



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 03:03 PM EST

PDB ID : 6DHO
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.07 Angstrom resolution
Authors : Kern, J.; Chatterjee, R.; Young, I.D.; Fuller, F.D.; Lassalle, L.; Ibrahim, M.; Gul, S.; Fransson, T.; Brewster, A.S.; Alonso-Mori, R.; Hussein, R.; Zhang, M.; Douthit, L.; de Lichtenberg, C.; Cheah, M.H.; Shevela, D.; Wersig, J.; Seufert, I.; Sokaras, D.; Pastor, E.; Weninger, C.; Kroll, T.; Sierra, R.G.; Aller, P.; Butryn, A.; Orville, A.M.; Liang, M.; Batyuk, A.; Koglin, J.E.; Carbajo, S.; Boutet, S.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Zouni, A.; Messinger, J.; Yano, J.; Yachandra, V.K.
Deposited on : 2018-05-20
Resolution : 2.07 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)

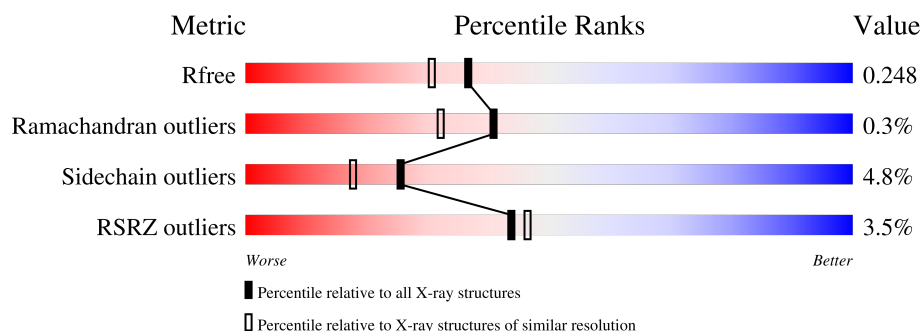
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	2684 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

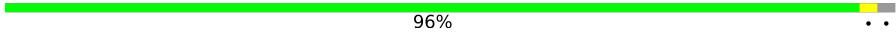
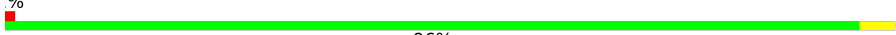
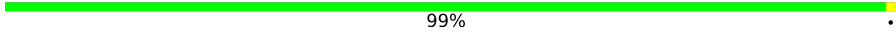
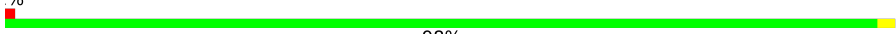
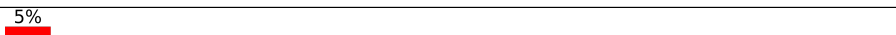
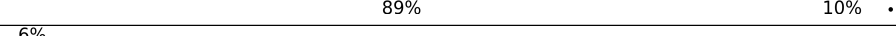
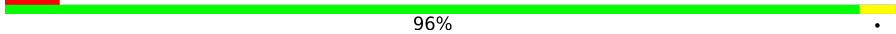

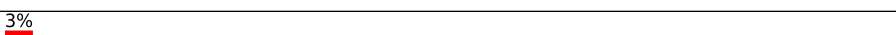
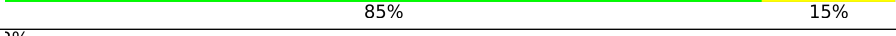


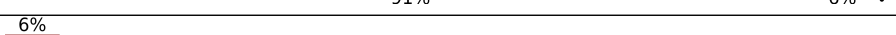

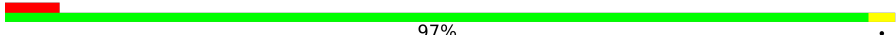

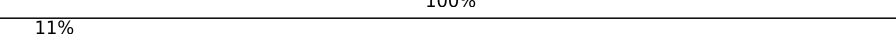
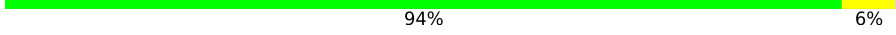



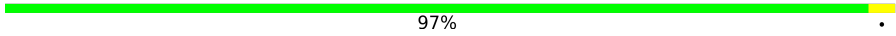


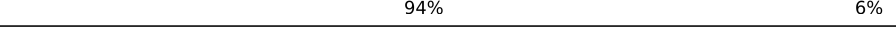
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	334	<div> <div>98%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	a	334	<div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	B	505	<div> <div>97%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
2	b	505	<div> <div>98%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

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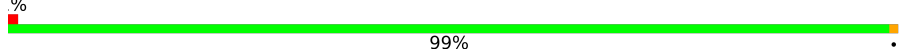
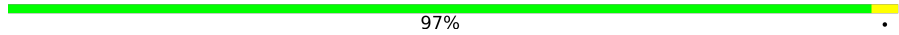
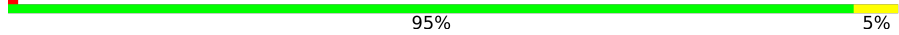


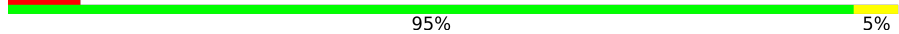





Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.17.1

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Mol	Chain	Length	Quality of chain
3	C	451	 96%
3	c	451	 96%
4	D	341	 99%
4	d	341	 98%
5	E	82	 89% 10%
5	e	82	 96%
6	F	34	 100%
6	f	34	 85% 15%
7	H	65	 94% 6%
7	h	65	 91% 6%
8	I	36	 86% 14%
8	i	36	 97%
9	J	36	 100%
9	j	36	 94% 6%
10	K	37	 89% 11%
10	k	37	 89% 11%
11	L	37	 97%
11	l	37	 89% 8%
12	M	33	 94% 6%
12	m	33	 91% 6%
13	O	244	 95% 5%
13	o	244	 92% 7%
14	T	30	 87% 10%
14	t	30	 93% 7%
15	U	97	 97%

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Mol	Chain	Length	Quality of chain
15	u	97	
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	38	
18	x	38	
19	Z	62	
19	z	62	
20	R	34	
20	r	34	

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
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	616	X	-	-	-
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	408	X	-	-	-
23	CLA	a	411	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
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23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	h	101	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105756 atoms, of which 52470 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	59	0
			6018	2010	2937	507	545	19			
1	a	334	Total	C	H	N	O	S	0	59	0
			6006	2007	2928	507	545	19			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7849	2631	3845	666	694	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7789	2610	3811	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	7	0
			6868	2282	3392	579	601	14			
3	c	451	Total	C	H	N	O	S	0	8	0
			7017	2324	3464	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	H	N	O	0	1	0
			1309	434	647	106	122			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1030	338	523	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			516	172	261	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	1	0
			620	209	318	46	47			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	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	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3730	1174	1850	317	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	H	N	O	0	0	0
			519	181	261	36	39			
14	t	30	Total	C	H	N	O	0	0	0
			512	180	256	36	38			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			
15	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	129	154			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	V	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			
16	v	137	Total	C	H	N	O	S	0	0	0
			2134	675	1070	177	208	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	Y	27	Total	C	H	N	O	S	0	0	0
			404	128	208	35	30	3			
17	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				
18	x	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Z	62	Total	C	H	N	O	S	0	0	0
			988	328	509	72	77	2			
19	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	R	34	Total	C	H	N	O		0	0	0
			569	184	298	47	40				
20	r	31	Total	C	H	N	O		0	0	0
			461	154	234	40	33				

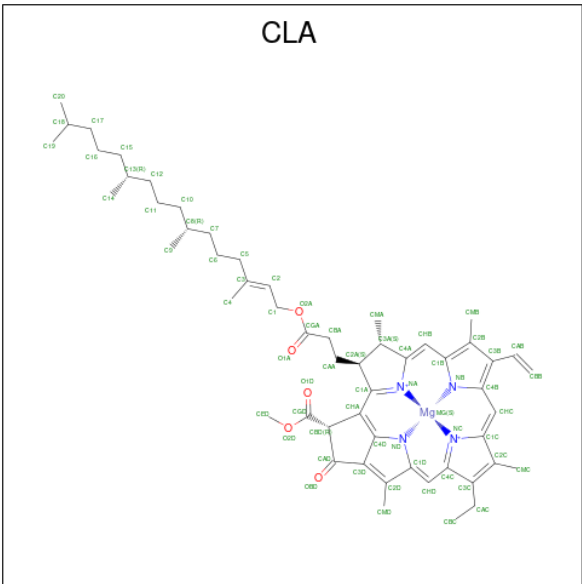
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
23	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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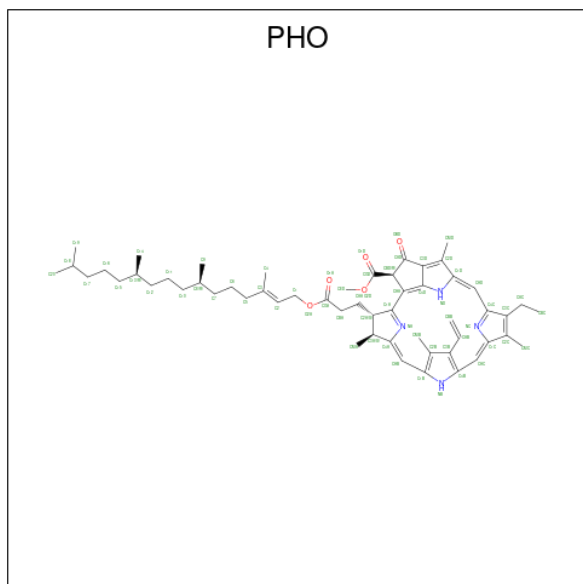
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
23	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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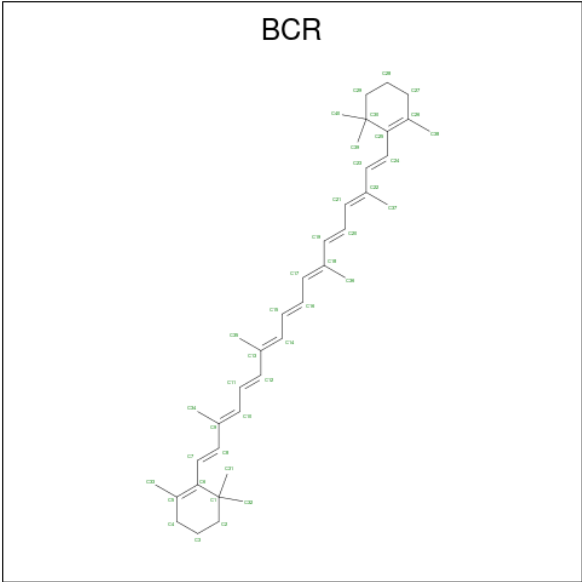
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
23	h	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
24	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



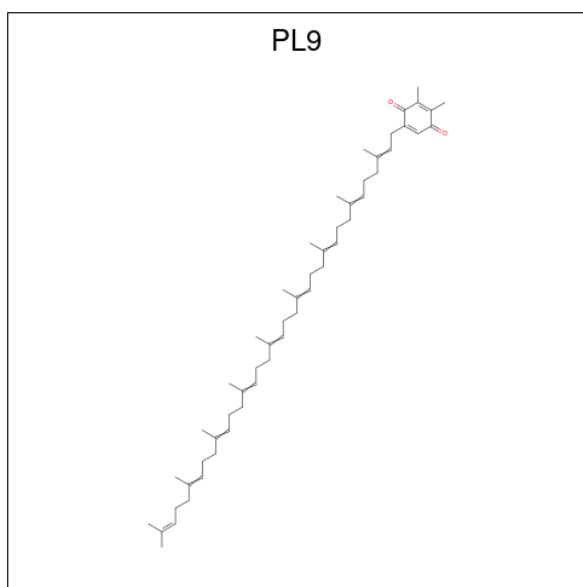
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	B	1	Total	C	H	0	0
			96	40	56		
25	C	1	Total	C	H	0	0
			96	40	56		
25	D	1	Total	C	H	0	0
			96	40	56		
25	H	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	K	1	Total	C	H	0	0
			96	40	56		
25	T	1	Total	C	H	0	0
			96	40	56		
25	Z	1	Total	C	H	0	0
			96	40	56		
25	a	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		
25	b	1	Total	C	H	0	0
			96	40	56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	b	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	c	1	Total	C	H	0	0
			96	40	56		
25	d	1	Total	C	H	0	0
			96	40	56		
25	k	1	Total	C	H	0	0
			96	40	56		
25	k	1	Total	C	H	0	0
			96	40	56		
25	t	1	Total	C	H	0	0
			96	40	56		
25	x	1	Total	C	H	0	0
			96	40	56		

- Molecule 26 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: $C_{53}H_{80}O_2$).



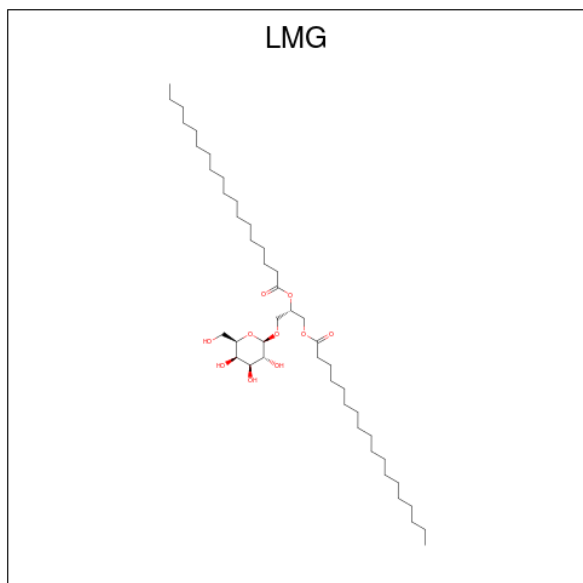
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



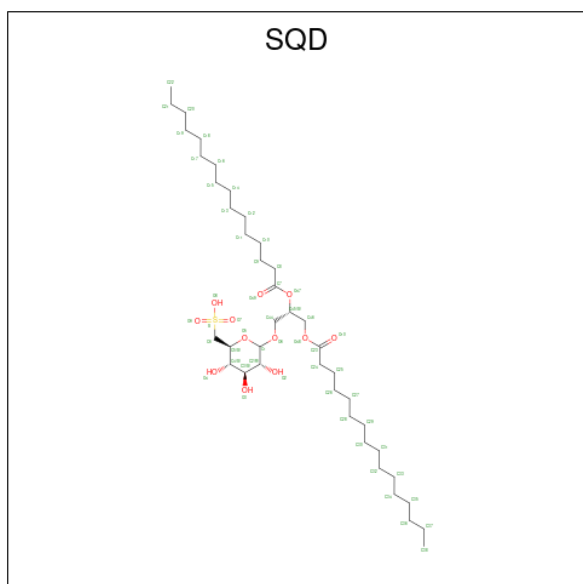
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			57	21	34	2		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



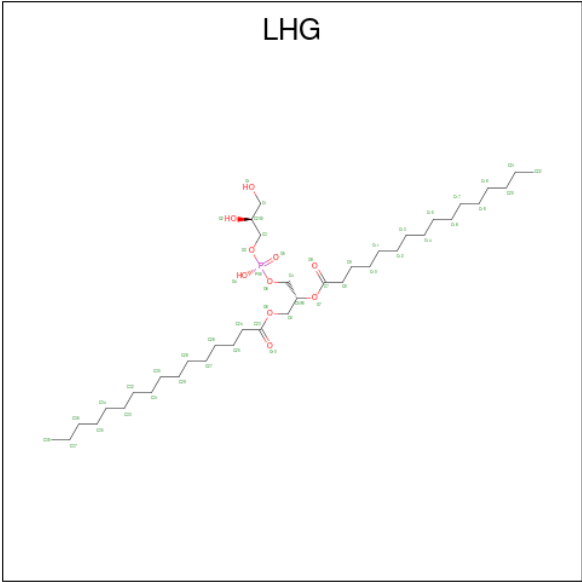
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		

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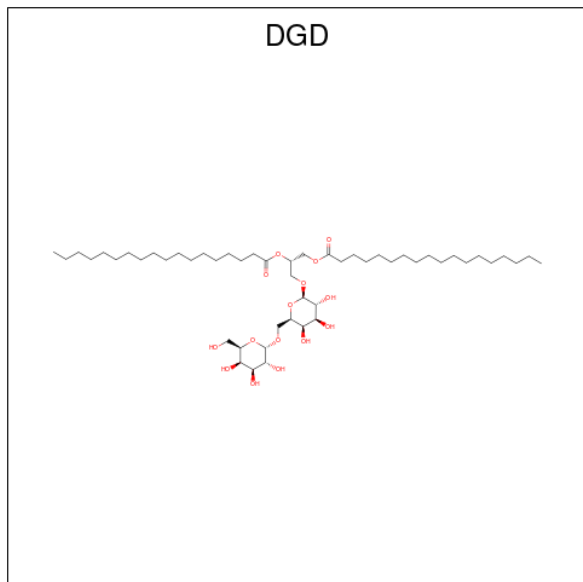
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	f	1	Total	C	H	O	S	0	0
			90	28	49	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



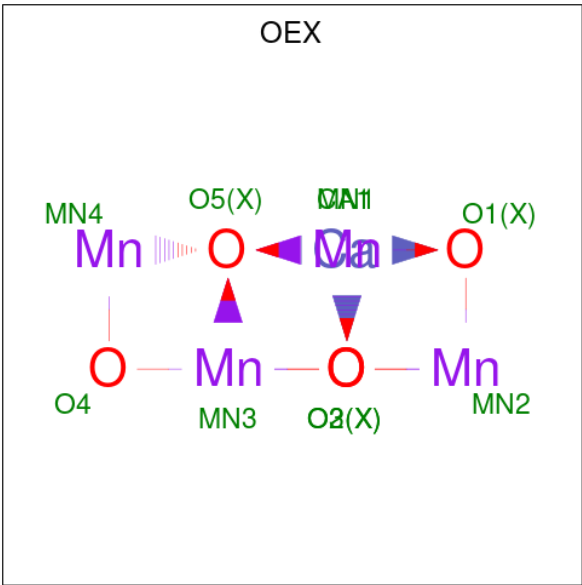
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
29	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
29	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



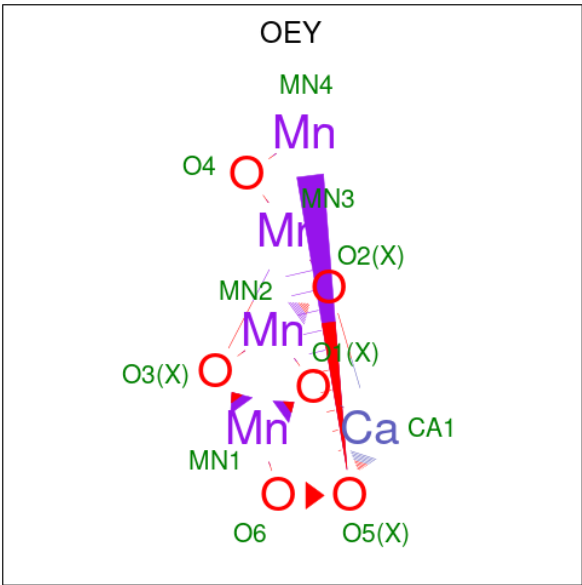
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	a	1	Total	C	H	O	0	0
			119	39	75	5		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



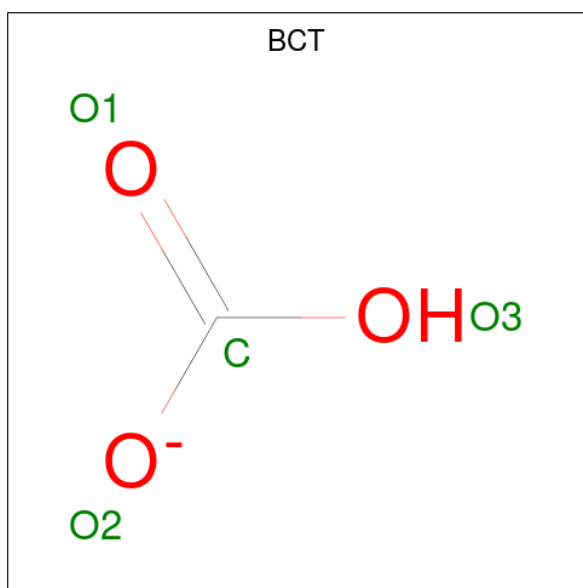
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
32	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

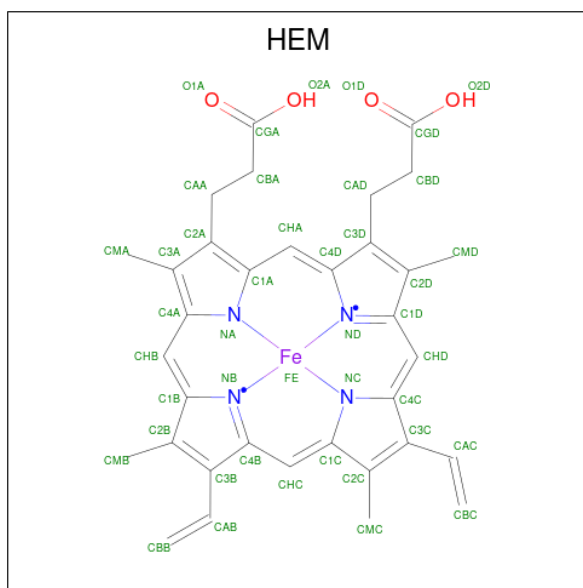
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	5	Total	C	H	O	0	0
			192	67	117	8		
34	C	3	Total	C	H	O	0	0
			103	36	63	4		
34	E	1	Total	C	H	O	0	0
			28	10	16	2		
34	H	1	Total	C	H		0	0
			53	18	35			
34	I	1	Total	C	H		0	0
			41	15	26			
34	J	1	Total	C	H	O	0	0
			28	10	16	2		
34	M	2	Total	C	H	O	0	0
			63	23	38	2		
34	X	1	Total	C	H	O	0	0
			55	18	35	2		
34	a	1	Total	C	H	O	0	0
			28	10	16	2		

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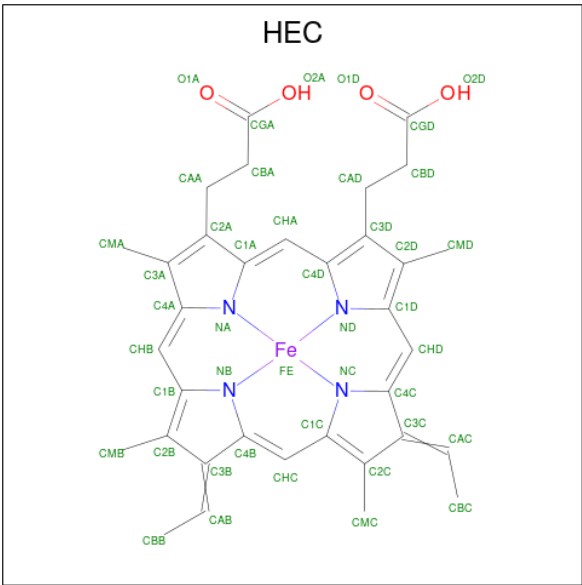
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	b	6	Total	C	H	O	0	0
			267	91	170	6		
34	c	2	Total	C	H	O	0	0
			83	28	51	4		
34	d	2	Total	C	H	O	0	0
			98	33	61	4		
34	j	1	Total	C	H	O	0	0
			28	10	16	2		
34	l	1	Total	C	H		0	0
			53	18	35			
34	m	1	Total	C	H	O	0	0
			28	10	16	2		
34	t	2	Total	C	H	O	0	0
			60	22	36	2		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
35	e	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	V	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
36	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	146	Total	O	0	8
			146	146		
37	B	213	Total	O	0	0
			213	213		
37	C	193	Total	O	0	0
			193	193		
37	D	129	Total	O	0	0
			129	129		
37	E	29	Total	O	0	0
			29	29		
37	F	14	Total	O	0	0
			14	14		
37	H	29	Total	O	0	0
			29	29		
37	I	14	Total	O	0	0
			14	14		
37	J	12	Total	O	0	0
			12	12		
37	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	8	Total 8	O 8	0	0
37	M	7	Total 7	O 7	0	0
37	O	123	Total 123	O 123	0	0
37	T	14	Total 14	O 14	0	0
37	U	49	Total 49	O 49	0	0
37	V	73	Total 73	O 73	0	0
37	Y	3	Total 3	O 3	0	0
37	X	8	Total 8	O 8	0	0
37	Z	4	Total 4	O 4	0	0
37	R	3	Total 3	O 3	0	0
37	a	125	Total 125	O 125	0	8
37	b	188	Total 188	O 188	0	0
37	c	159	Total 159	O 159	0	0
37	d	123	Total 123	O 123	0	0
37	e	22	Total 22	O 22	0	0
37	f	5	Total 5	O 5	0	0
37	h	20	Total 20	O 20	0	0
37	i	12	Total 12	O 12	0	0
37	j	8	Total 8	O 8	0	0
37	k	4	Total 4	O 4	0	0
37	l	10	Total 10	O 10	0	0

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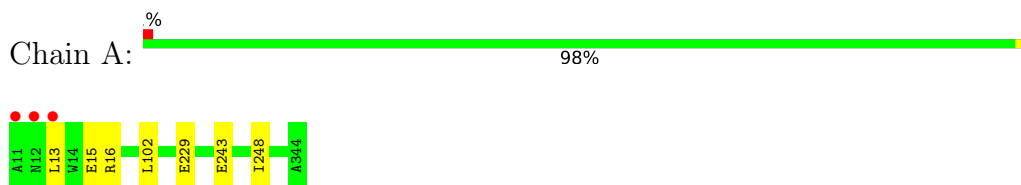
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	6	Total 6	O 6	0	0
37	o	120	Total 120	O 120	0	0
37	t	12	Total 12	O 12	0	0
37	u	50	Total 50	O 50	0	0
37	v	68	Total 68	O 68	0	0
37	y	4	Total 4	O 4	0	0
37	x	11	Total 11	O 11	0	0
37	z	1	Total 1	O 1	0	0
37	r	6	Total 6	O 6	0	0

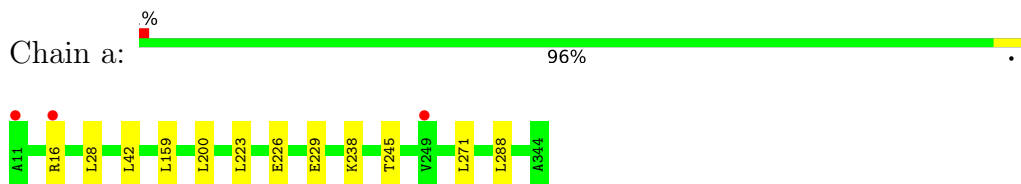
3 Residue-property plots [i](#)

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.

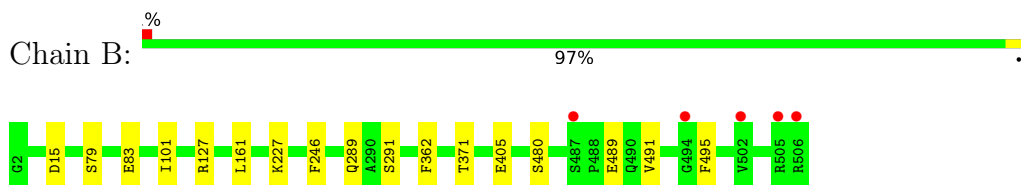
- Molecule 1: Photosystem II protein D1 1



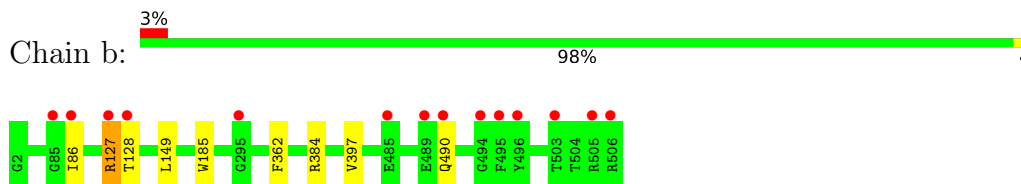
- Molecule 1: Photosystem II protein D1 1



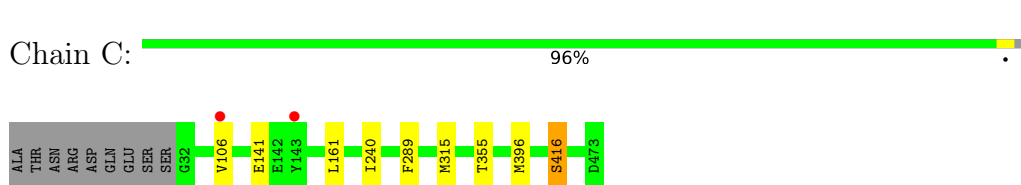
- Molecule 2: Photosystem II CP47 reaction center protein



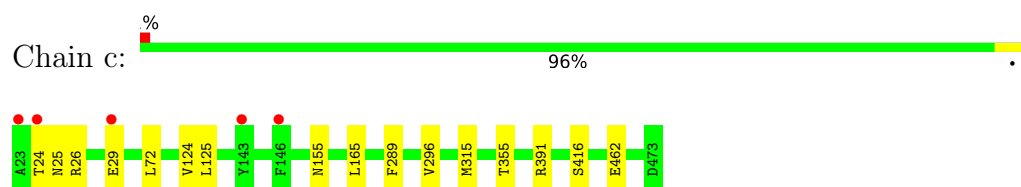
- Molecule 2: Photosystem II CP47 reaction center protein



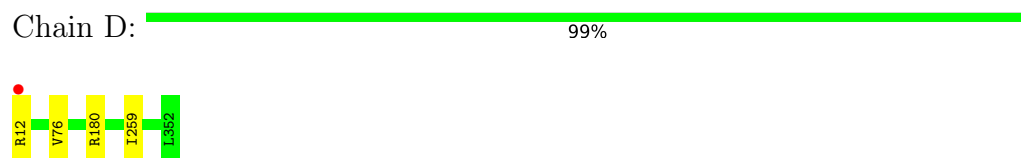
- Molecule 3: Photosystem II CP43 reaction center protein



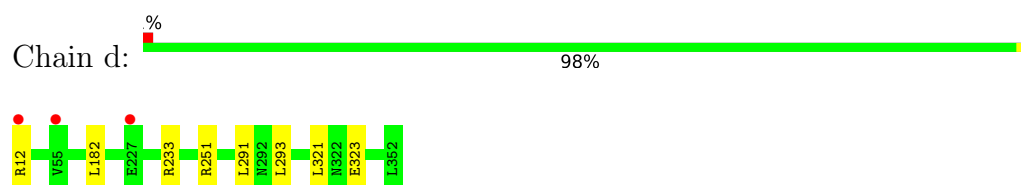
- Molecule 3: Photosystem II CP43 reaction center protein



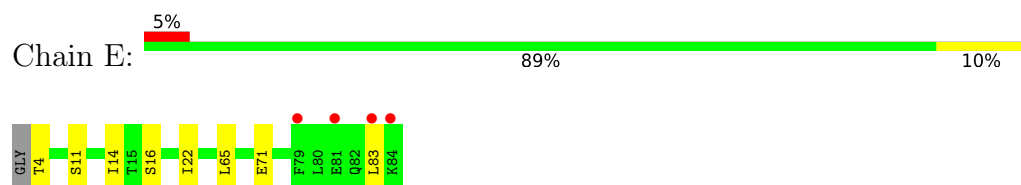
- Molecule 4: Photosystem II D2 protein



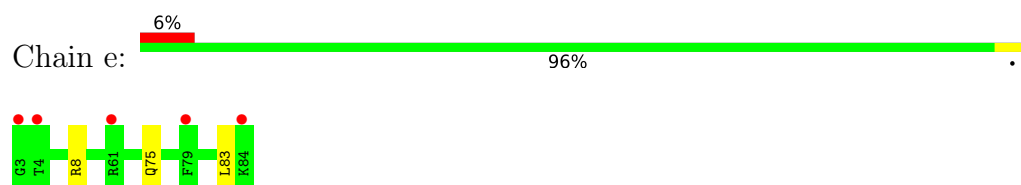
- Molecule 4: Photosystem II D2 protein



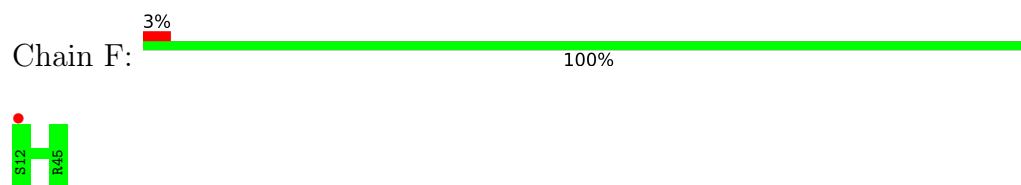
- Molecule 5: Cytochrome b559 subunit alpha



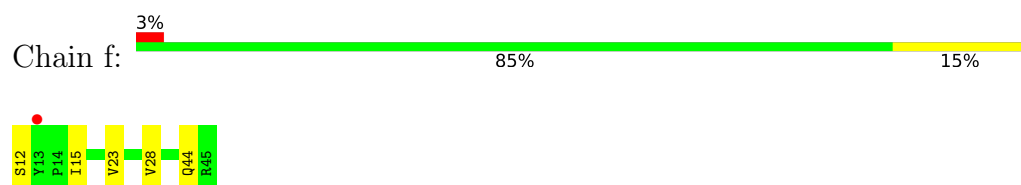
- Molecule 5: Cytochrome b559 subunit alpha



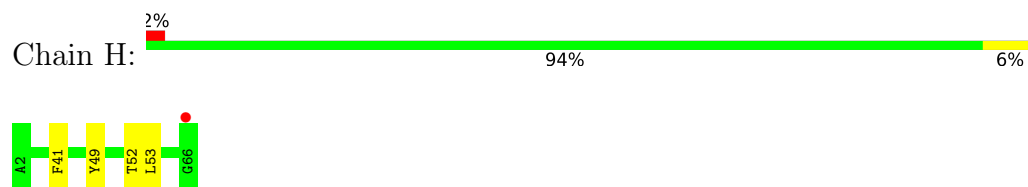
- Molecule 6: Cytochrome b559 subunit beta



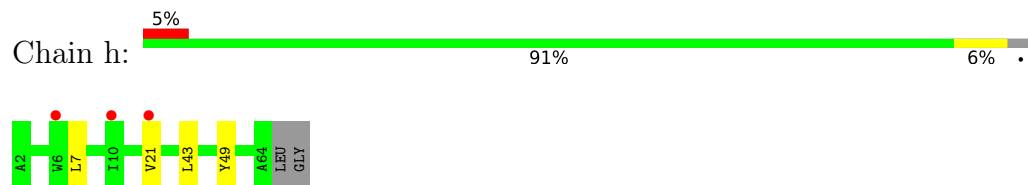
- Molecule 6: Cytochrome b559 subunit beta



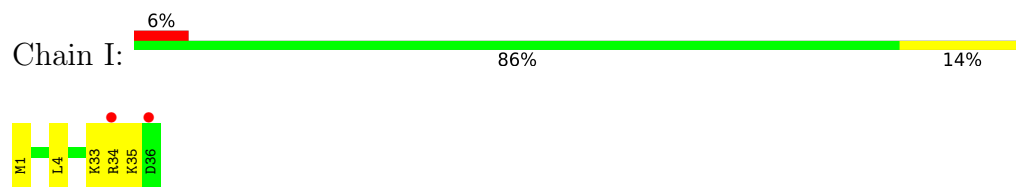
• Molecule 7: Photosystem II reaction center protein H



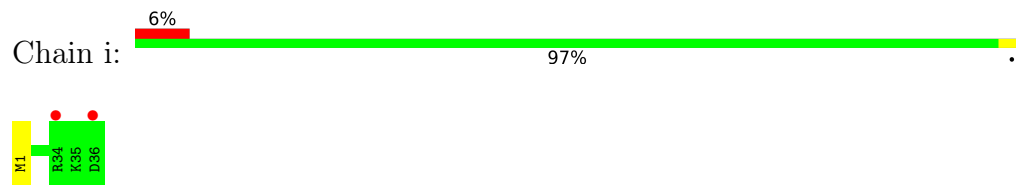
• Molecule 7: Photosystem II reaction center protein H



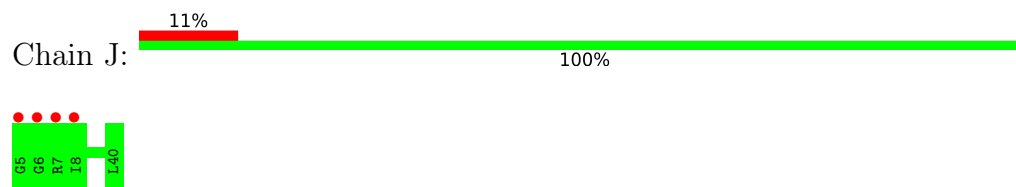
• Molecule 8: Photosystem II reaction center protein I



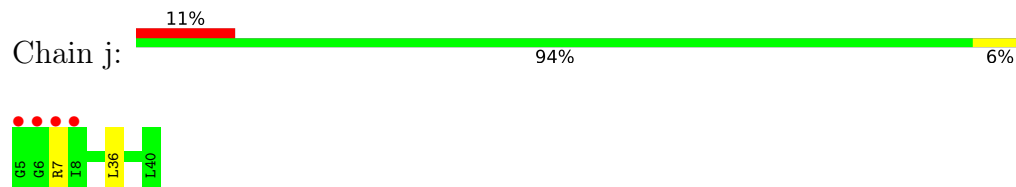
• Molecule 8: Photosystem II reaction center protein I



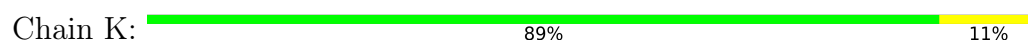
• Molecule 9: Photosystem II reaction center protein J

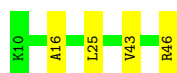


• Molecule 9: Photosystem II reaction center protein J

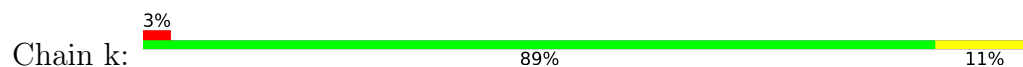


• Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



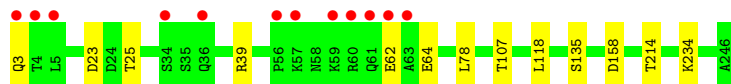
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

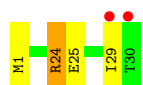
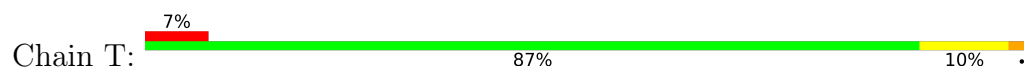


- Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 14: Photosystem II reaction center protein T



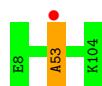
- Molecule 14: Photosystem II reaction center protein T



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



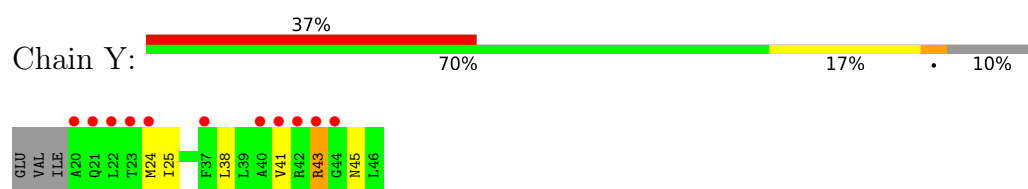
- Molecule 16: Cytochrome c-550



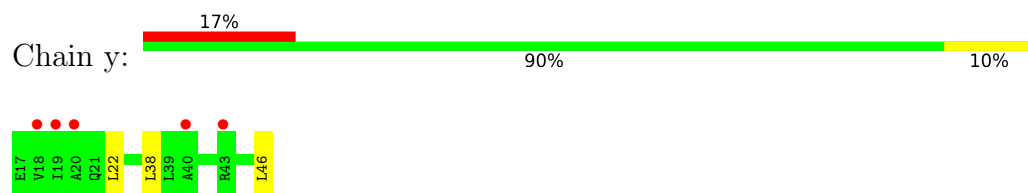
- Molecule 16: Cytochrome c-550



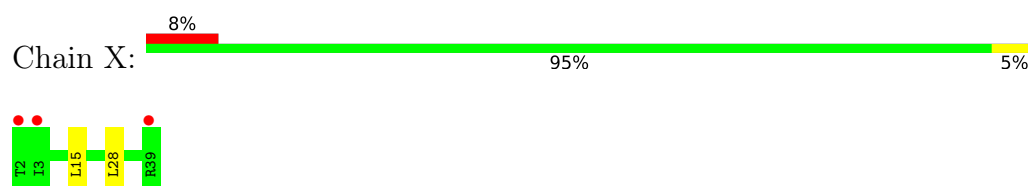
- Molecule 17: Photosystem II reaction center protein Ycf12



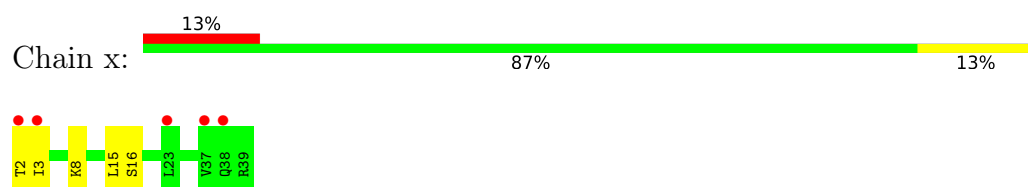
- Molecule 17: Photosystem II reaction center protein Ycf12



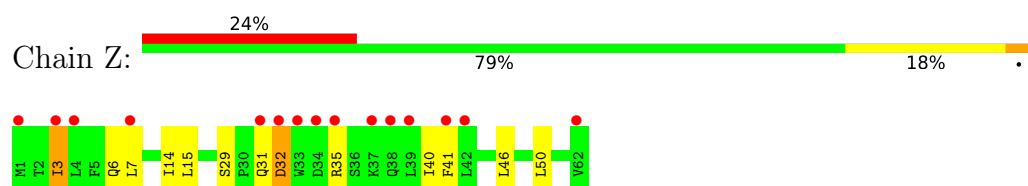
- Molecule 18: Photosystem II reaction center X protein



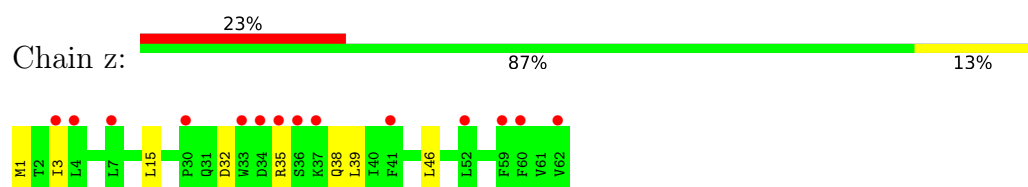
- Molecule 18: Photosystem II reaction center X protein



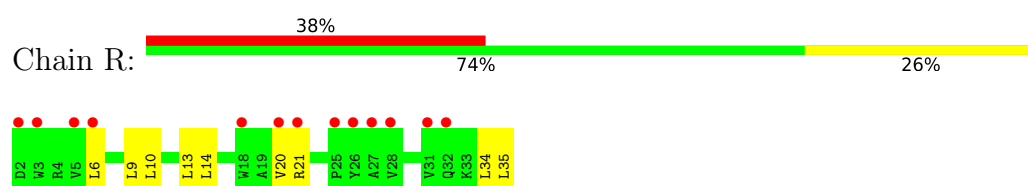
- Molecule 19: Photosystem II reaction center protein Z



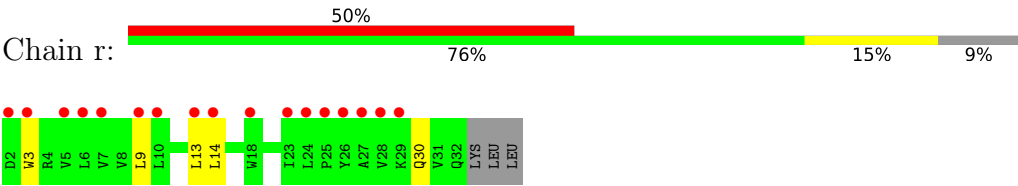
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.01Å 221.54Å 308.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.58 – 2.07 30.58 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.58-2.07) 87.1 (30.58-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 2.06Å)	Xtriage
Refinement program	PHENIX dev_svn	Depositor
R, R_{free}	0.184 , 0.247 0.184 , 0.248	Depositor DCC
R_{free} test set	4294 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	105756	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: FME, LMG, DGD, PHO, HEC, FE2, SQD, CLA, OEX, BCT, HEM, LHG, CL, OEY, BCR, UNL, PL9

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	0.69	0/3179	0.73	0/4331
1	a	0.65	0/3176	0.70	0/4327
2	B	0.63	0/4160	0.67	1/5668 (0.0%)
2	b	0.62	1/4118 (0.0%)	0.68	1/5611 (0.0%)
3	C	0.60	0/3593	0.66	1/4891 (0.0%)
3	c	0.59	1/3673 (0.0%)	0.67	0/4998
4	D	0.64	0/2820	0.66	0/3840
4	d	0.63	1/2829 (0.0%)	0.67	1/3852 (0.0%)
5	E	0.51	0/684	0.61	0/935
5	e	0.50	0/683	0.61	0/932
6	F	0.51	0/284	0.58	0/387
6	f	0.45	0/284	0.58	0/387
7	H	0.59	0/520	0.67	0/709
7	h	0.57	0/511	0.67	0/697
8	I	0.64	0/293	0.63	0/396
8	i	0.66	0/293	0.74	0/396
9	J	0.55	0/263	0.67	0/356
9	j	0.47	0/261	0.63	0/353
10	K	0.49	0/314	0.66	0/427
10	k	0.47	0/303	0.61	0/416
11	L	0.60	0/311	0.66	0/422
11	l	0.62	0/303	0.68	0/412
12	M	0.60	0/249	0.67	0/341
12	m	0.64	0/244	0.65	0/334
13	O	0.59	0/1914	0.73	1/2596 (0.0%)
13	o	0.56	0/1905	0.71	1/2583 (0.0%)
14	T	0.69	0/257	0.75	1/349 (0.3%)
14	t	0.69	0/255	0.62	0/346
15	U	0.53	0/785	0.65	0/1064
15	u	0.59	0/785	0.68	0/1064
16	V	0.56	0/1085	0.64	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.53	0/1085	0.64	0/1473
17	Y	0.40	0/197	0.60	0/264
17	y	0.35	0/219	0.54	0/294
18	X	0.52	0/284	0.59	0/384
18	x	0.38	0/284	0.55	0/384
19	Z	0.47	0/490	0.60	0/669
19	z	0.42	0/488	0.56	0/666
20	R	0.41	0/277	0.63	0/380
20	r	0.33	0/233	0.48	0/323
All	All	0.60	3/43891 (0.0%)	0.67	7/59730 (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
15	u	0	1
19	Z	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	323	GLU	CB-CG	5.85	1.63	1.52
3	c	296	VAL	CB-CG1	-5.38	1.41	1.52
2	b	185	TRP	CB-CG	-5.00	1.41	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.63	123.37	118.30
2	b	384	ARG	NE-CZ-NH2	5.59	123.10	120.30
2	B	15	ASP	CB-CG-OD2	-5.55	113.30	118.30
13	O	158	ASP	CB-CG-OD1	5.45	123.21	118.30
14	T	24	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	C	396	MET	CG-SD-CE	-5.20	91.89	100.20
4	d	251	ARG	NE-CZ-NH2	-5.18	117.71	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	Z	32	ASP	Peptide
15	u	53	ALA	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/334 (117%)	381 (98%)	9 (2%)	0	100	100
1	a	390/334 (117%)	382 (98%)	8 (2%)	0	100	100
2	B	508/505 (101%)	497 (98%)	11 (2%)	0	100	100
2	b	503/505 (100%)	495 (98%)	7 (1%)	1 (0%)	47	39
3	C	447/451 (99%)	435 (97%)	11 (2%)	1 (0%)	47	39
3	c	457/451 (101%)	442 (97%)	14 (3%)	1 (0%)	47	39
4	D	339/341 (99%)	330 (97%)	9 (3%)	0	100	100
4	d	340/341 (100%)	329 (97%)	11 (3%)	0	100	100
5	E	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
5	e	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	55 (90%)	6 (10%)	0	100	100
8	I	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
9	J	34/36 (94%)	31 (91%)	3 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	0	1 (3%)	4	1
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/33 (94%)	31 (100%)	0	0	100	100
12	m	30/33 (91%)	29 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	226 (93%)	16 (7%)	1 (0%)	34	25
13	o	242/244 (99%)	230 (95%)	8 (3%)	4 (2%)	9	2
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	28 (100%)	0	0	100	100
15	U	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
15	u	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	14	5
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	Y	25/30 (83%)	19 (76%)	4 (16%)	2 (8%)	1	0
17	y	28/30 (93%)	24 (86%)	4 (14%)	0	100	100
18	X	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
18	x	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	50 (83%)	7 (12%)	3 (5%)	2	0
19	z	60/62 (97%)	50 (83%)	9 (15%)	1 (2%)	9	2
20	R	32/34 (94%)	30 (94%)	1 (3%)	1 (3%)	4	0
20	r	29/34 (85%)	22 (76%)	6 (21%)	1 (3%)	3	0
All	All	5365/5326 (101%)	5164 (96%)	183 (3%)	18 (0%)	41	32

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	62	GLU
3	c	416	SER
13	o	60	ARG
13	o	61	GLN
15	u	53	ALA

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Mol	Chain	Res	Type
19	z	15	LEU
20	r	30	GLN
10	K	16	ALA
17	Y	41	VAL
17	Y	43	ARG
20	R	34	LEU
19	Z	3	ILE
13	o	57	LYS
19	Z	6	GLN
2	b	127	ARG
13	o	62	GLU
19	Z	14	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	319/270 (118%)	312 (98%)	7 (2%)	52	46
1	a	318/270 (118%)	306 (96%)	12 (4%)	33	26
2	B	407/403 (101%)	390 (96%)	17 (4%)	30	23
2	b	402/403 (100%)	395 (98%)	7 (2%)	60	57
3	C	351/352 (100%)	342 (97%)	9 (3%)	46	40
3	c	360/352 (102%)	344 (96%)	16 (4%)	28	21
4	D	277/276 (100%)	273 (99%)	4 (1%)	67	64
4	d	278/276 (101%)	272 (98%)	6 (2%)	52	46
5	E	72/72 (100%)	63 (88%)	9 (12%)	4	1
5	e	71/72 (99%)	68 (96%)	3 (4%)	30	23
6	F	28/28 (100%)	28 (100%)	0	100	100
6	f	28/28 (100%)	23 (82%)	5 (18%)	2	0
7	H	53/54 (98%)	49 (92%)	4 (8%)	13	6
7	h	53/54 (98%)	49 (92%)	4 (8%)	13	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	32/32 (100%)	28 (88%)	4 (12%)	4	1
8	i	32/32 (100%)	32 (100%)	0	100	100
9	J	24/24 (100%)	24 (100%)	0	100	100
9	j	23/24 (96%)	21 (91%)	2 (9%)	10	4
10	K	31/30 (103%)	27 (87%)	4 (13%)	4	1
10	k	30/30 (100%)	26 (87%)	4 (13%)	4	1
11	L	35/35 (100%)	34 (97%)	1 (3%)	42	36
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	4
12	M	28/29 (97%)	26 (93%)	2 (7%)	14	7
12	m	28/29 (97%)	27 (96%)	1 (4%)	35	28
13	O	208/207 (100%)	197 (95%)	11 (5%)	22	14
13	o	207/207 (100%)	191 (92%)	16 (8%)	13	5
14	T	26/26 (100%)	23 (88%)	3 (12%)	5	1
14	t	25/26 (96%)	24 (96%)	1 (4%)	31	24
15	U	84/84 (100%)	81 (96%)	3 (4%)	35	28
15	u	84/84 (100%)	84 (100%)	0	100	100
16	V	117/117 (100%)	113 (97%)	4 (3%)	37	30
16	v	117/117 (100%)	110 (94%)	7 (6%)	19	11
17	Y	19/23 (83%)	14 (74%)	5 (26%)	0	0
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
18	X	31/31 (100%)	29 (94%)	2 (6%)	17	9
18	x	31/31 (100%)	26 (84%)	5 (16%)	2	0
19	Z	52/52 (100%)	41 (79%)	11 (21%)	1	0
19	z	51/52 (98%)	44 (86%)	7 (14%)	3	1
20	R	28/29 (97%)	20 (71%)	8 (29%)	0	0
20	r	19/29 (66%)	15 (79%)	4 (21%)	1	0
All	All	4435/4348 (102%)	4221 (95%)	214 (5%)	25	18

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	15	GLU

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Mol	Chain	Res	Type
1	A	16	ARG
1	A	102	LEU
1	A	229	GLU
1	A	243	GLU
1	A	248	ILE
2	B	79	SER
2	B	83	GLU
2	B	101	ILE
2	B	127	ARG
2	B	161	LEU
2	B	227	LYS
2	B	246	PHE
2	B	289	GLN
2	B	291	SER
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	480[A]	SER
2	B	480[B]	SER
2	B	489	GLU
2	B	491	VAL
2	B	495	PHE
3	C	106	VAL
3	C	141	GLU
3	C	161	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355[A]	THR
3	C	355[B]	THR
3	C	416	SER
4	D	12	ARG
4	D	76	VAL
4	D	180	ARG
4	D	259	ILE
5	E	4	THR
5	E	11	SER
5	E	14	ILE
5	E	16	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	65	LEU

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Mol	Chain	Res	Type
5	E	71	GLU
5	E	83	LEU
7	H	41	PHE
7	H	49	TYR
7	H	52	THR
7	H	53	LEU
8	I	4	LEU
8	I	33	LYS
8	I	34	ARG
8	I	35	LYS
10	K	25	LEU
10	K	43	VAL
10	K	46[A]	ARG
10	K	46[B]	ARG
11	L	2	GLU
12	M	3	VAL
12	M	13	LEU
13	O	3	GLN
13	O	23	ASP
13	O	25	THR
13	O	39	ARG
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	214	THR
13	O	234	LYS
14	T	24	ARG
14	T	25	GLU
14	T	29	ILE
15	U	10	VAL
15	U	39	ARG
15	U	67	LEU
16	V	3	LEU
16	V	7	VAL
16	V	14	SER
16	V	110	LYS
17	Y	24	MET
17	Y	25	ILE
17	Y	38	LEU
17	Y	43	ARG

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Mol	Chain	Res	Type
17	Y	45	ASN
18	X	15	LEU
18	X	28	LEU
19	Z	3	ILE
19	Z	7	LEU
19	Z	15	LEU
19	Z	29	SER
19	Z	31	GLN
19	Z	32	ASP
19	Z	35	ARG
19	Z	40	ILE
19	Z	41	PHE
19	Z	46	LEU
19	Z	50	LEU
20	R	6	LEU
20	R	9	LEU
20	R	10	LEU
20	R	13	LEU
20	R	14	LEU
20	R	20	VAL
20	R	21	ARG
20	R	35	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	238	LYS
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	86	ILE
2	b	127	ARG
2	b	128	THR
2	b	149	LEU
2	b	362	PHE
2	b	397	VAL
2	b	490	GLN
3	c	24	THR

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Mol	Chain	Res	Type
3	c	25	ASN
3	c	26	ARG
3	c	29	GLU
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	155	ASN
3	c	165	LEU
3	c	289	PHE
3	c	315	MET
3	c	355[A]	THR
3	c	355[B]	THR
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	462	GLU
4	d	12	ARG
4	d	182	LEU
4	d	233	ARG
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	8	ARG
5	e	75	GLN
5	e	83	LEU
6	f	12	SER
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
6	f	44	GLN
7	h	7	LEU
7	h	21	VAL
7	h	43	LEU
7	h	49	TYR
9	j	7	ARG
9	j	36	LEU
10	k	10	LYS
10	k	11	LEU
10	k	23	ASP
10	k	30	VAL
11	l	2	GLU
11	l	21	LEU
11	l	30	LEU

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Mol	Chain	Res	Type
12	m	13	LEU
13	o	4	THR
13	o	18	LYS
13	o	39	ARG
13	o	49	THR
13	o	53	LYS
13	o	57	LYS
13	o	59	LYS
13	o	60	ARG
13	o	97	GLU
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	135	SER
13	o	181	GLU
13	o	198	SER
13	o	207	ARG
14	t	25	GLU
16	v	15	GLU
16	v	24	LYS
16	v	52	LEU
16	v	106	ASN
16	v	107	LEU
16	v	109	GLU
16	v	112	LEU
17	y	22	LEU
17	y	38	LEU
17	y	46	LEU
18	x	2	THR
18	x	3	ILE
18	x	8	LYS
18	x	15	LEU
18	x	16	SER
19	z	1	MET
19	z	3	ILE
19	z	32	ASP
19	z	35	ARG
19	z	38	GLN
19	z	39	LEU
19	z	46	LEU
20	r	3	TRP
20	r	9	LEU

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Mol	Chain	Res	Type
20	r	13	LEU
20	r	14	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	289	GLN
2	B	490	GLN
13	O	82	GLN
13	O	231	HIS
17	Y	21	GLN
2	b	497	GLN
3	c	418	ASN
13	o	58	ASN
19	z	38	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
12	FME	m	1	12	8,9,10	1.02	1 (12%)	7,9,11	0.67	0
8	FME	i	1	8	8,9,10	1.01	0	7,9,11	1.15	1 (14%)
14	FME	T	1	14	8,9,10	1.11	1 (12%)	7,9,11	1.62	2 (28%)
14	FME	t	1	14	8,9,10	1.07	1 (12%)	7,9,11	1.97	1 (14%)
12	FME	M	1	12	8,9,10	0.92	0	7,9,11	1.02	0
8	FME	I	1	8	8,9,10	0.87	0	7,9,11	1.47	2 (28%)

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
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	t	1	FME	CA-N	-2.69	1.42	1.46
14	T	1	FME	CA-N	-2.32	1.43	1.46
12	m	1	FME	CA-N	-2.08	1.43	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-4.32	116.18	122.82
8	I	1	FME	CA-N-CN	-3.12	118.02	122.82
14	T	1	FME	CA-N-CN	-2.62	118.79	122.82
8	i	1	FME	C-CA-N	2.40	114.07	109.73
14	T	1	FME	O1-CN-N	-2.12	119.68	125.27
8	I	1	FME	O1-CN-N	-2.02	119.96	125.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	1	FME	CB-CG-SD-CE
14	t	1	FME	CB-CG-SD-CE
12	M	1	FME	CB-CA-N-CN
8	i	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic and 31 are unknown - leaving 151 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
23	CLA	D	402	-	59,73,73	1.19	8 (13%)	67,113,113	1.35	10 (14%)
33	BCT	A	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	614	-	59,73,73	1.50	8 (13%)	67,113,113	1.67	16 (23%)
23	CLA	c	504	37	54,68,73	1.46	6 (11%)	61,107,113	1.63	11 (18%)
24	PHO	A	406	-	67,69,69	1.18	10 (14%)	85,99,99	1.11	4 (4%)
25	BCR	x	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	6 (10%)
27	LMG	c	523	-	49,49,55	0.89	1 (2%)	57,57,63	1.31	7 (12%)
24	PHO	a	407	-	67,69,69	1.29	9 (13%)	85,99,99	1.04	4 (4%)
23	CLA	C	508	-	59,73,73	1.37	6 (10%)	67,113,113	1.58	12 (17%)
23	CLA	b	605	-	59,73,73	1.40	6 (10%)	67,113,113	1.58	14 (20%)
23	CLA	c	501	-	59,73,73	1.49	9 (15%)	67,113,113	1.79	11 (16%)
27	LMG	C	518	-	48,48,55	1.02	3 (6%)	56,56,63	1.34	8 (14%)
29	LHG	D	408	-	46,46,48	1.07	4 (8%)	49,52,54	1.30	5 (10%)
23	CLA	B	609	-	59,73,73	1.61	10 (16%)	67,113,113	1.68	15 (22%)
23	CLA	C	503	-	59,73,73	1.82	9 (15%)	67,113,113	1.85	11 (16%)
23	CLA	C	505	-	59,73,73	1.42	5 (8%)	67,113,113	1.38	9 (13%)
23	CLA	c	510	-	59,73,73	1.51	8 (13%)	67,113,113	1.67	13 (19%)
26	PL9	A	410	-	55,55,55	1.14	2 (3%)	68,69,69	1.69	15 (22%)
23	CLA	C	501	-	59,73,73	1.68	6 (10%)	67,113,113	1.51	9 (13%)
27	LMG	b	622	-	55,55,55	1.03	3 (5%)	63,63,63	1.45	8 (12%)
23	CLA	C	504	37	53,67,73	1.48	9 (16%)	59,105,113	1.39	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	506	-	59,73,73	1.34	6 (10%)	67,113,113	1.49	9 (13%)
23	CLA	b	608	37	59,73,73	1.53	8 (13%)	67,113,113	1.36	8 (11%)
30	DGD	H	102	-	63,63,67	1.32	9 (14%)	77,77,81	1.45	11 (14%)
32	OEY	a	417[B]	3,37,1	0,16,16	0.00	-	-		
23	CLA	c	513	-	59,73,73	1.45	8 (13%)	67,113,113	1.28	7 (10%)
26	PL9	d	405	-	55,55,55	1.37	10 (18%)	68,69,69	1.79	20 (29%)
23	CLA	A	404	-	59,73,73	1.59	7 (11%)	67,113,113	1.62	13 (19%)
23	CLA	b	614	-	59,73,73	1.67	6 (10%)	67,113,113	1.56	13 (19%)
27	LMG	c	521	-	48,48,55	1.12	6 (12%)	56,56,63	1.36	7 (12%)
23	CLA	C	509	-	59,73,73	1.33	7 (11%)	67,113,113	1.37	7 (10%)
27	LMG	D	406	-	51,51,55	0.98	2 (3%)	59,59,63	1.28	8 (13%)
35	HEM	e	102	6,5	27,50,50	1.98	4 (14%)	17,82,82	2.46	6 (35%)
25	BCR	c	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	12 (21%)
23	CLA	b	604	-	59,73,73	1.44	8 (13%)	67,113,113	1.69	13 (19%)
23	CLA	c	502	-	59,73,73	1.52	7 (11%)	67,113,113	1.60	10 (14%)
25	BCR	k	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.22	5 (8%)
29	LHG	d	408	-	38,38,48	0.88	1 (2%)	41,44,54	1.21	4 (9%)
23	CLA	C	513	-	59,73,73	1.37	8 (13%)	67,113,113	1.64	7 (10%)
23	CLA	a	408	-	59,73,73	1.41	6 (10%)	67,113,113	1.62	14 (20%)
23	CLA	c	508	-	58,72,73	1.32	7 (12%)	65,111,113	1.52	9 (13%)
31	OEX	a	416[A]	3,37,1	0,15,15	0.00	-	-		
23	CLA	D	403	-	59,73,73	1.41	10 (16%)	67,113,113	1.42	9 (13%)
23	CLA	a	405	-	59,73,73	1.27	7 (11%)	67,113,113	1.66	12 (17%)
30	DGD	c	518	-	63,63,67	1.10	6 (9%)	77,77,81	1.46	15 (19%)
23	CLA	B	615	-	59,73,73	1.71	12 (20%)	67,113,113	1.42	7 (10%)
25	BCR	B	618	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	10 (17%)
23	CLA	A	408	-	48,62,73	1.68	6 (12%)	53,99,113	1.70	12 (22%)
25	BCR	c	515	-	41,41,41	1.27	3 (7%)	56,56,56	1.44	10 (17%)
27	LMG	A	411	-	48,48,55	0.94	2 (4%)	56,56,63	1.39	9 (16%)
23	CLA	C	507	37	59,73,73	1.51	8 (13%)	67,113,113	1.59	11 (16%)
23	CLA	c	512	-	59,73,73	1.48	8 (13%)	67,113,113	1.53	13 (19%)
23	CLA	B	606	-	59,73,73	1.77	8 (13%)	67,113,113	1.65	12 (17%)
23	CLA	a	411	37	59,73,73	1.47	7 (11%)	67,113,113	1.80	11 (16%)
26	PL9	a	410	-	55,55,55	1.08	4 (7%)	68,69,69	1.73	12 (17%)
23	CLA	b	606	-	59,73,73	1.31	6 (10%)	67,113,113	1.67	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	511	3	59,73,73	1.71	9 (15%)	67,113,113	1.75	10 (14%)
29	LHG	D	407	-	48,48,48	0.98	3 (6%)	51,54,54	1.32	7 (13%)
28	SQD	A	412	-	51,52,54	1.06	4 (7%)	60,63,65	2.29	15 (25%)
31	OEX	A	416[A]	3,37,1	0,15,15	0.00	-	-		
26	PL9	D	405	-	55,55,55	1.57	8 (14%)	68,69,69	1.47	11 (16%)
23	CLA	A	405	37	59,73,73	1.37	10 (16%)	67,113,113	1.57	9 (13%)
32	OXY	A	417[B]	3,37,1	0,16,16	0.00	-	-		
23	CLA	C	510	-	59,73,73	1.46	8 (13%)	67,113,113	1.47	9 (13%)
30	DGD	C	515	-	63,63,67	1.40	9 (14%)	77,77,81	1.33	9 (11%)
23	CLA	C	512	-	59,73,73	1.39	7 (11%)	67,113,113	1.57	14 (20%)
25	BCR	k	102	-	41,41,41	0.90	1 (2%)	56,56,56	1.15	3 (5%)
25	BCR	H	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.40	6 (10%)
23	CLA	B	605	-	59,73,73	1.31	6 (10%)	67,113,113	1.70	14 (20%)
27	LMG	b	623	-	18,21,55	0.73	0	16,20,63	0.92	1 (6%)
23	CLA	B	613	-	59,73,73	1.46	9 (15%)	67,113,113	1.53	10 (14%)
24	PHO	d	401	-	67,69,69	1.23	11 (16%)	85,99,99	1.27	10 (11%)
23	CLA	D	401	37	59,73,73	1.33	7 (11%)	67,113,113	1.47	11 (16%)
29	LHG	d	407	-	48,48,48	0.78	1 (2%)	51,54,54	1.29	6 (11%)
23	CLA	c	507	37	59,73,73	1.46	9 (15%)	67,113,113	1.57	10 (14%)
25	BCR	T	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.53	10 (17%)
23	CLA	B	611	-	59,73,73	1.35	9 (15%)	67,113,113	1.55	13 (19%)
23	CLA	d	402	-	59,73,73	1.53	7 (11%)	67,113,113	1.76	9 (13%)
36	HEC	v	201	16	26,50,50	2.42	4 (15%)	18,82,82	1.45	4 (22%)
25	BCR	b	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	6 (10%)
30	DGD	A	415	-	67,67,67	1.25	8 (11%)	81,81,81	1.48	11 (13%)
27	LMG	D	409	-	31,31,55	0.99	3 (9%)	33,33,63	1.24	3 (9%)
23	CLA	B	616	-	54,68,73	1.54	8 (14%)	61,107,113	1.60	14 (22%)
23	CLA	a	406	37	59,73,73	1.78	9 (15%)	67,113,113	1.66	12 (17%)
23	CLA	b	616	-	59,73,73	1.73	10 (16%)	67,113,113	1.40	6 (8%)
23	CLA	b	609	-	59,73,73	1.48	8 (13%)	67,113,113	1.64	17 (25%)
28	SQD	f	101	-	40,41,54	1.16	5 (12%)	49,52,65	1.75	9 (18%)
23	CLA	B	604	-	59,73,73	1.47	6 (10%)	67,113,113	1.69	12 (17%)
23	CLA	c	505	-	59,73,73	1.46	6 (10%)	67,113,113	1.66	14 (20%)
25	BCR	b	620	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	9 (16%)
27	LMG	M	101	-	51,51,55	0.99	3 (5%)	59,59,63	1.50	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	d	404	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	5 (8%)
30	DGD	a	414	-	43,43,67	1.45	5 (11%)	45,45,81	1.49	7 (15%)
23	CLA	B	612	-	59,73,73	1.24	6 (10%)	67,113,113	1.61	11 (16%)
23	CLA	b	613	-	59,73,73	1.31	6 (10%)	67,113,113	1.56	12 (17%)
30	DGD	c	516	-	63,63,67	1.28	6 (9%)	77,77,81	1.39	12 (15%)
23	CLA	B	608	-	59,73,73	1.33	8 (13%)	67,113,113	1.51	13 (19%)
25	BCR	Z	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
29	LHG	e	101	-	41,41,48	0.92	3 (7%)	44,47,54	1.37	4 (9%)
25	BCR	C	514	-	41,41,41	1.16	4 (9%)	56,56,56	1.31	8 (14%)
25	BCR	A	409	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	6 (10%)
23	CLA	b	617	-	54,68,73	1.41	5 (9%)	61,107,113	1.54	11 (18%)
28	SQD	a	413	-	35,35,54	1.11	2 (5%)	37,37,65	1.39	5 (13%)
28	SQD	a	412	-	53,54,54	0.98	4 (7%)	62,65,65	1.90	11 (17%)
25	BCR	b	618	-	41,41,41	1.15	3 (7%)	56,56,56	1.40	10 (17%)
27	LMG	B	621	-	20,26,55	0.64	0	18,26,63	1.00	0
23	CLA	b	615	-	59,73,73	1.62	8 (13%)	67,113,113	1.71	11 (16%)
23	CLA	d	403	-	59,73,73	1.47	9 (15%)	67,113,113	1.31	10 (14%)
24	PHO	A	407	-	67,69,69	1.26	10 (14%)	85,99,99	1.20	10 (11%)
25	BCR	B	617	-	41,41,41	1.19	4 (9%)	56,56,56	1.38	8 (14%)
29	LHG	A	413	-	48,48,48	0.99	4 (8%)	51,54,54	1.21	2 (3%)
29	LHG	B	623	-	48,48,48	0.86	2 (4%)	51,54,54	1.43	6 (11%)
27	LMG	c	519	-	37,37,55	1.15	4 (10%)	45,45,63	1.26	6 (13%)
28	SQD	B	624	-	53,54,54	0.93	2 (3%)	62,65,65	1.83	12 (19%)
33	BCT	a	404	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	c	511	3	59,73,73	1.74	6 (10%)	67,113,113	1.57	10 (14%)
23	CLA	c	506	-	59,73,73	1.38	6 (10%)	67,113,113	1.57	14 (20%)
27	LMG	m	101	-	51,51,55	0.82	1 (1%)	59,59,63	1.54	12 (20%)
35	HEM	E	101	6,5	27,50,50	1.89	4 (14%)	17,82,82	2.09	8 (47%)
29	LHG	d	406	-	48,48,48	0.72	0	51,54,54	1.29	6 (11%)
23	CLA	c	509	-	59,73,73	1.36	5 (8%)	67,113,113	1.72	11 (16%)
36	HEC	V	201	16	26,50,50	2.33	5 (19%)	18,82,82	1.76	6 (33%)
23	CLA	B	601	37	59,73,73	1.71	7 (11%)	67,113,113	1.84	9 (13%)
25	BCR	a	409	-	41,41,41	0.99	2 (4%)	56,56,56	1.34	10 (17%)
28	SQD	A	414	-	38,38,54	1.04	3 (7%)	40,40,65	1.30	3 (7%)
23	CLA	b	607	-	59,73,73	1.68	7 (11%)	67,113,113	1.80	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	h	101	37	59,73,73	1.74	10 (16%)	67,113,113	1.52	13 (19%)
28	SQD	b	601	-	48,49,54	0.95	3 (6%)	57,60,65	1.96	13 (22%)
23	CLA	B	602	-	59,73,73	1.75	9 (15%)	67,113,113	1.49	11 (16%)
29	LHG	B	622	-	48,48,48	0.69	1 (2%)	51,54,54	1.12	5 (9%)
30	DGD	C	517	-	63,63,67	1.13	8 (12%)	77,77,81	1.37	8 (10%)
30	DGD	h	102	-	63,63,67	1.03	5 (7%)	77,77,81	1.53	14 (18%)
25	BCR	D	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.25	5 (8%)
25	BCR	t	101	-	41,41,41	1.01	2 (4%)	56,56,56	1.43	9 (16%)
23	CLA	B	610	37	59,73,73	1.59	7 (11%)	67,113,113	1.55	9 (13%)
23	CLA	B	607	37	59,73,73	1.40	8 (13%)	67,113,113	1.55	10 (14%)
29	LHG	l	101	-	48,48,48	0.78	1 (2%)	51,54,54	1.22	5 (9%)
23	CLA	c	503	-	59,73,73	1.51	6 (10%)	67,113,113	1.68	10 (14%)
23	CLA	B	603	-	59,73,73	1.47	11 (18%)	67,113,113	1.42	13 (19%)
23	CLA	b	610	-	59,73,73	1.64	8 (13%)	67,113,113	1.24	8 (11%)
30	DGD	c	517	-	63,63,67	1.09	6 (9%)	77,77,81	1.41	9 (11%)
25	BCR	B	619	-	41,41,41	1.23	3 (7%)	56,56,56	1.32	8 (14%)
23	CLA	b	611	37	59,73,73	1.33	6 (10%)	67,113,113	1.45	12 (17%)
23	CLA	b	612	-	59,73,73	1.49	7 (11%)	67,113,113	1.47	11 (16%)
23	CLA	b	603	-	59,73,73	1.49	8 (13%)	67,113,113	1.50	9 (13%)
28	SQD	F	101	-	35,36,54	1.02	3 (8%)	42,45,65	1.79	9 (21%)
27	LMG	d	409	-	44,44,55	1.02	3 (6%)	52,52,63	1.33	7 (13%)
25	BCR	K	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.41	9 (16%)
23	CLA	C	502	-	59,73,73	1.43	7 (11%)	67,113,113	1.43	11 (16%)
25	BCR	K	102	-	41,41,41	1.10	2 (4%)	56,56,56	1.18	6 (10%)
30	DGD	C	516	-	63,63,67	1.07	4 (6%)	77,77,81	1.44	12 (15%)

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
23	CLA	D	402	-	1/1/25/25	5/37/135/135	-
23	CLA	B	614	-	3/3/25/25	13/37/135/135	-
23	CLA	c	504	37	3/3/24/25	6/31/129/135	-
24	PHO	A	406	-	-	7/53/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	x	101	-	-	6/29/63/63	0/2/2/2
27	LMG	c	523	-	-	27/44/64/70	0/1/1/1
24	PHO	a	407	-	-	6/53/103/103	0/5/6/6
23	CLA	C	508	-	3/3/25/25	5/37/135/135	-
23	CLA	b	605	-	3/3/25/25	13/37/135/135	-
23	CLA	c	501	-	3/3/25/25	7/37/135/135	-
27	LMG	C	518	-	-	15/43/63/70	0/1/1/1
29	LHG	D	408	-	-	21/51/51/53	-
23	CLA	B	609	-	1/1/25/25	3/37/135/135	-
23	CLA	C	503	-	3/3/25/25	5/37/135/135	-
23	CLA	C	505	-	3/3/25/25	13/37/135/135	-
23	CLA	c	510	-	3/3/25/25	15/37/135/135	-
26	PL9	A	410	-	-	27/53/73/73	0/1/1/1
23	CLA	C	501	-	3/3/25/25	6/37/135/135	-
27	LMG	b	622	-	-	26/50/70/70	0/1/1/1
23	CLA	C	504	37	3/3/23/25	8/30/128/135	-
23	CLA	C	506	-	2/2/25/25	11/37/135/135	-
23	CLA	b	608	37	3/3/25/25	13/37/135/135	-
30	DGD	H	102	-	-	13/51/91/95	0/2/2/2
23	CLA	c	513	-	3/3/25/25	7/37/135/135	-
26	PL9	d	405	-	-	17/53/73/73	0/1/1/1
23	CLA	A	404	-	2/2/25/25	4/37/135/135	-
23	CLA	b	614	-	3/3/25/25	4/37/135/135	-
27	LMG	c	521	-	-	19/43/63/70	0/1/1/1
23	CLA	C	509	-	3/3/25/25	9/37/135/135	-
27	LMG	D	406	-	-	14/46/66/70	0/1/1/1
35	HEM	e	102	6,5	-	0/6/54/54	-
25	BCR	c	514	-	-	16/29/63/63	0/2/2/2
23	CLA	b	604	-	2/2/25/25	9/37/135/135	-
23	CLA	c	502	-	1/1/25/25	5/37/135/135	-
25	BCR	k	101	-	-	11/29/63/63	0/2/2/2
29	LHG	d	408	-	-	12/43/43/53	-
23	CLA	C	513	-	3/3/25/25	10/37/135/135	-
23	CLA	a	408	-	3/3/25/25	14/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	508	-	2/2/24/25	12/36/134/135	-
23	CLA	D	403	-	2/2/25/25	13/37/135/135	-
23	CLA	a	405	-	3/3/25/25	3/37/135/135	-
30	DGD	c	518	-	-	19/51/91/95	0/2/2/2
23	CLA	B	615	-	3/3/25/25	10/37/135/135	-
25	BCR	B	618	-	-	6/29/63/63	0/2/2/2
23	CLA	A	408	-	3/3/22/25	3/24/122/135	-
25	BCR	c	515	-	-	10/29/63/63	0/2/2/2
27	LMG	A	411	-	-	19/43/63/70	0/1/1/1
23	CLA	C	507	37	3/3/25/25	9/37/135/135	-
23	CLA	c	512	-	3/3/25/25	20/37/135/135	-
23	CLA	B	606	-	3/3/25/25	12/37/135/135	-
23	CLA	a	411	37	2/2/25/25	5/37/135/135	-
26	PL9	a	410	-	-	25/53/73/73	0/1/1/1
23	CLA	b	606	-	3/3/25/25	9/37/135/135	-
23	CLA	C	511	3	3/3/25/25	7/37/135/135	-
29	LHG	D	407	-	-	25/53/53/53	-
28	SQD	A	412	-	-	21/47/67/69	0/1/1/1
26	PL9	D	405	-	-	12/53/73/73	0/1/1/1
23	CLA	A	405	37	3/3/25/25	7/37/135/135	-
23	CLA	C	510	-	3/3/25/25	11/37/135/135	-
30	DGD	C	515	-	-	20/51/91/95	0/2/2/2
23	CLA	C	512	-	3/3/25/25	7/37/135/135	-
25	BCR	k	102	-	-	4/29/63/63	0/2/2/2
25	BCR	H	101	-	-	4/29/63/63	0/2/2/2
23	CLA	B	605	-	3/3/25/25	10/37/135/135	-
27	LMG	b	623	-	-	9/15/17/70	-
23	CLA	B	613	-	3/3/25/25	8/37/135/135	-
24	PHO	d	401	-	-	5/53/103/103	0/5/6/6
23	CLA	D	401	37	1/1/25/25	5/37/135/135	-
29	LHG	d	407	-	-	26/53/53/53	-
23	CLA	c	507	37	3/3/25/25	10/37/135/135	-
25	BCR	T	101	-	-	6/29/63/63	0/2/2/2
23	CLA	B	611	-	3/3/25/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	402	-	1/1/25/25	9/37/135/135	-
36	HEC	v	201	16	-	0/6/54/54	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
30	DGD	A	415	-	-	25/55/95/95	0/2/2/2
27	LMG	D	409	-	-	13/33/33/70	-
23	CLA	B	616	-	3/3/24/25	8/31/129/135	-
23	CLA	a	406	37	2/2/25/25	11/37/135/135	-
23	CLA	b	616	-	3/3/25/25	6/37/135/135	-
23	CLA	b	609	-	2/2/25/25	6/37/135/135	-
28	SQD	f	101	-	-	13/36/56/69	0/1/1/1
23	CLA	B	604	-	2/2/25/25	11/37/135/135	-
23	CLA	c	505	-	2/2/25/25	10/37/135/135	-
25	BCR	b	620	-	-	4/29/63/63	0/2/2/2
27	LMG	M	101	-	-	19/46/66/70	0/1/1/1
25	BCR	d	404	-	-	7/29/63/63	0/2/2/2
30	DGD	a	414	-	-	25/45/45/95	-
23	CLA	B	612	-	3/3/25/25	6/37/135/135	-
23	CLA	b	613	-	3/3/25/25	11/37/135/135	-
30	DGD	c	516	-	-	27/51/91/95	0/2/2/2
23	CLA	B	608	-	1/1/25/25	0/37/135/135	-
25	BCR	Z	101	-	-	10/29/63/63	0/2/2/2
29	LHG	e	101	-	-	28/46/46/53	-
25	BCR	C	514	-	-	2/29/63/63	0/2/2/2
25	BCR	A	409	-	-	12/29/63/63	0/2/2/2
23	CLA	b	617	-	3/3/24/25	10/31/129/135	-
28	SQD	a	413	-	-	19/37/37/69	-
28	SQD	a	412	-	-	25/49/69/69	0/1/1/1
25	BCR	b	618	-	-	6/29/63/63	0/2/2/2
27	LMG	B	621	-	-	9/18/22/70	-
23	CLA	b	615	-	3/3/25/25	16/37/135/135	-
23	CLA	d	403	-	3/3/25/25	7/37/135/135	-
24	PHO	A	407	-	-	2/53/103/103	0/5/6/6
25	BCR	B	617	-	-	11/29/63/63	0/2/2/2
29	LHG	A	413	-	-	27/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	B	623	-	-	21/53/53/53	-
27	LMG	c	519	-	-	12/31/51/70	0/1/1/1
28	SQD	B	624	-	-	24/49/69/69	0/1/1/1
23	CLA	c	511	3	3/3/25/25	10/37/135/135	-
23	CLA	c	506	-	3/3/25/25	16/37/135/135	-
27	LMG	m	101	-	-	19/46/66/70	0/1/1/1
35	HEM	E	101	6,5	-	0/6/54/54	-
29	LHG	d	406	-	-	23/53/53/53	-
23	CLA	c	509	-	3/3/25/25	15/37/135/135	-
36	HEC	V	201	16	-	0/6/54/54	-
23	CLA	B	601	37	3/3/25/25	13/37/135/135	-
25	BCR	a	409	-	-	6/29/63/63	0/2/2/2
28	SQD	A	414	-	-	18/39/39/69	-
23	CLA	b	607	-	3/3/25/25	13/37/135/135	-
23	CLA	h	101	37	2/2/25/25	17/37/135/135	-
28	SQD	b	601	-	-	18/44/64/69	0/1/1/1
23	CLA	B	602	-	3/3/25/25	5/37/135/135	-
29	LHG	B	622	-	-	20/53/53/53	-
30	DGD	C	517	-	-	15/51/91/95	0/2/2/2
30	DGD	h	102	-	-	17/51/91/95	0/2/2/2
25	BCR	D	404	-	-	5/29/63/63	0/2/2/2
25	BCR	t	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	610	37	3/3/25/25	8/37/135/135	-
23	CLA	B	607	37	3/3/25/25	12/37/135/135	-
29	LHG	l	101	-	-	19/53/53/53	-
23	CLA	c	503	-	3/3/25/25	7/37/135/135	-
23	CLA	B	603	-	3/3/25/25	14/37/135/135	-
23	CLA	b	610	-	2/2/25/25	10/37/135/135	-
30	DGD	c	517	-	-	19/51/91/95	0/2/2/2
25	BCR	B	619	-	-	7/29/63/63	0/2/2/2
23	CLA	b	611	37	3/3/25/25	10/37/135/135	-
23	CLA	b	612	-	2/2/25/25	7/37/135/135	-
23	CLA	b	603	-	2/2/25/25	10/37/135/135	-
28	SQD	F	101	-	-	16/28/48/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	d	409	-	-	13/39/59/70	0/1/1/1
25	BCR	K	101	-	-	7/29/63/63	0/2/2/2
23	CLA	C	502	-	2/2/25/25	9/37/135/135	-
25	BCR	K	102	-	-	12/29/63/63	0/2/2/2
30	DGD	C	516	-	-	21/51/91/95	0/2/2/2

All (804) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C4B-NB	9.93	1.44	1.35
23	b	614	CLA	C4B-NB	9.72	1.43	1.35
23	B	601	CLA	C4B-NB	8.67	1.42	1.35
23	C	501	CLA	C4B-NB	8.46	1.42	1.35
23	b	615	CLA	C4B-NB	8.15	1.42	1.35
23	b	610	CLA	C4B-NB	8.04	1.42	1.35
23	C	511	CLA	C4B-NB	7.91	1.42	1.35
23	b	616	CLA	C4B-NB	7.81	1.42	1.35
23	a	406	CLA	C4B-NB	7.77	1.42	1.35
23	B	614	CLA	C4B-NB	7.67	1.42	1.35
23	c	501	CLA	C4B-NB	7.64	1.42	1.35
23	b	607	CLA	MG-NA	7.60	2.24	2.06
23	c	512	CLA	C4B-NB	7.49	1.41	1.35
23	B	610	CLA	C4B-NB	7.41	1.41	1.35
23	C	503	CLA	C4B-NB	7.41	1.41	1.35
23	a	408	CLA	C4B-NB	7.34	1.41	1.35
23	B	606	CLA	MG-NA	7.33	2.23	2.06
23	h	101	CLA	C4B-NB	7.31	1.41	1.35
23	B	609	CLA	C4B-NB	7.26	1.41	1.35
23	b	603	CLA	C4B-NB	7.22	1.41	1.35
23	C	503	CLA	MG-NA	7.18	2.23	2.06
23	c	505	CLA	C4B-NB	7.10	1.41	1.35
23	B	615	CLA	C4B-NB	7.10	1.41	1.35
23	c	513	CLA	C4B-NB	7.08	1.41	1.35
23	B	613	CLA	C4B-NB	7.07	1.41	1.35
23	c	511	CLA	C4B-NB	7.03	1.41	1.35
23	C	505	CLA	C4B-NB	7.01	1.41	1.35
36	V	201	HEC	C3B-C2B	-7.00	1.33	1.40
23	c	504	CLA	C4B-NB	6.97	1.41	1.35
23	c	510	CLA	C4B-NB	6.94	1.41	1.35
23	C	510	CLA	C4B-NB	6.86	1.41	1.35
23	b	608	CLA	C4B-NB	6.81	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	MG-NC	6.79	2.22	2.06
23	d	403	CLA	C4B-NB	6.74	1.41	1.35
36	v	201	HEC	C3B-C2B	-6.73	1.33	1.40
23	c	506	CLA	C4B-NB	6.66	1.41	1.35
23	b	605	CLA	C4B-NB	6.62	1.41	1.35
23	b	604	CLA	C4B-NB	6.61	1.41	1.35
23	C	513	CLA	C4B-NB	6.61	1.41	1.35
23	A	408	CLA	C4B-NB	6.60	1.41	1.35
23	c	503	CLA	C4B-NB	6.58	1.41	1.35
23	C	502	CLA	C4B-NB	6.53	1.41	1.35
23	B	606	CLA	C4B-NB	6.51	1.41	1.35
23	d	402	CLA	C4B-NB	6.46	1.41	1.35
36	v	201	HEC	C3C-C2C	-6.42	1.34	1.40
23	c	511	CLA	MG-NA	6.36	2.21	2.06
23	c	509	CLA	C4B-NB	6.34	1.40	1.35
23	C	504	CLA	C4B-NB	6.27	1.40	1.35
36	V	201	HEC	C3C-C2C	-6.25	1.34	1.40
23	b	617	CLA	C4B-NB	6.20	1.40	1.35
23	h	101	CLA	MG-NA	6.19	2.21	2.06
23	A	405	CLA	C4B-NB	6.19	1.40	1.35
23	D	403	CLA	C4B-NB	6.16	1.40	1.35
23	C	506	CLA	C4B-NB	6.16	1.40	1.35
23	b	606	CLA	C4B-NB	6.15	1.40	1.35
23	b	612	CLA	C4B-NB	6.15	1.40	1.35
23	b	616	CLA	MG-NA	6.10	2.20	2.06
23	C	509	CLA	C4B-NB	6.04	1.40	1.35
23	c	507	CLA	C4B-NB	6.03	1.40	1.35
23	b	607	CLA	C4B-NB	5.99	1.40	1.35
23	B	604	CLA	MG-NA	5.96	2.20	2.06
23	A	404	CLA	C4B-NB	5.95	1.40	1.35
35	e	102	HEM	C3B-C2B	-5.93	1.32	1.40
23	C	511	CLA	MG-NA	5.86	2.20	2.06
23	D	401	CLA	C4B-NB	5.85	1.40	1.35
23	c	502	CLA	MG-NA	5.84	2.20	2.06
23	C	507	CLA	C4B-NB	5.82	1.40	1.35
23	A	408	CLA	MG-NC	-5.76	1.92	2.06
23	c	502	CLA	C4B-NB	5.71	1.40	1.35
23	b	613	CLA	C4B-NB	5.68	1.40	1.35
23	b	611	CLA	C4B-NB	5.65	1.40	1.35
23	C	508	CLA	C4B-NB	5.61	1.40	1.35
23	B	616	CLA	C4B-NB	5.61	1.40	1.35
23	B	608	CLA	C4B-NB	5.60	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C4B-NB	5.59	1.40	1.35
23	C	512	CLA	C4B-NB	5.54	1.40	1.35
23	C	507	CLA	MG-NA	5.53	2.19	2.06
23	a	411	CLA	MG-NA	5.52	2.19	2.06
23	B	603	CLA	C4B-NB	5.49	1.40	1.35
23	B	601	CLA	MG-NA	5.42	2.19	2.06
23	B	607	CLA	C4B-NB	5.38	1.40	1.35
23	B	611	CLA	C4B-NB	5.37	1.40	1.35
23	B	616	CLA	MG-NA	5.35	2.19	2.06
23	A	404	CLA	MG-NA	5.32	2.18	2.06
30	a	414	DGD	O2G-C1B	5.28	1.49	1.34
23	c	508	CLA	C4B-NB	5.25	1.39	1.35
23	c	503	CLA	MG-NC	5.06	2.18	2.06
35	E	101	HEM	C3B-C2B	-5.01	1.33	1.40
23	B	612	CLA	C4B-NB	4.93	1.39	1.35
23	a	411	CLA	C4B-NB	4.92	1.39	1.35
23	b	609	CLA	C4B-NB	4.91	1.39	1.35
26	D	405	PL9	C11-C9	-4.89	1.41	1.51
23	C	501	CLA	MG-NA	4.88	2.17	2.06
26	A	410	PL9	C7-C3	-4.87	1.46	1.51
30	A	415	DGD	C4D-C5D	4.85	1.63	1.53
30	C	515	DGD	C4E-C3E	4.85	1.64	1.52
23	d	402	CLA	MG-NA	4.66	2.17	2.06
23	c	510	CLA	MG-NA	4.62	2.17	2.06
23	B	609	CLA	MG-NA	4.58	2.17	2.06
23	A	404	CLA	MG-NC	-4.58	1.95	2.06
35	E	101	HEM	C3C-C2C	-4.56	1.34	1.40
23	B	604	CLA	C4B-NB	4.50	1.39	1.35
23	b	609	CLA	MG-NA	4.44	2.16	2.06
25	c	515	BCR	C1-C6	-4.44	1.47	1.53
26	D	405	PL9	C6-C1	-4.43	1.40	1.48
23	b	610	CLA	MG-NA	4.38	2.16	2.06
35	e	102	HEM	C3C-C2C	-4.37	1.34	1.40
26	d	405	PL9	C6-C1	-4.25	1.41	1.48
23	B	615	CLA	MG-NC	4.20	2.16	2.06
25	A	409	BCR	C1-C6	-4.17	1.48	1.53
25	x	101	BCR	C30-C25	-4.07	1.48	1.53
23	c	511	CLA	MG-NC	4.07	2.15	2.06
25	D	404	BCR	C30-C25	-4.06	1.48	1.53
23	B	610	CLA	MG-NC	-4.04	1.96	2.06
30	c	516	DGD	O2G-C2G	-3.98	1.36	1.46
29	D	407	LHG	O7-C5	-3.96	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C1-C6	-3.92	1.48	1.53
36	v	201	HEC	CBC-CAC	-3.89	1.34	1.49
23	c	505	CLA	CHC-C1C	3.89	1.44	1.35
30	c	516	DGD	O2E-C2E	-3.88	1.33	1.43
29	D	408	LHG	P-O6	3.88	1.75	1.59
23	C	502	CLA	MG-NC	3.86	2.15	2.06
30	h	102	DGD	C4D-C3D	3.86	1.62	1.52
27	d	409	LMG	O7-C8	-3.86	1.36	1.46
23	b	605	CLA	MG-NA	3.85	2.15	2.06
25	K	101	BCR	C1-C6	-3.85	1.48	1.53
23	a	406	CLA	CHC-C1C	3.84	1.44	1.35
23	C	508	CLA	MG-NA	3.83	2.15	2.06
36	V	201	HEC	CBB-CAB	-3.83	1.35	1.49
23	B	605	CLA	CHC-C1C	3.82	1.44	1.35
23	b	612	CLA	MG-NA	3.81	2.15	2.06
23	B	610	CLA	C3B-C2B	-3.80	1.35	1.40
28	a	413	SQD	O47-C7	3.79	1.45	1.34
23	B	605	CLA	C3B-C2B	-3.79	1.35	1.40
25	d	404	BCR	C1-C6	-3.77	1.48	1.53
25	H	101	BCR	C30-C25	-3.76	1.48	1.53
23	c	503	CLA	CHC-C1C	3.75	1.44	1.35
30	A	415	DGD	C4D-C3D	3.72	1.61	1.52
23	B	606	CLA	CHC-C1C	3.70	1.44	1.35
23	c	511	CLA	CHC-C1C	3.69	1.44	1.35
25	b	619	BCR	C1-C6	-3.66	1.48	1.53
23	d	402	CLA	C3B-C2B	-3.66	1.35	1.40
23	c	507	CLA	MG-NC	-3.63	1.97	2.06
23	b	609	CLA	CHC-C1C	3.59	1.44	1.35
23	B	611	CLA	MG-NC	-3.59	1.97	2.06
23	b	605	CLA	CHC-C1C	3.59	1.44	1.35
23	b	615	CLA	CHC-C1C	3.58	1.44	1.35
30	A	415	DGD	C1E-C2E	3.58	1.62	1.52
25	C	514	BCR	C1-C6	-3.56	1.48	1.53
25	K	102	BCR	C30-C25	-3.55	1.48	1.53
36	v	201	HEC	CBB-CAB	-3.54	1.36	1.49
23	b	609	CLA	C3B-CAB	-3.54	1.40	1.47
25	K	101	BCR	C30-C25	-3.54	1.48	1.53
28	f	101	SQD	O47-C7	3.53	1.44	1.34
25	B	617	BCR	C1-C6	-3.52	1.48	1.53
27	c	521	LMG	O1-C1	3.51	1.46	1.40
23	b	608	CLA	MG-NC	3.51	2.14	2.06
23	a	411	CLA	CHC-C1C	3.50	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	516	DGD	C4D-C3D	3.50	1.61	1.52
23	B	605	CLA	C4B-NB	3.49	1.38	1.35
28	A	414	SQD	O48-C23	3.48	1.43	1.33
28	a	412	SQD	O48-C23	3.48	1.43	1.33
24	A	406	PHO	C4C-C3C	3.48	1.51	1.45
28	a	413	SQD	O48-C23	3.44	1.43	1.33
25	Z	101	BCR	C30-C25	-3.44	1.49	1.53
25	k	101	BCR	C1-C6	-3.43	1.49	1.53
26	D	405	PL9	C41-C39	-3.43	1.44	1.51
25	b	618	BCR	C1-C6	-3.41	1.49	1.53
26	d	405	PL9	C46-C44	-3.41	1.44	1.51
25	c	515	BCR	C30-C25	-3.40	1.49	1.53
23	C	510	CLA	CHC-C1C	3.40	1.43	1.35
30	C	517	DGD	O1G-C1G	-3.40	1.37	1.45
23	d	402	CLA	CMB-C2B	-3.40	1.44	1.51
36	V	201	HEC	CBC-CAC	-3.39	1.36	1.49
23	B	603	CLA	MG-NA	3.38	2.14	2.06
23	b	612	CLA	C1D-C2D	3.38	1.50	1.42
23	b	607	CLA	C1B-NB	3.36	1.38	1.35
23	C	501	CLA	C1D-C2D	3.35	1.50	1.42
25	x	101	BCR	C1-C6	-3.35	1.49	1.53
30	a	414	DGD	C3G-C2G	3.34	1.59	1.51
23	c	508	CLA	CHC-C1C	3.34	1.43	1.35
23	C	503	CLA	C1D-C2D	3.34	1.50	1.42
26	d	405	PL9	C3-C4	-3.34	1.44	1.49
25	B	619	BCR	C30-C25	-3.33	1.49	1.53
23	B	602	CLA	MG-NA	3.32	2.14	2.06
30	C	515	DGD	O5D-C1E	3.31	1.45	1.40
23	C	503	CLA	CHC-C1C	3.31	1.43	1.35
23	D	402	CLA	C4B-NB	3.31	1.38	1.35
28	A	414	SQD	O47-C7	3.31	1.43	1.34
23	B	606	CLA	MG-NC	-3.31	1.98	2.06
23	B	615	CLA	C3B-C2B	-3.30	1.35	1.40
28	F	101	SQD	O48-C23	3.30	1.43	1.33
25	b	618	BCR	C30-C25	-3.30	1.49	1.53
25	b	619	BCR	C30-C25	-3.30	1.49	1.53
24	a	407	PHO	C3B-C4B	3.30	1.50	1.43
23	b	614	CLA	MG-NA	3.28	2.14	2.06
23	D	402	CLA	CHC-C1C	3.27	1.43	1.35
23	B	612	CLA	MG-NA	3.27	2.14	2.06
28	b	601	SQD	O48-C23	3.27	1.42	1.33
23	C	512	CLA	CHC-C1C	3.26	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	MG-NA	3.25	2.14	2.06
23	c	509	CLA	CHC-C1C	3.24	1.43	1.35
28	B	624	SQD	O47-C7	3.23	1.43	1.34
23	C	503	CLA	CMB-C2B	-3.22	1.44	1.51
30	c	516	DGD	C3G-C2G	3.22	1.60	1.50
23	B	615	CLA	CMB-C2B	-3.22	1.44	1.51
23	C	507	CLA	CHC-C1C	3.21	1.43	1.35
23	B	606	CLA	C3B-C2B	-3.21	1.35	1.40
23	B	614	CLA	CHC-C1C	3.21	1.43	1.35
30	C	516	DGD	C4D-C3D	3.20	1.60	1.52
27	c	523	LMG	C4-C5	3.20	1.59	1.53
23	b	617	CLA	C3B-C2B	-3.20	1.35	1.40
27	C	518	LMG	O7-C8	-3.19	1.38	1.46
30	H	102	DGD	C4D-C5D	3.19	1.59	1.53
24	d	401	PHO	C3B-C4B	3.19	1.49	1.43
25	c	514	BCR	C1-C6	-3.19	1.49	1.53
23	b	606	CLA	CHC-C1C	3.18	1.43	1.35
28	A	412	SQD	O48-C23	3.18	1.42	1.33
23	B	601	CLA	CHC-C1C	3.18	1.43	1.35
23	b	611	CLA	C3B-C2B	-3.18	1.36	1.40
23	C	508	CLA	C1D-C2D	3.17	1.49	1.42
23	B	607	CLA	C3B-C2B	-3.16	1.36	1.40
23	C	507	CLA	MG-NC	-3.15	1.98	2.06
27	M	101	LMG	C9-C8	3.15	1.60	1.50
23	C	506	CLA	CHC-C1C	3.14	1.43	1.35
25	d	404	BCR	C30-C25	-3.13	1.49	1.53
29	d	408	LHG	P-O6	3.13	1.72	1.59
23	c	511	CLA	C1D-C2D	3.13	1.49	1.42
23	c	513	CLA	MG-NA	3.13	2.13	2.06
23	C	501	CLA	CHC-C1C	3.13	1.43	1.35
23	c	502	CLA	CHC-C1C	3.13	1.43	1.35
23	c	510	CLA	CHC-C1C	3.12	1.43	1.35
23	a	411	CLA	CMB-C2B	-3.12	1.45	1.51
23	c	501	CLA	MG-NC	3.11	2.13	2.06
30	a	414	DGD	O1G-C1A	3.11	1.42	1.33
23	c	504	CLA	CHC-C1C	3.10	1.42	1.35
23	b	603	CLA	CHC-C1C	3.09	1.42	1.35
29	A	413	LHG	O8-C23	3.09	1.42	1.33
23	d	403	CLA	C1B-NB	3.09	1.38	1.35
23	C	511	CLA	C1D-C2D	3.08	1.49	1.42
23	c	505	CLA	C3B-C2B	-3.07	1.36	1.40
27	A	411	LMG	C1-C2	3.07	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	517	DGD	O3G-C3G	-3.06	1.38	1.43
28	A	412	SQD	O47-C7	3.05	1.42	1.34
27	b	622	LMG	C4-C3	3.05	1.60	1.52
23	c	512	CLA	CHC-C1C	3.05	1.42	1.35
30	c	516	DGD	O6D-C1D	3.05	1.49	1.41
30	c	517	DGD	O2G-C2G	-3.05	1.39	1.46
30	H	102	DGD	O5D-C1E	3.04	1.45	1.40
35	e	102	HEM	C3C-CAC	3.04	1.54	1.47
30	H	102	DGD	C4E-C5E	3.04	1.59	1.53
23	b	616	CLA	CHC-C1C	3.03	1.42	1.35
23	c	509	CLA	MG-NC	3.03	2.13	2.06
23	B	602	CLA	CHC-C1C	3.03	1.42	1.35
23	B	612	CLA	CHC-C1C	3.03	1.42	1.35
23	b	610	CLA	CMB-C2B	-3.02	1.45	1.51
23	B	610	CLA	CMB-C2B	-3.02	1.45	1.51
23	c	503	CLA	C1D-C2D	3.02	1.49	1.42
23	B	604	CLA	CHC-C1C	3.01	1.42	1.35
23	B	610	CLA	CHC-C1C	3.01	1.42	1.35
23	b	617	CLA	C3B-CAB	-3.01	1.41	1.47
23	B	603	CLA	C3B-CAB	-3.00	1.41	1.47
25	a	409	BCR	C1-C6	-3.00	1.49	1.53
23	B	615	CLA	CMD-C2D	-3.00	1.44	1.51
24	a	407	PHO	C4C-NC	3.00	1.43	1.36
35	E	101	HEM	C3B-CAB	2.99	1.54	1.47
23	B	609	CLA	CMD-C2D	-2.99	1.44	1.51
30	c	518	DGD	C6D-C5D	2.98	1.60	1.51
28	B	624	SQD	O48-C23	2.98	1.42	1.33
23	b	614	CLA	CMB-C2B	-2.98	1.45	1.51
23	A	404	CLA	CHC-C1C	2.98	1.42	1.35
30	C	517	DGD	O2G-C2G	-2.98	1.39	1.46
23	b	610	CLA	CHC-C1C	2.98	1.42	1.35
35	e	102	HEM	C3B-CAB	2.97	1.54	1.47
25	k	101	BCR	C30-C25	-2.97	1.49	1.53
23	h	101	CLA	CHC-C1C	2.97	1.42	1.35
23	b	608	CLA	C1D-C2D	2.97	1.49	1.42
23	C	505	CLA	C3B-C2B	-2.97	1.36	1.40
23	c	512	CLA	CMB-C2B	-2.96	1.45	1.51
23	C	508	CLA	CHC-C1C	2.96	1.42	1.35
28	f	101	SQD	O48-C23	2.95	1.42	1.33
23	A	405	CLA	MG-NA	2.95	2.13	2.06
23	h	101	CLA	C1D-C2D	2.95	1.49	1.42
24	A	407	PHO	C1A-NA	2.95	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	CMB-C2B	-2.95	1.45	1.51
25	Z	101	BCR	C1-C6	-2.94	1.49	1.53
23	C	505	CLA	CHC-C1C	2.94	1.42	1.35
24	A	406	PHO	C1C-NC	-2.94	1.32	1.38
24	a	407	PHO	C4C-C3C	2.94	1.50	1.45
28	b	601	SQD	O47-C7	2.94	1.42	1.34
24	a	407	PHO	O2D-CGD	2.93	1.40	1.33
23	B	614	CLA	CMB-C2B	-2.93	1.45	1.51
23	B	601	CLA	C1D-C2D	2.93	1.49	1.42
30	C	515	DGD	O4D-C4D	2.92	1.49	1.43
25	b	620	BCR	C30-C25	-2.92	1.49	1.53
23	D	401	CLA	CHC-C1C	2.92	1.42	1.35
23	c	508	CLA	MG-NC	2.92	2.13	2.06
25	D	404	BCR	C1-C6	-2.91	1.49	1.53
23	h	101	CLA	C1B-NB	2.91	1.37	1.35
30	C	517	DGD	C1D-C2D	2.91	1.60	1.52
23	b	604	CLA	CHC-C1C	2.91	1.42	1.35
23	c	507	CLA	CMB-C2B	-2.91	1.45	1.51
23	b	615	CLA	CMC-C2C	-2.90	1.44	1.50
23	b	612	CLA	CMD-C2D	-2.90	1.44	1.51
23	c	501	CLA	MG-NA	2.90	2.13	2.06
27	M	101	LMG	C1-C2	2.89	1.60	1.52
25	b	620	BCR	C1-C6	-2.89	1.49	1.53
23	C	504	CLA	CMB-C2B	-2.88	1.45	1.51
23	b	611	CLA	CHC-C1C	2.88	1.42	1.35
27	b	622	LMG	C4-C5	2.87	1.59	1.53
23	b	604	CLA	C3B-CAB	-2.87	1.42	1.47
23	a	406	CLA	C3B-C2B	-2.87	1.36	1.40
23	c	512	CLA	C1D-C2D	2.86	1.49	1.42
26	a	410	PL9	C53-C6	-2.86	1.44	1.50
23	B	603	CLA	CMC-C2C	-2.86	1.44	1.50
23	B	608	CLA	C3B-C2B	-2.86	1.36	1.40
25	T	101	BCR	C30-C25	-2.86	1.49	1.53
25	B	618	BCR	C1-C6	-2.85	1.49	1.53
23	C	511	CLA	CHC-C1C	2.85	1.42	1.35
23	C	512	CLA	C1D-C2D	2.85	1.49	1.42
23	a	405	CLA	CHC-C1C	2.85	1.42	1.35
28	a	412	SQD	O47-C7	2.85	1.42	1.34
23	c	507	CLA	C3B-CAB	-2.84	1.42	1.47
23	c	507	CLA	CMC-C2C	-2.83	1.44	1.50
27	c	519	LMG	C7-C8	2.83	1.59	1.50
23	c	513	CLA	CHC-C1C	2.83	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	CMB-C2B	-2.83	1.45	1.51
23	B	607	CLA	CAC-C3C	-2.82	1.43	1.51
26	D	405	PL9	C7-C3	-2.82	1.48	1.51
25	B	617	BCR	C33-C5	-2.81	1.46	1.50
23	C	503	CLA	MG-NC	2.81	2.12	2.06
25	B	618	BCR	C30-C25	-2.81	1.49	1.53
23	B	610	CLA	C1D-C2D	2.80	1.48	1.42
23	b	615	CLA	MG-NA	2.80	2.12	2.06
23	b	611	CLA	C1D-C2D	2.80	1.48	1.42
23	a	406	CLA	CMB-C2B	-2.80	1.45	1.51
29	B	623	LHG	O7-C5	-2.79	1.39	1.46
23	C	512	CLA	MG-NA	2.79	2.12	2.06
23	b	608	CLA	C3B-C2B	-2.79	1.36	1.40
23	A	405	CLA	C3B-C2B	-2.78	1.36	1.40
27	D	409	LMG	C7-C8	2.78	1.58	1.51
27	d	409	LMG	C4-C3	2.78	1.59	1.52
23	b	607	CLA	CHC-C1C	2.77	1.42	1.35
23	B	615	CLA	C1D-C2D	2.77	1.48	1.42
23	B	615	CLA	C3B-CAB	-2.77	1.42	1.47
25	K	102	BCR	C1-C6	-2.77	1.50	1.53
23	D	402	CLA	CMD-C2D	-2.76	1.45	1.51
23	b	613	CLA	CHC-C1C	2.76	1.42	1.35
24	A	407	PHO	C3B-C4B	2.76	1.49	1.43
23	B	605	CLA	C1D-C2D	2.75	1.48	1.42
23	b	604	CLA	C1D-C2D	2.75	1.48	1.42
23	B	613	CLA	CHC-C1C	2.74	1.42	1.35
30	c	517	DGD	C4D-C3D	2.73	1.59	1.52
23	C	502	CLA	CHC-C1C	2.72	1.41	1.35
23	C	509	CLA	CHC-C1C	2.72	1.41	1.35
23	C	511	CLA	C1B-NB	2.72	1.37	1.35
23	b	604	CLA	C3B-C2B	-2.71	1.36	1.40
29	B	623	LHG	C24-C23	2.71	1.58	1.50
23	b	604	CLA	CMC-C2C	-2.71	1.45	1.50
23	a	408	CLA	C3B-C2B	-2.71	1.36	1.40
23	C	510	CLA	MG-NA	2.70	2.12	2.06
23	B	603	CLA	C1A-CHA	-2.70	1.31	1.43
23	c	510	CLA	CMB-C2B	-2.70	1.46	1.51
23	a	408	CLA	CMD-C2D	-2.70	1.45	1.51
25	B	617	BCR	C30-C25	-2.68	1.50	1.53
30	C	516	DGD	O3E-C3E	-2.68	1.36	1.43
23	c	513	CLA	CMB-C2B	-2.68	1.46	1.51
28	a	412	SQD	O3-C3	-2.68	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406	CLA	C1D-C2D	2.67	1.48	1.42
23	b	616	CLA	CMB-C2B	-2.67	1.46	1.51
23	b	608	CLA	MG-NA	2.67	2.12	2.06
30	c	518	DGD	C2A-C1A	-2.67	1.42	1.50
30	c	518	DGD	O4D-C4D	-2.66	1.36	1.43
23	c	506	CLA	CAC-C3C	-2.66	1.44	1.51
23	b	617	CLA	CMB-C2B	-2.66	1.46	1.51
23	c	507	CLA	MG-NA	2.66	2.12	2.06
23	B	609	CLA	CHC-C1C	2.66	1.41	1.35
29	D	408	LHG	O3-C3	-2.66	1.34	1.44
30	C	515	DGD	C6E-C5E	2.66	1.60	1.51
30	c	517	DGD	O3E-C3E	-2.65	1.36	1.43
30	c	518	DGD	C1D-C2D	2.65	1.60	1.52
24	d	401	PHO	C1A-NA	2.64	1.42	1.37
23	c	502	CLA	C3B-C2B	-2.64	1.36	1.40
23	b	608	CLA	CHC-C1C	2.64	1.41	1.35
23	D	403	CLA	C1D-C2D	2.64	1.48	1.42
23	B	609	CLA	C4B-CHC	-2.64	1.33	1.41
26	d	405	PL9	C46-C47	-2.62	1.44	1.53
24	A	406	PHO	C1A-NA	2.62	1.42	1.37
23	b	608	CLA	CMD-C2D	-2.62	1.45	1.51
24	A	407	PHO	CHC-C1C	2.62	1.43	1.38
23	c	511	CLA	CMB-C2B	-2.62	1.46	1.51
23	b	603	CLA	MG-NC	-2.62	2.00	2.06
23	B	613	CLA	CMB-C2B	-2.61	1.46	1.51
23	a	411	CLA	CMD-C2D	-2.61	1.45	1.51
35	E	101	HEM	C3C-CAC	2.61	1.53	1.47
28	A	412	SQD	O2-C2	-2.61	1.36	1.43
30	H	102	DGD	C6E-C5E	2.61	1.60	1.51
24	d	401	PHO	CMC-C2C	-2.61	1.45	1.50
23	B	602	CLA	C1D-C2D	2.61	1.48	1.42
23	B	611	CLA	CMB-C2B	-2.61	1.46	1.51
23	b	612	CLA	CHC-C1C	2.60	1.41	1.35
23	A	405	CLA	CHC-C1C	2.60	1.41	1.35
23	b	603	CLA	C1D-C2D	2.60	1.48	1.42
23	D	403	CLA	CMB-C2B	-2.60	1.46	1.51
28	A	414	SQD	O47-C45	-2.60	1.42	1.47
23	B	615	CLA	CAC-C3C	-2.60	1.44	1.51
23	C	510	CLA	CMD-C2D	-2.59	1.45	1.51
23	b	606	CLA	CMB-C2B	-2.59	1.46	1.51
30	C	515	DGD	O1G-C1A	2.59	1.40	1.33
26	a	410	PL9	C6-C1	-2.59	1.44	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	CMB-C2B	-2.59	1.46	1.51
30	H	102	DGD	C1E-C2E	2.59	1.59	1.52
30	C	515	DGD	C2A-C1A	-2.58	1.43	1.50
23	B	608	CLA	CHC-C1C	2.58	1.41	1.35
23	D	401	CLA	C1D-C2D	2.58	1.48	1.42
23	a	405	CLA	C1D-C2D	2.58	1.48	1.42
27	C	518	LMG	C1-C2	2.58	1.59	1.52
27	M	101	LMG	O3-C3	-2.58	1.36	1.43
23	C	504	CLA	C1D-C2D	2.58	1.48	1.42
23	C	513	CLA	CMB-C2B	-2.58	1.46	1.51
27	b	622	LMG	C9-C8	2.57	1.58	1.50
23	a	406	CLA	C3B-CAB	-2.57	1.42	1.47
23	B	612	CLA	C1D-C2D	2.57	1.48	1.42
27	c	521	LMG	C7-C8	2.57	1.58	1.50
23	d	403	CLA	MG-NA	2.57	2.12	2.06
23	B	611	CLA	MG-NA	2.57	2.12	2.06
29	e	101	LHG	C24-C23	2.56	1.58	1.50
23	b	606	CLA	C1D-C2D	2.56	1.48	1.42
27	c	519	LMG	C3-C2	2.55	1.58	1.52
23	c	501	CLA	CMB-C2B	-2.55	1.46	1.51
23	h	101	CLA	O2A-CGA	2.55	1.40	1.33
27	D	406	LMG	C4-C3	2.55	1.58	1.52
25	C	514	BCR	C30-C25	-2.55	1.50	1.53
23	c	502	CLA	CMC-C2C	-2.55	1.45	1.50
23	A	404	CLA	CMC-C2C	-2.54	1.45	1.50
23	B	603	CLA	CMB-C2B	-2.54	1.46	1.51
23	B	605	CLA	MG-NC	-2.54	2.00	2.06
30	H	102	DGD	C3E-C2E	2.54	1.58	1.52
27	D	409	LMG	C9-C8	2.53	1.58	1.50
28	f	101	SQD	O3-C3	-2.53	1.37	1.43
23	B	601	CLA	C3B-C2B	-2.53	1.36	1.40
25	a	409	BCR	C30-C25	-2.53	1.50	1.53
23	B	604	CLA	C1D-C2D	2.53	1.48	1.42
23	B	613	CLA	CMD-C2D	-2.53	1.45	1.51
23	D	403	CLA	CMD-C2D	-2.53	1.45	1.51
23	C	501	CLA	CMB-C2B	-2.53	1.46	1.51
29	e	101	LHG	O8-C23	2.53	1.40	1.33
23	B	603	CLA	C3B-C2B	-2.53	1.36	1.40
23	d	402	CLA	MG-NC	2.52	2.12	2.06
23	A	404	CLA	CMD-C2D	-2.52	1.45	1.51
23	d	403	CLA	CMD-C2D	-2.52	1.45	1.51
23	C	504	CLA	CHC-C1C	2.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	CMD-C2D	-2.52	1.45	1.51
23	C	503	CLA	C3B-C2B	-2.51	1.36	1.40
23	b	611	CLA	CMB-C2B	-2.51	1.46	1.51
23	B	608	CLA	C1D-C2D	2.51	1.48	1.42
24	d	401	PHO	C4C-NC	2.51	1.42	1.36
23	b	613	CLA	C1D-C2D	2.51	1.48	1.42
23	d	402	CLA	CHC-C1C	2.50	1.41	1.35
23	c	510	CLA	C1D-C2D	2.50	1.48	1.42
23	A	404	CLA	C5-C3	-2.50	1.46	1.51
23	B	613	CLA	MG-NA	2.50	2.12	2.06
23	B	609	CLA	CMC-C2C	-2.49	1.45	1.50
23	A	408	CLA	C1D-C2D	2.49	1.48	1.42
23	B	606	CLA	C3B-CAB	-2.49	1.42	1.47
23	A	408	CLA	CMD-C2D	-2.49	1.45	1.51
23	C	502	CLA	CMB-C2B	-2.49	1.46	1.51
30	H	102	DGD	O2D-C2D	-2.49	1.37	1.43
23	b	609	CLA	C3B-C2B	-2.48	1.36	1.40
23	b	611	CLA	CMD-C2D	-2.48	1.45	1.51
23	C	513	CLA	C1D-C2D	2.48	1.48	1.42
23	B	607	CLA	C4B-CHC	-2.48	1.34	1.41
23	C	502	CLA	C1D-C2D	2.48	1.48	1.42
23	c	507	CLA	CHC-C1C	2.47	1.41	1.35
29	D	407	LHG	C24-C23	2.47	1.57	1.50
23	B	607	CLA	CMD-C2D	-2.47	1.45	1.51
23	B	602	CLA	CMB-C2B	-2.47	1.46	1.51
23	a	406	CLA	CMD-C2D	-2.47	1.45	1.51
23	b	616	CLA	CMD-C2D	-2.47	1.45	1.51
23	B	614	CLA	CMC-C2C	-2.46	1.45	1.50
23	C	513	CLA	C4B-CHC	-2.46	1.34	1.41
23	b	610	CLA	CMD-C2D	-2.46	1.45	1.51
23	a	411	CLA	C1D-C2D	2.46	1.48	1.42
27	c	521	LMG	C4-C3	2.46	1.58	1.52
24	A	407	PHO	CHC-C4B	-2.46	1.34	1.40
23	B	613	CLA	C3B-CAB	-2.45	1.42	1.47
23	B	603	CLA	CHC-C1C	2.45	1.41	1.35
23	b	615	CLA	C1D-C2D	2.45	1.48	1.42
23	c	508	CLA	CMB-C2B	-2.44	1.46	1.51
23	C	503	CLA	CMD-C2D	-2.44	1.45	1.51
27	d	409	LMG	O6-C5	-2.44	1.38	1.44
23	b	613	CLA	CMC-C2C	-2.44	1.45	1.50
23	b	609	CLA	C1D-C2D	2.44	1.48	1.42
23	C	513	CLA	CHC-C1C	2.44	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C4B-CHC	-2.44	1.34	1.41
23	B	609	CLA	C3B-CAB	-2.44	1.43	1.47
24	A	406	PHO	CMD-C2D	-2.44	1.45	1.50
23	a	411	CLA	C3B-C2B	-2.43	1.37	1.40
23	B	614	CLA	MG-NA	2.43	2.12	2.06
23	a	408	CLA	CMB-C2B	-2.43	1.46	1.51
24	d	401	PHO	CHD-C4C	-2.43	1.34	1.40
23	C	512	CLA	CMB-C2B	-2.43	1.46	1.51
30	a	414	DGD	C1G-C2G	2.43	1.58	1.50
23	c	506	CLA	C3B-CAB	-2.42	1.43	1.47
29	l	101	LHG	O7-C5	-2.42	1.40	1.46
23	h	101	CLA	CMC-C2C	-2.42	1.45	1.50
23	C	506	CLA	C1D-C2D	2.42	1.48	1.42
24	a	407	PHO	C1C-NC	-2.41	1.33	1.38
23	c	508	CLA	CMC-C2C	-2.41	1.45	1.50
23	d	403	CLA	C1D-C2D	2.41	1.48	1.42
23	C	511	CLA	CMB-C2B	-2.41	1.46	1.51
23	D	401	CLA	C4B-CHC	-2.41	1.34	1.41
24	a	407	PHO	CHC-C4B	-2.40	1.34	1.40
23	d	403	CLA	CHC-C1C	2.40	1.41	1.35
23	a	408	CLA	C4B-CHC	-2.40	1.34	1.41
23	B	616	CLA	C1D-C2D	2.40	1.48	1.42
23	b	613	CLA	CMB-C2B	-2.40	1.46	1.51
23	C	511	CLA	MG-NC	2.40	2.12	2.06
23	c	502	CLA	CMD-C2D	-2.40	1.45	1.51
23	b	607	CLA	CAC-C3C	-2.40	1.45	1.51
26	d	405	PL9	C7-C3	2.40	1.53	1.51
23	B	610	CLA	CMD-C2D	-2.39	1.45	1.51
23	B	611	CLA	C1D-C2D	2.39	1.48	1.42
30	c	516	DGD	C6D-C5D	2.39	1.59	1.51
23	C	510	CLA	C1D-C2D	2.39	1.48	1.42
23	D	402	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	515	BCR	C33-C5	-2.38	1.47	1.50
23	C	507	CLA	C3B-CAB	-2.38	1.43	1.47
23	b	603	CLA	MG-NA	2.38	2.11	2.06
23	C	502	CLA	C3B-C2B	-2.38	1.37	1.40
23	c	512	CLA	C3B-CAB	-2.38	1.43	1.47
24	d	401	PHO	CHC-C1C	2.38	1.43	1.38
23	b	607	CLA	MG-NC	2.38	2.11	2.06
24	a	407	PHO	C1B-C2B	2.37	1.50	1.45
23	b	610	CLA	C1D-C2D	2.37	1.47	1.42
23	b	603	CLA	C1B-NB	2.37	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	PHO	CHC-C4B	-2.37	1.34	1.40
30	C	516	DGD	C1E-C2E	2.37	1.59	1.52
23	d	403	CLA	C3B-CAB	-2.37	1.43	1.47
26	A	410	PL9	C7-C8	-2.36	1.47	1.50
23	c	506	CLA	CMD-C2D	-2.35	1.46	1.51
28	F	101	SQD	O2-C2	-2.35	1.37	1.43
23	h	101	CLA	CMD-C2D	-2.35	1.46	1.51
23	B	607	CLA	MG-NA	2.35	2.11	2.06
24	a	407	PHO	CHD-C1D	2.35	1.43	1.38
23	c	503	CLA	CMB-C2B	-2.35	1.46	1.51
30	A	415	DGD	O1G-C1G	-2.35	1.39	1.45
28	f	101	SQD	O2-C2	-2.35	1.37	1.43
23	c	512	CLA	CMD-C2D	-2.35	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.34	1.46	1.51
23	C	505	CLA	CMB-C2B	-2.34	1.46	1.51
23	B	603	CLA	C1D-C2D	2.34	1.47	1.42
23	b	617	CLA	CHC-C1C	2.34	1.41	1.35
30	c	517	DGD	C6E-C5E	2.33	1.59	1.51
23	D	403	CLA	C4B-CHC	-2.33	1.34	1.41
23	c	506	CLA	C3B-C2B	-2.33	1.37	1.40
23	b	615	CLA	C1B-NB	2.33	1.37	1.35
23	C	505	CLA	C3B-CAB	-2.33	1.43	1.47
23	B	611	CLA	CHC-C1C	2.33	1.40	1.35
23	b	610	CLA	O2D-CGD	2.33	1.38	1.33
29	D	408	LHG	O8-C6	2.32	1.50	1.45
23	c	501	CLA	CAC-C3C	-2.32	1.45	1.51
23	b	615	CLA	CMB-C2B	-2.32	1.46	1.51
23	c	507	CLA	C4B-CHC	-2.32	1.34	1.41
23	c	507	CLA	C3B-C2B	-2.32	1.37	1.40
28	a	412	SQD	O2-C2	-2.32	1.37	1.43
23	B	604	CLA	CMB-C2B	-2.32	1.46	1.51
29	A	413	LHG	O7-C5	-2.32	1.40	1.46
23	b	604	CLA	CMB-C2B	-2.31	1.46	1.51
23	B	615	CLA	CHC-C1C	2.31	1.40	1.35
23	c	508	CLA	C3B-CAB	-2.31	1.43	1.47
30	C	517	DGD	C4E-C3E	2.31	1.58	1.52
23	B	613	CLA	C1D-C2D	2.31	1.47	1.42
25	k	102	BCR	C1-C6	-2.30	1.50	1.53
23	B	601	CLA	CMB-C2B	-2.30	1.46	1.51
23	B	607	CLA	C1D-C2D	2.30	1.47	1.42
23	C	509	CLA	CMB-C2B	-2.30	1.46	1.51
23	C	504	CLA	C3B-C2B	-2.30	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	CMB-C2B	-2.30	1.46	1.51
23	B	609	CLA	CMB-C2B	-2.30	1.46	1.51
23	B	608	CLA	MG-NA	2.30	2.11	2.06
23	A	405	CLA	CMC-C2C	-2.30	1.45	1.50
29	A	413	LHG	C24-C23	2.29	1.57	1.50
23	B	606	CLA	CMB-C2B	-2.29	1.46	1.51
25	c	514	BCR	C30-C25	-2.29	1.50	1.53
25	b	618	BCR	C33-C5	-2.29	1.47	1.50
23	b	606	CLA	C4B-CHC	-2.29	1.34	1.41
23	b	616	CLA	CMC-C2C	-2.29	1.45	1.50
23	b	616	CLA	CAC-C3C	-2.29	1.45	1.51
26	d	405	PL9	C53-C6	-2.28	1.46	1.50
23	c	505	CLA	C1D-C2D	2.28	1.47	1.42
23	B	608	CLA	MG-NC	2.28	2.11	2.06
25	C	514	BCR	C33-C5	-2.28	1.47	1.50
25	k	101	BCR	C33-C5	-2.28	1.47	1.50
28	F	101	SQD	O3-C3	-2.27	1.37	1.43
23	B	615	CLA	C4B-CHC	-2.27	1.34	1.41
23	B	616	CLA	O2D-CGD	2.27	1.38	1.33
24	A	407	PHO	C1C-NC	-2.27	1.33	1.38
23	B	614	CLA	C1A-CHA	-2.27	1.33	1.43
24	d	401	PHO	CMD-C2D	-2.27	1.46	1.50
23	b	614	CLA	CMC-C2C	-2.27	1.46	1.50
30	C	516	DGD	O2G-C2G	-2.27	1.40	1.46
23	a	408	CLA	MG-NA	2.27	2.11	2.06
23	c	509	CLA	C3C-C2C	2.26	1.41	1.36
30	h	102	DGD	C3G-C2G	2.26	1.57	1.50
23	C	506	CLA	CMB-C2B	-2.26	1.46	1.51
23	h	101	CLA	CMB-C2B	-2.26	1.46	1.51
30	C	517	DGD	O4E-C4E	-2.26	1.37	1.43
23	a	405	CLA	C3B-C2B	-2.26	1.37	1.40
24	A	407	PHO	C4C-C3C	2.26	1.49	1.45
23	b	610	CLA	C3B-CAB	-2.26	1.43	1.47
26	D	405	PL9	C27-C28	-2.25	1.43	1.50
26	D	405	PL9	C45-C44	-2.25	1.44	1.50
25	t	101	BCR	C30-C25	-2.25	1.50	1.53
27	m	101	LMG	O6-C1	2.25	1.47	1.41
23	c	504	CLA	CMD-C2D	-2.24	1.46	1.51
30	A	415	DGD	O2G-C1B	2.24	1.40	1.34
23	A	405	CLA	CMD-C2D	-2.24	1.46	1.51
23	b	603	CLA	CMD-C2D	-2.24	1.46	1.51
26	d	405	PL9	C31-C29	-2.24	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	O2A-CGA	2.24	1.39	1.33
29	D	408	LHG	O7-C7	2.24	1.40	1.34
23	C	507	CLA	C3B-C2B	-2.23	1.37	1.40
23	C	503	CLA	C3B-CAB	-2.23	1.43	1.47
29	D	407	LHG	O8-C6	-2.23	1.40	1.45
23	b	612	CLA	CMB-C2B	-2.23	1.47	1.51
23	c	510	CLA	CMD-C2D	-2.23	1.46	1.51
23	B	616	CLA	CMD-C2D	-2.23	1.46	1.51
23	b	604	CLA	C1A-CHA	-2.23	1.33	1.43
24	A	407	PHO	CMD-C2D	-2.23	1.46	1.50
23	b	615	CLA	O2D-CGD	2.22	1.38	1.33
30	C	515	DGD	O2G-C2G	-2.22	1.41	1.46
23	b	609	CLA	C3C-C2C	2.22	1.41	1.36
23	B	615	CLA	CMC-C2C	-2.22	1.46	1.50
24	d	401	PHO	CMB-C2B	-2.22	1.46	1.50
30	A	415	DGD	C3G-C2G	2.22	1.57	1.50
23	b	606	CLA	CMD-C2D	-2.22	1.46	1.51
24	A	407	PHO	CMB-C2B	-2.22	1.46	1.50
23	c	508	CLA	C1D-C2D	2.22	1.47	1.42
23	C	504	CLA	O2D-CGD	2.22	1.38	1.33
23	C	507	CLA	CMB-C2B	-2.22	1.47	1.51
23	c	504	CLA	CMC-C2C	-2.22	1.46	1.50
30	c	517	DGD	C6D-C5D	2.22	1.58	1.51
29	e	101	LHG	P-O6	2.21	1.68	1.59
23	C	509	CLA	CMD-C2D	-2.21	1.46	1.51
23	c	513	CLA	C1D-C2D	2.21	1.47	1.42
23	a	405	CLA	CMB-C2B	-2.21	1.47	1.51
26	d	405	PL9	C16-C14	-2.21	1.46	1.51
23	c	513	CLA	CMD-C2D	-2.21	1.46	1.51
23	b	612	CLA	CMC-C2C	-2.21	1.46	1.50
23	C	511	CLA	CMC-C2C	-2.21	1.46	1.50
23	c	501	CLA	CMD-C2D	-2.21	1.46	1.51
23	B	603	CLA	CMA-C3A	-2.20	1.48	1.53
23	B	614	CLA	C1D-C2D	2.20	1.47	1.42
23	c	512	CLA	C3B-C2B	-2.20	1.37	1.40
23	d	402	CLA	CMD-C2D	-2.20	1.46	1.51
23	B	608	CLA	CMB-C2B	-2.20	1.47	1.51
23	c	504	CLA	MG-NA	2.20	2.11	2.06
23	c	502	CLA	O2D-CGD	2.20	1.38	1.33
23	c	501	CLA	C1D-C2D	2.20	1.47	1.42
23	c	501	CLA	CHC-C1C	2.19	1.40	1.35
23	B	601	CLA	CMC-C2C	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	601	SQD	O2-C2	-2.19	1.37	1.43
25	H	101	BCR	C1-C6	-2.19	1.50	1.53
23	B	608	CLA	CMC-C2C	-2.19	1.46	1.50
23	a	405	CLA	MG-NA	2.19	2.11	2.06
26	a	410	PL9	C52-C5	-2.19	1.46	1.50
23	D	401	CLA	MG-NA	2.18	2.11	2.06
25	C	514	BCR	C36-C18	-2.18	1.46	1.50
24	A	406	PHO	C4C-NC	2.18	1.41	1.36
25	d	404	BCR	C33-C5	-2.18	1.47	1.50
23	c	501	CLA	CMC-C2C	-2.18	1.46	1.50
30	C	515	DGD	C2B-C1B	-2.18	1.44	1.50
23	C	513	CLA	MG-NC	2.18	2.11	2.06
23	C	508	CLA	CMC-C2C	-2.17	1.46	1.50
27	c	519	LMG	C4-C5	2.17	1.57	1.53
23	C	501	CLA	CMD-C2D	-2.17	1.46	1.51
26	a	410	PL9	C41-C39	2.17	1.55	1.51
23	B	616	CLA	C4B-CHC	-2.17	1.35	1.41
23	c	510	CLA	C3B-C2B	-2.17	1.37	1.40
23	C	513	CLA	CMD-C2D	-2.17	1.46	1.51
26	D	405	PL9	C5-C4	-2.16	1.39	1.47
23	C	502	CLA	CMC-C2C	-2.16	1.46	1.50
23	D	402	CLA	CMC-C2C	-2.16	1.46	1.50
23	D	403	CLA	C3B-C2B	-2.16	1.37	1.40
30	C	515	DGD	O2G-C1B	2.15	1.40	1.34
30	H	102	DGD	C4E-C3E	2.15	1.57	1.52
29	d	407	LHG	P-O3	2.15	1.68	1.59
30	c	518	DGD	O5D-C1E	2.15	1.43	1.40
23	B	609	CLA	C3B-C2B	-2.15	1.37	1.40
23	b	616	CLA	MG-NC	-2.15	2.01	2.06
23	C	513	CLA	MG-NA	2.15	2.11	2.06
23	C	512	CLA	CMD-C2D	-2.14	1.46	1.51
23	C	510	CLA	C3B-C2B	-2.14	1.37	1.40
26	d	405	PL9	C16-C17	2.14	1.60	1.53
23	C	509	CLA	MG-NC	-2.14	2.01	2.06
26	D	405	PL9	C53-C6	-2.14	1.46	1.50
23	B	616	CLA	CMC-C2C	-2.14	1.46	1.50
27	c	521	LMG	C4-C5	2.14	1.57	1.53
23	B	602	CLA	C1C-C2C	2.14	1.48	1.44
23	b	603	CLA	CMB-C2B	-2.13	1.47	1.51
23	B	616	CLA	CMB-C2B	-2.13	1.47	1.51
24	A	406	PHO	CMC-C2C	-2.13	1.46	1.50
27	C	518	LMG	O8-C28	2.13	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CMD-C2D	-2.13	1.46	1.51
23	B	609	CLA	O2D-CGD	2.13	1.38	1.33
24	A	406	PHO	C3B-C4B	2.13	1.47	1.43
23	D	403	CLA	CHC-C1C	2.13	1.40	1.35
23	C	509	CLA	O2D-CGD	2.12	1.38	1.33
30	A	415	DGD	C6E-C5E	2.12	1.59	1.51
23	b	613	CLA	C1B-NB	2.12	1.37	1.35
23	B	611	CLA	C3B-CAB	-2.12	1.43	1.47
23	B	605	CLA	CMB-C2B	-2.12	1.47	1.51
23	C	508	CLA	CMB-C2B	-2.12	1.47	1.51
23	h	101	CLA	C3B-CAB	-2.12	1.43	1.47
23	D	401	CLA	CMD-C2D	-2.12	1.46	1.51
23	C	504	CLA	C4B-CHC	-2.12	1.35	1.41
30	h	102	DGD	C6D-C5D	2.12	1.58	1.51
30	H	102	DGD	O3E-C3E	-2.11	1.38	1.43
23	D	401	CLA	CMB-C2B	-2.11	1.47	1.51
23	B	614	CLA	C3B-CAB	-2.11	1.43	1.47
36	V	201	HEC	CMB-C2B	2.11	1.56	1.51
24	d	401	PHO	CHC-C4B	-2.11	1.35	1.40
23	B	615	CLA	C5-C3	-2.11	1.46	1.51
23	C	506	CLA	MG-NA	2.10	2.11	2.06
23	c	506	CLA	CHC-C1C	2.10	1.40	1.35
23	D	403	CLA	CMC-C2C	-2.10	1.46	1.50
23	C	509	CLA	C1D-C2D	2.10	1.47	1.42
23	b	605	CLA	CMC-C2C	-2.10	1.46	1.50
23	B	613	CLA	C3B-C2B	-2.10	1.37	1.40
24	A	407	PHO	CAA-C2A	-2.09	1.50	1.54
23	d	403	CLA	C1A-CHA	-2.09	1.34	1.43
23	D	402	CLA	C1C-NC	-2.09	1.34	1.37
27	A	411	LMG	O1-C1	2.09	1.43	1.40
23	C	512	CLA	C3B-C2B	-2.09	1.37	1.40
30	h	102	DGD	C1E-C2E	2.09	1.58	1.52
23	b	605	CLA	CMB-C2B	-2.08	1.47	1.51
30	h	102	DGD	C3D-C2D	2.08	1.57	1.52
23	c	510	CLA	CMC-C2C	-2.08	1.46	1.50
23	B	612	CLA	CMB-C2B	-2.08	1.47	1.51
23	c	513	CLA	C3B-C2B	-2.08	1.37	1.40
23	C	510	CLA	MG-NC	2.08	2.11	2.06
23	b	614	CLA	C5-C3	-2.08	1.47	1.51
23	a	405	CLA	C3B-CAB	-2.08	1.43	1.47
25	B	617	BCR	C36-C18	-2.08	1.46	1.50
27	c	519	LMG	C4-C3	2.07	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C4B-CHC	-2.07	1.35	1.41
23	C	507	CLA	CMC-C2C	-2.07	1.46	1.50
23	b	607	CLA	C3B-C2B	-2.07	1.37	1.40
27	D	406	LMG	C6-C5	2.07	1.58	1.51
28	f	101	SQD	O4-C4	-2.06	1.38	1.43
23	b	616	CLA	C3B-CAB	-2.06	1.43	1.47
23	B	603	CLA	CMD-C2D	-2.06	1.46	1.51
23	B	602	CLA	C3C-C2C	2.06	1.41	1.36
23	C	510	CLA	C3B-CAB	-2.06	1.43	1.47
27	c	521	LMG	C1-C2	2.06	1.58	1.52
23	d	403	CLA	CMC-C2C	-2.06	1.46	1.50
23	D	403	CLA	C3B-CAB	-2.05	1.43	1.47
23	B	612	CLA	CMC-C2C	-2.05	1.46	1.50
23	C	506	CLA	CAC-C3C	-2.05	1.45	1.51
23	c	505	CLA	C3B-CAB	-2.05	1.43	1.47
23	D	402	CLA	C1A-CHA	-2.05	1.34	1.43
30	A	415	DGD	C3E-C2E	2.05	1.57	1.52
23	A	405	CLA	CMB-C2B	-2.05	1.47	1.51
23	B	602	CLA	MG-NC	2.05	2.11	2.06
24	A	406	PHO	CHD-C4C	-2.05	1.35	1.40
30	a	414	DGD	C2B-C1B	2.05	1.56	1.50
25	B	619	BCR	C33-C5	-2.05	1.47	1.50
23	c	512	CLA	CMC-C2C	-2.05	1.46	1.50
30	C	517	DGD	C6D-C5D	2.04	1.58	1.51
23	A	405	CLA	C1D-C2D	2.04	1.47	1.42
23	C	511	CLA	C4B-CHC	-2.04	1.35	1.41
30	c	517	DGD	O1G-C1G	-2.04	1.40	1.45
27	D	409	LMG	O8-C28	2.03	1.39	1.33
23	c	504	CLA	CAC-C3C	-2.03	1.45	1.51
23	c	513	CLA	CMC-C2C	-2.03	1.46	1.50
25	A	409	BCR	C33-C5	-2.03	1.47	1.50
27	c	521	LMG	O7-C10	2.03	1.40	1.34
24	A	407	PHO	CMC-C2C	-2.03	1.46	1.50
29	B	622	LHG	O7-C5	-2.03	1.41	1.46
23	B	613	CLA	OBD-CAD	2.03	1.25	1.22
30	c	518	DGD	O1G-C1G	-2.03	1.40	1.45
23	b	605	CLA	C3B-C2B	-2.03	1.37	1.40
23	D	403	CLA	C1A-CHA	-2.03	1.34	1.43
23	c	503	CLA	CMC-C2C	-2.02	1.46	1.50
23	A	408	CLA	CMB-C2B	-2.02	1.47	1.51
24	d	401	PHO	C1B-C2B	2.02	1.50	1.45
24	A	406	PHO	C1D-C2D	-2.02	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	101	BCR	C1-C6	-2.02	1.51	1.53
26	d	405	PL9	C52-C5	-2.02	1.46	1.50
23	B	602	CLA	C4B-CHC	-2.02	1.35	1.41
23	a	406	CLA	C4B-CHC	-2.02	1.35	1.41
24	d	401	PHO	C1C-NC	-2.02	1.34	1.38
23	b	616	CLA	OBD-CAD	2.01	1.25	1.22
23	D	402	CLA	MG-NA	2.01	2.11	2.06
23	B	606	CLA	CMD-C2D	-2.01	1.46	1.51
24	a	407	PHO	CMD-C2D	-2.01	1.46	1.50
23	C	504	CLA	CMD-C2D	-2.01	1.46	1.51
23	A	405	CLA	CAC-C3C	-2.01	1.46	1.51
25	t	101	BCR	C1-C6	-2.01	1.51	1.53
23	A	405	CLA	C3B-CAB	-2.01	1.43	1.47
29	A	413	LHG	P-O3	2.01	1.67	1.59
30	C	517	DGD	C3E-C2E	-2.00	1.47	1.52
28	A	412	SQD	O3-C3	-2.00	1.38	1.43

All (1377) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C4A-NA-C1A	9.88	111.15	106.71
23	C	511	CLA	C4A-NA-C1A	9.86	111.14	106.71
23	d	402	CLA	C4A-NA-C1A	9.84	111.13	106.71
23	C	503	CLA	C4A-NA-C1A	9.73	111.08	106.71
23	a	411	CLA	C4A-NA-C1A	9.62	111.03	106.71
28	A	412	SQD	O6-C1-C2	9.26	122.77	108.30
28	A	412	SQD	O7-S-C6	8.94	117.56	106.94
23	b	607	CLA	C4A-NA-C1A	8.49	110.52	106.71
23	c	503	CLA	C4A-NA-C1A	8.49	110.52	106.71
28	a	412	SQD	O6-C1-C2	8.32	121.29	108.30
26	a	410	PL9	C7-C3-C4	7.85	123.26	116.88
23	C	513	CLA	C4A-NA-C1A	7.79	110.21	106.71
23	B	606	CLA	C4A-NA-C1A	7.68	110.16	106.71
23	c	501	CLA	C4A-NA-C1A	7.50	110.08	106.71
23	c	511	CLA	C4A-NA-C1A	7.22	109.95	106.71
28	b	601	SQD	O6-C1-C2	7.11	119.41	108.30
23	B	607	CLA	C4A-NA-C1A	7.08	109.89	106.71
23	B	604	CLA	C4A-NA-C1A	7.07	109.88	106.71
23	b	615	CLA	C4A-NA-C1A	7.06	109.88	106.71
23	c	509	CLA	C4A-NA-C1A	6.80	109.76	106.71
23	c	508	CLA	C4A-NA-C1A	6.72	109.73	106.71
23	C	501	CLA	C4A-NA-C1A	6.71	109.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	C	507	CLA	C4A-NA-C1A	6.60	109.67	106.71
23	C	510	CLA	C4A-NA-C1A	6.58	109.66	106.71
23	a	405	CLA	C4A-NA-C1A	6.34	109.56	106.71
23	B	612	CLA	C4A-NA-C1A	6.26	109.52	106.71
23	B	609	CLA	C4A-NA-C1A	6.21	109.50	106.71
23	c	510	CLA	C4A-NA-C1A	6.20	109.49	106.71
28	B	624	SQD	O6-C1-C2	6.13	117.88	108.30
35	e	102	HEM	CBD-CAD-C3D	-6.11	101.21	112.48
26	A	410	PL9	C7-C3-C4	6.09	121.83	116.88
23	b	605	CLA	C4A-NA-C1A	6.08	109.44	106.71
28	f	101	SQD	O9-S-C6	6.04	114.11	106.94
23	c	502	CLA	C4A-NA-C1A	5.93	109.37	106.71
23	C	506	CLA	C4A-NA-C1A	5.90	109.36	106.71
28	F	101	SQD	O8-S-C6	5.90	115.14	105.74
23	c	507	CLA	C4A-NA-C1A	5.85	109.34	106.71
23	c	513	CLA	C4A-NA-C1A	5.80	109.31	106.71
23	c	505	CLA	C4A-NA-C1A	5.57	109.21	106.71
23	B	614	CLA	O2D-CGD-O1D	-5.53	113.03	123.84
23	D	401	CLA	C4A-NA-C1A	5.53	109.19	106.71
23	B	608	CLA	C4A-NA-C1A	5.45	109.16	106.71
23	a	408	CLA	C4A-NA-C1A	5.45	109.16	106.71
23	b	606	CLA	C4A-NA-C1A	5.34	109.11	106.71
23	B	616	CLA	C4A-NA-C1A	5.30	109.09	106.71
23	C	508	CLA	C4A-NA-C1A	5.30	109.09	106.71
23	c	501	CLA	O2D-CGD-O1D	-5.27	113.54	123.84
23	B	602	CLA	C4A-NA-C1A	5.22	109.05	106.71
28	B	624	SQD	O7-S-C6	5.21	113.14	106.94
23	c	504	CLA	C4A-NA-C1A	5.21	109.05	106.71
23	A	404	CLA	C4A-NA-C1A	5.19	109.04	106.71
23	B	605	CLA	C4D-C3D-CAD	-5.14	105.60	108.47
23	C	502	CLA	C4A-NA-C1A	5.14	109.02	106.71
23	b	616	CLA	C4A-NA-C1A	5.11	109.00	106.71
28	A	414	SQD	C45-O47-C7	5.06	124.39	117.88
35	E	101	HEM	CBD-CAD-C3D	-5.05	103.17	112.48
28	B	624	SQD	O47-C7-C8	5.03	122.34	111.50
23	B	604	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
30	H	102	DGD	O3G-C3G-C2G	-4.99	98.87	110.90
23	c	512	CLA	C4A-NA-C1A	4.97	108.94	106.71
23	a	406	CLA	C4A-NA-C1A	4.95	108.93	106.71
23	C	512	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
23	B	601	CLA	O2D-CGD-O1D	-4.88	114.29	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	413	SQD	O47-C7-C8	4.87	121.99	111.50
23	h	101	CLA	O2D-CGD-O1D	-4.84	114.37	123.84
23	b	614	CLA	C4A-NA-C1A	4.83	108.88	106.71
28	F	101	SQD	O6-C1-C2	4.81	115.81	108.30
27	b	622	LMG	O1-C1-C2	-4.80	100.81	108.30
23	b	604	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
23	c	505	CLA	C4D-C3D-CAD	-4.70	105.85	108.47
35	e	102	HEM	CBA-CAA-C2A	-4.70	103.81	112.49
28	A	412	SQD	O9-S-O7	-4.69	97.73	113.95
23	c	509	CLA	C4D-C3D-CAD	-4.68	105.86	108.47
26	a	410	PL9	C7-C3-C2	-4.67	117.16	123.30
28	f	101	SQD	O6-C1-C2	4.66	115.58	108.30
23	A	408	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
23	c	501	CLA	CMB-C2B-C1B	-4.65	121.31	128.46
30	C	516	DGD	O3G-C3G-C2G	-4.60	99.80	110.90
23	b	612	CLA	CMB-C2B-C1B	-4.57	121.43	128.46
23	C	512	CLA	CMB-C2B-C3B	4.57	133.22	124.68
23	b	615	CLA	OBD-CAD-CBD	-4.57	119.37	125.89
23	C	505	CLA	OBD-CAD-CBD	-4.56	119.38	125.89
23	C	513	CLA	CMB-C2B-C1B	-4.54	121.48	128.46
30	a	414	DGD	C2G-O2G-C1B	4.52	128.92	117.79
23	B	605	CLA	OBD-CAD-CBD	-4.52	119.44	125.89
28	a	412	SQD	O9-S-C6	4.51	112.30	106.94
23	b	604	CLA	O2D-CGD-O1D	-4.51	115.02	123.84
23	B	609	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
23	a	406	CLA	O2D-CGD-CBD	4.49	119.25	111.27
23	b	608	CLA	C4A-NA-C1A	4.49	108.72	106.71
23	B	610	CLA	CHB-C4A-NA	4.49	130.72	124.51
23	C	503	CLA	C7-C6-C5	-4.47	101.23	113.36
23	c	504	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
23	b	613	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
23	c	502	CLA	CMD-C2D-C3D	4.42	132.95	124.68
23	b	613	CLA	C4A-NA-C1A	4.41	108.69	106.71
23	b	603	CLA	O2D-CGD-CBD	4.40	119.09	111.27
23	b	615	CLA	CMB-C2B-C1B	-4.40	121.70	128.46
23	A	405	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
28	F	101	SQD	O9-S-C6	4.35	112.11	106.94
23	B	610	CLA	C4A-NA-C1A	4.33	108.65	106.71
28	b	601	SQD	O5-C5-C4	4.32	117.53	109.69
23	c	510	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
26	d	405	PL9	C7-C3-C4	4.31	120.38	116.88
27	m	101	LMG	O7-C10-O9	-4.30	113.30	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	C4D-C3D-CAD	-4.28	106.08	108.47
23	c	501	CLA	O2D-CGD-CBD	4.26	118.84	111.27
23	b	611	CLA	O2D-CGD-O1D	-4.26	115.52	123.84
23	c	511	CLA	C1D-CHD-C4C	4.25	128.16	122.56
23	b	613	CLA	CMB-C2B-C3B	4.25	132.62	124.68
29	e	101	LHG	O4-P-O5	4.25	133.23	112.24
23	b	614	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
29	B	623	LHG	O4-P-O5	4.21	133.06	112.24
23	b	604	CLA	CMB-C2B-C3B	4.20	132.54	124.68
23	D	403	CLA	C1B-CHB-C4A	-4.20	121.81	130.12
23	A	404	CLA	CMD-C2D-C3D	4.19	132.52	124.68
23	C	508	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
23	A	405	CLA	CMD-C2D-C3D	4.17	132.48	124.68
30	h	102	DGD	O6E-C5E-C4E	4.17	117.26	109.69
23	B	610	CLA	O2D-CGD-O1D	-4.16	115.70	123.84
23	D	403	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
23	C	506	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
23	C	509	CLA	C4A-NA-C1A	4.15	108.57	106.71
23	b	617	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
29	d	406	LHG	O4-P-O5	4.13	132.67	112.24
29	D	408	LHG	O4-P-O5	4.12	132.61	112.24
23	A	408	CLA	CMB-C2B-C3B	4.10	132.35	124.68
23	B	615	CLA	C4A-NA-C1A	4.10	108.55	106.71
23	b	603	CLA	C4A-NA-C1A	4.09	108.55	106.71
29	d	407	LHG	O4-P-O5	4.09	132.48	112.24
23	b	603	CLA	CHB-C4A-NA	4.09	130.17	124.51
28	A	412	SQD	C1-C2-C3	-4.09	101.48	110.00
25	c	515	BCR	C36-C18-C17	-4.09	117.20	122.92
23	B	615	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
23	a	406	CLA	CHB-C4A-NA	4.06	130.13	124.51
23	B	605	CLA	CMD-C2D-C3D	4.06	132.28	124.68
23	b	616	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
23	C	509	CLA	CHB-C4A-NA	4.05	130.11	124.51
23	B	611	CLA	O2D-CGD-O1D	-4.04	115.93	123.84
23	c	506	CLA	C4A-NA-C1A	4.04	108.52	106.71
28	b	601	SQD	O7-S-C6	4.03	111.73	106.94
29	l	101	LHG	O4-P-O5	4.02	132.09	112.24
23	c	509	CLA	CMD-C2D-C3D	4.00	132.17	124.68
30	C	517	DGD	O3G-C3G-C2G	-4.00	101.24	110.90
23	B	604	CLA	CMB-C2B-C3B	4.00	132.16	124.68
23	D	403	CLA	CMB-C2B-C3B	4.00	132.16	124.68
24	d	401	PHO	CMC-C2C-C1C	-3.98	118.94	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
23	b	607	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
23	B	610	CLA	C1B-CHB-C4A	-3.96	122.27	130.12
23	B	603	CLA	O2D-CGD-O1D	-3.96	116.09	123.84
27	b	622	LMG	C1-O6-C5	-3.96	105.91	113.69
23	c	502	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
30	H	102	DGD	C1D-O6D-C5D	-3.93	105.97	113.69
26	d	405	PL9	C45-C44-C46	-3.93	108.67	115.27
29	A	413	LHG	O4-P-O5	3.90	131.54	112.24
25	b	618	BCR	C2-C1-C6	3.90	116.49	110.48
30	C	515	DGD	C3D-C4D-C5D	-3.90	103.29	110.24
29	d	408	LHG	O4-P-O5	3.90	131.50	112.24
25	a	409	BCR	C35-C13-C14	-3.89	117.47	122.92
29	e	101	LHG	O8-C23-C24	3.89	124.11	111.91
23	B	612	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
23	b	608	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
23	B	601	CLA	O1D-CGD-CBD	3.88	132.42	124.48
23	c	512	CLA	C1-C2-C3	-3.86	119.37	126.04
23	a	406	CLA	O2D-CGD-O1D	-3.84	116.34	123.84
28	a	412	SQD	C1-C2-C3	-3.82	102.04	110.00
23	B	611	CLA	O2D-CGD-CBD	3.82	118.06	111.27
29	D	407	LHG	O4-P-O5	3.82	131.12	112.24
23	b	612	CLA	CMB-C2B-C3B	3.82	131.82	124.68
25	K	101	BCR	C39-C30-C25	-3.82	104.11	110.30
28	B	624	SQD	O8-S-C6	3.81	111.81	105.74
29	B	623	LHG	O8-C23-O10	-3.81	113.98	123.59
23	b	617	CLA	C4A-NA-C1A	3.80	108.42	106.71
26	D	405	PL9	C37-C38-C39	-3.80	118.50	127.66
23	C	513	CLA	CMB-C2B-C3B	3.80	131.79	124.68
23	b	609	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
23	B	614	CLA	CAC-C3C-C4C	3.79	129.72	124.81
23	b	607	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
26	D	405	PL9	C7-C3-C4	3.77	119.94	116.88
23	B	606	CLA	CHD-C4C-NC	3.76	130.12	124.20
23	b	609	CLA	CMB-C2B-C3B	3.75	131.70	124.68
28	a	412	SQD	O9-S-O7	-3.75	100.98	113.95
23	A	404	CLA	CMB-C2B-C3B	3.75	131.69	124.68
28	b	601	SQD	O8-S-C6	3.74	111.70	105.74
23	D	401	CLA	CMD-C2D-C3D	3.73	131.66	124.68
30	A	415	DGD	C3G-C2G-C1G	-3.73	102.97	111.79
23	b	606	CLA	C4D-C3D-CAD	-3.73	106.39	108.47
23	c	504	CLA	CMB-C2B-C3B	3.73	131.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	518	DGD	O3G-C3G-C2G	-3.73	101.91	110.90
23	a	408	CLA	CMD-C2D-C3D	3.73	131.65	124.68
25	H	101	BCR	C29-C30-C25	3.72	116.20	110.48
26	A	410	PL9	C40-C39-C41	3.72	121.52	115.27
23	B	602	CLA	O2D-CGD-CBD	3.71	117.87	111.27
28	A	412	SQD	O47-C7-C8	3.71	119.49	111.50
23	C	504	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
23	A	405	CLA	C1B-CHB-C4A	-3.70	122.78	130.12
25	B	617	BCR	C29-C30-C25	3.69	116.16	110.48
23	A	405	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
23	h	101	CLA	O2D-CGD-CBD	3.68	117.81	111.27
30	h	102	DGD	O2D-C2D-C1D	-3.68	101.12	110.05
23	c	506	CLA	CMB-C2B-C3B	3.68	131.55	124.68
26	A	410	PL9	C7-C3-C2	-3.67	118.47	123.30
30	c	516	DGD	O3G-C3G-C2G	-3.67	102.04	110.90
23	B	612	CLA	CMB-C2B-C3B	3.67	131.54	124.68
23	c	501	CLA	CMB-C2B-C3B	3.66	131.52	124.68
23	a	405	CLA	CAC-C3C-C4C	3.64	129.54	124.81
23	c	510	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
23	b	603	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
23	b	604	CLA	C1B-CHB-C4A	-3.63	122.94	130.12
23	C	513	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	C	508	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	b	617	CLA	CMB-C2B-C3B	3.61	131.42	124.68
23	B	602	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
23	B	608	CLA	C4D-C3D-CAD	-3.60	106.46	108.47
23	a	406	CLA	C4D-C3D-CAD	-3.59	106.47	108.47
23	A	405	CLA	CMB-C2B-C3B	3.59	131.40	124.68
23	a	405	CLA	C4D-C3D-CAD	-3.58	106.47	108.47
23	c	505	CLA	C1D-CHD-C4C	3.58	127.28	122.56
23	A	404	CLA	CMB-C2B-C1B	-3.58	122.97	128.46
23	a	411	CLA	CHB-C4A-NA	3.58	129.46	124.51
23	c	509	CLA	CMB-C2B-C3B	3.57	131.36	124.68
23	c	505	CLA	OBD-CAD-CBD	-3.56	120.80	125.89
26	d	405	PL9	C35-C34-C36	3.56	121.27	115.27
28	b	601	SQD	C3-C4-C5	3.56	116.60	110.24
35	e	102	HEM	CMD-C2D-C1D	-3.56	122.99	128.46
23	b	609	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	B	605	CLA	C16-C15-C13	-3.55	104.44	115.92
30	C	517	DGD	O3E-C3E-C2E	-3.55	102.15	110.35
23	a	408	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	k	101	BCR	C33-C5-C6	-3.54	120.56	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
23	c	507	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
23	B	616	CLA	C1B-CHB-C4A	-3.52	123.15	130.12
23	c	507	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
29	A	413	LHG	O8-C23-C24	3.51	122.91	111.91
24	d	401	PHO	O1D-CGD-CBD	3.50	131.65	124.48
23	D	401	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
23	B	609	CLA	CMB-C2B-C3B	3.49	131.20	124.68
23	c	509	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
25	T	101	BCR	C35-C13-C14	-3.46	118.07	122.92
23	a	406	CLA	CED-O2D-CGD	-3.46	108.11	115.94
23	C	504	CLA	C4A-NA-C1A	3.46	108.26	106.71
23	B	610	CLA	O2A-CGA-O1A	-3.45	114.88	123.59
23	A	404	CLA	CHB-C4A-NA	3.45	129.28	124.51
23	B	610	CLA	O1D-CGD-CBD	3.45	131.53	124.48
23	B	602	CLA	CHB-C4A-NA	3.44	129.27	124.51
23	a	408	CLA	OBD-CAD-CBD	-3.43	121.00	125.89
23	c	503	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
23	B	605	CLA	C4-C3-C5	3.43	121.03	115.27
30	A	415	DGD	O5D-C1E-C2E	3.42	113.64	108.30
23	c	512	CLA	CHB-C4A-NA	3.42	129.24	124.51
28	A	412	SQD	O47-C7-O49	-3.42	115.44	123.70
25	t	101	BCR	C35-C13-C14	-3.41	118.15	122.92
26	A	410	PL9	C36-C34-C33	-3.40	114.23	121.12
23	B	611	CLA	OBD-CAD-CBD	-3.40	121.03	125.89
23	C	512	CLA	OBD-CAD-CBD	-3.40	121.03	125.89
23	C	506	CLA	CMB-C2B-C3B	3.40	131.03	124.68
30	A	415	DGD	O3G-C3G-C2G	-3.39	102.72	110.90
25	T	101	BCR	C15-C14-C13	-3.39	122.47	127.31
23	d	403	CLA	C4A-NA-C1A	3.37	108.22	106.71
23	D	401	CLA	CMB-C2B-C3B	3.37	130.99	124.68
25	c	515	BCR	C33-C5-C6	-3.37	120.75	124.53
23	B	615	CLA	C6-C7-C8	-3.37	105.04	115.92
23	B	611	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
23	b	606	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
25	B	617	BCR	C34-C9-C10	-3.36	118.22	122.92
23	A	408	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
23	b	614	CLA	CMD-C2D-C3D	3.35	130.95	124.68
27	c	523	LMG	C1-O6-C5	-3.35	107.11	113.69
28	f	101	SQD	O9-S-O7	-3.35	102.35	113.95
23	b	612	CLA	C4A-NA-C1A	3.35	108.21	106.71
23	c	502	CLA	CMB-C2B-C3B	3.34	130.94	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C4D-C3D-CAD	-3.34	106.61	108.47
28	a	412	SQD	O7-S-C6	3.34	110.90	106.94
29	D	408	LHG	O8-C23-O10	-3.33	115.18	123.59
23	c	507	CLA	CMB-C2B-C3B	3.33	130.91	124.68
23	b	617	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
23	b	608	CLA	CMB-C2B-C3B	3.33	130.91	124.68
25	H	101	BCR	C27-C26-C25	3.33	127.56	122.73
26	d	405	PL9	C50-C49-C48	-3.33	113.03	122.65
23	b	614	CLA	C4D-C3D-CAD	-3.33	106.61	108.47
23	C	503	CLA	C1D-CHD-C4C	3.33	126.95	122.56
23	B	605	CLA	OBD-CAD-C3D	3.33	133.50	127.98
26	d	405	PL9	C22-C23-C24	-3.32	119.66	127.66
28	a	413	SQD	O48-C23-O10	-3.32	115.21	123.59
23	c	505	CLA	CMD-C2D-C3D	3.32	130.89	124.68
23	b	617	CLA	C1B-CHB-C4A	-3.31	123.55	130.12
23	c	508	CLA	CHB-C4A-NA	3.31	129.09	124.51
23	a	405	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
25	A	409	BCR	C2-C1-C6	3.30	115.56	110.48
23	C	505	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	C	514	BCR	C15-C14-C13	-3.30	122.60	127.31
23	b	611	CLA	C4A-NA-C1A	3.29	108.19	106.71
28	b	601	SQD	C45-O47-C7	3.29	125.90	117.79
23	c	509	CLA	O2A-CGA-O1A	-3.29	115.28	123.59
23	b	612	CLA	C1D-CHD-C4C	3.29	126.90	122.56
23	C	501	CLA	O2A-CGA-O1A	-3.29	115.30	123.59
25	D	404	BCR	C2-C1-C6	3.28	115.53	110.48
30	a	414	DGD	O1G-C1A-O1A	-3.28	115.32	123.59
25	D	404	BCR	C38-C26-C25	-3.27	120.85	124.53
23	b	606	CLA	CMD-C2D-C3D	3.27	130.79	124.68
28	B	624	SQD	O9-S-O7	-3.27	102.65	113.95
23	a	411	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
27	A	411	LMG	C38-C37-C36	-3.26	97.87	114.42
23	C	508	CLA	CMB-C2B-C3B	3.25	130.77	124.68
23	b	615	CLA	CMB-C2B-C3B	3.25	130.76	124.68
30	h	102	DGD	O3G-C3G-C2G	-3.25	103.06	110.90
23	c	511	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	C	508	CLA	OBD-CAD-CBD	-3.25	121.25	125.89
23	B	601	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
30	c	518	DGD	C3G-C2G-C1G	-3.24	104.13	111.79
23	b	613	CLA	CMD-C2D-C3D	3.24	130.73	124.68
25	B	619	BCR	C33-C5-C6	-3.23	120.90	124.53
25	b	618	BCR	C11-C10-C9	-3.23	122.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C4-C3-C5	3.23	120.70	115.27
23	b	611	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
23	c	509	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
30	c	517	DGD	O3G-C3G-C2G	-3.21	103.14	110.90
23	C	510	CLA	C7-C6-C5	-3.21	104.64	113.36
23	C	508	CLA	C1D-CHD-C4C	3.21	126.79	122.56
23	D	403	CLA	OBD-CAD-CBD	-3.21	121.31	125.89
30	A	415	DGD	C1D-C2D-C3D	-3.20	103.33	110.00
24	a	407	PHO	C1-C2-C3	-3.20	120.51	126.04
25	Z	101	BCR	C11-C10-C9	-3.19	122.75	127.31
23	a	405	CLA	CMD-C2D-C3D	3.19	130.65	124.68
23	C	509	CLA	CMB-C2B-C3B	3.19	130.64	124.68
23	A	408	CLA	O2D-CGD-CBD	3.18	116.92	111.27
23	D	402	CLA	CMD-C2D-C3D	3.18	130.63	124.68
25	T	101	BCR	C2-C1-C6	3.18	115.38	110.48
23	c	507	CLA	CHB-C4A-NA	3.18	128.91	124.51
25	t	101	BCR	C15-C16-C17	-3.18	116.96	123.47
30	H	102	DGD	C1D-C2D-C3D	-3.18	103.38	110.00
23	C	501	CLA	O2D-CGD-O1D	-3.17	117.63	123.84
23	a	408	CLA	CMB-C2B-C3B	3.17	130.62	124.68
23	B	612	CLA	CHB-C4A-NA	3.17	128.90	124.51
23	C	507	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
23	d	402	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
23	C	507	CLA	CMB-C2B-C3B	3.17	130.61	124.68
23	B	608	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
27	c	521	LMG	O3-C3-C2	-3.17	103.02	110.35
29	B	623	LHG	O8-C23-C24	3.16	121.82	111.91
23	B	616	CLA	C1-O2A-CGA	3.16	124.73	116.44
30	A	415	DGD	C4E-C3E-C2E	-3.16	105.31	110.82
28	a	412	SQD	O47-C7-C8	3.16	118.30	111.50
28	A	412	SQD	O8-S-C6	3.15	110.76	105.74
23	c	504	CLA	O2D-CGD-CBD	3.15	116.86	111.27
23	D	402	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
30	C	517	DGD	CDB-CCB-CBB	-3.14	98.46	114.42
25	Z	101	BCR	C34-C9-C10	-3.14	118.52	122.92
29	B	622	LHG	O4-P-O5	3.14	127.77	112.24
25	b	620	BCR	C37-C22-C21	-3.14	118.52	122.92
23	B	602	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
23	C	507	CLA	CHB-C4A-NA	3.14	128.85	124.51
23	A	408	CLA	CHB-C4A-NA	3.13	128.84	124.51
30	C	516	DGD	O6D-C1D-O3G	-3.13	102.57	109.97
23	B	616	CLA	C2C-C1C-NC	3.13	112.90	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	402	CLA	CHB-C4A-NA	3.13	128.84	124.51
27	c	521	LMG	C9-C8-C7	-3.13	104.39	111.79
26	d	405	PL9	C40-C39-C41	3.13	120.53	115.27
23	c	507	CLA	CMD-C2D-C3D	3.12	130.52	124.68
23	b	604	CLA	C4A-NA-C1A	3.12	108.11	106.71
23	C	512	CLA	CHB-C4A-NA	3.12	128.82	124.51
26	d	405	PL9	C46-C47-C48	-3.11	101.66	111.88
23	b	613	CLA	O1D-CGD-CBD	3.11	130.85	124.48
26	a	410	PL9	C22-C23-C24	-3.11	120.17	127.66
23	C	506	CLA	CHB-C4A-NA	3.11	128.81	124.51
30	c	517	DGD	O3G-C1D-C2D	-3.10	103.46	108.30
23	b	609	CLA	O2D-CGD-CBD	3.10	116.78	111.27
23	c	510	CLA	CHB-C4A-NA	3.10	128.80	124.51
23	c	508	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
23	B	607	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
23	C	501	CLA	O2D-CGD-CBD	3.10	116.77	111.27
23	C	511	CLA	CAC-C3C-C4C	3.10	128.83	124.81
25	T	101	BCR	C38-C26-C27	-3.09	107.67	113.62
23	b	616	CLA	CMB-C2B-C3B	3.09	130.47	124.68
23	c	511	CLA	OBD-CAD-CBD	-3.09	121.48	125.89
27	d	409	LMG	O2-C2-C1	-3.09	102.55	110.05
23	b	614	CLA	C1D-CHD-C4C	3.09	126.63	122.56
25	B	619	BCR	C29-C30-C25	3.09	115.23	110.48
23	B	615	CLA	CHB-C4A-NA	3.09	128.78	124.51
23	A	405	CLA	O2D-CGD-CBD	3.07	116.73	111.27
23	D	403	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
23	c	512	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
27	c	521	LMG	O6-C1-O1	-3.07	102.70	109.97
30	C	516	DGD	O3E-C3E-C2E	-3.06	103.27	110.35
30	c	517	DGD	C8B-C7B-C6B	-3.06	98.90	114.42
23	b	607	CLA	CMB-C2B-C3B	3.06	130.39	124.68
23	C	502	CLA	C4D-C3D-CAD	-3.05	106.77	108.47
30	h	102	DGD	O5E-C6E-C5E	-3.05	100.84	111.29
23	b	609	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
30	c	518	DGD	O6D-C1D-O3G	-3.05	102.76	109.97
23	c	506	CLA	CGD-CBD-CAD	-3.05	100.87	110.73
25	b	619	BCR	C30-C25-C26	-3.04	118.33	122.61
23	C	504	CLA	C1D-CHD-C4C	3.04	126.58	122.56
23	b	605	CLA	CHB-C4A-NA	3.04	128.71	124.51
23	b	615	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
23	d	402	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
25	H	101	BCR	C38-C26-C25	-3.03	121.13	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4D-C3D-CAD	-3.03	106.78	108.47
23	A	404	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
25	T	101	BCR	C27-C26-C25	3.02	127.12	122.73
25	C	514	BCR	C15-C16-C17	-3.02	117.28	123.47
23	B	603	CLA	CHD-C4C-NC	3.02	128.96	124.20
23	b	611	CLA	O1D-CGD-CBD	3.02	130.66	124.48
26	d	405	PL9	C37-C38-C39	-3.02	120.39	127.66
23	b	604	CLA	O2D-CGD-CBD	3.02	116.63	111.27
23	B	603	CLA	OBD-CAD-CBD	-3.02	121.59	125.89
24	A	406	PHO	O2D-CGD-O1D	-3.01	117.94	123.84
28	A	412	SQD	O2-C2-C1	3.01	117.37	110.05
27	D	406	LMG	O6-C1-O1	-3.01	102.84	109.97
25	A	409	BCR	C11-C10-C9	-3.01	123.02	127.31
24	A	407	PHO	O2D-CGD-O1D	-3.01	117.96	123.84
25	x	101	BCR	C30-C25-C26	-3.01	118.38	122.61
25	b	618	BCR	C33-C5-C6	-3.01	121.15	124.53
23	C	501	CLA	C1D-CHD-C4C	3.00	126.52	122.56
23	c	512	CLA	CMD-C2D-C3D	3.00	130.29	124.68
23	B	616	CLA	C5-C3-C2	3.00	127.18	121.12
23	a	405	CLA	O1D-CGD-CBD	3.00	130.62	124.48
23	C	509	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
23	B	606	CLA	CHD-C4C-C3C	-2.99	120.44	124.84
28	b	601	SQD	O2-C2-C1	2.99	117.31	110.05
35	E	101	HEM	CAD-CBD-CGD	2.99	117.69	112.67
23	B	612	CLA	C11-C12-C13	-2.99	106.26	115.92
24	A	407	PHO	C3A-C4A-CHB	-2.98	116.68	121.83
23	B	615	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
23	c	506	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
24	A	407	PHO	C1-C2-C3	-2.97	120.91	126.04
23	C	505	CLA	OBD-CAD-C3D	2.97	132.91	127.98
26	D	405	PL9	C22-C23-C24	-2.96	120.52	127.66
23	c	510	CLA	O2A-C1-C2	-2.96	100.85	108.64
23	c	508	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	B	608	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	c	513	CLA	CHB-C4A-NA	2.95	128.60	124.51
23	B	606	CLA	CGD-CBD-CAD	-2.95	101.17	110.73
27	M	101	LMG	O1-C1-C2	-2.95	103.70	108.30
23	c	510	CLA	C1D-CHD-C4C	2.95	126.45	122.56
23	D	402	CLA	C4A-NA-C1A	2.95	108.03	106.71
27	D	406	LMG	O3-C3-C2	-2.95	103.54	110.35
23	D	402	CLA	CMB-C2B-C3B	2.95	130.19	124.68
23	B	602	CLA	CHA-C1A-NA	-2.95	119.65	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	DGD	O2D-C2D-C1D	-2.94	102.90	110.05
29	d	407	LHG	O8-C23-C24	2.94	121.13	111.91
28	B	624	SQD	C1-C2-C3	-2.94	103.88	110.00
23	A	405	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
23	B	614	CLA	O1D-CGD-CBD	2.94	130.49	124.48
25	K	102	BCR	C37-C22-C21	-2.94	118.81	122.92
23	B	614	CLA	O2D-CGD-CBD	2.93	116.48	111.27
23	B	614	CLA	C1-C2-C3	-2.93	120.97	126.04
23	c	503	CLA	CAC-C3C-C4C	2.93	128.61	124.81
29	D	408	LHG	O8-C23-C24	2.93	121.10	111.91
23	B	614	CLA	O2A-CGA-O1A	-2.93	116.20	123.59
25	c	514	BCR	C27-C26-C25	2.92	126.97	122.73
23	c	507	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	B	618	BCR	C3-C4-C5	-2.92	108.86	114.08
23	B	616	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
23	b	610	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
23	C	502	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	B	603	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
28	B	624	SQD	C3-C4-C5	2.91	115.43	110.24
23	B	611	CLA	CMB-C2B-C3B	2.91	130.12	124.68
23	b	603	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
23	B	615	CLA	CMB-C2B-C3B	2.90	130.11	124.68
25	Z	101	BCR	C33-C5-C6	-2.90	121.27	124.53
23	c	503	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
25	c	514	BCR	C37-C22-C21	-2.90	118.86	122.92
23	b	609	CLA	OBD-CAD-CBD	-2.90	121.75	125.89
23	c	510	CLA	C4D-C3D-CAD	-2.90	106.86	108.47
23	b	603	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
25	b	619	BCR	C15-C14-C13	-2.89	123.18	127.31
23	B	614	CLA	C1D-CHD-C4C	2.89	126.38	122.56
23	b	612	CLA	O2D-CGD-CBD	2.89	116.41	111.27
23	C	511	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
36	V	201	HEC	CMB-C2B-C3B	2.89	129.22	125.82
23	C	507	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	b	611	CLA	OBD-CAD-CBD	-2.88	121.78	125.89
23	c	508	CLA	O2A-CGA-O1A	-2.88	116.33	123.59
25	B	619	BCR	C38-C26-C25	-2.88	121.30	124.53
25	B	618	BCR	C15-C14-C13	-2.88	123.20	127.31
28	f	101	SQD	O47-C7-C8	2.88	118.82	110.80
23	B	609	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
23	b	611	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	b	616	CLA	CMD-C2D-C3D	2.87	130.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
28	a	412	SQD	C1-O5-C5	-2.87	108.06	113.69
23	c	509	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
28	b	601	SQD	C1-C2-C3	-2.86	104.03	110.00
23	B	609	CLA	C7-C6-C5	-2.86	105.59	113.36
23	D	401	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	k	101	BCR	C27-C26-C25	2.86	126.88	122.73
30	C	517	DGD	O6D-C1D-O3G	-2.85	103.23	109.97
28	B	624	SQD	C1-O5-C5	-2.84	108.11	113.69
23	b	605	CLA	CHC-C1C-NC	2.84	128.51	124.20
23	c	504	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	a	405	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
23	B	614	CLA	CMB-C2B-C3B	2.84	129.98	124.68
23	C	512	CLA	C1B-CHB-C4A	-2.83	124.50	130.12
23	B	609	CLA	OBD-CAD-CBD	-2.83	121.85	125.89
25	K	101	BCR	C33-C5-C6	-2.83	121.35	124.53
23	d	402	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
23	b	604	CLA	O2A-CGA-O1A	-2.82	116.46	123.59
30	h	102	DGD	C1E-O6E-C5E	2.82	119.23	113.69
23	C	510	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	a	408	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
23	b	615	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
23	d	403	CLA	CMB-C2B-C3B	2.82	129.96	124.68
23	b	605	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
23	B	607	CLA	C2C-C1C-NC	2.82	112.61	109.97
23	c	512	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
35	E	101	HEM	C1D-C2D-C3D	2.81	108.95	107.00
23	D	402	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	h	101	CLA	CBA-CAA-C2A	2.80	122.14	113.86
23	b	609	CLA	CMD-C2D-C3D	2.80	129.92	124.68
36	V	201	HEC	CMB-C2B-C1B	-2.80	124.16	128.46
25	K	102	BCR	C29-C30-C25	2.80	114.79	110.48
29	d	408	LHG	O8-C23-O10	-2.80	116.53	123.59
23	c	504	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	a	408	CLA	C4D-C3D-CAD	-2.79	106.91	108.47
23	B	614	CLA	CMD-C2D-C3D	2.79	129.90	124.68
26	A	410	PL9	O2-C1-C2	-2.79	115.38	121.78
30	C	515	DGD	O1G-C1A-C2A	-2.79	103.15	111.91
23	B	608	CLA	CMD-C2D-C3D	2.79	129.89	124.68
23	h	101	CLA	C4A-NA-C1A	2.79	107.96	106.71
23	c	503	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	t	101	BCR	C36-C18-C19	2.79	122.47	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	413	SQD	O49-C7-C8	-2.79	112.86	123.73
23	B	603	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	a	411	CLA	CMD-C2D-C3D	2.78	129.88	124.68
25	b	618	BCR	C34-C9-C10	-2.78	119.03	122.92
27	M	101	LMG	O7-C10-O9	-2.78	116.99	123.70
29	d	406	LHG	O8-C6-C5	-2.78	100.35	108.43
23	b	605	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
25	C	514	BCR	C29-C30-C25	2.77	114.75	110.48
25	c	515	BCR	C35-C13-C14	-2.77	119.04	122.92
26	a	410	PL9	C35-C34-C36	2.77	119.93	115.27
23	c	508	CLA	C1D-CHD-C4C	2.77	126.21	122.56
25	b	620	BCR	C29-C30-C25	2.77	114.75	110.48
23	b	606	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	e	101	LHG	O8-C23-O10	-2.77	116.61	123.59
26	d	405	PL9	C31-C32-C33	-2.77	102.79	111.88
23	c	510	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	B	605	CLA	C1D-CHD-C4C	2.76	126.20	122.56
23	B	609	CLA	C4-C3-C5	-2.76	110.63	115.27
26	a	410	PL9	C12-C13-C14	-2.76	121.02	127.66
23	C	502	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
28	B	624	SQD	O48-C23-C24	2.75	120.55	111.91
23	c	513	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	d	406	LHG	C11-C10-C9	-2.75	100.45	114.42
27	m	101	LMG	O1-C7-C8	-2.75	104.27	110.90
25	t	101	BCR	C35-C13-C12	2.75	122.41	118.08
23	b	617	CLA	CHB-C4A-NA	2.74	128.31	124.51
23	b	614	CLA	C7-C6-C5	-2.74	105.92	113.36
28	A	412	SQD	O5-C1-C2	-2.74	104.55	110.35
23	C	505	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
23	B	614	CLA	OBD-CAD-CBD	-2.74	121.98	125.89
23	B	606	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
25	k	102	BCR	C27-C26-C25	2.73	126.70	122.73
25	d	404	BCR	C38-C26-C25	-2.73	121.46	124.53
23	b	603	CLA	CMB-C2B-C3B	2.73	129.79	124.68
30	C	515	DGD	O2D-C2D-C1D	-2.73	103.41	110.05
23	b	609	CLA	CMA-C3A-C4A	-2.73	104.43	111.77
28	a	412	SQD	O8-S-C6	2.73	110.09	105.74
36	V	201	HEC	CMC-C2C-C1C	-2.73	124.27	128.46
23	b	607	CLA	C6-C5-C3	2.73	120.61	113.45
23	B	608	CLA	C1D-CHD-C4C	2.73	126.16	122.56
23	C	507	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
23	b	609	CLA	CHA-C1A-NA	-2.73	120.15	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	CHB-C4A-NA	2.73	128.28	124.51
23	a	411	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
29	D	407	LHG	O8-C23-O10	-2.72	116.72	123.59
26	d	405	PL9	C20-C19-C21	2.72	119.85	115.27
28	F	101	SQD	O9-S-O7	-2.72	104.53	113.95
26	A	410	PL9	C22-C23-C24	-2.72	121.11	127.66
30	C	515	DGD	O3G-C1D-C2D	-2.72	104.06	108.30
23	a	408	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
23	C	503	CLA	O2A-C1-C2	-2.72	101.50	108.64
25	x	101	BCR	C27-C26-C25	2.71	126.67	122.73
27	C	518	LMG	O1-C7-C8	-2.71	104.36	110.90
29	d	406	LHG	O8-C23-C24	2.71	120.41	111.91
23	D	401	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	T	101	BCR	C15-C16-C17	-2.71	117.93	123.47
23	B	612	CLA	CMD-C2D-C3D	2.71	129.74	124.68
23	A	404	CLA	CAA-CBA-CGA	-2.70	105.35	113.25
25	c	515	BCR	C27-C26-C25	2.70	126.66	122.73
28	B	624	SQD	C45-O47-C7	2.70	124.44	117.79
27	m	101	LMG	C9-C8-C7	-2.70	105.41	111.79
23	b	613	CLA	C1-C2-C3	-2.70	121.38	126.04
27	C	518	LMG	O1-C1-C2	-2.70	104.09	108.30
23	A	404	CLA	C7-C6-C5	-2.70	106.04	113.36
23	c	512	CLA	CMB-C2B-C3B	2.70	129.72	124.68
23	B	613	CLA	CMB-C2B-C1B	-2.69	124.32	128.46
23	b	606	CLA	OBD-CAD-CBD	-2.69	122.05	125.89
27	d	409	LMG	O6-C1-O1	-2.69	103.60	109.97
23	c	504	CLA	CMD-C2D-C3D	2.69	129.71	124.68
23	C	510	CLA	OBD-CAD-CBD	-2.69	122.05	125.89
23	a	411	CLA	C4D-C3D-CAD	-2.69	106.97	108.47
23	c	509	CLA	CHB-C4A-NA	2.69	128.23	124.51
28	f	101	SQD	C45-O47-C7	2.69	124.40	117.79
27	A	411	LMG	C40-C39-C38	-2.68	100.80	114.42
23	b	610	CLA	OBD-CAD-CBD	-2.68	122.06	125.89
23	b	604	CLA	OBD-CAD-CBD	-2.68	122.06	125.89
27	c	519	LMG	C40-C39-C38	-2.68	100.81	114.42
29	d	407	LHG	O7-C7-C8	-2.68	105.72	111.50
23	B	601	CLA	CAA-CBA-CGA	-2.68	105.42	113.25
23	c	509	CLA	OBD-CAD-CBD	-2.68	122.07	125.89
29	D	407	LHG	O8-C23-C24	2.68	120.31	111.91
23	c	501	CLA	CED-O2D-CGD	-2.68	109.88	115.94
28	b	601	SQD	O48-C23-C24	2.68	120.31	111.91
23	D	402	CLA	C3B-C4B-NB	-2.67	105.75	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C4D-C3D-CAD	-2.67	106.98	108.47
25	K	101	BCR	C27-C26-C25	2.67	126.61	122.73
23	C	510	CLA	CMD-C2D-C3D	2.67	129.67	124.68
23	C	512	CLA	C4A-NA-C1A	2.67	107.91	106.71
25	K	101	BCR	C15-C16-C17	-2.67	118.01	123.47
25	B	618	BCR	C27-C26-C25	2.67	126.60	122.73
30	C	517	DGD	C3G-C2G-C1G	-2.67	105.48	111.79
25	K	101	BCR	C23-C24-C25	-2.66	119.72	127.20
23	a	411	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	C	511	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	b	613	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
30	C	516	DGD	C1D-C2D-C3D	-2.66	104.47	110.00
23	B	611	CLA	C2C-C1C-NC	2.65	112.46	109.97
23	a	408	CLA	O2D-CGD-CBD	2.65	115.98	111.27
25	Z	101	BCR	C27-C26-C25	2.65	126.58	122.73
27	c	523	LMG	O1-C7-C8	-2.65	104.50	110.90
23	a	406	CLA	OBD-CAD-CBD	-2.65	122.11	125.89
30	c	516	DGD	CDB-CCB-CBB	-2.65	100.98	114.42
27	D	406	LMG	O8-C28-O10	-2.65	116.91	123.59
28	b	601	SQD	O9-S-C6	2.65	110.08	106.94
28	A	412	SQD	O48-C23-O10	-2.65	116.91	123.59
25	B	618	BCR	C40-C30-C25	2.65	114.59	110.30
30	c	516	DGD	C3D-C4D-C5D	-2.64	105.53	110.24
23	b	611	CLA	CHB-C4A-NA	2.64	128.16	124.51
26	D	405	PL9	C12-C13-C14	-2.64	121.30	127.66
30	a	414	DGD	O3G-C3G-C2G	-2.64	104.79	111.78
36	v	201	HEC	CBD-CAD-C3D	-2.64	107.62	112.49
23	b	612	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	c	508	CLA	CMB-C2B-C3B	2.64	129.61	124.68
30	c	517	DGD	C1D-C2D-C3D	-2.64	104.50	110.00
28	A	414	SQD	O47-C7-C8	2.63	117.18	111.50
28	a	412	SQD	O48-C23-C24	2.63	120.16	111.91
28	f	101	SQD	O5-C5-C4	2.63	114.47	109.69
27	d	409	LMG	O1-C7-C8	-2.63	104.56	110.90
24	d	401	PHO	CMC-C2C-C3C	2.63	133.25	126.12
23	b	613	CLA	C11-C12-C13	-2.63	107.43	115.92
23	B	602	CLA	CMB-C2B-C3B	2.63	129.59	124.68
23	b	611	CLA	CMB-C2B-C3B	2.63	129.59	124.68
23	B	602	CLA	C2A-C1A-CHA	2.62	128.45	123.86
23	c	506	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	b	604	CLA	CHB-C4A-NA	2.62	128.14	124.51
28	F	101	SQD	C1-C2-C3	-2.62	104.54	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	407	LHG	C18-C17-C16	-2.62	101.12	114.42
23	B	614	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
23	b	615	CLA	OBD-CAD-C3D	2.62	132.33	127.98
30	c	516	DGD	O3G-C1D-C2D	-2.62	104.21	108.30
23	B	601	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	c	505	CLA	O2A-CGA-O1A	-2.61	116.99	123.59
26	A	410	PL9	C35-C34-C36	2.61	119.67	115.27
23	C	504	CLA	CMB-C2B-C3B	2.61	129.57	124.68
23	b	609	CLA	C3B-C4B-NB	-2.61	105.83	109.21
23	c	505	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
23	B	602	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
23	c	506	CLA	CBC-CAC-C3C	-2.61	105.24	112.43
27	m	101	LMG	O1-C1-C2	-2.61	104.23	108.30
23	b	605	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
23	A	404	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
23	A	408	CLA	C2C-C1C-NC	2.60	112.41	109.97
27	D	406	LMG	O7-C10-O9	-2.60	117.42	123.70
27	m	101	LMG	O8-C28-O10	-2.59	117.05	123.59
23	C	511	CLA	C1D-CHD-C4C	2.59	125.98	122.56
25	t	101	BCR	C27-C26-C25	2.59	126.50	122.73
23	B	608	CLA	OBD-CAD-CBD	-2.59	122.19	125.89
24	d	401	PHO	C1B-NB-C4B	2.59	111.39	106.51
30	A	415	DGD	O3G-C1D-C2D	-2.59	104.27	108.30
23	b	609	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
29	d	407	LHG	C18-C17-C16	-2.58	101.31	114.42
30	c	518	DGD	C3D-C4D-C5D	-2.58	105.64	110.24
25	K	102	BCR	C2-C1-C6	2.58	114.45	110.48
25	c	514	BCR	C15-C16-C17	-2.58	118.19	123.47
25	c	515	BCR	C2-C1-C6	2.58	114.45	110.48
26	d	405	PL9	C7-C3-C2	-2.58	119.91	123.30
23	C	511	CLA	OBD-CAD-CBD	-2.57	122.22	125.89
29	B	622	LHG	O8-C23-O10	-2.57	117.10	123.59
23	C	513	CLA	O2D-CGD-CBD	2.57	115.84	111.27
30	H	102	DGD	C8B-C7B-C6B	-2.57	101.38	114.42
30	C	515	DGD	O3G-C3G-C2G	-2.57	104.70	110.90
23	B	611	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
24	A	406	PHO	C1-O2A-CGA	2.57	123.19	116.44
23	B	616	CLA	O2D-CGD-CBD	2.57	115.83	111.27
24	A	407	PHO	CBD-CHA-C1A	2.57	132.36	126.40
23	b	606	CLA	C16-C15-C13	-2.57	107.63	115.92
30	c	516	DGD	O5D-C6D-C5D	-2.56	104.31	109.05
23	B	613	CLA	OBD-CAD-C3D	2.56	132.24	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	d	402	CLA	C1-C2-C3	-2.56	121.62	126.04
27	A	411	LMG	C36-C35-C34	-2.56	101.44	114.42
29	D	407	LHG	C20-C19-C18	-2.55	101.46	114.42
26	D	405	PL9	C7-C8-C9	-2.55	122.55	126.79
23	C	507	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
23	B	609	CLA	CMD-C2D-C3D	2.55	129.45	124.68
25	B	617	BCR	C11-C10-C9	-2.55	123.67	127.31
25	b	620	BCR	C33-C5-C6	-2.55	121.67	124.53
25	K	101	BCR	C40-C30-C25	2.54	114.42	110.30
27	b	622	LMG	C8-O7-C10	2.54	124.05	117.79
25	d	404	BCR	C27-C26-C25	2.54	126.42	122.73
25	c	514	BCR	C7-C8-C9	-2.54	122.40	126.23
23	c	501	CLA	CMD-C2D-C3D	2.54	129.43	124.68
29	d	407	LHG	C20-C19-C18	-2.54	101.55	114.42
23	B	608	CLA	C6-C7-C8	-2.54	107.72	115.92
23	c	506	CLA	CMC-C2C-C1C	2.54	128.90	125.04
27	A	411	LMG	O6-C1-O1	-2.54	103.97	109.97
28	b	601	SQD	C44-O6-C1	2.53	118.69	113.74
27	m	101	LMG	O3-C3-C2	-2.53	104.49	110.35
23	c	505	CLA	O2D-CGD-CBD	2.53	115.77	111.27
27	D	409	LMG	O1-C7-C8	-2.53	105.06	111.78
30	A	415	DGD	C3E-C4E-C5E	-2.53	105.72	110.24
23	C	502	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
23	C	501	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
23	C	510	CLA	O2D-CGD-CBD	2.53	115.76	111.27
23	b	608	CLA	O1D-CGD-CBD	2.53	129.66	124.48
23	C	503	CLA	C6-C5-C3	2.53	120.09	113.45
23	c	512	CLA	O1D-CGD-CBD	2.53	129.65	124.48
25	a	409	BCR	C27-C26-C25	2.53	126.40	122.73
25	b	618	BCR	C15-C16-C17	-2.53	118.30	123.47
25	T	101	BCR	C30-C25-C26	-2.52	119.06	122.61
23	c	510	CLA	CMD-C2D-C3D	2.52	129.40	124.68
23	B	610	CLA	CMD-C2D-C3D	2.52	129.40	124.68
35	e	102	HEM	CMC-C2C-C3C	2.52	129.39	124.68
28	F	101	SQD	C46-C45-C44	-2.52	105.31	113.70
23	A	404	CLA	CAA-C2A-C1A	-2.52	103.72	111.97
23	c	505	CLA	OBD-CAD-C3D	2.52	132.16	127.98
23	b	607	CLA	C3C-C4C-NC	-2.52	107.75	110.57
23	B	616	CLA	C1-C2-C3	2.51	130.39	126.04
23	D	403	CLA	C4-C3-C5	2.51	119.50	115.27
23	C	510	CLA	C1D-CHD-C4C	2.51	125.88	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	622	LMG	O3-C3-C2	-2.51	104.54	110.35
23	C	508	CLA	O2D-CGD-CBD	2.51	115.73	111.27
35	E	101	HEM	CMD-C2D-C1D	-2.51	124.60	128.46
36	V	201	HEC	CBD-CAD-C3D	-2.51	107.85	112.49
27	M	101	LMG	O8-C28-O10	-2.51	117.25	123.59
23	a	406	CLA	CMA-C3A-C4A	-2.51	105.03	111.77
23	C	509	CLA	CED-O2D-CGD	2.51	121.61	115.94
26	d	405	PL9	C36-C34-C33	-2.51	116.04	121.12
23	B	612	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
23	d	403	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
26	a	410	PL9	C40-C39-C38	-2.50	117.27	123.68
25	k	101	BCR	C30-C25-C26	-2.50	119.10	122.61
23	d	402	CLA	C4-C3-C5	2.50	119.47	115.27
26	a	410	PL9	C27-C28-C29	-2.49	121.65	127.66
30	C	515	DGD	C4E-C3E-C2E	-2.49	106.47	110.82
23	B	604	CLA	C1D-CHD-C4C	2.49	125.85	122.56
23	c	511	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	h	101	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	D	405	PL9	C50-C49-C48	-2.49	115.46	122.65
23	B	611	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	a	406	CLA	CMD-C2D-C3D	2.49	129.33	124.68
23	b	615	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
30	c	517	DGD	C6B-C5B-C4B	-2.49	101.81	114.42
26	D	405	PL9	C31-C32-C33	-2.48	103.72	111.88
30	c	518	DGD	C4D-C3D-C2D	-2.48	106.49	110.82
23	C	501	CLA	OBD-CAD-CBD	-2.48	122.35	125.89
23	b	604	CLA	C6-C5-C3	2.48	119.96	113.45
23	d	402	CLA	C6-C5-C3	2.48	119.95	113.45
25	b	619	BCR	C35-C13-C14	-2.48	119.45	122.92
30	h	102	DGD	C1D-C2D-C3D	-2.48	104.83	110.00
23	B	616	CLA	CMB-C2B-C3B	2.48	129.31	124.68
23	B	605	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
23	C	506	CLA	CMD-C2D-C3D	2.48	129.31	124.68
23	b	609	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	b	605	CLA	C1-C2-C3	-2.47	121.77	126.04
25	D	404	BCR	C27-C26-C25	2.47	126.32	122.73
23	a	408	CLA	CAA-CBA-CGA	-2.47	106.04	113.25
23	b	607	CLA	O2D-CGD-CBD	2.47	115.65	111.27
23	B	604	CLA	O2A-C1-C2	2.47	115.11	108.64
23	b	614	CLA	CHA-C1A-NA	-2.46	120.75	126.40
23	h	101	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
35	E	101	HEM	CBA-CAA-C2A	-2.46	107.95	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	O1D-CGD-CBD	2.46	129.52	124.48
25	B	619	BCR	C15-C16-C17	-2.46	118.44	123.47
26	a	410	PL9	C37-C38-C39	-2.46	121.74	127.66
25	C	514	BCR	C2-C1-C6	2.46	114.26	110.48
25	B	618	BCR	C11-C10-C9	-2.46	123.80	127.31
25	a	409	BCR	C38-C26-C27	-2.46	108.90	113.62
23	b	605	CLA	CMD-C2D-C3D	2.46	129.28	124.68
23	D	401	CLA	O2D-CGD-CBD	2.46	115.63	111.27
25	T	101	BCR	C3-C4-C5	-2.46	109.69	114.08
29	d	408	LHG	C26-C25-C24	2.46	122.02	113.19
23	a	405	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	t	101	BCR	C36-C18-C17	-2.46	119.48	122.92
23	D	403	CLA	OBD-CAD-C3D	2.46	132.06	127.98
23	B	603	CLA	CMD-C2D-C3D	2.46	129.27	124.68
23	c	504	CLA	C1D-CHD-C4C	2.46	125.80	122.56
23	B	612	CLA	C4D-C3D-CAD	-2.45	107.10	108.47
30	c	516	DGD	O3E-C3E-C2E	-2.45	104.67	110.35
23	C	512	CLA	OBD-CAD-C3D	2.45	132.06	127.98
23	C	507	CLA	CMD-C2D-C3D	2.45	129.27	124.68
27	C	518	LMG	O6-C1-O1	-2.45	104.17	109.97
23	b	613	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
27	d	409	LMG	C3-C4-C5	-2.45	105.87	110.24
28	b	601	SQD	O9-S-O7	-2.45	105.48	113.95
25	D	404	BCR	C16-C15-C14	-2.45	118.46	123.47
23	a	408	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
25	T	101	BCR	C7-C8-C9	-2.44	122.54	126.23
23	B	603	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	b	605	CLA	OBD-CAD-CBD	-2.44	122.41	125.89
23	b	617	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	B	611	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	C	503	CLA	C2A-C1A-CHA	2.44	128.12	123.86
30	a	414	DGD	C1G-O1G-C1A	2.44	126.14	117.12
23	b	612	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
27	C	518	LMG	O8-C28-O10	-2.44	117.45	123.59
29	B	623	LHG	O3-P-O5	-2.43	99.55	109.07
23	c	509	CLA	O1D-CGD-CBD	2.43	129.47	124.48
27	c	523	LMG	O6-C1-O1	-2.43	104.21	109.97
23	c	505	CLA	C3B-C4B-NB	-2.43	106.06	109.21
24	d	401	PHO	CBD-CHA-C4D	-2.43	105.80	108.54
23	B	606	CLA	OBD-CAD-CBD	-2.43	122.42	125.89
30	A	415	DGD	CDB-CCB-CBB	-2.43	102.10	114.42
27	M	101	LMG	C40-C39-C38	-2.43	102.11	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	b	612	CLA	OBD-CAD-C3D	2.42	132.01	127.98
23	d	402	CLA	CMD-C2D-C3D	2.42	129.21	124.68
23	B	604	CLA	C6-C5-C3	-2.42	107.10	113.45
27	D	406	LMG	O2-C2-C1	-2.42	104.16	110.05
23	A	404	CLA	O1D-CGD-CBD	2.42	129.44	124.48
23	a	406	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	B	607	CLA	OBD-CAD-CBD	-2.42	122.44	125.89
23	A	408	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
36	v	201	HEC	CMB-C2B-C1B	-2.42	124.74	128.46
26	a	410	PL9	O2-C1-C2	-2.42	116.23	121.78
23	c	504	CLA	O1A-CGA-CBA	2.42	133.17	123.73
23	c	502	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	A	409	BCR	C24-C23-C22	-2.42	122.58	126.23
23	b	615	CLA	C4D-C3D-CAD	-2.41	107.12	108.47
36	V	201	HEC	CMD-C2D-C1D	-2.41	124.75	128.46
26	d	405	PL9	C8-C7-C3	2.41	118.80	111.98
23	B	605	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
26	A	410	PL9	C40-C39-C38	-2.41	117.49	123.68
23	b	607	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
23	c	507	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
23	D	401	CLA	O2D-CGD-O1D	-2.41	119.14	123.84
27	A	411	LMG	O3-C3-C2	-2.40	104.79	110.35
23	C	512	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
30	C	516	DGD	CCB-CBB-CAB	-2.40	102.22	114.42
24	a	407	PHO	C2C-C1C-NC	2.40	113.42	109.79
23	B	613	CLA	OBD-CAD-CBD	-2.40	122.46	125.89
23	C	508	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
23	A	408	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	d	403	CLA	CAC-C3C-C4C	2.40	127.92	124.81
27	d	409	LMG	O1-C1-C2	-2.40	104.56	108.30
28	B	624	SQD	O5-C5-C4	2.39	114.04	109.69
23	B	616	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
23	h	101	CLA	C1D-CHD-C4C	2.39	125.71	122.56
23	C	510	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	c	502	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	A	408	CLA	CHC-C1C-C2C	-2.39	120.11	126.72
23	b	604	CLA	C5-C3-C2	-2.39	116.28	121.12
25	H	101	BCR	C35-C13-C14	-2.39	119.58	122.92
23	a	406	CLA	CMB-C2B-C1B	-2.39	124.80	128.46
27	C	518	LMG	C3-C4-C5	-2.39	105.98	110.24
23	C	501	CLA	OBD-CAD-C3D	2.39	131.94	127.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	617	BCR	C30-C25-C26	-2.38	119.25	122.61
25	b	618	BCR	C29-C30-C25	2.38	114.15	110.48
23	b	607	CLA	C4-C3-C5	2.38	119.28	115.27
25	B	617	BCR	C35-C13-C14	-2.38	119.58	122.92
23	B	609	CLA	O2D-CGD-CBD	2.38	115.50	111.27
23	b	610	CLA	CHA-C1A-NA	-2.38	120.94	126.40
23	B	607	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
36	v	201	HEC	CMC-C2C-C1C	-2.38	124.80	128.46
27	M	101	LMG	C1-O6-C5	-2.38	109.01	113.69
30	c	516	DGD	C2G-O2G-C1B	2.38	123.65	117.79
25	a	409	BCR	C30-C25-C26	-2.38	119.26	122.61
24	A	407	PHO	C3C-C4C-NC	-2.38	106.59	110.28
23	b	607	CLA	C4D-C3D-CAD	-2.38	107.14	108.47
23	a	406	CLA	C1D-CHD-C4C	2.38	125.70	122.56
30	c	516	DGD	C1D-C2D-C3D	-2.38	105.04	110.00
23	B	607	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	B	617	BCR	C37-C22-C21	-2.38	119.59	122.92
25	C	514	BCR	C33-C5-C6	-2.38	121.86	124.53
23	C	504	CLA	C6-C5-C3	2.38	119.68	113.45
30	a	414	DGD	O2G-C2G-C1G	2.37	117.00	108.40
23	B	613	CLA	O2A-C1-C2	-2.37	102.39	108.64
23	a	411	CLA	O2D-CGD-CBD	2.37	115.49	111.27
23	b	606	CLA	CHD-C4C-NC	2.37	127.94	124.20
25	b	619	BCR	C8-C7-C6	-2.37	120.55	127.20
23	C	505	CLA	C1D-CHD-C4C	2.37	125.68	122.56
23	c	511	CLA	CHA-C1A-NA	-2.37	120.97	126.40
23	h	101	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
23	c	510	CLA	O1D-CGD-CBD	2.36	129.32	124.48
29	B	623	LHG	C18-C17-C16	-2.36	102.43	114.42
23	b	614	CLA	C1-C2-C3	-2.36	121.96	126.04
23	b	614	CLA	C2C-C1C-NC	2.36	112.18	109.97
30	c	517	DGD	O5D-C6D-C5D	-2.36	104.68	109.05
23	A	408	CLA	OBD-CAD-C3D	2.36	131.90	127.98
23	c	510	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
23	B	602	CLA	C1-C2-C3	-2.36	121.96	126.04
25	B	617	BCR	C2-C1-C6	2.36	114.11	110.48
25	b	620	BCR	C2-C1-C6	2.36	114.11	110.48
26	A	410	PL9	O2-C1-C6	2.36	124.67	120.59
28	a	412	SQD	O5-C5-C4	2.35	113.97	109.69
23	C	506	CLA	C4D-C3D-CAD	-2.35	107.16	108.47
23	B	613	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
23	c	503	CLA	C1B-CHB-C4A	-2.35	125.46	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	CLA	C4D-C3D-CAD	-2.35	107.16	108.47
28	A	412	SQD	O48-C46-C45	2.35	115.27	108.43
23	c	512	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
27	m	101	LMG	C1-O6-C5	-2.35	109.08	113.69
23	b	607	CLA	CMD-C2D-C3D	2.34	129.06	124.68
23	b	609	CLA	C4D-C3D-CAD	-2.34	107.16	108.47
25	Z	101	BCR	C2-C1-C6	2.34	114.09	110.48
25	A	409	BCR	C8-C7-C6	-2.34	120.62	127.20
25	A	409	BCR	C33-C5-C6	-2.34	121.90	124.53
23	D	403	CLA	O1D-CGD-CBD	2.34	129.28	124.48
23	A	404	CLA	CHD-C4C-C3C	-2.34	121.40	124.84
27	A	411	LMG	C1-O6-C5	-2.34	109.09	113.69
25	A	409	BCR	C27-C26-C25	2.34	126.13	122.73
26	D	405	PL9	C8-C7-C3	2.34	118.59	111.98
30	A	415	DGD	O6E-C1E-O5D	-2.34	104.44	109.97
23	b	611	CLA	CAA-CBA-CGA	-2.34	106.42	113.25
27	A	411	LMG	O7-C10-O9	-2.34	118.05	123.70
23	a	408	CLA	CGD-CBD-CAD	-2.34	103.17	110.73
26	d	405	PL9	C45-C44-C43	-2.34	117.69	123.68
23	b	606	CLA	C6-C7-C8	-2.33	108.38	115.92
26	d	405	PL9	C7-C8-C9	-2.33	122.91	126.79
23	b	616	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	B	605	CLA	CHB-C4A-NA	2.33	127.74	124.51
26	A	410	PL9	C36-C37-C38	-2.33	104.22	111.88
27	b	622	LMG	C1-C2-C3	-2.33	105.14	110.00
23	C	512	CLA	CAA-CBA-CGA	-2.33	106.46	113.25
23	C	512	CLA	C1D-CHD-C4C	2.33	125.63	122.56
23	c	513	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
29	D	408	LHG	C11-C10-C9	-2.32	102.62	114.42
25	b	618	BCR	C24-C23-C22	-2.32	122.72	126.23
30	H	102	DGD	CDB-CCB-CBB	-2.32	102.63	114.42
23	a	411	CLA	C1D-CHD-C4C	2.32	125.62	122.56
23	D	401	CLA	C16-C15-C13	-2.32	108.42	115.92
26	D	405	PL9	C42-C43-C44	-2.32	122.07	127.66
23	c	503	CLA	C7-C6-C5	-2.32	107.06	113.36
30	h	102	DGD	CAB-C9B-C8B	-2.32	102.64	114.42
23	b	608	CLA	C4-C3-C5	2.32	119.17	115.27
23	b	611	CLA	CMD-C2D-C3D	2.32	129.02	124.68
23	a	411	CLA	C1-O2A-CGA	2.32	122.53	116.44
23	b	611	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
23	b	610	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
25	Z	101	BCR	C38-C26-C25	-2.31	121.93	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	101	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
25	x	101	BCR	C35-C13-C14	-2.31	119.68	122.92
30	C	515	DGD	C7B-C6B-C5B	-2.31	102.70	114.42
28	A	412	SQD	O48-C23-C24	2.31	119.16	111.91
23	C	513	CLA	C6-C7-C8	-2.31	108.45	115.92
23	B	605	CLA	O1D-CGD-CBD	2.31	129.21	124.48
23	B	614	CLA	O1A-CGA-CBA	2.31	132.73	123.73
23	C	508	CLA	CHC-C1C-NC	2.30	127.70	124.20
30	h	102	DGD	C4E-C3E-C2E	-2.30	106.80	110.82
30	C	515	DGD	CBB-CAB-C9B	-2.30	102.73	114.42
23	d	403	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	b	606	CLA	C1-C2-C3	-2.30	122.06	126.04
30	H	102	DGD	C6D-C5D-C4D	2.30	116.90	112.09
23	c	506	CLA	CMD-C2D-C3D	2.30	128.98	124.68
23	b	609	CLA	CHD-C4C-C3C	-2.30	121.46	124.84
25	b	620	BCR	C38-C26-C25	-2.30	121.94	124.53
23	c	505	CLA	C6-C7-C8	-2.30	108.49	115.92
23	B	606	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
27	M	101	LMG	C38-C37-C36	-2.30	102.76	114.42
27	A	411	LMG	O1-C7-C8	-2.30	105.35	110.90
23	D	402	CLA	C4D-C3D-CAD	-2.30	107.19	108.47
23	a	408	CLA	C2A-C1A-CHA	2.30	127.87	123.86
23	b	612	CLA	C3C-C4C-NC	-2.29	108.00	110.57
23	C	503	CLA	CHA-C1A-NA	-2.29	121.14	126.40
30	h	102	DGD	C3E-C4E-C5E	-2.29	106.15	110.24
30	c	518	DGD	O3E-C3E-C2E	-2.29	105.05	110.35
23	C	509	CLA	C2A-C3A-C4A	2.29	105.57	101.87
23	b	613	CLA	CHB-C4A-NA	2.29	127.68	124.51
30	C	516	DGD	CDB-CCB-CBB	-2.29	102.80	114.42
23	C	505	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
23	b	613	CLA	C9-C8-C10	-2.29	103.02	111.29
23	b	611	CLA	OBD-CAD-C3D	2.28	131.77	127.98
26	d	405	PL9	C32-C33-C34	-2.28	122.16	127.66
23	B	614	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
25	a	409	BCR	C29-C30-C25	2.28	113.99	110.48
23	c	508	CLA	C1-C2-C3	-2.28	122.10	126.04
23	c	503	CLA	O1D-CGD-CBD	2.28	129.15	124.48
23	B	604	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	b	620	BCR	C36-C18-C17	-2.28	119.73	122.92
28	F	101	SQD	O48-C23-C24	2.28	119.06	111.91
26	D	405	PL9	C36-C34-C33	-2.28	116.51	121.12
28	A	412	SQD	O47-C45-C46	2.28	116.64	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	411	LMG	O8-C28-O10	-2.28	117.85	123.59
23	b	617	CLA	O1D-CGD-CBD	2.27	129.14	124.48
23	C	505	CLA	C4D-C3D-CAD	-2.27	107.20	108.47
30	H	102	DGD	O2D-C2D-C1D	-2.27	104.53	110.05
23	c	505	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
23	C	502	CLA	C6-C5-C3	-2.27	107.51	113.45
29	l	101	LHG	C5-O7-C7	-2.27	112.21	117.79
23	b	606	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
27	d	409	LMG	O7-C10-O9	-2.27	118.22	123.70
23	c	512	CLA	C4D-C3D-CAD	-2.27	107.21	108.47
23	C	502	CLA	C1D-CHD-C4C	2.27	125.55	122.56
30	a	414	DGD	C1G-C2G-C3G	-2.27	106.50	111.80
23	b	617	CLA	CMD-C2D-C3D	2.27	128.92	124.68
26	A	410	PL9	C27-C28-C29	-2.26	122.21	127.66
27	M	101	LMG	C8-O7-C10	2.26	123.36	117.79
23	c	502	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
29	D	407	LHG	C11-C10-C9	-2.26	102.94	114.42
30	c	517	DGD	CDB-CCB-CBB	-2.26	102.96	114.42
23	B	611	CLA	C1-C2-C3	-2.26	122.14	126.04
23	b	609	CLA	CAC-C3C-C2C	2.25	131.38	127.53
23	C	503	CLA	O1D-CGD-CBD	2.25	129.09	124.48
23	c	503	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	K	101	BCR	C8-C7-C6	-2.25	120.88	127.20
23	B	603	CLA	CHA-C1A-NA	-2.25	121.25	126.40
25	H	101	BCR	C16-C15-C14	-2.25	118.87	123.47
23	d	403	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
25	C	514	BCR	C7-C8-C9	-2.25	122.84	126.23
23	C	505	CLA	CMB-C2B-C3B	2.25	128.88	124.68
27	c	523	LMG	O2-C2-C1	-2.25	104.59	110.05
30	h	102	DGD	O6E-C5E-C6E	-2.24	100.85	106.44
25	a	409	BCR	C15-C14-C13	-2.24	124.11	127.31
23	b	605	CLA	CMB-C2B-C3B	2.24	128.87	124.68
27	m	101	LMG	C21-C20-C19	-2.24	103.04	114.42
23	b	610	CLA	CMB-C2B-C3B	2.24	128.87	124.68
26	a	410	PL9	C11-C12-C13	-2.24	104.52	111.88
35	e	102	HEM	C1D-C2D-C3D	2.24	108.56	107.00
25	a	409	BCR	C33-C5-C6	-2.24	122.01	124.53
23	C	507	CLA	CAC-C3C-C4C	-2.24	121.91	124.81
23	C	512	CLA	CMD-C2D-C3D	2.23	128.86	124.68
23	b	614	CLA	CMB-C2B-C3B	2.23	128.86	124.68
25	c	515	BCR	C1-C6-C5	-2.23	119.47	122.61
27	M	101	LMG	O1-C7-C8	-2.23	105.51	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	K	102	BCR	C27-C26-C25	2.23	125.97	122.73
23	D	402	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
30	c	516	DGD	O6E-C5E-C6E	-2.23	100.89	106.44
28	f	101	SQD	O48-C23-O10	-2.23	117.96	123.59
23	B	611	CLA	C11-C10-C8	-2.23	108.72	115.92
25	B	619	BCR	C2-C1-C6	2.23	113.91	110.48
28	B	624	SQD	O47-C7-O49	-2.23	118.32	123.70
27	c	523	LMG	O5-C6-C5	-2.23	103.65	111.29
28	A	412	SQD	C1-O5-C5	-2.23	109.32	113.69
23	C	512	CLA	C6-C5-C3	-2.23	107.62	113.45
29	d	407	LHG	O8-C6-C5	-2.23	101.95	108.43
29	B	622	LHG	C12-C11-C10	-2.23	103.13	114.42
23	B	603	CLA	CMB-C2B-C3B	2.22	128.84	124.68
25	B	618	BCR	C35-C13-C14	-2.22	119.81	122.92
26	a	410	PL9	C30-C29-C28	-2.22	117.98	123.68
30	c	518	DGD	C1D-C2D-C3D	-2.22	105.38	110.00
23	B	616	CLA	C4D-C3D-CAD	-2.22	107.23	108.47
23	b	608	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
23	B	601	CLA	C2A-C1A-CHA	2.22	127.73	123.86
23	C	501	CLA	CAC-C3C-C4C	2.22	127.69	124.81
30	C	517	DGD	O6E-C1E-O5D	-2.22	104.73	109.97
23	C	512	CLA	C11-C12-C13	-2.22	108.76	115.92
23	C	502	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
23	c	502	CLA	OBD-CAD-CBD	-2.22	122.73	125.89
27	c	521	LMG	O8-C28-O10	-2.21	118.00	123.59
29	d	406	LHG	O8-C23-O10	-2.21	118.01	123.59
30	C	516	DGD	O5D-C6D-C5D	-2.21	104.96	109.05
23	B	607	CLA	CMD-C2D-C3D	2.21	128.81	124.68
30	c	518	DGD	C7B-C6B-C5B	-2.21	103.21	114.42
23	a	405	CLA	CMB-C2B-C3B	2.21	128.81	124.68
27	M	101	LMG	O6-C1-O1	-2.21	104.75	109.97
27	b	622	LMG	O2-C2-C1	-2.21	104.69	110.05
30	c	518	DGD	O6E-C1E-O5D	-2.21	104.75	109.97
23	c	510	CLA	O2D-CGD-CBD	2.21	115.19	111.27
23	B	613	CLA	C16-C15-C13	-2.20	108.79	115.92
23	c	511	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
27	C	518	LMG	C9-C8-C7	-2.20	106.58	111.79
26	A	410	PL9	C30-C29-C28	-2.20	118.03	123.68
30	c	518	DGD	CDB-CCB-CBB	-2.20	103.25	114.42
27	m	101	LMG	C40-C39-C38	-2.20	103.25	114.42
23	C	506	CLA	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CHA-C1A-NA	-2.20	121.36	126.40
23	h	101	CLA	C3C-C4C-NC	-2.20	108.10	110.57
24	a	407	PHO	CAC-C3C-C4C	-2.20	122.82	125.22
23	B	606	CLA	C7-C6-C5	-2.20	107.39	113.36
30	H	102	DGD	O3E-C3E-C2E	-2.20	105.27	110.35
23	c	513	CLA	CMD-C2D-C3D	2.20	128.79	124.68
25	c	514	BCR	C33-C5-C6	-2.20	122.06	124.53
27	c	519	LMG	O2-C2-C1	-2.20	104.71	110.05
23	B	609	CLA	C1-O2A-CGA	2.20	122.21	116.44
23	b	614	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
23	B	616	CLA	CED-O2D-CGD	-2.20	110.97	115.94
23	B	612	CLA	CED-O2D-CGD	-2.19	110.97	115.94
23	B	603	CLA	O1D-CGD-CBD	2.19	128.97	124.48
23	B	608	CLA	CMB-C2B-C3B	2.19	128.78	124.68
23	C	510	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
23	B	616	CLA	CMD-C2D-C3D	2.19	128.78	124.68
28	a	413	SQD	O47-C45-C44	2.19	116.22	108.36
25	B	618	BCR	C8-C7-C6	-2.19	121.05	127.20
23	c	506	CLA	C6-C5-C3	-2.19	107.71	113.45
23	C	502	CLA	CMB-C2B-C3B	2.19	128.78	124.68
23	B	605	CLA	CAC-C3C-C4C	2.19	127.65	124.81
25	B	619	BCR	C15-C14-C13	-2.19	124.19	127.31
23	c	513	CLA	CAC-C3C-C4C	2.19	127.65	124.81
30	H	102	DGD	O2G-C1B-O1B	-2.19	118.42	123.70
29	d	406	LHG	C20-C19-C18	-2.19	103.33	114.42
35	E	101	HEM	C4C-C3C-C2C	2.19	108.42	106.90
23	B	607	CLA	C4D-C3D-CAD	-2.19	107.25	108.47
29	B	622	LHG	C20-C19-C18	-2.19	103.33	114.42
23	B	616	CLA	C4-C3-C2	-2.19	118.07	123.68
23	c	512	CLA	C1D-CHD-C4C	2.18	125.44	122.56
25	K	102	BCR	C8-C7-C6	-2.18	121.08	127.20
23	b	608	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	c	503	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
25	C	514	BCR	C35-C13-C14	-2.18	119.87	122.92
23	b	617	CLA	O2D-CGD-CBD	2.18	115.14	111.27
23	c	507	CLA	C4D-C3D-CAD	-2.18	107.26	108.47
27	m	101	LMG	O6-C1-O1	-2.18	104.82	109.97
23	b	615	CLA	C1D-CHD-C4C	2.17	125.43	122.56
23	b	603	CLA	CGD-CBD-CAD	-2.17	103.70	110.73
27	D	406	LMG	O1-C7-C8	-2.17	105.66	110.90
23	C	502	CLA	CAC-C3C-C4C	2.17	127.63	124.81
24	d	401	PHO	CHB-C4A-NA	2.17	128.67	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	CBA-CAA-C2A	-2.17	107.46	113.86
23	B	602	CLA	C1D-CHD-C4C	2.17	125.42	122.56
25	c	515	BCR	C30-C25-C26	-2.17	119.56	122.61
30	c	518	DGD	C7A-C6A-C5A	-2.17	103.42	114.42
23	B	609	CLA	CED-O2D-CGD	2.17	120.84	115.94
23	B	613	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
27	D	409	LMG	O7-C10-O9	-2.17	118.47	123.70
30	c	518	DGD	O5E-C6E-C5E	-2.17	103.86	111.29
23	B	607	CLA	C6-C5-C3	-2.17	107.78	113.45
23	B	609	CLA	CHA-C1A-NA	-2.16	121.44	126.40
23	A	408	CLA	C3D-CAD-CBD	-2.16	104.75	107.61
23	B	604	CLA	CAC-C3C-C4C	2.16	127.62	124.81
29	l	101	LHG	C27-C26-C25	-2.16	103.44	114.42
29	D	408	LHG	O8-C6-C5	-2.16	102.14	108.43
23	B	606	CLA	CMD-C2D-C3D	2.16	128.72	124.68
27	M	101	LMG	C6-C5-C4	-2.16	107.94	113.00
23	B	608	CLA	OBD-CAD-C3D	2.16	131.57	127.98
23	c	511	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
23	C	505	CLA	CAC-C3C-C4C	2.16	127.61	124.81
23	c	501	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	C	506	CLA	CHA-C1A-NA	-2.16	121.45	126.40
24	A	407	PHO	CHB-C4A-NA	2.16	128.65	124.94
23	b	606	CLA	CMB-C2B-C3B	2.16	128.71	124.68
23	B	609	CLA	OBD-CAD-C3D	2.16	131.56	127.98
23	b	612	CLA	C1-C2-C3	-2.16	122.31	126.04
23	B	608	CLA	O2A-C1-C2	-2.16	102.97	108.64
27	c	523	LMG	O3-C3-C2	-2.16	105.37	110.35
30	C	516	DGD	O3D-C3D-C4D	-2.15	105.37	110.35
23	b	604	CLA	O2A-C1-C2	-2.15	102.98	108.64
23	b	603	CLA	CHC-C1C-NC	2.15	127.47	124.20
27	c	521	LMG	C42-C41-C40	-2.15	103.50	114.42
23	d	402	CLA	CMB-C2B-C3B	2.15	128.70	124.68
25	x	101	BCR	C11-C10-C9	-2.15	124.24	127.31
23	b	609	CLA	C4C-C3C-C2C	-2.15	103.76	106.90
23	d	403	CLA	C1-C2-C3	-2.15	122.32	126.04
23	b	606	CLA	CMC-C2C-C1C	2.15	128.31	125.04
23	a	405	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
23	b	606	CLA	O1A-CGA-CBA	2.15	132.11	123.73
25	c	514	BCR	C15-C14-C13	-2.15	124.24	127.31
25	B	619	BCR	C27-C26-C25	2.15	125.85	122.73
23	B	614	CLA	CHA-C1A-NA	-2.15	121.48	126.40
26	d	405	PL9	C12-C13-C14	-2.15	122.49	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	PHO	CMA-C3A-C4A	-2.15	105.97	112.36
25	c	515	BCR	C4-C5-C6	2.15	125.85	122.73
25	H	101	BCR	C1-C6-C5	-2.15	119.59	122.61
25	B	618	BCR	C15-C16-C17	-2.15	119.08	123.47
25	d	404	BCR	C39-C30-C25	-2.15	106.82	110.30
23	c	508	CLA	O2D-CGD-CBD	2.14	115.08	111.27
27	c	521	LMG	C40-C39-C38	-2.14	103.54	114.42
23	D	402	CLA	CBA-CAA-C2A	-2.14	107.54	113.86
23	A	405	CLA	CED-O2D-CGD	-2.14	111.09	115.94
25	B	618	BCR	C30-C25-C26	-2.14	119.60	122.61
25	b	619	BCR	C15-C16-C17	-2.14	119.09	123.47
28	A	412	SQD	C3-C4-C5	2.14	114.05	110.24
23	b	614	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
23	b	609	CLA	C11-C10-C8	-2.14	109.01	115.92
23	A	408	CLA	CHA-C1A-NA	-2.14	121.51	126.40
24	d	401	PHO	C2B-C1B-NB	-2.14	106.57	109.79
26	D	405	PL9	C40-C39-C38	-2.13	118.21	123.68
30	h	102	DGD	C3G-C2G-C1G	-2.13	106.74	111.79
23	b	605	CLA	C3B-C4B-NB	-2.13	106.45	109.21
23	b	614	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	b	619	BCR	C27-C26-C25	2.13	125.82	122.73
27	c	519	LMG	O8-C28-O10	-2.13	118.22	123.59
30	h	102	DGD	C3D-C4D-C5D	-2.13	106.44	110.24
25	K	102	BCR	C15-C16-C17	-2.13	119.12	123.47
25	Z	101	BCR	C15-C16-C17	-2.13	119.12	123.47
23	B	613	CLA	CMB-C2B-C3B	2.13	128.65	124.68
23	C	513	CLA	O2A-C1-C2	-2.13	103.05	108.64
26	d	405	PL9	C11-C9-C8	-2.12	116.82	121.12
25	t	101	BCR	C2-C1-C6	2.12	113.75	110.48
25	k	101	BCR	C38-C26-C25	-2.12	122.15	124.53
23	B	611	CLA	CGD-CBD-CAD	-2.12	103.86	110.73
24	A	407	PHO	C1B-NB-C4B	2.12	110.50	106.51
23	B	612	CLA	C16-C15-C13	-2.12	109.07	115.92
25	k	102	BCR	C40-C30-C25	2.12	113.73	110.30
23	B	609	CLA	CMC-C2C-C1C	2.12	128.26	125.04
26	A	410	PL9	C11-C9-C8	-2.12	116.84	121.12
23	c	512	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
23	B	606	CLA	O2D-CGD-CBD	2.11	115.02	111.27
25	c	514	BCR	C38-C26-C25	-2.11	122.16	124.53
30	c	518	DGD	CBB-CAB-C9B	-2.11	103.71	114.42
30	C	517	DGD	O3D-C3D-C4D	-2.11	105.47	110.35
27	b	622	LMG	C24-C23-C22	-2.11	103.72	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C27-C26-C25	2.11	125.79	122.73
27	D	406	LMG	C3-C4-C5	-2.11	106.48	110.24
23	h	101	CLA	O2A-C1-C2	2.11	114.17	108.64
26	d	405	PL9	C41-C39-C38	-2.11	116.86	121.12
23	b	605	CLA	C4-C3-C5	2.10	118.81	115.27
23	C	511	CLA	O2A-C1-C2	-2.10	103.11	108.64
25	T	101	BCR	C40-C30-C25	2.10	113.71	110.30
23	h	101	CLA	C3A-C2A-C1A	-2.10	98.19	101.34
23	c	512	CLA	CHA-C1A-NA	-2.10	121.59	126.40
27	D	406	LMG	C9-C8-C7	-2.10	106.82	111.79
23	B	605	CLA	CHA-C1A-NA	-2.10	121.59	126.40
23	b	615	CLA	O2D-CGD-CBD	2.10	115.00	111.27
28	A	414	SQD	O48-C23-C24	2.10	118.49	111.91
25	t	101	BCR	C29-C30-C25	2.10	113.71	110.48
27	m	101	LMG	C6-C5-C4	-2.10	108.09	113.00
24	A	407	PHO	O1D-CGD-CBD	2.10	128.78	124.48
23	B	604	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
23	h	101	CLA	CMD-C2D-C3D	2.10	128.60	124.68
23	a	405	CLA	C4-C3-C5	2.09	118.79	115.27
30	c	518	DGD	O1G-C1A-C2A	-2.09	105.33	111.91
23	b	612	CLA	OBD-CAD-CBD	-2.09	122.90	125.89
30	a	414	DGD	C5B-C4B-C3B	-2.09	103.80	114.42
30	c	517	DGD	O2G-C1B-O1B	-2.09	118.65	123.70
23	A	404	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
23	b	613	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
23	B	606	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
27	c	523	LMG	C39-C38-C37	-2.09	103.81	114.42
30	C	516	DGD	CAB-C9B-C8B	-2.09	103.81	114.42
26	A	410	PL9	C42-C43-C44	-2.09	122.63	127.66
27	c	519	LMG	O6-C1-O1	-2.09	105.02	109.97
23	B	606	CLA	CHA-C1A-NA	-2.09	121.61	126.40
25	B	618	BCR	C2-C1-C6	2.09	113.70	110.48
25	b	620	BCR	C16-C15-C14	-2.09	119.20	123.47
26	d	405	PL9	O1-C4-C3	-2.09	118.42	120.72
30	C	515	DGD	C5B-C4B-C3B	-2.09	103.83	114.42
23	b	605	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
25	c	514	BCR	C24-C23-C22	-2.09	123.08	126.23
24	d	401	PHO	O2A-CGA-O1A	-2.08	118.33	123.59
23	c	501	CLA	CAC-C3C-C4C	2.08	127.51	124.81
30	c	516	DGD	O6D-C1D-O3G	-2.08	105.04	109.97
23	B	604	CLA	CHA-C1A-NA	-2.08	121.63	126.40
23	b	608	CLA	CHA-C1A-NA	-2.08	121.63	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	C6-C7-C8	-2.08	109.19	115.92
23	C	502	CLA	CHA-C1A-NA	-2.08	121.63	126.40
35	E	101	HEM	CMC-C2C-C3C	2.08	128.57	124.68
25	Z	101	BCR	C24-C23-C22	-2.08	123.09	126.23
30	C	516	DGD	C7B-C6B-C5B	-2.08	103.86	114.42
30	h	102	DGD	CDB-CCB-CBB	-2.08	103.87	114.42
29	B	623	LHG	C20-C19-C18	-2.08	103.87	114.42
23	C	511	CLA	O2D-CGD-CBD	2.08	114.96	111.27
23	c	506	CLA	CHA-C1A-NA	-2.08	121.64	126.40
25	x	101	BCR	C34-C9-C8	-2.08	114.81	118.08
25	a	409	BCR	C7-C8-C9	-2.07	123.10	126.23
23	c	505	CLA	CHC-C1C-NC	2.07	127.35	124.20
23	B	609	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
35	e	102	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
25	x	101	BCR	C38-C26-C25	-2.07	122.20	124.53
28	f	101	SQD	O7-S-C6	2.07	109.40	106.94
23	c	510	CLA	OBD-CAD-CBD	-2.07	122.94	125.89
23	C	512	CLA	C1-C2-C3	-2.07	122.46	126.04
30	C	517	DGD	C8B-C7B-C6B	-2.07	103.91	114.42
23	B	604	CLA	C11-C10-C8	-2.07	109.23	115.92
23	D	403	CLA	CMD-C2D-C3D	2.07	128.55	124.68
23	B	611	CLA	OBD-CAD-C3D	2.07	131.42	127.98
23	D	401	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	C	503	CLA	CMD-C2D-C3D	2.07	128.55	124.68
23	b	610	CLA	O1D-CGD-CBD	2.07	128.71	124.48
23	c	502	CLA	C1-C2-C3	-2.07	122.47	126.04
23	c	507	CLA	CHD-C4C-NC	2.07	127.46	124.20
25	c	515	BCR	C15-C14-C13	-2.07	124.36	127.31
29	D	407	LHG	C27-C26-C25	-2.07	103.94	114.42
25	B	617	BCR	C39-C30-C25	-2.07	106.95	110.30
28	a	413	SQD	O48-C23-C24	2.07	118.39	111.91
23	a	411	CLA	CAA-C2A-C3A	-2.06	107.12	112.78
25	b	620	BCR	C27-C26-C25	2.06	125.73	122.73
30	A	415	DGD	C3G-O3G-C1D	2.06	117.77	113.74
30	H	102	DGD	C3E-C4E-C5E	-2.06	106.56	110.24
27	C	518	LMG	O2-C2-C1	-2.06	105.04	110.05
27	d	409	LMG	C1-C2-C3	-2.06	105.70	110.00
23	C	507	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
23	c	501	CLA	CHA-C1A-NA	-2.06	121.68	126.40
25	b	618	BCR	C38-C26-C25	-2.06	122.21	124.53
25	K	101	BCR	C1-C6-C5	-2.06	119.71	122.61
23	B	603	CLA	O2D-CGD-CBD	2.06	114.93	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
27	b	622	LMG	C7-O1-C1	-2.06	109.72	113.74
23	C	507	CLA	O1D-CGD-CBD	2.06	128.70	124.48
23	a	408	CLA	CHA-C1A-NA	-2.06	121.69	126.40
25	d	404	BCR	C1-C6-C5	-2.06	119.72	122.61
27	C	518	LMG	C38-C37-C36	-2.06	103.98	114.42
27	m	101	LMG	O2-C2-C1	-2.06	105.05	110.05
23	B	610	CLA	C1-C2-C3	-2.06	122.49	126.04
36	v	201	HEC	CBA-CAA-C2A	-2.06	108.69	112.48
23	B	610	CLA	O1A-CGA-CBA	2.06	131.75	123.73
28	f	101	SQD	O8-S-C6	2.05	109.01	105.74
30	c	516	DGD	C4D-C3D-C2D	-2.05	107.24	110.82
29	e	101	LHG	C11-C10-C9	-2.05	104.00	114.42
29	l	101	LHG	O8-C23-C24	2.05	118.34	111.91
25	a	409	BCR	C2-C1-C6	2.05	113.64	110.48
25	c	514	BCR	C10-C11-C12	-2.05	116.82	123.22
23	b	610	CLA	C1D-CHD-C4C	2.05	125.26	122.56
27	c	521	LMG	O1-C1-C2	-2.05	105.11	108.30
23	B	604	CLA	C11-C12-C13	-2.05	109.30	115.92
24	a	407	PHO	CBD-CHA-C4D	-2.05	106.23	108.54
23	C	509	CLA	CMD-C2D-C3D	2.05	128.51	124.68
23	B	601	CLA	C1-C2-C3	-2.05	122.50	126.04
26	A	410	PL9	C20-C19-C21	2.05	118.71	115.27
23	b	616	CLA	C3D-CAD-CBD	-2.05	104.91	107.61
30	C	516	DGD	C1E-O6E-C5E	2.04	117.70	113.69
23	b	605	CLA	CHD-C4C-NC	2.04	127.42	124.20
23	c	506	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
25	t	101	BCR	C38-C26-C27	-2.04	109.69	113.62
29	l	101	LHG	O8-C6-C5	-2.04	102.49	108.43
28	F	101	SQD	C1-O5-C5	-2.04	109.68	113.69
28	b	601	SQD	C1-O5-C5	2.04	117.69	113.69
28	a	412	SQD	O5-C1-C2	-2.04	106.03	110.35
25	a	409	BCR	C35-C13-C12	2.04	121.29	118.08
23	b	606	CLA	OBD-CAD-C3D	2.04	131.37	127.98
24	d	401	PHO	CAC-C3C-C2C	2.04	131.01	127.53
23	d	403	CLA	CHA-C1A-NA	-2.04	121.73	126.40
23	c	501	CLA	C2C-C1C-NC	2.04	111.88	109.97
30	c	516	DGD	C4A-C3A-C2A	-2.04	105.87	113.19
25	c	514	BCR	C30-C25-C26	-2.04	119.75	122.61
23	c	504	CLA	C7-C6-C5	-2.04	107.83	113.36
23	b	610	CLA	CMD-C2D-C3D	2.04	128.49	124.68
23	d	403	CLA	C1D-CHD-C4C	2.04	125.24	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	518	DGD	C9B-C8B-C7B	-2.03	104.10	114.42
30	A	415	DGD	O5D-C6D-C5D	-2.03	105.28	109.05
35	E	101	HEM	C3C-C4C-NC	-2.03	107.11	110.94
23	C	504	CLA	O2D-CGD-CBD	2.03	114.88	111.27
23	c	511	CLA	CHB-C4A-NA	2.03	127.32	124.51
26	a	410	PL9	C26-C24-C23	-2.03	117.01	121.12
23	B	608	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
28	F	101	SQD	C3-C4-C5	2.03	113.86	110.24
23	b	617	CLA	C4-C3-C5	2.03	118.69	115.27
23	c	505	CLA	CHB-C4A-NA	2.03	127.32	124.51
29	d	408	LHG	C25-C24-C23	2.03	121.00	113.62
23	B	615	CLA	C1C-C2C-C3C	-2.03	104.83	106.96
23	a	405	CLA	CMC-C2C-C1C	2.03	128.12	125.04
30	h	102	DGD	CCB-CBB-CAB	-2.03	104.14	114.42
25	k	102	BCR	C33-C5-C6	-2.03	122.25	124.53
27	b	623	LMG	C37-C36-C35	-2.02	104.15	114.42
25	b	620	BCR	C15-C16-C17	-2.02	119.33	123.47
23	b	607	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
30	C	516	DGD	O2D-C2D-C1D	-2.02	105.13	110.05
23	C	504	CLA	CMD-C2D-C3D	2.02	128.46	124.68
25	K	101	BCR	C23-C22-C21	-2.02	115.84	118.94
25	b	618	BCR	C15-C14-C13	-2.02	124.42	127.31
23	C	511	CLA	OBD-CAD-C3D	2.02	131.34	127.98
23	B	613	CLA	CHB-C4A-NA	2.02	127.31	124.51
25	c	514	BCR	C2-C1-C6	2.02	113.59	110.48
25	k	101	BCR	C1-C6-C5	-2.02	119.77	122.61
23	C	504	CLA	CHD-C4C-NC	2.02	127.39	124.20
24	A	406	PHO	C5-C3-C2	2.02	125.20	121.12
29	B	622	LHG	C25-C24-C23	2.02	120.96	113.62
23	B	601	CLA	C1D-CHD-C4C	2.02	125.22	122.56
24	A	407	PHO	C3A-C2A-C1A	2.02	104.05	101.64
27	D	409	LMG	C38-C37-C36	-2.01	104.20	114.42
25	d	404	BCR	C8-C7-C6	-2.01	121.55	127.20
23	B	603	CLA	CHD-C4C-C3C	-2.01	121.88	124.84
24	d	401	PHO	C1-C2-C3	-2.01	122.56	126.04
25	c	514	BCR	C3-C4-C5	-2.01	110.49	114.08
23	c	511	CLA	OBD-CAD-C3D	2.01	131.32	127.98
23	c	513	CLA	C1-C2-C3	-2.01	122.57	126.04
23	C	508	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
36	V	201	HEC	C4B-C3B-C2B	2.01	108.52	106.35
25	c	515	BCR	C34-C9-C10	-2.01	120.11	122.92
23	b	606	CLA	CBC-CAC-C3C	-2.01	106.90	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	C1C-C2C-C3C	-2.01	104.85	106.96
27	c	519	LMG	C9-C8-C7	-2.00	107.05	111.79
25	B	619	BCR	C11-C10-C9	-2.00	124.45	127.31
23	C	503	CLA	CMB-C2B-C1B	-2.00	125.38	128.46
25	D	404	BCR	C24-C23-C22	-2.00	123.21	126.23
23	C	511	CLA	CMD-C2D-C3D	2.00	128.43	124.68
27	c	519	LMG	O7-C10-O9	-2.00	118.98	122.96
23	C	506	CLA	C1D-CHD-C4C	2.00	125.20	122.56
25	C	514	BCR	C36-C18-C17	-2.00	120.12	122.92
23	C	508	CLA	OBD-CAD-C3D	2.00	131.30	127.98
30	H	102	DGD	CAB-C9B-C8B	-2.00	104.27	114.42

All (183) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404	CLA	ND
23	A	404	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	ND
23	A	408	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	607	CLA	NA
23	B	608	CLA	NA
23	B	609	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	NA
23	B	612	CLA	ND
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	NA
23	B	616	CLA	ND
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND

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Mol	Chain	Res	Type	Atom
23	C	507	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	D	401	CLA	NA
23	D	402	CLA	NA
23	D	403	CLA	NC
23	D	403	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	NA
23	a	408	CLA	NC
23	a	408	CLA	ND
23	a	408	CLA	NA
23	a	411	CLA	NA
23	a	411	CLA	ND
23	b	603	CLA	NC
23	b	603	CLA	ND
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	606	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	b	609	CLA	ND
23	b	609	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	NA
23	b	614	CLA	ND
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	NA
23	b	617	CLA	ND
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	c	502	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	c	505	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	505	CLA	NA
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	509	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	d	402	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	h	101	CLA	NA
23	h	101	CLA	ND

All (1694) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	614	CLA	CBD-CGD-O2D-CED
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	508	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	512	CLA	O2A-C1-C2-C3
23	D	401	CLA	CHA-CBD-CGD-O1D
23	D	401	CLA	CHA-CBD-CGD-O2D
23	D	403	CLA	C2-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
23	b	603	CLA	CHA-CBD-CGD-O1D
23	b	603	CLA	CHA-CBD-CGD-O2D
23	b	604	CLA	C2-C3-C5-C6
23	b	604	CLA	C4-C3-C5-C6
23	b	606	CLA	C2-C3-C5-C6
23	b	606	CLA	C4-C3-C5-C6
23	b	607	CLA	CHA-CBD-CGD-O1D
23	b	608	CLA	C2-C3-C5-C6
23	b	608	CLA	C4-C3-C5-C6
23	b	615	CLA	CHA-CBD-CGD-O1D
23	b	615	CLA	CHA-CBD-CGD-O2D
23	b	615	CLA	CAD-CBD-CGD-O1D
23	b	615	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	C2-C3-C5-C6
23	c	507	CLA	C4-C3-C5-C6
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	C11-C12-C13-C14
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	CBD-CGD-O2D-CED
25	A	409	BCR	C35-C13-C14-C15
25	A	409	BCR	C16-C17-C18-C36
25	A	409	BCR	C36-C18-C19-C20
25	B	617	BCR	C35-C13-C14-C15
25	B	617	BCR	C16-C17-C18-C19
25	B	617	BCR	C20-C21-C22-C37
25	B	618	BCR	C11-C12-C13-C35
25	B	619	BCR	C16-C17-C18-C19
25	D	404	BCR	C22-C23-C24-C25
25	H	101	BCR	C16-C17-C18-C36
25	K	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C37-C22-C23-C24
25	K	102	BCR	C7-C8-C9-C34
25	K	102	BCR	C37-C22-C23-C24
25	K	102	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
25	T	101	BCR	C7-C8-C9-C10
25	T	101	BCR	C7-C8-C9-C34
25	Z	101	BCR	C10-C11-C12-C13
25	Z	101	BCR	C16-C17-C18-C19
25	Z	101	BCR	C16-C17-C18-C36
25	a	409	BCR	C21-C22-C23-C24
25	b	618	BCR	C1-C6-C7-C8
25	b	620	BCR	C36-C18-C19-C20
25	b	620	BCR	C37-C22-C23-C24
25	c	514	BCR	C1-C6-C7-C8
25	c	514	BCR	C7-C8-C9-C10
25	c	514	BCR	C7-C8-C9-C34
25	c	514	BCR	C11-C12-C13-C14
25	c	514	BCR	C36-C18-C19-C20
25	c	514	BCR	C20-C21-C22-C37
25	c	515	BCR	C7-C8-C9-C34
25	c	515	BCR	C36-C18-C19-C20
25	c	515	BCR	C20-C21-C22-C37
25	d	404	BCR	C11-C12-C13-C35
25	d	404	BCR	C21-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C34
25	k	101	BCR	C21-C22-C23-C24
25	k	101	BCR	C37-C22-C23-C24
25	k	101	BCR	C23-C24-C25-C30
25	k	102	BCR	C7-C8-C9-C10
25	x	101	BCR	C11-C12-C13-C14
25	x	101	BCR	C11-C12-C13-C35
26	A	410	PL9	C9-C11-C12-C13
26	A	410	PL9	C13-C14-C16-C17
26	A	410	PL9	C18-C19-C21-C22
26	A	410	PL9	C20-C19-C21-C22
26	A	410	PL9	C32-C33-C34-C35
26	A	410	PL9	C35-C34-C36-C37
26	A	410	PL9	C37-C38-C39-C40
26	A	410	PL9	C37-C38-C39-C41
26	A	410	PL9	C38-C39-C41-C42
26	D	405	PL9	C22-C23-C24-C25
26	D	405	PL9	C32-C33-C34-C36
26	a	410	PL9	C17-C18-C19-C20
26	a	410	PL9	C22-C23-C24-C25
26	a	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	a	410	PL9	C27-C28-C29-C31
26	a	410	PL9	C30-C29-C31-C32
26	a	410	PL9	C32-C33-C34-C35
26	a	410	PL9	C33-C34-C36-C37
26	d	405	PL9	C32-C33-C34-C36
26	d	405	PL9	C37-C38-C39-C40
26	d	405	PL9	C38-C39-C41-C42
27	A	411	LMG	O6-C1-O1-C7
27	A	411	LMG	O9-C10-O7-C8
27	B	621	LMG	C28-C29-C30-C31
27	C	518	LMG	C11-C10-O7-C8
27	D	409	LMG	O9-C10-O7-C8
27	D	409	LMG	C11-C10-O7-C8
27	b	622	LMG	C2-C1-O1-C7
27	b	622	LMG	O6-C1-O1-C7
27	b	622	LMG	C11-C10-O7-C8
27	c	523	LMG	O6-C1-O1-C7
28	A	412	SQD	O6-C44-C45-O47
28	B	624	SQD	O5-C1-O6-C44
28	B	624	SQD	O6-C44-C45-O47
28	B	624	SQD	O49-C7-O47-C45
28	B	624	SQD	C8-C7-O47-C45
28	F	101	SQD	C45-C44-O6-C1
28	a	413	SQD	O6-C44-C45-O47
28	f	101	SQD	O5-C1-O6-C44
29	A	413	LHG	C4-O6-P-O3
29	A	413	LHG	O10-C23-O8-C6
29	A	413	LHG	C24-C23-O8-C6
29	B	622	LHG	C3-O3-P-O4
29	B	622	LHG	C4-O6-P-O4
29	B	622	LHG	C4-O6-P-O5
29	B	623	LHG	O1-C1-C2-C3
29	B	623	LHG	C3-O3-P-O4
29	D	407	LHG	O1-C1-C2-O2
29	D	407	LHG	O1-C1-C2-C3
29	D	407	LHG	C3-O3-P-O4
29	D	407	LHG	C3-O3-P-O6
29	D	407	LHG	C4-O6-P-O4
29	d	406	LHG	O1-C1-C2-C3
29	d	406	LHG	C3-O3-P-O4
29	d	407	LHG	C4-O6-P-O4
29	d	407	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	C3-O3-P-O4
29	e	101	LHG	C3-O3-P-O5
29	e	101	LHG	C3-O3-P-O6
29	e	101	LHG	O6-C4-C5-O7
29	e	101	LHG	O10-C23-O8-C6
29	e	101	LHG	C24-C23-O8-C6
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
30	a	414	DGD	O1G-C1G-C2G-O2G
23	b	617	CLA	O1D-CGD-O2D-CED
23	h	101	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	O1D-CGD-O2D-CED
23	b	617	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	h	101	CLA	CBD-CGD-O2D-CED
27	c	523	LMG	O10-C28-O8-C9
30	a	414	DGD	O1A-C1A-O1G-C1G
23	B	614	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	O1D-CGD-O2D-CED
23	d	402	CLA	C3-C5-C6-C7
26	d	405	PL9	C47-C48-C49-C51
23	B	601	CLA	CBD-CGD-O2D-CED
23	B	607	CLA	CBD-CGD-O2D-CED
23	b	608	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
24	d	401	PHO	CBD-CGD-O2D-CED
27	M	101	LMG	O10-C28-O8-C9
28	b	601	SQD	O10-C23-O48-C46
23	c	510	CLA	O1D-CGD-O2D-CED
27	C	518	LMG	O9-C10-O7-C8
27	b	622	LMG	O9-C10-O7-C8
28	a	413	SQD	O49-C7-O47-C45
23	C	512	CLA	C3-C5-C6-C7
23	b	615	CLA	C3-C5-C6-C7
27	c	519	LMG	C29-C28-O8-C9
27	c	523	LMG	C29-C28-O8-C9
28	a	413	SQD	C24-C23-O48-C46
28	b	601	SQD	C24-C23-O48-C46
30	a	414	DGD	C2A-C1A-O1G-C1G
23	b	613	CLA	C13-C15-C16-C17
27	A	411	LMG	C11-C10-O7-C8
28	a	413	SQD	C8-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
26	d	405	PL9	C47-C48-C49-C50
27	A	411	LMG	O6-C5-C6-O5
23	B	614	CLA	C4-C3-C5-C6
26	a	410	PL9	C28-C29-C31-C32
23	B	606	CLA	C2A-CAA-CBA-CGA
30	h	102	DGD	O6E-C5E-C6E-O5E
26	A	410	PL9	C22-C23-C24-C25
26	d	405	PL9	C32-C33-C34-C35
26	A	410	PL9	C12-C13-C14-C16
26	A	410	PL9	C22-C23-C24-C26
26	a	410	PL9	C32-C33-C34-C36
26	d	405	PL9	C42-C43-C44-C46
27	c	521	LMG	O10-C28-O8-C9
28	F	101	SQD	O10-C23-O48-C46
28	a	413	SQD	O10-C23-O48-C46
23	c	509	CLA	C13-C15-C16-C17
23	C	501	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CBD-CGD-O2D-CED
23	b	604	CLA	CBD-CGD-O2D-CED
29	d	406	LHG	O2-C2-C3-O3
23	b	603	CLA	C3-C5-C6-C7
23	B	601	CLA	CBA-CGA-O2A-C1
27	M	101	LMG	C29-C28-O8-C9
28	f	101	SQD	C24-C23-O48-C46
29	A	413	LHG	C28-C29-C30-C31
29	A	413	LHG	C8-C7-O7-C5
23	c	501	CLA	CBD-CGD-O2D-CED
27	A	411	LMG	C28-C29-C30-C31
29	D	407	LHG	C28-C29-C30-C31
23	b	605	CLA	C3-C5-C6-C7
26	D	405	PL9	C47-C48-C49-C51
23	B	604	CLA	C13-C15-C16-C17
26	A	410	PL9	C40-C39-C41-C42
27	A	411	LMG	C4-C5-C6-O5
26	A	410	PL9	C33-C34-C36-C37
23	c	512	CLA	C2A-CAA-CBA-CGA
23	B	601	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	O1A-C1A-O1G-C1G
26	A	410	PL9	C34-C36-C37-C38
26	a	410	PL9	C19-C21-C22-C23
26	a	410	PL9	C34-C36-C37-C38
26	d	405	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
30	h	102	DGD	C4E-C5E-C6E-O5E
23	c	511	CLA	O1D-CGD-O2D-CED
23	B	601	CLA	O1D-CGD-O2D-CED
24	d	401	PHO	O1D-CGD-O2D-CED
29	d	406	LHG	C1-C2-C3-O3
23	b	613	CLA	C3-C5-C6-C7
23	B	607	CLA	O1D-CGD-O2D-CED
23	B	614	CLA	CBA-CGA-O2A-C1
23	a	408	CLA	CBA-CGA-O2A-C1
27	C	518	LMG	C29-C28-O8-C9
27	c	521	LMG	C29-C28-O8-C9
28	F	101	SQD	C24-C23-O48-C46
29	A	413	LHG	C26-C27-C28-C29
23	c	510	CLA	C8-C10-C11-C12
27	M	101	LMG	O6-C5-C6-O5
27	A	411	LMG	O10-C28-O8-C9
23	A	404	CLA	C15-C16-C17-C18
23	C	505	CLA	C5-C6-C7-C8
23	c	512	CLA	C13-C15-C16-C17
29	D	407	LHG	O2-C2-C3-O3
29	d	406	LHG	C7-C8-C9-C10
27	c	523	LMG	C2-C1-O1-C7
28	B	624	SQD	C2-C1-O6-C44
28	f	101	SQD	C2-C1-O6-C44
28	a	412	SQD	O6-C44-C45-O47
30	A	415	DGD	O2G-C2G-C3G-O3G
26	A	410	PL9	C15-C14-C16-C17
26	a	410	PL9	C35-C34-C36-C37
23	B	614	CLA	C2-C3-C5-C6
26	A	410	PL9	C23-C24-C26-C27
23	B	610	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	C	502	CLA	C6-C7-C8-C9
23	C	507	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C12-C13-C14
23	a	411	CLA	C14-C13-C15-C16
23	b	607	CLA	C6-C7-C8-C9
23	b	611	CLA	C14-C13-C15-C16
23	b	617	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C12-C13-C14
23	c	511	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	h	101	CLA	C11-C10-C8-C9
24	A	406	PHO	C14-C13-C15-C16
23	b	607	CLA	C2A-CAA-CBA-CGA
23	h	101	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C36-C18-C19-C20
25	Z	101	BCR	C7-C8-C9-C34
25	Z	101	BCR	C37-C22-C23-C24
25	c	514	BCR	C11-C12-C13-C35
25	d	404	BCR	C37-C22-C23-C24
25	A	409	BCR	C17-C18-C19-C20
29	B	622	LHG	C29-C30-C31-C32
27	c	523	LMG	C28-C29-C30-C31
30	a	414	DGD	C1B-C2B-C3B-C4B
30	c	518	DGD	O1A-C1A-O1G-C1G
23	B	614	CLA	C8-C10-C11-C12
23	C	513	CLA	C13-C15-C16-C17
27	c	519	LMG	O6-C5-C6-O5
27	c	523	LMG	C4-C5-C6-O5
23	B	606	CLA	C15-C16-C17-C18
23	B	611	CLA	C8-C10-C11-C12
23	B	614	CLA	C13-C15-C16-C17
23	C	505	CLA	C8-C10-C11-C12
23	b	608	CLA	C10-C11-C12-C13
23	b	609	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	c	506	CLA	C5-C6-C7-C8
23	c	508	CLA	C13-C15-C16-C17
23	c	513	CLA	C8-C10-C11-C12
23	d	403	CLA	C8-C10-C11-C12
27	d	409	LMG	C28-C29-C30-C31
29	d	406	LHG	C23-C24-C25-C26
23	b	608	CLA	O1D-CGD-O2D-CED
23	a	408	CLA	O1A-CGA-O2A-C1
23	B	611	CLA	C13-C15-C16-C17
23	B	612	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
23	b	617	CLA	C10-C11-C12-C13
23	c	504	CLA	C5-C6-C7-C8
23	h	101	CLA	C8-C10-C11-C12
29	B	623	LHG	O1-C1-C2-O2
26	D	405	PL9	C32-C33-C34-C35
27	D	409	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C10-C11-C12-C13
28	A	412	SQD	C7-C8-C9-C10
29	B	623	LHG	C7-C8-C9-C10
23	B	607	CLA	C8-C10-C11-C12
23	C	509	CLA	C13-C15-C16-C17
23	a	411	CLA	C15-C16-C17-C18
23	b	612	CLA	C8-C10-C11-C12
23	b	612	CLA	C13-C15-C16-C17
23	c	512	CLA	C5-C6-C7-C8
23	d	403	CLA	C5-C6-C7-C8
28	a	412	SQD	C24-C23-O48-C46
23	b	617	CLA	C2-C1-O2A-CGA
23	B	605	CLA	C5-C6-C7-C8
23	B	606	CLA	C8-C10-C11-C12
23	a	408	CLA	C13-C15-C16-C17
23	b	608	CLA	C5-C6-C7-C8
27	c	519	LMG	O10-C28-O8-C9
27	b	622	LMG	C10-C11-C12-C13
30	c	517	DGD	C1B-C2B-C3B-C4B
23	b	613	CLA	CBD-CGD-O2D-CED
23	b	610	CLA	C15-C16-C17-C18
23	b	606	CLA	C11-C10-C8-C7
23	b	617	CLA	C11-C10-C8-C7
23	B	607	CLA	C13-C15-C16-C17
23	C	506	CLA	C15-C16-C17-C18
23	c	510	CLA	C15-C16-C17-C18
26	A	410	PL9	C44-C46-C47-C48
26	a	410	PL9	C44-C46-C47-C48
26	d	405	PL9	C44-C46-C47-C48
25	K	102	BCR	C18-C19-C20-C21
25	b	619	BCR	C10-C11-C12-C13
25	d	404	BCR	C18-C19-C20-C21
25	k	101	BCR	C18-C19-C20-C21
25	x	101	BCR	C18-C19-C20-C21
29	A	413	LHG	O2-C2-C3-O3
30	a	414	DGD	O1B-C1B-O2G-C2G
23	C	502	CLA	C3-C5-C6-C7
23	B	612	CLA	C10-C11-C12-C13
23	B	613	CLA	C8-C10-C11-C12
23	C	504	CLA	C8-C10-C11-C12
23	D	403	CLA	C5-C6-C7-C8
23	b	612	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	B	614	CLA	O1A-CGA-O2A-C1
23	C	508	CLA	C13-C15-C16-C17
23	a	408	CLA	C10-C11-C12-C13
23	b	607	CLA	C15-C16-C17-C18
23	c	503	CLA	C8-C10-C11-C12
23	h	101	CLA	C15-C16-C17-C18
23	B	603	CLA	C5-C6-C7-C8
23	b	604	CLA	C8-C10-C11-C12
23	b	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C13-C15-C16-C17
29	B	622	LHG	C4-O6-P-O3
29	D	408	LHG	C3-O3-P-O6
29	d	407	LHG	C4-O6-P-O3
23	c	512	CLA	CBA-CGA-O2A-C1
30	A	415	DGD	C2A-C1A-O1G-C1G
23	c	505	CLA	CBD-CGD-O2D-CED
23	B	605	CLA	C15-C16-C17-C18
27	M	101	LMG	C4-C5-C6-O5
29	D	408	LHG	C7-C8-C9-C10
23	C	506	CLA	C4-C3-C5-C6
26	A	410	PL9	C25-C24-C26-C27
23	B	607	CLA	C5-C6-C7-C8
23	C	509	CLA	C10-C11-C12-C13
23	B	616	CLA	CBD-CGD-O2D-CED
23	A	405	CLA	C16-C17-C18-C20
27	b	622	LMG	O6-C5-C6-O5
30	C	517	DGD	C2A-C1A-O1G-C1G
29	e	101	LHG	C23-C24-C25-C26
30	C	515	DGD	C1B-C2B-C3B-C4B
27	c	521	LMG	C36-C37-C38-C39
27	d	409	LMG	C30-C31-C32-C33
25	B	617	BCR	C11-C10-C9-C34
25	B	617	BCR	C16-C17-C18-C36
25	B	618	BCR	C11-C10-C9-C34
25	B	619	BCR	C35-C13-C14-C15
25	B	619	BCR	C16-C17-C18-C36
25	K	101	BCR	C20-C21-C22-C37
25	K	102	BCR	C20-C21-C22-C37
25	Z	101	BCR	C11-C10-C9-C34
25	Z	101	BCR	C35-C13-C14-C15
25	a	409	BCR	C35-C13-C14-C15
25	a	409	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
25	a	409	BCR	C20-C21-C22-C37
25	c	515	BCR	C11-C10-C9-C34
25	c	515	BCR	C35-C13-C14-C15
25	d	404	BCR	C16-C17-C18-C36
25	d	404	BCR	C20-C21-C22-C37
25	k	101	BCR	C16-C17-C18-C36
25	x	101	BCR	C20-C21-C22-C37
30	C	515	DGD	O6D-C5D-C6D-O5D
27	B	621	LMG	C29-C30-C31-C32
27	D	406	LMG	C11-C12-C13-C14
27	D	406	LMG	C14-C15-C16-C17
27	c	523	LMG	C32-C33-C34-C35
27	c	523	LMG	C34-C35-C36-C37
28	A	414	SQD	C28-C29-C30-C31
28	a	412	SQD	C18-C19-C20-C21
28	a	412	SQD	C26-C27-C28-C29
28	b	601	SQD	C18-C19-C20-C21
29	A	413	LHG	C32-C33-C34-C35
29	d	407	LHG	C11-C12-C13-C14
28	f	101	SQD	O10-C23-O48-C46
23	C	509	CLA	C16-C17-C18-C19
23	c	507	CLA	C16-C17-C18-C20
27	M	101	LMG	C39-C40-C41-C42
27	d	409	LMG	C34-C35-C36-C37
28	a	412	SQD	C10-C11-C12-C13
28	b	601	SQD	C16-C17-C18-C19
29	A	413	LHG	C33-C34-C35-C36
29	d	406	LHG	C16-C17-C18-C19
29	d	408	LHG	C26-C27-C28-C29
30	C	516	DGD	C6A-C7A-C8A-C9A
30	C	516	DGD	C8B-C9B-CAB-CBB
23	c	511	CLA	C15-C16-C17-C18
28	A	412	SQD	C23-C24-C25-C26
29	d	407	LHG	C23-C24-C25-C26
27	B	621	LMG	C36-C37-C38-C39
27	D	406	LMG	C18-C19-C20-C21
28	A	414	SQD	C14-C15-C16-C17
28	a	412	SQD	C15-C16-C17-C18
28	a	413	SQD	C15-C16-C17-C18
29	B	622	LHG	C14-C15-C16-C17
30	C	517	DGD	CCA-CDA-CEA-CFA
28	A	412	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	B	624	SQD	C11-C10-C9-C8
29	B	622	LHG	C27-C28-C29-C30
29	e	101	LHG	C26-C27-C28-C29
23	b	611	CLA	C2C-C3C-CAC-CBC
27	B	621	LMG	C33-C34-C35-C36
27	M	101	LMG	C13-C14-C15-C16
27	c	523	LMG	C12-C13-C14-C15
30	A	415	DGD	C9B-CAB-CBB-CCB
30	h	102	DGD	C9A-CAA-CBA-CCA
30	h	102	DGD	C2B-C3B-C4B-C5B
25	A	409	BCR	C16-C17-C18-C19
25	B	617	BCR	C12-C13-C14-C15
25	B	617	BCR	C20-C21-C22-C23
25	B	618	BCR	C12-C13-C14-C15
25	B	618	BCR	C16-C17-C18-C19
25	B	619	BCR	C11-C10-C9-C8
25	K	102	BCR	C16-C17-C18-C19
25	b	619	BCR	C12-C13-C14-C15
25	b	620	BCR	C16-C17-C18-C19
25	c	514	BCR	C20-C21-C22-C23
25	x	101	BCR	C11-C10-C9-C8
30	c	517	DGD	C2E-C1E-O5D-C6D
28	a	412	SQD	O47-C45-C46-O48
27	M	101	LMG	C16-C17-C18-C19
27	b	622	LMG	C15-C16-C17-C18
28	b	601	SQD	C10-C11-C12-C13
29	B	623	LHG	C12-C13-C14-C15
29	d	406	LHG	C32-C33-C34-C35
29	l	101	LHG	C9-C10-C11-C12
30	C	515	DGD	C4A-C5A-C6A-C7A
23	C	502	CLA	C16-C17-C18-C19
26	d	405	PL9	C42-C43-C44-C45
27	b	622	LMG	C16-C17-C18-C19
27	b	622	LMG	C34-C35-C36-C37
28	B	624	SQD	C17-C18-C19-C20
30	A	415	DGD	C5B-C6B-C7B-C8B
30	c	518	DGD	C3A-C4A-C5A-C6A
23	C	506	CLA	C2-C3-C5-C6
26	d	405	PL9	C13-C14-C16-C17
23	B	602	CLA	C11-C12-C13-C14
23	B	604	CLA	C11-C10-C8-C9
23	a	406	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	D	406	LMG	C30-C31-C32-C33
27	b	623	LMG	C32-C33-C34-C35
27	c	521	LMG	C34-C35-C36-C37
28	a	413	SQD	C10-C11-C12-C13
29	D	408	LHG	C34-C35-C36-C37
29	d	407	LHG	C26-C27-C28-C29
29	e	101	LHG	C17-C18-C19-C20
29	l	101	LHG	C32-C33-C34-C35
30	A	415	DGD	CDB-CEB-CFB-CGB
30	c	516	DGD	C4B-C5B-C6B-C7B
30	c	517	DGD	C7B-C8B-C9B-CAB
30	h	102	DGD	CAB-CBB-CCB-CDB
23	c	512	CLA	O1A-CGA-O2A-C1
25	A	409	BCR	C7-C8-C9-C34
28	A	414	SQD	C12-C13-C14-C15
28	f	101	SQD	C24-C25-C26-C27
29	D	407	LHG	C29-C30-C31-C32
29	D	408	LHG	C11-C12-C13-C14
29	d	407	LHG	C30-C31-C32-C33
30	C	517	DGD	C2A-C3A-C4A-C5A
29	d	408	LHG	O1-C1-C2-C3
25	c	514	BCR	C17-C18-C19-C20
27	c	521	LMG	O9-C10-O7-C8
27	b	622	LMG	C11-C12-C13-C14
27	b	622	LMG	C31-C32-C33-C34
30	C	516	DGD	C9A-CAA-CBA-CCA
30	c	518	DGD	C5B-C6B-C7B-C8B
28	B	624	SQD	C24-C23-O48-C46
29	A	413	LHG	C23-C24-C25-C26
28	A	412	SQD	C25-C26-C27-C28
28	a	412	SQD	C30-C31-C32-C33
28	b	601	SQD	C26-C27-C28-C29
28	f	101	SQD	C32-C33-C34-C35
29	A	413	LHG	C16-C17-C18-C19
29	B	623	LHG	C25-C26-C27-C28
29	B	623	LHG	C29-C30-C31-C32
29	D	407	LHG	C12-C13-C14-C15
29	d	406	LHG	C25-C26-C27-C28
29	d	406	LHG	C29-C30-C31-C32
29	l	101	LHG	C28-C29-C30-C31
30	C	517	DGD	C8B-C9B-CAB-CBB
30	H	102	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
30	a	414	DGD	C7B-C8B-C9B-CAB
30	c	517	DGD	C6A-C7A-C8A-C9A
30	h	102	DGD	C5B-C6B-C7B-C8B
23	A	405	CLA	C16-C17-C18-C19
30	c	517	DGD	O6E-C1E-O5D-C6D
23	B	604	CLA	C10-C11-C12-C13
26	a	410	PL9	C14-C16-C17-C18
27	A	411	LMG	C16-C17-C18-C19
27	b	623	LMG	C36-C37-C38-C39
27	c	521	LMG	C11-C12-C13-C14
29	D	407	LHG	C11-C10-C9-C8
30	H	102	DGD	C3B-C4B-C5B-C6B
30	c	516	DGD	C5B-C6B-C7B-C8B
30	c	518	DGD	C2A-C3A-C4A-C5A
28	B	624	SQD	C26-C27-C28-C29
28	f	101	SQD	C28-C29-C30-C31
29	A	413	LHG	C10-C11-C12-C13
29	d	407	LHG	C29-C30-C31-C32
30	A	415	DGD	C2A-C3A-C4A-C5A
30	A	415	DGD	CAA-CBA-CCA-CDA
30	H	102	DGD	CBA-CCA-CDA-CEA
27	B	621	LMG	C32-C33-C34-C35
27	c	519	LMG	C35-C36-C37-C38
30	A	415	DGD	C6B-C7B-C8B-C9B
30	C	516	DGD	C8A-C9A-CAA-CBA
28	a	413	SQD	C12-C13-C14-C15
23	b	604	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	C3A-C2A-CAA-CBA
23	h	101	CLA	C3A-C2A-CAA-CBA
23	b	616	CLA	C8-C10-C11-C12
30	C	517	DGD	C5A-C6A-C7A-C8A
23	c	510	CLA	C16-C17-C18-C19
27	m	101	LMG	C29-C30-C31-C32
28	A	412	SQD	C26-C27-C28-C29
28	a	413	SQD	C11-C10-C9-C8
29	A	413	LHG	C12-C13-C14-C15
29	d	407	LHG	C12-C13-C14-C15
29	e	101	LHG	C13-C14-C15-C16
29	e	101	LHG	C27-C28-C29-C30
30	C	517	DGD	C8A-C9A-CAA-CBA
30	a	414	DGD	C4A-C5A-C6A-C7A
30	c	516	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
30	h	102	DGD	C7A-C8A-C9A-CAA
28	a	412	SQD	C44-C45-C46-O48
27	c	519	LMG	C11-C10-O7-C8
27	c	521	LMG	C32-C33-C34-C35
28	A	412	SQD	C11-C12-C13-C14
28	b	601	SQD	C12-C13-C14-C15
28	b	601	SQD	C24-C25-C26-C27
29	d	408	LHG	C33-C34-C35-C36
30	c	518	DGD	C7A-C8A-C9A-CAA
30	c	516	DGD	O6D-C5D-C6D-O5D
27	c	523	LMG	O6-C5-C6-O5
30	a	414	DGD	C1A-C2A-C3A-C4A
23	b	610	CLA	C4-C3-C5-C6
23	b	610	CLA	C2-C3-C5-C6
26	d	405	PL9	C28-C29-C31-C32
27	M	101	LMG	C18-C19-C20-C21
29	e	101	LHG	C12-C13-C14-C15
29	d	406	LHG	O1-C1-C2-O2
23	B	603	CLA	C8-C10-C11-C12
27	D	406	LMG	C20-C21-C22-C23
27	c	521	LMG	C38-C39-C40-C41
29	D	407	LHG	C30-C31-C32-C33
30	c	517	DGD	CCA-CDA-CEA-CFA
30	h	102	DGD	C7B-C8B-C9B-CAB
23	c	513	CLA	C13-C15-C16-C17
27	D	409	LMG	C33-C34-C35-C36
28	F	101	SQD	C26-C27-C28-C29
27	m	101	LMG	C31-C32-C33-C34
29	A	413	LHG	C1-C2-C3-O3
23	b	611	CLA	C4C-C3C-CAC-CBC
27	D	406	LMG	C33-C34-C35-C36
27	D	406	LMG	C34-C35-C36-C37
28	b	601	SQD	C13-C14-C15-C16
30	a	414	DGD	CBA-CCA-CDA-CEA
29	e	101	LHG	O9-C7-O7-C5
23	B	601	CLA	C2-C1-O2A-CGA
28	B	624	SQD	C9-C10-C11-C12
29	B	622	LHG	C30-C31-C32-C33
29	d	406	LHG	C10-C11-C12-C13
27	C	518	LMG	C32-C33-C34-C35
27	c	519	LMG	C31-C32-C33-C34
28	B	624	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
28	F	101	SQD	C33-C34-C35-C36
29	d	406	LHG	C31-C32-C33-C34
23	h	101	CLA	C3-C5-C6-C7
25	D	404	BCR	C23-C24-C25-C26
25	D	404	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	K	102	BCR	C23-C24-C25-C26
25	T	101	BCR	C1-C6-C7-C8
25	T	101	BCR	C5-C6-C7-C8
25	b	618	BCR	C5-C6-C7-C8
25	c	514	BCR	C5-C6-C7-C8
25	k	101	BCR	C1-C6-C7-C8
25	k	101	BCR	C5-C6-C7-C8
30	c	516	DGD	C7A-C8A-C9A-CAA
30	c	516	DGD	C8B-C9B-CAB-CBB
23	B	603	CLA	C10-C11-C12-C13
23	C	507	CLA	C13-C15-C16-C17
23	b	615	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
27	c	521	LMG	C11-C10-O7-C8
27	c	523	LMG	C14-C15-C16-C17
27	d	409	LMG	C35-C36-C37-C38
28	B	624	SQD	C25-C26-C27-C28
29	B	622	LHG	C32-C33-C34-C35
30	h	102	DGD	CCA-CDA-CEA-CFA
27	c	521	LMG	C10-C11-C12-C13
30	A	415	DGD	CDA-CEA-CFA-CGA
26	a	410	PL9	C47-C48-C49-C50
23	B	602	CLA	C13-C15-C16-C17
23	c	509	CLA	C10-C11-C12-C13
27	c	519	LMG	C34-C35-C36-C37
26	D	405	PL9	C30-C29-C31-C32
23	B	604	CLA	C11-C10-C8-C7
23	B	604	CLA	C11-C12-C13-C15
23	B	605	CLA	C11-C12-C13-C15
23	B	606	CLA	C6-C7-C8-C10
23	C	506	CLA	C11-C12-C13-C15
23	a	406	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C7
27	b	623	LMG	C31-C32-C33-C34
28	B	624	SQD	C34-C35-C36-C37
23	C	501	CLA	O1D-CGD-O2D-CED
30	c	518	DGD	C1A-C2A-C3A-C4A
27	A	411	LMG	C29-C28-O8-C9
27	m	101	LMG	C29-C28-O8-C9
30	c	518	DGD	C2A-C1A-O1G-C1G
27	c	523	LMG	C30-C31-C32-C33
27	m	101	LMG	C15-C16-C17-C18
23	B	616	CLA	C5-C6-C7-C8
23	C	503	CLA	C5-C6-C7-C8
23	c	509	CLA	C15-C16-C17-C18
27	b	623	LMG	C34-C35-C36-C37
29	D	408	LHG	C27-C28-C29-C30
30	H	102	DGD	C4B-C5B-C6B-C7B
27	B	621	LMG	C34-C35-C36-C37
28	A	414	SQD	C32-C33-C34-C35
30	c	516	DGD	C9A-CAA-CBA-CCA
29	A	413	LHG	C7-C8-C9-C10
30	A	415	DGD	C1A-C2A-C3A-C4A
27	M	101	LMG	C12-C13-C14-C15
27	M	101	LMG	C32-C33-C34-C35
28	F	101	SQD	C34-C35-C36-C37
30	A	415	DGD	C2B-C3B-C4B-C5B
30	C	516	DGD	C5A-C6A-C7A-C8A
30	H	102	DGD	C9A-CAA-CBA-CCA
30	c	518	DGD	C8B-C9B-CAB-CBB
25	Z	101	BCR	C22-C23-C24-C25
23	b	610	CLA	CBD-CGD-O2D-CED
30	C	515	DGD	C4D-C5D-C6D-O5D
30	c	516	DGD	C4D-C5D-C6D-O5D
23	B	603	CLA	C16-C17-C18-C20
23	a	405	CLA	C16-C17-C18-C20
30	C	516	DGD	O6E-C1E-O5D-C6D
27	A	411	LMG	C14-C15-C16-C17
28	a	413	SQD	C11-C12-C13-C14
29	B	622	LHG	C33-C34-C35-C36
30	a	414	DGD	C2B-C1B-O2G-C2G
25	B	617	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	A	415	DGD	C8B-C9B-CAB-CBB
30	C	517	DGD	CAA-CBA-CCA-CDA
27	b	623	LMG	C11-C12-C13-C14
27	m	101	LMG	C11-C12-C13-C14
29	D	408	LHG	O2-C2-C3-O3
29	A	413	LHG	O9-C7-O7-C5
30	c	517	DGD	O1B-C1B-O2G-C2G
29	D	408	LHG	C23-C24-C25-C26
28	f	101	SQD	C33-C34-C35-C36
29	d	407	LHG	C14-C15-C16-C17
29	d	407	LHG	C32-C33-C34-C35
30	c	516	DGD	C4A-C5A-C6A-C7A
30	C	516	DGD	C2E-C1E-O5D-C6D
23	b	607	CLA	C10-C11-C12-C13
27	c	519	LMG	O7-C8-C9-O8
23	b	615	CLA	CBA-CGA-O2A-C1
29	A	413	LHG	C11-C10-C9-C8
29	D	408	LHG	C25-C26-C27-C28
30	c	518	DGD	CCB-CDB-CEB-CFB
30	h	102	DGD	C6A-C7A-C8A-C9A
23	B	611	CLA	C16-C17-C18-C20
23	C	509	CLA	C16-C17-C18-C20
23	c	507	CLA	C16-C17-C18-C19
23	h	101	CLA	C16-C17-C18-C20
29	D	407	LHG	C32-C33-C34-C35
23	c	512	CLA	C8-C10-C11-C12
26	a	410	PL9	C15-C14-C16-C17
26	d	405	PL9	C15-C14-C16-C17
26	d	405	PL9	C30-C29-C31-C32
29	e	101	LHG	C7-C8-C9-C10
26	A	410	PL9	C43-C44-C46-C47
26	D	405	PL9	C4-C3-C7-C8
28	a	413	SQD	C24-C25-C26-C27
29	d	407	LHG	C33-C34-C35-C36
23	B	604	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C12-C13-C14
23	C	506	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C9
23	D	401	CLA	C11-C12-C13-C14
23	a	408	CLA	C11-C10-C8-C9
23	b	603	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C11-C12-C13-C14
23	b	613	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C12-C13-C14
23	b	611	CLA	CBD-CGD-O2D-CED
28	a	412	SQD	C13-C14-C15-C16
29	D	408	LHG	C16-C17-C18-C19
30	a	414	DGD	CEA-CFA-CGA-CHA
30	C	516	DGD	O6E-C5E-C6E-O5E
25	B	619	BCR	C7-C8-C9-C34
23	C	512	CLA	C10-C11-C12-C13
23	c	506	CLA	C13-C15-C16-C17
27	b	622	LMG	C39-C40-C41-C42
27	c	523	LMG	C11-C12-C13-C14
25	b	618	BCR	C21-C22-C23-C24
23	b	613	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	C1A-C2A-CAA-CBA
23	a	408	CLA	C1A-C2A-CAA-CBA
23	h	101	CLA	C1A-C2A-CAA-CBA
23	B	603	CLA	C16-C17-C18-C19
23	a	405	CLA	C16-C17-C18-C19
27	d	409	LMG	C14-C15-C16-C17
29	B	623	LHG	C14-C15-C16-C17
25	c	514	BCR	C13-C14-C15-C16
23	B	613	CLA	C13-C15-C16-C17
23	b	605	CLA	C10-C11-C12-C13
23	b	608	CLA	C8-C10-C11-C12
29	B	623	LHG	C3-O3-P-O6
29	d	406	LHG	C3-O3-P-O6
23	D	403	CLA	O1D-CGD-O2D-CED
27	M	101	LMG	C36-C37-C38-C39
23	B	611	CLA	C15-C16-C17-C18
23	C	503	CLA	C8-C10-C11-C12
23	d	403	CLA	C13-C15-C16-C17
27	C	518	LMG	C34-C35-C36-C37
30	h	102	DGD	CBA-CCA-CDA-CEA
23	B	606	CLA	C13-C15-C16-C17
23	c	510	CLA	C16-C17-C18-C20
29	D	407	LHG	C25-C26-C27-C28
23	B	616	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
28	A	412	SQD	C15-C16-C17-C18
29	B	622	LHG	C18-C19-C20-C21
23	b	611	CLA	O1D-CGD-O2D-CED
23	b	614	CLA	C15-C16-C17-C18
27	D	406	LMG	C17-C18-C19-C20
27	b	622	LMG	C18-C19-C20-C21
27	c	523	LMG	C38-C39-C40-C41
27	d	409	LMG	O6-C5-C6-O5
29	B	623	LHG	C1-C2-C3-O3
29	D	407	LHG	C1-C2-C3-O3
30	c	516	DGD	O6E-C5E-C6E-O5E
23	C	510	CLA	C4-C3-C5-C6
23	c	510	CLA	C4-C3-C5-C6
23	c	510	CLA	C2-C3-C5-C6
26	D	405	PL9	C28-C29-C31-C32
27	A	411	LMG	C17-C18-C19-C20
28	a	413	SQD	C19-C20-C21-C22
30	H	102	DGD	CAA-CBA-CCA-CDA
27	M	101	LMG	C35-C36-C37-C38
28	a	413	SQD	C18-C19-C20-C21
29	e	101	LHG	C11-C10-C9-C8
23	C	502	CLA	C16-C17-C18-C20
23	D	402	CLA	C3-C5-C6-C7
27	D	409	LMG	C7-C8-C9-O8
27	b	622	LMG	O1-C7-C8-C9
27	c	519	LMG	C7-C8-C9-O8
27	c	521	LMG	C7-C8-C9-O8
28	A	412	SQD	O6-C44-C45-C46
28	B	624	SQD	O6-C44-C45-C46
28	a	412	SQD	C12-C13-C14-C15
28	a	413	SQD	C44-C45-C46-O48
28	b	601	SQD	C44-C45-C46-O48
30	C	515	DGD	O1G-C1G-C2G-C3G
27	c	521	LMG	O6-C5-C6-O5
28	A	412	SQD	C35-C36-C37-C38
28	B	624	SQD	C45-C44-O6-C1
30	C	516	DGD	C2G-C3G-O3G-C1D
30	C	516	DGD	C5D-C6D-O5D-C1E
30	c	517	DGD	C2G-C3G-O3G-C1D
30	c	517	DGD	C5D-C6D-O5D-C1E
28	F	101	SQD	C25-C26-C27-C28
30	a	414	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
27	D	409	LMG	C37-C38-C39-C40
29	A	413	LHG	C19-C20-C21-C22
23	c	505	CLA	C16-C17-C18-C20
26	A	410	PL9	C19-C21-C22-C23
23	c	508	CLA	C16-C17-C18-C19
29	D	408	LHG	C9-C10-C11-C12
30	C	515	DGD	O6E-C5E-C6E-O5E
27	d	409	LMG	C33-C34-C35-C36
27	m	101	LMG	C40-C41-C42-C43
23	c	503	CLA	C5-C6-C7-C8
25	Z	101	BCR	C20-C21-C22-C37
25	c	514	BCR	C16-C17-C18-C36
25	k	102	BCR	C35-C13-C14-C15
25	t	101	BCR	C11-C10-C9-C34
27	D	406	LMG	O6-C5-C6-O5
27	b	623	LMG	C37-C38-C39-C40
27	c	519	LMG	C36-C37-C38-C39
23	C	505	CLA	C2-C3-C5-C6
23	b	608	CLA	C16-C17-C18-C20
29	d	406	LHG	C24-C25-C26-C27
29	e	101	LHG	C28-C29-C30-C31
27	D	409	LMG	C9-C8-O7-C10
27	b	622	LMG	C9-C8-O7-C10
23	a	408	CLA	C5-C6-C7-C8
23	c	506	CLA	C2-C1-O2A-CGA
26	a	410	PL9	C17-C18-C19-C21
28	A	414	SQD	C46-C45-O47-C7
27	c	523	LMG	C13-C14-C15-C16
29	B	623	LHG	C32-C33-C34-C35
23	b	608	CLA	C16-C17-C18-C19
27	b	623	LMG	C30-C31-C32-C33
23	c	501	CLA	O1D-CGD-O2D-CED
23	D	401	CLA	C13-C15-C16-C17
25	c	514	BCR	C12-C13-C14-C15
27	A	411	LMG	O1-C7-C8-O7
27	d	409	LMG	C40-C41-C42-C43
30	C	517	DGD	C3A-C4A-C5A-C6A
30	C	516	DGD	O1B-C1B-O2G-C2G
26	A	410	PL9	C47-C48-C49-C50
23	b	615	CLA	O1A-CGA-O2A-C1
27	C	518	LMG	O10-C28-O8-C9
30	C	517	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C10-C11-C12-C13
23	C	505	CLA	C4-C3-C5-C6
23	B	603	CLA	C6-C7-C8-C10
23	C	504	CLA	C11-C10-C8-C7
23	C	506	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C10-C8-C7
23	C	510	CLA	C2-C3-C5-C6
23	C	510	CLA	C11-C10-C8-C7
23	D	401	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	b	603	CLA	C6-C7-C8-C10
23	b	605	CLA	C11-C10-C8-C7
23	b	607	CLA	C11-C10-C8-C7
23	b	613	CLA	C6-C7-C8-C10
23	b	616	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C10-C8-C7
23	c	509	CLA	C6-C7-C8-C10
23	c	512	CLA	C11-C12-C13-C15
30	H	102	DGD	O2G-C1B-C2B-C3B
23	B	603	CLA	C6-C7-C8-C9
23	B	615	CLA	C11-C12-C13-C14
23	C	504	CLA	C11-C10-C8-C9
23	C	512	CLA	C11-C10-C8-C9
23	C	513	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	605	CLA	C11-C10-C8-C9
23	b	605	CLA	C14-C13-C15-C16
23	b	607	CLA	C11-C10-C8-C9
23	b	610	CLA	C14-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
28	A	414	SQD	C30-C31-C32-C33
29	D	408	LHG	C33-C34-C35-C36
29	l	101	LHG	C29-C30-C31-C32
23	c	503	CLA	CBA-CGA-O2A-C1
23	c	508	CLA	CBA-CGA-O2A-C1
29	B	623	LHG	C19-C20-C21-C22
29	D	408	LHG	C24-C25-C26-C27
23	c	506	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	k	101	BCR	C17-C18-C19-C20
28	f	101	SQD	C31-C32-C33-C34
30	C	515	DGD	CBA-CCA-CDA-CEA
23	c	510	CLA	C5-C6-C7-C8
27	D	406	LMG	C15-C16-C17-C18
30	H	102	DGD	CCB-CDB-CEB-CFB
26	a	410	PL9	C12-C13-C14-C16
30	A	415	DGD	CCB-CDB-CEB-CFB
30	c	516	DGD	CAB-CBB-CCB-CDB
27	D	406	LMG	C35-C36-C37-C38
29	l	101	LHG	O6-C4-C5-C6
30	c	518	DGD	CCA-CDA-CEA-CFA
23	C	511	CLA	C8-C10-C11-C12
28	B	624	SQD	C11-C12-C13-C14
30	a	414	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	CBB-CCB-CDB-CEB
23	c	512	CLA	C4-C3-C5-C6
26	d	405	PL9	C40-C39-C41-C42
23	c	512	CLA	C2-C3-C5-C6
26	a	410	PL9	C13-C14-C16-C17
23	c	507	CLA	C8-C10-C11-C12
23	h	101	CLA	C10-C11-C12-C13
23	A	404	CLA	C2C-C3C-CAC-CBC
30	c	518	DGD	C5A-C6A-C7A-C8A
23	B	602	CLA	C3A-C2A-CAA-CBA
23	b	604	CLA	C13-C15-C16-C17
23	h	101	CLA	C16-C17-C18-C19
27	M	101	LMG	C7-C8-C9-O8
28	a	412	SQD	O6-C44-C45-C46
30	A	415	DGD	C1G-C2G-C3G-O3G
30	a	414	DGD	O1G-C1G-C2G-C3G
27	c	521	LMG	C40-C41-C42-C43
29	B	622	LHG	C19-C20-C21-C22
29	d	406	LHG	C19-C20-C21-C22
29	d	406	LHG	C33-C34-C35-C36
30	c	516	DGD	C9B-CAB-CBB-CCB
23	b	606	CLA	C5-C6-C7-C8
29	d	408	LHG	C29-C30-C31-C32
30	c	518	DGD	C6B-C7B-C8B-C9B
23	c	511	CLA	C13-C15-C16-C17
23	a	408	CLA	C16-C17-C18-C19
23	A	408	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	c	521	LMG	C35-C36-C37-C38
29	d	407	LHG	C25-C26-C27-C28
29	B	622	LHG	C23-C24-C25-C26
27	M	101	LMG	C40-C41-C42-C43
29	D	407	LHG	C15-C16-C17-C18
30	C	515	DGD	C9B-CAB-CBB-CCB
27	D	406	LMG	C39-C40-C41-C42
29	d	406	LHG	C17-C18-C19-C20
29	l	101	LHG	O6-C4-C5-O7
23	c	506	CLA	CBA-CGA-O2A-C1
23	c	503	CLA	O1A-CGA-O2A-C1
23	B	615	CLA	C16-C17-C18-C19
23	b	612	CLA	C16-C17-C18-C19
27	b	622	LMG	C42-C43-C44-C45
30	C	516	DGD	CCB-CDB-CEB-CFB
30	C	515	DGD	O1G-C1A-C2A-C3A
27	c	523	LMG	C33-C34-C35-C36
29	B	623	LHG	C27-C28-C29-C30
28	A	414	SQD	O47-C45-C46-O48
27	m	101	LMG	C17-C18-C19-C20
27	D	409	LMG	O7-C8-C9-O8
27	c	523	LMG	O7-C8-C9-O8
23	c	509	CLA	CAA-CBA-CGA-O2A
27	c	523	LMG	C40-C41-C42-C43
30	C	516	DGD	CDA-CEA-CFA-CGA
30	c	518	DGD	C9A-CAA-CBA-CCA
26	A	410	PL9	C29-C31-C32-C33
26	A	410	PL9	C39-C41-C42-C43
29	e	101	LHG	C1-C2-C3-O3
27	c	521	LMG	C13-C14-C15-C16
29	d	407	LHG	C28-C29-C30-C31
30	a	414	DGD	C5B-C6B-C7B-C8B
23	b	610	CLA	O1D-CGD-O2D-CED
27	A	411	LMG	C12-C13-C14-C15
23	B	615	CLA	C6-C7-C8-C9
23	C	508	CLA	C11-C10-C8-C9
23	C	509	CLA	C14-C13-C15-C16
23	C	510	CLA	C14-C13-C15-C16
23	C	511	CLA	C6-C7-C8-C9
23	a	406	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C14-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C9
23	d	402	CLA	C6-C7-C8-C9
28	A	414	SQD	C16-C17-C18-C19
28	F	101	SQD	C27-C28-C29-C30
30	c	517	DGD	CDB-CEB-CFB-CGB
27	C	518	LMG	C37-C38-C39-C40
29	D	408	LHG	C30-C31-C32-C33
30	H	102	DGD	C8B-C9B-CAB-CBB
29	A	413	LHG	C2-C3-O3-P
29	d	408	LHG	C2-C3-O3-P
28	F	101	SQD	O6-C44-C45-C46
30	C	517	DGD	CBA-CCA-CDA-CEA
23	B	616	CLA	C11-C12-C13-C14
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	k	101	BCR	C23-C24-C25-C26
23	B	610	CLA	C8-C10-C11-C12
27	D	406	LMG	C40-C41-C42-C43
27	m	101	LMG	C22-C23-C24-C25
23	a	405	CLA	C15-C16-C17-C18
30	a	414	DGD	CFA-CGA-CHA-CIA
29	l	101	LHG	O9-C7-O7-C5
25	D	404	BCR	C14-C15-C16-C17
25	a	409	BCR	C14-C15-C16-C17
29	B	623	LHG	C9-C10-C11-C12
23	B	611	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	c	506	CLA	C16-C17-C18-C20
28	A	412	SQD	C10-C11-C12-C13
29	D	407	LHG	C11-C12-C13-C14
29	e	101	LHG	O6-C4-C5-C6
28	F	101	SQD	O48-C23-C24-C25
28	A	412	SQD	C11-C10-C9-C8
29	e	101	LHG	C14-C15-C16-C17
27	c	519	LMG	C4-C5-C6-O5
23	B	602	CLA	C11-C12-C13-C15
23	B	615	CLA	C6-C7-C8-C10
23	B	615	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	C	509	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C12-C13-C15
23	a	406	CLA	C11-C10-C8-C7
23	a	406	CLA	C12-C13-C15-C16
23	a	411	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C12-C13-C15
23	b	609	CLA	C11-C10-C8-C7
23	b	609	CLA	C11-C12-C13-C15
23	b	610	CLA	C12-C13-C15-C16
23	b	611	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	505	CLA	C6-C7-C8-C10
23	c	508	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C12-C13-C15
23	d	402	CLA	C6-C7-C8-C10
28	a	413	SQD	C9-C10-C11-C12
23	B	607	CLA	C16-C17-C18-C19
23	b	612	CLA	C16-C17-C18-C20
29	d	407	LHG	C34-C35-C36-C37
28	F	101	SQD	C45-C46-O48-C23
29	B	623	LHG	C24-C25-C26-C27
23	c	508	CLA	O1A-CGA-O2A-C1
27	b	622	LMG	C41-C42-C43-C44
30	C	516	DGD	C3B-C4B-C5B-C6B
25	A	409	BCR	C20-C21-C22-C37
25	B	619	BCR	C11-C10-C9-C34
25	K	102	BCR	C16-C17-C18-C36
25	b	618	BCR	C16-C17-C18-C36
25	b	618	BCR	C20-C21-C22-C37
25	b	620	BCR	C20-C21-C22-C37
25	c	514	BCR	C11-C10-C9-C34
25	k	102	BCR	C20-C21-C22-C37
25	t	101	BCR	C16-C17-C18-C36
25	t	101	BCR	C20-C21-C22-C37
29	D	407	LHG	C23-C24-C25-C26
23	B	616	CLA	C11-C12-C13-C15
23	d	403	CLA	C16-C17-C18-C19
29	d	408	LHG	C24-C23-O8-C6
29	d	407	LHG	C31-C32-C33-C34
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	b	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	406	PHO	CAD-CBD-CGD-O2D
24	a	407	PHO	CAD-CBD-CGD-O2D
27	A	411	LMG	C9-C8-O7-C10
28	b	601	SQD	C44-C45-O47-C7
30	a	414	DGD	C1G-C2G-O2G-C1B
28	A	414	SQD	C44-C45-O47-C7
28	A	412	SQD	C14-C15-C16-C17
29	e	101	LHG	C10-C11-C12-C13
25	T	101	BCR	C6-C7-C8-C9
25	d	404	BCR	C22-C23-C24-C25
23	b	617	CLA	CBA-CGA-O2A-C1
27	B	621	LMG	C14-C15-C16-C17
28	A	414	SQD	C17-C18-C19-C20
23	c	507	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	C10-C11-C12-C13
28	b	601	SQD	C15-C16-C17-C18
23	C	511	CLA	CBA-CGA-O2A-C1
29	l	101	LHG	C11-C12-C13-C14
23	C	505	CLA	C16-C17-C18-C19
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O2D
24	d	401	PHO	CHA-CBD-CGD-O1D
24	d	401	PHO	CHA-CBD-CGD-O2D
29	e	101	LHG	C19-C20-C21-C22
23	C	511	CLA	O1A-CGA-O2A-C1
28	a	412	SQD	O10-C23-O48-C46
30	c	516	DGD	O1A-C1A-O1G-C1G
25	A	409	BCR	C11-C10-C9-C8
25	A	409	BCR	C20-C21-C22-C23
25	c	514	BCR	C11-C10-C9-C8
27	b	622	LMG	O1-C7-C8-O7
28	A	412	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
27	D	409	LMG	C12-C13-C14-C15
23	c	506	CLA	O1A-CGA-O2A-C1
27	b	622	LMG	C13-C14-C15-C16
30	H	102	DGD	C5A-C6A-C7A-C8A
23	c	507	CLA	O1D-CGD-O2D-CED
30	A	415	DGD	O6D-C5D-C6D-O5D
29	B	622	LHG	O10-C23-O8-C6
30	c	517	DGD	O1A-C1A-O1G-C1G
26	a	410	PL9	C4-C3-C7-C8
29	d	407	LHG	C19-C20-C21-C22
27	d	409	LMG	O9-C10-O7-C8
23	B	616	CLA	C6-C7-C8-C9
23	b	608	CLA	C11-C12-C13-C14
23	b	609	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C6-C7-C8-C9
28	A	414	SQD	C10-C11-C12-C13
30	H	102	DGD	C9B-CAB-CBB-CCB
28	A	414	SQD	C7-C8-C9-C10
29	d	407	LHG	C17-C18-C19-C20
28	a	412	SQD	C5-C6-S-O8
29	d	408	LHG	C32-C33-C34-C35
23	B	603	CLA	CBD-CGD-O2D-CED
27	C	518	LMG	C29-C30-C31-C32
28	a	412	SQD	C32-C33-C34-C35
25	H	101	BCR	C21-C22-C23-C24
25	k	101	BCR	C7-C8-C9-C10
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
27	C	518	LMG	O6-C5-C6-O5
23	B	610	CLA	C16-C17-C18-C19
23	c	505	CLA	C16-C17-C18-C19
29	d	407	LHG	C3-O3-P-O6
30	A	415	DGD	CEB-CFB-CGB-CHB
30	c	516	DGD	C1A-C2A-C3A-C4A
30	a	414	DGD	C7A-C8A-C9A-CAA
30	c	517	DGD	CBB-CCB-CDB-CEB
23	B	601	CLA	C4-C3-C5-C6
23	C	504	CLA	C4-C3-C5-C6
29	D	408	LHG	C2-C3-O3-P
27	D	406	LMG	C37-C38-C39-C40
27	d	409	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
27	m	101	LMG	C38-C39-C40-C41
28	a	412	SQD	C17-C18-C19-C20
28	a	412	SQD	C34-C35-C36-C37
30	C	515	DGD	CBB-CCB-CDB-CEB
30	C	517	DGD	C2B-C3B-C4B-C5B
30	a	414	DGD	C4B-C5B-C6B-C7B
29	A	413	LHG	C3-O3-P-O4
29	A	413	LHG	C4-O6-P-O5
29	B	623	LHG	C3-O3-P-O5
29	D	408	LHG	C3-O3-P-O5
29	d	407	LHG	C3-O3-P-O4
28	F	101	SQD	C23-C24-C25-C26
30	C	515	DGD	C6A-C7A-C8A-C9A
23	B	611	CLA	CBA-CGA-O2A-C1
23	c	505	CLA	O1D-CGD-O2D-CED
30	h	102	DGD	O2G-C1B-C2B-C3B
23	C	506	CLA	C13-C15-C16-C17
23	b	603	CLA	C13-C15-C16-C17
23	b	611	CLA	C2A-CAA-CBA-CGA
30	A	415	DGD	CFA-CGA-CHA-CIA
30	c	516	DGD	C6A-C7A-C8A-C9A
30	h	102	DGD	CBB-CCB-CDB-CEB
29	D	407	LHG	C27-C28-C29-C30
30	C	516	DGD	C3A-C4A-C5A-C6A
23	B	614	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	b	610	CLA	CAD-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
28	a	412	SQD	C5-C6-S-O7
28	a	412	SQD	C5-C6-S-O9
23	B	613	CLA	C5-C6-C7-C8
28	A	414	SQD	C15-C16-C17-C18
30	c	518	DGD	C7B-C8B-C9B-CAB
29	D	407	LHG	C33-C34-C35-C36
23	b	617	CLA	C5-C6-C7-C8
27	b	622	LMG	C35-C36-C37-C38
28	A	414	SQD	C9-C10-C11-C12
23	D	403	CLA	C16-C17-C18-C20
23	B	603	CLA	C12-C13-C15-C16
23	B	604	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C12-C13-C15-C16
23	B	616	CLA	C6-C7-C8-C10
23	C	505	CLA	C11-C12-C13-C15
23	C	507	CLA	C11-C10-C8-C7
23	C	510	CLA	C12-C13-C15-C16
23	C	512	CLA	C12-C13-C15-C16
23	D	402	CLA	C6-C7-C8-C10
23	b	608	CLA	C11-C12-C13-C15
23	c	501	CLA	C11-C12-C13-C15
23	c	509	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
23	h	101	CLA	C11-C10-C8-C7
24	A	406	PHO	C12-C13-C15-C16
24	a	407	PHO	C6-C7-C8-C10
23	B	610	CLA	C2C-C3C-CAC-CBC
29	B	622	LHG	C15-C16-C17-C18
27	D	409	LMG	C15-C16-C17-C18
29	e	101	LHG	C8-C7-O7-C5
23	b	617	CLA	O1A-CGA-O2A-C1
27	m	101	LMG	C14-C15-C16-C17
29	e	101	LHG	C15-C16-C17-C18
30	C	516	DGD	C7A-C8A-C9A-CAA
27	c	523	LMG	C7-C8-C9-O8
28	A	412	SQD	C44-C45-C46-O48
27	M	101	LMG	O7-C8-C9-O8
27	c	521	LMG	O7-C8-C9-O8
28	a	413	SQD	O47-C45-C46-O48
28	b	601	SQD	O6-C44-C45-O47
28	b	601	SQD	O47-C45-C46-O48
28	f	101	SQD	O6-C44-C45-O47
29	e	101	LHG	O7-C5-C6-O8
30	C	515	DGD	O1G-C1G-C2G-O2G
23	A	405	CLA	C2C-C3C-CAC-CBC
29	A	413	LHG	C13-C14-C15-C16
29	D	408	LHG	C11-C10-C9-C8
23	B	601	CLA	C3-C5-C6-C7
23	C	502	CLA	C15-C16-C17-C18
23	B	603	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14
23	C	505	CLA	C14-C13-C15-C16
23	a	406	CLA	C11-C10-C8-C9
23	b	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C6-C7-C8-C9
23	c	508	CLA	C11-C12-C13-C14
23	c	509	CLA	C14-C13-C15-C16
30	c	516	DGD	C1B-C2B-C3B-C4B
25	B	619	BCR	C22-C23-C24-C25
23	C	506	CLA	C3-C5-C6-C7
23	B	611	CLA	O1A-CGA-O2A-C1
30	A	415	DGD	C8A-C9A-CAA-CBA
25	t	101	BCR	C7-C8-C9-C34
23	B	606	CLA	C16-C17-C18-C19
25	K	102	BCR	C7-C8-C9-C10
30	A	415	DGD	C4B-C5B-C6B-C7B
23	c	506	CLA	C10-C11-C12-C13
29	D	408	LHG	C29-C30-C31-C32
23	B	601	CLA	C2-C3-C5-C6
23	c	510	CLA	C10-C11-C12-C13
27	C	518	LMG	C28-C29-C30-C31
29	D	407	LHG	C35-C36-C37-C38
28	A	414	SQD	C18-C19-C20-C21
28	f	101	SQD	C46-C45-O47-C7
23	b	603	CLA	C2A-CAA-CBA-CGA
30	a	414	DGD	CEB-CFB-CGB-CHB
23	A	404	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	D	402	CLA	C2-C1-O2A-CGA
30	c	517	DGD	C9B-CAB-CBB-CCB
23	a	408	CLA	C16-C17-C18-C20
23	B	607	CLA	O1A-CGA-O2A-C1
30	A	415	DGD	O1A-C1A-O1G-C1G
28	f	101	SQD	C25-C26-C27-C28
29	l	101	LHG	C33-C34-C35-C36
23	B	615	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
25	b	619	BCR	C23-C24-C25-C30
27	c	523	LMG	C35-C36-C37-C38
29	l	101	LHG	C24-C25-C26-C27
30	C	516	DGD	C6B-C7B-C8B-C9B
23	B	607	CLA	CBA-CGA-O2A-C1
23	D	402	CLA	C2C-C3C-CAC-CBC
27	m	101	LMG	O6-C1-O1-C7
30	C	515	DGD	O6E-C1E-O5D-C6D
28	B	624	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	CDA-CEA-CFA-CGA
23	a	406	CLA	C8-C10-C11-C12
25	c	515	BCR	C12-C13-C14-C15
30	C	515	DGD	C2E-C1E-O5D-C6D
30	c	516	DGD	O1G-C1G-C2G-O2G
27	B	621	LMG	C35-C36-C37-C38
29	l	101	LHG	C4-O6-P-O3
30	c	516	DGD	C2A-C3A-C4A-C5A
30	c	518	DGD	C8A-C9A-CAA-CBA
30	H	102	DGD	C7B-C8B-C9B-CAB
28	F	101	SQD	C30-C31-C32-C33
30	C	515	DGD	C5B-C6B-C7B-C8B
29	e	101	LHG	C4-C5-C6-O8
29	l	101	LHG	C4-C5-C6-O8
30	A	415	DGD	C4D-C5D-C6D-O5D
23	C	502	CLA	C6-C7-C8-C10
23	C	511	CLA	C6-C7-C8-C10
23	c	509	CLA	C11-C12-C13-C15
23	d	402	CLA	C2C-C3C-CAC-CBC
23	B	614	CLA	C14-C13-C15-C16
23	C	513	CLA	C14-C13-C15-C16
23	D	403	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	501	CLA	C11-C12-C13-C14
29	d	407	LHG	C35-C36-C37-C38
29	d	408	LHG	C23-C24-C25-C26
30	C	516	DGD	C9B-CAB-CBB-CCB
23	c	510	CLA	CBA-CGA-O2A-C1
29	D	407	LHG	C34-C35-C36-C37
29	l	101	LHG	C13-C14-C15-C16
30	h	102	DGD	C5A-C6A-C7A-C8A
29	d	406	LHG	C27-C28-C29-C30
29	l	101	LHG	C35-C36-C37-C38
30	h	102	DGD	CDA-CEA-CFA-CGA
29	B	622	LHG	C25-C26-C27-C28
23	C	507	CLA	C5-C6-C7-C8
23	b	609	CLA	C5-C6-C7-C8
23	c	513	CLA	C3-C5-C6-C7
29	B	623	LHG	C31-C32-C33-C34
28	a	412	SQD	O49-C7-O47-C45
29	d	407	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	B	609	CLA	C2-C3-C5-C6
23	C	504	CLA	C2-C3-C5-C6
27	c	521	LMG	C30-C31-C32-C33
29	B	622	LHG	C12-C13-C14-C15
27	m	101	LMG	C16-C17-C18-C19
30	h	102	DGD	C3A-C4A-C5A-C6A
25	A	409	BCR	C13-C14-C15-C16
25	k	102	BCR	C15-C16-C17-C18
30	A	415	DGD	C4A-C5A-C6A-C7A
26	d	405	PL9	C34-C36-C37-C38
23	c	510	CLA	O1A-CGA-O2A-C1
27	C	518	LMG	C18-C19-C20-C21
23	B	609	CLA	C4-C3-C5-C6
23	B	604	CLA	C2C-C3C-CAC-CBC
23	C	507	CLA	C15-C16-C17-C18
28	F	101	SQD	C32-C33-C34-C35
29	A	413	LHG	C35-C36-C37-C38
30	c	517	DGD	C8A-C9A-CAA-CBA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
23	d	402	CLA	C2-C1-O2A-CGA
23	a	406	CLA	C13-C15-C16-C17
23	b	615	CLA	C2A-CAA-CBA-CGA
28	A	412	SQD	C17-C18-C19-C20
28	B	624	SQD	C18-C19-C20-C21
27	D	409	LMG	C11-C12-C13-C14
23	d	403	CLA	C3A-C2A-CAA-CBA
23	c	503	CLA	C15-C16-C17-C18
23	b	603	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C19
27	b	622	LMG	C19-C20-C21-C22
28	A	414	SQD	C11-C12-C13-C14
28	a	413	SQD	C27-C28-C29-C30
23	A	404	CLA	O1D-CGD-O2D-CED
27	B	621	LMG	C37-C38-C39-C40
27	b	622	LMG	C17-C18-C19-C20
26	d	405	PL9	C45-C44-C46-C47
30	c	518	DGD	C4B-C5B-C6B-C7B
26	A	410	PL9	C4-C3-C7-C8
27	m	101	LMG	C36-C37-C38-C39
29	l	101	LHG	C30-C31-C32-C33
30	a	414	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	C6-C7-C8-C9
23	B	606	CLA	C11-C10-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	C	509	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
29	D	407	LHG	C10-C11-C12-C13
27	c	521	LMG	C41-C42-C43-C44
27	c	523	LMG	C31-C32-C33-C34
28	A	414	SQD	C26-C27-C28-C29
27	b	622	LMG	C7-C8-C9-O8
29	d	407	LHG	O9-C7-O7-C5
29	d	406	LHG	O10-C23-O8-C6
26	A	410	PL9	C12-C13-C14-C15
23	d	402	CLA	C16-C17-C18-C20
24	a	407	PHO	O2A-C1-C2-C3
27	b	622	LMG	C4-C5-C6-O5
30	C	516	DGD	O6D-C1D-O3G-C3G
25	b	618	BCR	C11-C12-C13-C35
23	b	607	CLA	C3-C5-C6-C7
23	B	602	CLA	C1A-C2A-CAA-CBA
23	d	403	CLA	C16-C17-C18-C20
23	B	601	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	b	607	CLA	C11-C12-C13-C15
23	d	402	CLA	C11-C12-C13-C15
23	h	101	CLA	C12-C13-C15-C16
29	B	622	LHG	C28-C29-C30-C31
23	b	605	CLA	C13-C15-C16-C17
27	b	623	LMG	C33-C34-C35-C36
30	C	515	DGD	C2B-C3B-C4B-C5B
30	a	414	DGD	C5A-C6A-C7A-C8A
23	c	501	CLA	C2A-CAA-CBA-CGA
29	d	408	LHG	O1-C1-C2-O2
27	c	523	LMG	C18-C19-C20-C21
23	C	510	CLA	C10-C11-C12-C13
30	c	517	DGD	C3B-C4B-C5B-C6B
23	c	512	CLA	C16-C17-C18-C19
23	b	604	CLA	C5-C6-C7-C8
29	A	413	LHG	C9-C10-C11-C12
23	c	508	CLA	C4-C3-C5-C6
26	A	410	PL9	C30-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
28	a	413	SQD	C31-C32-C33-C34
29	B	623	LHG	C23-C24-C25-C26
27	A	411	LMG	C39-C40-C41-C42
28	a	412	SQD	C24-C25-C26-C27
23	C	501	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	O1D-CGD-O2D-CED
25	c	514	BCR	C15-C16-C17-C18
25	c	515	BCR	C15-C16-C17-C18
30	c	516	DGD	C3B-C4B-C5B-C6B
30	c	518	DGD	C4A-C5A-C6A-C7A
23	B	607	CLA	C16-C17-C18-C20
23	C	505	CLA	C16-C17-C18-C20
26	D	405	PL9	C24-C26-C27-C28
27	D	409	LMG	O1-C7-C8-C9
29	D	407	LHG	C13-C14-C15-C16
30	C	515	DGD	C9A-CAA-CBA-CCA
23	B	615	CLA	C2-C3-C5-C6
23	B	610	CLA	C15-C16-C17-C18
23	A	405	CLA	C4C-C3C-CAC-CBC
30	c	516	DGD	O1G-C1A-C2A-C3A
23	B	606	CLA	C16-C17-C18-C20
23	a	408	CLA	C6-C7-C8-C9
23	b	616	CLA	C14-C13-C15-C16
24	A	407	PHO	C6-C7-C8-C9
27	d	409	LMG	C32-C33-C34-C35
23	B	616	CLA	O1A-CGA-O2A-C1
29	B	623	LHG	O2-C2-C3-O3
30	C	517	DGD	CBB-CCB-CDB-CEB
23	a	406	CLA	C10-C11-C12-C13
23	b	615	CLA	C16-C17-C18-C19
23	c	502	CLA	O1A-CGA-O2A-C1
25	A	409	BCR	C23-C24-C25-C30
25	B	618	BCR	C23-C24-C25-C30
25	K	101	BCR	C23-C24-C25-C30
25	K	102	BCR	C1-C6-C7-C8
25	Z	101	BCR	C23-C24-C25-C30
25	x	101	BCR	C23-C24-C25-C30
27	m	101	LMG	C35-C36-C37-C38
30	c	516	DGD	O1G-C1G-C2G-C3G
25	K	102	BCR	C13-C14-C15-C16
23	B	613	CLA	C4-C3-C5-C6
23	B	607	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	a	408	CLA	C2-C3-C5-C6
28	B	624	SQD	O10-C23-O48-C46
25	A	409	BCR	C14-C15-C16-C17
30	c	516	DGD	C5D-C6D-O5D-C1E
30	A	415	DGD	CBB-CCB-CDB-CEB
23	C	513	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C20
23	C	510	CLA	C15-C16-C17-C18
23	B	603	CLA	C13-C15-C16-C17
28	F	101	SQD	C35-C36-C37-C38
28	b	601	SQD	C29-C30-C31-C32
29	d	408	LHG	C9-C10-C11-C12
24	A	406	PHO	C15-C16-C17-C18
23	C	505	CLA	C6-C7-C8-C10
23	b	605	CLA	C6-C7-C8-C10
23	b	616	CLA	C12-C13-C15-C16
23	c	506	CLA	C6-C7-C8-C10
23	c	508	CLA	C2-C3-C5-C6
23	B	615	CLA	C13-C15-C16-C17
23	b	610	CLA	C13-C15-C16-C17
27	c	523	LMG	C15-C16-C17-C18
30	c	516	DGD	C3A-C4A-C5A-C6A
27	D	409	LMG	O1-C7-C8-O7
23	c	511	CLA	C16-C17-C18-C19
29	d	407	LHG	C15-C16-C17-C18
29	l	101	LHG	O7-C5-C6-O8
28	f	101	SQD	C26-C27-C28-C29
25	C	514	BCR	C35-C13-C14-C15
25	C	514	BCR	C16-C17-C18-C36
25	D	404	BCR	C20-C21-C22-C37
25	T	101	BCR	C35-C13-C14-C15
25	c	515	BCR	C16-C17-C18-C36
28	B	624	SQD	O47-C7-C8-C9
23	c	506	CLA	C4-C3-C5-C6
26	D	405	PL9	C45-C44-C46-C47
26	a	410	PL9	C20-C19-C21-C22
26	a	410	PL9	C25-C24-C26-C27
23	C	509	CLA	C8-C10-C11-C12
29	D	408	LHG	C35-C36-C37-C38
30	c	517	DGD	CAA-CBA-CCA-CDA
26	D	405	PL9	C43-C44-C46-C47
23	B	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	C14-C13-C15-C16
23	B	605	CLA	C14-C13-C15-C16
23	C	505	CLA	C6-C7-C8-C9
23	D	402	CLA	C6-C7-C8-C9
23	b	613	CLA	C11-C10-C8-C9
24	a	407	PHO	C6-C7-C8-C9
28	b	601	SQD	C17-C18-C19-C20
23	C	501	CLA	O1A-CGA-O2A-C1
30	C	517	DGD	O6D-C5D-C6D-O5D
28	A	412	SQD	O47-C7-C8-C9
30	a	414	DGD	O2G-C1B-C2B-C3B
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	b	605	CLA	CAD-CBD-CGD-O2D
23	b	608	CLA	CAD-CBD-CGD-O2D
23	b	617	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CAD-CBD-CGD-O2D
23	c	510	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
26	a	410	PL9	C37-C38-C39-C40
28	A	414	SQD	C27-C28-C29-C30
29	D	408	LHG	C15-C16-C17-C18
23	b	615	CLA	C8-C10-C11-C12
23	b	611	CLA	C8-C10-C11-C12
29	A	413	LHG	C34-C35-C36-C37
26	a	410	PL9	C40-C39-C41-C42
23	c	506	CLA	C3-C5-C6-C7
27	C	518	LMG	C15-C16-C17-C18
27	b	622	LMG	O7-C10-C11-C12
27	m	101	LMG	O7-C10-C11-C12
27	A	411	LMG	O1-C7-C8-C9
27	C	518	LMG	O1-C7-C8-C9
27	c	523	LMG	O1-C7-C8-C9
27	m	101	LMG	O1-C7-C8-C9
30	c	516	DGD	C1G-C2G-C3G-O3G
30	a	414	DGD	C8B-C9B-CAB-CBB
29	d	408	LHG	C30-C31-C32-C33
23	B	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	c	518	DGD	O1G-C1A-C2A-C3A
23	C	509	CLA	O2A-C1-C2-C3
23	D	403	CLA	O2A-C1-C2-C3
23	h	101	CLA	O2A-C1-C2-C3
24	A	406	PHO	O2A-C1-C2-C3
23	C	501	CLA	C2A-CAA-CBA-CGA
28	a	412	SQD	O47-C7-C8-C9
23	c	509	CLA	CAA-CBA-CGA-O1A
23	B	601	CLA	C16-C17-C18-C20
23	b	603	CLA	C16-C17-C18-C20
23	c	504	CLA	C11-C12-C13-C15
29	l	101	LHG	C16-C17-C18-C19
23	B	604	CLA	CBD-CGD-O2D-CED
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	a	411	CLA	CHA-CBD-CGD-O1D
23	a	411	CLA	CHA-CBD-CGD-O2D
23	b	607	CLA	CHA-CBD-CGD-O2D
23	b	610	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
24	A	407	PHO	CHA-CBD-CGD-O2D
24	A	406	PHO	C4-C3-C5-C6
30	c	516	DGD	O2G-C1B-C2B-C3B
28	B	624	SQD	C32-C33-C34-C35
25	c	515	BCR	C20-C21-C22-C23
27	m	101	LMG	C2-C1-O1-C7
23	B	607	CLA	C15-C16-C17-C18
23	C	513	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12
29	B	622	LHG	O7-C7-C8-C9
28	A	412	SQD	C27-C28-C29-C30
23	C	510	CLA	C8-C10-C11-C12
30	C	515	DGD	O2G-C1B-C2B-C3B
27	d	409	LMG	C15-C16-C17-C18
29	D	407	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	h	101	CLA	C4-C3-C5-C6
23	B	615	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	c	509	CLA	C11-C10-C8-C7
23	c	512	CLA	C12-C13-C15-C16
23	b	615	CLA	C16-C17-C18-C20
28	b	601	SQD	C11-C12-C13-C14
23	B	603	CLA	C14-C13-C15-C16
23	B	604	CLA	C14-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C14
23	C	512	CLA	C14-C13-C15-C16
23	b	604	CLA	C11-C12-C13-C14
23	b	612	CLA	C6-C7-C8-C9
23	c	503	CLA	C11-C10-C8-C9
23	h	101	CLA	C14-C13-C15-C16
29	l	101	LHG	C7-C8-C9-C10
28	A	412	SQD	C12-C13-C14-C15
28	B	624	SQD	C12-C13-C14-C15
27	c	523	LMG	C17-C18-C19-C20
27	C	518	LMG	C19-C20-C21-C22
23	B	603	CLA	C2A-CAA-CBA-CGA
26	D	405	PL9	C36-C37-C38-C39
28	B	624	SQD	O49-C7-C8-C9
28	a	413	SQD	C29-C30-C31-C32
23	c	504	CLA	C11-C12-C13-C14
23	c	512	CLA	C16-C17-C18-C20
29	B	622	LHG	C24-C25-C26-C27
27	c	521	LMG	C37-C38-C39-C40
30	C	516	DGD	CAA-CBA-CCA-CDA
23	b	612	CLA	C1A-C2A-CAA-CBA
23	d	403	CLA	C1A-C2A-CAA-CBA
24	a	407	PHO	C1A-C2A-CAA-CBA
27	c	519	LMG	C37-C38-C39-C40
30	H	102	DGD	CCA-CDA-CEA-CFA
28	a	412	SQD	O10-C23-C24-C25
23	c	512	CLA	C2C-C3C-CAC-CBC
28	B	624	SQD	C30-C31-C32-C33
29	d	408	LHG	C28-C29-C30-C31
29	d	406	LHG	O10-C23-C24-C25
23	B	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C2A-CAA-CBA-CGA
29	A	413	LHG	C11-C12-C13-C14
30	h	102	DGD	CDB-CEB-CFB-CGB
29	e	101	LHG	O2-C2-C3-O3
23	C	501	CLA	C16-C17-C18-C20
28	a	412	SQD	O49-C7-C8-C9
28	F	101	SQD	C44-C45-C46-O48
23	A	405	CLA	C13-C15-C16-C17
23	C	512	CLA	C8-C10-C11-C12
29	D	407	LHG	C26-C27-C28-C29
29	A	413	LHG	C3-O3-P-O5
29	d	406	LHG	C3-O3-P-O5
29	l	101	LHG	C4-O6-P-O5
24	a	407	PHO	O1D-CGD-O2D-CED
30	c	516	DGD	O1B-C1B-C2B-C3B
25	a	409	BCR	C11-C10-C9-C34
27	A	411	LMG	C33-C34-C35-C36
25	K	102	BCR	C5-C6-C7-C8
25	b	619	BCR	C23-C24-C25-C26
23	c	507	CLA	C5-C6-C7-C8
29	e	101	LHG	O10-C23-C24-C25
29	B	623	LHG	C18-C19-C20-C21
30	C	517	DGD	C4E-C5E-C6E-O5E
23	b	613	CLA	CAA-CBA-CGA-O2A
28	A	412	SQD	C32-C33-C34-C35
27	d	409	LMG	O7-C10-C11-C12
27	M	101	LMG	C28-C29-C30-C31
23	B	612	CLA	CAA-CBA-CGA-O1A
29	d	406	LHG	C11-C10-C9-C8
23	B	606	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
27	c	523	LMG	C7-C8-O7-C10
23	B	612	CLA	C11-C10-C8-C9
23	C	507	CLA	C6-C7-C8-C9
23	C	510	CLA	C11-C12-C13-C14
23	C	513	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
23	b	613	CLA	C14-C13-C15-C16
23	b	614	CLA	C14-C13-C15-C16
23	c	511	CLA	C6-C7-C8-C9
23	c	512	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	d	402	CLA	C11-C12-C13-C14
30	C	515	DGD	C4B-C5B-C6B-C7B
30	c	517	DGD	C2A-C3A-C4A-C5A
29	d	407	LHG	O1-C1-C2-O2
24	A	406	PHO	C8-C10-C11-C12
23	B	609	CLA	C3-C5-C6-C7
27	M	101	LMG	C38-C39-C40-C41
23	c	502	CLA	C15-C16-C17-C18
23	c	506	CLA	C8-C10-C11-C12
27	A	411	LMG	C38-C39-C40-C41
30	C	515	DGD	CDB-CEB-CFB-CGB
27	A	411	LMG	C8-C9-O8-C28
23	B	613	CLA	CAA-CBA-CGA-O2A
27	m	101	LMG	O8-C28-C29-C30
29	D	408	LHG	C31-C32-C33-C34
23	C	511	CLA	C11-C12-C13-C15
23	a	408	CLA	C6-C7-C8-C10
23	b	607	CLA	C6-C7-C8-C10
23	b	613	CLA	C12-C13-C15-C16
28	b	601	SQD	O49-C7-C8-C9
29	B	623	LHG	C16-C17-C18-C19
23	c	501	CLA	CAA-CBA-CGA-O2A
28	a	412	SQD	O48-C23-C24-C25
25	B	618	BCR	C11-C12-C13-C14
25	K	101	BCR	C7-C8-C9-C10
25	c	515	BCR	C17-C18-C19-C20
28	A	412	SQD	O49-C7-C8-C9
25	t	101	BCR	C13-C14-C15-C16
27	C	518	LMG	O7-C10-C11-C12
30	C	516	DGD	O1G-C1A-C2A-C3A
30	c	516	DGD	O6E-C1E-O5D-C6D
30	c	517	DGD	O6D-C1D-O3G-C3G
24	d	401	PHO	C2C-C3C-CAC-CBC
23	B	613	CLA	CAA-CBA-CGA-O1A
23	c	501	CLA	CAA-CBA-CGA-O1A
29	d	407	LHG	O9-C7-C8-C9
27	M	101	LMG	C14-C15-C16-C17
30	a	414	DGD	C9B-CAB-CBB-CCB
23	b	615	CLA	C13-C15-C16-C17
26	D	405	PL9	C21-C22-C23-C24
27	c	523	LMG	O8-C28-C29-C30
29	D	408	LHG	O10-C23-C24-C25

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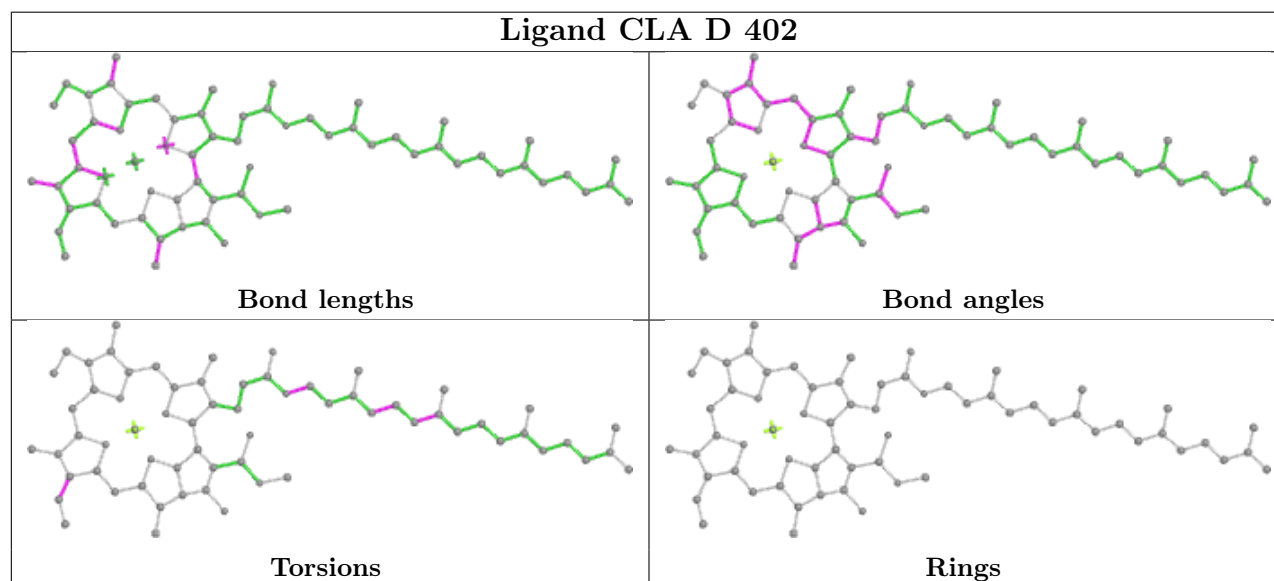
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Mol	Chain	Res	Type	Atoms
23	B	605	CLA	C16-C17-C18-C20
27	b	623	LMG	C39-C40-C41-C42
23	C	503	CLA	C15-C16-C17-C18
23	b	613	CLA	CAA-CBA-CGA-O1A
27	b	622	LMG	O9-C10-C11-C12
29	e	101	LHG	O8-C23-C24-C25

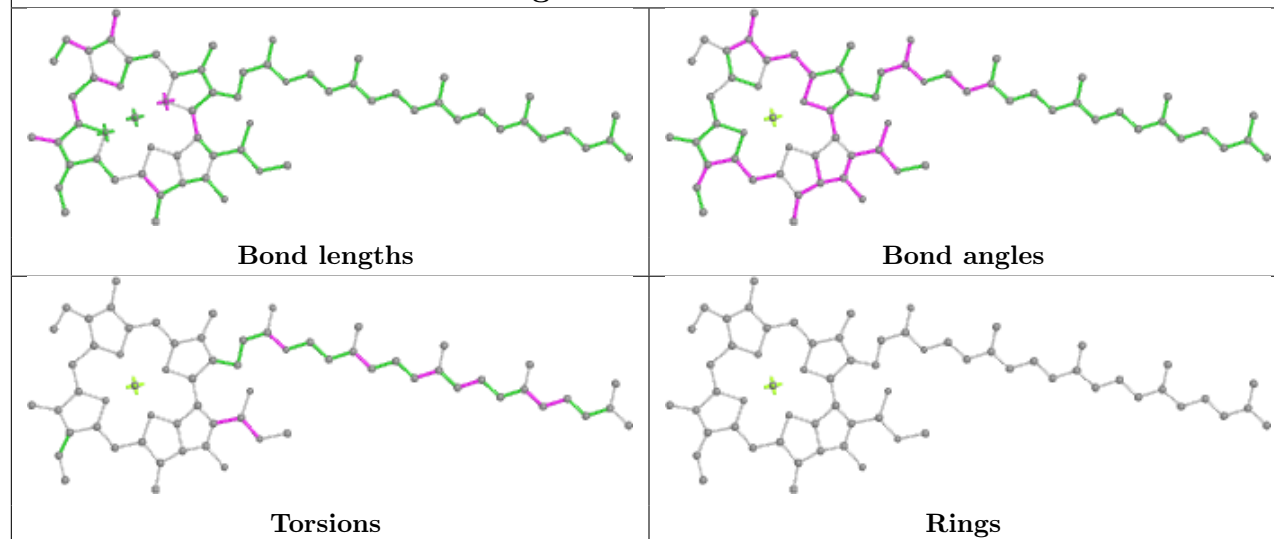
There are no ring outliers.

No monomer is involved in short contacts.

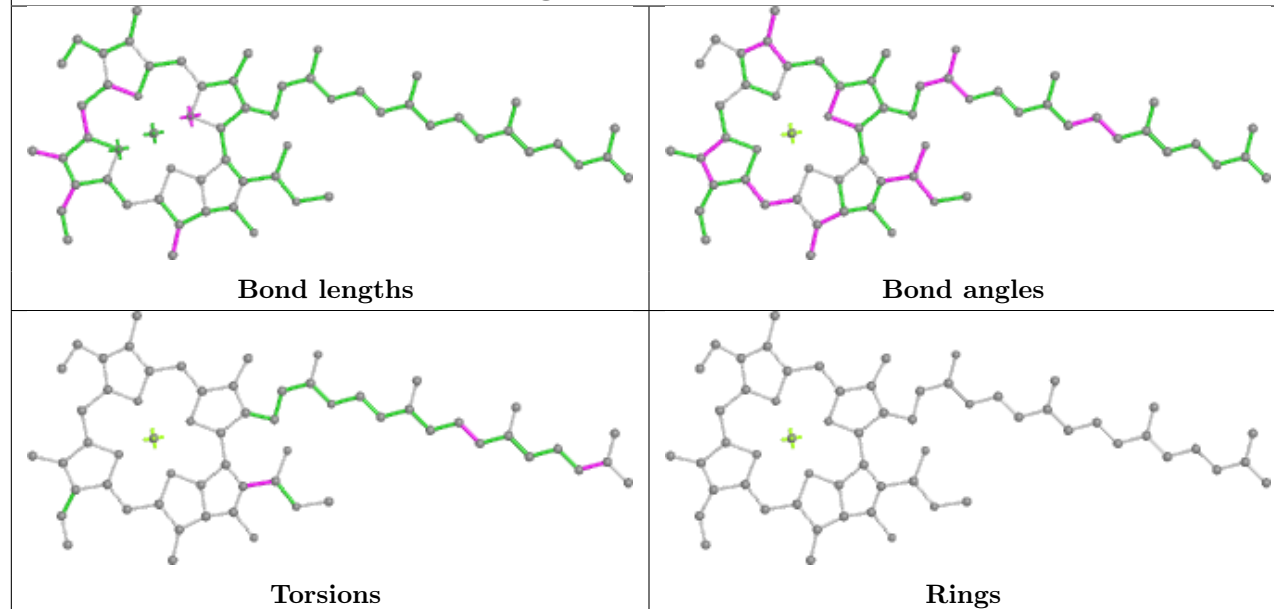
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



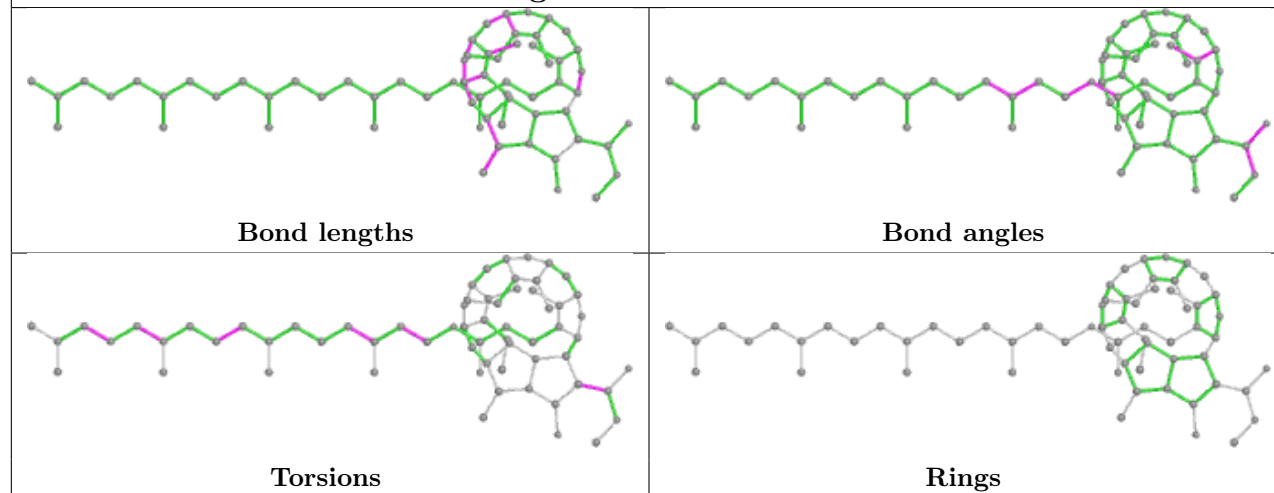
Ligand CLA B 614

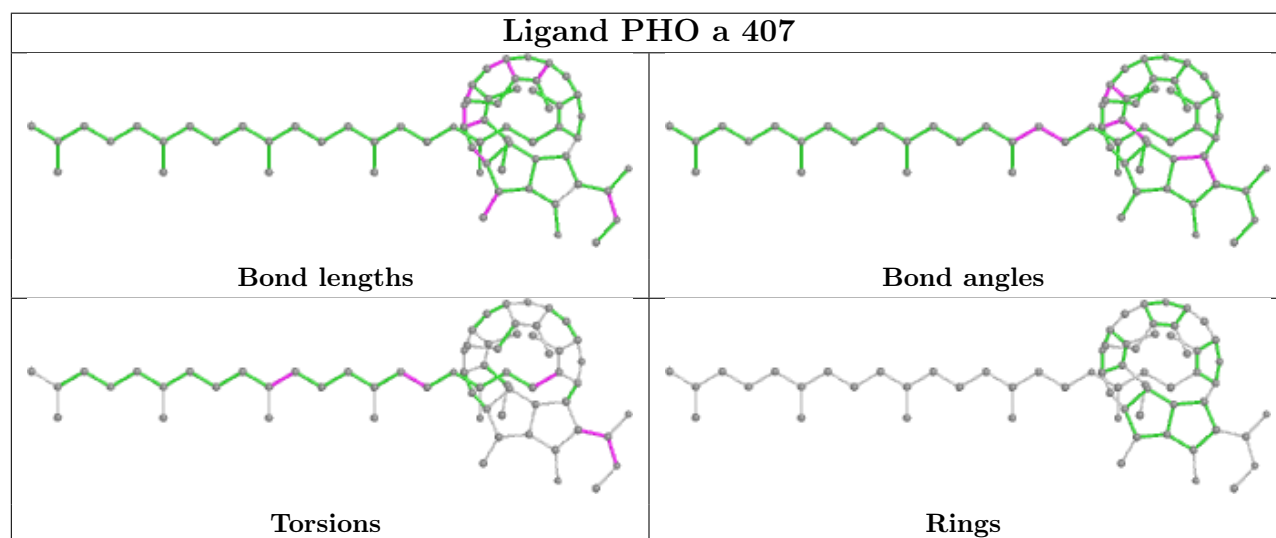
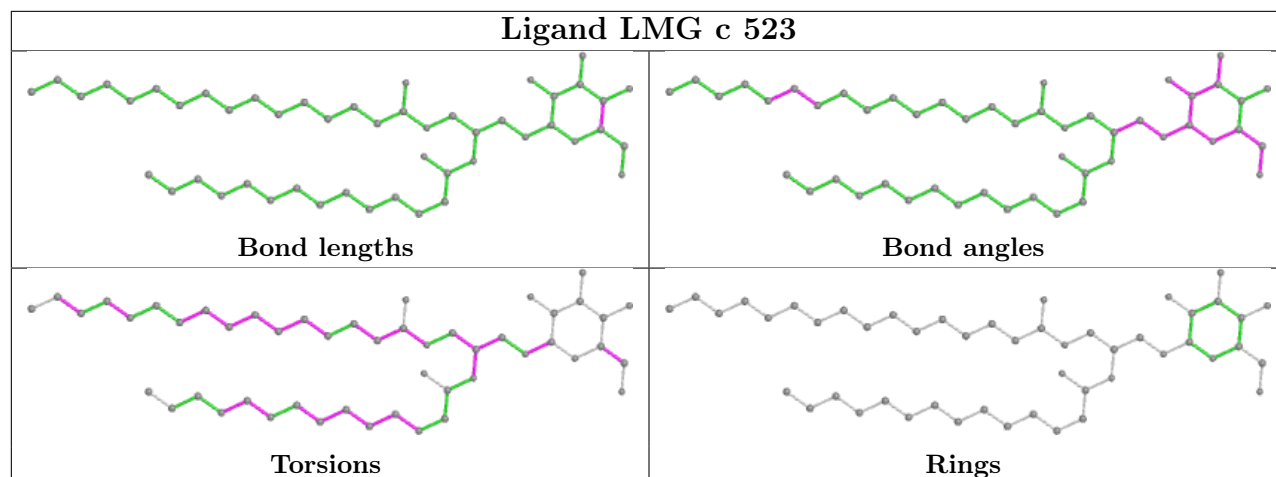
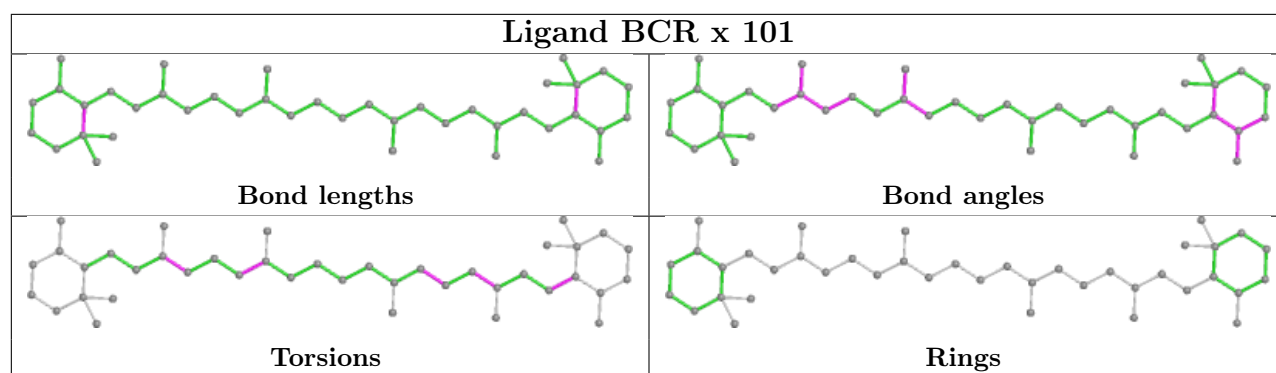


Ligand CLA c 504

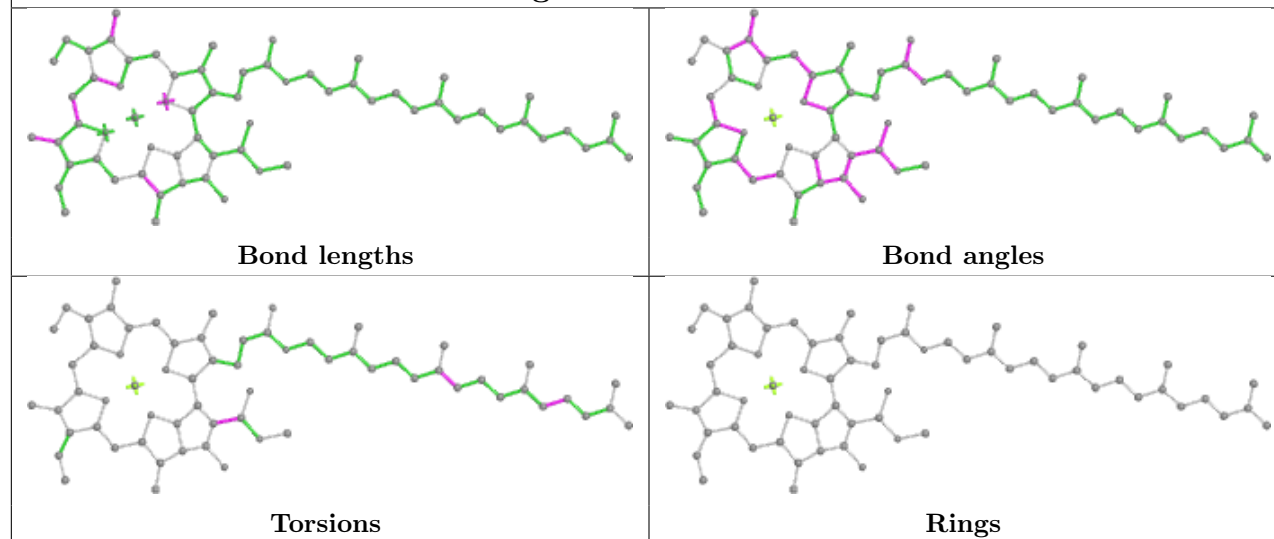


Ligand PHO A 406

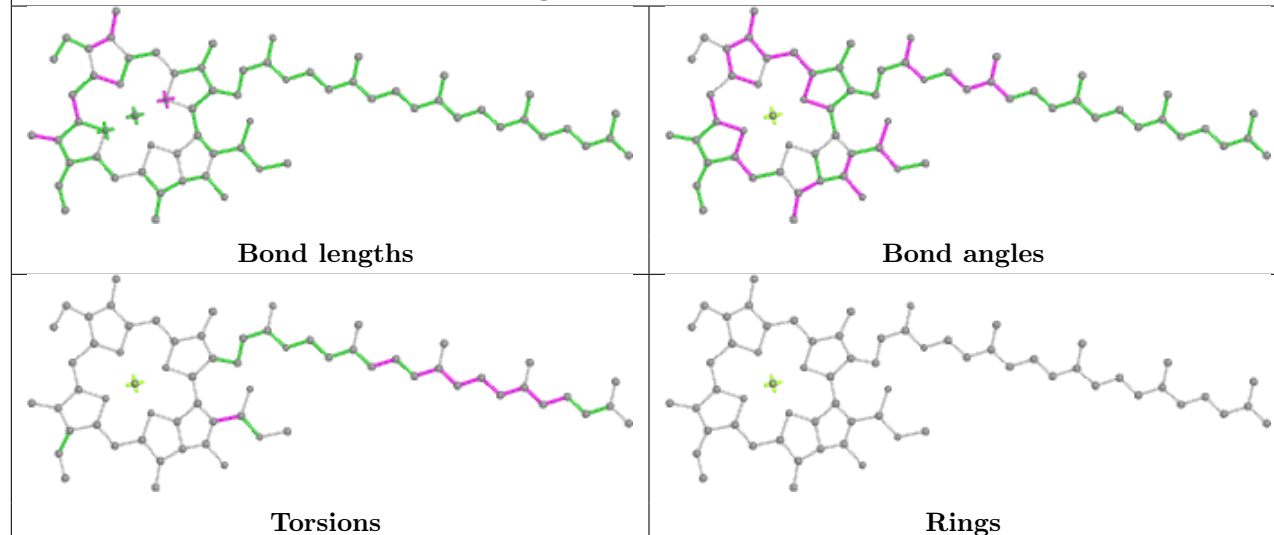




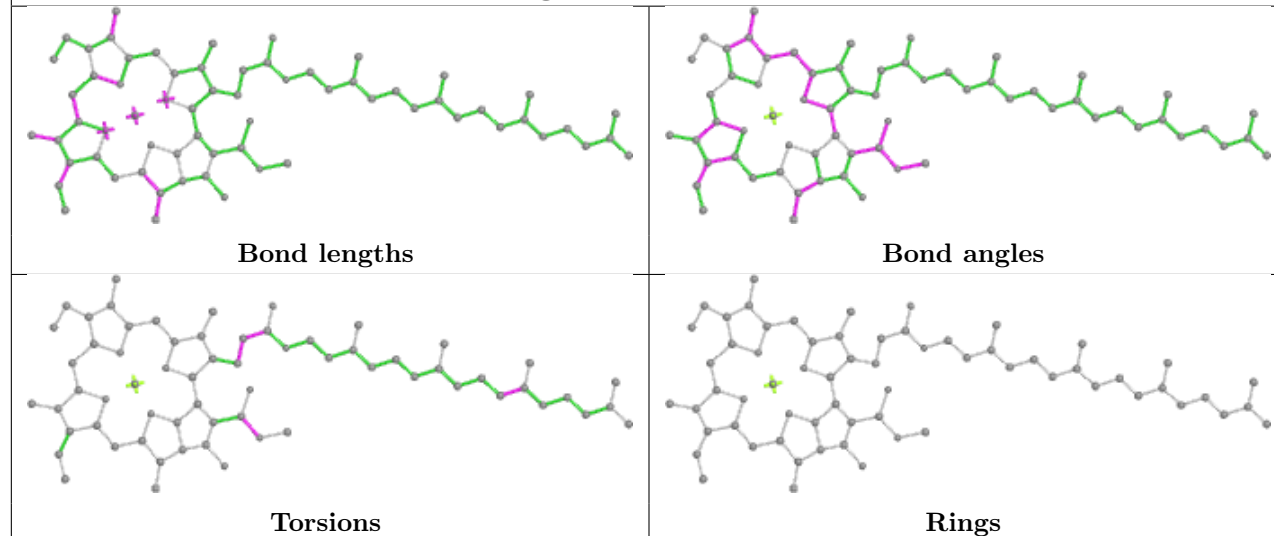
Ligand CLA C 508

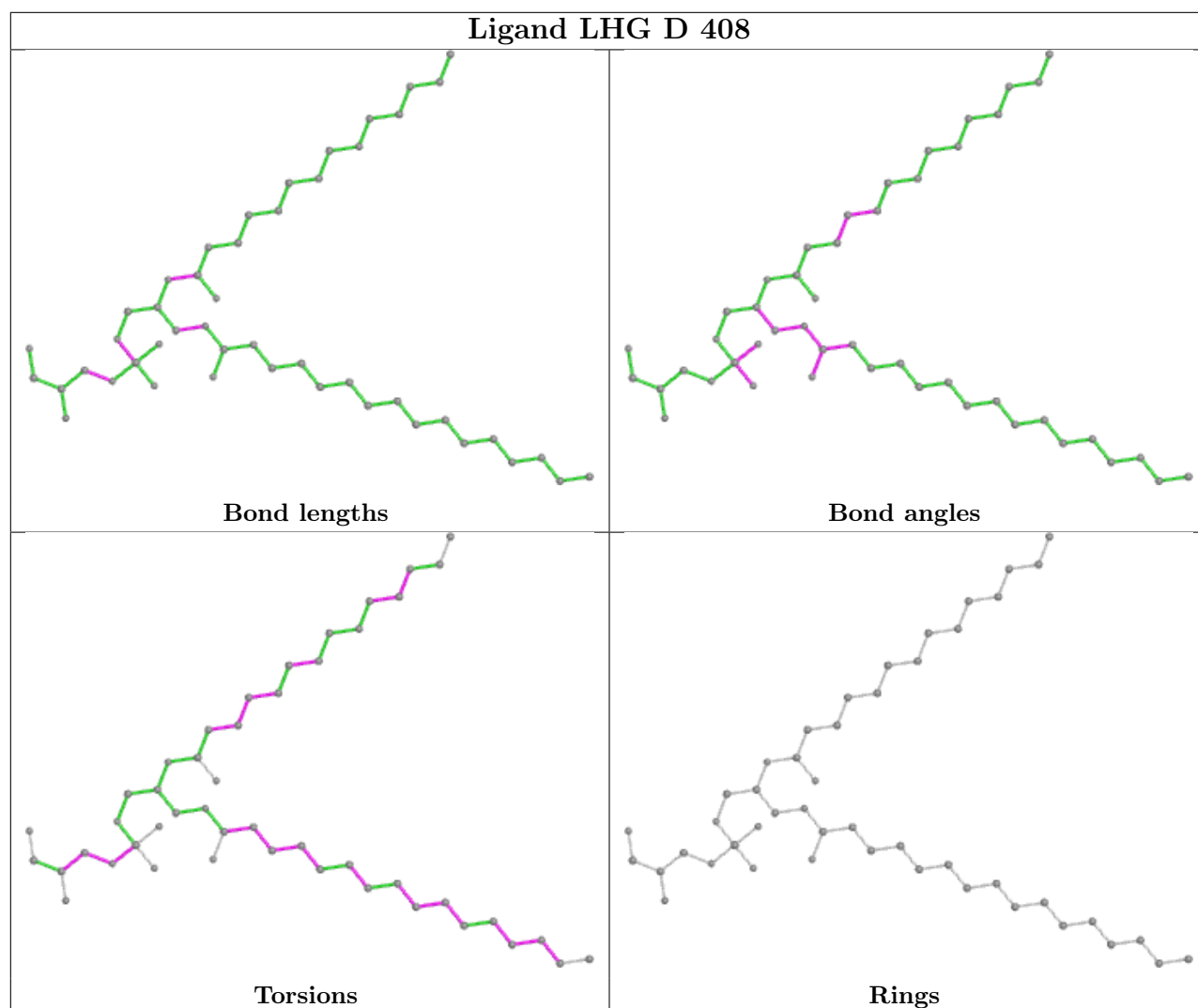
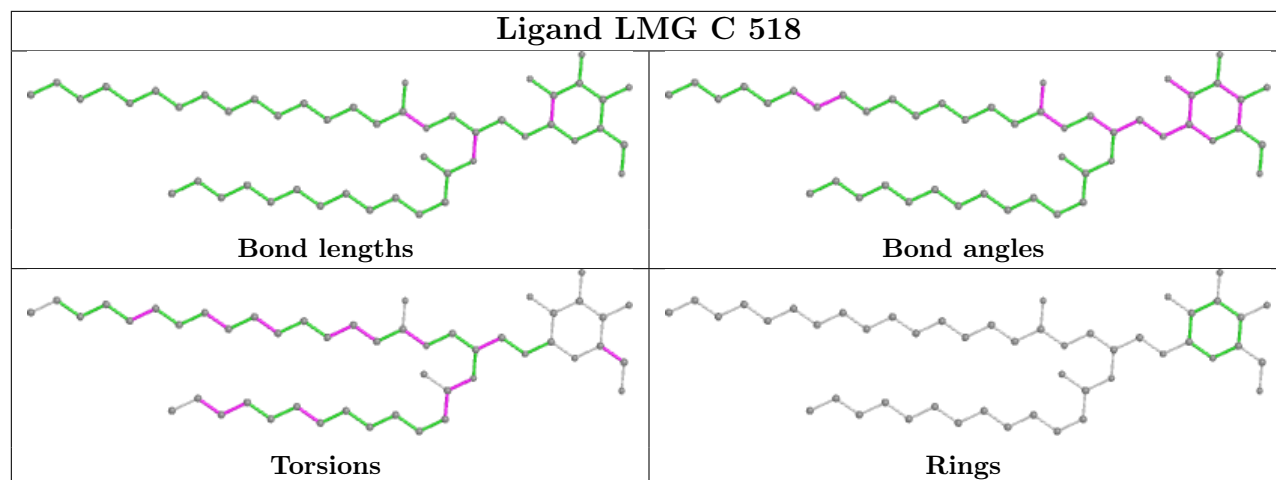


Ligand CLA b 605

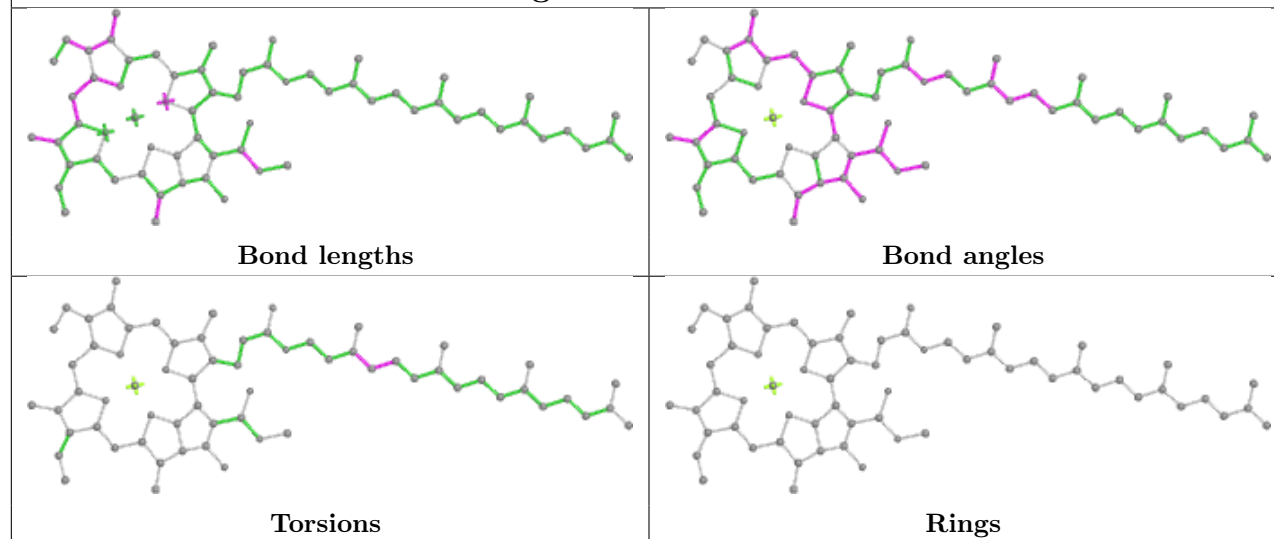


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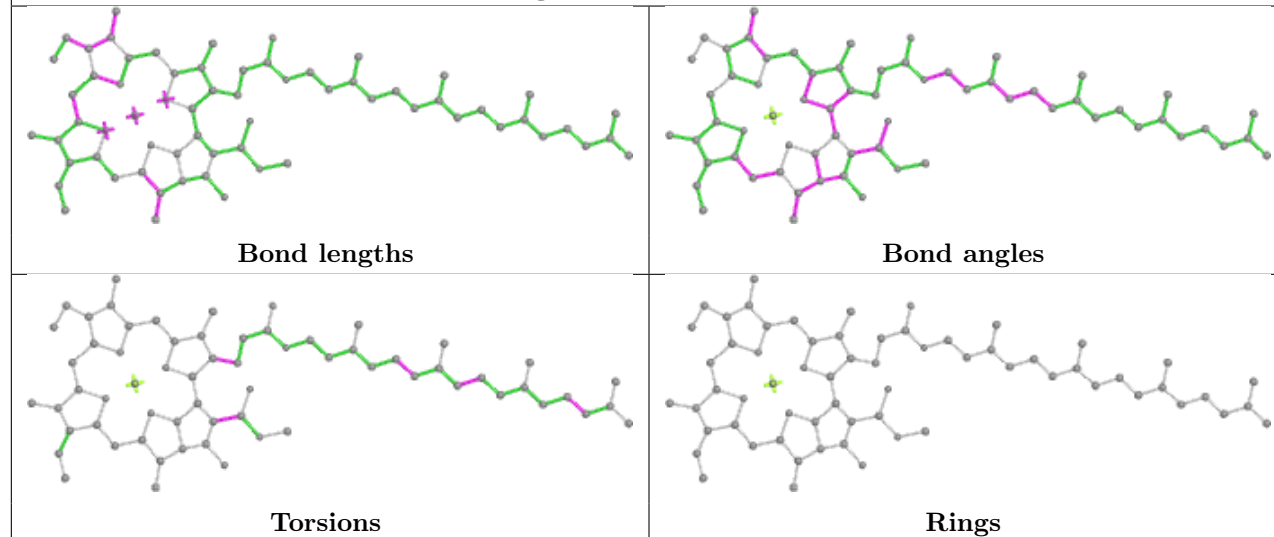




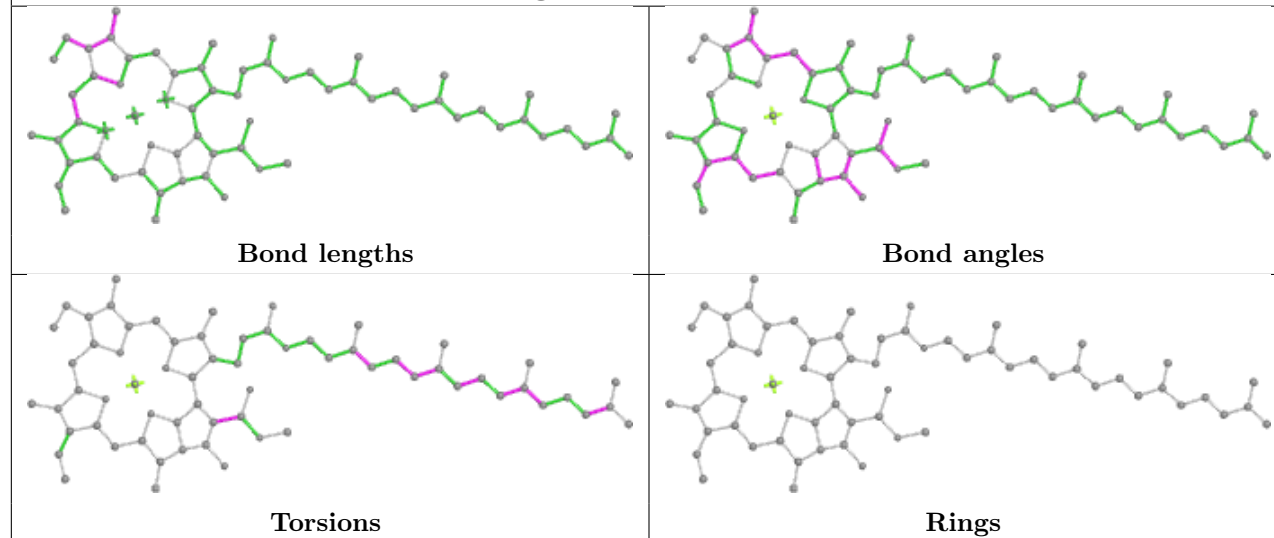
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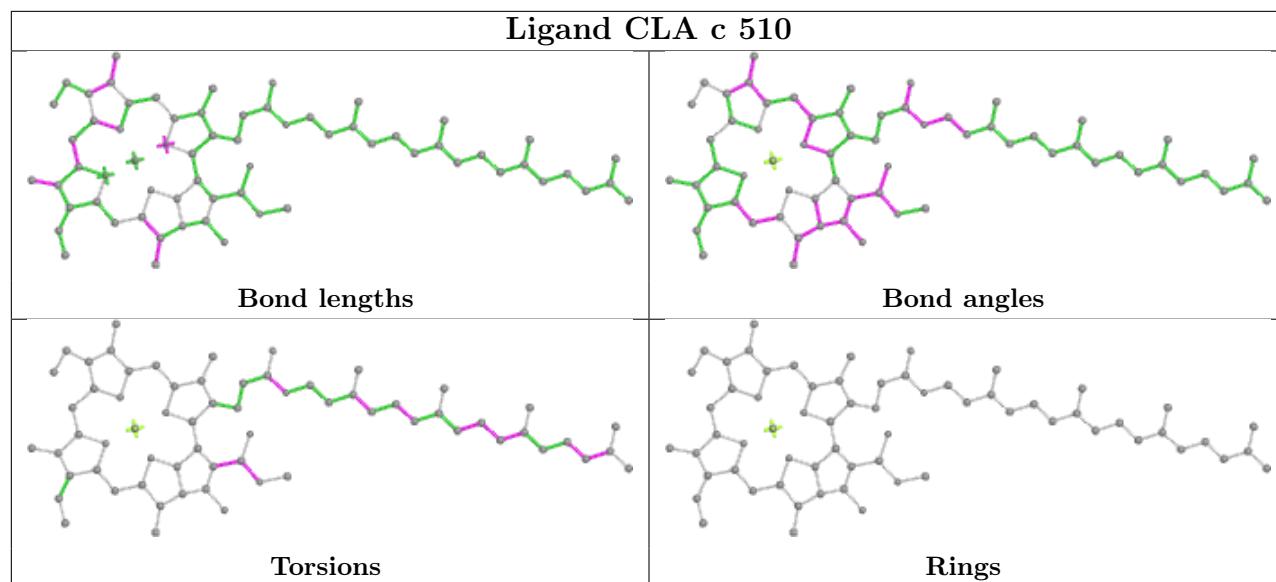
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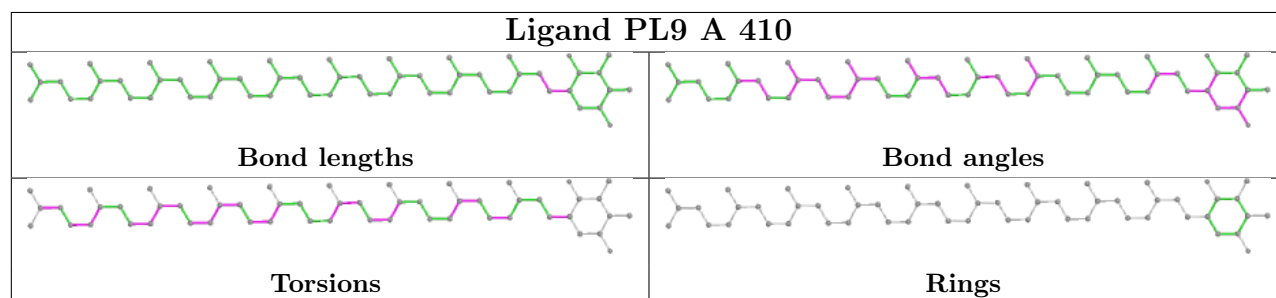
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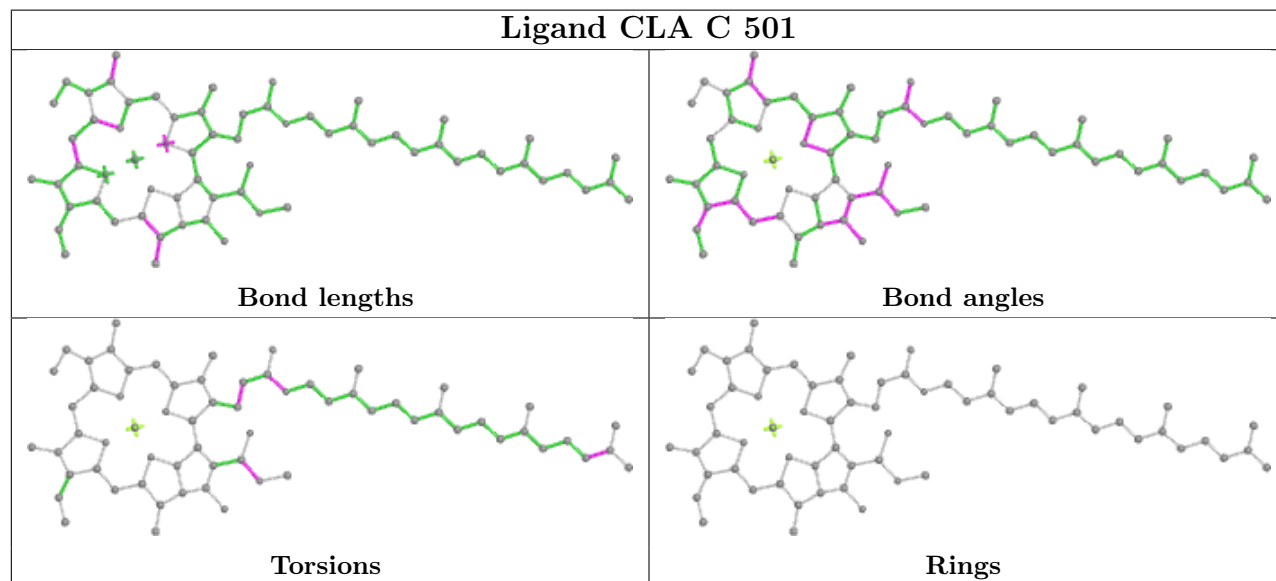
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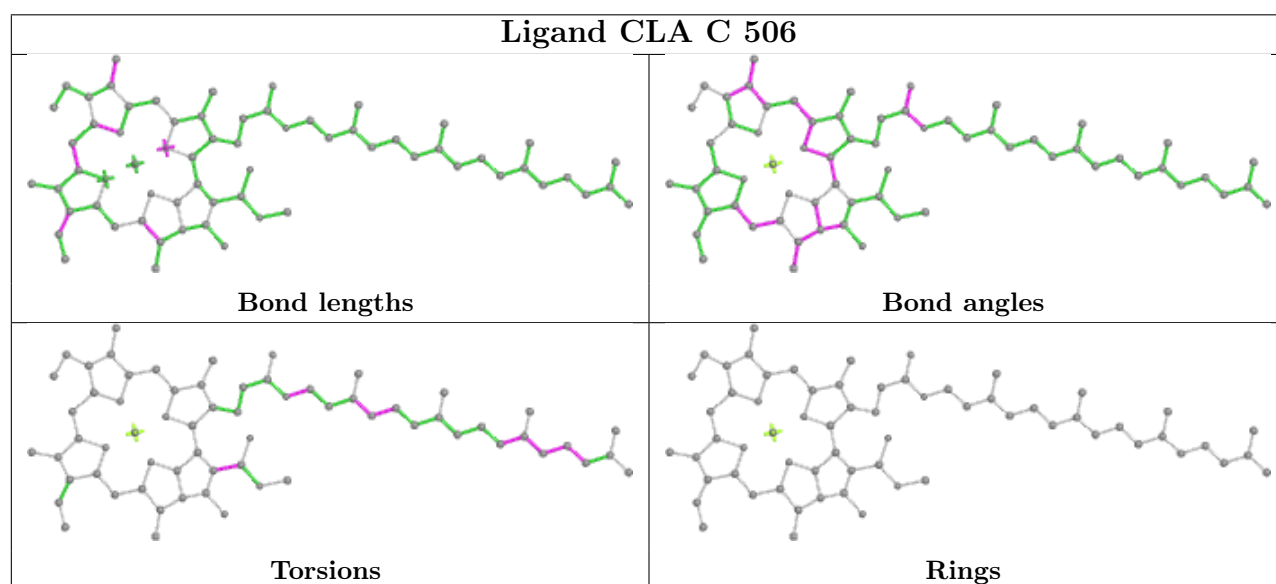
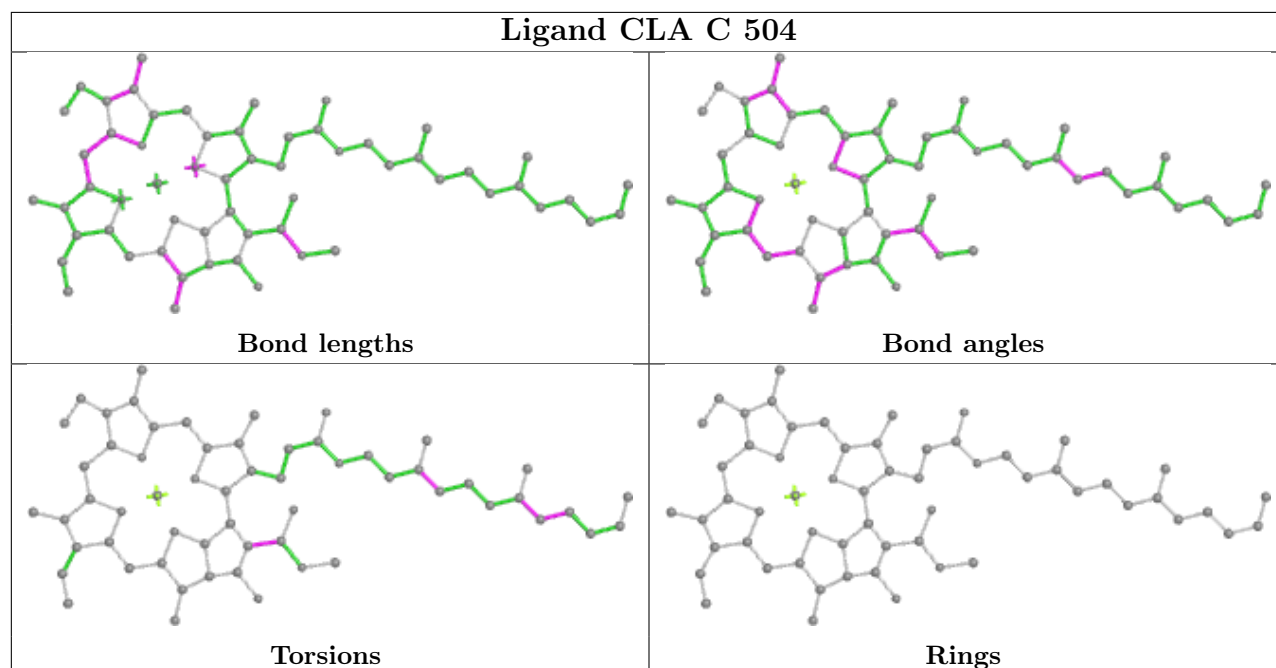
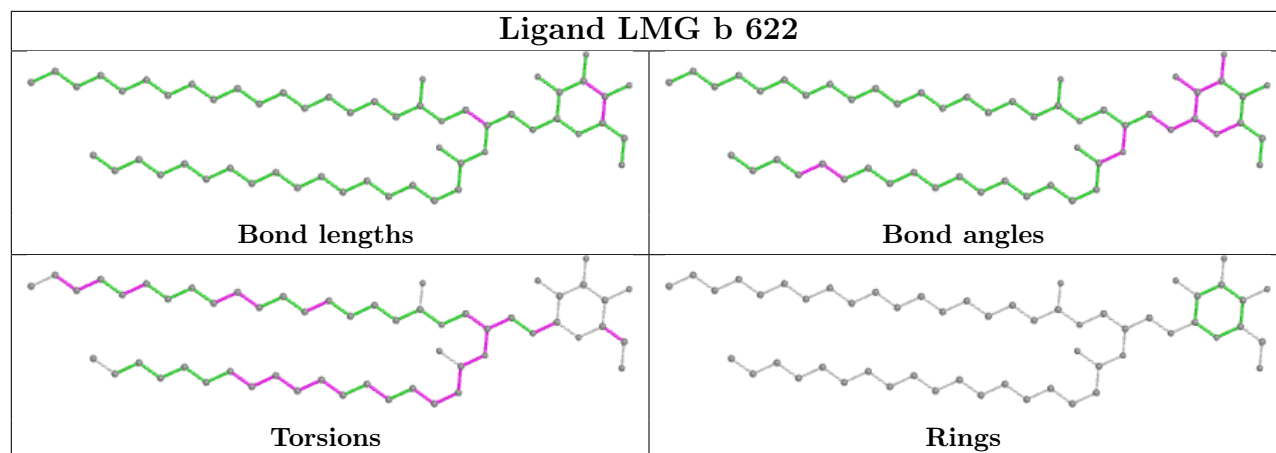


Ligand PL9 A 410

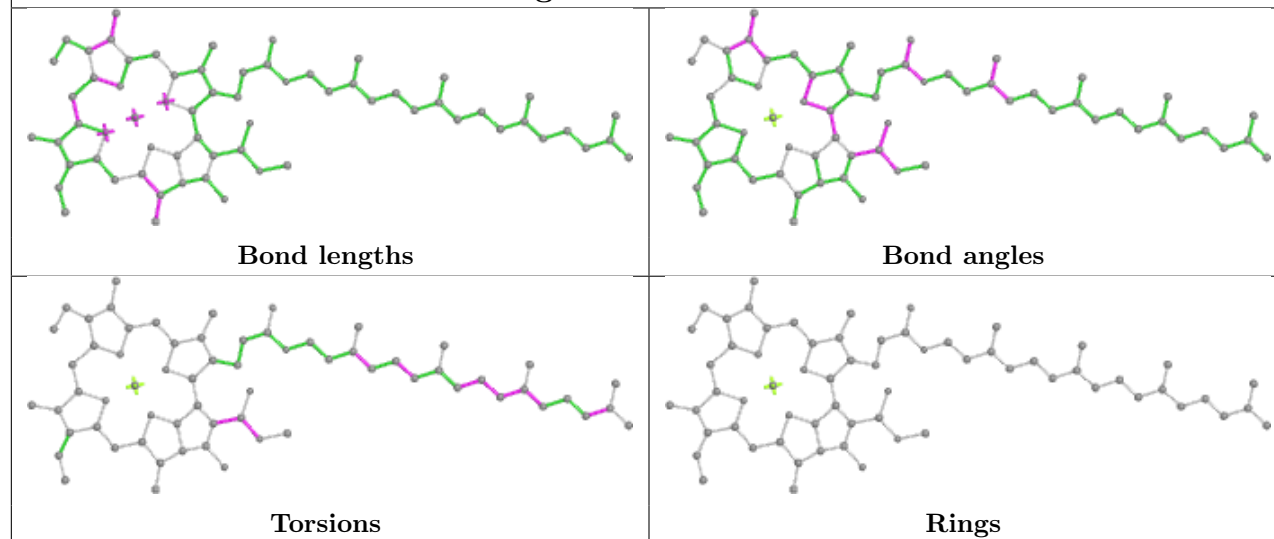


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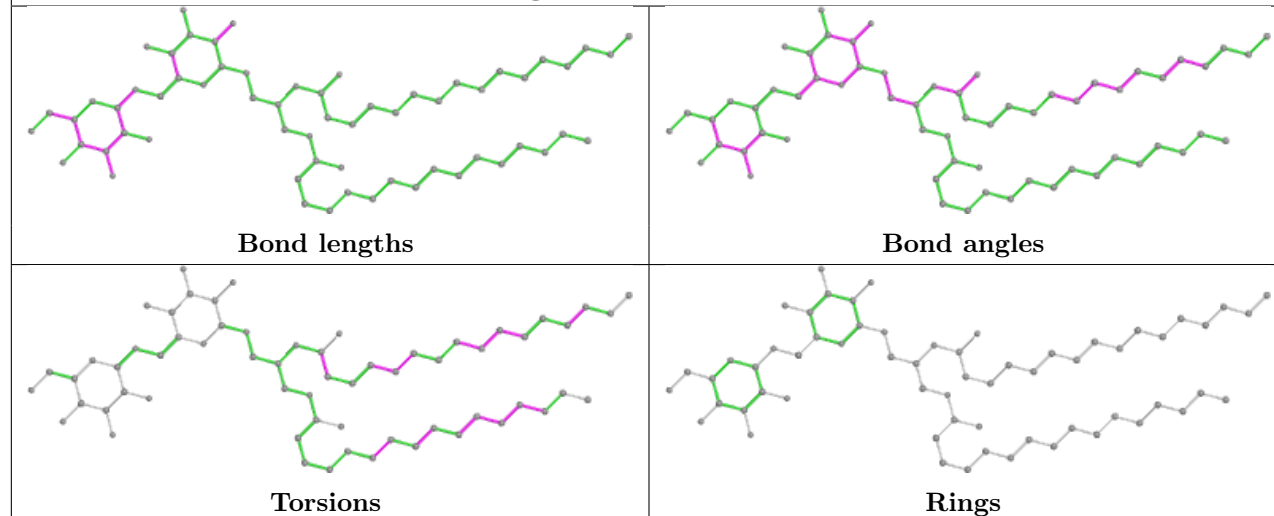




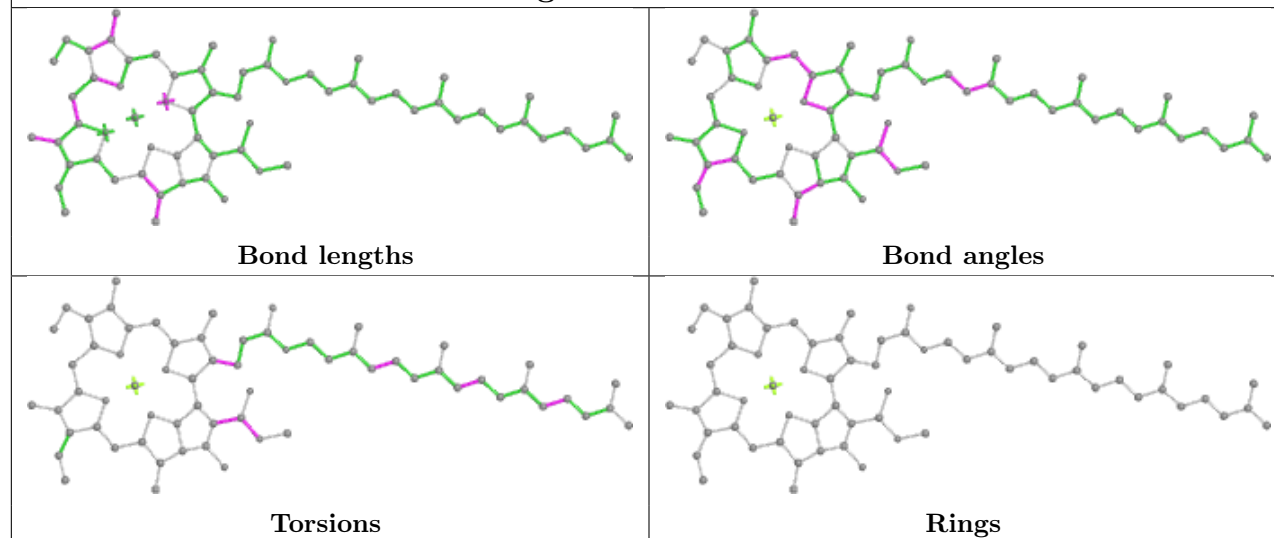
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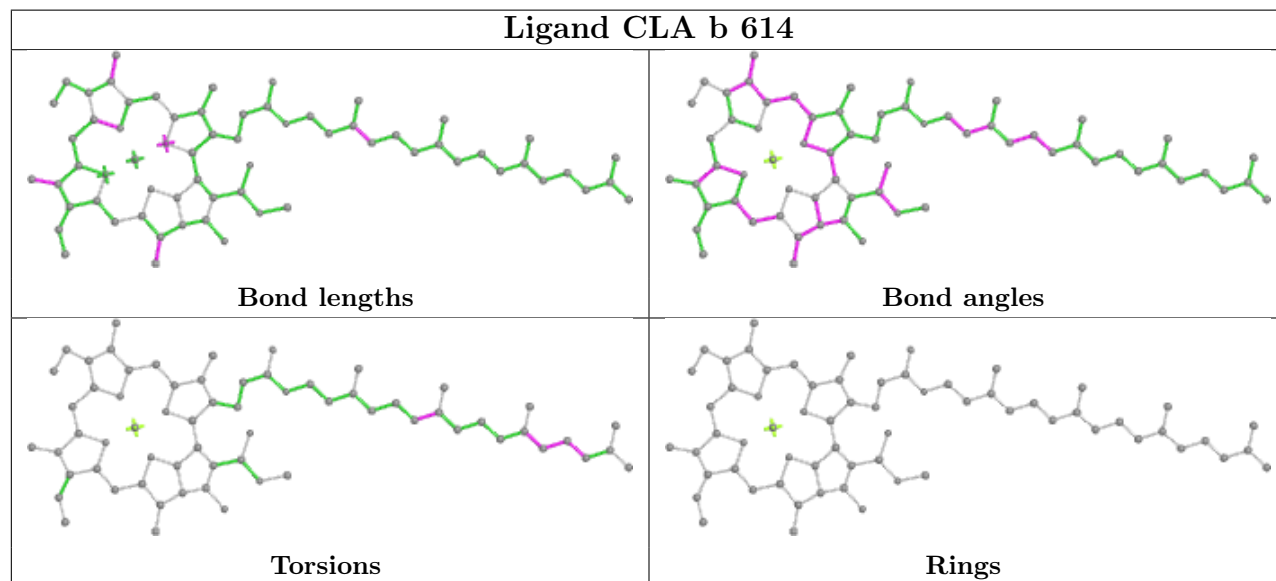
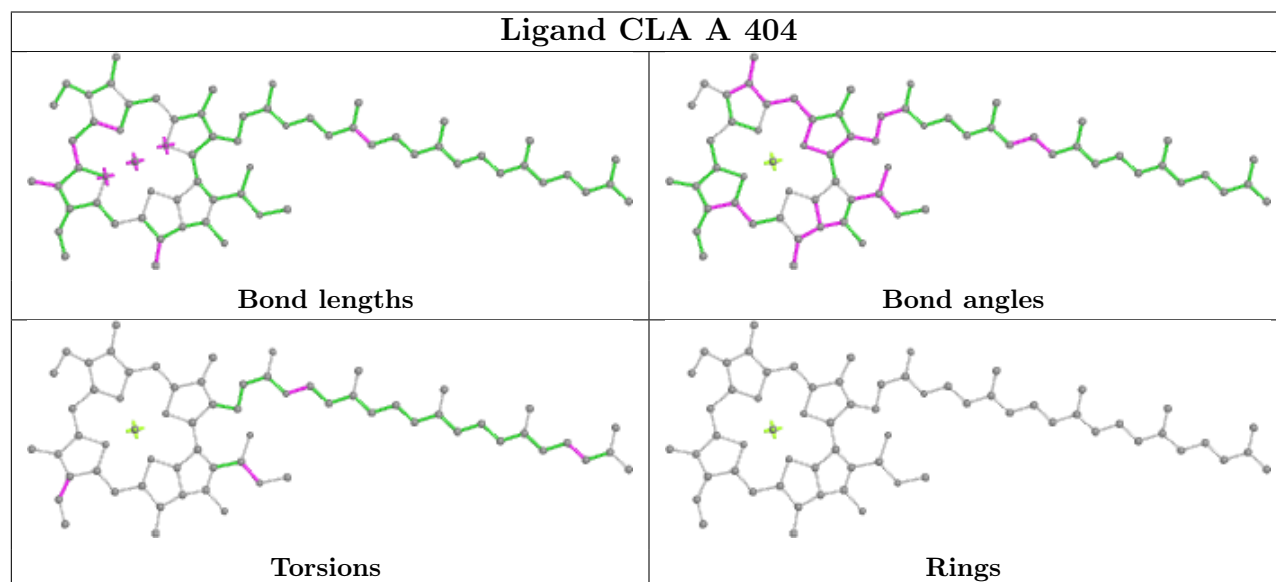
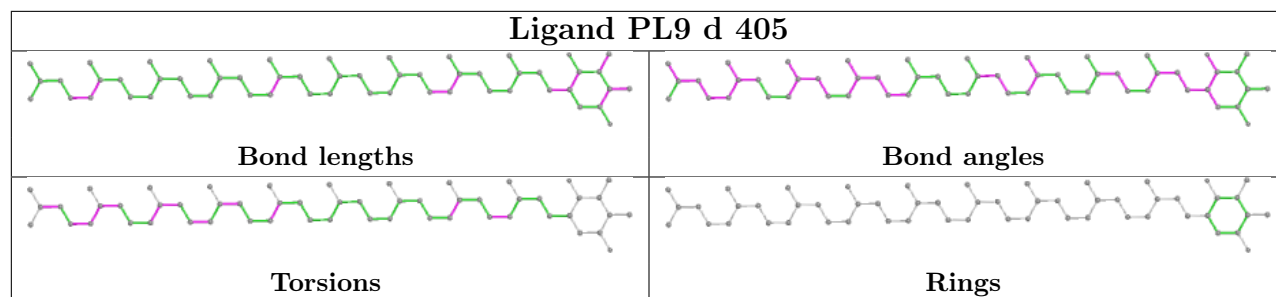


Ligand DGD H 102

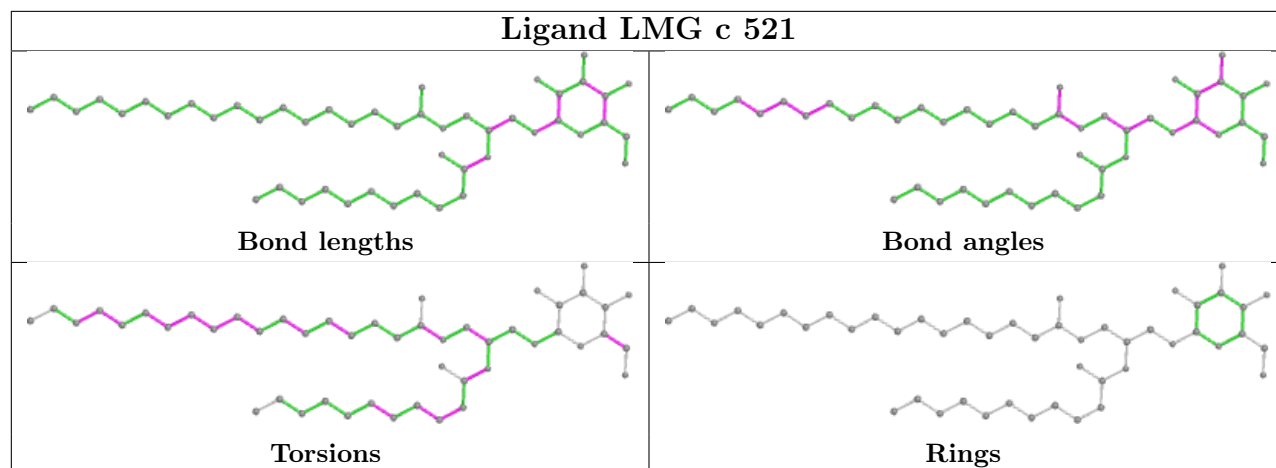


Ligand CLA c 513

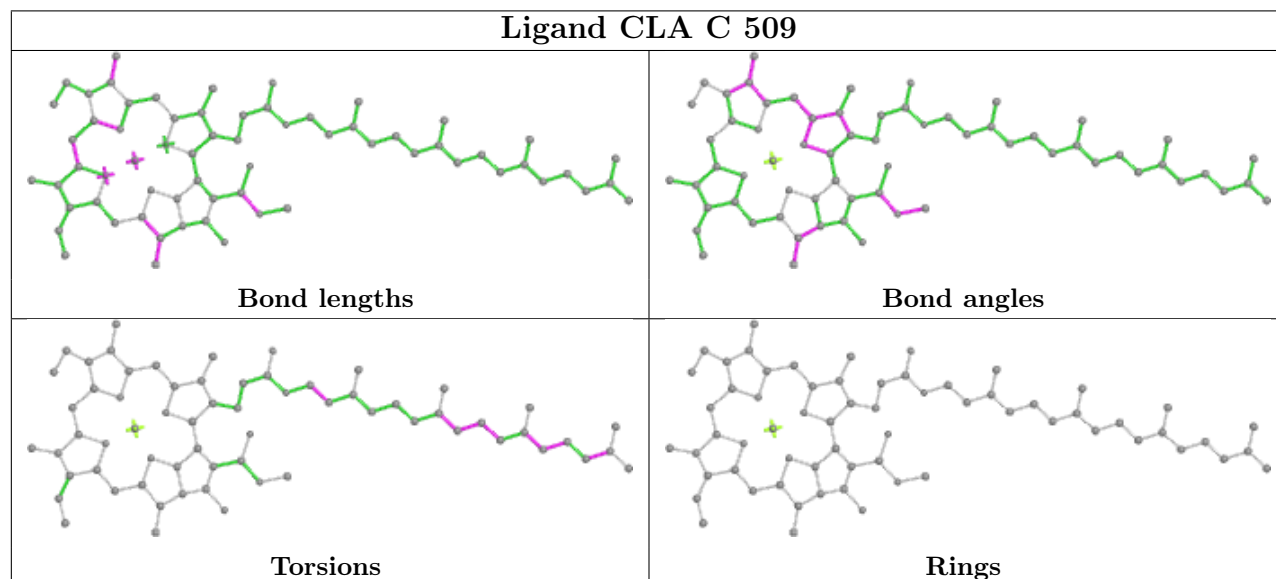




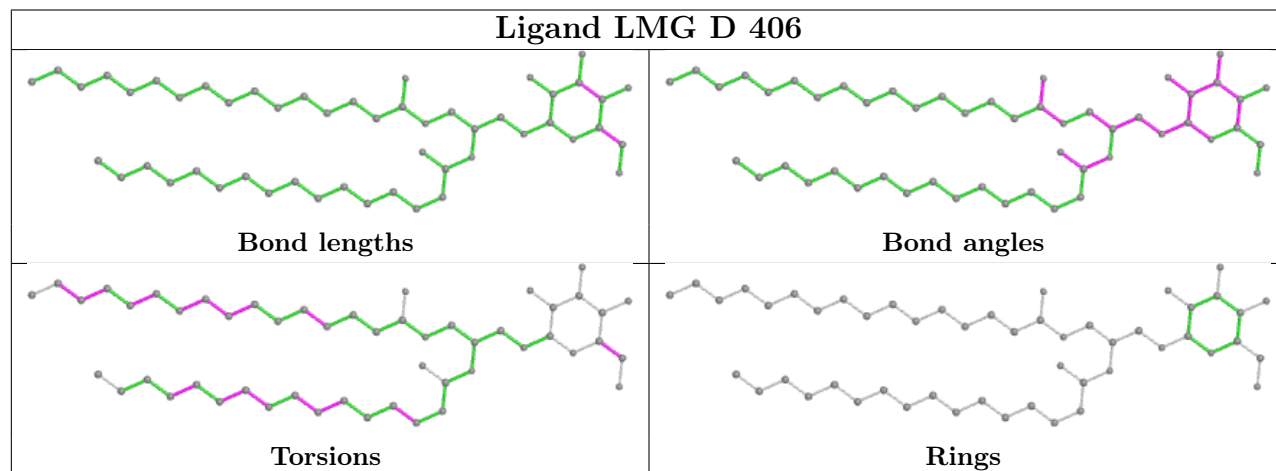
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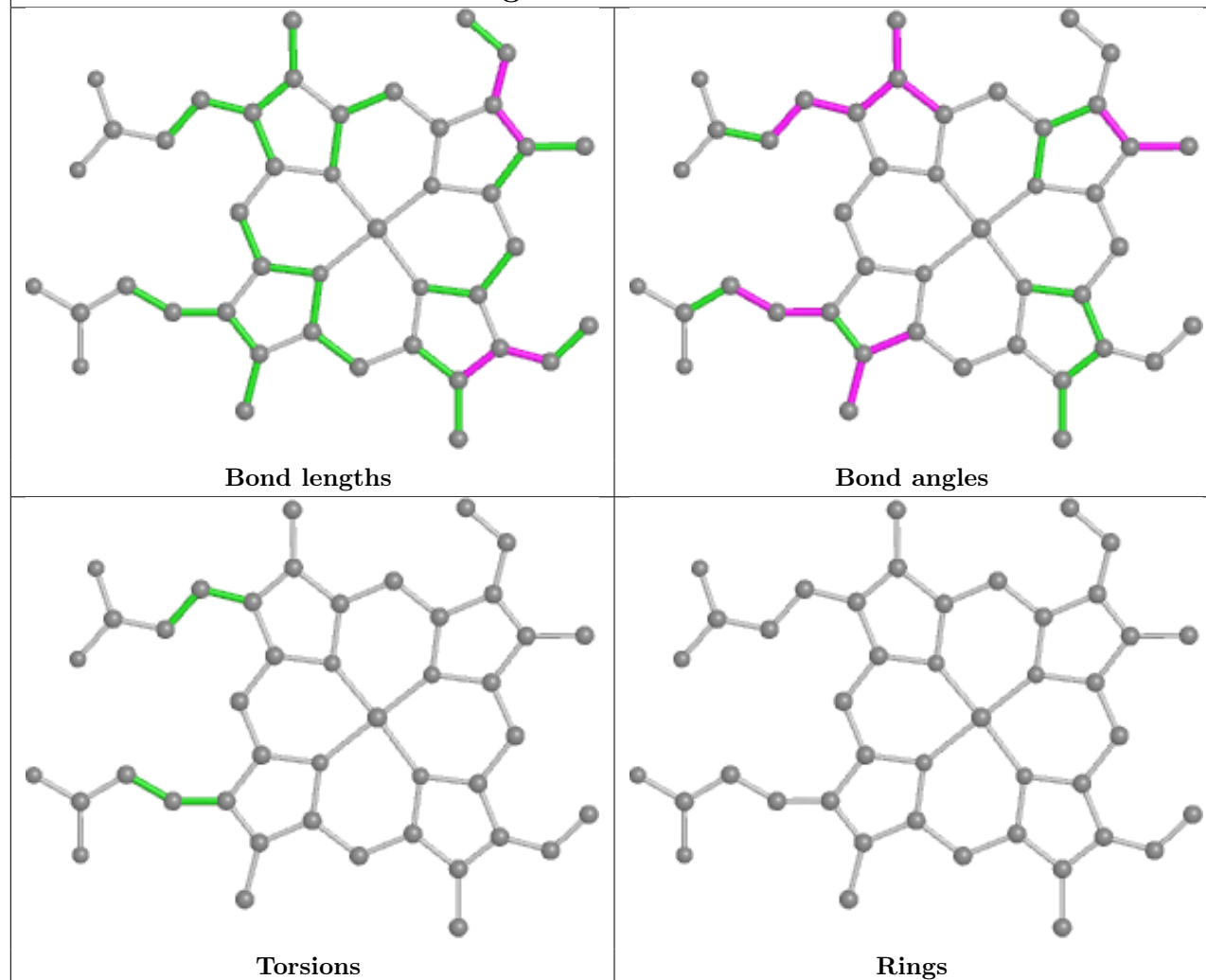
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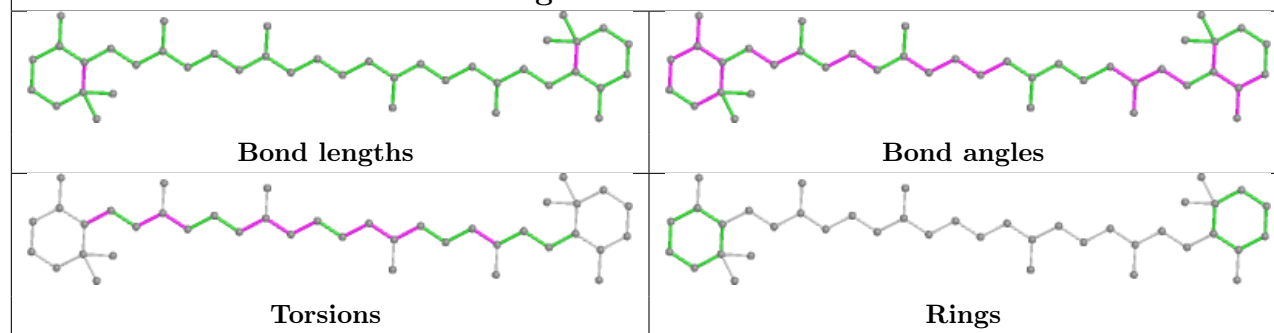
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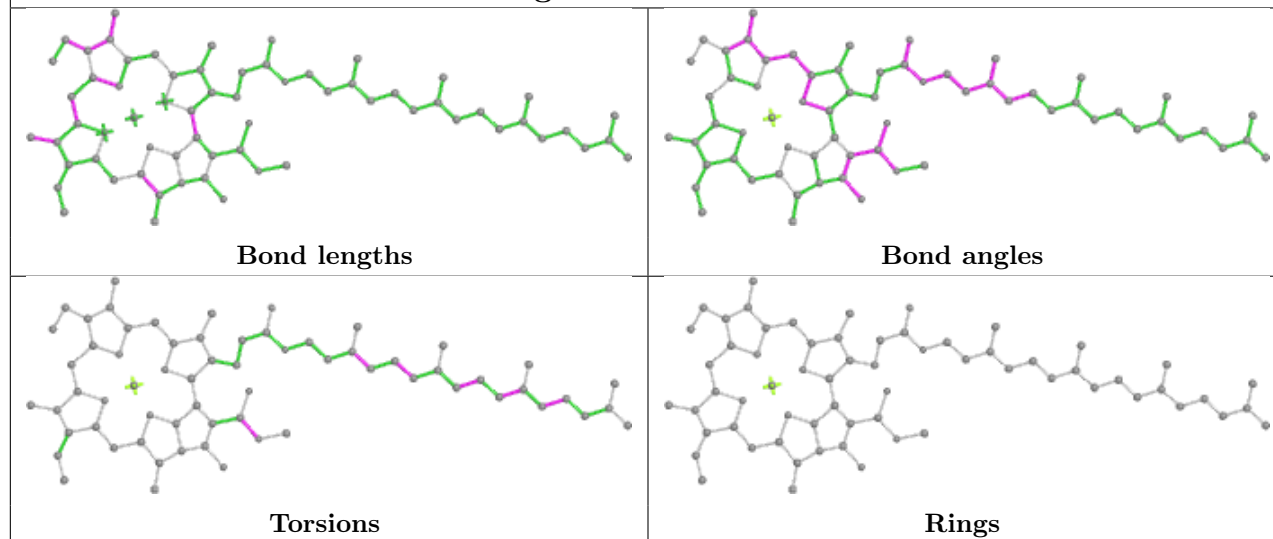
Ligand HEM e 102



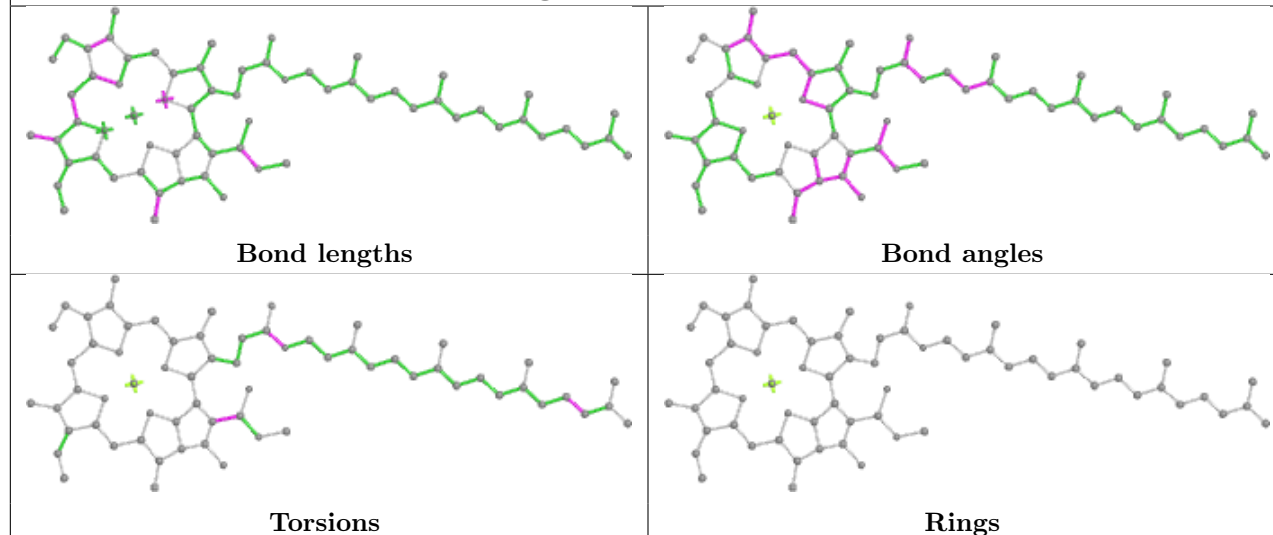
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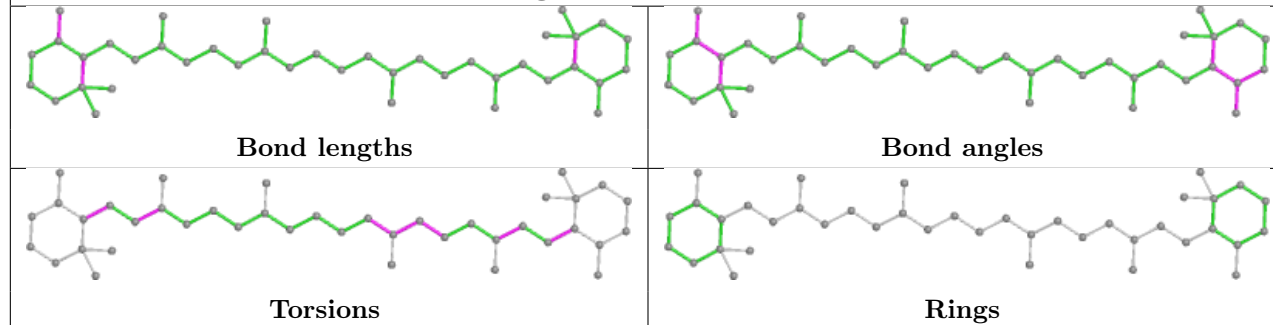
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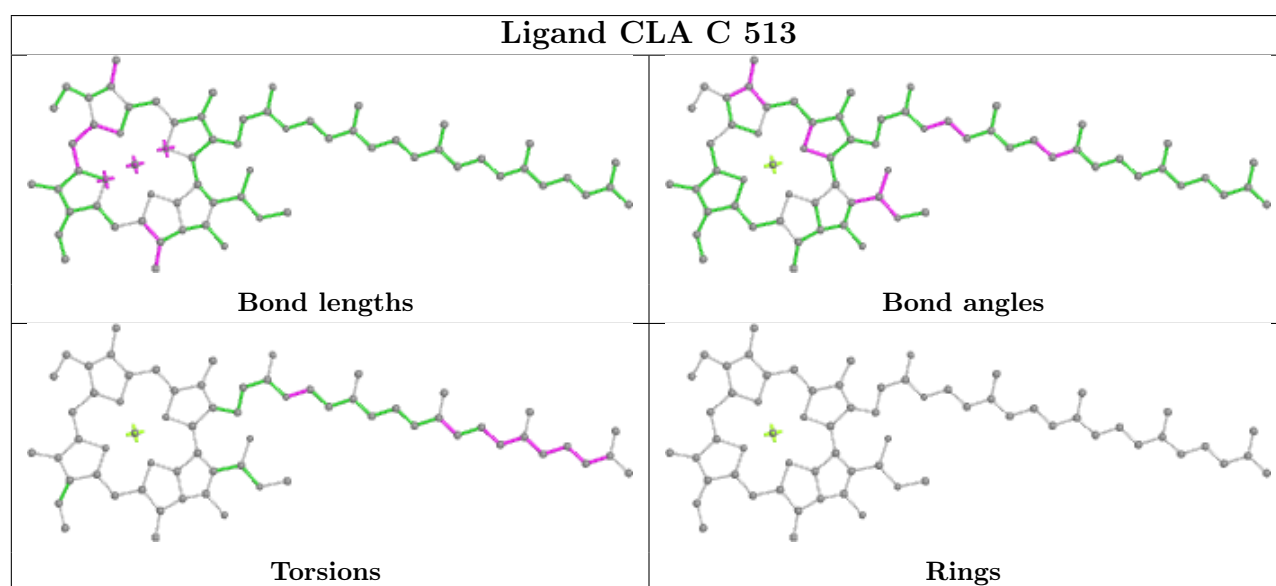
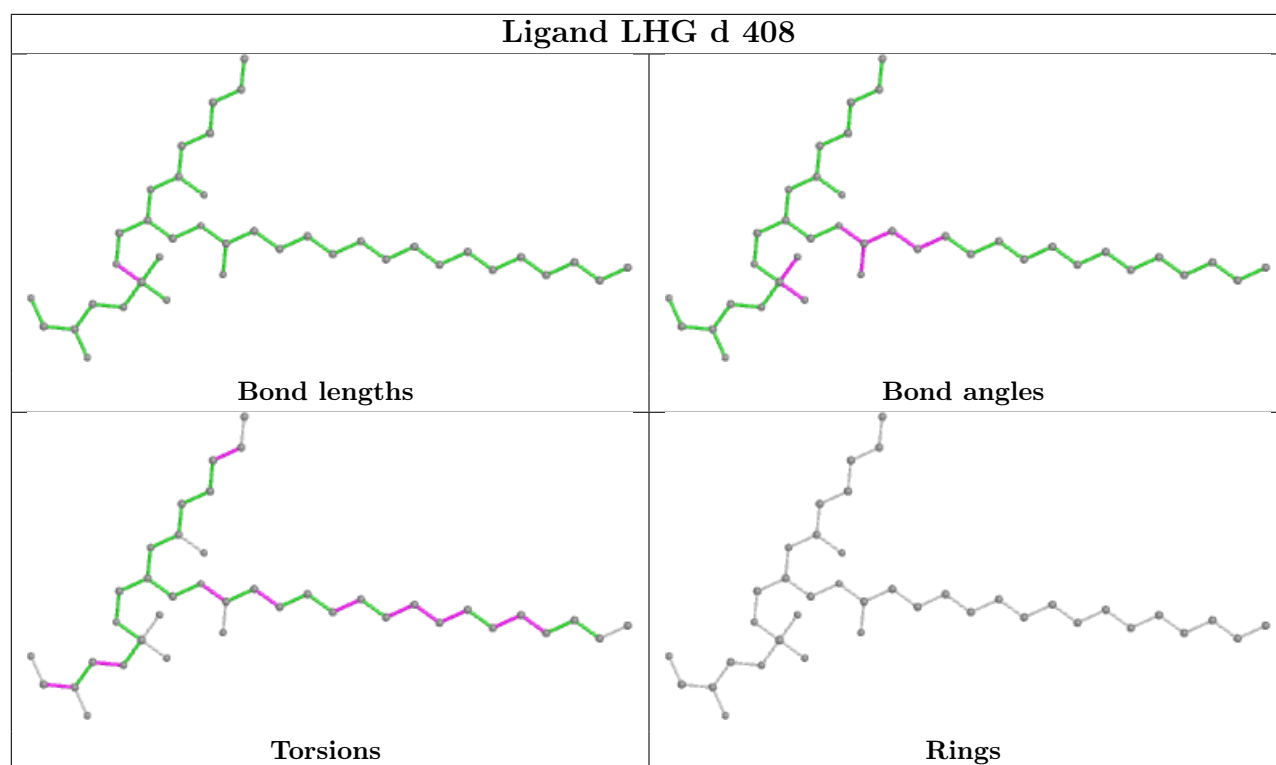


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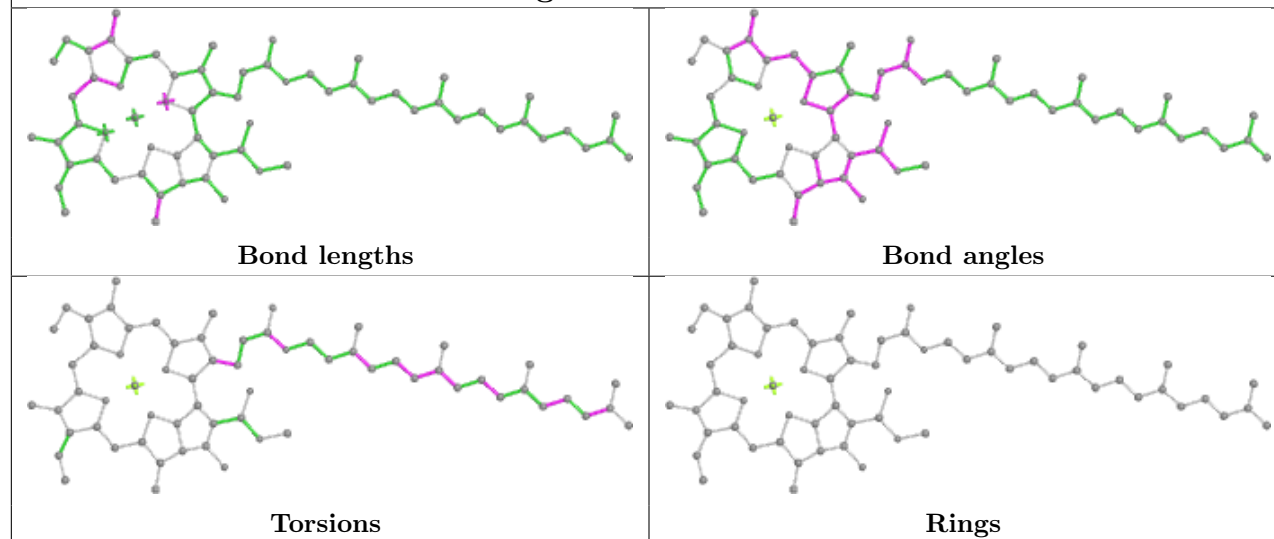


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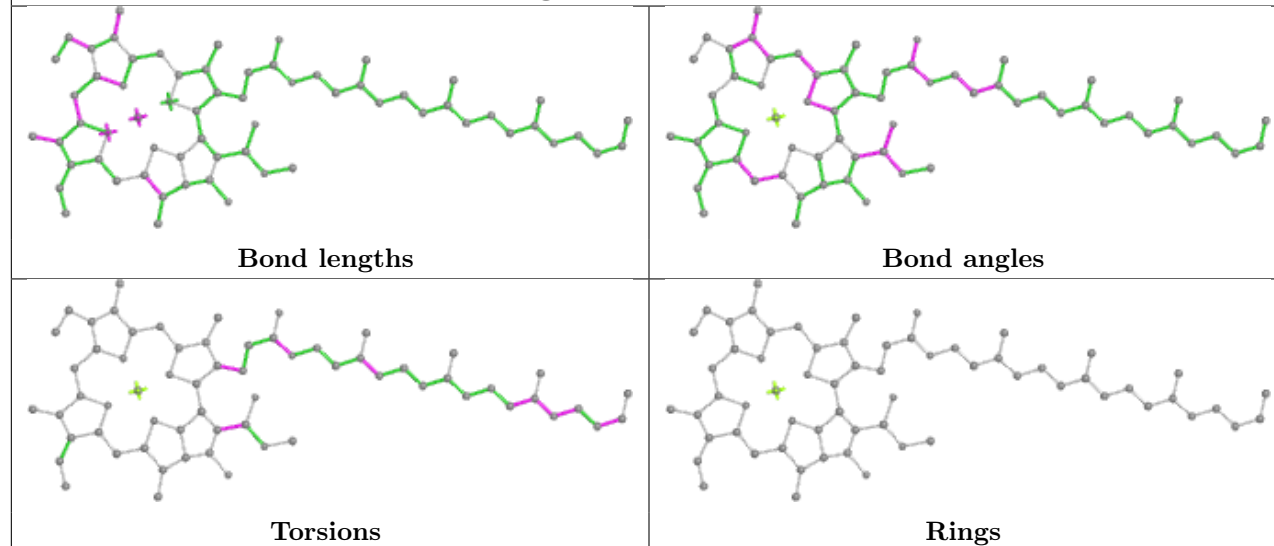




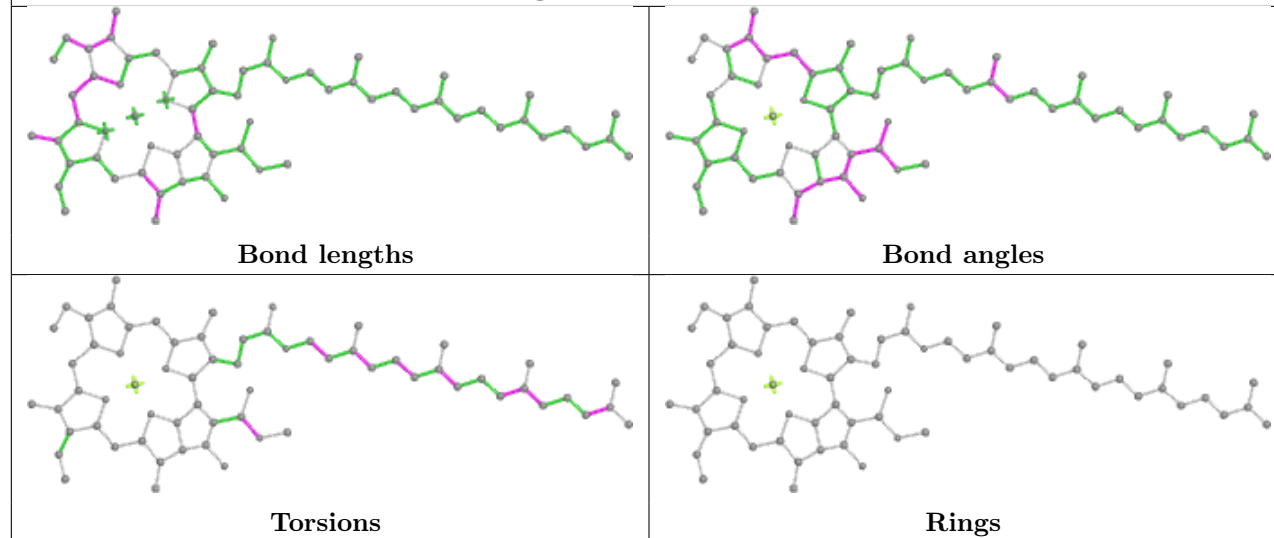
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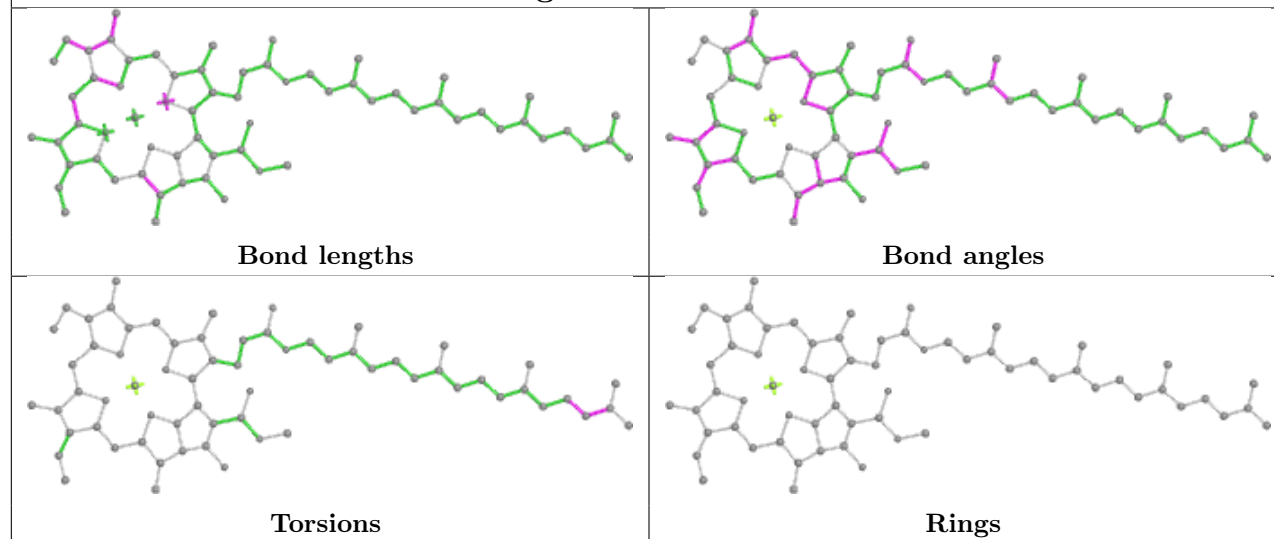
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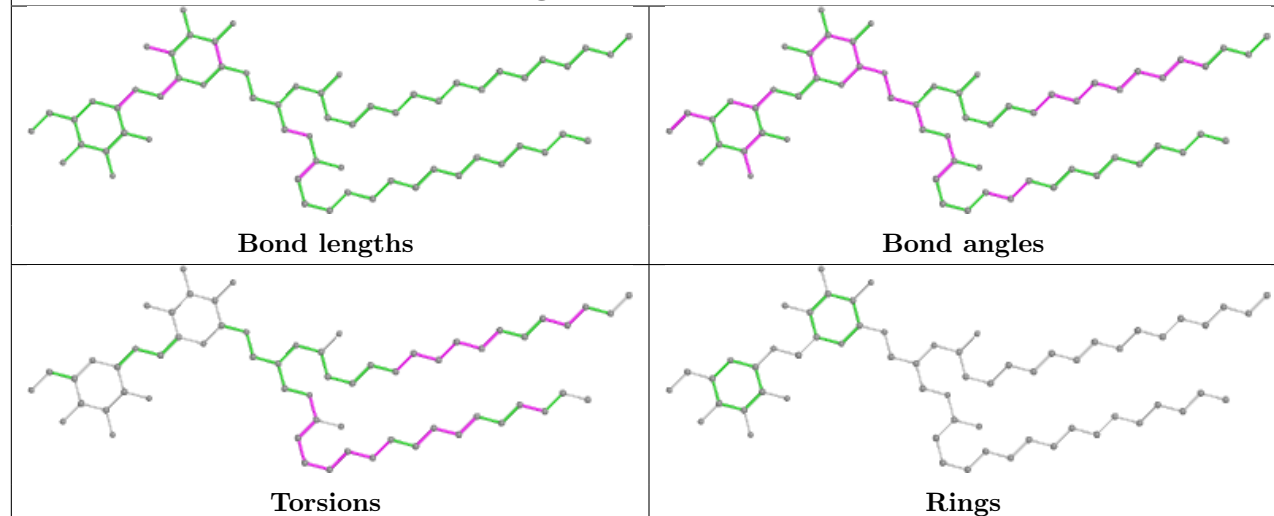
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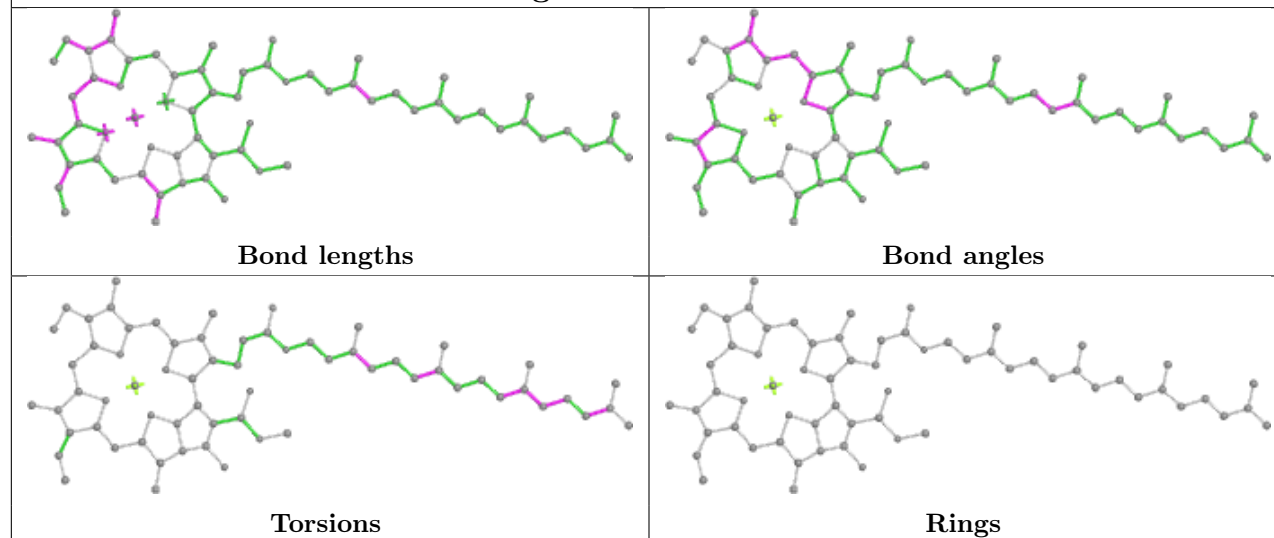
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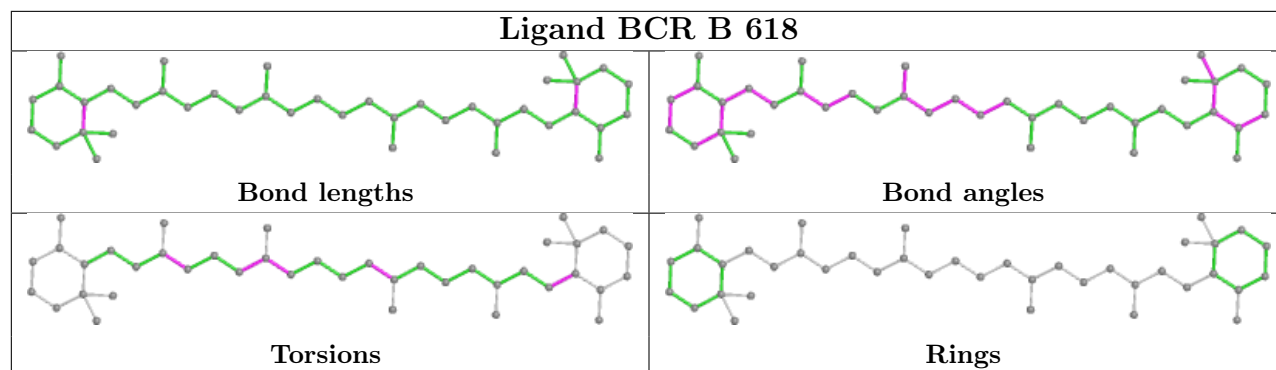
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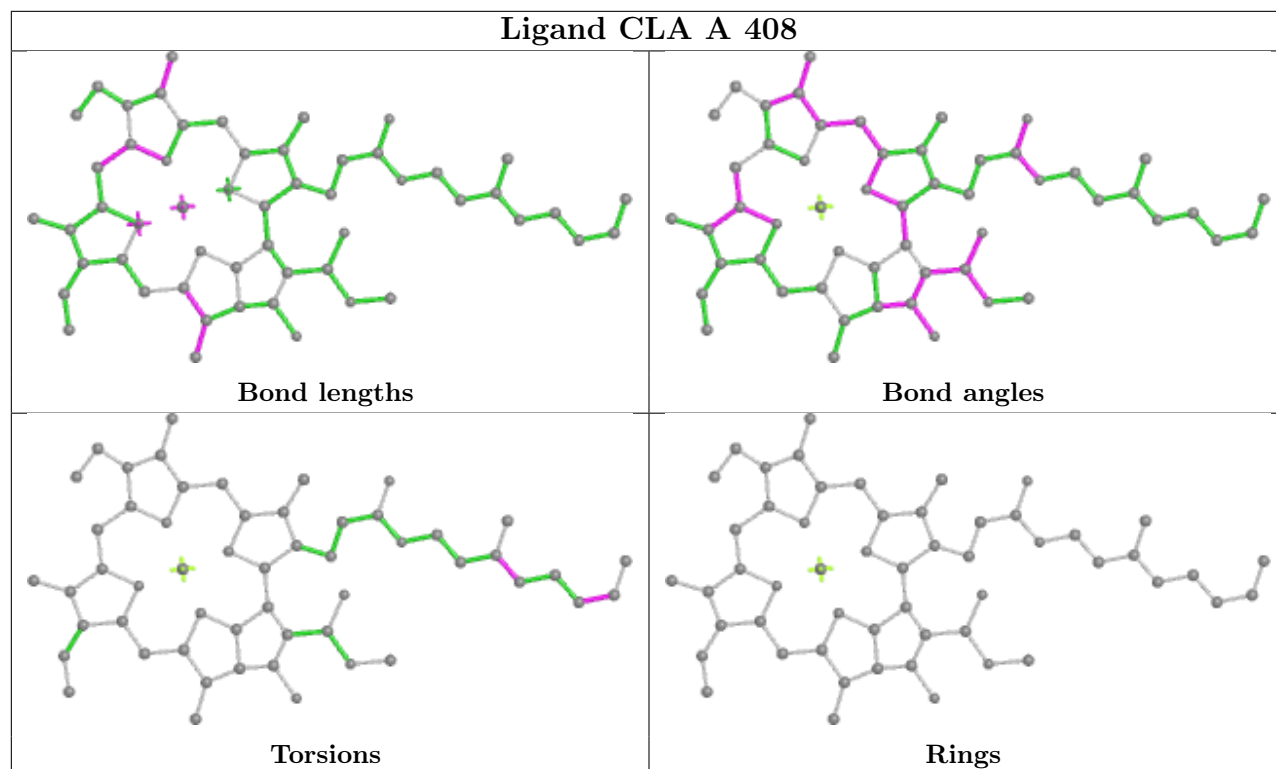
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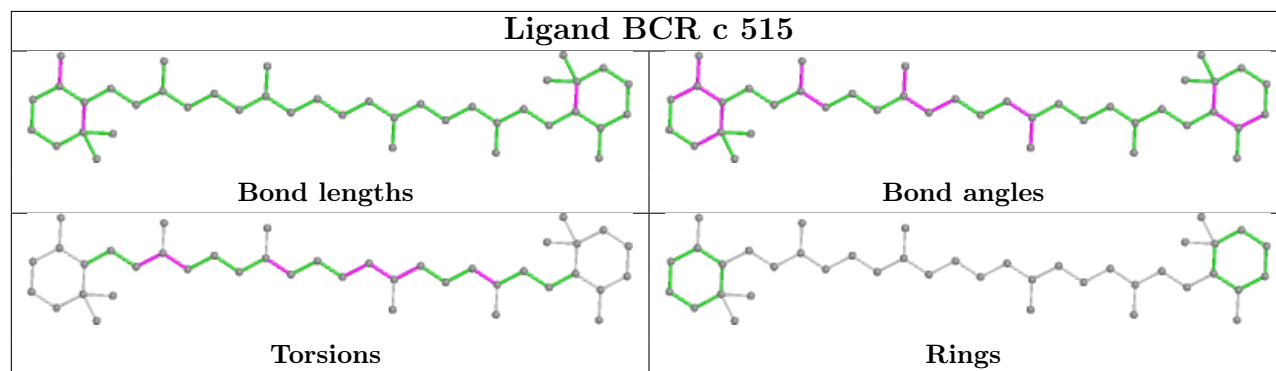
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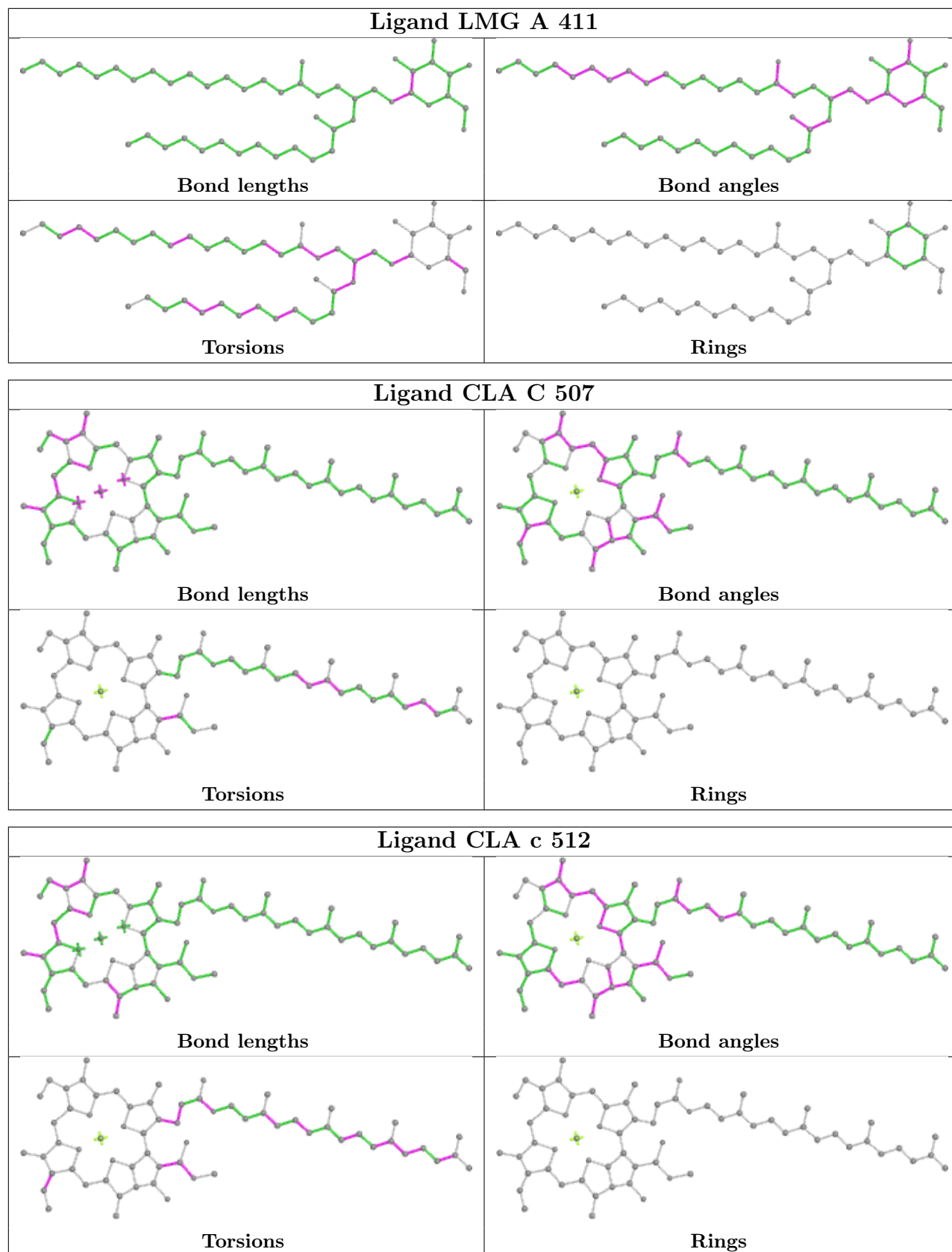


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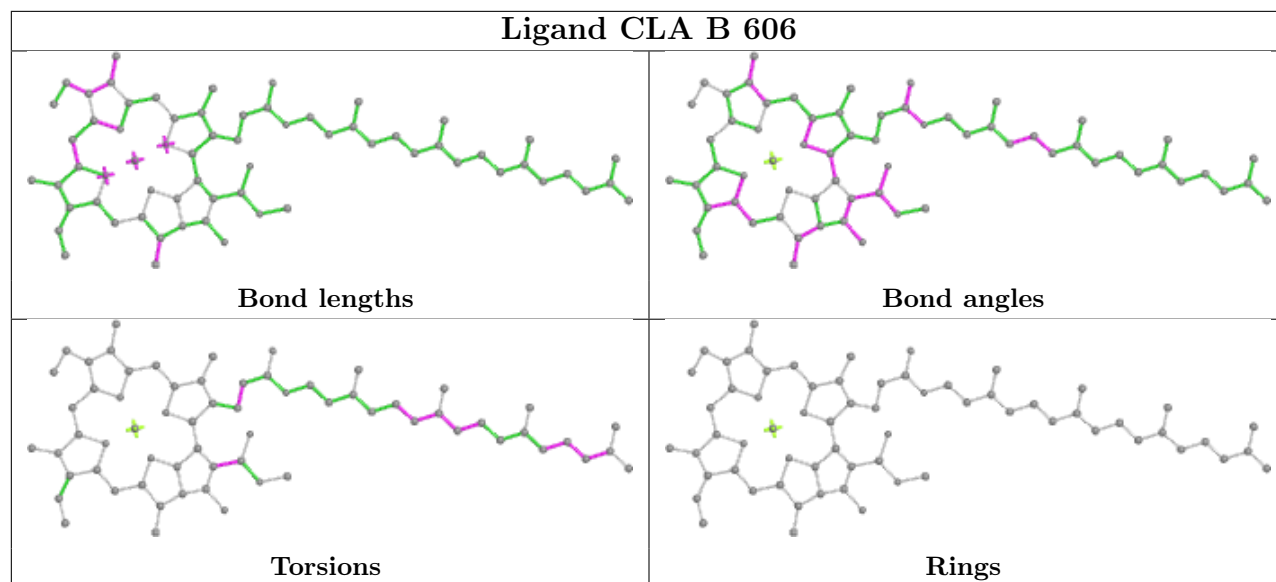


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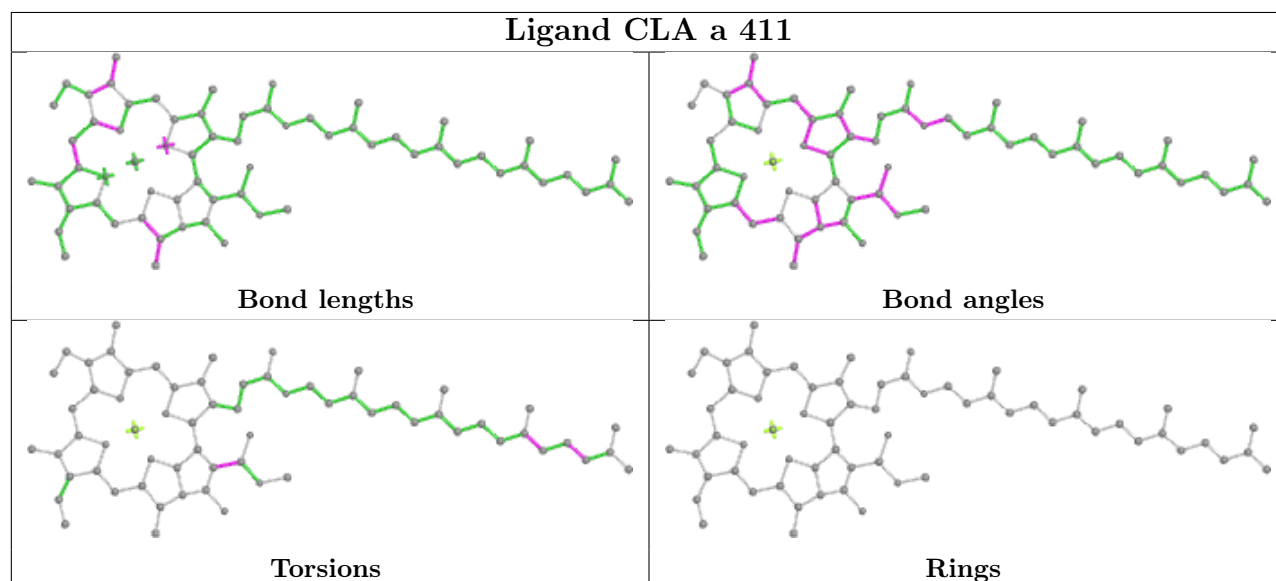




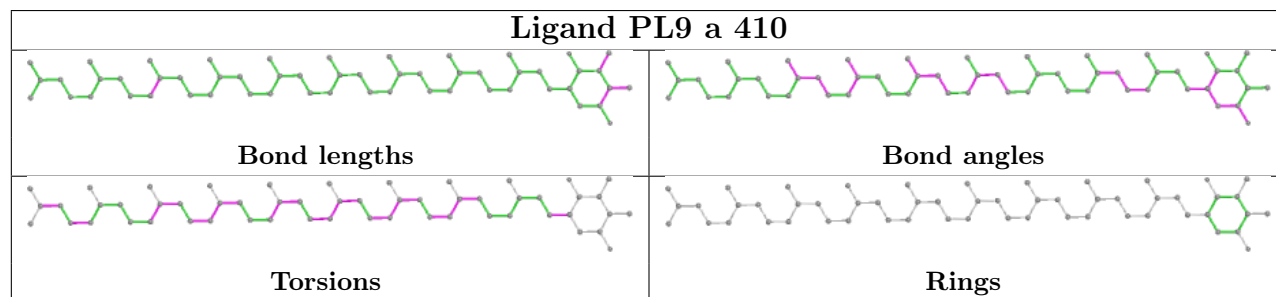
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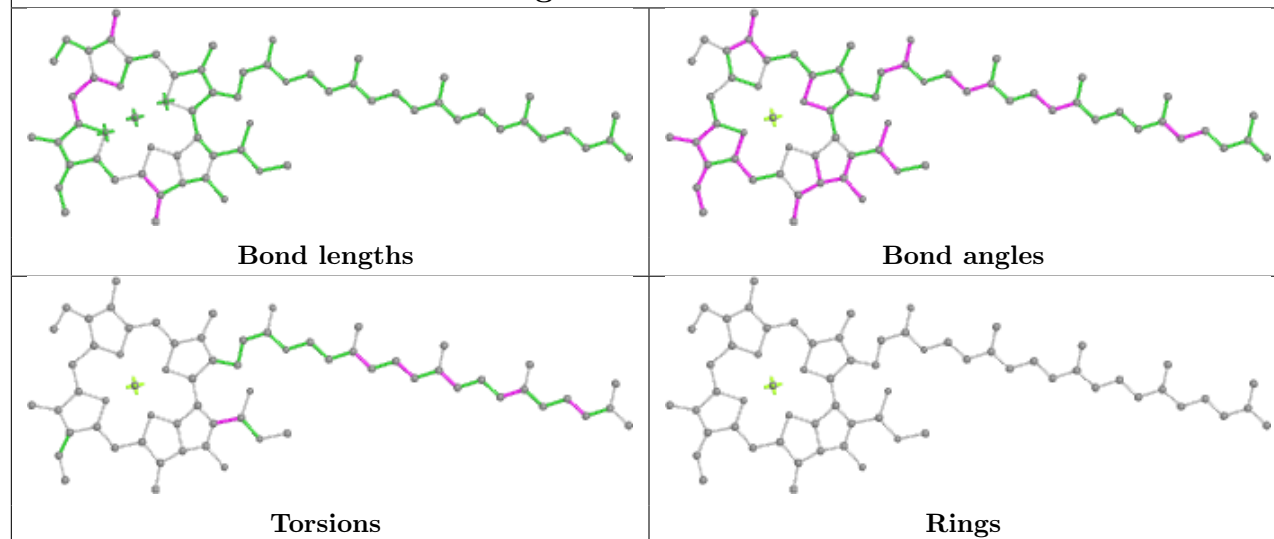
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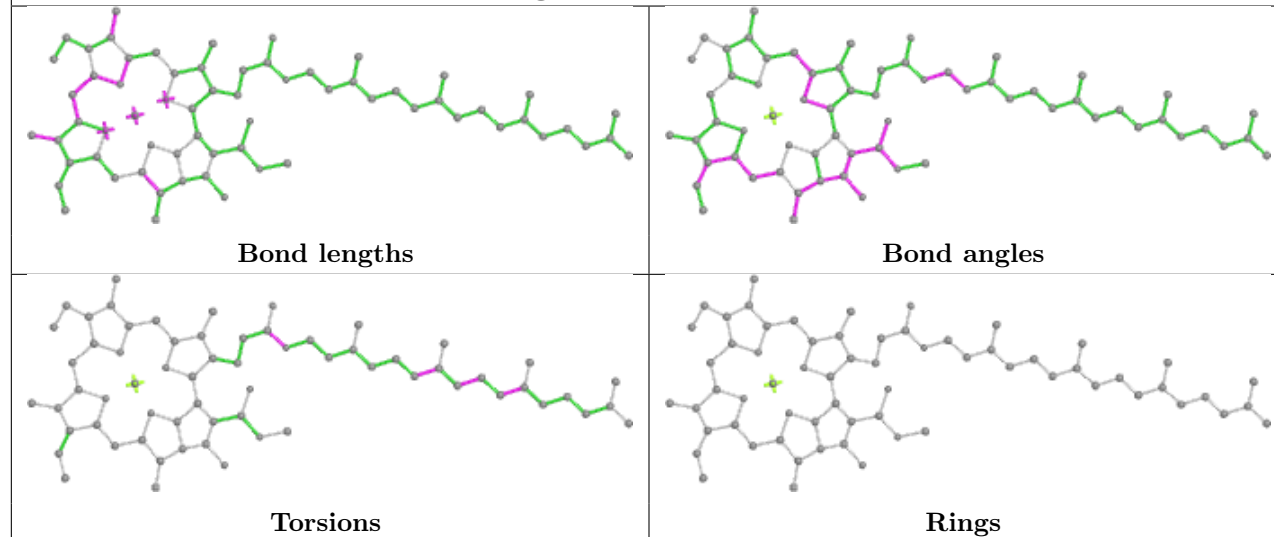
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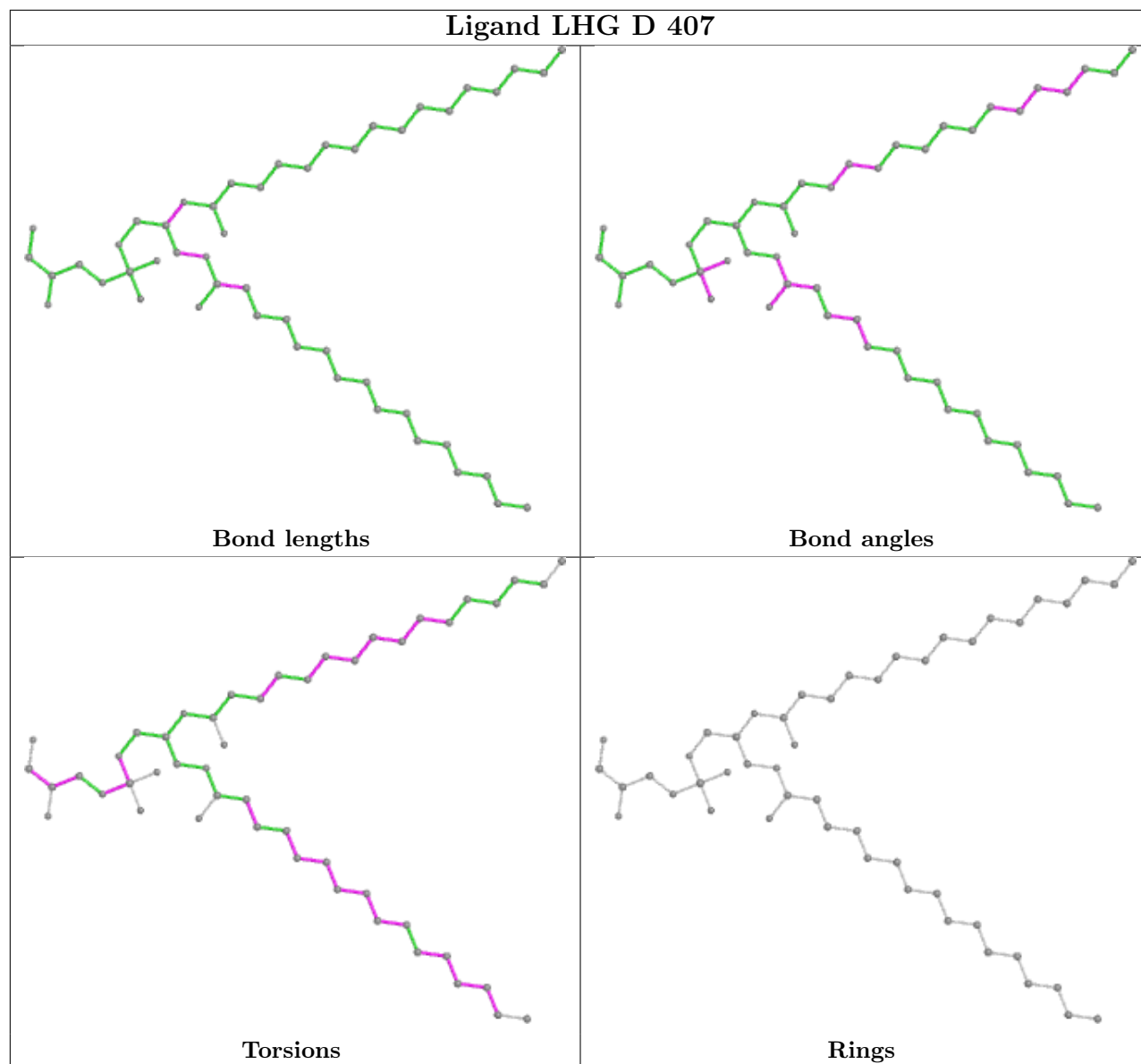


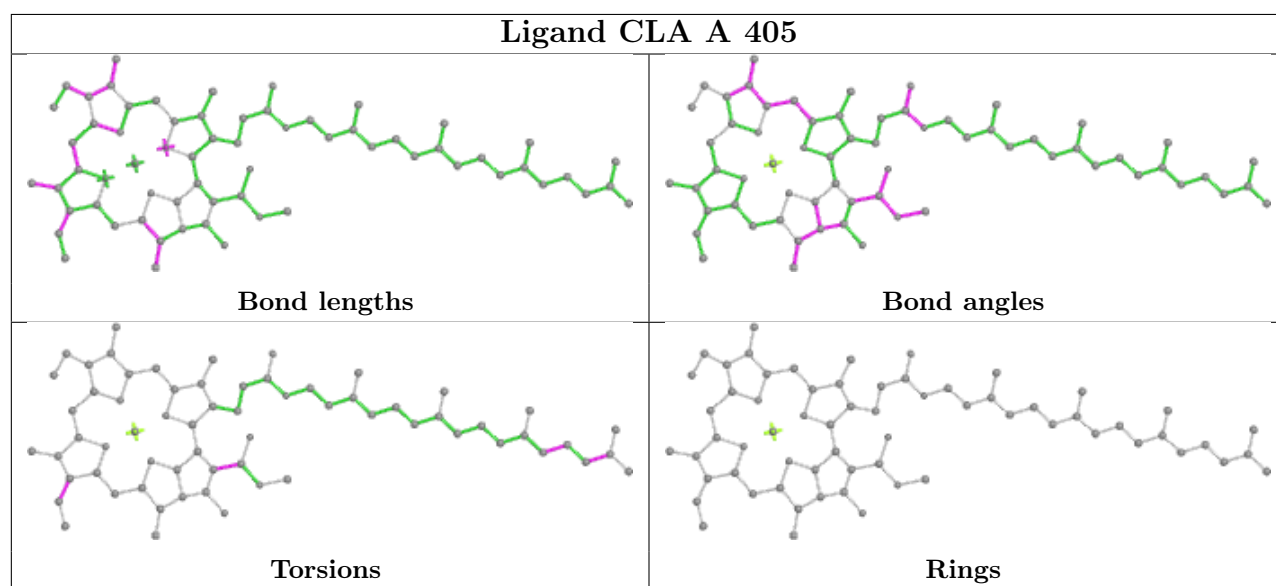
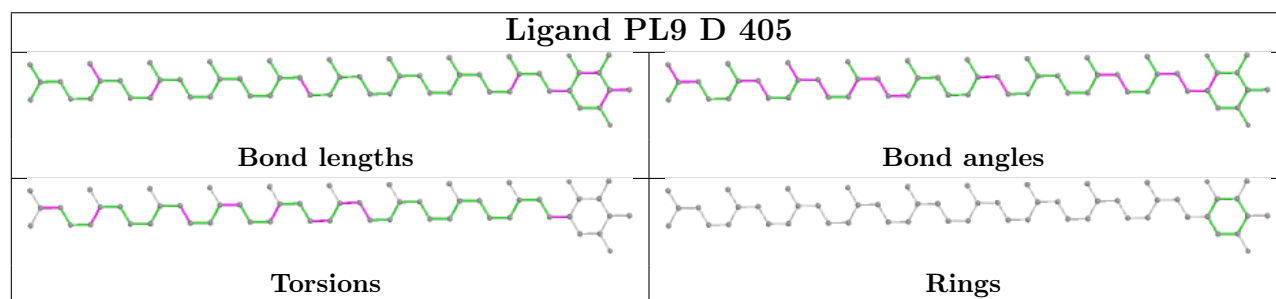
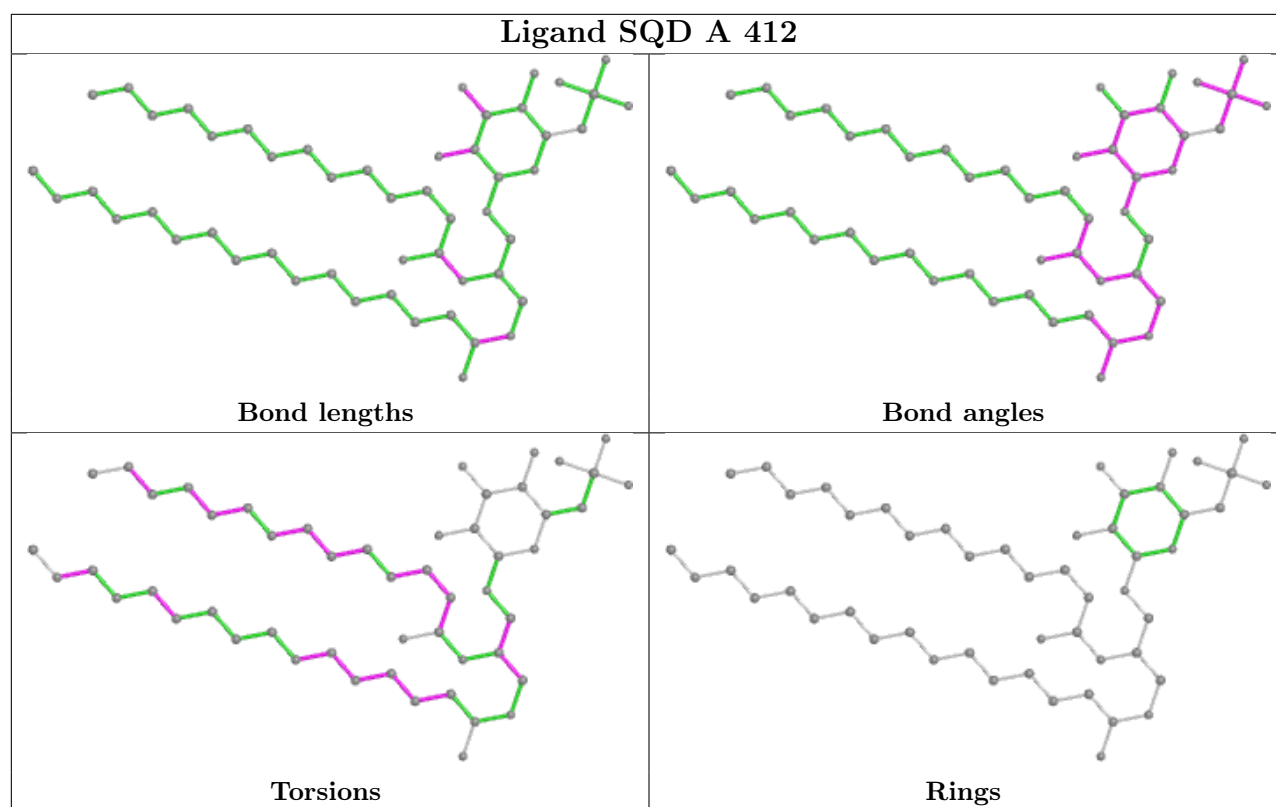
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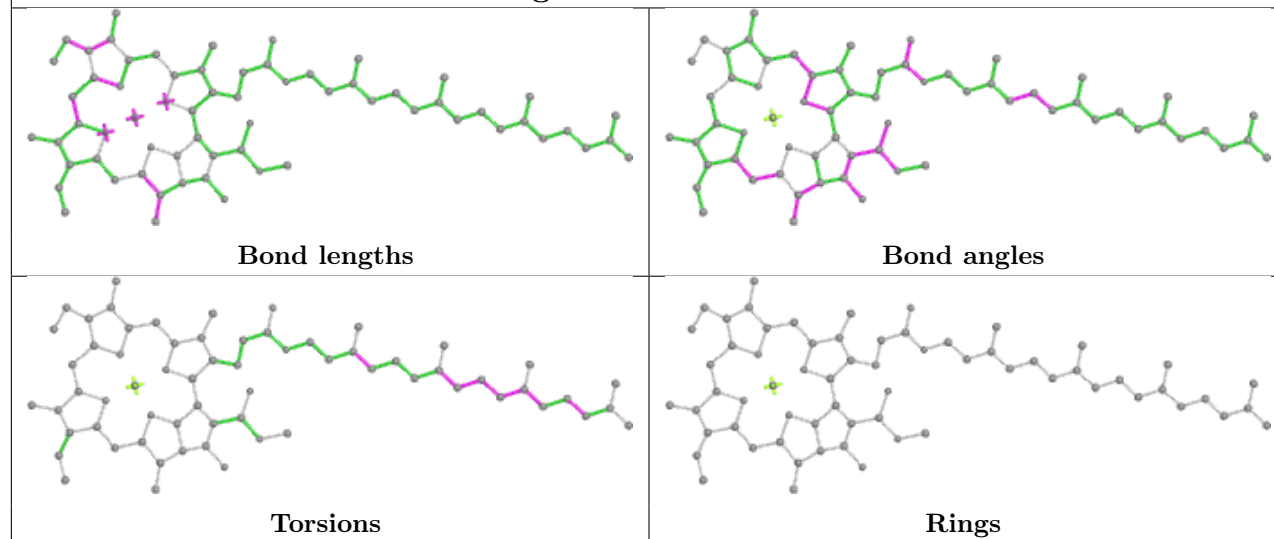
Ligand CLA C 511



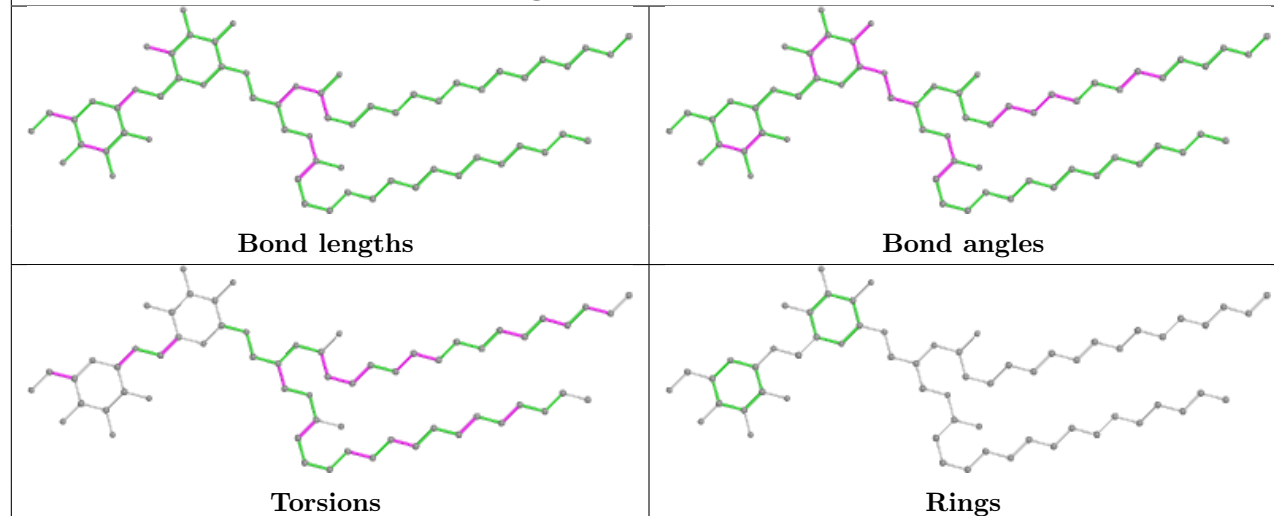




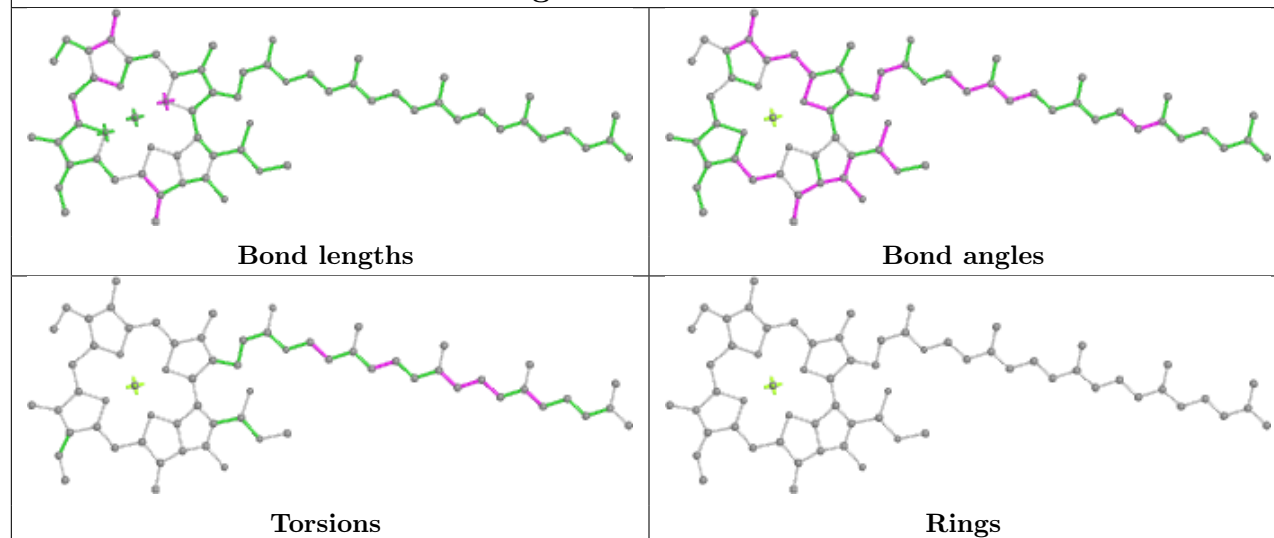
Ligand CLA C 510

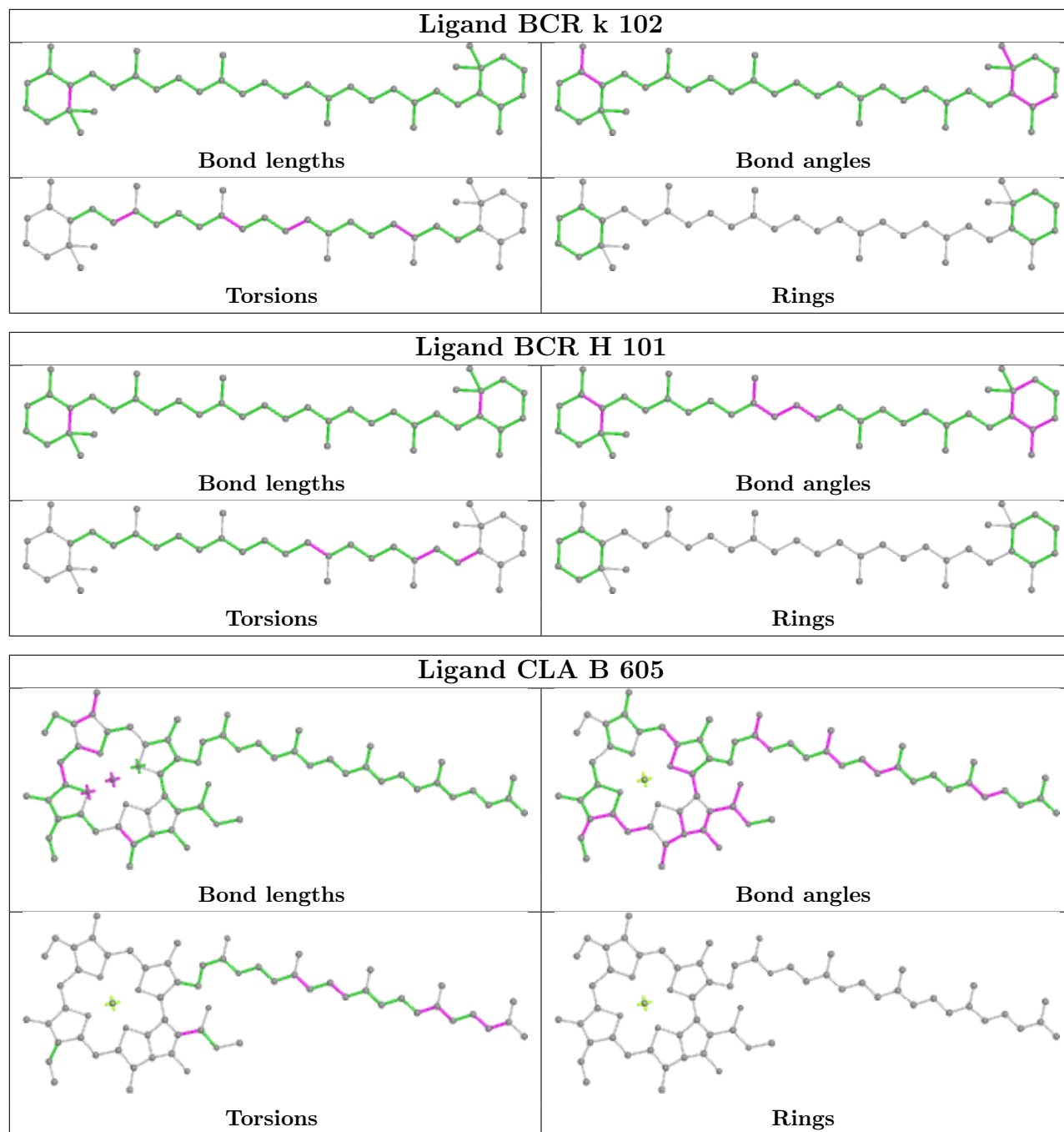


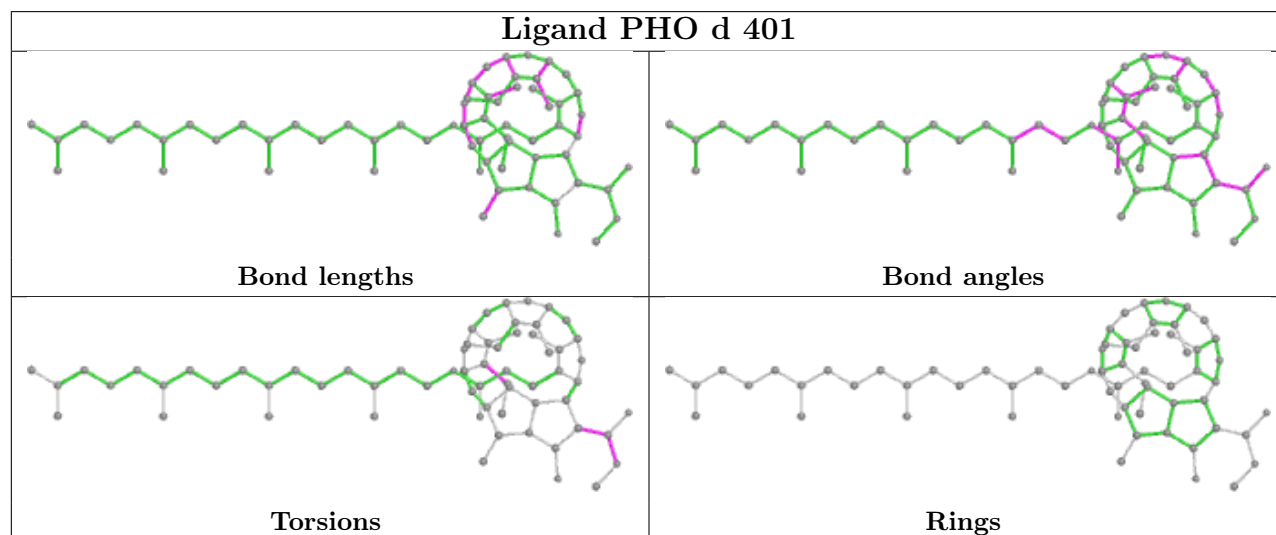
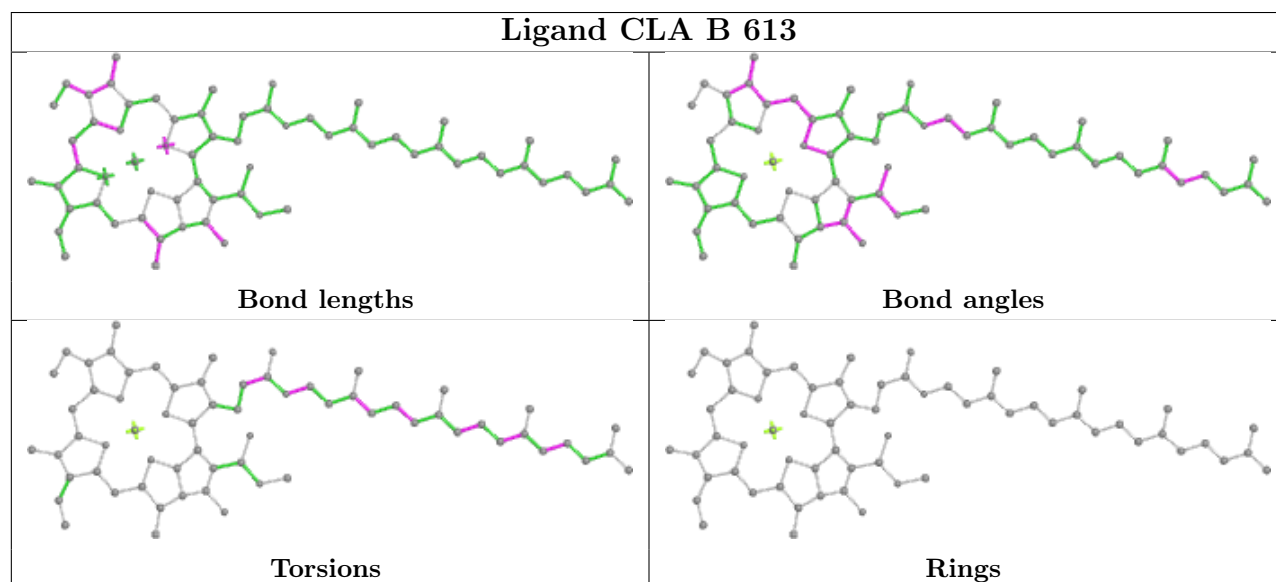
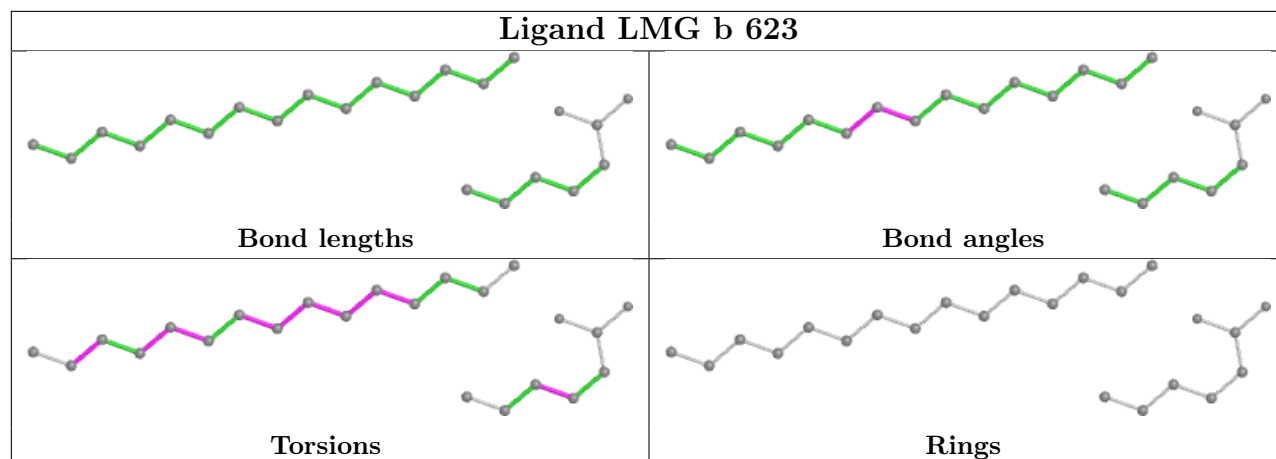
Ligand DGD C 515

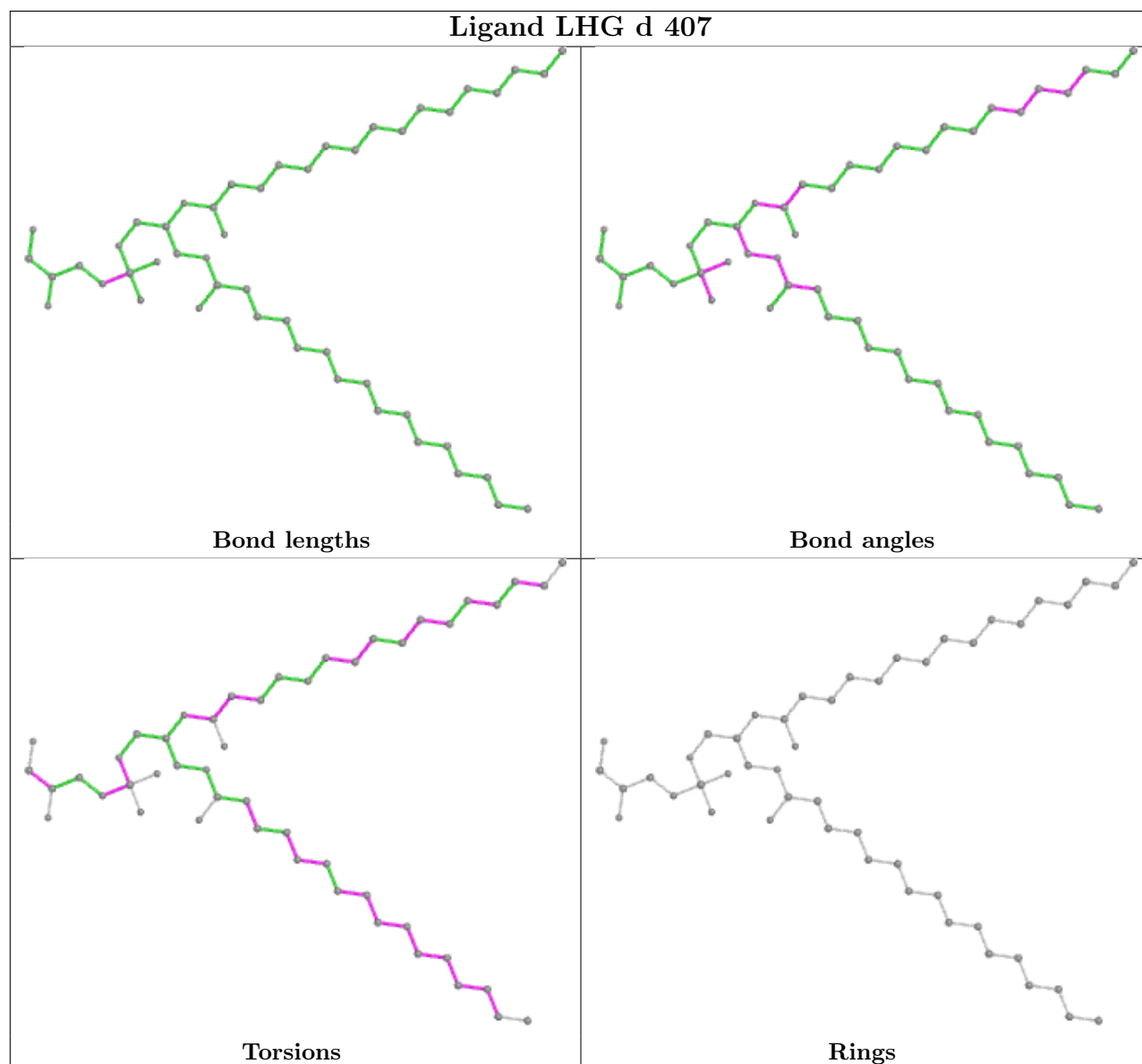
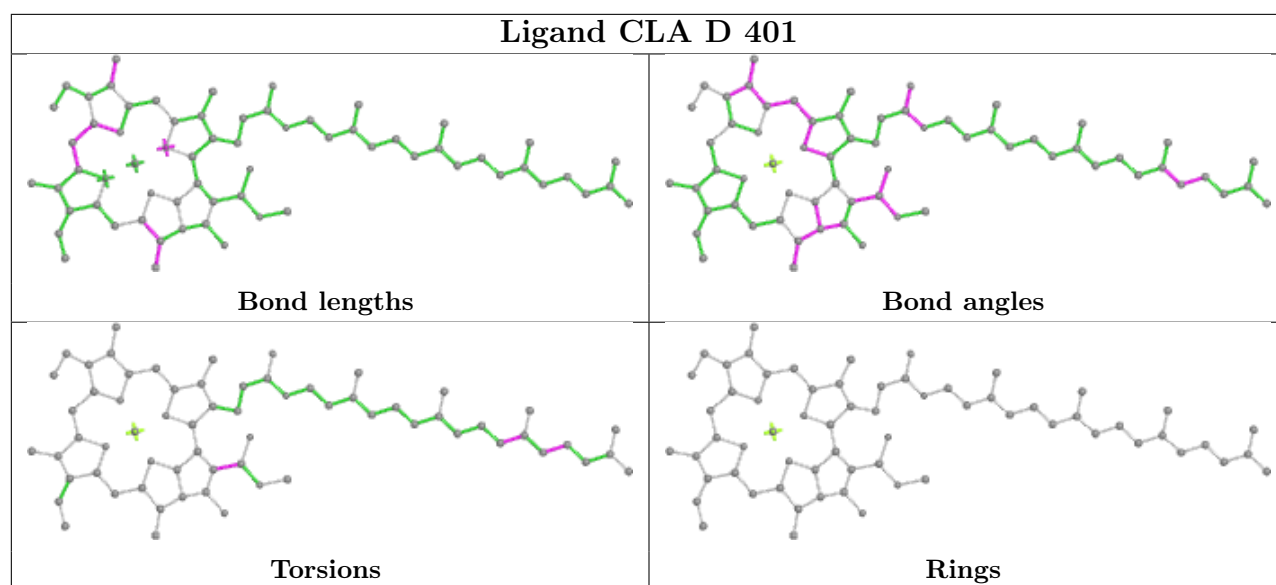


Ligand CLA C 512

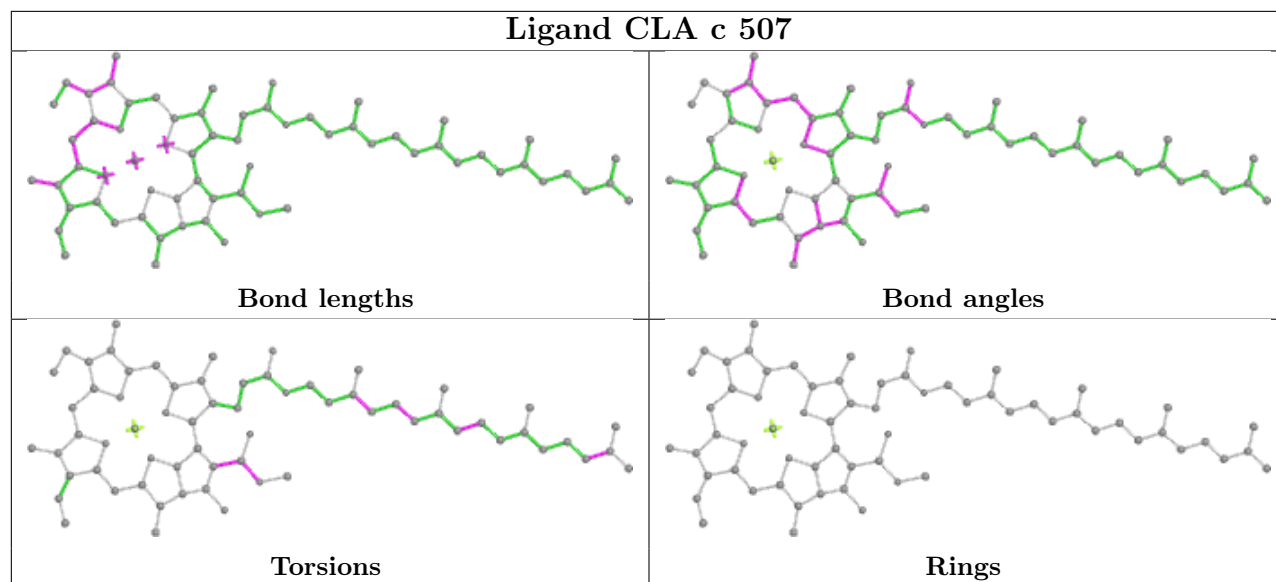




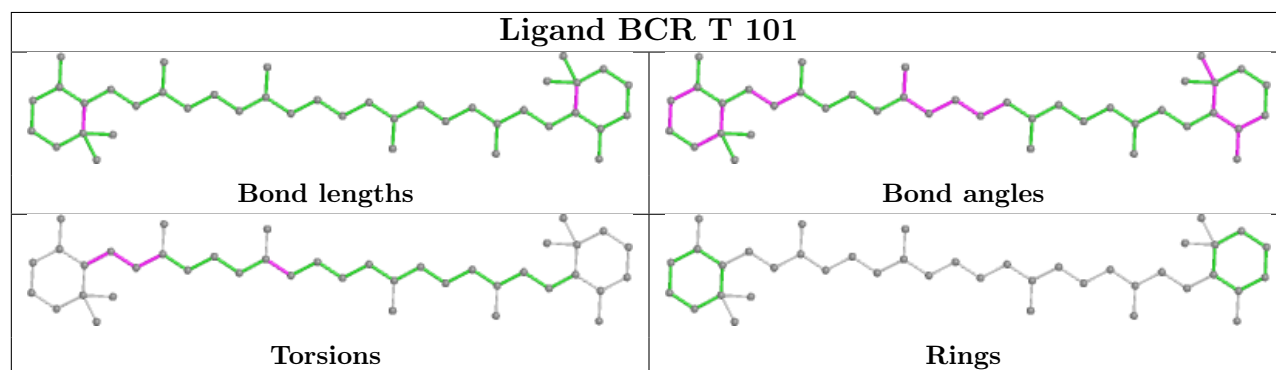




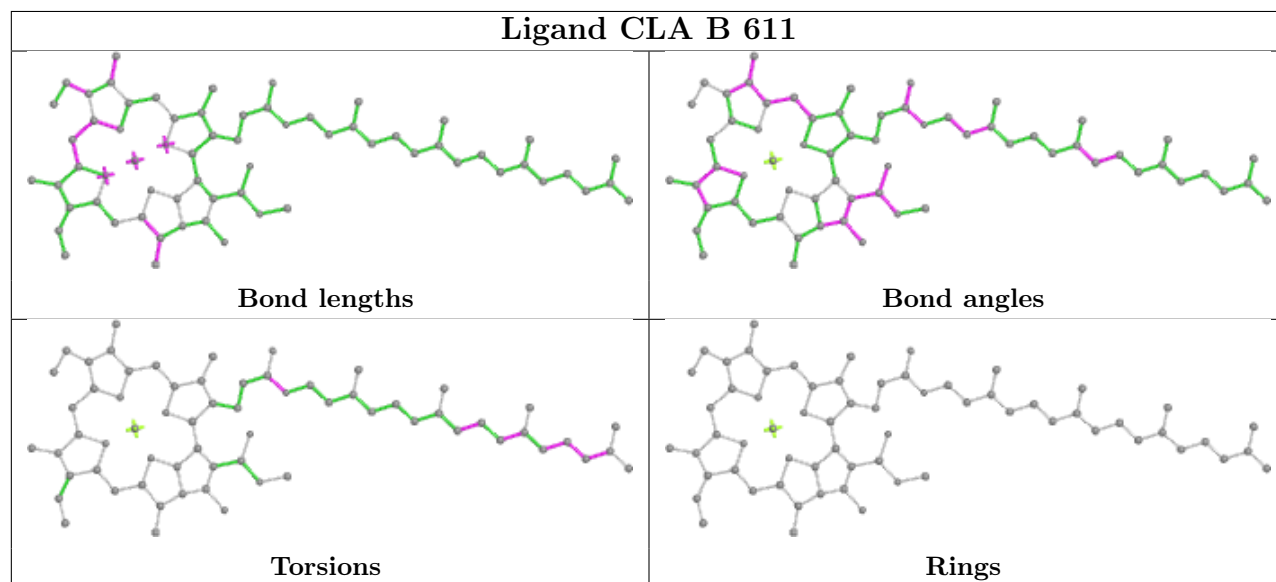
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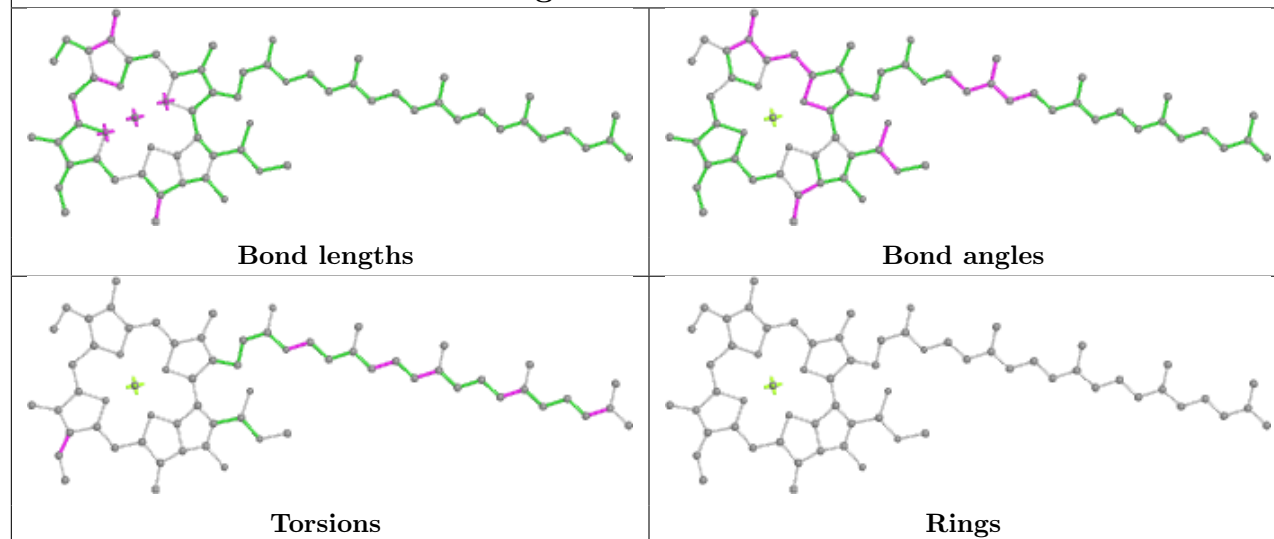
Ligand BCR T 101



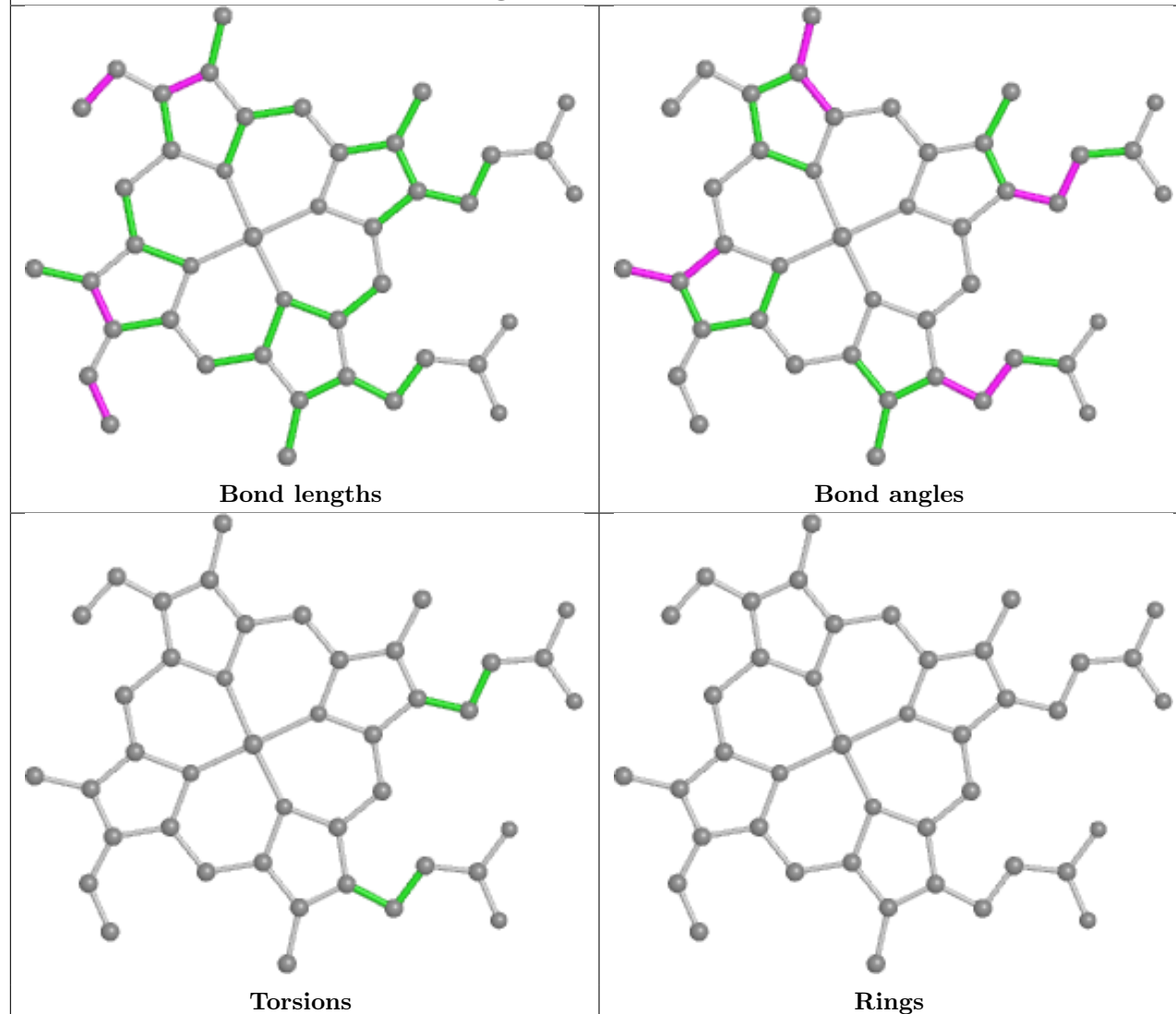
Ligand CLA B 611



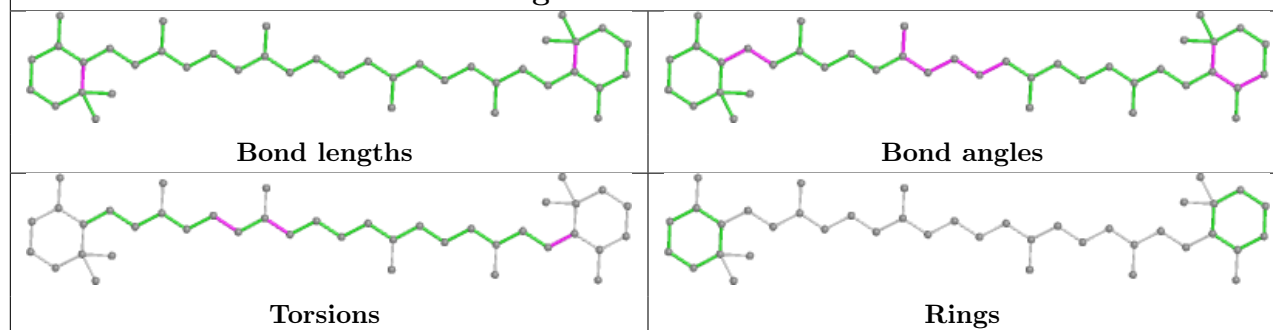
Ligand CLA d 402



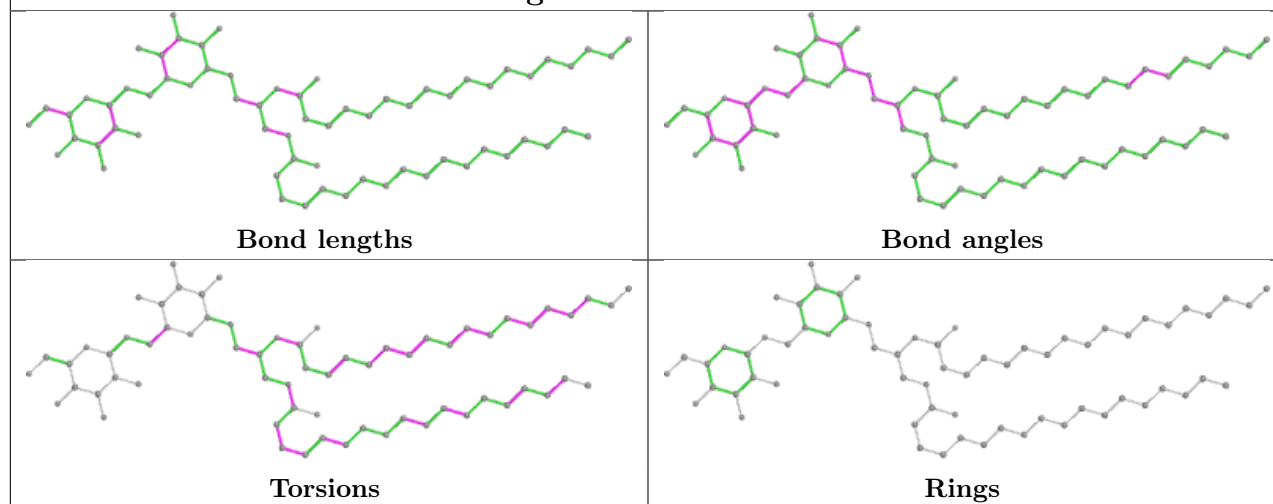
Ligand HEC v 201



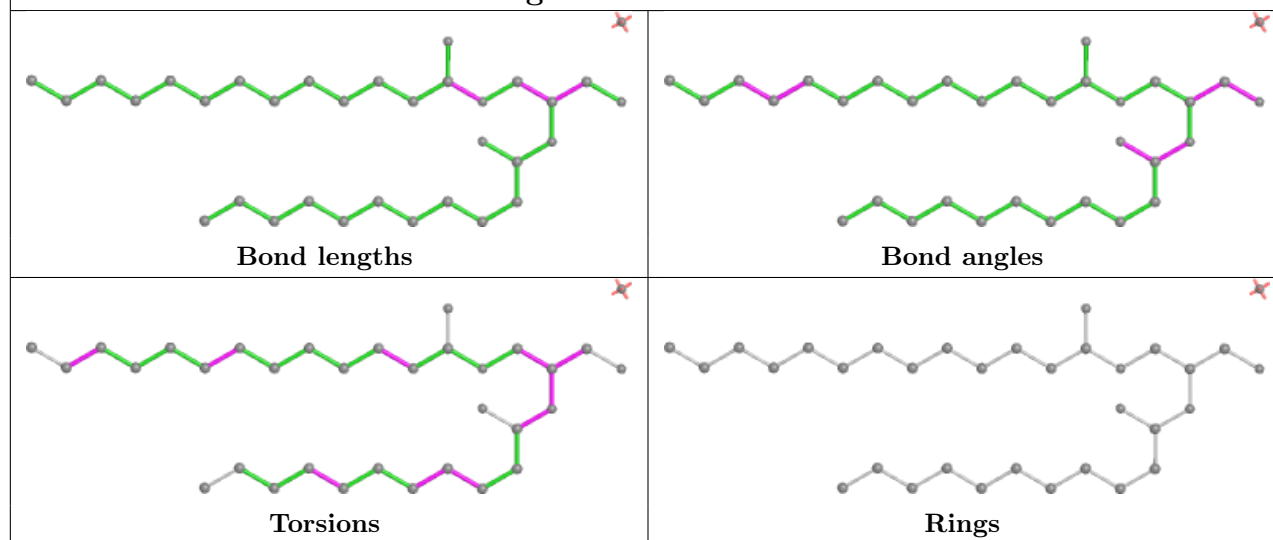
Ligand BCR b 619



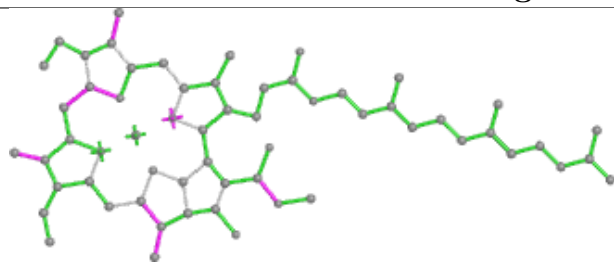
Ligand DGD A 415



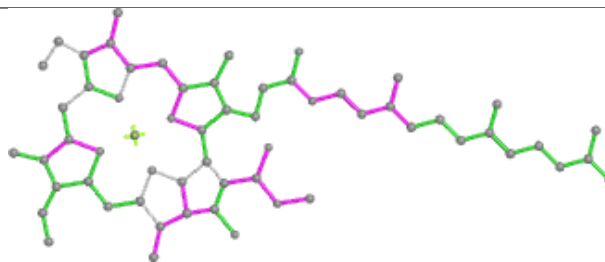
Ligand LMG D 409



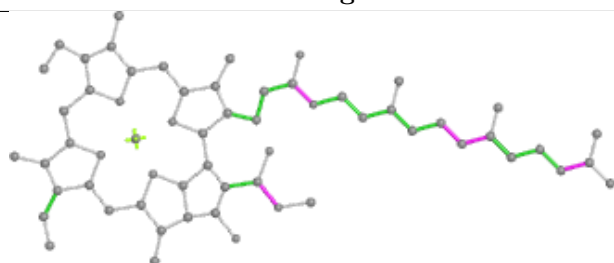
Ligand CLA B 616



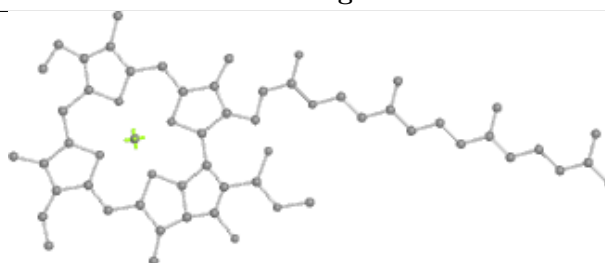
Bond lengths



Bond angles

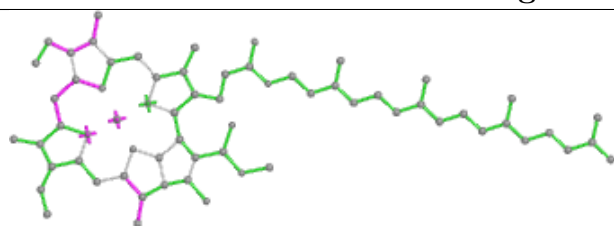


Torsions

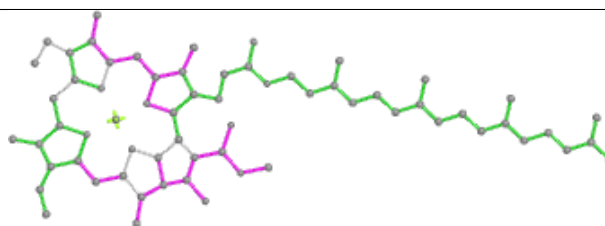


Rings

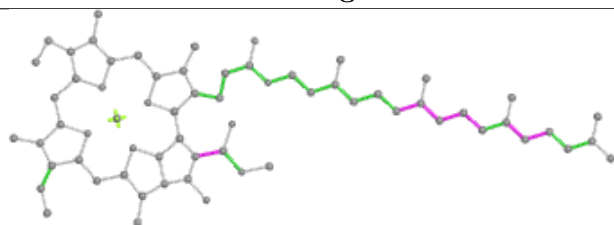
Ligand CLA a 406



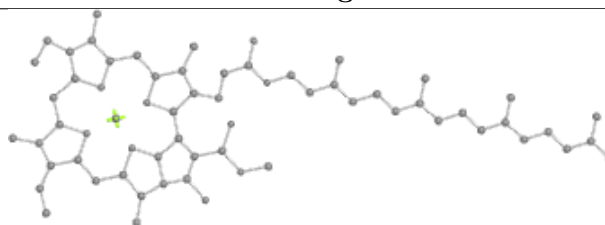
Bond lengths



Bond angles

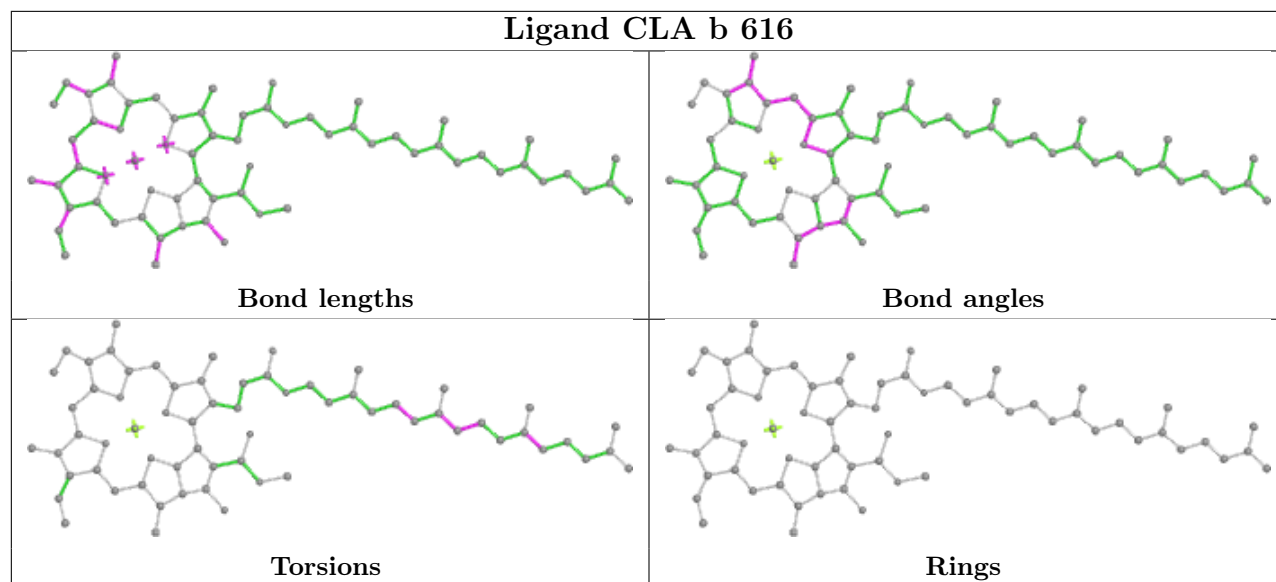


Torsions

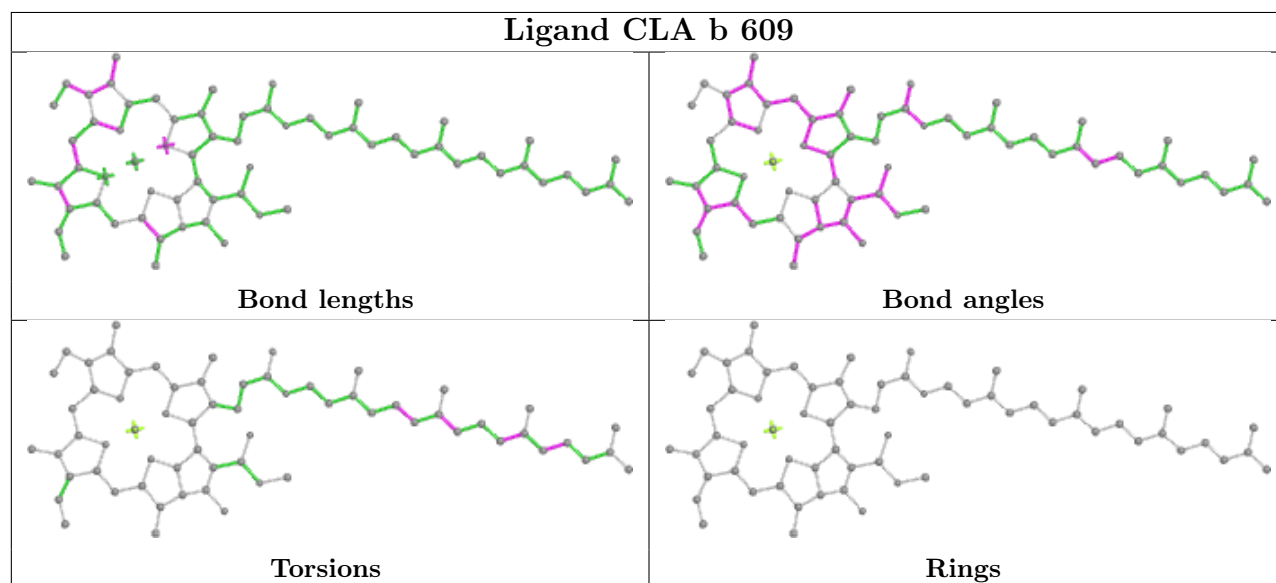


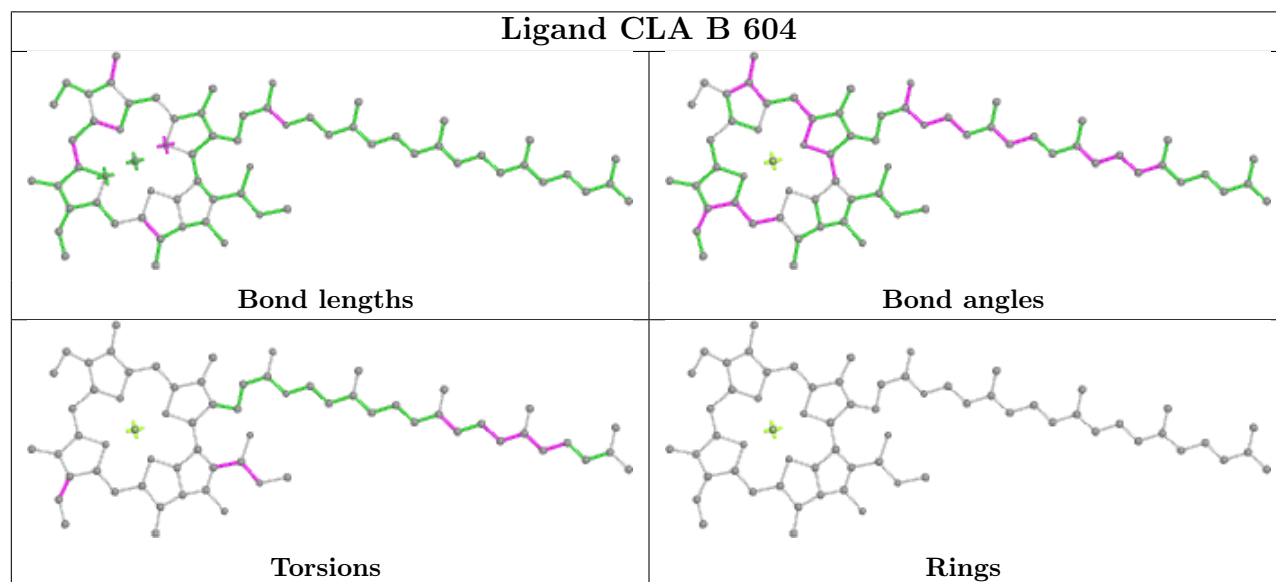
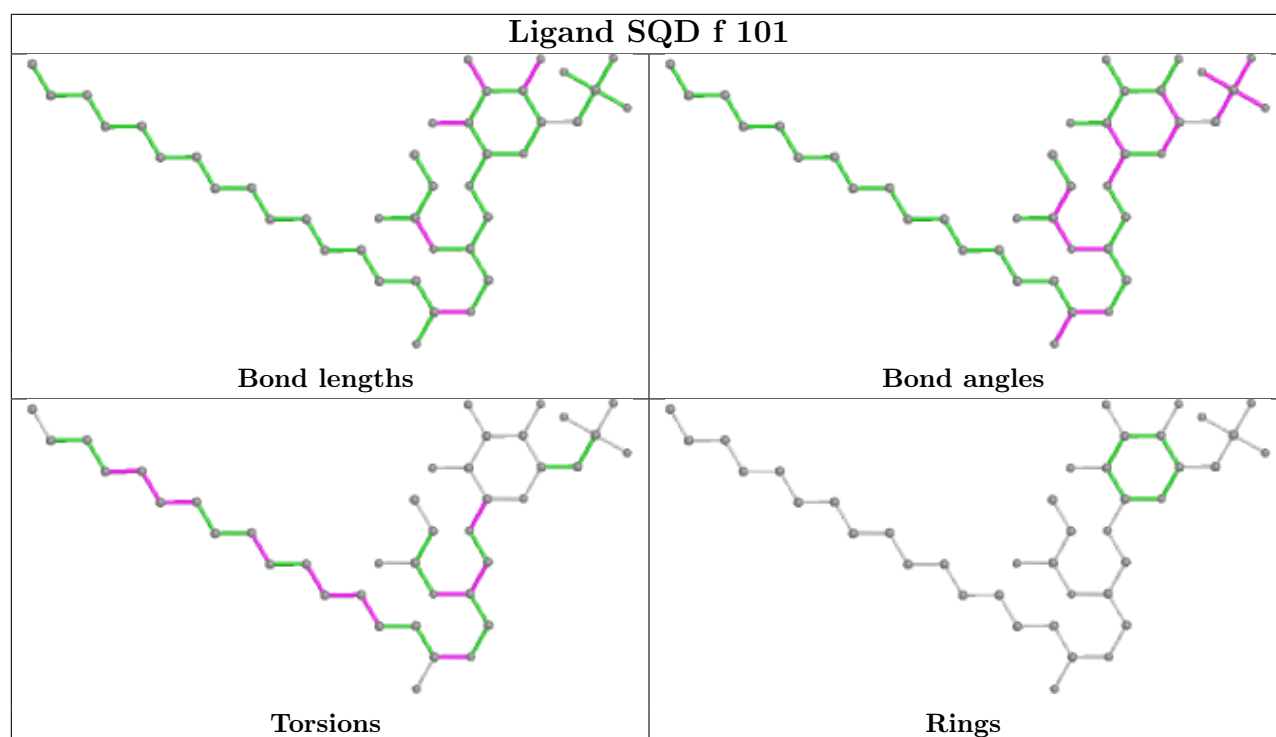
Rings

Ligand CLA b 616

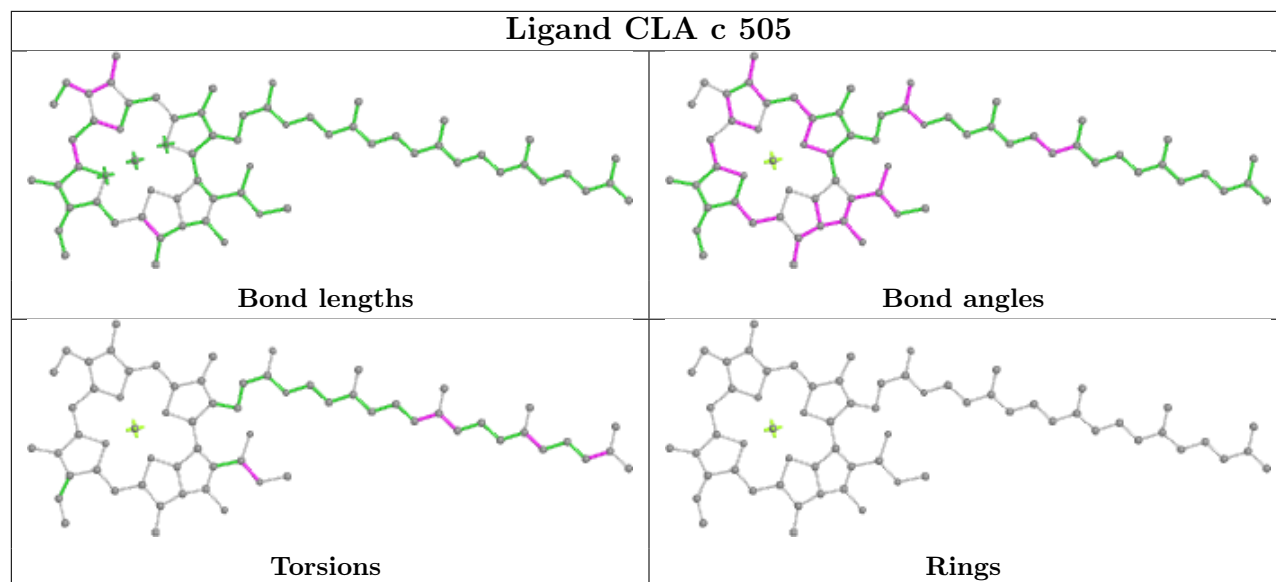


Ligand CLA b 609

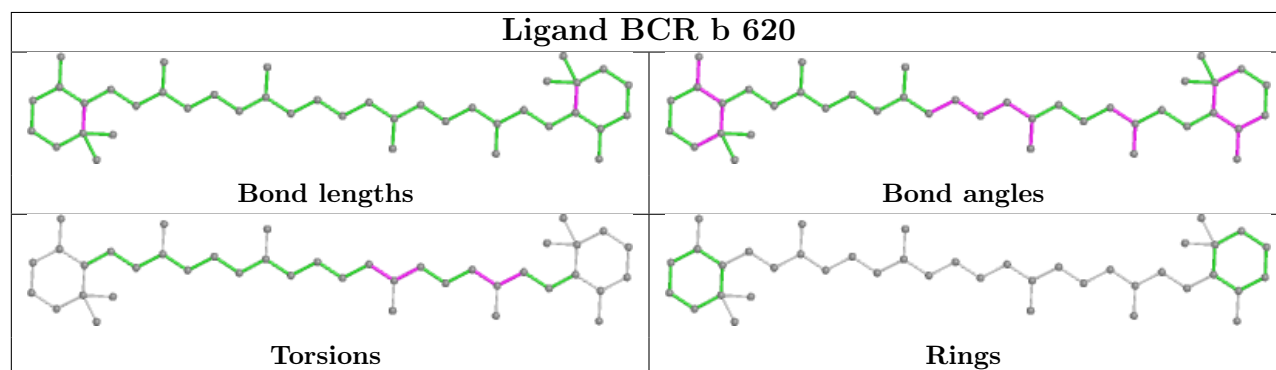




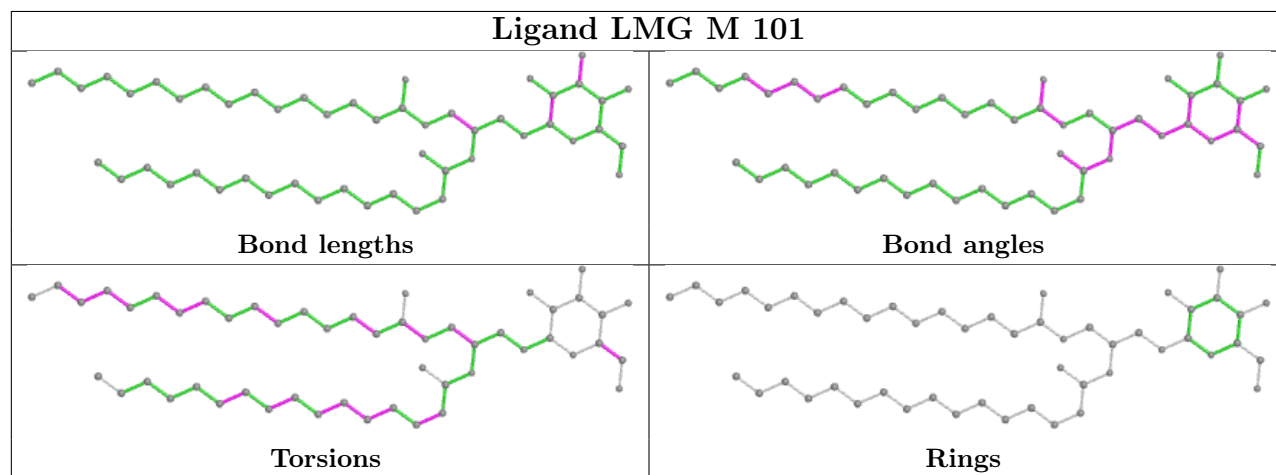
Ligand CLA c 505



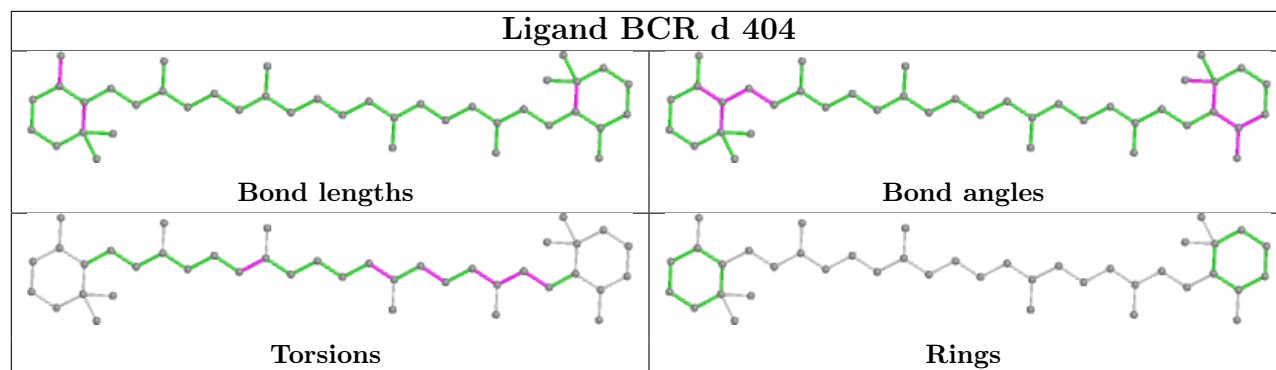
Ligand BCR b 620



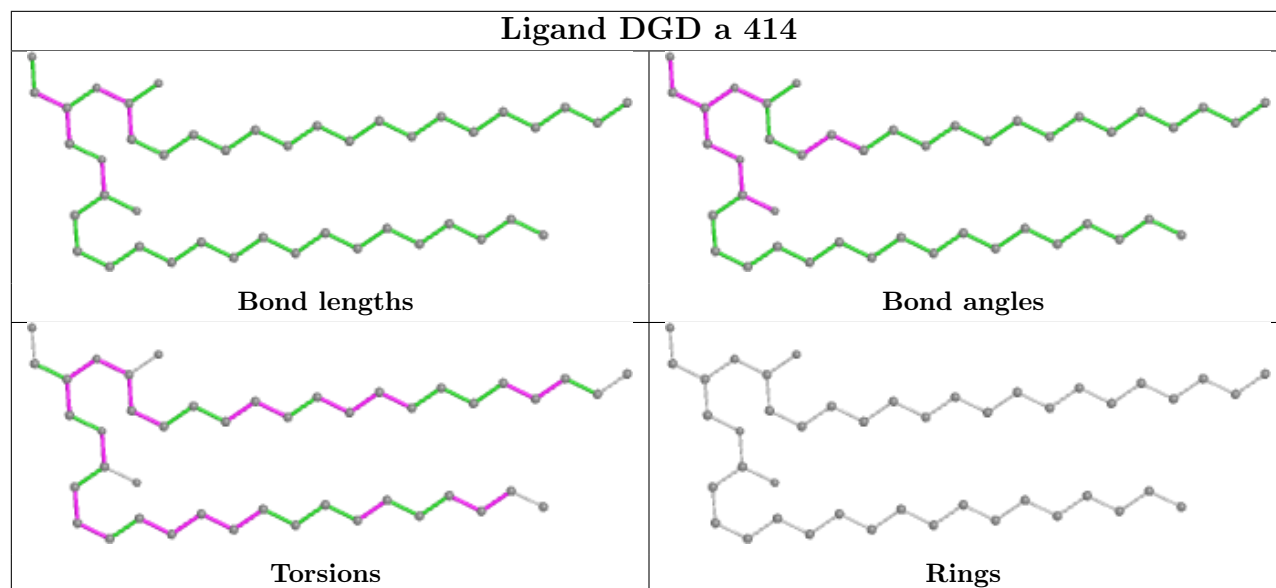
Ligand LMG M 101



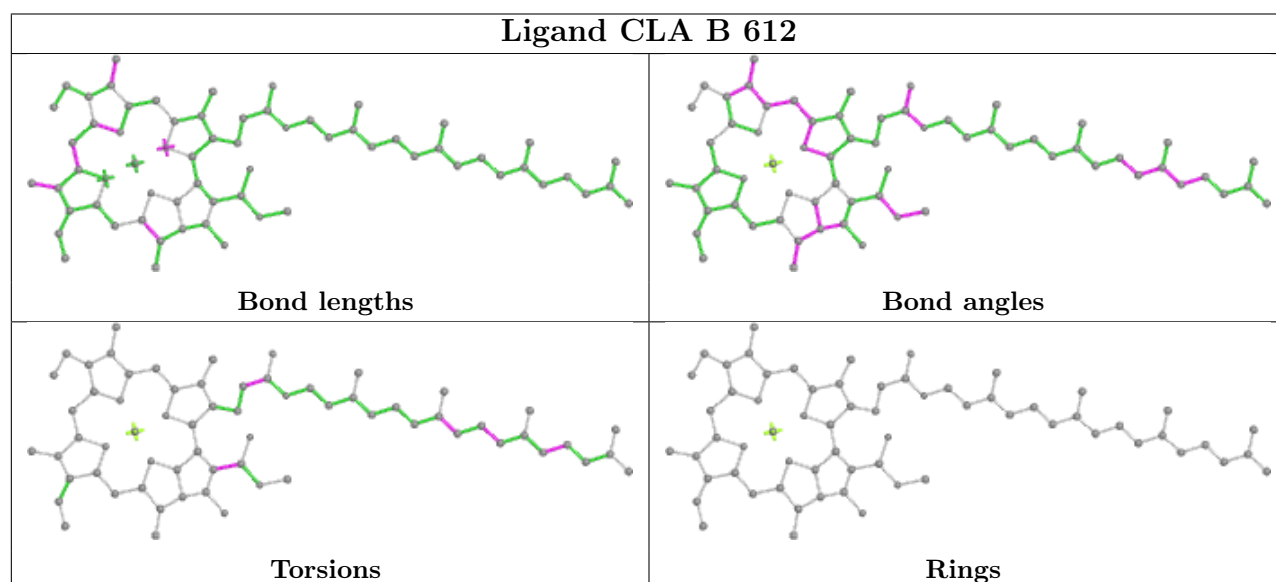
Ligand BCR d 404



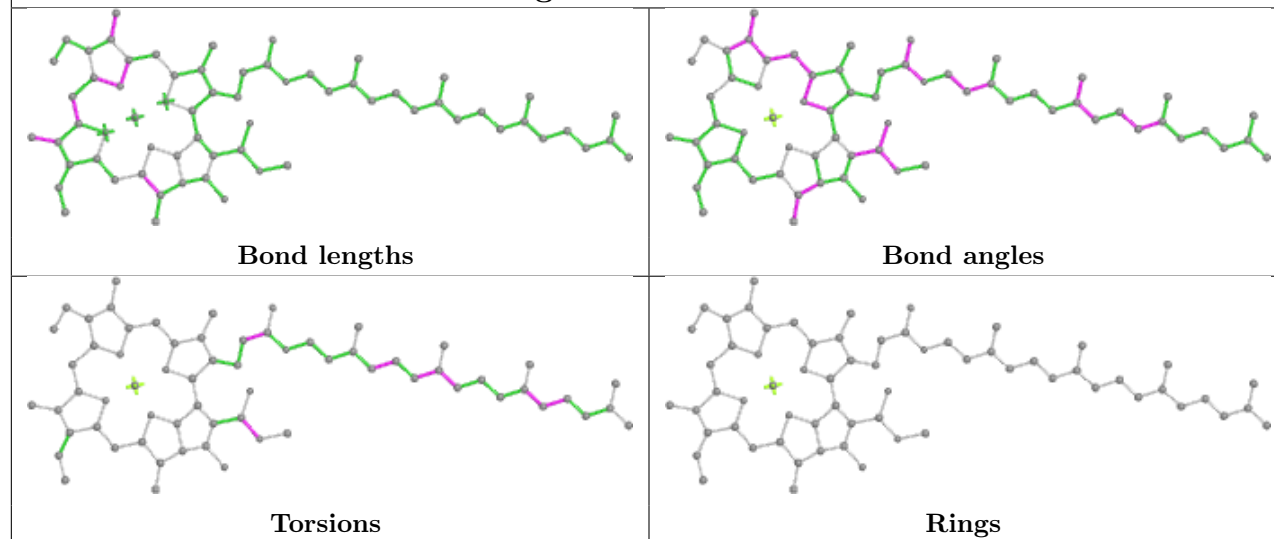
Ligand DGD a 414



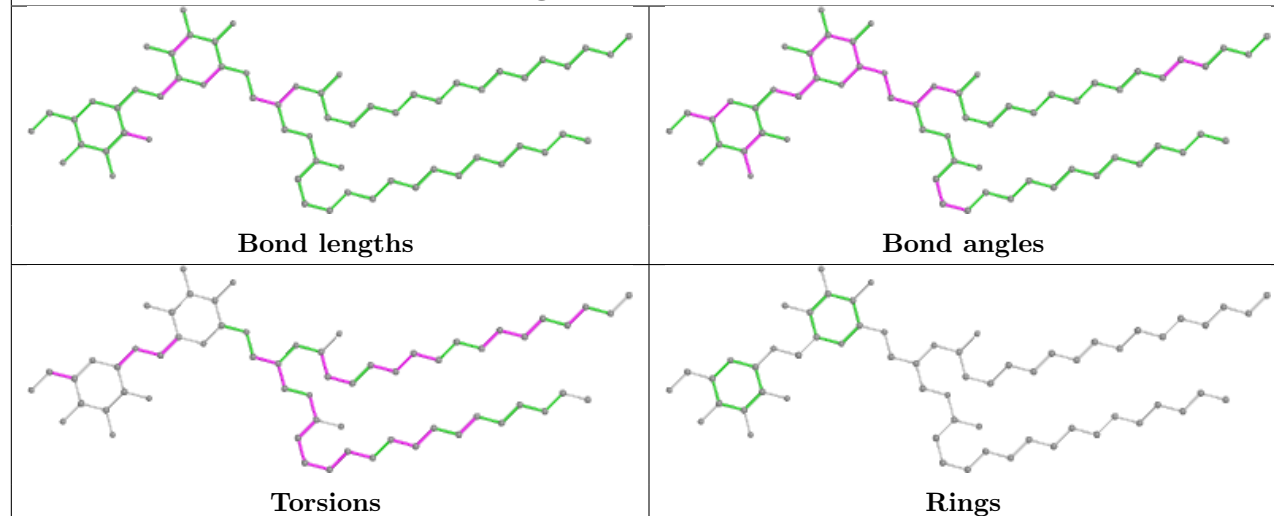
Ligand CLA B 612



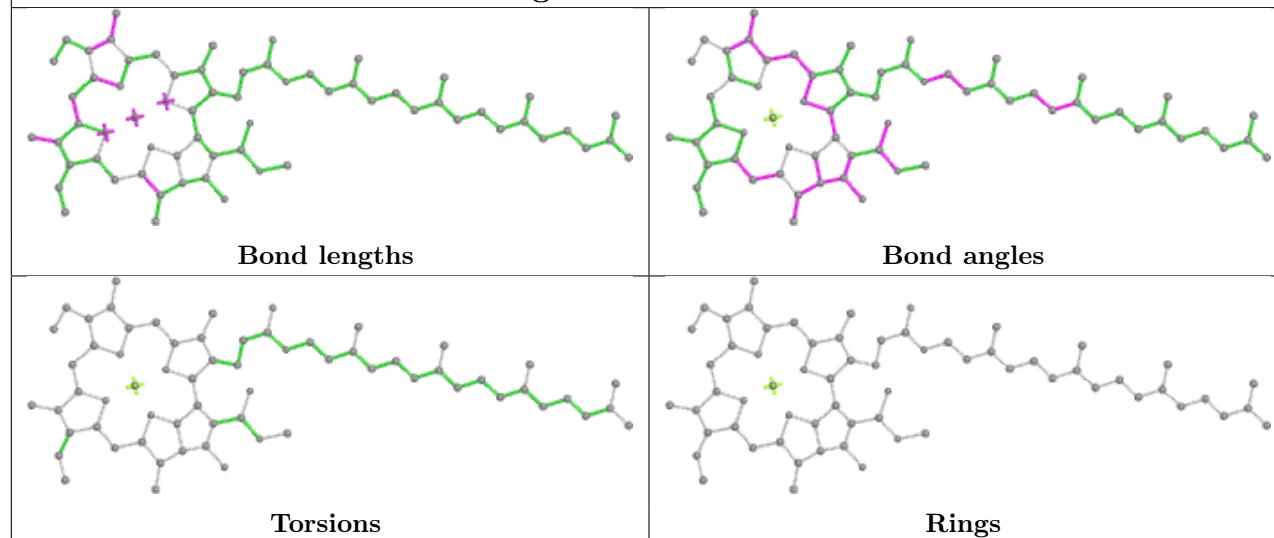
Ligand CLA b 613

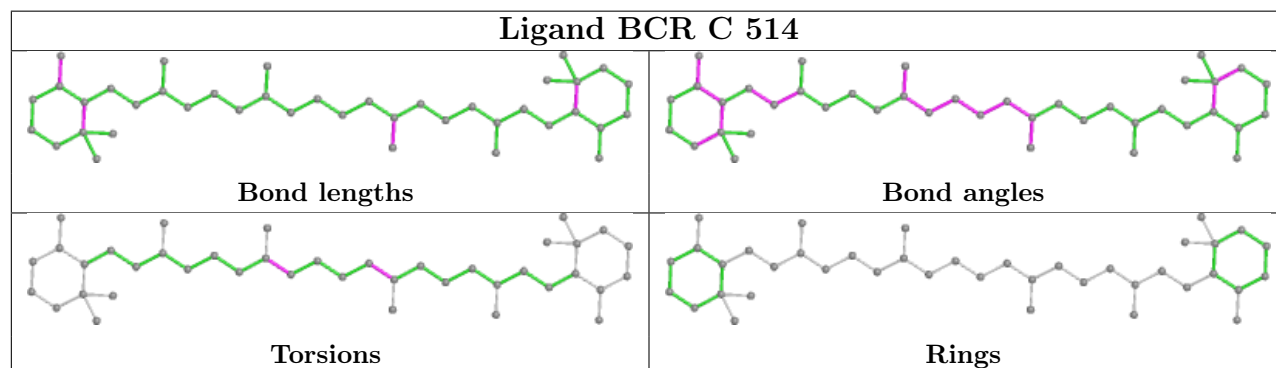
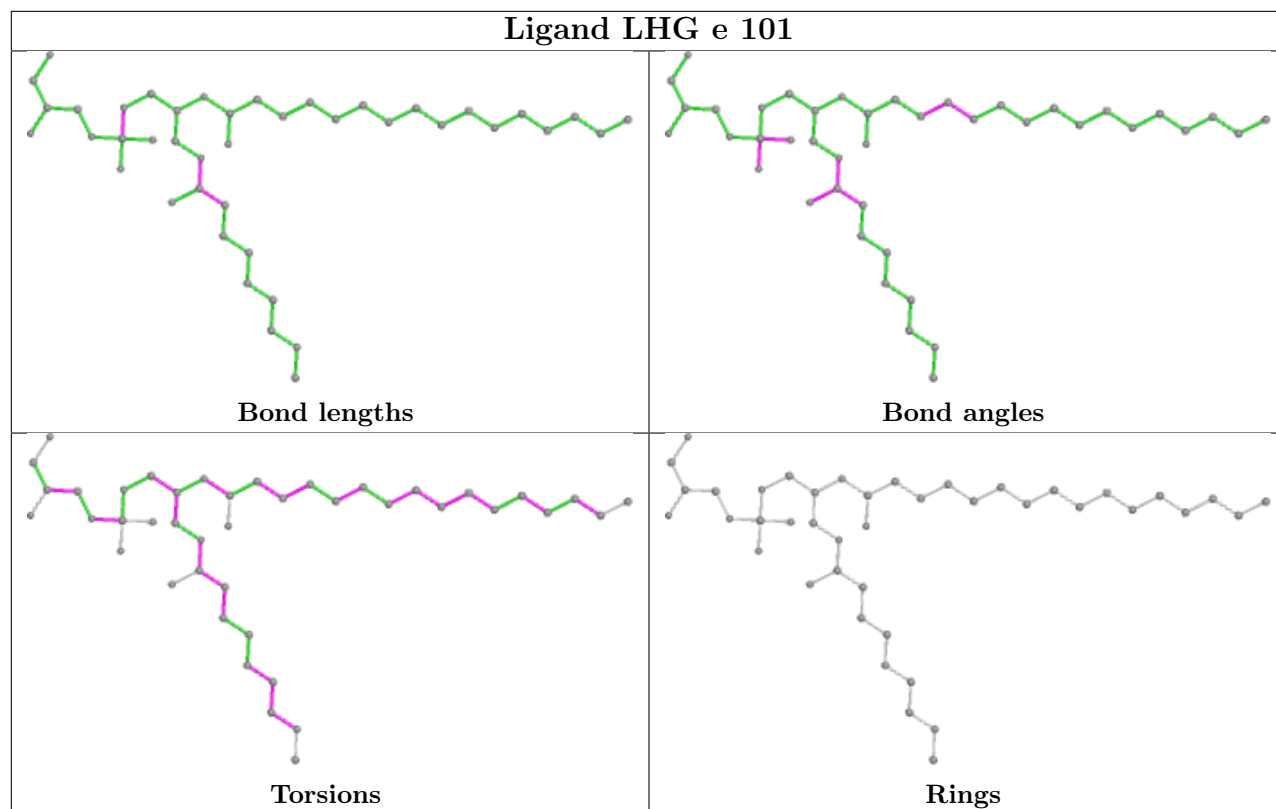
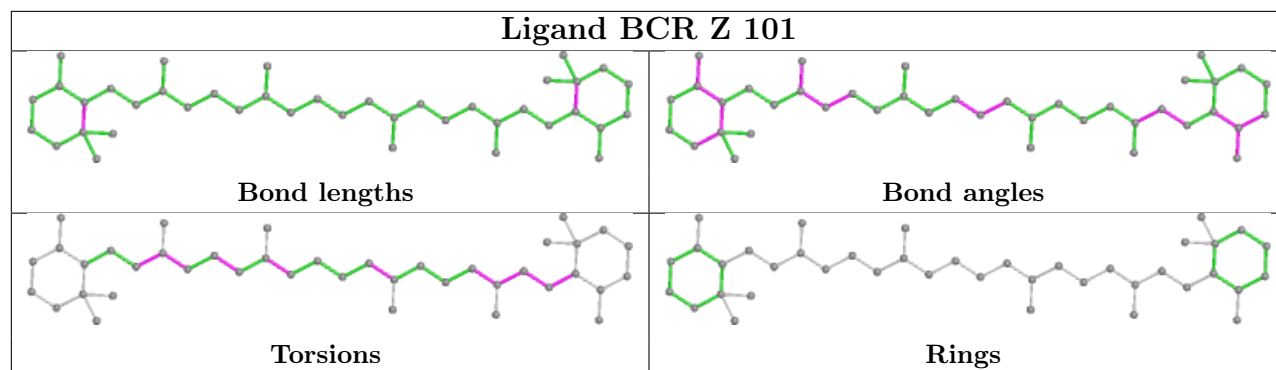


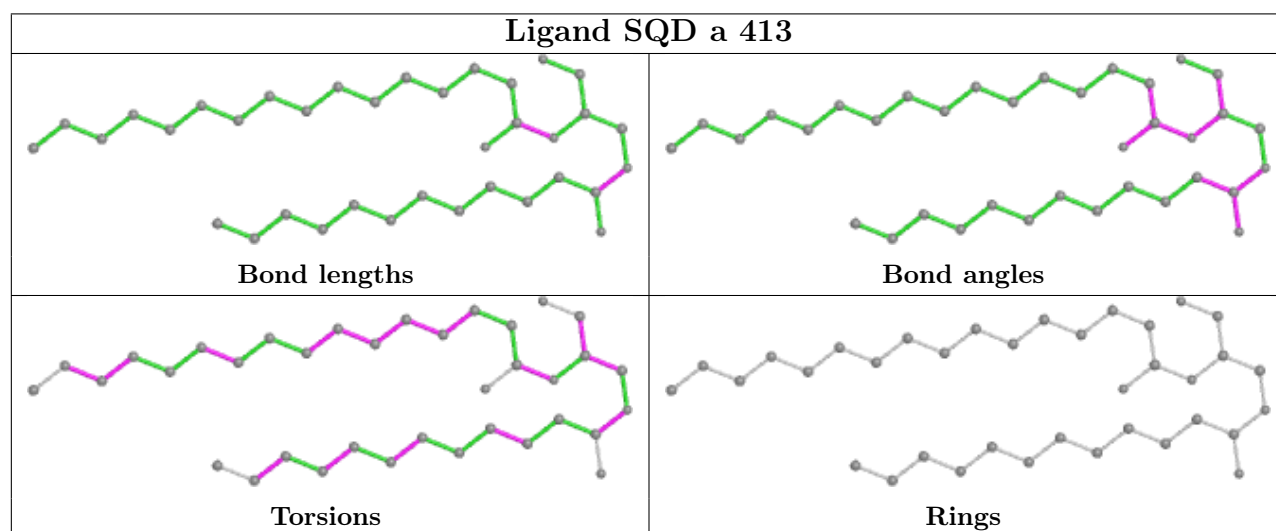
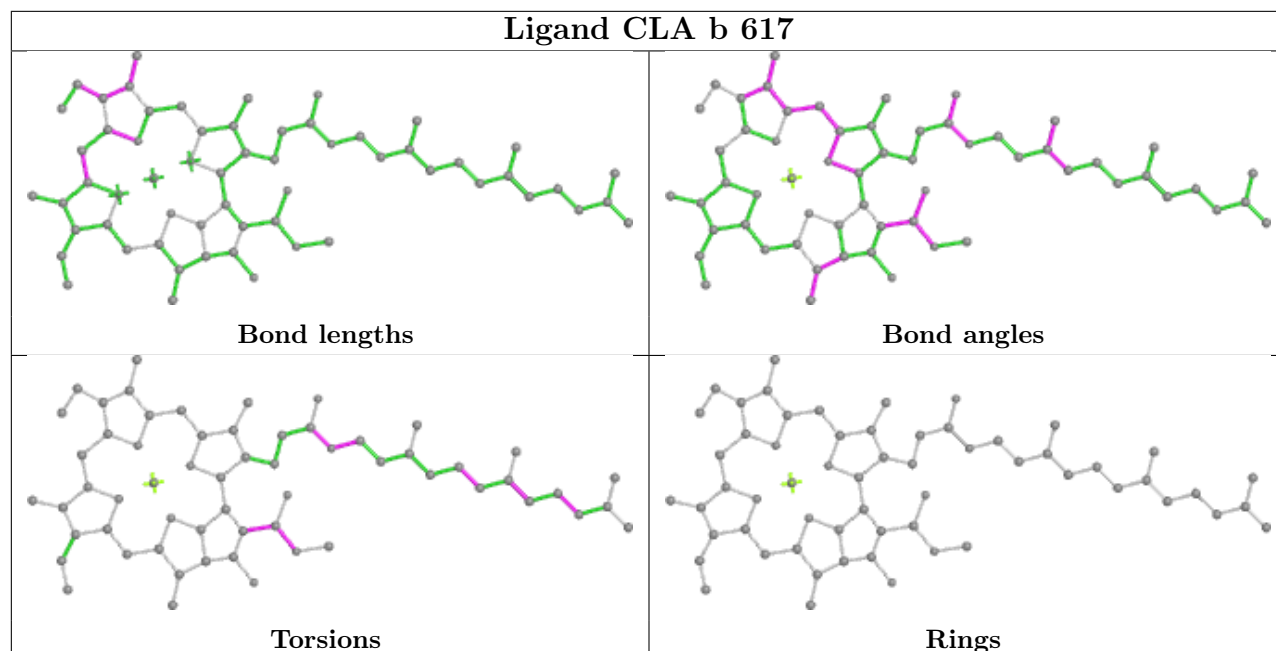
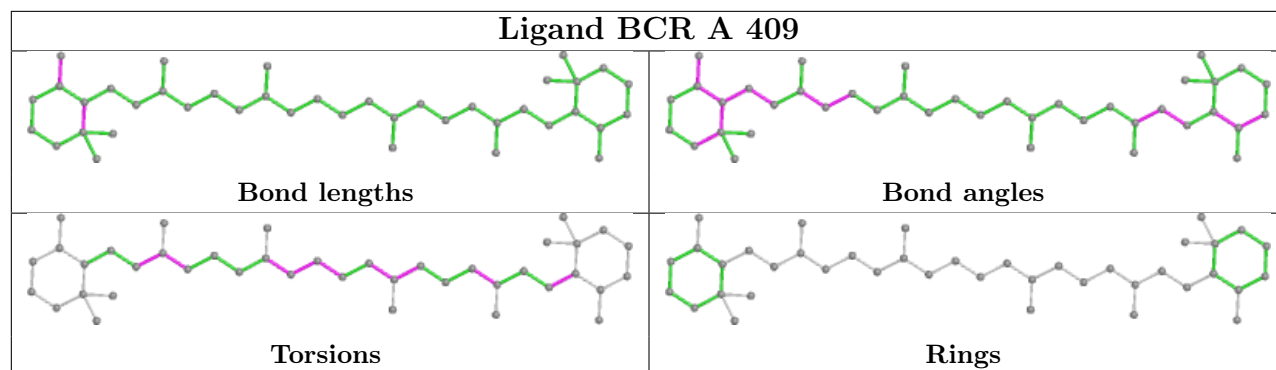
Ligand DGD c 516

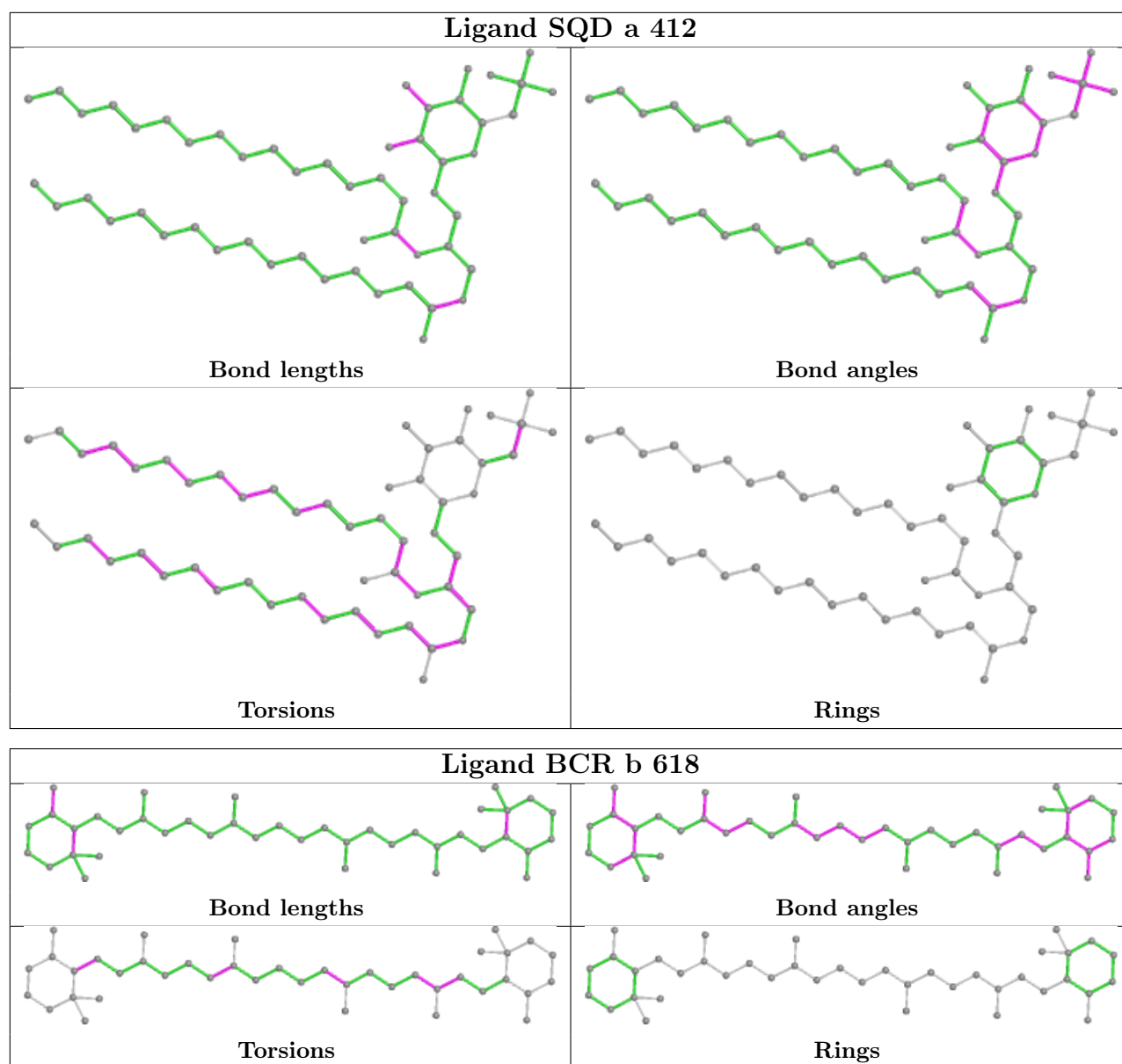


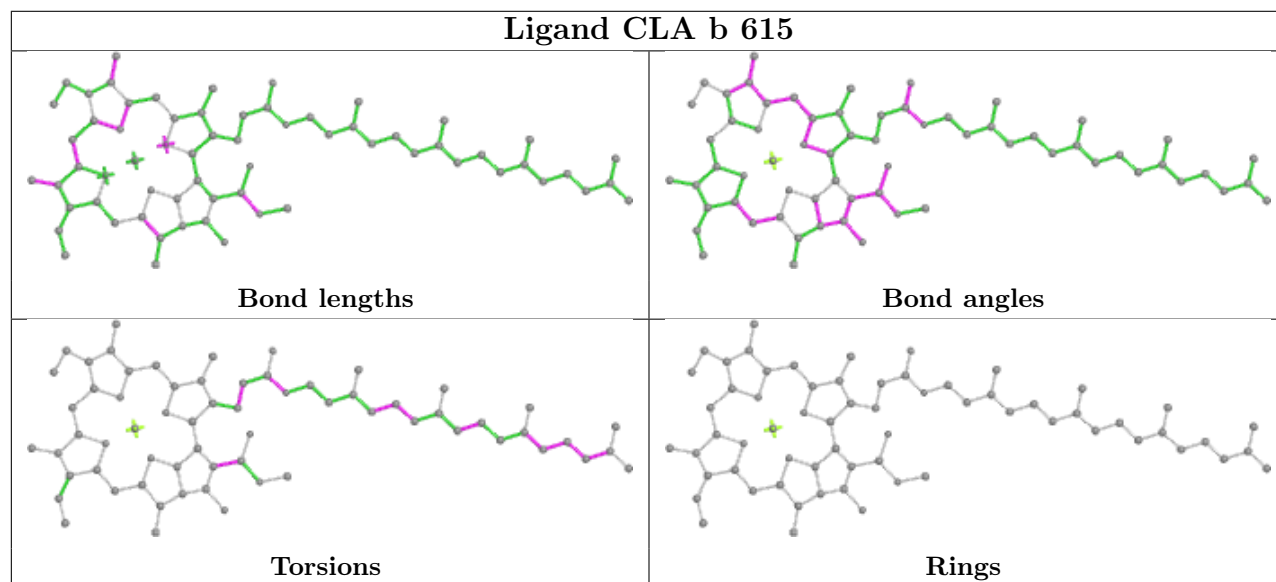
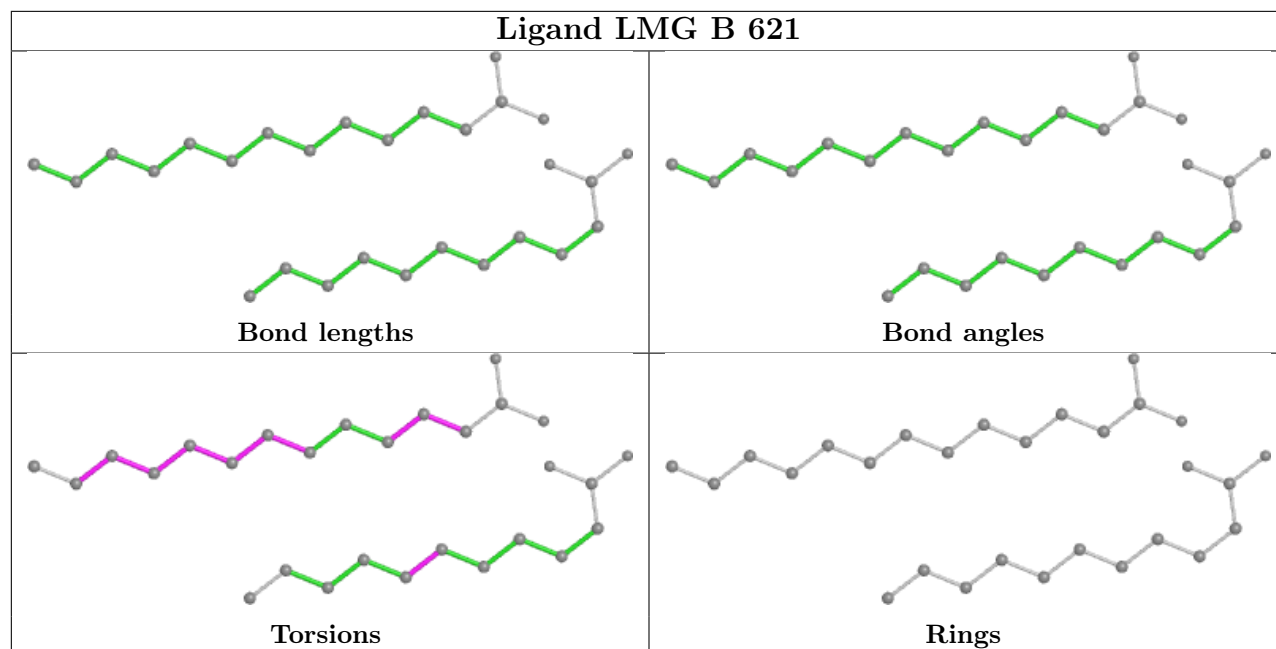
Ligand CLA B 608



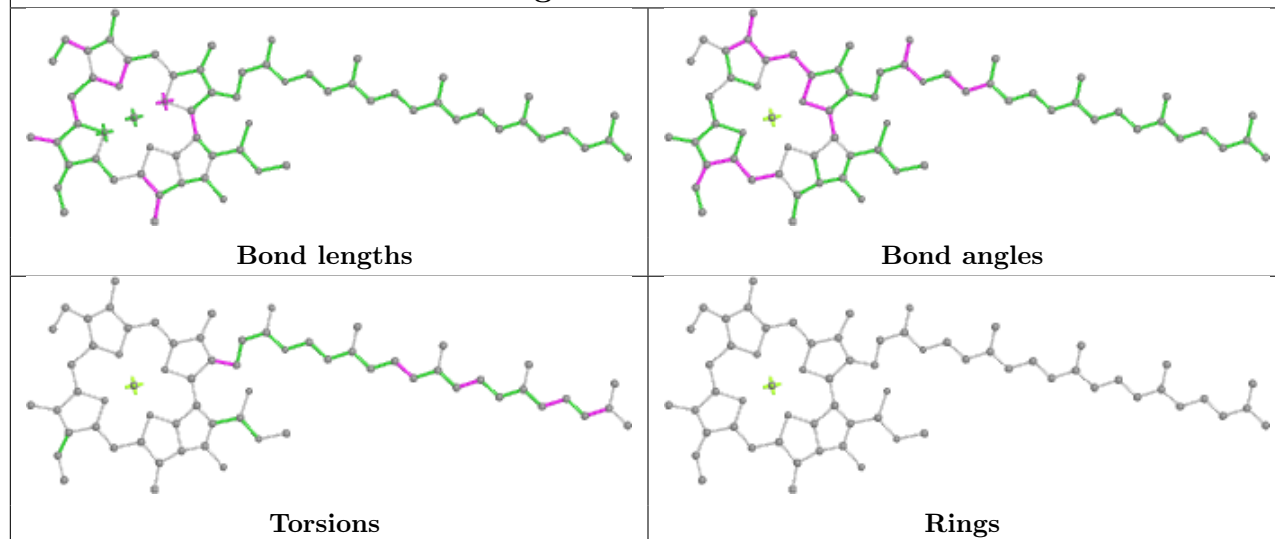




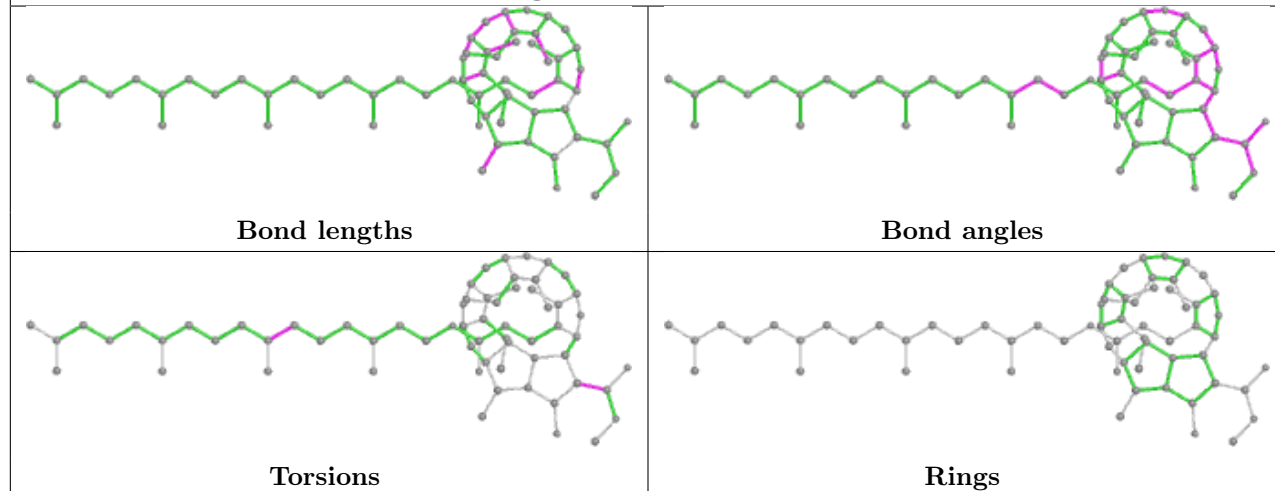




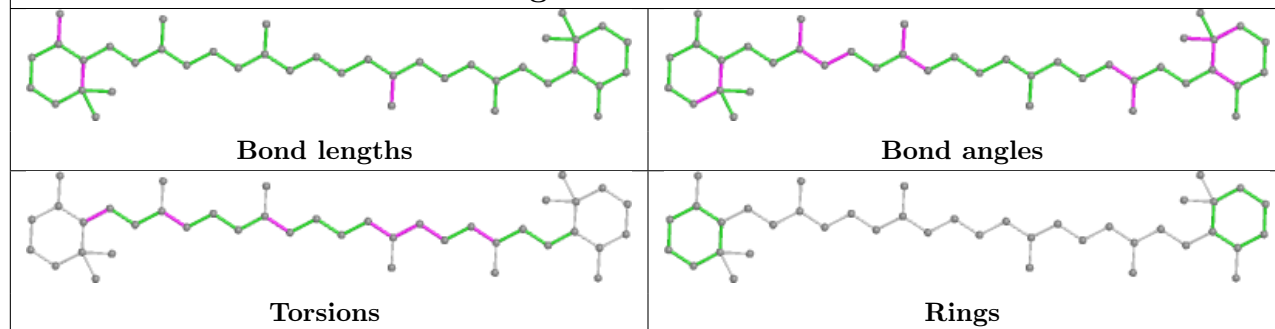
Ligand CLA d 403

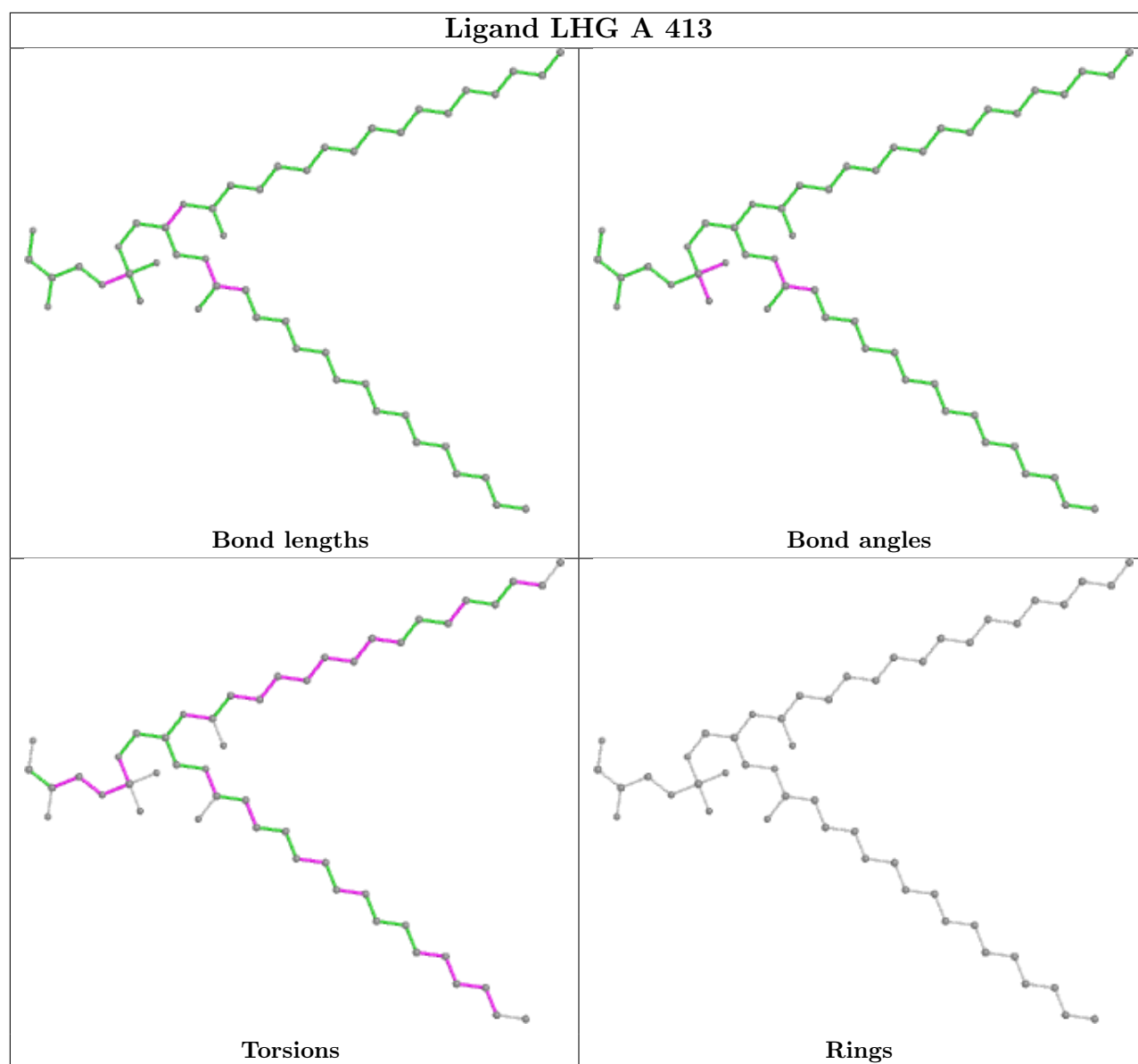


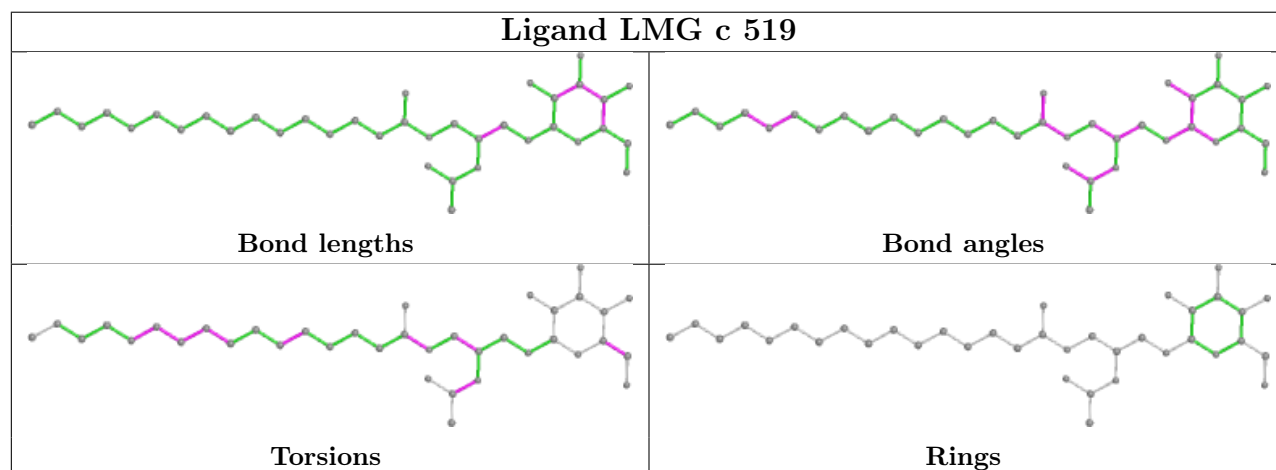
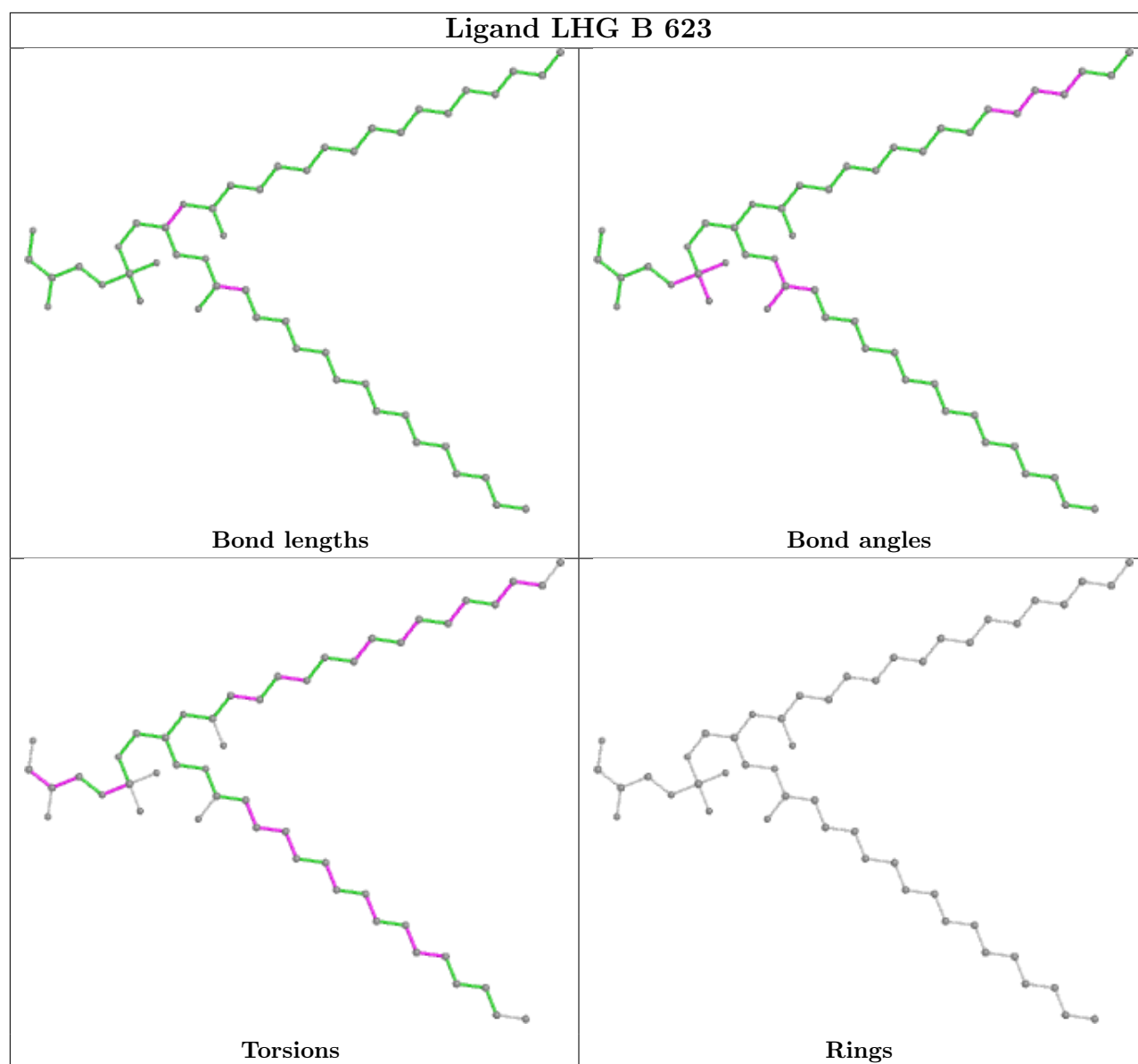
Ligand PHO A 407

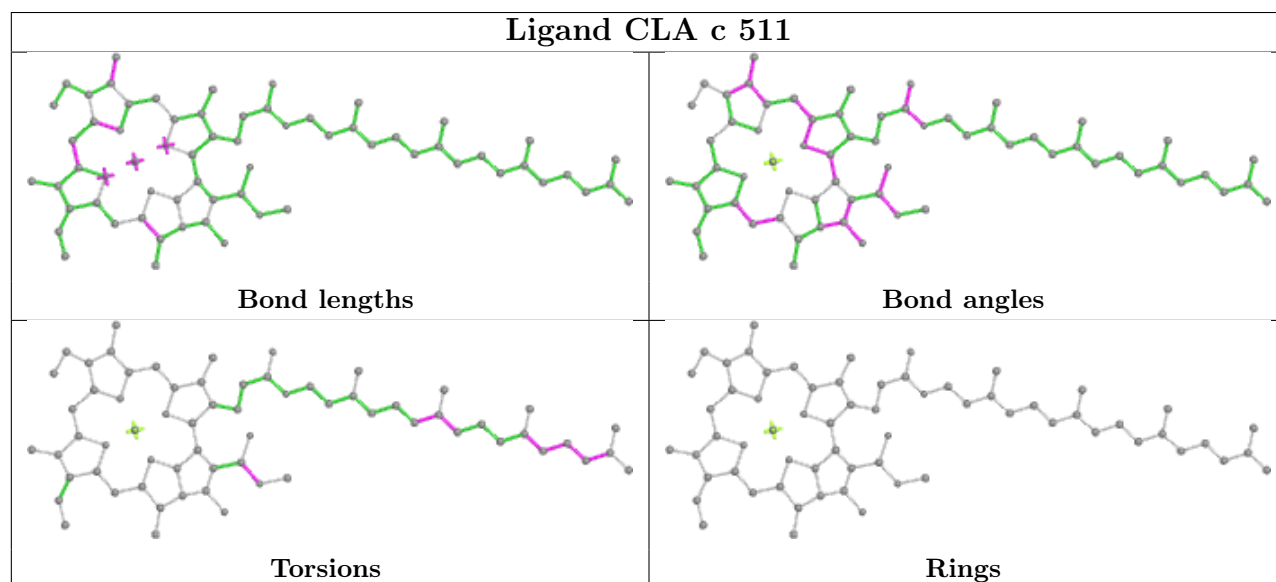
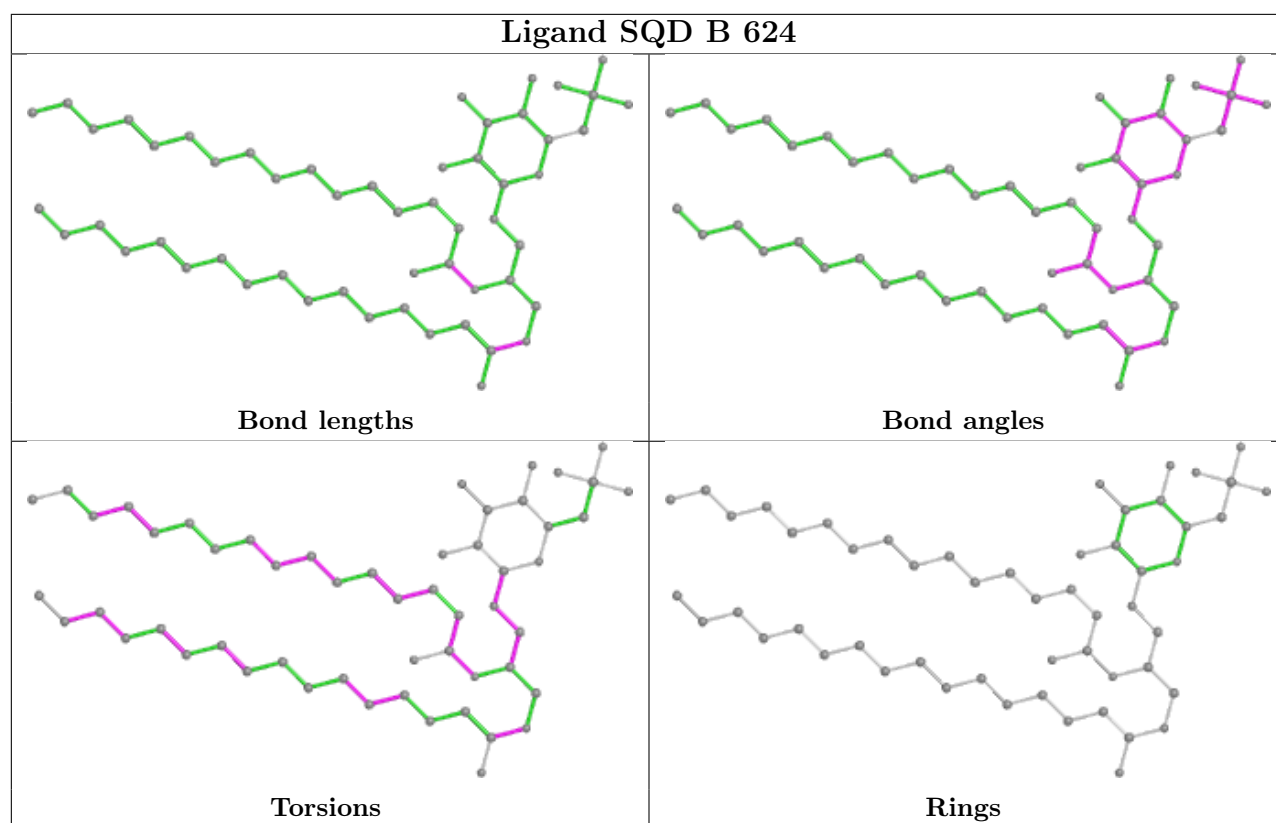


Ligand BCR B 617

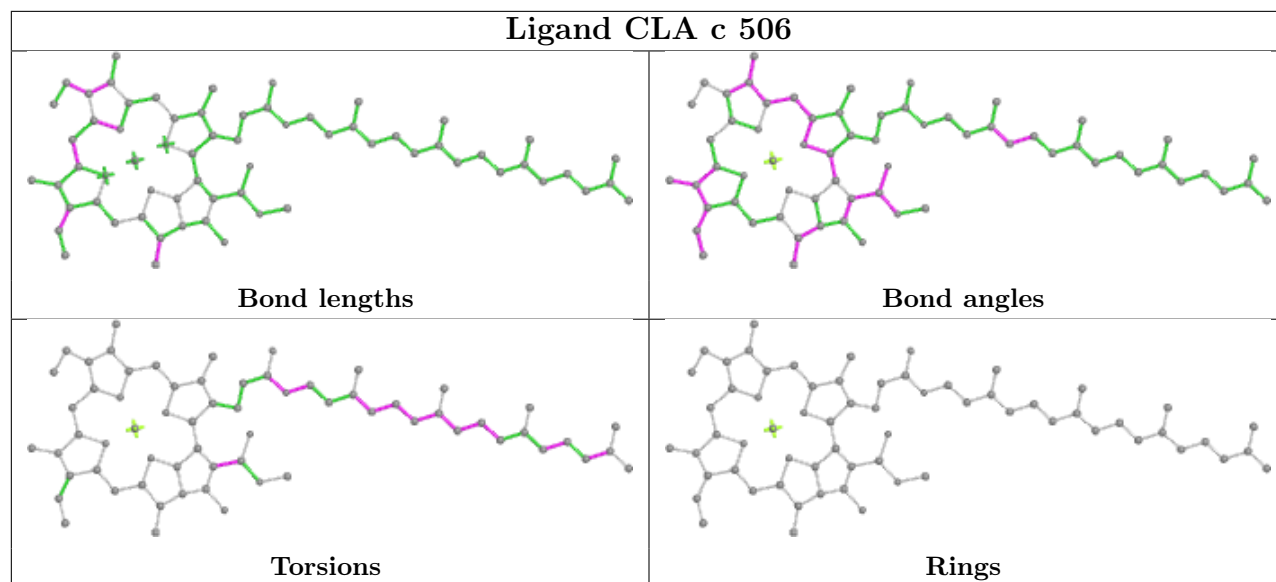




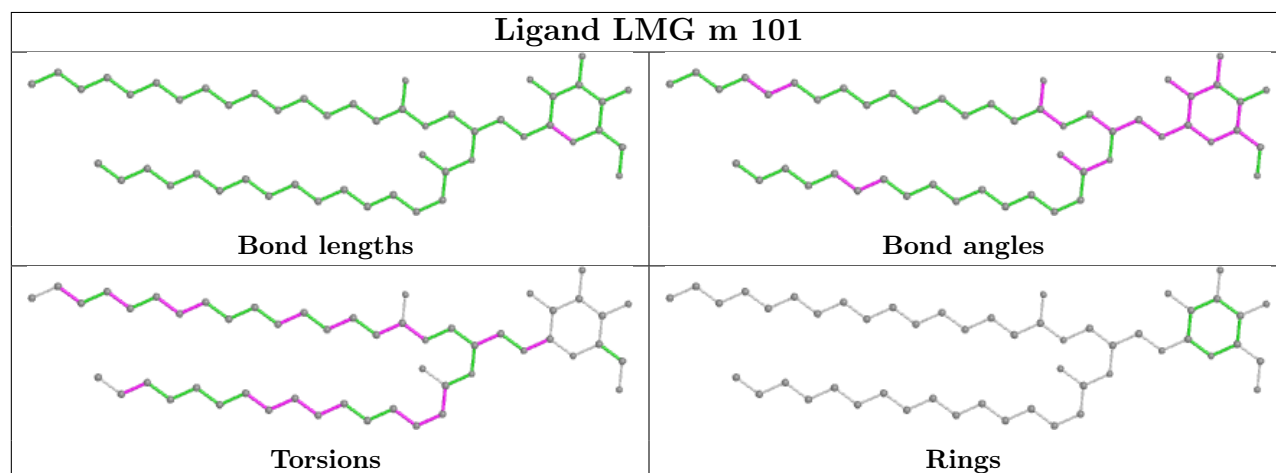


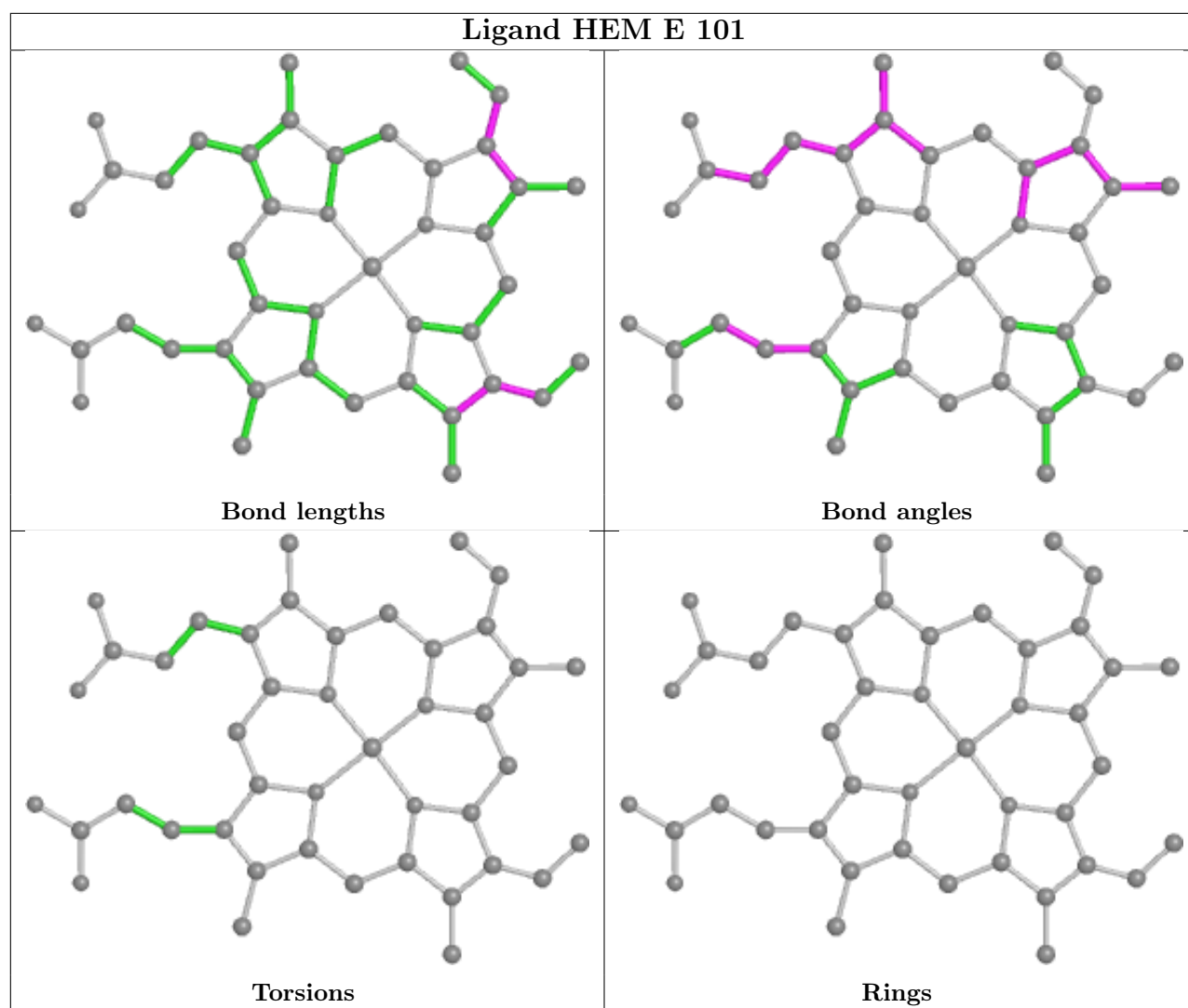


Ligand CLA c 506

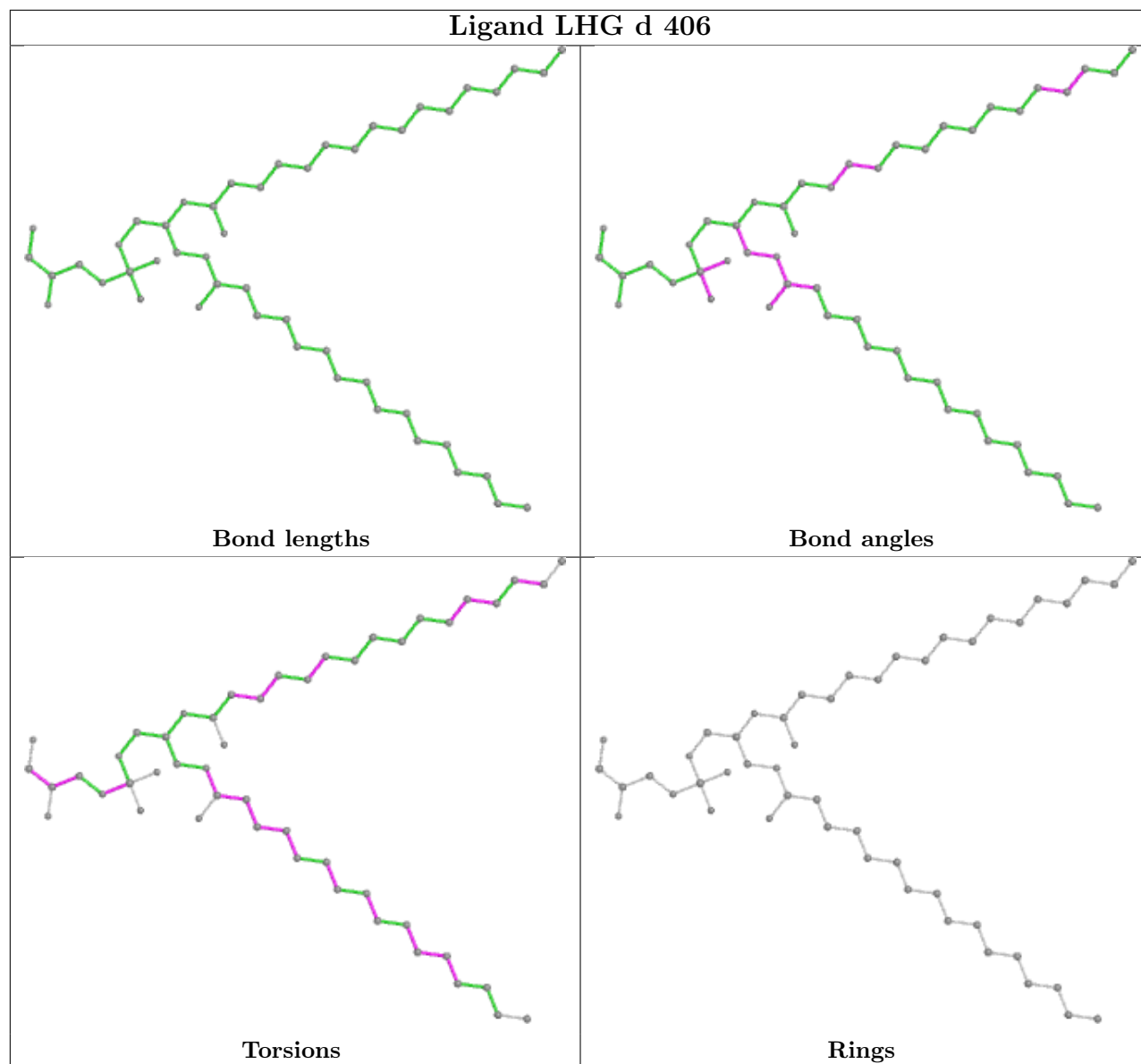


Ligand LMG m 101

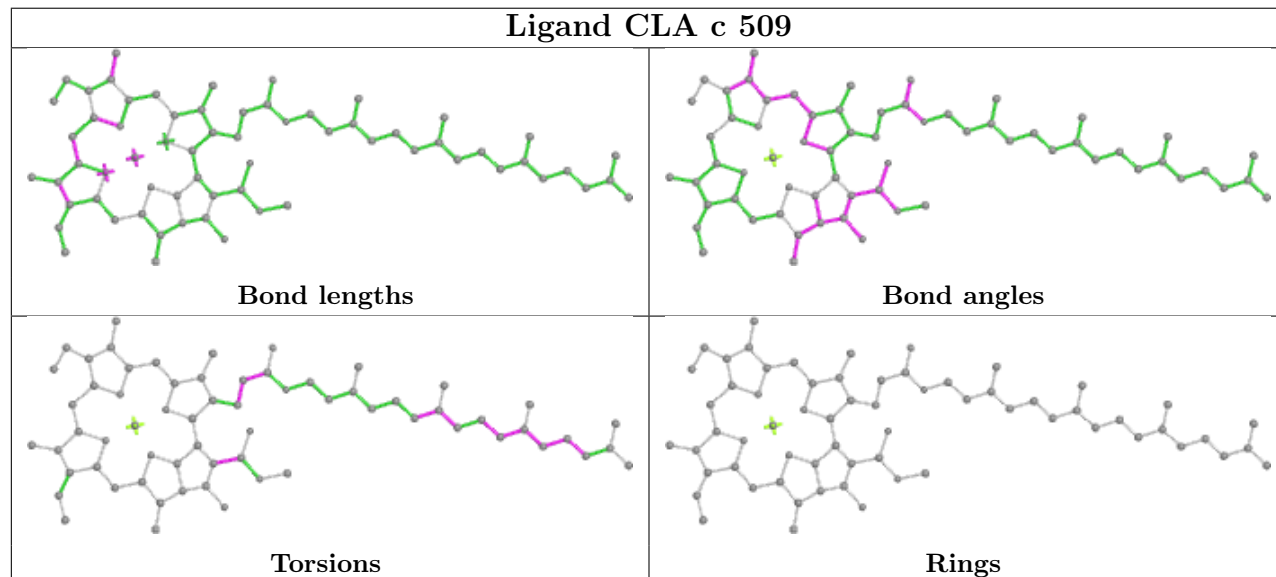




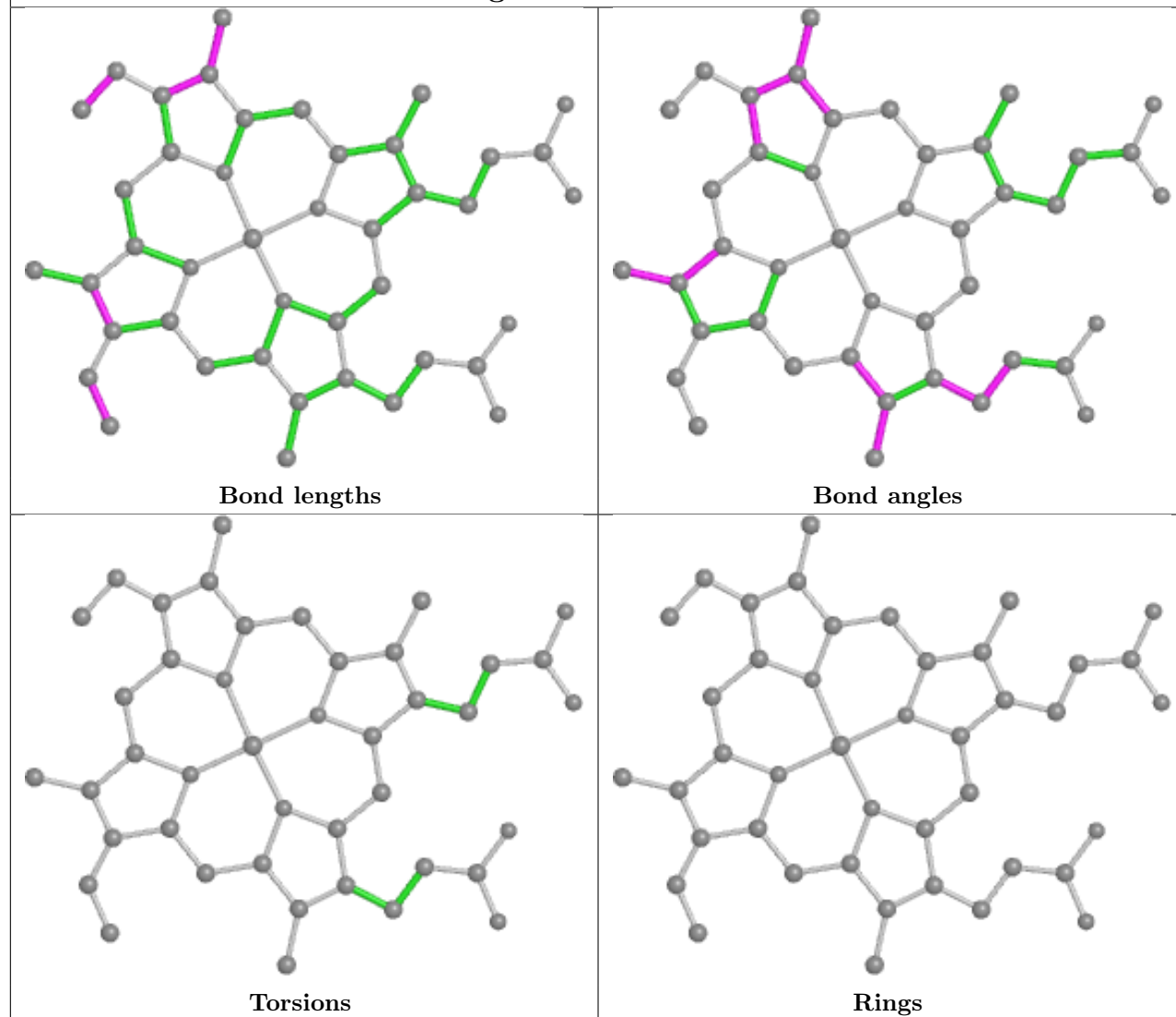
Ligand LHG d 406



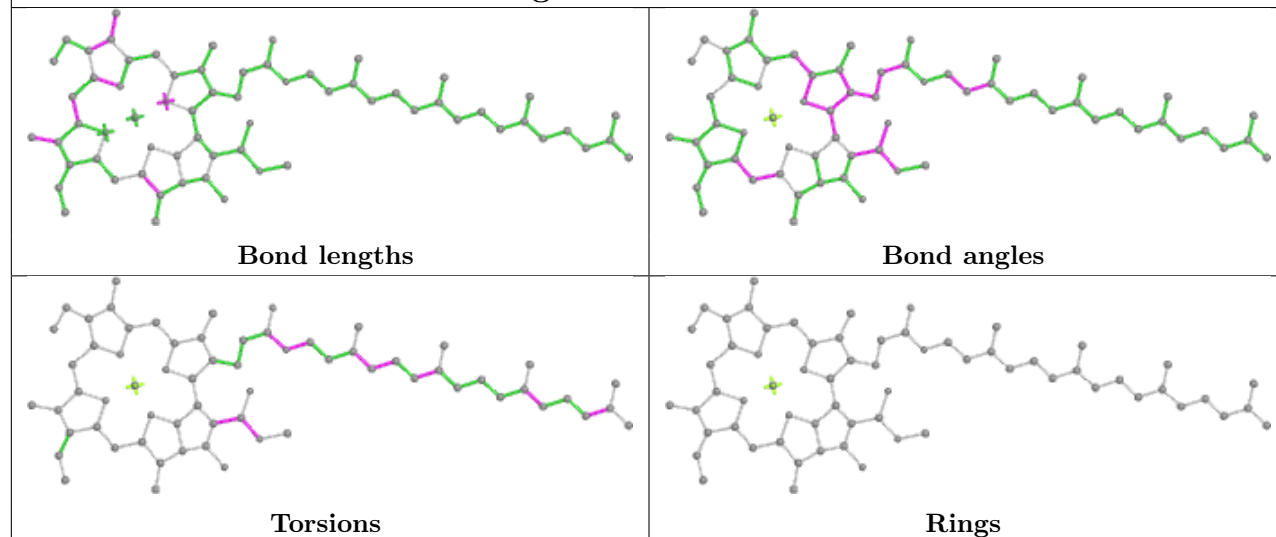
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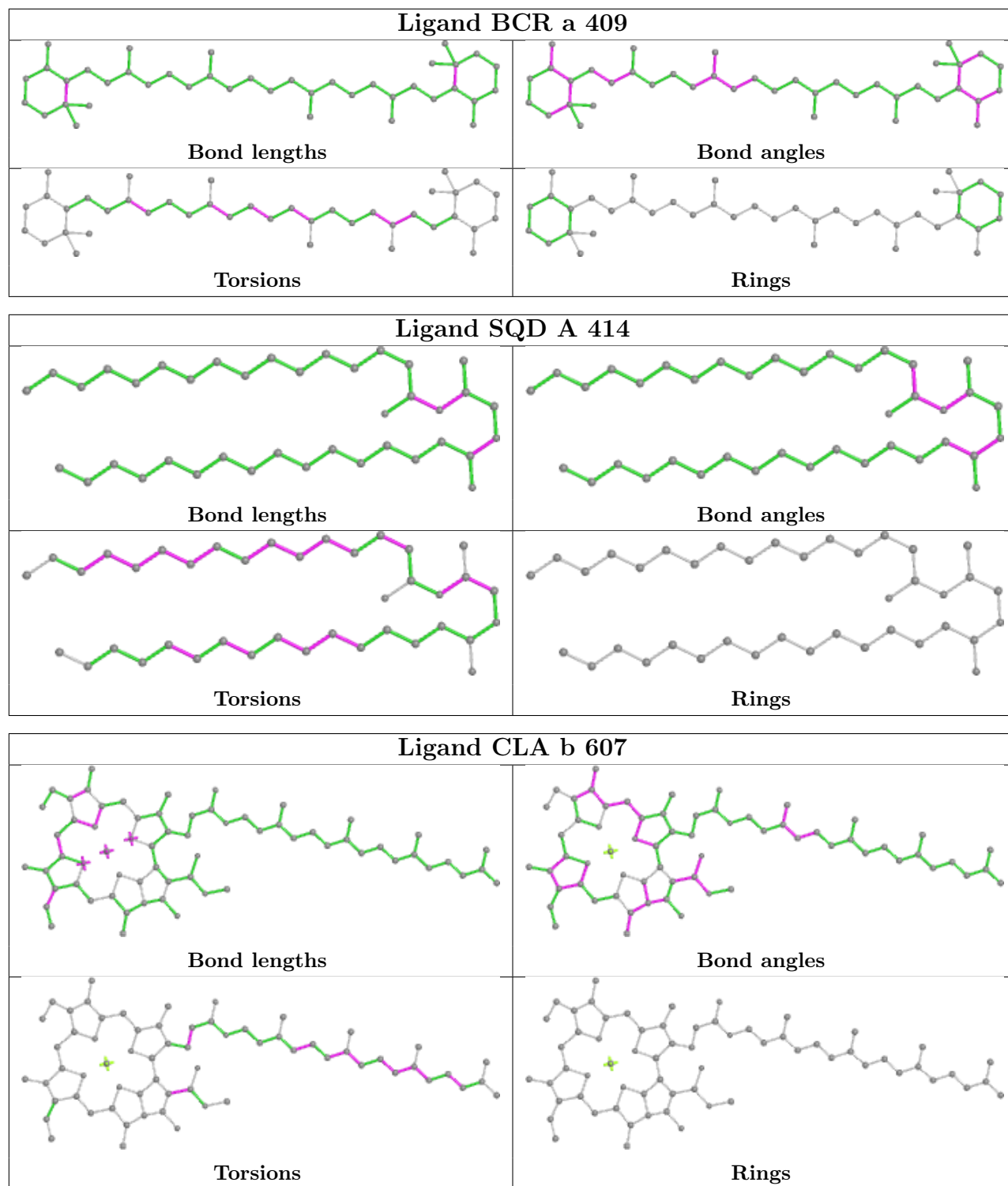


Ligand HEC V 201

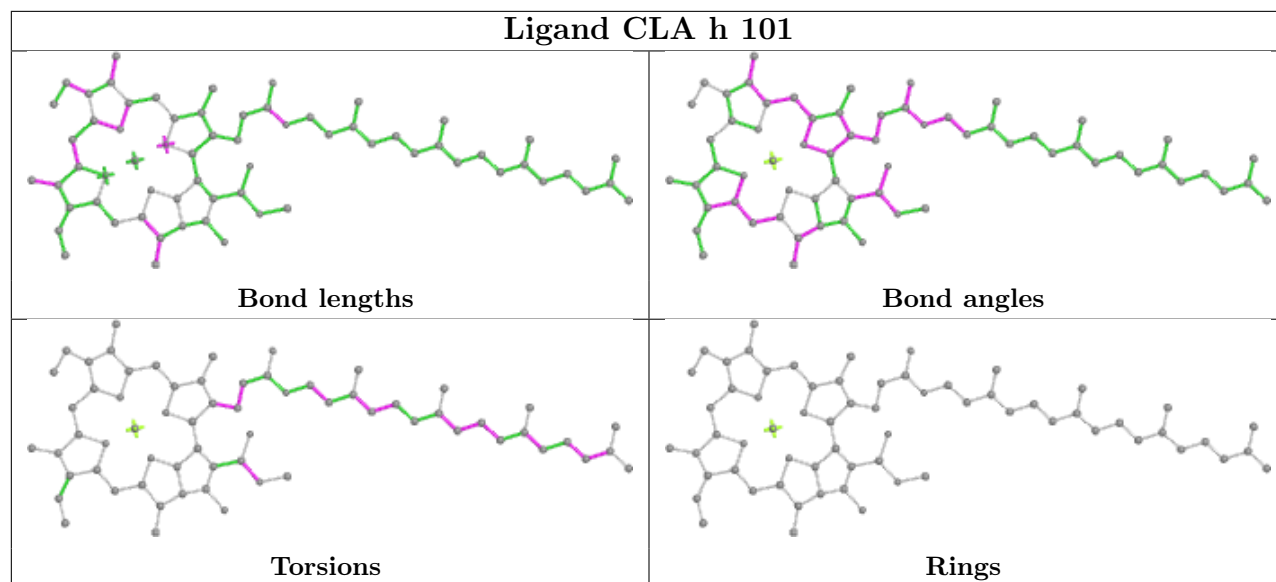


Ligand CLA B 601

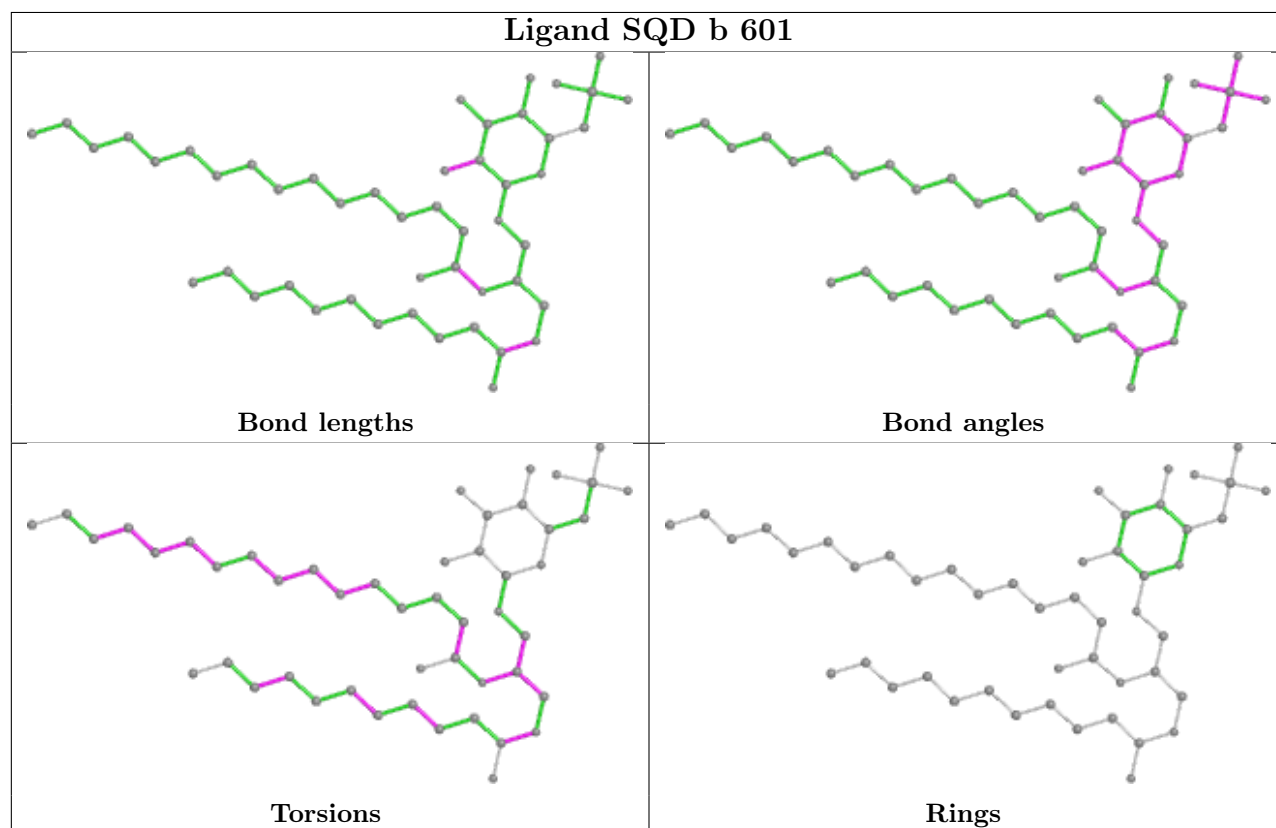


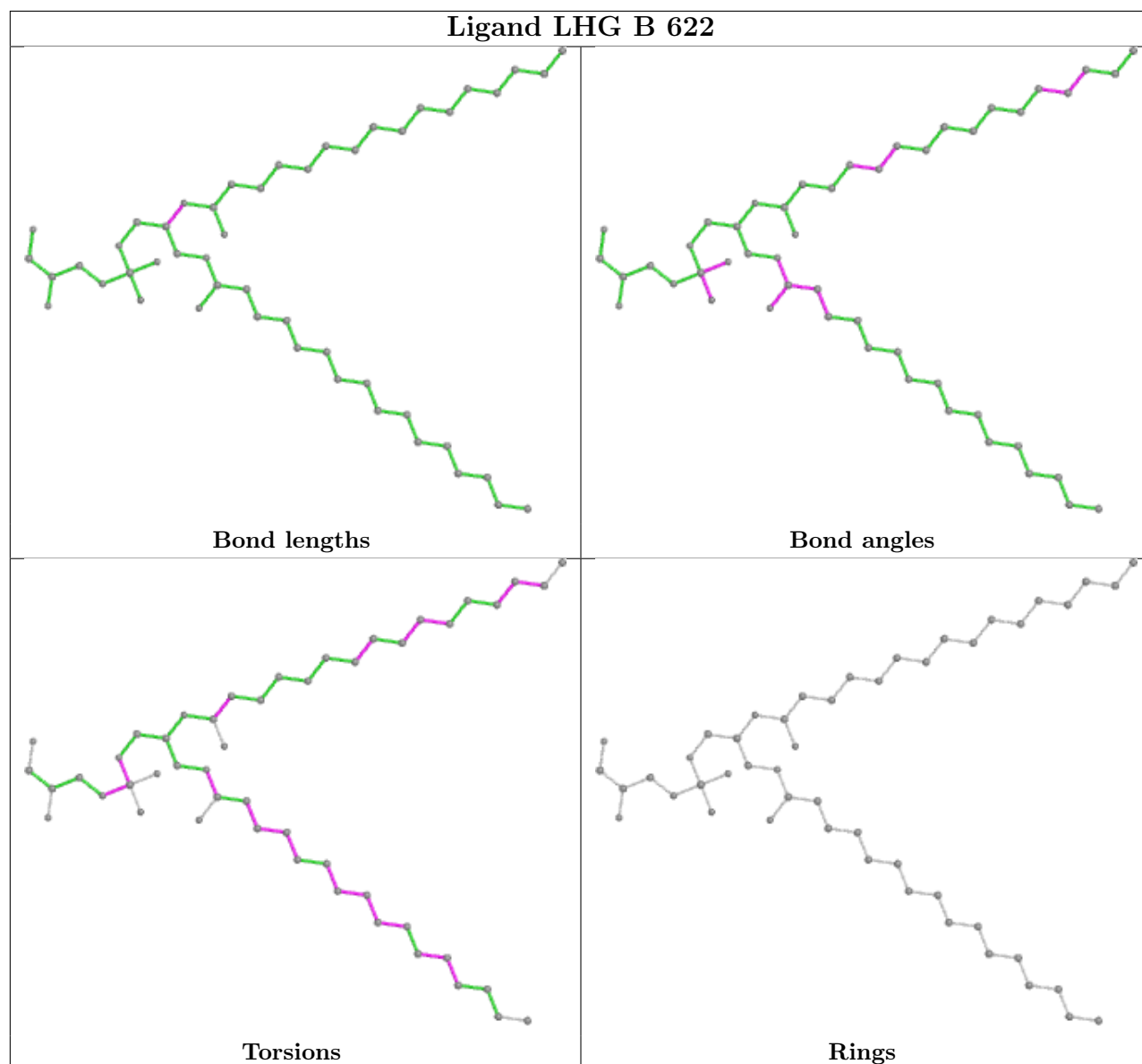
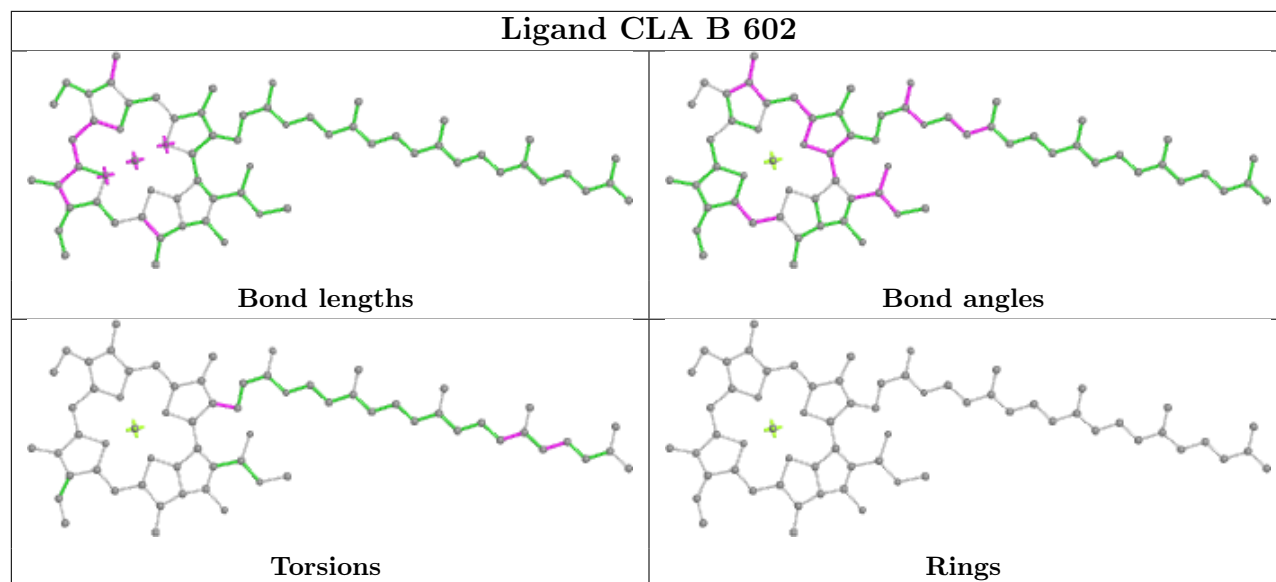


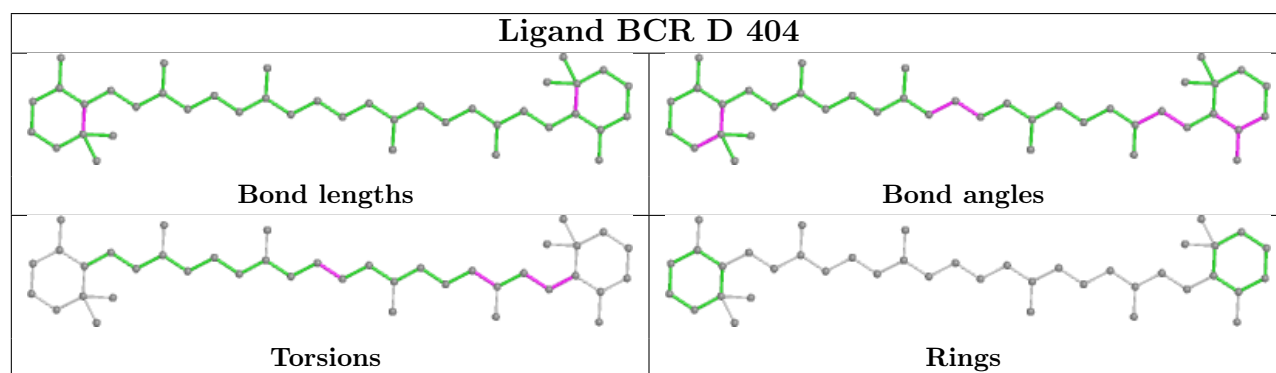
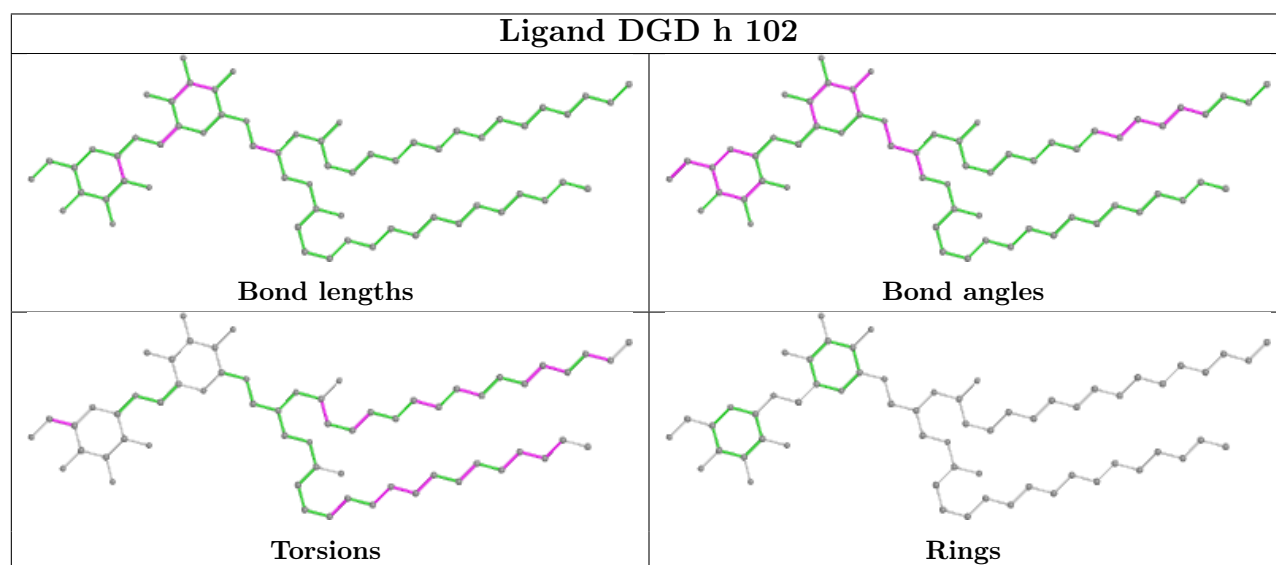
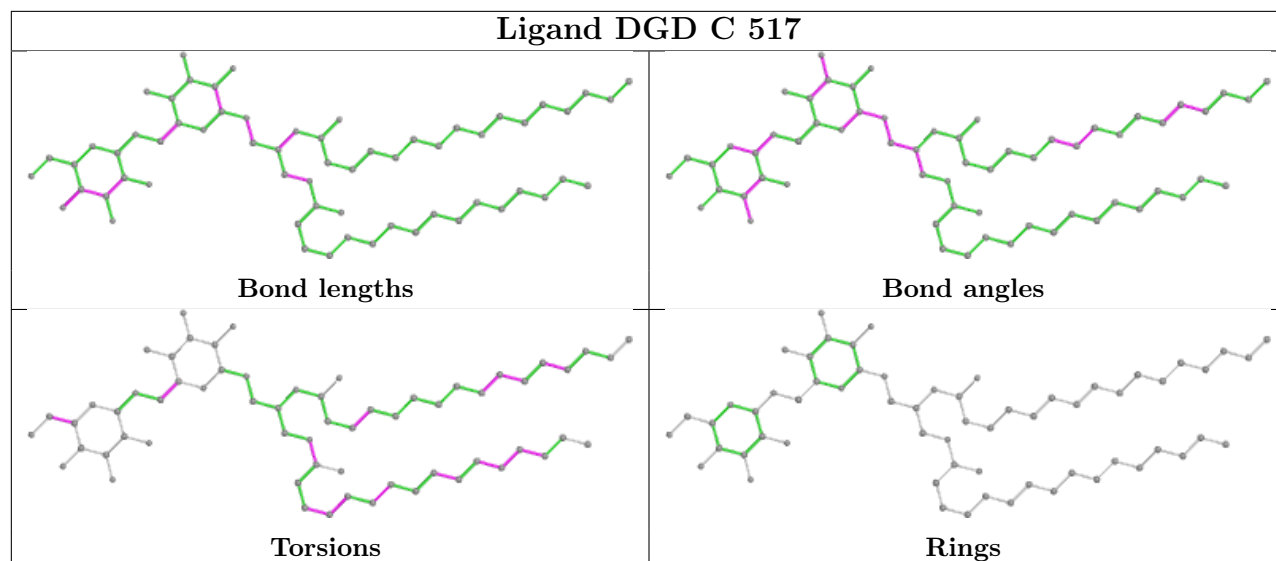
Ligand CLA h 101



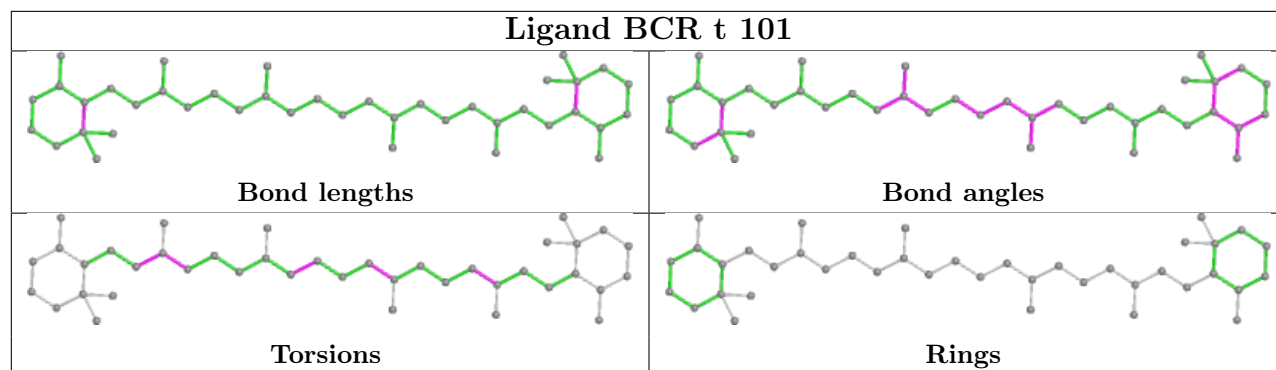
Ligand SQD b 601



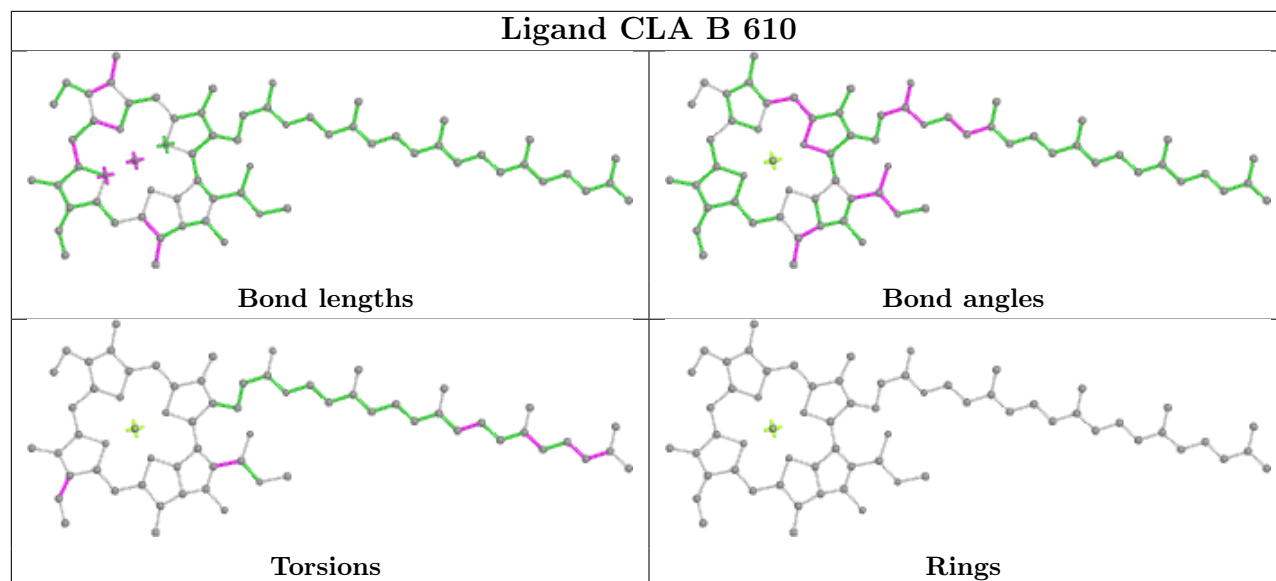




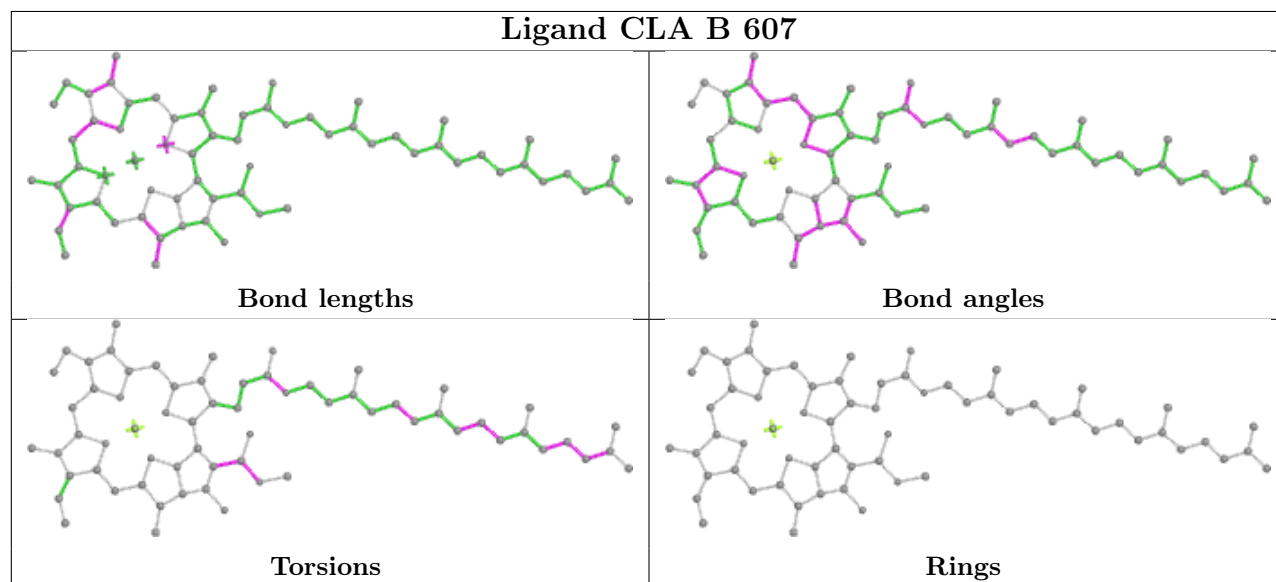
Ligand BCR t 101

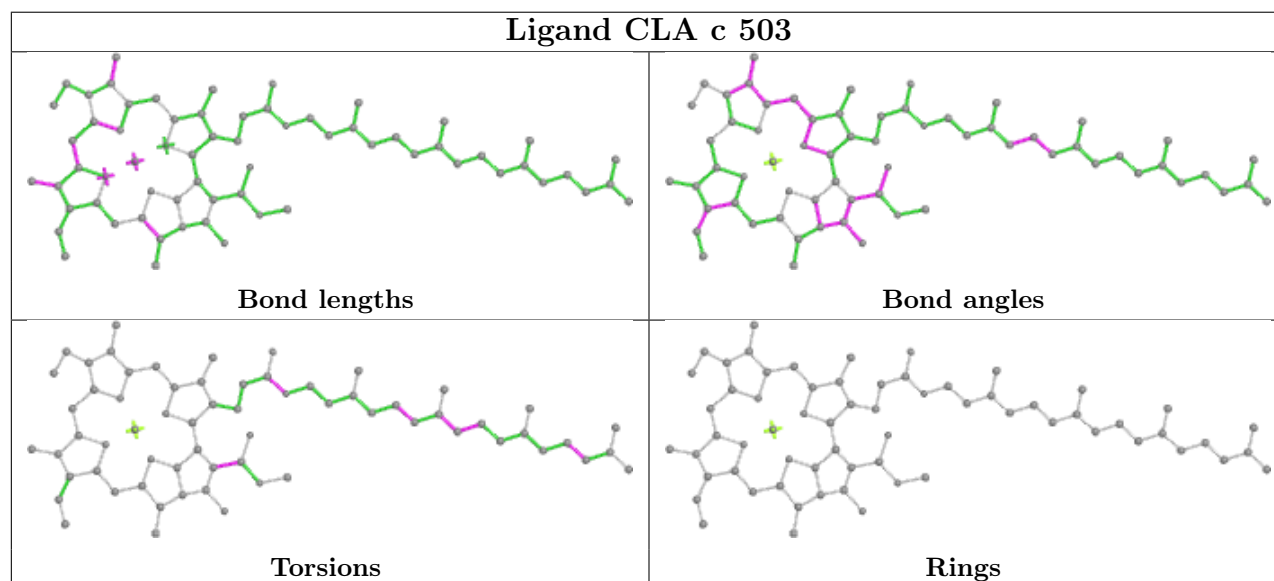
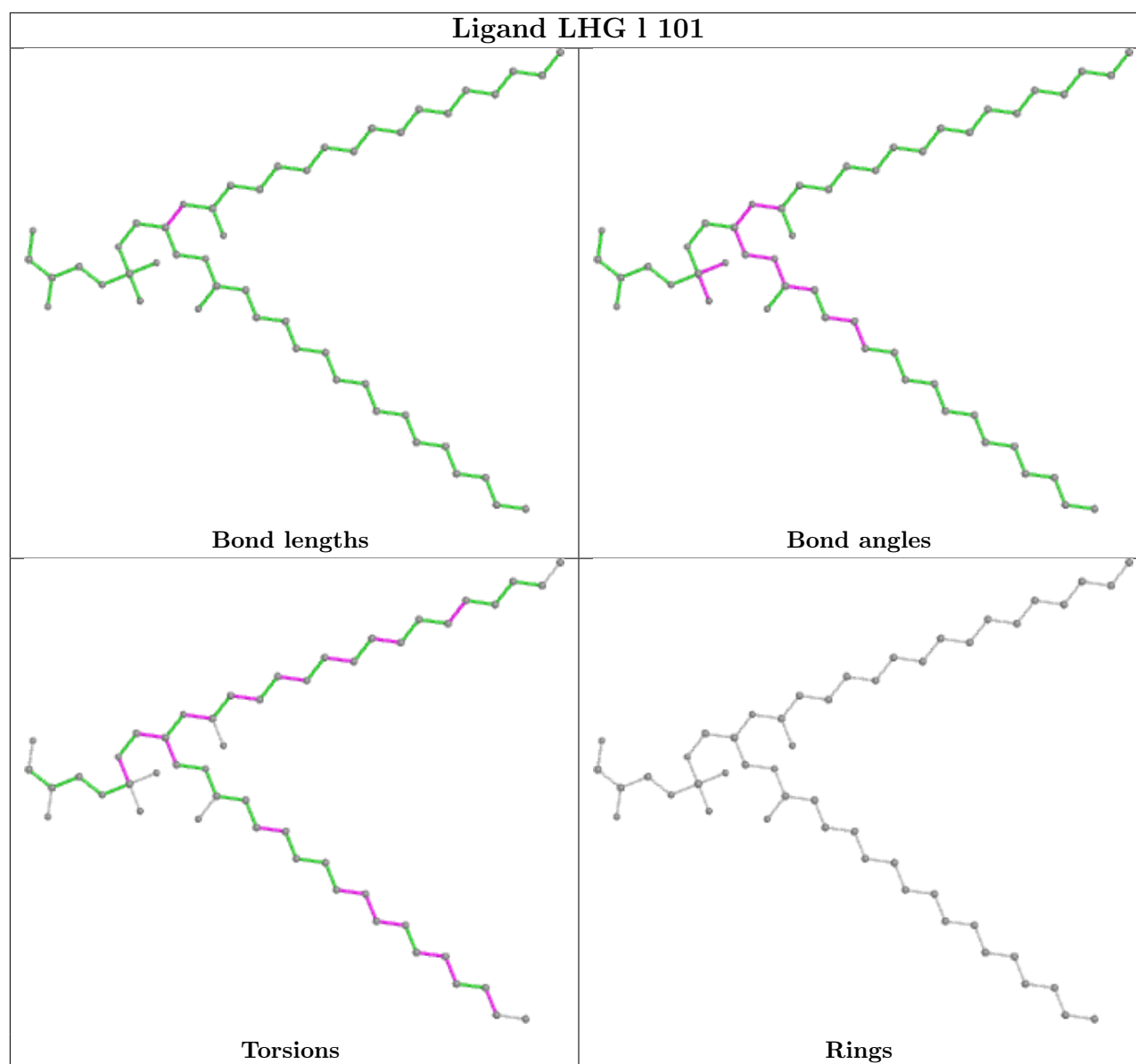


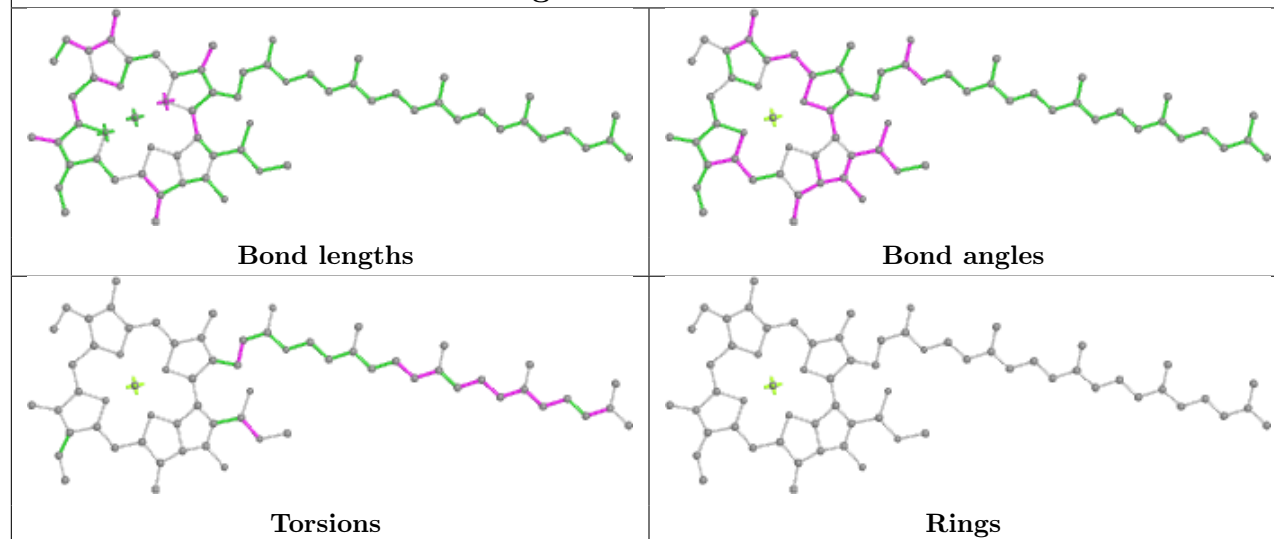
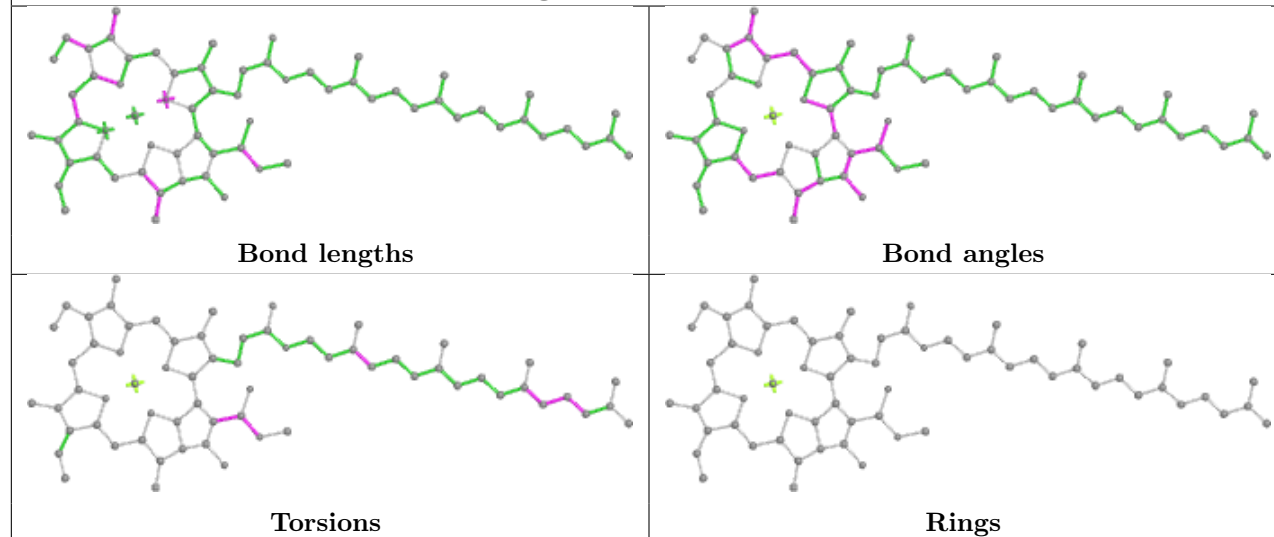
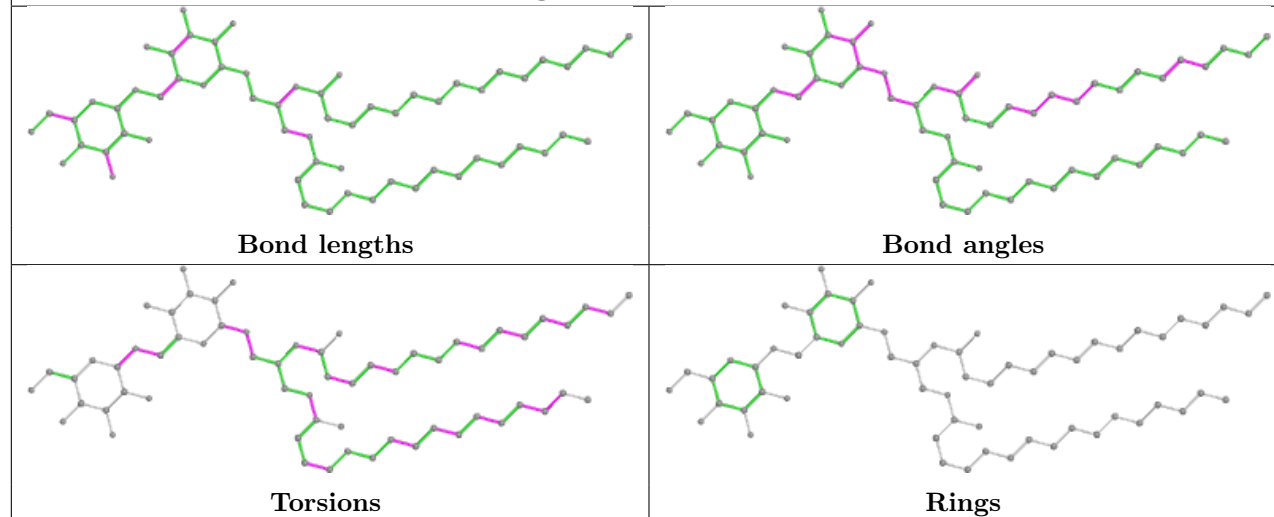
Ligand CLA B 610

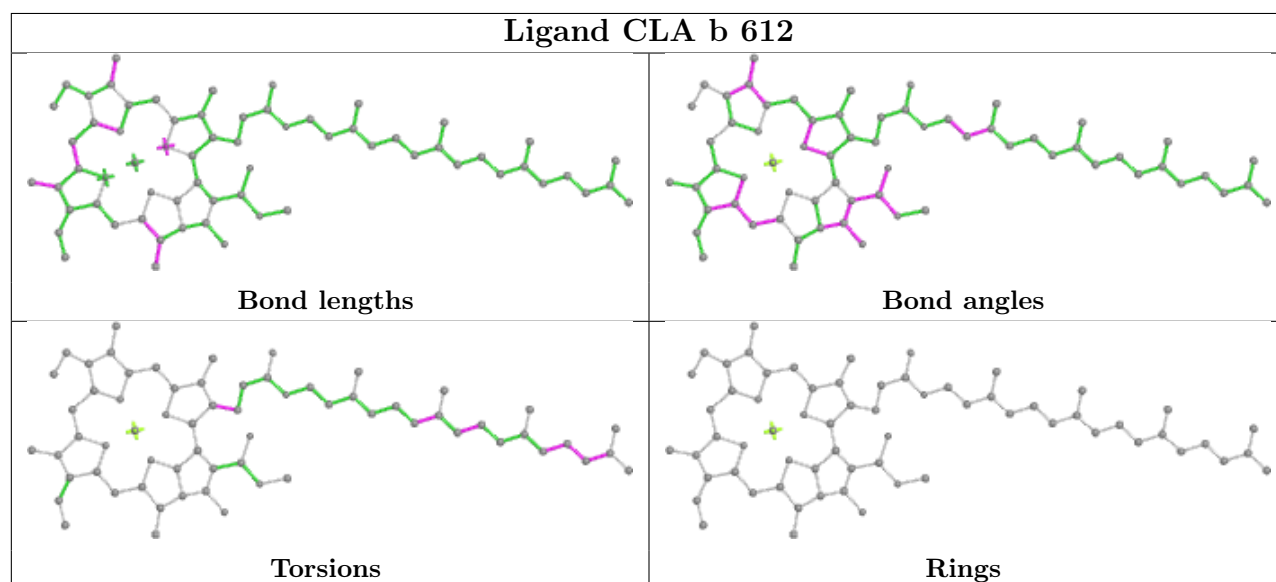
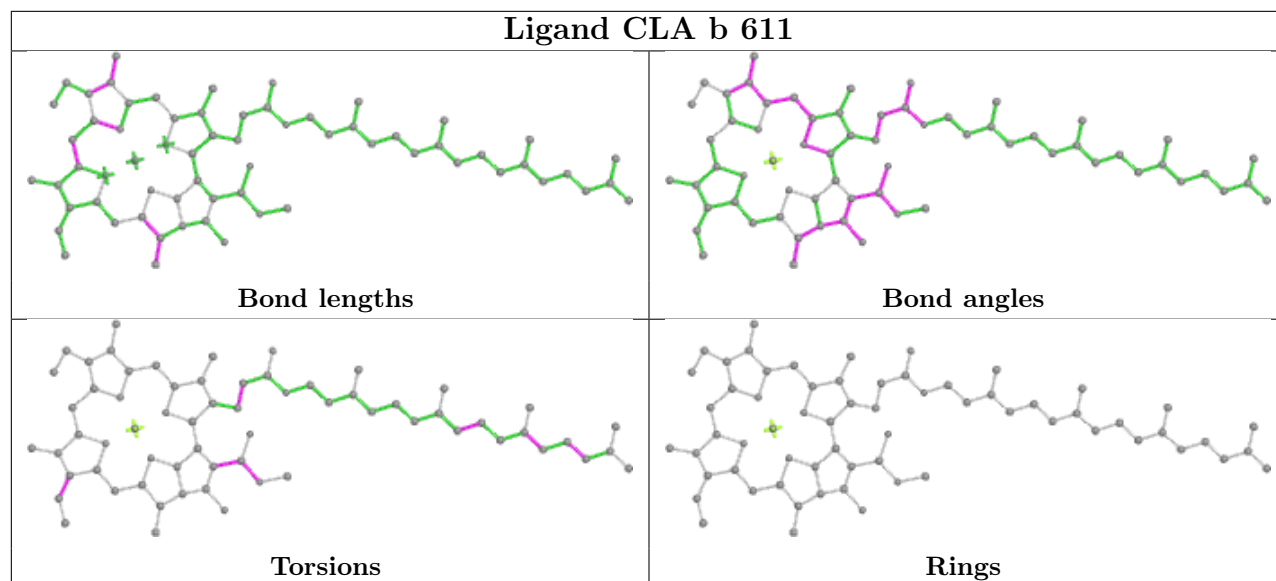
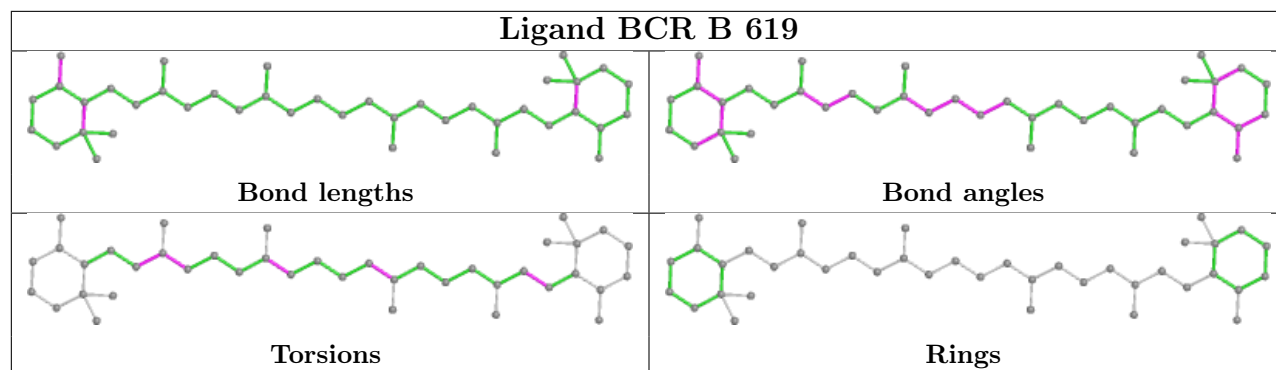


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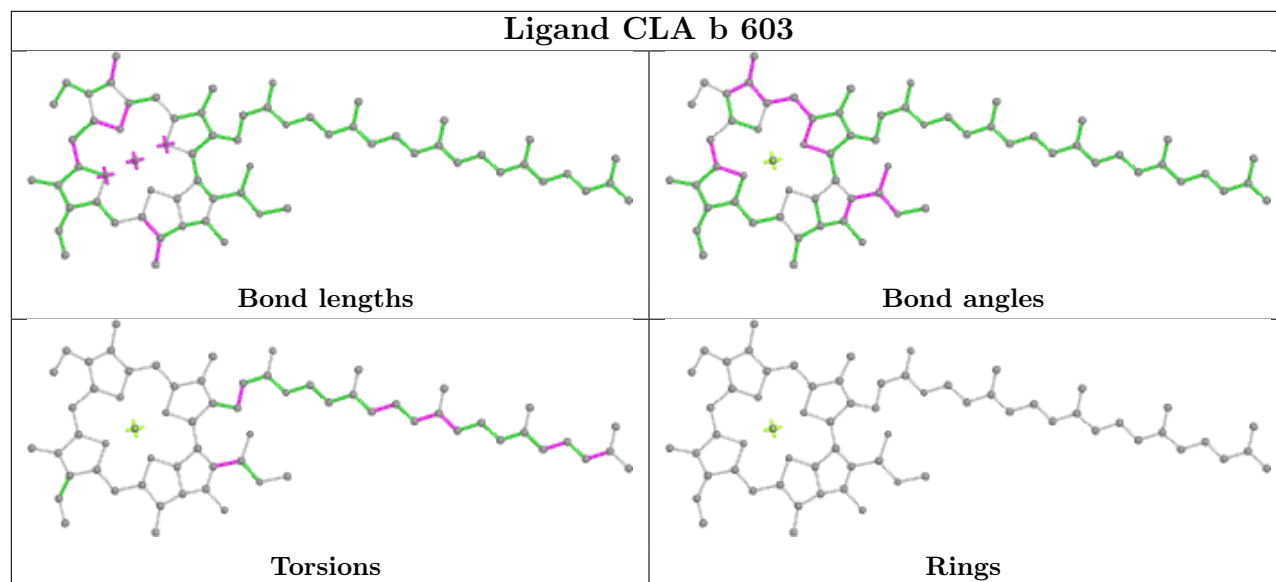




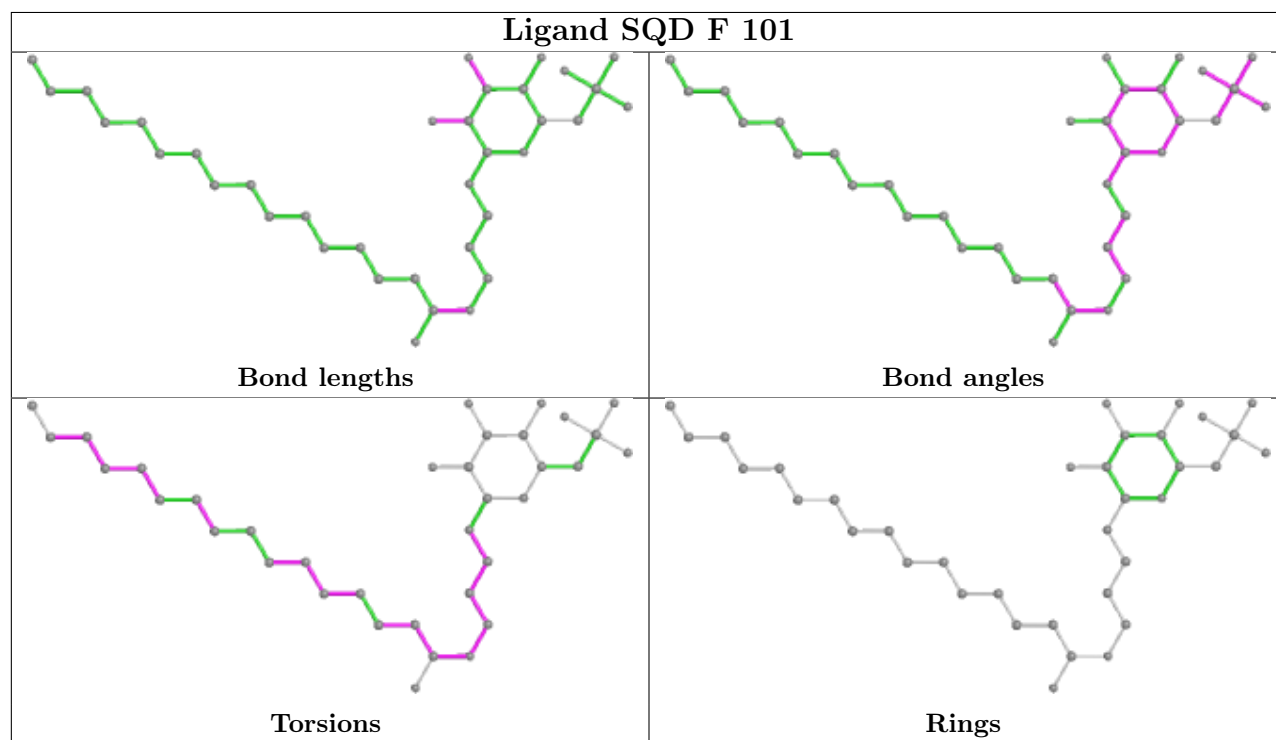
Ligand CLA B 603**Ligand CLA b 610****Ligand DGD c 517**

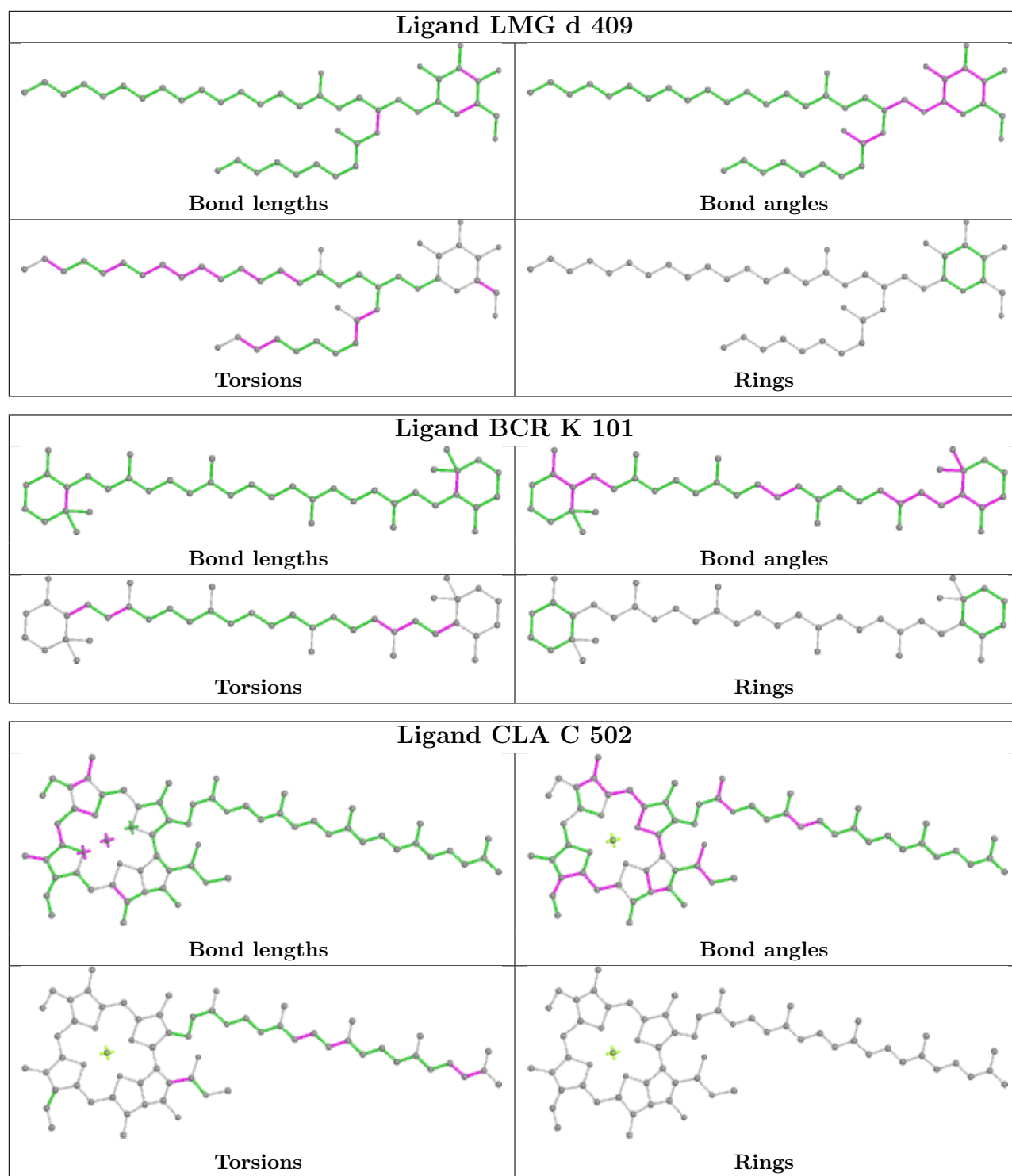


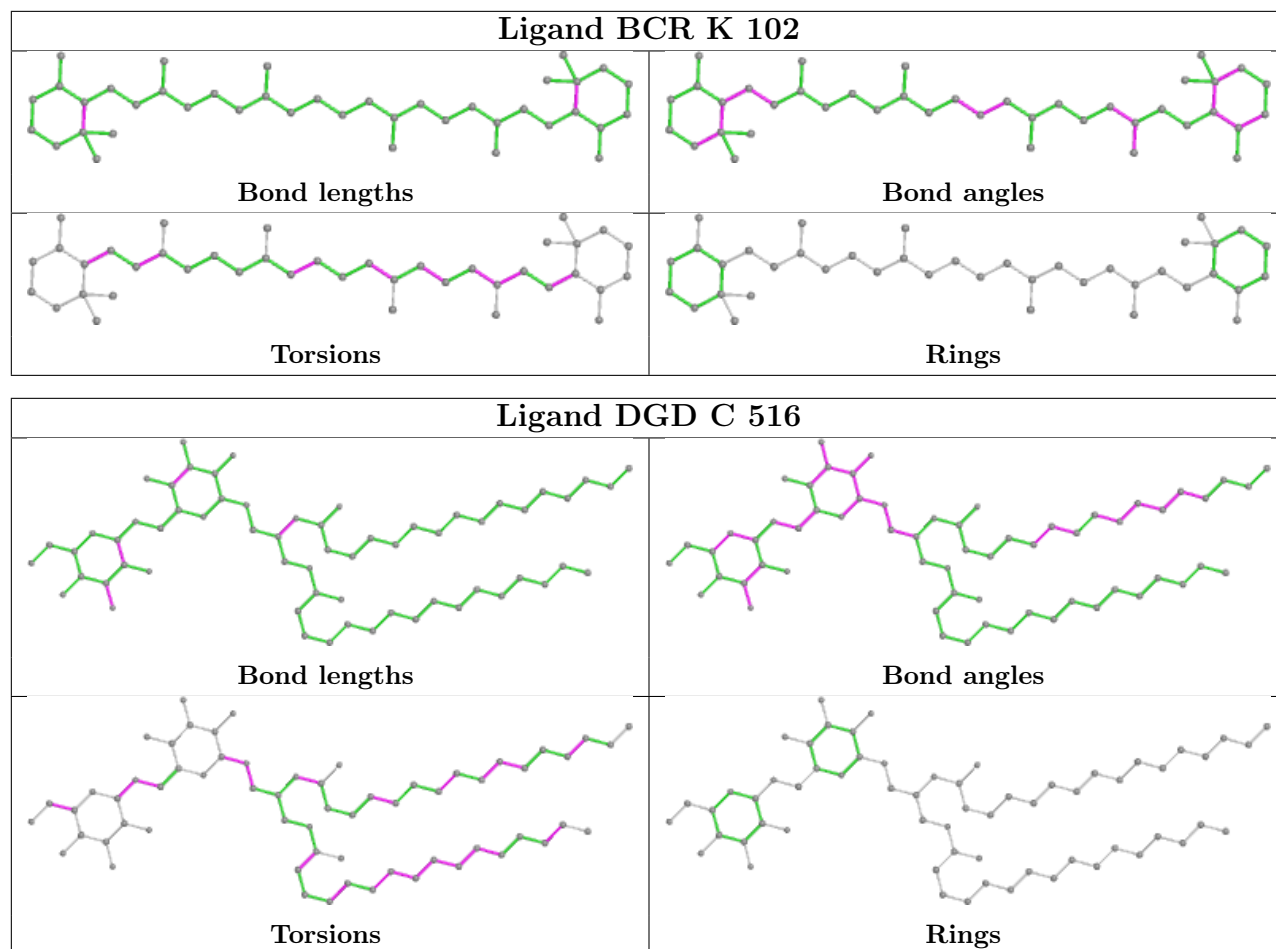
Ligand CLA b 603



Ligand SQD F 101







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	334/334 (100%)	-0.48	3 (0%) 84 85	19, 28, 48, 74	0
1	a	334/334 (100%)	-0.45	3 (0%) 84 85	21, 30, 59, 80	0
2	B	505/505 (100%)	-0.43	5 (0%) 82 83	21, 31, 61, 96	0
2	b	505/505 (100%)	-0.31	14 (2%) 53 56	19, 35, 74, 106	0
3	C	442/451 (98%)	-0.36	2 (0%) 91 91	24, 35, 53, 76	0
3	c	451/451 (100%)	-0.31	5 (1%) 80 81	24, 38, 61, 96	0
4	D	341/341 (100%)	-0.40	1 (0%) 94 94	21, 29, 48, 89	0
4	d	341/341 (100%)	-0.35	3 (0%) 84 85	23, 33, 58, 82	0
5	E	81/82 (98%)	0.14	4 (4%) 29 30	31, 50, 69, 85	0
5	e	82/82 (100%)	0.22	5 (6%) 21 21	38, 59, 80, 92	0
6	F	34/34 (100%)	-0.41	1 (2%) 51 54	34, 42, 61, 82	0
6	f	34/34 (100%)	-0.19	1 (2%) 51 54	41, 50, 73, 87	0
7	H	65/65 (100%)	-0.11	1 (1%) 73 75	33, 39, 57, 77	0
7	h	63/65 (96%)	0.17	3 (4%) 30 31	38, 47, 61, 70	0
8	I	35/36 (97%)	-0.35	2 (5%) 23 24	30, 37, 72, 79	0
8	i	35/36 (97%)	-0.16	2 (5%) 23 24	31, 38, 70, 80	0
9	J	36/36 (100%)	0.12	4 (11%) 5 5	35, 48, 76, 93	0
9	j	36/36 (100%)	0.23	4 (11%) 5 5	38, 51, 85, 92	0
10	K	37/37 (100%)	-0.21	0 100 100	40, 51, 68, 72	0
10	k	37/37 (100%)	0.12	1 (2%) 54 57	44, 55, 72, 84	0
11	L	37/37 (100%)	-0.41	0 100 100	23, 29, 67, 69	0
11	l	36/37 (97%)	-0.35	0 100 100	24, 29, 73, 81	0
12	M	32/33 (96%)	-0.31	1 (3%) 49 52	26, 32, 60, 73	0
12	m	31/33 (93%)	-0.28	0 100 100	26, 31, 50, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/244 (100%)	-0.12	12 (4%) 29 30	21, 40, 84, 142	0
13	o	244/244 (100%)	-0.14	14 (5%) 23 24	24, 39, 80, 131	0
14	T	29/30 (96%)	-0.62	2 (6%) 16 17	24, 31, 58, 71	0
14	t	29/30 (96%)	-0.44	3 (10%) 6 6	23, 31, 78, 92	0
15	U	97/97 (100%)	-0.23	3 (3%) 49 52	31, 42, 68, 95	0
15	u	97/97 (100%)	-0.47	1 (1%) 82 83	28, 38, 57, 90	0
16	V	137/137 (100%)	-0.57	0 100 100	27, 39, 56, 83	0
16	v	137/137 (100%)	-0.26	1 (0%) 87 88	33, 46, 66, 78	0
17	Y	27/30 (90%)	1.79	11 (40%) 0 0	53, 74, 115, 119	0
17	y	30/30 (100%)	0.78	5 (16%) 1 1	59, 73, 90, 105	0
18	X	38/38 (100%)	0.15	3 (7%) 12 13	38, 48, 74, 78	0
18	x	38/38 (100%)	0.50	5 (13%) 3 2	46, 56, 87, 99	0
19	Z	62/62 (100%)	0.60	15 (24%) 0 0	48, 66, 110, 124	0
19	z	62/62 (100%)	0.98	14 (22%) 0 0	53, 69, 107, 122	0
20	R	34/34 (100%)	1.82	13 (38%) 0 0	59, 70, 89, 97	0
20	r	31/34 (91%)	2.38	17 (54%) 0 0	71, 85, 98, 104	0
All	All	5300/5326 (99%)	-0.23	184 (3%) 44 46	19, 37, 74, 142	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	59	LYS	9.8
17	Y	20	ALA	8.4
19	z	33	TRP	7.4
13	o	3	GLN	7.3
13	o	58	ASN	7.3
1	A	13	LEU	7.2
13	O	3	GLN	7.1
13	O	60	ARG	6.5
19	z	35	ARG	5.8
18	x	2	THR	5.4
20	R	3	TRP	5.3
13	O	4	THR	5.3
20	r	14	LEU	5.2
17	Y	22	LEU	5.1
5	E	79	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
18	X	2	THR	5.0
6	F	12	SER	4.9
2	b	127	ARG	4.8
13	o	61	GLN	4.8
20	R	6	LEU	4.5
13	o	4	THR	4.5
13	O	62	GLU	4.5
9	j	5	GLY	4.5
13	o	62	GLU	4.5
17	Y	23	THR	4.4
19	z	60	PHE	4.2
13	o	59	LYS	4.1
17	Y	41	VAL	4.1
20	r	3	TRP	4.1
14	t	30	THR	4.1
20	r	6	LEU	4.0
20	r	13	LEU	4.0
19	z	34	ASP	4.0
9	J	5	GLY	4.0
3	c	23	ALA	3.9
13	O	56	PRO	3.8
13	o	56	PRO	3.8
13	o	57	LYS	3.8
7	H	66	GLY	3.8
20	r	24	LEU	3.8
20	R	26	TYR	3.7
20	r	5	VAL	3.7
15	U	8	GLU	3.7
2	B	505	ARG	3.7
2	b	128	THR	3.7
20	R	32	GLN	3.7
2	b	490	GLN	3.6
9	J	8	ILE	3.6
2	b	506	ARG	3.6
17	y	19	ILE	3.6
20	r	10	LEU	3.6
18	X	3	ILE	3.5
9	J	7	ARG	3.5
19	Z	35	ARG	3.5
20	r	28	VAL	3.5
19	Z	33	TRP	3.5
13	o	5	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
17	Y	24	MET	3.4
19	z	30	PRO	3.4
20	r	7	VAL	3.4
1	A	11	ALA	3.4
19	z	37	LYS	3.4
8	i	36	ASP	3.3
20	r	9	LEU	3.3
13	O	61	GLN	3.3
13	o	60	ARG	3.3
19	Z	38	GLN	3.3
17	Y	42	ARG	3.3
17	y	43	ARG	3.3
3	c	24	THR	3.2
17	Y	21	GLN	3.2
20	r	26	TYR	3.2
13	O	5	LEU	3.2
17	Y	43	ARG	3.1
20	R	31	VAL	3.1
1	A	12	ASN	3.1
5	e	79	PHE	3.1
3	C	143	TYR	3.1
9	J	6	GLY	3.1
2	b	495	PHE	3.1
19	Z	62	VAL	3.1
20	r	29	LYS	3.0
1	a	11	ALA	3.0
9	j	7	ARG	3.0
2	B	506	ARG	3.0
2	b	505	ARG	3.0
20	R	28	VAL	3.0
20	R	21	ARG	3.0
3	c	143	TYR	3.0
5	e	4	THR	3.0
19	Z	7	LEU	3.0
2	B	502	VAL	2.9
13	o	55	GLU	2.9
9	j	6	GLY	2.9
18	x	3	ILE	2.9
19	Z	41	PHE	2.9
5	e	84	LYS	2.9
7	h	6	TRP	2.9
6	f	13	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	b	503	THR	2.9
20	r	18	TRP	2.9
3	c	146	PHE	2.8
17	Y	40	ALA	2.8
18	x	23	LEU	2.8
19	z	3	ILE	2.8
19	Z	1	MET	2.8
19	z	62	VAL	2.8
4	d	227[A]	GLU	2.8
15	U	9	LEU	2.7
17	Y	37	PHE	2.7
3	C	106	VAL	2.7
20	r	2	ASP	2.7
19	z	4	LEU	2.7
19	z	7	LEU	2.7
2	b	489	GLU	2.7
8	I	36	ASP	2.7
5	e	3	GLY	2.6
9	j	8	ILE	2.6
2	B	494	GLY	2.6
13	o	246	ALA	2.6
13	O	57	LYS	2.6
20	r	25	PRO	2.6
17	y	20	ALA	2.6
20	R	5	VAL	2.5
1	a	16	ARG	2.5
5	E	84	LYS	2.5
15	u	53	ALA	2.5
19	Z	34	ASP	2.5
20	R	2	ASP	2.5
2	b	494	GLY	2.5
5	E	83	LEU	2.5
14	t	28	ARG	2.5
19	Z	4	LEU	2.5
20	r	27	ALA	2.5
13	O	34	SER	2.5
5	e	61	ARG	2.5
14	t	29	ILE	2.5
19	z	41	PHE	2.5
2	b	496	TYR	2.4
20	r	23	ILE	2.4
7	h	10	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
10	k	17	ILE	2.4
19	Z	3	ILE	2.4
14	T	30	THR	2.4
17	y	18	VAL	2.4
18	X	39	ARG	2.4
20	R	25	PRO	2.4
14	T	29	ILE	2.4
20	R	27	ALA	2.4
8	I	34	ARG	2.4
15	U	67	LEU	2.3
19	Z	37	LYS	2.3
8	i	34	ARG	2.3
13	O	36	GLN	2.3
2	B	487	SER	2.3
2	b	85	GLY	2.3
17	Y	44	GLY	2.3
20	R	20	VAL	2.3
4	D	12	ARG	2.3
19	Z	32	ASP	2.2
18	x	38	GLN	2.2
19	Z	42	LEU	2.2
19	z	59	PHE	2.2
7	h	21	VAL	2.2
18	x	37	VAL	2.1
13	o	207	ARG	2.1
3	c	29	GLU	2.1
20	R	18	TRP	2.1
13	O	63	ALA	2.1
17	y	40	ALA	2.1
12	M	33	GLN	2.1
13	o	64	GLU	2.1
16	v	15	GLU	2.1
2	b	86	ILE	2.1
2	b	295	GLY	2.1
1	a	249	VAL	2.1
4	d	55	VAL	2.1
19	Z	39	LEU	2.1
5	E	81	GLU	2.1
19	Z	31	GLN	2.0
19	z	52	LEU	2.0
19	z	36	SER	2.0
2	b	485	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
4	d	12	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.95	0.13	35,48,60,64	0
14	FME	t	1	10/11	0.95	0.09	29,37,64,69	0
12	FME	M	1	10/11	0.96	0.13	34,48,63,68	0
14	FME	T	1	10/11	0.96	0.10	27,44,65,71	0
12	FME	m	1	10/11	0.97	0.12	31,46,65,72	0
8	FME	I	1	10/11	0.97	0.13	35,54,65,68	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	UNL	a	415	28/-	0.70	0.27	39,66,77,79	0
34	UNL	E	102	28/-	0.72	0.29	52,79,91,94	0
34	UNL	H	103	53/-	0.73	0.22	43,73,86,90	0
34	UNL	c	520	55/-	0.77	0.17	39,61,79,86	0
27	LMG	b	623	23/55	0.78	0.24	43,70,95,98	0
34	UNL	c	522	28/-	0.78	0.19	46,66,88,93	0
29	LHG	A	413	49/49	0.79	0.24	51,85,125,130	0
26	PL9	A	410	55/55	0.81	0.24	39,62,83,94	135
34	UNL	B	627	28/-	0.81	0.39	42,64,86,91	0
34	UNL	C	521	47/-	0.81	0.13	37,56,73,74	0
28	SQD	a	413	36/54	0.81	0.15	31,67,87,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	UNL	b	624	40/-	0.82	0.18	46,63,83,85	0
34	UNL	b	626	55/-	0.82	0.17	44,61,77,81	0
23	CLA	h	101	65/65	0.82	0.16	45,69,93,104	0
27	LMG	D	409	33/55	0.82	0.17	32,54,107,111	0
34	UNL	t	103	26/-	0.82	0.17	42,64,76,81	0
30	DGD	A	415	66/66	0.83	0.19	45,68,93,108	0
25	BCR	x	101	40/40	0.83	0.15	35,57,76,82	0
34	UNL	B	628	47/-	0.83	0.24	47,65,78,89	0
27	LMG	c	521	48/55	0.83	0.24	44,77,121,128	0
34	UNL	B	626	46/-	0.85	0.14	44,64,84,93	0
28	SQD	f	101	41/54	0.85	0.22	54,87,117,125	0
26	PL9	a	410	55/55	0.85	0.22	36,67,91,98	0
29	LHG	e	101	42/49	0.85	0.27	57,87,116,139	0
28	SQD	b	601	49/54	0.85	0.14	38,60,102,112	0
34	UNL	d	411	55/-	0.85	0.19	42,58,72,73	0
34	UNL	m	102	28/-	0.85	0.14	42,59,73,78	0
30	DGD	a	414	44/66	0.85	0.16	36,58,84,92	0
34	UNL	X	101	55/-	0.86	0.20	34,49,75,79	0
23	CLA	c	512	65/65	0.86	0.14	40,58,97,107	0
25	BCR	k	101	40/40	0.86	0.12	39,65,81,83	0
34	UNL	l	102	53/-	0.86	0.16	33,50,87,91	0
27	LMG	b	622	55/55	0.86	0.27	35,73,101,104	0
34	UNL	b	627	26/-	0.86	0.21	42,58,69,74	0
34	UNL	b	621	55/-	0.87	0.21	39,57,86,91	0
34	UNL	j	101	28/-	0.87	0.13	42,56,67,67	0
34	UNL	B	620	43/-	0.87	0.11	34,51,68,74	0
34	UNL	I	101	41/-	0.87	0.13	37,53,75,79	0
34	UNL	d	410	43/-	0.87	0.16	39,58,70,78	0
27	LMG	A	411	48/55	0.88	0.17	37,62,78,103	0
23	CLA	c	513	65/65	0.88	0.20	47,72,109,114	0
27	LMG	c	519	37/55	0.88	0.17	44,70,88,97	0
23	CLA	C	513	65/65	0.89	0.16	45,68,95,101	0
27	LMG	c	523	49/55	0.89	0.13	32,56,87,111	0
28	SQD	B	624	54/54	0.89	0.13	39,58,90,100	0
27	LMG	C	518	48/55	0.89	0.14	43,72,96,103	0
23	CLA	C	512	65/65	0.89	0.15	33,56,102,109	0
34	UNL	t	102	34/-	0.89	0.14	35,50,58,65	0
34	UNL	b	602	47/-	0.89	0.15	35,50,64,73	0
34	UNL	M	102	37/-	0.90	0.12	26,45,54,69	0
23	CLA	a	408	65/65	0.90	0.14	16,36,95,107	0
28	SQD	A	414	39/54	0.90	0.19	36,69,93,99	0
23	CLA	b	617	60/65	0.90	0.14	28,44,105,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	BCR	H	101	40/40	0.90	0.10	31,47,57,62	0
25	BCR	K	101	40/40	0.90	0.12	36,53,73,79	0
34	UNL	b	625	44/-	0.90	0.16	34,58,80,84	0
23	CLA	B	616	60/65	0.90	0.16	23,41,93,102	0
34	UNL	J	101	28/-	0.90	0.15	52,64,78,86	0
27	LMG	m	101	51/55	0.91	0.11	30,51,81,97	0
27	LMG	M	101	51/55	0.91	0.11	25,47,72,84	0
25	BCR	D	404	40/40	0.91	0.12	25,46,103,108	0
34	UNL	B	625	28/-	0.91	0.09	31,46,69,70	0
23	CLA	B	601	65/65	0.91	0.13	32,61,99,105	0
25	BCR	c	514	40/40	0.92	0.17	40,59,77,79	0
23	CLA	b	616	65/65	0.92	0.13	26,39,62,68	0
27	LMG	B	621	28/55	0.92	0.14	31,47,60,70	0
23	CLA	D	403	65/65	0.92	0.14	23,40,121,137	0
28	SQD	a	412	54/54	0.92	0.14	34,69,91,95	0
25	BCR	Z	101	40/40	0.92	0.12	34,57,72,75	0
30	DGD	h	102	62/66	0.92	0.12	33,52,65,70	0
30	DGD	H	102	62/66	0.93	0.10	30,49,61,74	0
23	CLA	d	403	65/65	0.93	0.12	29,49,97,109	0
23	CLA	C	505	65/65	0.93	0.17	25,43,73,83	0
25	BCR	C	514	40/40	0.93	0.10	27,39,54,59	0
23	CLA	c	502	65/65	0.93	0.12	27,43,65,69	0
23	CLA	c	503	65/65	0.93	0.14	32,45,56,62	0
23	CLA	c	508	64/65	0.93	0.13	30,45,93,113	0
27	LMG	D	406	51/55	0.93	0.15	26,56,89,97	0
23	CLA	c	510	65/65	0.93	0.13	33,50,69,76	0
25	BCR	b	619	40/40	0.93	0.09	27,39,55,58	0
23	CLA	B	615	65/65	0.93	0.12	24,36,70,87	0
25	BCR	d	404	40/40	0.93	0.10	36,54,90,102	0
23	CLA	B	606	65/65	0.93	0.10	21,35,73,83	0
30	DGD	C	515	62/66	0.93	0.13	21,40,86,103	0
34	UNL	M	103	26/-	0.93	0.16	24,49,57,63	0
30	DGD	C	516	62/66	0.93	0.11	30,54,108,129	0
25	BCR	B	617	40/40	0.94	0.10	26,40,54,56	0
25	BCR	B	618	40/40	0.94	0.09	23,39,54,56	0
23	CLA	C	510	65/65	0.94	0.12	29,46,75,87	0
23	CLA	C	503	65/65	0.94	0.11	29,42,52,55	0
34	UNL	C	519	28/-	0.94	0.09	34,46,55,56	0
34	UNL	C	520	28/-	0.94	0.09	42,51,64,65	0
23	CLA	C	502	65/65	0.94	0.11	24,44,56,64	0
23	CLA	C	506	65/65	0.94	0.11	27,42,95,110	0
25	BCR	K	102	40/40	0.94	0.15	34,58,73,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
27	LMG	d	409	44/55	0.94	0.11	31,58,89,105	0
25	BCR	T	101	40/40	0.94	0.09	27,40,60,62	0
23	CLA	c	504	60/65	0.94	0.12	30,44,86,93	0
25	BCR	b	618	40/40	0.94	0.10	22,43,54,58	0
28	SQD	F	101	36/54	0.94	0.14	41,71,87,95	0
23	CLA	c	505	65/65	0.94	0.14	23,43,68,72	0
23	CLA	c	506	65/65	0.94	0.13	28,51,111,120	0
23	CLA	c	507	65/65	0.94	0.14	21,43,62,66	0
23	CLA	a	406	65/65	0.94	0.11	24,40,100,112	0
25	BCR	k	102	40/40	0.94	0.15	37,57,66,73	0
29	LHG	d	408	39/49	0.94	0.11	26,47,73,78	0
23	CLA	c	509	65/65	0.94	0.17	30,48,67,68	0
23	CLA	C	507	65/65	0.94	0.12	23,40,57,62	0
26	PL9	D	405	55/55	0.94	0.12	17,32,48,52	0
23	CLA	c	511	65/65	0.94	0.14	34,57,74,76	0
23	CLA	b	605	65/65	0.94	0.15	21,34,88,99	0
23	CLA	b	607	65/65	0.94	0.10	24,40,74,83	0
30	DGD	c	517	62/66	0.94	0.09	31,52,86,96	0
30	DGD	c	518	62/66	0.94	0.10	29,52,82,94	0
23	CLA	b	610	65/65	0.94	0.11	30,46,71,89	0
23	CLA	b	615	65/65	0.94	0.14	20,37,81,97	0
25	BCR	c	515	40/40	0.95	0.11	31,48,64,72	0
28	SQD	A	412	52/54	0.95	0.14	32,61,93,101	0
23	CLA	b	614	65/65	0.95	0.12	18,32,77,84	0
23	CLA	A	405	65/65	0.95	0.11	18,34,99,118	0
23	CLA	C	511	65/65	0.95	0.10	35,51,67,69	0
25	BCR	t	101	40/40	0.95	0.07	25,36,53,61	0
24	PHO	a	407	64/64	0.95	0.11	22,31,40,48	0
25	BCR	A	409	40/40	0.95	0.09	24,34,43,47	0
23	CLA	B	604	65/65	0.95	0.11	18,31,79,87	0
23	CLA	A	408	54/65	0.95	0.12	16,30,74,77	0
29	LHG	D	408	47/49	0.95	0.10	26,46,84,100	0
29	LHG	d	406	49/49	0.95	0.12	36,52,82,94	0
26	PL9	d	405	55/55	0.95	0.10	21,35,44,47	0
25	BCR	B	619	40/40	0.95	0.09	27,42,65,78	0
29	LHG	l	101	49/49	0.95	0.11	29,48,59,64	0
23	CLA	D	402	65/65	0.95	0.11	15,32,58,67	0
23	CLA	B	609	65/65	0.95	0.10	24,35,57,66	0
23	CLA	B	610	65/65	0.95	0.14	16,31,44,48	0
30	DGD	C	517	62/66	0.95	0.09	23,45,82,93	0
23	CLA	B	612	65/65	0.95	0.14	21,32,46,51	0
23	CLA	b	603	65/65	0.95	0.15	26,42,73,83	0

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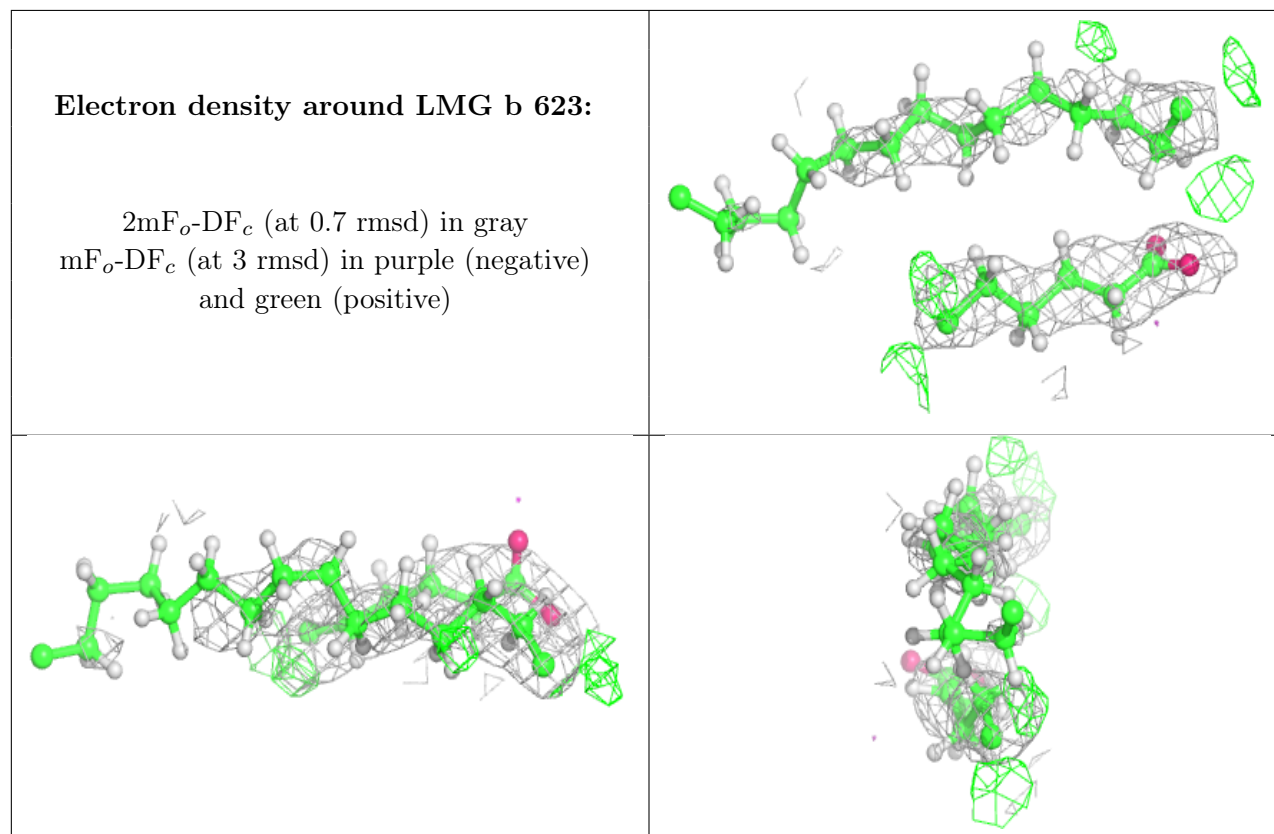
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	DGD	c	516	62/66	0.95	0.10	21,43,78,84	0
23	CLA	B	614	65/65	0.95	0.14	21,38,83,95	0
23	CLA	C	508	65/65	0.95	0.12	23,41,119,127	0
23	CLA	C	509	65/65	0.95	0.14	26,45,65,79	0
23	CLA	b	611	65/65	0.95	0.13	24,38,51,57	0
25	BCR	b	620	40/40	0.95	0.10	28,47,61,67	0
23	CLA	b	613	65/65	0.95	0.15	20,34,49,55	0
29	LHG	B	623	49/49	0.96	0.11	25,44,76,87	0
23	CLA	b	604	65/65	0.96	0.12	18,37,70,77	0
23	CLA	B	605	65/65	0.96	0.14	18,30,44,46	0
29	LHG	d	407	49/49	0.96	0.11	24,44,61,72	0
23	CLA	b	606	65/65	0.96	0.11	21,35,52,57	0
23	CLA	C	504	59/65	0.96	0.13	24,44,83,93	0
23	CLA	b	608	65/65	0.96	0.11	18,35,66,74	0
23	CLA	b	609	65/65	0.96	0.12	24,41,70,74	0
23	CLA	B	613	65/65	0.96	0.11	13,30,63,74	0
25	BCR	a	409	40/40	0.96	0.08	22,33,42,46	0
23	CLA	D	401	65/65	0.96	0.11	18,29,53,61	0
23	CLA	b	612	65/65	0.96	0.10	20,33,51,57	0
23	CLA	B	602	65/65	0.96	0.11	22,36,61,63	0
23	CLA	d	402	65/65	0.96	0.10	19,33,64,73	0
23	CLA	B	607	65/65	0.96	0.10	14,33,65,72	0
23	CLA	a	405	65/65	0.96	0.09	17,29,50,61	0
24	PHO	A	406	64/64	0.96	0.10	15,28,37,41	0
24	PHO	A	407	64/64	0.96	0.08	22,32,44,50	0
23	CLA	B	603	65/65	0.96	0.12	16,32,70,72	0
24	PHO	d	401	64/64	0.96	0.10	27,38,50,59	0
23	CLA	C	501	65/65	0.96	0.11	18,34,52,58	0
23	CLA	c	501	65/65	0.96	0.12	25,39,52,59	0
23	CLA	a	411	65/65	0.96	0.10	17,31,44,50	0
23	CLA	A	404	65/65	0.96	0.10	17,27,47,57	0
35	HEM	E	101	43/43	0.96	0.12	35,50,67,72	0
35	HEM	e	102	43/43	0.96	0.11	43,57,78,80	0
29	LHG	B	622	49/49	0.97	0.11	26,42,57,74	0
23	CLA	B	608	65/65	0.97	0.10	19,35,56,61	0
29	LHG	D	407	49/49	0.97	0.10	21,41,54,68	0
23	CLA	B	611	65/65	0.97	0.11	17,30,46,53	0
36	HEC	v	201	43/43	0.97	0.12	27,35,51,54	0
31	OEX	A	416[A]	10/10	0.98	0.10	21,30,34,35	10
36	HEC	V	201	43/43	0.98	0.12	24,31,41,41	0
33	BCT	a	404	4/4	0.98	0.13	23,23,41,49	0
22	CL	A	403	1/1	0.99	0.03	24,24,24,24	0

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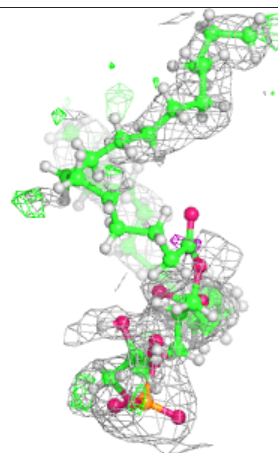
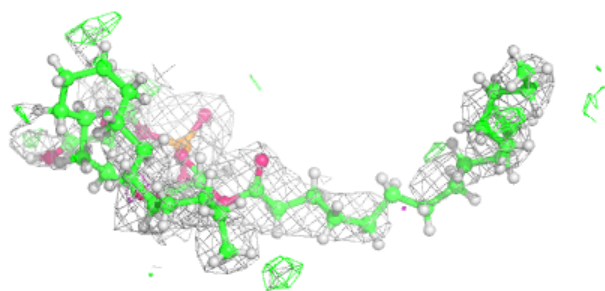
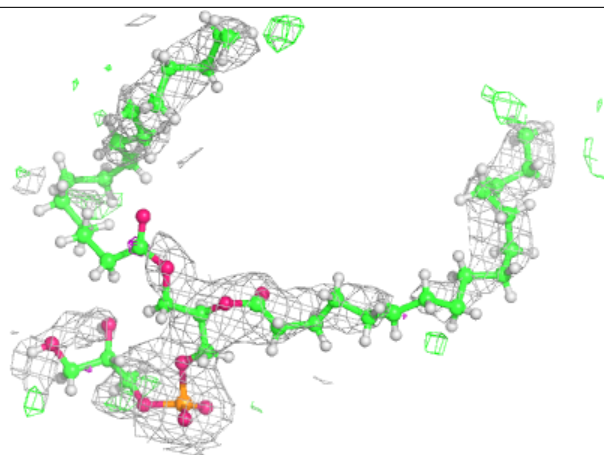
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CL	a	402	1/1	0.99	0.04	28,28,28,28	0
22	CL	a	403	1/1	0.99	0.04	27,27,27,27	0
21	FE2	a	401	1/1	0.99	0.07	35,35,35,35	0
22	CL	A	402	1/1	0.99	0.10	29,29,29,29	0
31	OEX	a	416[A]	10/10	0.99	0.11	25,31,34,35	10
32	OEY	A	417[B]	11/11	0.99	0.10	22,26,29,30	11
32	OEY	a	417[B]	11/11	0.99	0.11	22,28,30,30	11
33	BCT	A	418	4/4	0.99	0.17	26,33,39,47	0
21	FE2	A	401	1/1	1.00	0.09	30,30,30,30	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.

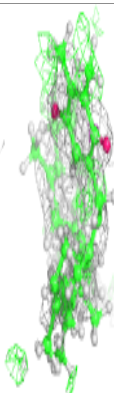
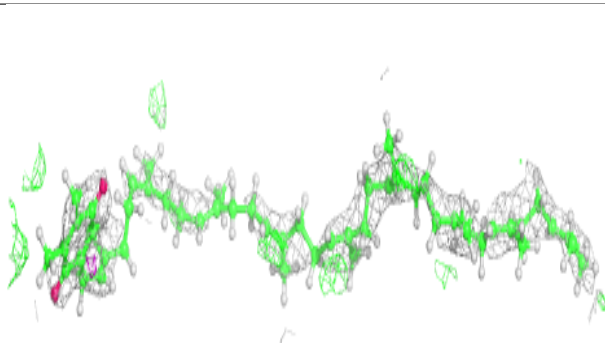
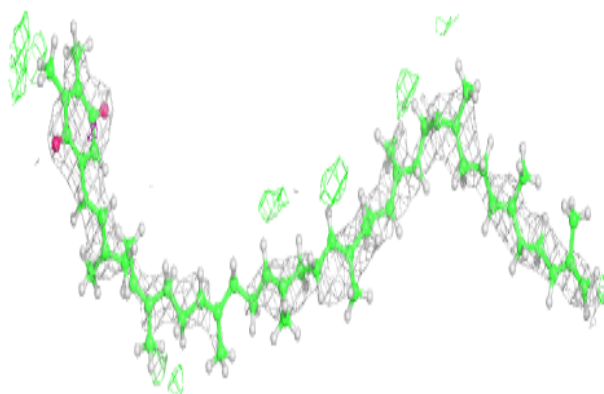


Electron density around LHG A 413:

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

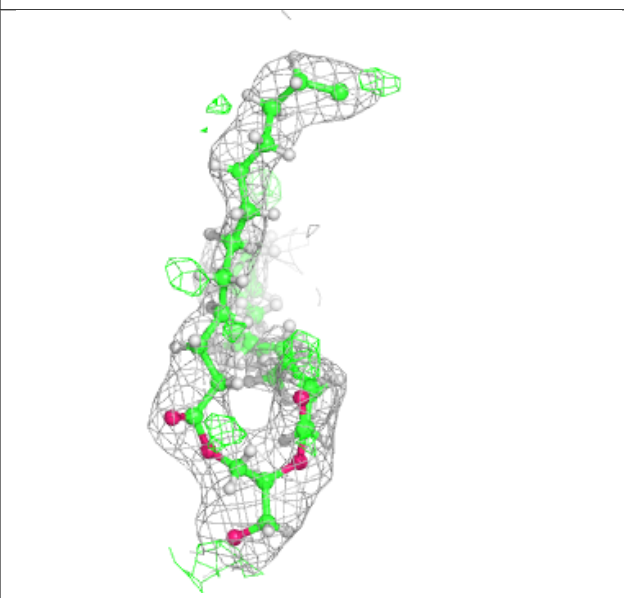
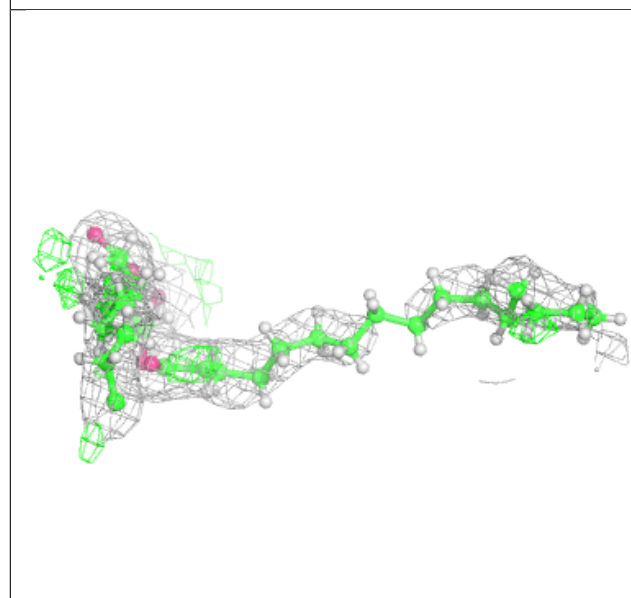
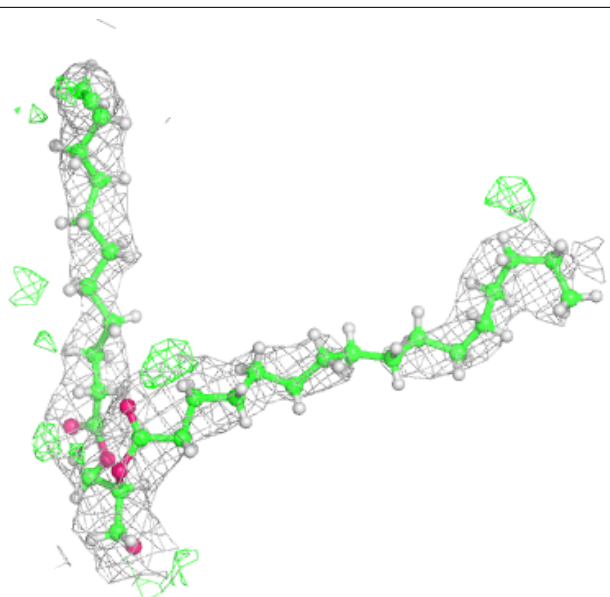
**Electron density around PL9 A 410:**

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



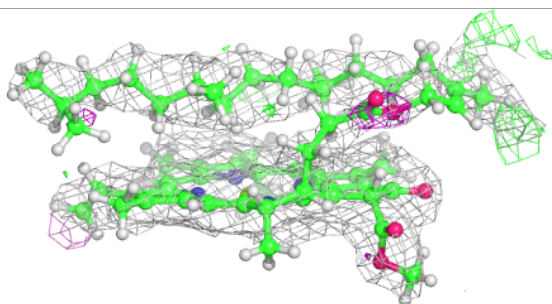
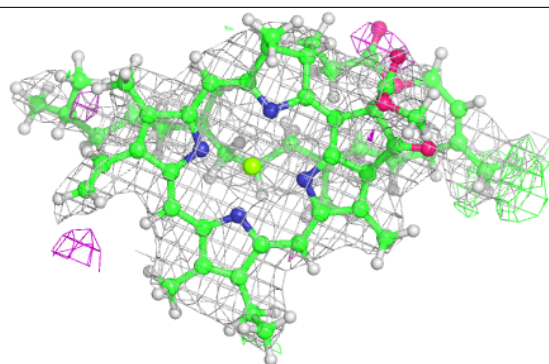
Electron density around SQD a 413:

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

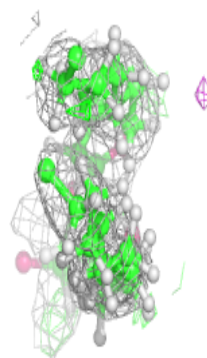
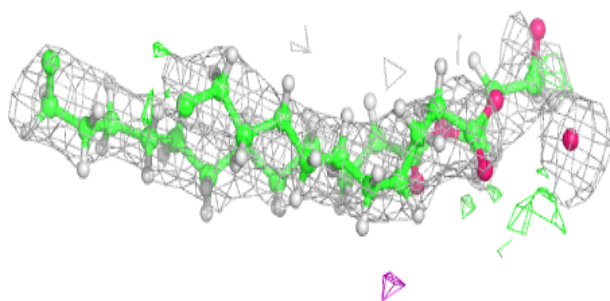
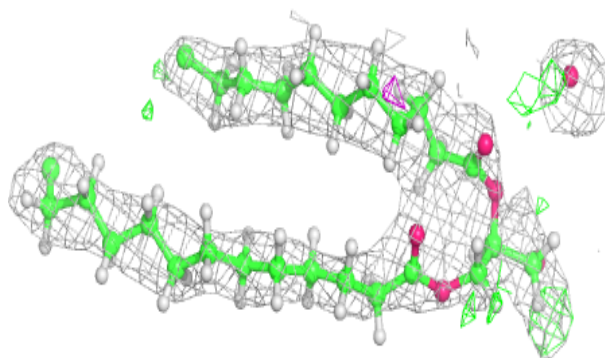


Electron density around CLA h 101:

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

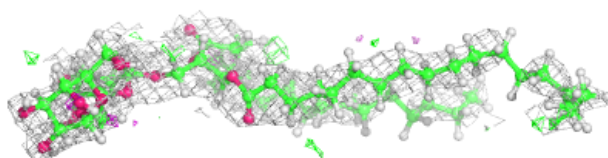
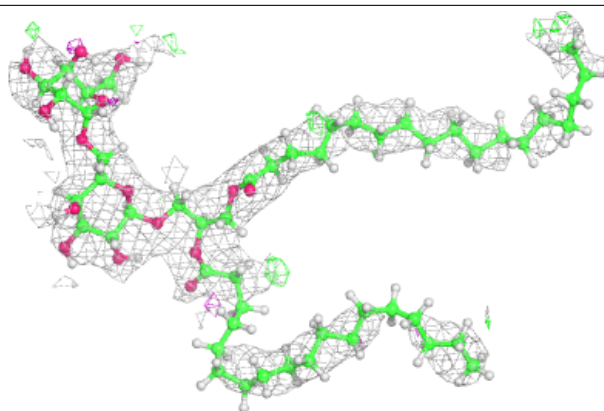
**Electron density around LMG D 409:**

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

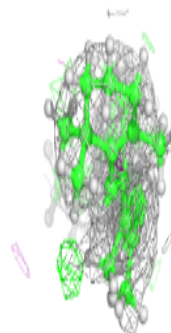
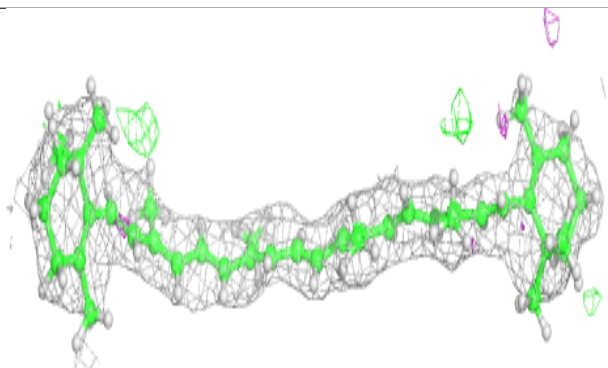
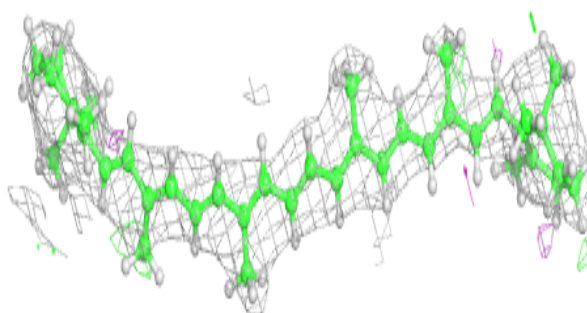


Electron density around DGD A 415:

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

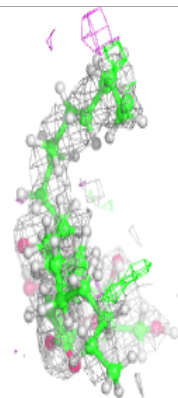
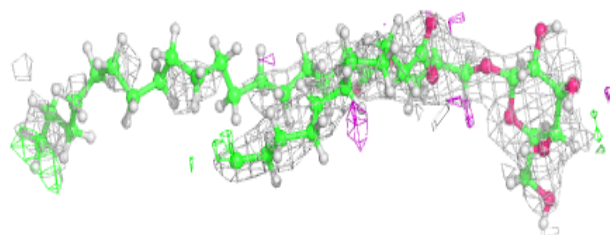
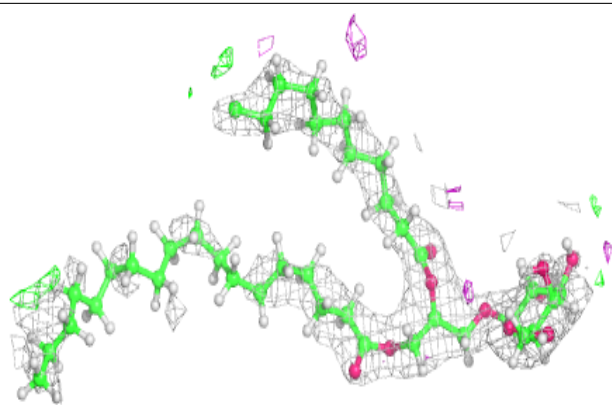
**Electron density around BCR x 101:**

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

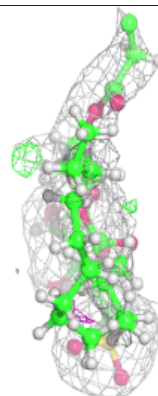
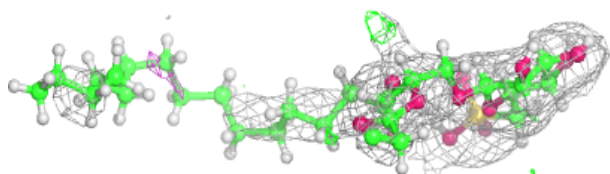
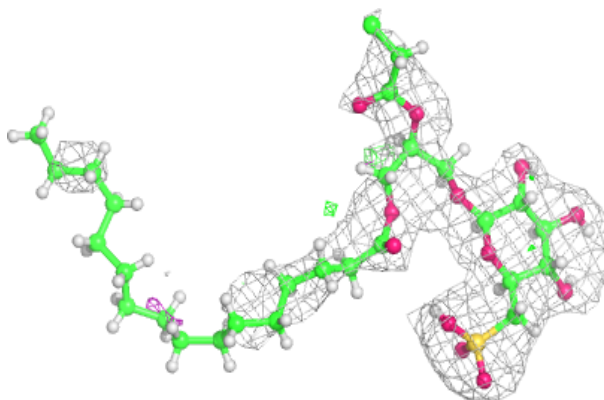


Electron density around LMG c 521:

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

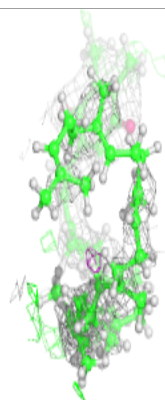
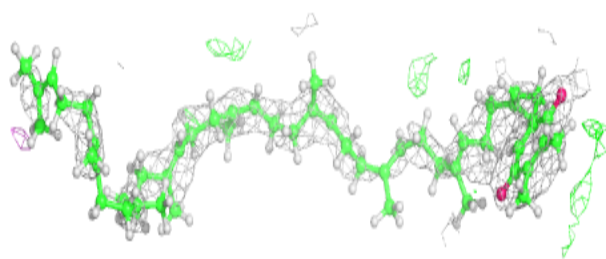
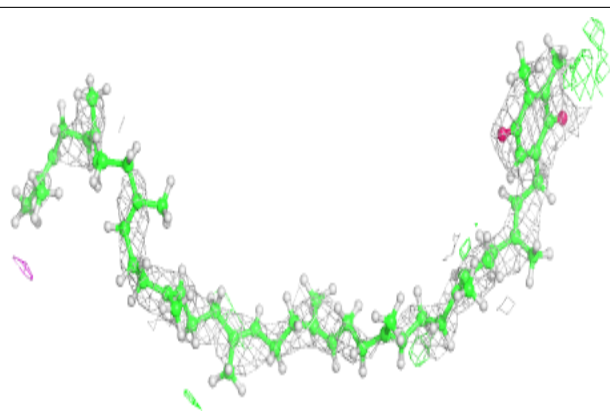
**Electron density around SQD f 101:**

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

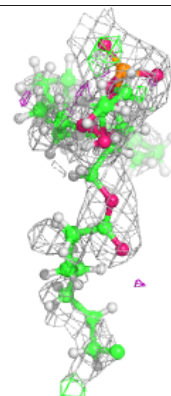
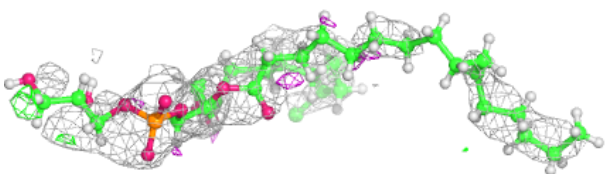
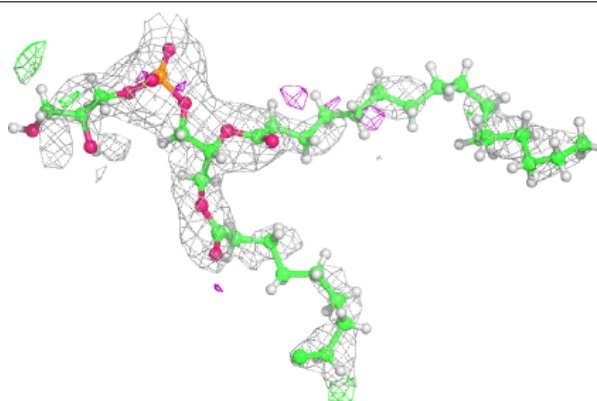


Electron density around PL9 a 410:

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

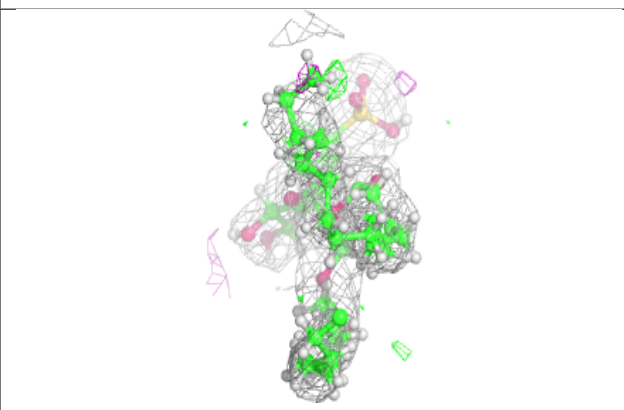
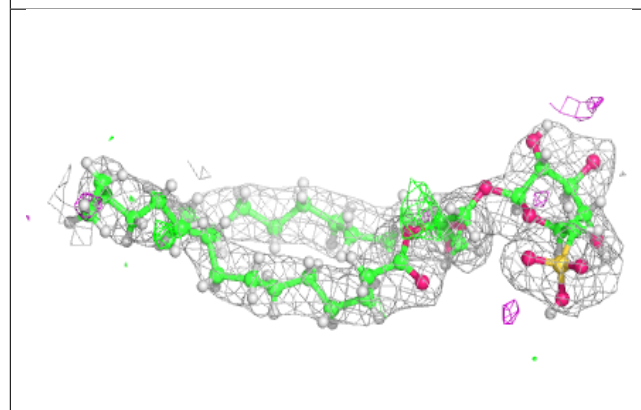
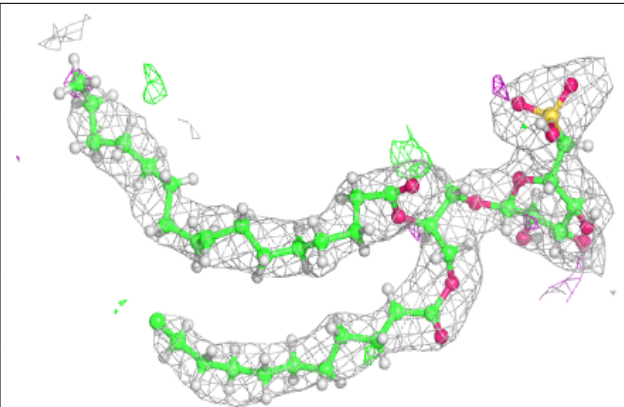
**Electron density around LHG e 101:**

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

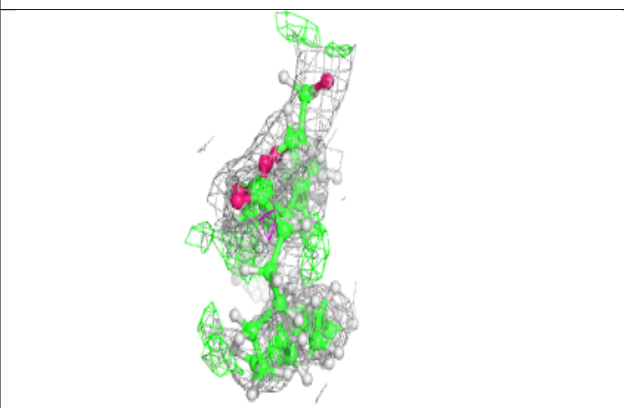
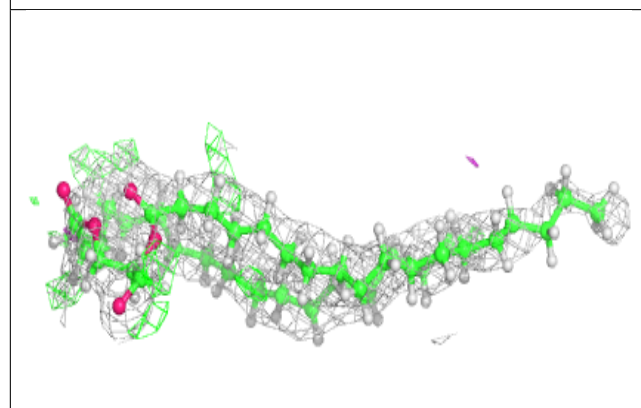
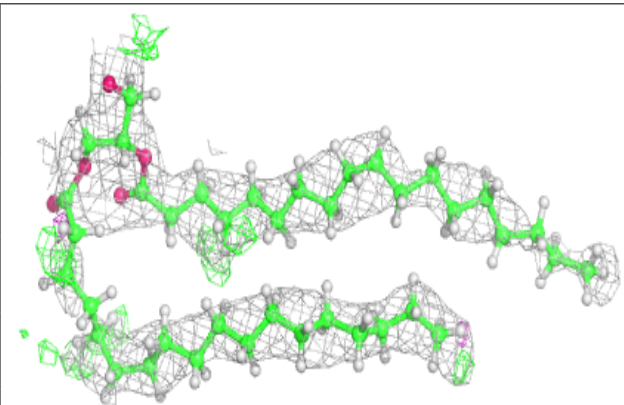


Electron density around SQD b 601:

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

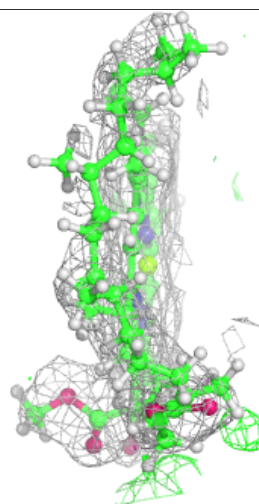
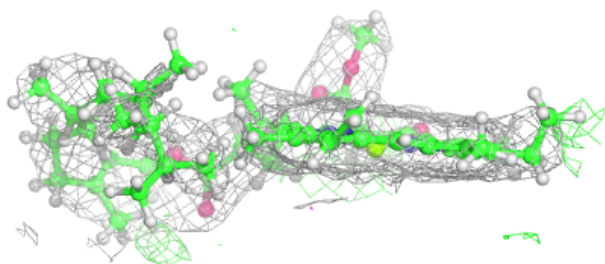
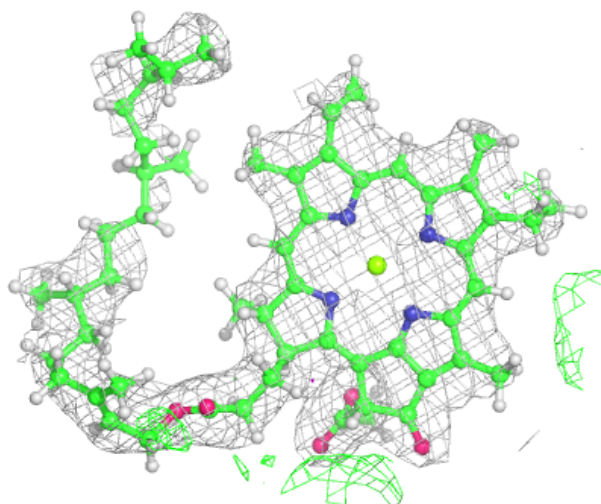
**Electron density around DGD a 414:**

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



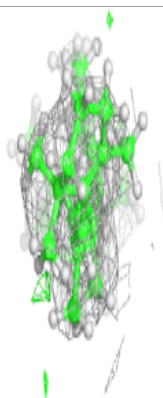
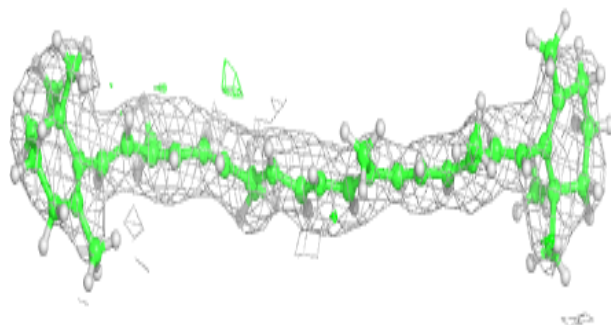
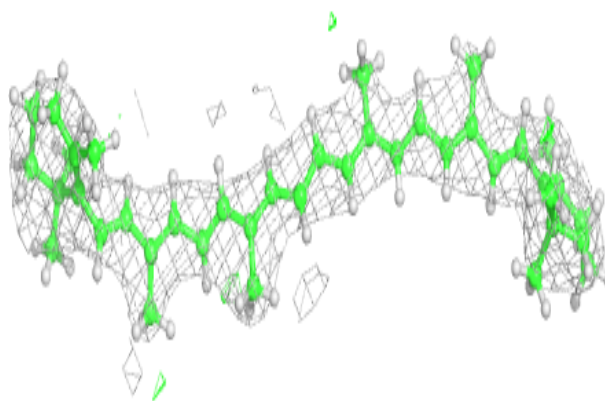
Electron density around CLA c 512:

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

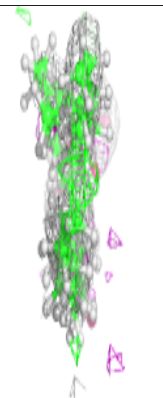
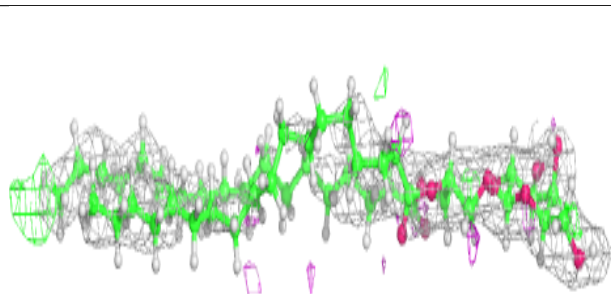
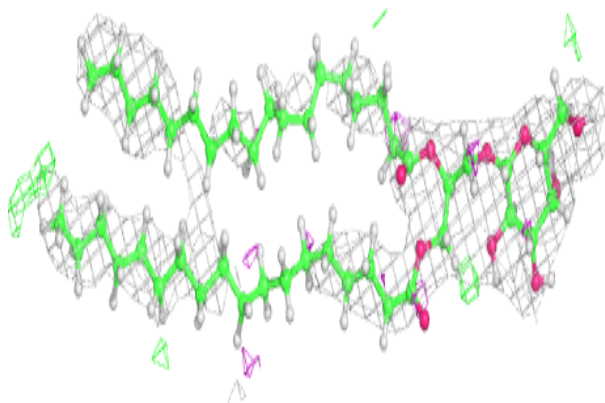


Electron density around BCR k 101:

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

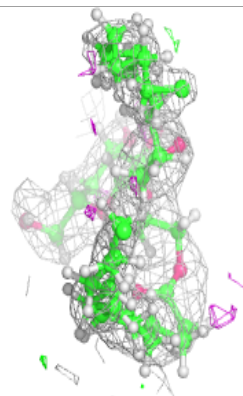
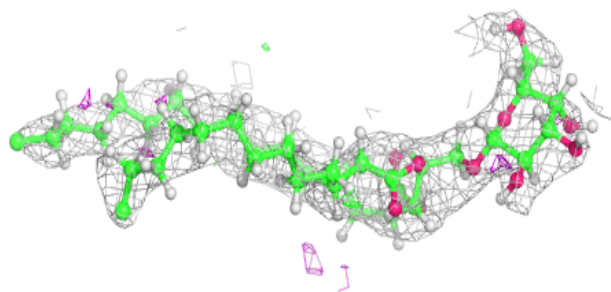
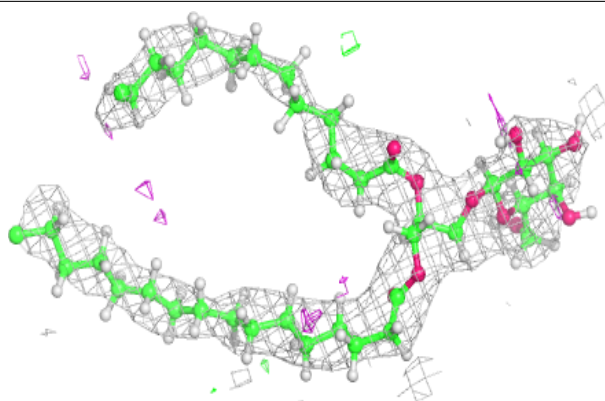
**Electron density around LMG b 622:**

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

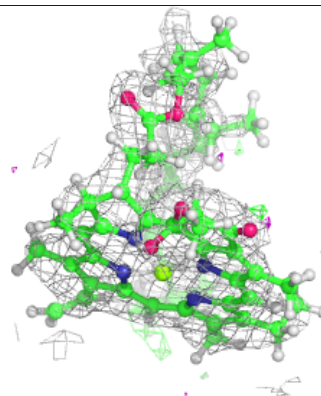
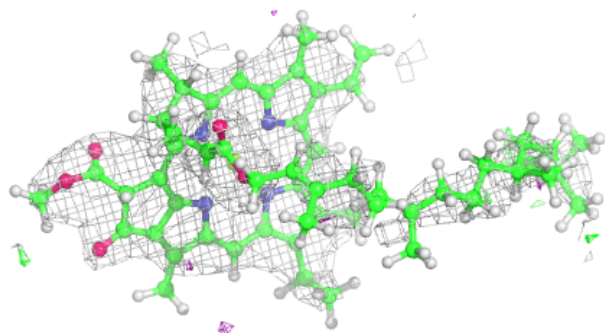
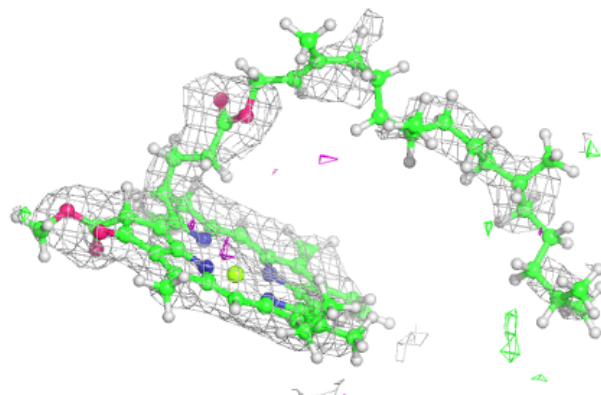


Electron density around LMG A 411:

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

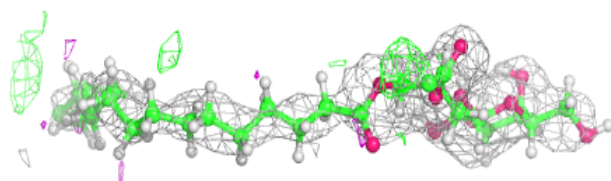
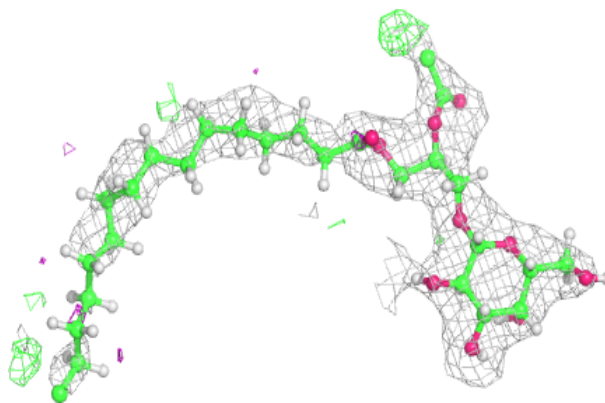
**Electron density around CLA c 513:**

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

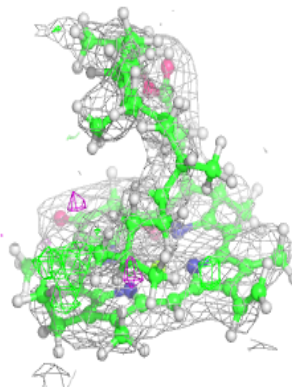
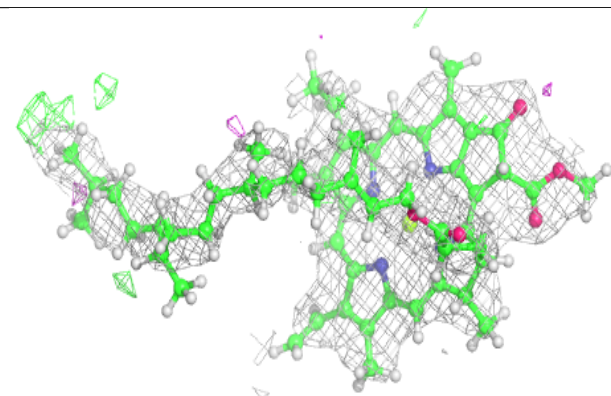
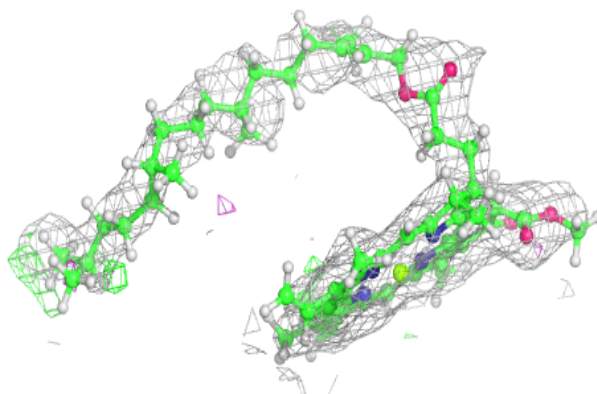


Electron density around LMG c 519:

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

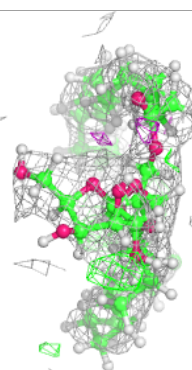
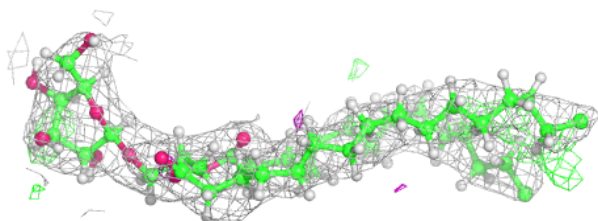
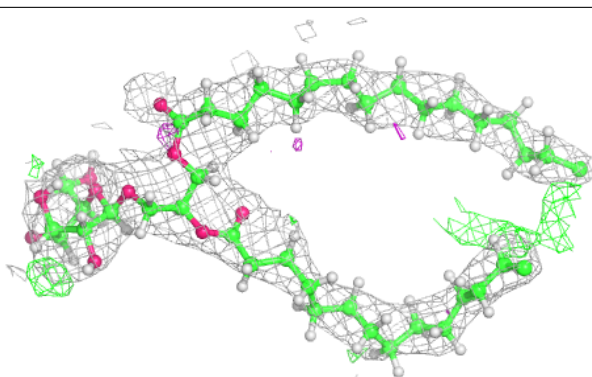
**Electron density around CLA C 513:**

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

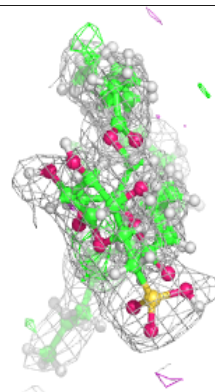
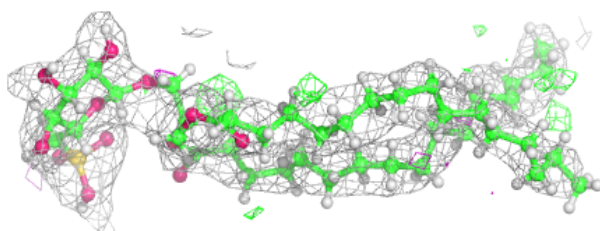
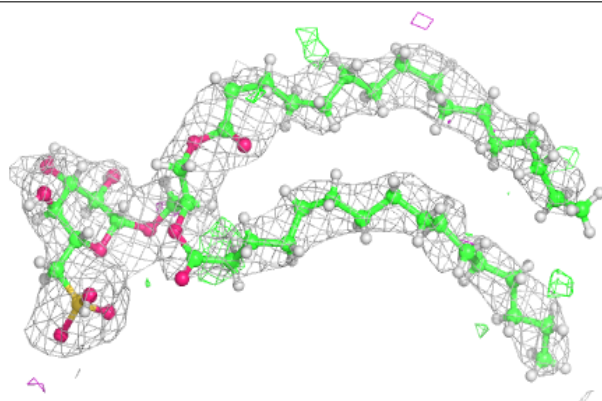


Electron density around LMG c 523:

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

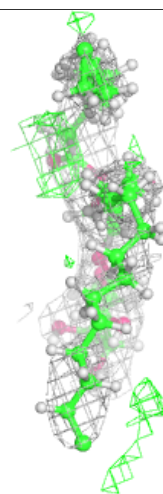
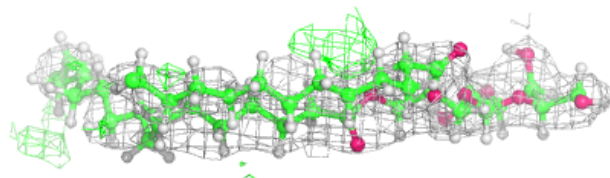
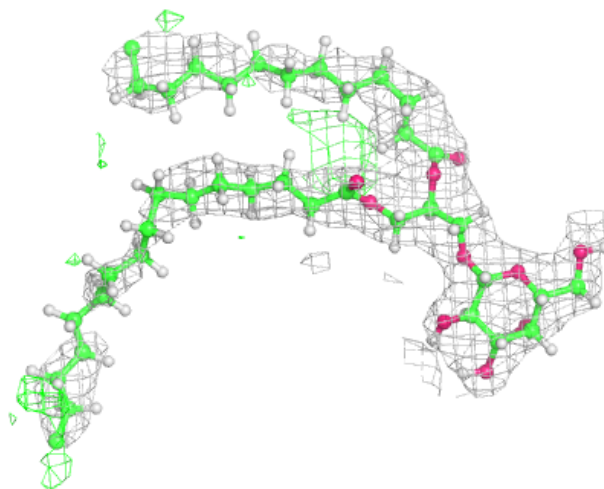
**Electron density around SQD B 624:**

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



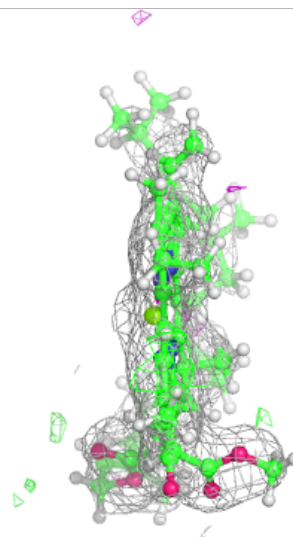
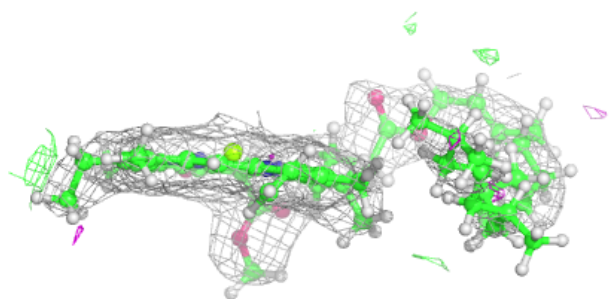
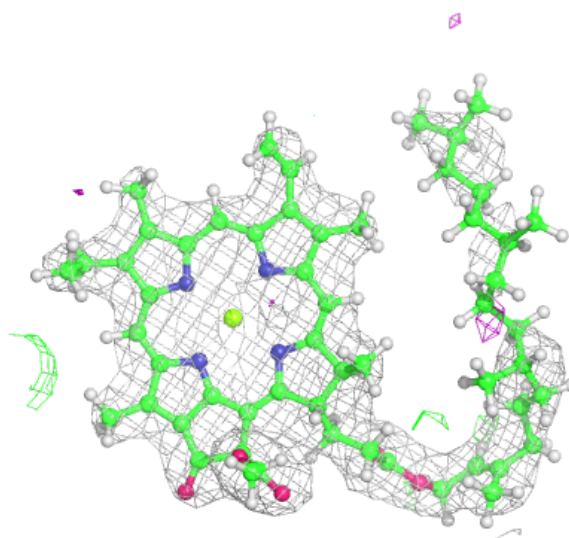
Electron density around LMG C 518:

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



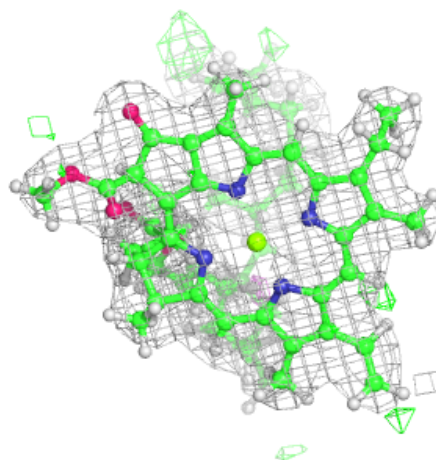
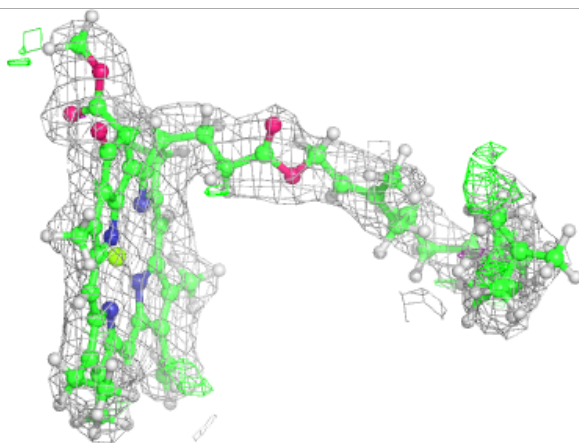
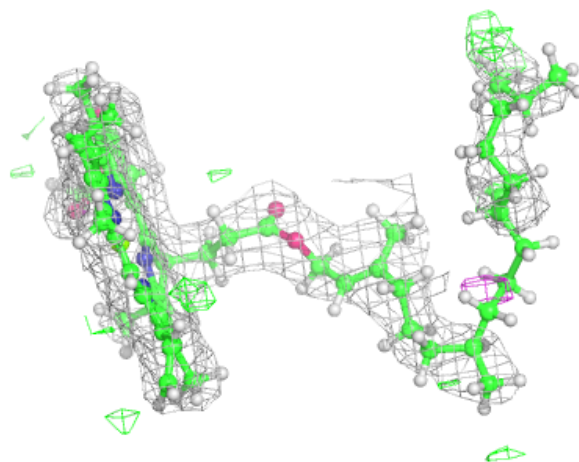
Electron density around CLA C 512:

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



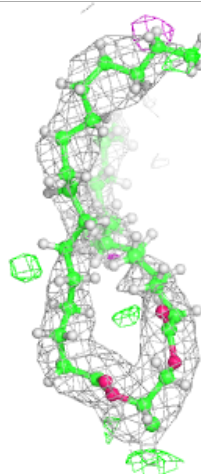
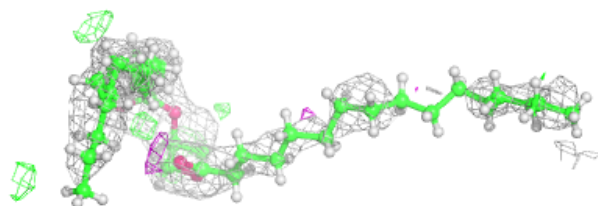
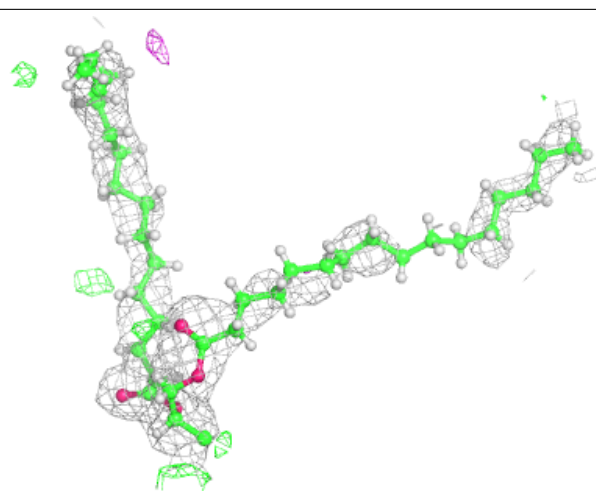
Electron density around CLA a 408:

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



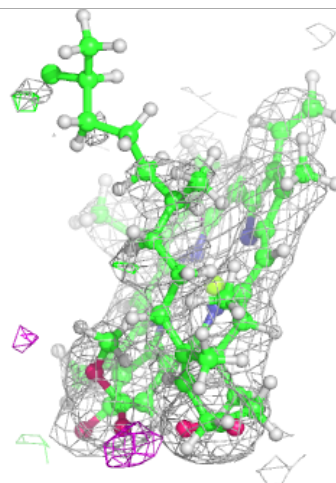
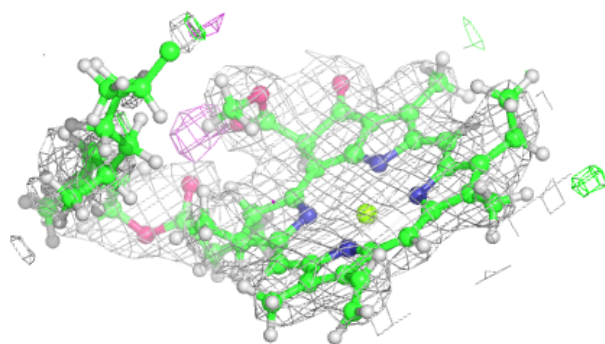
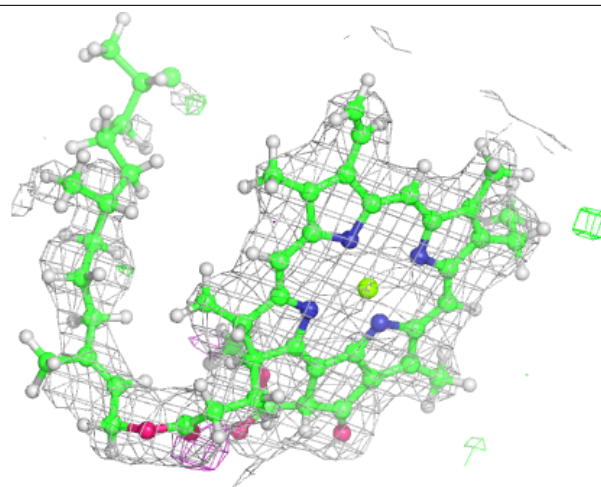
Electron density around SQD A 414:

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



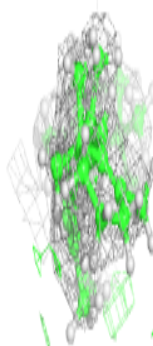
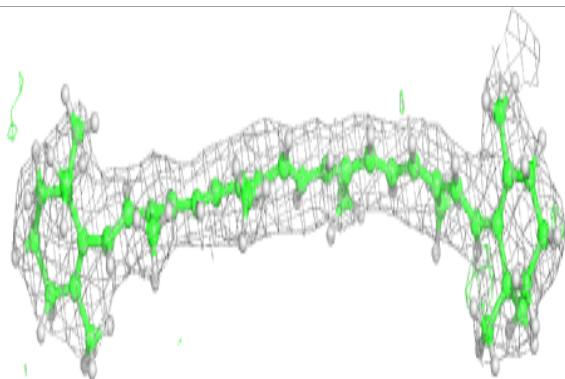
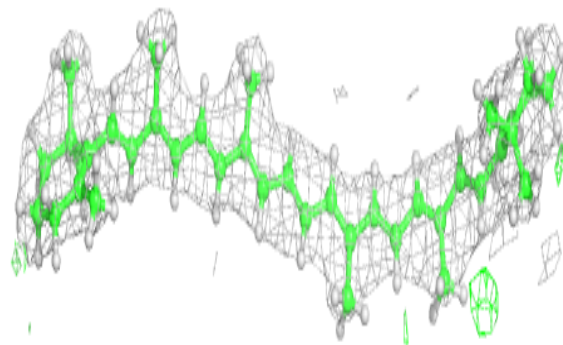
Electron density around CLA b 617:

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

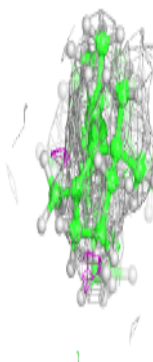
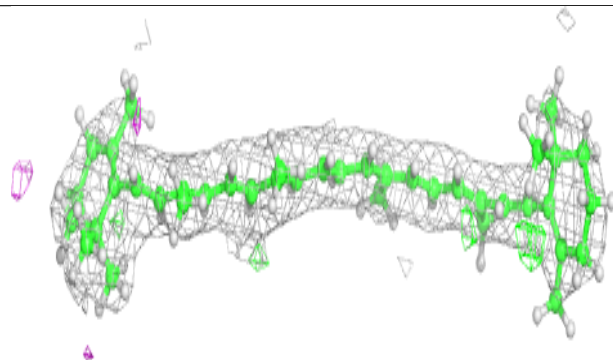
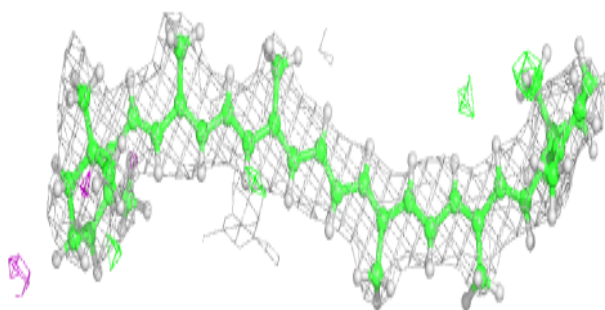


Electron density around BCR H 101:

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

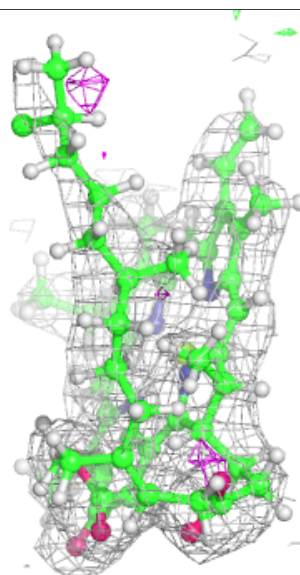
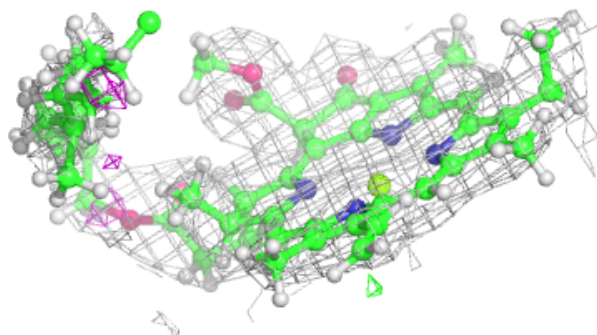
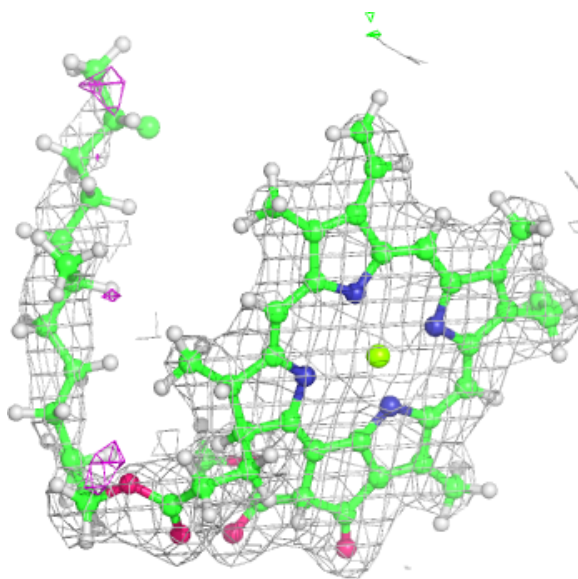
**Electron density around BCR K 101:**

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



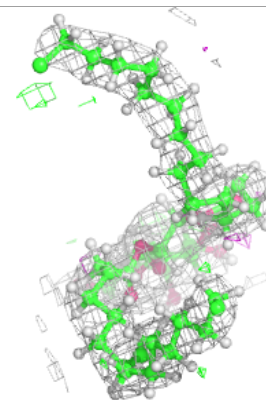
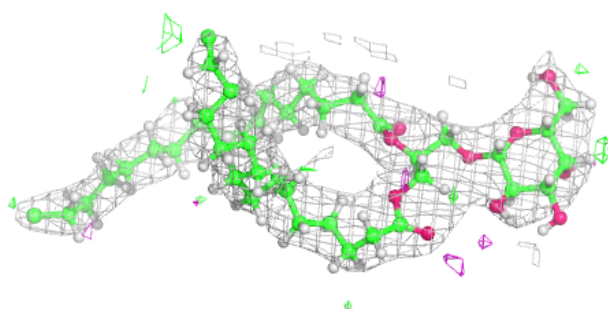
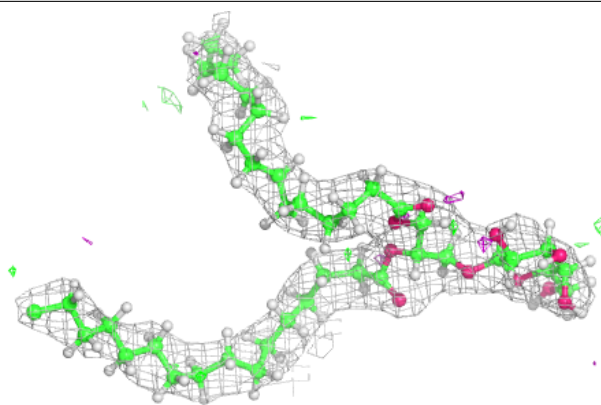
Electron density around CLA B 616:

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

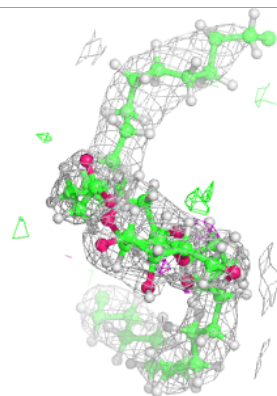
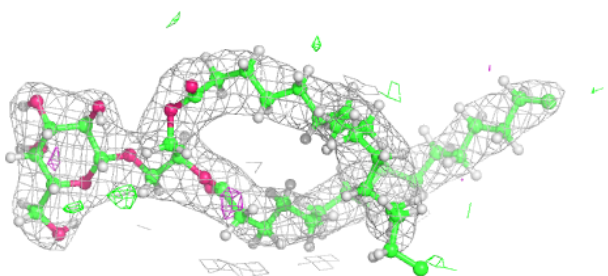
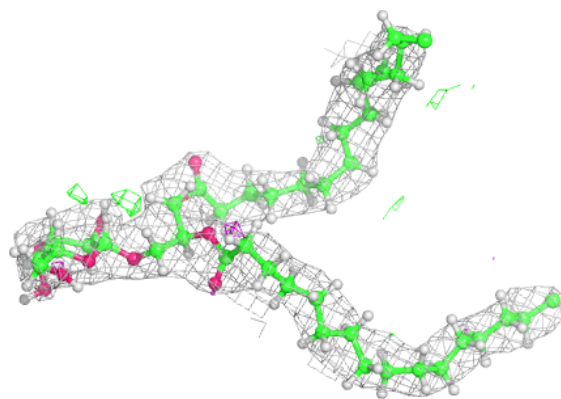


Electron density around LMG m 101:

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

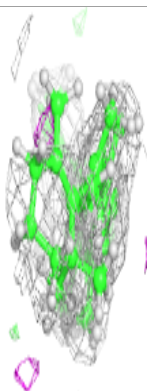
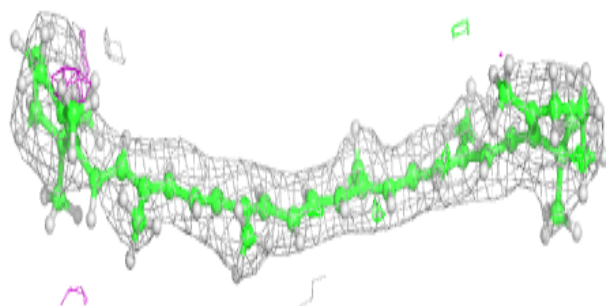
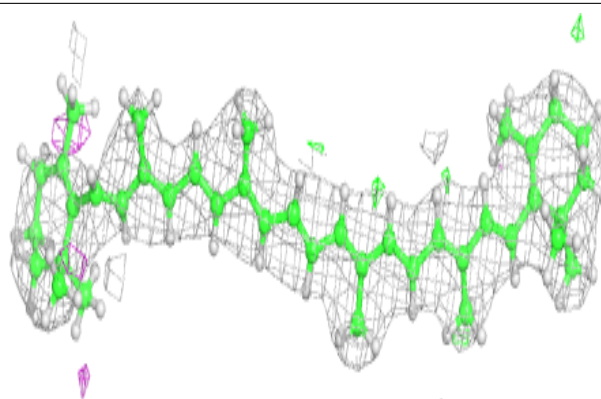
**Electron density around LMG M 101:**

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

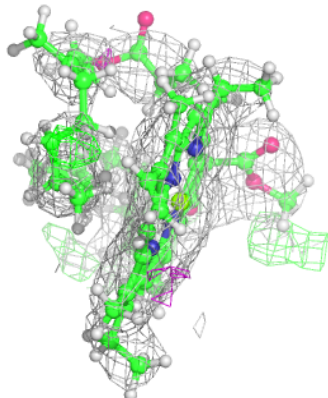
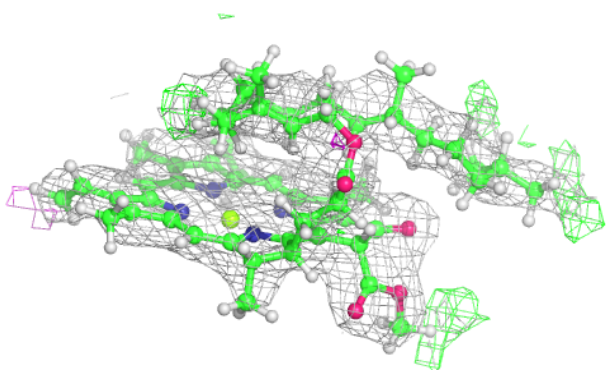
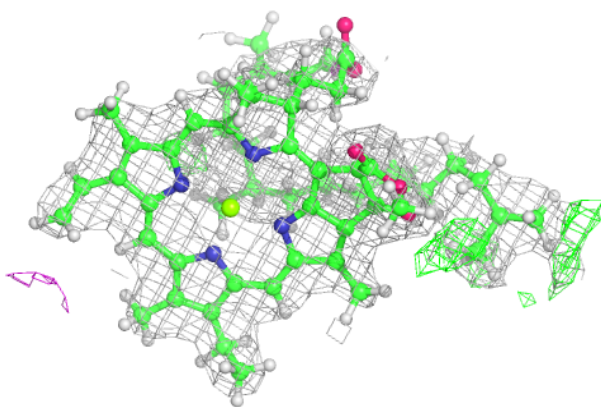


Electron density around BCR D 404:

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

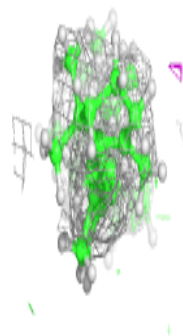
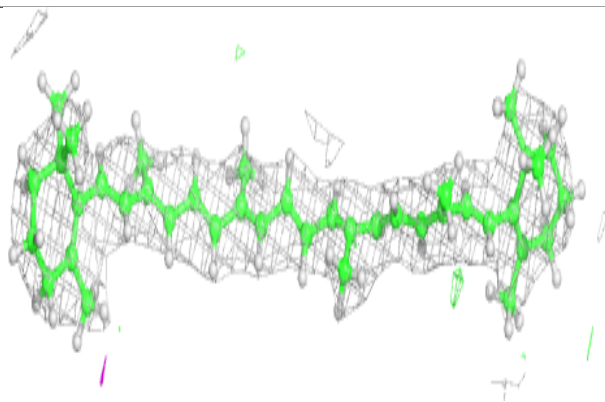
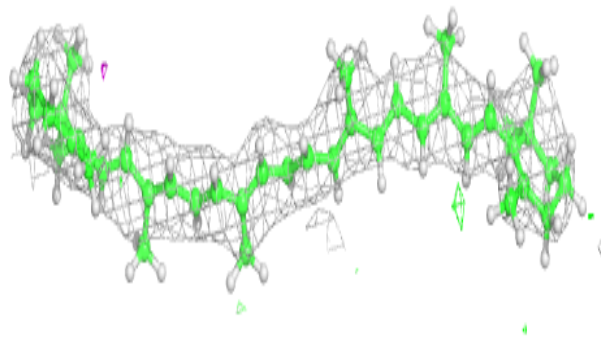
**Electron density around CLA B 601:**

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



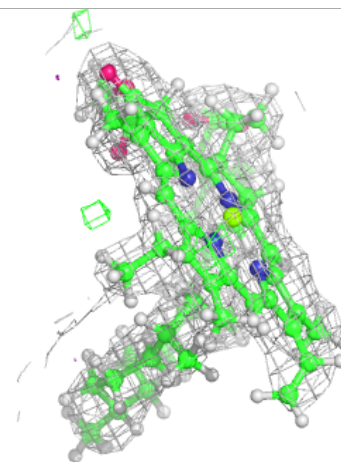
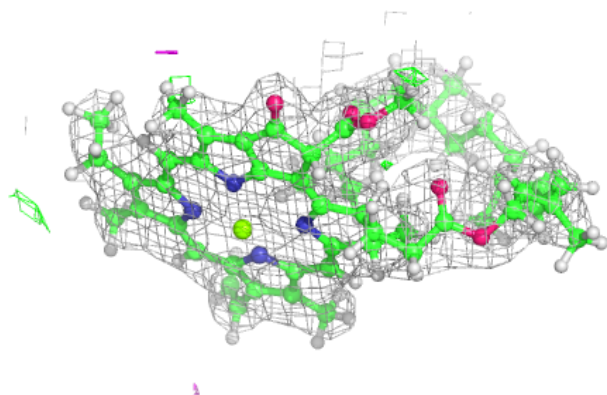
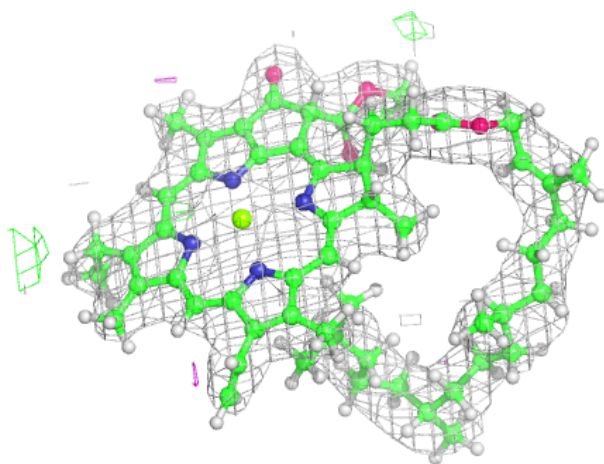
Electron density around BCR c 514:

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



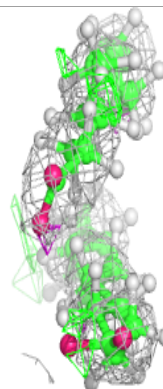
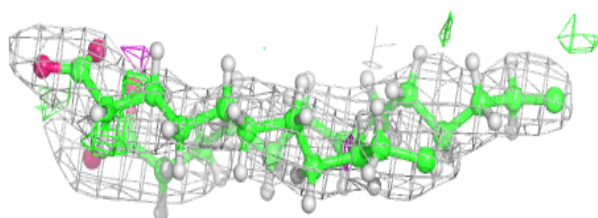
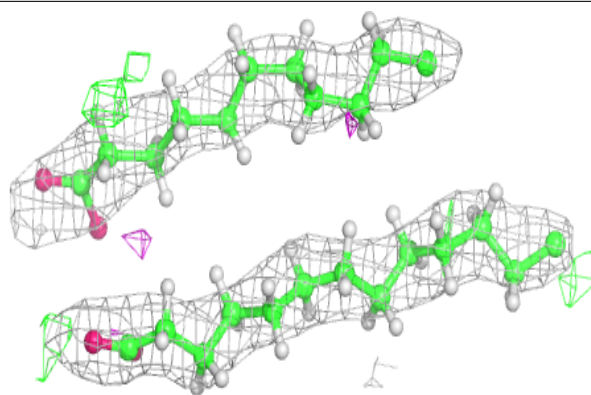
Electron density around CLA b 616:

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

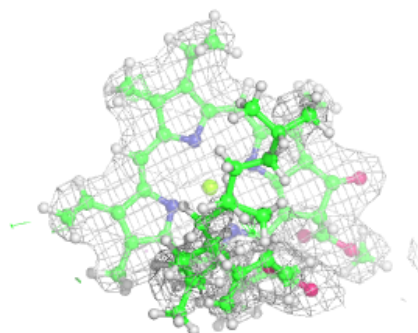
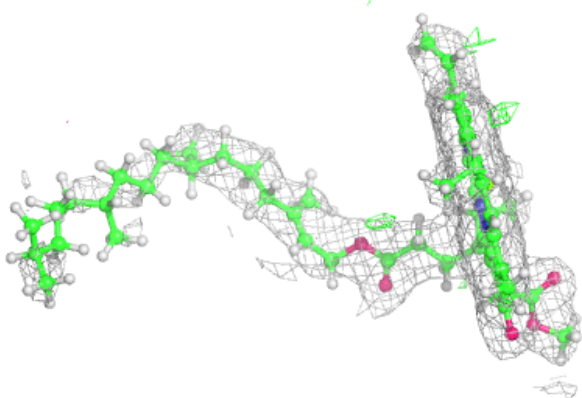
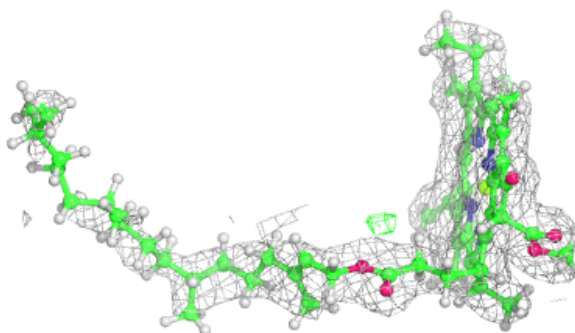


Electron density around LMG B 621:

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

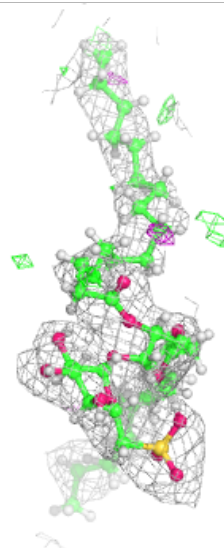
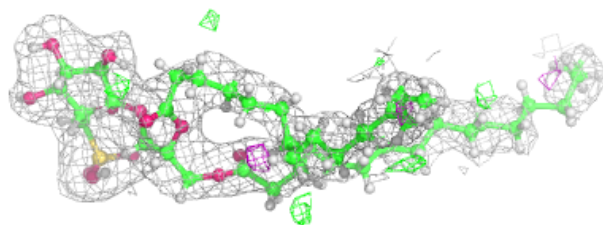
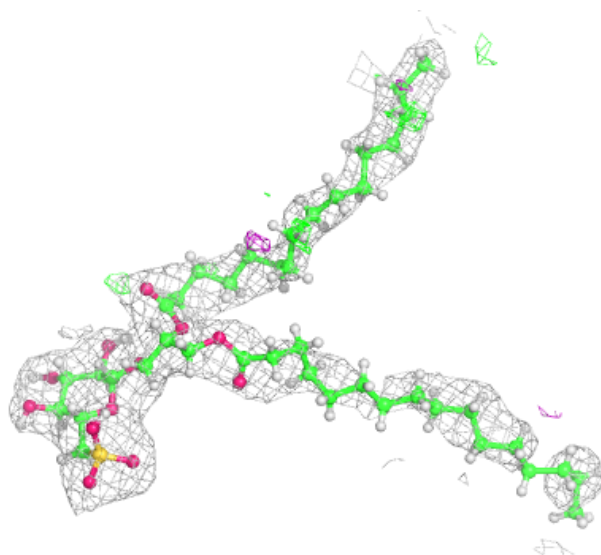
**Electron density around CLA D 403:**

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



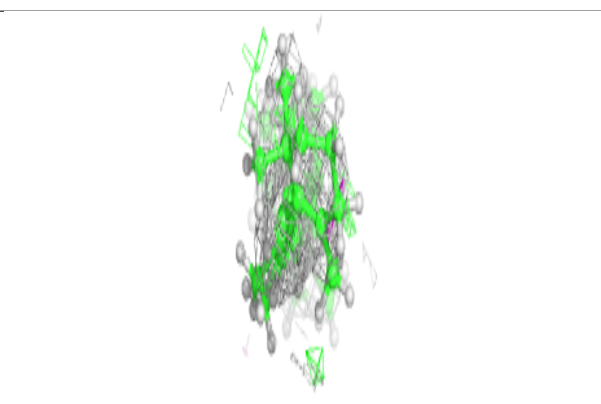
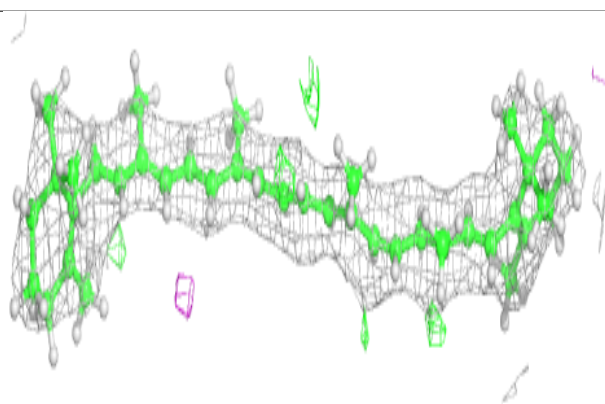
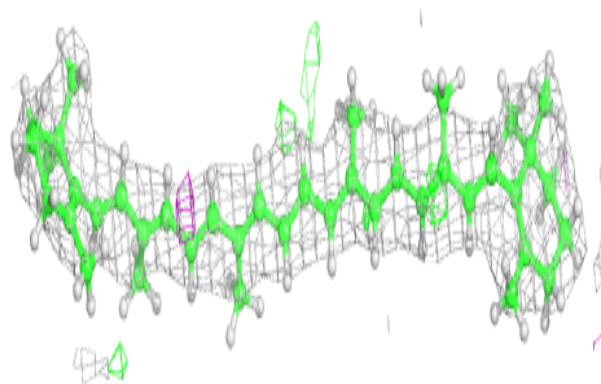
Electron density around SQD a 412:

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

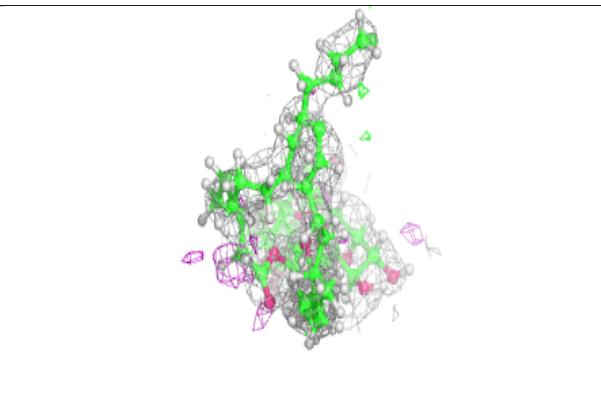
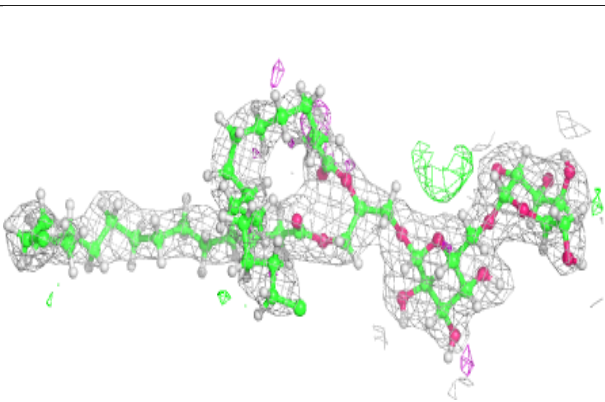
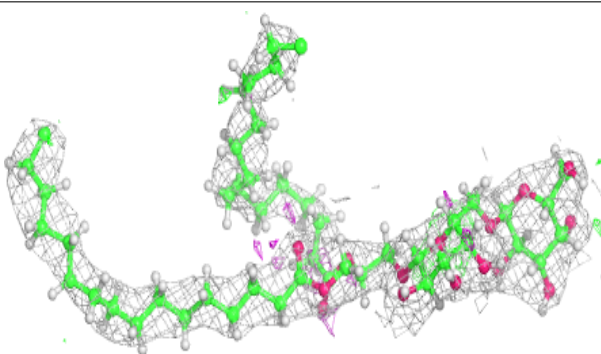


Electron density around BCR Z 101:

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

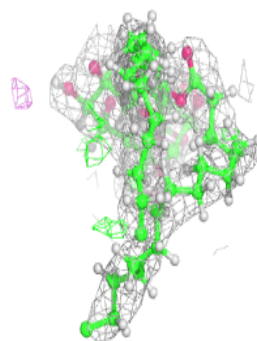
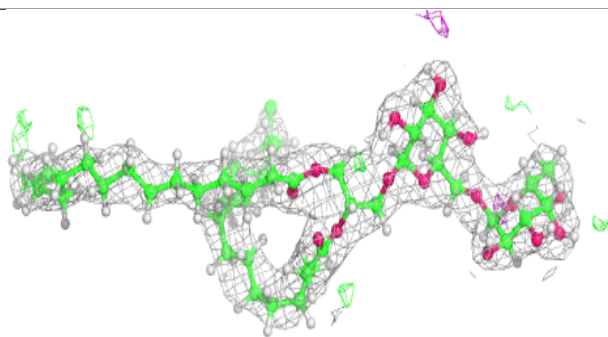
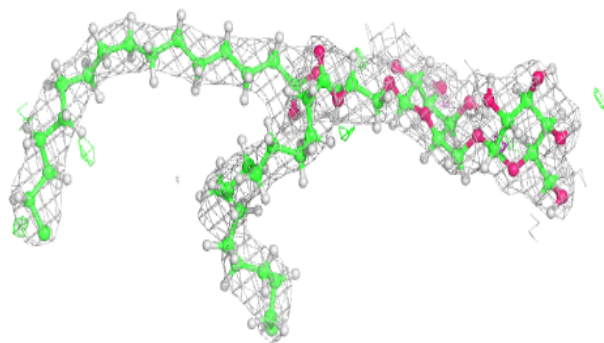
**Electron density around DGD h 102:**

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

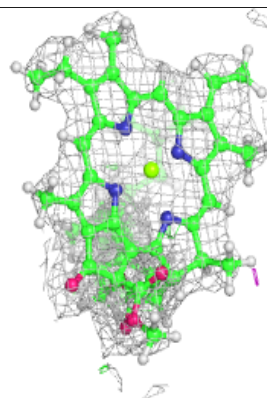
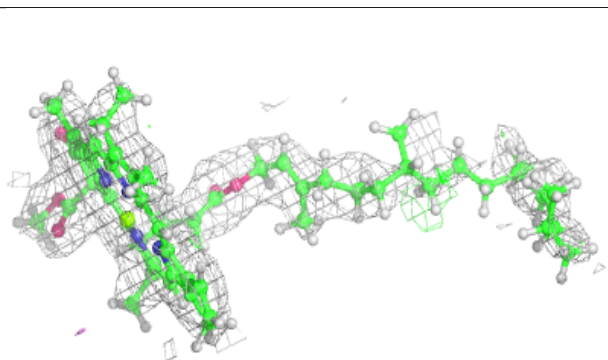
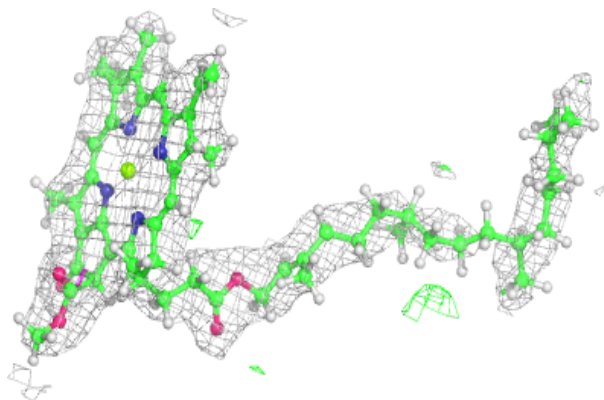


Electron density around DGD H 102:

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

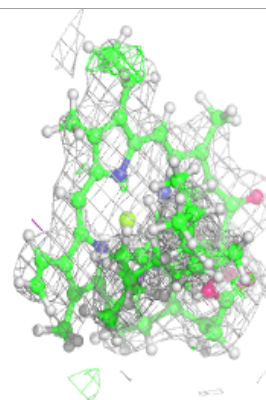
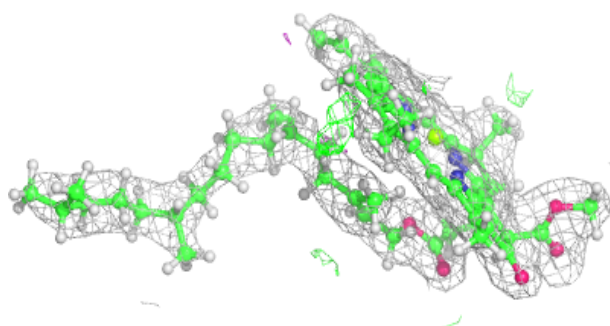
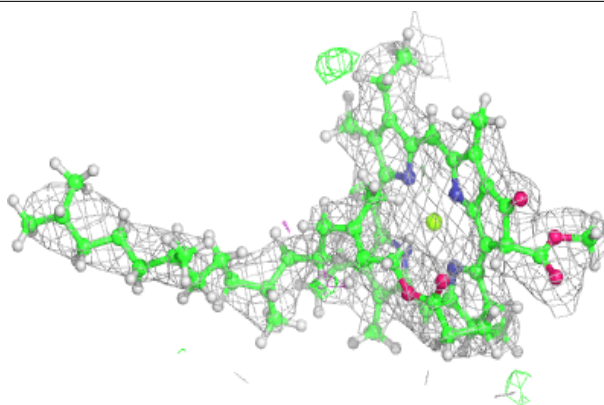
**Electron density around CLA d 403:**

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

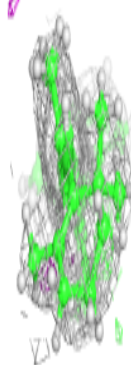
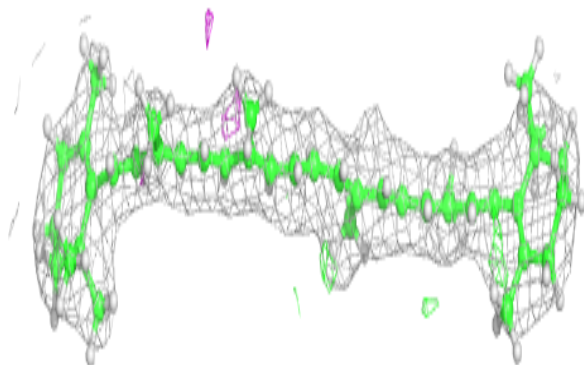
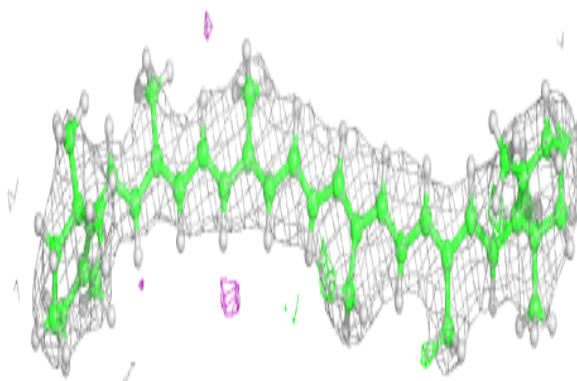


Electron density around CLA C 505:

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

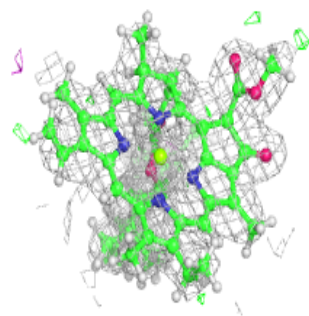
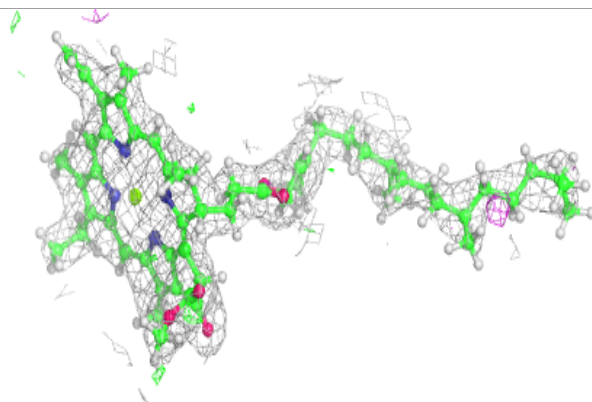
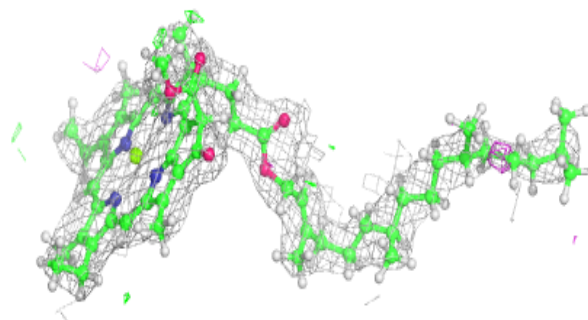
**Electron density around BCR C 514:**

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



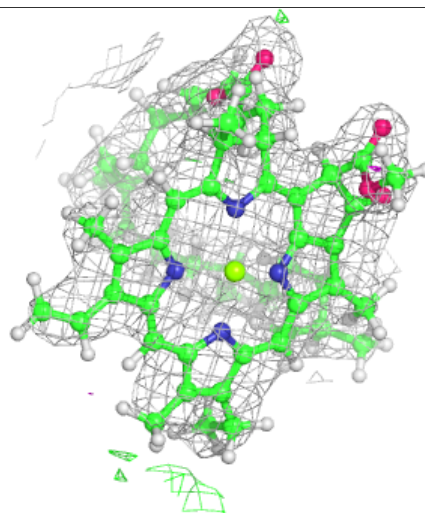
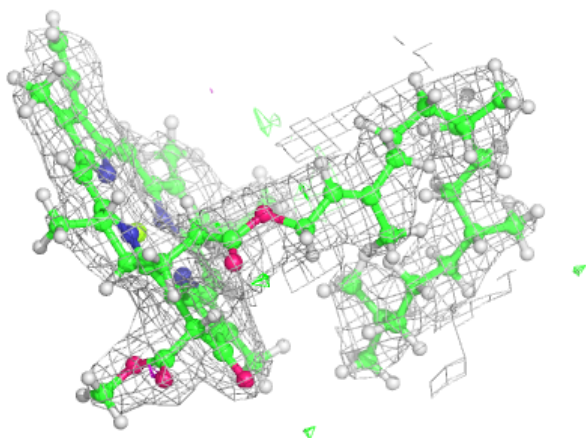
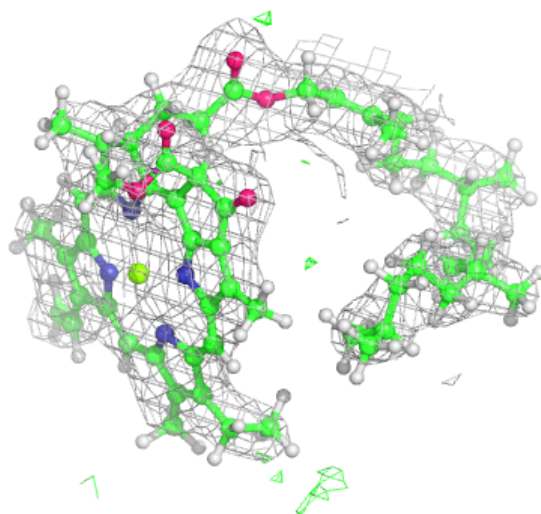
Electron density around CLA c 502:

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



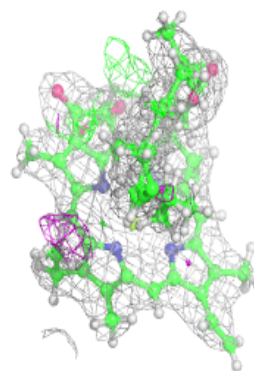
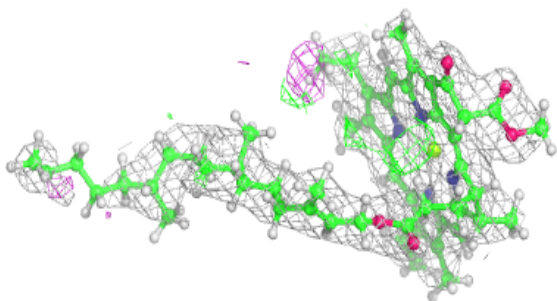
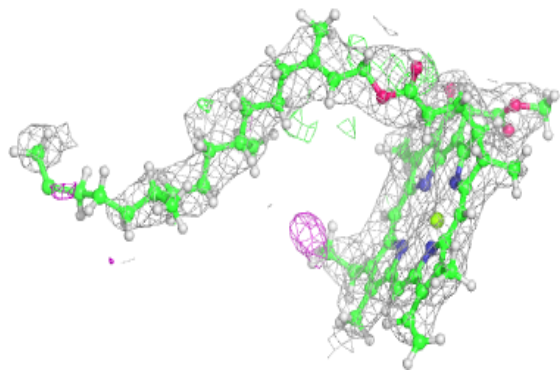
Electron density around CLA c 503:

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

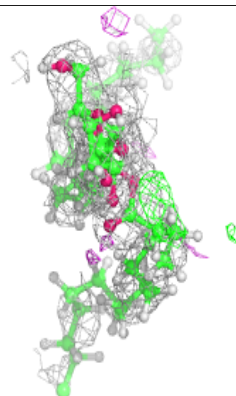
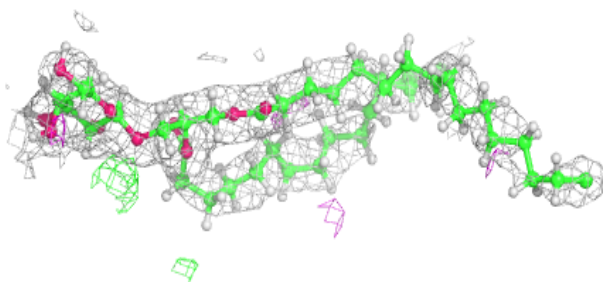
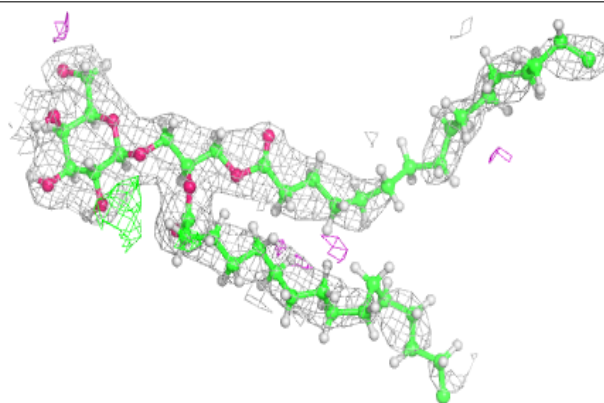


Electron density around CLA c 508:

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

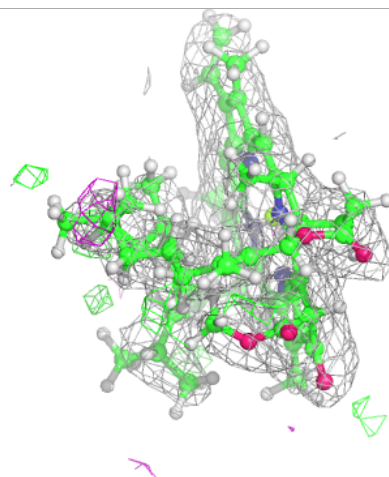
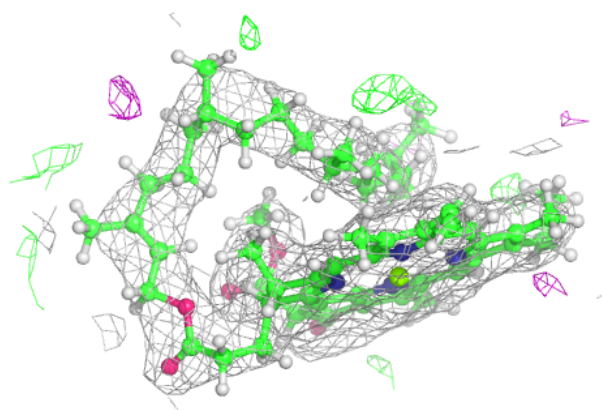
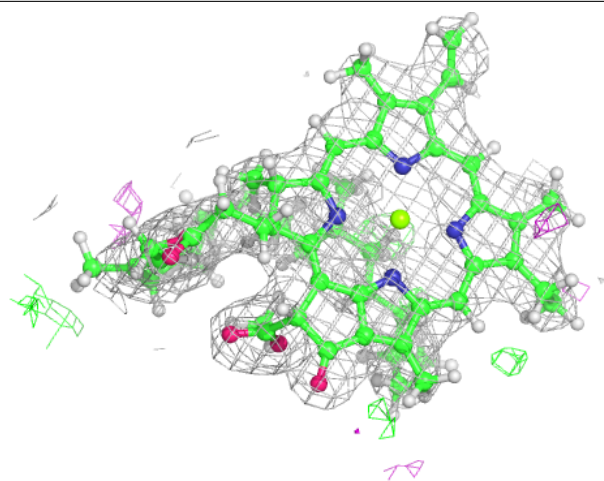
**Electron density around LMG D 406:**

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



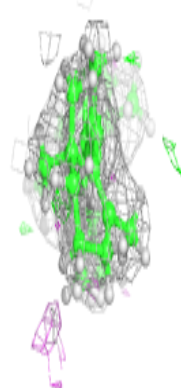
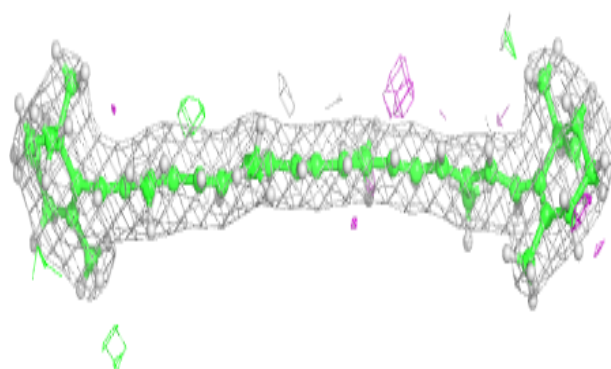
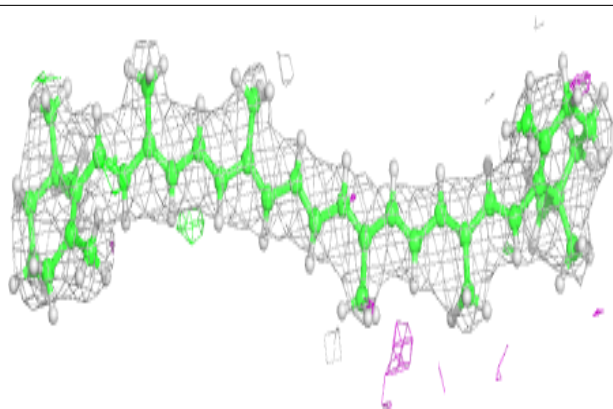
Electron density around CLA c 510:

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



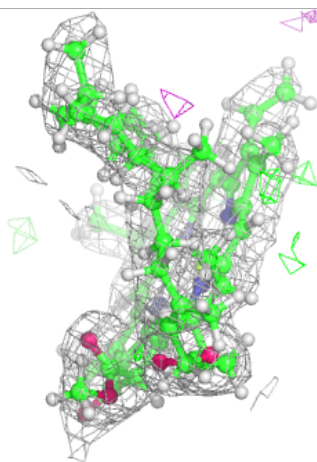
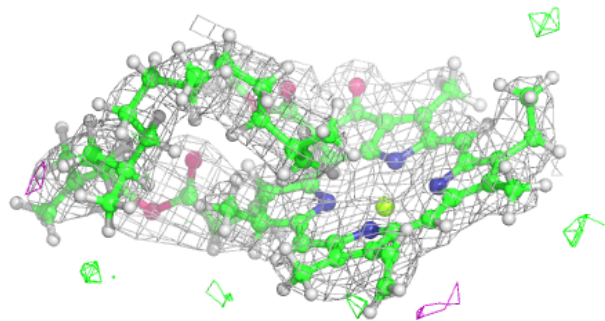
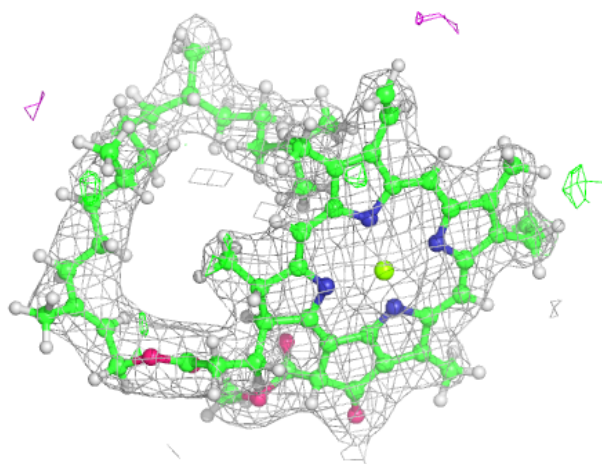
Electron density around BCR b 619:

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



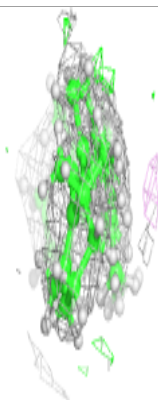
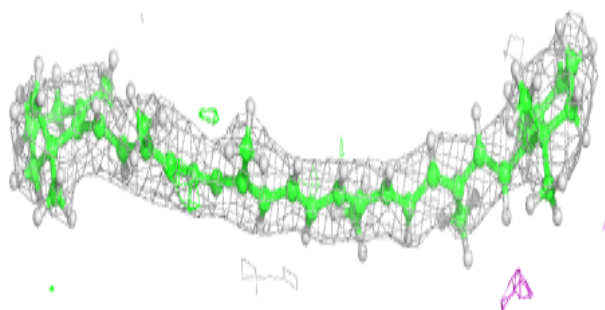
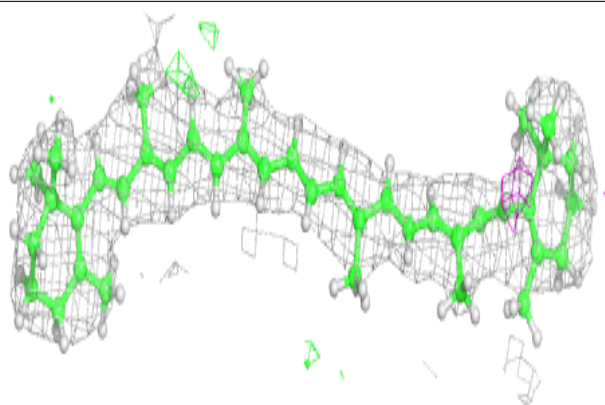
Electron density around CLA B 615:

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

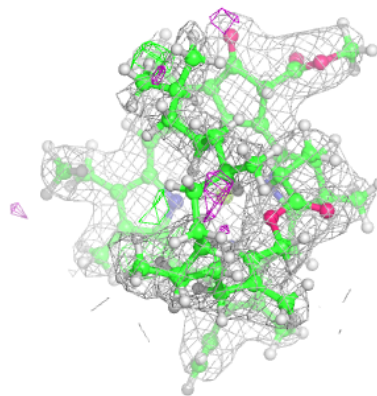
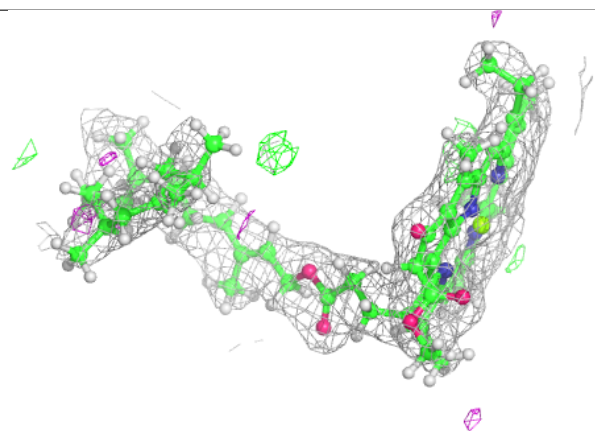
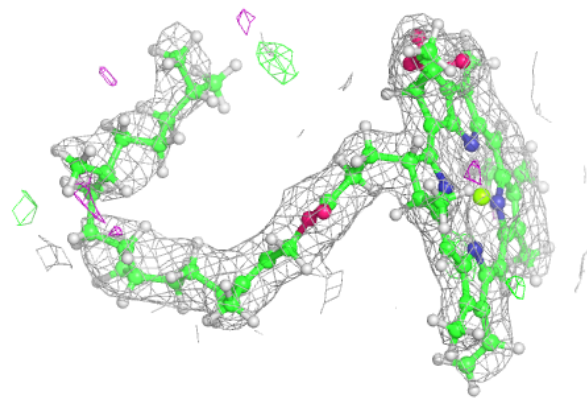


Electron density around BCR d 404:

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

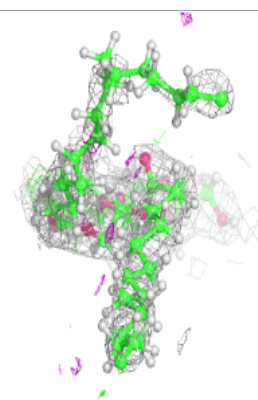
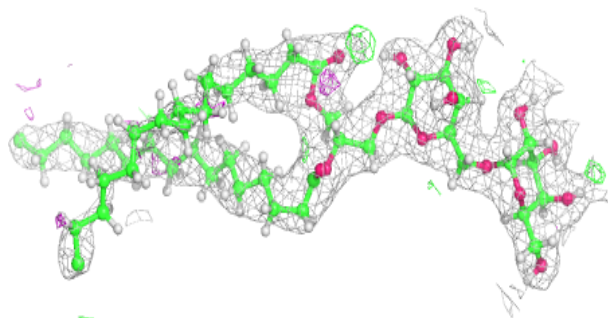
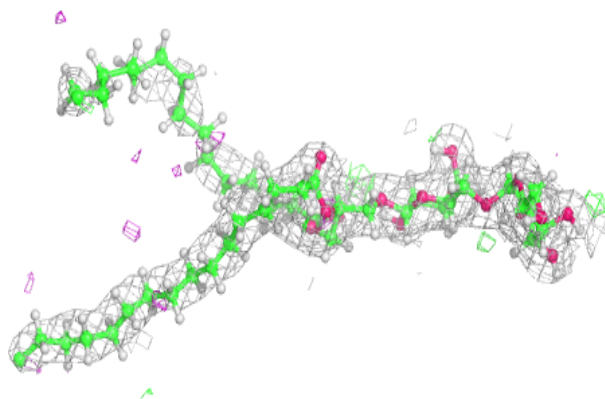
**Electron density around CLA B 606:**

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

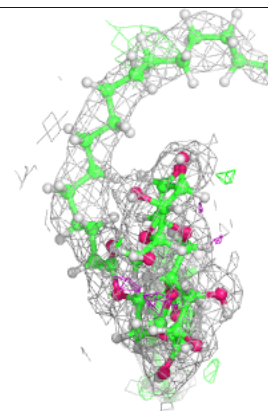
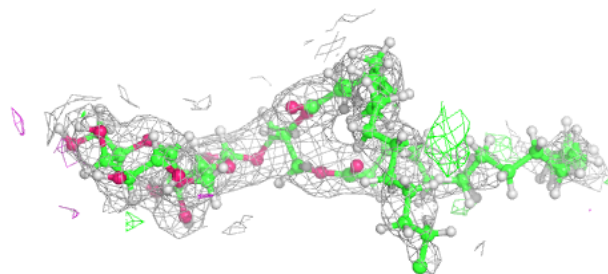
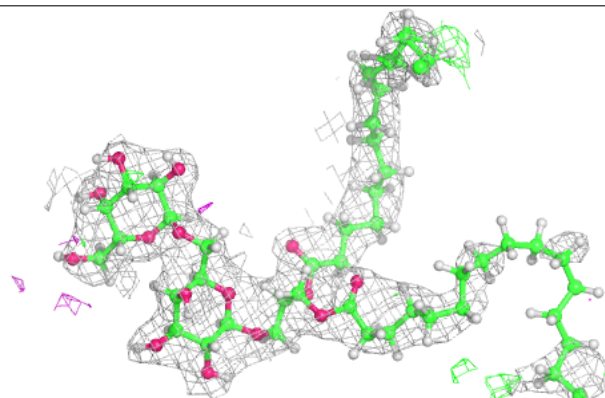


Electron density around DGD C 515:

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

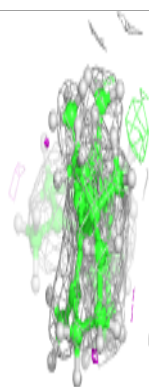
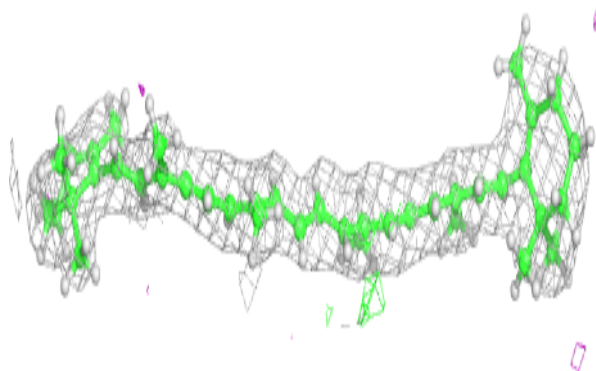
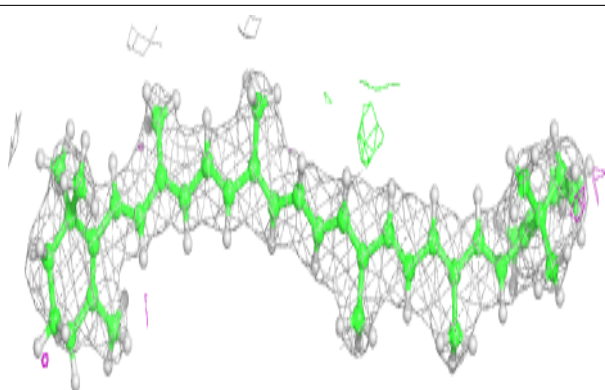
**Electron density around DGD C 516:**

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

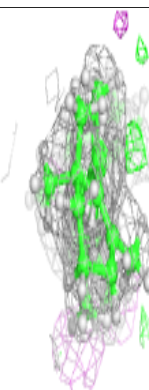
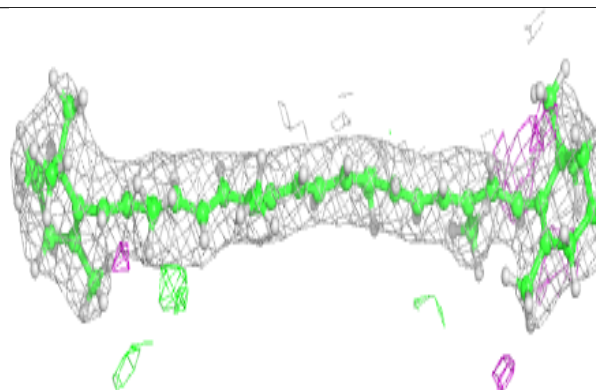
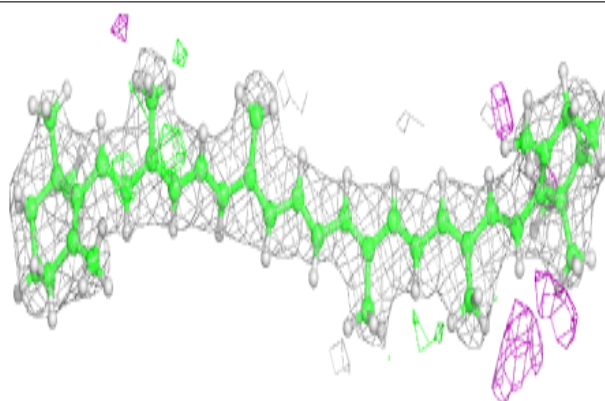


Electron density around BCR B 617:

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

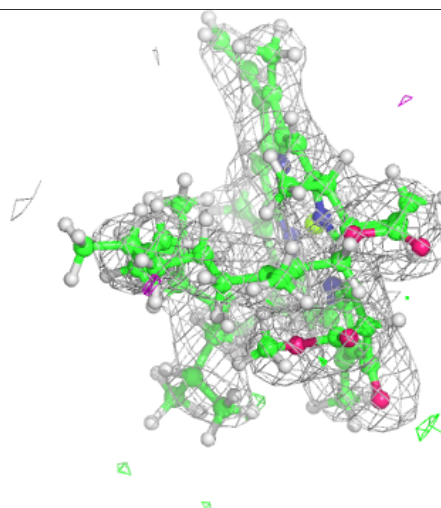
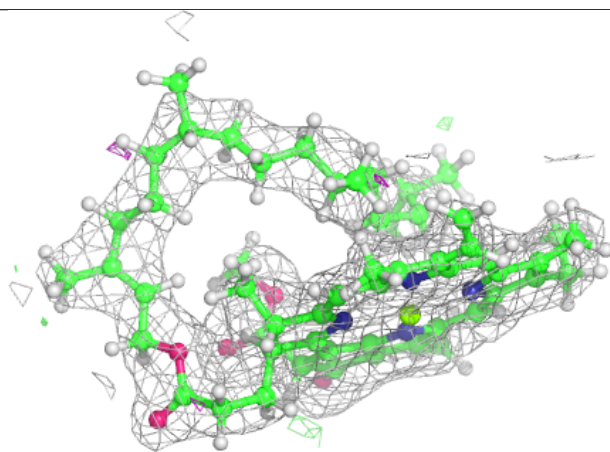
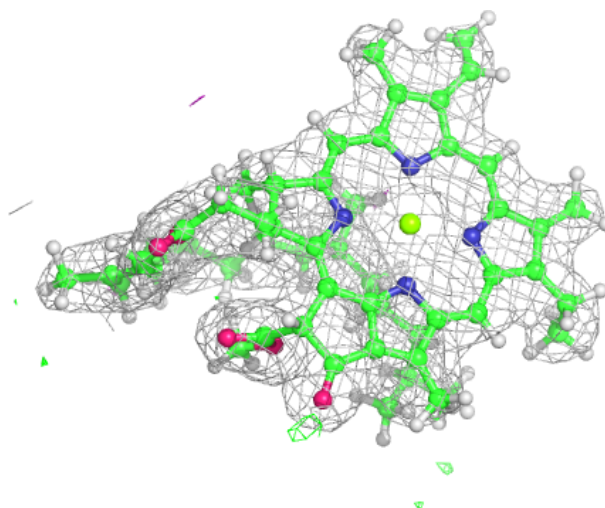
**Electron density around BCR B 618:**

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



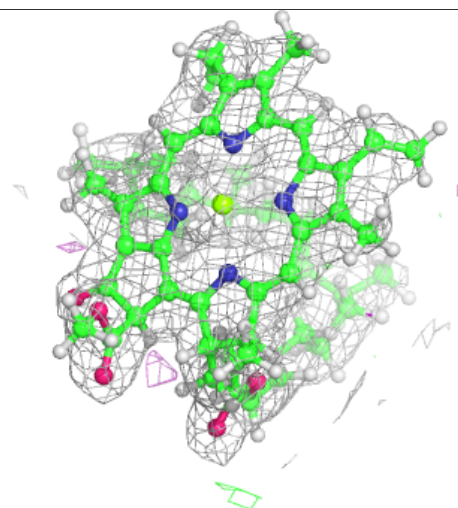
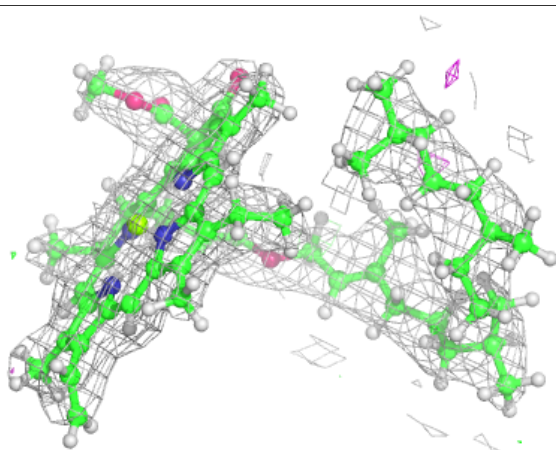
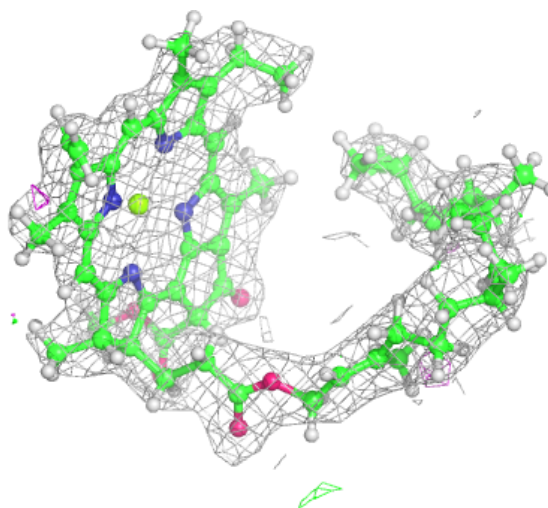
Electron density around CLA C 510:

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



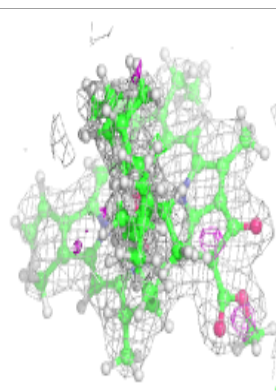
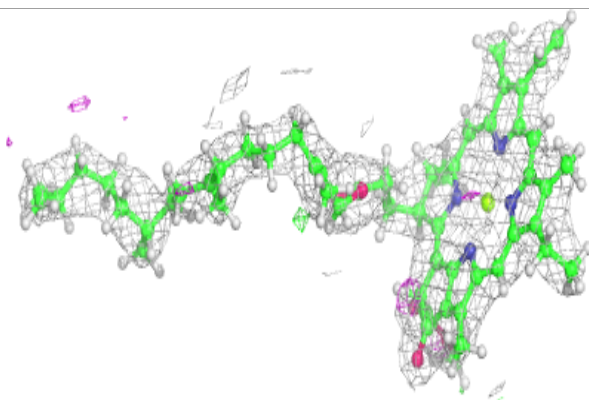
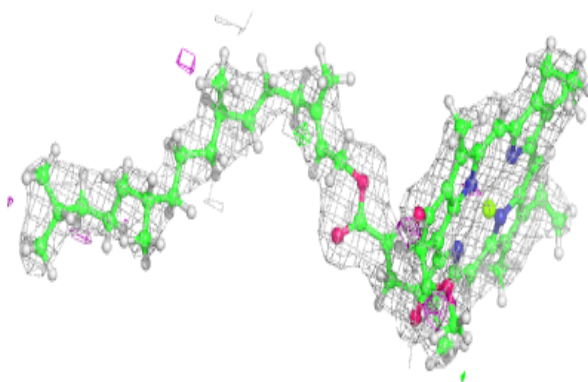
Electron density around CLA C 503:

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

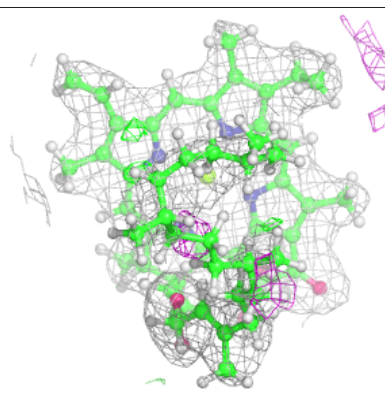
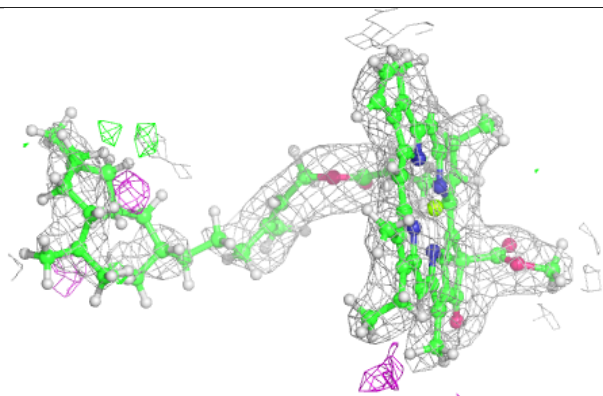
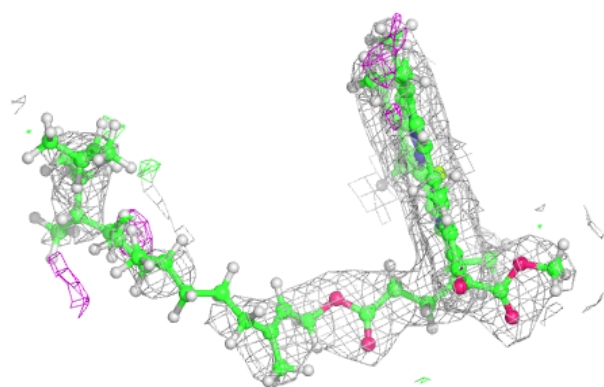


Electron density around CLA C 502:

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

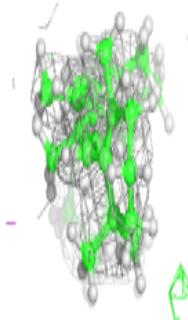
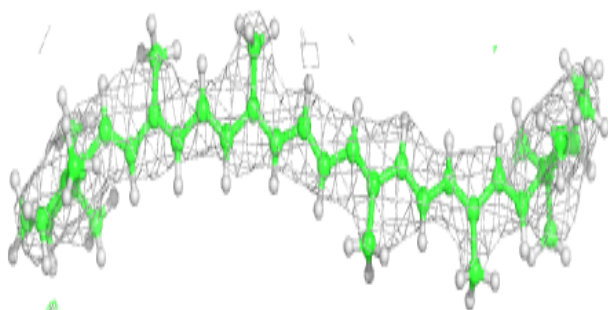
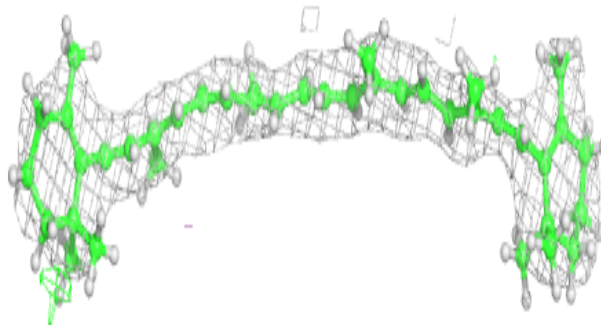
**Electron density around CLA C 506:**

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

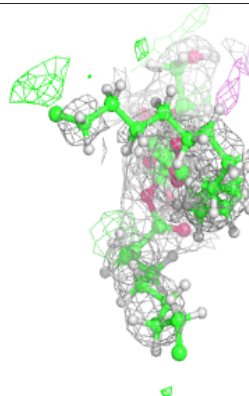
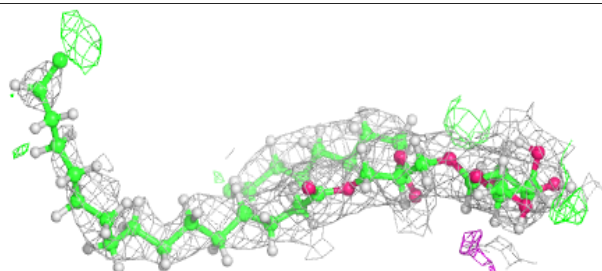
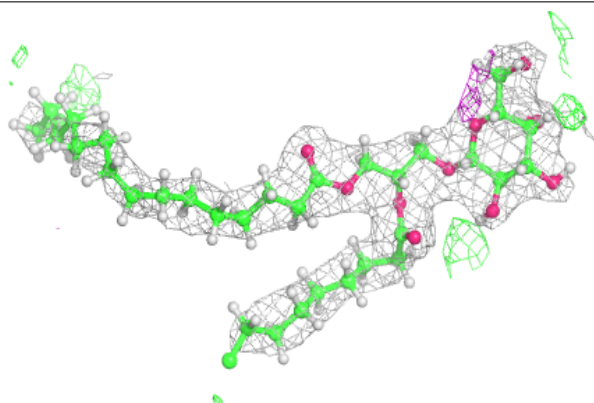


Electron density around BCR K 102:

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

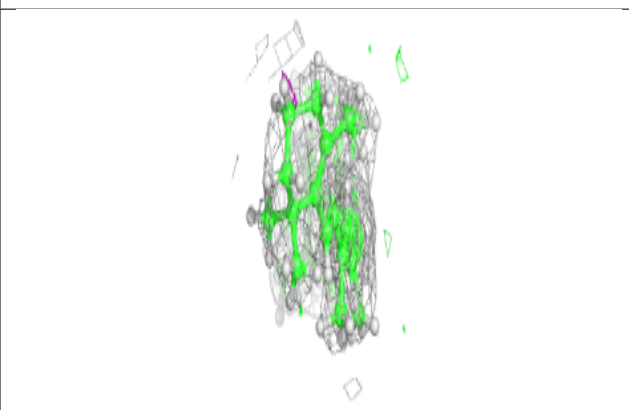
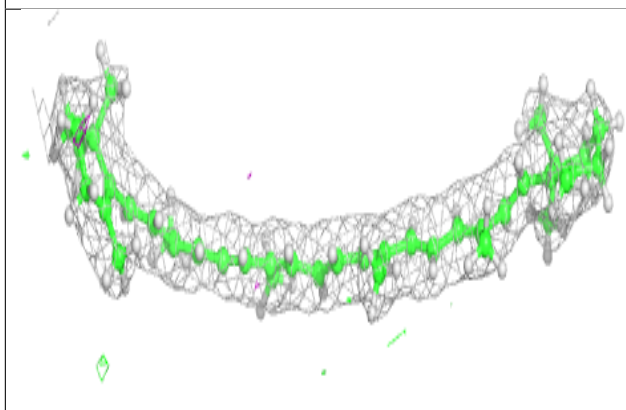
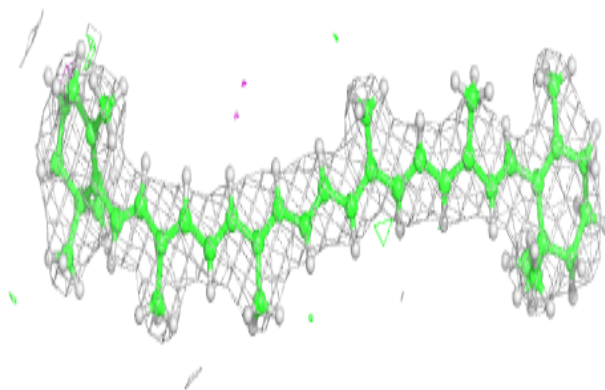
**Electron density around LMG d 409:**

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

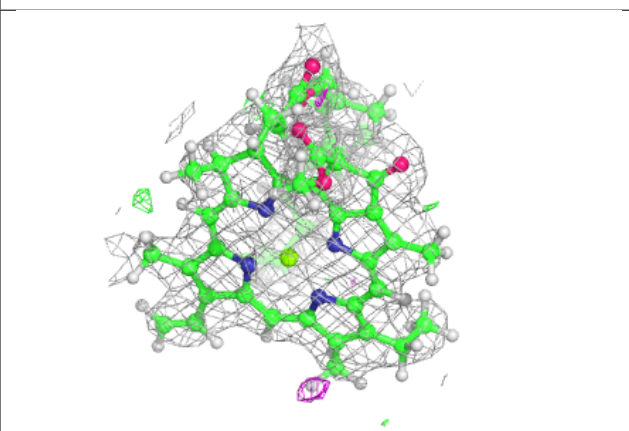
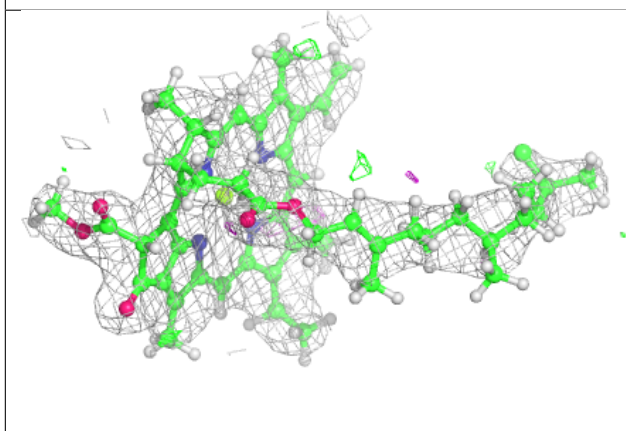
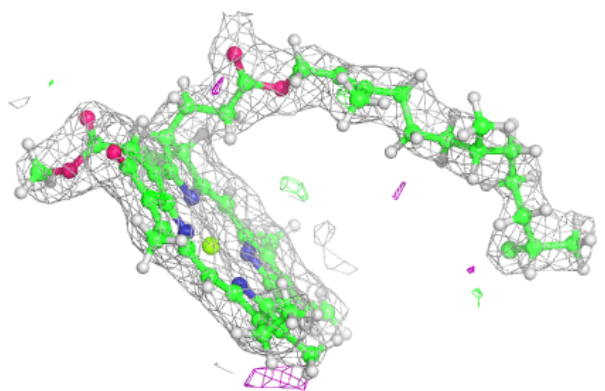


Electron density around BCR T 101:

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

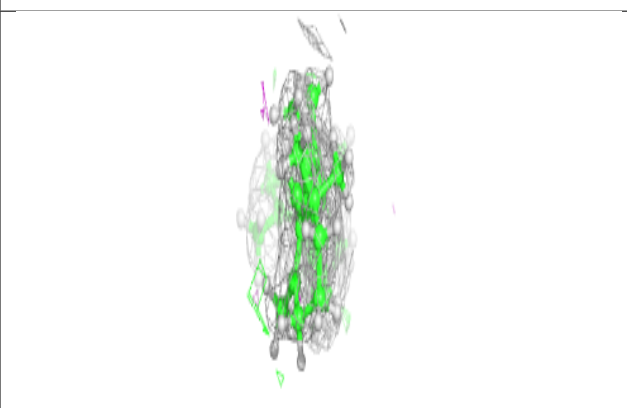
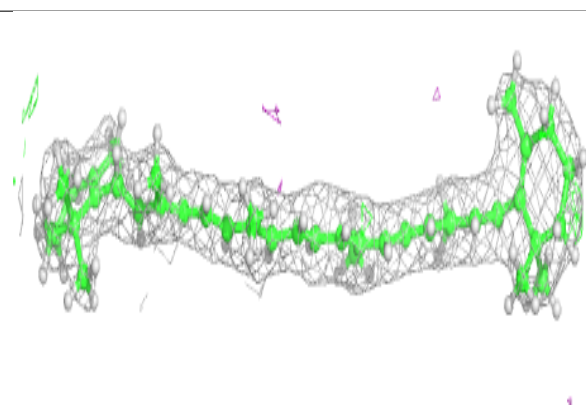
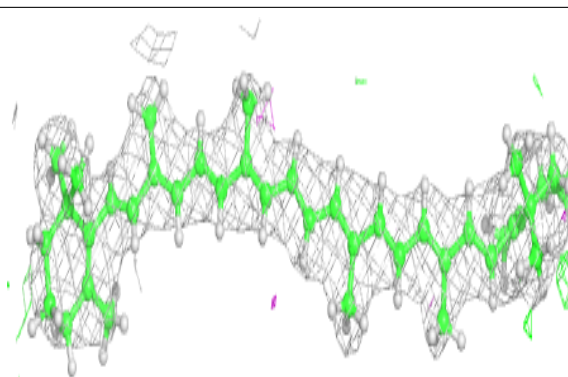
**Electron density around CLA c 504:**

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

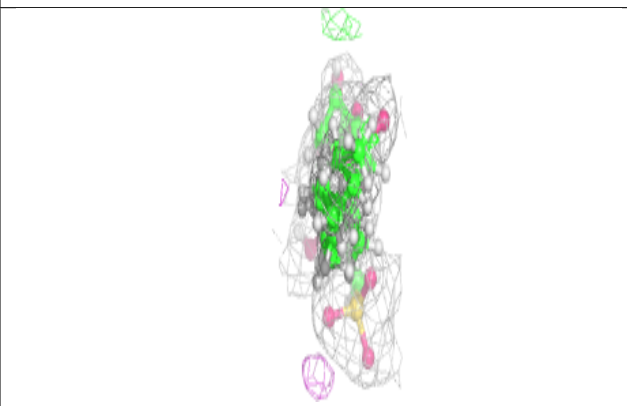
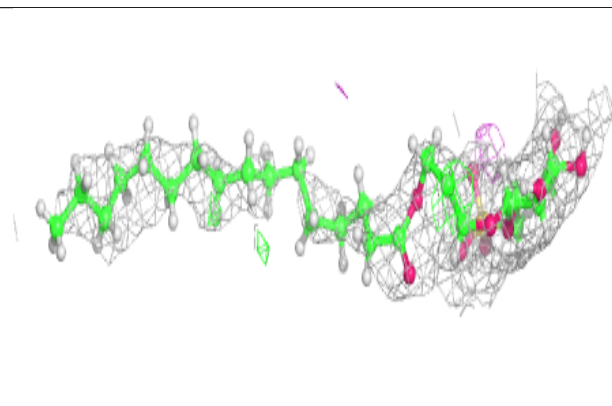
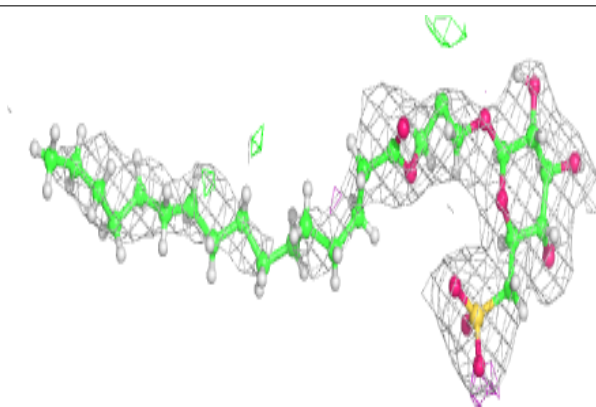


Electron density around BCR b 618:

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

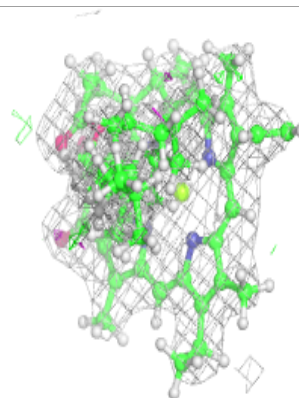
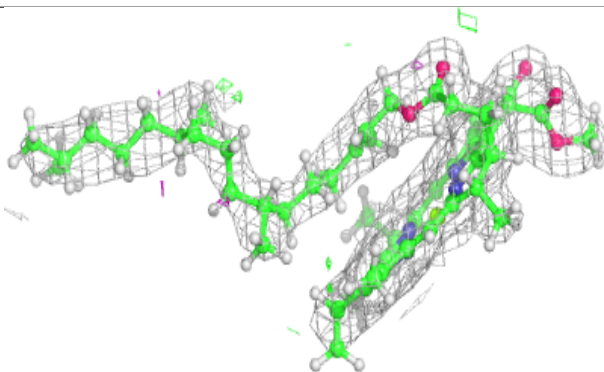
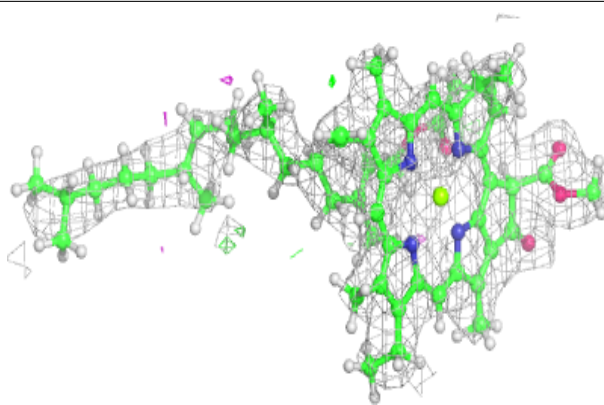
**Electron density around SQD F 101:**

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

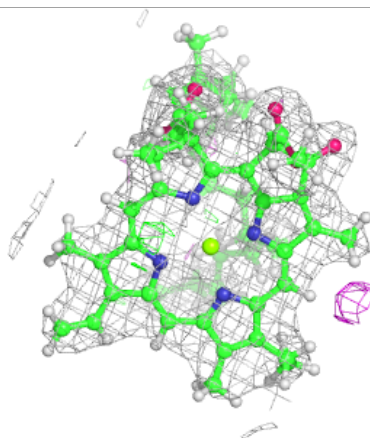
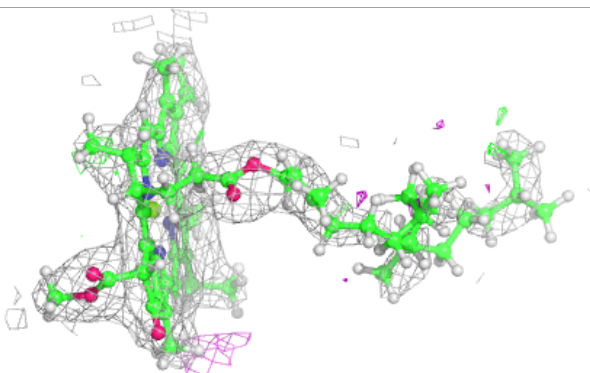
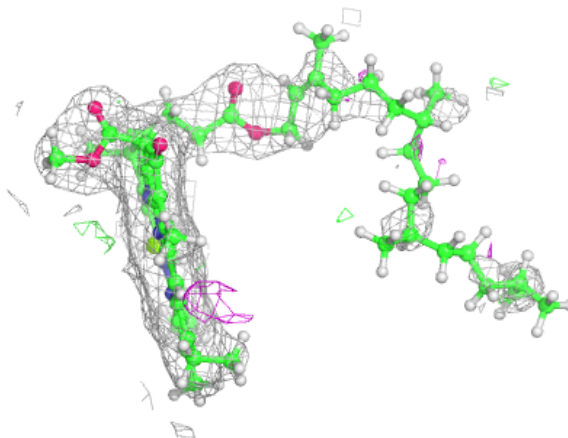


Electron density around CLA c 505:

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

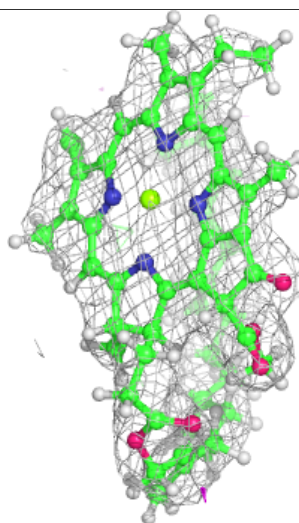
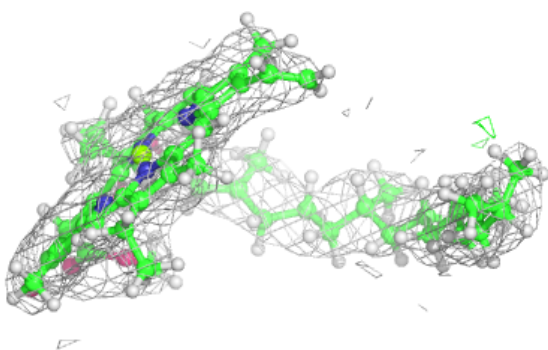
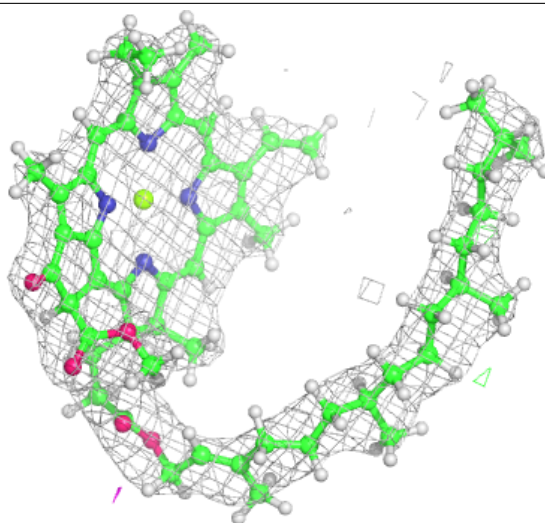
**Electron density around CLA c 506:**

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



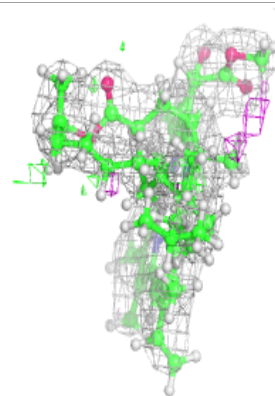
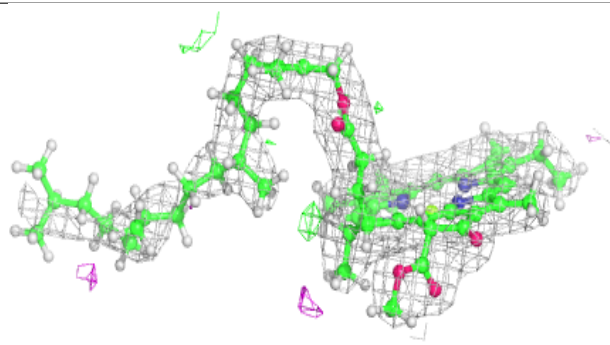
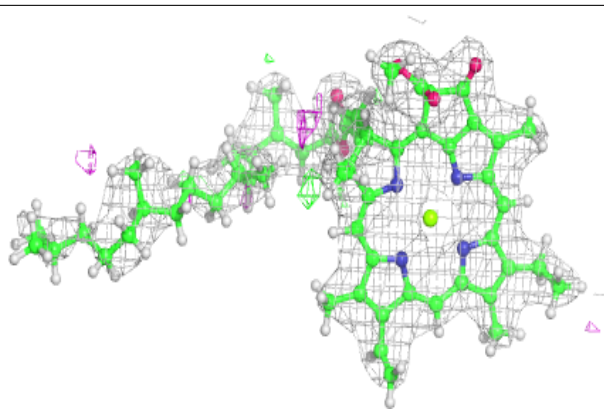
Electron density around CLA c 507:

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

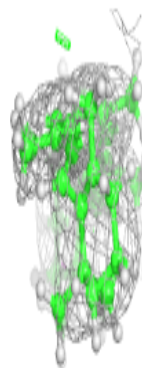
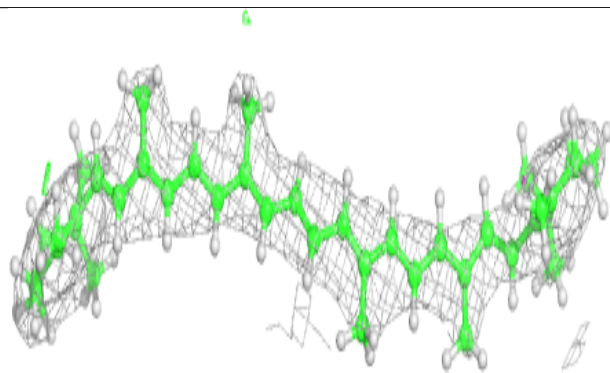
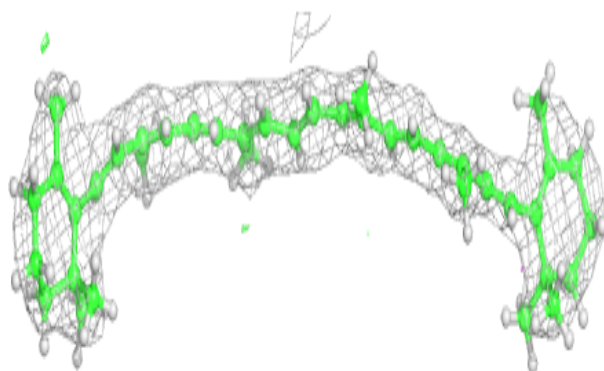


Electron density around CLA a 406:

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

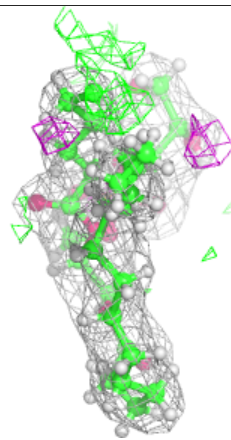
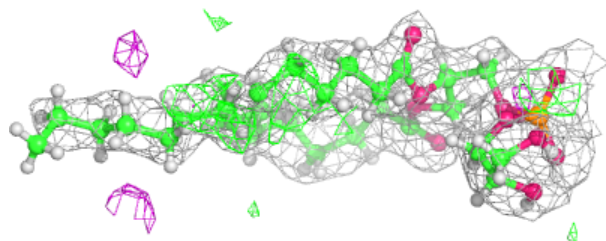
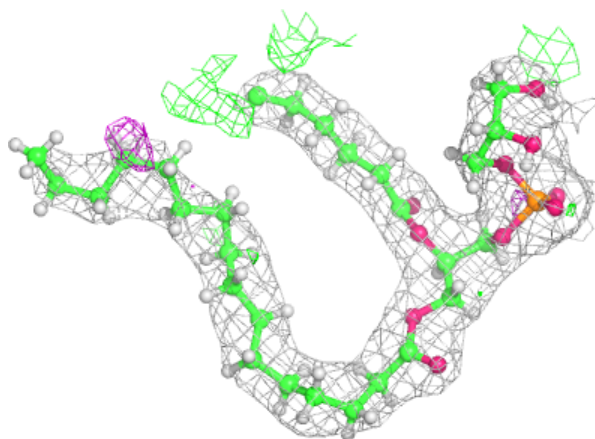
**Electron density around BCR k 102:**

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



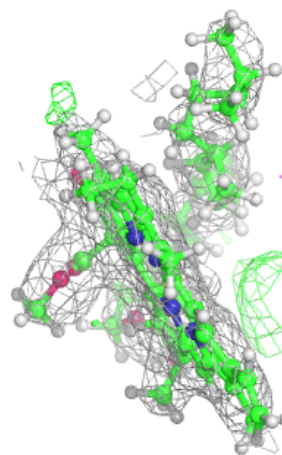
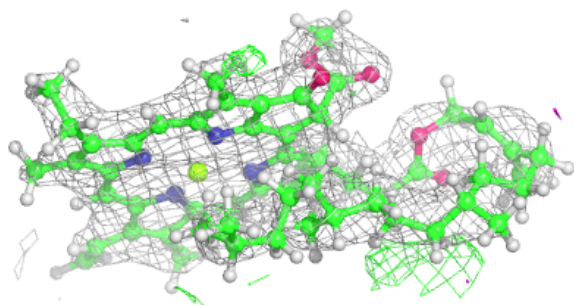
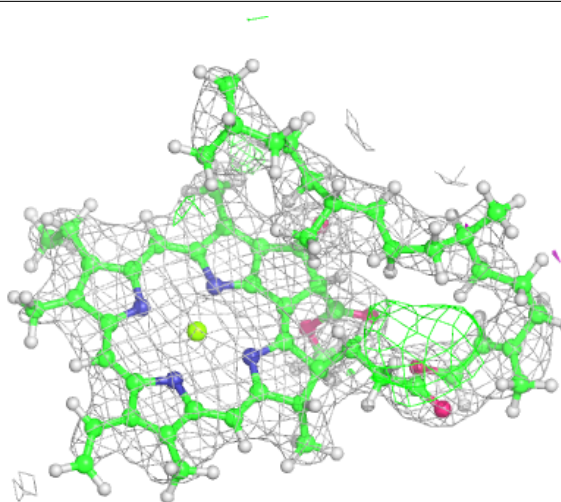
Electron density around LHG d 408:

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



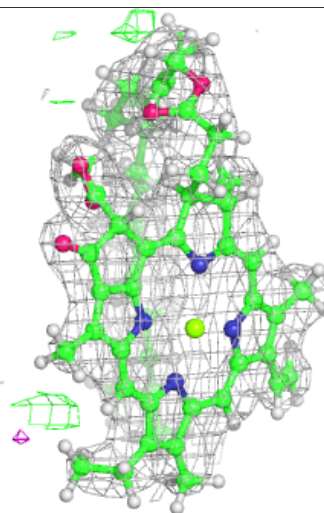
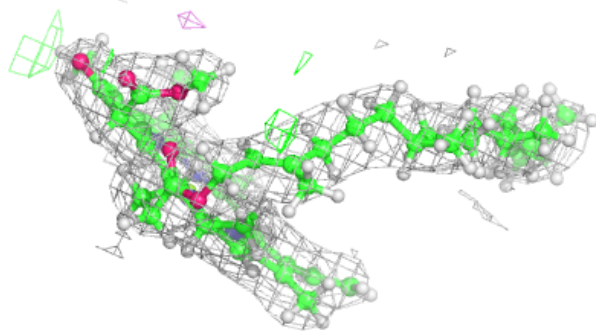
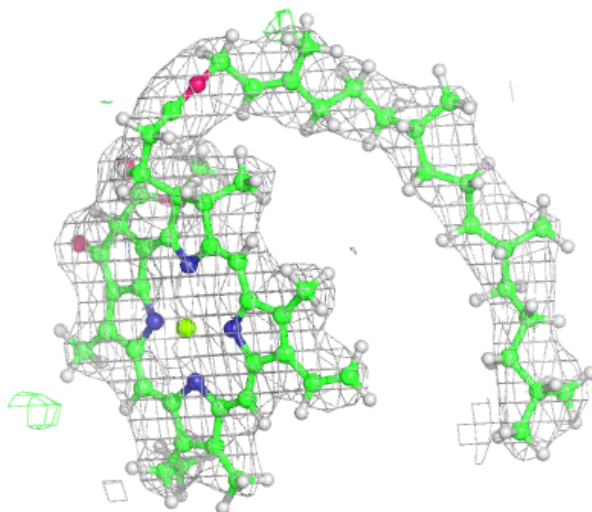
Electron density around CLA c 509:

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



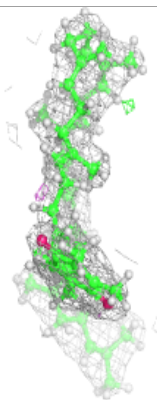
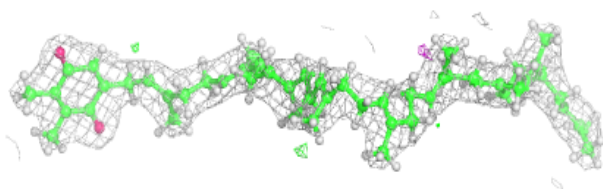
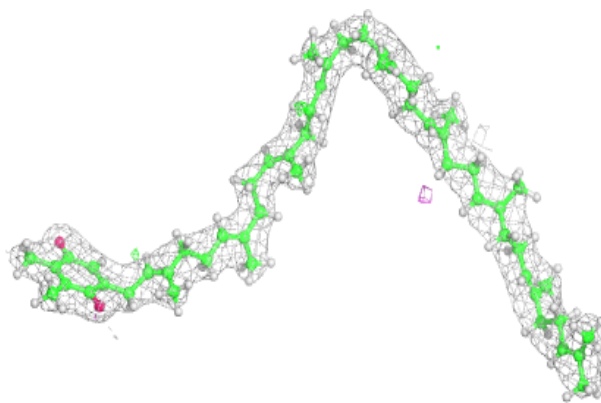
Electron density around CLA C 507:

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



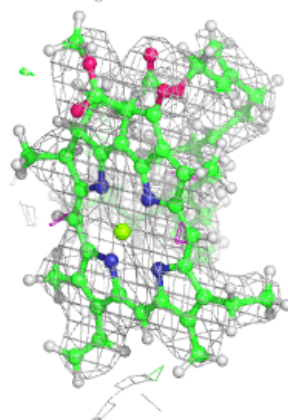
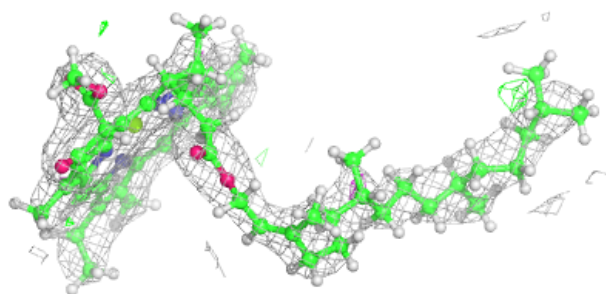
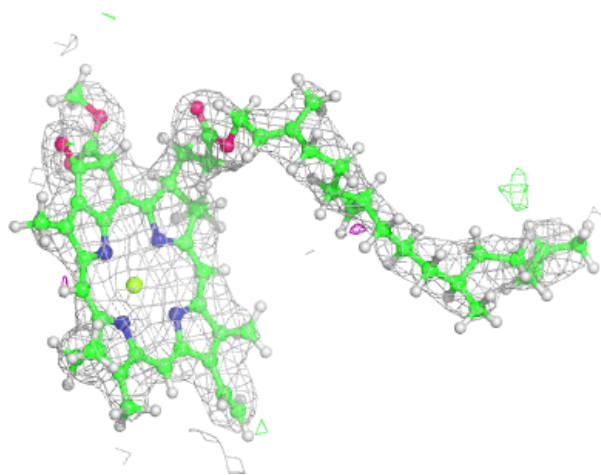
Electron density around PL9 D 405:

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



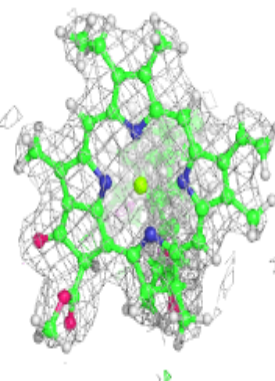
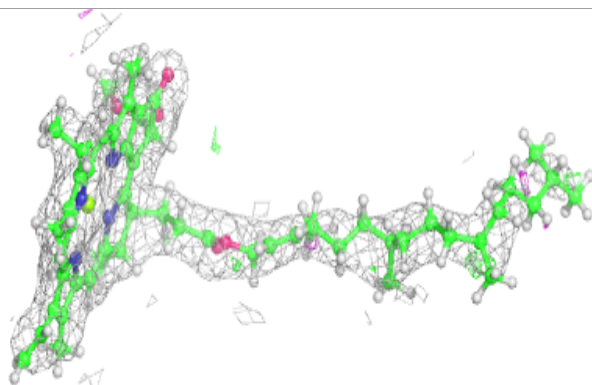
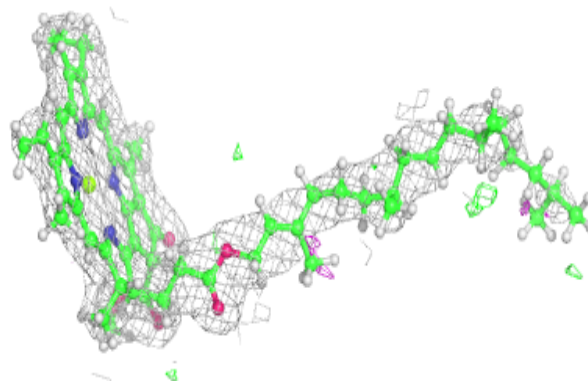
Electron density around CLA c 511:

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

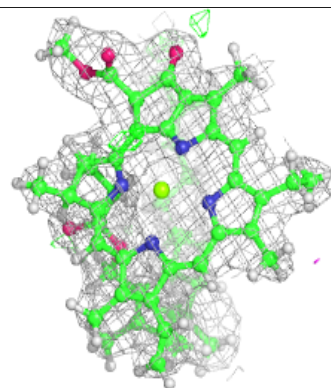
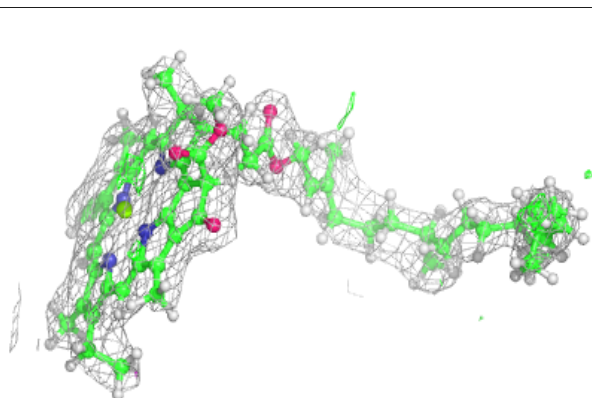
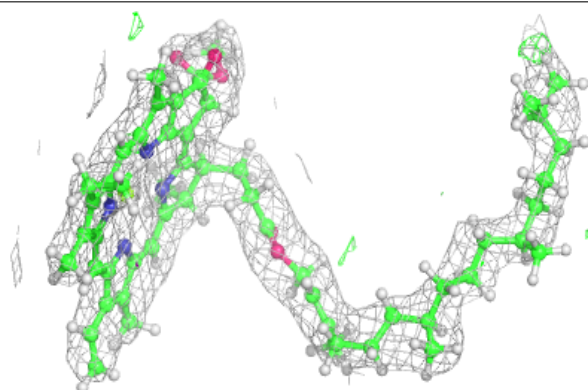


Electron density around CLA b 605:

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

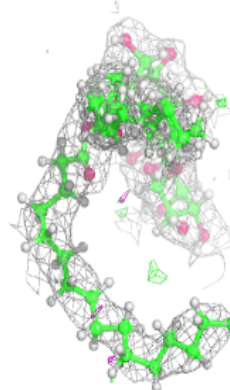
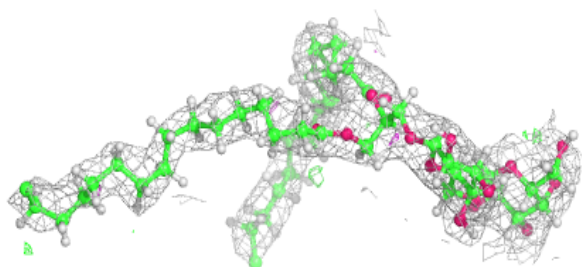
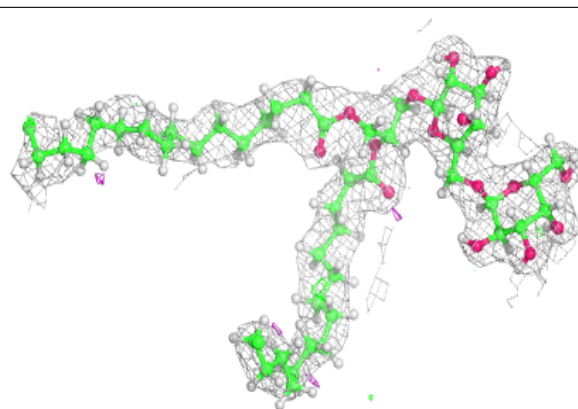
**Electron density around CLA b 607:**

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

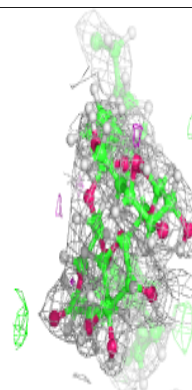
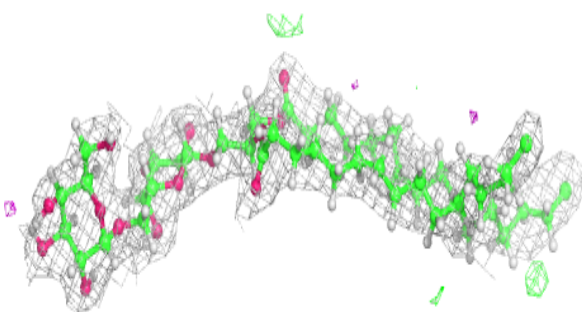
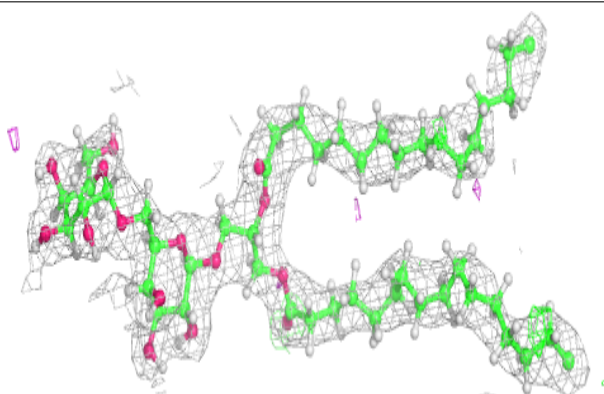


Electron density around DGD c 517:

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

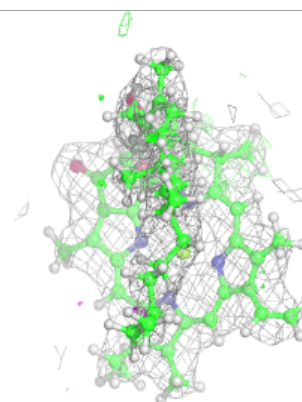
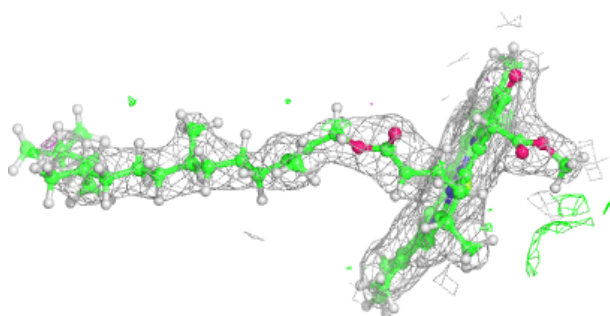
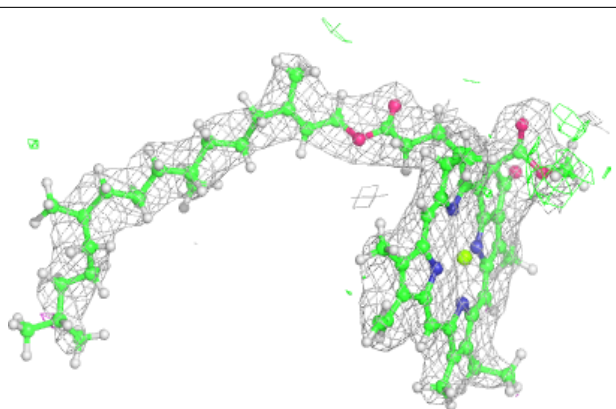
**Electron density around DGD c 518:**

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

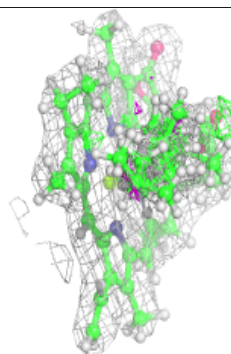
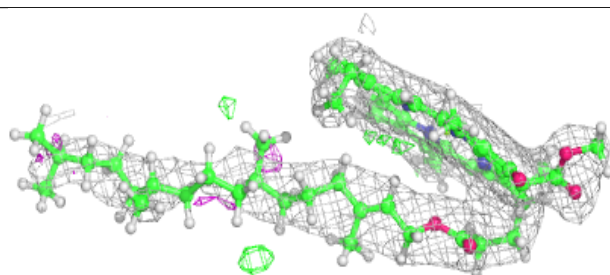
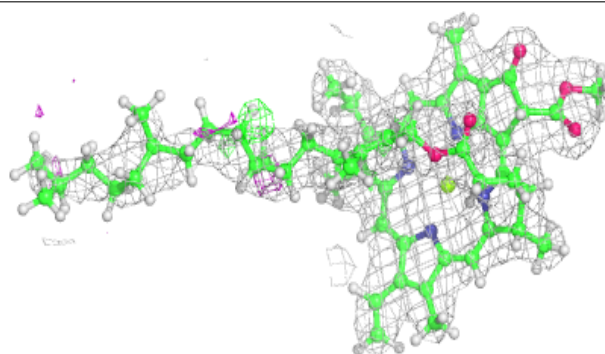


Electron density around CLA b 610:

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

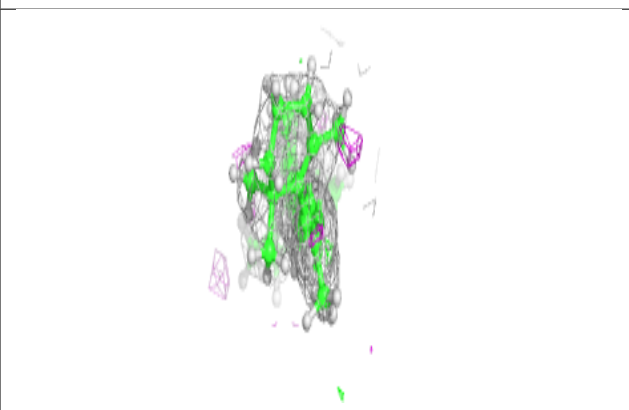
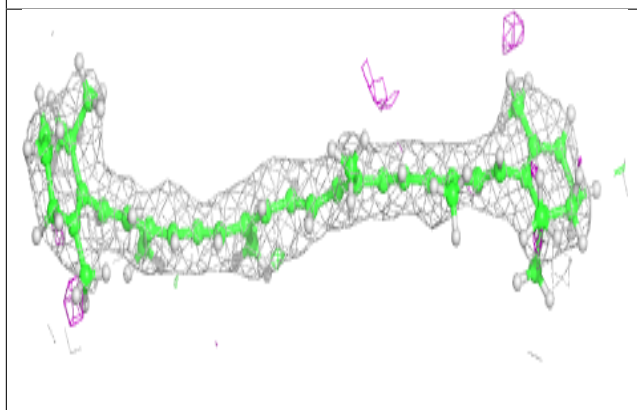
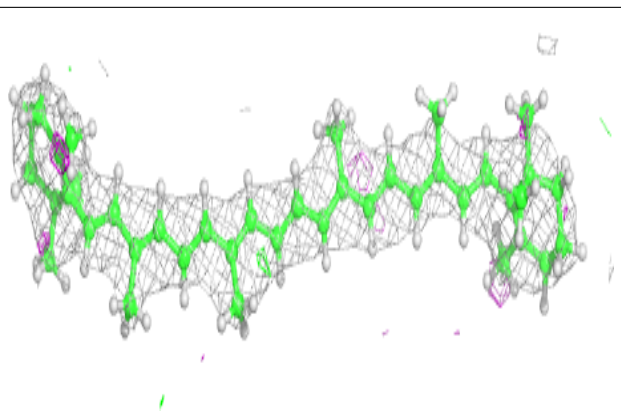
**Electron density around CLA b 615:**

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



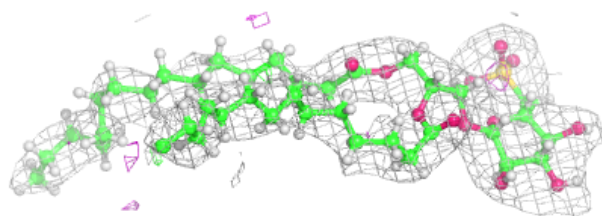
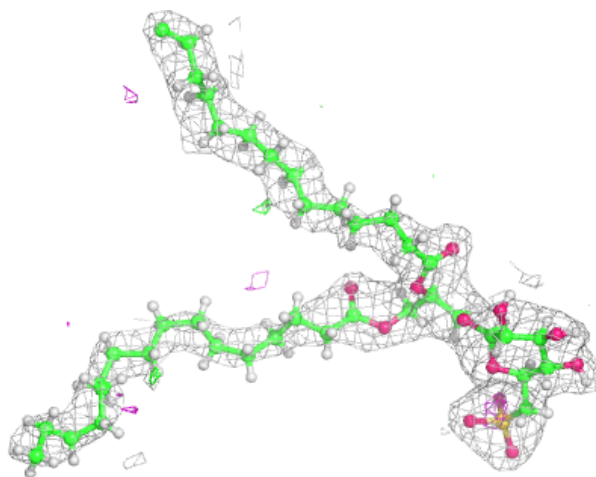
Electron density around BCR c 515:

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



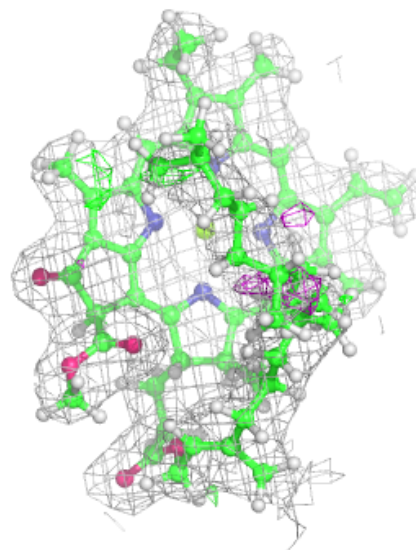
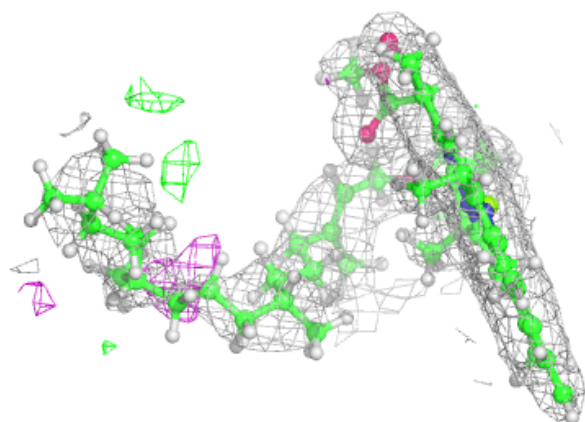
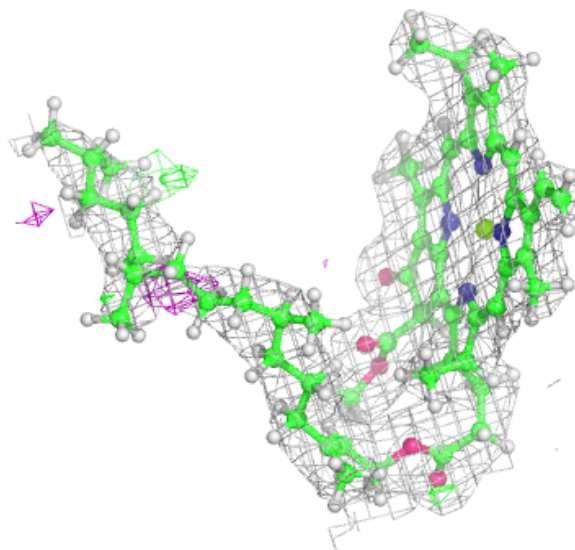
Electron density around SQD A 412:

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



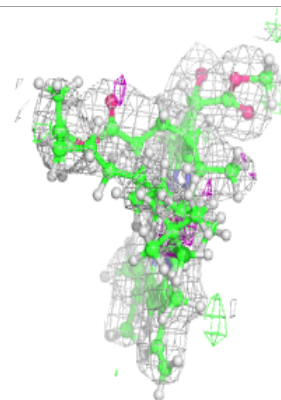
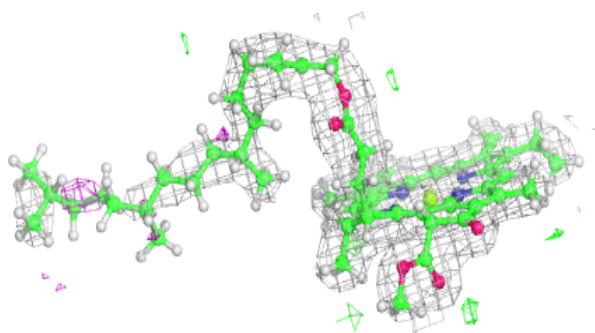
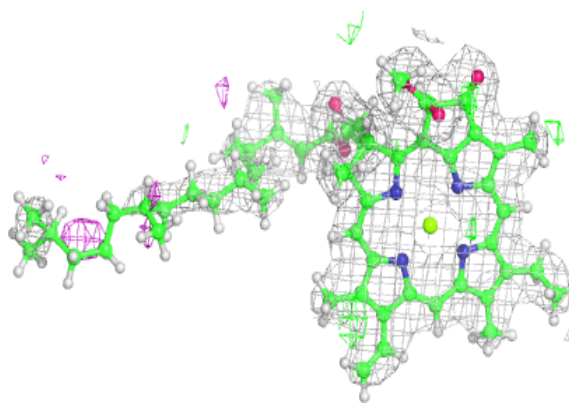
Electron density around CLA b 614:

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

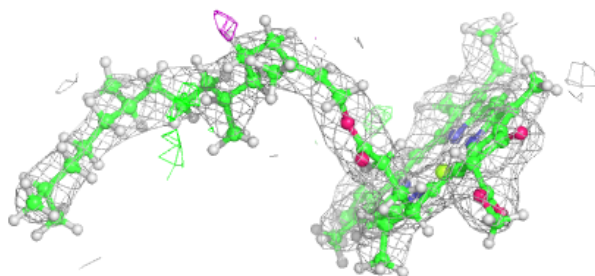
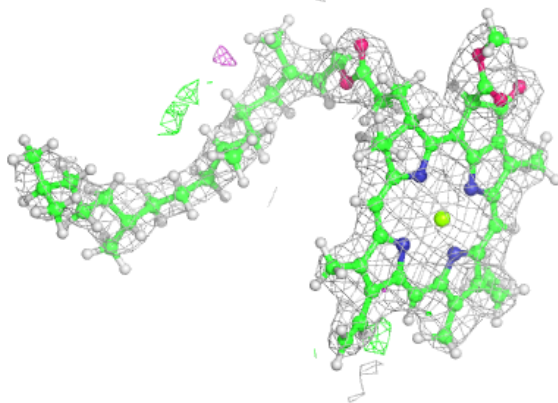


Electron density around CLA A 405:

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

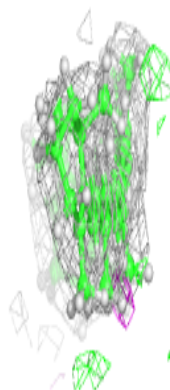
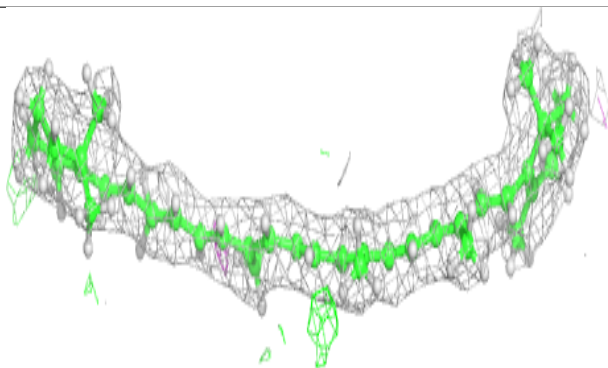
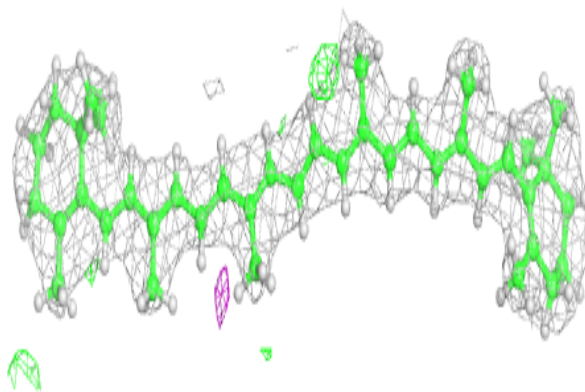
**Electron density around CLA C 511:**

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



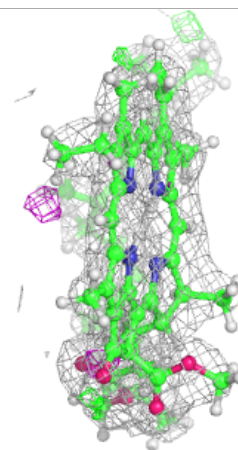
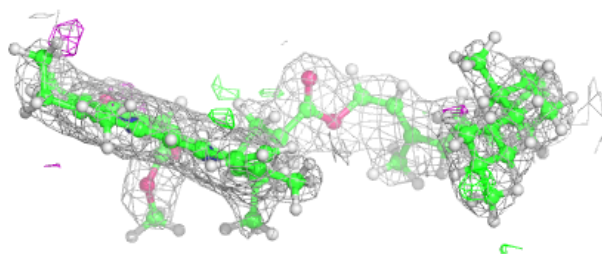
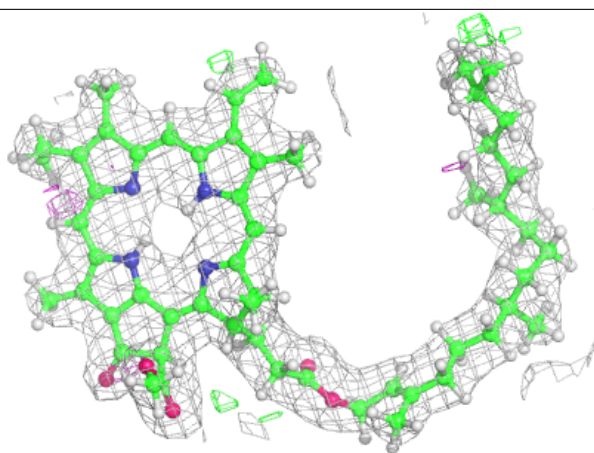
Electron density around BCR t 101:

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



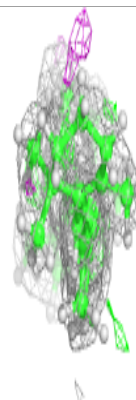
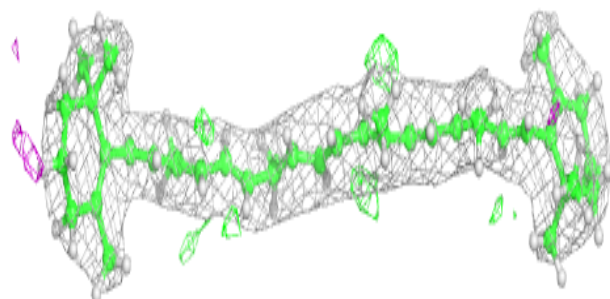
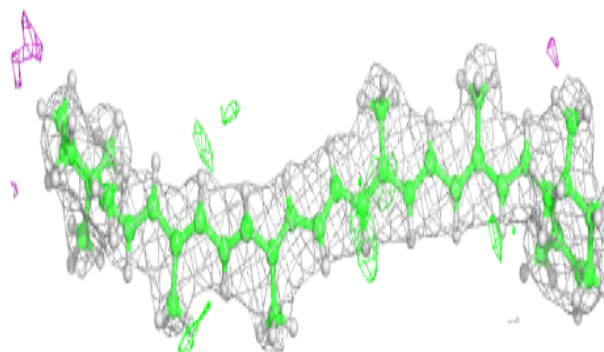
Electron density around PHO a 407:

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

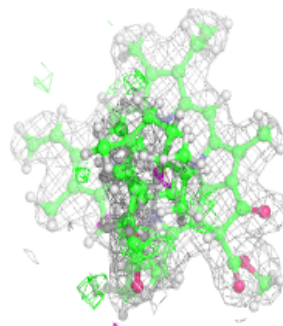
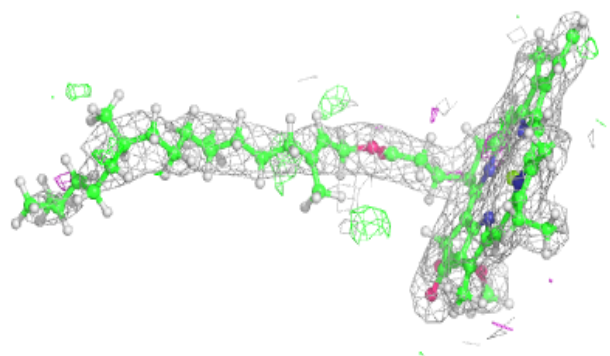
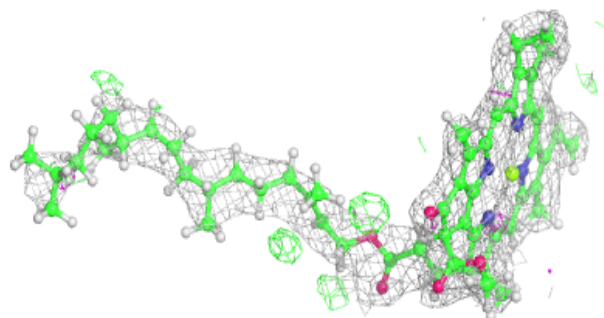


Electron density around BCR A 409:

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

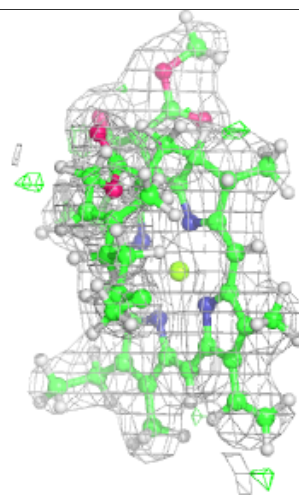
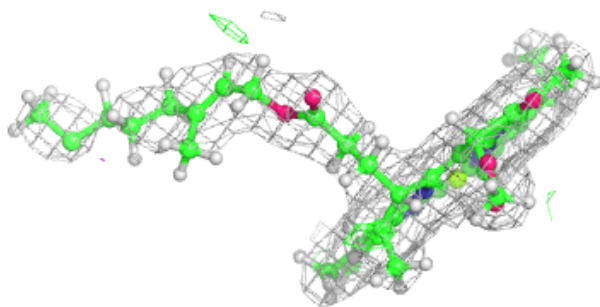
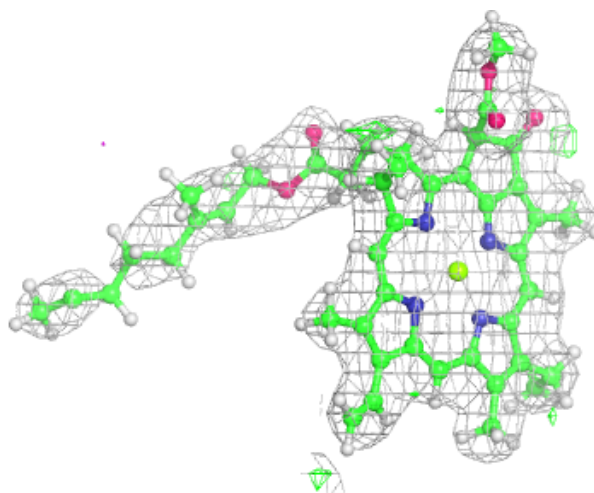
**Electron density around CLA B 604:**

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



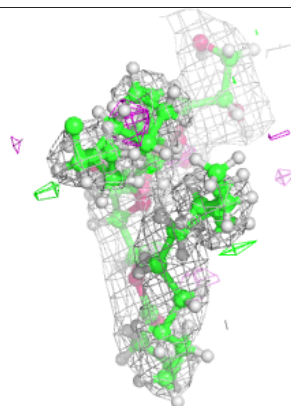
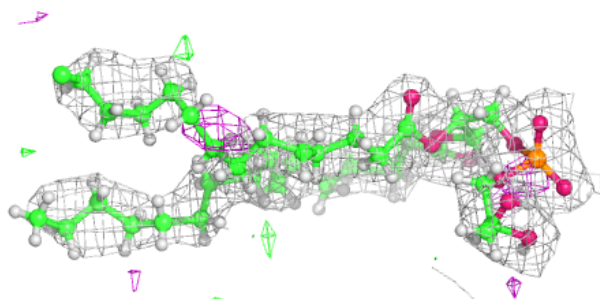
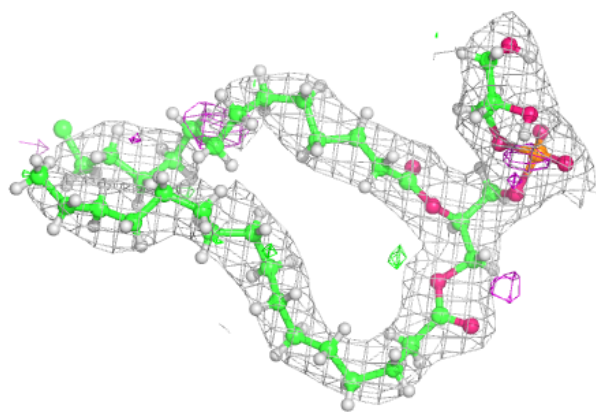
Electron density around CLA A 408:

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

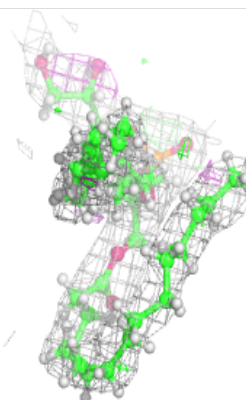
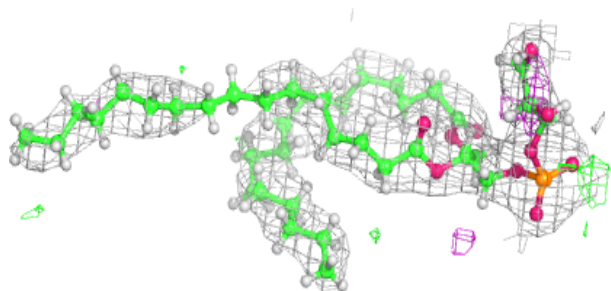
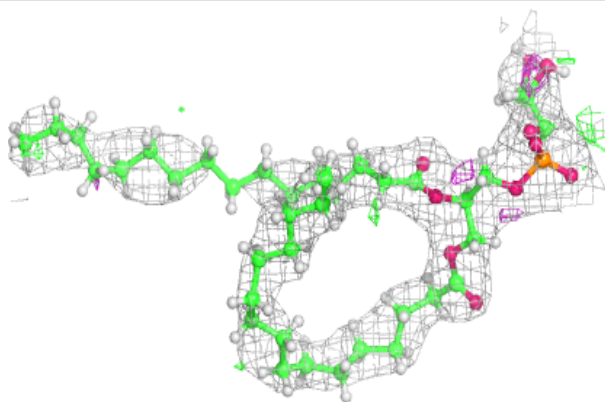


Electron density around LHG D 408:

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

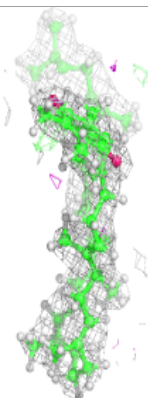
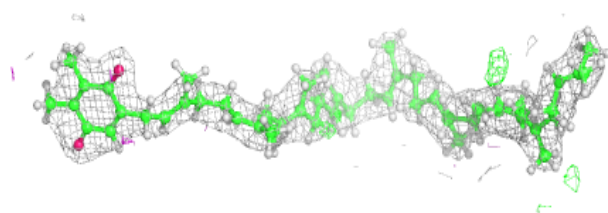
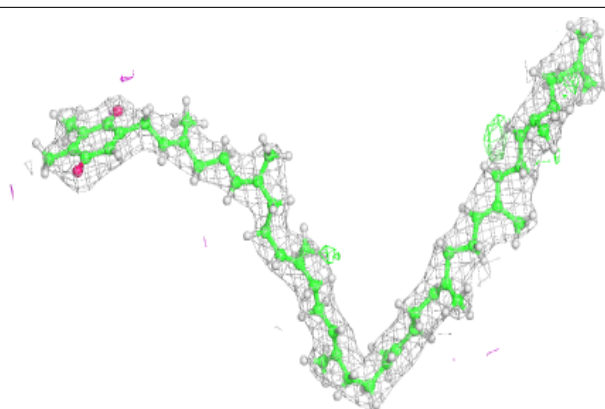
**Electron density around LHG d 406:**

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

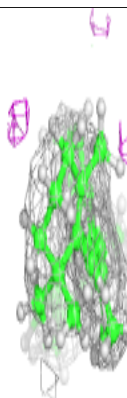
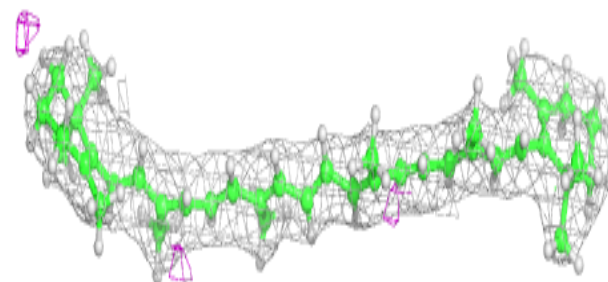
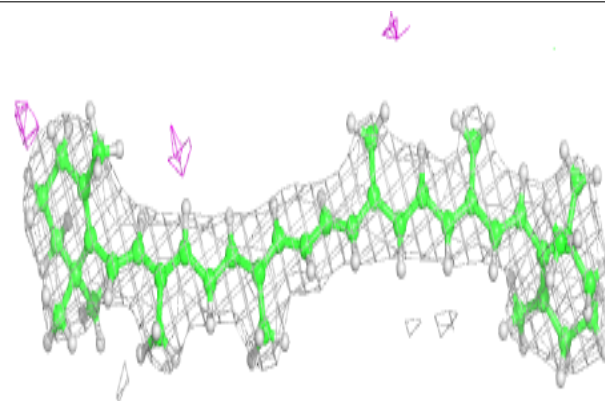


Electron density around PL9 d 405:

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

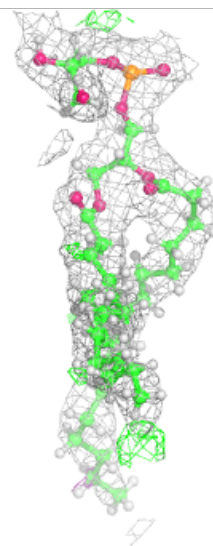
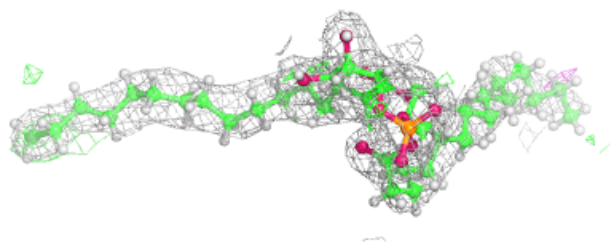
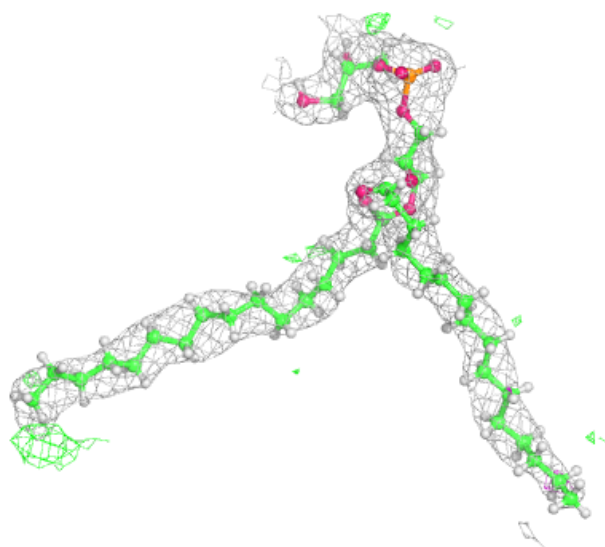
**Electron density around BCR B 619:**

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



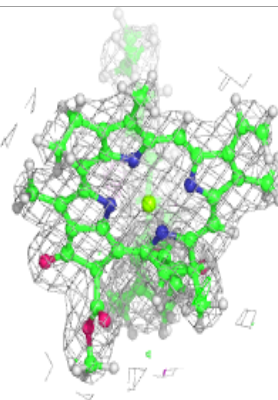
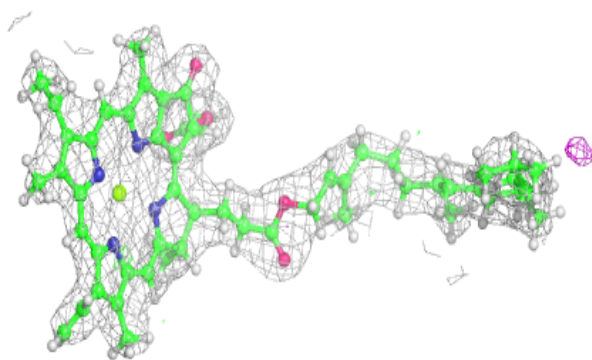
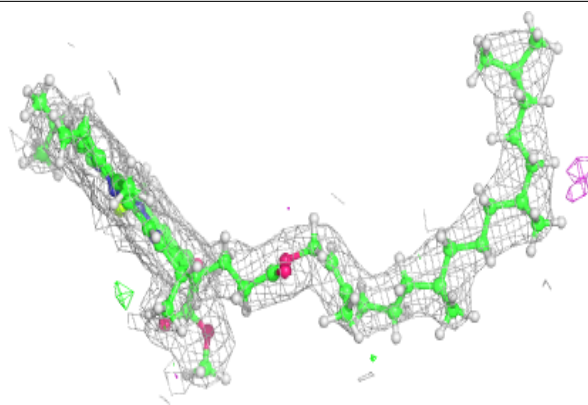
Electron density around LHG 1 101:

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

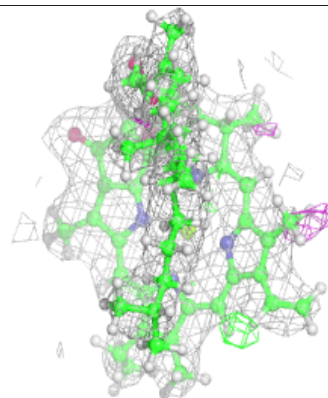
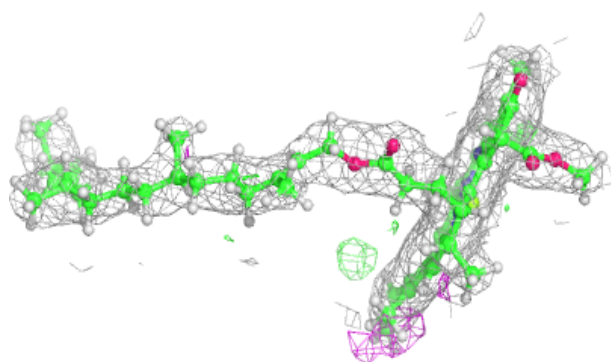
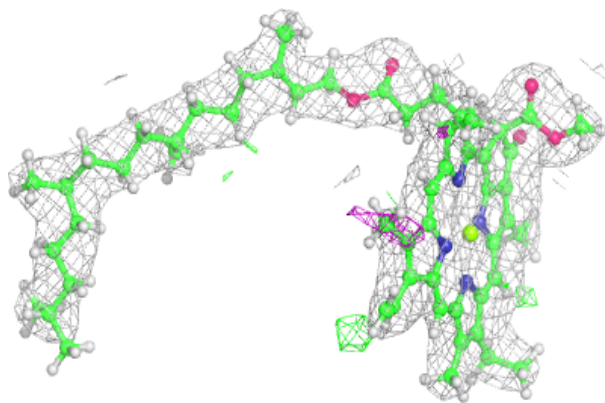


Electron density around CLA D 402:

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

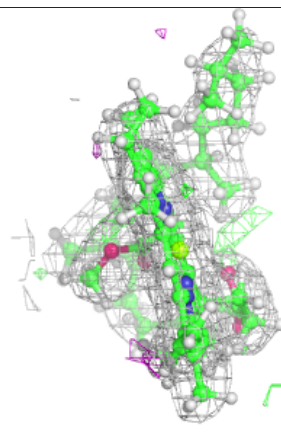
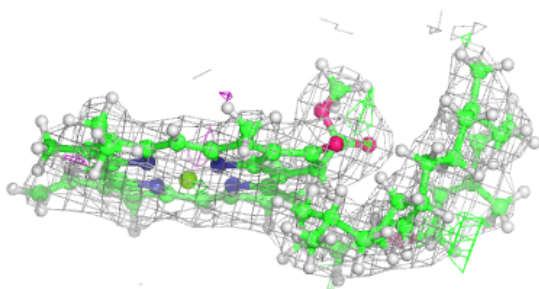
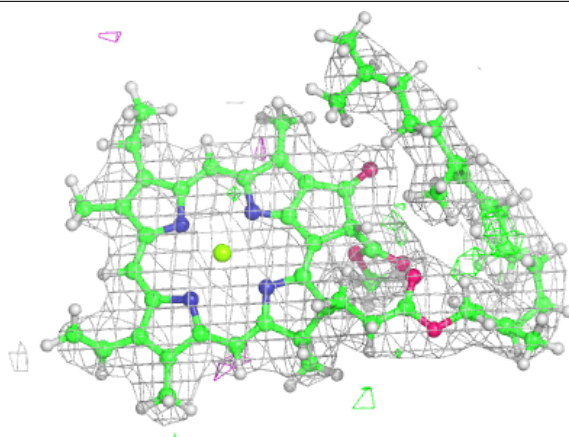
**Electron density around CLA B 609:**

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

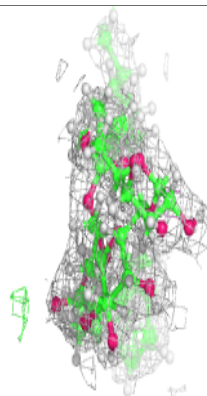
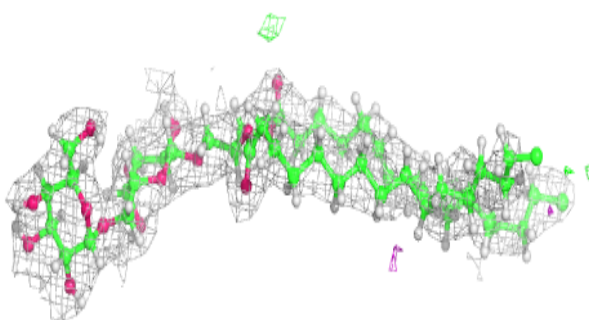
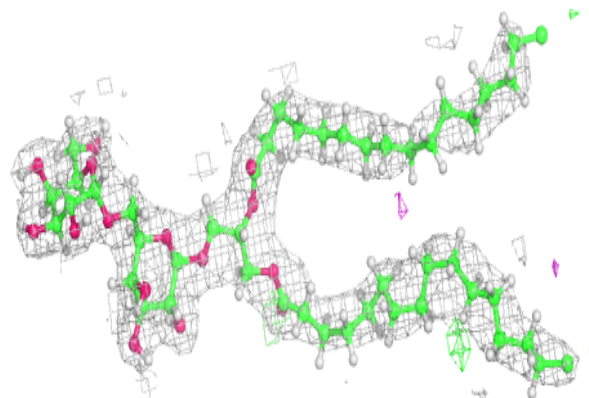


Electron density around CLA B 610:

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

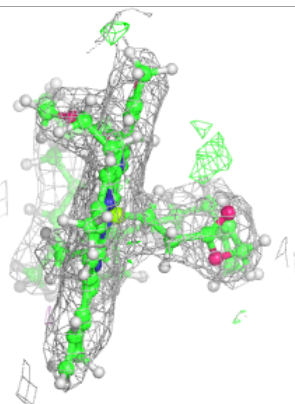
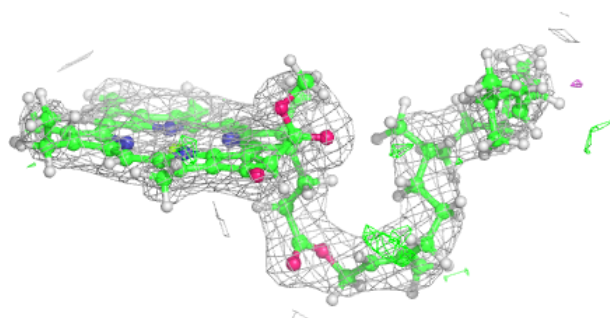
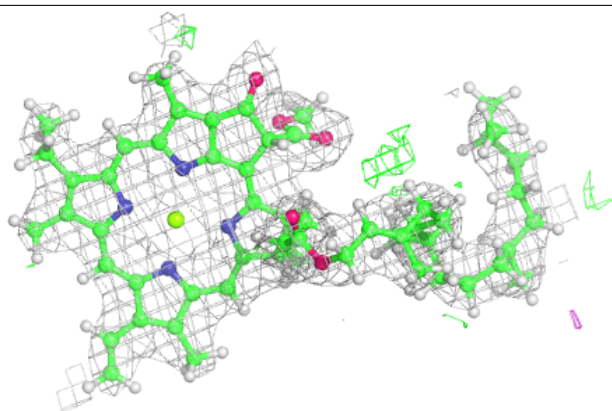
**Electron density around DGD C 517:**

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

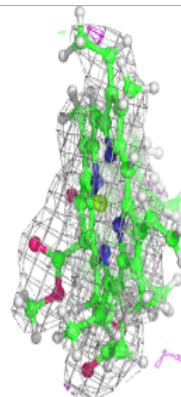
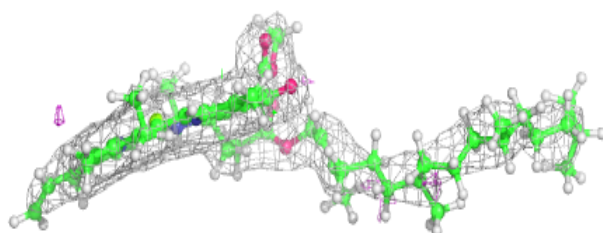
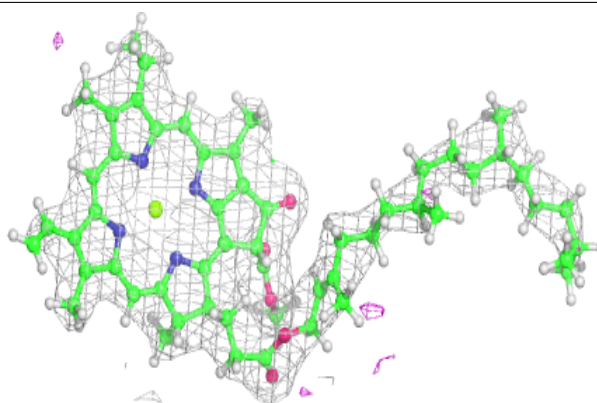


Electron density around CLA B 612:

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

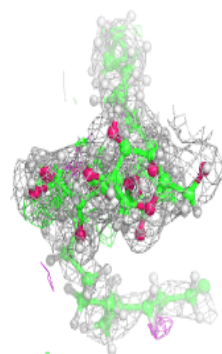
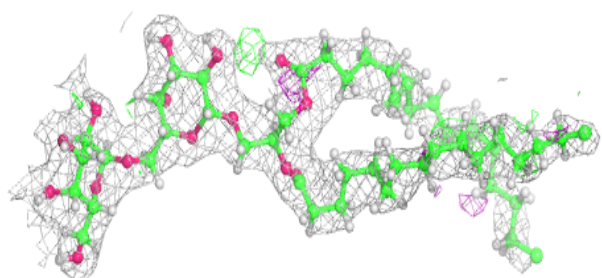
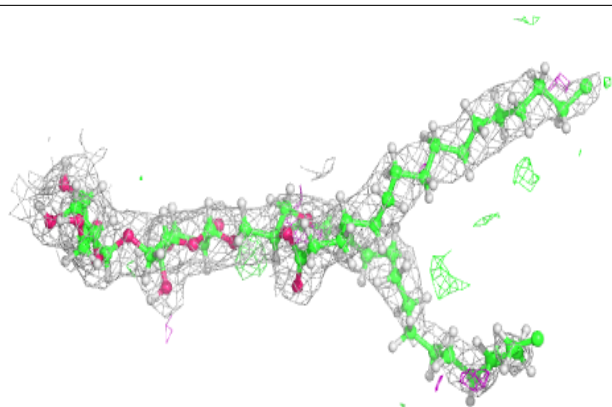
**Electron density around CLA b 603:**

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

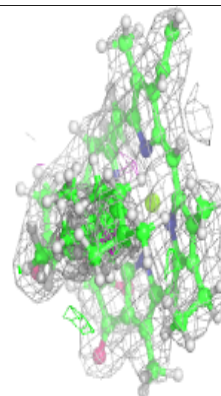
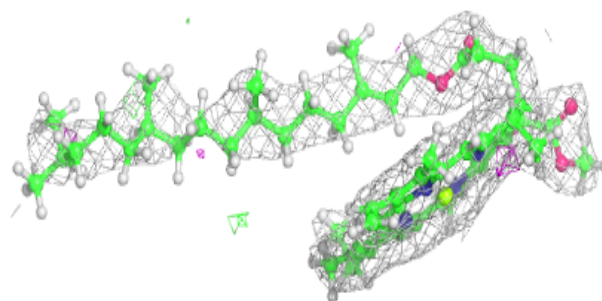
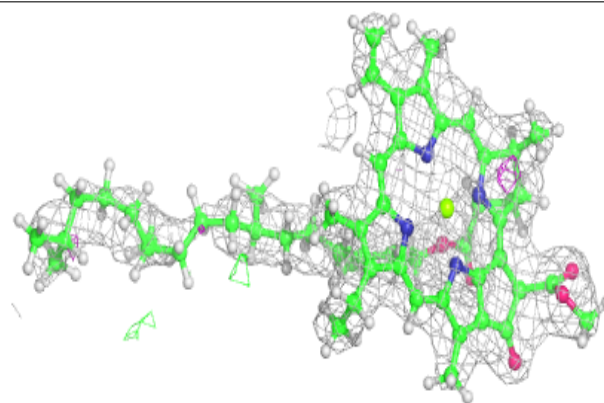


Electron density around DGD c 516:

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

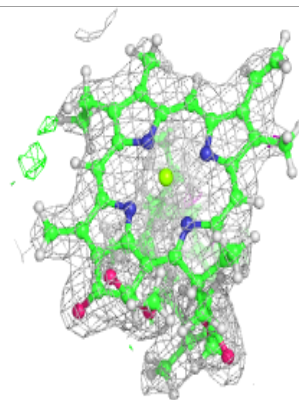
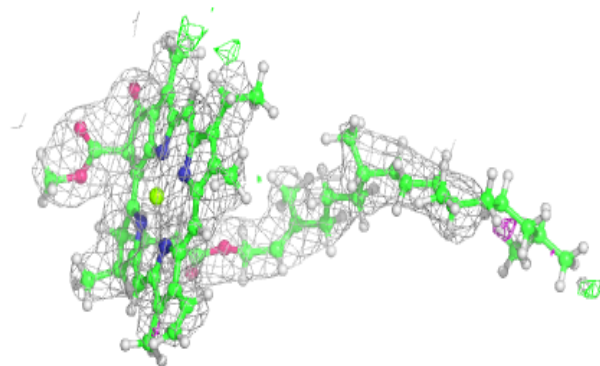
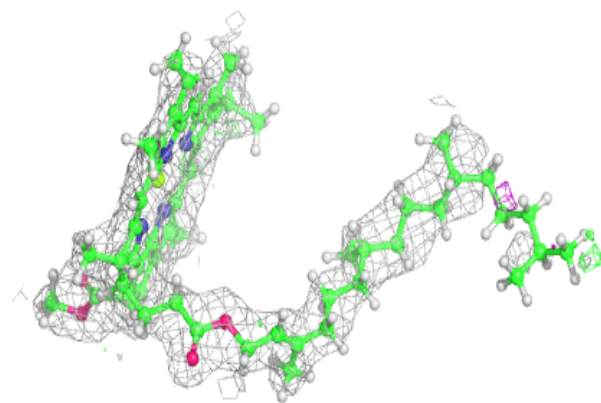
**Electron density around CLA B 614:**

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



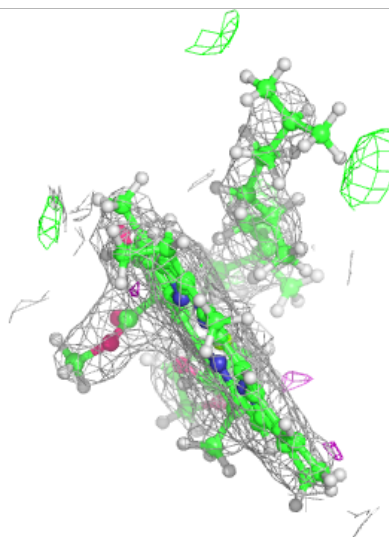
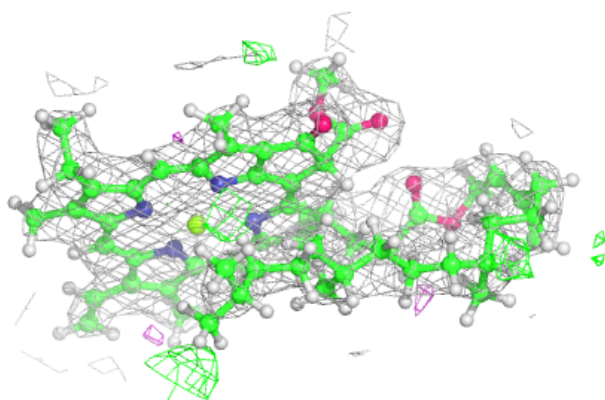
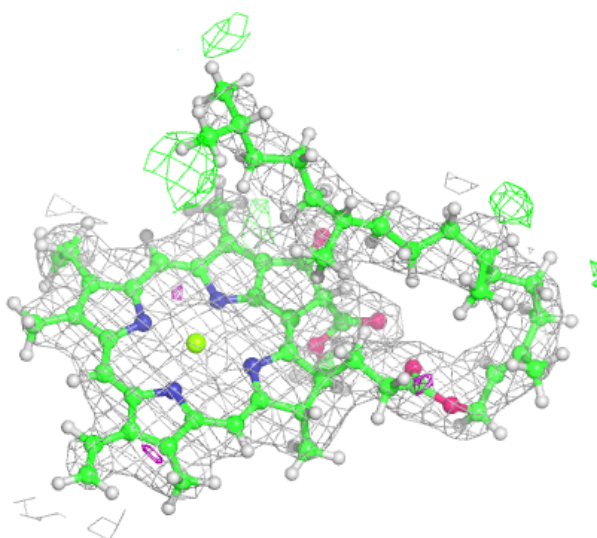
Electron density around CLA C 508:

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



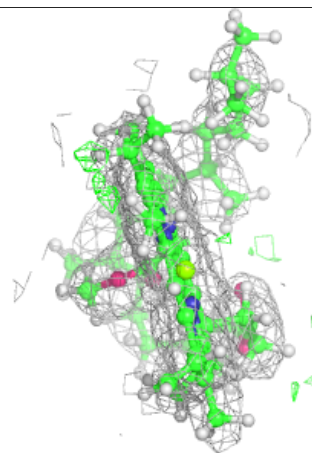
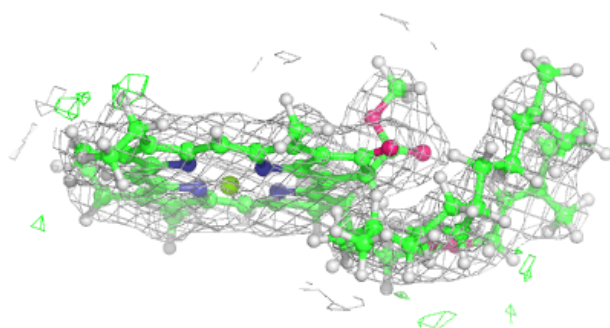
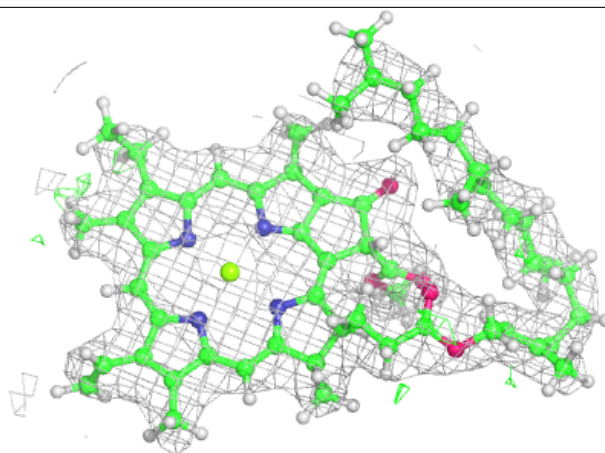
Electron density around CLA C 509:

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

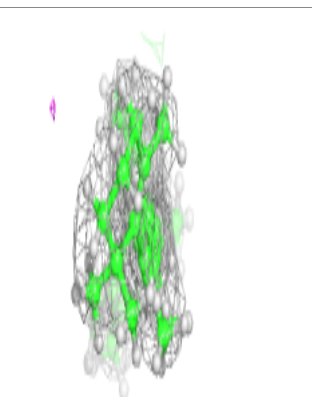
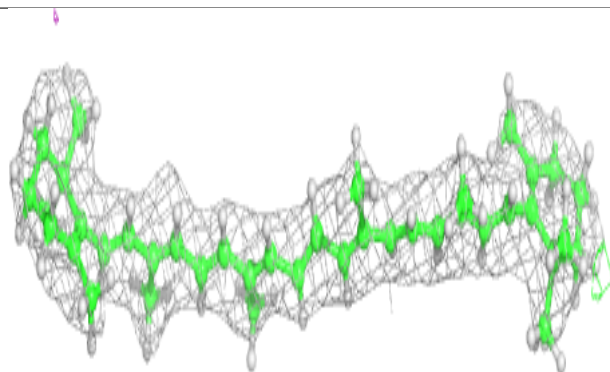
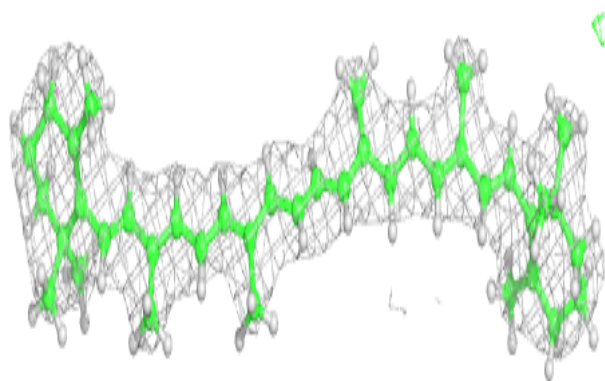


Electron density around CLA b 611:

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

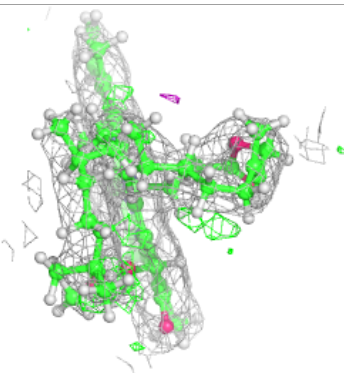
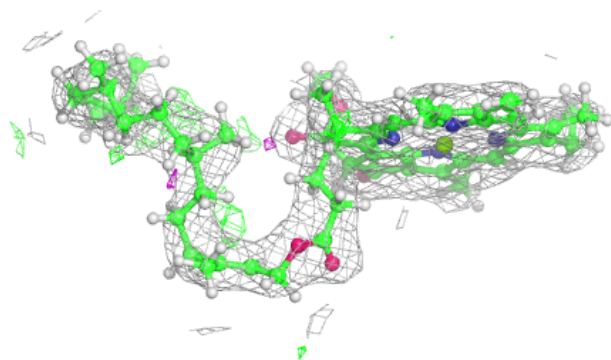
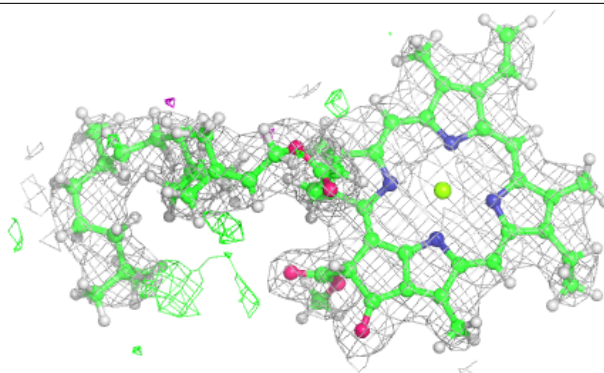
**Electron density around BCR b 620:**

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

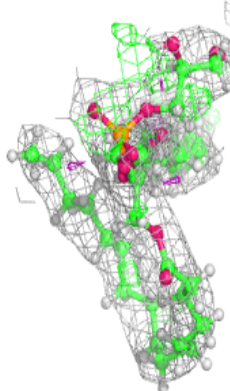
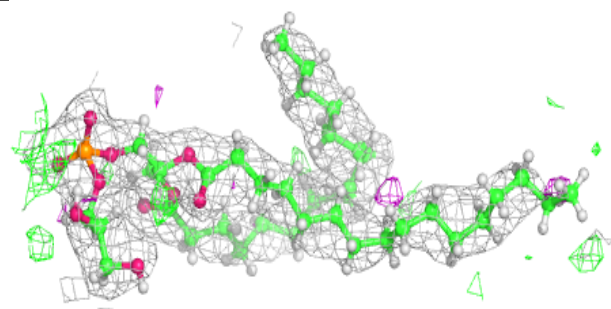
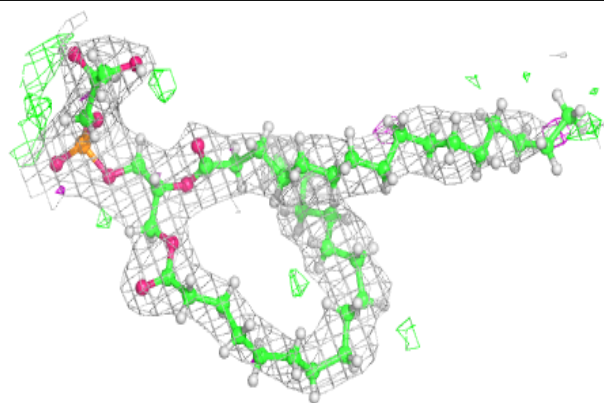


Electron density around CLA b 613:

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

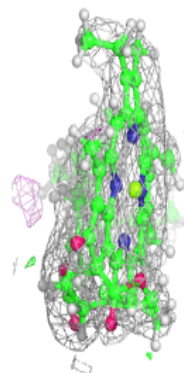
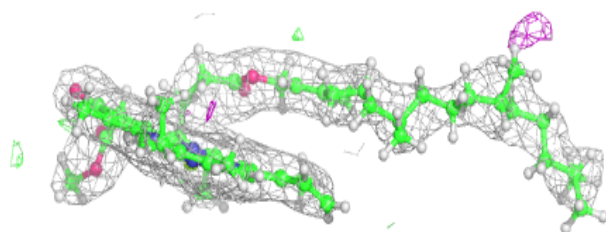
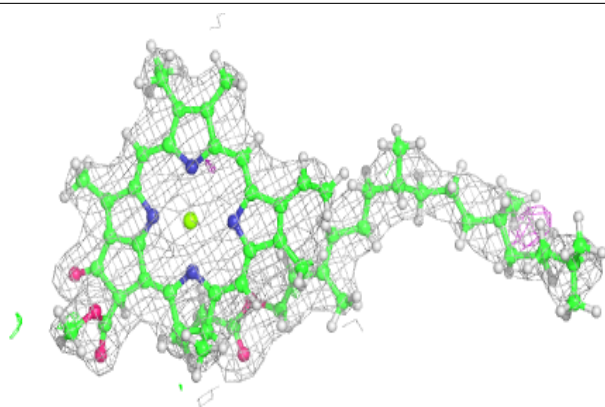
**Electron density around LHG B 623:**

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

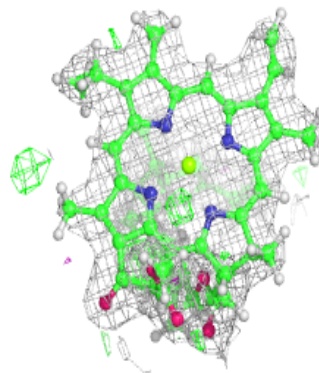
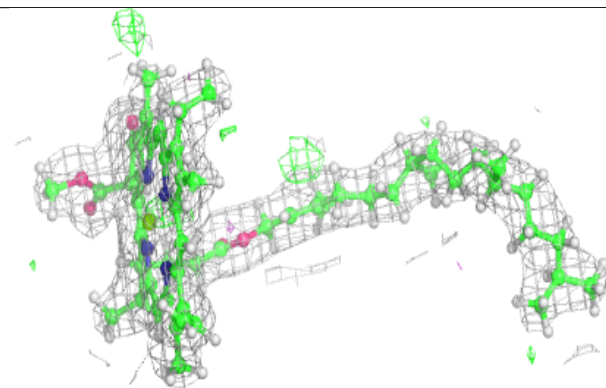
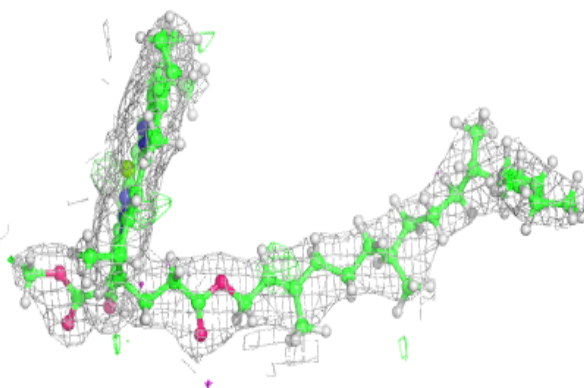


Electron density around CLA b 604:

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

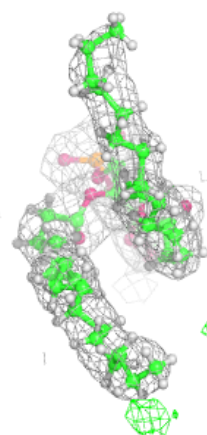
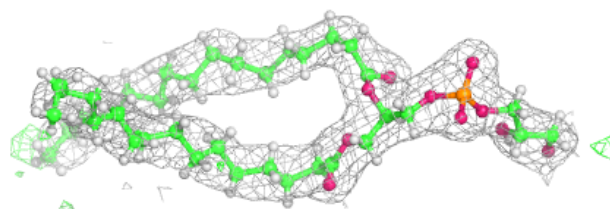
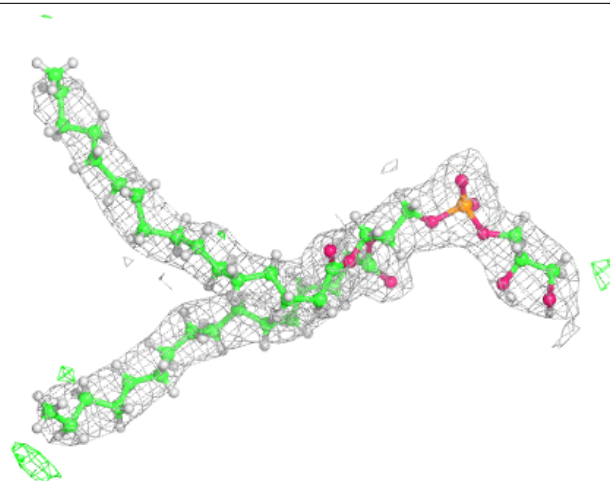
**Electron density around CLA B 605:**

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



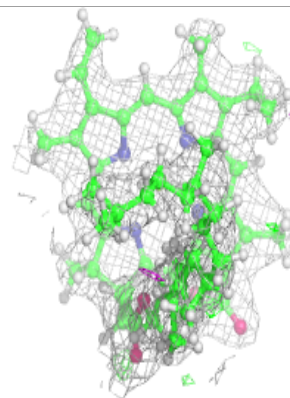
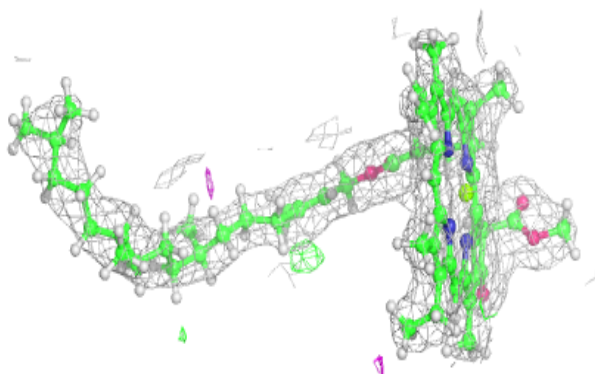
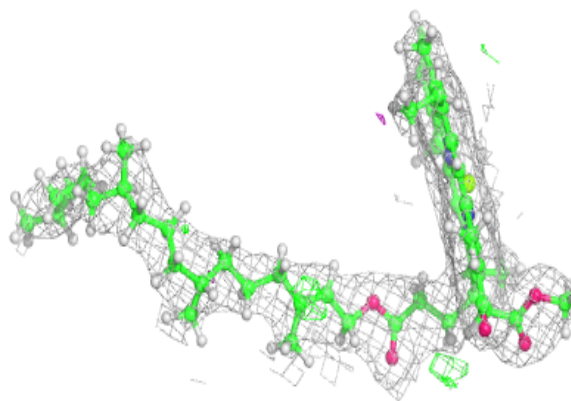
Electron density around LHG d 407:

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

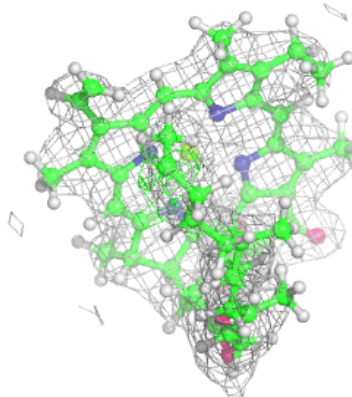
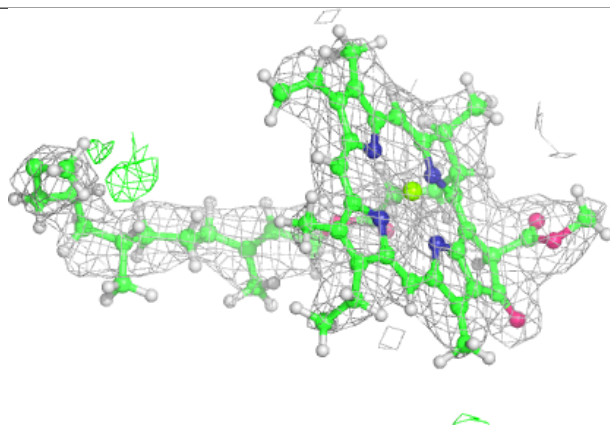
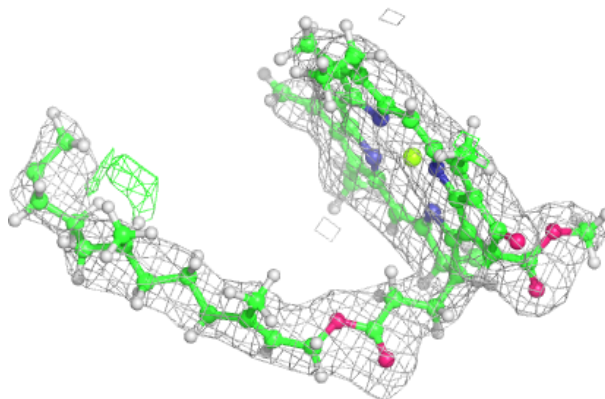


Electron density around CLA b 606:

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

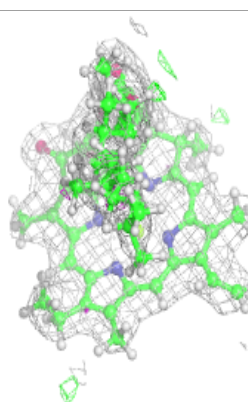
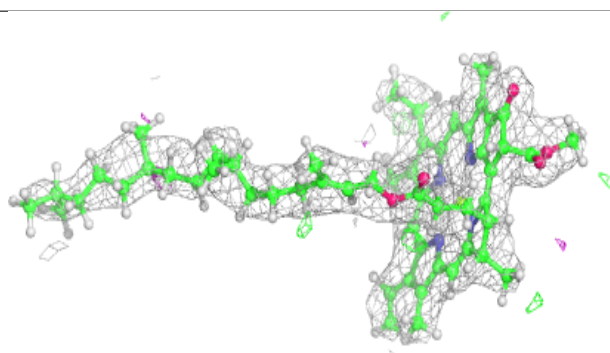
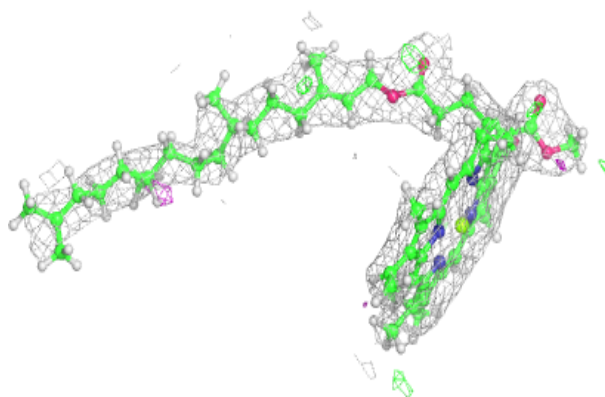
**Electron density around CLA C 504:**

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

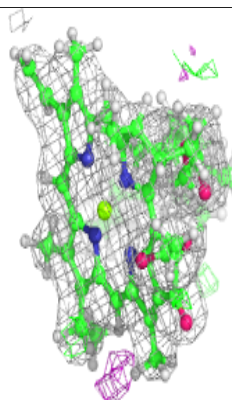
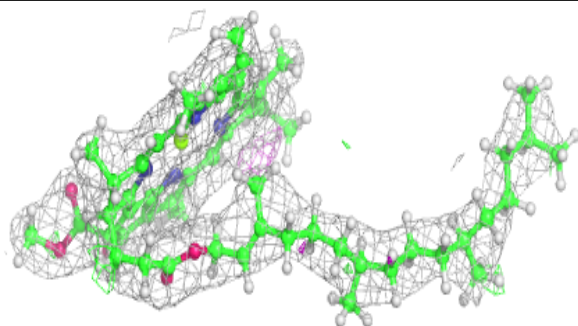
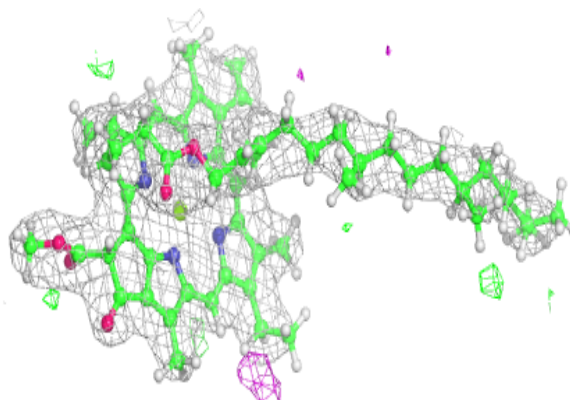


Electron density around CLA b 608:

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

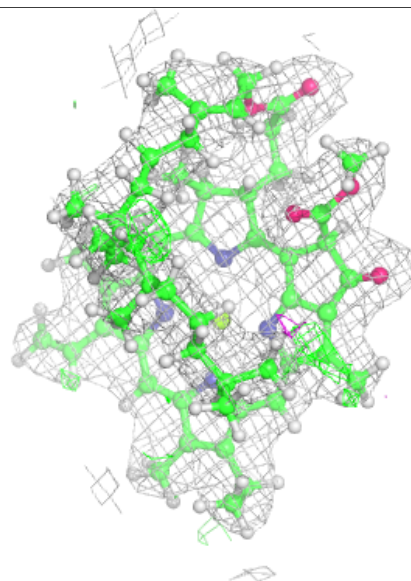
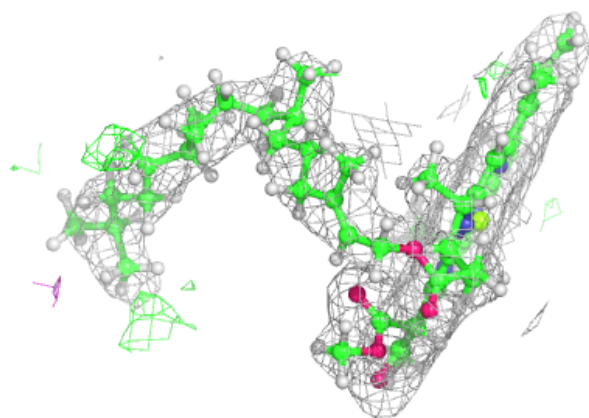
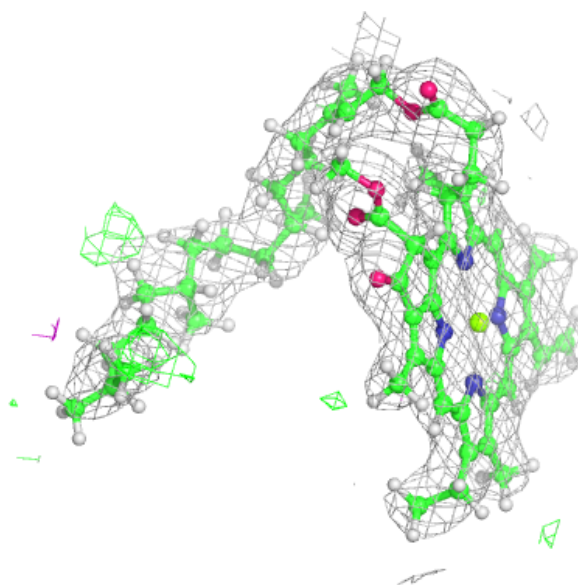
**Electron density around CLA b 609:**

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



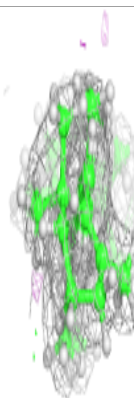
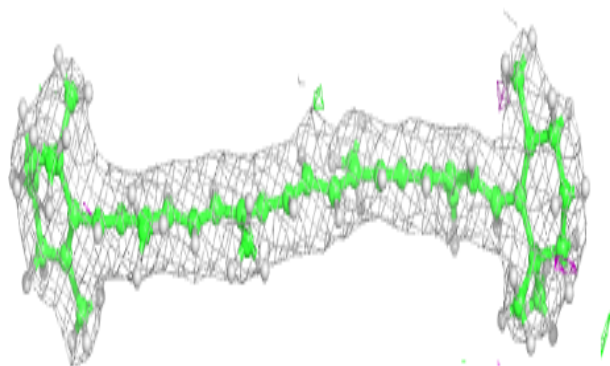
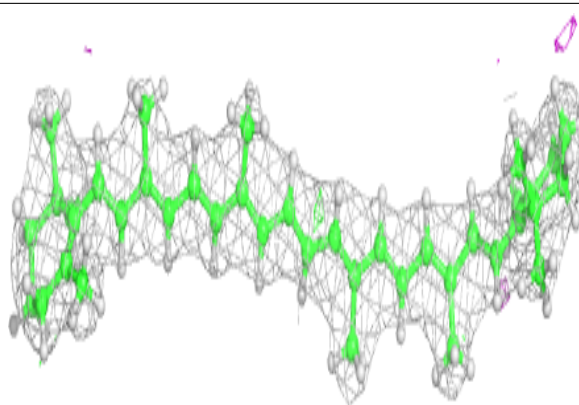
Electron density around CLA B 613:

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

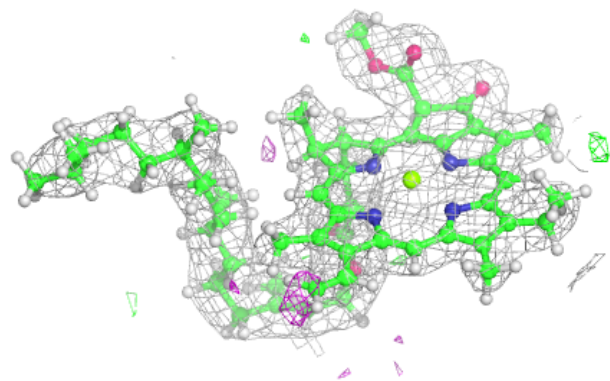
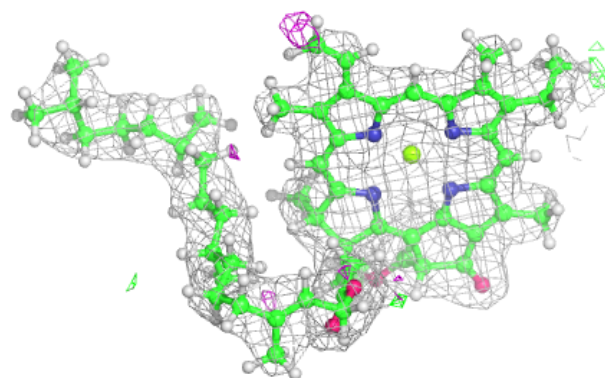


Electron density around BCR a 409:

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

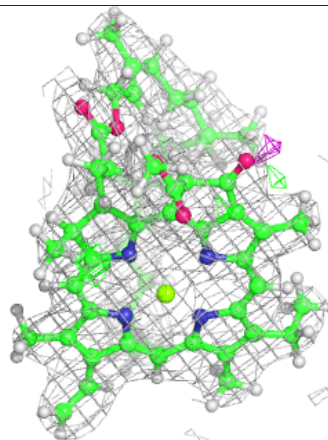
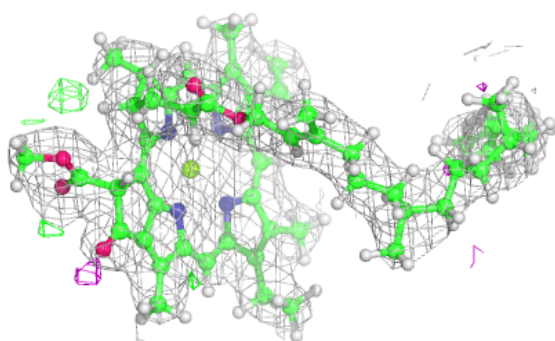
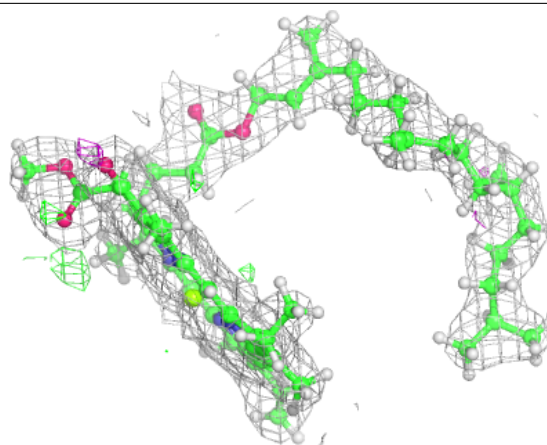
**Electron density around CLA D 401:**

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

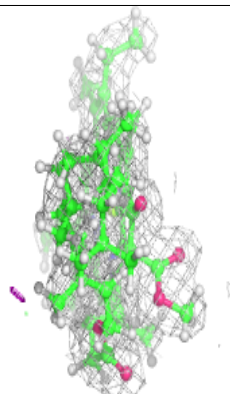
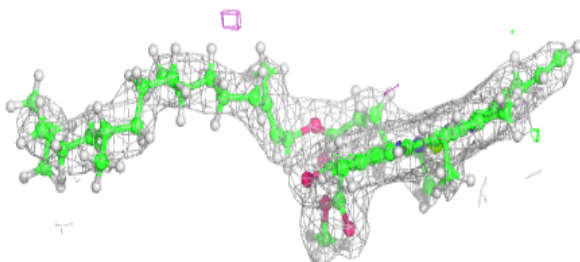
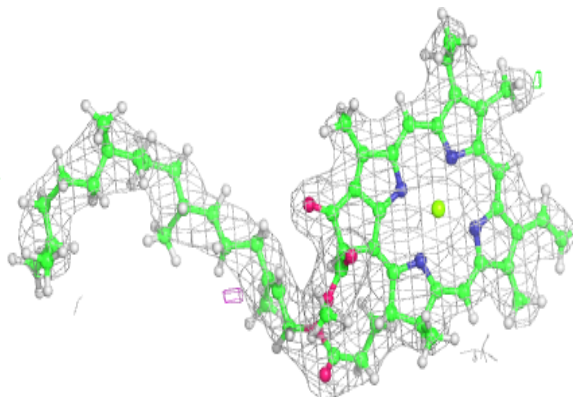


Electron density around CLA b 612:

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

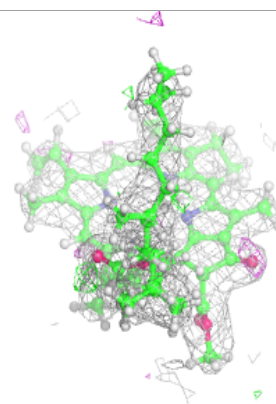
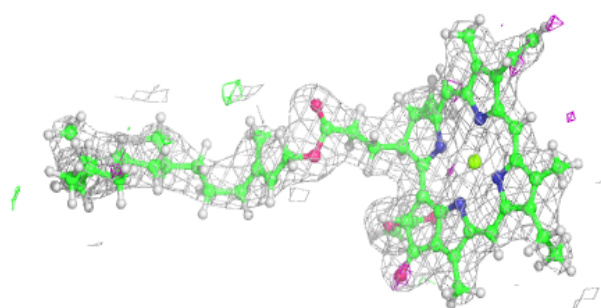
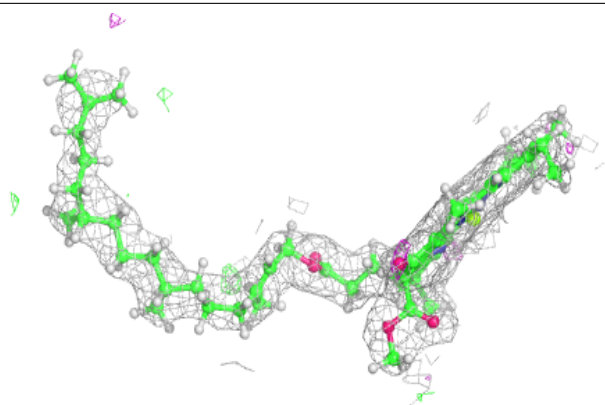
**Electron density around CLA B 602:**

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

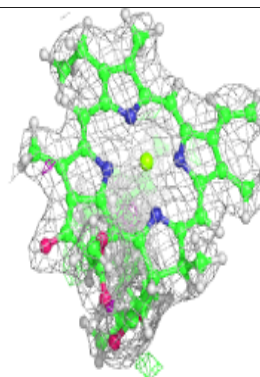
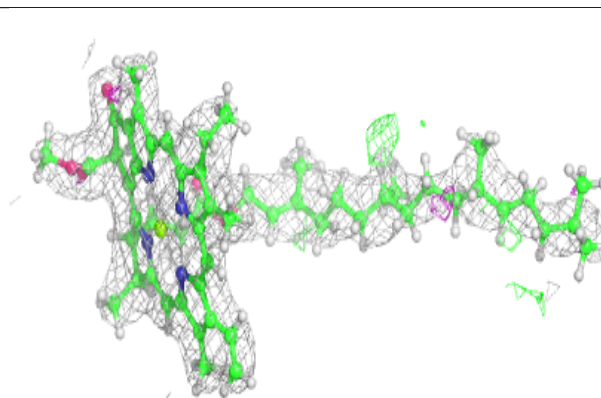
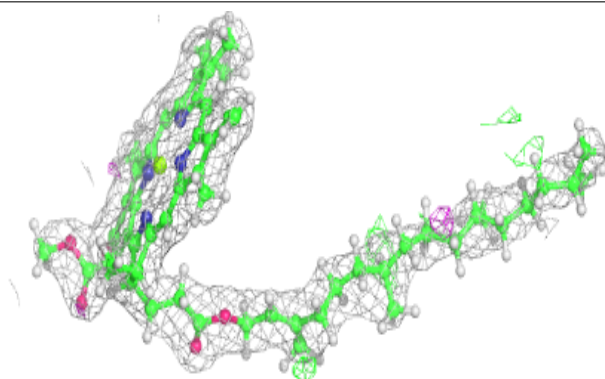


Electron density around CLA d 402:

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

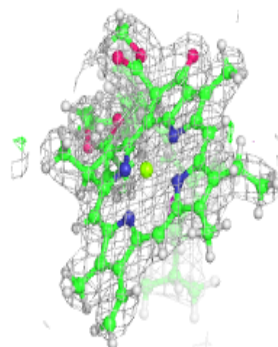
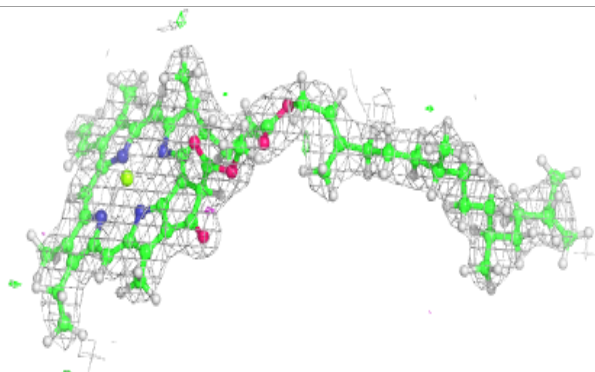
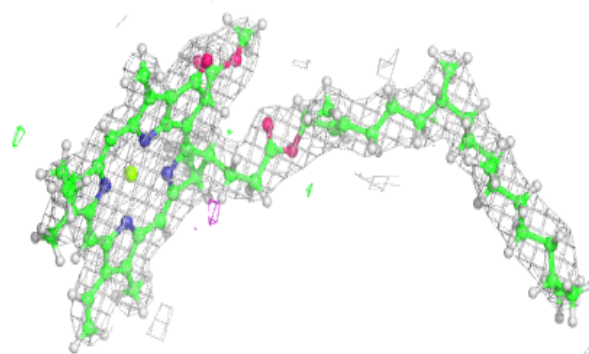
**Electron density around CLA B 607:**

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

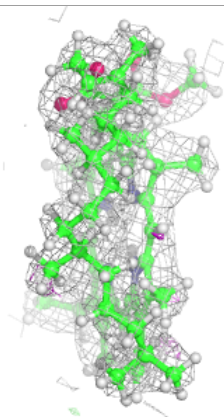
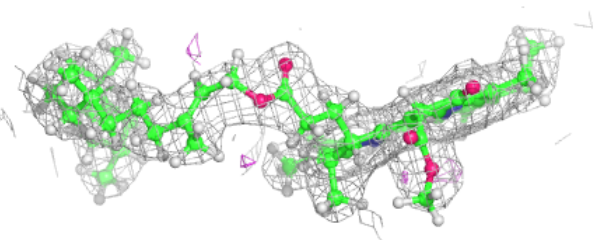
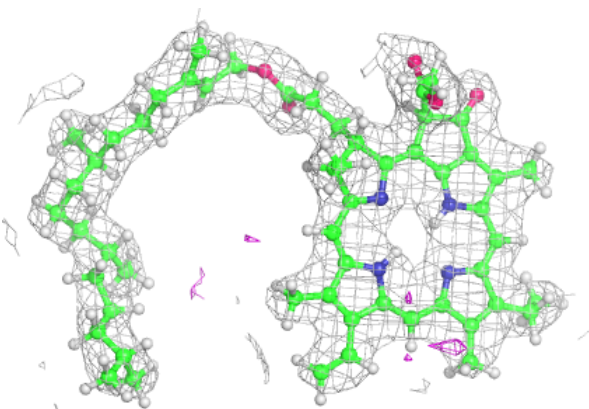


Electron density around CLA a 405:

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

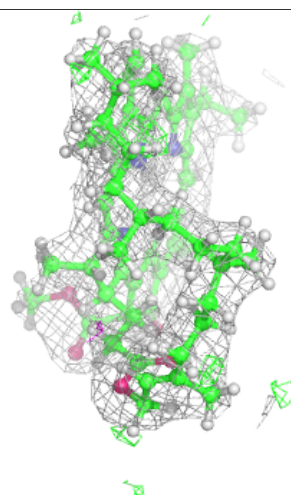
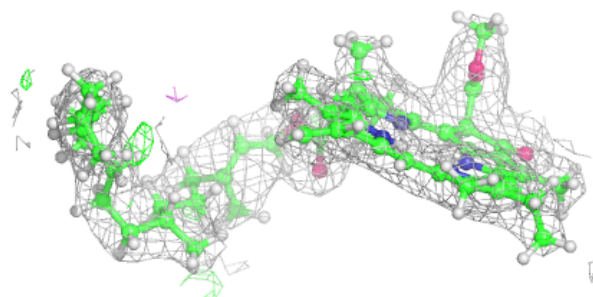
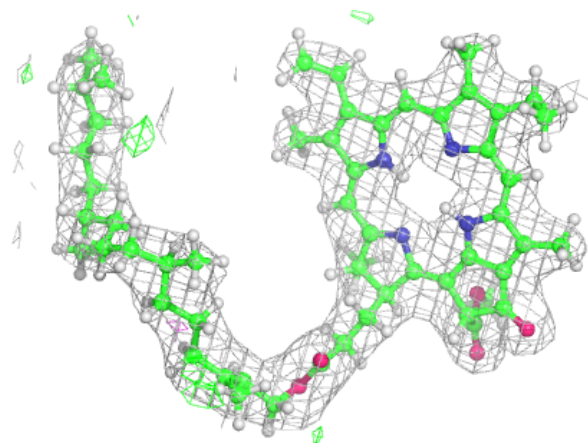
**Electron density around PHO A 406:**

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



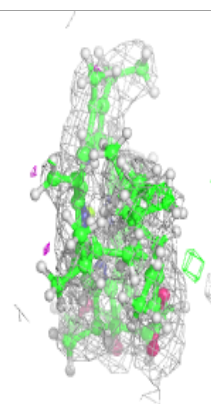
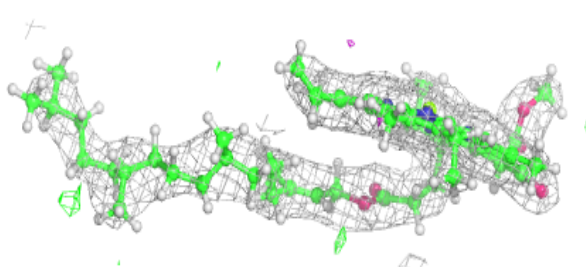
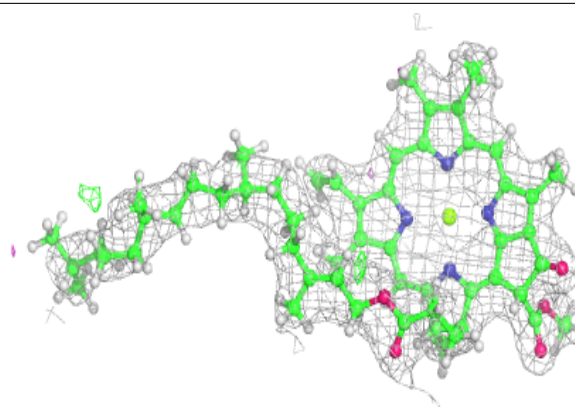
Electron density around PHO A 407:

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

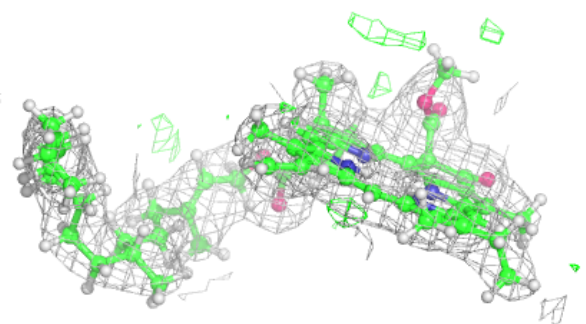
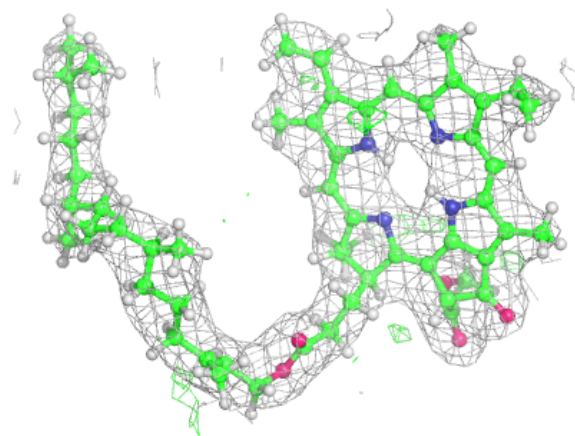


Electron density around CLA B 603:

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

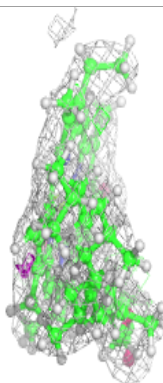
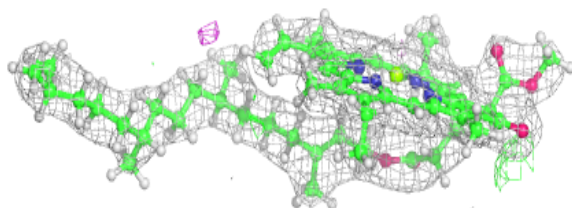
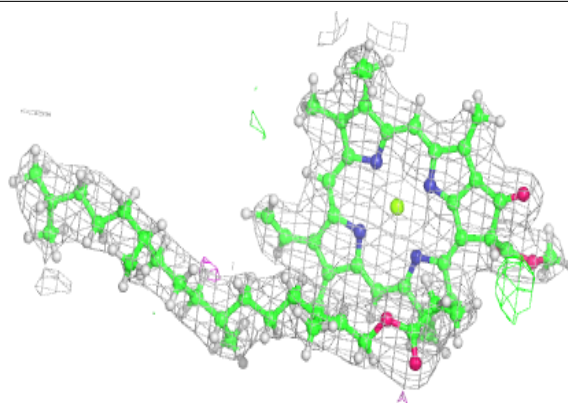
**Electron density around PHO d 401:**

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

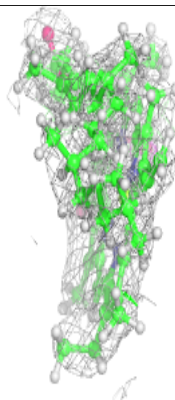
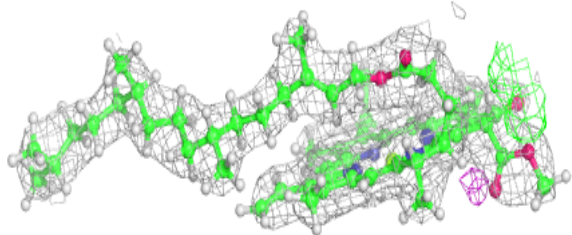
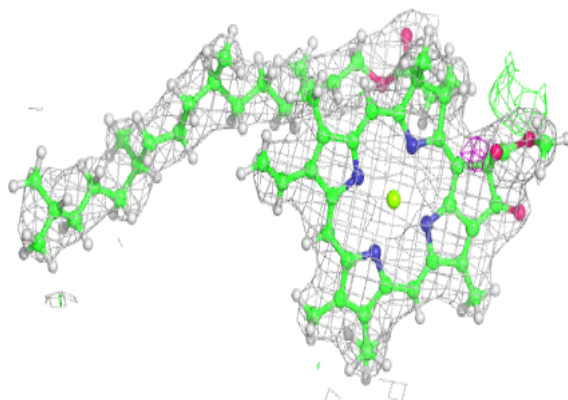


Electron density around CLA C 501:

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

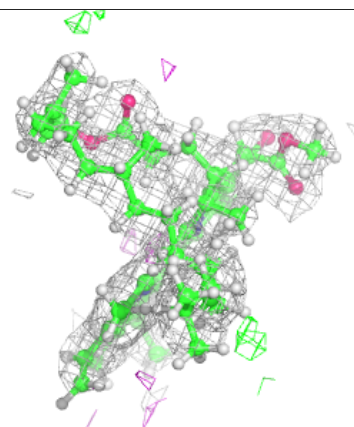
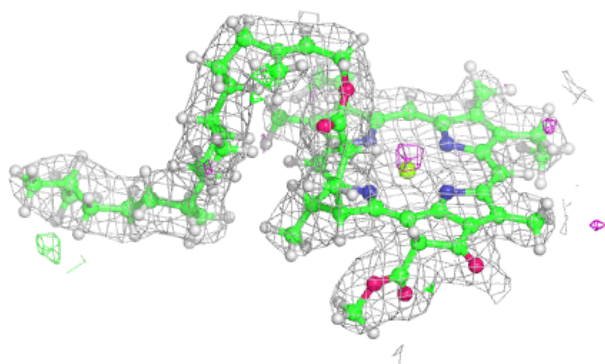
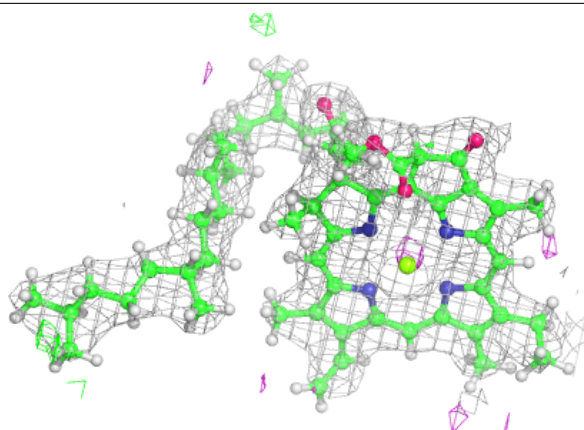
**Electron density around CLA c 501:**

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

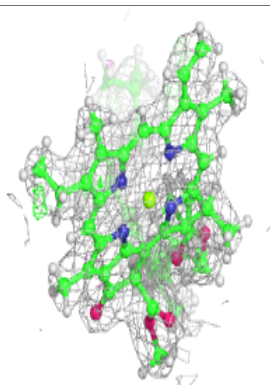
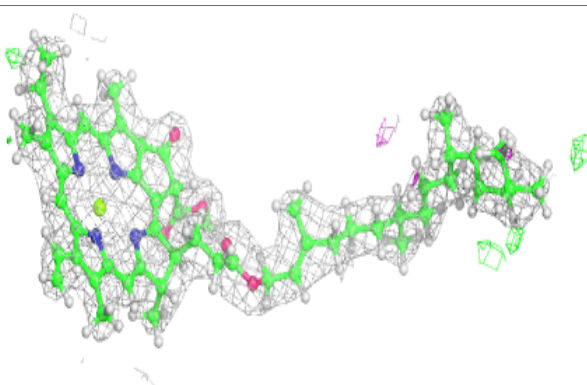
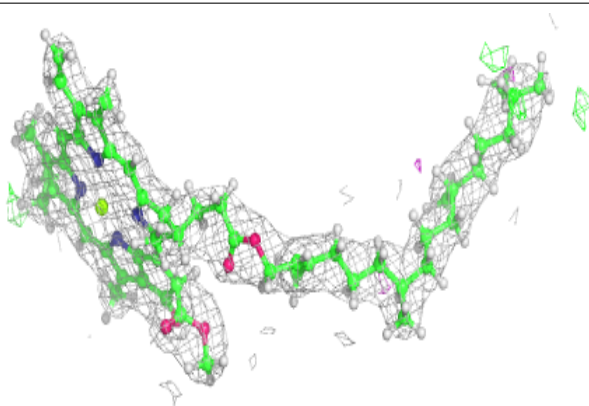


Electron density around CLA a 411:

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

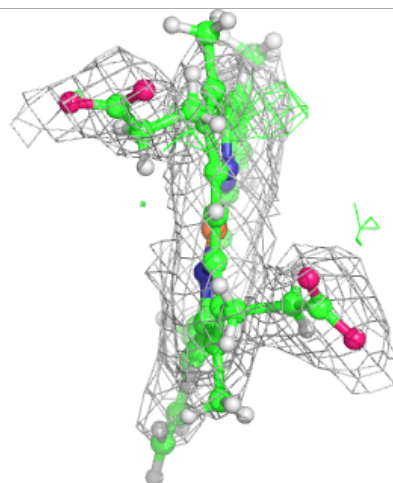
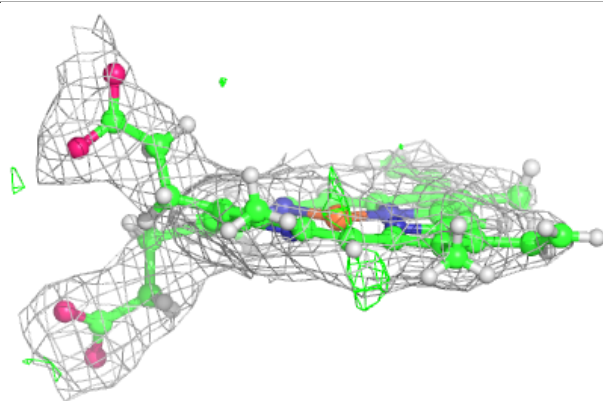
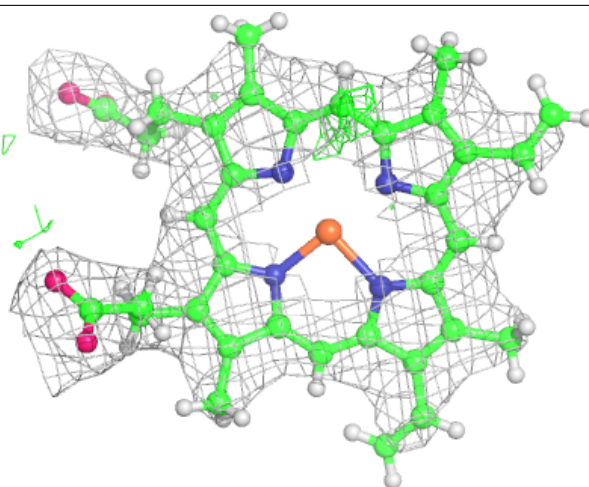
**Electron density around CLA A 404:**

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



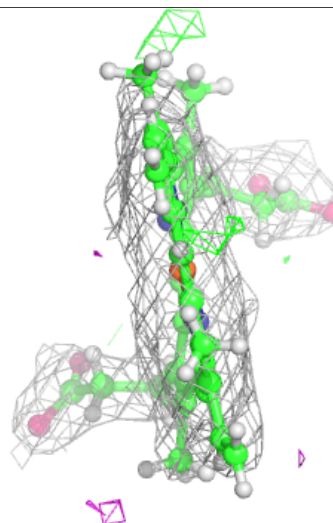
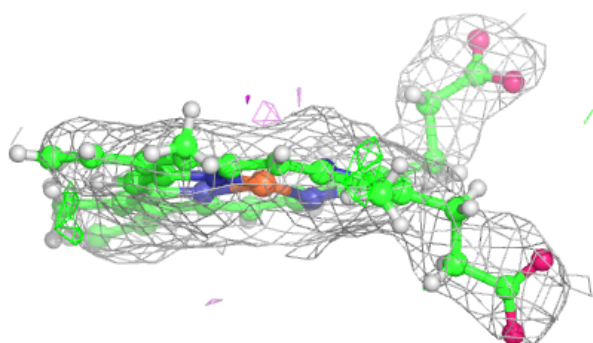
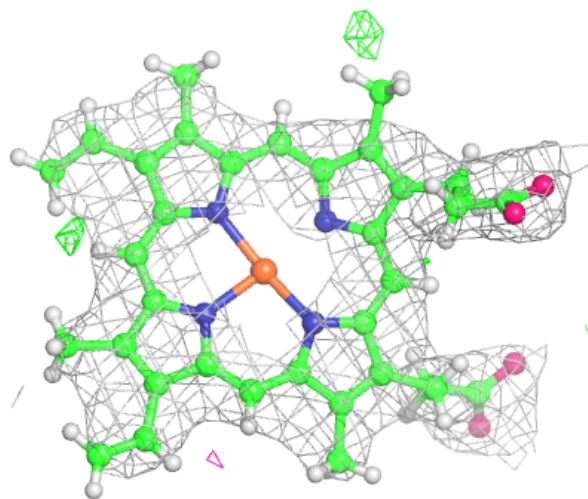
Electron density around HEM E 101:

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



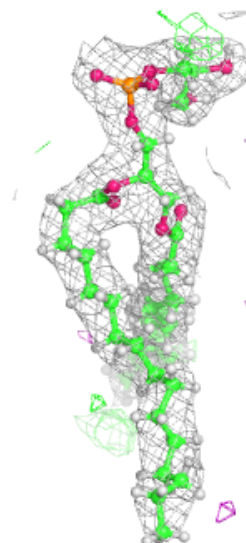
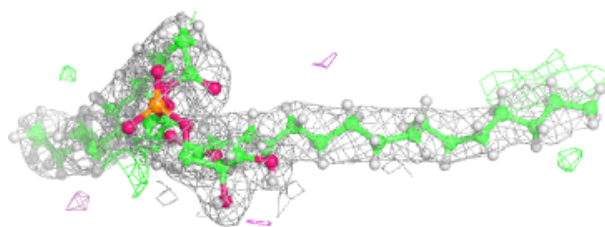
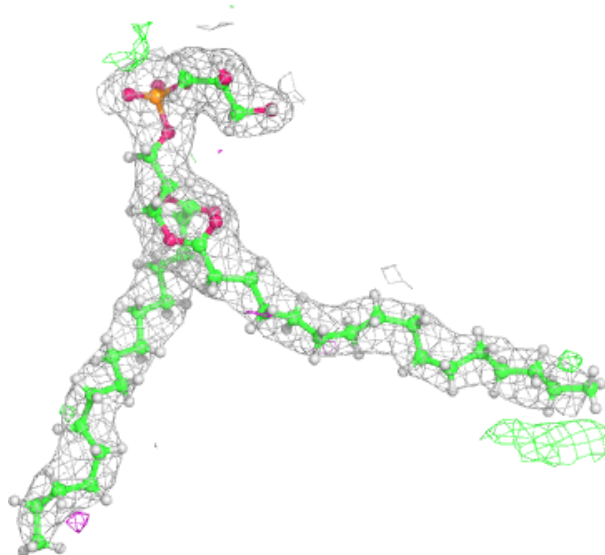
Electron density around HEM e 102:

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



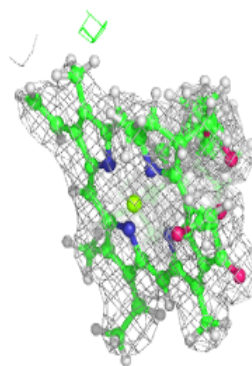
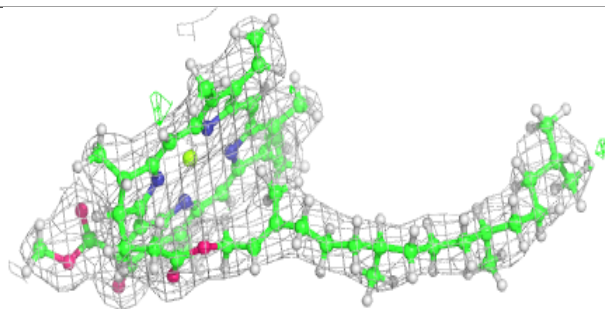
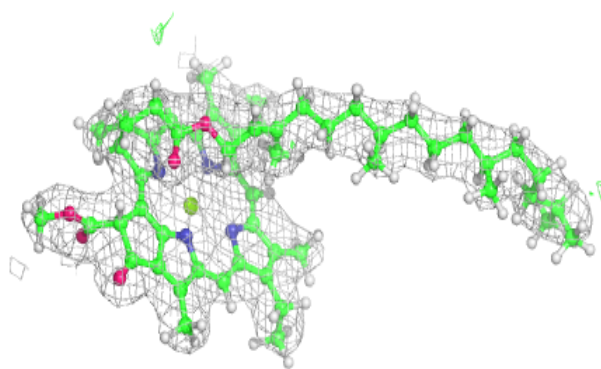
Electron density around LHG B 622:

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

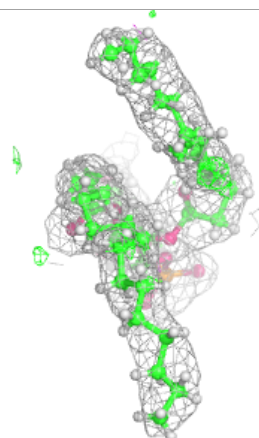
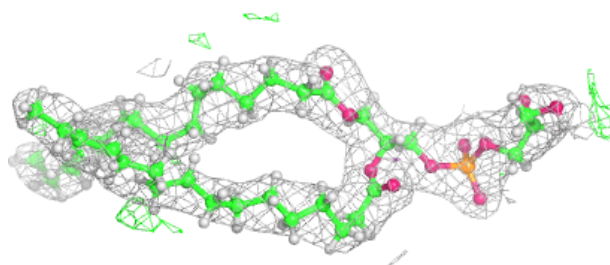
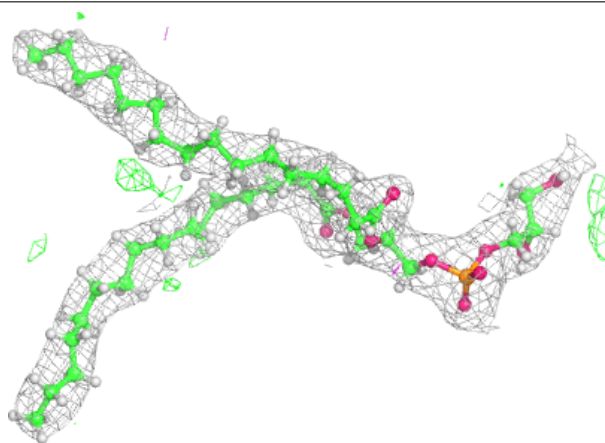


Electron density around CLA B 608:

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

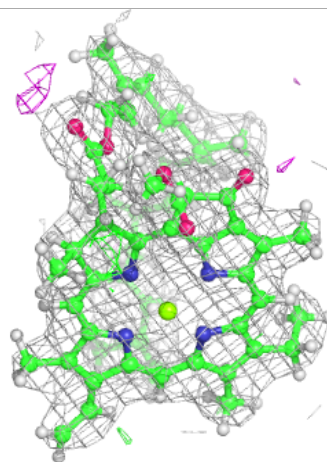
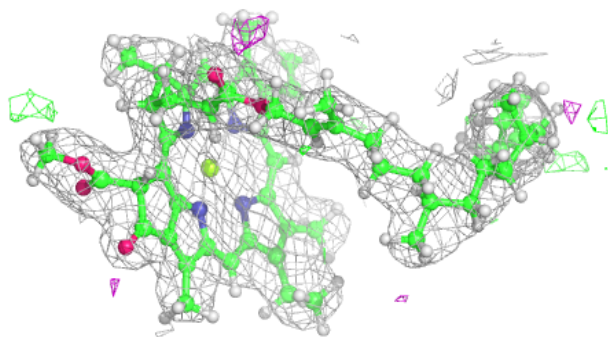
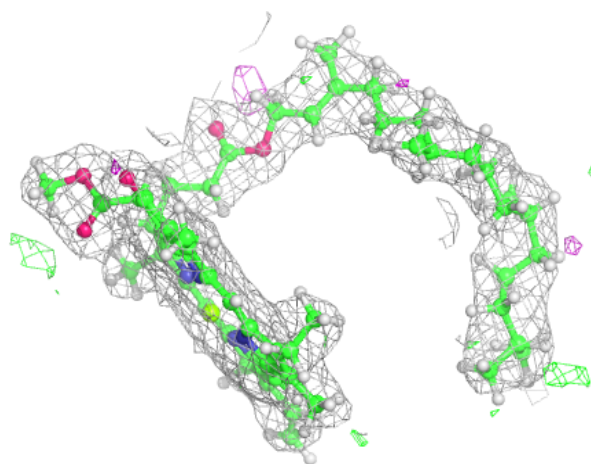
**Electron density around LHG D 407:**

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



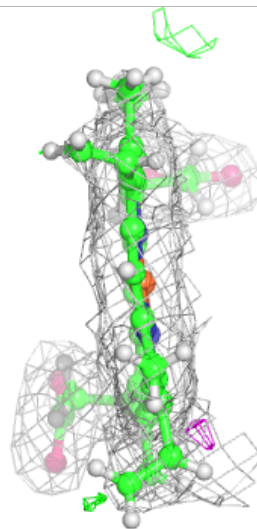
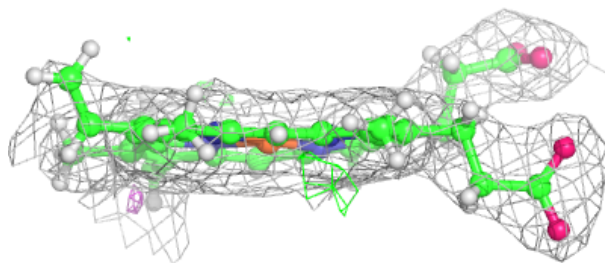
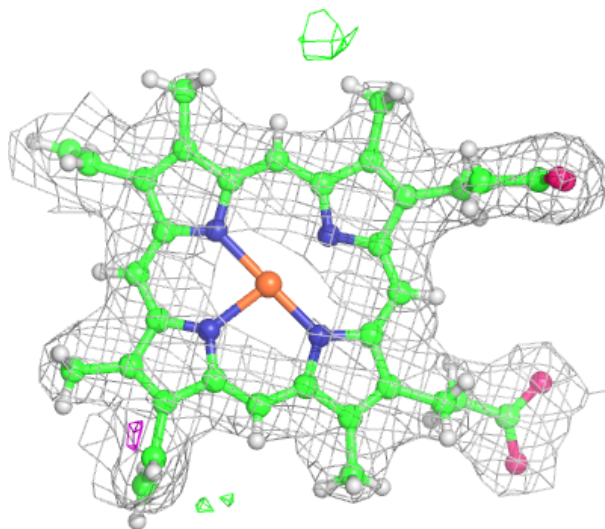
Electron density around CLA B 611:

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



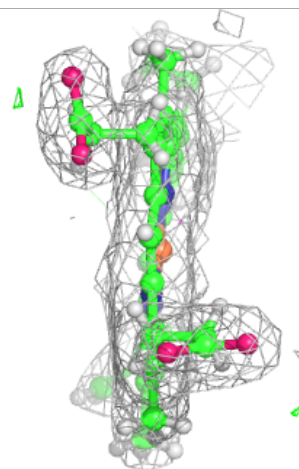
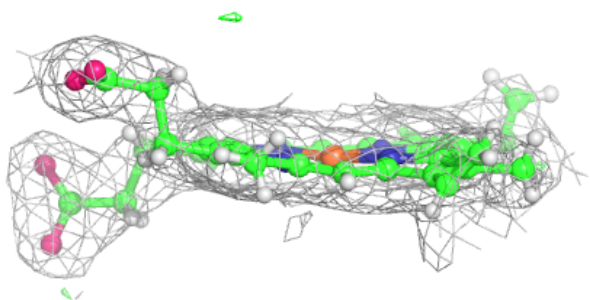
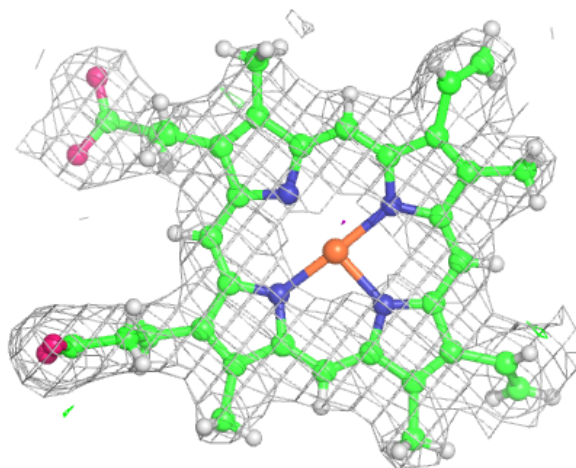
Electron density around HEC v 201:

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



Electron density around HEC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.