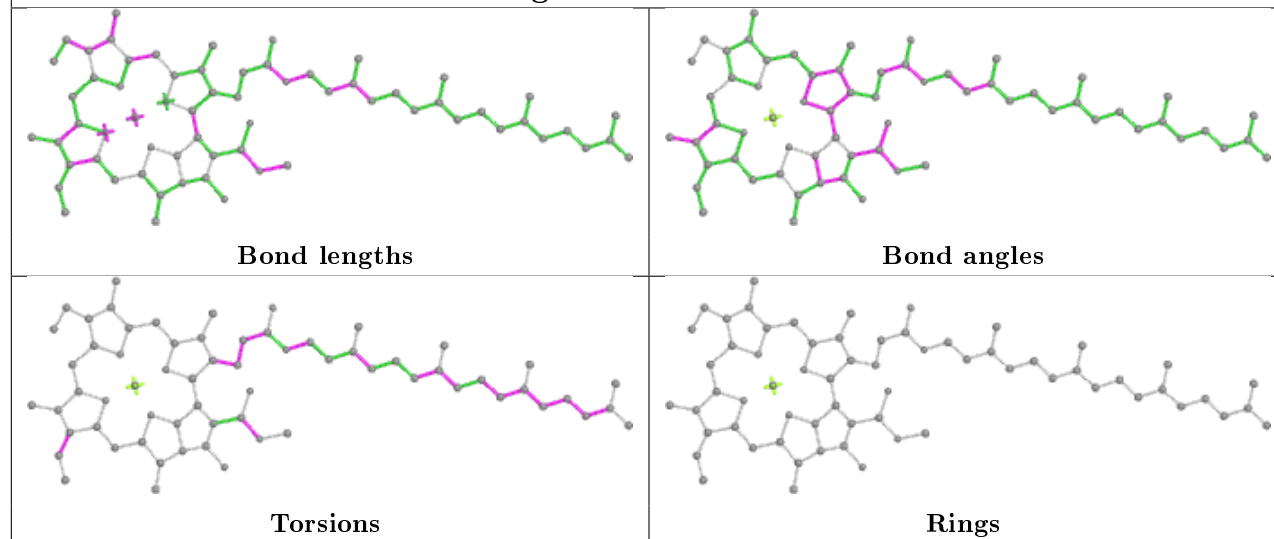
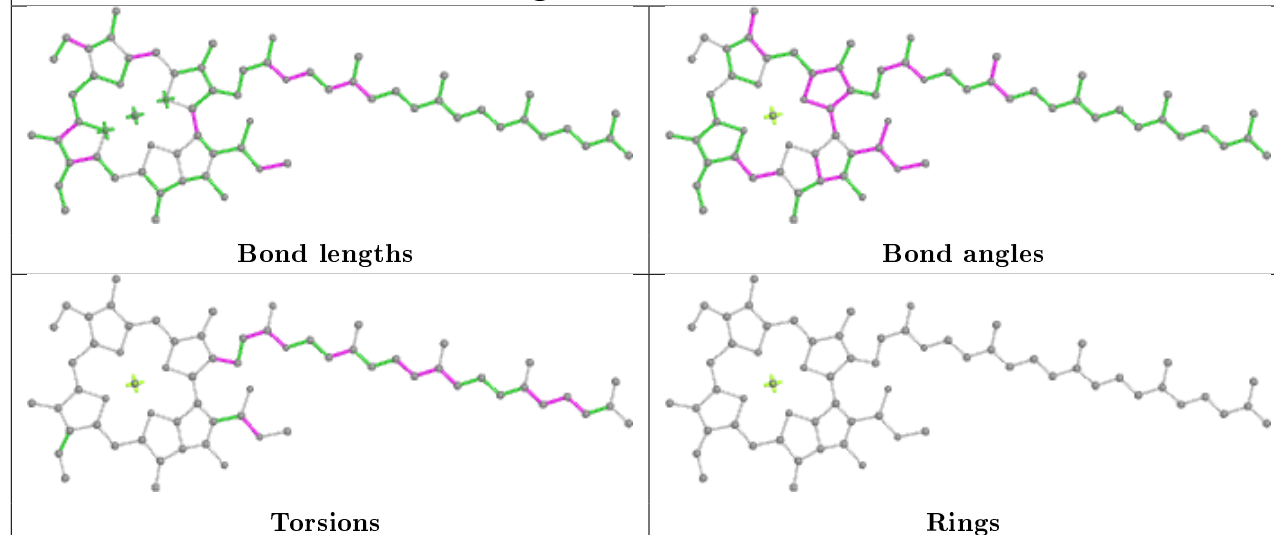
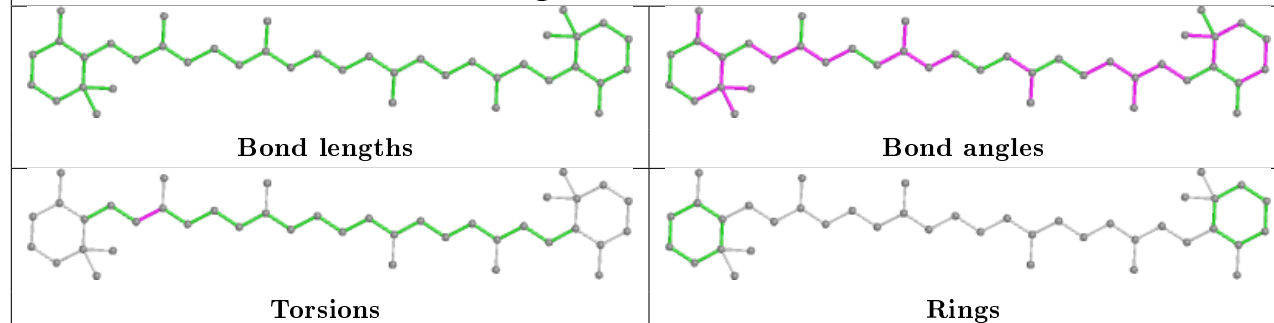




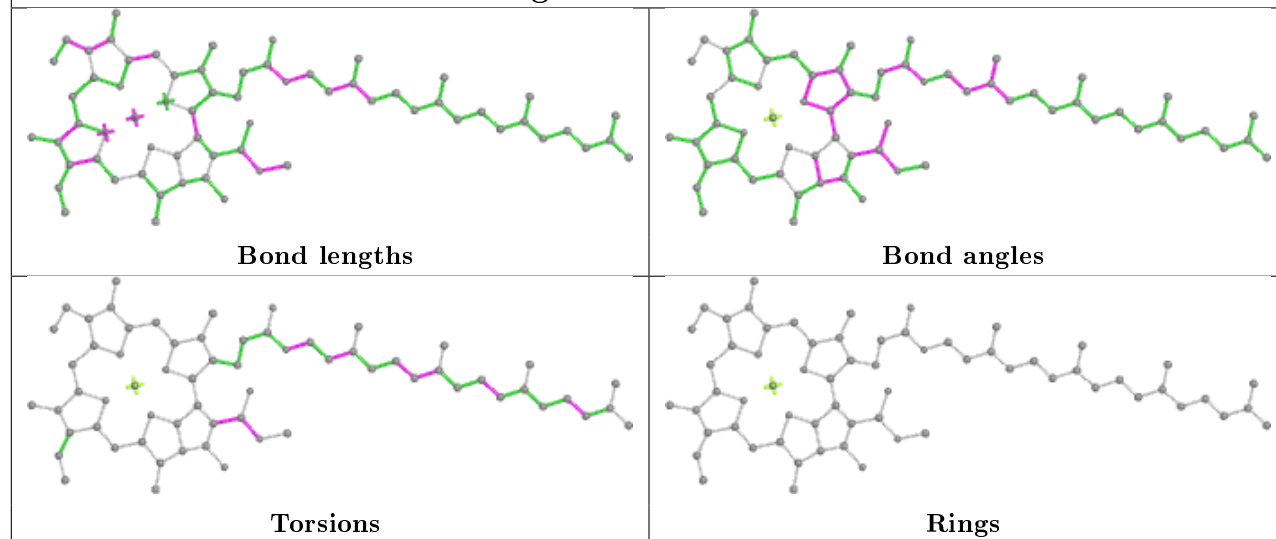
Ligand CLA B 609**Ligand CLA P 502****Ligand BCR H 101**



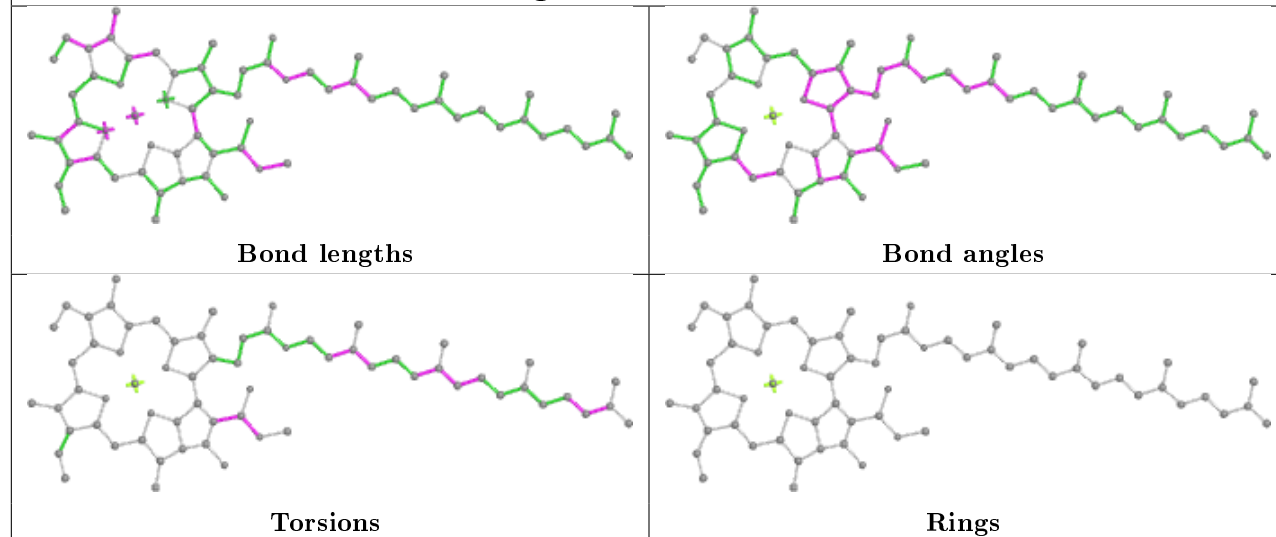
Ligand CLA C 503**Ligand BCR Z 101****Ligand LMG N 622**

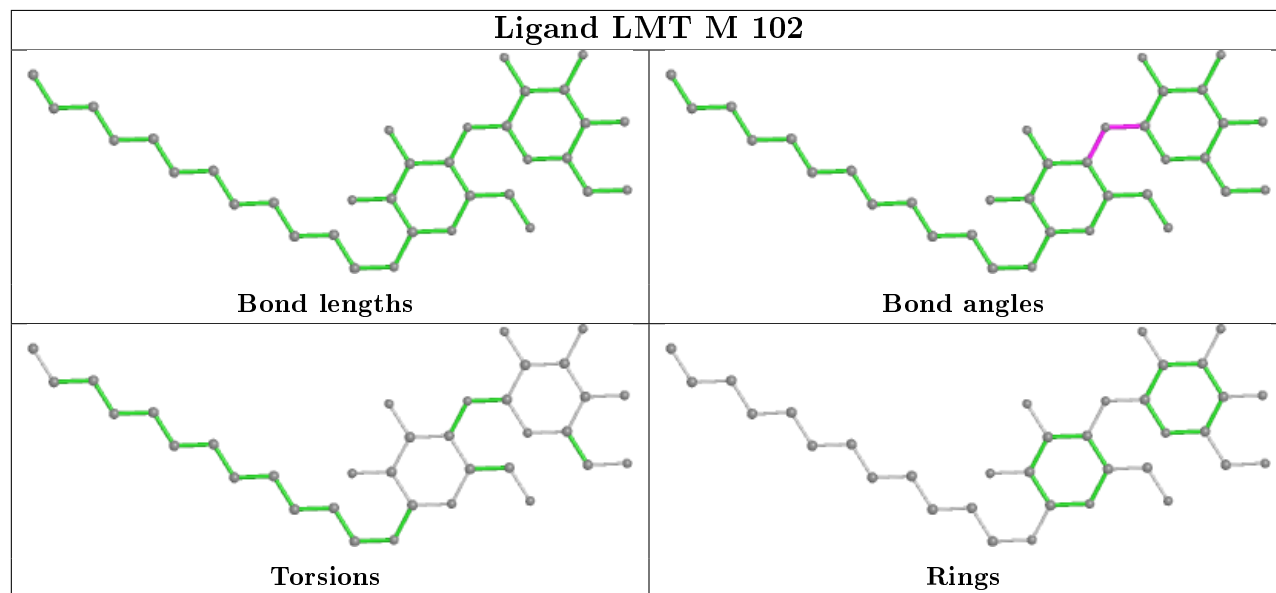
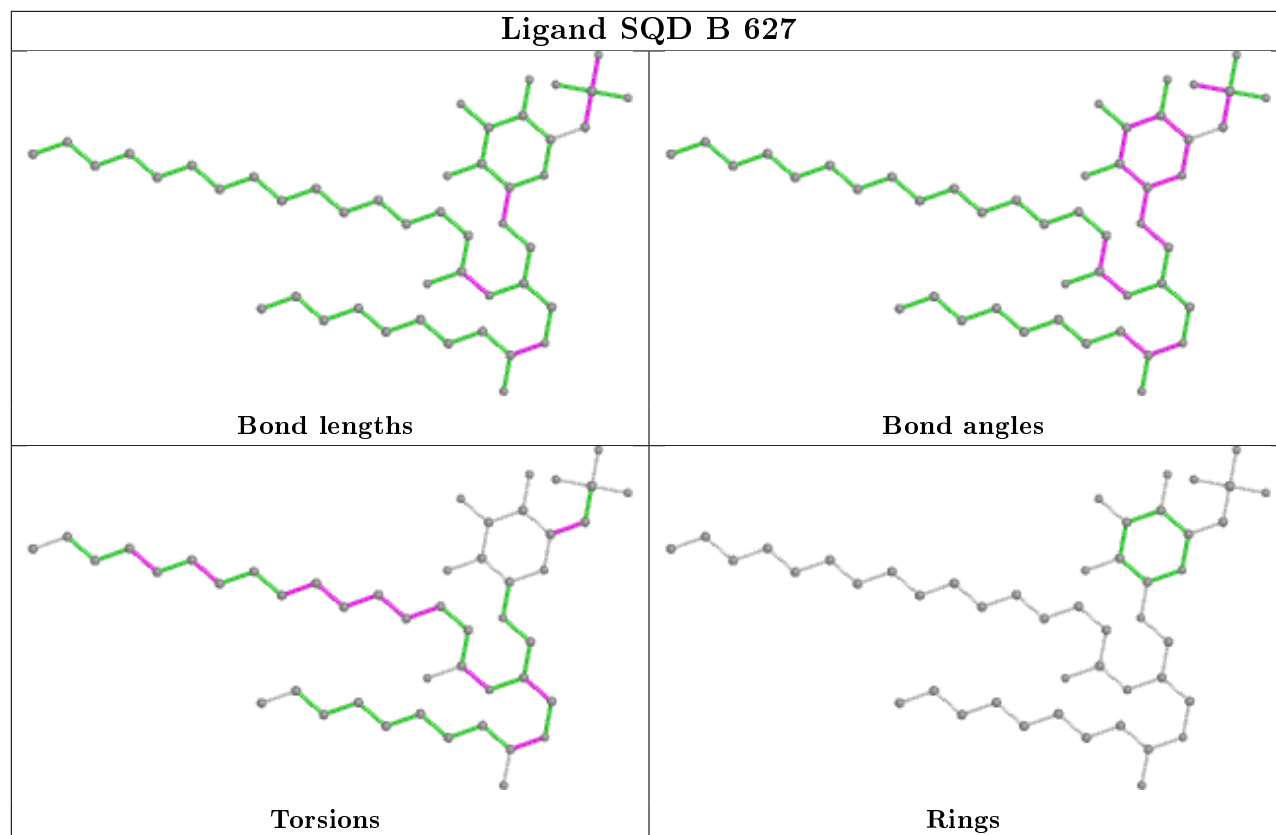
Ligand CLA N 605**Ligand CLA D 401****Ligand BCR b 102**

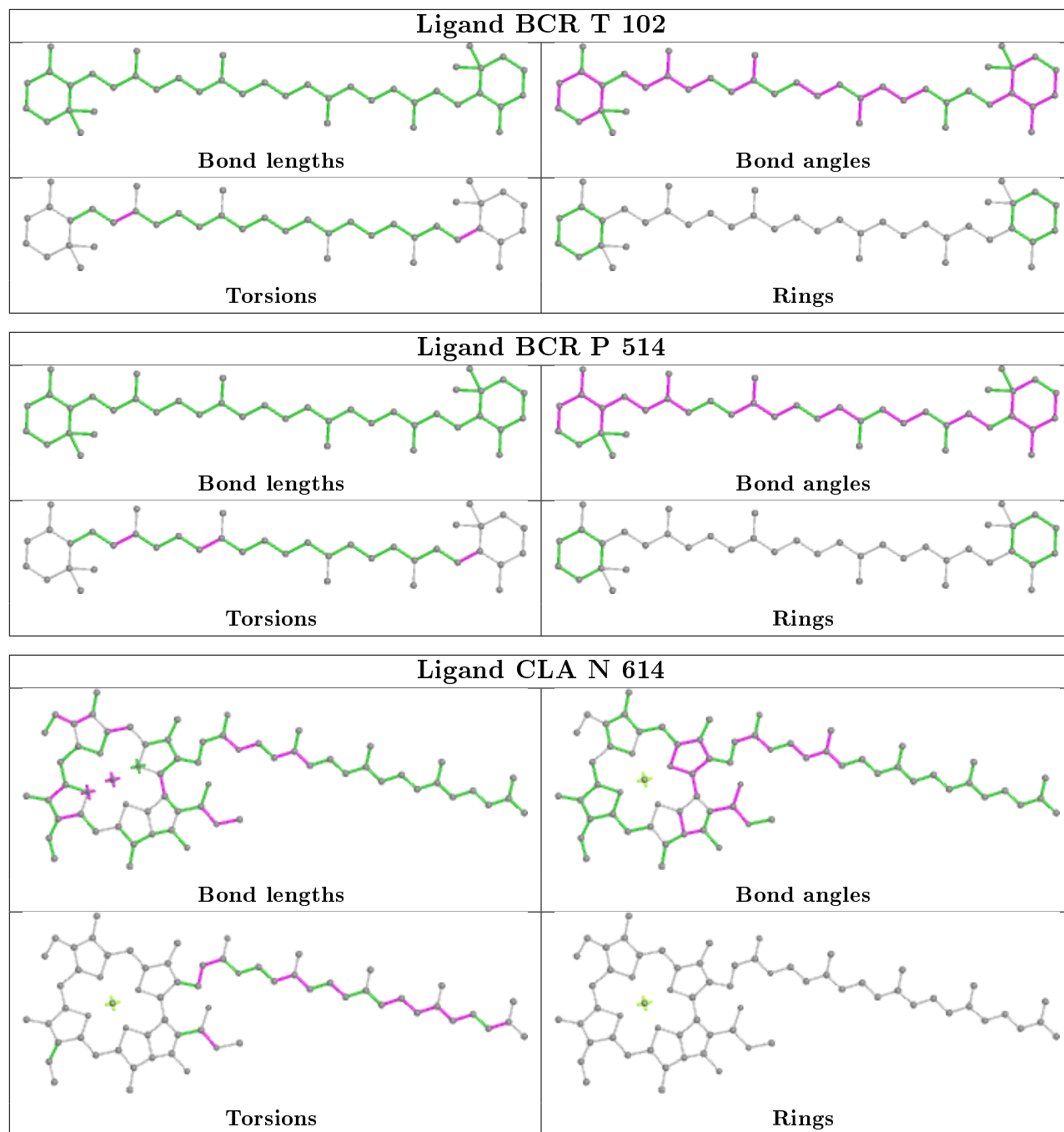
Ligand CLA G 404

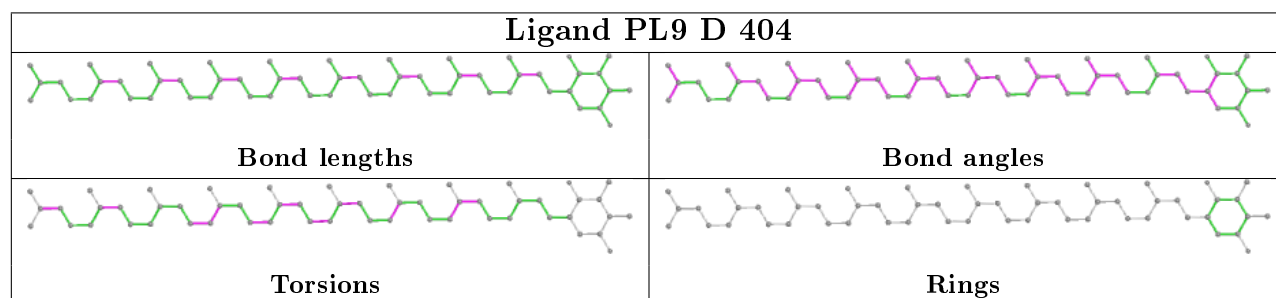
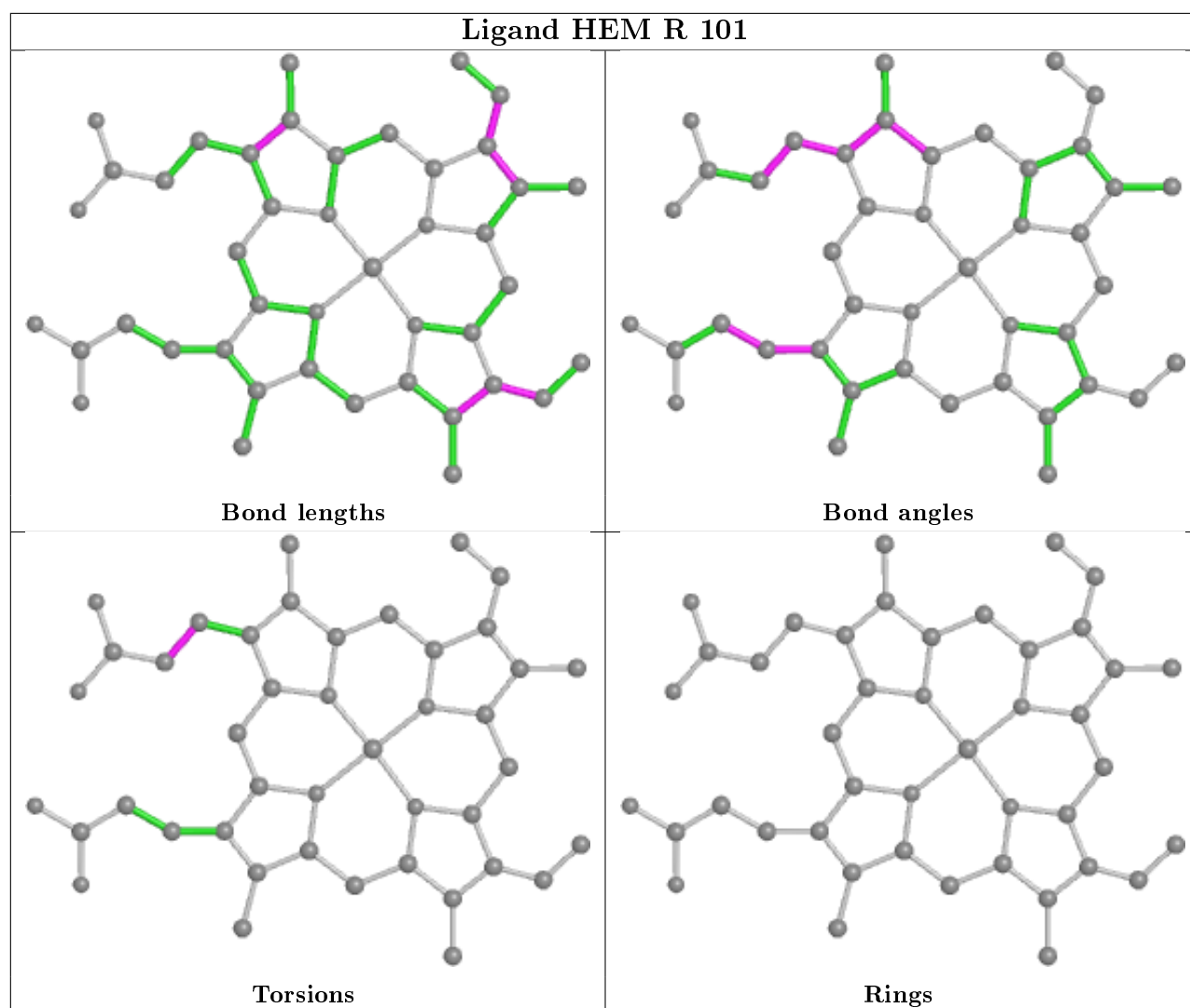


Ligand CLA B 611

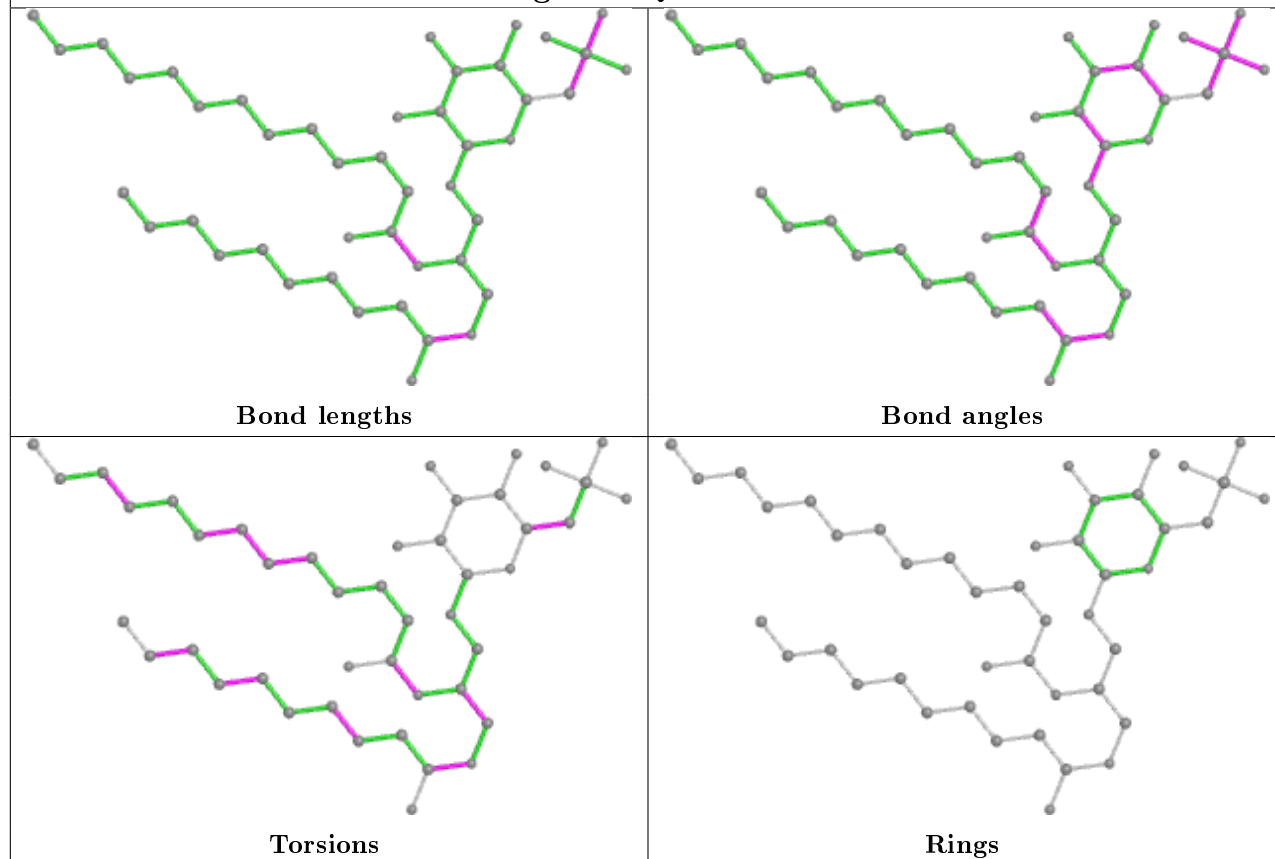




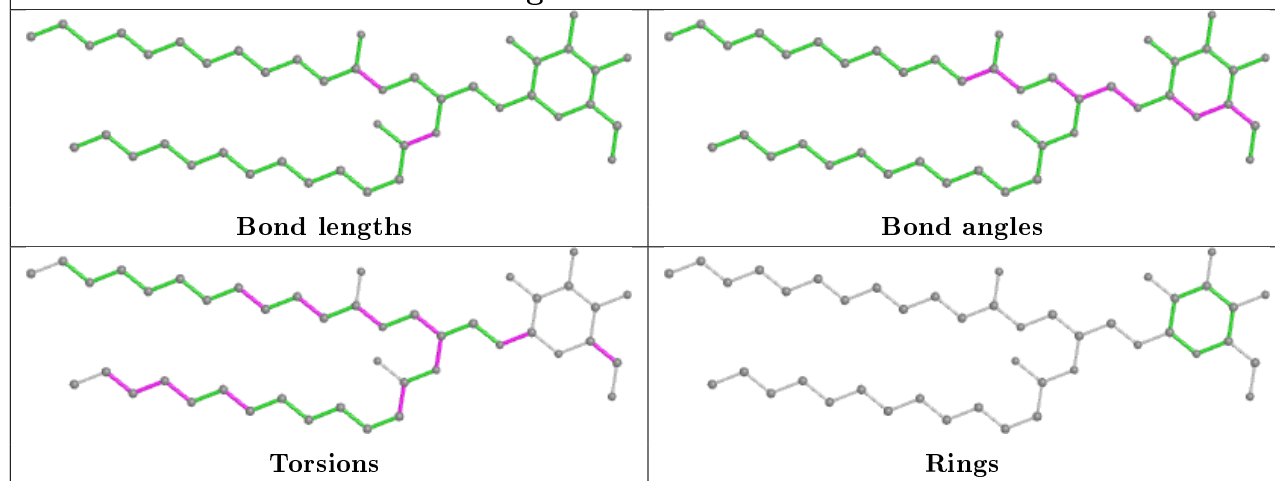


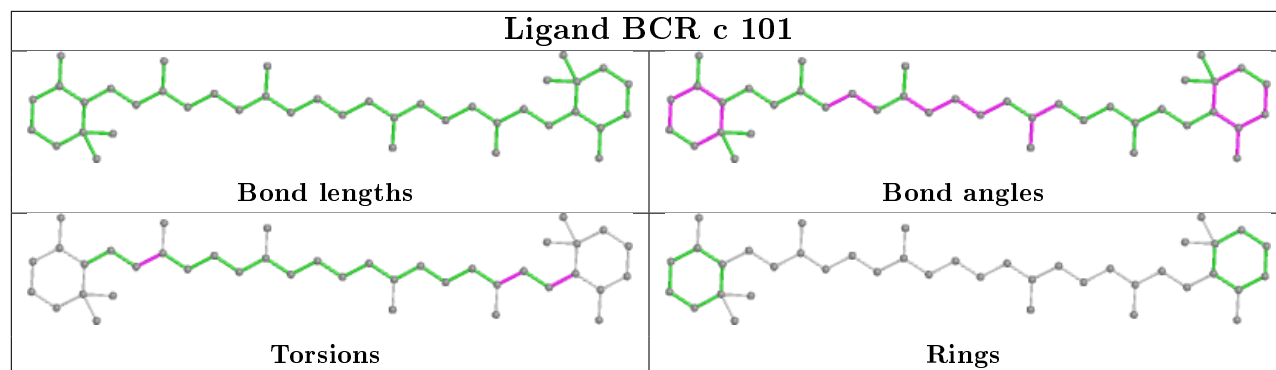
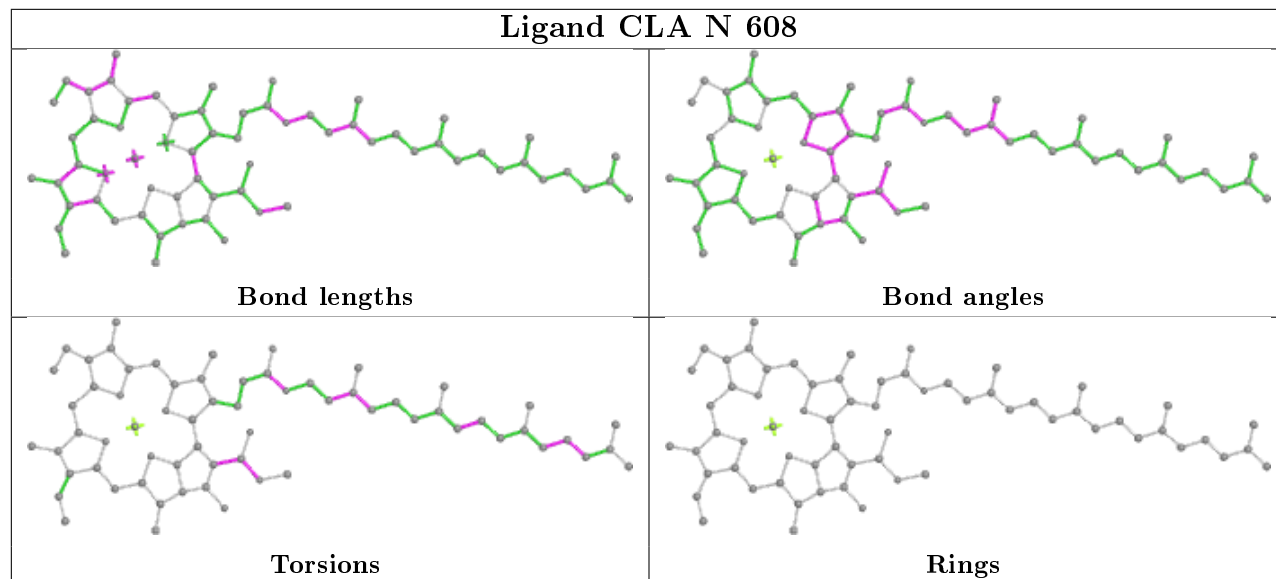
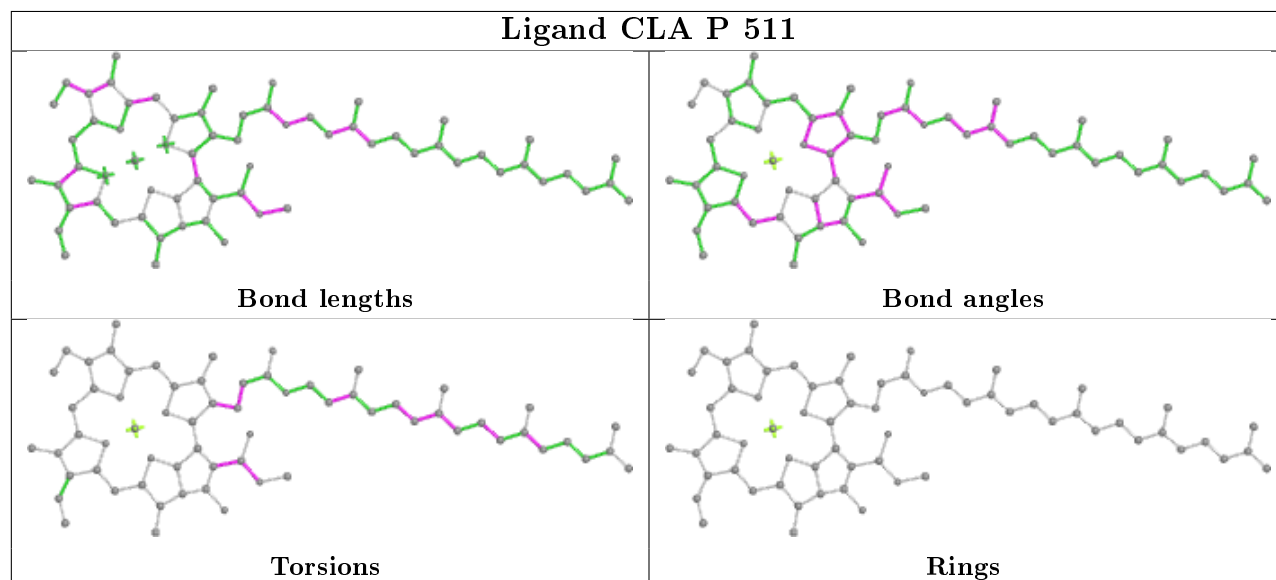


Ligand SQD F 101

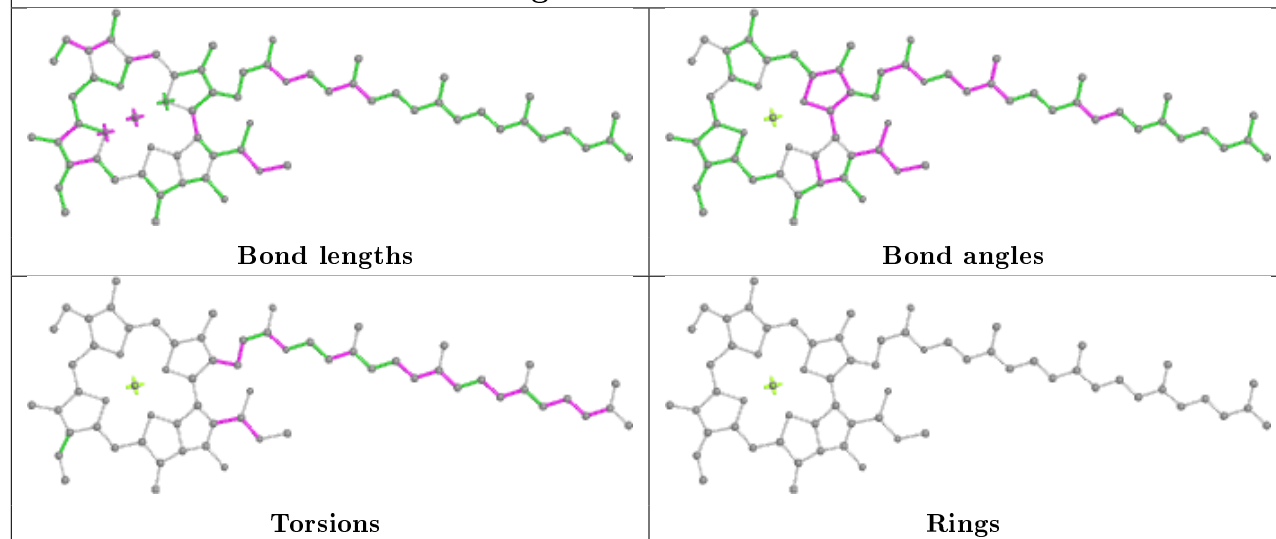


Ligand LMG R 102

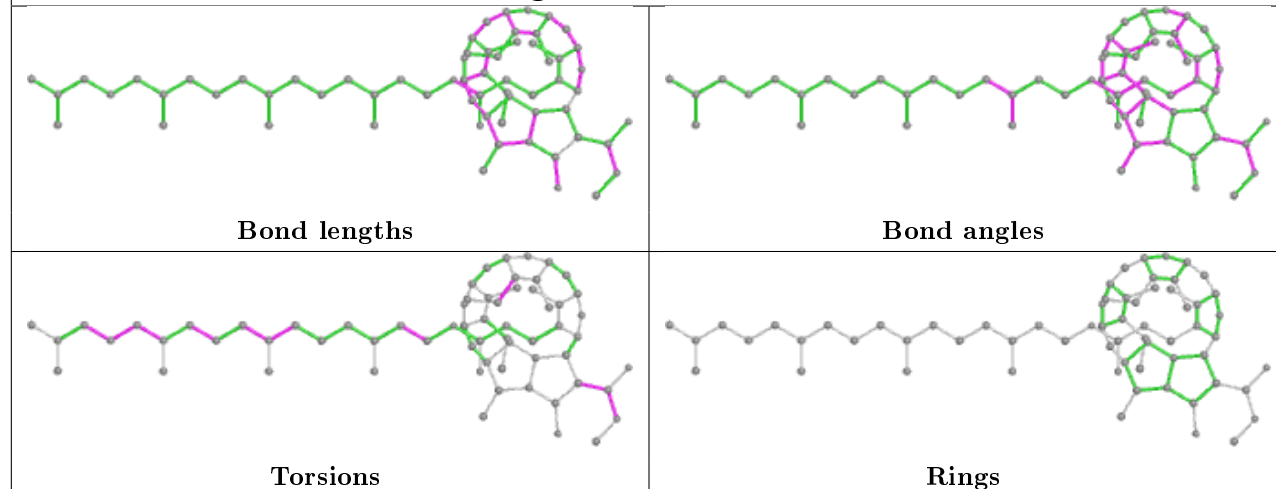


Ligand BCR c 101**Ligand CLA N 608****Ligand CLA P 511**

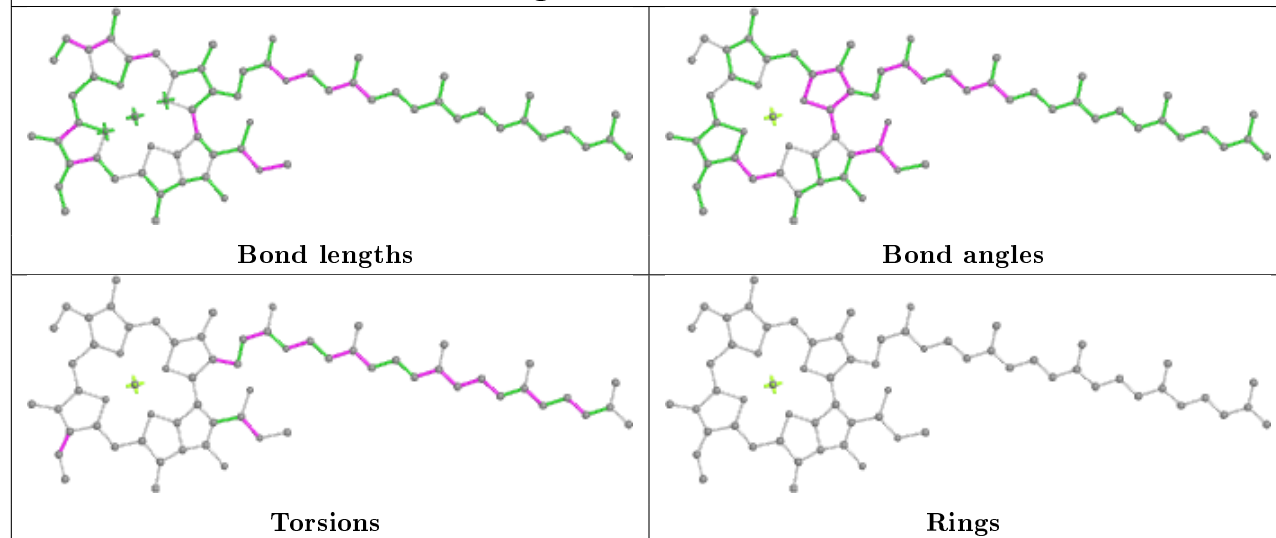
Ligand CLA N 609

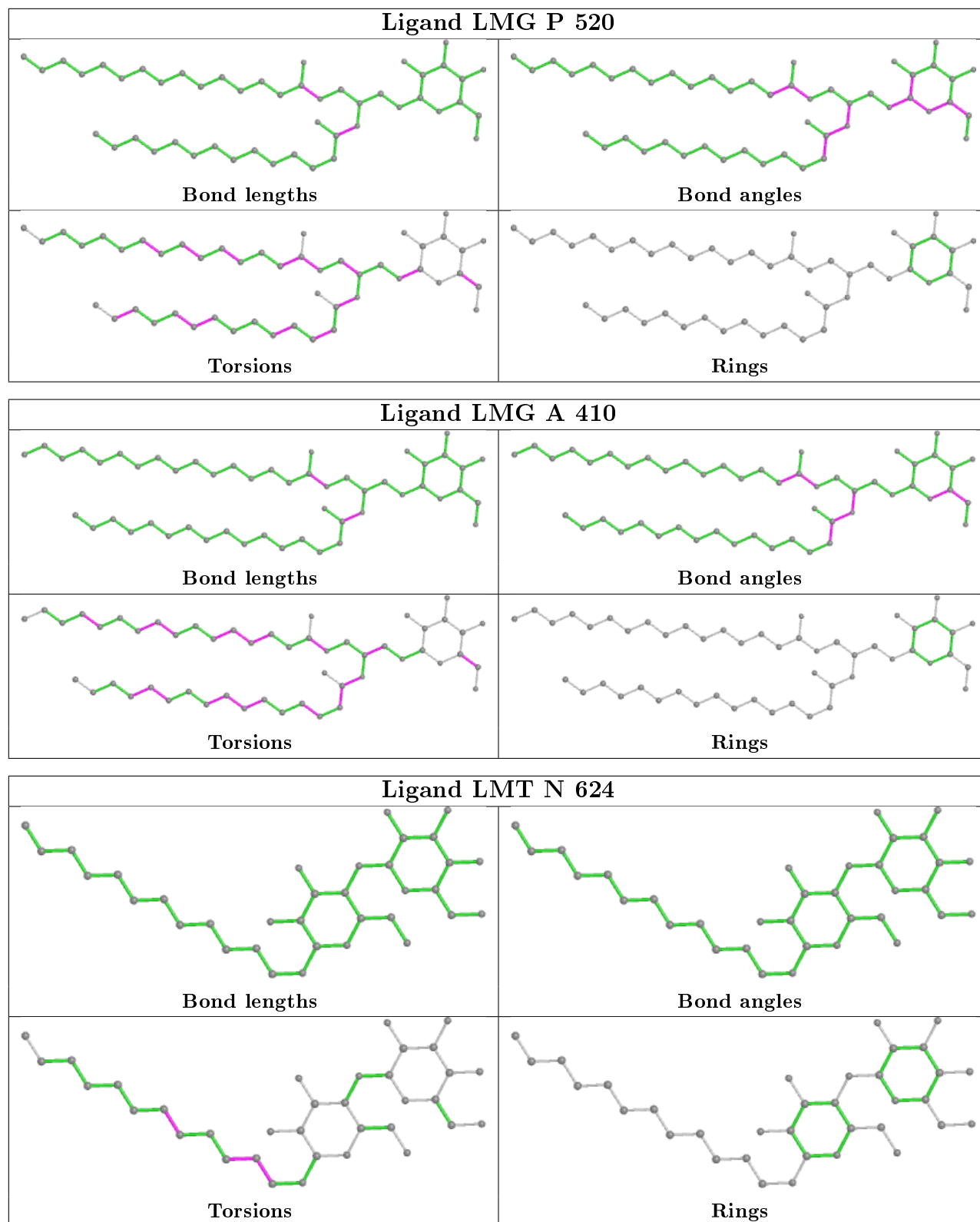


Ligand PHO Q 403

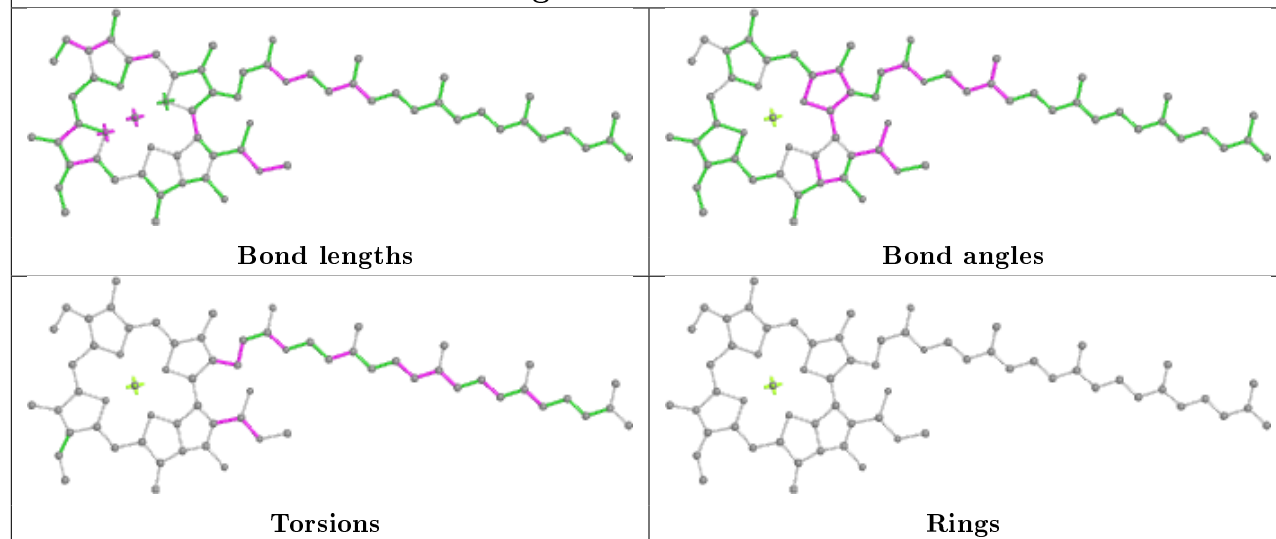


Ligand CLA C 505

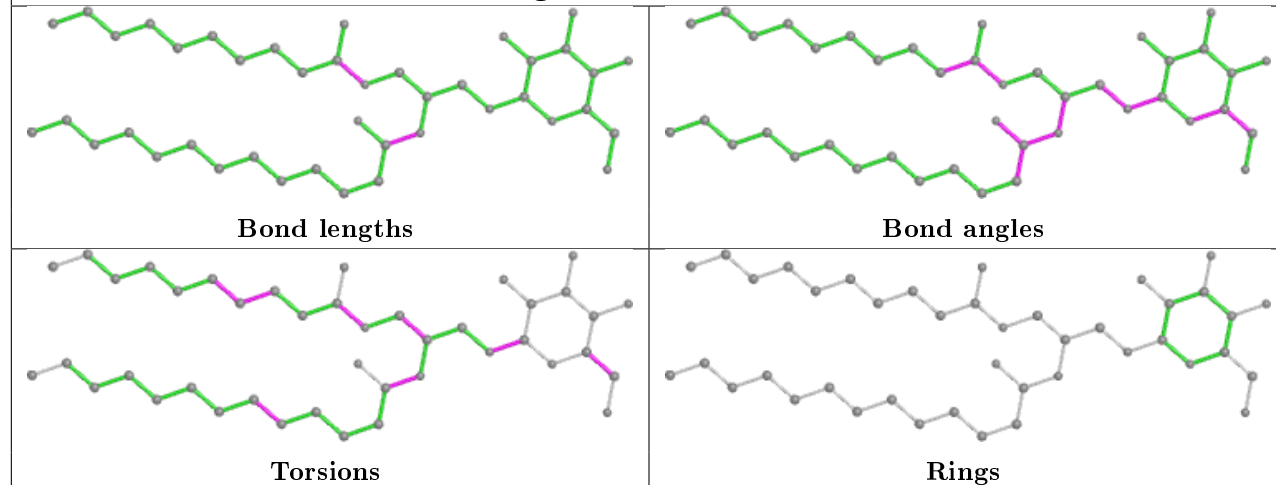




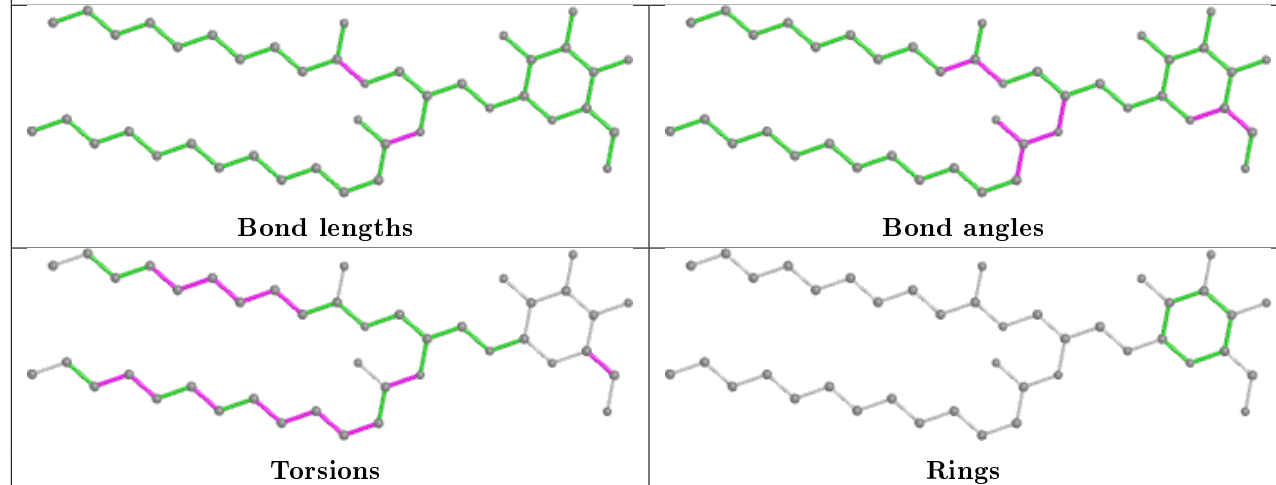
Ligand CLA C 511



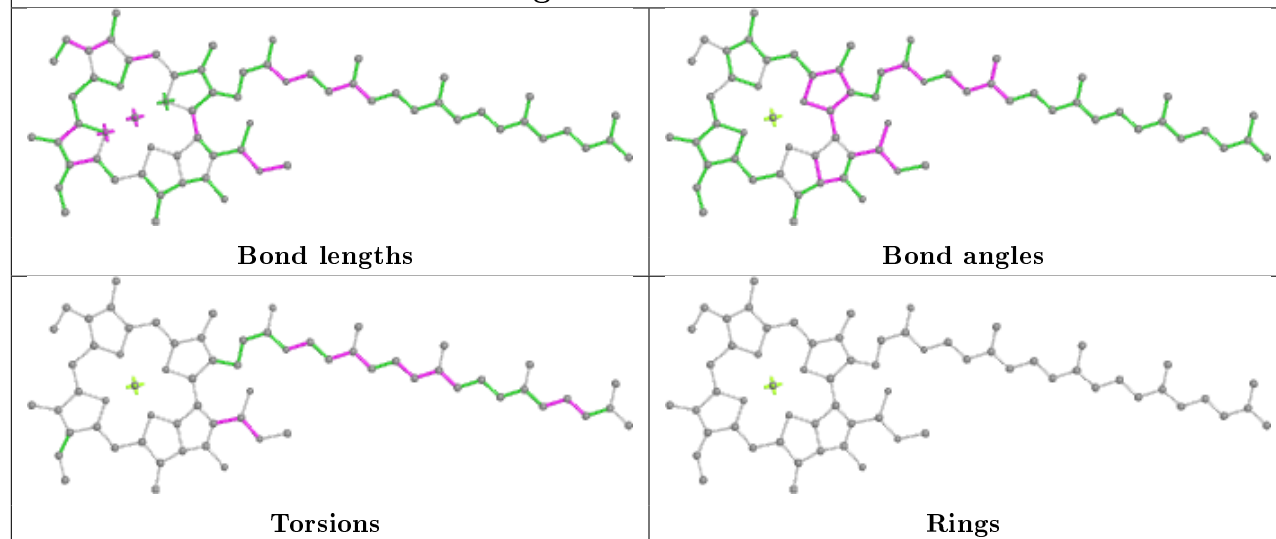
Ligand LMG e 102



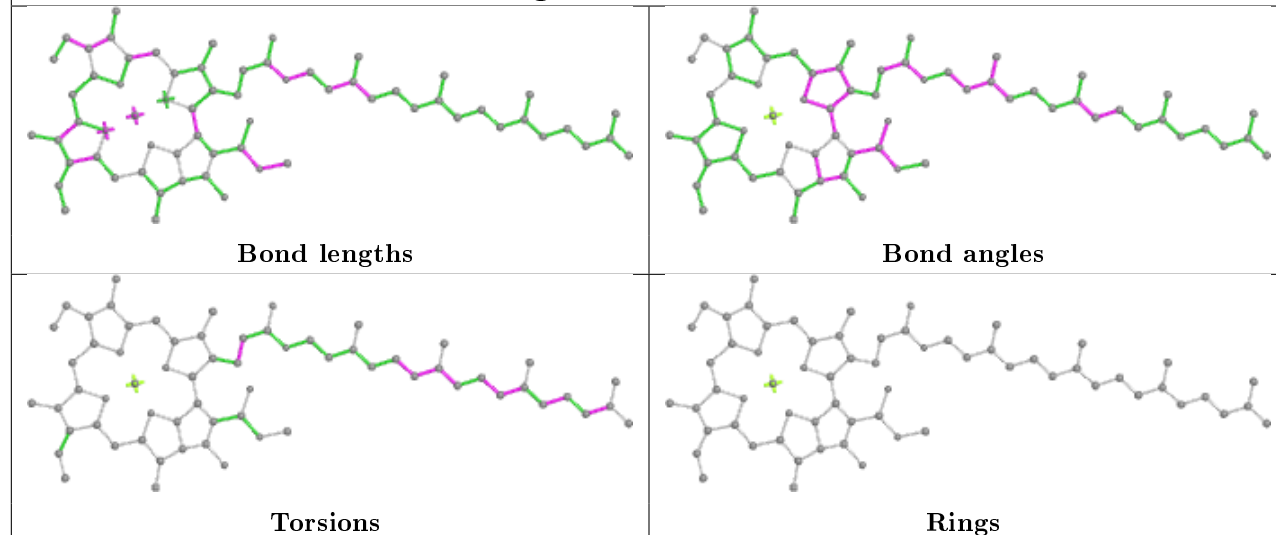
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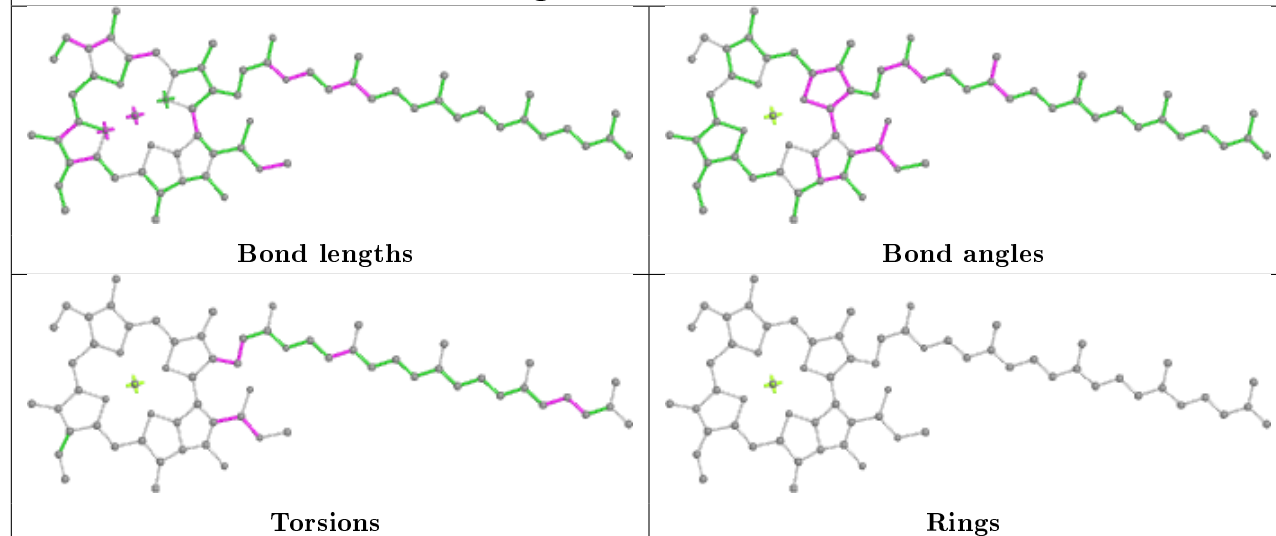
Ligand CLA P 510



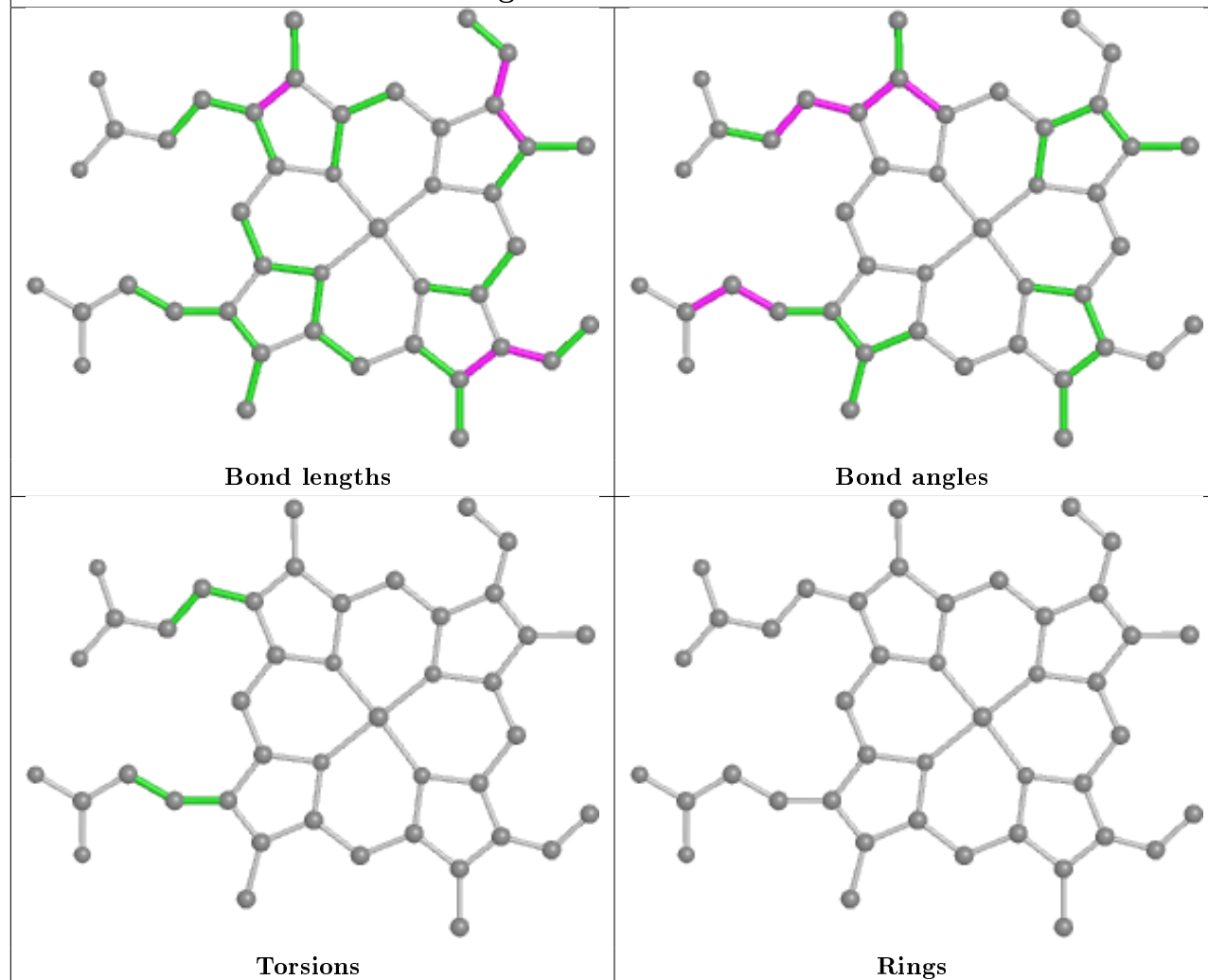
Ligand CLA A 405



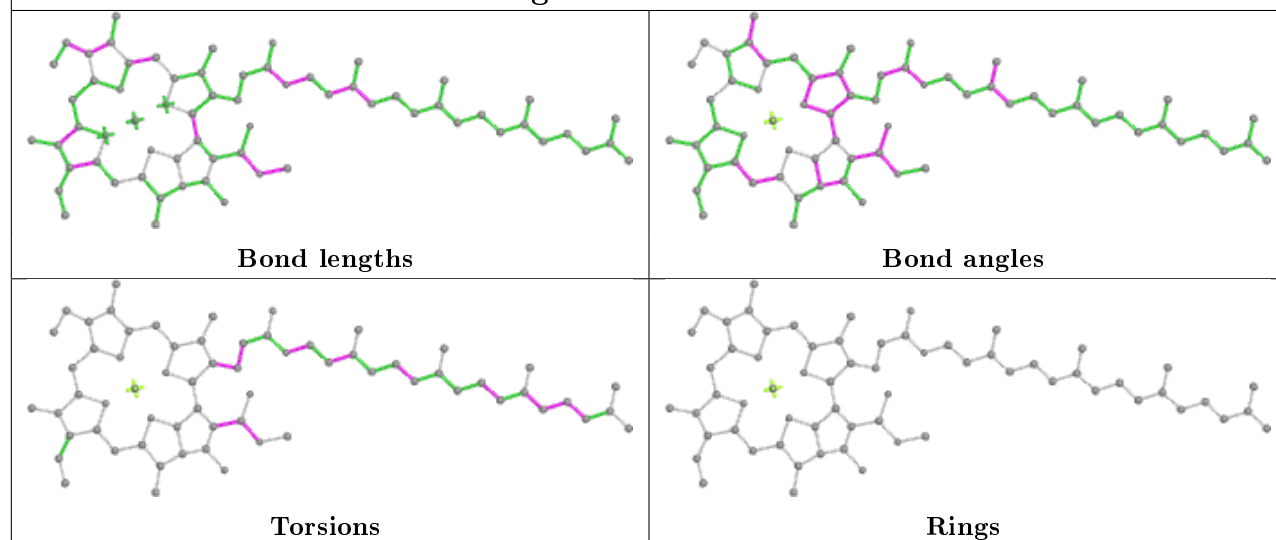
Ligand CLA B 607

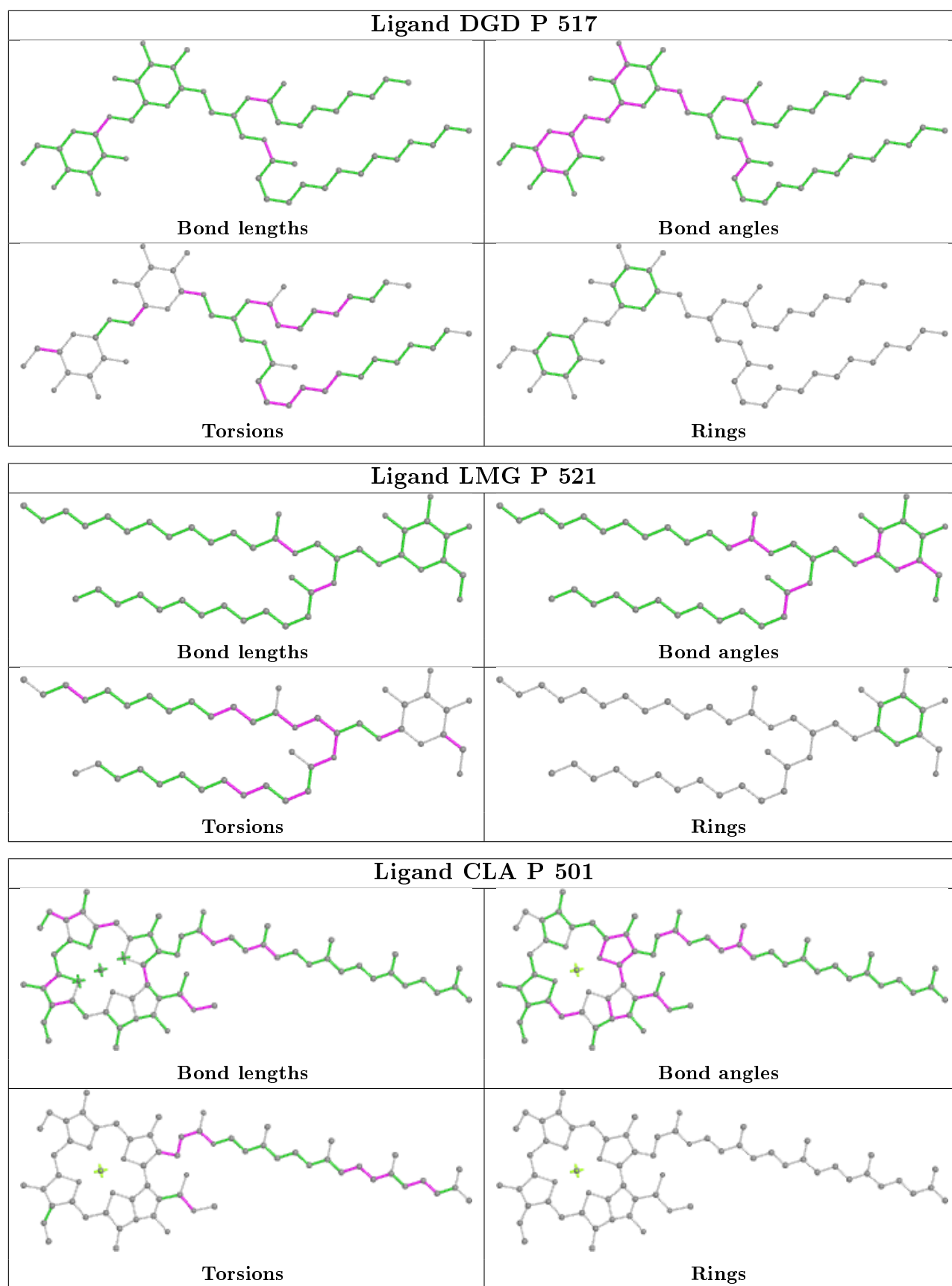


Ligand HEM V 201

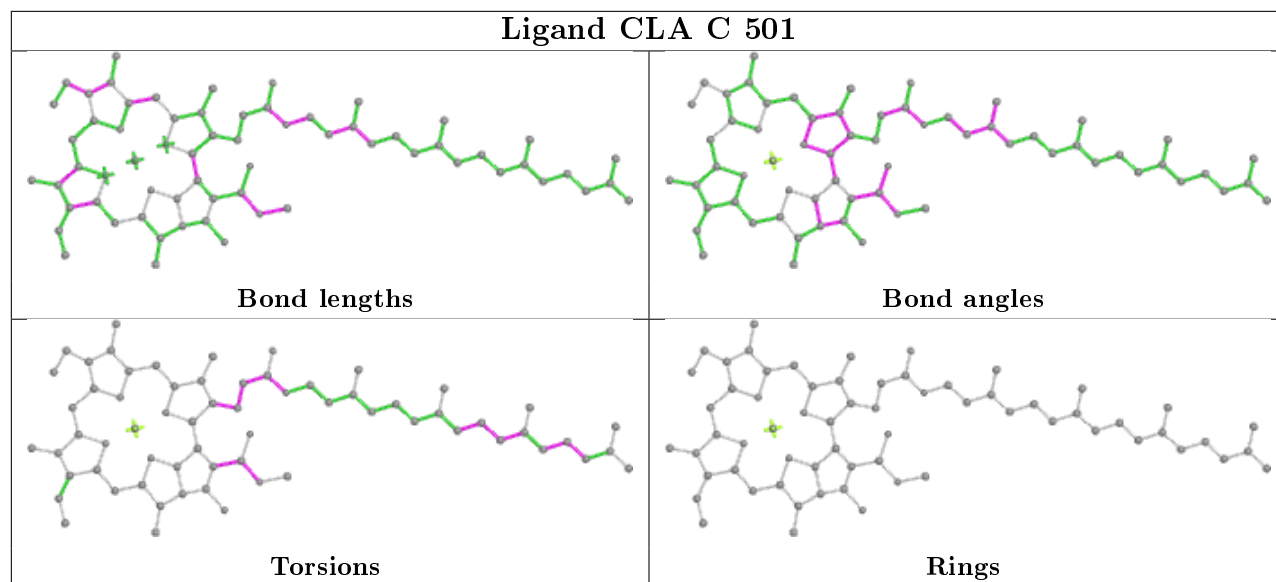


Ligand CLA N 610

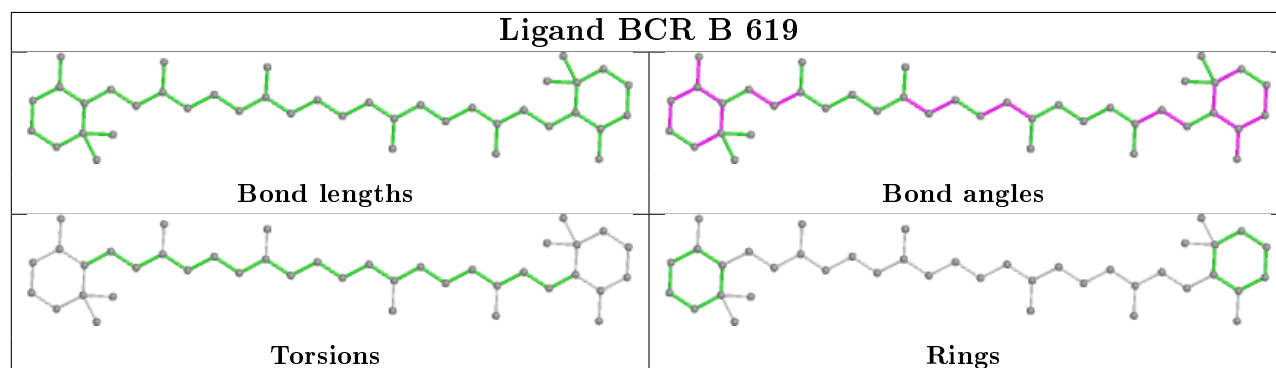




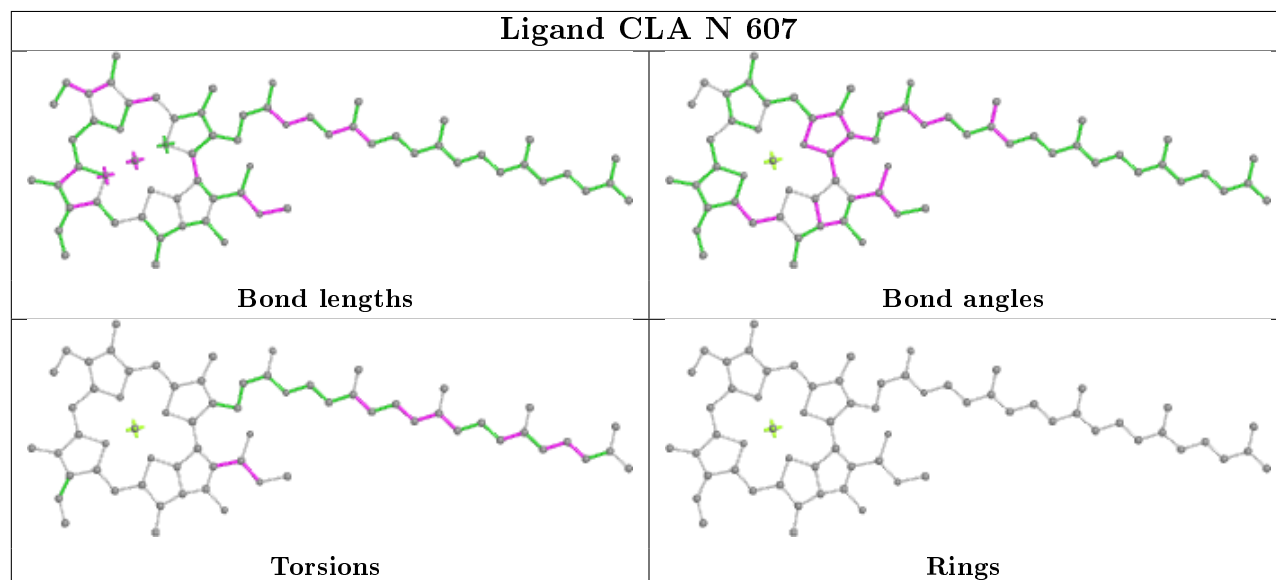
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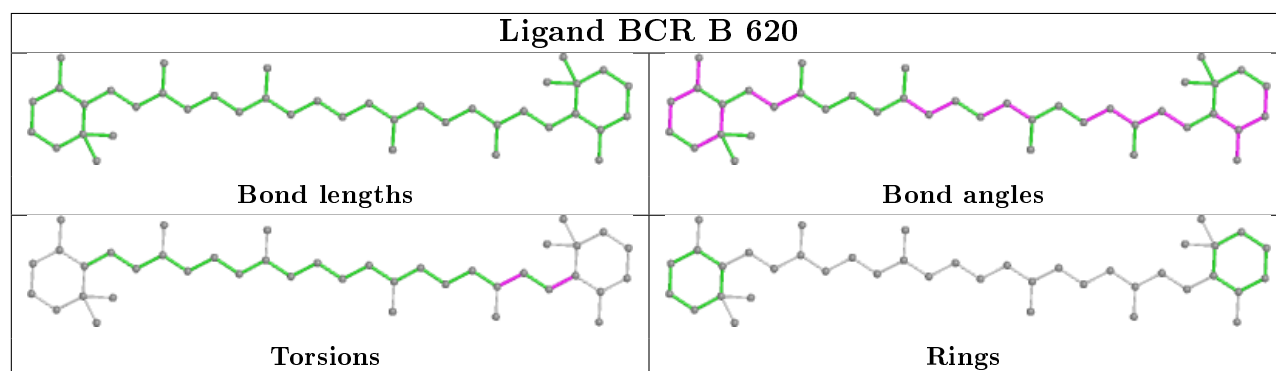
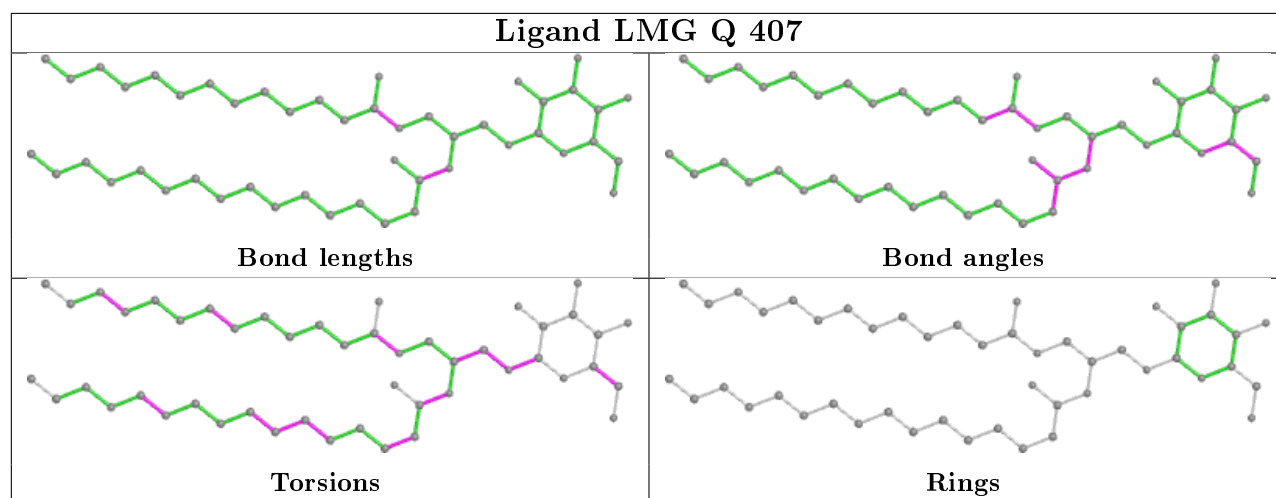
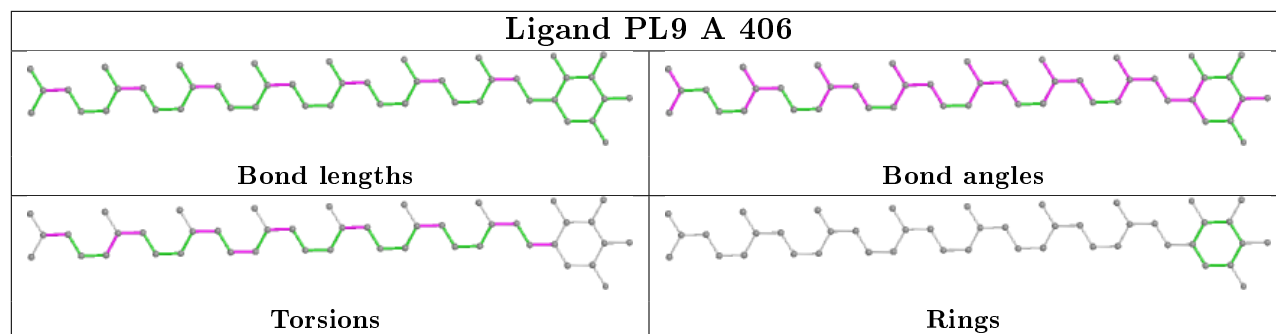


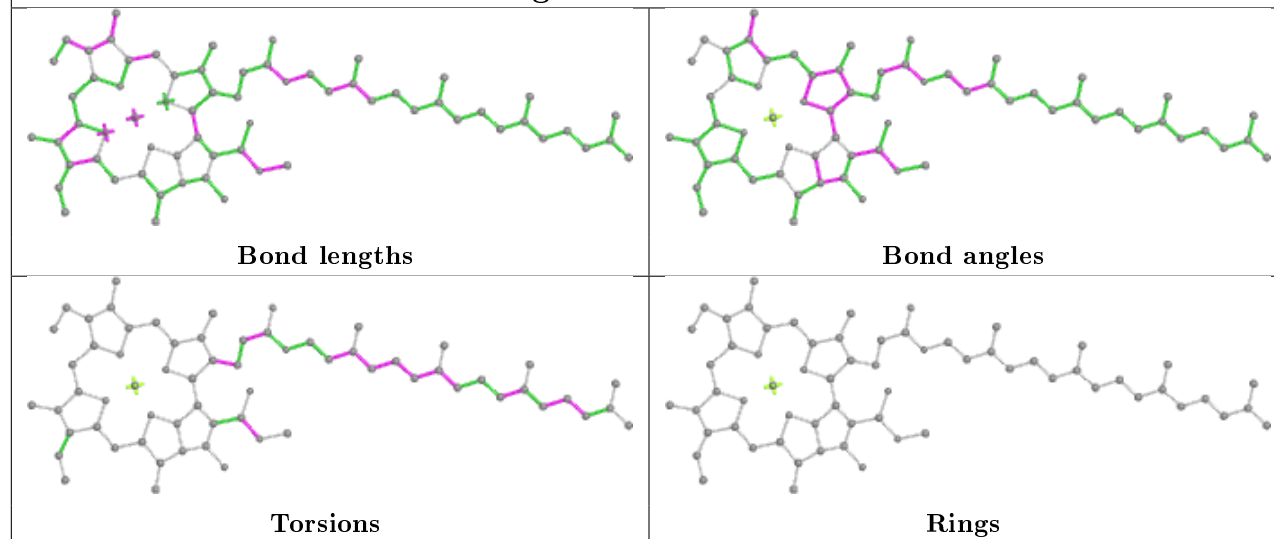
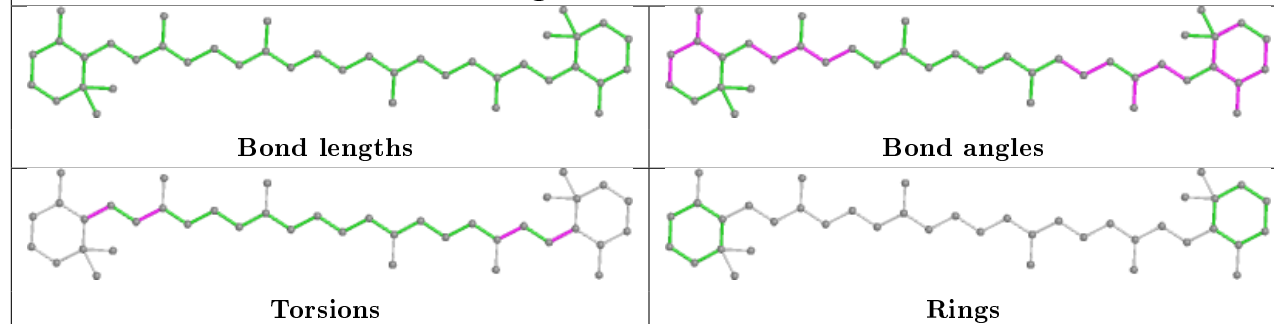
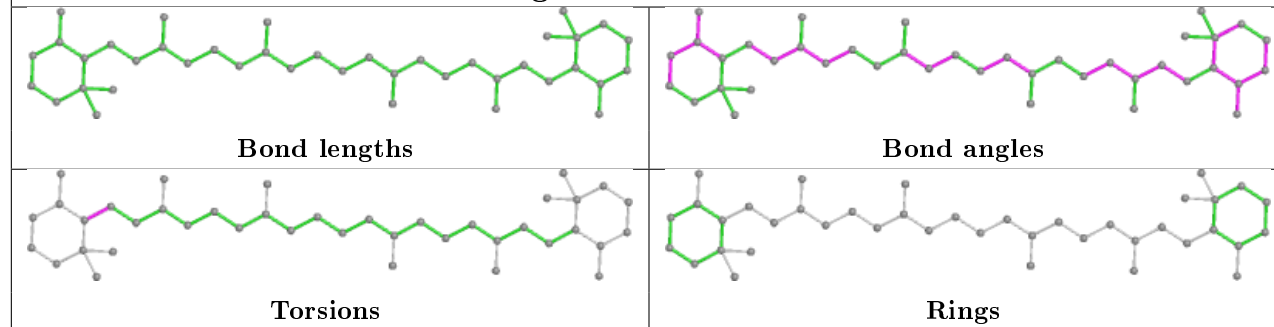
Ligand BCR B 619



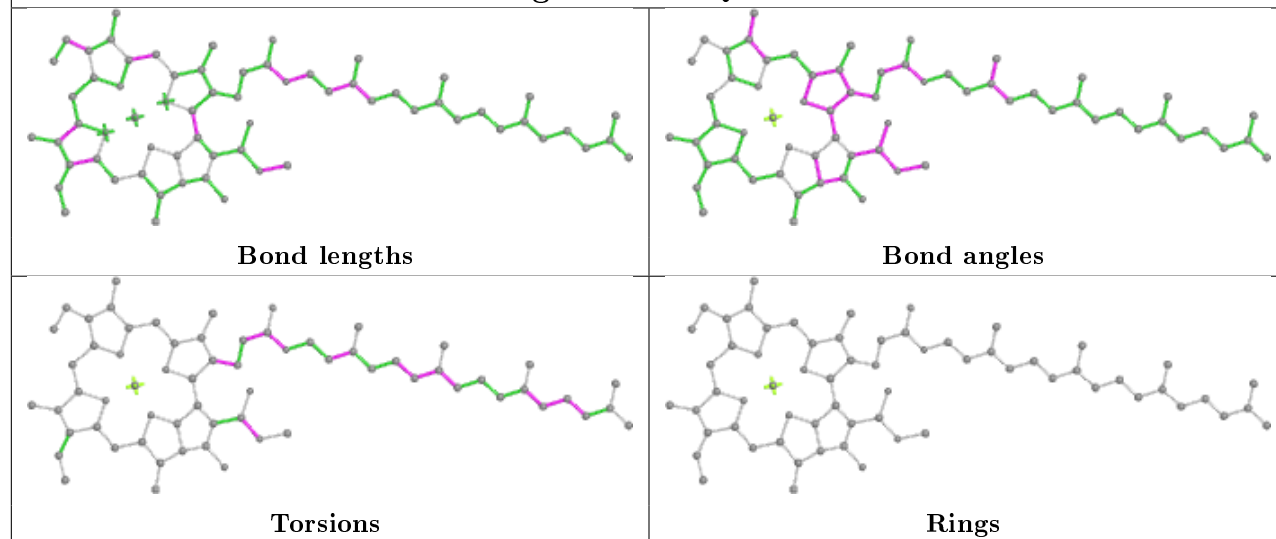
Ligand CLA N 607



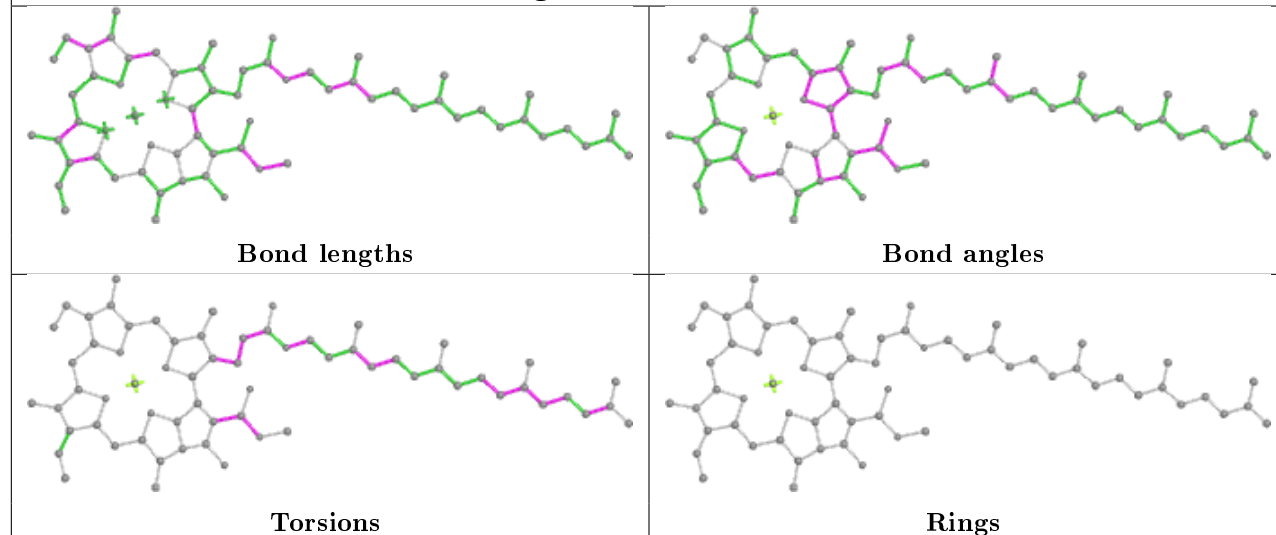


Ligand CLA B 608**Ligand BCR D 405****Ligand BCR B 617**

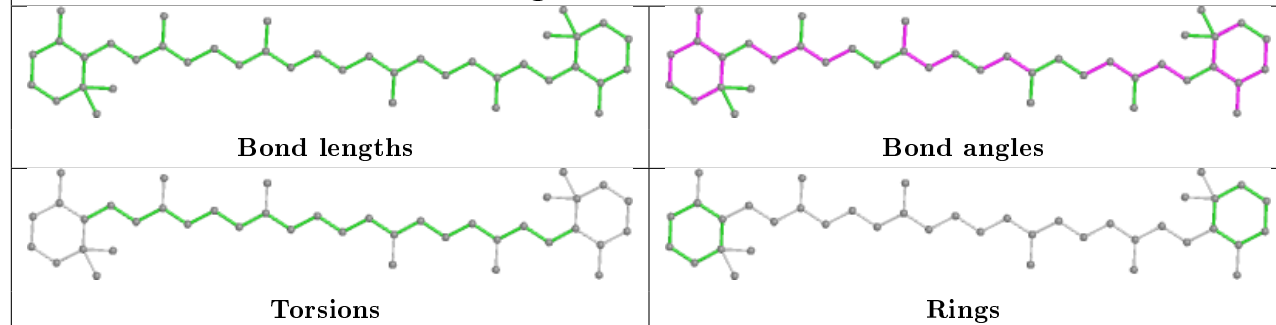
Ligand CLA Q 402

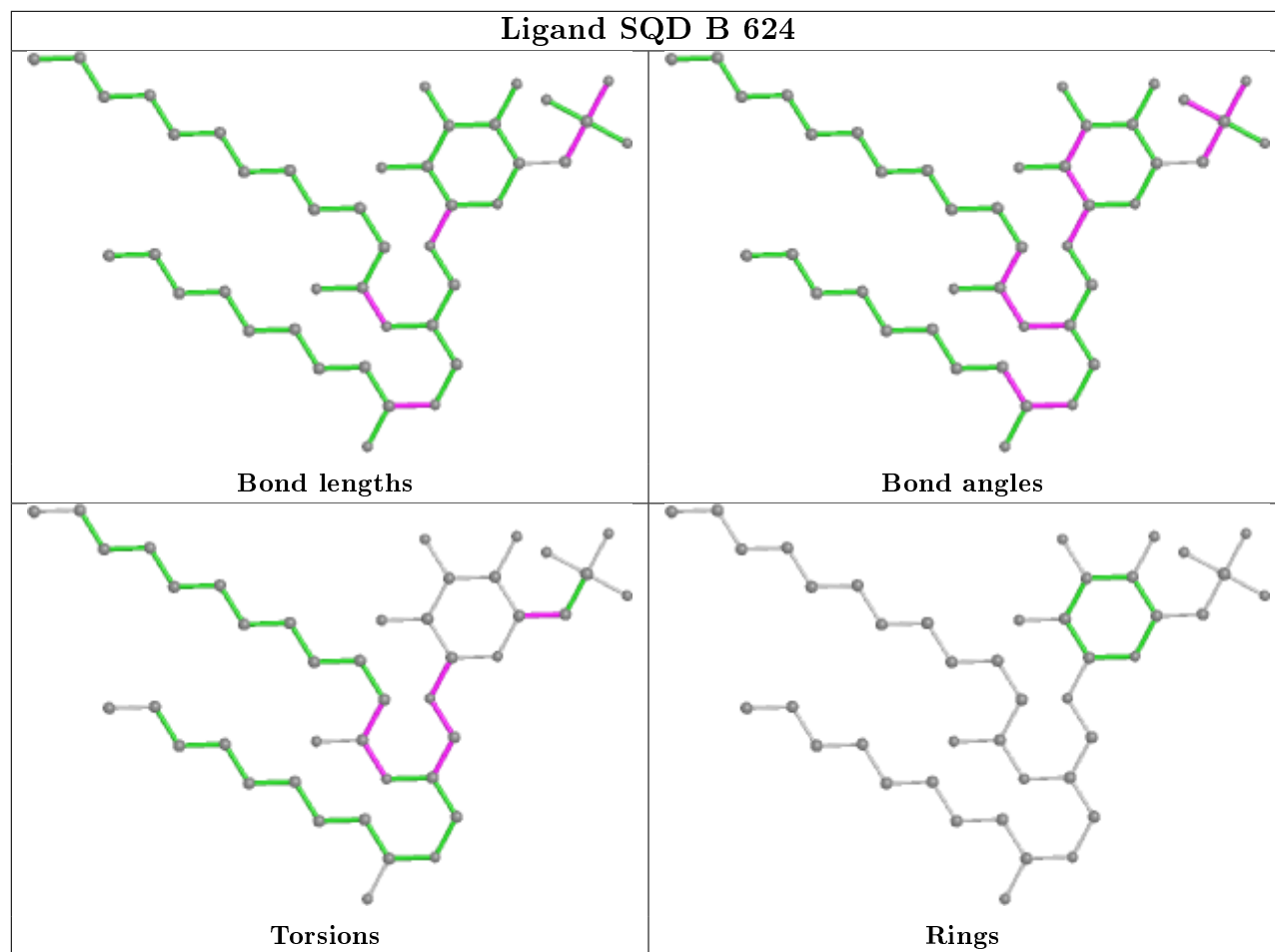
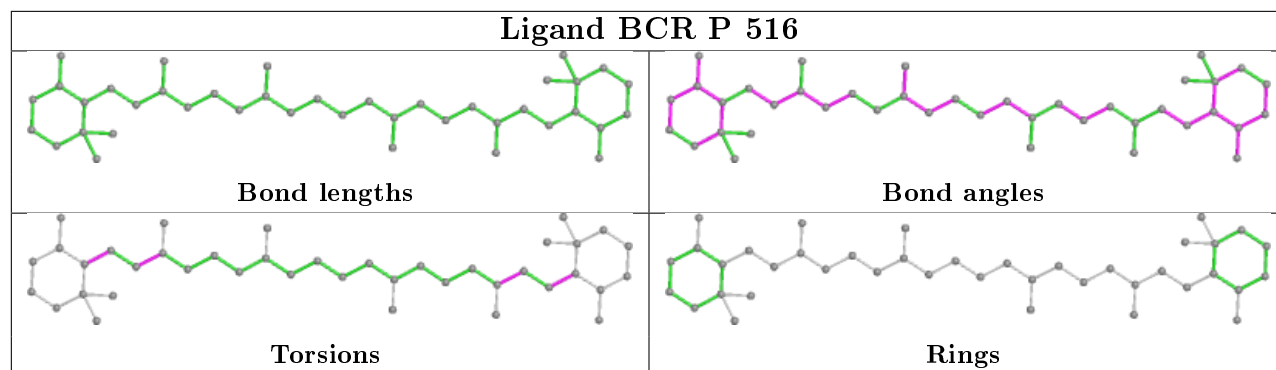


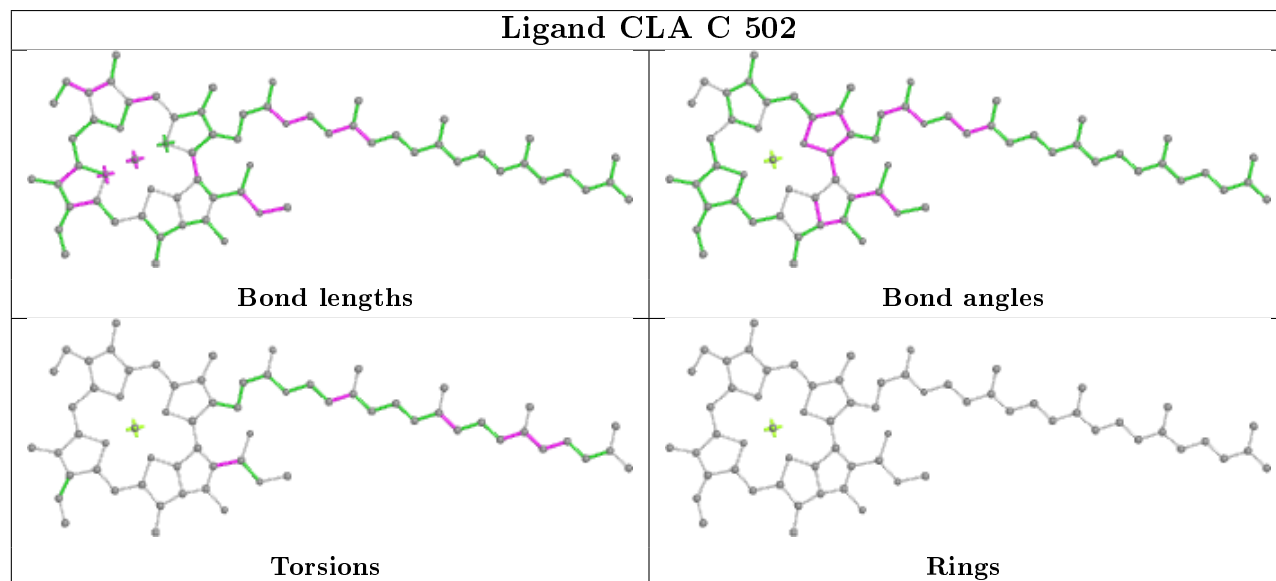
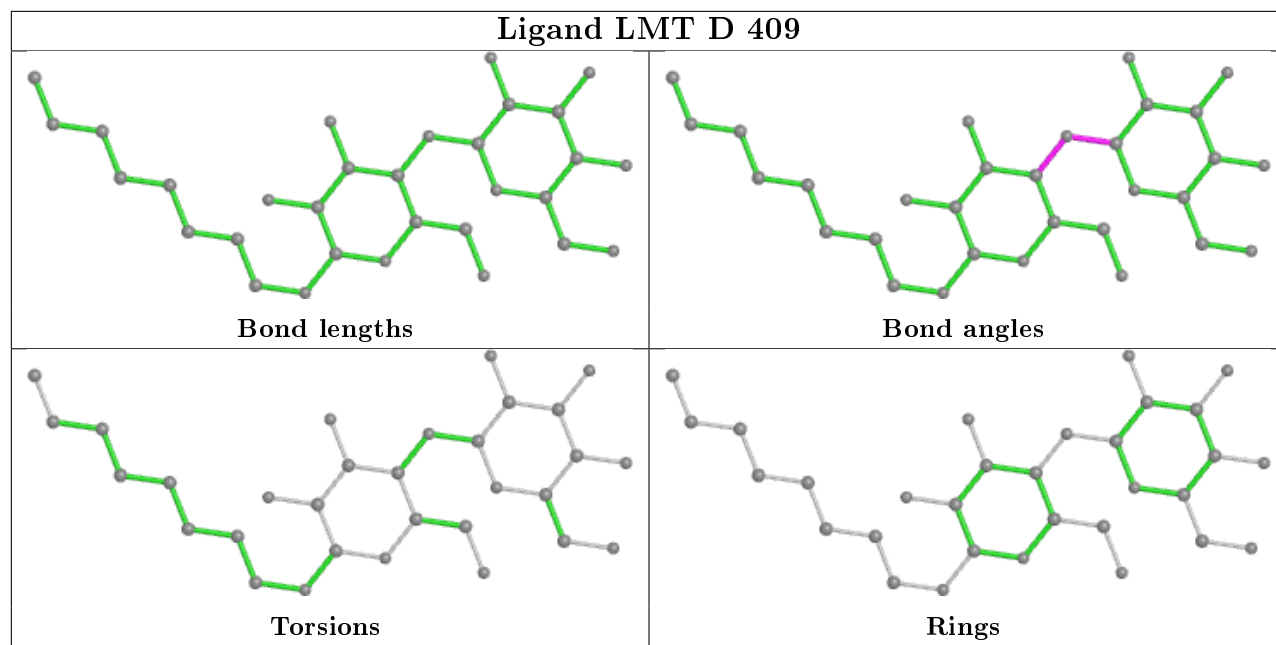
Ligand CLA C 512



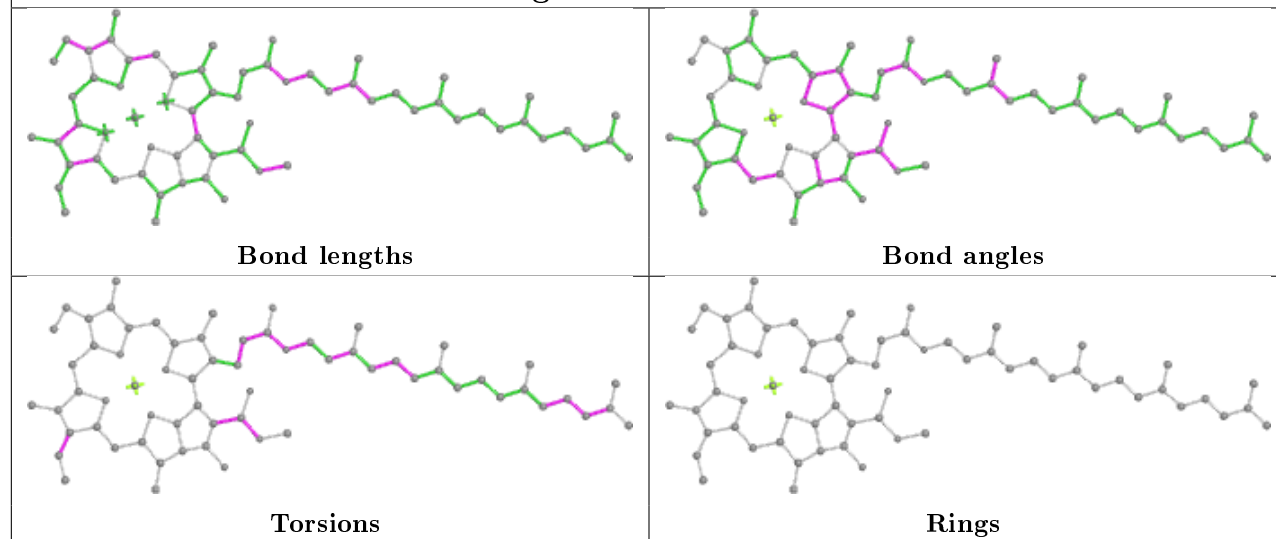
Ligand BCR N 621



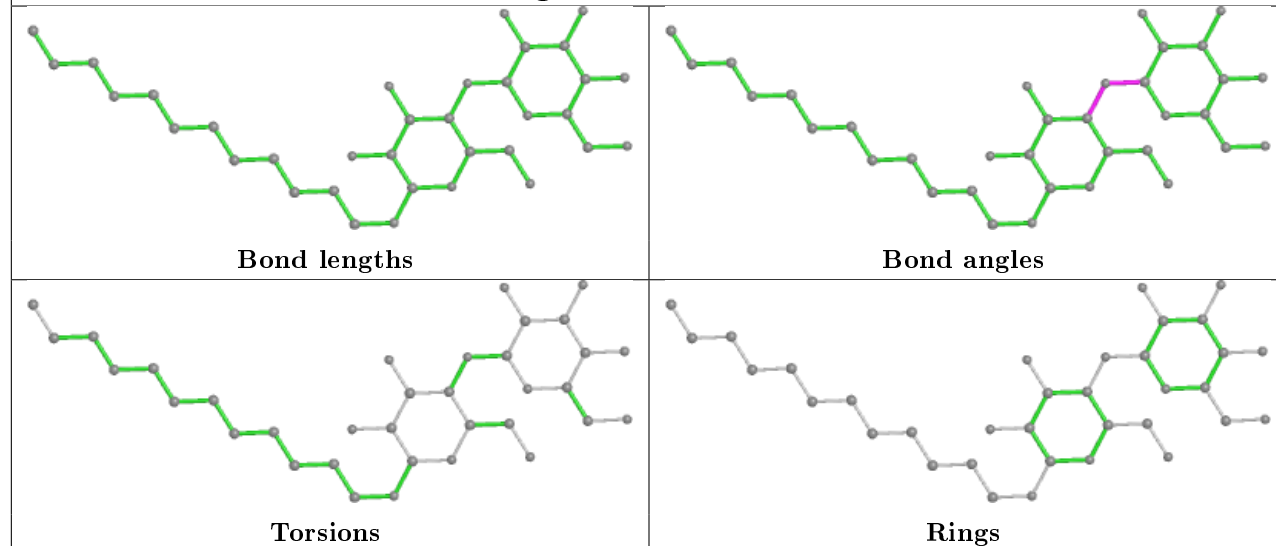




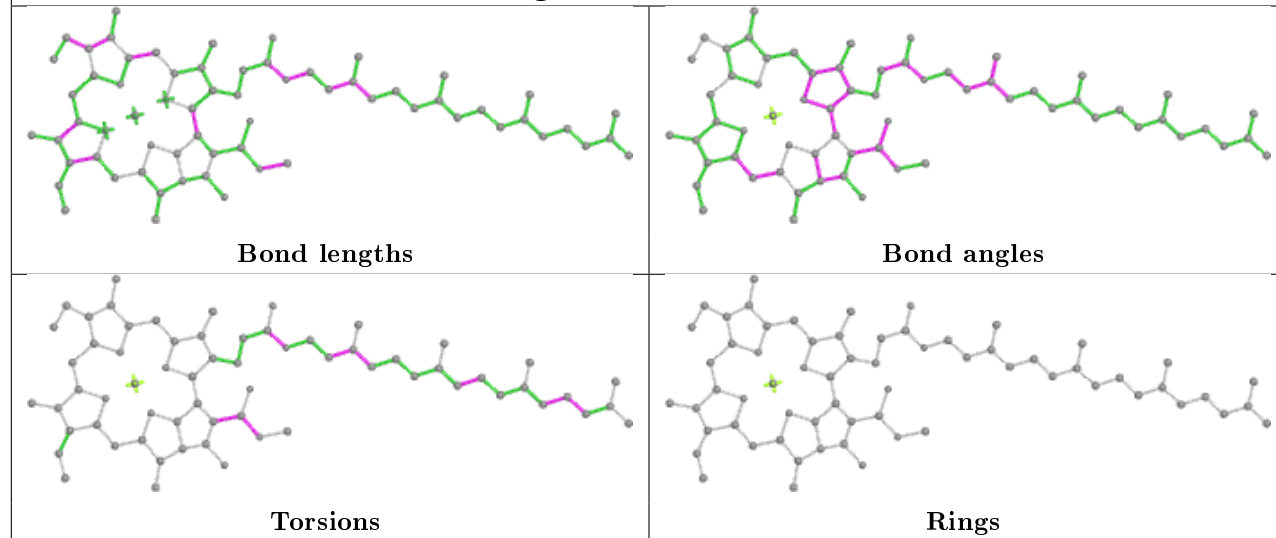
Ligand CLA B 614



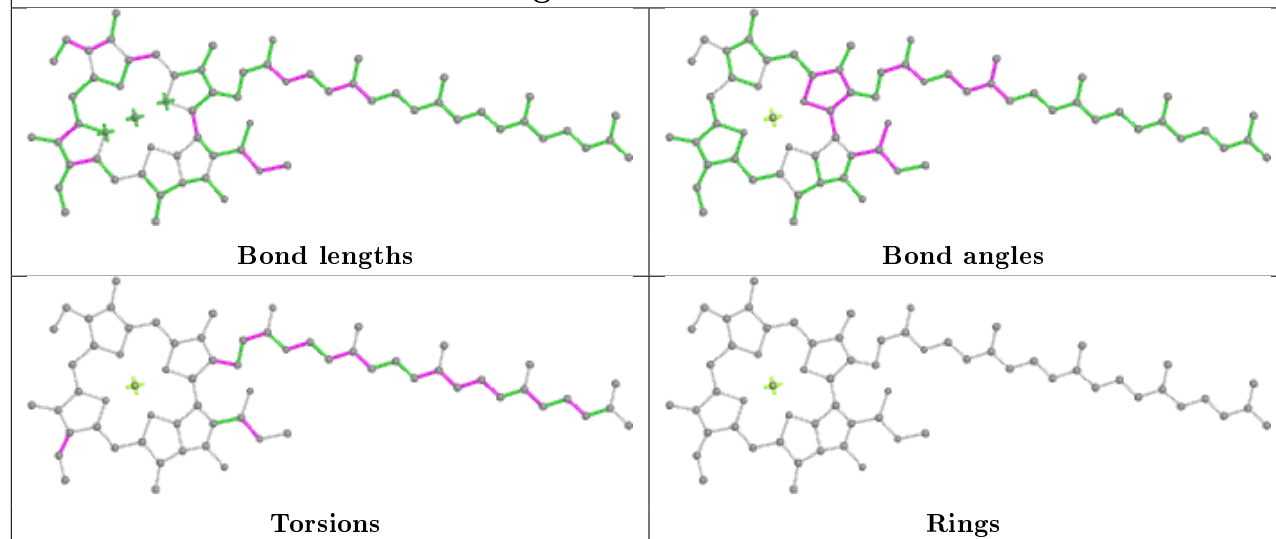
Ligand LMT e 101



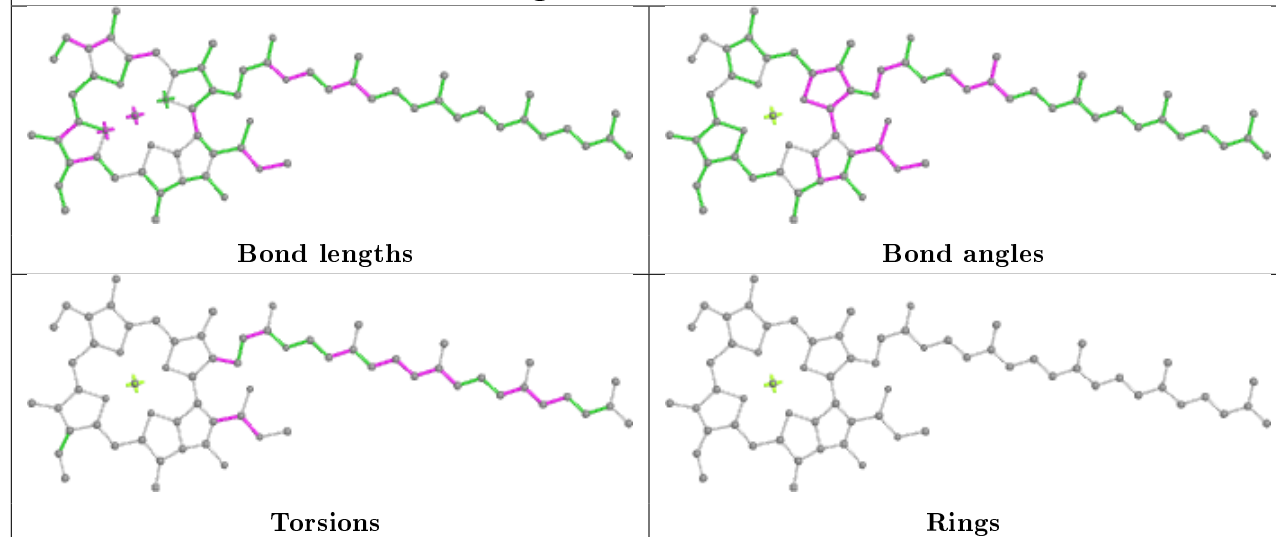
Ligand CLA B 604

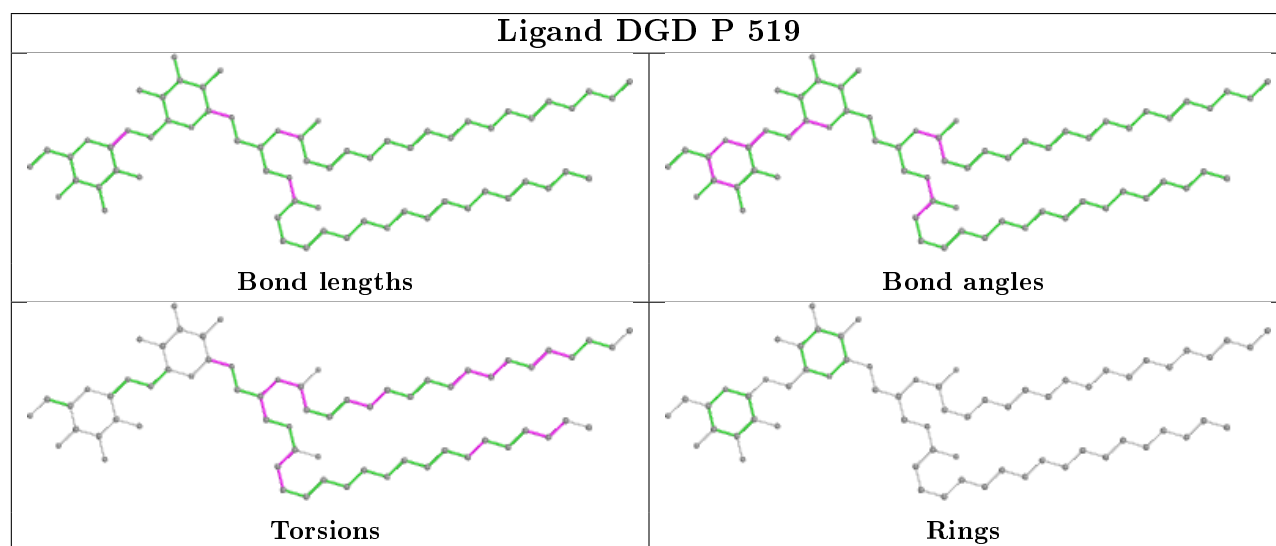
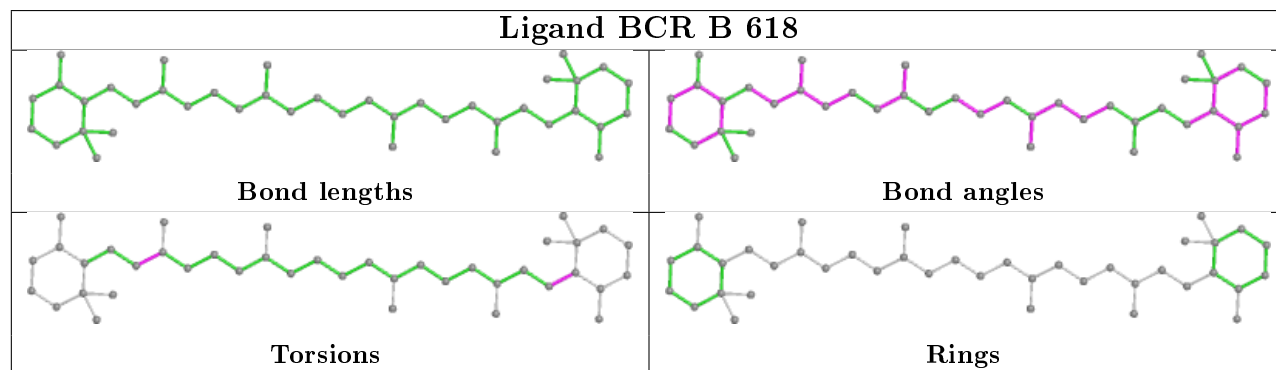
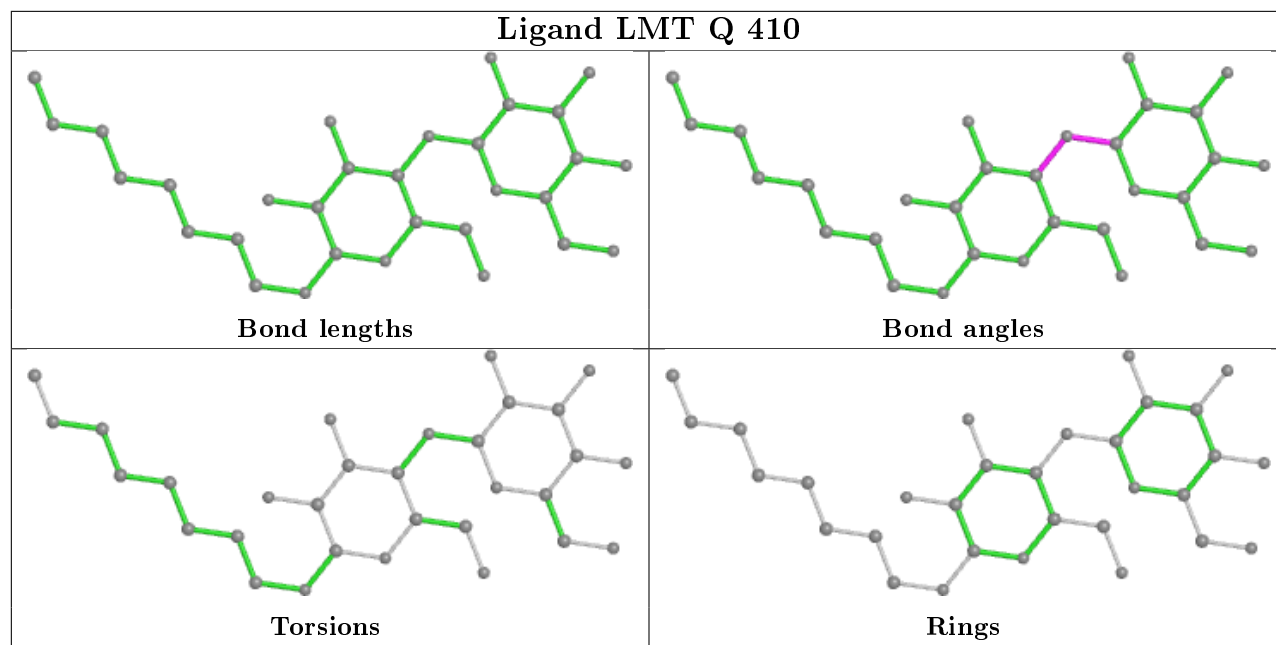


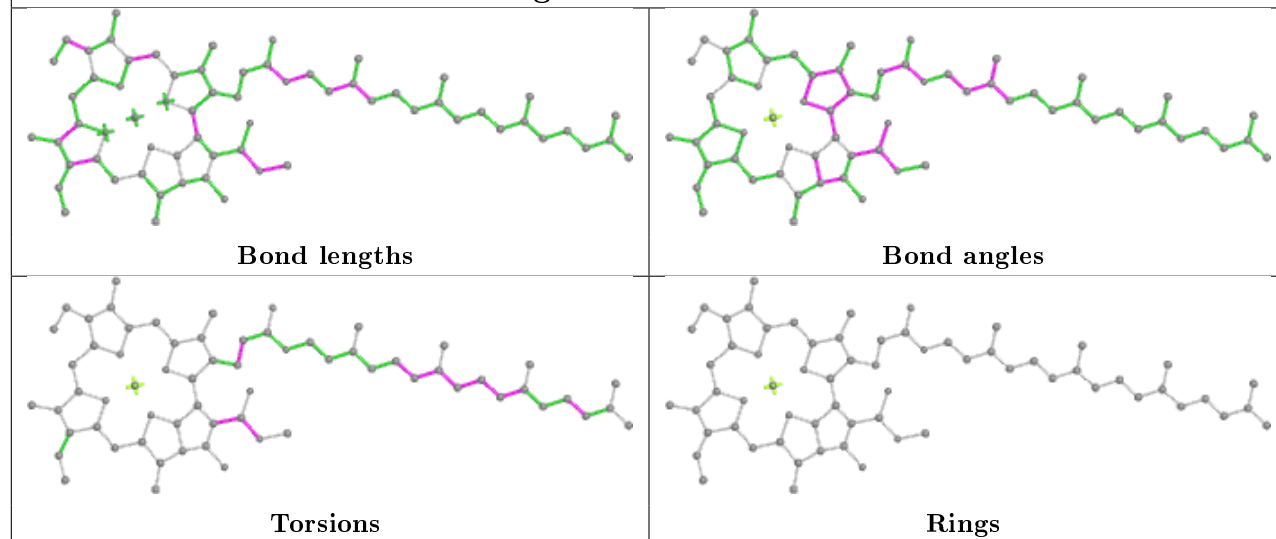
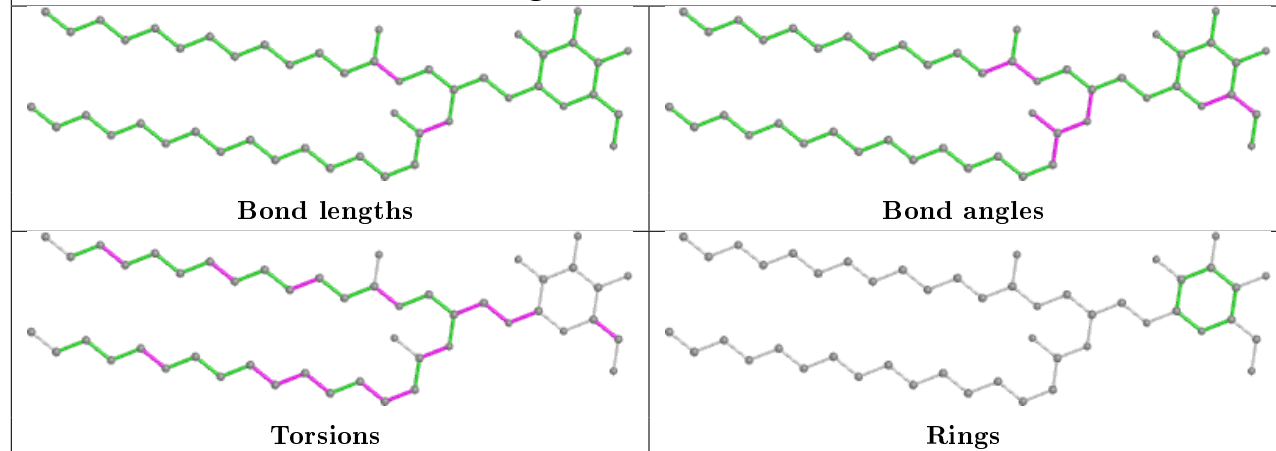
Ligand CLA P 505

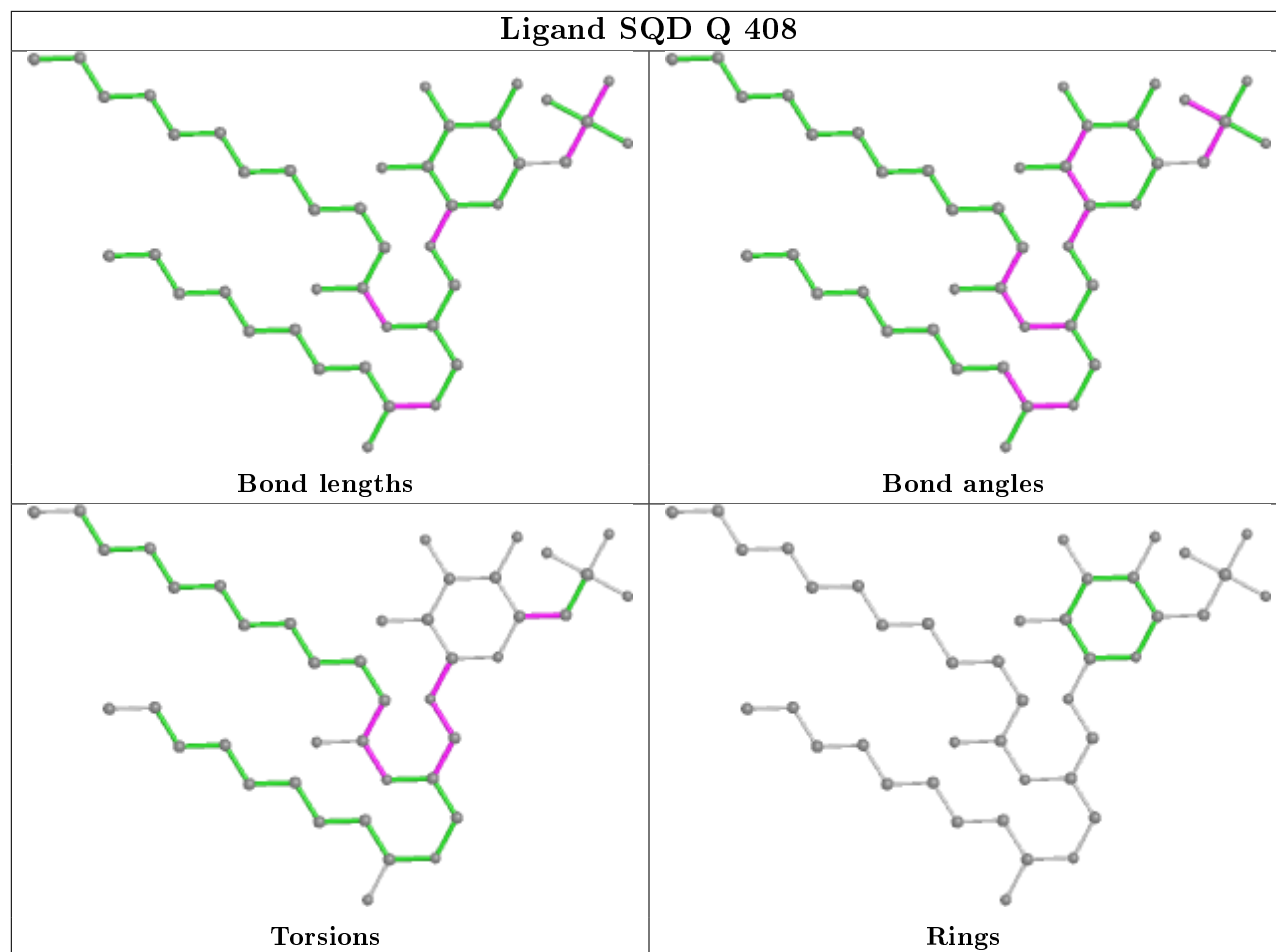


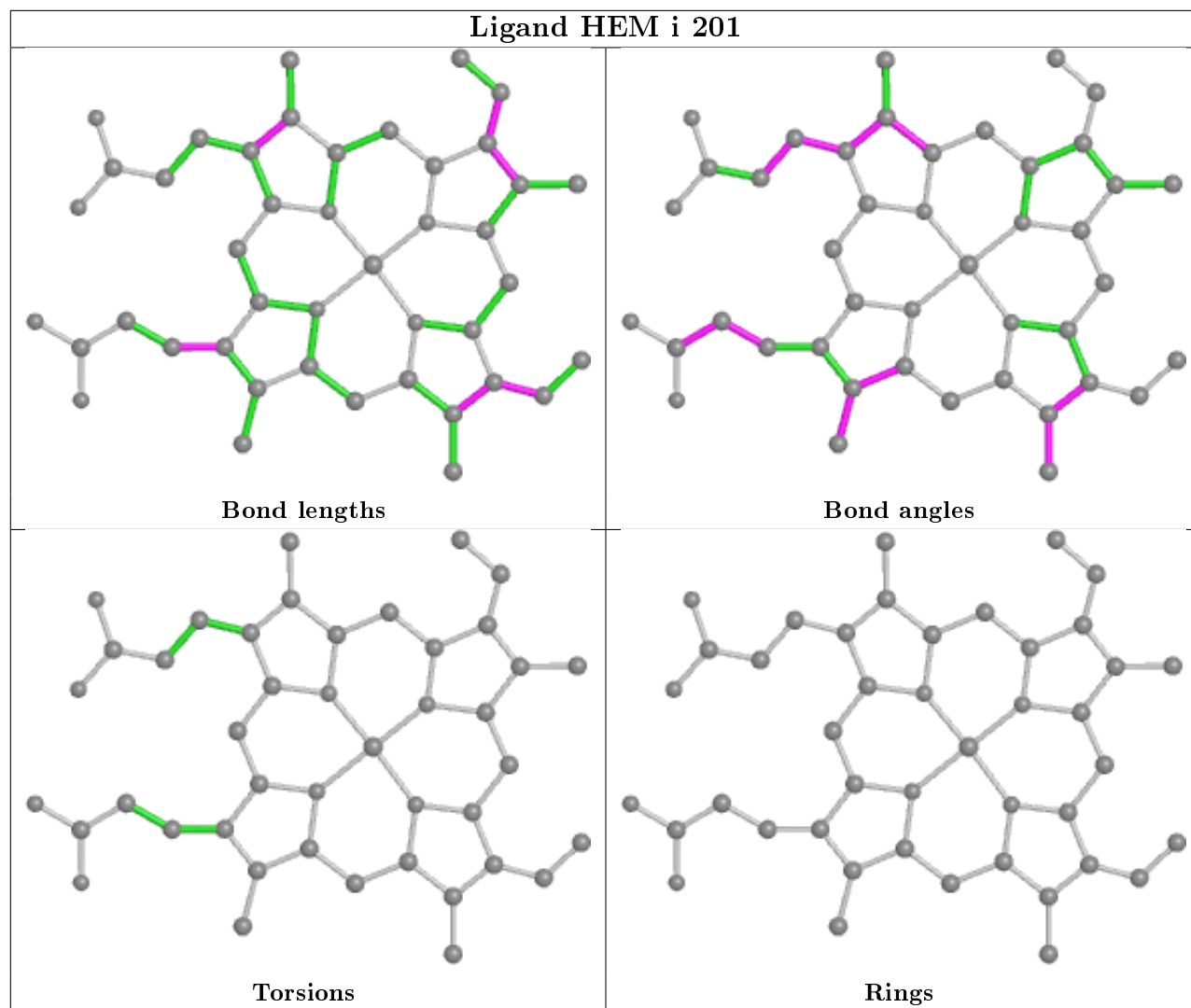
Ligand CLA N 606

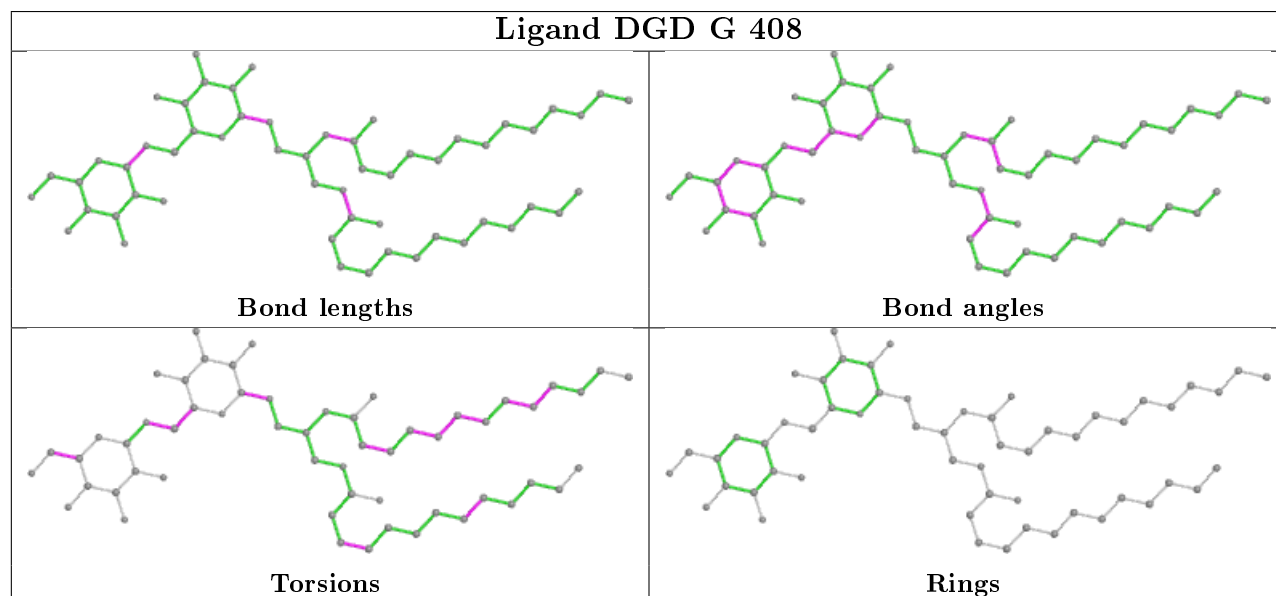
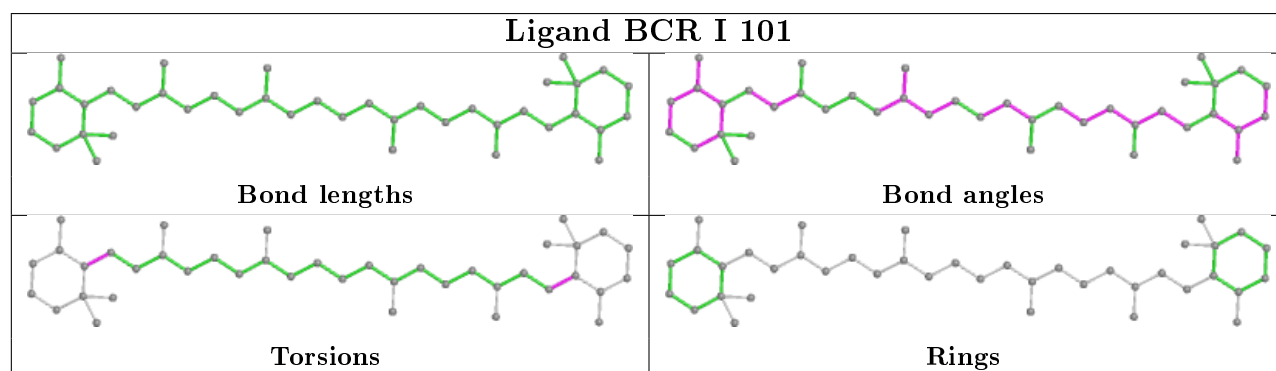
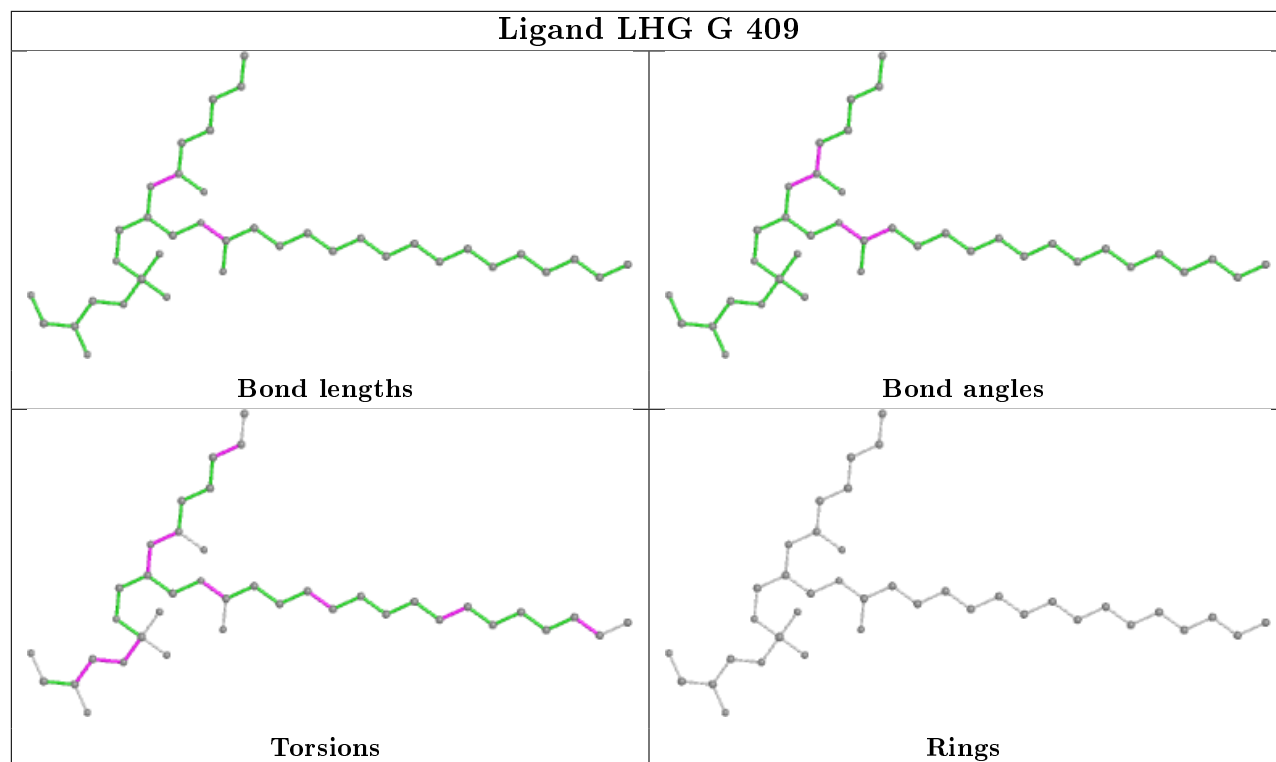




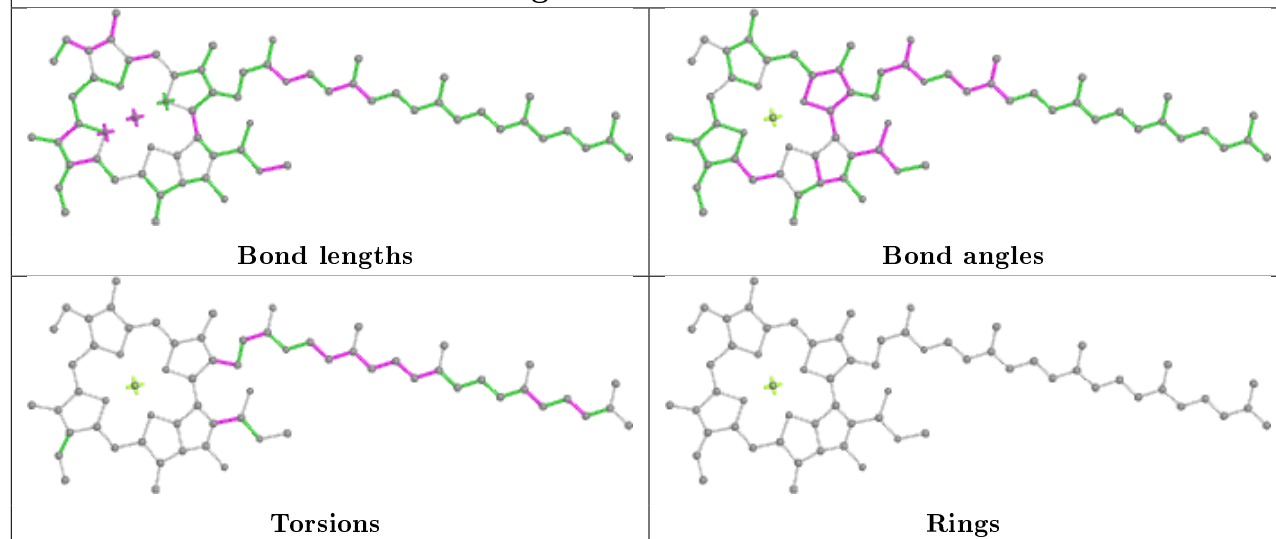
Ligand CLA P 503**Ligand LMG D 407**



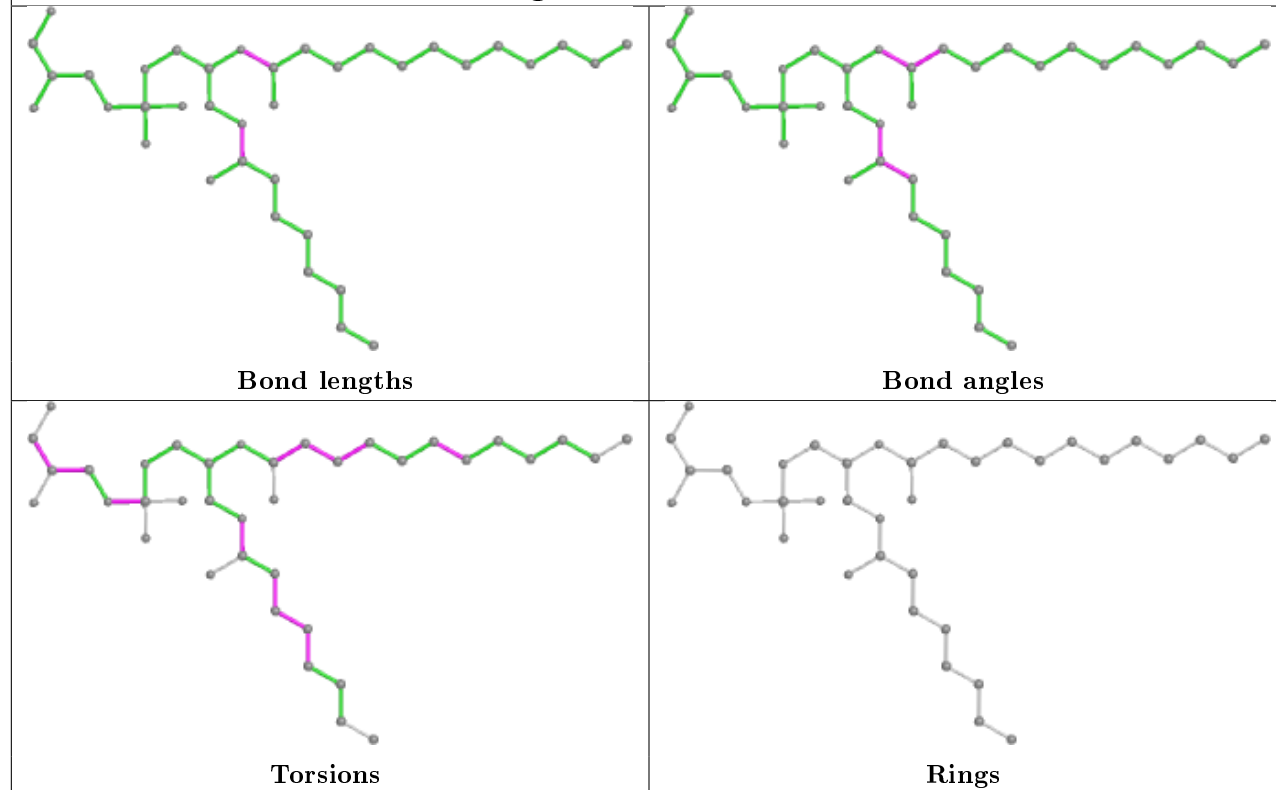




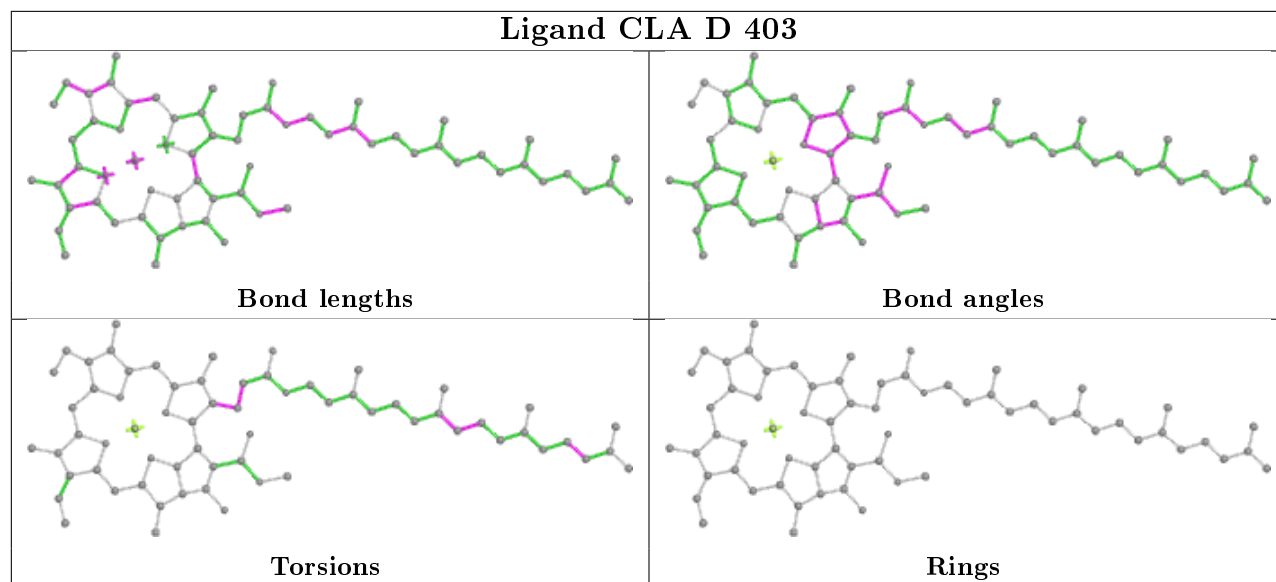
Ligand CLA G 403



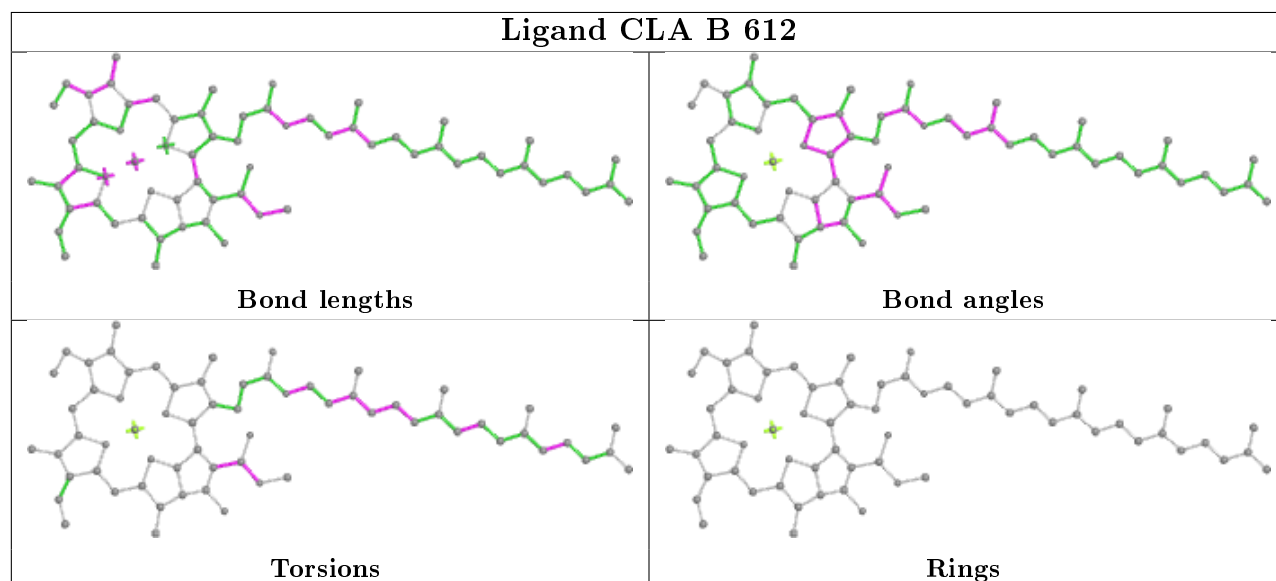
Ligand LHG G 412



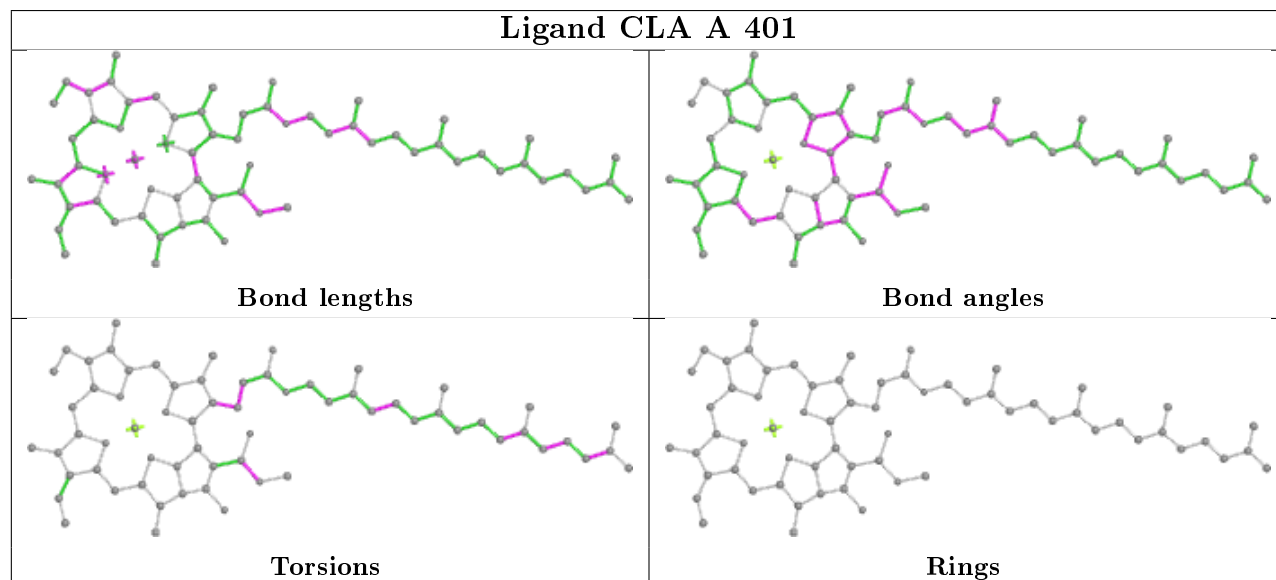
Ligand CLA D 403

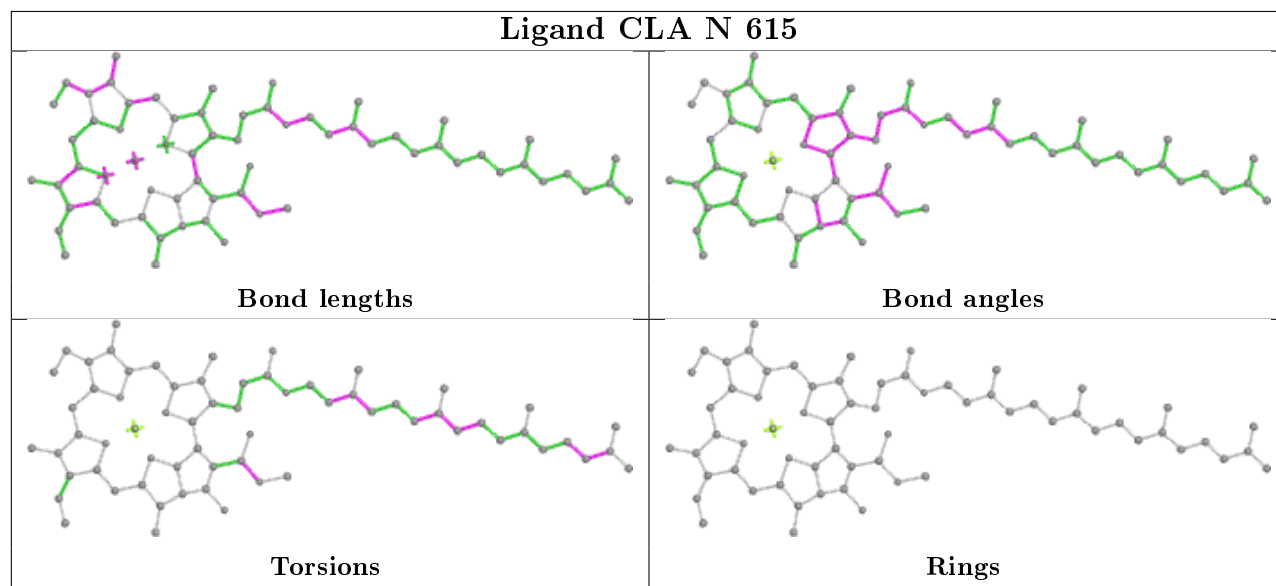
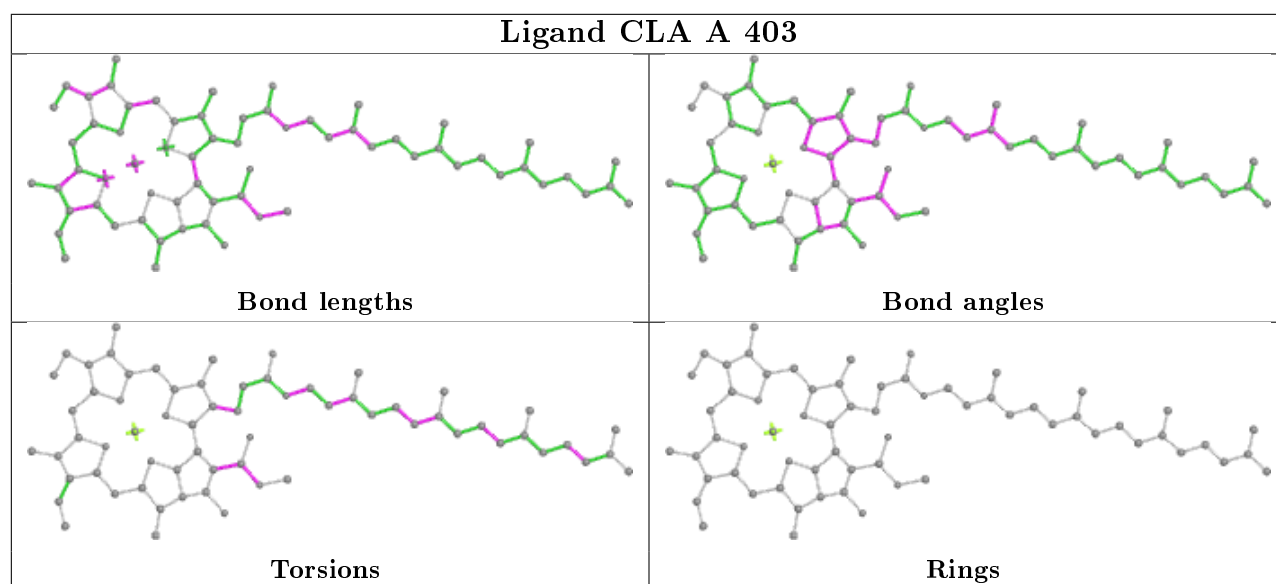
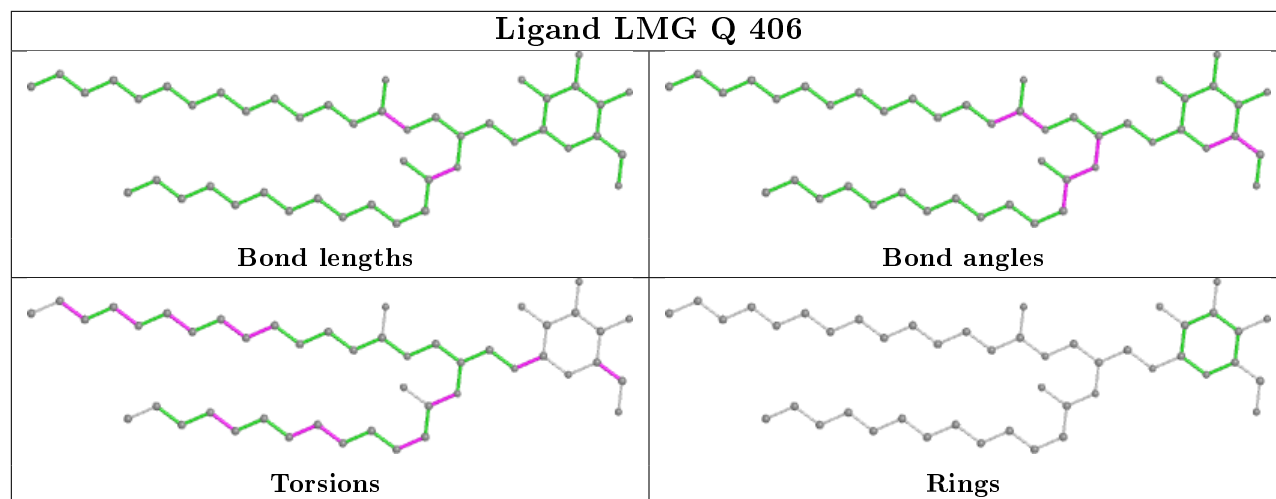


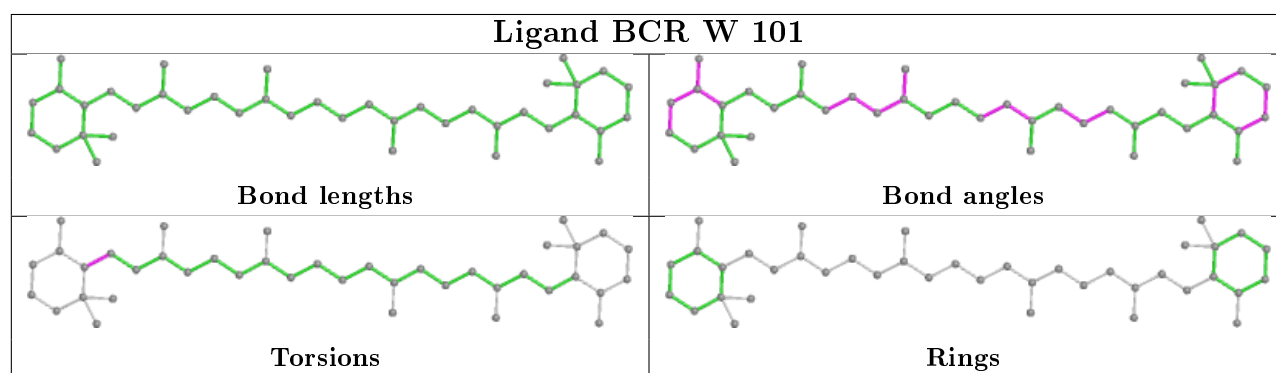
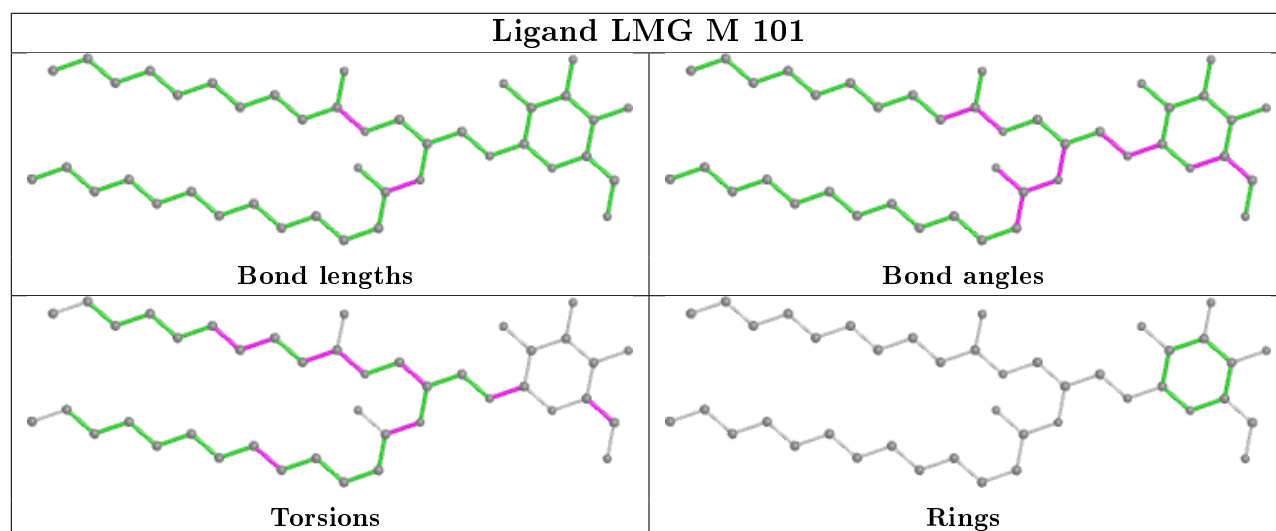
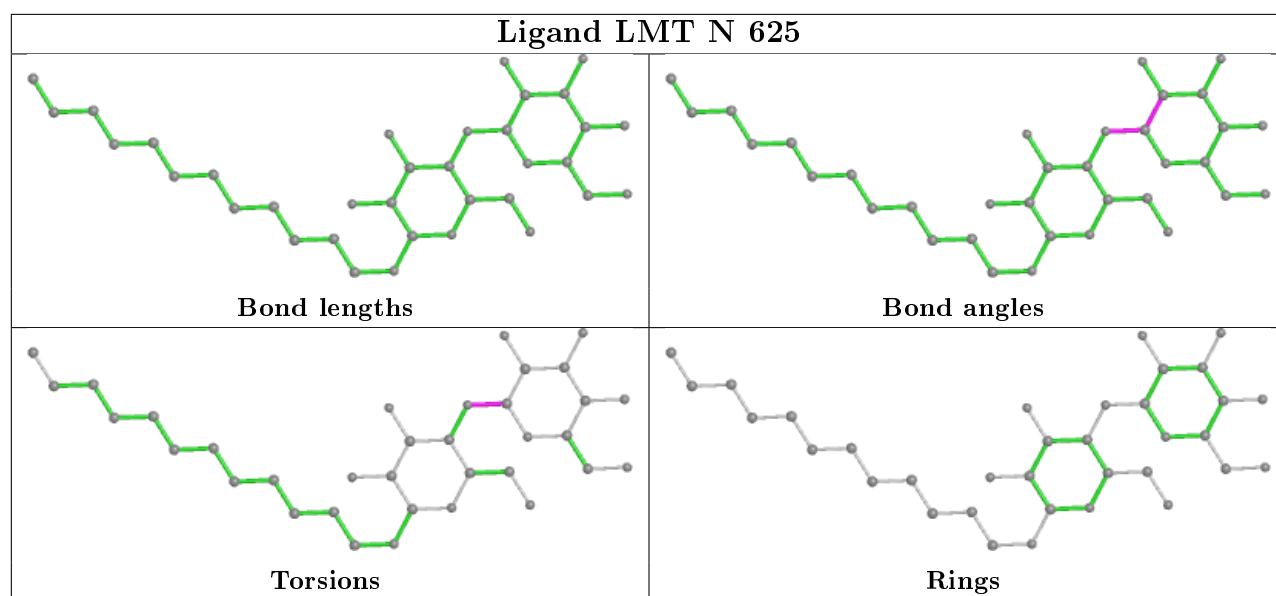
Ligand CLA B 612

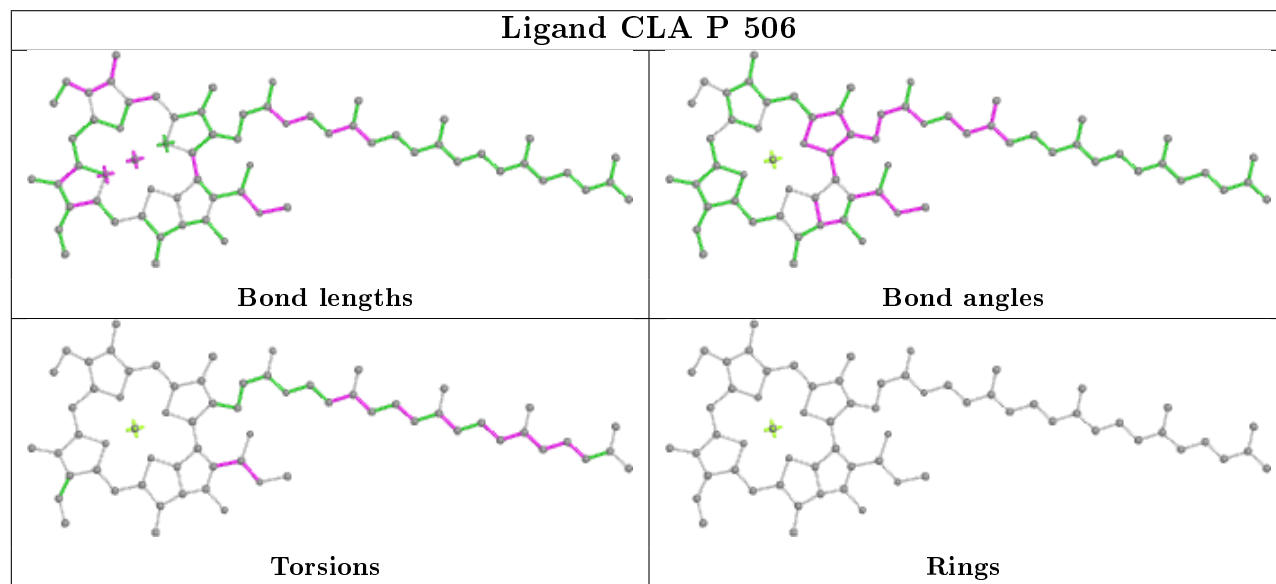
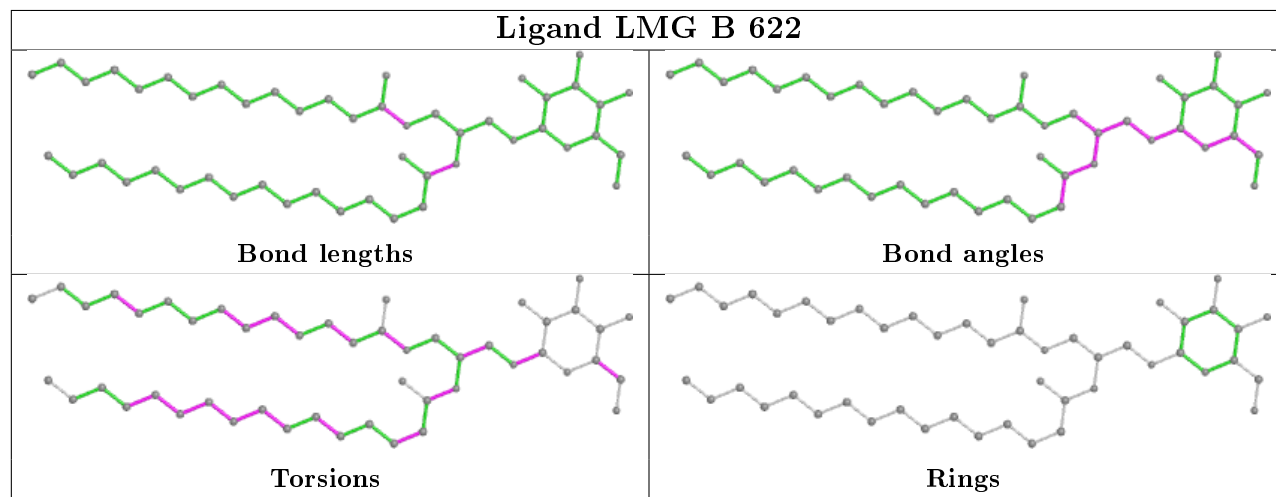
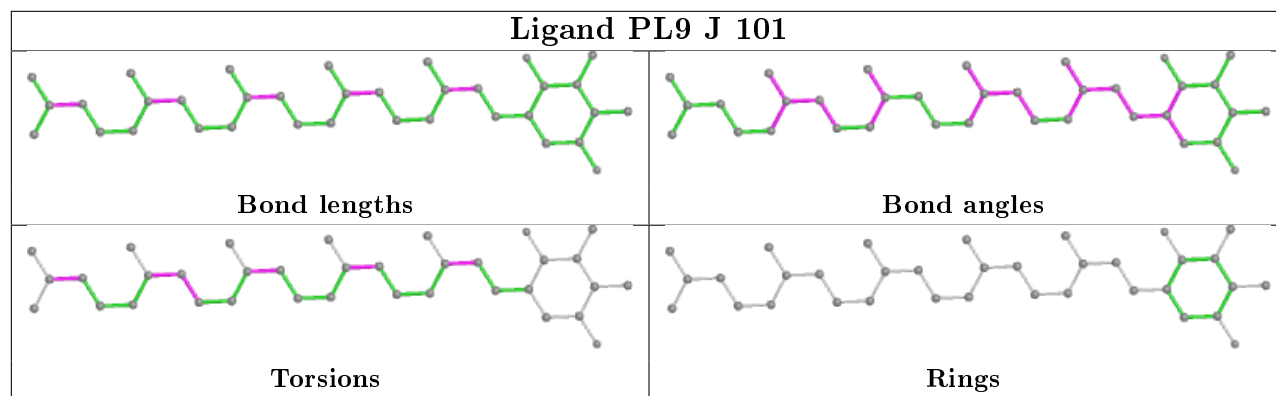


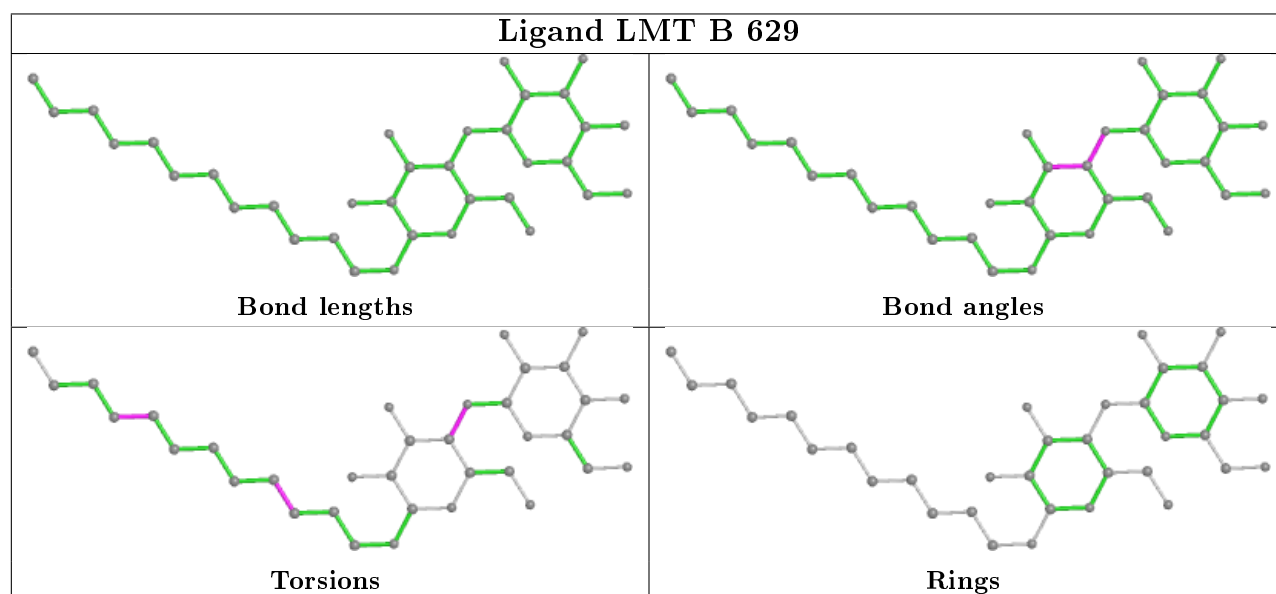
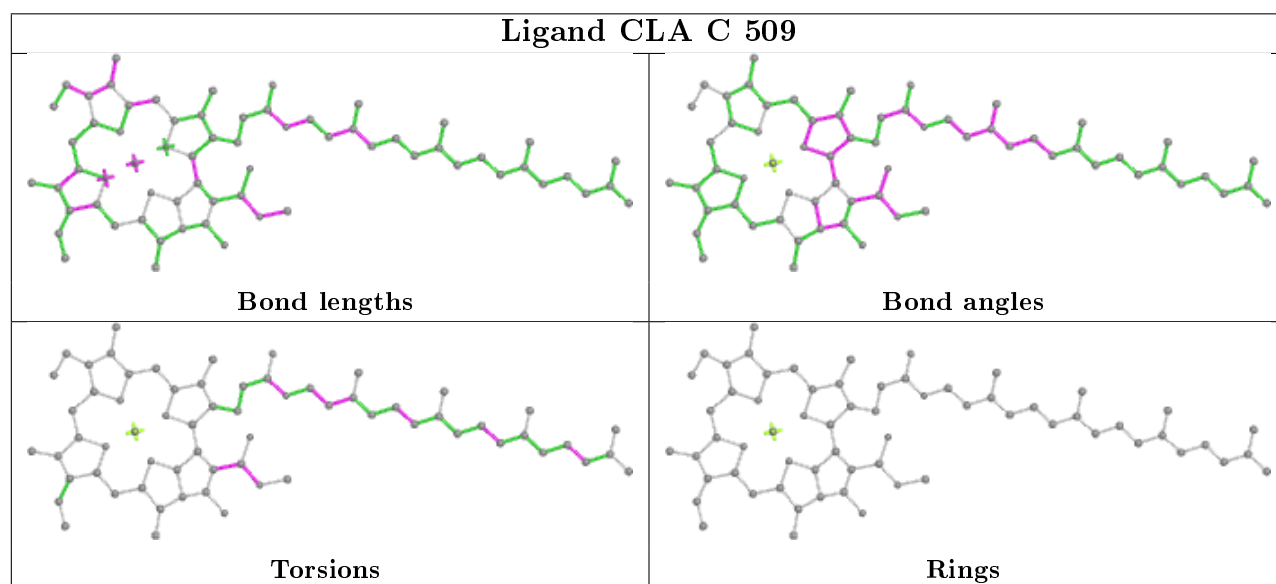
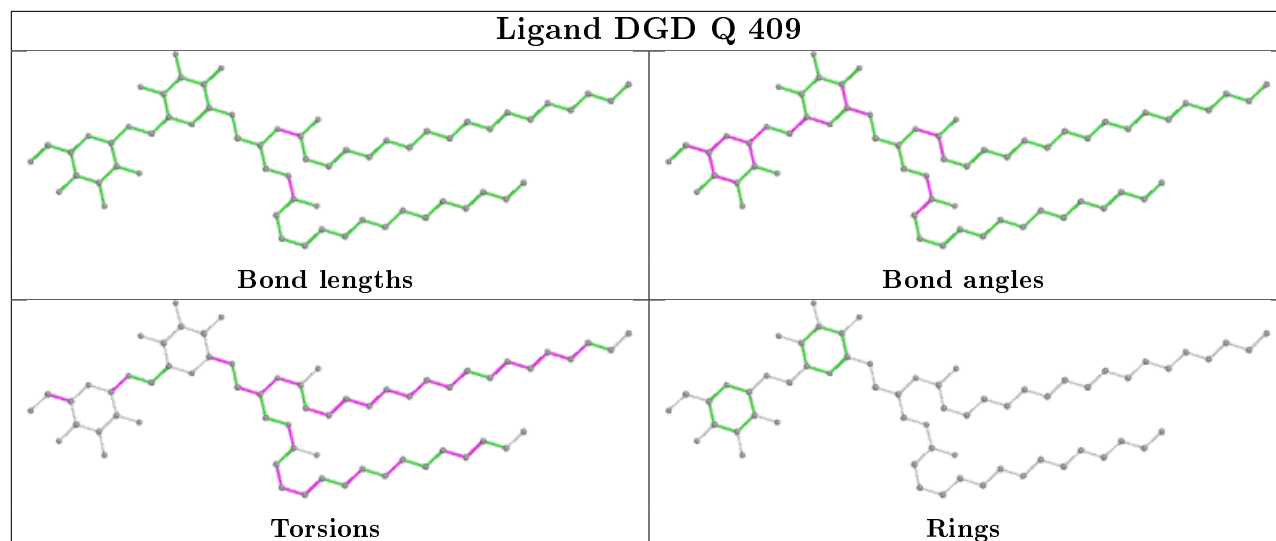
Ligand CLA A 401

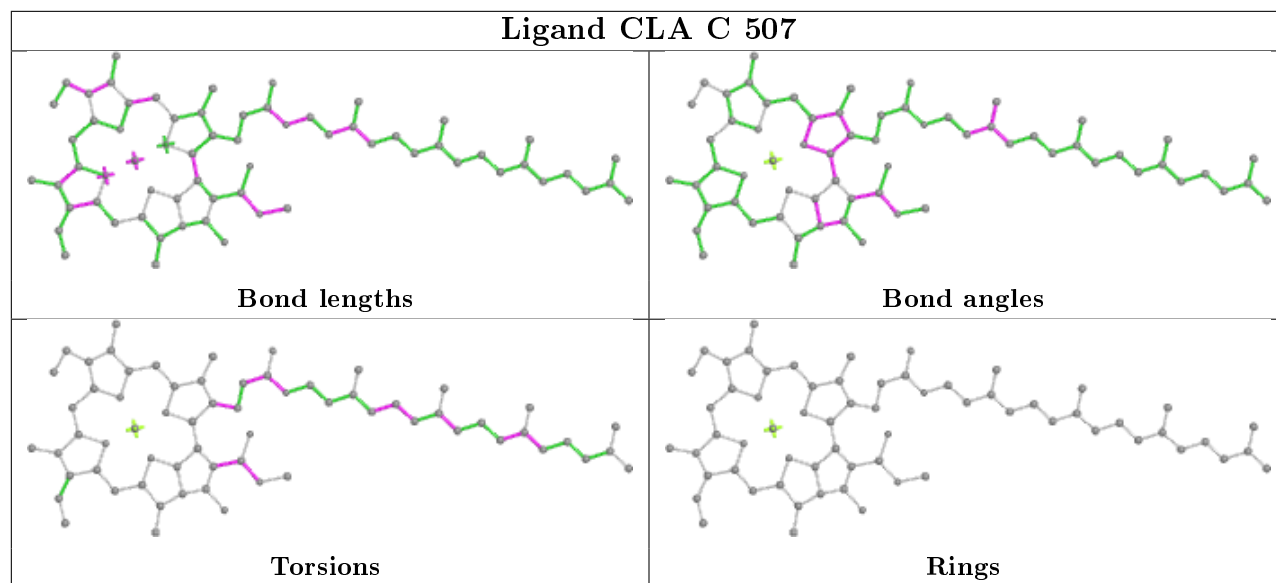
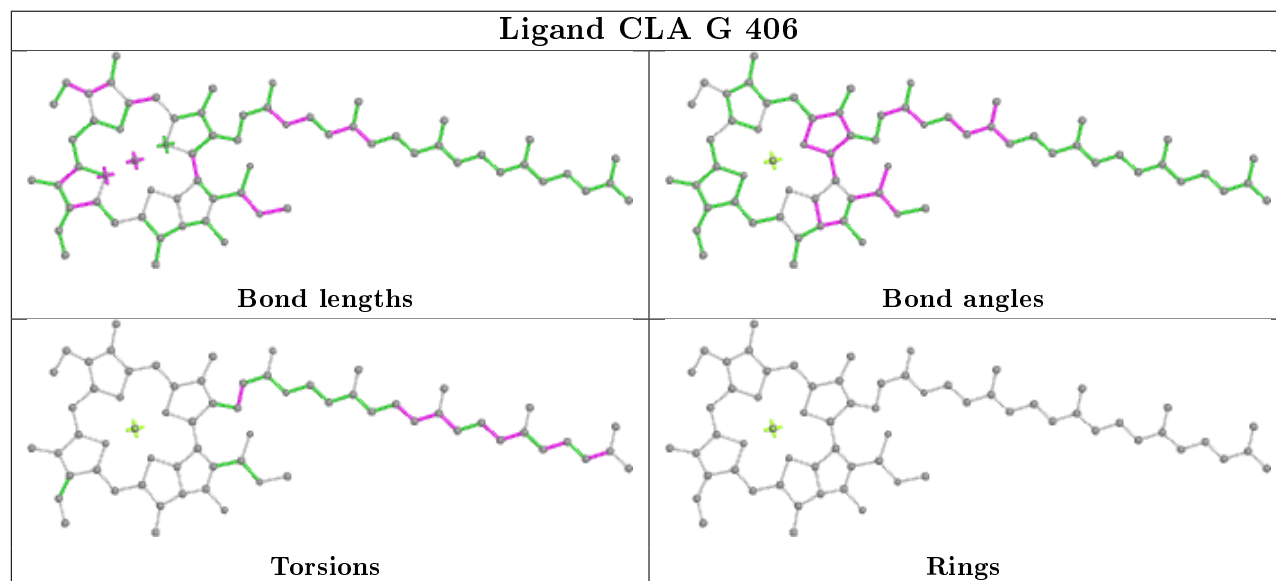
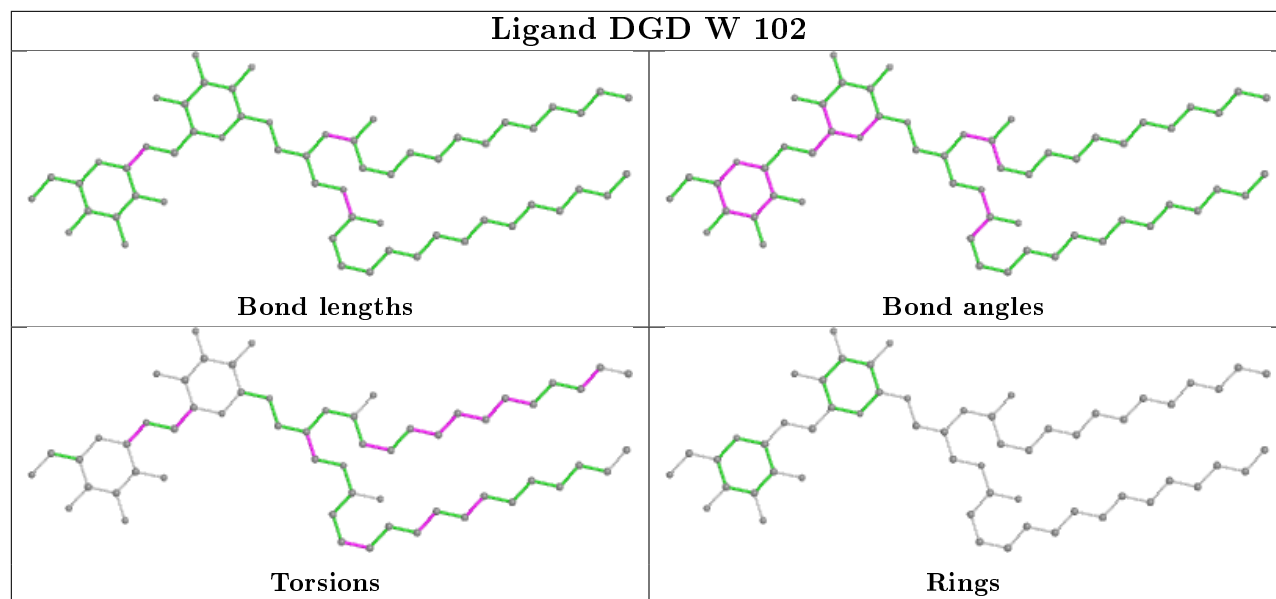




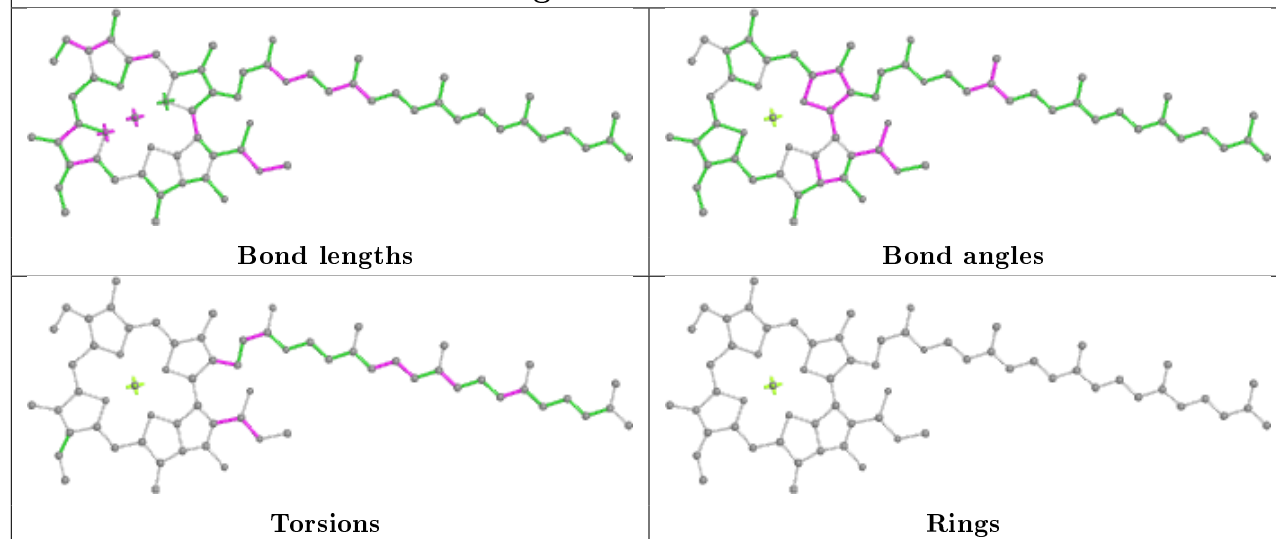




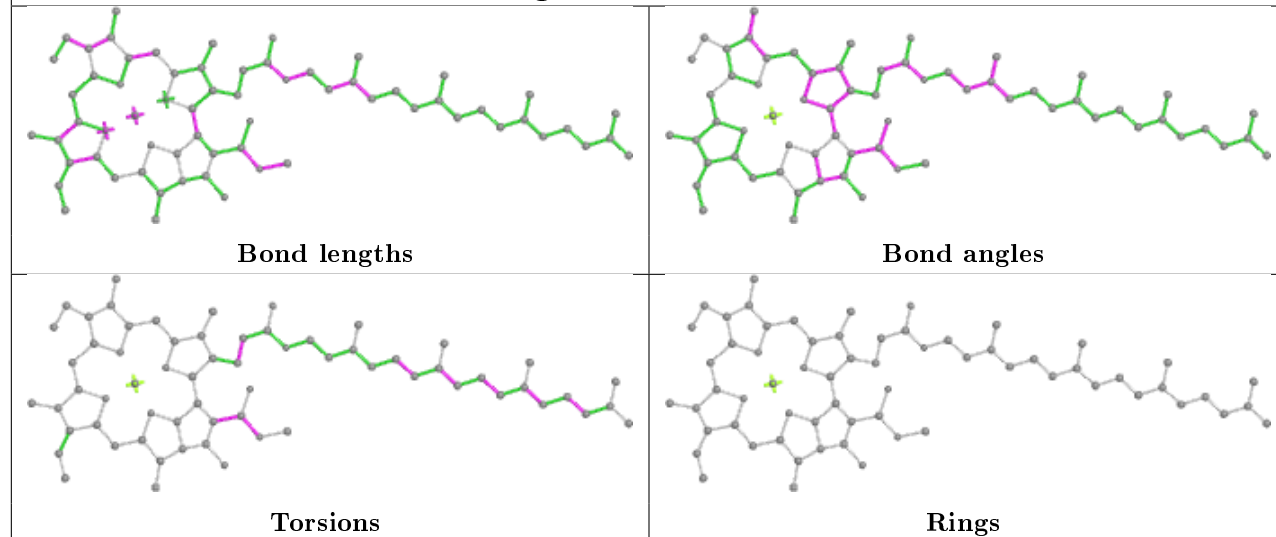




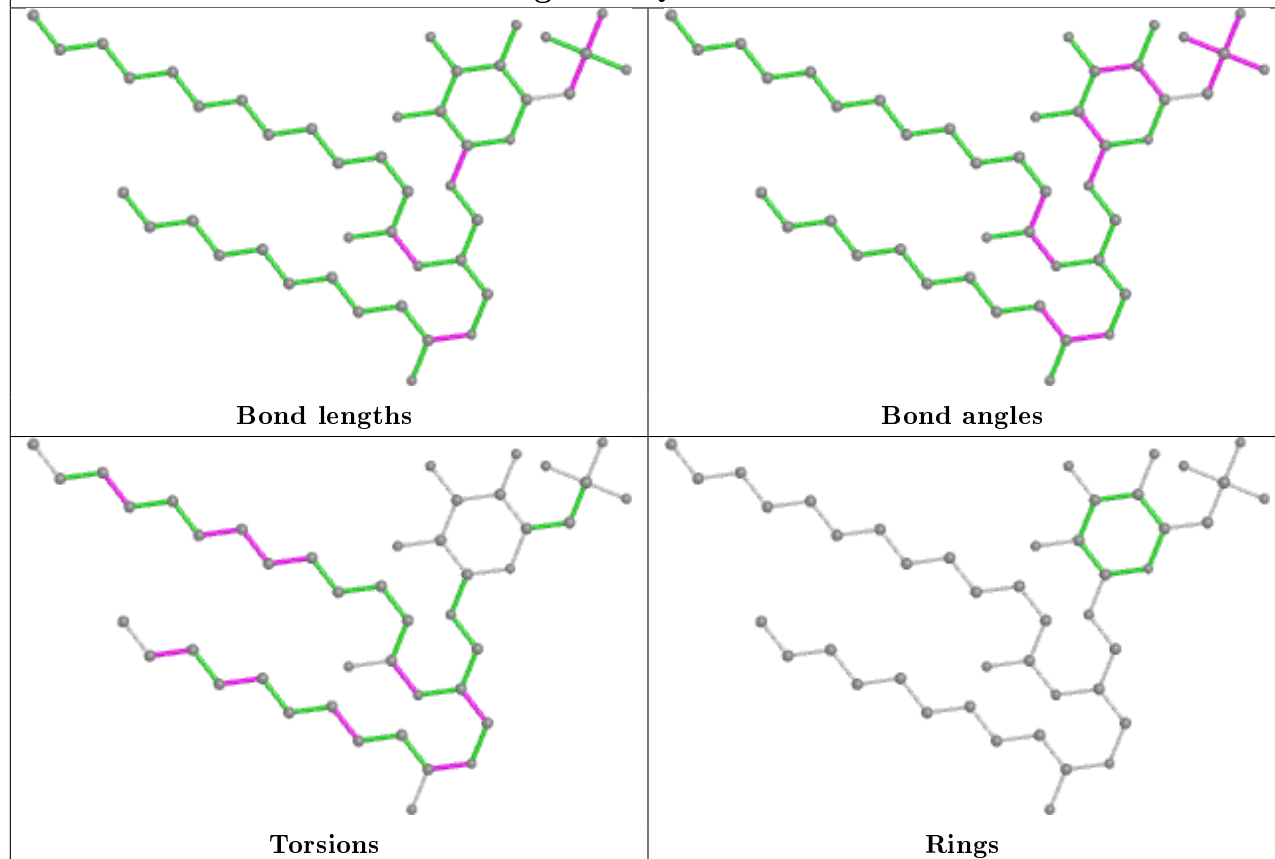
Ligand CLA P 507



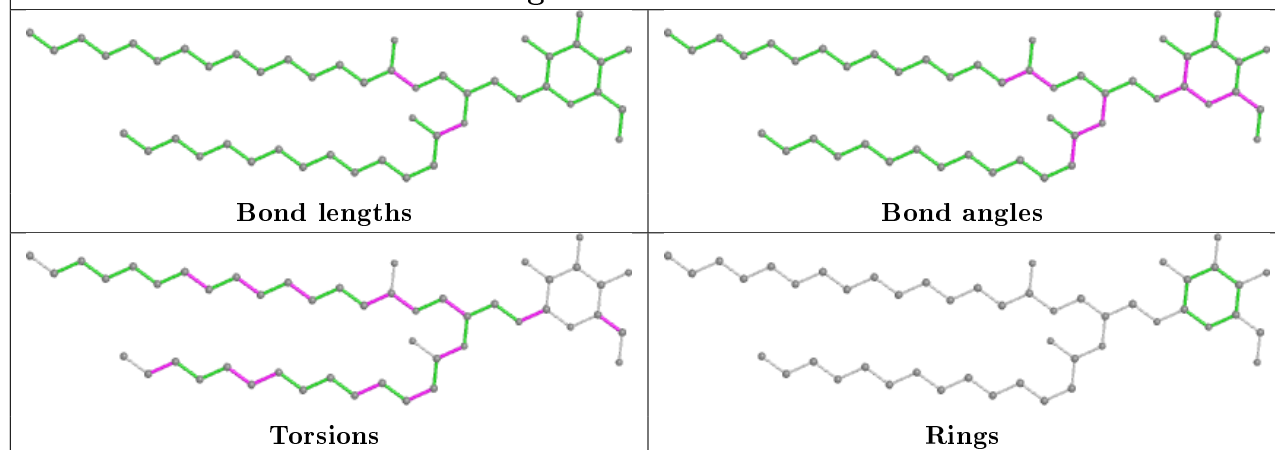
Ligand CLA P 508

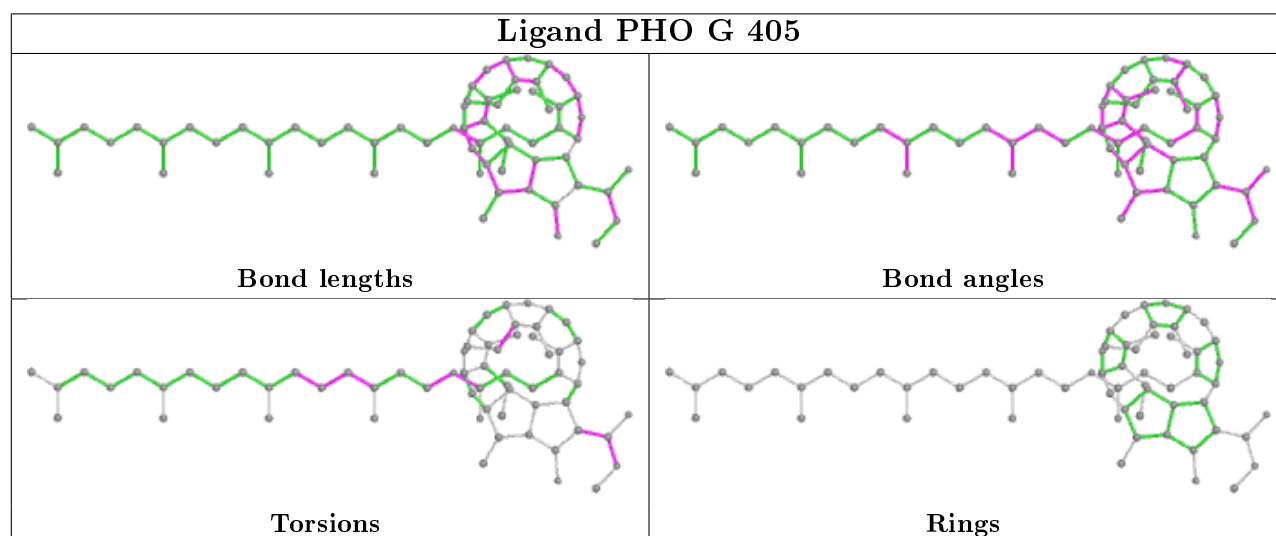
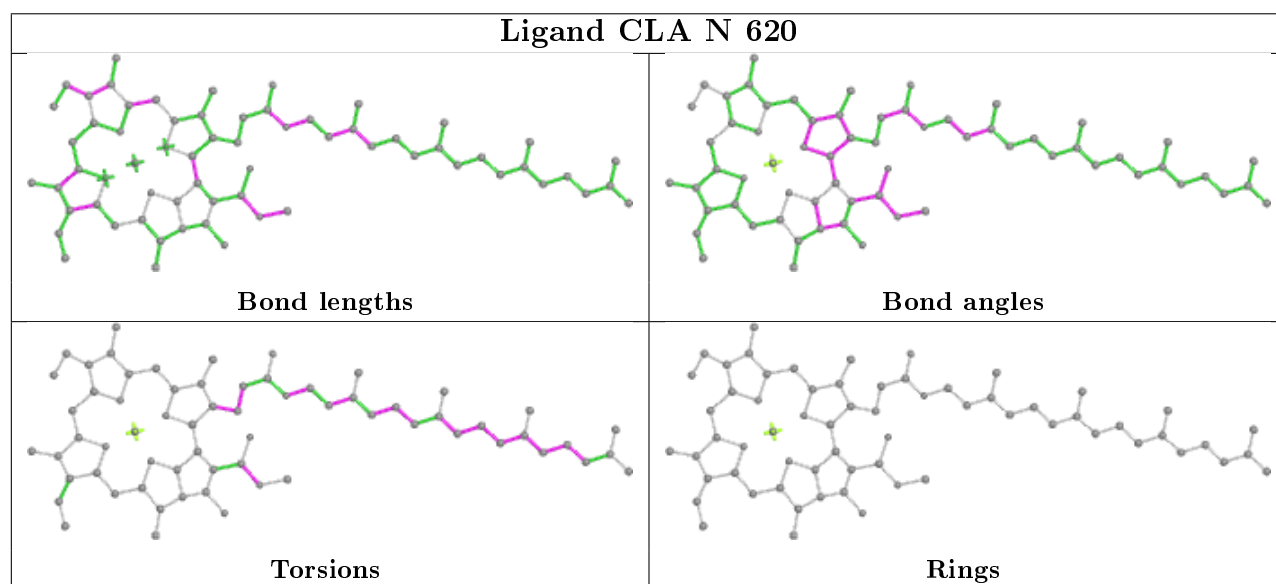
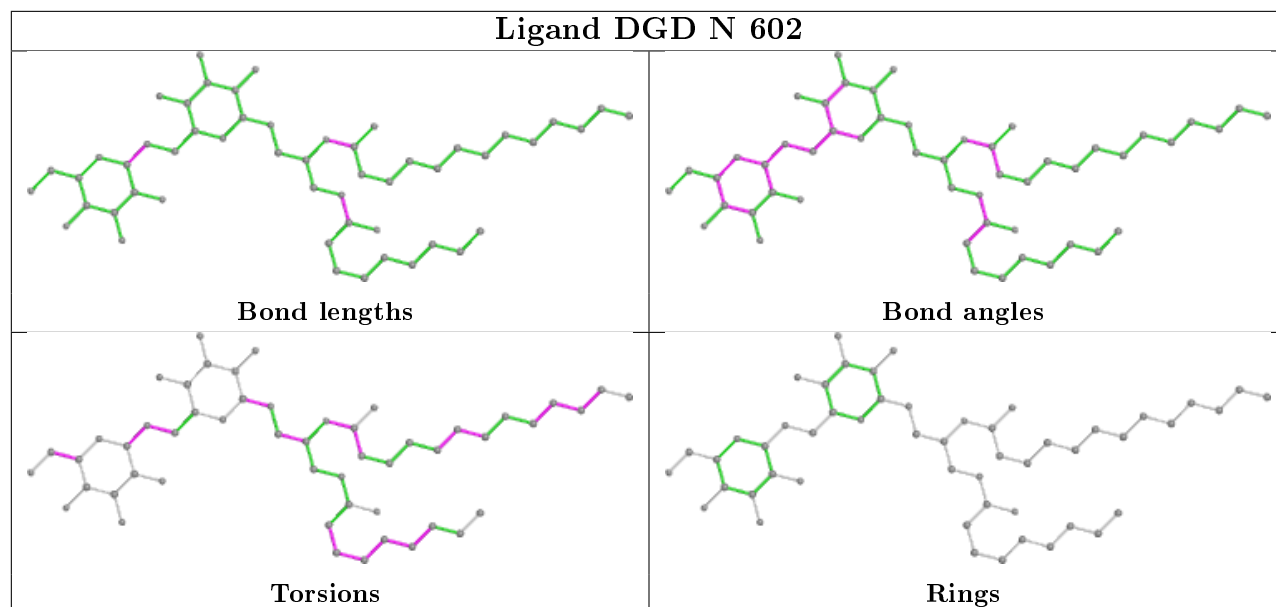


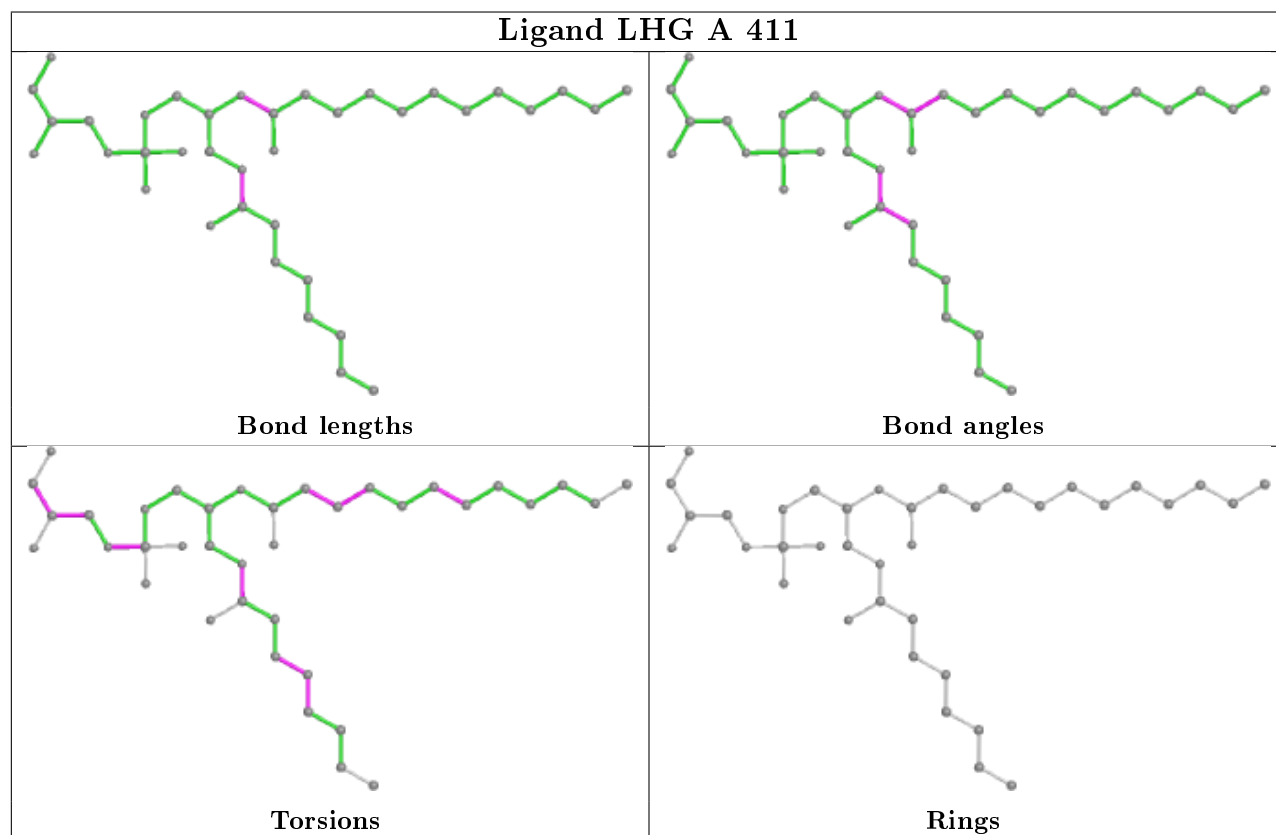
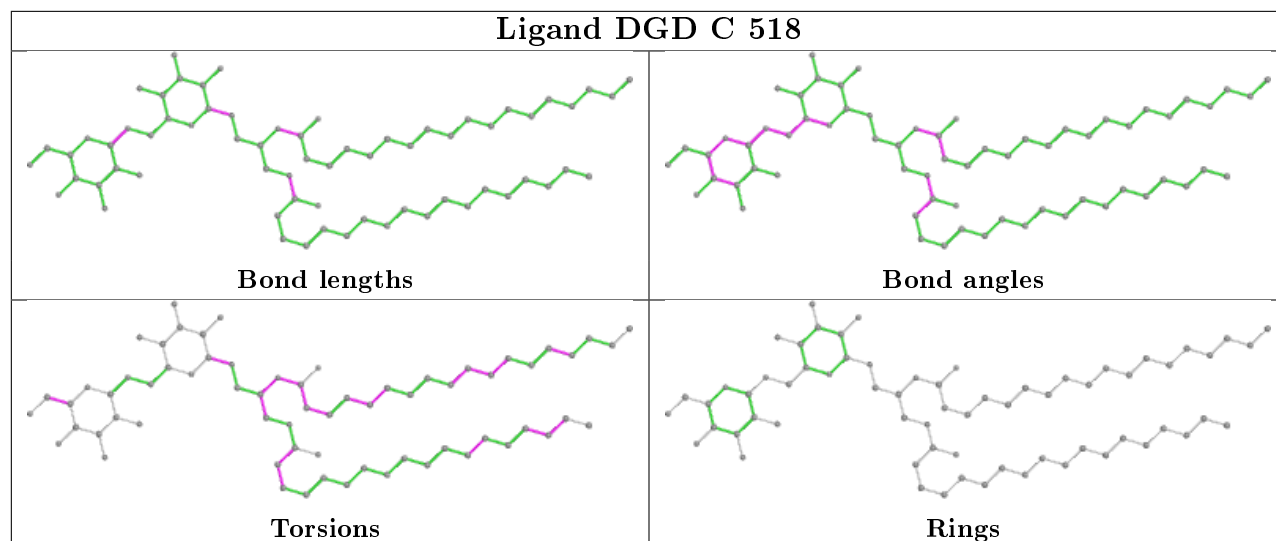
Ligand SQD S 102

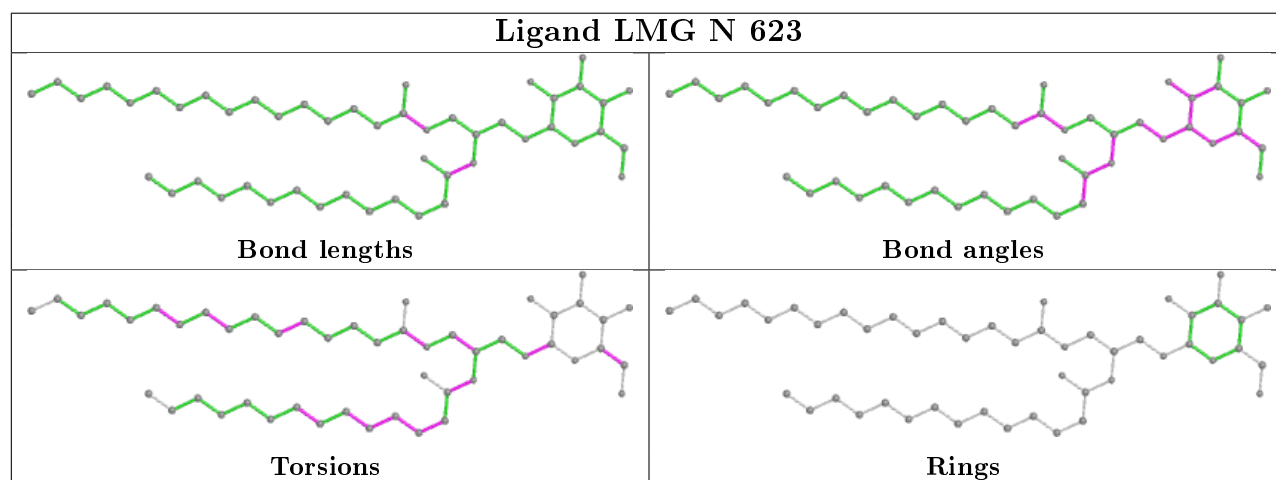
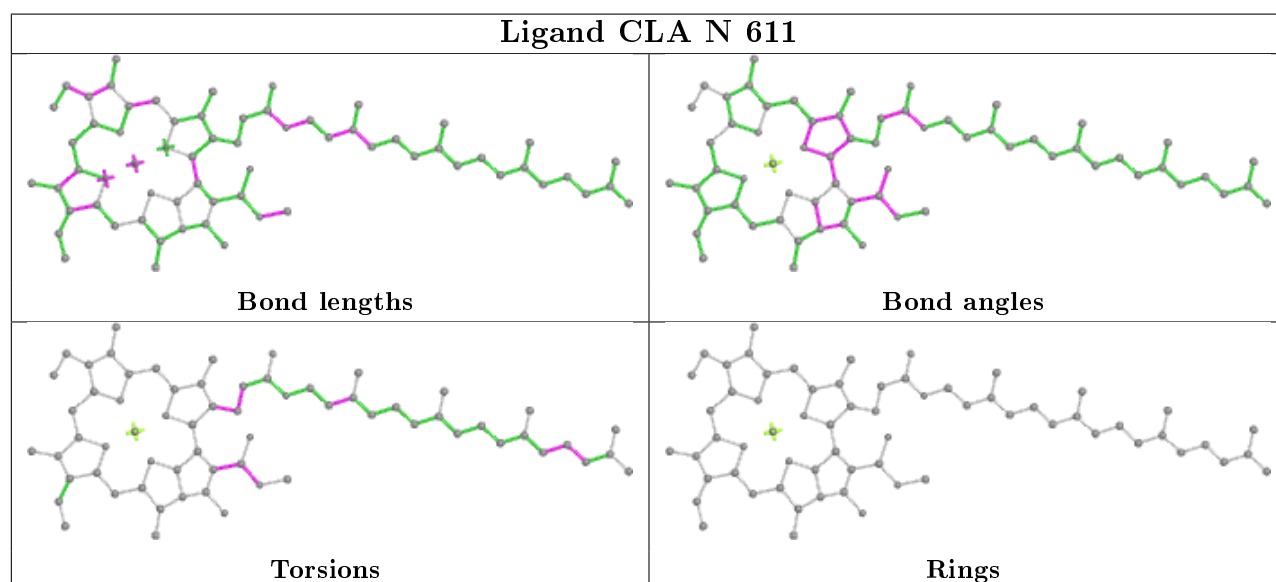
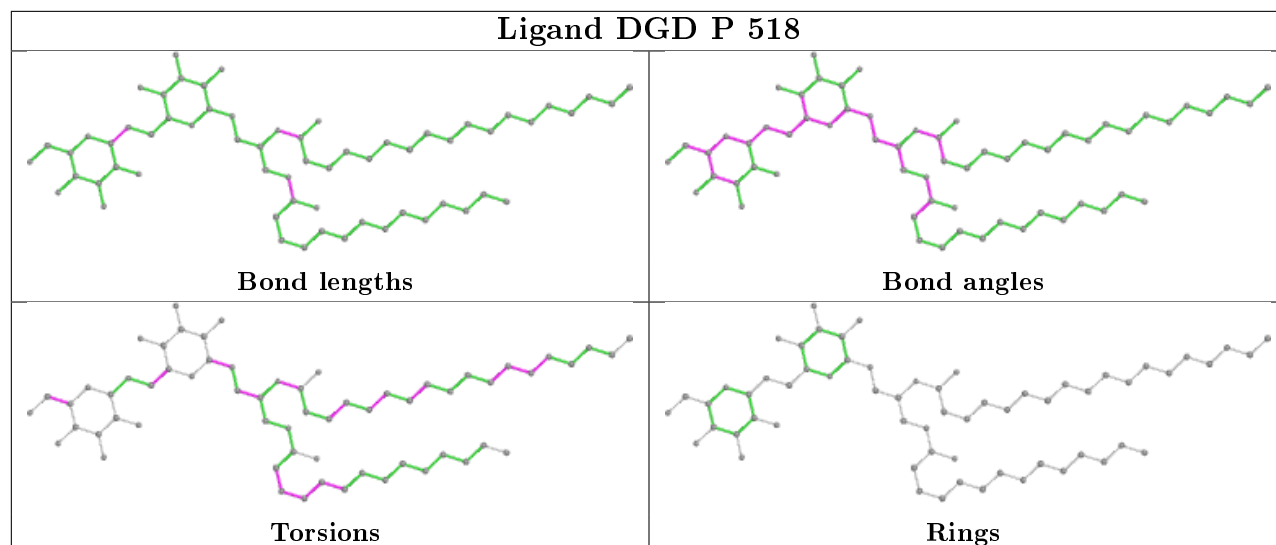


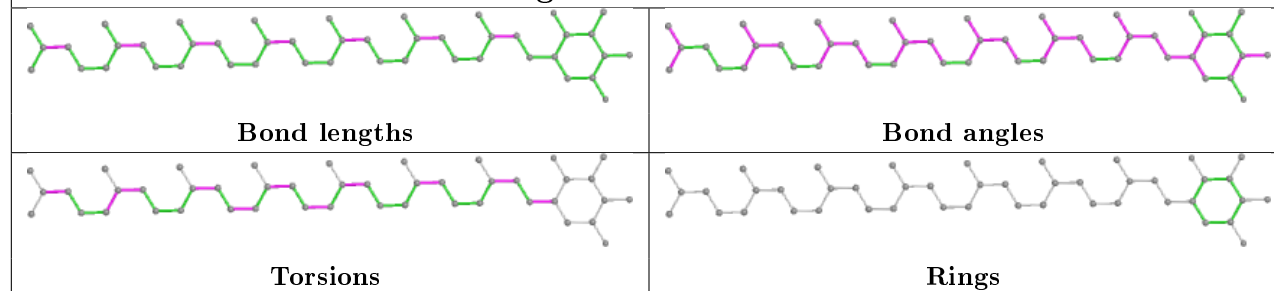
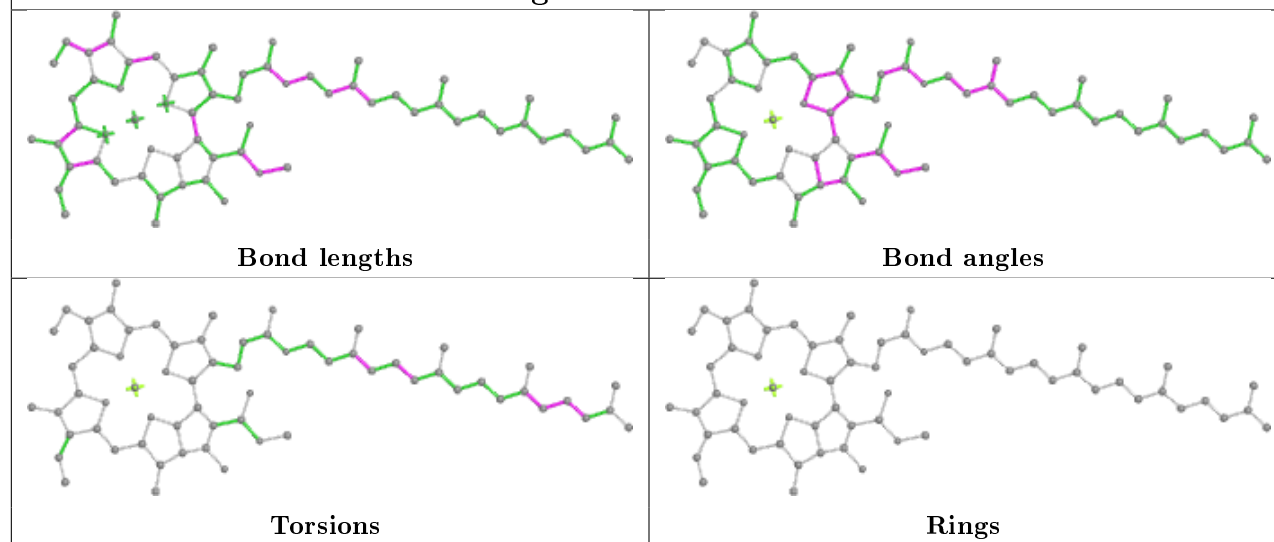
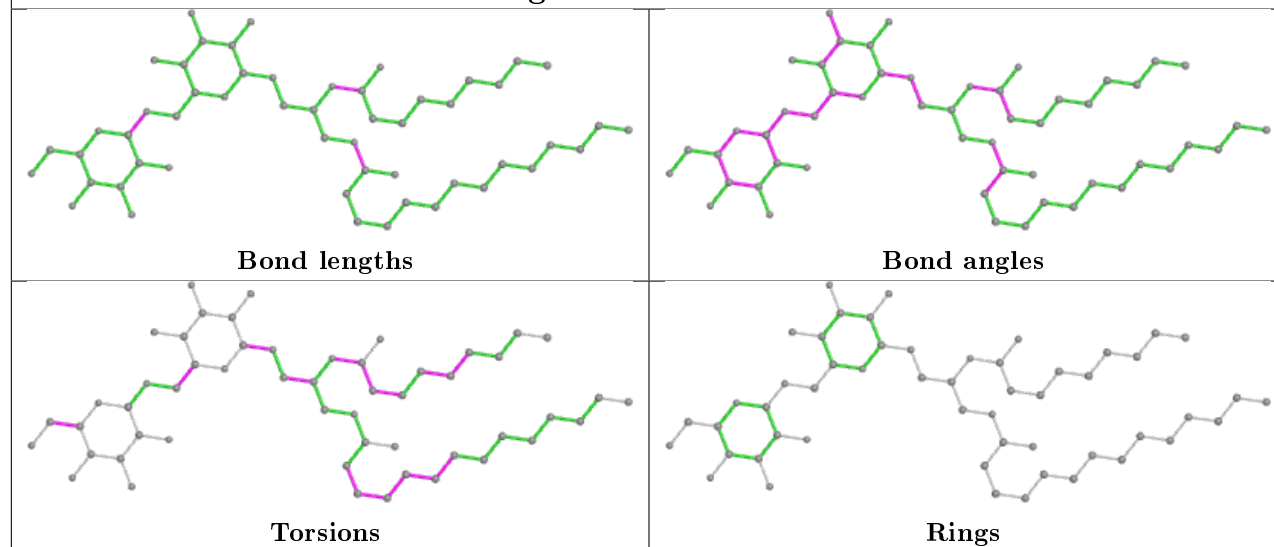
Ligand LMG C 519



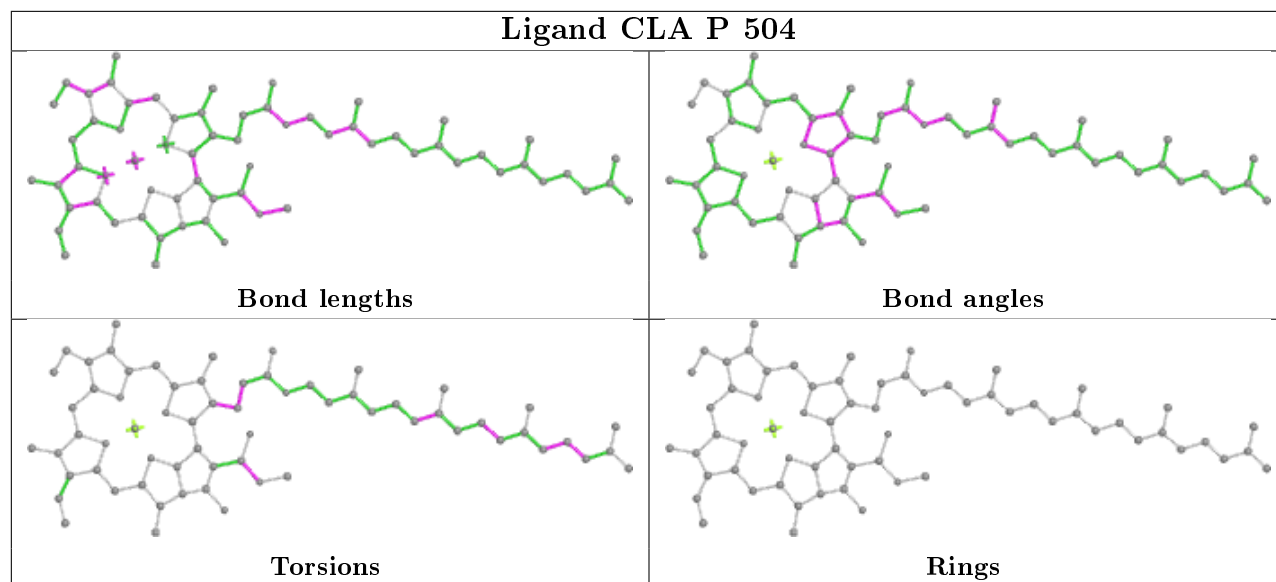




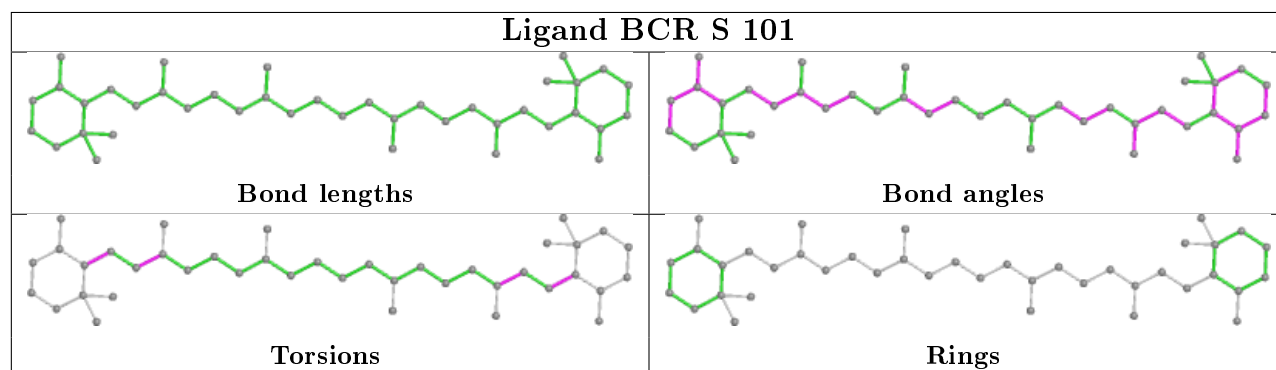


Ligand PL9 G 407**Ligand CLA N 613****Ligand DGD C 516**

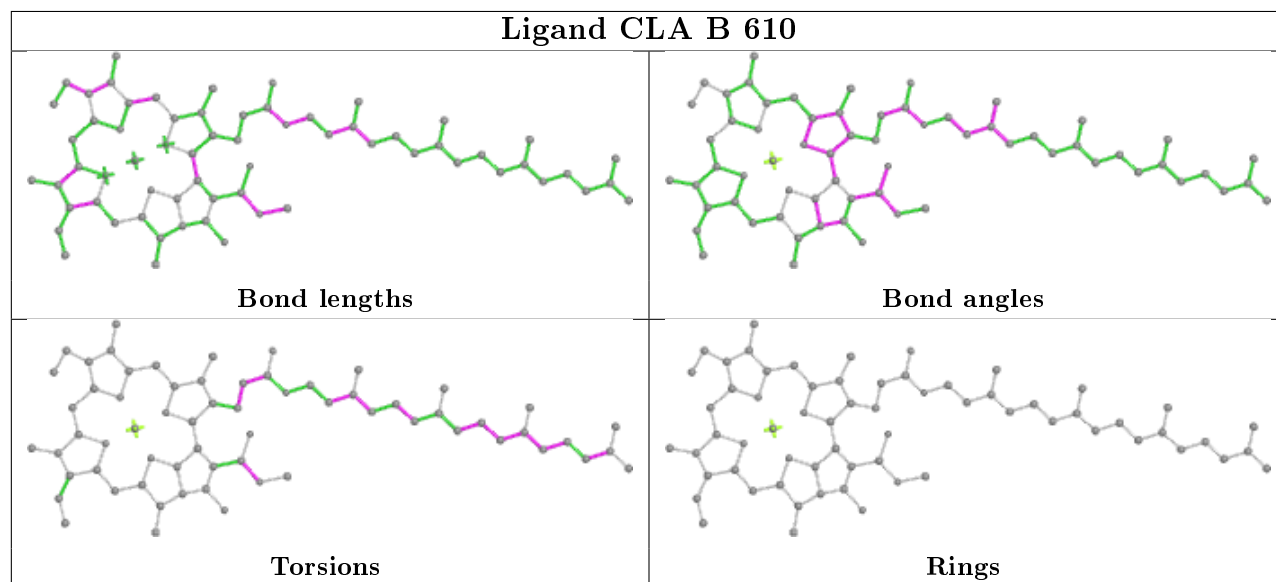
Ligand CLA P 504



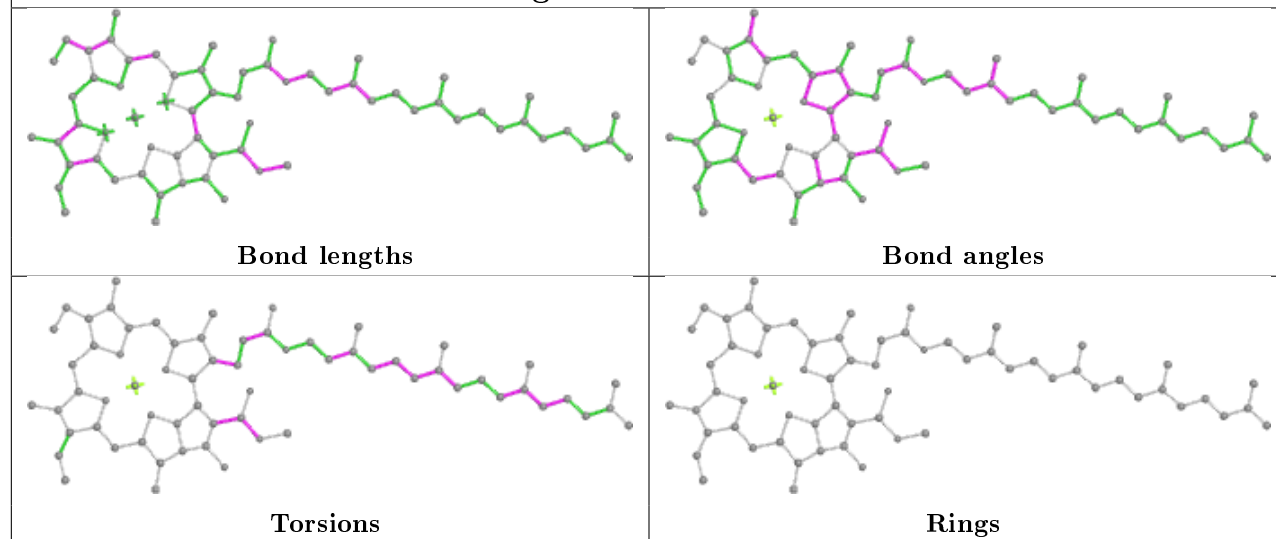
Ligand BCR S 101



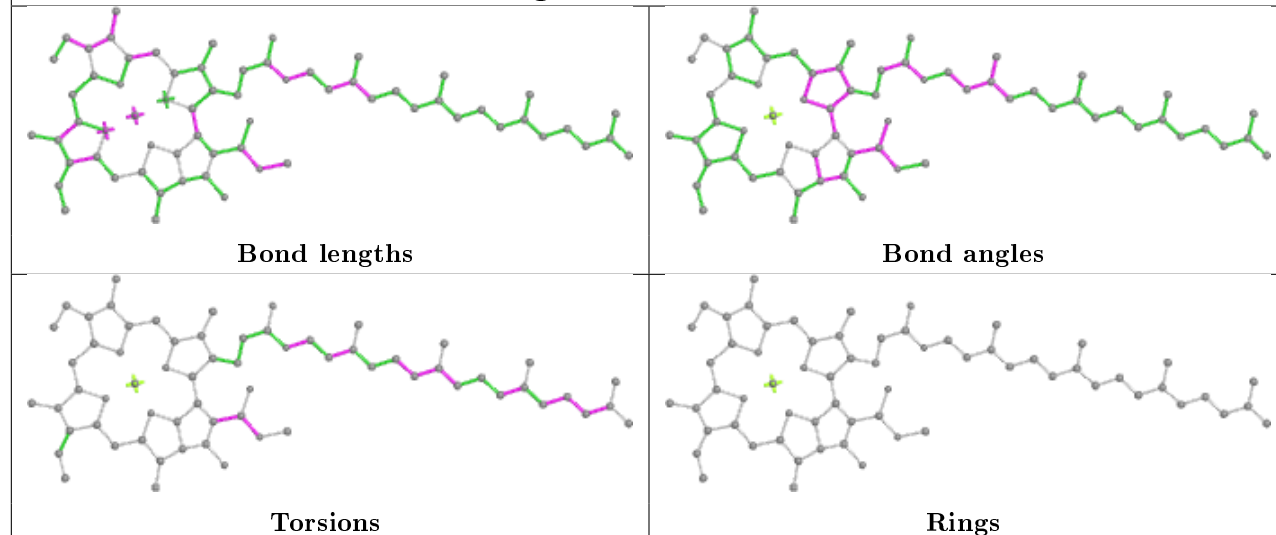
Ligand CLA B 610



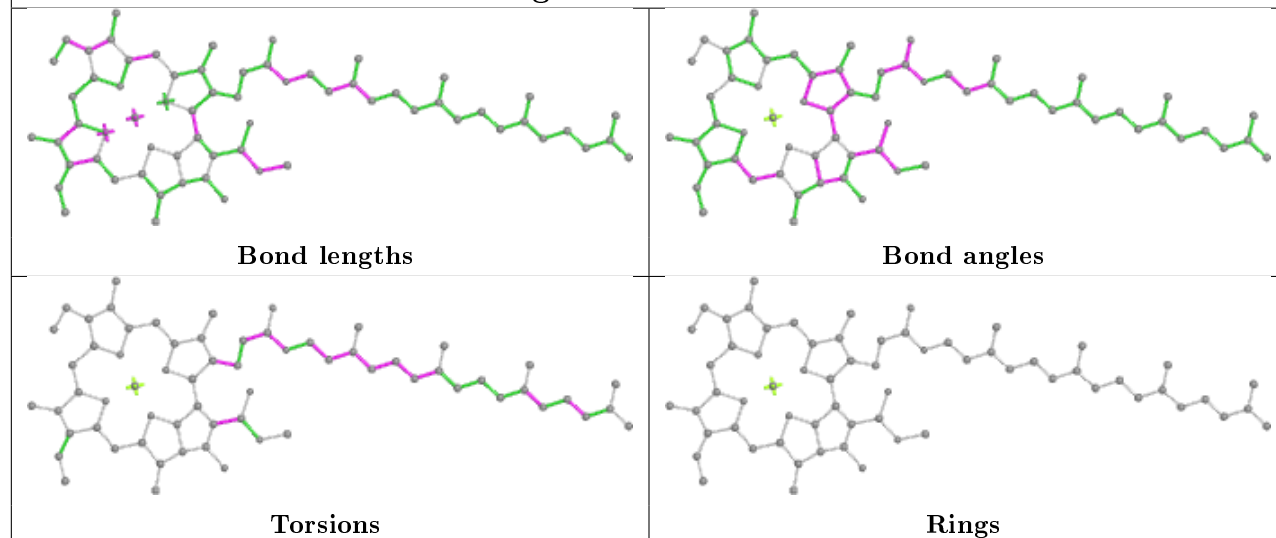
Ligand CLA B 602

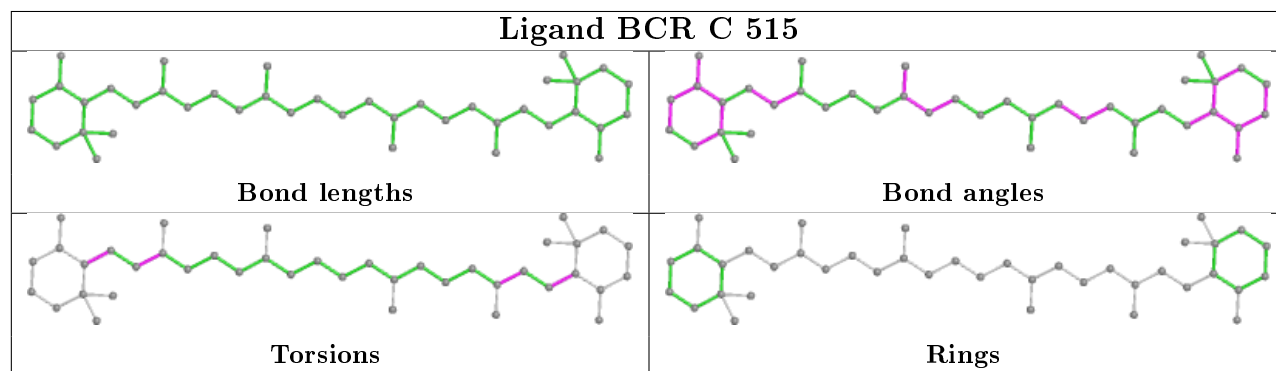
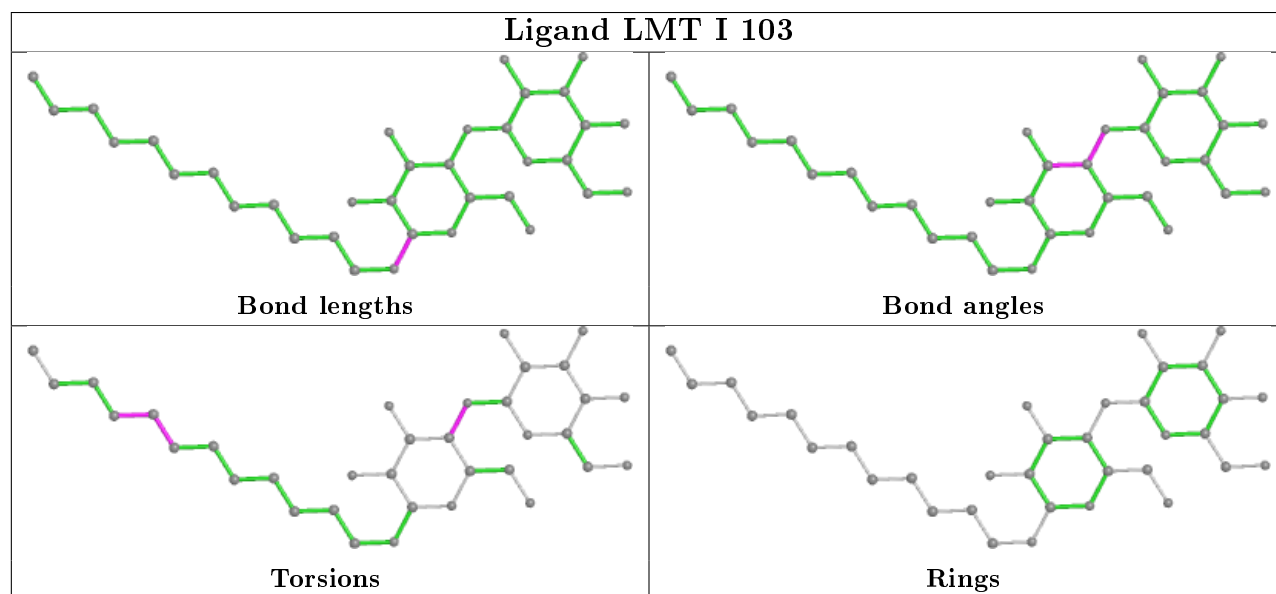
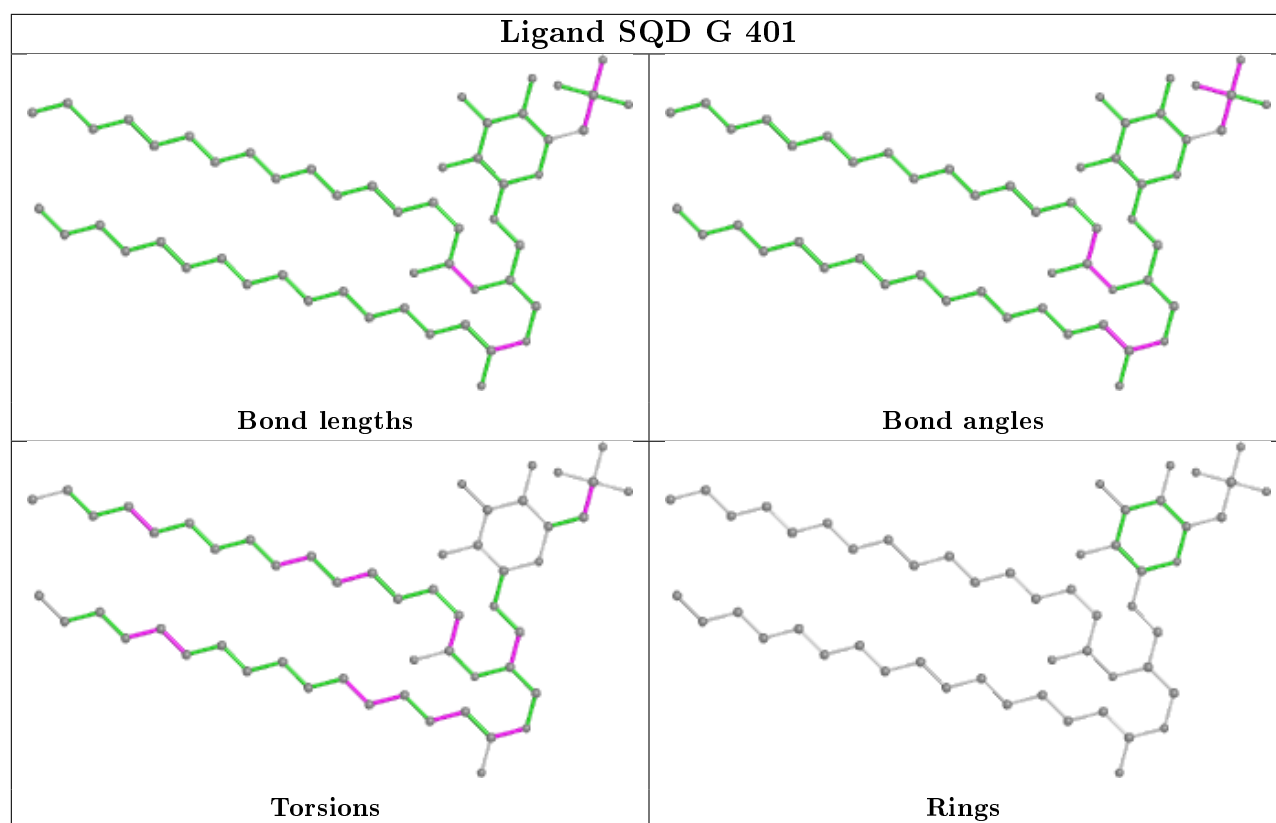


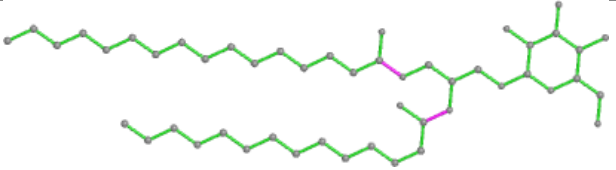
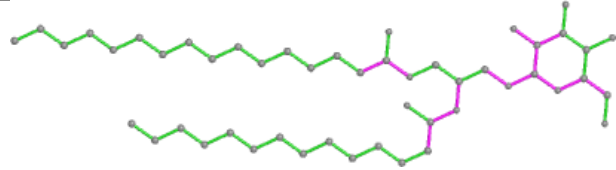
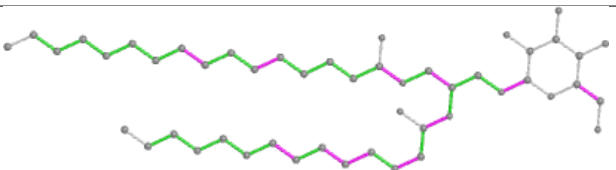
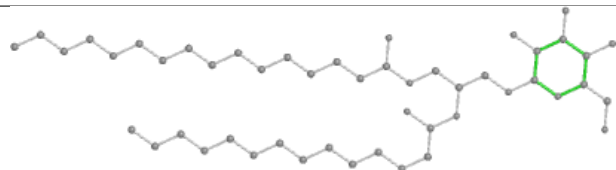
Ligand CLA C 510

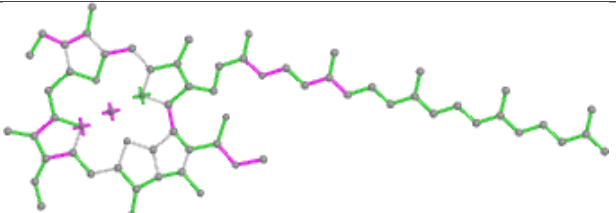
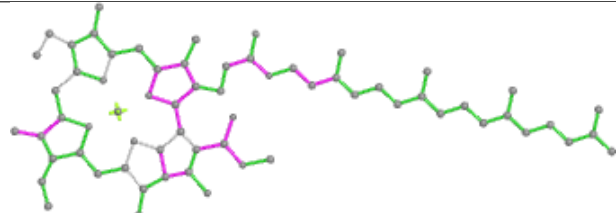
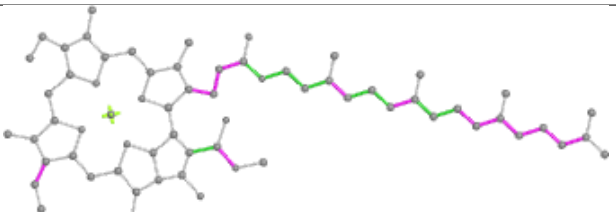
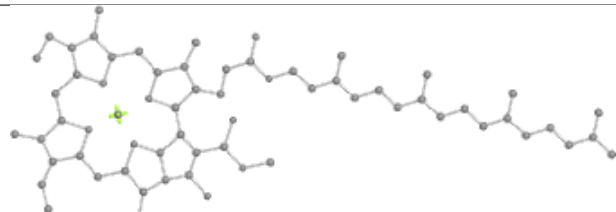


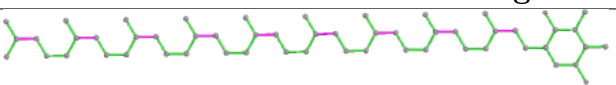
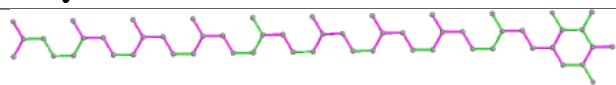
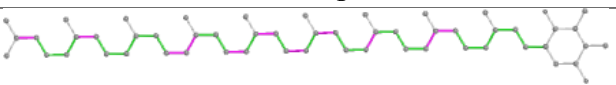
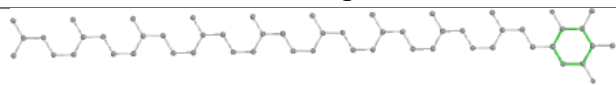
Ligand CLA A 402

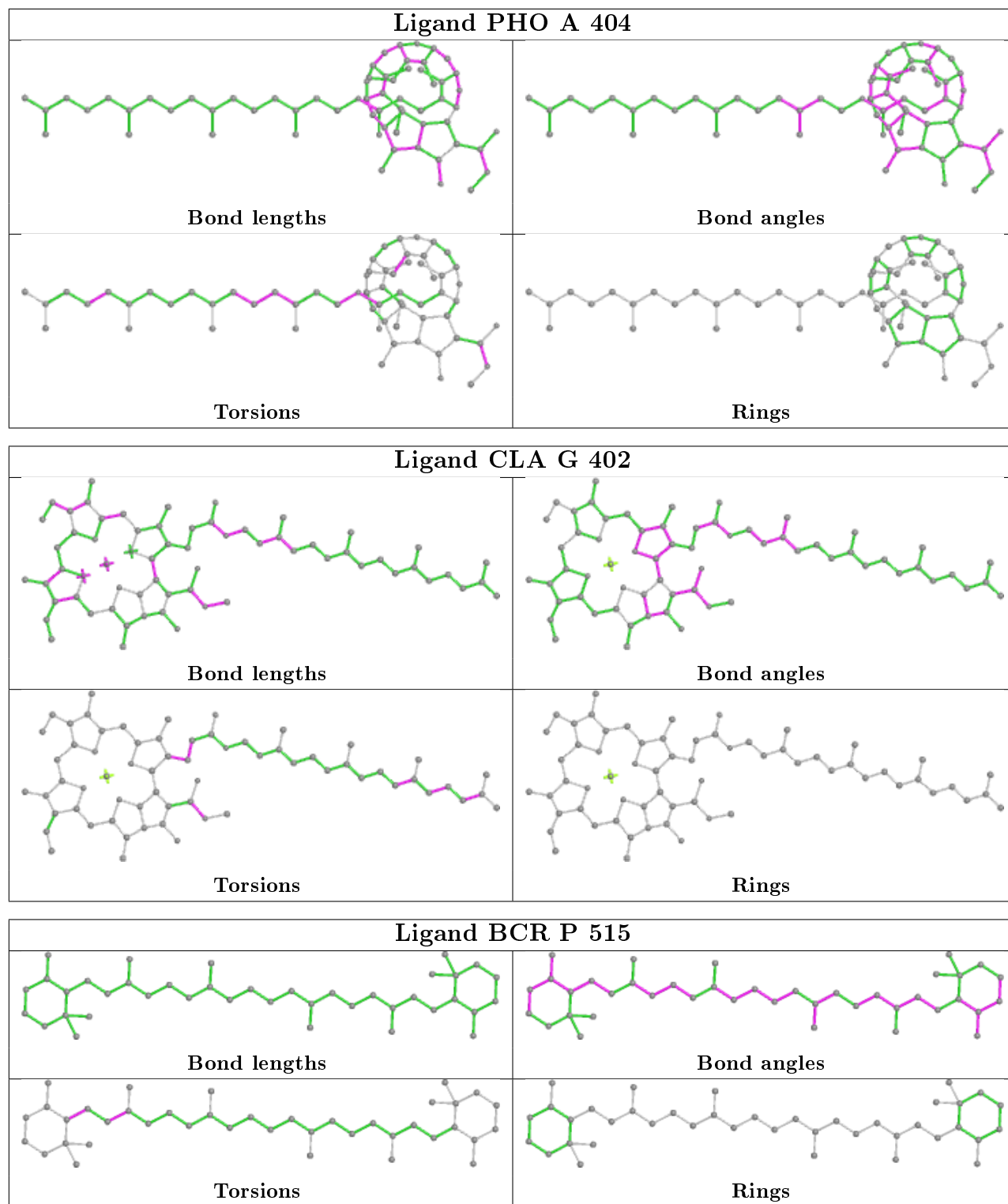


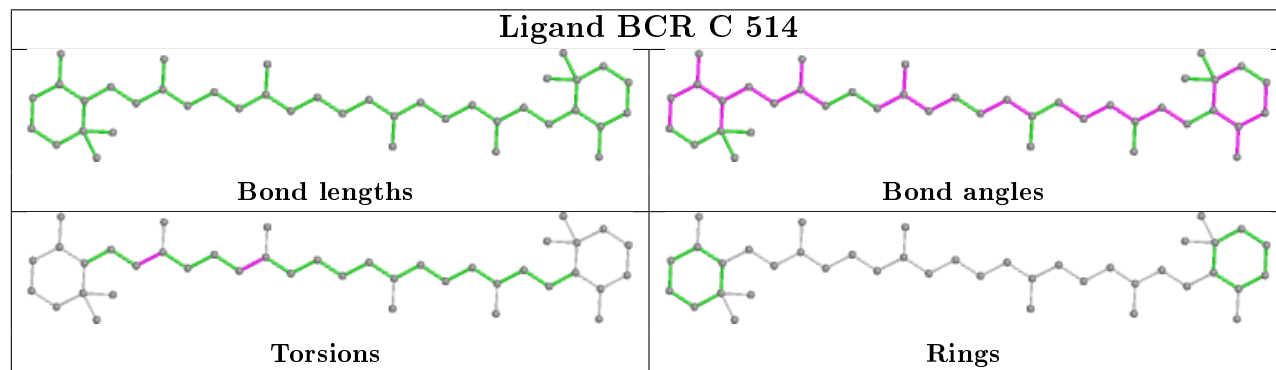
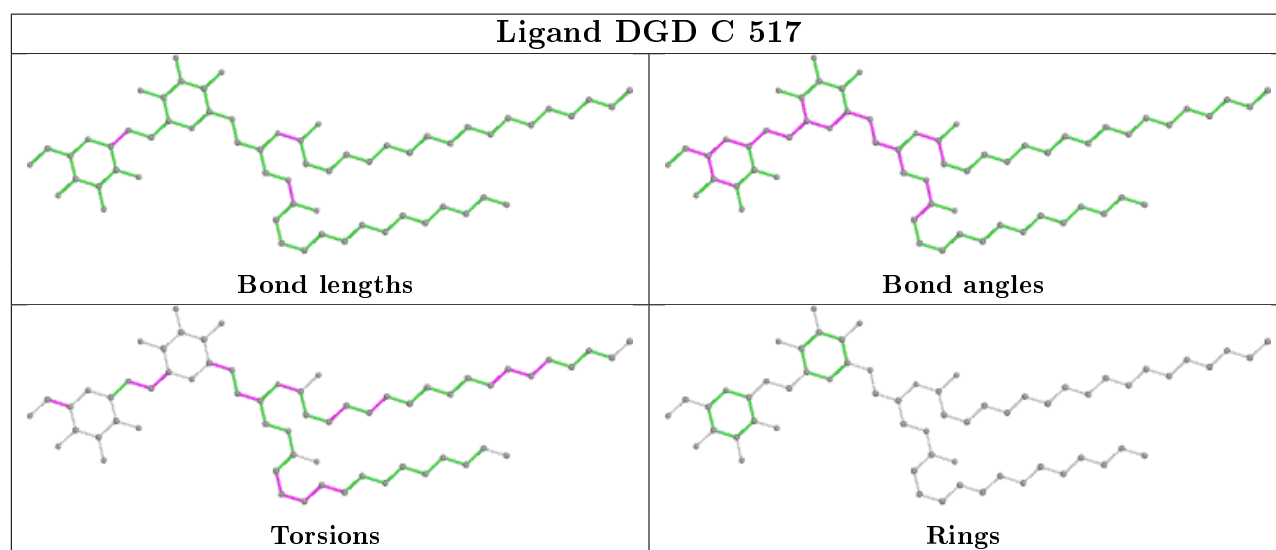
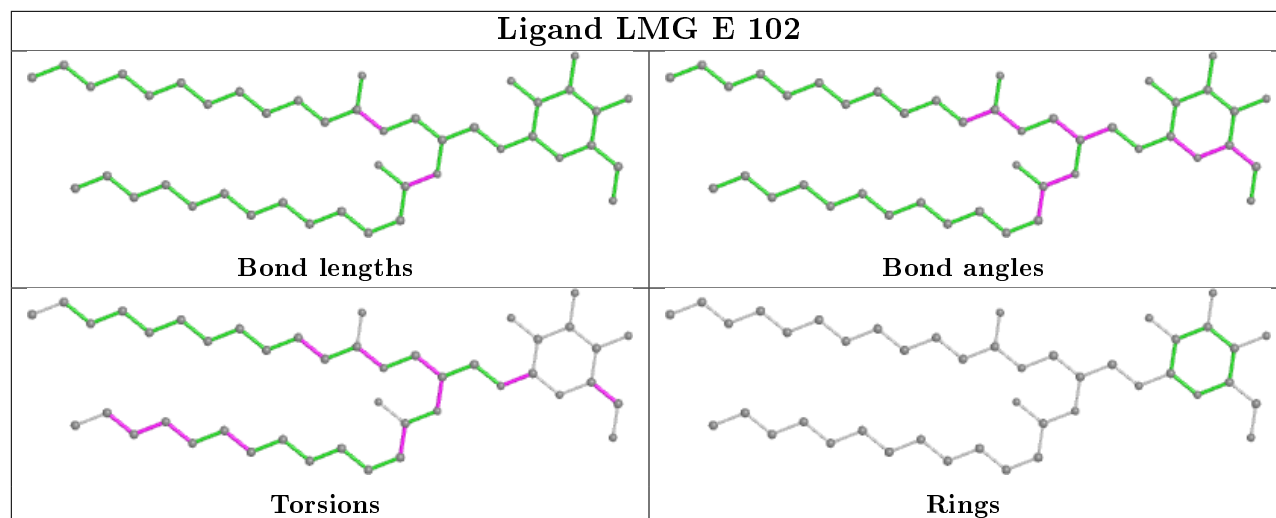


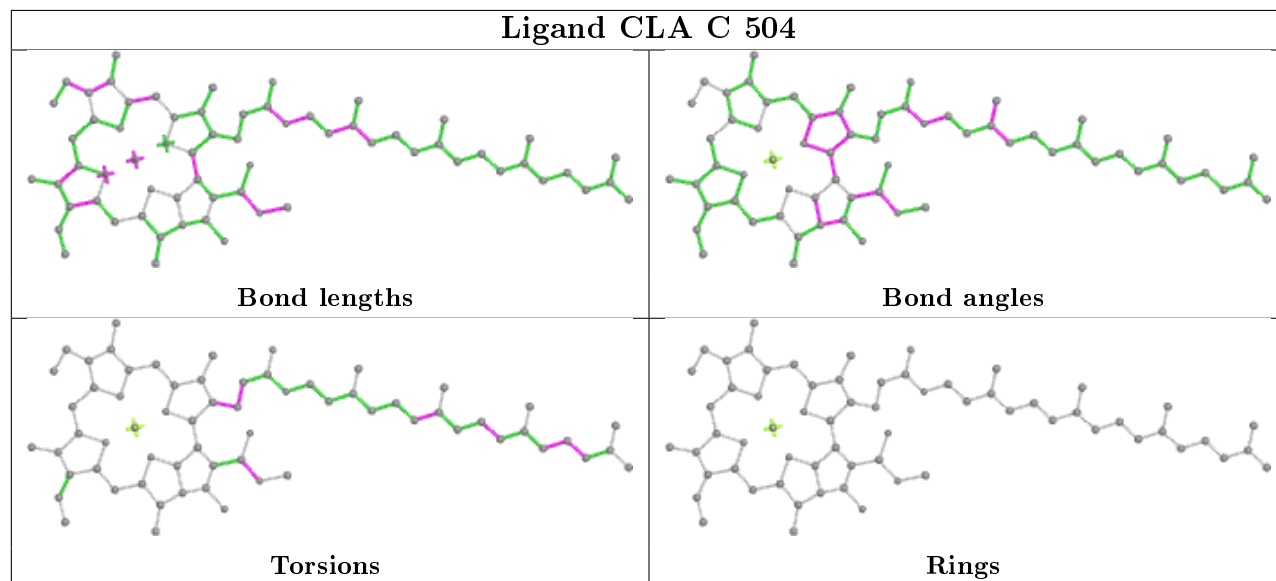
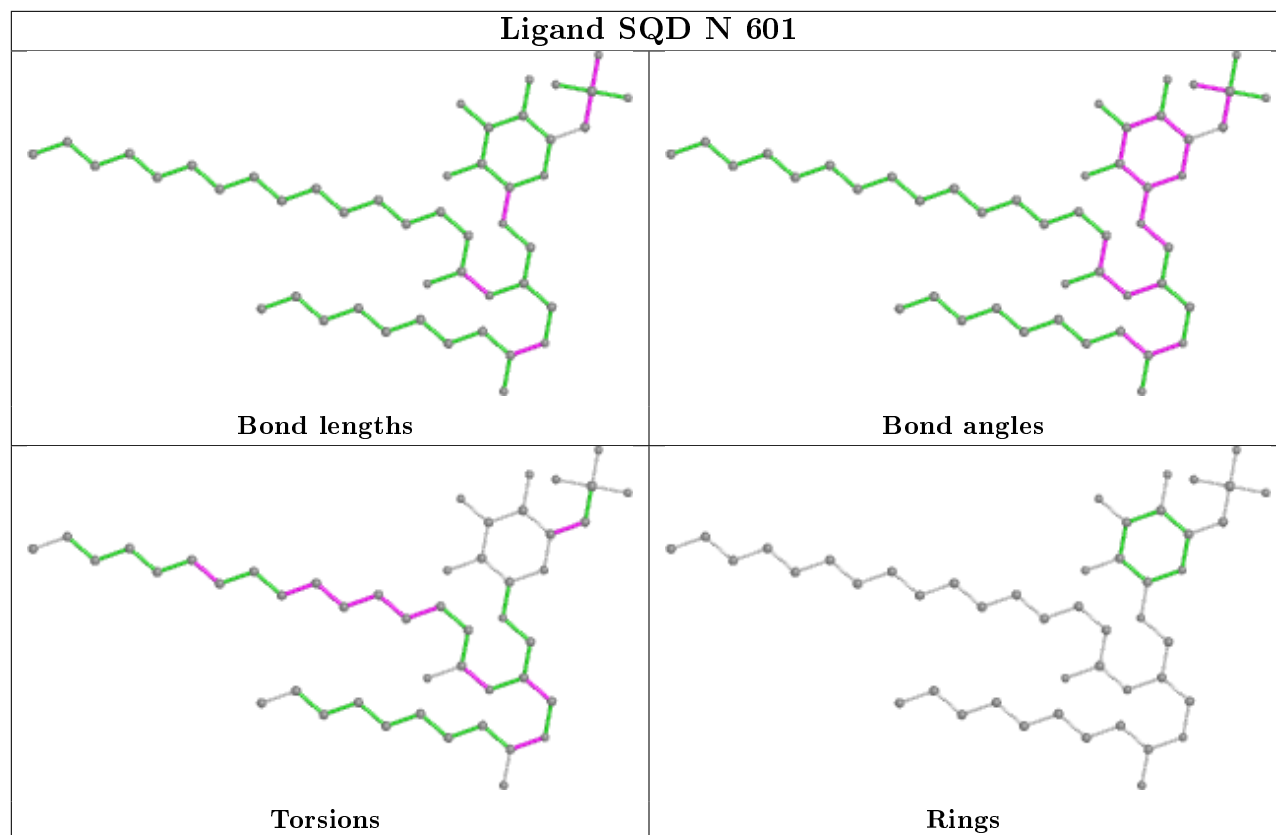
Ligand LMG B 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

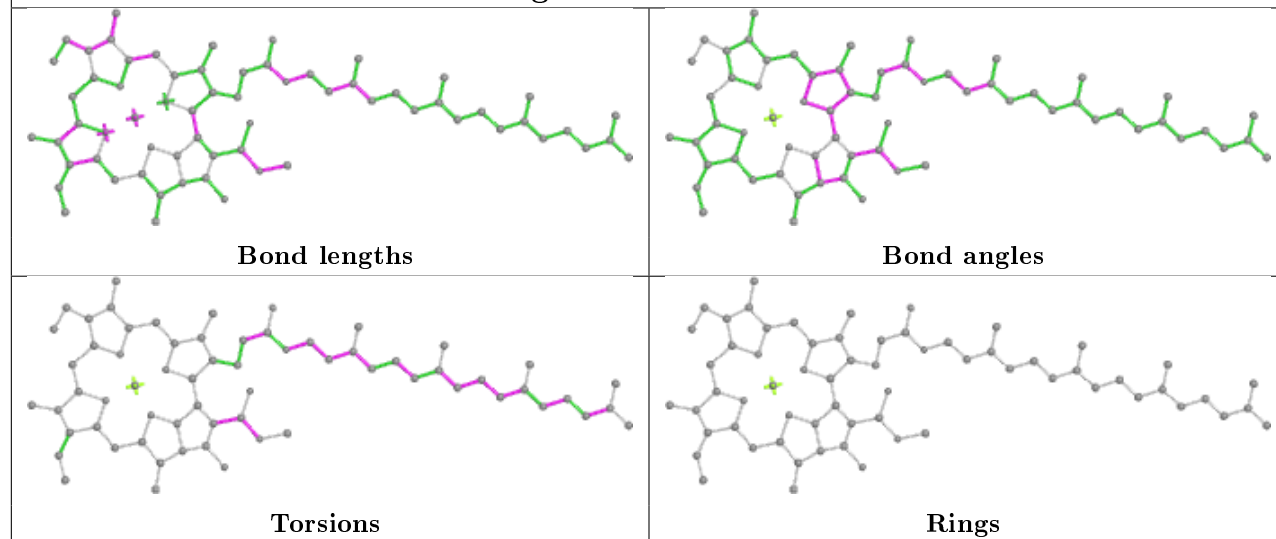
Ligand PL9 Q 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



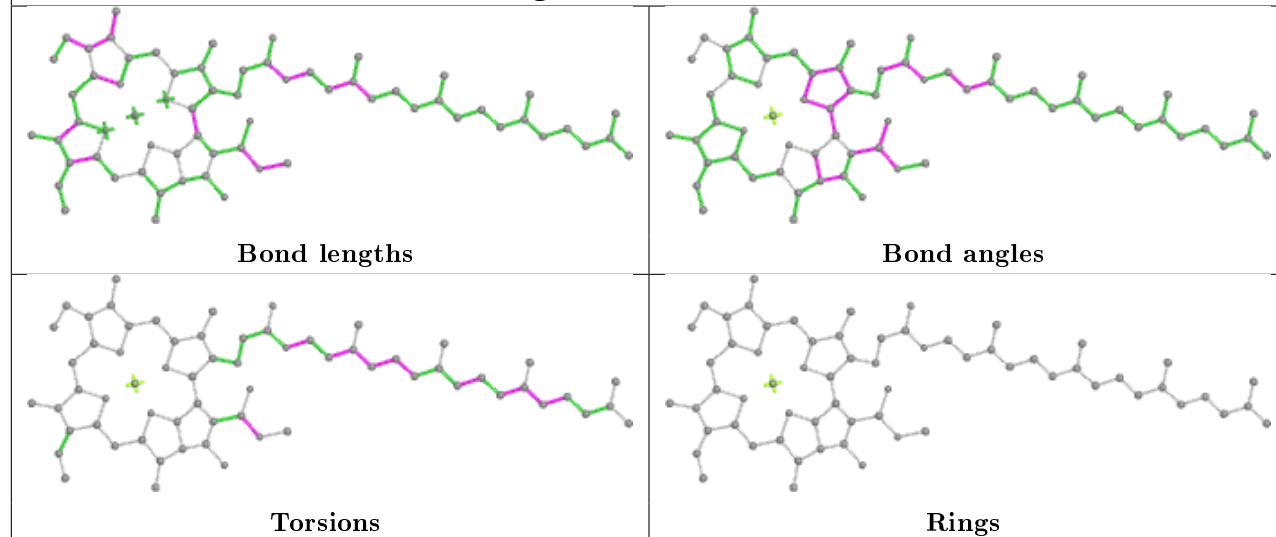




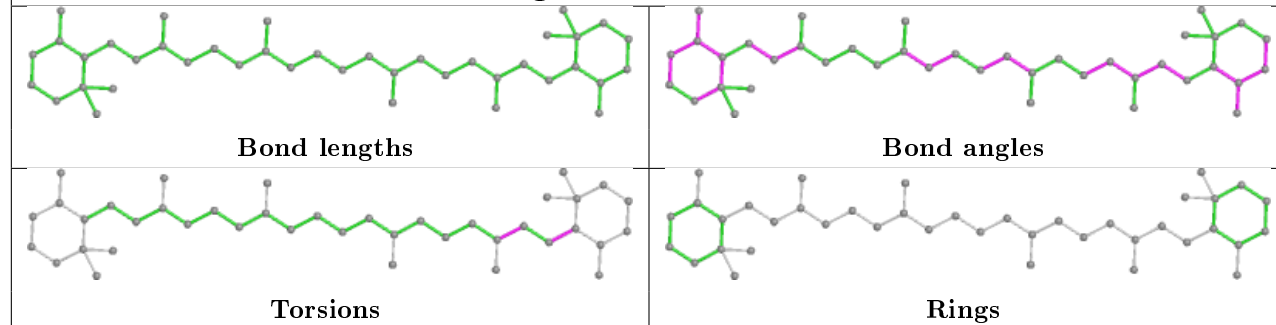
Ligand CLA N 617

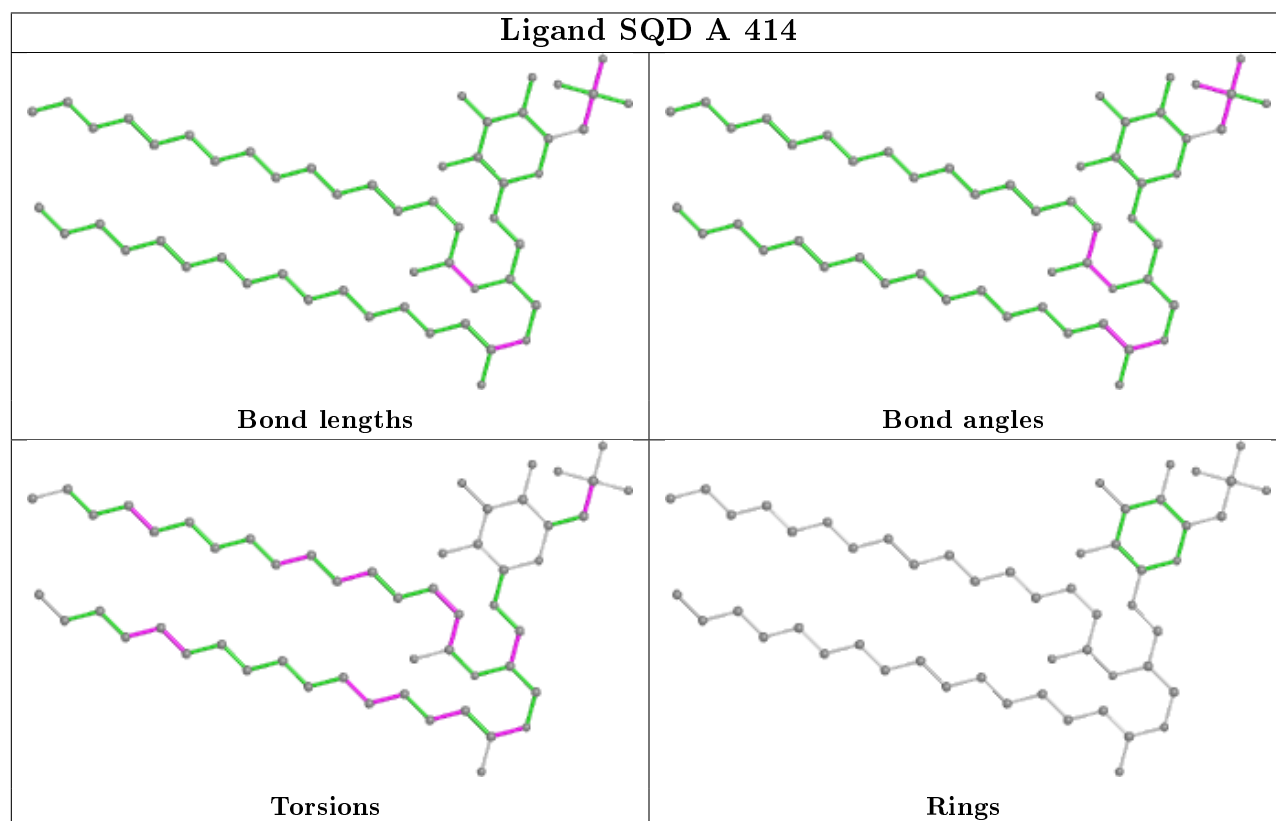
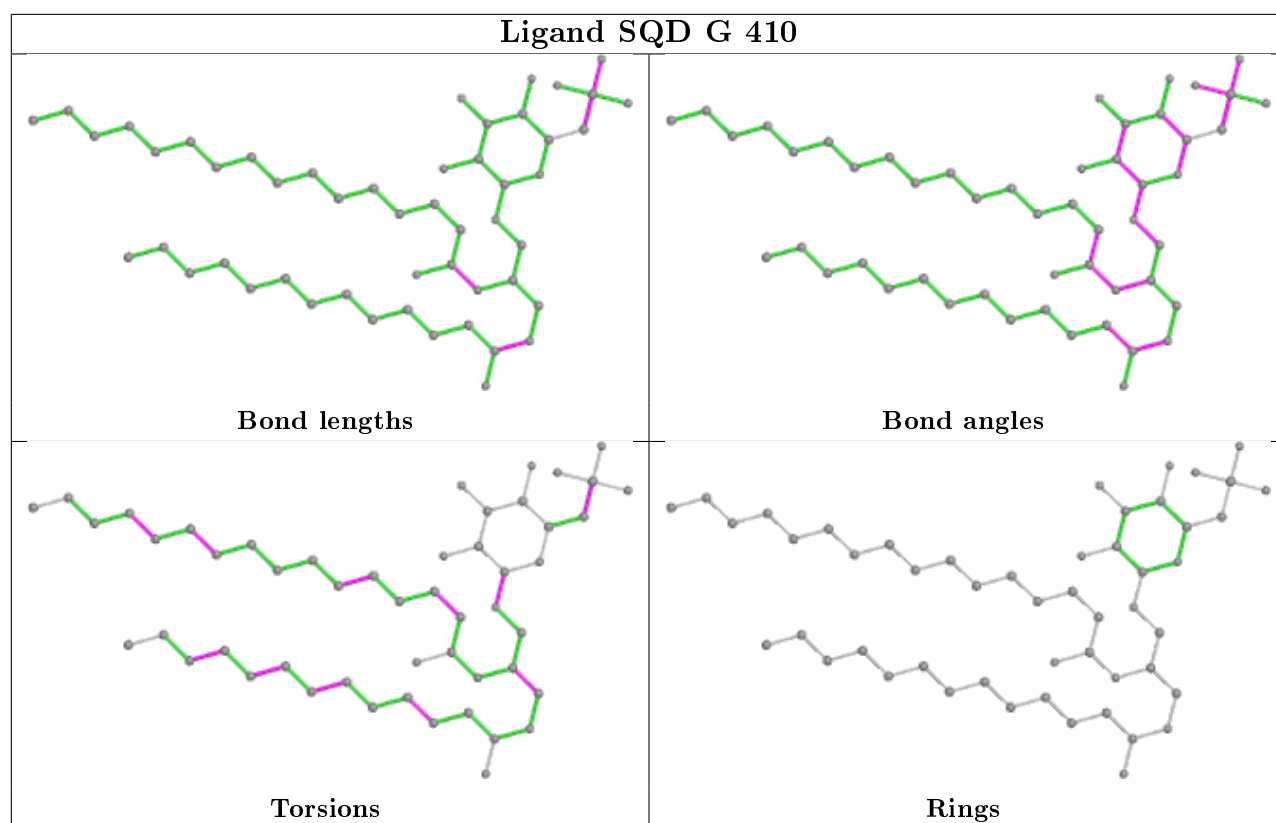


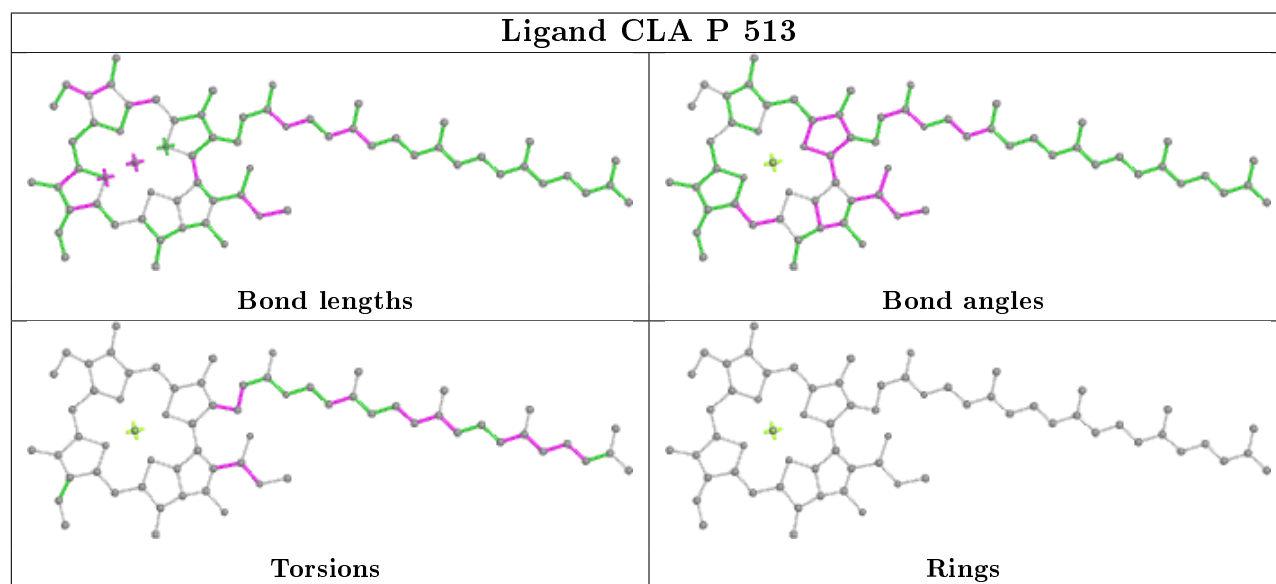
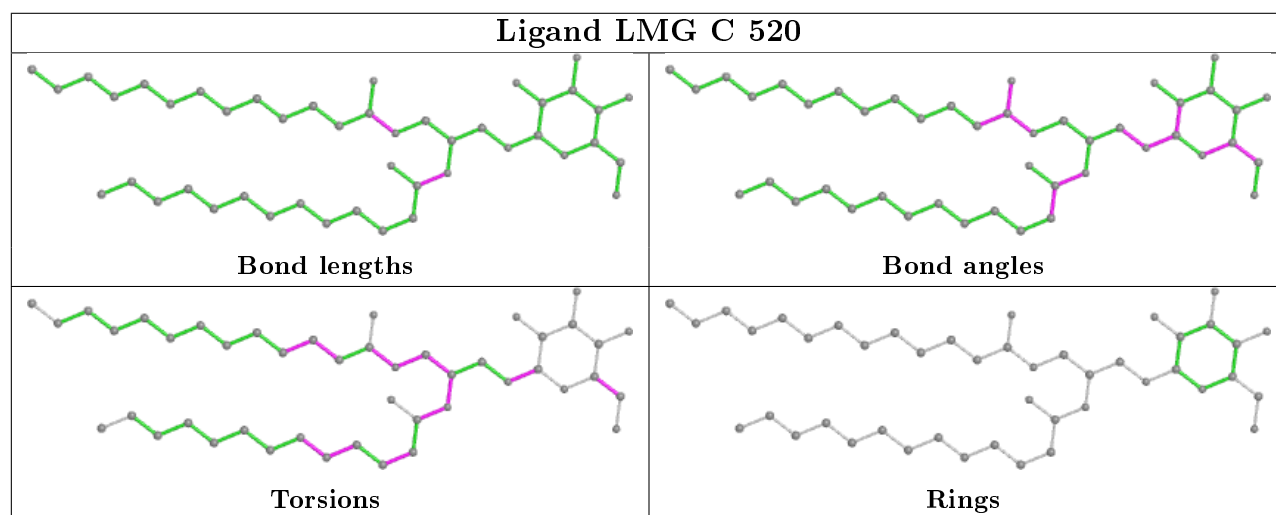
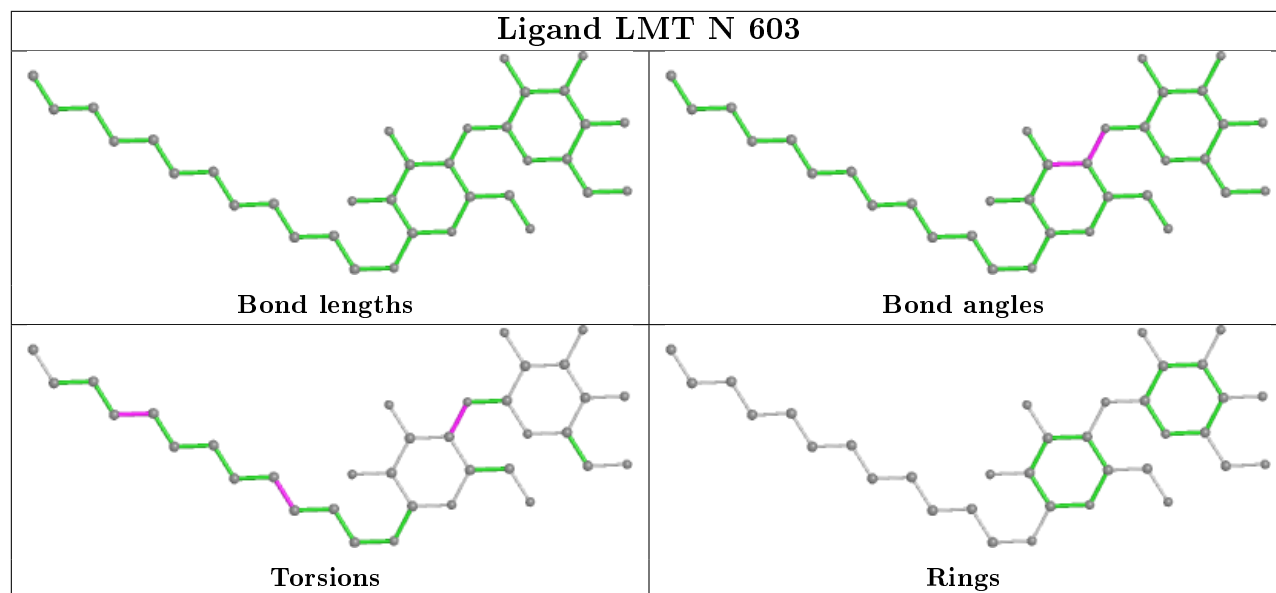
Ligand CLA N 616

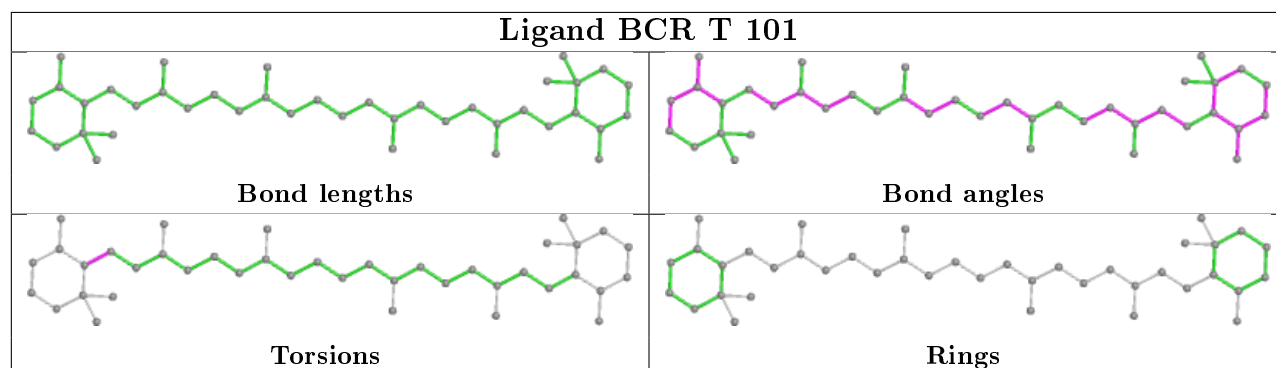
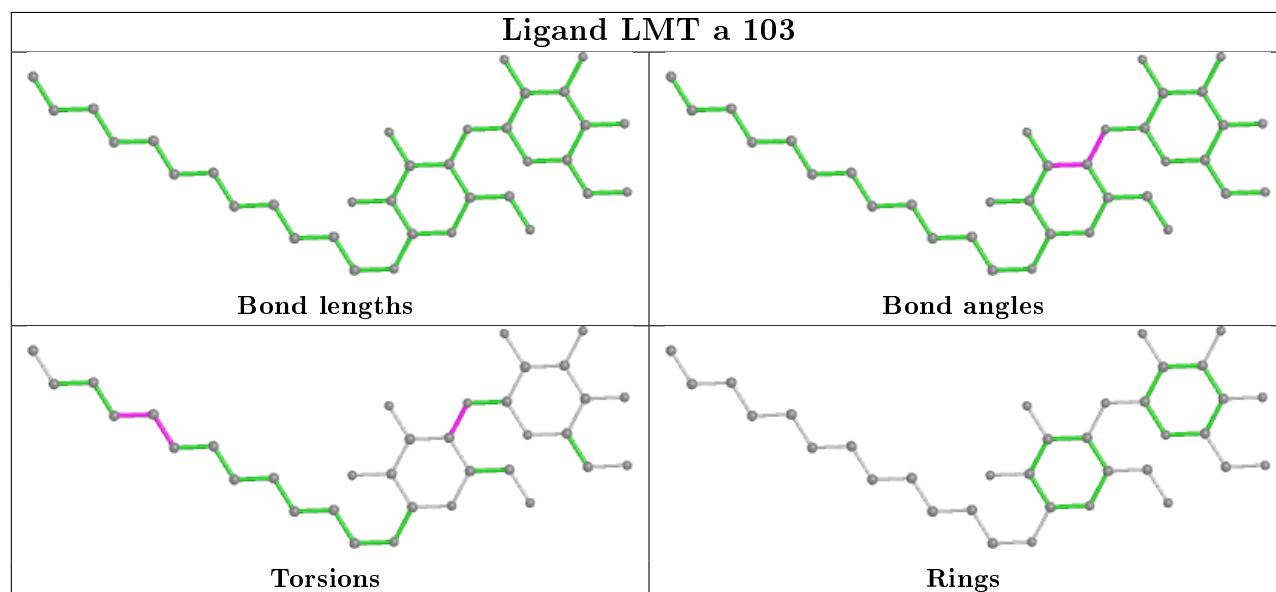
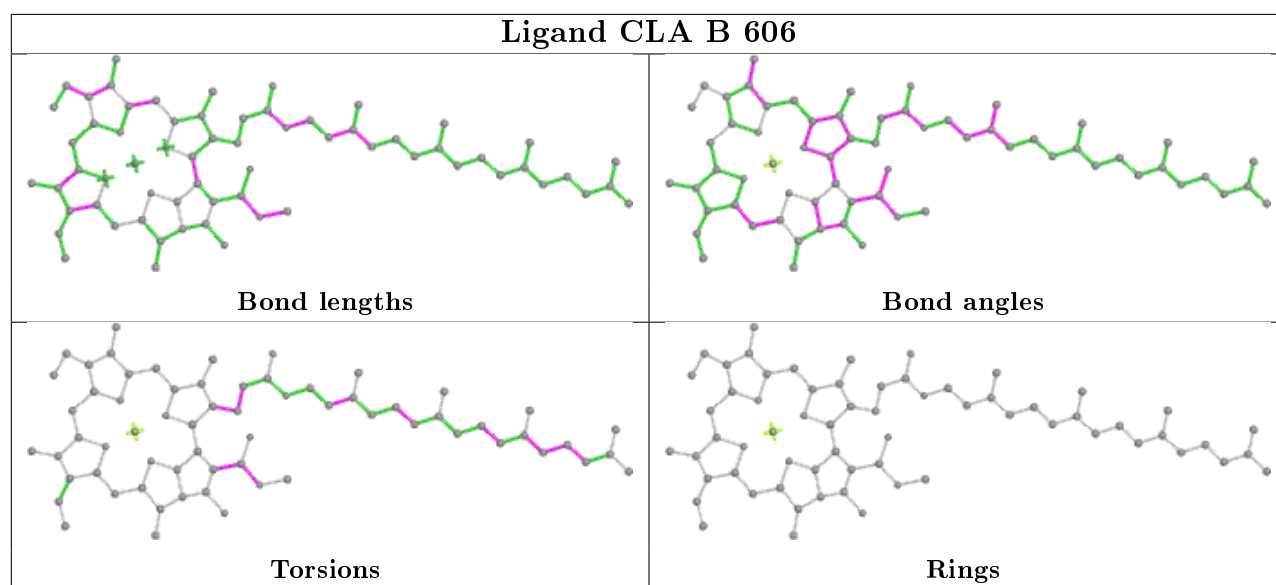


Ligand BCR T 103

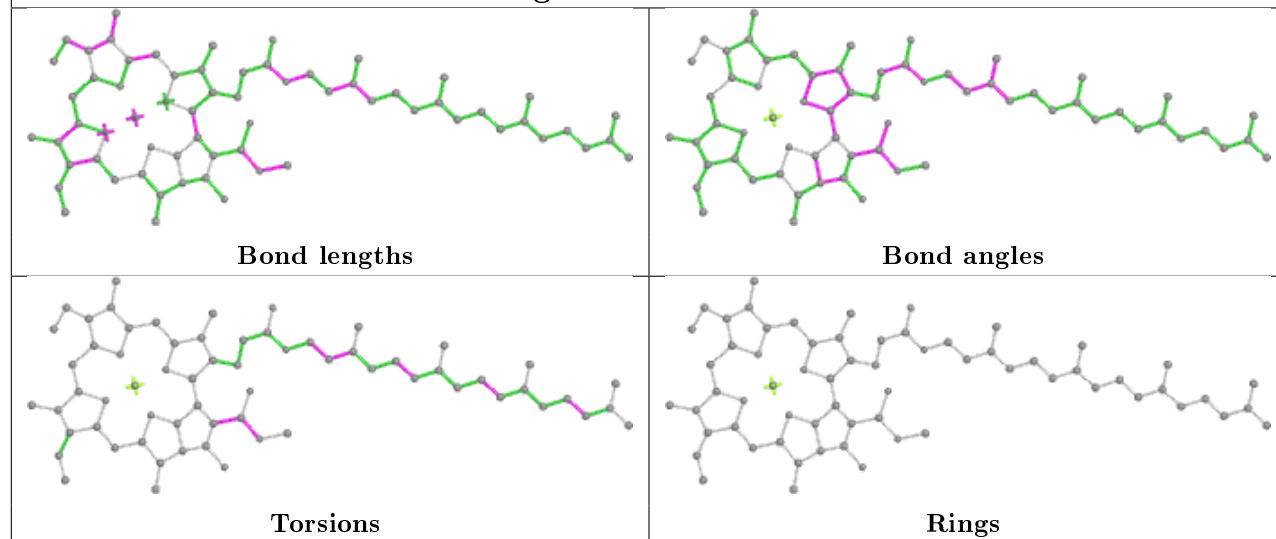




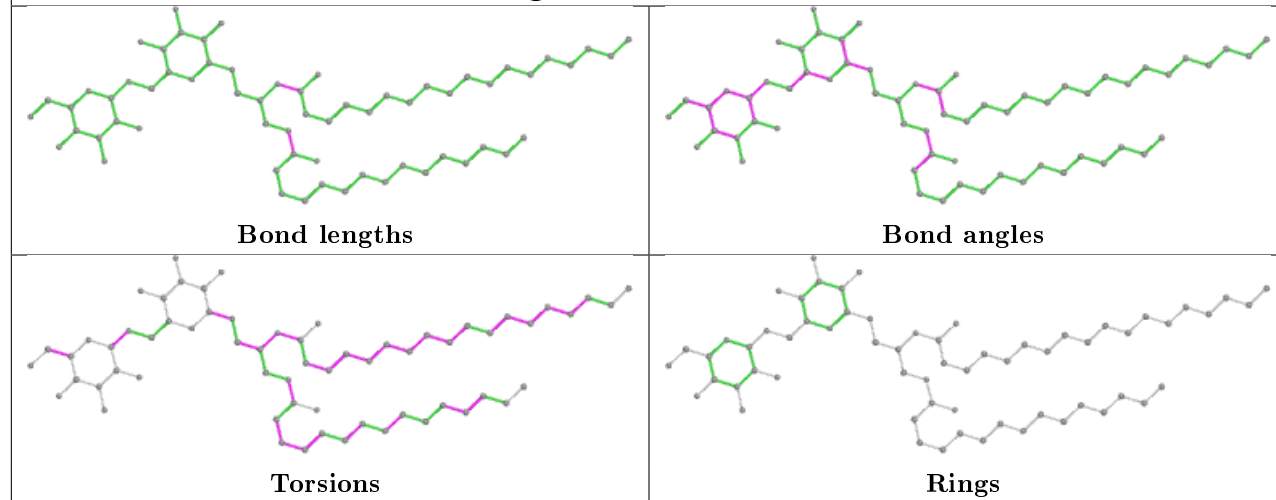


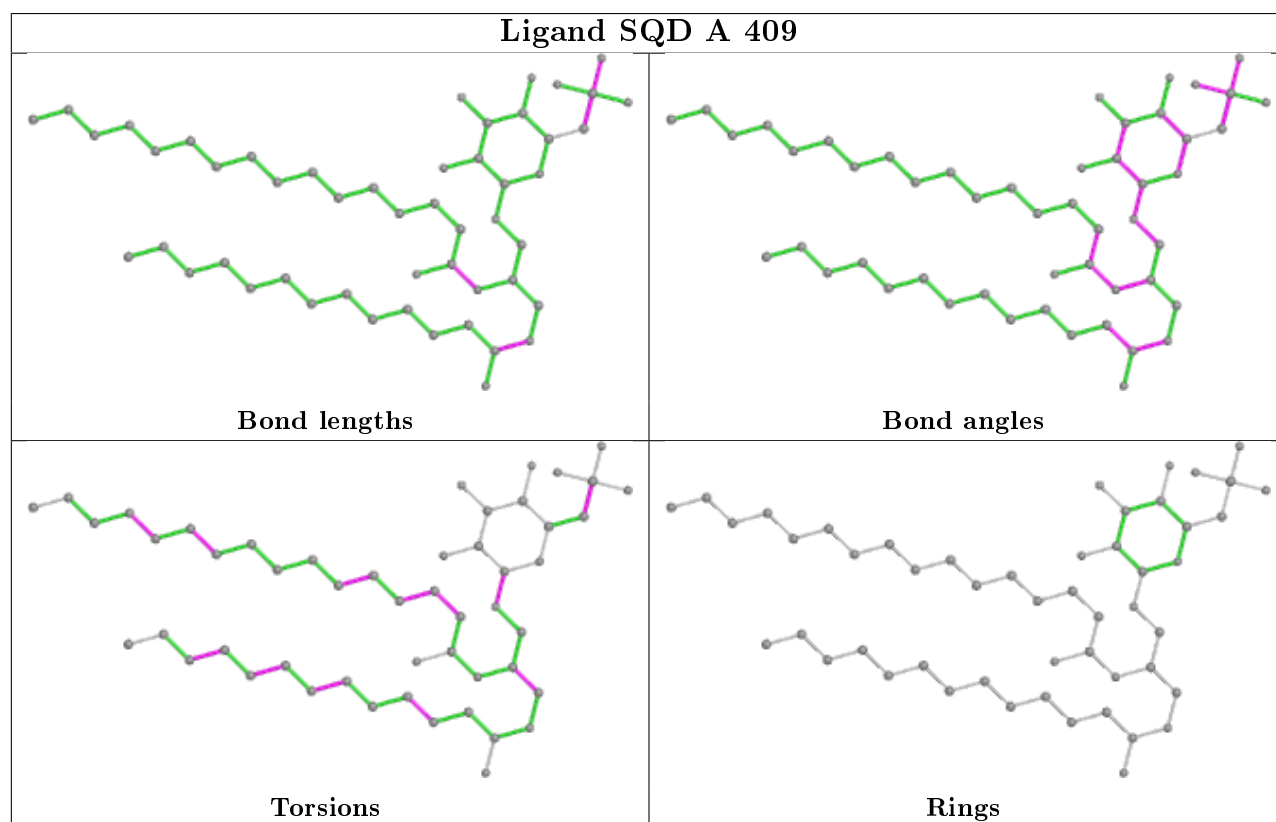
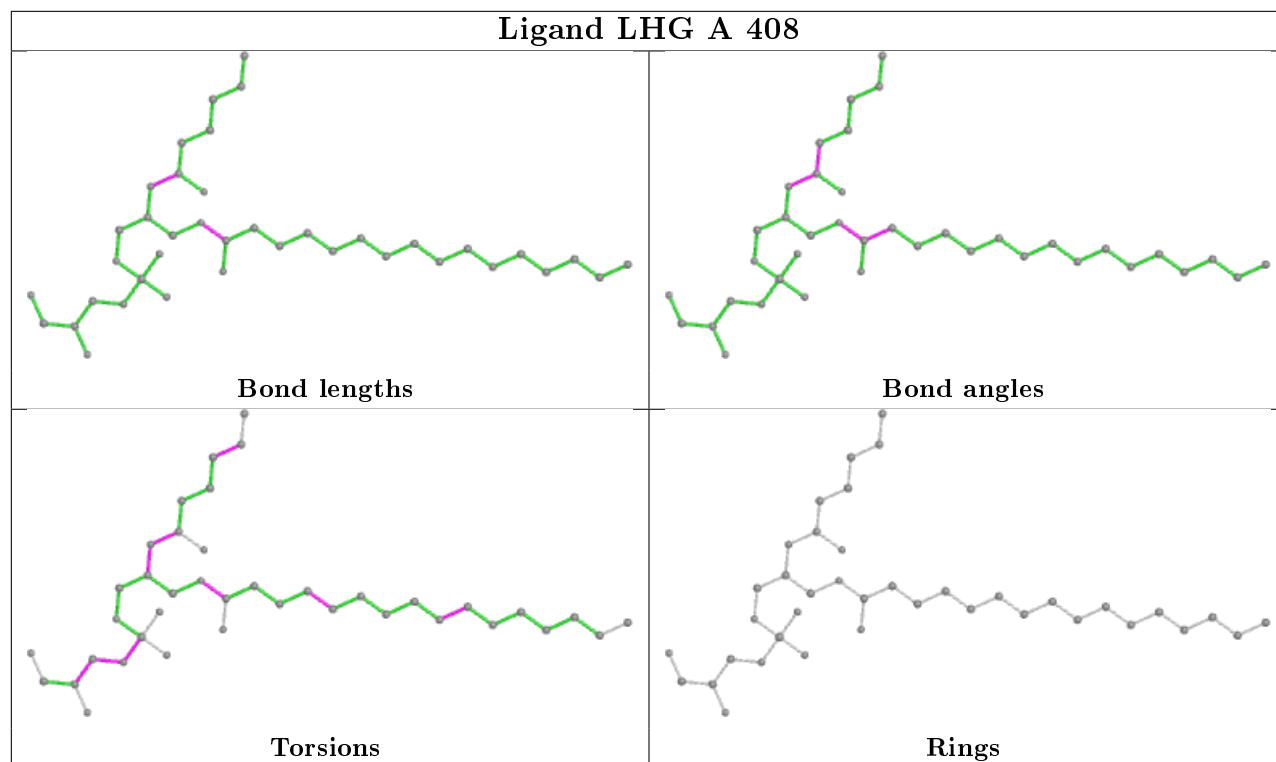


Ligand CLA P 509

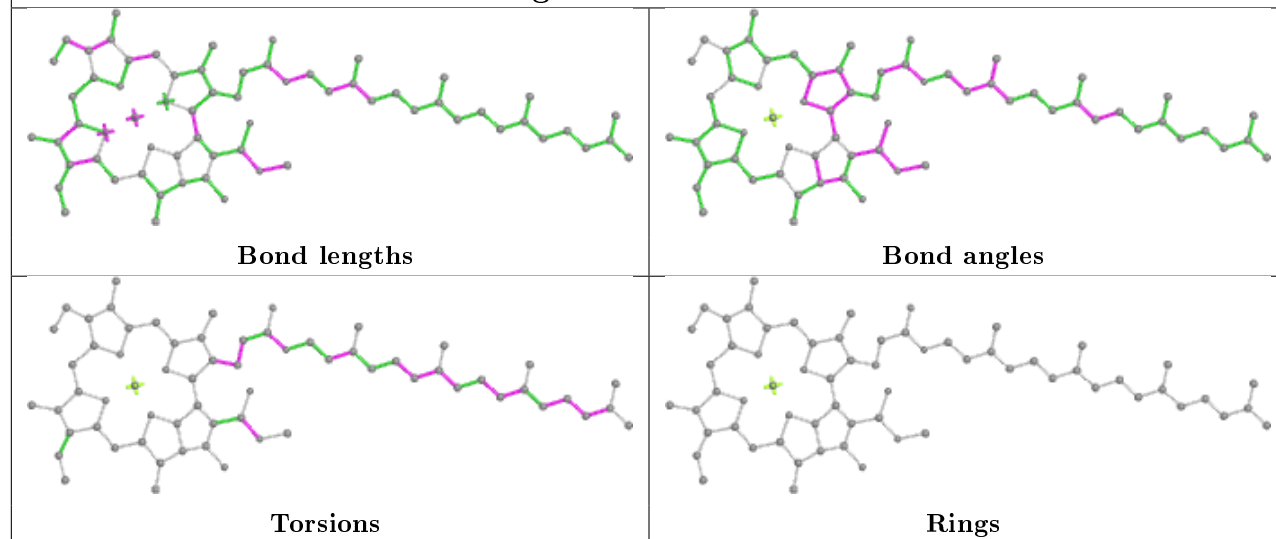


Ligand DGD D 408

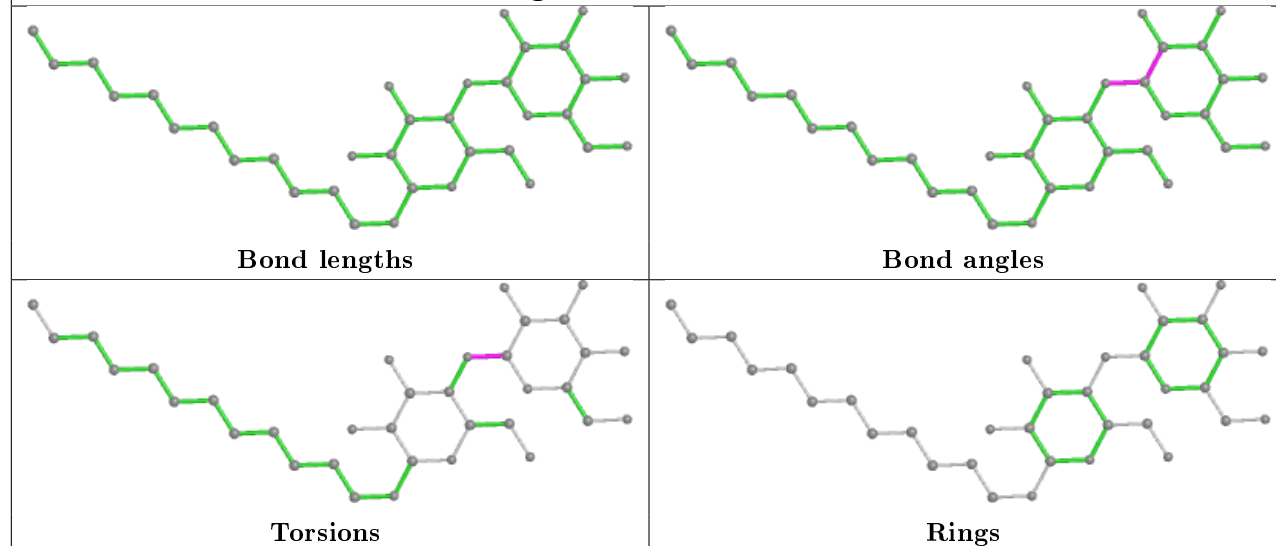




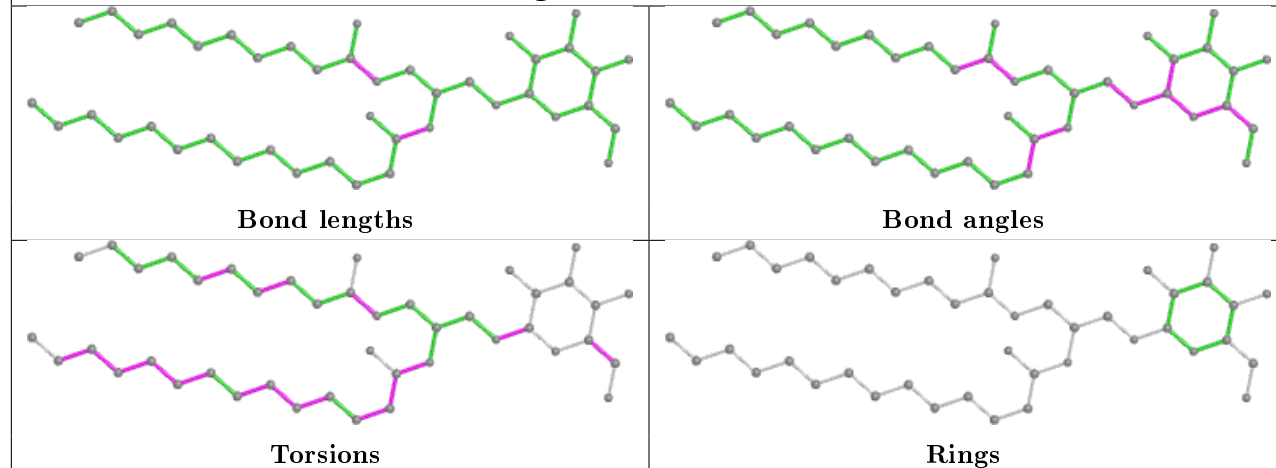
Ligand CLA B 605



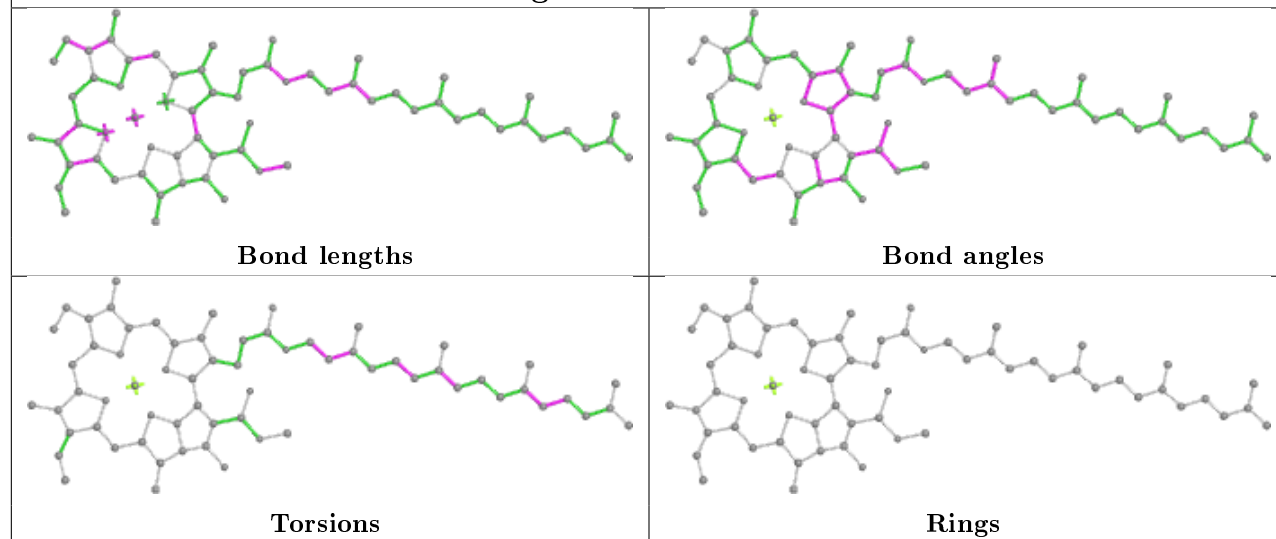
Ligand LMT B 626



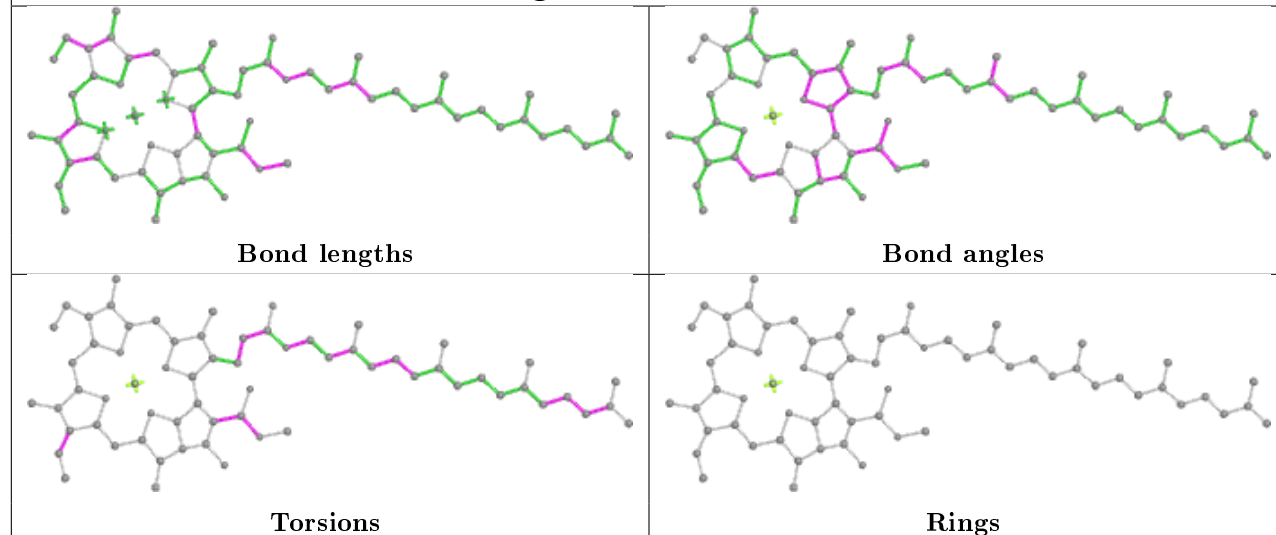
Ligand LMG a 102



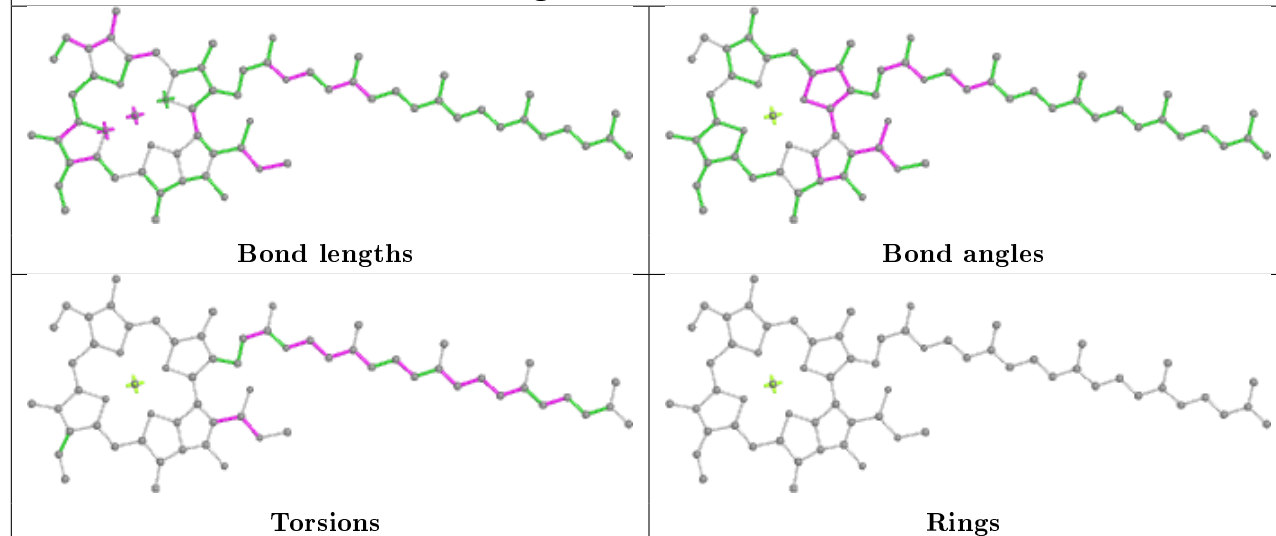
Ligand CLA N 619



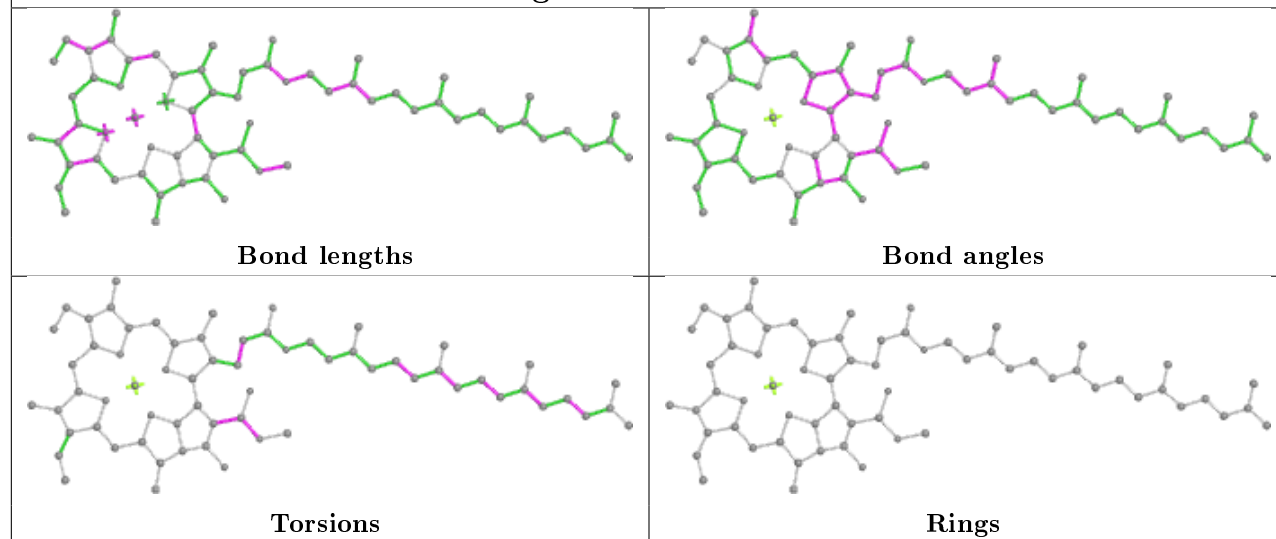
Ligand CLA N 618



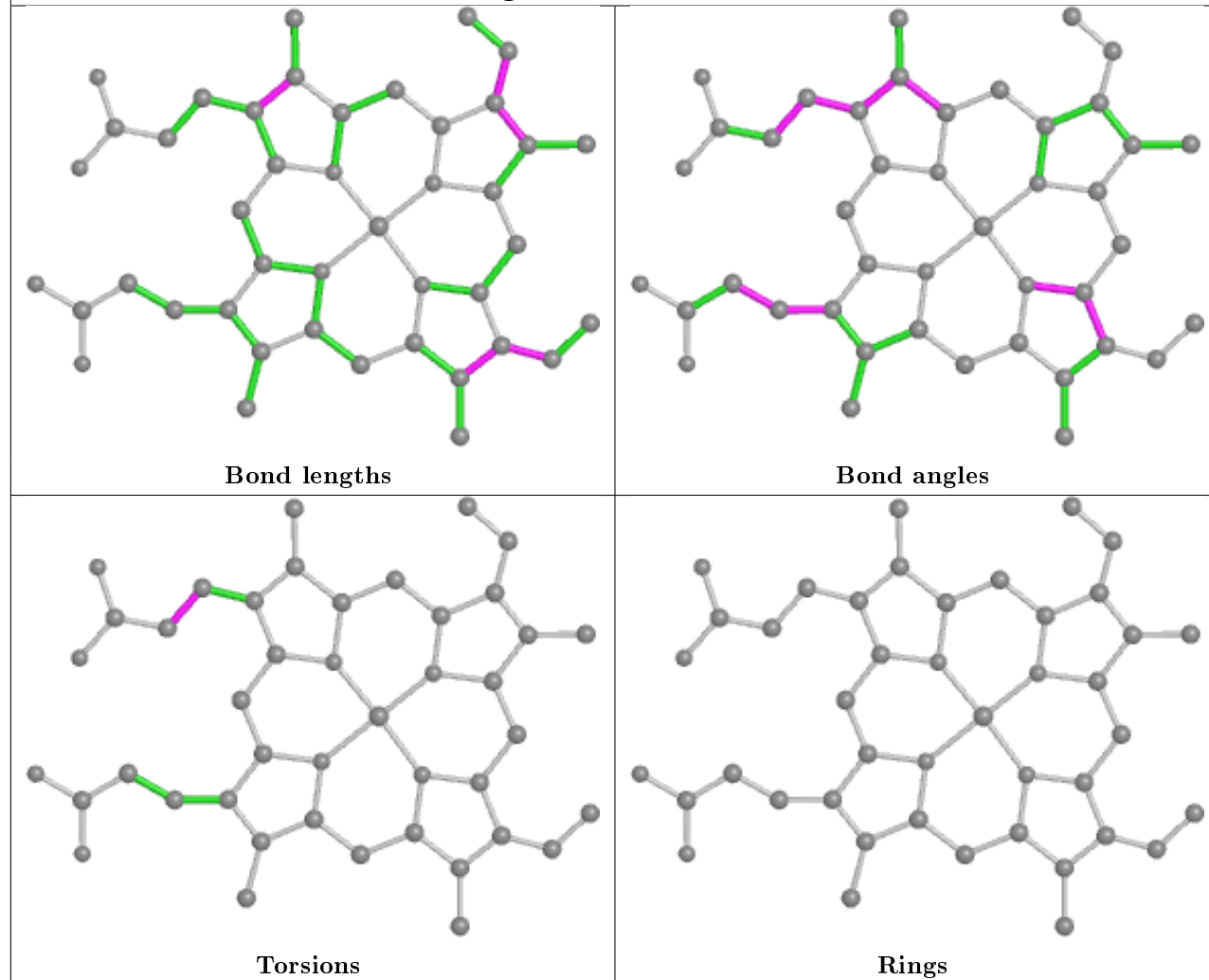
Ligand CLA B 613

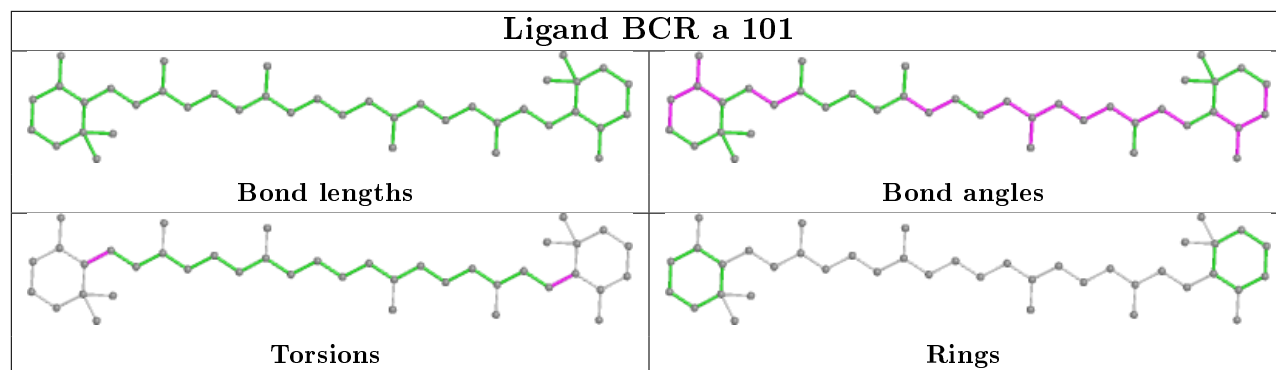
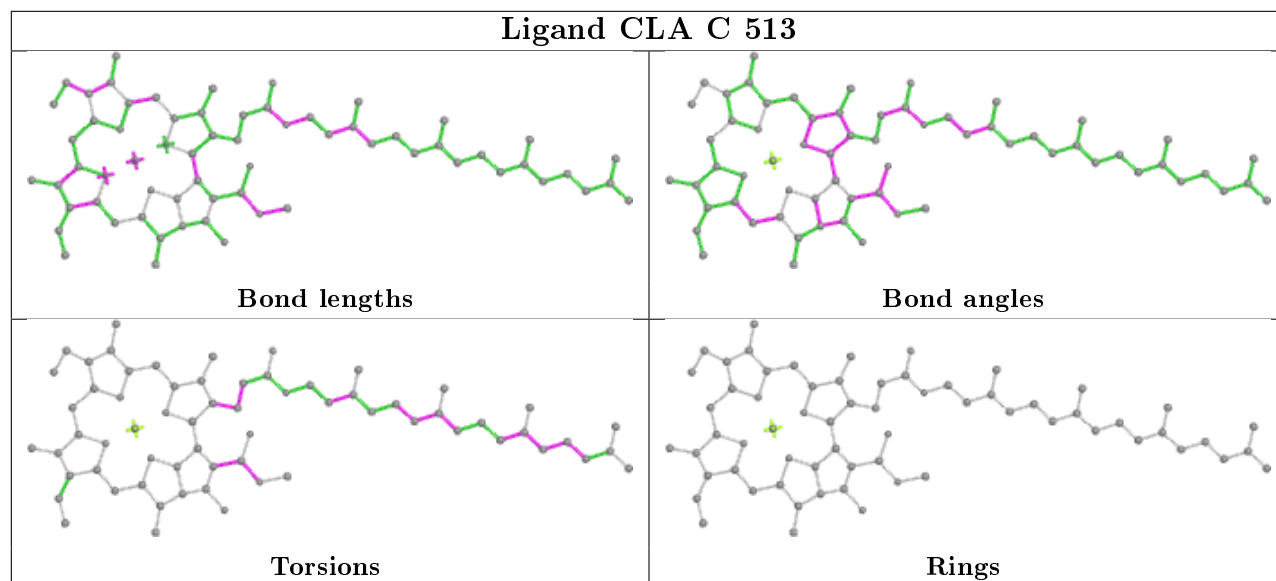
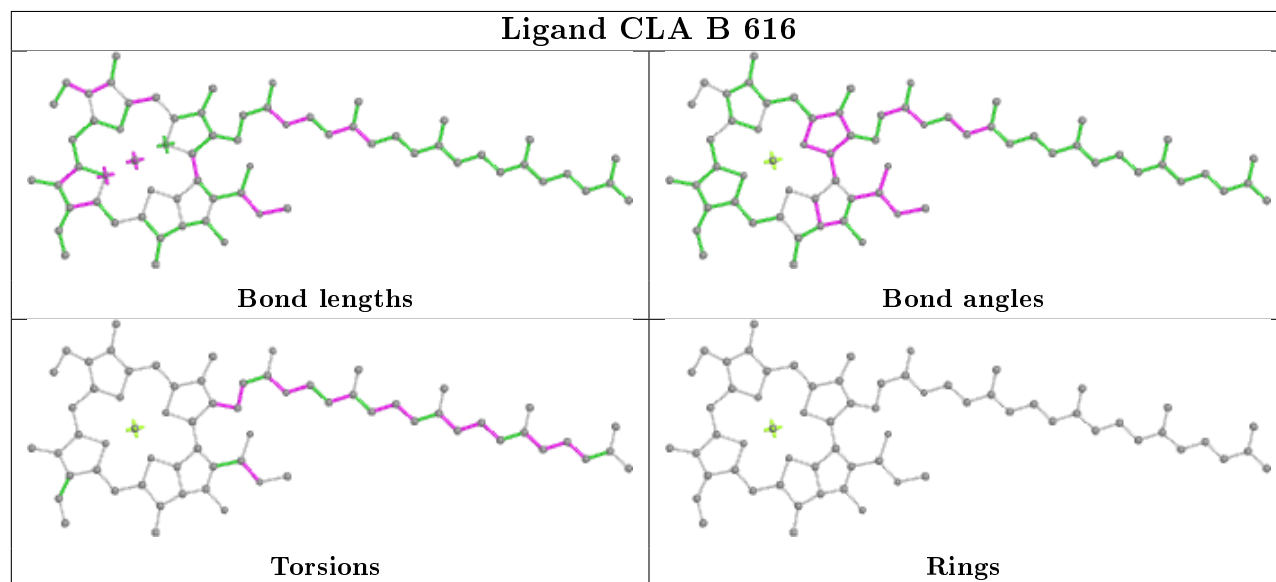


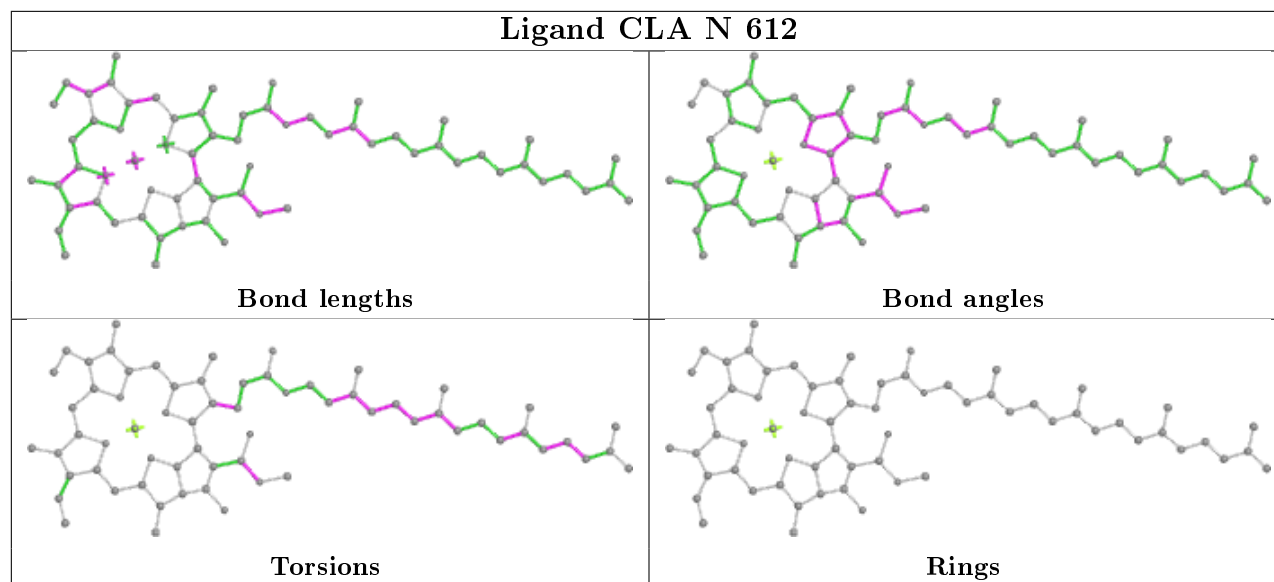
Ligand CLA C 508



Ligand HEM E 101



Ligand BCR a 101**Ligand CLA C 513****Ligand CLA B 616**



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%)	0.46	29 (8%) 10 12	131, 152, 182, 204	0
1	G	335/344 (97%)	0.29	20 (5%) 21 21	128, 156, 184, 213	0
2	B	490/510 (96%)	0.58	56 (11%) 5 8	128, 158, 178, 195	0
2	N	490/510 (96%)	0.63	64 (13%) 3 7	129, 160, 180, 207	0
3	C	447/461 (96%)	0.30	23 (5%) 28 27	129, 164, 183, 211	0
3	P	447/461 (96%)	0.66	70 (15%) 2 5	139, 165, 183, 197	0
4	D	340/352 (96%)	0.33	25 (7%) 14 15	125, 152, 176, 198	0
4	Q	340/352 (96%)	0.18	13 (3%) 40 36	130, 155, 175, 184	0
5	E	82/83 (98%)	0.17	3 (3%) 41 37	148, 171, 188, 198	0
5	R	82/83 (98%)	-0.15	0 100 100	148, 171, 188, 195	0
6	F	35/44 (79%)	-0.18	1 (2%) 51 44	140, 168, 185, 199	0
6	S	35/44 (79%)	0.37	0 100 100	148, 165, 187, 188	0
7	H	65/65 (100%)	0.78	7 (10%) 5 9	154, 172, 189, 195	0
7	W	65/65 (100%)	0.86	16 (24%) 0 2	154, 173, 188, 196	0
8	I	35/38 (92%)	0.20	1 (2%) 51 44	147, 163, 174, 178	0
8	a	35/38 (92%)	0.03	0 100 100	148, 164, 179, 190	0
9	J	34/39 (87%)	0.03	0 100 100	155, 165, 183, 189	0
9	b	34/39 (87%)	1.19	8 (23%) 0 2	156, 176, 190, 190	0
10	K	37/37 (100%)	0.21	3 (8%) 12 14	158, 170, 181, 185	0
10	c	37/37 (100%)	1.36	10 (27%) 0 2	152, 171, 187, 195	0
11	L	37/37 (100%)	0.27	4 (10%) 5 9	137, 155, 186, 190	0
11	d	37/37 (100%)	0.26	4 (10%) 5 9	143, 158, 194, 201	0
12	M	34/36 (94%)	0.38	5 (14%) 2 5	147, 163, 179, 195	0
12	e	34/36 (94%)	0.45	7 (20%) 1 3	147, 159, 176, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/246 (98%)	0.84	39 (16%) 1 4	132, 162, 190, 201	0
13	f	243/246 (98%)	0.55	15 (6%) 20 20	127, 164, 191, 211	0
14	T	32/32 (100%)	0.21	0 100 100	144, 157, 187, 198	0
14	g	32/32 (100%)	0.28	3 (9%) 8 11	145, 158, 179, 198	0
15	U	97/104 (93%)	0.88	10 (10%) 6 9	136, 154, 173, 177	0
15	h	97/104 (93%)	1.74	33 (34%) 0 2	140, 154, 165, 174	0
16	V	137/137 (100%)	0.45	10 (7%) 15 16	135, 156, 170, 180	0
16	i	137/137 (100%)	0.54	11 (8%) 12 14	131, 158, 176, 185	0
17	m	28/46 (60%)	2.12	17 (60%) 0 0	167, 183, 198, 205	0
17	y	28/46 (60%)	0.46	2 (7%) 16 16	164, 182, 197, 201	0
18	X	37/40 (92%)	1.21	6 (16%) 1 4	158, 173, 188, 190	0
18	j	37/40 (92%)	0.77	3 (8%) 12 14	161, 175, 191, 202	0
19	Y	0/28	-	-	-	-
19	k	0/28	-	-	-	-
20	Z	62/62 (100%)	1.56	18 (29%) 0 2	159, 178, 198, 208	0
20	l	62/62 (100%)	0.97	5 (8%) 12 14	164, 178, 199, 208	0
All	All	5214/5482 (95%)	0.53	541 (10%) 6 9	125, 161, 185, 213	0

All (541) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	295	SER	7.7
12	M	2	GLU	6.5
16	i	132	ASN	6.3
15	U	123	GLU	6.3
2	N	393	GLU	6.1
9	b	15	THR	6.1
2	B	412	THR	5.9
2	N	388	SER	5.9
4	Q	295	SER	5.7
2	B	438	ASN	5.6
12	M	4	ASN	5.5
2	N	483	ASP	5.4
2	N	306	PRO	5.4
13	O	269	ILE	5.4
18	X	47	GLN	5.3
13	f	175	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
2	N	305	ILE	5.2
2	B	322	GLY	5.1
2	N	382	PRO	5.0
15	h	44	ASP	5.0
3	P	328	VAL	4.9
15	U	38	GLU	4.9
13	O	56	TYR	4.8
3	P	329	GLY	4.8
15	U	39	LEU	4.8
13	f	176	SER	4.8
2	N	484	PRO	4.7
17	m	29	GLY	4.7
3	P	340	TYR	4.7
13	O	176	SER	4.6
2	N	408	GLY	4.6
15	U	40	VAL	4.6
13	O	161	SER	4.6
4	D	294	ARG	4.6
3	C	137	PRO	4.5
2	B	326	ARG	4.5
11	L	37	ASN	4.5
3	P	330	SER	4.4
12	e	5	GLN	4.4
2	B	305	ILE	4.4
1	A	69	GLY	4.4
3	P	373	ASN	4.4
2	N	407	ASN	4.2
4	D	194	ASN	4.2
2	B	417	VAL	4.2
9	b	18	GLY	4.1
3	P	228	ASN	4.1
13	O	57	PRO	4.1
2	B	421	ALA	4.1
2	B	411	PHE	4.1
2	B	397	VAL	4.0
2	B	420	TYR	4.0
2	B	323	GLY	4.0
7	W	14	LEU	4.0
18	X	46	VAL	4.0
12	M	5	GLN	4.0
13	O	175	PRO	4.0
11	L	33	SER	3.9

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Mol	Chain	Res	Type	RSRZ
4	D	296	TYR	3.9
2	B	306	PRO	3.9
17	m	32	GLY	3.9
12	e	7	GLY	3.9
13	O	162	ILE	3.9
2	B	418	LYS	3.8
3	P	44	ASN	3.8
13	f	221	GLY	3.8
3	P	341	LEU	3.8
13	O	90	GLU	3.8
2	N	405	GLU	3.8
2	B	127	ARG	3.8
17	m	28	ILE	3.8
10	c	32	PHE	3.8
15	h	52	GLY	3.7
2	B	327	THR	3.7
1	A	79	THR	3.7
17	m	21	GLN	3.7
13	O	84	ASN	3.7
1	A	81	ALA	3.7
3	C	167	VAL	3.7
13	O	58	ILE	3.7
7	H	2	ALA	3.7
2	B	347	ARG	3.7
1	G	69	GLY	3.6
2	B	128	THR	3.6
13	O	235	GLY	3.6
13	O	217	SER	3.6
17	m	31	ALA	3.6
15	U	121	LEU	3.6
3	P	369	LEU	3.6
17	m	27	MET	3.6
1	G	75	ASN	3.6
4	D	297	ASP	3.6
9	b	20	GLY	3.6
15	U	124	GLY	3.6
16	i	49	GLU	3.6
1	G	81	ALA	3.5
9	b	14	ALA	3.5
3	C	27	ASP	3.5
4	Q	294	ARG	3.5
3	C	328	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
3	P	325	GLY	3.5
2	N	381	ILE	3.5
15	U	122	VAL	3.5
15	h	113	THR	3.5
20	Z	1	MET	3.5
13	f	190	LEU	3.5
2	N	343	HIS	3.5
7	W	9	ASP	3.5
9	b	17	ALA	3.5
2	N	385	ARG	3.5
3	P	146	PHE	3.5
11	L	34	TYR	3.5
13	f	216	PHE	3.5
7	W	27	THR	3.5
2	N	409	GLN	3.4
1	G	80	GLY	3.4
2	N	212	ALA	3.4
2	N	307	GLU	3.4
3	P	138	GLU	3.4
3	C	327	ASN	3.4
10	K	14	ALA	3.4
3	P	147	PHE	3.4
2	N	219	VAL	3.3
17	m	33	PRO	3.3
20	Z	4	LEU	3.3
2	B	352	GLU	3.3
2	N	394	GLN	3.3
13	O	85	LYS	3.3
4	Q	194	ASN	3.3
1	A	266	ASN	3.3
2	B	346	PHE	3.3
15	h	47	LEU	3.3
3	C	149	TYR	3.3
3	P	367	GLU	3.3
2	N	404	GLY	3.3
5	E	3	GLY	3.3
1	A	10	SER	3.3
17	m	35	ILE	3.3
2	B	348	ASN	3.3
1	G	76	ASN	3.3
16	i	78	LEU	3.3
13	O	88	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
3	P	385	GLN	3.3
13	O	268	SER	3.2
13	O	87	GLN	3.2
7	W	11	LEU	3.2
18	X	45	LYS	3.2
1	A	229	GLU	3.2
17	m	34	MET	3.2
2	B	296	ALA	3.2
2	N	380	ASP	3.2
5	E	4	THR	3.2
16	V	49	GLU	3.2
20	Z	2	THR	3.2
3	P	370	ARG	3.2
3	P	139	THR	3.2
8	I	3	THR	3.2
13	O	55	ALA	3.2
15	h	51	TYR	3.2
2	N	414	PRO	3.2
2	B	345	VAL	3.2
13	O	89	ALA	3.2
20	Z	62	VAL	3.2
2	N	403	GLY	3.1
14	g	2	GLU	3.1
17	m	26	ALA	3.1
2	B	398	THR	3.1
3	P	331	ALA	3.1
3	C	326	ALA	3.1
15	U	110	GLU	3.1
2	N	295	GLY	3.1
2	N	489	GLU	3.1
2	N	488	PRO	3.1
2	N	302	TRP	3.1
15	h	108	ASN	3.1
7	W	5	THR	3.1
2	N	410	THR	3.1
2	N	304	ALA	3.1
2	N	490	GLN	3.0
7	W	6	TRP	3.0
2	N	487	SER	3.0
3	P	326	ALA	3.0
7	H	56	ASP	3.0
13	O	216	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
15	h	115	THR	3.0
2	B	295	GLY	3.0
4	Q	282	SER	3.0
10	c	26	PRO	3.0
1	G	79	THR	3.0
3	C	332	GLN	3.0
4	Q	344	GLU	3.0
15	h	74	THR	3.0
7	W	4	ARG	3.0
1	A	75	ASN	3.0
17	m	24	MET	3.0
1	A	268	SER	3.0
7	H	57	GLY	3.0
10	c	29	PRO	3.0
13	O	160	THR	3.0
3	P	324	LEU	3.0
16	i	131	ARG	3.0
1	G	10	SER	2.9
2	N	136	PRO	2.9
10	c	23	ASP	2.9
4	D	227	GLU	2.9
3	C	449	ARG	2.9
3	P	315	MET	2.9
7	W	13	PRO	2.9
3	P	116	VAL	2.9
1	A	298	ASN	2.9
20	Z	57	LEU	2.9
1	G	171	GLY	2.9
13	O	86	ARG	2.9
13	O	82	PRO	2.9
3	P	351	PHE	2.9
7	W	10	ILE	2.9
9	b	26	GLY	2.9
2	B	413	ASP	2.9
2	N	402	TYR	2.9
16	i	47	LEU	2.9
20	Z	17	PHE	2.9
2	N	294	SER	2.9
3	P	342	MET	2.9
2	B	382	PRO	2.9
2	B	396	GLY	2.9
15	h	69	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	132	ILE	2.9
2	B	350	GLU	2.8
4	D	140	PRO	2.8
4	D	190	ASN	2.8
13	O	244	GLU	2.8
13	O	243	SER	2.8
13	f	191	ALA	2.8
2	N	368	VAL	2.8
13	O	236	GLU	2.8
1	A	177	SER	2.8
16	i	158	GLY	2.8
1	A	80	GLY	2.8
2	B	444	ARG	2.8
2	N	204	ALA	2.8
3	P	27	ASP	2.8
2	B	353	GLU	2.8
3	P	365	TRP	2.8
1	A	178	GLY	2.8
3	P	362	ARG	2.8
3	P	137	PRO	2.8
13	O	207	GLU	2.8
7	H	6	TRP	2.8
1	A	254	TYR	2.8
16	i	77	SER	2.7
12	M	3	VAL	2.7
20	l	23	VAL	2.7
2	B	388	SER	2.7
3	P	142	GLU	2.7
2	B	491	VAL	2.7
15	h	55	ILE	2.7
20	Z	6	GLN	2.7
15	h	54	LYS	2.7
3	P	388	GLN	2.7
2	B	304	ALA	2.7
2	B	126	PRO	2.7
2	N	232	GLY	2.7
3	C	164	HIS	2.7
3	P	363	GLY	2.7
16	V	78	LEU	2.7
2	B	410	THR	2.7
20	Z	3	ILE	2.7
2	B	416	THR	2.7

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Mol	Chain	Res	Type	RSRZ
12	e	1	MET	2.7
13	f	217	SER	2.7
3	P	140	LEU	2.7
1	G	179	THR	2.7
2	B	351	GLY	2.7
6	F	44	GLN	2.7
2	B	354	LEU	2.7
2	N	391	SER	2.7
7	W	30	LEU	2.7
12	e	4	ASN	2.7
2	N	392	PHE	2.7
4	D	59	TYR	2.7
1	G	173	PRO	2.7
10	c	24	VAL	2.7
2	N	435	GLU	2.7
3	P	210	PHE	2.7
1	A	175	GLY	2.7
2	B	414	PRO	2.7
2	N	398	THR	2.7
2	B	439	SER	2.7
1	G	43	ALA	2.7
15	U	120	ALA	2.7
2	B	307	GLU	2.7
15	h	75	LEU	2.6
2	N	386	ALA	2.6
3	P	145	SER	2.6
13	f	153	ALA	2.6
3	P	368	PRO	2.6
4	D	193	LEU	2.6
3	P	372	PRO	2.6
3	C	148	GLY	2.6
1	A	267	ASN	2.6
3	P	180	MET	2.6
11	d	33	SER	2.6
3	P	349	ILE	2.6
13	f	220	LYS	2.6
1	A	179	THR	2.6
7	H	3	ARG	2.6
2	N	412	THR	2.6
17	m	19	ILE	2.6
1	A	247	ASN	2.6
1	A	16	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	P	295	THR	2.6
7	H	4	ARG	2.6
13	O	68	ARG	2.6
15	h	101	GLN	2.6
4	D	197	HIS	2.6
4	D	313	THR	2.6
2	N	340	TRP	2.6
1	A	222	SER	2.6
3	P	211	GLY	2.6
15	h	56	ASP	2.6
3	P	213	LEU	2.6
3	P	45	LEU	2.6
3	P	375	LEU	2.6
11	d	37	ASN	2.6
2	B	392	PHE	2.5
11	L	2	GLU	2.5
12	e	2	GLU	2.5
20	l	17	PHE	2.5
15	h	60	THR	2.5
17	m	23	THR	2.5
20	l	20	VAL	2.5
4	Q	197	HIS	2.5
20	Z	8	ALA	2.5
16	i	111	GLU	2.5
4	D	292	ASN	2.5
4	Q	342	PRO	2.5
2	N	322	GLY	2.5
15	h	68	TYR	2.5
1	G	68	SER	2.5
7	W	29	PRO	2.5
3	P	321	ASP	2.5
11	d	36	PHE	2.5
4	D	195	PRO	2.5
13	f	207	GLU	2.5
7	W	8	GLY	2.5
3	P	62	PHE	2.5
3	P	209	ILE	2.5
4	D	241	GLU	2.5
13	O	67	ALA	2.5
2	N	387	GLU	2.5
7	W	35	MET	2.5
17	m	30	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
9	b	16	VAL	2.4
13	f	222	GLN	2.4
3	P	371	GLY	2.4
7	W	7	LEU	2.4
15	h	43	VAL	2.4
2	B	297	THR	2.4
1	A	190	HIS	2.4
10	c	20	PRO	2.4
14	g	1	MET	2.4
12	M	7	GLY	2.4
15	h	70	GLY	2.4
20	Z	5	PHE	2.4
4	D	239	GLN	2.4
13	O	46	PRO	2.4
3	P	208	VAL	2.4
14	g	3	THR	2.4
3	P	126	GLY	2.4
7	H	55	LEU	2.4
10	c	28	ILE	2.4
16	i	159	GLY	2.4
4	D	198	MET	2.4
2	N	406	LEU	2.4
2	N	438	ASN	2.4
16	V	77	SER	2.4
9	b	19	MET	2.4
13	O	234	THR	2.4
3	P	332	GLN	2.4
15	h	41	ASN	2.4
17	y	45	ASN	2.3
3	C	268	GLY	2.3
3	P	117	VAL	2.3
20	Z	61	VAL	2.3
13	O	218	LEU	2.3
2	N	211	ILE	2.3
3	P	374	GLY	2.3
20	Z	43	GLY	2.3
3	P	78	GLU	2.3
3	P	174	LEU	2.3
4	Q	191	TRP	2.3
13	O	64	TYR	2.3
1	G	175	GLY	2.3
2	N	68	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
12	e	34	LYS	2.3
15	h	46	LYS	2.3
3	P	296	VAL	2.3
13	O	270	GLU	2.3
20	Z	7	LEU	2.3
3	C	400	PRO	2.3
3	P	350	ILE	2.3
2	B	405	GLU	2.3
1	A	11	ALA	2.3
4	D	142	ASN	2.3
16	i	51	GLN	2.3
13	O	91	PHE	2.3
1	G	61	ASP	2.3
15	h	97	LEU	2.3
7	W	15	ASN	2.3
16	V	48	THR	2.3
10	c	25	LEU	2.3
1	A	258	LEU	2.2
20	l	21	ILE	2.2
10	c	19	ASP	2.2
16	i	48	THR	2.2
2	B	472	ARG	2.2
3	C	470	PRO	2.2
2	B	187	PRO	2.2
3	C	453	ALA	2.2
3	C	135	ARG	2.2
2	N	418	LYS	2.2
2	B	325	PHE	2.2
2	N	485	GLU	2.2
3	P	389	GLU	2.2
1	A	12	ASN	2.2
1	A	70	SER	2.2
4	D	192	THR	2.2
2	N	299	GLU	2.2
4	Q	313	THR	2.2
2	B	309	LEU	2.2
2	N	70	GLY	2.2
4	D	130	PHE	2.2
16	V	37	PRO	2.2
1	G	198	HIS	2.2
13	f	35	ASP	2.2
13	O	232	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
17	m	36	ILE	2.2
10	K	13	GLU	2.2
1	A	27	ARG	2.2
3	C	147	PHE	2.2
1	A	230	THR	2.2
1	G	11	ALA	2.2
4	D	264	LYS	2.2
3	P	318	LEU	2.2
10	K	12	PRO	2.2
13	O	271	PRO	2.2
15	h	111	HIS	2.2
17	m	20	ALA	2.2
4	Q	200	GLY	2.2
16	V	47	LEU	2.2
15	h	116	GLU	2.2
18	X	44	ASP	2.2
12	e	3	VAL	2.2
3	P	212	TYR	2.2
1	A	74	GLY	2.2
3	P	229	ASN	2.2
3	P	361	PHE	2.2
2	B	44	THR	2.2
2	N	303	SER	2.2
15	h	59	ASN	2.2
2	N	482	ILE	2.2
2	N	215	PHE	2.1
2	B	332	LYS	2.1
3	C	121	SER	2.1
20	Z	53	VAL	2.1
15	U	119	THR	2.1
15	h	53	GLU	2.1
20	Z	27	TYR	2.1
1	G	189	GLU	2.1
3	P	114	VAL	2.1
2	B	381	ILE	2.1
13	f	34	ASP	2.1
15	h	67	GLN	2.1
2	N	491	VAL	2.1
18	j	42	GLN	2.1
2	N	326	ARG	2.1
16	V	50	LYS	2.1
2	N	283	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	293	ALA	2.1
13	O	233	ARG	2.1
13	O	66	ILE	2.1
20	Z	38	GLN	2.1
3	C	151	TRP	2.1
3	P	202	PRO	2.1
3	P	227	VAL	2.1
15	h	106	ARG	2.1
20	l	44	SER	2.1
17	m	25	ILE	2.1
1	G	56	PRO	2.1
4	D	300	SER	2.1
2	B	368	VAL	2.1
2	B	287	ARG	2.1
16	V	45	ILE	2.1
3	C	473	ASP	2.1
4	D	129	GLN	2.1
15	h	112	PHE	2.1
2	B	435	GLU	2.1
2	N	218	LEU	2.1
2	N	421	ALA	2.1
15	h	92	LEU	2.1
4	D	298	PHE	2.1
18	j	11	THR	2.1
10	c	31	LEU	2.1
2	B	395	GLN	2.1
11	d	32	SER	2.1
7	W	2	ALA	2.1
4	Q	192	THR	2.1
2	B	409	GLN	2.1
2	N	296	ALA	2.1
3	C	265	ILE	2.1
5	E	50	PRO	2.0
3	P	141	GLU	2.0
13	f	173	ASN	2.0
3	P	339	LYS	2.0
15	h	120	ALA	2.0
13	O	177	TYR	2.0
3	P	207	ARG	2.0
3	P	112	PHE	2.0
4	Q	300	SER	2.0
3	C	409	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	P	179	ALA	2.0
13	f	32	THR	2.0
15	h	82	ASN	2.0
3	P	144	SER	2.0
15	h	57	LEU	2.0
16	V	40	SER	2.0
4	Q	296	TYR	2.0
20	Z	58	ASN	2.0
20	Z	56	VAL	2.0
1	G	226	GLU	2.0
1	G	74	GLY	2.0
3	C	325	GLY	2.0
17	y	31	ALA	2.0
1	A	76	ASN	2.0
16	V	36	VAL	2.0
18	X	20	PHE	2.0
18	j	34	PHE	2.0
18	X	32	LEU	2.0
1	A	173	PRO	2.0
2	N	137	LYS	2.0
15	h	124	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CA	O	301	1/1	0.05	0.78	138,138,138,138	0
23	PL9	b	101	35/55	0.28	0.47	168,188,199,208	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	CA	f	301	1/1	0.28	0.81	210,210,210,210	0
27	LMG	C	520	45/55	0.29	1.14	164,178,186,187	0
31	LMT	I	103	35/35	0.31	1.02	153,189,201,206	0
31	LMT	Q	410	31/35	0.39	0.73	165,182,193,197	0
30	BCR	a	101	40/40	0.39	0.56	139,159,176,181	0
30	BCR	c	101	40/40	0.40	1.10	151,171,188,190	0
27	LMG	P	521	45/55	0.43	1.10	149,175,191,198	0
31	LMT	N	624	35/35	0.44	0.92	166,201,210,213	0
21	CLA	N	605	65/65	0.46	0.79	170,189,202,205	0
23	PL9	J	101	35/55	0.46	0.49	177,190,200,204	0
30	BCR	I	101	40/40	0.47	0.54	143,155,171,183	0
31	LMT	a	103	35/35	0.48	0.86	169,180,206,216	0
30	BCR	T	103	40/40	0.49	0.88	155,168,181,184	0
21	CLA	B	601	65/65	0.49	1.00	167,188,199,203	0
30	BCR	J	102	40/40	0.50	0.47	167,182,207,208	0
31	LMT	B	625	35/35	0.50	0.89	163,196,218,227	0
31	LMT	N	603	35/35	0.53	0.61	153,179,189,190	0
27	LMG	D	412	42/55	0.53	0.42	147,178,195,199	0
31	LMT	D	409	31/35	0.56	1.06	162,187,202,208	0
31	LMT	B	629	35/35	0.57	0.74	153,166,181,185	0
24	DGD	D	408	63/66	0.58	0.78	167,181,198,212	0
31	LMT	N	625	35/35	0.59	0.87	165,184,206,216	0
25	LHG	G	412	37/49	0.59	0.52	147,176,193,204	0
31	LMT	N	604	35/35	0.59	0.51	145,180,209,212	0
27	LMG	I	102	43/55	0.60	0.79	152,184,203,207	0
30	BCR	B	620	40/40	0.61	0.76	161,168,186,196	0
27	LMG	Q	401	42/55	0.61	0.65	131,168,174,183	0
30	BCR	H	101	40/40	0.62	0.96	165,178,188,190	0
21	CLA	N	608	65/65	0.63	0.59	146,158,176,191	0
26	SQD	A	414	54/54	0.63	0.57	139,173,190,200	0
30	BCR	b	102	40/40	0.63	0.54	158,178,202,203	0
26	SQD	Q	408	43/54	0.64	0.59	143,180,193,194	0
31	LMT	e	101	35/35	0.65	0.52	164,176,191,195	0
21	CLA	P	502	65/65	0.65	0.87	146,161,175,182	0
30	BCR	D	405	40/40	0.65	0.69	145,161,176,179	0
31	LMT	B	630	35/35	0.65	0.53	157,169,199,220	0
21	CLA	N	620	65/65	0.65	0.79	156,175,192,194	0
21	CLA	C	513	65/65	0.66	1.15	173,193,206,213	0
27	LMG	R	102	44/55	0.67	0.42	161,177,189,192	0
21	CLA	P	513	65/65	0.67	1.02	168,182,207,216	0
24	DGD	Q	409	63/66	0.67	0.54	157,183,208,238	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	C	502	65/65	0.68	0.51	142,157,179,185	0
21	CLA	N	609	65/65	0.68	0.68	148,165,174,178	0
21	CLA	C	507	65/65	0.68	0.82	159,172,185,187	0
21	CLA	C	505	65/65	0.68	0.50	147,172,186,188	0
26	SQD	B	627	47/54	0.68	0.41	143,179,209,227	0
26	SQD	B	624	43/54	0.68	0.45	150,181,199,206	0
21	CLA	A	403	65/65	0.68	0.40	142,161,183,185	0
21	CLA	D	401	65/65	0.68	0.42	137,149,176,181	0
31	LMT	M	102	35/35	0.69	0.59	134,165,196,205	0
21	CLA	B	604	65/65	0.69	0.69	148,158,172,182	0
21	CLA	N	607	65/65	0.69	0.71	133,163,170,175	0
27	LMG	C	519	48/55	0.69	0.39	132,169,183,188	0
30	BCR	P	516	40/40	0.69	0.85	164,173,180,187	0
25	LHG	A	411	37/49	0.69	0.41	156,178,214,232	0
21	CLA	N	610	65/65	0.70	0.77	152,178,191,194	0
21	CLA	G	406	65/65	0.70	0.61	145,159,181,186	0
31	LMT	B	626	35/35	0.70	0.41	163,194,202,213	0
21	CLA	C	509	65/65	0.70	0.80	145,170,180,183	0
26	SQD	N	601	47/54	0.70	0.44	141,176,198,202	0
33	CL	D	411	1/1	0.71	0.86	121,121,121,121	0
30	BCR	B	618	40/40	0.71	0.30	149,162,168,169	0
24	DGD	C	518	66/66	0.71	0.34	139,157,179,185	0
22	PHO	D	402	64/64	0.72	0.49	135,155,161,168	0
23	PL9	G	407	45/55	0.72	0.44	148,160,183,188	0
27	LMG	a	102	43/55	0.72	0.64	160,179,196,200	0
21	CLA	P	511	65/65	0.72	1.03	156,174,184,187	0
30	BCR	P	514	40/40	0.72	1.53	139,152,173,175	0
24	DGD	B	628	52/66	0.73	0.47	148,173,194,200	0
22	PHO	A	404	64/64	0.73	0.32	129,151,167,177	0
21	CLA	C	503	65/65	0.74	0.54	155,171,181,183	0
30	BCR	T	101	40/40	0.74	0.29	144,167,181,184	0
24	DGD	N	602	52/66	0.74	0.46	154,176,204,206	0
27	LMG	B	623	49/55	0.74	0.36	128,147,164,167	0
24	DGD	B	621	58/66	0.74	0.49	142,158,168,171	0
24	DGD	G	408	56/66	0.74	0.42	163,179,188,193	0
21	CLA	G	404	65/65	0.74	0.36	141,159,179,181	0
21	CLA	P	509	65/65	0.75	0.84	152,174,181,184	0
22	PHO	G	405	64/64	0.75	0.37	131,149,159,162	0
21	CLA	B	605	65/65	0.75	0.76	156,167,176,179	0
21	CLA	A	405	65/65	0.75	0.51	144,155,176,187	0
30	BCR	C	514	40/40	0.75	0.84	153,160,171,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	CLA	N	619	65/65	0.75	0.86	158,180,190,193	0
30	BCR	B	617	40/40	0.75	0.28	151,158,176,180	0
24	DGD	A	407	56/66	0.75	0.35	147,171,188,195	0
21	CLA	C	512	65/65	0.76	1.23	173,183,196,199	0
30	BCR	K	101	40/40	0.76	0.81	154,167,176,181	0
21	CLA	N	613	65/65	0.76	0.78	160,170,177,182	0
21	CLA	P	507	65/65	0.76	0.66	162,172,191,194	0
21	CLA	C	501	65/65	0.76	0.55	160,174,184,185	0
26	SQD	F	101	45/54	0.77	0.61	157,176,196,198	0
27	LMG	E	102	44/55	0.77	0.44	168,188,198,203	0
26	SQD	G	410	51/54	0.77	0.39	161,172,184,190	0
21	CLA	Q	402	65/65	0.77	0.50	136,144,158,169	0
21	CLA	C	506	65/65	0.78	0.45	159,175,202,211	0
27	LMG	B	622	49/55	0.78	0.36	148,163,174,176	0
24	DGD	C	517	62/66	0.78	0.35	145,169,193,200	0
21	CLA	B	607	65/65	0.78	0.30	135,152,161,165	0
21	CLA	P	503	65/65	0.78	1.06	144,174,187,195	0
21	CLA	N	616	65/65	0.78	0.57	156,167,181,184	0
30	BCR	W	101	40/40	0.78	0.79	164,176,182,186	0
30	BCR	B	619	40/40	0.79	0.25	140,156,169,178	0
27	LMG	P	520	48/55	0.79	0.58	147,168,177,184	0
30	BCR	C	515	40/40	0.79	0.66	139,164,177,180	0
21	CLA	B	608	65/65	0.79	0.72	147,165,180,186	0
21	CLA	C	511	65/65	0.79	0.47	155,172,181,184	0
21	CLA	G	403	65/65	0.79	0.32	123,139,149,162	0
30	BCR	N	621	40/40	0.79	0.21	132,154,165,172	0
26	SQD	G	401	54/54	0.80	0.37	158,176,209,210	0
26	SQD	A	409	51/54	0.80	0.35	156,178,191,194	0
21	CLA	B	615	65/65	0.80	0.67	162,178,191,194	0
21	CLA	N	614	65/65	0.80	0.75	150,162,173,178	0
23	PL9	Q	405	55/55	0.80	0.22	137,146,166,170	0
21	CLA	B	612	65/65	0.80	0.55	152,163,174,176	0
30	BCR	T	102	40/40	0.80	0.30	143,167,176,178	0
22	PHO	Q	403	64/64	0.80	0.37	144,155,164,168	0
21	CLA	B	616	65/65	0.80	0.46	155,166,199,214	0
21	CLA	Q	404	65/65	0.81	0.60	152,162,187,194	0
21	CLA	P	501	65/65	0.81	0.96	149,170,185,188	0
21	CLA	P	512	65/65	0.81	1.30	172,184,194,199	0
34	HEM	V	201	43/43	0.81	0.43	139,151,166,173	0
21	CLA	A	402	65/65	0.81	0.25	139,147,158,164	0
27	LMG	Q	407	48/55	0.82	0.25	142,156,168,176	0
21	CLA	B	603	65/65	0.82	1.03	147,166,178,179	0

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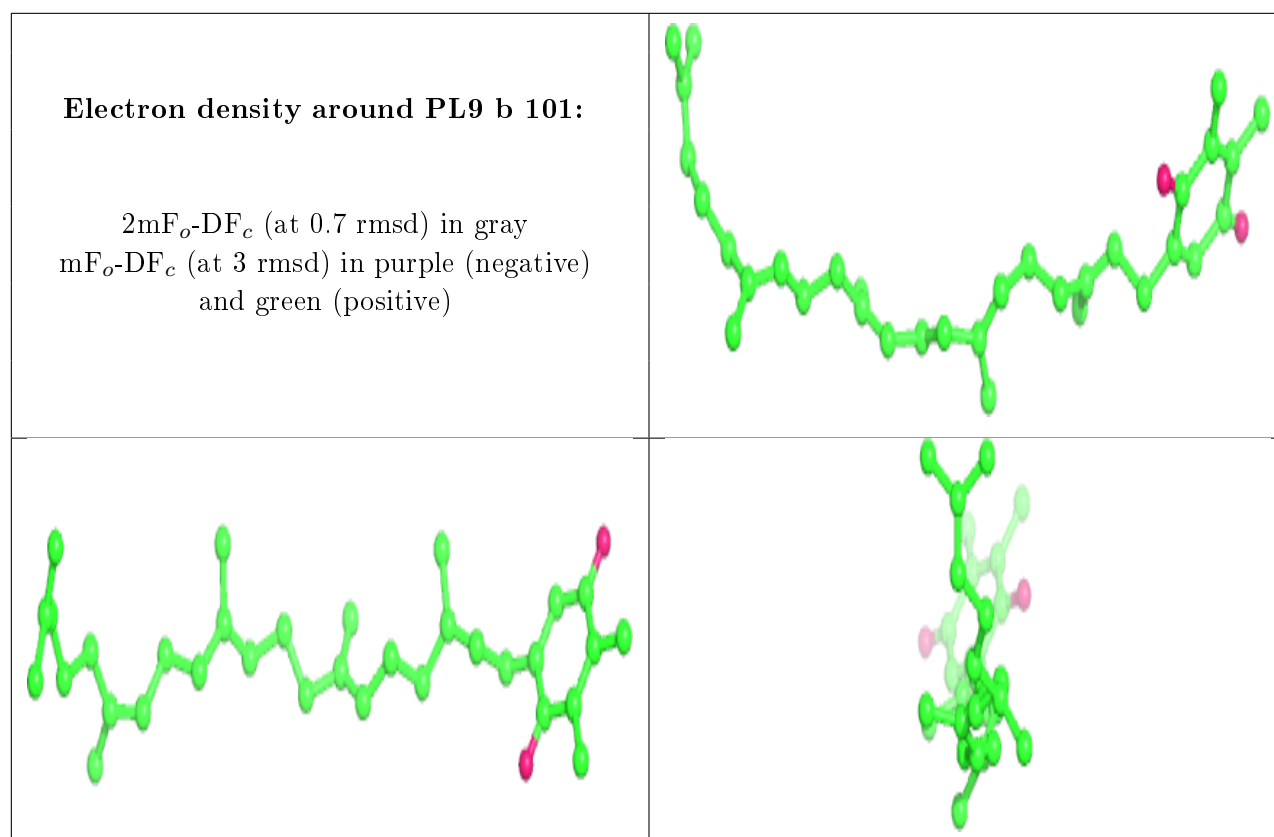
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LMG	N	623	49/55	0.82	0.27	139,152,164,171	0
26	SQD	S	102	45/54	0.82	0.58	160,188,201,203	0
27	LMG	D	407	48/55	0.82	0.32	145,159,169,175	0
21	CLA	B	610	65/65	0.82	0.58	146,163,174,176	0
21	CLA	P	505	65/65	0.82	0.37	134,164,180,183	0
21	CLA	B	606	65/65	0.82	0.55	156,173,194,204	0
21	CLA	B	609	65/65	0.82	0.79	162,177,185,186	0
21	CLA	P	510	65/65	0.82	0.69	145,161,170,178	0
21	CLA	B	614	65/65	0.83	0.28	157,172,181,184	0
24	DGD	C	516	53/66	0.83	0.34	141,158,168,170	0
21	CLA	P	504	65/65	0.83	0.46	155,169,181,186	0
24	DGD	P	519	66/66	0.83	0.32	142,157,177,186	0
24	DGD	P	518	62/66	0.83	0.44	144,168,195,200	0
21	CLA	D	403	65/65	0.83	0.89	153,160,181,189	0
34	HEM	i	201	43/43	0.83	0.49	131,158,169,172	0
25	LHG	A	408	39/49	0.83	0.35	146,167,179,179	0
24	DGD	W	102	58/66	0.84	0.34	145,157,168,172	0
21	CLA	G	402	65/65	0.84	0.43	136,148,155,166	0
30	BCR	P	515	40/40	0.84	1.38	165,176,185,189	0
30	BCR	S	101	40/40	0.84	0.63	145,159,176,178	0
27	LMG	M	101	42/55	0.84	0.32	166,174,184,188	0
27	LMG	Q	406	46/55	0.84	0.41	135,162,171,180	0
21	CLA	P	506	65/65	0.84	0.43	159,176,194,202	0
21	CLA	N	612	65/65	0.84	0.50	151,164,181,190	0
27	LMG	G	411	51/55	0.85	0.24	152,164,177,178	0
21	CLA	B	602	65/65	0.85	0.72	152,172,182,185	0
21	CLA	N	618	65/65	0.85	0.31	153,171,180,185	0
34	HEM	E	101	43/43	0.85	0.36	166,179,188,190	0
21	CLA	C	504	65/65	0.85	0.29	153,172,198,204	0
30	BCR	Z	101	40/40	0.85	1.17	163,178,192,197	0
27	LMG	e	102	42/55	0.85	0.30	155,166,183,191	0
24	DGD	P	517	53/66	0.85	0.33	141,160,173,176	0
21	CLA	A	401	65/65	0.86	0.27	138,146,156,160	0
23	PL9	D	404	55/55	0.86	0.23	129,150,158,160	0
21	CLA	N	606	65/65	0.86	0.37	152,172,178,182	0
33	CL	G	415	1/1	0.86	0.89	122,122,122,122	0
32	BCT	D	410	4/4	0.87	0.35	166,167,167,169	0
27	LMG	A	410	51/55	0.87	0.30	138,157,168,171	0
23	PL9	A	406	45/55	0.88	0.51	152,174,185,188	0
21	CLA	N	611	65/65	0.88	0.29	145,156,164,166	0
25	LHG	G	409	39/49	0.88	0.39	156,168,188,191	0
27	LMG	N	622	49/55	0.88	0.28	145,154,172,174	0

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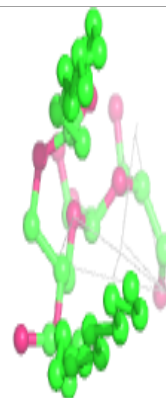
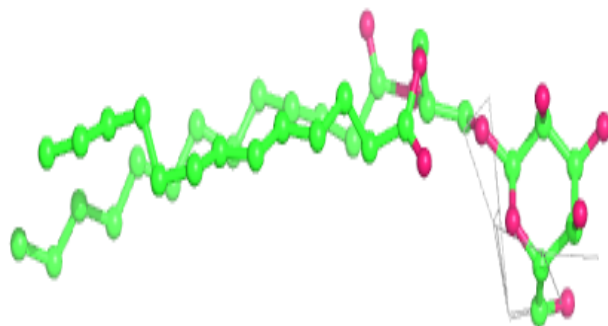
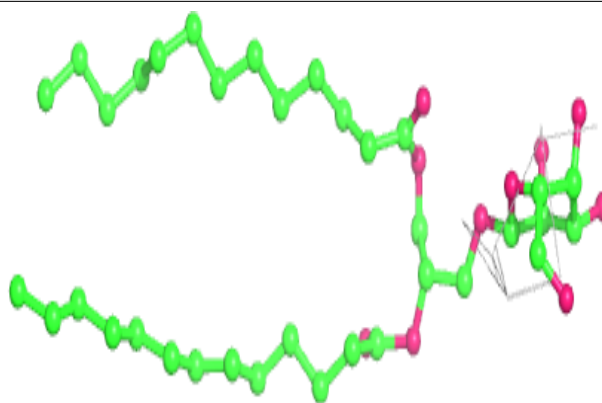
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
21	CLA	N	615	65/65	0.88	0.30	152,158,168,173	0
21	CLA	B	613	65/65	0.88	0.30	148,160,171,175	0
32	BCT	Q	411	4/4	0.89	0.41	164,166,168,173	0
27	LMG	D	406	46/55	0.89	0.36	140,153,176,181	0
21	CLA	N	617	65/65	0.89	0.29	149,168,182,188	0
21	CLA	C	510	65/65	0.89	0.28	149,161,171,178	0
29	FE2	A	413	1/1	0.89	0.17	166,166,166,166	0
21	CLA	B	611	65/65	0.89	0.32	149,160,167,169	0
21	CLA	P	508	65/65	0.89	0.43	157,168,182,193	0
28	OEC	G	413	5/9	0.90	0.47	91,102,115,124	0
34	HEM	R	101	43/43	0.90	0.50	164,184,192,199	0
21	CLA	C	508	65/65	0.90	0.34	154,170,194,203	0
29	FE2	G	414	1/1	0.92	0.16	149,149,149,149	0
28	OEC	A	412	5/9	0.96	0.47	122,122,126,129	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.

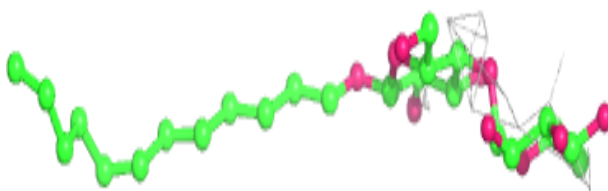
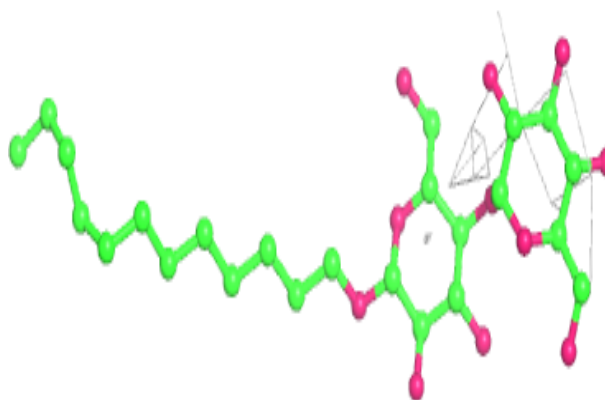


Electron density around LMG C 520:

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

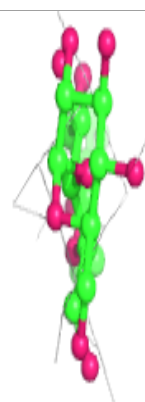
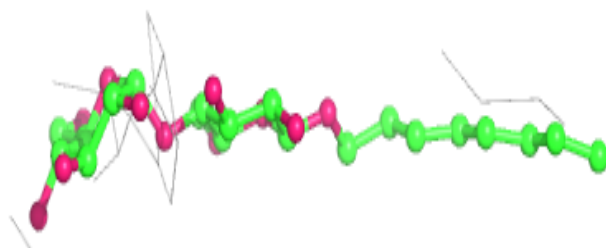
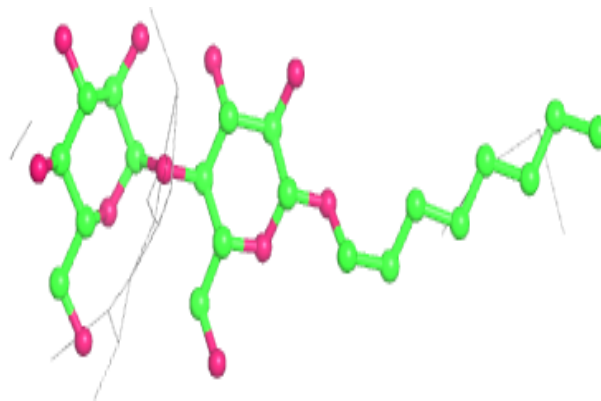
**Electron density around LMT I 103:**

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

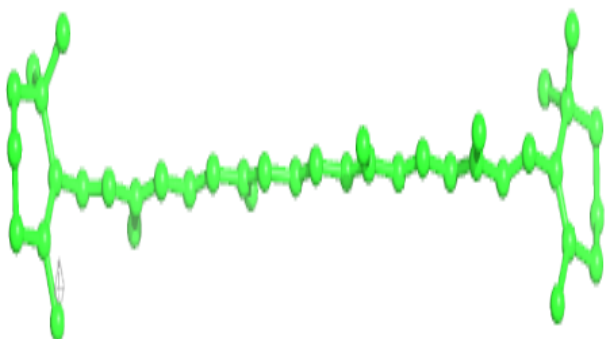
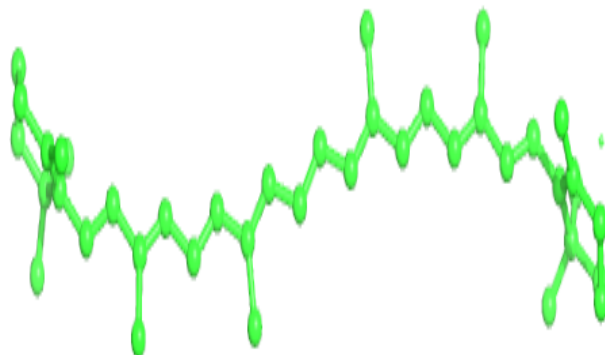


Electron density around LMT Q 410:

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

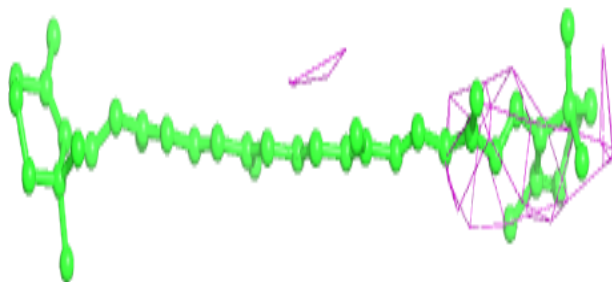
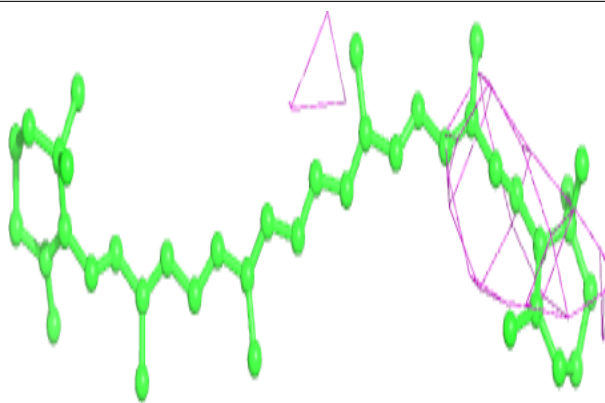
**Electron density around BCR a 101:**

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

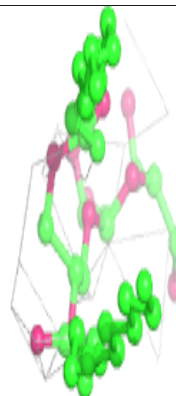
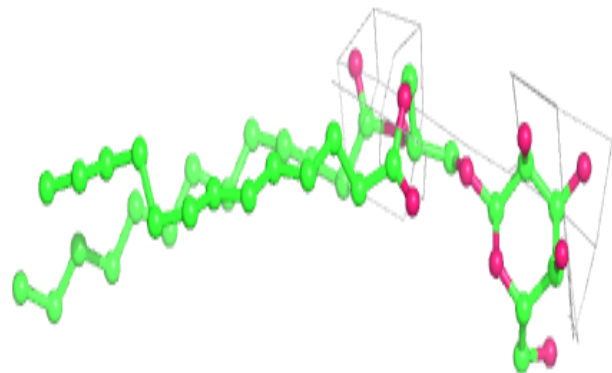
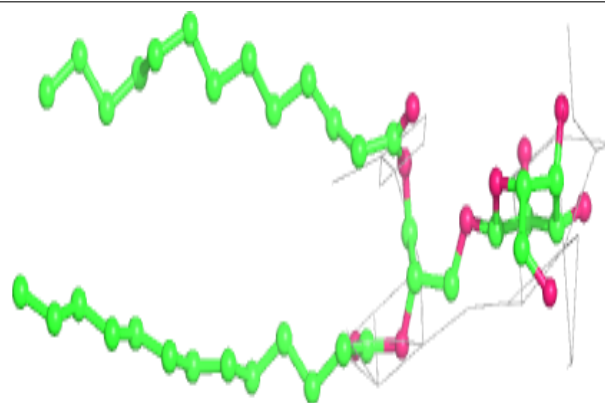


Electron density around BCR c 101:

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

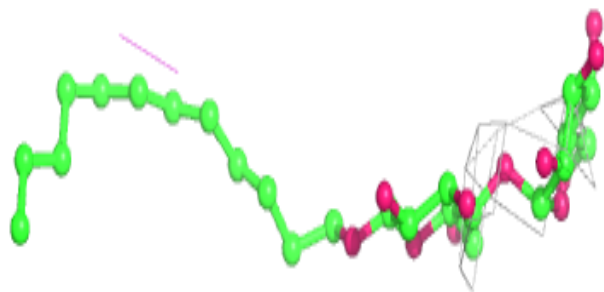
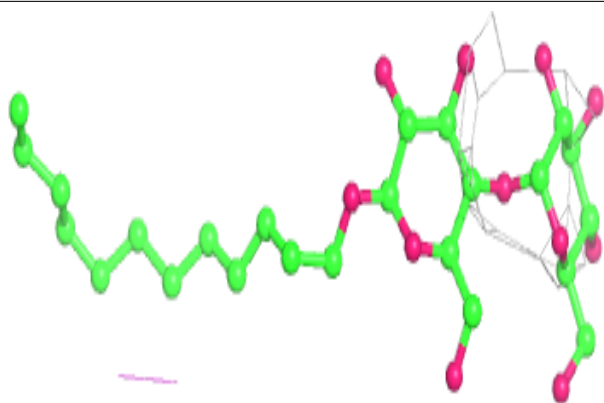
**Electron density around LMG P 521:**

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



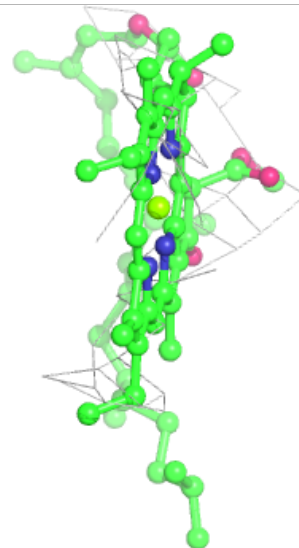
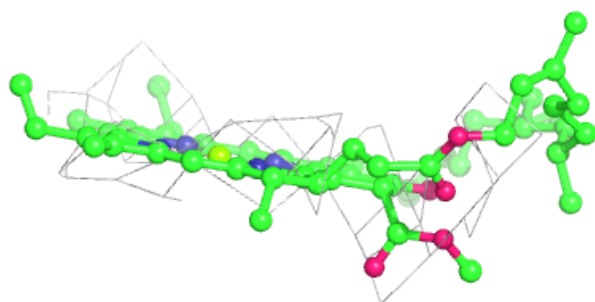
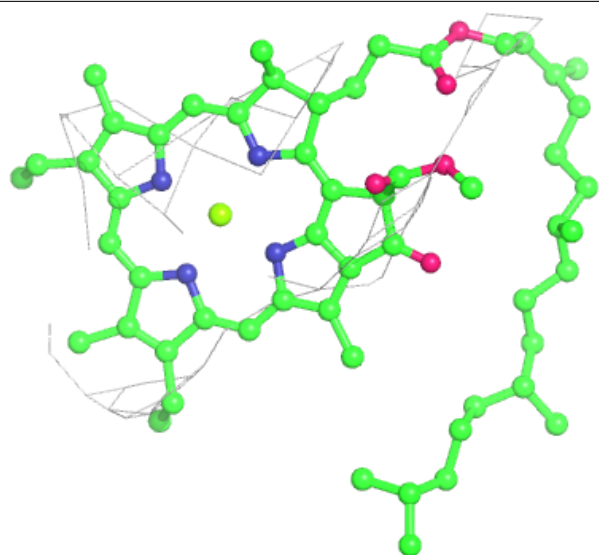
Electron density around LMT N 624:

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



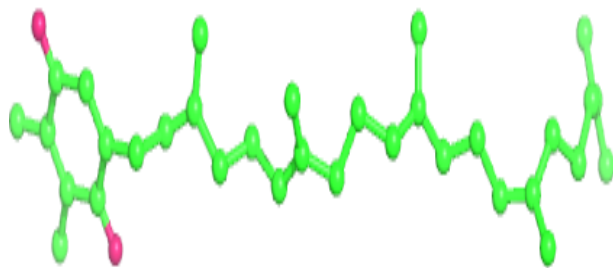
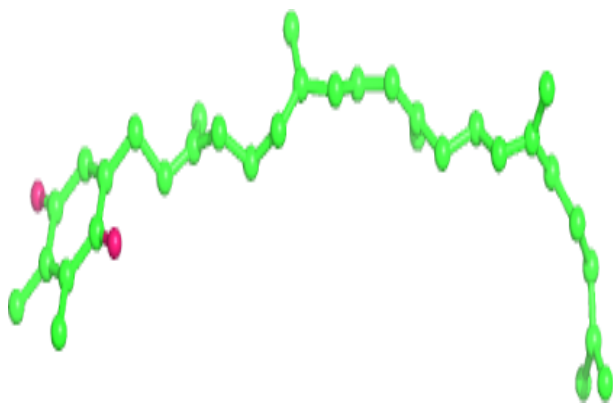
Electron density around CLA N 605:

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

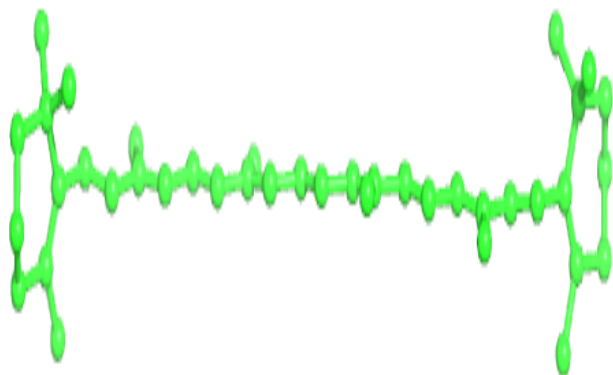
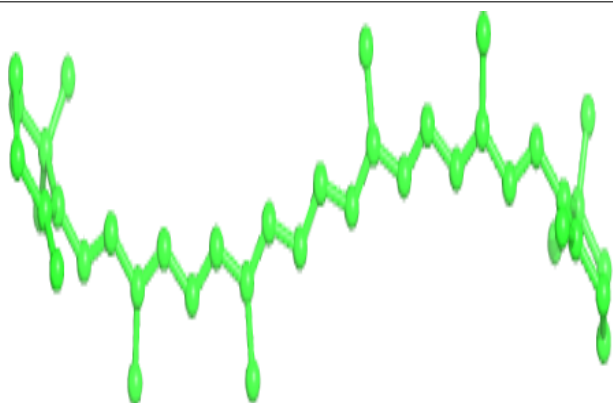


Electron density around PL9 J 101:

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

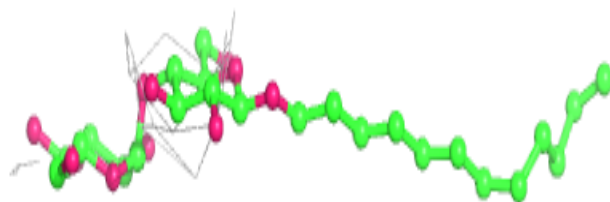
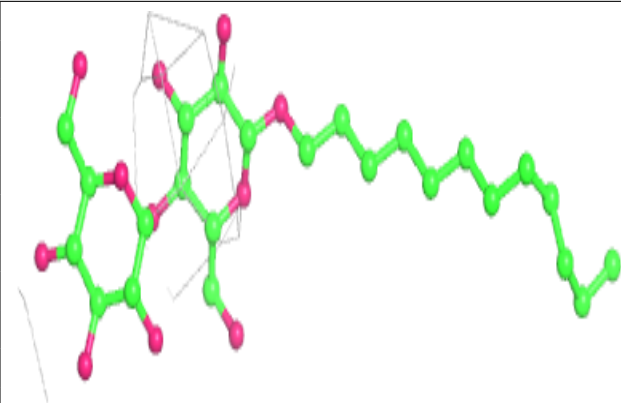
**Electron density around BCR I 101:**

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

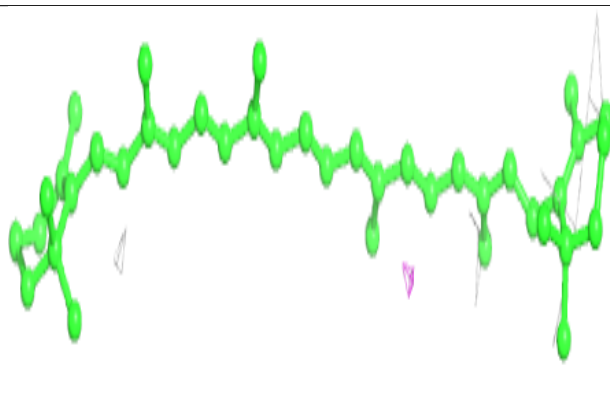
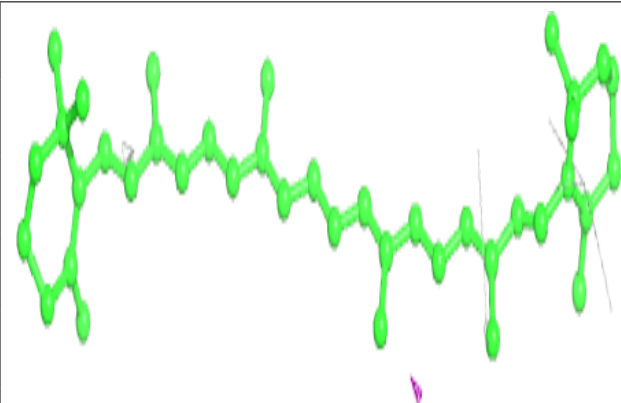


Electron density around LMT a 103:

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

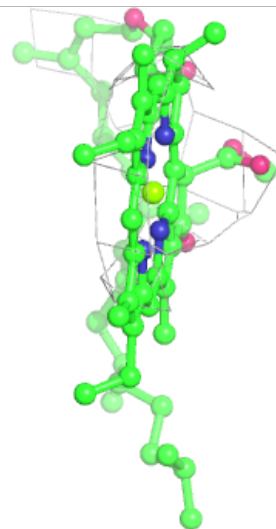
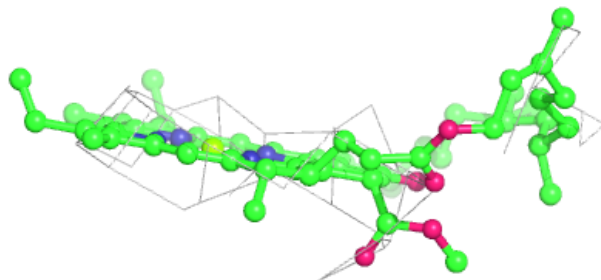
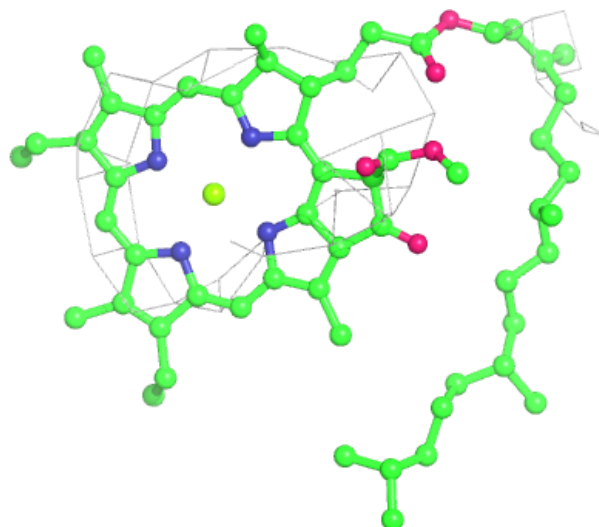
**Electron density around BCR T 103:**

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



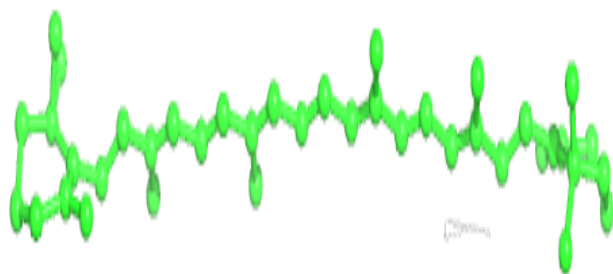
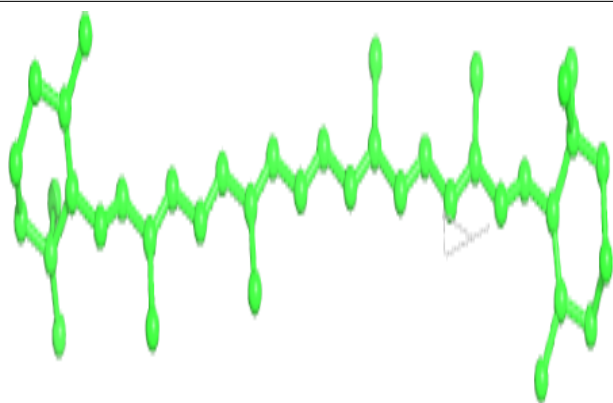
Electron density around CLA B 601:

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

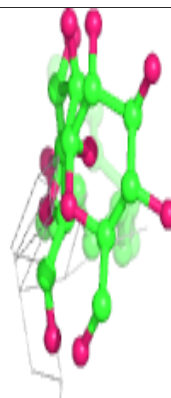
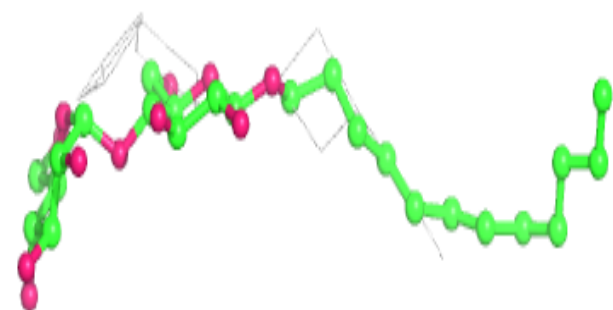
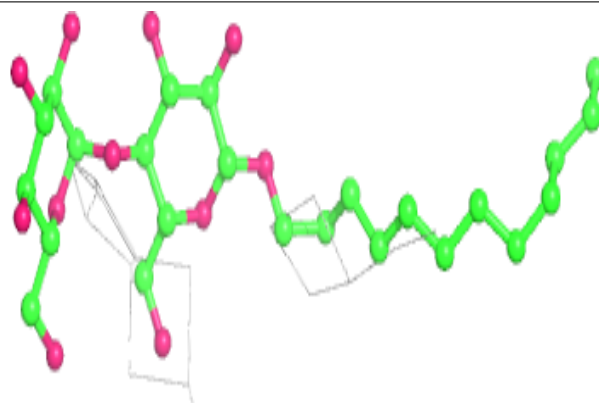


Electron density around BCR J 102:

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

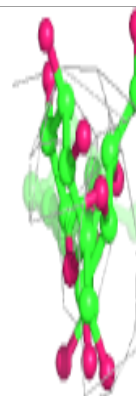
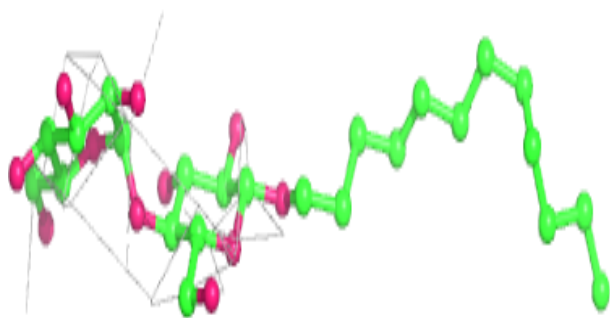
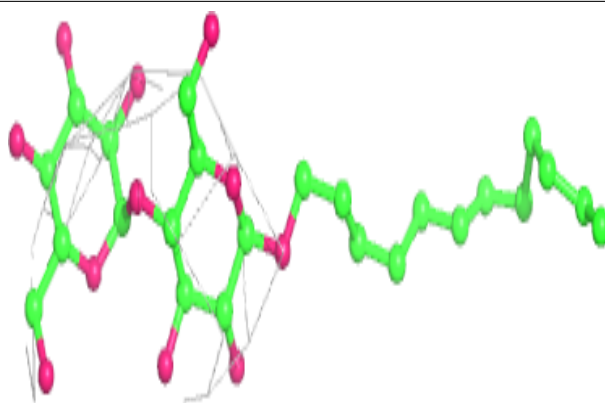
**Electron density around LMT B 625:**

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

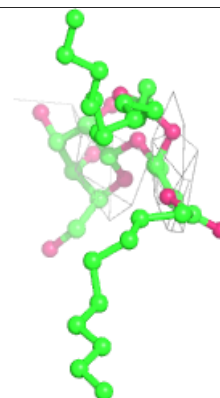
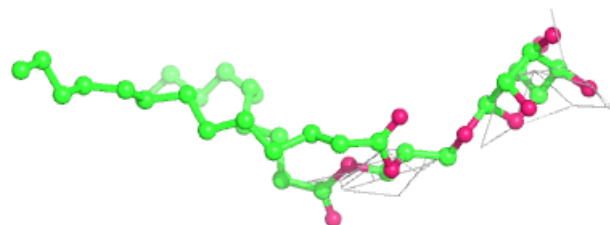
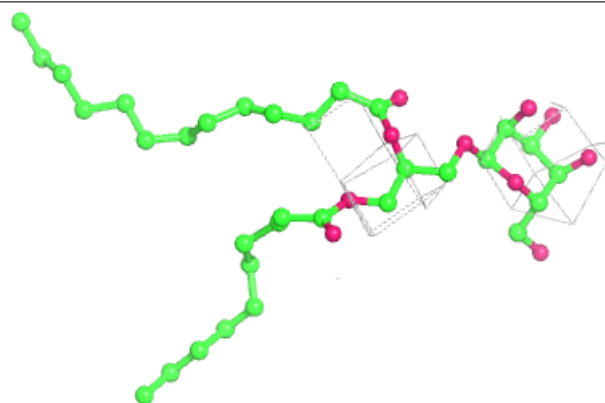


Electron density around LMT N 603:

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

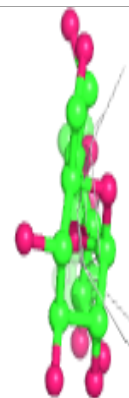
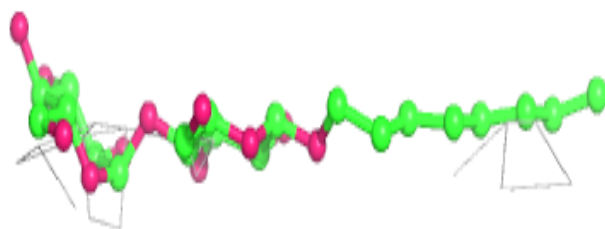
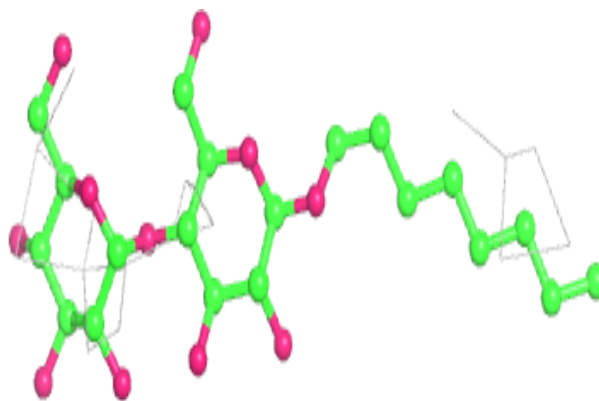
**Electron density around LMG D 412:**

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

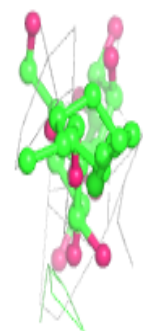
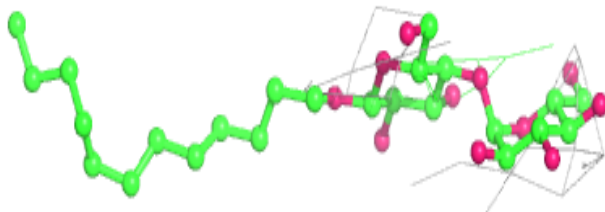
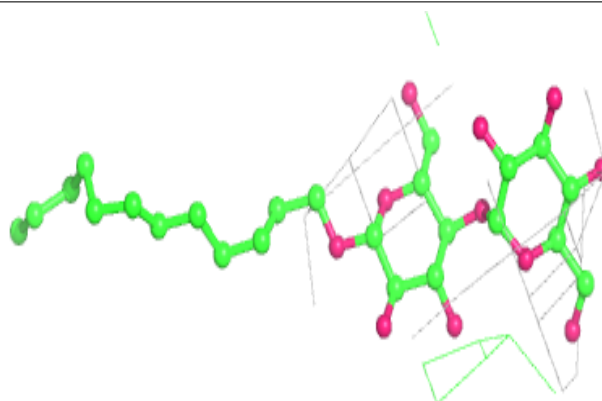


Electron density around LMT D 409:

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

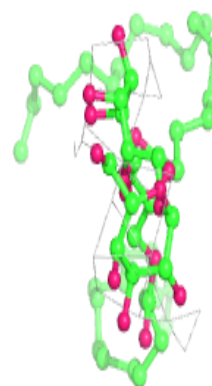
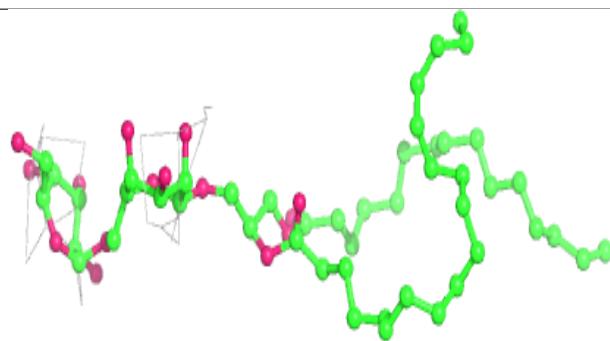
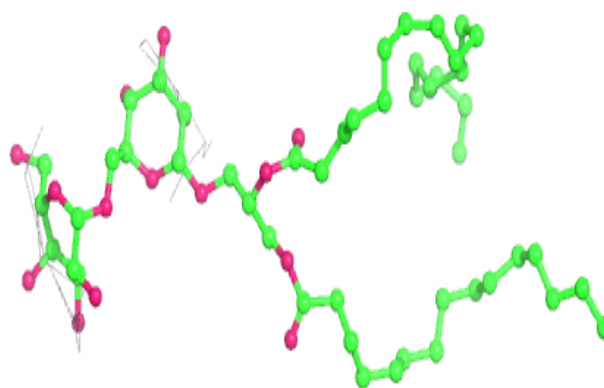
**Electron density around LMT B 629:**

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

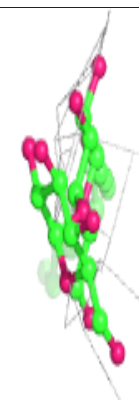
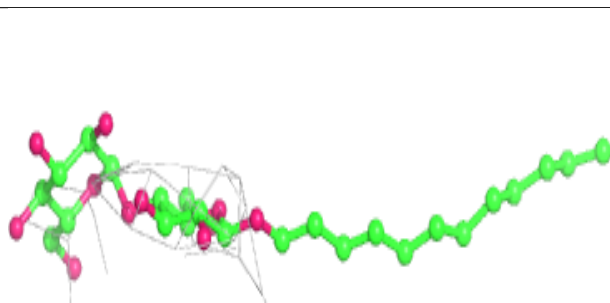
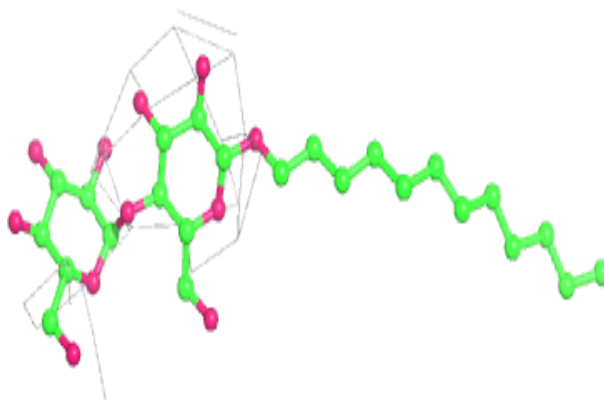


Electron density around DGD D 408:

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

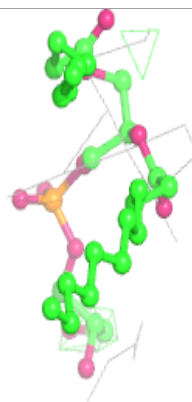
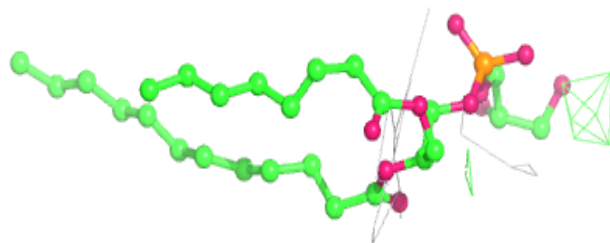
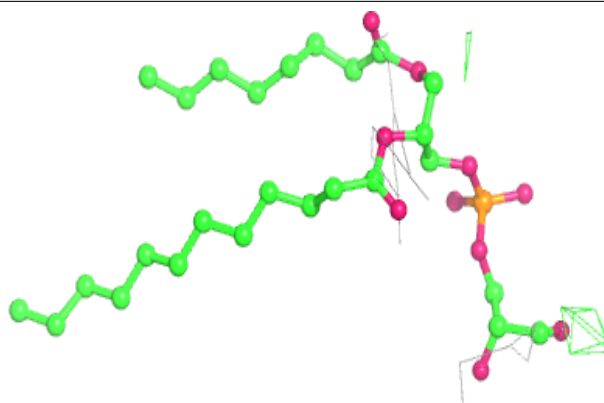
**Electron density around LMT N 625:**

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

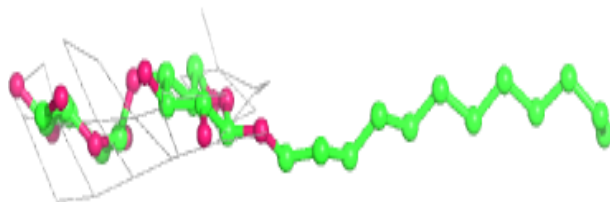
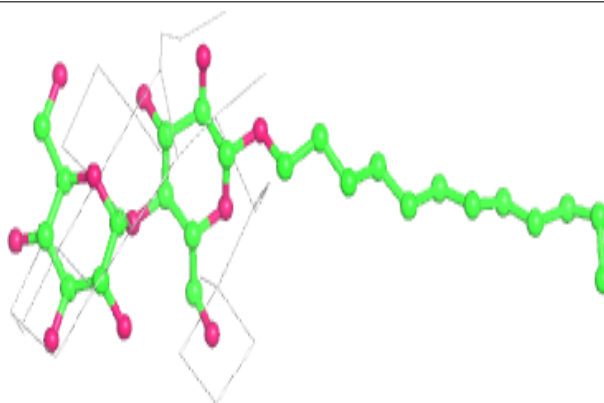


Electron density around LHG G 412:

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

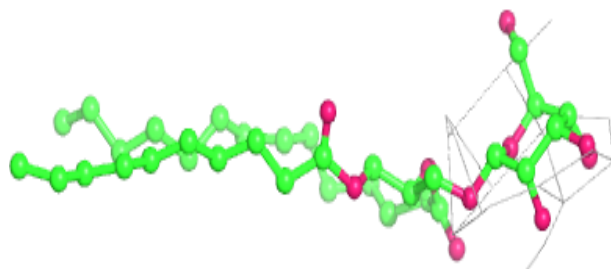
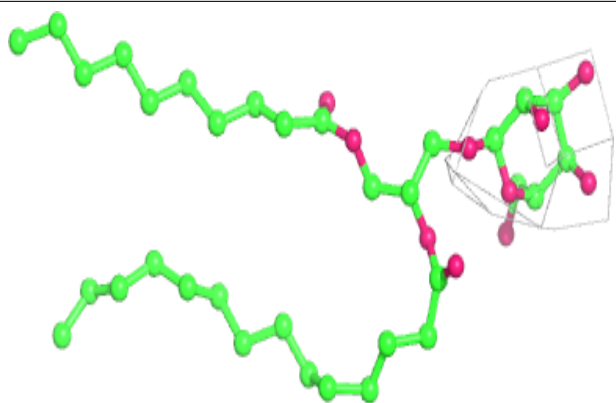
**Electron density around LMT N 604:**

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

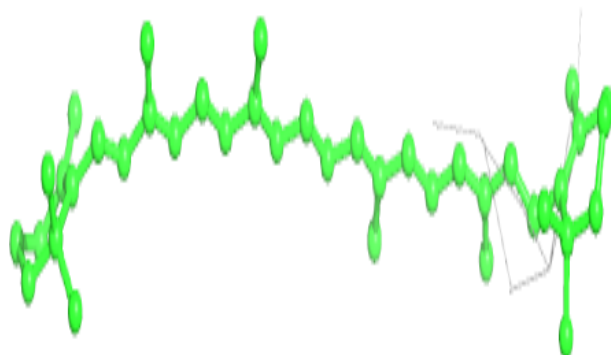
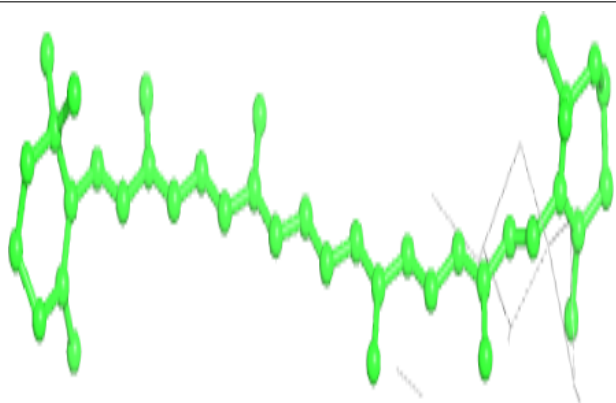


Electron density around LMG I 102:

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

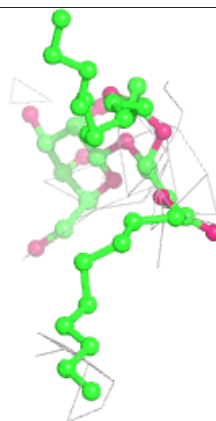
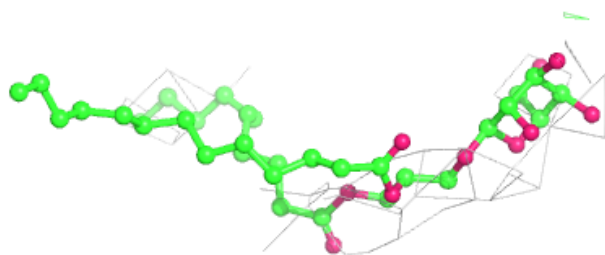
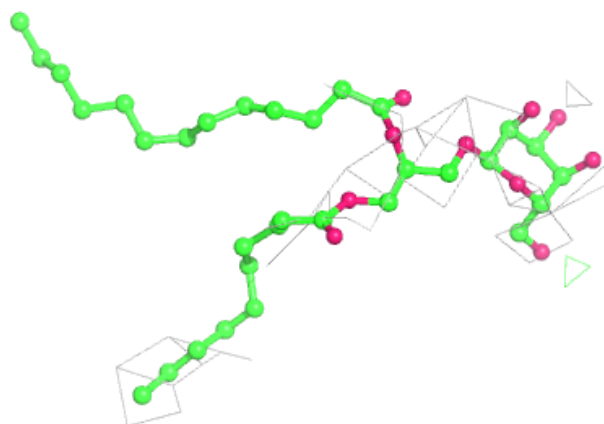
**Electron density around BCR B 620:**

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

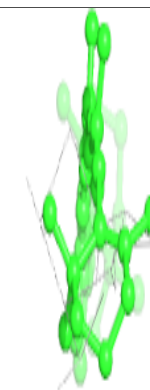
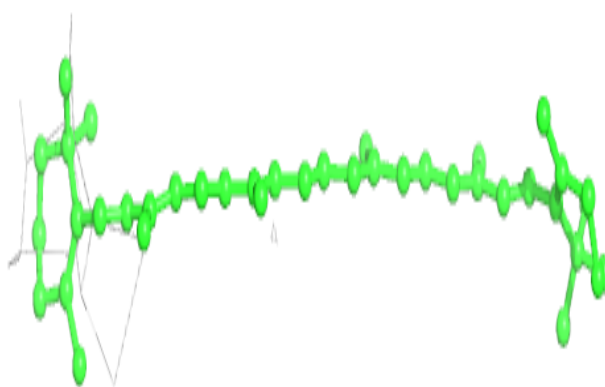
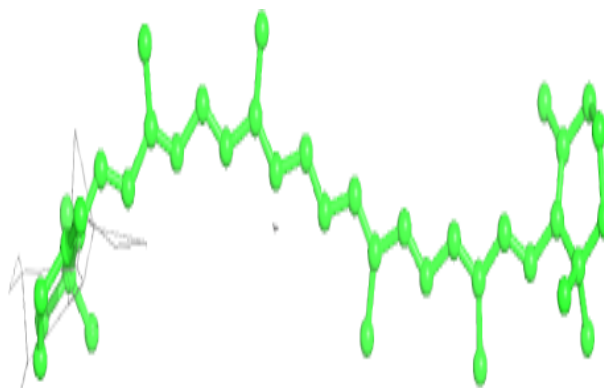


Electron density around LMG Q 401:

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

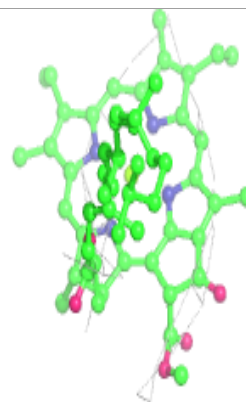
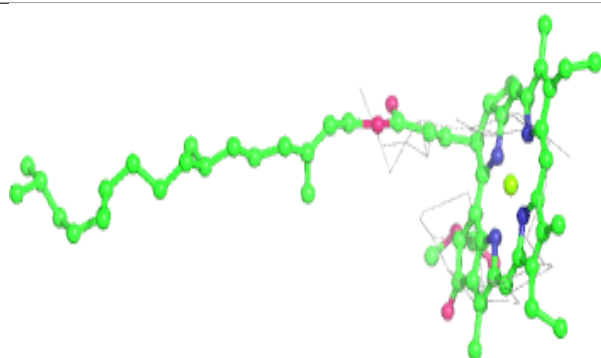
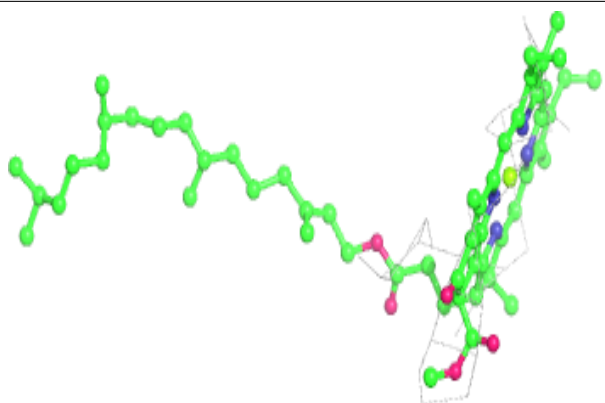
**Electron density around BCR H 101:**

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



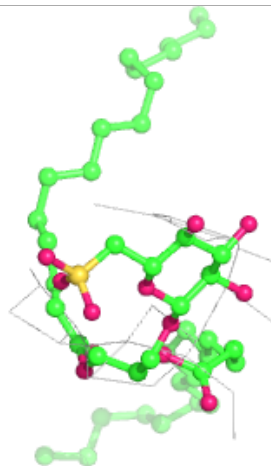
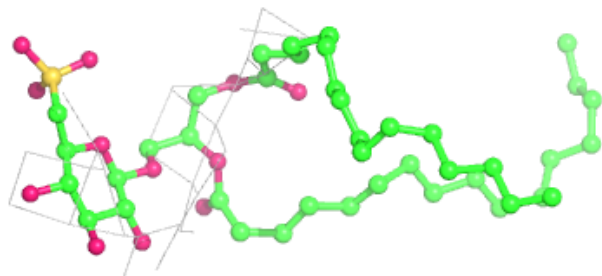
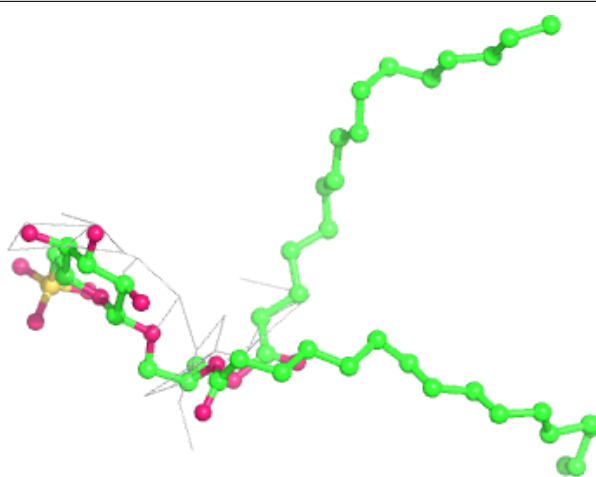
Electron density around CLA N 608:

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



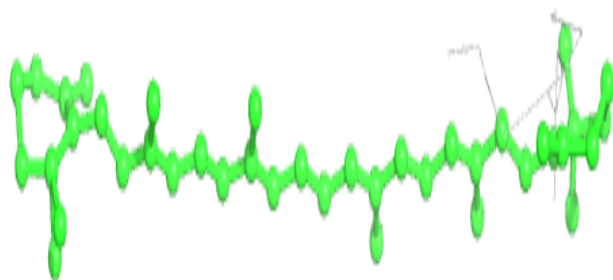
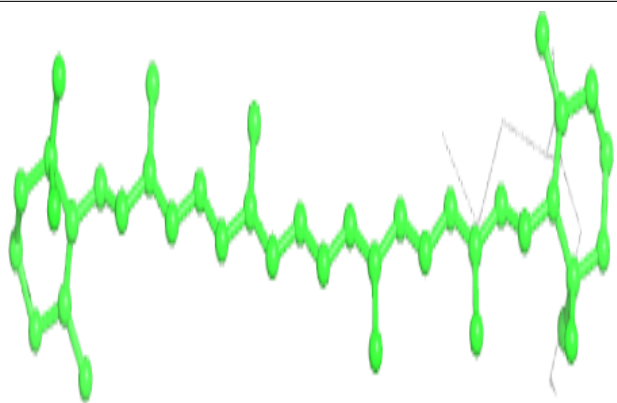
Electron density around SQD A 414:

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

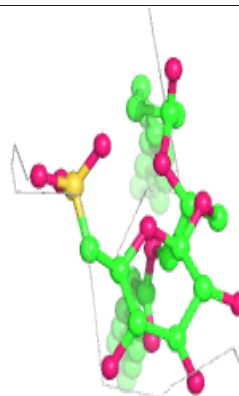
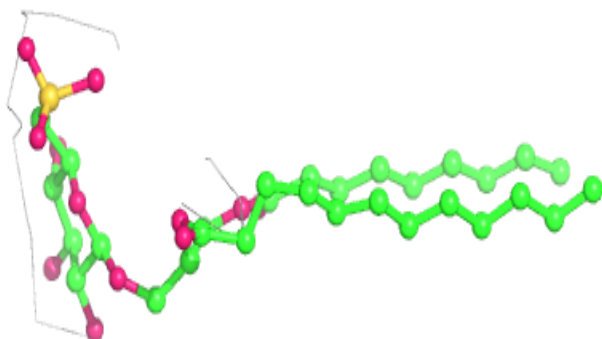
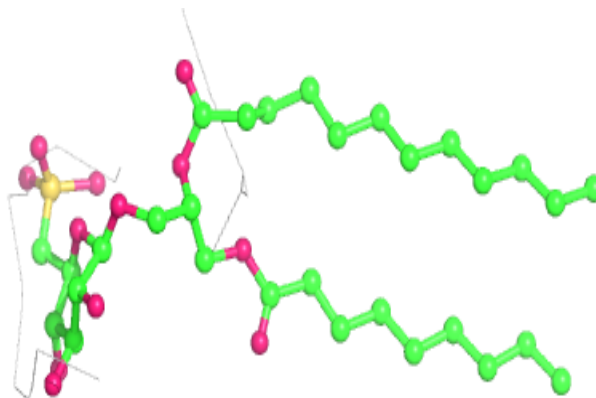


Electron density around BCR b 102:

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

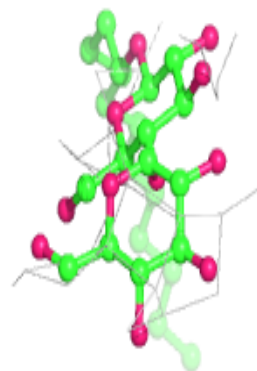
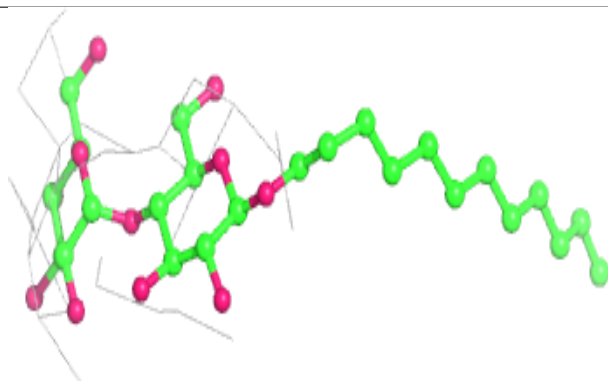
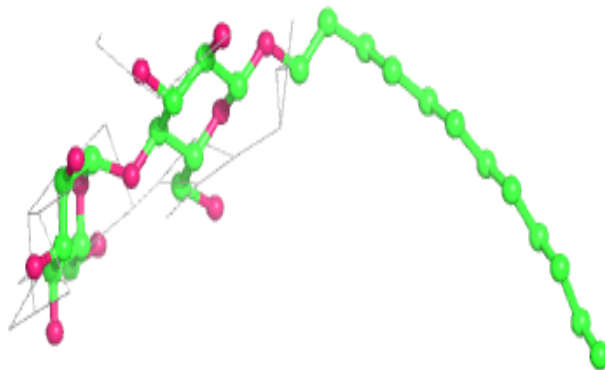
**Electron density around SQD Q 408:**

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

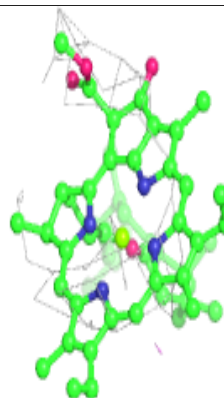
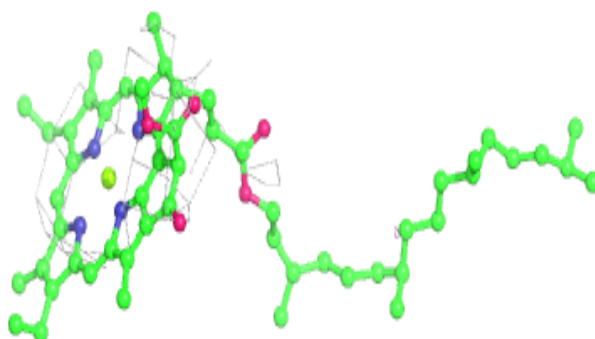
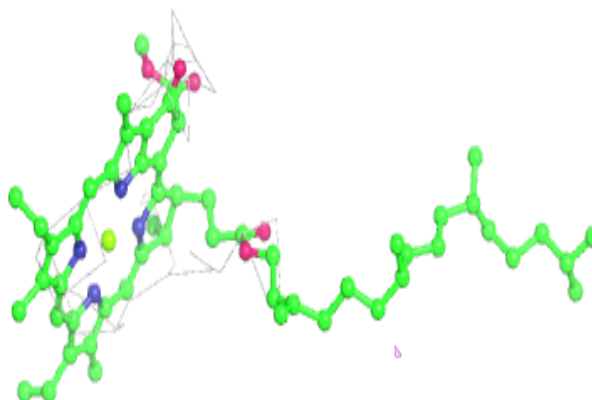


Electron density around LMT e 101:

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

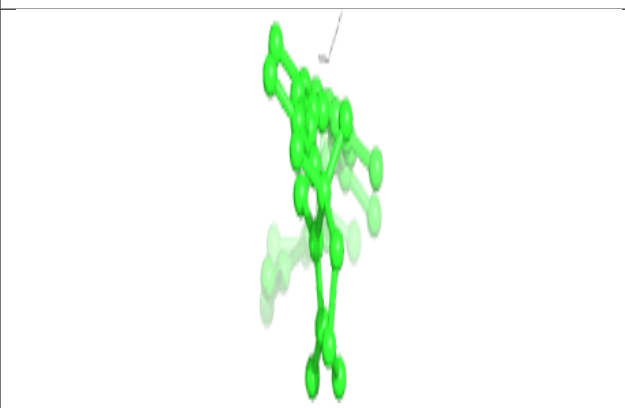
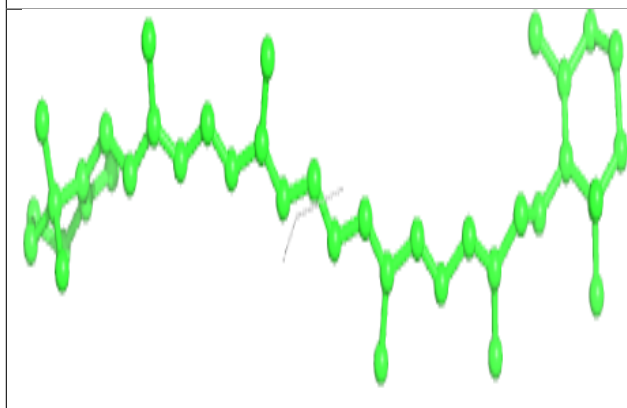
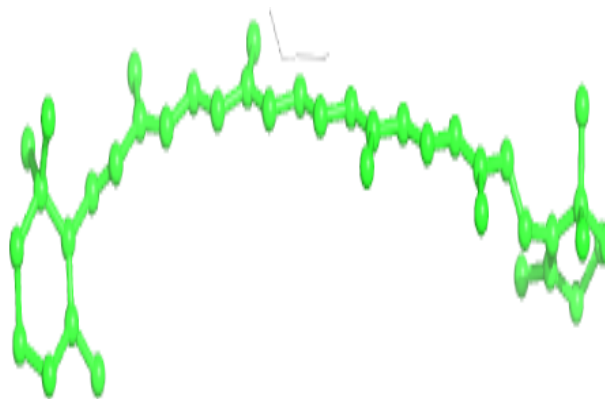
**Electron density around CLA P 502:**

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

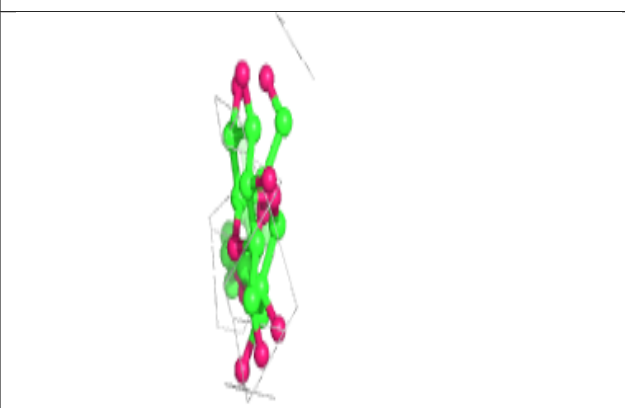
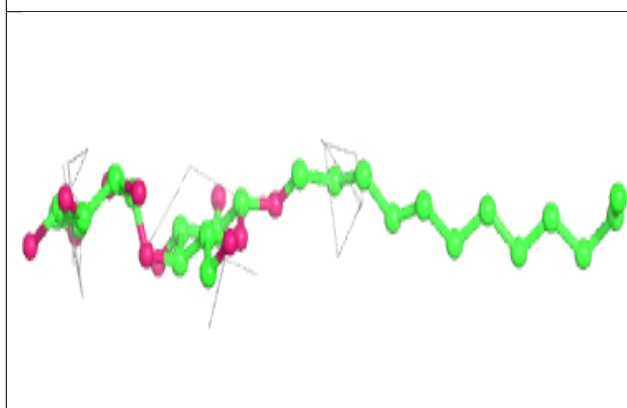
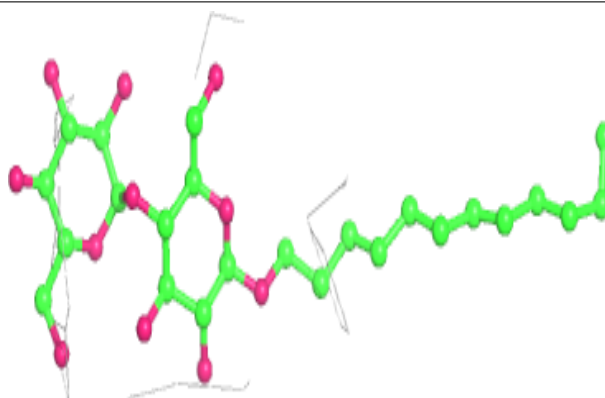


Electron density around BCR D 405:

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

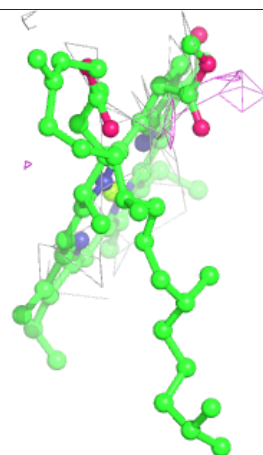
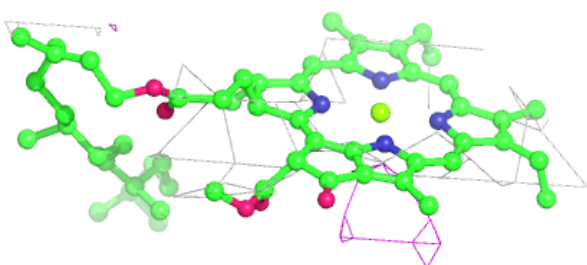
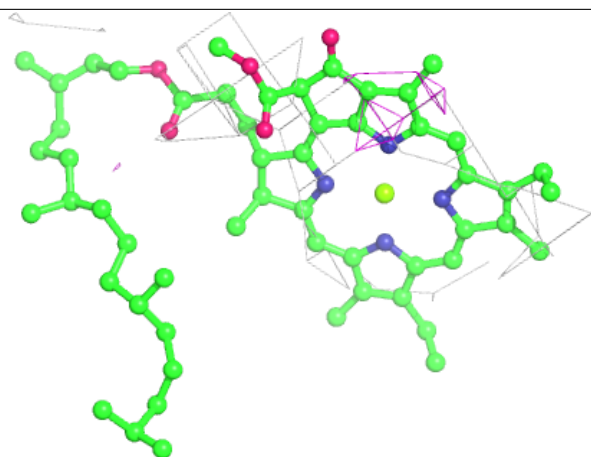
**Electron density around LMT B 630:**

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

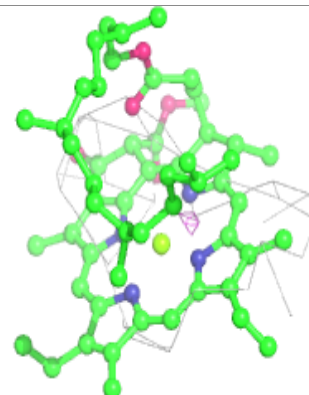
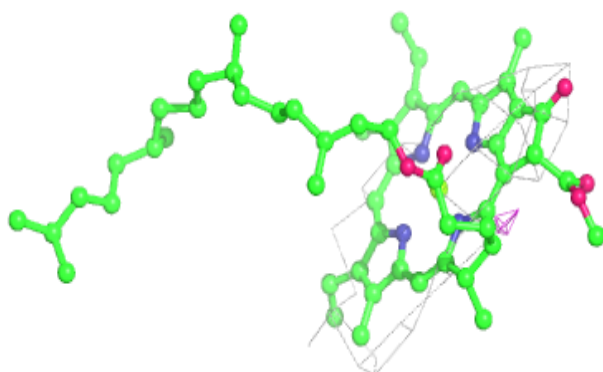
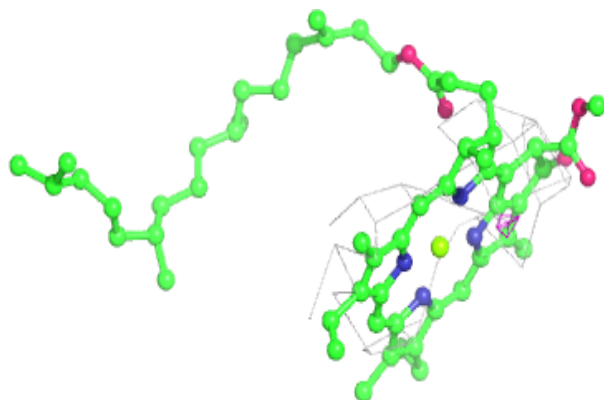


Electron density around CLA N 620:

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

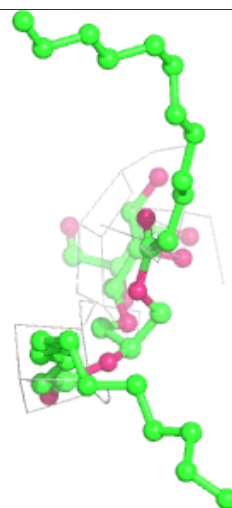
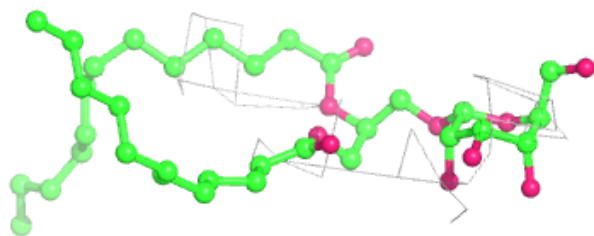
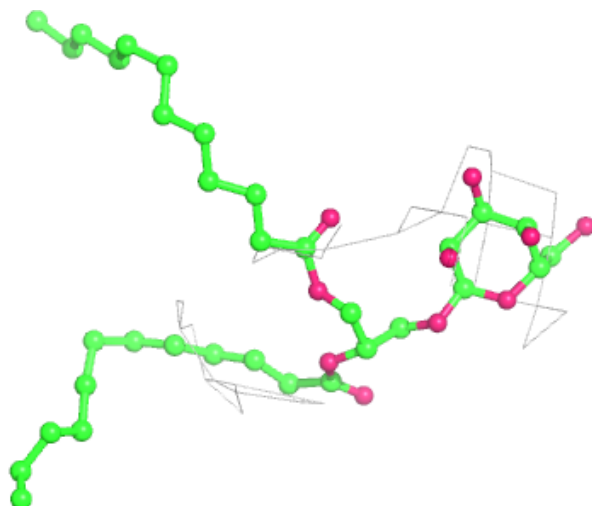
**Electron density around CLA C 513:**

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



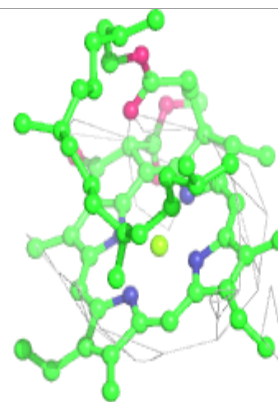
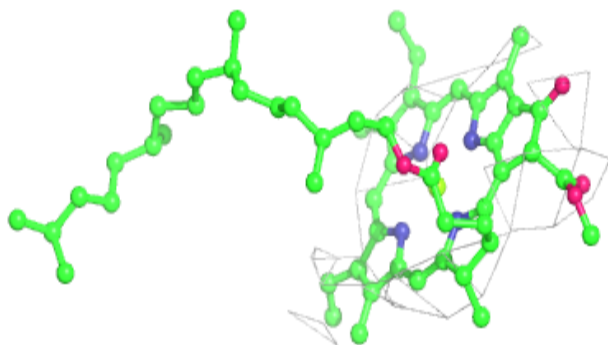
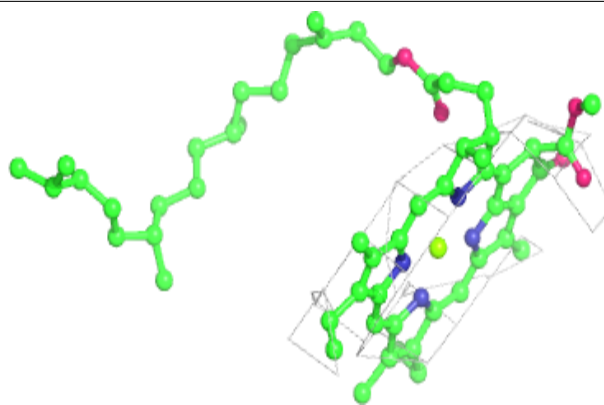
Electron density around LMG R 102:

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

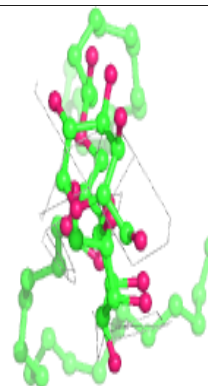
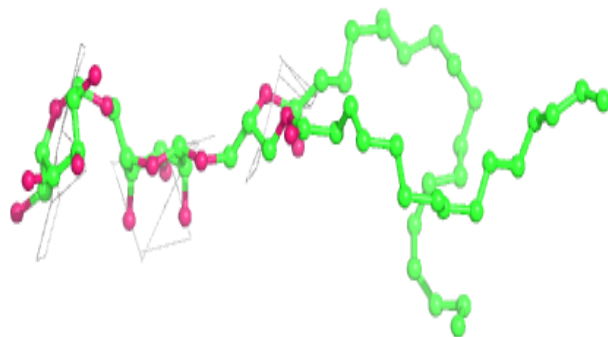
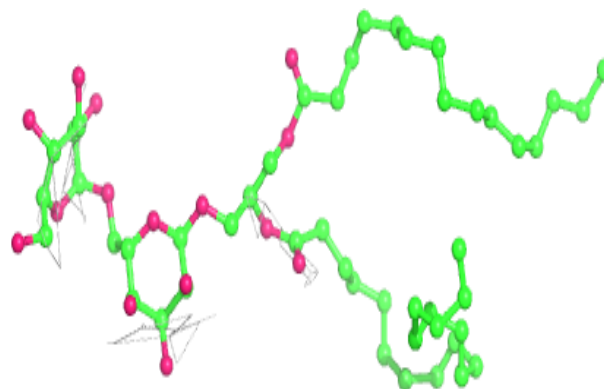


Electron density around CLA P 513:

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

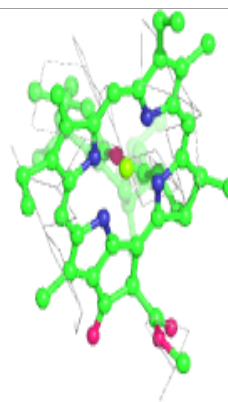
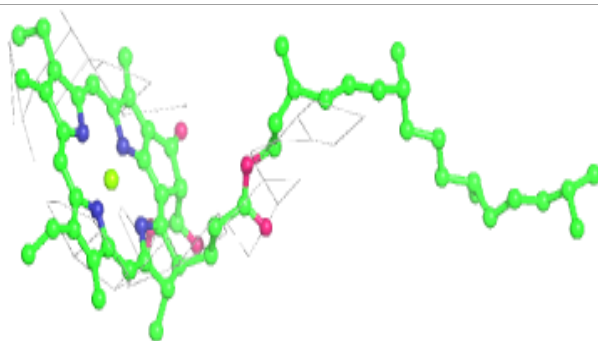
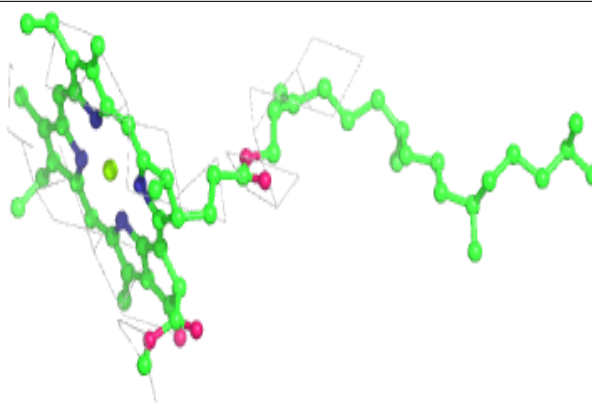
**Electron density around DGD Q 409:**

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

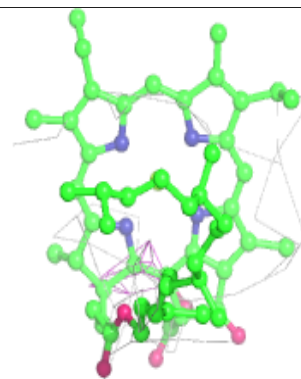
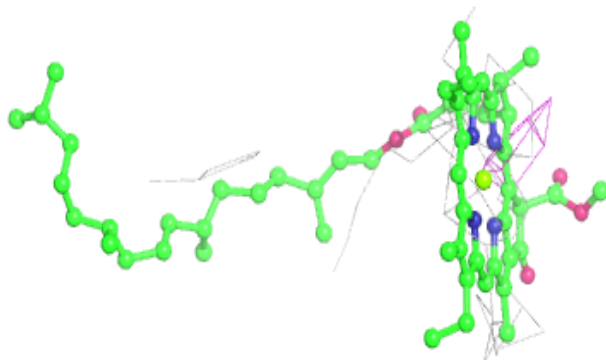
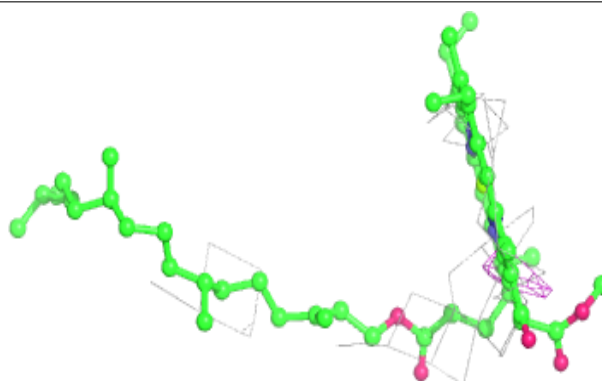


Electron density around CLA C 502:

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

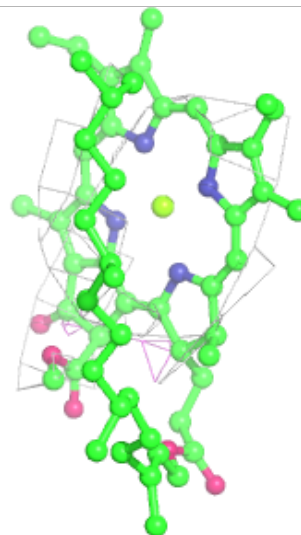
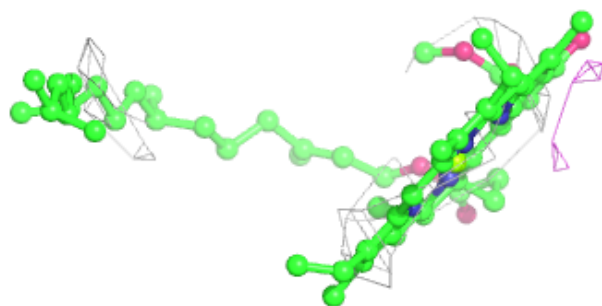
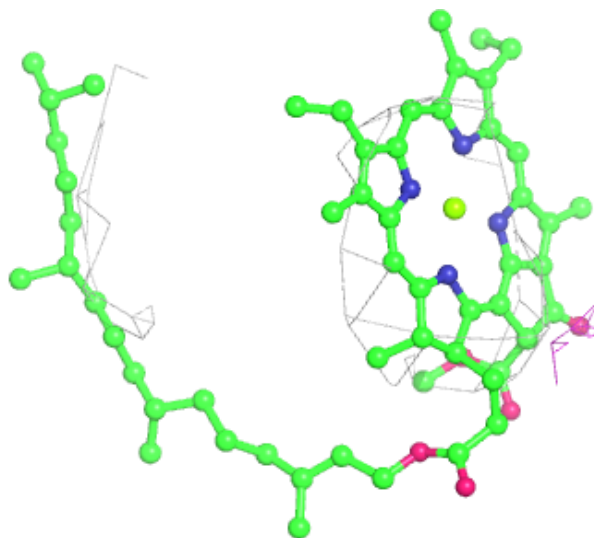
**Electron density around CLA N 609:**

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



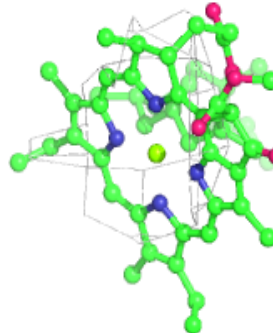
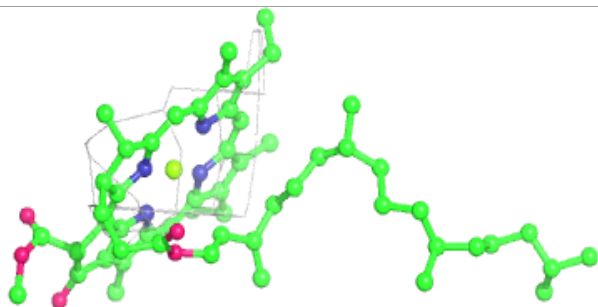
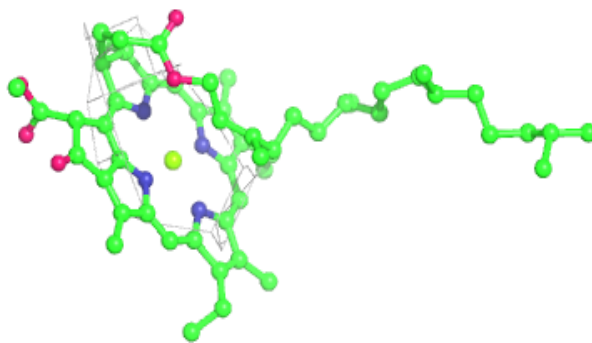
Electron density around CLA C 507:

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

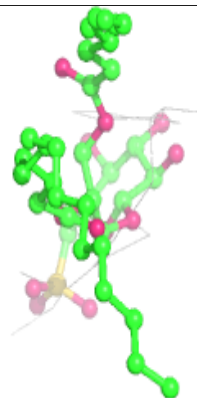
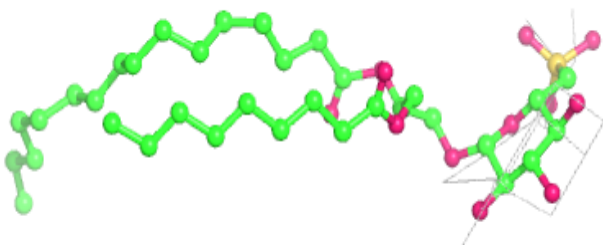
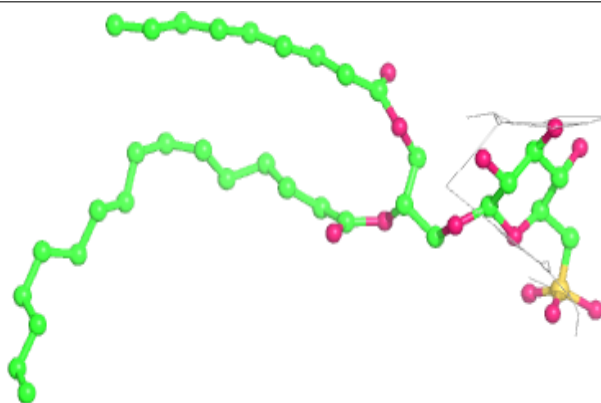


Electron density around CLA C 505:

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

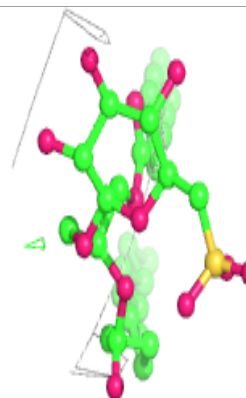
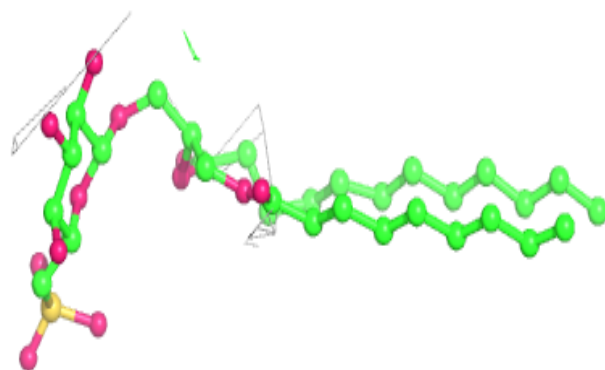
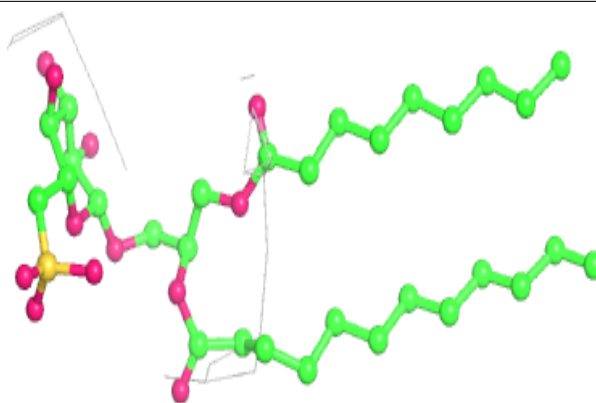
**Electron density around SQD B 627:**

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

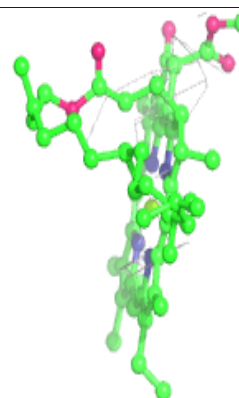
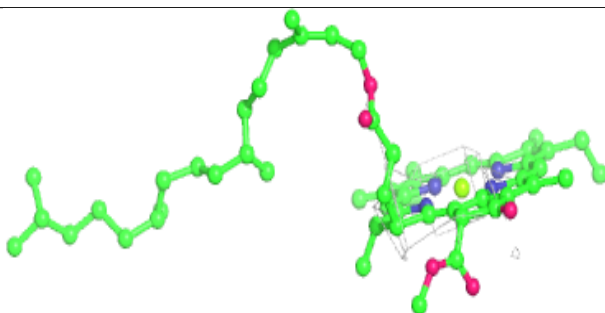
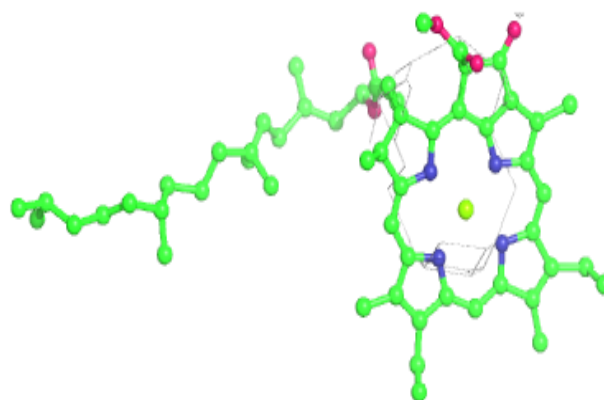


Electron density around SQD B 624:

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

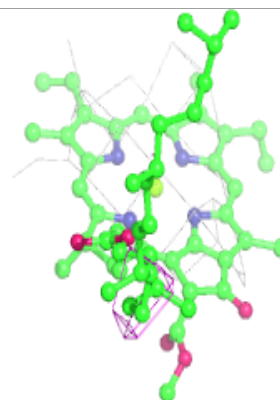
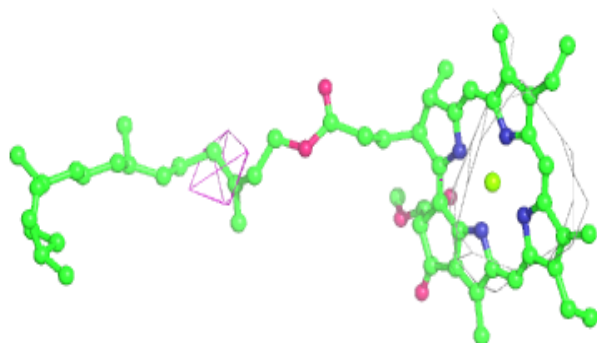
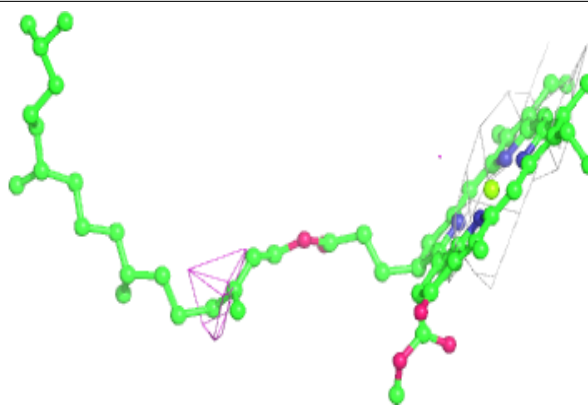
**Electron density around CLA A 403:**

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

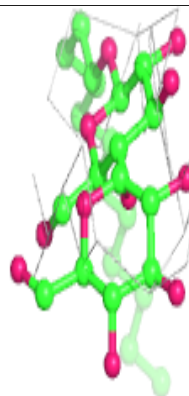
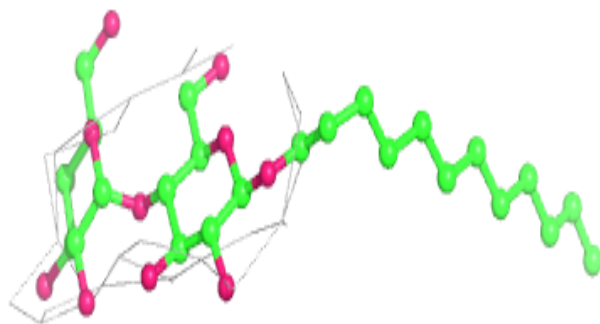
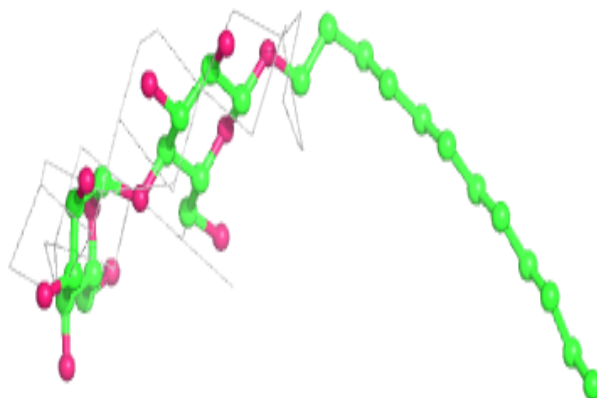


Electron density around CLA D 401:

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

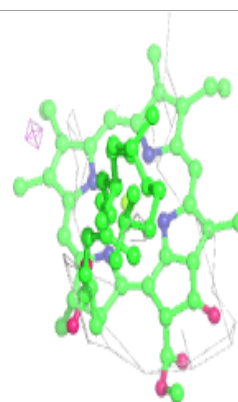
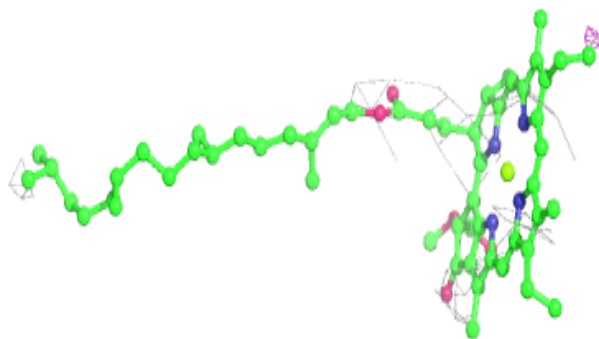
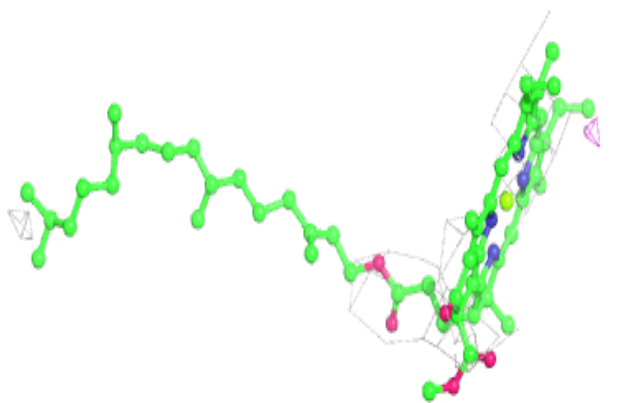
**Electron density around LMT M 102:**

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

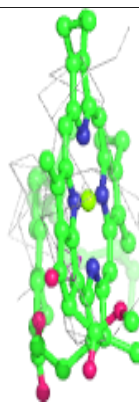
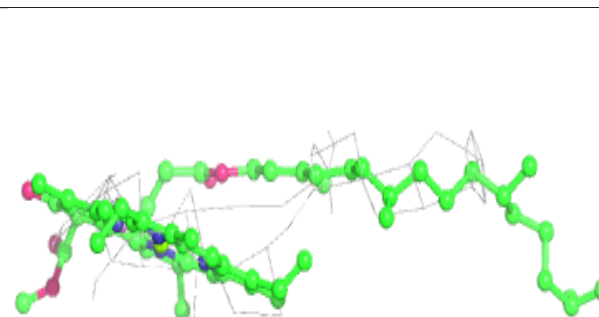
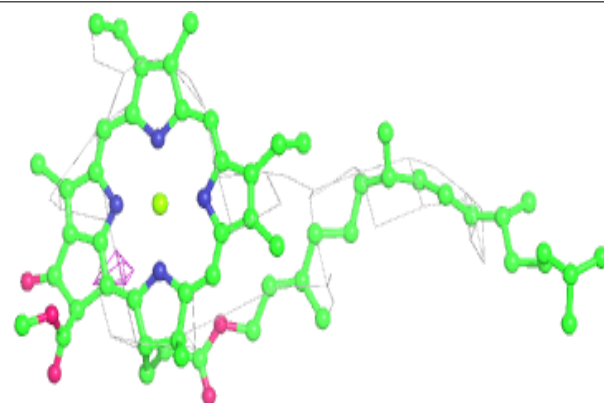


Electron density around CLA B 604:

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

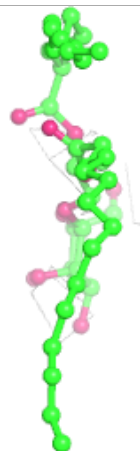
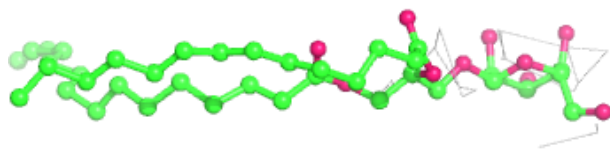
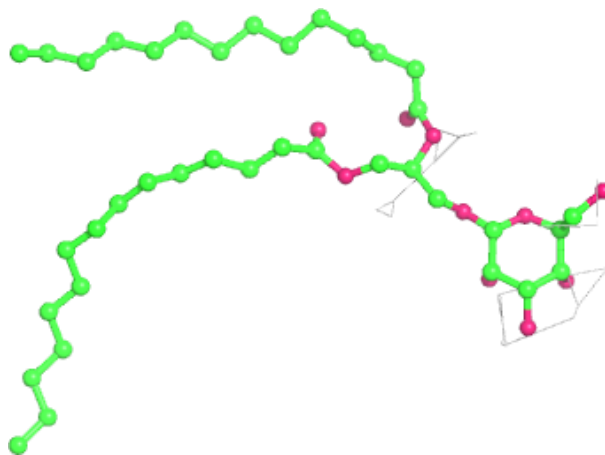
**Electron density around CLA N 607:**

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



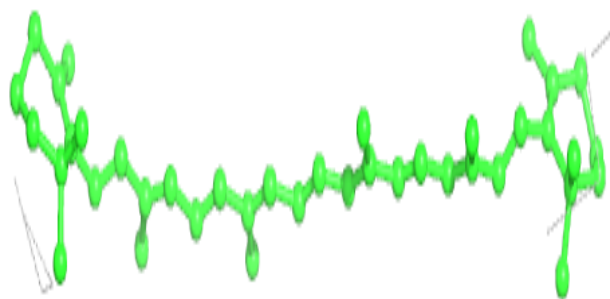
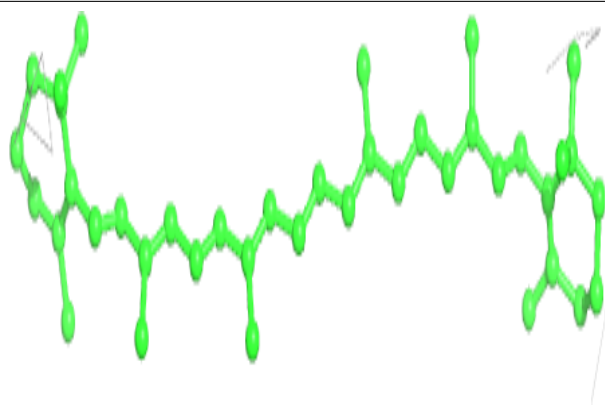
Electron density around LMG C 519:

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

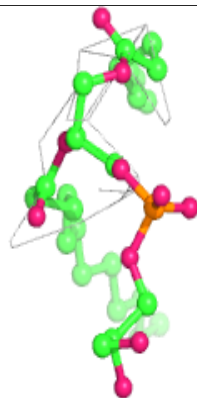
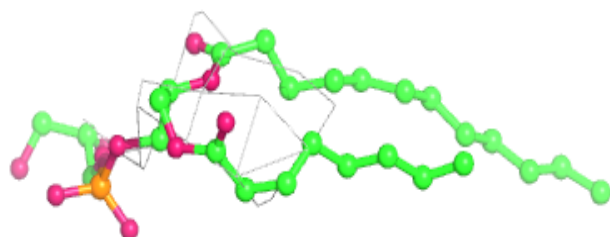
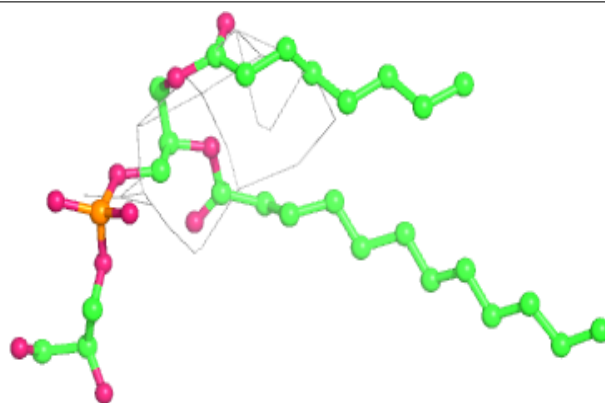


Electron density around BCR P 516:

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

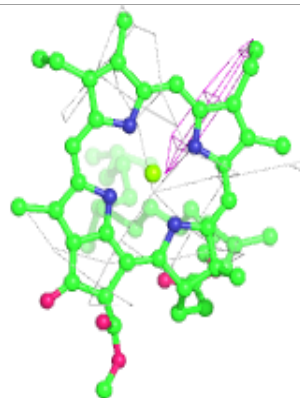
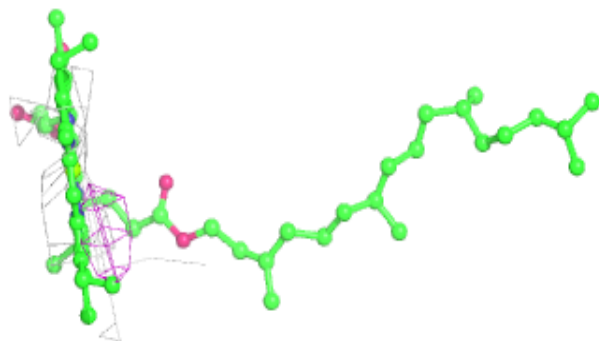
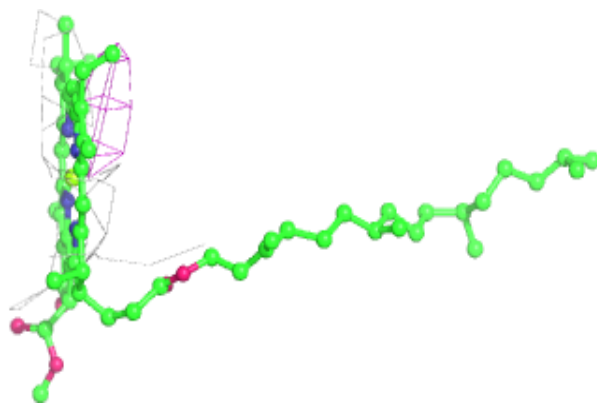
**Electron density around LHG A 411:**

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

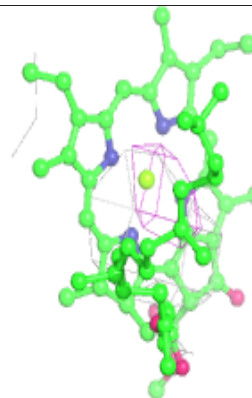
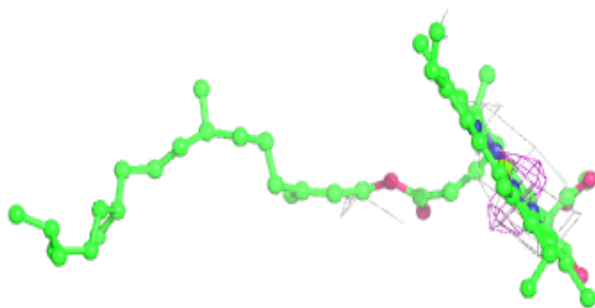
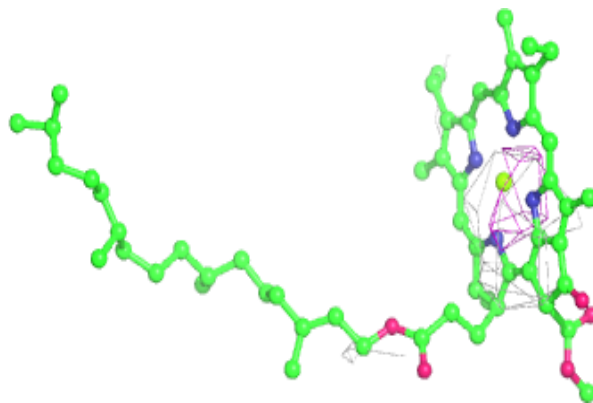


Electron density around CLA N 610:

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

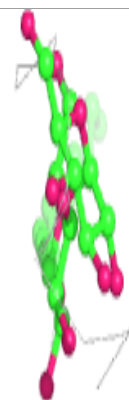
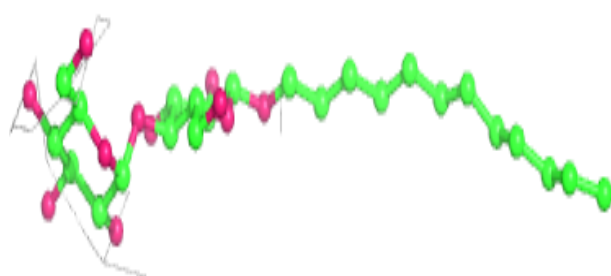
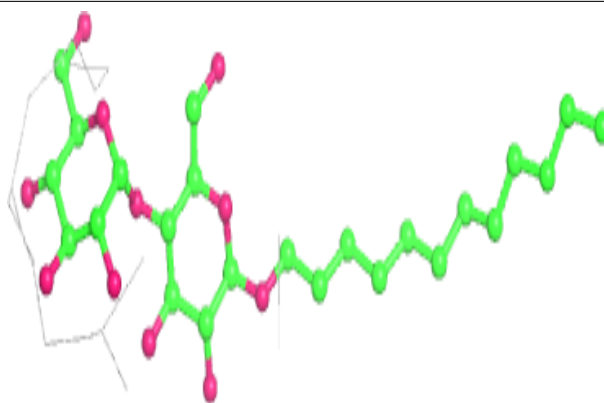
**Electron density around CLA G 406:**

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

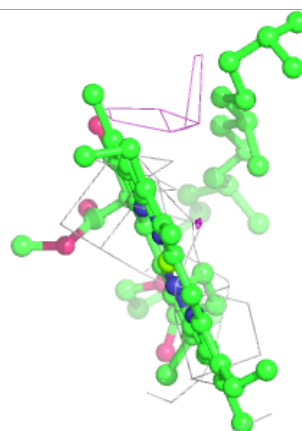
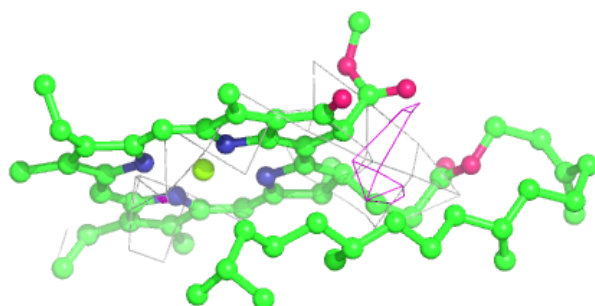
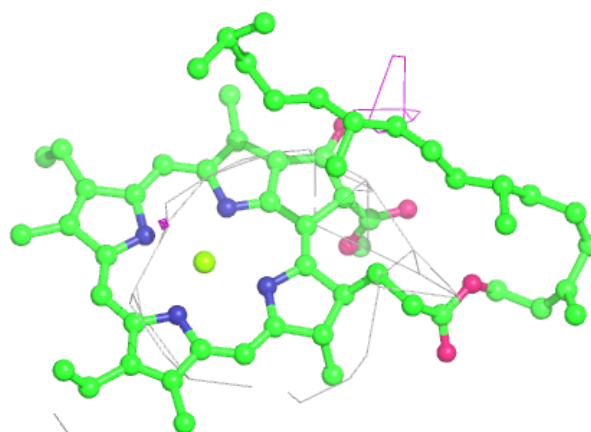


Electron density around LMT B 626:

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

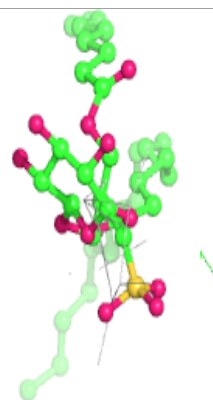
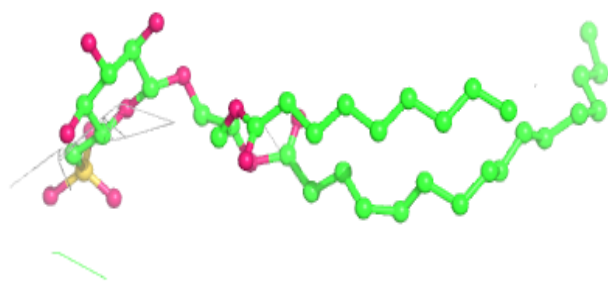
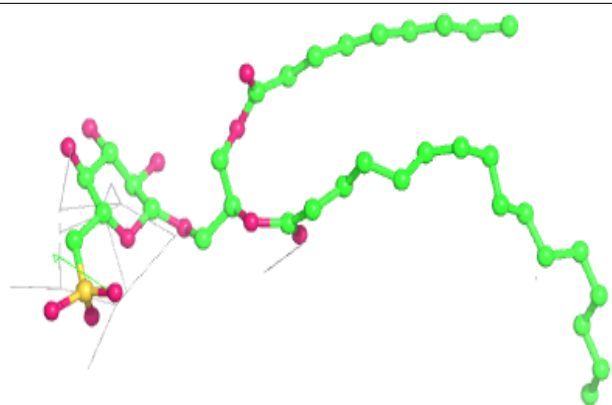
**Electron density around CLA C 509:**

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

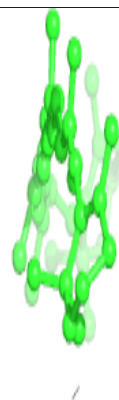
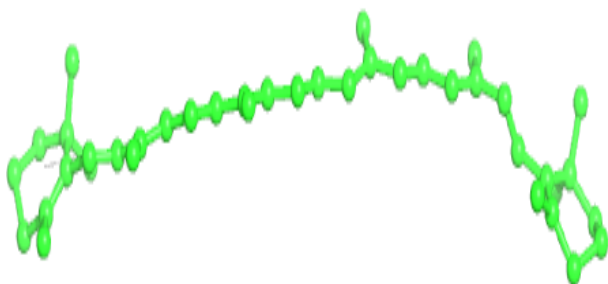
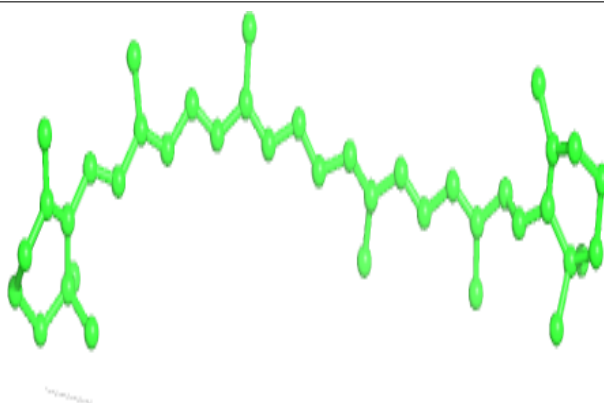


Electron density around SQD N 601:

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

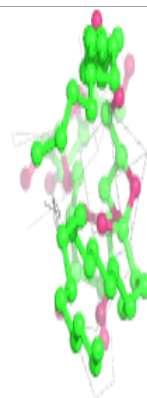
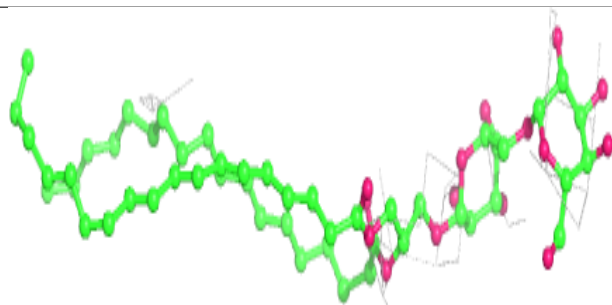
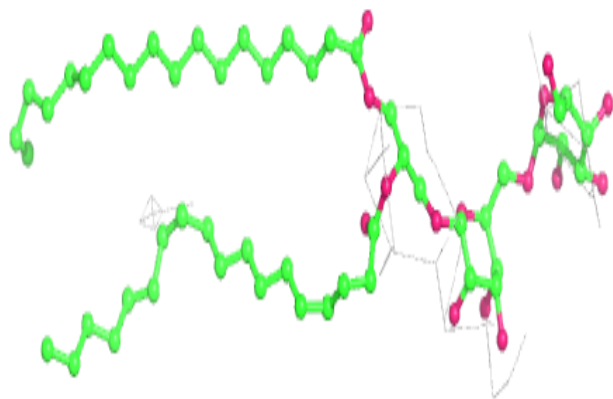
**Electron density around BCR B 618:**

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



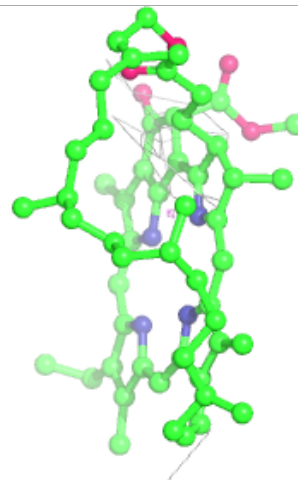
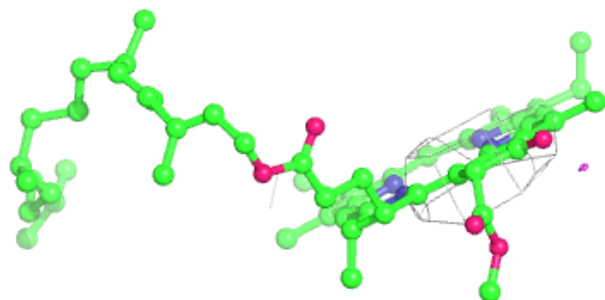
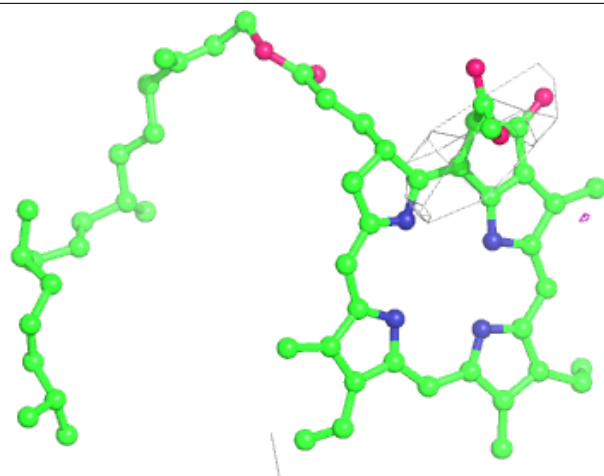
Electron density around DGD C 518:

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



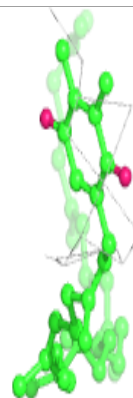
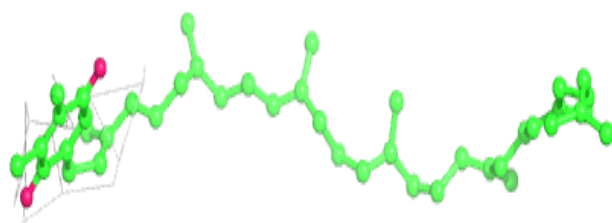
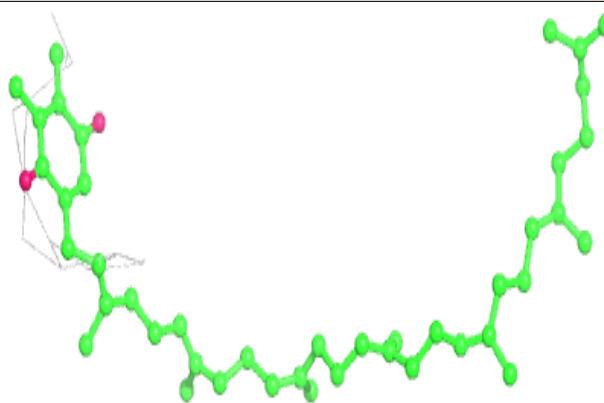
Electron density around PHO D 402:

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

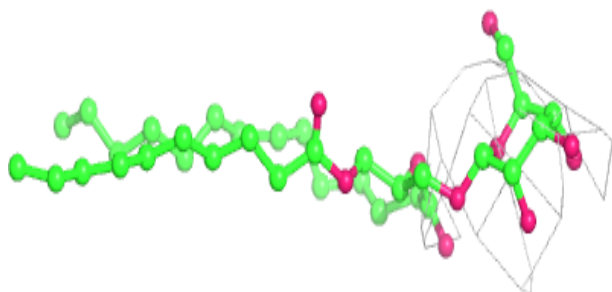
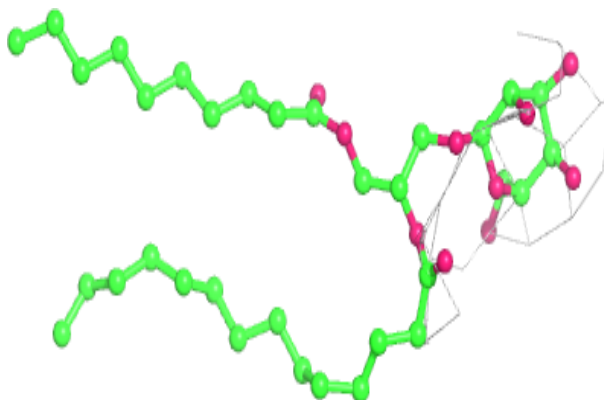


Electron density around PL9 G 407:

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

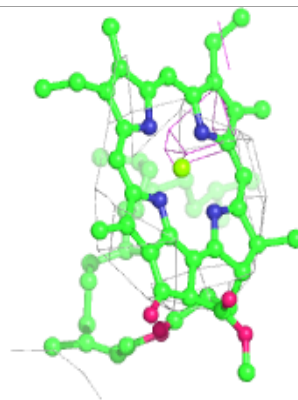
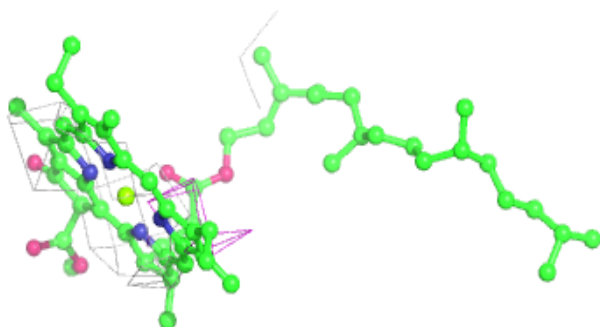
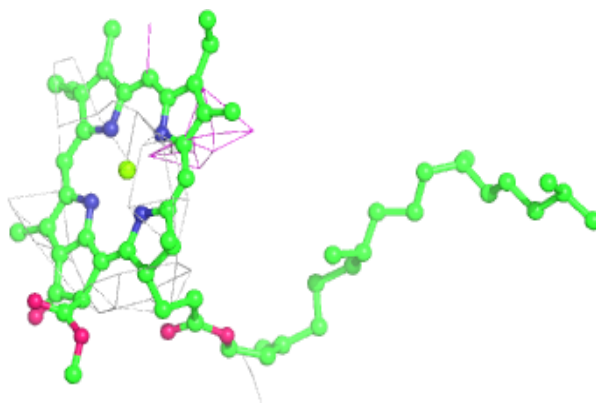
**Electron density around LMG a 102:**

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

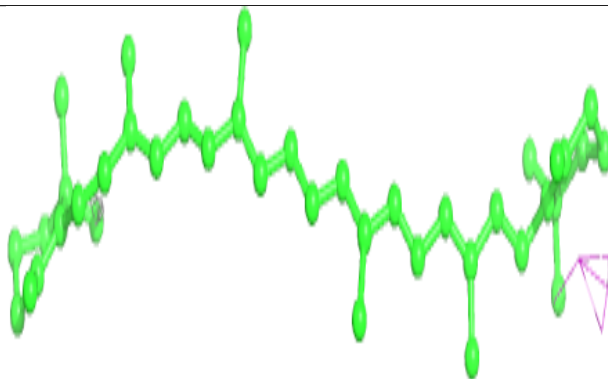
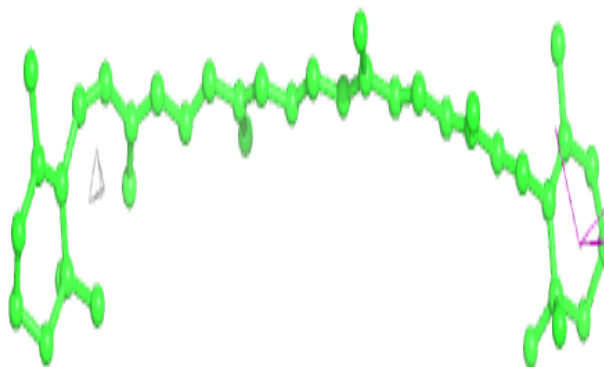


Electron density around CLA P 511:

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

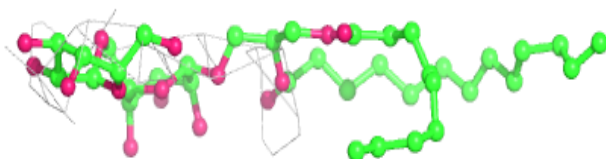
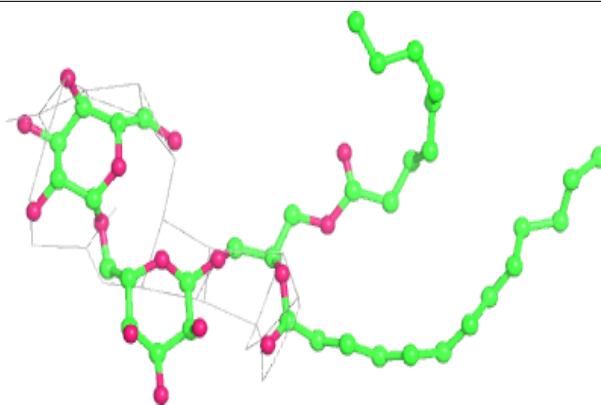
**Electron density around BCR P 514:**

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

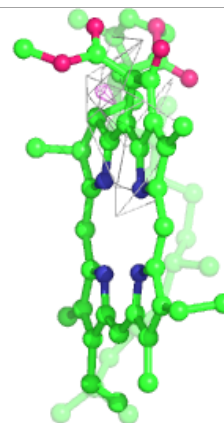
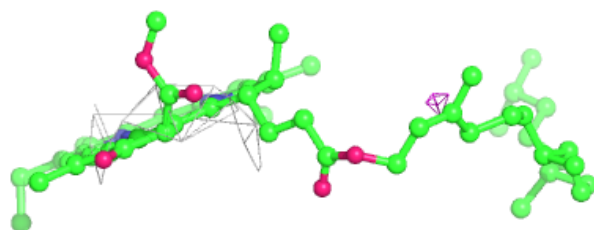
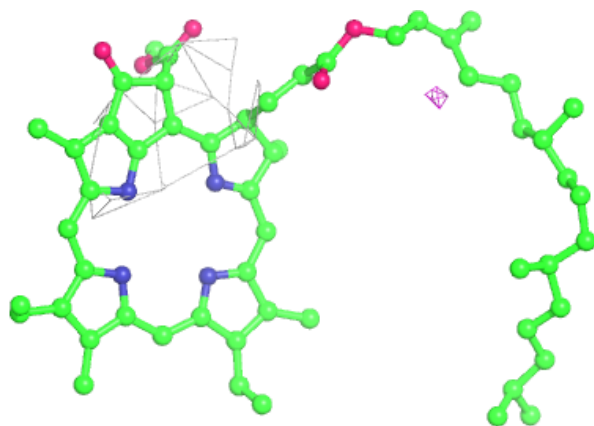


Electron density around DGD B 628:

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

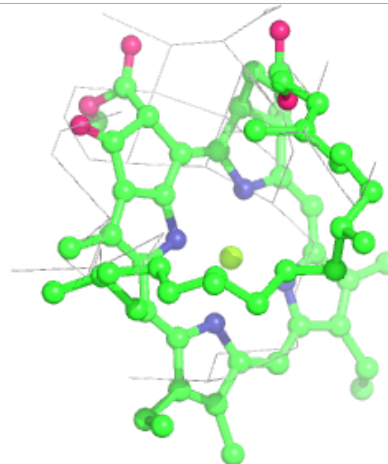
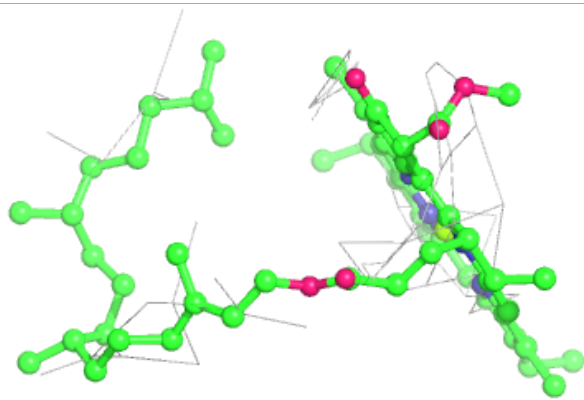
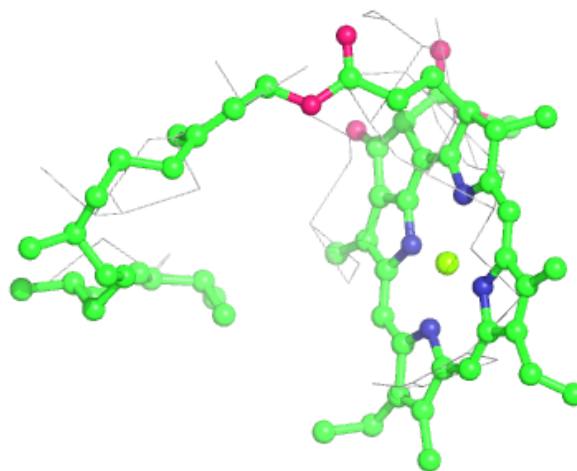
**Electron density around PHO A 404:**

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



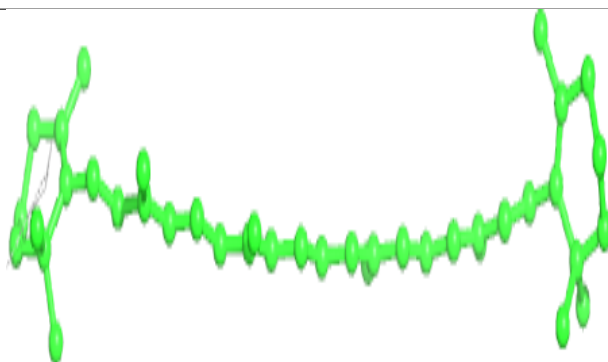
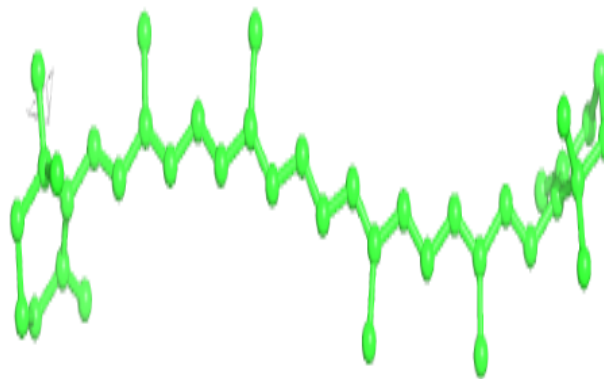
Electron density around CLA C 503:

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

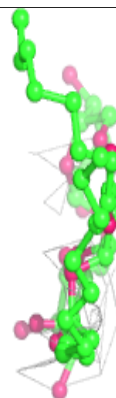
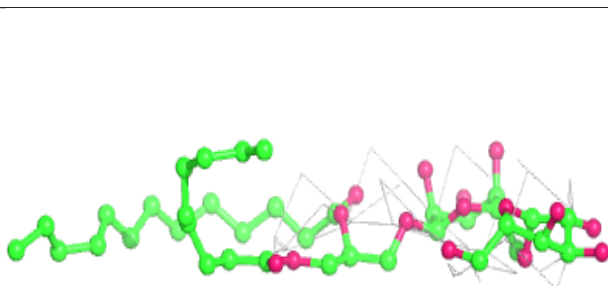
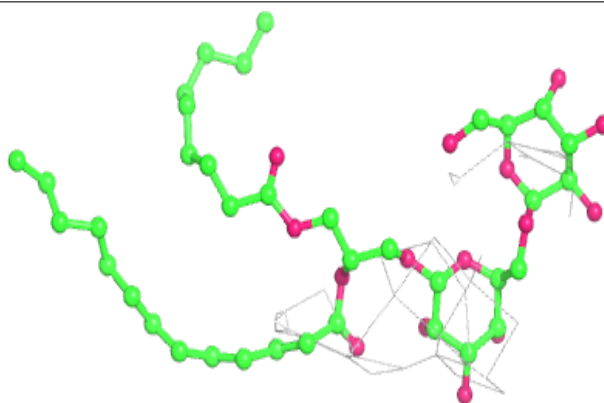


Electron density around BCR T 101:

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

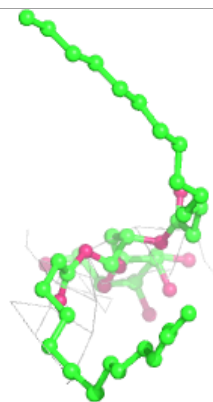
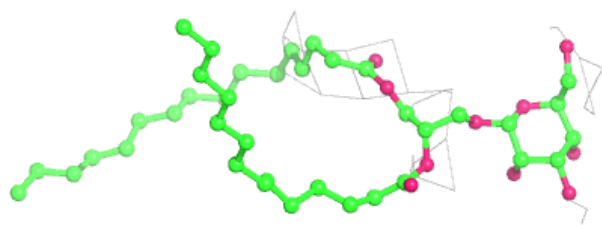
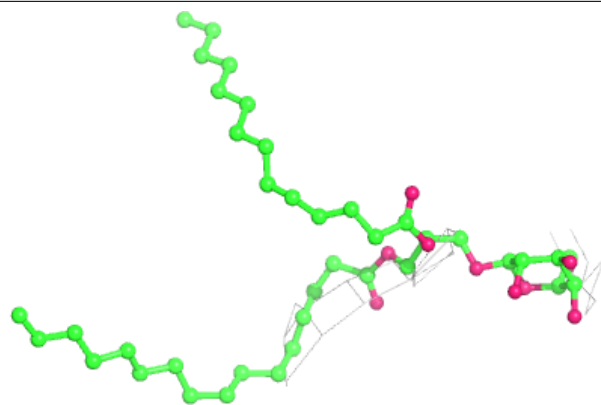
**Electron density around DGD N 602:**

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

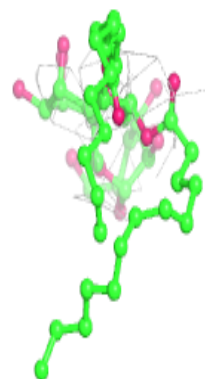
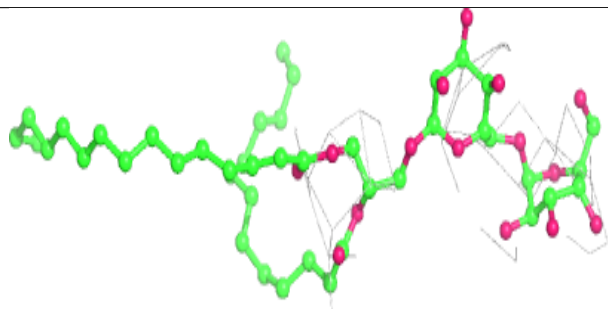
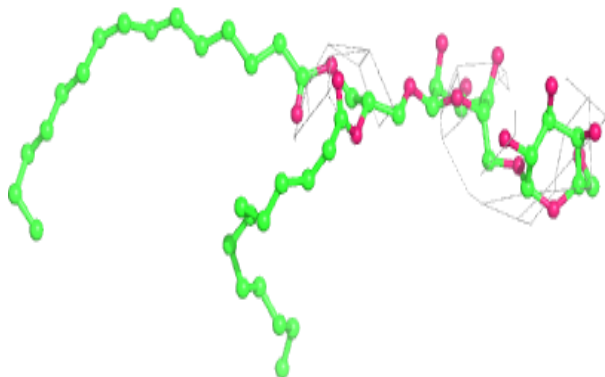


Electron density around LMG B 623:

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

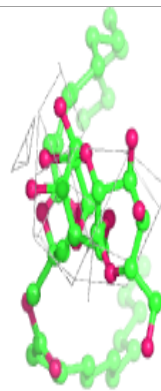
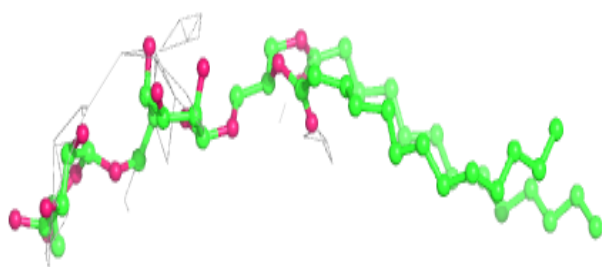
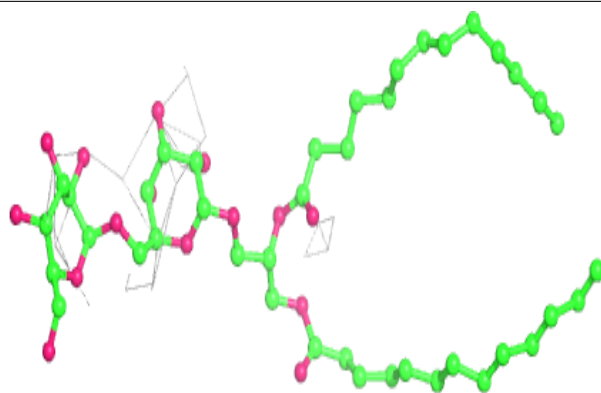
**Electron density around DGD B 621:**

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

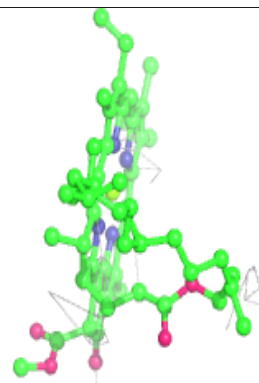
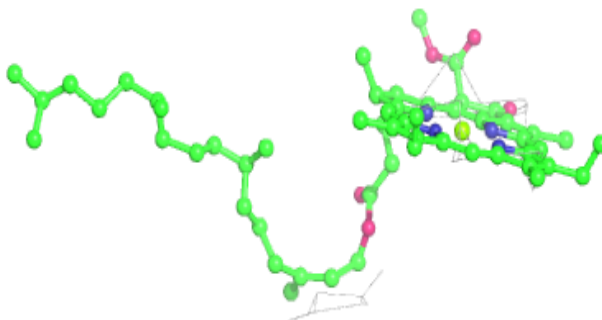
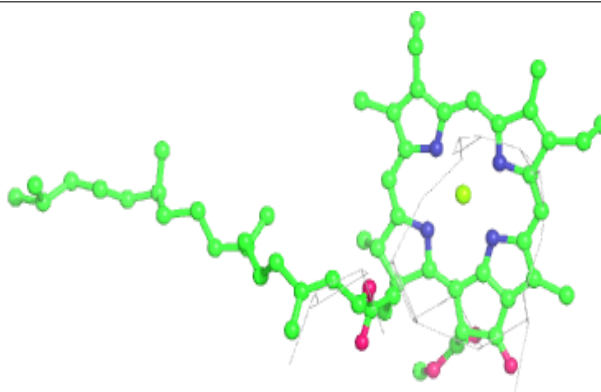


Electron density around DGD G 408:

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

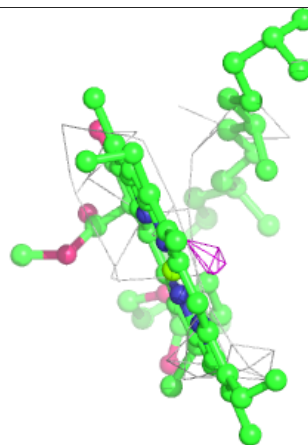
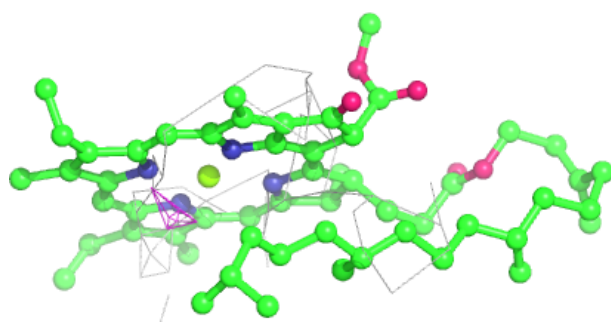
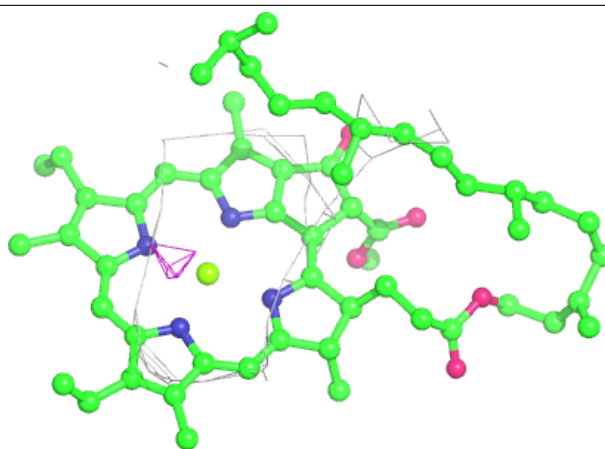
**Electron density around CLA G 404:**

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



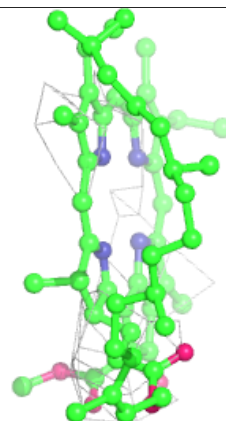
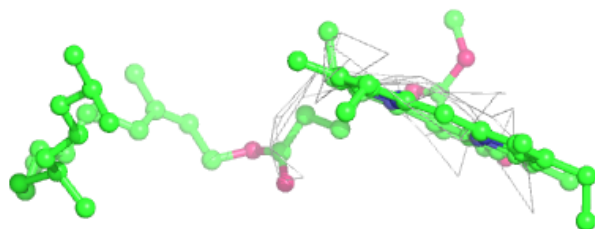
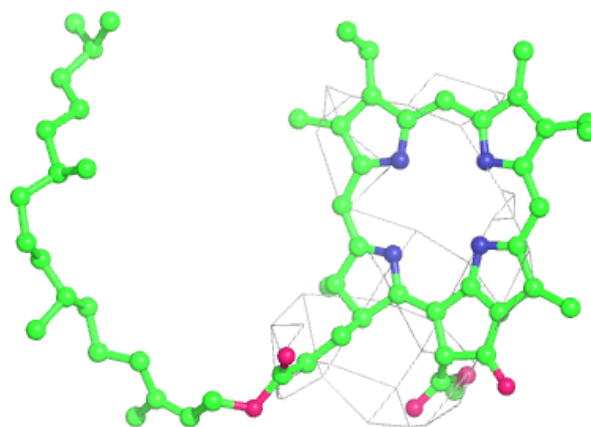
Electron density around CLA P 509:

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

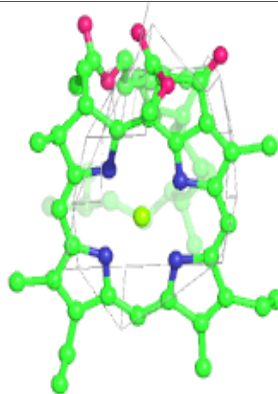
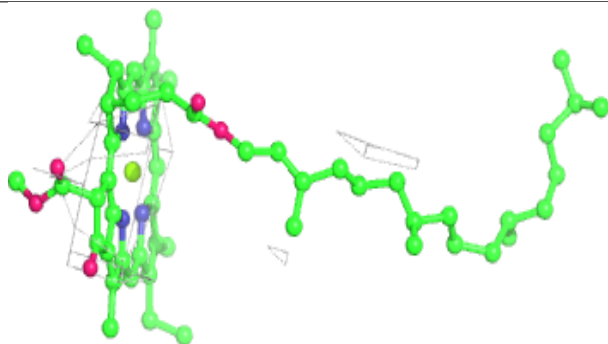
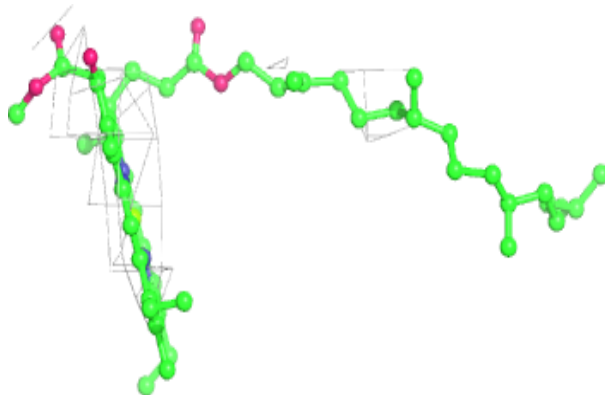


Electron density around PHO G 405:

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

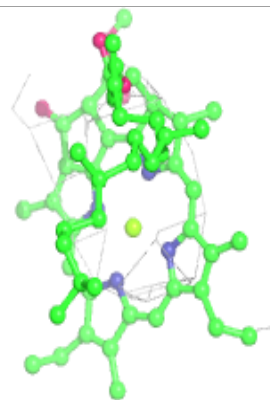
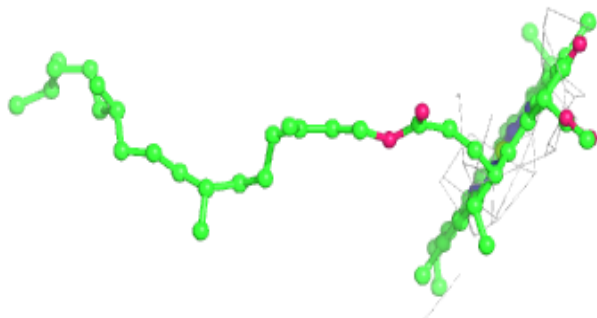
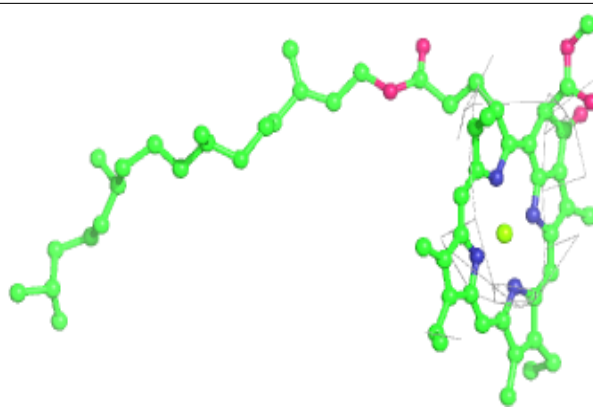
**Electron density around CLA B 605:**

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

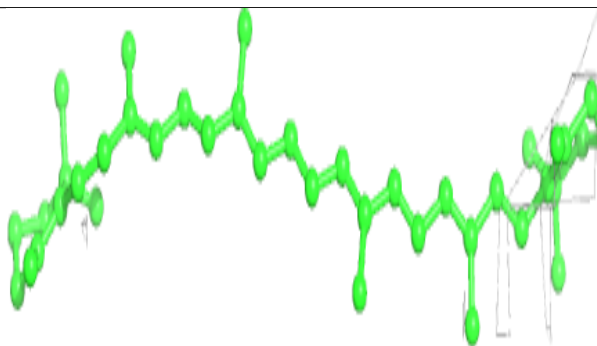
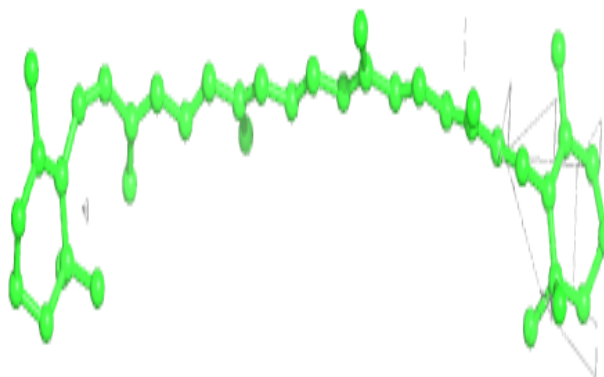


Electron density around CLA A 405:

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

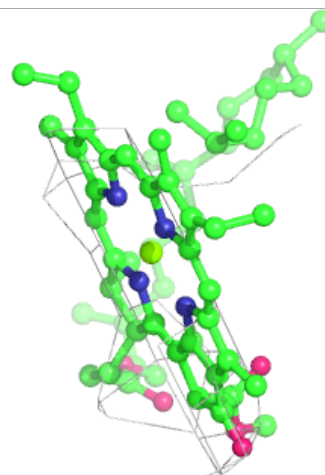
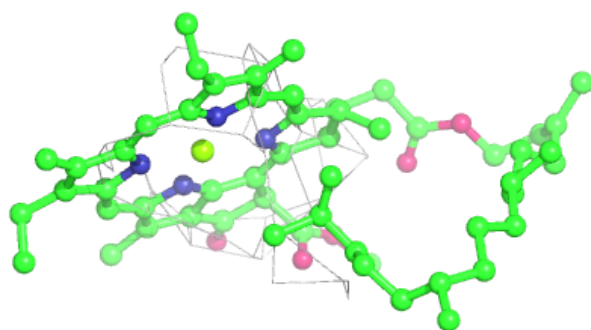
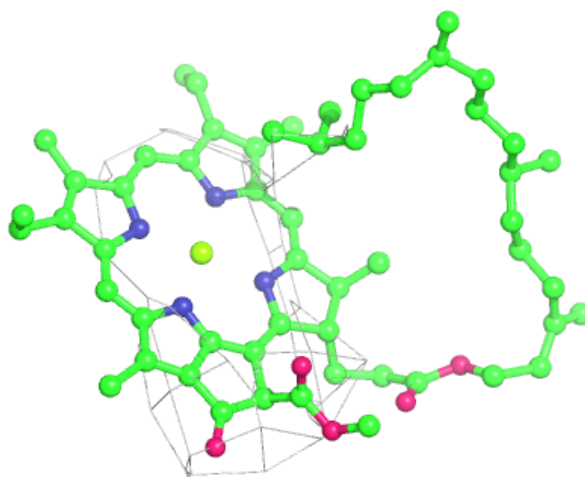
**Electron density around BCR C 514:**

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



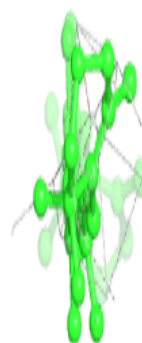
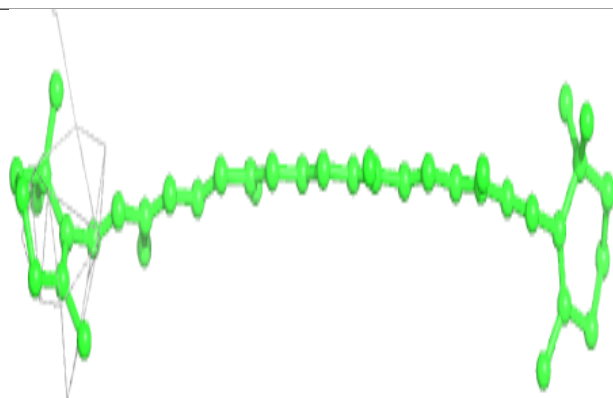
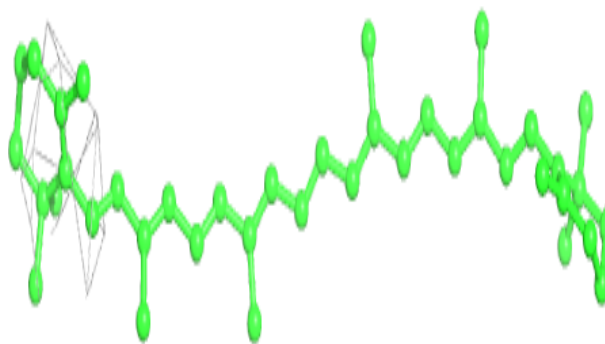
Electron density around CLA N 619:

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

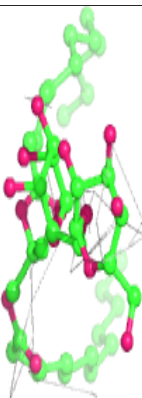
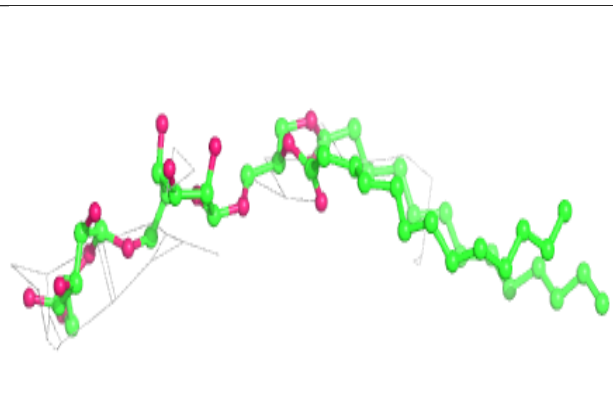
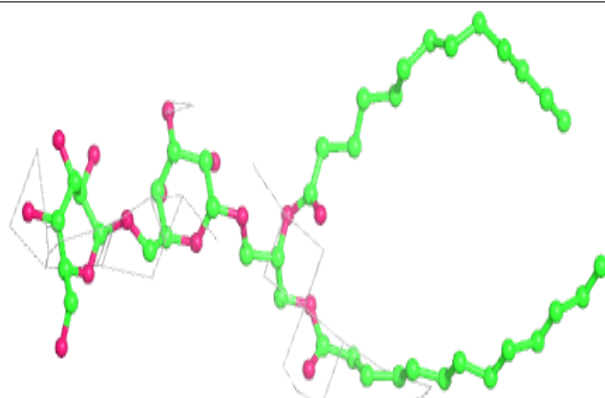


Electron density around BCR B 617:

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

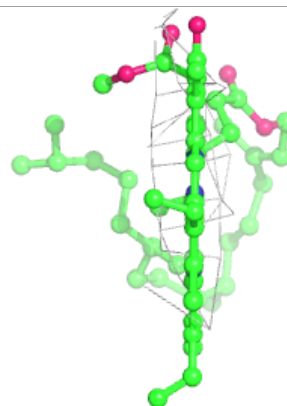
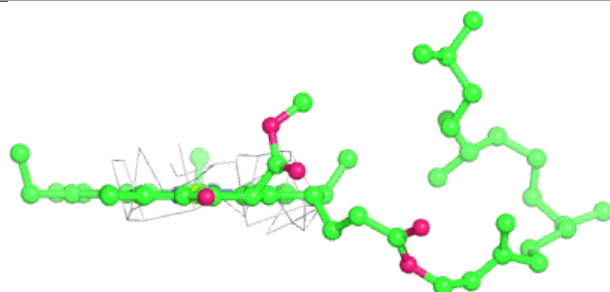
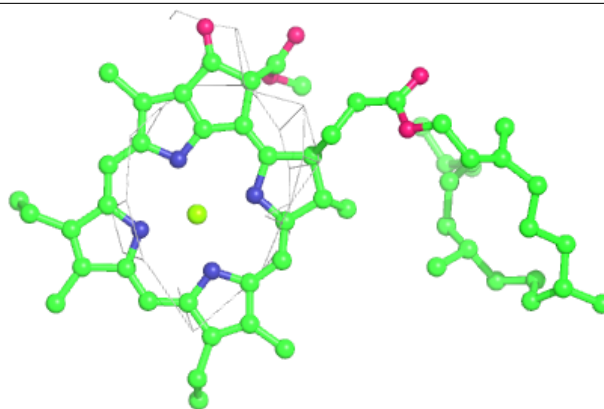
**Electron density around DGD A 407:**

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

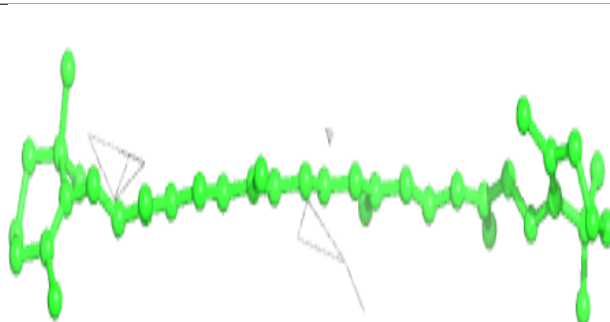
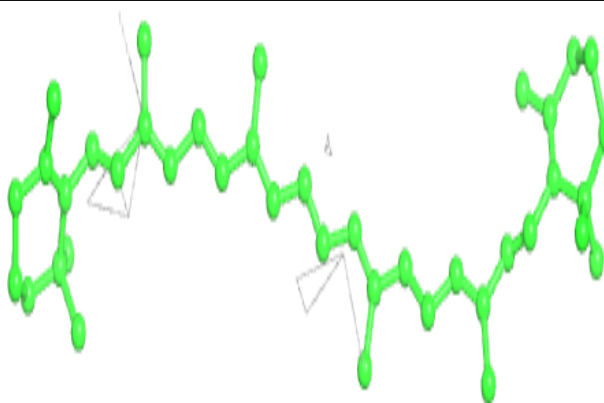


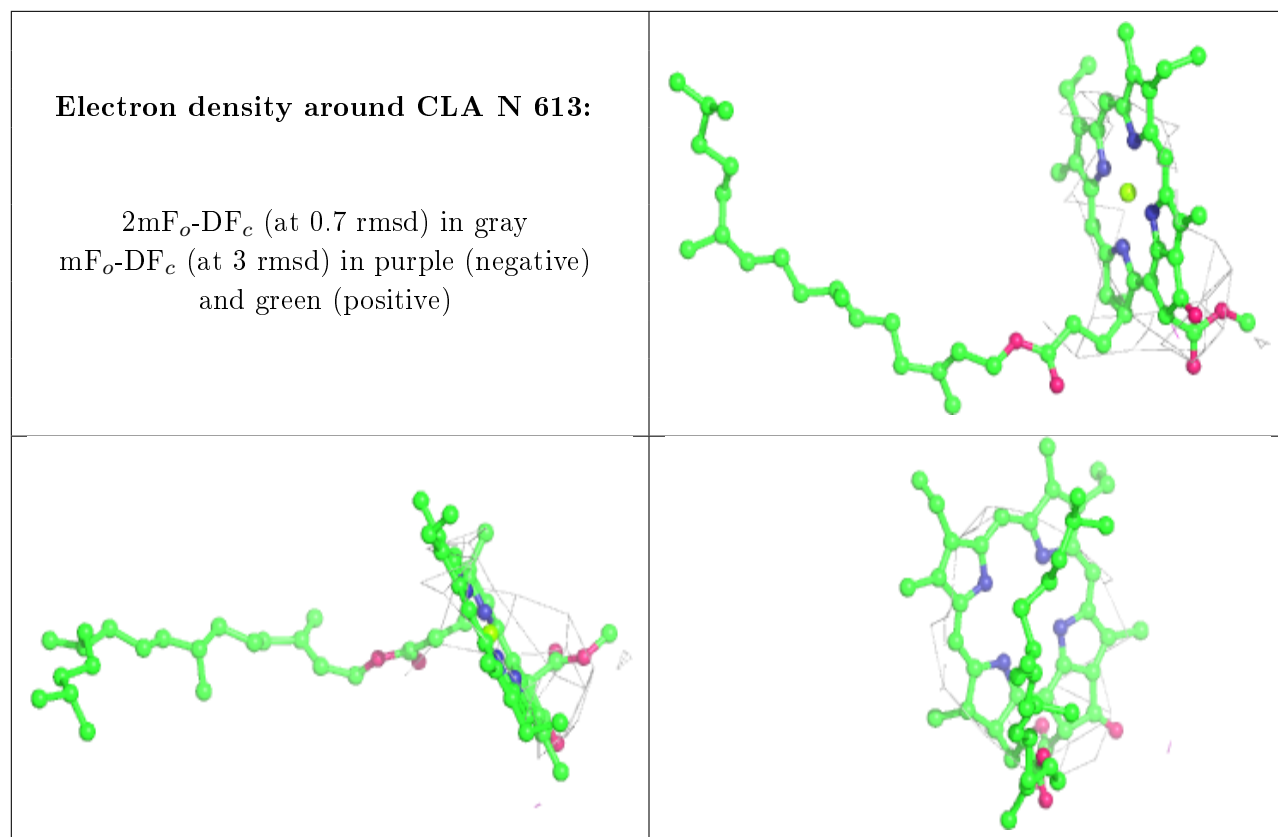
Electron density around CLA C 512:

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

**Electron density around BCR K 101:**

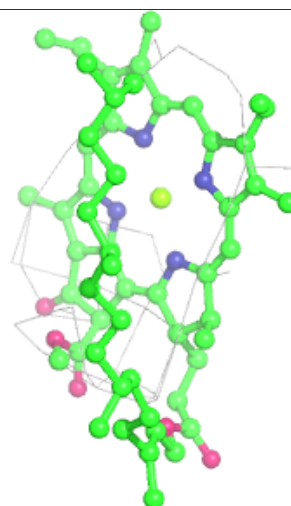
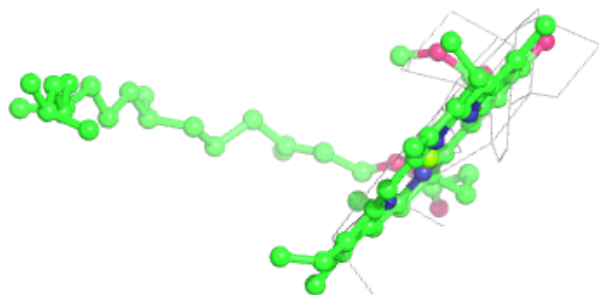
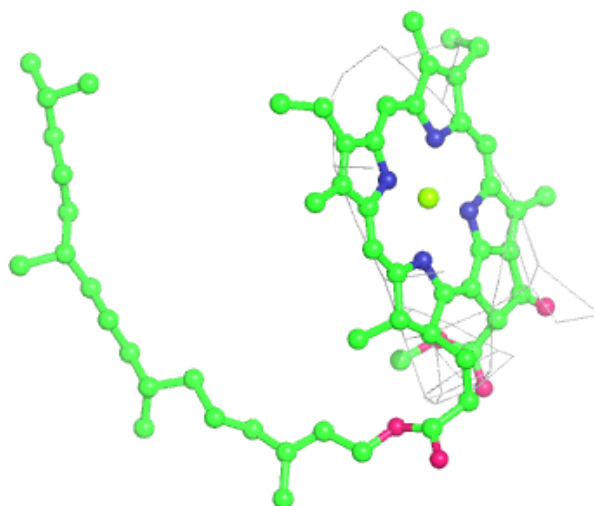
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





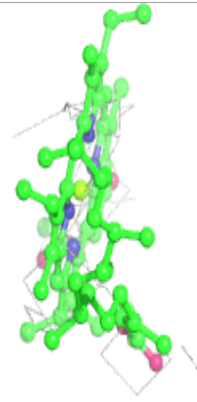
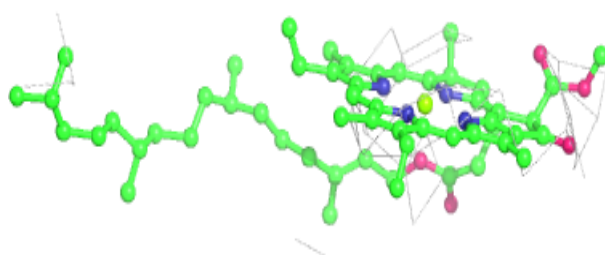
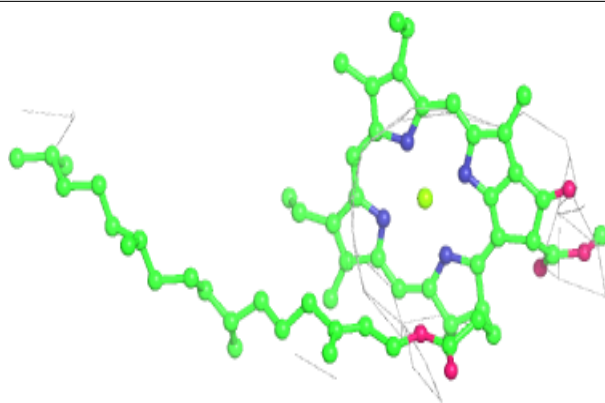
Electron density around CLA P 507:

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

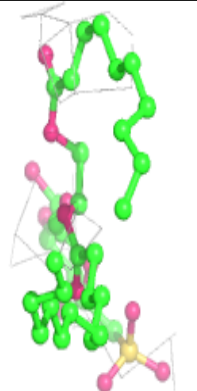
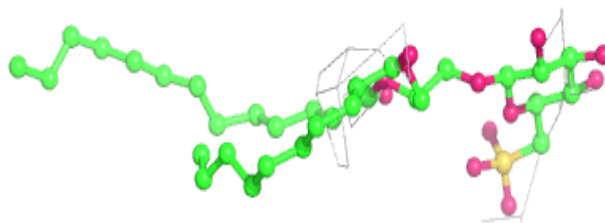
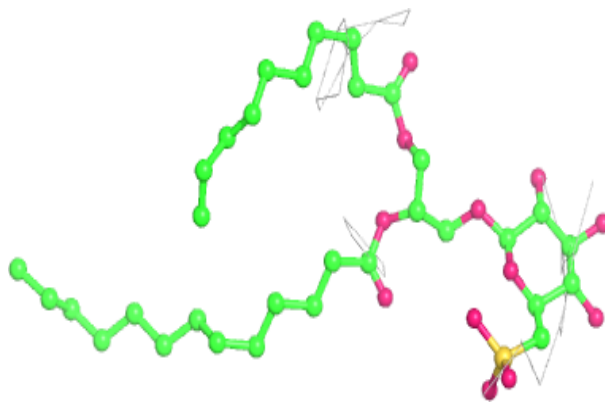


Electron density around CLA C 501:

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

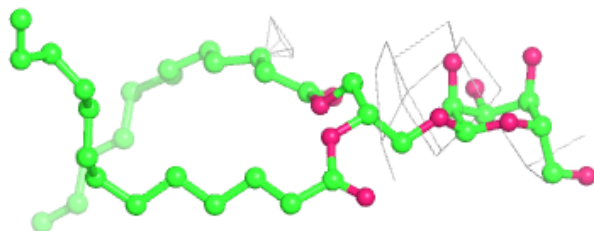
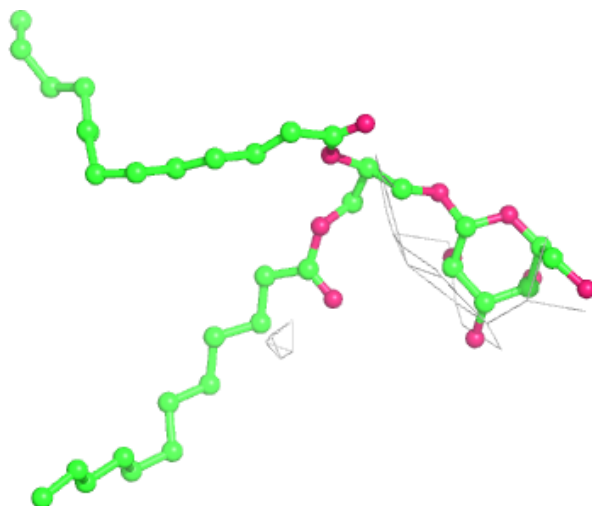
**Electron density around SQD F 101:**

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



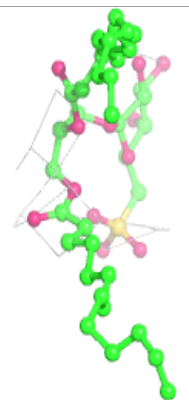
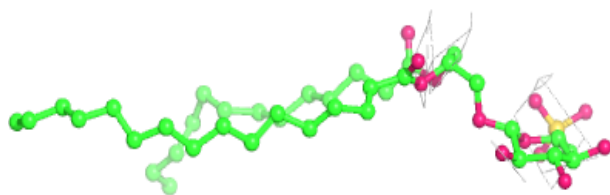
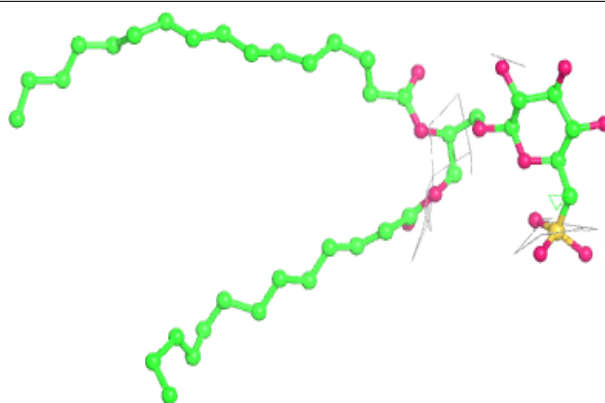
Electron density around LMG E 102:

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

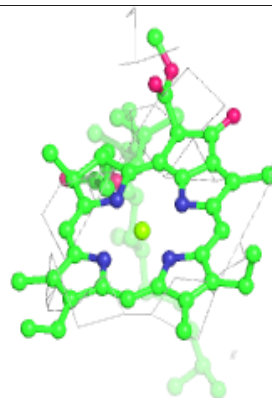
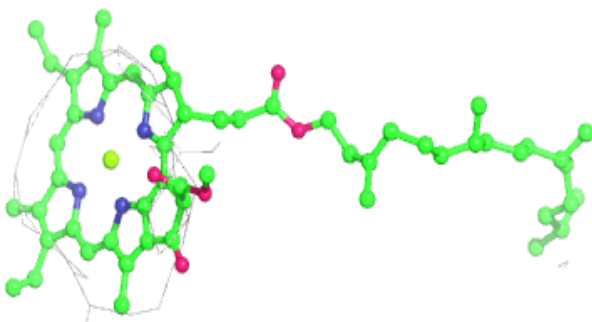
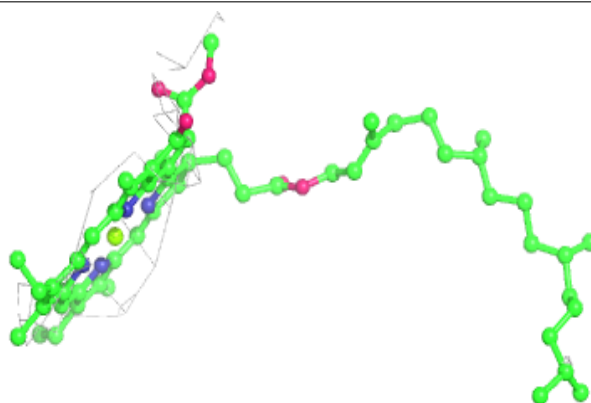


Electron density around SQD G 410:

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

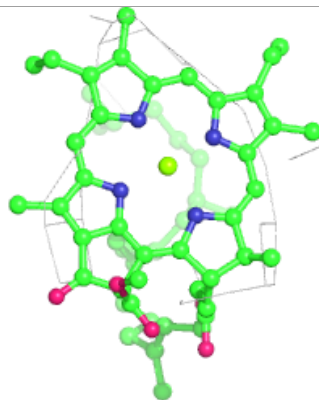
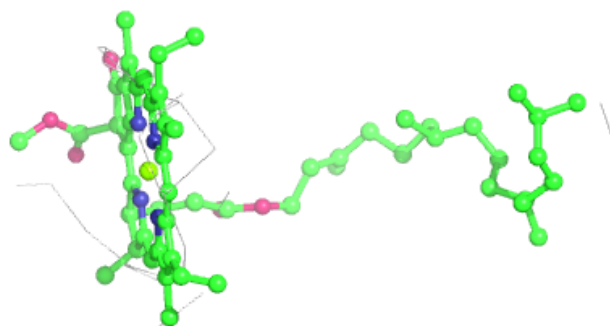
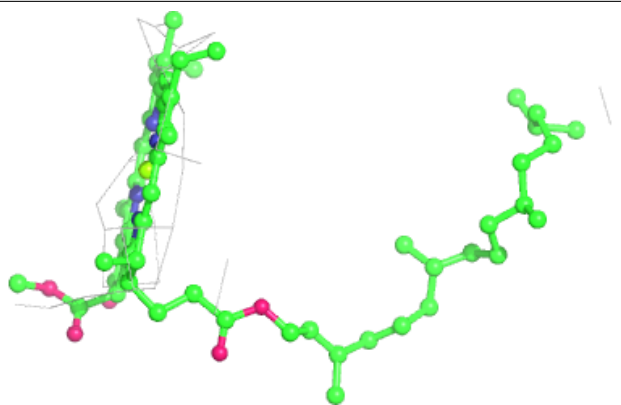
**Electron density around CLA Q 402:**

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

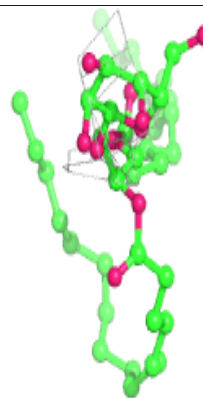
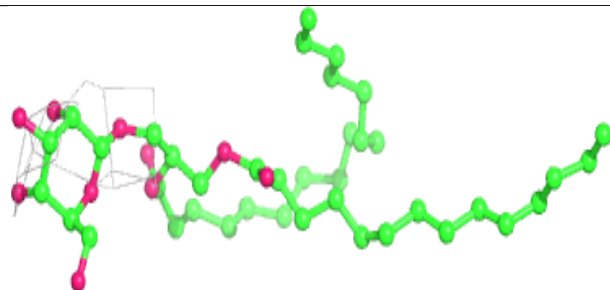
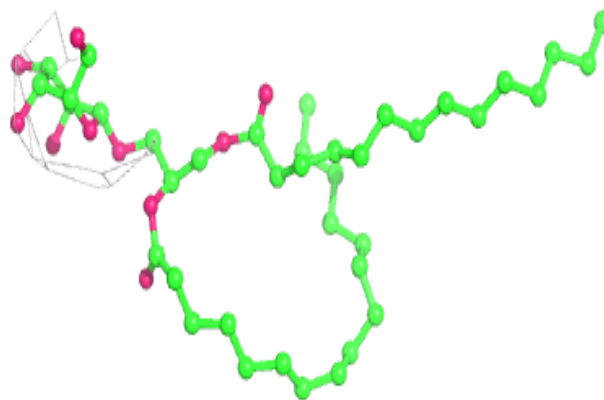


Electron density around CLA C 506:

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

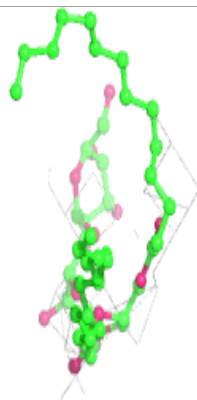
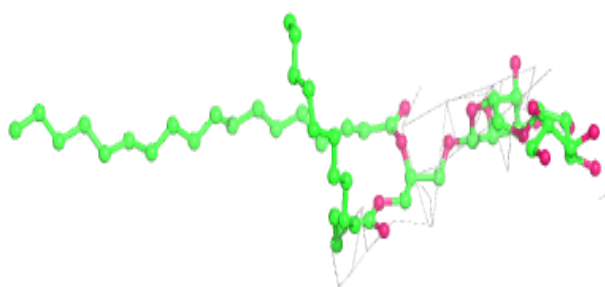
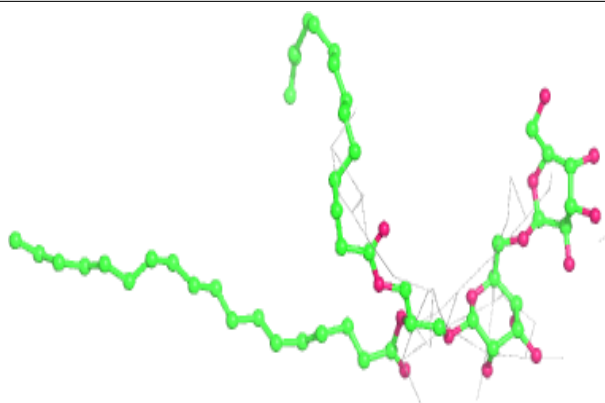
**Electron density around LMG B 622:**

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

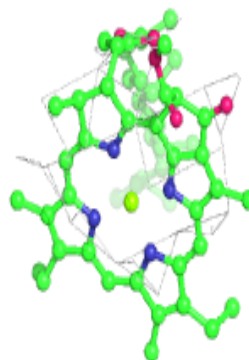
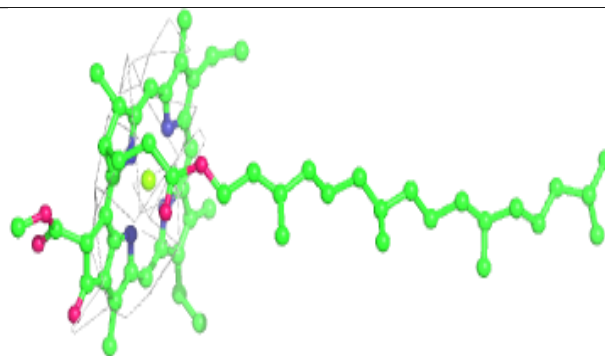
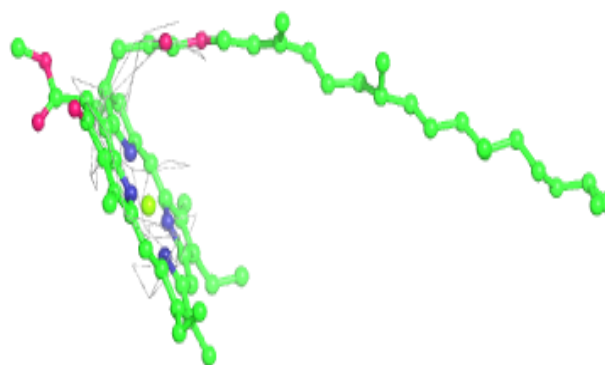


Electron density around DGD C 517:

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

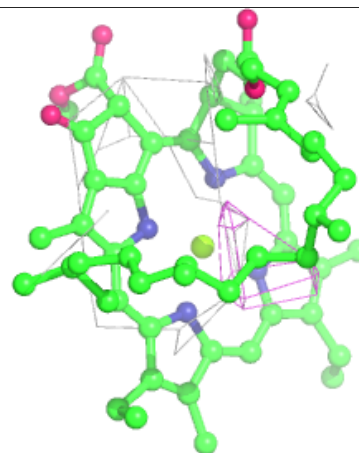
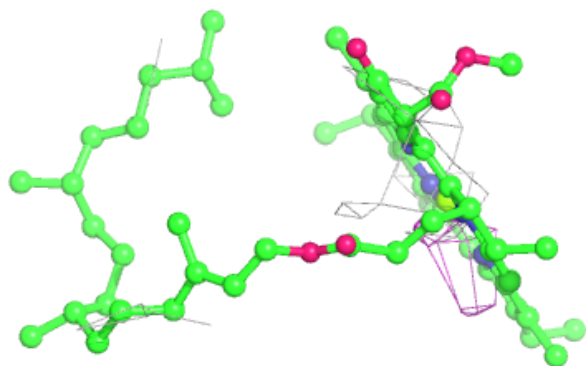
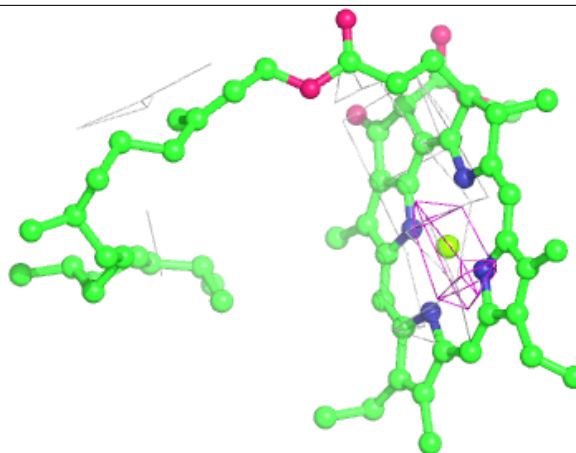
**Electron density around CLA B 607:**

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

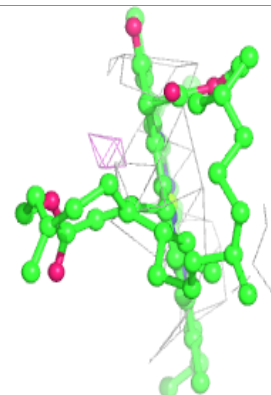
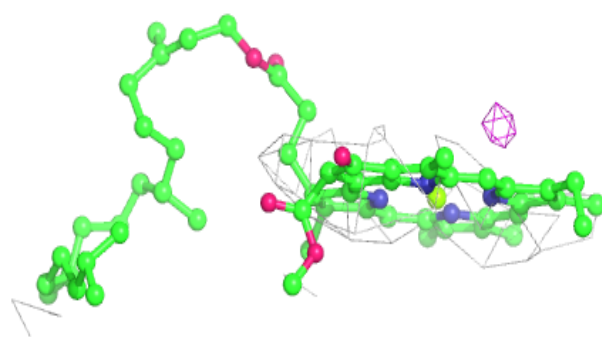
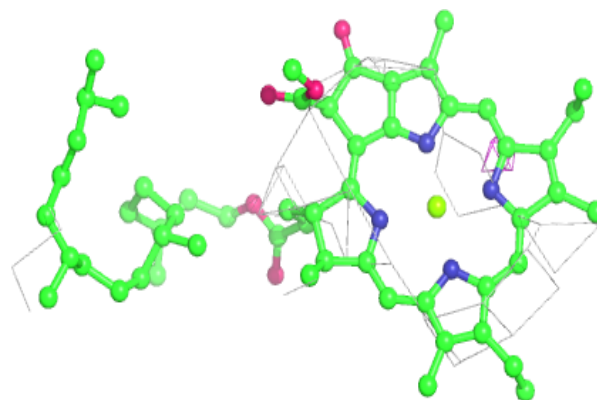


Electron density around CLA P 503:

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

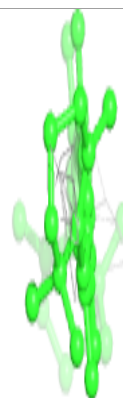
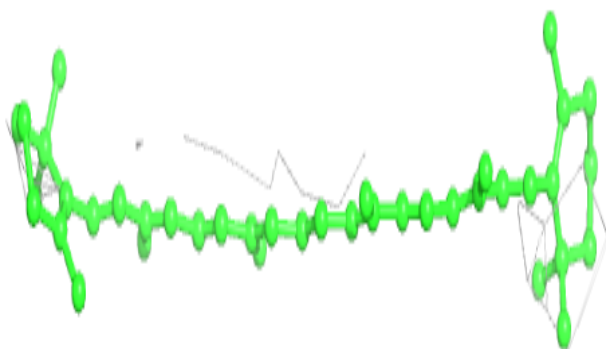
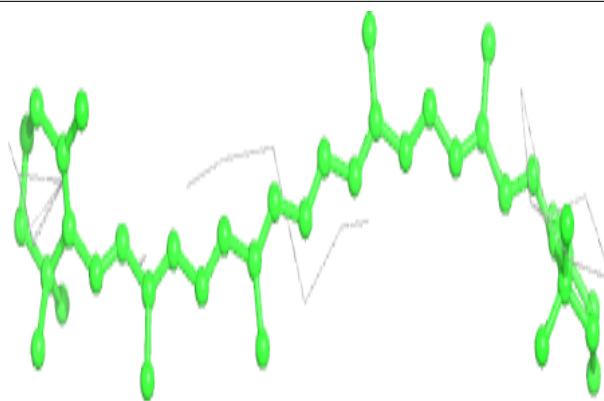
**Electron density around CLA N 616:**

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

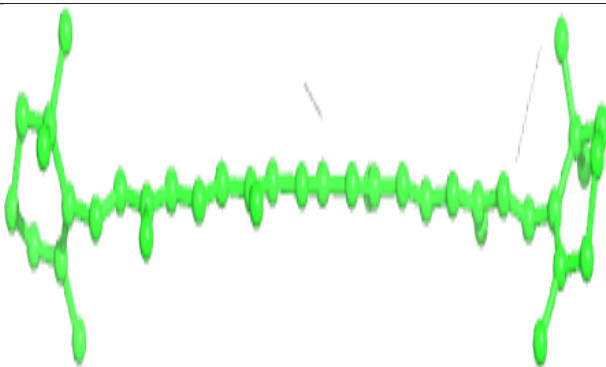
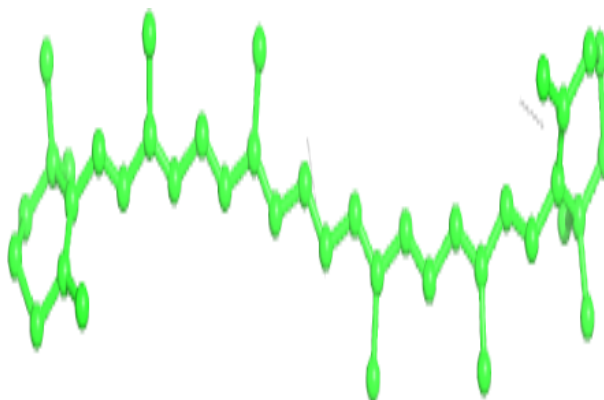


Electron density around BCR W 101:

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

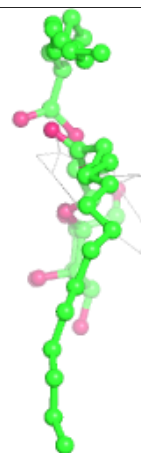
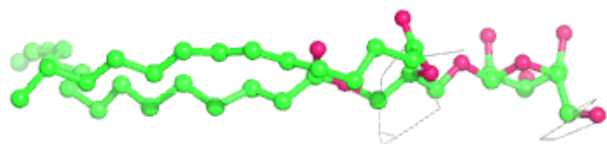
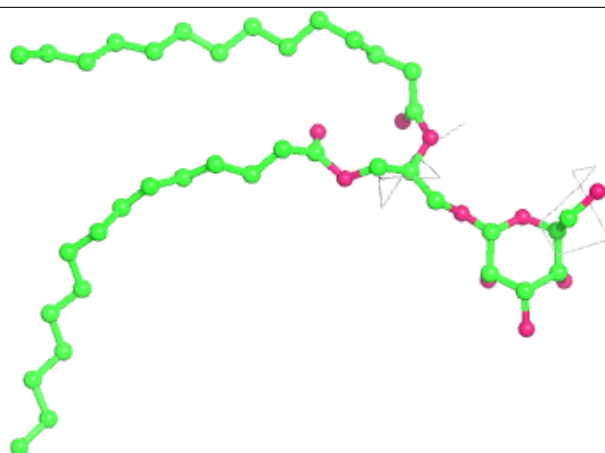
**Electron density around BCR B 619:**

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

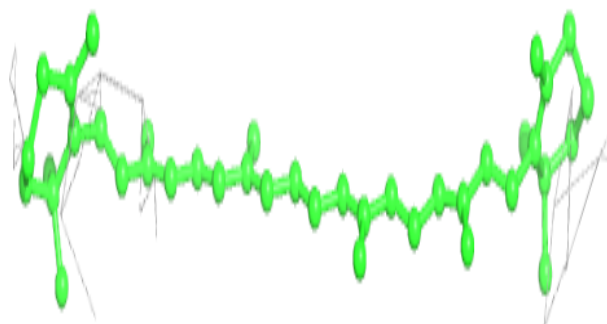
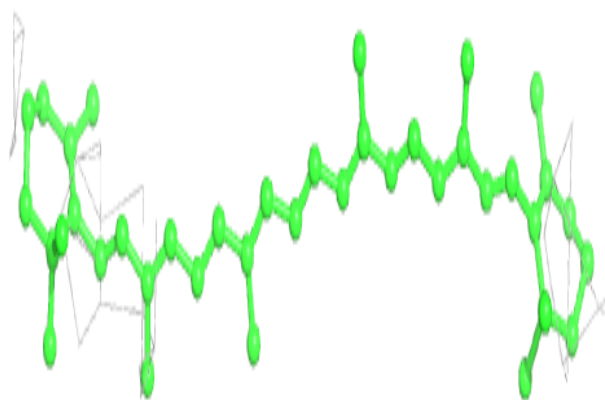


Electron density around LMG P 520:

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

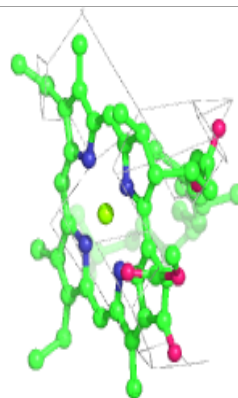
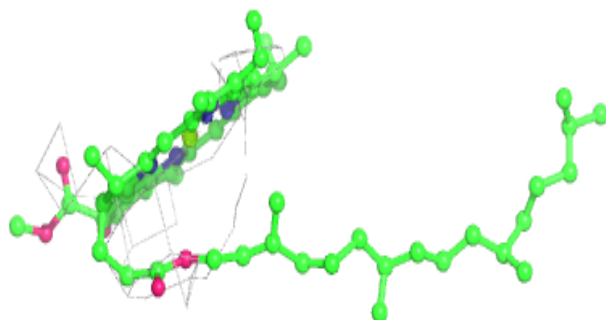
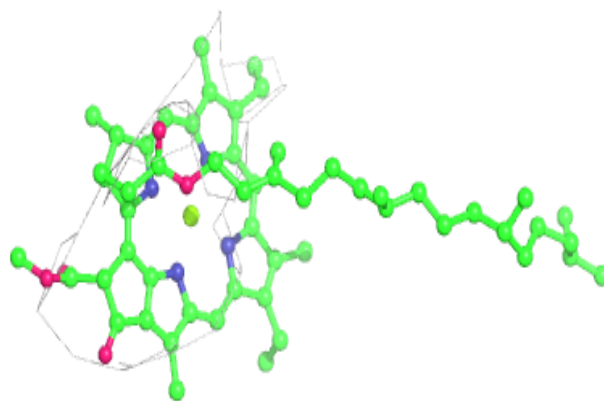
**Electron density around BCR C 515:**

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

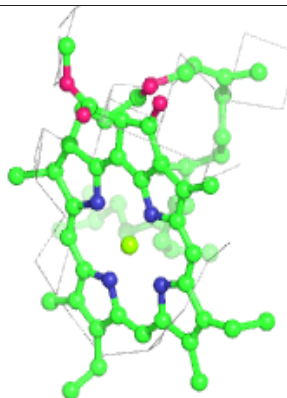
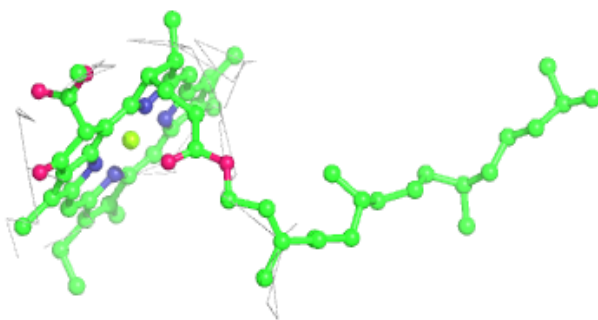
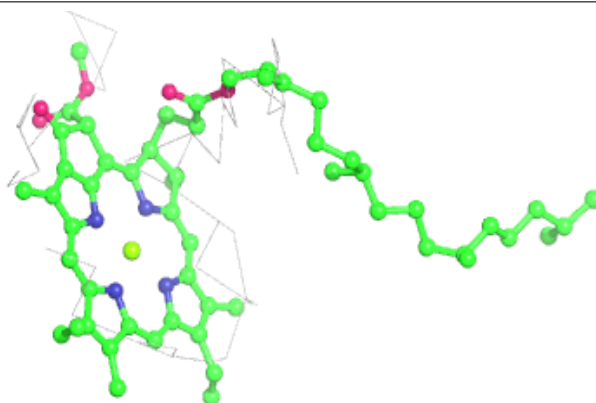


Electron density around CLA B 608:

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

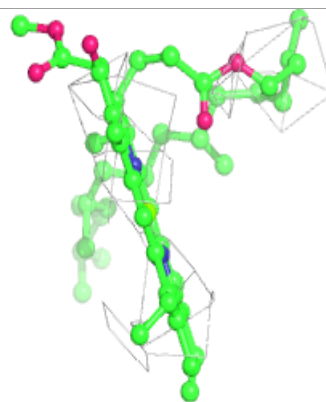
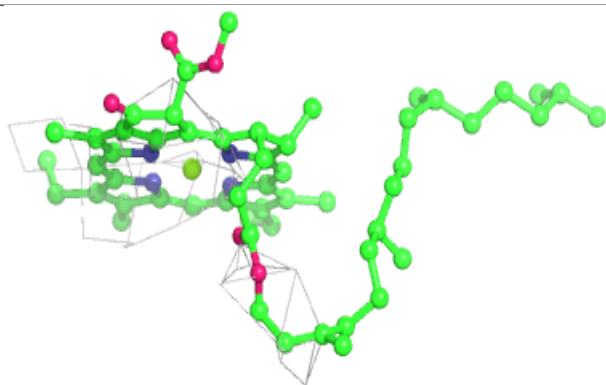
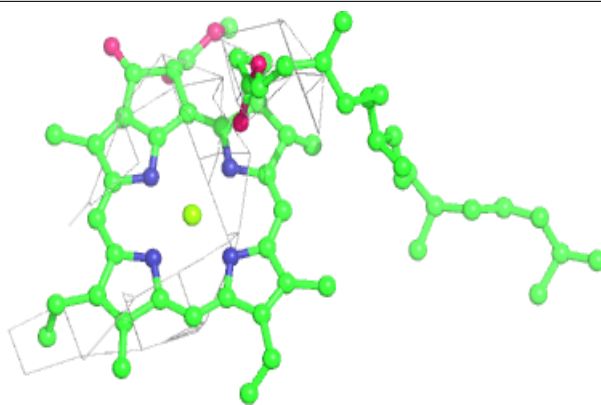
**Electron density around CLA C 511:**

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

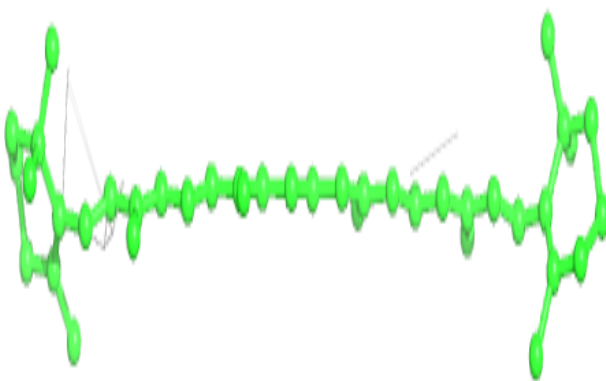
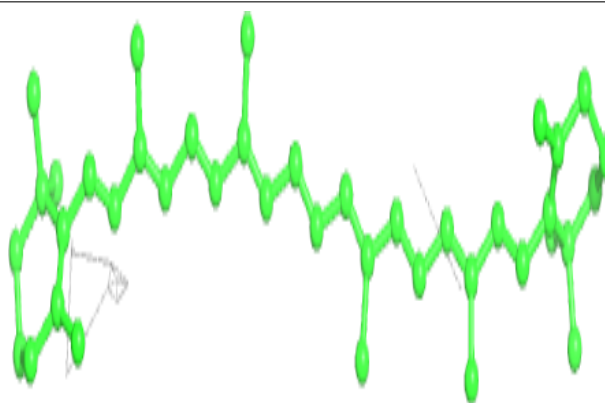


Electron density around CLA G 403:

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

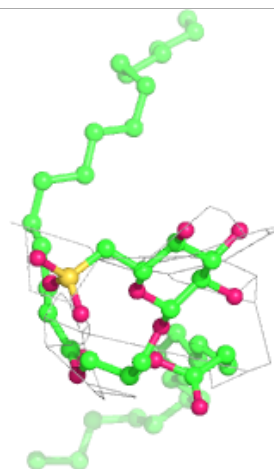
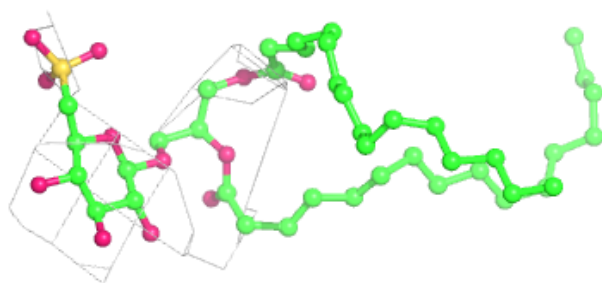
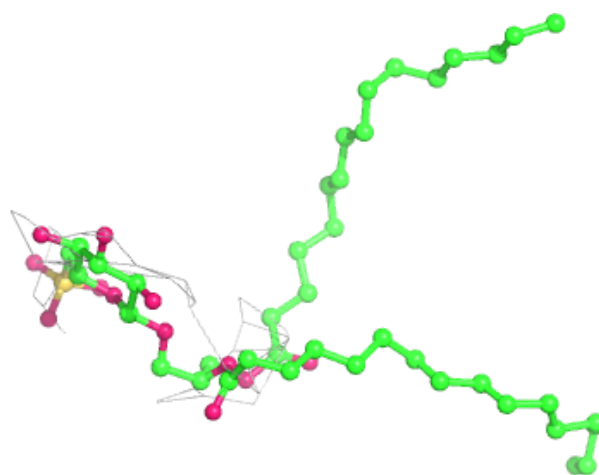
**Electron density around BCR N 621:**

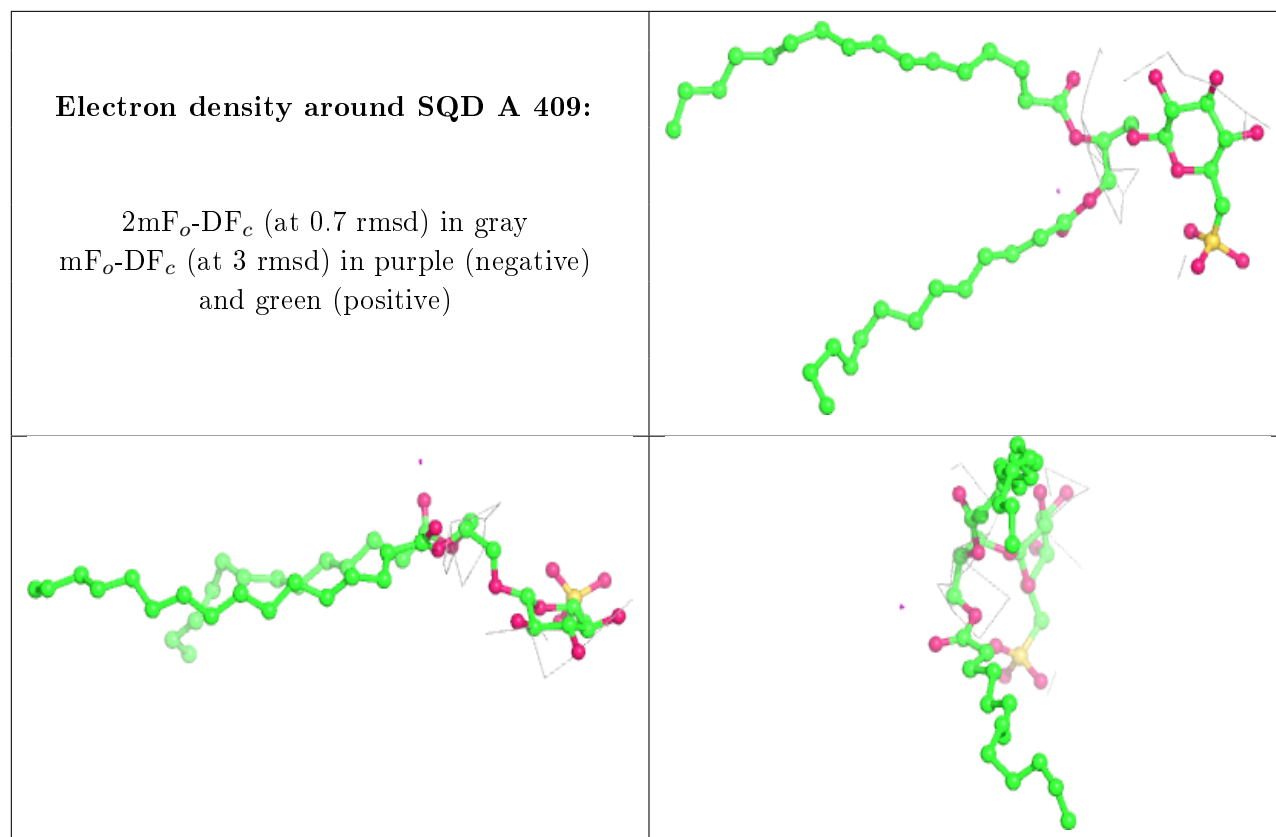
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SQD G 401:

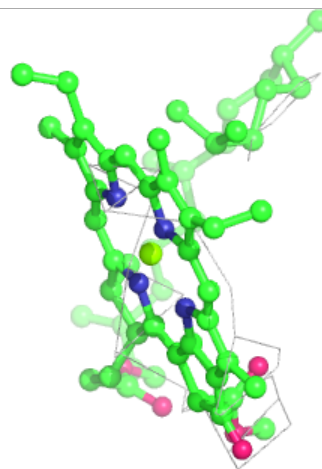
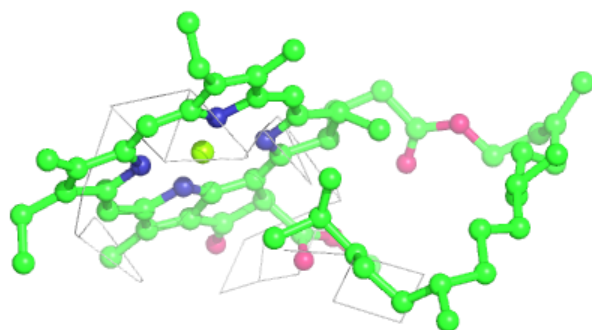
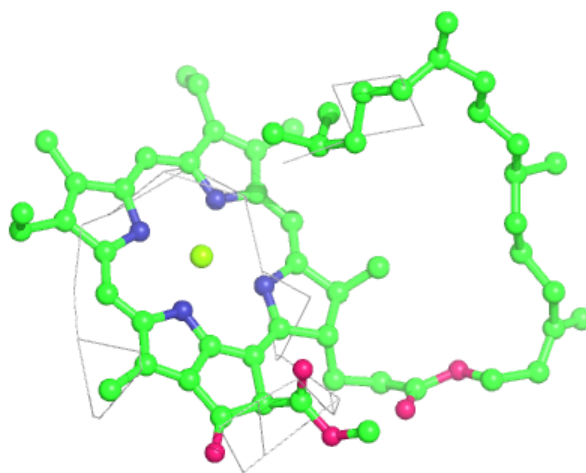
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





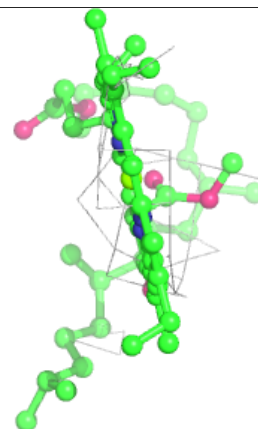
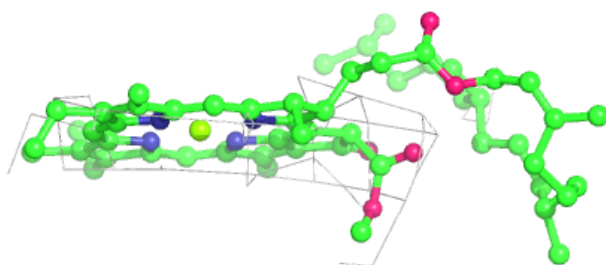
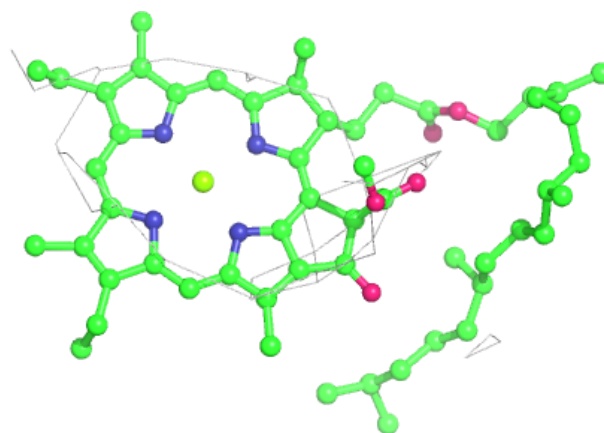
Electron density around CLA B 615:

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

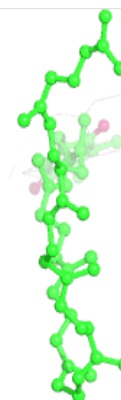
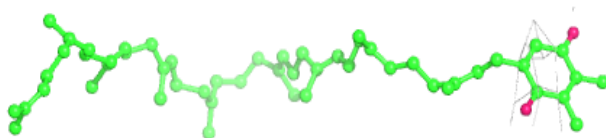
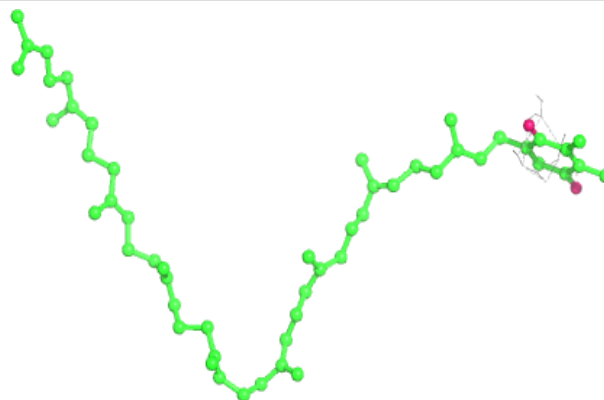


Electron density around CLA N 614:

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

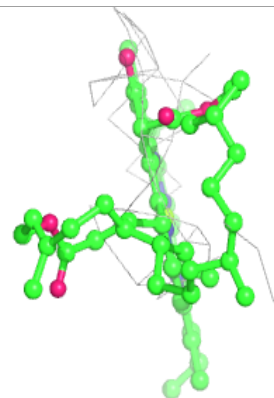
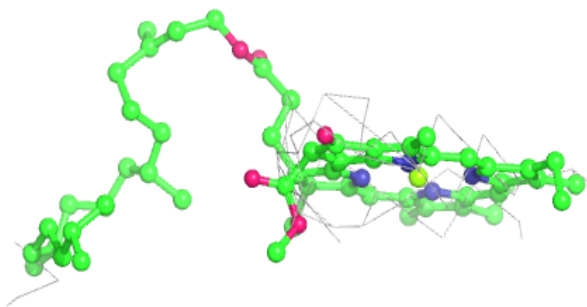
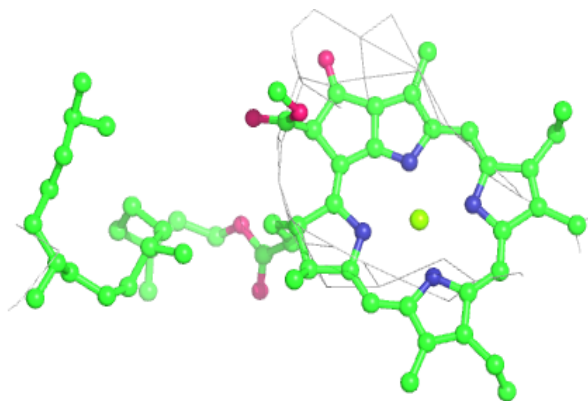
**Electron density around PL9 Q 405:**

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

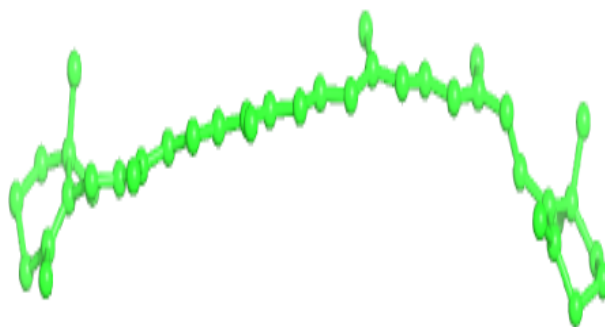
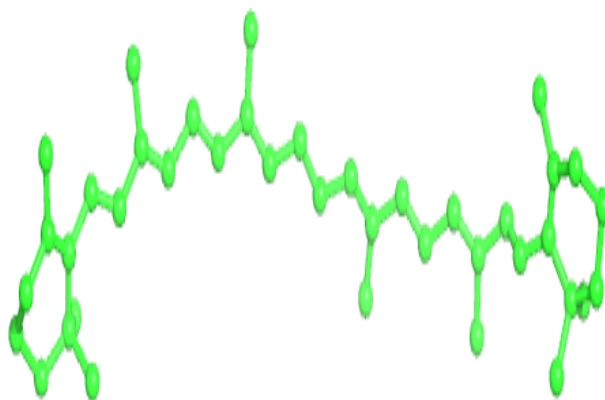


Electron density around CLA B 612:

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

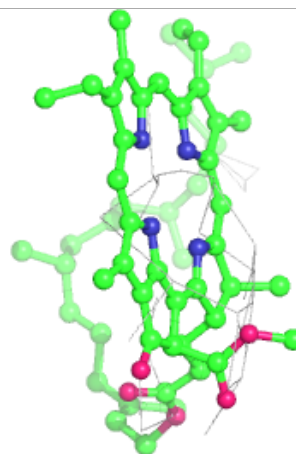
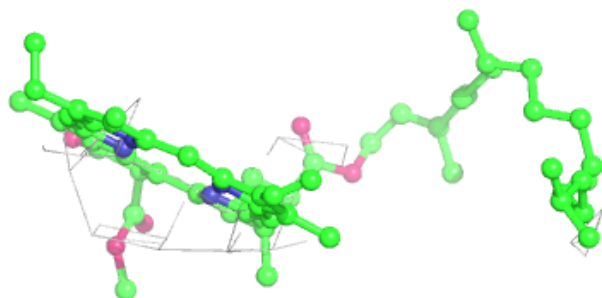
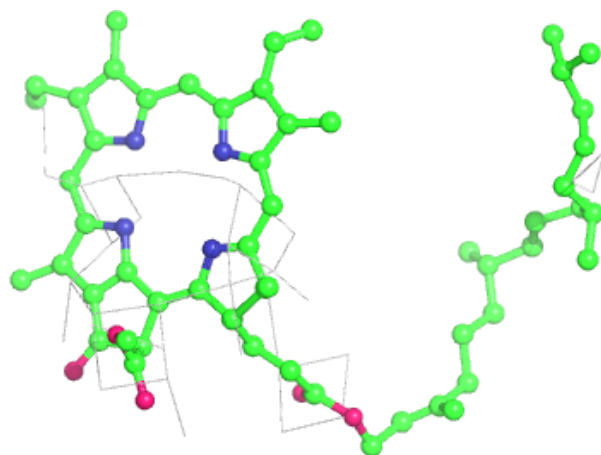
**Electron density around BCR T 102:**

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



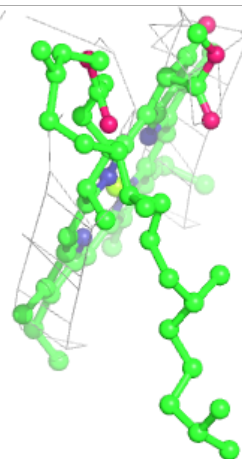
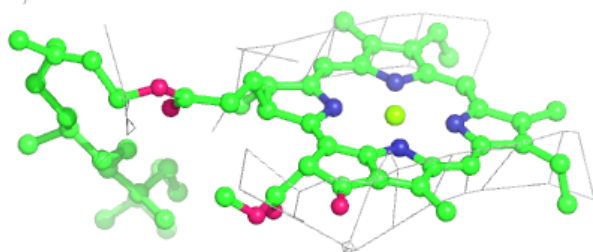
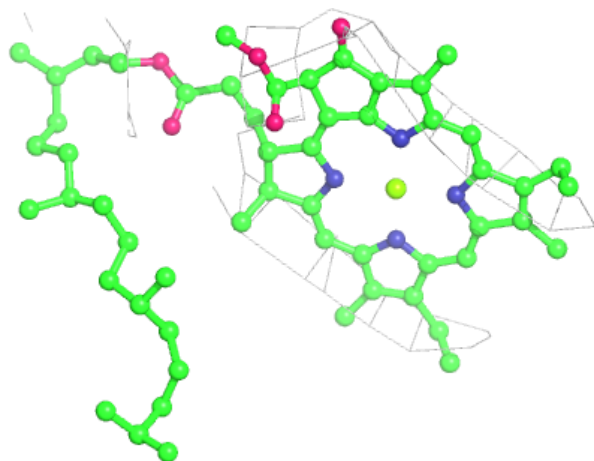
Electron density around PHO Q 403:

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



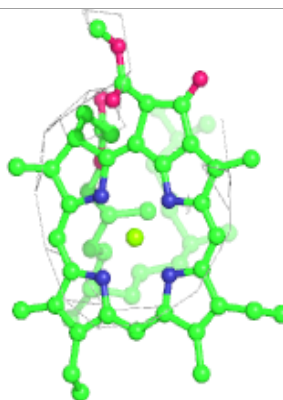
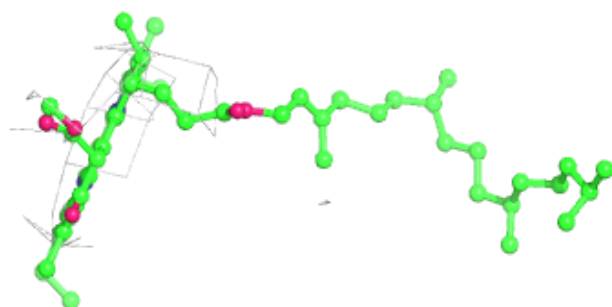
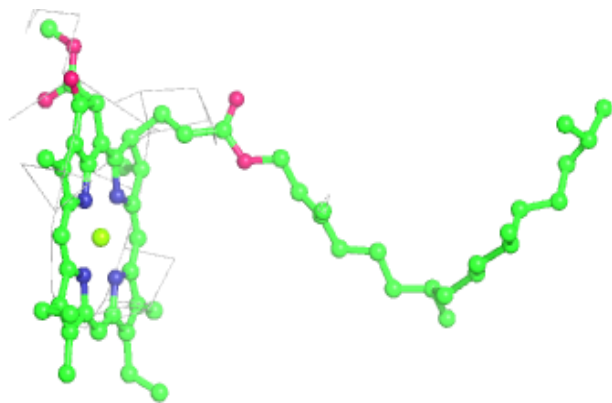
Electron density around CLA B 616:

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

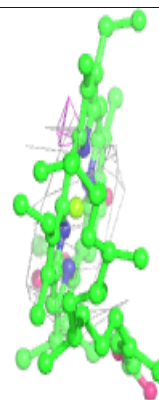
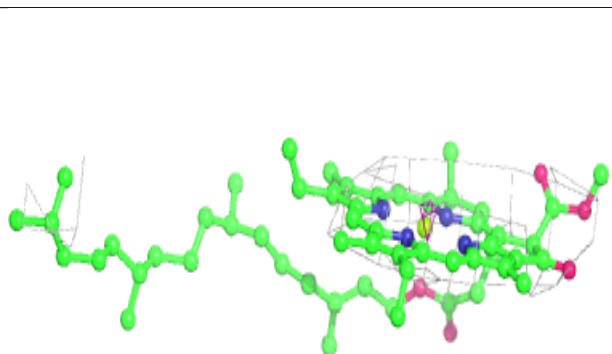
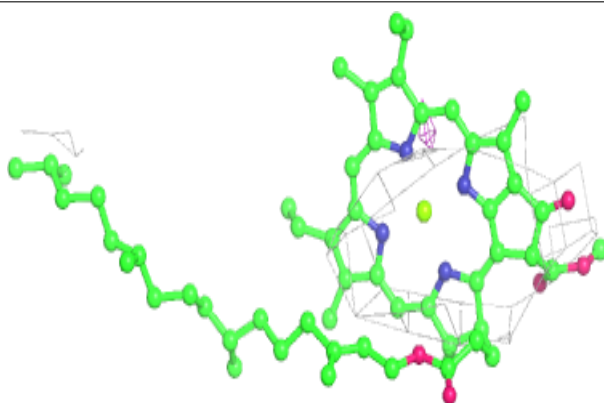


Electron density around CLA Q 404:

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

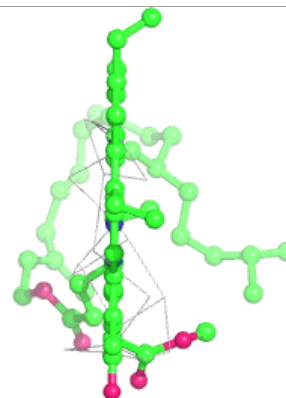
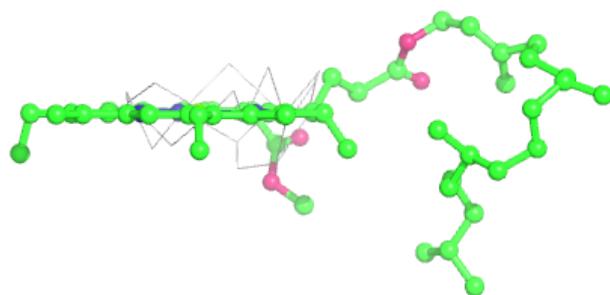
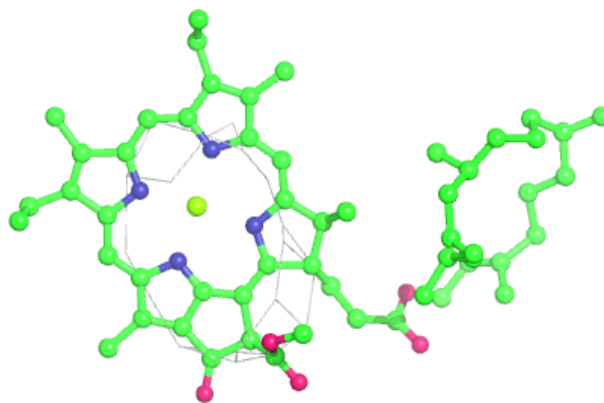
**Electron density around CLA P 501:**

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



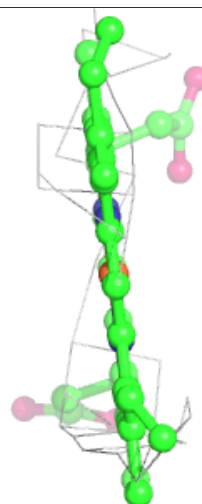
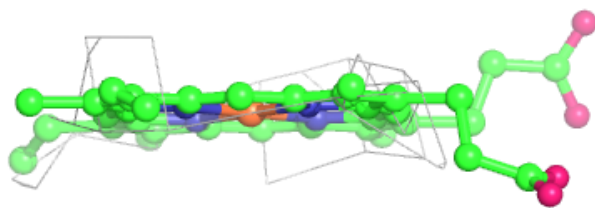
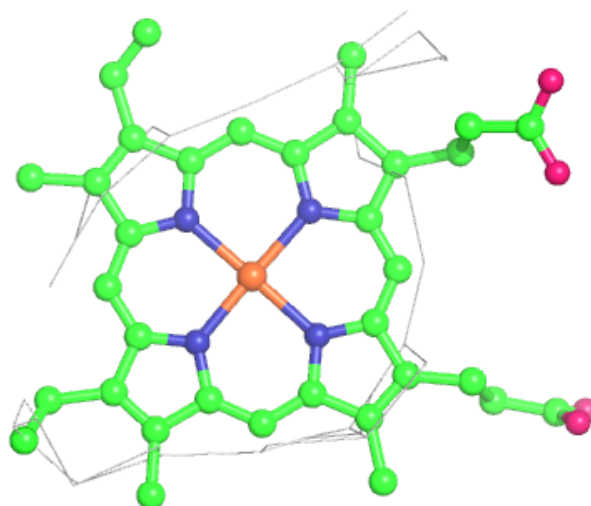
Electron density around CLA P 512:

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



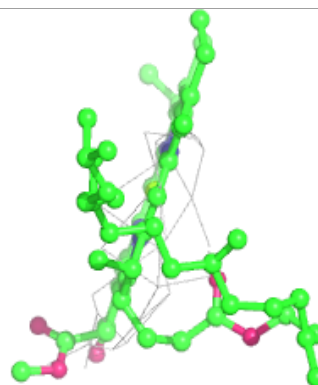
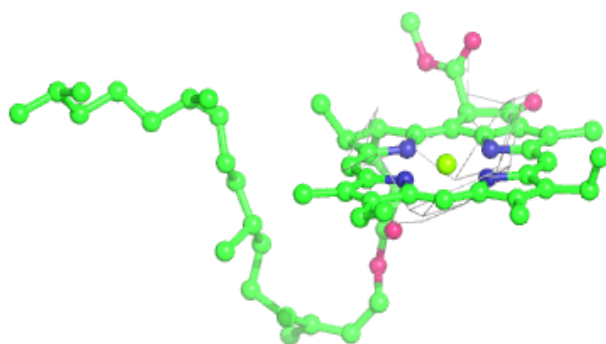
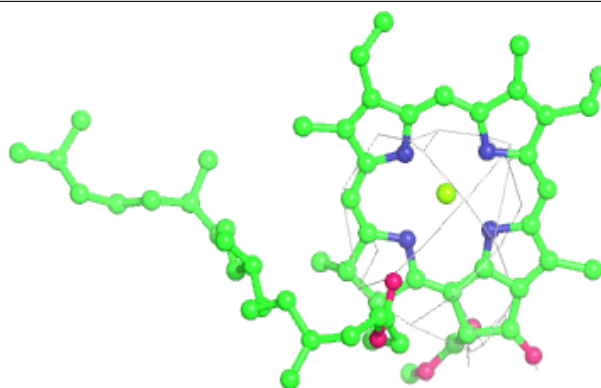
Electron density around HEM V 201:

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

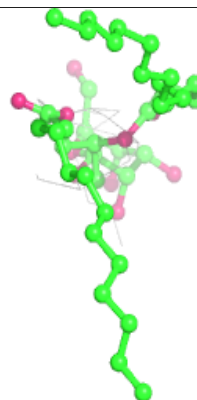
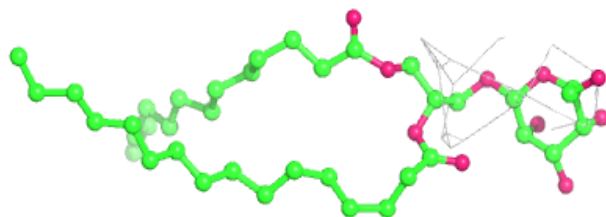
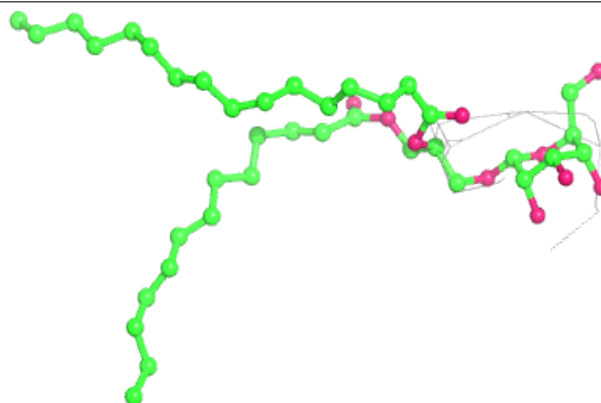


Electron density around CLA A 402:

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

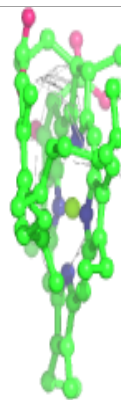
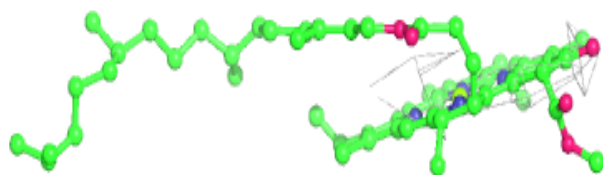
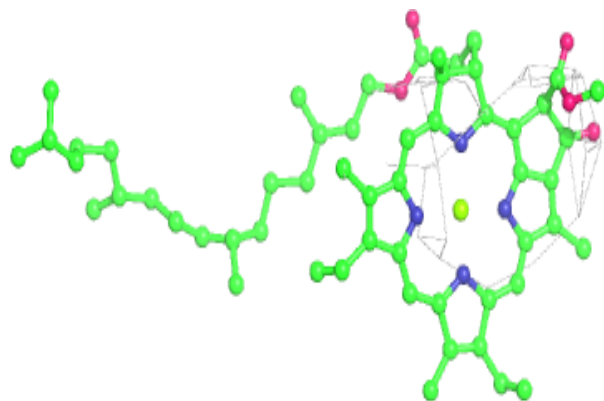
**Electron density around LMG Q 407:**

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

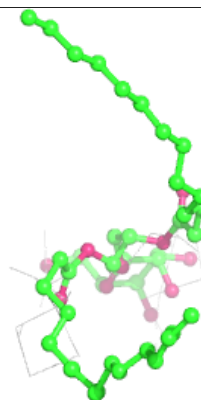
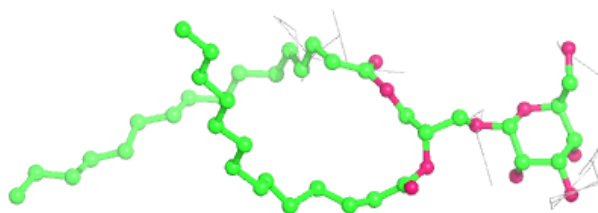
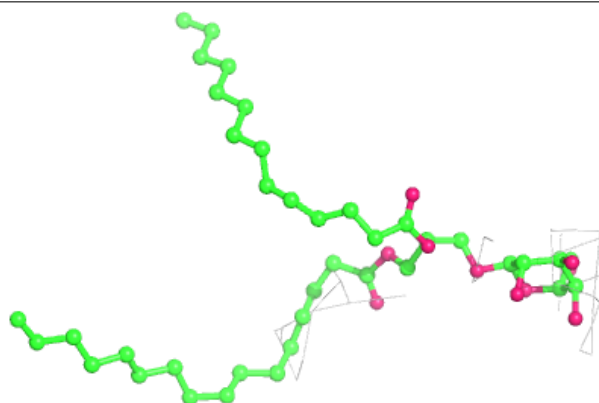


Electron density around CLA B 603:

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

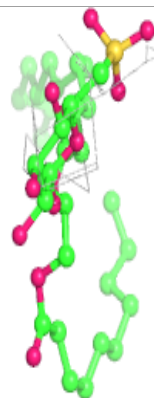
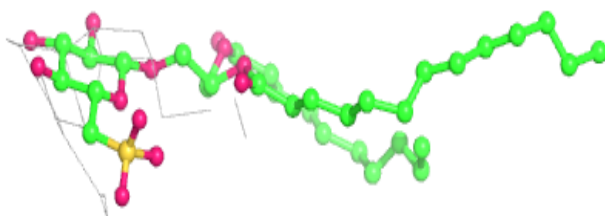
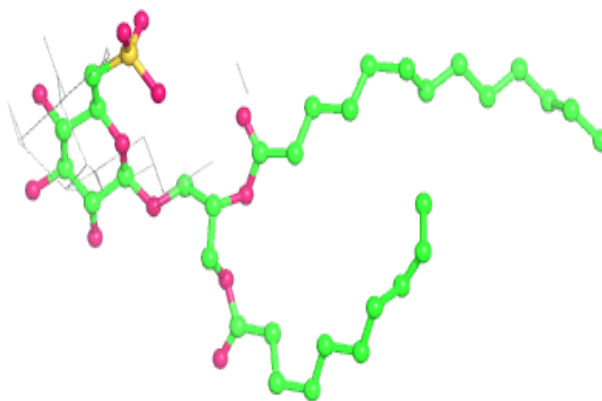
**Electron density around LMG N 623:**

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

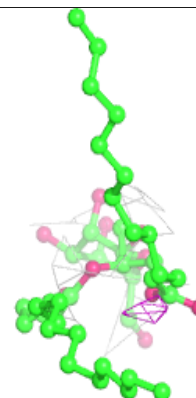
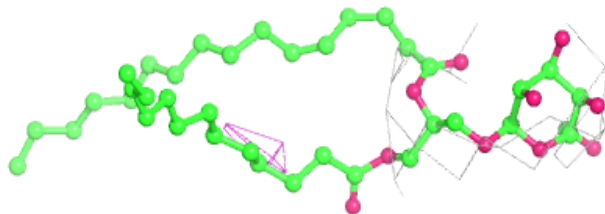
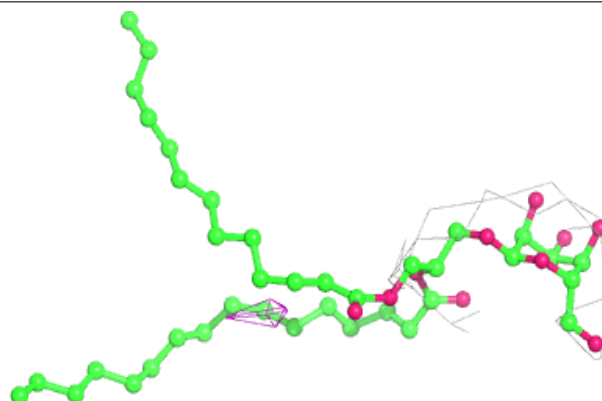


Electron density around SQD S 102:

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

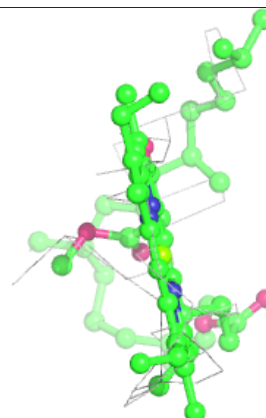
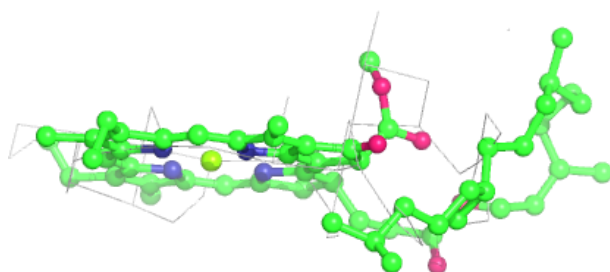
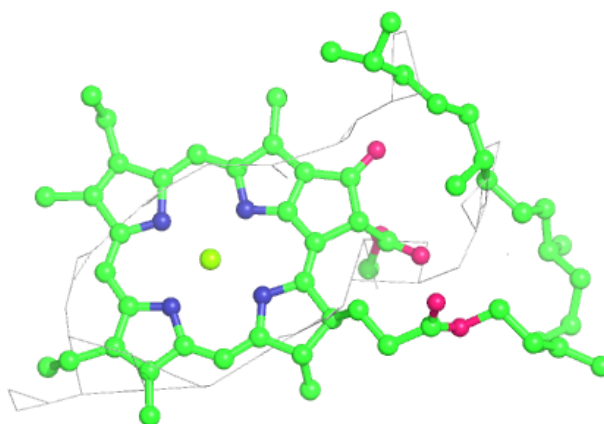
**Electron density around LMG D 407:**

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

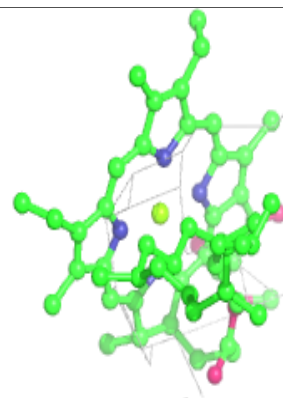
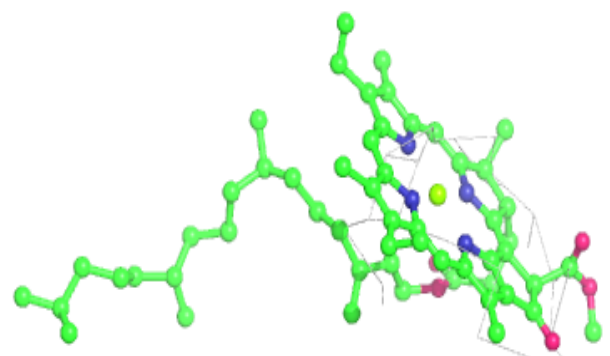
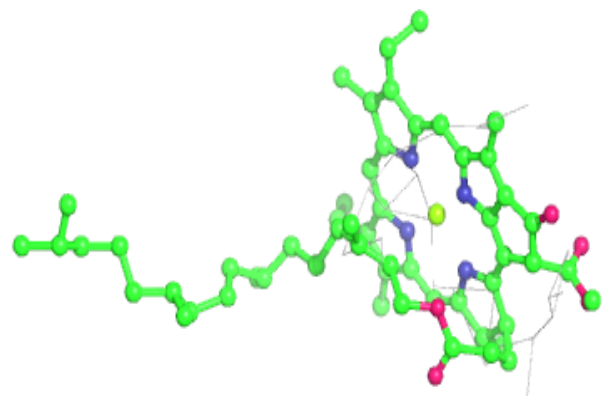


Electron density around CLA B 610:

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

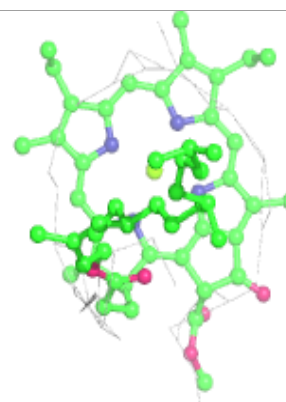
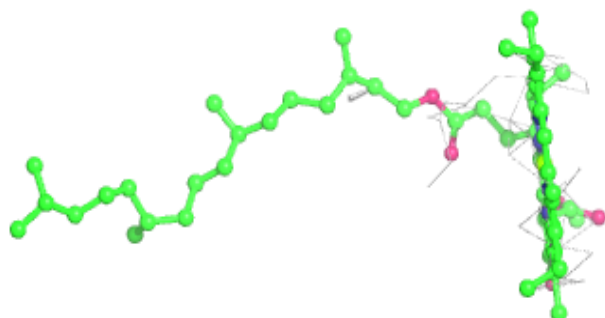
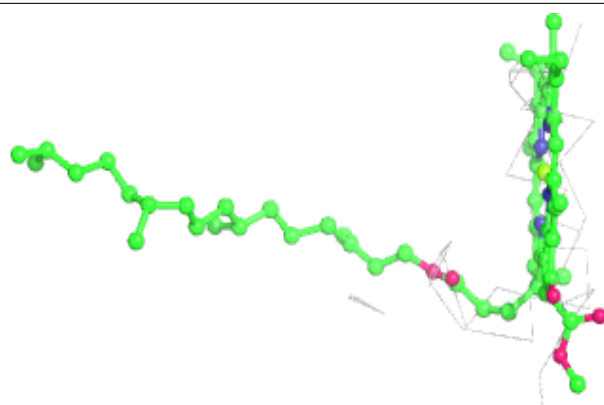
**Electron density around CLA P 505:**

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

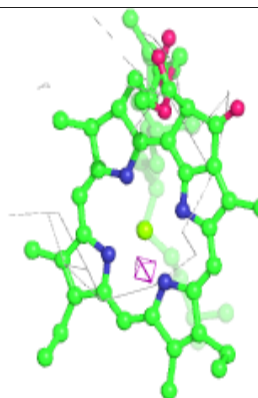
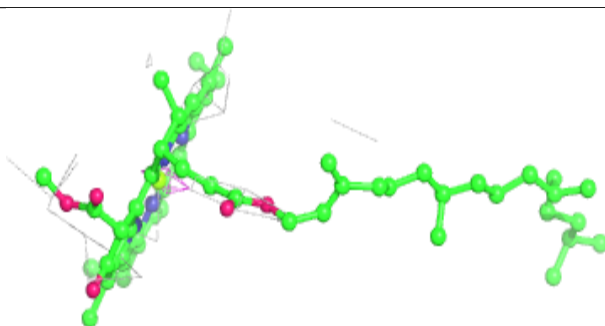
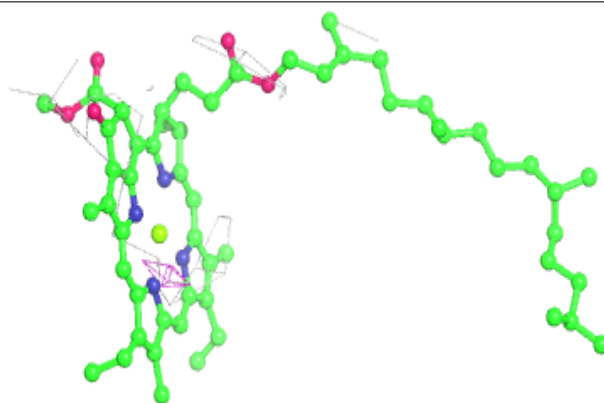


Electron density around CLA B 606:

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

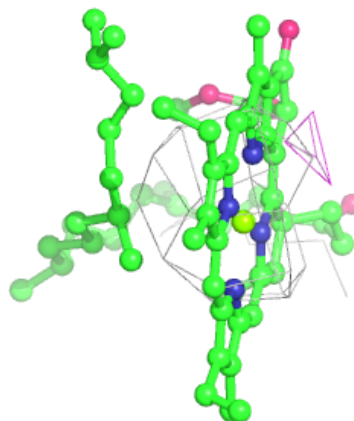
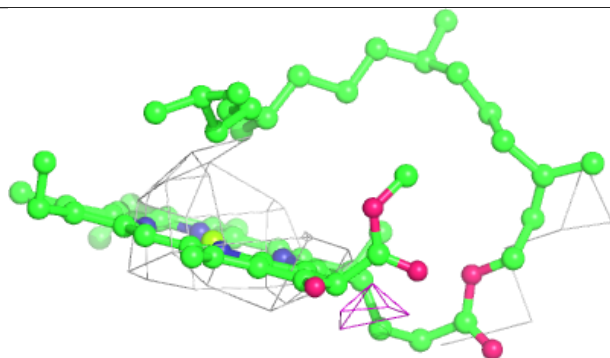
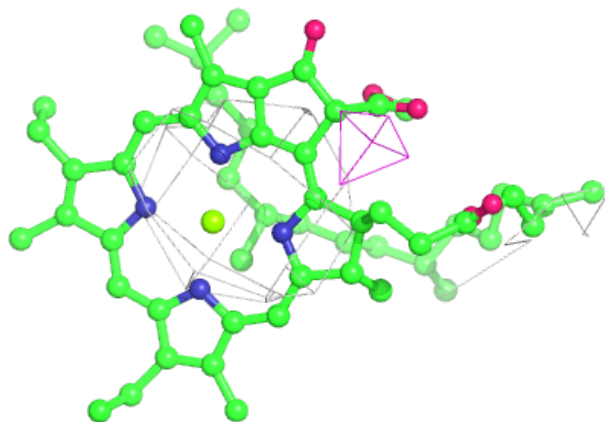
**Electron density around CLA B 609:**

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

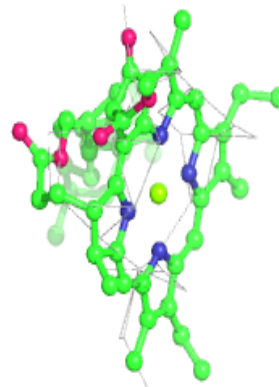
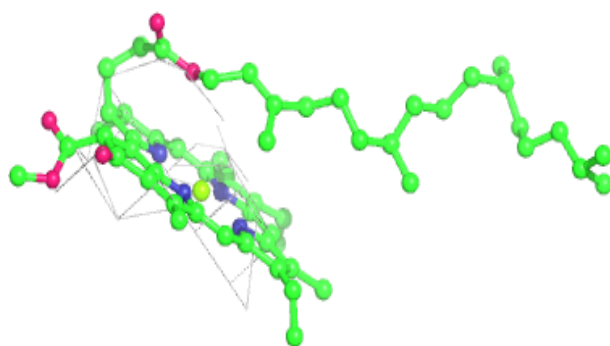
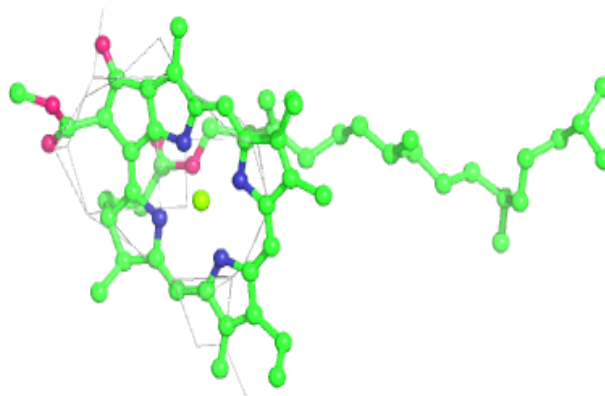


Electron density around CLA P 510:

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

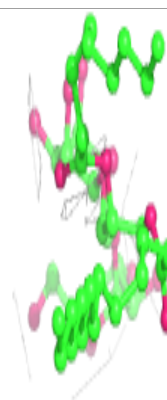
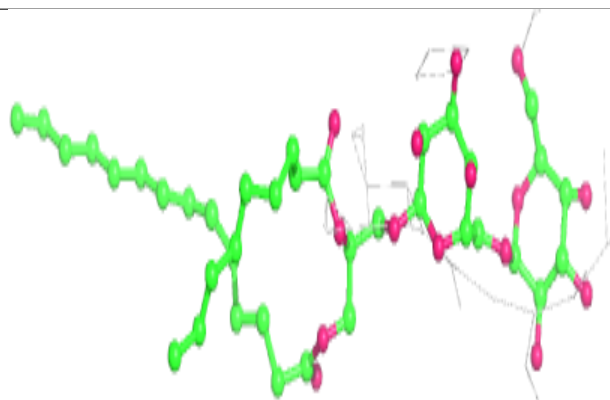
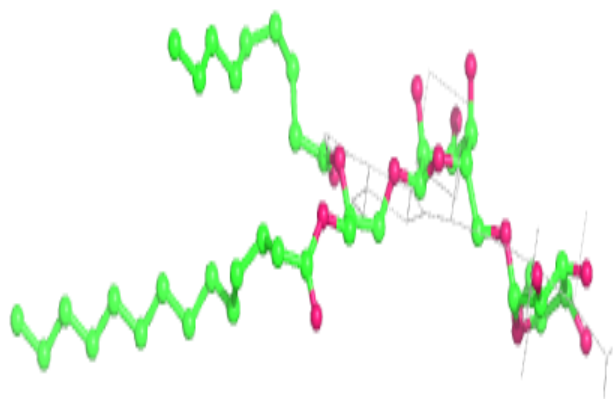
**Electron density around CLA B 614:**

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

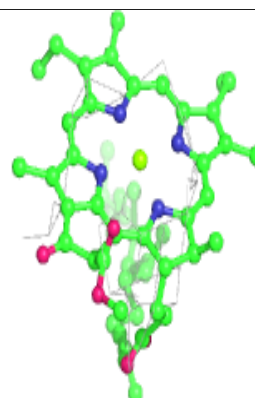
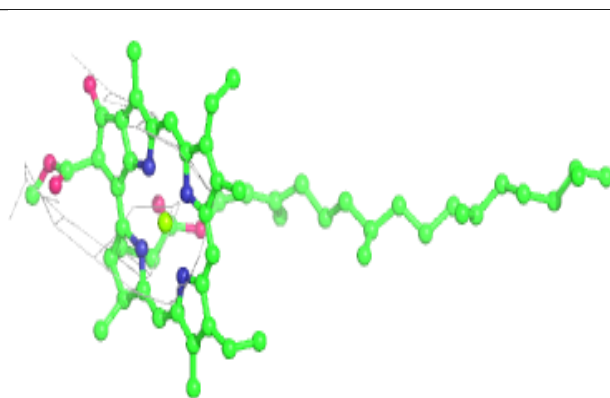
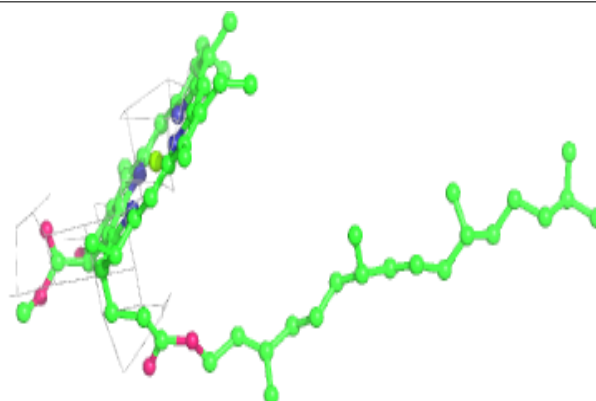


Electron density around DGD C 516:

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

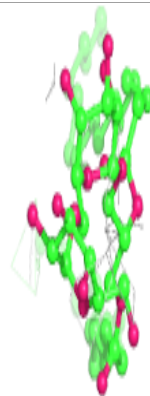
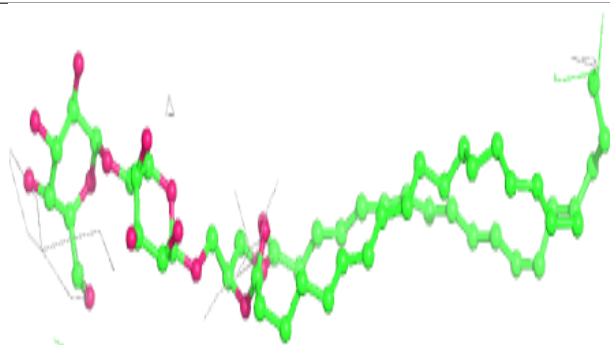
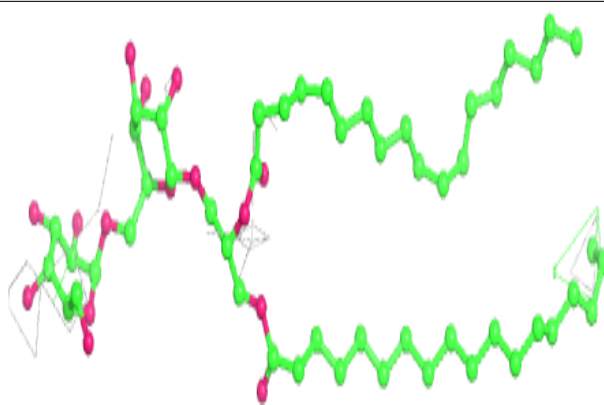
**Electron density around CLA P 504:**

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

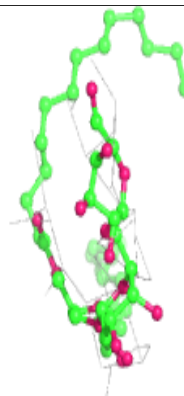
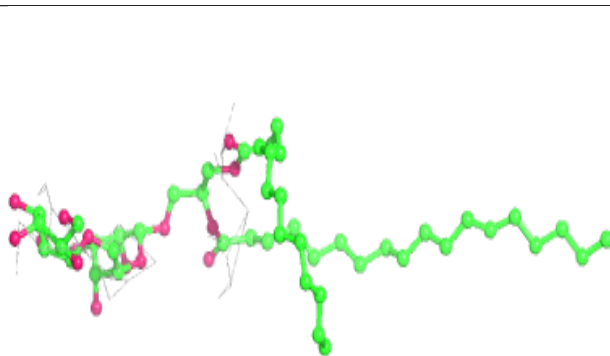
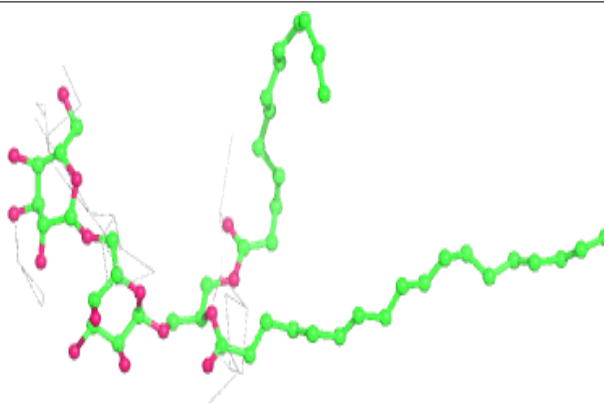


Electron density around DGD P 519:

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

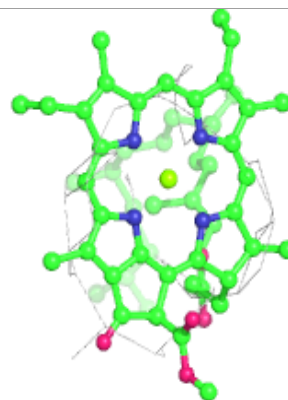
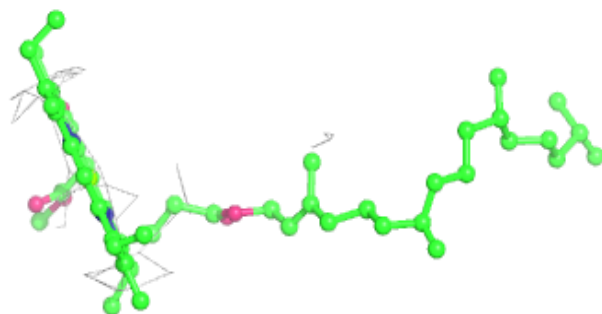
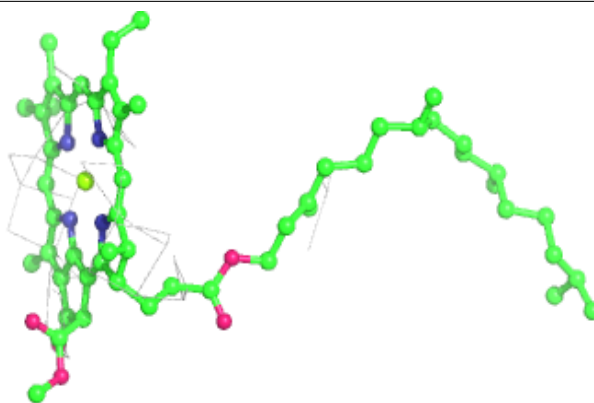
**Electron density around DGD P 518:**

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



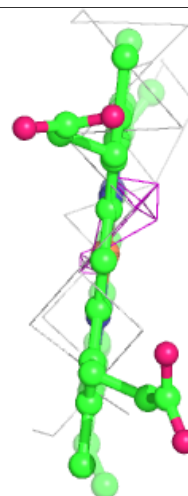
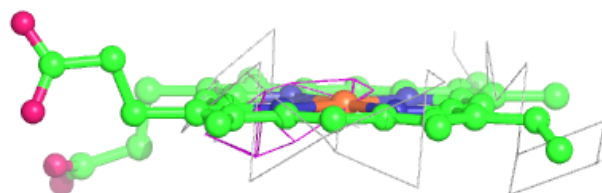
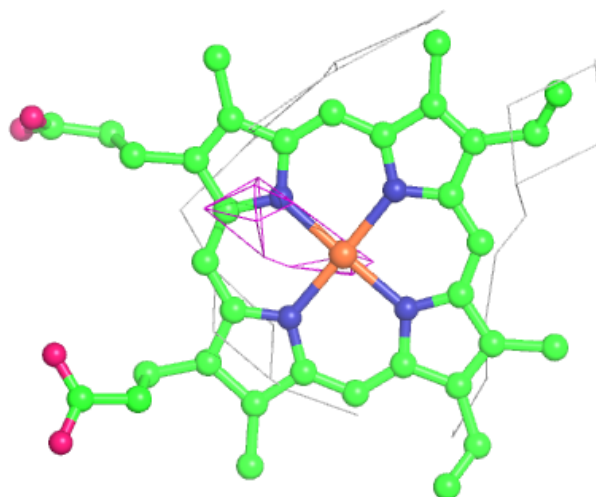
Electron density around CLA D 403:

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



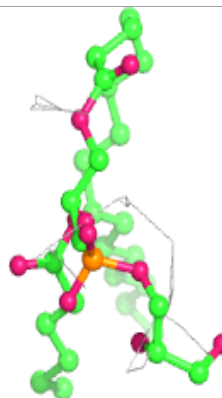
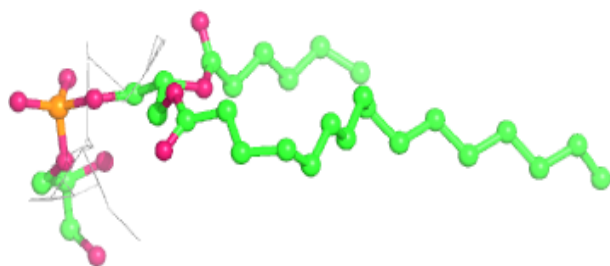
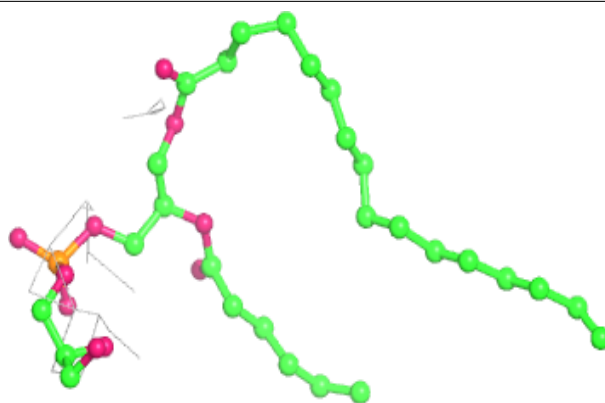
Electron density around HEM i 201:

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

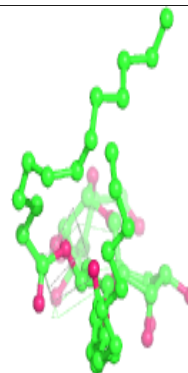
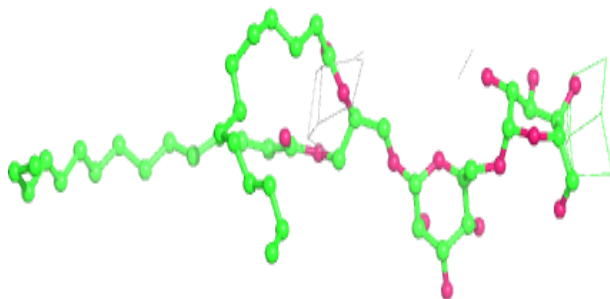
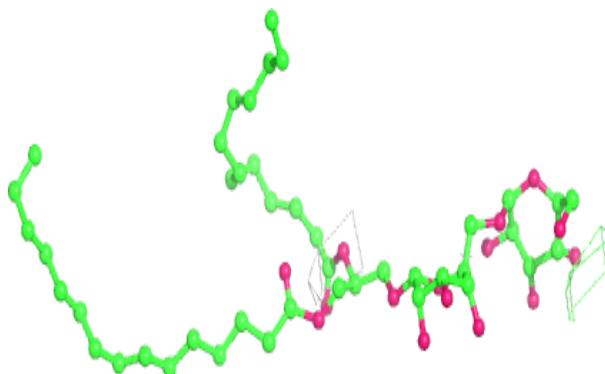


Electron density around LHG A 408:

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

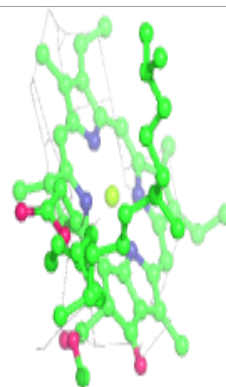
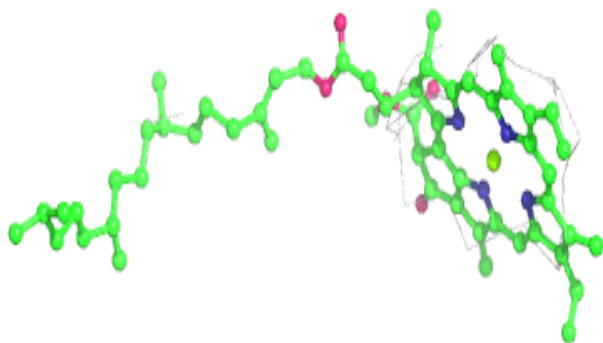
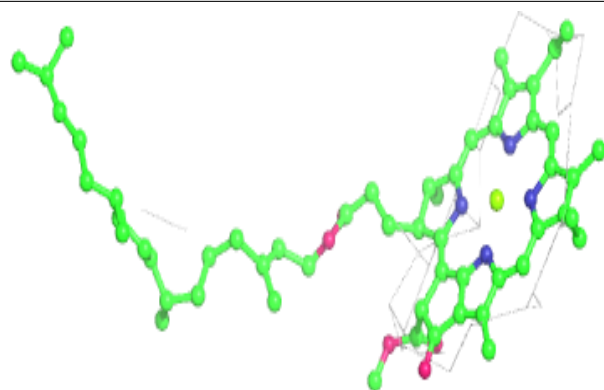
**Electron density around DGD W 102:**

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

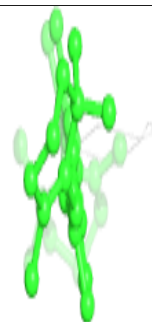
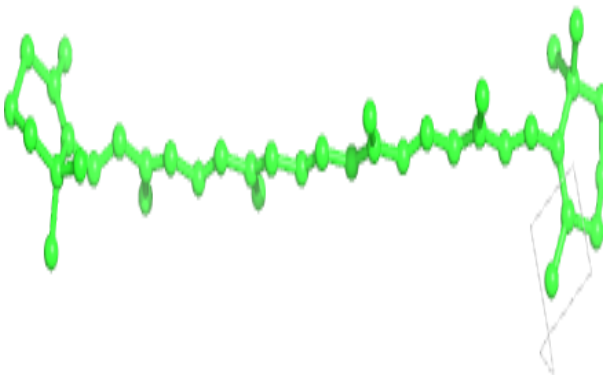
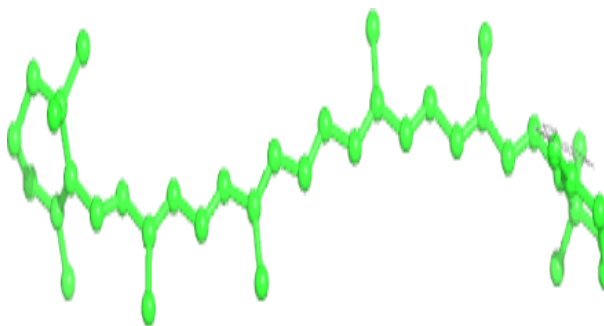


Electron density around CLA G 402:

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

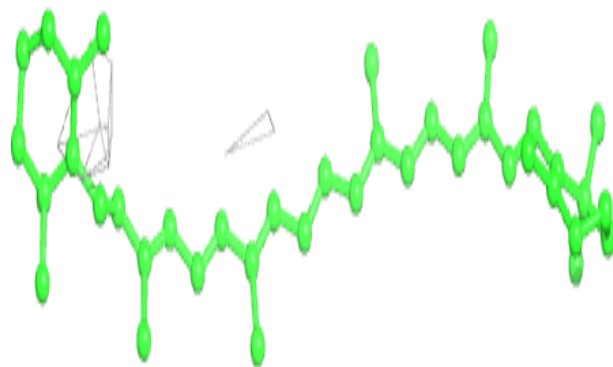
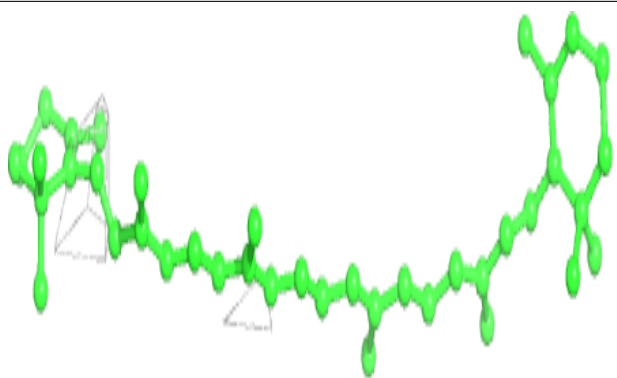
**Electron density around BCR P 515:**

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

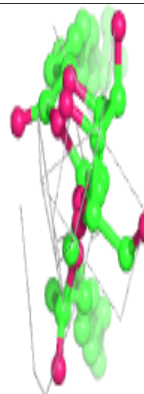
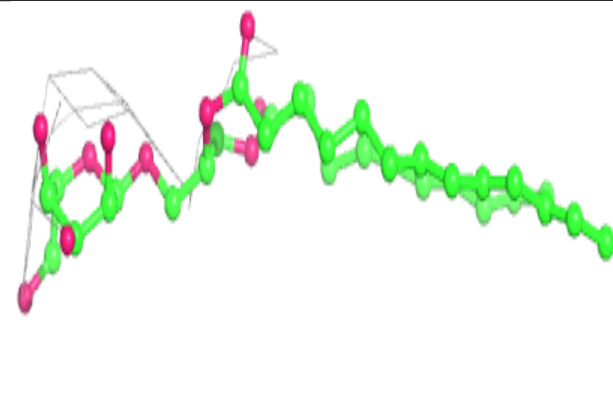
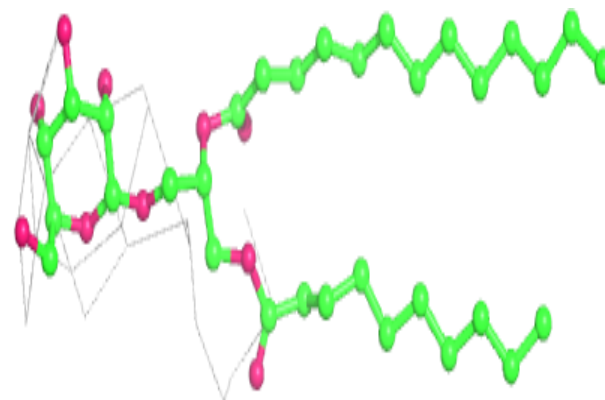


Electron density around BCR S 101:

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

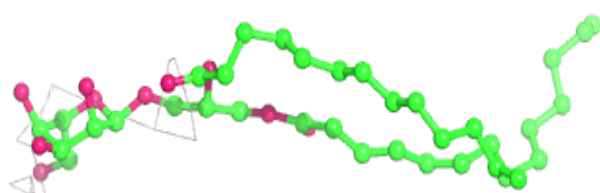
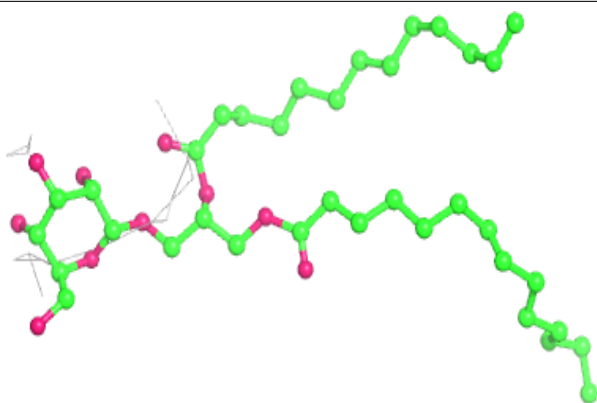
**Electron density around LMG M 101:**

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

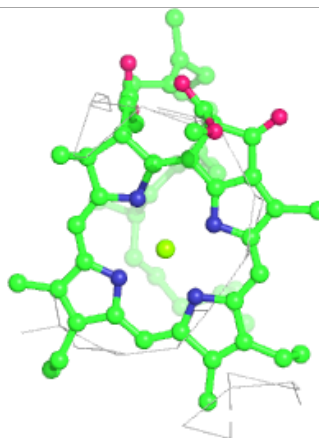
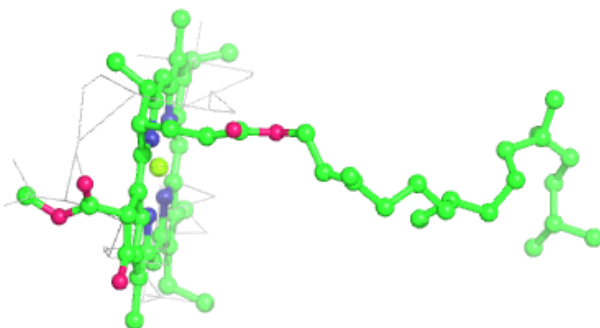
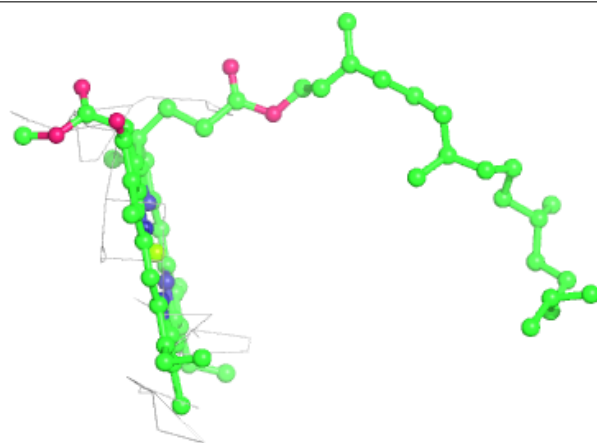


Electron density around LMG Q 406:

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

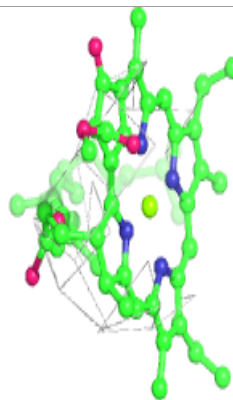
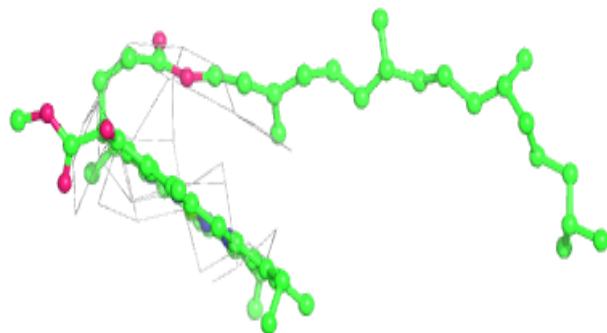
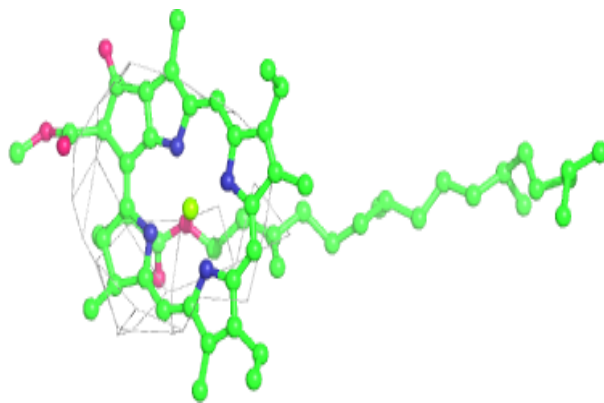
**Electron density around CLA P 506:**

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



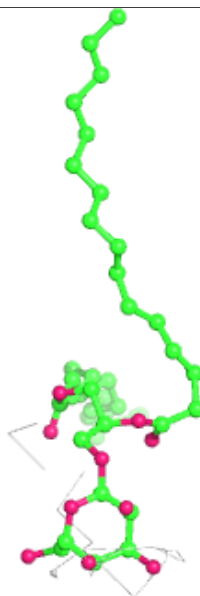
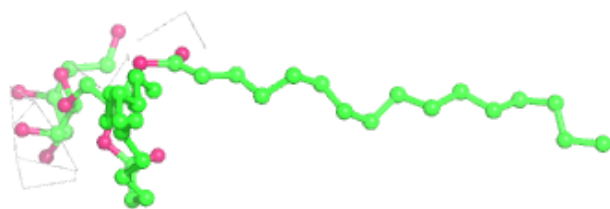
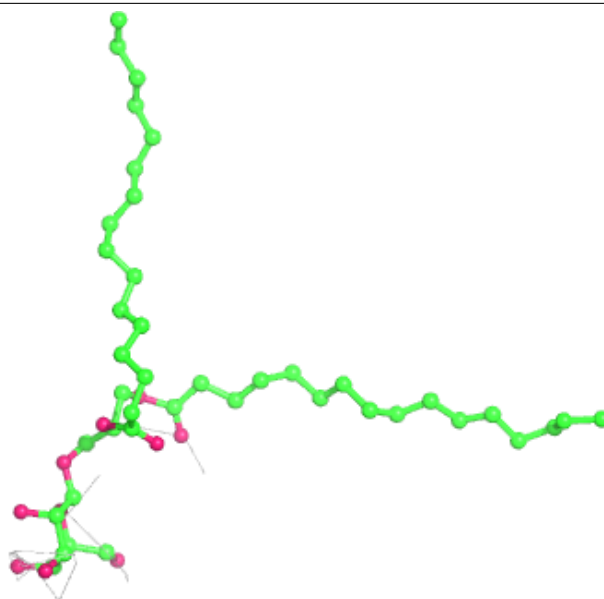
Electron density around CLA N 612:

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



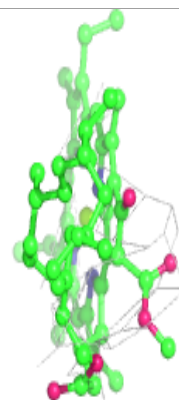
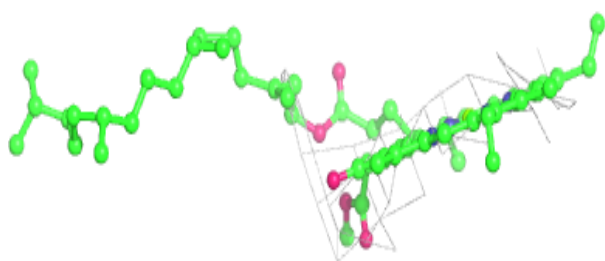
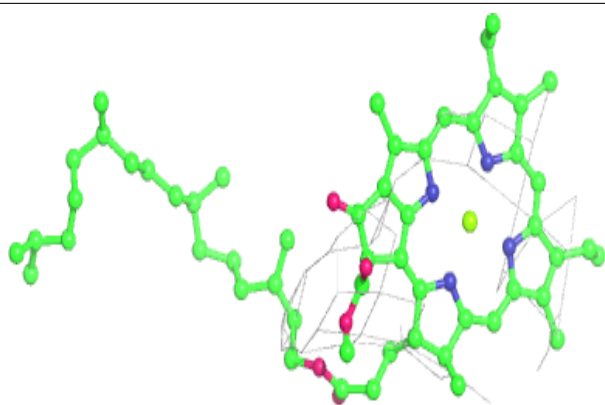
Electron density around LMG G 411:

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

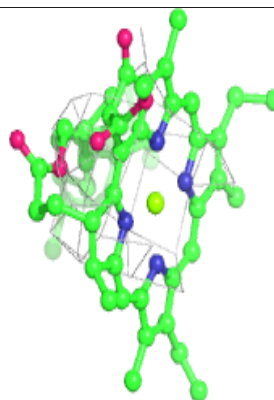
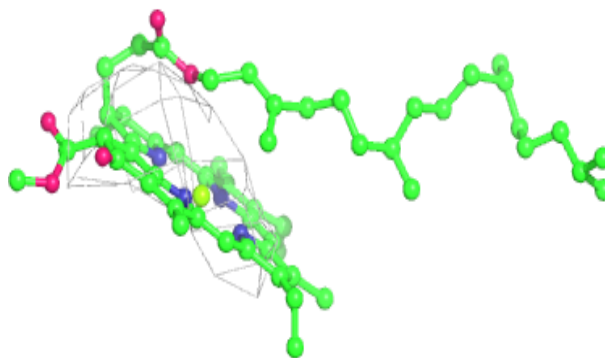
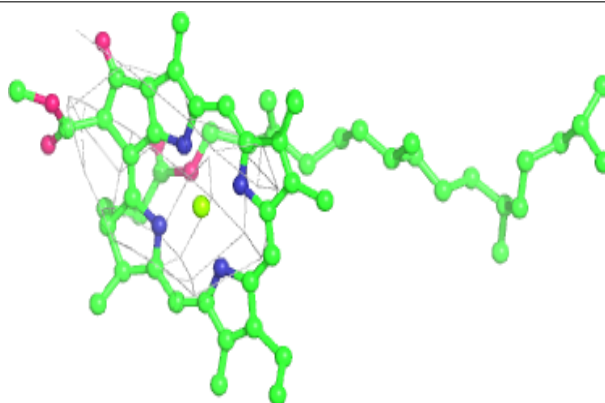


Electron density around CLA B 602:

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

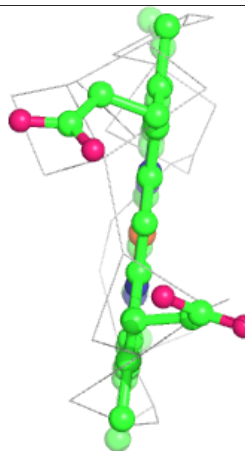
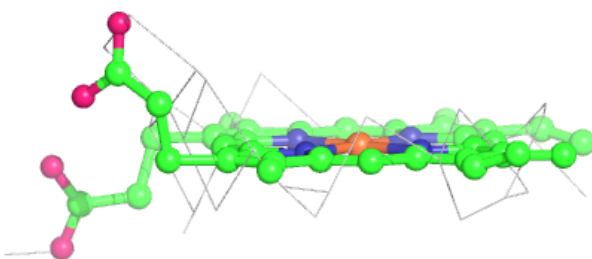
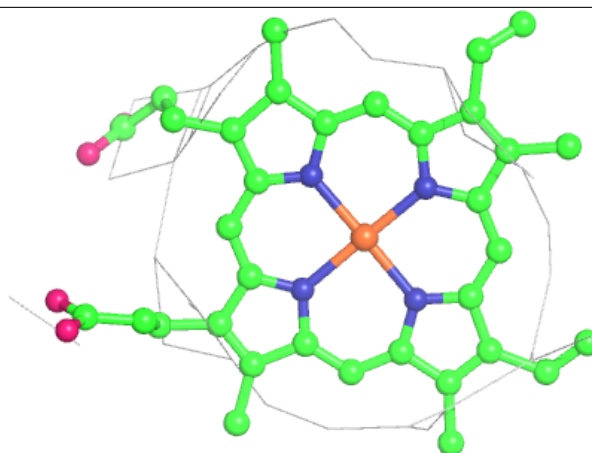
**Electron density around CLA N 618:**

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

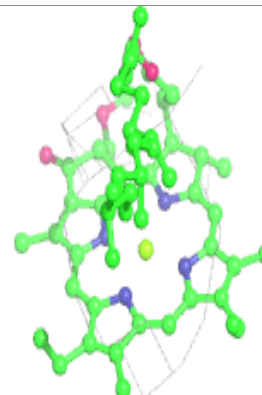
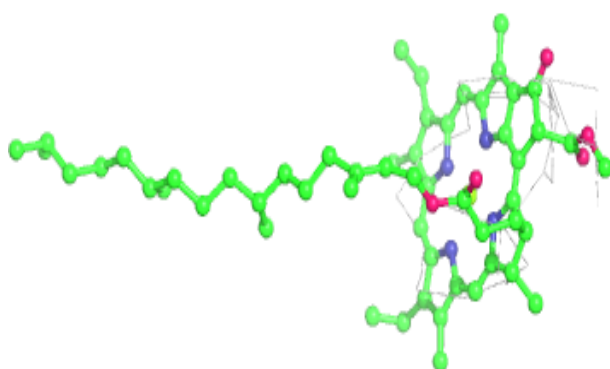
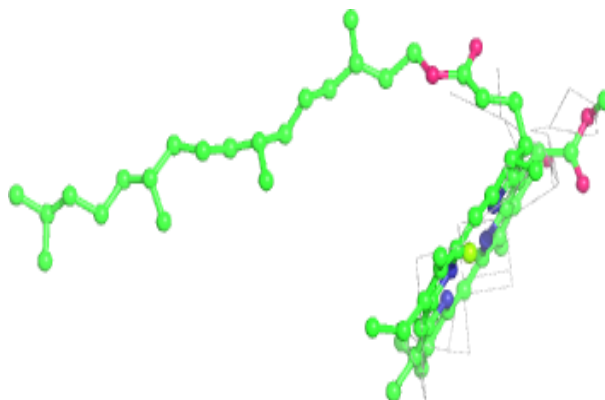


Electron density around HEM E 101:

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

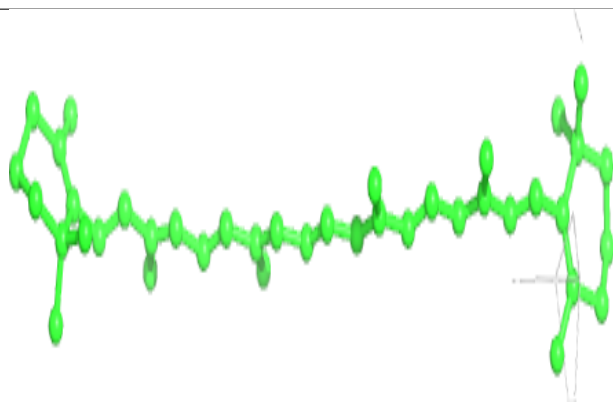
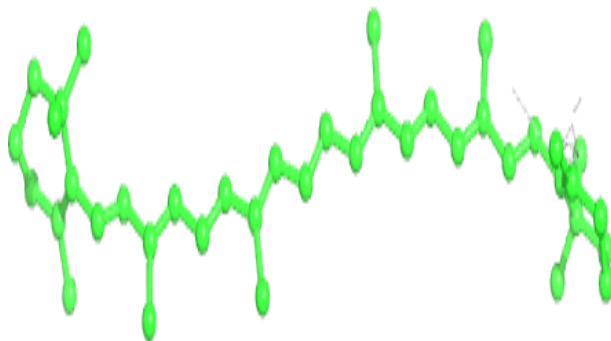
**Electron density around CLA C 504:**

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

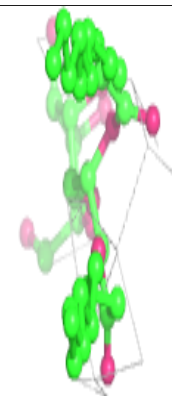
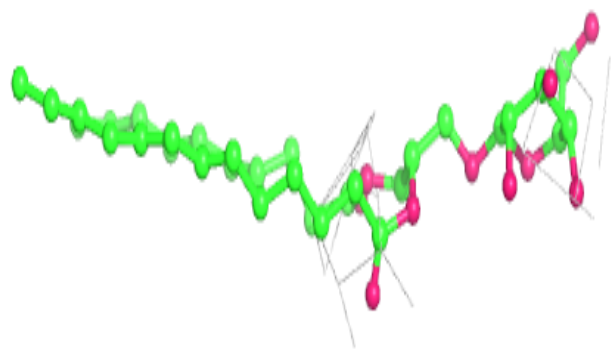
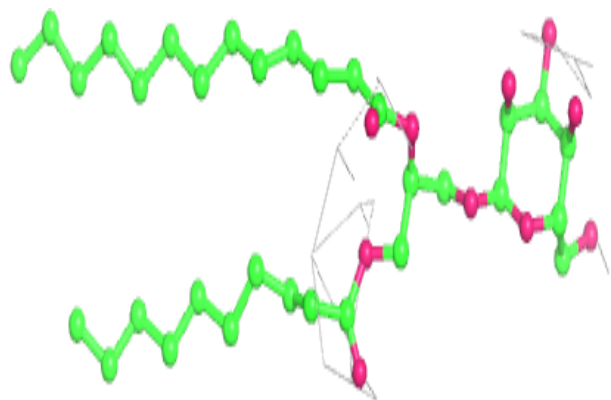


Electron density around BCR Z 101:

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

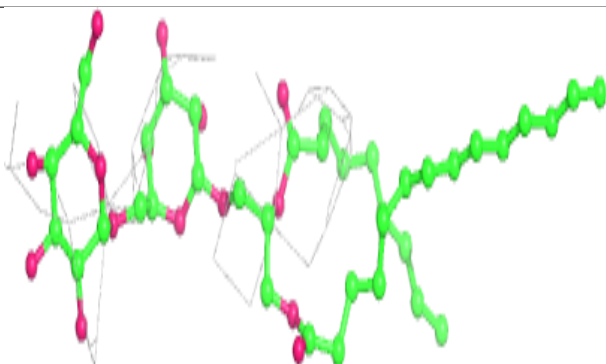
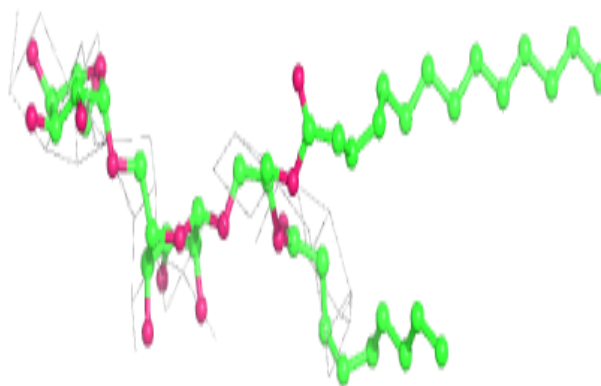
**Electron density around LMG e 102:**

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

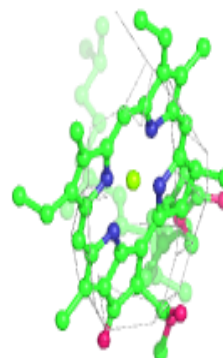
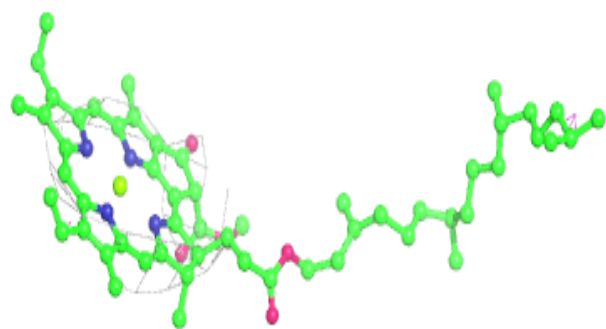
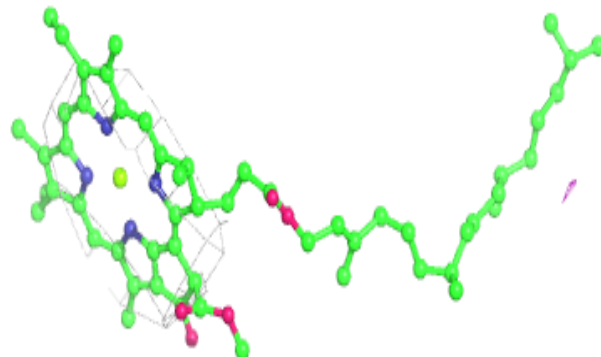


Electron density around DGD P 517:

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

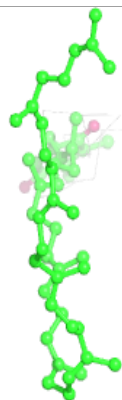
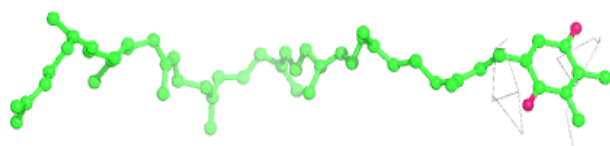
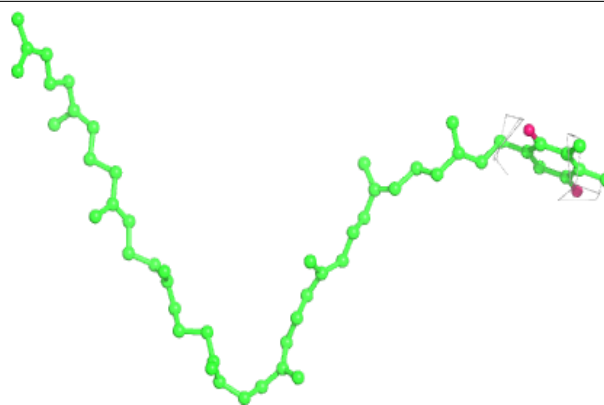
**Electron density around CLA A 401:**

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

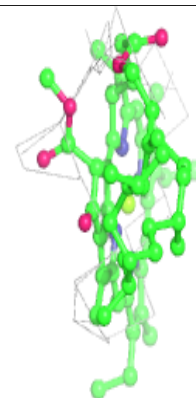
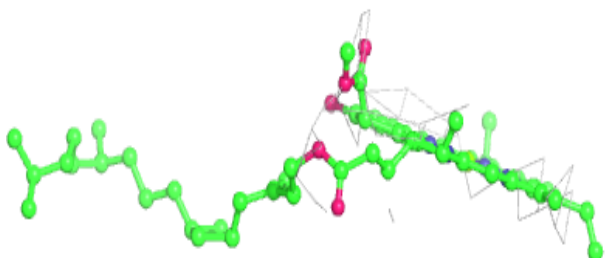
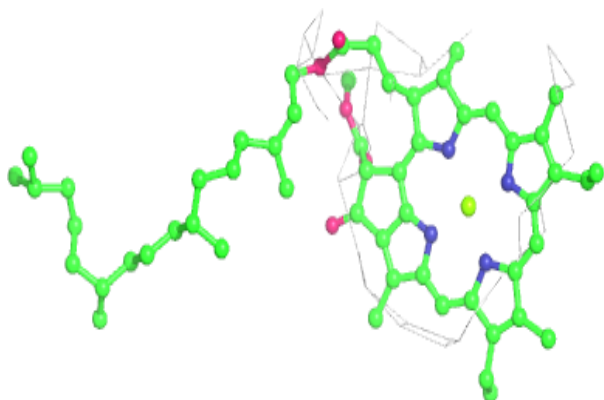


Electron density around PL9 D 404:

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

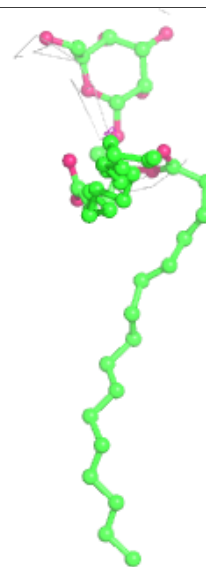
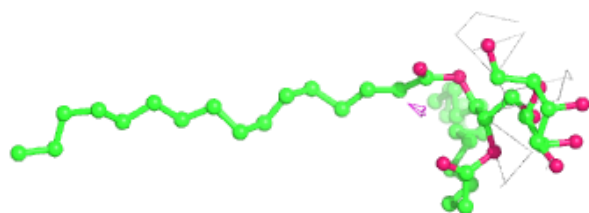
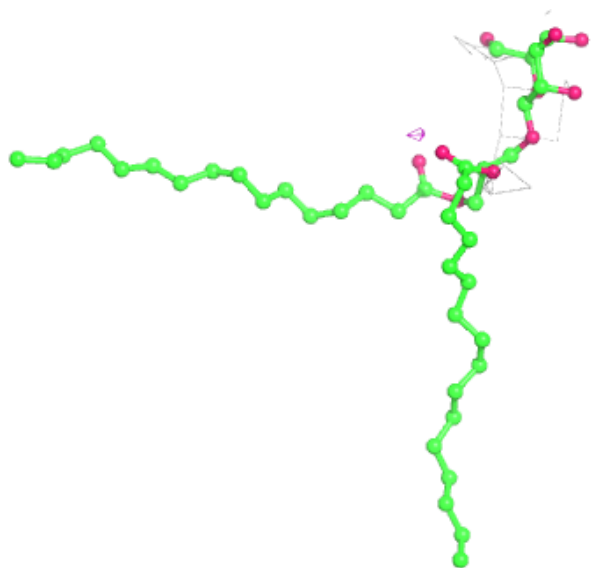
**Electron density around CLA N 606:**

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



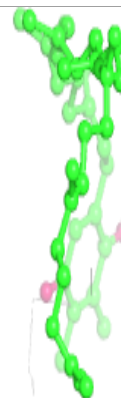
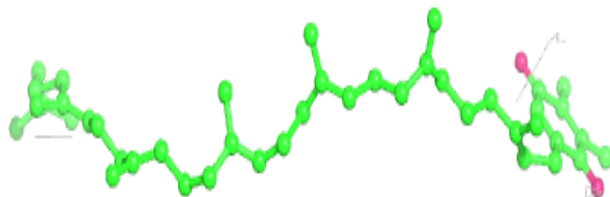
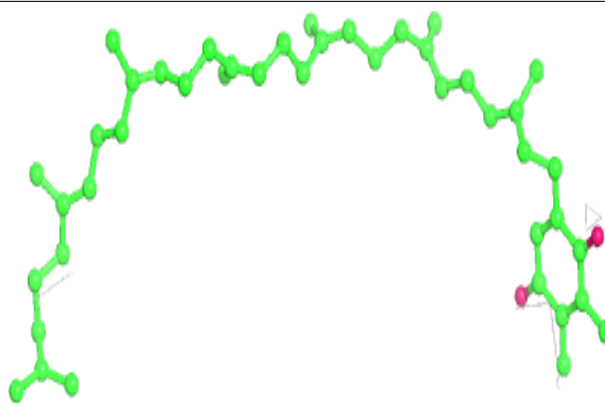
Electron density around LMG A 410:

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

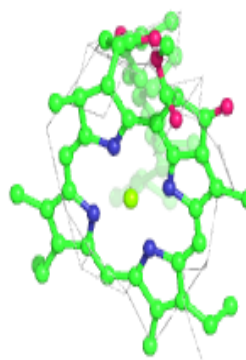
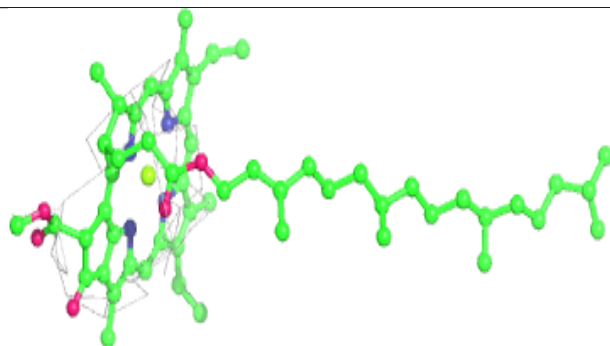
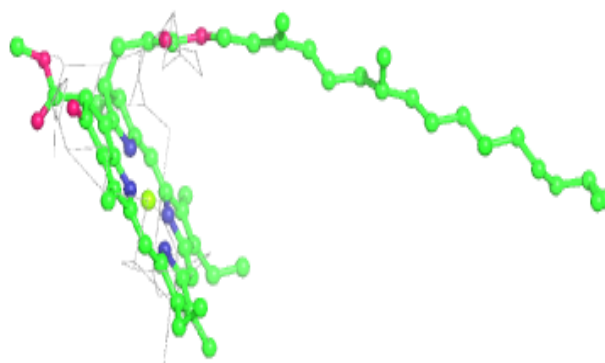


Electron density around PL9 A 406:

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

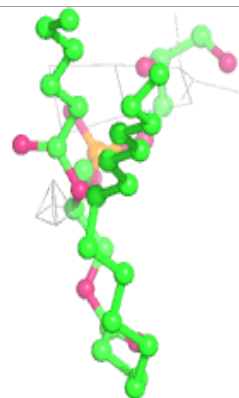
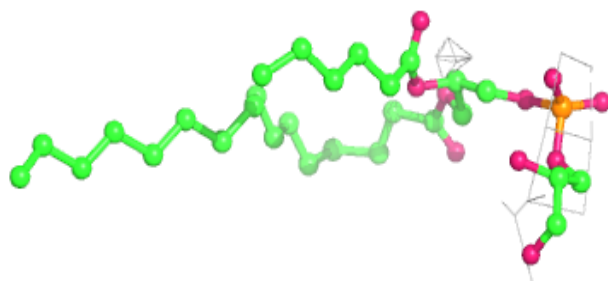
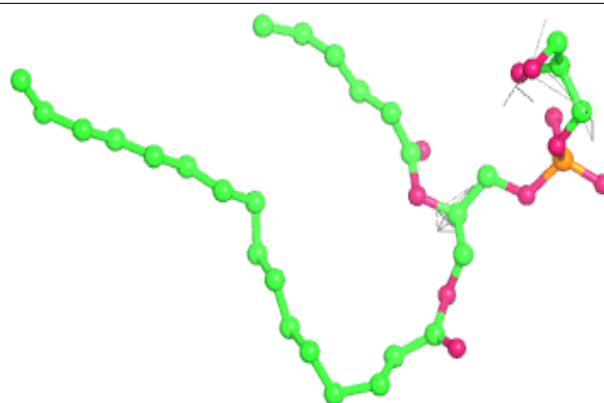
**Electron density around CLA N 611:**

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

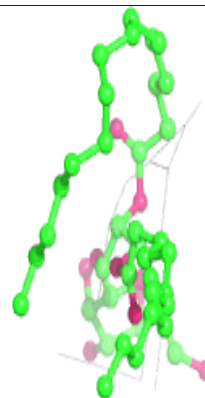
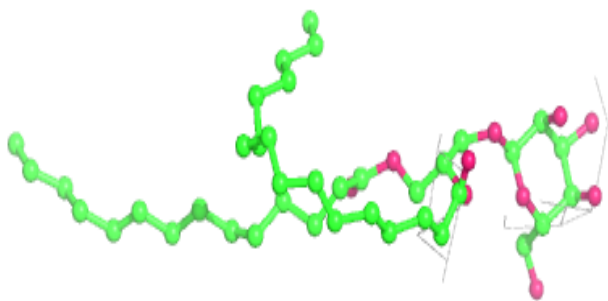
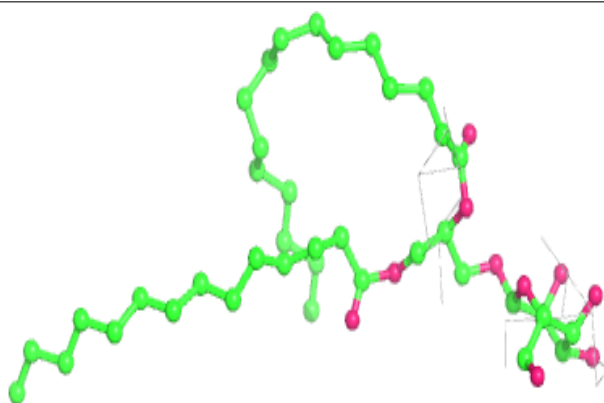


Electron density around LHG G 409:

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

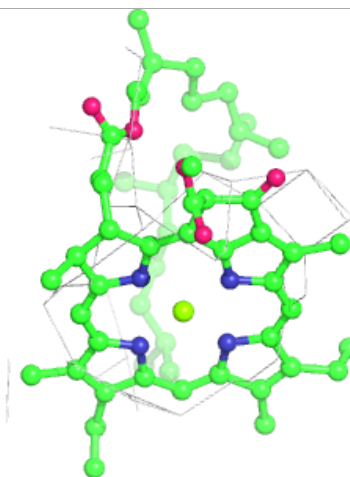
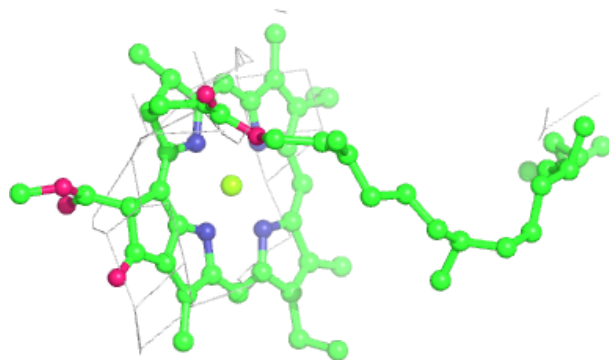
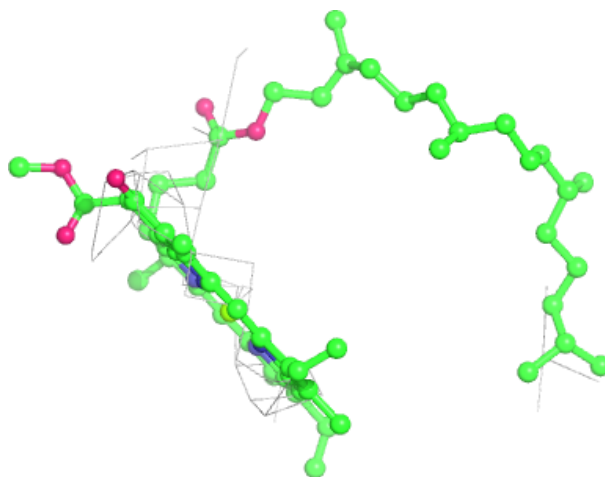
**Electron density around LMG N 622:**

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



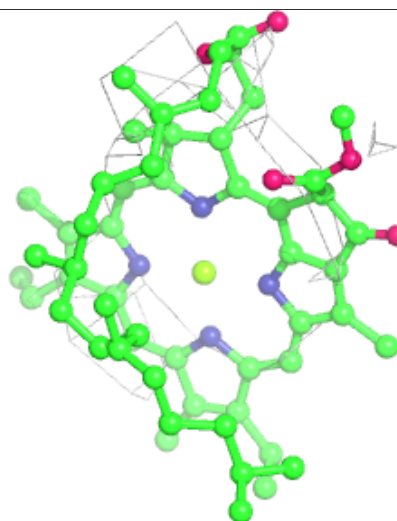
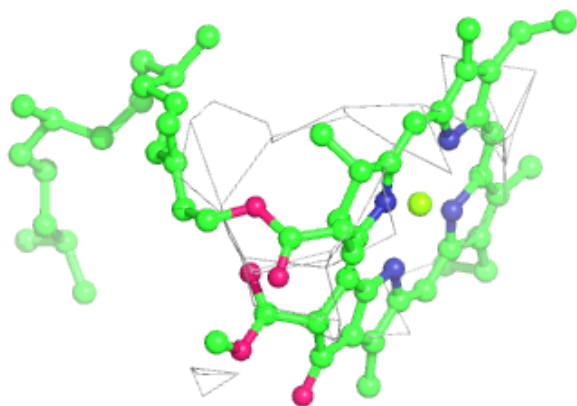
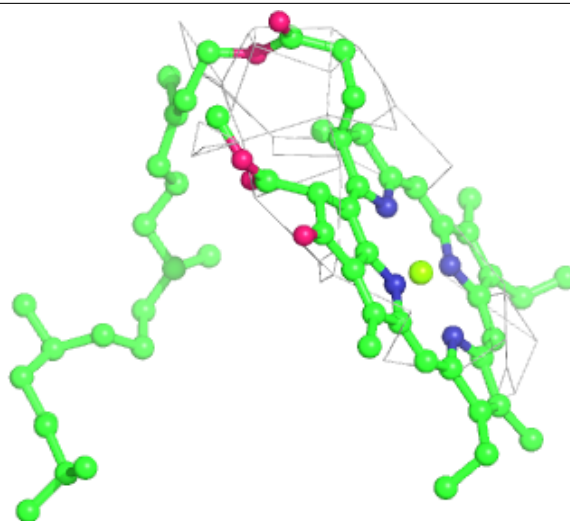
Electron density around CLA N 615:

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



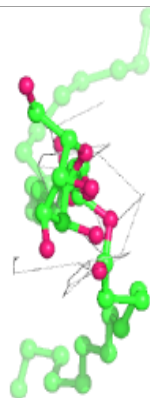
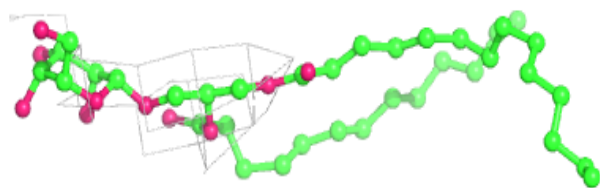
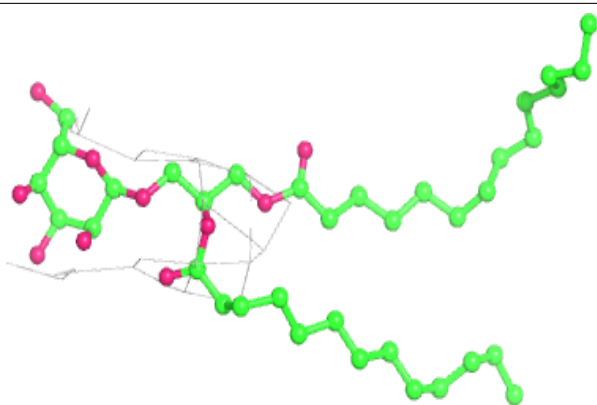
Electron density around CLA B 613:

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



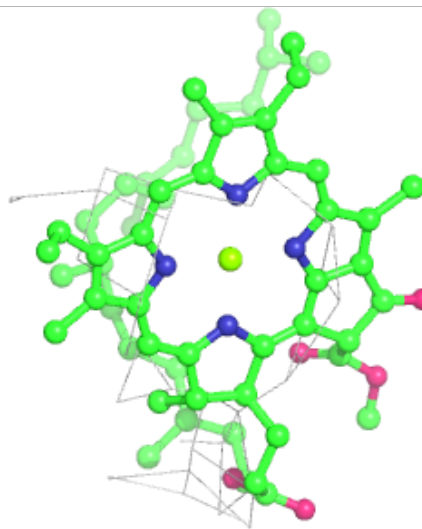
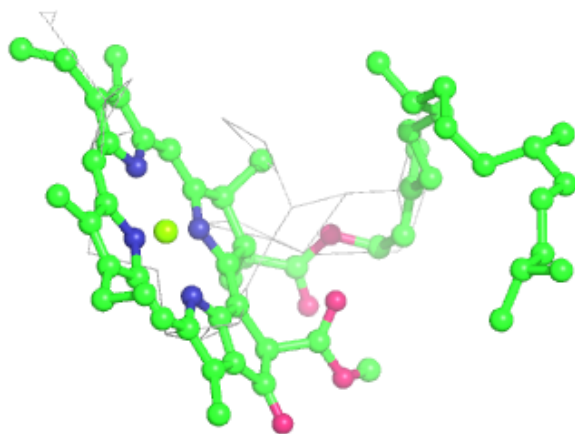
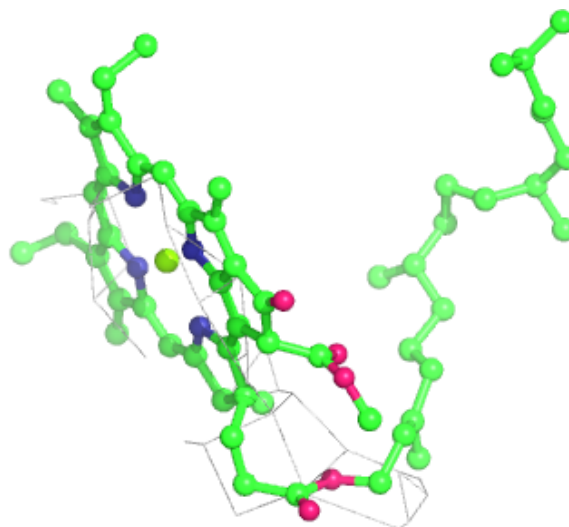
Electron density around LMG D 406:

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



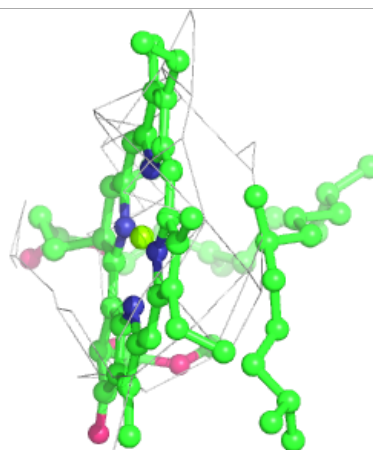
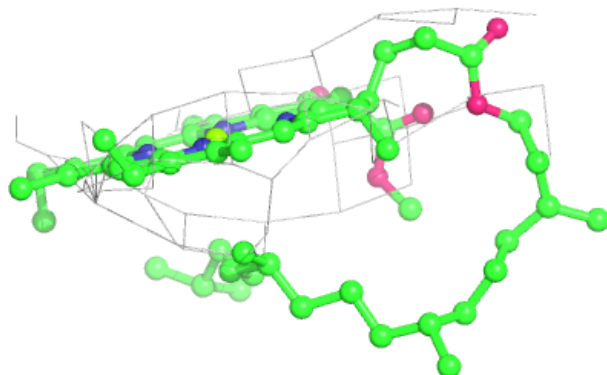
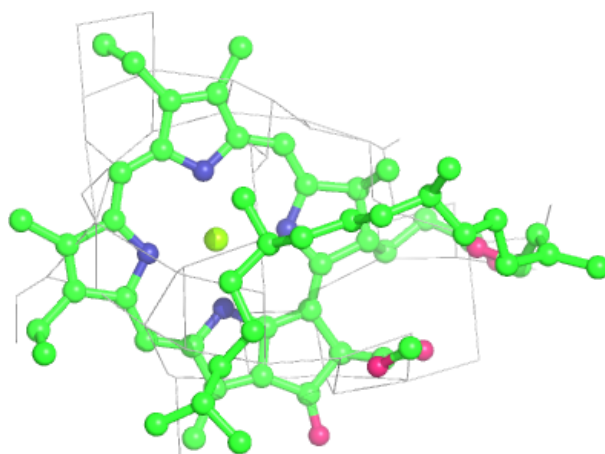
Electron density around CLA N 617:

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



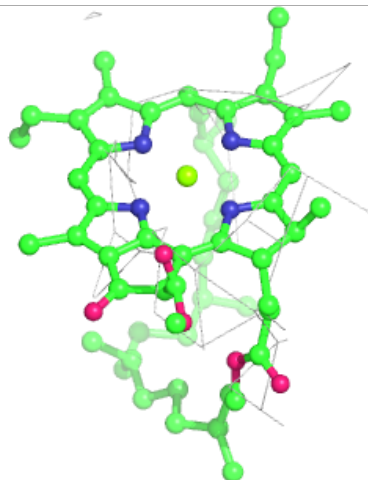
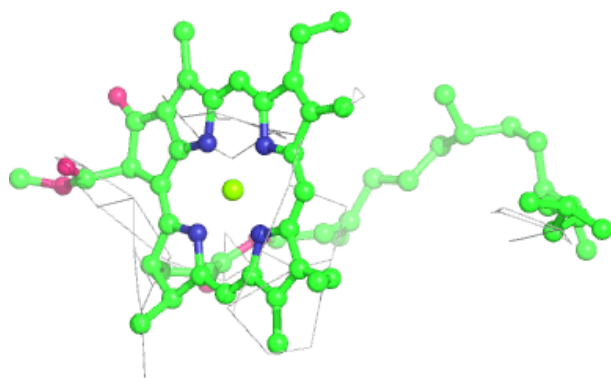
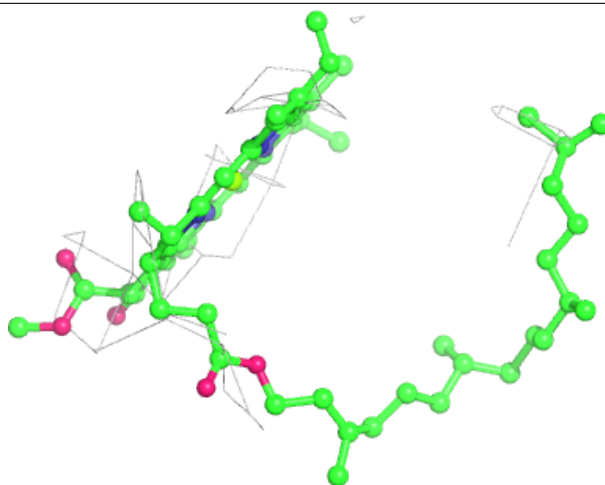
Electron density around CLA C 510:

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



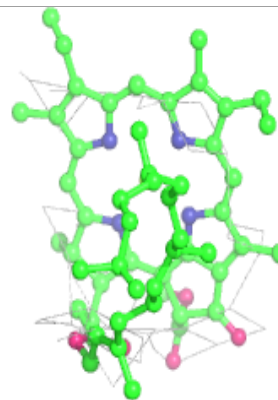
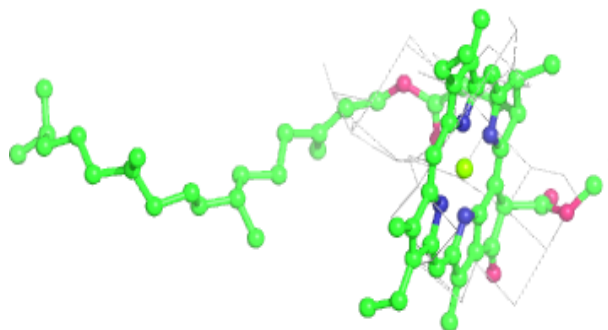
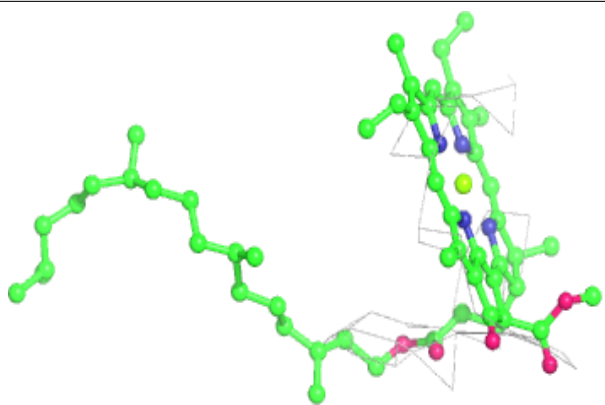
Electron density around CLA B 611:

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



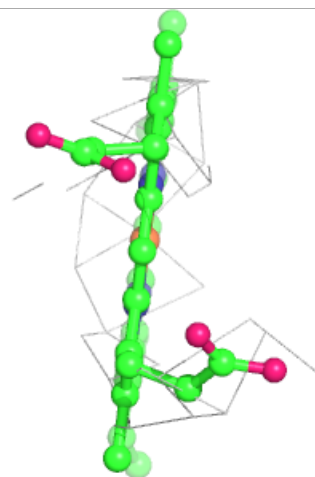
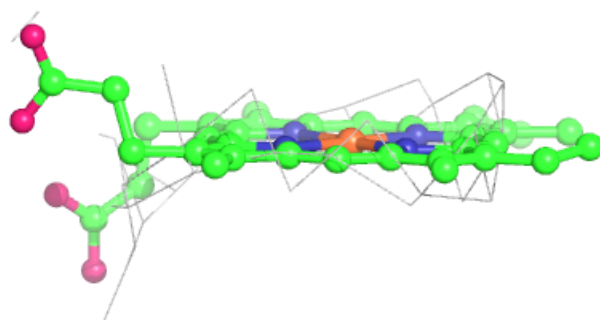
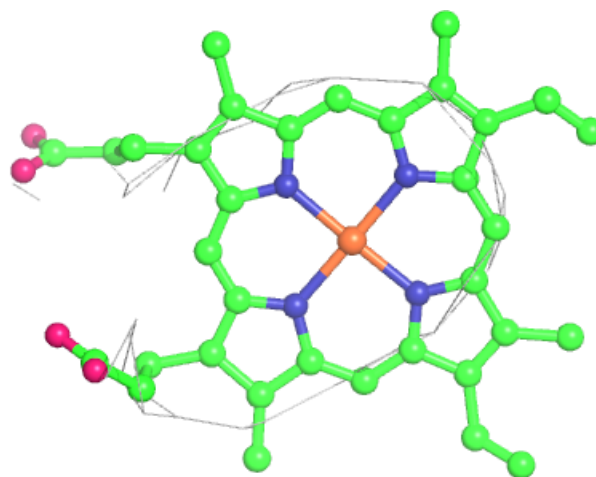
Electron density around CLA P 508:

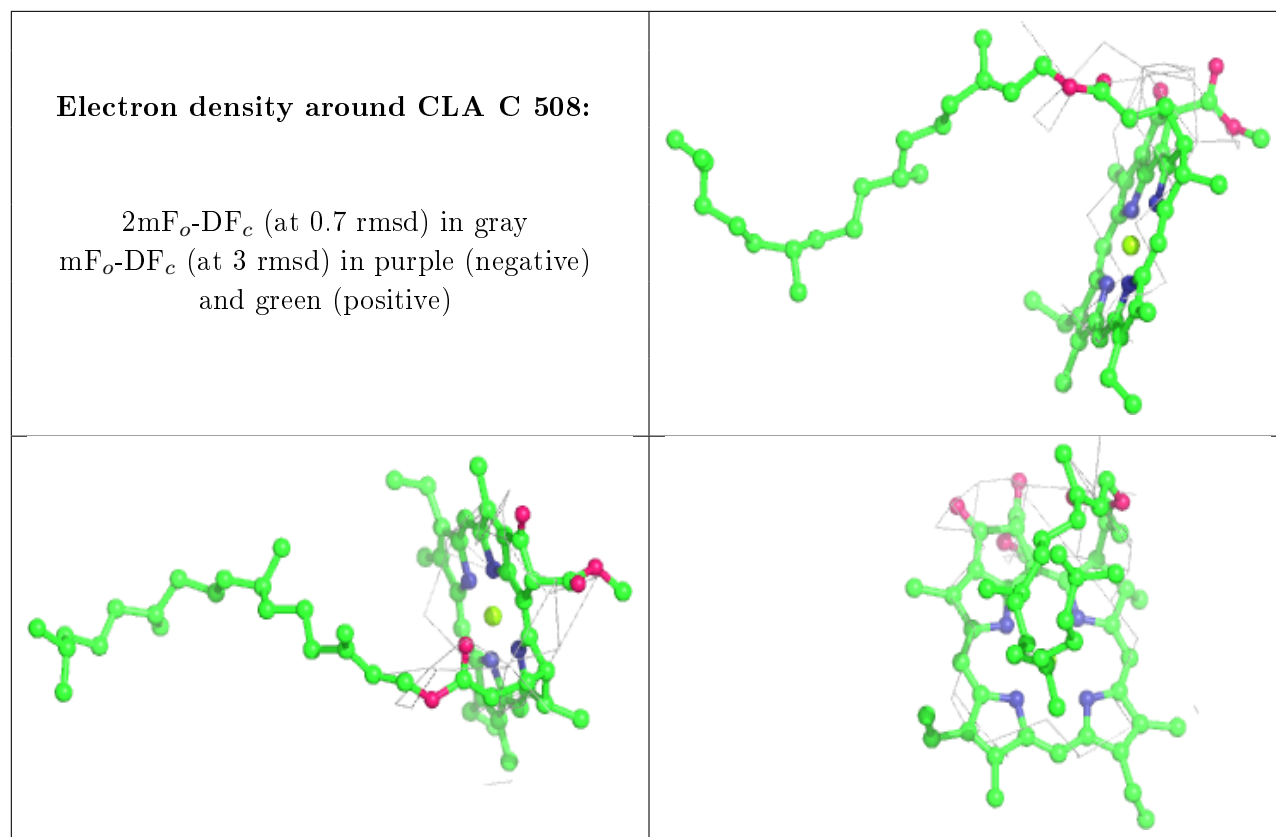
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM R 101:

$2mF_o-DF_c$ (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.