



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 03:14 AM BST

PDB ID : 6W1R
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.23 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	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

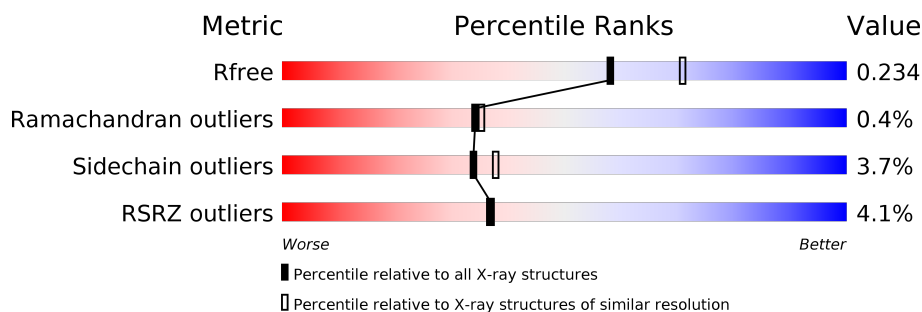
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	2391 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

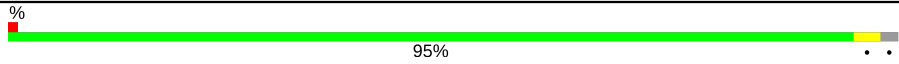
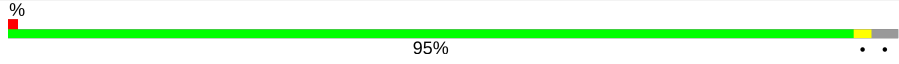
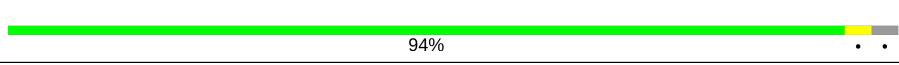
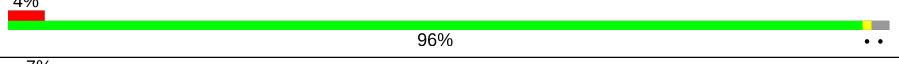
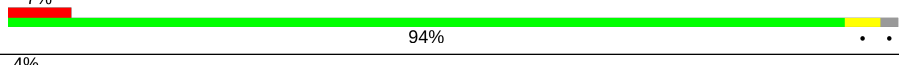
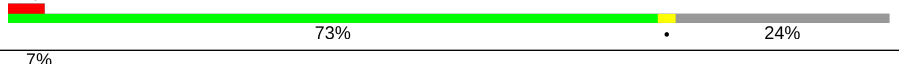
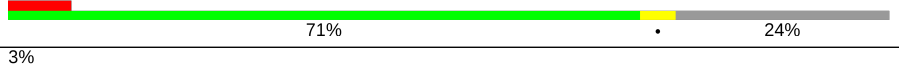
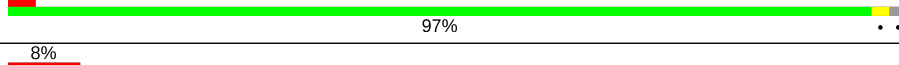
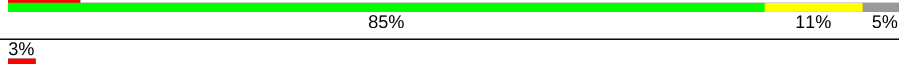
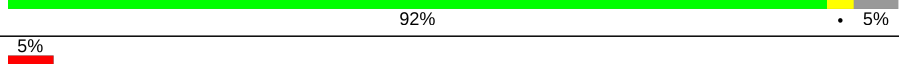
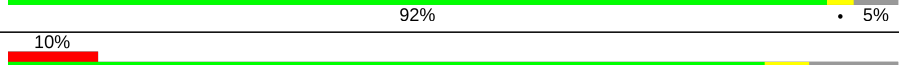
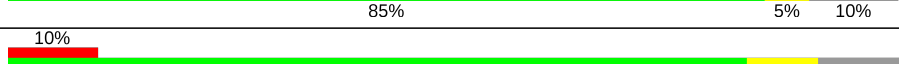

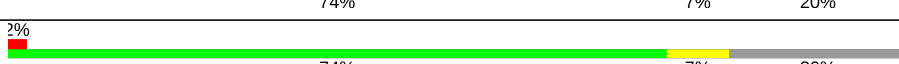
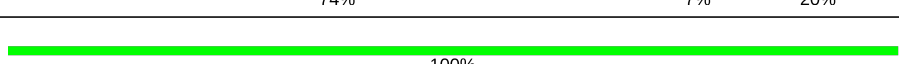
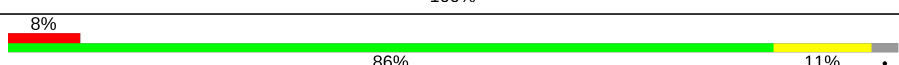
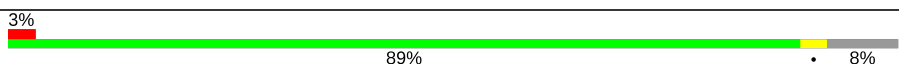
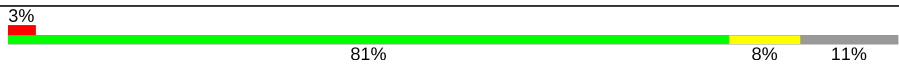
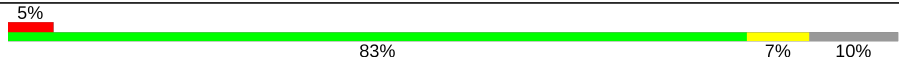

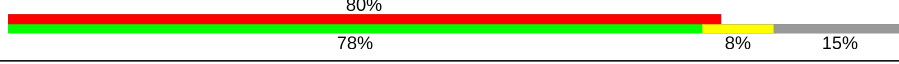
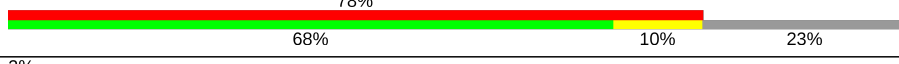
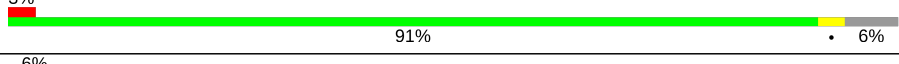
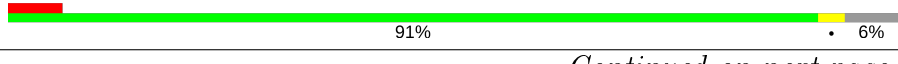

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div style="width: 96%;"></div> <div>96%</div> </div>
1	a	344	<div> <div style="width: 94%;"></div> <div>94%</div> </div>
2	B	506	<div> <div style="width: 97%;"></div> <div>97%</div> </div>
2	b	506	<div> <div style="width: 97%;"></div> <div>97%</div> </div>
3	C	461	<div> <div style="width: 93%;"></div> <div>93%</div> </div>

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

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Mol	Chain	Length	Quality of chain
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	40	
14	r	40	
15	T	32	
15	t	32	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	409	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	D	405	X	-	-	-
22	CLA	H	101	X	-	-	-
22	CLA	a	402	X	-	-	-
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	a	411	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
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22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	c	513	X	-	-	-
22	CLA	c	514	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105311 atoms, of which 52566 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	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
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	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	82	Total	C	H	N	O	0	1	0
			1316	436	650	107	123			
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
			1042	341	532	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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
			525	174	268	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	0	0
			598	204	305	43	46			
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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

- 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
			3698	1168	1828	313	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 protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

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

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	177	208	4		

- 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	39	Total	C	H	N	O	0	0	0
			602	191	316	46	49			

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

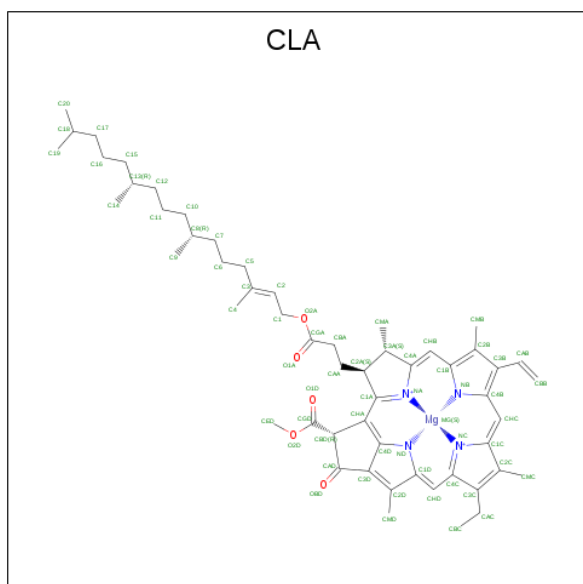
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	A	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0	0
22	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	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
22	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	H	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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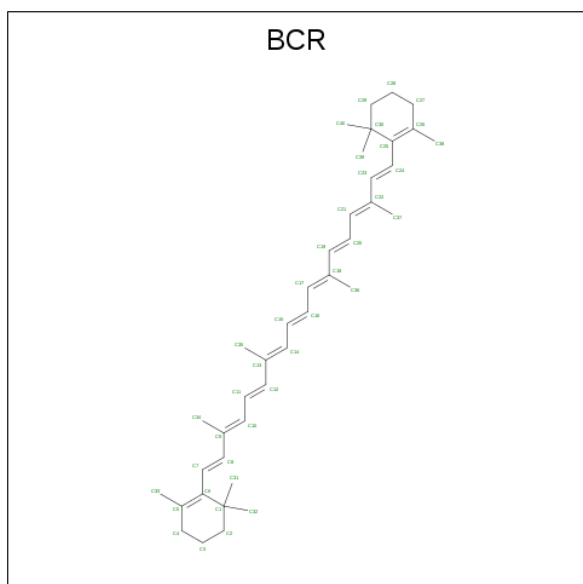
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	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
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	H	0	0
			96	40	56		
23	B	1	Total	C	H	0	0
			96	40	56		
23	B	1	Total	C	H	0	0
			96	40	56		
23	B	1	Total	C	H	0	0
			96	40	56		
23	C	1	Total	C	H	0	0
			96	40	56		

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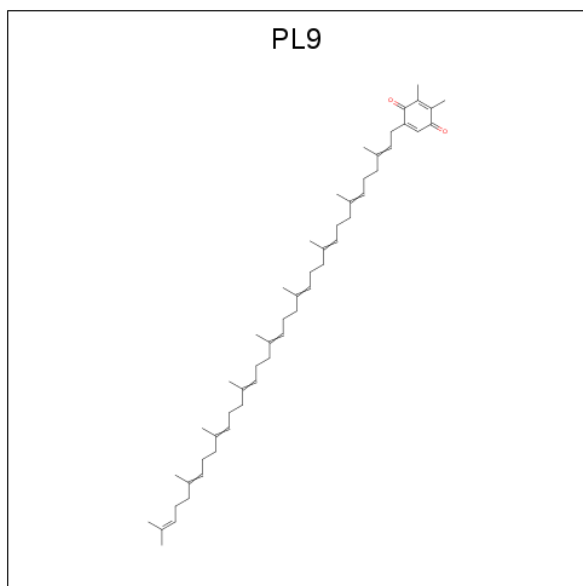
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	H	0	0
			96	40	56		
23	D	1	Total	C	H	0	0
			96	40	56		
23	K	1	Total	C	H	0	0
			96	40	56		
23	K	1	Total	C	H	0	0
			96	40	56		
23	T	1	Total	C	H	0	0
			96	40	56		
23	X	1	Total	C	H	0	0
			96	40	56		
23	a	1	Total	C	H	0	0
			96	40	56		
23	b	1	Total	C	H	0	0
			96	40	56		
23	b	1	Total	C	H	0	0
			96	40	56		
23	b	1	Total	C	H	0	0
			96	40	56		
23	c	1	Total	C	H	0	0
			96	40	56		
23	c	1	Total	C	H	0	0
			96	40	56		
23	d	1	Total	C	H	0	0
			96	40	56		
23	h	1	Total	C	H	0	0
			96	40	56		
23	k	1	Total	C	H	0	0
			96	40	56		
23	k	1	Total	C	H	0	0
			96	40	56		
23	t	1	Total	C	H	0	0
			96	40	56		

- Molecule 24 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

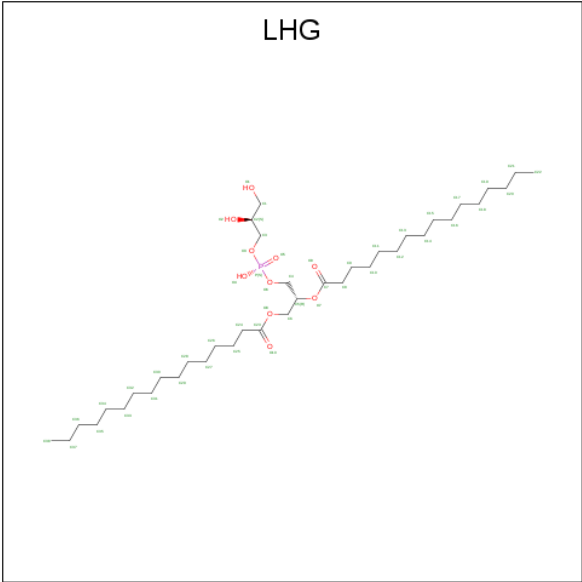
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	2	Total	Cl	0	0
			2	2		
24	a	2	Total	Cl	0	0
			2	2		

- Molecule 25 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by author).



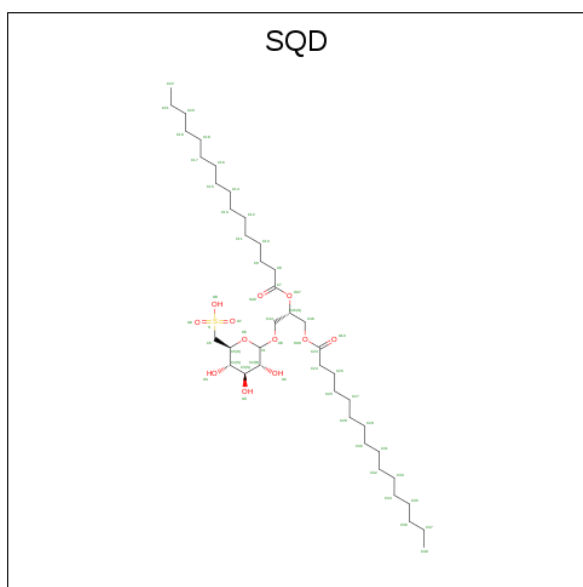
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	H	O	0	0
			135	53	80	2		
25	D	1	Total	C	H	O	0	0
			135	53	80	2		
25	a	1	Total	C	H	O	0	0
			135	53	80	2		
25	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



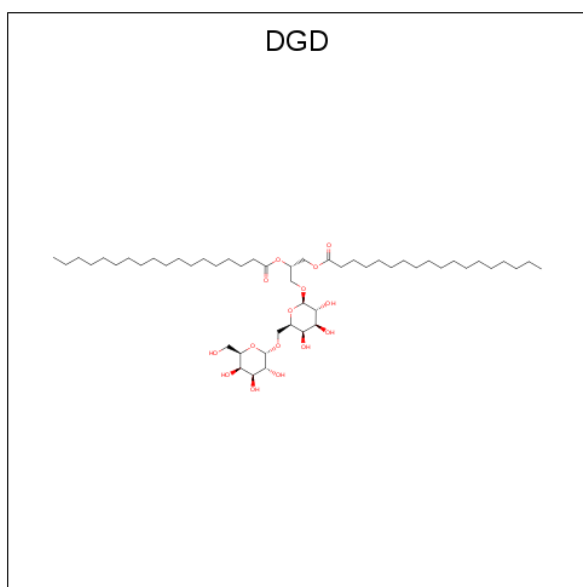
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	A	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
26	A	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	D	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
26	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	L	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	a	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
26	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
26	d	1	Total	C	H	O	P	0	0
			89	28	50	10	1		
26	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
26	l	1	Total	C	H	O	P	0	0
			121	38	72	10	1		

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



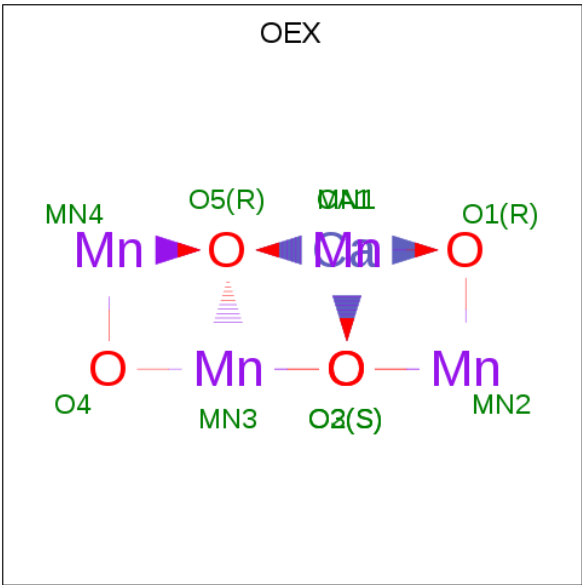
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
27	F	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			130	41	76	12	1		
27	a	1	Total	C	H	O		0	0
			92	31	56	5			
27	d	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



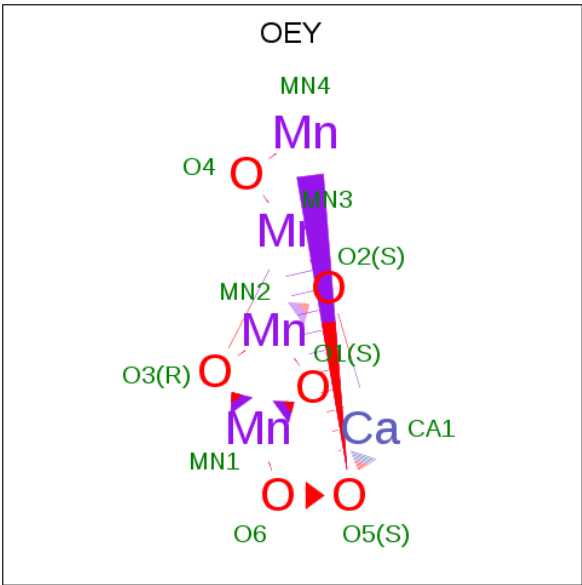
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			160	51	94	15		
28	C	1	Total	C	H	O	0	0
			144	47	82	15		
28	C	1	Total	C	H	O	0	0
			142	47	80	15		
28	C	1	Total	C	H	O	0	0
			141	47	79	15		
28	H	1	Total	C	H	O	0	0
			141	47	79	15		
28	c	1	Total	C	H	O	0	0
			141	47	79	15		
28	c	1	Total	C	H	O	0	0
			141	47	79	15		
28	c	1	Total	C	H	O	0	0
			141	47	79	15		
28	h	1	Total	C	H	O	0	0
			141	47	79	15		

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



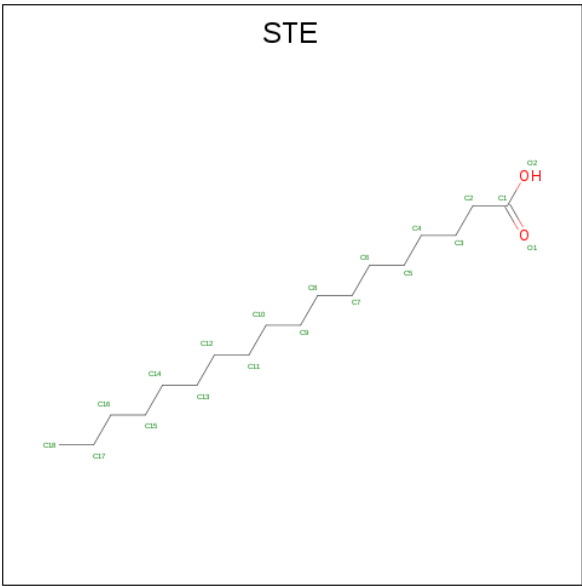
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



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

- Molecule 31 is STEARIC ACID (three-letter code: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			43	15	26	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		
31	B	1	Total	C	H		0	0
			47	16	31			
31	B	1	Total	C	H		0	0
			41	15	26			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	C	1	Total	C	H		0	0
			47	16	31			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	D	1	Total	C	H	O	0	0
			55	18	35	2		
31	H	1	Total	C	H		0	0
			53	18	35			
31	I	1	Total	C	H		0	0
			41	15	26			
31	J	1	Total	C	H	O	0	0
			28	10	16	2		

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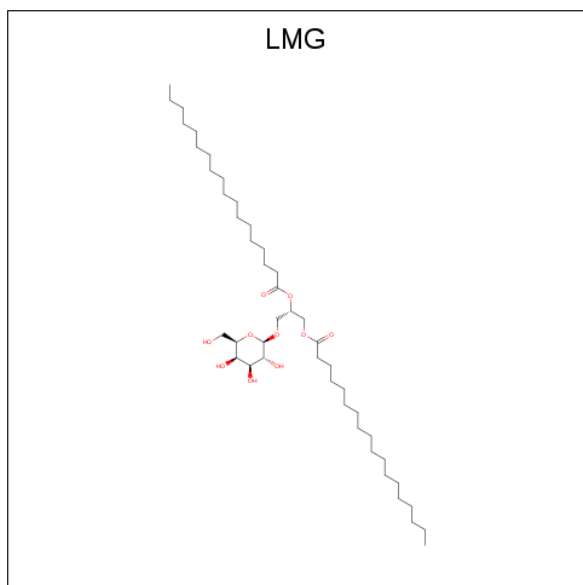
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	L	1	Total	C	H	O	0	0
			28	10	16	2		
31	M	1	Total	C	H	O	0	0
			37	13	22	2		
31	M	1	Total	C	H		0	0
			26	10	16			
31	M	1	Total	C	H		0	0
			53	18	35			
31	R	1	Total	C	H	O	0	0
			28	10	16	2		
31	T	1	Total	C	H		0	0
			47	16	31			
31	T	1	Total	C	H		0	0
			44	15	29			
31	Z	1	Total	C	H		0	0
			20	8	12			
31	a	1	Total	C	H		0	0
			26	10	16			
31	a	1	Total	C	H	O	0	0
			28	10	16	2		
31	b	1	Total	C	H	O	0	0
			55	18	35	2		
31	b	1	Total	C	H	O	0	0
			40	14	24	2		
31	b	1	Total	C	H	O	0	0
			55	18	35	2		
31	b	1	Total	C	H		0	0
			26	10	16			
31	c	1	Total	C	H	O	0	0
			28	10	16	2		
31	c	1	Total	C	H	O	0	0
			55	18	35	2		
31	d	1	Total	C	H	O	0	0
			43	15	26	2		
31	d	1	Total	C	H	O	0	0
			55	18	35	2		
31	d	1	Total	C	H	O	0	0
			55	18	35	2		
31	h	1	Total	C	H		0	0
			41	14	27			
31	j	1	Total	C	H	O	0	0
			28	10	16	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total	C	H	O	0	0
			34	12	20	2		

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



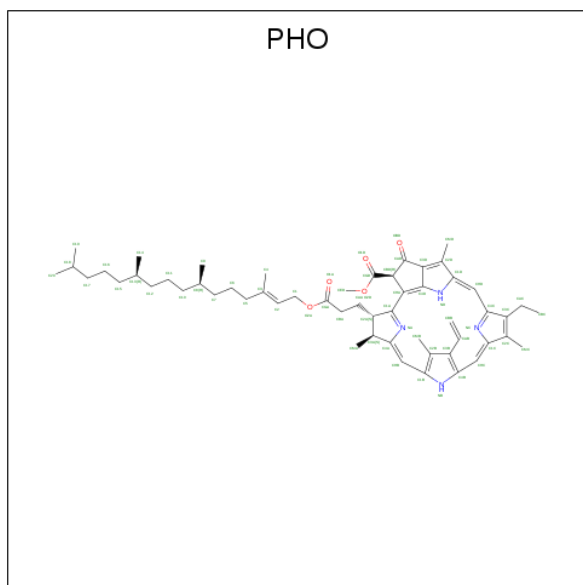
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	C	1	Total	C	H	O	0	0
			114	38	66	10		
32	D	1	Total	C	H	O	0	0
			122	41	71	10		
32	D	1	Total	C	H	O	0	0
			78	27	45	6		
32	D	1	Total	C	H	O	0	0
			68	24	40	4		
32	M	1	Total	C	H	O	0	0
			122	41	71	10		
32	Y	1	Total	C	H	O	0	0
			113	38	65	10		
32	a	1	Total	C	H	O	0	0
			140	45	85	10		
32	b	1	Total	C	H	O	0	0
			141	45	86	10		
32	c	1	Total	C	H	O	0	0
			80	27	43	10		
32	c	1	Total	C	H	O	0	0
			117	38	69	10		

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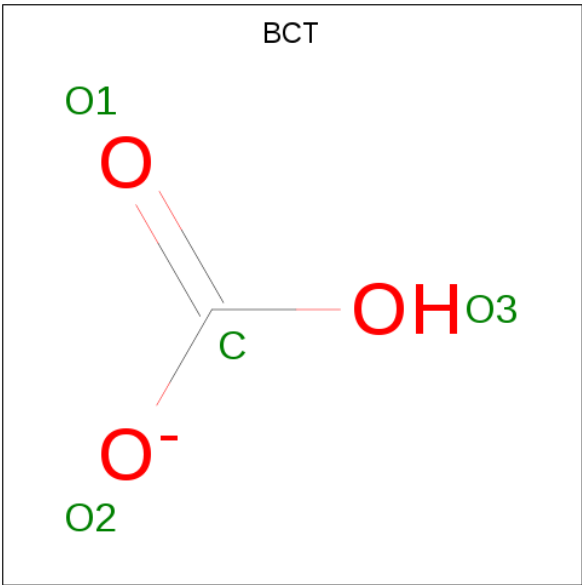
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	c	1	Total	C	H	O	0	0
			116	39	67	10		
32	d	1	Total	C	H	O	0	0
			101	34	57	10		
32	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



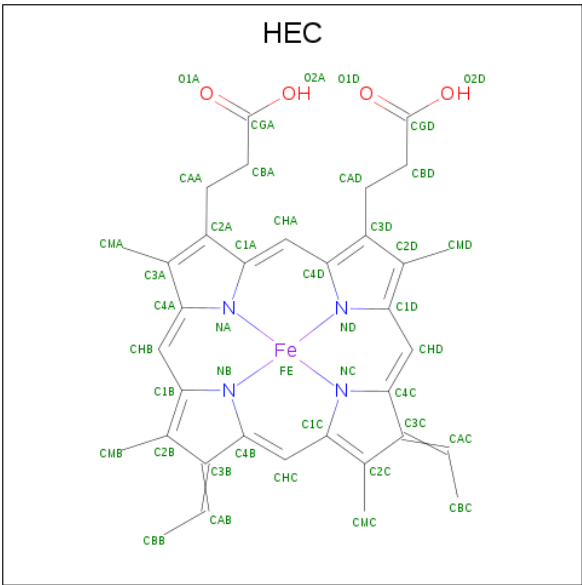
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
33	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
33	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
33	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	f	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	119	Total	O	0	8
			119	119		
36	B	148	Total	O	0	0
			148	148		
36	C	118	Total	O	0	0
			118	118		
36	D	98	Total	O	0	0
			98	98		
36	E	21	Total	O	0	0
			21	21		
36	F	2	Total	O	0	0
			2	2		
36	H	26	Total	O	0	0
			26	26		
36	I	7	Total	O	0	0
			7	7		
36	J	6	Total	O	0	0
			6	6		
36	K	4	Total	O	0	0
			4	4		
36	L	9	Total	O	0	0
			9	9		
36	M	3	Total	O	0	0
			3	3		
36	O	71	Total	O	0	0
			71	71		
36	R	1	Total	O	0	0
			1	1		
36	T	2	Total	O	0	0
			2	2		
36	U	31	Total	O	0	0
			31	31		
36	V	51	Total	O	0	0
			51	51		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	9	Total O 9 9	0	0
36	Y	4	Total O 4 4	0	0
36	Z	2	Total O 2 2	0	0
36	a	114	Total O 114 114	0	8
36	b	126	Total O 126 126	0	0
36	c	122	Total O 122 122	0	0
36	d	94	Total O 94 94	0	0
36	e	13	Total O 13 13	0	0
36	f	2	Total O 2 2	0	0
36	h	21	Total O 21 21	0	0
36	i	8	Total O 8 8	0	0
36	j	8	Total O 8 8	0	0
36	k	6	Total O 6 6	0	0
36	l	8	Total O 8 8	0	0
36	m	7	Total O 7 7	0	0
36	o	67	Total O 67 67	0	0
36	r	1	Total O 1 1	0	0
36	t	5	Total O 5 5	0	0
36	u	41	Total O 41 41	0	0
36	v	31	Total O 31 31	0	0
36	x	9	Total O 9 9	0	0

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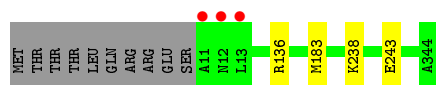
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	y	1	Total	O	0	0
			1	1		
36	z	1	Total	O	0	0
			1	1		

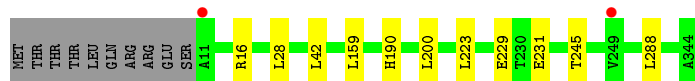
3 Residue-property plots [i](#)

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

- Molecule 1: Photosystem II protein D1 1



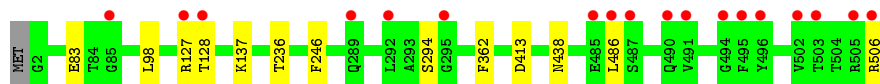
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



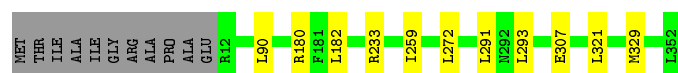
- Molecule 3: Photosystem II CP43 reaction center protein



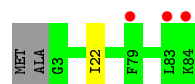
- Molecule 4: Photosystem II D2 protein



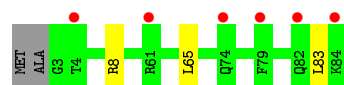
- Molecule 4: Photosystem II D2 protein



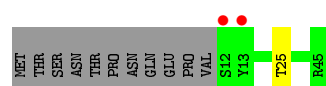
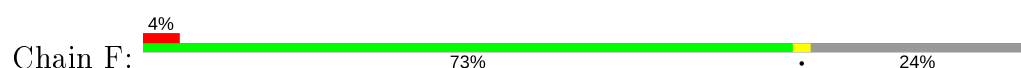
- Molecule 5: Cytochrome b559 subunit alpha



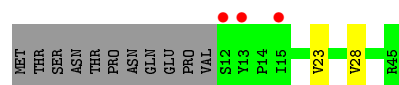
- Molecule 5: Cytochrome b559 subunit alpha



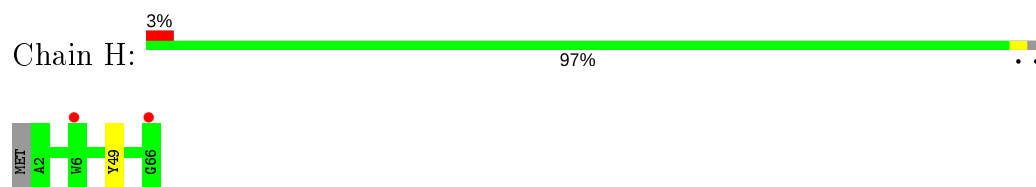
- Molecule 6: Cytochrome b559 subunit beta



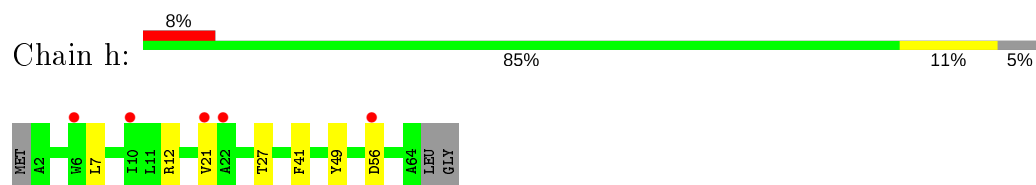
- Molecule 6: Cytochrome b559 subunit beta



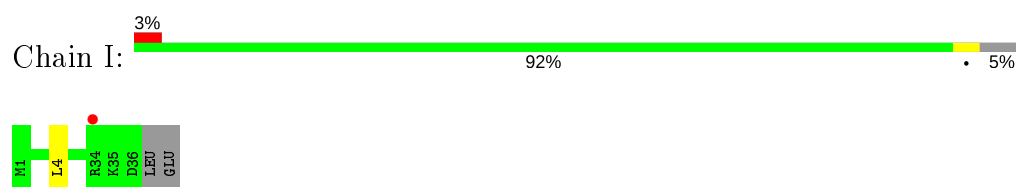
- Molecule 7: Photosystem II reaction center protein H



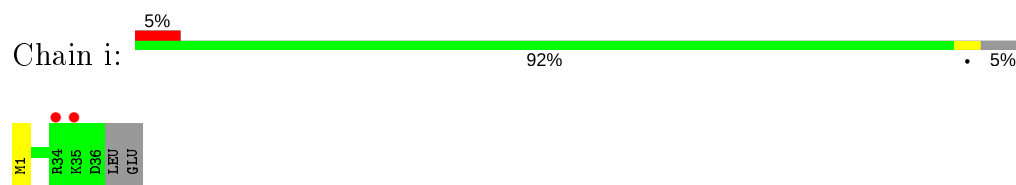
- Molecule 7: Photosystem II reaction center protein H



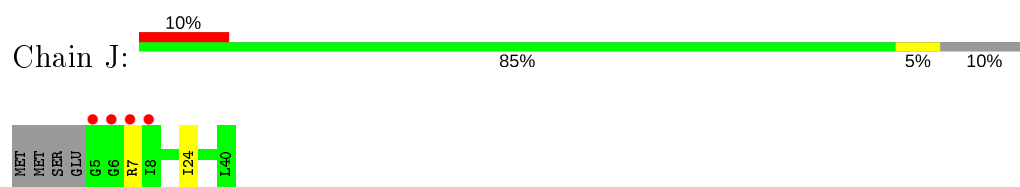
- Molecule 8: Photosystem II reaction center protein I



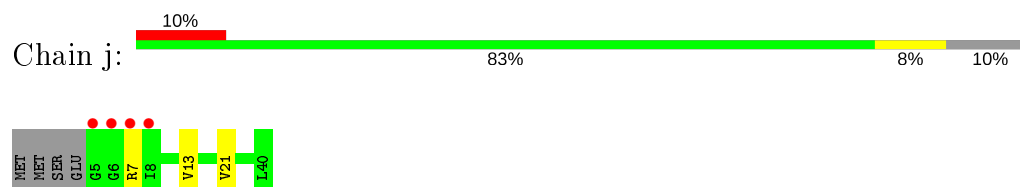
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

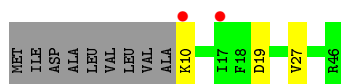


- Molecule 9: Photosystem II reaction center protein J

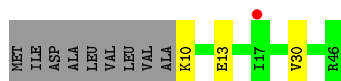
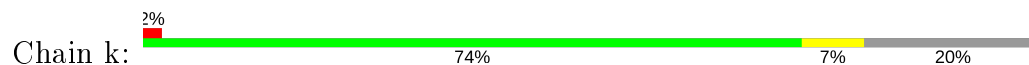


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

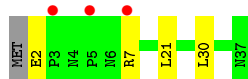
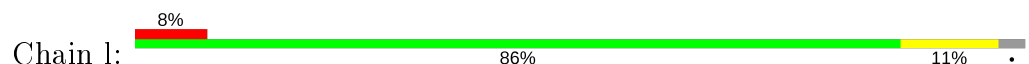


- Molecule 11: Photosystem II reaction center protein L

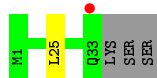
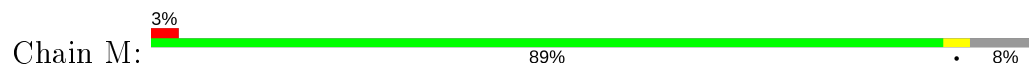


There are no outlier residues recorded for this chain.

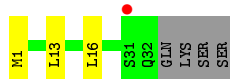
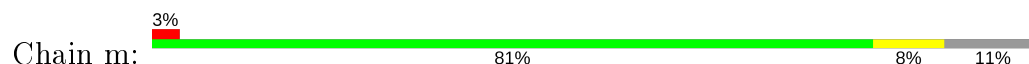
- Molecule 11: Photosystem II reaction center protein L



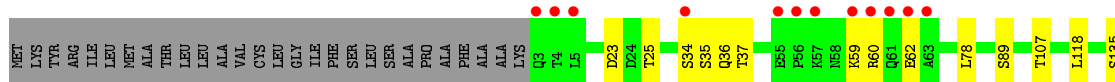
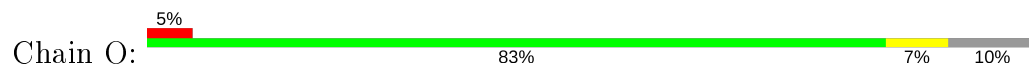
- Molecule 12: Photosystem II reaction center protein M



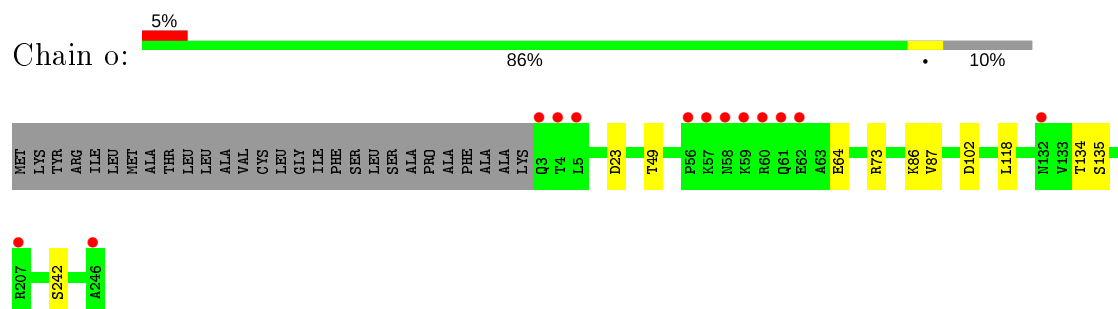
- Molecule 12: Photosystem II reaction center protein M



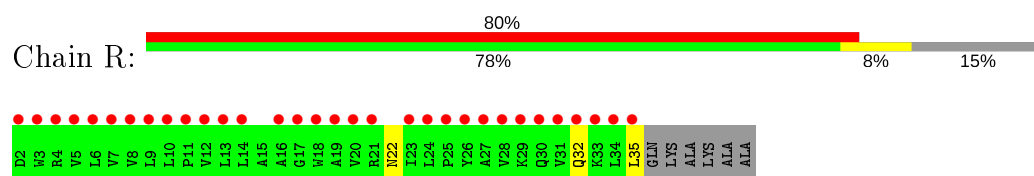
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



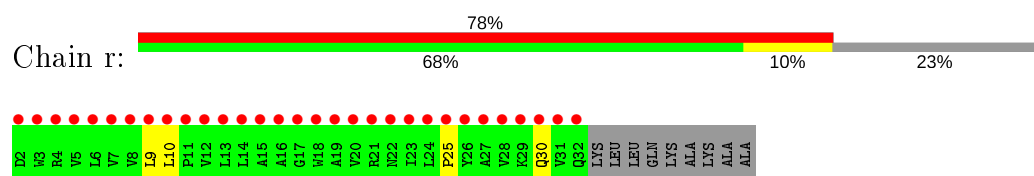
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



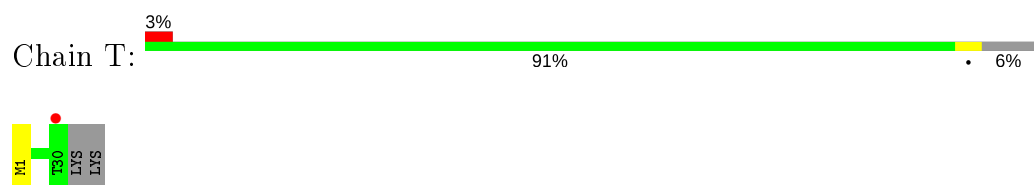
- Molecule 14: Photosystem II protein Y



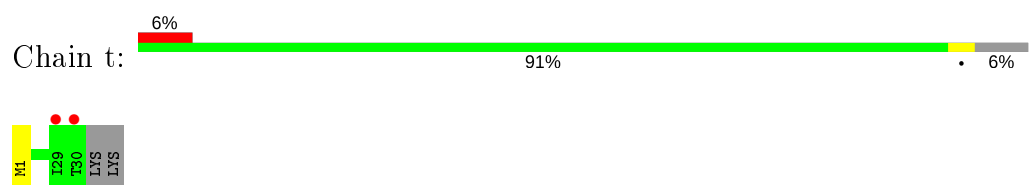
- Molecule 14: Photosystem II protein Y



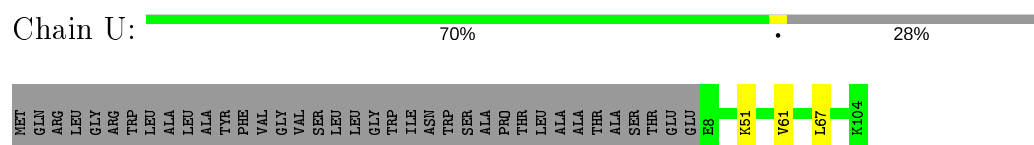
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

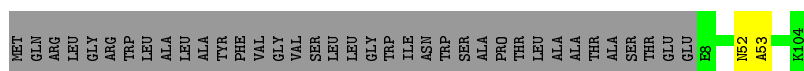


- Molecule 16: Photosystem II 12 kDa extrinsic protein



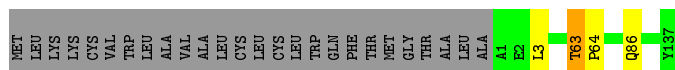
- Molecule 16: Photosystem II 12 kDa extrinsic protein





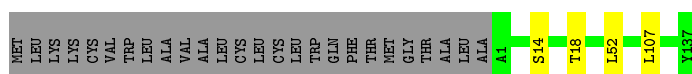
- Molecule 17: Cytochrome c-550

Chain V: 82% 16%



- Molecule 17: Cytochrome c-550

Chain v: 82% 16%



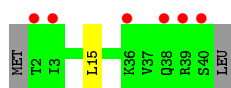
- Molecule 18: Photosystem II reaction center X protein

Chain X: 5% 88% 5% 7%



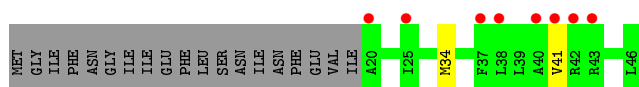
- Molecule 18: Photosystem II reaction center X protein

Chain x: 15% 93% 5%



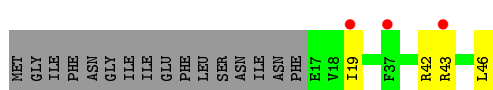
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 17% 54% 41%



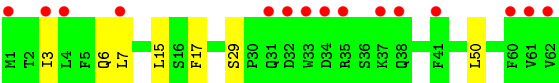
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y: 7% 57% 9% 35%

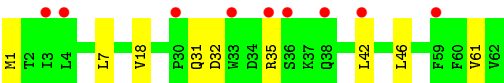
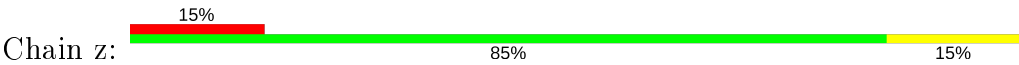


- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 24% 89% 11%



● Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.23 33.70 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.70-2.23) 85.1 (33.70-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.172 , 0.235 0.172 , 0.234	Depositor DCC
R_{free} test set	3445 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	105311	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, STE, OEY, OEX, PHO, DGD, CL, SQD, CLA, PL9, FE2, HEC, BCT, FME, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.59	0/3187	0.69	4/4342 (0.1%)
1	a	0.59	0/3184	0.73	6/4338 (0.1%)
2	B	0.65	1/4161 (0.0%)	0.70	3/5669 (0.1%)
2	b	0.61	0/4118	0.69	0/5611
3	C	0.62	0/3621	0.69	2/4930 (0.0%)
3	c	0.59	0/3693	0.66	0/5026
4	D	0.68	0/2820	0.69	1/3840 (0.0%)
4	d	0.63	0/2829	0.70	0/3852
5	E	0.55	0/688	0.60	0/940
5	e	0.50	0/683	0.60	0/932
6	F	0.49	0/284	0.60	0/387
6	f	0.50	0/284	0.61	0/387
7	H	0.59	0/523	0.66	0/713
7	h	0.57	0/511	0.69	0/697
8	I	0.63	0/293	0.70	0/396
8	i	0.70	0/293	0.63	0/396
9	J	0.53	0/263	0.63	0/356
9	j	0.53	0/263	0.65	0/356
10	K	0.49	0/303	0.60	0/416
10	k	0.54	0/303	0.66	0/416
11	L	0.72	0/311	0.76	0/422
11	l	0.65	0/303	0.66	0/412
12	M	0.69	0/249	0.69	0/341
12	m	0.70	0/244	0.73	0/334
13	O	0.61	0/1904	0.75	1/2585 (0.0%)
13	o	0.63	0/1905	0.75	1/2583 (0.0%)
14	R	0.45	0/277	0.53	0/380
14	r	0.38	0/246	0.48	0/339
15	T	0.78	0/257	0.69	0/349
15	t	0.73	0/255	0.69	0/346
16	U	0.56	0/785	0.69	0/1064
16	u	0.62	0/785	0.72	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.61	0/1085	0.73	1/1473 (0.1%)
17	v	0.53	0/1085	0.65	0/1473
18	X	0.51	0/284	0.63	0/384
18	x	0.43	0/289	0.56	0/391
19	Y	0.52	0/197	0.62	0/264
19	y	0.40	0/219	0.62	0/294
20	Z	0.47	0/490	0.54	0/669
20	z	0.44	0/488	0.55	0/666
All	All	0.61	1/43962 (0.0%)	0.69	19/59833 (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
16	u	0	1
17	V	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	129	GLY	C-N	-5.76	1.20	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	190[A]	HIS	O-C-N	-10.10	106.55	122.70
1	a	190[B]	HIS	O-C-N	-10.10	106.55	122.70
1	a	190[A]	HIS	CA-C-N	8.05	134.92	117.20
1	a	190[B]	HIS	CA-C-N	8.05	134.92	117.20
1	a	190[A]	HIS	C-N-CA	7.16	139.60	121.70
1	a	190[B]	HIS	C-N-CA	7.16	139.60	121.70
13	o	102	ASP	CB-CG-OD1	6.60	124.24	118.30
17	V	63	THR	C-N-CD	-6.45	106.41	120.60
4	D	294	ARG	NE-CZ-NH1	-6.44	117.08	120.30
3	C	396	MET	CG-SD-CE	-6.28	90.15	100.20
2	B	230	ARG	NE-CZ-NH1	6.09	123.34	120.30
2	B	476	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	136	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	136	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	315	MET	CG-SD-CE	-5.43	91.51	100.20
2	B	380	ASP	CB-CG-OD1	5.38	123.14	118.30
13	O	158	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	183[A]	MET	CA-CB-CG	5.29	122.29	113.30
1	A	183[B]	MET	CA-CB-CG	5.29	122.29	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	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	391/344 (114%)	379 (97%)	12 (3%)	0	100	100
1	a	391/344 (114%)	381 (97%)	10 (3%)	0	100	100
2	B	508/506 (100%)	498 (98%)	10 (2%)	0	100	100
2	b	503/506 (99%)	486 (97%)	15 (3%)	2 (0%)	34	35
3	C	450/461 (98%)	438 (97%)	11 (2%)	1 (0%)	47	53
3	c	459/461 (100%)	445 (97%)	13 (3%)	1 (0%)	47	53
4	D	339/352 (96%)	330 (97%)	9 (3%)	0	100	100
4	d	340/352 (97%)	330 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	80/84 (95%)	75 (94%)	4 (5%)	1 (1%)	12	7
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	56 (89%)	7 (11%)	0	100	100
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	4	1
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	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	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	223 (92%)	13 (5%)	7 (3%)	4	1
13	o	242/272 (89%)	229 (95%)	12 (5%)	1 (0%)	34	35
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	23 (79%)	4 (14%)	2 (7%)	1	0
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	89 (94%)	5 (5%)	1 (1%)	14	9
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	20
17	v	135/163 (83%)	127 (94%)	8 (6%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	24 (86%)	2 (7%)	2 (7%)	1	0
20	Z	60/62 (97%)	48 (80%)	12 (20%)	0	100	100
20	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	9	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5374/5690 (94%)	5161 (96%)	192 (4%)	21 (0%)	34	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	36	GLN
13	O	59	LYS
13	O	60	ARG
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
14	r	30	GLN
16	u	53	ALA
3	C	416	SER
2	b	294	SER
13	o	73	ARG
19	y	43	ARG
9	J	7	ARG
13	O	35	SER
2	b	127	ARG
13	O	34	SER
13	O	138	THR
5	e	83	LEU
19	y	42	ARG
20	z	61	VAL
14	r	25	PRO

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	320/280 (114%)	318 (99%)	2 (1%)	86	90
1	a	319/280 (114%)	309 (97%)	10 (3%)	40	46
2	B	408/404 (101%)	399 (98%)	9 (2%)	52	59
2	b	402/404 (100%)	391 (97%)	11 (3%)	44	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	353/362 (98%)	343 (97%)	10 (3%)	43	49
3	c	361/362 (100%)	345 (96%)	16 (4%)	28	30
4	D	277/283 (98%)	272 (98%)	5 (2%)	59	66
4	d	278/283 (98%)	267 (96%)	11 (4%)	31	34
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	49
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	49
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	39
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	11
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	64
7	h	53/55 (96%)	46 (87%)	7 (13%)	4	2
8	I	32/34 (94%)	31 (97%)	1 (3%)	40	46
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	32
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	2
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	27 (96%)	1 (4%)	35	39
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	195 (95%)	11 (5%)	22	21
13	o	207/228 (91%)	198 (96%)	9 (4%)	29	31
14	R	28/32 (88%)	25 (89%)	3 (11%)	6	3
14	r	23/32 (72%)	21 (91%)	2 (9%)	10	6
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	81 (96%)	3 (4%)	35	39
16	u	84/112 (75%)	84 (100%)	0	100	100
17	V	117/138 (85%)	115 (98%)	2 (2%)	60	68
17	v	117/138 (85%)	113 (97%)	4 (3%)	37	42
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	44
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	3
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
20	z	51/52 (98%)	43 (84%)	8 (16%)	2	1
All	All	4444/4646 (96%)	4281 (96%)	163 (4%)	34	38

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LYS
1	A	243	GLU
2	B	87	ASP
2	B	98	LEU
2	B	127	ARG
2	B	177	SER
2	B	246	PHE
2	B	362	PHE
2	B	371	THR
2	B	388	SER
2	B	476	ARG
3	C	104	GLU
3	C	106	VAL
3	C	108	THR
3	C	130	VAL
3	C	141	GLU
3	C	185	LEU
3	C	201	ASN
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	154	VAL
4	D	180	ARG
4	D	264	LYS
4	D	329	MET
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR

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Mol	Chain	Res	Type
8	I	4	LEU
9	J	24	ILE
10	K	10	LYS
10	K	19	ASP
10	K	27	VAL
12	M	25	LEU
13	O	23	ASP
13	O	25	THR
13	O	37	THR
13	O	78	LEU
13	O	89	SER
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	184	ARG
13	O	189	ARG
13	O	214	THR
14	R	22	ASN
14	R	32	GLN
14	R	35	LEU
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	86	GLN
18	X	3	ILE
18	X	15	LEU
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	6	GLN
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	29	SER
20	Z	50	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

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Mol	Chain	Res	Type
1	a	229	GLU
1	a	231	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	137	LYS
2	b	236	THR
2	b	246	PHE
2	b	362	PHE
2	b	413	ASP
2	b	438	ASN
2	b	486	LEU
2	b	506	ARG
3	c	24	THR
3	c	30	SER
3	c	72	LEU
3	c	79	LYS
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	165	LEU
3	c	240	ILE
3	c	289	PHE
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	413[A]	GLU
3	c	413[B]	GLU
3	c	468	SER
4	d	90	LEU
4	d	180	ARG
4	d	182	LEU
4	d	233	ARG
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET

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Mol	Chain	Res	Type
5	e	8	ARG
5	e	65	LEU
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	12	ARG
7	h	21	VAL
7	h	27	THR
7	h	41	PHE
7	h	49	TYR
7	h	56	ASP
9	j	7	ARG
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	30	VAL
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	23	ASP
13	o	49	THR
13	o	64	GLU
13	o	86	LYS
13	o	87	VAL
13	o	118	LEU
13	o	134	THR
13	o	135	SER
13	o	242	SER
14	r	9	LEU
14	r	10	LEU
17	v	14	SER
17	v	18	THR
17	v	52	LEU
17	v	107	LEU
18	x	15	LEU
19	y	19	ILE
19	y	46	LEU
20	z	1	MET

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Mol	Chain	Res	Type
20	z	7	LEU
20	z	18	VAL
20	z	31	GLN
20	z	32	ASP
20	z	35	ARG
20	z	42	LEU
20	z	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	409	GLN
3	C	74	HIS
3	C	201	ASN
13	O	88	ASN
13	O	231	HIS
17	V	86	GLN
18	X	38	GLN
20	Z	38	GLN
1	a	19	ASN
1	a	234	ASN
2	b	490	GLN
4	d	61	HIS
13	o	61	GLN
13	o	200	ASN

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
15	FME	T	1	15	8,9,10	1.11	1 (12%)	7,9,11	1.40	2 (28%)
8	FME	I	1	8	8,9,10	1.00	0	7,9,11	0.97	0
12	FME	M	1	12	8,9,10	0.86	0	7,9,11	0.92	0
8	FME	i	1	8	8,9,10	1.15	1 (12%)	7,9,11	0.52	0
15	FME	t	1	15	8,9,10	1.34	1 (12%)	7,9,11	0.78	0
12	FME	m	1	12	8,9,10	1.02	1 (12%)	7,9,11	1.21	1 (14%)

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
15	FME	T	1	15	-	1/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.00	1.42	1.46
12	m	1	FME	CA-N	-2.24	1.43	1.46
8	i	1	FME	CA-N	-2.09	1.43	1.46
15	T	1	FME	CB-CA	2.06	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	CA-N-CN	2.91	127.29	122.82
12	m	1	FME	CA-N-CN	-2.35	119.21	122.82
15	T	1	FME	CG-CB-CA	2.03	118.59	112.95

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
8	i	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
12	M	1	FME	CB-CA-N-CN
8	I	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 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	LMG	b	621	-	55,55,55	0.91	3 (5%)	63,63,63	1.52	10 (15%)
22	CLA	c	514	-	59,73,73	1.42	6 (10%)	67,113,113	1.46	7 (10%)
26	LHG	D	412	-	48,48,48	0.96	3 (6%)	51,54,54	1.34	7 (13%)
23	BCR	b	618	-	41,41,41	1.25	2 (4%)	56,56,56	1.37	7 (12%)
27	SQD	F	102	-	35,36,54	1.03	3 (8%)	42,45,65	1.88	9 (21%)
31	STE	a	415	-	9,9,19	0.53	0	8,8,19	0.54	0
28	DGD	H	102	-	63,63,67	1.30	8 (12%)	77,77,81	1.34	7 (9%)
22	CLA	B	604	-	59,73,73	1.50	8 (13%)	67,113,113	2.19	14 (20%)
31	STE	b	620	-	16,19,19	0.45	0	15,19,19	0.83	0
33	PHO	a	404	-	67,69,69	1.08	7 (10%)	85,99,99	1.13	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	513	-	59,73,73	1.52	6 (10%)	67,113,113	1.66	14 (20%)
22	CLA	B	616	-	54,68,73	1.79	10 (18%)	61,107,113	1.75	10 (16%)
31	STE	C	521	-	15,15,19	0.53	0	14,14,19	0.52	0
22	CLA	c	506	-	59,73,73	1.57	7 (11%)	67,113,113	1.82	15 (22%)
23	BCR	t	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.47	11 (19%)
22	CLA	A	402	-	59,73,73	1.51	7 (11%)	67,113,113	1.69	13 (19%)
23	BCR	X	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.36	8 (14%)
31	STE	R	101	-	8,11,19	0.49	0	7,11,19	0.70	0
26	LHG	D	409	-	48,48,48	1.30	5 (10%)	51,54,54	1.25	7 (13%)
23	BCR	d	404	-	41,41,41	1.10	2 (4%)	56,56,56	1.14	6 (10%)
32	LMG	C	516	-	48,48,55	1.19	3 (6%)	56,56,63	1.53	9 (16%)
31	STE	T	103	-	14,14,19	0.50	0	13,13,19	0.71	0
31	STE	M	104	-	17,17,19	0.36	0	16,16,19	0.88	0
22	CLA	C	506	-	59,73,73	1.64	7 (11%)	67,113,113	1.66	12 (17%)
23	BCR	K	102	-	41,41,41	1.06	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	c	508	36	59,73,73	1.41	6 (10%)	67,113,113	1.68	14 (20%)
25	PL9	A	408	-	55,55,55	1.65	12 (21%)	68,69,69	1.75	18 (26%)
31	STE	c	501	-	8,11,19	0.45	0	7,11,19	0.60	0
31	STE	T	102	-	15,15,19	0.45	0	14,14,19	0.81	0
22	CLA	c	509	-	58,72,73	1.64	7 (12%)	65,111,113	1.57	9 (13%)
35	HEC	F	101	5,6	26,50,50	2.50	5 (19%)	18,82,82	2.37	6 (33%)
23	BCR	c	516	-	41,41,41	1.16	4 (9%)	56,56,56	1.56	9 (16%)
22	CLA	C	510	-	59,73,73	1.47	7 (11%)	67,113,113	1.47	8 (11%)
33	PHO	d	401	-	67,69,69	1.22	8 (11%)	85,99,99	1.30	9 (10%)
22	CLA	c	511	-	59,73,73	1.56	6 (10%)	67,113,113	1.70	14 (20%)
22	CLA	C	503	-	59,73,73	1.71	9 (15%)	67,113,113	1.74	10 (14%)
22	CLA	C	508	-	59,73,73	1.57	8 (13%)	67,113,113	1.41	7 (10%)
22	CLA	b	610	36	59,73,73	1.20	7 (11%)	67,113,113	1.51	13 (19%)
23	BCR	B	618	-	41,41,41	1.07	3 (7%)	56,56,56	1.43	10 (17%)
35	HEC	v	201	17	26,50,50	2.37	3 (11%)	18,82,82	2.08	6 (33%)
22	CLA	b	602	-	59,73,73	1.36	9 (15%)	67,113,113	1.56	10 (14%)
22	CLA	c	505	36	54,68,73	1.48	6 (11%)	61,107,113	1.57	12 (19%)
27	SQD	a	414	-	35,35,54	1.10	2 (5%)	37,37,65	1.30	3 (8%)
28	DGD	h	102	-	63,63,67	1.28	9 (14%)	77,77,81	1.40	9 (11%)
31	STE	I	101	-	14,14,19	0.62	0	13,13,19	0.43	0
29	OEX	A	415[A]	1,3,36	0,15,15	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	d	402	-	59,73,73	1.21	7 (11%)	67,113,113	1.27	11 (16%)
32	LMG	c	523	-	49,49,55	1.06	5 (10%)	57,57,63	1.30	4 (7%)
25	PL9	a	410	-	55,55,55	0.94	3 (5%)	68,69,69	1.61	9 (13%)
32	LMG	d	408	-	44,44,55	1.03	4 (9%)	52,52,63	1.27	6 (11%)
22	CLA	b	608	-	59,73,73	1.87	10 (16%)	67,113,113	1.43	11 (16%)
31	STE	B	625	-	14,14,19	0.46	0	13,13,19	0.79	0
22	CLA	B	606	-	59,73,73	1.73	8 (13%)	67,113,113	1.51	10 (14%)
22	CLA	B	614	-	59,73,73	1.53	6 (10%)	67,113,113	1.34	11 (16%)
31	STE	C	520	-	8,11,19	0.57	0	7,11,19	0.47	0
27	SQD	d	409	-	40,41,54	1.14	4 (10%)	49,52,65	1.99	13 (26%)
28	DGD	C	518	-	63,63,67	1.11	5 (7%)	77,77,81	1.37	11 (14%)
28	DGD	C	519	-	63,63,67	1.15	10 (15%)	77,77,81	1.38	8 (10%)
23	BCR	b	619	-	41,41,41	1.00	2 (4%)	56,56,56	1.40	7 (12%)
22	CLA	C	507	36	59,73,73	1.56	8 (13%)	67,113,113	1.69	9 (13%)
22	CLA	b	606	-	59,73,73	1.62	5 (8%)	67,113,113	1.83	13 (19%)
22	CLA	b	611	-	59,73,73	1.39	8 (13%)	67,113,113	1.64	14 (20%)
31	STE	j	101	-	8,11,19	0.52	0	7,11,19	0.48	0
22	CLA	C	513	-	59,73,73	1.48	7 (11%)	67,113,113	1.74	13 (19%)
22	CLA	b	616	-	54,68,73	1.53	8 (14%)	61,107,113	1.63	12 (19%)
35	HEC	V	201	17	26,50,50	2.29	3 (11%)	18,82,82	2.01	9 (50%)
31	STE	M	103	-	9,9,19	0.53	0	8,8,19	0.51	0
31	STE	B	620	-	13,16,19	0.48	0	12,16,19	0.68	0
23	BCR	k	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.08	4 (7%)
22	CLA	c	503	-	59,73,73	1.37	6 (10%)	67,113,113	1.63	14 (20%)
22	CLA	B	610	36	59,73,73	1.51	8 (13%)	67,113,113	1.44	12 (17%)
31	STE	b	622	-	12,15,19	0.64	0	11,15,19	0.56	0
22	CLA	a	411	36	59,73,73	1.66	6 (10%)	67,113,113	1.40	9 (13%)
22	CLA	C	512	-	59,73,73	1.58	8 (13%)	67,113,113	1.45	10 (14%)
26	LHG	d	407	-	38,38,48	1.03	2 (5%)	41,44,54	1.14	2 (4%)
31	STE	B	624	-	15,15,19	0.56	0	14,14,19	0.51	0
26	LHG	A	412	-	48,48,48	0.84	2 (4%)	51,54,54	1.17	5 (9%)
22	CLA	b	615	-	59,73,73	1.52	7 (11%)	67,113,113	1.46	12 (17%)
23	BCR	b	617	-	41,41,41	0.98	3 (7%)	56,56,56	1.30	8 (14%)
27	SQD	A	413	-	38,38,54	1.09	4 (10%)	40,40,65	1.43	4 (10%)
22	CLA	B	613	-	59,73,73	1.67	7 (11%)	67,113,113	1.64	16 (23%)
23	BCR	h	101	-	41,41,41	0.97	2 (4%)	56,56,56	1.36	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	SQD	a	413	-	53,54,54	0.94	4 (7%)	62,65,65	1.94	12 (19%)
26	LHG	L	102	-	48,48,48	0.75	2 (4%)	51,54,54	1.15	2 (3%)
35	HEC	f	101	5,6	26,50,50	2.33	3 (11%)	18,82,82	2.54	4 (22%)
32	LMG	Y	101	-	48,48,55	1.20	5 (10%)	56,56,63	1.21	5 (8%)
31	STE	D	413	-	16,19,19	0.38	0	15,19,19	0.94	0
27	SQD	L	101	-	48,49,54	0.95	2 (4%)	57,60,65	2.50	18 (31%)
22	CLA	B	605	-	59,73,73	1.31	6 (10%)	67,113,113	1.43	13 (19%)
22	CLA	D	405	-	59,73,73	1.20	5 (8%)	67,113,113	1.50	11 (16%)
22	CLA	b	607	36	59,73,73	1.48	4 (6%)	67,113,113	1.64	12 (17%)
32	LMG	a	417	-	55,55,55	1.57	10 (18%)	63,63,63	1.50	12 (19%)
22	CLA	b	612	-	59,73,73	1.33	5 (8%)	67,113,113	1.86	13 (19%)
22	CLA	C	504	36	53,67,73	1.63	6 (11%)	59,105,113	1.44	9 (15%)
32	LMG	m	101	-	51,51,55	1.14	4 (7%)	59,59,63	1.59	9 (15%)
22	CLA	b	613	-	59,73,73	1.57	7 (11%)	67,113,113	1.43	10 (14%)
31	STE	c	521	-	16,19,19	0.52	0	15,19,19	0.51	0
23	BCR	c	515	-	41,41,41	1.00	3 (7%)	56,56,56	1.28	9 (16%)
22	CLA	B	603	-	59,73,73	1.27	7 (11%)	67,113,113	1.57	13 (19%)
22	CLA	C	511	3	59,73,73	1.71	9 (15%)	67,113,113	1.36	7 (10%)
31	STE	H	103	-	17,17,19	0.47	0	16,16,19	0.69	0
23	BCR	T	101	-	41,41,41	1.05	3 (7%)	56,56,56	1.22	3 (5%)
22	CLA	a	402	-	59,73,73	1.61	5 (8%)	67,113,113	1.35	13 (19%)
22	CLA	C	505	-	59,73,73	1.66	7 (11%)	67,113,113	1.56	11 (16%)
22	CLA	b	605	-	59,73,73	1.35	6 (10%)	67,113,113	1.74	11 (16%)
31	STE	Z	101	-	7,7,19	0.50	0	6,6,19	0.33	0
26	LHG	a	412	-	48,48,48	1.07	5 (10%)	51,54,54	1.42	9 (17%)
22	CLA	B	615	-	59,73,73	1.69	7 (11%)	67,113,113	1.69	8 (11%)
28	DGD	c	518	-	63,63,67	1.08	3 (4%)	77,77,81	1.23	5 (6%)
23	BCR	B	617	-	41,41,41	1.05	2 (4%)	56,56,56	1.55	11 (19%)
31	STE	a	416	-	8,11,19	0.45	0	7,11,19	0.74	0
28	DGD	c	519	-	63,63,67	1.10	4 (6%)	77,77,81	1.38	13 (16%)
28	DGD	C	517	-	63,63,67	1.39	9 (14%)	77,77,81	1.39	12 (15%)
22	CLA	d	403	-	59,73,73	1.64	9 (15%)	67,113,113	1.22	4 (5%)
26	LHG	A	410	-	46,46,48	1.19	5 (10%)	49,52,54	1.16	4 (8%)
31	STE	L	103	-	8,11,19	0.51	0	7,11,19	0.73	0
30	OXY	a	419[B]	1,3,36	0,16,16	0.00	-	-	-	-
34	BCT	a	409	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PHO	D	401	-	67,69,69	1.20	11 (16%)	85,99,99	1.13	8 (9%)
32	LMG	c	522	-	48,48,55	1.19	4 (8%)	56,56,63	1.25	6 (10%)
22	CLA	A	403	36	59,73,73	1.56	7 (11%)	67,113,113	1.48	10 (14%)
22	CLA	A	409	36	59,73,73	1.30	5 (8%)	67,113,113	1.47	10 (14%)
22	CLA	a	405	-	59,73,73	1.44	8 (13%)	67,113,113	1.34	10 (14%)
31	STE	B	623	-	14,17,19	0.47	0	13,17,19	0.77	0
32	LMG	D	408	-	51,51,55	0.99	3 (5%)	59,59,63	1.47	7 (11%)
22	CLA	B	607	36	59,73,73	1.45	8 (13%)	67,113,113	1.65	11 (16%)
22	CLA	B	608	-	59,73,73	1.52	11 (18%)	67,113,113	1.73	12 (17%)
26	LHG	e	101	-	41,41,48	1.11	4 (9%)	44,47,54	1.24	3 (6%)
23	BCR	k	102	-	41,41,41	1.02	3 (7%)	56,56,56	1.17	6 (10%)
22	CLA	C	502	-	59,73,73	1.42	6 (10%)	67,113,113	1.44	10 (14%)
31	STE	M	102	-	11,14,19	0.54	0	10,14,19	0.57	0
27	SQD	A	411	-	51,52,54	1.09	5 (9%)	60,63,65	2.18	15 (25%)
33	PHO	D	402	-	67,69,69	1.25	9 (13%)	85,99,99	1.14	8 (9%)
22	CLA	D	404	-	59,73,73	1.49	7 (11%)	67,113,113	1.57	11 (16%)
22	CLA	A	404	-	48,62,73	1.41	10 (20%)	53,99,113	1.57	7 (13%)
34	BCT	D	403	21	0,3,3	0.00	-	0,3,3	0.00	-
31	STE	d	412	-	16,19,19	0.43	0	15,19,19	0.62	0
23	BCR	B	619	-	41,41,41	1.08	3 (7%)	56,56,56	1.55	13 (23%)
31	STE	d	411	-	16,19,19	0.44	0	15,19,19	0.67	0
22	CLA	c	507	-	59,73,73	1.33	7 (11%)	67,113,113	1.50	11 (16%)
32	LMG	D	411	-	20,26,55	0.83	0	18,26,63	1.05	0
26	LHG	l	101	-	48,48,48	0.79	1 (2%)	51,54,54	1.25	6 (11%)
23	BCR	C	514	-	41,41,41	1.25	4 (9%)	56,56,56	1.30	5 (8%)
22	CLA	B	611	-	59,73,73	1.41	8 (13%)	67,113,113	1.44	10 (14%)
22	CLA	b	601	36	59,73,73	1.64	7 (11%)	67,113,113	1.70	9 (13%)
31	STE	J	101	-	8,11,19	0.33	0	7,11,19	0.77	0
31	STE	B	601	-	8,11,19	0.38	0	7,11,19	0.70	0
30	OEY	A	416[B]	1,3,36	0,16,16	0.00	-	-		
32	LMG	M	101	-	51,51,55	0.86	1 (1%)	59,59,63	1.37	11 (18%)
23	BCR	C	515	-	41,41,41	1.11	2 (4%)	56,56,56	1.36	8 (14%)
23	BCR	K	101	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	9 (16%)
22	CLA	b	603	-	59,73,73	1.62	10 (16%)	67,113,113	1.58	11 (16%)
31	STE	h	103	-	13,13,19	0.43	0	12,12,19	0.61	0
31	STE	B	622	-	8,11,19	0.49	0	7,11,19	0.78	0
22	CLA	b	614	-	59,73,73	1.40	10 (16%)	67,113,113	1.39	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	512	3	59,73,73	1.65	6 (10%)	67,113,113	1.51	6 (8%)
23	BCR	a	406	-	41,41,41	1.03	3 (7%)	56,56,56	1.35	5 (8%)
22	CLA	C	501	-	59,73,73	1.66	8 (13%)	67,113,113	1.35	9 (13%)
22	CLA	b	604	-	59,73,73	1.50	5 (8%)	67,113,113	2.19	17 (25%)
23	BCR	A	405	-	41,41,41	1.16	1 (2%)	56,56,56	1.42	10 (17%)
22	CLA	a	403	36	59,73,73	1.43	9 (15%)	67,113,113	1.69	11 (16%)
22	CLA	c	510	-	59,73,73	1.42	6 (10%)	67,113,113	1.77	11 (16%)
27	SQD	B	621	-	53,54,54	0.94	2 (3%)	62,65,65	2.19	16 (25%)
22	CLA	c	502	-	59,73,73	1.33	7 (11%)	67,113,113	1.51	13 (19%)
29	OEX	a	418[A]	1,3,36	0,15,15	0.00	-	-		
25	PL9	d	405	-	55,55,55	1.47	7 (12%)	68,69,69	1.62	11 (16%)
22	CLA	B	602	-	59,73,73	1.51	6 (10%)	67,113,113	1.70	13 (19%)
28	DGD	A	414	-	67,67,67	1.41	9 (13%)	81,81,81	1.41	13 (16%)
31	STE	C	522	-	8,11,19	0.49	0	7,11,19	0.87	0
22	CLA	B	612	-	59,73,73	1.43	7 (11%)	67,113,113	1.54	7 (10%)
22	CLA	c	504	-	59,73,73	1.44	8 (13%)	67,113,113	1.35	4 (5%)
22	CLA	B	609	-	59,73,73	1.50	7 (11%)	67,113,113	1.87	9 (13%)
25	PL9	D	407	-	55,55,55	1.18	3 (5%)	68,69,69	1.88	18 (26%)
32	LMG	D	410	-	31,31,55	1.23	4 (12%)	33,33,63	1.14	3 (9%)
23	BCR	D	406	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	8 (14%)
22	CLA	H	101	36	59,73,73	1.68	8 (13%)	67,113,113	1.42	8 (11%)
26	LHG	d	406	-	48,48,48	0.79	2 (4%)	51,54,54	1.16	1 (1%)
31	STE	b	623	-	16,19,19	0.60	0	15,19,19	0.58	0
31	STE	d	410	-	13,16,19	0.34	0	12,16,19	1.00	0
32	LMG	c	520	-	37,37,55	1.13	4 (10%)	45,45,63	1.36	7 (15%)
31	STE	t	102	-	10,13,19	0.53	0	9,13,19	0.69	0
31	STE	b	624	-	9,9,19	0.46	0	8,8,19	0.48	0
22	CLA	C	509	-	59,73,73	1.46	8 (13%)	67,113,113	1.53	10 (14%)
22	CLA	b	609	-	59,73,73	1.80	8 (13%)	67,113,113	1.66	14 (20%)
28	DGD	c	517	-	63,63,67	1.35	8 (12%)	77,77,81	1.42	13 (16%)

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
32	LMG	b	621	-	-	25/50/70/70	0/1/1/1
22	CLA	c	514	-	3/3/25/25	9/37/135/135	-
26	LHG	D	412	-	-	15/53/53/53	-
23	BCR	b	618	-	-	4/29/63/63	0/2/2/2
27	SQD	F	102	-	-	15/28/48/69	0/1/1/1
31	STE	a	415	-	-	3/7/7/17	-
28	DGD	H	102	-	-	17/51/91/95	0/2/2/2
22	CLA	B	604	-	3/3/25/25	10/37/135/135	-
31	STE	b	620	-	-	8/15/17/17	-
33	PHO	a	404	-	-	8/53/103/103	0/5/6/6
22	CLA	c	513	-	3/3/25/25	18/37/135/135	-
22	CLA	B	616	-	3/3/24/25	8/31/129/135	-
31	STE	C	521	-	-	6/13/13/17	-
22	CLA	c	506	-	2/2/25/25	12/37/135/135	-
23	BCR	t	101	-	-	6/29/63/63	0/2/2/2
22	CLA	A	402	-	3/3/25/25	8/37/135/135	-
23	BCR	X	101	-	-	6/29/63/63	0/2/2/2
31	STE	R	101	-	-	3/7/9/17	-
23	BCR	c	516	-	-	5/29/63/63	0/2/2/2
23	BCR	d	404	-	-	5/29/63/63	0/2/2/2
32	LMG	C	516	-	-	16/43/63/70	0/1/1/1
31	STE	T	103	-	-	8/12/12/17	-
31	STE	M	104	-	-	7/15/15/17	-
22	CLA	C	506	-	3/3/25/25	13/37/135/135	-
23	BCR	K	102	-	-	11/29/63/63	0/2/2/2
22	CLA	c	508	36	3/3/25/25	12/37/135/135	-
25	PL9	A	408	-	-	21/53/73/73	0/1/1/1
31	STE	c	501	-	-	5/7/9/17	-
31	STE	T	102	-	-	10/13/13/17	-
22	CLA	c	509	-	3/3/24/25	5/36/134/135	-
35	HEC	F	101	5,6	-	0/6/54/54	-
26	LHG	D	409	-	-	22/53/53/53	-
22	CLA	C	510	-	3/3/25/25	6/37/135/135	-
33	PHO	d	401	-	-	9/53/103/103	0/5/6/6
22	CLA	c	511	-	3/3/25/25	11/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	503	-	3/3/25/25	3/37/135/135	-
22	CLA	C	508	-	2/2/25/25	8/37/135/135	-
22	CLA	b	610	36	3/3/25/25	5/37/135/135	-
23	BCR	B	618	-	-	4/29/63/63	0/2/2/2
35	HEC	v	201	17	-	0/6/54/54	-
22	CLA	b	602	-	1/1/25/25	6/37/135/135	-
22	CLA	c	505	36	3/3/24/25	5/31/129/135	-
27	SQD	a	414	-	-	16/37/37/69	-
28	DGD	h	102	-	-	15/51/91/95	0/2/2/2
31	STE	I	101	-	-	4/12/12/17	-
31	STE	B	620	-	-	9/12/14/17	-
31	STE	M	102	-	-	8/10/12/17	-
32	LMG	c	523	-	-	22/44/64/70	0/1/1/1
27	SQD	a	413	-	-	25/49/69/69	0/1/1/1
32	LMG	d	408	-	-	11/39/59/70	0/1/1/1
22	CLA	b	608	-	2/2/25/25	7/37/135/135	-
31	STE	B	625	-	-	7/12/12/17	-
22	CLA	B	606	-	3/3/25/25	10/37/135/135	-
22	CLA	B	614	-	3/3/25/25	14/37/135/135	-
31	STE	C	520	-	-	3/7/9/17	-
27	SQD	d	409	-	-	13/36/56/69	0/1/1/1
28	DGD	C	518	-	-	22/51/91/95	0/2/2/2
28	DGD	C	519	-	-	18/51/91/95	0/2/2/2
23	BCR	b	619	-	-	8/29/63/63	0/2/2/2
22	CLA	C	507	36	3/3/25/25	5/37/135/135	-
22	CLA	b	606	-	3/3/25/25	4/37/135/135	-
22	CLA	b	611	-	3/3/25/25	8/37/135/135	-
31	STE	j	101	-	-	4/7/9/17	-
22	CLA	C	513	-	3/3/25/25	10/37/135/135	-
22	CLA	b	616	-	3/3/24/25	5/31/129/135	-
35	HEC	V	201	17	-	0/6/54/54	-
31	STE	M	103	-	-	2/7/7/17	-
23	BCR	k	101	-	-	10/29/63/63	0/2/2/2
22	CLA	c	503	-	2/2/25/25	8/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	610	36	3/3/25/25	5/37/135/135	-
31	STE	b	622	-	-	4/11/13/17	-
22	CLA	a	411	36	2/2/25/25	5/37/135/135	-
22	CLA	C	512	-	3/3/25/25	10/37/135/135	-
26	LHG	d	407	-	-	15/43/43/53	-
31	STE	B	624	-	-	10/13/13/17	-
26	LHG	A	412	-	-	28/53/53/53	-
22	CLA	b	615	-	3/3/25/25	3/37/135/135	-
23	BCR	b	617	-	-	6/29/63/63	0/2/2/2
27	SQD	A	413	-	-	18/39/39/69	-
22	CLA	B	613	-	3/3/25/25	12/37/135/135	-
23	BCR	h	101	-	-	8/29/63/63	0/2/2/2
25	PL9	a	410	-	-	19/53/73/73	0/1/1/1
26	LHG	L	102	-	-	17/53/53/53	-
32	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
31	STE	D	413	-	-	12/15/17/17	-
27	SQD	L	101	-	-	18/44/64/69	0/1/1/1
22	CLA	B	605	-	2/2/25/25	14/37/135/135	-
22	CLA	D	405	-	3/3/25/25	13/37/135/135	-
23	BCR	B	619	-	-	7/29/63/63	0/2/2/2
32	LMG	a	417	-	-	30/50/70/70	0/1/1/1
22	CLA	b	612	-	3/3/25/25	4/37/135/135	-
22	CLA	C	504	36	3/3/23/25	7/30/128/135	-
32	LMG	m	101	-	-	20/46/66/70	0/1/1/1
22	CLA	b	613	-	3/3/25/25	8/37/135/135	-
31	STE	c	521	-	-	8/15/17/17	-
23	BCR	c	515	-	-	8/29/63/63	0/2/2/2
22	CLA	B	603	-	3/3/25/25	12/37/135/135	-
22	CLA	C	511	3	3/3/25/25	8/37/135/135	-
31	STE	H	103	-	-	8/15/15/17	-
23	BCR	T	101	-	-	10/29/63/63	0/2/2/2
22	CLA	a	402	-	3/3/25/25	5/37/135/135	-
22	CLA	C	505	-	1/1/25/25	8/37/135/135	-
22	CLA	b	605	-	3/3/25/25	7/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	Z	101	-	-	2/5/5/17	-
26	LHG	a	412	-	-	20/53/53/53	-
22	CLA	B	615	-	3/3/25/25	7/37/135/135	-
28	DGD	c	518	-	-	18/51/91/95	0/2/2/2
23	BCR	B	617	-	-	9/29/63/63	0/2/2/2
31	STE	a	416	-	-	4/7/9/17	-
28	DGD	c	519	-	-	18/51/91/95	0/2/2/2
28	DGD	C	517	-	-	18/51/91/95	0/2/2/2
22	CLA	d	403	-	2/2/25/25	6/37/135/135	-
26	LHG	A	410	-	-	23/51/51/53	-
31	STE	L	103	-	-	4/7/9/17	-
33	PHO	D	401	-	-	5/53/103/103	0/5/6/6
32	LMG	c	522	-	-	25/43/63/70	0/1/1/1
22	CLA	A	403	36	3/3/25/25	11/37/135/135	-
22	CLA	A	409	36	3/3/25/25	7/37/135/135	-
22	CLA	a	405	-	3/3/25/25	12/37/135/135	-
31	STE	B	623	-	-	8/13/15/17	-
32	LMG	D	408	-	-	15/46/66/70	0/1/1/1
22	CLA	B	607	36	3/3/25/25	14/37/135/135	-
22	CLA	B	608	-	3/3/25/25	3/37/135/135	-
26	LHG	e	101	-	-	24/46/46/53	-
23	BCR	k	102	-	-	9/29/63/63	0/2/2/2
22	CLA	C	502	-	3/3/25/25	8/37/135/135	-
22	CLA	d	402	-	1/1/25/25	6/37/135/135	-
27	SQD	A	411	-	-	24/47/67/69	0/1/1/1
33	PHO	D	402	-	-	4/53/103/103	0/5/6/6
22	CLA	D	404	-	1/1/25/25	8/37/135/135	-
22	CLA	A	404	-	3/3/22/25	1/24/122/135	-
35	HEC	f	101	5,6	-	0/6/54/54	-
31	STE	d	412	-	-	9/15/17/17	-
22	CLA	b	607	36	3/3/25/25	12/37/135/135	-
31	STE	d	411	-	-	9/15/17/17	-
22	CLA	c	507	-	3/3/25/25	14/37/135/135	-
32	LMG	D	411	-	-	8/18/22/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	l	101	-	-	15/53/53/53	-
23	BCR	C	514	-	-	5/29/63/63	0/2/2/2
22	CLA	B	611	-	3/3/25/25	4/37/135/135	-
22	CLA	b	601	36	2/2/25/25	21/37/135/135	-
31	STE	J	101	-	-	2/7/9/17	-
31	STE	B	601	-	-	5/7/9/17	-
32	LMG	M	101	-	-	25/46/66/70	0/1/1/1
23	BCR	C	515	-	-	11/29/63/63	0/2/2/2
23	BCR	K	101	-	-	9/29/63/63	0/2/2/2
22	CLA	b	603	-	3/3/25/25	4/37/135/135	-
31	STE	h	103	-	-	6/11/11/17	-
31	STE	B	622	-	-	5/7/9/17	-
22	CLA	b	614	-	3/3/25/25	17/37/135/135	-
22	CLA	c	512	3	3/3/25/25	3/37/135/135	-
23	BCR	a	406	-	-	7/29/63/63	0/2/2/2
22	CLA	C	501	-	3/3/25/25	2/37/135/135	-
22	CLA	b	604	-	3/3/25/25	10/37/135/135	-
23	BCR	A	405	-	-	9/29/63/63	0/2/2/2
22	CLA	a	403	36	2/2/25/25	10/37/135/135	-
22	CLA	c	510	-	3/3/25/25	11/37/135/135	-
27	SQD	B	621	-	-	24/49/69/69	0/1/1/1
22	CLA	c	502	-	3/3/25/25	5/37/135/135	-
25	PL9	d	405	-	-	17/53/73/73	0/1/1/1
22	CLA	B	602	-	3/3/25/25	9/37/135/135	-
28	DGD	A	414	-	-	27/55/95/95	0/2/2/2
31	STE	C	522	-	-	1/7/9/17	-
22	CLA	B	612	-	3/3/25/25	8/37/135/135	-
22	CLA	c	504	-	3/3/25/25	7/37/135/135	-
22	CLA	B	609	-	1/1/25/25	2/37/135/135	-
25	PL9	D	407	-	-	12/53/73/73	0/1/1/1
32	LMG	D	410	-	-	13/33/33/70	-
23	BCR	D	406	-	-	4/29/63/63	0/2/2/2
22	CLA	H	101	36	3/3/25/25	18/37/135/135	-
26	LHG	d	406	-	-	23/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	STE	b	623	-	-	9/15/17/17	-
31	STE	d	410	-	-	9/12/14/17	-
32	LMG	c	520	-	-	7/31/51/70	0/1/1/1
31	STE	t	102	-	-	4/9/11/17	-
31	STE	b	624	-	-	2/7/7/17	-
22	CLA	C	509	-	3/3/25/25	11/37/135/135	-
22	CLA	b	609	-	1/1/25/25	8/37/135/135	-
28	DGD	c	517	-	-	28/51/91/95	0/2/2/2

All (804) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	101	CLA	C4B-NB	8.96	1.43	1.35
22	B	613	CLA	C4B-NB	8.96	1.43	1.35
22	C	503	CLA	C4B-NB	8.41	1.42	1.35
22	A	403	CLA	C4B-NB	8.23	1.42	1.35
22	b	604	CLA	C4B-NB	8.15	1.42	1.35
22	B	606	CLA	MG-NA	8.08	2.25	2.06
22	b	601	CLA	C4B-NB	8.02	1.42	1.35
35	F	101	HEC	C3C-C2C	-8.01	1.32	1.40
22	B	602	CLA	C4B-NB	7.93	1.42	1.35
22	b	609	CLA	C4B-NB	7.88	1.42	1.35
22	C	504	CLA	C4B-NB	7.79	1.42	1.35
22	B	614	CLA	C4B-NB	7.76	1.42	1.35
35	V	201	HEC	C3B-C2B	-7.73	1.32	1.40
22	b	607	CLA	C4B-NB	7.70	1.42	1.35
22	C	501	CLA	C4B-NB	7.65	1.42	1.35
22	C	506	CLA	C4B-NB	7.60	1.42	1.35
22	a	402	CLA	C4B-NB	7.46	1.41	1.35
22	b	613	CLA	C4B-NB	7.45	1.41	1.35
22	b	606	CLA	C4B-NB	7.35	1.41	1.35
22	B	610	CLA	C4B-NB	7.34	1.41	1.35
22	a	411	CLA	MG-NA	7.34	2.23	2.06
22	c	514	CLA	C4B-NB	7.32	1.41	1.35
22	c	506	CLA	C4B-NB	7.30	1.41	1.35
22	C	511	CLA	MG-NA	7.27	2.23	2.06
22	c	509	CLA	C4B-NB	7.26	1.41	1.35
22	b	608	CLA	C4B-NB	7.25	1.41	1.35
22	C	505	CLA	MG-NA	7.24	2.23	2.06
22	c	512	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	C4B-NB	7.19	1.41	1.35
22	B	615	CLA	C4B-NB	7.18	1.41	1.35
35	f	101	HEC	C3B-C2B	-7.17	1.33	1.40
22	C	512	CLA	MG-NA	7.16	2.23	2.06
22	B	616	CLA	MG-NA	7.16	2.23	2.06
22	C	510	CLA	C4B-NB	7.15	1.41	1.35
22	B	616	CLA	C4B-NB	7.07	1.41	1.35
22	b	608	CLA	MG-NA	6.98	2.22	2.06
22	c	510	CLA	C4B-NB	6.96	1.41	1.35
22	c	505	CLA	C4B-NB	6.94	1.41	1.35
22	b	616	CLA	C4B-NB	6.94	1.41	1.35
22	c	513	CLA	C4B-NB	6.92	1.41	1.35
22	b	603	CLA	C4B-NB	6.85	1.41	1.35
22	c	503	CLA	C4B-NB	6.83	1.41	1.35
22	A	402	CLA	C4B-NB	6.77	1.41	1.35
22	C	513	CLA	C4B-NB	6.75	1.41	1.35
22	d	403	CLA	C4B-NB	6.71	1.41	1.35
35	v	201	HEC	C3B-C2B	-6.70	1.33	1.40
22	c	511	CLA	MG-NA	6.66	2.22	2.06
22	c	512	CLA	MG-NA	6.62	2.22	2.06
25	d	405	PL9	C6-C1	-6.58	1.36	1.48
35	v	201	HEC	C3C-C2C	-6.56	1.33	1.40
22	B	609	CLA	MG-NA	6.55	2.21	2.06
22	C	508	CLA	C4B-NB	6.54	1.41	1.35
22	b	612	CLA	C4B-NB	6.45	1.41	1.35
35	F	101	HEC	C3B-C2B	-6.45	1.34	1.40
22	C	505	CLA	C4B-NB	6.37	1.40	1.35
22	c	504	CLA	C4B-NB	6.34	1.40	1.35
22	b	615	CLA	C4B-NB	6.33	1.40	1.35
22	C	502	CLA	C4B-NB	6.33	1.40	1.35
22	a	411	CLA	C4B-NB	6.29	1.40	1.35
22	b	605	CLA	C4B-NB	6.29	1.40	1.35
22	B	612	CLA	C4B-NB	6.29	1.40	1.35
22	c	508	CLA	C4B-NB	6.29	1.40	1.35
22	B	604	CLA	MG-NA	6.28	2.21	2.06
22	C	509	CLA	C4B-NB	6.26	1.40	1.35
22	c	502	CLA	C4B-NB	6.21	1.40	1.35
22	a	405	CLA	C4B-NB	6.12	1.40	1.35
22	C	507	CLA	C4B-NB	6.12	1.40	1.35
22	A	409	CLA	C4B-NB	5.98	1.40	1.35
22	B	607	CLA	C4B-NB	5.94	1.40	1.35
22	C	506	CLA	MG-NA	5.85	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	C4B-NB	5.84	1.40	1.35
22	c	507	CLA	C4B-NB	5.83	1.40	1.35
22	c	509	CLA	MG-NA	5.82	2.20	2.06
22	c	511	CLA	C4B-NB	5.76	1.40	1.35
35	f	101	HEC	C3C-C2C	-5.72	1.34	1.40
22	C	508	CLA	MG-NA	5.69	2.19	2.06
22	b	609	CLA	MG-NC	5.69	2.19	2.06
25	A	408	PL9	C7-C3	-5.65	1.45	1.51
22	B	608	CLA	MG-NA	5.61	2.19	2.06
22	d	403	CLA	MG-NA	5.56	2.19	2.06
22	D	404	CLA	MG-NA	5.31	2.18	2.06
22	C	503	CLA	MG-NA	5.28	2.18	2.06
22	b	614	CLA	C4B-NB	5.26	1.39	1.35
22	B	615	CLA	MG-NA	5.22	2.18	2.06
22	B	609	CLA	C4B-NB	5.16	1.39	1.35
22	a	402	CLA	MG-NA	5.13	2.18	2.06
22	C	507	CLA	MG-NC	-5.05	1.94	2.06
22	B	605	CLA	C4B-NB	5.03	1.39	1.35
22	b	608	CLA	MG-NC	-5.03	1.94	2.06
22	b	606	CLA	MG-NC	5.03	2.18	2.06
22	B	613	CLA	MG-NA	5.01	2.18	2.06
22	D	404	CLA	C4B-NB	4.99	1.39	1.35
22	C	513	CLA	MG-NA	4.98	2.18	2.06
28	A	414	DGD	C4D-C5D	4.95	1.63	1.53
22	b	615	CLA	MG-NA	4.94	2.18	2.06
22	B	607	CLA	MG-NA	4.80	2.17	2.06
35	f	101	HEC	C3D-C2D	4.79	1.51	1.37
32	a	417	LMG	C4-C5	4.78	1.63	1.53
22	b	613	CLA	MG-NA	4.75	2.17	2.06
22	b	601	CLA	MG-NA	4.75	2.17	2.06
22	B	611	CLA	C4B-NB	4.74	1.39	1.35
22	B	608	CLA	C4B-NB	4.74	1.39	1.35
35	V	201	HEC	C3C-C2C	-4.71	1.35	1.40
35	F	101	HEC	C3D-C2D	4.70	1.51	1.37
22	b	611	CLA	MG-NA	4.68	2.17	2.06
22	a	403	CLA	C4B-NB	4.68	1.39	1.35
22	D	405	CLA	C4B-NB	4.67	1.39	1.35
22	C	504	CLA	MG-NA	4.67	2.17	2.06
26	D	409	LHG	O8-C6	-4.63	1.34	1.45
35	v	201	HEC	C3D-C2D	4.62	1.51	1.37
22	b	609	CLA	MG-NA	4.60	2.17	2.06
22	c	513	CLA	MG-NC	4.55	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	501	CLA	MG-NA	4.54	2.17	2.06
22	B	606	CLA	C4B-NB	4.53	1.39	1.35
35	V	201	HEC	C3D-C2D	4.50	1.51	1.37
22	B	611	CLA	MG-NC	4.46	2.16	2.06
22	c	506	CLA	MG-NA	4.42	2.16	2.06
32	C	516	LMG	C4-C3	4.42	1.63	1.52
23	C	514	BCR	C1-C6	-4.38	1.47	1.53
23	b	618	BCR	C30-C25	-4.38	1.47	1.53
25	A	408	PL9	C21-C19	4.34	1.60	1.51
22	C	507	CLA	MG-NA	4.30	2.16	2.06
22	A	404	CLA	C4B-NB	4.27	1.39	1.35
22	b	603	CLA	MG-NC	4.22	2.16	2.06
22	B	612	CLA	MG-NA	4.21	2.16	2.06
22	B	606	CLA	C3B-C2B	-4.20	1.34	1.40
22	A	402	CLA	CHC-C1C	4.18	1.45	1.35
22	B	604	CLA	C4B-NB	4.14	1.38	1.35
23	d	404	BCR	C1-C6	-4.14	1.48	1.53
32	a	417	LMG	C7-C8	4.13	1.63	1.50
22	a	403	CLA	MG-NC	4.12	2.16	2.06
22	d	402	CLA	C4B-NB	4.11	1.38	1.35
22	b	604	CLA	MG-NA	4.10	2.16	2.06
22	b	606	CLA	MG-NA	4.09	2.16	2.06
22	b	611	CLA	C4B-NB	4.01	1.38	1.35
23	K	102	BCR	C1-C6	-4.01	1.48	1.53
22	C	502	CLA	C3B-C2B	-4.01	1.34	1.40
22	b	610	CLA	C4B-NB	4.00	1.38	1.35
28	A	414	DGD	C3E-C2E	4.00	1.62	1.52
28	C	517	DGD	O5D-C6D	-4.00	1.36	1.43
22	C	512	CLA	MG-NC	-3.98	1.96	2.06
23	K	101	BCR	C1-C6	-3.97	1.48	1.53
22	B	615	CLA	CHC-C1C	3.94	1.45	1.35
26	D	409	LHG	O7-C5	-3.93	1.36	1.46
23	X	101	BCR	C30-C25	-3.92	1.48	1.53
27	a	414	SQD	O47-C7	3.91	1.45	1.34
32	Y	101	LMG	C4-C5	3.90	1.61	1.53
22	C	512	CLA	C4B-NB	3.89	1.38	1.35
22	B	603	CLA	C3B-C2B	-3.89	1.35	1.40
32	m	101	LMG	O7-C8	-3.89	1.36	1.46
28	H	102	DGD	C4E-C5E	3.89	1.61	1.53
26	a	412	LHG	O7-C5	-3.87	1.36	1.46
27	F	102	SQD	O48-C23	3.84	1.44	1.33
22	C	505	CLA	CHC-C1C	3.84	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	MG-NC	3.83	2.15	2.06
22	C	509	CLA	MG-NA	3.79	2.15	2.06
23	D	406	BCR	C1-C6	-3.79	1.48	1.53
22	c	508	CLA	MG-NA	3.78	2.15	2.06
23	C	514	BCR	C30-C25	-3.75	1.48	1.53
22	C	501	CLA	C3B-C2B	-3.72	1.35	1.40
22	A	402	CLA	MG-NA	3.70	2.15	2.06
23	B	617	BCR	C1-C6	-3.65	1.48	1.53
28	c	517	DGD	O2G-C2G	-3.65	1.37	1.46
22	a	403	CLA	MG-NA	-3.64	1.97	2.06
22	c	513	CLA	CHC-C1C	3.64	1.44	1.35
32	m	101	LMG	C4-C3	3.64	1.61	1.52
22	B	614	CLA	MG-NC	3.61	2.14	2.06
28	C	518	DGD	C4D-C3D	3.61	1.61	1.52
26	d	407	LHG	P-O6	3.58	1.73	1.59
28	A	414	DGD	C1E-C2E	3.56	1.62	1.52
27	A	413	SQD	O48-C23	3.56	1.43	1.33
22	d	403	CLA	CHC-C1C	3.55	1.44	1.35
22	b	609	CLA	CMB-C2B	-3.54	1.44	1.51
23	c	516	BCR	C1-C6	-3.53	1.48	1.53
22	C	510	CLA	CHC-C1C	3.52	1.44	1.35
23	A	405	BCR	C1-C6	-3.52	1.48	1.53
23	D	406	BCR	C30-C25	-3.52	1.48	1.53
28	c	518	DGD	O5D-C1E	3.52	1.46	1.40
23	k	101	BCR	C30-C25	-3.49	1.49	1.53
22	B	604	CLA	CHC-C1C	3.49	1.43	1.35
26	A	410	LHG	P-O6	3.47	1.73	1.59
23	C	515	BCR	C30-C25	-3.46	1.49	1.53
28	A	414	DGD	C3G-C2G	3.45	1.61	1.50
22	b	607	CLA	CHC-C1C	3.44	1.43	1.35
28	H	102	DGD	C1E-C2E	3.44	1.62	1.52
22	c	510	CLA	CHC-C1C	3.43	1.43	1.35
22	H	101	CLA	MG-NA	3.43	2.14	2.06
27	L	101	SQD	O48-C23	3.43	1.43	1.33
22	c	509	CLA	CHC-C1C	3.41	1.43	1.35
22	b	601	CLA	CHC-C1C	3.41	1.43	1.35
22	D	405	CLA	CMD-C2D	-3.41	1.43	1.51
27	B	621	SQD	O48-C23	3.41	1.43	1.33
27	A	411	SQD	O48-C23	3.40	1.43	1.33
32	D	408	LMG	O2-C2	-3.39	1.35	1.43
32	c	522	LMG	C7-C8	3.39	1.61	1.50
22	b	608	CLA	C1B-NB	3.39	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	CHC-C1C	3.38	1.43	1.35
27	A	413	SQD	O47-C7	3.37	1.43	1.34
22	D	404	CLA	CMB-C2B	-3.37	1.44	1.51
28	c	517	DGD	O6E-C1E	-3.37	1.33	1.41
27	B	621	SQD	O47-C7	3.36	1.43	1.34
27	d	409	SQD	O47-C7	3.31	1.43	1.34
22	c	512	CLA	CHC-C1C	3.30	1.43	1.35
22	B	606	CLA	C3B-CAB	-3.30	1.41	1.47
22	B	608	CLA	C1D-C2D	3.28	1.50	1.42
22	B	602	CLA	CHC-C1C	3.27	1.43	1.35
26	e	101	LHG	P-O6	3.27	1.72	1.59
23	B	619	BCR	C1-C6	-3.26	1.49	1.53
28	C	517	DGD	O1G-C1G	-3.26	1.37	1.45
23	k	102	BCR	C30-C25	-3.26	1.49	1.53
22	C	508	CLA	C1B-NB	3.25	1.38	1.35
22	b	604	CLA	CHC-C1C	3.25	1.43	1.35
22	B	610	CLA	C3B-C2B	-3.23	1.35	1.40
32	a	417	LMG	C4-C3	3.23	1.60	1.52
32	a	417	LMG	O7-C10	3.22	1.43	1.34
22	A	403	CLA	CMD-C2D	-3.22	1.43	1.51
22	B	605	CLA	CHC-C1C	3.22	1.43	1.35
23	t	101	BCR	C30-C25	-3.20	1.49	1.53
22	b	616	CLA	MG-NA	3.20	2.13	2.06
22	a	405	CLA	CMC-C2C	-3.20	1.44	1.50
22	b	608	CLA	CHC-C1C	3.20	1.43	1.35
28	c	517	DGD	O3E-C3E	-3.18	1.35	1.43
22	a	411	CLA	CMB-C2B	-3.18	1.45	1.51
22	c	511	CLA	CHC-C1C	3.18	1.43	1.35
22	A	403	CLA	CHC-C1C	3.18	1.43	1.35
32	c	520	LMG	C4-C3	3.18	1.60	1.52
22	B	606	CLA	MG-NC	-3.18	1.98	2.06
25	D	407	PL9	C52-C5	-3.18	1.44	1.50
22	c	514	CLA	CHC-C1C	3.17	1.43	1.35
28	h	102	DGD	O2G-C1B	3.17	1.43	1.34
22	c	513	CLA	C1D-C2D	3.17	1.49	1.42
22	b	615	CLA	CHC-C1C	3.15	1.43	1.35
22	B	603	CLA	C3B-CAB	-3.15	1.41	1.47
22	C	510	CLA	MG-NC	3.15	2.13	2.06
27	a	414	SQD	O48-C23	3.15	1.42	1.33
22	C	504	CLA	CHC-C1C	3.15	1.43	1.35
22	H	101	CLA	CHC-C1C	3.15	1.43	1.35
22	B	610	CLA	CMB-C2B	-3.15	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	CHC-C1C	3.15	1.43	1.35
23	K	101	BCR	C30-C25	-3.14	1.49	1.53
26	a	412	LHG	C24-C23	3.14	1.59	1.50
22	b	611	CLA	C1D-C2D	3.13	1.49	1.42
32	m	101	LMG	O1-C7	-3.13	1.38	1.43
22	b	603	CLA	MG-NA	3.13	2.13	2.06
22	b	615	CLA	C3B-C2B	-3.13	1.36	1.40
28	h	102	DGD	C4E-C5E	3.13	1.59	1.53
33	d	401	PHO	CHC-C1C	3.12	1.44	1.38
22	b	614	CLA	C3B-C2B	-3.12	1.36	1.40
27	d	409	SQD	O48-C23	3.12	1.42	1.33
23	k	101	BCR	C1-C6	-3.12	1.49	1.53
22	b	603	CLA	C3B-C2B	-3.11	1.36	1.40
22	a	402	CLA	CHC-C1C	3.10	1.42	1.35
22	C	501	CLA	CMB-C2B	-3.09	1.45	1.51
22	b	609	CLA	C3B-C2B	-3.09	1.36	1.40
22	C	501	CLA	CHC-C1C	3.09	1.42	1.35
27	a	413	SQD	O48-C23	3.08	1.42	1.33
26	D	412	LHG	C24-C23	3.08	1.59	1.50
22	b	608	CLA	C1D-C2D	3.08	1.49	1.42
22	C	502	CLA	CHC-C1C	3.08	1.42	1.35
22	b	615	CLA	CMB-C2B	-3.07	1.45	1.51
26	A	410	LHG	O3-C3	-3.07	1.33	1.44
22	B	615	CLA	CMB-C2B	-3.06	1.45	1.51
28	H	102	DGD	C4D-C3D	3.06	1.60	1.52
22	B	610	CLA	C1D-C2D	3.04	1.49	1.42
32	D	410	LMG	C7-C8	3.03	1.58	1.51
22	C	511	CLA	CHC-C1C	3.02	1.42	1.35
26	A	410	LHG	C24-C23	-3.02	1.41	1.50
32	c	522	LMG	O1-C1	3.01	1.45	1.40
23	d	404	BCR	C30-C25	-3.00	1.49	1.53
23	T	101	BCR	C1-C6	-3.00	1.49	1.53
22	B	606	CLA	CHC-C1C	3.00	1.42	1.35
22	c	505	CLA	C3B-C2B	-3.00	1.36	1.40
32	m	101	LMG	C1-C2	2.99	1.61	1.52
25	a	410	PL9	C53-C6	-2.99	1.44	1.50
22	c	505	CLA	CHC-C1C	2.99	1.42	1.35
22	b	603	CLA	CMD-C2D	-2.99	1.44	1.51
22	H	101	CLA	CMB-C2B	-2.99	1.45	1.51
22	D	404	CLA	CAA-C2A	-2.98	1.48	1.54
22	C	503	CLA	CHC-C1C	2.98	1.42	1.35
22	C	506	CLA	CMC-C2C	-2.98	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	616	CLA	CHC-C1C	2.97	1.42	1.35
28	C	519	DGD	O6D-C5D	-2.97	1.37	1.44
22	B	615	CLA	C3B-C2B	-2.97	1.36	1.40
23	a	406	BCR	C30-C25	-2.96	1.49	1.53
22	B	616	CLA	CMC-C2C	-2.96	1.44	1.50
22	C	507	CLA	CMD-C2D	-2.96	1.44	1.51
33	D	402	PHO	C1A-NA	2.96	1.43	1.37
22	B	604	CLA	CMB-C2B	-2.96	1.45	1.51
22	A	409	CLA	C1D-C2D	2.95	1.49	1.42
28	C	517	DGD	C6E-C5E	2.95	1.61	1.51
28	C	518	DGD	O3E-C3E	-2.94	1.36	1.43
22	C	513	CLA	CHC-C1C	2.94	1.42	1.35
28	h	102	DGD	C1E-C2E	2.94	1.60	1.52
22	a	402	CLA	CMB-C2B	-2.94	1.45	1.51
22	c	514	CLA	C1D-C2D	2.93	1.49	1.42
22	a	405	CLA	CMD-C2D	-2.93	1.44	1.51
22	A	402	CLA	MG-NC	-2.93	1.99	2.06
22	B	609	CLA	C3B-CAB	-2.92	1.42	1.47
23	C	515	BCR	C1-C6	-2.92	1.49	1.53
22	b	616	CLA	C1D-C2D	2.92	1.49	1.42
22	b	612	CLA	CHC-C1C	2.92	1.42	1.35
22	A	404	CLA	CMB-C2B	-2.92	1.45	1.51
22	a	411	CLA	CHC-C1C	2.92	1.42	1.35
33	D	401	PHO	C4C-C3C	2.90	1.50	1.45
22	b	602	CLA	MG-NA	2.89	2.13	2.06
22	c	505	CLA	CMD-C2D	-2.89	1.44	1.51
22	d	402	CLA	CMB-C2B	-2.88	1.45	1.51
33	D	402	PHO	C4C-NC	2.88	1.43	1.36
28	A	414	DGD	C4E-C5E	2.88	1.59	1.53
22	C	503	CLA	C1D-C2D	2.88	1.49	1.42
22	c	502	CLA	CMB-C2B	-2.87	1.45	1.51
22	a	403	CLA	CMB-C2B	-2.87	1.45	1.51
22	b	614	CLA	CHC-C1C	2.86	1.42	1.35
32	c	522	LMG	C3-C2	2.86	1.59	1.52
28	C	517	DGD	O5D-C1E	2.86	1.45	1.40
22	C	501	CLA	CMD-C2D	-2.86	1.44	1.51
22	B	605	CLA	C1D-C2D	2.86	1.49	1.42
22	c	514	CLA	CMB-C2B	-2.85	1.45	1.51
28	C	518	DGD	C6D-C5D	2.85	1.60	1.51
33	D	401	PHO	CMC-C2C	-2.85	1.44	1.50
32	D	410	LMG	C9-C8	2.85	1.59	1.50
22	b	604	CLA	C1D-C2D	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	C3B-CAB	-2.85	1.42	1.47
22	d	403	CLA	C3B-C2B	-2.84	1.36	1.40
22	b	613	CLA	CMD-C2D	-2.83	1.44	1.51
22	c	506	CLA	CHC-C1C	2.83	1.42	1.35
22	B	603	CLA	CHC-C1C	2.83	1.42	1.35
28	C	517	DGD	C4E-C3E	2.83	1.59	1.52
28	c	517	DGD	C4D-C3D	2.83	1.59	1.52
33	a	404	PHO	C3B-C4B	2.82	1.49	1.43
23	b	619	BCR	C1-C6	-2.82	1.49	1.53
27	L	101	SQD	O47-C7	2.82	1.42	1.34
28	A	414	DGD	C4D-C3D	2.82	1.59	1.52
22	c	512	CLA	C1D-C2D	2.81	1.48	1.42
22	b	613	CLA	CHC-C1C	2.81	1.42	1.35
22	C	507	CLA	C1D-C2D	2.81	1.48	1.42
22	C	509	CLA	CHC-C1C	2.81	1.42	1.35
22	b	605	CLA	CHC-C1C	2.80	1.42	1.35
22	C	506	CLA	CHC-C1C	2.80	1.42	1.35
22	C	512	CLA	CHC-C1C	2.80	1.42	1.35
28	c	519	DGD	C3E-C2E	2.80	1.59	1.52
23	h	101	BCR	C30-C25	-2.79	1.49	1.53
23	T	101	BCR	C30-C25	-2.78	1.49	1.53
22	C	511	CLA	CMB-C2B	-2.78	1.45	1.51
28	h	102	DGD	O1G-C1G	-2.78	1.38	1.45
22	c	511	CLA	CMB-C2B	-2.78	1.45	1.51
22	D	404	CLA	CHC-C1C	2.78	1.42	1.35
33	d	401	PHO	C3B-C4B	2.77	1.49	1.43
22	B	608	CLA	C3B-CAB	-2.77	1.42	1.47
23	a	406	BCR	C1-C6	-2.77	1.50	1.53
22	A	403	CLA	CMB-C2B	-2.76	1.45	1.51
32	C	516	LMG	C6-C5	2.76	1.61	1.51
25	d	405	PL9	C3-C4	-2.76	1.45	1.49
22	c	511	CLA	MG-NC	-2.76	1.99	2.06
22	B	602	CLA	C1D-C2D	2.75	1.48	1.42
23	k	102	BCR	C1-C6	-2.75	1.50	1.53
28	c	517	DGD	O3G-C3G	-2.75	1.38	1.43
22	a	403	CLA	CMD-C2D	-2.75	1.45	1.51
22	b	603	CLA	CHC-C1C	2.75	1.42	1.35
28	C	519	DGD	C6D-C5D	2.75	1.60	1.51
22	A	402	CLA	CMB-C2B	-2.74	1.45	1.51
22	B	606	CLA	CMB-C2B	-2.74	1.45	1.51
22	B	604	CLA	C3B-C2B	-2.74	1.36	1.40
22	a	405	CLA	MG-NA	2.73	2.12	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	523	LMG	C7-C8	2.73	1.59	1.50
28	C	519	DGD	O1G-C1G	-2.72	1.38	1.45
22	B	616	CLA	C3B-C2B	-2.72	1.36	1.40
28	C	519	DGD	O5D-C1E	2.71	1.44	1.40
22	B	612	CLA	C1D-C2D	2.71	1.48	1.42
22	d	402	CLA	C1D-C2D	2.71	1.48	1.42
22	c	507	CLA	CHC-C1C	2.71	1.41	1.35
22	b	610	CLA	C3B-C2B	-2.71	1.36	1.40
28	H	102	DGD	O5D-C1E	2.70	1.44	1.40
22	b	616	CLA	CMB-C2B	-2.70	1.46	1.51
22	B	616	CLA	CMB-C2B	-2.70	1.46	1.51
23	b	619	BCR	C30-C25	-2.69	1.50	1.53
33	D	401	PHO	CHD-C4C	-2.69	1.34	1.40
26	D	409	LHG	P-O6	2.69	1.70	1.59
25	d	405	PL9	C11-C9	-2.69	1.45	1.51
22	c	510	CLA	MG-NC	2.69	2.12	2.06
32	D	408	LMG	C4-C5	2.69	1.58	1.53
22	c	508	CLA	C3B-C2B	-2.68	1.36	1.40
22	B	605	CLA	MG-NC	-2.68	1.99	2.06
22	B	603	CLA	C4B-NB	2.68	1.37	1.35
22	b	601	CLA	C1B-NB	2.68	1.37	1.35
22	c	504	CLA	CHC-C1C	2.67	1.41	1.35
22	c	510	CLA	CMB-C2B	-2.67	1.46	1.51
22	a	411	CLA	C3B-C2B	-2.67	1.36	1.40
22	b	613	CLA	CMB-C2B	-2.67	1.46	1.51
22	c	507	CLA	CMB-C2B	-2.67	1.46	1.51
28	c	518	DGD	O3E-C3E	-2.67	1.36	1.43
22	c	506	CLA	C3B-CAB	-2.67	1.42	1.47
22	B	616	CLA	CHC-C1C	2.67	1.41	1.35
22	B	614	CLA	C3B-C2B	-2.67	1.36	1.40
22	a	402	CLA	C1D-C2D	2.66	1.48	1.42
28	h	102	DGD	C1G-C2G	2.66	1.58	1.50
22	c	504	CLA	C1D-C2D	2.66	1.48	1.42
32	Y	101	LMG	C1-C2	2.66	1.60	1.52
22	b	602	CLA	CMD-C2D	-2.66	1.45	1.51
22	b	605	CLA	MG-NA	2.66	2.12	2.06
22	C	513	CLA	CMB-C2B	-2.66	1.46	1.51
22	b	601	CLA	C1D-C2D	2.66	1.48	1.42
22	C	509	CLA	CMD-C2D	-2.66	1.45	1.51
22	C	511	CLA	MG-NC	-2.65	2.00	2.06
32	c	520	LMG	C4-C5	2.65	1.58	1.53
22	C	501	CLA	C1D-C2D	2.65	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	515	BCR	C1-C6	-2.65	1.50	1.53
32	C	516	LMG	O6-C5	-2.65	1.37	1.44
22	c	506	CLA	MG-NC	2.65	2.12	2.06
22	B	609	CLA	CMD-C2D	-2.65	1.45	1.51
23	B	618	BCR	C30-C25	-2.64	1.50	1.53
22	B	613	CLA	C3B-CAB	-2.64	1.42	1.47
22	b	603	CLA	CMC-C2C	-2.64	1.45	1.50
26	D	409	LHG	P-O3	2.64	1.70	1.59
22	c	502	CLA	CHC-C1C	2.64	1.41	1.35
22	B	614	CLA	CMB-C2B	-2.63	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.63	1.46	1.51
33	D	402	PHO	CMB-C2B	-2.63	1.45	1.50
32	Y	101	LMG	C3-C2	2.63	1.59	1.52
22	A	403	CLA	C1D-C2D	2.62	1.48	1.42
22	b	606	CLA	CMB-C2B	-2.62	1.46	1.51
33	D	401	PHO	O2D-CGD	2.62	1.39	1.33
28	C	517	DGD	C6D-C5D	2.62	1.59	1.51
22	b	608	CLA	CMB-C2B	-2.61	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.60	1.46	1.51
23	b	617	BCR	C1-C6	-2.60	1.50	1.53
22	C	508	CLA	C1D-C2D	2.60	1.48	1.42
32	c	523	LMG	C4-C5	2.60	1.58	1.53
32	c	522	LMG	O7-C10	2.59	1.41	1.34
32	c	523	LMG	C1-C2	2.59	1.59	1.52
27	d	409	SQD	O2-C2	-2.59	1.36	1.43
22	B	611	CLA	C3B-C2B	-2.59	1.36	1.40
27	A	411	SQD	O47-C7	2.59	1.41	1.34
32	d	408	LMG	C4-C5	2.59	1.58	1.53
26	L	102	LHG	O7-C5	-2.59	1.40	1.46
22	A	409	CLA	CHC-C1C	2.58	1.41	1.35
32	Y	101	LMG	C4-C3	2.58	1.58	1.52
22	A	404	CLA	C3B-C2B	-2.58	1.36	1.40
22	c	504	CLA	C3B-C2B	-2.58	1.36	1.40
22	c	503	CLA	CMD-C2D	-2.58	1.45	1.51
22	B	610	CLA	CHC-C1C	2.58	1.41	1.35
28	c	517	DGD	O1G-C1G	-2.58	1.39	1.45
28	C	517	DGD	C3D-C2D	2.58	1.58	1.52
22	c	512	CLA	CMB-C2B	-2.57	1.46	1.51
22	C	502	CLA	CMB-C2B	-2.57	1.46	1.51
33	d	401	PHO	C4C-NC	2.57	1.42	1.36
22	c	505	CLA	C1D-C2D	2.57	1.48	1.42
22	d	403	CLA	CMD-C2D	-2.56	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	CMB-C2B	-2.56	1.46	1.51
22	B	608	CLA	CMD-C2D	-2.55	1.45	1.51
22	B	611	CLA	CMB-C2B	-2.55	1.46	1.51
27	A	413	SQD	O47-C45	-2.55	1.42	1.47
22	a	405	CLA	CMB-C2B	-2.55	1.46	1.51
22	A	404	CLA	C4B-CHC	-2.55	1.33	1.41
28	A	414	DGD	O5D-C6D	-2.55	1.39	1.43
22	B	605	CLA	C3B-C2B	-2.54	1.36	1.40
23	C	514	BCR	C33-C5	-2.54	1.46	1.50
22	H	101	CLA	C3B-CAB	-2.54	1.42	1.47
22	B	611	CLA	C1D-C2D	2.54	1.48	1.42
22	B	605	CLA	CMB-C2B	-2.54	1.46	1.51
22	c	502	CLA	C4B-CHC	-2.54	1.33	1.41
23	K	102	BCR	C30-C25	-2.54	1.50	1.53
22	b	613	CLA	C1C-NC	-2.53	1.34	1.37
25	d	405	PL9	C53-C6	-2.53	1.45	1.50
22	c	513	CLA	CMB-C2B	-2.53	1.46	1.51
22	b	605	CLA	C4B-CHC	-2.53	1.34	1.41
33	d	401	PHO	CHD-C1D	2.52	1.43	1.38
22	b	610	CLA	CMB-C2B	-2.52	1.46	1.51
33	a	404	PHO	CHD-C4C	-2.52	1.34	1.40
22	c	502	CLA	CMD-C2D	-2.52	1.45	1.51
26	A	412	LHG	P-O6	2.52	1.69	1.59
22	b	614	CLA	CMC-C2C	-2.52	1.45	1.50
28	C	517	DGD	C4D-C3D	2.51	1.58	1.52
22	C	512	CLA	CMD-C2D	-2.51	1.45	1.51
23	c	516	BCR	C33-C5	-2.51	1.46	1.50
22	B	612	CLA	CMD-C2D	-2.51	1.45	1.51
22	H	101	CLA	C1D-C2D	2.50	1.48	1.42
22	B	613	CLA	CMB-C2B	-2.50	1.46	1.51
23	B	619	BCR	C30-C25	-2.50	1.50	1.53
22	d	402	CLA	CMC-C2C	-2.50	1.45	1.50
22	B	608	CLA	CMB-C2B	-2.50	1.46	1.51
23	a	406	BCR	C38-C26	-2.50	1.46	1.50
22	C	512	CLA	C1D-C2D	2.50	1.48	1.42
22	B	614	CLA	CHC-C1C	2.49	1.41	1.35
22	d	403	CLA	C3B-CAB	-2.49	1.42	1.47
27	a	413	SQD	O3-C3	-2.49	1.37	1.43
22	b	614	CLA	MG-NC	2.49	2.12	2.06
22	b	603	CLA	C3B-CAB	-2.49	1.42	1.47
22	d	403	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	511	CLA	CMC-C2C	-2.49	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C1D-C2D	2.49	1.48	1.42
33	a	404	PHO	C1C-NC	-2.48	1.33	1.38
22	b	615	CLA	CMD-C2D	-2.48	1.45	1.51
22	b	602	CLA	CHC-C1C	2.48	1.41	1.35
22	b	613	CLA	C1D-C2D	2.48	1.48	1.42
22	b	609	CLA	C1D-C2D	2.48	1.48	1.42
22	C	502	CLA	C1D-C2D	2.47	1.48	1.42
22	C	511	CLA	CMD-C2D	-2.47	1.45	1.51
22	C	503	CLA	CMD-C2D	-2.47	1.45	1.51
22	C	506	CLA	C1D-C2D	2.46	1.48	1.42
22	B	603	CLA	CMB-C2B	-2.46	1.46	1.51
23	B	618	BCR	C1-C6	-2.46	1.50	1.53
22	a	405	CLA	MG-NC	-2.46	2.00	2.06
22	c	507	CLA	C1D-C2D	2.46	1.48	1.42
22	b	608	CLA	C3C-C2C	2.46	1.41	1.36
22	c	503	CLA	CHC-C1C	2.46	1.41	1.35
22	c	502	CLA	CMC-C2C	-2.46	1.45	1.50
32	Y	101	LMG	C6-C5	2.45	1.60	1.51
23	B	617	BCR	C33-C5	-2.45	1.46	1.50
26	d	406	LHG	O7-C5	-2.44	1.40	1.46
22	B	603	CLA	CMD-C2D	-2.44	1.45	1.51
22	B	613	CLA	CHC-C1C	2.44	1.41	1.35
22	c	506	CLA	C1D-C2D	2.44	1.48	1.42
22	C	509	CLA	C1D-C2D	2.44	1.48	1.42
26	A	410	LHG	O8-C23	2.44	1.40	1.33
28	h	102	DGD	C4D-C3D	2.44	1.58	1.52
22	b	601	CLA	O2A-CGA	2.43	1.40	1.33
22	b	611	CLA	MG-NC	-2.43	2.00	2.06
22	B	608	CLA	C3B-C2B	-2.43	1.37	1.40
22	c	510	CLA	MG-NA	-2.43	2.00	2.06
25	A	408	PL9	C46-C47	2.43	1.61	1.53
22	a	405	CLA	CHC-C1C	2.42	1.41	1.35
23	c	516	BCR	C30-C25	-2.42	1.50	1.53
22	b	611	CLA	CMD-C2D	-2.42	1.45	1.51
33	d	401	PHO	C1C-NC	-2.41	1.33	1.38
25	A	408	PL9	C22-C23	2.41	1.58	1.50
28	H	102	DGD	O3D-C3D	-2.41	1.37	1.43
22	b	603	CLA	C1D-C2D	2.40	1.48	1.42
22	C	509	CLA	O2D-CGD	2.40	1.39	1.33
22	b	607	CLA	C1D-C2D	2.40	1.48	1.42
22	B	610	CLA	CMC-C2C	-2.40	1.45	1.50
25	D	407	PL9	C7-C8	-2.40	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	101	CLA	C3B-C2B	-2.40	1.37	1.40
22	c	502	CLA	C1D-C2D	2.39	1.48	1.42
33	D	401	PHO	CMA-C3A	-2.39	1.48	1.53
22	C	509	CLA	MG-NC	-2.39	2.00	2.06
28	h	102	DGD	C4E-C3E	2.38	1.58	1.52
26	D	412	LHG	O7-C5	-2.38	1.40	1.46
22	C	510	CLA	C1D-C2D	2.38	1.48	1.42
22	d	402	CLA	MG-NC	2.38	2.11	2.06
22	C	508	CLA	CHC-C1C	2.38	1.41	1.35
22	c	503	CLA	C4B-CHC	-2.38	1.34	1.41
26	D	409	LHG	O6-C4	-2.37	1.35	1.44
22	A	404	CLA	MG-NC	-2.37	2.00	2.06
22	b	616	CLA	CMD-C2D	-2.37	1.45	1.51
33	D	402	PHO	CHC-C1C	2.37	1.43	1.38
22	c	504	CLA	C3B-CAB	-2.37	1.43	1.47
22	c	504	CLA	CMB-C2B	-2.37	1.46	1.51
22	B	607	CLA	C1D-C2D	2.36	1.47	1.42
22	c	509	CLA	CMD-C2D	-2.36	1.45	1.51
26	a	412	LHG	P-O6	2.36	1.68	1.59
27	a	413	SQD	O47-C7	2.36	1.41	1.34
22	b	607	CLA	CMD-C2D	-2.36	1.46	1.51
32	c	520	LMG	C7-C8	2.36	1.57	1.50
32	D	410	LMG	O8-C28	2.36	1.40	1.33
22	C	501	CLA	CMC-C2C	-2.35	1.45	1.50
28	c	519	DGD	C6D-C5D	2.35	1.58	1.51
27	A	413	SQD	C46-C45	2.35	1.56	1.50
28	c	519	DGD	O1G-C1G	-2.35	1.39	1.45
22	B	607	CLA	C3B-C2B	-2.35	1.37	1.40
22	A	404	CLA	C1D-C2D	2.35	1.47	1.42
22	B	607	CLA	C3B-CAB	-2.35	1.43	1.47
27	A	411	SQD	O4-C4	-2.35	1.37	1.43
22	c	513	CLA	MG-NA	2.34	2.11	2.06
22	b	614	CLA	C5-C3	-2.34	1.46	1.51
22	B	608	CLA	CHC-C1C	2.33	1.41	1.35
33	d	401	PHO	CMD-C2D	-2.33	1.45	1.50
22	C	504	CLA	CMD-C2D	-2.33	1.46	1.51
32	d	408	LMG	C7-C8	2.33	1.57	1.50
22	b	604	CLA	CMB-C2B	-2.33	1.46	1.51
22	C	513	CLA	C1D-C2D	2.33	1.47	1.42
22	a	403	CLA	CHC-C1C	2.33	1.40	1.35
22	C	503	CLA	CMB-C2B	-2.33	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.32	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	CMB-C2B	-2.32	1.46	1.51
22	b	616	CLA	C3B-CAB	-2.32	1.43	1.47
22	b	614	CLA	MG-NA	2.32	2.11	2.06
22	b	602	CLA	C1D-C2D	2.32	1.47	1.42
23	c	515	BCR	C30-C25	-2.32	1.50	1.53
22	A	403	CLA	CAA-C2A	-2.32	1.49	1.54
28	C	519	DGD	O2G-C2G	-2.31	1.40	1.46
28	H	102	DGD	O6E-C1E	2.31	1.47	1.41
22	C	504	CLA	C1D-C2D	2.31	1.47	1.42
22	b	602	CLA	CAC-C3C	-2.31	1.45	1.51
32	a	417	LMG	C9-C8	2.31	1.57	1.50
26	d	406	LHG	C1-C2	-2.31	1.42	1.51
32	c	523	LMG	C3-C2	2.31	1.58	1.52
22	b	608	CLA	O2A-CGA	2.30	1.40	1.33
32	d	408	LMG	O2-C2	-2.30	1.37	1.43
22	c	508	CLA	CHC-C1C	2.30	1.40	1.35
22	c	503	CLA	C1D-C2D	2.30	1.47	1.42
22	D	404	CLA	C1D-C2D	2.30	1.47	1.42
32	a	417	LMG	C3-C2	2.29	1.58	1.52
23	T	101	BCR	C38-C26	-2.29	1.47	1.50
22	a	403	CLA	C4B-CHC	-2.29	1.34	1.41
22	C	505	CLA	CMC-C2C	-2.29	1.45	1.50
22	A	404	CLA	CMD-C2D	-2.29	1.46	1.51
22	B	612	CLA	CMC-C2C	-2.29	1.45	1.50
33	D	402	PHO	CHC-C4B	-2.29	1.35	1.40
25	a	410	PL9	C7-C3	2.28	1.53	1.51
22	B	616	CLA	CMD-C2D	-2.28	1.46	1.51
25	d	405	PL9	C23-C24	2.28	1.38	1.33
22	c	511	CLA	C1D-C2D	2.28	1.47	1.42
26	L	102	LHG	P-O6	2.28	1.68	1.59
26	A	412	LHG	O8-C23	2.27	1.40	1.33
25	A	408	PL9	C23-C24	2.27	1.38	1.33
22	c	504	CLA	MG-NC	2.27	2.11	2.06
22	b	614	CLA	C1D-C2D	2.27	1.47	1.42
22	b	614	CLA	O2D-CGD	2.27	1.38	1.33
22	C	510	CLA	MG-NA	2.27	2.11	2.06
22	B	616	CLA	C4B-CHC	-2.26	1.34	1.41
32	d	408	LMG	O7-C8	-2.26	1.40	1.46
25	A	408	PL9	C41-C42	2.26	1.61	1.53
23	k	102	BCR	C38-C26	-2.26	1.47	1.50
33	D	402	PHO	C3B-C4B	2.26	1.47	1.43
22	H	101	CLA	CMC-C2C	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	403	CLA	C3B-C2B	-2.26	1.37	1.40
22	c	509	CLA	CMB-C2B	-2.25	1.47	1.51
22	C	507	CLA	CMC-C2C	-2.25	1.46	1.50
22	B	607	CLA	O2D-CGD	2.25	1.38	1.33
28	A	414	DGD	O5D-C1E	2.25	1.44	1.40
22	B	608	CLA	O2A-CGA	2.25	1.39	1.33
28	A	414	DGD	O2G-C1B	2.25	1.40	1.34
32	D	408	LMG	C1-C2	2.24	1.59	1.52
22	d	402	CLA	CHC-C1C	2.24	1.40	1.35
25	A	408	PL9	C37-C38	2.24	1.57	1.50
23	t	101	BCR	C38-C26	-2.24	1.47	1.50
28	C	518	DGD	C1E-C2E	2.24	1.58	1.52
22	c	510	CLA	C1D-C2D	2.24	1.47	1.42
22	b	606	CLA	CHC-C1C	2.24	1.40	1.35
33	a	404	PHO	C1B-C2B	2.24	1.50	1.45
22	B	610	CLA	CMD-C2D	-2.24	1.46	1.51
22	A	403	CLA	C3B-CAB	-2.24	1.43	1.47
28	c	517	DGD	C3G-C2G	2.24	1.57	1.50
33	d	401	PHO	C1A-NA	2.24	1.41	1.37
22	B	611	CLA	C3B-CAB	-2.24	1.43	1.47
22	d	402	CLA	CMD-C2D	-2.23	1.46	1.51
22	A	409	CLA	C3C-C2C	2.23	1.41	1.36
23	b	617	BCR	C4-C5	-2.23	1.46	1.51
22	D	404	CLA	CMD-C2D	-2.23	1.46	1.51
25	A	408	PL9	C35-C34	-2.23	1.45	1.50
22	d	403	CLA	CMC-C2C	-2.23	1.46	1.50
25	A	408	PL9	C42-C43	2.22	1.57	1.50
28	C	519	DGD	C6E-C5E	2.22	1.59	1.51
28	c	519	DGD	C2A-C1A	-2.22	1.44	1.50
26	A	410	LHG	C3-C2	2.22	1.59	1.51
22	A	402	CLA	C3C-C2C	2.22	1.41	1.36
33	D	402	PHO	CMD-C2D	-2.22	1.46	1.50
22	B	614	CLA	C3B-CAB	-2.22	1.43	1.47
33	D	401	PHO	CAC-C3C	-2.22	1.45	1.51
22	C	505	CLA	C1D-C2D	2.21	1.47	1.42
22	C	513	CLA	C4B-CHC	-2.21	1.34	1.41
22	a	405	CLA	C3B-C2B	-2.21	1.37	1.40
22	D	405	CLA	C4B-CHC	-2.21	1.34	1.41
27	A	411	SQD	O3-C3	-2.21	1.37	1.43
28	C	519	DGD	C4D-C5D	2.21	1.57	1.53
22	B	613	CLA	C1C-NC	-2.21	1.34	1.37
22	b	610	CLA	C1D-C2D	2.21	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	BCR	C38-C26	-2.20	1.47	1.50
22	b	602	CLA	CMC-C2C	-2.20	1.46	1.50
22	c	514	CLA	CMC-C2C	-2.20	1.46	1.50
22	A	404	CLA	CMC-C2C	-2.20	1.46	1.50
22	D	405	CLA	CMB-C2B	-2.20	1.47	1.51
22	d	403	CLA	C1D-C2D	2.20	1.47	1.42
22	c	507	CLA	C4B-CHC	-2.20	1.34	1.41
28	H	102	DGD	C4D-C5D	2.19	1.57	1.53
22	B	609	CLA	MG-NC	-2.19	2.01	2.06
22	b	610	CLA	CHC-C1C	2.19	1.40	1.35
22	c	509	CLA	C3C-C2C	2.19	1.41	1.36
32	c	520	LMG	O1-C1	2.18	1.43	1.40
22	b	602	CLA	C4B-CHC	-2.18	1.34	1.41
22	b	610	CLA	C1C-NC	-2.18	1.34	1.37
22	B	608	CLA	CMC-C2C	-2.18	1.46	1.50
22	c	507	CLA	O2D-CGD	2.18	1.38	1.33
35	F	101	HEC	C1B-NB	2.18	1.40	1.36
27	F	102	SQD	O3-C3	-2.18	1.37	1.43
22	a	403	CLA	C3B-CAB	-2.18	1.43	1.47
22	b	605	CLA	MG-NC	-2.17	2.01	2.06
22	C	505	CLA	CMB-C2B	-2.17	1.47	1.51
22	b	610	CLA	CMD-C2D	-2.17	1.46	1.51
33	D	401	PHO	C1C-NC	-2.17	1.33	1.38
22	C	504	CLA	O2D-CGD	2.17	1.38	1.33
22	b	612	CLA	CMC-C2C	-2.17	1.46	1.50
22	C	510	CLA	CMD-C2D	-2.17	1.46	1.51
25	A	408	PL9	C21-C22	2.17	1.60	1.53
23	B	618	BCR	C36-C18	-2.17	1.46	1.50
26	e	101	LHG	C24-C23	2.17	1.57	1.50
25	A	408	PL9	C41-C39	2.16	1.55	1.51
28	c	518	DGD	C6D-C5D	2.16	1.58	1.51
22	b	612	CLA	CMD-C2D	-2.16	1.46	1.51
22	B	602	CLA	C4B-CHC	-2.15	1.35	1.41
22	D	405	CLA	C3B-C2B	-2.15	1.37	1.40
32	M	101	LMG	C4-C3	2.15	1.57	1.52
23	C	514	BCR	C36-C18	-2.15	1.46	1.50
33	a	404	PHO	CHC-C1C	2.15	1.42	1.38
22	b	608	CLA	C3B-CAB	-2.15	1.43	1.47
27	a	413	SQD	O4-C4	-2.15	1.37	1.43
22	A	404	CLA	C3B-CAB	-2.15	1.43	1.47
22	B	610	CLA	CMA-C3A	-2.14	1.48	1.53
22	b	609	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	CHC-C1C	2.14	1.40	1.35
22	a	411	CLA	C5-C3	-2.14	1.46	1.51
22	c	514	CLA	C3B-C2B	-2.14	1.37	1.40
25	D	407	PL9	C36-C34	2.14	1.55	1.51
22	B	612	CLA	CMB-C2B	-2.14	1.47	1.51
22	C	503	CLA	C3B-C2B	-2.14	1.37	1.40
23	b	618	BCR	C1-C6	-2.14	1.50	1.53
22	b	609	CLA	C3B-CAB	-2.14	1.43	1.47
25	a	410	PL9	C50-C49	2.14	1.56	1.50
28	C	519	DGD	O2E-C2E	-2.14	1.37	1.43
35	F	101	HEC	C1D-CHD	-2.14	1.35	1.41
32	b	621	LMG	C3-C2	2.13	1.57	1.52
27	A	411	SQD	O2-C2	-2.13	1.38	1.43
22	b	611	CLA	C4B-CHC	-2.13	1.35	1.41
28	C	519	DGD	O4E-C4E	-2.13	1.38	1.43
26	a	412	LHG	C8-C7	-2.13	1.44	1.50
26	e	101	LHG	C4-C5	2.13	1.57	1.50
33	D	401	PHO	C1A-NA	2.13	1.41	1.37
27	F	102	SQD	O4-C4	-2.13	1.38	1.43
22	A	402	CLA	O2D-CGD	2.13	1.38	1.33
22	b	601	CLA	CMD-C2D	-2.13	1.46	1.51
23	h	101	BCR	C33-C5	-2.13	1.47	1.50
22	c	508	CLA	C1D-C2D	2.12	1.47	1.42
22	b	605	CLA	C1D-C2D	2.12	1.47	1.42
22	c	509	CLA	C3B-C2B	-2.12	1.37	1.40
22	b	614	CLA	CMD-C2D	-2.12	1.46	1.51
22	B	611	CLA	CMD-C2D	-2.11	1.46	1.51
33	a	404	PHO	C4C-C3C	2.11	1.49	1.45
22	B	603	CLA	MG-NA	2.11	2.11	2.06
26	e	101	LHG	O8-C23	2.11	1.39	1.33
22	C	510	CLA	CAC-C3C	-2.11	1.45	1.51
33	d	401	PHO	CMC-C2C	-2.11	1.46	1.50
25	d	405	PL9	C7-C3	2.11	1.53	1.51
22	c	504	CLA	MG-NA	2.11	2.11	2.06
32	b	621	LMG	O8-C28	2.10	1.39	1.33
26	a	412	LHG	O8-C6	2.10	1.49	1.45
25	d	405	PL9	C25-C24	-2.10	1.45	1.50
22	B	604	CLA	CMD-C2D	-2.10	1.46	1.51
26	l	101	LHG	O8-C6	-2.10	1.40	1.45
22	C	507	CLA	C3B-C2B	-2.10	1.37	1.40
22	C	502	CLA	CMD-C2D	-2.10	1.46	1.51
32	a	417	LMG	O8-C28	2.10	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	CMB-C2B	-2.09	1.47	1.51
22	b	615	CLA	CMC-C2C	-2.09	1.46	1.50
32	a	417	LMG	C14-C13	2.09	1.63	1.51
22	C	508	CLA	CMD-C2D	-2.08	1.46	1.51
33	D	401	PHO	C4C-NC	2.08	1.41	1.36
22	B	608	CLA	C4B-CHC	-2.08	1.35	1.41
28	C	517	DGD	C3G-C2G	2.08	1.57	1.50
22	C	511	CLA	C1D-C2D	2.08	1.47	1.42
22	C	512	CLA	C4B-CHC	-2.08	1.35	1.41
22	b	611	CLA	CHC-C1C	2.08	1.40	1.35
22	C	503	CLA	C3B-CAB	-2.08	1.43	1.47
22	B	602	CLA	O2D-CGD	2.08	1.38	1.33
22	C	507	CLA	CMB-C2B	-2.08	1.47	1.51
28	c	517	DGD	C6D-C5D	2.07	1.58	1.51
32	c	523	LMG	O8-C9	-2.07	1.40	1.45
23	c	515	BCR	C38-C26	-2.07	1.47	1.50
26	d	407	LHG	O8-C6	2.07	1.49	1.45
33	D	402	PHO	C1C-NC	-2.06	1.34	1.38
22	c	508	CLA	CMB-C2B	-2.06	1.47	1.51
33	D	402	PHO	CHD-C1D	2.06	1.42	1.38
22	b	612	CLA	CAC-C3C	-2.06	1.45	1.51
22	B	604	CLA	CMC-C2C	-2.05	1.46	1.50
22	b	616	CLA	CAC-C3C	-2.05	1.45	1.51
22	B	607	CLA	CHC-C1C	2.05	1.40	1.35
22	C	512	CLA	CMB-C2B	-2.05	1.47	1.51
32	D	410	LMG	C30-C29	2.04	1.59	1.52
33	D	401	PHO	CMD-C2D	-2.04	1.46	1.50
32	b	621	LMG	C4-C3	2.04	1.57	1.52
23	B	619	BCR	C31-C1	-2.04	1.49	1.53
32	a	417	LMG	C11-C10	2.04	1.56	1.50
22	c	512	CLA	CMD-C2D	-2.04	1.46	1.51
33	a	404	PHO	CAA-C2A	-2.04	1.50	1.54
22	A	409	CLA	OBD-CAD	2.04	1.25	1.22
33	D	401	PHO	CHC-C1C	2.04	1.42	1.38
28	C	518	DGD	C3G-C2G	2.04	1.57	1.50
22	B	604	CLA	O2A-CGA	2.04	1.39	1.33
22	b	611	CLA	CMB-C2B	-2.04	1.47	1.51
22	C	506	CLA	C3B-C2B	-2.04	1.37	1.40
27	d	409	SQD	O3-C3	-2.04	1.38	1.43
22	C	506	CLA	CAC-C3C	-2.03	1.45	1.51
28	h	102	DGD	O2D-C2D	-2.03	1.38	1.43
22	B	616	CLA	C3B-CAB	-2.03	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	O2D-CGD	2.03	1.38	1.33
32	a	417	LMG	C6-C5	2.03	1.58	1.51
22	A	404	CLA	CHC-C1C	2.03	1.40	1.35
22	C	508	CLA	C4B-CHC	-2.03	1.35	1.41
22	C	513	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	616	CLA	C1D-C2D	2.03	1.47	1.42
22	B	606	CLA	C1D-C2D	2.03	1.47	1.42
22	C	503	CLA	CMC-C2C	-2.03	1.46	1.50
28	h	102	DGD	C6D-C5D	2.02	1.57	1.51
28	H	102	DGD	C1G-C2G	2.02	1.56	1.50
22	C	511	CLA	C3B-C2B	-2.02	1.37	1.40
26	D	412	LHG	P-O4	-2.02	1.45	1.55
28	C	519	DGD	O3D-C3D	-2.01	1.38	1.43
22	c	506	CLA	C3C-C2C	2.01	1.41	1.36
22	c	507	CLA	CMD-C2D	-2.01	1.46	1.51
23	b	617	BCR	C30-C25	-2.00	1.51	1.53
22	b	602	CLA	CMB-C2B	-2.00	1.47	1.51
25	A	408	PL9	C7-C8	-2.00	1.47	1.50
22	B	613	CLA	CMD-C2D	-2.00	1.46	1.51
22	c	505	CLA	CMB-C2B	-2.00	1.47	1.51

All (1359) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	C4A-NA-C1A	11.79	112.01	106.71
27	L	101	SQD	O6-C1-C2	11.45	126.19	108.30
22	b	604	CLA	C4A-NA-C1A	10.51	111.43	106.71
22	B	615	CLA	C4A-NA-C1A	9.02	110.76	106.71
22	B	607	CLA	C4A-NA-C1A	8.90	110.71	106.71
22	B	609	CLA	C4A-NA-C1A	8.88	110.70	106.71
27	a	413	SQD	O6-C1-C2	8.83	122.10	108.30
22	b	606	CLA	C4A-NA-C1A	8.74	110.64	106.71
22	b	601	CLA	C4A-NA-C1A	8.70	110.62	106.71
27	B	621	SQD	O6-C1-C2	8.47	121.52	108.30
22	C	513	CLA	C4A-NA-C1A	8.43	110.50	106.71
22	c	512	CLA	C4A-NA-C1A	8.39	110.48	106.71
22	C	507	CLA	C4A-NA-C1A	8.07	110.34	106.71
22	c	506	CLA	C4A-NA-C1A	7.84	110.23	106.71
22	c	510	CLA	C4A-NA-C1A	7.59	110.12	106.71
22	B	608	CLA	C4A-NA-C1A	7.54	110.09	106.71
27	A	411	SQD	O6-C1-C2	7.19	119.53	108.30
25	a	410	PL9	C7-C3-C4	7.15	122.69	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	C4A-NA-C1A	7.04	109.87	106.71
22	C	503	CLA	C4A-NA-C1A	7.03	109.87	106.71
22	B	612	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	c	509	CLA	C4A-NA-C1A	7.00	109.85	106.71
27	A	411	SQD	O7-S-C6	6.98	115.23	106.94
35	f	101	HEC	CBD-CAD-C3D	-6.93	99.70	112.49
22	C	510	CLA	C4A-NA-C1A	6.84	109.78	106.71
22	c	504	CLA	C4A-NA-C1A	6.75	109.74	106.71
27	d	409	SQD	O7-S-C6	6.65	114.85	106.94
22	B	616	CLA	C4A-NA-C1A	6.49	109.63	106.71
22	H	101	CLA	C4A-NA-C1A	6.31	109.54	106.71
22	C	506	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	C	511	CLA	C4A-NA-C1A	6.12	109.46	106.71
22	c	513	CLA	C4A-NA-C1A	6.11	109.45	106.71
27	F	102	SQD	O9-S-C6	6.06	114.14	106.94
22	b	609	CLA	C4A-NA-C1A	6.02	109.41	106.71
22	b	605	CLA	C4A-NA-C1A	5.95	109.38	106.71
22	b	603	CLA	C4A-NA-C1A	5.92	109.37	106.71
35	F	101	HEC	CBD-CAD-C3D	-5.88	101.64	112.49
22	d	403	CLA	C4A-NA-C1A	5.83	109.33	106.71
22	A	402	CLA	C4A-NA-C1A	5.81	109.32	106.71
22	b	614	CLA	C4A-NA-C1A	5.78	109.30	106.71
22	c	511	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	d	405	PL9	C7-C3-C4	5.71	121.52	116.88
22	b	607	CLA	C4A-NA-C1A	5.69	109.27	106.71
22	B	616	CLA	O2D-CGD-O1D	-5.68	112.74	123.84
22	C	502	CLA	C4A-NA-C1A	5.51	109.18	106.71
22	b	604	CLA	OBD-CAD-CBD	-5.51	118.02	125.89
35	f	101	HEC	CBA-CAA-C2A	-5.47	102.40	112.48
28	C	519	DGD	O3G-C3G-C2G	-5.43	97.80	110.90
22	B	611	CLA	C4A-NA-C1A	5.39	109.13	106.71
27	L	101	SQD	O7-S-C6	5.39	113.34	106.94
22	c	503	CLA	CMB-C2B-C1B	-5.36	120.22	128.46
22	c	502	CLA	O2D-CGD-O1D	-5.32	113.43	123.84
27	d	409	SQD	O6-C1-C2	5.31	116.60	108.30
22	C	509	CLA	C4A-NA-C1A	5.30	109.09	106.71
25	D	407	PL9	C36-C34-C33	-5.30	110.39	121.12
22	D	404	CLA	CMB-C2B-C1B	-5.29	120.34	128.46
27	A	411	SQD	C1-C2-C3	-5.28	99.00	110.00
25	D	407	PL9	C7-C3-C4	5.27	121.16	116.88
22	a	403	CLA	C4A-NA-C1A	5.22	109.06	106.71
22	b	612	CLA	CMB-C2B-C1B	-5.17	120.52	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	CMD-C2D-C3D	5.15	134.32	124.68
27	B	621	SQD	O8-S-C6	5.14	113.93	105.74
22	B	613	CLA	C4A-NA-C1A	5.13	109.01	106.71
27	L	101	SQD	C1-C2-C3	-5.12	99.33	110.00
22	b	604	CLA	C4D-C3D-CAD	-5.07	105.64	108.47
22	b	605	CLA	O1D-CGD-CBD	5.05	134.82	124.48
27	F	102	SQD	O6-C1-C2	5.01	116.13	108.30
22	b	616	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
27	L	101	SQD	O9-S-C6	4.99	112.87	106.94
27	A	411	SQD	O47-C7-C8	4.98	122.24	111.50
22	b	602	CLA	C4A-NA-C1A	4.97	108.94	106.71
22	B	609	CLA	C4D-C3D-CAD	-4.97	105.70	108.47
22	a	403	CLA	CMB-C2B-C1B	-4.93	120.88	128.46
22	b	611	CLA	O2D-CGD-O1D	-4.92	114.21	123.84
22	B	606	CLA	C4A-NA-C1A	4.91	108.91	106.71
22	c	506	CLA	C4D-C3D-CAD	-4.88	105.75	108.47
22	B	602	CLA	O2D-CGD-CBD	4.79	119.77	111.27
27	A	413	SQD	C45-O47-C7	4.78	124.03	117.88
22	B	602	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
27	a	413	SQD	C1-O5-C5	-4.75	104.36	113.69
33	d	401	PHO	O2D-CGD-O1D	-4.75	114.55	123.84
22	A	403	CLA	CMB-C2B-C1B	-4.75	121.17	128.46
22	c	514	CLA	C4A-NA-C1A	4.73	108.83	106.71
22	b	611	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
22	c	505	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
22	C	508	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
22	c	503	CLA	CMB-C2B-C3B	4.67	133.41	124.68
22	a	403	CLA	CMB-C2B-C3B	4.65	133.38	124.68
22	C	505	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
27	A	411	SQD	O8-S-C6	4.63	113.12	105.74
22	b	616	CLA	C4A-NA-C1A	4.63	108.79	106.71
22	b	607	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
22	c	507	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
22	C	506	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
22	B	608	CLA	CMB-C2B-C1B	-4.60	121.40	128.46
22	C	508	CLA	C4A-NA-C1A	4.57	108.76	106.71
25	A	408	PL9	C7-C3-C4	4.56	120.59	116.88
22	B	606	CLA	C4D-C3D-CAD	-4.55	105.93	108.47
22	b	612	CLA	CMD-C2D-C3D	4.54	133.18	124.68
22	c	511	CLA	O2D-CGD-O1D	-4.53	114.97	123.84
22	A	404	CLA	CMB-C2B-C1B	-4.53	121.51	128.46
27	a	413	SQD	C1-C2-C3	-4.52	100.58	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	614	CLA	O2D-CGD-O1D	-4.52	115.01	123.84
27	B	621	SQD	C1-C2-C3	-4.50	100.62	110.00
22	C	512	CLA	C4A-NA-C1A	4.49	108.72	106.71
25	D	407	PL9	C30-C29-C31	-4.49	107.72	115.27
35	F	101	HEC	C1D-C2D-C3D	-4.47	103.88	107.00
28	H	102	DGD	O3G-C3G-C2G	-4.46	100.13	110.90
22	D	405	CLA	C4A-NA-C1A	4.46	108.71	106.71
22	B	604	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
22	A	409	CLA	C4A-NA-C1A	4.40	108.69	106.71
22	b	610	CLA	C4A-NA-C1A	4.40	108.68	106.71
23	c	516	BCR	C35-C13-C14	-4.39	116.78	122.92
23	a	406	BCR	C37-C22-C21	-4.37	116.80	122.92
22	B	603	CLA	OBD-CAD-CBD	-4.34	119.69	125.89
22	b	612	CLA	OBD-CAD-CBD	-4.32	119.72	125.89
22	C	513	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
28	C	518	DGD	O3G-C3G-C2G	-4.31	100.50	110.90
22	B	603	CLA	C4D-C3D-CAD	-4.30	106.07	108.47
22	C	505	CLA	OBD-CAD-CBD	-4.29	119.77	125.89
27	d	409	SQD	O9-S-O7	-4.29	99.11	113.95
22	b	612	CLA	C4D-C3D-CAD	-4.28	106.08	108.47
22	a	411	CLA	C4A-NA-C1A	4.28	108.63	106.71
22	C	509	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
22	C	505	CLA	CMB-C2B-C3B	4.27	132.66	124.68
32	b	621	LMG	O1-C1-C2	-4.25	101.66	108.30
27	L	101	SQD	O2-C2-C1	4.24	120.34	110.05
22	b	602	CLA	O2D-CGD-CBD	4.22	118.76	111.27
27	B	621	SQD	C1-O5-C5	-4.21	105.42	113.69
26	d	406	LHG	O4-P-O5	4.21	133.05	112.24
27	d	409	SQD	O9-S-C6	4.21	111.94	106.94
22	b	605	CLA	C4D-C3D-CAD	-4.21	106.12	108.47
27	B	621	SQD	O47-C7-C8	4.19	120.54	111.50
26	D	409	LHG	O4-P-O5	4.19	132.97	112.24
32	m	101	LMG	O6-C1-O1	-4.18	100.08	109.97
35	v	201	HEC	CBA-CAA-C2A	-4.17	104.79	112.48
22	C	504	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
22	A	403	CLA	CMB-C2B-C3B	4.17	132.47	124.68
22	B	602	CLA	C4D-C3D-CAD	-4.16	106.15	108.47
22	b	612	CLA	CMB-C2B-C3B	4.15	132.45	124.68
27	a	414	SQD	O47-C7-C8	4.15	120.45	111.50
22	B	602	CLA	CMB-C2B-C3B	4.15	132.44	124.68
22	b	607	CLA	CMB-C2B-C3B	4.13	132.41	124.68
22	b	612	CLA	C4A-NA-C1A	4.13	108.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	CMB-C2B-C3B	4.11	132.37	124.68
22	c	510	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
26	A	412	LHG	O4-P-O5	4.10	132.51	112.24
22	c	514	CLA	CMB-C2B-C1B	-4.09	122.19	128.46
22	a	403	CLA	CHB-C4A-NA	4.08	130.16	124.51
22	A	404	CLA	O2D-CGD-O1D	-4.08	115.85	123.84
22	b	616	CLA	CMB-C2B-C3B	4.07	132.30	124.68
22	A	402	CLA	C4D-C3D-CAD	-4.07	106.20	108.47
26	L	102	LHG	O4-P-O5	4.07	132.36	112.24
22	D	404	CLA	C4A-NA-C1A	4.06	108.53	106.71
22	b	602	CLA	O2D-CGD-O1D	-4.06	115.90	123.84
22	B	616	CLA	O2D-CGD-CBD	4.06	118.48	111.27
22	b	615	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
22	C	512	CLA	CMB-C2B-C3B	4.05	132.25	124.68
22	c	511	CLA	CMD-C2D-C3D	4.04	132.23	124.68
32	m	101	LMG	O1-C1-C2	-4.03	102.00	108.30
27	a	413	SQD	O7-S-C6	4.03	111.73	106.94
26	e	101	LHG	O4-P-O5	4.03	132.16	112.24
35	V	201	HEC	CMC-C2C-C1C	-4.02	122.28	128.46
32	C	516	LMG	O6-C1-O1	-4.02	100.45	109.97
23	B	618	BCR	C15-C14-C13	-4.01	121.58	127.31
22	C	506	CLA	CMB-C2B-C3B	4.01	132.18	124.68
22	c	510	CLA	CHB-C4A-NA	4.00	130.05	124.51
22	C	512	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
22	b	601	CLA	CHB-C4A-NA	3.99	130.03	124.51
22	C	503	CLA	C4D-C3D-CAD	-3.98	106.25	108.47
22	B	610	CLA	CHB-C4A-NA	3.97	130.00	124.51
22	C	508	CLA	CMB-C2B-C3B	3.96	132.09	124.68
22	B	612	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
26	l	101	LHG	O4-P-O5	3.95	131.79	112.24
22	C	502	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
26	A	410	LHG	O4-P-O5	3.94	131.69	112.24
27	A	411	SQD	O47-C7-O49	-3.93	114.19	123.70
22	A	402	CLA	CHB-C4A-NA	3.93	129.94	124.51
22	b	610	CLA	CHB-C4A-NA	3.92	129.94	124.51
27	B	621	SQD	O7-S-C6	3.92	111.60	106.94
22	B	604	CLA	OBD-CAD-CBD	-3.91	120.31	125.89
27	F	102	SQD	O8-S-C6	3.91	111.96	105.74
26	d	407	LHG	O4-P-O5	3.88	131.44	112.24
22	D	404	CLA	CMB-C2B-C3B	3.88	131.93	124.68
23	B	617	BCR	C2-C1-C6	3.88	116.45	110.48
26	D	412	LHG	O4-P-O5	3.87	131.38	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	102	DGD	O3G-C3G-C2G	-3.86	101.59	110.90
22	D	405	CLA	C2C-C1C-NC	3.85	113.58	109.97
32	b	621	LMG	C1-O6-C5	-3.85	106.13	113.69
26	a	412	LHG	O4-P-O5	3.85	131.26	112.24
27	B	621	SQD	O2-C2-C1	3.83	119.36	110.05
22	c	505	CLA	CMB-C2B-C3B	3.83	131.85	124.68
35	v	201	HEC	CMC-C2C-C1C	-3.82	122.59	128.46
22	C	509	CLA	CMB-C2B-C3B	3.82	131.82	124.68
27	B	621	SQD	C3-C4-C5	3.81	117.04	110.24
22	B	609	CLA	OBD-CAD-CBD	-3.81	120.45	125.89
25	a	410	PL9	C7-C3-C2	-3.80	118.30	123.30
22	c	507	CLA	CMB-C2B-C3B	3.80	131.79	124.68
22	B	608	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
22	c	510	CLA	O2A-CGA-O1A	-3.80	114.01	123.59
27	A	411	SQD	C1-O5-C5	-3.79	106.25	113.69
22	c	513	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
28	C	517	DGD	O5D-C6D-C5D	-3.77	102.07	109.05
22	b	608	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
22	A	404	CLA	CMB-C2B-C3B	3.77	131.73	124.68
22	A	402	CLA	CMD-C2D-C3D	3.77	131.72	124.68
22	C	501	CLA	C4A-NA-C1A	3.76	108.40	106.71
32	a	417	LMG	C1-O6-C5	-3.75	106.32	113.69
35	F	101	HEC	CBA-CAA-C2A	-3.75	105.57	112.48
22	b	612	CLA	C1B-CHB-C4A	-3.73	122.73	130.12
22	b	613	CLA	OBD-CAD-CBD	-3.72	120.58	125.89
22	b	613	CLA	C1-C2-C3	-3.70	119.64	126.04
22	a	405	CLA	C4A-NA-C1A	3.70	108.37	106.71
23	B	617	BCR	C37-C22-C23	3.70	123.90	118.08
22	A	404	CLA	C1B-CHB-C4A	-3.69	122.82	130.12
22	B	610	CLA	C1B-CHB-C4A	-3.68	122.82	130.12
22	c	513	CLA	C1-C2-C3	-3.68	119.68	126.04
22	c	502	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
22	b	610	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
25	d	405	PL9	C40-C39-C41	3.66	121.42	115.27
22	b	613	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
25	D	407	PL9	C20-C19-C21	3.64	121.39	115.27
32	b	621	LMG	C1-C2-C3	-3.64	102.42	110.00
22	c	511	CLA	C4D-C3D-CAD	-3.63	106.44	108.47
22	b	611	CLA	CMB-C2B-C3B	3.63	131.47	124.68
35	f	101	HEC	C1D-C2D-C3D	-3.62	104.48	107.00
22	c	506	CLA	OBD-CAD-CBD	-3.62	120.72	125.89
22	c	513	CLA	CMB-C2B-C1B	-3.61	122.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PL9	O1-C4-C3	-3.61	116.74	120.72
22	b	604	CLA	OBD-CAD-C3D	3.60	133.96	127.98
23	t	101	BCR	C15-C16-C17	-3.60	116.10	123.47
22	C	509	CLA	CHB-C4A-NA	3.59	129.48	124.51
22	C	503	CLA	CMD-C2D-C3D	3.59	131.40	124.68
22	C	507	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
22	c	502	CLA	O2D-CGD-CBD	3.59	117.64	111.27
35	v	201	HEC	C1D-C2D-C3D	-3.59	104.50	107.00
22	b	608	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
23	C	515	BCR	C15-C16-C17	-3.58	116.14	123.47
22	b	613	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
23	b	619	BCR	C36-C18-C17	-3.57	117.93	122.92
32	m	101	LMG	O7-C10-O9	-3.56	115.10	123.70
25	A	408	PL9	C36-C34-C33	-3.56	113.92	121.12
22	B	604	CLA	CMB-C2B-C3B	3.56	131.33	124.68
22	C	507	CLA	CHB-C4A-NA	3.56	129.43	124.51
23	b	617	BCR	C3-C4-C5	-3.55	107.73	114.08
22	B	613	CLA	CAC-C3C-C4C	3.55	129.42	124.81
25	A	408	PL9	C20-C19-C21	3.55	121.24	115.27
22	c	508	CLA	OBD-CAD-CBD	-3.55	120.82	125.89
22	C	503	CLA	O2A-C1-C2	-3.54	99.33	108.64
23	c	516	BCR	C2-C1-C6	3.54	115.93	110.48
22	b	614	CLA	C1-C2-C3	-3.54	119.92	126.04
22	B	612	CLA	C11-C12-C13	-3.54	104.49	115.92
23	B	617	BCR	C37-C22-C21	-3.53	117.98	122.92
23	B	619	BCR	C2-C1-C6	3.52	115.91	110.48
22	b	603	CLA	OBD-CAD-CBD	-3.51	120.88	125.89
27	d	409	SQD	O5-C5-C4	3.51	116.06	109.69
23	C	514	BCR	C34-C9-C10	-3.50	118.02	122.92
22	B	604	CLA	CHB-C4A-NA	3.49	129.34	124.51
22	b	606	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
22	b	615	CLA	CMD-C2D-C3D	3.49	131.21	124.68
26	a	412	LHG	O8-C23-C24	3.49	122.85	111.91
22	B	603	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
32	c	523	LMG	O6-C1-O1	-3.49	101.72	109.97
32	a	417	LMG	C1-C2-C3	-3.48	102.74	110.00
22	D	404	CLA	CMD-C2D-C3D	3.48	131.19	124.68
23	b	618	BCR	C36-C18-C17	-3.47	118.06	122.92
22	B	603	CLA	O2D-CGD-CBD	3.47	117.43	111.27
22	c	506	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
22	B	604	CLA	CMD-C2D-C3D	3.46	131.15	124.68
32	a	417	LMG	C9-C8-C7	-3.45	103.62	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	O2D-CGD-CBD	3.45	117.39	111.27
28	A	414	DGD	C4E-C3E-C2E	-3.45	104.81	110.82
22	b	605	CLA	CMD-C2D-C3D	3.45	131.12	124.68
22	D	405	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	B	613	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
22	a	402	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	C	501	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
27	a	414	SQD	O48-C23-O10	-3.42	114.95	123.59
33	D	401	PHO	CED-O2D-CGD	3.42	123.68	115.94
22	A	403	CLA	C1B-CHB-C4A	-3.42	123.35	130.12
27	L	101	SQD	C3-C4-C5	3.42	116.33	110.24
22	c	511	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	a	410	PL9	C22-C23-C24	-3.40	119.47	127.66
22	b	604	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
22	a	402	CLA	C4A-NA-C1A	3.40	108.23	106.71
23	T	101	BCR	C7-C8-C9	-3.40	121.10	126.23
22	C	505	CLA	C1B-CHB-C4A	-3.39	123.39	130.12
22	C	511	CLA	CMD-C2D-C3D	3.39	131.01	124.68
23	K	101	BCR	C15-C16-C17	-3.39	116.54	123.47
27	B	621	SQD	O9-S-O7	-3.37	102.28	113.95
22	B	602	CLA	OBD-CAD-CBD	-3.37	121.08	125.89
27	F	102	SQD	C1-C2-C3	-3.37	102.98	110.00
22	b	605	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
22	B	610	CLA	C4A-NA-C1A	3.37	108.22	106.71
22	c	502	CLA	C4A-NA-C1A	3.37	108.22	106.71
22	b	610	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
22	b	601	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
22	b	602	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
22	A	409	CLA	CHB-C4A-NA	3.36	129.15	124.51
23	K	102	BCR	C37-C22-C21	-3.35	118.22	122.92
22	B	606	CLA	CMD-C2D-C3D	3.35	130.95	124.68
28	h	102	DGD	C3E-C4E-C5E	-3.35	104.26	110.24
23	B	619	BCR	C15-C16-C17	-3.35	116.61	123.47
27	B	621	SQD	O48-C23-O10	-3.35	115.14	123.59
22	c	503	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
22	b	608	CLA	OBD-CAD-CBD	-3.34	121.12	125.89
22	a	403	CLA	C4D-C3D-CAD	-3.34	106.61	108.47
22	b	612	CLA	C11-C12-C13	-3.34	105.14	115.92
23	b	619	BCR	C2-C1-C6	3.34	115.62	110.48
22	c	508	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
22	b	603	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
22	b	605	CLA	O2D-CGD-O1D	-3.32	117.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	C16-C15-C13	-3.32	105.18	115.92
33	D	401	PHO	CMB-C2B-C1B	-3.31	119.96	125.06
23	b	619	BCR	C29-C30-C25	3.31	115.57	110.48
27	B	621	SQD	O48-C23-C24	3.31	122.29	111.91
22	B	615	CLA	CHB-C4A-NA	3.31	129.09	124.51
35	v	201	HEC	CBD-CAD-C3D	-3.31	106.39	112.49
23	B	619	BCR	C36-C18-C17	-3.30	118.29	122.92
23	X	101	BCR	C30-C25-C26	-3.30	117.96	122.61
22	B	608	CLA	O2D-CGD-CBD	3.30	117.14	111.27
22	A	409	CLA	CMB-C2B-C3B	3.30	130.85	124.68
22	D	404	CLA	C4-C3-C5	3.30	120.82	115.27
22	b	609	CLA	C4D-C3D-CAD	-3.29	106.63	108.47
22	c	505	CLA	C4-C3-C5	3.29	120.81	115.27
22	a	405	CLA	O2D-CGD-CBD	3.29	117.12	111.27
33	a	404	PHO	C1-C2-C3	-3.29	120.35	126.04
23	X	101	BCR	C27-C26-C25	3.29	127.51	122.73
23	B	619	BCR	C33-C5-C6	-3.29	120.84	124.53
22	c	514	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
27	a	414	SQD	O48-C23-C24	3.28	122.20	111.91
22	b	603	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
22	A	409	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
22	a	405	CLA	CMD-C2D-C3D	3.28	130.81	124.68
22	c	506	CLA	CMB-C2B-C3B	3.27	130.80	124.68
22	c	514	CLA	CHB-C4A-NA	3.27	129.04	124.51
22	B	604	CLA	C4D-C3D-CAD	-3.27	106.65	108.47
22	C	510	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
22	B	615	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
22	C	505	CLA	O2A-CGA-O1A	-3.26	115.35	123.59
22	C	501	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
22	c	506	CLA	CMD-C2D-C3D	3.26	130.78	124.68
22	C	513	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
22	b	604	CLA	CHB-C4A-NA	3.25	129.00	124.51
23	D	406	BCR	C24-C23-C22	-3.25	121.33	126.23
22	b	608	CLA	O2D-CGD-CBD	3.23	117.01	111.27
22	c	512	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
32	C	516	LMG	C3-C4-C5	-3.23	104.48	110.24
28	c	518	DGD	O6D-C1D-O3G	-3.22	102.34	109.97
25	D	407	PL9	C35-C34-C36	3.22	120.68	115.27
22	d	402	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
22	B	604	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
26	a	412	LHG	O8-C23-O10	-3.21	115.50	123.59
22	c	511	CLA	CMB-C2B-C3B	3.21	130.68	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	BCR	C2-C1-C6	3.21	115.42	110.48
22	C	512	CLA	C1-C2-C3	-3.20	120.51	126.04
25	A	408	PL9	C7-C3-C2	-3.20	119.09	123.30
22	c	503	CLA	C4A-NA-C1A	3.20	108.14	106.71
25	a	410	PL9	C26-C24-C23	-3.19	114.66	121.12
22	b	605	CLA	CHB-C4A-NA	3.19	128.92	124.51
27	A	411	SQD	O8-S-O7	-3.17	103.52	111.27
32	D	408	LMG	O1-C7-C8	-3.17	103.25	110.90
22	b	615	CLA	C4A-NA-C1A	3.17	108.13	106.71
22	C	503	CLA	C1-O2A-CGA	3.17	124.76	116.44
22	C	513	CLA	CMD-C2D-C3D	3.16	130.60	124.68
22	b	614	CLA	O2A-CGA-O1A	-3.16	115.62	123.59
22	B	605	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
22	b	612	CLA	C1-C2-C3	-3.15	120.59	126.04
22	c	510	CLA	CMB-C2B-C3B	3.15	130.57	124.68
23	c	516	BCR	C34-C9-C10	-3.15	118.52	122.92
28	C	517	DGD	C6D-O5D-C1E	3.15	119.88	113.74
22	C	504	CLA	C4-C3-C5	3.15	120.56	115.27
22	c	505	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
35	F	101	HEC	CMB-C2B-C1B	-3.14	123.63	128.46
35	f	101	HEC	CMC-C2C-C1C	-3.14	123.64	128.46
23	A	405	BCR	C40-C30-C25	3.14	115.39	110.30
25	A	408	PL9	C35-C34-C36	3.14	120.55	115.27
22	b	604	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	D	407	PL9	C31-C29-C28	3.13	127.46	121.12
22	c	513	CLA	CMB-C2B-C3B	3.13	130.54	124.68
27	L	101	SQD	O9-S-O7	-3.13	103.12	113.95
22	C	504	CLA	C4A-NA-C1A	3.13	108.11	106.71
22	c	514	CLA	CMB-C2B-C3B	3.12	130.52	124.68
22	B	613	CLA	CMD-C2D-C3D	3.12	130.52	124.68
25	A	408	PL9	C40-C39-C38	-3.12	115.67	123.68
22	b	606	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	A	402	CLA	CAA-CBA-CGA	-3.12	104.14	113.25
22	b	602	CLA	CMB-C2B-C3B	3.11	130.51	124.68
22	D	405	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
22	a	411	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
32	a	417	LMG	O7-C10-O9	-3.11	116.19	123.70
23	b	618	BCR	C35-C13-C14	-3.11	118.57	122.92
26	D	412	LHG	O8-C23-O10	-3.11	115.75	123.59
22	C	506	CLA	CMD-C2D-C3D	3.11	130.49	124.68
22	D	405	CLA	CMB-C2B-C3B	3.10	130.49	124.68
22	C	513	CLA	C4D-C3D-CAD	-3.10	106.74	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	403	CLA	CMD-C2D-C3D	3.10	130.48	124.68
22	B	605	CLA	C1D-CHD-C4C	3.10	126.65	122.56
27	A	413	SQD	O47-C7-C8	3.10	118.18	111.50
32	m	101	LMG	O3-C3-C2	-3.10	103.19	110.35
28	C	518	DGD	O5D-C6D-C5D	-3.10	103.32	109.05
23	B	618	BCR	C15-C16-C17	-3.09	117.14	123.47
23	b	617	BCR	C2-C1-C6	3.09	115.24	110.48
32	m	101	LMG	O1-C7-C8	-3.09	103.45	110.90
22	b	602	CLA	CHB-C4A-NA	3.09	128.78	124.51
25	d	405	PL9	C22-C23-C24	-3.09	120.23	127.66
22	c	507	CLA	C4A-NA-C1A	3.09	108.09	106.71
22	B	602	CLA	CHB-C4A-NA	3.08	128.77	124.51
32	C	516	LMG	O6-C5-C4	-3.08	104.11	109.69
26	e	101	LHG	O8-C23-C24	3.07	121.55	111.91
26	D	412	LHG	O8-C23-C24	3.07	121.55	111.91
22	B	616	CLA	CHB-C4A-NA	3.07	128.75	124.51
22	a	403	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
22	c	505	CLA	C4A-NA-C1A	3.06	108.08	106.71
22	b	616	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
22	B	613	CLA	C1D-CHD-C4C	3.06	126.59	122.56
23	b	618	BCR	C15-C14-C13	-3.05	122.95	127.31
22	B	616	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
22	B	612	CLA	CMB-C2B-C3B	3.05	130.39	124.68
27	A	411	SQD	O9-S-O7	-3.05	103.38	113.95
22	B	607	CLA	C1-C2-C3	-3.05	120.77	126.04
22	a	411	CLA	C1D-CHD-C4C	3.05	126.58	122.56
22	B	605	CLA	C4D-C3D-CAD	-3.04	106.77	108.47
22	B	616	CLA	CMD-C2D-C3D	3.04	130.36	124.68
22	C	501	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
26	d	407	LHG	O8-C23-C24	3.04	121.44	111.91
22	b	605	CLA	CMB-C2B-C3B	3.04	130.36	124.68
25	A	408	PL9	C12-C13-C14	-3.03	120.35	127.66
23	c	516	BCR	C27-C26-C25	3.03	127.14	122.73
28	A	414	DGD	C1D-C2D-C3D	-3.03	103.68	110.00
22	a	405	CLA	CHB-C4A-NA	3.03	128.70	124.51
27	a	413	SQD	O47-C7-C8	3.03	118.03	111.50
22	B	609	CLA	CMB-C2B-C3B	3.02	130.34	124.68
28	c	517	DGD	O6D-C1D-O3G	-3.02	102.82	109.97
22	b	606	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
22	B	614	CLA	C4A-NA-C1A	3.02	108.06	106.71
28	A	414	DGD	O3G-C3G-C2G	-3.01	103.63	110.90
22	B	610	CLA	O2A-CGA-O1A	-3.01	116.00	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	CMB-C2B-C3B	3.01	130.31	124.68
22	b	604	CLA	CAA-CBA-CGA	-3.01	104.46	113.25
22	b	601	CLA	C1D-CHD-C4C	3.01	126.53	122.56
22	C	512	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
22	b	609	CLA	O1D-CGD-CBD	3.00	130.62	124.48
22	c	503	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
22	B	605	CLA	OBD-CAD-CBD	-3.00	121.61	125.89
22	b	615	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
32	c	523	LMG	O8-C28-O10	-2.99	116.04	123.59
23	K	101	BCR	C11-C10-C9	-2.99	123.04	127.31
22	c	507	CLA	C4-C3-C5	2.99	120.30	115.27
22	b	609	CLA	C5-C3-C2	2.99	127.17	121.12
22	b	608	CLA	CMB-C2B-C3B	2.99	130.26	124.68
22	c	514	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
28	h	102	DGD	CDB-CCB-CBB	-2.98	99.32	114.42
22	C	506	CLA	CHB-C4A-NA	2.98	128.63	124.51
22	b	602	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
22	C	506	CLA	C1D-CHD-C4C	2.97	126.47	122.56
22	c	509	CLA	CMD-C2D-C3D	2.96	130.22	124.68
25	D	407	PL9	C22-C23-C24	-2.96	120.53	127.66
32	c	523	LMG	O7-C10-O9	-2.96	116.55	123.70
28	A	414	DGD	O6D-C1D-O3G	-2.96	102.97	109.97
22	B	608	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
23	B	617	BCR	C35-C13-C14	-2.95	118.79	122.92
27	a	413	SQD	O9-S-O7	-2.95	103.75	113.95
27	L	101	SQD	O8-S-C6	2.94	110.43	105.74
22	B	613	CLA	CHA-C1A-NA	-2.94	119.66	126.40
22	b	616	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	B	617	BCR	C29-C30-C25	2.94	115.00	110.48
22	a	402	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	b	607	CLA	OBD-CAD-CBD	-2.94	121.70	125.89
23	K	101	BCR	C2-C1-C6	2.94	115.00	110.48
22	B	610	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
22	b	610	CLA	CAA-CBA-CGA	-2.93	104.68	113.25
22	B	603	CLA	CMB-C2B-C3B	2.93	130.16	124.68
27	A	413	SQD	O47-C45-C46	2.93	112.92	106.13
27	L	101	SQD	O5-C1-C2	-2.93	104.15	110.35
32	D	408	LMG	O1-C1-C2	-2.93	103.73	108.30
22	H	101	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
28	c	519	DGD	C3D-C4D-C5D	-2.93	105.02	110.24
22	d	402	CLA	O2A-CGA-O1A	-2.92	116.21	123.59
33	d	401	PHO	O1D-CGD-CBD	2.92	130.47	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	402	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
22	a	405	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
22	B	603	CLA	O2A-CGA-O1A	-2.92	116.23	123.59
32	D	408	LMG	O3-C3-C2	-2.91	103.62	110.35
25	A	408	PL9	O2-C1-C2	-2.91	115.12	121.78
32	m	101	LMG	O8-C28-O10	-2.91	116.26	123.59
22	b	611	CLA	C2C-C1C-NC	2.91	112.69	109.97
22	b	609	CLA	CHA-C1A-NA	-2.90	119.75	126.40
23	T	101	BCR	C27-C26-C25	2.90	126.94	122.73
22	b	608	CLA	C4D-C3D-CAD	-2.90	106.85	108.47
25	d	405	PL9	C41-C39-C38	-2.90	115.25	121.12
33	D	402	PHO	C5-C3-C2	2.89	126.97	121.12
22	C	512	CLA	CHB-C4A-NA	2.89	128.51	124.51
22	c	507	CLA	OBD-CAD-CBD	-2.89	121.77	125.89
22	b	609	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
22	c	504	CLA	CMA-C3A-C4A	2.89	119.54	111.77
22	c	514	CLA	O2A-CGA-O1A	-2.89	116.31	123.59
33	D	402	PHO	O1D-CGD-CBD	2.88	130.38	124.48
23	A	405	BCR	C27-C26-C25	2.88	126.91	122.73
22	b	603	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
28	C	518	DGD	O6D-C1D-O3G	-2.88	103.16	109.97
22	C	503	CLA	C7-C6-C5	-2.88	105.55	113.36
22	C	510	CLA	CMB-C2B-C3B	2.88	130.06	124.68
22	C	505	CLA	OBD-CAD-C3D	2.88	132.75	127.98
22	A	402	CLA	C7-C6-C5	-2.87	105.55	113.36
22	B	613	CLA	OBD-CAD-CBD	-2.87	121.79	125.89
22	c	509	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
23	d	404	BCR	C38-C26-C25	-2.87	121.30	124.53
22	c	510	CLA	CMD-C2D-C3D	2.87	130.05	124.68
25	A	408	PL9	C40-C39-C41	2.87	120.10	115.27
22	c	503	CLA	O1D-CGD-CBD	2.87	130.36	124.48
23	b	618	BCR	C37-C22-C21	-2.87	118.91	122.92
22	A	403	CLA	CMD-C2D-C3D	2.87	130.04	124.68
22	b	612	CLA	CAA-CBA-CGA	-2.87	104.88	113.25
22	c	508	CLA	CMB-C2B-C3B	2.87	130.04	124.68
22	d	402	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
33	a	404	PHO	O2D-CGD-O1D	-2.86	118.24	123.84
22	b	603	CLA	CMB-C2B-C3B	2.86	130.03	124.68
23	c	516	BCR	C11-C10-C9	-2.86	123.23	127.31
27	d	409	SQD	O5-C1-C2	-2.86	104.30	110.35
28	c	519	DGD	O3G-C3G-C2G	-2.86	104.00	110.90
27	L	101	SQD	O5-C5-C4	2.85	114.88	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C1D-CHD-C4C	2.85	126.32	122.56
35	F	101	HEC	CMB-C2B-C3B	2.84	129.16	125.82
32	d	408	LMG	O2-C2-C1	-2.84	103.14	110.05
22	C	512	CLA	O2A-CGA-O1A	-2.84	116.41	123.59
25	A	408	PL9	C31-C32-C33	-2.84	102.54	111.88
27	a	413	SQD	O8-S-C6	2.84	110.27	105.74
28	C	517	DGD	O5D-C1E-C2E	-2.84	103.87	108.30
32	C	516	LMG	O3-C3-C2	-2.84	103.78	110.35
32	d	408	LMG	O6-C1-O1	-2.84	103.25	109.97
22	B	602	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
23	C	514	BCR	C36-C18-C17	-2.84	118.95	122.92
22	a	403	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
22	H	101	CLA	C5-C3-C2	-2.84	115.38	121.12
28	h	102	DGD	O6D-C1D-O3G	-2.83	103.26	109.97
23	K	102	BCR	C33-C5-C6	-2.83	121.35	124.53
22	a	411	CLA	CMD-C2D-C3D	2.83	129.98	124.68
22	b	612	CLA	CHB-C4A-NA	2.83	128.43	124.51
22	D	405	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
22	C	501	CLA	OBD-CAD-CBD	-2.83	121.85	125.89
28	c	517	DGD	O2D-C2D-C1D	-2.83	103.18	110.05
35	V	201	HEC	CMD-C2D-C1D	-2.83	124.12	128.46
22	B	611	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
28	A	414	DGD	O5D-C6D-C5D	-2.82	103.82	109.05
22	c	508	CLA	CMD-C2D-C3D	2.82	129.96	124.68
22	D	404	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
28	H	102	DGD	C3D-C4D-C5D	-2.82	105.21	110.24
27	B	621	SQD	O9-S-C6	2.82	110.29	106.94
26	D	412	LHG	C11-C10-C9	-2.81	100.14	114.42
27	d	409	SQD	O47-C7-C8	2.81	118.65	110.80
22	b	601	CLA	O2D-CGD-CBD	2.81	116.26	111.27
22	b	615	CLA	CED-O2D-CGD	2.81	122.29	115.94
22	H	101	CLA	O2D-CGD-CBD	2.81	116.26	111.27
27	F	102	SQD	C1-O5-C5	-2.80	108.18	113.69
25	d	405	PL9	C7-C3-C2	-2.80	119.62	123.30
27	F	102	SQD	C3-C4-C5	2.80	115.23	110.24
26	D	409	LHG	C18-C17-C16	-2.80	100.22	114.42
35	v	201	HEC	CMB-C2B-C1B	-2.79	124.17	128.46
22	B	604	CLA	C1D-CHD-C4C	2.79	126.24	122.56
22	c	506	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
22	C	508	CLA	C1D-CHD-C4C	2.79	126.24	122.56
23	t	101	BCR	C33-C5-C6	-2.79	121.40	124.53
25	d	405	PL9	C7-C8-C9	-2.78	122.16	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	H	101	CLA	C4-C3-C5	2.78	119.95	115.27
23	c	515	BCR	C3-C4-C5	-2.78	109.12	114.08
22	C	503	CLA	O1D-CGD-CBD	2.77	130.16	124.48
28	C	517	DGD	O1G-C1A-C2A	-2.77	103.20	111.91
22	c	508	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
22	B	607	CLA	CHB-C4A-NA	2.77	128.34	124.51
27	a	413	SQD	O48-C23-C24	2.77	120.59	111.91
22	B	611	CLA	C14-C13-C15	-2.77	101.27	111.29
22	b	613	CLA	CMB-C2B-C3B	2.77	129.85	124.68
22	B	602	CLA	C1D-CHD-C4C	2.77	126.21	122.56
22	b	605	CLA	C1-C2-C3	-2.77	121.26	126.04
22	a	405	CLA	CMB-C2B-C3B	2.77	129.85	124.68
22	b	615	CLA	CHB-C4A-NA	2.76	128.33	124.51
22	B	606	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
22	B	609	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
22	C	502	CLA	CMD-C2D-C3D	2.76	129.84	124.68
25	a	410	PL9	C32-C33-C34	-2.76	121.02	127.66
23	X	101	BCR	C35-C13-C14	-2.76	119.06	122.92
23	c	516	BCR	C8-C9-C10	2.75	123.17	118.94
22	B	613	CLA	C1-C2-C3	-2.75	121.28	126.04
22	C	513	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	b	616	CLA	CHB-C4A-NA	2.75	128.32	124.51
22	c	507	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
32	Y	101	LMG	O6-C1-O1	-2.75	103.47	109.97
35	V	201	HEC	CMC-C2C-C3C	2.75	129.05	125.82
22	b	604	CLA	CMD-C2D-C3D	2.75	129.82	124.68
23	B	618	BCR	C29-C30-C25	2.75	114.71	110.48
28	c	519	DGD	O6E-C1E-O5D	-2.75	103.47	109.97
22	C	512	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
28	c	519	DGD	O6D-C1D-O3G	-2.74	103.48	109.97
33	D	402	PHO	C1B-NB-C4B	2.74	111.67	106.51
28	h	102	DGD	O3E-C3E-C2E	-2.74	104.02	110.35
22	b	611	CLA	O1D-CGD-CBD	2.74	130.09	124.48
28	c	517	DGD	O3G-C3G-C2G	-2.74	104.29	110.90
32	c	522	LMG	O8-C28-O10	-2.74	116.69	123.59
32	D	410	LMG	O8-C28-O10	-2.73	116.69	123.59
22	b	614	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
22	c	509	CLA	C4D-C3D-CAD	-2.73	106.95	108.47
22	c	506	CLA	C11-C10-C8	-2.73	107.11	115.92
32	m	101	LMG	O6-C1-C2	2.72	116.12	110.35
22	c	511	CLA	O1D-CGD-CBD	2.72	130.06	124.48
22	C	513	CLA	O2D-CGD-CBD	2.72	116.10	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	h	101	BCR	C27-C26-C25	2.72	126.68	122.73
22	b	604	CLA	C11-C10-C8	-2.72	107.14	115.92
25	A	408	PL9	C11-C9-C8	-2.72	115.62	121.12
28	h	102	DGD	C1D-C2D-C3D	-2.72	104.34	110.00
28	C	519	DGD	O6D-C1D-O3G	-2.71	103.56	109.97
25	D	407	PL9	C8-C7-C3	2.71	119.63	111.98
33	d	401	PHO	C1B-NB-C4B	2.71	111.61	106.51
22	c	503	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
22	b	615	CLA	C11-C10-C8	-2.71	107.17	115.92
23	A	405	BCR	C15-C14-C13	-2.70	123.45	127.31
23	B	618	BCR	C36-C18-C17	-2.70	119.14	122.92
22	B	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	B	607	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
22	b	612	CLA	OBD-CAD-C3D	2.70	132.46	127.98
23	k	102	BCR	C24-C23-C22	-2.70	122.16	126.23
33	d	401	PHO	CAC-C3C-C4C	-2.70	122.28	125.22
22	B	606	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
22	B	614	CLA	CMD-C2D-C3D	2.69	129.71	124.68
22	B	608	CLA	CMD-C2D-C3D	2.69	129.71	124.68
22	c	513	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	B	615	CLA	CMD-C2D-C3D	2.68	129.70	124.68
22	d	402	CLA	CMB-C2B-C3B	2.68	129.69	124.68
22	A	409	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
22	C	511	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
23	B	617	BCR	C33-C5-C6	-2.68	121.52	124.53
22	b	610	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
25	A	408	PL9	C27-C28-C29	-2.67	121.22	127.66
33	D	402	PHO	O2D-CGD-O1D	-2.67	118.62	123.84
23	C	515	BCR	C37-C22-C21	-2.67	119.18	122.92
22	b	611	CLA	C4A-NA-C1A	2.67	107.91	106.71
22	B	602	CLA	CMD-C2D-C3D	2.66	129.66	124.68
22	b	616	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
27	a	413	SQD	O47-C7-O49	-2.66	117.27	123.70
22	b	606	CLA	OBD-CAD-CBD	-2.66	122.09	125.89
22	c	503	CLA	C1D-CHD-C4C	2.66	126.06	122.56
22	B	614	CLA	C1D-CHD-C4C	2.66	126.06	122.56
23	b	618	BCR	C30-C25-C26	-2.65	118.88	122.61
22	b	601	CLA	CMD-C2D-C3D	2.65	129.64	124.68
22	b	603	CLA	C7-C6-C5	-2.65	106.16	113.36
23	b	617	BCR	C15-C14-C13	-2.65	123.53	127.31
27	F	102	SQD	O9-S-O7	-2.64	104.80	113.95
28	A	414	DGD	C3G-C2G-C1G	-2.64	105.54	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	101	BCR	C29-C30-C25	2.64	114.55	110.48
22	B	614	CLA	O2D-CGD-CBD	2.64	115.96	111.27
22	B	610	CLA	CMB-C2B-C3B	2.64	129.62	124.68
22	C	503	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
22	b	604	CLA	C1D-CHD-C4C	2.64	126.04	122.56
23	h	101	BCR	C36-C18-C17	-2.64	119.23	122.92
22	B	613	CLA	C2A-C1A-CHA	2.64	128.47	123.86
22	c	510	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	a	406	BCR	C27-C26-C25	2.63	126.55	122.73
23	K	101	BCR	C24-C23-C22	-2.63	122.26	126.23
22	C	505	CLA	CMD-C2D-C3D	2.62	129.58	124.68
33	d	401	PHO	C1-C2-C3	-2.62	121.51	126.04
23	K	102	BCR	C27-C26-C25	2.62	126.53	122.73
22	b	613	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
22	A	403	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
25	D	407	PL9	C42-C43-C44	-2.62	121.36	127.66
22	b	604	CLA	CHD-C4C-NC	2.62	128.33	124.20
25	A	408	PL9	C36-C37-C38	-2.61	103.29	111.88
22	C	508	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	B	606	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
22	A	404	CLA	O1D-CGD-CBD	2.61	129.83	124.48
22	b	615	CLA	CMB-C2B-C3B	2.61	129.56	124.68
32	a	417	LMG	C7-O1-C1	2.61	118.83	113.74
33	D	402	PHO	C2B-C1B-NB	-2.61	105.86	109.79
22	c	507	CLA	OBD-CAD-C3D	2.60	132.31	127.98
22	C	503	CLA	CMB-C2B-C1B	-2.60	124.46	128.46
32	M	101	LMG	O6-C1-O1	-2.60	103.81	109.97
22	D	405	CLA	C4-C3-C5	2.60	119.65	115.27
22	A	403	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	a	410	PL9	C20-C19-C21	2.60	119.64	115.27
22	c	513	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
28	H	102	DGD	O2D-C2D-C1D	-2.59	103.75	110.05
26	A	412	LHG	O8-C23-C24	2.59	120.03	111.91
22	C	504	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	B	607	CLA	CMB-C2B-C3B	2.59	129.52	124.68
22	c	505	CLA	C6-C7-C8	-2.59	107.55	115.92
22	c	509	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
22	a	405	CLA	CAA-CBA-CGA	-2.59	105.69	113.25
22	a	402	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	b	607	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
22	b	606	CLA	CMD-C2D-C3D	2.58	129.51	124.68
22	b	613	CLA	C1B-CHB-C4A	-2.58	125.00	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	517	DGD	O6D-C1D-O3G	-2.58	103.86	109.97
23	a	406	BCR	C30-C25-C26	-2.58	118.98	122.61
32	a	417	LMG	O7-C10-C11	2.58	117.06	111.50
27	L	101	SQD	O47-C7-C8	2.58	117.06	111.50
25	D	407	PL9	C7-C3-C2	-2.58	119.91	123.30
25	D	407	PL9	C7-C8-C9	-2.57	122.51	126.79
28	c	517	DGD	C3G-C2G-C1G	-2.57	105.70	111.79
22	B	605	CLA	OBD-CAD-C3D	2.57	132.25	127.98
22	c	504	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
22	b	606	CLA	CMB-C2B-C3B	2.57	129.49	124.68
32	M	101	LMG	C40-C39-C38	-2.57	101.38	114.42
22	c	512	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
22	c	509	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	b	619	BCR	C3-C4-C5	-2.57	109.50	114.08
22	b	614	CLA	OBD-CAD-CBD	-2.56	122.23	125.89
26	a	412	LHG	C20-C19-C18	-2.56	101.41	114.42
26	l	101	LHG	C20-C19-C18	-2.56	101.41	114.42
22	a	411	CLA	C4D-C3D-CAD	-2.56	107.04	108.47
33	d	401	PHO	CMD-C2D-C1D	2.56	129.01	125.06
23	b	618	BCR	C27-C26-C25	2.56	126.45	122.73
27	L	101	SQD	O48-C23-C24	2.56	119.94	111.91
32	b	621	LMG	C3-C4-C5	-2.56	105.68	110.24
32	b	621	LMG	C4-C3-C2	-2.56	106.36	110.82
22	A	403	CLA	CHB-C4A-NA	2.56	128.05	124.51
28	C	517	DGD	O3G-C3G-C2G	-2.55	104.74	110.90
22	b	601	CLA	CBA-CAA-C2A	2.55	121.39	113.86
22	B	604	CLA	C6-C5-C3	-2.55	106.77	113.45
23	a	406	BCR	C20-C21-C22	-2.55	123.67	127.31
33	d	401	PHO	C11-C10-C8	-2.55	107.69	115.92
22	a	402	CLA	CMD-C2D-C3D	2.55	129.44	124.68
22	c	511	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	d	404	BCR	C11-C10-C9	-2.54	123.68	127.31
22	c	503	CLA	O2A-C1-C2	-2.54	101.96	108.64
22	B	610	CLA	CAA-C2A-C3A	-2.54	105.82	112.78
23	A	405	BCR	C37-C22-C21	-2.54	119.36	122.92
22	C	507	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
22	C	513	CLA	CMB-C2B-C3B	2.54	129.42	124.68
22	b	615	CLA	OBD-CAD-CBD	-2.54	122.27	125.89
22	c	508	CLA	C2C-C1C-NC	2.54	112.35	109.97
28	c	518	DGD	O3G-C3G-C2G	-2.53	104.78	110.90
22	b	614	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
22	B	609	CLA	CMC-C2C-C1C	2.53	128.90	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	BCR	C3-C4-C5	-2.53	109.56	114.08
22	b	616	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
22	B	615	CLA	C11-C10-C8	-2.53	107.74	115.92
22	D	405	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
28	c	517	DGD	CDB-CCB-CBB	-2.53	101.59	114.42
22	C	506	CLA	OBD-CAD-CBD	-2.53	122.29	125.89
33	a	404	PHO	C3A-C4A-CHB	-2.53	117.47	121.83
22	B	611	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
28	C	517	DGD	O2E-C2E-C1E	-2.52	103.91	110.05
23	t	101	BCR	C1-C6-C7	2.52	122.92	115.78
22	D	405	CLA	CMD-C2D-C3D	2.52	129.40	124.68
22	D	405	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
22	c	512	CLA	C1D-CHD-C4C	2.52	125.89	122.56
28	C	517	DGD	C3D-C4D-C5D	-2.52	105.74	110.24
22	c	507	CLA	CAC-C3C-C4C	2.52	128.08	124.81
22	d	402	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	d	404	BCR	C16-C15-C14	-2.52	118.32	123.47
26	a	412	LHG	C11-C10-C9	-2.51	101.66	114.42
22	A	409	CLA	O2D-CGD-CBD	2.51	115.73	111.27
22	b	607	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	d	403	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
22	B	607	CLA	C2A-C1A-CHA	2.51	128.25	123.86
22	B	613	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
23	t	101	BCR	C1-C6-C5	-2.51	119.08	122.61
22	C	511	CLA	C4-C3-C5	2.51	119.49	115.27
22	b	605	CLA	CHD-C4C-NC	2.51	128.15	124.20
22	d	402	CLA	C4A-NA-C1A	2.50	107.83	106.71
25	a	410	PL9	C21-C19-C18	-2.50	116.05	121.12
22	C	504	CLA	CHD-C4C-NC	2.50	128.14	124.20
22	B	614	CLA	C4D-C3D-CAD	-2.50	107.08	108.47
22	B	604	CLA	C11-C10-C8	-2.50	107.85	115.92
23	b	619	BCR	C28-C27-C26	-2.49	109.62	114.08
32	c	520	LMG	O6-C1-O1	-2.49	104.07	109.97
22	B	611	CLA	CMB-C2B-C3B	2.49	129.34	124.68
35	V	201	HEC	C4B-C3B-C2B	2.49	109.04	106.35
22	B	605	CLA	CMB-C2B-C3B	2.49	129.34	124.68
23	C	515	BCR	C27-C26-C25	2.49	126.35	122.73
22	b	609	CLA	C1D-CHD-C4C	2.49	125.84	122.56
32	D	408	LMG	C3-C4-C5	-2.49	105.80	110.24
22	B	613	CLA	C4-C3-C5	2.48	119.45	115.27
27	L	101	SQD	O8-S-O7	-2.48	105.20	111.27
22	c	505	CLA	C1B-CHB-C4A	-2.48	125.20	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	401	PHO	C2B-C1B-NB	-2.48	106.05	109.79
22	C	509	CLA	C1-O2A-CGA	2.48	122.96	116.44
23	b	618	BCR	C15-C16-C17	-2.48	118.39	123.47
22	D	404	CLA	C1-C2-C3	-2.48	121.75	126.04
22	B	606	CLA	OBD-CAD-CBD	-2.48	122.35	125.89
23	B	617	BCR	C27-C26-C25	2.48	126.33	122.73
32	Y	101	LMG	O2-C2-C1	-2.48	104.02	110.05
22	b	615	CLA	C4D-C3D-CAD	-2.48	107.09	108.47
22	b	610	CLA	CMB-C2B-C3B	2.48	129.32	124.68
23	K	101	BCR	C33-C5-C6	-2.48	121.75	124.53
26	l	101	LHG	C5-O7-C7	-2.48	111.70	117.79
22	b	606	CLA	O2D-CGD-CBD	2.47	115.67	111.27
22	B	602	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
23	k	101	BCR	C38-C26-C25	-2.47	121.75	124.53
35	V	201	HEC	CMB-C2B-C1B	-2.47	124.67	128.46
22	b	608	CLA	C1D-CHD-C4C	2.47	125.81	122.56
27	d	409	SQD	C45-O47-C7	2.47	123.87	117.79
23	a	406	BCR	C2-C1-C6	2.47	114.28	110.48
22	B	613	CLA	C2C-C1C-NC	2.47	112.28	109.97
23	c	515	BCR	C11-C10-C9	-2.47	123.79	127.31
23	C	515	BCR	C2-C1-C6	2.46	114.28	110.48
27	A	413	SQD	O48-C23-C24	2.46	119.64	111.91
23	k	102	BCR	C8-C7-C6	-2.46	120.28	127.20
28	C	517	DGD	O3E-C3E-C2E	-2.46	104.66	110.35
22	B	610	CLA	CMD-C2D-C3D	2.46	129.28	124.68
26	D	409	LHG	O7-C7-C8	-2.46	106.19	111.50
22	B	602	CLA	CHA-C1A-NA	-2.46	120.76	126.40
28	C	519	DGD	CDB-CCB-CBB	-2.46	101.94	114.42
22	B	603	CLA	OBD-CAD-C3D	2.46	132.06	127.98
23	B	617	BCR	C15-C14-C13	-2.46	123.80	127.31
33	D	402	PHO	CAC-C3C-C4C	-2.46	122.54	125.22
22	c	510	CLA	C1D-CHD-C4C	2.46	125.80	122.56
27	L	101	SQD	O10-C23-C24	-2.46	114.14	123.73
22	B	608	CLA	CHB-C4A-NA	2.46	127.91	124.51
22	b	611	CLA	O2D-CGD-CBD	2.46	115.63	111.27
23	C	514	BCR	C15-C16-C17	-2.46	118.44	123.47
23	c	515	BCR	C33-C5-C6	-2.45	121.78	124.53
28	C	517	DGD	CBB-CAB-C9B	-2.45	101.99	114.42
22	C	511	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
23	k	102	BCR	C27-C26-C25	2.45	126.28	122.73
22	b	601	CLA	O2A-CGA-O1A	-2.44	117.42	123.59
32	M	101	LMG	C1-O6-C5	-2.44	108.89	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	X	101	BCR	C37-C22-C23	2.44	121.93	118.08
23	b	617	BCR	C29-C30-C25	2.44	114.24	110.48
22	c	508	CLA	C4D-C3D-CAD	-2.44	107.11	108.47
23	k	102	BCR	C38-C26-C25	-2.44	121.79	124.53
32	c	520	LMG	O8-C28-O10	-2.44	117.43	123.59
22	B	613	CLA	CMB-C2B-C3B	2.44	129.24	124.68
22	c	512	CLA	CHB-C4A-NA	2.44	127.88	124.51
33	D	401	PHO	C5-C3-C2	2.44	126.05	121.12
22	D	404	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
22	b	606	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
25	A	408	PL9	C22-C23-C24	-2.43	121.80	127.66
23	b	619	BCR	C15-C16-C17	-2.43	118.49	123.47
23	t	101	BCR	C36-C18-C19	2.43	121.91	118.08
22	B	615	CLA	C1D-CHD-C4C	2.43	125.76	122.56
22	C	507	CLA	CAA-CBA-CGA	-2.43	106.17	113.25
23	c	515	BCR	C15-C16-C17	-2.42	118.51	123.47
22	B	608	CLA	C1D-CHD-C4C	2.42	125.75	122.56
23	c	516	BCR	C33-C5-C6	-2.42	121.81	124.53
22	b	609	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	B	608	CLA	C11-C12-C13	-2.42	108.10	115.92
22	B	602	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
35	V	201	HEC	CMD-C2D-C3D	2.42	129.50	124.94
23	K	102	BCR	C30-C25-C26	-2.41	119.21	122.61
22	b	609	CLA	OBD-CAD-CBD	-2.41	122.45	125.89
22	b	606	CLA	CHB-C4A-NA	2.41	127.85	124.51
23	c	515	BCR	C15-C14-C13	-2.41	123.87	127.31
22	b	603	CLA	OBD-CAD-C3D	2.41	131.99	127.98
32	b	621	LMG	O2-C2-C1	-2.41	104.19	110.05
22	C	513	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
22	b	606	CLA	C1D-CHD-C4C	2.41	125.74	122.56
23	t	101	BCR	C7-C8-C9	-2.41	122.59	126.23
22	c	513	CLA	O2A-CGA-O1A	-2.41	117.51	123.59
22	b	610	CLA	C2C-C1C-NC	2.41	112.23	109.97
22	B	615	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
22	c	511	CLA	OBD-CAD-CBD	-2.41	122.45	125.89
22	b	607	CLA	CHD-C4C-NC	2.41	128.00	124.20
22	b	602	CLA	CMD-C2D-C3D	2.41	129.18	124.68
25	d	405	PL9	C8-C7-C3	2.40	118.78	111.98
23	K	102	BCR	C16-C15-C14	-2.40	118.55	123.47
23	A	405	BCR	C30-C25-C26	-2.40	119.23	122.61
28	c	517	DGD	C3E-C4E-C5E	-2.40	105.96	110.24
23	B	619	BCR	C29-C30-C25	2.40	114.18	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	517	DGD	O2G-C1B-C2B	-2.40	106.33	111.50
22	b	606	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
28	c	519	DGD	C6D-O5D-C1E	2.40	118.43	113.74
23	k	101	BCR	C33-C5-C6	-2.40	121.83	124.53
22	b	610	CLA	CHA-C1A-NA	-2.40	120.91	126.40
22	c	505	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
22	b	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
28	c	519	DGD	CBB-CAB-C9B	-2.39	102.27	114.42
22	B	614	CLA	C1-C2-C3	-2.39	121.90	126.04
32	D	408	LMG	O2-C2-C3	-2.39	104.82	110.35
32	M	101	LMG	O3-C3-C2	-2.39	104.82	110.35
22	B	605	CLA	CMD-C2D-C3D	2.39	129.16	124.68
22	a	411	CLA	CHA-C1A-NA	-2.39	120.92	126.40
22	b	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
22	B	605	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
22	c	502	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
22	C	509	CLA	C1-C2-C3	-2.39	121.91	126.04
28	c	518	DGD	O2D-C2D-C1D	-2.39	104.24	110.05
22	c	513	CLA	C1D-CHD-C4C	2.39	125.71	122.56
33	D	402	PHO	CMB-C2B-C1B	-2.39	121.39	125.06
22	a	402	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
22	b	604	CLA	CMB-C2B-C3B	2.38	129.14	124.68
32	C	516	LMG	C9-C8-C7	-2.38	106.15	111.79
22	d	402	CLA	CMD-C2D-C3D	2.38	129.14	124.68
22	A	409	CLA	C3D-CAD-CBD	-2.38	104.47	107.61
25	A	408	PL9	C20-C19-C18	-2.38	117.56	123.68
22	C	501	CLA	CAA-CBA-CGA	-2.38	106.30	113.25
23	D	406	BCR	C16-C15-C14	-2.38	118.60	123.47
22	A	402	CLA	CMB-C2B-C3B	2.38	129.13	124.68
27	F	102	SQD	C46-O48-C23	2.38	124.60	116.92
22	b	607	CLA	C4D-C3D-CAD	-2.37	107.15	108.47
26	D	412	LHG	O8-C6-C5	-2.37	101.52	108.43
32	C	516	LMG	C1-O6-C5	-2.37	109.03	113.69
22	b	607	CLA	C6-C7-C8	-2.37	108.25	115.92
22	c	507	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	b	608	CLA	C3C-C4C-NC	-2.37	107.91	110.57
22	B	606	CLA	C1D-CHD-C4C	2.37	125.69	122.56
23	c	515	BCR	C24-C23-C22	-2.37	122.66	126.23
33	D	402	PHO	C1-C2-C3	-2.37	121.95	126.04
22	B	609	CLA	OBD-CAD-C3D	2.37	131.91	127.98
22	b	615	CLA	CAA-CBA-CGA	-2.37	106.34	113.25
23	K	102	BCR	C8-C7-C6	-2.37	120.56	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	CLA	O2D-CGD-CBD	2.36	115.47	111.27
32	a	417	LMG	O6-C1-C2	-2.36	105.35	110.35
22	C	505	CLA	C4D-C3D-CAD	-2.36	107.15	108.47
22	C	505	CLA	CHA-C1A-NA	-2.36	120.99	126.40
22	b	611	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
22	C	510	CLA	CMD-C2D-C3D	2.36	129.09	124.68
22	B	608	CLA	C6-C7-C8	-2.36	108.30	115.92
22	c	506	CLA	OBD-CAD-C3D	2.36	131.90	127.98
23	K	102	BCR	C16-C17-C18	-2.36	123.95	127.31
22	C	507	CLA	O2D-CGD-CBD	2.35	115.45	111.27
26	D	409	LHG	C20-C19-C18	-2.35	102.48	114.42
22	B	614	CLA	CHB-C4A-NA	2.35	127.76	124.51
28	c	517	DGD	O1G-C1A-C2A	-2.35	104.53	111.91
22	C	505	CLA	C16-C15-C13	-2.35	108.32	115.92
22	a	411	CLA	CMC-C2C-C1C	2.35	128.62	125.04
22	c	513	CLA	CMD-C2D-C3D	2.35	129.07	124.68
22	c	513	CLA	O1D-CGD-CBD	2.35	129.29	124.48
28	H	102	DGD	C3E-C4E-C5E	-2.35	106.05	110.24
28	c	517	DGD	O3G-C1D-C2D	-2.35	104.64	108.30
32	c	520	LMG	C9-C8-C7	-2.35	106.24	111.79
22	b	604	CLA	C3C-C4C-NC	-2.35	107.94	110.57
28	A	414	DGD	CBB-CAB-C9B	-2.35	102.51	114.42
32	c	522	LMG	C9-C8-C7	-2.35	106.24	111.79
23	C	515	BCR	C15-C14-C13	-2.35	123.96	127.31
32	D	408	LMG	O8-C28-O10	-2.35	117.67	123.59
22	C	508	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
28	A	414	DGD	CDB-CCB-CBB	-2.34	102.52	114.42
28	c	519	DGD	C3G-C2G-C1G	-2.34	106.24	111.79
23	D	406	BCR	C27-C26-C25	2.34	126.13	122.73
22	b	601	CLA	C4-C3-C5	2.34	119.21	115.27
22	B	605	CLA	C7-C6-C5	-2.34	107.02	113.36
33	a	404	PHO	O2A-CGA-O1A	-2.33	117.70	123.59
22	H	101	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
23	d	404	BCR	C8-C7-C6	-2.33	120.64	127.20
25	D	407	PL9	C12-C13-C14	-2.33	122.05	127.66
22	b	611	CLA	CHB-C4A-NA	2.33	127.73	124.51
32	c	522	LMG	O3-C3-C2	-2.33	104.97	110.35
22	a	405	CLA	CMA-C3A-C4A	-2.33	105.52	111.77
23	c	516	BCR	C1-C6-C5	-2.33	119.34	122.61
28	C	517	DGD	CDB-CCB-CBB	-2.32	102.62	114.42
22	B	603	CLA	CMD-C2D-C3D	2.32	129.03	124.68
22	C	513	CLA	CHC-C1C-NC	2.32	127.73	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	102	DGD	C3D-C4D-C5D	-2.32	106.10	110.24
28	A	414	DGD	O5E-C6E-C5E	-2.32	103.33	111.29
32	c	523	LMG	O2-C2-C3	-2.32	104.99	110.35
23	C	515	BCR	C7-C8-C9	-2.32	122.73	126.23
32	m	101	LMG	C37-C36-C35	-2.32	102.65	114.42
22	a	411	CLA	C2A-C1A-CHA	2.32	127.91	123.86
22	c	508	CLA	O1A-CGA-CBA	2.32	132.77	123.73
22	a	411	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	A	405	BCR	C15-C16-C17	-2.32	118.73	123.47
22	c	505	CLA	CHD-C4C-NC	2.31	127.85	124.20
23	b	617	BCR	C8-C7-C6	-2.31	120.70	127.20
22	A	409	CLA	C1D-CHD-C4C	2.31	125.61	122.56
28	A	414	DGD	C3E-C4E-C5E	-2.31	106.11	110.24
23	B	618	BCR	C35-C13-C14	-2.31	119.69	122.92
32	Y	101	LMG	O8-C28-O10	-2.31	117.76	123.59
22	c	513	CLA	C4-C3-C5	2.31	119.16	115.27
28	C	517	DGD	C9B-C8B-C7B	-2.31	102.71	114.42
25	A	408	PL9	O2-C1-C6	2.31	124.58	120.59
23	k	101	BCR	C27-C26-C25	2.30	126.08	122.73
23	D	406	BCR	C35-C13-C12	2.30	121.71	118.08
22	b	616	CLA	CHD-C4C-NC	2.30	127.83	124.20
22	c	508	CLA	OBD-CAD-C3D	2.30	131.81	127.98
22	B	606	CLA	CHA-C1A-NA	-2.30	121.13	126.40
23	h	101	BCR	C40-C30-C25	2.30	114.03	110.30
22	C	506	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	h	101	BCR	C38-C26-C25	-2.30	121.95	124.53
22	b	604	CLA	O2D-CGD-CBD	2.30	115.35	111.27
22	b	609	CLA	CMD-C2D-C3D	2.30	128.98	124.68
22	c	505	CLA	O2D-CGD-CBD	2.30	115.35	111.27
22	C	501	CLA	C1D-CHD-C4C	2.30	125.59	122.56
25	D	407	PL9	C26-C24-C23	-2.29	116.47	121.12
32	Y	101	LMG	O1-C7-C8	-2.29	105.36	110.90
22	C	504	CLA	CHC-C1C-NC	2.29	127.68	124.20
22	c	511	CLA	C1-O2A-CGA	2.29	122.46	116.44
22	B	603	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
22	C	504	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
32	b	621	LMG	O8-C28-O10	-2.29	117.82	123.59
22	b	609	CLA	C2A-C1A-CHA	2.29	127.86	123.86
22	C	502	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
23	B	619	BCR	C28-C27-C26	-2.28	110.00	114.08
23	A	405	BCR	C35-C13-C14	-2.28	119.73	122.92
22	C	507	CLA	C3C-C4C-NC	-2.28	108.01	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	414	DGD	O1G-C1A-O1A	-2.28	117.83	123.59
22	B	603	CLA	CMB-C2B-C1B	-2.28	124.96	128.46
22	B	608	CLA	C11-C10-C8	-2.28	108.55	115.92
22	C	507	CLA	CMB-C2B-C3B	2.28	128.94	124.68
22	C	510	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
22	c	506	CLA	C6-C7-C8	-2.28	108.56	115.92
23	b	619	BCR	C30-C25-C26	-2.28	119.41	122.61
23	B	619	BCR	C36-C18-C19	2.28	121.66	118.08
32	c	522	LMG	C6-C5-C4	-2.28	107.67	113.00
22	c	506	CLA	C3A-C2A-C1A	2.27	104.75	101.34
32	M	101	LMG	O7-C10-O9	-2.27	118.21	123.70
22	c	508	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
22	b	603	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
22	c	508	CLA	C6-C7-C8	-2.27	108.58	115.92
22	C	509	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
22	A	409	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
32	d	408	LMG	O7-C10-O9	-2.27	118.22	123.70
27	d	409	SQD	O5-C1-O6	2.27	115.35	109.97
22	B	612	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
23	h	101	BCR	C2-C1-C6	2.27	113.97	110.48
22	b	613	CLA	C7-C6-C5	-2.27	107.21	113.36
22	b	607	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
22	A	403	CLA	O2D-CGD-CBD	2.26	115.29	111.27
22	b	603	CLA	C3C-C4C-NC	-2.26	108.03	110.57
23	c	516	BCR	C15-C16-C17	-2.26	118.84	123.47
25	D	407	PL9	C37-C38-C39	-2.26	122.21	127.66
22	A	402	CLA	C11-C10-C8	-2.26	108.62	115.92
27	A	411	SQD	O5-C1-C2	-2.26	105.57	110.35
28	c	519	DGD	C3A-C2A-C1A	-2.26	105.41	113.62
22	d	402	CLA	C1-C2-C3	-2.26	122.14	126.04
32	c	522	LMG	O7-C10-O9	-2.25	118.25	123.70
22	d	402	CLA	O1D-CGD-CBD	2.25	129.10	124.48
22	a	405	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
22	B	603	CLA	C3C-C4C-NC	-2.25	108.05	110.57
22	c	502	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
22	B	609	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
23	B	619	BCR	C29-C28-C27	-2.25	106.36	111.38
28	C	519	DGD	O3G-C1D-C2D	-2.25	104.80	108.30
22	C	502	CLA	C4D-C3D-CAD	-2.25	107.22	108.47
22	b	611	CLA	O2A-C1-C2	-2.24	102.74	108.64
22	B	605	CLA	C5-C3-C2	-2.24	116.58	121.12
22	c	507	CLA	C4-C3-C2	-2.24	117.93	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	610	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
22	b	609	CLA	C1-O2A-CGA	2.24	122.32	116.44
22	B	615	CLA	CMB-C2B-C3B	2.24	128.87	124.68
25	A	408	PL9	C45-C44-C46	-2.24	111.51	115.27
22	B	612	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	C	503	CLA	OBD-CAD-CBD	-2.24	122.70	125.89
22	b	610	CLA	O2D-CGD-CBD	2.24	115.24	111.27
23	B	617	BCR	C15-C16-C17	-2.23	118.90	123.47
22	A	404	CLA	C2C-C1C-NC	2.23	112.06	109.97
27	a	413	SQD	O9-S-C6	2.23	109.59	106.94
22	A	402	CLA	OBD-CAD-C3D	-2.23	124.27	127.98
23	D	406	BCR	C35-C13-C14	-2.23	119.80	122.92
23	A	405	BCR	C36-C18-C19	2.23	121.59	118.08
27	L	101	SQD	C26-C25-C24	-2.23	105.17	113.19
23	t	101	BCR	C24-C23-C22	-2.23	122.87	126.23
23	B	618	BCR	C38-C26-C27	-2.23	109.33	113.62
22	b	616	CLA	C1D-CHD-C4C	2.23	125.50	122.56
32	c	522	LMG	O2-C2-C1	-2.23	104.63	110.05
27	A	411	SQD	O5-C1-O6	2.23	115.25	109.97
27	L	101	SQD	C1-O5-C5	-2.23	109.32	113.69
35	v	201	HEC	CAD-CBD-CGD	-2.23	108.94	112.67
33	a	404	PHO	C4-C3-C2	-2.22	117.97	123.68
23	K	101	BCR	C3-C4-C5	-2.22	110.11	114.08
22	b	611	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
22	C	502	CLA	O2D-CGD-CBD	2.22	115.22	111.27
32	m	101	LMG	C40-C39-C38	-2.22	103.15	114.42
22	d	403	CLA	OBD-CAD-CBD	-2.22	122.72	125.89
26	A	412	LHG	C11-C10-C9	-2.22	103.15	114.42
22	B	614	CLA	O1D-CGD-CBD	2.22	129.02	124.48
22	b	611	CLA	C1D-CHD-C4C	2.22	125.49	122.56
32	d	408	LMG	C3-C4-C5	-2.22	106.28	110.24
22	b	604	CLA	CGD-CBD-CAD	-2.22	103.55	110.73
35	V	201	HEC	CBD-CAD-C3D	-2.22	108.40	112.49
22	b	616	CLA	OBD-CAD-C3D	2.22	131.66	127.98
23	t	101	BCR	C4-C5-C6	2.22	125.95	122.73
28	c	517	DGD	O4D-C4D-C5D	-2.21	103.80	109.30
28	H	102	DGD	CEB-CDB-CCB	-2.21	103.19	114.42
22	C	510	CLA	C1D-CHD-C4C	2.21	125.48	122.56
25	D	407	PL9	C40-C39-C41	2.21	118.99	115.27
28	A	414	DGD	C7A-C6A-C5A	-2.21	103.21	114.42
33	D	401	PHO	C1B-NB-C4B	2.21	110.67	106.51
27	B	621	SQD	C46-C45-C44	-2.21	106.57	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	413	SQD	O10-C23-C24	-2.21	115.12	123.73
32	M	101	LMG	O2-C2-C1	-2.21	104.68	110.05
22	D	404	CLA	CHB-C4A-NA	2.21	127.56	124.51
22	B	611	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
22	d	402	CLA	C4-C3-C5	2.21	118.98	115.27
22	c	505	CLA	CMC-C2C-C1C	2.21	128.40	125.04
25	d	405	PL9	C12-C13-C14	-2.21	122.35	127.66
22	D	404	CLA	O2D-CGD-CBD	2.21	115.19	111.27
23	t	101	BCR	C34-C9-C10	-2.21	119.83	122.92
32	c	520	LMG	C40-C39-C38	-2.20	103.23	114.42
28	C	518	DGD	C1D-C2D-C3D	-2.20	105.41	110.00
22	H	101	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
22	c	502	CLA	OBD-CAD-CBD	-2.20	122.75	125.89
23	t	101	BCR	C16-C15-C14	-2.20	118.97	123.47
23	B	618	BCR	C30-C25-C26	-2.20	119.52	122.61
22	c	513	CLA	C4D-C3D-CAD	-2.20	107.25	108.47
23	X	101	BCR	C39-C30-C25	-2.20	106.74	110.30
28	c	519	DGD	O5D-C1E-C2E	2.20	111.73	108.30
22	C	509	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	C	514	BCR	C11-C10-C9	-2.19	124.18	127.31
22	b	610	CLA	C2A-C1A-CHA	2.19	127.69	123.86
22	c	503	CLA	C1-C2-C3	-2.19	122.25	126.04
22	c	503	CLA	CED-O2D-CGD	2.19	120.90	115.94
32	c	520	LMG	O7-C10-O9	-2.19	118.61	122.96
22	c	502	CLA	C2C-C1C-NC	2.19	112.03	109.97
23	t	101	BCR	C31-C1-C6	2.19	113.86	110.30
28	C	518	DGD	CDB-CCB-CBB	-2.19	103.30	114.42
22	B	611	CLA	C4D-C3D-CAD	2.19	109.69	108.47
32	b	621	LMG	O6-C5-C6	2.19	111.88	106.44
27	A	411	SQD	O48-C23-C24	2.19	118.78	111.91
23	B	618	BCR	C2-C1-C6	2.19	113.85	110.48
22	a	402	CLA	OBD-CAD-CBD	-2.19	122.77	125.89
22	A	409	CLA	CMC-C2C-C3C	2.19	132.06	126.12
23	A	405	BCR	C38-C26-C27	-2.18	109.42	113.62
22	a	403	CLA	CMA-C3A-C4A	-2.18	105.90	111.77
23	C	515	BCR	C8-C7-C6	-2.18	121.07	127.20
23	b	617	BCR	C27-C26-C25	2.18	125.90	122.73
28	A	414	DGD	O5D-C1E-C2E	2.18	111.71	108.30
23	B	619	BCR	C30-C25-C26	-2.18	119.54	122.61
22	B	603	CLA	CHD-C4C-NC	2.18	127.64	124.20
35	V	201	HEC	CAD-CBD-CGD	-2.18	109.02	112.67
22	C	504	CLA	O2A-CGA-O1A	-2.18	118.09	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	O47-C45-C46	2.18	116.29	108.40
22	C	506	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
27	d	409	SQD	O48-C23-C24	2.18	118.74	111.91
23	X	101	BCR	C16-C15-C14	-2.17	119.02	123.47
22	B	616	CLA	CMB-C2B-C1B	-2.17	125.12	128.46
25	d	405	PL9	C15-C14-C16	-2.17	111.62	115.27
22	c	504	CLA	O1D-CGD-CBD	2.17	128.93	124.48
33	D	401	PHO	CMD-C2D-C1D	2.17	128.41	125.06
22	B	613	CLA	OBD-CAD-C3D	2.17	131.58	127.98
26	e	101	LHG	C11-C10-C9	-2.17	103.42	114.42
27	F	102	SQD	O5-C5-C4	2.17	113.63	109.69
22	A	402	CLA	CBA-CAA-C2A	-2.16	107.47	113.86
32	M	101	LMG	C6-C5-C4	-2.16	107.93	113.00
23	c	515	BCR	C38-C26-C25	-2.16	122.10	124.53
22	C	510	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	B	614	CLA	CHA-C1A-NA	-2.16	121.44	126.40
25	d	405	PL9	C36-C34-C33	-2.16	116.74	121.12
22	b	610	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
22	B	606	CLA	CMB-C2B-C3B	2.16	128.72	124.68
25	D	407	PL9	C16-C14-C13	2.16	125.49	121.12
23	c	515	BCR	C28-C27-C26	-2.16	110.22	114.08
22	c	510	CLA	C2A-C3A-C4A	2.16	105.35	101.87
23	A	405	BCR	C8-C7-C6	-2.16	121.14	127.20
23	k	102	BCR	C16-C15-C14	-2.16	119.06	123.47
25	a	410	PL9	O2-C1-C2	-2.16	116.84	121.78
22	a	402	CLA	C4-C3-C5	2.16	118.90	115.27
22	a	405	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
22	C	504	CLA	O2D-CGD-CBD	2.15	115.10	111.27
22	b	607	CLA	OBD-CAD-C3D	2.15	131.56	127.98
23	B	619	BCR	C8-C7-C6	-2.15	121.16	127.20
35	F	101	HEC	CMC-C2C-C1C	-2.15	125.16	128.46
26	a	412	LHG	C25-C24-C23	2.15	121.44	113.62
35	V	201	HEC	C3B-C4B-NB	-2.15	106.89	110.94
22	b	609	CLA	CMB-C2B-C3B	2.15	128.69	124.68
32	D	410	LMG	C38-C37-C36	-2.14	103.54	114.42
26	D	409	LHG	C27-C26-C25	-2.14	103.54	114.42
32	c	520	LMG	C38-C37-C36	-2.14	103.54	114.42
22	B	603	CLA	CHB-C4A-NA	2.14	127.47	124.51
23	h	101	BCR	C35-C13-C14	-2.14	119.92	122.92
22	C	512	CLA	CAA-CBA-CGA	-2.14	107.00	113.25
28	C	518	DGD	O2G-C1B-O1B	-2.14	118.53	123.70
22	C	502	CLA	C3A-C2A-C1A	2.14	104.54	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	101	BCR	C15-C14-C13	-2.14	124.26	127.31
22	C	511	CLA	CHB-C4A-NA	2.14	127.47	124.51
32	a	417	LMG	C32-C31-C30	-2.14	103.58	114.42
22	b	608	CLA	C1B-CHB-C4A	-2.14	125.89	130.12
22	B	605	CLA	C4A-NA-C1A	2.14	107.67	106.71
22	B	611	CLA	C1-C2-C3	-2.13	122.35	126.04
32	C	516	LMG	C36-C35-C34	-2.13	103.59	114.42
28	c	519	DGD	CDB-CCB-CBB	-2.13	103.59	114.42
32	D	410	LMG	O1-C7-C8	-2.13	106.12	111.78
28	h	102	DGD	C7B-C6B-C5B	-2.13	103.59	114.42
28	C	518	DGD	C7B-C6B-C5B	-2.13	103.60	114.42
22	C	511	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
22	c	511	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
32	M	101	LMG	O1-C7-C8	-2.13	105.76	110.90
26	a	412	LHG	C18-C17-C16	-2.13	103.61	114.42
32	a	417	LMG	O8-C28-O10	-2.13	118.22	123.59
22	c	502	CLA	CHC-C1C-C2C	-2.13	120.83	126.72
22	c	503	CLA	CMC-C2C-C3C	2.13	131.89	126.12
22	c	502	CLA	O1D-CGD-CBD	2.13	128.84	124.48
23	d	404	BCR	C27-C26-C25	2.13	125.82	122.73
23	D	406	BCR	C19-C18-C17	-2.13	115.68	118.94
23	B	619	BCR	C34-C9-C10	-2.12	119.95	122.92
22	b	609	CLA	O2D-CGD-CBD	-2.12	107.49	111.27
28	C	518	DGD	O3E-C3E-C4E	-2.12	105.44	110.35
22	b	611	CLA	OBD-CAD-CBD	-2.12	122.86	125.89
22	B	616	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
25	d	405	PL9	C32-C33-C34	-2.12	122.55	127.66
22	C	501	CLA	OBD-CAD-C3D	2.12	131.50	127.98
22	b	607	CLA	C1-O2A-CGA	2.12	122.00	116.44
28	c	519	DGD	CAB-C9B-C8B	-2.12	103.67	114.42
22	B	607	CLA	CMD-C2D-C3D	2.12	128.64	124.68
22	c	509	CLA	CGD-CBD-CAD	-2.12	103.87	110.73
22	c	506	CLA	CMC-C2C-C1C	-2.12	121.81	125.04
26	L	102	LHG	C12-C11-C10	-2.12	103.68	114.42
22	b	608	CLA	CMD-C2D-C3D	2.12	128.64	124.68
22	B	610	CLA	C4-C3-C2	-2.11	118.25	123.68
23	h	101	BCR	C3-C4-C5	-2.11	110.30	114.08
28	C	518	DGD	O6E-C1E-O5D	-2.11	104.97	109.97
22	b	606	CLA	OBD-CAD-C3D	2.11	131.49	127.98
22	C	509	CLA	O2D-CGD-CBD	2.11	115.02	111.27
27	d	409	SQD	O47-C7-O49	-2.11	118.60	123.70
26	a	412	LHG	C15-C14-C13	-2.11	103.71	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	CMB-C2B-C3B	2.11	128.62	124.68
25	D	407	PL9	C27-C28-C29	-2.10	122.59	127.66
22	C	513	CLA	C2A-C1A-CHA	2.10	127.54	123.86
22	c	506	CLA	C1-C2-C3	-2.10	122.41	126.04
23	B	618	BCR	C27-C26-C25	2.10	125.78	122.73
27	A	411	SQD	C46-C45-C44	-2.10	106.82	111.79
26	A	412	LHG	C18-C17-C16	-2.10	103.76	114.42
22	B	616	CLA	O1D-CGD-CBD	2.10	128.78	124.48
22	B	612	CLA	C9-C8-C7	-2.10	103.69	111.29
27	B	621	SQD	O5-C5-C4	2.10	113.50	109.69
23	b	617	BCR	C24-C23-C22	-2.10	123.07	126.23
22	c	509	CLA	CMB-C2B-C1B	-2.09	125.24	128.46
22	B	610	CLA	C1-C2-C3	-2.09	122.42	126.04
22	a	402	CLA	C3C-C4C-NC	-2.09	108.22	110.57
27	B	621	SQD	O10-C23-C24	-2.09	115.57	123.73
22	a	402	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
33	d	401	PHO	O2D-CGD-CBD	2.09	114.98	111.27
23	k	101	BCR	C8-C7-C6	-2.09	121.33	127.20
22	B	607	CLA	CHA-C1A-NA	-2.09	121.61	126.40
22	A	403	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
26	A	410	LHG	C11-C10-C9	-2.09	103.81	114.42
27	L	101	SQD	O48-C23-O10	-2.09	118.32	123.59
22	B	605	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
33	D	401	PHO	C1-O2A-CGA	2.09	121.92	116.44
22	D	405	CLA	C4D-C3D-CAD	-2.09	107.31	108.47
22	d	402	CLA	C6-C5-C3	2.08	118.92	113.45
25	D	407	PL9	O2-C1-C2	-2.08	117.00	121.78
23	C	515	BCR	C3-C4-C5	-2.08	110.36	114.08
22	A	402	CLA	C11-C12-C13	-2.08	109.19	115.92
23	X	101	BCR	C38-C26-C27	-2.08	109.62	113.62
22	a	403	CLA	CHC-C1C-C2C	-2.08	120.97	126.72
26	D	412	LHG	C20-C19-C18	-2.08	103.87	114.42
23	T	101	BCR	C1-C6-C5	-2.08	119.69	122.61
22	b	616	CLA	C2A-C3A-C4A	2.08	105.23	101.87
26	a	412	LHG	O10-C23-C24	-2.08	115.63	123.73
22	B	614	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
22	c	506	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
28	c	518	DGD	CDB-CCB-CBB	-2.08	103.88	114.42
22	c	511	CLA	O2D-CGD-CBD	2.08	114.96	111.27
27	d	409	SQD	C26-C25-C24	-2.08	105.73	113.19
32	M	101	LMG	C37-C36-C35	-2.08	103.89	114.42
22	c	513	CLA	O2A-C1-C2	-2.08	103.18	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	417	LMG	O7-C8-C7	2.07	115.91	108.40
26	D	409	LHG	C15-C14-C13	-2.07	103.90	114.42
23	h	101	BCR	C16-C17-C18	-2.07	124.35	127.31
32	c	520	LMG	O3-C3-C2	-2.07	105.56	110.35
28	C	519	DGD	C6B-C5B-C4B	-2.07	103.91	114.42
22	B	604	CLA	OBD-CAD-C3D	2.07	131.42	127.98
22	B	604	CLA	O1D-CGD-CBD	2.07	128.72	124.48
32	b	621	LMG	O7-C10-O9	-2.07	118.70	123.70
32	a	417	LMG	O6-C5-C6	2.07	111.58	106.44
28	h	102	DGD	C6D-C5D-C4D	2.07	116.41	112.09
22	c	503	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	C	510	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	D	406	BCR	C15-C16-C17	-2.07	119.24	123.47
32	b	621	LMG	C9-C8-C7	-2.07	106.90	111.79
26	l	101	LHG	C11-C10-C9	-2.07	103.94	114.42
28	C	519	DGD	O3E-C3E-C2E	-2.07	105.57	110.35
23	K	102	BCR	C35-C13-C14	-2.07	120.03	122.92
27	A	411	SQD	C3-C4-C5	2.07	113.92	110.24
22	C	513	CLA	C4-C3-C5	2.06	118.74	115.27
27	d	409	SQD	O6-C44-C45	2.06	115.88	110.90
32	C	516	LMG	O7-C10-C11	2.06	115.95	111.50
22	d	403	CLA	CHA-C1A-NA	-2.06	121.68	126.40
26	l	101	LHG	C27-C26-C25	-2.06	103.96	114.42
23	h	101	BCR	C37-C22-C21	-2.06	120.04	122.92
22	A	403	CLA	C7-C6-C5	-2.06	107.76	113.36
28	H	102	DGD	C1D-C2D-C3D	-2.06	105.71	110.00
22	b	613	CLA	O1D-CGD-CBD	2.06	128.69	124.48
27	A	411	SQD	O48-C23-O10	-2.06	118.40	123.59
22	c	510	CLA	OBD-CAD-CBD	-2.05	122.96	125.89
23	K	101	BCR	C28-C27-C26	-2.05	110.41	114.08
28	c	517	DGD	O5D-C1E-C2E	2.05	111.51	108.30
23	B	619	BCR	C40-C30-C29	-2.05	100.69	108.91
25	a	410	PL9	C35-C34-C36	2.05	118.72	115.27
22	C	512	CLA	O2D-CGD-CBD	2.05	114.91	111.27
23	b	617	BCR	C11-C10-C9	-2.05	124.39	127.31
32	M	101	LMG	C31-C30-C29	-2.05	105.82	113.19
26	A	410	LHG	O8-C6-C5	-2.05	102.47	108.43
32	M	101	LMG	C38-C37-C36	-2.05	104.04	114.42
26	D	412	LHG	C18-C17-C16	-2.05	104.04	114.42
22	c	503	CLA	CMD-C2D-C3D	2.05	128.50	124.68
22	C	506	CLA	OBD-CAD-C3D	2.04	131.38	127.98
32	d	408	LMG	O1-C1-C2	-2.04	105.11	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	C1D-CHD-C4C	2.04	125.25	122.56
22	c	502	CLA	CHB-C4A-NA	2.04	127.33	124.51
22	B	611	CLA	OBD-CAD-C3D	2.04	131.37	127.98
22	c	508	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	B	621	SQD	C46-O48-C23	2.04	124.67	117.12
22	b	602	CLA	C1-O2A-CGA	2.04	121.80	116.44
28	c	517	DGD	C6D-O5D-C1E	2.04	117.72	113.74
22	B	613	CLA	O1D-CGD-CBD	2.04	128.66	124.48
22	b	608	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	B	607	CLA	C4-C3-C5	2.04	118.70	115.27
22	B	613	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	C	506	CLA	CHA-C1A-NA	-2.03	121.74	126.40
22	C	502	CLA	CHC-C1C-NC	2.03	127.29	124.20
28	H	102	DGD	CAB-C9B-C8B	-2.03	104.10	114.42
22	B	610	CLA	CED-O2D-CGD	2.03	120.53	115.94
22	b	615	CLA	C3B-C4B-NB	-2.03	106.58	109.21
22	C	506	CLA	CED-O2D-CGD	2.03	120.53	115.94
32	D	408	LMG	C12-C11-C10	-2.03	106.23	113.62
22	c	511	CLA	C11-C12-C13	-2.03	109.36	115.92
22	C	507	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
23	d	404	BCR	C33-C5-C6	-2.03	122.25	124.53
32	d	408	LMG	O1-C7-C8	-2.03	106.00	110.90
22	A	402	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
22	b	604	CLA	C11-C12-C13	-2.03	109.37	115.92
26	A	410	LHG	C5-O7-C7	-2.03	112.80	117.79
22	B	610	CLA	C4-C3-C5	2.03	118.68	115.27
22	A	404	CLA	CMA-C3A-C2A	-2.03	105.65	113.83
22	C	502	CLA	O1D-CGD-CBD	2.03	128.63	124.48
33	a	404	PHO	C2C-C1C-NC	2.03	112.85	109.79
22	c	508	CLA	CHD-C4C-NC	2.03	127.39	124.20
22	B	605	CLA	CHB-C4A-NA	2.02	127.31	124.51
22	c	507	CLA	CHA-C1A-NA	-2.02	121.76	126.40
22	c	510	CLA	O1D-CGD-CBD	2.02	128.62	124.48
28	C	518	DGD	O2D-C2D-C1D	-2.02	105.13	110.05
26	D	409	LHG	C29-C28-C27	-2.02	104.15	114.42
33	D	401	PHO	C1-C2-C3	-2.02	122.54	126.04
22	a	402	CLA	CHA-C1A-NA	-2.02	121.77	126.40
22	C	513	CLA	C3A-C2A-C1A	2.02	104.37	101.34
22	b	603	CLA	O2A-C1-C2	-2.02	103.32	108.64
22	a	403	CLA	CHC-C1C-NC	2.02	127.27	124.20
22	b	602	CLA	C4D-C3D-CAD	-2.02	107.34	108.47
28	c	519	DGD	C5B-C4B-C3B	-2.02	104.17	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	BCR	C30-C25-C26	-2.02	119.77	122.61
23	B	618	BCR	C8-C7-C6	-2.02	121.53	127.20
22	B	607	CLA	C1D-CHD-C4C	2.02	125.22	122.56
22	b	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
28	C	518	DGD	C5B-C4B-C3B	-2.02	104.17	114.42
22	C	502	CLA	CHD-C4C-NC	2.02	127.39	124.20
28	C	519	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
32	Y	101	LMG	O7-C10-O9	-2.02	118.82	123.70
22	b	611	CLA	C1-C2-C3	-2.02	122.55	126.04
22	a	402	CLA	C2A-C1A-CHA	2.02	127.39	123.86
28	c	519	DGD	O6E-C5E-C4E	2.02	113.36	109.69
22	B	616	CLA	CMB-C2B-C3B	2.02	128.45	124.68
22	C	509	CLA	CHC-C1C-NC	2.02	127.26	124.20
28	C	519	DGD	O5D-C6D-C5D	-2.02	105.32	109.05
27	a	413	SQD	O2-C2-C1	2.02	114.94	110.05
22	c	511	CLA	C1D-CHD-C4C	2.01	125.22	122.56
26	l	101	LHG	C33-C32-C31	-2.01	104.20	114.42
23	K	102	BCR	C38-C26-C27	-2.01	109.75	113.62
22	c	505	CLA	CHB-C4A-NA	2.01	127.30	124.51
22	C	508	CLA	C3C-C4C-NC	-2.01	108.31	110.57
22	a	402	CLA	O1D-CGD-CBD	2.01	128.60	124.48
32	C	516	LMG	C35-C34-C33	-2.01	104.21	114.42
22	H	101	CLA	C3B-C4B-NB	-2.01	106.61	109.21
23	C	514	BCR	C15-C14-C13	-2.01	124.44	127.31
22	D	404	CLA	C6-C5-C3	2.01	118.72	113.45
22	B	604	CLA	CGD-CBD-CAD	-2.01	104.23	110.73
23	K	101	BCR	C27-C26-C25	2.01	125.64	122.73
33	D	401	PHO	CMB-C2B-C3B	2.01	133.21	128.30
23	D	406	BCR	C7-C8-C9	-2.01	123.20	126.23
23	h	101	BCR	C36-C18-C19	2.00	121.24	118.08
23	B	619	BCR	C35-C13-C12	2.00	121.24	118.08
23	k	102	BCR	C2-C1-C6	2.00	113.57	110.48
22	B	607	CLA	C1C-C2C-C3C	-2.00	104.85	106.96
22	c	502	CLA	CMC-C2C-C3C	2.00	131.56	126.12
26	A	412	LHG	C20-C19-C18	-2.00	104.26	114.42
32	a	417	LMG	C12-C11-C10	2.00	120.90	113.62
28	c	517	DGD	O3E-C3E-C2E	-2.00	105.72	110.35
22	C	505	CLA	C3B-C4B-NB	-2.00	106.62	109.21
28	c	518	DGD	C7A-C6A-C5A	-2.00	104.27	114.42

All (189) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	c	514	CLA	NC
22	c	514	CLA	ND
22	c	514	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	c	513	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	ND
22	B	616	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND
22	c	506	CLA	ND
22	c	506	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	c	508	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	NA
22	b	610	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	602	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	505	CLA	NA
22	b	608	CLA	ND
22	b	608	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	NA
22	C	507	CLA	ND
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	C	513	CLA	NC
22	C	513	CLA	ND
22	C	513	CLA	NA
22	b	616	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	c	503	CLA	ND
22	c	503	CLA	NA
22	B	610	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	a	411	CLA	ND
22	a	411	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	605	CLA	ND
22	B	605	CLA	NA

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Mol	Chain	Res	Type	Atom
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	b	612	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	a	402	CLA	NC
22	a	402	CLA	ND
22	a	402	CLA	NA
22	C	505	CLA	ND
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	d	403	CLA	NC
22	d	403	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	A	409	CLA	NC
22	A	409	CLA	ND
22	A	409	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA

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Mol	Chain	Res	Type	Atom
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	d	402	CLA	NA
22	D	404	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	601	CLA	NA
22	b	601	CLA	ND
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	a	403	CLA	NC
22	a	403	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA

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Mol	Chain	Res	Type	Atom
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	NA
22	B	612	CLA	ND
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	B	609	CLA	NC
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	b	609	CLA	NC

All (1829) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	b	621	LMG	C2-C1-O1-C7
32	b	621	LMG	O6-C1-O1-C7
26	D	412	LHG	C1-C2-C3-O3
26	D	412	LHG	C3-O3-P-O4
26	D	412	LHG	C3-O3-P-O5
23	b	618	BCR	C35-C13-C14-C15
23	b	618	BCR	C37-C22-C23-C24
22	B	616	CLA	CBD-CGD-O2D-CED
23	t	101	BCR	C11-C10-C9-C34
23	t	101	BCR	C11-C12-C13-C35
23	X	101	BCR	C11-C12-C13-C35
31	R	101	STE	C1-C2-C3-C4
26	D	409	LHG	O1-C1-C2-C3
26	D	409	LHG	O2-C2-C3-O3
26	D	409	LHG	C3-O3-P-O5
26	D	409	LHG	C4-O6-P-O4
23	d	404	BCR	C22-C23-C24-C25
32	C	516	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
23	K	102	BCR	C1-C6-C7-C8
23	K	102	BCR	C5-C6-C7-C8
23	K	102	BCR	C11-C12-C13-C35
23	K	102	BCR	C20-C21-C22-C37
23	K	102	BCR	C37-C22-C23-C24
25	A	408	PL9	C18-C19-C21-C22
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C37-C38-C39-C41
31	c	501	STE	C1-C2-C3-C4
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
23	c	516	BCR	C11-C12-C13-C35
23	c	516	BCR	C35-C13-C14-C15
23	c	516	BCR	C16-C17-C18-C36
33	d	401	PHO	CHA-CBD-CGD-O1D
33	d	401	PHO	CHA-CBD-CGD-O2D
33	d	401	PHO	CBD-CGD-O2D-CED
23	B	618	BCR	C11-C10-C9-C34
23	B	618	BCR	C16-C17-C18-C36
22	c	505	CLA	C2-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
27	a	414	SQD	C8-C7-O47-C45
32	c	523	LMG	O6-C1-O1-C7
25	a	410	PL9	C12-C13-C14-C16
25	a	410	PL9	C22-C23-C24-C26
25	a	410	PL9	C39-C41-C42-C43
22	B	614	CLA	CHA-CBD-CGD-O1D
22	B	614	CLA	CHA-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O1D
27	d	409	SQD	O5-C1-O6-C44
23	b	619	BCR	C35-C13-C14-C15
22	C	513	CLA	CAD-CBD-CGD-O1D
31	B	620	STE	C1-C2-C3-C4
23	k	101	BCR	C1-C6-C7-C8
23	k	101	BCR	C5-C6-C7-C8
23	k	101	BCR	C7-C8-C9-C34
23	k	101	BCR	C36-C18-C19-C20
23	k	101	BCR	C21-C22-C23-C24
23	k	101	BCR	C37-C22-C23-C24
23	k	101	BCR	C23-C24-C25-C30
22	a	411	CLA	CHA-CBD-CGD-O1D
22	a	411	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	A	412	LHG	O1-C1-C2-C3
26	A	412	LHG	C4-O6-P-O4
27	A	413	SQD	C46-C45-O47-C7
23	h	101	BCR	C7-C8-C9-C34
23	h	101	BCR	C11-C10-C9-C8
23	h	101	BCR	C11-C12-C13-C35
26	L	102	LHG	C3-O3-P-O4
26	L	102	LHG	C4-O6-P-O4
32	Y	101	LMG	C11-C10-O7-C8
27	L	101	SQD	C8-C7-O47-C45
27	L	101	SQD	O10-C23-O48-C46
27	L	101	SQD	C24-C23-O48-C46
32	a	417	LMG	O7-C8-C9-O8
31	c	521	STE	C1-C2-C3-C4
23	c	515	BCR	C11-C12-C13-C35
26	a	412	LHG	O1-C1-C2-C3
26	a	412	LHG	C3-O3-P-O6
23	B	617	BCR	C16-C17-C18-C36
31	L	103	STE	C1-C2-C3-C4
32	c	522	LMG	C11-C10-O7-C8
22	A	403	CLA	C14-C13-C15-C16
22	A	409	CLA	CHA-CBD-CGD-O1D
22	A	409	CLA	CHA-CBD-CGD-O2D
26	e	101	LHG	C3-O3-P-O5
23	k	102	BCR	C11-C12-C13-C35
22	D	404	CLA	C14-C13-C15-C16
23	B	619	BCR	C35-C13-C14-C15
23	B	619	BCR	C37-C22-C23-C24
32	D	411	LMG	C28-C29-C30-C31
26	l	101	LHG	C4-O6-P-O5
23	C	514	BCR	C36-C18-C19-C20
23	C	514	BCR	C23-C24-C25-C30
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	CAD-CBD-CGD-O1D
22	b	601	CLA	CAD-CBD-CGD-O2D
22	b	601	CLA	CBD-CGD-O2D-CED
31	B	601	STE	C1-C2-C3-C4
23	C	515	BCR	C10-C11-C12-C13
23	C	515	BCR	C11-C12-C13-C35
23	C	515	BCR	C18-C19-C20-C21
23	C	515	BCR	C20-C21-C22-C23
23	C	515	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	C	515	BCR	C21-C22-C23-C24
23	K	101	BCR	C16-C17-C18-C19
23	K	101	BCR	C16-C17-C18-C36
23	K	101	BCR	C18-C19-C20-C21
31	B	622	STE	C1-C2-C3-C4
22	b	614	CLA	CHA-CBD-CGD-O1D
22	b	614	CLA	CHA-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	C6-C7-C8-C9
23	a	406	BCR	C37-C22-C23-C24
22	C	501	CLA	CBD-CGD-O2D-CED
23	A	405	BCR	C11-C12-C13-C14
23	A	405	BCR	C35-C13-C14-C15
23	A	405	BCR	C20-C21-C22-C37
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
27	B	621	SQD	C2-C1-O6-C44
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	C8-C7-O47-C45
27	B	621	SQD	O10-C23-O48-C46
25	d	405	PL9	C32-C33-C34-C36
25	d	405	PL9	C37-C38-C39-C41
25	d	405	PL9	C38-C39-C41-C42
28	A	414	DGD	C2B-C1B-O2G-C2G
28	A	414	DGD	O1B-C1B-O2G-C2G
28	A	414	DGD	O2G-C2G-C3G-O3G
25	D	407	PL9	C32-C33-C34-C35
25	D	407	PL9	C33-C34-C36-C37
25	D	407	PL9	C35-C34-C36-C37
31	M	102	STE	C1-C2-C3-C4
32	D	410	LMG	O1-C7-C8-C9
32	D	410	LMG	O1-C7-C8-O7
23	D	406	BCR	C23-C24-C25-C26
23	D	406	BCR	C23-C24-C25-C30
22	H	101	CLA	CHA-CBD-CGD-O1D
22	H	101	CLA	CHA-CBD-CGD-O2D
22	H	101	CLA	CAD-CBD-CGD-O1D
26	d	406	LHG	O1-C1-C2-C3
26	d	406	LHG	C3-O3-P-O6
31	b	623	STE	C1-C2-C3-C4
22	B	616	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	O1D-CGD-O2D-CED
22	B	603	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
22	b	609	CLA	CBD-CGD-O2D-CED
32	c	523	LMG	O10-C28-O8-C9
32	c	522	LMG	O10-C28-O8-C9
32	M	101	LMG	O10-C28-O8-C9
32	c	520	LMG	C11-C10-O7-C8
27	B	621	SQD	C45-C46-O48-C23
22	C	501	CLA	O1D-CGD-O2D-CED
25	a	410	PL9	C47-C48-C49-C50
25	a	410	PL9	C47-C48-C49-C51
22	c	513	CLA	CBD-CGD-O2D-CED
22	C	513	CLA	CBD-CGD-O2D-CED
27	a	414	SQD	O10-C23-O48-C46
26	A	412	LHG	O10-C23-O8-C6
33	d	401	PHO	O1D-CGD-O2D-CED
32	c	520	LMG	O9-C10-O7-C8
22	b	607	CLA	CBD-CGD-O2D-CED
27	a	414	SQD	O49-C7-O47-C45
27	L	101	SQD	O49-C7-O47-C45
32	c	522	LMG	O9-C10-O7-C8
27	B	621	SQD	O49-C7-O47-C45
22	B	616	CLA	C3-C5-C6-C7
22	C	506	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
22	B	605	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
27	a	414	SQD	C24-C23-O48-C46
32	c	523	LMG	C29-C28-O8-C9
32	c	522	LMG	C29-C28-O8-C9
32	M	101	LMG	C29-C28-O8-C9
32	C	516	LMG	C11-C10-O7-C8
22	B	614	CLA	CBD-CGD-O2D-CED
25	A	408	PL9	C20-C19-C21-C22
22	c	507	CLA	C4-C3-C5-C6
25	A	408	PL9	C23-C24-C26-C27
22	C	511	CLA	CBD-CGD-O2D-CED
22	b	606	CLA	C2A-CAA-CBA-CGA
22	B	603	CLA	O1D-CGD-O2D-CED
22	b	603	CLA	C3-C5-C6-C7
27	d	409	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
32	a	417	LMG	C29-C28-O8-C9
27	B	621	SQD	C24-C23-O48-C46
25	a	410	PL9	C22-C23-C24-C25
25	d	405	PL9	C32-C33-C34-C35
22	H	101	CLA	CBD-CGD-O2D-CED
27	d	409	SQD	O49-C7-O47-C45
32	D	410	LMG	O9-C10-O7-C8
25	A	408	PL9	C12-C13-C14-C16
25	D	407	PL9	C32-C33-C34-C36
27	F	102	SQD	O10-C23-O48-C46
27	d	409	SQD	O10-C23-O48-C46
32	a	417	LMG	O10-C28-O8-C9
26	D	412	LHG	O2-C2-C3-O3
26	e	101	LHG	O2-C2-C3-O3
22	C	509	CLA	C3-C5-C6-C7
27	d	409	SQD	C8-C7-O47-C45
28	C	517	DGD	O6E-C5E-C6E-O5E
28	c	519	DGD	CAA-CBA-CCA-CDA
22	b	609	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	C3-C5-C6-C7
22	a	403	CLA	C3-C5-C6-C7
26	A	412	LHG	C24-C23-O8-C6
28	A	414	DGD	CEB-CFB-CGB-CHB
26	e	101	LHG	O10-C23-O8-C6
25	A	408	PL9	C40-C39-C41-C42
25	a	410	PL9	C20-C19-C21-C22
22	C	513	CLA	C4-C3-C5-C6
22	D	405	CLA	C4-C3-C5-C6
25	a	410	PL9	C18-C19-C21-C22
22	C	513	CLA	C2-C3-C5-C6
22	D	405	CLA	C2-C3-C5-C6
22	B	606	CLA	C2A-CAA-CBA-CGA
32	c	522	LMG	O6-C5-C6-O5
32	Y	101	LMG	O6-C1-O1-C7
25	A	408	PL9	C39-C41-C42-C43
25	A	408	PL9	C44-C46-C47-C48
25	a	410	PL9	C34-C36-C37-C38
31	B	624	STE	C9-C10-C11-C12
32	m	101	LMG	O6-C5-C6-O5
22	c	513	CLA	O1D-CGD-O2D-CED
26	A	412	LHG	C1-C2-C3-O3
26	e	101	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	T	103	STE	C3-C4-C5-C6
27	F	102	SQD	C24-C23-O48-C46
26	e	101	LHG	C24-C23-O8-C6
31	d	412	STE	C9-C10-C11-C12
23	k	102	BCR	C9-C10-C11-C12
27	A	413	SQD	C23-C24-C25-C26
22	B	612	CLA	C8-C10-C11-C12
31	c	521	STE	C2-C3-C4-C5
31	b	623	STE	C4-C5-C6-C7
32	c	522	LMG	C4-C5-C6-O5
22	B	604	CLA	C10-C11-C12-C13
26	A	412	LHG	O2-C2-C3-O3
27	A	411	SQD	C7-C8-C9-C10
27	d	409	SQD	C2-C1-O6-C44
27	B	621	SQD	O6-C44-C45-O47
22	c	513	CLA	C6-C7-C8-C9
33	d	401	PHO	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	C	507	CLA	C14-C13-C15-C16
22	b	616	CLA	C11-C10-C8-C9
22	B	605	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
33	D	401	PHO	C14-C13-C15-C16
22	B	607	CLA	C14-C13-C15-C16
22	b	601	CLA	C11-C10-C8-C9
22	c	510	CLA	C6-C7-C8-C9
22	H	101	CLA	C14-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C9
22	B	608	CLA	C13-C15-C16-C17
23	t	101	BCR	C7-C8-C9-C34
23	K	102	BCR	C7-C8-C9-C34
23	b	619	BCR	C36-C18-C19-C20
23	b	619	BCR	C37-C22-C23-C24
23	k	102	BCR	C7-C8-C9-C34
23	c	515	BCR	C11-C12-C13-C14
32	a	417	LMG	C11-C10-O7-C8
32	D	410	LMG	C11-C10-O7-C8
32	D	410	LMG	C10-C11-C12-C13
22	C	513	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	CBA-CGA-O2A-C1
22	c	513	CLA	C8-C10-C11-C12
22	b	614	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C8-C10-C11-C12
27	a	414	SQD	C7-C8-C9-C10
32	c	523	LMG	C10-C11-C12-C13
27	A	411	SQD	C23-C24-C25-C26
32	m	101	LMG	C4-C5-C6-O5
22	c	514	CLA	C10-C11-C12-C13
22	B	616	CLA	C5-C6-C7-C8
22	c	509	CLA	C10-C11-C12-C13
22	C	503	CLA	C5-C6-C7-C8
22	b	602	CLA	C8-C10-C11-C12
22	b	602	CLA	C15-C16-C17-C18
22	c	505	CLA	C10-C11-C12-C13
22	B	606	CLA	C15-C16-C17-C18
22	D	405	CLA	C5-C6-C7-C8
22	b	607	CLA	C10-C11-C12-C13
22	B	607	CLA	C10-C11-C12-C13
22	b	601	CLA	C8-C10-C11-C12
22	c	510	CLA	C10-C11-C12-C13
22	B	612	CLA	C10-C11-C12-C13
22	H	101	CLA	C10-C11-C12-C13
22	C	509	CLA	C5-C6-C7-C8
25	D	407	PL9	C37-C38-C39-C40
32	d	408	LMG	C28-C29-C30-C31
28	C	519	DGD	C1A-C2A-C3A-C4A
27	L	101	SQD	C7-C8-C9-C10
26	a	412	LHG	C23-C24-C25-C26
28	c	518	DGD	C1B-C2B-C3B-C4B
22	A	402	CLA	C2C-C3C-CAC-CBC
22	b	608	CLA	C5-C6-C7-C8
22	b	611	CLA	C8-C10-C11-C12
22	b	611	CLA	C15-C16-C17-C18
22	B	607	CLA	C5-C6-C7-C8
22	b	603	CLA	C10-C11-C12-C13
32	b	621	LMG	O6-C5-C6-O5
22	C	509	CLA	C2-C1-O2A-CGA
22	C	506	CLA	C15-C16-C17-C18
22	B	606	CLA	C8-C10-C11-C12
22	B	614	CLA	C15-C16-C17-C18
32	D	408	LMG	C10-C11-C12-C13
26	e	101	LHG	C23-C24-C25-C26
31	B	625	STE	C4-C5-C6-C7
33	d	401	PHO	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C12-C13-C15-C16
22	C	508	CLA	C12-C13-C15-C16
22	A	403	CLA	C12-C13-C15-C16
33	D	402	PHO	C12-C13-C15-C16
22	c	507	CLA	C11-C12-C13-C15
22	b	614	CLA	C11-C12-C13-C15
22	C	512	CLA	C3-C5-C6-C7
22	d	402	CLA	C3-C5-C6-C7
32	Y	101	LMG	C10-C11-C12-C13
22	b	601	CLA	C2A-CAA-CBA-CGA
22	b	611	CLA	C13-C15-C16-C17
22	B	613	CLA	C15-C16-C17-C18
22	B	607	CLA	C15-C16-C17-C18
22	c	507	CLA	C10-C11-C12-C13
22	c	507	CLA	O1A-CGA-O2A-C1
28	C	518	DGD	O6E-C1E-O5D-C6D
28	A	414	DGD	O6D-C1D-O3G-C3G
25	A	408	PL9	C34-C36-C37-C38
25	a	410	PL9	C24-C26-C27-C28
25	a	410	PL9	C44-C46-C47-C48
25	D	407	PL9	C29-C31-C32-C33
31	L	103	STE	C6-C7-C8-C9
26	D	412	LHG	C23-C24-C25-C26
28	A	414	DGD	C1B-C2B-C3B-C4B
23	t	101	BCR	C18-C19-C20-C21
23	k	102	BCR	C10-C11-C12-C13
22	B	614	CLA	C5-C6-C7-C8
22	b	605	CLA	C10-C11-C12-C13
28	c	519	DGD	O1A-C1A-O1G-C1G
28	c	518	DGD	C1A-C2A-C3A-C4A
22	C	513	CLA	C15-C16-C17-C18
22	b	607	CLA	C8-C10-C11-C12
22	a	405	CLA	C5-C6-C7-C8
22	B	607	CLA	C8-C10-C11-C12
22	c	507	CLA	C8-C10-C11-C12
22	C	506	CLA	C8-C10-C11-C12
22	C	505	CLA	C10-C11-C12-C13
22	a	403	CLA	C10-C11-C12-C13
26	D	412	LHG	C3-O3-P-O6
26	D	409	LHG	C3-O3-P-O6
26	A	410	LHG	C3-O3-P-O6
26	d	406	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	CBA-CGA-O2A-C1
22	d	403	CLA	C8-C10-C11-C12
22	d	403	CLA	C13-C15-C16-C17
22	B	614	CLA	O1D-CGD-O2D-CED
22	b	607	CLA	O1D-CGD-O2D-CED
26	D	409	LHG	C1-C2-C3-O3
22	a	402	CLA	C16-C17-C18-C20
22	d	402	CLA	C16-C17-C18-C20
28	h	102	DGD	O6E-C5E-C6E-O5E
32	Y	101	LMG	C29-C28-O8-C9
22	a	405	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C5-C6-C7-C8
26	D	412	LHG	C28-C29-C30-C31
28	h	102	DGD	C7A-C8A-C9A-CAA
27	d	409	SQD	C32-C33-C34-C35
31	b	622	STE	C3-C4-C5-C6
32	a	417	LMG	C12-C13-C14-C15
32	b	621	LMG	C11-C10-O7-C8
23	X	101	BCR	C16-C17-C18-C36
23	K	102	BCR	C11-C10-C9-C34
23	K	102	BCR	C16-C17-C18-C36
23	c	516	BCR	C20-C21-C22-C37
23	b	617	BCR	C35-C13-C14-C15
23	b	617	BCR	C20-C21-C22-C37
23	h	101	BCR	C20-C21-C22-C37
23	c	515	BCR	C35-C13-C14-C15
23	c	515	BCR	C16-C17-C18-C36
23	T	101	BCR	C11-C10-C9-C34
23	T	101	BCR	C16-C17-C18-C36
23	T	101	BCR	C20-C21-C22-C37
23	B	617	BCR	C20-C21-C22-C37
23	k	102	BCR	C11-C10-C9-C34
23	k	102	BCR	C35-C13-C14-C15
23	k	102	BCR	C20-C21-C22-C37
23	C	514	BCR	C16-C17-C18-C36
23	C	515	BCR	C11-C10-C9-C34
23	C	515	BCR	C16-C17-C18-C36
23	K	101	BCR	C20-C21-C22-C37
23	a	406	BCR	C35-C13-C14-C15
23	a	406	BCR	C16-C17-C18-C36
23	a	406	BCR	C20-C21-C22-C37
23	A	405	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
26	D	409	LHG	C18-C19-C20-C21
26	D	409	LHG	C30-C31-C32-C33
32	C	516	LMG	C35-C36-C37-C38
31	T	103	STE	C5-C6-C7-C8
31	c	501	STE	C6-C7-C8-C9
31	T	102	STE	C7-C8-C9-C10
28	h	102	DGD	C9A-CAA-CBA-CCA
28	C	519	DGD	C6A-C7A-C8A-C9A
26	d	407	LHG	C32-C33-C34-C35
32	Y	101	LMG	C18-C19-C20-C21
27	L	101	SQD	C25-C26-C27-C28
32	a	417	LMG	C15-C16-C17-C18
28	C	517	DGD	C6A-C7A-C8A-C9A
26	A	410	LHG	C11-C12-C13-C14
31	B	623	STE	C10-C11-C12-C13
28	c	517	DGD	C4A-C5A-C6A-C7A
22	B	604	CLA	C16-C17-C18-C19
22	A	403	CLA	C16-C17-C18-C20
32	b	621	LMG	C40-C41-C42-C43
31	T	103	STE	C6-C7-C8-C9
31	D	413	STE	C5-C6-C7-C8
31	H	103	STE	C3-C4-C5-C6
28	c	519	DGD	CCB-CDB-CEB-CFB
26	A	410	LHG	C24-C25-C26-C27
32	D	411	LMG	C32-C33-C34-C35
31	h	103	STE	C11-C12-C13-C14
27	B	621	SQD	C25-C26-C27-C28
32	b	621	LMG	C9-C8-O7-C10
27	L	101	SQD	C46-C45-O47-C7
32	Y	101	LMG	O9-C10-O7-C8
22	b	614	CLA	C13-C15-C16-C17
31	b	620	STE	C14-C15-C16-C17
32	C	516	LMG	C33-C34-C35-C36
28	C	519	DGD	C5A-C6A-C7A-C8A
27	A	413	SQD	C10-C11-C12-C13
27	a	413	SQD	C17-C18-C19-C20
26	a	412	LHG	C14-C15-C16-C17
28	c	519	DGD	CCA-CDA-CEA-CFA
28	c	519	DGD	C3B-C4B-C5B-C6B
26	A	410	LHG	C9-C10-C11-C12
26	A	410	LHG	C33-C34-C35-C36
32	D	408	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	D	408	LMG	C21-C22-C23-C24
32	D	411	LMG	C33-C34-C35-C36
32	M	101	LMG	C32-C33-C34-C35
22	H	101	CLA	O1D-CGD-O2D-CED
28	h	102	DGD	C2B-C3B-C4B-C5B
28	h	102	DGD	C5B-C6B-C7B-C8B
27	A	411	SQD	C12-C13-C14-C15
26	l	101	LHG	C14-C15-C16-C17
31	I	101	STE	C11-C10-C9-C8
27	A	413	SQD	C11-C10-C9-C8
27	A	413	SQD	C12-C13-C14-C15
27	a	413	SQD	C28-C29-C30-C31
27	a	413	SQD	C34-C35-C36-C37
32	m	101	LMG	C16-C17-C18-C19
28	c	519	DGD	C9B-CAB-CBB-CCB
32	c	522	LMG	C33-C34-C35-C36
27	B	621	SQD	C13-C14-C15-C16
26	d	406	LHG	C33-C34-C35-C36
23	b	618	BCR	C12-C13-C14-C15
23	X	101	BCR	C11-C10-C9-C8
28	C	518	DGD	C2E-C1E-O5D-C6D
23	b	617	BCR	C12-C13-C14-C15
27	a	413	SQD	C2-C1-O6-C44
32	Y	101	LMG	C2-C1-O1-C7
23	c	515	BCR	C11-C10-C9-C8
23	T	101	BCR	C12-C13-C14-C15
28	c	518	DGD	C2E-C1E-O5D-C6D
23	B	617	BCR	C16-C17-C18-C19
23	B	617	BCR	C20-C21-C22-C23
23	k	102	BCR	C20-C21-C22-C23
23	B	619	BCR	C11-C10-C9-C8
23	B	619	BCR	C12-C13-C14-C15
23	K	101	BCR	C11-C10-C9-C8
23	A	405	BCR	C12-C13-C14-C15
23	A	405	BCR	C16-C17-C18-C19
31	B	624	STE	C7-C8-C9-C10
31	c	521	STE	C7-C8-C9-C10
26	A	410	LHG	C14-C15-C16-C17
32	c	522	LMG	C15-C16-C17-C18
27	A	411	SQD	C30-C31-C32-C33
31	J	101	STE	C5-C6-C7-C8
22	A	409	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	c	508	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C19
25	a	410	PL9	C12-C13-C14-C15
25	d	405	PL9	C37-C38-C39-C40
32	b	621	LMG	C16-C17-C18-C19
28	H	102	DGD	CAB-CBB-CCB-CDB
31	B	625	STE	C7-C8-C9-C10
31	B	624	STE	C6-C7-C8-C9
31	B	624	STE	C12-C13-C14-C15
27	a	413	SQD	C30-C31-C32-C33
32	Y	101	LMG	C17-C18-C19-C20
32	Y	101	LMG	C33-C34-C35-C36
32	Y	101	LMG	C37-C38-C39-C40
32	M	101	LMG	C33-C34-C35-C36
32	D	410	LMG	C34-C35-C36-C37
25	A	408	PL9	C38-C39-C41-C42
25	D	407	PL9	C38-C39-C41-C42
22	b	607	CLA	C11-C10-C8-C9
22	B	603	CLA	C14-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C14
22	c	512	CLA	C6-C7-C8-C9
22	b	604	CLA	C14-C13-C15-C16
22	C	511	CLA	O1D-CGD-O2D-CED
28	c	517	DGD	O6D-C5D-C6D-O5D
31	a	415	STE	C5-C6-C7-C8
31	b	620	STE	C3-C4-C5-C6
31	b	620	STE	C13-C14-C15-C16
31	c	501	STE	C3-C4-C5-C6
27	d	409	SQD	C28-C29-C30-C31
26	A	412	LHG	C18-C19-C20-C21
31	D	413	STE	C4-C5-C6-C7
32	a	417	LMG	C39-C40-C41-C42
31	H	103	STE	C5-C6-C7-C8
31	Z	101	STE	C11-C12-C13-C14
28	c	519	DGD	C2A-C3A-C4A-C5A
26	A	410	LHG	C27-C28-C29-C30
31	B	623	STE	C3-C4-C5-C6
32	D	408	LMG	C15-C16-C17-C18
31	d	411	STE	C6-C7-C8-C9
26	l	101	LHG	C27-C28-C29-C30
31	b	623	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	O1A-CGA-O2A-C1
26	D	412	LHG	C25-C26-C27-C28
26	D	409	LHG	C32-C33-C34-C35
32	c	523	LMG	C32-C33-C34-C35
31	B	620	STE	C2-C3-C4-C5
26	L	102	LHG	C12-C13-C14-C15
28	c	519	DGD	C3A-C4A-C5A-C6A
26	e	101	LHG	C27-C28-C29-C30
27	B	621	SQD	C33-C34-C35-C36
31	b	623	STE	C10-C11-C12-C13
26	d	407	LHG	O1-C1-C2-C3
26	A	410	LHG	O1-C1-C2-C3
32	b	621	LMG	C32-C33-C34-C35
32	C	516	LMG	C11-C12-C13-C14
27	d	409	SQD	C25-C26-C27-C28
28	c	519	DGD	C4B-C5B-C6B-C7B
31	B	623	STE	C11-C10-C9-C8
27	A	411	SQD	C10-C11-C12-C13
26	l	101	LHG	C16-C17-C18-C19
31	d	410	STE	C5-C6-C7-C8
32	b	621	LMG	C10-C11-C12-C13
26	a	412	LHG	C7-C8-C9-C10
32	C	516	LMG	C13-C14-C15-C16
31	c	501	STE	C4-C5-C6-C7
27	a	414	SQD	C15-C16-C17-C18
31	C	520	STE	C3-C4-C5-C6
28	C	519	DGD	CBA-CCA-CDA-CEA
31	B	620	STE	C9-C10-C11-C12
26	A	412	LHG	C11-C10-C9-C8
26	A	412	LHG	C12-C13-C14-C15
27	A	413	SQD	C9-C10-C11-C12
27	A	413	SQD	C31-C32-C33-C34
27	L	101	SQD	C10-C11-C12-C13
26	a	412	LHG	C11-C10-C9-C8
32	c	522	LMG	C16-C17-C18-C19
26	e	101	LHG	C11-C10-C9-C8
27	A	411	SQD	C25-C26-C27-C28
31	d	412	STE	C6-C7-C8-C9
31	d	411	STE	C11-C12-C13-C14
26	l	101	LHG	C29-C30-C31-C32
28	A	414	DGD	C7B-C8B-C9B-CAB
28	c	517	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	C4B-C5B-C6B-C7B
22	B	608	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C19
28	c	518	DGD	O6E-C1E-O5D-C6D
22	C	513	CLA	C10-C11-C12-C13
22	b	616	CLA	C10-C11-C12-C13
22	b	615	CLA	C15-C16-C17-C18
22	c	504	CLA	C15-C16-C17-C18
31	T	103	STE	C11-C12-C13-C14
31	B	625	STE	C3-C4-C5-C6
26	e	101	LHG	C26-C27-C28-C29
31	B	622	STE	C2-C3-C4-C5
31	b	624	STE	C2-C3-C4-C5
28	c	517	DGD	C4D-C5D-C6D-O5D
22	A	402	CLA	CBD-CGD-O2D-CED
27	F	102	SQD	C32-C33-C34-C35
32	c	523	LMG	C17-C18-C19-C20
31	D	413	STE	C11-C12-C13-C14
32	D	411	LMG	C31-C32-C33-C34
31	M	102	STE	C9-C10-C11-C12
26	d	406	LHG	C29-C30-C31-C32
31	d	410	STE	C4-C5-C6-C7
27	A	413	SQD	C7-C8-C9-C10
27	F	102	SQD	C25-C26-C27-C28
27	F	102	SQD	C29-C30-C31-C32
31	a	415	STE	C4-C5-C6-C7
31	T	102	STE	C4-C5-C6-C7
32	c	523	LMG	C18-C19-C20-C21
28	C	518	DGD	CCB-CDB-CEB-CFB
31	L	103	STE	C2-C3-C4-C5
31	b	623	STE	C12-C13-C14-C15
31	t	102	STE	C6-C7-C8-C9
31	T	103	STE	C7-C8-C9-C10
27	d	409	SQD	C27-C28-C29-C30
28	C	518	DGD	C6A-C7A-C8A-C9A
32	a	417	LMG	C33-C34-C35-C36
26	A	410	LHG	C26-C27-C28-C29
31	d	411	STE	C13-C14-C15-C16
32	M	101	LMG	C39-C40-C41-C42
28	A	414	DGD	CBB-CCB-CDB-CEB
22	b	601	CLA	C3A-C2A-CAA-CBA
22	H	101	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	C	512	CLA	C8-C10-C11-C12
22	b	601	CLA	C10-C11-C12-C13
22	b	614	CLA	C8-C10-C11-C12
22	c	510	CLA	C5-C6-C7-C8
28	H	102	DGD	C6B-C7B-C8B-C9B
32	c	523	LMG	C31-C32-C33-C34
28	C	519	DGD	CCA-CDA-CEA-CFA
31	D	413	STE	C6-C7-C8-C9
27	L	101	SQD	C9-C10-C11-C12
32	a	417	LMG	C13-C14-C15-C16
32	m	101	LMG	C20-C21-C22-C23
32	D	408	LMG	C35-C36-C37-C38
32	M	101	LMG	C19-C20-C21-C22
22	c	511	CLA	C16-C17-C18-C19
22	B	610	CLA	C16-C17-C18-C20
22	B	615	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C20
31	b	620	STE	C11-C12-C13-C14
32	C	516	LMG	C16-C17-C18-C19
32	c	523	LMG	C14-C15-C16-C17
28	C	519	DGD	C9A-CAA-CBA-CCA
32	m	101	LMG	C18-C19-C20-C21
32	m	101	LMG	C37-C38-C39-C40
28	C	517	DGD	CBA-CCA-CDA-CEA
32	c	522	LMG	O1-C7-C8-C9
32	b	621	LMG	O9-C10-O7-C8
28	h	102	DGD	C7B-C8B-C9B-CAB
27	a	413	SQD	C24-C25-C26-C27
28	C	517	DGD	C4B-C5B-C6B-C7B
32	D	408	LMG	C30-C31-C32-C33
28	H	102	DGD	CCB-CDB-CEB-CFB
31	H	103	STE	C6-C7-C8-C9
31	H	103	STE	C13-C14-C15-C16
22	D	405	CLA	C10-C11-C12-C13
22	C	511	CLA	CBA-CGA-O2A-C1
25	A	408	PL9	C43-C44-C46-C47
22	B	605	CLA	C2-C3-C5-C6
26	d	407	LHG	C25-C26-C27-C28
27	B	621	SQD	C9-C10-C11-C12
26	A	412	LHG	O1-C1-C2-O2
26	a	412	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C15-C16-C17-C18
22	d	403	CLA	C10-C11-C12-C13
27	a	413	SQD	C12-C13-C14-C15
27	a	413	SQD	C14-C15-C16-C17
31	d	411	STE	C3-C4-C5-C6
32	M	101	LMG	C13-C14-C15-C16
31	B	622	STE	C5-C6-C7-C8
26	d	406	LHG	C28-C29-C30-C31
22	a	405	CLA	O1A-CGA-O2A-C1
22	c	514	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
22	d	402	CLA	C16-C17-C18-C19
26	d	406	LHG	C15-C16-C17-C18
26	A	410	LHG	O2-C2-C3-O3
26	e	101	LHG	C25-C26-C27-C28
22	D	404	CLA	C3-C5-C6-C7
22	A	402	CLA	C4C-C3C-CAC-CBC
31	T	102	STE	C10-C11-C12-C13
32	c	523	LMG	C12-C13-C14-C15
28	C	518	DGD	C5A-C6A-C7A-C8A
31	M	103	STE	C3-C4-C5-C6
27	a	413	SQD	C11-C12-C13-C14
31	T	103	STE	C11-C10-C9-C8
31	C	520	STE	C2-C3-C4-C5
27	B	621	SQD	C11-C12-C13-C14
22	b	616	CLA	C2-C1-O2A-CGA
26	A	410	LHG	C25-C26-C27-C28
32	c	522	LMG	C32-C33-C34-C35
28	A	414	DGD	CCB-CDB-CEB-CFB
26	d	406	LHG	C31-C32-C33-C34
31	b	624	STE	C3-C4-C5-C6
22	B	606	CLA	C10-C11-C12-C13
22	a	405	CLA	C10-C11-C12-C13
26	D	412	LHG	C14-C15-C16-C17
31	a	415	STE	C2-C3-C4-C5
28	H	102	DGD	C8B-C9B-CAB-CBB
31	C	521	STE	C10-C11-C12-C13
32	c	523	LMG	C33-C34-C35-C36
31	D	413	STE	C13-C14-C15-C16
28	c	519	DGD	C5B-C6B-C7B-C8B
26	e	101	LHG	C12-C13-C14-C15
23	k	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	b	617	BCR	C1-C6-C7-C8
23	c	515	BCR	C1-C6-C7-C8
23	c	515	BCR	C5-C6-C7-C8
23	T	101	BCR	C1-C6-C7-C8
23	B	617	BCR	C1-C6-C7-C8
23	B	617	BCR	C5-C6-C7-C8
23	C	514	BCR	C23-C24-C25-C26
23	C	515	BCR	C1-C6-C7-C8
23	C	515	BCR	C5-C6-C7-C8
22	b	604	CLA	C3-C5-C6-C7
28	H	102	DGD	CCA-CDA-CEA-CFA
32	C	516	LMG	C14-C15-C16-C17
32	Y	101	LMG	C38-C39-C40-C41
22	H	101	CLA	CBA-CGA-O2A-C1
22	c	503	CLA	C15-C16-C17-C18
28	A	414	DGD	O6D-C5D-C6D-O5D
32	m	101	LMG	C11-C10-O7-C8
32	b	621	LMG	C31-C32-C33-C34
31	R	101	STE	C7-C8-C9-C10
32	a	417	LMG	C10-C11-C12-C13
28	C	517	DGD	C4E-C5E-C6E-O5E
32	b	621	LMG	C41-C42-C43-C44
31	J	101	STE	C6-C7-C8-C9
22	C	509	CLA	C13-C15-C16-C17
32	c	523	LMG	C19-C20-C21-C22
31	Z	101	STE	C13-C14-C15-C16
28	c	518	DGD	C4B-C5B-C6B-C7B
28	c	518	DGD	CAB-CBB-CCB-CDB
26	d	406	LHG	C13-C14-C15-C16
22	C	510	CLA	C4-C3-C5-C6
25	d	405	PL9	C30-C29-C31-C32
22	c	506	CLA	C11-C10-C8-C7
22	A	402	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C15
22	C	510	CLA	C2-C3-C5-C6
22	c	511	CLA	C11-C12-C13-C15
22	b	610	CLA	C12-C13-C15-C16
22	B	603	CLA	C12-C13-C15-C16
22	C	502	CLA	C11-C12-C13-C15
22	D	404	CLA	C12-C13-C15-C16
22	c	507	CLA	C2-C3-C5-C6
22	b	604	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	d	405	PL9	C28-C29-C31-C32
22	B	602	CLA	C11-C12-C13-C15
25	D	407	PL9	C28-C29-C31-C32
22	H	101	CLA	C11-C10-C8-C7
22	C	511	CLA	O1A-CGA-O2A-C1
26	a	412	LHG	C32-C33-C34-C35
22	c	507	CLA	C13-C15-C16-C17
23	T	101	BCR	C13-C14-C15-C16
22	b	615	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C19
26	A	412	LHG	C23-C24-C25-C26
22	C	506	CLA	CBA-CGA-O2A-C1
32	m	101	LMG	C29-C28-O8-C9
32	b	621	LMG	C38-C39-C40-C41
26	D	409	LHG	C25-C26-C27-C28
31	B	624	STE	C3-C4-C5-C6
31	d	412	STE	C7-C8-C9-C10
22	c	507	CLA	C5-C6-C7-C8
32	a	417	LMG	C21-C22-C23-C24
32	M	101	LMG	C36-C37-C38-C39
31	h	103	STE	C7-C8-C9-C10
28	A	414	DGD	C5B-C6B-C7B-C8B
26	d	406	LHG	C11-C10-C9-C8
28	C	517	DGD	C1B-C2B-C3B-C4B
22	A	409	CLA	C13-C15-C16-C17
32	C	516	LMG	C31-C32-C33-C34
31	B	620	STE	C11-C12-C13-C14
27	A	413	SQD	C15-C16-C17-C18
32	m	101	LMG	C39-C40-C41-C42
32	c	522	LMG	C36-C37-C38-C39
27	A	411	SQD	C14-C15-C16-C17
32	D	411	LMG	C29-C30-C31-C32
32	M	101	LMG	C29-C30-C31-C32
28	A	414	DGD	CAA-CBA-CCA-CDA
32	Y	101	LMG	C11-C12-C13-C14
32	D	408	LMG	C11-C12-C13-C14
22	b	616	CLA	C11-C12-C13-C14
28	c	517	DGD	O6E-C1E-O5D-C6D
22	B	610	CLA	C15-C16-C17-C18
31	T	102	STE	C11-C12-C13-C14
32	a	417	LMG	C38-C39-C40-C41
27	A	411	SQD	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	c	523	LMG	C11-C10-O7-C8
23	B	619	BCR	C10-C11-C12-C13
31	b	620	STE	C2-C3-C4-C5
31	C	521	STE	C5-C6-C7-C8
32	C	516	LMG	C38-C39-C40-C41
31	B	623	STE	C5-C6-C7-C8
28	A	414	DGD	C4B-C5B-C6B-C7B
22	B	603	CLA	C8-C10-C11-C12
22	A	403	CLA	C10-C11-C12-C13
26	D	409	LHG	C15-C16-C17-C18
26	d	407	LHG	C26-C27-C28-C29
26	e	101	LHG	C16-C17-C18-C19
31	B	622	STE	C4-C5-C6-C7
27	B	621	SQD	C11-C10-C9-C8
31	d	410	STE	C11-C12-C13-C14
27	A	413	SQD	O49-C7-O47-C45
26	a	412	LHG	C15-C16-C17-C18
32	c	523	LMG	C2-C1-O1-C7
28	c	517	DGD	C2E-C1E-O5D-C6D
27	a	413	SQD	O6-C44-C45-O47
27	A	411	SQD	O6-C44-C45-O47
26	L	102	LHG	C13-C14-C15-C16
26	l	101	LHG	C32-C33-C34-C35
22	B	604	CLA	C16-C17-C18-C20
26	L	102	LHG	C18-C19-C20-C21
32	a	417	LMG	C41-C42-C43-C44
25	D	407	PL9	C30-C29-C31-C32
25	A	408	PL9	C4-C3-C7-C8
31	b	620	STE	C11-C10-C9-C8
31	c	521	STE	C9-C10-C11-C12
26	a	412	LHG	C25-C26-C27-C28
32	M	101	LMG	C31-C32-C33-C34
22	c	506	CLA	C11-C10-C8-C9
22	C	506	CLA	C11-C12-C13-C14
22	c	511	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	C	508	CLA	C14-C13-C15-C16
22	b	610	CLA	C14-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C9
22	b	612	CLA	C14-C13-C15-C16
33	D	402	PHO	C14-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C12-C13-C14
22	b	609	CLA	C14-C13-C15-C16
31	d	412	STE	C12-C13-C14-C15
31	b	623	STE	C11-C12-C13-C14
32	a	417	LMG	C30-C31-C32-C33
32	a	417	LMG	O6-C5-C6-O5
32	D	410	LMG	C29-C28-O8-C9
22	B	605	CLA	C8-C10-C11-C12
28	C	517	DGD	CAB-CBB-CCB-CDB
32	D	408	LMG	C33-C34-C35-C36
31	d	411	STE	C9-C10-C11-C12
22	C	506	CLA	O1A-CGA-O2A-C1
22	H	101	CLA	O1A-CGA-O2A-C1
22	c	514	CLA	C1A-C2A-CAA-CBA
22	B	604	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C1A-C2A-CAA-CBA
22	a	411	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
28	H	102	DGD	C4B-C5B-C6B-C7B
32	m	101	LMG	C32-C33-C34-C35
28	c	518	DGD	C6B-C7B-C8B-C9B
31	d	410	STE	C11-C10-C9-C8
27	A	411	SQD	C32-C33-C34-C35
22	c	513	CLA	C13-C15-C16-C17
26	d	406	LHG	O6-C4-C5-C6
27	a	413	SQD	C9-C10-C11-C12
32	a	417	LMG	C23-C24-C25-C26
28	A	414	DGD	C6B-C7B-C8B-C9B
22	b	612	CLA	C10-C11-C12-C13
22	A	403	CLA	C16-C17-C18-C19
22	a	405	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
28	H	102	DGD	C5A-C6A-C7A-C8A
31	d	412	STE	C14-C15-C16-C17
27	L	101	SQD	C13-C14-C15-C16
28	c	518	DGD	C7A-C8A-C9A-CAA
28	c	518	DGD	C9A-CAA-CBA-CCA

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Mol	Chain	Res	Type	Atoms
26	A	410	LHG	C29-C30-C31-C32
27	A	411	SQD	C34-C35-C36-C37
31	d	410	STE	C2-C3-C4-C5
22	B	615	CLA	C10-C11-C12-C13
26	D	412	LHG	C27-C28-C29-C30
28	c	517	DGD	O6E-C5E-C6E-O5E
22	C	506	CLA	C4-C3-C5-C6
25	A	408	PL9	C25-C24-C26-C27
25	a	410	PL9	C40-C39-C41-C42
22	C	506	CLA	C2-C3-C5-C6
31	M	104	STE	C4-C5-C6-C7
31	B	625	STE	C2-C3-C4-C5
27	A	413	SQD	C16-C17-C18-C19
27	L	101	SQD	C27-C28-C29-C30
31	h	103	STE	C10-C11-C12-C13
22	C	502	CLA	C13-C15-C16-C17
22	c	510	CLA	C13-C15-C16-C17
31	I	101	STE	C10-C11-C12-C13
31	a	416	STE	C4-C5-C6-C7
31	a	416	STE	C6-C7-C8-C9
28	A	414	DGD	C8A-C9A-CAA-CBA
28	C	519	DGD	O1A-C1A-O1G-C1G
28	C	519	DGD	CDB-CEB-CFB-CGB
31	c	521	STE	C6-C7-C8-C9
32	c	522	LMG	C29-C30-C31-C32
27	a	414	SQD	C12-C13-C14-C15
32	c	523	LMG	O1-C7-C8-C9
26	L	102	LHG	C19-C20-C21-C22
32	Y	101	LMG	O1-C7-C8-C9
32	a	417	LMG	C7-C8-C9-O8
31	c	521	STE	C4-C5-C6-C7
28	C	517	DGD	O1G-C1G-C2G-C3G
32	c	522	LMG	C34-C35-C36-C37
27	A	411	SQD	O6-C44-C45-C46
27	B	621	SQD	O6-C44-C45-C46
26	d	406	LHG	C26-C27-C28-C29
32	m	101	LMG	C22-C23-C24-C25
28	C	517	DGD	CDA-CEA-CFA-CGA
26	l	101	LHG	C19-C20-C21-C22
28	C	518	DGD	C2G-C3G-O3G-C1D
28	C	518	DGD	C5D-C6D-O5D-C1E
28	c	518	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
28	c	518	DGD	C5D-C6D-O5D-C1E
31	C	521	STE	C1-C2-C3-C4
31	M	104	STE	C15-C16-C17-C18
27	a	413	SQD	C25-C26-C27-C28
32	Y	101	LMG	C40-C41-C42-C43
32	D	408	LMG	C36-C37-C38-C39
31	d	411	STE	C12-C13-C14-C15
22	B	611	CLA	C13-C15-C16-C17
28	H	102	DGD	CDB-CEB-CFB-CGB
31	d	412	STE	C2-C3-C4-C5
27	a	414	SQD	C31-C32-C33-C34
22	D	405	CLA	C2C-C3C-CAC-CBC
31	B	622	STE	C7-C8-C9-C10
32	a	417	LMG	C42-C43-C44-C45
32	D	411	LMG	C37-C38-C39-C40
32	d	408	LMG	O6-C5-C6-O5
26	d	407	LHG	O1-C1-C2-O2
26	d	406	LHG	O1-C1-C2-O2
26	L	102	LHG	C11-C12-C13-C14
26	e	101	LHG	C28-C29-C30-C31
31	B	601	STE	C2-C3-C4-C5
22	b	608	CLA	C13-C15-C16-C17
31	C	520	STE	C7-C8-C9-C10
28	A	414	DGD	CBA-CCA-CDA-CEA
28	c	517	DGD	CBA-CCA-CDA-CEA
32	b	621	LMG	C19-C20-C21-C22
32	Y	101	LMG	C35-C36-C37-C38
31	H	103	STE	C1-C2-C3-C4
23	B	617	BCR	C11-C10-C9-C34
23	a	406	BCR	C11-C10-C9-C34
32	c	520	LMG	O6-C5-C6-O5
26	D	412	LHG	C19-C20-C21-C22
31	h	103	STE	C14-C15-C16-C17
25	d	405	PL9	C43-C44-C46-C47
27	B	621	SQD	C23-C24-C25-C26
32	D	408	LMG	O6-C5-C6-O5
28	C	517	DGD	C5B-C6B-C7B-C8B
26	A	410	LHG	C35-C36-C37-C38
27	A	411	SQD	C17-C18-C19-C20
27	F	102	SQD	C31-C32-C33-C34
26	D	409	LHG	C33-C34-C35-C36
32	a	417	LMG	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
31	h	103	STE	C9-C10-C11-C12
27	B	621	SQD	C46-C45-O47-C7
22	c	507	CLA	C2-C1-O2A-CGA
31	B	624	STE	C5-C6-C7-C8
27	A	413	SQD	C32-C33-C34-C35
26	a	412	LHG	C29-C30-C31-C32
26	d	406	LHG	C35-C36-C37-C38
28	c	517	DGD	C7A-C8A-C9A-CAA
28	C	518	DGD	C1B-C2B-C3B-C4B
31	M	104	STE	C13-C14-C15-C16
28	C	519	DGD	CAB-CBB-CCB-CDB
32	Y	101	LMG	C39-C40-C41-C42
26	A	410	LHG	C17-C18-C19-C20
31	B	625	STE	C1-C2-C3-C4
28	c	519	DGD	CDA-CEA-CFA-CGA
27	A	411	SQD	C9-C10-C11-C12
28	A	414	DGD	C2A-C1A-O1G-C1G
26	L	102	LHG	O10-C23-O8-C6
28	H	102	DGD	O2G-C1B-C2B-C3B
31	L	103	STE	C4-C5-C6-C7
22	C	507	CLA	C13-C15-C16-C17
22	B	605	CLA	C13-C15-C16-C17
28	C	518	DGD	CAA-CBA-CCA-CDA
22	A	402	CLA	O1D-CGD-O2D-CED
22	c	514	CLA	C5-C6-C7-C8
22	b	604	CLA	C10-C11-C12-C13
23	b	617	BCR	C11-C10-C9-C8
31	M	104	STE	C10-C11-C12-C13
32	c	522	LMG	O1-C7-C8-O7
32	c	522	LMG	C11-C12-C13-C14
22	b	616	CLA	C11-C12-C13-C15
28	h	102	DGD	CDA-CEA-CFA-CGA
31	B	625	STE	C5-C6-C7-C8
22	C	505	CLA	C4-C3-C5-C6
22	B	604	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C10
22	c	511	CLA	C6-C7-C8-C10
22	b	602	CLA	C11-C12-C13-C15
22	c	505	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	B	613	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C12-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C10
33	D	401	PHO	C12-C13-C15-C16
22	d	402	CLA	C6-C7-C8-C10
22	D	404	CLA	C6-C7-C8-C10
22	c	507	CLA	C11-C10-C8-C7
22	B	611	CLA	C11-C10-C8-C7
22	B	602	CLA	C12-C13-C15-C16
22	H	101	CLA	C12-C13-C15-C16
22	b	609	CLA	C12-C13-C15-C16
27	L	101	SQD	C30-C31-C32-C33
31	c	521	STE	C10-C11-C12-C13
28	A	414	DGD	C2B-C3B-C4B-C5B
22	B	604	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	c	505	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C12-C13-C14
22	B	603	CLA	C6-C7-C8-C9
22	a	405	CLA	C14-C13-C15-C16
22	B	607	CLA	C11-C10-C8-C9
22	d	402	CLA	C6-C7-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	B	602	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
28	H	102	DGD	CDA-CEA-CFA-CGA
32	D	408	LMG	C38-C39-C40-C41
31	M	102	STE	C2-C3-C4-C5
31	d	410	STE	C7-C8-C9-C10
31	T	103	STE	C9-C10-C11-C12
26	d	406	LHG	C17-C18-C19-C20
22	a	405	CLA	C16-C17-C18-C19
32	c	523	LMG	C29-C30-C31-C32
23	T	101	BCR	C7-C8-C9-C10
27	L	101	SQD	C29-C30-C31-C32
22	C	511	CLA	C3-C5-C6-C7
22	B	606	CLA	C5-C6-C7-C8
22	b	604	CLA	C15-C16-C17-C18
27	A	413	SQD	C28-C29-C30-C31
32	D	408	LMG	C39-C40-C41-C42
25	A	408	PL9	C32-C33-C34-C36
25	a	410	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	CBA-CGA-O2A-C1
32	c	523	LMG	C37-C38-C39-C40
22	C	510	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C16-C17-C18-C19
26	l	101	LHG	O6-C4-C5-C6
31	B	620	STE	C6-C7-C8-C9
28	c	518	DGD	CCA-CDA-CEA-CFA
32	M	101	LMG	C30-C31-C32-C33
22	A	403	CLA	C15-C16-C17-C18
31	M	104	STE	C7-C8-C9-C10
31	I	101	STE	C2-C3-C4-C5
22	B	605	CLA	C4-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
32	b	621	LMG	C11-C12-C13-C14
28	C	519	DGD	C3B-C4B-C5B-C6B
31	B	601	STE	C5-C6-C7-C8
27	F	102	SQD	C28-C29-C30-C31
28	C	519	DGD	C4A-C5A-C6A-C7A
27	a	413	SQD	C35-C36-C37-C38
26	e	101	LHG	C7-C8-C9-C10
31	B	620	STE	C7-C8-C9-C10
26	d	407	LHG	C29-C30-C31-C32
22	a	403	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	C8-C10-C11-C12
22	a	403	CLA	C13-C15-C16-C17
32	b	621	LMG	C13-C14-C15-C16
32	M	101	LMG	C14-C15-C16-C17
28	c	517	DGD	C6B-C7B-C8B-C9B
27	F	102	SQD	C45-C44-O6-C1
26	A	412	LHG	C13-C14-C15-C16
31	d	410	STE	C9-C10-C11-C12
22	c	502	CLA	CBA-CGA-O2A-C1
27	a	413	SQD	C19-C20-C21-C22
22	D	405	CLA	C13-C15-C16-C17
32	b	621	LMG	O1-C7-C8-C9
27	a	414	SQD	C44-C45-C46-O48
26	A	412	LHG	C4-C5-C6-O8
27	A	413	SQD	C44-C45-C46-O48
32	c	522	LMG	C7-C8-C9-O8
26	e	101	LHG	C4-C5-C6-O8
32	M	101	LMG	C7-C8-C9-O8
28	A	414	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
28	c	517	DGD	O1B-C1B-O2G-C2G
28	c	518	DGD	C3A-C4A-C5A-C6A
28	A	414	DGD	C4D-C5D-C6D-O5D
27	F	102	SQD	C30-C31-C32-C33
31	j	101	STE	C5-C6-C7-C8
28	c	518	DGD	CDA-CEA-CFA-CGA
31	d	412	STE	C15-C16-C17-C18
27	F	102	SQD	C44-C45-C46-O48
28	H	102	DGD	C7A-C8A-C9A-CAA
32	b	621	LMG	C18-C19-C20-C21
22	A	409	CLA	C16-C17-C18-C19
31	d	412	STE	C13-C14-C15-C16
26	D	412	LHG	C29-C30-C31-C32
32	c	522	LMG	C31-C32-C33-C34
26	d	406	LHG	C25-C26-C27-C28
22	c	513	CLA	C2A-CAA-CBA-CGA
32	C	516	LMG	C39-C40-C41-C42
26	A	410	LHG	C12-C13-C14-C15
25	d	405	PL9	C22-C23-C24-C25
32	D	411	LMG	C35-C36-C37-C38
32	d	408	LMG	C32-C33-C34-C35
32	d	408	LMG	C39-C40-C41-C42
32	c	522	LMG	C30-C31-C32-C33
32	b	621	LMG	C39-C40-C41-C42
32	c	523	LMG	C11-C12-C13-C14
27	A	413	SQD	O47-C45-C46-O48
32	D	408	LMG	C19-C20-C21-C22
27	L	101	SQD	O6-C44-C45-O47
32	c	522	LMG	O7-C8-C9-O8
22	B	612	CLA	CBA-CGA-O2A-C1
27	a	414	SQD	C19-C20-C21-C22
31	h	103	STE	C5-C6-C7-C8
22	c	514	CLA	C16-C17-C18-C19
28	C	519	DGD	C5B-C6B-C7B-C8B
31	M	103	STE	C1-C2-C3-C4
32	m	101	LMG	C15-C16-C17-C18
31	d	410	STE	C10-C11-C12-C13
25	A	408	PL9	C19-C21-C22-C23
25	a	410	PL9	C29-C31-C32-C33
31	R	101	STE	C3-C4-C5-C6
26	A	412	LHG	C10-C11-C12-C13
31	D	413	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	m	101	LMG	C33-C34-C35-C36
31	B	623	STE	C6-C7-C8-C9
26	e	101	LHG	O9-C7-O7-C5
22	A	402	CLA	C2-C1-O2A-CGA
22	b	607	CLA	C5-C6-C7-C8
22	c	513	CLA	C11-C12-C13-C14
22	C	510	CLA	C11-C10-C8-C9
22	c	503	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	C	511	CLA	C6-C7-C8-C9
22	d	403	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	604	CLA	C6-C7-C8-C9
22	C	509	CLA	C14-C13-C15-C16
31	B	620	STE	C4-C5-C6-C7
32	c	520	LMG	C33-C34-C35-C36
28	c	517	DGD	CAB-CBB-CCB-CDB
22	B	613	CLA	C13-C15-C16-C17
32	a	417	LMG	C32-C33-C34-C35
32	M	101	LMG	C15-C16-C17-C18
28	A	414	DGD	C4A-C5A-C6A-C7A
22	c	508	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C19
22	A	409	CLA	C16-C17-C18-C20
22	B	608	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C20
22	c	504	CLA	C16-C17-C18-C19
23	X	101	BCR	C23-C24-C25-C26
23	T	101	BCR	C5-C6-C7-C8
23	a	406	BCR	C23-C24-C25-C26
23	a	406	BCR	C23-C24-C25-C30
22	c	508	CLA	C10-C11-C12-C13
32	d	408	LMG	C37-C38-C39-C40
26	A	412	LHG	C27-C28-C29-C30
23	b	619	BCR	C7-C8-C9-C34
23	A	405	BCR	C11-C12-C13-C35
23	D	406	BCR	C37-C22-C23-C24
28	H	102	DGD	C9A-CAA-CBA-CCA
23	K	102	BCR	C17-C18-C19-C20
22	B	614	CLA	C8-C10-C11-C12
22	B	610	CLA	C8-C10-C11-C12
22	B	603	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C10-C11-C12-C13
22	A	409	CLA	O1D-CGD-O2D-CED
26	A	412	LHG	C14-C15-C16-C17
22	B	610	CLA	C16-C17-C18-C19
22	b	609	CLA	C3-C5-C6-C7
31	I	101	STE	C3-C4-C5-C6
28	C	518	DGD	CDA-CEA-CFA-CGA
28	c	517	DGD	C9B-CAB-CBB-CCB
31	b	620	STE	C6-C7-C8-C9
27	a	414	SQD	C11-C10-C9-C8
26	A	412	LHG	O6-C4-C5-C6
22	B	604	CLA	C12-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
22	C	510	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C12-C13-C15
22	B	613	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	B	603	CLA	C6-C7-C8-C10
22	A	403	CLA	C11-C12-C13-C15
22	a	405	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C10-C8-C7
22	B	607	CLA	C12-C13-C15-C16
22	b	601	CLA	C11-C12-C13-C15
22	b	614	CLA	C6-C7-C8-C10
22	a	403	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
23	K	101	BCR	C13-C14-C15-C16
28	h	102	DGD	CCA-CDA-CEA-CFA
28	C	518	DGD	C3A-C4A-C5A-C6A
31	D	413	STE	C10-C11-C12-C13
22	C	507	CLA	C10-C11-C12-C13
31	a	416	STE	C3-C4-C5-C6
23	X	101	BCR	C11-C10-C9-C34
23	b	619	BCR	C16-C17-C18-C36
23	b	619	BCR	C20-C21-C22-C37
23	h	101	BCR	C11-C10-C9-C34
23	h	101	BCR	C35-C13-C14-C15
23	B	617	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	K	101	BCR	C11-C10-C9-C34
23	D	406	BCR	C20-C21-C22-C37
31	b	622	STE	C11-C10-C9-C8
22	B	613	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBA-CGA-O2A-C1
22	b	601	CLA	CBA-CGA-O2A-C1
27	B	621	SQD	C18-C19-C20-C21
26	D	409	LHG	C12-C13-C14-C15
32	d	408	LMG	C33-C34-C35-C36
22	c	514	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
22	c	511	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	B	603	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
32	D	410	LMG	C9-C8-O7-C10
31	b	622	STE	C4-C5-C6-C7
31	B	624	STE	C1-C2-C3-C4
27	L	101	SQD	C28-C29-C30-C31
28	A	414	DGD	CEA-CFA-CGA-CHA
28	c	517	DGD	CDA-CEA-CFA-CGA
22	a	402	CLA	C15-C16-C17-C18
27	A	413	SQD	C44-C45-O47-C7
32	C	516	LMG	O6-C1-O1-C7
28	C	518	DGD	O6D-C1D-O3G-C3G
27	L	101	SQD	O5-C1-O6-C44
32	a	417	LMG	O6-C1-O1-C7
31	H	103	STE	C11-C12-C13-C14
26	d	406	LHG	C30-C31-C32-C33
27	a	413	SQD	O6-C44-C45-C46
26	A	410	LHG	C2-C3-O3-P
28	c	517	DGD	O1G-C1G-C2G-C3G
22	B	605	CLA	O1A-CGA-O2A-C1
31	M	102	STE	C3-C4-C5-C6
26	l	101	LHG	O6-C4-C5-O7
31	B	624	STE	C13-C14-C15-C16
23	X	101	BCR	C14-C15-C16-C17
22	B	611	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
32	a	417	LMG	C16-C17-C18-C19
22	c	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
22	C	502	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	O1A-CGA-O2A-C1
22	B	612	CLA	O1A-CGA-O2A-C1
32	m	101	LMG	C31-C32-C33-C34
23	h	101	BCR	C20-C21-C22-C23
23	C	514	BCR	C20-C21-C22-C23
26	d	406	LHG	C14-C15-C16-C17
32	b	621	LMG	O1-C7-C8-O7
27	a	414	SQD	O47-C45-C46-O48
32	c	523	LMG	O1-C7-C8-O7
26	A	412	LHG	O7-C5-C6-O8
32	Y	101	LMG	O1-C7-C8-O7
28	C	517	DGD	O1G-C1G-C2G-O2G
26	D	412	LHG	C24-C25-C26-C27
28	c	517	DGD	O1A-C1A-O1G-C1G
27	A	411	SQD	C11-C12-C13-C14
22	c	504	CLA	C16-C17-C18-C20
26	D	409	LHG	O1-C1-C2-O2
26	A	410	LHG	O1-C1-C2-O2
28	C	519	DGD	O6D-C5D-C6D-O5D
27	a	413	SQD	C32-C33-C34-C35
25	d	405	PL9	C35-C34-C36-C37
25	d	405	PL9	C45-C44-C46-C47
22	c	506	CLA	C6-C7-C8-C9
22	a	403	CLA	C6-C7-C8-C9
26	L	102	LHG	C16-C17-C18-C19
22	c	508	CLA	O1A-CGA-O2A-C1
28	H	102	DGD	C7B-C8B-C9B-CAB
27	B	621	SQD	C24-C25-C26-C27
27	B	621	SQD	C28-C29-C30-C31
26	L	102	LHG	C26-C27-C28-C29
31	b	623	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	CBD-CGD-O2D-CED
22	b	605	CLA	C5-C6-C7-C8
31	C	521	STE	C2-C3-C4-C5
32	c	520	LMG	C39-C40-C41-C42
31	D	413	STE	C15-C16-C17-C18
31	d	411	STE	C1-C2-C3-C4
32	D	411	LMG	C10-C11-C12-C13
22	a	403	CLA	C1A-C2A-CAA-CBA
22	H	101	CLA	C16-C17-C18-C19
32	d	408	LMG	C14-C15-C16-C17
31	D	413	STE	C2-C3-C4-C5
26	a	412	LHG	C31-C32-C33-C34
26	A	412	LHG	C4-O6-P-O3
26	e	101	LHG	C3-O3-P-O6
28	c	517	DGD	CDB-CEB-CFB-CGB
27	d	409	SQD	C29-C30-C31-C32
31	j	101	STE	C3-C4-C5-C6
25	A	408	PL9	C33-C34-C36-C37
31	B	620	STE	C11-C10-C9-C8
26	D	409	LHG	C3-O3-P-O4
26	a	412	LHG	C3-O3-P-O5
26	A	410	LHG	C3-O3-P-O5
26	d	406	LHG	C3-O3-P-O5
26	d	406	LHG	C4-O6-P-O5
22	b	610	CLA	C2C-C3C-CAC-CBC
32	a	417	LMG	C36-C37-C38-C39
28	C	517	DGD	CDB-CEB-CFB-CGB
32	M	101	LMG	O6-C1-O1-C7
28	c	519	DGD	C2A-C1A-O1G-C1G
22	b	609	CLA	C15-C16-C17-C18
31	d	412	STE	C4-C5-C6-C7
26	A	412	LHG	C17-C18-C19-C20
32	D	410	LMG	C12-C13-C14-C15
22	c	503	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
31	B	624	STE	C2-C3-C4-C5
31	M	102	STE	C4-C5-C6-C7
26	A	412	LHG	C16-C17-C18-C19
33	D	402	PHO	C8-C10-C11-C12
32	c	523	LMG	C39-C40-C41-C42
31	b	623	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C20
22	c	513	CLA	C4-C3-C5-C6
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15
33	d	401	PHO	C11-C12-C13-C15
22	C	508	CLA	C11-C10-C8-C7
26	A	412	LHG	O6-C4-C5-O7
22	C	504	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	c	510	CLA	C6-C7-C8-C10
26	d	406	LHG	O6-C4-C5-O7
26	a	412	LHG	C26-C27-C28-C29
27	L	101	SQD	C19-C20-C21-C22
22	B	616	CLA	C10-C11-C12-C13
22	b	612	CLA	C13-C15-C16-C17
28	H	102	DGD	C9B-CAB-CBB-CCB
31	M	102	STE	C6-C7-C8-C9
28	C	517	DGD	O1A-C1A-O1G-C1G
22	b	601	CLA	O1A-CGA-O2A-C1
26	d	407	LHG	C27-C28-C29-C30
27	a	413	SQD	C26-C27-C28-C29
31	b	623	STE	C13-C14-C15-C16
32	c	520	LMG	C35-C36-C37-C38
26	L	102	LHG	C33-C34-C35-C36
32	b	621	LMG	C4-C5-C6-O5
28	c	517	DGD	C1G-C2G-C3G-O3G
27	a	413	SQD	O10-C23-O48-C46
26	A	412	LHG	O9-C7-O7-C5
26	e	101	LHG	O7-C5-C6-O8
32	M	101	LMG	O7-C8-C9-O8
28	c	517	DGD	O1G-C1G-C2G-O2G
26	d	406	LHG	C16-C17-C18-C19
28	c	517	DGD	C7B-C8B-C9B-CAB
22	c	503	CLA	O1A-CGA-O2A-C1
22	b	610	CLA	C4C-C3C-CAC-CBC
32	a	417	LMG	C8-C7-O1-C1
22	H	101	CLA	C8-C10-C11-C12
22	B	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	A	412	LHG	C2-C3-O3-P
28	h	102	DGD	C6B-C7B-C8B-C9B
26	d	407	LHG	C35-C36-C37-C38
26	a	412	LHG	C27-C28-C29-C30
22	B	603	CLA	C4-C3-C5-C6
31	T	102	STE	C2-C3-C4-C5
31	T	102	STE	C5-C6-C7-C8
27	a	414	SQD	C9-C10-C11-C12
32	c	522	LMG	C38-C39-C40-C41
28	c	517	DGD	C2A-C3A-C4A-C5A
22	B	604	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
22	C	513	CLA	C6-C7-C8-C9
22	B	613	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	A	403	CLA	C11-C12-C13-C14
22	D	404	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C12-C13-C14
23	K	102	BCR	C22-C23-C24-C25
32	a	417	LMG	C35-C36-C37-C38
22	b	608	CLA	C16-C17-C18-C20
22	c	504	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
27	F	102	SQD	O6-C44-C45-C46
23	B	618	BCR	C37-C22-C23-C24
25	D	407	PL9	C22-C23-C24-C25
25	D	407	PL9	C42-C43-C44-C45
28	C	517	DGD	CCB-CDB-CEB-CFB
28	c	518	DGD	CCB-CDB-CEB-CFB
26	A	410	LHG	C8-C7-O7-C5
32	a	417	LMG	C17-C18-C19-C20
28	c	518	DGD	CBB-CCB-CDB-CEB
32	D	410	LMG	C36-C37-C38-C39
28	h	102	DGD	O2G-C1B-C2B-C3B
26	a	412	LHG	C13-C14-C15-C16
26	L	102	LHG	C29-C30-C31-C32
32	c	522	LMG	C42-C43-C44-C45
26	a	412	LHG	C12-C13-C14-C15
26	L	102	LHG	C7-C8-C9-C10
31	T	102	STE	C13-C14-C15-C16
31	j	101	STE	C4-C5-C6-C7
28	c	517	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	c	523	LMG	C7-C8-O7-C10
22	B	613	CLA	O1D-CGD-O2D-CED
22	c	503	CLA	CBA-CGA-O2A-C1
22	d	402	CLA	C2-C1-O2A-CGA
22	D	404	CLA	C2-C1-O2A-CGA
22	B	614	CLA	O1A-CGA-O2A-C1
26	L	102	LHG	C10-C11-C12-C13
26	d	407	LHG	C2-C3-O3-P
32	m	101	LMG	C30-C31-C32-C33
32	D	408	LMG	C17-C18-C19-C20
22	B	614	CLA	CBA-CGA-O2A-C1
31	d	410	STE	C6-C7-C8-C9
22	B	607	CLA	C16-C17-C18-C19
22	b	611	CLA	C10-C11-C12-C13
26	D	412	LHG	C7-C8-C9-C10
23	d	404	BCR	C23-C24-C25-C30
23	b	617	BCR	C5-C6-C7-C8
32	c	522	LMG	C13-C14-C15-C16
28	C	518	DGD	CAB-CBB-CCB-CDB
28	C	517	DGD	O1G-C1A-C2A-C3A
22	D	405	CLA	C4C-C3C-CAC-CBC
27	A	411	SQD	C15-C16-C17-C18
26	e	101	LHG	C8-C7-O7-C5
28	A	414	DGD	O6E-C1E-O5D-C6D
32	b	621	LMG	C30-C31-C32-C33
26	A	410	LHG	C32-C33-C34-C35
23	b	619	BCR	C12-C13-C14-C15
28	A	414	DGD	C2E-C1E-O5D-C6D
27	d	409	SQD	O47-C45-C46-O48
27	a	414	SQD	C29-C30-C31-C32
32	M	101	LMG	C17-C18-C19-C20
26	l	101	LHG	C4-O6-P-O3
31	b	622	STE	C9-C10-C11-C12
26	A	412	LHG	C33-C34-C35-C36
31	j	101	STE	C7-C8-C9-C10
22	B	615	CLA	C5-C6-C7-C8
27	A	411	SQD	C16-C17-C18-C19
26	d	407	LHG	C4-C5-C6-O8
26	l	101	LHG	C4-C5-C6-O8
32	M	101	LMG	O1-C7-C8-C9
22	H	101	CLA	C4-C3-C5-C6
22	D	405	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C6-C7-C8-C10
22	b	609	CLA	C11-C12-C13-C15
31	C	521	STE	C9-C10-C11-C12
22	c	508	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	C	505	CLA	C6-C7-C8-C9
23	b	619	BCR	C15-C16-C17-C18
22	b	601	CLA	C16-C17-C18-C19
32	m	101	LMG	C17-C18-C19-C20
26	A	410	LHG	C31-C32-C33-C34
22	c	510	CLA	CAA-CBA-CGA-O2A
28	H	102	DGD	C4A-C5A-C6A-C7A
22	A	403	CLA	C2C-C3C-CAC-CBC
25	a	410	PL9	C15-C14-C16-C17
25	A	408	PL9	C42-C43-C44-C46
32	m	101	LMG	C36-C37-C38-C39
28	C	518	DGD	O1A-C1A-O1G-C1G
28	c	517	DGD	C5B-C6B-C7B-C8B
32	Y	101	LMG	C30-C31-C32-C33
28	c	517	DGD	CBB-CCB-CDB-CEB
22	b	613	CLA	C15-C16-C17-C18
22	c	502	CLA	C2A-CAA-CBA-CGA
23	A	405	BCR	C9-C10-C11-C12
32	c	522	LMG	C17-C18-C19-C20
31	t	102	STE	C4-C5-C6-C7
22	b	603	CLA	C13-C15-C16-C17
26	a	412	LHG	C18-C19-C20-C21
31	T	103	STE	C10-C11-C12-C13
28	h	102	DGD	C8B-C9B-CAB-CBB
26	d	407	LHG	C30-C31-C32-C33
27	F	102	SQD	C45-C46-O48-C23
22	C	504	CLA	C4-C3-C5-C6
22	B	609	CLA	C4-C3-C5-C6
27	A	411	SQD	C28-C29-C30-C31
22	B	609	CLA	C2-C3-C5-C6
26	D	412	LHG	C31-C32-C33-C34
31	C	521	STE	C6-C7-C8-C9
28	c	518	DGD	C4A-C5A-C6A-C7A
22	B	614	CLA	C13-C15-C16-C17
27	a	413	SQD	C18-C19-C20-C21
27	A	413	SQD	C29-C30-C31-C32
33	d	401	PHO	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C3A-C2A-CAA-CBA
33	a	404	PHO	C16-C17-C18-C20
31	B	620	STE	C12-C13-C14-C15
22	a	402	CLA	C4C-C3C-CAC-CBC
31	d	411	STE	C5-C6-C7-C8
23	C	515	BCR	C15-C16-C17-C18
22	c	511	CLA	C4-C3-C5-C6
28	C	518	DGD	C8B-C9B-CAB-CBB
28	C	519	DGD	C7B-C8B-C9B-CAB
25	a	410	PL9	C4-C3-C7-C8
32	d	408	LMG	C11-C12-C13-C14
22	c	514	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	C	505	CLA	C14-C13-C15-C16
22	b	601	CLA	C14-C13-C15-C16
22	a	411	CLA	C4C-C3C-CAC-CBC
23	b	618	BCR	C20-C21-C22-C37
31	B	601	STE	C3-C4-C5-C6
33	a	404	PHO	O2A-C1-C2-C3
22	b	608	CLA	O2A-C1-C2-C3
22	C	512	CLA	O2A-C1-C2-C3
22	D	405	CLA	O2A-C1-C2-C3
33	D	401	PHO	O2A-C1-C2-C3
28	H	102	DGD	C5B-C6B-C7B-C8B
32	D	410	LMG	C14-C15-C16-C17
23	B	619	BCR	C7-C8-C9-C34
23	K	102	BCR	C11-C12-C13-C14
26	A	412	LHG	C34-C35-C36-C37
26	L	102	LHG	C30-C31-C32-C33
31	B	623	STE	C2-C3-C4-C5
32	a	417	LMG	C9-C8-O7-C10
32	M	101	LMG	C7-C8-O7-C10
22	b	614	CLA	C15-C16-C17-C18
22	c	513	CLA	C1A-C2A-CAA-CBA
33	d	401	PHO	C1A-C2A-CAA-CBA
22	C	508	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C11-C12-C13-C15
22	c	506	CLA	C2-C3-C5-C6
25	a	410	PL9	C38-C39-C41-C42
22	D	405	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
32	D	408	LMG	C18-C19-C20-C21
32	b	621	LMG	C42-C43-C44-C45
31	C	522	STE	C6-C7-C8-C9
31	T	102	STE	C9-C10-C11-C12
22	B	614	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C10-C11-C12-C13
22	a	405	CLA	C15-C16-C17-C18
22	c	510	CLA	C8-C10-C11-C12
31	T	102	STE	C6-C7-C8-C9
26	e	101	LHG	C14-C15-C16-C17
28	c	519	DGD	C9A-CAA-CBA-CCA
28	h	102	DGD	CDB-CEB-CFB-CGB
31	D	413	STE	C9-C10-C11-C12
32	d	408	LMG	C10-C11-C12-C13
22	c	511	CLA	C2-C3-C5-C6
22	D	405	CLA	C15-C16-C17-C18
31	B	601	STE	C4-C5-C6-C7
32	D	410	LMG	C33-C34-C35-C36
31	B	623	STE	C11-C12-C13-C14
26	l	101	LHG	O7-C5-C6-O8
23	c	515	BCR	C9-C10-C11-C12
23	K	101	BCR	C9-C10-C11-C12
33	D	401	PHO	C10-C11-C12-C13
26	D	409	LHG	C23-C24-C25-C26
28	C	519	DGD	C9B-CAB-CBB-CCB
26	e	101	LHG	C11-C12-C13-C14
22	B	603	CLA	C5-C6-C7-C8
28	h	102	DGD	C9B-CAB-CBB-CCB
32	M	101	LMG	C38-C39-C40-C41
22	c	513	CLA	C2-C3-C5-C6
22	H	101	CLA	C2-C3-C5-C6
23	d	404	BCR	C10-C11-C12-C13
27	A	411	SQD	C31-C32-C33-C34
22	c	503	CLA	C13-C15-C16-C17
22	B	616	CLA	C11-C12-C13-C15
27	F	102	SQD	O10-C23-C24-C25
23	d	404	BCR	C23-C24-C25-C26
23	B	619	BCR	C23-C24-C25-C30
23	K	101	BCR	C23-C24-C25-C30
22	c	513	CLA	C15-C16-C17-C18
31	M	104	STE	C9-C10-C11-C12
26	D	409	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
32	C	516	LMG	C36-C37-C38-C39
23	t	101	BCR	C13-C14-C15-C16
23	c	516	BCR	C9-C10-C11-C12
22	c	506	CLA	C4-C3-C5-C6
22	b	610	CLA	C8-C10-C11-C12
28	C	518	DGD	C4A-C5A-C6A-C7A
22	a	402	CLA	C2C-C3C-CAC-CBC
28	A	414	DGD	C5A-C6A-C7A-C8A
25	a	410	PL9	C43-C44-C46-C47
22	B	603	CLA	C2-C3-C5-C6
28	c	519	DGD	C6A-C7A-C8A-C9A
28	C	517	DGD	C9A-CAA-CBA-CCA
32	M	101	LMG	C8-C7-O1-C1
27	a	413	SQD	C11-C10-C9-C8
31	c	521	STE	C3-C4-C5-C6
27	B	621	SQD	C10-C11-C12-C13
27	A	411	SQD	C13-C14-C15-C16
28	h	102	DGD	CAA-CBA-CCA-CDA
27	B	621	SQD	C35-C36-C37-C38
22	B	607	CLA	C13-C15-C16-C17
28	C	518	DGD	C3B-C4B-C5B-C6B
32	m	101	LMG	C13-C14-C15-C16
32	C	516	LMG	C37-C38-C39-C40
32	M	101	LMG	C34-C35-C36-C37
32	c	520	LMG	C37-C38-C39-C40
27	A	413	SQD	C27-C28-C29-C30
32	D	410	LMG	O10-C28-O8-C9
22	b	614	CLA	C4-C3-C5-C6
22	a	405	CLA	C11-C10-C8-C7
22	b	601	CLA	C2-C3-C5-C6
22	c	502	CLA	C11-C12-C13-C15
31	H	103	STE	C11-C10-C9-C8
32	M	101	LMG	C10-C11-C12-C13
32	Y	101	LMG	C12-C13-C14-C15
22	c	506	CLA	C13-C15-C16-C17
23	T	101	BCR	C15-C16-C17-C18
28	c	517	DGD	O1G-C1A-C2A-C3A
28	C	518	DGD	C2D-C1D-O3G-C3G
32	M	101	LMG	C2-C1-O1-C7
26	A	410	LHG	C16-C17-C18-C19
32	M	101	LMG	C22-C23-C24-C25
31	t	102	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C5-C6-C7-C8
26	d	406	LHG	C34-C35-C36-C37
31	M	102	STE	C5-C6-C7-C8
26	D	409	LHG	C9-C10-C11-C12
28	A	414	DGD	C2A-C3A-C4A-C5A
22	C	512	CLA	C5-C6-C7-C8
22	C	512	CLA	C13-C15-C16-C17
26	D	409	LHG	C35-C36-C37-C38
28	h	102	DGD	CBA-CCA-CDA-CEA
23	h	101	BCR	C16-C17-C18-C36
28	A	414	DGD	CDB-CEB-CFB-CGB
22	b	613	CLA	CAA-CBA-CGA-O2A
22	c	509	CLA	C4-C3-C5-C6
22	B	614	CLA	C4-C3-C5-C6
22	A	404	CLA	C4-C3-C5-C6
22	b	601	CLA	C4-C3-C5-C6
25	d	405	PL9	C40-C39-C41-C42
31	T	102	STE	C11-C10-C9-C8
25	A	408	PL9	C13-C14-C16-C17
22	B	604	CLA	CBD-CGD-O2D-CED
28	C	517	DGD	C1A-C2A-C3A-C4A
28	C	518	DGD	C6B-C7B-C8B-C9B
22	c	508	CLA	C14-C13-C15-C16
22	D	405	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C12-C13-C14
32	m	101	LMG	C40-C41-C42-C43
22	c	506	CLA	O1A-CGA-O2A-C1
22	B	604	CLA	CAD-CBD-CGD-O2D
33	a	404	PHO	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	513	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	B	612	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	C16-C17-C18-C19
31	B	624	STE	C11-C10-C9-C8
22	b	602	CLA	C2A-CAA-CBA-CGA
32	Y	101	LMG	C16-C17-C18-C19
22	a	405	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
26	d	407	LHG	C33-C34-C35-C36
28	c	519	DGD	O1G-C1A-C2A-C3A
28	C	517	DGD	O2G-C1B-C2B-C3B
31	M	102	STE	C7-C8-C9-C10
32	Y	101	LMG	C34-C35-C36-C37
22	b	613	CLA	C8-C10-C11-C12
25	d	405	PL9	C13-C14-C16-C17
27	A	411	SQD	O47-C7-C8-C9
31	t	102	STE	C2-C3-C4-C5
31	M	104	STE	C6-C7-C8-C9
26	e	101	LHG	O6-C4-C5-O7
32	a	417	LMG	O8-C28-C29-C30
23	B	618	BCR	C18-C19-C20-C21
33	D	402	PHO	C2C-C3C-CAC-CBC
26	l	101	LHG	C9-C10-C11-C12
26	l	101	LHG	C7-C8-C9-C10
22	b	611	CLA	CBD-CGD-O2D-CED
27	a	414	SQD	C18-C19-C20-C21
26	L	102	LHG	C15-C16-C17-C18
22	C	504	CLA	C11-C12-C13-C14
33	a	404	PHO	C16-C17-C18-C19
28	C	518	DGD	C9B-CAB-CBB-CCB
32	a	417	LMG	O9-C10-O7-C8
22	B	616	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CHA-CBD-CGD-O2D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O2D
22	b	611	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O1D
22	A	403	CLA	CHA-CBD-CGD-O2D
23	k	102	BCR	C19-C20-C21-C22
22	b	609	CLA	CHA-CBD-CGD-O2D
25	d	405	PL9	C42-C43-C44-C46
28	c	519	DGD	C7A-C8A-C9A-CAA
22	c	508	CLA	C13-C15-C16-C17
31	D	413	STE	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
23	d	404	BCR	C16-C17-C18-C19
23	T	101	BCR	C16-C17-C18-C19
23	B	617	BCR	C12-C13-C14-C15
33	D	401	PHO	C2C-C3C-CAC-CBC
22	C	508	CLA	C16-C17-C18-C19
27	F	102	SQD	O48-C23-C24-C25
32	m	101	LMG	O8-C28-C29-C30
27	B	621	SQD	O47-C7-C8-C9
27	a	413	SQD	O47-C45-C46-O48
28	c	517	DGD	O2G-C2G-C3G-O3G
22	a	411	CLA	C2C-C3C-CAC-CBC
26	a	412	LHG	C33-C34-C35-C36
26	a	412	LHG	C9-C10-C11-C12
22	B	613	CLA	C5-C6-C7-C8
28	C	519	DGD	O1G-C1A-C2A-C3A
26	l	101	LHG	C34-C35-C36-C37
32	C	516	LMG	C17-C18-C19-C20
22	B	607	CLA	C11-C12-C13-C15
25	d	405	PL9	C33-C34-C36-C37
22	C	509	CLA	C11-C10-C8-C7
26	D	409	LHG	O9-C7-O7-C5
32	b	621	LMG	O7-C10-C11-C12
22	B	613	CLA	CAA-CBA-CGA-O2A
28	c	517	DGD	O2G-C1B-C2B-C3B
31	a	416	STE	C2-C3-C4-C5
22	c	514	CLA	C11-C12-C13-C14
22	c	506	CLA	C11-C12-C13-C14
22	b	611	CLA	C6-C7-C8-C9
22	C	513	CLA	C11-C10-C8-C9
22	D	405	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
23	k	101	BCR	C19-C20-C21-C22
32	c	522	LMG	C41-C42-C43-C44
26	D	409	LHG	C11-C10-C9-C8
23	t	101	BCR	C14-C15-C16-C17
28	C	519	DGD	C8B-C9B-CAB-CBB
26	A	412	LHG	C15-C16-C17-C18
31	B	623	STE	C4-C5-C6-C7
25	A	408	PL9	C21-C22-C23-C24
25	D	407	PL9	C21-C22-C23-C24
22	c	506	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	d	411	STE	C4-C5-C6-C7
23	A	405	BCR	C21-C22-C23-C24
32	C	516	LMG	C4-C5-C6-O5
22	d	403	CLA	C1A-C2A-CAA-CBA
22	B	602	CLA	C1A-C2A-CAA-CBA
27	d	409	SQD	C34-C35-C36-C37
25	d	405	PL9	C21-C22-C23-C24
22	C	506	CLA	C2-C1-O2A-CGA
27	a	413	SQD	C29-C30-C31-C32
22	b	613	CLA	CAA-CBA-CGA-O1A
27	L	101	SQD	O6-C44-C45-C46
27	A	411	SQD	C29-C30-C31-C32
22	B	605	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
26	d	407	LHG	O10-C23-C24-C25
22	B	615	CLA	C13-C15-C16-C17
33	a	404	PHO	C4-C3-C5-C6
27	B	621	SQD	O49-C7-C8-C9
22	A	402	CLA	C15-C16-C17-C18
26	A	412	LHG	C4-O6-P-O5
27	a	413	SQD	C13-C14-C15-C16
27	a	414	SQD	O10-C23-C24-C25
22	B	612	CLA	CAA-CBA-CGA-O2A
28	C	518	DGD	CCA-CDA-CEA-CFA
22	C	509	CLA	C10-C11-C12-C13
31	b	620	STE	C12-C13-C14-C15
26	e	101	LHG	O8-C23-C24-C25
26	D	409	LHG	C19-C20-C21-C22
22	c	504	CLA	C5-C6-C7-C8
28	c	518	DGD	CAA-CBA-CCA-CDA
22	C	504	CLA	C2-C3-C5-C6
22	B	605	CLA	C16-C17-C18-C19
31	D	413	STE	C14-C15-C16-C17
32	c	523	LMG	C9-C8-O7-C10
22	B	606	CLA	CAD-CBD-CGD-O1D
26	d	407	LHG	C4-C5-O7-C7
22	C	504	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	CAD-CBD-CGD-O1D
32	Y	101	LMG	O10-C28-O8-C9
28	C	518	DGD	O1B-C1B-C2B-C3B
22	b	604	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	a	404	PHO	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	a	405	CLA	C11-C10-C8-C9
22	c	504	CLA	C14-C13-C15-C16
22	H	101	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C12-C13-C14
32	a	417	LMG	C34-C35-C36-C37
31	H	103	STE	C2-C3-C4-C5
32	d	408	LMG	C15-C16-C17-C18
22	B	616	CLA	C11-C12-C13-C14
28	c	519	DGD	C6B-C7B-C8B-C9B
31	c	501	STE	C2-C3-C4-C5
22	D	404	CLA	C2C-C3C-CAC-CBC
22	b	614	CLA	C2A-CAA-CBA-CGA
26	e	101	LHG	C15-C16-C17-C18
28	H	102	DGD	C3B-C4B-C5B-C6B
31	B	625	STE	C9-C10-C11-C12
33	a	404	PHO	C2-C3-C5-C6
33	a	404	PHO	C6-C7-C8-C10
22	c	513	CLA	C3A-C2A-CAA-CBA
22	b	611	CLA	C6-C7-C8-C10
22	B	605	CLA	C11-C10-C8-C7
22	b	613	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C15
22	B	602	CLA	C3A-C2A-CAA-CBA
26	A	410	LHG	O10-C23-C24-C25
27	A	411	SQD	O49-C7-C8-C9
32	d	408	LMG	O7-C10-C11-C12
27	a	413	SQD	O47-C7-C8-C9
26	L	102	LHG	O7-C7-C8-C9
27	A	411	SQD	C35-C36-C37-C38
27	F	102	SQD	C23-C24-C25-C26
23	k	101	BCR	C7-C8-C9-C10
28	c	519	DGD	O1B-C1B-C2B-C3B
26	d	407	LHG	O8-C23-C24-C25
22	B	611	CLA	C8-C10-C11-C12
22	b	603	CLA	C8-C10-C11-C12
28	C	519	DGD	C8A-C9A-CAA-CBA
32	b	621	LMG	O9-C10-C11-C12
22	B	613	CLA	CAA-CBA-CGA-O1A
22	C	512	CLA	C10-C11-C12-C13
22	b	613	CLA	C13-C15-C16-C17

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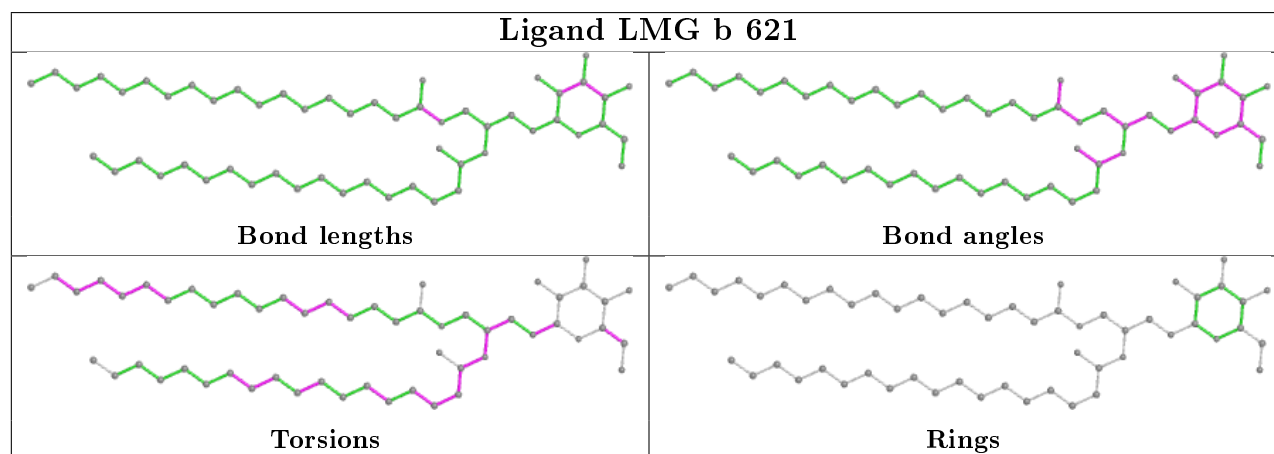
Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	a	413	SQD	O49-C7-C8-C9
25	A	408	PL9	C12-C13-C14-C15
22	c	508	CLA	C5-C6-C7-C8
25	d	405	PL9	C15-C14-C16-C17
22	A	403	CLA	C4C-C3C-CAC-CBC

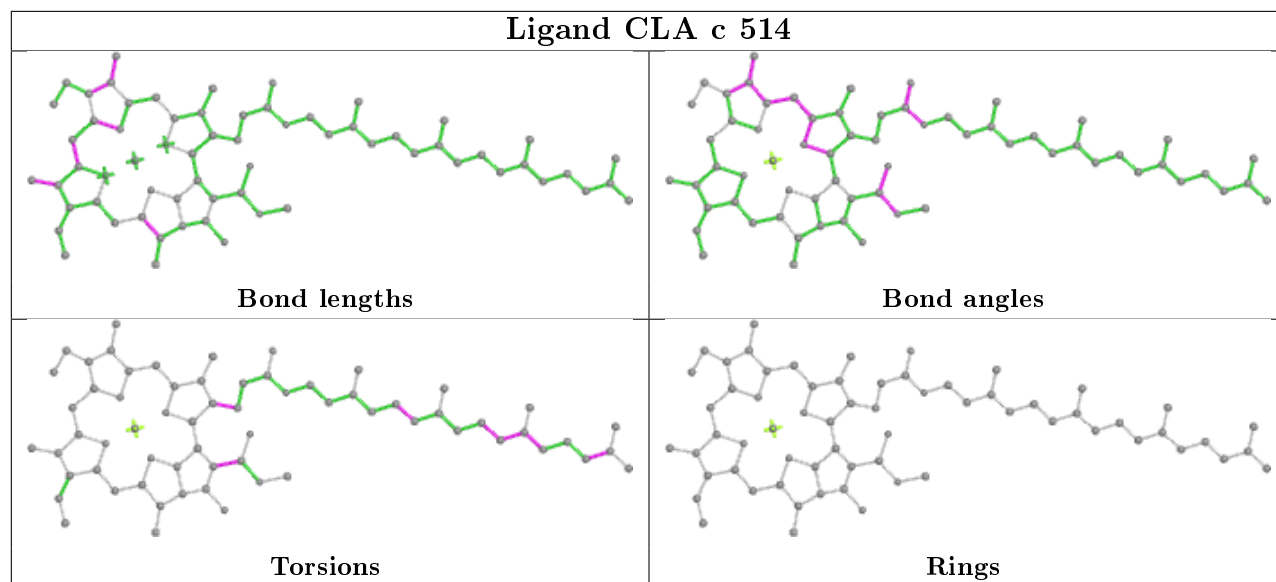
There are no ring outliers.

No monomer is involved in short contacts.

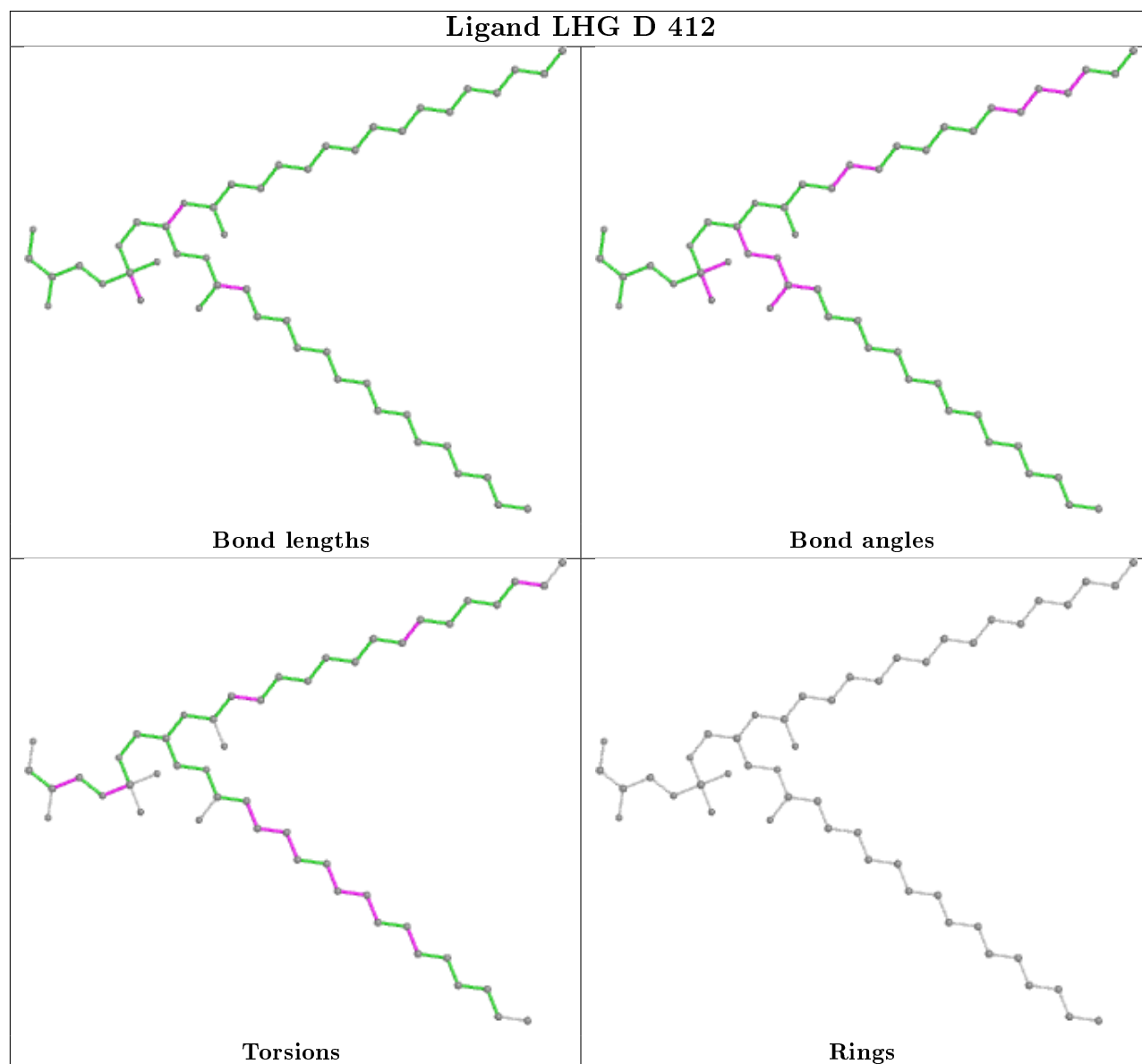
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

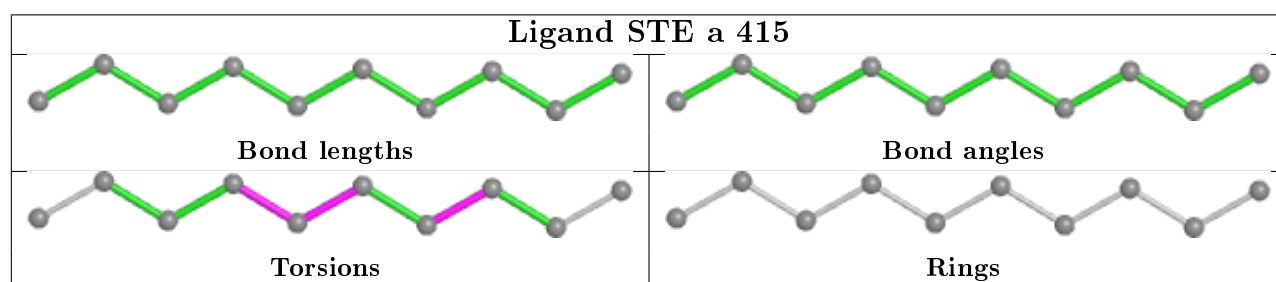
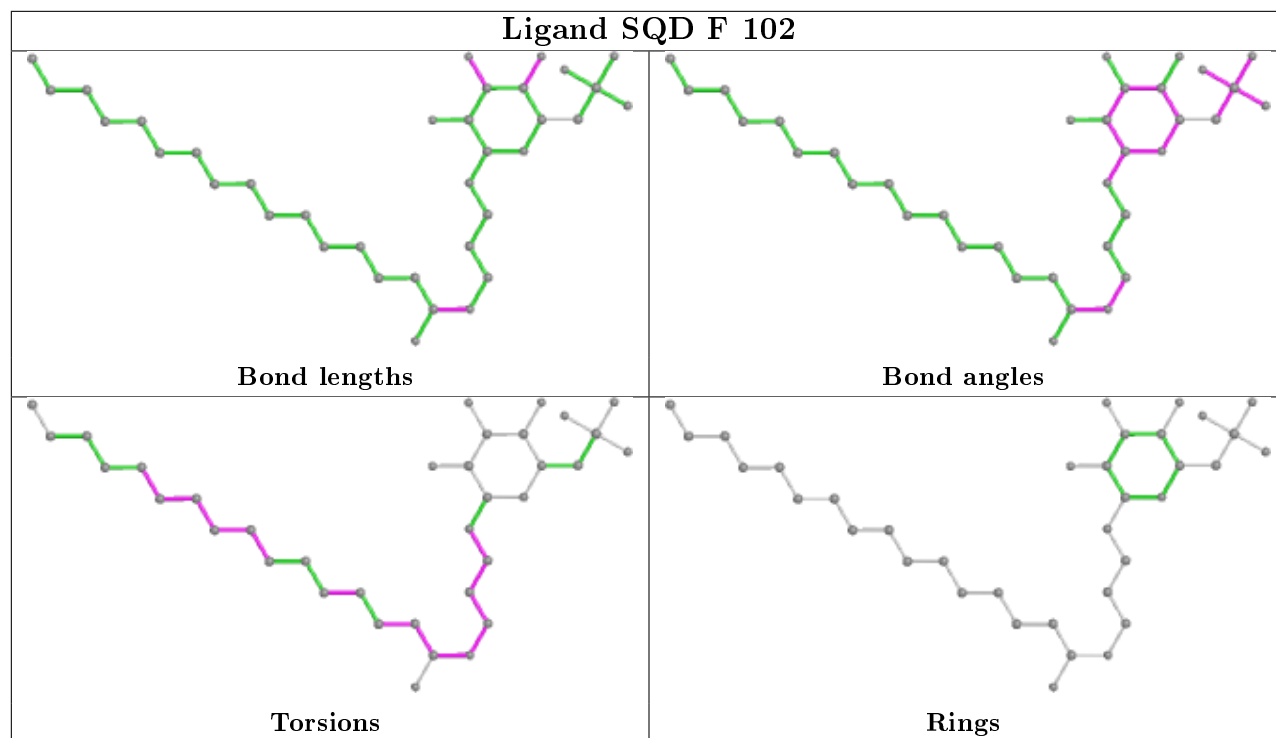
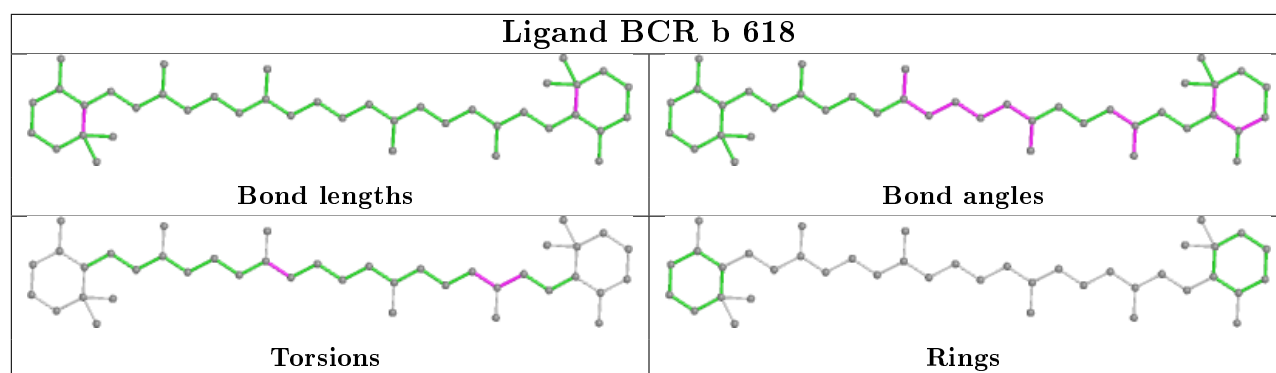


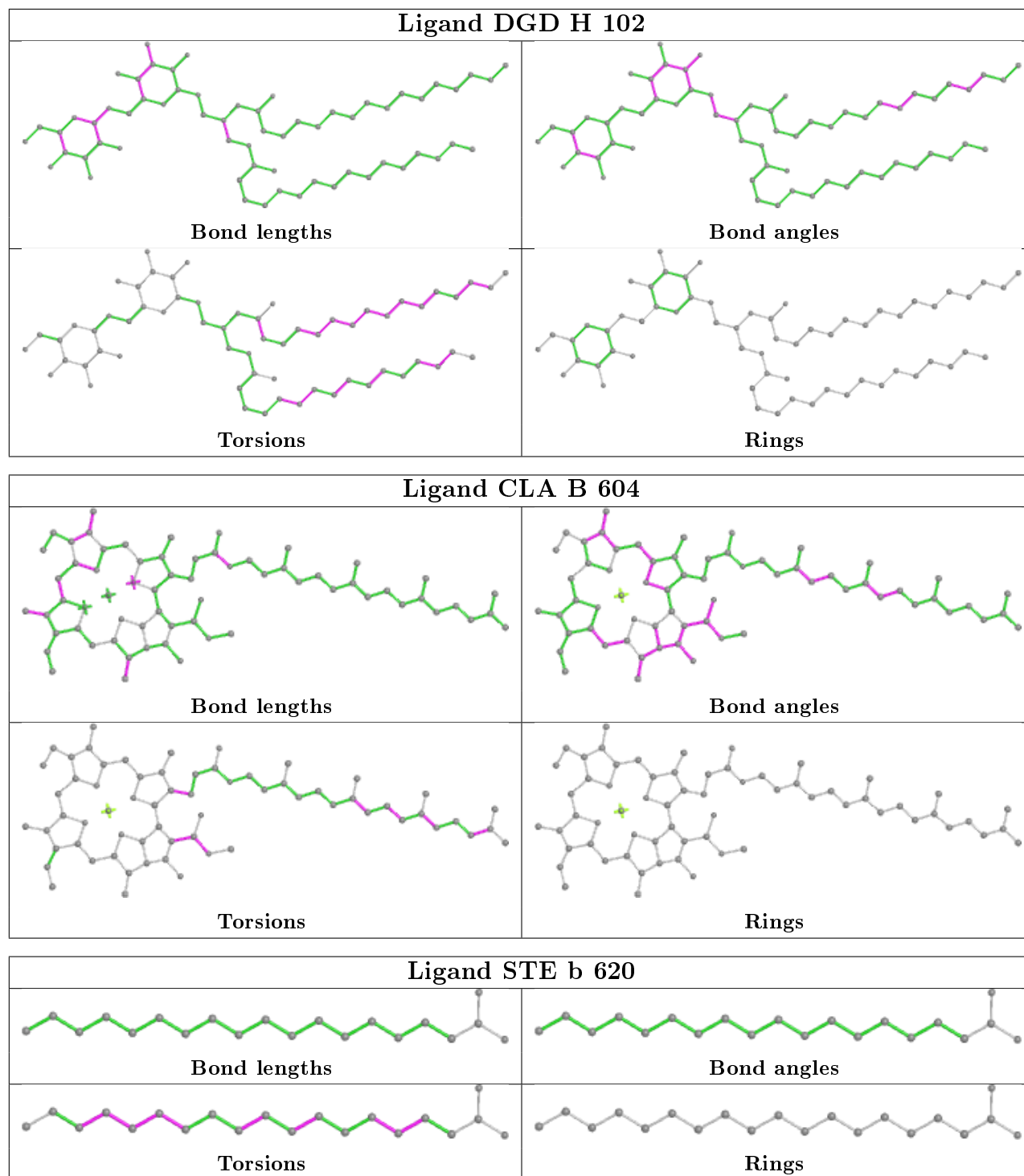
Ligand CLA c 514

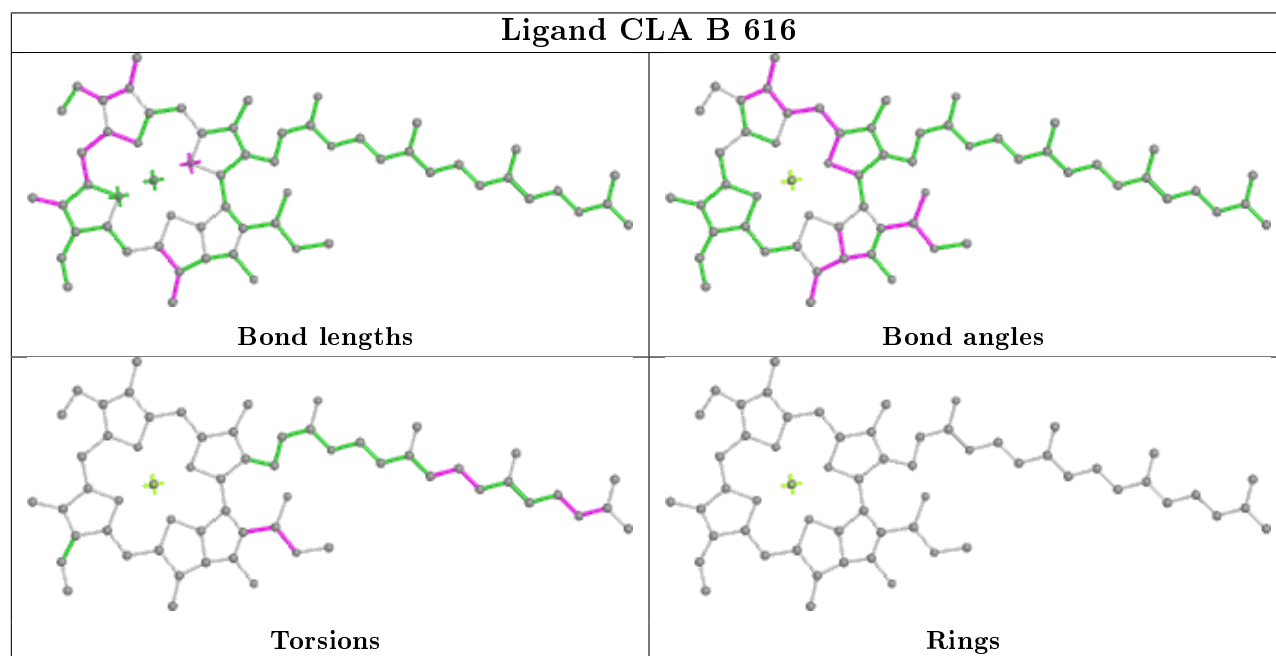
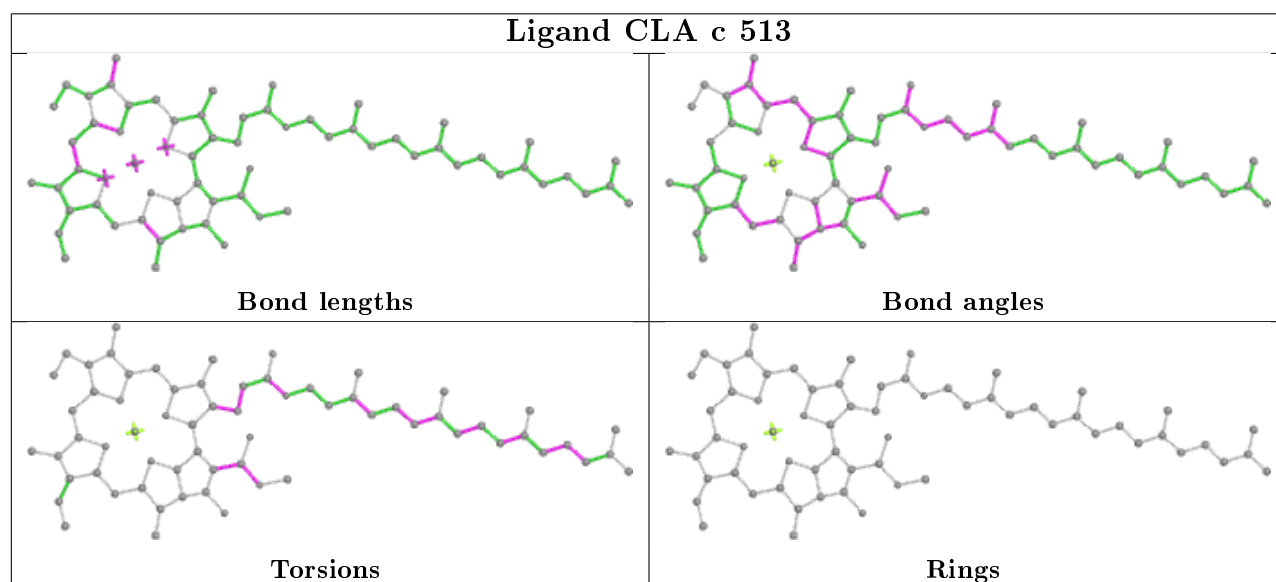
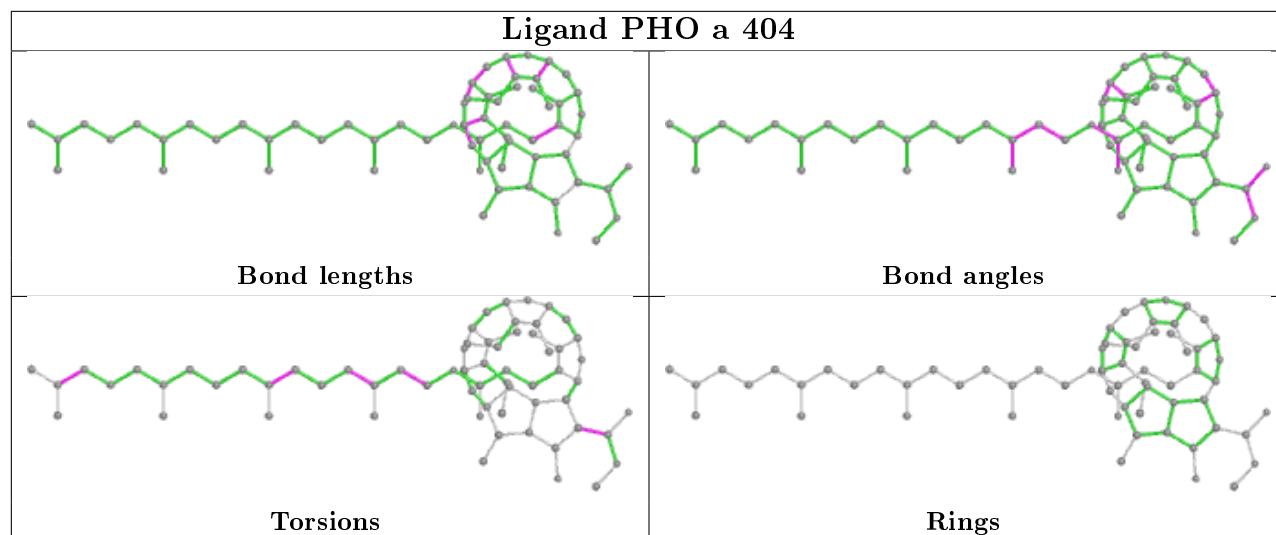


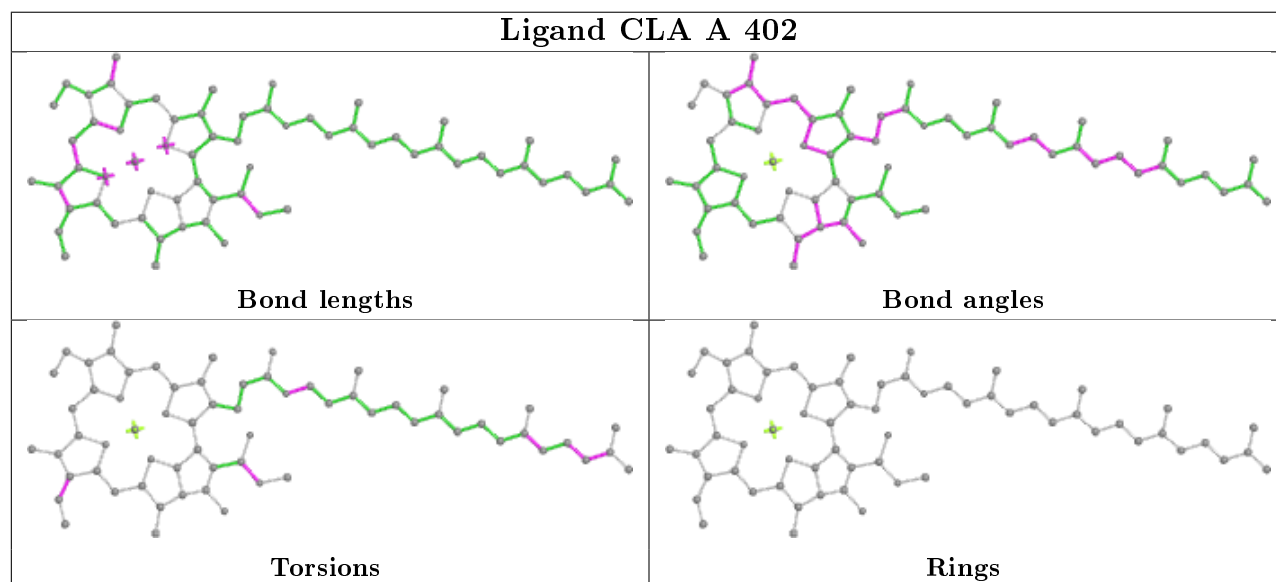
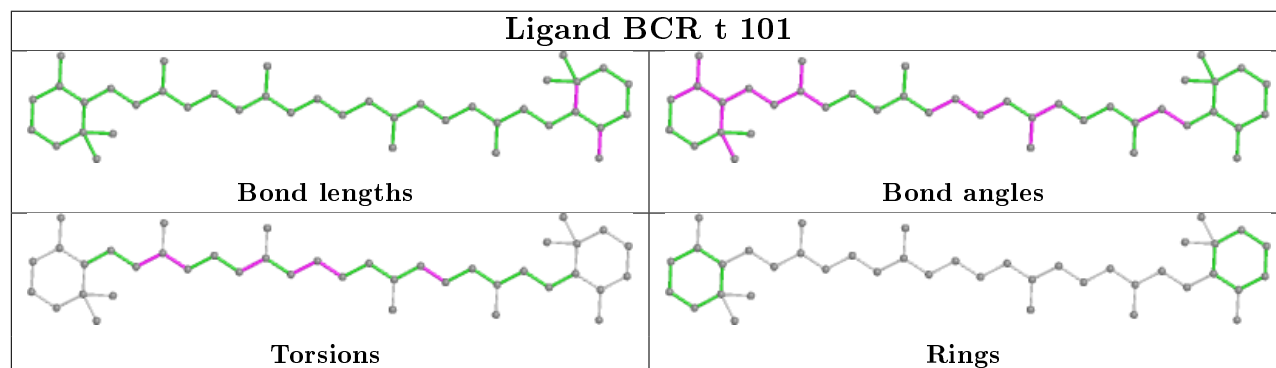
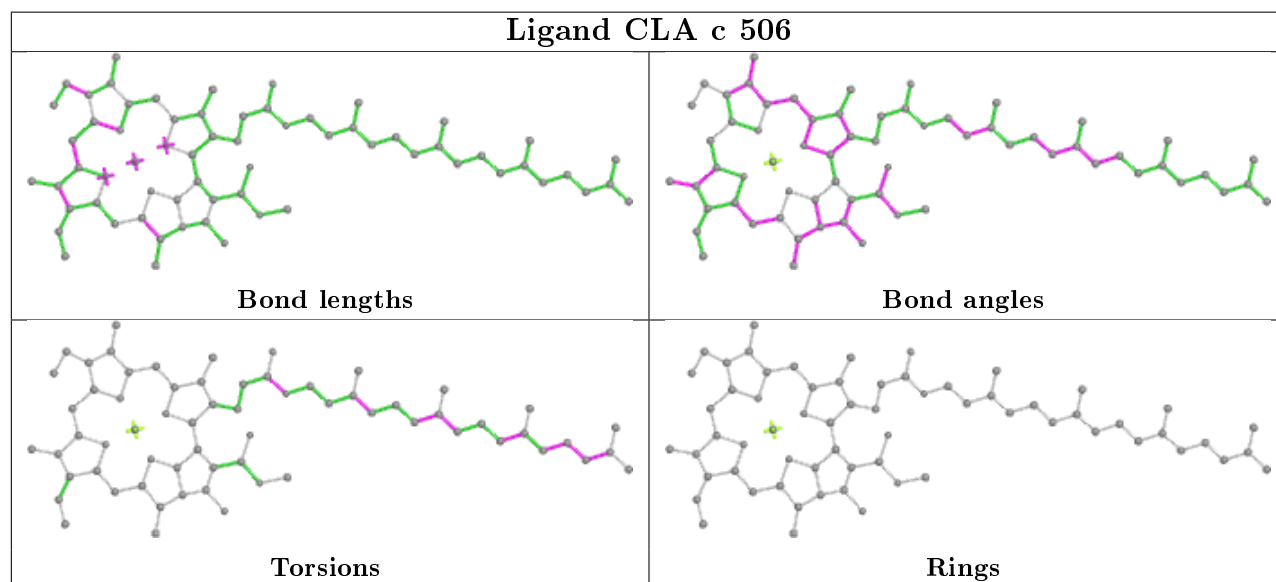
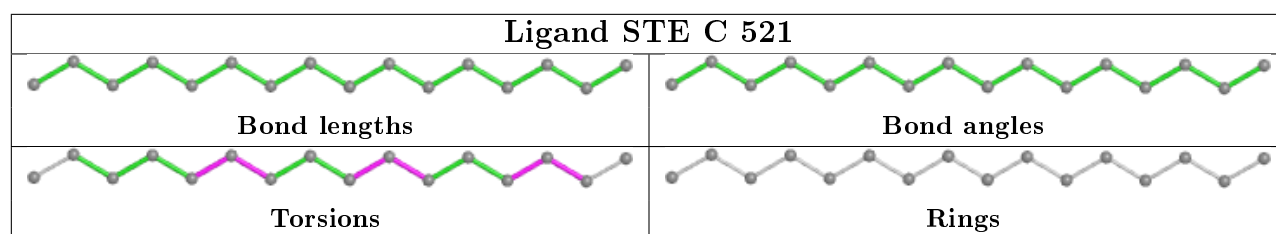
Ligand LHG D 412

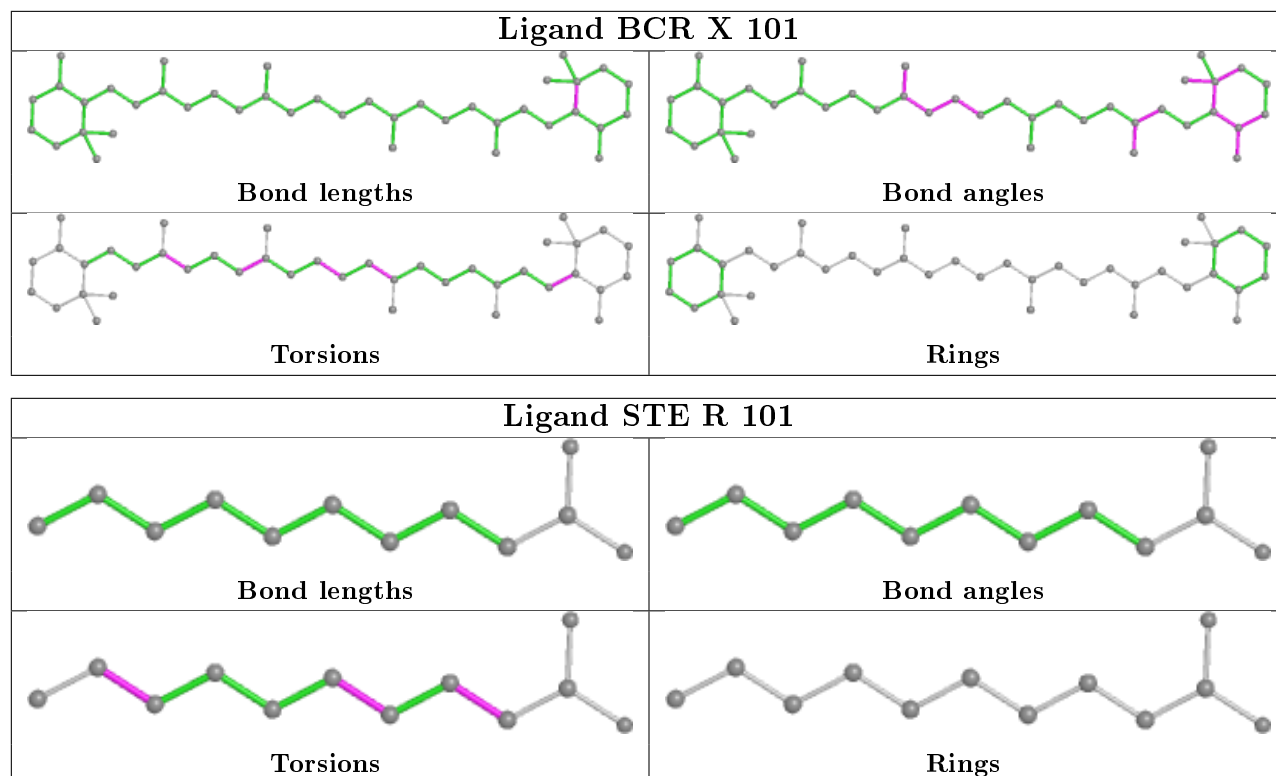


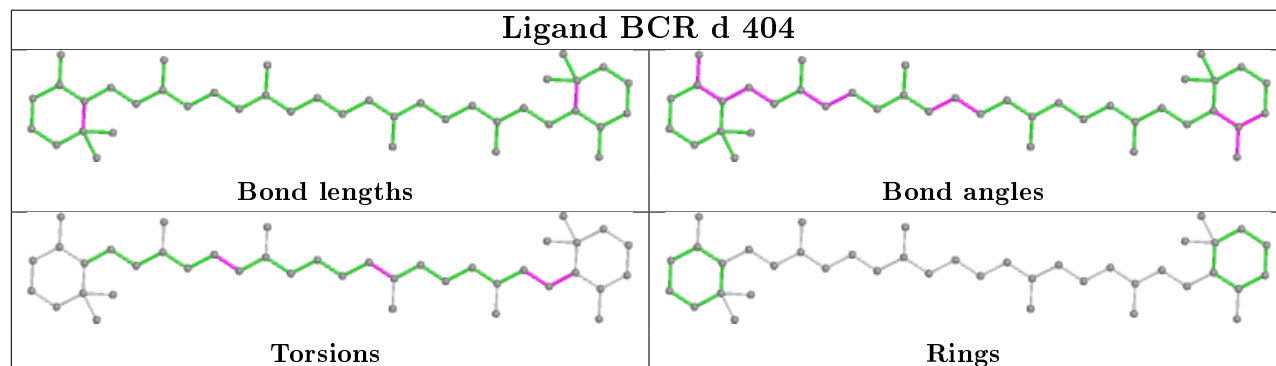
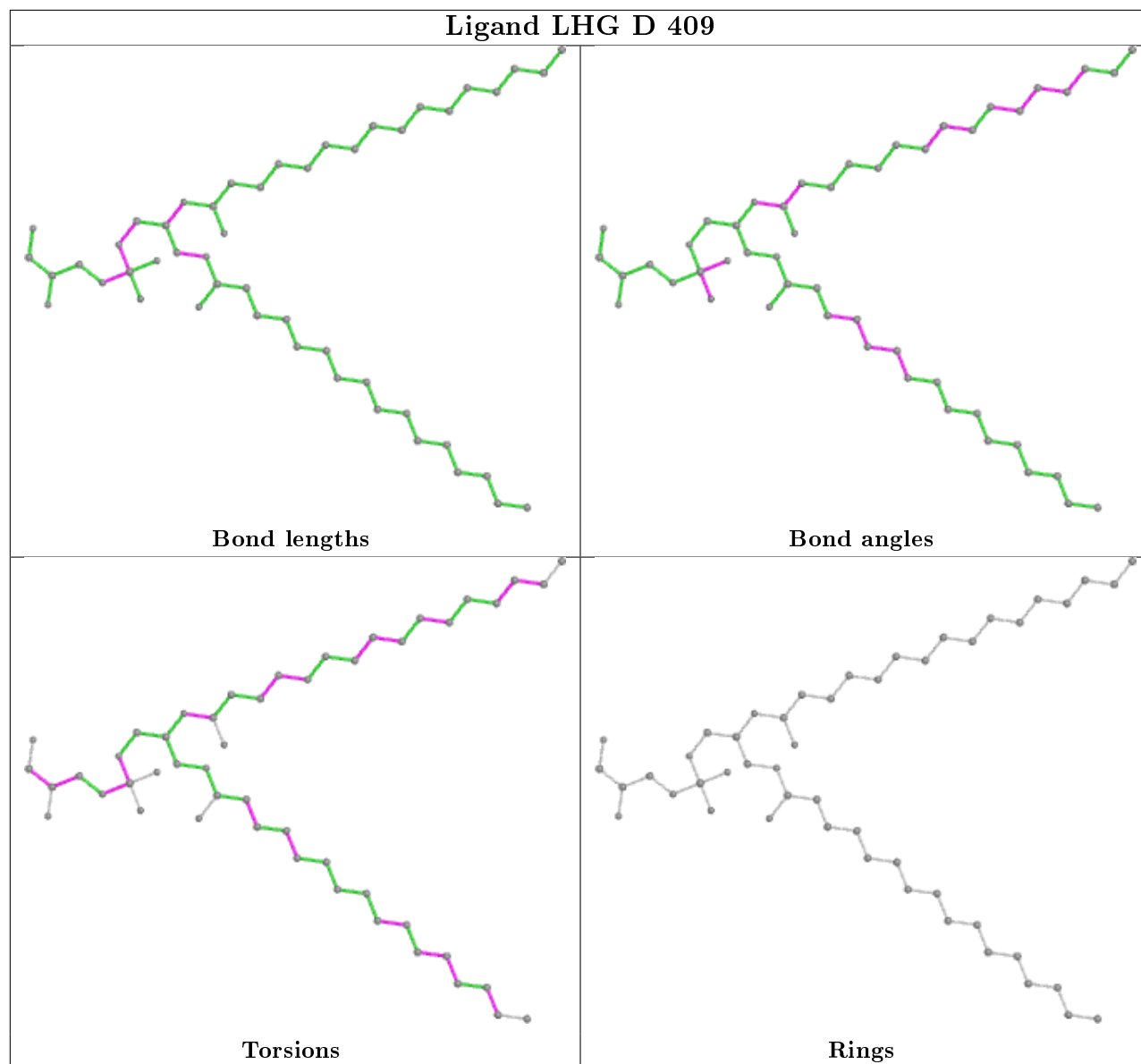


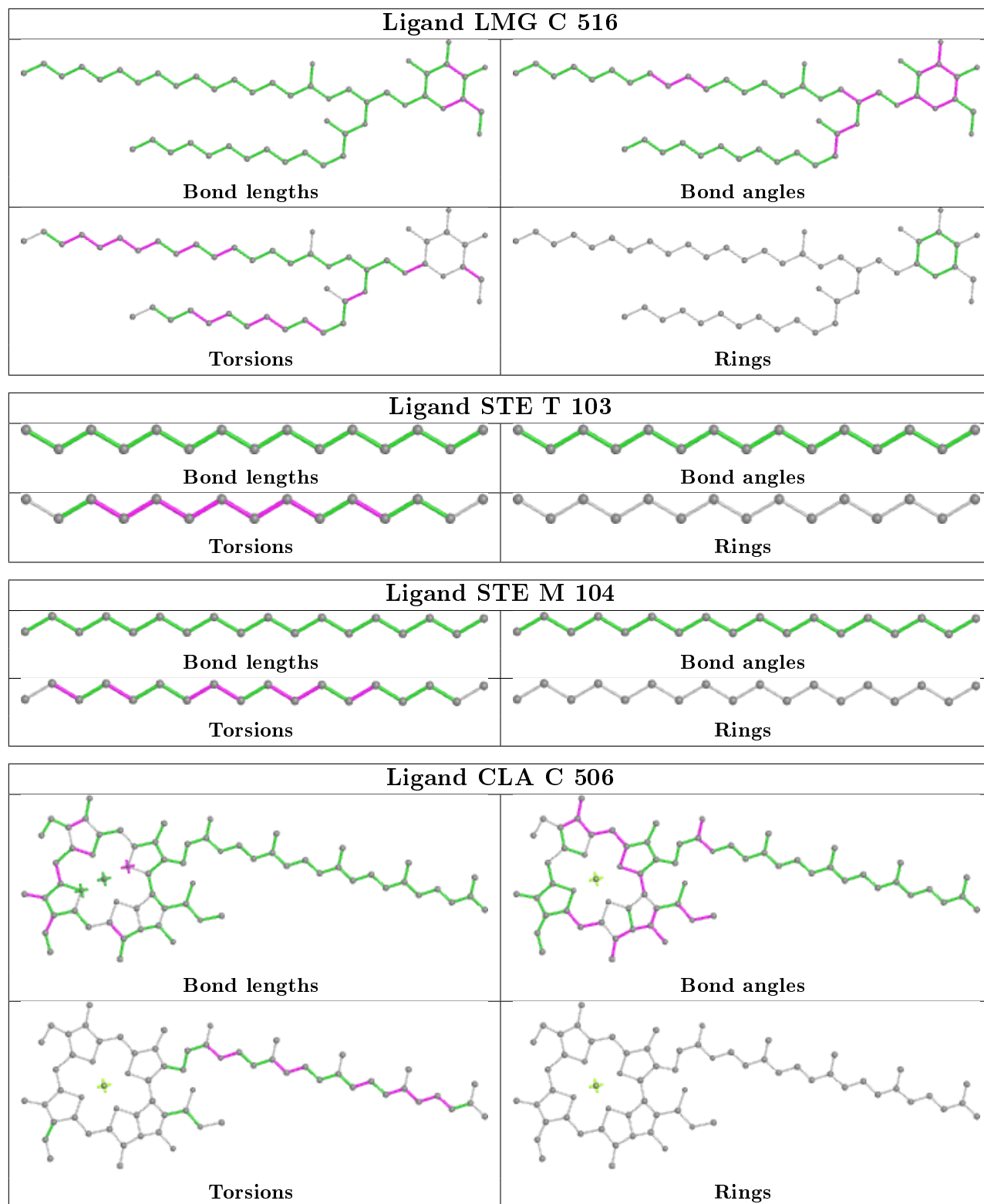


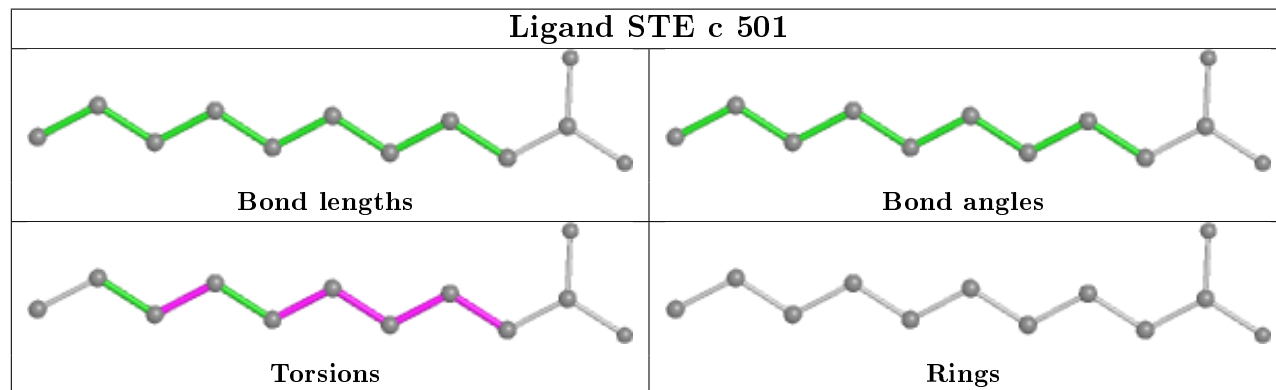
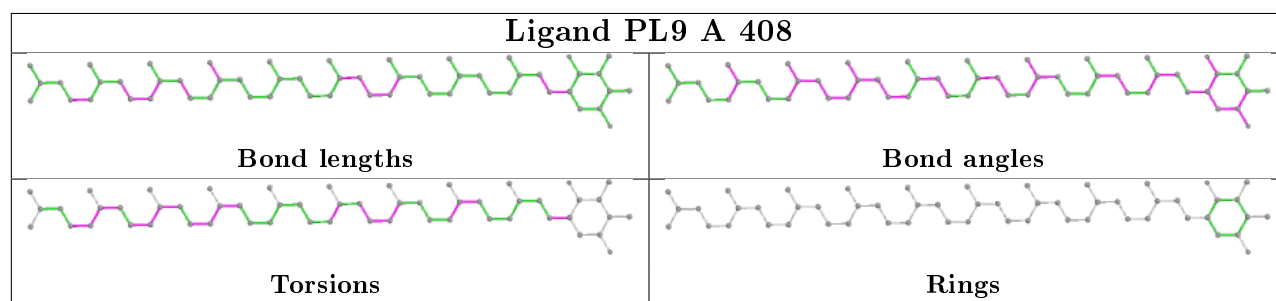
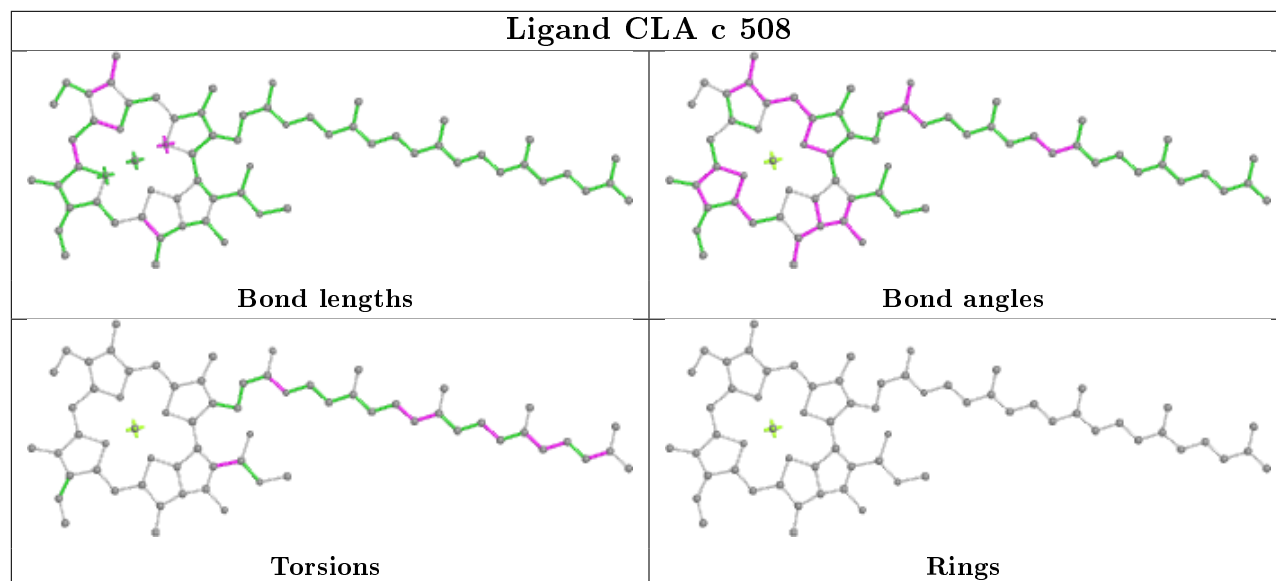
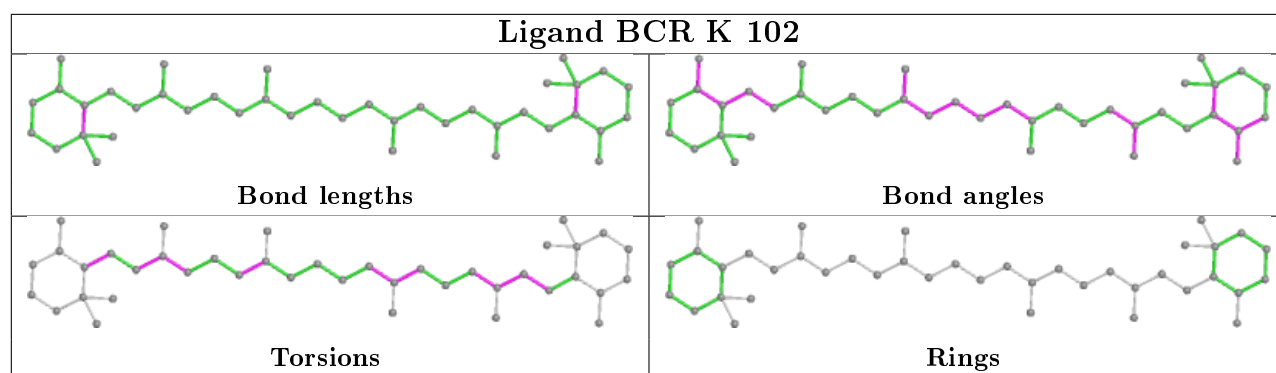


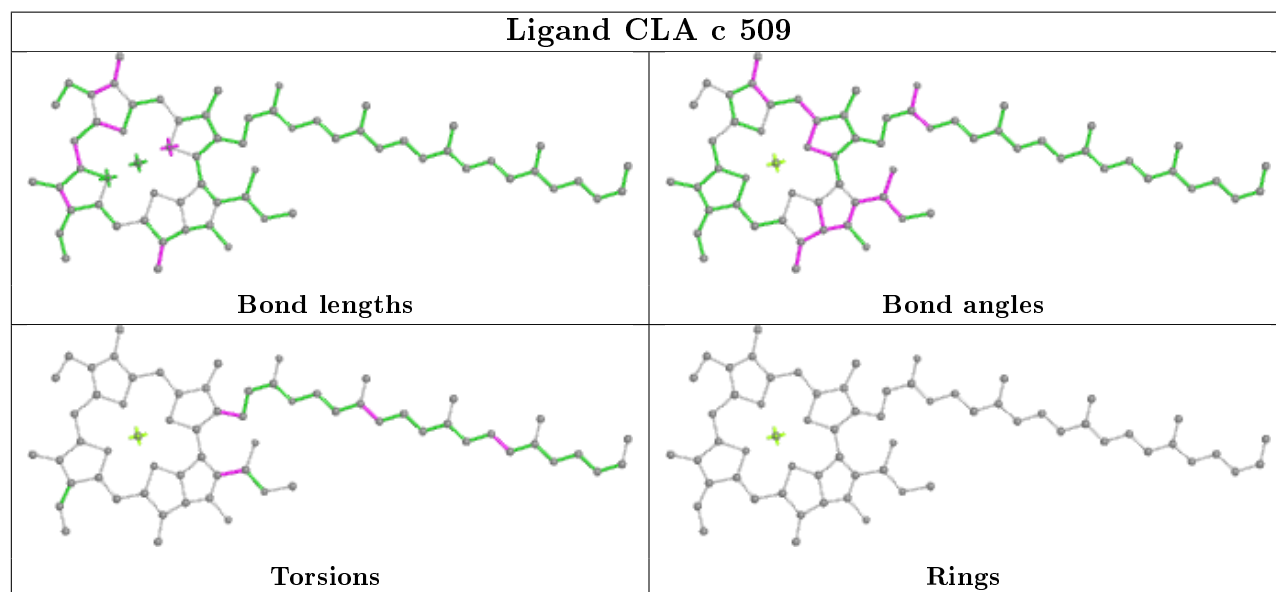
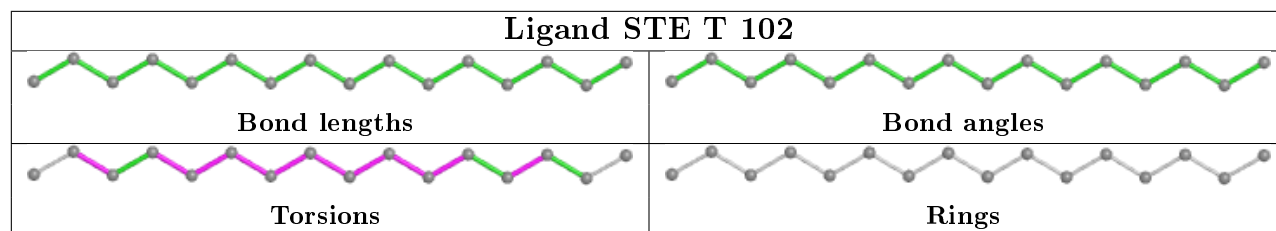




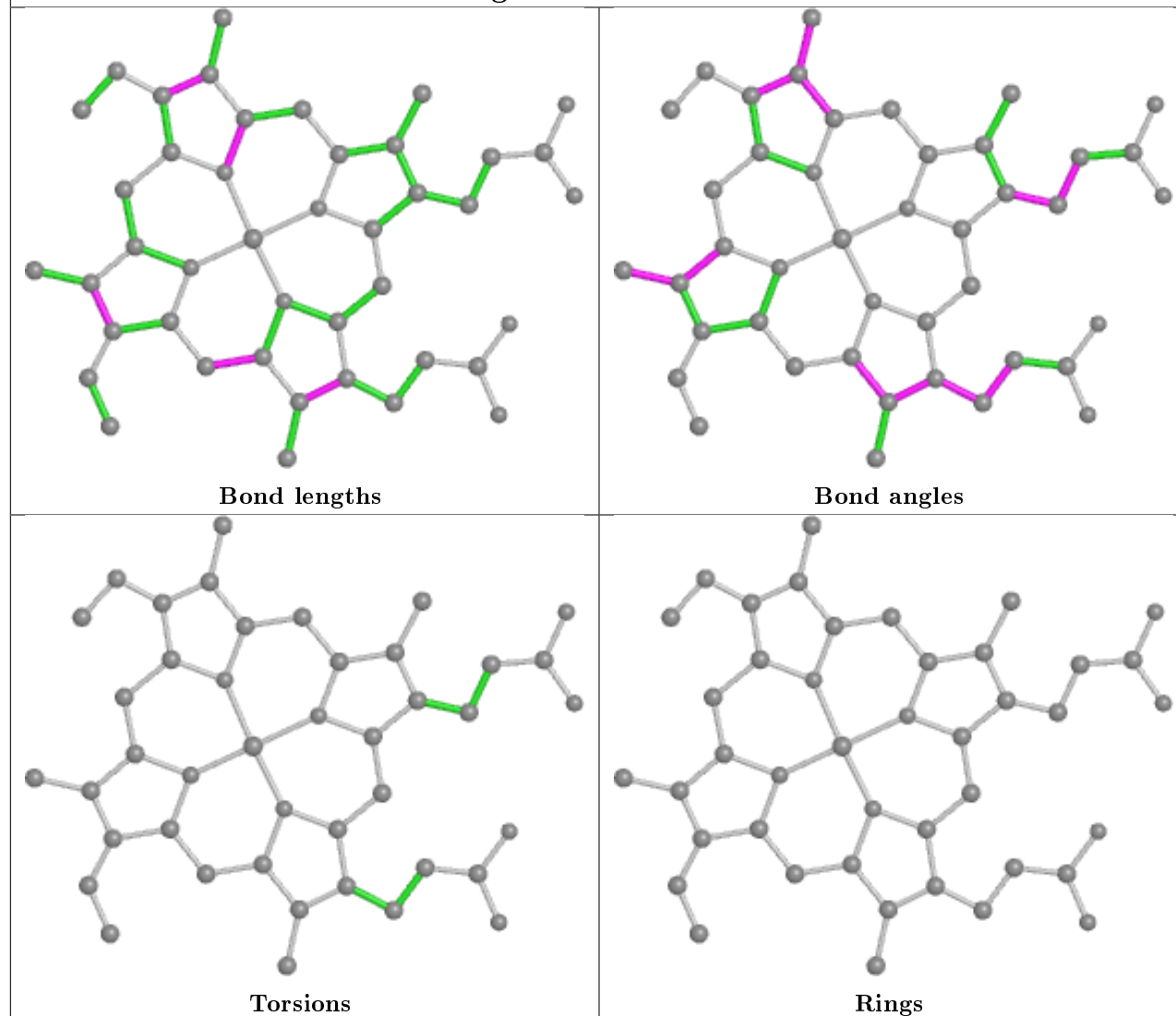




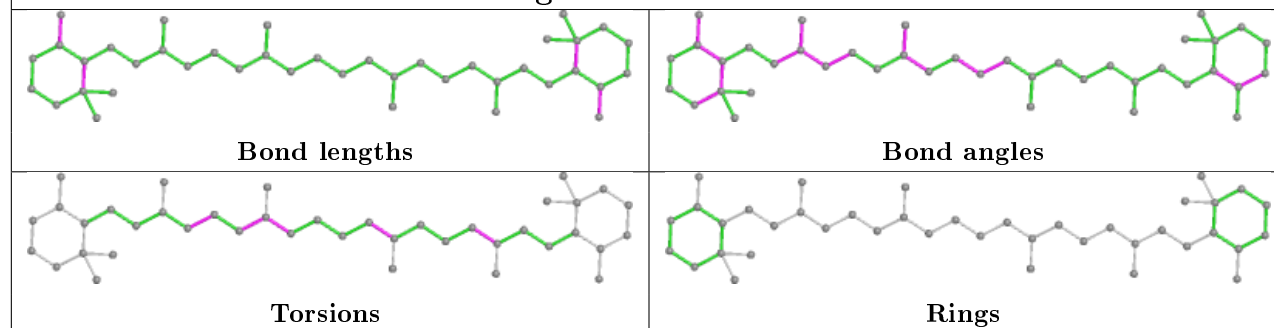




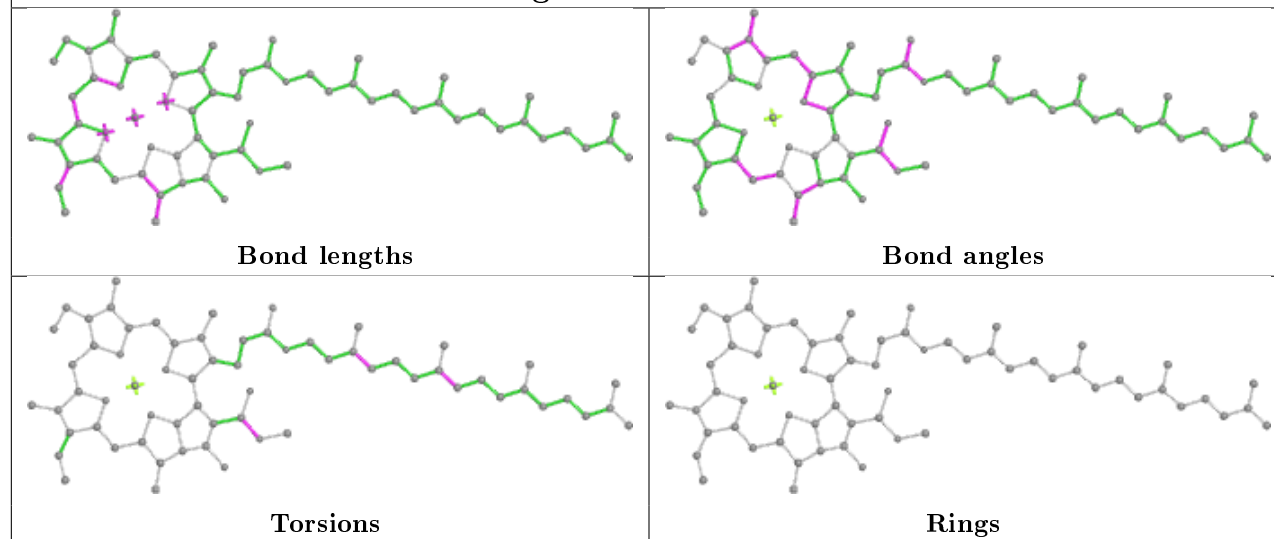
Ligand HEC F 101



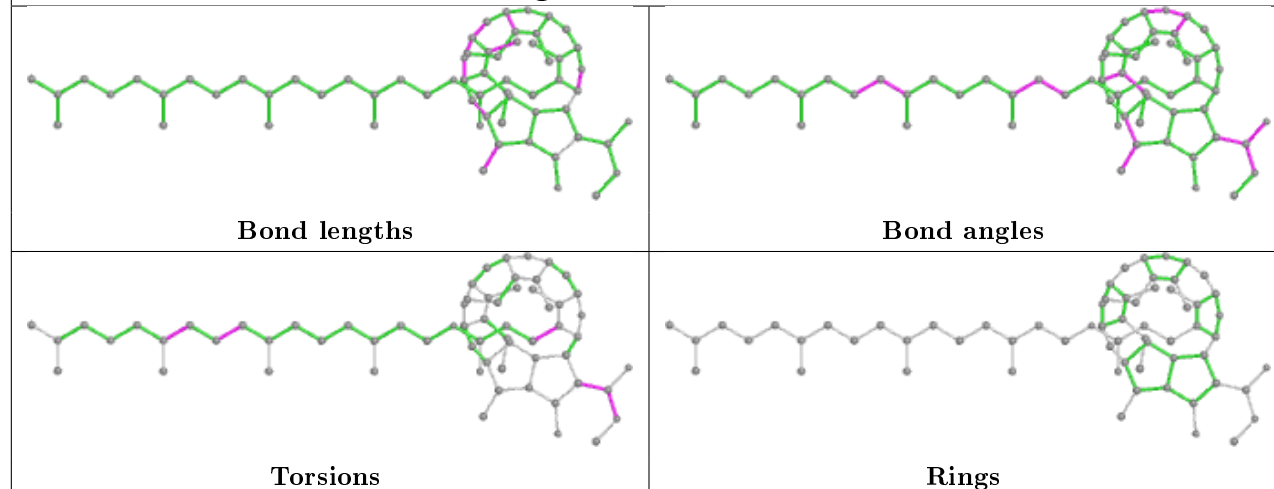
Ligand BCR c 516



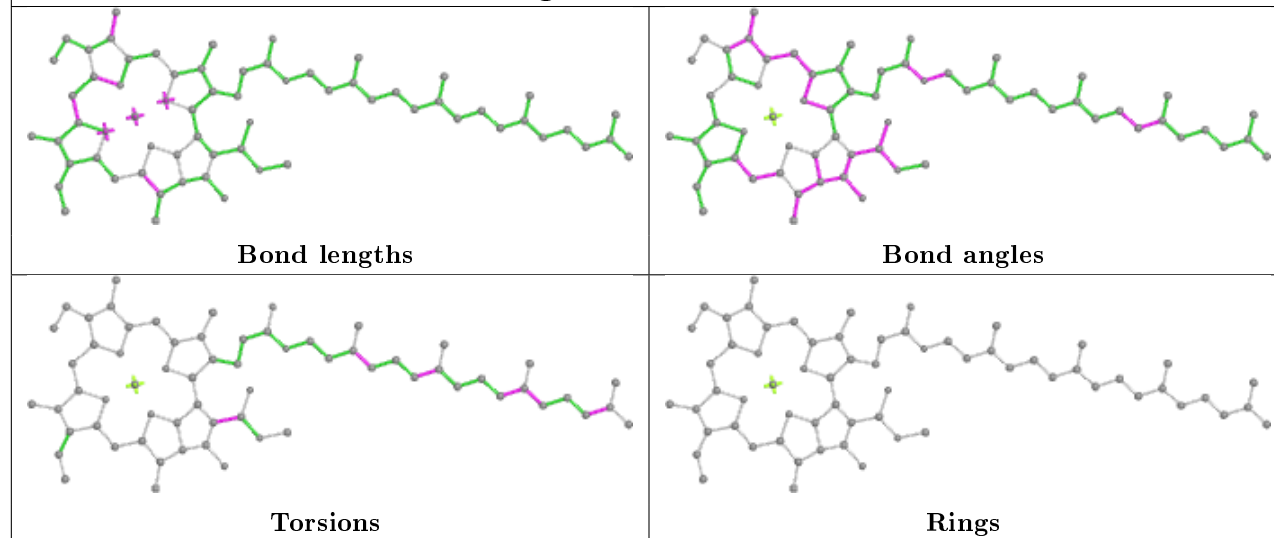
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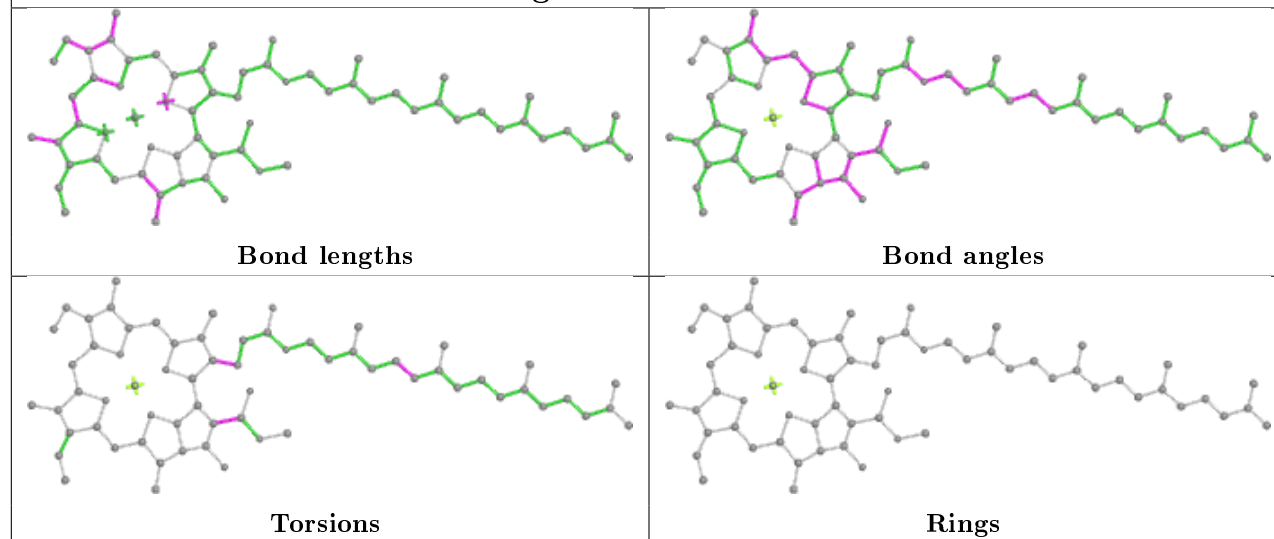
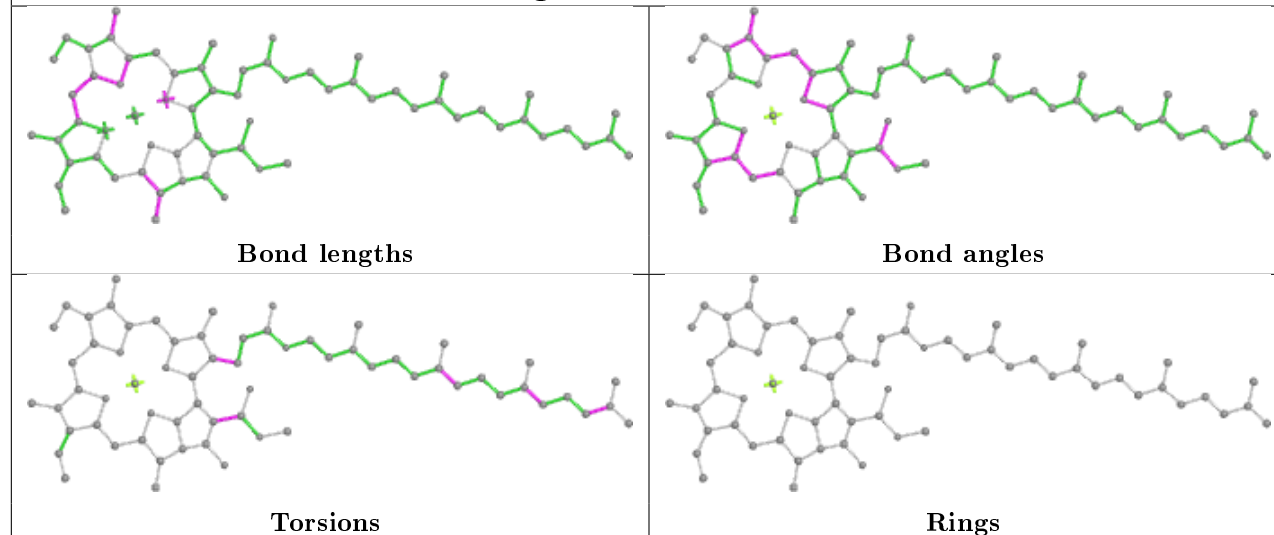
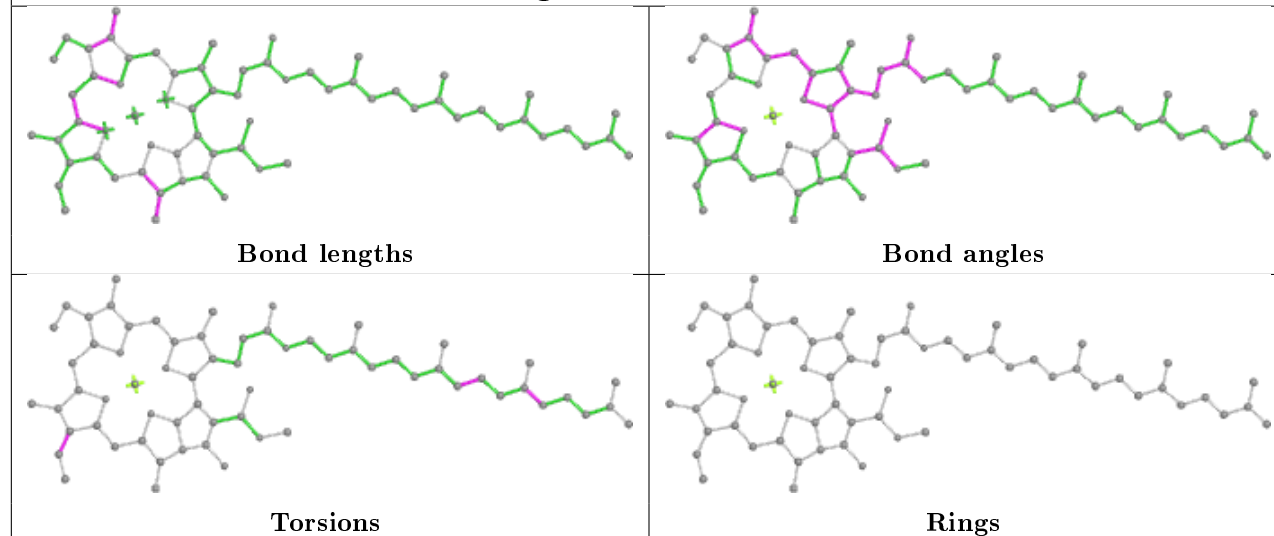


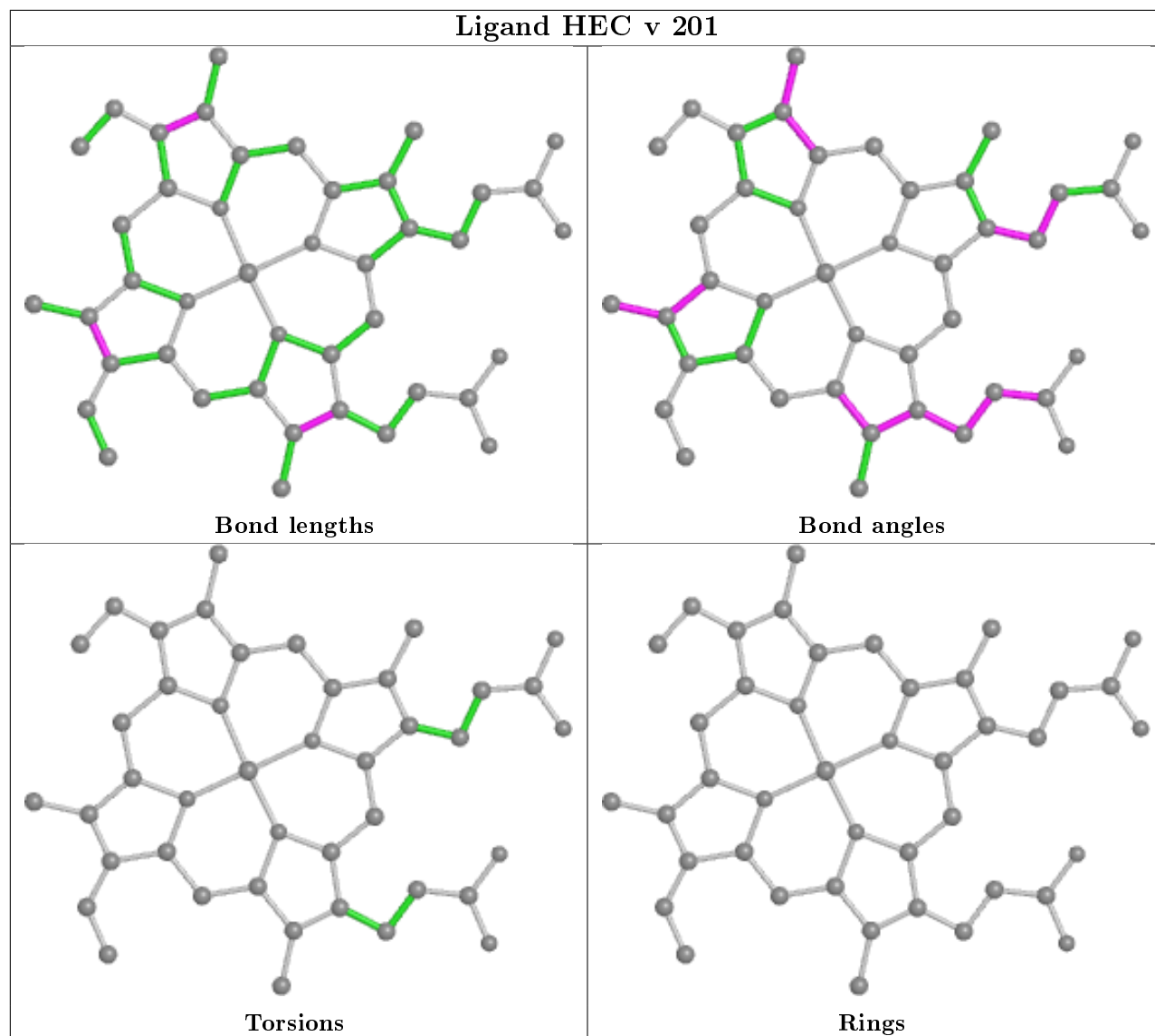
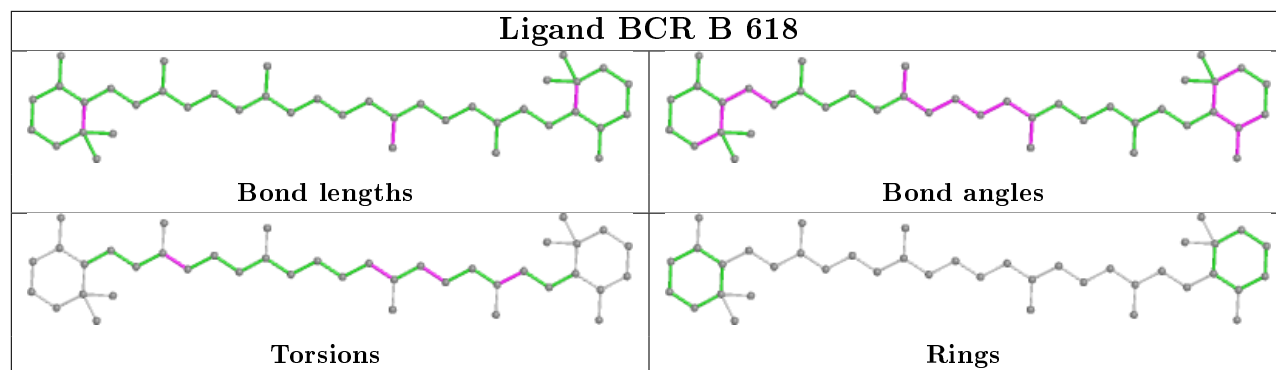
Ligand PHO d 401



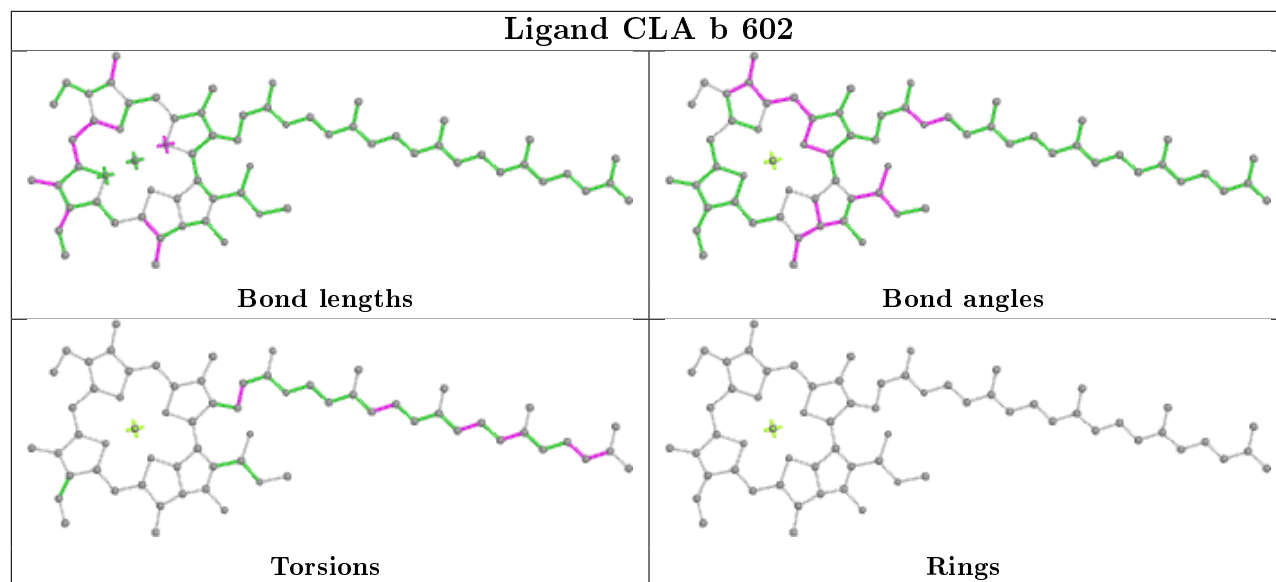
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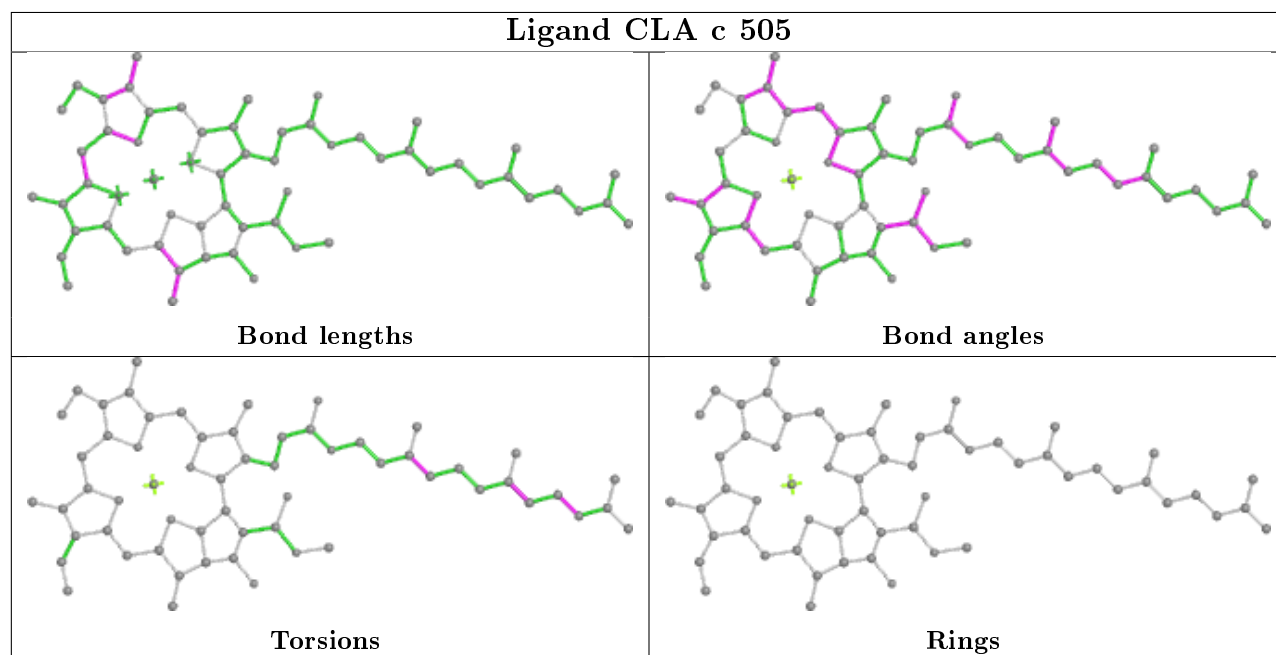
Ligand CLA C 503**Ligand CLA C 508****Ligand CLA b 610**



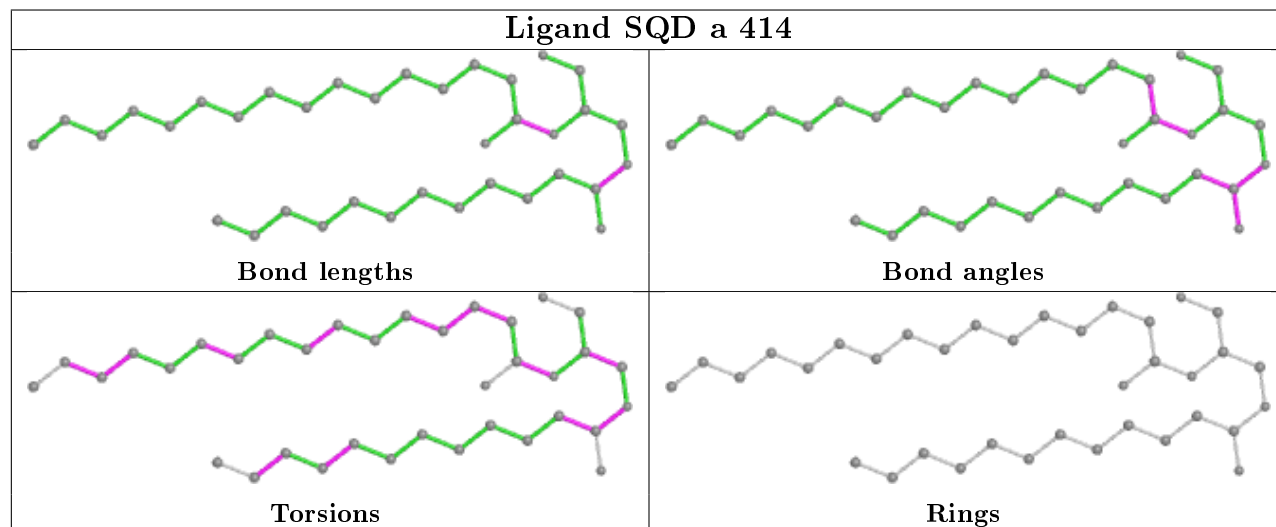
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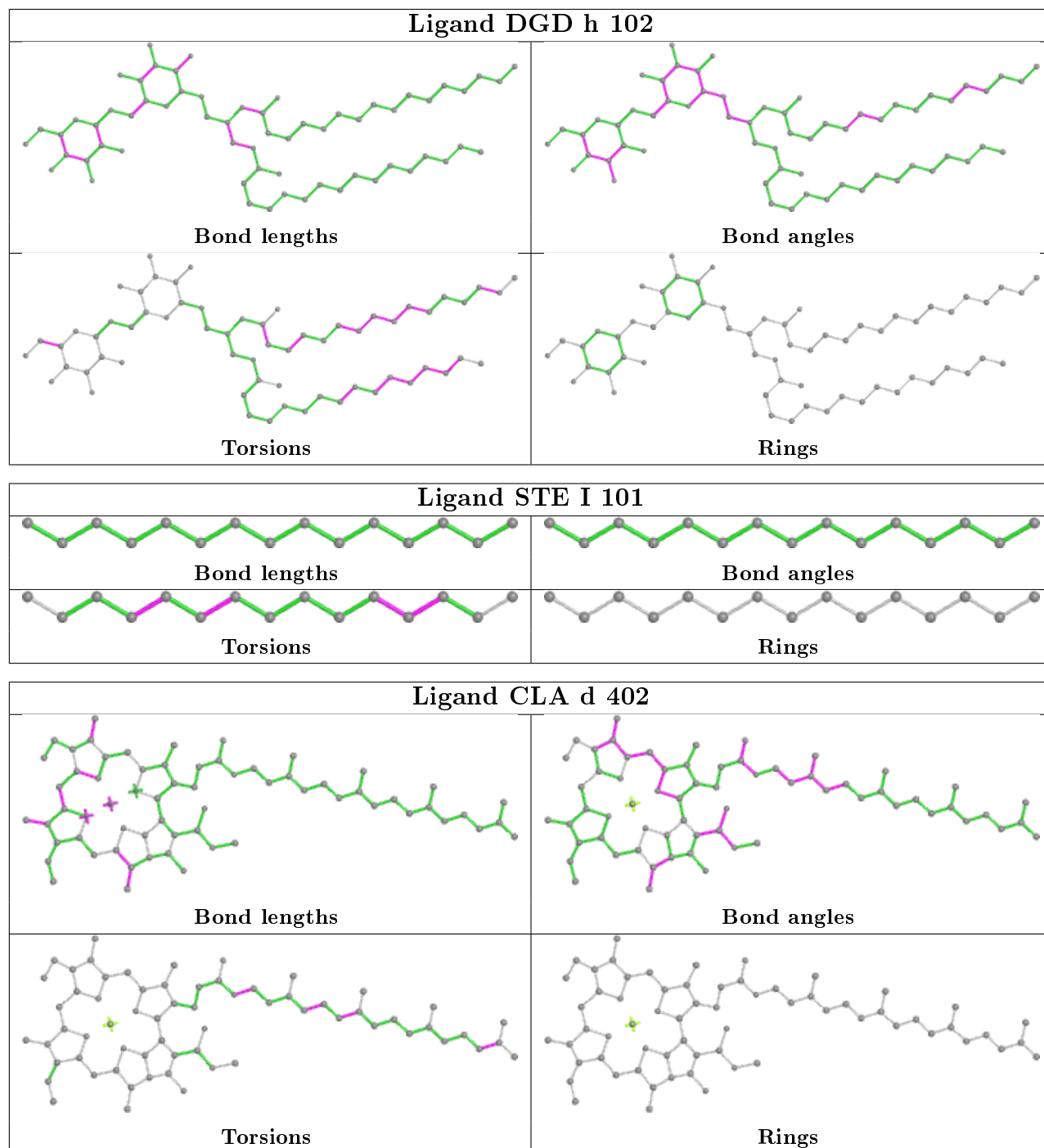


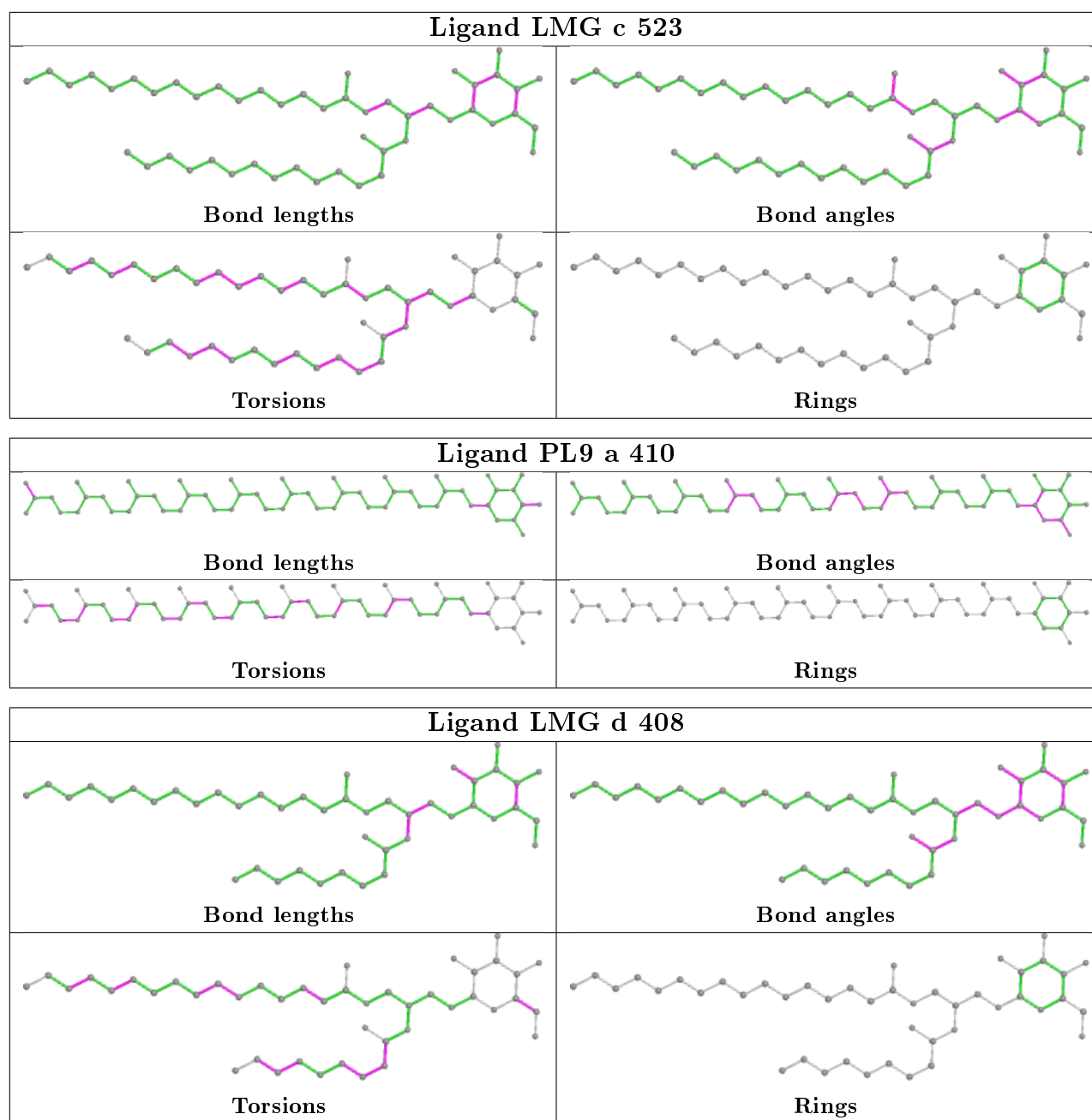
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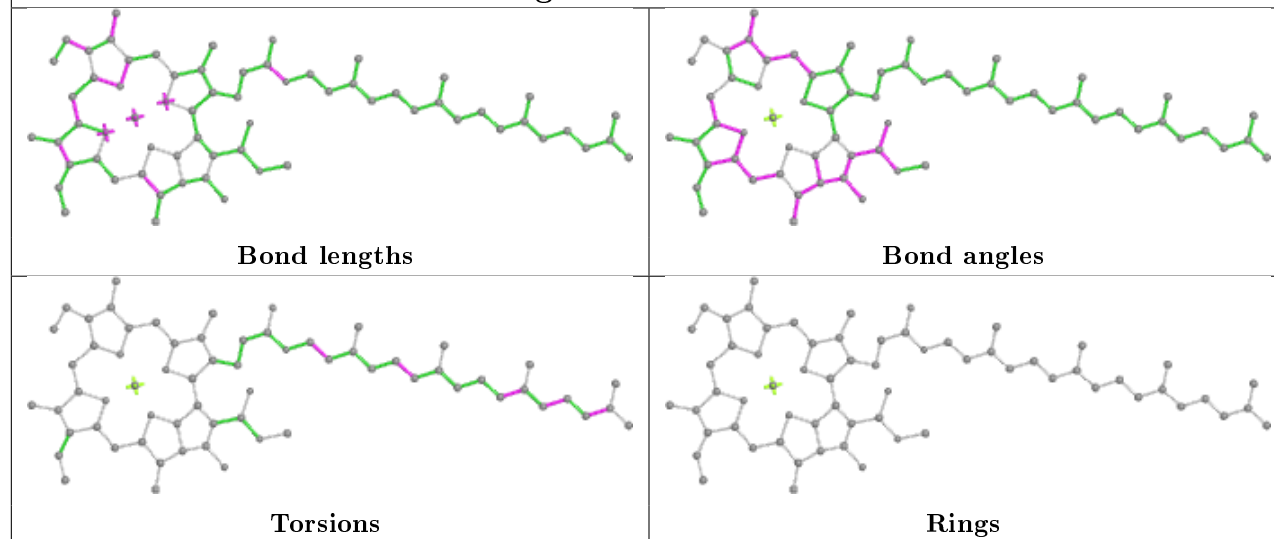
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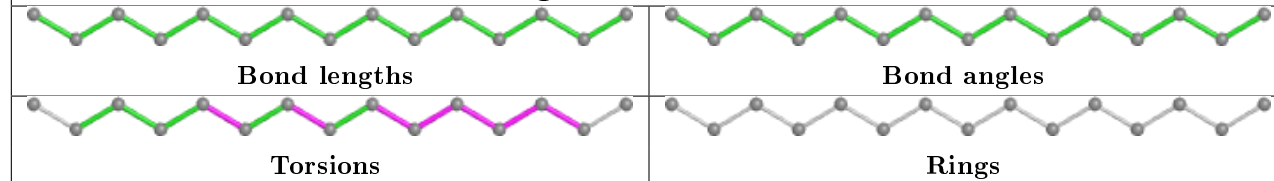




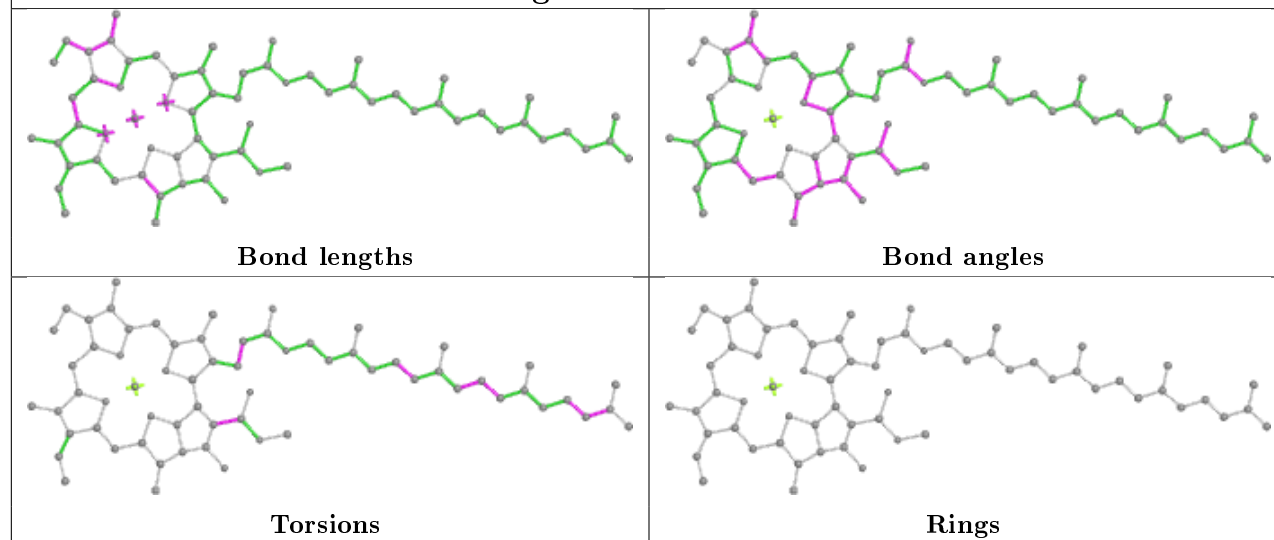
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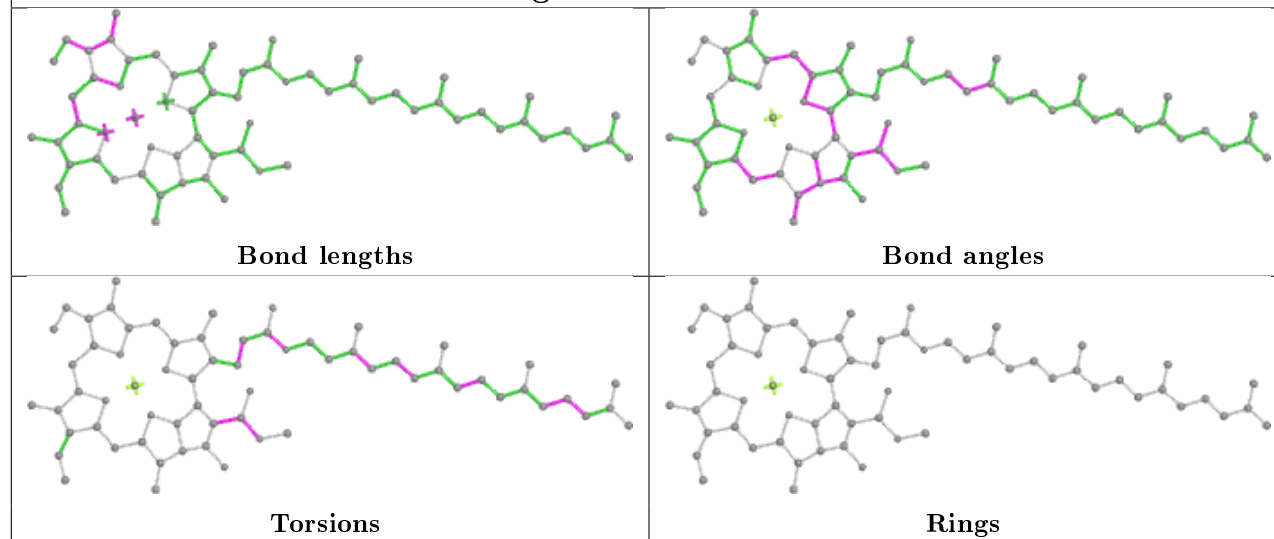
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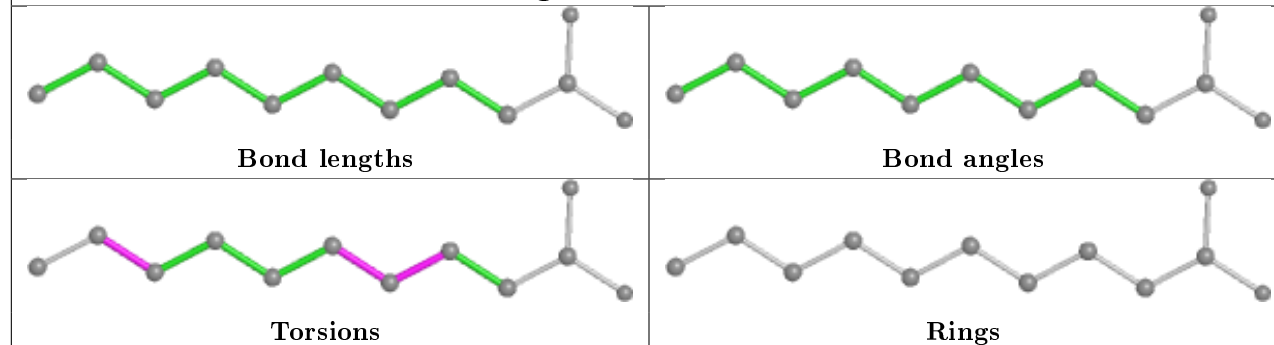
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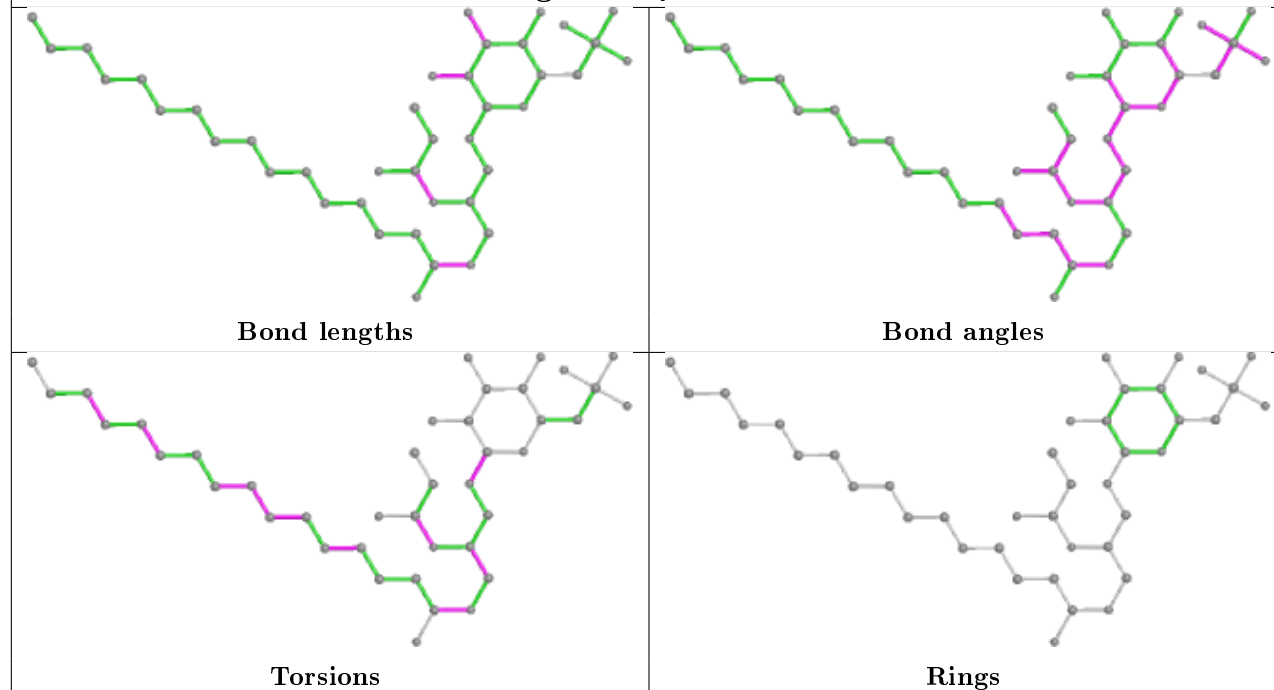
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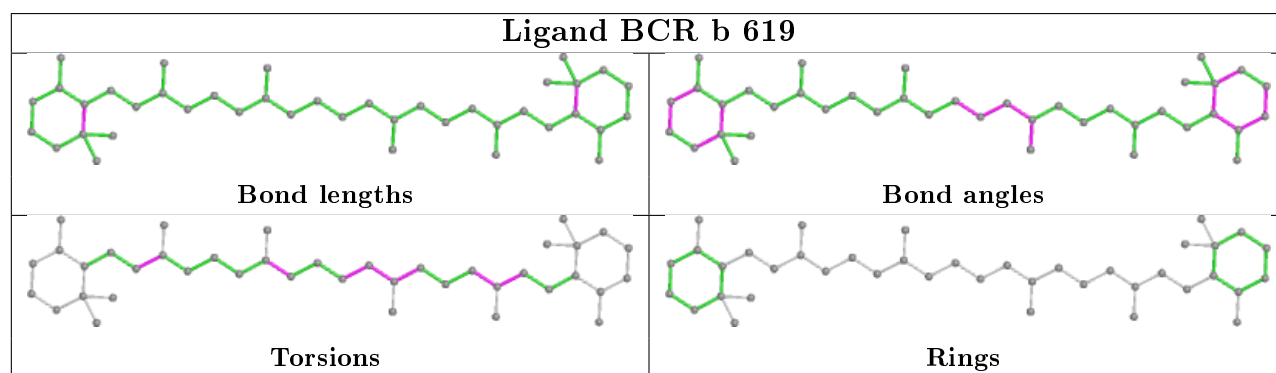
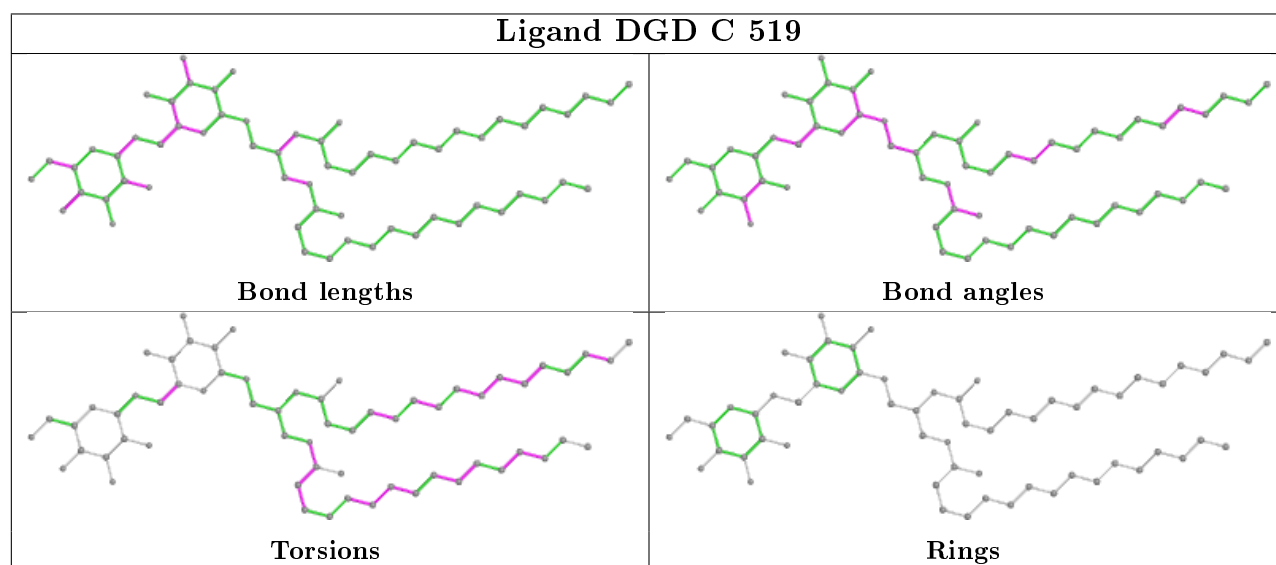
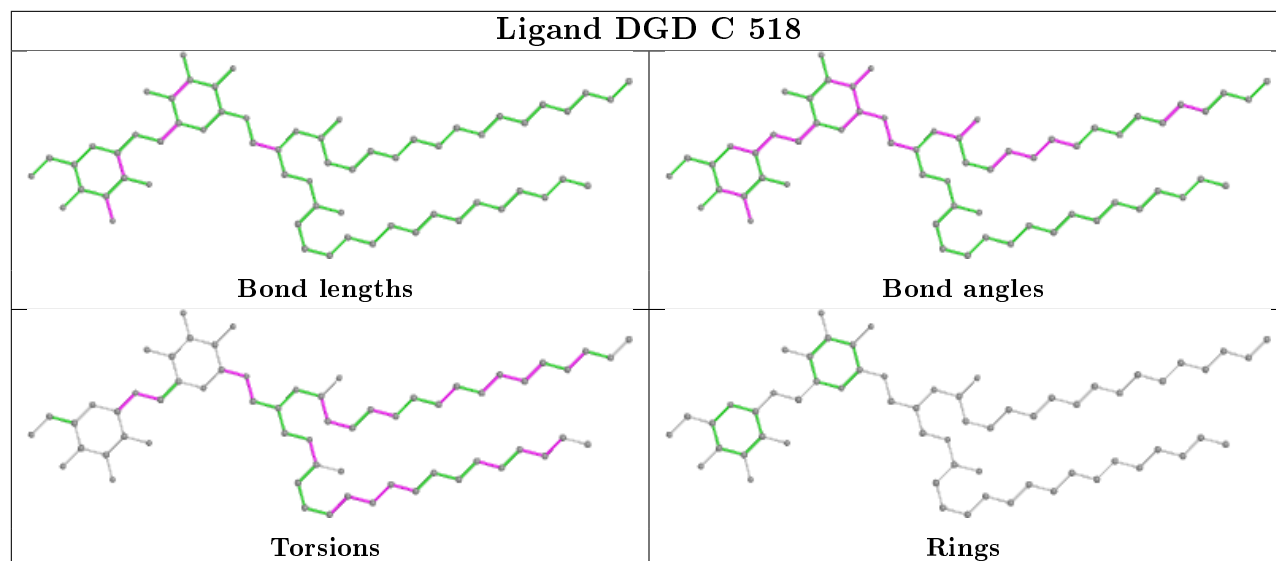


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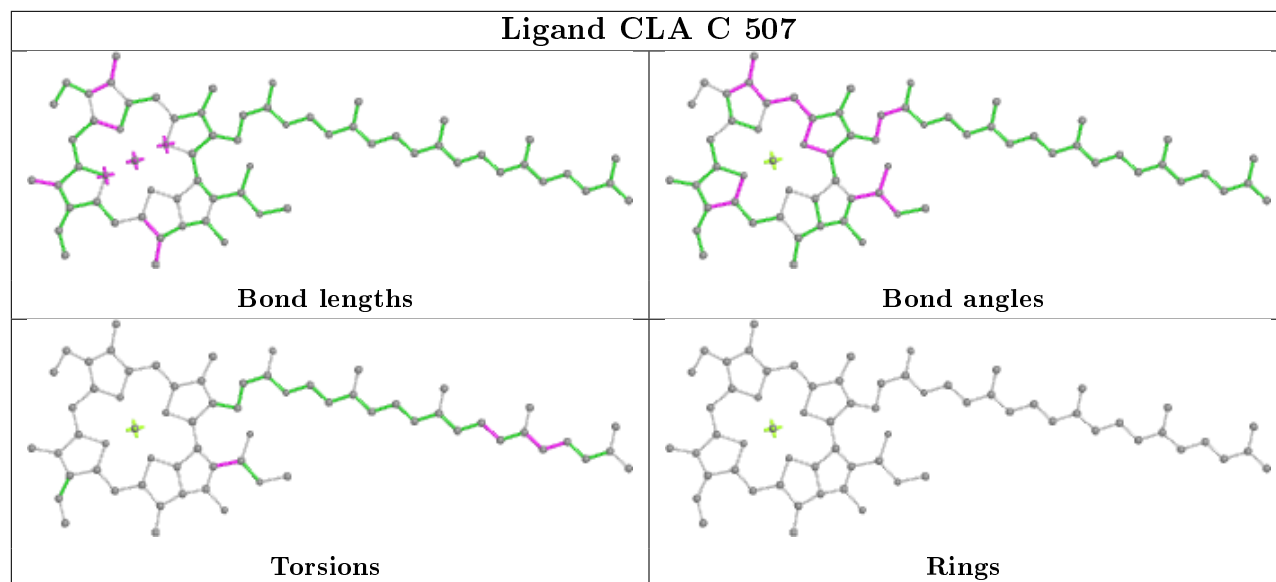


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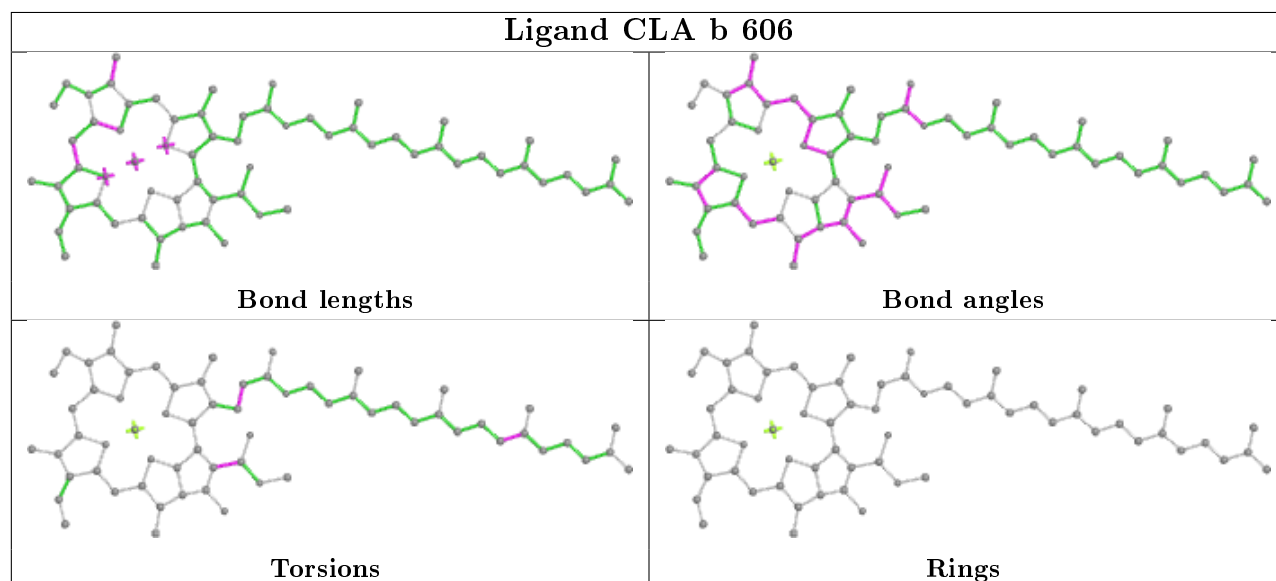




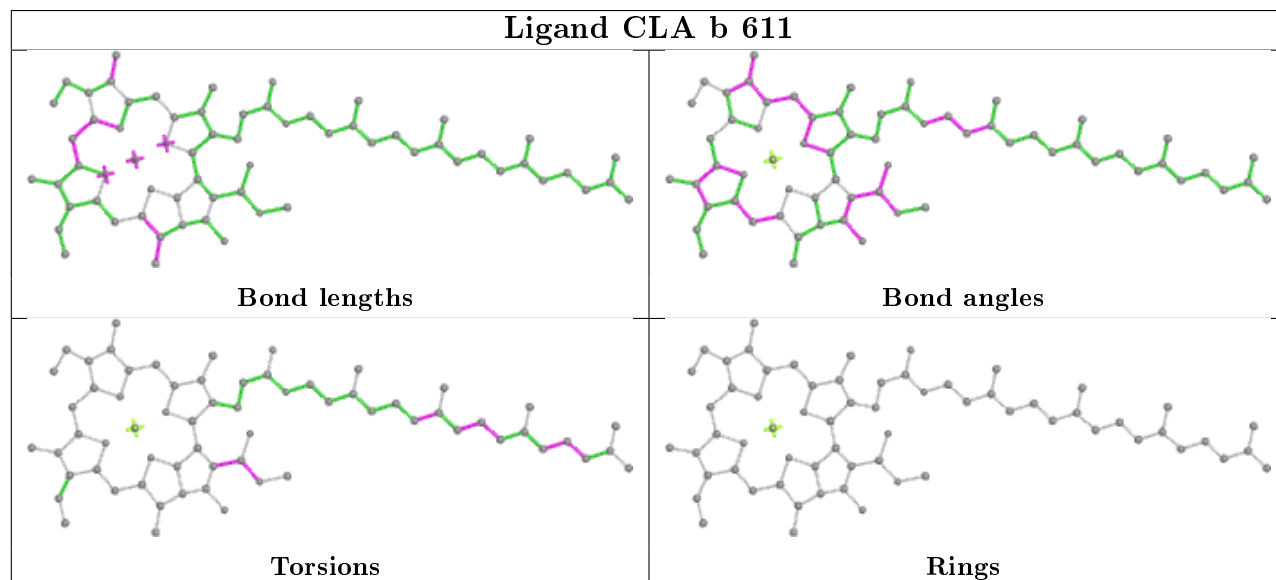
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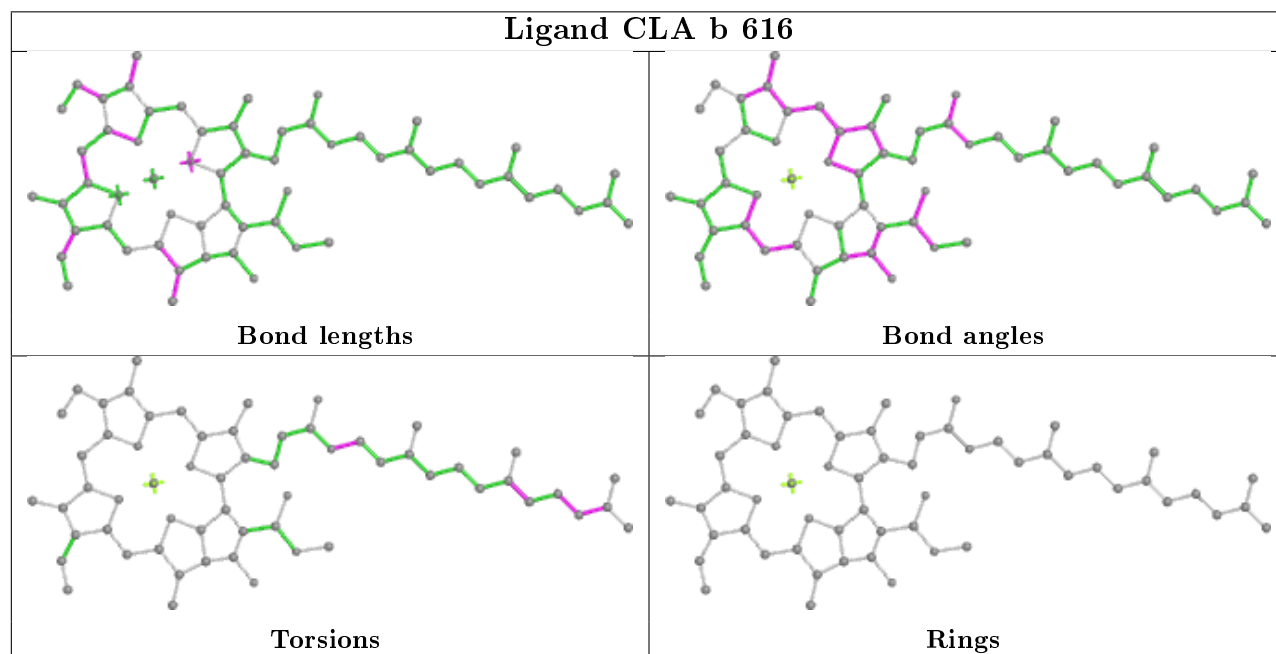
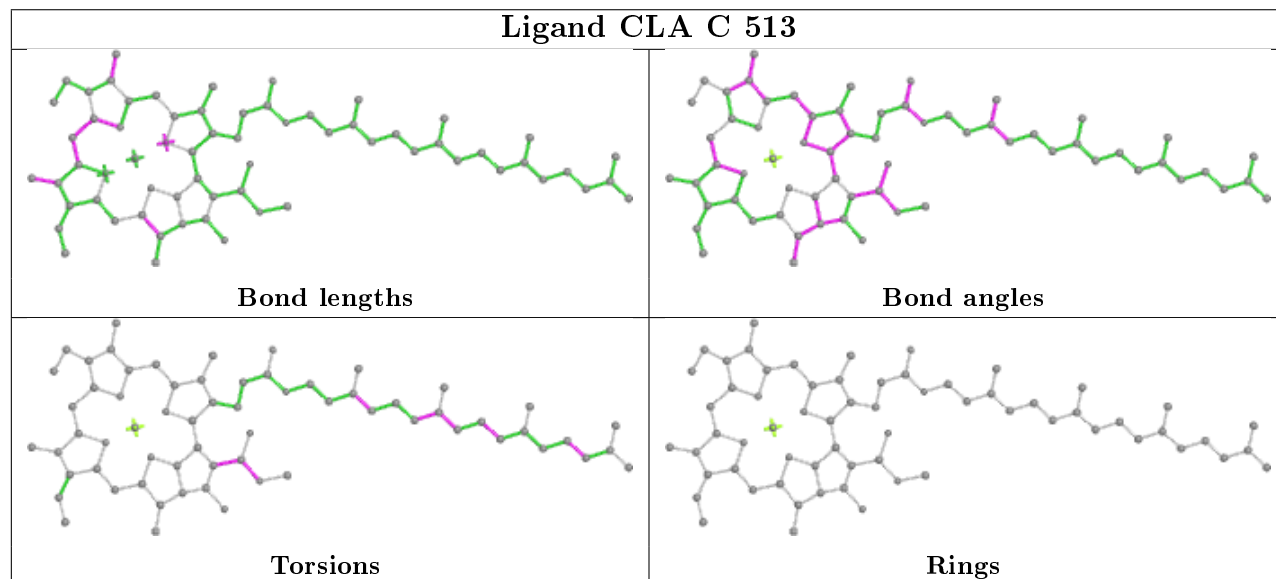
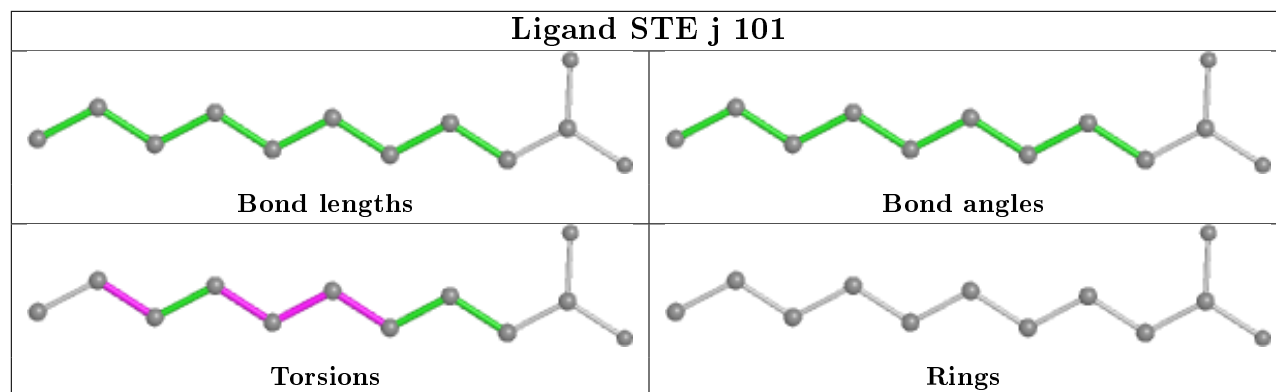


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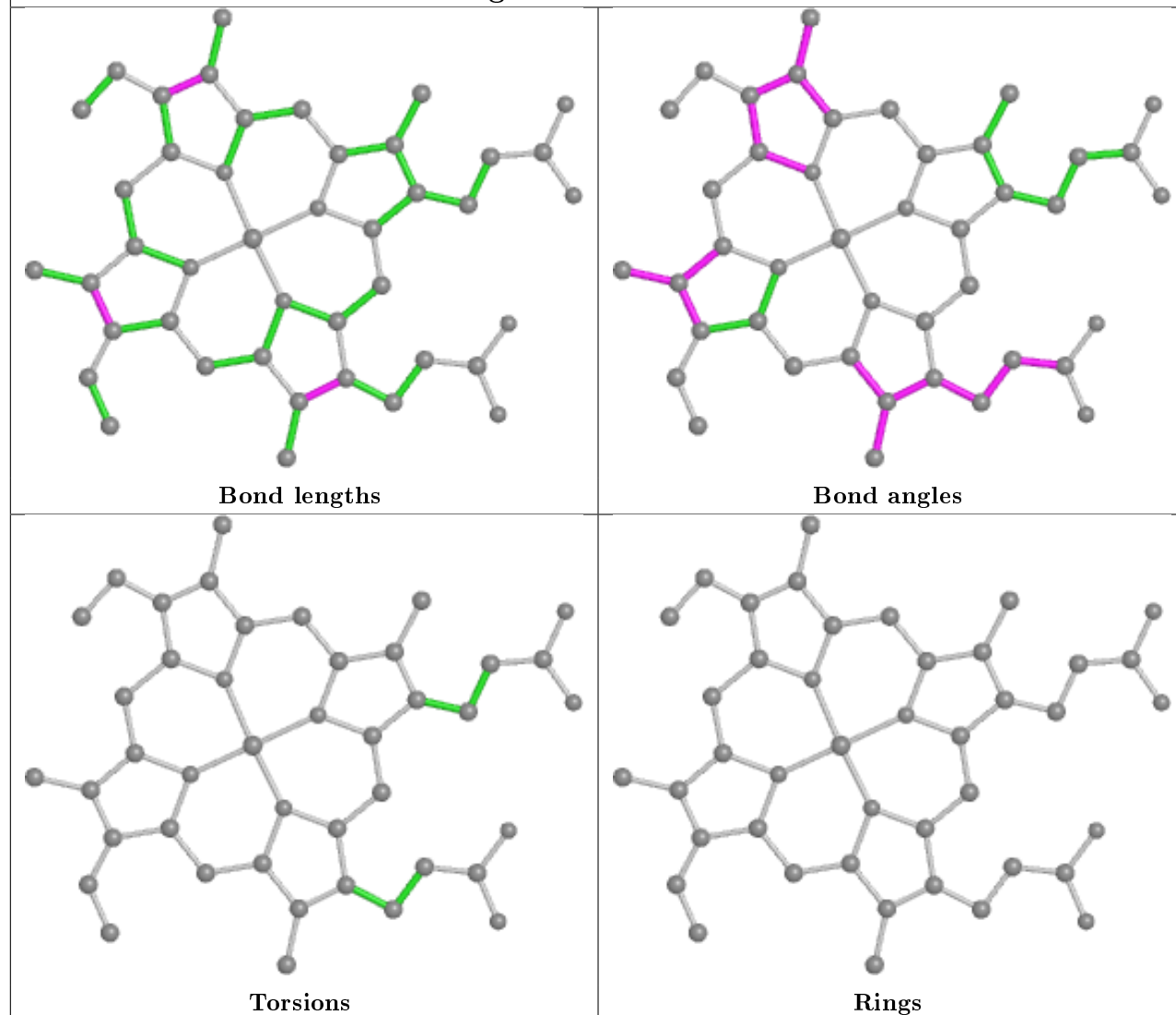


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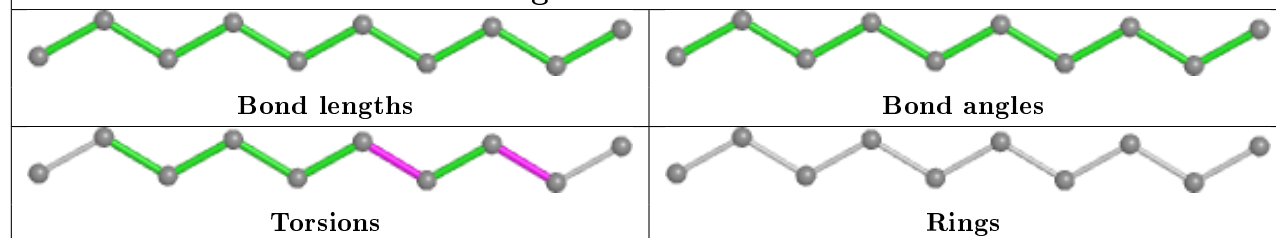




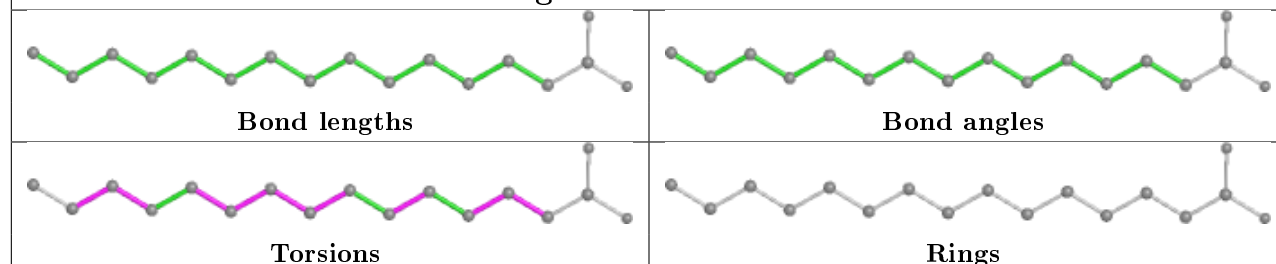
Ligand HEC V 201



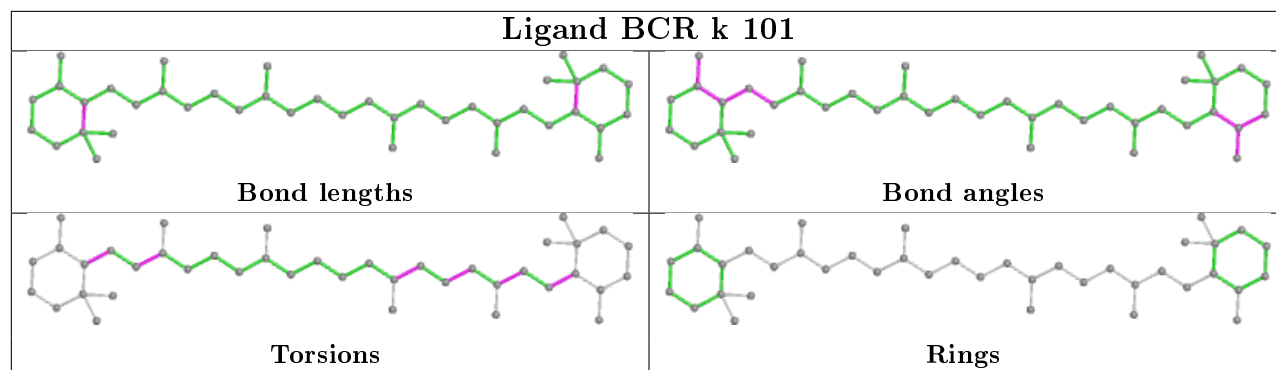
Ligand STE M 103



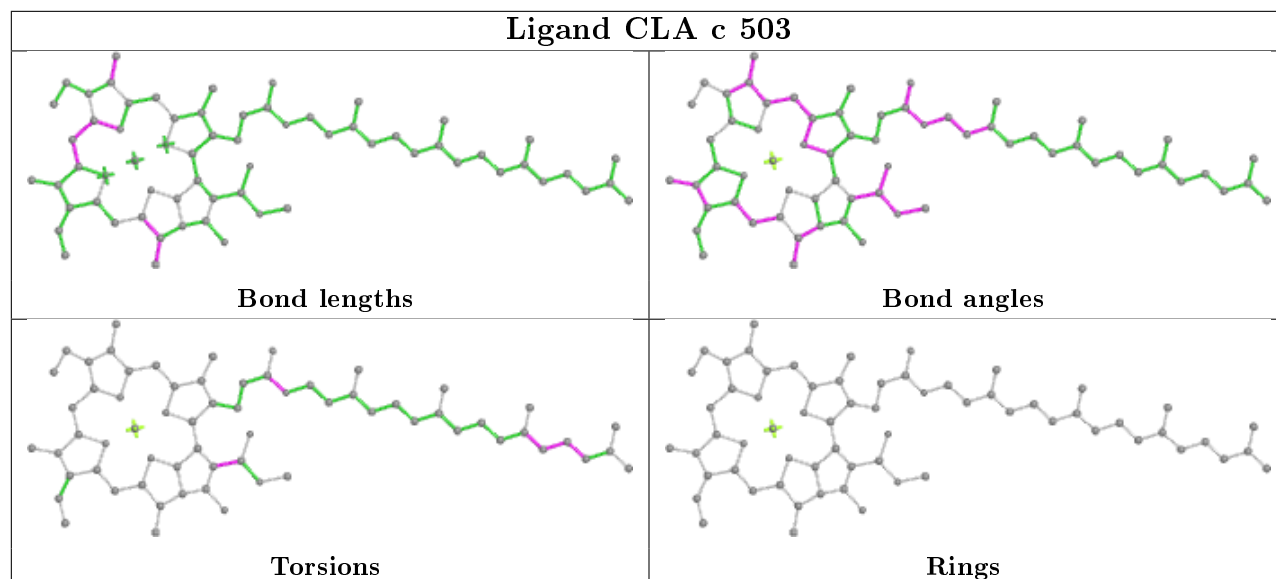
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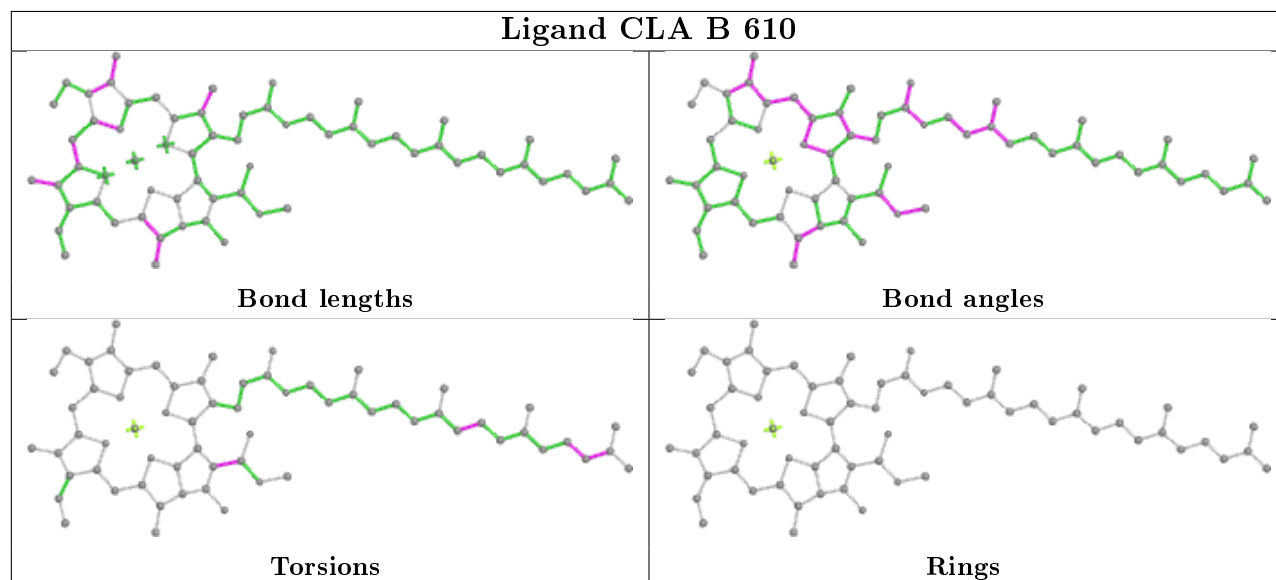
Ligand BCR k 101



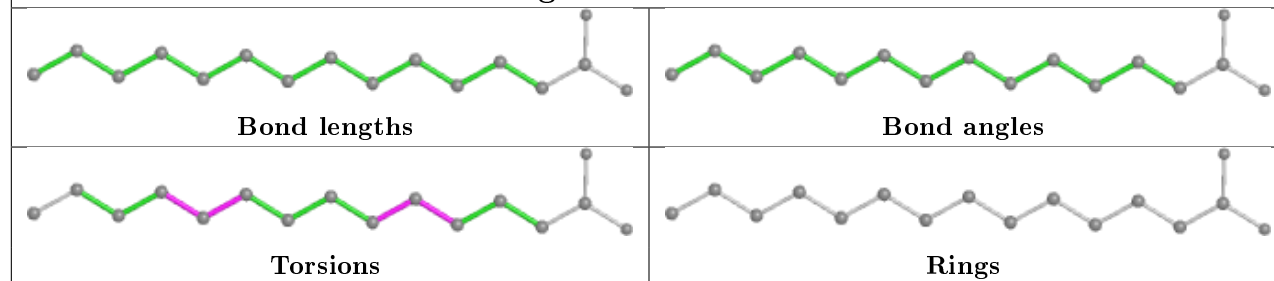
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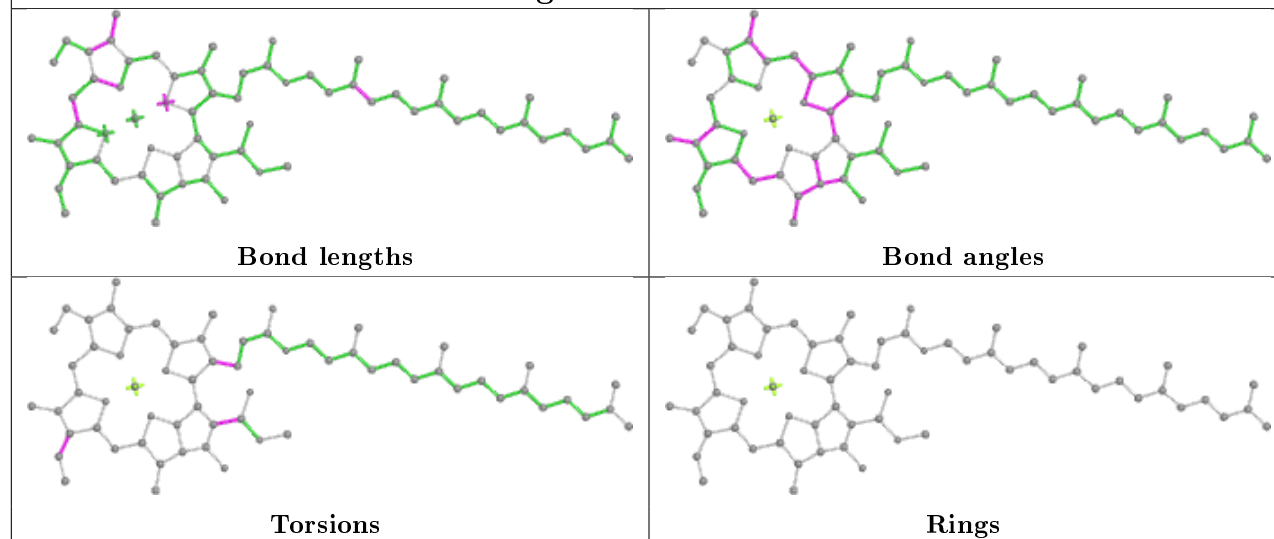
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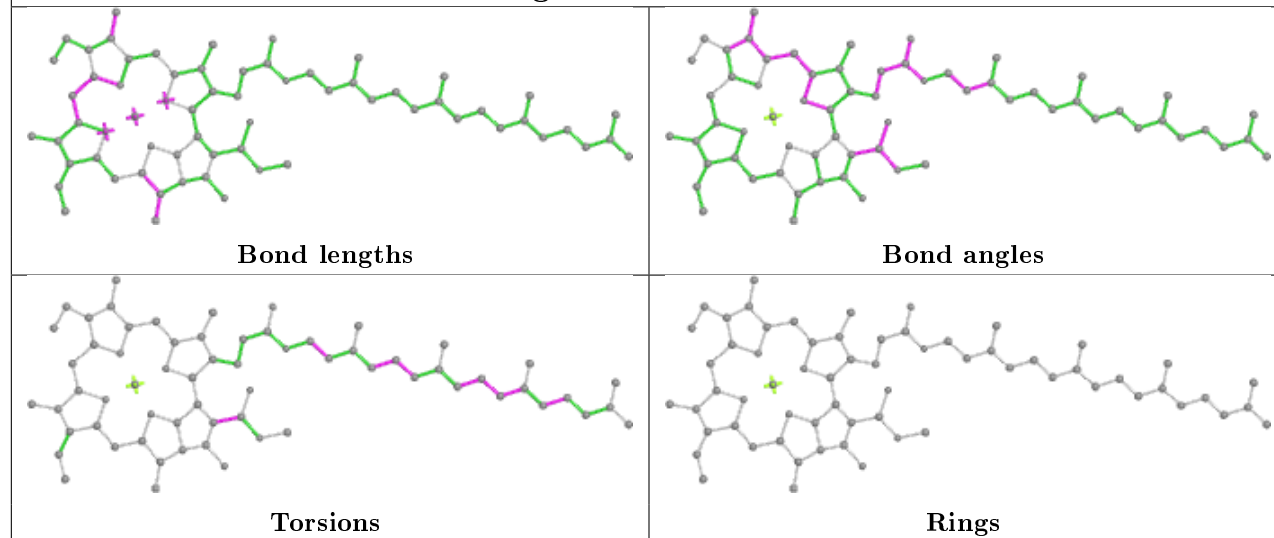
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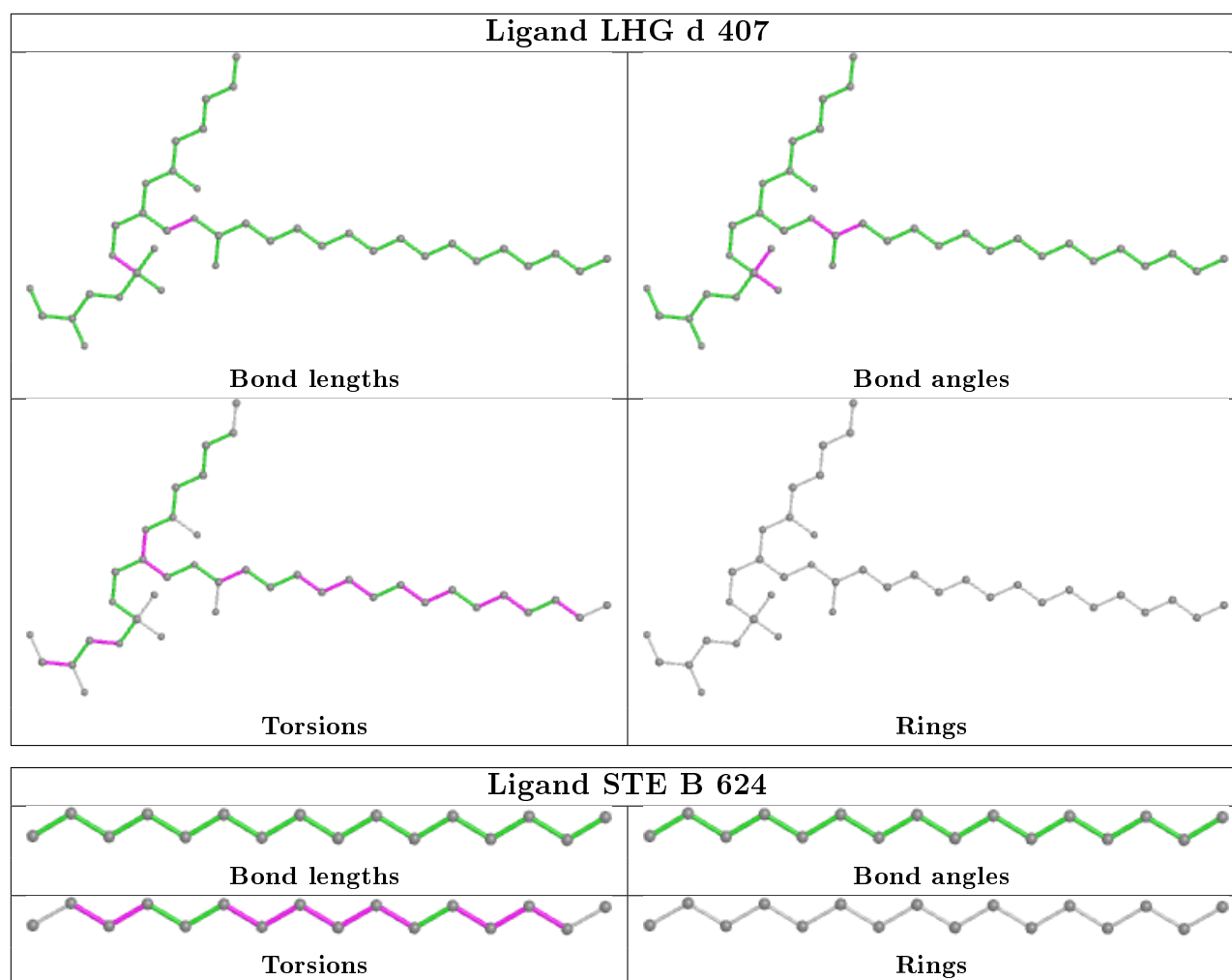


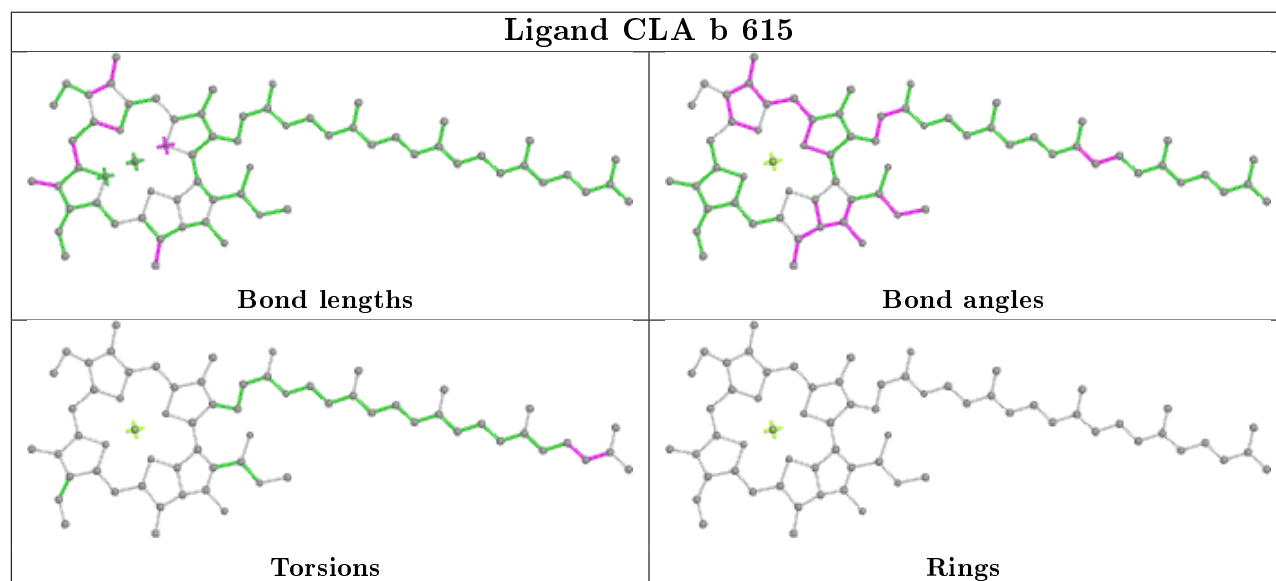
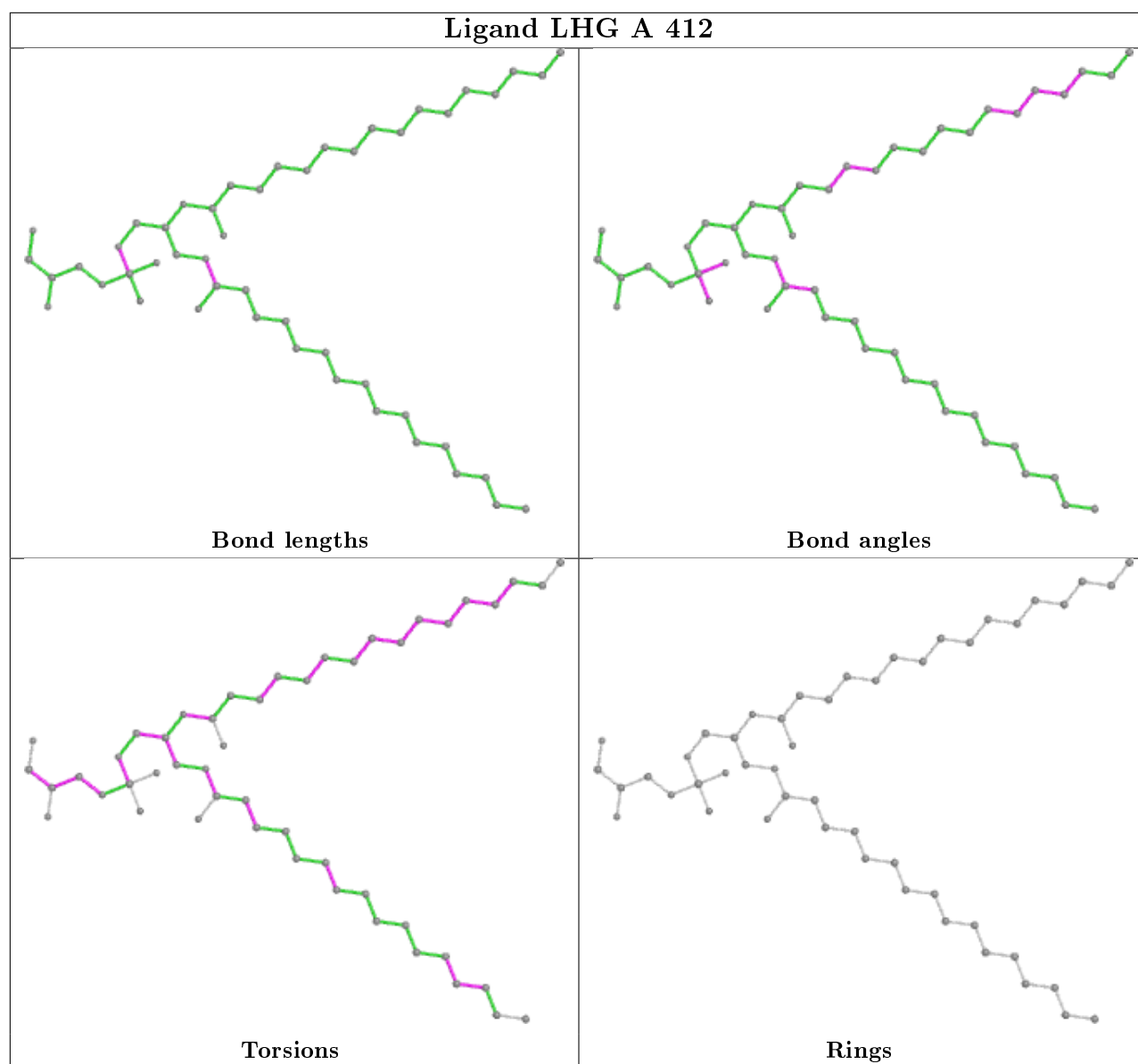
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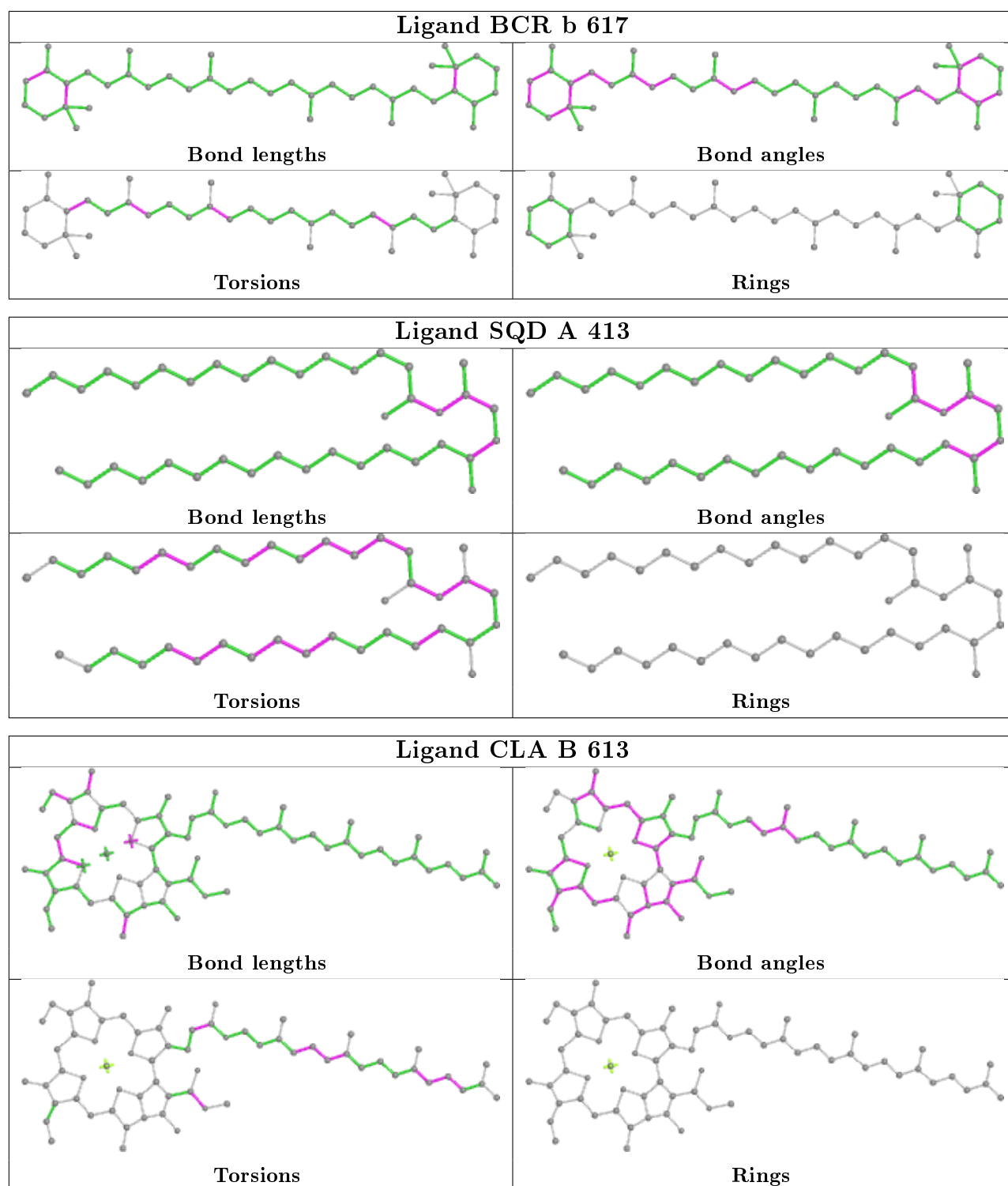


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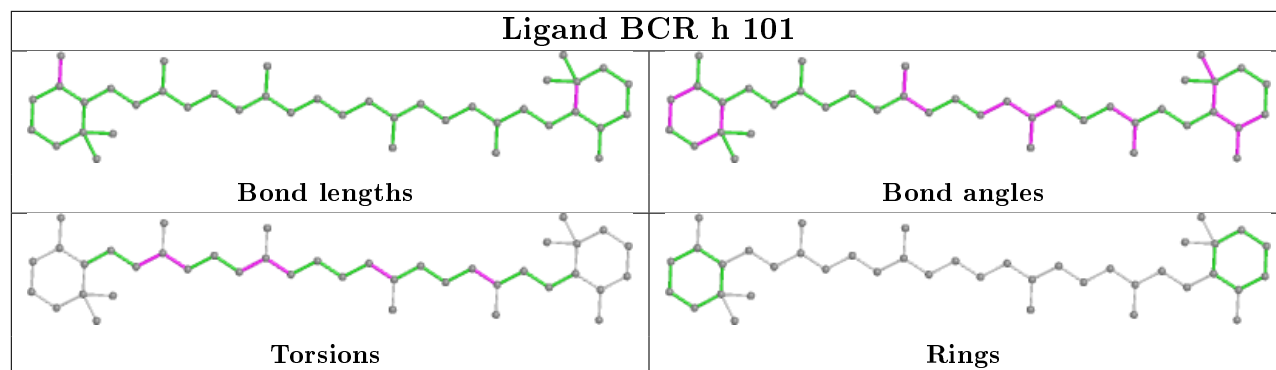




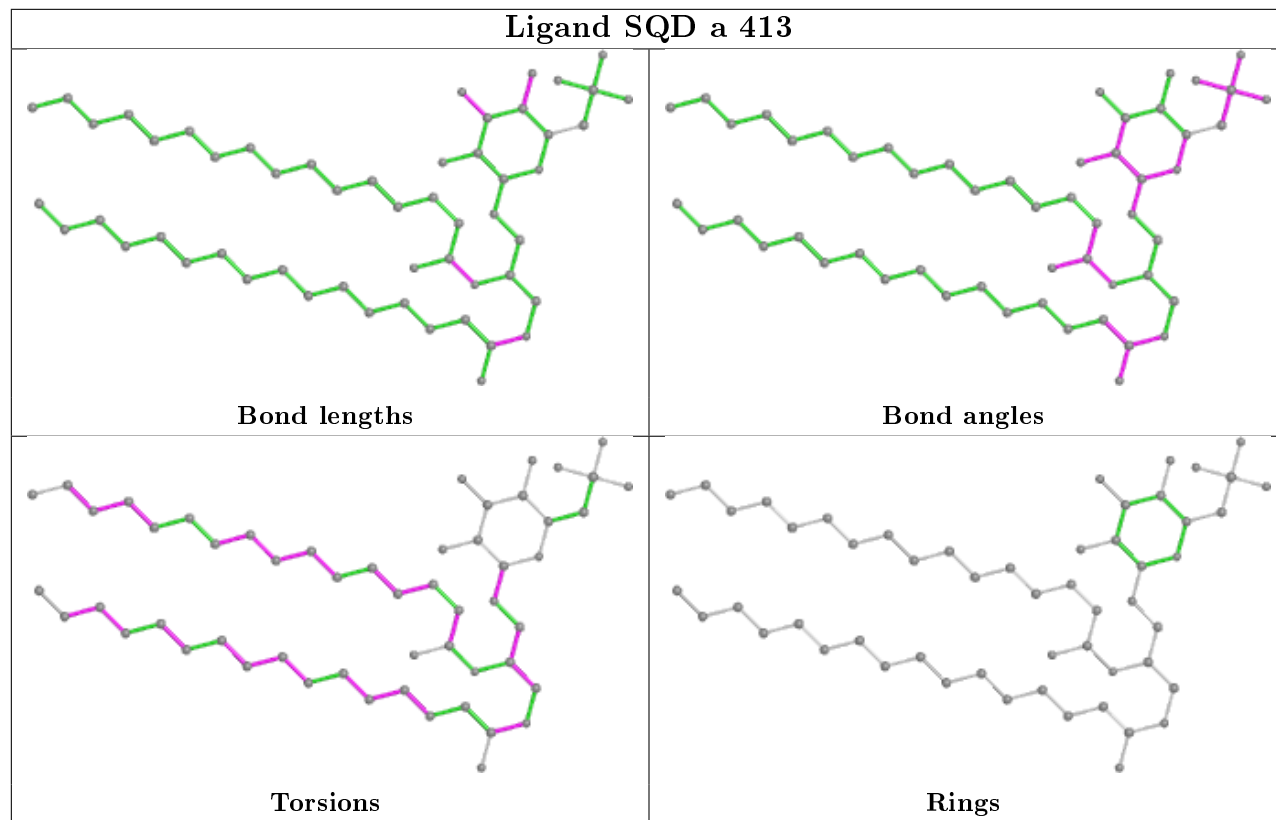


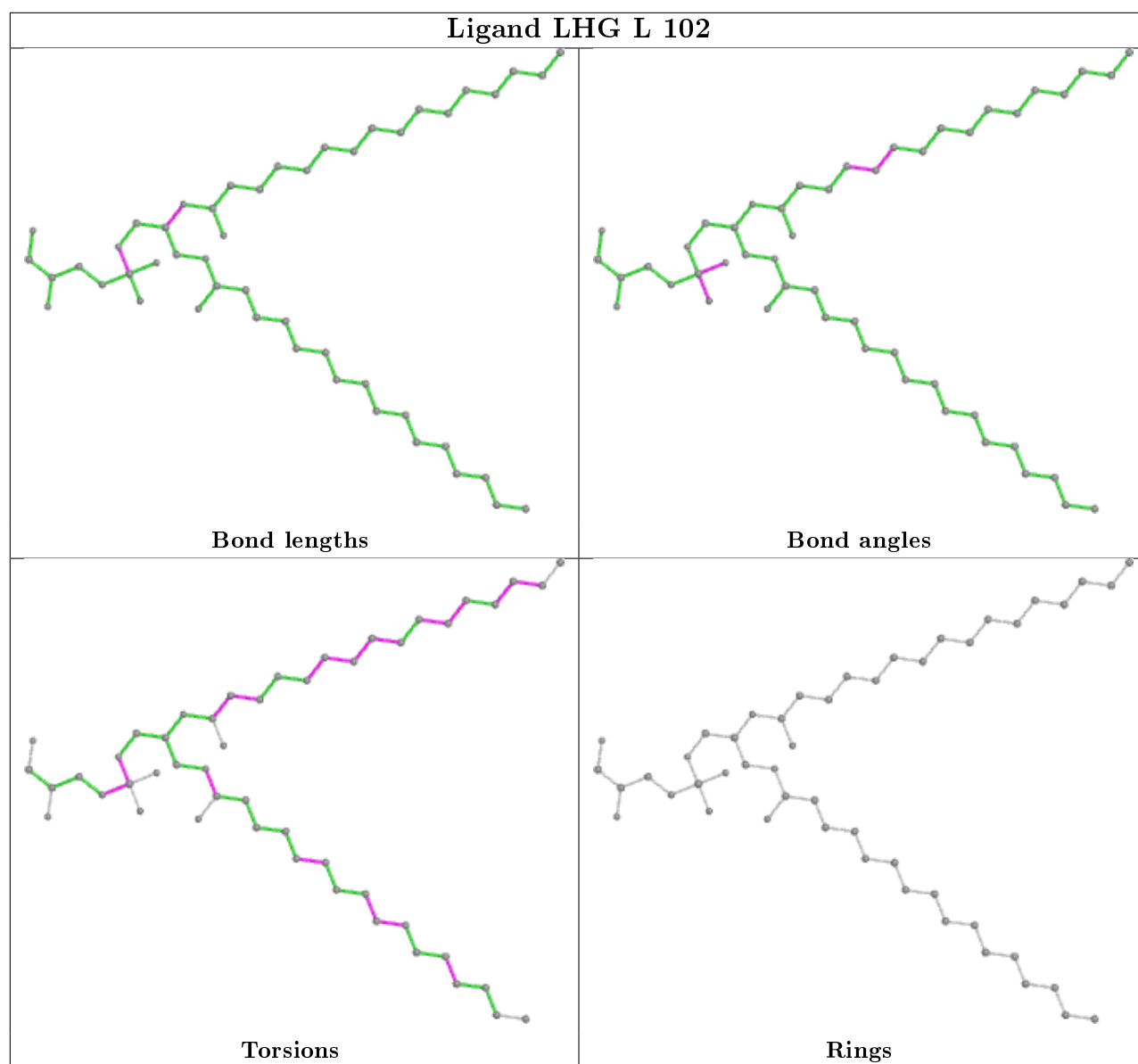


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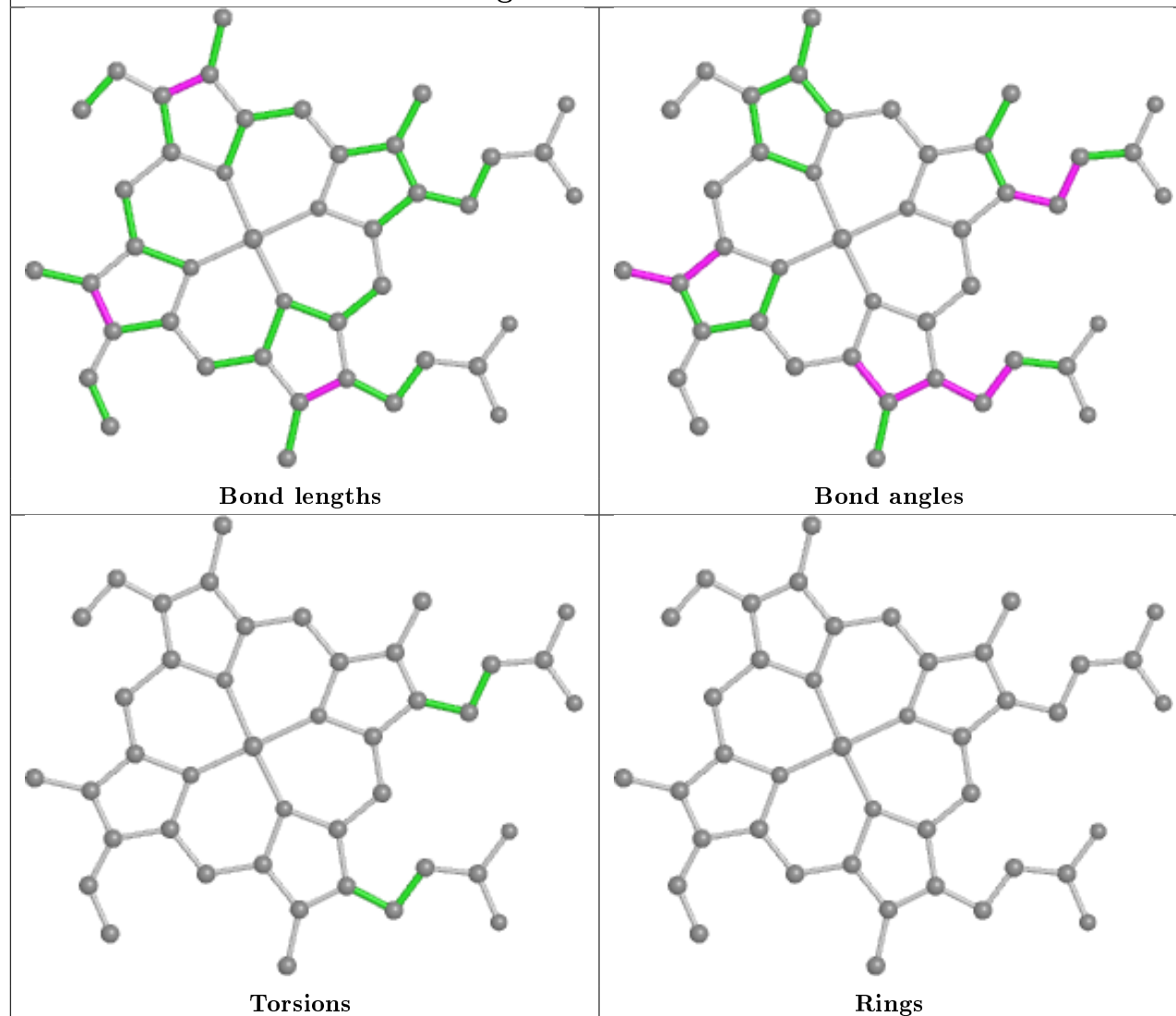


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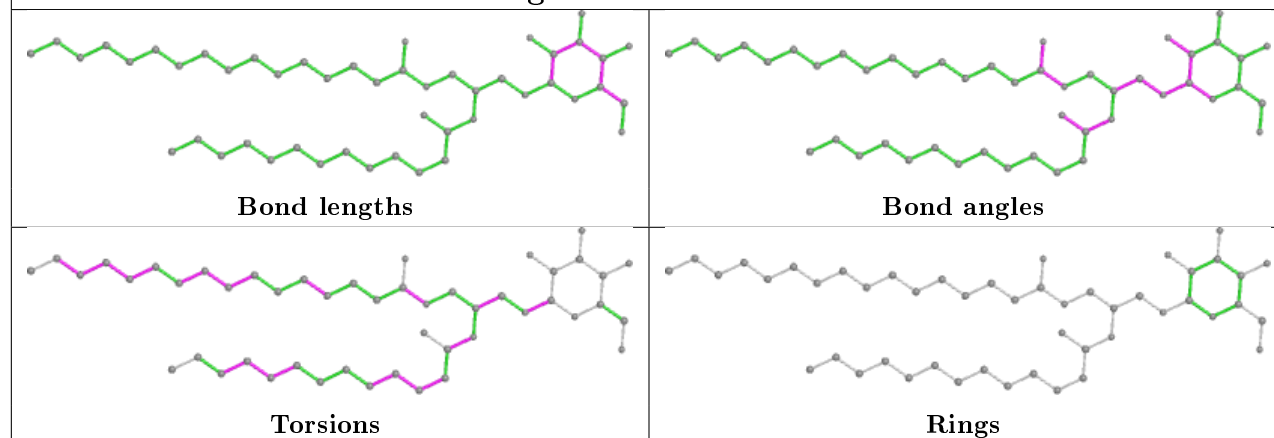


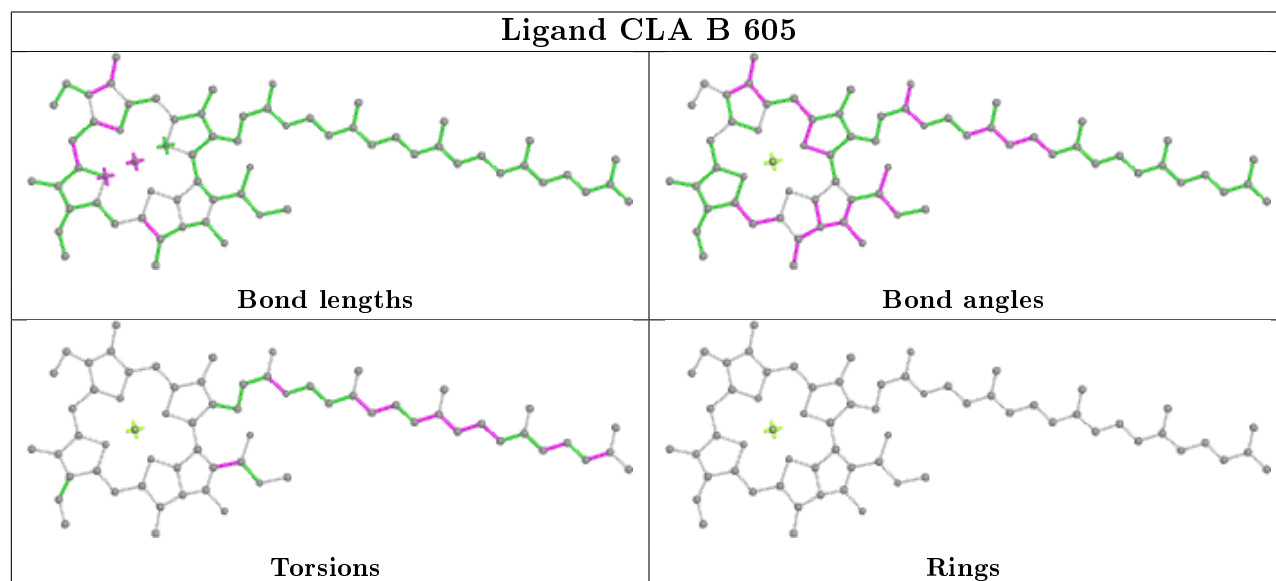
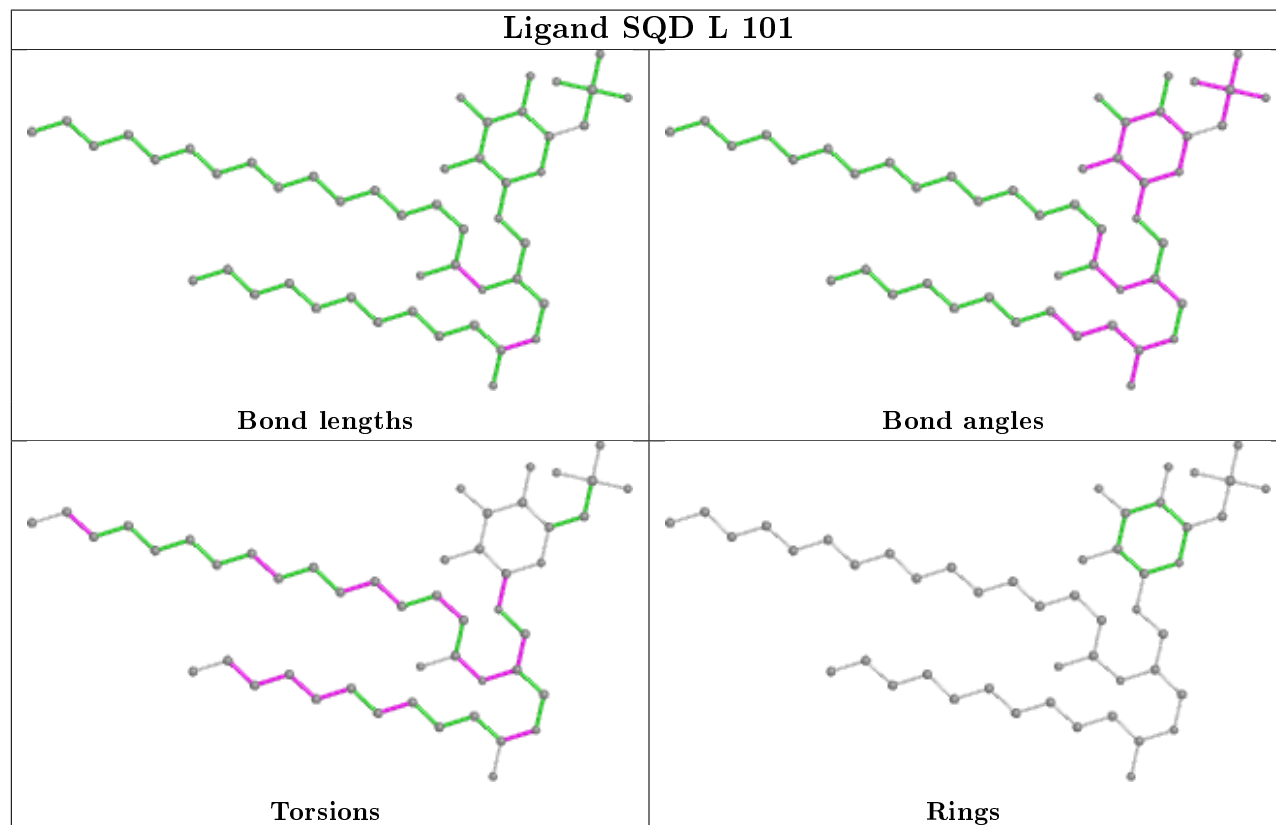
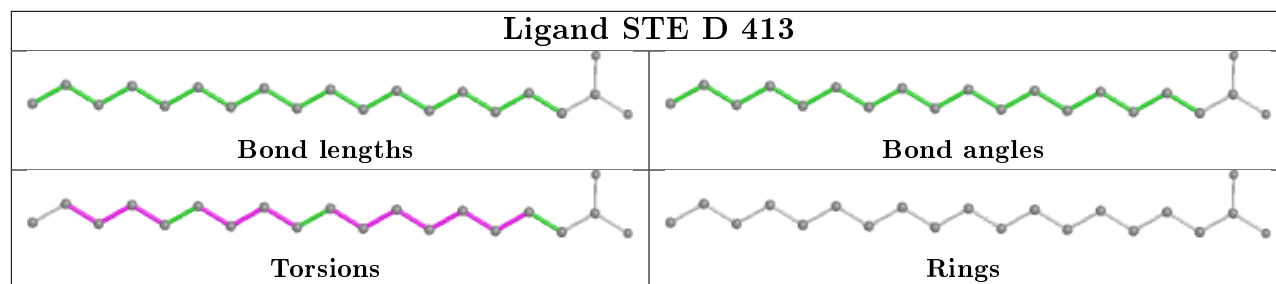


Ligand HEC f 101

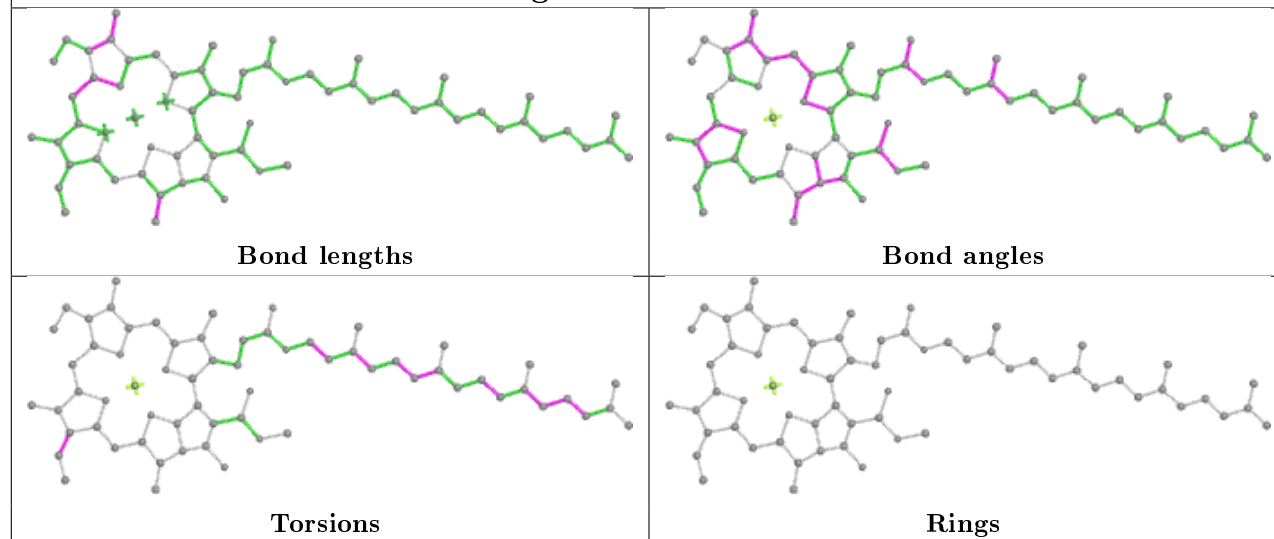


Ligand LMG Y 101

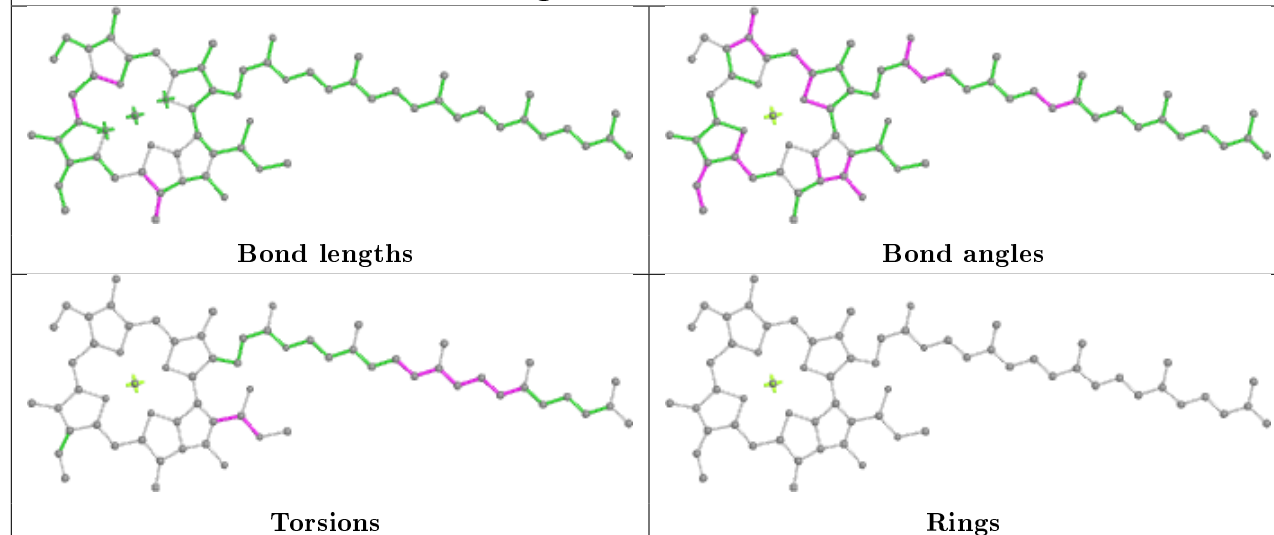




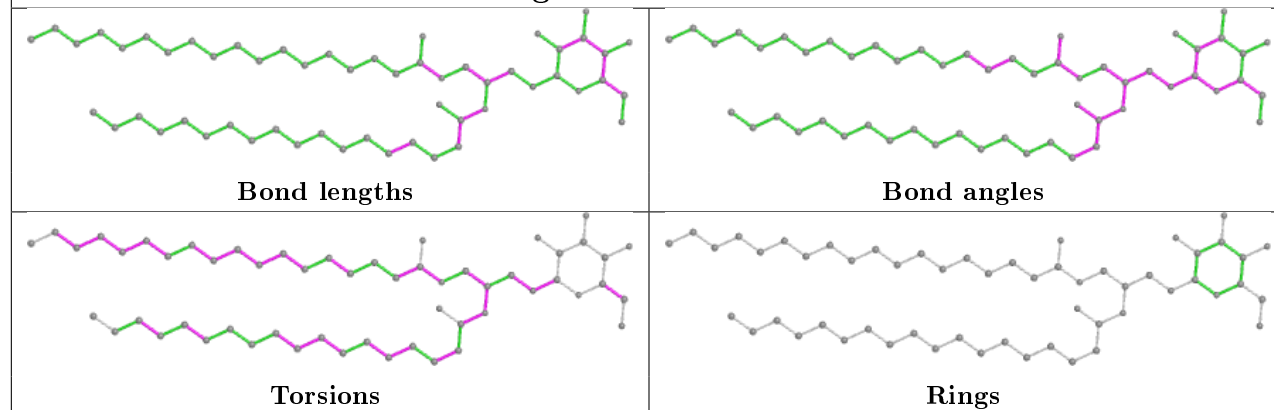
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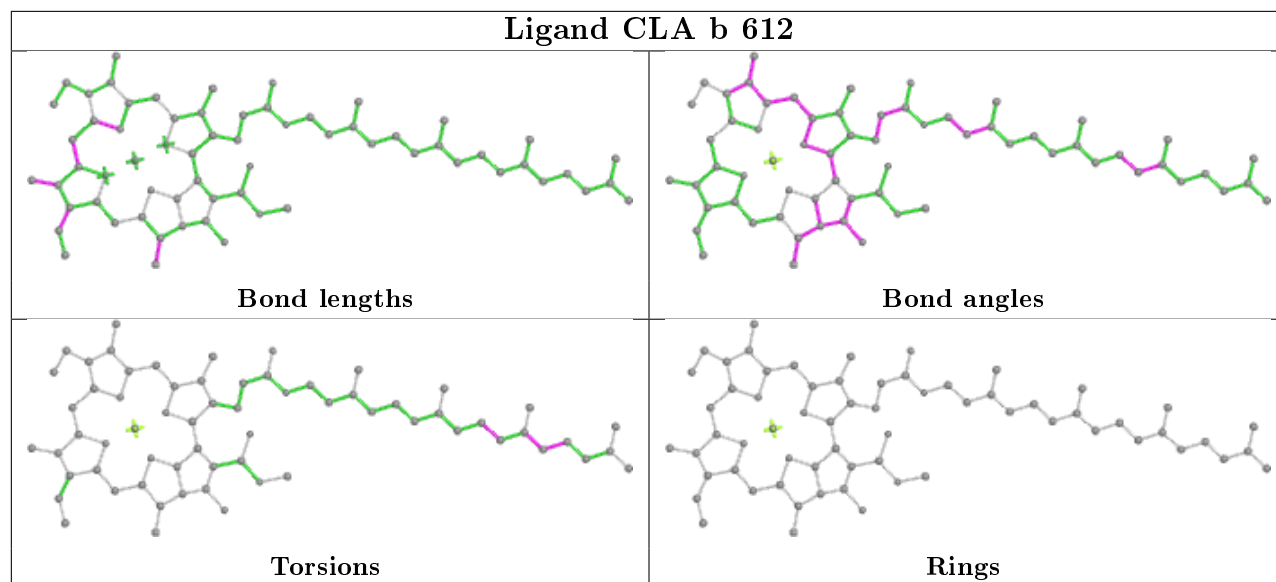
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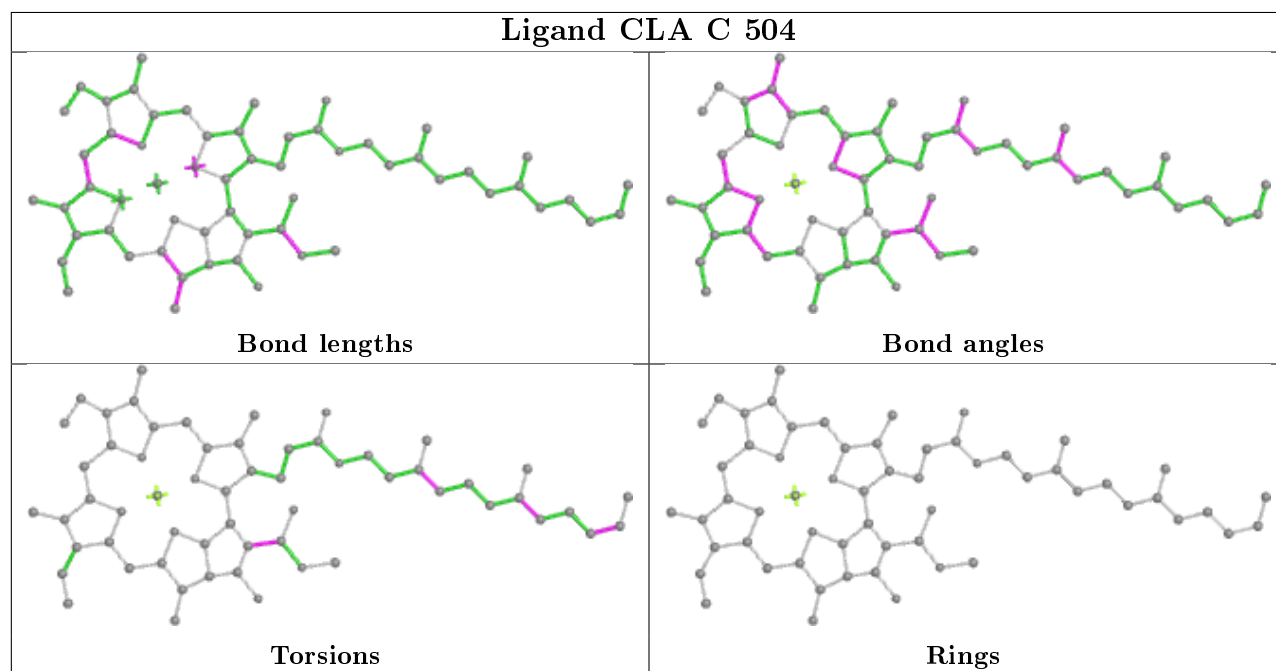
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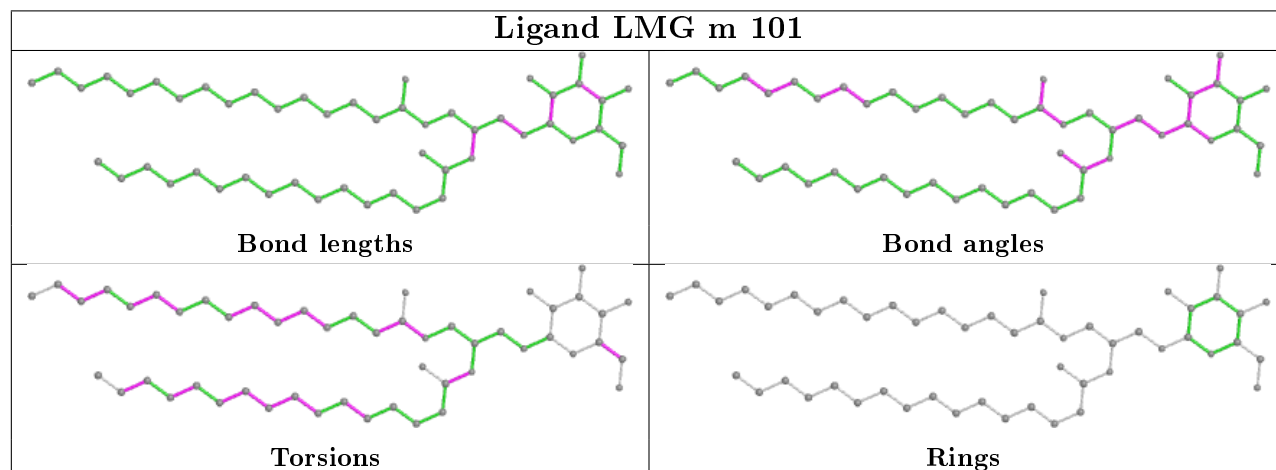
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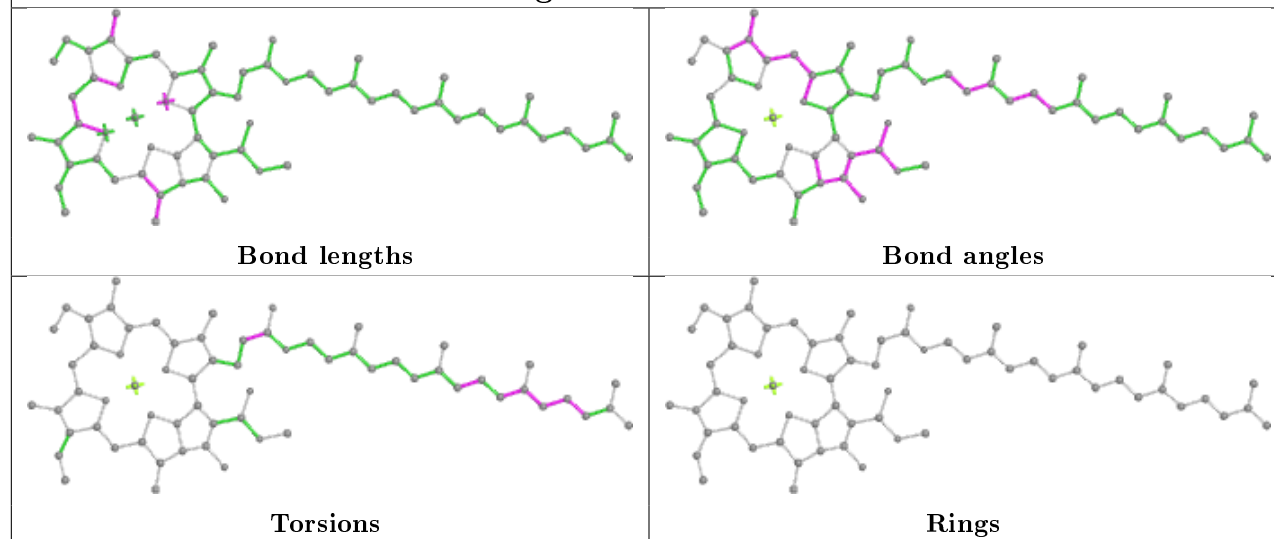
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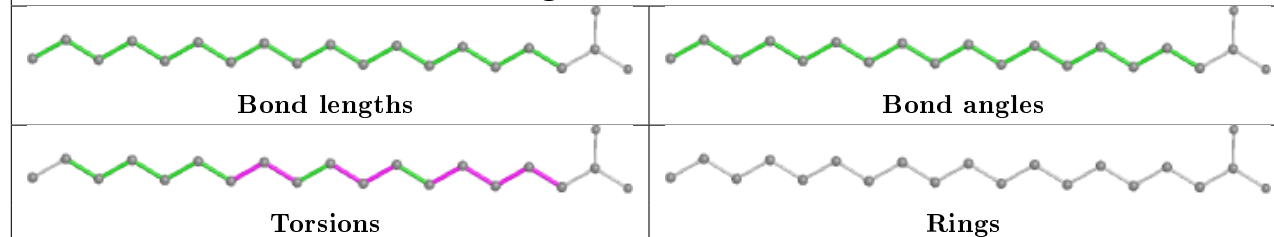
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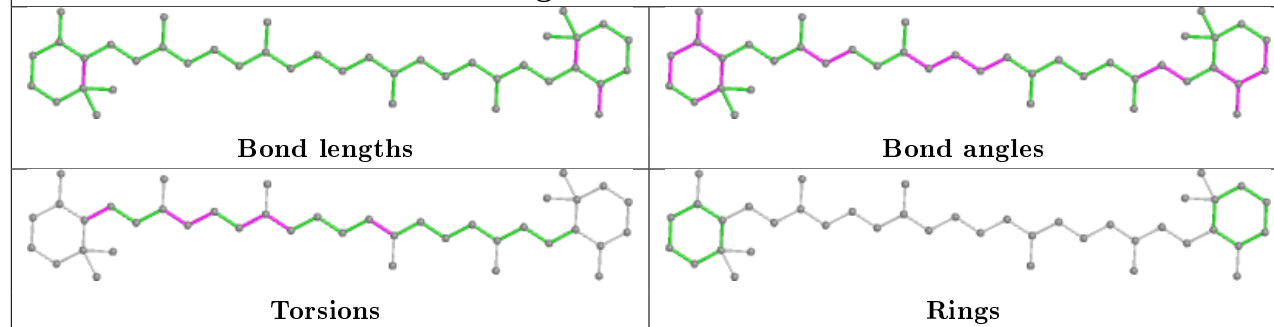
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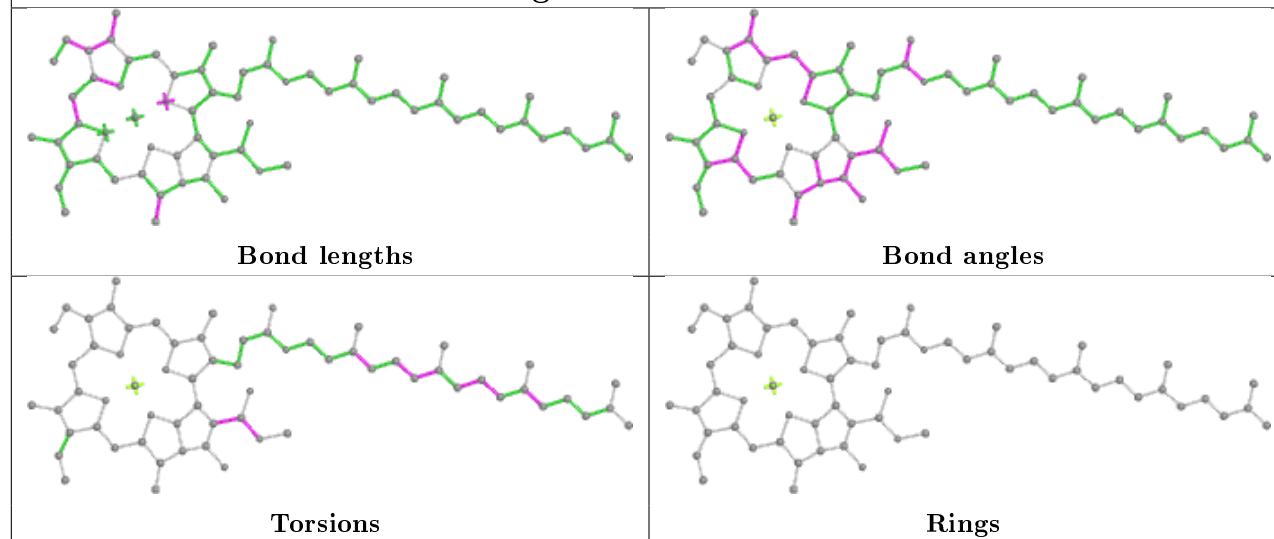
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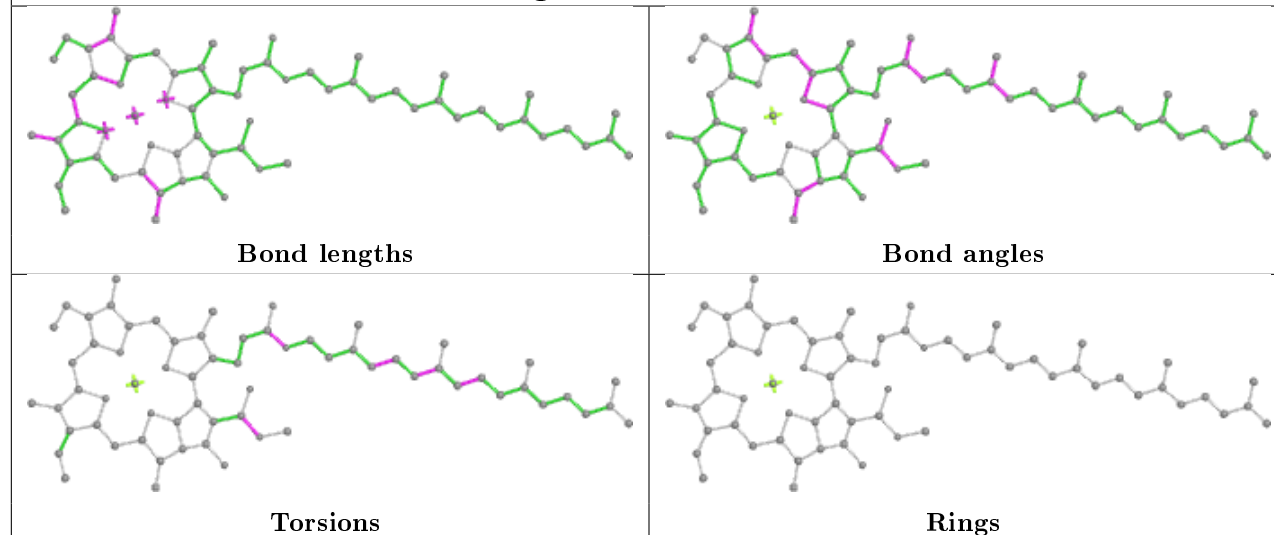
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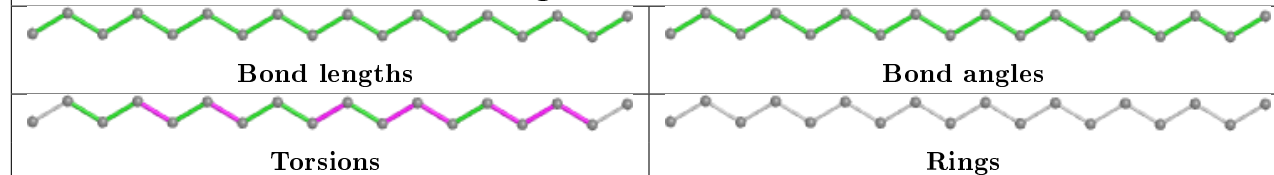
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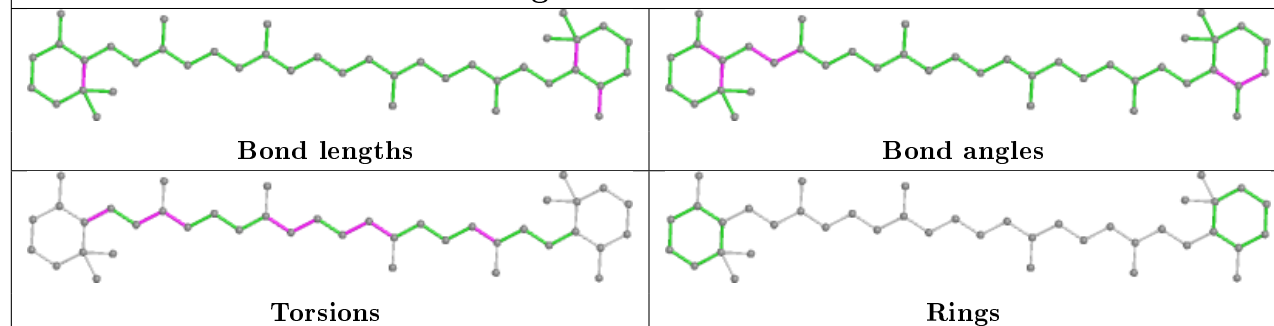
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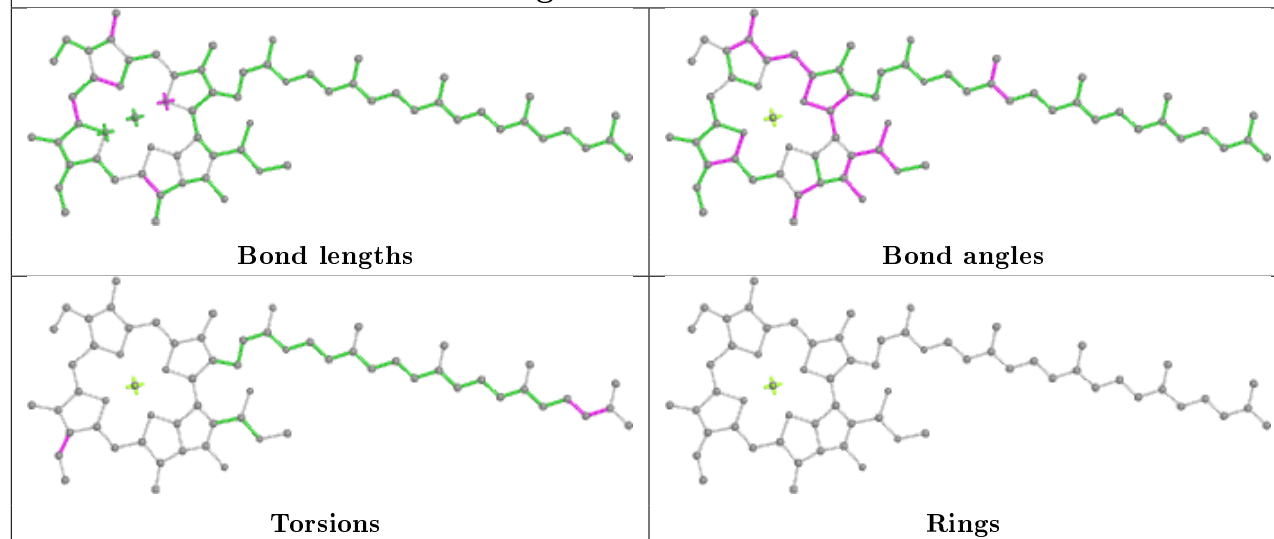
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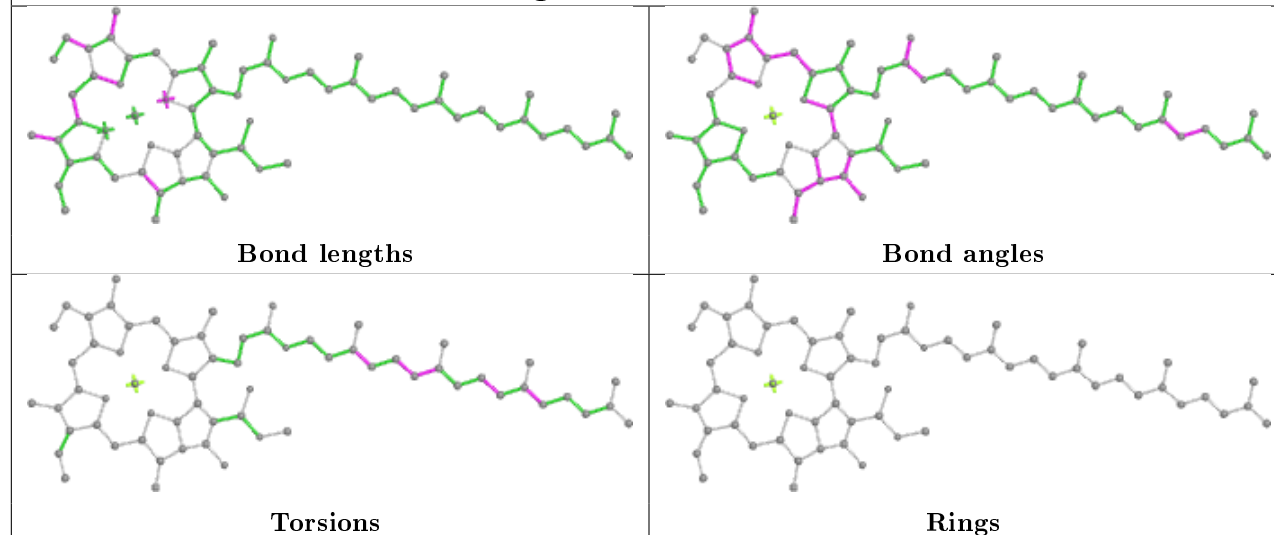
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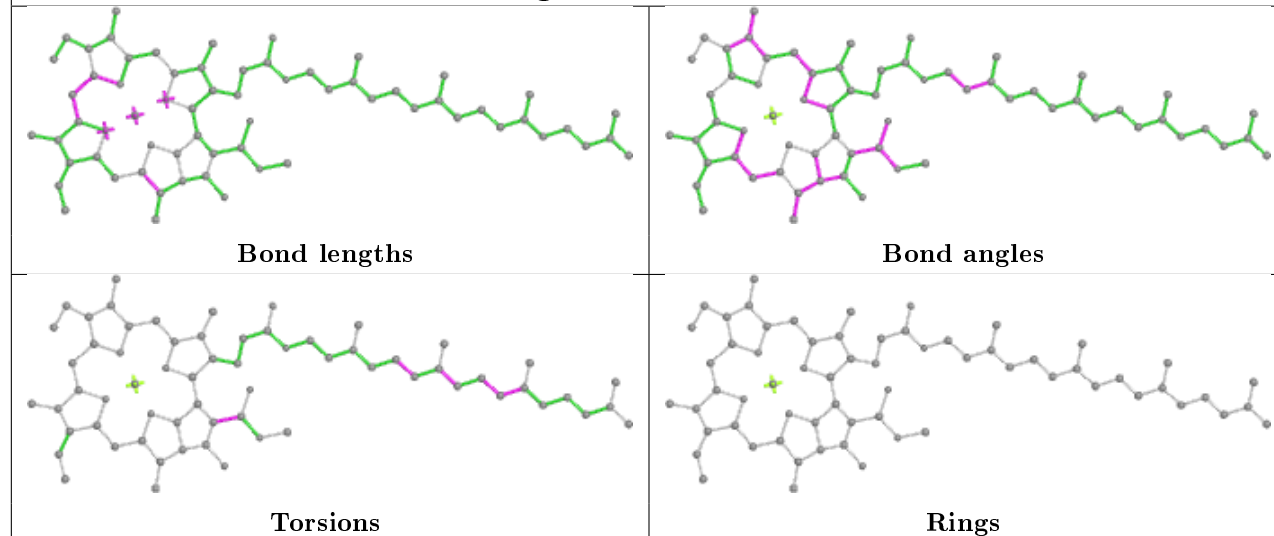
Ligand CLA a 402

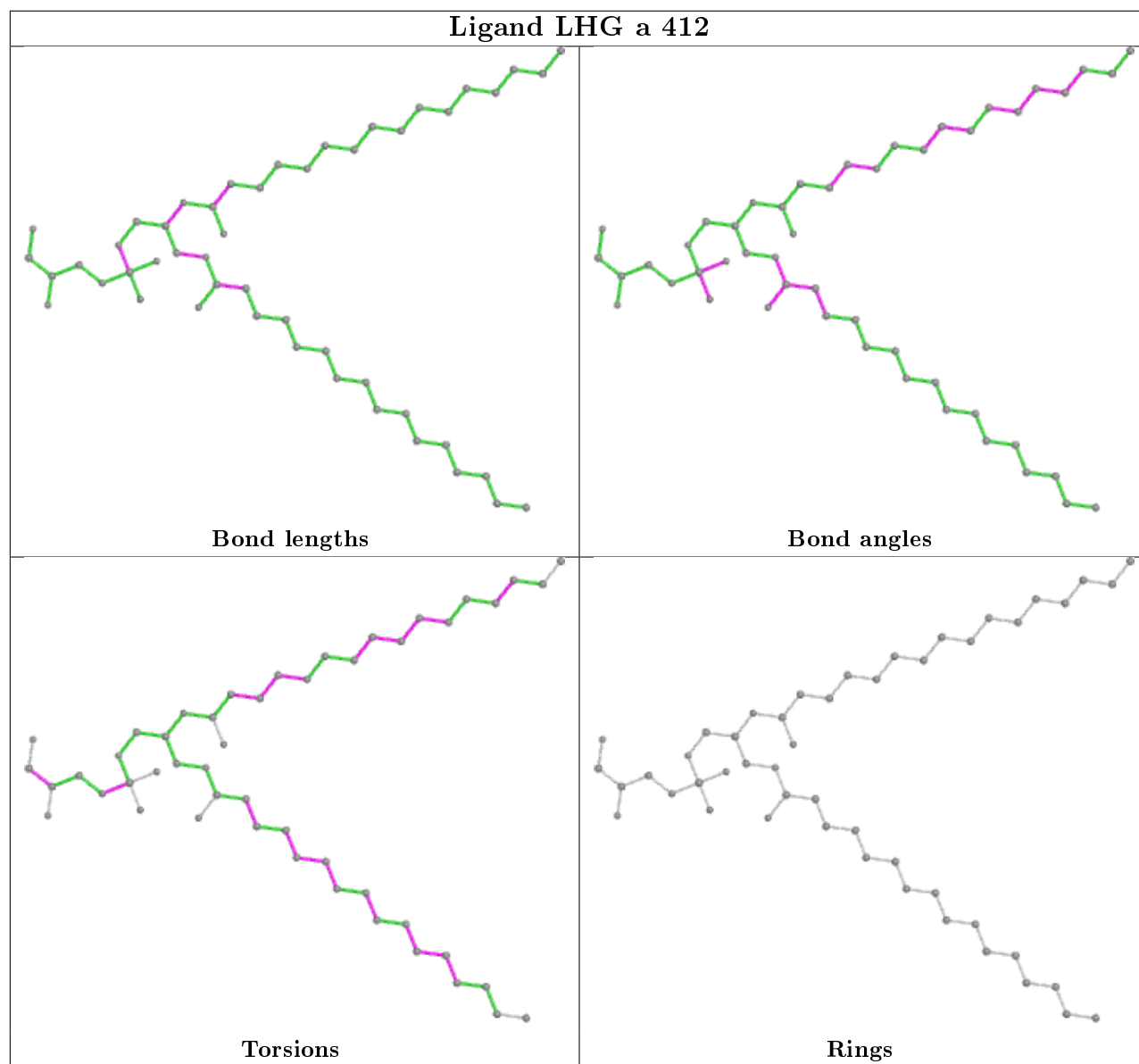
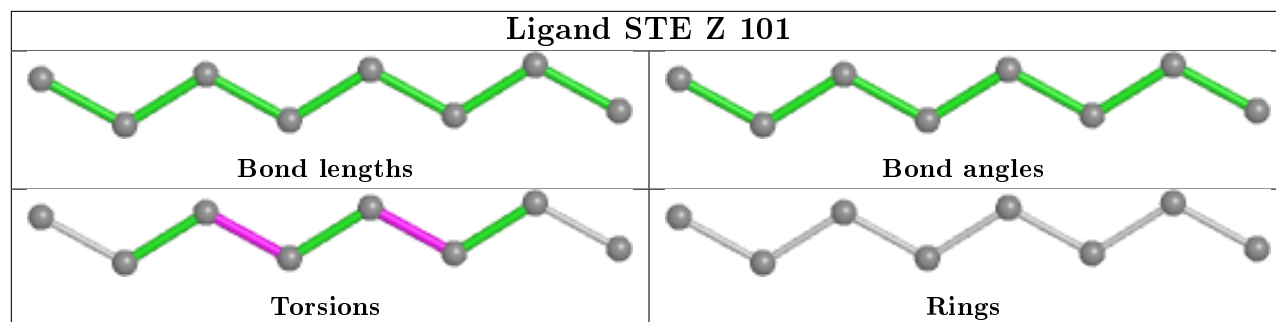


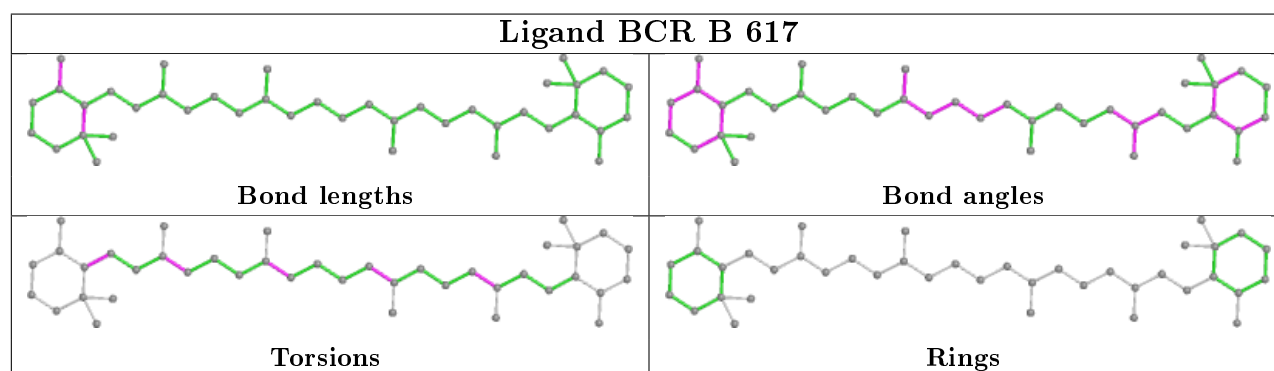
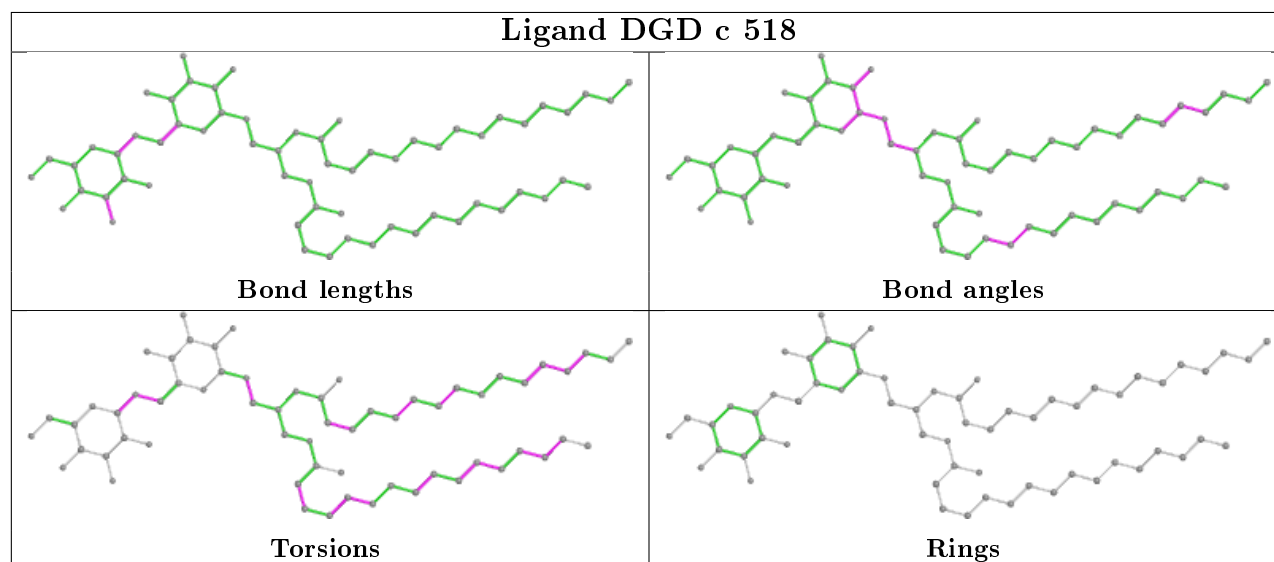
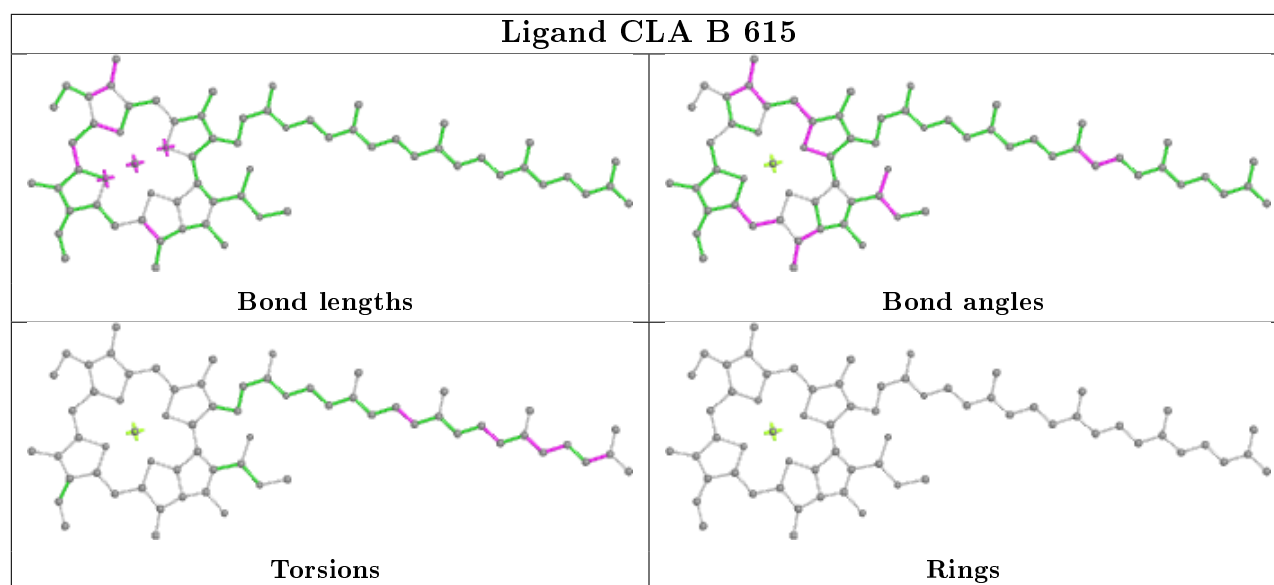
Ligand CLA C 505

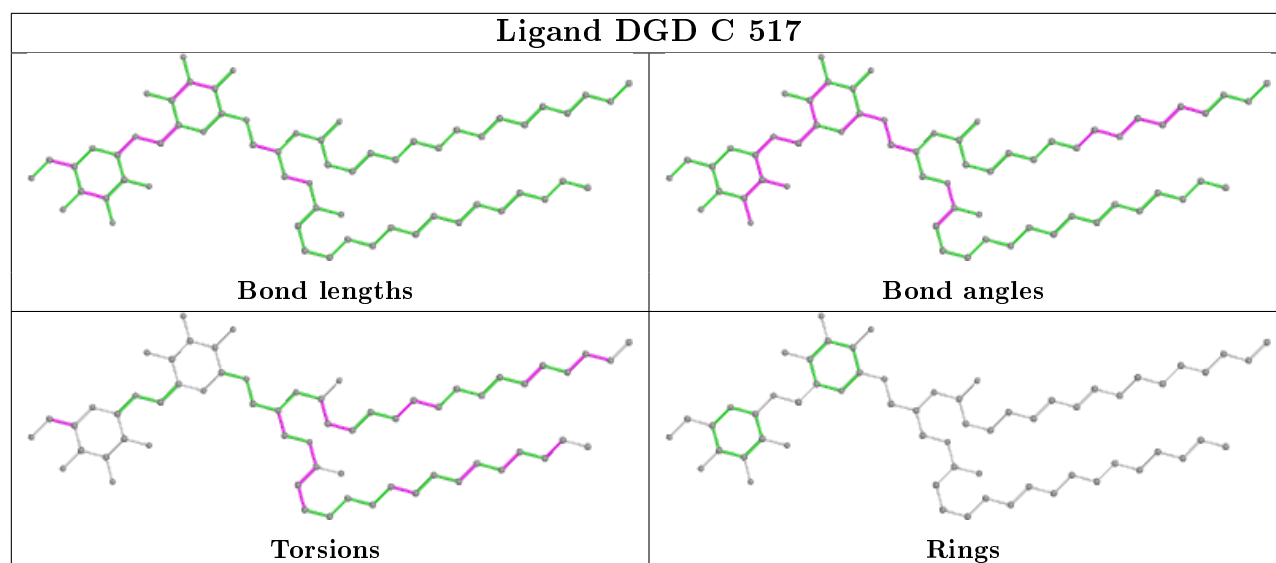
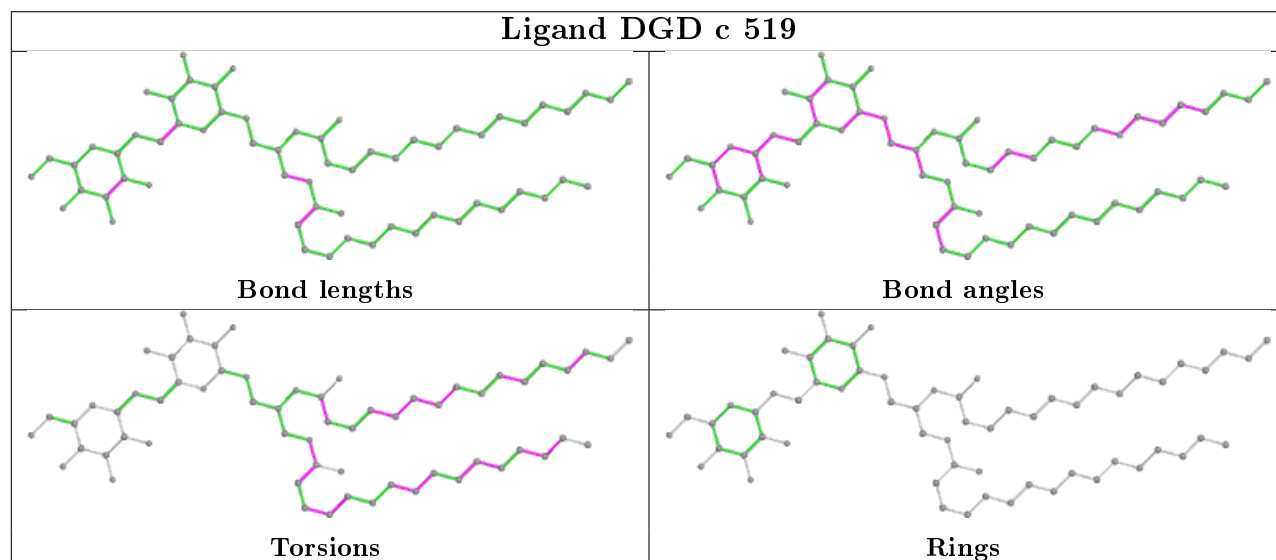
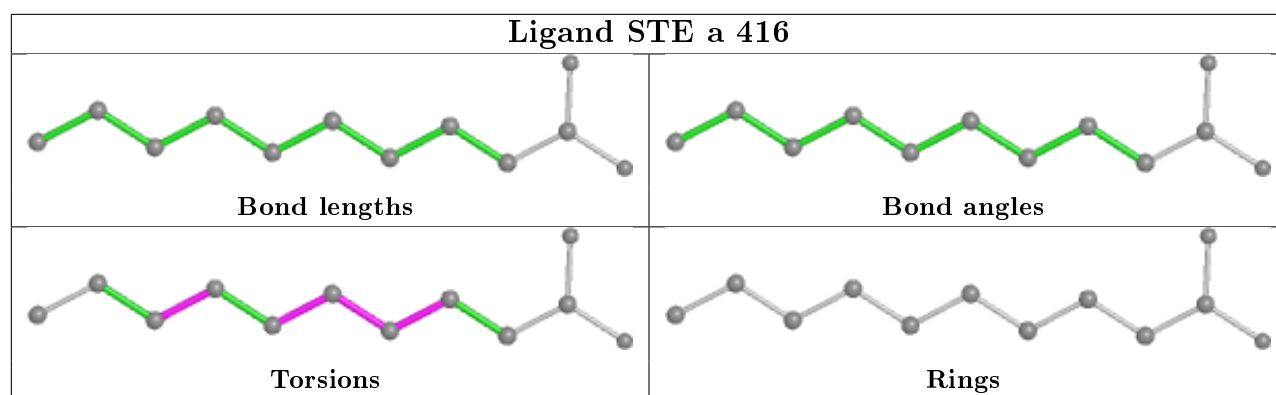


Ligand CLA b 605

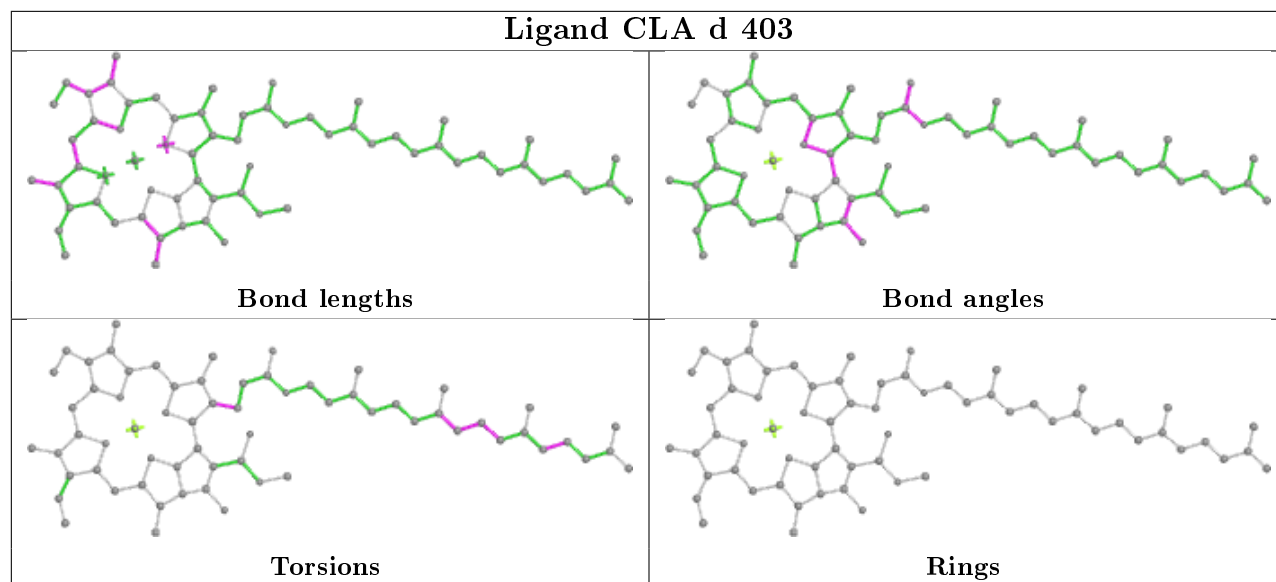




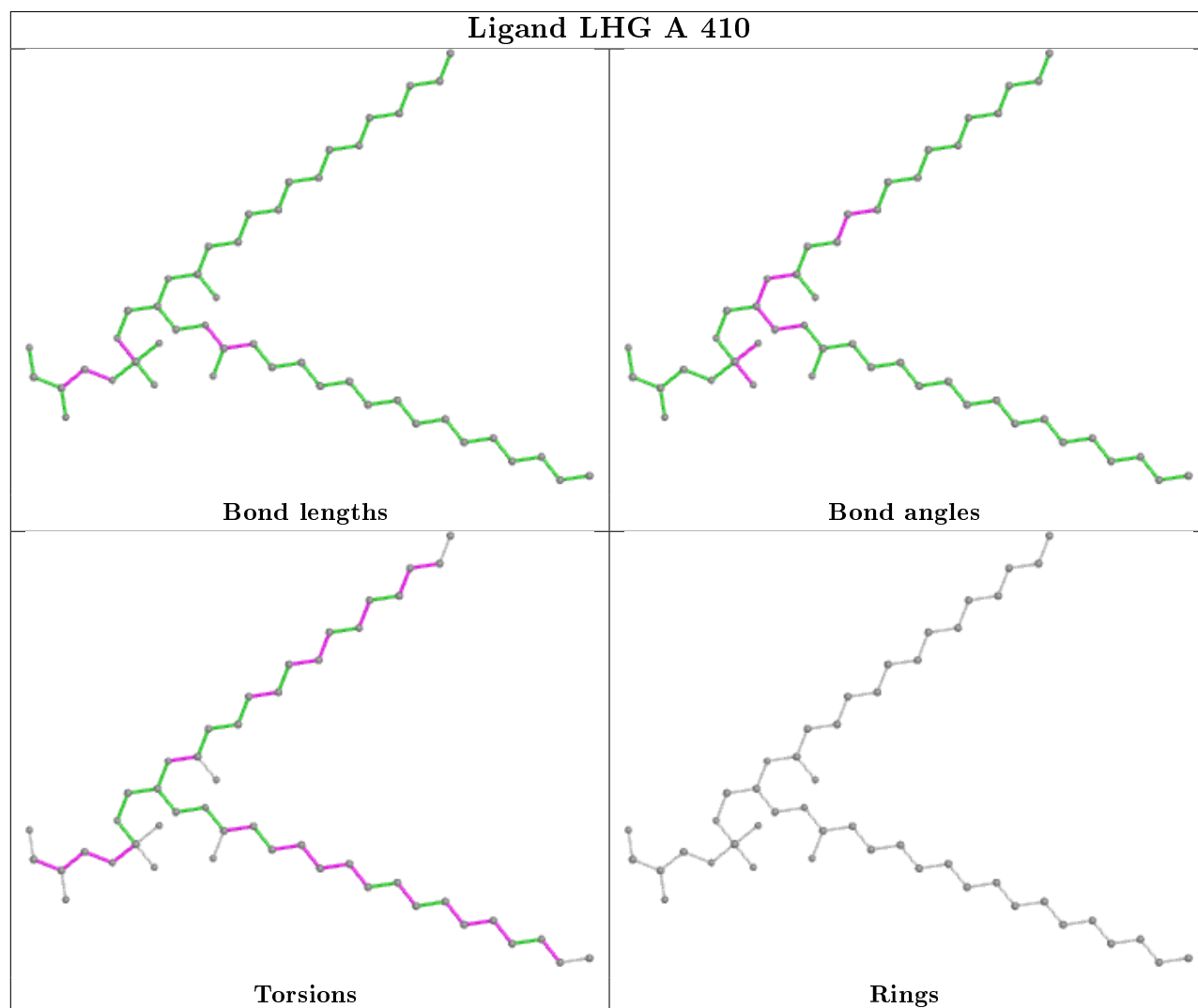


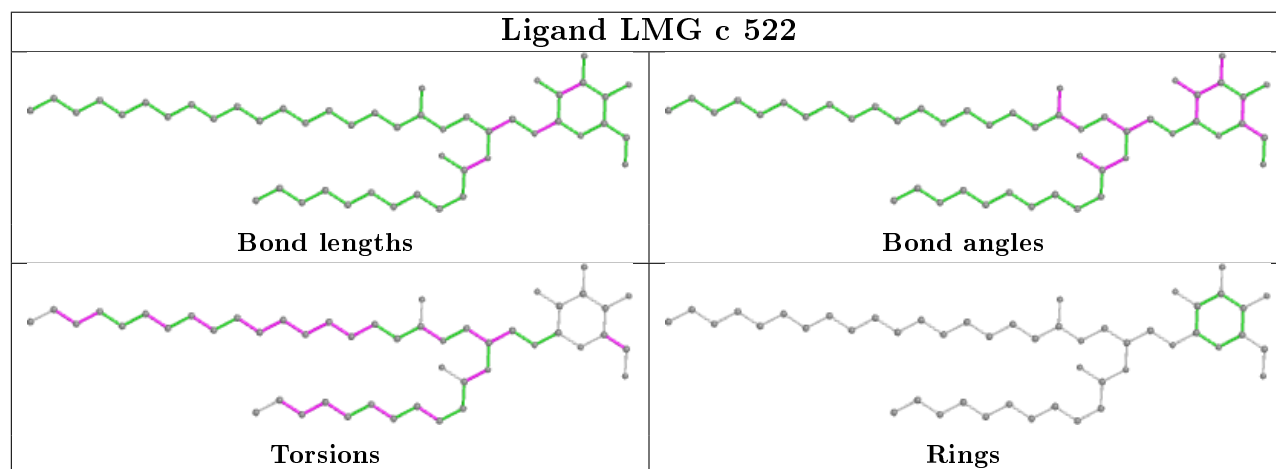
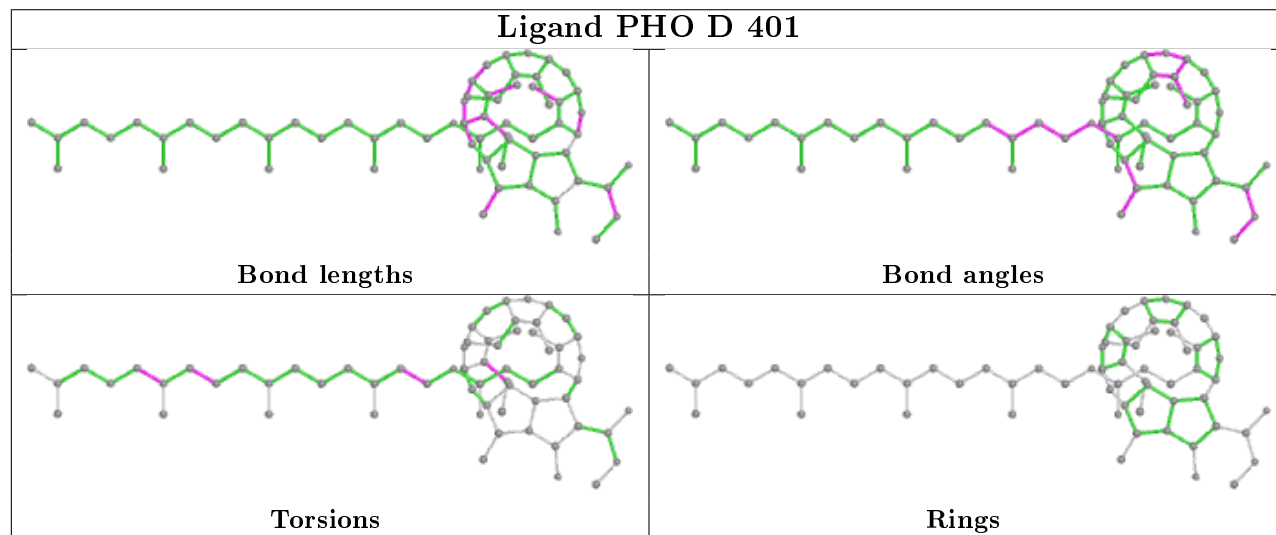
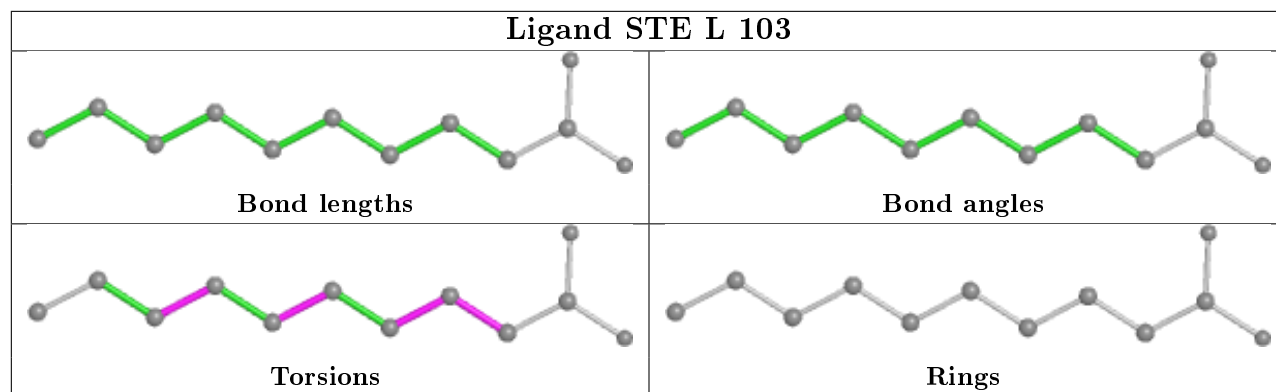


Ligand CLA d 403

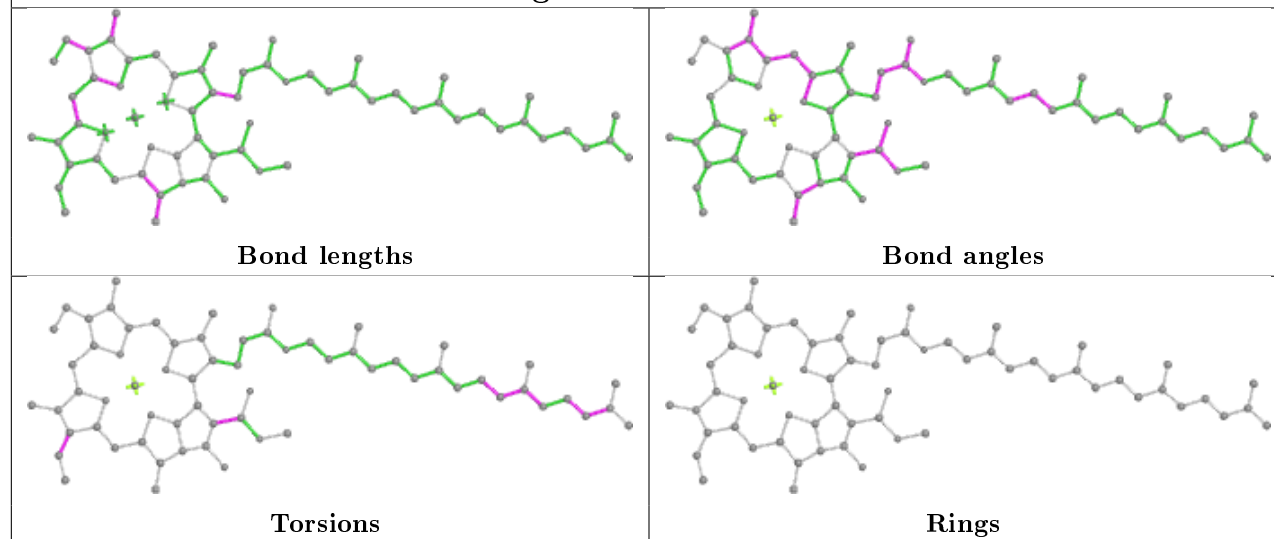


Ligand LHG A 410

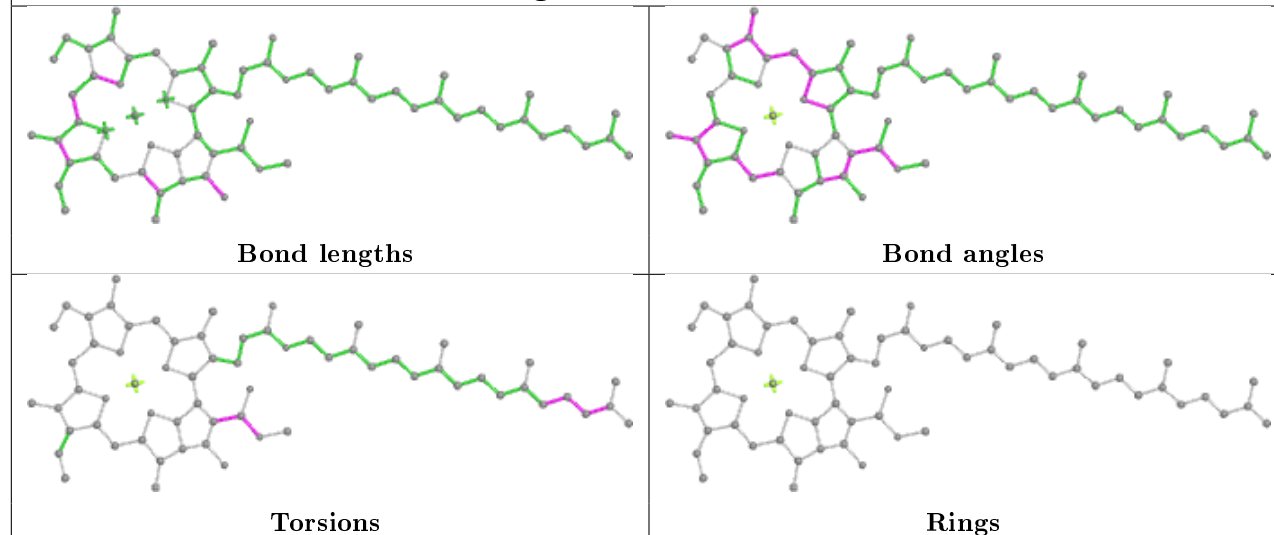




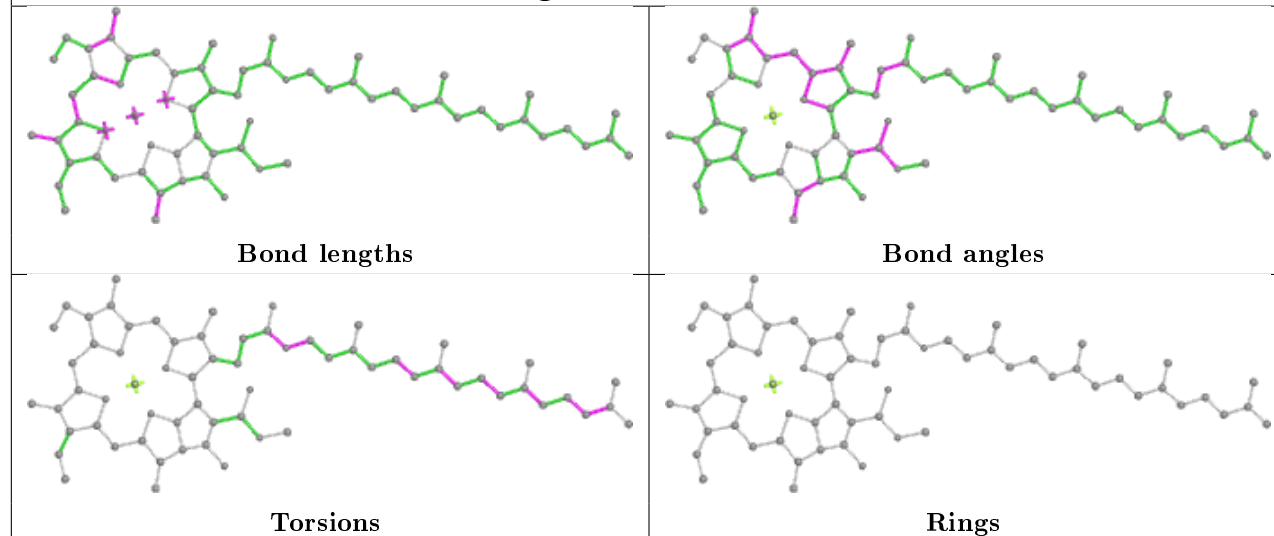
Ligand CLA A 403

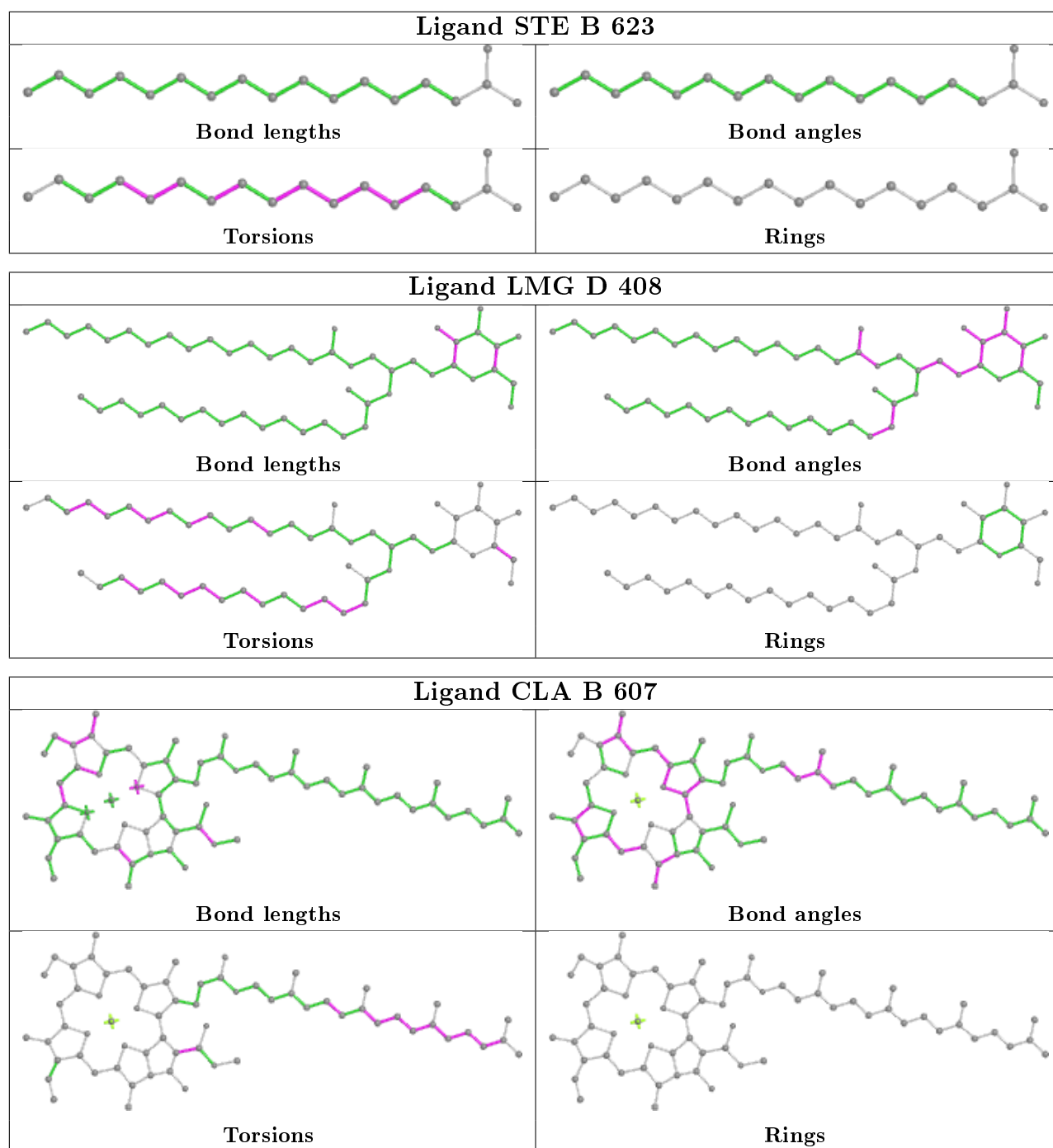


Ligand CLA A 409

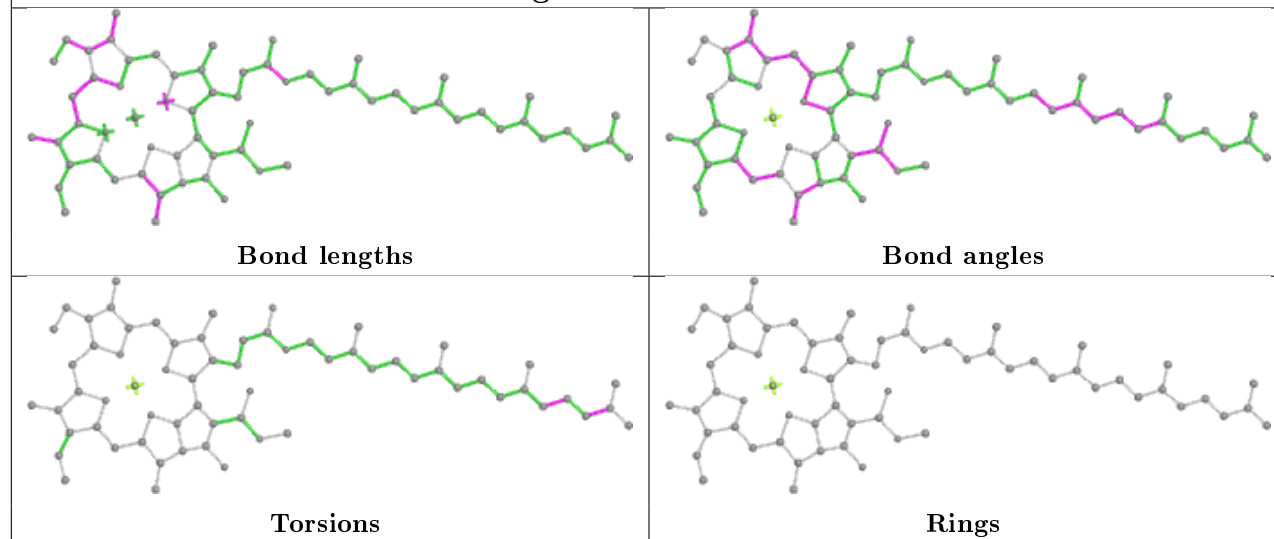


Ligand CLA a 405

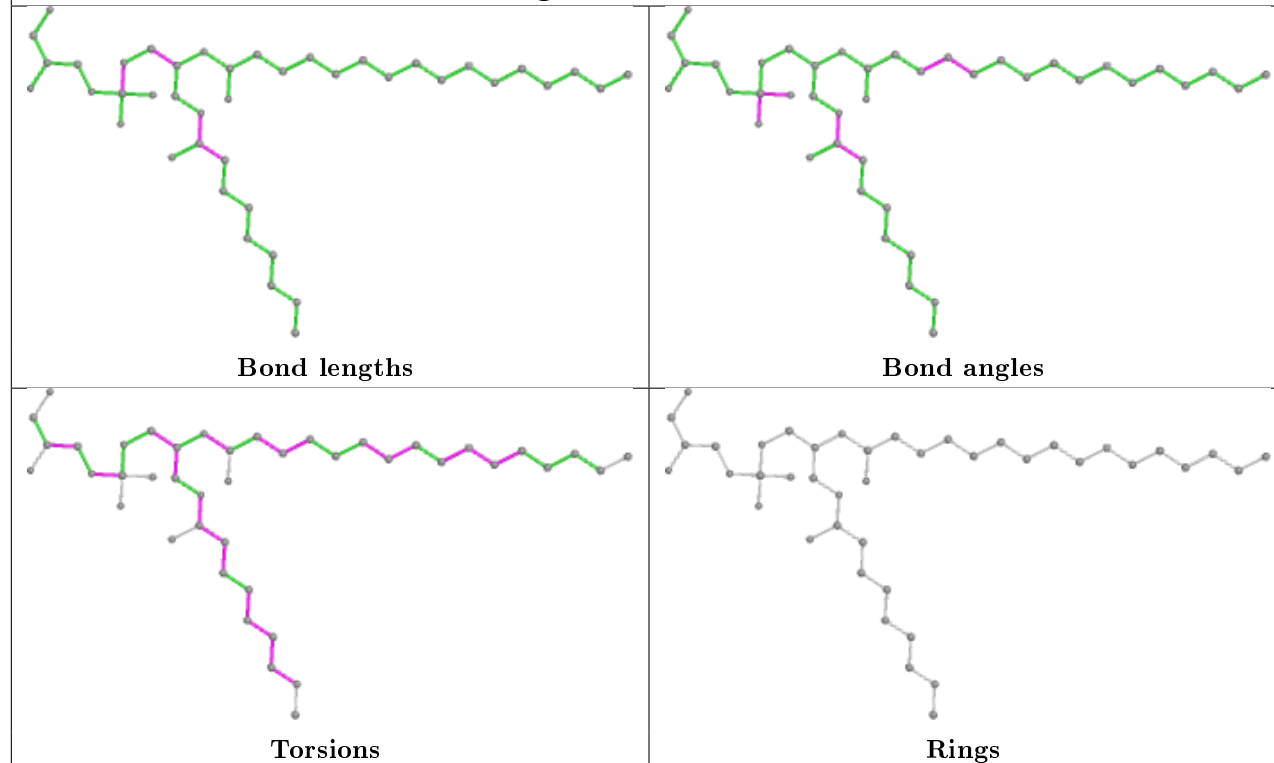




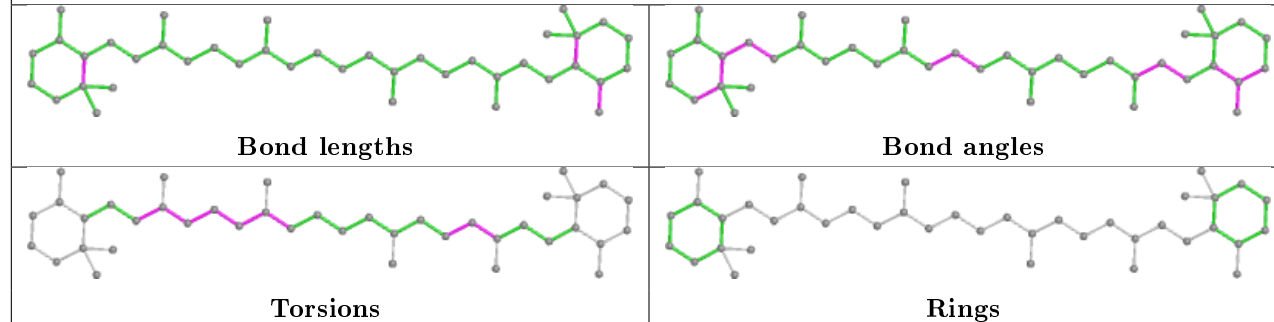
Ligand CLA B 608

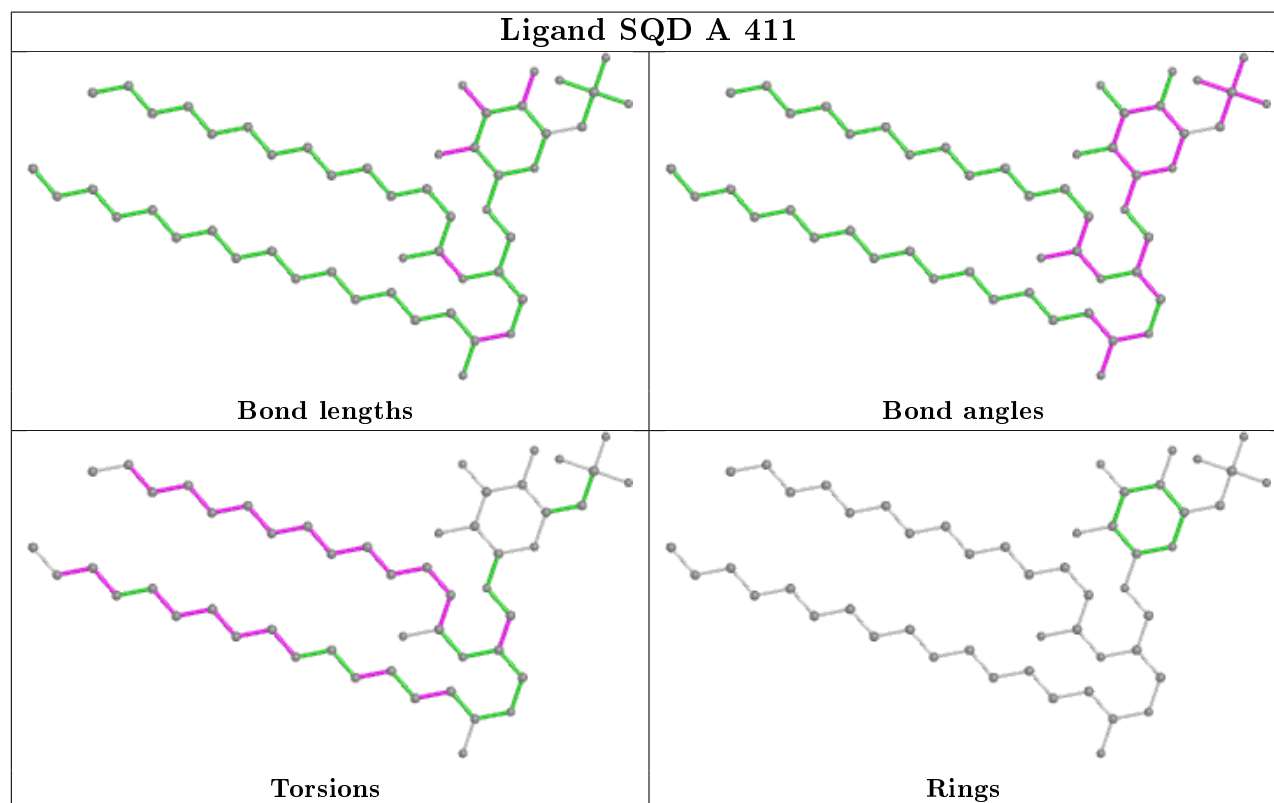
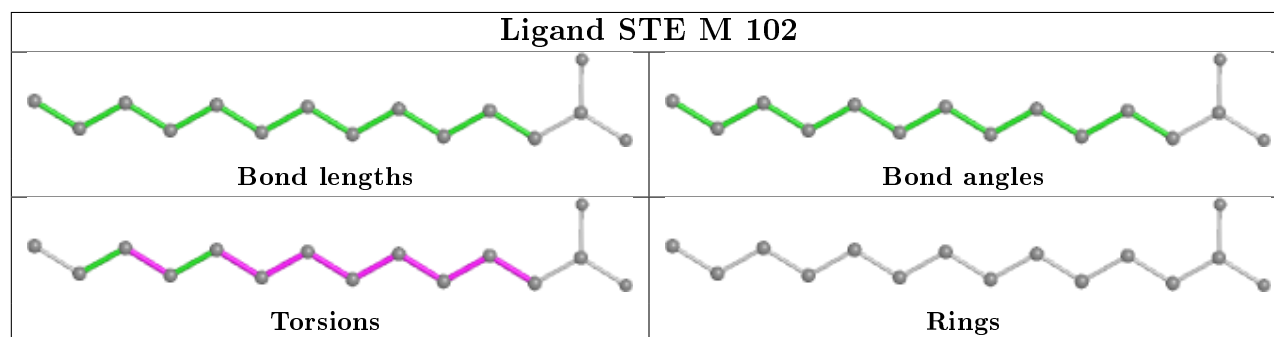
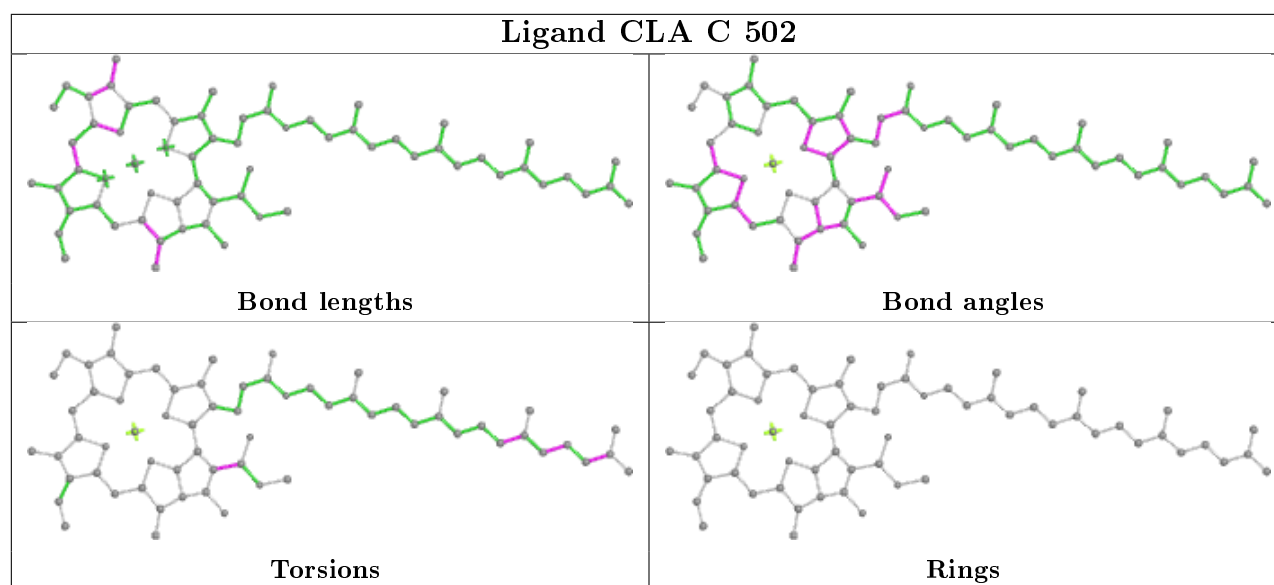


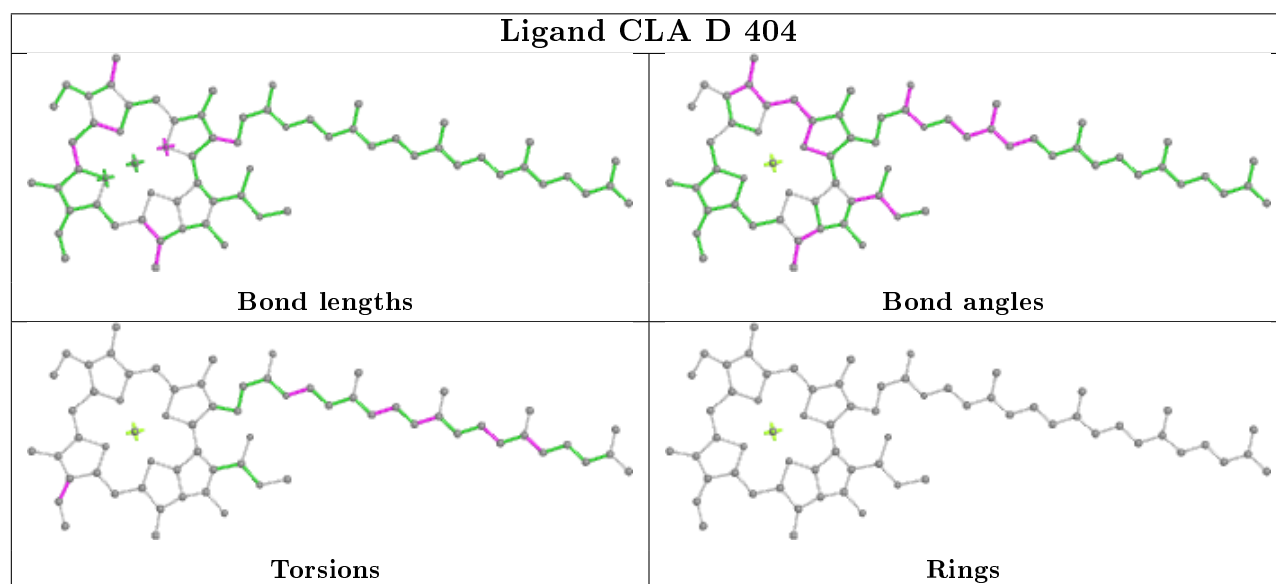
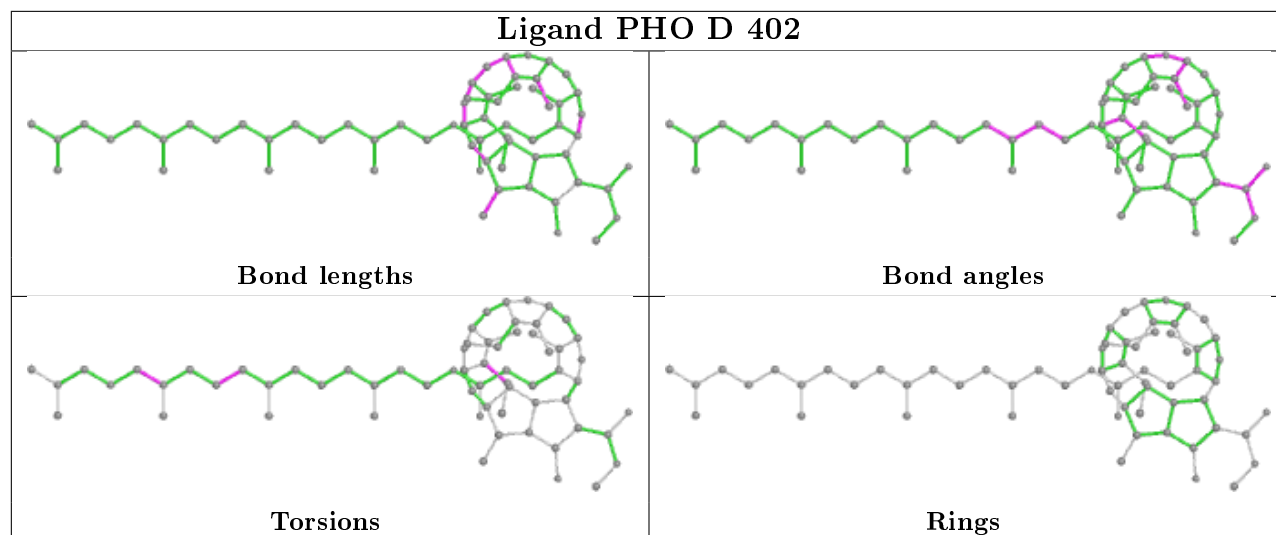
Ligand LHG e 101

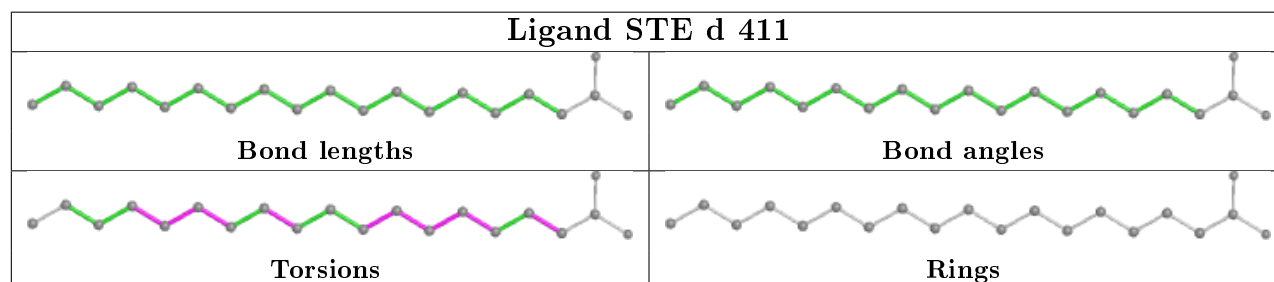
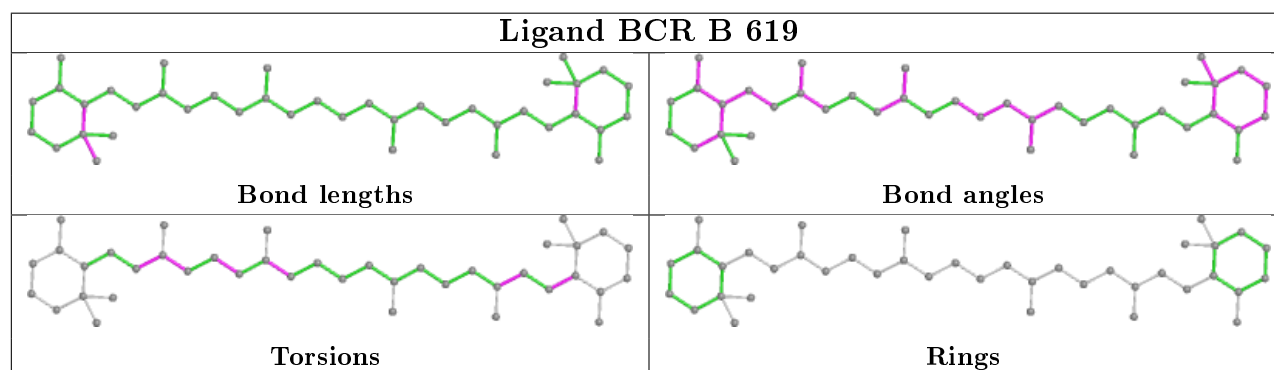
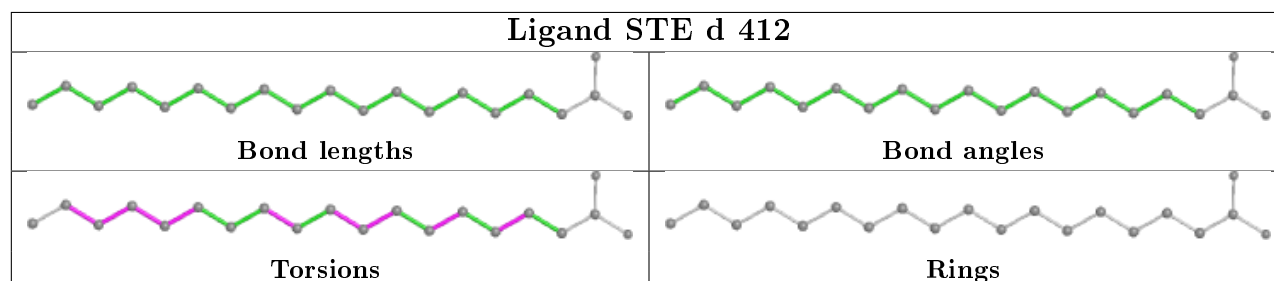
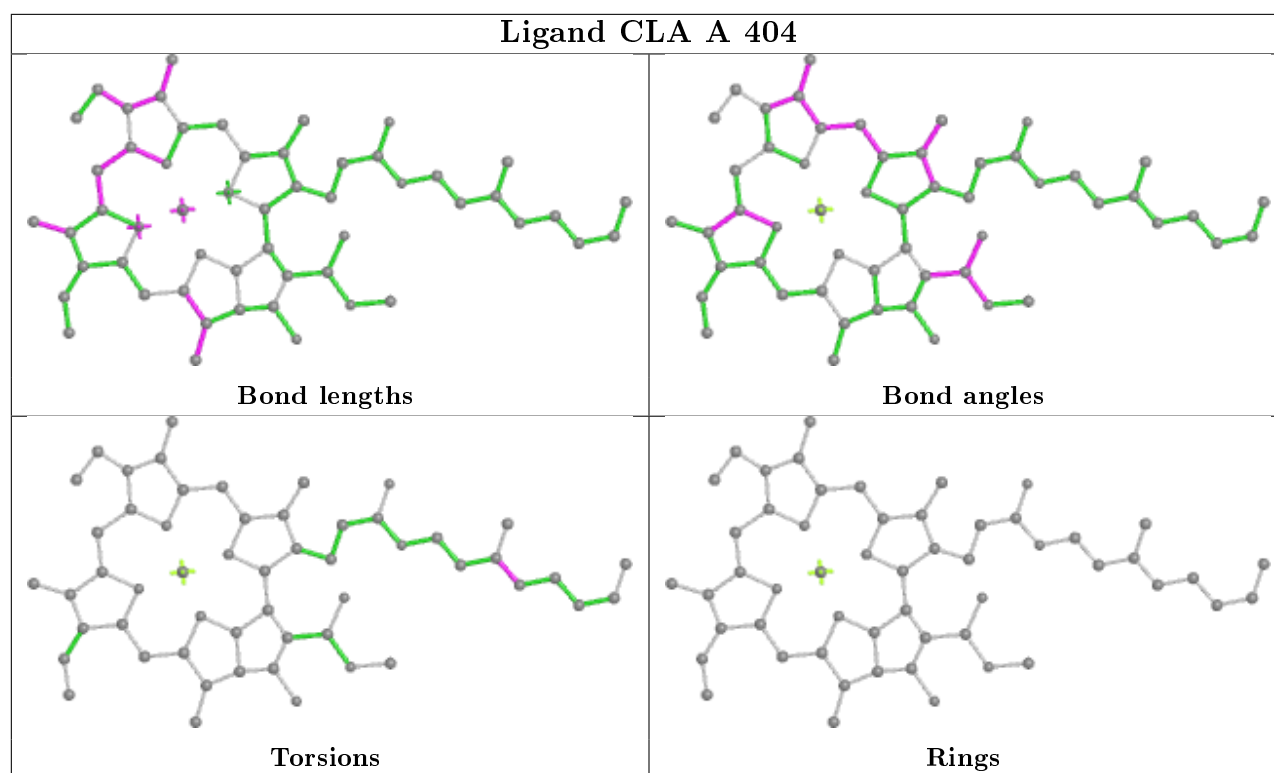


Ligand BCR k 102

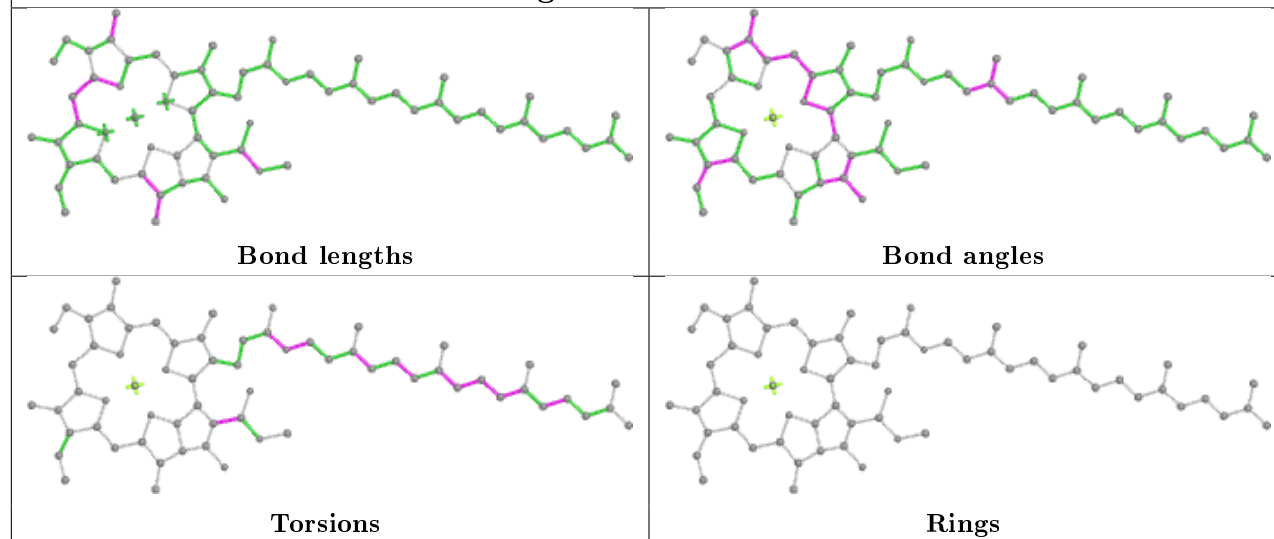




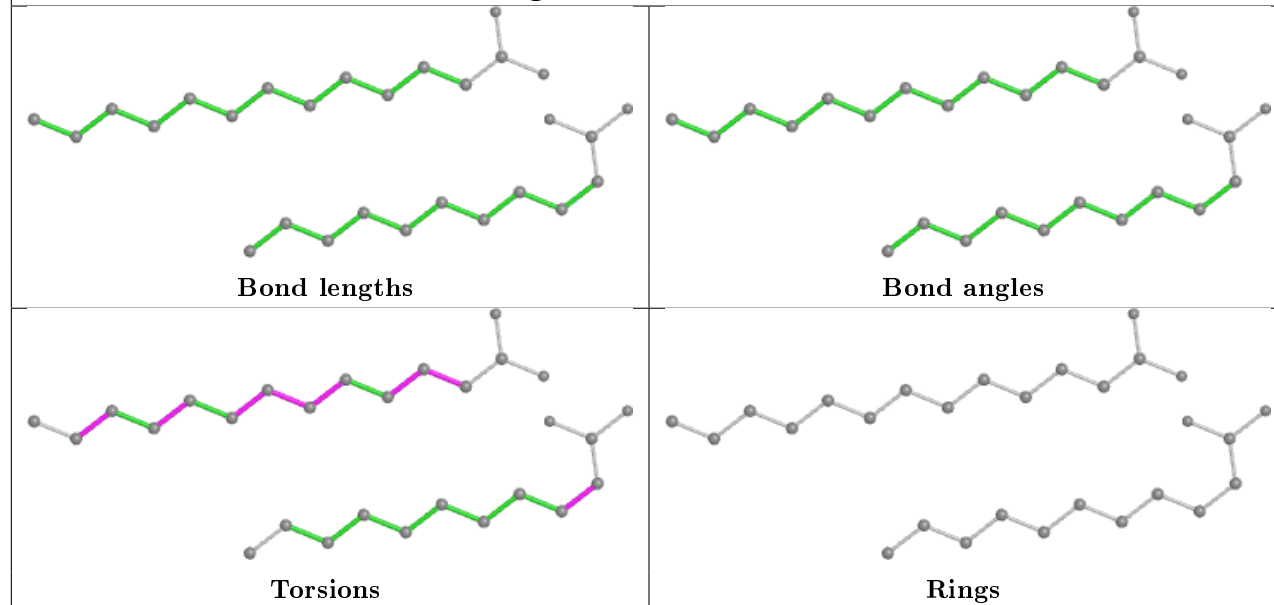




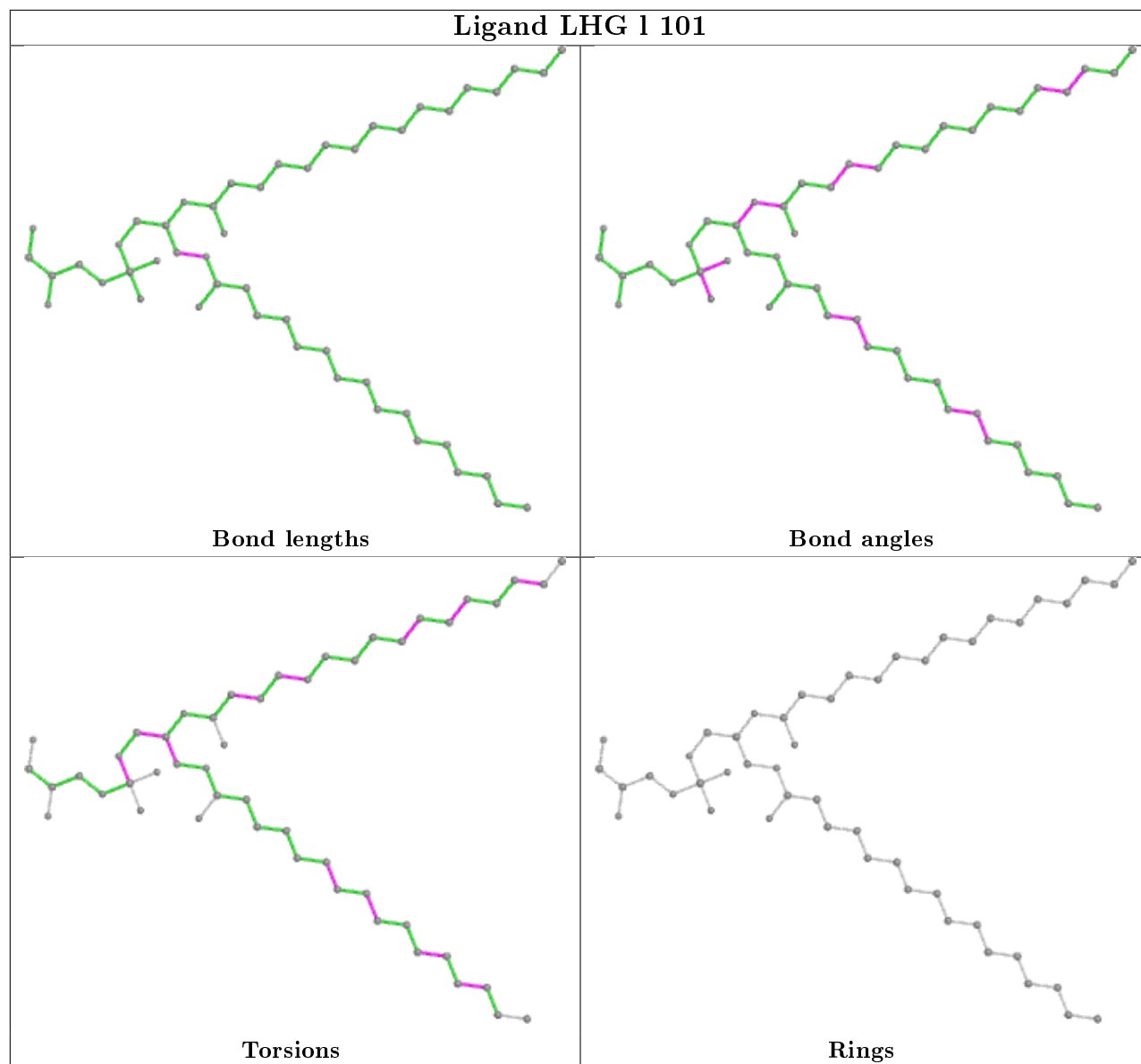
Ligand CLA c 507



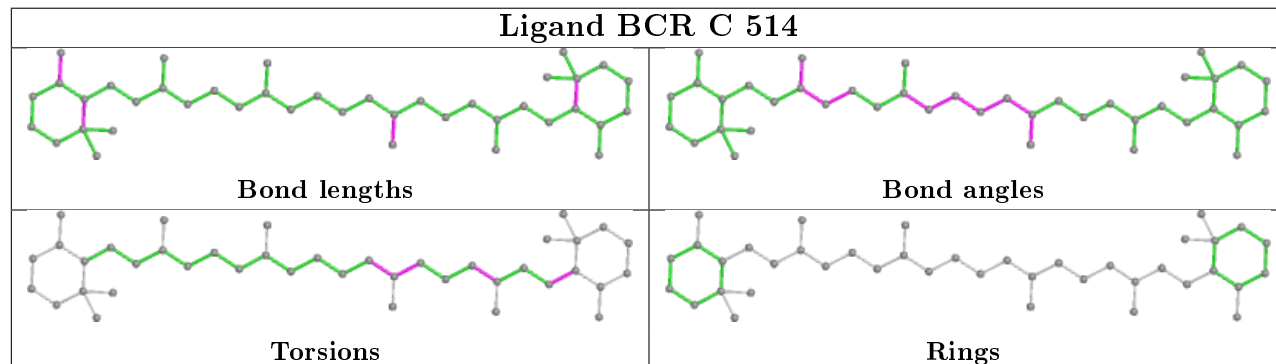
Ligand LMG D 411



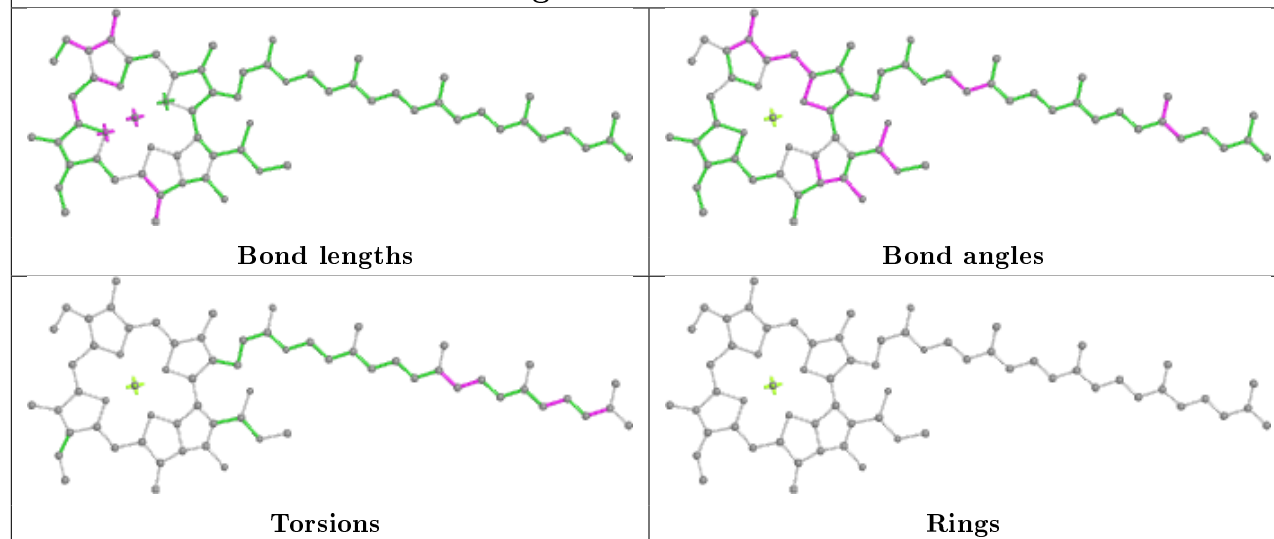
Ligand LHG 1 101



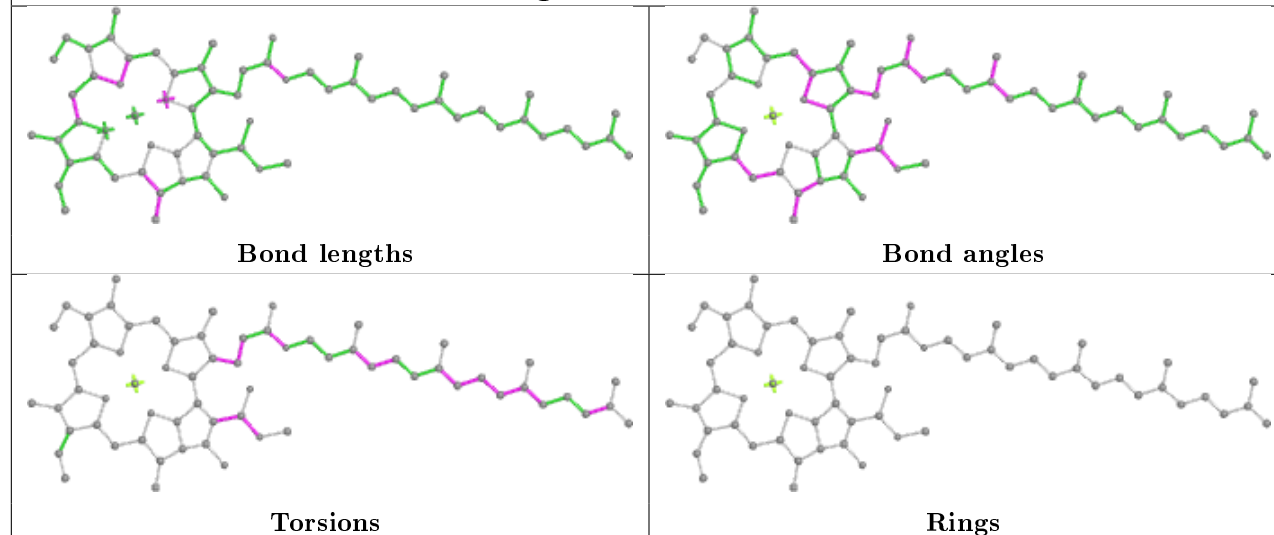
Ligand BCR C 514



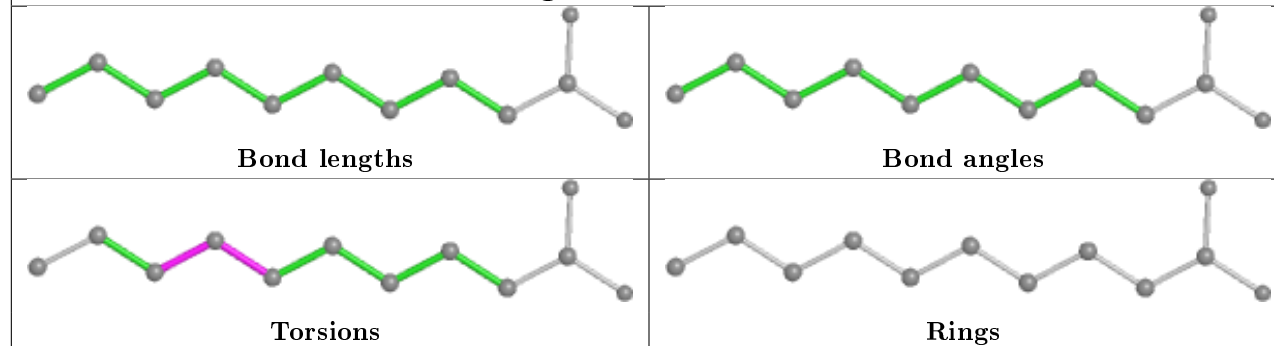
Ligand CLA B 611

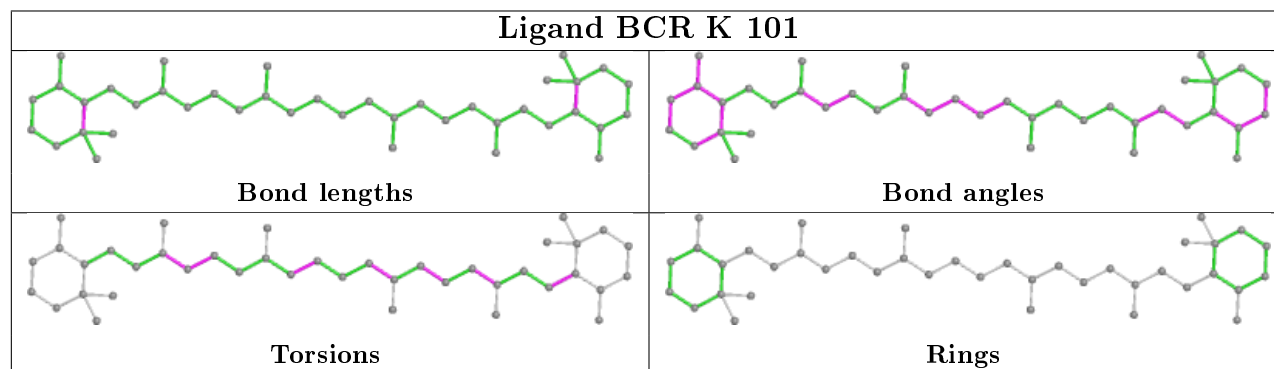
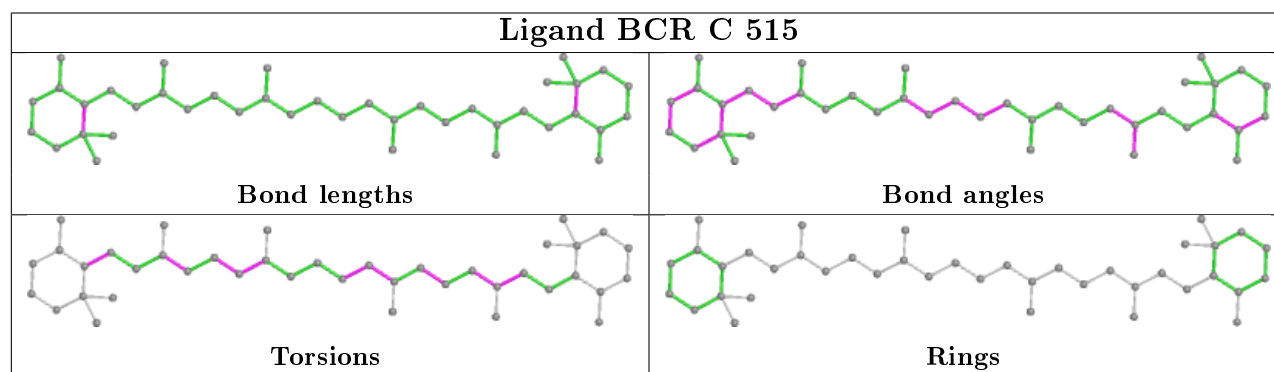
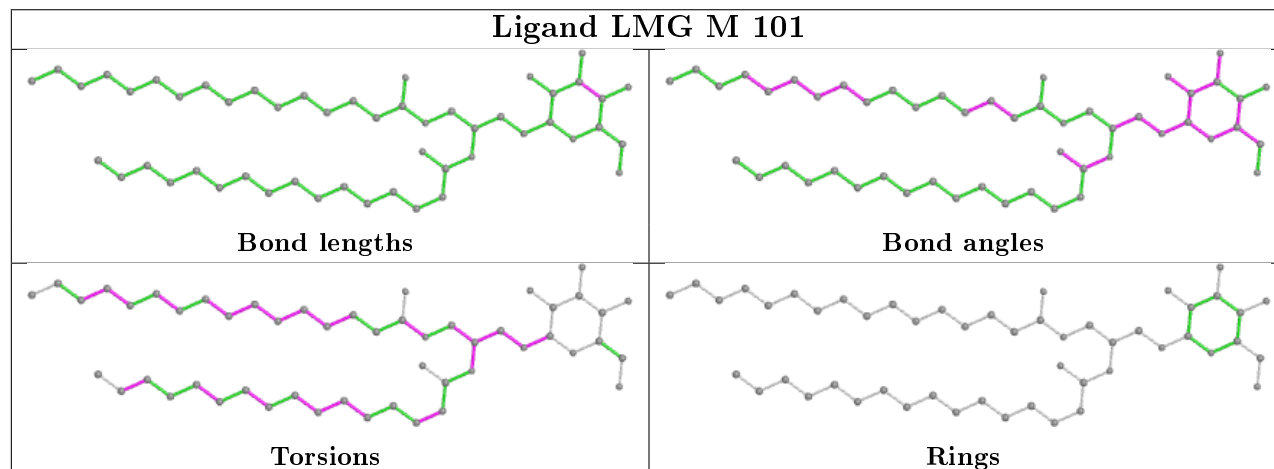
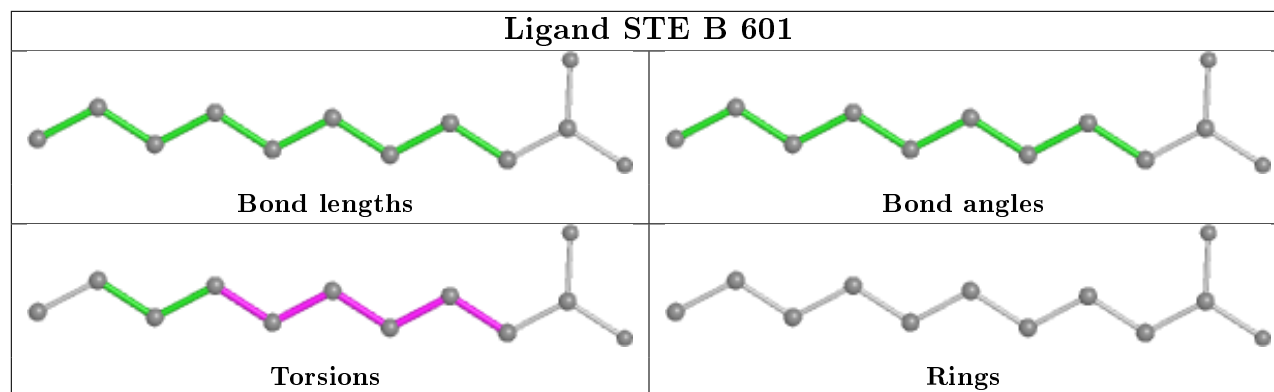


Ligand CLA b 601

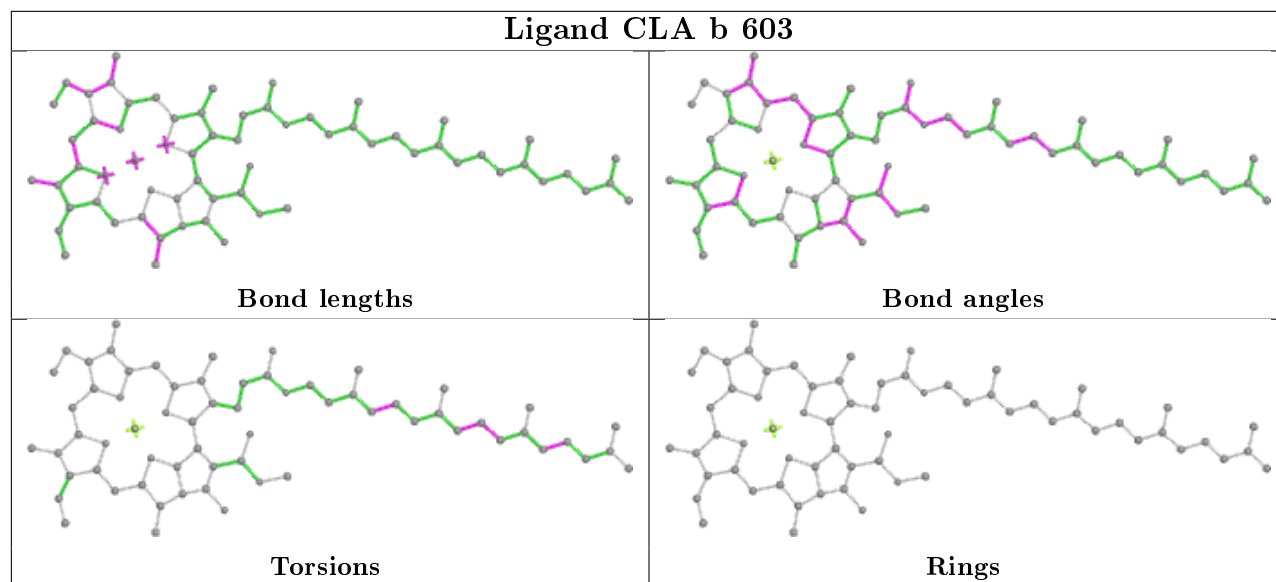


Ligand STE J 101

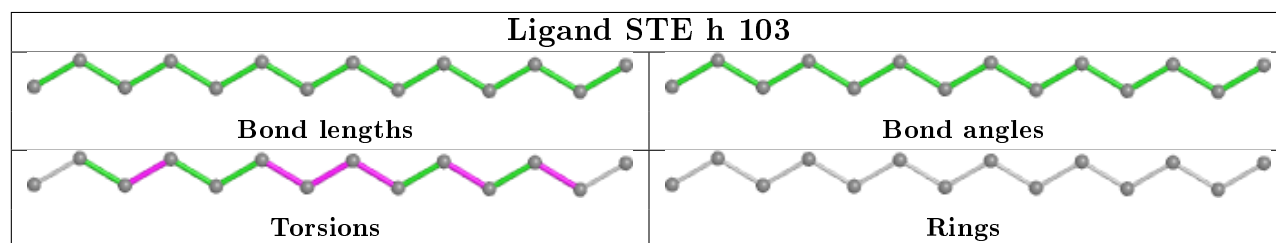




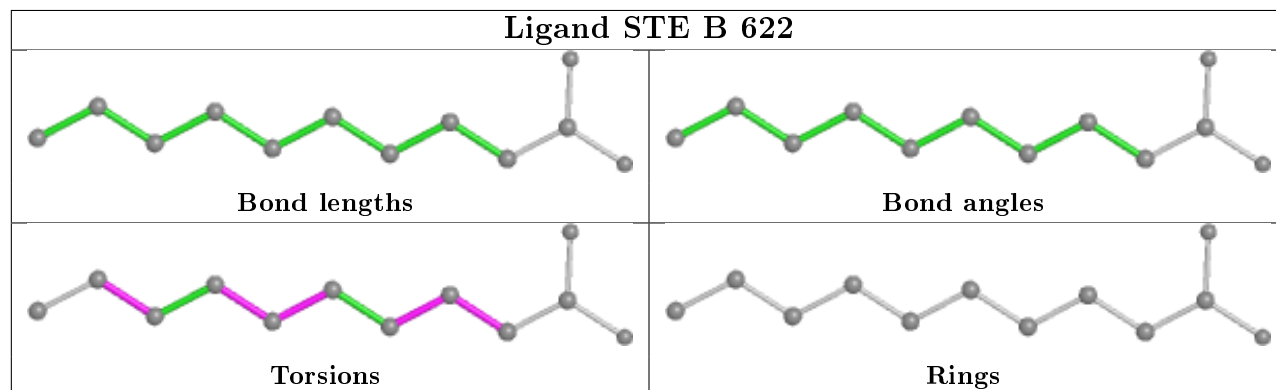
Ligand CLA b 603



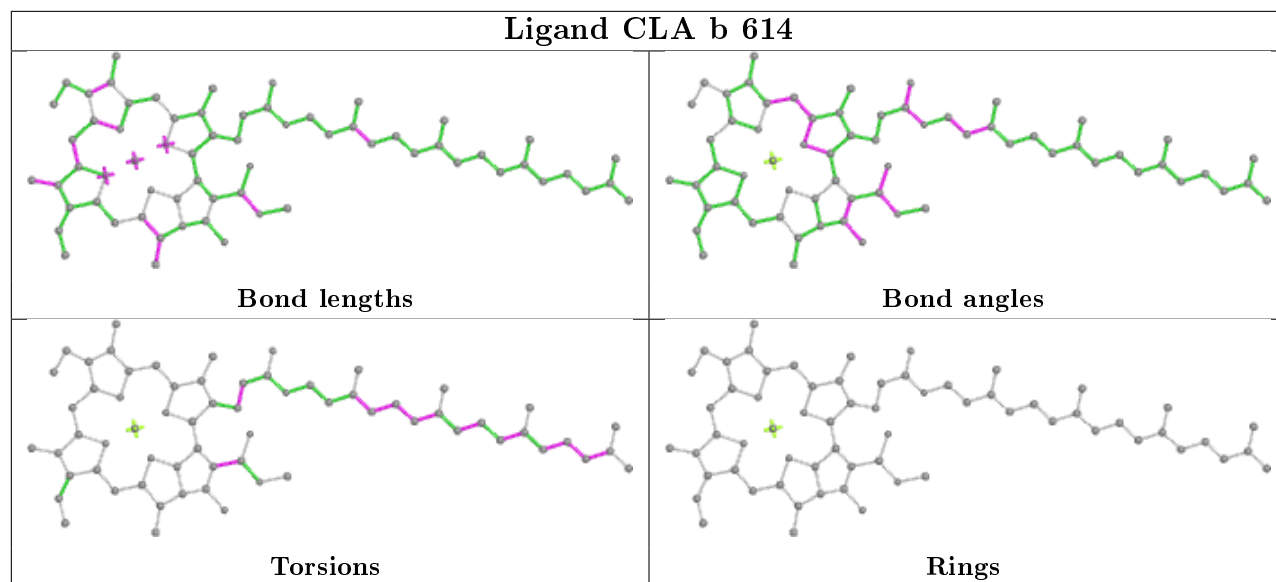
Ligand STE h 103



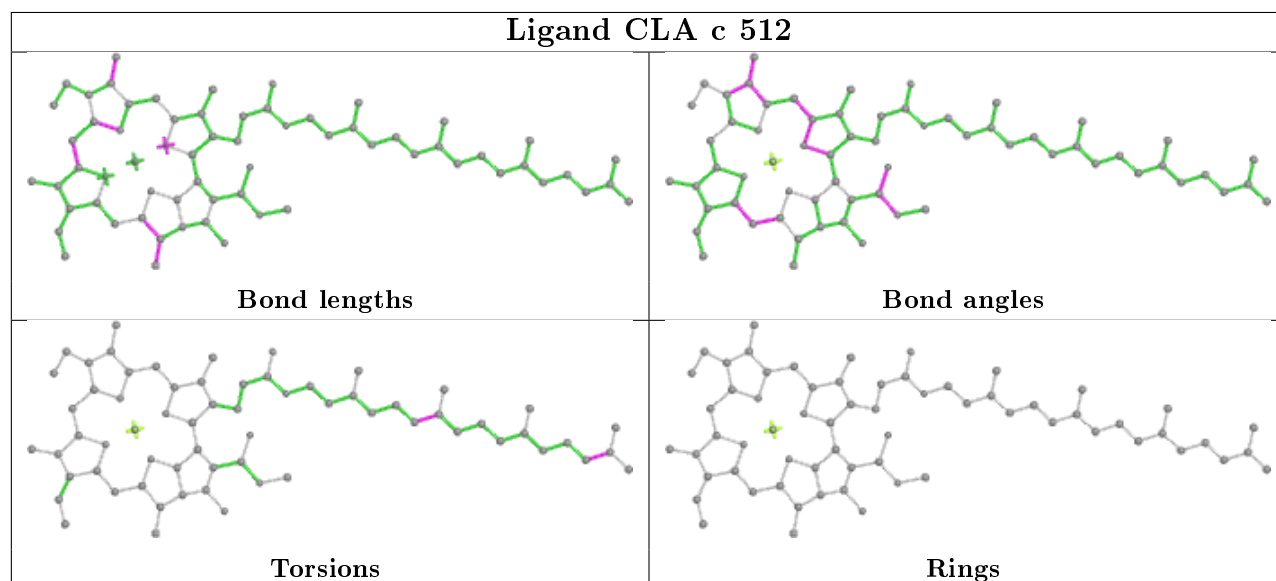
Ligand STE B 622



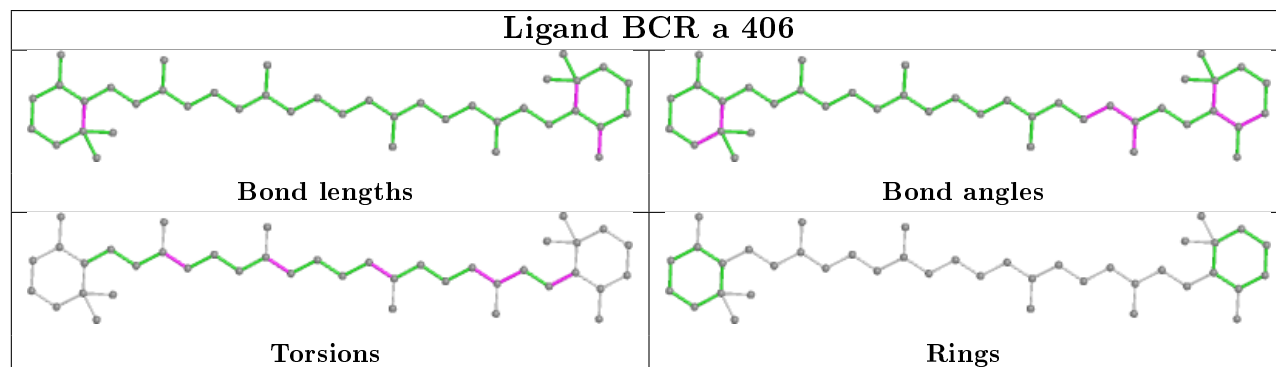
Ligand CLA b 614



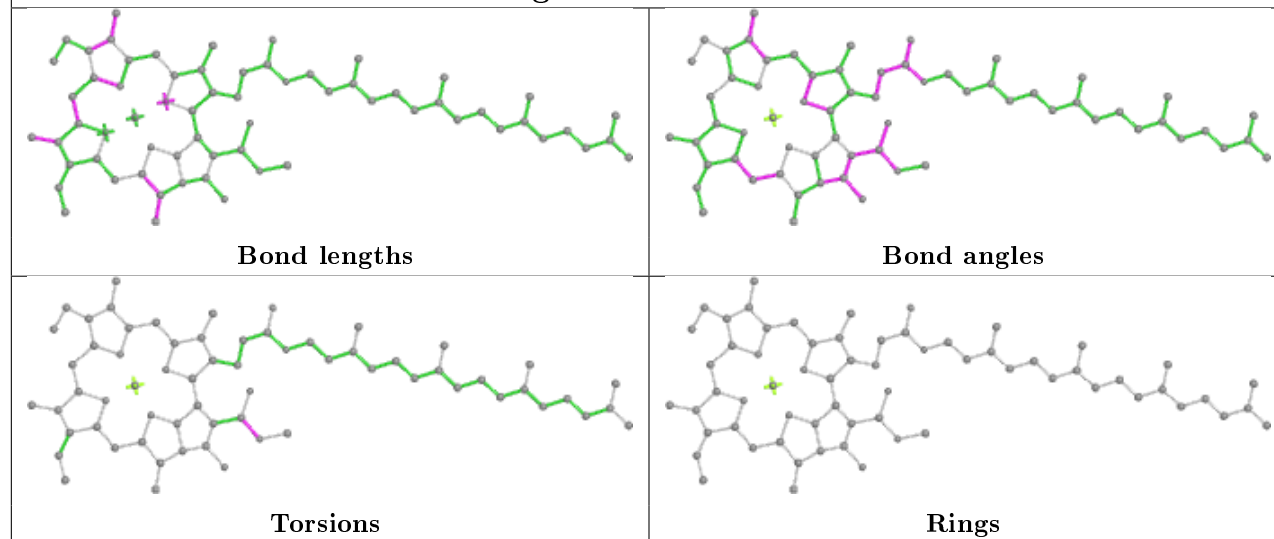
Ligand CLA c 512



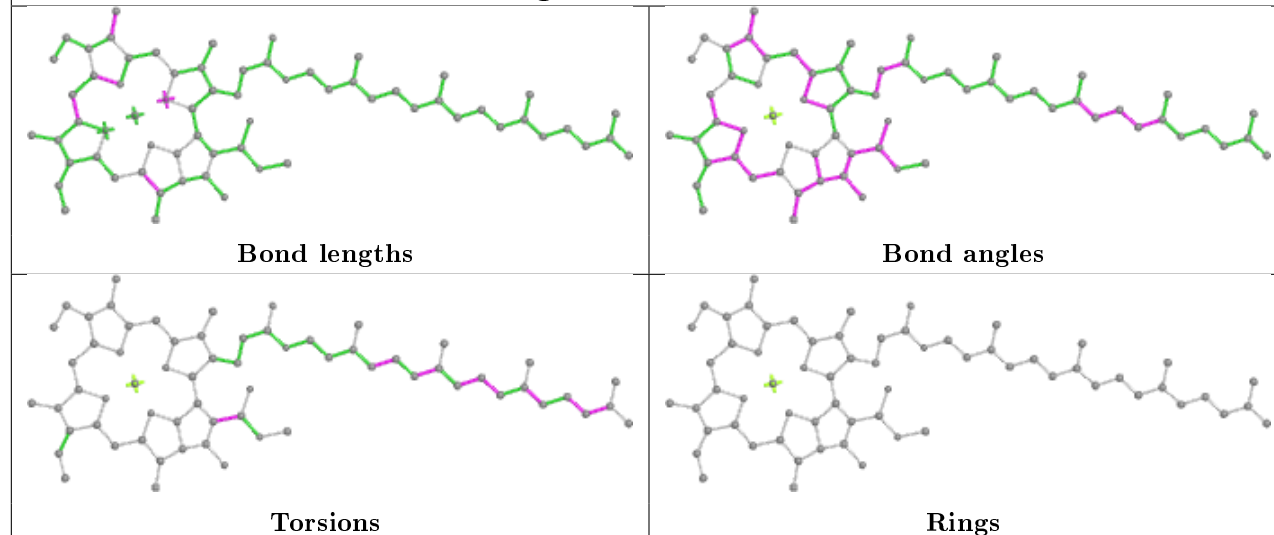
Ligand BCR a 406



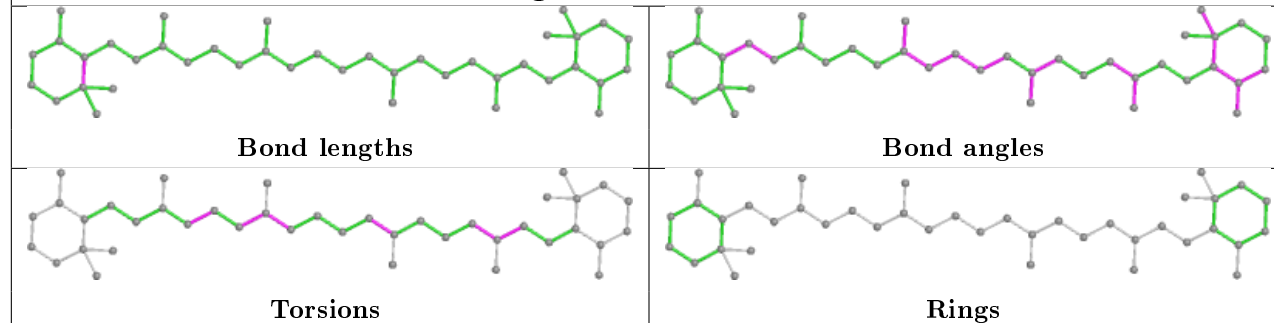
Ligand CLA C 501

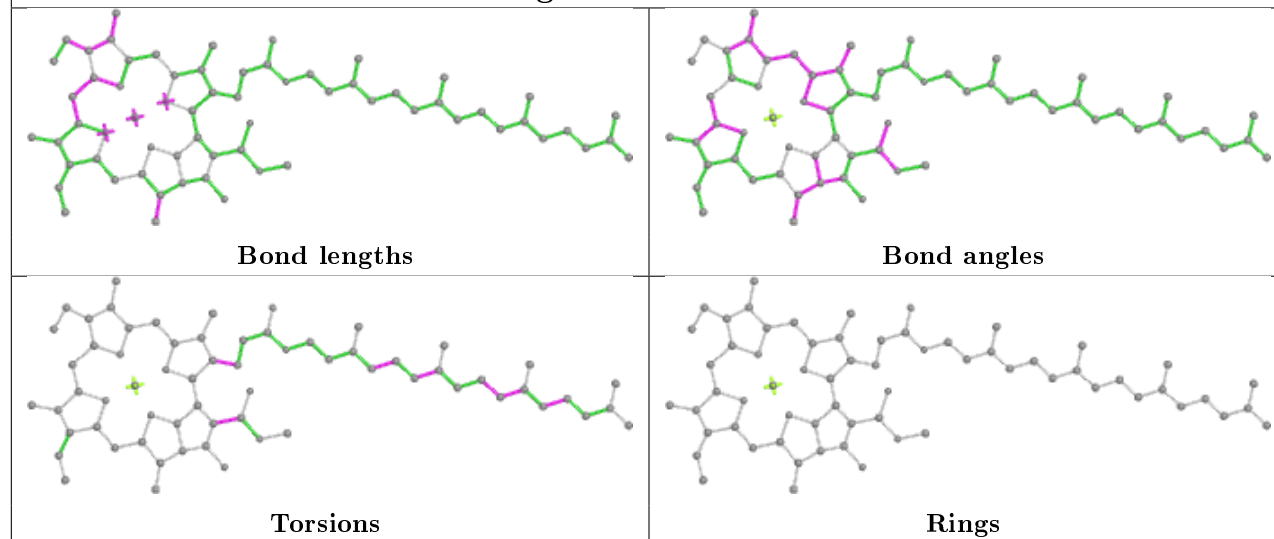
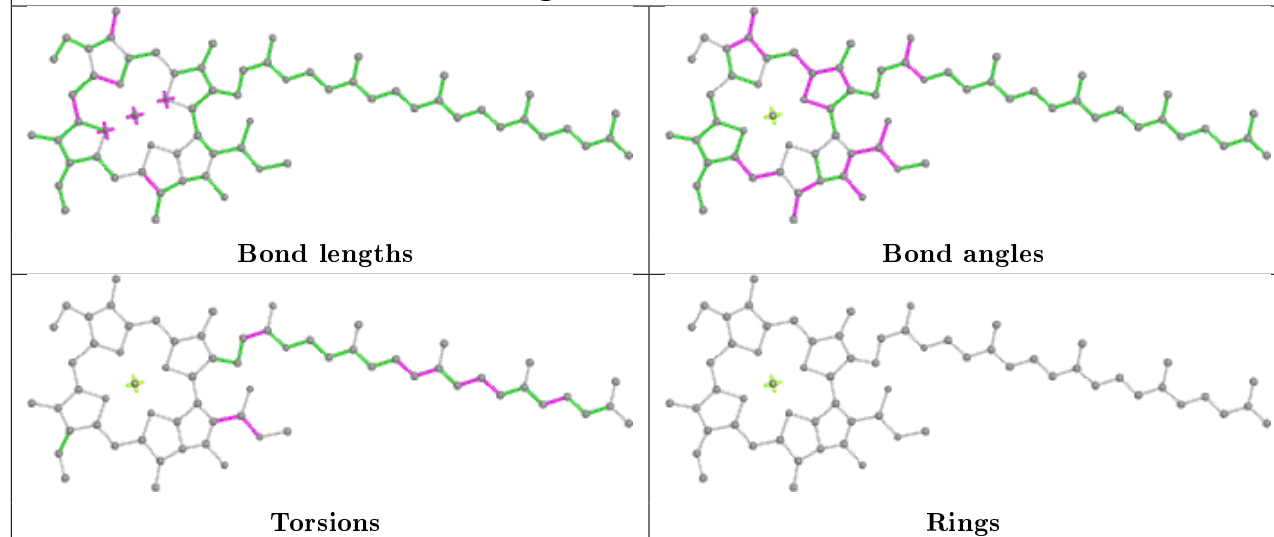


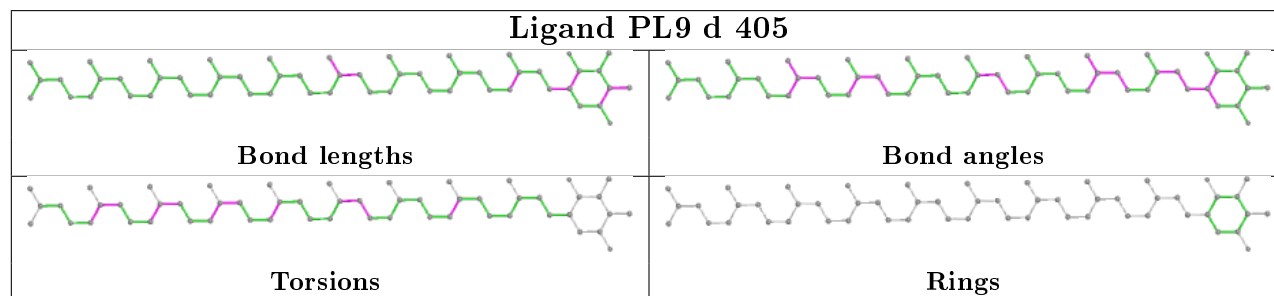
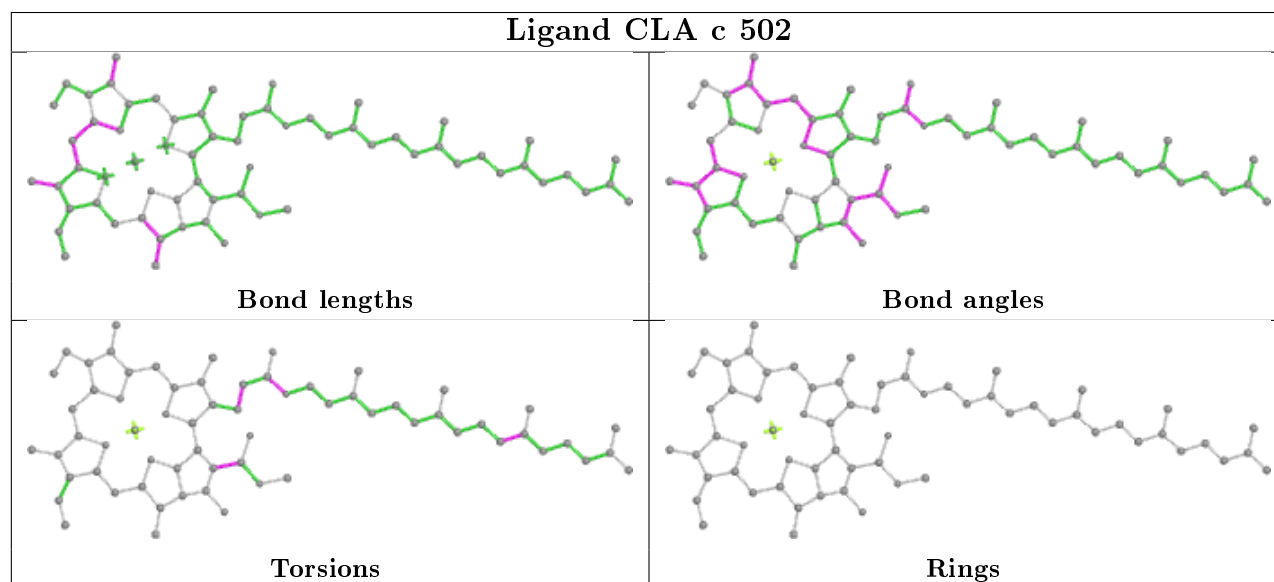
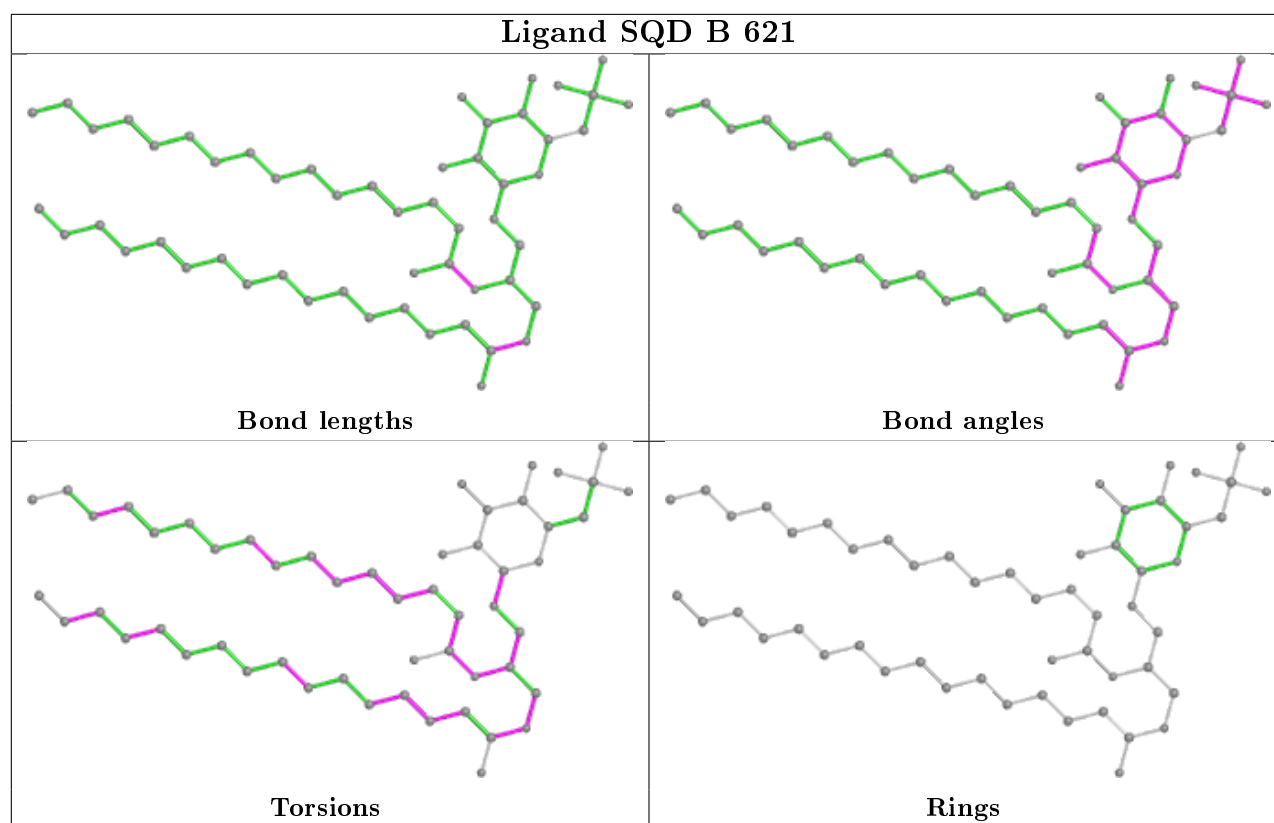
Ligand CLA b 604



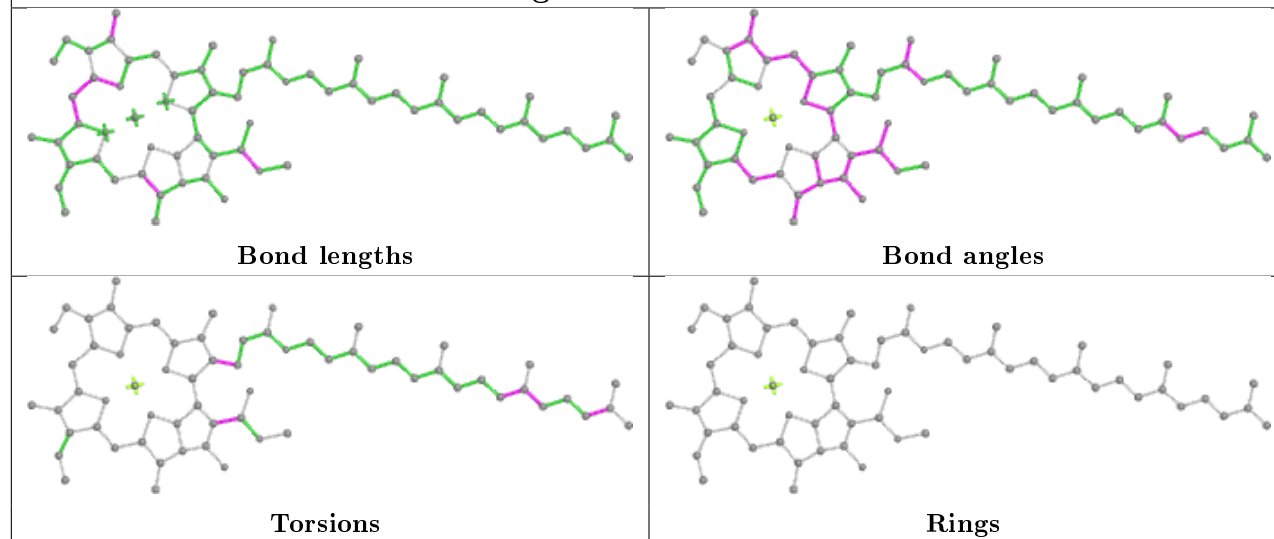
Ligand BCR A 405



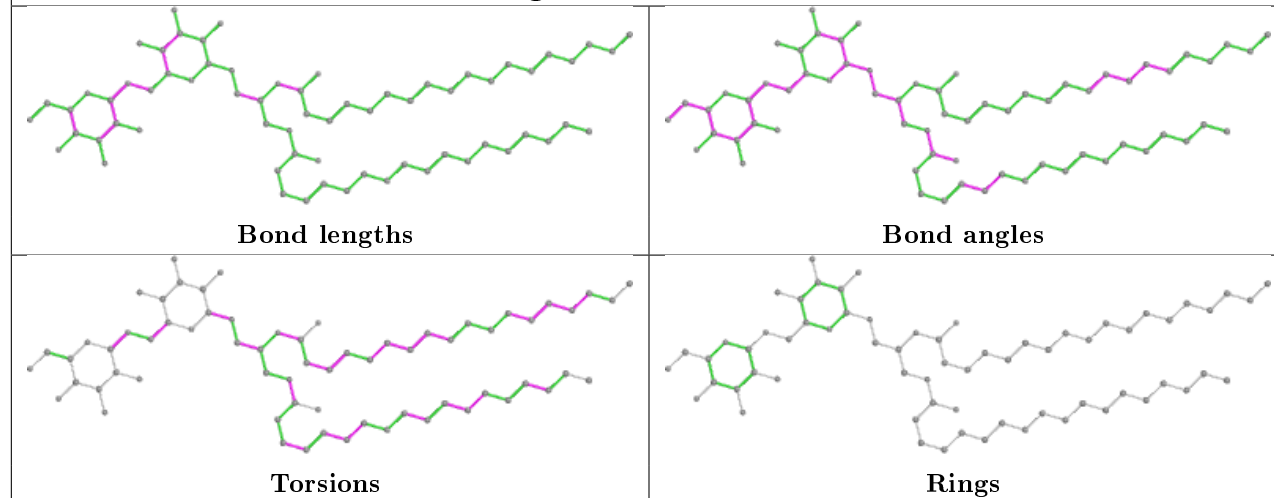
Ligand CLA a 403**Ligand CLA c 510**



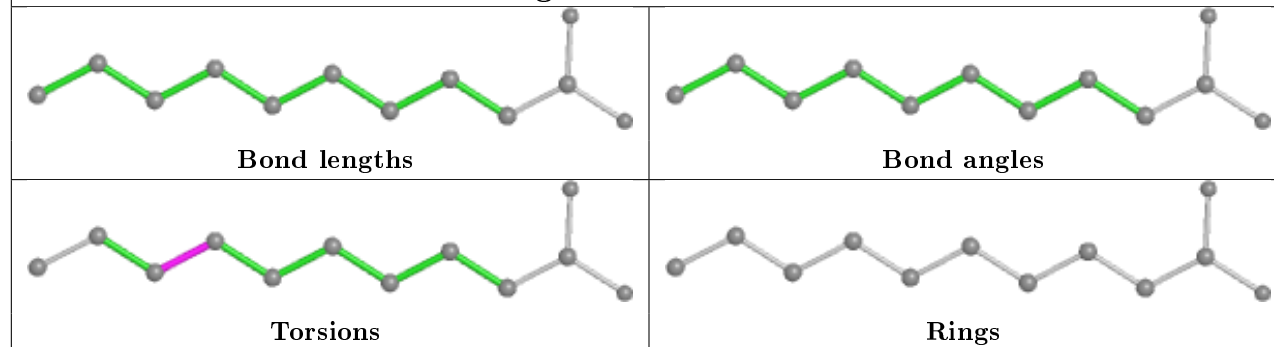
Ligand CLA B 602



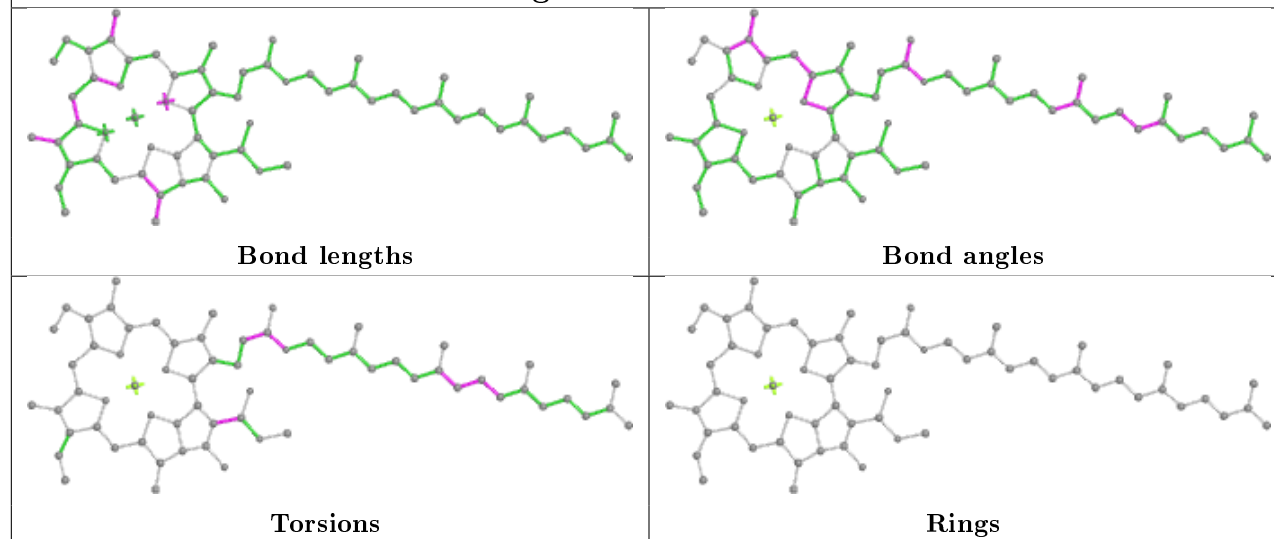
Ligand DGD A 414



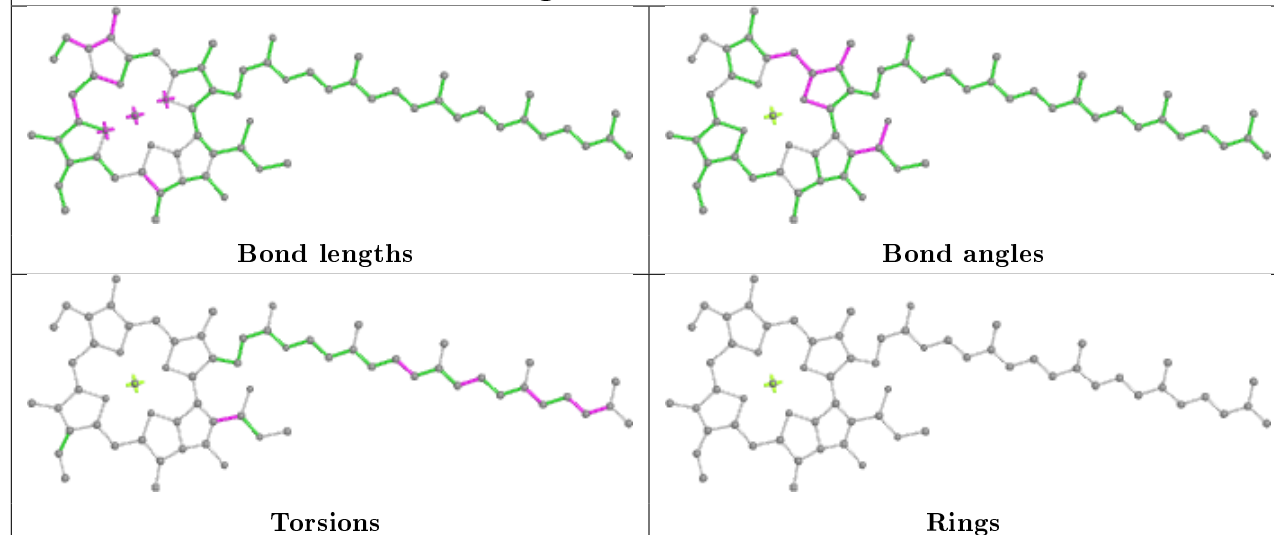
Ligand STE C 522



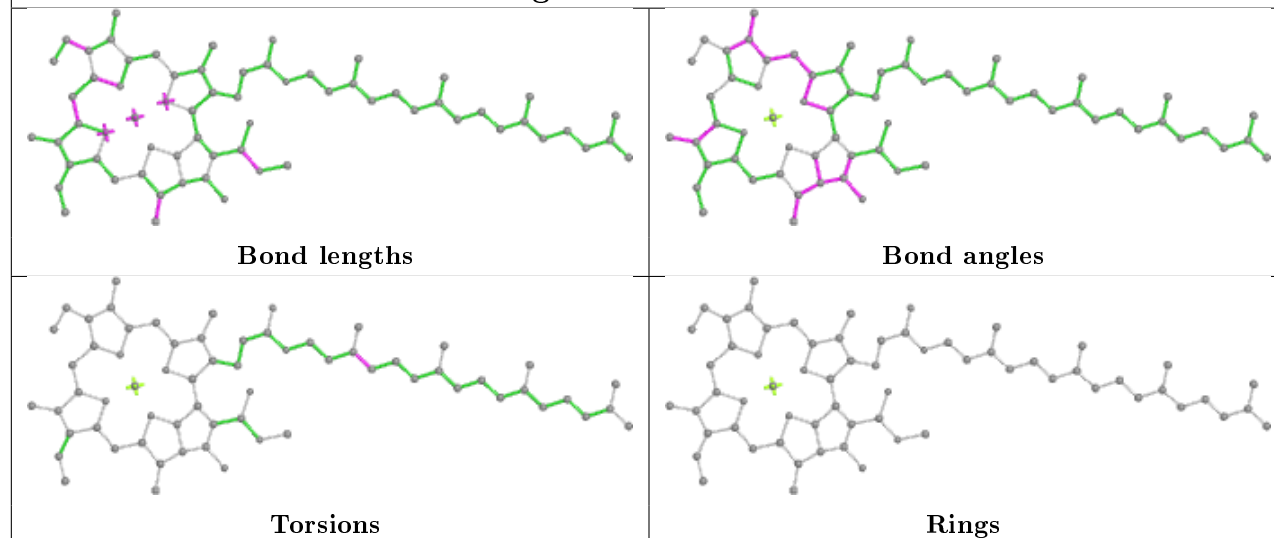
Ligand CLA B 612

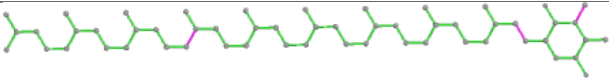
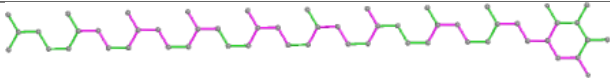
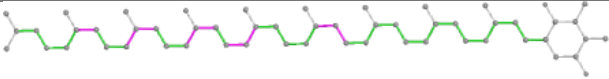
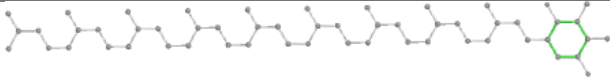


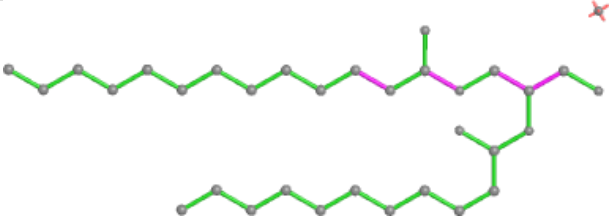
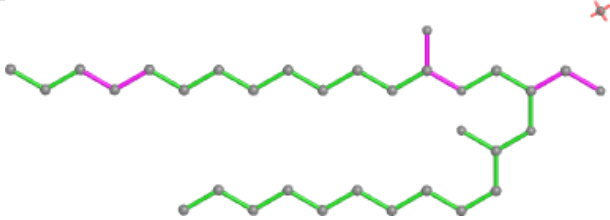
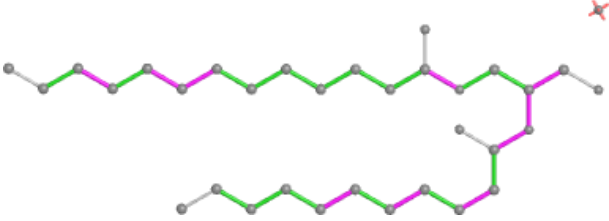
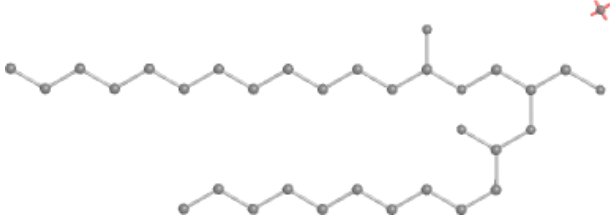
Ligand CLA c 504

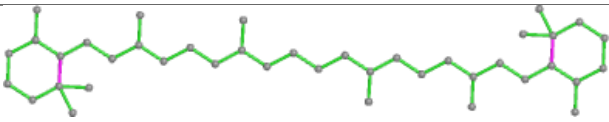
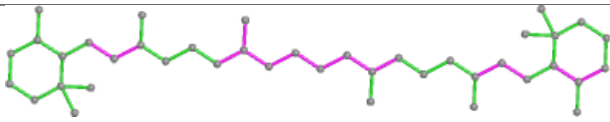
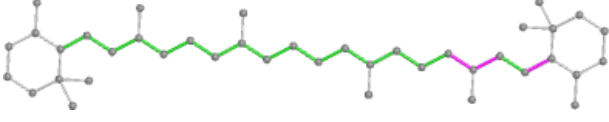
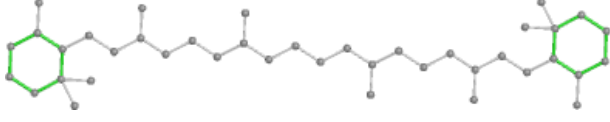


Ligand CLA B 609

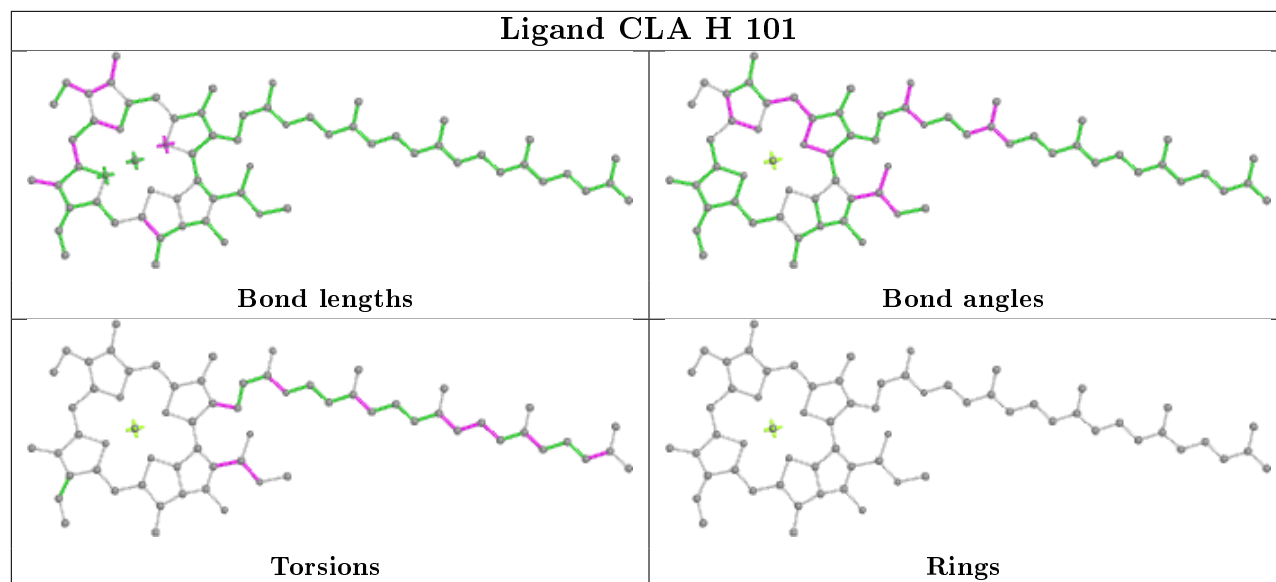


Ligand PL9 D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

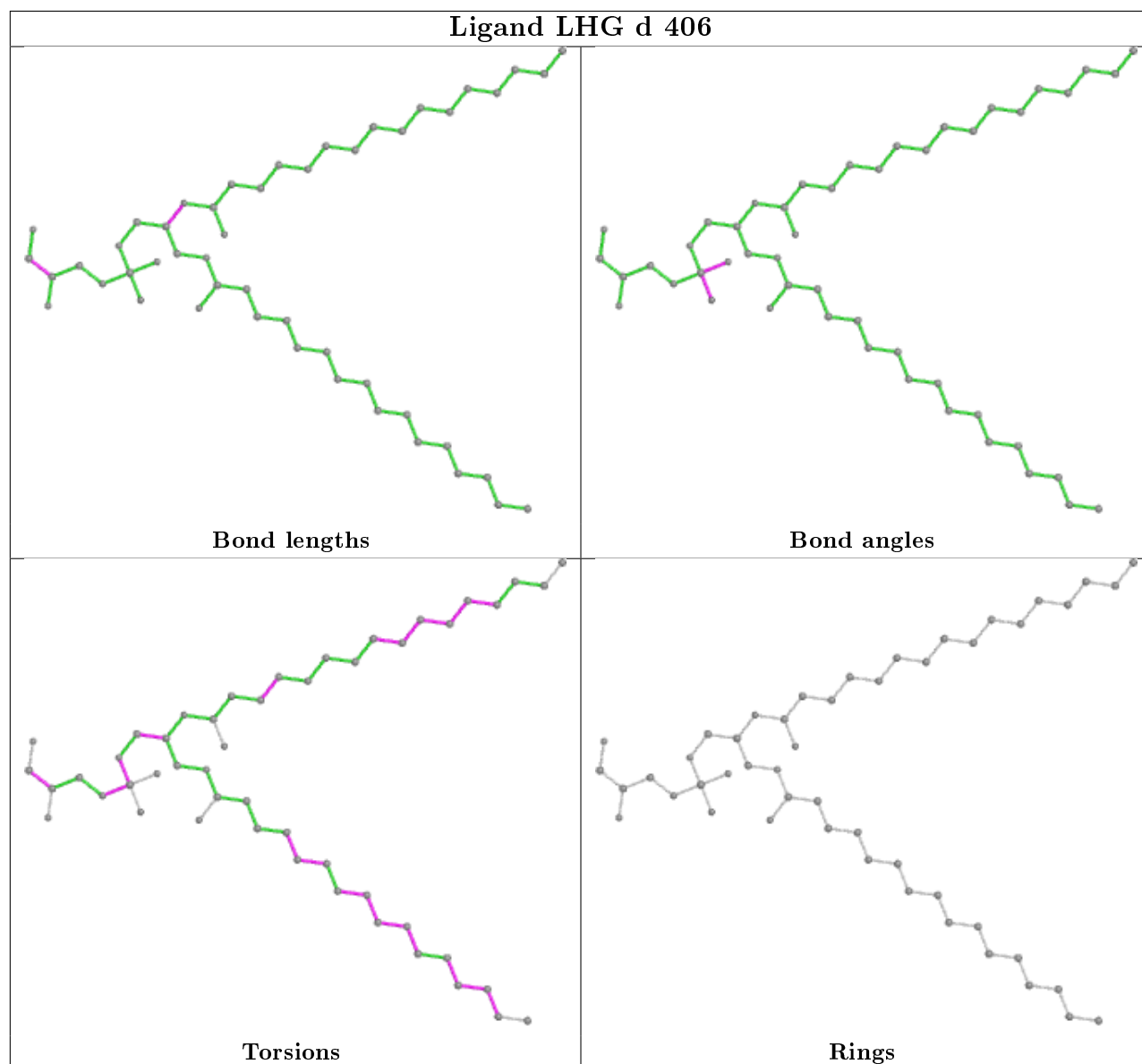
Ligand LMG D 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

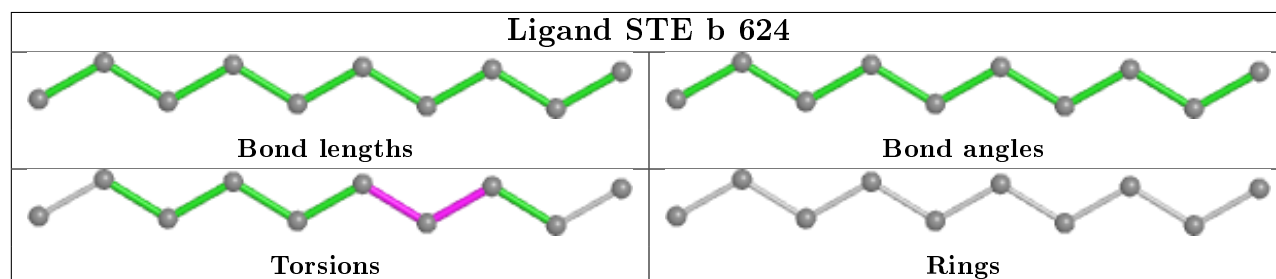
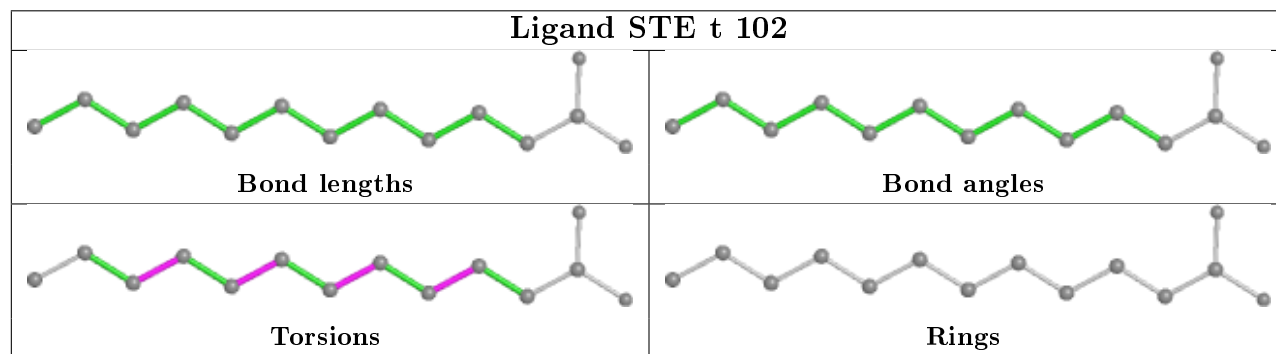
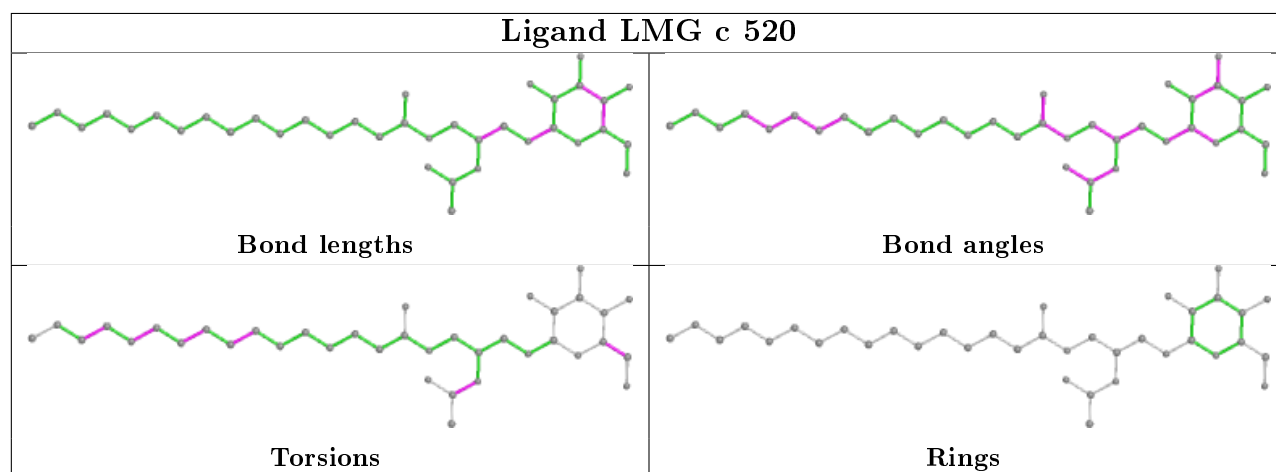
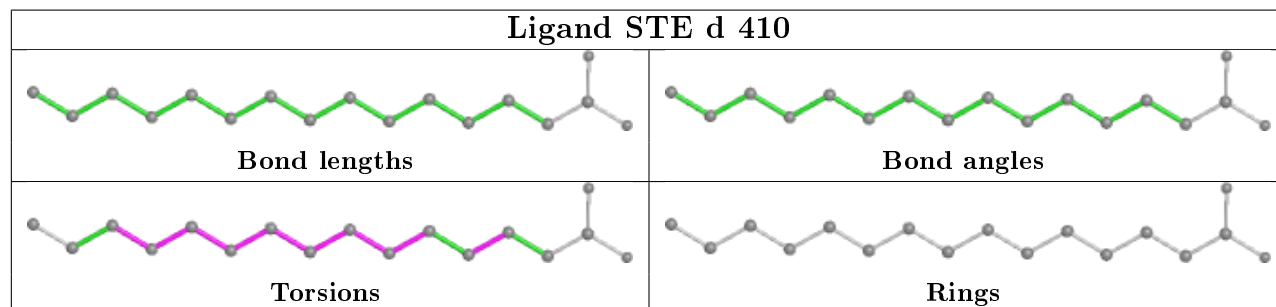
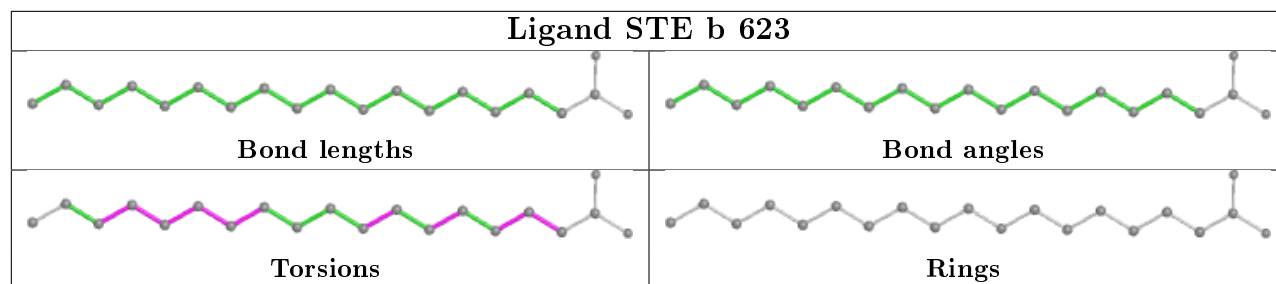
Ligand BCR D 406	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA H 101

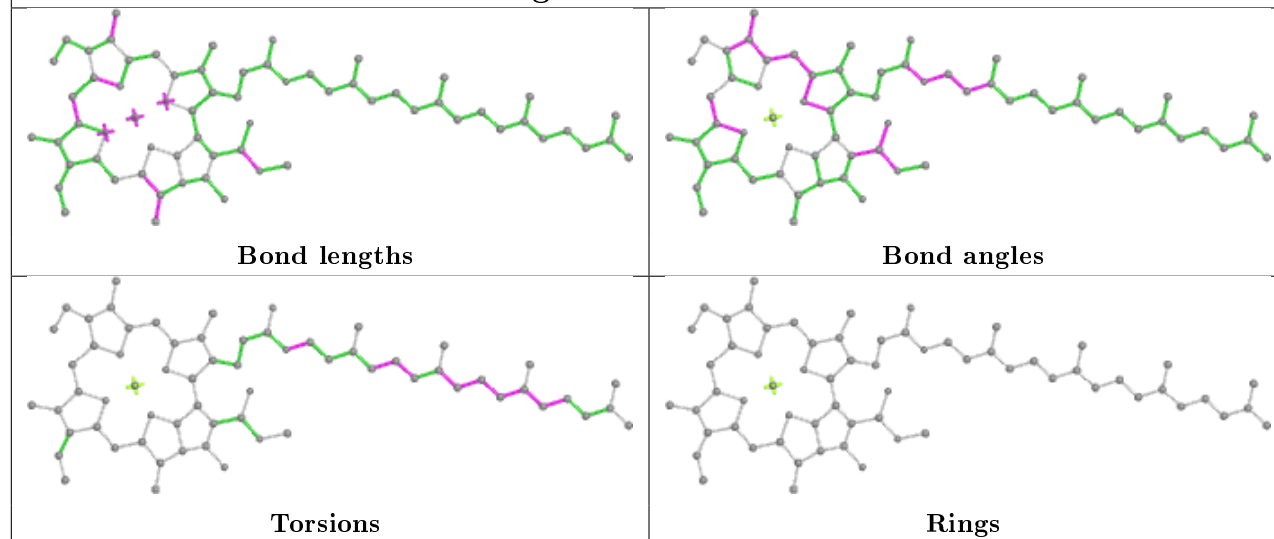


Ligand LHG d 406

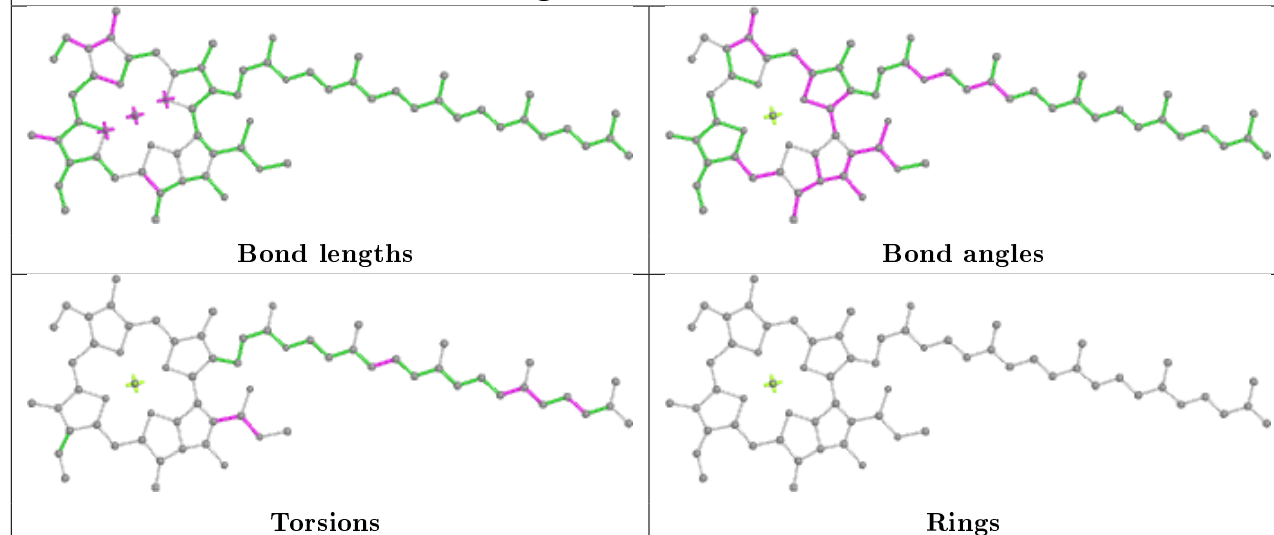




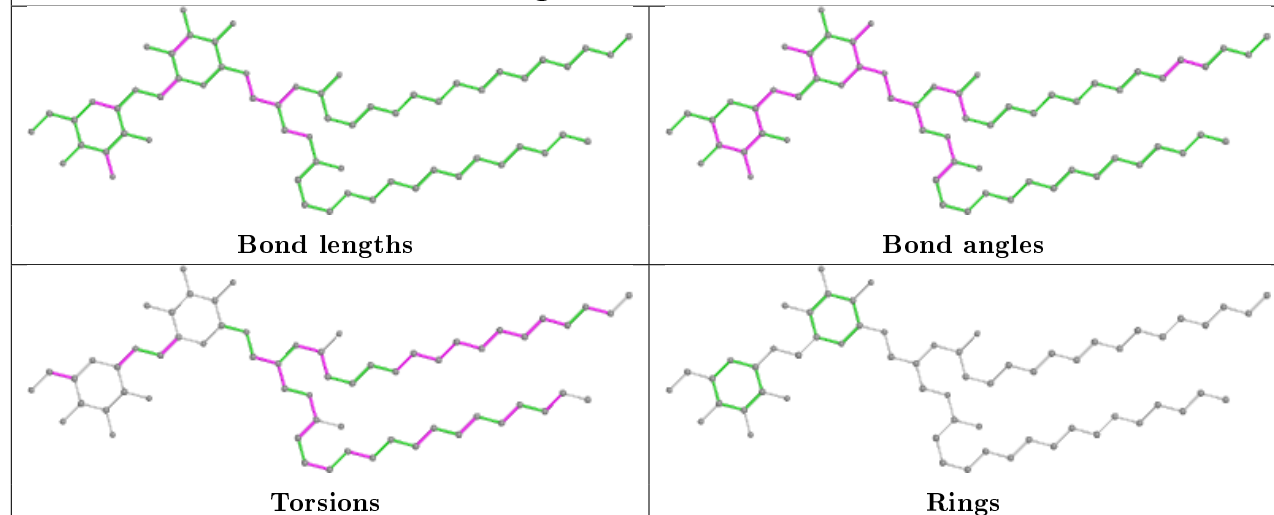
Ligand CLA C 509



Ligand CLA b 609



Ligand DGD c 517



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	334/344 (97%)	-0.40	3 (0%) 84 84	26, 34, 55, 81	0
1	a	334/344 (97%)	-0.38	2 (0%) 89 89	24, 36, 62, 82	0
2	B	505/506 (99%)	-0.42	7 (1%) 75 76	26, 37, 68, 99	0
2	b	505/506 (99%)	-0.26	18 (3%) 42 42	28, 40, 77, 107	0
3	C	442/461 (95%)	-0.32	7 (1%) 72 73	29, 41, 58, 78	0
3	c	451/461 (97%)	-0.28	6 (1%) 77 78	29, 43, 66, 101	0
4	D	341/352 (96%)	-0.43	2 (0%) 89 89	25, 34, 55, 86	0
4	d	341/352 (96%)	-0.34	0 100 100	27, 38, 63, 82	0
5	E	82/84 (97%)	-0.05	3 (3%) 41 41	37, 58, 77, 85	0
5	e	82/84 (97%)	0.18	6 (7%) 15 14	41, 65, 83, 99	0
6	F	34/45 (75%)	-0.39	2 (5%) 22 21	40, 48, 72, 95	0
6	f	34/45 (75%)	-0.23	3 (8%) 10 9	45, 53, 92, 104	0
7	H	65/66 (98%)	-0.12	2 (3%) 49 49	38, 46, 63, 76	0
7	h	63/66 (95%)	0.21	5 (7%) 12 12	46, 55, 66, 75	0
8	I	35/38 (92%)	-0.33	1 (2%) 51 52	35, 42, 73, 88	0
8	i	35/38 (92%)	-0.20	2 (5%) 23 23	36, 44, 80, 82	0
9	J	36/40 (90%)	0.03	4 (11%) 5 4	38, 52, 79, 96	0
9	j	36/40 (90%)	0.10	4 (11%) 5 4	43, 56, 89, 104	0
10	K	37/46 (80%)	0.13	2 (5%) 25 25	48, 58, 76, 86	0
10	k	37/46 (80%)	-0.12	1 (2%) 54 55	53, 60, 79, 83	0
11	L	37/37 (100%)	-0.55	0 100 100	29, 33, 65, 77	0
11	l	36/37 (97%)	-0.31	3 (8%) 11 11	27, 34, 72, 86	0
12	M	32/36 (88%)	-0.26	1 (3%) 49 49	30, 37, 66, 78	0
12	m	31/36 (86%)	-0.31	1 (3%) 47 47	30, 37, 59, 71	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.15	13 (5%) 26 26	28, 45, 86, 126	0
13	o	244/272 (89%)	-0.22	13 (5%) 26 26	28, 44, 83, 124	0
14	R	34/40 (85%)	3.40	32 (94%) 0 0	80, 93, 105, 110	0
14	r	31/40 (77%)	5.55	31 (100%) 0 0	87, 118, 131, 136	0
15	T	29/32 (90%)	-0.42	1 (3%) 45 45	30, 35, 65, 81	0
15	t	29/32 (90%)	-0.30	2 (6%) 16 16	31, 37, 80, 81	0
16	U	97/134 (72%)	-0.40	0 100 100	36, 46, 68, 94	0
16	u	97/134 (72%)	-0.54	0 100 100	34, 44, 61, 85	0
17	V	137/163 (84%)	-0.65	0 100 100	31, 44, 59, 77	0
17	v	137/163 (84%)	-0.30	0 100 100	37, 50, 70, 80	0
18	X	38/41 (92%)	0.13	2 (5%) 26 26	46, 58, 80, 85	0
18	x	39/41 (95%)	0.41	6 (15%) 2 1	52, 65, 94, 106	0
19	Y	27/46 (58%)	1.20	8 (29%) 0 0	58, 78, 89, 100	0
19	y	30/46 (65%)	0.56	3 (10%) 7 6	63, 75, 92, 95	0
20	Z	62/62 (100%)	0.73	15 (24%) 0 0	55, 73, 112, 128	0
20	z	62/62 (100%)	0.75	9 (14%) 2 2	61, 73, 107, 119	0
All	All	5302/5690 (93%)	-0.20	220 (4%) 37 37	24, 42, 79, 136	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	14	LEU	12.2
14	r	9	LEU	9.0
14	r	10	LEU	8.5
14	r	28	VAL	8.2
2	b	495	PHE	7.8
13	o	58	ASN	7.6
14	R	3	TRP	7.3
14	r	3	TRP	7.0
13	o	3	GLN	7.0
14	r	18	TRP	6.6
1	A	13	LEU	6.4
14	r	15	ALA	6.4
13	O	60	ARG	6.4
14	r	6	LEU	6.3
14	r	13	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
20	Z	33	TRP	6.2
14	r	24	LEU	6.1
14	r	31	VAL	6.0
13	o	60	ARG	6.0
13	O	3	GLN	5.9
14	r	12	VAL	5.9
14	r	26	TYR	5.8
14	r	22	ASN	5.8
14	R	6	LEU	5.7
14	r	25	PRO	5.7
14	R	13	LEU	5.7
13	O	56	PRO	5.5
14	r	29	LYS	5.5
14	R	32	GLN	5.5
6	F	12	SER	5.5
14	r	11	PRO	5.3
9	J	5	GLY	5.2
13	o	61	GLN	5.2
2	b	487	SER	5.2
14	r	2	ASP	5.0
2	b	502	VAL	5.0
14	r	4	ARG	4.9
20	z	33	TRP	4.9
13	O	61	GLN	4.8
20	Z	1	MET	4.8
9	j	6	GLY	4.8
13	o	4	THR	4.8
13	O	4	THR	4.8
14	R	20	VAL	4.8
14	r	19	ALA	4.7
20	Z	34	ASP	4.7
14	R	26	TYR	4.7
14	r	5	VAL	4.6
20	z	35	ARG	4.5
14	r	7	VAL	4.5
14	R	21	ARG	4.5
20	z	30	PRO	4.5
13	o	57	LYS	4.4
14	r	16	ALA	4.4
5	e	79	PHE	4.4
9	j	7	ARG	4.4
9	j	8	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
13	O	62	GLU	4.3
14	r	23	ILE	4.3
9	J	7	ARG	4.2
18	X	2	THR	4.1
19	Y	43	ARG	4.0
20	Z	35	ARG	4.0
3	c	23	ALA	4.0
3	c	24	THR	4.0
13	o	56	PRO	4.0
14	r	17	GLY	4.0
6	f	12	SER	4.0
20	Z	62	VAL	3.9
2	b	127	ARG	3.9
1	A	11	ALA	3.9
2	b	505	ARG	3.9
19	y	19	ILE	3.9
14	r	27	ALA	3.9
14	R	25	PRO	3.8
13	o	62	GLU	3.7
14	R	9	LEU	3.7
14	R	31	VAL	3.7
14	R	10	LEU	3.6
14	R	14	LEU	3.6
14	R	28	VAL	3.6
2	B	505	ARG	3.6
9	J	6	GLY	3.5
14	r	21	ARG	3.5
3	C	146	PHE	3.5
20	Z	32	ASP	3.5
3	c	143	TYR	3.5
10	k	17	ILE	3.5
13	O	59	LYS	3.5
15	T	30	THR	3.4
9	J	8	ILE	3.4
15	t	29	ILE	3.4
14	R	24	LEU	3.4
18	X	3	ILE	3.3
11	l	3	PRO	3.3
14	R	29	LYS	3.3
7	H	66	GLY	3.3
8	i	35	LYS	3.3
2	b	486	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
14	R	5	VAL	3.3
14	R	18	TRP	3.2
5	e	61	ARG	3.2
8	I	34	ARG	3.2
20	Z	31	GLN	3.2
2	B	127	ARG	3.2
20	Z	3	ILE	3.2
2	B	495	PHE	3.2
14	R	2	ASP	3.2
14	r	8	VAL	3.2
7	h	21	VAL	3.2
13	o	132	ASN	3.1
13	O	246	ALA	3.1
7	h	10	ILE	3.1
19	Y	42	ARG	3.1
13	o	59	LYS	3.1
15	t	30	THR	3.1
14	R	27	ALA	3.1
2	b	506	ARG	3.0
14	R	35	LEU	3.0
2	b	503	THR	3.0
8	i	34	ARG	3.0
5	E	84	LYS	3.0
3	C	57	ALA	2.9
19	Y	40	ALA	2.9
3	c	146	PHE	2.9
14	r	30	GLN	2.9
19	Y	41	VAL	2.9
14	R	8	VAL	2.9
18	x	38	GLN	2.9
9	j	5	GLY	2.8
14	r	32	GLN	2.8
20	z	3	ILE	2.8
19	Y	37	PHE	2.8
20	Z	4	LEU	2.8
18	x	2	THR	2.8
5	e	82	GLN	2.8
13	O	63	ALA	2.8
18	x	40	SER	2.8
13	O	57	LYS	2.8
7	h	56	ASP	2.7
14	R	7	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
14	R	17	GLY	2.7
5	E	83	LEU	2.7
1	a	11	ALA	2.7
3	C	58	GLY	2.7
14	R	34	LEU	2.7
11	l	7	ARG	2.6
14	R	23	ILE	2.6
14	r	20	VAL	2.6
2	b	490	GLN	2.6
19	Y	25	ILE	2.6
2	b	295	GLY	2.6
7	h	6	TRP	2.6
1	A	12	ASN	2.6
6	f	13	TYR	2.6
2	b	494	GLY	2.6
14	R	30	GLN	2.6
2	b	491	VAL	2.6
2	b	496	TYR	2.6
13	O	5	LEU	2.5
5	e	4	THR	2.5
3	C	143	TYR	2.5
2	B	293	ALA	2.5
2	b	292	LEU	2.5
20	Z	7	LEU	2.5
5	E	79	PHE	2.5
5	e	74	GLN	2.5
2	b	85	GLY	2.5
13	O	34	SER	2.5
14	R	19	ALA	2.5
5	e	84	LYS	2.5
3	c	262	ARG	2.4
13	o	207	ARG	2.4
19	Y	20	ALA	2.4
20	Z	60	PHE	2.4
7	H	6	TRP	2.4
4	D	227	GLU	2.4
20	z	36	SER	2.4
13	o	5	LEU	2.4
14	R	11	PRO	2.4
20	z	42	LEU	2.3
2	b	289	GLN	2.3
14	R	16	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
14	R	12	VAL	2.3
19	y	37	PHE	2.3
14	R	33	LYS	2.3
3	c	25	ASN	2.3
12	m	31	SER	2.3
18	x	3	ILE	2.3
13	O	55	GLU	2.3
13	o	246	ALA	2.3
10	K	10	LYS	2.2
20	Z	37	LYS	2.2
3	C	61	VAL	2.2
2	b	128	THR	2.2
12	M	33	GLN	2.2
14	R	4	ARG	2.2
20	z	4	LEU	2.2
6	F	13	TYR	2.2
20	z	38	GLN	2.2
3	C	60	ILE	2.2
18	x	36	LYS	2.1
20	Z	61	VAL	2.1
6	f	15	ILE	2.1
3	C	122	SER	2.1
11	l	5	PRO	2.1
20	Z	41	PHE	2.1
7	h	22	ALA	2.1
19	Y	38	LEU	2.1
2	b	485	GLU	2.1
19	y	43	ARG	2.1
4	D	229	ALA	2.1
2	B	502	VAL	2.1
2	B	485	GLU	2.0
2	B	486	LEU	2.0
10	K	17	ILE	2.0
18	x	39	ARG	2.0
20	Z	38	GLN	2.0
1	a	249	VAL	2.0
20	z	59	PHE	2.0

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

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
15	FME	T	1	10/11	0.94	0.10	36,48,68,68	0
15	FME	t	1	10/11	0.95	0.09	34,48,77,77	0
12	FME	M	1	10/11	0.96	0.10	47,57,75,77	0
8	FME	I	1	10/11	0.96	0.15	48,61,80,82	0
8	FME	i	1	10/11	0.97	0.15	46,59,70,75	0
12	FME	m	1	10/11	0.97	0.13	40,57,76,89	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
31	STE	R	101	12/20	0.67	0.32	68,87,105,110	0
31	STE	H	103	18/20	0.69	0.32	56,85,97,102	0
26	LHG	A	412	49/49	0.79	0.26	46,87,119,124	0
23	BCR	X	101	40/40	0.79	0.17	34,54,70,73	0
32	LMG	c	522	48/55	0.79	0.24	42,81,110,115	0
31	STE	a	416	12/20	0.81	0.27	35,72,80,82	0
25	PL9	A	408	55/55	0.81	0.27	42,71,90,93	0
26	LHG	e	101	42/49	0.81	0.28	60,94,114,125	0
31	STE	T	103	15/20	0.82	0.18	40,62,91,93	0
31	STE	c	521	20/20	0.82	0.22	45,65,94,110	0
31	STE	B	624	16/20	0.82	0.24	40,64,83,86	0
31	STE	h	103	14/20	0.82	0.26	57,74,88,95	0
32	LMG	D	410	33/55	0.82	0.19	42,60,95,106	0
22	CLA	C	512	65/65	0.83	0.20	41,62,105,110	0
31	STE	b	622	16/20	0.83	0.17	44,66,87,93	0
31	STE	b	623	20/20	0.83	0.21	44,66,96,98	0
31	STE	B	623	18/20	0.84	0.16	45,65,90,95	0
32	LMG	c	523	49/55	0.84	0.18	37,62,105,119	0
31	STE	d	412	20/20	0.84	0.19	53,75,97,103	0
25	PL9	a	410	55/55	0.84	0.21	43,76,96,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	STE	C	522	12/20	0.84	0.14	40,56,65,69	0
22	CLA	c	513	65/65	0.84	0.16	47,65,103,110	0
23	BCR	h	101	40/40	0.84	0.17	41,63,87,90	0
31	STE	I	101	15/20	0.85	0.15	43,64,86,87	0
31	STE	d	411	20/20	0.85	0.25	49,67,82,86	0
22	CLA	b	601	65/65	0.85	0.19	52,76,101,103	0
31	STE	b	620	20/20	0.85	0.24	44,61,82,88	0
32	LMG	b	621	55/55	0.85	0.29	50,79,102,113	0
31	STE	B	625	15/20	0.85	0.19	43,66,83,92	0
31	STE	a	415	10/20	0.85	0.20	33,67,81,83	0
32	LMG	a	417	55/55	0.86	0.15	39,61,90,107	0
31	STE	M	103	10/20	0.86	0.18	40,54,63,72	0
28	DGD	A	414	66/66	0.86	0.17	43,67,92,99	0
31	STE	c	501	12/20	0.86	0.17	44,72,81,86	0
31	STE	Z	101	8/20	0.86	0.18	42,63,77,77	0
22	CLA	C	513	65/65	0.86	0.21	51,69,108,113	0
31	STE	B	620	17/20	0.87	0.14	39,56,72,81	0
31	STE	B	601	12/20	0.87	0.41	56,74,93,94	0
31	STE	M	102	15/20	0.87	0.15	43,60,73,74	0
23	BCR	K	102	40/40	0.87	0.13	42,61,76,76	0
22	CLA	H	101	65/65	0.87	0.16	43,68,99,105	0
31	STE	B	622	12/20	0.87	0.13	35,58,68,76	0
27	SQD	B	621	54/54	0.88	0.15	41,64,93,101	0
22	CLA	c	514	65/65	0.88	0.20	47,72,110,119	0
27	SQD	d	409	41/54	0.88	0.20	59,95,120,123	0
32	LMG	Y	101	48/55	0.88	0.18	50,77,102,109	0
27	SQD	L	101	49/54	0.88	0.13	42,64,97,117	0
31	STE	C	521	16/20	0.88	0.15	46,61,71,77	0
27	SQD	a	414	36/54	0.88	0.17	24,66,100,107	0
31	STE	b	624	10/20	0.88	0.28	41,58,71,73	0
31	STE	D	413	20/20	0.89	0.17	38,56,85,86	0
31	STE	M	104	18/20	0.89	0.15	37,51,85,94	0
32	LMG	C	516	48/55	0.89	0.15	37,60,85,102	0
31	STE	C	520	12/20	0.89	0.13	45,63,73,76	0
27	SQD	A	413	39/54	0.89	0.17	45,70,99,104	0
32	LMG	D	411	28/55	0.89	0.15	35,54,68,74	0
23	BCR	k	101	40/40	0.89	0.14	40,67,80,83	0
31	STE	T	102	16/20	0.89	0.15	40,55,78,91	0
31	STE	L	103	12/20	0.89	0.19	55,70,86,96	0
23	BCR	k	102	40/40	0.90	0.18	40,58,70,72	0
22	CLA	C	502	65/65	0.90	0.16	32,48,65,66	0
31	STE	t	102	14/20	0.90	0.12	39,51,63,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	BCR	D	406	40/40	0.90	0.14	33,49,89,93	0
22	CLA	a	405	65/65	0.91	0.14	22,40,94,108	0
23	BCR	d	404	40/40	0.91	0.13	36,56,96,97	0
22	CLA	c	503	65/65	0.91	0.16	35,47,65,71	0
32	LMG	M	101	51/55	0.91	0.13	34,54,82,89	0
28	DGD	C	518	62/66	0.91	0.14	38,59,101,119	0
22	CLA	D	405	65/65	0.91	0.14	24,45,110,127	0
31	STE	j	101	12/20	0.91	0.17	47,65,78,79	0
32	LMG	m	101	51/55	0.91	0.14	31,58,83,98	0
22	CLA	C	507	65/65	0.92	0.15	30,48,65,71	0
27	SQD	F	102	36/54	0.92	0.18	53,78,93,101	0
22	CLA	c	509	64/65	0.92	0.15	36,53,103,122	0
23	BCR	K	101	40/40	0.92	0.15	45,63,78,89	0
22	CLA	b	616	60/65	0.92	0.15	33,50,91,95	0
23	BCR	c	515	40/40	0.92	0.18	46,65,82,84	0
22	CLA	b	615	65/65	0.92	0.14	30,46,67,79	0
23	BCR	C	514	40/40	0.92	0.12	30,47,59,73	0
32	LMG	D	408	51/55	0.93	0.18	33,65,95,99	0
28	DGD	c	519	62/66	0.93	0.14	31,59,86,90	0
22	CLA	c	504	65/65	0.93	0.15	35,50,61,64	0
22	CLA	d	403	65/65	0.93	0.14	32,55,102,112	0
23	BCR	b	619	40/40	0.93	0.10	34,53,64,73	0
23	BCR	C	515	40/40	0.93	0.16	45,60,79,83	0
22	CLA	B	616	60/65	0.93	0.14	27,46,107,121	0
22	CLA	B	615	65/65	0.93	0.13	26,43,65,70	0
32	LMG	c	520	37/55	0.93	0.15	49,70,89,90	0
22	CLA	c	507	65/65	0.93	0.13	33,54,91,108	0
32	LMG	d	408	44/55	0.93	0.15	36,61,95,103	0
22	CLA	C	503	65/65	0.94	0.15	35,51,62,64	0
22	CLA	C	505	65/65	0.94	0.15	27,47,70,73	0
22	CLA	C	508	65/65	0.94	0.14	30,51,113,130	0
23	BCR	B	618	40/40	0.94	0.10	30,43,56,61	0
28	DGD	c	518	62/66	0.94	0.12	37,57,94,108	0
23	BCR	B	617	40/40	0.94	0.13	29,46,63,67	0
23	BCR	b	617	40/40	0.94	0.12	31,49,60,63	0
22	CLA	b	602	65/65	0.94	0.15	29,47,70,76	0
23	BCR	b	618	40/40	0.94	0.11	26,46,60,67	0
22	CLA	a	403	65/65	0.94	0.14	29,45,101,111	0
22	CLA	c	510	65/65	0.94	0.19	32,54,72,73	0
27	SQD	a	413	54/54	0.94	0.15	47,66,94,98	0
22	CLA	B	602	65/65	0.94	0.17	27,41,68,77	0
28	DGD	h	102	62/66	0.94	0.12	37,53,67,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	c	508	65/65	0.94	0.14	33,48,64,75	0
22	CLA	c	506	65/65	0.94	0.17	30,49,70,81	0
25	PL9	D	407	55/55	0.94	0.12	25,39,51,66	0
28	DGD	H	102	62/66	0.94	0.11	31,51,65,77	0
22	CLA	B	604	65/65	0.94	0.13	22,37,79,93	0
22	CLA	C	504	59/65	0.94	0.12	33,47,84,103	0
22	CLA	C	506	65/65	0.94	0.12	28,48,91,99	0
22	CLA	B	606	65/65	0.94	0.11	20,41,72,78	0
31	STE	d	410	17/20	0.94	0.12	44,60,69,76	0
23	BCR	B	619	40/40	0.94	0.10	28,47,61,74	0
22	CLA	C	510	65/65	0.94	0.15	31,52,70,74	0
22	CLA	C	511	65/65	0.94	0.11	38,56,75,80	0
22	CLA	C	509	65/65	0.94	0.19	29,50,70,77	0
22	CLA	b	609	65/65	0.94	0.14	32,51,76,78	0
22	CLA	b	614	65/65	0.95	0.12	29,43,84,94	0
22	CLA	c	512	65/65	0.95	0.12	40,61,79,85	0
22	CLA	C	501	65/65	0.95	0.12	28,42,53,62	0
22	CLA	b	604	65/65	0.95	0.14	28,41,91,114	0
23	BCR	A	405	40/40	0.95	0.09	26,40,48,51	0
22	CLA	b	608	65/65	0.95	0.15	29,48,70,87	0
22	CLA	b	613	65/65	0.95	0.14	22,41,82,90	0
27	SQD	A	411	52/54	0.95	0.16	41,66,102,108	0
22	CLA	A	404	54/65	0.95	0.11	21,36,64,77	0
23	BCR	c	516	40/40	0.95	0.11	31,50,77,78	0
22	CLA	b	606	65/65	0.95	0.12	30,45,78,87	0
22	CLA	B	603	65/65	0.95	0.17	23,38,66,74	0
22	CLA	B	609	65/65	0.95	0.13	28,46,66,74	0
28	DGD	C	517	62/66	0.95	0.13	27,42,78,88	0
22	CLA	b	611	65/65	0.95	0.13	20,39,63,71	0
26	LHG	l	101	49/49	0.95	0.11	34,51,60,72	0
26	LHG	A	410	47/49	0.95	0.13	34,53,93,105	0
22	CLA	c	511	65/65	0.95	0.15	35,54,72,75	0
31	STE	J	101	12/20	0.95	0.12	48,64,78,79	0
23	BCR	T	101	40/40	0.95	0.09	27,46,64,66	0
22	CLA	A	403	65/65	0.95	0.14	24,40,103,110	0
28	DGD	C	519	62/66	0.95	0.12	29,55,84,94	0
22	CLA	b	605	65/65	0.95	0.15	29,41,60,66	0
22	CLA	a	411	65/65	0.95	0.13	21,37,47,52	0
26	LHG	a	412	49/49	0.95	0.13	33,53,75,84	0
28	DGD	c	517	62/66	0.95	0.12	28,46,79,95	0
23	BCR	a	406	40/40	0.96	0.08	24,37,48,58	0
33	PHO	d	401	64/64	0.96	0.09	27,44,54,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	d	402	65/65	0.96	0.12	25,40,65,80	0
22	CLA	b	612	65/65	0.96	0.17	22,39,54,60	0
33	PHO	D	402	64/64	0.96	0.14	26,37,46,47	0
22	CLA	D	404	65/65	0.96	0.12	19,33,58,67	0
22	CLA	c	505	60/65	0.96	0.11	37,54,82,90	0
22	CLA	c	502	65/65	0.96	0.13	29,44,56,62	0
25	PL9	d	405	55/55	0.96	0.11	26,40,51,54	0
22	CLA	A	402	65/65	0.96	0.10	18,33,51,69	0
26	LHG	D	412	49/49	0.96	0.12	34,48,69,76	0
22	CLA	B	613	65/65	0.96	0.14	21,38,77,88	0
22	CLA	B	612	65/65	0.96	0.15	24,37,51,56	0
22	CLA	B	610	65/65	0.96	0.14	22,36,47,54	0
22	CLA	B	614	65/65	0.96	0.15	24,41,87,101	0
35	HEC	f	101	43/43	0.96	0.12	48,65,89,92	0
33	PHO	D	401	64/64	0.96	0.10	21,34,45,48	0
33	PHO	a	404	64/64	0.96	0.13	24,34,44,44	0
22	CLA	b	610	65/65	0.96	0.17	27,43,56,64	0
22	CLA	A	409	65/65	0.96	0.10	23,34,56,61	0
22	CLA	a	402	65/65	0.96	0.11	22,34,48,60	0
26	LHG	d	407	39/49	0.96	0.10	35,53,78,84	0
22	CLA	B	605	65/65	0.96	0.15	25,37,51,53	0
22	CLA	b	603	65/65	0.96	0.15	25,43,77,92	0
22	CLA	B	607	65/65	0.96	0.11	22,35,71,80	0
22	CLA	B	608	65/65	0.96	0.12	23,39,63,69	0
23	BCR	t	101	40/40	0.96	0.09	25,43,56,57	0
22	CLA	b	607	65/65	0.96	0.11	22,43,71,75	0
35	HEC	v	201	43/43	0.97	0.12	30,41,55,57	0
26	LHG	L	102	49/49	0.97	0.13	30,47,62,69	0
35	HEC	V	201	43/43	0.97	0.12	28,37,45,54	0
22	CLA	B	611	65/65	0.97	0.15	23,34,51,51	0
26	LHG	D	409	49/49	0.97	0.10	26,43,55,62	0
26	LHG	d	406	49/49	0.97	0.10	30,46,60,68	0
35	HEC	F	101	43/43	0.97	0.11	40,57,70,79	0
34	BCT	a	409	4/4	0.98	0.21	32,35,48,57	0
34	BCT	D	403	4/4	0.98	0.17	33,37,44,45	0
24	CL	A	407	1/1	0.99	0.04	36,36,36,36	0
24	CL	A	406	1/1	0.99	0.09	34,34,34,34	0
29	OEX	a	418[A]	10/10	0.99	0.11	33,39,42,43	10
24	CL	a	407	1/1	0.99	0.03	32,32,32,32	0
29	OEX	A	415[A]	10/10	0.99	0.14	36,38,42,43	10
24	CL	a	408	1/1	0.99	0.03	34,34,34,34	0
30	OXY	a	419[B]	11/11	0.99	0.12	18,23,28,29	11

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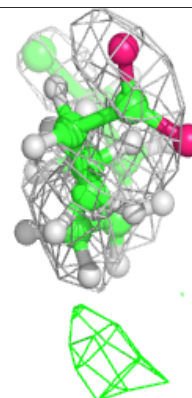
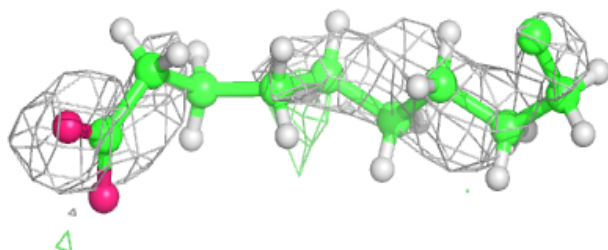
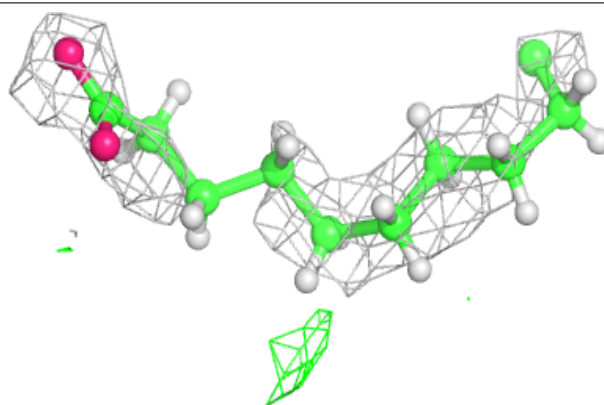
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	OEY	A	416[B]	11/11	0.99	0.14	18,23,28,28	11
21	FE2	a	401	1/1	1.00	0.11	38,38,38,38	0
21	FE2	A	401	1/1	1.00	0.14	37,37,37,37	0

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.

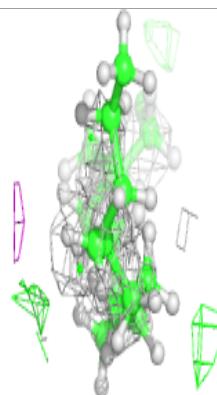
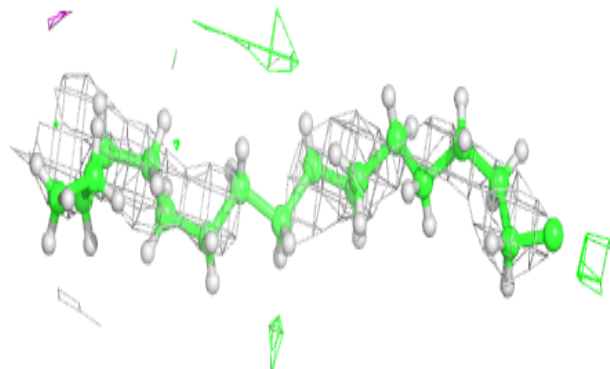
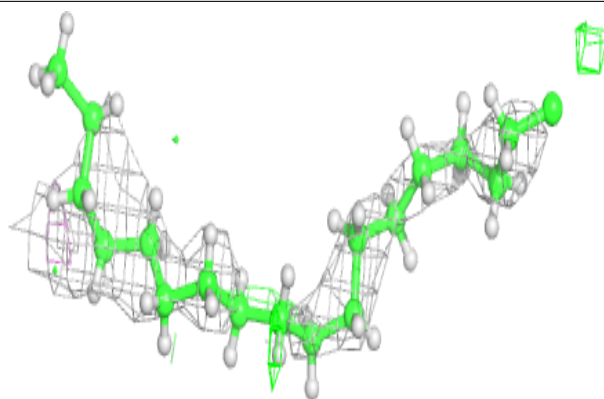
Electron density around STE R 101:

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



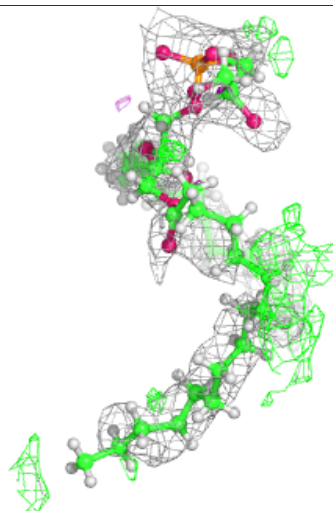
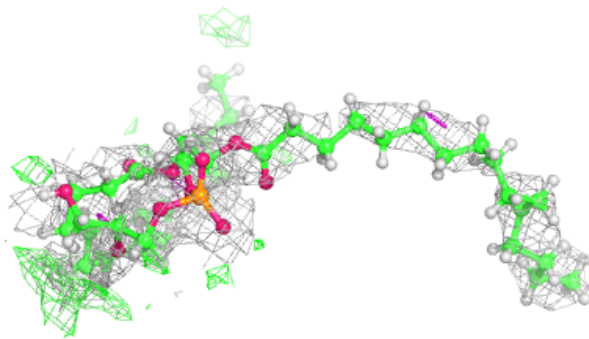
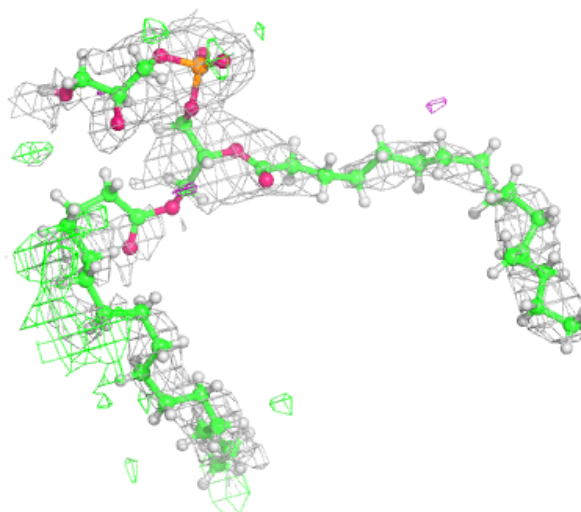
Electron density around STE H 103:

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



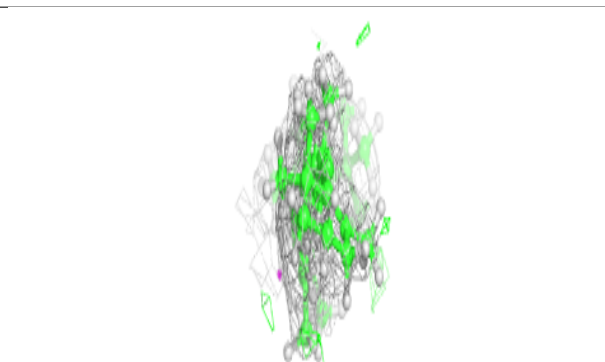
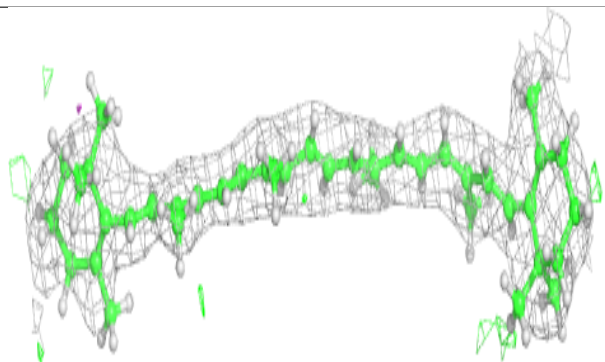
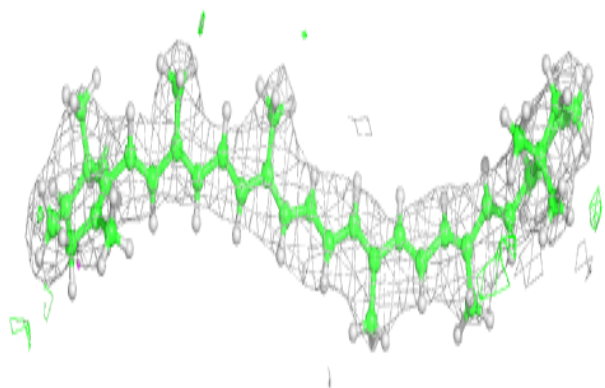
Electron density around LHG A 412:

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

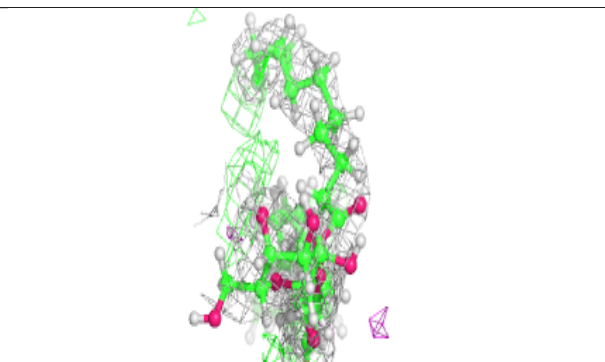
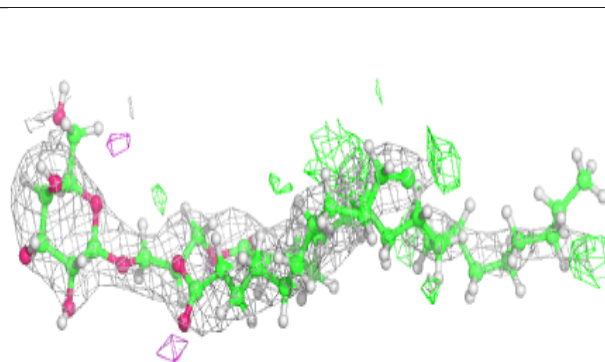
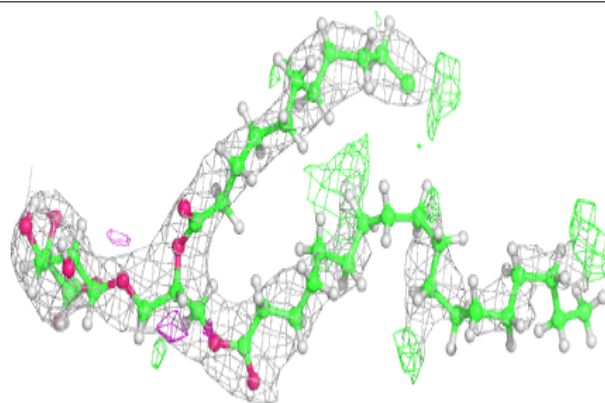


Electron density around BCR X 101:

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

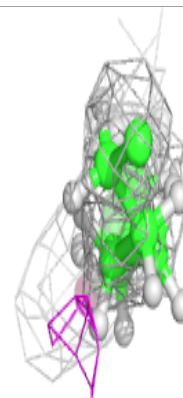
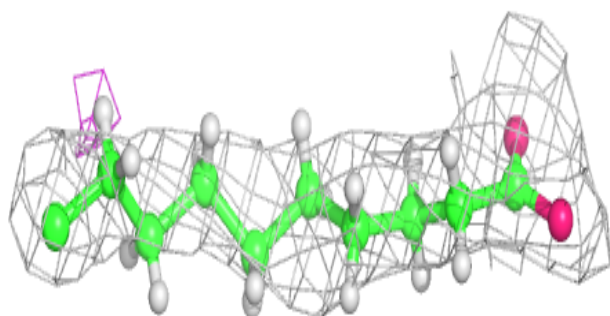
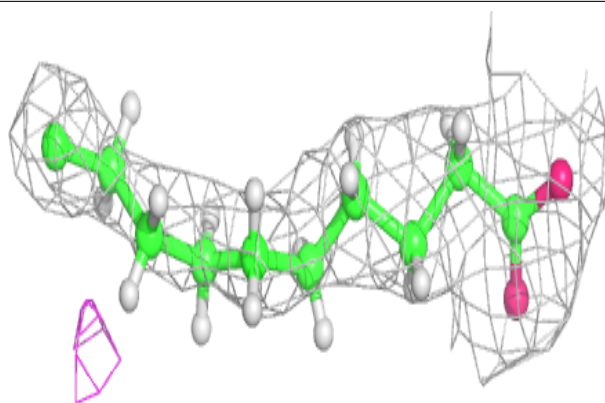
**Electron density around LMG c 522:**

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

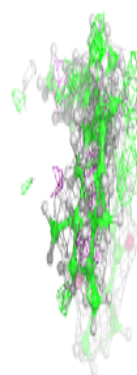
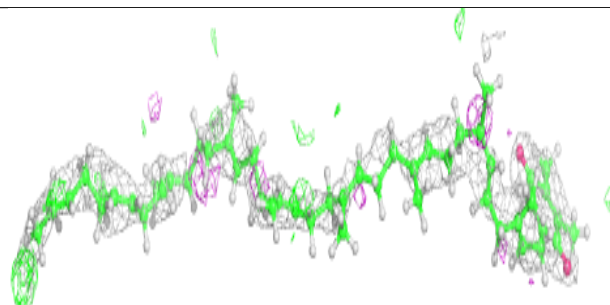
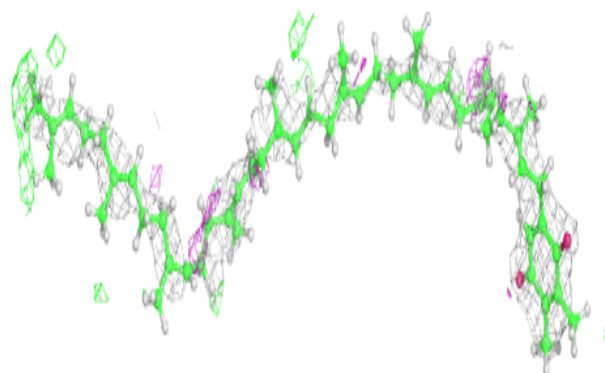


Electron density around STE a 416:

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

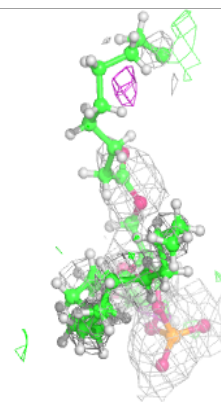
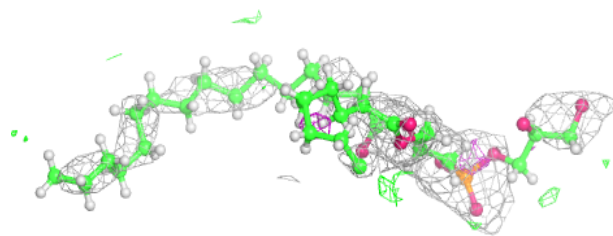
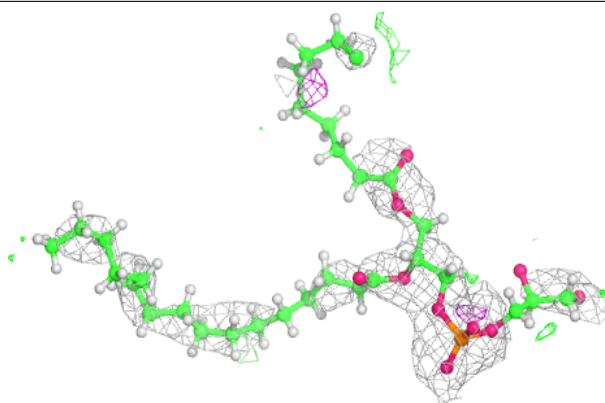
**Electron density around PL9 A 408:**

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

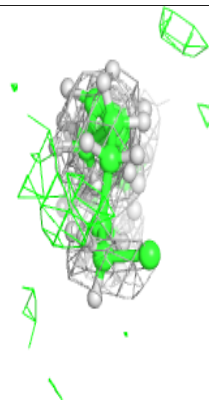
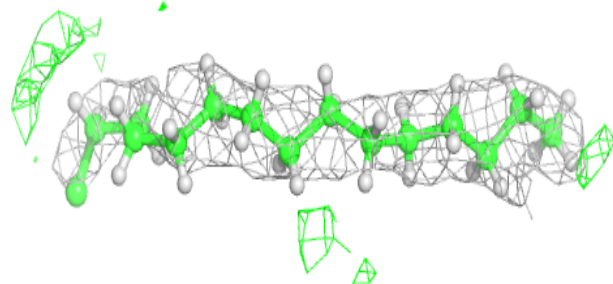
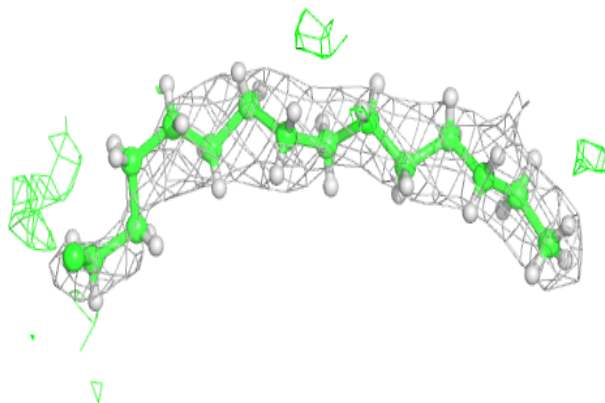


Electron density around LHG e 101:

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

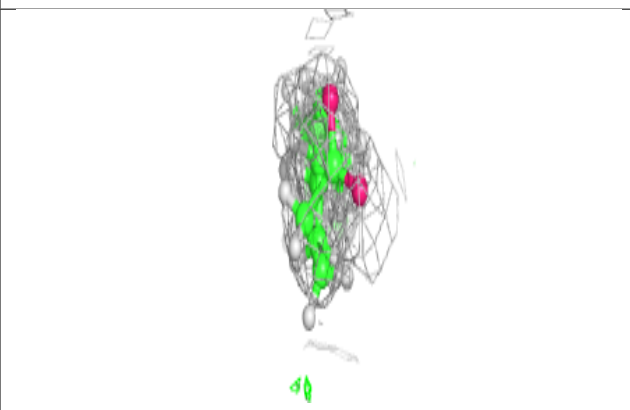
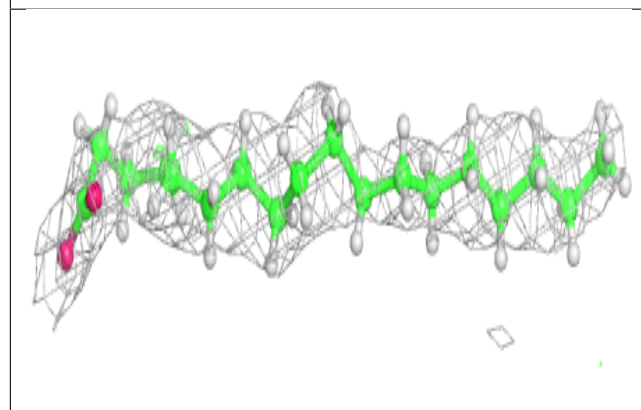
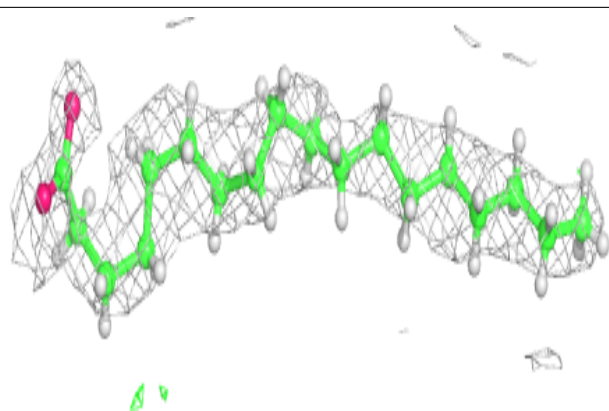
**Electron density around STE T 103:**

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

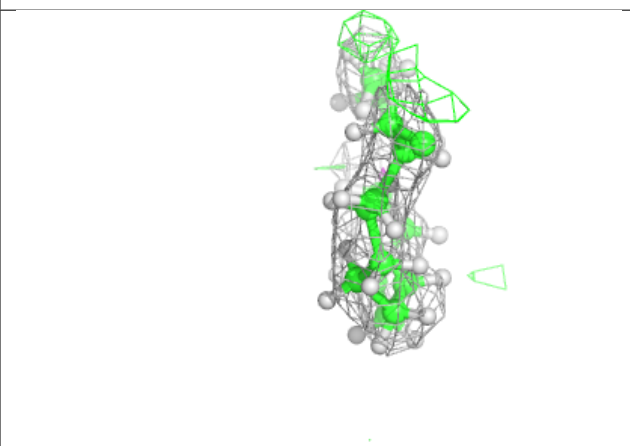
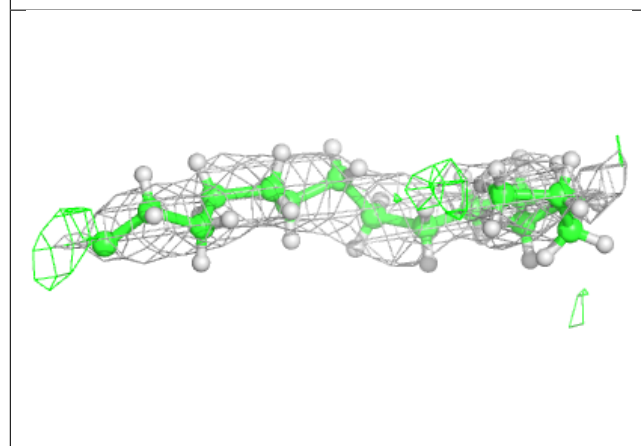
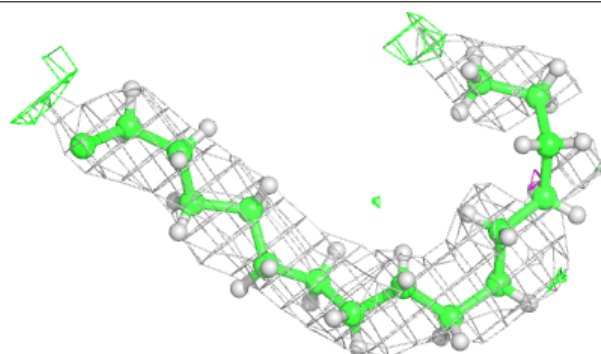


Electron density around STE c 521:

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

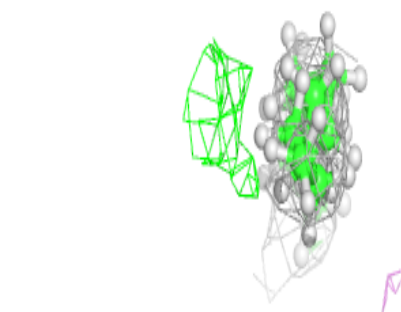
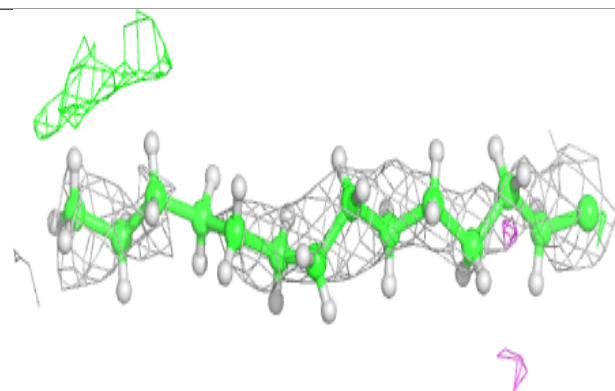
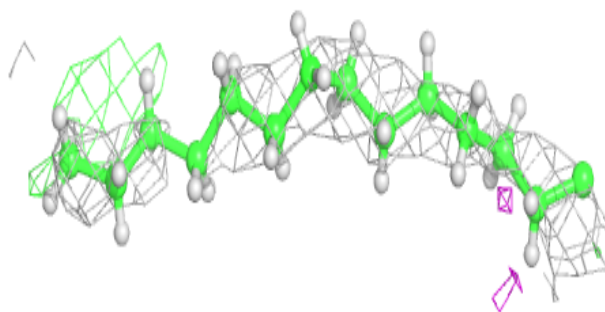
**Electron density around STE B 624:**

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and green (positive)

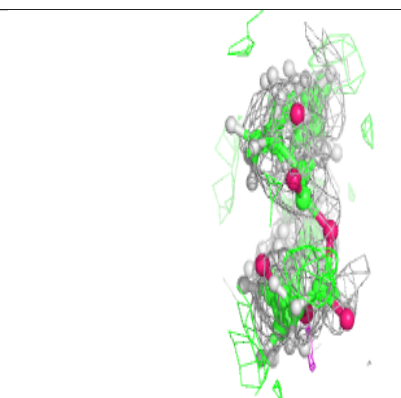
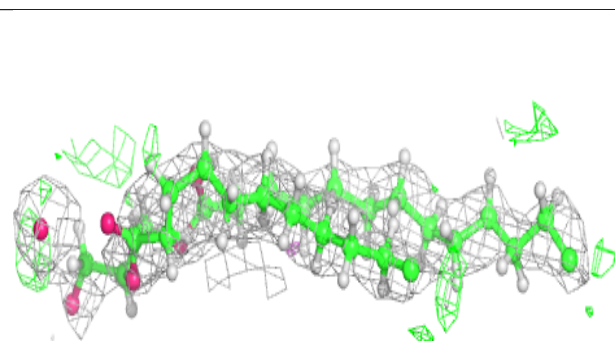
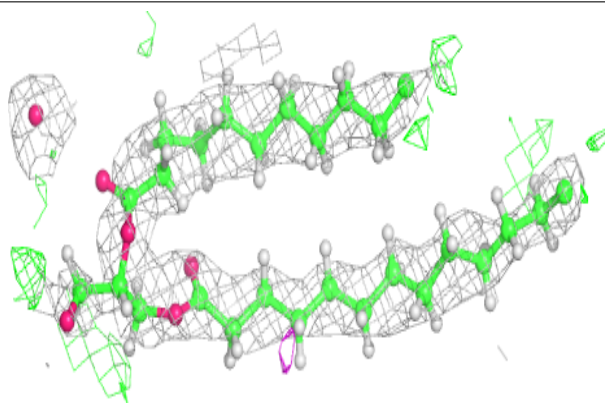


Electron density around STE h 103:

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and green (positive)

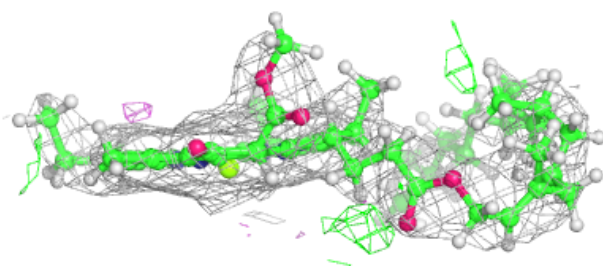
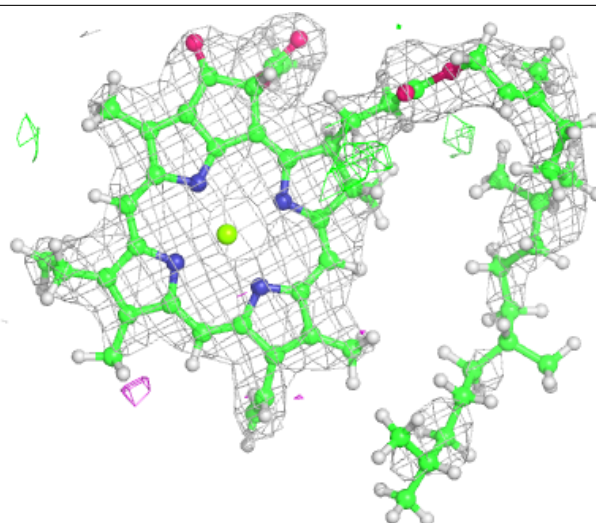
**Electron density around LMG D 410:**

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



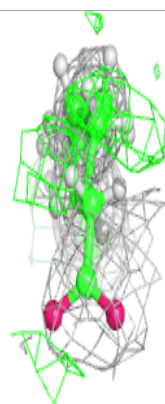
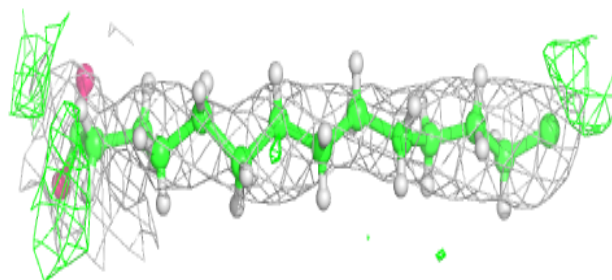
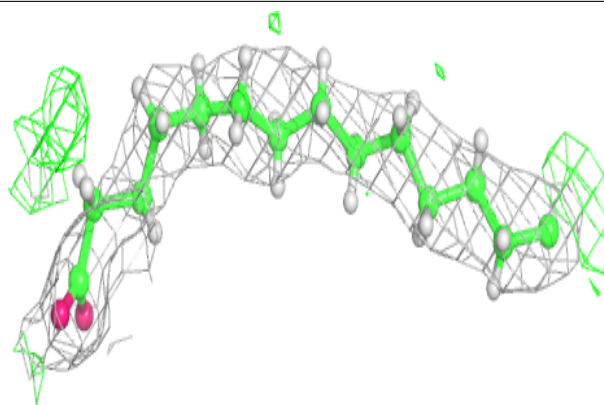
Electron density around CLA C 512:

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and green (positive)

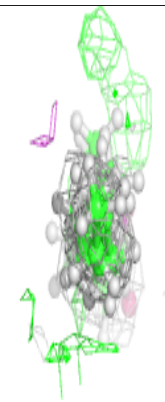
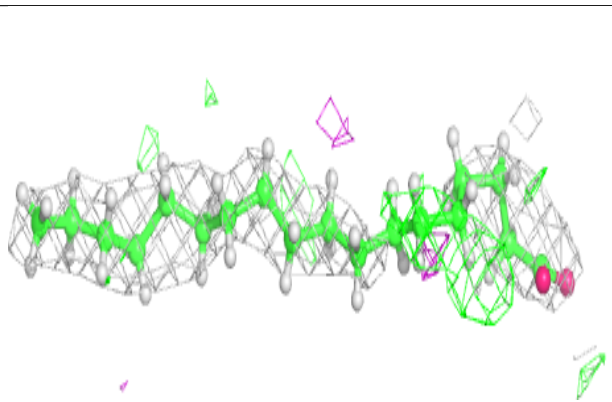
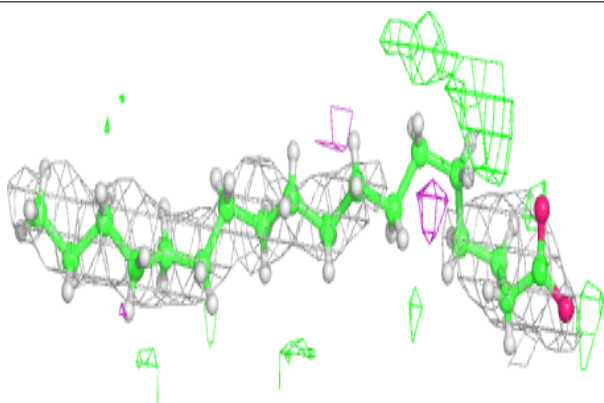


Electron density around STE b 622:

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

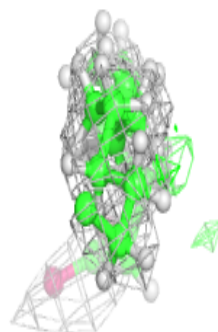
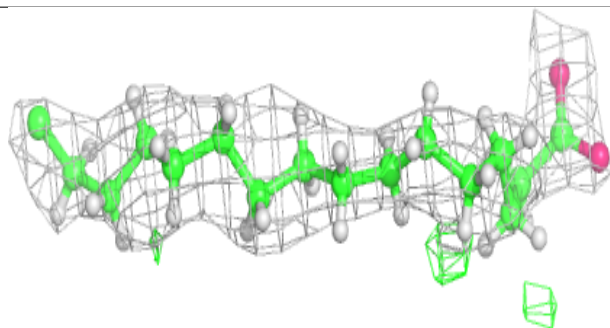
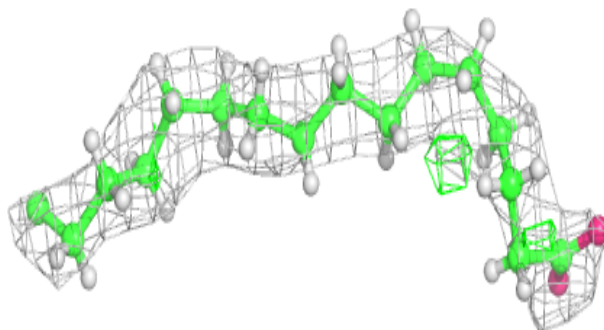
**Electron density around STE b 623:**

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

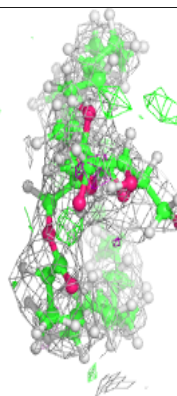
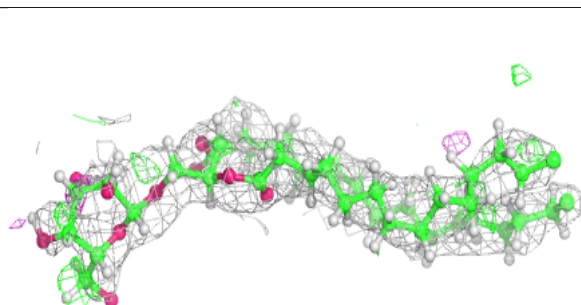
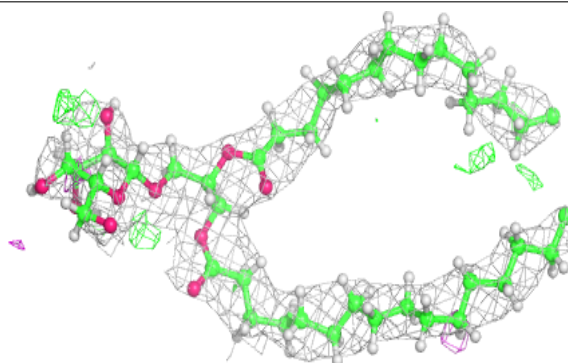


Electron density around STE B 623:

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and green (positive)

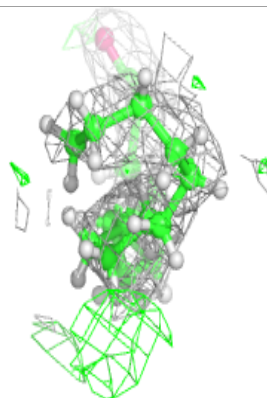
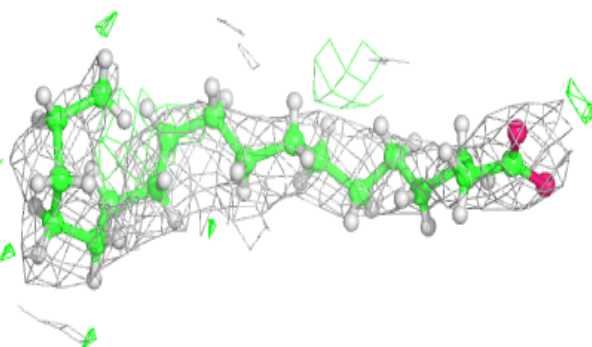
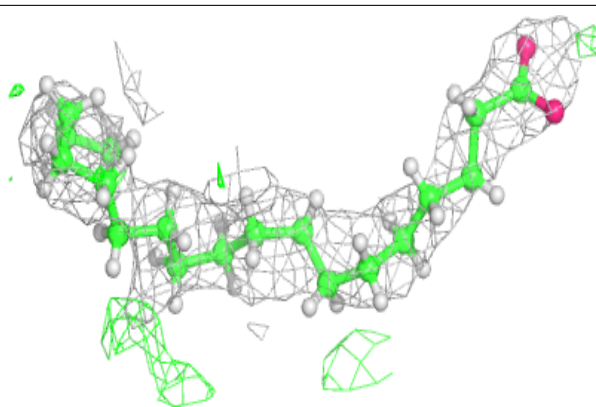
**Electron density around LMG c 523:**

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

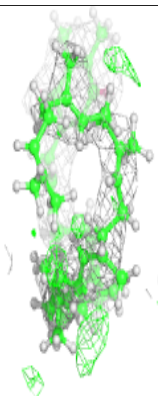
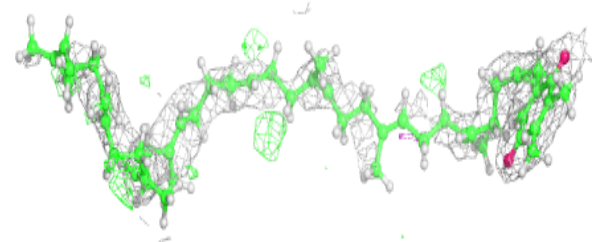
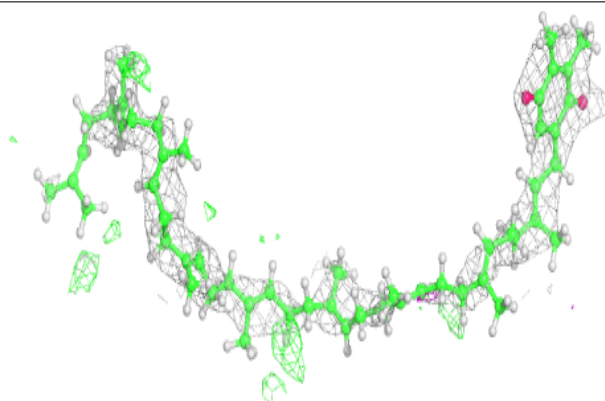


Electron density around STE d 412:

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

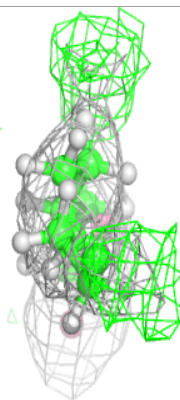
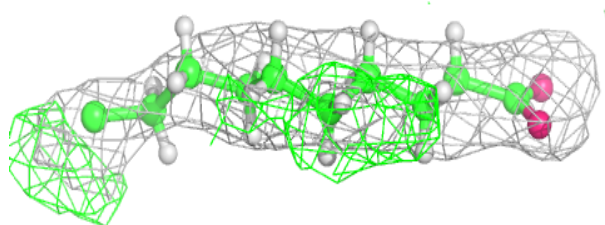
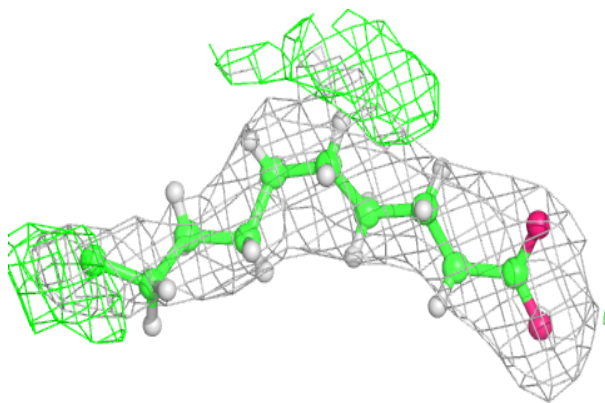
**Electron density around PL9 a 410:**

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



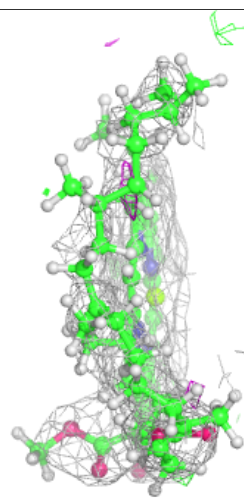
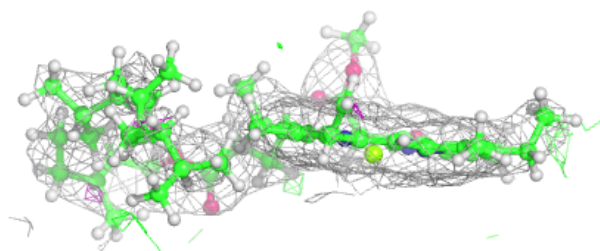
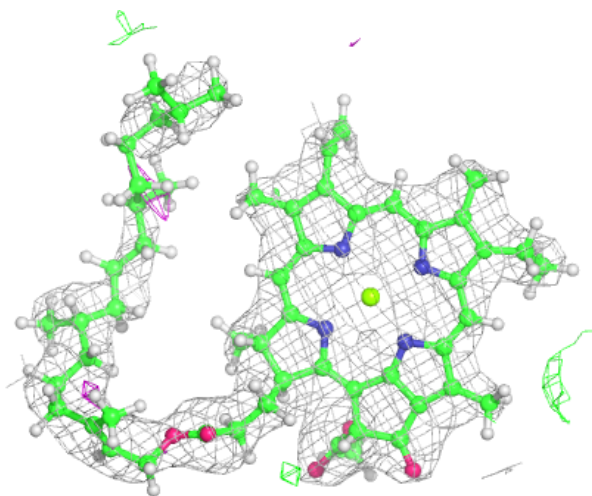
Electron density around STE C 522:

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



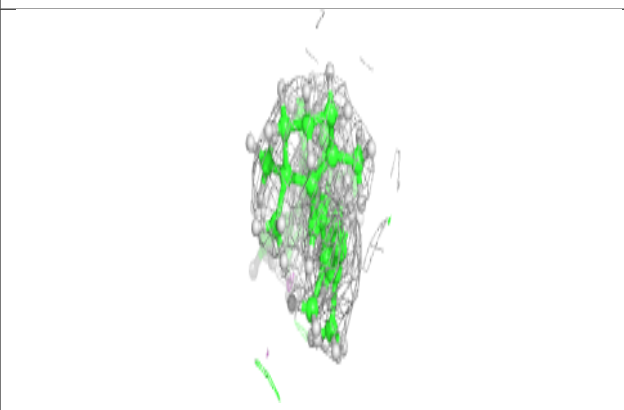
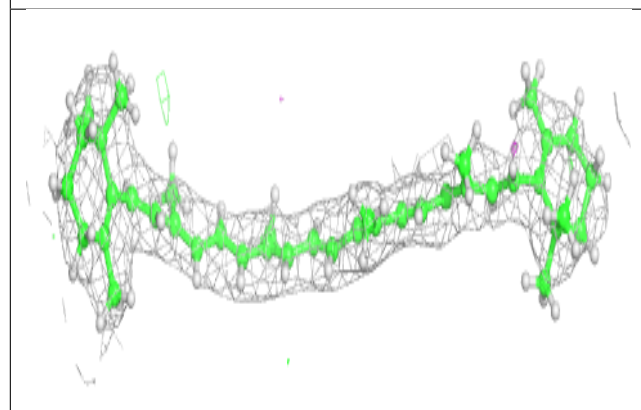
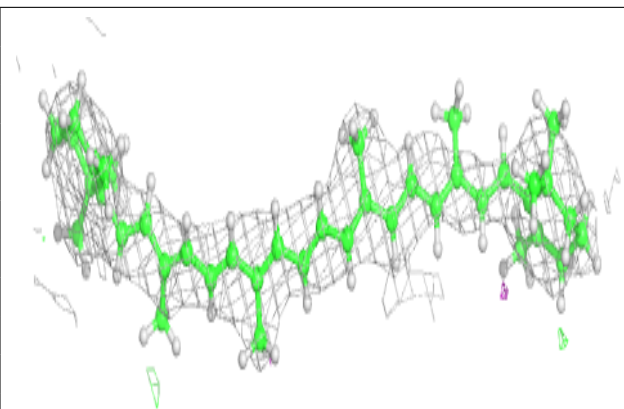
Electron density around CLA c 513:

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

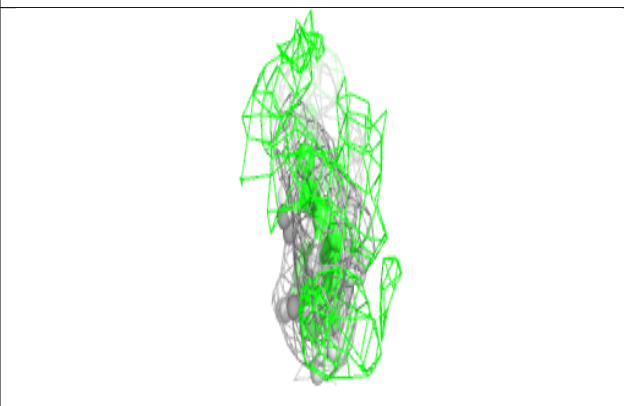
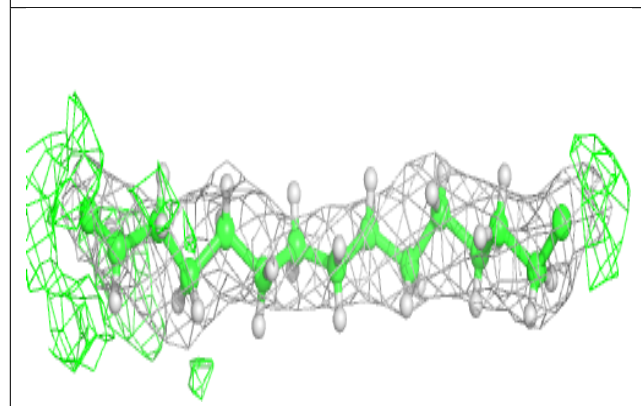
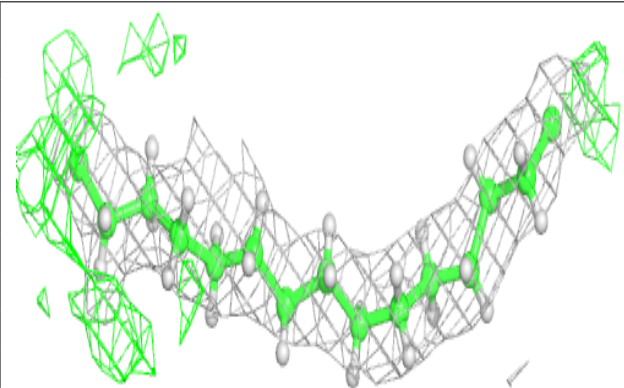


Electron density around BCR h 101:

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

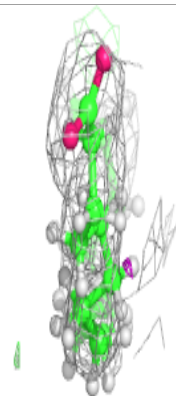
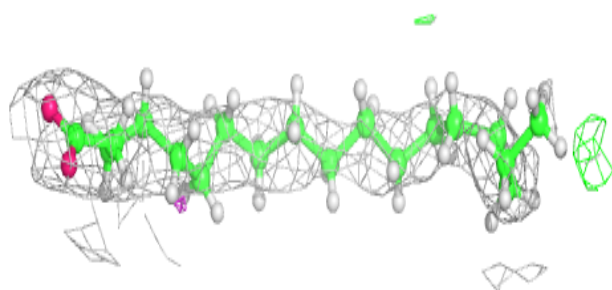
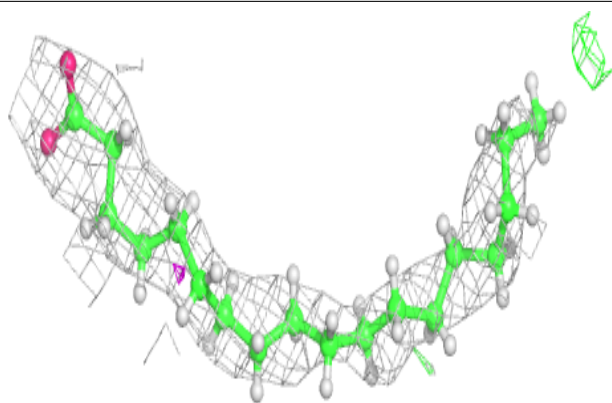
**Electron density around STE I 101:**

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

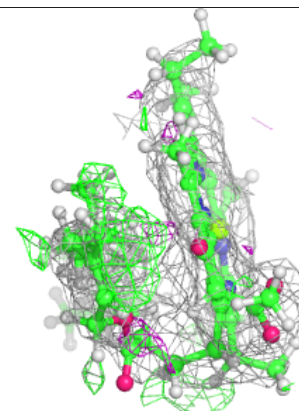
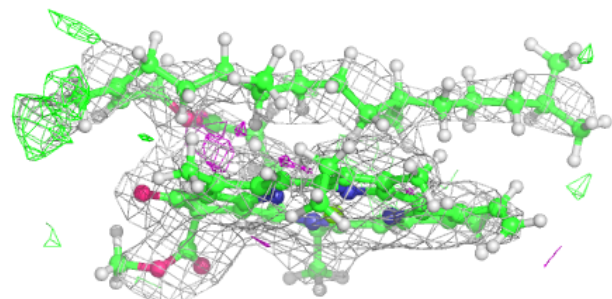
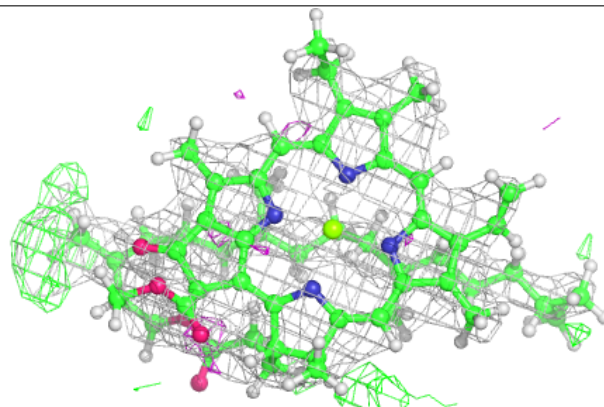


Electron density around STE d 411:

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

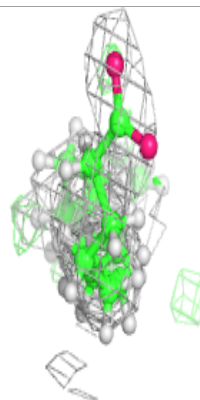
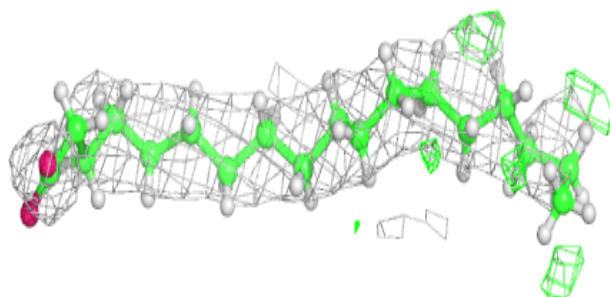
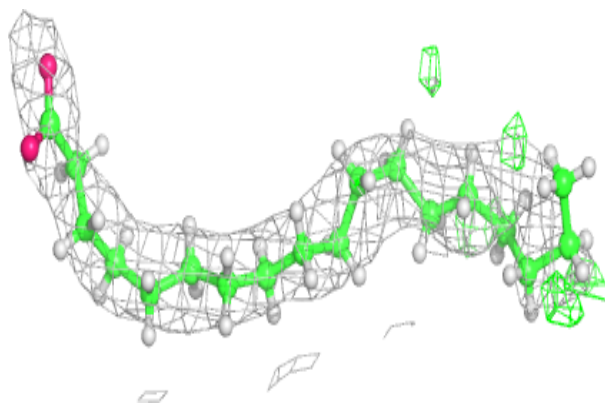
**Electron density around CLA b 601:**

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

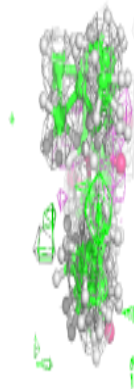
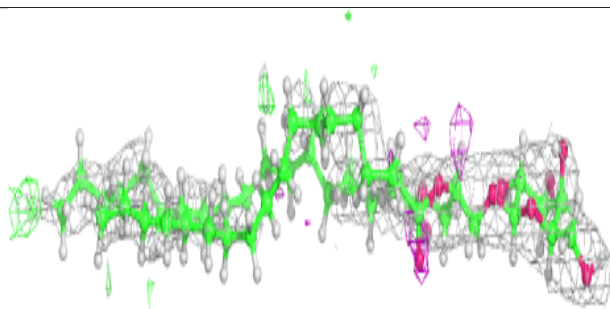
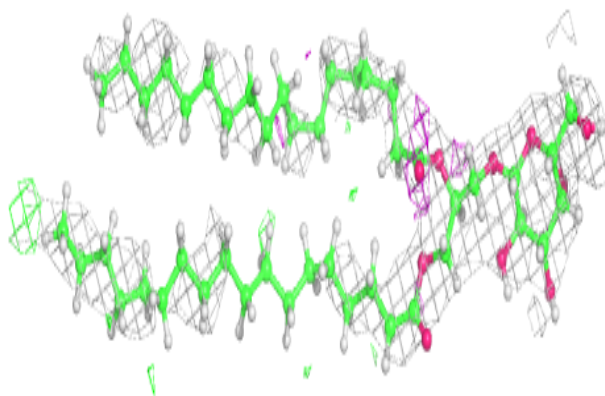


Electron density around STE b 620:

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

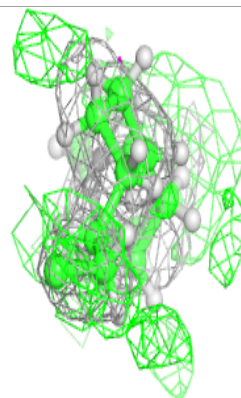
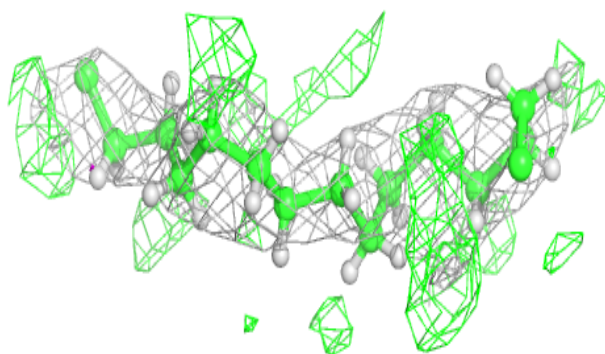
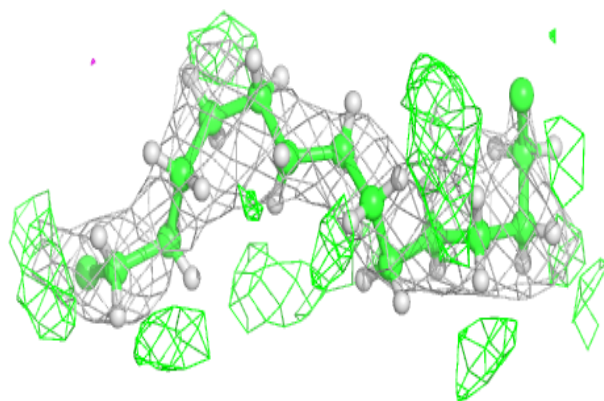
**Electron density around LMG b 621:**

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

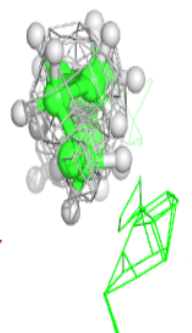
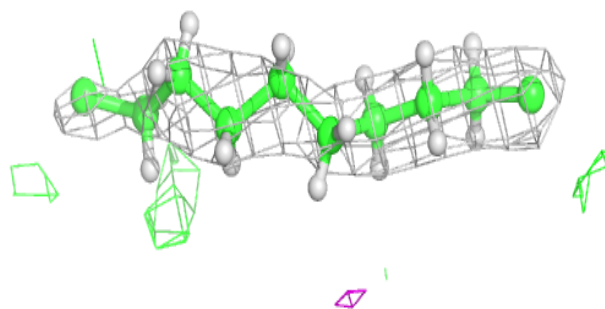
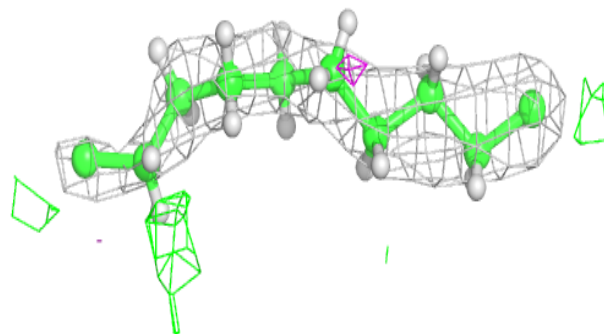


Electron density around STE B 625:

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

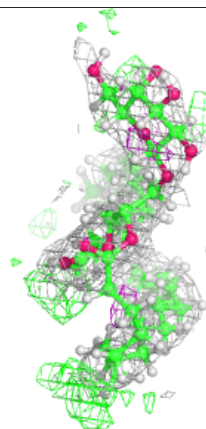
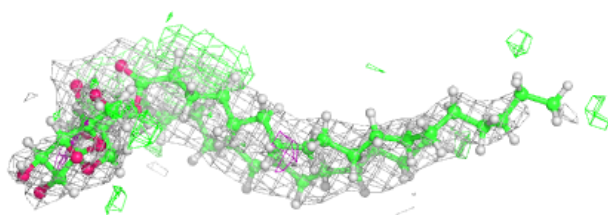
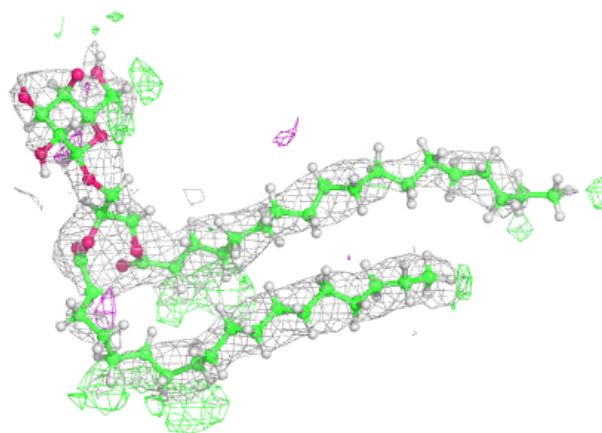
**Electron density around STE a 415:**

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

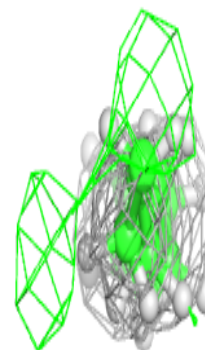
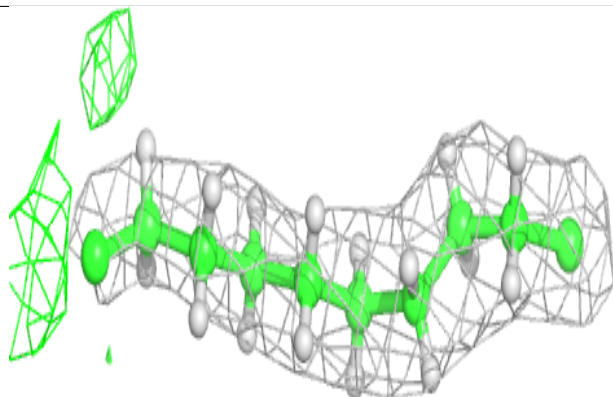
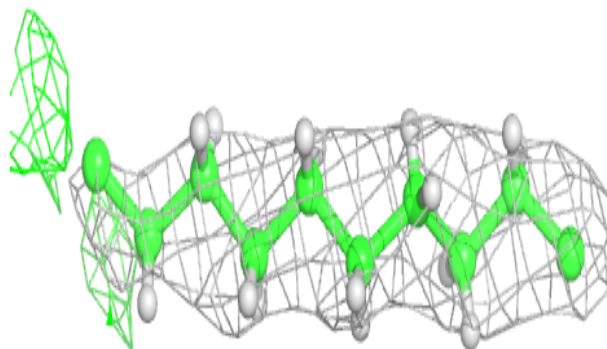


Electron density around LMG a 417:

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

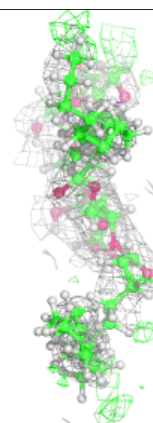
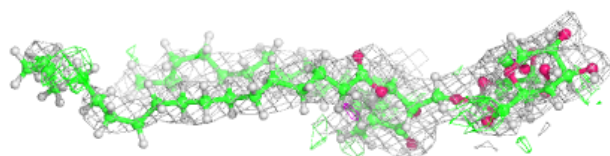
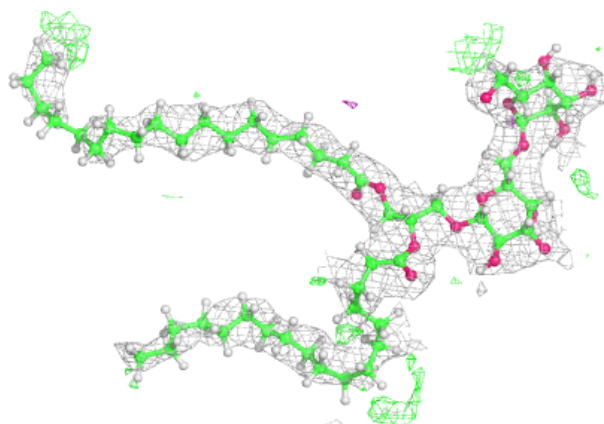
**Electron density around STE M 103:**

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

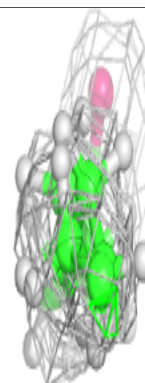
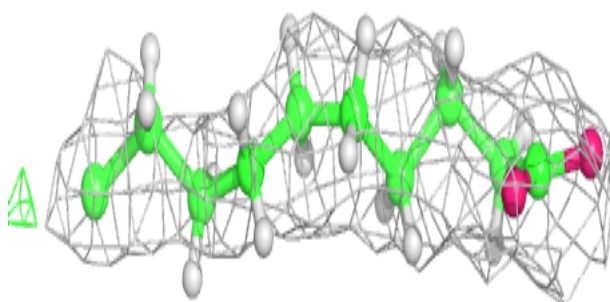
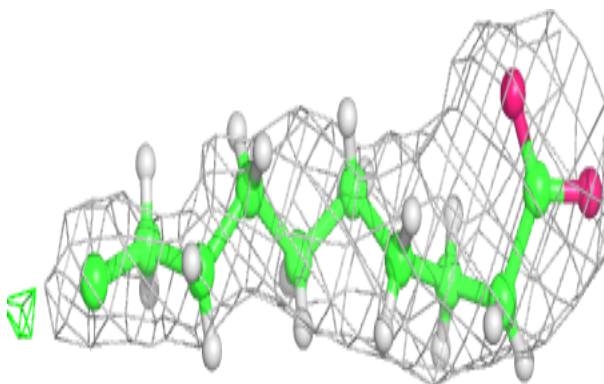


Electron density around DGD A 414:

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

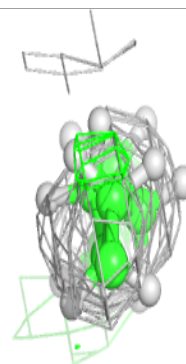
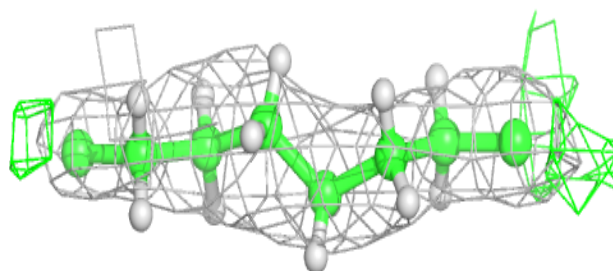
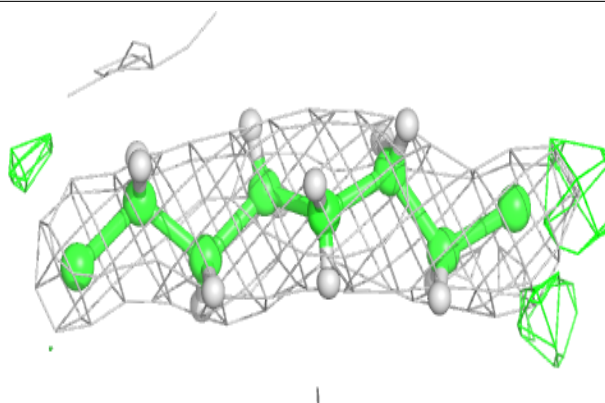
**Electron density around STE c 501:**

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

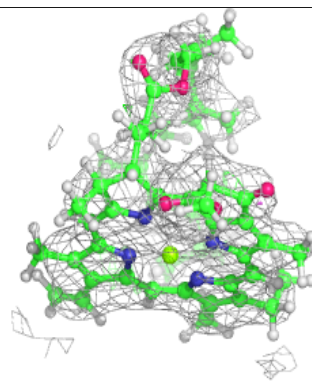
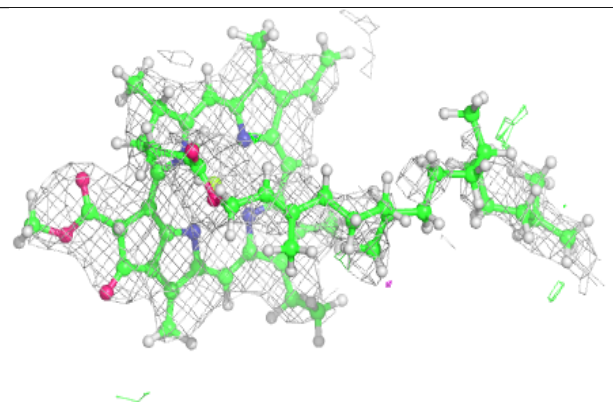
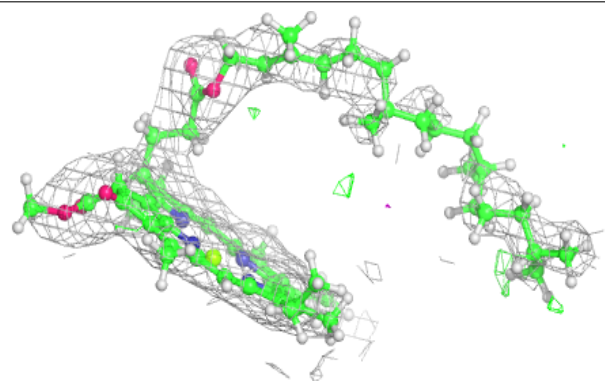


Electron density around STE Z 101:

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

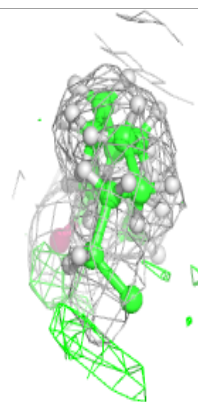
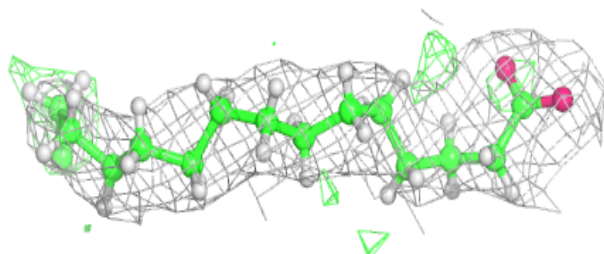
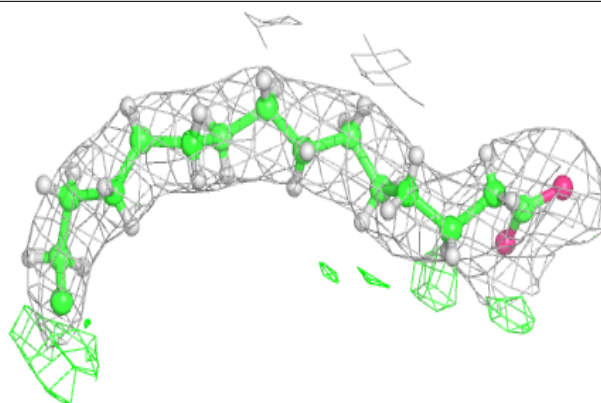
**Electron density around CLA C 513:**

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

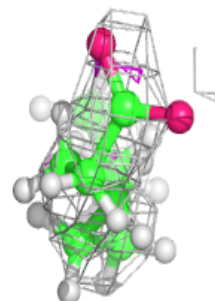
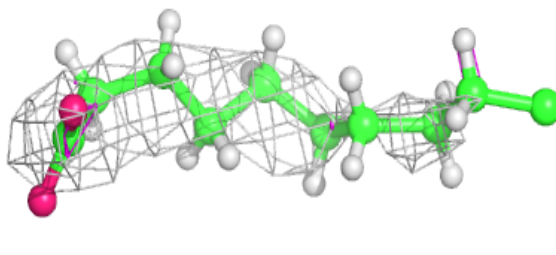
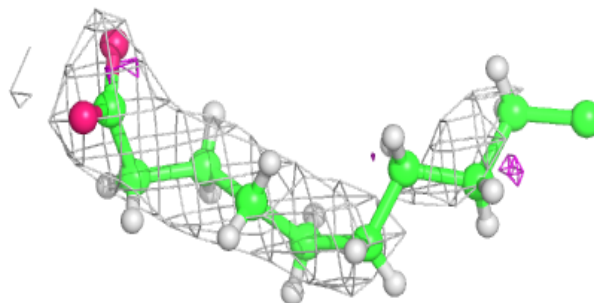


Electron density around STE B 620:

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

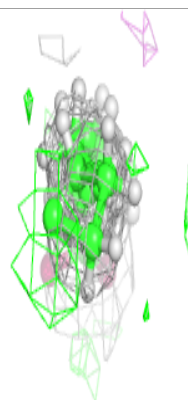
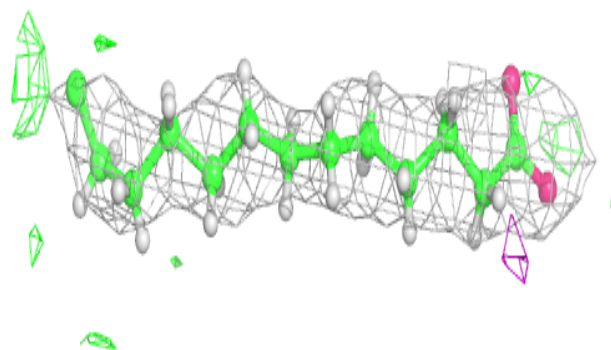
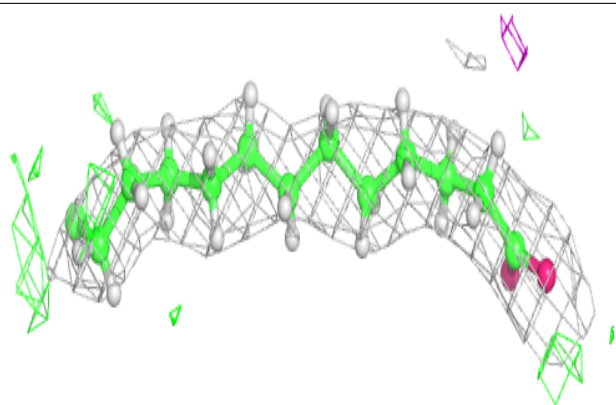
**Electron density around STE B 601:**

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

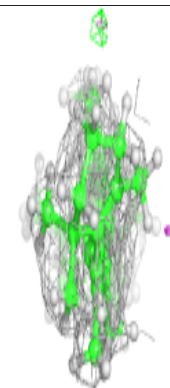
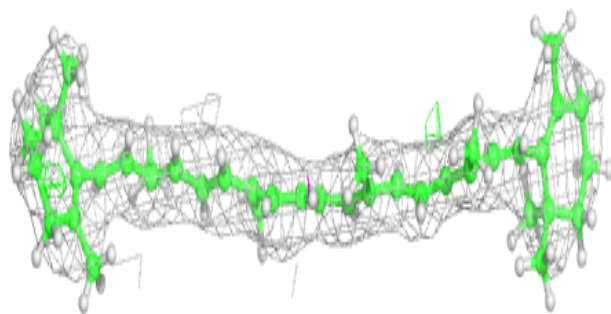
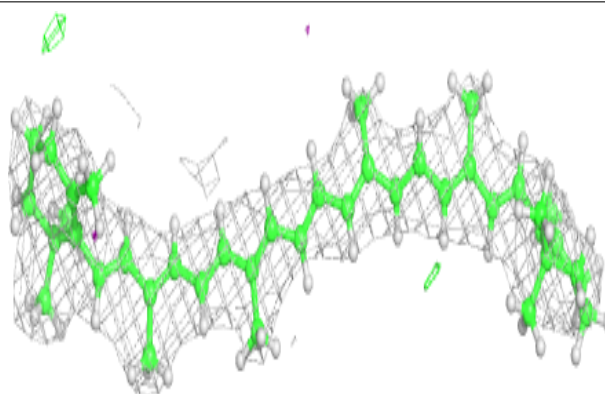


Electron density around STE M 102:

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

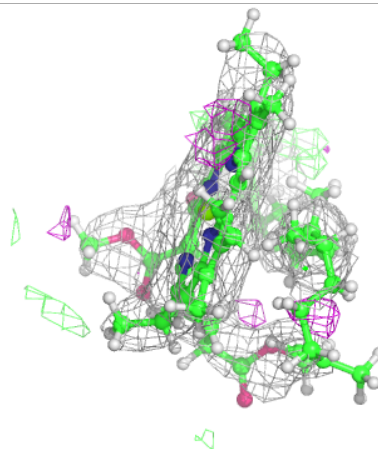
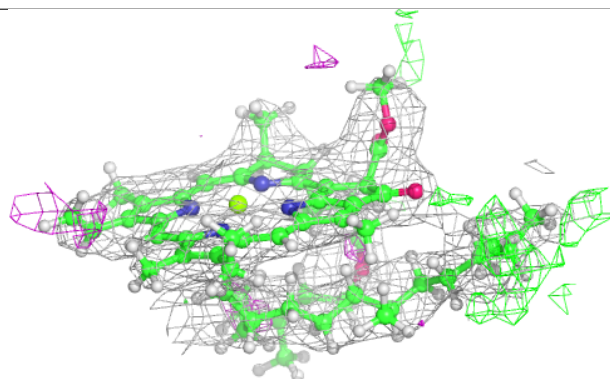
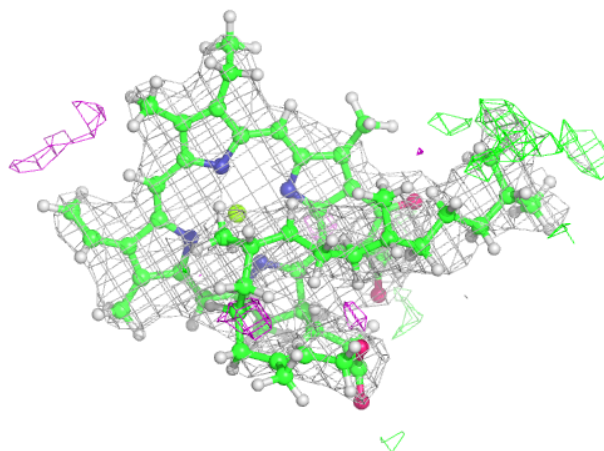
**Electron density around BCR K 102:**

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



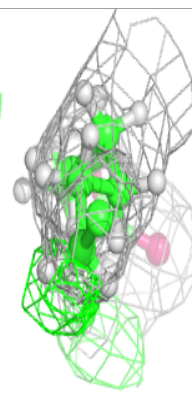
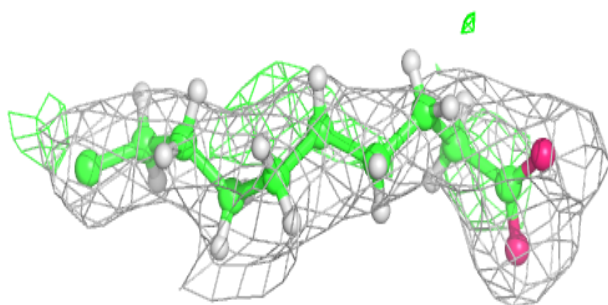
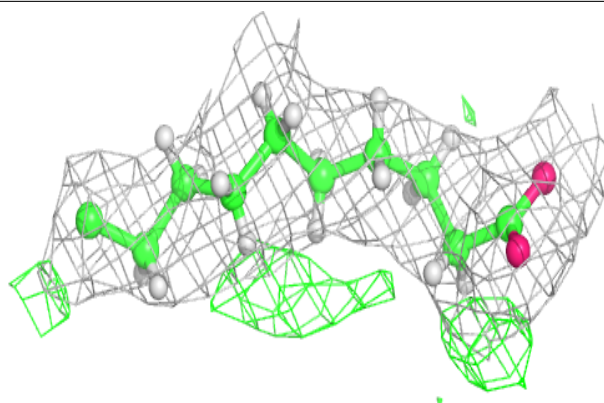
Electron density around CLA H 101:

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

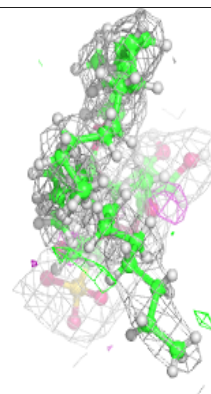
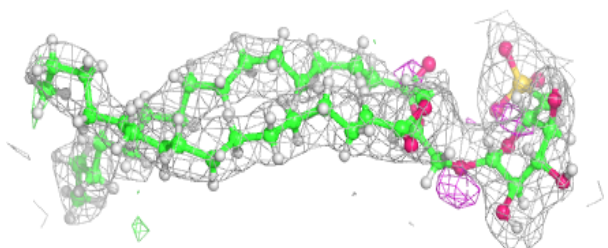
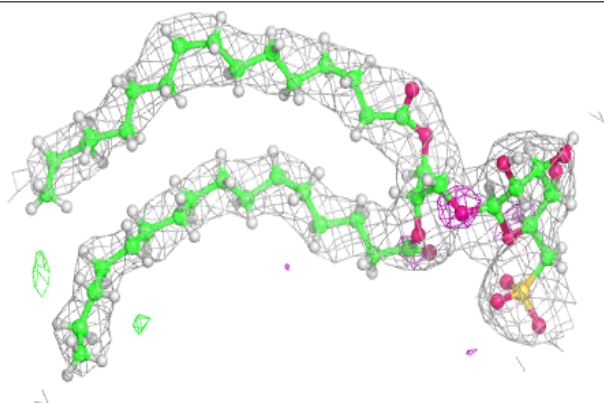


Electron density around STE B 622:

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

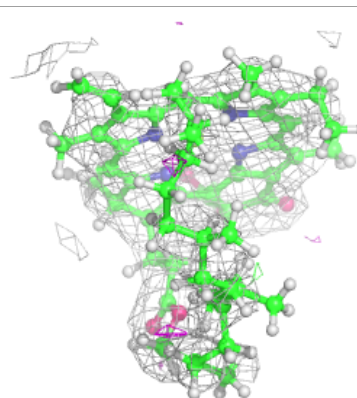
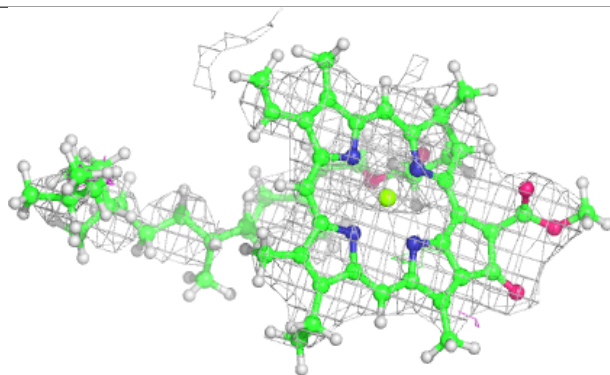
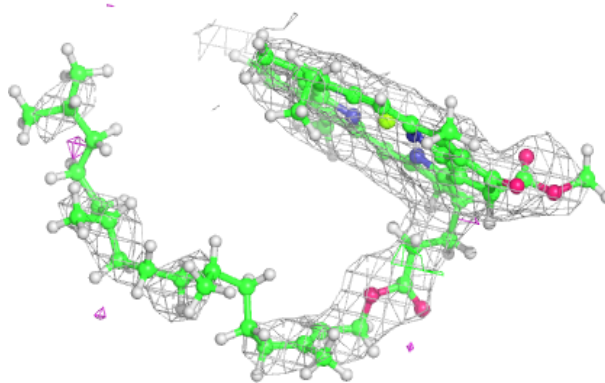
**Electron density around SQD B 621:**

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

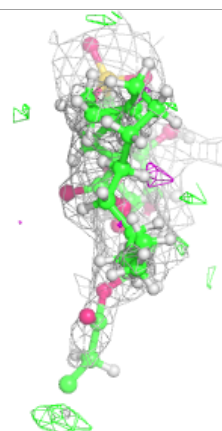
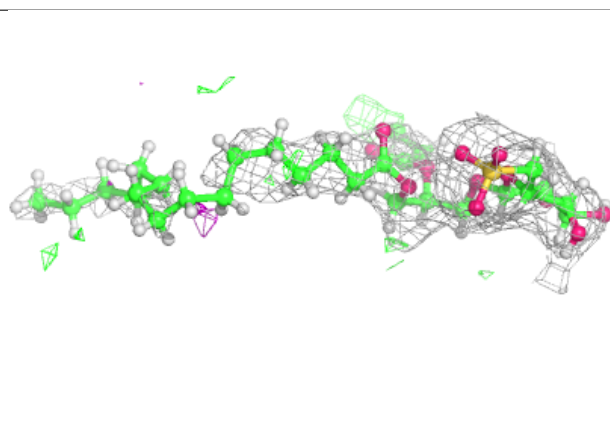
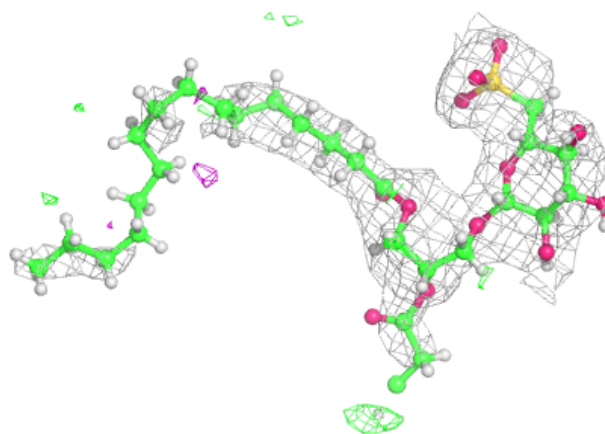


Electron density around CLA c 514:

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

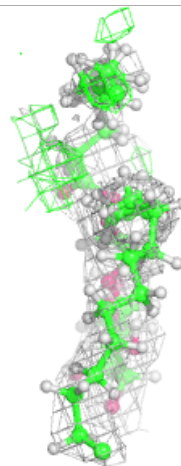
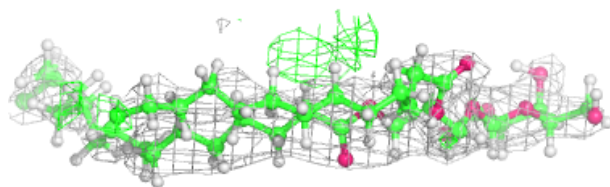
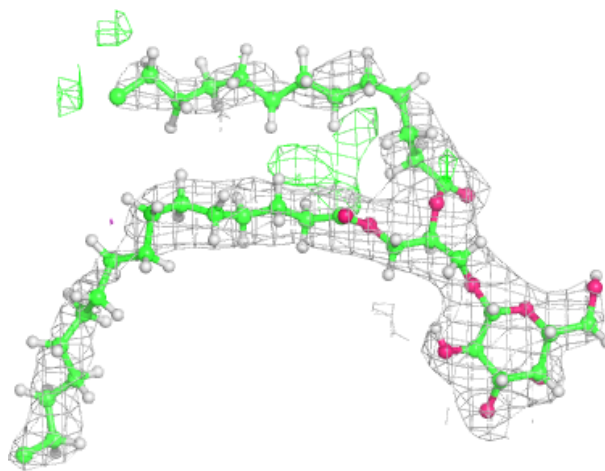
**Electron density around SQD d 409:**

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



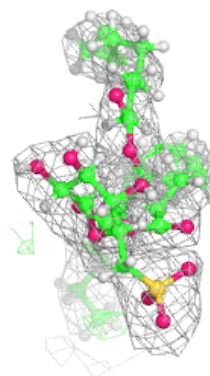
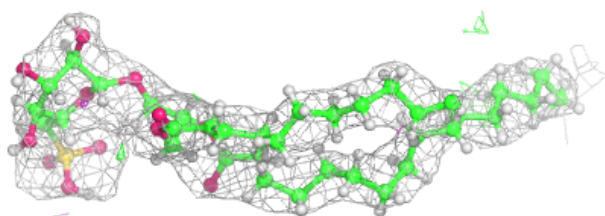
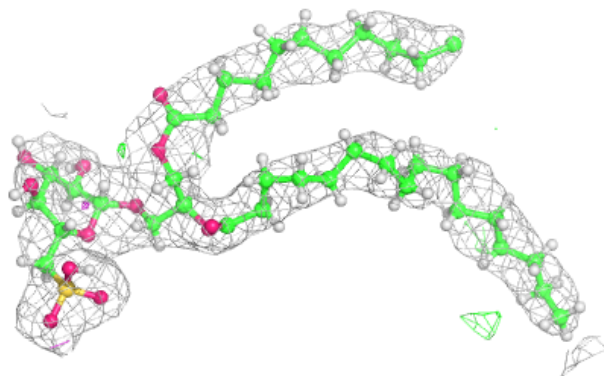
Electron density around LMG Y 101:

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

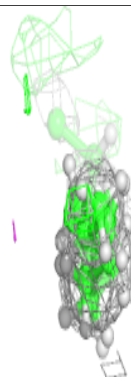
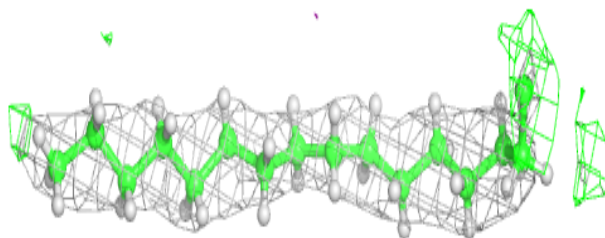
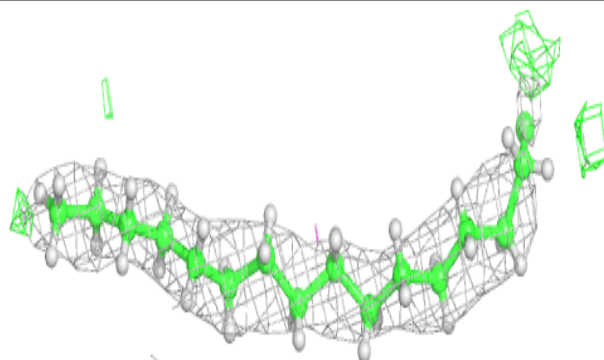


Electron density around SQD L 101:

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

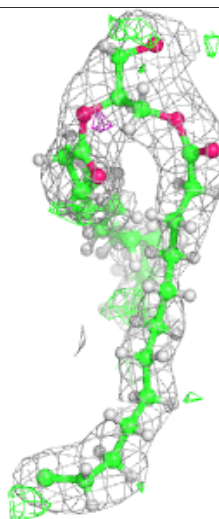
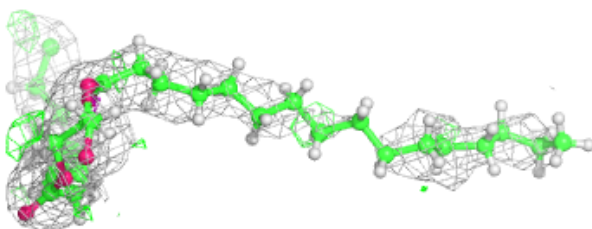
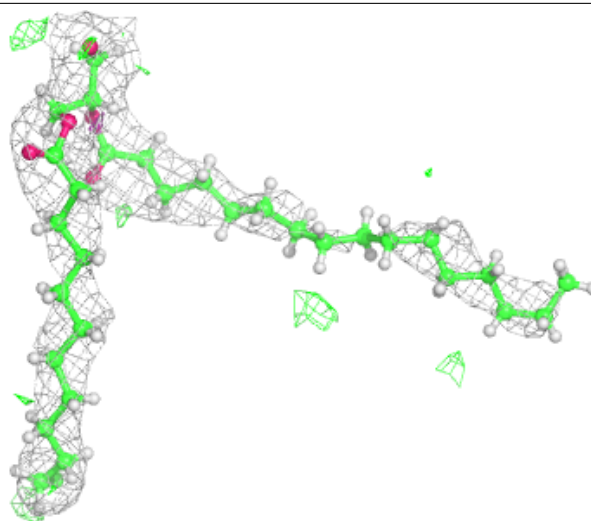
**Electron density around STE C 521:**

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



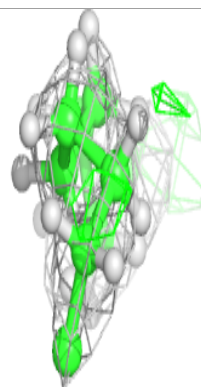
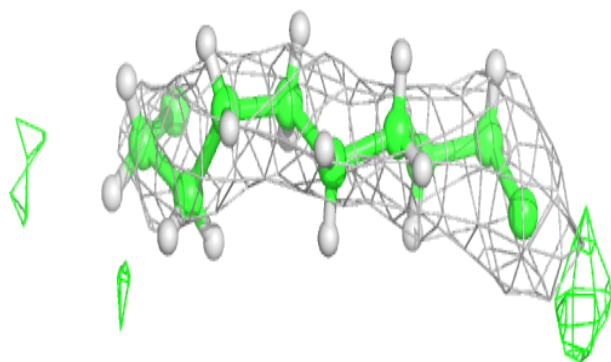
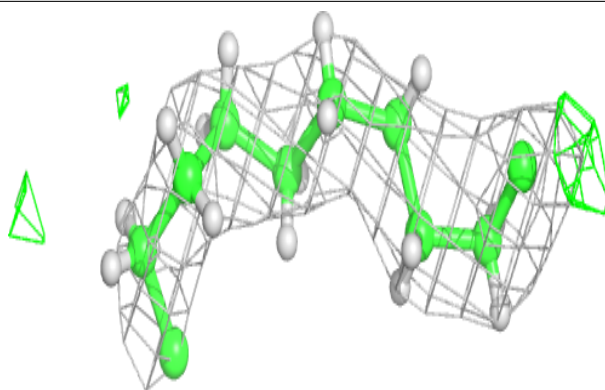
Electron density around SQD a 414:

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

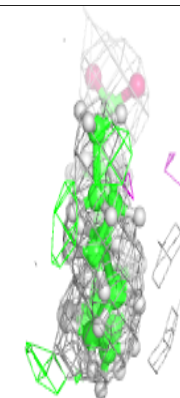
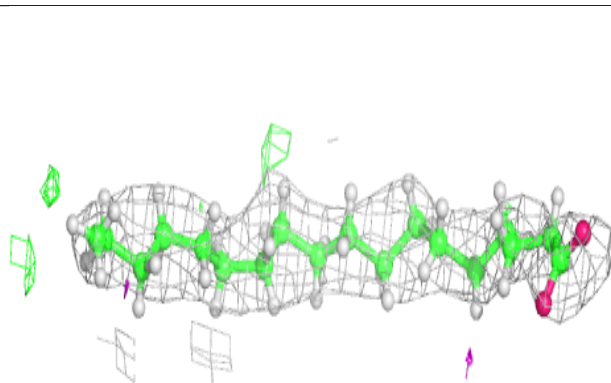
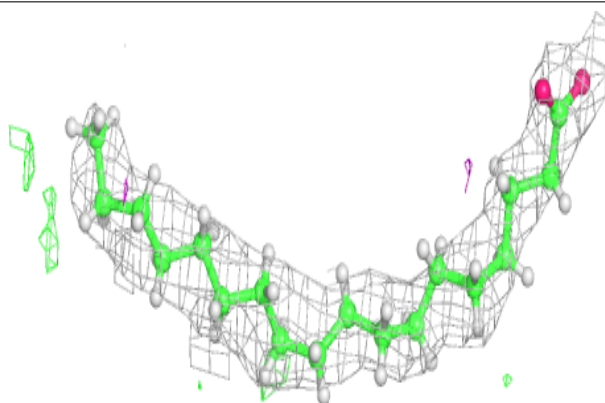


Electron density around STE b 624:

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

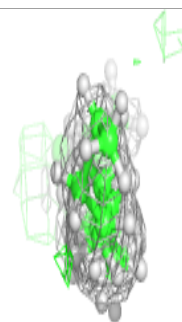
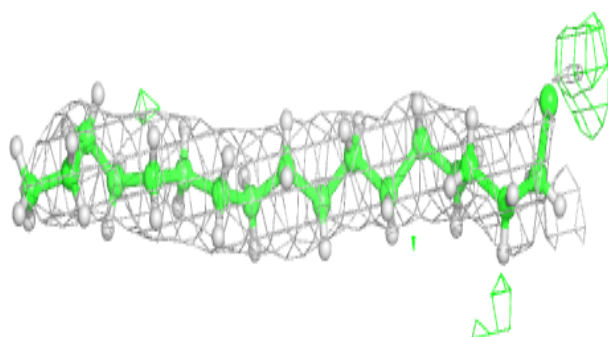
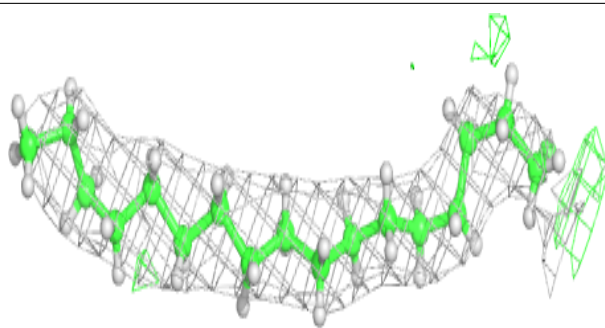
**Electron density around STE D 413:**

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

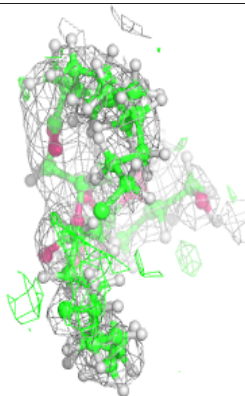
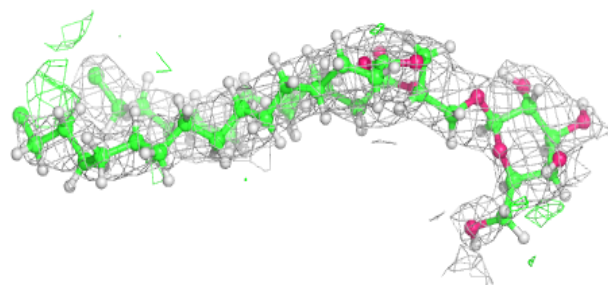
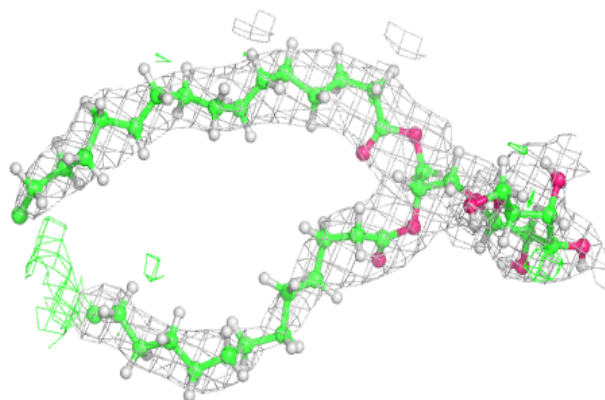


Electron density around STE M 104:

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

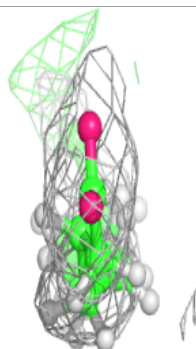
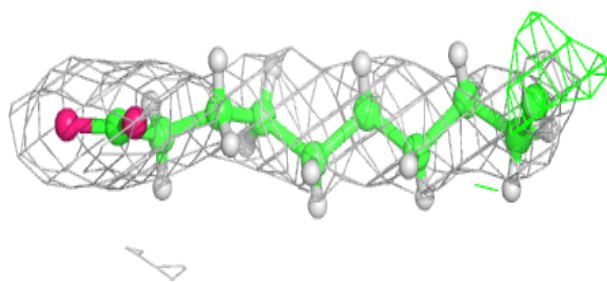
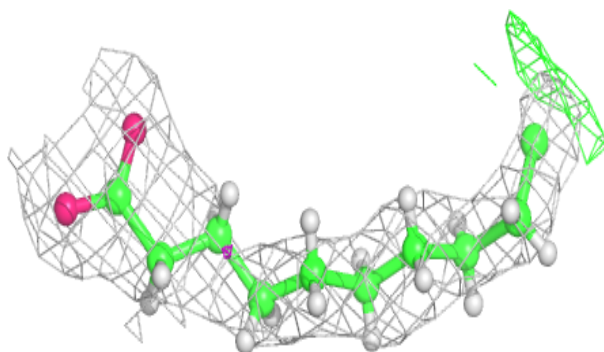
**Electron density around LMG C 516:**

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



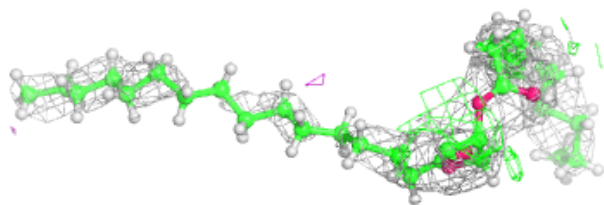
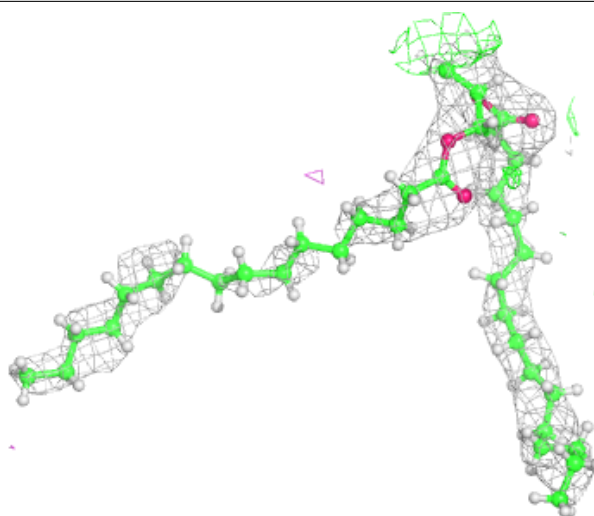
Electron density around STE C 520:

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



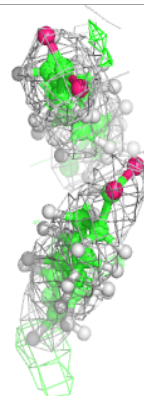
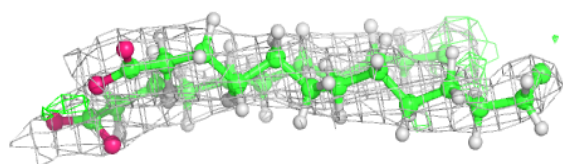
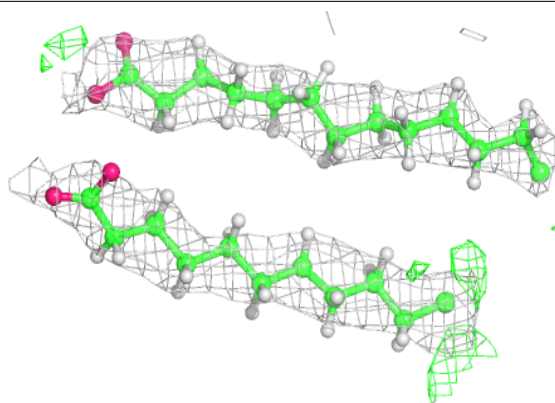
Electron density around SQD A 413:

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

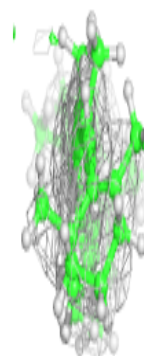
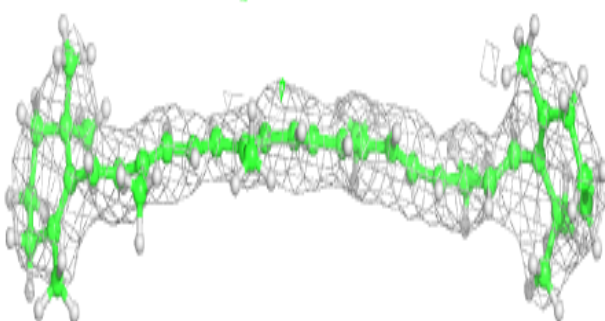
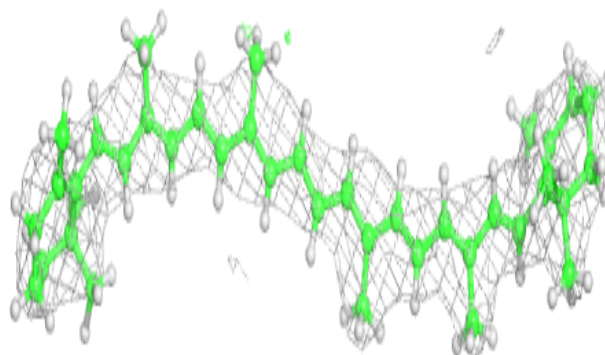


Electron density around LMG D 411:

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

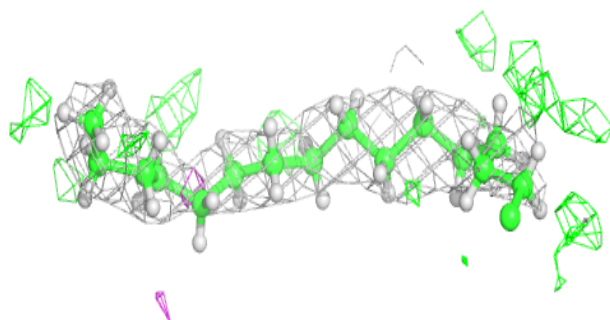
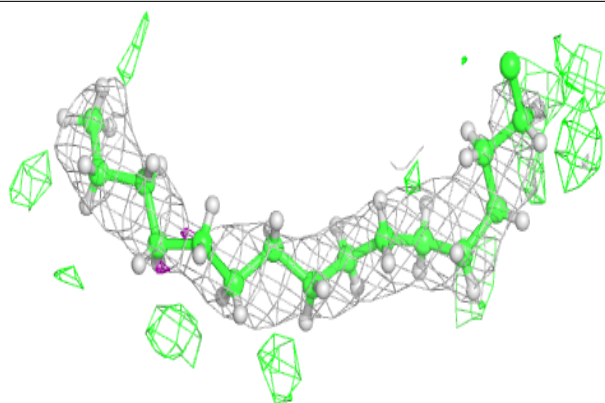
**Electron density around BCR k 101:**

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

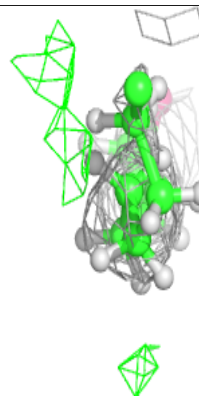
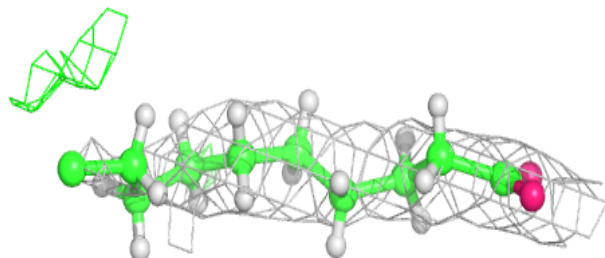
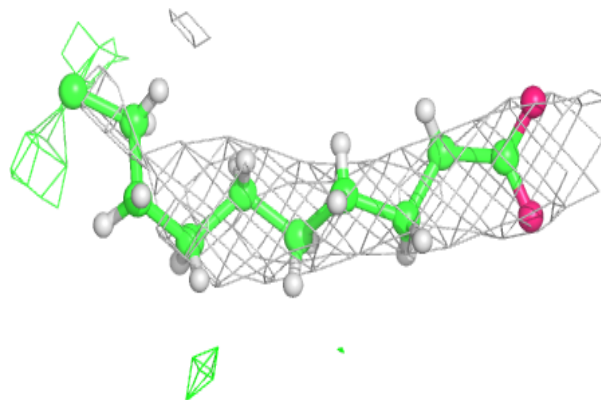


Electron density around STE T 102:

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

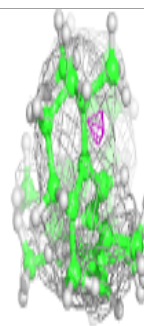
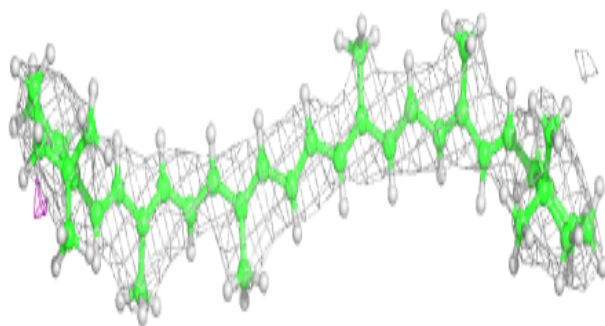
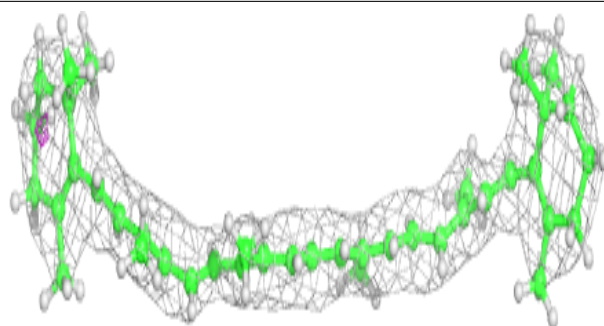
**Electron density around STE L 103:**

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

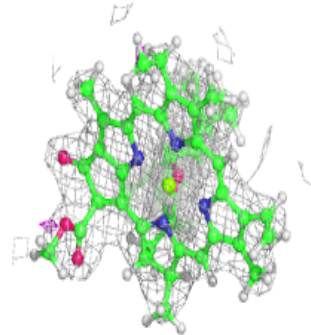
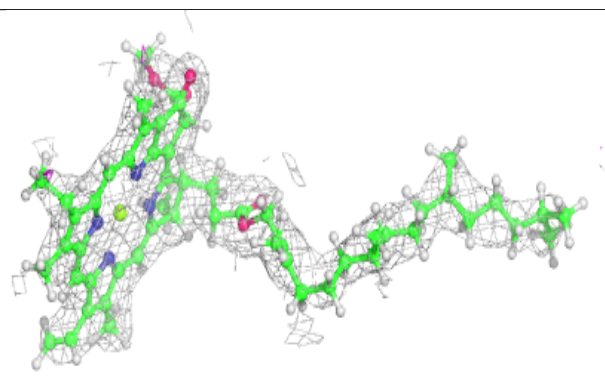
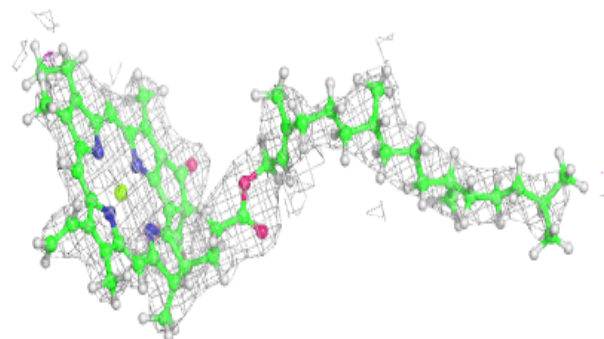


Electron density around BCR k 102:

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

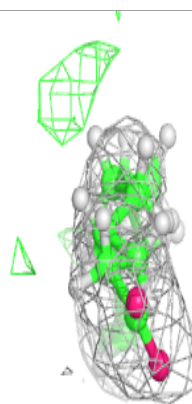
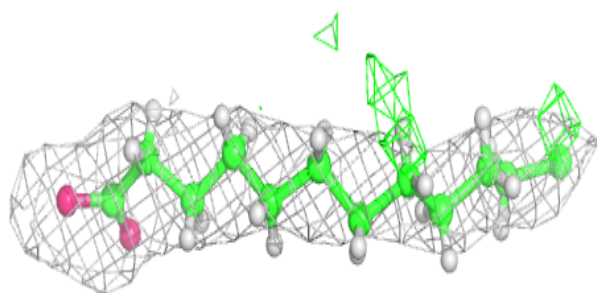
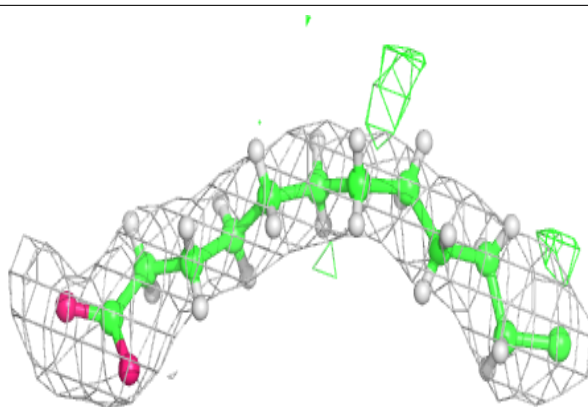
**Electron density around CLA C 502:**

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

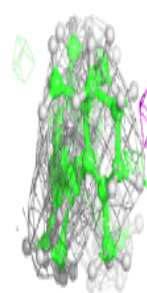
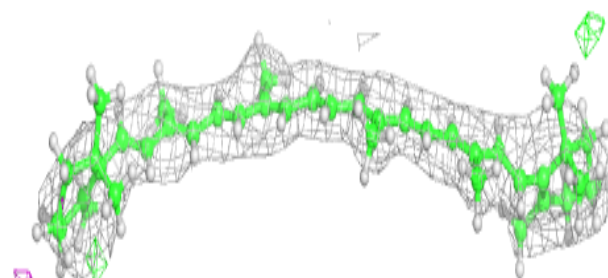
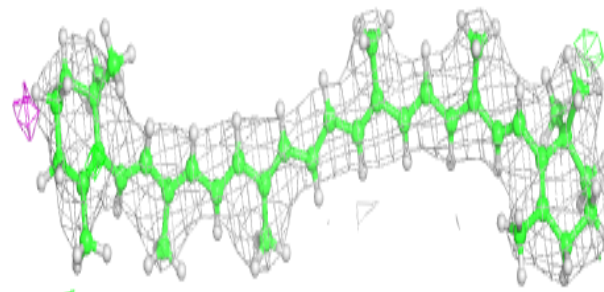


Electron density around STE t 102:

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

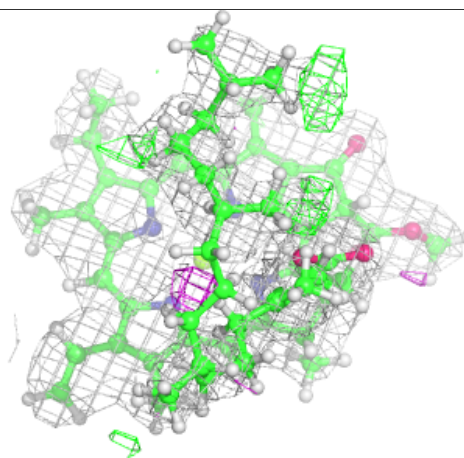
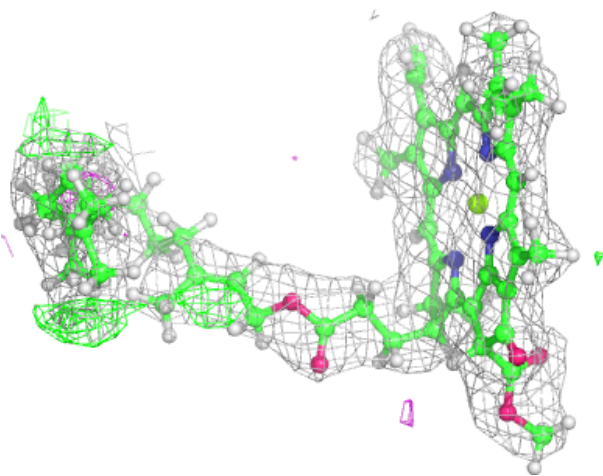
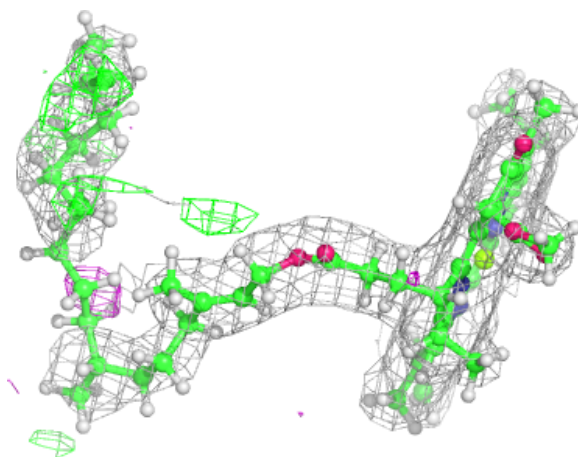
**Electron density around BCR D 406:**

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



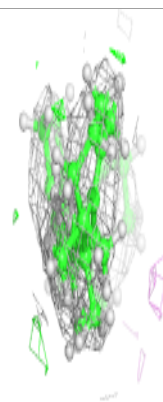
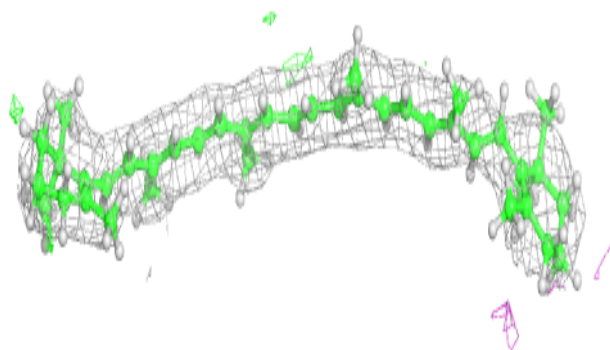
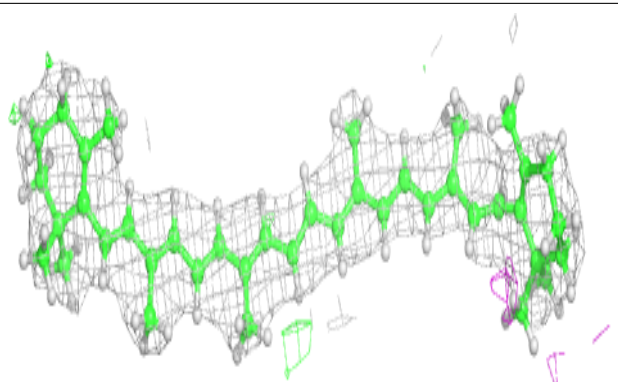
Electron density around CLA a 405:

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

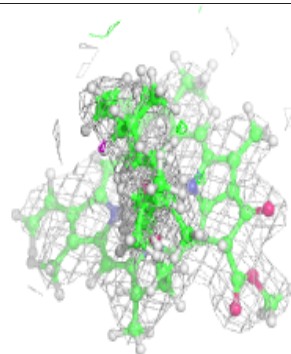
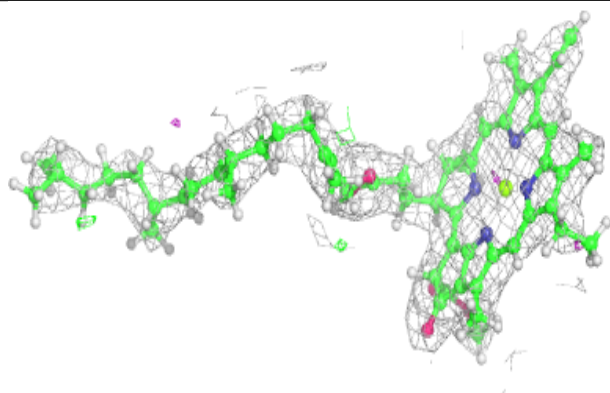
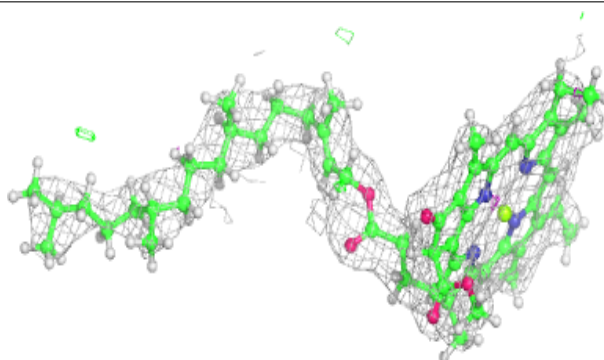


Electron density around BCR d 404:

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

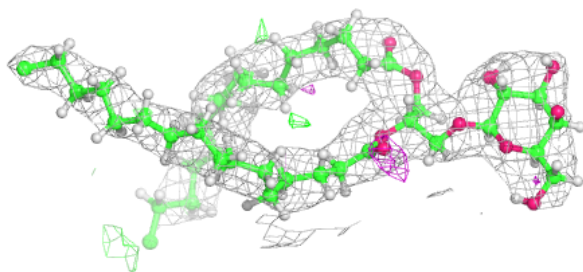
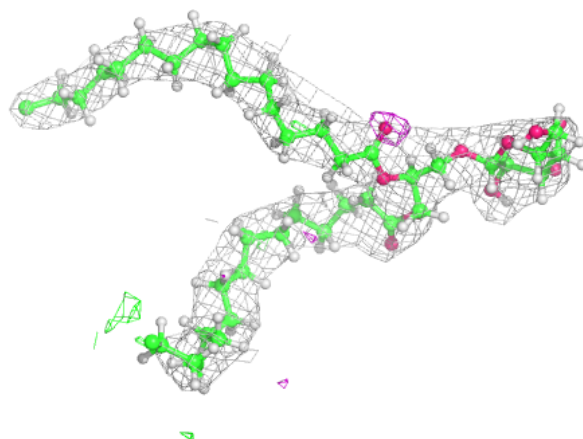
**Electron density around CLA c 503:**

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



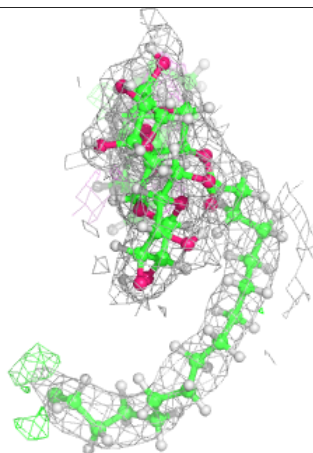
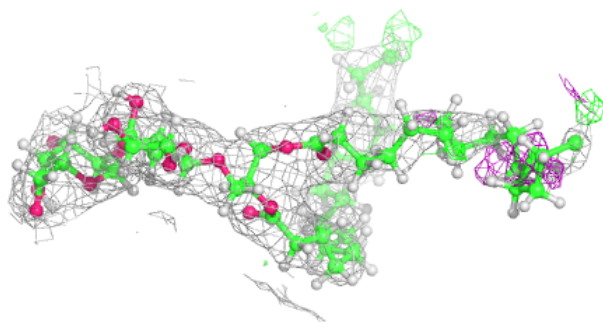
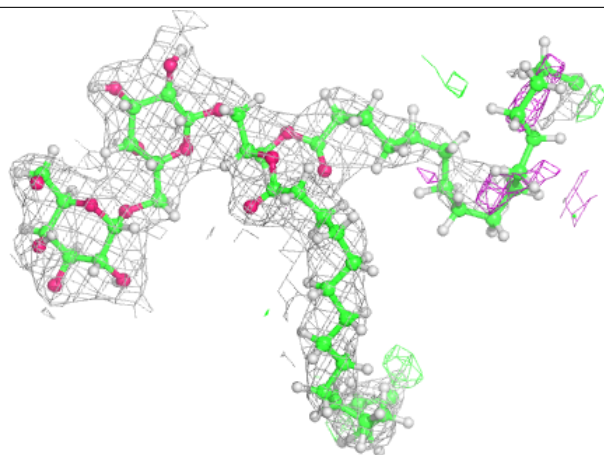
Electron density around LMG M 101:

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



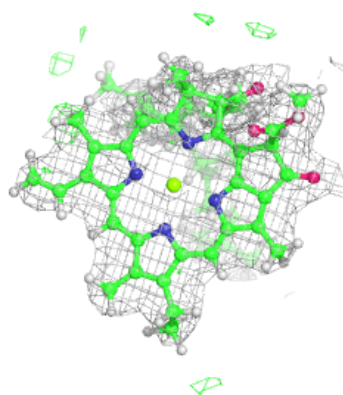
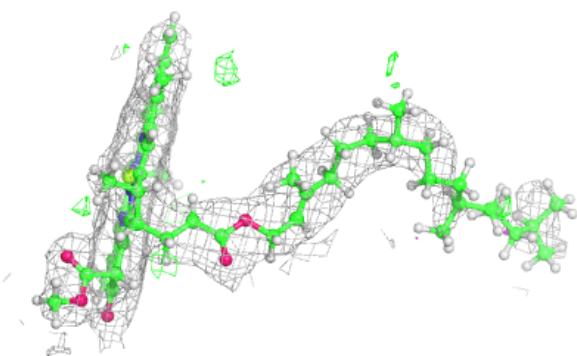
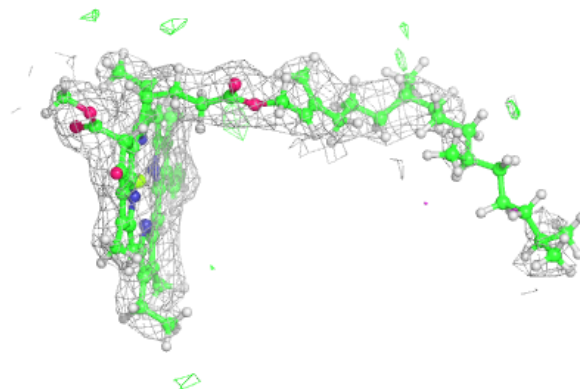
Electron density around DGD C 518:

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

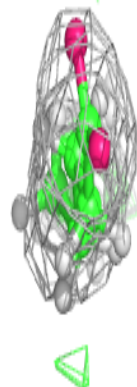
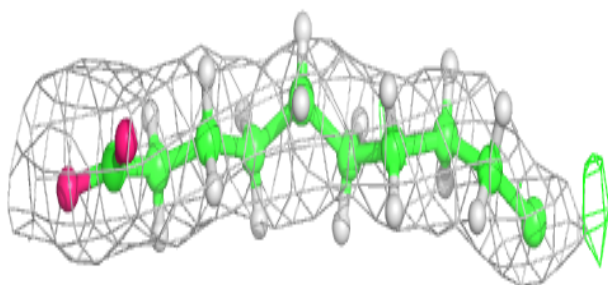
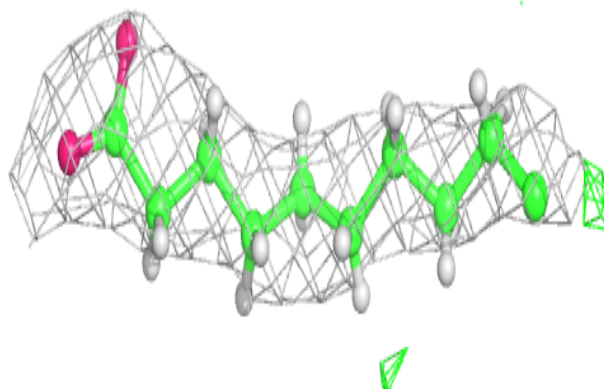


Electron density around CLA D 405:

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

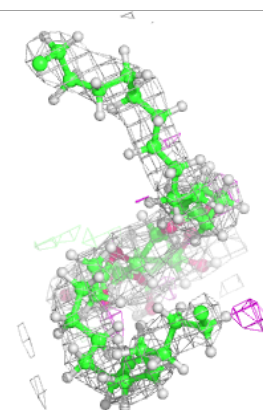
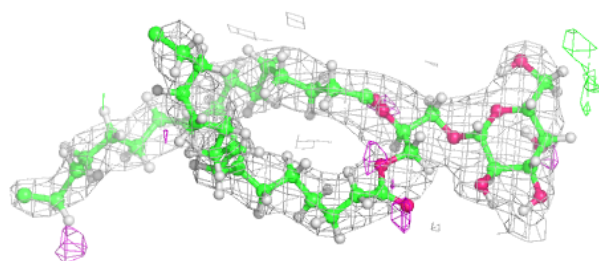
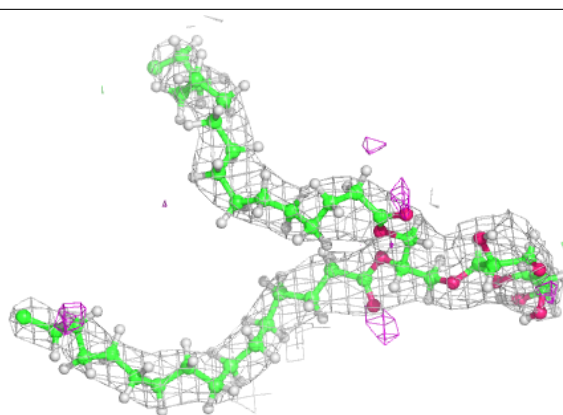
**Electron density around STE j 101:**

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



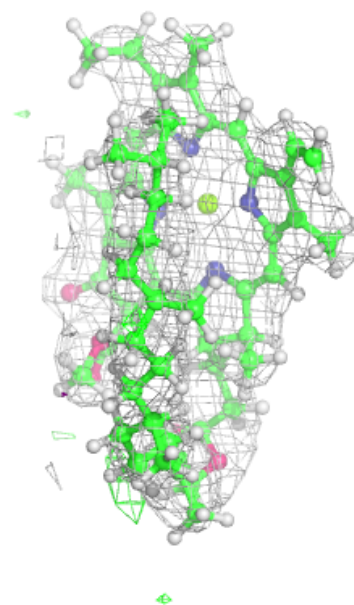
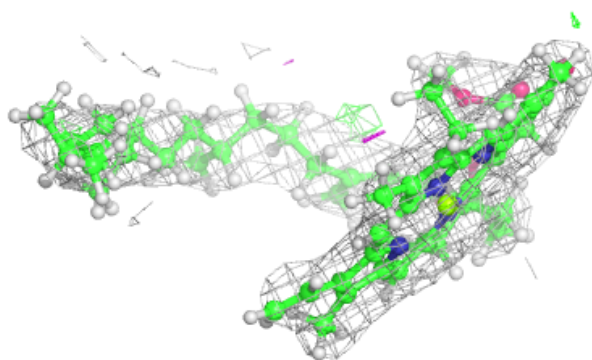
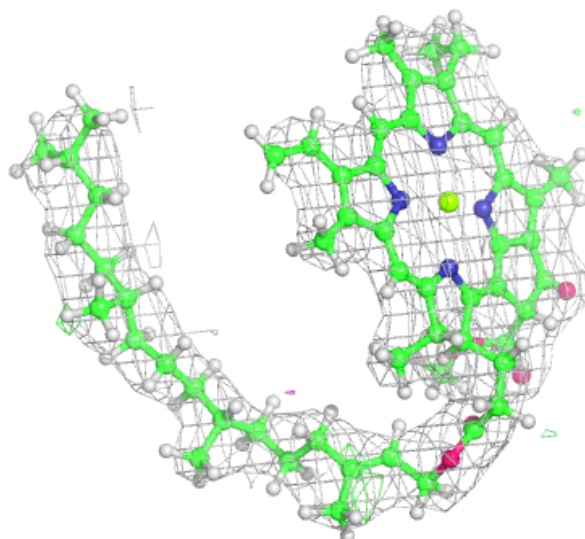
Electron density around LMG m 101:

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



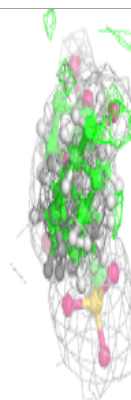
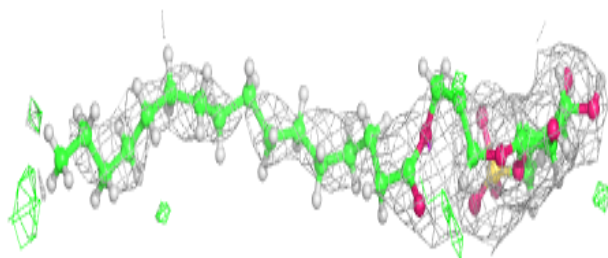
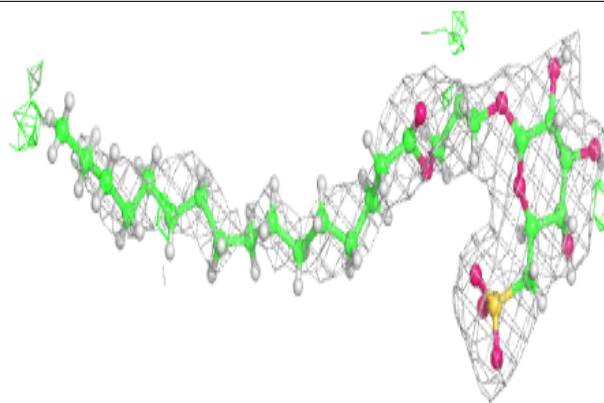
Electron density around CLA C 507:

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

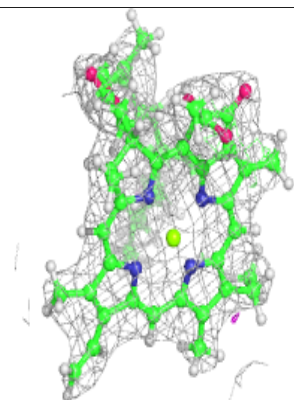
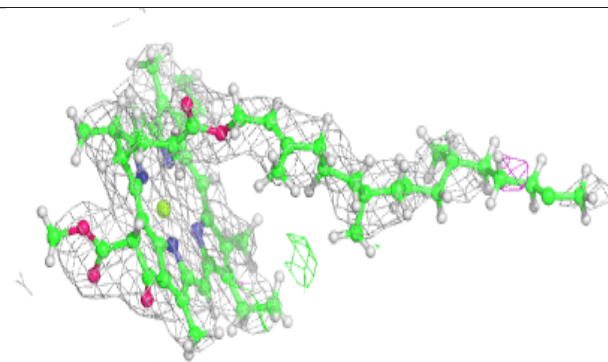
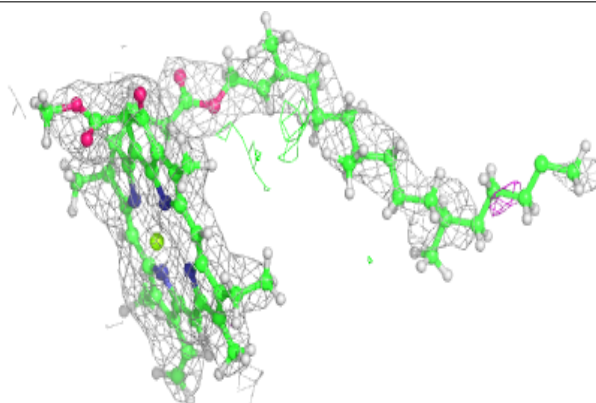


Electron density around SQD F 102:

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

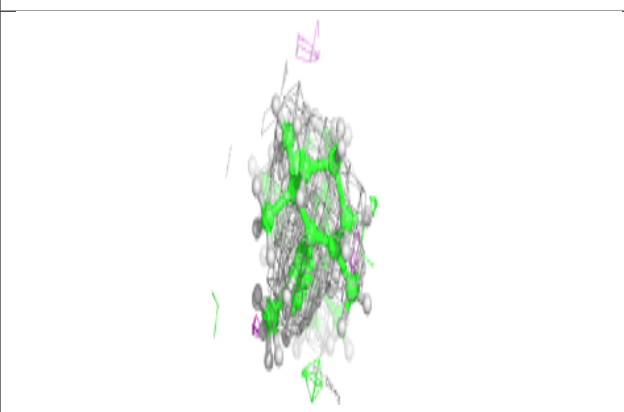
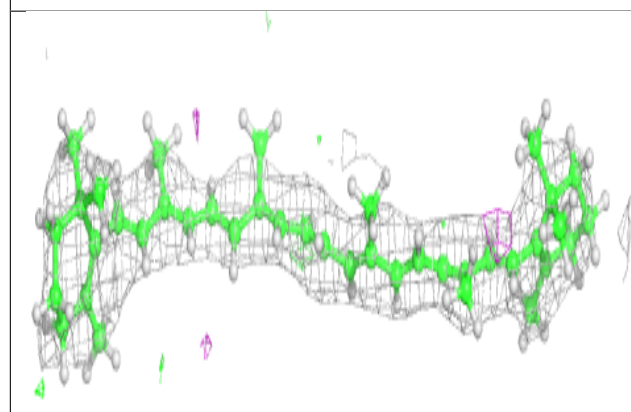
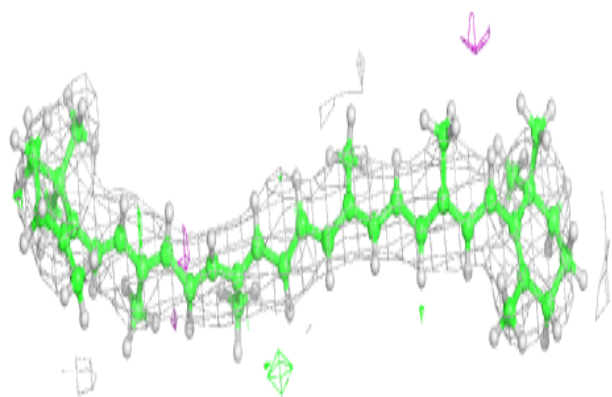
**Electron density around CLA c 509:**

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



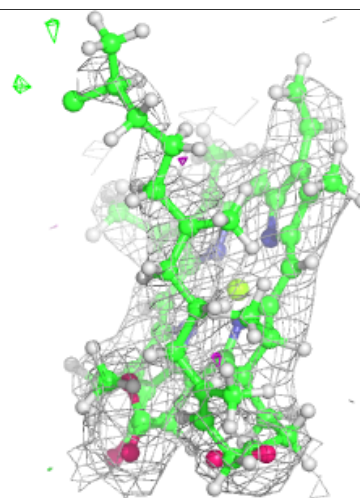
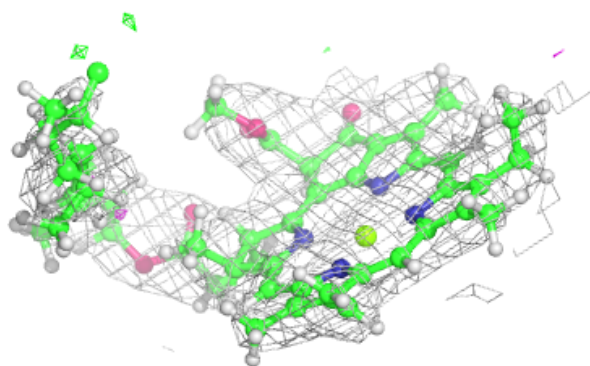
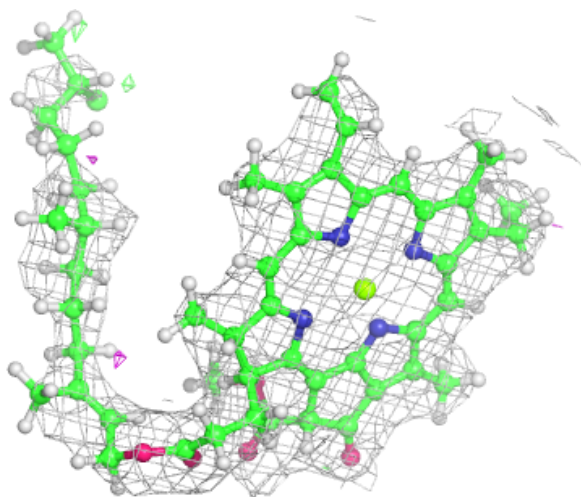
Electron density around BCR K 101:

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



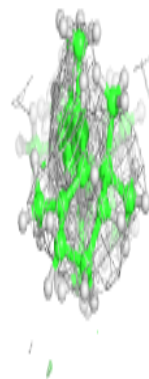
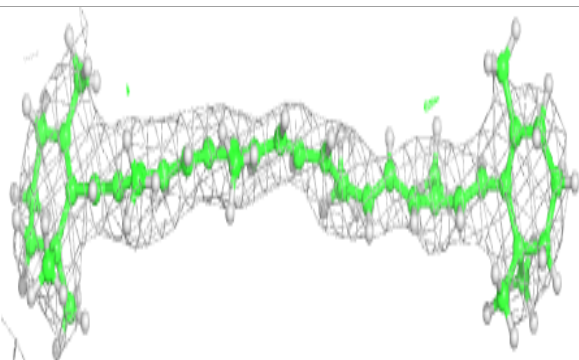
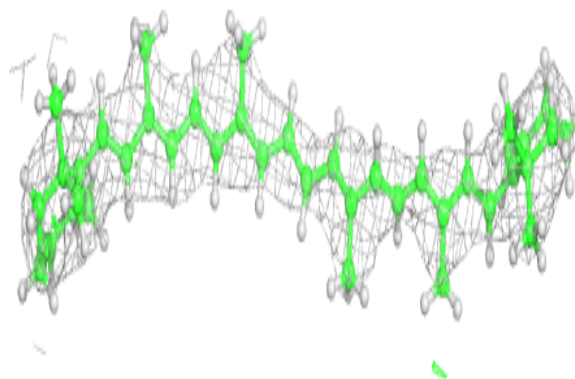
Electron density around CLA b 616:

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



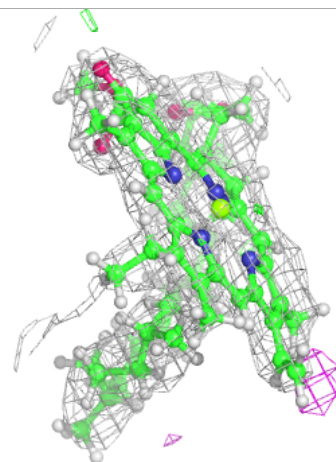
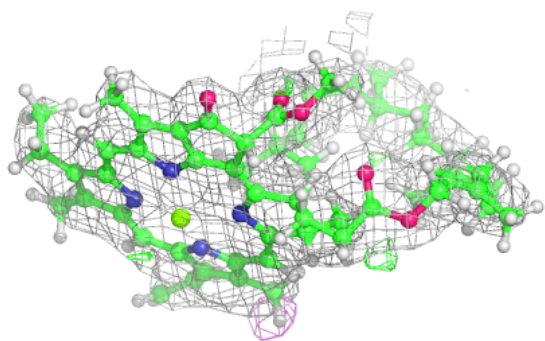
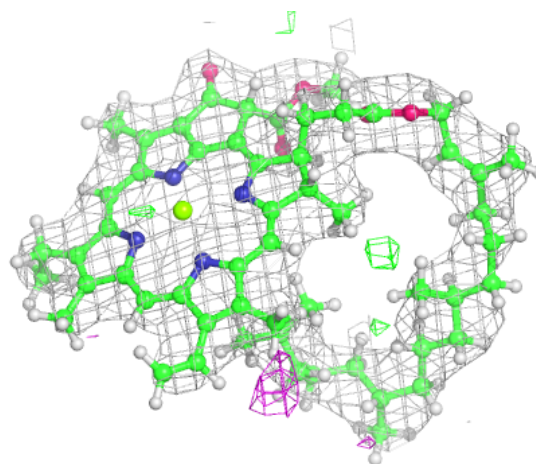
Electron density around BCR c 515:

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



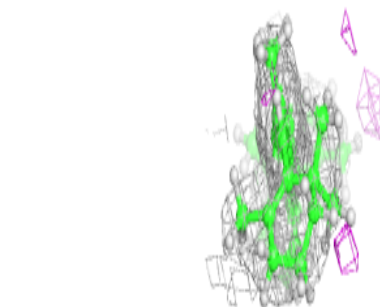
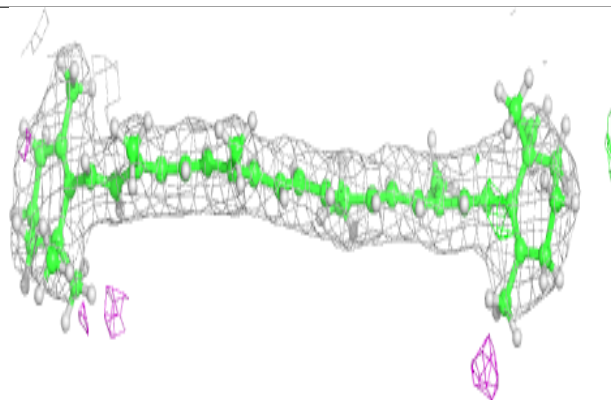
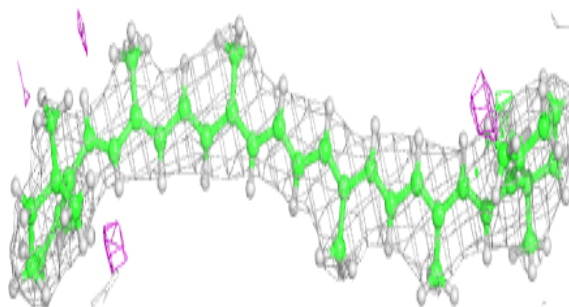
Electron density around CLA b 615:

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

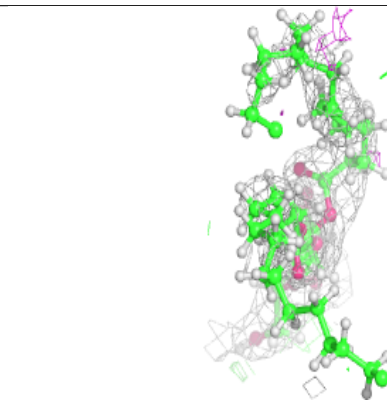
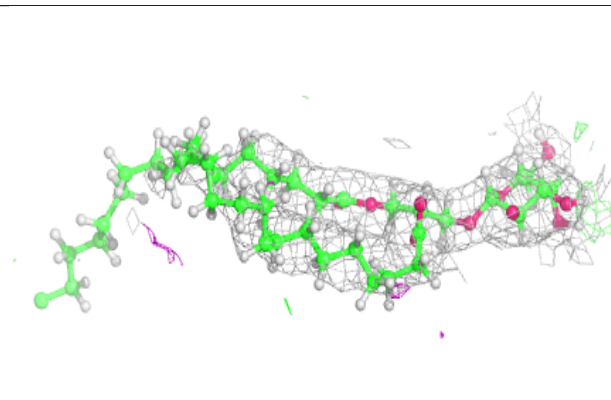
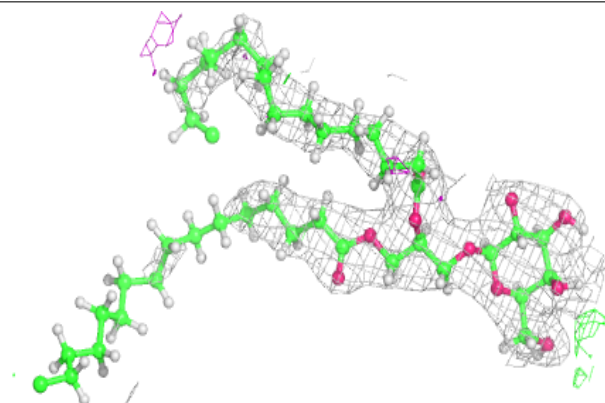


Electron density around BCR C 514:

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

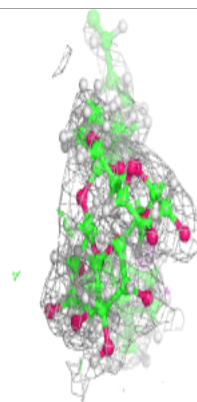
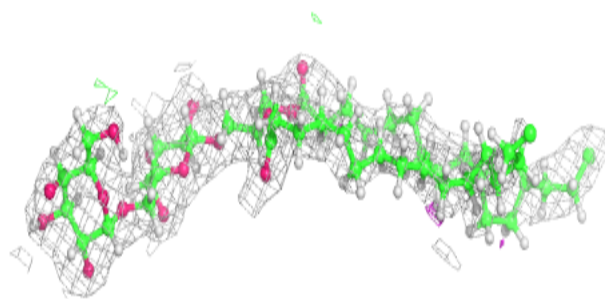
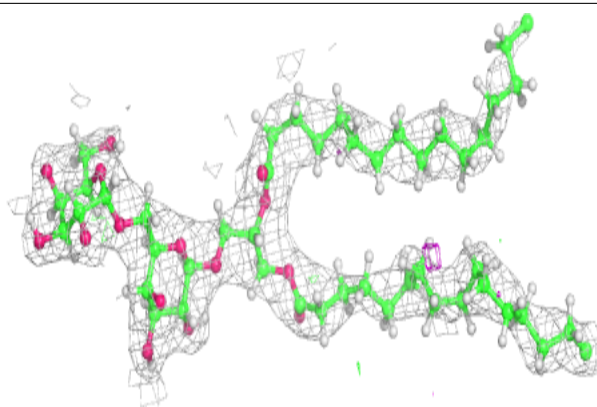
**Electron density around LMG D 408:**

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



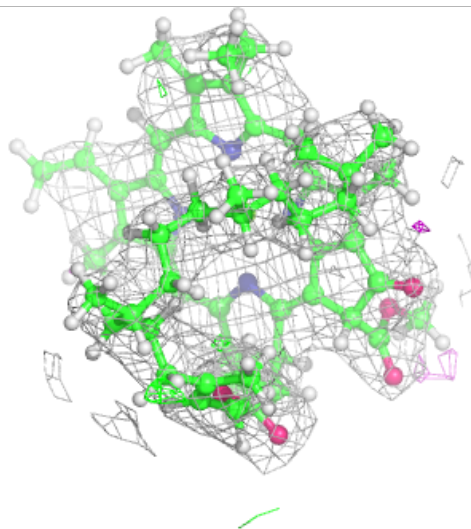
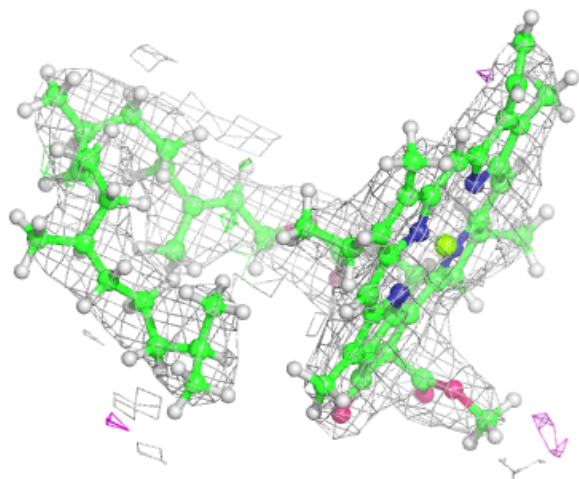
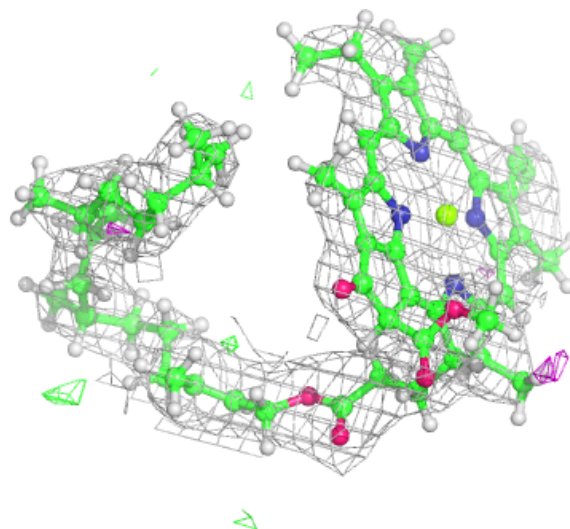
Electron density around DGD c 519:

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



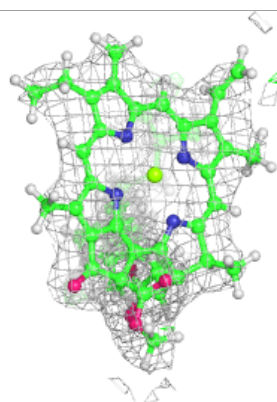
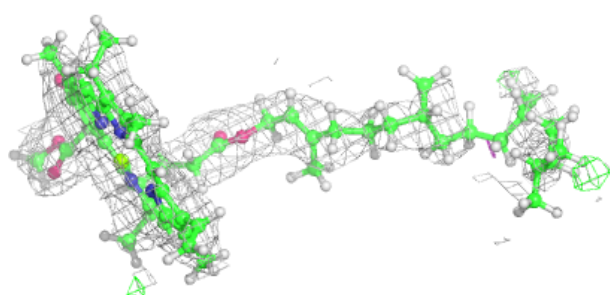
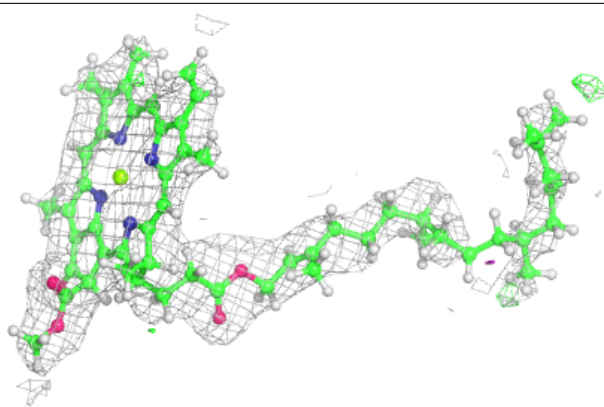
Electron density around CLA c 504:

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

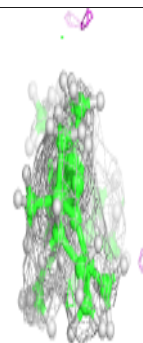
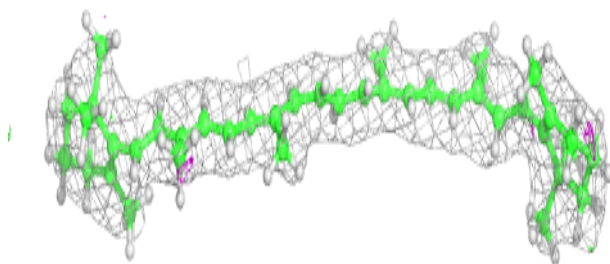
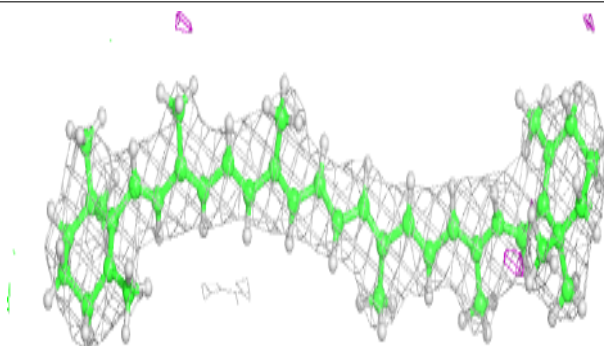


Electron density around CLA d 403:

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

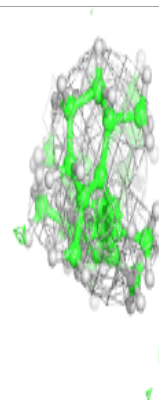
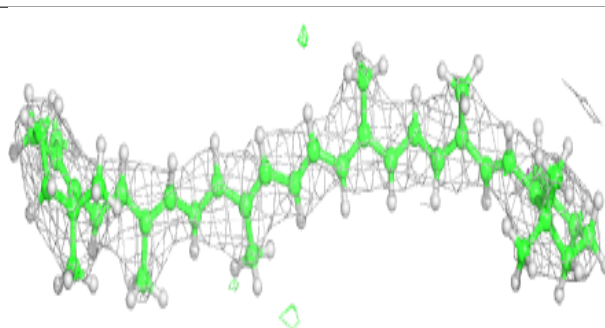
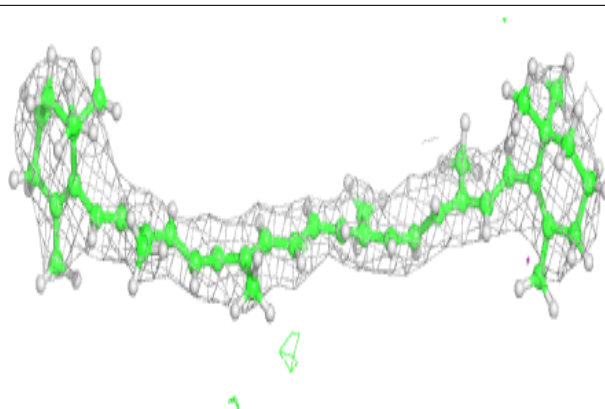
**Electron density around BCR b 619:**

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



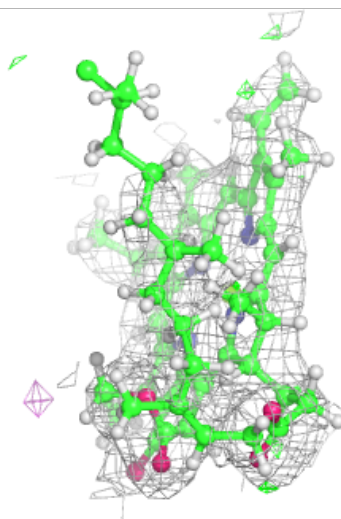
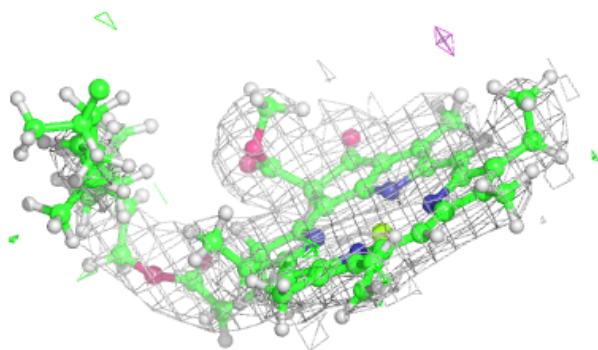
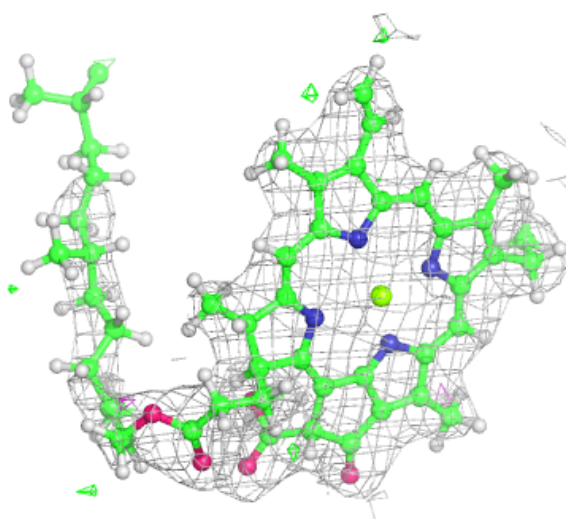
Electron density around BCR C 515:

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



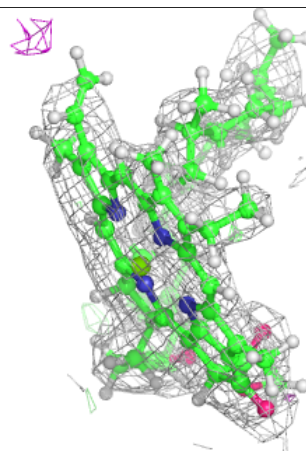
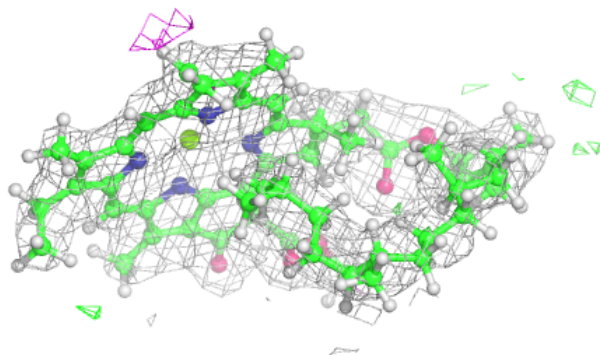
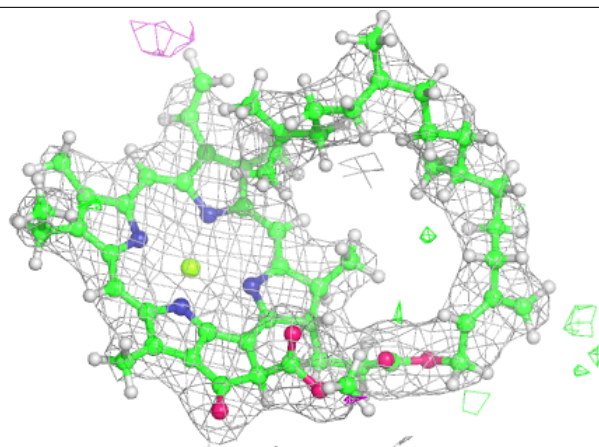
Electron density around CLA B 616:

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

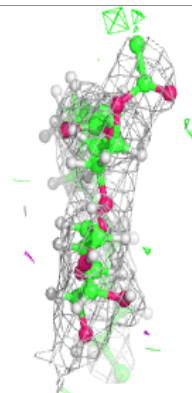
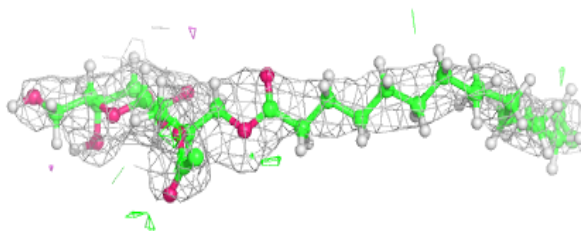
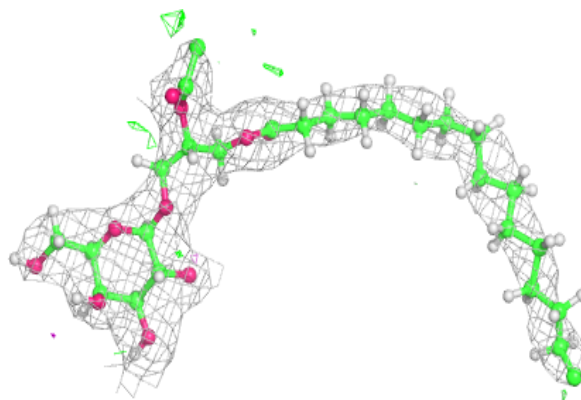


Electron density around CLA B 615:

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

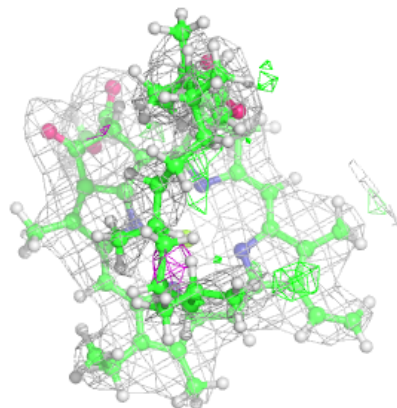
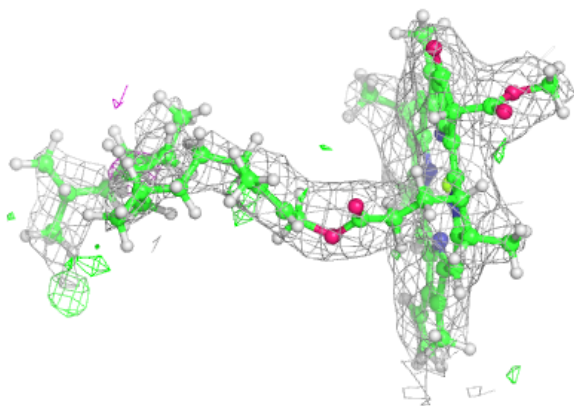
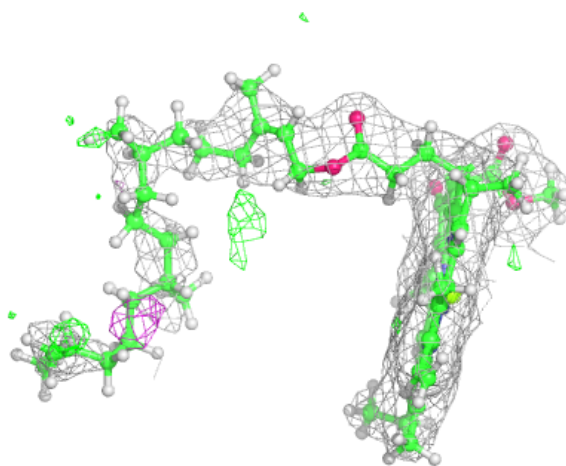
**Electron density around LMG c 520:**

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



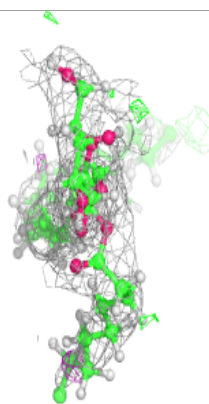
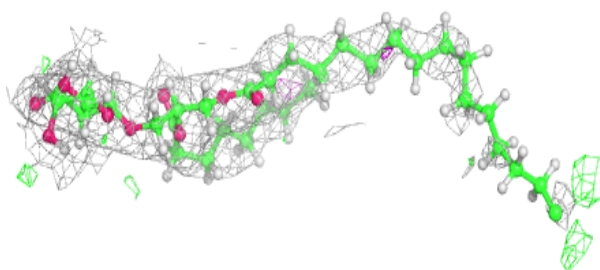
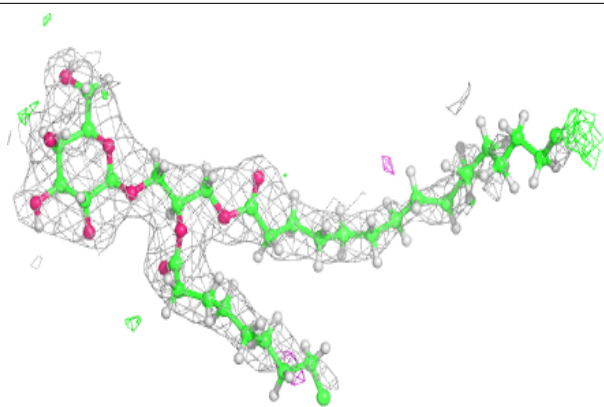
Electron density around CLA c 507:

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



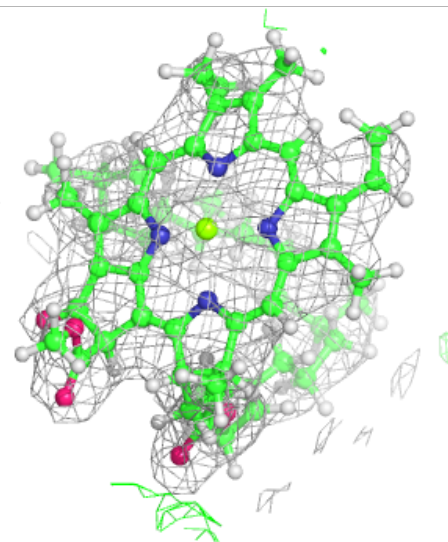
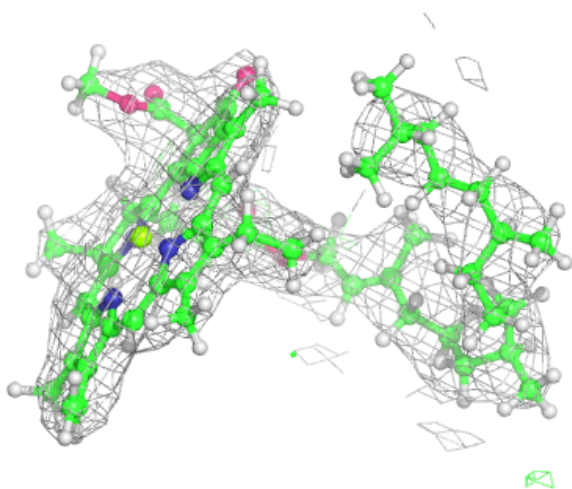
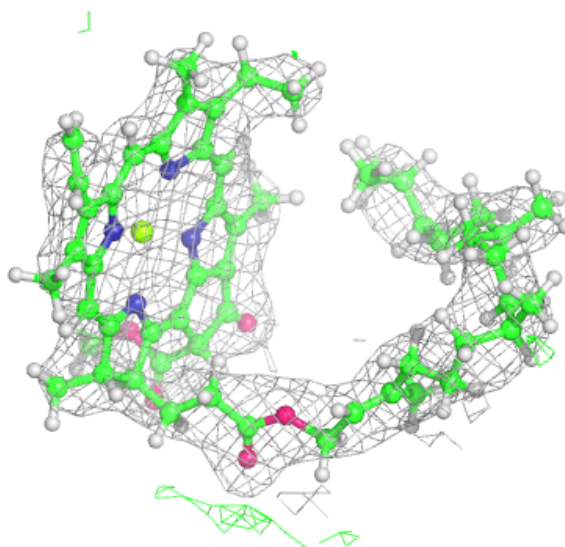
Electron density around LMG d 408:

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



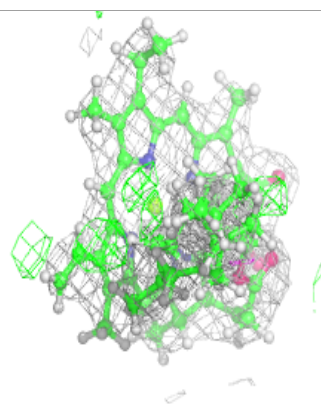
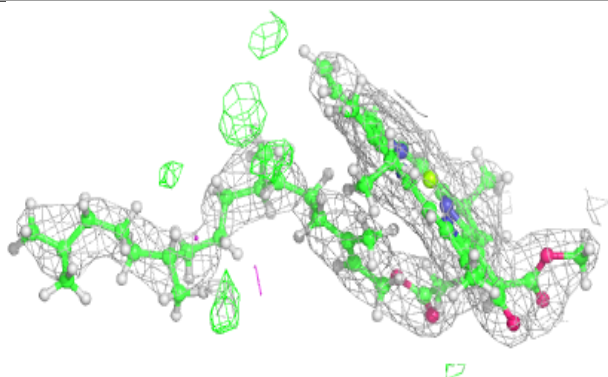
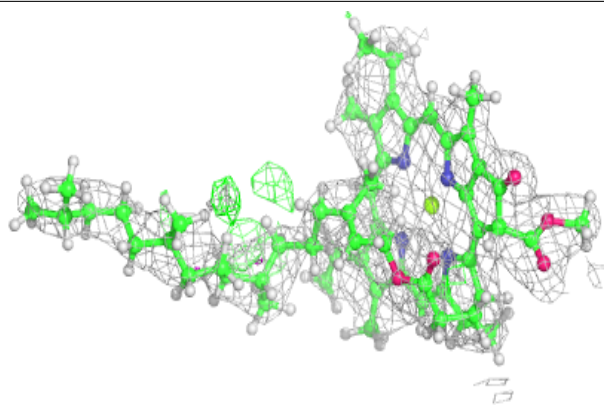
Electron density around CLA C 503:

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

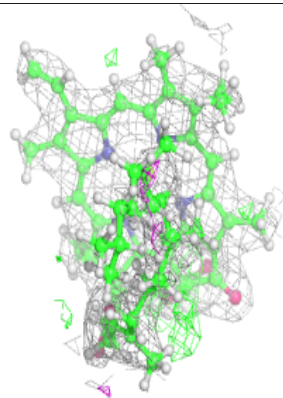
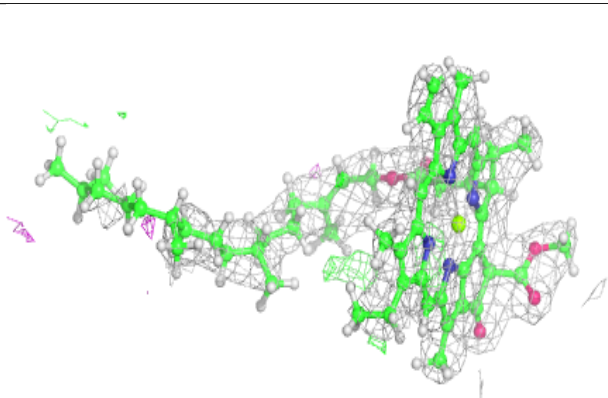
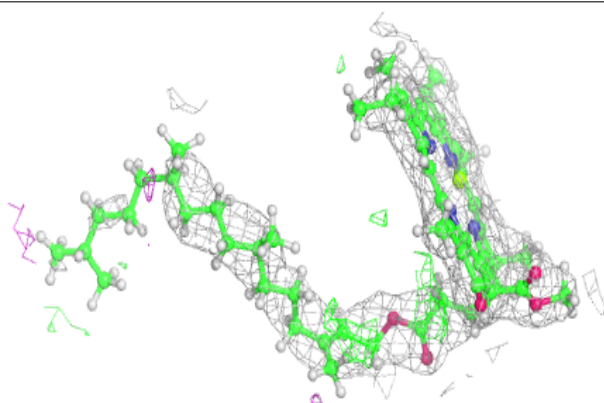


Electron density around CLA C 505:

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

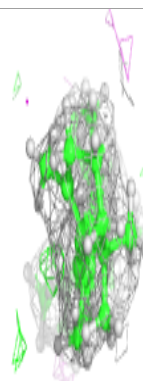
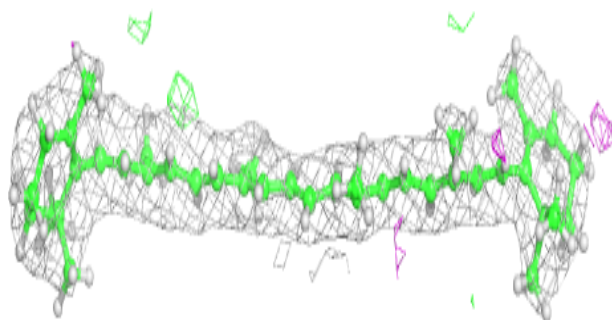
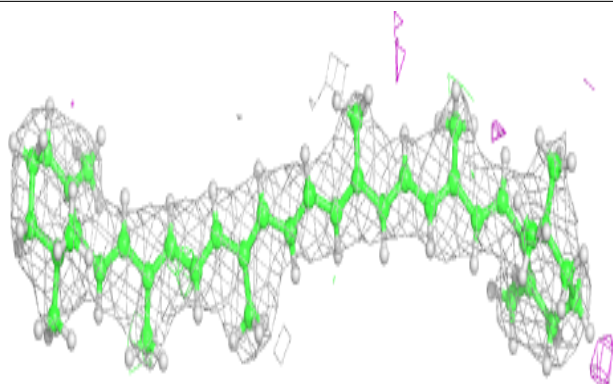
**Electron density around CLA C 508:**

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

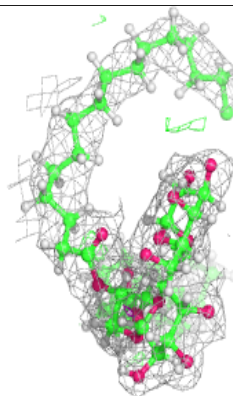
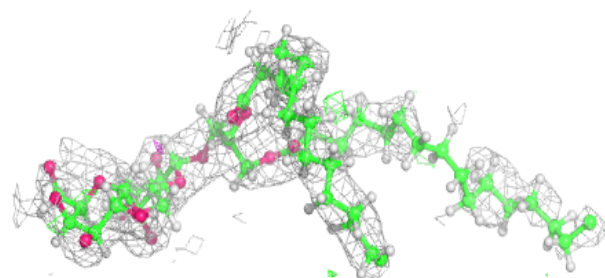
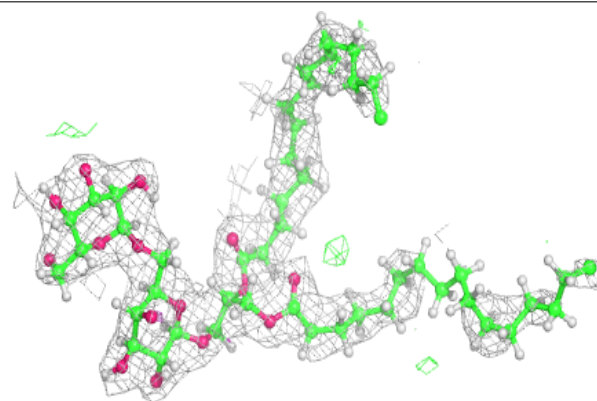


Electron density around BCR B 618:

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

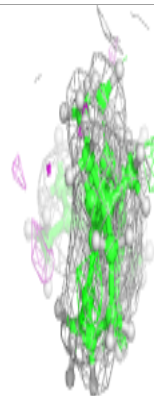
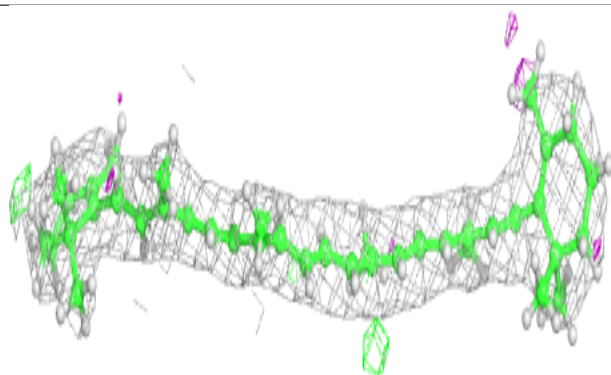
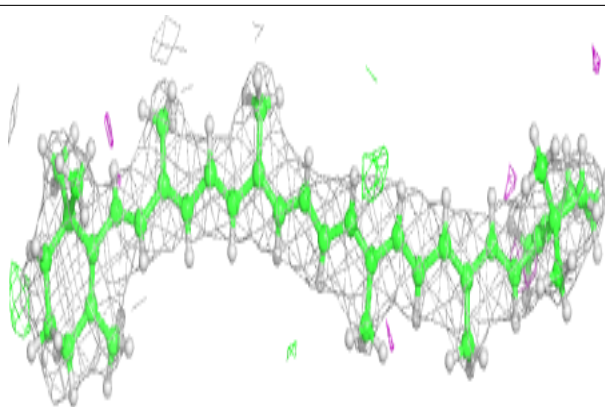
**Electron density around DGD c 518:**

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

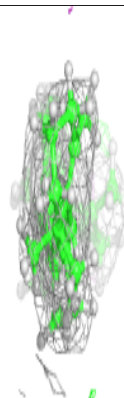
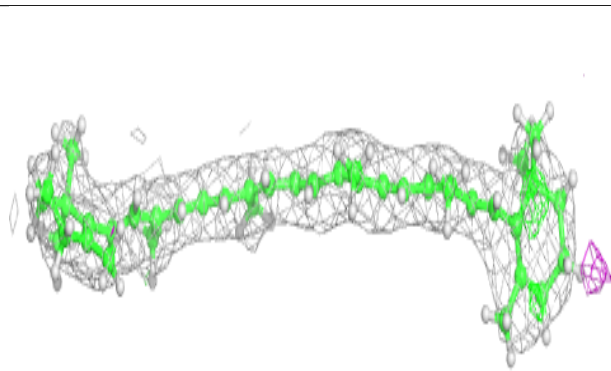
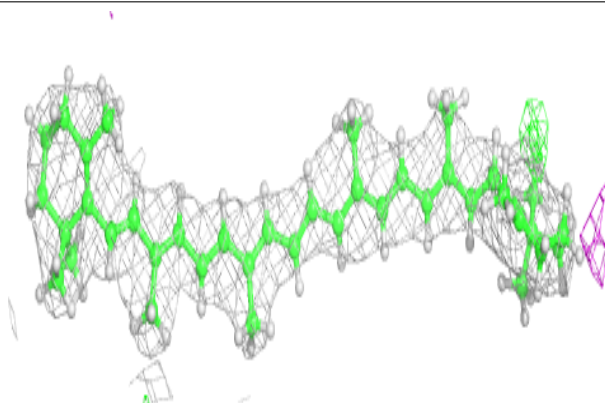


Electron density around BCR B 617:

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

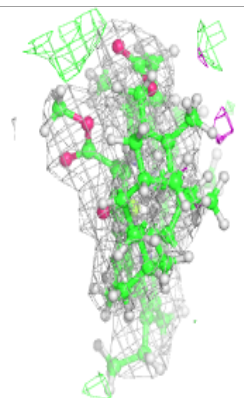
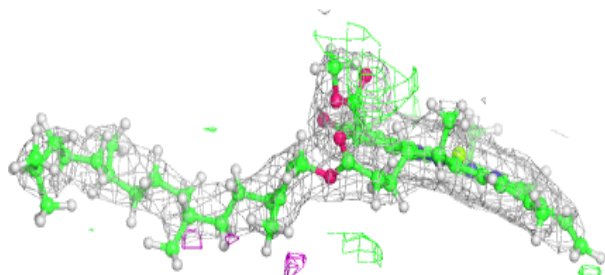
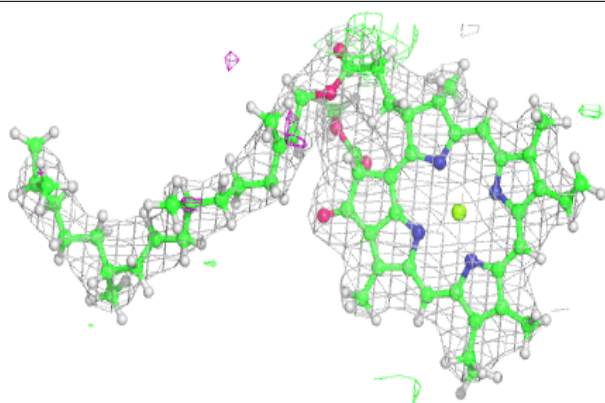
**Electron density around BCR b 617:**

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

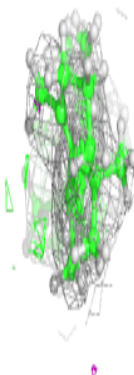
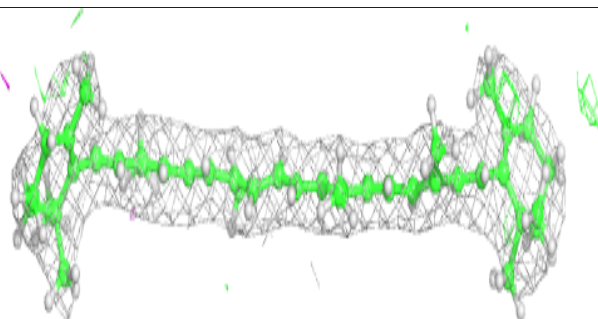
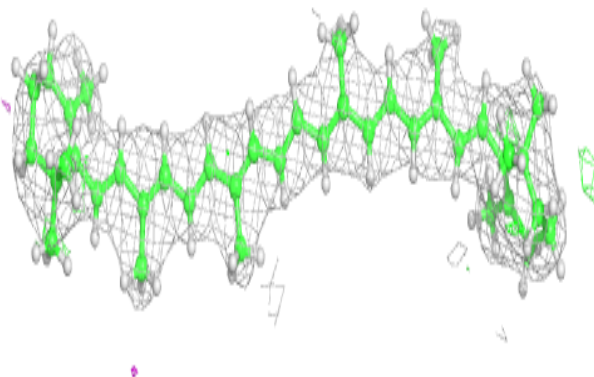


Electron density around CLA b 602:

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

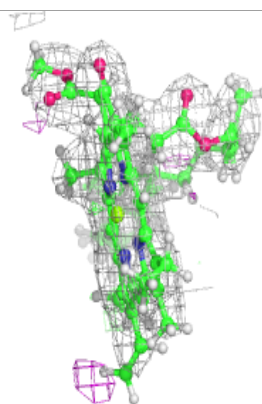
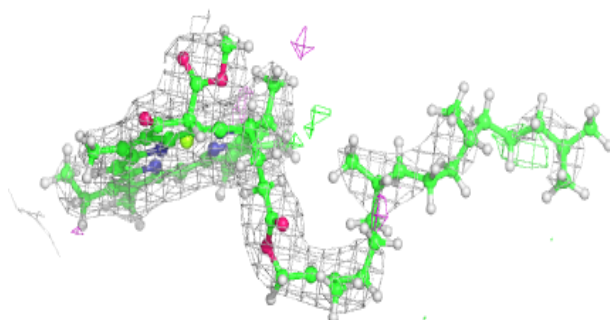
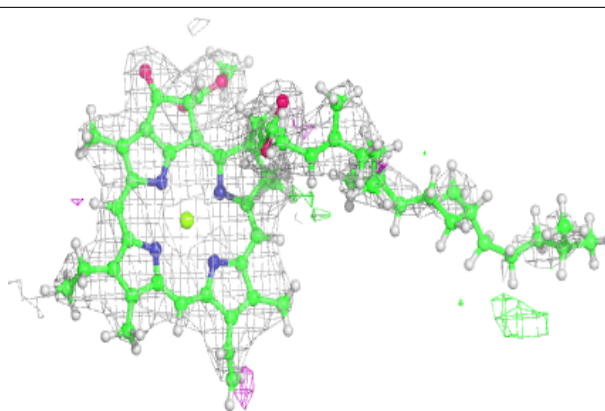
**Electron density around BCR b 618:**

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



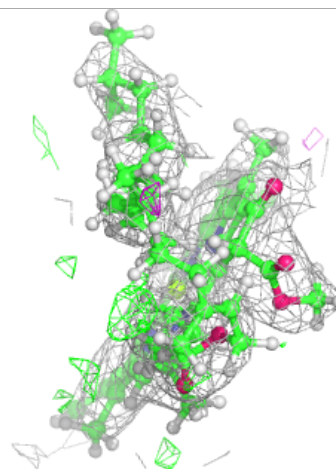
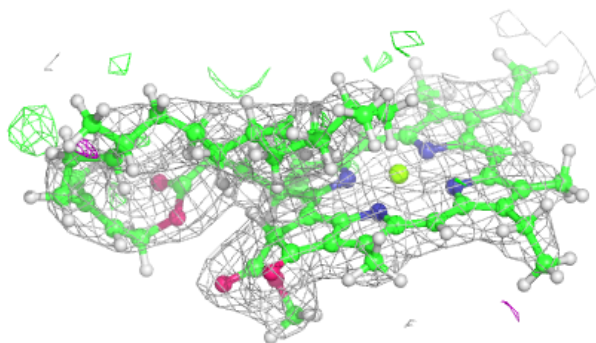
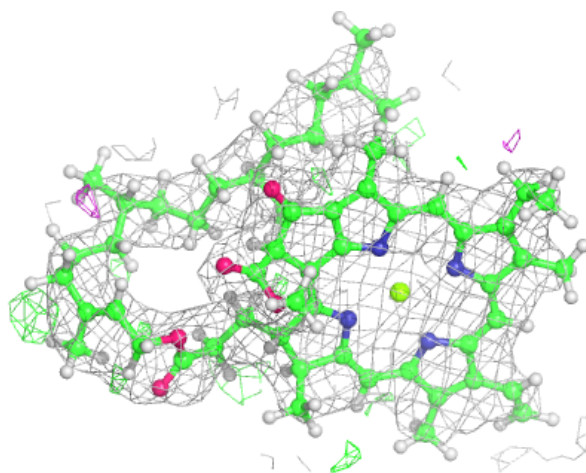
Electron density around CLA a 403:

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



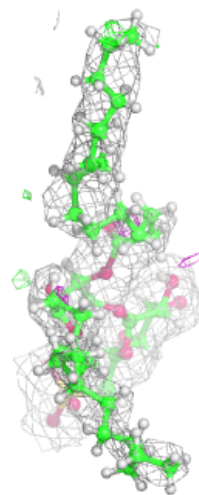
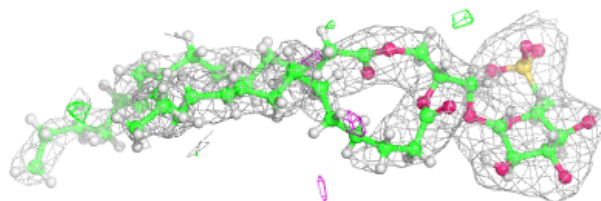
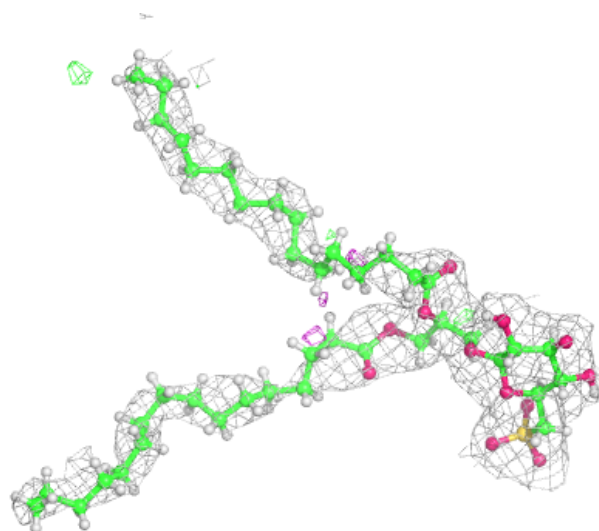
Electron density around CLA c 510:

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



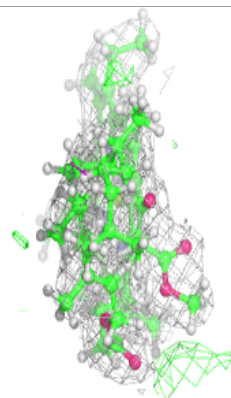
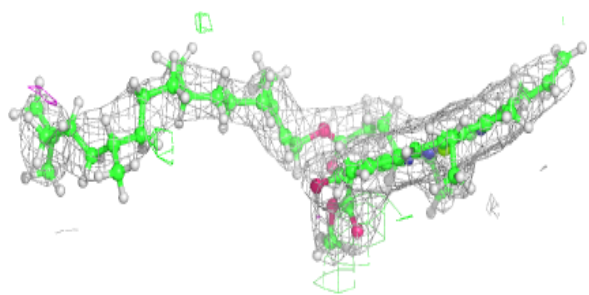
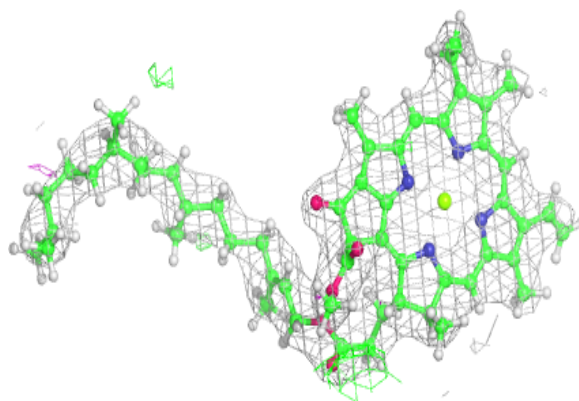
Electron density around SQD a 413:

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

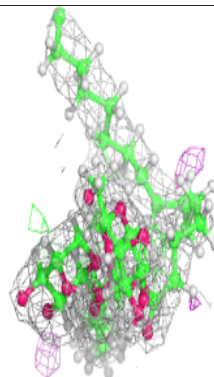
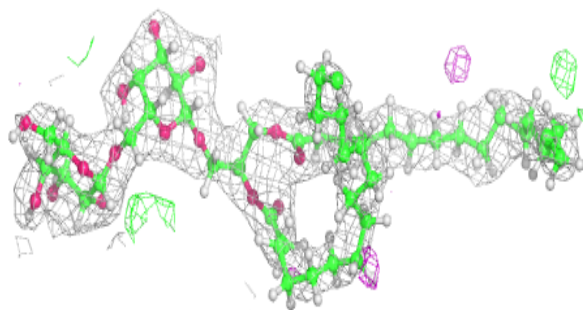
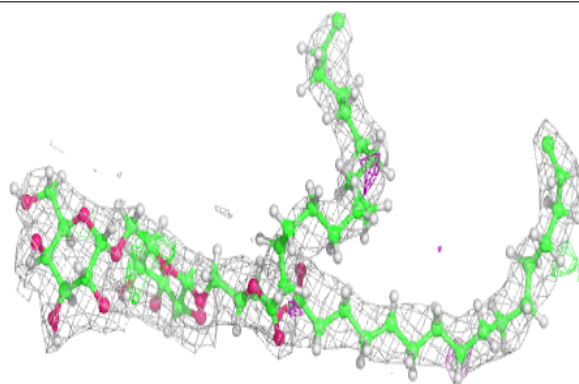


Electron density around CLA B 602:

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

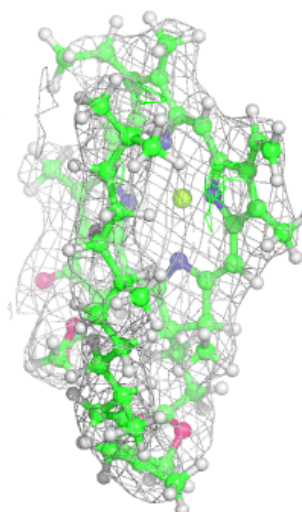
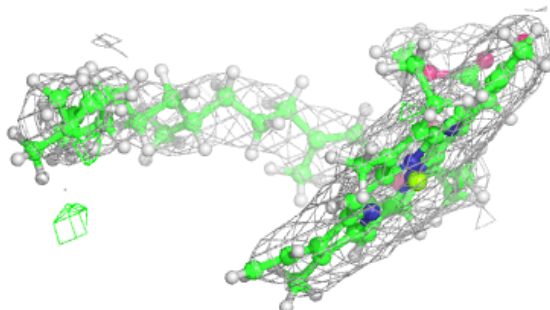
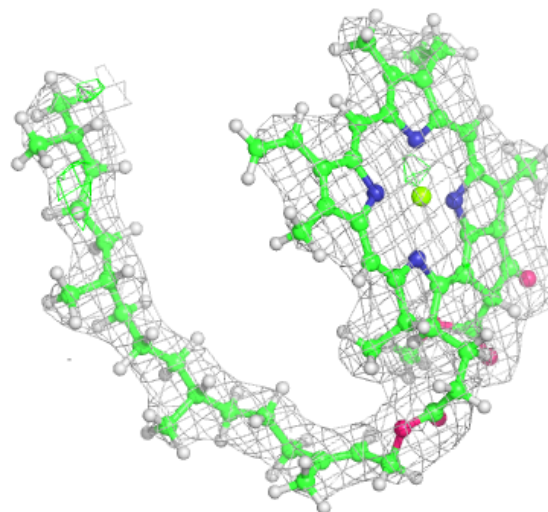
**Electron density around DGD h 102:**

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



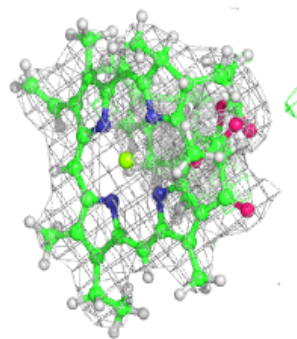
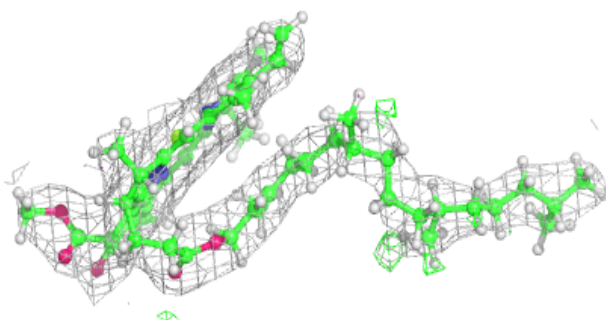
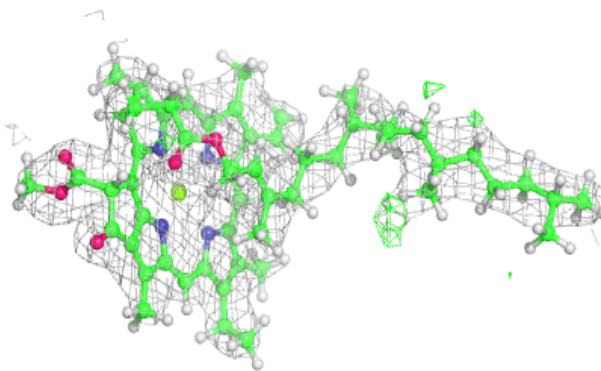
Electron density around CLA c 508:

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

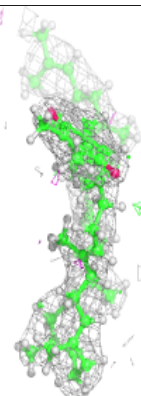
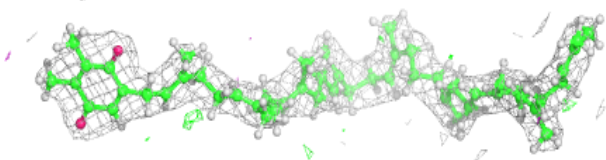
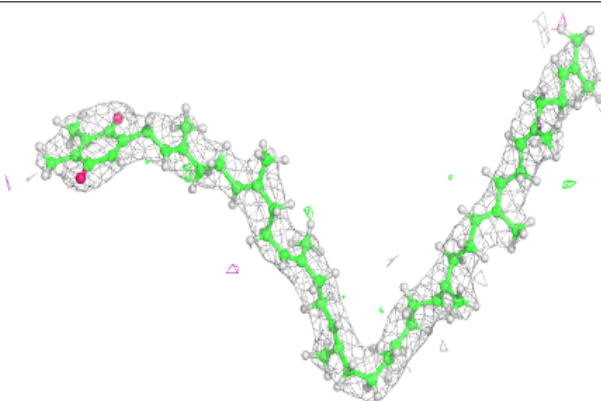


Electron density around CLA c 506:

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

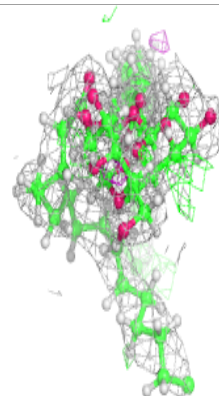
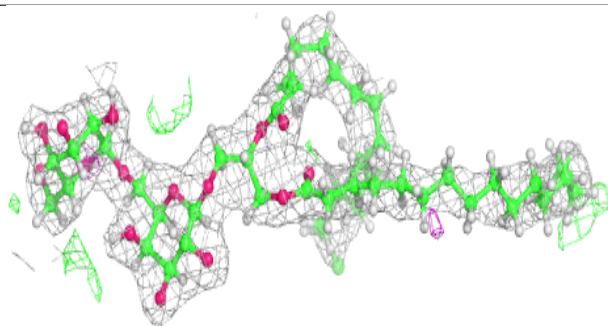
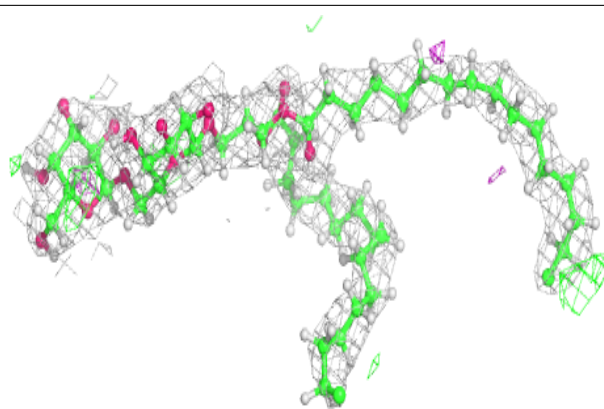
**Electron density around PL9 D 407:**

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

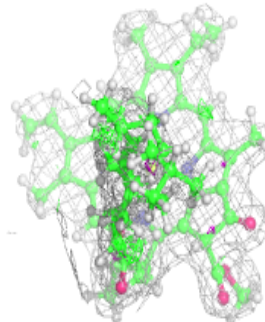
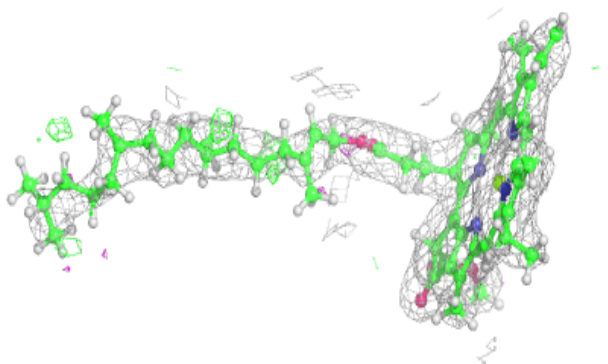
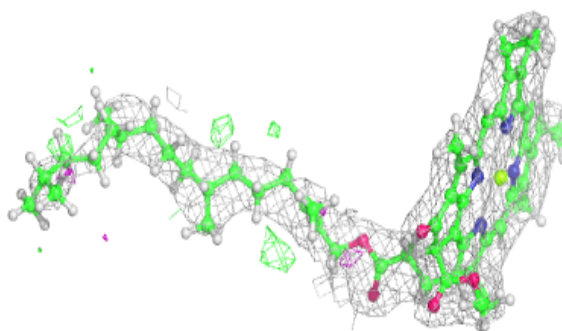


Electron density around DGD H 102:

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

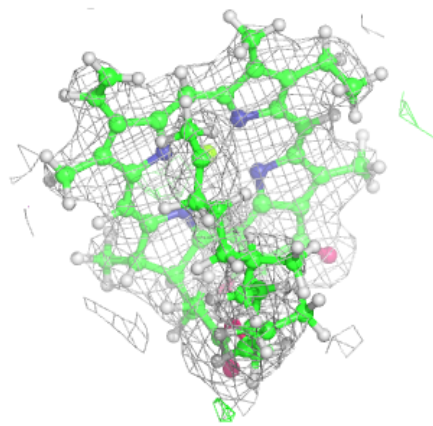
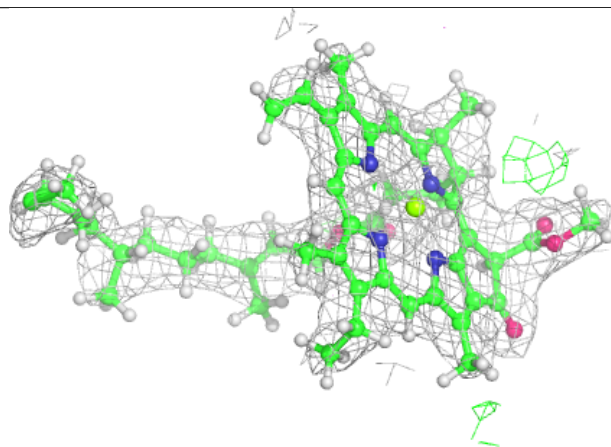
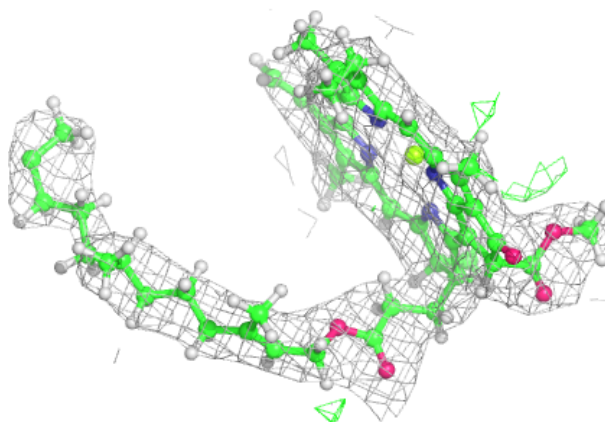
**Electron density around CLA B 604:**

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



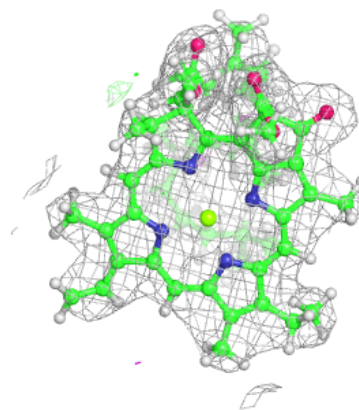
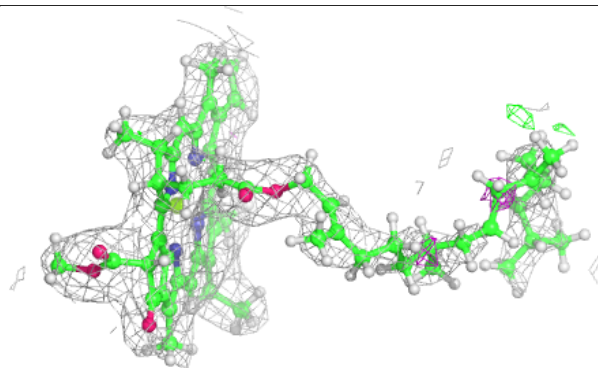
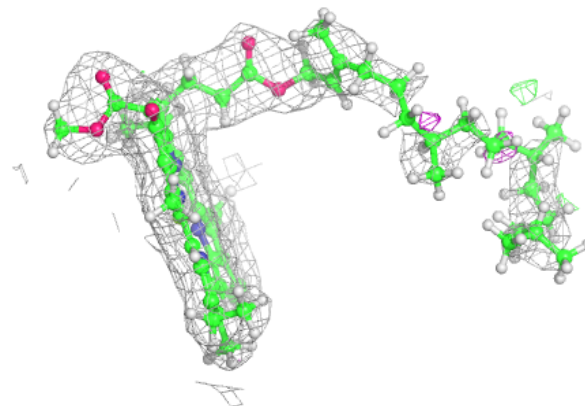
Electron density around CLA C 504:

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



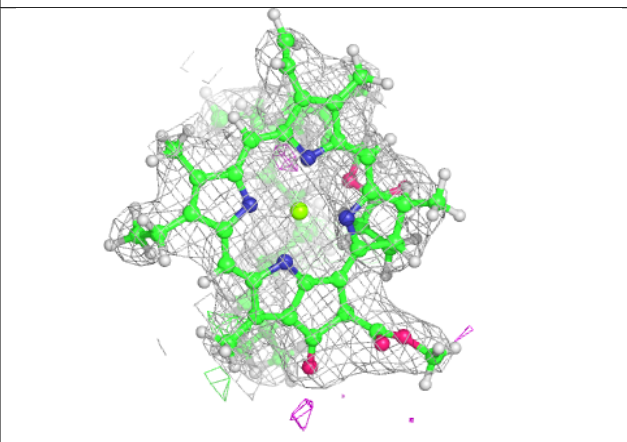
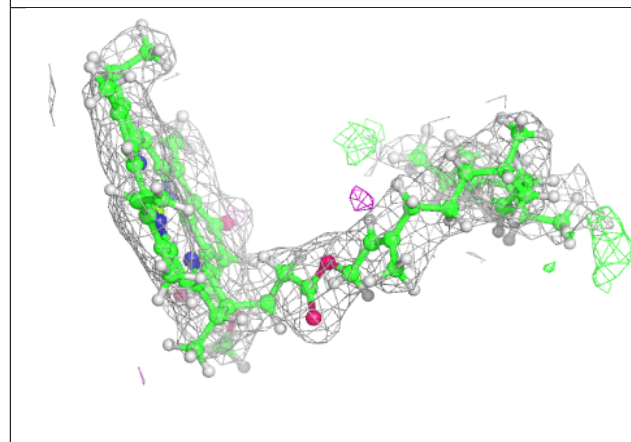
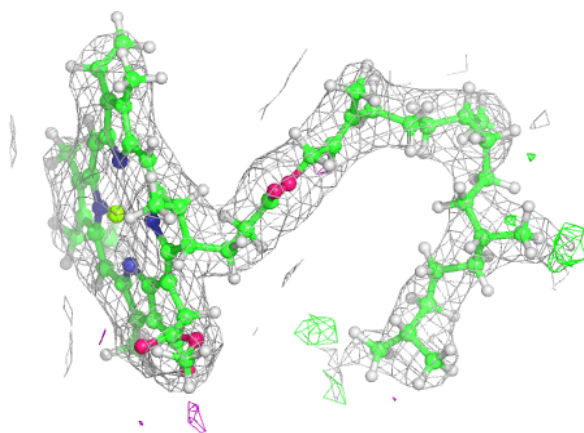
Electron density around CLA C 506:

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

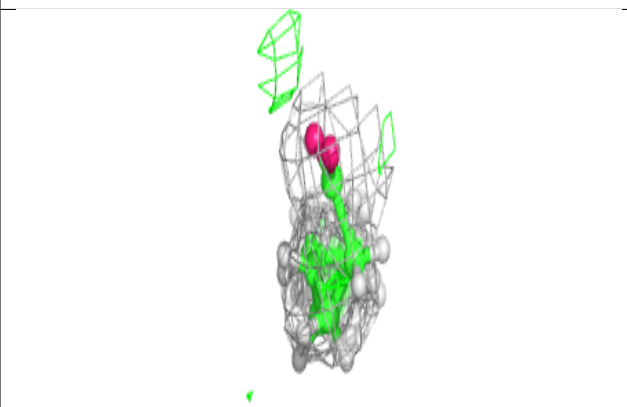
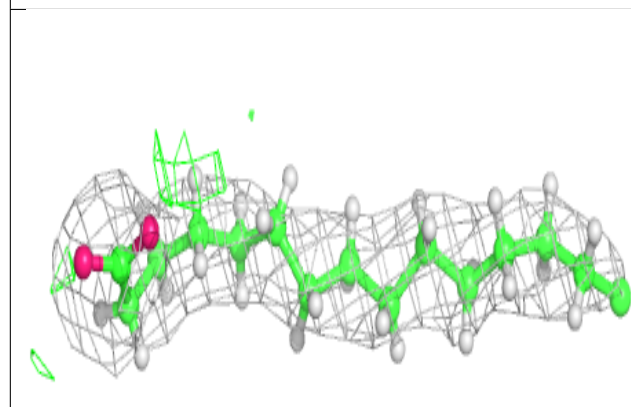
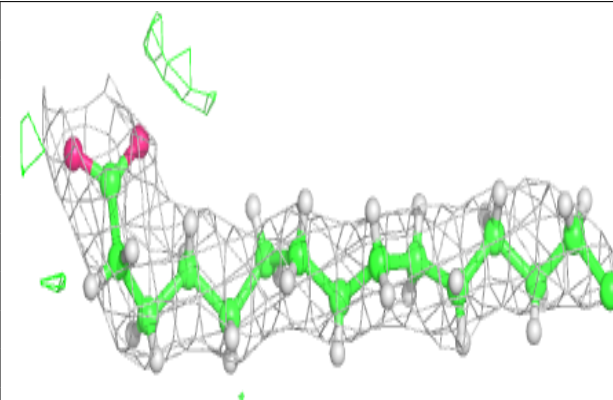


Electron density around CLA B 606:

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

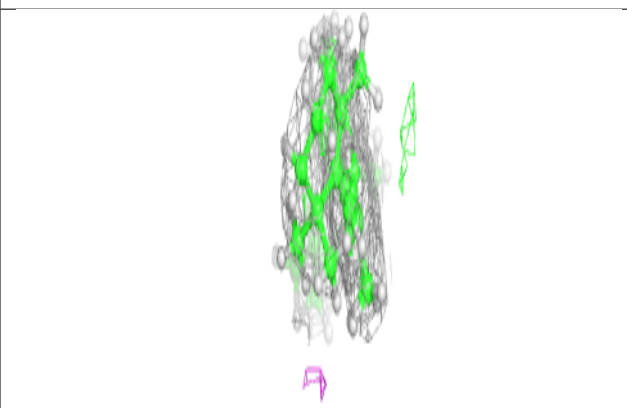
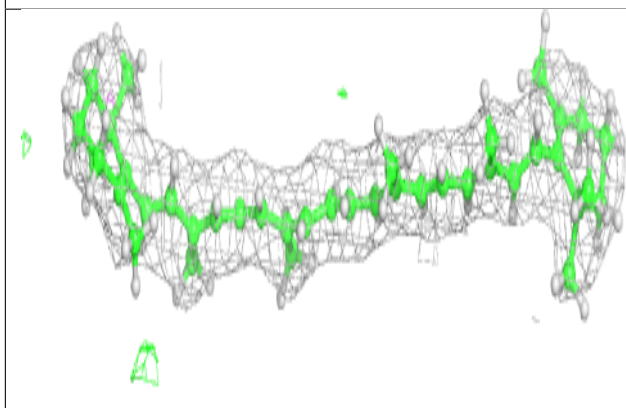
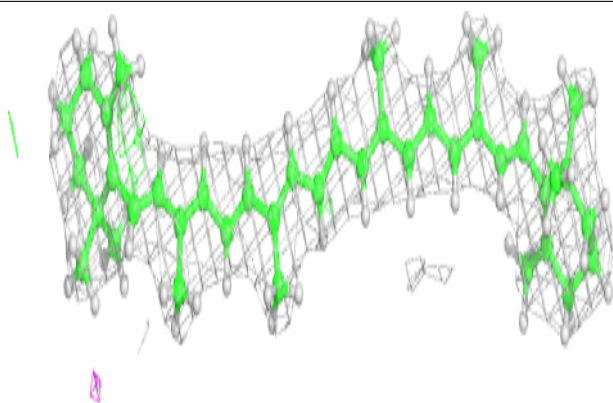
**Electron density around STE d 410:**

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



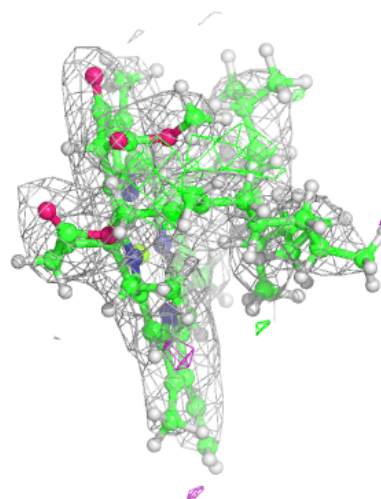
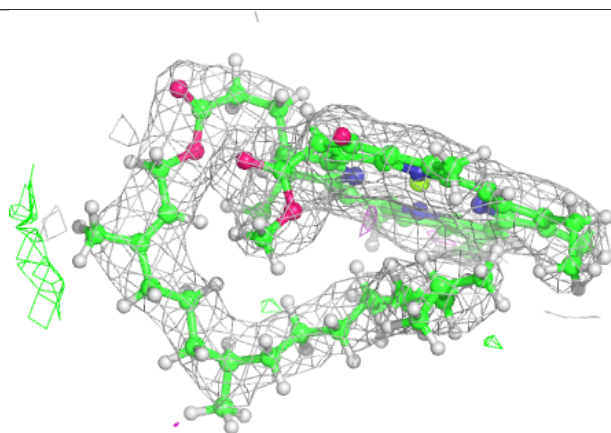
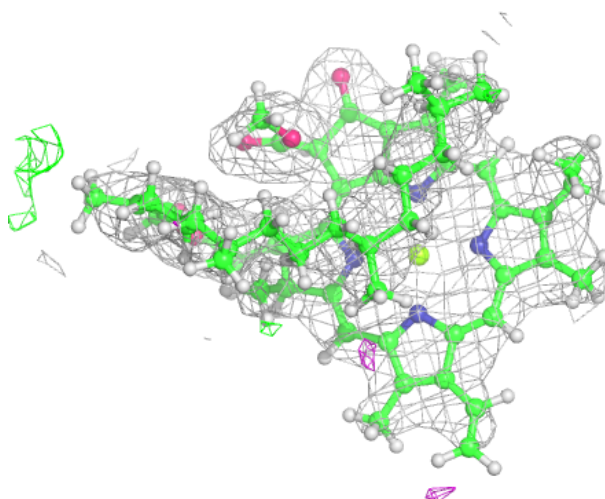
Electron density around BCR B 619:

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



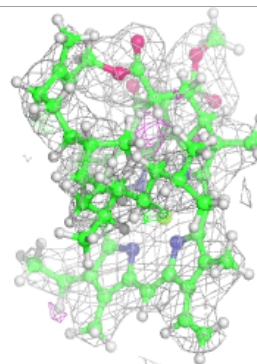
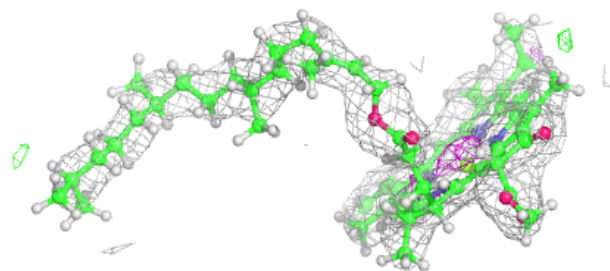
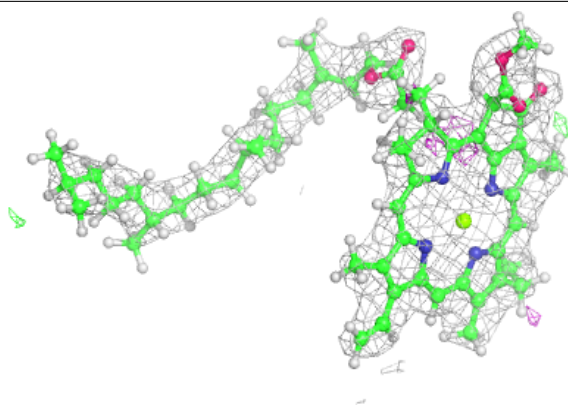
Electron density around CLA C 510:

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



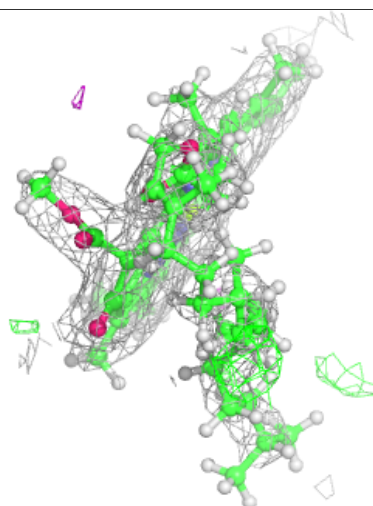
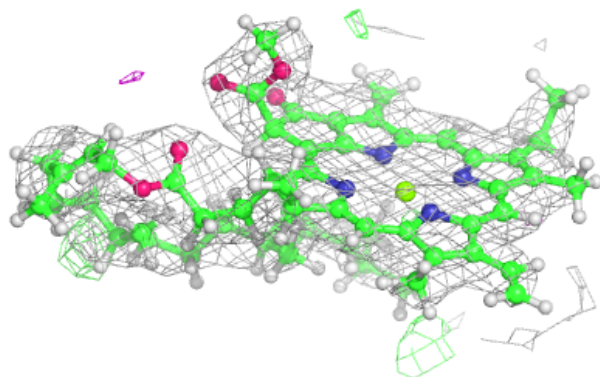
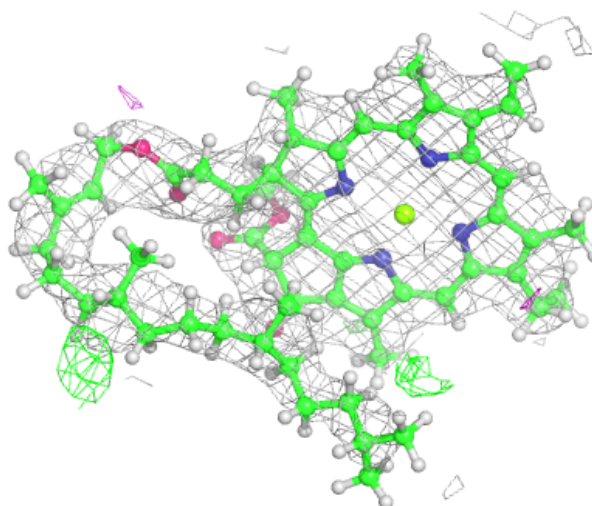
Electron density around CLA C 511:

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



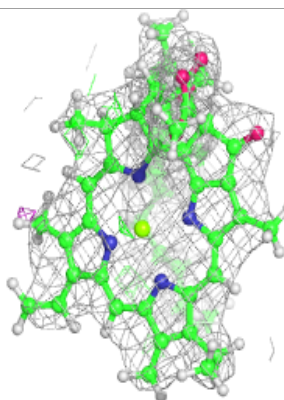
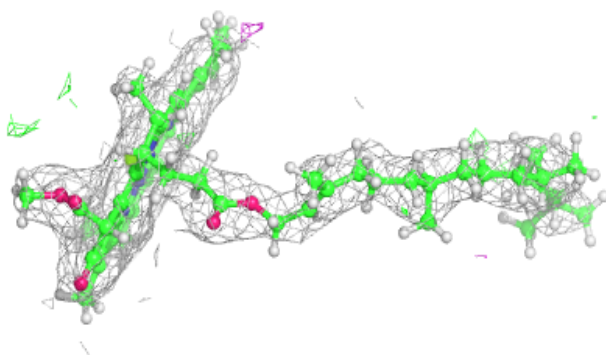
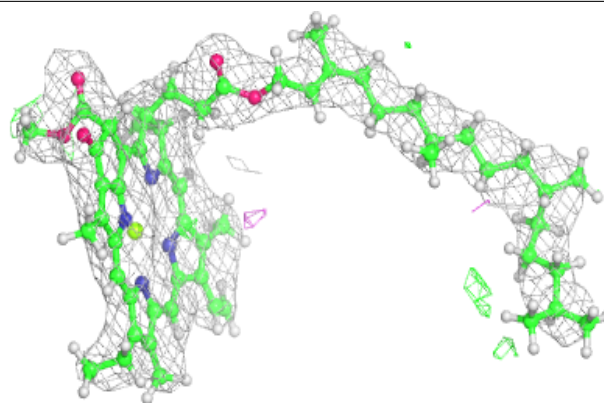
Electron density around CLA C 509:

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

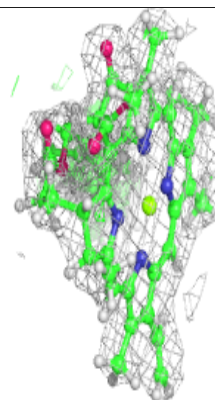
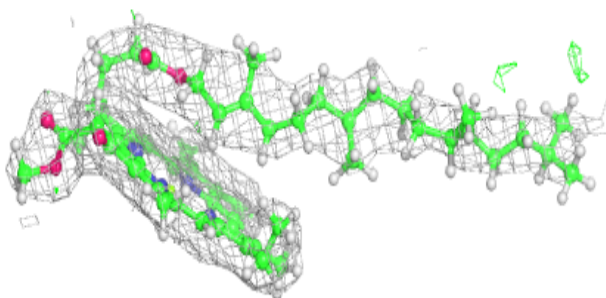
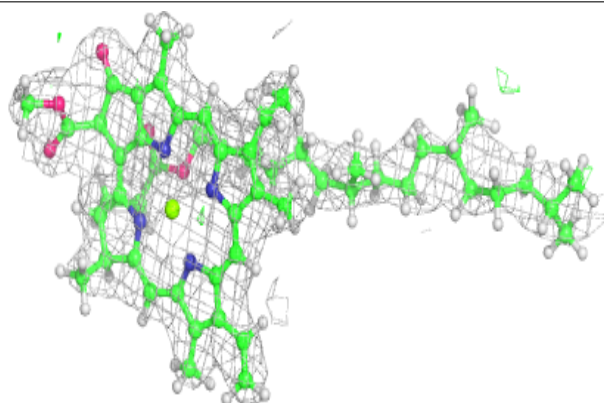


Electron density around CLA b 609:

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

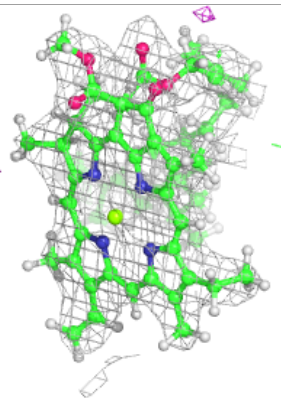
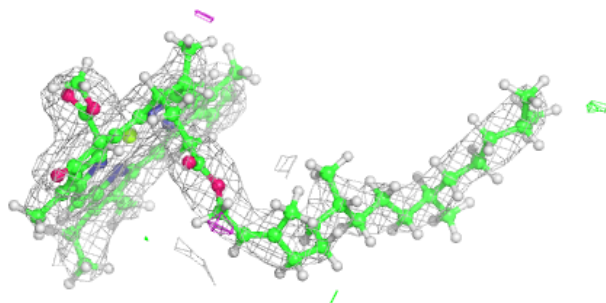
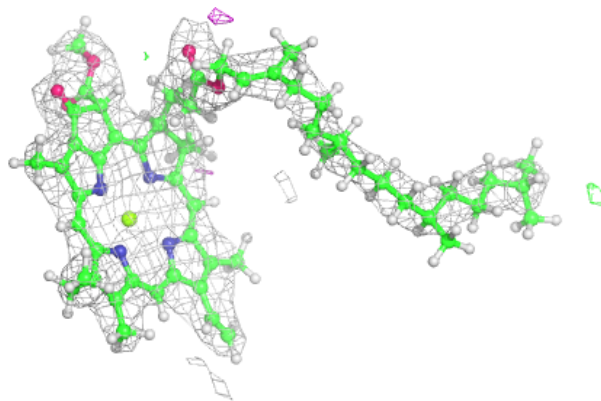
**Electron density around CLA b 614:**

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

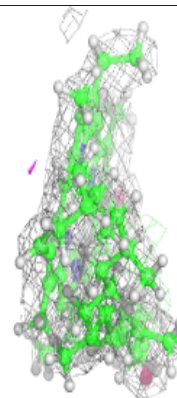
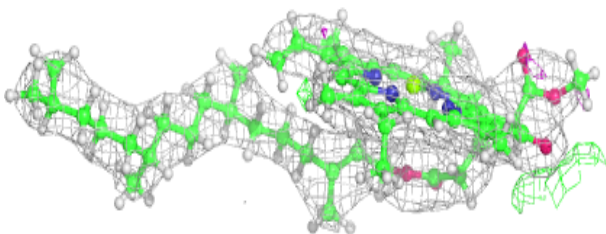
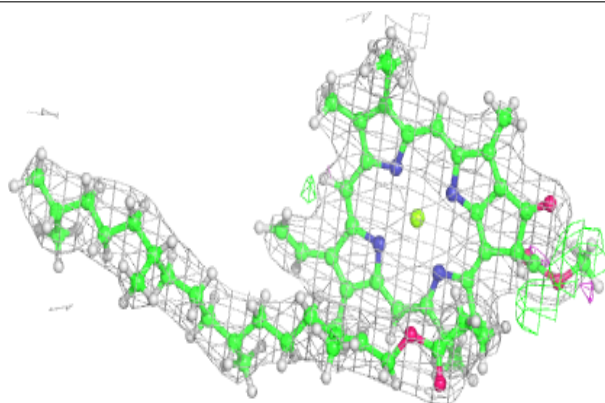


Electron density around CLA c 512:

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

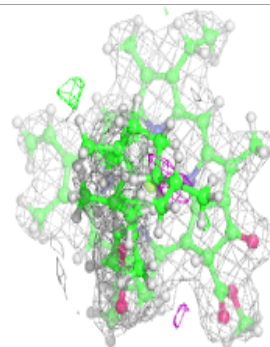
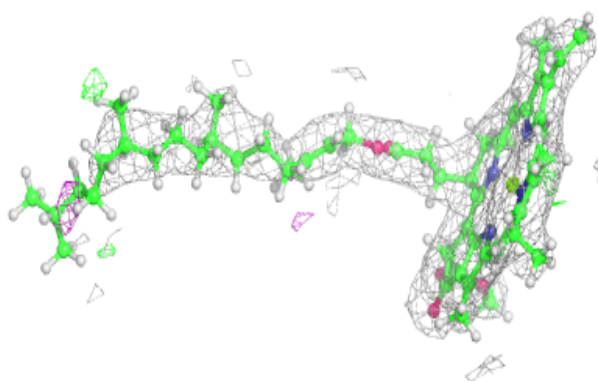
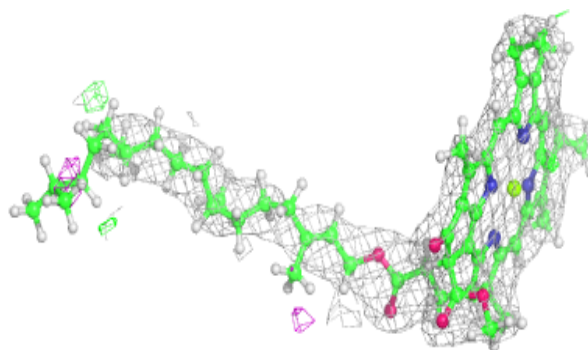
**Electron density around CLA C 501:**

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

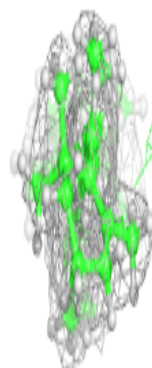
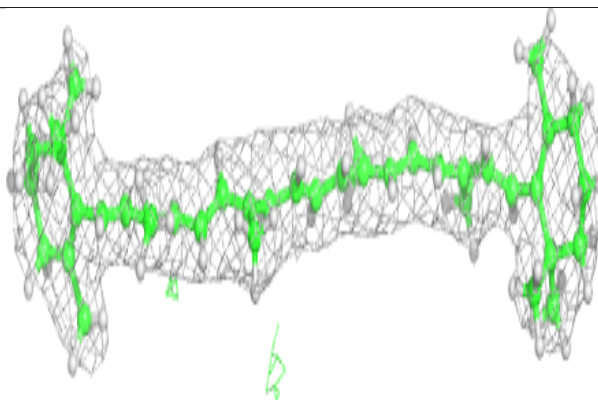
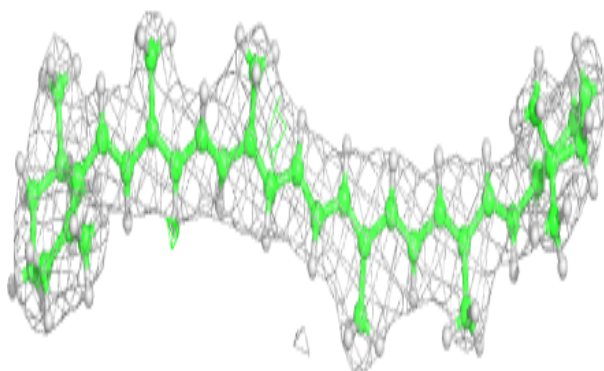


Electron density around CLA b 604:

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

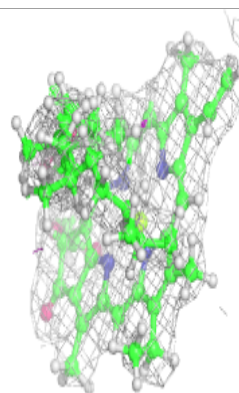
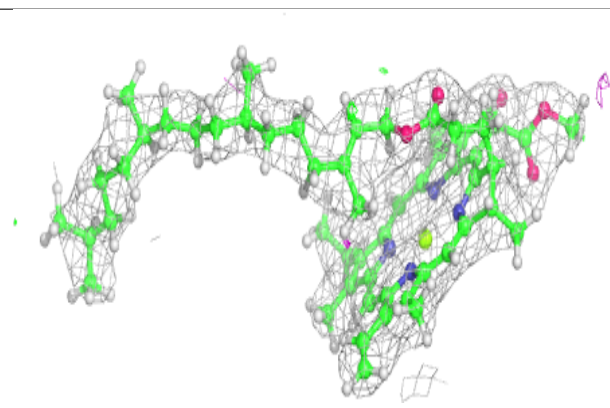
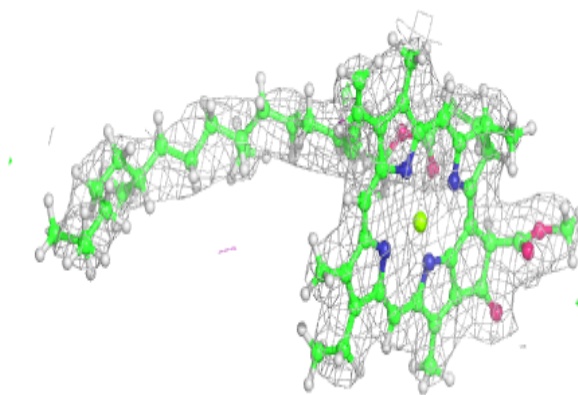
**Electron density around BCR A 405:**

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



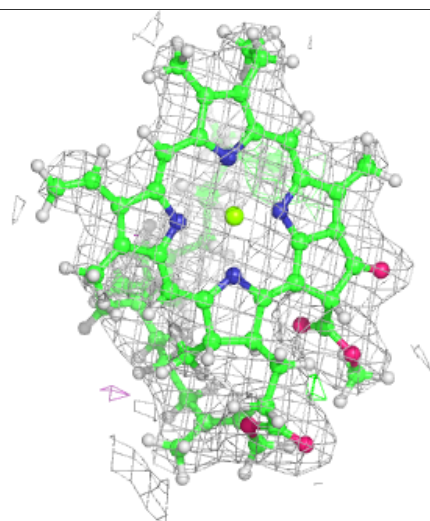
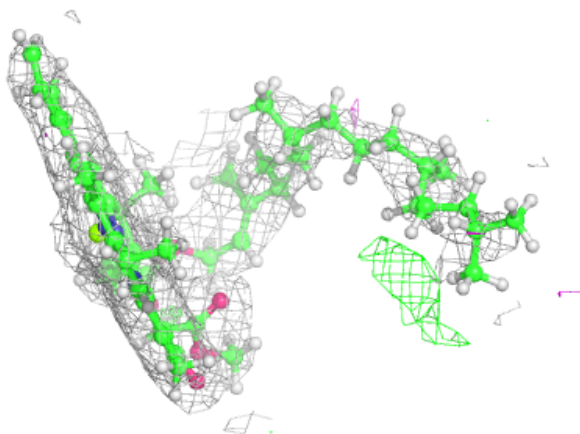
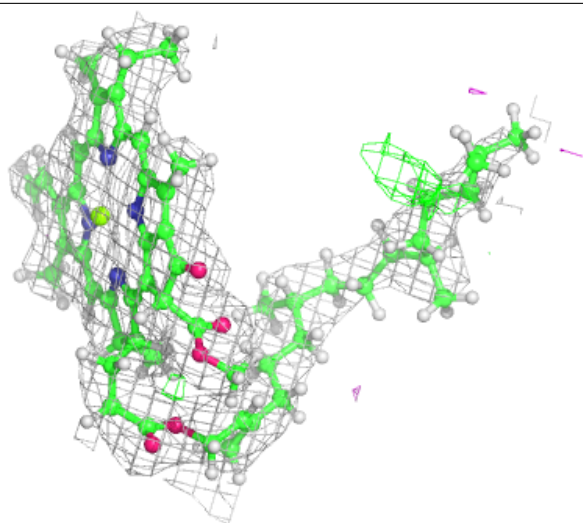
Electron density around CLA b 608:

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



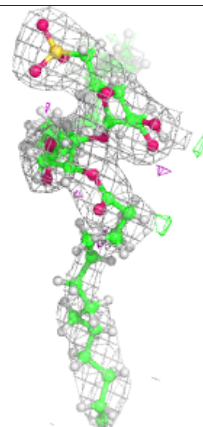
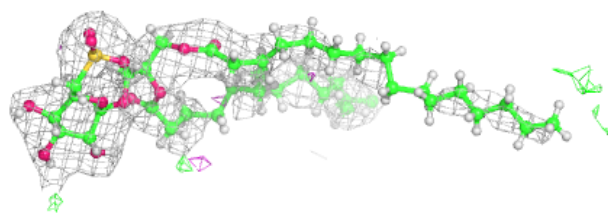
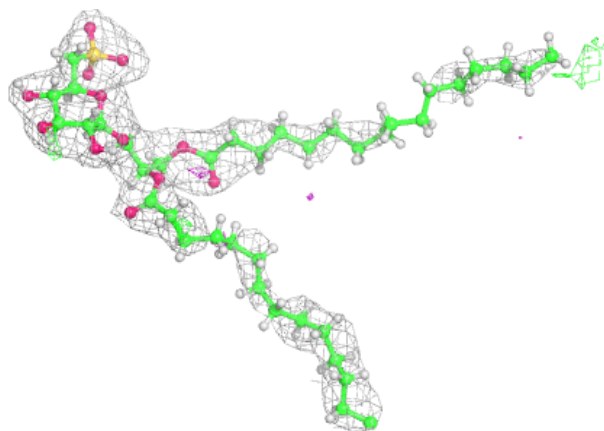
Electron density around CLA b 613:

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



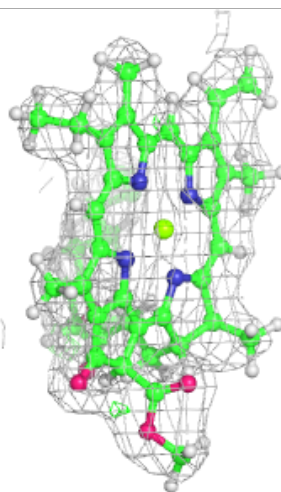
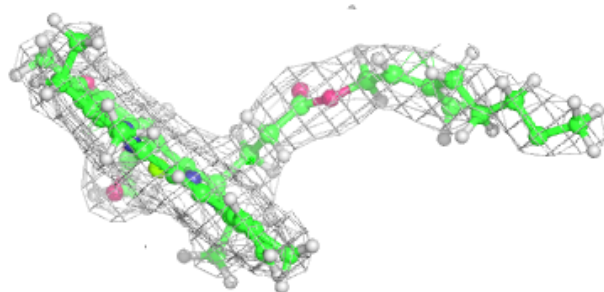
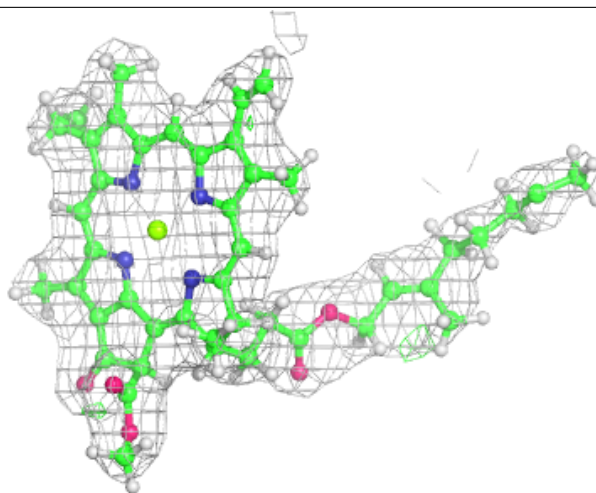
Electron density around SQD A 411:

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



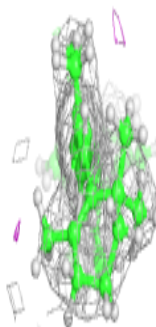
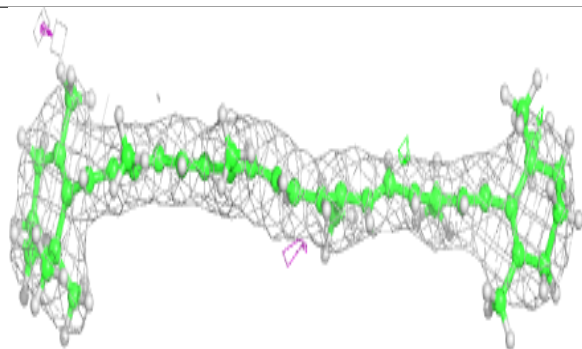
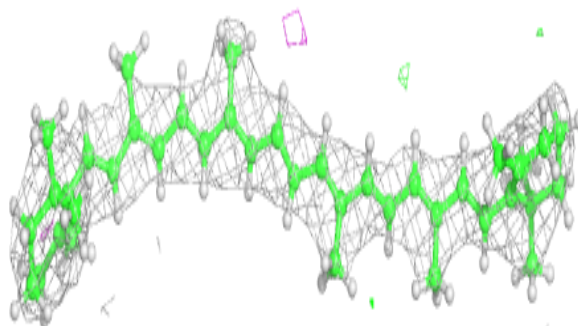
Electron density around CLA A 404:

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

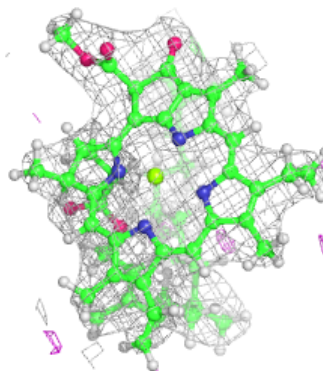
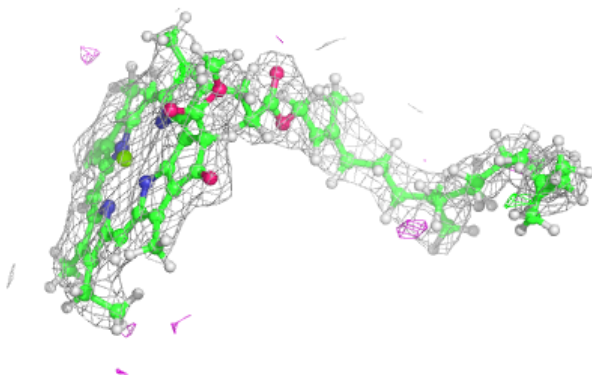
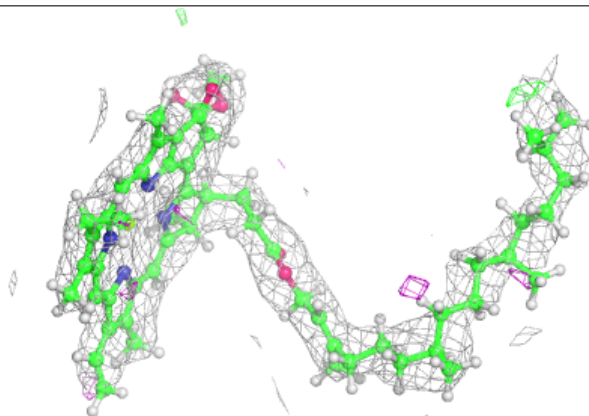


Electron density around BCR c 516:

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

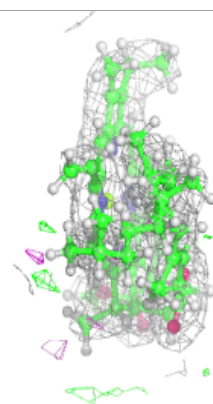
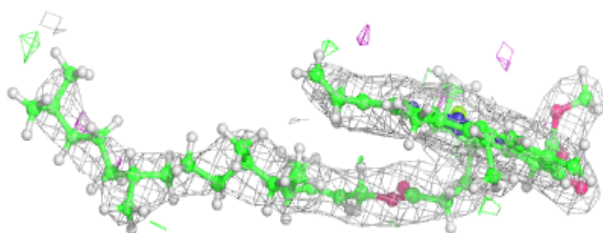
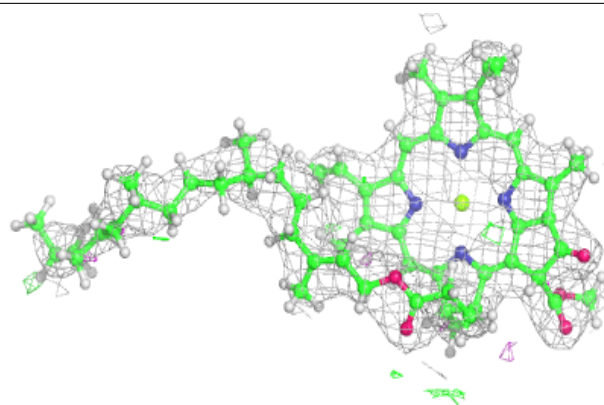
**Electron density around CLA b 606:**

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

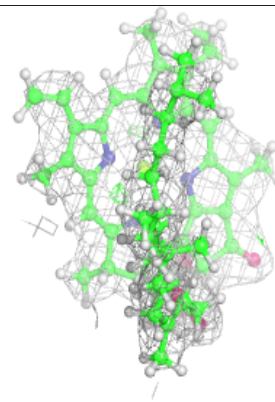
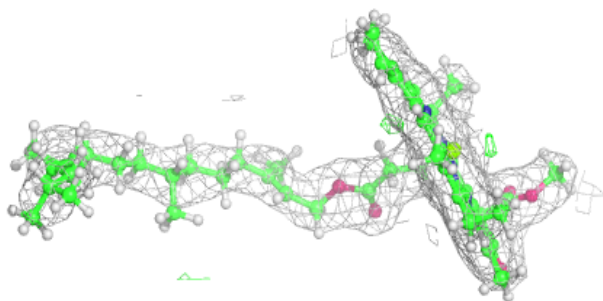
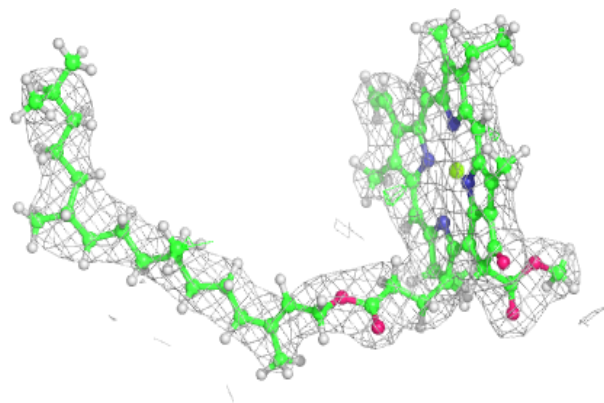


Electron density around CLA B 603:

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

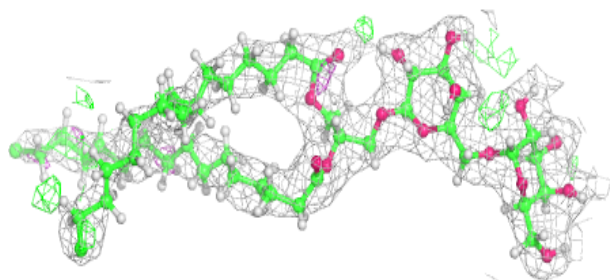
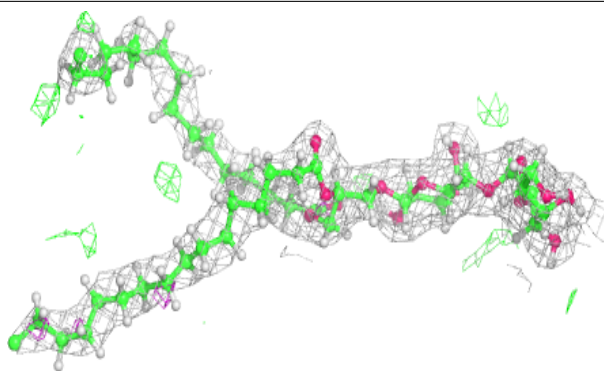
**Electron density around CLA B 609:**

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



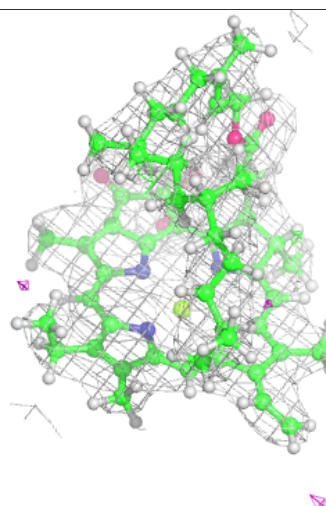
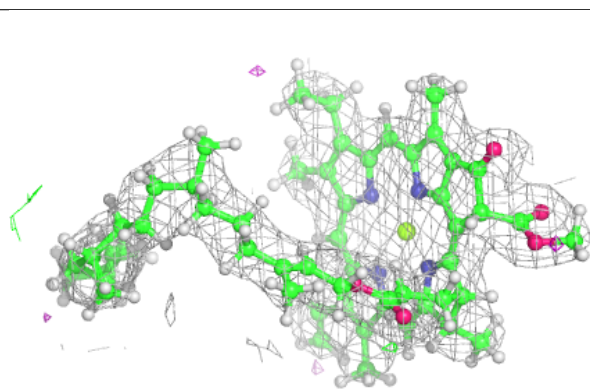
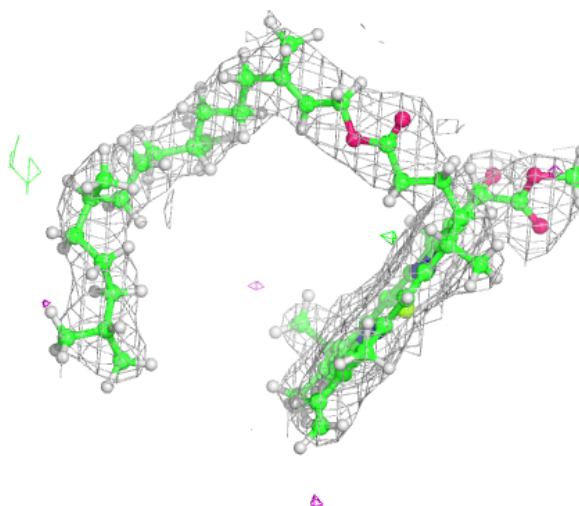
Electron density around DGD C 517:

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



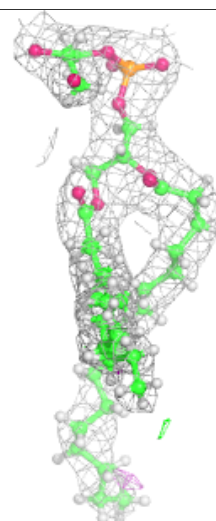
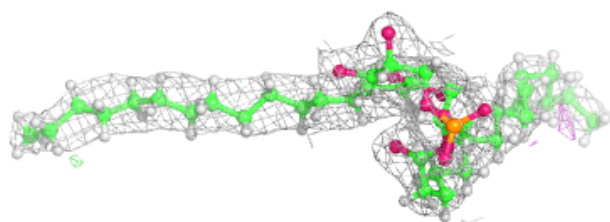
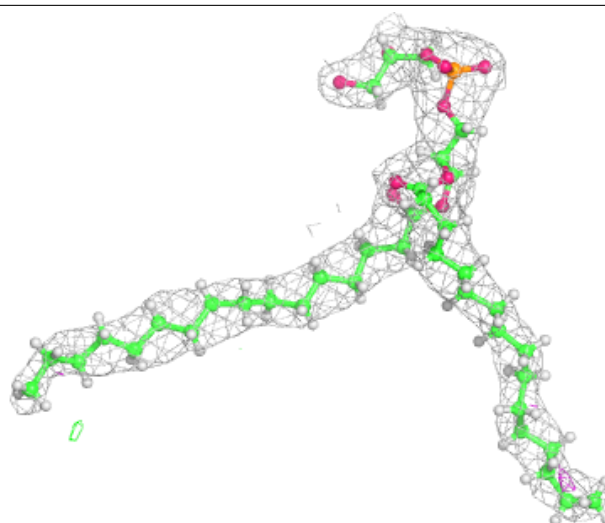
Electron density around CLA b 611:

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



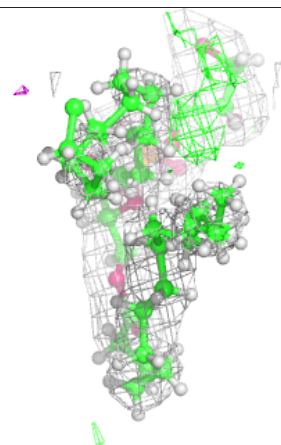
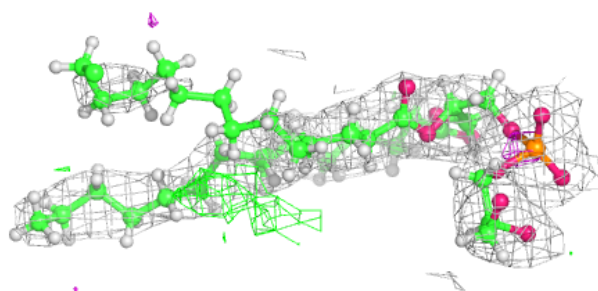
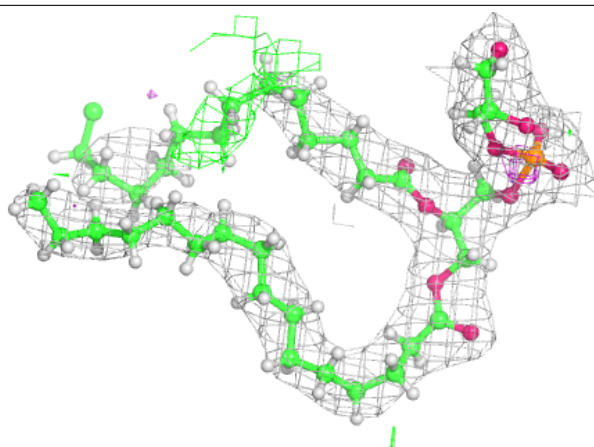
Electron density around LHG 1 101:

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



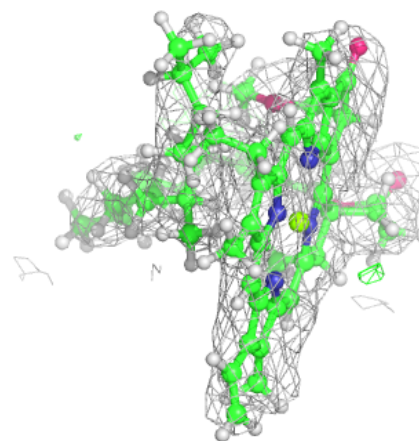
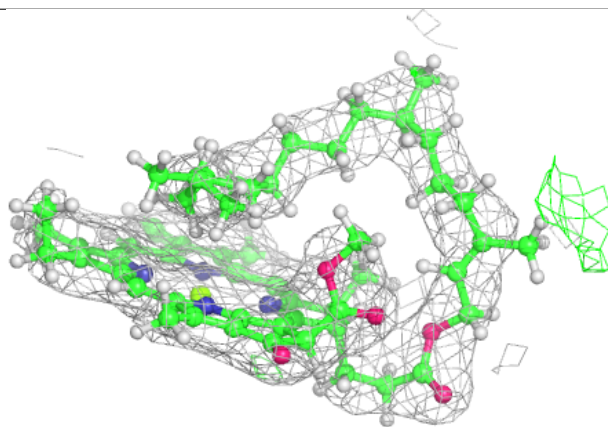
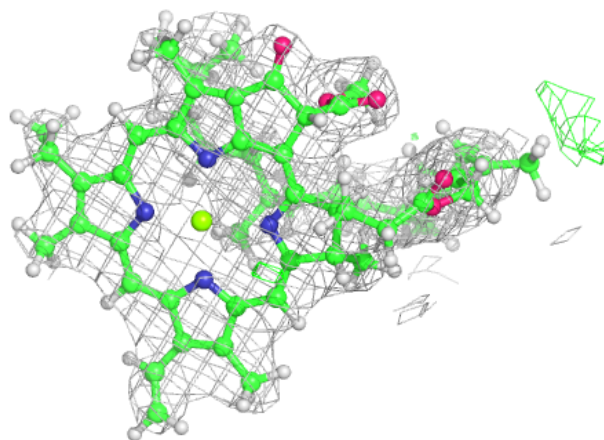
Electron density around LHG A 410:

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



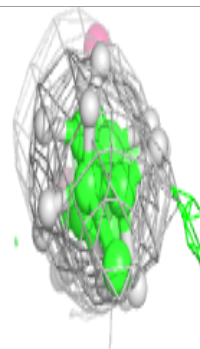
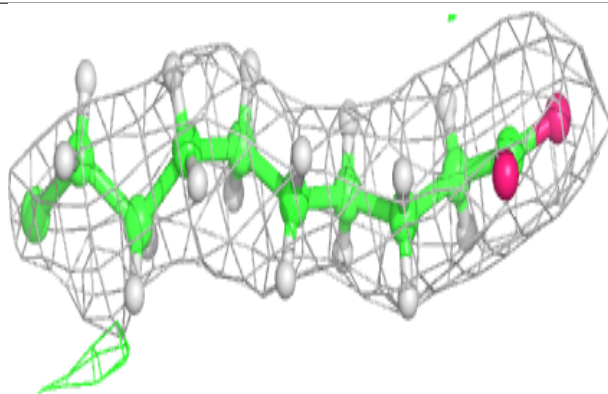
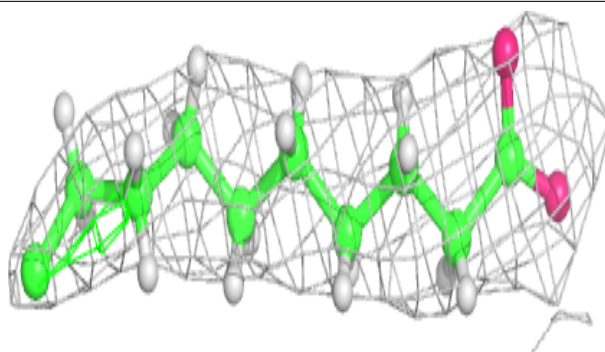
Electron density around CLA c 511:

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

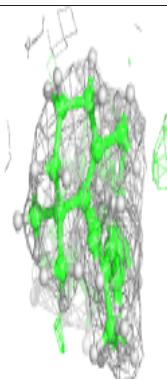
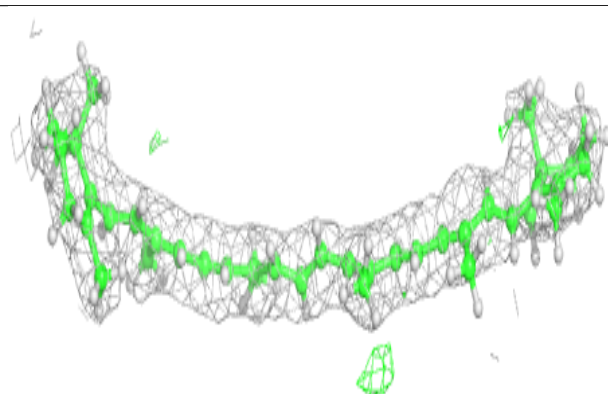
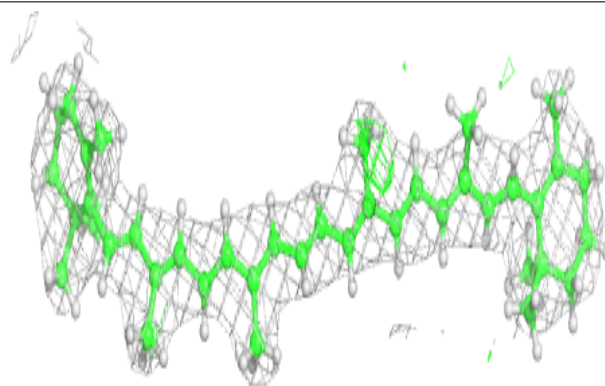


Electron density around STE J 101:

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

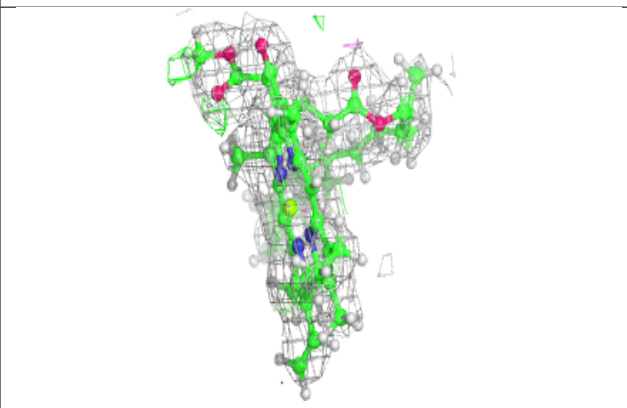
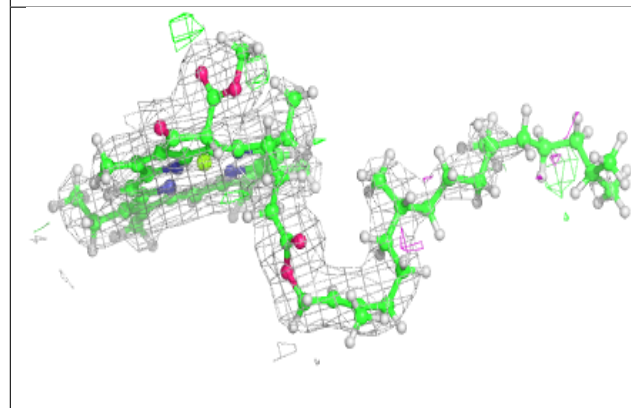
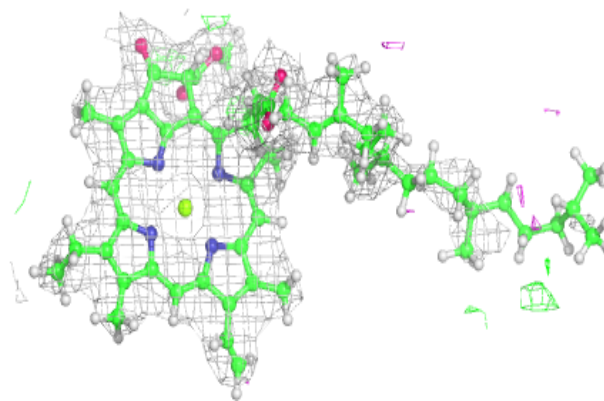
**Electron density around BCR T 101:**

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

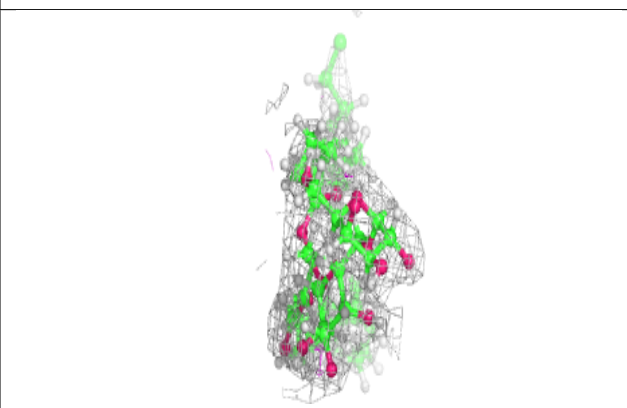
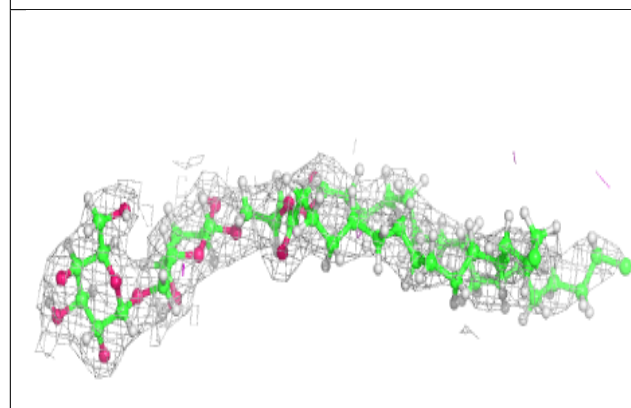
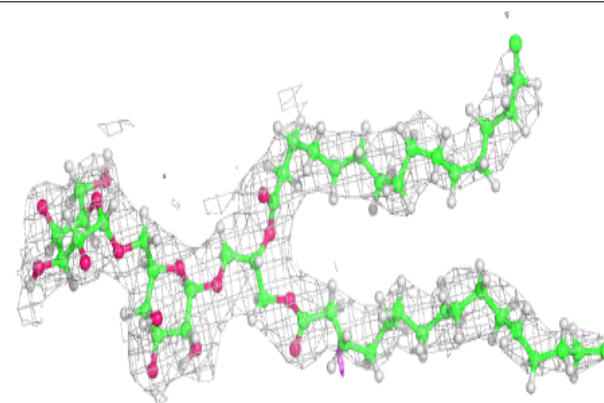


Electron density around CLA A 403:

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

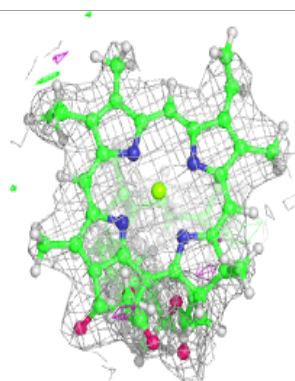
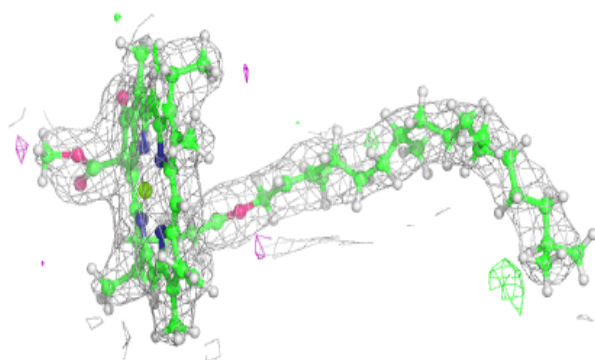
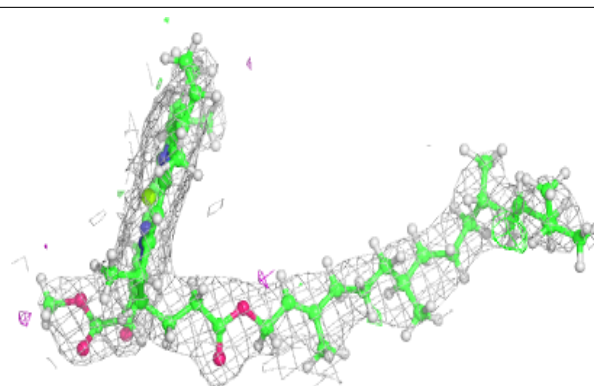
**Electron density around DGD C 519:**

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

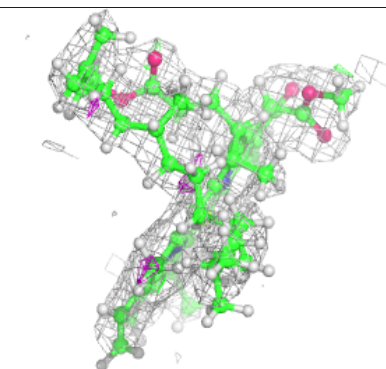
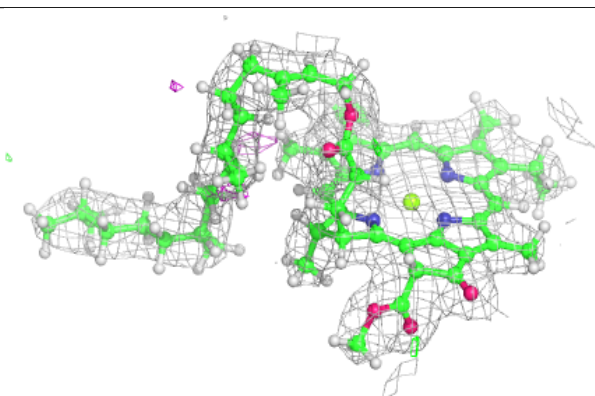
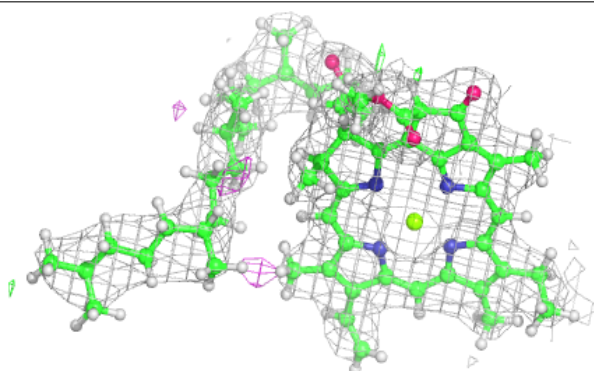


Electron density around CLA b 605:

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

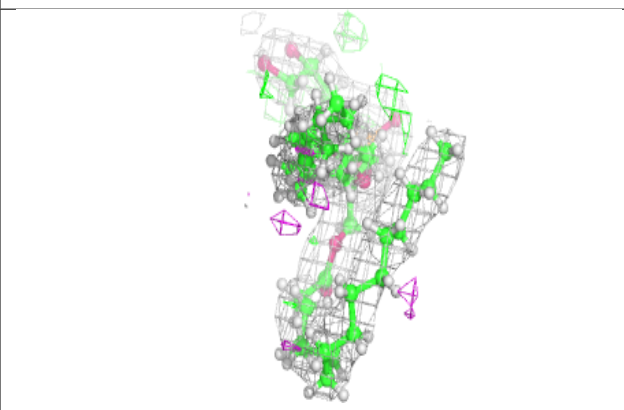
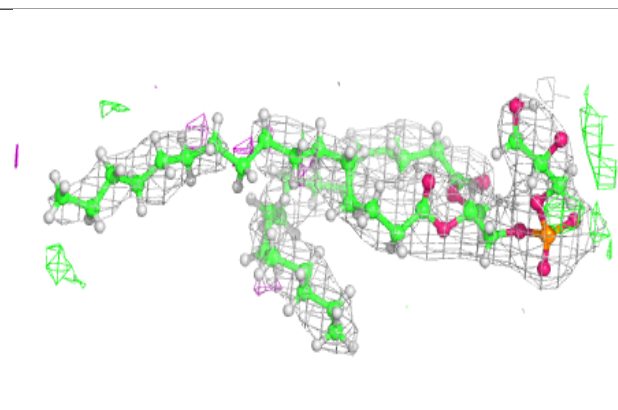
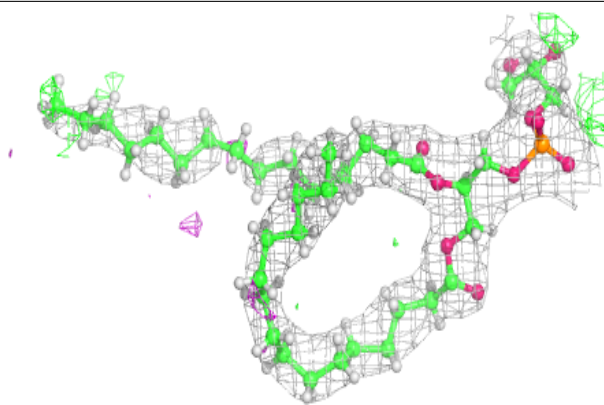
**Electron density around CLA a 411:**

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

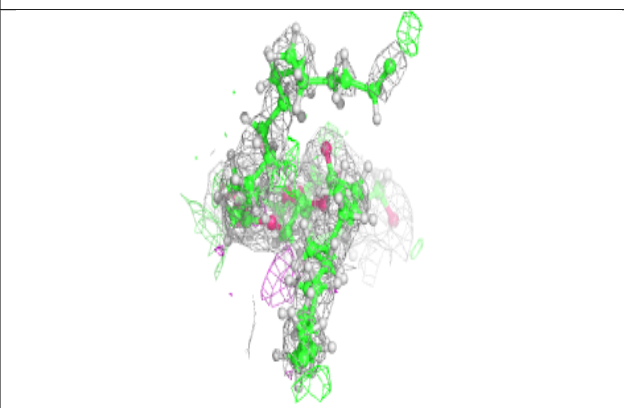
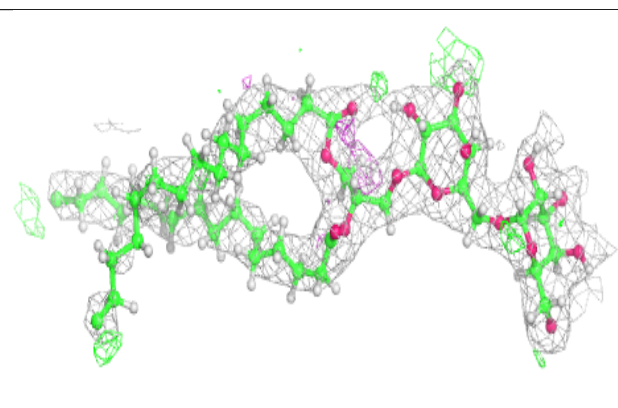
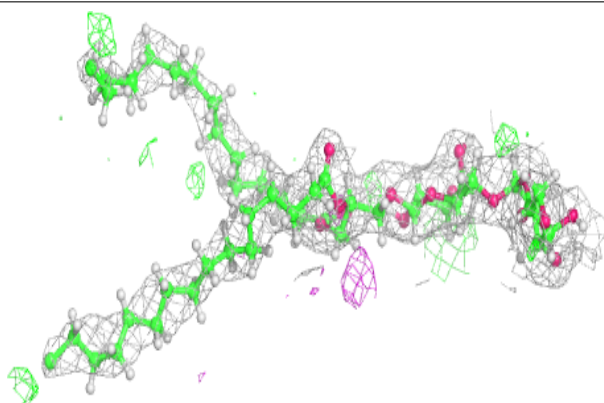


Electron density around LHG a 412:

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

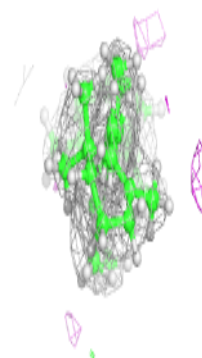
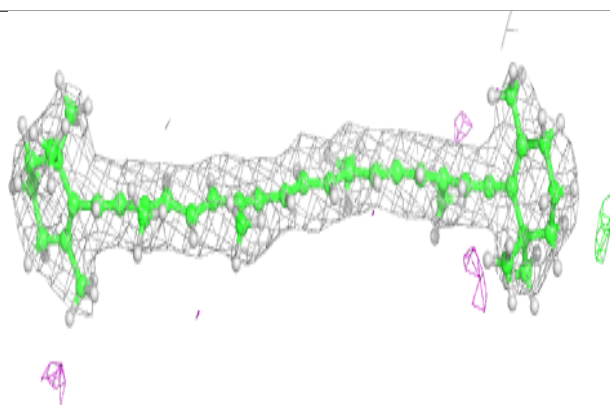
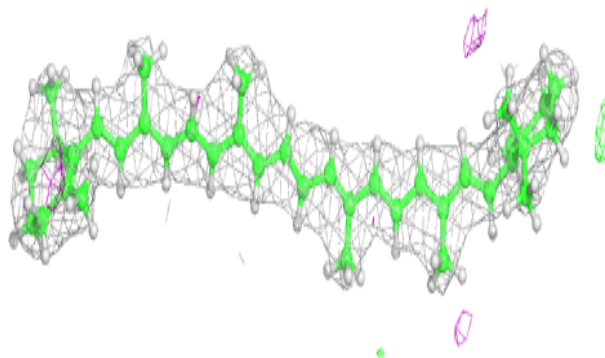
**Electron density around DGD c 517:**

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



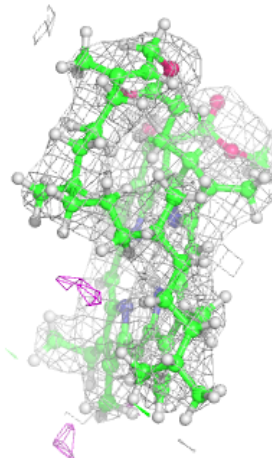
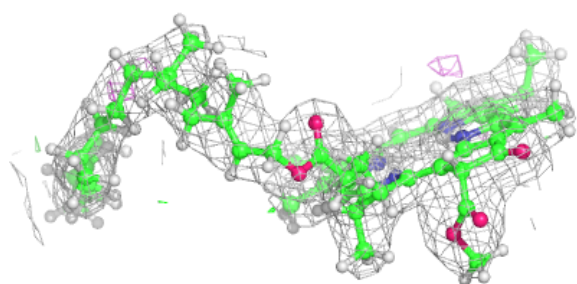
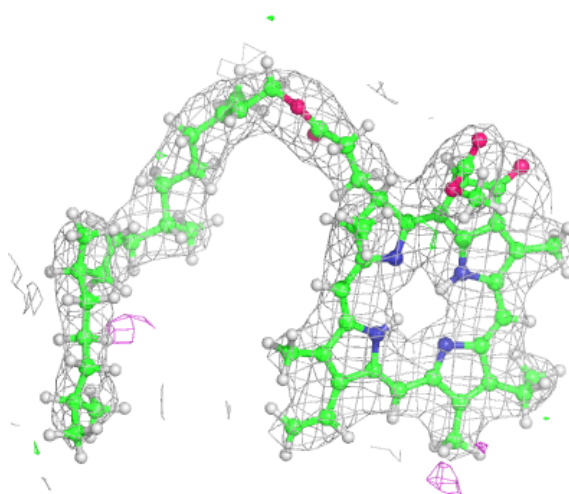
Electron density around BCR a 406:

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



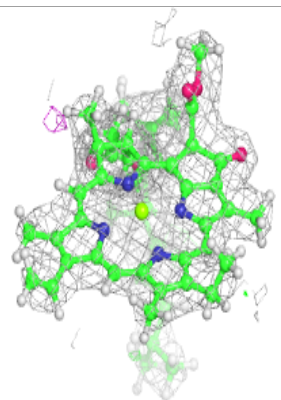
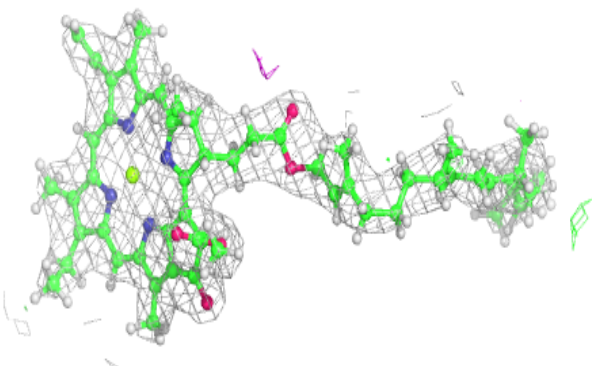
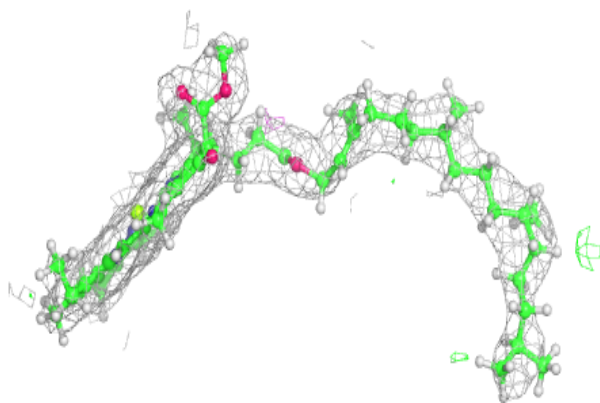
Electron density around PHO d 401:

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

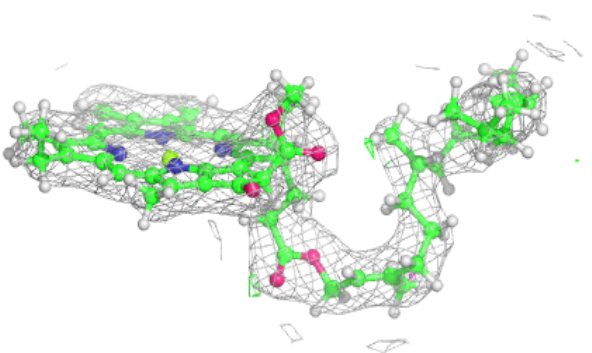
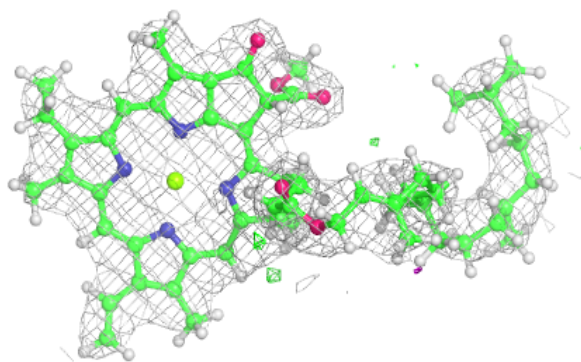


Electron density around CLA d 402:

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

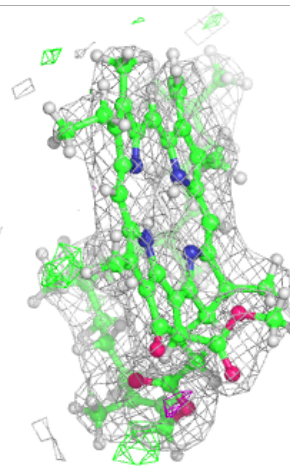
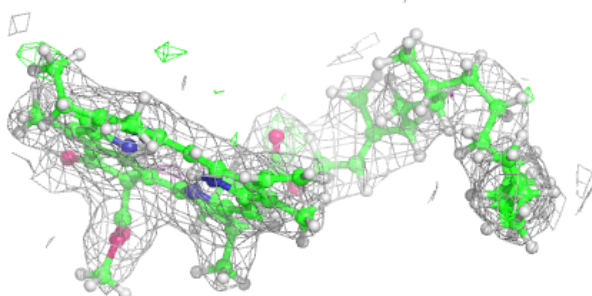
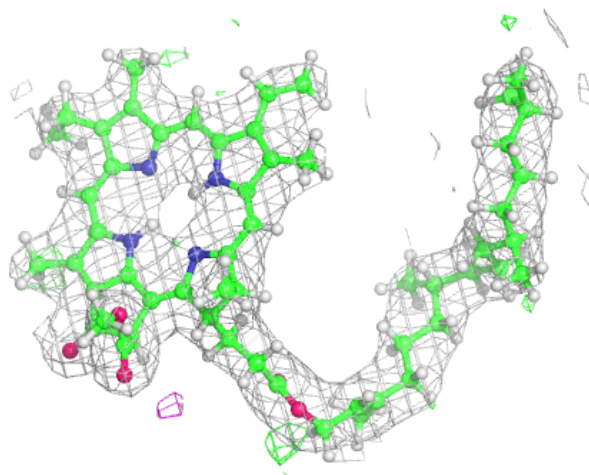
**Electron density around CLA b 612:**

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



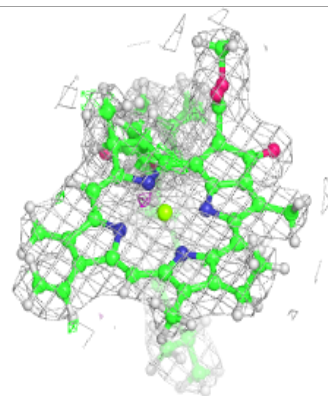
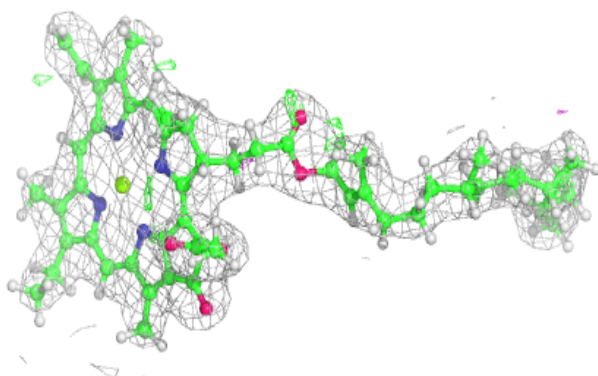
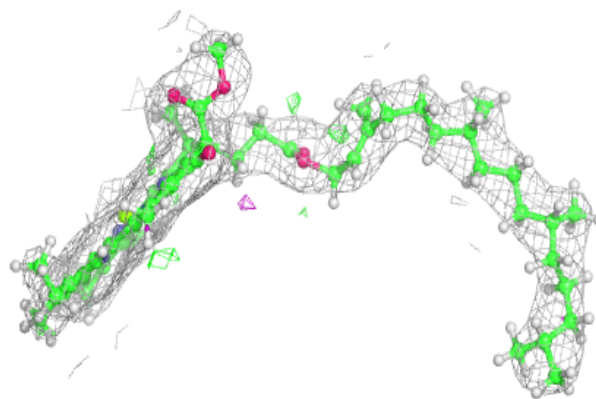
Electron density around PHO D 402:

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

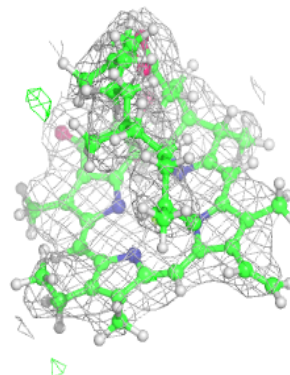
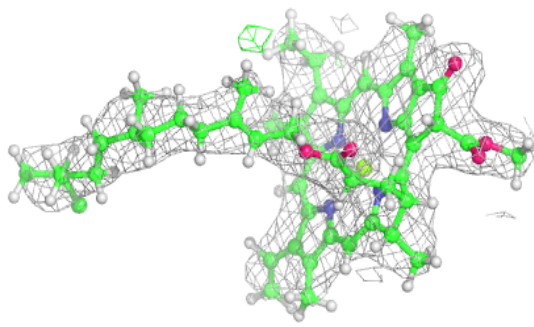
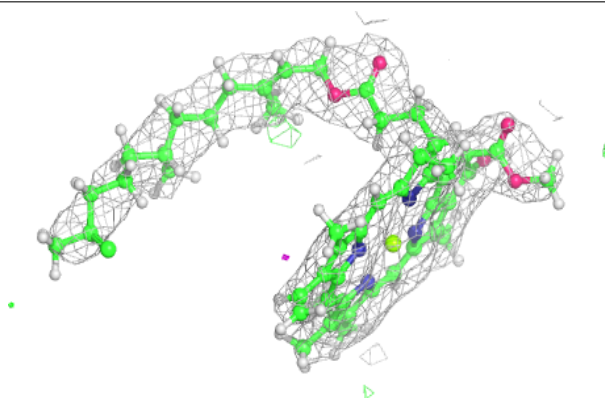


Electron density around CLA D 404:

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

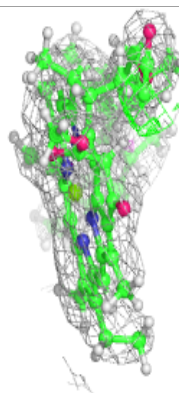
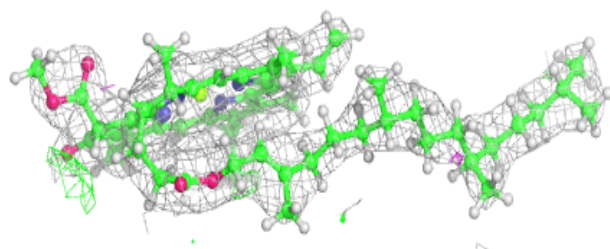
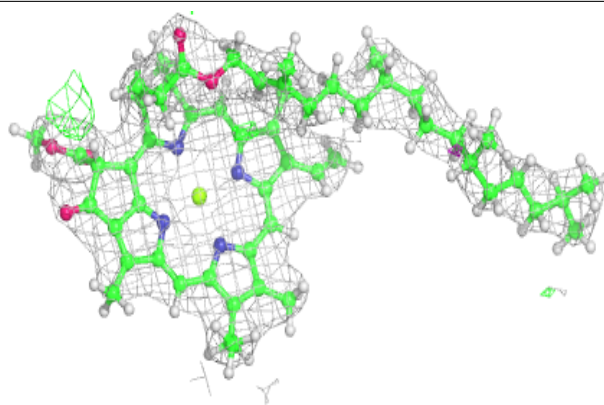
**Electron density around CLA c 505:**

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

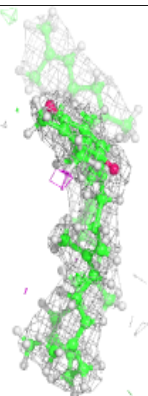
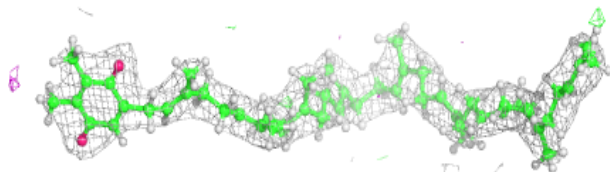
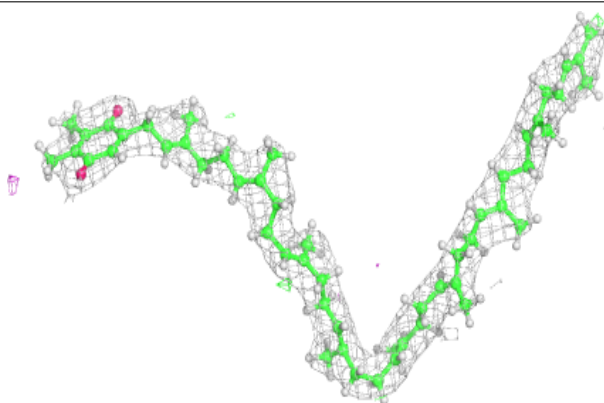


Electron density around CLA c 502:

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

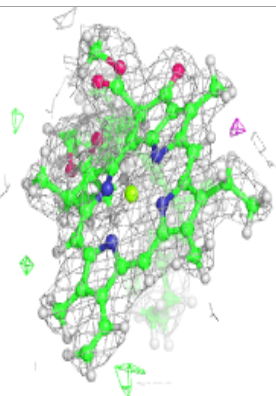
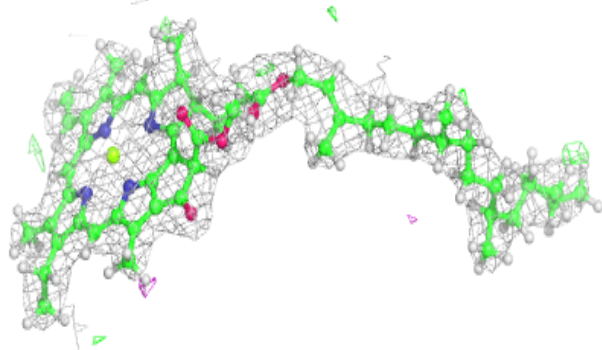
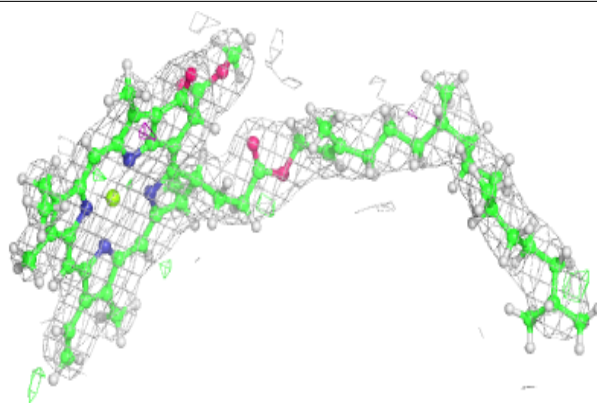
**Electron density around PL9 d 405:**

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

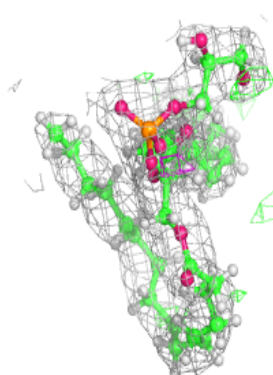
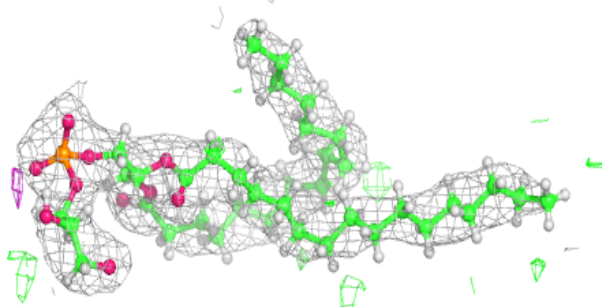
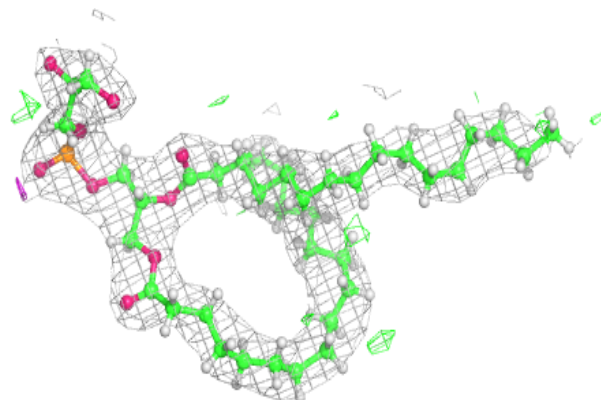


Electron density around CLA A 402:

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

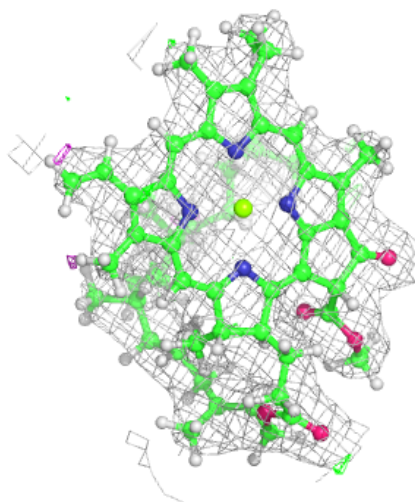
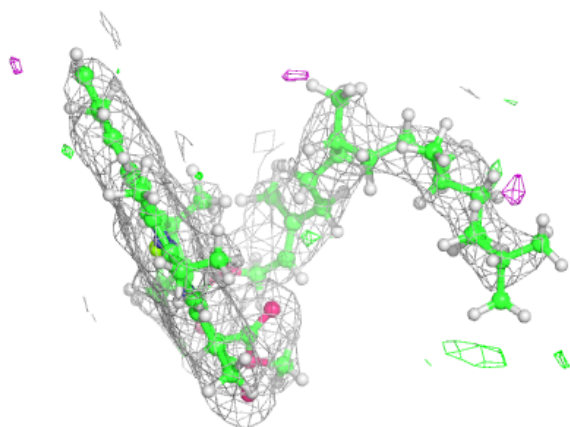
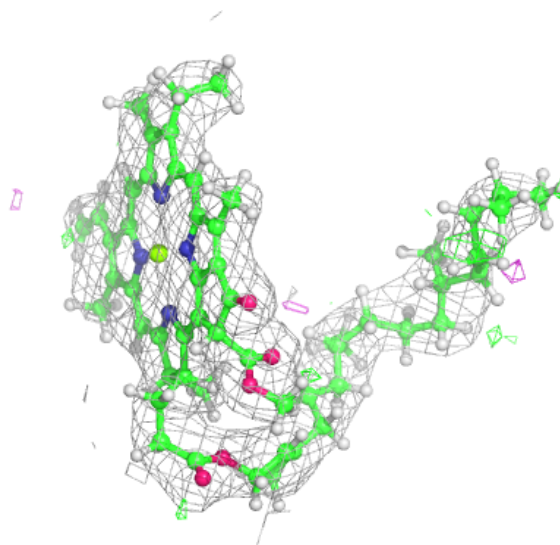
**Electron density around LHG D 412:**

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



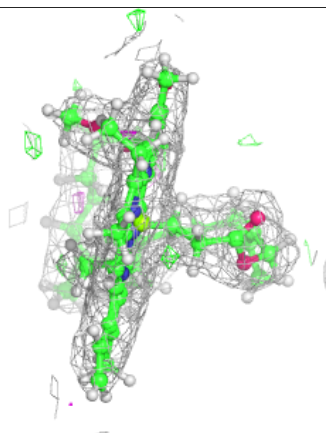
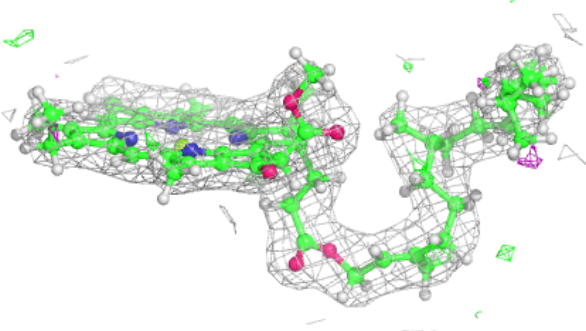
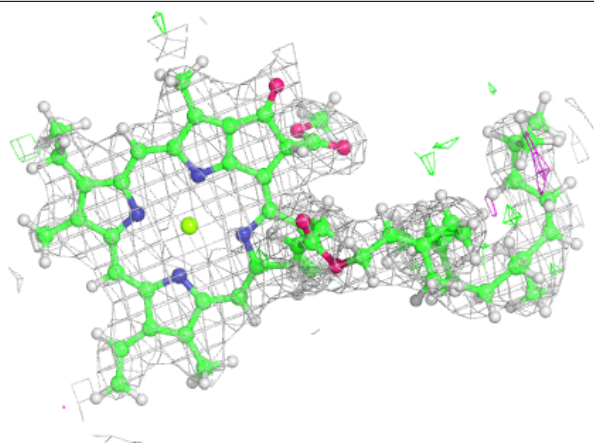
Electron density around CLA B 613:

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



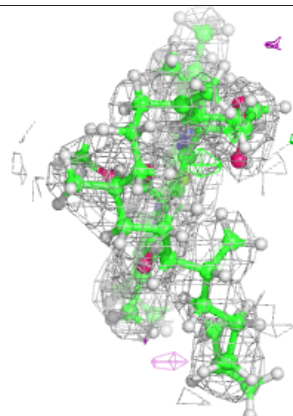
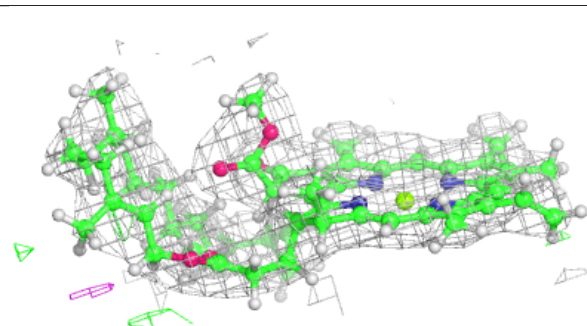
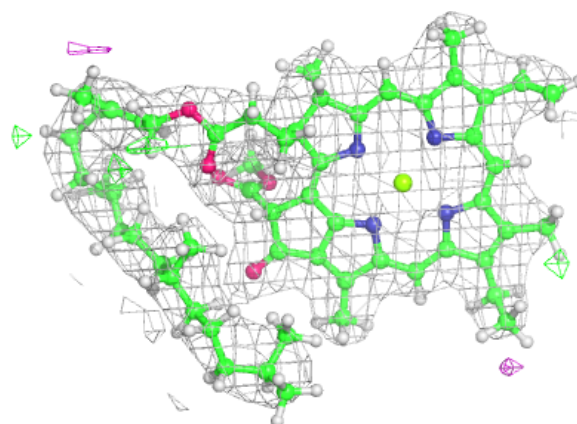
Electron density around CLA B 612:

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

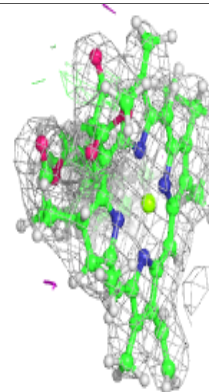
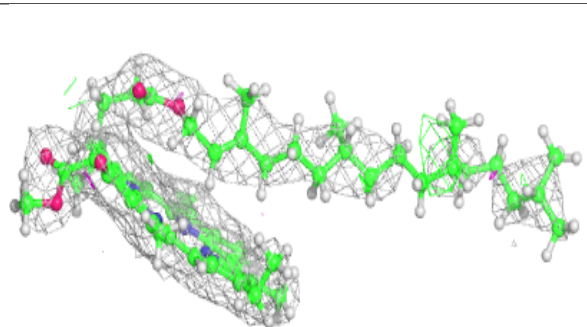
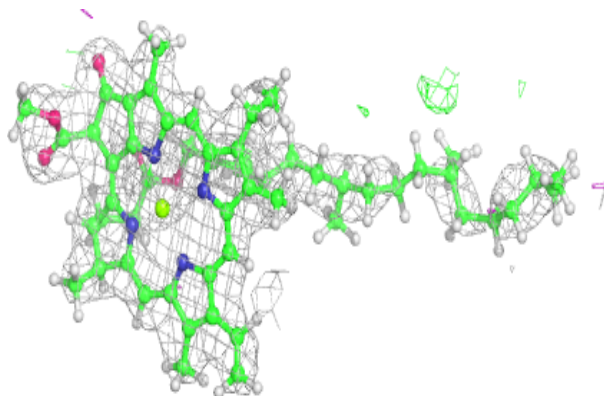


Electron density around CLA B 610:

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

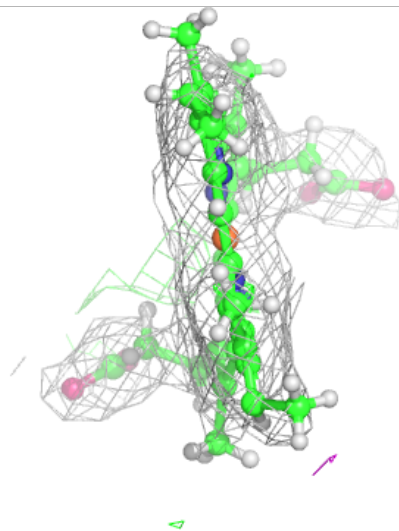
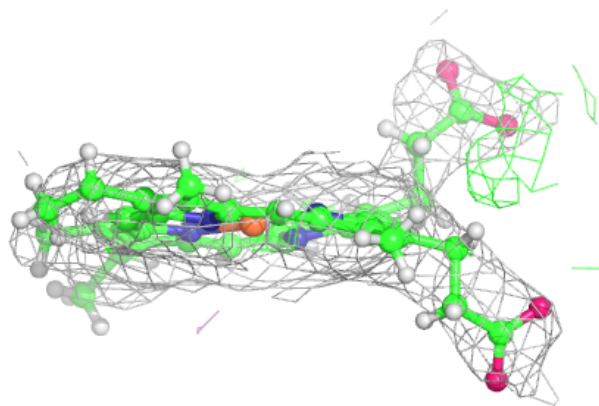
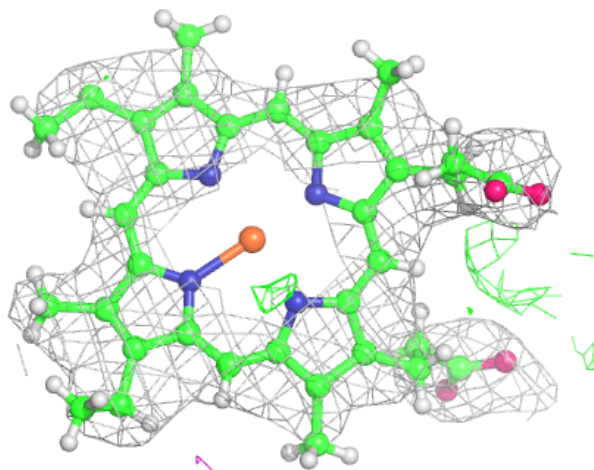
**Electron density around CLA B 614:**

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



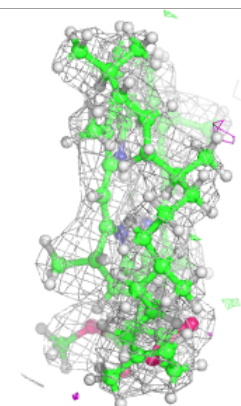
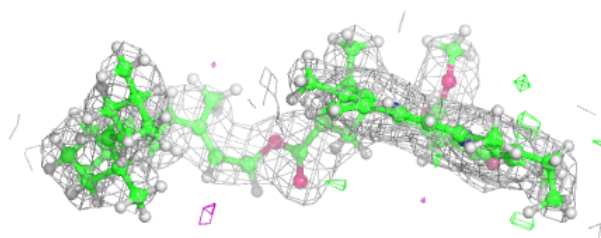
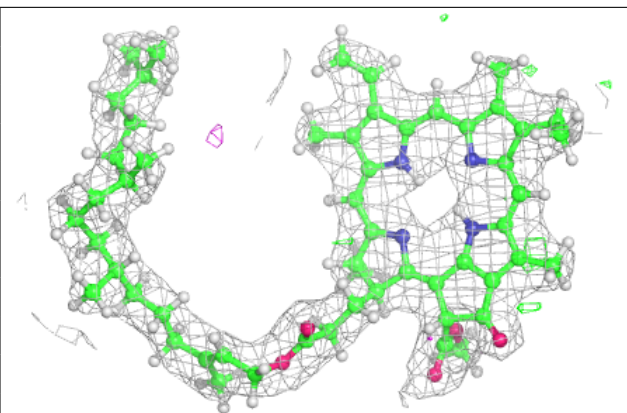
Electron density around HEC f 101:

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

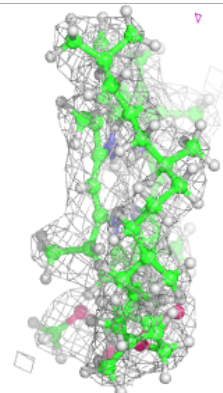
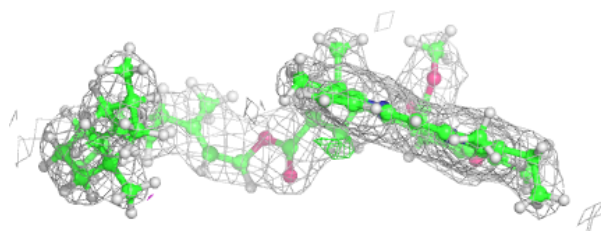
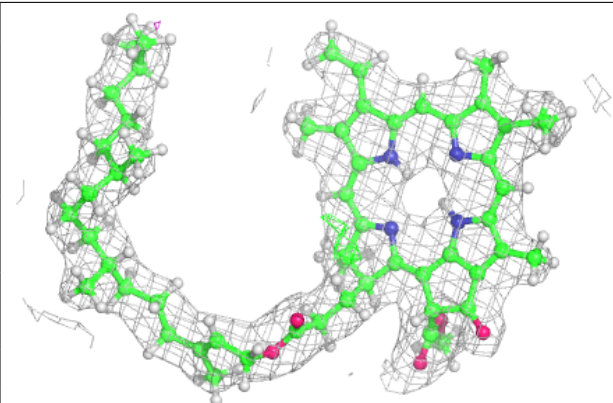


Electron density around PHO D 401:

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

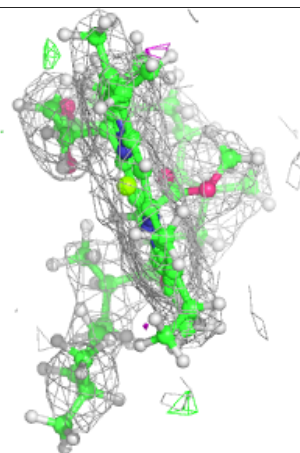
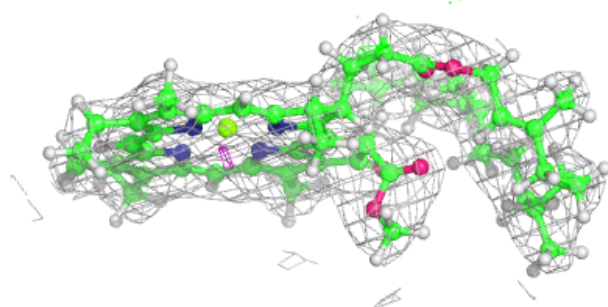
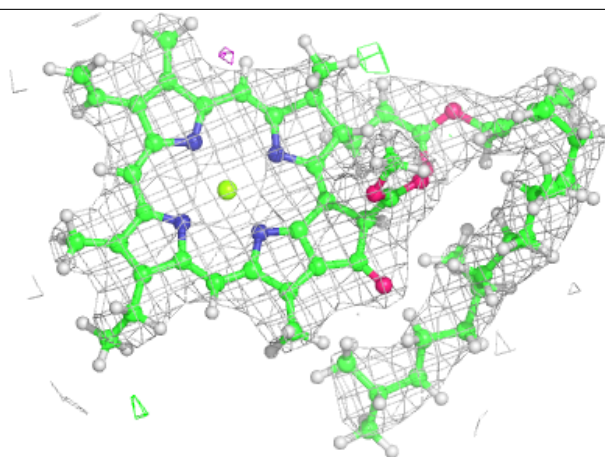
**Electron density around PHO a 404:**

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



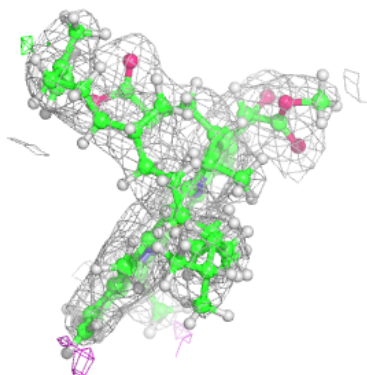
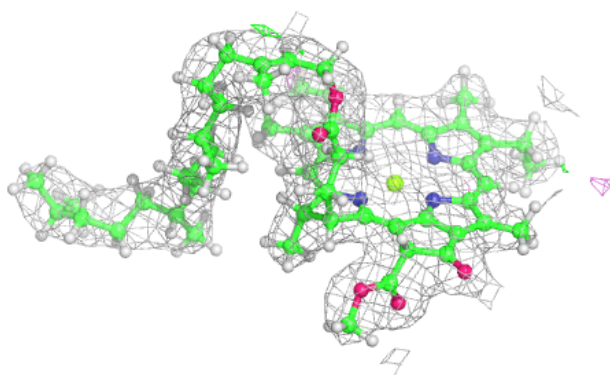
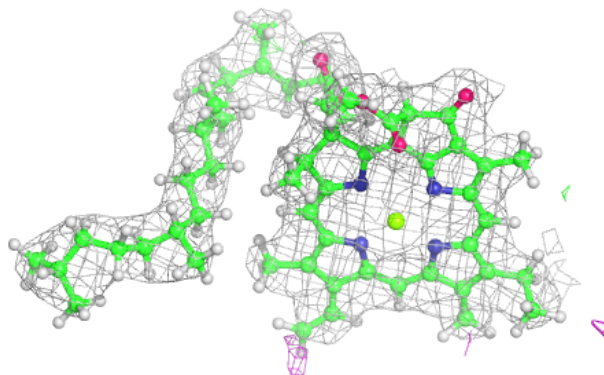
Electron density around CLA b 610:

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

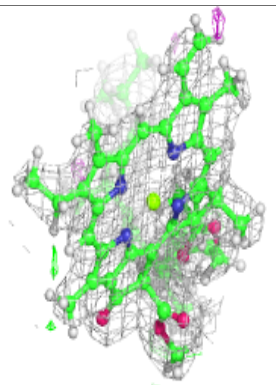
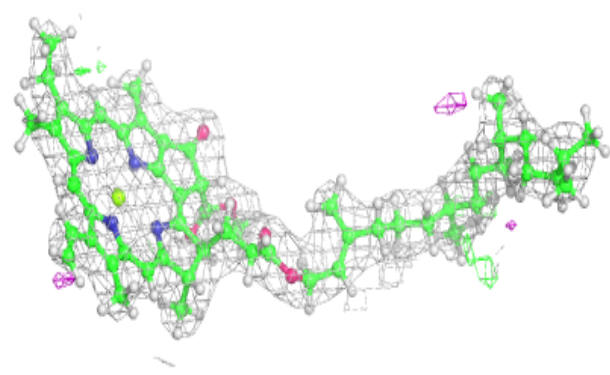
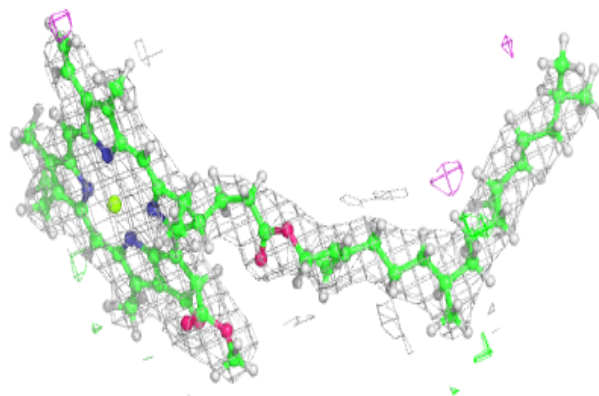


Electron density around CLA A 409:

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

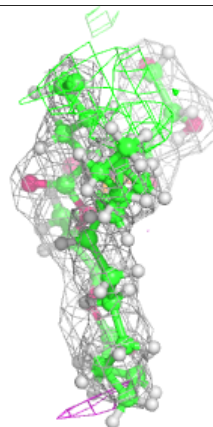
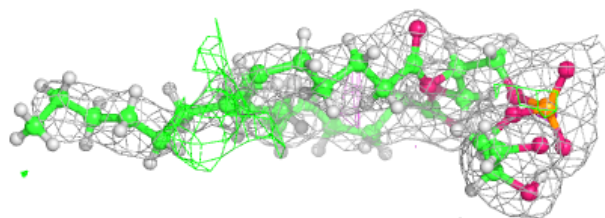
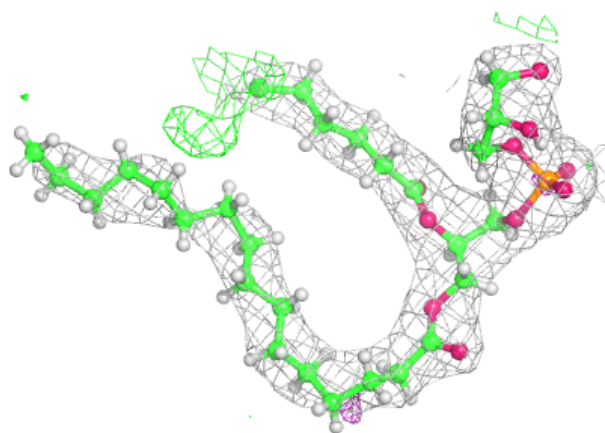
**Electron density around CLA a 402:**

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

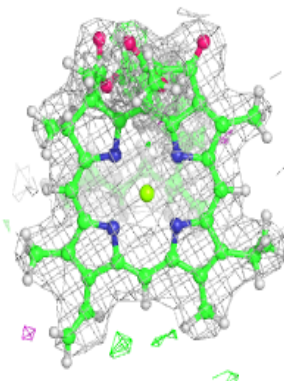
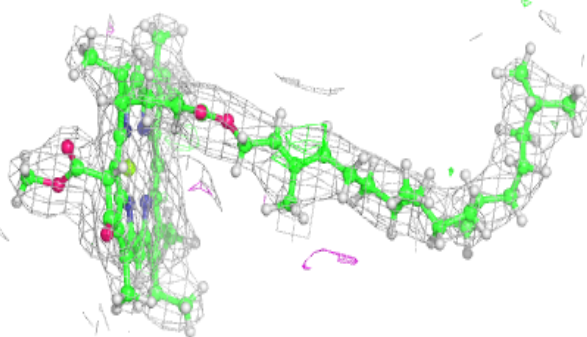
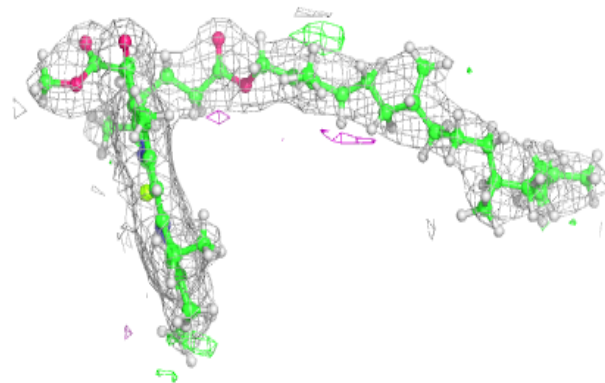


Electron density around LHG d 407:

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

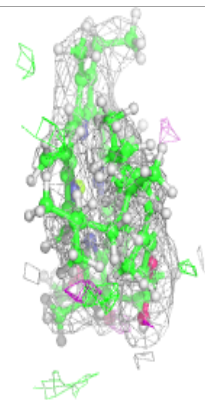
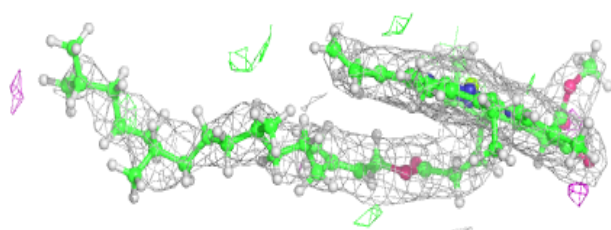
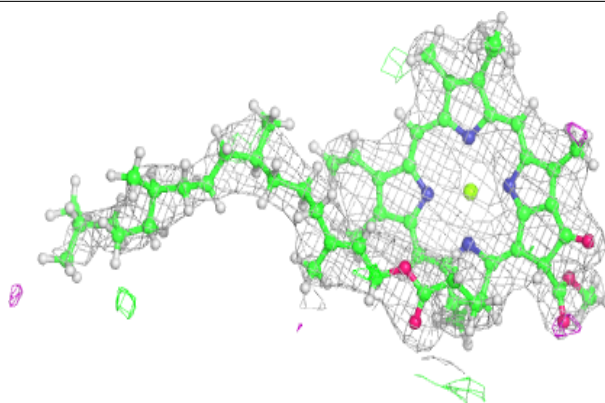
**Electron density around CLA B 605:**

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

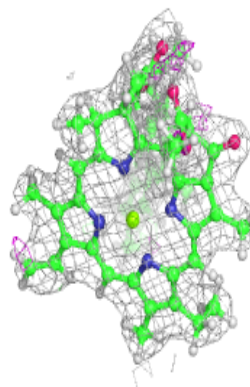
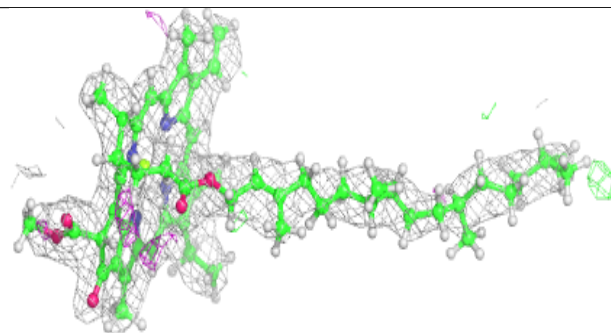
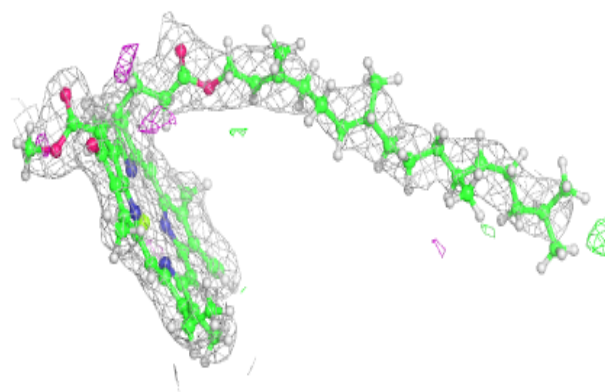


Electron density around CLA b 603:

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

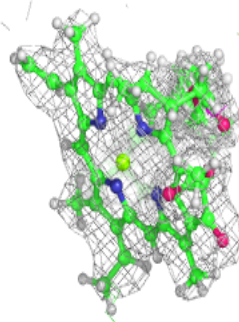
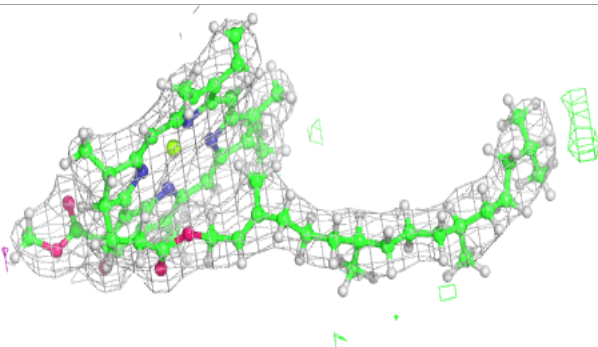
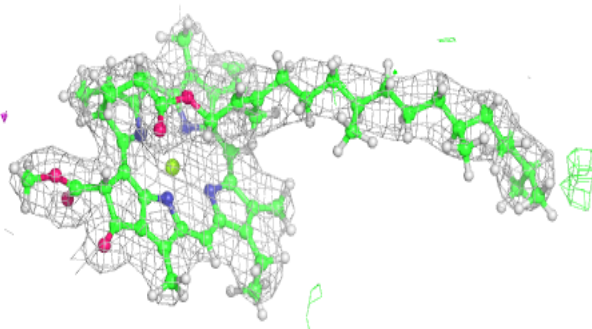
**Electron density around CLA B 607:**

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

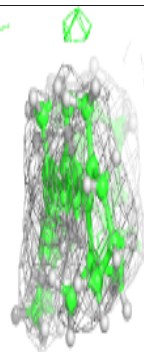
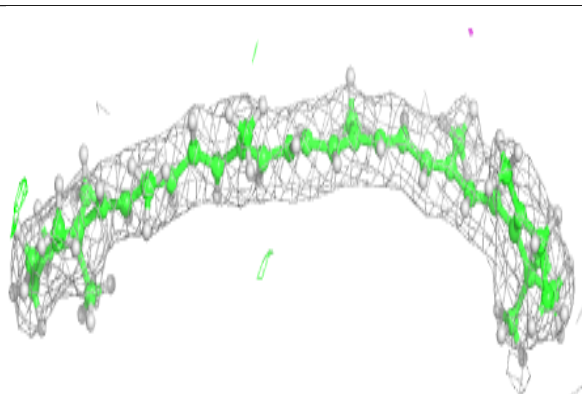
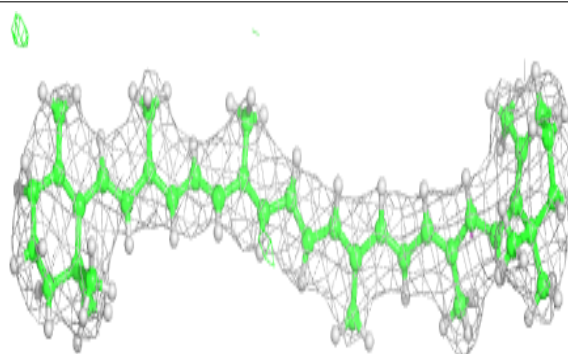


Electron density around CLA B 608:

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

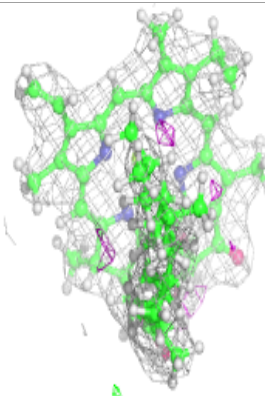
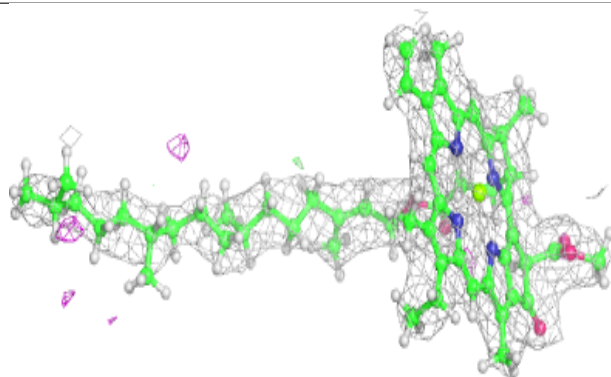
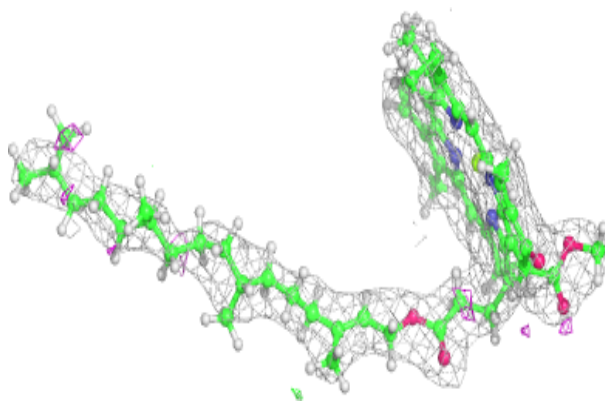
**Electron density around BCR t 101:**

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



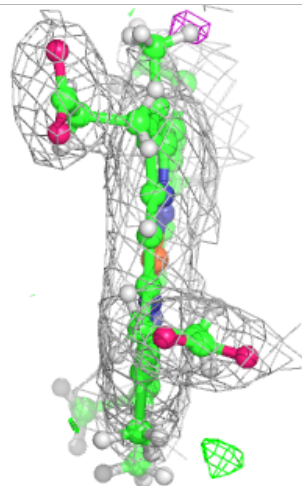
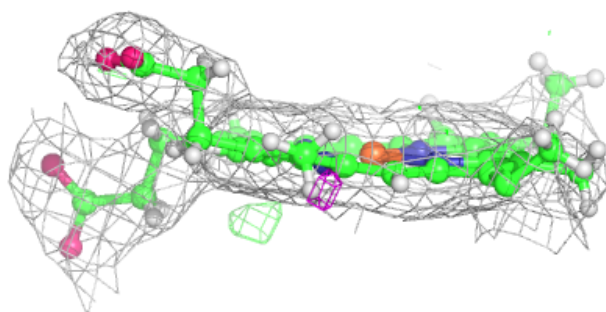
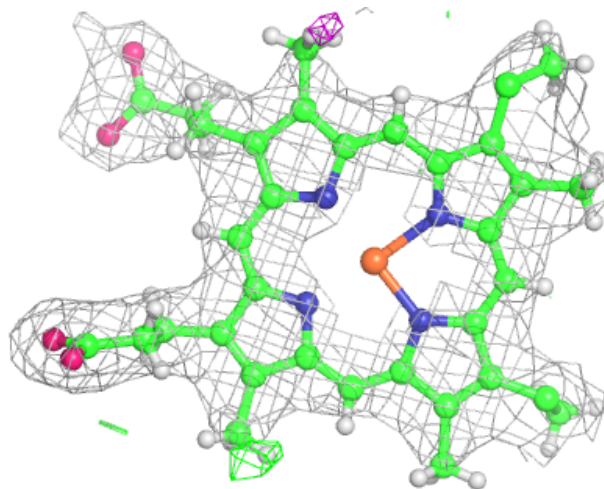
Electron density around CLA b 607:

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



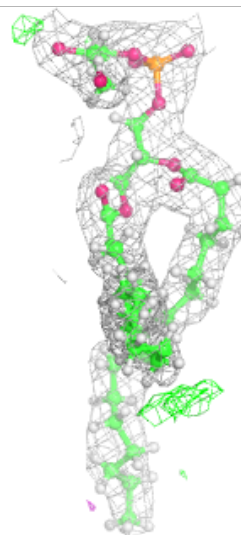
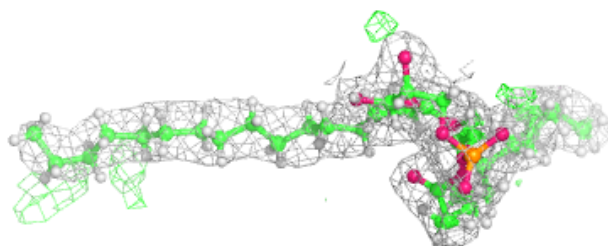
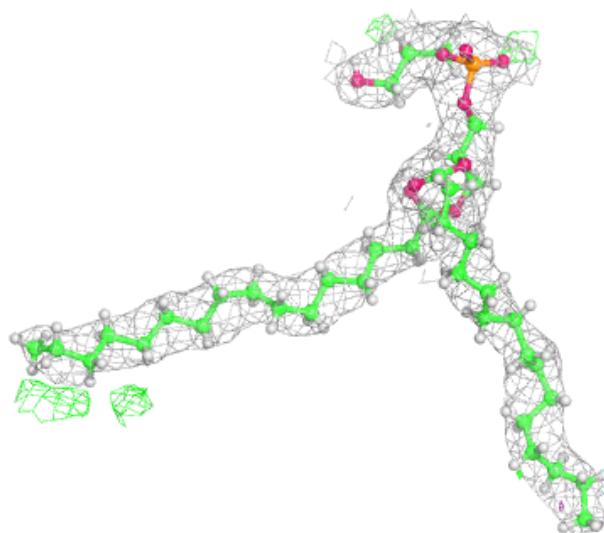
Electron density around HEC v 201:

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



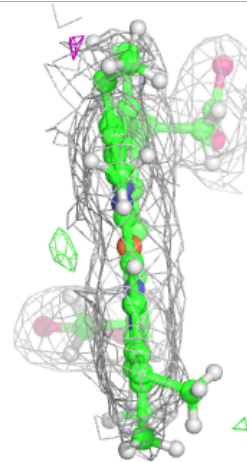
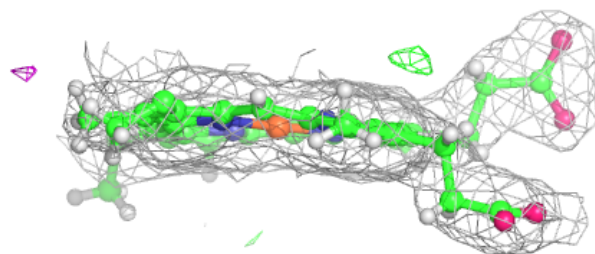
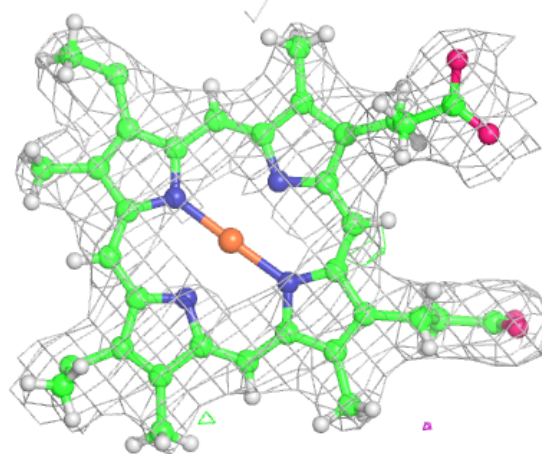
Electron density around LHG L 102:

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



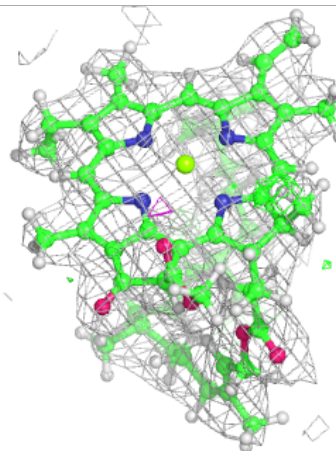
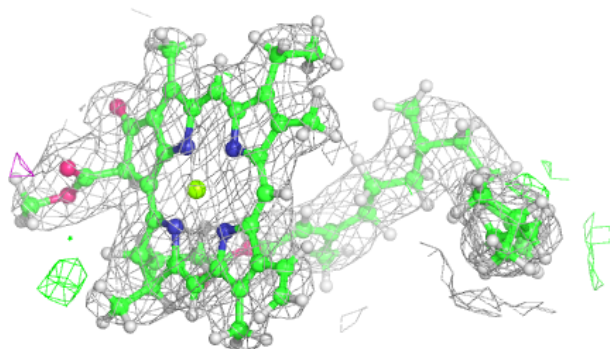
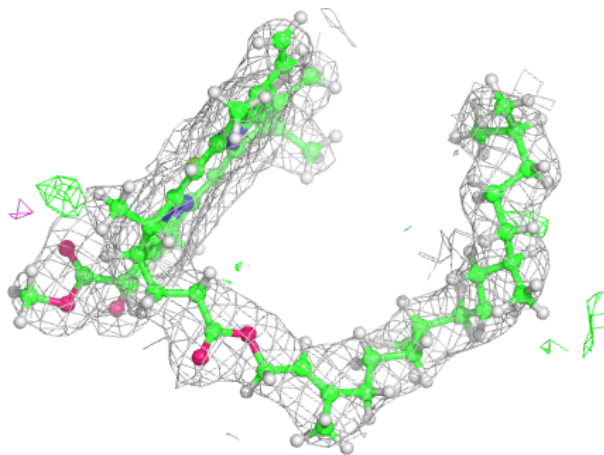
Electron density around HEC V 201:

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



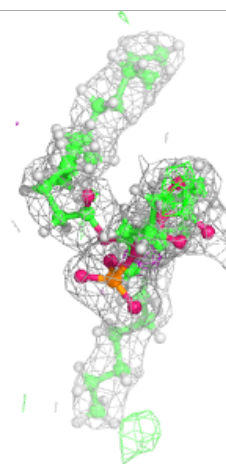
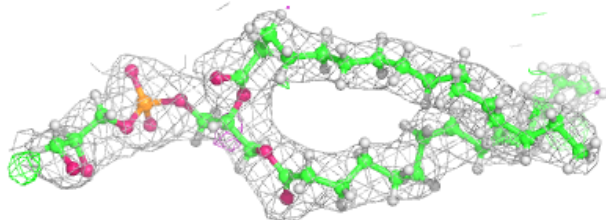
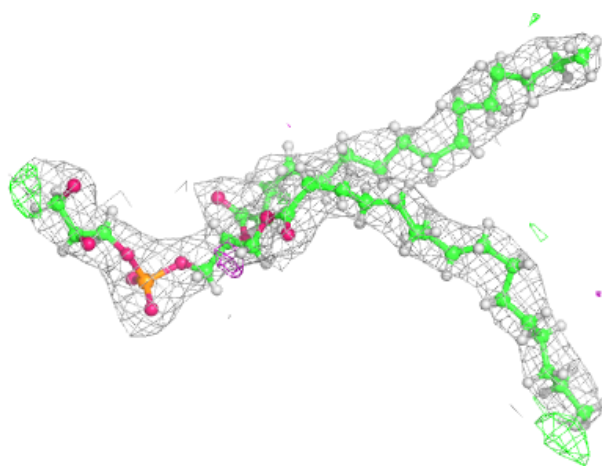
Electron density around CLA B 611:

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



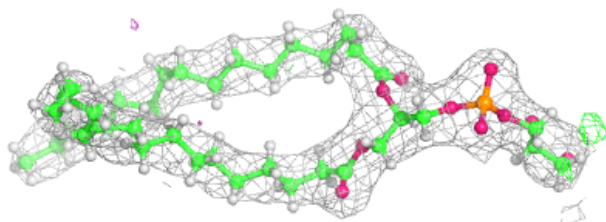
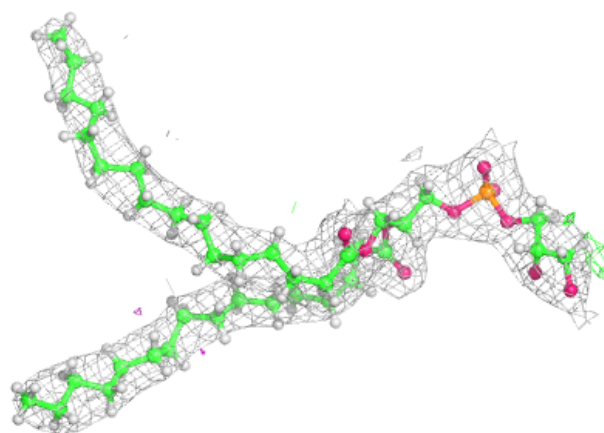
Electron density around LHG D 409:

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



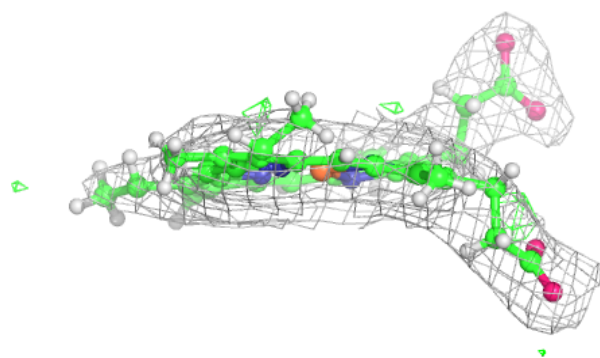
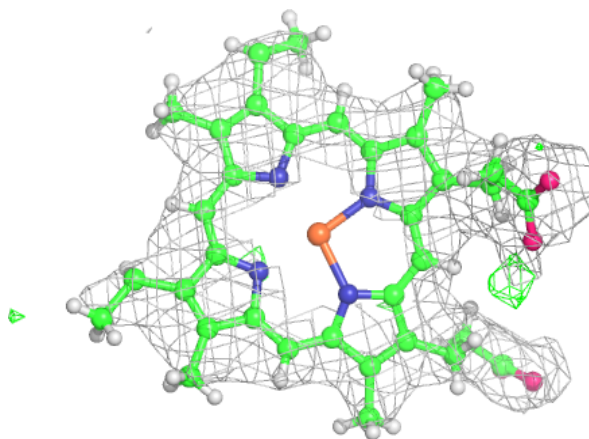
Electron density around LHG d 406:

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



Electron density around HEC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.