



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:33 PM BST

PDB ID : 6W1O
Title : RT XFEL structure of the dark-stable state of Photosystem II (0F, S1-rich) at 2.08 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 : 2.08 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)

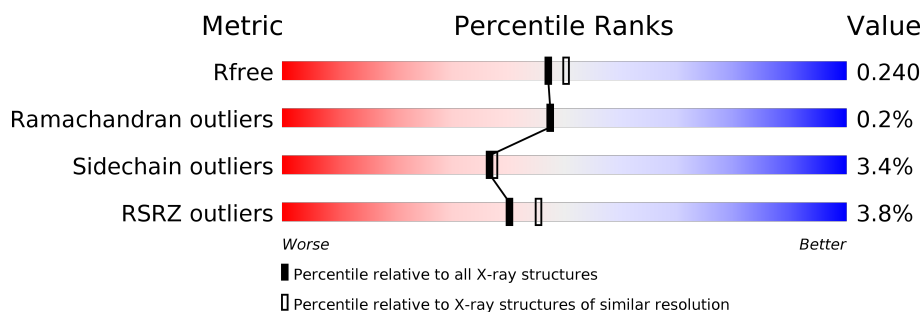
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	334	<div> <div>%</div> <div>99%</div> <div>.</div> </div>
1	a	334	<div> <div>96%</div> <div>.</div> </div>
2	B	506	<div> <div>%</div> <div>98%</div> <div>.</div> </div>
2	b	506	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
3	C	461	<div> <div>%</div> <div>94%</div> <div>.</div> <div>.</div> </div>

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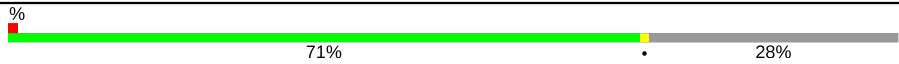

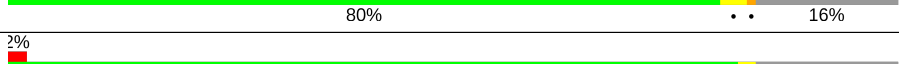
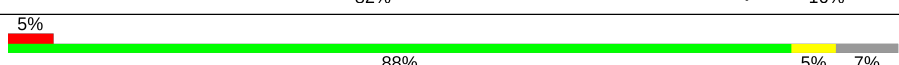
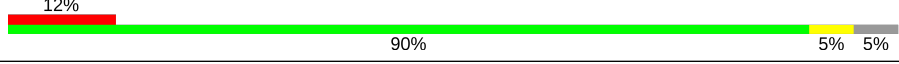

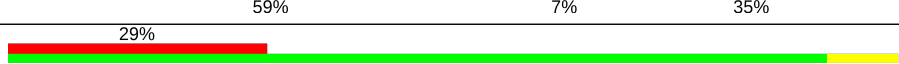
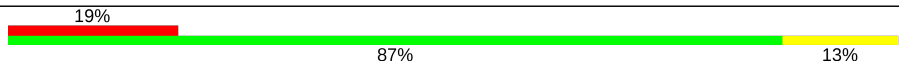
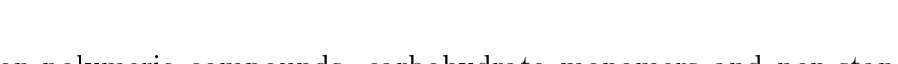
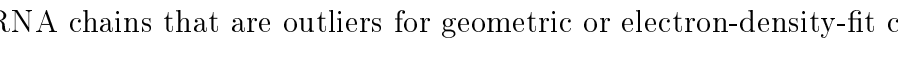
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

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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	30	
15	t	30	

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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	405	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	-	-	-
22	CLA	C	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	403	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	410	X	-	-	-
22	CLA	b	601	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	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	403	X	-	-	-
22	CLA	d	404	X	-	-	-
31	STE	E	102	-	-	-	X

2 Entry composition [i](#)

There are 35 unique types of molecules in this entry. The entry contains 103895 atoms, of which 51610 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	0	0
			5130	1717	2508	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5118	1714	2499	431	459	15			

- 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	2	0
			6768	2249	3342	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6913	2290	3413	587	610	13			

- 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	0	0
			5330	1800	2613	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5342	1804	2619	444	463	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			

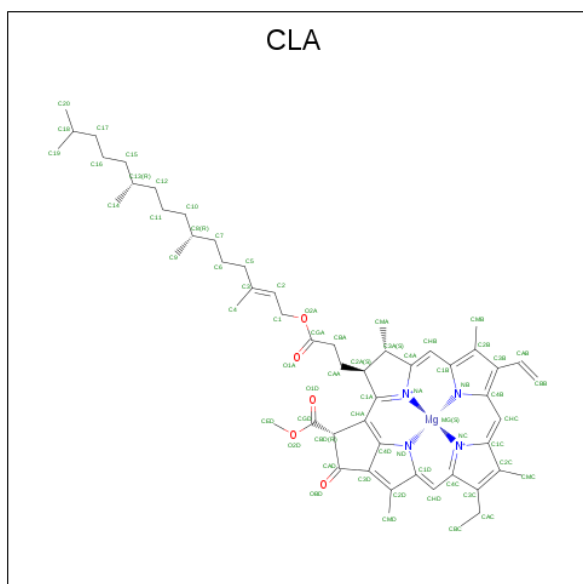
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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).



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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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	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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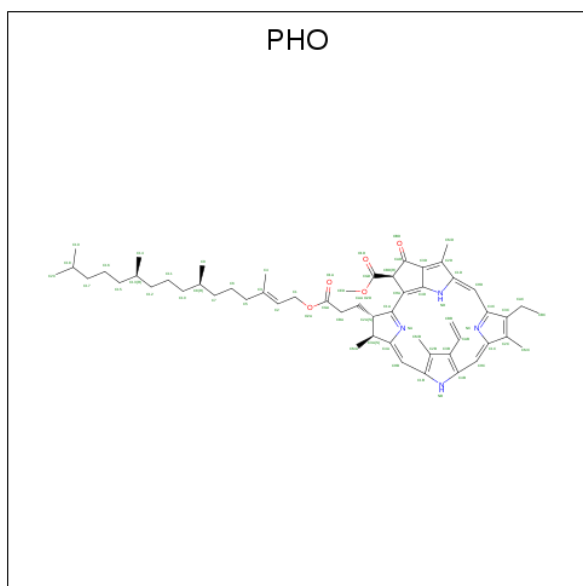
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	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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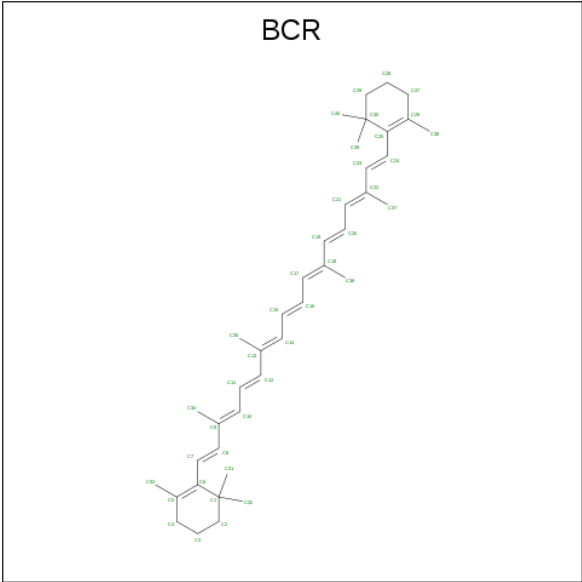
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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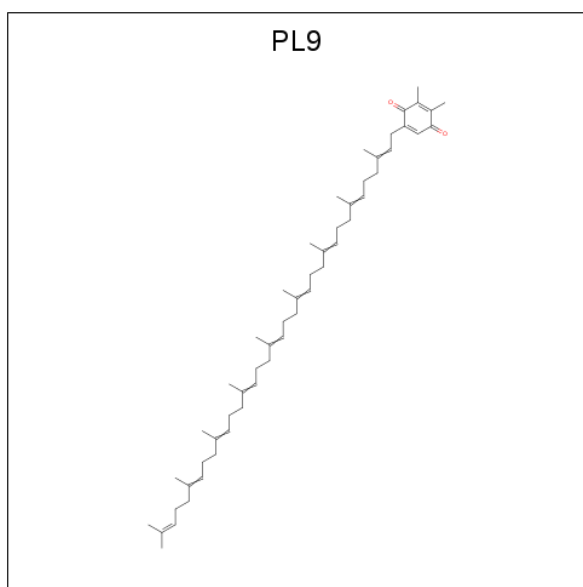
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

- Molecule 25 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

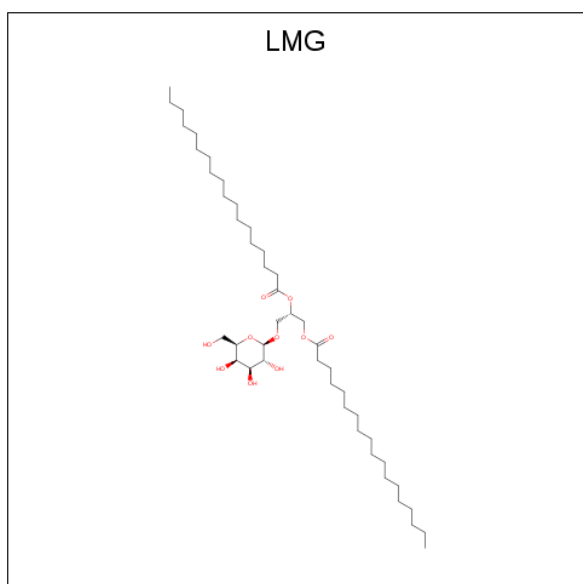
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by author).



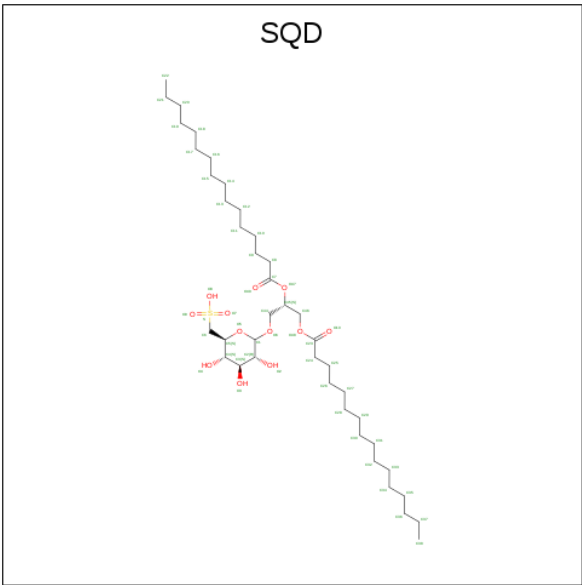
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



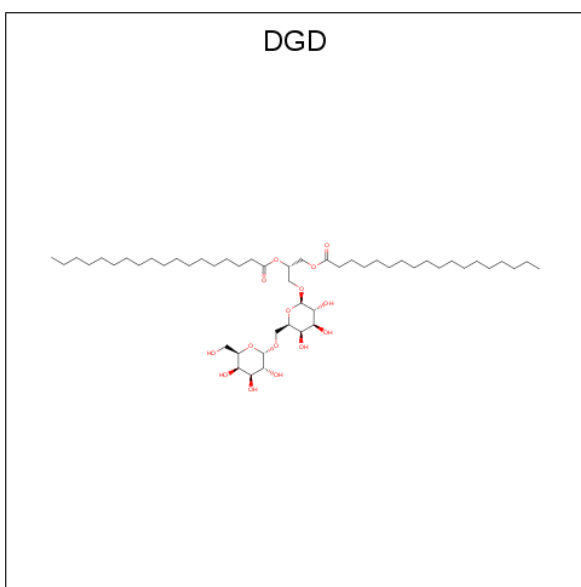
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			141	45	86	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

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



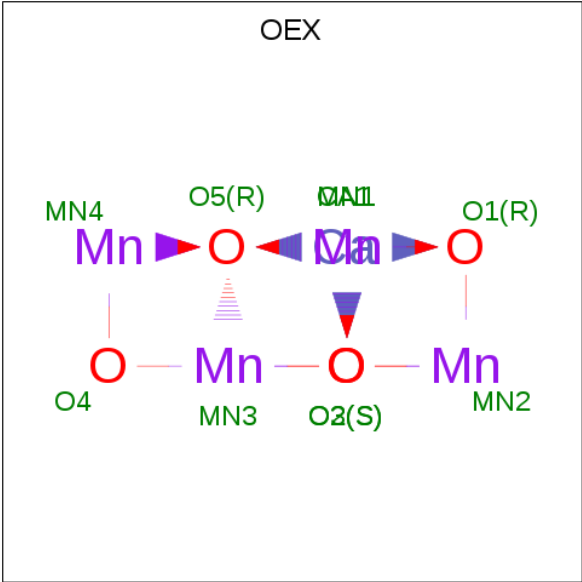
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



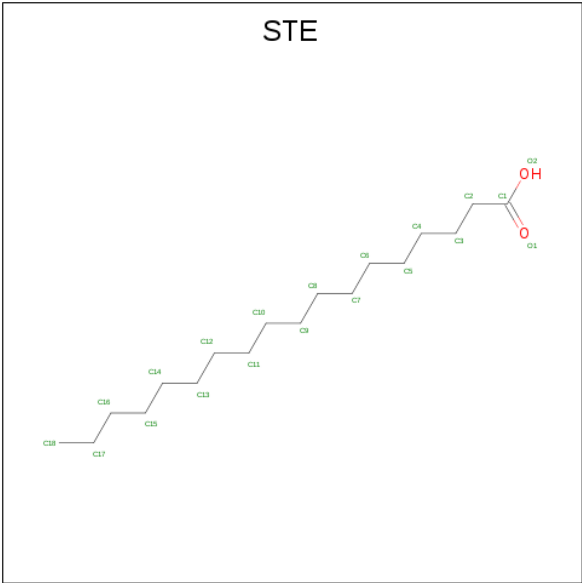
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- 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		

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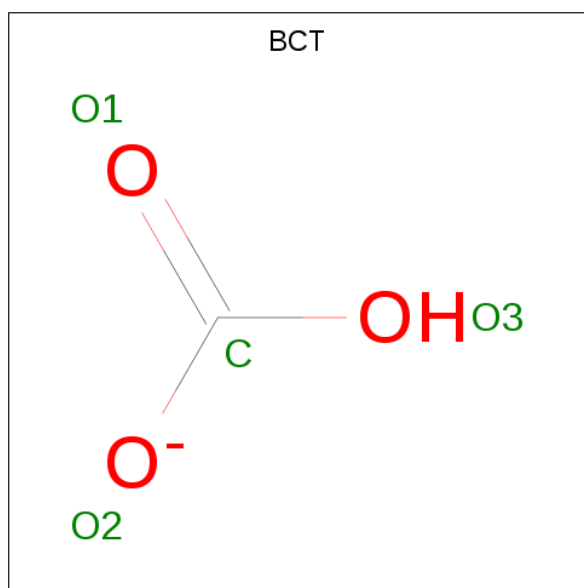
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total	C	H	O	0	0
			34	12	20	2		
31	B	1	Total	C	H	O	0	0
			28	10	16	2		
31	B	1	Total	C	H	O	0	0
			46	16	28	2		
31	B	1	Total	C	H		0	0
			47	16	31			
31	B	1	Total	C	H		0	0
			41	15	26			
31	C	1	Total	C	H	O	0	0
			28	10	16	2		
31	C	1	Total	C	H		0	0
			47	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	E	1	Total	C	H	O	0	0
			28	10	16	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		
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	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		0	0
			47	16	31			
31	b	1	Total	C	H	O	0	0
			55	18	35	2		

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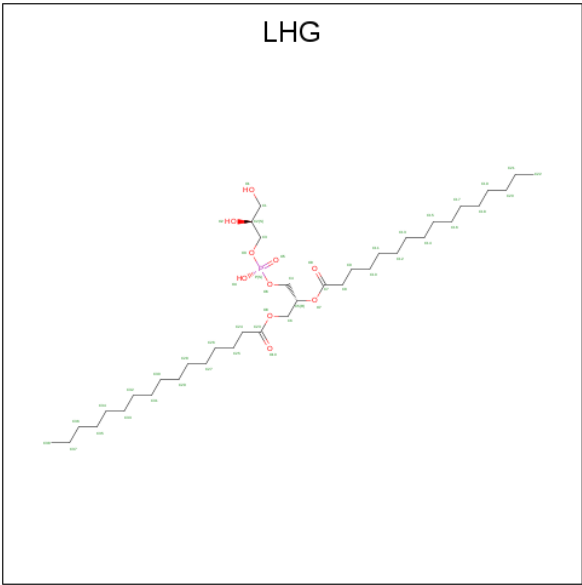
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	b	1	Total C H O 55 18 35 2	0	0
31	b	1	Total C H 26 10 16	0	0
31	b	1	Total C H 41 14 27	0	0
31	b	1	Total C H O 55 18 35 2	0	0
31	c	1	Total C H O 28 10 16 2	0	0
31	c	1	Total C H O 55 18 35 2	0	0
31	d	1	Total C H O 40 14 24 2	0	0
31	d	1	Total C H O 43 15 26 2	0	0
31	d	1	Total C H O 55 18 35 2	0	0
31	j	1	Total C H O 28 10 16 2	0	0
31	m	1	Total C H 53 18 35	0	0
31	m	1	Total C H O 28 10 16 2	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	D	1	Total	C	H	O	0	0
			5	1	1	3		
32	d	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



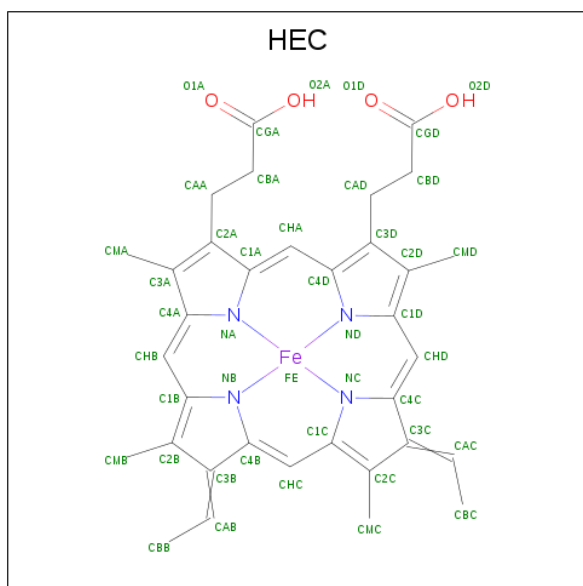
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	1	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 34 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 35 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	142	Total O 142 142	0	0
35	B	212	Total O 212 212	0	0
35	C	184	Total O 184 184	0	0
35	D	138	Total O 138 138	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	E	36	Total O 36 36	0	0
35	F	8	Total O 8 8	0	0
35	H	40	Total O 40 40	0	0
35	I	24	Total O 24 24	0	0
35	J	15	Total O 15 15	0	0
35	K	7	Total O 7 7	0	0
35	L	9	Total O 9 9	0	0
35	M	11	Total O 11 11	0	0
35	O	104	Total O 104 104	0	0
35	R	4	Total O 4 4	0	0
35	T	10	Total O 10 10	0	0
35	U	52	Total O 52 52	0	0
35	V	59	Total O 59 59	0	0
35	X	15	Total O 15 15	0	0
35	Y	5	Total O 5 5	0	0
35	Z	6	Total O 6 6	0	0
35	a	116	Total O 116 116	0	0
35	b	201	Total O 201 201	0	0
35	c	187	Total O 187 187	0	0
35	d	115	Total O 115 115	0	0
35	e	21	Total O 21 21	0	0

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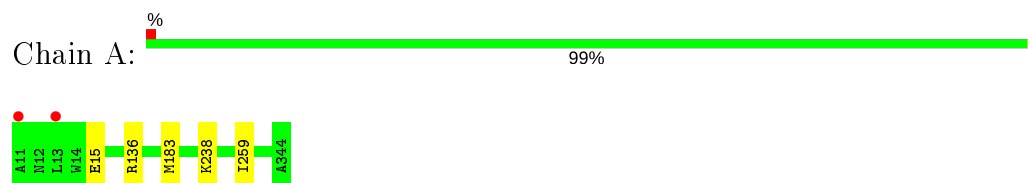
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	f	6	Total 6	O 6	0	0
35	h	31	Total 31	O 31	0	0
35	i	12	Total 12	O 12	0	0
35	j	6	Total 6	O 6	0	0
35	k	7	Total 7	O 7	0	0
35	l	5	Total 5	O 5	0	0
35	m	10	Total 10	O 10	0	0
35	o	86	Total 86	O 86	0	0
35	r	6	Total 6	O 6	0	0
35	t	9	Total 9	O 9	0	0
35	u	53	Total 53	O 53	0	0
35	v	62	Total 62	O 62	0	0
35	x	8	Total 8	O 8	0	0
35	y	4	Total 4	O 4	0	0
35	z	11	Total 11	O 11	0	0

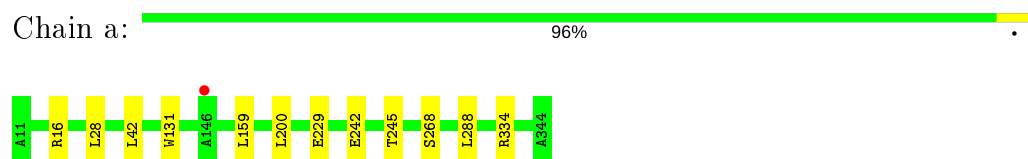
3 Residue-property plots [i](#)

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

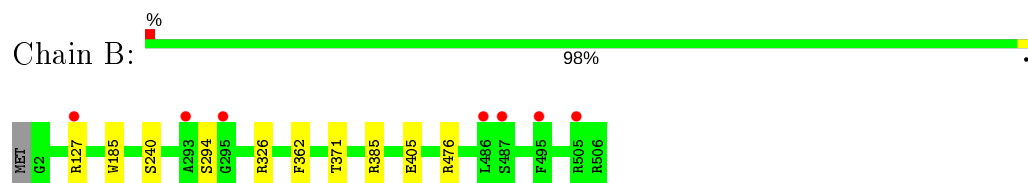
- Molecule 1: Photosystem II protein D1 1



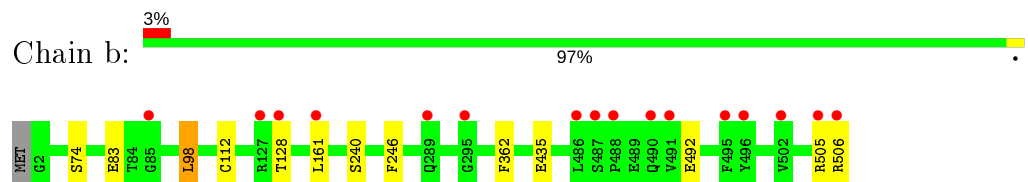
- Molecule 1: Photosystem II protein D1 1



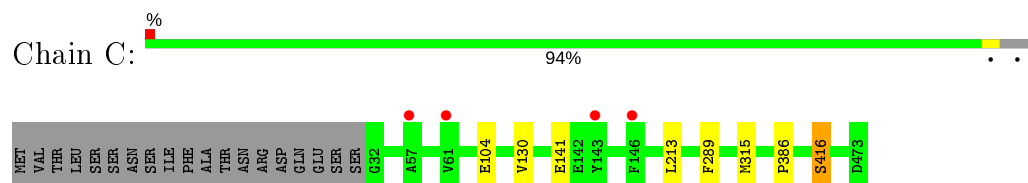
- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein



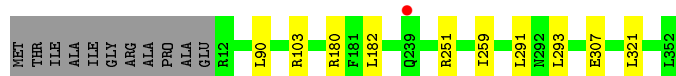
- Molecule 3: Photosystem II CP43 reaction center protein



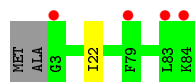
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



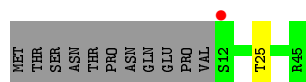
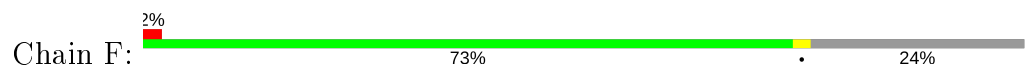
- Molecule 5: Cytochrome b559 subunit alpha



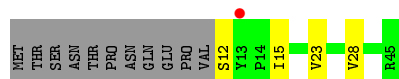
- Molecule 5: Cytochrome b559 subunit alpha



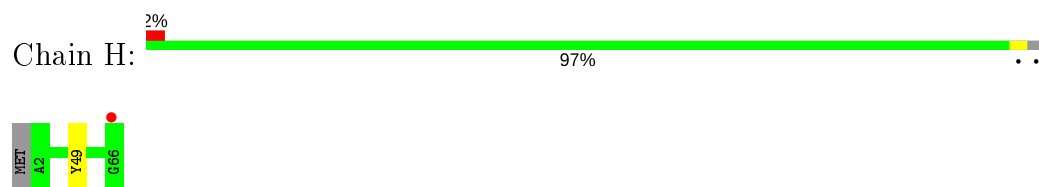
- Molecule 6: Cytochrome b559 subunit beta



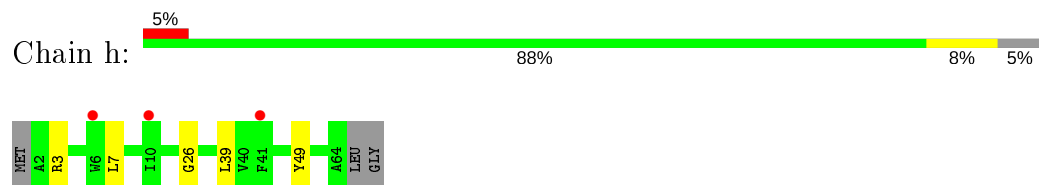
- Molecule 6: Cytochrome b559 subunit beta



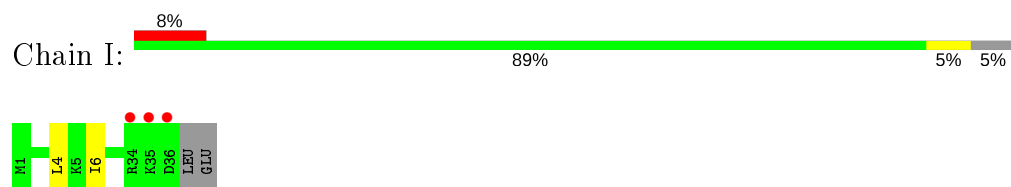
- Molecule 7: Photosystem II reaction center protein H



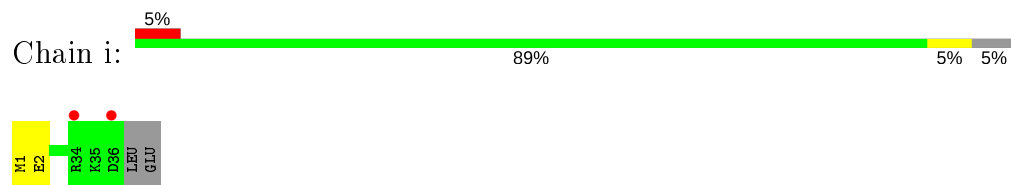
- Molecule 7: Photosystem II reaction center protein H



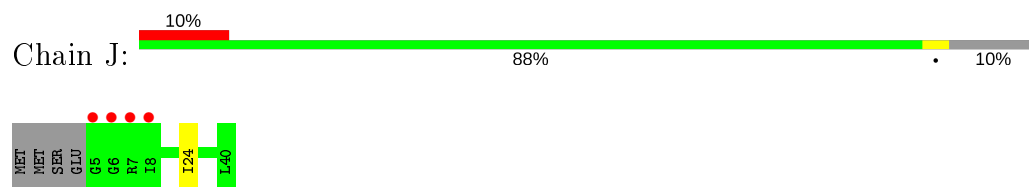
- Molecule 8: Photosystem II reaction center protein I



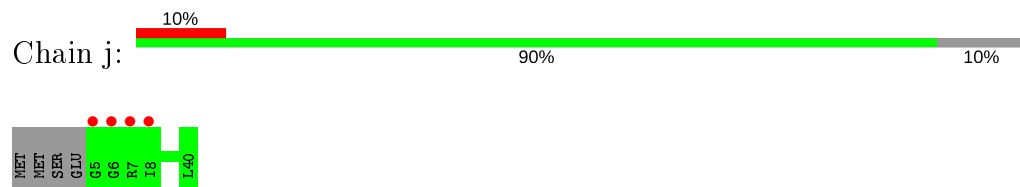
- Molecule 8: Photosystem II reaction center protein I



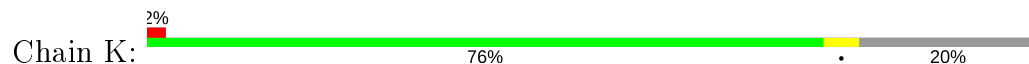
- Molecule 9: Photosystem II reaction center protein J

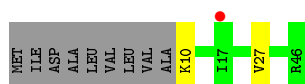


- Molecule 9: Photosystem II reaction center protein J

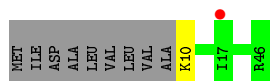
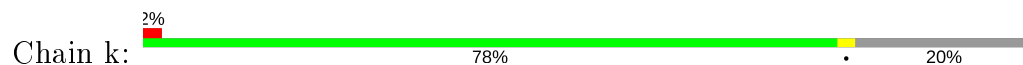


- Molecule 10: Photosystem II reaction center protein K

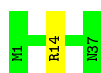




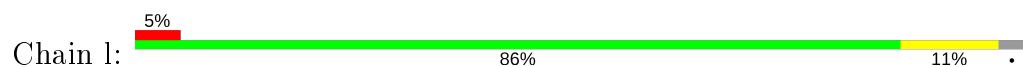
- Molecule 10: Photosystem II reaction center protein K



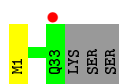
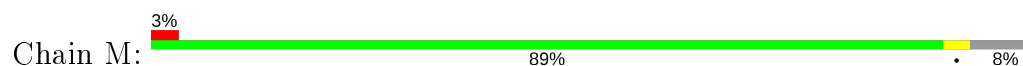
- Molecule 11: Photosystem II reaction center protein L



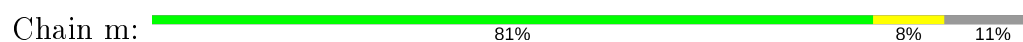
- Molecule 11: Photosystem II reaction center protein L



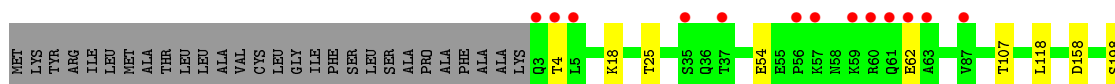
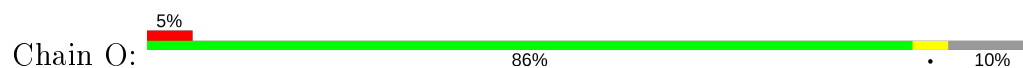
- Molecule 12: Photosystem II reaction center protein M



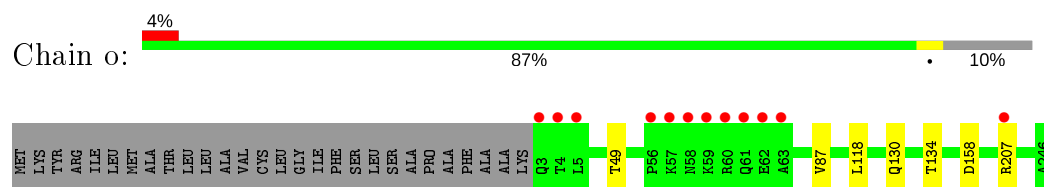
- Molecule 12: Photosystem II reaction center protein M



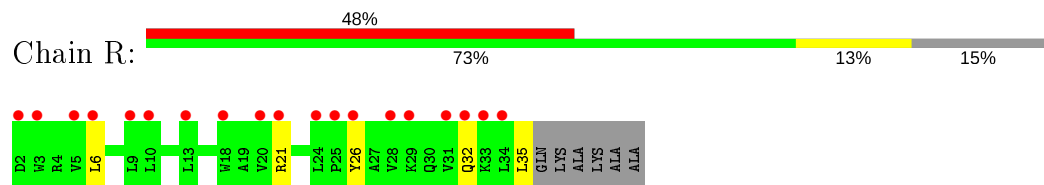
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



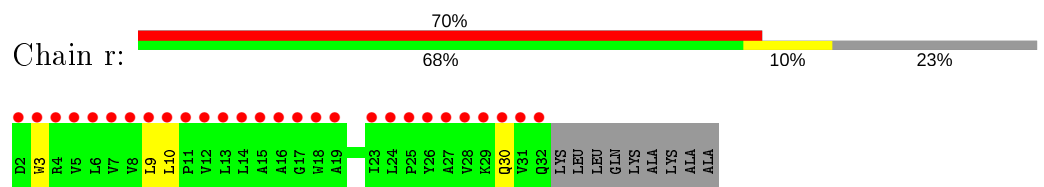
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



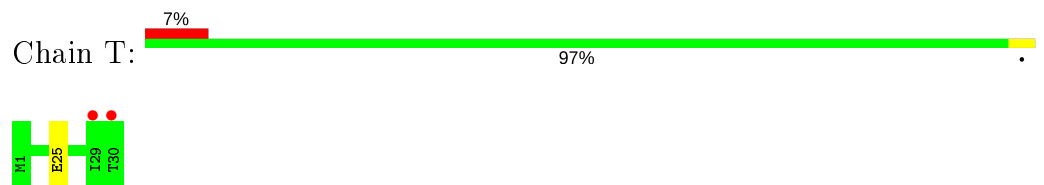
- Molecule 14: Photosystem II protein Y



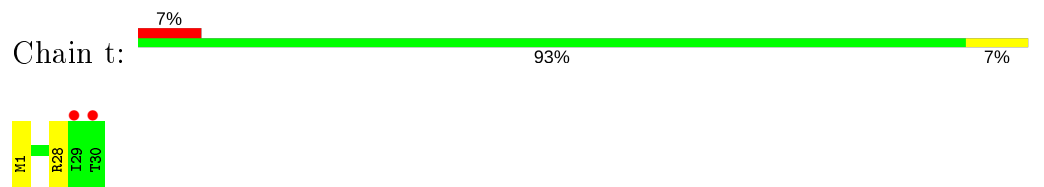
- Molecule 14: Photosystem II protein Y



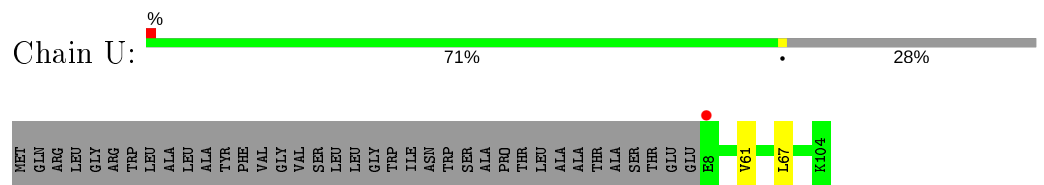
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

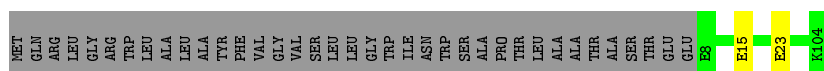


- Molecule 16: Photosystem II 12 kDa extrinsic protein



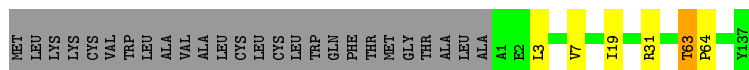
- Molecule 16: Photosystem II 12 kDa extrinsic protein





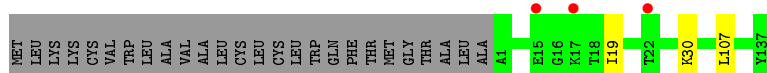
- Molecule 17: Cytochrome c-550

Chain V: 80% 16%



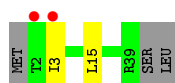
- Molecule 17: Cytochrome c-550

Chain v: 82% 16%



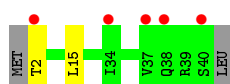
- Molecule 18: Photosystem II reaction center X protein

Chain X: 88% 5% 7%



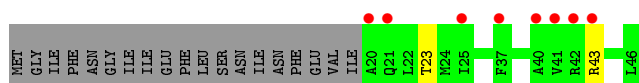
- Molecule 18: Photosystem II reaction center X protein

Chain x: 90% 5% 5%



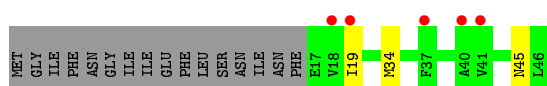
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 54% 41%

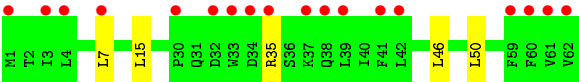


- Molecule 19: Photosystem II reaction center protein Ycf12

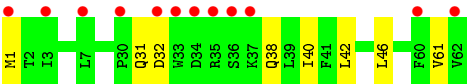
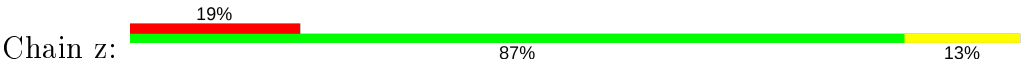
Chain y: 59% 7% 35%



- Molecule 20: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.1 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.240 0.181 , 0.240	Depositor DCC
R_{free} test set	4226 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103895	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	0/2707	0.70	2/3692 (0.1%)
1	a	0.66	0/2704	0.71	2/3688 (0.1%)
2	B	0.65	1/4161 (0.0%)	0.68	1/5669 (0.0%)
2	b	0.63	1/4118 (0.0%)	0.68	1/5611 (0.0%)
3	C	0.62	0/3547	0.68	0/4830
3	c	0.59	0/3619	0.66	0/4926
4	D	0.66	1/2812 (0.0%)	0.69	1/3832 (0.0%)
4	d	0.64	0/2821	0.69	1/3844 (0.0%)
5	E	0.55	0/688	0.62	0/940
5	e	0.50	0/683	0.59	0/932
6	F	0.55	0/284	0.56	0/387
6	f	0.46	0/284	0.60	0/387
7	H	0.63	0/523	0.69	0/713
7	h	0.58	0/511	0.67	0/697
8	I	0.61	0/293	0.65	0/396
8	i	0.69	0/293	0.71	0/396
9	J	0.54	0/263	0.64	0/356
9	j	0.50	0/263	0.62	0/356
10	K	0.51	0/303	0.62	0/416
10	k	0.55	0/303	0.65	0/416
11	L	0.70	0/311	0.73	1/422 (0.2%)
11	l	0.71	0/303	0.70	0/412
12	M	0.71	0/249	0.77	0/341
12	m	0.65	0/244	0.76	0/334
13	O	0.62	0/1904	0.73	1/2585 (0.0%)
13	o	0.60	0/1905	0.75	1/2583 (0.0%)
14	R	0.45	0/277	0.53	0/380
14	r	0.43	0/246	0.52	0/339
15	T	0.68	0/257	0.69	0/349
15	t	0.69	0/255	0.63	0/346
16	U	0.54	0/785	0.69	0/1064
16	u	0.64	0/785	0.74	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.60	0/1085	0.72	1/1473 (0.1%)
17	v	0.55	0/1085	0.64	0/1473
18	X	0.51	0/284	0.63	0/384
18	x	0.39	0/289	0.55	0/391
19	Y	0.45	0/197	0.63	0/264
19	y	0.39	0/219	0.54	0/294
20	Z	0.46	0/490	0.55	0/669
20	z	0.45	0/488	0.55	0/666
All	All	0.62	3/42838 (0.0%)	0.68	12/58317 (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
17	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	211	CYS	CB-SG	-5.77	1.72	1.81
2	B	185	TRP	CB-CG	-5.58	1.40	1.50
2	b	112	CYS	CB-SG	-5.16	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	334	ARG	NE-CZ-NH1	6.96	123.78	120.30
17	V	63	THR	C-N-CD	-6.82	105.61	120.60
13	o	158	ASP	CB-CG-OD1	6.30	123.97	118.30
2	B	326	ARG	NE-CZ-NH2	-5.80	117.40	120.30
4	d	251	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	b	98	LEU	CA-CB-CG	5.48	127.91	115.30
4	D	294	ARG	NE-CZ-NH1	-5.38	117.61	120.30
13	O	158	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	183	MET	CA-CB-CG	5.26	122.25	113.30
1	a	131	TRP	CA-CB-CG	-5.16	103.89	113.70
1	A	136	ARG	NE-CZ-NH2	-5.12	117.74	120.30
11	L	14	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	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	332/334 (99%)	325 (98%)	6 (2%)	1 (0%)	41	39
1	a	332/334 (99%)	326 (98%)	6 (2%)	0	100	100
2	B	508/506 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/506 (99%)	490 (97%)	13 (3%)	0	100	100
3	C	442/461 (96%)	433 (98%)	8 (2%)	1 (0%)	47	47
3	c	451/461 (98%)	435 (96%)	15 (3%)	1 (0%)	47	47
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	333 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
7	h	61/66 (92%)	56 (92%)	4 (7%)	1 (2%)	9	4
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	30 (88%)	4 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	224 (92%)	18 (7%)	1 (0%)	34	31
13	o	242/272 (89%)	230 (95%)	12 (5%)	0	100	100
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	26 (90%)	2 (7%)	1 (3%)	3	1
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	22	17
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	3	1
19	y	28/46 (61%)	25 (89%)	3 (11%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	9	4
All	All	5240/5666 (92%)	5072 (97%)	159 (3%)	9 (0%)	47	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
19	Y	43	ARG
14	r	30	GLN

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Mol	Chain	Res	Type
20	z	61	VAL
1	A	259	ILE
7	h	26	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/270 (100%)	268 (99%)	2 (1%)	84	87
1	a	269/270 (100%)	259 (96%)	10 (4%)	34	34
2	B	408/404 (101%)	400 (98%)	8 (2%)	55	59
2	b	402/404 (100%)	390 (97%)	12 (3%)	41	43
3	C	346/362 (96%)	338 (98%)	8 (2%)	50	53
3	c	354/362 (98%)	342 (97%)	12 (3%)	37	37
4	D	276/283 (98%)	270 (98%)	6 (2%)	52	55
4	d	277/283 (98%)	268 (97%)	9 (3%)	39	40
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	46
5	e	71/73 (97%)	69 (97%)	2 (3%)	43	46
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	35
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	61
7	h	53/55 (96%)	49 (92%)	4 (8%)	13	9
8	I	32/34 (94%)	30 (94%)	2 (6%)	18	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	40	41
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	29
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/37 (81%)	28 (93%)	2 (7%)	16	12
10	k	30/37 (81%)	29 (97%)	1 (3%)	38	39
11	L	35/35 (100%)	35 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	2
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	198 (96%)	8 (4%)	32	32
13	o	207/228 (91%)	201 (97%)	6 (3%)	42	44
14	R	28/32 (88%)	23 (82%)	5 (18%)	2	1
14	r	23/32 (72%)	20 (87%)	3 (13%)	4	2
15	T	26/26 (100%)	25 (96%)	1 (4%)	33	33
15	t	25/26 (96%)	24 (96%)	1 (4%)	31	31
16	U	84/112 (75%)	82 (98%)	2 (2%)	49	52
16	u	84/112 (75%)	82 (98%)	2 (2%)	49	52
17	V	117/138 (85%)	113 (97%)	4 (3%)	37	37
17	v	117/138 (85%)	114 (97%)	3 (3%)	46	49
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	13
18	x	31/34 (91%)	29 (94%)	2 (6%)	17	13
19	Y	19/37 (51%)	18 (95%)	1 (5%)	22	20
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	1
20	Z	52/52 (100%)	47 (90%)	5 (10%)	8	5
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	1
All	All	4328/4622 (94%)	4179 (97%)	149 (3%)	37	37

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	238	LYS
2	B	127	ARG
2	B	240	SER
2	B	294	SER
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	405	GLU
2	B	476	ARG
3	C	104	GLU

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Mol	Chain	Res	Type
3	C	130	VAL
3	C	141	GLU
3	C	213	LEU
3	C	289	PHE
3	C	315	MET
3	C	386	PRO
3	C	416	SER
4	D	26	ARG
4	D	43	LEU
4	D	171	PRO
4	D	180	ARG
4	D	264	LYS
4	D	295	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR
8	I	4	LEU
8	I	6	ILE
9	J	24	ILE
10	K	10	LYS
10	K	27	VAL
13	O	4	THR
13	O	18	LYS
13	O	25	THR
13	O	54	GLU
13	O	107	THR
13	O	118	LEU
13	O	198	SER
13	O	214	THR
14	R	6	LEU
14	R	21	ARG
14	R	26	TYR
14	R	32	GLN
14	R	35	LEU
15	T	25	GLU
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	19	ILE
17	V	31	ARG

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Mol	Chain	Res	Type
18	X	3	ILE
18	X	15	LEU
19	Y	23	THR
20	Z	7	LEU
20	Z	15	LEU
20	Z	35	ARG
20	Z	46	LEU
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	229	GLU
1	a	242	GLU
1	a	245	THR
1	a	268	SER
1	a	288	LEU
2	b	74	SER
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	161	LEU
2	b	240	SER
2	b	246	PHE
2	b	362	PHE
2	b	435	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	135	ARG
3	c	165	LEU
3	c	289	PHE
3	c	315	MET
3	c	346	THR
3	c	416	SER

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Mol	Chain	Res	Type
4	d	90	LEU
4	d	103	ARG
4	d	180	ARG
4	d	182	LEU
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	66	VAL
5	e	83	LEU
6	f	12	SER
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	3	ARG
7	h	7	LEU
7	h	39	LEU
7	h	49	TYR
8	i	2	GLU
10	k	10	LYS
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	49	THR
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	207	ARG
14	r	3	TRP
14	r	9	LEU
14	r	10	LEU
15	t	28	ARG
16	u	15	GLU
16	u	23	GLU
17	v	19	ILE
17	v	30	LYS
17	v	107	LEU

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Mol	Chain	Res	Type
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	34	MET
19	y	45	ASN
20	z	1	MET
20	z	31	GLN
20	z	32	ASP
20	z	38	GLN
20	z	40	ILE
20	z	42	LEU
20	z	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	338	ASN
11	L	8	GLN
13	O	3	GLN
13	O	36	GLN
13	O	88	ASN
20	Z	6	GLN
20	Z	31	GLN
1	a	181	ASN
1	a	234	ASN
2	b	409	GLN
3	c	28	GLN
3	c	373	ASN
5	e	60	GLN
16	u	37	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
12	FME	M	1	12	8,9,10	1.07	1 (12%)	7,9,11	0.79	0
15	FME	T	1	15	8,9,10	1.18	0	7,9,11	0.65	0
15	FME	t	1	15	8,9,10	1.06	0	7,9,11	1.26	1 (14%)
12	FME	m	1	12	8,9,10	1.12	1 (12%)	7,9,11	0.44	0
8	FME	i	1	8	8,9,10	1.20	1 (12%)	7,9,11	1.20	1 (14%)
8	FME	I	1	8	8,9,10	1.01	0	7,9,11	0.97	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
15	FME	T	1	15	-	2/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-2.76	1.42	1.46
12	m	1	FME	CA-N	-2.32	1.43	1.46
12	M	1	FME	CA-N	-2.05	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CA-N-CN	-2.41	119.12	122.82
15	t	1	FME	C-CA-N	2.40	114.06	109.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	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
8	I	1	FME	C-CA-CB-CG
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 189 ligands modelled in this entry, 6 are monoatomic - leaving 183 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	A	413	-	67,67,67	1.31	10 (14%)	81,81,81	1.53	13 (16%)
34	HEC	v	201	17	26,50,50	2.35	4 (15%)	18,82,82	1.95	4 (22%)
28	SQD	L	101	-	48,49,54	0.94	2 (4%)	57,60,65	2.40	16 (28%)
22	CLA	B	605	-	59,73,73	1.29	8 (13%)	67,113,113	1.91	15 (22%)
24	BCR	a	406	-	41,41,41	1.22	3 (7%)	56,56,56	1.22	6 (10%)
27	LMG	c	520	-	37,37,55	1.17	4 (10%)	45,45,63	1.27	5 (11%)
31	STE	B	601	-	8,11,19	0.36	0	7,11,19	0.97	0
27	LMG	d	410	-	44,44,55	1.15	4 (9%)	52,52,63	1.31	5 (9%)
27	LMG	c	523	-	49,49,55	1.04	5 (10%)	57,57,63	1.30	5 (8%)
22	CLA	C	512	-	59,73,73	1.36	6 (10%)	67,113,113	1.45	13 (19%)
31	STE	C	518	-	8,11,19	0.46	0	7,11,19	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	t	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.47	12 (21%)
31	STE	b	620	-	15,15,19	0.43	0	14,14,19	0.82	0
28	SQD	B	622	-	53,54,54	1.00	3 (5%)	62,65,65	1.87	13 (20%)
31	STE	b	625	-	9,9,19	0.50	0	8,8,19	0.54	0
22	CLA	C	507	35	59,73,73	1.47	6 (10%)	67,113,113	1.84	12 (17%)
22	CLA	c	502	-	59,73,73	1.42	8 (13%)	67,113,113	1.74	9 (13%)
24	BCR	k	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.10	3 (5%)
22	CLA	b	613	-	59,73,73	1.35	8 (13%)	67,113,113	1.68	14 (20%)
31	STE	m	101	-	17,17,19	0.42	0	16,16,19	0.80	0
31	STE	b	627	-	16,19,19	0.32	0	15,19,19	1.01	0
22	CLA	a	405	-	59,73,73	1.34	6 (10%)	67,113,113	1.63	14 (20%)
32	BCT	D	402	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	c	510	-	59,73,73	1.26	6 (10%)	67,113,113	1.87	12 (17%)
22	CLA	C	509	-	59,73,73	1.45	10 (16%)	67,113,113	1.41	9 (13%)
34	HEC	V	201	17	26,50,50	2.27	4 (15%)	18,82,82	1.86	5 (27%)
24	BCR	c	515	-	41,41,41	1.08	2 (4%)	56,56,56	1.17	2 (3%)
22	CLA	B	608	-	59,73,73	1.76	8 (13%)	67,113,113	1.66	10 (14%)
26	PL9	d	406	-	55,55,55	1.54	10 (18%)	68,69,69	1.84	16 (23%)
30	OEX	A	414	1,3,35	0,15,15	0.00	-	-	-	-
24	BCR	F	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	5 (8%)
29	DGD	c	519	-	63,63,67	1.22	8 (12%)	77,77,81	1.41	8 (10%)
22	CLA	A	405	-	48,62,73	1.80	9 (18%)	53,99,113	1.73	12 (22%)
24	BCR	b	619	-	41,41,41	1.08	2 (4%)	56,56,56	1.28	10 (17%)
22	CLA	C	508	-	59,73,73	1.61	6 (10%)	67,113,113	1.70	9 (13%)
27	LMG	D	407	-	51,51,55	0.91	2 (3%)	59,59,63	1.37	8 (13%)
29	DGD	c	518	-	63,63,67	1.15	6 (9%)	77,77,81	1.41	11 (14%)
23	PHO	a	404	-	67,69,69	1.05	5 (7%)	85,99,99	1.18	8 (9%)
22	CLA	C	506	-	59,73,73	1.62	6 (10%)	67,113,113	1.51	10 (14%)
22	CLA	c	506	-	59,73,73	1.40	5 (8%)	67,113,113	1.65	11 (16%)
22	CLA	b	610	35	59,73,73	1.30	9 (15%)	67,113,113	1.57	17 (25%)
22	CLA	C	510	-	59,73,73	1.30	8 (13%)	67,113,113	1.40	10 (14%)
31	STE	J	101	-	8,11,19	0.30	0	7,11,19	0.95	0
22	CLA	c	508	35	59,73,73	1.33	7 (11%)	67,113,113	1.45	8 (11%)
26	PL9	D	406	-	55,55,55	1.35	6 (10%)	68,69,69	1.64	14 (20%)
22	CLA	C	504	35	53,67,73	1.53	7 (13%)	59,105,113	1.64	14 (23%)
31	STE	H	104	-	17,17,19	0.40	0	16,16,19	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	d	403	-	59,73,73	1.48	8 (13%)	67,113,113	1.31	7 (10%)
22	CLA	B	615	-	59,73,73	1.61	10 (16%)	67,113,113	1.41	8 (11%)
31	STE	a	413	-	9,9,19	0.53	0	8,8,19	0.56	0
22	CLA	b	604	-	59,73,73	1.85	6 (10%)	67,113,113	1.99	13 (19%)
22	CLA	D	405	-	59,73,73	1.32	7 (11%)	67,113,113	1.26	8 (11%)
22	CLA	B	613	-	59,73,73	1.65	10 (16%)	67,113,113	1.57	12 (17%)
26	PL9	a	409	-	55,55,55	1.07	4 (7%)	68,69,69	1.61	11 (16%)
31	STE	j	101	-	8,11,19	0.61	0	7,11,19	0.62	0
31	STE	d	412	-	13,16,19	0.37	0	12,16,19	0.72	0
27	LMG	A	410	-	48,48,55	0.99	2 (4%)	56,56,63	1.43	7 (12%)
22	CLA	B	616	-	54,68,73	1.72	8 (14%)	61,107,113	1.84	15 (24%)
23	PHO	D	401	-	67,69,69	1.23	9 (13%)	85,99,99	1.10	6 (7%)
31	STE	B	627	-	14,14,19	0.51	0	13,13,19	0.64	0
24	BCR	H	102	-	41,41,41	0.96	1 (2%)	56,56,56	1.36	7 (12%)
22	CLA	b	611	-	59,73,73	1.27	7 (11%)	67,113,113	1.88	10 (14%)
27	LMG	B	621	-	20,26,55	0.53	0	18,26,63	1.11	0
23	PHO	A	404	-	67,69,69	1.25	10 (14%)	85,99,99	1.03	4 (4%)
28	SQD	a	412	-	35,35,54	1.19	2 (5%)	37,37,65	1.46	4 (10%)
24	BCR	K	102	-	41,41,41	0.99	3 (7%)	56,56,56	1.26	5 (8%)
22	CLA	c	511	-	59,73,73	1.38	7 (11%)	67,113,113	1.64	11 (16%)
34	HEC	f	101	5,6	26,50,50	2.55	5 (19%)	18,82,82	2.33	5 (27%)
26	PL9	A	409	-	55,55,55	0.95	1 (1%)	68,69,69	1.60	14 (20%)
31	STE	m	102	-	8,11,19	0.46	0	7,11,19	0.79	0
28	SQD	A	411	-	51,52,54	1.11	5 (9%)	60,63,65	1.70	11 (18%)
29	DGD	C	517	-	63,63,67	1.16	7 (11%)	77,77,81	1.47	12 (15%)
31	STE	B	624	-	8,11,19	0.39	0	7,11,19	0.97	0
22	CLA	c	505	35	54,68,73	1.55	6 (11%)	61,107,113	1.71	14 (22%)
33	LHG	E	101	-	48,48,48	0.86	3 (6%)	51,54,54	1.20	6 (11%)
22	CLA	B	603	-	59,73,73	1.23	5 (8%)	67,113,113	1.61	11 (16%)
24	BCR	k	102	-	41,41,41	0.94	2 (4%)	56,56,56	1.20	5 (8%)
22	CLA	H	101	35	59,73,73	1.72	9 (15%)	67,113,113	1.57	7 (10%)
22	CLA	B	610	35	59,73,73	1.50	10 (16%)	67,113,113	1.52	12 (17%)
22	CLA	C	502	-	59,73,73	1.46	6 (10%)	67,113,113	1.44	11 (16%)
31	STE	E	102	-	8,11,19	0.54	0	7,11,19	0.40	0
22	CLA	b	601	35	59,73,73	1.68	7 (11%)	67,113,113	1.47	10 (14%)
22	CLA	c	504	-	59,73,73	1.43	9 (15%)	67,113,113	1.78	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	T	101	-	41,41,41	1.18	4 (9%)	56,56,56	1.19	4 (7%)
29	DGD	c	517	-	63,63,67	1.37	7 (11%)	77,77,81	1.34	8 (10%)
22	CLA	b	607	35	59,73,73	1.48	6 (10%)	67,113,113	1.44	11 (16%)
22	CLA	C	501	-	59,73,73	1.60	8 (13%)	67,113,113	1.57	10 (14%)
22	CLA	B	614	-	59,73,73	1.46	7 (11%)	67,113,113	1.48	13 (19%)
28	SQD	D	408	-	35,36,54	0.94	2 (5%)	42,45,65	1.87	9 (21%)
24	BCR	h	101	-	41,41,41	1.00	2 (4%)	56,56,56	1.38	9 (16%)
22	CLA	b	608	-	59,73,73	1.61	7 (11%)	67,113,113	1.58	14 (20%)
24	BCR	b	618	-	41,41,41	1.14	2 (4%)	56,56,56	1.33	5 (8%)
24	BCR	c	516	-	41,41,41	1.21	4 (9%)	56,56,56	1.29	6 (10%)
22	CLA	c	512	3	59,73,73	1.73	7 (11%)	67,113,113	1.65	8 (11%)
31	STE	C	520	-	8,11,19	0.33	0	7,11,19	1.20	0
31	STE	B	625	-	14,17,19	0.41	0	13,17,19	0.83	0
22	CLA	c	507	-	59,73,73	1.44	5 (8%)	67,113,113	1.47	13 (19%)
22	CLA	b	614	-	59,73,73	1.43	8 (13%)	67,113,113	1.32	7 (10%)
24	BCR	K	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.44	9 (16%)
22	CLA	A	403	35	59,73,73	1.54	8 (13%)	67,113,113	1.46	11 (16%)
22	CLA	c	513	-	59,73,73	1.42	7 (11%)	67,113,113	1.53	10 (14%)
27	LMG	a	415	-	55,55,55	1.42	7 (12%)	63,63,63	1.46	6 (9%)
27	LMG	D	411	-	31,31,55	1.11	3 (9%)	33,33,63	1.15	2 (6%)
22	CLA	a	402	-	59,73,73	1.62	5 (8%)	67,113,113	1.67	15 (22%)
31	STE	C	519	-	15,15,19	0.56	0	14,14,19	0.50	0
22	CLA	b	615	-	59,73,73	1.95	6 (10%)	67,113,113	1.53	10 (14%)
27	LMG	c	522	-	48,48,55	1.12	5 (10%)	56,56,63	1.19	3 (5%)
22	CLA	b	605	-	59,73,73	1.28	4 (6%)	67,113,113	1.76	17 (25%)
22	CLA	c	509	-	58,72,73	1.44	9 (15%)	65,111,113	1.54	12 (18%)
24	BCR	A	406	-	41,41,41	1.14	3 (7%)	56,56,56	1.42	8 (14%)
22	CLA	c	503	-	59,73,73	1.27	8 (13%)	67,113,113	1.54	10 (14%)
31	STE	T	102	-	14,14,19	0.42	0	13,13,19	0.85	0
31	STE	I	101	-	14,14,19	0.53	0	13,13,19	0.45	0
27	LMG	M	101	-	51,51,55	1.13	3 (5%)	59,59,63	1.48	10 (16%)
24	BCR	B	619	-	41,41,41	1.11	1 (2%)	56,56,56	1.47	9 (16%)
31	STE	B	620	-	13,16,19	0.59	0	12,16,19	0.57	0
32	BCT	d	402	21	0,3,3	0.00	-	0,3,3	0.00	-
29	DGD	h	102	-	63,63,67	1.16	10 (15%)	77,77,81	1.38	10 (12%)
31	STE	c	521	-	16,19,19	0.37	0	15,19,19	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	STE	d	413	-	16,19,19	0.41	0	15,19,19	0.65	0
33	LHG	d	408	-	48,48,48	0.98	1 (2%)	51,54,54	1.15	3 (5%)
24	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.40	9 (16%)
33	LHG	L	102	-	48,48,48	0.79	2 (4%)	51,54,54	1.18	3 (5%)
28	SQD	A	412	-	38,38,54	1.03	3 (7%)	40,40,65	1.30	4 (10%)
34	HEC	F	102	5,6	26,50,50	2.57	5 (19%)	18,82,82	2.22	6 (33%)
22	CLA	B	604	-	59,73,73	1.31	7 (11%)	67,113,113	1.91	19 (28%)
29	DGD	C	515	-	63,63,67	1.44	11 (17%)	77,77,81	1.46	12 (15%)
22	CLA	c	514	-	59,73,73	1.73	9 (15%)	67,113,113	1.38	11 (16%)
31	STE	b	626	-	13,13,19	0.40	0	12,12,19	0.77	0
31	STE	b	622	-	16,19,19	0.39	0	15,19,19	0.81	0
22	CLA	b	606	-	59,73,73	1.70	9 (15%)	67,113,113	1.70	9 (13%)
33	LHG	l	101	-	48,48,48	0.60	0	51,54,54	1.14	4 (7%)
22	CLA	B	602	-	59,73,73	1.51	6 (10%)	67,113,113	1.61	12 (17%)
27	LMG	b	621	-	51,51,55	1.00	4 (7%)	59,59,63	1.42	10 (16%)
22	CLA	a	403	35	59,73,73	1.53	7 (11%)	67,113,113	1.62	12 (17%)
24	BCR	C	514	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	8 (14%)
31	STE	c	501	-	8,11,19	0.39	0	7,11,19	0.84	0
30	OEX	a	416	1,3,35	0,15,15	0.00	-	-	-	-
22	CLA	D	404	35	59,73,73	1.61	8 (13%)	67,113,113	1.49	8 (11%)
27	LMG	b	623	-	55,55,55	0.87	3 (5%)	63,63,63	1.60	11 (17%)
22	CLA	B	612	-	59,73,73	1.30	6 (10%)	67,113,113	1.67	13 (19%)
31	STE	M	102	-	11,14,19	0.57	0	10,14,19	0.39	0
29	DGD	H	103	-	63,63,67	1.32	8 (12%)	77,77,81	1.53	14 (18%)
22	CLA	b	602	-	59,73,73	1.65	10 (16%)	67,113,113	1.44	10 (14%)
24	BCR	B	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	5 (8%)
31	STE	B	623	-	10,13,19	0.49	0	9,13,19	0.74	0
22	CLA	D	403	-	59,73,73	1.34	4 (6%)	67,113,113	1.64	12 (17%)
31	STE	Z	101	-	7,7,19	0.42	0	6,6,19	0.55	0
33	LHG	d	409	-	38,38,48	0.99	1 (2%)	41,44,54	1.06	2 (4%)
22	CLA	a	410	35	59,73,73	1.49	7 (11%)	67,113,113	1.58	13 (19%)
22	CLA	b	612	-	59,73,73	1.21	4 (6%)	67,113,113	1.70	14 (20%)
22	CLA	C	513	-	59,73,73	1.38	9 (15%)	67,113,113	1.66	13 (19%)
22	CLA	b	616	-	54,68,73	1.38	8 (14%)	61,107,113	1.92	11 (18%)
23	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.29	9 (10%)
24	BCR	b	617	-	41,41,41	1.10	3 (7%)	56,56,56	1.38	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	402	-	59,73,73	1.40	8 (13%)	67,113,113	1.47	7 (10%)
33	LHG	d	407	-	48,48,48	1.00	2 (4%)	51,54,54	1.44	5 (9%)
22	CLA	B	607	35	59,73,73	1.19	8 (13%)	67,113,113	1.57	10 (14%)
31	STE	d	411	-	12,15,19	0.46	0	11,15,19	0.58	0
22	CLA	C	511	3	59,73,73	1.45	8 (13%)	67,113,113	1.37	6 (8%)
28	SQD	f	102	-	40,41,54	1.11	4 (10%)	49,52,65	1.91	10 (20%)
33	LHG	D	409	-	48,48,48	0.92	2 (4%)	51,54,54	1.28	6 (11%)
22	CLA	C	503	-	59,73,73	1.67	10 (16%)	67,113,113	1.60	11 (16%)
31	STE	B	626	-	15,15,19	0.45	0	14,14,19	0.71	0
33	LHG	D	412	-	48,48,48	0.76	1 (2%)	51,54,54	1.32	5 (9%)
22	CLA	B	609	-	59,73,73	1.45	8 (13%)	67,113,113	1.56	12 (17%)
28	SQD	a	411	-	53,54,54	1.02	5 (9%)	62,65,65	2.18	16 (25%)
31	STE	b	624	-	16,19,19	0.46	0	15,19,19	0.69	0
31	STE	M	103	-	9,9,19	0.47	0	8,8,19	0.72	0
22	CLA	B	606	-	59,73,73	1.77	9 (15%)	67,113,113	1.60	9 (13%)
22	CLA	C	505	-	59,73,73	1.56	7 (11%)	67,113,113	1.59	12 (17%)
33	LHG	D	410	-	46,46,48	1.03	3 (6%)	49,52,54	1.21	4 (8%)
22	CLA	b	603	-	59,73,73	1.47	8 (13%)	67,113,113	1.64	11 (16%)
33	LHG	e	101	-	41,41,48	0.91	1 (2%)	44,47,54	1.22	4 (9%)
24	BCR	d	405	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	5 (8%)
31	STE	a	414	-	8,11,19	0.40	0	7,11,19	0.81	0
22	CLA	d	404	-	59,73,73	1.40	7 (11%)	67,113,113	1.42	10 (14%)
27	LMG	Y	101	-	48,48,55	0.96	2 (4%)	56,56,63	1.35	6 (10%)
31	STE	D	413	-	16,19,19	0.31	0	15,19,19	0.92	0
22	CLA	b	609	-	59,73,73	1.72	8 (13%)	67,113,113	1.49	12 (17%)
24	BCR	K	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	8 (14%)
22	CLA	B	611	-	59,73,73	1.47	8 (13%)	67,113,113	1.79	16 (23%)
29	DGD	C	516	-	63,63,67	1.20	9 (14%)	77,77,81	1.40	11 (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
29	DGD	A	413	-	-	30/55/95/95	0/2/2/2
34	HEC	v	201	17	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	L	101	-	-	22/44/64/69	0/1/1/1
22	CLA	B	605	-	3/3/25/25	9/37/135/135	-
24	BCR	a	406	-	-	3/29/63/63	0/2/2/2
27	LMG	c	520	-	-	10/31/51/70	0/1/1/1
31	STE	B	601	-	-	4/7/9/17	-
31	STE	d	412	-	-	5/12/14/17	-
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
22	CLA	C	512	-	3/3/25/25	15/37/135/135	-
31	STE	C	518	-	-	4/7/9/17	-
22	CLA	C	508	-	1/1/25/25	9/37/135/135	-
28	SQD	B	622	-	-	19/49/69/69	0/1/1/1
31	STE	b	625	-	-	6/7/7/17	-
22	CLA	C	507	35	3/3/25/25	5/37/135/135	-
22	CLA	c	502	-	3/3/25/25	1/37/135/135	-
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
22	CLA	b	613	-	3/3/25/25	7/37/135/135	-
31	STE	m	101	-	-	7/15/15/17	-
31	STE	b	627	-	-	9/15/17/17	-
22	CLA	a	405	-	3/3/25/25	7/37/135/135	-
22	CLA	c	510	-	3/3/25/25	15/37/135/135	-
22	CLA	C	509	-	3/3/25/25	11/37/135/135	-
22	CLA	b	610	35	3/3/25/25	3/37/135/135	-
24	BCR	c	515	-	-	10/29/63/63	0/2/2/2
22	CLA	B	608	-	2/2/25/25	4/37/135/135	-
26	PL9	d	406	-	-	15/53/73/73	0/1/1/1
24	BCR	F	101	-	-	5/29/63/63	0/2/2/2
29	DGD	c	519	-	-	18/51/91/95	0/2/2/2
22	CLA	A	405	-	3/3/22/25	3/24/122/135	-
24	BCR	b	619	-	-	8/29/63/63	0/2/2/2
31	STE	b	620	-	-	7/13/13/17	-
27	LMG	D	407	-	-	16/46/66/70	0/1/1/1
29	DGD	c	518	-	-	21/51/91/95	0/2/2/2
31	STE	d	411	-	-	7/11/13/17	-
22	CLA	c	506	-	2/2/25/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HEC	V	201	17	-	0/6/54/54	-
22	CLA	C	510	-	3/3/25/25	8/37/135/135	-
31	STE	J	101	-	-	3/7/9/17	-
26	PL9	D	406	-	-	12/53/73/73	0/1/1/1
22	CLA	C	504	35	3/3/23/25	8/30/128/135	-
31	STE	H	104	-	-	9/15/15/17	-
22	CLA	d	403	-	1/1/25/25	10/37/135/135	-
22	CLA	B	615	-	3/3/25/25	9/37/135/135	-
31	STE	a	413	-	-	5/7/7/17	-
22	CLA	b	604	-	3/3/25/25	7/37/135/135	-
22	CLA	D	405	-	3/3/25/25	7/37/135/135	-
22	CLA	B	613	-	3/3/25/25	13/37/135/135	-
26	PL9	a	409	-	-	21/53/73/73	0/1/1/1
31	STE	j	101	-	-	4/7/9/17	-
27	LMG	d	410	-	-	11/39/59/70	0/1/1/1
27	LMG	A	410	-	-	18/43/63/70	0/1/1/1
22	CLA	B	616	-	3/3/24/25	10/31/129/135	-
23	PHO	D	401	-	-	1/53/103/103	0/5/6/6
31	STE	B	627	-	-	5/12/12/17	-
24	BCR	H	102	-	-	6/29/63/63	0/2/2/2
22	CLA	b	611	-	2/2/25/25	7/37/135/135	-
27	LMG	B	621	-	-	9/18/22/70	-
23	PHO	A	404	-	-	4/53/103/103	0/5/6/6
28	SQD	a	412	-	-	15/37/37/69	-
24	BCR	K	102	-	-	6/29/63/63	0/2/2/2
22	CLA	c	511	-	3/3/25/25	7/37/135/135	-
34	HEC	f	101	5,6	-	1/6/54/54	-
26	PL9	A	409	-	-	22/53/73/73	0/1/1/1
31	STE	m	102	-	-	4/7/9/17	-
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2
28	SQD	A	411	-	-	9/47/67/69	0/1/1/1
29	DGD	C	517	-	-	14/51/91/95	0/2/2/2
31	STE	B	624	-	-	3/7/9/17	-
22	CLA	c	505	35	3/3/24/25	7/31/129/135	-
33	LHG	E	101	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	603	-	3/3/25/25	14/37/135/135	-
24	BCR	k	102	-	-	6/29/63/63	0/2/2/2
22	CLA	H	101	35	2/2/25/25	20/37/135/135	-
22	CLA	B	610	35	3/3/25/25	6/37/135/135	-
22	CLA	C	502	-	3/3/25/25	10/37/135/135	-
31	STE	E	102	-	-	5/7/9/17	-
22	CLA	b	601	35	2/2/25/25	16/37/135/135	-
22	CLA	c	504	-	2/2/25/25	11/37/135/135	-
23	PHO	a	404	-	-	6/53/103/103	0/5/6/6
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
29	DGD	c	517	-	-	24/51/91/95	0/2/2/2
22	CLA	b	607	35	3/3/25/25	15/37/135/135	-
22	CLA	C	501	-	3/3/25/25	3/37/135/135	-
22	CLA	B	614	-	3/3/25/25	10/37/135/135	-
28	SQD	D	408	-	-	13/28/48/69	0/1/1/1
24	BCR	h	101	-	-	6/29/63/63	0/2/2/2
22	CLA	b	608	-	1/1/25/25	5/37/135/135	-
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
24	BCR	c	516	-	-	6/29/63/63	0/2/2/2
22	CLA	c	512	3	3/3/25/25	11/37/135/135	-
31	STE	C	520	-	-	2/7/9/17	-
31	STE	B	625	-	-	12/13/15/17	-
22	CLA	c	507	-	3/3/25/25	16/37/135/135	-
22	CLA	b	614	-	3/3/25/25	16/37/135/135	-
24	BCR	K	101	-	-	9/29/63/63	0/2/2/2
22	CLA	A	403	35	1/1/25/25	14/37/135/135	-
22	CLA	c	513	-	3/3/25/25	19/37/135/135	-
27	LMG	a	415	-	-	31/50/70/70	0/1/1/1
27	LMG	D	411	-	-	15/33/33/70	-
22	CLA	a	402	-	3/3/25/25	7/37/135/135	-
31	STE	C	519	-	-	5/13/13/17	-
22	CLA	b	615	-	3/3/25/25	8/37/135/135	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
27	LMG	Y	101	-	-	24/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	605	-	3/3/25/25	8/37/135/135	-
22	CLA	c	509	-	2/2/24/25	7/36/134/135	-
24	BCR	A	406	-	-	11/29/63/63	0/2/2/2
22	CLA	c	503	-	2/2/25/25	8/37/135/135	-
31	STE	T	102	-	-	7/12/12/17	-
31	STE	I	101	-	-	7/12/12/17	-
27	LMG	M	101	-	-	27/46/66/70	0/1/1/1
24	BCR	B	619	-	-	5/29/63/63	0/2/2/2
31	STE	B	620	-	-	8/12/14/17	-
24	BCR	t	101	-	-	4/29/63/63	0/2/2/2
29	DGD	h	102	-	-	18/51/91/95	0/2/2/2
33	LHG	D	412	-	-	20/53/53/53	-
31	STE	c	521	-	-	9/15/17/17	-
31	STE	d	413	-	-	9/15/17/17	-
33	LHG	d	408	-	-	20/53/53/53	-
24	BCR	B	618	-	-	9/29/63/63	0/2/2/2
33	LHG	L	102	-	-	20/53/53/53	-
28	SQD	A	412	-	-	17/39/39/69	-
34	HEC	F	102	5,6	-	0/6/54/54	-
22	CLA	B	604	-	3/3/25/25	12/37/135/135	-
29	DGD	C	515	-	-	22/51/91/95	0/2/2/2
22	CLA	c	514	-	3/3/25/25	10/37/135/135	-
31	STE	b	626	-	-	5/11/11/17	-
31	STE	b	622	-	-	6/15/17/17	-
22	CLA	b	606	-	3/3/25/25	7/37/135/135	-
33	LHG	l	101	-	-	17/53/53/53	-
22	CLA	B	602	-	3/3/25/25	8/37/135/135	-
27	LMG	b	621	-	-	14/46/66/70	0/1/1/1
22	CLA	C	506	-	2/2/25/25	8/37/135/135	-
31	STE	c	501	-	-	3/7/9/17	-
22	CLA	D	404	35	1/1/25/25	10/37/135/135	-
27	LMG	b	623	-	-	26/50/70/70	0/1/1/1
22	CLA	B	612	-	3/3/25/25	12/37/135/135	-
31	STE	M	102	-	-	5/10/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	DGD	H	103	-	-	17/51/91/95	0/2/2/2
22	CLA	b	602	-	1/1/25/25	6/37/135/135	-
24	BCR	B	617	-	-	7/29/63/63	0/2/2/2
31	STE	B	623	-	-	3/9/11/17	-
22	CLA	D	403	-	1/1/25/25	5/37/135/135	-
31	STE	Z	101	-	-	2/5/5/17	-
33	LHG	d	409	-	-	12/43/43/53	-
22	CLA	a	410	35	1/1/25/25	6/37/135/135	-
22	CLA	b	612	-	3/3/25/25	8/37/135/135	-
22	CLA	C	513	-	3/3/25/25	17/37/135/135	-
22	CLA	b	616	-	3/3/24/25	10/31/129/135	-
23	PHO	d	401	-	-	5/53/103/103	0/5/6/6
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
22	CLA	A	402	-	3/3/25/25	5/37/135/135	-
33	LHG	d	407	-	-	14/53/53/53	-
22	CLA	B	607	35	3/3/25/25	7/37/135/135	-
22	CLA	c	508	35	3/3/25/25	8/37/135/135	-
22	CLA	C	511	3	3/3/25/25	9/37/135/135	-
28	SQD	f	102	-	-	15/36/56/69	0/1/1/1
33	LHG	D	409	-	-	28/53/53/53	-
22	CLA	C	503	-	3/3/25/25	5/37/135/135	-
31	STE	B	626	-	-	8/13/13/17	-
22	CLA	B	606	-	3/3/25/25	13/37/135/135	-
22	CLA	B	609	-	1/1/25/25	8/37/135/135	-
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
31	STE	b	624	-	-	8/15/17/17	-
31	STE	M	103	-	-	3/7/7/17	-
22	CLA	C	505	-	2/2/25/25	12/37/135/135	-
33	LHG	D	410	-	-	22/51/51/53	-
22	CLA	b	603	-	3/3/25/25	10/37/135/135	-
33	LHG	e	101	-	-	23/46/46/53	-
24	BCR	d	405	-	-	8/29/63/63	0/2/2/2
31	STE	a	414	-	-	2/7/9/17	-
22	CLA	d	404	-	2/2/25/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	403	35	2/2/25/25	11/37/135/135	-
31	STE	D	413	-	-	7/15/17/17	-
22	CLA	b	609	-	1/1/25/25	8/37/135/135	-
24	BCR	K	103	-	-	7/29/63/63	0/2/2/2
22	CLA	B	611	-	3/3/25/25	2/37/135/135	-
29	DGD	C	516	-	-	21/51/91/95	0/2/2/2

All (799) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	C4B-NB	9.07	1.43	1.35
22	b	615	CLA	MG-NA	8.66	2.26	2.06
22	b	615	CLA	C4B-NB	8.52	1.42	1.35
22	A	405	CLA	C4B-NB	8.31	1.42	1.35
22	c	505	CLA	C4B-NB	8.28	1.42	1.35
34	f	101	HEC	C3B-C2B	-8.12	1.32	1.40
22	B	613	CLA	C4B-NB	8.06	1.42	1.35
22	B	602	CLA	C4B-NB	7.98	1.42	1.35
22	B	616	CLA	MG-NA	7.90	2.25	2.06
22	C	505	CLA	C4B-NB	7.87	1.42	1.35
22	C	506	CLA	C4B-NB	7.85	1.42	1.35
22	b	606	CLA	MG-NA	7.76	2.24	2.06
22	A	403	CLA	C4B-NB	7.66	1.42	1.35
22	H	101	CLA	C4B-NB	7.64	1.42	1.35
22	b	604	CLA	MG-NA	7.64	2.24	2.06
22	B	608	CLA	MG-NA	7.61	2.24	2.06
22	C	501	CLA	C4B-NB	7.48	1.41	1.35
34	F	102	HEC	C3B-C2B	-7.36	1.33	1.40
22	c	512	CLA	C4B-NB	7.33	1.41	1.35
34	v	201	HEC	C3B-C2B	-7.33	1.33	1.40
22	C	503	CLA	C4B-NB	7.31	1.41	1.35
34	V	201	HEC	C3B-C2B	-7.26	1.33	1.40
22	b	609	CLA	C4B-NB	7.25	1.41	1.35
22	a	402	CLA	C4B-NB	7.21	1.41	1.35
22	b	601	CLA	C4B-NB	7.17	1.41	1.35
22	B	606	CLA	C4B-NB	7.15	1.41	1.35
22	a	403	CLA	C4B-NB	7.13	1.41	1.35
22	c	507	CLA	C4B-NB	7.11	1.41	1.35
22	d	403	CLA	C4B-NB	7.04	1.41	1.35
22	c	514	CLA	MG-NC	-7.03	1.89	2.06
22	d	404	CLA	C4B-NB	7.03	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	MG-NA	7.01	2.22	2.06
34	F	102	HEC	C3C-C2C	-6.99	1.33	1.40
22	C	511	CLA	C4B-NB	6.94	1.41	1.35
22	c	502	CLA	C4B-NB	6.93	1.41	1.35
22	D	403	CLA	C4B-NB	6.89	1.41	1.35
22	C	502	CLA	C4B-NB	6.86	1.41	1.35
22	C	508	CLA	C4B-NB	6.68	1.41	1.35
22	c	513	CLA	C4B-NB	6.66	1.41	1.35
22	b	614	CLA	C4B-NB	6.53	1.41	1.35
22	C	504	CLA	C4B-NB	6.53	1.41	1.35
22	C	512	CLA	C4B-NB	6.50	1.41	1.35
22	c	504	CLA	C4B-NB	6.50	1.41	1.35
22	b	609	CLA	MG-NA	6.44	2.21	2.06
22	b	608	CLA	MG-NA	6.43	2.21	2.06
22	D	404	CLA	C4B-NB	6.41	1.40	1.35
22	D	404	CLA	MG-NA	6.36	2.21	2.06
22	b	605	CLA	C4B-NB	6.35	1.40	1.35
22	B	615	CLA	C4B-NB	6.33	1.40	1.35
22	c	514	CLA	C4B-NB	6.31	1.40	1.35
22	b	613	CLA	C4B-NB	6.30	1.40	1.35
22	b	608	CLA	C4B-NB	6.29	1.40	1.35
22	C	513	CLA	C4B-NB	6.27	1.40	1.35
22	b	601	CLA	MG-NA	6.26	2.21	2.06
22	B	608	CLA	MG-NC	-6.25	1.91	2.06
22	B	614	CLA	C4B-NB	6.17	1.40	1.35
22	C	508	CLA	MG-NA	6.06	2.20	2.06
22	b	602	CLA	MG-NA	6.06	2.20	2.06
22	a	405	CLA	C4B-NB	6.05	1.40	1.35
22	C	509	CLA	C4B-NB	6.04	1.40	1.35
22	a	402	CLA	MG-NA	6.02	2.20	2.06
22	C	507	CLA	MG-NA	6.00	2.20	2.06
22	B	606	CLA	MG-NC	5.96	2.20	2.06
22	b	607	CLA	C4B-NB	5.96	1.40	1.35
22	b	612	CLA	C4B-NB	5.95	1.40	1.35
22	c	506	CLA	C4B-NB	5.93	1.40	1.35
22	a	410	CLA	MG-NA	5.92	2.20	2.06
22	B	611	CLA	C4B-NB	5.92	1.40	1.35
22	c	508	CLA	C4B-NB	5.91	1.40	1.35
22	C	503	CLA	MG-NA	5.87	2.20	2.06
22	B	616	CLA	C4B-NB	5.74	1.40	1.35
22	H	101	CLA	MG-NA	5.72	2.19	2.06
22	C	506	CLA	MG-NA	5.70	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C4B-NB	5.69	1.40	1.35
22	D	405	CLA	C4B-NB	5.68	1.40	1.35
27	a	415	LMG	C4-C5	5.67	1.65	1.53
22	B	609	CLA	C4B-NB	5.65	1.40	1.35
22	c	511	CLA	C4B-NB	5.64	1.40	1.35
22	C	507	CLA	C4B-NB	5.63	1.40	1.35
22	b	616	CLA	C4B-NB	5.62	1.40	1.35
22	c	510	CLA	C4B-NB	5.60	1.40	1.35
34	v	201	HEC	C3C-C2C	-5.59	1.34	1.40
22	B	609	CLA	MG-NA	5.57	2.19	2.06
34	f	101	HEC	C3C-C2C	-5.51	1.35	1.40
22	A	402	CLA	C4B-NB	5.49	1.40	1.35
34	V	201	HEC	C3C-C2C	-5.48	1.35	1.40
22	B	610	CLA	C4B-NB	5.40	1.40	1.35
22	b	606	CLA	C4B-NB	5.40	1.40	1.35
22	b	603	CLA	C4B-NB	5.38	1.40	1.35
22	c	514	CLA	MG-NA	5.13	2.18	2.06
22	B	606	CLA	MG-NA	5.01	2.18	2.06
22	b	610	CLA	C4B-NB	5.01	1.39	1.35
22	c	503	CLA	C4B-NB	4.97	1.39	1.35
22	B	612	CLA	C4B-NB	4.93	1.39	1.35
22	b	602	CLA	C4B-NB	4.91	1.39	1.35
22	c	509	CLA	C4B-NB	4.87	1.39	1.35
22	C	510	CLA	C4B-NB	4.86	1.39	1.35
22	b	602	CLA	MG-NC	-4.82	1.94	2.06
22	B	604	CLA	MG-NA	4.77	2.17	2.06
22	b	607	CLA	MG-NA	4.68	2.17	2.06
22	B	608	CLA	C4B-NB	4.67	1.39	1.35
22	a	410	CLA	C4B-NB	4.65	1.39	1.35
29	c	517	DGD	C3G-C2G	4.64	1.64	1.50
26	d	406	PL9	C6-C1	-4.63	1.40	1.48
22	B	615	CLA	MG-NC	4.57	2.17	2.06
22	B	603	CLA	C4B-NB	4.54	1.39	1.35
22	c	509	CLA	MG-NA	4.54	2.17	2.06
29	H	103	DGD	C4E-C5E	4.48	1.62	1.53
26	D	406	PL9	C7-C3	-4.45	1.46	1.51
27	M	101	LMG	O7-C8	-4.45	1.35	1.46
34	f	101	HEC	CBB-CAB	-4.42	1.32	1.49
33	d	408	LHG	O8-C6	-4.39	1.35	1.45
34	F	102	HEC	CBC-CAC	-4.35	1.33	1.49
22	c	506	CLA	MG-NA	4.31	2.16	2.06
24	C	514	BCR	C1-C6	-4.30	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	BCR	C30-C25	-4.30	1.47	1.53
22	C	505	CLA	CHC-C1C	4.26	1.45	1.35
22	B	607	CLA	C4B-NB	4.26	1.39	1.35
24	c	516	BCR	C1-C6	-4.23	1.48	1.53
29	c	517	DGD	O3E-C3E	-4.18	1.33	1.43
22	b	603	CLA	MG-NA	4.15	2.16	2.06
22	B	610	CLA	MG-NC	-4.13	1.96	2.06
22	c	509	CLA	CHC-C1C	4.10	1.45	1.35
28	a	412	SQD	O47-C7	4.10	1.45	1.34
24	T	101	BCR	C1-C6	-4.07	1.48	1.53
22	B	613	CLA	MG-NA	4.07	2.15	2.06
24	a	406	BCR	C1-C6	-4.05	1.48	1.53
29	C	515	DGD	C6E-C5E	4.04	1.65	1.51
28	a	411	SQD	O48-C23	4.04	1.45	1.33
26	D	406	PL9	C52-C5	-4.03	1.42	1.50
34	F	102	HEC	CBB-CAB	-4.03	1.34	1.49
22	B	611	CLA	MG-NA	4.03	2.15	2.06
34	f	101	HEC	CBC-CAC	-4.03	1.34	1.49
22	B	604	CLA	C4B-NB	4.02	1.38	1.35
29	C	517	DGD	O2G-C2G	-4.00	1.36	1.46
27	d	410	LMG	C4-C5	3.97	1.61	1.53
26	a	409	PL9	C7-C3	3.97	1.55	1.51
29	c	518	DGD	C4D-C3D	3.97	1.62	1.52
33	D	410	LHG	P-O6	3.92	1.75	1.59
24	d	405	BCR	C30-C25	-3.90	1.48	1.53
29	C	515	DGD	O2G-C2G	-3.89	1.36	1.46
22	B	610	CLA	C3B-C2B	-3.88	1.35	1.40
22	c	511	CLA	MG-NA	3.87	2.15	2.06
22	b	611	CLA	C4B-NB	3.85	1.38	1.35
34	V	201	HEC	CBB-CAB	-3.85	1.35	1.49
27	A	410	LMG	O1-C7	-3.83	1.36	1.43
27	D	407	LMG	C4-C5	3.82	1.61	1.53
22	c	512	CLA	CHC-C1C	3.82	1.44	1.35
22	C	502	CLA	MG-NA	3.82	2.15	2.06
22	C	511	CLA	MG-NA	3.77	2.15	2.06
34	v	201	HEC	CBC-CAC	-3.75	1.35	1.49
29	c	519	DGD	O2E-C2E	-3.75	1.34	1.43
29	A	413	DGD	C3E-C2E	3.71	1.61	1.52
22	B	610	CLA	CMB-C2B	-3.70	1.43	1.51
28	a	412	SQD	O48-C23	3.68	1.44	1.33
33	D	409	LHG	O7-C5	-3.68	1.37	1.46
22	a	402	CLA	CHC-C1C	3.65	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	517	DGD	O2G-C2G	-3.65	1.37	1.46
22	b	608	CLA	CHC-C1C	3.65	1.44	1.35
22	C	501	CLA	MG-NA	3.64	2.14	2.06
27	D	411	LMG	C9-C8	3.63	1.61	1.50
22	b	611	CLA	MG-NA	3.63	2.14	2.06
22	D	404	CLA	CHC-C1C	3.63	1.44	1.35
22	b	603	CLA	CMD-C2D	-3.63	1.42	1.51
22	a	403	CLA	CHC-C1C	3.63	1.44	1.35
29	c	519	DGD	O3D-C3D	-3.62	1.34	1.43
33	d	407	LHG	C24-C23	3.61	1.61	1.50
22	c	507	CLA	CHC-C1C	3.59	1.44	1.35
22	d	403	CLA	MG-NA	3.58	2.14	2.06
24	c	515	BCR	C1-C6	-3.55	1.48	1.53
22	b	615	CLA	CMD-C2D	-3.54	1.43	1.51
22	c	502	CLA	MG-NA	3.53	2.14	2.06
29	C	515	DGD	C4E-C3E	3.52	1.61	1.52
22	c	506	CLA	MG-NC	-3.52	1.97	2.06
24	K	102	BCR	C30-C25	-3.52	1.48	1.53
23	d	401	PHO	CHC-C1C	3.51	1.45	1.38
24	F	101	BCR	C1-C6	-3.51	1.48	1.53
22	A	405	CLA	MG-NC	-3.51	1.97	2.06
22	a	410	CLA	C3B-C2B	-3.51	1.35	1.40
27	c	522	LMG	O1-C1	3.50	1.46	1.40
26	d	406	PL9	C46-C44	-3.50	1.44	1.51
22	b	601	CLA	CHC-C1C	3.48	1.43	1.35
22	C	501	CLA	C3B-C2B	-3.48	1.35	1.40
22	B	614	CLA	MG-NA	3.48	2.14	2.06
22	C	509	CLA	MG-NA	3.46	2.14	2.06
28	B	622	SQD	O48-C23	3.45	1.43	1.33
22	C	501	CLA	CHC-C1C	3.44	1.43	1.35
24	B	619	BCR	C1-C6	-3.44	1.49	1.53
22	C	505	CLA	MG-NA	3.43	2.14	2.06
22	b	611	CLA	CHC-C1C	3.43	1.43	1.35
22	A	405	CLA	MG-NA	3.42	2.14	2.06
22	C	502	CLA	CHC-C1C	3.40	1.43	1.35
24	b	619	BCR	C30-C25	-3.40	1.49	1.53
22	c	510	CLA	CHC-C1C	3.39	1.43	1.35
28	B	622	SQD	O47-C7	3.38	1.43	1.34
24	A	406	BCR	C1-C6	-3.38	1.49	1.53
28	f	102	SQD	O48-C23	3.38	1.43	1.33
24	K	101	BCR	C30-C25	-3.38	1.49	1.53
28	A	412	SQD	O48-C23	3.37	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEC	CBC-CAC	-3.37	1.36	1.49
26	d	406	PL9	C26-C24	-3.36	1.44	1.51
24	d	405	BCR	C1-C6	-3.35	1.49	1.53
22	c	514	CLA	CHC-C1C	3.35	1.43	1.35
34	v	201	HEC	CBB-CAB	-3.35	1.36	1.49
22	C	503	CLA	CHC-C1C	3.34	1.43	1.35
22	B	615	CLA	MG-NA	3.33	2.14	2.06
22	b	606	CLA	C3B-C2B	-3.30	1.35	1.40
24	b	617	BCR	C30-C25	-3.29	1.49	1.53
27	c	523	LMG	C4-C5	3.29	1.60	1.53
27	a	415	LMG	O8-C9	-3.29	1.37	1.45
22	D	405	CLA	CMD-C2D	-3.29	1.43	1.51
22	C	504	CLA	CHC-C1C	3.28	1.43	1.35
22	C	501	CLA	C1D-C2D	3.28	1.50	1.42
28	A	411	SQD	O48-C23	3.28	1.42	1.33
27	b	621	LMG	O7-C8	-3.27	1.38	1.46
24	h	101	BCR	C30-C25	-3.27	1.49	1.53
22	B	613	CLA	CHC-C1C	3.27	1.43	1.35
22	a	403	CLA	CMB-C2B	-3.25	1.44	1.51
22	B	606	CLA	CHC-C1C	3.25	1.43	1.35
22	H	101	CLA	C3B-C2B	-3.25	1.35	1.40
29	A	413	DGD	C4D-C3D	3.24	1.60	1.52
29	H	103	DGD	C3E-C2E	3.23	1.60	1.52
29	A	413	DGD	C1E-C2E	3.23	1.61	1.52
22	a	405	CLA	C4B-CHC	-3.22	1.32	1.41
29	H	103	DGD	C4D-C5D	3.22	1.59	1.53
22	c	511	CLA	CMB-C2B	-3.22	1.45	1.51
22	a	402	CLA	CMB-C2B	-3.21	1.45	1.51
22	C	512	CLA	CHC-C1C	3.21	1.43	1.35
22	c	506	CLA	CHC-C1C	3.21	1.43	1.35
22	b	615	CLA	CHC-C1C	3.20	1.43	1.35
24	B	617	BCR	C30-C25	-3.20	1.49	1.53
22	a	403	CLA	C3B-C2B	-3.20	1.35	1.40
22	b	614	CLA	CHC-C1C	3.20	1.43	1.35
27	d	410	LMG	O7-C8	-3.19	1.38	1.46
24	H	102	BCR	C30-C25	-3.19	1.49	1.53
28	L	101	SQD	O48-C23	3.19	1.42	1.33
22	b	610	CLA	C3B-C2B	-3.18	1.36	1.40
22	b	601	CLA	C1D-C2D	3.18	1.49	1.42
24	b	619	BCR	C1-C6	-3.18	1.49	1.53
29	A	413	DGD	C4E-C5E	3.17	1.59	1.53
22	C	509	CLA	CMB-C2B	-3.17	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	CHC-C1C	3.17	1.43	1.35
22	H	101	CLA	C1D-C2D	3.16	1.49	1.42
22	A	402	CLA	MG-NA	3.15	2.13	2.06
22	B	608	CLA	C1D-C2D	3.15	1.49	1.42
24	k	101	BCR	C1-C6	-3.13	1.49	1.53
22	C	508	CLA	C1D-C2D	3.13	1.49	1.42
23	d	401	PHO	C3B-C4B	3.13	1.49	1.43
33	d	409	LHG	P-O6	3.12	1.71	1.59
22	b	613	CLA	CMB-C2B	-3.12	1.45	1.51
22	B	614	CLA	CHC-C1C	3.12	1.43	1.35
22	A	403	CLA	C1B-NB	3.11	1.38	1.35
22	B	615	CLA	CMD-C2D	-3.11	1.44	1.51
29	H	103	DGD	C1G-C2G	3.10	1.60	1.50
22	b	609	CLA	CMB-C2B	-3.10	1.45	1.51
22	D	403	CLA	CHC-C1C	3.10	1.42	1.35
27	Y	101	LMG	O7-C8	-3.09	1.38	1.46
22	a	403	CLA	MG-NA	3.09	2.13	2.06
22	b	607	CLA	C3B-C2B	-3.09	1.36	1.40
26	d	406	PL9	C31-C29	-3.09	1.44	1.51
22	b	602	CLA	C3B-C2B	-3.09	1.36	1.40
22	c	513	CLA	CHC-C1C	3.08	1.42	1.35
22	b	604	CLA	C1B-NB	3.08	1.38	1.35
28	A	412	SQD	O47-C45	-3.07	1.41	1.47
22	C	506	CLA	CHC-C1C	3.07	1.42	1.35
28	f	102	SQD	O47-C7	3.07	1.43	1.34
22	b	606	CLA	CHC-C1C	3.06	1.42	1.35
22	a	405	CLA	CMC-C2C	-3.06	1.44	1.50
22	b	602	CLA	CMD-C2D	-3.06	1.44	1.51
28	D	408	SQD	O48-C23	3.05	1.42	1.33
26	d	406	PL9	C3-C4	-3.05	1.44	1.49
22	a	410	CLA	CMB-C2B	-3.04	1.45	1.51
22	C	513	CLA	CHC-C1C	3.04	1.42	1.35
22	A	403	CLA	CHC-C1C	3.04	1.42	1.35
29	c	519	DGD	O4D-C4D	-3.03	1.35	1.43
22	B	611	CLA	CHC-C1C	3.02	1.42	1.35
22	c	507	CLA	CMD-C2D	-3.02	1.44	1.51
22	b	604	CLA	CHC-C1C	3.01	1.42	1.35
23	A	404	PHO	CMD-C2D	-3.01	1.44	1.50
22	C	511	CLA	CHC-C1C	3.01	1.42	1.35
22	C	513	CLA	MG-NA	3.01	2.13	2.06
23	A	404	PHO	CHB-C1B	-3.00	1.33	1.38
28	L	101	SQD	O47-C7	3.00	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406	BCR	C38-C26	-3.00	1.46	1.50
22	B	611	CLA	CMB-C2B	-3.00	1.45	1.51
26	d	406	PL9	C25-C24	-2.99	1.43	1.50
22	b	606	CLA	CMB-C2B	-2.99	1.45	1.51
28	A	412	SQD	O47-C7	2.98	1.42	1.34
24	K	101	BCR	C1-C6	-2.98	1.49	1.53
22	c	503	CLA	CHC-C1C	2.97	1.42	1.35
22	B	603	CLA	CMB-C2B	-2.97	1.45	1.51
22	B	614	CLA	C3B-C2B	-2.96	1.36	1.40
29	A	413	DGD	O1G-C1G	-2.96	1.38	1.45
22	b	613	CLA	MG-NA	2.96	2.13	2.06
28	A	411	SQD	O2-C2	-2.96	1.36	1.43
22	B	615	CLA	CHC-C1C	2.94	1.42	1.35
22	C	503	CLA	C1D-C2D	2.94	1.49	1.42
22	b	607	CLA	CMB-C2B	-2.94	1.45	1.51
22	H	101	CLA	CHC-C1C	2.93	1.42	1.35
22	b	609	CLA	CHC-C1C	2.93	1.42	1.35
22	b	606	CLA	C1B-NB	2.93	1.37	1.35
29	C	515	DGD	O5D-C1E	2.93	1.45	1.40
22	b	604	CLA	C1D-C2D	2.93	1.49	1.42
22	C	510	CLA	MG-NC	2.93	2.13	2.06
22	b	614	CLA	C3B-CAB	-2.92	1.42	1.47
22	b	603	CLA	CMC-C2C	-2.92	1.44	1.50
22	B	603	CLA	CMD-C2D	-2.92	1.44	1.51
22	B	602	CLA	CMB-C2B	-2.92	1.45	1.51
22	B	612	CLA	C1C-NC	-2.91	1.33	1.37
22	b	605	CLA	CHC-C1C	2.91	1.42	1.35
22	B	612	CLA	CMC-C2C	-2.91	1.44	1.50
24	B	618	BCR	C30-C25	-2.90	1.49	1.53
24	T	101	BCR	C30-C25	-2.90	1.49	1.53
22	C	507	CLA	CHC-C1C	2.90	1.42	1.35
22	B	602	CLA	MG-NA	2.89	2.13	2.06
22	B	615	CLA	C3B-C2B	-2.89	1.36	1.40
29	A	413	DGD	O5D-C6D	-2.89	1.38	1.43
22	B	606	CLA	C3B-C2B	-2.89	1.36	1.40
22	B	605	CLA	CHC-C1C	2.88	1.42	1.35
29	c	518	DGD	C3E-C2E	2.88	1.59	1.52
22	B	615	CLA	CMB-C2B	-2.88	1.45	1.51
22	c	512	CLA	C1D-C2D	2.87	1.49	1.42
27	c	520	LMG	O1-C1	2.87	1.45	1.40
22	C	513	CLA	CMB-C2B	-2.86	1.45	1.51
22	b	609	CLA	C1D-C2D	2.86	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	MG-NA	2.86	2.13	2.06
22	b	603	CLA	C3B-C2B	-2.85	1.36	1.40
27	M	101	LMG	C4-C3	2.85	1.59	1.52
22	c	508	CLA	CHC-C1C	2.85	1.42	1.35
23	D	401	PHO	CHC-C1C	2.85	1.44	1.38
26	D	406	PL9	C31-C29	-2.84	1.45	1.51
27	b	621	LMG	C4-C3	2.84	1.59	1.52
22	c	511	CLA	CHC-C1C	2.84	1.42	1.35
24	b	617	BCR	C1-C6	-2.84	1.49	1.53
22	D	403	CLA	CMB-C2B	-2.83	1.45	1.51
29	C	517	DGD	C6E-C5E	2.82	1.61	1.51
24	c	515	BCR	C30-C25	-2.82	1.49	1.53
22	b	607	CLA	CMD-C2D	-2.82	1.44	1.51
22	C	508	CLA	CHC-C1C	2.82	1.42	1.35
22	c	504	CLA	CMB-C2B	-2.82	1.45	1.51
23	D	401	PHO	CHC-C4B	-2.82	1.33	1.40
22	B	608	CLA	CHC-C1C	2.81	1.42	1.35
24	B	617	BCR	C1-C6	-2.81	1.49	1.53
22	C	504	CLA	MG-NC	2.81	2.12	2.06
27	c	522	LMG	C4-C3	2.81	1.59	1.52
33	E	101	LHG	P-O6	2.81	1.70	1.59
27	D	411	LMG	C7-C8	2.81	1.58	1.51
22	c	509	CLA	CMB-C2B	-2.81	1.45	1.51
22	b	608	CLA	C1D-C2D	2.81	1.48	1.42
28	A	411	SQD	O47-C7	2.80	1.42	1.34
22	B	607	CLA	MG-NA	2.80	2.12	2.06
22	B	614	CLA	C3B-CAB	-2.80	1.42	1.47
22	B	607	CLA	CHC-C1C	2.79	1.42	1.35
22	B	603	CLA	C1D-C2D	2.79	1.48	1.42
23	D	401	PHO	CMB-C2B	-2.78	1.44	1.50
22	b	610	CLA	C1D-C2D	2.78	1.48	1.42
22	C	509	CLA	MG-NC	-2.77	1.99	2.06
22	B	606	CLA	CMB-C2B	-2.77	1.45	1.51
29	A	413	DGD	O2G-C2G	-2.77	1.39	1.46
23	D	401	PHO	C4C-NC	2.77	1.43	1.36
22	b	612	CLA	CHC-C1C	2.77	1.42	1.35
24	T	101	BCR	C38-C26	-2.76	1.46	1.50
22	B	612	CLA	C1D-C2D	2.76	1.48	1.42
22	C	503	CLA	CMB-C2B	-2.76	1.45	1.51
22	a	405	CLA	CMD-C2D	-2.75	1.45	1.51
27	c	523	LMG	O1-C7	-2.75	1.38	1.43
23	A	404	PHO	C1A-NA	2.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	CHC-C1C	2.74	1.42	1.35
22	c	502	CLA	CHC-C1C	2.74	1.42	1.35
22	a	410	CLA	C1D-C2D	2.74	1.48	1.42
27	a	415	LMG	C3-C2	2.73	1.59	1.52
22	c	505	CLA	CMB-C2B	-2.72	1.46	1.51
29	c	517	DGD	O3D-C3D	-2.71	1.36	1.43
29	C	516	DGD	C1E-C2E	2.71	1.60	1.52
22	b	616	CLA	CMB-C2B	-2.71	1.46	1.51
23	A	404	PHO	C4C-NC	2.71	1.42	1.36
27	c	520	LMG	C4-C3	2.70	1.59	1.52
22	B	615	CLA	C1D-C2D	2.70	1.48	1.42
24	K	102	BCR	C1-C6	-2.70	1.50	1.53
22	c	514	CLA	C1D-C2D	2.70	1.48	1.42
29	c	517	DGD	C4D-C3D	2.70	1.59	1.52
24	K	103	BCR	C1-C6	-2.70	1.50	1.53
22	b	614	CLA	CMC-C2C	-2.69	1.45	1.50
22	A	402	CLA	CMB-C2B	-2.69	1.46	1.51
27	c	522	LMG	C3-C2	2.69	1.59	1.52
22	A	402	CLA	CHC-C1C	2.68	1.41	1.35
26	a	409	PL9	C53-C6	-2.68	1.45	1.50
23	A	404	PHO	C1C-NC	-2.68	1.32	1.38
22	C	508	CLA	C1B-NB	2.68	1.37	1.35
22	B	615	CLA	C3B-CAB	-2.68	1.42	1.47
22	b	616	CLA	C1D-C2D	2.67	1.48	1.42
29	C	517	DGD	O3G-C1D	2.67	1.44	1.40
22	d	403	CLA	CMB-C2B	-2.66	1.46	1.51
22	d	403	CLA	C3B-C2B	-2.66	1.36	1.40
22	c	508	CLA	CMD-C2D	-2.66	1.45	1.51
22	c	505	CLA	CHC-C1C	2.66	1.41	1.35
22	C	511	CLA	CMB-C2B	-2.66	1.46	1.51
22	C	510	CLA	CMD-C2D	-2.65	1.45	1.51
22	b	614	CLA	CMB-C2B	-2.65	1.46	1.51
29	A	413	DGD	C4D-C5D	2.65	1.58	1.53
22	B	606	CLA	C3B-CAB	-2.65	1.42	1.47
22	C	510	CLA	CHC-C1C	2.65	1.41	1.35
22	b	611	CLA	MG-NC	2.64	2.12	2.06
29	h	102	DGD	O3E-C3E	-2.64	1.36	1.43
27	c	522	LMG	C1-C2	2.64	1.60	1.52
22	B	602	CLA	CHC-C1C	2.64	1.41	1.35
29	c	518	DGD	O1G-C1G	-2.64	1.39	1.45
22	c	511	CLA	C1D-C2D	2.64	1.48	1.42
22	c	513	CLA	CMB-C2B	-2.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	410	LHG	O7-C5	-2.63	1.40	1.46
22	C	509	CLA	CHC-C1C	2.63	1.41	1.35
22	A	405	CLA	CMD-C2D	-2.62	1.45	1.51
22	b	609	CLA	C3B-CAB	-2.62	1.42	1.47
24	k	102	BCR	C30-C25	-2.62	1.50	1.53
22	C	504	CLA	O2D-CGD	2.61	1.39	1.33
22	b	603	CLA	CMB-C2B	-2.61	1.46	1.51
22	B	613	CLA	C1D-C2D	2.61	1.48	1.42
22	C	503	CLA	C3B-C2B	-2.61	1.36	1.40
22	d	403	CLA	CHC-C1C	2.61	1.41	1.35
22	b	607	CLA	C1D-C2D	2.61	1.48	1.42
22	D	404	CLA	C1D-C2D	2.60	1.48	1.42
22	c	504	CLA	C1D-C2D	2.60	1.48	1.42
22	B	604	CLA	CHC-C1C	2.60	1.41	1.35
22	c	512	CLA	MG-NC	2.60	2.12	2.06
24	F	101	BCR	C30-C25	-2.60	1.50	1.53
29	c	518	DGD	O3D-C3D	-2.60	1.36	1.43
22	b	602	CLA	CHC-C1C	2.59	1.41	1.35
22	B	611	CLA	MG-NC	-2.58	2.00	2.06
29	h	102	DGD	O1G-C1G	-2.58	1.39	1.45
22	B	616	CLA	CMC-C2C	-2.58	1.45	1.50
22	C	512	CLA	C1D-C2D	2.57	1.48	1.42
22	d	403	CLA	CMD-C2D	-2.57	1.45	1.51
23	A	404	PHO	C3B-C4B	2.57	1.48	1.43
22	b	601	CLA	O2A-CGA	2.57	1.40	1.33
29	H	103	DGD	C4E-C3E	2.57	1.58	1.52
24	k	101	BCR	C30-C25	-2.56	1.50	1.53
33	L	102	LHG	O7-C5	-2.56	1.40	1.46
22	c	513	CLA	CMD-C2D	-2.56	1.45	1.51
22	B	611	CLA	C3B-C2B	-2.56	1.36	1.40
22	a	410	CLA	CHC-C1C	2.56	1.41	1.35
29	C	516	DGD	O2G-C2G	-2.56	1.40	1.46
24	A	406	BCR	C33-C5	-2.55	1.46	1.50
22	b	602	CLA	CMB-C2B	-2.55	1.46	1.51
28	A	411	SQD	O3-C3	-2.55	1.37	1.43
22	c	502	CLA	CMD-C2D	-2.54	1.45	1.51
29	C	515	DGD	O1G-C1A	2.54	1.40	1.33
29	h	102	DGD	C4D-C3D	2.54	1.58	1.52
22	B	616	CLA	C3B-C2B	-2.54	1.36	1.40
22	b	613	CLA	CMD-C2D	-2.54	1.45	1.51
22	A	403	CLA	CMD-C2D	-2.54	1.45	1.51
22	B	609	CLA	C3B-C2B	-2.54	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	e	101	LHG	P-O6	2.53	1.69	1.59
33	D	412	LHG	O7-C5	-2.53	1.40	1.46
22	D	404	CLA	CMD-C2D	-2.53	1.45	1.51
24	A	406	BCR	C30-C25	-2.53	1.50	1.53
22	b	606	CLA	C4B-CHC	-2.53	1.34	1.41
22	c	509	CLA	CMD-C2D	-2.53	1.45	1.51
22	B	609	CLA	CMD-C2D	-2.53	1.45	1.51
24	c	516	BCR	C30-C25	-2.53	1.50	1.53
29	c	517	DGD	C3D-C2D	2.52	1.58	1.52
22	c	513	CLA	C1D-C2D	2.51	1.48	1.42
22	C	509	CLA	C3B-C2B	-2.51	1.36	1.40
22	c	510	CLA	C1D-C2D	2.51	1.48	1.42
24	K	103	BCR	C30-C25	-2.50	1.50	1.53
22	d	403	CLA	C4B-CHC	-2.50	1.34	1.41
22	B	614	CLA	CMC-C2C	-2.50	1.45	1.50
22	C	506	CLA	CMC-C2C	-2.50	1.45	1.50
34	F	102	HEC	CAD-C3D	2.49	1.55	1.52
27	d	410	LMG	O6-C5	-2.49	1.38	1.44
22	D	405	CLA	CMB-C2B	-2.49	1.46	1.51
22	b	614	CLA	O2D-CGD	2.49	1.39	1.33
29	h	102	DGD	O2D-C2D	-2.49	1.37	1.43
22	C	504	CLA	CMD-C2D	-2.49	1.45	1.51
22	b	608	CLA	C1B-NB	2.49	1.37	1.35
22	c	505	CLA	CMD-C2D	-2.48	1.45	1.51
33	d	407	LHG	O7-C5	-2.48	1.40	1.46
22	b	609	CLA	C3B-C2B	-2.48	1.36	1.40
22	b	615	CLA	CMB-C2B	-2.48	1.46	1.51
29	C	516	DGD	C6E-C5E	2.47	1.60	1.51
23	a	404	PHO	C3B-C4B	2.47	1.48	1.43
29	H	103	DGD	O6D-C5D	-2.47	1.38	1.44
29	C	515	DGD	C4D-C3D	2.46	1.58	1.52
28	B	622	SQD	O2-C2	-2.46	1.37	1.43
22	H	101	CLA	CMB-C2B	-2.45	1.46	1.51
22	C	504	CLA	C1B-NB	-2.45	1.33	1.35
23	D	401	PHO	C3B-C4B	2.45	1.48	1.43
27	c	523	LMG	C1-C2	2.45	1.59	1.52
22	d	404	CLA	CHC-C1C	2.45	1.41	1.35
22	B	615	CLA	O2D-CGD	2.44	1.39	1.33
22	c	503	CLA	CMD-C2D	-2.44	1.45	1.51
22	B	611	CLA	C1D-C2D	2.44	1.48	1.42
22	b	616	CLA	C3B-CAB	-2.44	1.43	1.47
22	C	505	CLA	C1D-C2D	2.43	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	610	CLA	MG-NA	2.43	2.12	2.06
22	B	612	CLA	CHC-C1C	2.43	1.41	1.35
22	c	503	CLA	MG-NA	2.43	2.12	2.06
22	C	512	CLA	CMD-C2D	-2.43	1.45	1.51
22	b	602	CLA	C4B-CHC	-2.43	1.34	1.41
22	b	612	CLA	CMB-C2B	-2.43	1.46	1.51
33	E	101	LHG	C24-C23	2.42	1.57	1.50
23	a	404	PHO	CHC-C4B	-2.42	1.34	1.40
22	b	610	CLA	MG-NC	2.42	2.12	2.06
23	A	404	PHO	CHC-C4B	-2.42	1.34	1.40
22	c	509	CLA	C1D-C2D	2.42	1.48	1.42
22	a	403	CLA	CMD-C2D	-2.42	1.45	1.51
22	b	611	CLA	C1D-C2D	2.42	1.48	1.42
22	B	614	CLA	CMB-C2B	-2.42	1.46	1.51
24	C	514	BCR	C30-C25	-2.41	1.50	1.53
22	A	405	CLA	C4B-CHC	-2.41	1.34	1.41
27	b	621	LMG	C1-C2	2.41	1.59	1.52
27	b	621	LMG	C4-C5	2.41	1.58	1.53
22	c	506	CLA	CMB-C2B	-2.41	1.46	1.51
22	C	504	CLA	C1D-C2D	2.41	1.48	1.42
28	f	102	SQD	O3-C3	-2.40	1.37	1.43
24	b	618	BCR	C1-C6	-2.40	1.50	1.53
22	C	507	CLA	CMB-C2B	-2.40	1.46	1.51
22	C	513	CLA	C1D-C2D	2.40	1.48	1.42
29	C	516	DGD	O3D-C3D	-2.40	1.37	1.43
22	c	510	CLA	CMB-C2B	-2.39	1.46	1.51
29	h	102	DGD	C4E-C5E	2.39	1.58	1.53
33	D	410	LHG	O3-C3	-2.39	1.35	1.44
22	c	507	CLA	C1D-C2D	2.39	1.48	1.42
22	b	606	CLA	CMD-C2D	-2.38	1.45	1.51
22	c	503	CLA	C3B-C2B	-2.38	1.37	1.40
22	C	513	CLA	CMC-C2C	-2.38	1.45	1.50
22	A	403	CLA	CMB-C2B	-2.38	1.46	1.51
26	d	406	PL9	C53-C6	-2.37	1.45	1.50
22	C	503	CLA	C4B-CHC	-2.37	1.34	1.41
22	A	402	CLA	C1D-C2D	2.37	1.47	1.42
23	d	401	PHO	C4C-C3C	2.37	1.49	1.45
22	B	616	CLA	CMD-C2D	-2.36	1.45	1.51
22	c	509	CLA	MG-NC	-2.36	2.00	2.06
24	c	516	BCR	C33-C5	-2.36	1.47	1.50
22	D	405	CLA	C4B-CHC	-2.35	1.34	1.41
22	c	504	CLA	C5-C3	-2.35	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	520	LMG	O2-C2	-2.35	1.37	1.43
22	B	610	CLA	CMD-C2D	-2.35	1.46	1.51
24	a	406	BCR	C30-C25	-2.35	1.50	1.53
27	b	623	LMG	C4-C5	2.35	1.58	1.53
27	a	415	LMG	C4-C3	2.35	1.58	1.52
22	B	606	CLA	CMC-C2C	-2.35	1.45	1.50
22	d	403	CLA	C1D-C2D	2.35	1.47	1.42
22	B	616	CLA	CMB-C2B	-2.35	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.34	1.46	1.51
22	b	609	CLA	O2D-CGD	2.34	1.38	1.33
26	d	406	PL9	C30-C29	-2.34	1.44	1.50
22	B	613	CLA	CMD-C2D	-2.33	1.46	1.51
22	B	616	CLA	CAC-C3C	-2.33	1.45	1.51
22	b	616	CLA	MG-NC	-2.33	2.00	2.06
27	c	523	LMG	O8-C9	-2.33	1.39	1.45
22	b	613	CLA	CAA-C2A	-2.33	1.49	1.54
22	c	504	CLA	MG-NC	2.33	2.11	2.06
29	c	519	DGD	O3G-C3G	-2.33	1.39	1.43
29	C	516	DGD	C4E-C3E	2.33	1.58	1.52
24	b	617	BCR	C33-C5	-2.33	1.47	1.50
22	B	605	CLA	C3B-C2B	-2.32	1.37	1.40
22	B	605	CLA	CMC-C2C	-2.32	1.45	1.50
22	c	509	CLA	C3B-C2B	-2.32	1.37	1.40
22	A	402	CLA	C5-C3	-2.32	1.46	1.51
29	c	519	DGD	C2A-C1A	-2.32	1.43	1.50
22	a	402	CLA	C1D-C2D	2.32	1.47	1.42
27	Y	101	LMG	C3-C2	2.32	1.58	1.52
22	b	605	CLA	C4B-CHC	-2.32	1.34	1.41
22	C	501	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	616	CLA	CMC-C2C	-2.32	1.45	1.50
22	B	609	CLA	C3B-CAB	-2.31	1.43	1.47
23	D	401	PHO	O2D-CGD	2.31	1.38	1.33
24	t	101	BCR	C30-C25	-2.31	1.50	1.53
22	d	404	CLA	C4B-CHC	-2.31	1.34	1.41
28	a	411	SQD	O3-C3	-2.31	1.37	1.43
22	C	508	CLA	CMC-C2C	-2.31	1.45	1.50
23	d	401	PHO	C1A-NA	2.30	1.42	1.37
22	A	405	CLA	CHC-C1C	2.30	1.40	1.35
29	c	517	DGD	C4E-C3E	2.30	1.58	1.52
22	b	610	CLA	C3B-CAB	-2.30	1.43	1.47
22	C	510	CLA	MG-NA	2.30	2.11	2.06
22	b	614	CLA	C1A-CHA	-2.30	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	CMB-C2B	-2.30	1.46	1.51
23	d	401	PHO	C1D-ND	2.30	1.43	1.38
29	C	517	DGD	C4E-C3E	2.30	1.58	1.52
29	A	413	DGD	C3G-C2G	2.29	1.57	1.50
22	b	605	CLA	CMD-C2D	-2.29	1.46	1.51
22	H	101	CLA	CMC-C2C	-2.29	1.45	1.50
29	c	519	DGD	O4E-C4E	-2.29	1.37	1.43
22	c	508	CLA	C3B-C2B	-2.29	1.37	1.40
22	C	503	CLA	C3B-CAB	-2.29	1.43	1.47
22	b	601	CLA	C1B-NB	2.29	1.37	1.35
22	b	610	CLA	CMD-C2D	-2.28	1.46	1.51
27	a	415	LMG	C14-C13	2.28	1.64	1.51
22	c	502	CLA	CMC-C2C	-2.28	1.46	1.50
22	c	505	CLA	CMC-C2C	-2.28	1.46	1.50
22	b	615	CLA	CMC-C2C	-2.28	1.46	1.50
22	b	612	CLA	CMC-C2C	-2.27	1.46	1.50
22	b	616	CLA	CHC-C1C	2.27	1.40	1.35
22	a	405	CLA	CHC-C1C	2.27	1.40	1.35
22	a	403	CLA	MG-NC	2.27	2.11	2.06
29	c	519	DGD	C1D-C2D	2.27	1.59	1.52
28	a	411	SQD	O47-C7	2.27	1.40	1.34
22	B	613	CLA	MG-NC	2.26	2.11	2.06
22	B	613	CLA	CMC-C2C	-2.26	1.46	1.50
27	c	523	LMG	O7-C8	-2.26	1.40	1.46
23	a	404	PHO	C4C-NC	2.26	1.41	1.36
27	b	623	LMG	C4-C3	2.26	1.58	1.52
22	b	613	CLA	CHC-C1C	2.25	1.40	1.35
22	C	511	CLA	CMC-C2C	-2.25	1.46	1.50
29	C	517	DGD	C3D-C2D	2.24	1.58	1.52
28	f	102	SQD	O2-C2	-2.24	1.37	1.43
24	C	514	BCR	C33-C5	-2.24	1.47	1.50
22	C	509	CLA	CMD-C2D	-2.24	1.46	1.51
22	C	511	CLA	C1D-C2D	2.23	1.47	1.42
22	a	410	CLA	MG-NC	-2.23	2.01	2.06
22	C	512	CLA	MG-NA	2.23	2.11	2.06
23	d	401	PHO	CHC-C4B	-2.23	1.35	1.40
24	T	101	BCR	C27-C26	-2.23	1.46	1.51
23	d	401	PHO	CMC-C2C	-2.22	1.46	1.50
22	d	404	CLA	CMB-C2B	-2.22	1.47	1.51
22	C	506	CLA	C3B-C2B	-2.22	1.37	1.40
22	c	503	CLA	CMC-C2C	-2.22	1.46	1.50
22	B	612	CLA	MG-NC	2.22	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	H	101	CLA	C4B-CHC	-2.22	1.34	1.41
22	D	404	CLA	O2D-CGD	2.22	1.38	1.33
22	b	608	CLA	CMB-C2B	-2.21	1.47	1.51
29	c	518	DGD	O2E-C2E	-2.21	1.37	1.43
22	c	508	CLA	C1D-C2D	2.21	1.47	1.42
24	c	516	BCR	C36-C18	-2.21	1.46	1.50
23	d	401	PHO	C1C-NC	-2.21	1.33	1.38
22	B	605	CLA	C5-C3	-2.21	1.46	1.51
27	a	415	LMG	O7-C10	2.21	1.40	1.34
22	b	602	CLA	CAC-C3C	-2.21	1.45	1.51
26	d	406	PL9	C45-C44	-2.21	1.45	1.50
22	a	405	CLA	CMB-C2B	-2.20	1.47	1.51
29	C	517	DGD	O6D-C5D	-2.20	1.39	1.44
22	B	616	CLA	C4B-CHC	-2.20	1.34	1.41
22	B	607	CLA	CMB-C2B	-2.20	1.47	1.51
22	B	603	CLA	CHC-C1C	2.20	1.40	1.35
22	B	608	CLA	C4B-CHC	-2.20	1.34	1.41
22	C	501	CLA	CMB-C2B	-2.20	1.47	1.51
22	B	605	CLA	C1D-C2D	2.19	1.47	1.42
22	D	404	CLA	C3B-CAB	-2.19	1.43	1.47
22	C	502	CLA	C3B-C2B	-2.19	1.37	1.40
23	D	401	PHO	C4C-C3C	2.19	1.49	1.45
22	c	504	CLA	CMC-C2C	-2.19	1.46	1.50
29	c	518	DGD	C6D-C5D	2.19	1.58	1.51
22	C	510	CLA	O2A-CGA	2.19	1.39	1.33
23	a	404	PHO	C1C-NC	-2.19	1.33	1.38
29	h	102	DGD	C4E-C3E	2.18	1.57	1.52
26	A	409	PL9	C31-C29	-2.18	1.46	1.51
22	B	602	CLA	OBD-CAD	2.18	1.25	1.22
22	C	510	CLA	CMC-C2C	-2.18	1.46	1.50
28	A	411	SQD	O47-C45	-2.18	1.41	1.46
22	b	601	CLA	C3B-CAB	-2.18	1.43	1.47
22	B	613	CLA	O2D-CED	-2.18	1.40	1.45
22	c	514	CLA	CMC-C2C	-2.18	1.46	1.50
29	C	516	DGD	O4E-C4E	-2.18	1.37	1.43
22	b	610	CLA	C4B-CHC	-2.18	1.34	1.41
29	H	103	DGD	O2D-C2D	-2.18	1.37	1.43
22	b	616	CLA	C3B-C2B	-2.18	1.37	1.40
22	B	613	CLA	C1C-NC	-2.17	1.34	1.37
29	h	102	DGD	O2E-C2E	-2.17	1.37	1.43
26	a	409	PL9	C18-C19	2.17	1.38	1.33
22	C	512	CLA	CMB-C2B	-2.17	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	C1B-NB	2.17	1.37	1.35
22	c	507	CLA	CMC-C2C	-2.17	1.46	1.50
22	A	402	CLA	C4B-CHC	-2.17	1.35	1.41
22	c	514	CLA	CMD-C2D	-2.17	1.46	1.51
22	c	505	CLA	C1D-C2D	2.17	1.47	1.42
27	c	520	LMG	C7-C8	2.16	1.57	1.50
22	D	405	CLA	C1D-C2D	2.16	1.47	1.42
22	C	501	CLA	CMC-C2C	-2.16	1.46	1.50
22	B	602	CLA	C1D-C2D	2.16	1.47	1.42
22	b	610	CLA	CMB-C2B	-2.16	1.47	1.51
22	c	508	CLA	CMB-C2B	-2.16	1.47	1.51
33	D	409	LHG	C3-C2	2.16	1.58	1.51
27	M	101	LMG	C9-C8	2.16	1.57	1.50
22	B	604	CLA	C1D-C2D	2.15	1.47	1.42
29	C	515	DGD	C3E-C2E	2.15	1.57	1.52
22	c	512	CLA	CMB-C2B	-2.15	1.47	1.51
23	D	401	PHO	C4B-NB	2.14	1.41	1.36
29	h	102	DGD	C1E-C2E	2.14	1.58	1.52
22	b	614	CLA	C1D-C2D	2.14	1.47	1.42
26	a	409	PL9	C3-C4	2.14	1.53	1.49
29	H	103	DGD	C1E-C2E	2.14	1.58	1.52
28	a	411	SQD	O2-C2	-2.14	1.37	1.43
28	D	408	SQD	O4-C4	-2.14	1.37	1.43
26	D	406	PL9	C26-C24	-2.14	1.46	1.51
22	c	514	CLA	CMB-C2B	-2.14	1.47	1.51
29	h	102	DGD	O3D-C3D	-2.13	1.37	1.43
22	B	604	CLA	CMB-C2B	-2.13	1.47	1.51
22	C	513	CLA	CMD-C2D	-2.13	1.46	1.51
23	a	404	PHO	C4C-C3C	2.13	1.49	1.45
33	L	102	LHG	O8-C23	2.12	1.39	1.33
22	B	604	CLA	CMD-C2D	-2.12	1.46	1.51
22	b	610	CLA	CHC-C1C	2.12	1.40	1.35
23	A	404	PHO	CMC-C2C	-2.12	1.46	1.50
22	D	403	CLA	C4B-CHC	-2.12	1.35	1.41
22	B	608	CLA	C3C-C2C	2.12	1.41	1.36
22	B	611	CLA	C3B-CAB	-2.12	1.43	1.47
22	B	604	CLA	O2A-CGA	2.12	1.39	1.33
29	A	413	DGD	O3G-C1D	2.11	1.43	1.40
22	c	514	CLA	C3B-C2B	-2.11	1.37	1.40
22	C	509	CLA	O2D-CGD	2.11	1.38	1.33
22	B	609	CLA	O2D-CGD	2.11	1.38	1.33
22	b	604	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	406	PL9	C36-C34	2.11	1.55	1.51
22	B	609	CLA	CHC-C1C	2.11	1.40	1.35
26	d	406	PL9	C21-C19	-2.11	1.46	1.51
22	C	505	CLA	C3B-CAB	-2.11	1.43	1.47
22	c	503	CLA	C1D-C2D	2.11	1.47	1.42
22	A	403	CLA	C3C-C2C	2.11	1.41	1.36
22	A	403	CLA	CAA-C2A	-2.11	1.50	1.54
22	C	507	CLA	C1D-C2D	2.10	1.47	1.42
22	B	613	CLA	C3B-CAB	-2.10	1.43	1.47
22	B	605	CLA	CMD-C2D	-2.10	1.46	1.51
22	C	505	CLA	CMC-C2C	-2.10	1.46	1.50
29	C	517	DGD	O2E-C2E	-2.10	1.38	1.43
22	c	510	CLA	C3B-CAB	-2.10	1.43	1.47
23	A	404	PHO	CMB-C2B	-2.10	1.46	1.50
29	C	515	DGD	O1G-C1G	-2.10	1.40	1.45
22	A	402	CLA	C3D-C2D	-2.10	1.35	1.39
26	D	406	PL9	C27-C28	-2.10	1.43	1.50
29	C	516	DGD	C1G-C2G	2.10	1.57	1.50
23	A	404	PHO	CHD-C4C	-2.09	1.35	1.40
22	A	405	CLA	CAC-C3C	-2.09	1.45	1.51
22	C	506	CLA	C1D-C2D	2.09	1.47	1.42
29	C	516	DGD	C4D-C3D	2.09	1.57	1.52
22	c	508	CLA	C3B-CAB	-2.09	1.43	1.47
22	B	607	CLA	CAC-C3C	-2.09	1.45	1.51
22	B	609	CLA	C1D-C2D	2.09	1.47	1.42
22	c	503	CLA	O2D-CGD	2.09	1.38	1.33
22	C	502	CLA	CMD-C2D	-2.08	1.46	1.51
22	D	405	CLA	CHC-C1C	2.08	1.40	1.35
29	C	516	DGD	O3G-C3G	-2.08	1.39	1.43
22	b	606	CLA	CMC-C2C	-2.08	1.46	1.50
24	F	101	BCR	C27-C26	-2.07	1.46	1.51
22	C	513	CLA	C4B-CHC	-2.07	1.35	1.41
27	A	410	LMG	C3-C2	2.07	1.57	1.52
22	d	404	CLA	C3B-C2B	-2.07	1.37	1.40
22	b	603	CLA	C1C-NC	-2.07	1.34	1.37
22	B	610	CLA	C1D-C2D	2.07	1.47	1.42
22	c	504	CLA	CMD-C2D	-2.07	1.46	1.51
22	H	101	CLA	C3B-CAB	-2.07	1.43	1.47
22	d	404	CLA	CMD-C2D	-2.07	1.46	1.51
22	b	613	CLA	CMC-C2C	-2.07	1.46	1.50
27	c	522	LMG	O7-C8	-2.06	1.41	1.46
29	c	519	DGD	O6D-C5D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	C5-C3	-2.06	1.47	1.51
22	C	511	CLA	C3B-C2B	-2.06	1.37	1.40
22	C	511	CLA	CMD-C2D	-2.06	1.46	1.51
24	h	101	BCR	C1-C6	-2.05	1.50	1.53
22	c	511	CLA	CMC-C2C	-2.05	1.46	1.50
22	b	611	CLA	CMD-C2D	-2.05	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.05	1.46	1.51
22	D	405	CLA	C3B-C2B	-2.05	1.37	1.40
22	C	513	CLA	C3B-C2B	-2.05	1.37	1.40
22	B	610	CLA	CMC-C2C	-2.05	1.46	1.50
22	B	608	CLA	C3B-CAB	-2.05	1.43	1.47
33	E	101	LHG	O8-C23	2.05	1.39	1.33
22	c	510	CLA	C4B-CHC	-2.04	1.35	1.41
27	D	407	LMG	O6-C5	-2.04	1.39	1.44
22	c	502	CLA	C3B-C2B	-2.04	1.37	1.40
24	k	102	BCR	C1-C6	-2.04	1.51	1.53
29	h	102	DGD	O2G-C1B	2.04	1.40	1.34
22	c	509	CLA	CMC-C2C	-2.04	1.46	1.50
29	C	515	DGD	O3G-C1D	-2.04	1.36	1.40
22	b	608	CLA	CMA-C3A	-2.04	1.48	1.53
27	D	411	LMG	O8-C28	2.03	1.39	1.33
22	A	405	CLA	CMB-C2B	-2.03	1.47	1.51
23	D	401	PHO	CMD-C2D	-2.03	1.46	1.50
22	b	602	CLA	C1D-C2D	2.03	1.47	1.42
34	f	101	HEC	C3B-C4B	2.03	1.46	1.43
28	a	411	SQD	O4-C4	-2.03	1.38	1.43
22	c	513	CLA	MG-NC	2.03	2.11	2.06
22	C	510	CLA	CMB-C2B	-2.03	1.47	1.51
22	C	505	CLA	CMB-C2B	-2.03	1.47	1.51
22	D	404	CLA	C3B-C2B	-2.03	1.37	1.40
22	c	502	CLA	CMB-C2B	-2.03	1.47	1.51
27	a	415	LMG	C7-C8	2.03	1.56	1.50
22	B	605	CLA	MG-NA	2.02	2.11	2.06
22	C	503	CLA	CMC-C2C	-2.02	1.46	1.50
22	b	603	CLA	CHC-C1C	2.02	1.40	1.35
22	b	613	CLA	C4B-CHC	-2.02	1.35	1.41
22	C	507	CLA	C3C-C2C	2.02	1.41	1.36
22	C	509	CLA	O2A-CGA	2.01	1.39	1.33
22	B	607	CLA	C1D-C2D	2.01	1.47	1.42
27	b	623	LMG	C3-C2	2.01	1.57	1.52
22	C	503	CLA	CMD-C2D	-2.01	1.46	1.51
22	A	403	CLA	C5-C3	-2.01	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	CMC-C2C	-2.01	1.46	1.50
29	C	515	DGD	O6D-C5D	-2.01	1.39	1.44
22	B	610	CLA	CMA-C3A	-2.01	1.48	1.53
22	c	512	CLA	C1C-C2C	2.01	1.48	1.44
22	d	404	CLA	C3B-CAB	-2.01	1.43	1.47
22	B	607	CLA	C3B-C2B	-2.00	1.37	1.40
27	d	410	LMG	O1-C7	-2.00	1.40	1.43
22	A	405	CLA	C1D-C2D	2.00	1.47	1.42
29	C	515	DGD	C1G-C2G	2.00	1.56	1.50
22	c	502	CLA	C1D-C2D	2.00	1.47	1.42
24	K	102	BCR	C38-C26	-2.00	1.47	1.50
22	c	504	CLA	MG-NA	2.00	2.11	2.06

All (1351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	101	SQD	O6-C1-C2	10.32	124.41	108.30
28	a	411	SQD	O6-C1-C2	9.80	123.61	108.30
22	b	604	CLA	C4A-NA-C1A	9.48	110.97	106.71
22	b	611	CLA	C4A-NA-C1A	9.46	110.96	106.71
22	c	510	CLA	C4A-NA-C1A	9.26	110.87	106.71
22	C	507	CLA	C4A-NA-C1A	8.60	110.57	106.71
22	c	512	CLA	C4A-NA-C1A	8.30	110.44	106.71
22	B	604	CLA	C4A-NA-C1A	8.26	110.42	106.71
22	c	504	CLA	C4A-NA-C1A	8.14	110.37	106.71
28	f	102	SQD	O9-S-C6	7.89	116.32	106.94
22	b	606	CLA	C4A-NA-C1A	7.86	110.24	106.71
22	B	616	CLA	C4A-NA-C1A	7.85	110.23	106.71
22	C	508	CLA	C4A-NA-C1A	7.73	110.18	106.71
22	H	101	CLA	C4A-NA-C1A	7.72	110.18	106.71
22	B	605	CLA	C4A-NA-C1A	7.56	110.10	106.71
22	C	511	CLA	C4A-NA-C1A	7.44	110.05	106.71
22	C	513	CLA	C4A-NA-C1A	7.40	110.03	106.71
22	c	502	CLA	C4A-NA-C1A	7.34	110.00	106.71
34	f	101	HEC	CBD-CAD-C3D	-7.16	99.27	112.49
28	L	101	SQD	O7-S-C6	7.16	115.45	106.94
22	c	511	CLA	C4A-NA-C1A	6.92	109.82	106.71
22	c	503	CLA	C4A-NA-C1A	6.86	109.79	106.71
22	B	606	CLA	C4A-NA-C1A	6.78	109.75	106.71
28	A	411	SQD	O6-C1-C2	6.71	118.78	108.30
26	a	409	PL9	C7-C3-C4	6.66	122.29	116.88
22	D	404	CLA	C4A-NA-C1A	6.66	109.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	609	CLA	C4A-NA-C1A	6.66	109.70	106.71
26	d	406	PL9	C7-C3-C4	6.62	122.26	116.88
22	a	410	CLA	C4A-NA-C1A	6.61	109.68	106.71
22	a	403	CLA	C4A-NA-C1A	6.60	109.67	106.71
28	D	408	SQD	O9-S-C6	6.51	114.67	106.94
22	C	503	CLA	C4A-NA-C1A	6.50	109.63	106.71
22	C	501	CLA	C4A-NA-C1A	6.21	109.50	106.71
28	a	411	SQD	O9-S-C6	6.12	114.22	106.94
28	B	622	SQD	O6-C1-C2	6.05	117.75	108.30
22	b	601	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	c	505	CLA	CMB-C2B-C1B	-6.02	119.22	128.46
22	B	607	CLA	C4A-NA-C1A	5.98	109.39	106.71
22	C	505	CLA	C4A-NA-C1A	5.90	109.36	106.71
22	b	615	CLA	C4A-NA-C1A	5.90	109.36	106.71
22	a	402	CLA	C4A-NA-C1A	5.85	109.34	106.71
22	c	513	CLA	C4A-NA-C1A	5.82	109.32	106.71
22	A	402	CLA	C4A-NA-C1A	5.75	109.29	106.71
22	D	403	CLA	C4A-NA-C1A	5.55	109.20	106.71
22	b	616	CLA	O2D-CGD-O1D	-5.55	112.99	123.84
22	c	502	CLA	O2D-CGD-O1D	-5.54	113.01	123.84
22	B	603	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
22	B	615	CLA	C4A-NA-C1A	5.38	109.12	106.71
22	b	616	CLA	C4A-NA-C1A	5.37	109.12	106.71
27	a	415	LMG	C1-C2-C3	-5.36	98.83	110.00
28	a	412	SQD	O47-C7-C8	5.35	123.03	111.50
27	b	623	LMG	O1-C1-C2	-5.33	99.98	108.30
22	B	608	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
22	B	602	CLA	C4A-NA-C1A	5.19	109.04	106.71
22	b	616	CLA	CMB-C2B-C1B	-5.17	120.51	128.46
22	b	604	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
22	a	402	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
22	b	616	CLA	CMB-C2B-C3B	5.14	134.29	124.68
22	B	608	CLA	C4A-NA-C1A	5.12	109.01	106.71
22	A	405	CLA	C4A-NA-C1A	5.08	108.99	106.71
22	b	605	CLA	C4A-NA-C1A	5.05	108.98	106.71
29	H	103	DGD	O3G-C3G-C2G	-5.03	98.76	110.90
22	b	603	CLA	C4A-NA-C1A	5.00	108.95	106.71
22	c	508	CLA	C4A-NA-C1A	4.99	108.95	106.71
22	B	612	CLA	CMB-C2B-C1B	-4.98	120.82	128.46
22	a	405	CLA	C4A-NA-C1A	4.98	108.94	106.71
22	b	613	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	A	409	PL9	C7-C3-C4	4.88	120.84	116.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	C4D-C3D-CAD	-4.84	105.77	108.47
22	B	608	CLA	CMB-C2B-C3B	4.76	133.59	124.68
22	B	616	CLA	C4D-C3D-CAD	-4.75	105.82	108.47
28	D	408	SQD	O6-C1-C2	4.74	115.71	108.30
22	b	615	CLA	CMB-C2B-C1B	-4.74	121.18	128.46
22	b	613	CLA	CMB-C2B-C1B	-4.73	121.19	128.46
34	F	102	HEC	CBD-CAD-C3D	-4.69	103.84	112.49
22	c	509	CLA	C4A-NA-C1A	4.68	108.81	106.71
22	c	502	CLA	O2D-CGD-CBD	4.67	119.56	111.27
28	L	101	SQD	C1-C2-C3	-4.65	100.31	110.00
22	b	602	CLA	C4A-NA-C1A	4.65	108.80	106.71
26	D	406	PL9	C7-C3-C4	4.64	120.64	116.88
28	B	622	SQD	O7-S-C6	4.63	112.44	106.94
22	B	602	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
29	C	517	DGD	O3G-C3G-C2G	-4.56	99.89	110.90
22	b	608	CLA	C4A-NA-C1A	4.56	108.75	106.71
22	B	612	CLA	CMB-C2B-C3B	4.54	133.18	124.68
22	b	612	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
22	C	507	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
22	c	505	CLA	C4A-NA-C1A	4.53	108.74	106.71
22	b	612	CLA	CMD-C2D-C3D	4.52	133.14	124.68
22	B	604	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
22	c	505	CLA	CMB-C2B-C3B	4.48	133.05	124.68
22	B	613	CLA	C4A-NA-C1A	4.47	108.71	106.71
22	C	502	CLA	C4A-NA-C1A	4.46	108.71	106.71
29	C	516	DGD	O3G-C3G-C2G	-4.44	100.19	110.90
22	D	403	CLA	CMD-C2D-C3D	4.44	132.98	124.68
22	B	603	CLA	CMB-C2B-C3B	4.42	132.95	124.68
22	C	506	CLA	C4A-NA-C1A	4.42	108.69	106.71
22	b	604	CLA	CMB-C2B-C3B	4.37	132.85	124.68
22	B	611	CLA	O2D-CGD-O1D	-4.36	115.31	123.84
22	c	507	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
22	b	611	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
22	C	510	CLA	C4A-NA-C1A	4.32	108.65	106.71
22	c	514	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
22	B	613	CLA	C1-C2-C3	-4.31	118.59	126.04
28	f	102	SQD	O6-C1-C2	4.31	115.03	108.30
22	b	616	CLA	O1D-CGD-CBD	4.30	133.28	124.48
28	B	622	SQD	O47-C7-C8	4.28	120.73	111.50
22	C	506	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
22	c	506	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
22	A	405	CLA	CMB-C2B-C1B	-4.25	121.94	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	O2D-CGD-O1D	-4.24	115.54	123.84
33	E	101	LHG	O4-P-O5	4.24	133.19	112.24
22	B	605	CLA	O2D-CGD-O1D	-4.24	115.55	123.84
28	A	411	SQD	C1-C2-C3	-4.22	101.21	110.00
22	c	506	CLA	CMD-C2D-C3D	4.21	132.56	124.68
34	v	201	HEC	CBD-CAD-C3D	-4.20	104.73	112.49
29	A	413	DGD	O3G-C3G-C2G	-4.19	100.79	110.90
34	F	102	HEC	CBA-CAA-C2A	-4.17	104.80	112.48
22	B	610	CLA	C4A-NA-C1A	4.16	108.58	106.71
22	B	611	CLA	O2D-CGD-CBD	4.16	118.66	111.27
22	B	602	CLA	O2D-CGD-CBD	4.16	118.66	111.27
33	D	410	LHG	O4-P-O5	4.16	132.79	112.24
22	C	509	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
22	B	605	CLA	OBD-CAD-CBD	-4.12	120.01	125.89
22	B	612	CLA	C11-C12-C13	-4.12	102.61	115.92
24	T	101	BCR	C7-C8-C9	-4.12	120.02	126.23
27	b	623	LMG	C1-O6-C5	-4.11	105.62	113.69
22	d	403	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
22	A	403	CLA	O2D-CGD-O1D	-4.10	115.83	123.84
22	C	510	CLA	CMB-C2B-C3B	4.10	132.34	124.68
22	B	614	CLA	C4D-C3D-CAD	-4.09	106.19	108.47
29	c	519	DGD	O3G-C3G-C2G	-4.09	101.03	110.90
33	e	101	LHG	O4-P-O5	4.08	132.42	112.24
28	D	408	SQD	O8-S-C6	4.08	112.24	105.74
28	f	102	SQD	O9-S-O7	-4.08	99.84	113.95
33	L	102	LHG	O4-P-O5	4.08	132.40	112.24
22	c	506	CLA	C4A-NA-C1A	4.07	108.54	106.71
22	b	605	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
22	A	402	CLA	CHB-C4A-NA	4.06	130.13	124.51
33	d	407	LHG	O4-P-O5	4.06	132.30	112.24
22	C	508	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
22	b	605	CLA	C4D-C3D-CAD	-4.05	106.21	108.47
22	b	603	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
22	A	405	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
22	C	507	CLA	CMB-C2B-C3B	4.03	132.21	124.68
22	b	609	CLA	CMB-C2B-C1B	-4.01	122.29	128.46
22	b	611	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
22	b	612	CLA	C4D-C3D-CAD	-4.01	106.24	108.47
22	C	504	CLA	C4D-C3D-CAD	-4.00	106.24	108.47
29	C	515	DGD	O6D-C1D-O3G	-4.00	100.50	109.97
28	A	412	SQD	O47-C7-C8	4.00	120.11	111.50
22	D	403	CLA	CMB-C2B-C1B	-3.97	122.37	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	O2D-CGD-O1D	-3.96	116.10	123.84
22	b	612	CLA	C1B-CHB-C4A	-3.94	122.31	130.12
22	b	604	CLA	CMD-C2D-C3D	3.94	132.05	124.68
26	D	406	PL9	C36-C34-C33	-3.93	113.17	121.12
33	d	408	LHG	O4-P-O5	3.93	131.66	112.24
22	H	101	CLA	CAA-CBA-CGA	-3.93	101.78	113.25
28	B	622	SQD	O8-S-C6	3.92	111.98	105.74
28	B	622	SQD	C1-O5-C5	-3.92	106.00	113.69
28	a	412	SQD	O48-C23-C24	3.91	124.18	111.91
22	C	510	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
22	C	503	CLA	O2A-C1-C2	-3.89	98.41	108.64
22	b	613	CLA	CMD-C2D-C3D	3.89	131.95	124.68
22	C	505	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
28	B	622	SQD	O5-C5-C4	3.88	116.75	109.69
22	C	501	CLA	OBD-CAD-CBD	-3.88	120.34	125.89
29	C	515	DGD	O3G-C3G-C2G	-3.88	101.54	110.90
22	B	611	CLA	OBD-CAD-CBD	-3.87	120.36	125.89
23	d	401	PHO	O1D-CGD-CBD	3.87	132.41	124.48
22	b	607	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
22	b	604	CLA	C4D-C3D-CAD	-3.85	106.32	108.47
22	C	502	CLA	C4D-C3D-CAD	-3.85	106.32	108.47
22	c	508	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
28	a	411	SQD	C1-O5-C5	-3.84	106.14	113.69
22	b	602	CLA	O2D-CGD-CBD	3.84	118.10	111.27
26	d	406	PL9	C41-C39-C38	-3.84	113.34	121.12
22	B	608	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
24	B	619	BCR	C2-C1-C6	3.84	116.39	110.48
33	d	407	LHG	O8-C23-C24	3.83	123.94	111.91
22	c	510	CLA	CHB-C4A-NA	3.83	129.81	124.51
22	d	404	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
22	C	504	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
33	d	409	LHG	O4-P-O5	3.81	131.08	112.24
26	a	409	PL9	C7-C3-C2	-3.81	118.29	123.30
22	c	511	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
22	c	504	CLA	C4D-C3D-CAD	-3.80	106.35	108.47
26	d	406	PL9	C22-C23-C24	-3.80	118.51	127.66
22	c	512	CLA	C4D-C3D-CAD	-3.80	106.35	108.47
29	c	517	DGD	O3G-C3G-C2G	-3.78	101.77	110.90
24	b	618	BCR	C35-C13-C14	-3.78	117.62	122.92
28	L	101	SQD	O2-C2-C1	3.78	119.22	110.05
22	C	505	CLA	C1D-CHD-C4C	3.77	127.53	122.56
28	A	411	SQD	O8-S-C6	3.77	111.75	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	l	101	LHG	O4-P-O5	3.76	130.85	112.24
22	B	612	CLA	C4A-NA-C1A	3.76	108.40	106.71
22	b	605	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
22	b	612	CLA	CMB-C2B-C3B	3.76	131.71	124.68
22	c	503	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
33	D	409	LHG	O4-P-O5	3.75	130.76	112.24
28	f	102	SQD	O5-C5-C4	3.74	116.48	109.69
24	K	101	BCR	C15-C16-C17	-3.73	115.83	123.47
28	a	411	SQD	O9-S-O7	-3.73	101.05	113.95
33	d	407	LHG	O8-C23-O10	-3.72	114.19	123.59
26	d	406	PL9	C7-C3-C2	-3.72	118.41	123.30
22	C	512	CLA	CHB-C4A-NA	3.72	129.66	124.51
22	c	508	CLA	CMB-C2B-C3B	3.72	131.64	124.68
33	D	412	LHG	O4-P-O5	3.72	130.63	112.24
22	D	404	CLA	CHB-C4A-NA	3.71	129.65	124.51
22	a	405	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
22	b	614	CLA	CMB-C2B-C3B	3.71	131.62	124.68
22	B	606	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
24	b	617	BCR	C2-C1-C6	3.70	116.17	110.48
27	a	415	LMG	O6-C1-C2	-3.69	102.55	110.35
22	c	506	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
22	C	501	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
22	C	502	CLA	CMD-C2D-C3D	3.68	131.56	124.68
22	d	404	CLA	CMB-C2B-C3B	3.67	131.55	124.68
22	b	606	CLA	CMD-C2D-C3D	3.67	131.55	124.68
22	b	603	CLA	C1B-CHB-C4A	-3.67	122.85	130.12
22	c	514	CLA	CMB-C2B-C3B	3.66	131.52	124.68
22	c	507	CLA	CMB-C2B-C3B	3.66	131.52	124.68
22	B	610	CLA	C1B-CHB-C4A	-3.65	122.88	130.12
28	a	411	SQD	C1-C2-C3	-3.65	102.39	110.00
23	d	401	PHO	O2D-CGD-O1D	-3.65	116.69	123.84
22	B	607	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
22	C	503	CLA	C7-C6-C5	-3.65	103.45	113.36
22	b	608	CLA	C4D-C3D-CAD	-3.65	106.44	108.47
22	c	506	CLA	C4D-C3D-CAD	-3.64	106.44	108.47
22	b	604	CLA	OBD-CAD-CBD	-3.64	120.69	125.89
22	b	607	CLA	C4A-NA-C1A	3.64	108.34	106.71
29	c	518	DGD	O3G-C3G-C2G	-3.64	102.12	110.90
22	a	402	CLA	CMB-C2B-C3B	3.63	131.47	124.68
28	L	101	SQD	O48-C23-C24	3.62	123.26	111.91
22	b	614	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	D	401	PHO	CMB-C2B-C1B	-3.61	119.51	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	411	SQD	O47-C7-O49	-3.61	114.99	123.70
22	B	604	CLA	CMB-C2B-C3B	3.60	131.41	124.68
24	b	618	BCR	C36-C18-C17	-3.59	117.89	122.92
22	B	613	CLA	C4-C3-C5	3.59	121.31	115.27
22	C	506	CLA	CMD-C2D-C3D	3.59	131.39	124.68
22	C	508	CLA	C4D-C3D-CAD	-3.58	106.47	108.47
22	C	513	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
34	F	102	HEC	C1D-C2D-C3D	3.58	109.49	107.00
28	a	411	SQD	O7-S-C6	3.58	111.19	106.94
22	b	613	CLA	CMB-C2B-C3B	3.58	131.37	124.68
28	B	622	SQD	C3-C4-C5	3.58	116.62	110.24
22	C	509	CLA	CMB-C2B-C3B	3.57	131.37	124.68
22	A	403	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
22	b	608	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
22	c	509	CLA	CHB-C4A-NA	3.56	129.44	124.51
34	v	201	HEC	CBA-CAA-C2A	-3.56	105.92	112.48
22	A	405	CLA	CMB-C2B-C3B	3.55	131.32	124.68
22	b	601	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
22	c	510	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
22	b	609	CLA	OBD-CAD-CBD	-3.54	120.83	125.89
22	B	602	CLA	CHB-C4A-NA	3.54	129.41	124.51
22	b	606	CLA	O2D-CGD-CBD	3.53	117.55	111.27
22	a	410	CLA	C4D-C3D-CAD	-3.53	106.50	108.47
24	A	406	BCR	C27-C26-C25	3.52	127.84	122.73
22	b	605	CLA	C1-C2-C3	-3.52	119.96	126.04
22	b	607	CLA	C4-C3-C5	3.52	121.19	115.27
22	C	504	CLA	C4A-NA-C1A	3.51	108.29	106.71
22	b	614	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
22	c	502	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
22	C	509	CLA	C4A-NA-C1A	3.50	108.28	106.71
22	C	512	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
22	H	101	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
24	K	101	BCR	C2-C1-C6	3.49	115.85	110.48
22	b	603	CLA	O2D-CGD-CBD	3.48	117.46	111.27
28	A	411	SQD	C1-O5-C5	-3.48	106.85	113.69
22	C	507	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
22	c	510	CLA	O2A-CGA-O1A	-3.48	114.81	123.59
34	V	201	HEC	CMC-C2C-C1C	-3.46	123.14	128.46
22	C	506	CLA	OBD-CAD-CBD	-3.46	120.95	125.89
22	B	608	CLA	O2D-CGD-CBD	3.46	117.41	111.27
22	b	607	CLA	C6-C7-C8	-3.45	104.75	115.92
26	A	409	PL9	C35-C34-C36	3.45	121.07	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
28	L	101	SQD	O9-S-O7	-3.44	102.03	113.95
22	C	501	CLA	O2D-CGD-CBD	3.44	117.38	111.27
26	D	406	PL9	C50-C49-C48	-3.44	112.71	122.65
22	C	513	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
24	K	101	BCR	C11-C10-C9	-3.44	122.41	127.31
22	B	614	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
22	b	616	CLA	CHB-C4A-NA	3.43	129.26	124.51
28	A	411	SQD	O47-C7-C8	3.43	118.90	111.50
22	c	510	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
22	b	610	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
22	c	511	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
24	F	101	BCR	C28-C27-C26	-3.42	107.97	114.08
22	B	613	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
34	V	201	HEC	CBD-CAD-C3D	-3.42	106.18	112.49
22	b	612	CLA	C11-C12-C13	-3.42	104.87	115.92
26	d	406	PL9	C36-C34-C33	-3.42	114.20	121.12
22	b	611	CLA	O2D-CGD-CBD	3.42	117.34	111.27
22	B	606	CLA	O2A-CGA-O1A	-3.41	114.98	123.59
29	C	516	DGD	O2D-C2D-C1D	-3.40	101.78	110.05
22	b	610	CLA	C4A-NA-C1A	3.40	108.23	106.71
22	c	506	CLA	C1D-CHD-C4C	3.40	127.04	122.56
22	c	514	CLA	O2D-CGD-O1D	-3.39	117.20	123.84
22	b	613	CLA	C4D-C3D-CAD	-3.39	106.58	108.47
22	a	410	CLA	CHB-C4A-NA	3.38	129.19	124.51
26	d	406	PL9	C35-C34-C36	3.38	120.96	115.27
22	B	602	CLA	CMB-C2B-C3B	3.37	130.98	124.68
22	B	614	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
22	B	615	CLA	O2D-CGD-CBD	3.37	117.25	111.27
24	t	101	BCR	C7-C8-C9	-3.36	121.15	126.23
22	C	508	CLA	CMB-C2B-C3B	3.36	130.97	124.68
24	b	619	BCR	C29-C30-C25	3.36	115.66	110.48
22	C	512	CLA	C4A-NA-C1A	3.36	108.22	106.71
22	D	403	CLA	C6-C5-C3	3.36	122.27	113.45
22	D	405	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
22	a	405	CLA	CMD-C2D-C3D	3.36	130.96	124.68
22	c	510	CLA	CMB-C2B-C3B	3.35	130.95	124.68
22	B	605	CLA	CMD-C2D-C3D	3.35	130.95	124.68
22	c	513	CLA	CMD-C2D-C3D	3.35	130.94	124.68
22	b	603	CLA	CMB-C2B-C3B	3.34	130.93	124.68
22	b	615	CLA	CMB-C2B-C3B	3.34	130.92	124.68
22	d	403	CLA	CMB-C2B-C3B	3.34	130.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C1D-CHD-C4C	3.33	126.95	122.56
29	H	103	DGD	O2D-C2D-C1D	-3.33	101.97	110.05
24	K	101	BCR	C33-C5-C6	-3.32	120.80	124.53
22	c	503	CLA	CMB-C2B-C3B	3.32	130.89	124.68
26	D	406	PL9	C22-C23-C24	-3.32	119.67	127.66
24	B	617	BCR	C2-C1-C6	3.31	115.58	110.48
23	a	404	PHO	C1-C2-C3	-3.31	120.32	126.04
27	b	621	LMG	O3-C3-C2	-3.31	102.71	110.35
22	H	101	CLA	O2D-CGD-CBD	3.30	117.14	111.27
22	B	606	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
22	a	403	CLA	CMD-C2D-C3D	3.30	130.85	124.68
22	C	507	CLA	O2D-CGD-CBD	3.30	117.13	111.27
22	b	616	CLA	C1B-CHB-C4A	-3.28	123.61	130.12
22	a	402	CLA	CMD-C2D-C3D	3.28	130.82	124.68
24	B	618	BCR	C29-C30-C25	3.28	115.53	110.48
22	B	615	CLA	CHB-C4A-NA	3.28	129.04	124.51
22	b	606	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
22	B	603	CLA	OBD-CAD-CBD	-3.27	121.23	125.89
22	C	506	CLA	O2D-CGD-O1D	-3.26	117.45	123.84
22	c	513	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
22	C	506	CLA	CMB-C2B-C3B	3.25	130.76	124.68
22	B	611	CLA	C14-C13-C15	-3.25	99.53	111.29
22	C	501	CLA	OBD-CAD-C3D	3.25	133.38	127.98
22	D	403	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
28	L	101	SQD	O9-S-C6	3.23	110.77	106.94
22	D	403	CLA	CHB-C4A-NA	3.23	128.97	124.51
22	A	405	CLA	C4-C3-C5	3.22	120.68	115.27
22	a	405	CLA	OBD-CAD-CBD	-3.21	121.30	125.89
22	a	405	CLA	CMB-C2B-C3B	3.21	130.68	124.68
29	c	517	DGD	C3D-C4D-C5D	-3.20	104.52	110.24
29	C	516	DGD	O5D-C6D-C5D	-3.20	103.12	109.05
22	c	504	CLA	CMD-C2D-C3D	3.20	130.67	124.68
22	c	508	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
26	A	409	PL9	C36-C34-C33	-3.19	114.65	121.12
27	M	101	LMG	O6-C1-O1	-3.19	102.41	109.97
22	b	608	CLA	OBD-CAD-CBD	-3.19	121.33	125.89
22	a	410	CLA	CMD-C2D-C3D	3.19	130.65	124.68
22	c	509	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
23	d	401	PHO	C1B-NB-C4B	3.19	112.52	106.51
22	c	509	CLA	C4D-C3D-CAD	-3.18	106.70	108.47
22	c	512	CLA	OBD-CAD-CBD	-3.18	121.35	125.89
22	B	614	CLA	C1B-CHB-C4A	-3.18	123.83	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	410	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
22	D	403	CLA	CMB-C2B-C3B	3.17	130.61	124.68
33	D	412	LHG	O8-C23-O10	-3.17	115.59	123.59
22	c	512	CLA	C1D-CHD-C4C	3.17	126.74	122.56
22	B	615	CLA	C1D-CHD-C4C	3.17	126.74	122.56
22	a	405	CLA	CHB-C4A-NA	3.17	128.89	124.51
22	b	612	CLA	CHB-C4A-NA	3.16	128.89	124.51
22	B	610	CLA	CMD-C2D-C3D	3.16	130.60	124.68
29	C	517	DGD	O3E-C3E-C2E	-3.16	103.04	110.35
22	C	504	CLA	OBD-CAD-CBD	-3.16	121.38	125.89
22	B	611	CLA	C1D-CHD-C4C	3.16	126.73	122.56
22	D	405	CLA	C4A-NA-C1A	3.16	108.13	106.71
22	b	601	CLA	CHB-C4A-NA	3.16	128.88	124.51
22	b	611	CLA	C4D-C3D-CAD	-3.16	106.71	108.47
22	D	404	CLA	C1D-CHD-C4C	3.16	126.72	122.56
22	C	505	CLA	CMB-C2B-C3B	3.16	130.58	124.68
22	A	405	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
22	B	611	CLA	CMD-C2D-C3D	3.15	130.58	124.68
22	B	604	CLA	OBD-CAD-CBD	-3.15	121.39	125.89
29	C	517	DGD	O6D-C1D-O3G	-3.15	102.52	109.97
24	h	101	BCR	C27-C26-C25	3.14	127.30	122.73
22	B	610	CLA	CHB-C4A-NA	3.14	128.86	124.51
22	B	604	CLA	C1-C2-C3	-3.14	120.61	126.04
26	A	409	PL9	C7-C3-C2	-3.14	119.17	123.30
22	a	405	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
29	h	102	DGD	C3D-C4D-C5D	-3.14	104.65	110.24
22	C	506	CLA	O1D-CGD-CBD	3.14	130.90	124.48
29	A	413	DGD	C4E-C3E-C2E	-3.13	105.35	110.82
29	h	102	DGD	O3G-C3G-C2G	-3.13	103.35	110.90
22	b	612	CLA	OBD-CAD-CBD	-3.13	121.43	125.89
22	B	616	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
22	c	504	CLA	CHB-C4A-NA	3.12	128.83	124.51
34	f	101	HEC	CBA-CAA-C2A	-3.12	106.73	112.48
22	b	606	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
22	B	611	CLA	OBD-CAD-C3D	3.12	133.16	127.98
28	B	622	SQD	O48-C23-C24	3.12	121.69	111.91
22	b	608	CLA	CMB-C2B-C3B	3.12	130.51	124.68
22	B	602	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
22	D	403	CLA	C4-C3-C5	3.10	120.48	115.27
33	D	412	LHG	O8-C23-C24	3.10	121.63	111.91
22	A	402	CLA	CAA-CBA-CGA	-3.10	104.20	113.25
34	v	201	HEC	CMC-C2C-C1C	-3.10	123.70	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	615	CLA	C1-C2-C3	3.09	131.40	126.04
22	B	605	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
22	B	607	CLA	CMB-C2B-C3B	3.09	130.47	124.68
26	d	406	PL9	C30-C29-C31	-3.09	110.07	115.27
29	A	413	DGD	O5E-C6E-C5E	-3.09	100.69	111.29
28	L	101	SQD	O47-C7-C8	3.09	118.16	111.50
24	c	516	BCR	C27-C26-C25	3.08	127.20	122.73
22	b	602	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
26	D	406	PL9	C37-C38-C39	-3.08	120.25	127.66
22	c	513	CLA	CHB-C4A-NA	3.08	128.77	124.51
24	B	619	BCR	C36-C18-C17	-3.08	118.61	122.92
29	c	519	DGD	C3G-C2G-C1G	-3.07	104.52	111.79
29	A	413	DGD	O5D-C6D-C5D	-3.07	103.36	109.05
27	b	623	LMG	O2-C2-C1	-3.07	102.58	110.05
26	D	406	PL9	C35-C34-C36	3.07	120.44	115.27
27	D	407	LMG	O6-C1-O1	-3.07	102.70	109.97
22	c	513	CLA	CMB-C2B-C3B	3.07	130.42	124.68
22	c	504	CLA	C7-C6-C5	-3.06	105.06	113.36
22	A	403	CLA	CMB-C2B-C3B	3.06	130.40	124.68
22	b	605	CLA	CMB-C2B-C3B	3.06	130.39	124.68
22	C	502	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
22	C	508	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
22	C	512	CLA	CMB-C2B-C3B	3.05	130.38	124.68
22	c	511	CLA	C6-C5-C3	-3.05	105.46	113.45
29	C	515	DGD	O5D-C6D-C5D	-3.05	103.40	109.05
29	C	516	DGD	O6E-C1E-O5D	-3.05	102.76	109.97
24	d	405	BCR	C38-C26-C25	-3.05	121.11	124.53
22	b	614	CLA	O2A-CGA-O1A	-3.05	115.91	123.59
22	C	509	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
26	a	409	PL9	C35-C34-C36	3.04	120.38	115.27
22	B	604	CLA	CHB-C4A-NA	3.04	128.71	124.51
24	k	102	BCR	C2-C1-C6	3.04	115.15	110.48
22	a	403	CLA	CAC-C3C-C4C	3.04	128.75	124.81
22	a	405	CLA	O2D-CGD-CBD	3.03	116.66	111.27
22	b	608	CLA	CMD-C2D-C3D	3.03	130.34	124.68
24	F	101	BCR	C7-C8-C9	-3.02	121.67	126.23
22	C	513	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	B	614	CLA	CMB-C2B-C3B	3.02	130.33	124.68
22	c	504	CLA	C5-C3-C2	-3.02	115.01	121.12
22	C	509	CLA	C1-C2-C3	-3.02	120.83	126.04
22	b	611	CLA	CMB-C2B-C3B	3.02	130.32	124.68
29	C	517	DGD	O6D-C5D-C6D	-3.02	100.58	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	CMD-C2D-C3D	3.01	130.31	124.68
22	b	602	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
22	c	514	CLA	CMD-C2D-C3D	3.01	130.30	124.68
22	C	504	CLA	O2A-CGA-O1A	-3.00	116.01	123.59
24	T	101	BCR	C27-C26-C25	3.00	127.09	122.73
22	B	612	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
27	d	410	LMG	O6-C1-O1	-3.00	102.87	109.97
34	f	101	HEC	CAD-CBD-CGD	3.00	117.70	112.67
22	B	604	CLA	C11-C10-C8	-3.00	106.23	115.92
29	c	519	DGD	C3D-C4D-C5D	-2.99	104.90	110.24
27	a	415	LMG	C9-C8-C7	-2.99	104.72	111.79
22	c	502	CLA	CMD-C2D-C3D	2.99	130.27	124.68
22	b	606	CLA	CHB-C4A-NA	2.99	128.64	124.51
22	c	511	CLA	CHB-C4A-NA	2.98	128.64	124.51
27	c	523	LMG	O6-C1-O1	-2.98	102.91	109.97
22	b	609	CLA	CMB-C2B-C3B	2.98	130.26	124.68
22	D	404	CLA	CMB-C2B-C3B	2.98	130.25	124.68
22	b	605	CLA	CMD-C2D-C3D	2.97	130.24	124.68
28	a	411	SQD	O5-C1-C2	-2.97	104.06	110.35
22	b	616	CLA	CMD-C2D-C3D	2.97	130.24	124.68
27	Y	101	LMG	O1-C1-C2	-2.97	103.67	108.30
22	C	512	CLA	O2D-CGD-CBD	2.97	116.54	111.27
29	h	102	DGD	O6E-C5E-C4E	2.97	115.08	109.69
22	c	506	CLA	C6-C7-C8	-2.96	106.35	115.92
27	a	415	LMG	O6-C5-C4	2.96	115.06	109.69
22	B	607	CLA	CED-O2D-CGD	2.96	122.62	115.94
22	b	613	CLA	CAC-C3C-C4C	2.95	128.64	124.81
22	b	605	CLA	C4-C3-C5	2.95	120.24	115.27
24	B	617	BCR	C3-C4-C5	-2.95	108.81	114.08
24	c	515	BCR	C24-C23-C22	-2.95	121.78	126.23
27	b	623	LMG	C8-O7-C10	2.95	125.04	117.79
24	b	617	BCR	C29-C30-C25	2.95	115.02	110.48
22	B	605	CLA	O1D-CGD-CBD	2.94	130.50	124.48
22	c	506	CLA	CMB-C2B-C3B	2.94	130.18	124.68
22	B	602	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
24	F	101	BCR	C24-C23-C22	-2.94	121.79	126.23
22	b	610	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
22	B	616	CLA	CMD-C2D-C3D	2.94	130.18	124.68
28	L	101	SQD	O5-C1-C2	-2.94	104.13	110.35
27	c	520	LMG	O3-C3-C2	-2.94	103.56	110.35
27	b	621	LMG	O1-C1-C2	-2.93	103.72	108.30
22	C	504	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	CHA-C1A-NA	-2.93	119.69	126.40
26	D	406	PL9	C31-C32-C33	-2.93	102.25	111.88
29	A	413	DGD	O6E-C5E-C4E	2.93	115.02	109.69
26	A	409	PL9	C22-C23-C24	-2.93	120.61	127.66
22	b	611	CLA	C1D-CHD-C4C	2.92	126.42	122.56
27	M	101	LMG	C1-O6-C5	-2.92	107.96	113.69
22	A	403	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
22	b	609	CLA	C4A-NA-C1A	2.92	108.02	106.71
22	a	403	CLA	C4D-C3D-CAD	-2.92	106.84	108.47
22	d	404	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
22	B	611	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
22	C	508	CLA	C1D-CHD-C4C	2.91	126.40	122.56
22	b	602	CLA	CMB-C2B-C3B	2.91	130.12	124.68
22	C	501	CLA	O2A-CGA-O1A	-2.91	116.26	123.59
29	c	517	DGD	CBB-CAB-C9B	-2.90	99.68	114.42
28	f	102	SQD	O47-C7-C8	2.90	118.90	110.80
22	C	507	CLA	C4-C3-C5	2.90	120.15	115.27
22	B	613	CLA	CMB-C2B-C3B	2.90	130.10	124.68
28	L	101	SQD	C3-C4-C5	2.90	115.41	110.24
28	A	412	SQD	O48-C23-C24	2.90	121.00	111.91
23	D	401	PHO	C1-C2-C3	-2.90	121.03	126.04
22	B	611	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
22	b	601	CLA	CMB-C2B-C3B	2.89	130.09	124.68
22	B	612	CLA	C16-C15-C13	-2.89	106.57	115.92
22	B	606	CLA	CGD-CBD-CAD	-2.89	101.37	110.73
22	b	610	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	A	406	BCR	C37-C22-C21	-2.89	118.88	122.92
22	b	614	CLA	CHB-C4A-NA	2.89	128.50	124.51
28	a	411	SQD	O48-C23-C24	2.88	120.96	111.91
22	b	604	CLA	C1D-CHD-C4C	2.88	126.36	122.56
28	a	411	SQD	O2-C2-C1	2.88	117.05	110.05
22	b	611	CLA	CHB-C4A-NA	2.88	128.50	124.51
22	B	608	CLA	C6-C7-C8	-2.88	106.61	115.92
22	B	605	CLA	OBD-CAD-C3D	2.88	132.76	127.98
22	C	513	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
34	F	102	HEC	CMD-C2D-C1D	-2.87	124.05	128.46
27	Y	101	LMG	O2-C2-C1	-2.87	103.07	110.05
22	b	610	CLA	CAC-C3C-C4C	2.87	128.54	124.81
22	b	605	CLA	CHB-C4A-NA	2.87	128.48	124.51
27	A	410	LMG	O6-C1-O1	-2.87	103.18	109.97
24	a	406	BCR	C27-C26-C25	2.87	126.89	122.73
27	b	621	LMG	O6-C1-O1	-2.87	103.18	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	CMD-C2D-C3D	2.87	130.04	124.68
24	h	101	BCR	C35-C13-C14	-2.87	118.91	122.92
22	B	612	CLA	CMD-C2D-C3D	2.87	130.04	124.68
27	A	410	LMG	C9-C8-C7	-2.86	105.01	111.79
28	A	411	SQD	O47-C7-O49	-2.86	116.78	123.70
24	b	619	BCR	C16-C15-C14	-2.86	117.61	123.47
24	F	101	BCR	C2-C1-C6	2.86	114.89	110.48
22	b	607	CLA	CMB-C2B-C3B	2.86	130.03	124.68
28	a	411	SQD	O47-C7-C8	2.85	117.65	111.50
24	H	102	BCR	C2-C1-C6	2.85	114.88	110.48
27	b	623	LMG	C3-C4-C5	-2.85	105.15	110.24
22	B	609	CLA	C2C-C1C-NC	2.85	112.64	109.97
24	B	618	BCR	C37-C22-C21	-2.85	118.93	122.92
22	a	403	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
22	c	507	CLA	C4-C3-C2	-2.85	116.37	123.68
22	B	613	CLA	C1D-CHD-C4C	2.84	126.31	122.56
22	b	613	CLA	CHB-C4A-NA	2.84	128.44	124.51
22	d	403	CLA	O1D-CGD-CBD	2.84	130.30	124.48
24	K	103	BCR	C15-C16-C17	-2.84	117.66	123.47
29	c	519	DGD	O6D-C1D-O3G	-2.84	103.26	109.97
22	c	503	CLA	C1-C2-C3	-2.83	121.14	126.04
22	B	602	CLA	C1-C2-C3	-2.83	121.14	126.04
22	B	604	CLA	OBD-CAD-C3D	2.83	132.69	127.98
26	d	406	PL9	C37-C38-C39	-2.83	120.84	127.66
22	C	502	CLA	CMB-C2B-C3B	2.83	129.98	124.68
22	c	502	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	c	510	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
27	d	410	LMG	O2-C2-C1	-2.82	103.19	110.05
22	c	511	CLA	C4-C3-C5	2.82	120.02	115.27
22	B	603	CLA	O2D-CGD-O1D	-2.81	118.33	123.84
24	H	102	BCR	C38-C26-C25	-2.81	121.37	124.53
29	H	103	DGD	C1D-C2D-C3D	-2.81	104.14	110.00
22	c	512	CLA	CMD-C2D-C3D	2.81	129.94	124.68
22	C	504	CLA	CMB-C2B-C3B	2.81	129.94	124.68
22	B	611	CLA	CHD-C4C-NC	2.81	128.63	124.20
22	B	613	CLA	CAC-C3C-C4C	2.81	128.46	124.81
22	A	402	CLA	C6-C5-C3	2.81	120.82	113.45
24	H	102	BCR	C35-C13-C14	-2.81	118.99	122.92
29	H	103	DGD	C6D-C5D-C4D	2.80	117.95	112.09
23	a	404	PHO	CMB-C2B-C1B	-2.80	120.75	125.06
22	B	605	CLA	CHB-C4A-NA	2.80	128.39	124.51
26	a	409	PL9	O2-C1-C2	-2.80	115.36	121.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CHB-C4A-NA	2.80	128.39	124.51
28	f	102	SQD	C1-C2-C3	-2.80	104.16	110.00
24	t	101	BCR	C3-C4-C5	-2.80	109.09	114.08
22	C	504	CLA	C4-C3-C5	2.79	119.96	115.27
22	B	613	CLA	C2A-C1A-CHA	2.79	128.73	123.86
22	c	505	CLA	O2D-CGD-CBD	2.79	116.22	111.27
28	D	408	SQD	O9-S-O7	-2.79	104.31	113.95
22	b	609	CLA	CHA-C1A-NA	-2.79	120.02	126.40
22	c	504	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
22	B	614	CLA	C4A-NA-C1A	2.78	107.95	106.71
22	c	509	CLA	O2A-CGA-O1A	-2.77	116.59	123.59
22	c	510	CLA	C4D-C3D-CAD	-2.77	106.92	108.47
22	b	610	CLA	CMB-C2B-C3B	2.77	129.87	124.68
22	b	601	CLA	O2D-CGD-CBD	2.77	116.19	111.27
22	C	508	CLA	CMD-C2D-C3D	2.77	129.86	124.68
34	V	201	HEC	CMB-C2B-C1B	-2.77	124.21	128.46
22	B	605	CLA	CMB-C2B-C3B	2.77	129.86	124.68
26	a	409	PL9	C22-C23-C24	-2.77	120.99	127.66
28	a	412	SQD	O48-C23-O10	-2.77	116.61	123.59
22	b	602	CLA	CHB-C4A-NA	2.77	128.34	124.51
27	d	410	LMG	O1-C1-C2	-2.76	103.99	108.30
23	D	401	PHO	C2B-C1B-NB	-2.76	105.63	109.79
28	L	101	SQD	C45-O47-C7	2.76	124.58	117.79
22	a	405	CLA	C4-C3-C5	2.76	119.91	115.27
22	B	616	CLA	CMB-C2B-C3B	2.76	129.83	124.68
22	C	511	CLA	CHB-C4A-NA	2.76	128.32	124.51
34	V	201	HEC	CAD-CBD-CGD	-2.75	108.06	112.67
22	A	405	CLA	O2D-CGD-CBD	2.75	116.15	111.27
22	B	610	CLA	O2D-CGD-CBD	2.75	116.15	111.27
22	a	410	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
22	B	605	CLA	C16-C15-C13	-2.74	107.05	115.92
24	B	618	BCR	C2-C1-C6	2.74	114.70	110.48
22	B	609	CLA	CMC-C2C-C1C	2.74	129.21	125.04
22	c	512	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
22	b	601	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
22	D	405	CLA	CMD-C2D-C3D	2.74	129.80	124.68
22	b	616	CLA	C4-C3-C5	2.74	119.87	115.27
24	k	102	BCR	C27-C26-C25	2.74	126.70	122.73
24	t	101	BCR	C2-C1-C6	2.73	114.68	110.48
22	D	403	CLA	CED-O2D-CGD	2.72	122.10	115.94
22	a	403	CLA	CHB-C4A-NA	2.72	128.28	124.51
22	B	607	CLA	O2A-CGA-O1A	-2.72	116.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	103	BCR	C3-C4-C5	-2.72	109.22	114.08
24	B	619	BCR	C29-C30-C25	2.72	114.67	110.48
22	C	505	CLA	C1-C2-C3	-2.72	121.34	126.04
27	M	101	LMG	C38-C37-C36	-2.72	100.64	114.42
24	h	101	BCR	C38-C26-C25	-2.71	121.48	124.53
22	b	610	CLA	C6-C5-C3	2.71	120.56	113.45
26	D	406	PL9	C7-C3-C2	-2.71	119.74	123.30
22	D	404	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
29	c	519	DGD	C1D-C2D-C3D	-2.71	104.36	110.00
22	C	511	CLA	CMB-C2B-C1B	-2.71	124.31	128.46
28	L	101	SQD	O5-C5-C4	2.70	114.60	109.69
22	A	402	CLA	CMD-C2D-C3D	2.70	129.73	124.68
24	h	101	BCR	C2-C1-C6	2.70	114.63	110.48
22	C	504	CLA	CED-O2D-CGD	2.70	122.03	115.94
22	c	508	CLA	C4-C3-C5	2.69	119.80	115.27
29	C	515	DGD	C2G-O2G-C1B	2.69	124.41	117.79
24	A	406	BCR	C2-C1-C6	2.69	114.62	110.48
22	d	404	CLA	OBD-CAD-CBD	-2.69	122.06	125.89
22	C	504	CLA	O2D-CGD-CBD	2.68	116.04	111.27
22	a	403	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
22	b	601	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
22	b	603	CLA	CMA-C3A-C4A	2.68	118.98	111.77
26	d	406	PL9	C20-C19-C21	2.68	119.78	115.27
22	B	608	CLA	C1D-CHD-C4C	2.68	126.09	122.56
29	c	517	DGD	O6D-C1D-O3G	-2.68	103.63	109.97
22	B	611	CLA	C4D-C3D-CAD	-2.68	106.98	108.47
22	B	612	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
27	c	522	LMG	O7-C10-O9	-2.68	117.23	123.70
22	a	410	CLA	C1B-CHB-C4A	-2.68	124.82	130.12
22	c	507	CLA	OBD-CAD-CBD	-2.68	122.07	125.89
22	b	605	CLA	OBD-CAD-CBD	-2.68	122.07	125.89
29	H	103	DGD	C3E-C4E-C5E	-2.67	105.47	110.24
29	A	413	DGD	C1D-C2D-C3D	-2.67	104.43	110.00
29	H	103	DGD	C3D-C4D-C5D	-2.67	105.47	110.24
22	B	609	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
22	b	610	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
22	C	510	CLA	OBD-CAD-CBD	-2.67	122.08	125.89
22	B	605	CLA	C7-C6-C5	-2.67	106.11	113.36
22	B	609	CLA	CMB-C2B-C3B	2.66	129.66	124.68
22	b	609	CLA	C3C-C4C-NC	-2.66	107.59	110.57
22	B	611	CLA	C11-C12-C13	-2.66	107.33	115.92
29	A	413	DGD	C3G-C2G-C1G	-2.66	105.50	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	BCR	C36-C18-C17	-2.66	119.20	122.92
27	c	522	LMG	O3-C3-C2	-2.65	104.21	110.35
22	a	402	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
24	H	102	BCR	C29-C30-C25	2.65	114.56	110.48
22	D	405	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
24	a	406	BCR	C2-C1-C6	2.65	114.56	110.48
33	D	409	LHG	O8-C23-O10	-2.65	116.91	123.59
33	D	409	LHG	C18-C17-C16	-2.65	100.99	114.42
24	t	101	BCR	C15-C16-C17	-2.65	118.05	123.47
28	L	101	SQD	O48-C23-O10	-2.65	116.91	123.59
22	B	609	CLA	CMB-C2B-C1B	-2.65	124.40	128.46
22	B	609	CLA	C4D-C3D-CAD	-2.64	107.00	108.47
22	c	504	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	c	518	DGD	O2G-C1B-O1B	-2.64	117.32	123.70
22	b	608	CLA	CHA-C1A-NA	-2.64	120.35	126.40
22	b	613	CLA	C7-C6-C5	-2.64	106.19	113.36
24	B	618	BCR	C35-C13-C14	-2.64	119.22	122.92
27	b	623	LMG	C4-C3-C2	-2.64	106.21	110.82
26	d	406	PL9	C40-C39-C41	2.64	119.71	115.27
22	A	403	CLA	C4A-NA-C1A	2.64	107.89	106.71
22	c	505	CLA	O2A-CGA-O1A	-2.63	116.94	123.59
22	A	403	CLA	O2D-CGD-CBD	2.63	115.95	111.27
27	Y	101	LMG	O1-C7-C8	-2.63	104.54	110.90
26	D	406	PL9	C30-C29-C31	-2.63	110.85	115.27
28	A	412	SQD	C45-O47-C7	2.63	121.25	117.88
23	A	404	PHO	C5-C3-C2	2.62	126.43	121.12
22	b	602	CLA	CED-O2D-CGD	2.62	121.87	115.94
22	D	403	CLA	C4D-C3D-CAD	-2.62	107.01	108.47
23	A	404	PHO	C1-O2A-CGA	2.62	123.32	116.44
22	b	602	CLA	CHC-C1C-NC	2.62	128.18	124.20
22	B	610	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
29	A	413	DGD	O2D-C2D-C1D	-2.62	103.69	110.05
26	d	406	PL9	C40-C39-C38	-2.62	116.97	123.68
22	B	606	CLA	CMD-C2D-C3D	2.62	129.57	124.68
22	c	505	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
22	D	405	CLA	CAC-C3C-C4C	2.61	128.20	124.81
22	a	403	CLA	O2D-CGD-CBD	2.61	115.91	111.27
22	B	609	CLA	CMD-C2D-C3D	2.61	129.57	124.68
27	b	623	LMG	O8-C28-O10	-2.61	117.00	123.59
22	B	603	CLA	C4-C3-C5	2.61	119.66	115.27
29	c	518	DGD	C3G-O3G-C1D	2.61	118.84	113.74
22	B	606	CLA	CMB-C2B-C3B	2.61	129.56	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O1G-C1A-C2A	-2.61	103.72	111.91
22	C	508	CLA	OBD-CAD-CBD	-2.61	122.17	125.89
27	c	522	LMG	O6-C1-O1	-2.60	103.81	109.97
24	C	514	BCR	C35-C13-C14	-2.60	119.28	122.92
22	b	604	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
22	B	603	CLA	CHD-C4C-NC	2.60	128.30	124.20
22	b	614	CLA	C4D-C3D-CAD	-2.60	107.02	108.47
22	b	603	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
27	b	623	LMG	O7-C10-O9	-2.60	117.42	123.70
22	c	506	CLA	C11-C10-C8	-2.60	107.53	115.92
22	c	511	CLA	CMB-C2B-C3B	2.59	129.53	124.68
26	A	409	PL9	C31-C32-C33	-2.59	103.35	111.88
22	B	610	CLA	CHC-C1C-NC	2.59	128.13	124.20
27	b	621	LMG	C38-C37-C36	-2.59	101.29	114.42
24	b	618	BCR	C15-C14-C13	-2.58	123.62	127.31
33	l	101	LHG	O8-C23-C24	2.58	120.01	111.91
22	c	503	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
33	d	409	LHG	C26-C25-C24	2.58	122.46	113.19
22	d	404	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
26	D	406	PL9	C7-C8-C9	-2.58	122.50	126.79
22	a	402	CLA	C3A-C2A-C1A	2.58	105.20	101.34
24	t	101	BCR	C34-C9-C10	-2.57	119.32	122.92
27	A	410	LMG	C1-O6-C5	-2.57	108.63	113.69
22	c	511	CLA	C1D-CHD-C4C	2.57	125.95	122.56
23	a	404	PHO	C3A-C4A-CHB	-2.57	117.38	121.83
28	D	408	SQD	O48-C23-O10	-2.57	117.11	123.59
22	B	611	CLA	CHB-C4A-NA	2.57	128.06	124.51
28	a	411	SQD	O10-C23-C24	-2.57	113.72	123.73
23	D	401	PHO	O2D-CGD-O1D	-2.57	118.82	123.84
22	b	603	CLA	OBD-CAD-CBD	-2.57	122.23	125.89
27	c	523	LMG	O8-C28-O10	-2.57	117.11	123.59
24	T	101	BCR	C38-C26-C27	-2.57	108.69	113.62
22	a	403	CLA	OBD-CAD-CBD	-2.57	122.23	125.89
28	A	411	SQD	O5-C1-O6	2.56	116.05	109.97
24	a	406	BCR	C8-C7-C6	-2.56	120.01	127.20
22	C	507	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
27	b	621	LMG	O7-C10-O9	-2.56	117.52	123.70
24	H	102	BCR	C16-C15-C14	-2.56	118.23	123.47
22	B	616	CLA	CHA-C1A-NA	-2.56	120.55	126.40
22	a	403	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
24	K	103	BCR	C16-C15-C14	-2.55	118.24	123.47
22	B	614	CLA	O2A-CGA-O1A	-2.55	117.16	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C38-C26-C25	-2.55	121.67	124.53
26	A	409	PL9	O2-C1-C2	-2.55	115.94	121.78
29	c	518	DGD	C3D-C4D-C5D	-2.55	105.70	110.24
22	b	613	CLA	C1-C2-C3	-2.54	121.64	126.04
22	B	616	CLA	C1-O2A-CGA	2.54	123.11	116.44
22	C	512	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
24	b	618	BCR	C38-C26-C25	-2.54	121.68	124.53
22	C	509	CLA	CHB-C4A-NA	2.54	128.02	124.51
24	d	405	BCR	C27-C26-C25	2.54	126.41	122.73
24	b	617	BCR	C37-C22-C21	-2.53	119.37	122.92
24	K	101	BCR	C7-C8-C9	-2.53	122.41	126.23
33	D	409	LHG	O8-C23-C24	2.53	119.85	111.91
22	B	603	CLA	C1D-CHD-C4C	2.53	125.90	122.56
26	d	406	PL9	C31-C32-C33	-2.53	103.57	111.88
22	c	509	CLA	CHC-C1C-NC	2.53	128.04	124.20
22	C	503	CLA	CMD-C2D-C3D	2.53	129.41	124.68
24	A	406	BCR	C15-C16-C17	-2.53	118.30	123.47
22	B	609	CLA	C1D-CHD-C4C	2.53	125.89	122.56
22	b	612	CLA	CBC-CAC-C3C	2.53	119.39	112.43
34	v	201	HEC	CMD-C2D-C1D	-2.53	124.58	128.46
27	Y	101	LMG	O6-C1-O1	-2.53	103.99	109.97
22	B	607	CLA	C2C-C1C-NC	2.52	112.33	109.97
22	C	513	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	B	614	CLA	CMD-C2D-C3D	2.52	129.39	124.68
22	B	614	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
26	A	409	PL9	O1-C4-C3	-2.52	117.95	120.72
29	c	518	DGD	O2D-C2D-C1D	-2.51	103.94	110.05
22	c	506	CLA	O2D-CGD-CBD	2.51	115.73	111.27
34	F	102	HEC	CAD-CBD-CGD	2.51	116.89	112.67
22	a	403	CLA	CHC-C1C-NC	2.51	128.01	124.20
22	c	510	CLA	CHC-C1C-NC	2.51	128.01	124.20
24	B	619	BCR	C15-C16-C17	-2.51	118.33	123.47
24	b	617	BCR	C3-C4-C5	-2.51	109.60	114.08
22	c	507	CLA	OBD-CAD-C3D	2.51	132.15	127.98
24	H	102	BCR	C27-C26-C25	2.51	126.37	122.73
27	D	407	LMG	C9-C8-C7	-2.51	105.86	111.79
22	D	404	CLA	CMD-C2D-C3D	2.50	129.36	124.68
22	C	512	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
23	d	401	PHO	CMC-C2C-C1C	-2.49	121.23	125.06
33	e	101	LHG	O8-C23-C24	2.49	119.73	111.91
22	c	512	CLA	O2D-CGD-CBD	2.49	115.69	111.27
22	c	505	CLA	C1D-CHD-C4C	2.49	125.84	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	407	LMG	C31-C30-C29	-2.49	104.25	113.19
22	a	410	CLA	CMB-C2B-C3B	2.48	129.32	124.68
24	d	405	BCR	C2-C1-C6	2.48	114.30	110.48
24	C	514	BCR	C34-C9-C10	-2.48	119.45	122.92
22	b	609	CLA	OBD-CAD-C3D	2.48	132.10	127.98
22	B	616	CLA	O1D-CGD-CBD	2.48	129.55	124.48
24	c	516	BCR	C2-C1-C6	2.47	114.29	110.48
24	k	101	BCR	C27-C26-C25	2.47	126.32	122.73
22	B	615	CLA	C1-O2A-CGA	2.47	122.94	116.44
22	b	610	CLA	C1-C2-C3	-2.47	121.77	126.04
22	B	610	CLA	C1-C2-C3	-2.47	121.77	126.04
28	A	411	SQD	O7-S-C6	2.47	109.88	106.94
27	Y	101	LMG	C40-C39-C38	-2.47	101.88	114.42
22	c	509	CLA	C11-C10-C8	-2.47	107.93	115.92
24	b	617	BCR	C36-C18-C17	-2.47	119.46	122.92
22	c	503	CLA	CMD-C2D-C3D	2.47	129.30	124.68
27	M	101	LMG	C1-C2-C3	-2.47	104.86	110.00
22	C	512	CLA	C6-C5-C3	-2.47	106.99	113.45
24	K	102	BCR	C36-C18-C17	-2.46	119.47	122.92
33	d	407	LHG	C11-C10-C9	-2.46	101.93	114.42
28	a	411	SQD	O8-S-C6	2.46	109.66	105.74
24	k	102	BCR	C40-C30-C25	2.46	114.29	110.30
24	b	619	BCR	C11-C10-C9	-2.46	123.80	127.31
22	b	613	CLA	CHA-C1A-NA	-2.46	120.76	126.40
27	A	410	LMG	C40-C39-C38	-2.46	101.95	114.42
23	A	404	PHO	CMD-C2D-C1D	2.46	128.85	125.06
22	b	610	CLA	CAA-CBA-CGA	-2.46	106.07	113.25
24	K	101	BCR	C27-C26-C25	2.46	126.30	122.73
22	B	608	CLA	CMD-C2D-C3D	2.46	129.27	124.68
22	c	512	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
22	b	605	CLA	CHC-C1C-NC	2.45	127.92	124.20
22	C	510	CLA	C11-C10-C8	-2.45	108.00	115.92
27	D	411	LMG	O8-C28-O10	-2.45	117.41	123.59
26	A	409	PL9	C20-C19-C21	2.45	119.39	115.27
22	a	402	CLA	C7-C6-C5	-2.45	106.71	113.36
22	c	509	CLA	CMD-C2D-C3D	2.45	129.26	124.68
22	B	612	CLA	CHB-C4A-NA	2.45	127.89	124.51
27	c	520	LMG	O2-C2-C3	-2.45	104.69	110.35
22	B	616	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
22	b	607	CLA	CHA-C1A-NA	-2.44	120.81	126.40
23	a	404	PHO	CBD-CHA-C4D	-2.44	105.79	108.54
22	C	513	CLA	C4D-C3D-CAD	-2.44	107.11	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C37-C22-C21	-2.44	119.51	122.92
22	B	605	CLA	C11-C10-C8	-2.43	108.05	115.92
29	c	517	DGD	C2G-O2G-C1B	2.43	123.78	117.79
26	a	409	PL9	C36-C34-C33	-2.43	116.20	121.12
22	b	601	CLA	C1D-CHD-C4C	2.43	125.77	122.56
22	C	512	CLA	C1-C2-C3	-2.43	121.84	126.04
24	K	102	BCR	C27-C26-C25	2.43	126.26	122.73
29	A	413	DGD	O3G-C1D-C2D	-2.43	104.51	108.30
24	a	406	BCR	C30-C25-C26	-2.43	119.20	122.61
22	b	607	CLA	C2C-C1C-NC	2.43	112.25	109.97
22	d	403	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
22	B	616	CLA	OBD-CAD-CBD	-2.42	122.43	125.89
22	c	503	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
26	A	409	PL9	C40-C39-C41	2.42	119.35	115.27
22	c	504	CLA	C11-C12-C13	-2.42	108.09	115.92
22	b	610	CLA	C3A-C2A-C1A	2.42	104.96	101.34
22	b	610	CLA	C4-C3-C5	2.42	119.34	115.27
22	C	507	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
22	C	503	CLA	C6-C7-C8	-2.42	108.11	115.92
28	B	622	SQD	O47-C45-C46	2.42	117.15	108.40
22	b	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
22	B	614	CLA	C4-C3-C5	2.41	119.33	115.27
28	D	408	SQD	C1-C2-C3	-2.41	104.98	110.00
22	c	511	CLA	O2A-C1-C2	-2.41	102.30	108.64
29	C	517	DGD	O3D-C3D-C4D	-2.41	104.78	110.35
29	C	516	DGD	C1D-C2D-C3D	-2.41	104.98	110.00
26	d	406	PL9	C7-C8-C9	-2.41	122.78	126.79
22	c	505	CLA	C7-C6-C5	-2.41	106.82	113.36
34	f	101	HEC	CMC-C2C-C1C	-2.41	124.76	128.46
29	C	515	DGD	O2G-C1B-C2B	-2.40	106.32	111.50
27	b	623	LMG	O6-C5-C6	2.40	112.41	106.44
24	F	101	BCR	C8-C7-C6	-2.40	120.45	127.20
23	a	404	PHO	C1B-NB-C4B	2.40	111.04	106.51
22	b	603	CLA	C7-C6-C5	-2.40	106.83	113.36
22	c	507	CLA	CED-O2D-CGD	2.40	121.37	115.94
27	M	101	LMG	C17-C16-C15	-2.40	102.23	114.42
22	A	403	CLA	C1D-CHD-C4C	2.40	125.73	122.56
22	B	607	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
22	a	410	CLA	C1-O2A-CGA	2.40	122.74	116.44
24	B	618	BCR	C15-C16-C17	-2.40	118.56	123.47
22	C	507	CLA	C4D-C3D-CAD	-2.40	107.13	108.47
29	c	517	DGD	C4A-C3A-C2A	-2.40	104.57	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	517	DGD	O2D-C2D-C1D	-2.40	104.22	110.05
24	K	103	BCR	C11-C10-C9	-2.40	123.89	127.31
22	a	403	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
28	D	408	SQD	O5-C5-C4	2.40	114.05	109.69
22	C	501	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
27	A	410	LMG	C38-C37-C36	-2.39	102.27	114.42
27	c	520	LMG	C1-O6-C5	-2.39	109.00	113.69
27	d	410	LMG	C3-C4-C5	-2.39	105.98	110.24
29	h	102	DGD	O5E-C6E-C5E	-2.39	103.11	111.29
22	C	505	CLA	CMD-C2D-C3D	2.39	129.14	124.68
29	C	516	DGD	O6D-C1D-O3G	-2.38	104.33	109.97
23	D	401	PHO	C1B-NB-C4B	2.38	111.00	106.51
29	C	515	DGD	O1G-C1A-C2A	-2.38	104.43	111.91
22	B	604	CLA	C6-C5-C3	-2.38	107.21	113.45
24	b	619	BCR	C2-C1-C6	2.38	114.15	110.48
29	c	518	DGD	O4D-C4D-C3D	2.38	115.85	110.35
27	M	101	LMG	O2-C2-C1	-2.38	104.27	110.05
22	d	403	CLA	C6-C5-C3	2.38	119.69	113.45
22	C	512	CLA	C1D-CHD-C4C	2.38	125.70	122.56
24	b	617	BCR	C38-C26-C25	-2.38	121.86	124.53
29	C	517	DGD	CAB-C9B-C8B	-2.38	102.36	114.42
24	A	406	BCR	C1-C6-C5	-2.38	119.27	122.61
24	K	103	BCR	C27-C26-C25	2.38	126.18	122.73
22	b	612	CLA	CAC-C3C-C4C	2.38	127.89	124.81
22	c	509	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
27	b	621	LMG	C20-C19-C18	-2.37	102.37	114.42
28	a	412	SQD	O49-C7-C8	-2.37	114.47	123.73
23	a	404	PHO	C2C-C1C-NC	2.37	113.37	109.79
28	A	411	SQD	O9-S-O7	-2.37	105.74	113.95
22	D	404	CLA	C3D-CAD-CBD	-2.37	104.48	107.61
28	D	408	SQD	O48-C23-C24	2.37	119.35	111.91
33	D	410	LHG	O8-C23-O10	-2.37	117.61	123.59
22	D	404	CLA	CMB-C2B-C1B	-2.37	124.83	128.46
22	c	514	CLA	CHB-C4A-NA	2.37	127.78	124.51
22	c	505	CLA	CMD-C2D-C3D	2.37	129.11	124.68
23	d	401	PHO	C1-C2-C3	-2.37	121.95	126.04
22	c	503	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
22	C	504	CLA	CMD-C2D-C3D	2.36	129.10	124.68
22	c	504	CLA	C4-C3-C5	2.36	119.25	115.27
22	C	501	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
22	D	405	CLA	O2D-CGD-CBD	2.36	115.46	111.27
22	b	615	CLA	O2D-CGD-O1D	-2.36	119.22	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	507	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
24	h	101	BCR	C36-C18-C17	-2.36	119.62	122.92
22	B	616	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
24	b	619	BCR	C28-C27-C26	-2.35	109.87	114.08
22	B	604	CLA	C1D-CHD-C4C	2.35	125.66	122.56
33	D	412	LHG	C20-C19-C18	-2.35	102.48	114.42
24	C	514	BCR	C15-C16-C17	-2.35	118.65	123.47
27	D	407	LMG	O2-C2-C1	-2.35	104.33	110.05
22	B	608	CLA	CHD-C4C-NC	2.35	127.91	124.20
22	B	607	CLA	C3A-C2A-C1A	2.35	104.86	101.34
22	b	610	CLA	C2C-C1C-NC	2.35	112.17	109.97
22	B	604	CLA	CHA-C1A-NA	-2.35	121.02	126.40
22	B	615	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
22	c	504	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
29	c	519	DGD	O3D-C3D-C4D	-2.34	104.94	110.35
29	A	413	DGD	O1G-C1A-O1A	-2.34	117.69	123.59
24	a	406	BCR	C38-C26-C27	-2.34	109.12	113.62
22	a	402	CLA	C4D-C3D-CAD	-2.34	107.17	108.47
22	A	405	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	k	101	BCR	C38-C26-C25	-2.34	121.90	124.53
29	C	517	DGD	CBB-CAB-C9B	-2.34	102.56	114.42
22	a	410	CLA	O2D-CGD-CBD	2.34	115.42	111.27
22	B	604	CLA	CGD-CBD-CAD	-2.33	103.17	110.73
22	H	101	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	b	606	CLA	C4-C3-C5	2.33	119.20	115.27
22	B	608	CLA	C4D-C3D-CAD	-2.33	107.17	108.47
26	D	406	PL9	O2-C1-C2	-2.33	116.44	121.78
22	C	505	CLA	C16-C15-C13	-2.33	108.38	115.92
22	c	503	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
22	c	510	CLA	CAC-C3C-C4C	2.33	127.83	124.81
22	b	605	CLA	C16-C15-C13	-2.33	108.39	115.92
29	c	518	DGD	O3G-C1D-C2D	-2.33	104.67	108.30
27	D	407	LMG	O8-C28-O10	-2.33	117.71	123.59
22	C	507	CLA	CHB-C4A-NA	2.33	127.73	124.51
22	b	611	CLA	CMD-C2D-C3D	2.33	129.04	124.68
22	B	607	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
22	c	514	CLA	C4A-NA-C1A	2.33	107.75	106.71
22	A	402	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
22	B	602	CLA	C11-C12-C13	-2.33	108.40	115.92
22	c	502	CLA	CED-O2D-CGD	-2.32	110.68	115.94
22	B	611	CLA	C3C-C4C-NC	-2.32	107.97	110.57
22	b	608	CLA	O2A-CGA-O1A	-2.32	117.73	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	CHA-C1A-NA	-2.32	121.08	126.40
22	C	509	CLA	CED-O2D-CGD	2.32	121.19	115.94
29	h	102	DGD	O3E-C3E-C2E	-2.32	104.98	110.35
26	D	406	PL9	C42-C43-C44	-2.32	122.07	127.66
22	b	615	CLA	C3B-C4B-NB	-2.32	106.21	109.21
22	c	507	CLA	C4-C3-C5	2.32	119.17	115.27
29	H	103	DGD	C7B-C6B-C5B	-2.32	102.66	114.42
26	a	409	PL9	O2-C1-C6	2.32	124.60	120.59
24	K	103	BCR	C37-C22-C21	-2.32	119.68	122.92
22	b	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	C	514	BCR	C33-C5-C6	-2.32	121.93	124.53
22	c	509	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
28	B	622	SQD	C46-C45-C44	-2.31	106.32	111.79
22	d	404	CLA	C1-C2-C3	-2.31	122.04	126.04
29	C	515	DGD	C3D-C4D-C5D	-2.31	106.12	110.24
24	d	405	BCR	C24-C23-C22	-2.31	122.75	126.23
22	B	614	CLA	CHA-C1A-NA	-2.31	121.12	126.40
24	d	405	BCR	C16-C15-C14	-2.31	118.75	123.47
22	B	612	CLA	C1D-CHD-C4C	2.30	125.60	122.56
27	M	101	LMG	O7-C10-C11	-2.30	106.53	111.50
22	c	504	CLA	C1D-CHD-C4C	2.30	125.60	122.56
29	h	102	DGD	C7B-C6B-C5B	-2.30	102.74	114.42
22	b	607	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	C	501	CLA	C9-C8-C10	-2.30	102.97	111.29
23	A	404	PHO	CBD-CHA-C4D	-2.30	105.95	108.54
22	C	502	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
22	b	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
22	C	505	CLA	CAA-CBA-CGA	-2.30	106.54	113.25
33	e	101	LHG	C11-C10-C9	-2.30	102.76	114.42
22	A	403	CLA	CMD-C2D-C3D	2.30	128.97	124.68
27	b	621	LMG	O8-C28-O10	-2.30	117.80	123.59
22	C	505	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
24	K	101	BCR	C36-C18-C17	-2.30	119.71	122.92
22	B	603	CLA	O2A-CGA-O1A	-2.30	117.80	123.59
24	t	101	BCR	C27-C26-C25	2.29	126.06	122.73
22	b	605	CLA	O1D-CGD-CBD	2.29	129.18	124.48
29	C	517	DGD	C8B-C7B-C6B	-2.29	102.78	114.42
29	C	515	DGD	C3B-C2B-C1B	-2.29	105.29	113.62
22	B	616	CLA	C2A-C1A-CHA	2.29	127.87	123.86
24	b	617	BCR	C8-C7-C6	-2.29	120.77	127.20
22	B	610	CLA	O1A-CGA-CBA	2.29	132.67	123.73
29	c	518	DGD	C6D-O5D-C1E	2.29	118.21	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	O2A-C1-C2	-2.29	102.62	108.64
29	C	517	DGD	C1D-C2D-C3D	-2.29	105.23	110.00
24	t	101	BCR	C38-C26-C27	-2.29	109.22	113.62
22	C	503	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
22	a	402	CLA	C1D-CHD-C4C	2.29	125.57	122.56
22	B	603	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
24	B	619	BCR	C28-C27-C26	-2.28	110.00	114.08
22	B	612	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
22	a	402	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
24	b	619	BCR	C8-C7-C6	-2.28	120.80	127.20
22	B	604	CLA	C1-O2A-CGA	-2.28	110.47	116.44
29	h	102	DGD	C1D-O6D-C5D	-2.28	109.22	113.69
22	a	402	CLA	C4-C3-C5	2.28	119.10	115.27
26	a	409	PL9	C12-C13-C14	-2.28	122.18	127.66
24	c	515	BCR	C15-C14-C13	-2.28	124.06	127.31
23	d	401	PHO	CBD-CHA-C4D	-2.28	105.98	108.54
27	c	523	LMG	C1-O6-C5	-2.27	109.22	113.69
29	H	103	DGD	C1D-O6D-C5D	-2.27	109.22	113.69
22	c	508	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
24	b	617	BCR	C27-C26-C25	2.27	126.03	122.73
22	C	509	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
33	L	102	LHG	C12-C11-C10	-2.27	102.90	114.42
22	B	602	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
24	B	617	BCR	C7-C8-C9	-2.27	122.81	126.23
28	A	411	SQD	O48-C23-C24	2.27	119.03	111.91
27	c	520	LMG	C40-C39-C38	-2.27	102.91	114.42
22	A	403	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	B	605	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
22	d	404	CLA	CHB-C4A-NA	2.27	127.65	124.51
29	H	103	DGD	C4D-C3D-C2D	-2.27	106.87	110.82
22	c	514	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
33	D	412	LHG	C11-C10-C9	-2.26	102.94	114.42
24	C	514	BCR	C2-C1-C6	2.26	113.96	110.48
22	b	613	CLA	C16-C15-C13	-2.26	108.61	115.92
26	A	409	PL9	C7-C8-C9	-2.26	123.03	126.79
22	C	512	CLA	CAA-CBA-CGA	-2.26	106.66	113.25
22	c	511	CLA	CMD-C2D-C3D	2.26	128.90	124.68
22	b	606	CLA	CMB-C2B-C3B	2.26	128.90	124.68
23	a	404	PHO	O2A-CGA-O1A	-2.25	117.90	123.59
22	b	604	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
22	b	608	CLA	C1D-CHD-C4C	2.25	125.53	122.56
22	A	402	CLA	CMB-C2B-C1B	-2.25	125.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	103	DGD	CAB-C9B-C8B	-2.25	103.02	114.42
28	B	622	SQD	O8-S-O7	-2.25	105.79	111.27
29	A	413	DGD	CDB-CCB-CBB	-2.24	103.03	114.42
22	b	605	CLA	C1D-CHD-C4C	2.24	125.52	122.56
22	c	503	CLA	OBD-CAD-CBD	-2.24	122.69	125.89
22	c	509	CLA	C1D-CHD-C4C	2.24	125.52	122.56
34	F	102	HEC	CMC-C2C-C1C	-2.24	125.02	128.46
24	t	101	BCR	C11-C10-C9	-2.24	124.12	127.31
33	E	101	LHG	O8-C23-C24	2.24	118.93	111.91
22	B	613	CLA	CMD-C2D-C3D	2.24	128.86	124.68
22	B	615	CLA	C1C-C2C-C3C	-2.24	104.61	106.96
22	C	503	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
22	B	610	CLA	CHC-C1C-C2C	-2.24	120.54	126.72
29	c	517	DGD	O3D-C3D-C4D	-2.23	105.18	110.35
24	B	619	BCR	C40-C30-C29	-2.23	99.97	108.91
22	C	504	CLA	CHC-C1C-NC	2.23	127.59	124.20
22	B	609	CLA	CHB-C4A-NA	2.23	127.60	124.51
24	h	101	BCR	C35-C13-C12	2.23	121.59	118.08
22	b	616	CLA	C4D-C3D-CAD	-2.23	107.22	108.47
24	K	101	BCR	C24-C23-C22	-2.23	122.87	126.23
22	A	405	CLA	CMD-C2D-C3D	2.23	128.84	124.68
26	A	409	PL9	C27-C28-C29	-2.23	122.30	127.66
27	A	410	LMG	C3-C4-C5	-2.22	106.27	110.24
22	D	403	CLA	C1-C2-C3	-2.22	122.20	126.04
22	C	506	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
24	b	617	BCR	C11-C10-C9	-2.22	124.14	127.31
22	c	505	CLA	O2A-C1-C2	-2.22	102.80	108.64
22	c	507	CLA	C4A-NA-C1A	2.22	107.70	106.71
22	B	612	CLA	C1-C2-C3	-2.22	122.20	126.04
26	A	409	PL9	C30-C29-C31	-2.22	111.54	115.27
22	b	611	CLA	C2A-C3A-C4A	2.22	105.45	101.87
33	d	408	LHG	C20-C19-C18	-2.22	103.17	114.42
22	a	402	CLA	CHB-C4A-NA	2.22	127.58	124.51
22	C	507	CLA	CMD-C2D-C3D	2.22	128.83	124.68
34	V	201	HEC	CMD-C2D-C1D	-2.22	125.06	128.46
22	c	505	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
22	b	602	CLA	O2D-CGD-O1D	-2.22	119.51	123.84
33	D	409	LHG	C27-C26-C25	-2.21	103.19	114.42
22	b	609	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
22	H	101	CLA	CAA-C2A-C1A	-2.21	104.72	111.97
22	b	609	CLA	CED-O2D-CGD	2.21	120.94	115.94
29	c	518	DGD	O6D-C1D-O3G	-2.21	104.73	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	101	LMG	C23-C22-C21	-2.21	103.20	114.42
22	C	509	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
27	b	621	LMG	C22-C21-C20	-2.21	103.21	114.42
29	h	102	DGD	C1D-C2D-C3D	-2.21	105.39	110.00
24	B	618	BCR	C38-C26-C25	-2.21	122.05	124.53
29	C	515	DGD	C1D-C2D-C3D	-2.21	105.40	110.00
24	B	619	BCR	C11-C10-C9	-2.21	124.16	127.31
34	f	101	HEC	C4C-C3C-C2C	2.21	108.73	106.35
22	a	402	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	a	409	PL9	C31-C32-C33	-2.20	104.64	111.88
22	b	602	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
29	h	102	DGD	O2D-C2D-C1D	-2.20	104.70	110.05
24	b	617	BCR	C15-C16-C17	-2.20	118.97	123.47
23	d	401	PHO	C2B-C1B-NB	-2.20	106.47	109.79
22	c	507	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	B	613	CLA	CHB-C4A-NA	2.20	127.55	124.51
22	D	403	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
22	C	510	CLA	CHB-C4A-NA	2.20	127.55	124.51
28	A	412	SQD	O47-C45-C46	2.20	111.22	106.13
26	A	409	PL9	C36-C37-C38	-2.20	104.67	111.88
27	Y	101	LMG	C3-C4-C5	-2.19	106.32	110.24
22	B	604	CLA	C2A-C3A-C4A	2.19	105.41	101.87
27	c	523	LMG	C4-C3-C2	-2.19	107.00	110.82
22	c	514	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
27	b	623	LMG	C40-C39-C38	-2.19	103.30	114.42
22	b	609	CLA	C7-C6-C5	-2.19	107.41	113.36
33	d	408	LHG	O8-C23-C24	2.19	118.78	111.91
33	E	101	LHG	C26-C25-C24	2.19	121.06	113.19
24	H	102	BCR	C1-C6-C5	-2.19	119.53	122.61
28	a	411	SQD	O4-C4-C3	-2.19	105.29	110.35
22	B	609	CLA	OBD-CAD-CBD	-2.19	122.77	125.89
22	B	616	CLA	C5-C3-C2	2.18	125.54	121.12
26	d	406	PL9	O2-C1-C2	-2.18	116.78	121.78
27	b	621	LMG	O1-C7-C8	-2.18	105.63	110.90
22	C	503	CLA	O1D-CGD-CBD	2.18	128.95	124.48
24	c	516	BCR	C7-C8-C9	-2.18	122.94	126.23
22	B	609	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
22	C	511	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
22	a	405	CLA	OBD-CAD-C3D	2.18	131.60	127.98
29	C	516	DGD	C1D-O6D-C5D	-2.18	109.41	113.69
22	B	616	CLA	C2C-C1C-NC	2.18	112.01	109.97
29	H	103	DGD	C9A-C8A-C7A	-2.18	103.36	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
22	C	513	CLA	C4-C3-C5	2.18	118.94	115.27
24	t	101	BCR	C36-C18-C19	2.18	121.50	118.08
29	C	515	DGD	C5B-C4B-C3B	-2.18	103.38	114.42
24	K	102	BCR	C33-C5-C6	-2.17	122.09	124.53
22	C	502	CLA	OBD-CAD-CBD	-2.17	122.79	125.89
22	B	604	CLA	C2A-C1A-CHA	2.17	127.66	123.86
29	H	103	DGD	C7A-C6A-C5A	-2.17	103.40	114.42
22	b	607	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
22	A	403	CLA	C1-C2-C3	-2.17	122.29	126.04
33	l	101	LHG	C11-C10-C9	-2.17	103.41	114.42
22	C	513	CLA	C3A-C2A-C1A	2.17	104.58	101.34
24	K	103	BCR	C7-C8-C9	-2.16	122.96	126.23
22	c	510	CLA	CMD-C2D-C3D	2.16	128.72	124.68
22	D	405	CLA	O2A-C1-C2	-2.16	102.96	108.64
22	b	615	CLA	CMD-C2D-C3D	2.16	128.72	124.68
22	c	508	CLA	CED-O2D-CGD	2.16	120.82	115.94
22	c	507	CLA	C1D-CHD-C4C	2.16	125.41	122.56
22	a	402	CLA	C17-C16-C15	-2.16	103.32	113.24
22	B	603	CLA	CMA-C3A-C4A	2.16	117.57	111.77
22	c	514	CLA	OBD-CAD-CBD	-2.16	122.81	125.89
22	C	506	CLA	CHA-C1A-NA	-2.16	121.46	126.40
22	c	504	CLA	O1D-CGD-CBD	2.16	128.90	124.48
24	b	617	BCR	C35-C13-C14	-2.16	119.90	122.92
27	c	523	LMG	O5-C6-C5	-2.16	103.90	111.29
22	A	405	CLA	O2A-CGA-O1A	-2.15	118.15	123.59
22	a	402	CLA	C2A-C1A-CHA	2.15	127.63	123.86
23	d	401	PHO	CMC-C2C-C3C	2.15	131.96	126.12
22	c	513	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
22	D	405	CLA	CHB-C4A-NA	2.15	127.49	124.51
24	B	618	BCR	C15-C14-C13	-2.15	124.24	127.31
29	H	103	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
26	D	406	PL9	C21-C19-C18	-2.15	116.77	121.12
28	L	101	SQD	O8-S-C6	2.15	109.16	105.74
27	b	623	LMG	C1-C2-C3	-2.15	105.53	110.00
29	c	518	DGD	CDB-CCB-CBB	-2.15	103.53	114.42
22	c	507	CLA	CHD-C4C-NC	2.15	127.58	124.20
22	H	101	CLA	C4-C3-C5	2.14	118.88	115.27
22	C	512	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
28	L	101	SQD	O47-C45-C46	2.14	116.16	108.40
22	b	601	CLA	C11-C12-C13	-2.14	108.99	115.92
22	B	614	CLA	OBD-CAD-CBD	-2.14	122.83	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	O2D-CGD-CBD	2.14	115.07	111.27
27	M	101	LMG	O3-C3-C2	-2.14	105.40	110.35
22	B	613	CLA	CED-O2D-CGD	2.14	120.78	115.94
29	h	102	DGD	C1E-O6E-C5E	2.14	117.89	113.69
24	h	101	BCR	C16-C15-C14	-2.14	119.09	123.47
33	D	410	LHG	O8-C6-C5	-2.14	102.22	108.43
24	k	102	BCR	C35-C13-C14	-2.14	119.93	122.92
22	b	604	CLA	CHB-C4A-NA	2.14	127.47	124.51
22	C	505	CLA	C4-C3-C2	-2.13	118.20	123.68
22	b	615	CLA	CHB-C4A-NA	2.13	127.46	124.51
24	C	514	BCR	C1-C6-C5	-2.13	119.61	122.61
22	b	610	CLA	CHA-C1A-NA	-2.13	121.52	126.40
24	K	103	BCR	C2-C1-C6	2.13	113.76	110.48
22	c	513	CLA	C1-C2-C3	-2.13	122.36	126.04
22	C	505	CLA	OBD-CAD-CBD	-2.13	122.85	125.89
22	a	410	CLA	C1D-CHD-C4C	2.13	125.37	122.56
22	A	405	CLA	C5-C3-C2	-2.13	116.81	121.12
22	d	403	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
22	a	405	CLA	CHC-C1C-NC	2.13	127.43	124.20
22	B	604	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
22	b	605	CLA	CHC-C1C-C2C	-2.12	120.84	126.72
33	E	101	LHG	C11-C10-C9	-2.12	103.64	114.42
22	a	405	CLA	CHD-C4C-NC	2.12	127.55	124.20
22	d	404	CLA	O1D-CGD-CBD	2.12	128.83	124.48
24	k	101	BCR	C1-C6-C5	-2.12	119.62	122.61
22	C	501	CLA	C2C-C1C-NC	-2.12	107.98	109.97
29	c	519	DGD	CAB-C9B-C8B	-2.12	103.65	114.42
26	a	409	PL9	C40-C39-C41	2.12	118.84	115.27
33	d	407	LHG	C25-C24-C23	2.12	121.34	113.62
27	d	410	LMG	O7-C10-O9	-2.12	118.58	123.70
24	c	516	BCR	C36-C18-C17	-2.12	119.95	122.92
24	K	101	BCR	C31-C1-C6	2.12	113.74	110.30
22	b	609	CLA	C1-C2-C3	-2.12	122.38	126.04
22	b	604	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
28	f	102	SQD	O7-S-C6	2.12	109.46	106.94
28	f	102	SQD	O5-C1-O6	2.12	114.99	109.97
24	k	102	BCR	C16-C15-C14	-2.12	119.14	123.47
22	d	404	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
22	B	614	CLA	O1D-CGD-CBD	2.12	128.82	124.48
33	e	101	LHG	C20-C19-C18	-2.12	103.68	114.42
29	C	515	DGD	CCB-CBB-CAB	-2.12	103.68	114.42
22	B	602	CLA	C2A-C1A-CHA	2.11	127.56	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	603	CLA	C5-C3-C2	-2.11	116.84	121.12
24	B	618	BCR	C3-C4-C5	-2.11	110.31	114.08
22	b	608	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
22	B	604	CLA	CMD-C2D-C3D	2.11	128.63	124.68
33	E	101	LHG	C20-C19-C18	-2.11	103.72	114.42
24	T	101	BCR	C30-C25-C26	-2.11	119.64	122.61
33	E	101	LHG	C18-C17-C16	-2.11	103.73	114.42
22	c	505	CLA	CMC-C2C-C1C	2.11	128.25	125.04
22	C	510	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
22	C	502	CLA	C2A-C1A-CHA	2.11	127.54	123.86
24	K	102	BCR	C16-C15-C14	-2.10	119.16	123.47
22	C	510	CLA	CHA-C1A-NA	-2.10	121.58	126.40
24	t	101	BCR	C2-C3-C4	-2.10	106.67	111.38
28	f	102	SQD	O47-C7-O49	-2.10	118.62	123.70
22	a	410	CLA	C3C-C4C-NC	-2.10	108.22	110.57
22	c	505	CLA	CHB-C4A-NA	2.10	127.42	124.51
22	b	610	CLA	C2A-C1A-CHA	2.10	127.53	123.86
24	b	619	BCR	C30-C25-C26	-2.10	119.66	122.61
24	b	618	BCR	C27-C26-C25	2.10	125.78	122.73
22	C	512	CLA	CHA-C1A-NA	-2.10	121.59	126.40
27	D	407	LMG	O3-C3-C2	-2.10	105.50	110.35
22	b	604	CLA	OBD-CAD-C3D	2.10	131.46	127.98
27	A	410	LMG	C1-C2-C3	-2.10	105.63	110.00
23	d	401	PHO	CAA-CBA-CGA	-2.10	107.13	113.25
22	c	502	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	c	516	BCR	C15-C16-C17	-2.09	119.18	123.47
22	C	503	CLA	C1-C2-C3	2.09	129.66	126.04
29	c	519	DGD	CDB-CCB-CBB	-2.09	103.80	114.42
22	C	510	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
27	a	415	LMG	C1-O6-C5	-2.09	109.58	113.69
22	B	611	CLA	C1-C2-C3	-2.09	122.43	126.04
33	D	409	LHG	C20-C19-C18	-2.09	103.83	114.42
26	D	406	PL9	C20-C19-C21	2.09	118.78	115.27
22	b	613	CLA	C2A-C1A-CHA	2.09	127.51	123.86
22	c	506	CLA	O1D-CGD-CBD	2.08	128.75	124.48
22	b	601	CLA	CBA-CAA-C2A	2.08	120.02	113.86
29	C	517	DGD	CDB-CCB-CBB	-2.08	103.84	114.42
28	B	622	SQD	C1-C2-C3	-2.08	105.66	110.00
22	b	608	CLA	C2A-C3A-C4A	2.08	105.23	101.87
22	C	502	CLA	O2D-CGD-O1D	-2.08	119.76	123.84
29	C	516	DGD	C4E-C3E-C2E	-2.08	107.19	110.82
29	A	413	DGD	C5B-C4B-C3B	-2.08	103.85	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	CHC-C1C-NC	2.08	127.36	124.20
23	D	401	PHO	C3C-C4C-NC	-2.08	107.05	110.28
22	b	615	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
22	b	608	CLA	OBD-CAD-C3D	2.08	131.43	127.98
26	d	406	PL9	O1-C4-C3	-2.07	118.44	120.72
27	b	621	LMG	C1-O6-C5	-2.07	109.62	113.69
24	c	516	BCR	C1-C6-C5	-2.07	119.70	122.61
24	b	619	BCR	C38-C26-C25	-2.07	122.20	124.53
24	h	101	BCR	C1-C6-C5	-2.07	119.70	122.61
29	C	516	DGD	C8B-C7B-C6B	-2.07	103.93	114.42
22	B	606	CLA	OBD-CAD-CBD	-2.07	122.94	125.89
22	C	511	CLA	C1D-CHD-C4C	2.07	125.28	122.56
22	b	616	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
24	h	101	BCR	C16-C17-C18	-2.07	124.36	127.31
24	a	406	BCR	C24-C23-C22	-2.07	123.11	126.23
29	c	517	DGD	O3E-C3E-C2E	-2.06	105.58	110.35
29	C	515	DGD	C9B-C8B-C7B	-2.06	103.95	114.42
29	A	413	DGD	O5D-C1E-C2E	2.06	111.52	108.30
22	a	410	CLA	C2A-C1A-CHA	2.06	127.46	123.86
22	C	503	CLA	C3A-C2A-C1A	2.06	104.42	101.34
33	l	101	LHG	C20-C19-C18	-2.06	103.98	114.42
22	b	606	CLA	C1D-CHD-C4C	2.06	125.27	122.56
22	b	605	CLA	O1A-CGA-CBA	2.06	131.75	123.73
22	b	614	CLA	C1D-CHD-C4C	2.06	125.27	122.56
22	B	606	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
22	c	513	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
22	d	403	CLA	C2C-C1C-NC	2.05	111.89	109.97
22	b	613	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
22	C	503	CLA	C5-C3-C2	-2.05	116.97	121.12
22	C	513	CLA	O1D-CGD-CBD	2.05	128.68	124.48
22	B	607	CLA	CHC-C1C-C2C	-2.05	121.06	126.72
22	C	508	CLA	CHB-C4A-NA	2.05	127.34	124.51
22	B	605	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
22	B	615	CLA	C3B-C4B-NB	-2.05	106.56	109.21
22	c	504	CLA	OBD-CAD-CBD	-2.05	122.97	125.89
26	d	406	PL9	C46-C47-C48	-2.05	105.16	111.88
22	c	505	CLA	OBD-CAD-CBD	-2.05	122.97	125.89
28	f	102	SQD	C45-O47-C7	2.05	122.83	117.79
23	a	404	PHO	CHC-C1C-C2C	-2.05	120.59	125.73
29	c	518	DGD	C8B-C7B-C6B	-2.04	104.05	114.42
22	b	607	CLA	OBD-CAD-CBD	-2.04	122.97	125.89
24	t	101	BCR	C1-C6-C5	-2.04	119.74	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	L	102	LHG	O6-P-O5	-2.04	101.09	109.07
28	a	411	SQD	O5-C5-C4	2.04	113.40	109.69
22	a	405	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
22	c	513	CLA	CHC-C1C-NC	2.04	127.30	124.20
22	c	514	CLA	CHD-C4C-NC	2.04	127.42	124.20
22	b	603	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
22	c	511	CLA	O2D-CGD-CBD	2.04	114.89	111.27
24	C	514	BCR	C15-C14-C13	-2.04	124.40	127.31
29	H	103	DGD	C8B-C7B-C6B	-2.04	104.08	114.42
27	D	407	LMG	C38-C37-C36	-2.04	104.09	114.42
22	B	612	CLA	C4C-C3C-C2C	-2.04	103.93	106.90
27	c	520	LMG	O6-C1-O1	-2.04	105.15	109.97
22	b	612	CLA	OBD-CAD-C3D	2.04	131.36	127.98
27	a	415	LMG	O1-C1-C2	2.04	111.48	108.30
22	b	607	CLA	O2A-C1-C2	-2.03	103.29	108.64
24	B	617	BCR	C37-C22-C23	2.03	121.28	118.08
22	c	507	CLA	CHA-C1A-NA	-2.03	121.74	126.40
28	D	408	SQD	C44-O6-C1	2.03	117.21	113.84
22	c	508	CLA	CHB-C4A-NA	2.03	127.32	124.51
22	b	605	CLA	O2D-CGD-CBD	2.03	114.88	111.27
26	a	409	PL9	C27-C28-C29	-2.03	122.77	127.66
22	b	613	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
22	B	616	CLA	CHB-C4A-NA	2.03	127.32	124.51
22	d	404	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
22	b	610	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
27	D	411	LMG	O7-C10-O9	-2.03	118.80	123.70
22	C	504	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
22	b	612	CLA	C1-C2-C3	-2.03	122.54	126.04
22	C	504	CLA	CHA-C1A-NA	-2.03	121.76	126.40
24	t	101	BCR	C16-C15-C14	-2.02	119.33	123.47
22	B	604	CLA	C11-C12-C13	-2.02	109.38	115.92
27	D	407	LMG	O1-C1-C2	-2.02	105.15	108.30
29	C	516	DGD	O3G-C1D-C2D	-2.02	105.15	108.30
22	b	604	CLA	C2A-C1A-CHA	2.02	127.39	123.86
22	C	506	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
22	B	610	CLA	CMA-C3A-C4A	-2.02	106.35	111.77
22	c	510	CLA	O2D-CGD-CBD	2.02	114.86	111.27
22	C	511	CLA	CMD-C2D-C3D	2.02	128.45	124.68
22	c	509	CLA	CMB-C2B-C3B	2.02	128.45	124.68
28	A	411	SQD	O5-C5-C4	2.02	113.36	109.69
22	A	405	CLA	C3D-CAD-CBD	-2.02	104.95	107.61
22	A	403	CLA	O2A-CGA-O1A	-2.02	118.50	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	514	CLA	O1D-CGD-CBD	2.02	128.61	124.48
29	C	516	DGD	O3D-C3D-C4D	-2.02	105.69	110.35
28	a	411	SQD	O8-S-O9	-2.01	106.35	111.27
28	B	622	SQD	O3-C3-C2	-2.01	105.69	110.35
24	b	619	BCR	C15-C16-C17	-2.01	119.35	123.47
28	L	101	SQD	O3-C3-C4	2.01	115.00	110.35
27	M	101	LMG	C32-C31-C30	-2.01	104.21	114.42
22	C	510	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
22	C	502	CLA	CED-O2D-CGD	2.01	120.49	115.94
24	C	514	BCR	C29-C30-C25	2.01	113.58	110.48
22	B	604	CLA	C6-C7-C8	-2.01	109.42	115.92
24	A	406	BCR	C38-C26-C27	-2.01	109.75	113.62
24	B	618	BCR	C40-C30-C25	2.01	113.56	110.30
22	b	610	CLA	O2D-CGD-CBD	2.01	114.84	111.27
22	c	502	CLA	OBD-CAD-CBD	-2.01	123.03	125.89
33	D	410	LHG	C6-C5-C4	2.01	116.53	111.79
24	K	102	BCR	C38-C26-C25	-2.00	122.28	124.53
22	a	405	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
22	b	615	CLA	C5-C3-C2	-2.00	117.06	121.12
24	B	617	BCR	C15-C16-C17	-2.00	119.37	123.47
22	B	611	CLA	C4A-NA-C1A	2.00	107.61	106.71
24	A	406	BCR	C4-C5-C6	2.00	125.64	122.73
24	b	619	BCR	C36-C18-C17	-2.00	120.12	122.92

All (178) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	b	613	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND

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Mol	Chain	Res	Type	Atom
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	C	508	CLA	NA
22	c	506	CLA	ND
22	c	506	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	C	510	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	d	403	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	D	405	CLA	NC
22	D	405	CLA	ND
22	D	405	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	B	616	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	611	CLA	NC
22	b	611	CLA	ND
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	610	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	b	601	CLA	ND
22	b	601	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	608	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA

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Mol	Chain	Res	Type	Atom
22	A	403	CLA	NA
22	c	513	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	ND
22	a	402	CLA	NC
22	a	402	CLA	ND
22	a	402	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	c	514	CLA	NC
22	c	514	CLA	ND
22	c	514	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	C	506	CLA	ND
22	C	506	CLA	NA
22	D	404	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	NA
22	B	612	CLA	ND
22	b	602	CLA	NA
22	D	403	CLA	NA
22	a	410	CLA	NA
22	b	612	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	C	513	CLA	NC

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Mol	Chain	Res	Type	Atom
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	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	NA
22	c	508	CLA	ND
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	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	609	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	d	404	CLA	ND
22	d	404	CLA	NA
22	a	403	CLA	NC
22	a	403	CLA	NA
22	b	609	CLA	NC
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA

All (1855) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	413	DGD	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
29	A	413	DGD	O1B-C1B-O2G-C2G
28	L	101	SQD	C8-C7-O47-C45
28	L	101	SQD	O10-C23-O48-C46
28	L	101	SQD	C24-C23-O48-C46
24	a	406	BCR	C36-C18-C19-C20
24	a	406	BCR	C37-C22-C23-C24
27	c	523	LMG	O6-C1-O1-C7
22	C	512	CLA	C11-C10-C8-C9
31	C	518	STE	C1-C2-C3-C4
28	B	622	SQD	C2-C1-O6-C44
28	B	622	SQD	O5-C1-O6-C44
28	B	622	SQD	O6-C44-C45-O47
28	B	622	SQD	O49-C7-O47-C45
28	B	622	SQD	C8-C7-O47-C45
24	k	101	BCR	C7-C8-C9-C34
24	k	101	BCR	C35-C13-C14-C15
24	k	101	BCR	C17-C18-C19-C20
24	k	101	BCR	C36-C18-C19-C20
24	k	101	BCR	C37-C22-C23-C24
22	c	510	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	C11-C10-C8-C9
24	c	515	BCR	C11-C12-C13-C35
24	c	515	BCR	C22-C23-C24-C25
26	d	406	PL9	C32-C33-C34-C36
26	d	406	PL9	C37-C38-C39-C41
26	d	406	PL9	C42-C43-C44-C45
26	d	406	PL9	C42-C43-C44-C46
26	d	406	PL9	C47-C48-C49-C51
24	F	101	BCR	C23-C24-C25-C26
24	F	101	BCR	C23-C24-C25-C30
22	A	405	CLA	C2-C3-C5-C6
22	A	405	CLA	C4-C3-C5-C6
24	b	619	BCR	C11-C12-C13-C35
24	b	619	BCR	C16-C17-C18-C36
24	b	619	BCR	C20-C21-C22-C37
31	J	101	STE	C1-C2-C3-C4
26	D	406	PL9	C32-C33-C34-C36
31	B	601	STE	C1-C2-C3-C4
31	j	101	STE	C1-C2-C3-C4
27	A	410	LMG	O9-C10-O7-C8
24	H	102	BCR	C11-C12-C13-C14
24	H	102	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
28	a	412	SQD	C8-C7-O47-C45
28	a	412	SQD	O10-C23-O48-C46
28	a	412	SQD	C24-C23-O48-C46
24	K	102	BCR	C1-C6-C7-C8
24	K	102	BCR	C5-C6-C7-C8
24	K	102	BCR	C21-C22-C23-C24
24	K	102	BCR	C37-C22-C23-C24
34	f	101	HEC	C2A-CAA-CBA-CGA
26	A	409	PL9	C23-C24-C26-C27
26	A	409	PL9	C32-C33-C34-C35
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C40
26	A	409	PL9	C37-C38-C39-C41
31	B	624	STE	C1-C2-C3-C4
33	E	101	LHG	O1-C1-C2-O2
33	E	101	LHG	O1-C1-C2-C3
33	E	101	LHG	C4-O6-P-O4
24	k	102	BCR	C35-C13-C14-C15
22	C	502	CLA	CHA-CBD-CGD-O1D
22	b	601	CLA	C1A-C2A-CAA-CBA
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C11-C12-C13-C35
24	T	101	BCR	C12-C13-C14-C15
24	T	101	BCR	C16-C17-C18-C36
24	T	101	BCR	C17-C18-C19-C20
24	T	101	BCR	C36-C18-C19-C20
24	T	101	BCR	C20-C21-C22-C37
22	b	607	CLA	C2-C3-C5-C6
22	b	607	CLA	C4-C3-C5-C6
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	CAD-CBD-CGD-O2D
22	B	614	CLA	C4-C3-C5-C6
28	D	408	SQD	C45-C44-O6-C1
28	D	408	SQD	C5-C6-S-O8
24	b	618	BCR	C23-C24-C25-C30
24	c	516	BCR	C36-C18-C19-C20
24	C	514	BCR	C16-C17-C18-C19
24	C	514	BCR	C36-C18-C19-C20
22	c	507	CLA	C12-C13-C15-C16
22	b	614	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	CAD-CBD-CGD-O2D
24	K	101	BCR	C16-C17-C18-C19
24	K	101	BCR	C16-C17-C18-C36
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C2A-CAA-CBA-CGA
27	c	522	LMG	O6-C1-O1-C7
24	A	406	BCR	C7-C8-C9-C34
24	A	406	BCR	C11-C12-C13-C14
24	A	406	BCR	C20-C21-C22-C37
24	A	406	BCR	C37-C22-C23-C24
33	L	102	LHG	C3-O3-P-O4
33	L	102	LHG	C4-O6-P-O4
33	D	412	LHG	O1-C1-C2-C3
31	c	521	STE	C1-C2-C3-C4
31	d	413	STE	C1-C2-C3-C4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C4-O6-P-O4
33	d	408	LHG	C4-O6-P-O5
24	B	618	BCR	C20-C21-C22-C37
24	B	618	BCR	C37-C22-C23-C24
24	B	618	BCR	C23-C24-C25-C30
22	c	514	CLA	CBD-CGD-O2D-CED
26	a	409	PL9	C12-C13-C14-C16
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C32-C33-C34-C36
26	a	409	PL9	C42-C43-C44-C45
26	a	409	PL9	C44-C46-C47-C48
26	a	409	PL9	C47-C48-C49-C50
22	b	606	CLA	CHA-CBD-CGD-O1D
22	b	606	CLA	CHA-CBD-CGD-O2D
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
22	D	404	CLA	CHA-CBD-CGD-O2D
27	b	623	LMG	C2-C1-O1-C7
27	b	623	LMG	O6-C1-O1-C7
31	M	102	STE	C1-C2-C3-C4
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C7-C8-C9-C34
24	B	617	BCR	C35-C13-C14-C15
22	a	410	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	a	410	CLA	CHA-CBD-CGD-O2D
24	b	617	BCR	C36-C18-C19-C20
24	b	617	BCR	C20-C21-C22-C37
22	c	508	CLA	C2-C3-C5-C6
22	c	508	CLA	C4-C3-C5-C6
28	f	102	SQD	O5-C1-O6-C44
28	f	102	SQD	O49-C7-O47-C45
33	D	409	LHG	O2-C2-C3-O3
33	D	409	LHG	C3-O3-P-O4
33	D	409	LHG	C4-O6-P-O4
22	B	606	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O2D
33	D	410	LHG	C1-C2-C3-O3
33	D	410	LHG	C3-O3-P-O4
33	e	101	LHG	O1-C1-C2-C3
33	e	101	LHG	C1-C2-C3-O3
33	e	101	LHG	C3-O3-P-O5
22	a	403	CLA	CHA-CBD-CGD-O1D
22	a	403	CLA	CHA-CBD-CGD-O2D
24	K	103	BCR	C7-C8-C9-C34
22	c	510	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	CBD-CGD-O2D-CED
27	c	523	LMG	O10-C28-O8-C9
27	M	101	LMG	O10-C28-O8-C9
28	f	102	SQD	O10-C23-O48-C46
33	e	101	LHG	O10-C23-O8-C6
22	b	601	CLA	O1D-CGD-O2D-CED
22	d	403	CLA	C3-C5-C6-C7
28	D	408	SQD	C24-C23-O48-C46
26	a	409	PL9	C47-C48-C49-C51
22	b	613	CLA	CBD-CGD-O2D-CED
22	d	403	CLA	CBD-CGD-O2D-CED
28	D	408	SQD	O10-C23-O48-C46
28	a	412	SQD	O49-C7-O47-C45
27	D	411	LMG	O9-C10-O7-C8
27	c	520	LMG	C11-C10-O7-C8
22	b	614	CLA	C3-C5-C6-C7
27	c	523	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9
33	e	101	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C11-C10-O7-C8
28	f	102	SQD	C8-C7-O47-C45
22	c	514	CLA	O1D-CGD-O2D-CED
26	A	409	PL9	C35-C34-C36-C37
22	C	513	CLA	C4-C3-C5-C6
26	d	406	PL9	C38-C39-C41-C42
22	B	614	CLA	C2-C3-C5-C6
22	C	511	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C3-C5-C6-C7
27	a	415	LMG	C29-C28-O8-C9
22	C	513	CLA	CBA-CGA-O2A-C1
29	h	102	DGD	O6E-C5E-C6E-O5E
22	c	512	CLA	O1D-CGD-O2D-CED
26	d	406	PL9	C47-C48-C49-C50
26	A	409	PL9	C12-C13-C14-C15
22	c	507	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	O1D-CGD-O2D-CED
26	A	409	PL9	C22-C23-C24-C26
27	c	522	LMG	O10-C28-O8-C9
27	c	520	LMG	O9-C10-O7-C8
22	B	613	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	b	616	CLA	CBD-CGD-O2D-CED
33	E	101	LHG	O2-C2-C3-O3
33	D	410	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
22	C	513	CLA	C3-C5-C6-C7
29	A	413	DGD	C2A-C1A-O1G-C1G
27	Y	101	LMG	C29-C28-O8-C9
26	A	409	PL9	C47-C48-C49-C50
22	c	503	CLA	CBD-CGD-O2D-CED
27	c	522	LMG	O6-C5-C6-O5
29	C	515	DGD	O6E-C5E-C6E-O5E
33	E	101	LHG	C24-C25-C26-C27
29	H	103	DGD	C4E-C5E-C6E-O5E
33	l	101	LHG	C7-C8-C9-C10
33	D	409	LHG	C23-C24-C25-C26
28	f	102	SQD	C24-C23-O48-C46
29	A	413	DGD	O6E-C5E-C6E-O5E
27	M	101	LMG	O6-C5-C6-O5
28	L	101	SQD	O49-C7-O47-C45
27	b	621	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
29	h	102	DGD	C4E-C5E-C6E-O5E
27	a	415	LMG	O10-C28-O8-C9
22	C	513	CLA	O1A-CGA-O2A-C1
26	D	406	PL9	C47-C48-C49-C51
26	A	409	PL9	C47-C48-C49-C51
26	a	409	PL9	C33-C34-C36-C37
26	d	406	PL9	C34-C36-C37-C38
26	A	409	PL9	C9-C11-C12-C13
26	A	409	PL9	C14-C16-C17-C18
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C34-C36-C37-C38
28	B	622	SQD	C24-C23-O48-C46
27	c	522	LMG	C29-C28-O8-C9
27	a	415	LMG	C4-C5-C6-O5
27	M	101	LMG	C4-C5-C6-O5
31	B	627	STE	C5-C6-C7-C8
27	Y	101	LMG	C11-C10-O7-C8
31	B	626	STE	C11-C12-C13-C14
26	A	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C42-C43-C44-C46
22	A	405	CLA	C3-C5-C6-C7
22	b	613	CLA	O1D-CGD-O2D-CED
29	c	519	DGD	C2A-C1A-O1G-C1G
22	c	507	CLA	CBA-CGA-O2A-C1
27	A	410	LMG	O6-C5-C6-O5
29	A	413	DGD	C4E-C5E-C6E-O5E
22	a	405	CLA	C10-C11-C12-C13
22	C	509	CLA	C13-C15-C16-C17
22	b	611	CLA	C13-C15-C16-C17
22	c	512	CLA	C15-C16-C17-C18
27	A	410	LMG	C28-C29-C30-C31
27	c	523	LMG	C2-C1-O1-C7
28	f	102	SQD	C2-C1-O6-C44
28	a	411	SQD	O6-C44-C45-O47
29	c	519	DGD	O1A-C1A-O1G-C1G
22	C	507	CLA	C4-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
22	C	513	CLA	C2-C3-C5-C6
22	c	510	CLA	C6-C7-C8-C9
22	c	510	CLA	C11-C12-C13-C14
23	A	404	PHO	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C11-C10-C8-C9
22	H	101	CLA	C11-C12-C13-C14
22	A	403	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C10-C8-C9
22	c	513	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	C10-C11-C12-C13
24	F	101	BCR	C37-C22-C23-C24
24	b	619	BCR	C7-C8-C9-C34
24	d	405	BCR	C37-C22-C23-C24
24	c	515	BCR	C11-C12-C13-C14
24	d	405	BCR	C21-C22-C23-C24
27	b	623	LMG	O9-C10-O7-C8
31	C	520	STE	C4-C5-C6-C7
33	d	409	LHG	C24-C25-C26-C27
27	A	410	LMG	C4-C5-C6-O5
27	M	101	LMG	C10-C11-C12-C13
33	e	101	LHG	C23-C24-C25-C26
27	b	623	LMG	O10-C28-O8-C9
22	A	402	CLA	C15-C16-C17-C18
22	b	601	CLA	C3-C5-C6-C7
22	C	504	CLA	C8-C10-C11-C12
22	b	608	CLA	C13-C15-C16-C17
22	D	403	CLA	C15-C16-C17-C18
22	B	609	CLA	C13-C15-C16-C17
22	b	603	CLA	C5-C6-C7-C8
28	B	622	SQD	C23-C24-C25-C26
28	A	411	SQD	C7-C8-C9-C10
29	c	517	DGD	C1B-C2B-C3B-C4B
22	c	504	CLA	CBD-CGD-O2D-CED
29	H	103	DGD	O6E-C5E-C6E-O5E
22	c	510	CLA	C10-C11-C12-C13
22	c	506	CLA	C13-C15-C16-C17
22	B	615	CLA	C5-C6-C7-C8
22	D	405	CLA	C13-C15-C16-C17
22	b	611	CLA	C8-C10-C11-C12
22	B	603	CLA	C8-C10-C11-C12
22	c	504	CLA	C8-C10-C11-C12
22	b	607	CLA	C10-C11-C12-C13
22	b	606	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C13-C15-C16-C17
22	C	513	CLA	C15-C16-C17-C18
22	b	616	CLA	C10-C11-C12-C13
22	B	606	CLA	C15-C16-C17-C18
22	C	505	CLA	C5-C6-C7-C8
22	a	403	CLA	C8-C10-C11-C12
22	d	403	CLA	O1D-CGD-O2D-CED
26	a	409	PL9	C12-C13-C14-C15
28	L	101	SQD	C23-C24-C25-C26
27	d	410	LMG	C28-C29-C30-C31
27	D	411	LMG	C10-C11-C12-C13
22	d	404	CLA	CBD-CGD-O2D-CED
22	B	605	CLA	C15-C16-C17-C18
22	c	506	CLA	C15-C16-C17-C18
22	A	403	CLA	C13-C15-C16-C17
22	B	612	CLA	C13-C15-C16-C17
22	C	512	CLA	C10-C11-C12-C13
22	B	614	CLA	C13-C15-C16-C17
22	b	606	CLA	C10-C11-C12-C13
22	C	513	CLA	C5-C6-C7-C8
22	C	505	CLA	C10-C11-C12-C13
27	D	407	LMG	C10-C11-C12-C13
22	b	605	CLA	C5-C6-C7-C8
22	B	607	CLA	C15-C16-C17-C18
22	C	508	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	a	402	CLA	C12-C13-C15-C16
22	c	507	CLA	O1A-CGA-O2A-C1
33	E	101	LHG	C27-C28-C29-C30
22	B	616	CLA	CBD-CGD-O2D-CED
22	a	405	CLA	C15-C16-C17-C18
22	b	614	CLA	C5-C6-C7-C8
22	b	605	CLA	C15-C16-C17-C18
22	B	607	CLA	C13-C15-C16-C17
22	C	511	CLA	C8-C10-C11-C12
22	B	606	CLA	C13-C15-C16-C17
29	C	515	DGD	C4E-C5E-C6E-O5E
28	A	412	SQD	C44-C45-O47-C7
28	A	412	SQD	C46-C45-O47-C7
22	C	513	CLA	CBD-CGD-O2D-CED
29	C	516	DGD	O6E-C1E-O5D-C6D
22	c	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C19-C21-C22-C23
26	A	409	PL9	C24-C26-C27-C28
26	A	409	PL9	C34-C36-C37-C38
26	A	409	PL9	C44-C46-C47-C48
29	c	518	DGD	C1A-C2A-C3A-C4A
27	c	522	LMG	C10-C11-C12-C13
24	c	515	BCR	C18-C19-C20-C21
24	K	102	BCR	C10-C11-C12-C13
24	K	101	BCR	C18-C19-C20-C21
24	B	618	BCR	C18-C19-C20-C21
24	d	405	BCR	C10-C11-C12-C13
33	d	407	LHG	O2-C2-C3-O3
22	B	603	CLA	C13-C15-C16-C17
22	C	506	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
22	b	616	CLA	C8-C10-C11-C12
22	a	405	CLA	C5-C6-C7-C8
22	C	502	CLA	C13-C15-C16-C17
22	b	615	CLA	C5-C6-C7-C8
22	B	606	CLA	C8-C10-C11-C12
27	a	415	LMG	C12-C13-C14-C15
33	d	408	LHG	C4-O6-P-O3
33	D	409	LHG	C3-O3-P-O6
33	D	410	LHG	C3-O3-P-O6
33	e	101	LHG	C3-O3-P-O6
29	C	515	DGD	C1B-C2B-C3B-C4B
22	B	608	CLA	C3-C5-C6-C7
22	b	605	CLA	C10-C11-C12-C13
22	b	602	CLA	C15-C16-C17-C18
33	E	101	LHG	C1-C2-C3-O3
33	d	407	LHG	C1-C2-C3-O3
33	D	409	LHG	C1-C2-C3-O3
22	c	513	CLA	C13-C15-C16-C17
22	b	606	CLA	C2A-CAA-CBA-CGA
22	B	606	CLA	C2A-CAA-CBA-CGA
22	B	615	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	D	403	CLA	C3-C5-C6-C7
27	c	522	LMG	C4-C5-C6-O5
27	c	520	LMG	C36-C37-C38-C39
29	c	519	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
29	C	517	DGD	C8A-C9A-CAA-CBA
29	h	102	DGD	C6B-C7B-C8B-C9B
31	c	521	STE	C9-C10-C11-C12
29	C	515	DGD	C3B-C4B-C5B-C6B
24	c	515	BCR	C35-C13-C14-C15
24	F	101	BCR	C35-C13-C14-C15
24	F	101	BCR	C20-C21-C22-C37
24	b	619	BCR	C35-C13-C14-C15
24	T	101	BCR	C35-C13-C14-C15
24	b	618	BCR	C35-C13-C14-C15
24	b	618	BCR	C16-C17-C18-C36
24	c	516	BCR	C16-C17-C18-C36
24	c	516	BCR	C20-C21-C22-C37
24	C	514	BCR	C16-C17-C18-C36
24	A	406	BCR	C11-C10-C9-C34
24	A	406	BCR	C35-C13-C14-C15
24	B	619	BCR	C11-C10-C9-C34
24	B	619	BCR	C20-C21-C22-C37
24	t	101	BCR	C11-C10-C9-C34
24	t	101	BCR	C35-C13-C14-C15
24	t	101	BCR	C16-C17-C18-C36
24	B	618	BCR	C35-C13-C14-C15
24	b	617	BCR	C35-C13-C14-C15
24	d	405	BCR	C35-C13-C14-C15
24	K	103	BCR	C11-C10-C9-C34
24	K	103	BCR	C35-C13-C14-C15
31	B	625	STE	C11-C12-C13-C14
27	c	523	LMG	C15-C16-C17-C18
31	C	518	STE	C4-C5-C6-C7
33	E	101	LHG	C18-C19-C20-C21
33	E	101	LHG	C32-C33-C34-C35
29	c	517	DGD	C4A-C5A-C6A-C7A
29	h	102	DGD	C6A-C7A-C8A-C9A
31	c	521	STE	C7-C8-C9-C10
33	d	408	LHG	C13-C14-C15-C16
29	C	515	DGD	C5B-C6B-C7B-C8B
33	l	101	LHG	C17-C18-C19-C20
27	b	621	LMG	C16-C17-C18-C19
27	b	623	LMG	C32-C33-C34-C35
33	d	407	LHG	C17-C18-C19-C20
33	d	407	LHG	C28-C29-C30-C31
28	a	411	SQD	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	C11-C12-C13-C15
22	c	504	CLA	C16-C17-C18-C20
22	B	604	CLA	CBA-CGA-O2A-C1
28	L	101	SQD	C26-C27-C28-C29
29	c	519	DGD	C4A-C5A-C6A-C7A
29	C	516	DGD	C7A-C8A-C9A-CAA
28	L	101	SQD	C46-C45-O47-C7
27	b	623	LMG	C9-C8-O7-C10
29	c	519	DGD	CCB-CDB-CEB-CFB
31	d	412	STE	C5-C6-C7-C8
27	A	410	LMG	C31-C32-C33-C34
29	c	517	DGD	C6B-C7B-C8B-C9B
33	d	408	LHG	C26-C27-C28-C29
31	Z	101	STE	C11-C12-C13-C14
28	a	411	SQD	C9-C10-C11-C12
33	D	410	LHG	C29-C30-C31-C32
22	B	613	CLA	O1D-CGD-O2D-CED
27	a	415	LMG	O6-C5-C6-O5
31	B	627	STE	C9-C10-C11-C12
33	E	101	LHG	C12-C13-C14-C15
31	E	102	STE	C6-C7-C8-C9
27	a	415	LMG	C36-C37-C38-C39
27	M	101	LMG	C37-C38-C39-C40
31	B	623	STE	C11-C10-C9-C8
22	c	503	CLA	O1D-CGD-O2D-CED
31	m	101	STE	C9-C10-C11-C12
31	m	101	STE	C10-C11-C12-C13
31	b	622	STE	C6-C7-C8-C9
28	a	412	SQD	C14-C15-C16-C17
28	A	411	SQD	C10-C11-C12-C13
33	L	102	LHG	C14-C15-C16-C17
31	H	104	STE	C4-C5-C6-C7
33	D	410	LHG	C25-C26-C27-C28
27	M	101	LMG	C28-C29-C30-C31
33	d	407	LHG	C23-C24-C25-C26
22	b	616	CLA	O1D-CGD-O2D-CED
22	C	511	CLA	O1D-CGD-O2D-CED
24	k	101	BCR	C12-C13-C14-C15
29	c	518	DGD	C2E-C1E-O5D-C6D
24	T	101	BCR	C16-C17-C18-C19
28	D	408	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
24	h	101	BCR	C11-C10-C9-C8
24	C	514	BCR	C12-C13-C14-C15
24	K	101	BCR	C11-C10-C9-C8
24	B	619	BCR	C12-C13-C14-C15
24	B	617	BCR	C11-C10-C9-C8
24	B	617	BCR	C12-C13-C14-C15
24	b	617	BCR	C20-C21-C22-C23
29	C	516	DGD	C2E-C1E-O5D-C6D
27	D	407	LMG	C15-C16-C17-C18
31	B	624	STE	C6-C7-C8-C9
27	a	415	LMG	C14-C15-C16-C17
31	I	101	STE	C7-C8-C9-C10
27	M	101	LMG	C32-C33-C34-C35
33	d	408	LHG	C29-C30-C31-C32
28	A	412	SQD	C15-C16-C17-C18
27	b	621	LMG	C33-C34-C35-C36
28	f	102	SQD	C33-C34-C35-C36
28	a	411	SQD	C34-C35-C36-C37
29	C	516	DGD	C3A-C4A-C5A-C6A
22	c	513	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C19
22	C	510	CLA	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
26	a	409	PL9	C15-C14-C16-C17
22	b	609	CLA	C4-C3-C5-C6
29	A	413	DGD	C5B-C6B-C7B-C8B
31	b	620	STE	C6-C7-C8-C9
29	c	518	DGD	C2A-C3A-C4A-C5A
31	d	412	STE	C3-C4-C5-C6
31	d	412	STE	C11-C12-C13-C14
27	A	410	LMG	C16-C17-C18-C19
27	c	522	LMG	C31-C32-C33-C34
33	d	408	LHG	C28-C29-C30-C31
22	C	510	CLA	C2-C3-C5-C6
22	b	616	CLA	C2-C3-C5-C6
22	C	512	CLA	C11-C12-C13-C14
22	C	508	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14
22	b	607	CLA	C11-C10-C8-C9
22	c	507	CLA	C14-C13-C15-C16
22	c	513	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	a	402	CLA	C14-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
27	b	623	LMG	C28-C29-C30-C31
28	L	101	SQD	C24-C25-C26-C27
28	B	622	SQD	C33-C34-C35-C36
33	E	101	LHG	C30-C31-C32-C33
29	c	517	DGD	C4B-C5B-C6B-C7B
27	c	522	LMG	C30-C31-C32-C33
31	T	102	STE	C10-C11-C12-C13
29	h	102	DGD	C2B-C3B-C4B-C5B
31	d	413	STE	C9-C10-C11-C12
31	d	413	STE	C10-C11-C12-C13
33	d	407	LHG	C16-C17-C18-C19
33	D	409	LHG	C31-C32-C33-C34
31	B	626	STE	C4-C5-C6-C7
22	C	512	CLA	C13-C15-C16-C17
22	c	507	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	b	603	CLA	C8-C10-C11-C12
27	c	520	LMG	C39-C40-C41-C42
27	A	410	LMG	C12-C13-C14-C15
29	C	517	DGD	C9A-CAA-CBA-CCA
27	a	415	LMG	C13-C14-C15-C16
27	D	411	LMG	C34-C35-C36-C37
27	Y	101	LMG	C36-C37-C38-C39
29	h	102	DGD	C5B-C6B-C7B-C8B
31	c	521	STE	C6-C7-C8-C9
33	l	101	LHG	C29-C30-C31-C32
27	b	623	LMG	C19-C20-C21-C22
31	B	626	STE	C5-C6-C7-C8
33	d	409	LHG	O1-C1-C2-C3
33	d	407	LHG	O1-C1-C2-C3
22	b	602	CLA	C3-C5-C6-C7
27	d	410	LMG	C38-C39-C40-C41
28	B	622	SQD	C11-C12-C13-C14
27	D	407	LMG	C17-C18-C19-C20
33	L	102	LHG	C30-C31-C32-C33
33	D	410	LHG	C34-C35-C36-C37
29	A	413	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
31	B	625	STE	C2-C3-C4-C5
27	c	523	LMG	C17-C18-C19-C20
27	c	523	LMG	C31-C32-C33-C34
31	b	627	STE	C10-C11-C12-C13
27	D	407	LMG	C12-C13-C14-C15
27	D	407	LMG	C30-C31-C32-C33
28	a	412	SQD	C11-C12-C13-C14
31	m	102	STE	C3-C4-C5-C6
29	C	517	DGD	CBA-CCA-CDA-CEA
27	M	101	LMG	C33-C34-C35-C36
31	B	620	STE	C10-C11-C12-C13
29	h	102	DGD	C3A-C4A-C5A-C6A
33	d	408	LHG	C34-C35-C36-C37
31	d	411	STE	C2-C3-C4-C5
33	l	101	LHG	C32-C33-C34-C35
31	H	104	STE	C6-C7-C8-C9
31	M	102	STE	C7-C8-C9-C10
31	M	102	STE	C11-C10-C9-C8
28	f	102	SQD	C24-C25-C26-C27
31	b	624	STE	C3-C4-C5-C6
33	e	101	LHG	C16-C17-C18-C19
29	C	516	DGD	C4A-C5A-C6A-C7A
29	C	516	DGD	C6A-C7A-C8A-C9A
22	c	513	CLA	C16-C17-C18-C19
22	B	609	CLA	C16-C17-C18-C20
29	c	518	DGD	O6E-C1E-O5D-C6D
29	c	519	DGD	C9A-CAA-CBA-CCA
27	Y	101	LMG	C13-C14-C15-C16
33	L	102	LHG	C12-C13-C14-C15
33	d	408	LHG	C11-C12-C13-C14
27	b	621	LMG	C37-C38-C39-C40
27	b	623	LMG	C18-C19-C20-C21
33	D	409	LHG	C29-C30-C31-C32
33	D	409	LHG	C34-C35-C36-C37
33	D	410	LHG	C13-C14-C15-C16
22	d	404	CLA	O1D-CGD-O2D-CED
29	A	413	DGD	C8B-C9B-CAB-CBB
27	d	410	LMG	C36-C37-C38-C39
29	c	518	DGD	C8B-C9B-CAB-CBB
31	B	601	STE	C5-C6-C7-C8
33	E	101	LHG	C13-C14-C15-C16
29	c	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
33	L	102	LHG	C26-C27-C28-C29
29	H	103	DGD	C7B-C8B-C9B-CAB
28	f	102	SQD	C23-C24-C25-C26
22	B	602	CLA	C13-C15-C16-C17
31	b	622	STE	C5-C6-C7-C8
28	D	408	SQD	C27-C28-C29-C30
28	a	411	SQD	C24-C23-O48-C46
27	a	415	LMG	C38-C39-C40-C41
31	d	411	STE	C4-C5-C6-C7
29	C	515	DGD	C4B-C5B-C6B-C7B
31	M	102	STE	C6-C7-C8-C9
33	d	409	LHG	C26-C27-C28-C29
28	a	411	SQD	C15-C16-C17-C18
31	D	413	STE	C4-C5-C6-C7
22	c	513	CLA	O1D-CGD-O2D-CED
22	H	101	CLA	C3A-C2A-CAA-CBA
22	b	601	CLA	C3A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
22	b	615	CLA	C8-C10-C11-C12
22	b	612	CLA	C13-C15-C16-C17
27	A	410	LMG	C35-C36-C37-C38
28	a	412	SQD	C15-C16-C17-C18
31	c	521	STE	C11-C12-C13-C14
29	H	103	DGD	C7A-C8A-C9A-CAA
33	D	410	LHG	C9-C10-C11-C12
22	a	402	CLA	C16-C17-C18-C19
31	b	620	STE	C9-C10-C11-C12
27	c	522	LMG	C14-C15-C16-C17
27	c	522	LMG	C39-C40-C41-C42
31	T	102	STE	C7-C8-C9-C10
27	M	101	LMG	C35-C36-C37-C38
29	H	103	DGD	C6B-C7B-C8B-C9B
33	e	101	LHG	C27-C28-C29-C30
31	d	411	STE	C6-C7-C8-C9
28	f	102	SQD	C28-C29-C30-C31
31	D	413	STE	C9-C10-C11-C12
29	C	516	DGD	C5A-C6A-C7A-C8A
28	L	101	SQD	C13-C14-C15-C16
31	b	622	STE	C12-C13-C14-C15
27	c	522	LMG	C38-C39-C40-C41
31	c	521	STE	C3-C4-C5-C6
31	d	413	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	b	623	LMG	C38-C39-C40-C41
22	B	613	CLA	C8-C10-C11-C12
22	C	507	CLA	C2-C3-C5-C6
27	D	411	LMG	C11-C10-O7-C8
31	b	622	STE	C14-C15-C16-C17
29	c	517	DGD	CBB-CCB-CDB-CEB
29	C	516	DGD	CCA-CDA-CEA-CFA
27	Y	101	LMG	O6-C5-C6-O5
33	D	412	LHG	O1-C1-C2-O2
33	e	101	LHG	O1-C1-C2-O2
28	B	622	SQD	C17-C18-C19-C20
29	c	518	DGD	CAA-CBA-CCA-CDA
31	b	622	STE	C13-C14-C15-C16
29	C	517	DGD	C5A-C6A-C7A-C8A
31	C	519	STE	C4-C5-C6-C7
33	D	412	LHG	C32-C33-C34-C35
31	a	414	STE	C4-C5-C6-C7
29	A	413	DGD	CBB-CCB-CDB-CEB
22	H	101	CLA	CBA-CGA-O2A-C1
28	A	411	SQD	C26-C27-C28-C29
31	H	104	STE	C2-C3-C4-C5
22	C	512	CLA	CBD-CGD-O2D-CED
27	c	520	LMG	C33-C34-C35-C36
28	A	411	SQD	C24-C25-C26-C27
28	D	408	SQD	C25-C26-C27-C28
27	Y	101	LMG	C35-C36-C37-C38
33	d	407	LHG	C11-C10-C9-C8
27	Y	101	LMG	O9-C10-O7-C8
29	A	413	DGD	CAA-CBA-CCA-CDA
27	c	523	LMG	C32-C33-C34-C35
31	b	627	STE	C13-C14-C15-C16
27	D	407	LMG	C35-C36-C37-C38
28	a	412	SQD	C24-C25-C26-C27
27	M	101	LMG	C34-C35-C36-C37
33	D	409	LHG	C14-C15-C16-C17
29	C	516	DGD	C8B-C9B-CAB-CBB
22	b	602	CLA	C8-C10-C11-C12
29	C	517	DGD	C4A-C5A-C6A-C7A
33	E	101	LHG	C28-C29-C30-C31
27	Y	101	LMG	C37-C38-C39-C40
33	l	101	LHG	C34-C35-C36-C37
33	d	409	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
24	k	101	BCR	C1-C6-C7-C8
24	k	101	BCR	C5-C6-C7-C8
24	c	515	BCR	C1-C6-C7-C8
24	c	515	BCR	C5-C6-C7-C8
24	H	102	BCR	C23-C24-C25-C26
24	H	102	BCR	C23-C24-C25-C30
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	b	618	BCR	C23-C24-C25-C26
24	A	406	BCR	C23-C24-C25-C26
24	A	406	BCR	C23-C24-C25-C30
24	B	617	BCR	C5-C6-C7-C8
31	B	625	STE	C7-C8-C9-C10
29	c	519	DGD	CBA-CCA-CDA-CEA
28	D	408	SQD	C32-C33-C34-C35
31	I	101	STE	C10-C11-C12-C13
33	D	412	LHG	C29-C30-C31-C32
27	b	621	LMG	C11-C10-O7-C8
31	m	101	STE	C4-C5-C6-C7
31	b	627	STE	C5-C6-C7-C8
29	C	517	DGD	C6B-C7B-C8B-C9B
27	a	415	LMG	C41-C42-C43-C44
27	Y	101	LMG	C17-C18-C19-C20
33	D	412	LHG	C28-C29-C30-C31
31	d	413	STE	C4-C5-C6-C7
33	D	409	LHG	C28-C29-C30-C31
28	B	622	SQD	O10-C23-O48-C46
22	c	511	CLA	CBD-CGD-O2D-CED
29	c	519	DGD	CCA-CDA-CEA-CFA
27	A	410	LMG	C33-C34-C35-C36
22	C	512	CLA	C11-C12-C13-C15
26	d	406	PL9	C43-C44-C46-C47
22	C	508	CLA	C11-C10-C8-C7
22	c	506	CLA	C6-C7-C8-C10
26	D	406	PL9	C13-C14-C16-C17
22	b	604	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	A	403	CLA	C11-C12-C13-C15
22	c	513	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	602	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C10-C8-C7
22	b	609	CLA	C2-C3-C5-C6
27	Y	101	LMG	O10-C28-O8-C9
33	L	102	LHG	O10-C23-O8-C6
22	B	604	CLA	O1A-CGA-O2A-C1
22	C	503	CLA	C5-C6-C7-C8
22	d	403	CLA	C16-C17-C18-C19
22	C	501	CLA	O1D-CGD-O2D-CED
27	c	522	LMG	O9-C10-O7-C8
31	B	620	STE	C11-C12-C13-C14
33	L	102	LHG	C13-C14-C15-C16
22	B	613	CLA	C5-C6-C7-C8
28	B	622	SQD	C9-C10-C11-C12
31	E	102	STE	C5-C6-C7-C8
27	a	415	LMG	C39-C40-C41-C42
29	c	518	DGD	C7A-C8A-C9A-CAA
28	a	411	SQD	C12-C13-C14-C15
29	H	103	DGD	C1A-C2A-C3A-C4A
33	E	101	LHG	C16-C17-C18-C19
33	e	101	LHG	C11-C10-C9-C8
26	d	406	PL9	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C35
22	c	504	CLA	O1D-CGD-O2D-CED
27	B	621	LMG	C16-C17-C18-C19
27	Y	101	LMG	C15-C16-C17-C18
33	D	412	LHG	C11-C12-C13-C14
29	C	515	DGD	C6A-C7A-C8A-C9A
33	l	101	LHG	C13-C14-C15-C16
22	A	402	CLA	C2C-C3C-CAC-CBC
24	B	617	BCR	C6-C7-C8-C9
24	d	405	BCR	C22-C23-C24-C25
22	B	614	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
27	b	621	LMG	C29-C28-O8-C9
28	L	101	SQD	O5-C1-O6-C44
26	d	406	PL9	C44-C46-C47-C48
27	c	520	LMG	C34-C35-C36-C37
27	c	520	LMG	C38-C39-C40-C41
29	C	515	DGD	CCB-CDB-CEB-CFB
31	b	626	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
28	a	411	SQD	C24-C25-C26-C27
33	E	101	LHG	C23-C24-C25-C26
27	M	101	LMG	C11-C10-O7-C8
27	b	623	LMG	C11-C10-O7-C8
33	D	409	LHG	C8-C7-O7-C5
29	c	518	DGD	CBB-CCB-CDB-CEB
33	D	412	LHG	C27-C28-C29-C30
28	A	412	SQD	C13-C14-C15-C16
31	M	102	STE	C9-C10-C11-C12
29	H	103	DGD	CCA-CDA-CEA-CFA
22	H	101	CLA	C5-C6-C7-C8
22	b	603	CLA	CBD-CGD-O2D-CED
31	b	620	STE	C11-C10-C9-C8
31	B	625	STE	C11-C10-C9-C8
27	c	523	LMG	C38-C39-C40-C41
29	h	102	DGD	C3B-C4B-C5B-C6B
29	A	413	DGD	O2G-C2G-C3G-O3G
27	a	415	LMG	O7-C8-C9-O8
22	c	513	CLA	CBA-CGA-O2A-C1
33	d	409	LHG	C34-C35-C36-C37
22	C	513	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C16-C17-C18-C19
22	H	101	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C20
22	D	404	CLA	C16-C17-C18-C20
33	L	102	LHG	C32-C33-C34-C35
22	C	505	CLA	C2-C3-C5-C6
29	A	413	DGD	C2B-C3B-C4B-C5B
27	M	101	LMG	C12-C13-C14-C15
29	H	103	DGD	CBB-CCB-CDB-CEB
22	b	604	CLA	C14-C13-C15-C16
22	b	601	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C10-C8-C9
22	A	403	CLA	C11-C12-C13-C14
22	c	513	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C12-C13-C14
22	D	404	CLA	C11-C12-C13-C14
22	b	612	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
31	d	413	STE	C3-C4-C5-C6
29	C	517	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
31	d	413	STE	C11-C12-C13-C14
33	D	410	LHG	C32-C33-C34-C35
29	h	102	DGD	C2A-C3A-C4A-C5A
24	h	101	BCR	C11-C12-C13-C14
22	H	101	CLA	O1A-CGA-O2A-C1
22	H	101	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	509	CLA	C1A-C2A-CAA-CBA
22	c	514	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C1A-C2A-CAA-CBA
22	B	616	CLA	C11-C12-C13-C14
22	b	611	CLA	C16-C17-C18-C19
22	c	504	CLA	C16-C17-C18-C19
27	c	523	LMG	O9-C10-O7-C8
27	d	410	LMG	C30-C31-C32-C33
31	j	101	STE	C3-C4-C5-C6
28	A	411	SQD	C16-C17-C18-C19
29	C	517	DGD	C4B-C5B-C6B-C7B
27	c	522	LMG	C15-C16-C17-C18
31	T	102	STE	C11-C10-C9-C8
33	L	102	LHG	C17-C18-C19-C20
29	H	103	DGD	C3A-C4A-C5A-C6A
33	D	409	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O3
29	A	413	DGD	C4A-C5A-C6A-C7A
29	c	518	DGD	C7B-C8B-C9B-CAB
31	T	102	STE	C12-C13-C14-C15
28	f	102	SQD	C32-C33-C34-C35
33	d	409	LHG	C23-C24-C25-C26
22	B	607	CLA	C3-C5-C6-C7
31	T	102	STE	C9-C10-C11-C12
29	C	516	DGD	CCB-CDB-CEB-CFB
22	C	509	CLA	C5-C6-C7-C8
22	c	504	CLA	C5-C6-C7-C8
22	b	607	CLA	C8-C10-C11-C12
29	c	517	DGD	O6E-C5E-C6E-O5E
27	B	621	LMG	C29-C30-C31-C32
29	c	519	DGD	C3A-C4A-C5A-C6A
27	D	407	LMG	C38-C39-C40-C41
27	b	623	LMG	C40-C41-C42-C43
29	A	413	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
33	D	410	LHG	C16-C17-C18-C19
33	E	101	LHG	C29-C30-C31-C32
31	b	626	STE	C10-C11-C12-C13
33	l	101	LHG	C14-C15-C16-C17
33	d	407	LHG	C29-C30-C31-C32
33	e	101	LHG	C12-C13-C14-C15
31	D	413	STE	C5-C6-C7-C8
23	a	404	PHO	C4-C3-C5-C6
31	b	620	STE	C5-C6-C7-C8
31	b	627	STE	C2-C3-C4-C5
31	H	104	STE	C11-C10-C9-C8
27	b	623	LMG	C15-C16-C17-C18
22	C	512	CLA	C8-C10-C11-C12
22	b	613	CLA	C10-C11-C12-C13
22	C	502	CLA	CBD-CGD-O2D-CED
31	C	518	STE	C2-C3-C4-C5
28	a	412	SQD	C17-C18-C19-C20
22	c	513	CLA	O1A-CGA-O2A-C1
29	c	517	DGD	C9B-CAB-CBB-CCB
27	c	522	LMG	C40-C41-C42-C43
27	M	101	LMG	C16-C17-C18-C19
33	l	101	LHG	C27-C28-C29-C30
33	e	101	LHG	C11-C12-C13-C14
22	d	403	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C20
27	D	407	LMG	O6-C5-C6-O5
29	A	413	DGD	C1G-C2G-C3G-O3G
27	c	523	LMG	O1-C7-C8-C9
28	B	622	SQD	O6-C44-C45-C46
27	M	101	LMG	C7-C8-C9-O8
28	a	411	SQD	O6-C44-C45-C46
33	e	101	LHG	C4-C5-C6-O8
27	b	623	LMG	O6-C5-C6-O5
22	b	616	CLA	C5-C6-C7-C8
28	L	101	SQD	C10-C11-C12-C13
33	d	408	LHG	C19-C20-C21-C22
31	H	104	STE	C14-C15-C16-C17
29	c	518	DGD	C5D-C6D-O5D-C1E
27	a	415	LMG	C8-C7-O1-C1
29	C	516	DGD	C2G-C3G-O3G-C1D
31	B	625	STE	C13-C14-C15-C16
29	h	102	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
33	d	409	LHG	C35-C36-C37-C38
27	d	410	LMG	C40-C41-C42-C43
28	a	412	SQD	C31-C32-C33-C34
33	L	102	LHG	C11-C12-C13-C14
33	D	409	LHG	C7-C8-C9-C10
22	b	610	CLA	C2C-C3C-CAC-CBC
22	d	403	CLA	C2C-C3C-CAC-CBC
33	d	407	LHG	O1-C1-C2-O2
31	m	101	STE	C14-C15-C16-C17
33	d	409	LHG	C33-C34-C35-C36
27	c	520	LMG	O6-C5-C6-O5
28	L	101	SQD	C27-C28-C29-C30
28	B	622	SQD	C13-C14-C15-C16
33	D	409	LHG	C17-C18-C19-C20
27	c	523	LMG	C11-C10-O7-C8
31	I	101	STE	C4-C5-C6-C7
31	b	626	STE	C5-C6-C7-C8
22	C	507	CLA	C5-C6-C7-C8
26	d	406	PL9	C45-C44-C46-C47
22	C	505	CLA	C4-C3-C5-C6
28	L	101	SQD	C19-C20-C21-C22
27	D	411	LMG	C11-C12-C13-C14
27	D	411	LMG	C36-C37-C38-C39
33	L	102	LHG	C18-C19-C20-C21
31	b	626	STE	C11-C10-C9-C8
27	D	411	LMG	C29-C28-O8-C9
31	b	625	STE	C7-C8-C9-C10
22	b	601	CLA	C10-C11-C12-C13
28	A	411	SQD	C11-C10-C9-C8
31	T	102	STE	C4-C5-C6-C7
33	e	101	LHG	C28-C29-C30-C31
27	d	410	LMG	O6-C5-C6-O5
22	B	616	CLA	C2-C1-O2A-CGA
31	m	102	STE	C5-C6-C7-C8
29	h	102	DGD	C4A-C5A-C6A-C7A
27	c	523	LMG	C18-C19-C20-C21
31	B	626	STE	C6-C7-C8-C9
22	c	510	CLA	C5-C6-C7-C8
31	B	620	STE	C9-C10-C11-C12
29	h	102	DGD	O2G-C1B-C2B-C3B
28	a	411	SQD	C29-C30-C31-C32
22	C	513	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	b	627	STE	C6-C7-C8-C9
28	L	101	SQD	C16-C17-C18-C19
27	c	523	LMG	C33-C34-C35-C36
29	C	516	DGD	CDB-CEB-CFB-CGB
24	H	102	BCR	C11-C10-C9-C8
24	b	617	BCR	C11-C10-C9-C8
27	M	101	LMG	C40-C41-C42-C43
31	d	413	STE	C2-C3-C4-C5
29	H	103	DGD	O2G-C1B-C2B-C3B
28	L	101	SQD	O6-C44-C45-O47
29	c	518	DGD	C5B-C6B-C7B-C8B
31	B	601	STE	C4-C5-C6-C7
31	M	103	STE	C1-C2-C3-C4
29	A	413	DGD	O6D-C5D-C6D-O5D
22	H	101	CLA	C16-C17-C18-C19
29	c	519	DGD	CBB-CCB-CDB-CEB
27	c	522	LMG	C33-C34-C35-C36
31	d	411	STE	C11-C10-C9-C8
27	b	623	LMG	C12-C13-C14-C15
27	b	623	LMG	C35-C36-C37-C38
28	f	102	SQD	C26-C27-C28-C29
29	c	518	DGD	C9B-CAB-CBB-CCB
27	b	621	LMG	C32-C33-C34-C35
22	C	512	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	d	403	CLA	C6-C7-C8-C10
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	c	507	CLA	C6-C7-C8-C10
22	A	403	CLA	C12-C13-C15-C16
22	c	509	CLA	C12-C13-C15-C16
22	D	404	CLA	C11-C12-C13-C15
22	C	513	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	B	611	CLA	C11-C10-C8-C7
33	e	101	LHG	C14-C15-C16-C17
22	b	613	CLA	C6-C7-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	c	506	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C11-C10-C8-C9
22	C	510	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	H	101	CLA	C11-C10-C8-C9
22	b	614	CLA	C6-C7-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	509	CLA	C14-C13-C15-C16
22	D	403	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	c	508	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	a	403	CLA	C6-C7-C8-C9
22	a	403	CLA	C11-C10-C8-C9
22	b	609	CLA	C14-C13-C15-C16
24	C	514	BCR	C13-C14-C15-C16
22	D	405	CLA	CBD-CGD-O2D-CED
24	K	101	BCR	C14-C15-C16-C17
29	C	516	DGD	CDA-CEA-CFA-CGA
22	H	101	CLA	C8-C10-C11-C12
22	b	609	CLA	C15-C16-C17-C18
24	B	618	BCR	C7-C8-C9-C34
24	b	617	BCR	C11-C12-C13-C35
22	b	607	CLA	C16-C17-C18-C19
22	A	403	CLA	C16-C17-C18-C20
29	C	517	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	CAA-CBA-CCA-CDA
33	D	412	LHG	C9-C10-C11-C12
27	b	621	LMG	C30-C31-C32-C33
29	c	517	DGD	CAB-CBB-CCB-CDB
27	a	415	LMG	C18-C19-C20-C21
29	C	515	DGD	O6D-C5D-C6D-O5D
22	B	612	CLA	C10-C11-C12-C13
31	I	101	STE	C12-C13-C14-C15
33	D	412	LHG	C24-C25-C26-C27
31	b	624	STE	C9-C10-C11-C12
29	C	516	DGD	CBB-CCB-CDB-CEB
27	c	523	LMG	C12-C13-C14-C15
29	c	519	DGD	CDA-CEA-CFA-CGA
27	a	415	LMG	C42-C43-C44-C45
33	D	410	LHG	C30-C31-C32-C33
22	b	604	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C8-C10-C11-C12
27	c	523	LMG	C29-C30-C31-C32
31	d	412	STE	C2-C3-C4-C5
27	Y	101	LMG	C18-C19-C20-C21
31	H	104	STE	C9-C10-C11-C12
27	D	407	LMG	C36-C37-C38-C39
31	I	101	STE	C2-C3-C4-C5
28	A	412	SQD	C18-C19-C20-C21
22	B	605	CLA	C10-C11-C12-C13
31	j	101	STE	C2-C3-C4-C5
27	Y	101	LMG	C29-C30-C31-C32
33	d	408	LHG	C12-C13-C14-C15
28	A	412	SQD	C16-C17-C18-C19
22	b	613	CLA	C13-C15-C16-C17
22	c	508	CLA	C10-C11-C12-C13
33	d	407	LHG	C7-C8-C9-C10
31	m	102	STE	C6-C7-C8-C9
27	Y	101	LMG	C32-C33-C34-C35
29	A	413	DGD	O1A-C1A-O1G-C1G
22	C	512	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C20
29	c	518	DGD	C4A-C5A-C6A-C7A
27	a	415	LMG	C16-C17-C18-C19
27	a	415	LMG	C29-C30-C31-C32
29	H	103	DGD	CBA-CCA-CDA-CEA
29	H	103	DGD	C3B-C4B-C5B-C6B
28	a	411	SQD	C16-C17-C18-C19
22	a	405	CLA	CBA-CGA-O2A-C1
29	c	517	DGD	O6D-C5D-C6D-O5D
29	H	103	DGD	CCB-CDB-CEB-CFB
31	b	624	STE	C12-C13-C14-C15
27	B	621	LMG	C30-C31-C32-C33
33	E	101	LHG	C11-C10-C9-C8
31	C	519	STE	C5-C6-C7-C8
24	K	101	BCR	C15-C16-C17-C18
28	B	622	SQD	C16-C17-C18-C19
27	a	415	LMG	C21-C22-C23-C24
31	c	501	STE	C2-C3-C4-C5
31	c	501	STE	C6-C7-C8-C9
33	D	410	LHG	C27-C28-C29-C30
27	D	407	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	a	415	LMG	C37-C38-C39-C40
28	a	411	SQD	C30-C31-C32-C33
27	b	623	LMG	C29-C28-O8-C9
22	B	616	CLA	C5-C6-C7-C8
28	a	412	SQD	C44-C45-C46-O48
27	Y	101	LMG	O1-C7-C8-C9
27	b	623	LMG	O1-C7-C8-C9
33	e	101	LHG	O9-C7-O7-C5
31	b	627	STE	C14-C15-C16-C17
27	D	407	LMG	C20-C21-C22-C23
31	B	620	STE	C3-C4-C5-C6
27	b	623	LMG	C29-C30-C31-C32
29	h	102	DGD	O1A-C1A-O1G-C1G
27	D	407	LMG	C37-C38-C39-C40
29	C	515	DGD	CDA-CEA-CFA-CGA
22	c	504	CLA	C15-C16-C17-C18
31	b	620	STE	C12-C13-C14-C15
28	A	412	SQD	C32-C33-C34-C35
29	H	103	DGD	CDB-CEB-CFB-CGB
22	B	616	CLA	O1D-CGD-O2D-CED
27	D	411	LMG	C28-C29-C30-C31
31	b	625	STE	C4-C5-C6-C7
33	l	101	LHG	C25-C26-C27-C28
31	c	501	STE	C5-C6-C7-C8
22	C	502	CLA	C16-C17-C18-C19
26	d	406	PL9	C33-C34-C36-C37
29	c	518	DGD	CDB-CEB-CFB-CGB
31	a	413	STE	C2-C3-C4-C5
27	Y	101	LMG	C14-C15-C16-C17
33	D	412	LHG	C25-C26-C27-C28
22	c	511	CLA	O1D-CGD-O2D-CED
33	L	102	LHG	C4-O6-P-O3
27	c	522	LMG	C17-C18-C19-C20
31	d	413	STE	C6-C7-C8-C9
33	d	408	LHG	O1-C1-C2-O2
33	D	409	LHG	O1-C1-C2-O2
31	D	413	STE	C10-C11-C12-C13
27	a	415	LMG	C30-C31-C32-C33
22	D	404	CLA	C16-C17-C18-C19
29	c	519	DGD	C8B-C9B-CAB-CBB
33	D	409	LHG	C24-C25-C26-C27
33	D	409	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
22	c	513	CLA	C8-C10-C11-C12
29	A	413	DGD	C8A-C9A-CAA-CBA
29	h	102	DGD	CAB-CBB-CCB-CDB
28	A	412	SQD	O47-C45-C46-O48
27	c	523	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
22	c	510	CLA	C8-C10-C11-C12
33	L	102	LHG	C31-C32-C33-C34
28	A	412	SQD	C9-C10-C11-C12
22	b	601	CLA	C16-C17-C18-C19
31	b	620	STE	C15-C16-C17-C18
27	d	410	LMG	O9-C10-O7-C8
22	B	613	CLA	C2-C1-O2A-CGA
22	C	506	CLA	C2-C1-O2A-CGA
31	a	413	STE	C1-C2-C3-C4
27	Y	101	LMG	C33-C34-C35-C36
22	C	504	CLA	C11-C10-C8-C9
22	d	403	CLA	C6-C7-C8-C9
22	B	613	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C10-C8-C9
22	b	601	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	c	512	CLA	C14-C13-C15-C16
22	A	403	CLA	C11-C10-C8-C9
22	c	514	CLA	C11-C12-C13-C14
22	c	508	CLA	C6-C7-C8-C9
28	L	101	SQD	C29-C30-C31-C32
27	M	101	LMG	C31-C32-C33-C34
33	D	409	LHG	C30-C31-C32-C33
27	a	415	LMG	C32-C33-C34-C35
29	h	102	DGD	CCA-CDA-CEA-CFA
33	D	412	LHG	C15-C16-C17-C18
33	d	408	LHG	C25-C26-C27-C28
22	b	601	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C20
24	k	102	BCR	C5-C6-C7-C8
24	c	516	BCR	C37-C22-C23-C24
31	C	519	STE	C9-C10-C11-C12
24	b	617	BCR	C21-C22-C23-C24
24	K	103	BCR	C7-C8-C9-C10
29	A	413	DGD	CEA-CFA-CGA-CHA

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Mol	Chain	Res	Type	Atoms
24	k	101	BCR	C14-C15-C16-C17
24	c	515	BCR	C14-C15-C16-C17
31	J	101	STE	C2-C3-C4-C5
27	c	522	LMG	C29-C30-C31-C32
29	C	515	DGD	C4D-C5D-C6D-O5D
22	B	604	CLA	C13-C15-C16-C17
27	c	523	LMG	C20-C21-C22-C23
27	d	410	LMG	C14-C15-C16-C17
27	b	623	LMG	C30-C31-C32-C33
33	l	101	LHG	O6-C4-C5-C6
29	A	413	DGD	C7A-C8A-C9A-CAA
31	d	412	STE	C10-C11-C12-C13
29	c	517	DGD	C7B-C8B-C9B-CAB
27	D	411	LMG	C16-C17-C18-C19
27	D	411	LMG	C32-C33-C34-C35
28	a	411	SQD	C17-C18-C19-C20
22	C	512	CLA	C12-C13-C15-C16
22	a	405	CLA	C11-C10-C8-C7
22	c	510	CLA	C6-C7-C8-C10
23	a	404	PHO	C2-C3-C5-C6
23	a	404	PHO	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
22	C	504	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C12-C13-C15
22	c	505	CLA	C11-C10-C8-C7
22	H	101	CLA	C11-C10-C8-C7
22	b	601	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
22	c	512	CLA	C12-C13-C15-C16
22	A	403	CLA	C11-C10-C8-C7
22	c	513	CLA	C6-C7-C8-C10
22	b	615	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	B	604	CLA	C11-C10-C8-C7
22	c	514	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C12-C13-C15
22	B	606	CLA	C11-C12-C13-C15
22	a	403	CLA	C6-C7-C8-C10
22	a	403	CLA	C11-C10-C8-C7
22	b	609	CLA	C12-C13-C15-C16
27	a	415	LMG	C34-C35-C36-C37
27	c	523	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	a	415	LMG	C23-C24-C25-C26
22	B	614	CLA	C8-C10-C11-C12
29	A	413	DGD	C2A-C3A-C4A-C5A
31	m	101	STE	C2-C3-C4-C5
24	c	515	BCR	C20-C21-C22-C37
24	K	102	BCR	C35-C13-C14-C15
24	k	102	BCR	C20-C21-C22-C37
24	h	101	BCR	C20-C21-C22-C37
24	K	101	BCR	C11-C10-C9-C34
22	C	512	CLA	C3-C5-C6-C7
27	M	101	LMG	C29-C30-C31-C32
31	b	626	STE	C11-C12-C13-C14
33	d	409	LHG	C32-C33-C34-C35
22	B	602	CLA	C16-C17-C18-C19
27	c	523	LMG	C37-C38-C39-C40
31	m	101	STE	C12-C13-C14-C15
33	D	412	LHG	C14-C15-C16-C17
29	A	413	DGD	C6B-C7B-C8B-C9B
27	M	101	LMG	C18-C19-C20-C21
28	f	102	SQD	C29-C30-C31-C32
31	B	626	STE	C11-C10-C9-C8
29	C	515	DGD	C9B-CAB-CBB-CCB
27	c	523	LMG	C9-C8-O7-C10
22	b	613	CLA	CAD-CBD-CGD-O2D
22	B	603	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
22	C	501	CLA	CAD-CBD-CGD-O2D
27	a	415	LMG	C9-C8-O7-C10
22	C	513	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	C	503	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	b	603	CLA	CAD-CBD-CGD-O2D
28	L	101	SQD	C18-C19-C20-C21
28	a	412	SQD	C29-C30-C31-C32
33	d	408	LHG	C9-C10-C11-C12
22	C	509	CLA	C10-C11-C12-C13
31	a	413	STE	C4-C5-C6-C7
27	D	411	LMG	C14-C15-C16-C17
29	C	516	DGD	CBA-CCA-CDA-CEA
22	c	512	CLA	CBA-CGA-O2A-C1
22	c	510	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	b	620	STE	C10-C11-C12-C13
27	c	522	LMG	C11-C12-C13-C14
26	a	409	PL9	C13-C14-C16-C17
28	L	101	SQD	C12-C13-C14-C15
28	A	412	SQD	C35-C36-C37-C38
33	E	101	LHG	C4-C5-C6-O8
33	d	409	LHG	C2-C3-O3-P
33	D	409	LHG	C4-C5-C6-O8
22	B	607	CLA	CBD-CGD-O2D-CED
33	D	409	LHG	O10-C23-O8-C6
31	T	102	STE	C11-C12-C13-C14
22	c	510	CLA	C16-C17-C18-C20
22	A	403	CLA	C16-C17-C18-C19
22	a	410	CLA	C4C-C3C-CAC-CBC
29	c	517	DGD	O1B-C1B-O2G-C2G
22	C	512	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O1D
22	c	510	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O1D
22	H	101	CLA	CHA-CBD-CGD-O1D
22	C	502	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O1D
22	c	509	CLA	CHA-CBD-CGD-O2D
22	c	503	CLA	CHA-CBD-CGD-O1D
22	c	503	CLA	CHA-CBD-CGD-O2D
22	b	603	CLA	CHA-CBD-CGD-O1D
22	B	612	CLA	C3-C5-C6-C7
22	a	405	CLA	O1A-CGA-O2A-C1
22	B	607	CLA	O1D-CGD-O2D-CED
24	t	101	BCR	C16-C17-C18-C19
28	A	411	SQD	O6-C44-C45-O47
33	E	101	LHG	O7-C5-C6-O8
29	c	517	DGD	O1G-C1G-C2G-O2G
29	C	515	DGD	O1G-C1G-C2G-O2G
33	D	409	LHG	O7-C5-C6-O8
22	B	603	CLA	CBD-CGD-O2D-CED
29	c	519	DGD	C9B-CAB-CBB-CCB
31	Z	101	STE	C13-C14-C15-C16
29	c	517	DGD	C4D-C5D-C6D-O5D
33	d	409	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	A	413	DGD	C6A-C7A-C8A-C9A
27	B	621	LMG	C12-C13-C14-C15
22	H	101	CLA	C4-C3-C5-C6
27	d	410	LMG	C32-C33-C34-C35
22	a	405	CLA	C11-C10-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	b	608	CLA	C11-C10-C8-C9
22	c	507	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	a	403	CLA	C14-C13-C15-C16
28	B	622	SQD	C45-C46-O48-C23
27	c	522	LMG	C34-C35-C36-C37
27	B	621	LMG	C33-C34-C35-C36
29	c	517	DGD	C5A-C6A-C7A-C8A
28	f	102	SQD	C25-C26-C27-C28
22	B	605	CLA	C3-C5-C6-C7
27	D	407	LMG	C39-C40-C41-C42
24	B	618	BCR	C36-C18-C19-C20
31	B	620	STE	C12-C13-C14-C15
33	d	407	LHG	C10-C11-C12-C13
33	D	409	LHG	C12-C13-C14-C15
31	D	413	STE	C2-C3-C4-C5
27	B	621	LMG	C28-C29-C30-C31
31	d	411	STE	C1-C2-C3-C4
31	b	624	STE	C1-C2-C3-C4
22	B	610	CLA	C16-C17-C18-C19
28	a	411	SQD	C25-C26-C27-C28
28	D	408	SQD	O6-C44-C45-C46
27	A	410	LMG	C19-C20-C21-C22
27	D	411	LMG	C37-C38-C39-C40
33	L	102	LHG	C33-C34-C35-C36
24	T	101	BCR	C13-C14-C15-C16
24	C	514	BCR	C15-C16-C17-C18
33	d	408	LHG	C3-O3-P-O6
33	D	410	LHG	C14-C15-C16-C17
31	b	627	STE	C12-C13-C14-C15
26	A	409	PL9	C33-C34-C36-C37
26	A	409	PL9	C43-C44-C46-C47
22	B	603	CLA	C2-C3-C5-C6
33	E	101	LHG	C3-O3-P-O4
33	d	408	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
33	D	410	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O4
22	d	404	CLA	C16-C17-C18-C19
27	b	621	LMG	C38-C39-C40-C41
28	a	411	SQD	C11-C12-C13-C14
33	D	410	LHG	C11-C12-C13-C14
27	Y	101	LMG	O6-C1-O1-C7
33	d	408	LHG	C10-C11-C12-C13
22	C	502	CLA	O1D-CGD-O2D-CED
33	E	101	LHG	C7-C8-C9-C10
22	B	616	CLA	C3-C5-C6-C7
22	a	410	CLA	C2C-C3C-CAC-CBC
22	D	404	CLA	C15-C16-C17-C18
33	D	410	LHG	C11-C10-C9-C8
22	C	508	CLA	C16-C17-C18-C20
22	B	603	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
22	C	502	CLA	CAD-CBD-CGD-O1D
28	D	408	SQD	C5-C6-S-O7
22	c	507	CLA	CAD-CBD-CGD-O1D
22	c	503	CLA	CAD-CBD-CGD-O1D
29	A	413	DGD	C4D-C5D-C6D-O5D
28	A	411	SQD	C32-C33-C34-C35
33	D	412	LHG	C26-C27-C28-C29
22	C	509	CLA	C3-C5-C6-C7
31	I	101	STE	C1-C2-C3-C4
31	B	625	STE	C4-C5-C6-C7
33	D	412	LHG	C33-C34-C35-C36
22	c	504	CLA	CBA-CGA-O2A-C1
22	D	405	CLA	O1D-CGD-O2D-CED
22	B	605	CLA	C11-C10-C8-C7
22	C	509	CLA	C12-C13-C15-C16
22	c	506	CLA	C12-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C10
22	c	511	CLA	C11-C10-C8-C7
22	H	101	CLA	C12-C13-C15-C16
22	b	601	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	b	614	CLA	C12-C13-C15-C16
22	B	604	CLA	C12-C13-C15-C16
22	c	514	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C11-C12-C13-C15
22	C	505	CLA	C6-C7-C8-C10
22	a	403	CLA	C12-C13-C15-C16
27	M	101	LMG	C22-C23-C24-C25
31	d	411	STE	C7-C8-C9-C10
22	B	609	CLA	O1A-CGA-O2A-C1
31	c	521	STE	C15-C16-C17-C18
22	c	510	CLA	CAA-CBA-CGA-O2A
29	c	518	DGD	C5A-C6A-C7A-C8A
27	D	411	LMG	C12-C13-C14-C15
22	a	402	CLA	C2C-C3C-CAC-CBC
31	b	624	STE	C7-C8-C9-C10
29	C	517	DGD	O1A-C1A-O1G-C1G
31	B	627	STE	C7-C8-C9-C10
22	C	505	CLA	CBD-CGD-O2D-CED
26	a	409	PL9	C32-C33-C34-C35
29	c	519	DGD	C3B-C4B-C5B-C6B
28	a	411	SQD	C7-C8-C9-C10
29	c	518	DGD	C4E-C5E-C6E-O5E
22	b	609	CLA	O1D-CGD-O2D-CED
27	a	415	LMG	C7-C8-C9-O8
29	C	515	DGD	C1G-C2G-C3G-O3G
27	Y	101	LMG	O1-C7-C8-O7
27	b	623	LMG	O1-C7-C8-O7
33	e	101	LHG	O7-C5-C6-O8
27	d	410	LMG	C15-C16-C17-C18
31	b	625	STE	C2-C3-C4-C5
29	c	518	DGD	C2G-C3G-O3G-C1D
29	C	516	DGD	C5D-C6D-O5D-C1E
29	C	515	DGD	O1G-C1A-C2A-C3A
26	d	406	PL9	C15-C14-C16-C17
26	D	406	PL9	C15-C14-C16-C17
27	D	407	LMG	C21-C22-C23-C24
33	E	101	LHG	C10-C11-C12-C13
33	D	412	LHG	C18-C19-C20-C21
22	A	402	CLA	C4C-C3C-CAC-CBC
26	d	406	PL9	C28-C29-C31-C32
22	C	512	CLA	C14-C13-C15-C16
23	a	404	PHO	C6-C7-C8-C9
22	c	511	CLA	C11-C12-C13-C14
22	H	101	CLA	C14-C13-C15-C16
22	c	507	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C11-C12-C13-C14
31	m	101	STE	C13-C14-C15-C16
27	c	522	LMG	C36-C37-C38-C39
31	B	626	STE	C7-C8-C9-C10
22	b	606	CLA	O1A-CGA-O2A-C1
28	B	622	SQD	C34-C35-C36-C37
24	B	619	BCR	C11-C12-C13-C35
29	A	413	DGD	CBA-CCA-CDA-CEA
33	D	412	LHG	C7-C8-C9-C10
31	B	625	STE	C12-C13-C14-C15
29	c	517	DGD	O1G-C1A-C2A-C3A
33	D	412	LHG	O9-C7-O7-C5
31	b	627	STE	C15-C16-C17-C18
22	B	604	CLA	C15-C16-C17-C18
33	d	409	LHG	C9-C10-C11-C12
22	H	101	CLA	C2-C3-C5-C6
31	M	103	STE	C3-C4-C5-C6
31	C	518	STE	C7-C8-C9-C10
28	A	412	SQD	C19-C20-C21-C22
27	A	410	LMG	C38-C39-C40-C41
29	c	517	DGD	CCB-CDB-CEB-CFB
31	D	413	STE	C6-C7-C8-C9
28	D	408	SQD	C28-C29-C30-C31
22	B	603	CLA	C10-C11-C12-C13
27	D	411	LMG	C9-C8-O7-C10
22	b	610	CLA	C2A-CAA-CBA-CGA
33	L	102	LHG	C27-C28-C29-C30
22	b	606	CLA	CBA-CGA-O2A-C1
22	d	403	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
22	B	612	CLA	C2-C1-O2A-CGA
33	D	412	LHG	C19-C20-C21-C22
22	B	603	CLA	C16-C17-C18-C19
31	a	413	STE	C7-C8-C9-C10
33	E	101	LHG	C2-C3-O3-P
33	l	101	LHG	C15-C16-C17-C18
31	D	413	STE	C12-C13-C14-C15
22	B	609	CLA	CBA-CGA-O2A-C1
33	l	101	LHG	O6-C4-C5-O7
22	b	612	CLA	C16-C17-C18-C20
26	A	409	PL9	C20-C19-C21-C22
22	c	505	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	h	102	DGD	CBA-CCA-CDA-CEA
24	B	618	BCR	C23-C24-C25-C26
22	B	610	CLA	O1D-CGD-O2D-CED
27	a	415	LMG	C31-C32-C33-C34
31	E	102	STE	C7-C8-C9-C10
31	c	521	STE	C11-C10-C9-C8
28	D	408	SQD	O5-C1-O6-C44
24	c	516	BCR	C20-C21-C22-C23
29	c	517	DGD	C7A-C8A-C9A-CAA
22	c	512	CLA	O1A-CGA-O2A-C1
28	a	412	SQD	O47-C45-C46-O48
27	c	522	LMG	O1-C7-C8-O7
27	M	101	LMG	O7-C8-C9-O8
29	A	413	DGD	C5A-C6A-C7A-C8A
31	b	624	STE	C15-C16-C17-C18
22	b	609	CLA	CBD-CGD-O2D-CED
33	E	101	LHG	C3-O3-P-O6
31	b	624	STE	C2-C3-C4-C5
29	c	519	DGD	O6D-C5D-C6D-O5D
27	D	407	LMG	C16-C17-C18-C19
28	A	412	SQD	C11-C10-C9-C8
22	B	612	CLA	O1D-CGD-O2D-CED
28	a	411	SQD	C14-C15-C16-C17
29	c	517	DGD	O1G-C1G-C2G-C3G
27	a	415	LMG	C35-C36-C37-C38
22	B	604	CLA	C10-C11-C12-C13
26	D	406	PL9	C28-C29-C31-C32
22	c	507	CLA	C11-C12-C13-C15
22	b	614	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C15
22	B	606	CLA	C6-C7-C8-C10
27	a	415	LMG	O8-C28-C29-C30
22	d	403	CLA	C4C-C3C-CAC-CBC
31	H	104	STE	C10-C11-C12-C13
28	a	411	SQD	C11-C10-C9-C8
22	B	605	CLA	C11-C10-C8-C9
22	B	616	CLA	C6-C7-C8-C9
22	B	614	CLA	C14-C13-C15-C16
28	f	102	SQD	O47-C7-C8-C9
22	B	606	CLA	C11-C12-C13-C14
24	k	101	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
24	c	515	BCR	C9-C10-C11-C12
24	B	618	BCR	C15-C16-C17-C18
22	C	510	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C20
27	c	520	LMG	C32-C33-C34-C35
22	A	403	CLA	CBA-CGA-O2A-C1
22	B	613	CLA	C15-C16-C17-C18
22	c	504	CLA	C10-C11-C12-C13
31	b	625	STE	C1-C2-C3-C4
31	B	626	STE	C3-C4-C5-C6
31	a	413	STE	C6-C7-C8-C9
24	b	618	BCR	C37-C22-C23-C24
24	K	103	BCR	C11-C12-C13-C35
33	E	101	LHG	C31-C32-C33-C34
27	Y	101	LMG	C31-C32-C33-C34
33	l	101	LHG	C11-C12-C13-C14
27	A	410	LMG	C13-C14-C15-C16
22	C	504	CLA	C4-C3-C5-C6
22	B	603	CLA	C4-C3-C5-C6
33	D	412	LHG	C24-C23-O8-C6
22	B	611	CLA	C13-C15-C16-C17
22	B	610	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBA-CGA-O2A-C1
29	C	515	DGD	O6E-C1E-O5D-C6D
33	E	101	LHG	O6-C4-C5-C6
33	d	408	LHG	O6-C4-C5-C6
29	A	413	DGD	CAB-CBB-CCB-CDB
23	d	401	PHO	C2C-C3C-CAC-CBC
27	c	523	LMG	C35-C36-C37-C38
26	D	406	PL9	C45-C44-C46-C47
22	b	614	CLA	C4-C3-C5-C6
27	B	621	LMG	C36-C37-C38-C39
29	C	517	DGD	C7A-C8A-C9A-CAA
28	a	411	SQD	C33-C34-C35-C36
22	c	504	CLA	O1A-CGA-O2A-C1
22	C	511	CLA	O1A-CGA-O2A-C1
28	B	622	SQD	C11-C10-C9-C8
31	B	627	STE	C11-C12-C13-C14
29	C	517	DGD	CDA-CEA-CFA-CGA
31	C	520	STE	C5-C6-C7-C8
29	C	517	DGD	C8B-C9B-CAB-CBB
22	D	403	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
27	A	410	LMG	C15-C16-C17-C18
22	c	502	CLA	C2A-CAA-CBA-CGA
31	B	625	STE	C10-C11-C12-C13
27	c	520	LMG	C30-C31-C32-C33
29	c	518	DGD	CCB-CDB-CEB-CFB
27	a	415	LMG	C11-C12-C13-C14
27	Y	101	LMG	C4-C5-C6-O5
26	A	409	PL9	C4-C3-C7-C8
26	a	409	PL9	C4-C3-C7-C8
22	B	605	CLA	C6-C7-C8-C9
23	D	401	PHO	C6-C7-C8-C9
22	B	610	CLA	C14-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C9
22	a	410	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
29	c	519	DGD	C2B-C3B-C4B-C5B
28	a	412	SQD	C30-C31-C32-C33
27	b	623	LMG	C31-C32-C33-C34
24	K	101	BCR	C35-C13-C14-C15
24	b	617	BCR	C16-C17-C18-C36
33	d	407	LHG	C31-C32-C33-C34
23	a	404	PHO	O2A-C1-C2-C3
22	b	601	CLA	O2A-C1-C2-C3
29	C	516	DGD	O6D-C1D-O3G-C3G
27	b	621	LMG	C18-C19-C20-C21
24	K	103	BCR	C37-C22-C23-C24
22	c	508	CLA	C5-C6-C7-C8
29	C	515	DGD	C2A-C3A-C4A-C5A
29	C	515	DGD	CBA-CCA-CDA-CEA
27	M	101	LMG	C9-C8-O7-C10
22	B	606	CLA	C10-C11-C12-C13
29	C	517	DGD	O6D-C5D-C6D-O5D
31	E	102	STE	C4-C5-C6-C7
31	a	414	STE	C5-C6-C7-C8
22	B	605	CLA	C12-C13-C15-C16
22	c	510	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	B	612	CLA	C11-C10-C8-C7
22	b	602	CLA	C11-C12-C13-C15
22	b	611	CLA	C15-C16-C17-C18
28	a	411	SQD	C32-C33-C34-C35
27	D	411	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C13-C15-C16-C17
33	D	410	LHG	O6-C4-C5-C6
22	c	513	CLA	C4-C3-C5-C6
22	c	511	CLA	C15-C16-C17-C18
31	B	625	STE	C5-C6-C7-C8
22	C	510	CLA	C13-C15-C16-C17
29	C	516	DGD	O1A-C1A-O1G-C1G
22	B	610	CLA	C16-C17-C18-C20
27	Y	101	LMG	C2-C1-O1-C7
31	j	101	STE	C7-C8-C9-C10
27	M	101	LMG	C36-C37-C38-C39
27	b	621	LMG	C39-C40-C41-C42
22	C	509	CLA	C16-C17-C18-C19
33	E	101	LHG	C34-C35-C36-C37
29	A	413	DGD	O6D-C1D-O3G-C3G
22	b	612	CLA	C10-C11-C12-C13
28	L	101	SQD	C14-C15-C16-C17
22	b	604	CLA	C3-C5-C6-C7
22	a	402	CLA	C2-C1-O2A-CGA
33	L	102	LHG	C29-C30-C31-C32
33	D	410	LHG	C17-C18-C19-C20
22	A	402	CLA	C14-C13-C15-C16
28	A	412	SQD	C24-C25-C26-C27
22	A	403	CLA	O1A-CGA-O2A-C1
28	B	622	SQD	C35-C36-C37-C38
27	c	522	LMG	C35-C36-C37-C38
26	D	406	PL9	C16-C17-C18-C19
29	H	103	DGD	C9B-CAB-CBB-CCB
24	k	102	BCR	C1-C6-C7-C8
24	k	102	BCR	C23-C24-C25-C26
24	k	102	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C30
24	A	406	BCR	C1-C6-C7-C8
24	A	406	BCR	C5-C6-C7-C8
24	d	405	BCR	C23-C24-C25-C30
24	K	103	BCR	C23-C24-C25-C30
29	c	518	DGD	C9A-CAA-CBA-CCA
29	c	518	DGD	CAB-CBB-CCB-CDB
33	D	409	LHG	O1-C1-C2-C3
31	b	627	STE	C4-C5-C6-C7
24	b	619	BCR	C9-C10-C11-C12
24	T	101	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C40-C39-C41-C42
23	A	404	PHO	C2C-C3C-CAC-CBC
27	a	415	LMG	C33-C34-C35-C36
31	c	521	STE	C10-C11-C12-C13
26	D	406	PL9	C33-C34-C36-C37
31	B	625	STE	C9-C10-C11-C12
27	M	101	LMG	C8-C7-O1-C1
33	D	410	LHG	O6-C4-C5-O7
31	B	624	STE	C4-C5-C6-C7
27	b	623	LMG	C17-C18-C19-C20
31	B	623	STE	C3-C4-C5-C6
22	b	603	CLA	C4-C3-C5-C6
22	B	608	CLA	C6-C7-C8-C10
22	C	510	CLA	C6-C7-C8-C10
22	b	611	CLA	C6-C7-C8-C10
26	a	409	PL9	C28-C29-C31-C32
22	B	612	CLA	C6-C7-C8-C10
31	b	625	STE	C5-C6-C7-C8
31	C	519	STE	C14-C15-C16-C17
33	E	101	LHG	C19-C20-C21-C22
31	B	623	STE	C9-C10-C11-C12
31	B	625	STE	C6-C7-C8-C9
28	L	101	SQD	O47-C45-C46-O48
27	A	410	LMG	O7-C8-C9-O8
29	C	515	DGD	O1A-C1A-O1G-C1G
29	H	103	DGD	CAB-CBB-CCB-CDB
22	D	405	CLA	C3-C5-C6-C7
27	d	410	LMG	O7-C10-C11-C12
22	B	612	CLA	CAA-CBA-CGA-O2A
24	d	405	BCR	C16-C17-C18-C36
29	C	516	DGD	C5B-C6B-C7B-C8B
26	a	409	PL9	C35-C34-C36-C37
22	B	616	CLA	C10-C11-C12-C13
27	c	523	LMG	C36-C37-C38-C39
31	m	102	STE	C4-C5-C6-C7
29	c	517	DGD	C5B-C6B-C7B-C8B
22	C	504	CLA	C2-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
22	c	513	CLA	C2-C3-C5-C6
28	a	411	SQD	O47-C7-C8-C9
22	c	506	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	604	CLA	C6-C7-C8-C9
22	b	611	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	c	512	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	514	CLA	C11-C10-C8-C9
22	B	609	CLA	C14-C13-C15-C16
22	C	505	CLA	C6-C7-C8-C9
22	A	403	CLA	C3A-C2A-CAA-CBA
27	M	101	LMG	C21-C22-C23-C24
22	B	605	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	CAD-CBD-CGD-O2D
22	C	508	CLA	CAD-CBD-CGD-O2D
22	b	610	CLA	CAD-CBD-CGD-O2D
22	b	604	CLA	CAD-CBD-CGD-O2D
22	c	511	CLA	CAD-CBD-CGD-O2D
22	B	610	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	c	514	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D
22	b	612	CLA	CAD-CBD-CGD-O2D
22	B	609	CLA	CAD-CBD-CGD-O2D
22	d	404	CLA	CAD-CBD-CGD-O2D
22	c	514	CLA	C13-C15-C16-C17
22	c	514	CLA	C2-C1-O2A-CGA
24	b	619	BCR	C6-C7-C8-C9
22	a	402	CLA	C4C-C3C-CAC-CBC
22	c	506	CLA	C2-C3-C5-C6
26	D	406	PL9	C43-C44-C46-C47
28	a	412	SQD	C16-C17-C18-C19
24	a	406	BCR	C21-C22-C23-C24
24	T	101	BCR	C11-C12-C13-C14
27	A	410	LMG	C7-C8-C9-O8
27	M	101	LMG	O1-C7-C8-C9
29	C	515	DGD	O1G-C1G-C2G-C3G
31	J	101	STE	C4-C5-C6-C7
26	a	409	PL9	C11-C12-C13-C14
24	A	406	BCR	C18-C19-C20-C21
24	B	619	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	B	625	STE	C3-C4-C5-C6
22	C	512	CLA	O2A-C1-C2-C3
22	C	509	CLA	O2A-C1-C2-C3
22	D	405	CLA	O2A-C1-C2-C3
22	d	404	CLA	O2A-C1-C2-C3
33	D	410	LHG	C24-C25-C26-C27
29	C	516	DGD	C2B-C3B-C4B-C5B
22	B	603	CLA	C2A-CAA-CBA-CGA
28	A	412	SQD	O48-C23-C24-C25
27	b	623	LMG	O7-C10-C11-C12
31	B	620	STE	C7-C8-C9-C10
31	b	624	STE	C14-C15-C16-C17
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	C	504	CLA	CHA-CBD-CGD-O1D
23	A	404	PHO	CHA-CBD-CGD-O1D
22	c	505	CLA	CHA-CBD-CGD-O2D
22	H	101	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O2D
24	K	101	BCR	C9-C10-C11-C12
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	D	404	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	CHA-CBD-CGD-O2D
23	d	401	PHO	CHA-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O2D
27	c	522	LMG	C42-C43-C44-C45
33	D	409	LHG	C18-C19-C20-C21
29	C	516	DGD	C8A-C9A-CAA-CBA
27	A	410	LMG	O1-C7-C8-O7
29	C	515	DGD	O2G-C2G-C3G-O3G
28	L	101	SQD	C11-C10-C9-C8
22	D	405	CLA	C10-C11-C12-C13
28	A	411	SQD	O47-C7-C8-C9
31	b	625	STE	C3-C4-C5-C6
27	M	101	LMG	C30-C31-C32-C33
29	h	102	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
27	a	415	LMG	C11-C10-O7-C8
29	C	515	DGD	O2G-C1B-C2B-C3B
22	B	615	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	C	506	CLA	C6-C7-C8-C10
22	B	606	CLA	C11-C10-C8-C7
22	b	603	CLA	C6-C7-C8-C10
22	c	509	CLA	O1D-CGD-O2D-CED
28	A	412	SQD	O49-C7-O47-C45
22	B	613	CLA	CAA-CBA-CGA-O2A
22	C	510	CLA	C6-C7-C8-C9
22	B	615	CLA	C6-C7-C8-C9
22	D	405	CLA	C6-C7-C8-C9
22	B	613	CLA	C6-C7-C8-C9
22	C	502	CLA	C14-C13-C15-C16
22	C	506	CLA	C14-C13-C15-C16
26	D	406	PL9	C34-C36-C37-C38
22	H	101	CLA	C15-C16-C17-C18
31	B	620	STE	C4-C5-C6-C7
33	l	101	LHG	O7-C7-C8-C9
22	B	603	CLA	O1D-CGD-O2D-CED
33	d	408	LHG	C30-C31-C32-C33
29	c	518	DGD	O1A-C1A-C2A-C3A
22	b	613	CLA	C16-C17-C18-C19
31	B	627	STE	C12-C13-C14-C15
22	a	403	CLA	CBD-CGD-O2D-CED
24	b	619	BCR	C7-C8-C9-C10
22	D	404	CLA	C2C-C3C-CAC-CBC
31	E	102	STE	C1-C2-C3-C4
22	A	403	CLA	C1A-C2A-CAA-CBA
31	B	620	STE	C1-C2-C3-C4
22	B	602	CLA	C1A-C2A-CAA-CBA
28	A	412	SQD	C31-C32-C33-C34
22	C	509	CLA	C16-C17-C18-C20
31	b	622	STE	C11-C10-C9-C8
33	E	101	LHG	C15-C16-C17-C18
23	A	404	PHO	C10-C11-C12-C13
27	b	623	LMG	O10-C28-C29-C30
31	B	601	STE	C3-C4-C5-C6
31	B	626	STE	C10-C11-C12-C13
28	L	101	SQD	O6-C44-C45-C46
29	h	102	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
33	E	101	LHG	C4-O6-P-O3
22	b	603	CLA	C13-C15-C16-C17
27	b	621	LMG	C36-C37-C38-C39
27	b	623	LMG	C16-C17-C18-C19
22	c	506	CLA	C4-C3-C5-C6
27	D	407	LMG	C18-C19-C20-C21
31	M	103	STE	C7-C8-C9-C10
22	B	612	CLA	CAA-CBA-CGA-O1A
33	E	101	LHG	C3-O3-P-O5
33	L	102	LHG	C4-O6-P-O5
33	D	409	LHG	C4-O6-P-O5
33	D	410	LHG	C4-O6-P-O4
33	e	101	LHG	C3-O3-P-O4
33	e	101	LHG	C4-O6-P-O5
29	c	519	DGD	O6D-C1D-O3G-C3G
24	h	101	BCR	C11-C10-C9-C34
31	C	519	STE	C11-C10-C9-C8
33	D	409	LHG	C19-C20-C21-C22
24	h	101	BCR	C23-C24-C25-C26
33	L	102	LHG	C28-C29-C30-C31
22	D	404	CLA	C4C-C3C-CAC-CBC
22	B	603	CLA	C15-C16-C17-C18
24	d	405	BCR	C18-C19-C20-C21
33	D	409	LHG	O10-C23-C24-C25
22	B	608	CLA	C13-C15-C16-C17
22	a	410	CLA	C15-C16-C17-C18
31	H	104	STE	C3-C4-C5-C6
27	b	621	LMG	C40-C41-C42-C43
29	H	103	DGD	C4A-C5A-C6A-C7A
23	a	404	PHO	C8-C10-C11-C12
22	c	509	CLA	C4-C3-C5-C6
33	D	412	LHG	C16-C17-C18-C19
22	B	608	CLA	C16-C17-C18-C19
29	c	519	DGD	C2A-C3A-C4A-C5A
22	C	504	CLA	CAD-CBD-CGD-O1D
22	c	505	CLA	CAD-CBD-CGD-O1D
22	H	101	CLA	CAD-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
28	D	408	SQD	C5-C6-S-O9
22	B	607	CLA	CAD-CBD-CGD-O1D
22	b	609	CLA	CAD-CBD-CGD-O1D
27	c	522	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
27	Y	101	LMG	C34-C35-C36-C37
22	B	606	CLA	C5-C6-C7-C8
22	B	605	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
22	B	603	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C14
22	b	612	CLA	C11-C10-C8-C9
22	b	603	CLA	C6-C7-C8-C9
22	c	510	CLA	CAA-CBA-CGA-O1A
29	c	517	DGD	O2G-C1B-C2B-C3B
27	A	410	LMG	C14-C15-C16-C17
29	A	413	DGD	O2G-C1B-C2B-C3B
22	c	503	CLA	C2C-C3C-CAC-CBC
22	b	605	CLA	C4-C3-C5-C6
27	B	621	LMG	C14-C15-C16-C17
22	B	613	CLA	C6-C7-C8-C10
22	B	603	CLA	C12-C13-C15-C16
22	H	101	CLA	C11-C12-C13-C15
22	c	512	CLA	C6-C7-C8-C10
22	b	602	CLA	C12-C13-C15-C16
22	A	402	CLA	C12-C13-C15-C16
22	C	505	CLA	C11-C12-C13-C15
22	b	603	CLA	C2-C3-C5-C6
28	A	412	SQD	O10-C23-C24-C25
22	b	601	CLA	CAA-CBA-CGA-O2A
27	b	621	LMG	O8-C28-C29-C30
33	d	407	LHG	O8-C23-C24-C25
22	D	403	CLA	C10-C11-C12-C13
24	H	102	BCR	C7-C8-C9-C10
24	c	516	BCR	C17-C18-C19-C20
31	I	101	STE	C6-C7-C8-C9
27	Y	101	LMG	O8-C28-C29-C30
29	A	413	DGD	O6E-C1E-O5D-C6D
29	c	517	DGD	O6E-C1E-O5D-C6D
22	C	503	CLA	C8-C10-C11-C12
22	B	612	CLA	O1A-CGA-O2A-C1
22	B	613	CLA	CAA-CBA-CGA-O1A
28	a	411	SQD	O10-C23-C24-C25
22	b	615	CLA	C13-C15-C16-C17
31	H	104	STE	C11-C12-C13-C14
33	L	102	LHG	O7-C7-C8-C9
27	B	621	LMG	C32-C33-C34-C35

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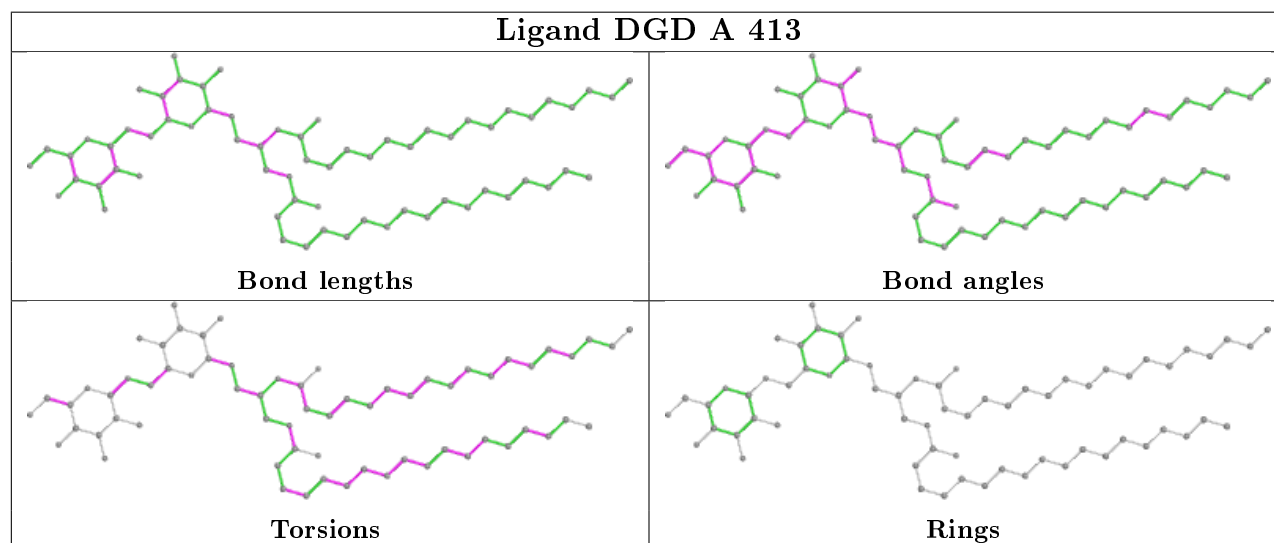
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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C13-C15-C16-C17
29	c	517	DGD	O1B-C1B-C2B-C3B
22	a	403	CLA	C16-C17-C18-C20
31	d	411	STE	C3-C4-C5-C6
22	C	504	CLA	C11-C12-C13-C14
22	b	612	CLA	CAA-CBA-CGA-O2A

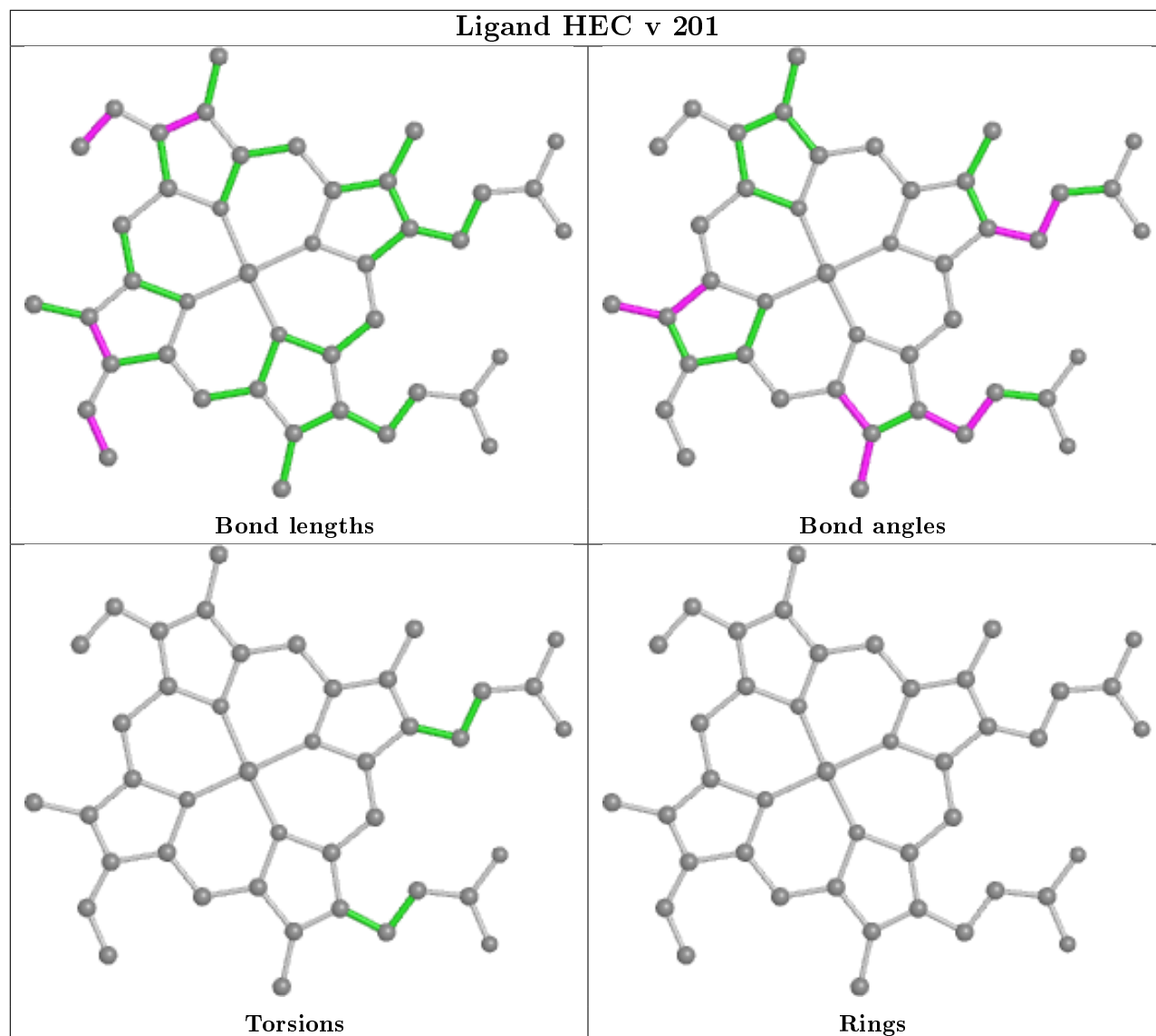
There are no ring outliers.

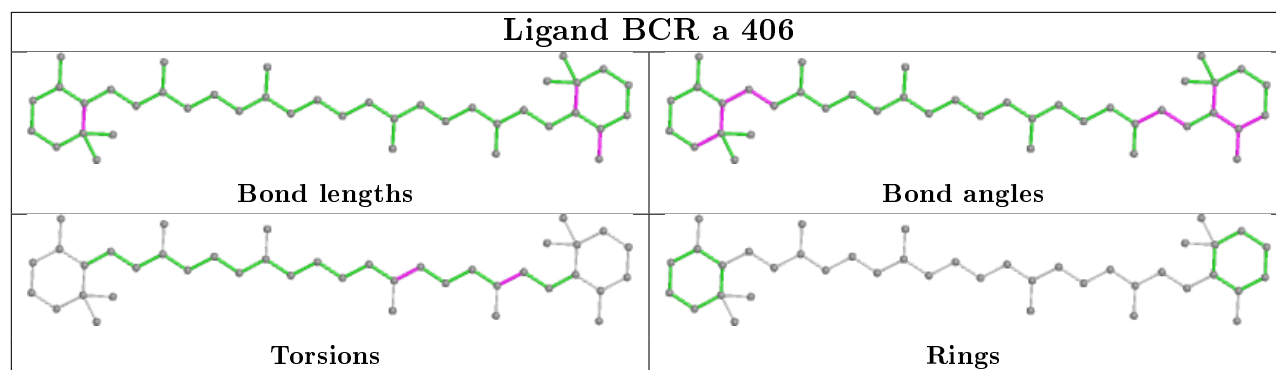
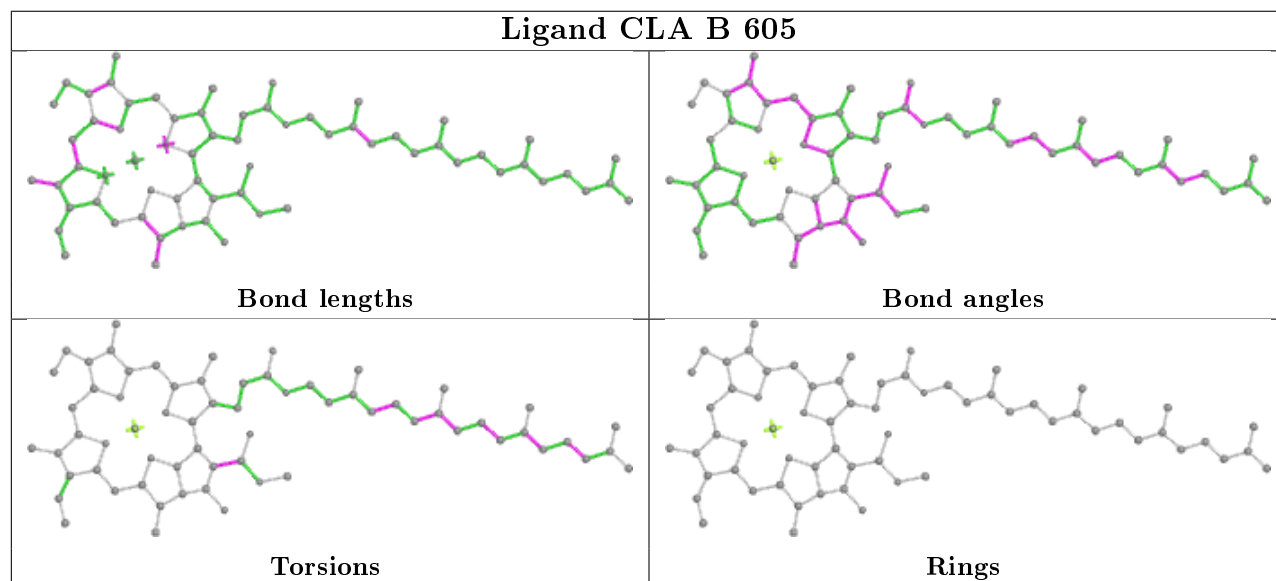
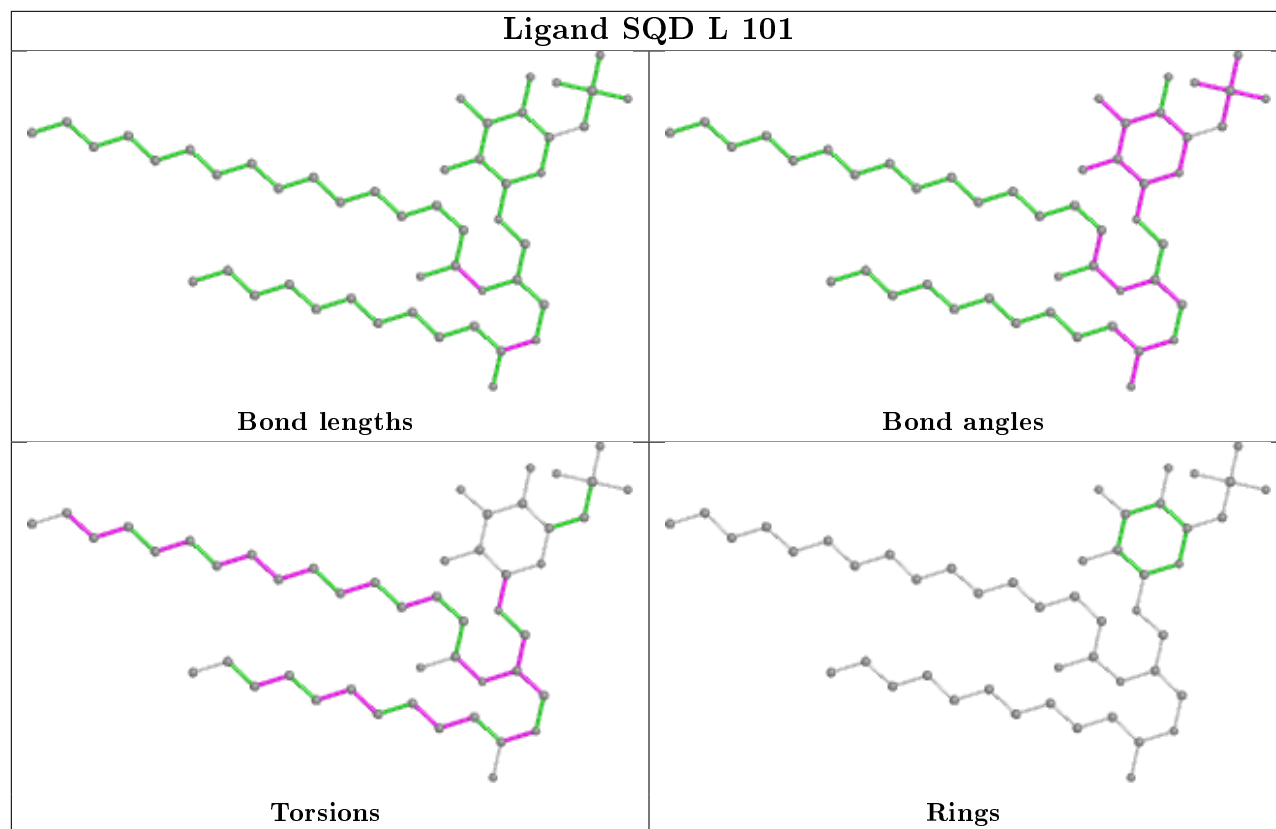
No monomer is involved in short contacts.

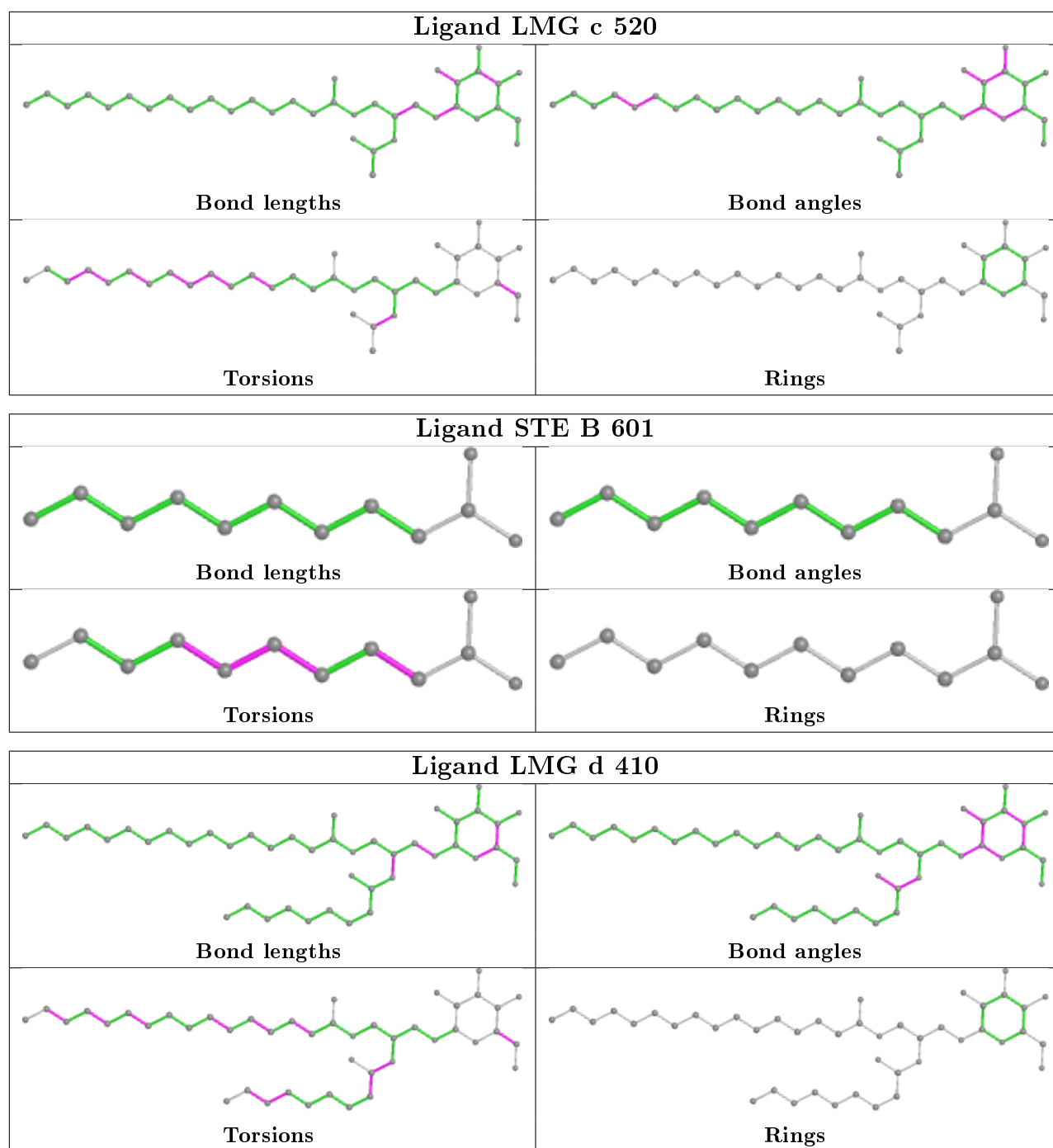
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

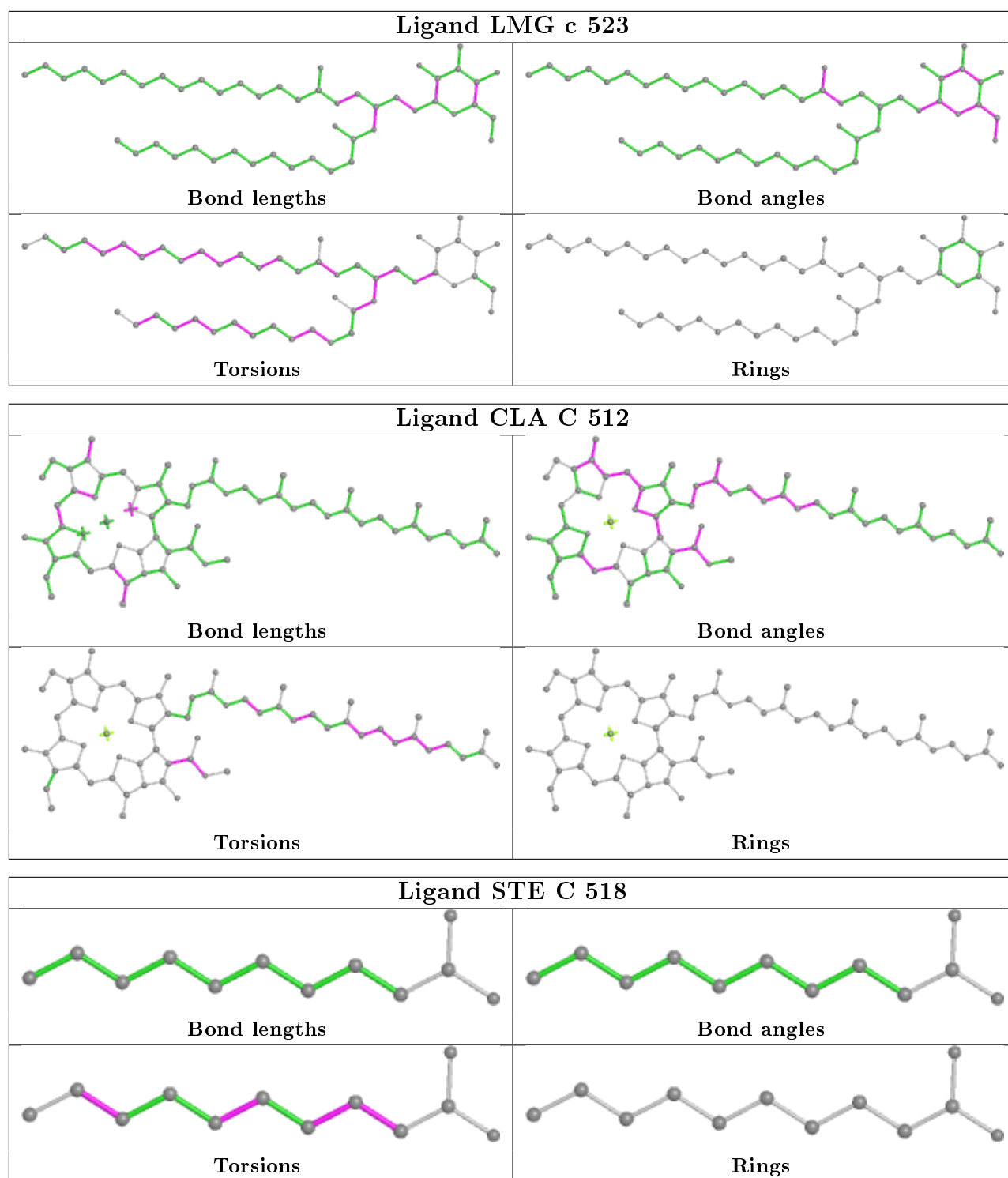


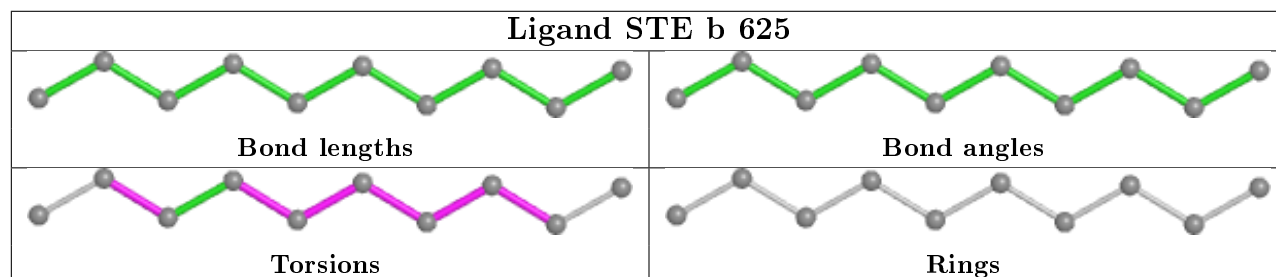
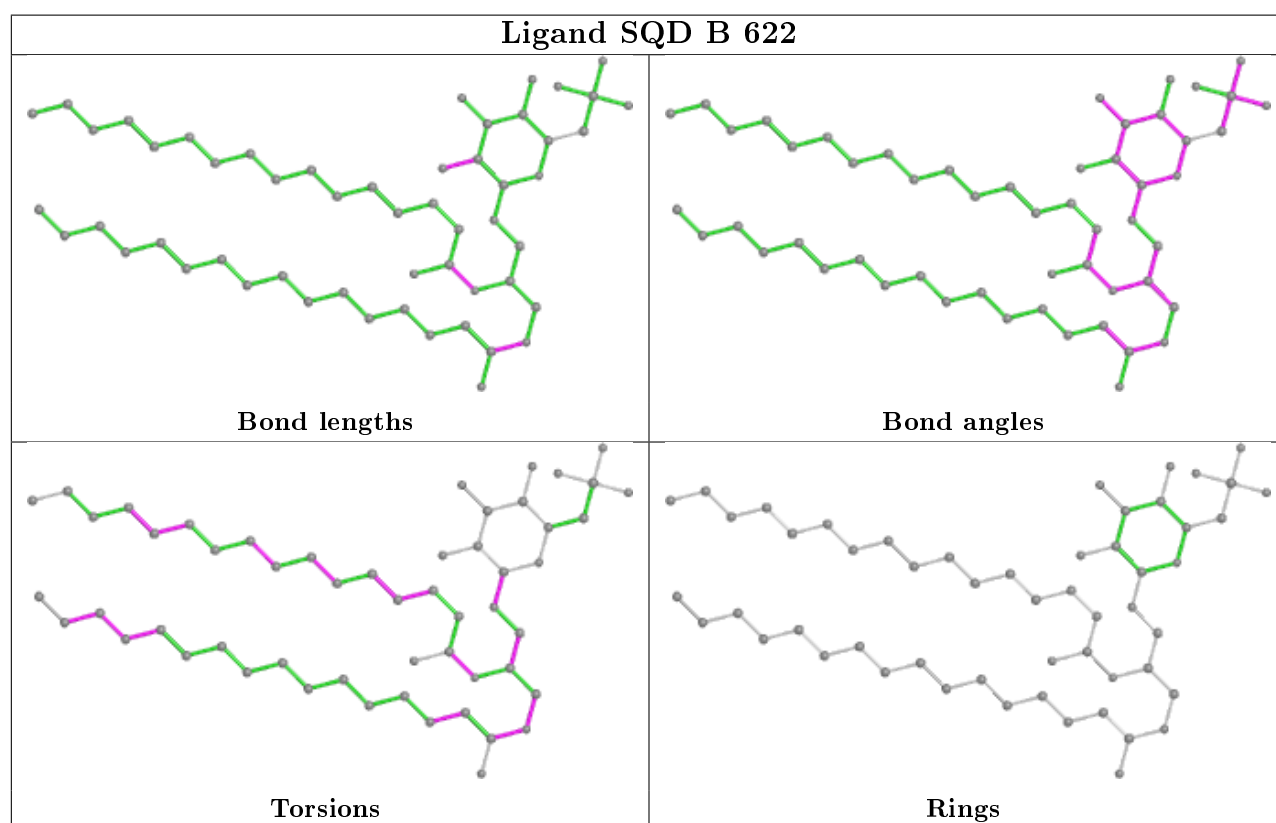
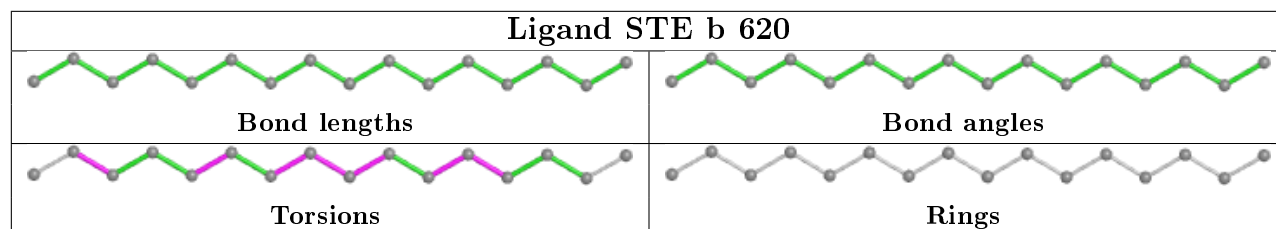
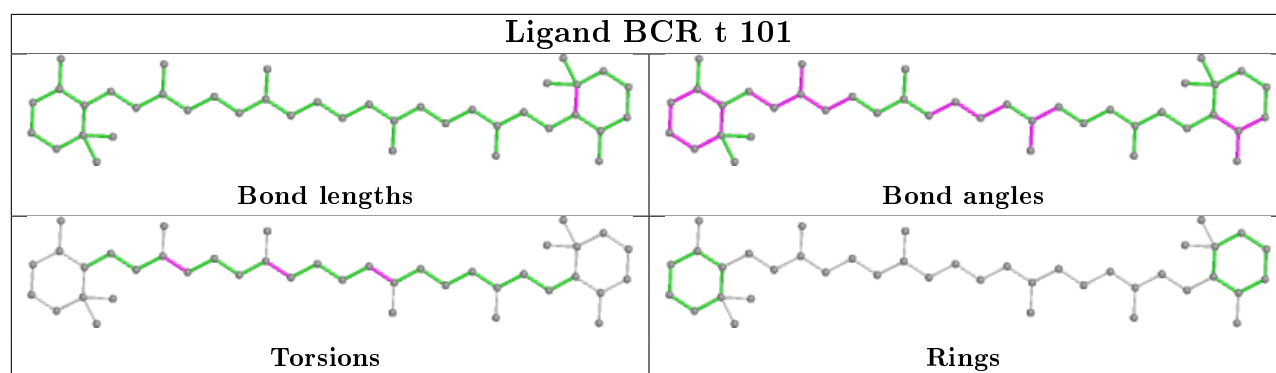
Ligand HEC v 201



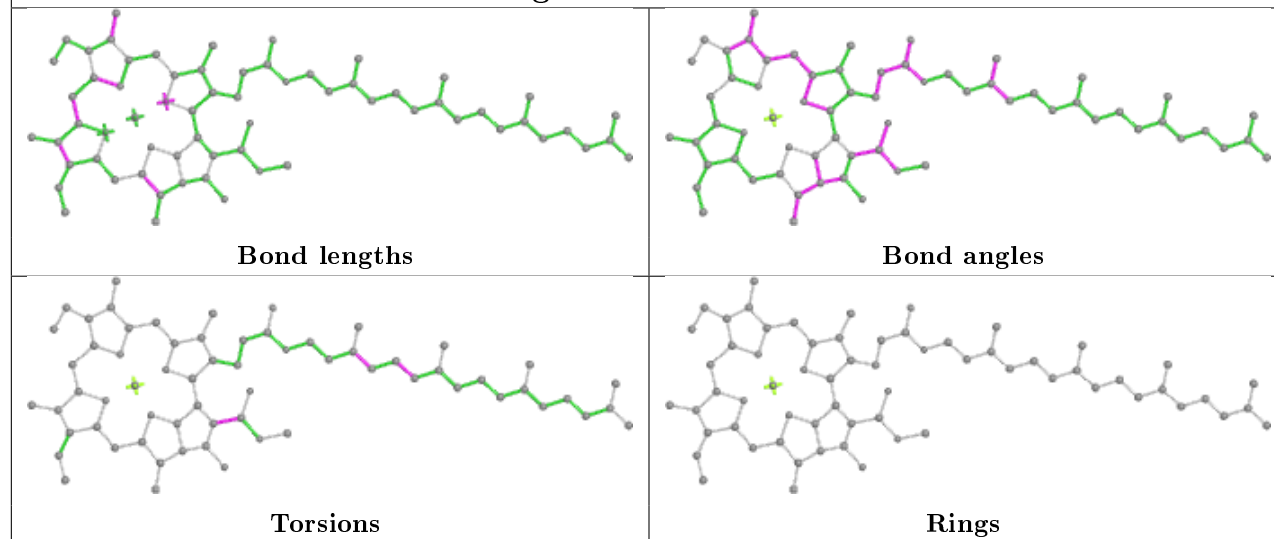




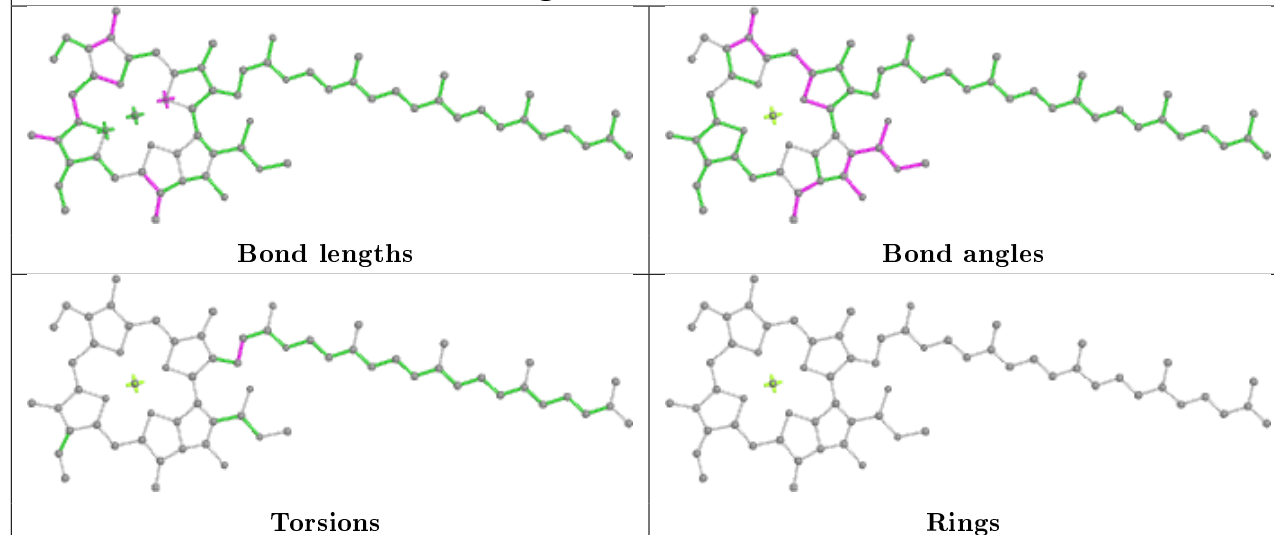




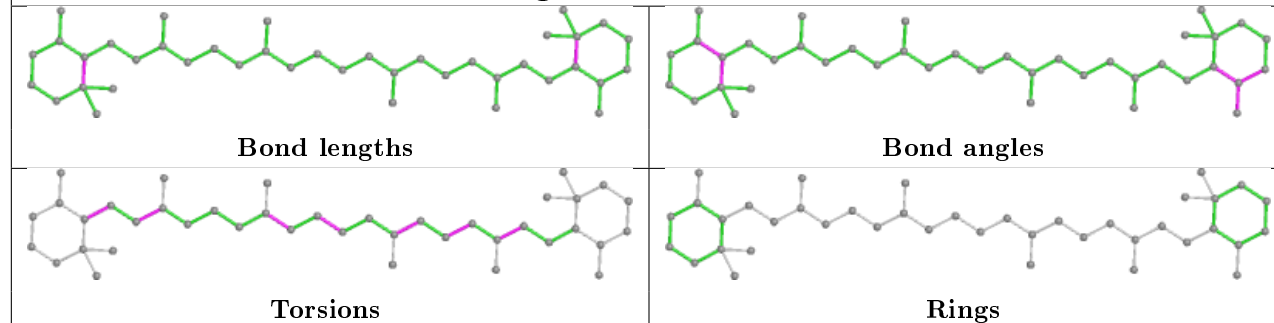
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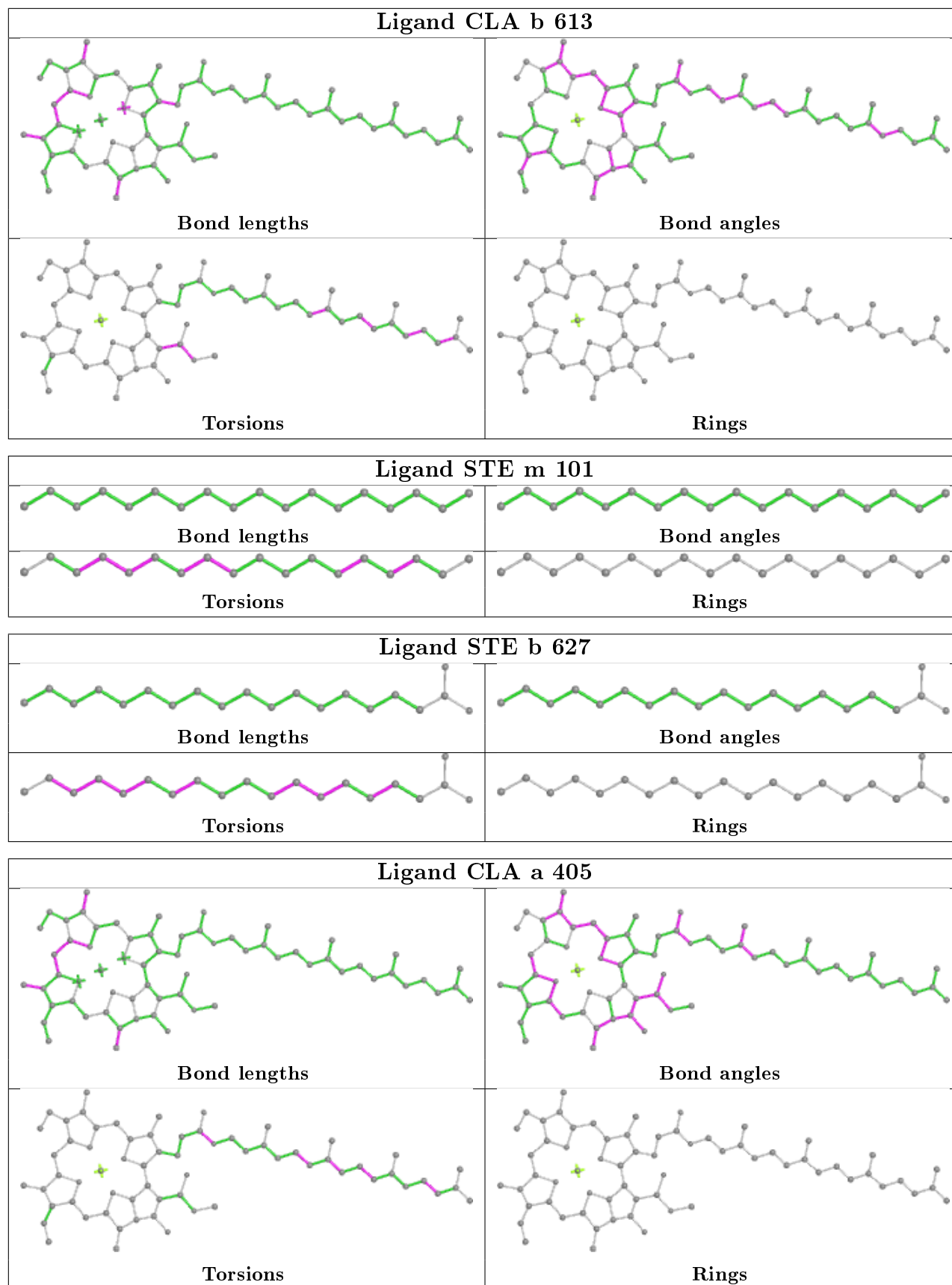


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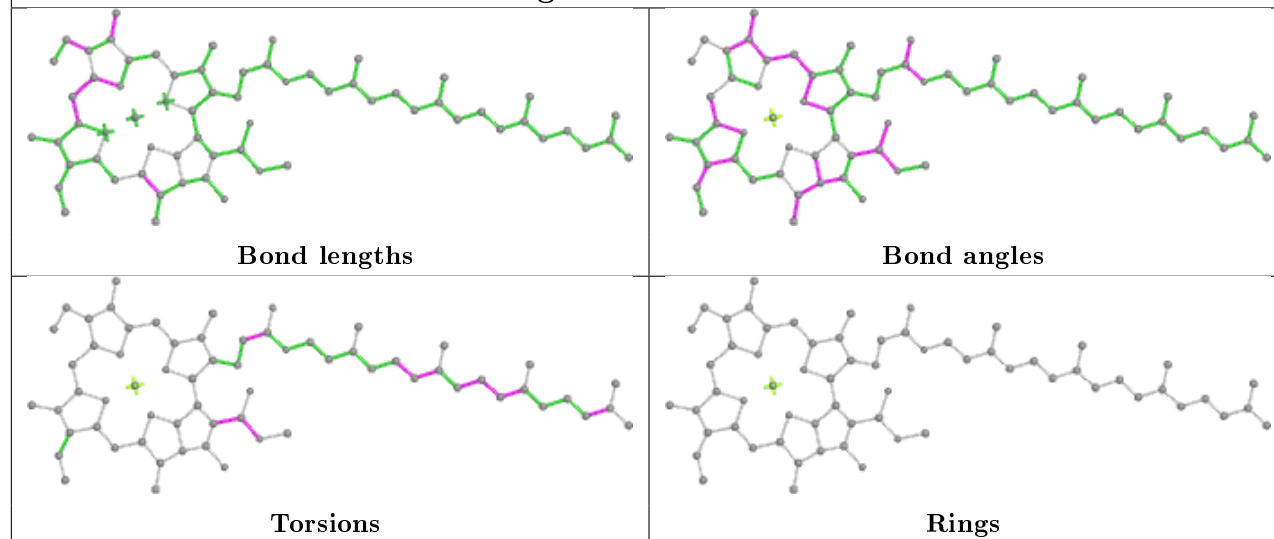


Ligand BCR k 101

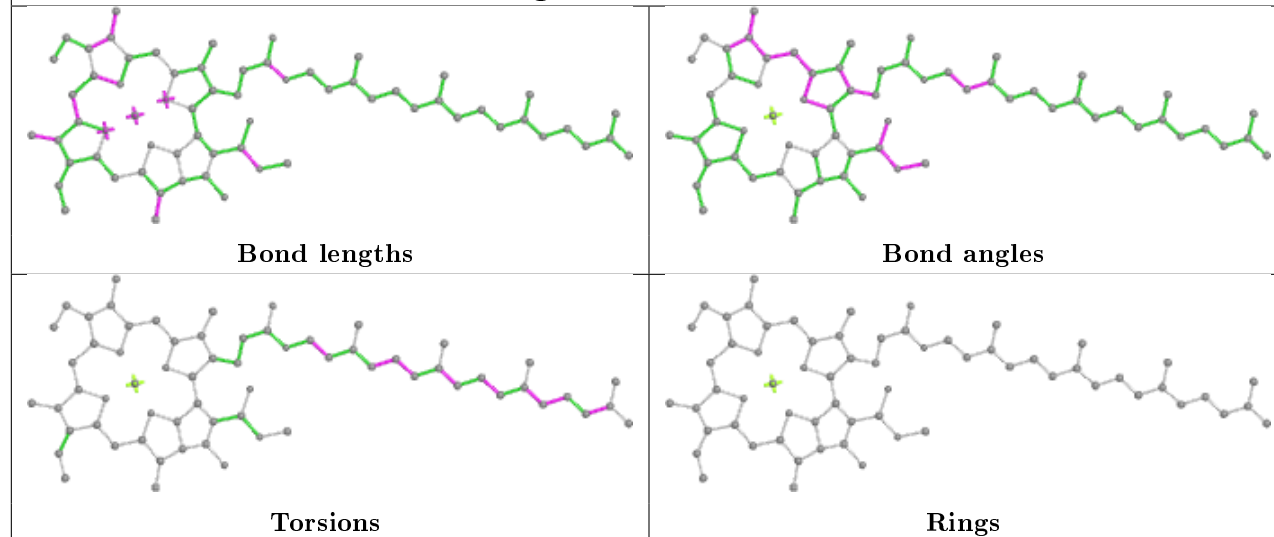




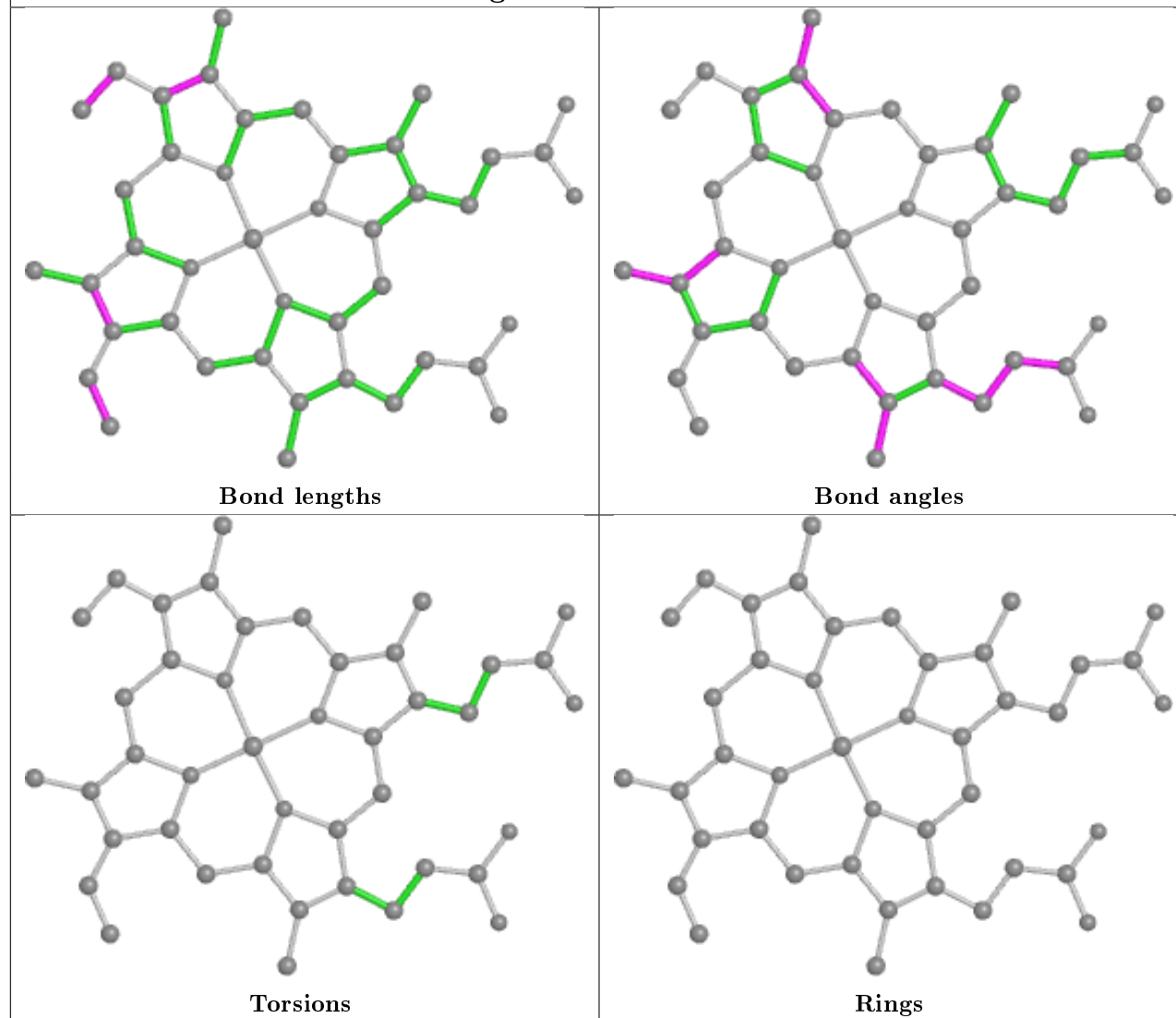
Ligand CLA c 510



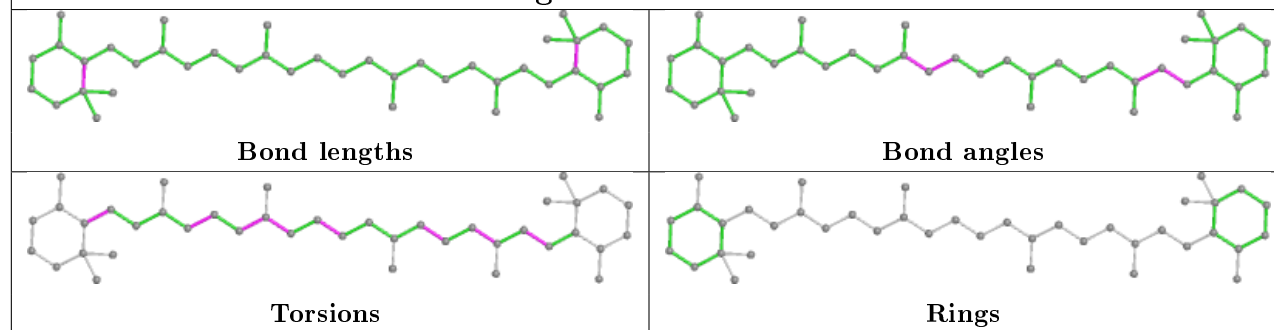
Ligand CLA C 509

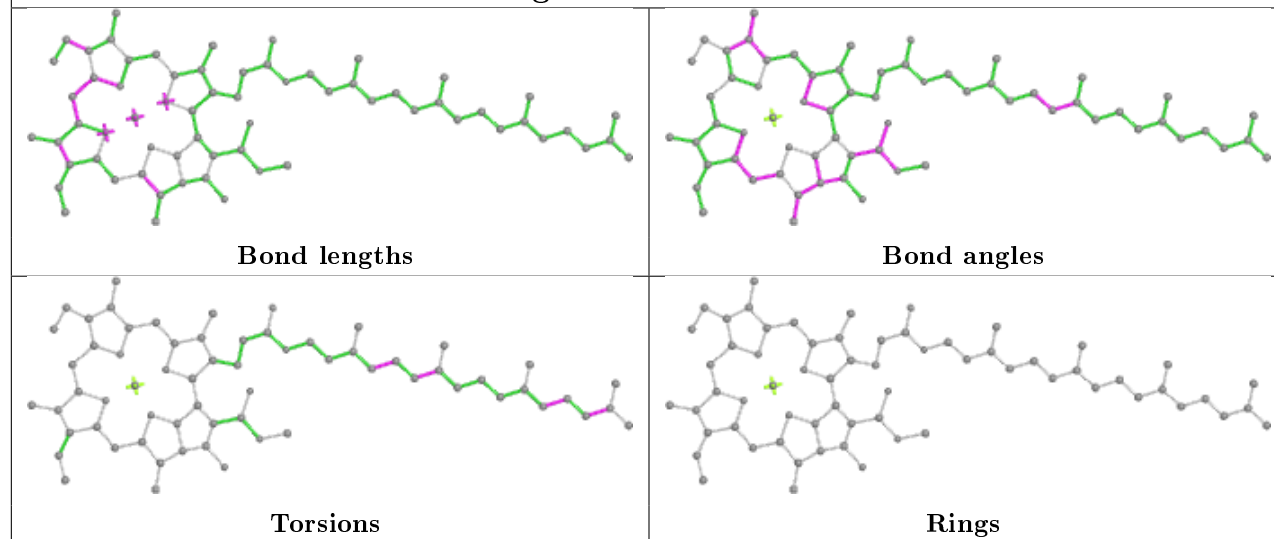
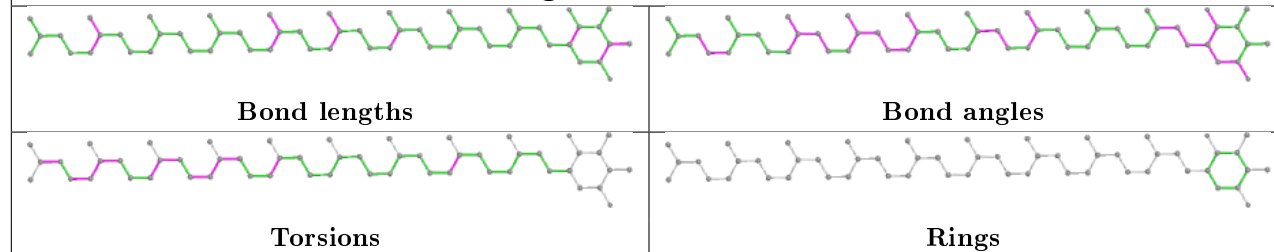
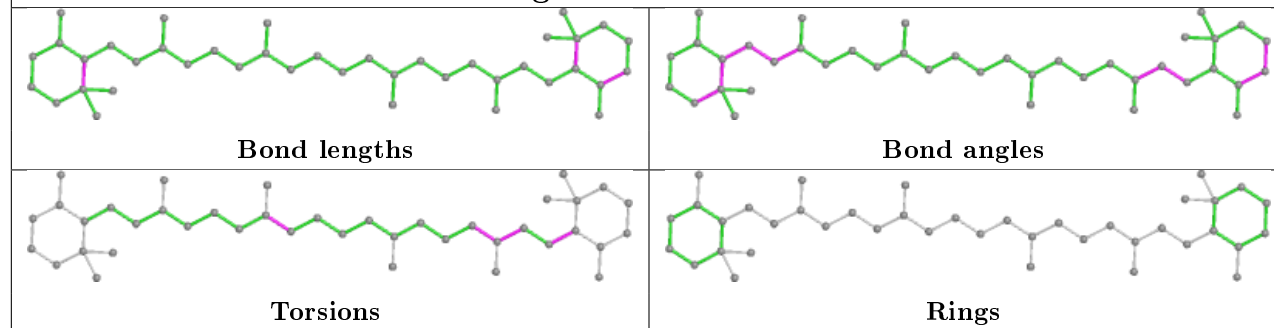


Ligand HEC V 201

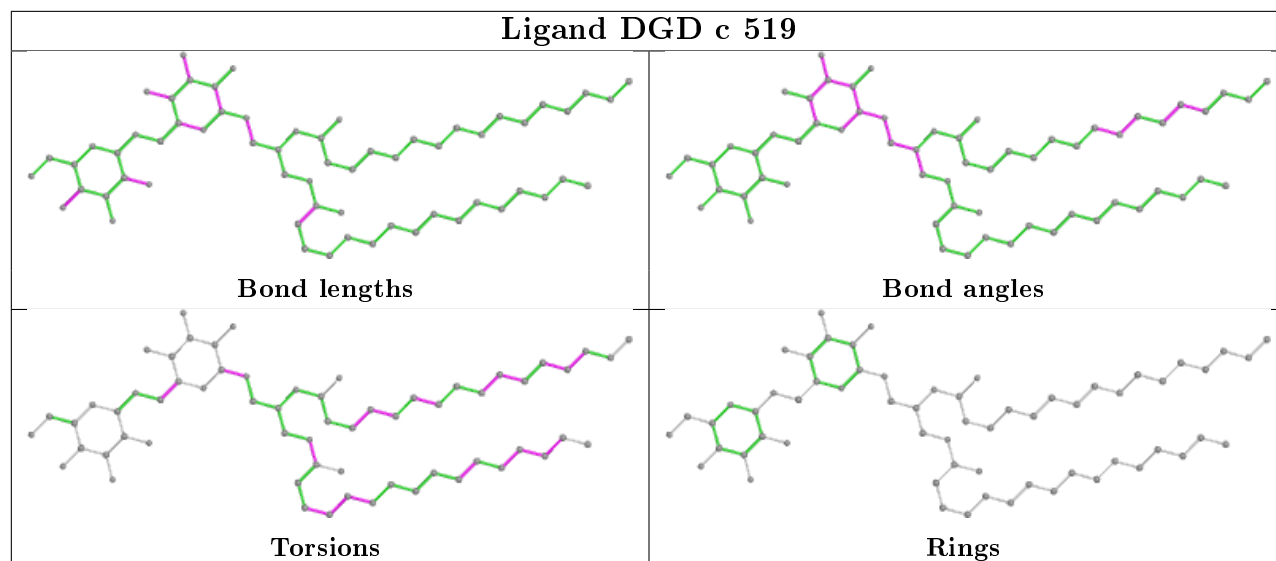


Ligand BCR c 515

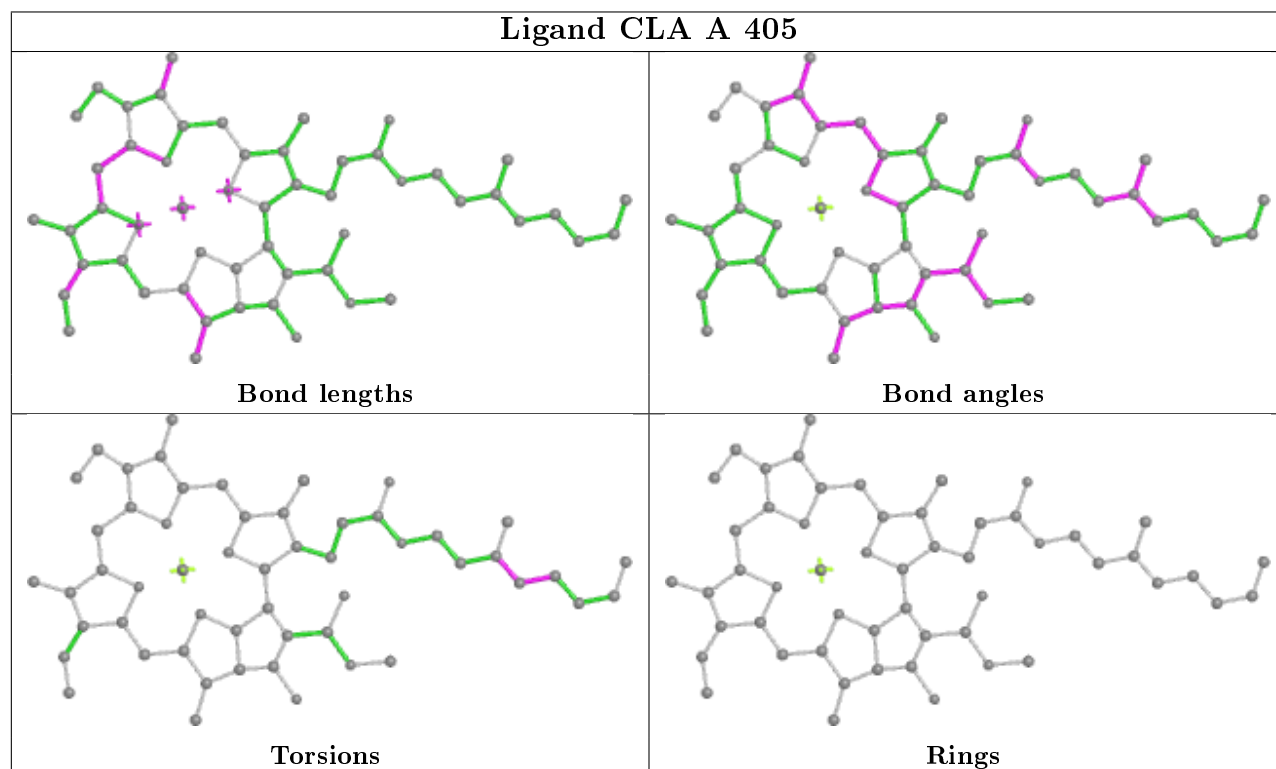


Ligand CLA B 608**Ligand PL9 d 406****Ligand BCR F 101**

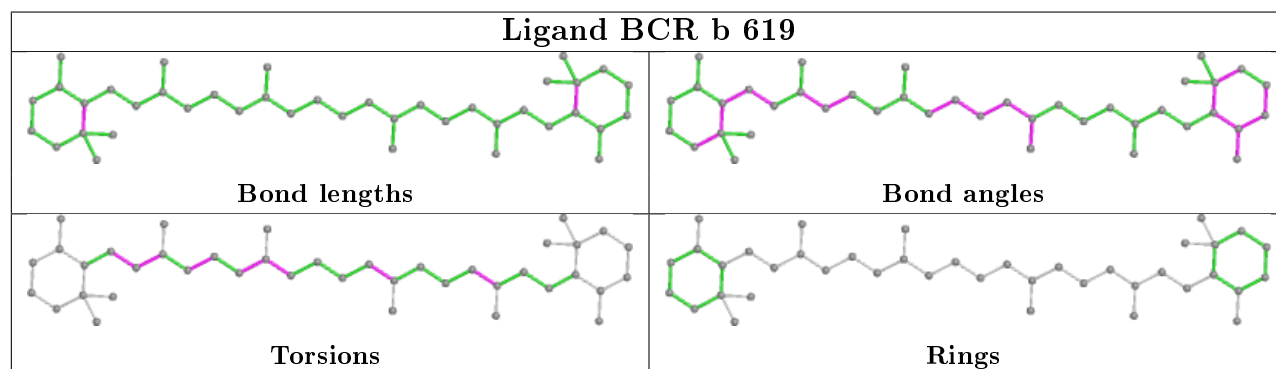
Ligand DGD c 519



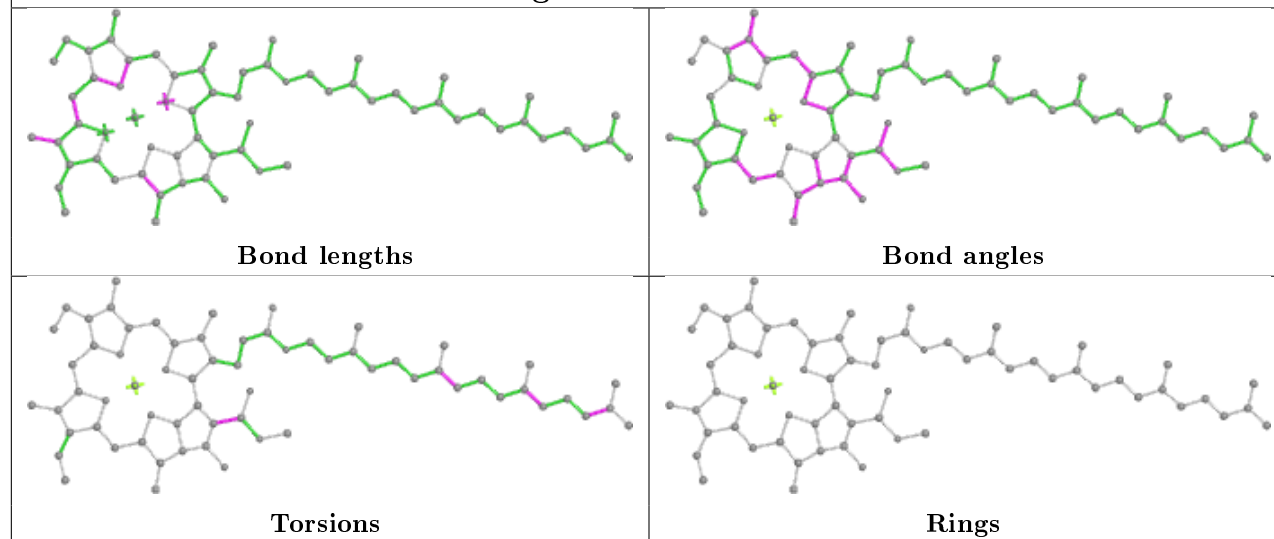
Ligand CLA A 405



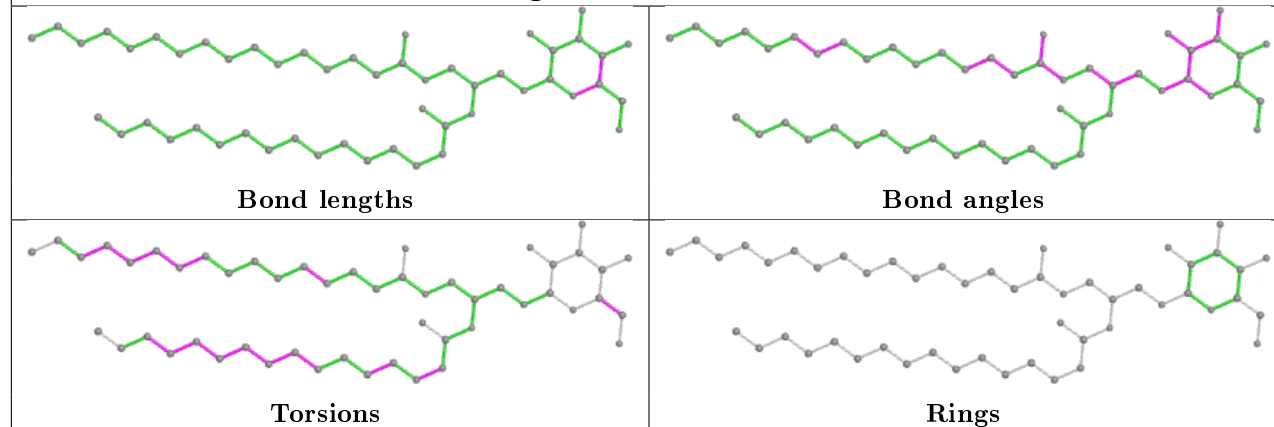
Ligand BCR b 619



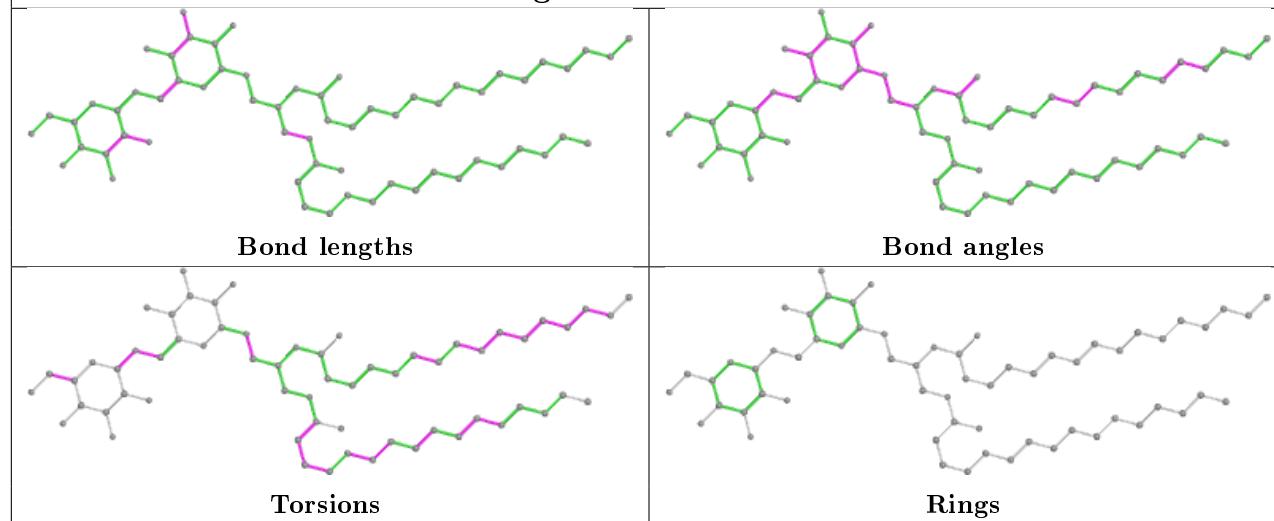
Ligand CLA C 508

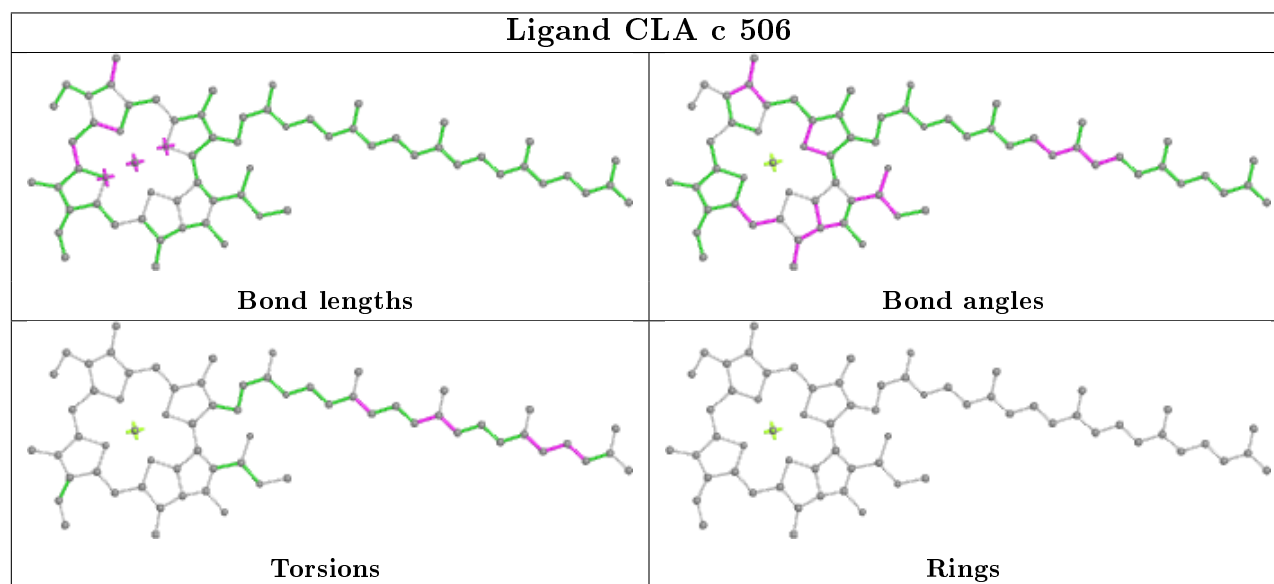
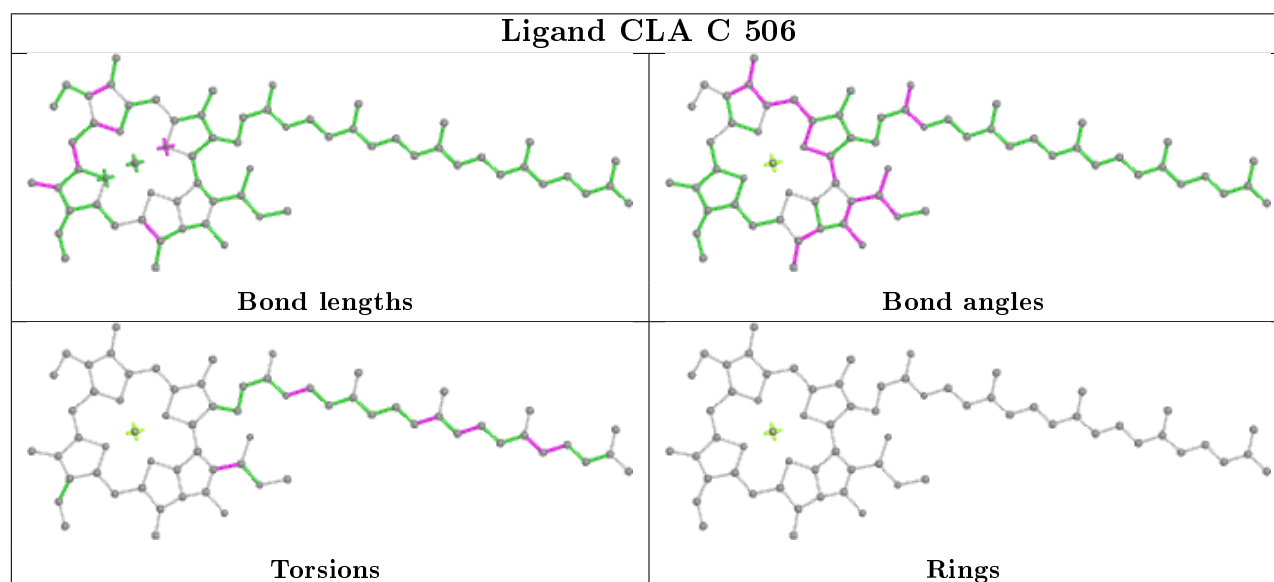
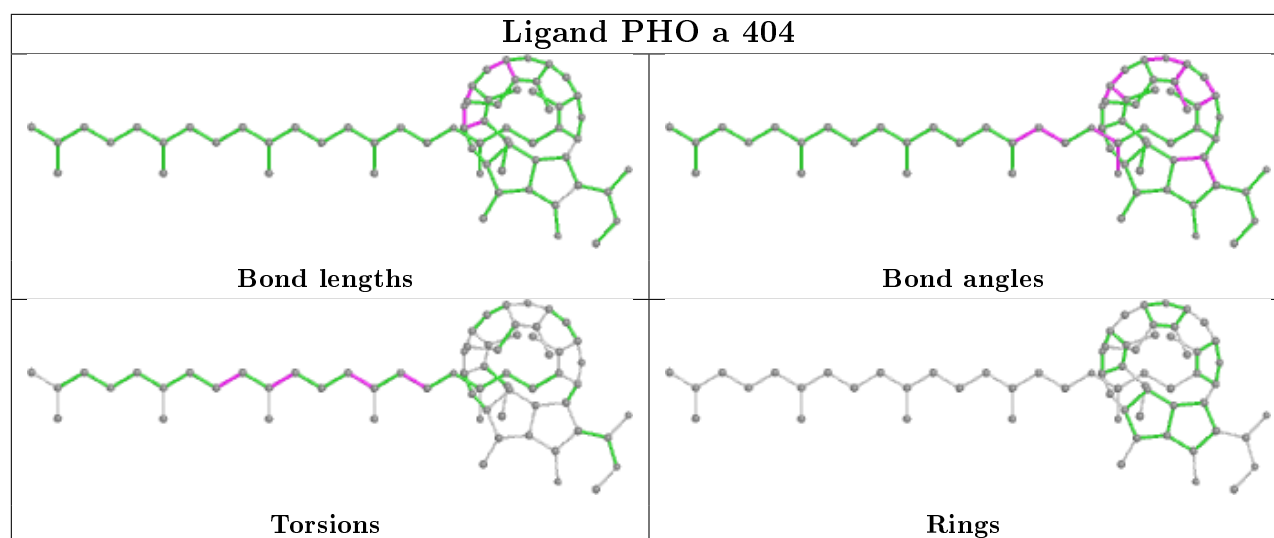


Ligand LMG D 407

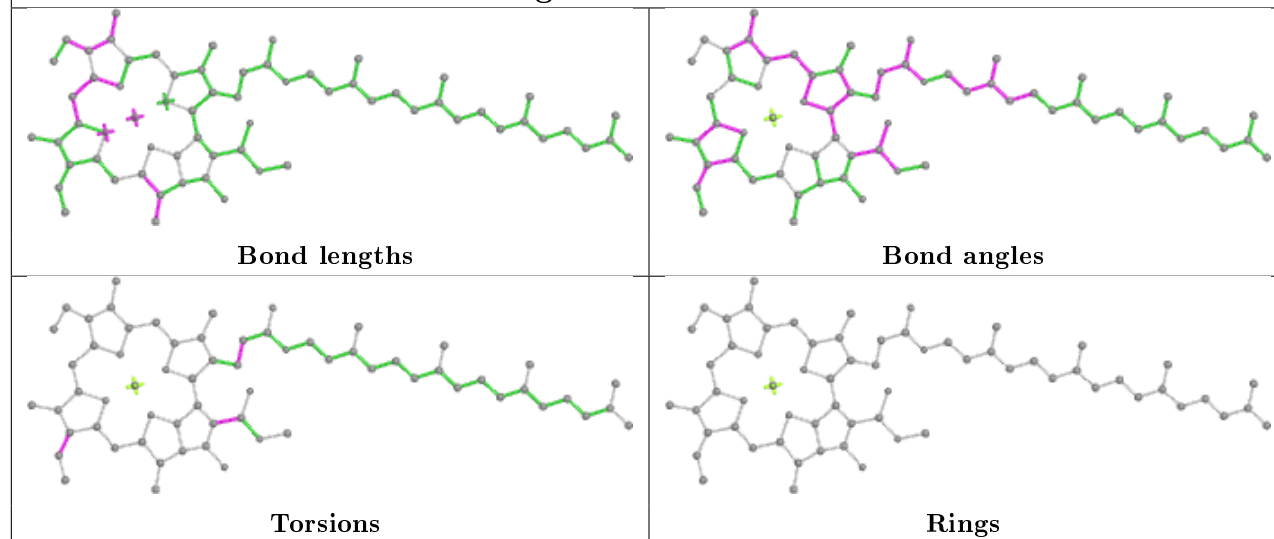


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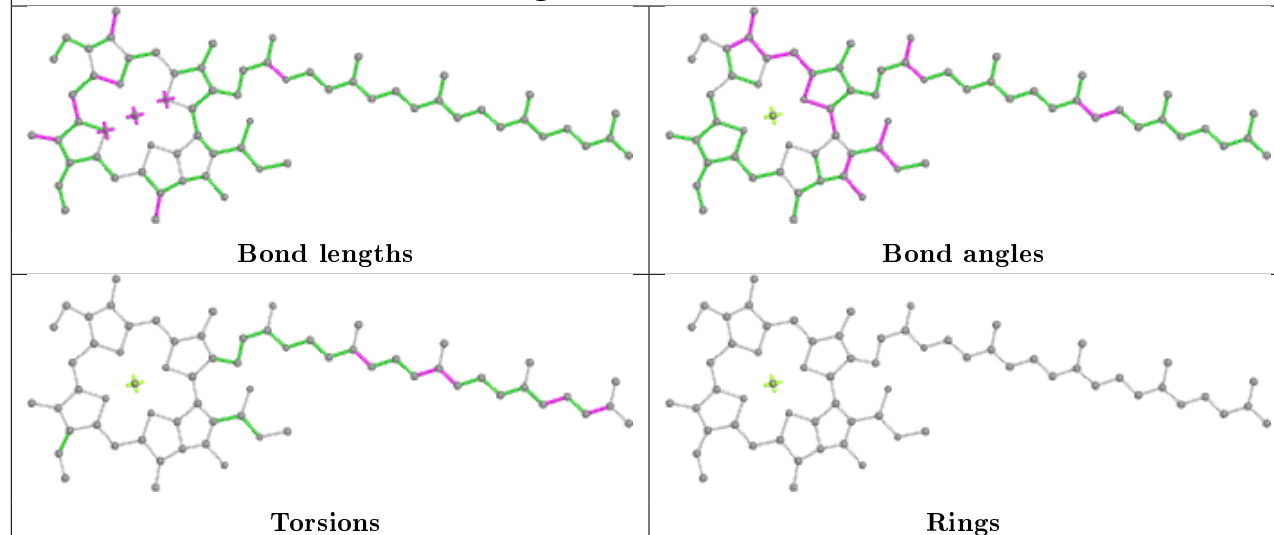




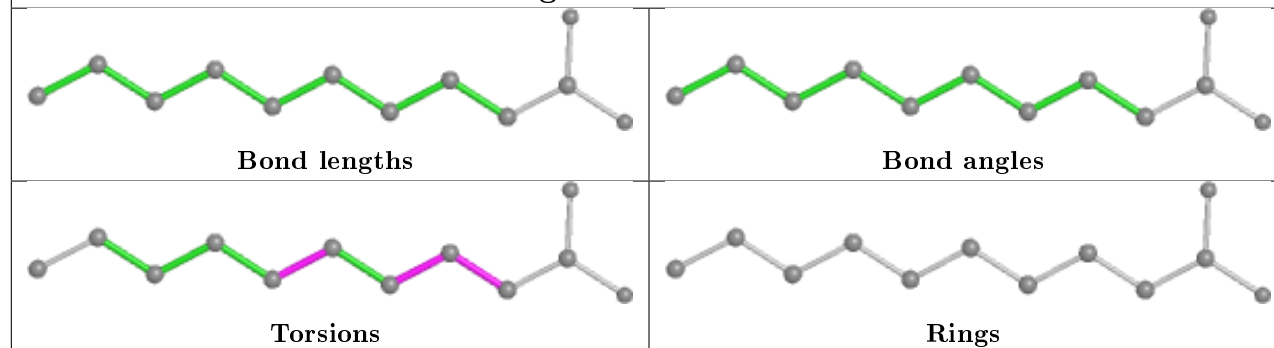
Ligand CLA b 610



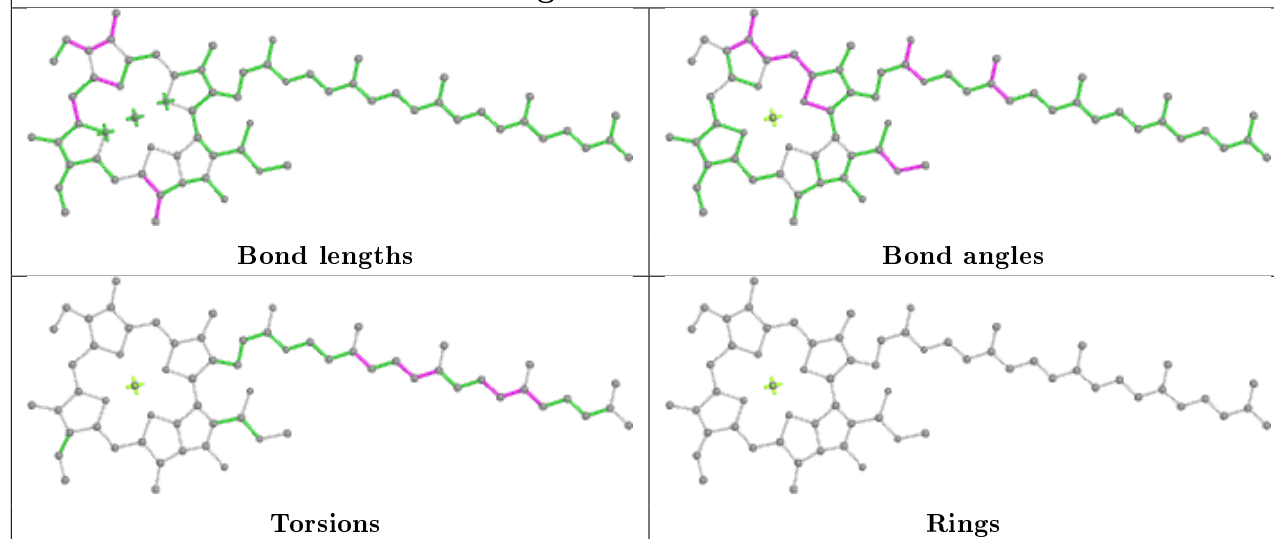
Ligand CLA C 510



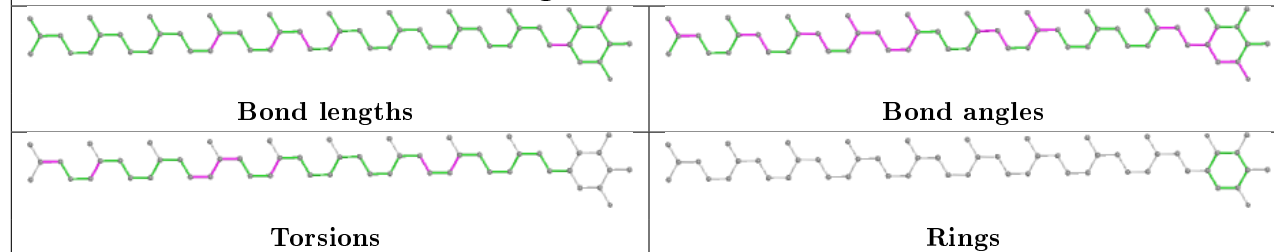
Ligand STE J 101



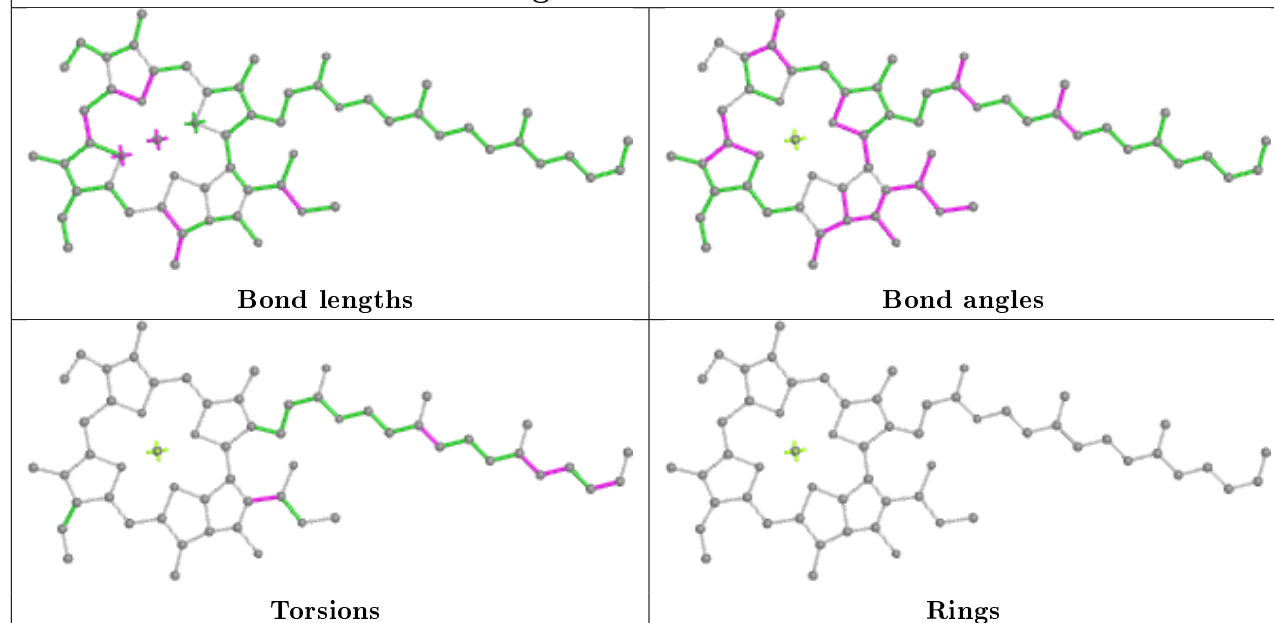
Ligand CLA c 508

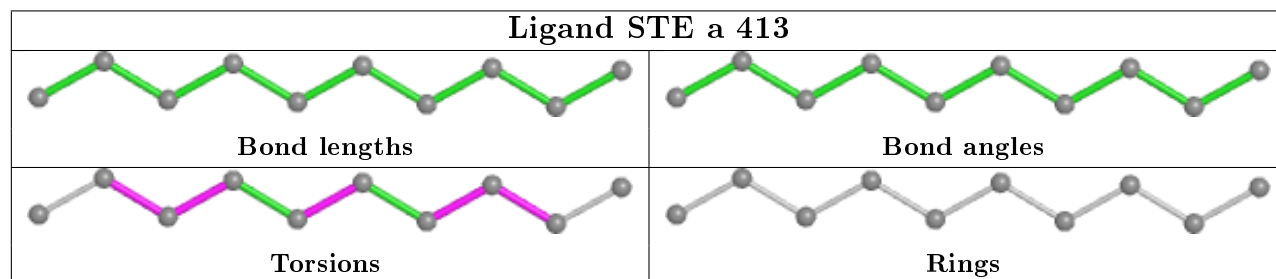
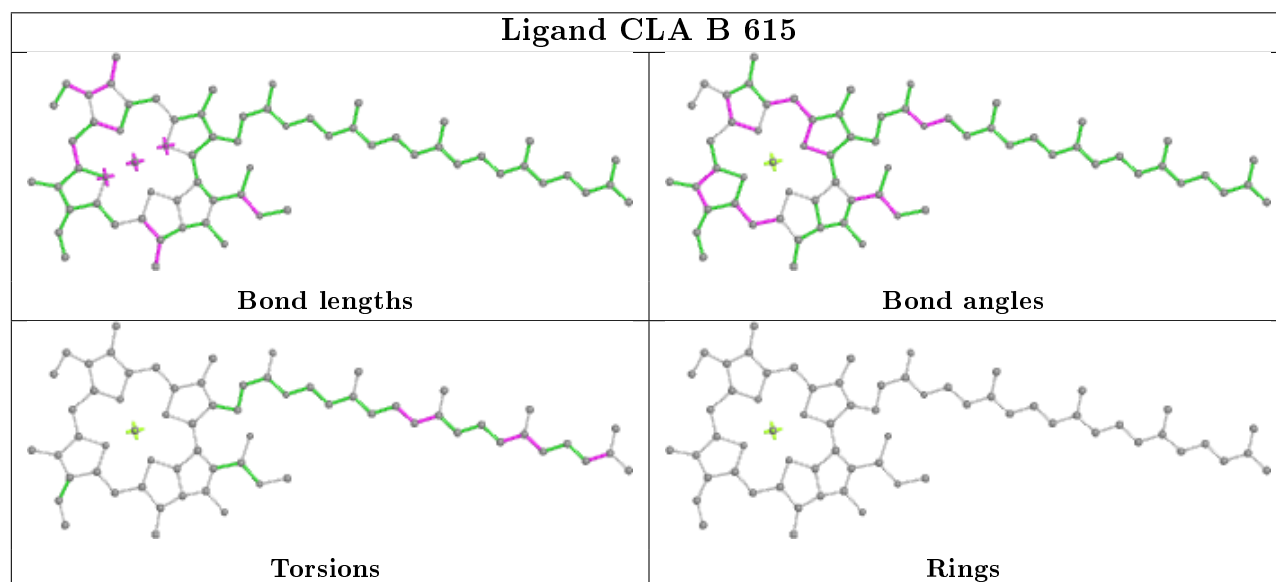
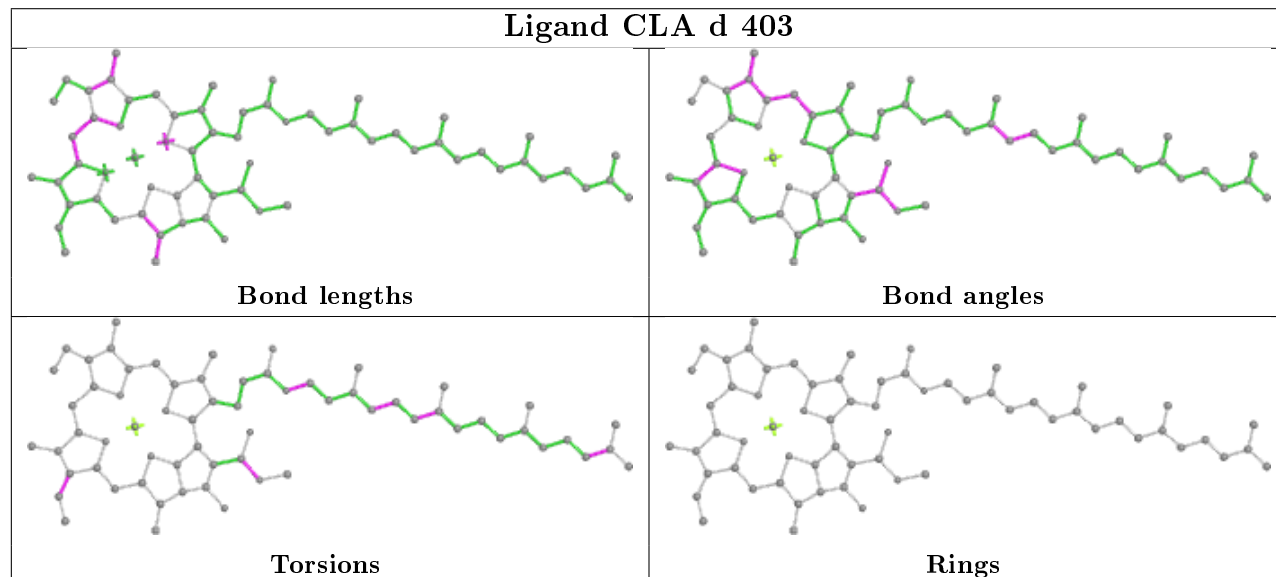
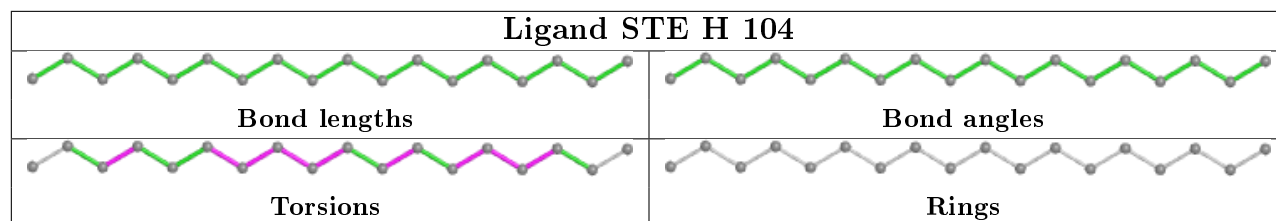


Ligand PL9 D 406

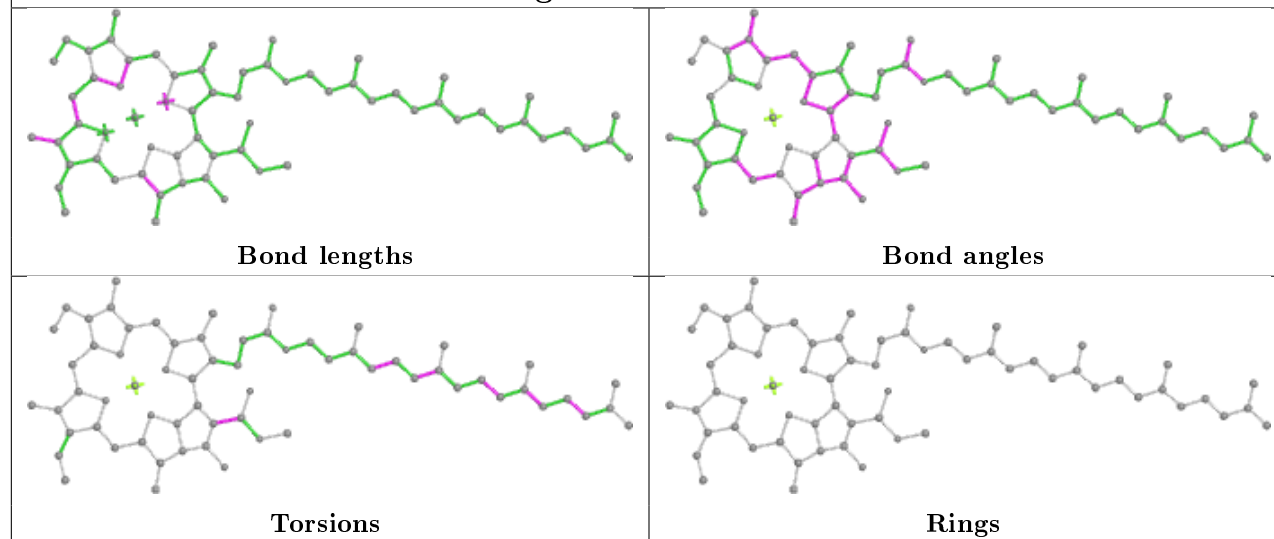


Ligand CLA C 504

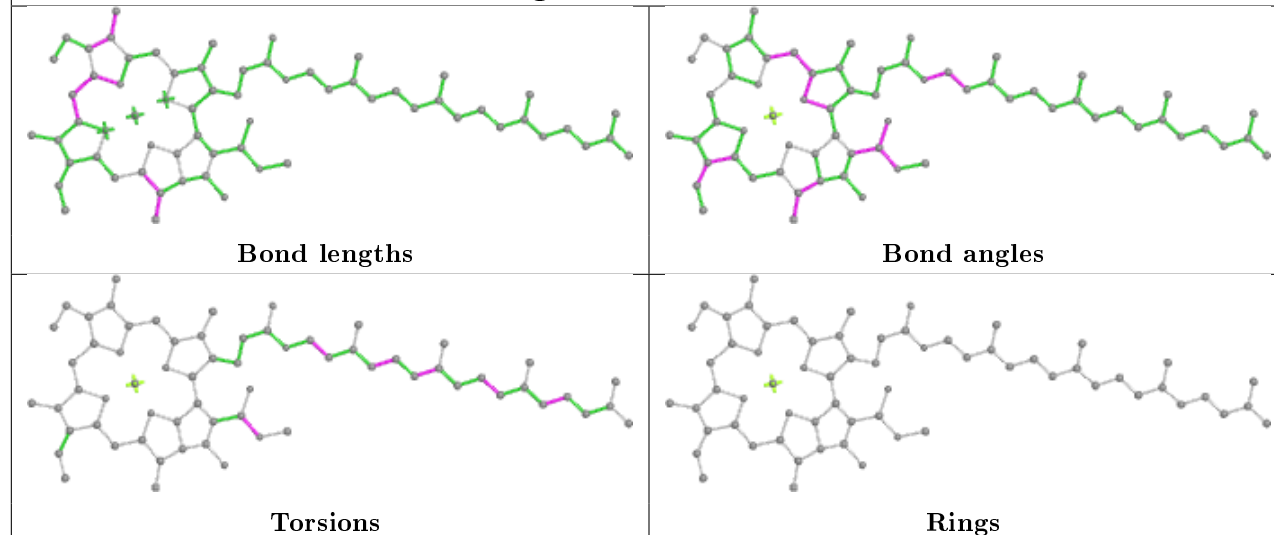




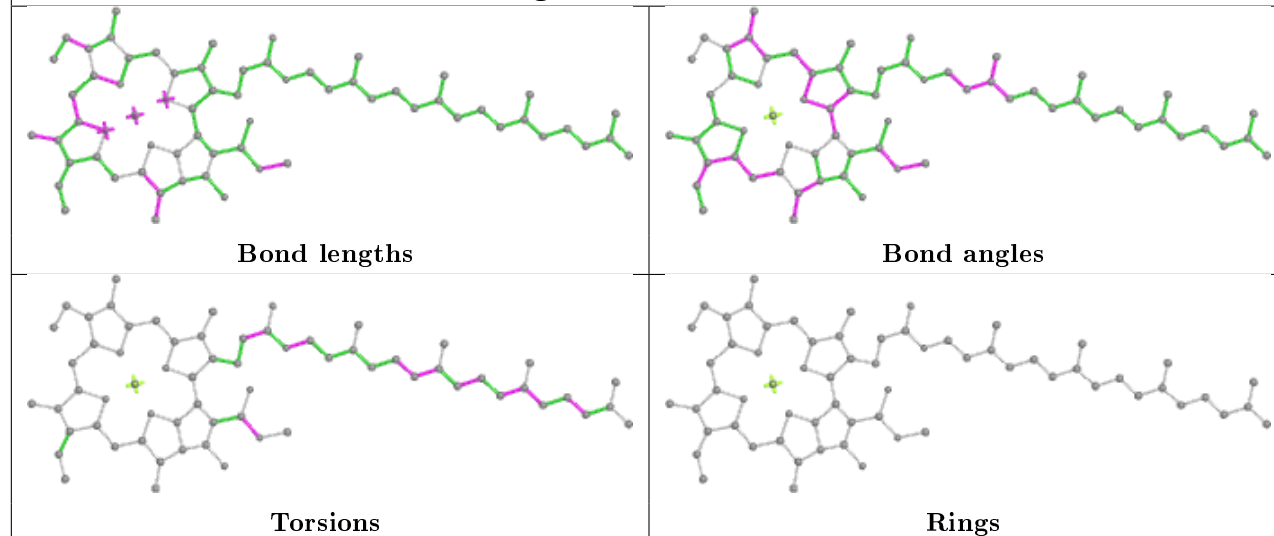
Ligand CLA b 604

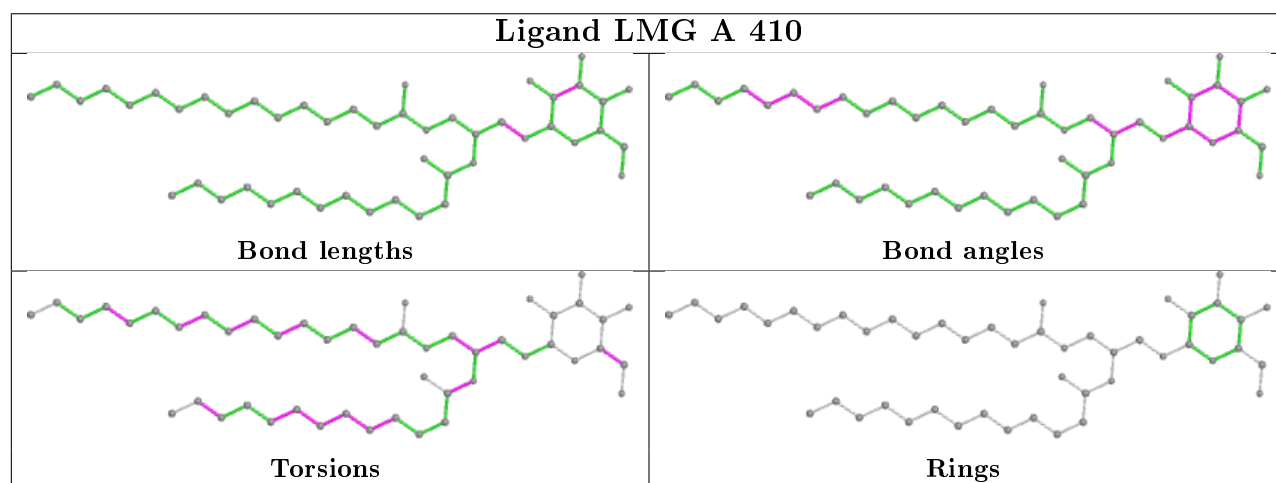
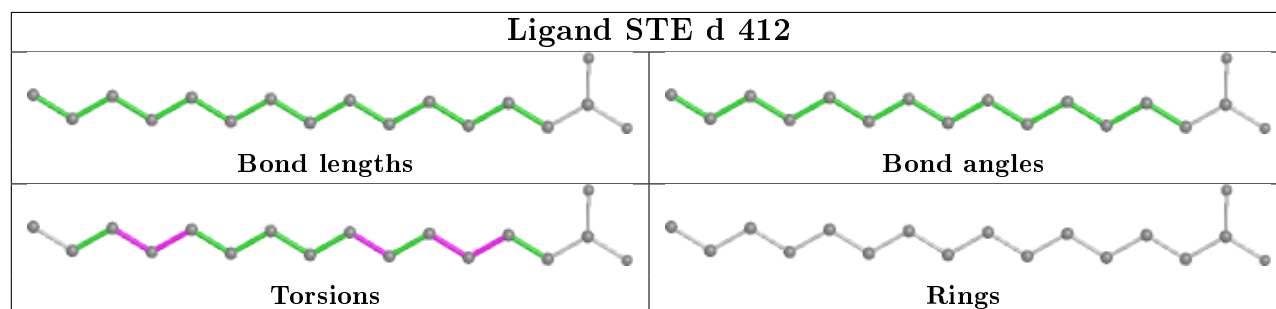
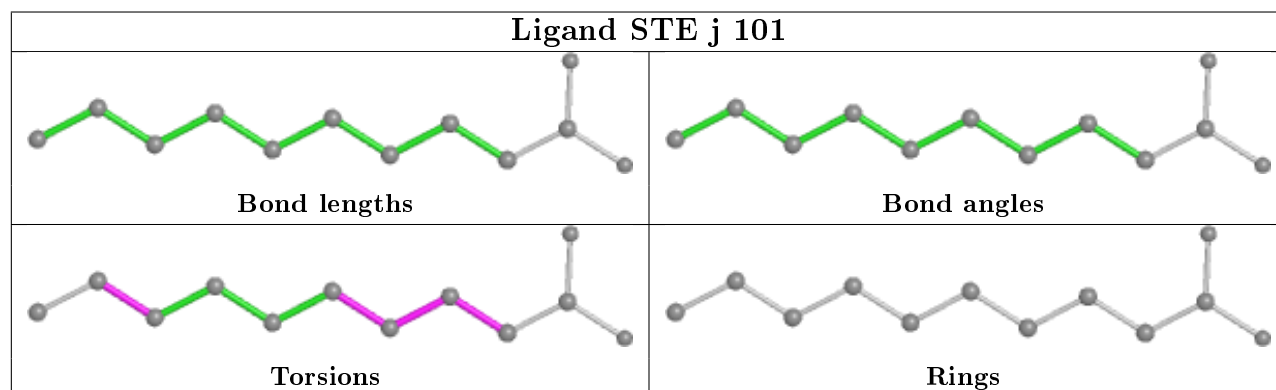
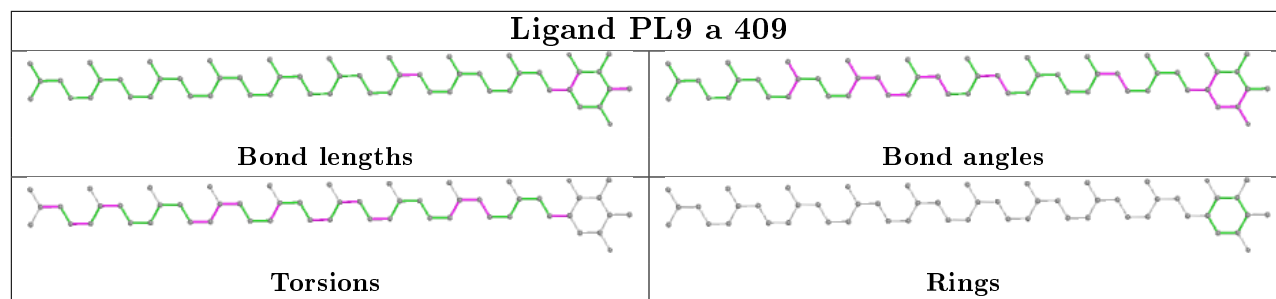


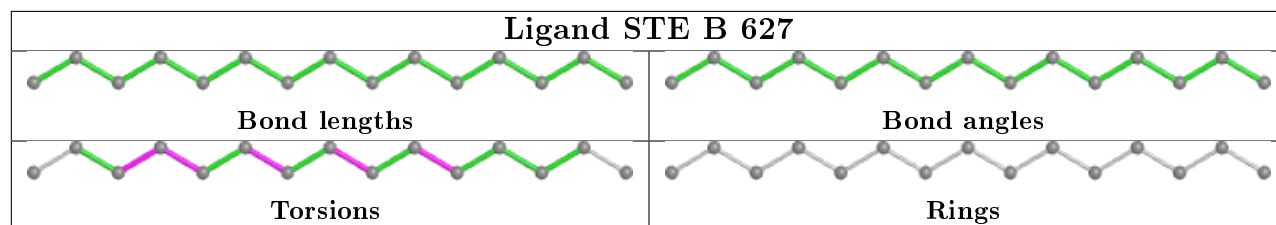
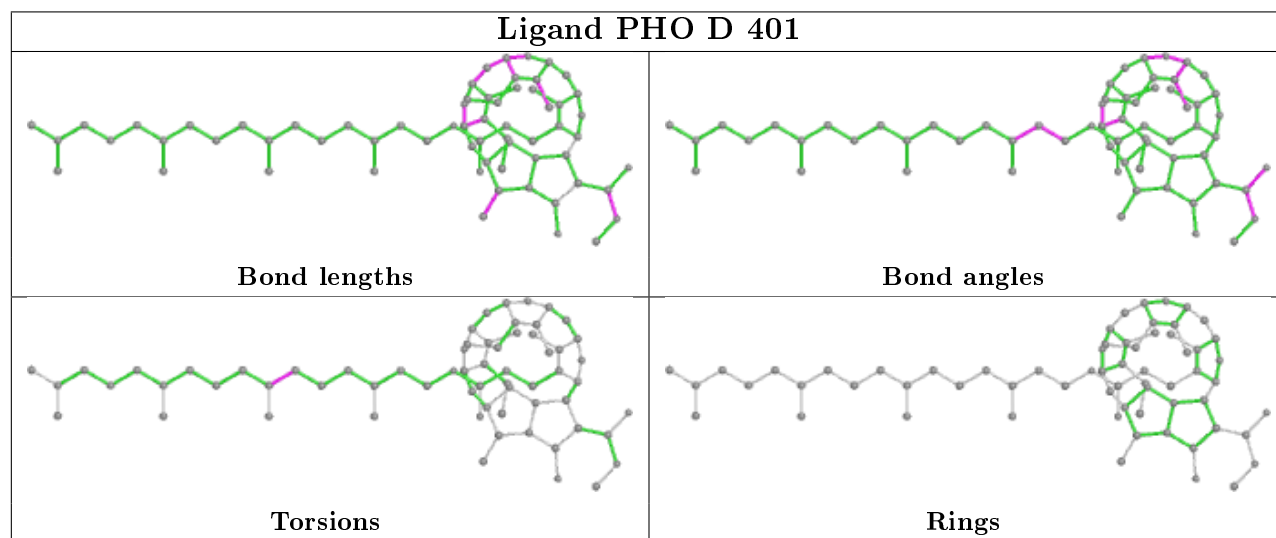
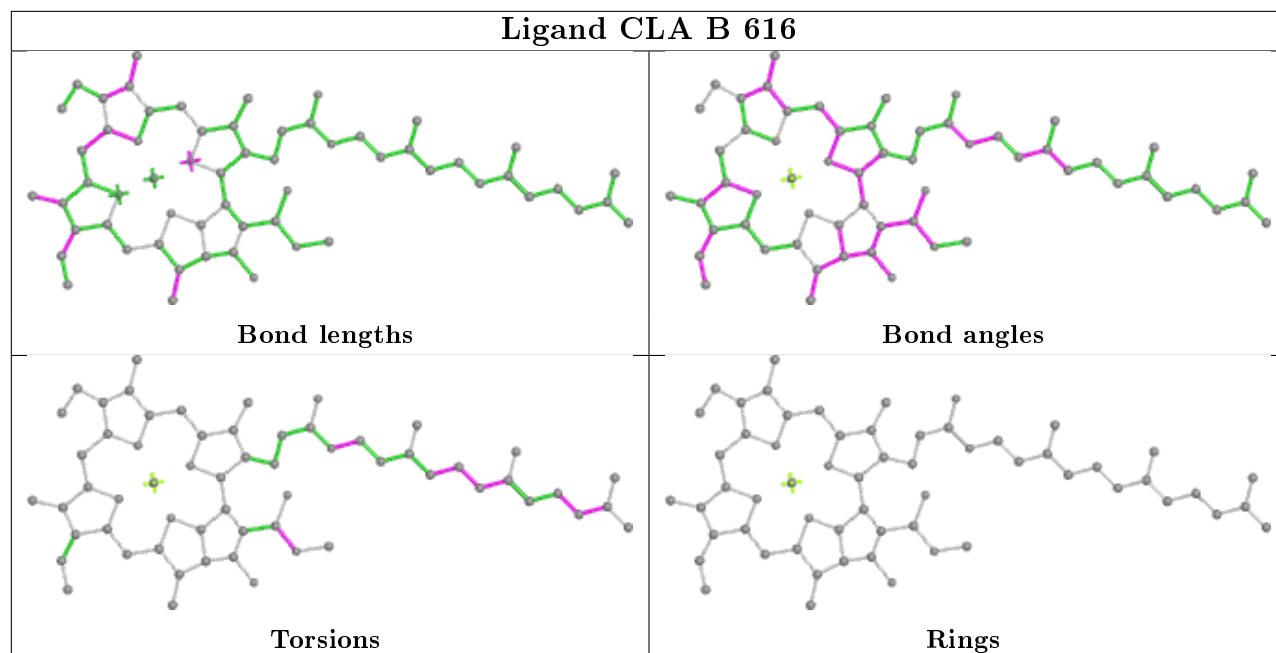
Ligand CLA D 405

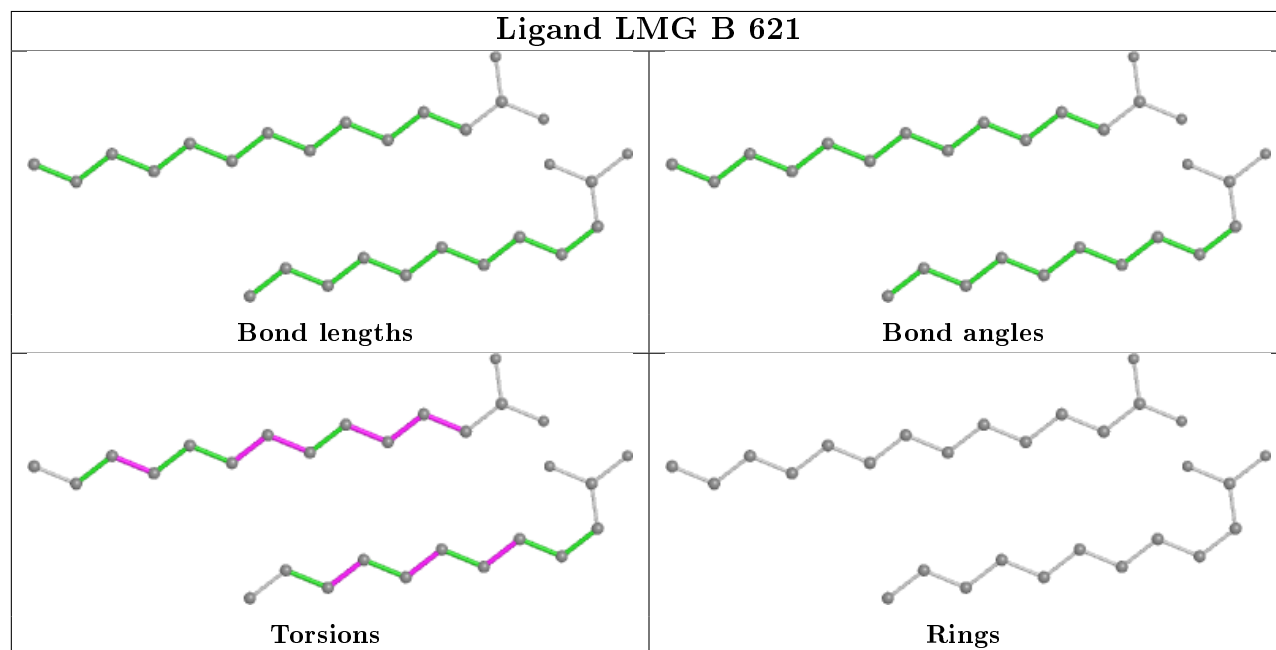
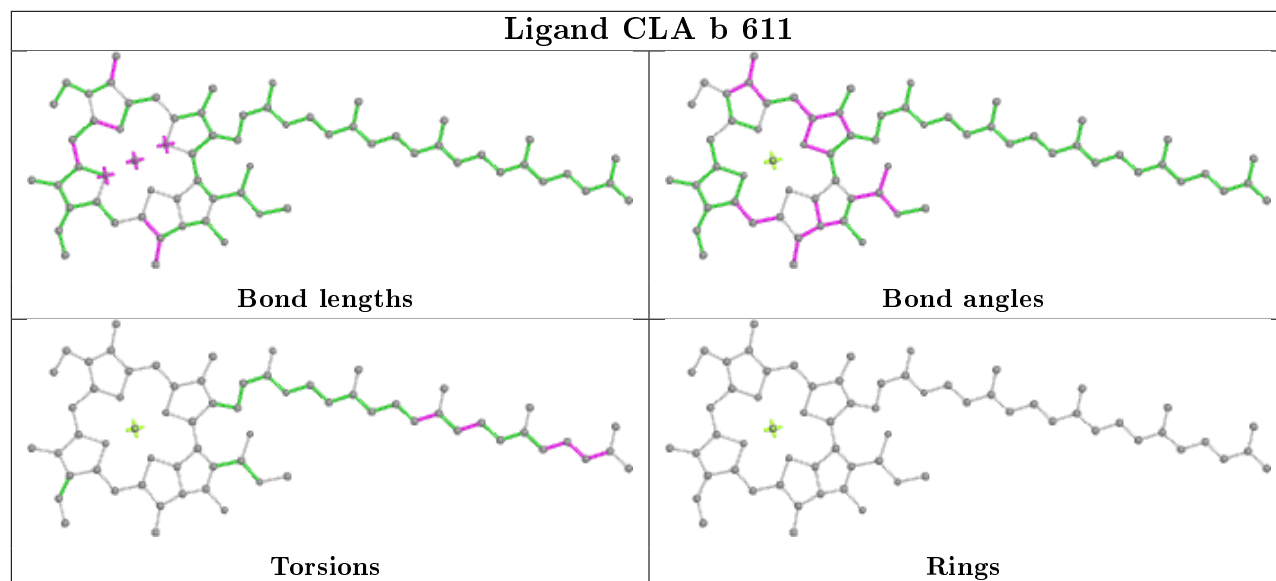
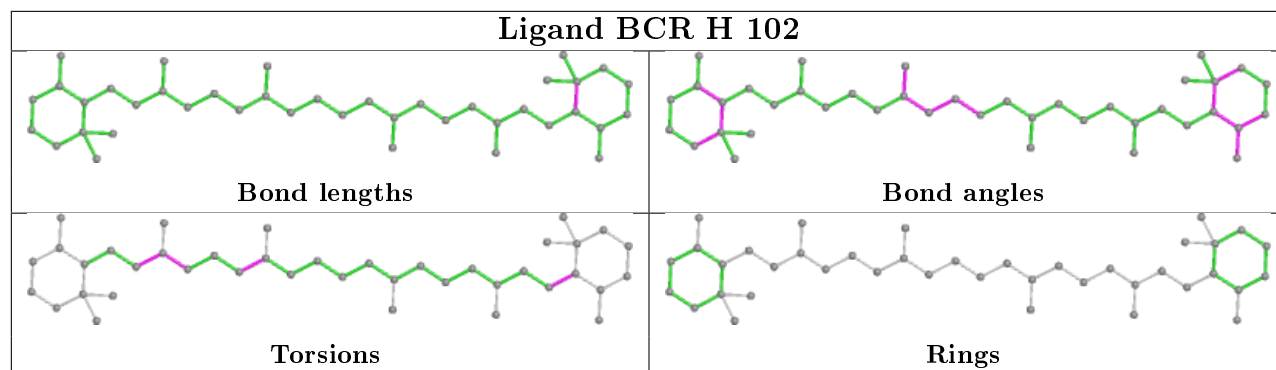


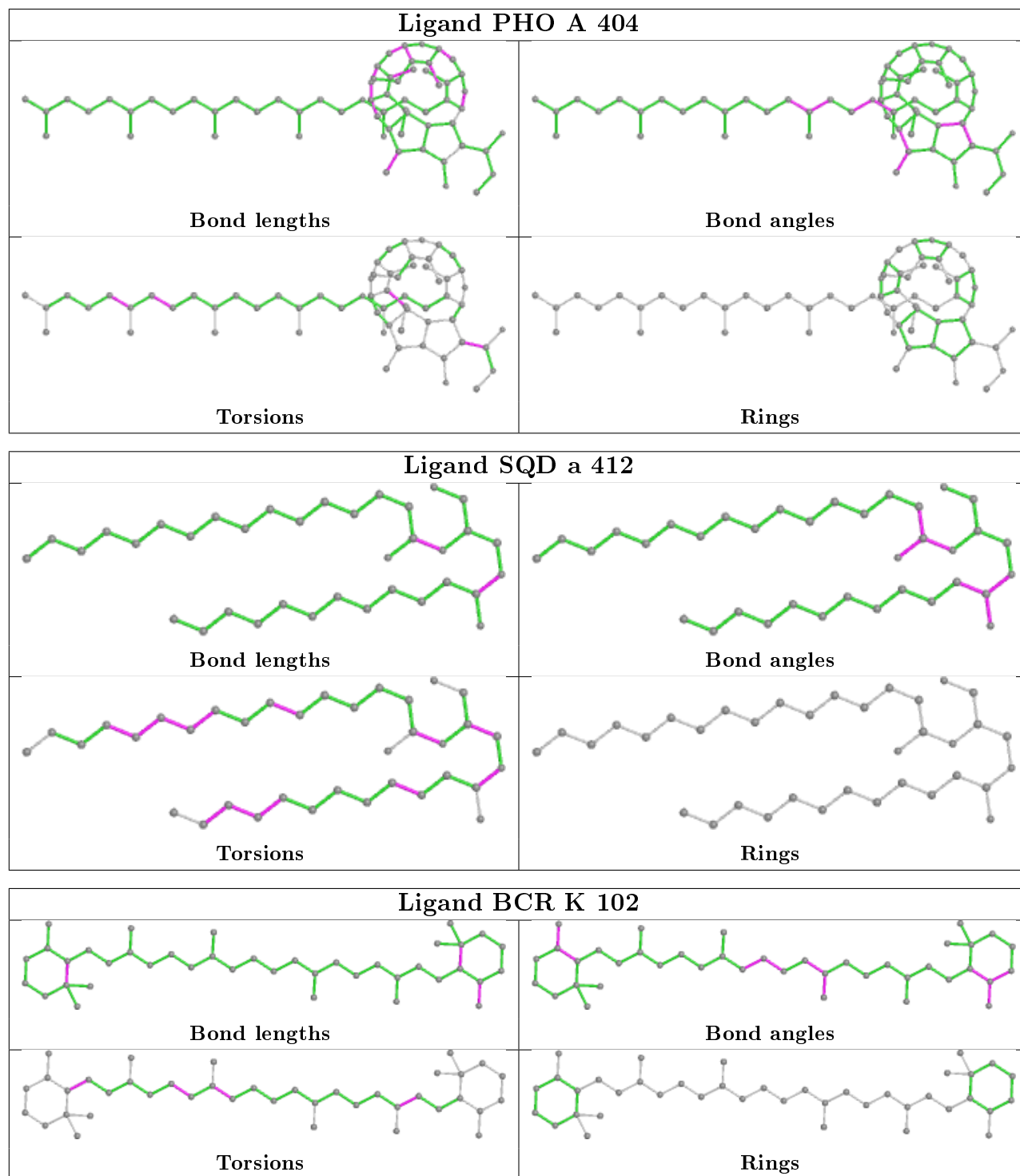
Ligand CLA B 613



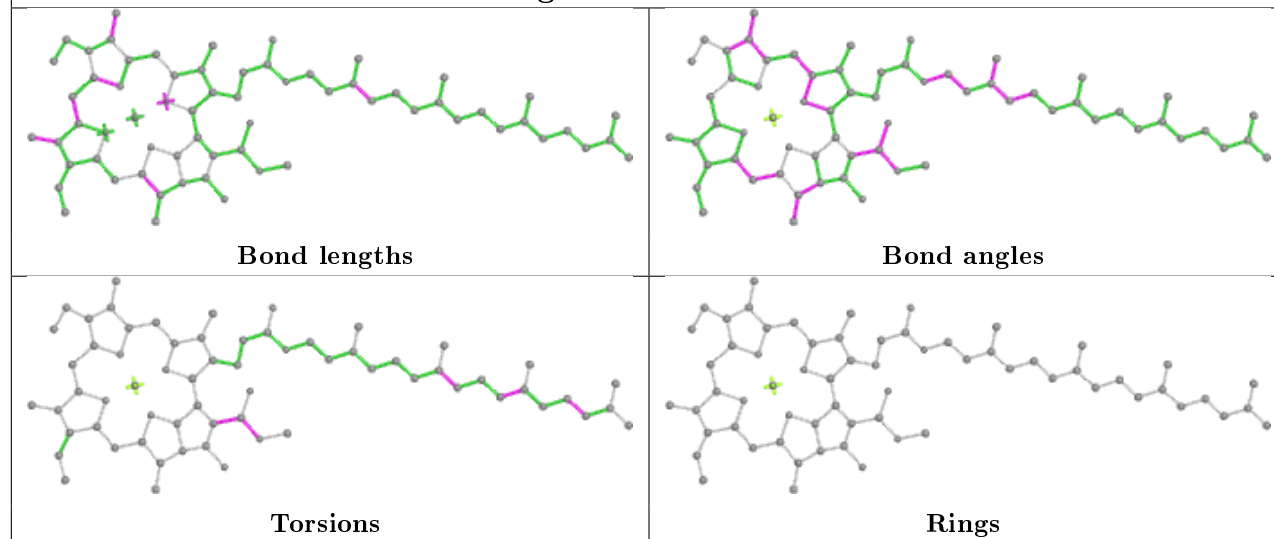




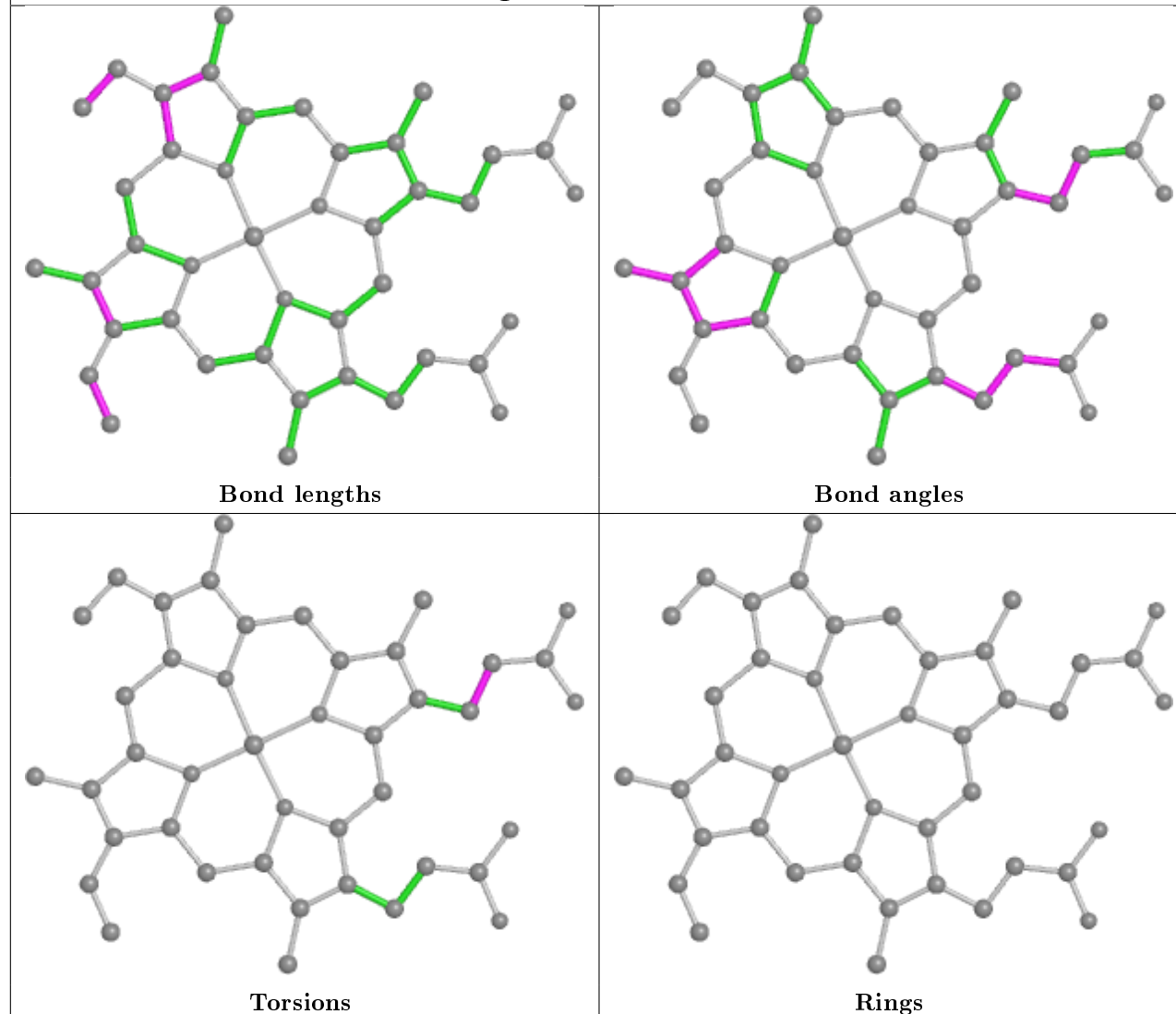


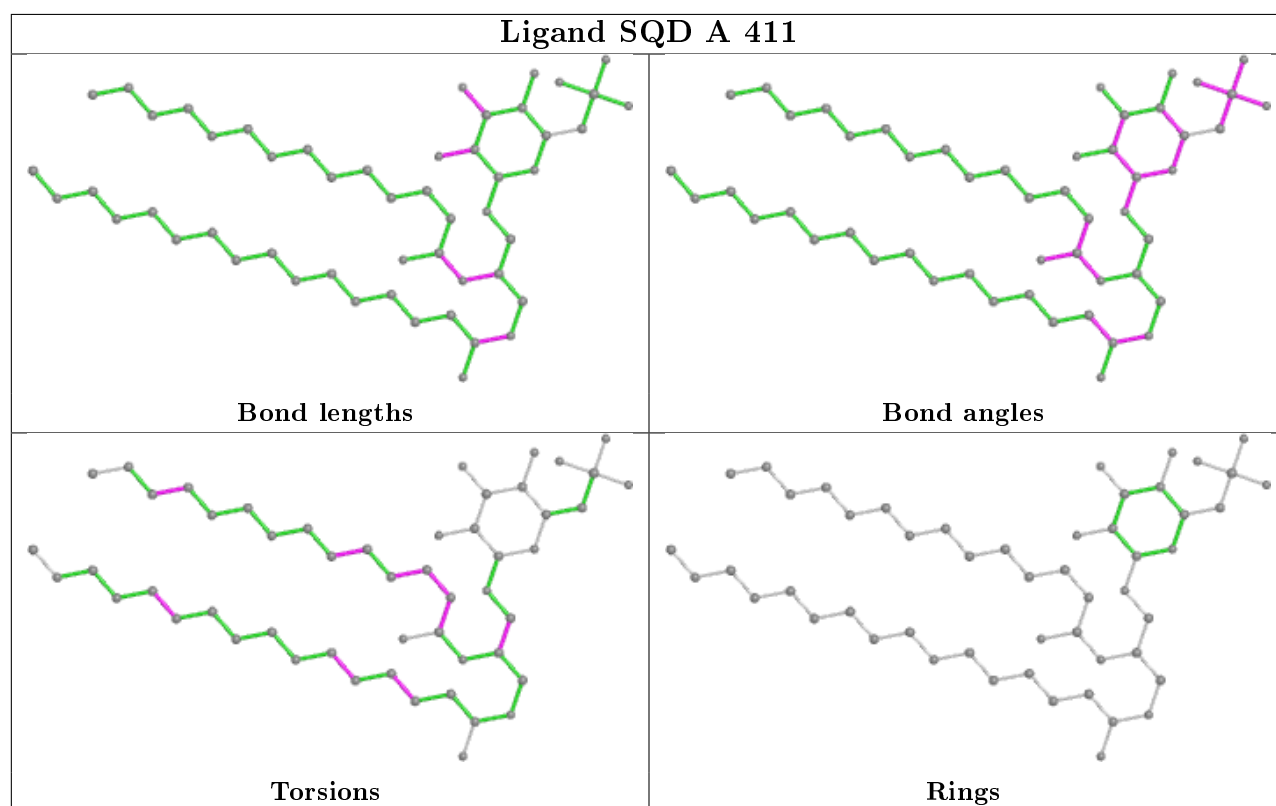
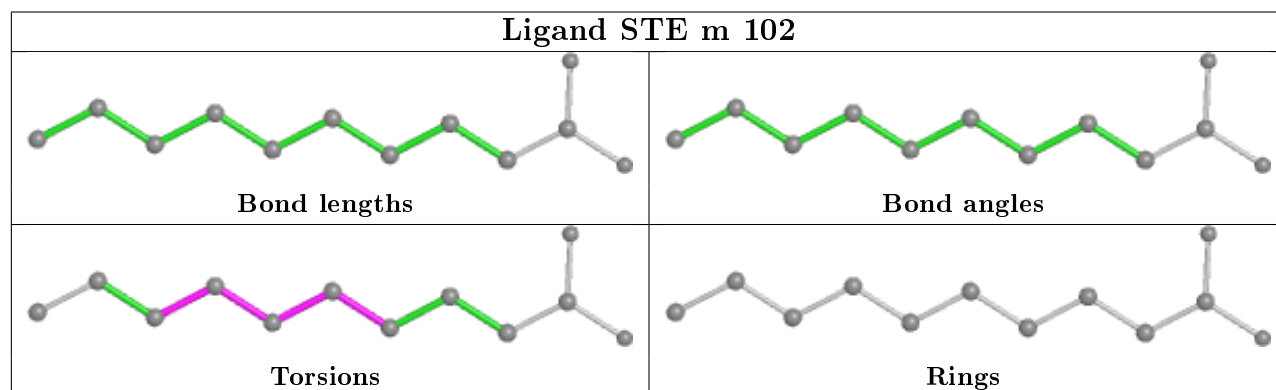
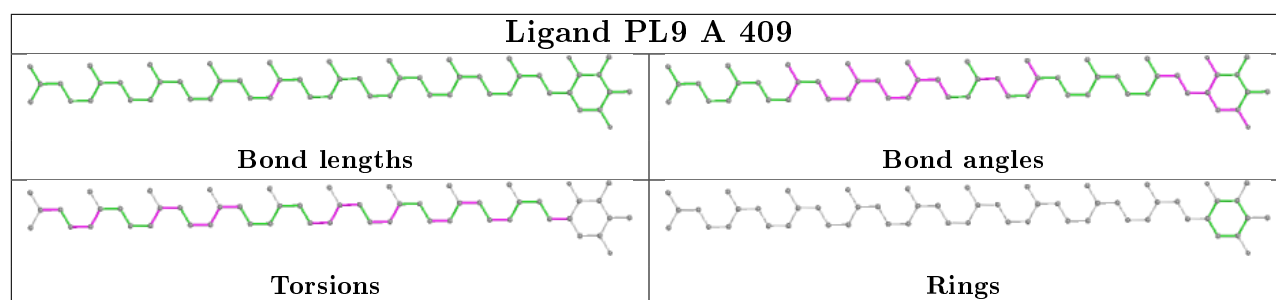


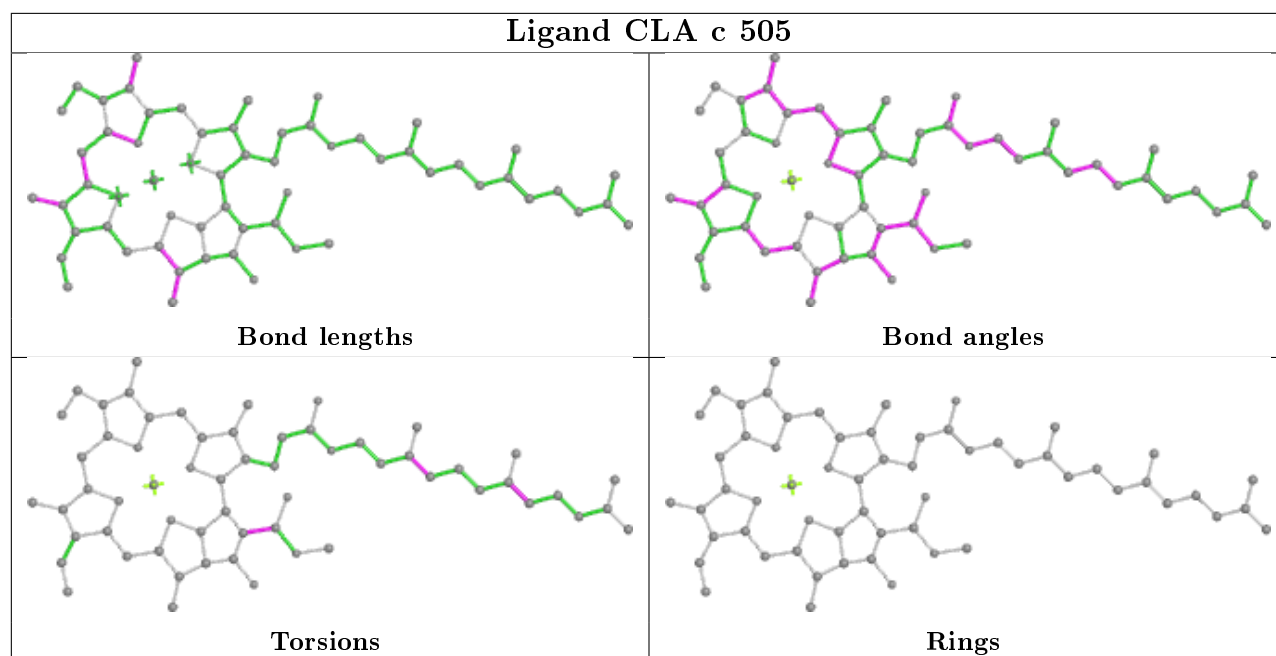
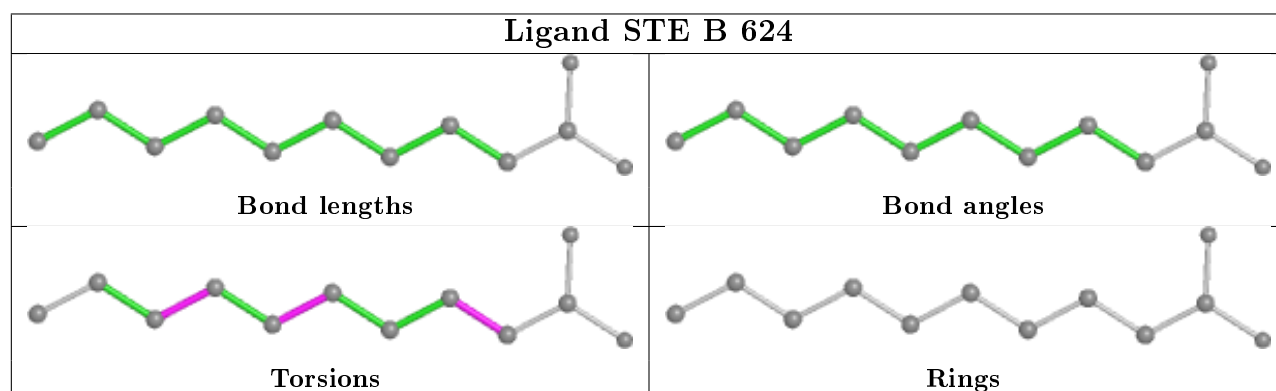
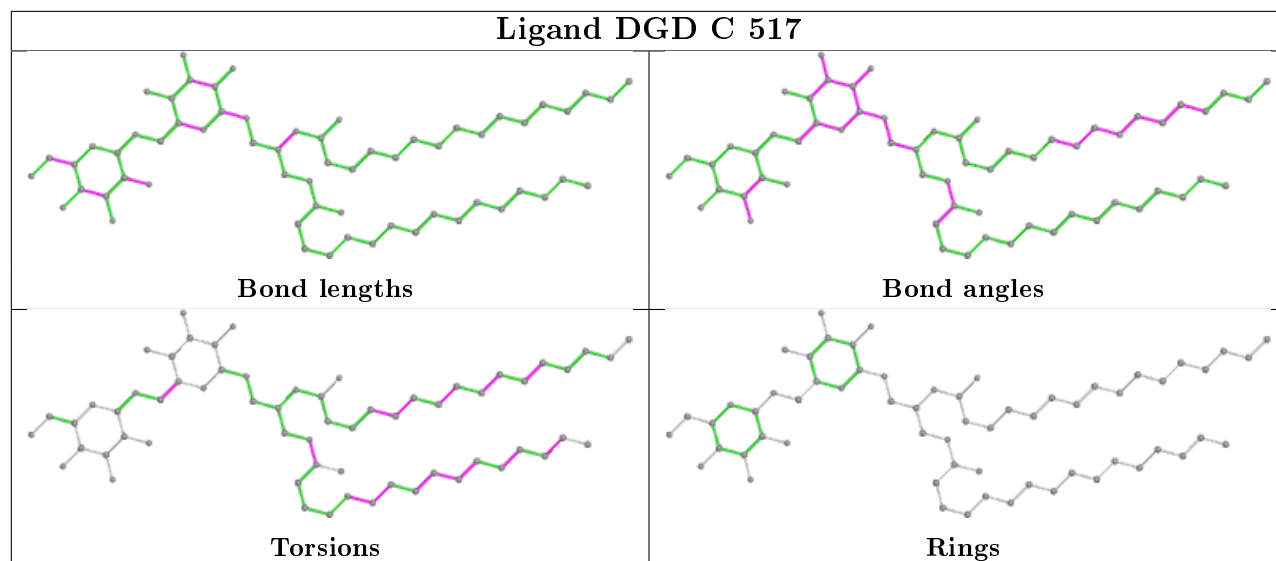
Ligand CLA c 511

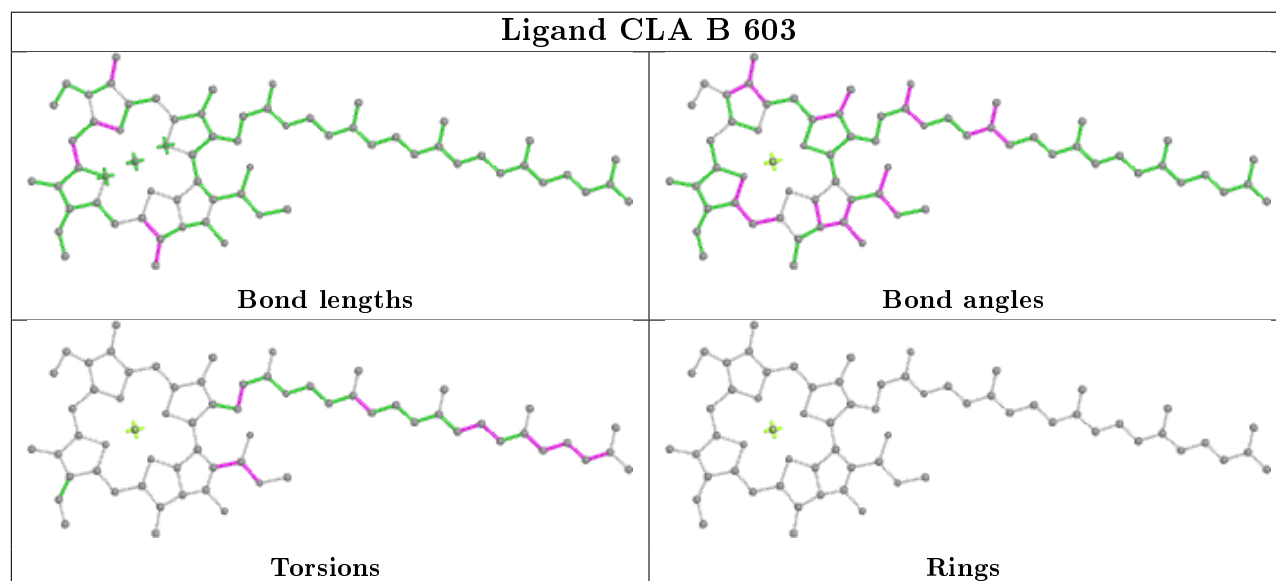
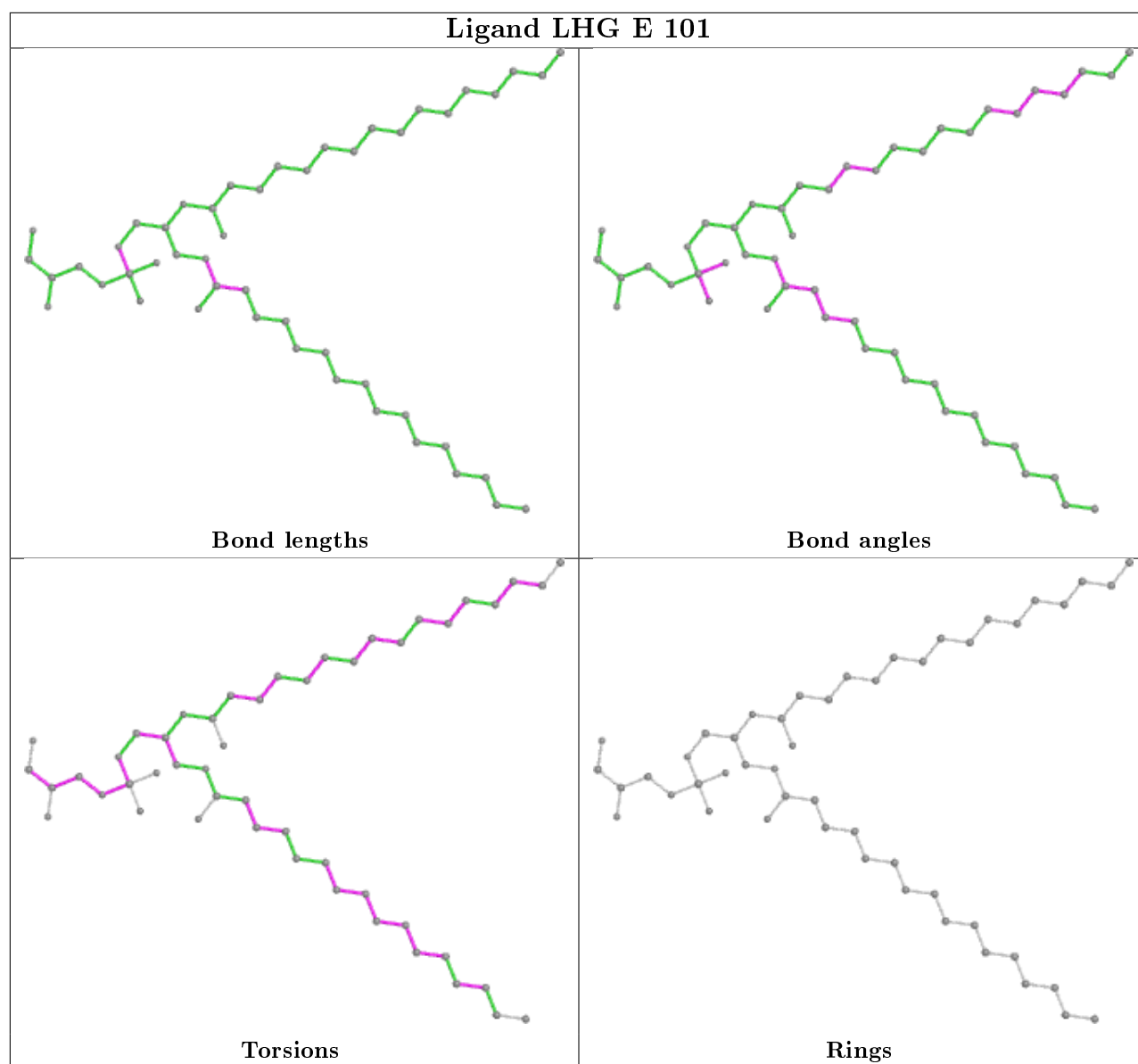


Ligand HEC f 101

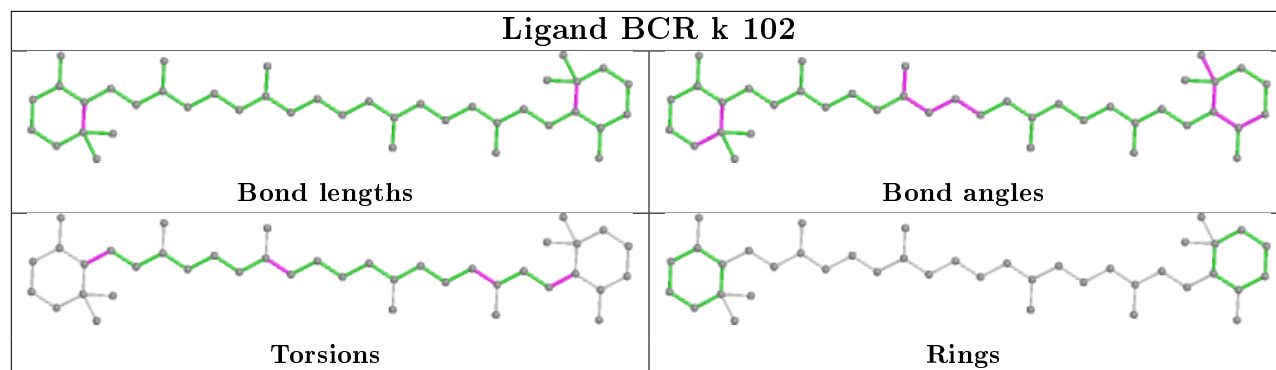




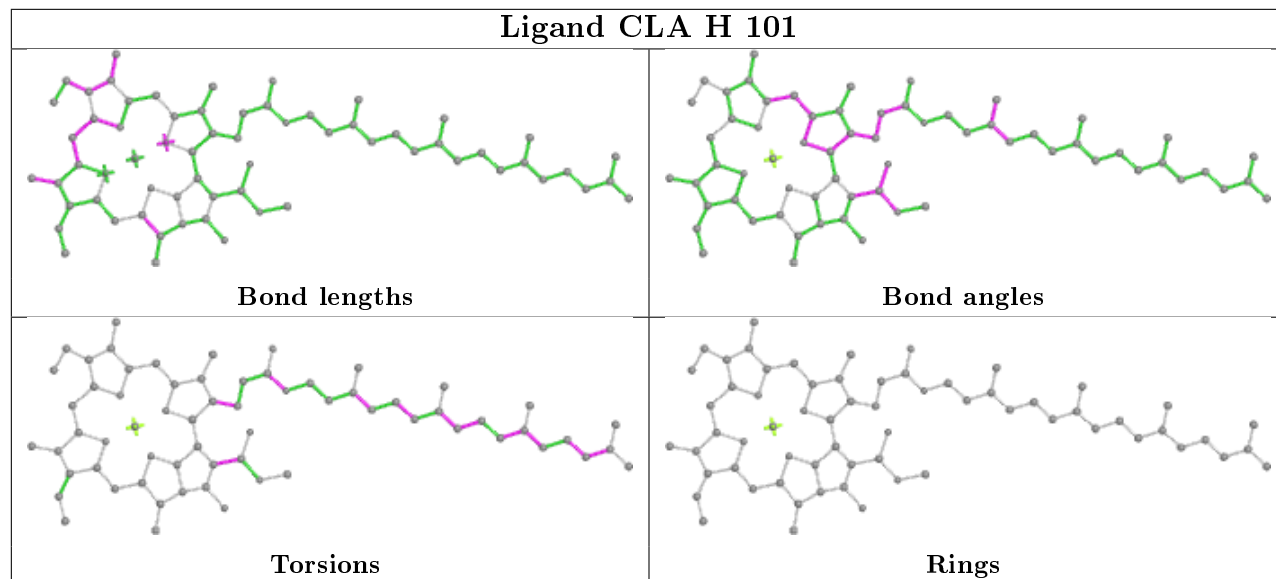




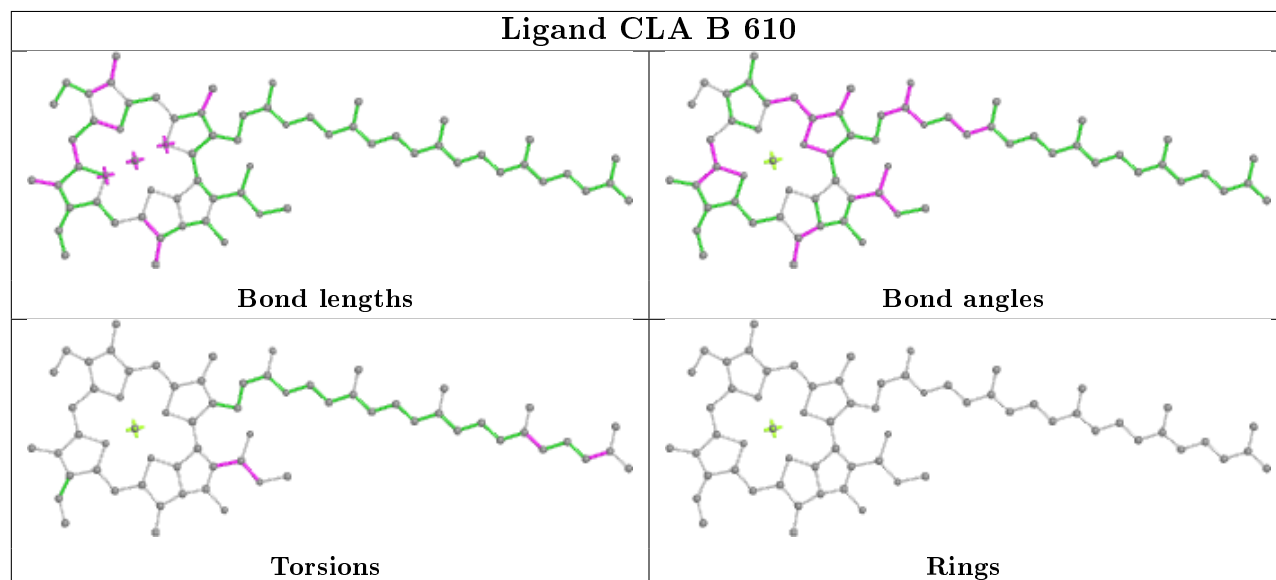
Ligand BCR k 102



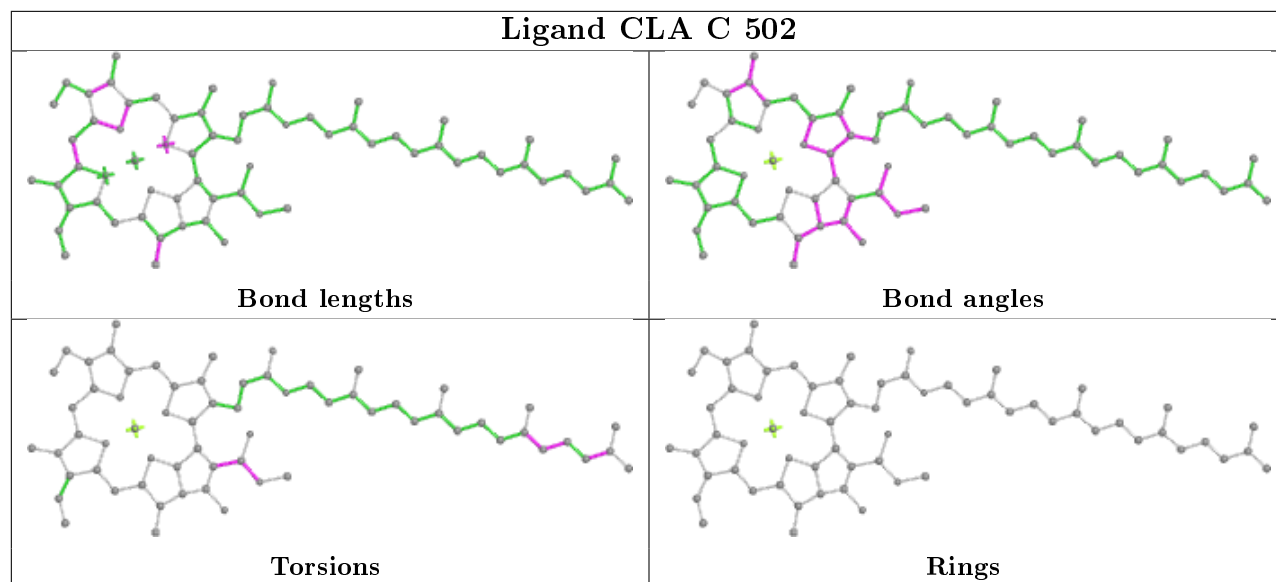
Ligand CLA H 101



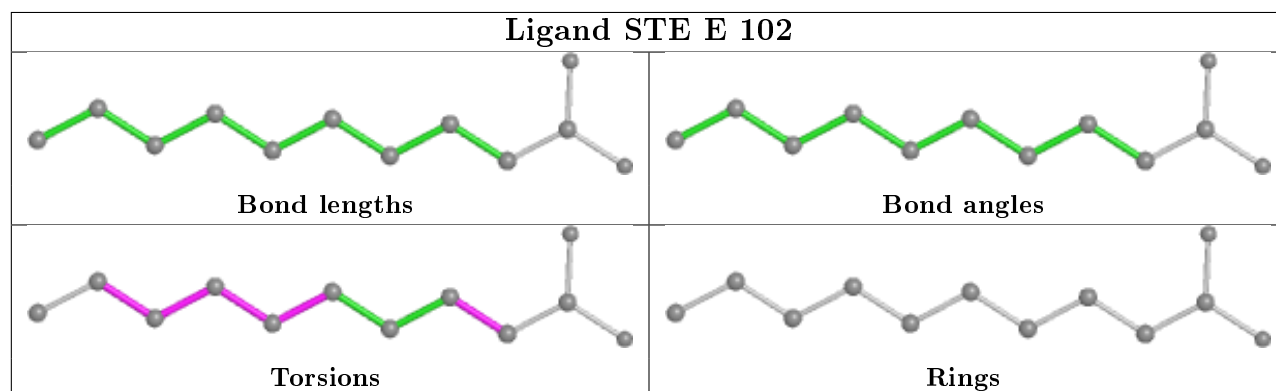
Ligand CLA B 610



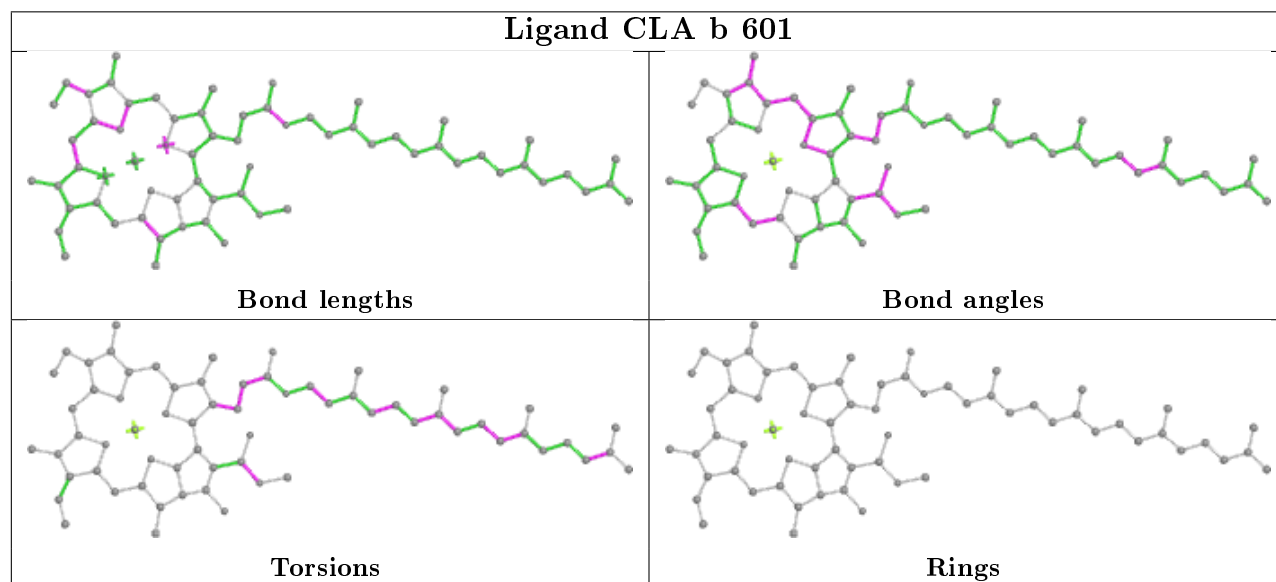
Ligand CLA C 502

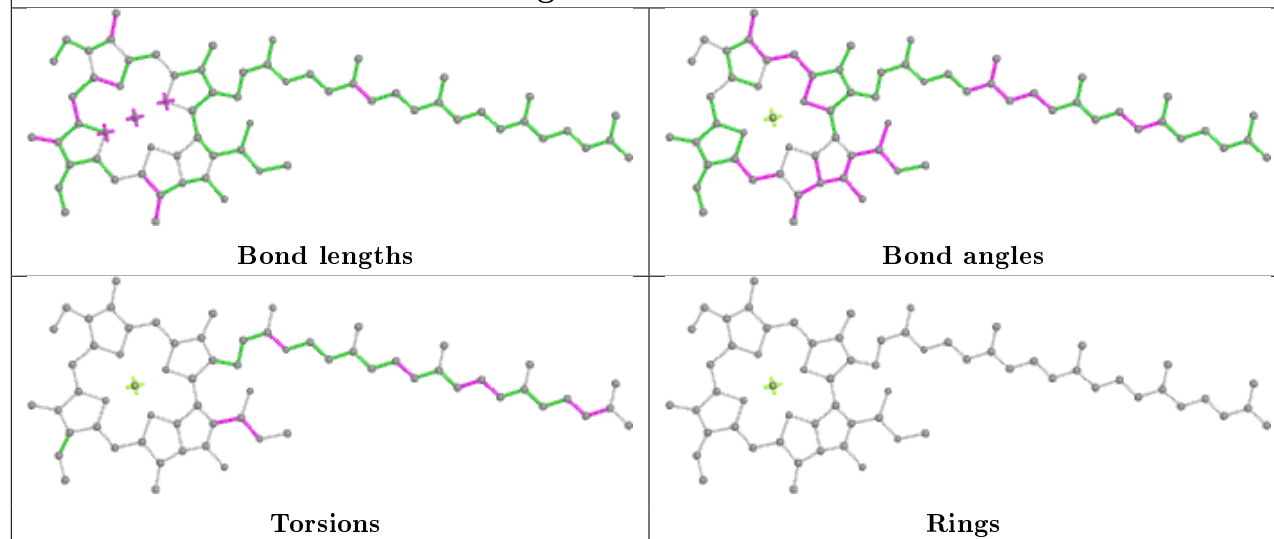
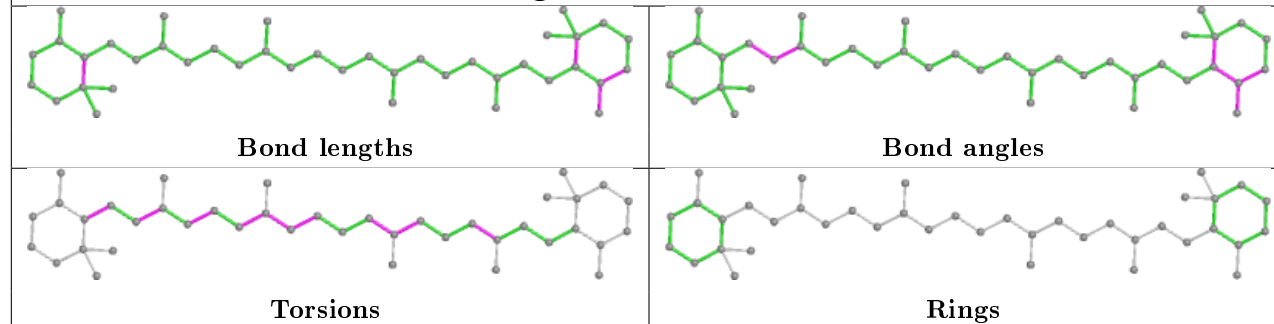
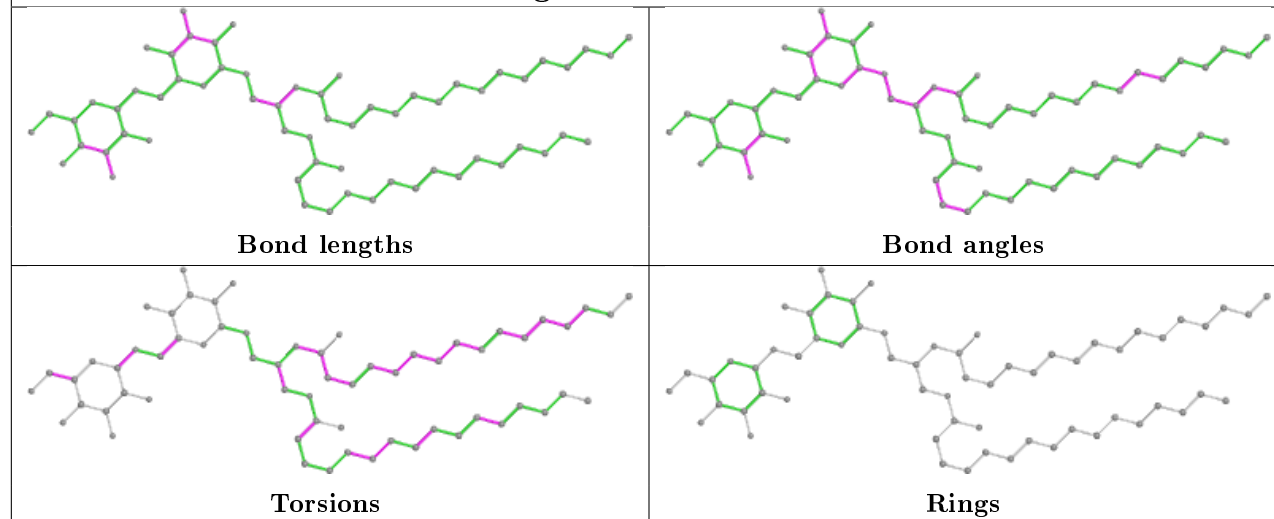


Ligand STE E 102

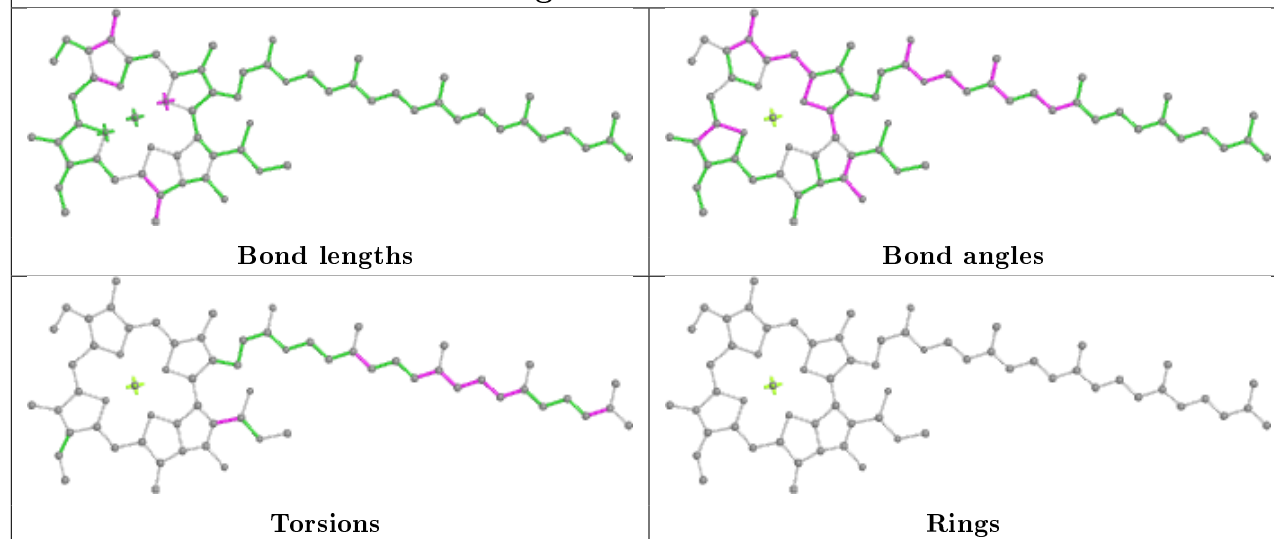


Ligand CLA b 601

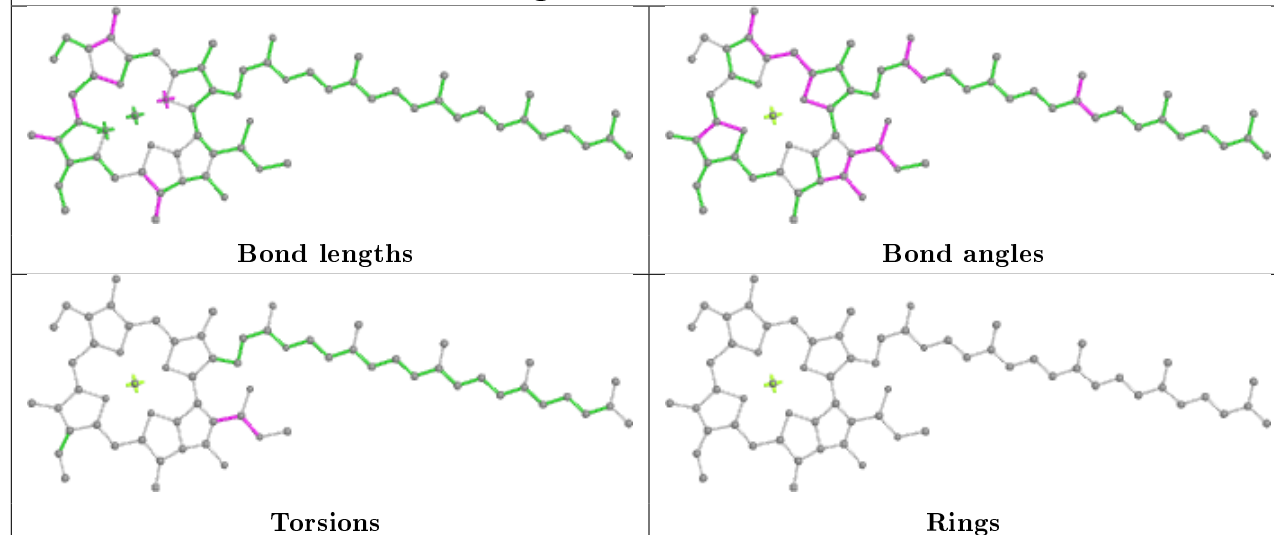


Ligand CLA c 504**Ligand BCR T 101****Ligand DGD c 517**

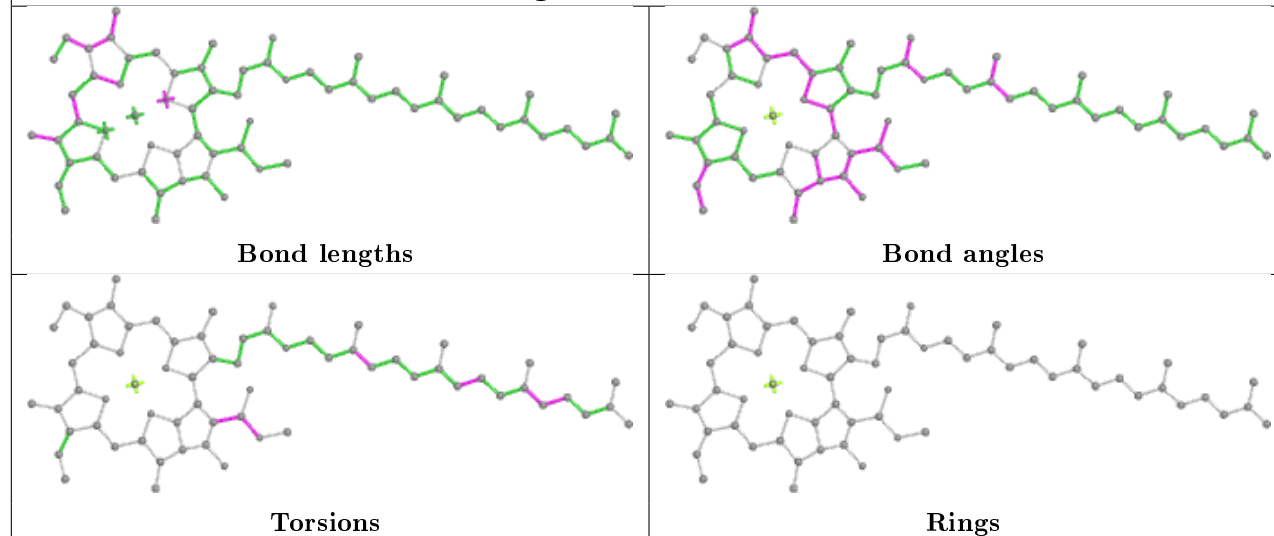
Ligand CLA b 607

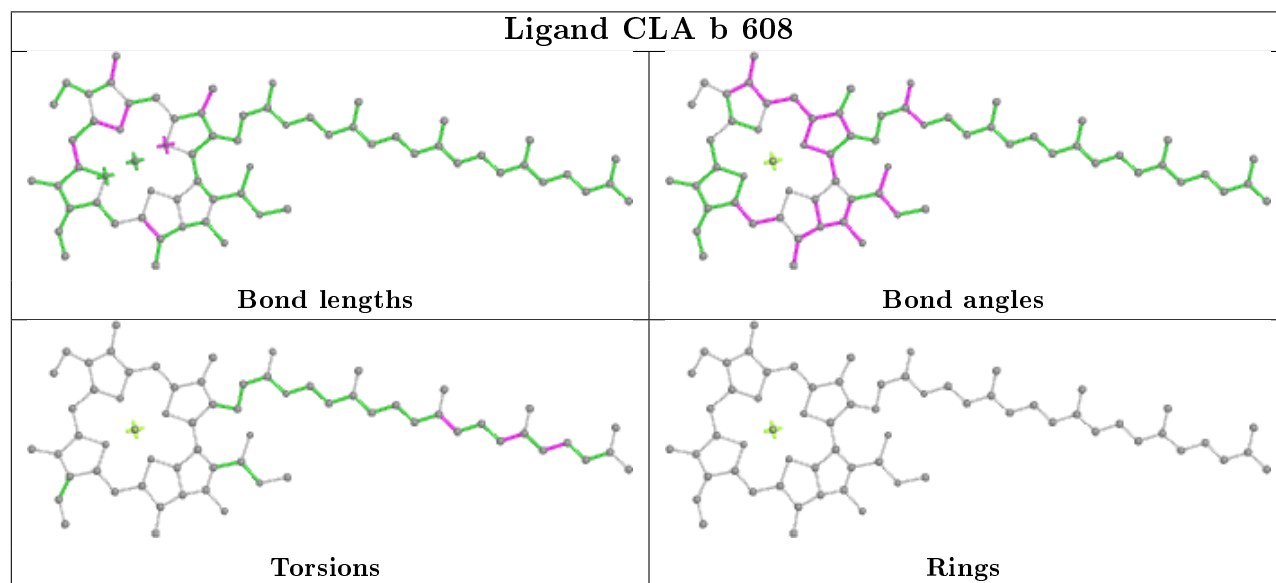
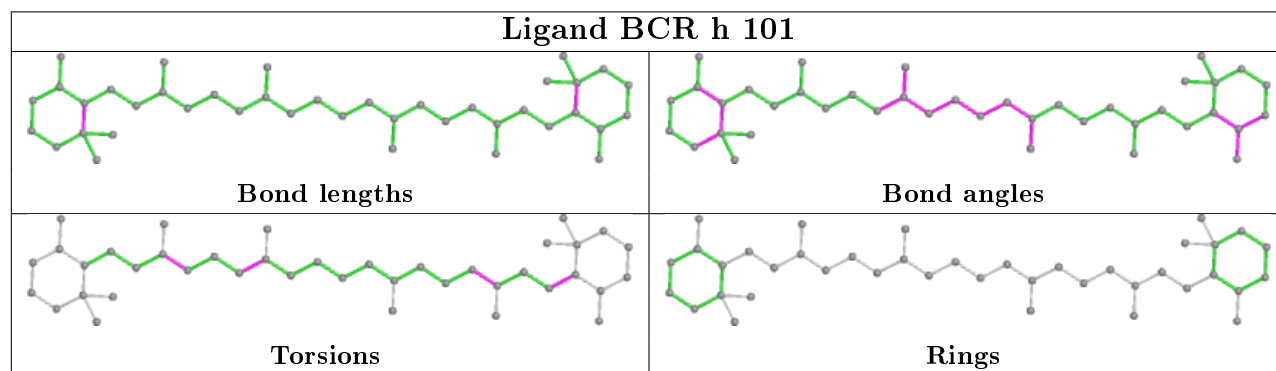
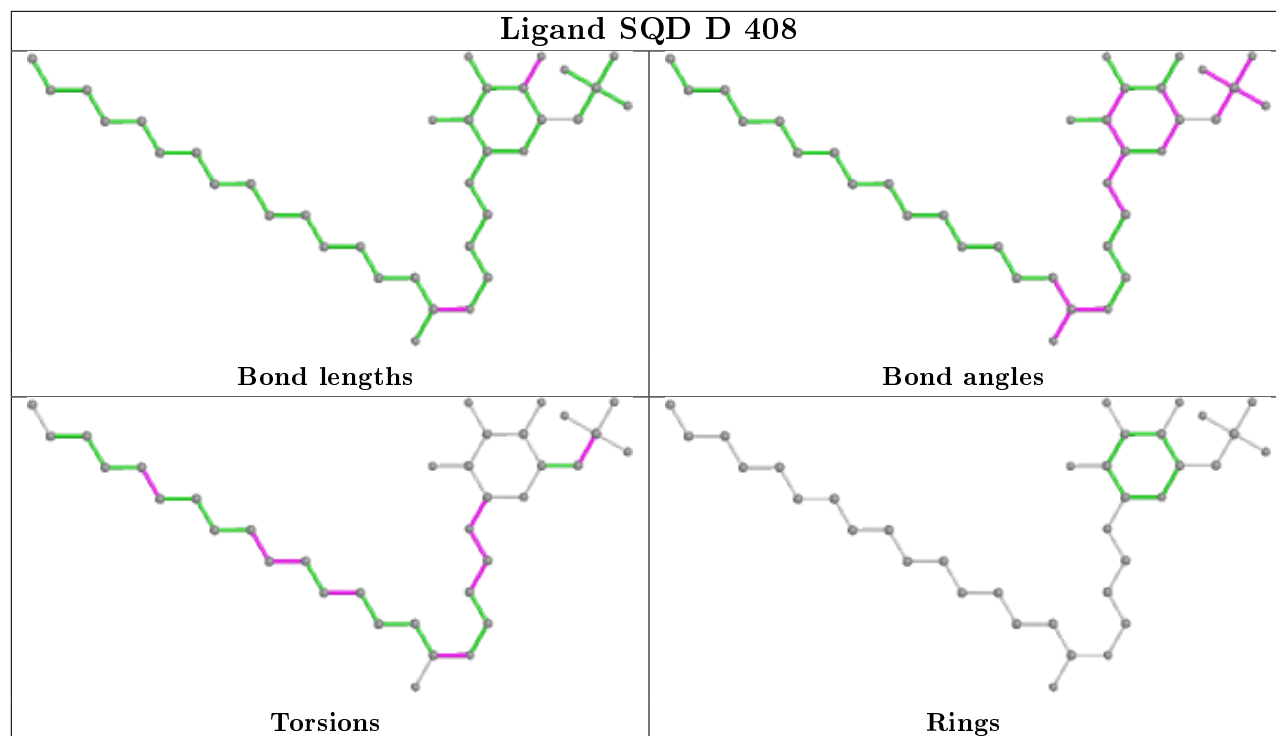


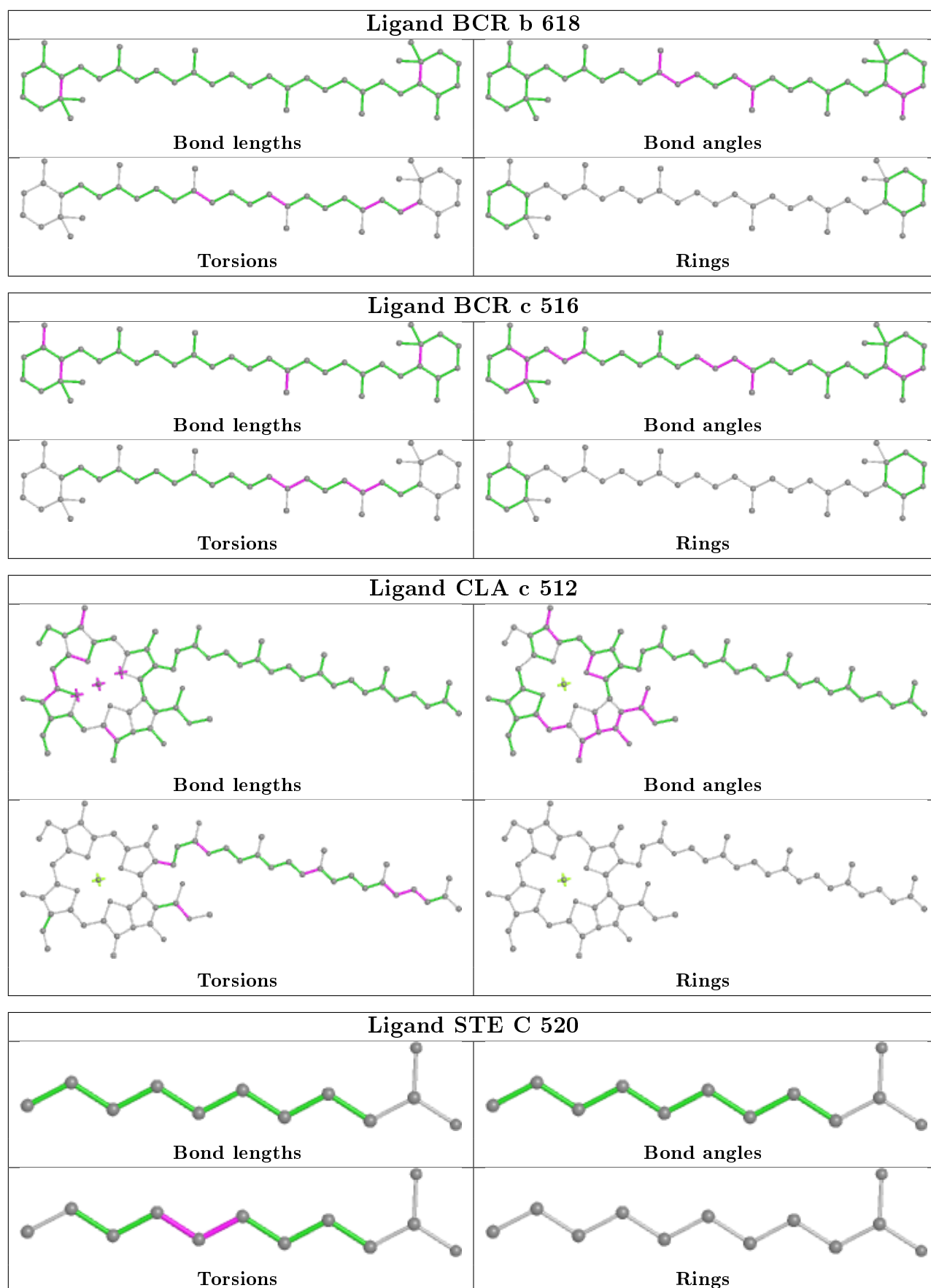
Ligand CLA C 501

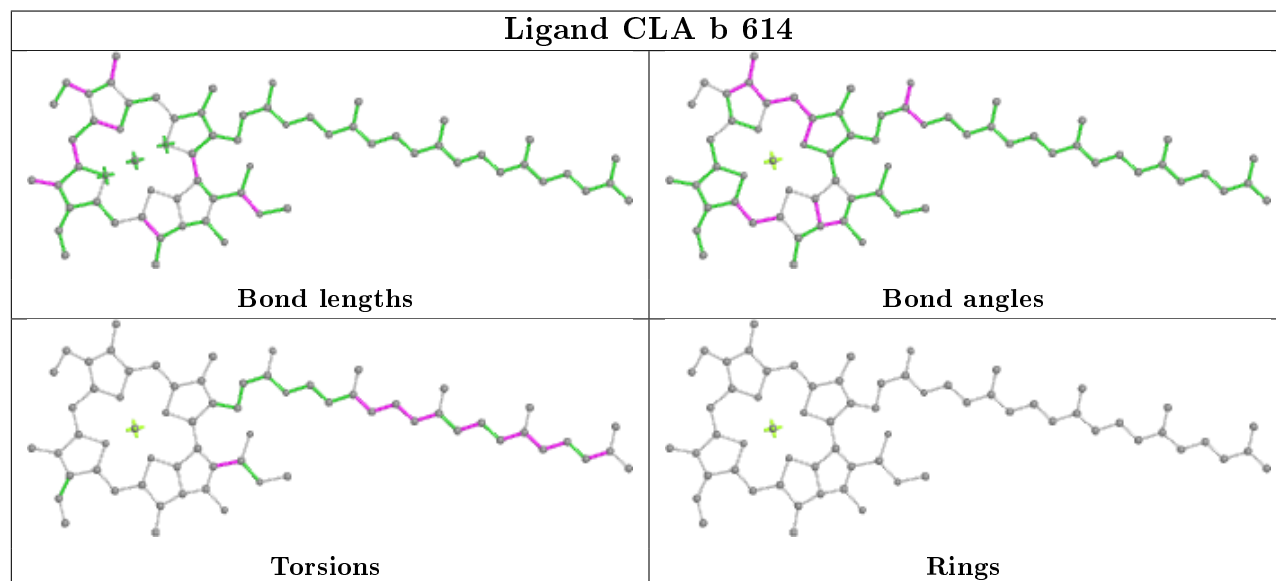
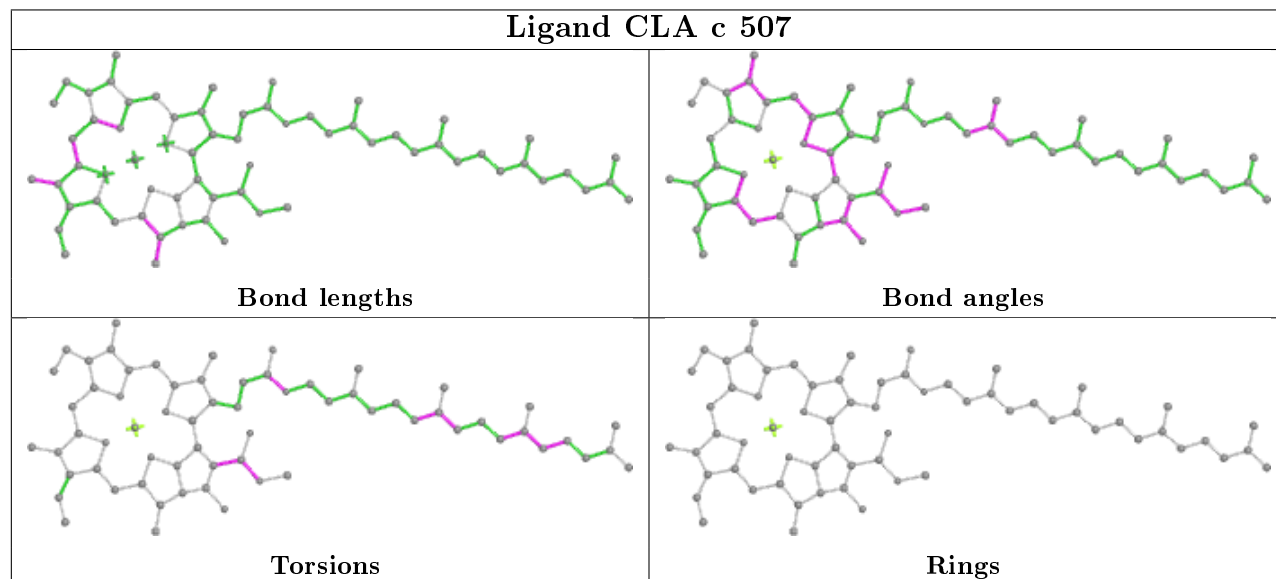
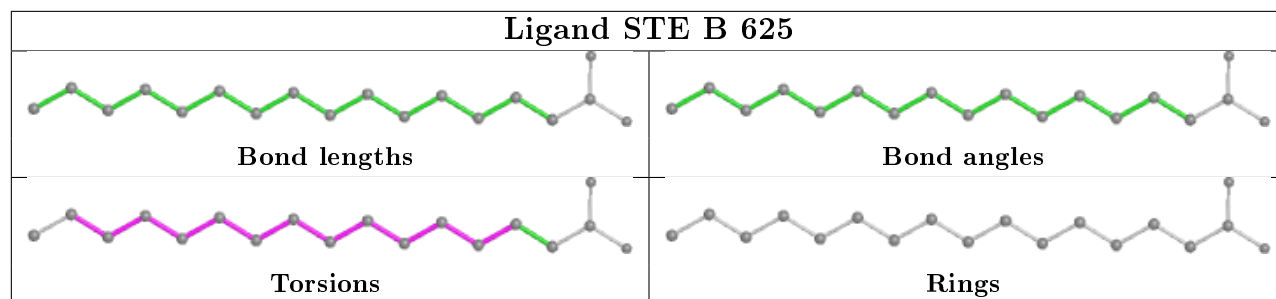


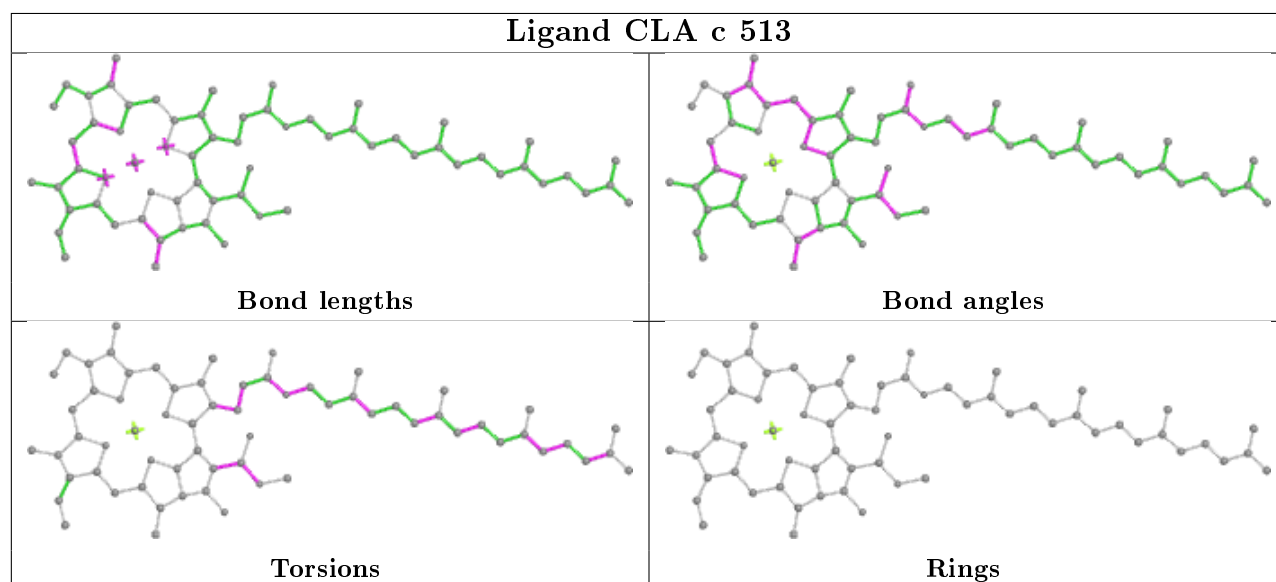
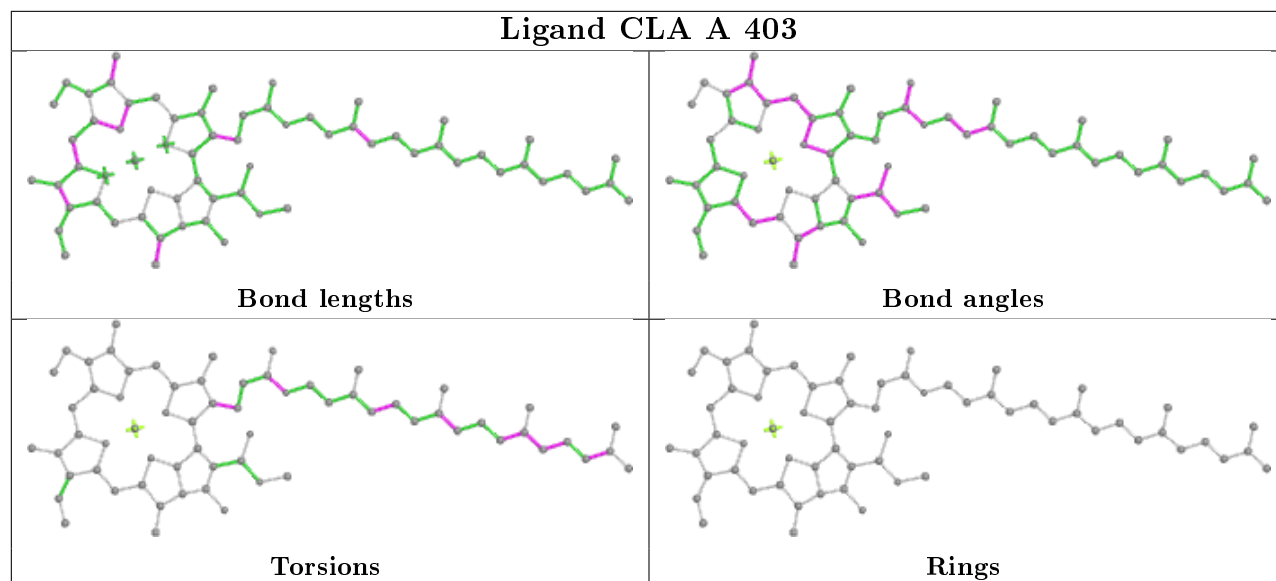
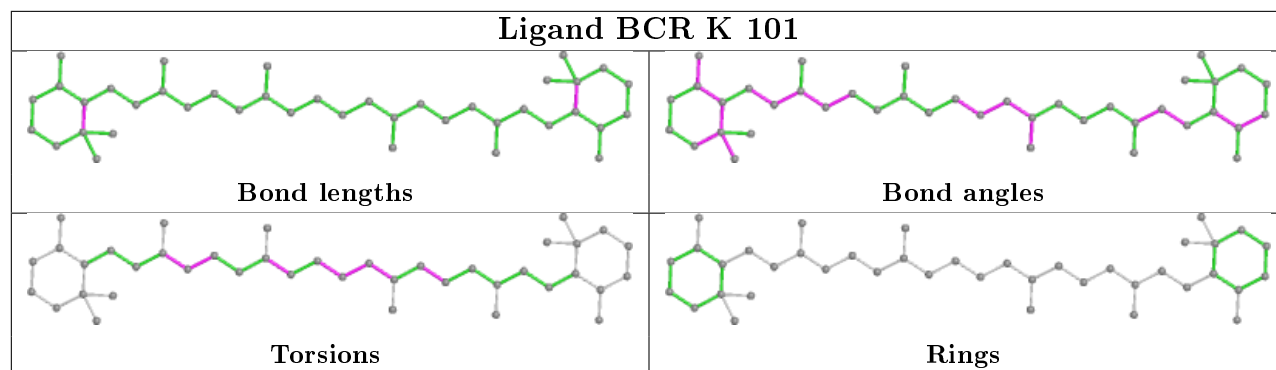
Ligand CLA B 614

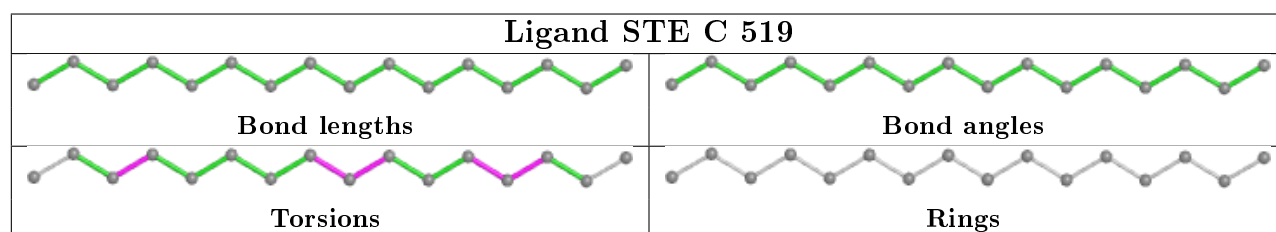
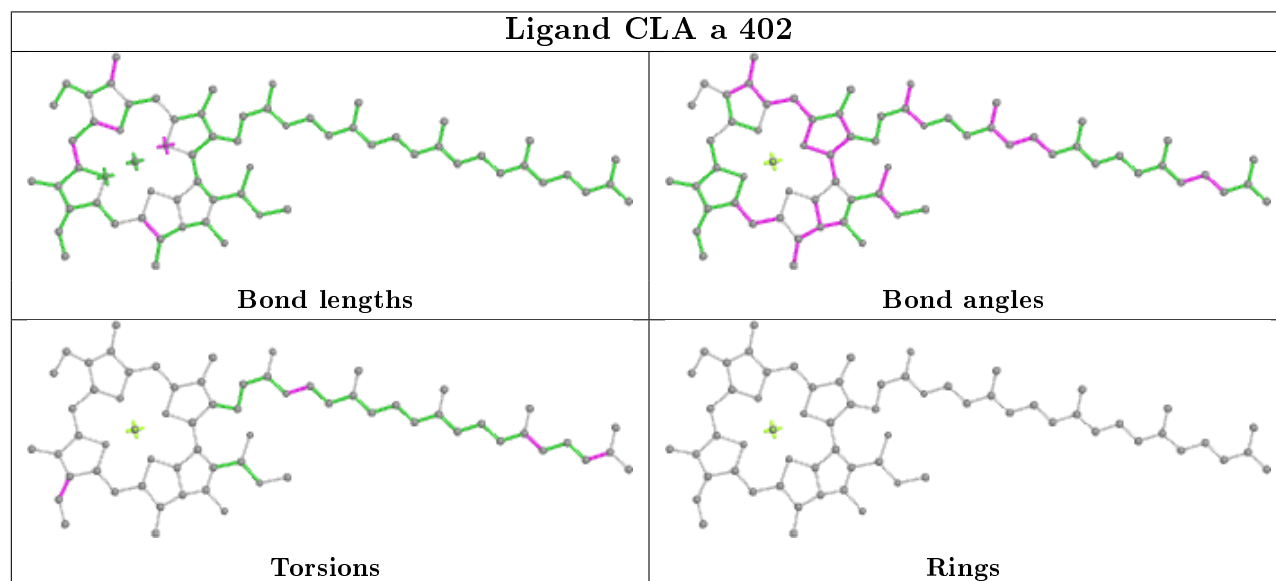
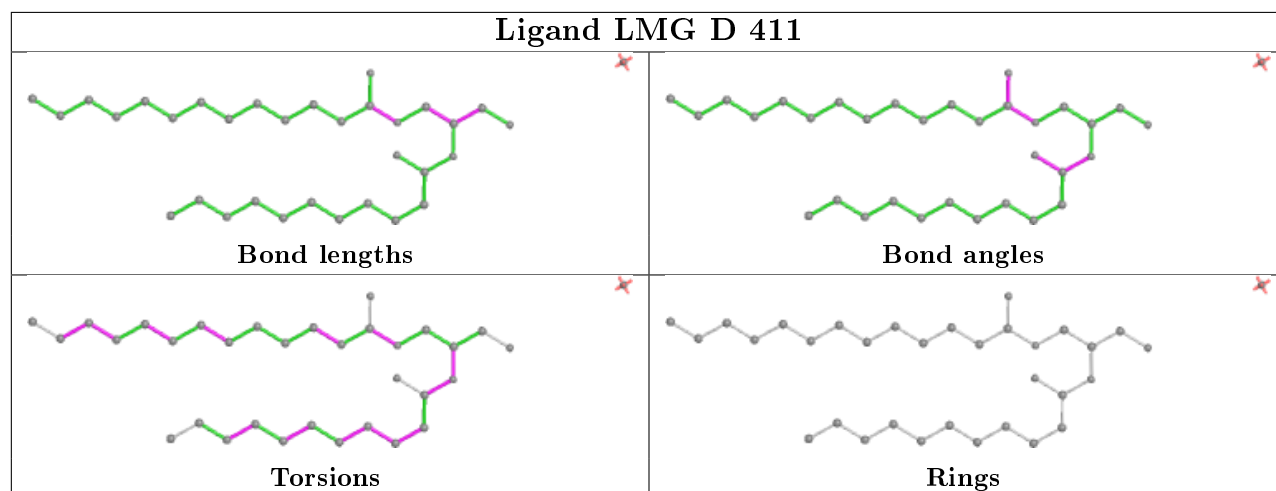
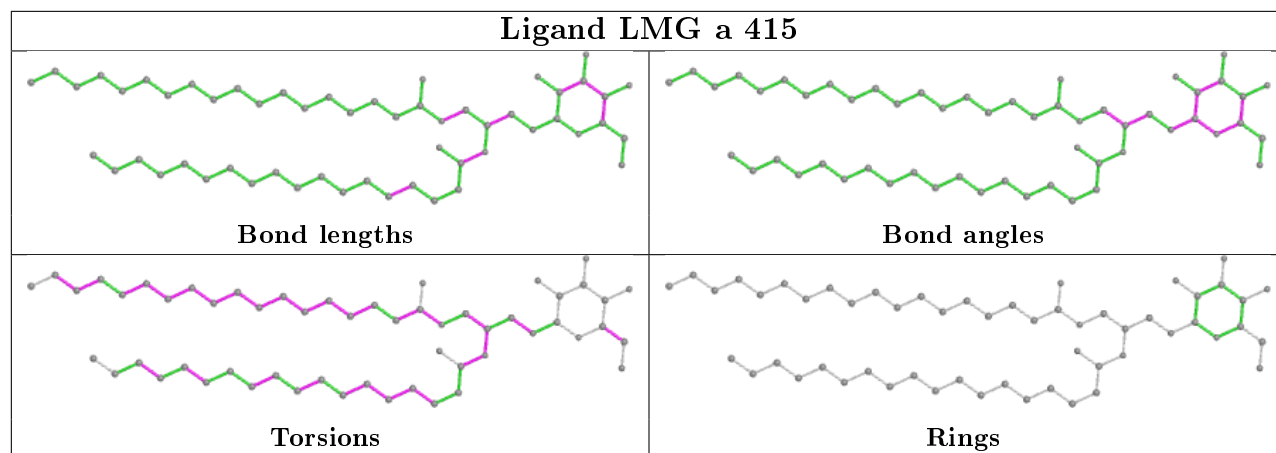




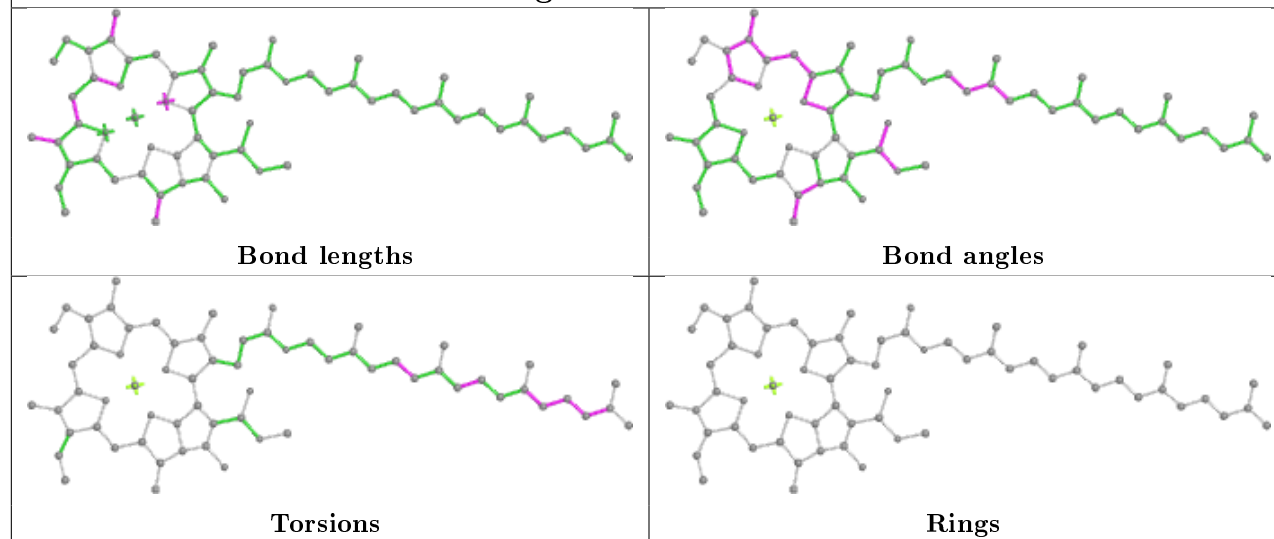




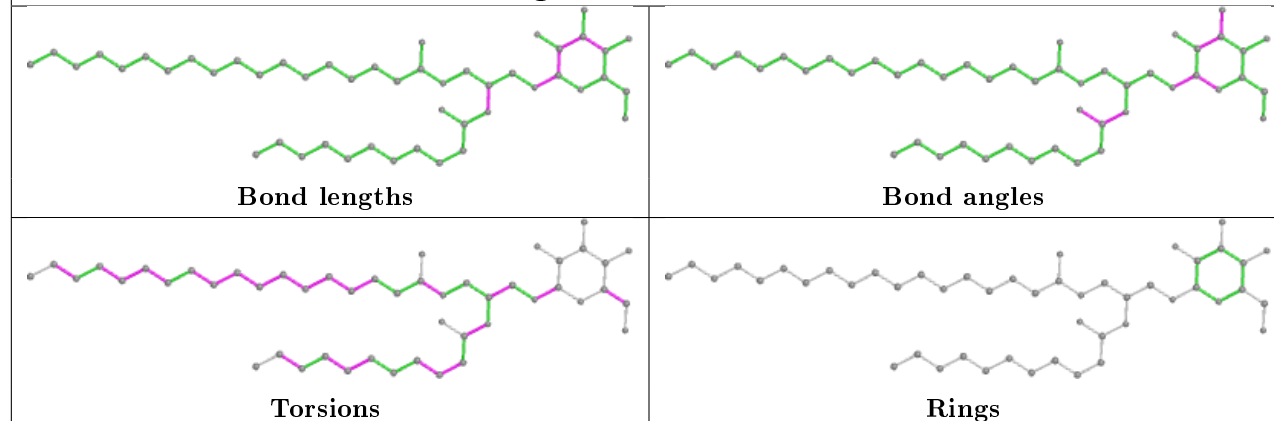




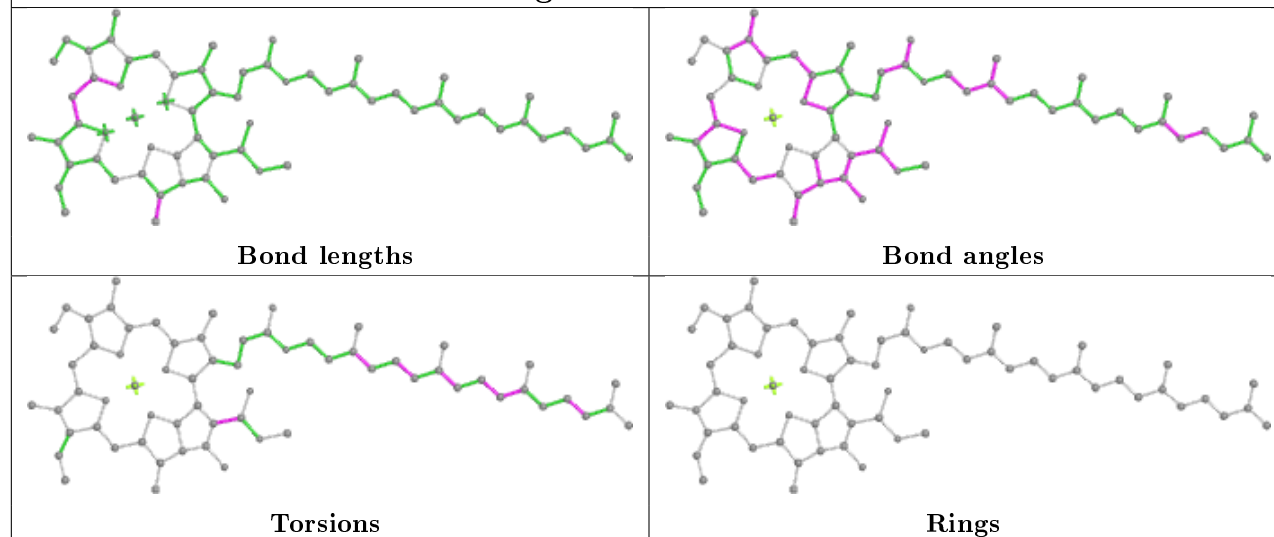
Ligand CLA b 615

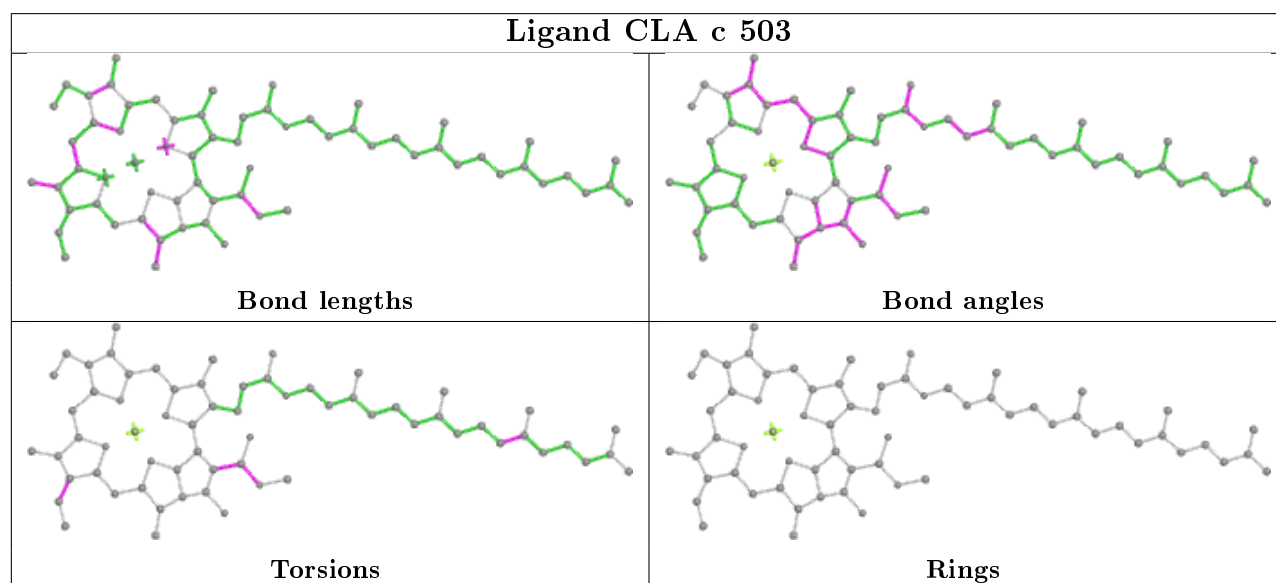
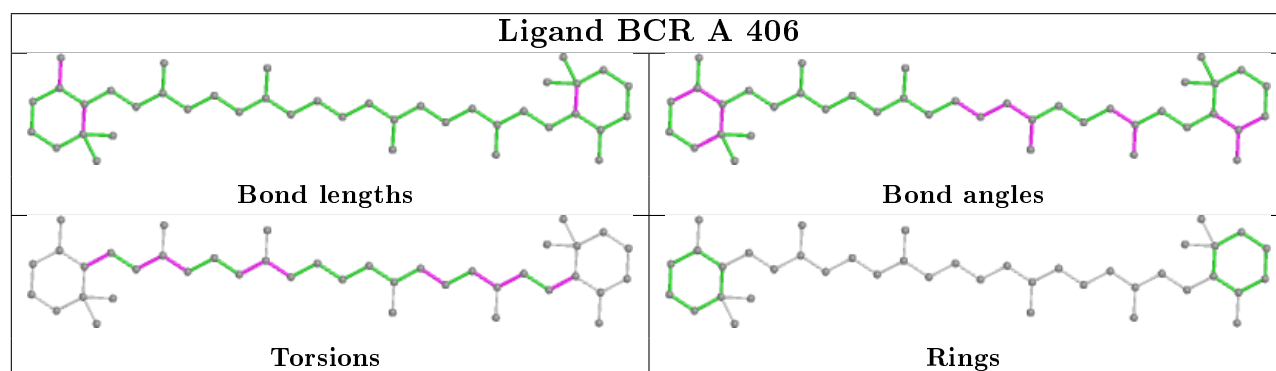
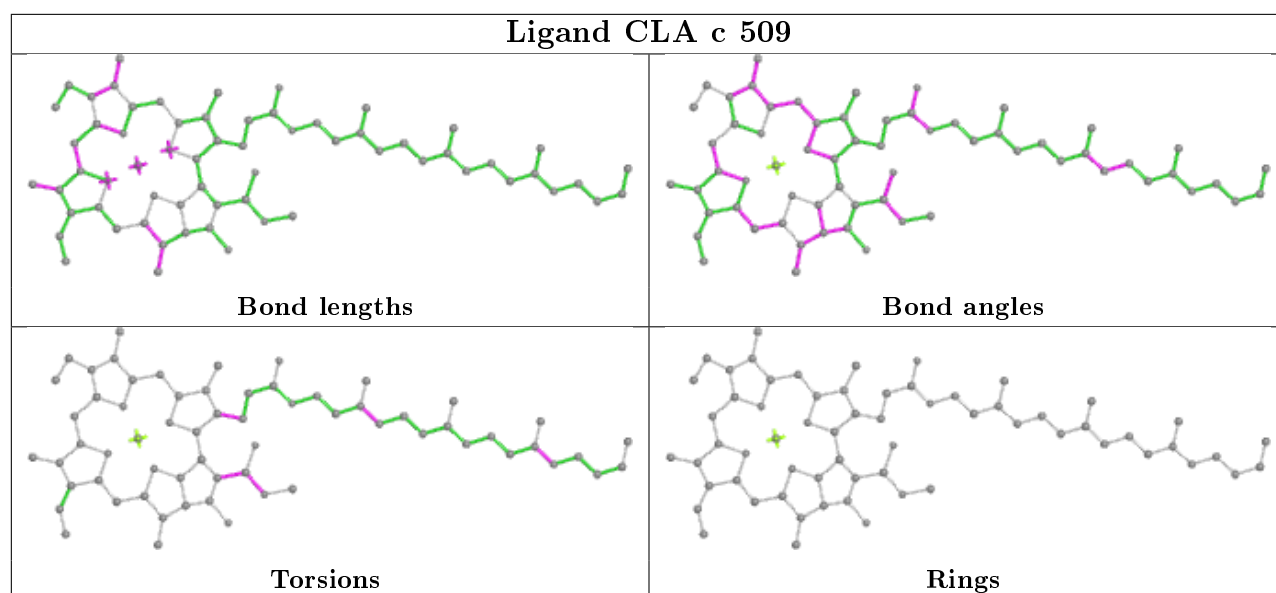


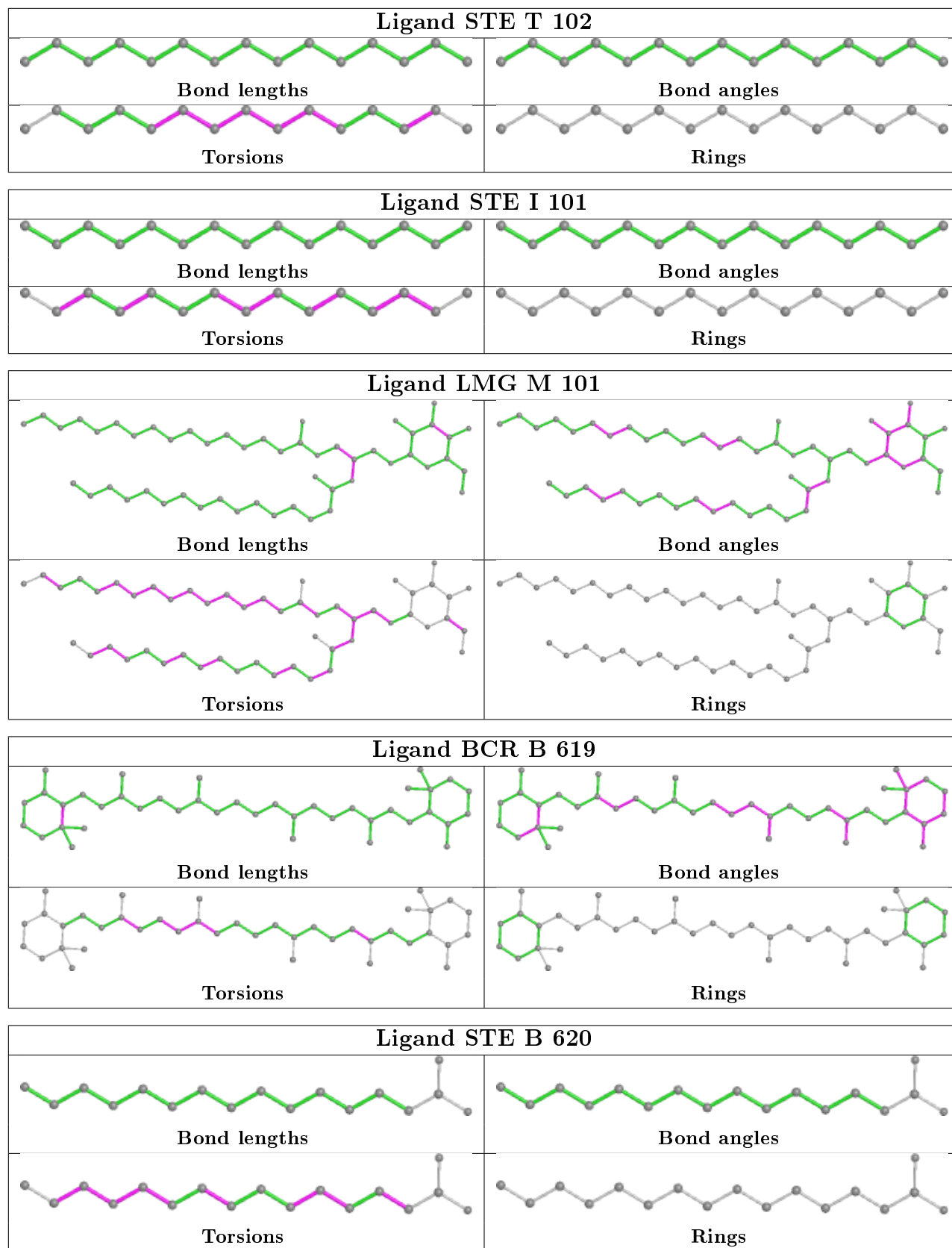
Ligand LMG c 522

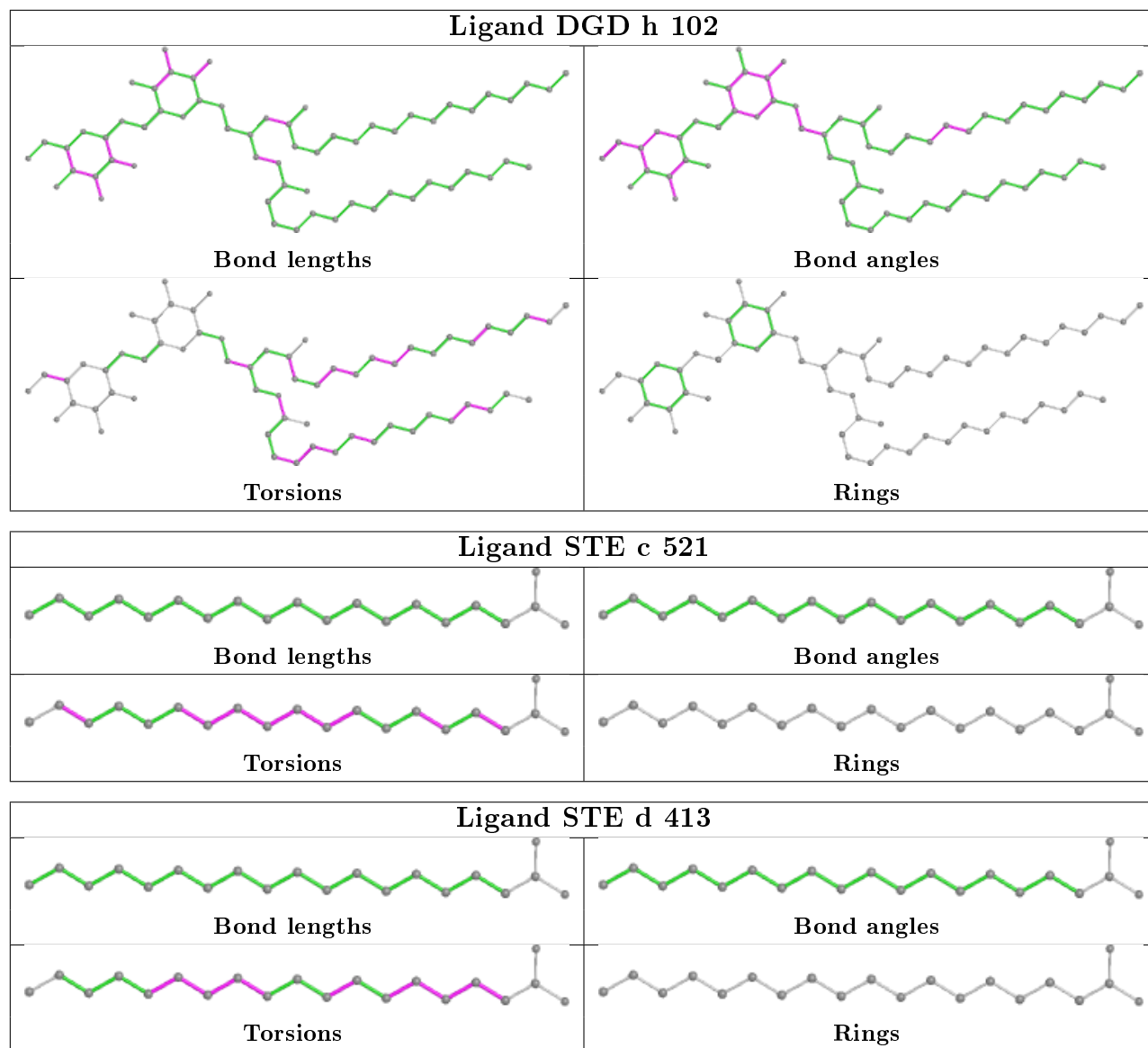


Ligand CLA b 605

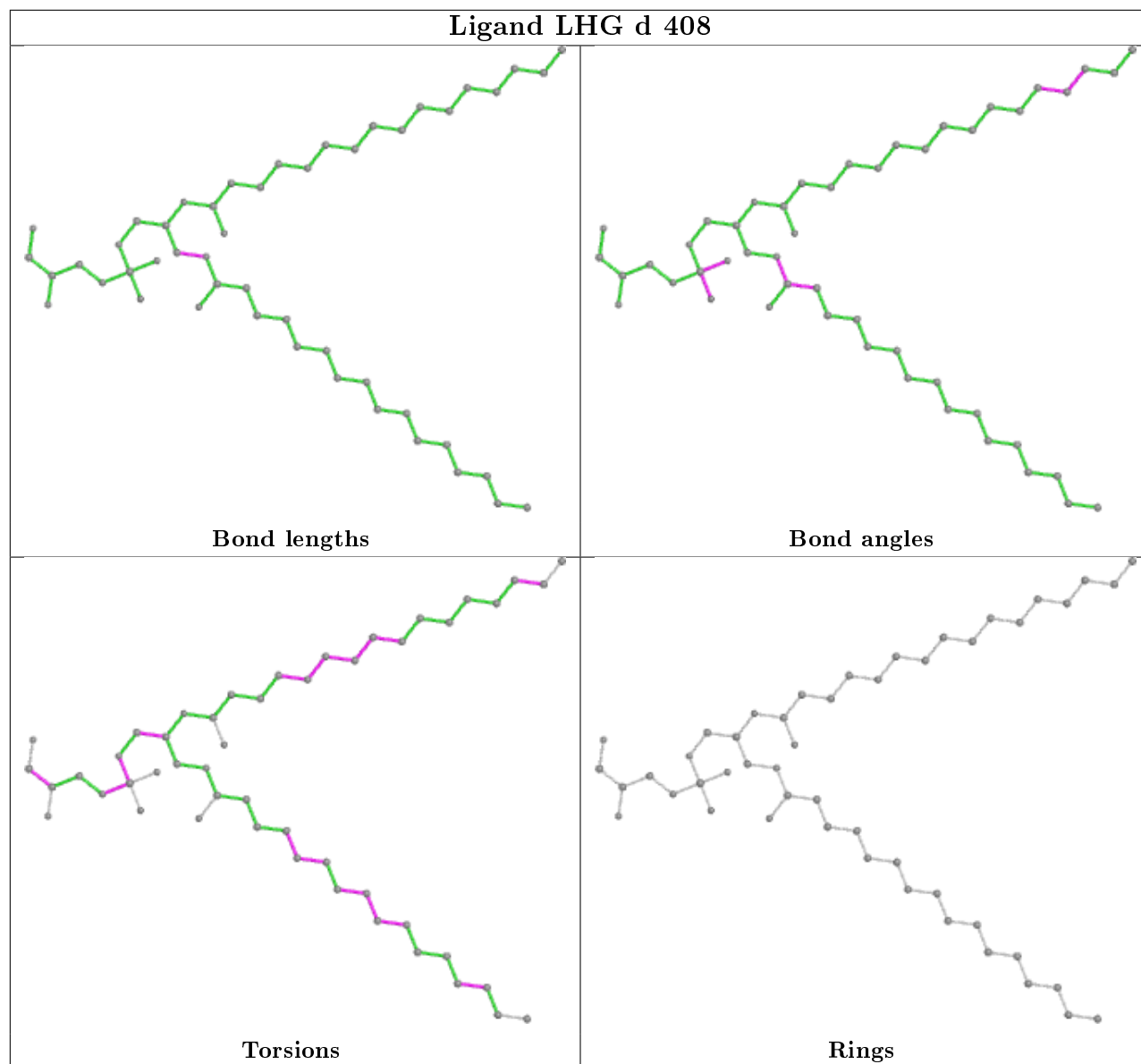




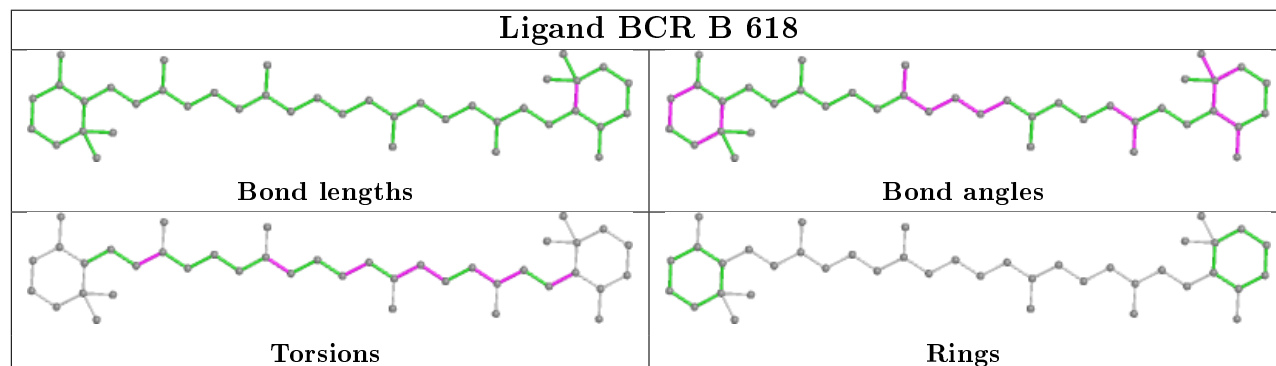


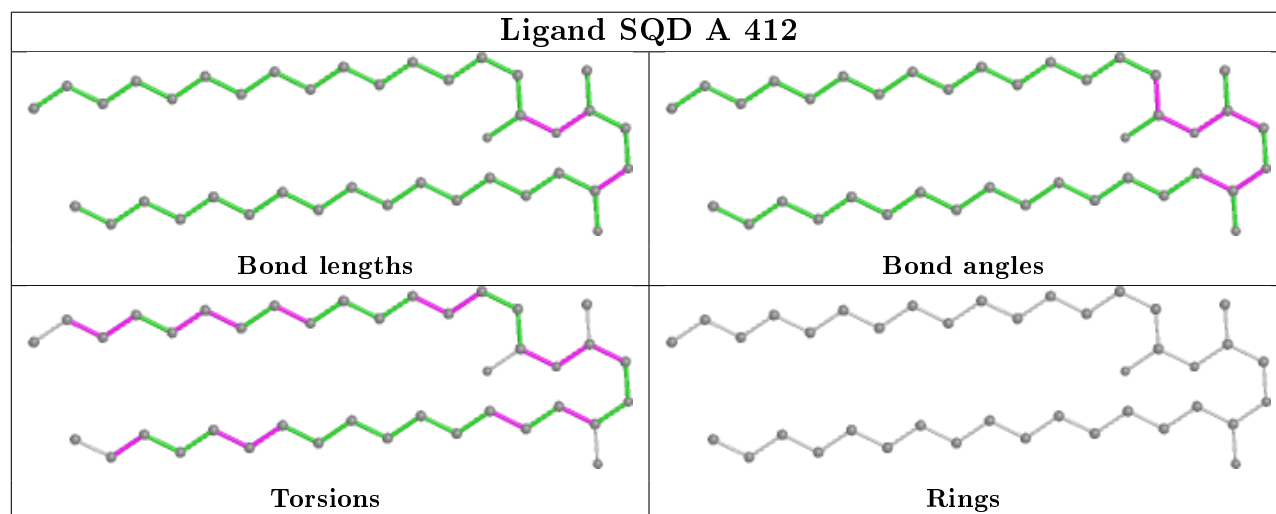
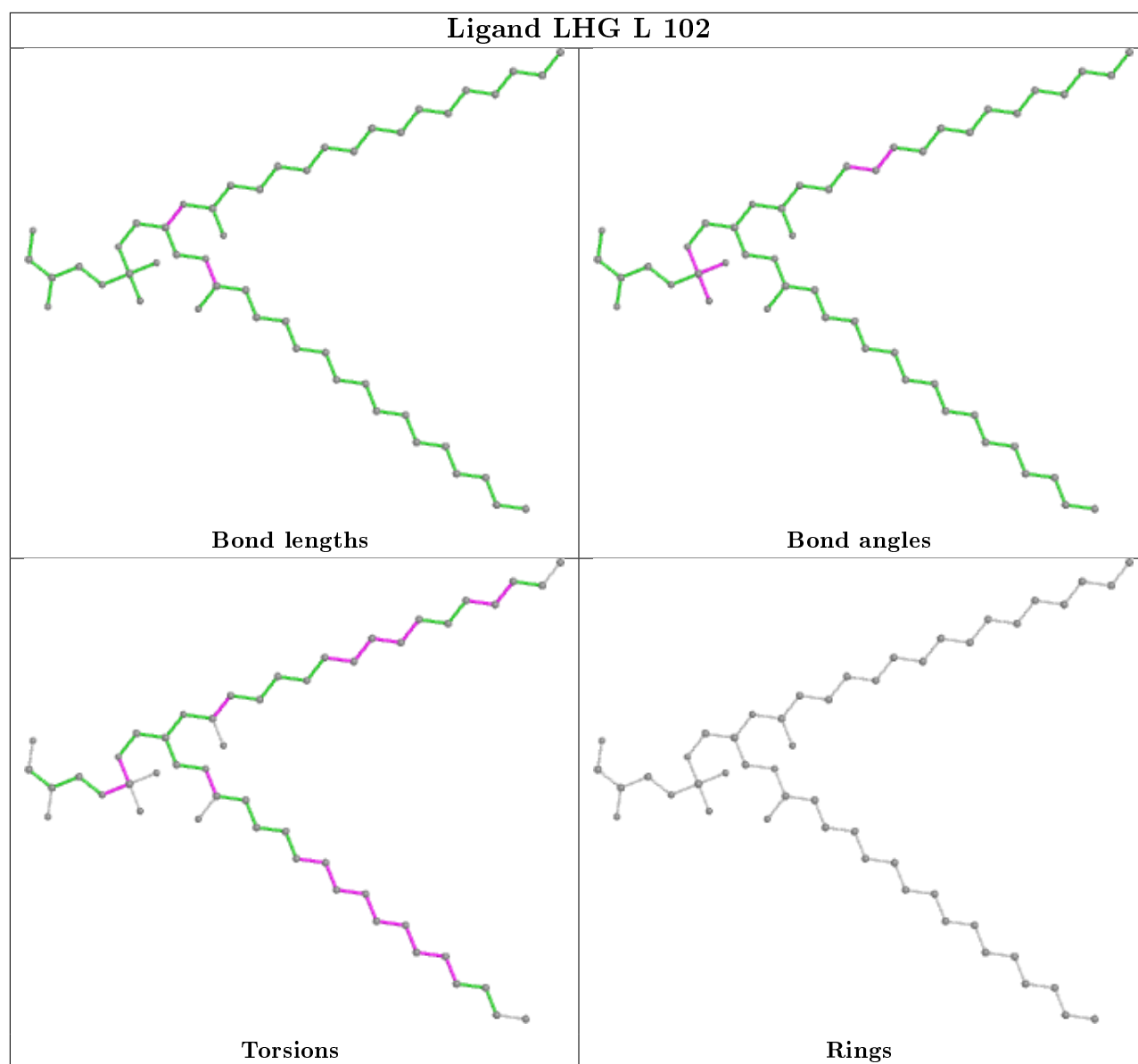


Ligand LHG d 408

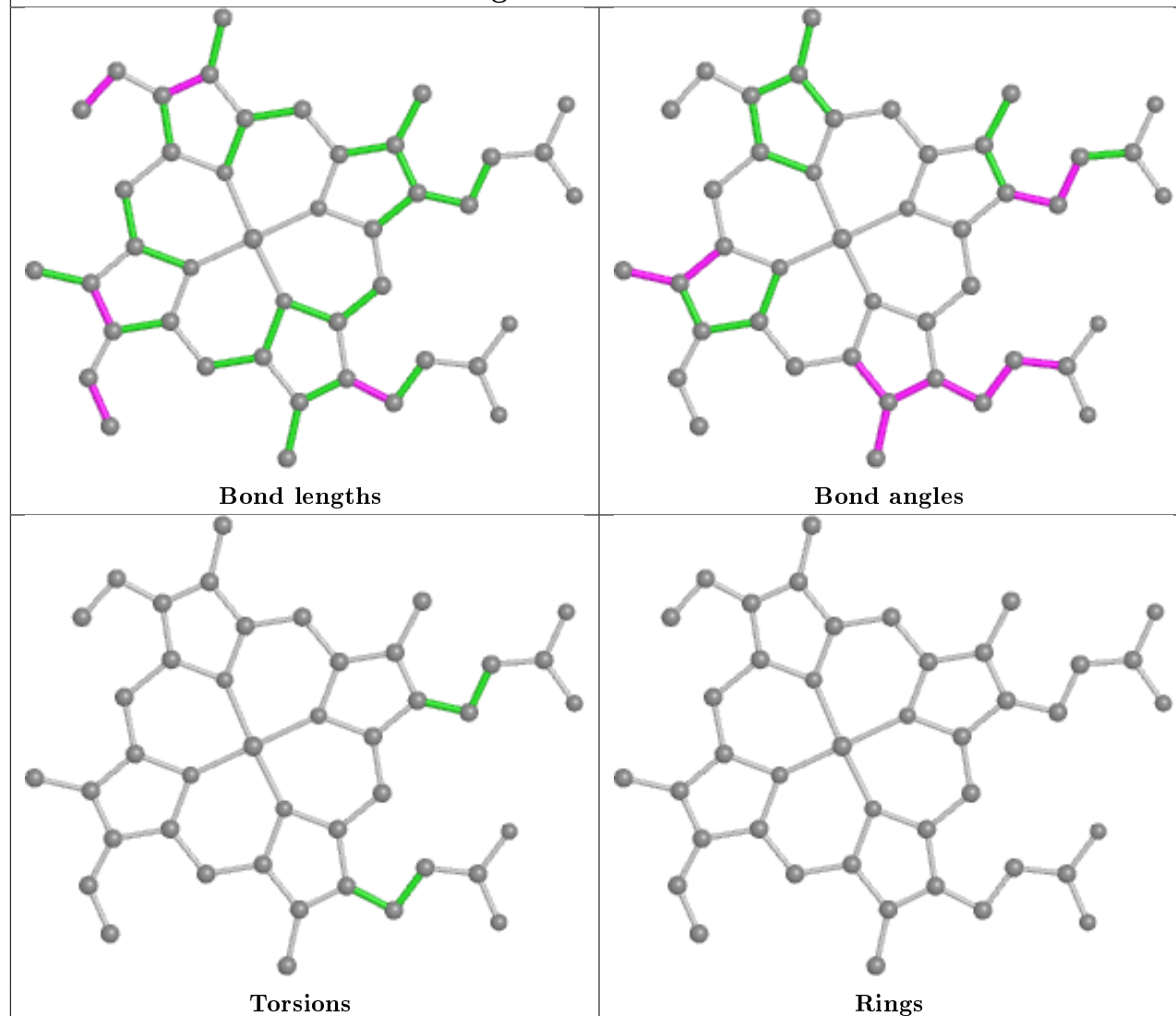


Ligand BCR B 618

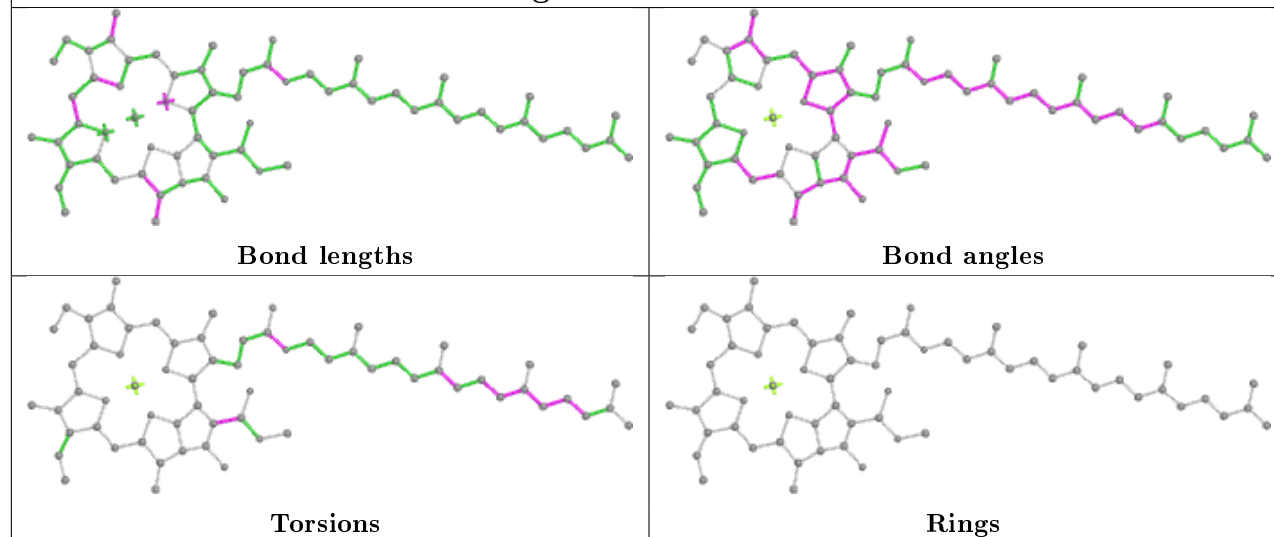


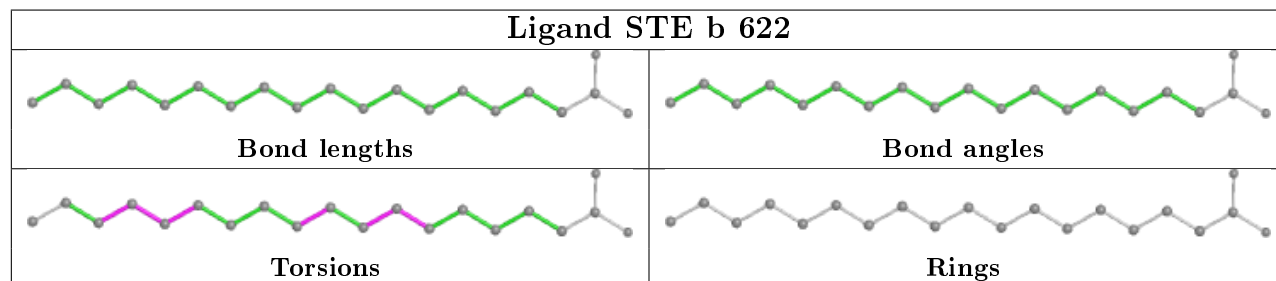
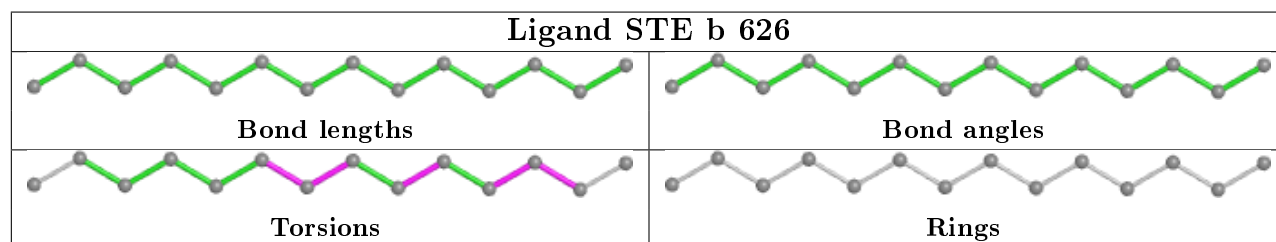
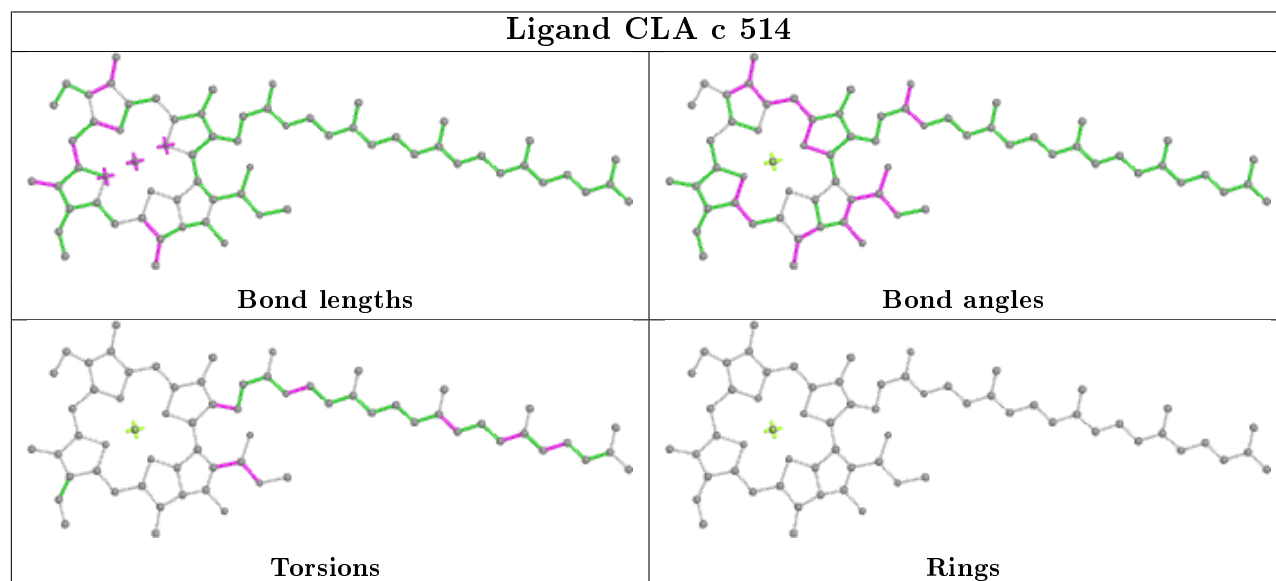
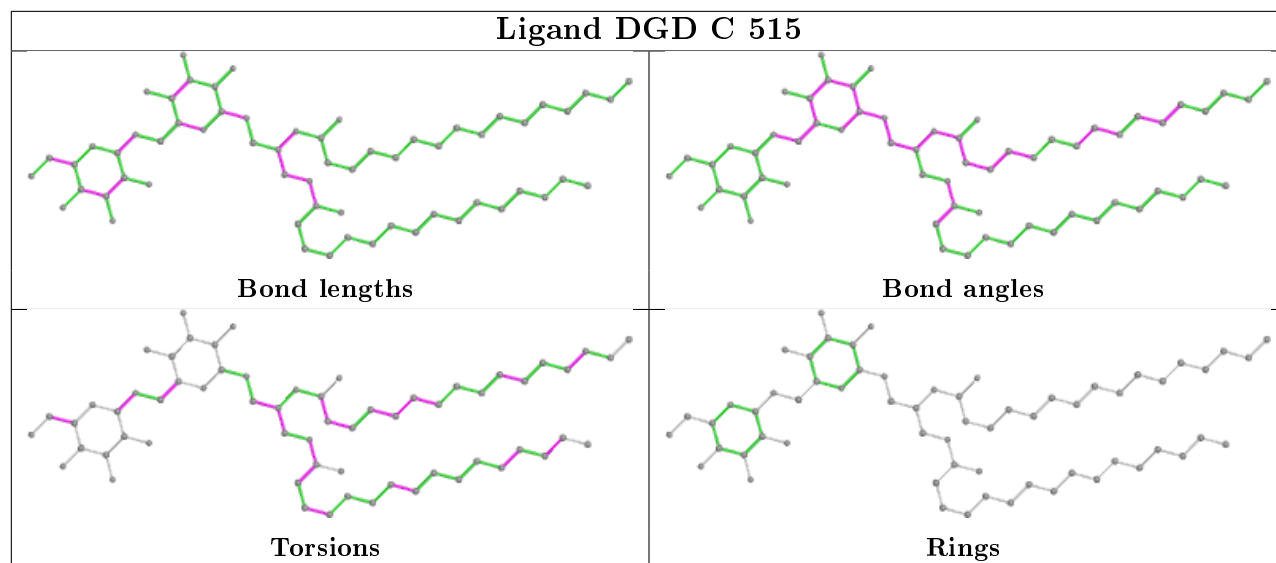


Ligand HEC F 102

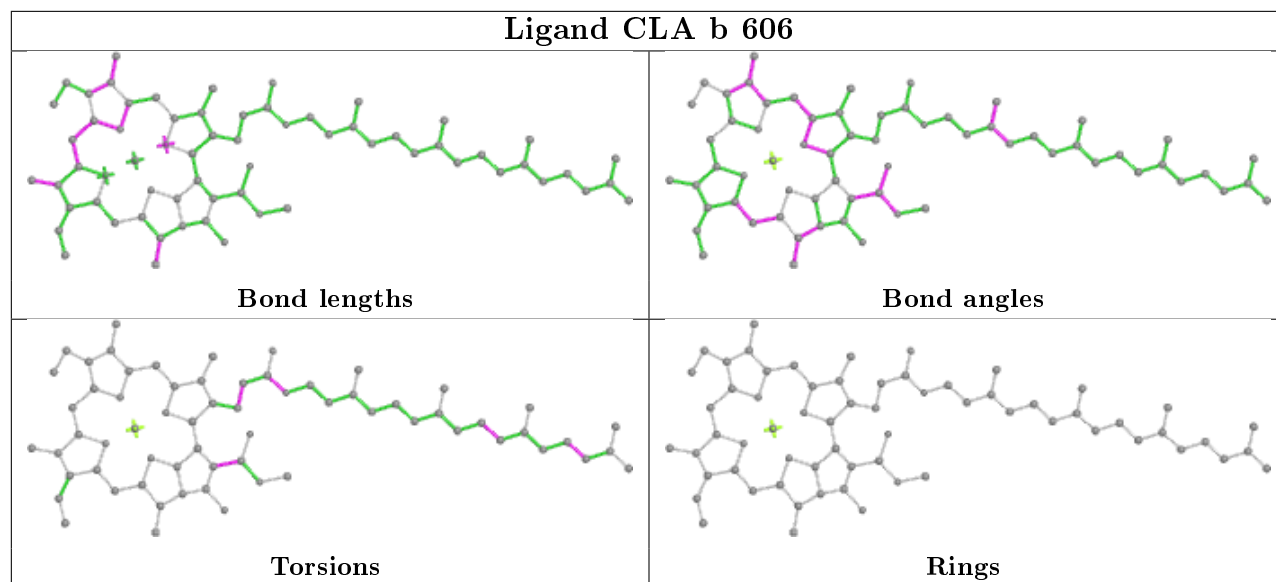


Ligand CLA B 604

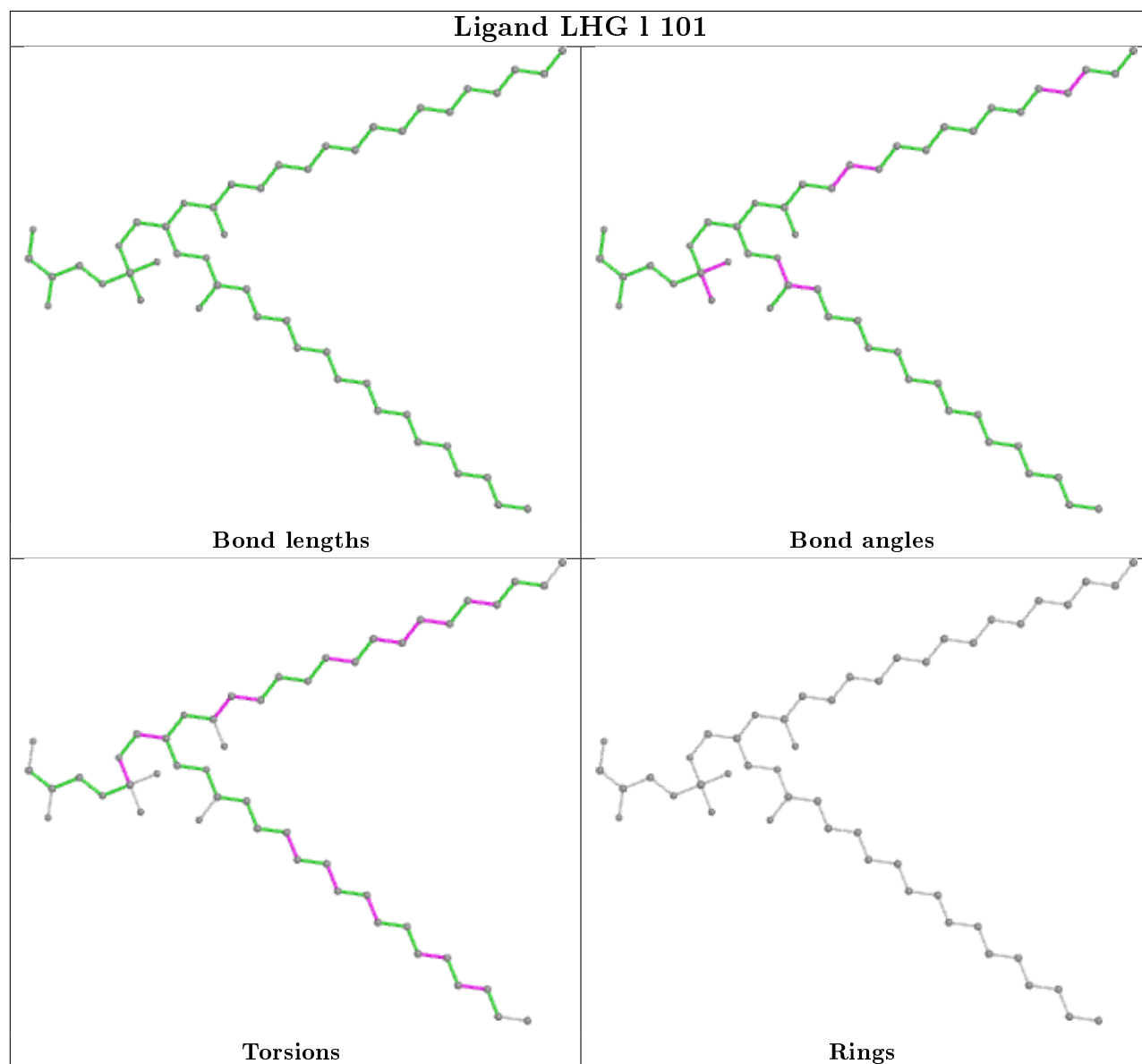


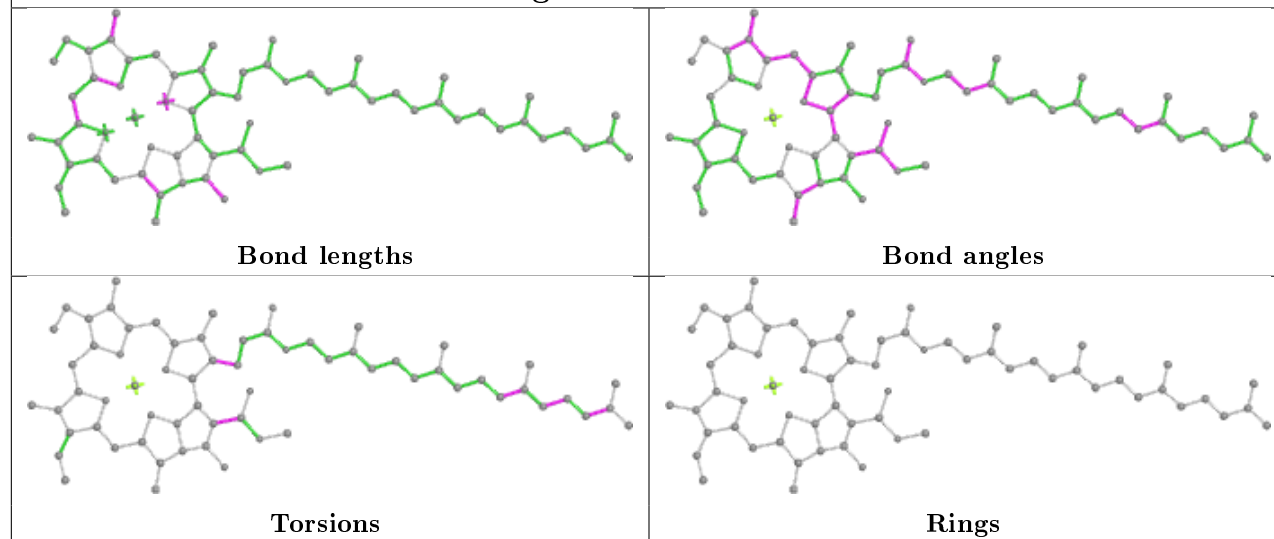
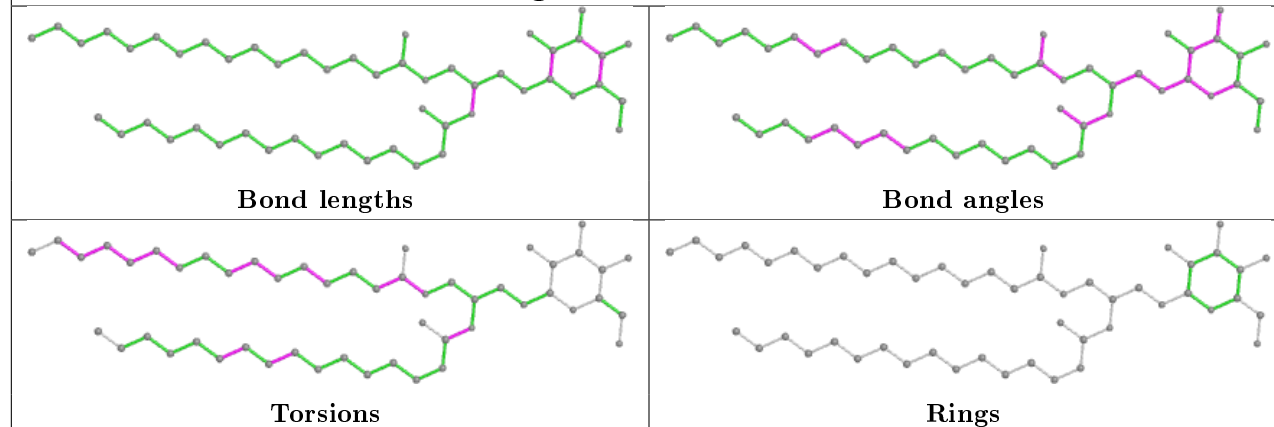
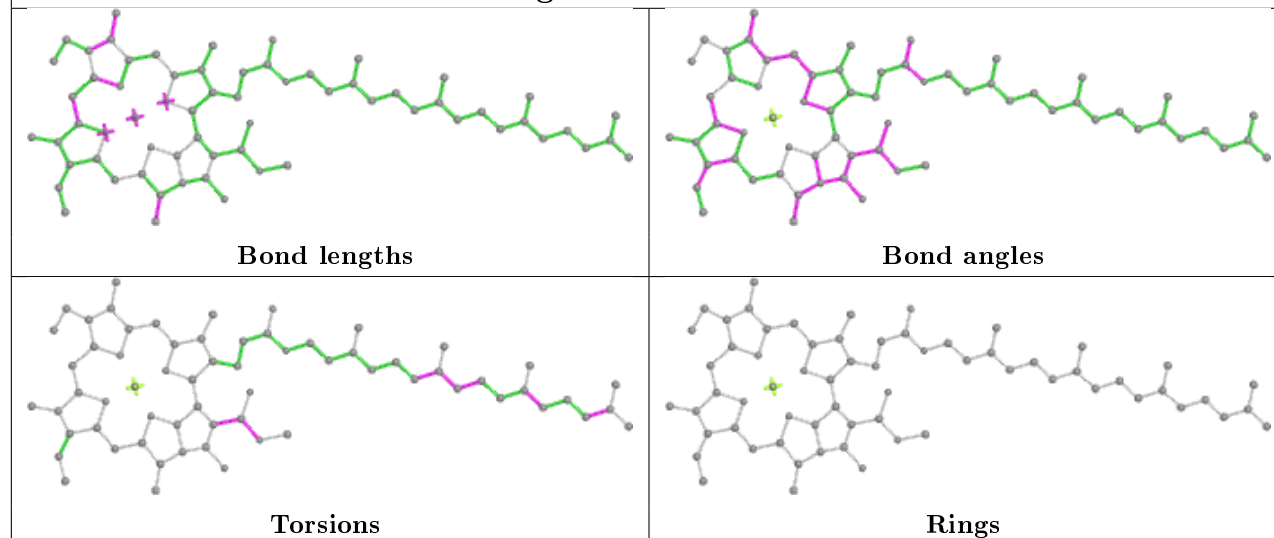


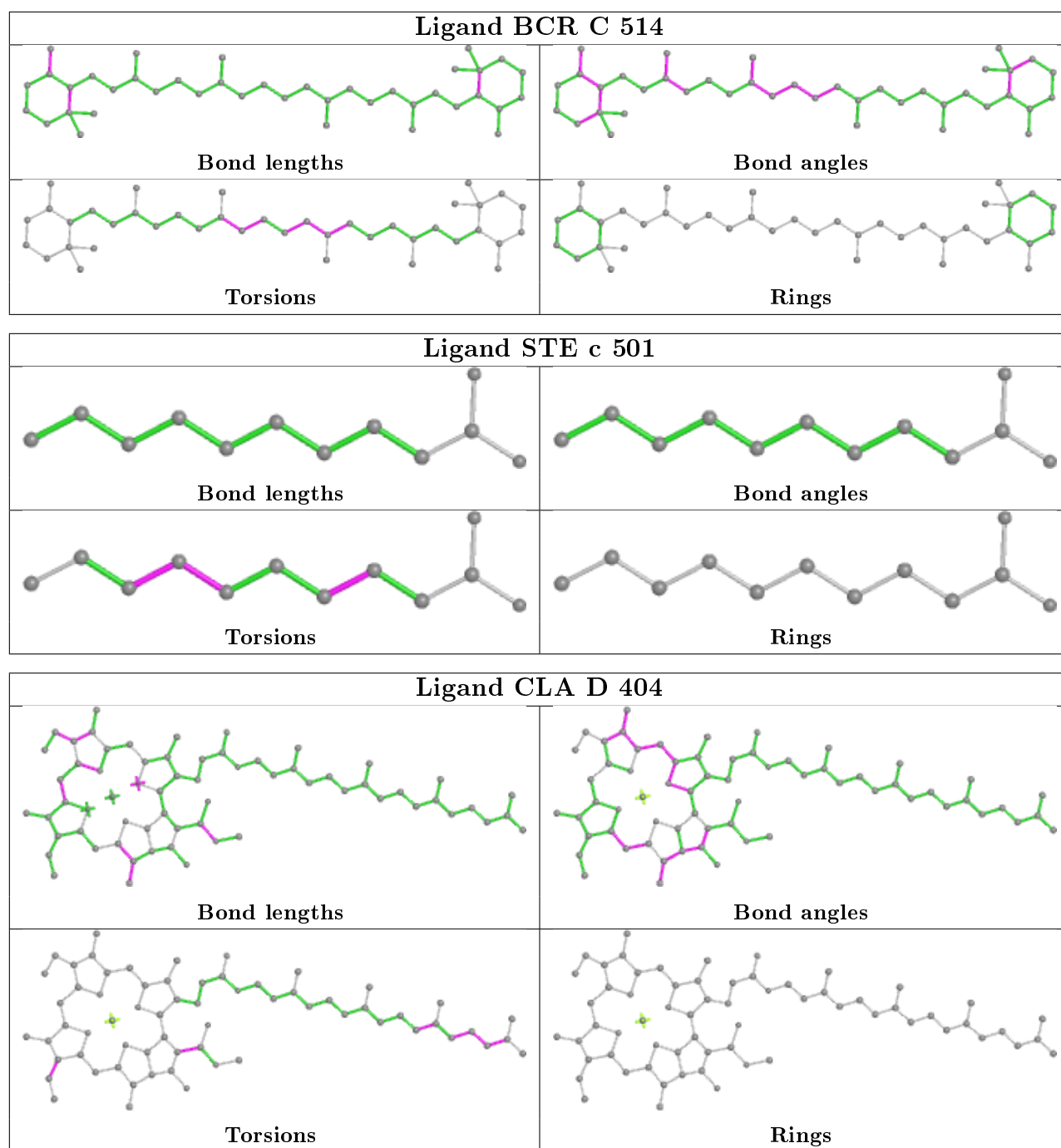
Ligand CLA b 606

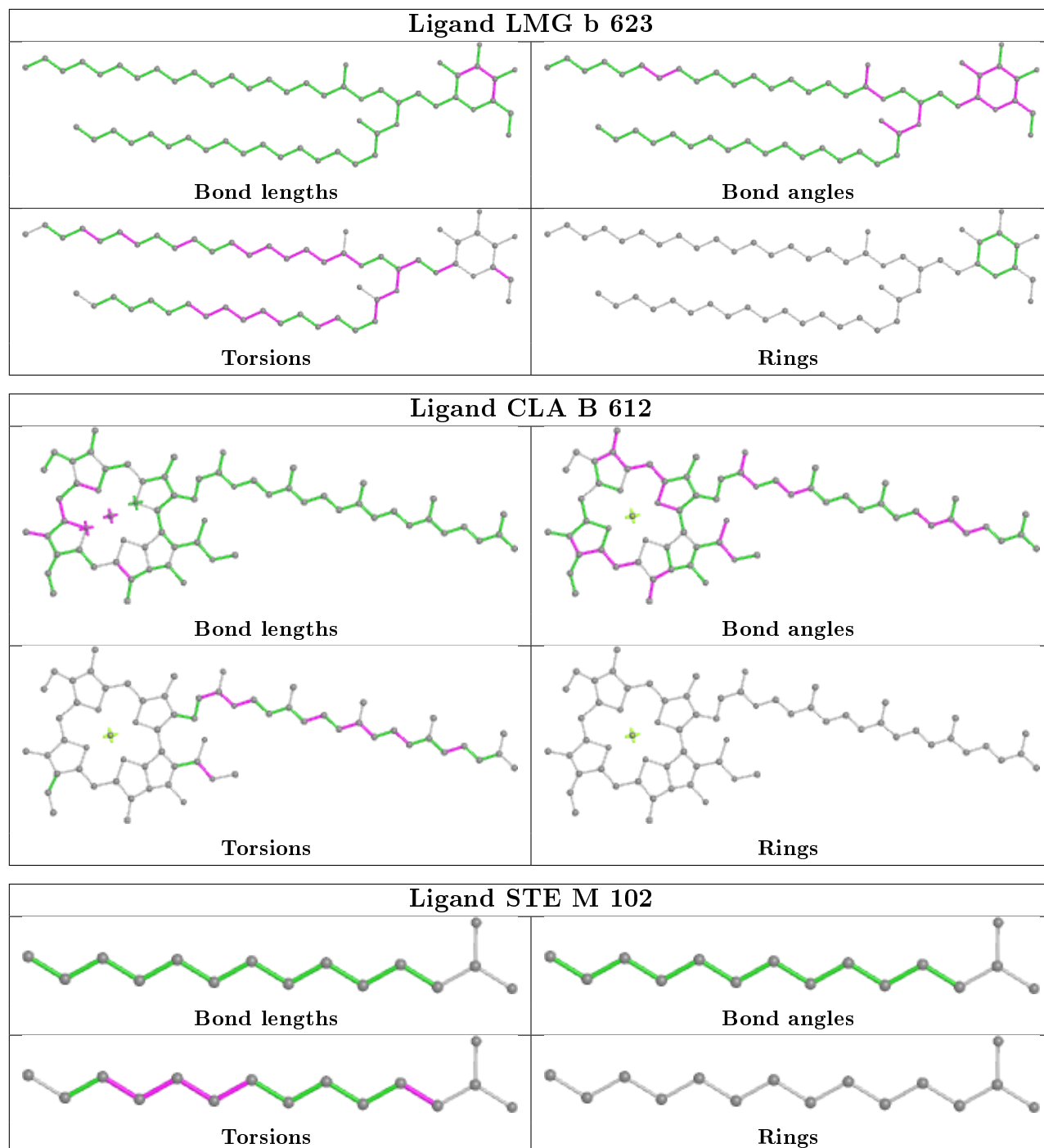


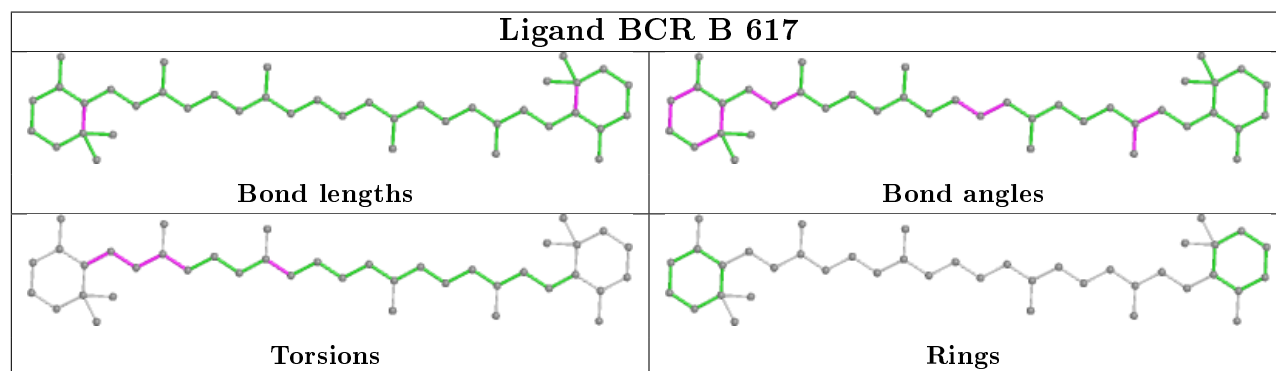
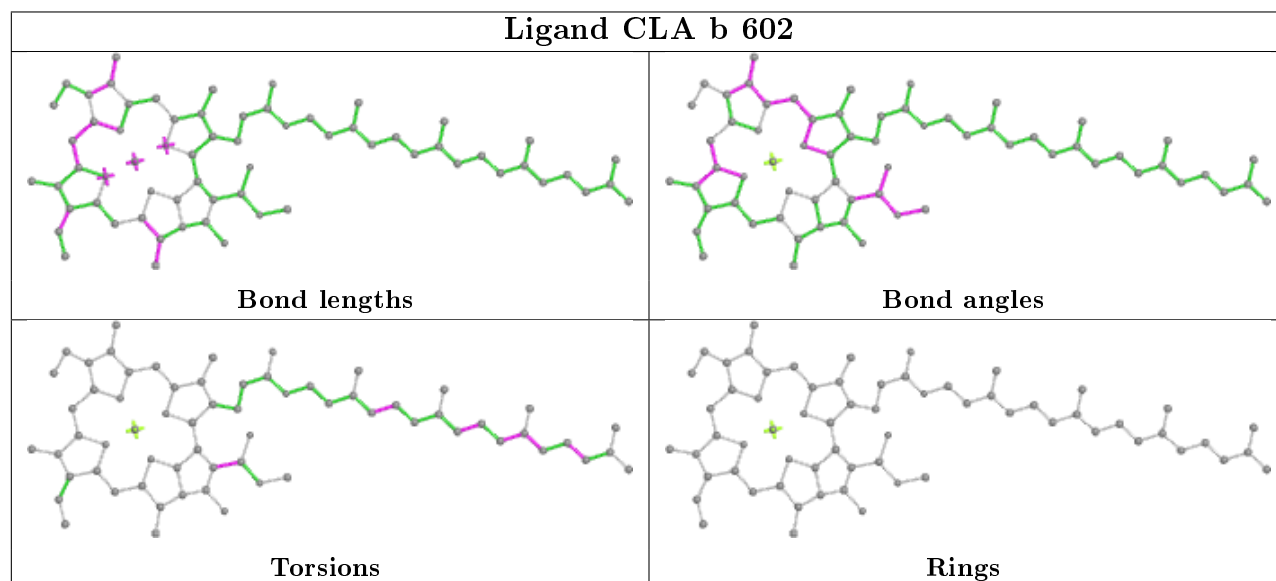
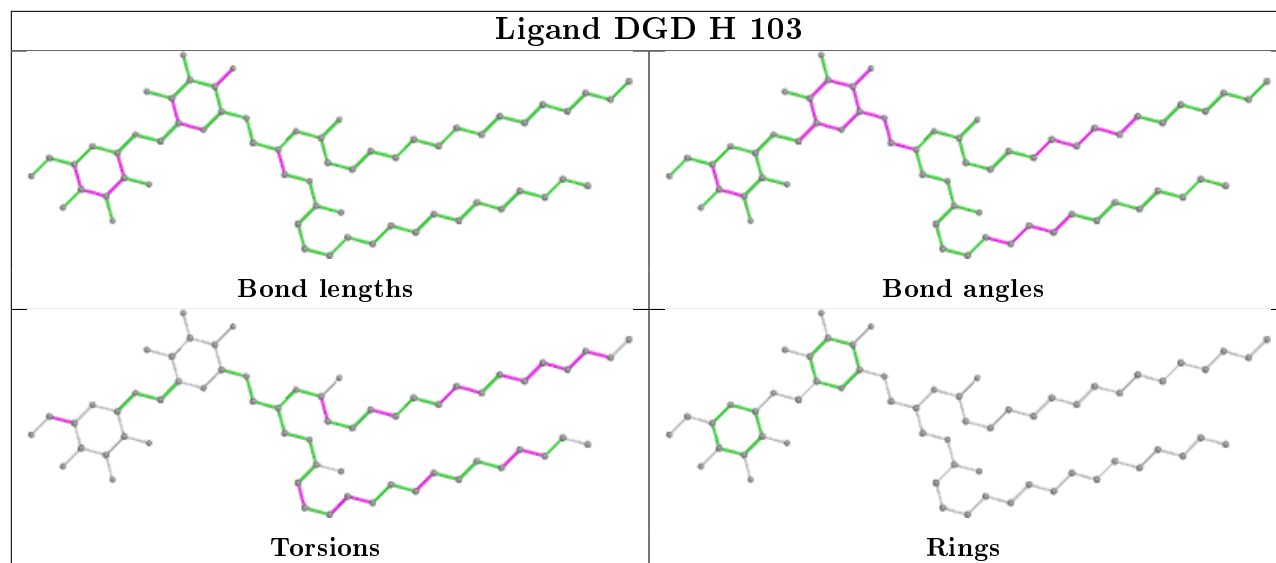
Ligand LHG 1 101

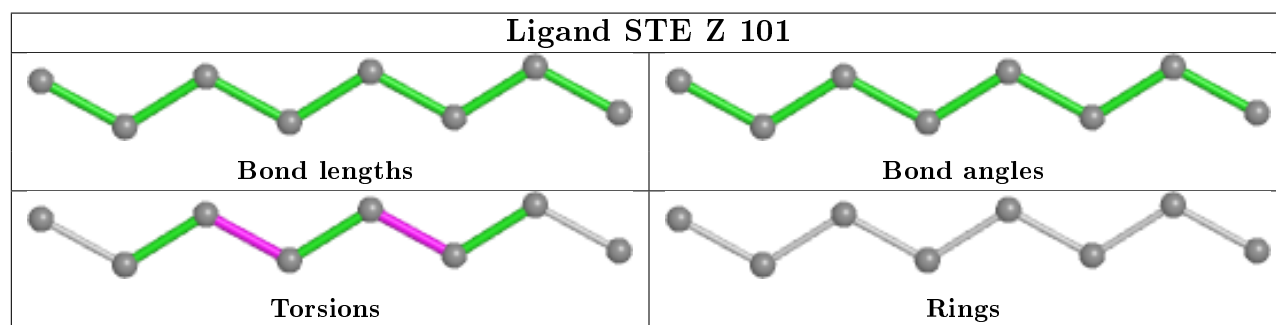
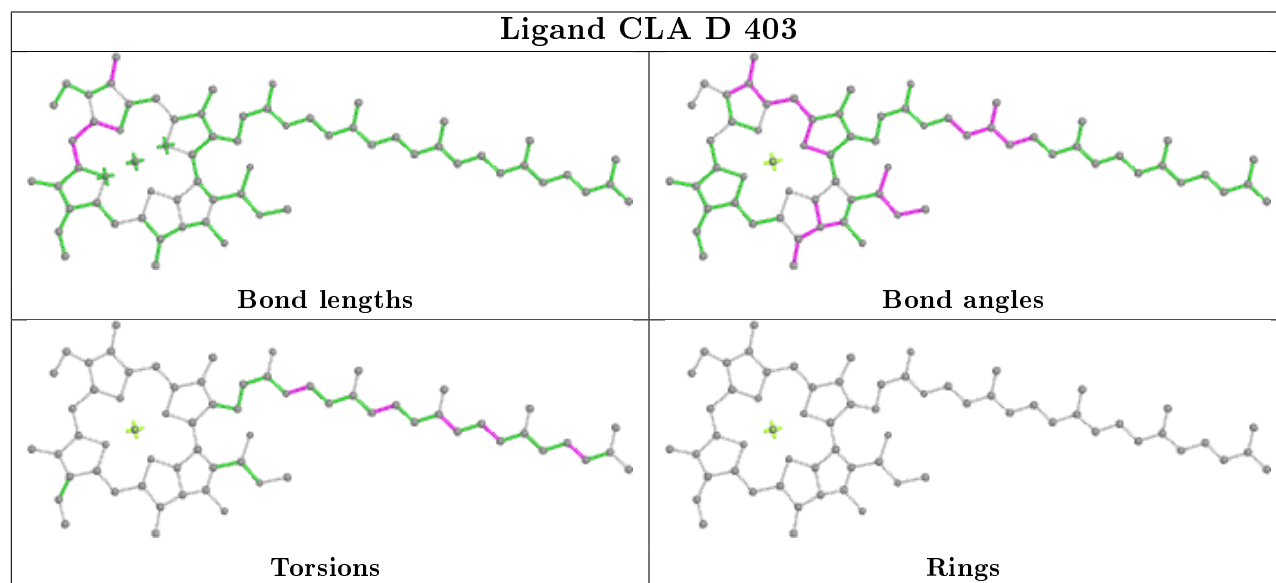
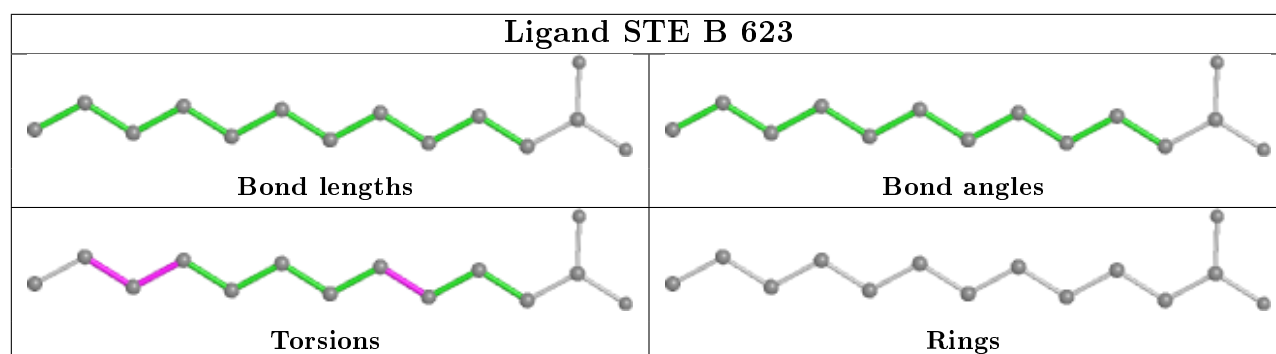


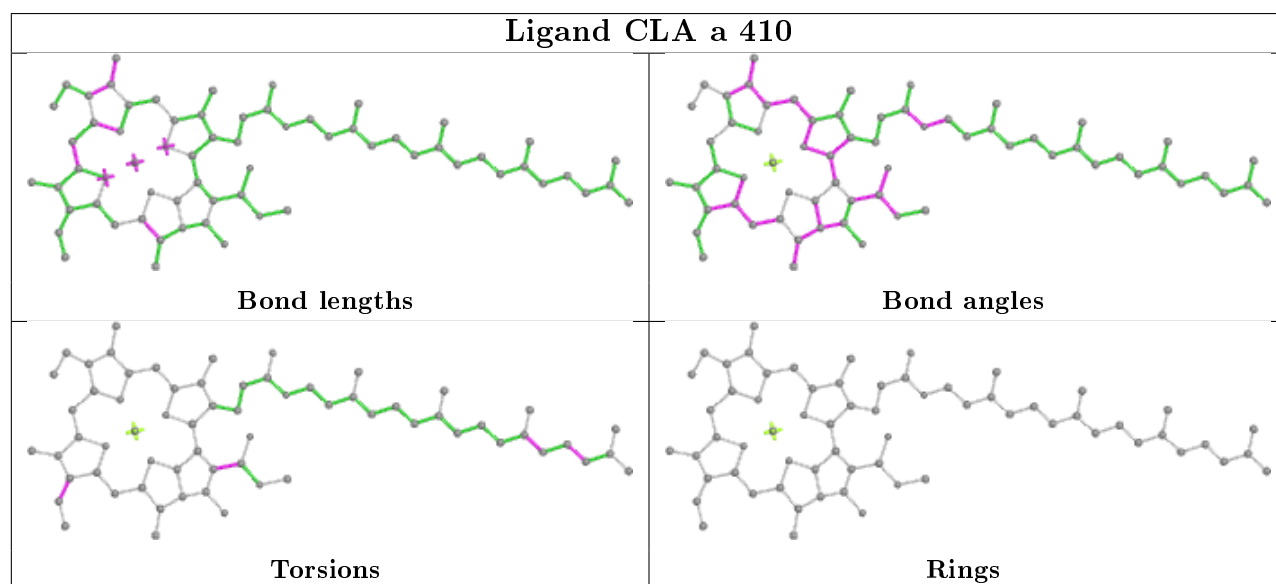
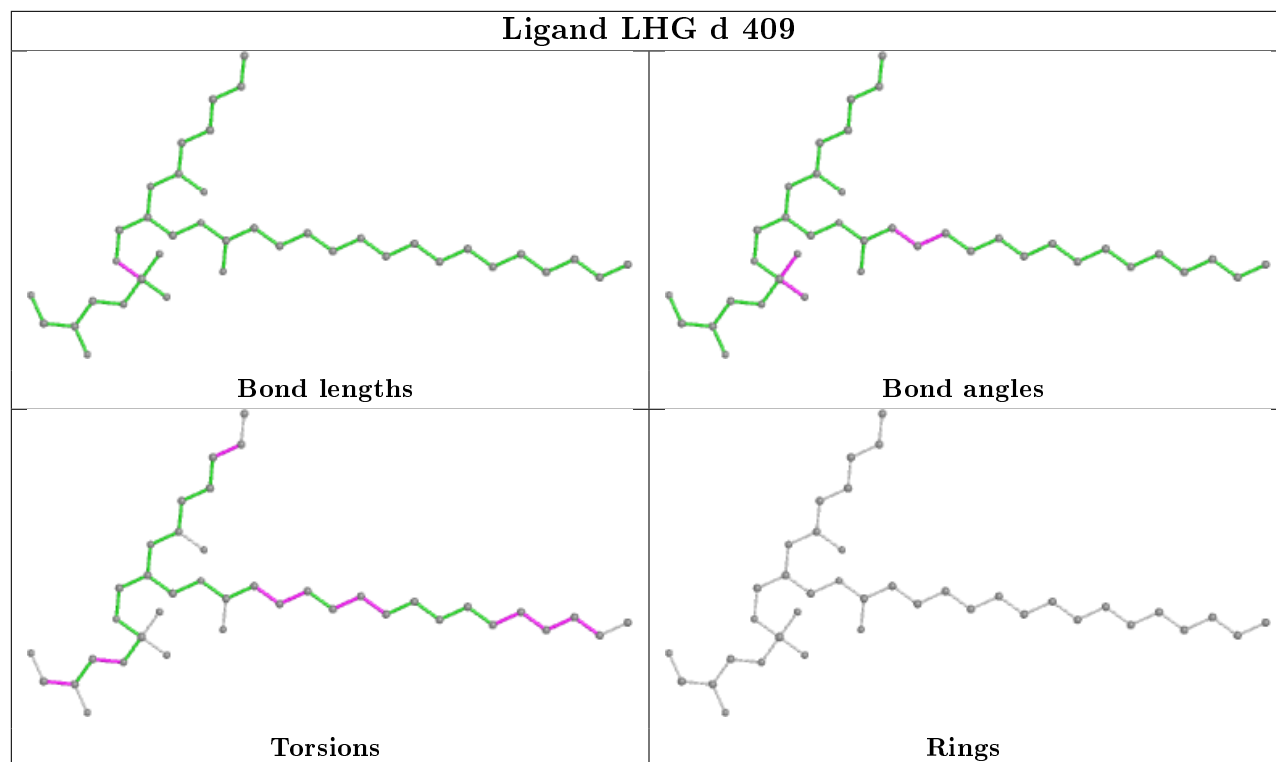
Ligand CLA B 602**Ligand LMG b 621****Ligand CLA a 403**

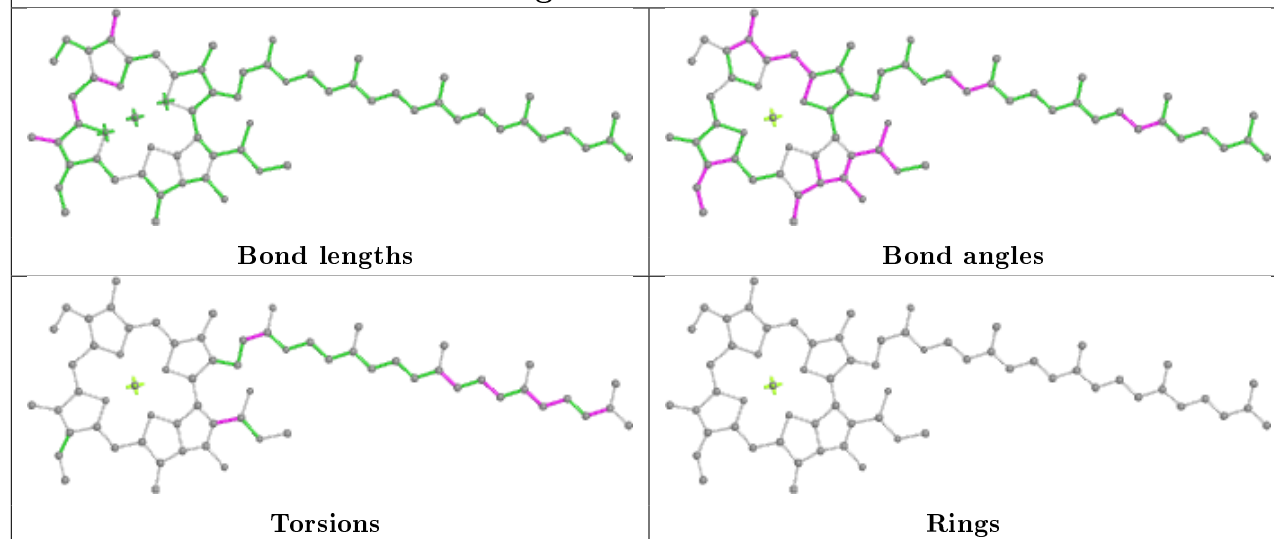
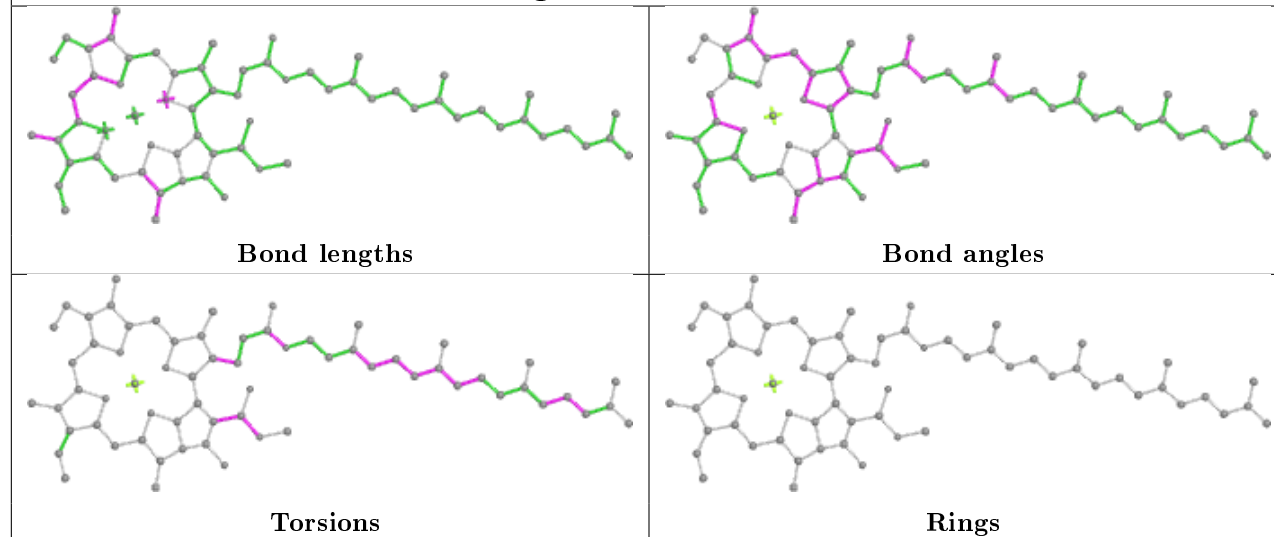




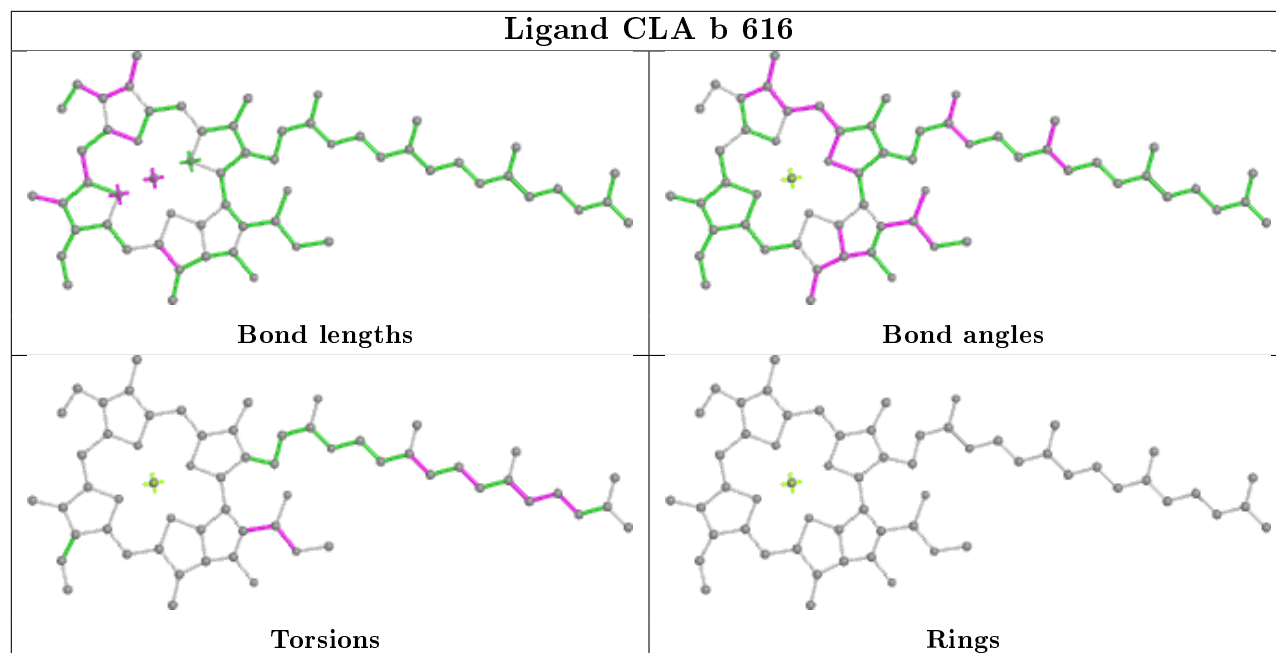




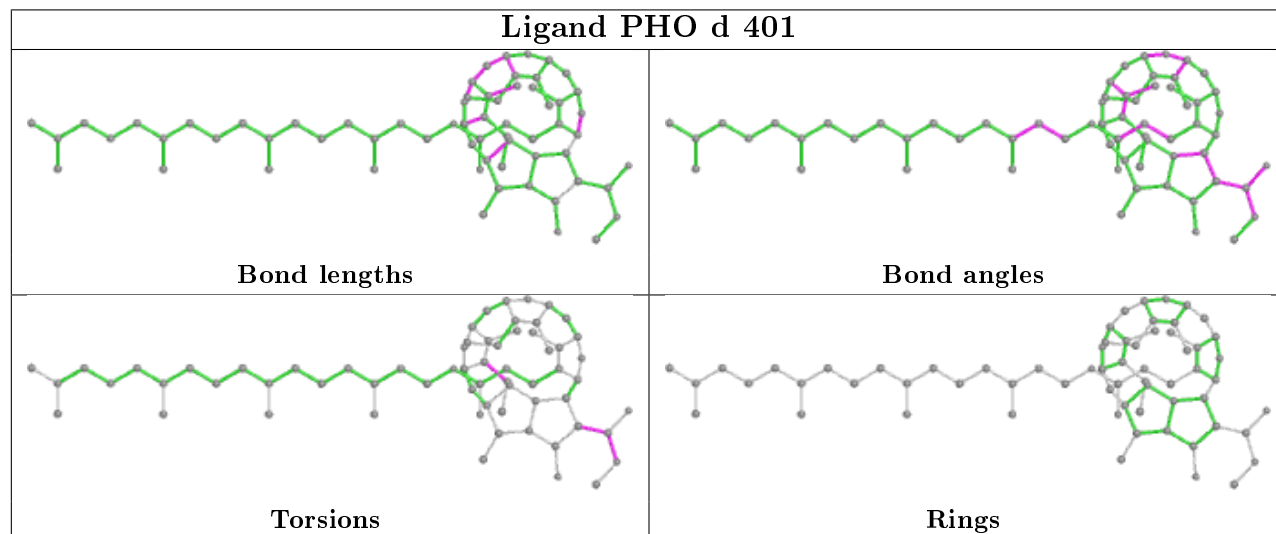


Ligand CLA b 612**Ligand CLA C 513**

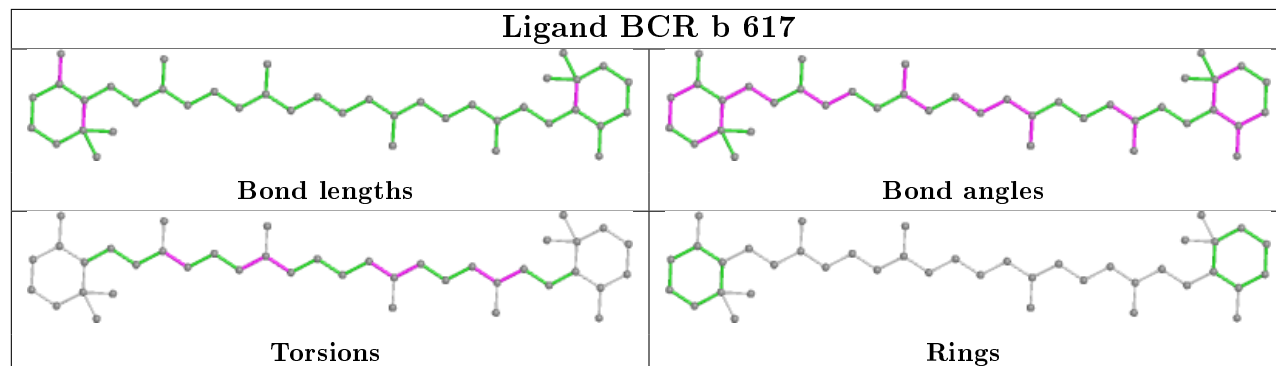
Ligand CLA b 616

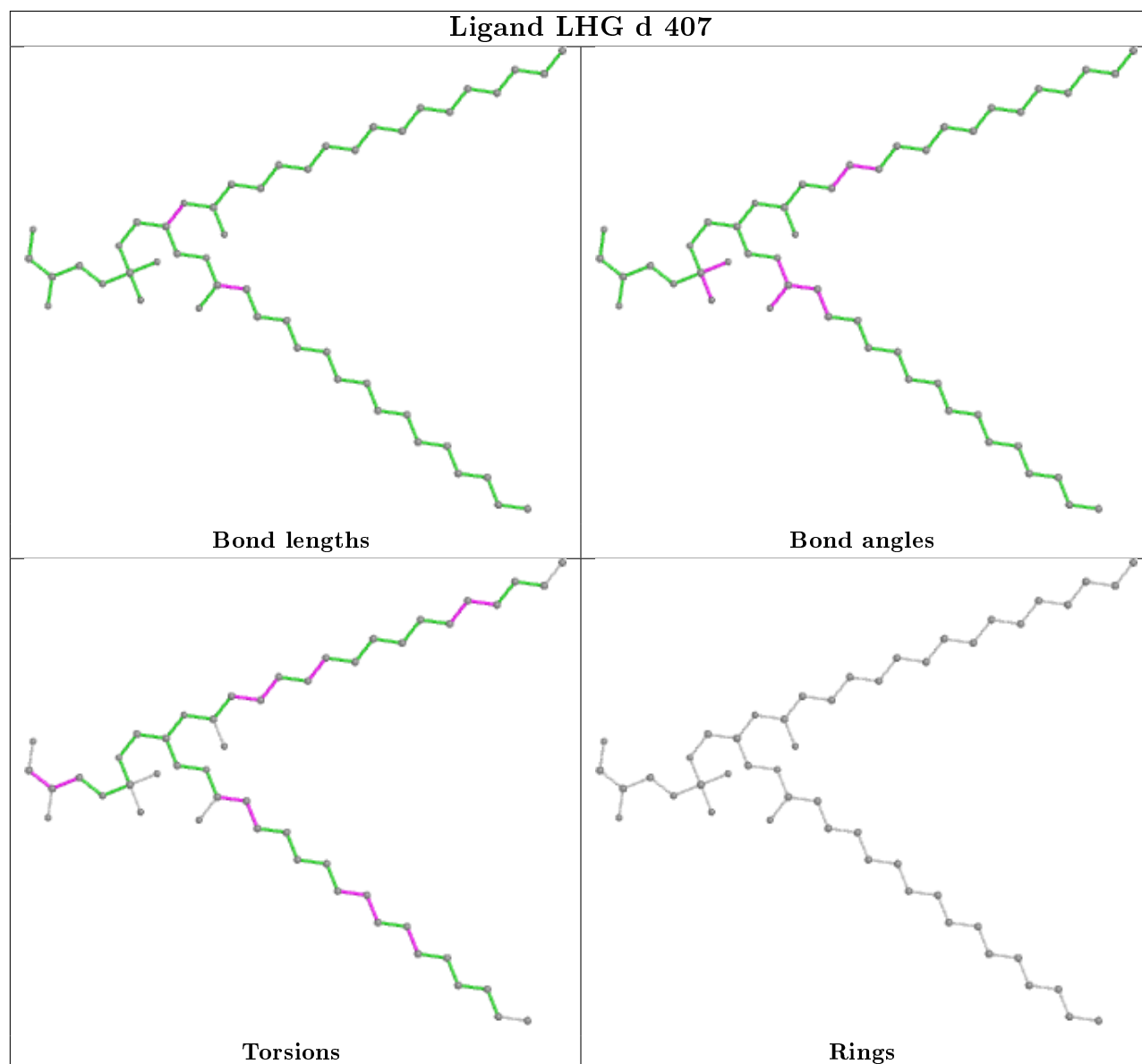
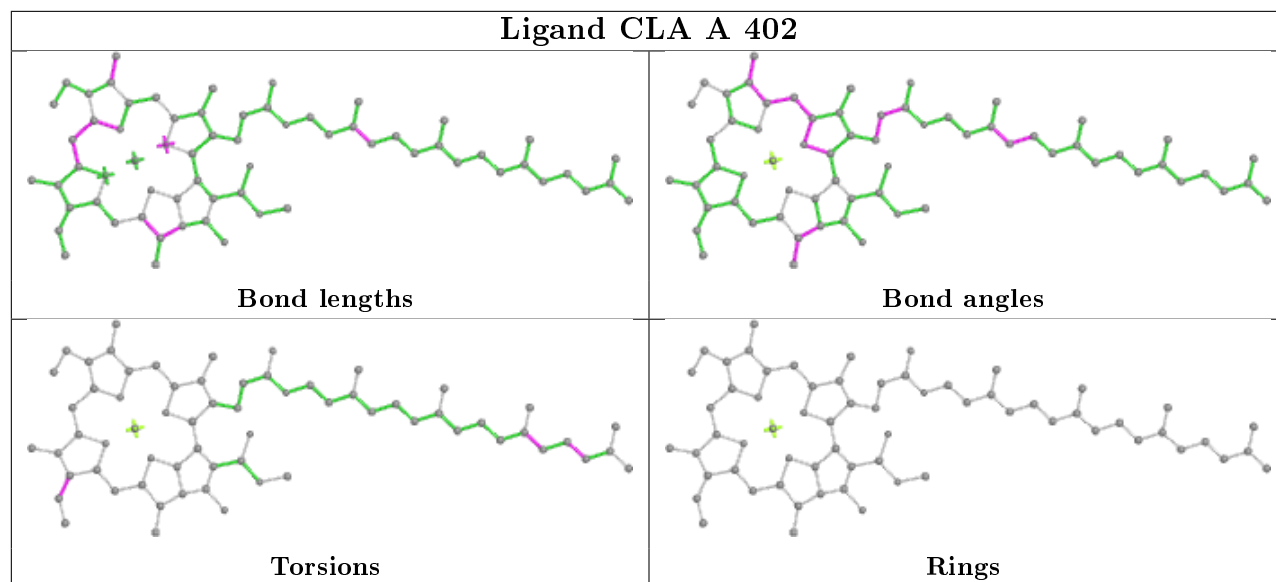


Ligand PHO d 401

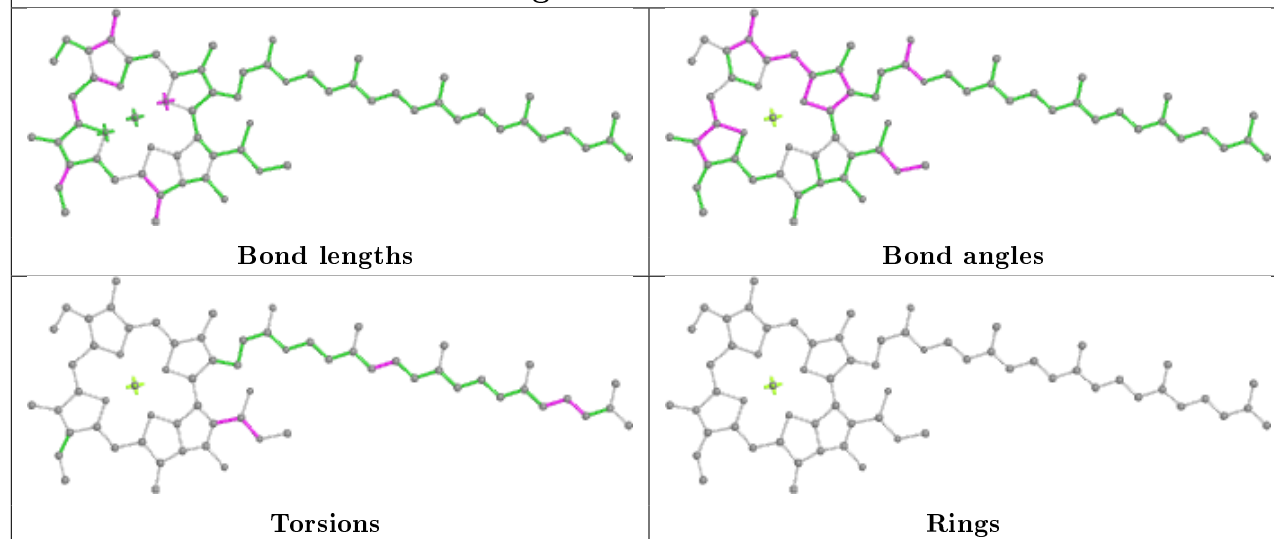


Ligand BCR b 617





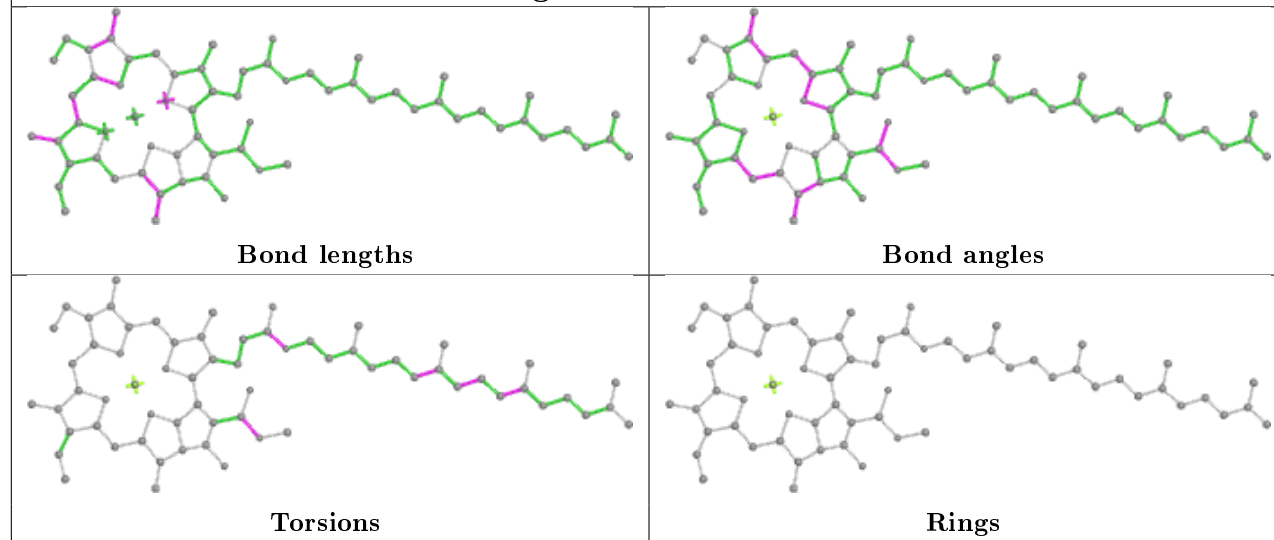
Ligand CLA B 607

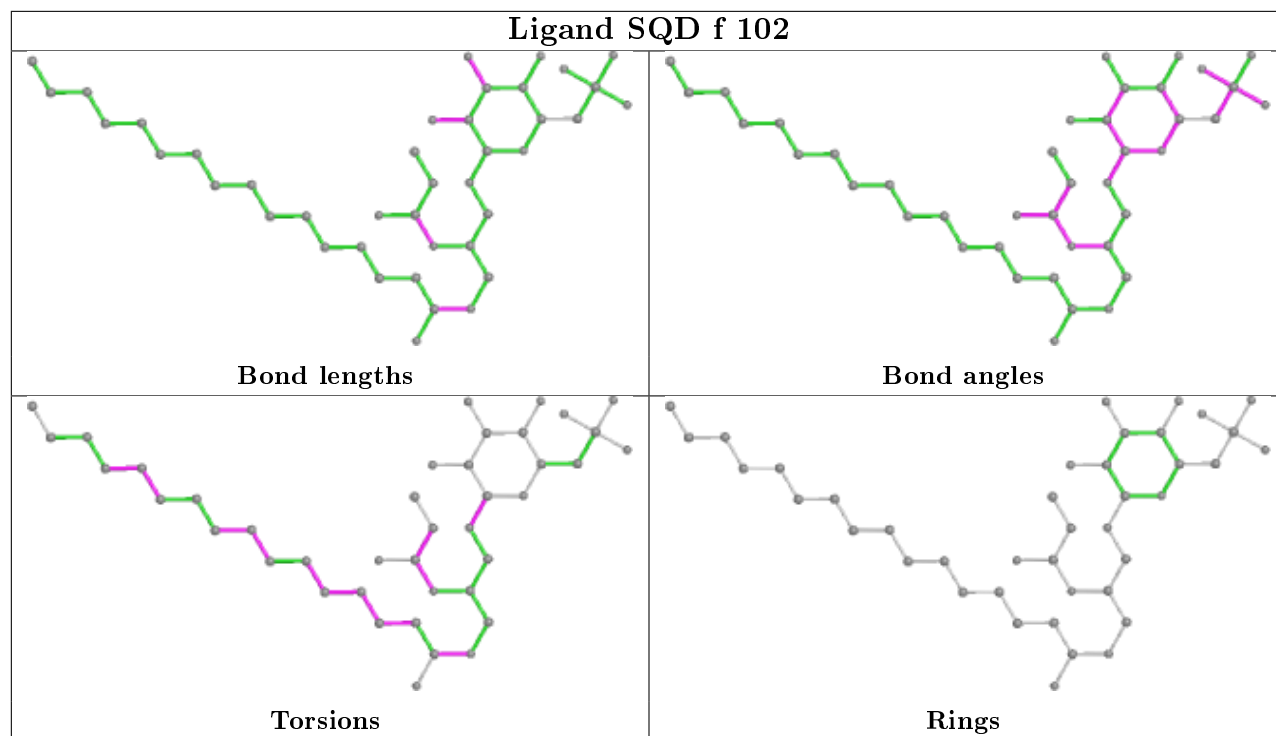


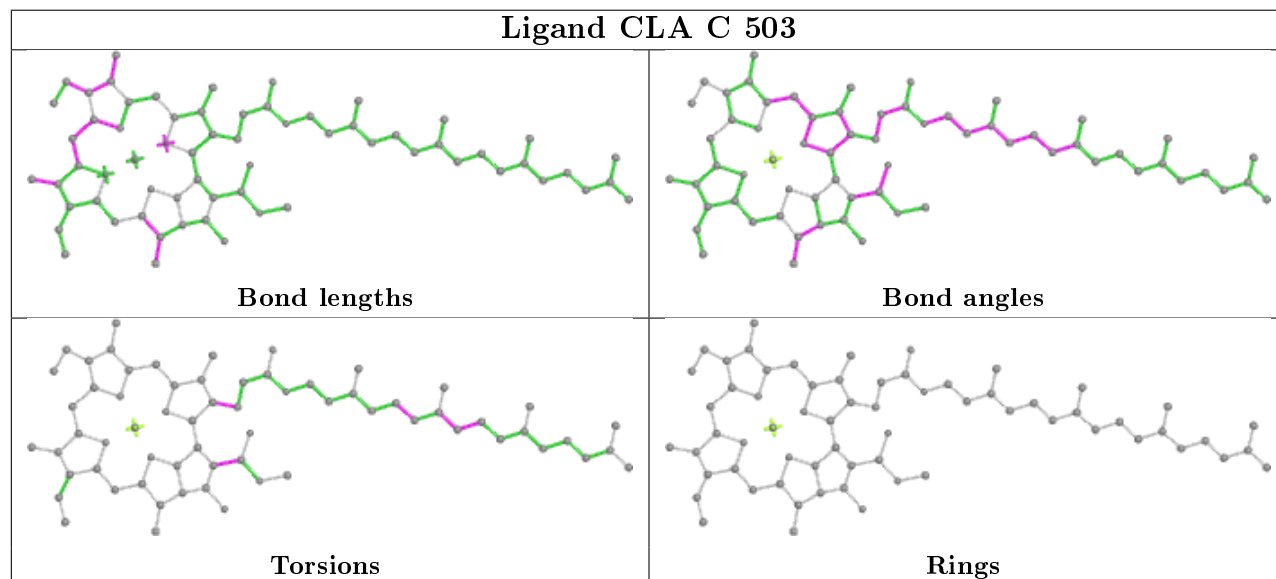
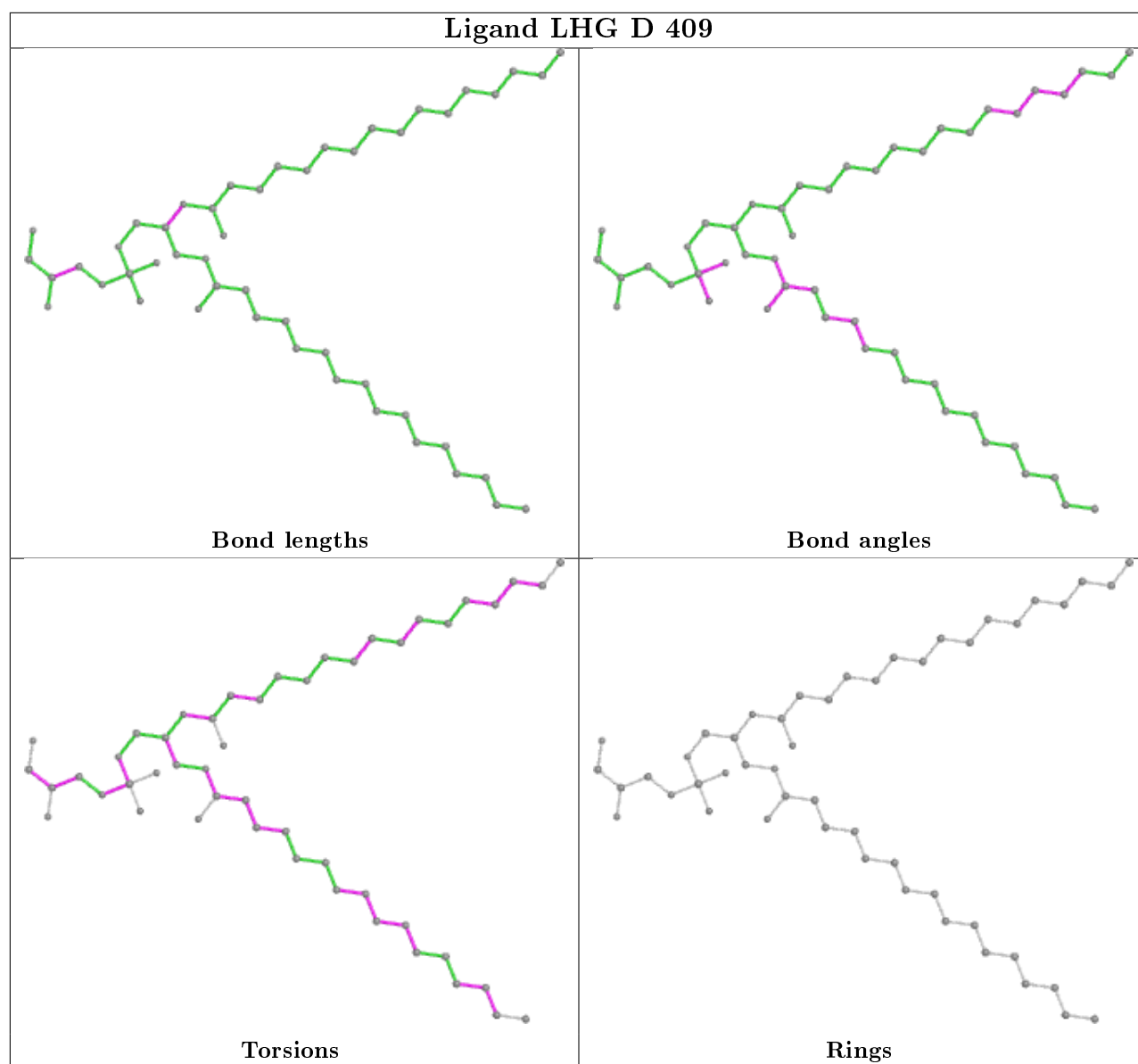
Ligand STE d 411

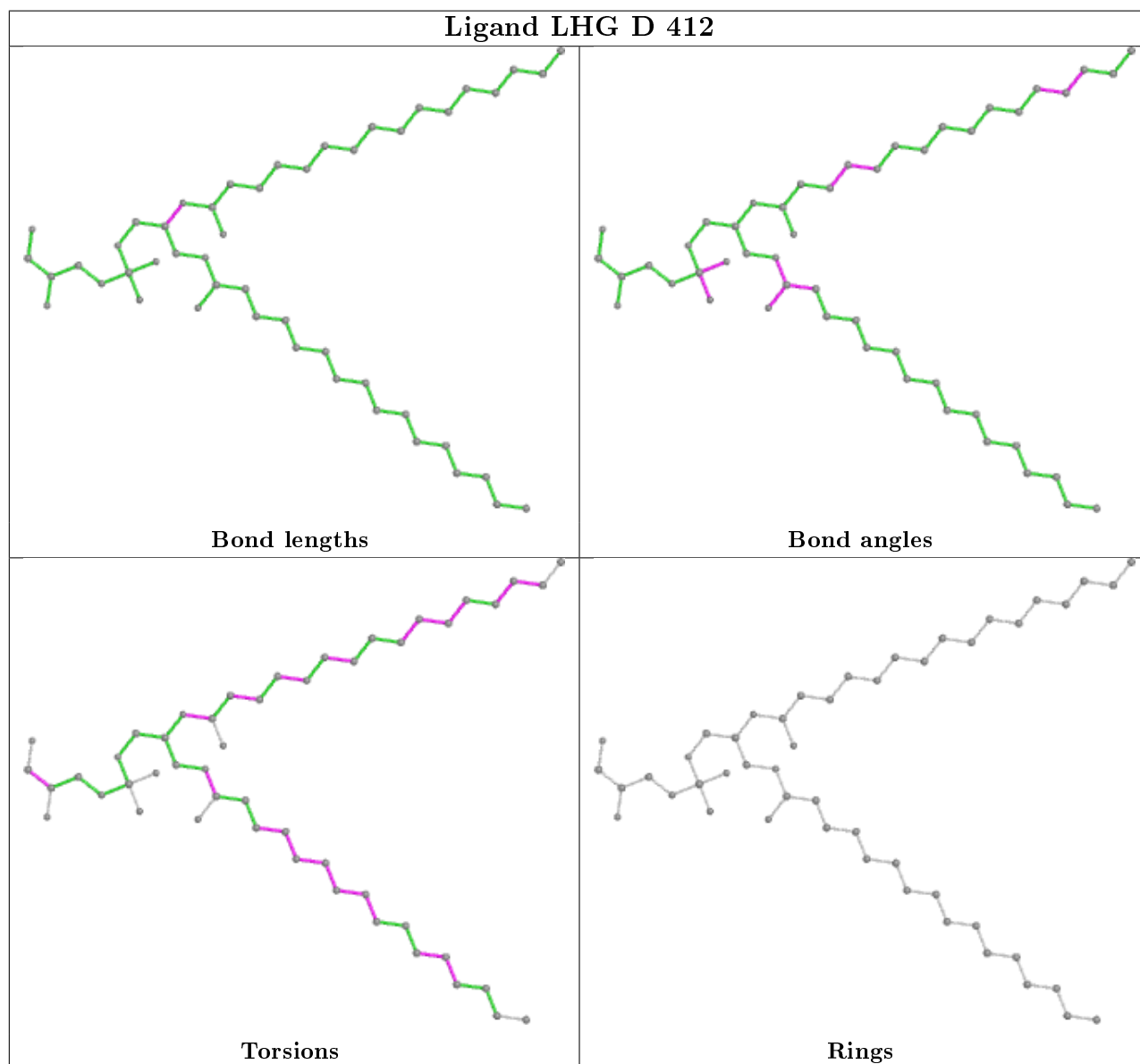
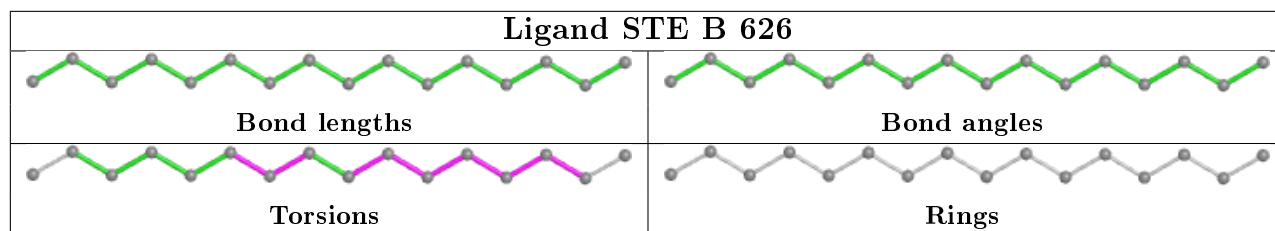


Ligand CLA C 511

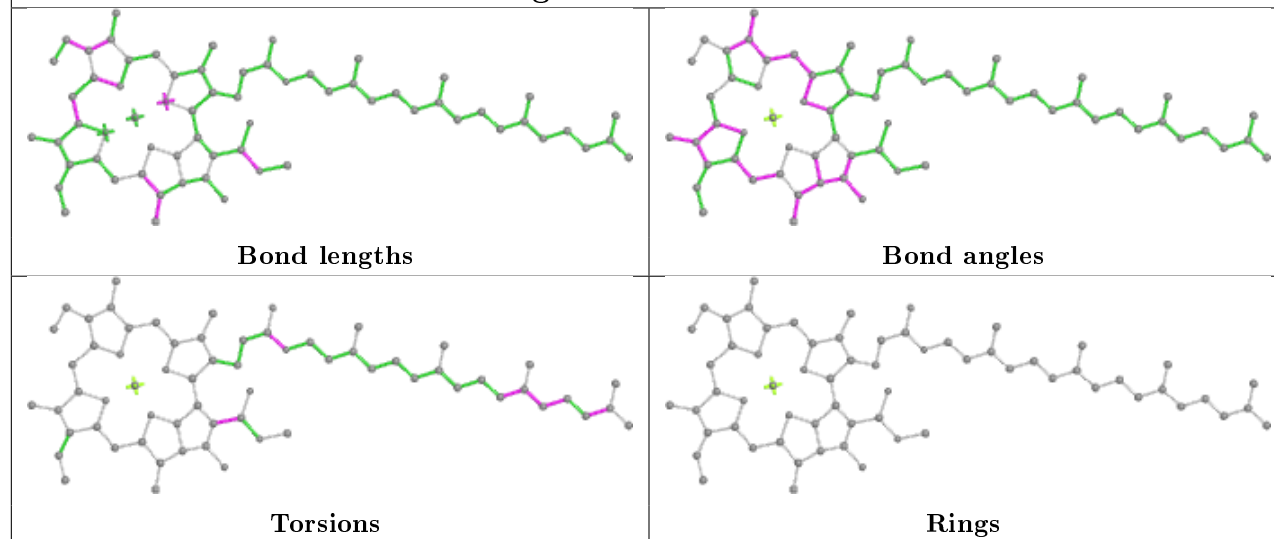




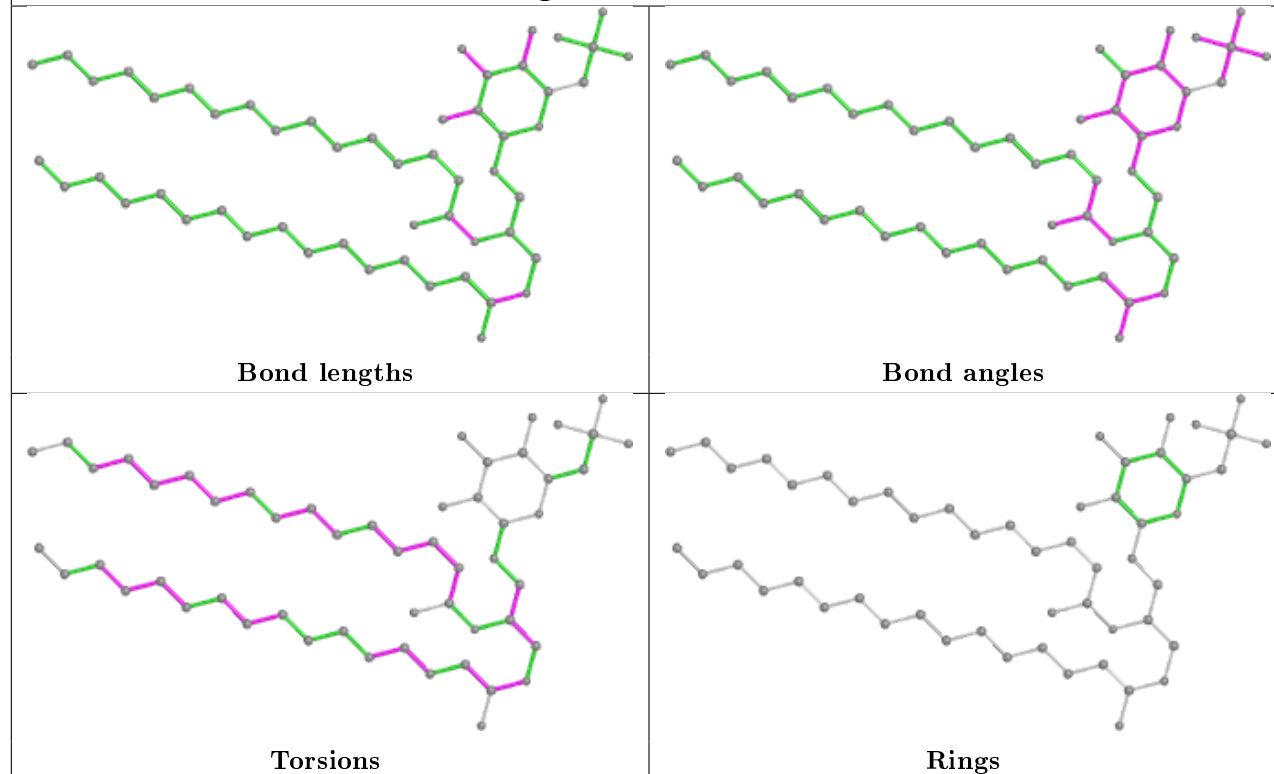




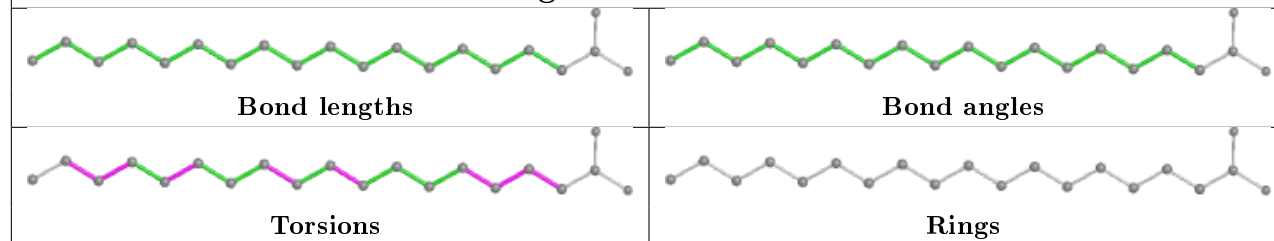
Ligand CLA B 609

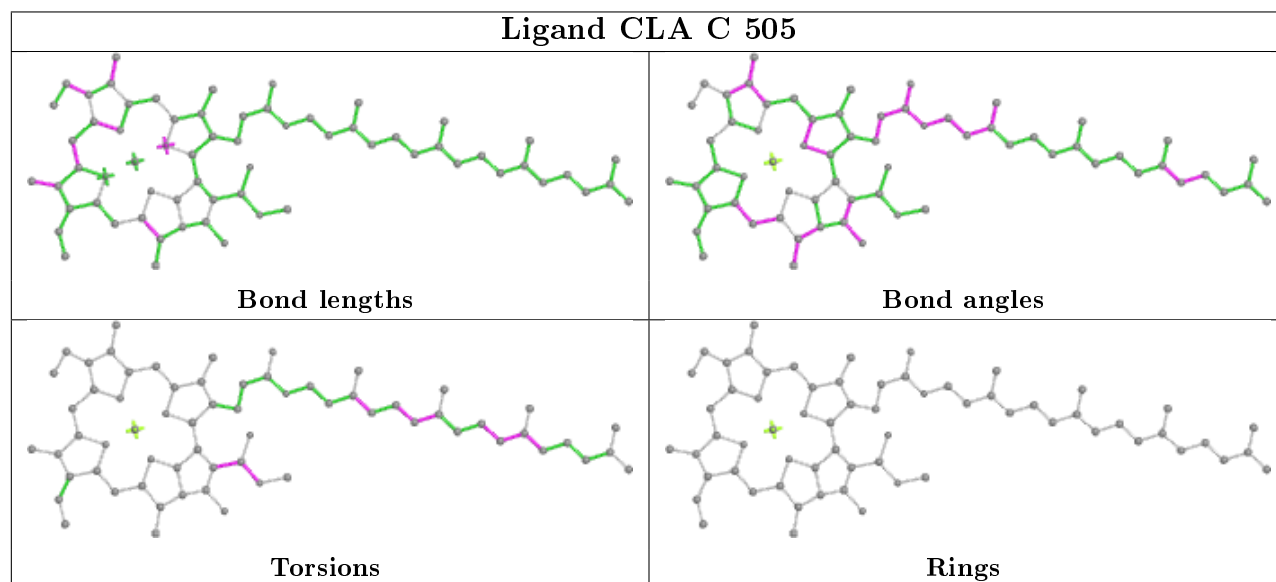
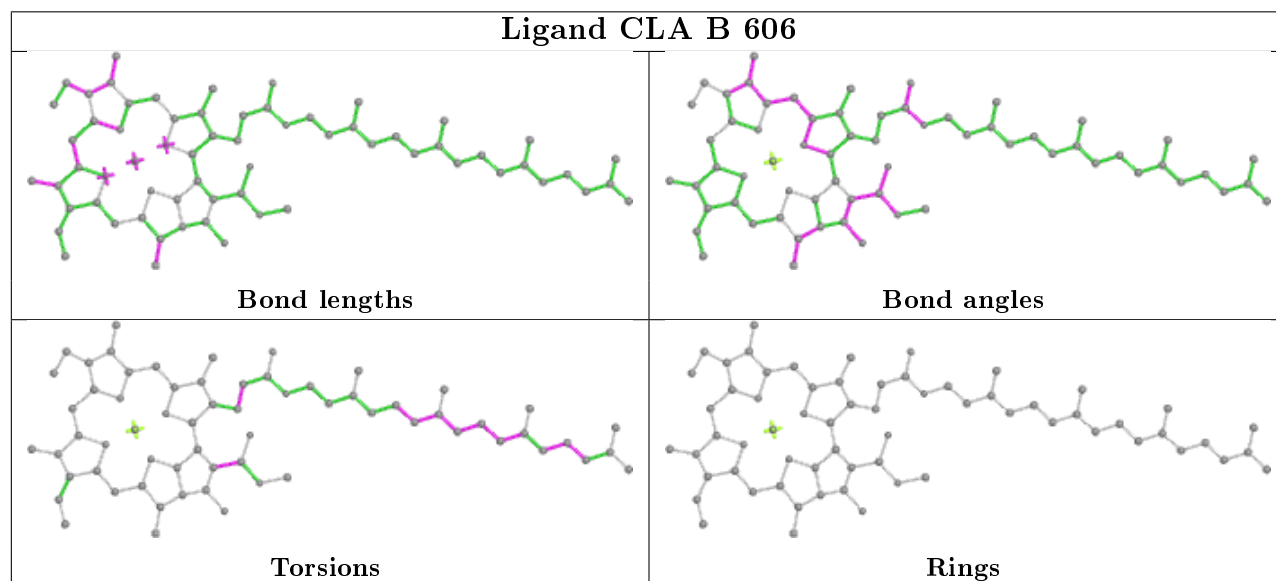
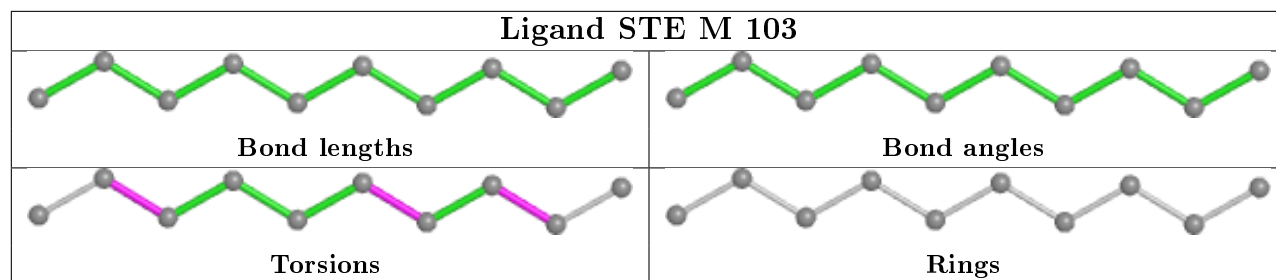


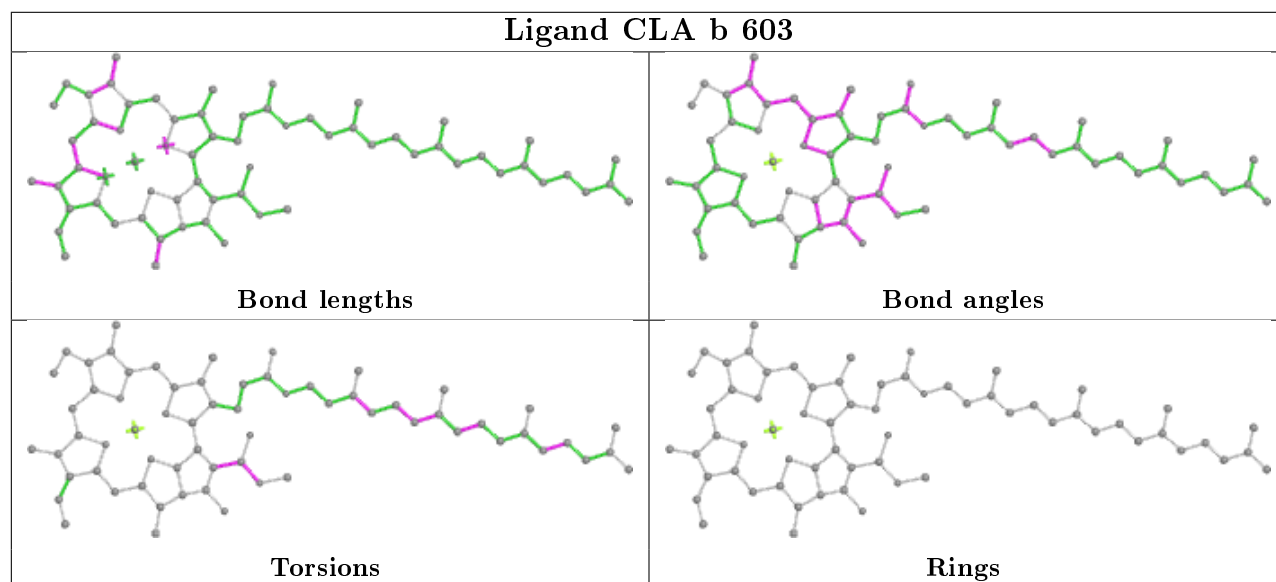
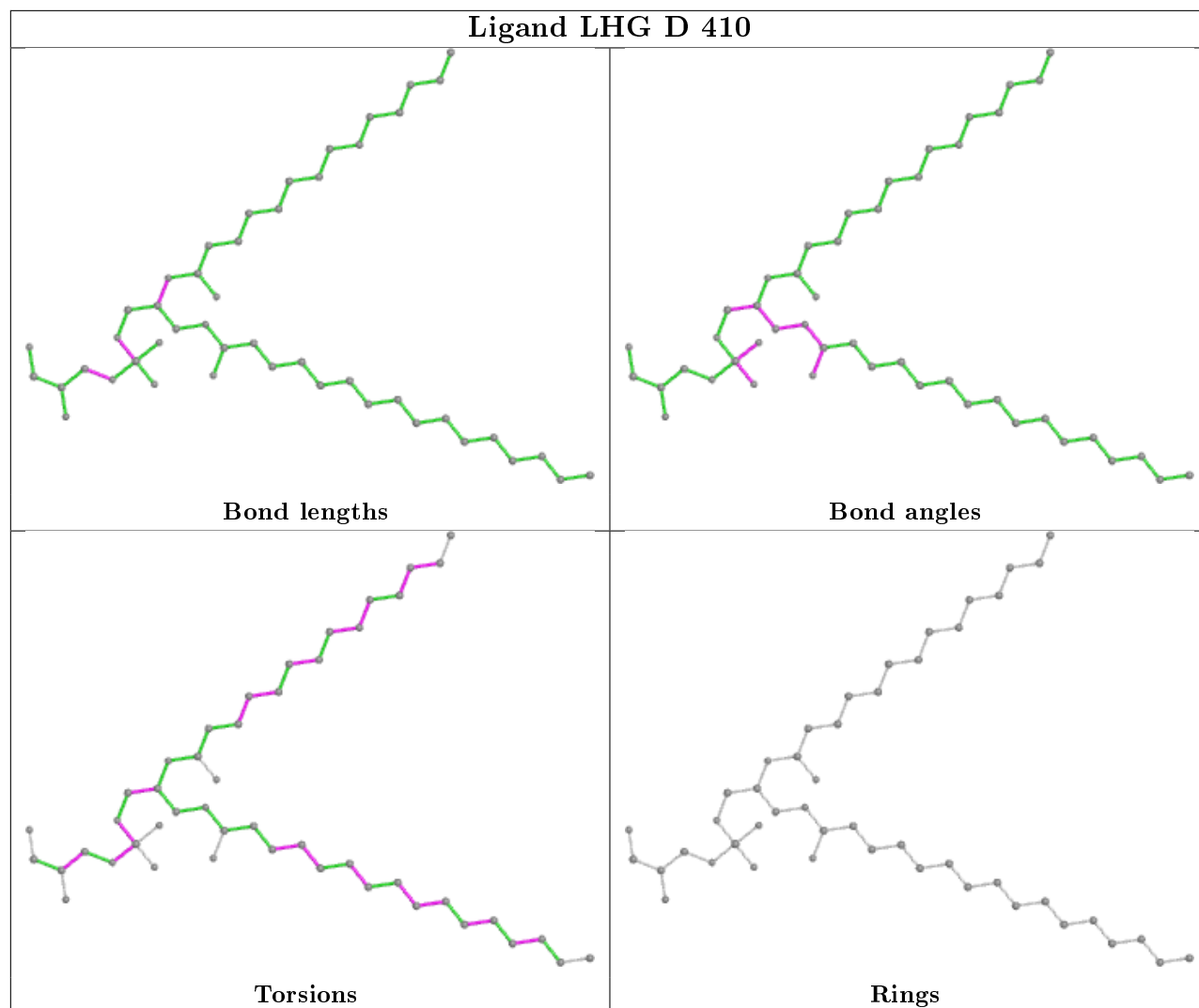
Ligand SQD a 411

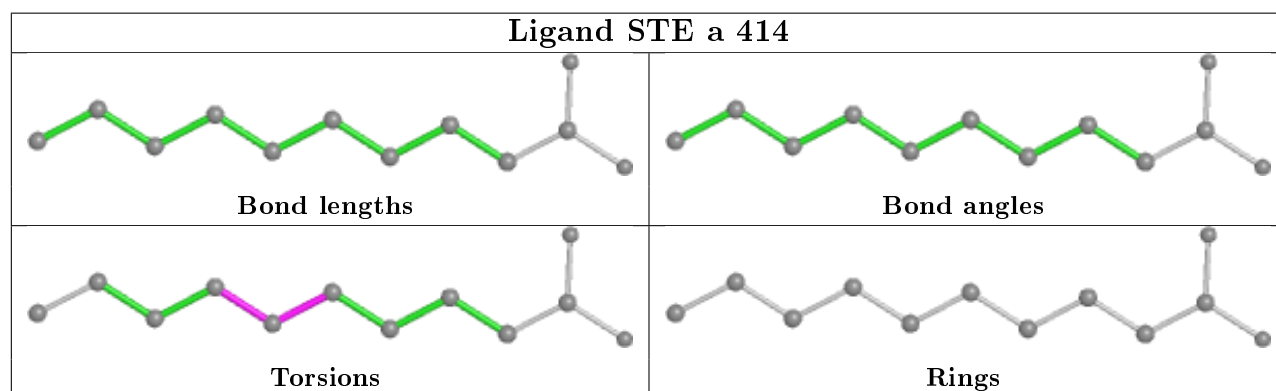
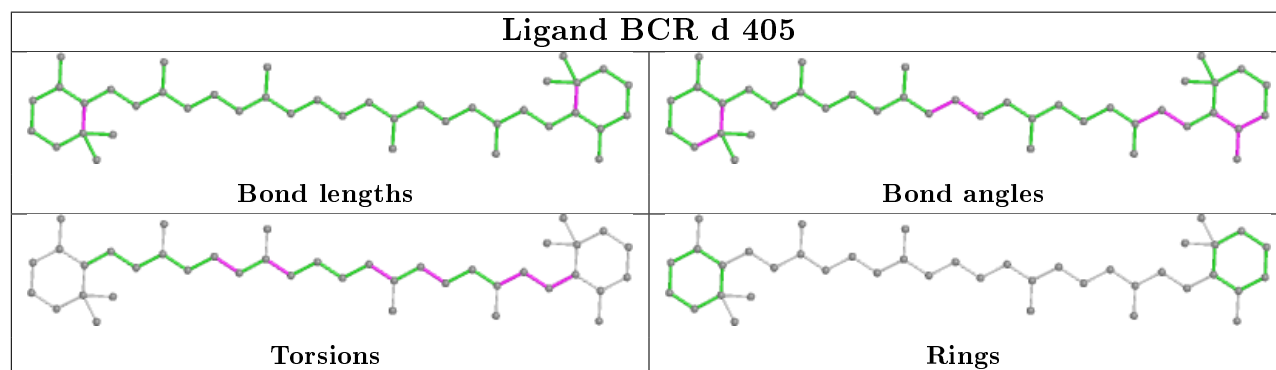
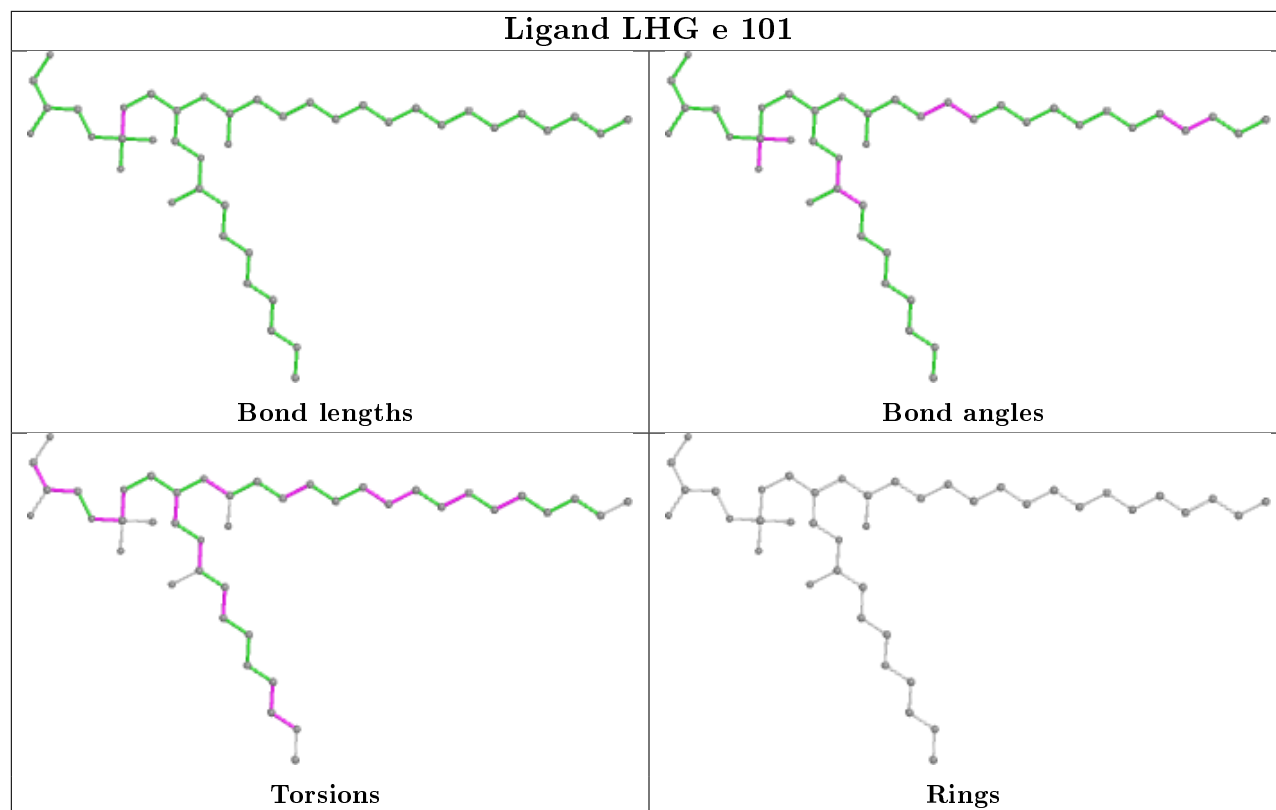


Ligand STE b 624

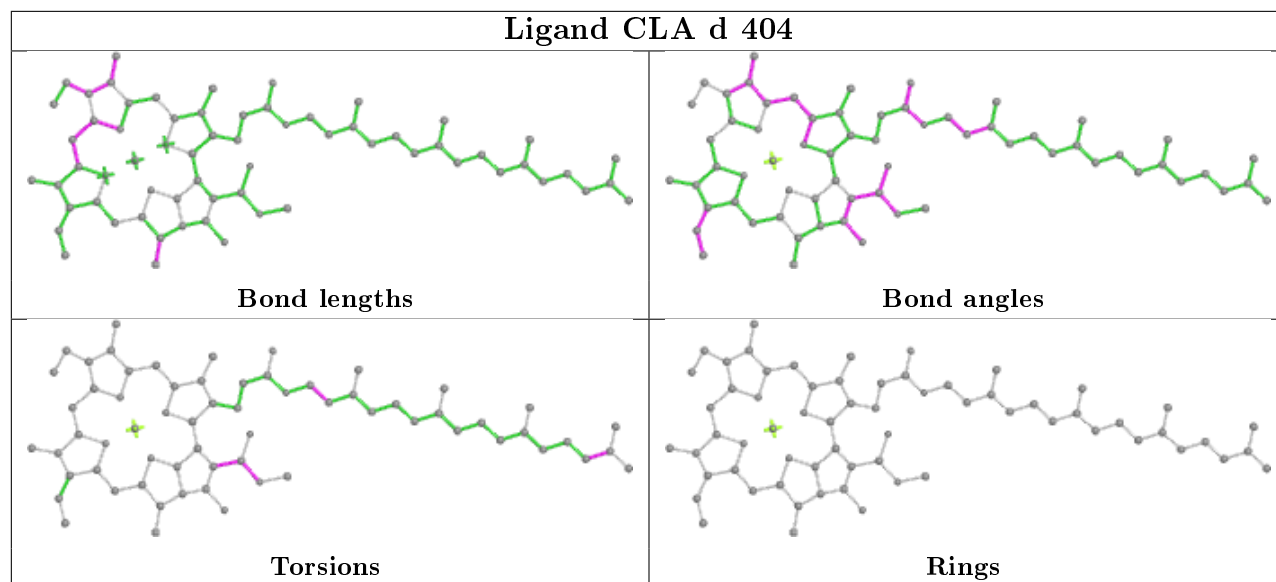




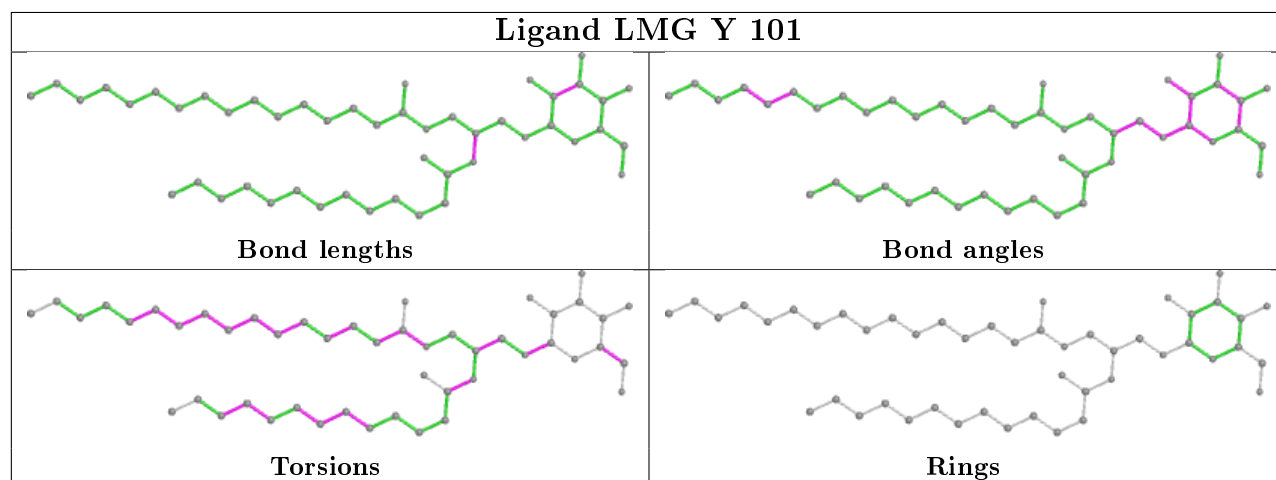




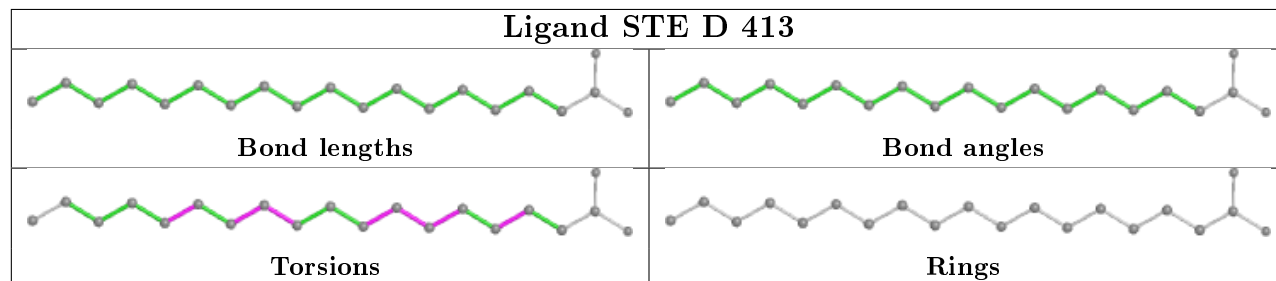
Ligand CLA d 404



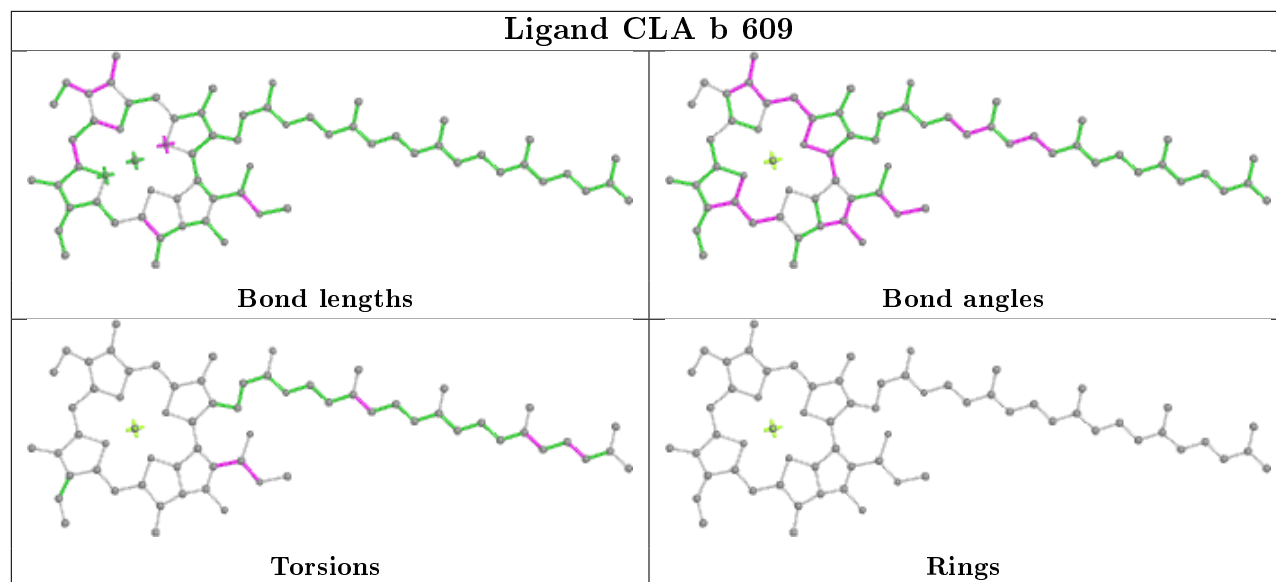
Ligand LMG Y 101



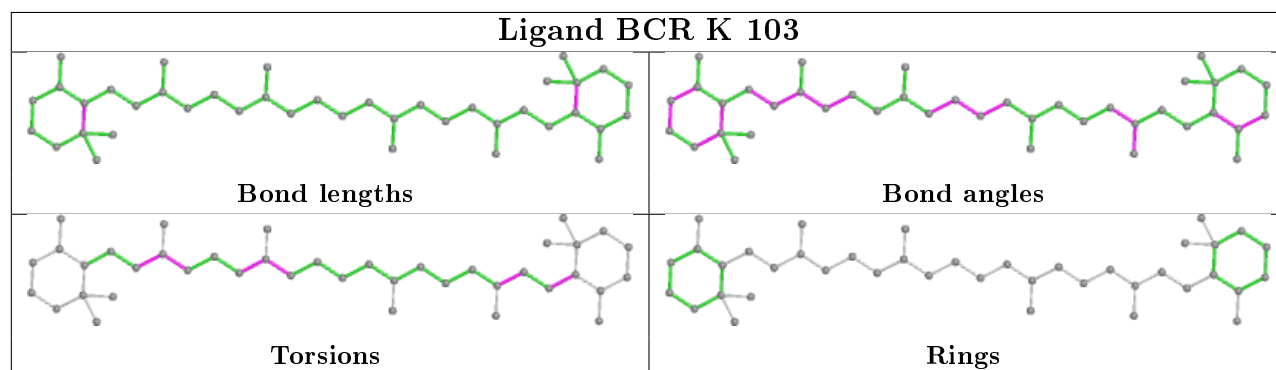
Ligand STE D 413



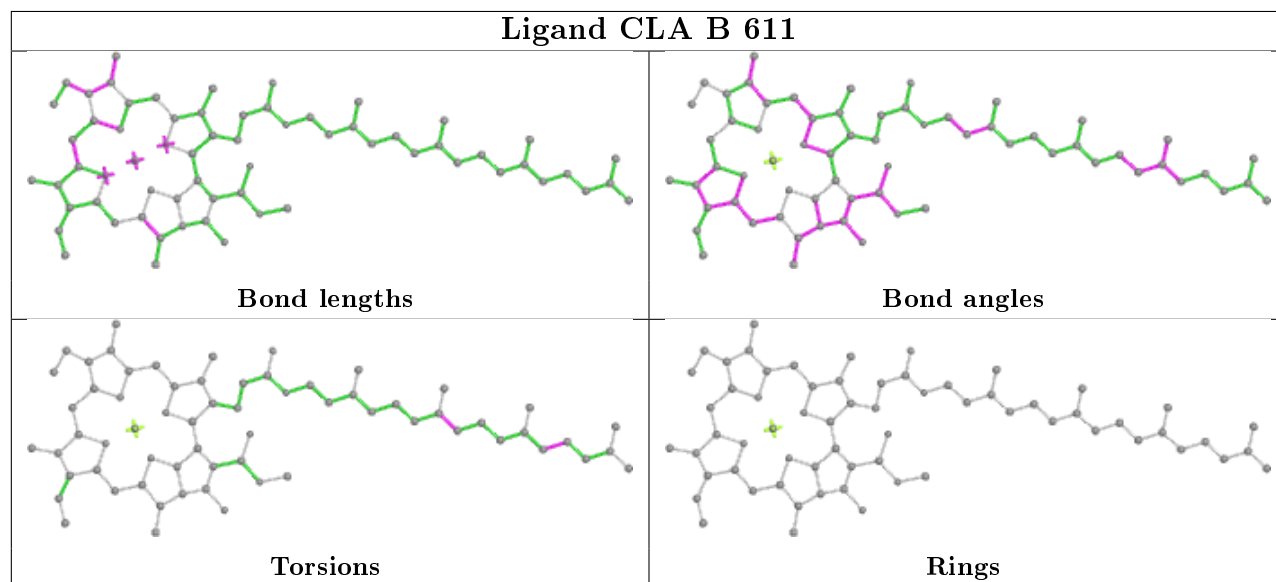
Ligand CLA b 609

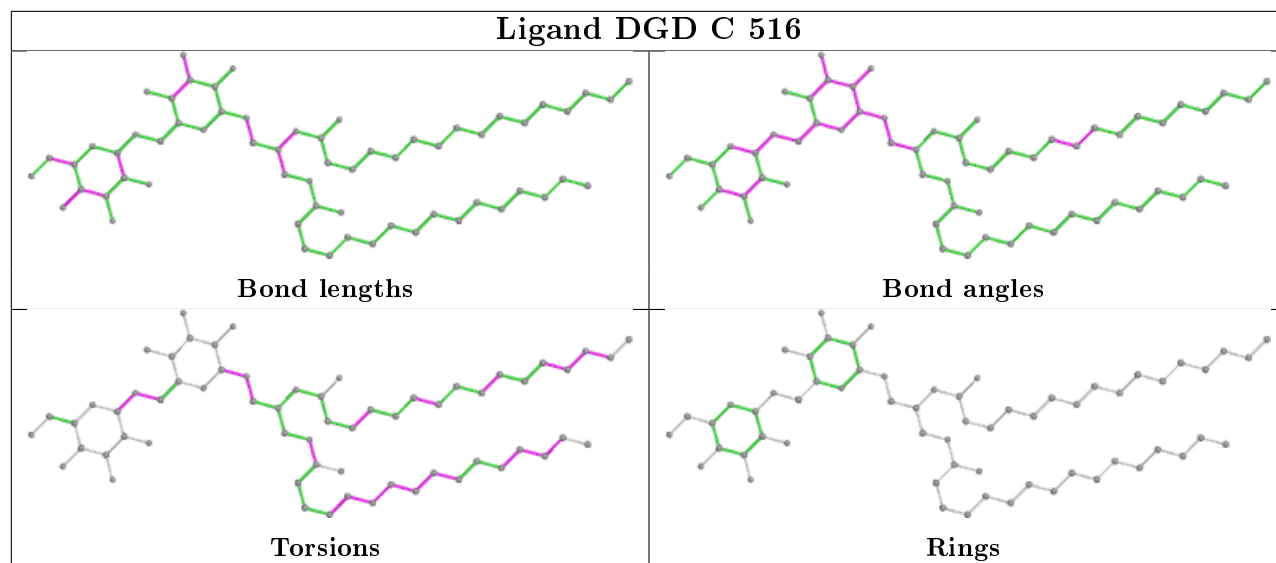


Ligand BCR K 103



Ligand CLA B 611





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.35	2 (0%) 89 91	21, 28, 49, 74	0
1	a	334/334 (100%)	-0.36	1 (0%) 94 94	22, 30, 56, 74	0
2	B	505/506 (99%)	-0.30	7 (1%) 75 78	22, 32, 61, 88	0
2	b	505/506 (99%)	-0.14	16 (3%) 47 53	21, 35, 69, 101	0
3	C	442/461 (95%)	-0.24	4 (0%) 84 86	23, 35, 51, 73	0
3	c	451/461 (97%)	-0.16	7 (1%) 72 75	25, 38, 59, 88	0
4	D	341/352 (96%)	-0.30	1 (0%) 94 94	20, 29, 48, 78	0
4	d	341/352 (96%)	-0.23	1 (0%) 94 94	22, 33, 55, 76	0
5	E	82/84 (97%)	0.05	4 (4%) 29 34	32, 50, 69, 76	0
5	e	82/84 (97%)	0.21	4 (4%) 29 34	38, 56, 76, 83	0
6	F	34/45 (75%)	-0.26	1 (2%) 51 56	34, 41, 62, 87	0
6	f	34/45 (75%)	-0.22	1 (2%) 51 56	41, 47, 75, 86	0
7	H	65/66 (98%)	-0.07	1 (1%) 73 76	30, 39, 57, 67	0
7	h	63/66 (95%)	0.22	3 (4%) 30 35	40, 48, 59, 71	0
8	I	35/38 (92%)	-0.09	3 (8%) 10 12	29, 37, 68, 80	0
8	i	35/38 (92%)	-0.24	2 (5%) 23 28	30, 39, 73, 77	0
9	J	36/40 (90%)	0.13	4 (11%) 5 6	33, 48, 73, 87	0
9	j	36/40 (90%)	0.21	4 (11%) 5 6	38, 50, 79, 91	0
10	K	37/46 (80%)	0.25	1 (2%) 54 59	42, 50, 66, 73	0
10	k	37/46 (80%)	0.08	1 (2%) 54 59	48, 54, 65, 75	0
11	L	37/37 (100%)	-0.44	0 100 100	23, 29, 59, 67	0
11	l	36/37 (97%)	-0.23	2 (5%) 24 28	24, 29, 69, 80	0
12	M	32/36 (88%)	-0.09	1 (3%) 49 54	26, 31, 56, 65	0
12	m	31/36 (86%)	-0.15	0 100 100	25, 32, 50, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.03	14 (5%) 23 28	25, 39, 76, 124	0
13	o	244/272 (89%)	-0.12	12 (4%) 29 34	23, 38, 72, 104	0
14	R	34/40 (85%)	2.46	19 (55%) 0 0	63, 73, 90, 102	0
14	r	31/40 (77%)	4.42	28 (90%) 0 0	70, 93, 109, 116	0
15	T	29/30 (96%)	-0.47	2 (6%) 16 20	24, 29, 58, 75	0
15	t	29/30 (96%)	-0.21	2 (6%) 16 20	25, 31, 72, 88	0
16	U	97/134 (72%)	-0.26	1 (1%) 82 84	30, 42, 64, 84	0
16	u	97/134 (72%)	-0.42	0 100 100	29, 38, 56, 78	0
17	V	137/163 (84%)	-0.45	0 100 100	29, 39, 55, 76	0
17	v	137/163 (84%)	-0.14	3 (2%) 62 66	30, 45, 65, 85	0
18	X	38/41 (92%)	-0.03	2 (5%) 26 31	38, 49, 71, 78	0
18	x	39/41 (95%)	0.54	5 (12%) 3 4	46, 57, 87, 100	0
19	Y	27/46 (58%)	1.31	8 (29%) 0 0	50, 69, 85, 92	0
19	y	30/46 (65%)	0.57	5 (16%) 1 1	58, 69, 81, 88	0
20	Z	62/62 (100%)	1.06	18 (29%) 0 0	53, 66, 109, 121	0
20	z	62/62 (100%)	0.95	12 (19%) 1 1	56, 67, 101, 116	0
All	All	5302/5666 (93%)	-0.11	202 (3%) 40 45	20, 36, 71, 124	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	14	LEU	9.0
2	b	495	PHE	7.7
13	o	58	ASN	7.4
14	r	9	LEU	7.2
20	z	33	TRP	7.0
14	r	10	LEU	6.9
13	O	60	ARG	6.8
14	r	29	LYS	6.6
14	r	28	VAL	6.4
20	Z	33	TRP	5.9
14	r	6	LEU	5.9
15	t	30	THR	5.7
13	O	56	PRO	5.7
20	z	35	ARG	5.7
14	r	3	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	13	LEU	5.6
13	o	4	THR	5.6
13	O	61	GLN	5.5
14	r	18	TRP	5.5
14	r	26	TYR	5.5
14	R	3	TRP	5.4
14	r	2	ASP	5.3
14	R	6	LEU	5.3
13	O	3	GLN	5.3
14	r	31	VAL	5.1
14	r	19	ALA	5.1
20	Z	7	LEU	5.1
14	r	13	LEU	5.1
20	Z	32	ASP	5.0
14	R	32	GLN	5.0
9	J	5	GLY	4.9
9	j	5	GLY	4.9
9	j	6	GLY	4.8
2	b	127	ARG	4.8
13	O	62	GLU	4.8
14	r	15	ALA	4.8
20	Z	62	VAL	4.7
14	r	25	PRO	4.6
20	Z	35	ARG	4.6
20	Z	34	ASP	4.6
13	O	59	LYS	4.5
13	o	3	GLN	4.5
14	r	7	VAL	4.4
14	r	11	PRO	4.4
13	O	4	THR	4.4
14	r	24	LEU	4.4
19	Y	41	VAL	4.4
3	c	147	PHE	4.3
2	b	487	SER	4.3
2	B	495	PHE	4.3
9	j	8	ILE	4.3
3	c	23	ALA	4.2
14	r	27	ALA	4.2
2	b	488	PRO	4.1
14	R	25	PRO	4.1
14	R	26	TYR	4.1
9	j	7	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
14	r	23	ILE	4.0
20	Z	42	LEU	3.9
14	R	21	ARG	3.9
19	Y	43	ARG	3.9
20	Z	61	VAL	3.9
7	H	66	GLY	3.9
3	c	146	PHE	3.9
5	e	79	PHE	3.9
13	o	61	GLN	3.8
18	X	2	THR	3.7
14	r	5	VAL	3.7
17	v	15	GLU	3.7
19	Y	42	ARG	3.6
20	Z	37	LYS	3.6
20	Z	3	ILE	3.5
14	R	2	ASP	3.5
5	E	79	PHE	3.5
2	b	505	ARG	3.5
8	I	36	ASP	3.5
19	y	37	PHE	3.5
13	O	63	ALA	3.5
13	o	59	LYS	3.5
10	K	17	ILE	3.5
20	z	1	MET	3.5
15	T	30	THR	3.4
9	J	7	ARG	3.4
14	r	16	ALA	3.4
19	Y	20	ALA	3.4
5	E	83	LEU	3.4
14	R	31	VAL	3.3
18	x	38	GLN	3.3
13	o	57	LYS	3.3
14	r	12	VAL	3.3
2	b	490	GLN	3.2
19	Y	37	PHE	3.2
7	h	6	TRP	3.2
14	R	24	LEU	3.1
9	J	8	ILE	3.1
6	F	12	SER	3.1
2	B	505	ARG	3.1
14	r	4	ARG	3.1
2	B	295	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
18	x	2	THR	3.1
13	o	5	LEU	3.1
20	Z	38	GLN	3.1
20	z	7	LEU	3.1
20	Z	59	PHE	3.1
14	R	10	LEU	3.0
14	R	18	TRP	3.0
14	R	13	LEU	3.0
14	R	29	LYS	3.0
2	b	502	VAL	3.0
8	I	34	ARG	3.0
2	b	85	GLY	3.0
19	y	19	ILE	3.0
16	U	8	GLU	3.0
2	b	491	VAL	2.9
20	z	3	ILE	2.9
2	B	293	ALA	2.9
18	x	40	SER	2.9
20	z	36	SER	2.9
20	z	37	LYS	2.9
20	Z	1	MET	2.9
19	Y	40	ALA	2.9
2	b	289	GLN	2.9
4	D	12	ARG	2.9
3	C	146	PHE	2.9
13	o	56	PRO	2.9
18	x	37	VAL	2.8
18	x	34	ILE	2.8
3	c	143	TYR	2.8
14	R	9	LEU	2.8
19	y	41	VAL	2.8
14	R	28	VAL	2.7
1	A	11	ALA	2.7
14	R	20	VAL	2.7
14	r	32	GLN	2.7
13	o	60	ARG	2.7
19	Y	25	ILE	2.7
13	O	57	LYS	2.7
2	B	127	ARG	2.7
18	X	3	ILE	2.7
19	y	18	VAL	2.6
2	b	295	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
8	i	34	ARG	2.6
20	Z	60	PHE	2.6
2	b	161	LEU	2.6
5	e	61	ARG	2.6
13	O	35	SER	2.6
15	t	29	ILE	2.6
9	J	6	GLY	2.6
14	r	30	GLN	2.5
20	z	30	PRO	2.5
19	y	40	ALA	2.5
3	c	25	ASN	2.5
13	O	5	LEU	2.5
11	l	3	PRO	2.5
2	b	496	TYR	2.5
13	o	207	ARG	2.4
11	l	2	GLU	2.4
5	E	3	GLY	2.4
10	k	17	ILE	2.4
14	r	17	GLY	2.4
3	C	143	TYR	2.4
13	o	62	GLU	2.4
14	R	5	VAL	2.4
13	O	87	VAL	2.4
14	R	33	LYS	2.4
20	Z	4	LEU	2.3
20	Z	39	LEU	2.3
20	z	62	VAL	2.3
19	Y	21	GLN	2.3
17	v	17	LYS	2.3
20	Z	41	PHE	2.3
5	E	84	LYS	2.3
2	b	128	THR	2.3
2	b	486	LEU	2.2
3	C	61	VAL	2.2
3	c	262	ARG	2.2
20	z	32	ASP	2.2
8	I	35	LYS	2.2
17	v	22	THR	2.2
6	f	13	TYR	2.2
8	i	36	ASP	2.2
7	h	10	ILE	2.2
7	h	41	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
13	o	63	ALA	2.2
20	Z	30	PRO	2.2
20	z	60	PHE	2.1
14	r	8	VAL	2.1
2	b	506	ARG	2.1
3	C	57	ALA	2.1
15	T	29	ILE	2.1
1	a	146	ALA	2.1
13	O	37	THR	2.1
14	R	34	LEU	2.0
20	z	34	ASP	2.0
13	O	246	ALA	2.0
4	d	239	GLN	2.0
12	M	33	GLN	2.0
2	B	486	LEU	2.0
3	c	261	ARG	2.0
2	B	487	SER	2.0
5	e	83	LEU	2.0
5	e	82	GLN	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
12	FME	M	1	10/11	0.95	0.12	40,53,69,79	0
15	FME	T	1	10/11	0.95	0.09	29,44,67,67	0
12	FME	m	1	10/11	0.95	0.10	33,47,65,76	0
8	FME	I	1	10/11	0.95	0.12	40,48,64,66	0
8	FME	i	1	10/11	0.96	0.18	40,50,65,66	0
15	FME	t	1	10/11	0.96	0.09	28,43,73,73	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	STE	E	102	12/20	0.68	0.42	46,78,92,94	0
31	STE	a	414	12/20	0.71	0.26	40,65,71,75	0
31	STE	b	624	20/20	0.75	0.21	41,60,75,89	0
31	STE	B	627	15/20	0.76	0.16	36,61,74,77	0
31	STE	B	626	16/20	0.76	0.29	35,58,78,79	0
31	STE	H	104	18/20	0.77	0.27	44,73,89,94	0
26	PL9	A	409	55/55	0.78	0.31	47,68,94,97	0
31	STE	j	101	12/20	0.78	0.17	42,56,74,75	0
31	STE	c	501	12/20	0.79	0.19	54,68,87,89	0
26	PL9	a	409	55/55	0.79	0.25	47,74,93,96	0
24	BCR	H	102	40/40	0.80	0.16	30,50,66,75	0
31	STE	C	519	16/20	0.80	0.17	42,58,73,77	0
27	LMG	c	522	48/55	0.80	0.23	46,80,104,108	0
31	STE	b	625	10/20	0.81	0.22	44,53,61,73	0
33	LHG	E	101	49/49	0.81	0.25	50,83,110,126	0
28	SQD	a	412	36/54	0.81	0.19	29,63,90,97	0
33	LHG	e	101	42/49	0.81	0.27	65,87,116,127	0
27	LMG	D	411	33/55	0.81	0.19	34,56,84,89	0
31	STE	I	101	15/20	0.82	0.17	37,55,73,76	0
27	LMG	a	415	55/55	0.82	0.17	34,58,80,92	0
31	STE	B	620	17/20	0.82	0.16	32,50,63,71	0
22	CLA	b	601	65/65	0.82	0.17	43,68,89,92	0
24	BCR	h	101	40/40	0.82	0.15	35,54,73,79	0
31	STE	m	101	18/20	0.83	0.13	34,51,78,79	0
31	STE	a	413	10/20	0.83	0.20	38,61,67,68	0
27	LMG	b	623	55/55	0.84	0.27	42,70,95,101	0
31	STE	d	413	20/20	0.84	0.21	42,57,76,84	0
22	CLA	C	512	65/65	0.84	0.17	35,55,82,95	0
31	STE	B	624	12/20	0.84	0.11	32,48,63,76	0
29	DGD	A	413	66/66	0.84	0.18	44,62,78,99	0
31	STE	c	521	20/20	0.85	0.20	37,55,93,103	0
31	STE	m	102	12/20	0.85	0.19	46,61,76,76	0
22	CLA	c	514	65/65	0.85	0.20	39,67,109,116	0
31	STE	b	626	14/20	0.85	0.22	51,65,84,88	0
31	STE	T	102	15/20	0.85	0.20	44,59,83,85	0
24	BCR	K	102	40/40	0.85	0.13	33,53,68,74	0
31	STE	B	623	14/20	0.86	0.13	36,47,56,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	c	513	65/65	0.86	0.16	38,56,91,106	0
28	SQD	A	412	39/54	0.86	0.19	42,61,90,93	0
22	CLA	H	101	65/65	0.86	0.16	33,63,91,110	0
31	STE	b	627	20/20	0.86	0.16	38,64,84,90	0
28	SQD	L	101	49/54	0.87	0.14	38,60,89,107	0
24	BCR	K	101	40/40	0.87	0.16	40,58,75,82	0
28	SQD	B	622	54/54	0.87	0.14	37,61,91,101	0
31	STE	d	411	16/20	0.87	0.16	45,62,78,83	0
31	STE	Z	101	8/20	0.88	0.14	50,61,70,70	0
22	CLA	C	513	65/65	0.88	0.18	38,64,97,109	0
31	STE	b	622	20/20	0.88	0.24	36,54,79,85	0
31	STE	B	625	18/20	0.88	0.11	40,58,76,83	0
31	STE	M	102	15/20	0.88	0.17	32,48,69,74	0
24	BCR	k	102	40/40	0.88	0.18	40,55,67,68	0
31	STE	D	413	20/20	0.88	0.15	34,54,71,79	0
31	STE	J	101	12/20	0.89	0.11	45,59,69,77	0
28	SQD	f	102	41/54	0.89	0.20	55,91,113,119	0
31	STE	d	412	17/20	0.89	0.14	41,56,67,74	0
31	STE	B	601	12/20	0.89	0.49	51,67,78,86	0
27	LMG	Y	101	48/55	0.89	0.14	34,68,86,99	0
27	LMG	c	523	49/55	0.89	0.14	30,56,82,98	0
24	BCR	k	101	40/40	0.89	0.13	42,60,81,85	0
22	CLA	c	503	65/65	0.90	0.16	29,41,62,66	0
27	LMG	A	410	48/55	0.90	0.14	38,57,72,87	0
31	STE	b	620	16/20	0.90	0.14	35,46,64,71	0
31	STE	M	103	10/20	0.90	0.13	34,47,64,70	0
31	STE	C	520	12/20	0.90	0.10	34,46,57,58	0
22	CLA	C	502	65/65	0.90	0.14	26,42,52,53	0
22	CLA	d	404	65/65	0.90	0.17	32,49,89,106	0
27	LMG	c	520	37/55	0.90	0.16	40,67,80,83	0
22	CLA	c	509	64/65	0.91	0.14	27,46,86,103	0
24	BCR	F	101	40/40	0.91	0.12	21,44,82,90	0
22	CLA	b	616	60/65	0.91	0.12	24,42,86,88	0
22	CLA	C	507	65/65	0.91	0.14	20,40,56,66	0
31	STE	C	518	12/20	0.91	0.10	41,55,62,66	0
27	LMG	M	101	51/55	0.91	0.12	31,48,72,90	0
27	LMG	b	621	51/55	0.91	0.12	32,53,76,97	0
22	CLA	a	405	65/65	0.91	0.14	18,35,82,91	0
24	BCR	d	405	40/40	0.91	0.12	28,54,85,95	0
22	CLA	D	405	65/65	0.91	0.13	22,42,107,119	0
24	BCR	c	515	40/40	0.91	0.15	41,62,76,77	0
24	BCR	C	514	40/40	0.91	0.11	23,38,55,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	DGD	C	516	62/66	0.91	0.13	34,51,97,119	0
24	BCR	B	619	40/40	0.92	0.09	25,42,61,72	0
22	CLA	b	615	65/65	0.92	0.13	24,39,59,63	0
22	CLA	c	506	65/65	0.92	0.16	24,40,64,70	0
24	BCR	b	619	40/40	0.92	0.11	31,47,63,67	0
27	LMG	B	621	28/55	0.92	0.14	35,51,65,73	0
22	CLA	b	602	65/65	0.92	0.15	26,44,65,72	0
27	LMG	D	407	51/55	0.92	0.16	27,56,86,93	0
28	SQD	D	408	36/54	0.92	0.17	46,75,89,100	0
22	CLA	B	616	60/65	0.92	0.15	25,39,94,110	0
24	BCR	K	103	40/40	0.92	0.17	36,54,67,69	0
22	CLA	c	512	65/65	0.92	0.12	39,52,65,74	0
29	DGD	c	518	62/66	0.93	0.11	33,50,90,96	0
22	CLA	c	508	65/65	0.93	0.14	28,44,59,63	0
22	CLA	c	504	65/65	0.93	0.14	28,41,54,58	0
29	DGD	h	102	62/66	0.93	0.11	29,48,65,68	0
28	SQD	a	411	54/54	0.93	0.15	39,62,94,96	0
22	CLA	C	506	65/65	0.93	0.12	28,45,83,99	0
22	CLA	c	507	65/65	0.93	0.13	29,48,102,109	0
22	CLA	C	505	65/65	0.93	0.16	19,39,71,77	0
24	BCR	T	101	40/40	0.93	0.10	23,39,52,52	0
24	BCR	B	618	40/40	0.93	0.10	23,39,50,52	0
29	DGD	H	103	62/66	0.93	0.11	29,46,61,73	0
22	CLA	C	510	65/65	0.93	0.14	27,46,62,66	0
22	CLA	B	615	65/65	0.93	0.12	21,38,60,69	0
22	CLA	b	609	65/65	0.93	0.13	27,43,64,74	0
24	BCR	c	516	40/40	0.93	0.11	22,44,60,72	0
22	CLA	c	511	65/65	0.93	0.15	29,47,64,68	0
22	CLA	B	614	65/65	0.94	0.15	20,36,75,87	0
22	CLA	c	510	65/65	0.94	0.17	33,47,70,77	0
24	BCR	A	406	40/40	0.94	0.09	23,35,43,47	0
22	CLA	B	613	65/65	0.94	0.14	17,31,71,73	0
22	CLA	b	608	65/65	0.94	0.15	25,42,60,69	0
24	BCR	b	618	40/40	0.94	0.10	22,38,51,52	0
22	CLA	C	509	65/65	0.94	0.17	25,46,62,69	0
29	DGD	C	517	62/66	0.94	0.11	26,46,77,87	0
22	CLA	a	410	65/65	0.94	0.12	17,29,48,54	0
22	CLA	b	612	65/65	0.94	0.17	15,33,48,57	0
27	LMG	d	410	44/55	0.94	0.13	31,51,89,104	0
24	BCR	t	101	40/40	0.94	0.09	23,38,51,52	0
24	BCR	b	617	40/40	0.94	0.11	25,41,54,59	0
22	CLA	c	505	60/65	0.94	0.11	32,45,76,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	511	65/65	0.94	0.11	27,49,66,77	0
22	CLA	b	610	65/65	0.94	0.18	23,36,50,56	0
22	CLA	C	503	65/65	0.94	0.13	32,42,51,61	0
22	CLA	b	614	65/65	0.94	0.12	21,38,78,86	0
22	CLA	B	606	65/65	0.94	0.10	23,36,69,86	0
22	CLA	B	609	65/65	0.94	0.13	24,39,57,69	0
24	BCR	a	406	40/40	0.94	0.09	19,32,50,55	0
22	CLA	A	403	65/65	0.94	0.14	21,34,97,110	0
29	DGD	c	519	62/66	0.94	0.13	28,54,83,91	0
22	CLA	B	604	65/65	0.94	0.12	19,32,79,84	0
29	DGD	C	515	62/66	0.94	0.12	21,40,73,87	0
26	PL9	D	406	55/55	0.94	0.10	21,34,49,54	0
22	CLA	C	504	59/65	0.94	0.12	27,41,81,83	0
22	CLA	A	405	54/65	0.94	0.11	18,31,66,72	0
22	CLA	a	403	65/65	0.94	0.14	25,40,97,106	0
22	CLA	b	606	65/65	0.94	0.11	22,37,73,77	0
22	CLA	B	602	65/65	0.94	0.15	20,36,55,66	0
22	CLA	b	613	65/65	0.94	0.14	17,34,73,87	0
22	CLA	C	508	65/65	0.94	0.11	25,42,97,107	0
26	PL9	d	406	55/55	0.95	0.10	22,33,42,53	0
33	LHG	d	407	49/49	0.95	0.12	33,49,76,80	0
29	DGD	c	517	62/66	0.95	0.11	24,42,84,94	0
22	CLA	C	501	65/65	0.95	0.12	19,36,51,56	0
22	CLA	b	611	65/65	0.95	0.13	19,34,53,61	0
22	CLA	B	605	65/65	0.95	0.14	19,31,47,52	0
23	PHO	A	404	64/64	0.95	0.10	18,28,40,48	0
22	CLA	D	404	65/65	0.95	0.10	19,28,52,62	0
22	CLA	B	603	65/65	0.95	0.14	15,32,63,67	0
22	CLA	B	612	65/65	0.95	0.14	19,31,47,56	0
22	CLA	d	403	65/65	0.95	0.11	19,34,54,65	0
22	CLA	c	502	65/65	0.95	0.13	26,41,53,57	0
22	CLA	b	605	65/65	0.95	0.11	21,34,49,53	0
33	LHG	D	410	47/49	0.95	0.12	24,46,82,99	0
24	BCR	B	617	40/40	0.95	0.11	24,38,59,60	0
34	HEC	F	102	43/43	0.95	0.12	37,48,64,66	0
22	CLA	D	403	65/65	0.95	0.12	15,29,52,61	0
22	CLA	B	610	65/65	0.95	0.15	18,33,46,50	0
33	LHG	d	409	39/49	0.95	0.10	29,45,72,80	0
22	CLA	B	608	65/65	0.95	0.12	20,34,56,61	0
22	CLA	b	604	65/65	0.95	0.12	20,33,81,91	0
23	PHO	a	404	64/64	0.95	0.13	19,29,40,44	0
22	CLA	B	611	65/65	0.95	0.13	19,30,46,50	0

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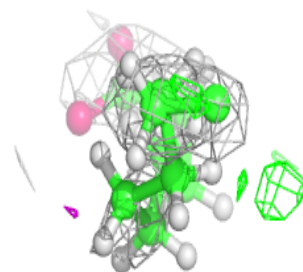
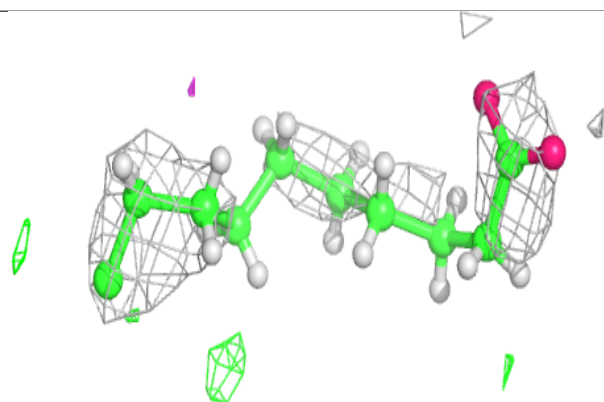
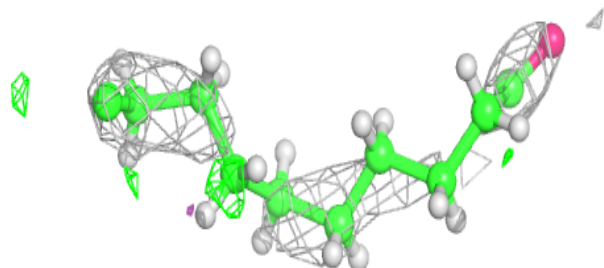
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	SQD	A	411	52/54	0.95	0.14	34,59,84,88	0
22	CLA	b	603	65/65	0.96	0.12	18,36,65,76	0
23	PHO	D	401	64/64	0.96	0.13	21,32,44,48	0
33	LHG	L	102	49/49	0.96	0.10	26,41,53,60	0
33	LHG	D	412	49/49	0.96	0.11	30,44,65,76	0
23	PHO	d	401	64/64	0.96	0.11	20,37,47,61	0
33	LHG	l	101	49/49	0.96	0.10	26,45,55,64	0
22	CLA	A	402	65/65	0.96	0.10	16,26,46,49	0
22	CLA	a	402	65/65	0.96	0.10	19,29,46,56	0
22	CLA	B	607	65/65	0.96	0.10	14,34,62,66	0
22	CLA	b	607	65/65	0.96	0.12	18,35,69,78	0
34	HEC	f	101	43/43	0.96	0.12	42,58,81,84	0
34	HEC	v	201	43/43	0.97	0.12	27,37,50,51	0
34	HEC	V	201	43/43	0.97	0.13	19,35,43,44	0
33	LHG	d	408	49/49	0.97	0.09	23,42,57,68	0
33	LHG	D	409	49/49	0.97	0.09	26,41,53,56	0
25	CL	A	407	1/1	0.98	0.06	29,29,29,29	0
32	BCT	d	402	4/4	0.98	0.17	31,35,44,53	0
32	BCT	D	402	4/4	0.98	0.17	22,26,32,36	0
21	FE2	A	401	1/1	0.99	0.10	26,26,26,26	0
30	OEX	A	414	10/10	0.99	0.11	22,26,28,29	0
25	CL	A	408	1/1	0.99	0.03	30,30,30,30	0
30	OEX	a	416	10/10	0.99	0.12	23,26,30,31	0
25	CL	a	408	1/1	0.99	0.05	28,28,28,28	0
21	FE2	a	401	1/1	0.99	0.08	34,34,34,34	0
25	CL	a	407	1/1	0.99	0.02	28,28,28,28	0

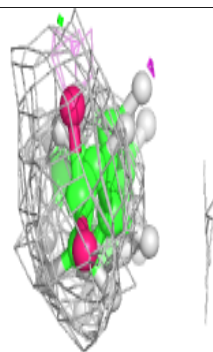
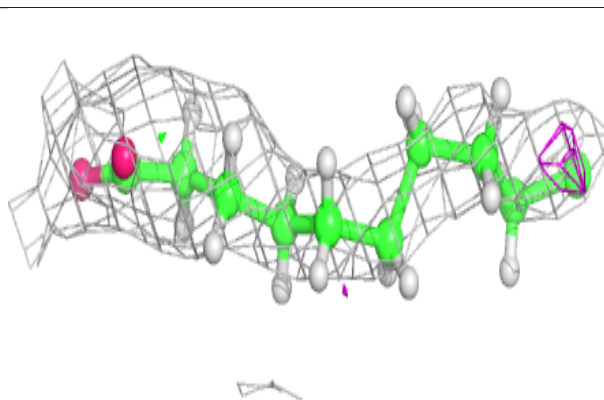
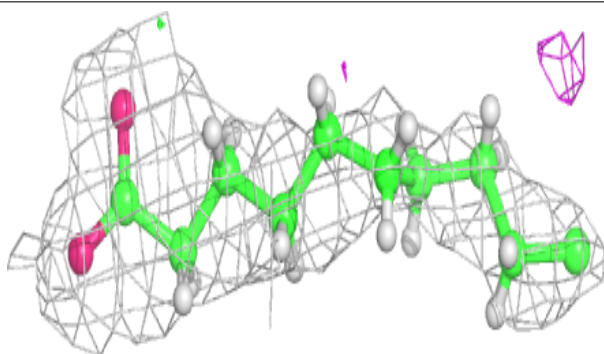
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE E 102:

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

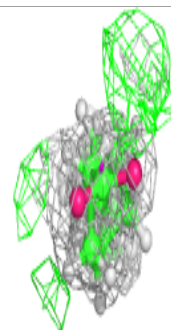
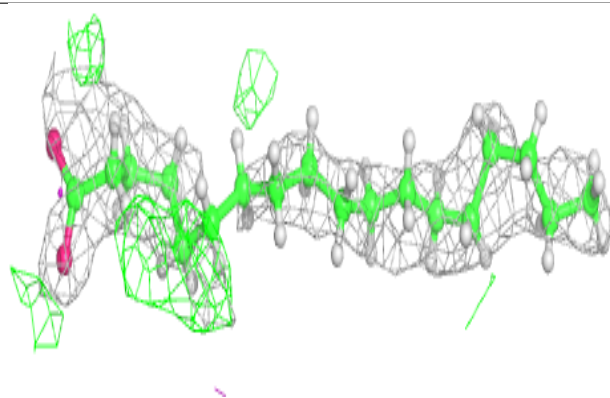
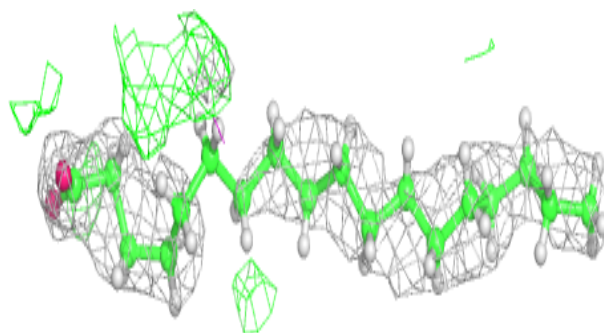
**Electron density around STE a 414:**

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

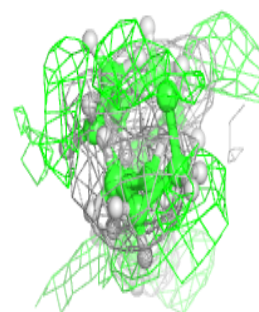
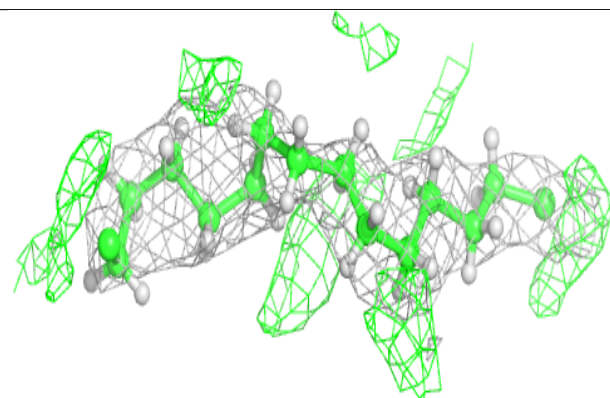
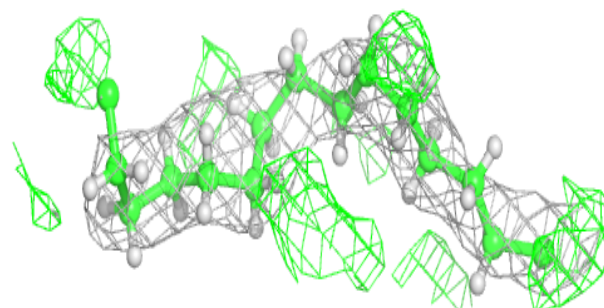


Electron density around STE b 624:

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

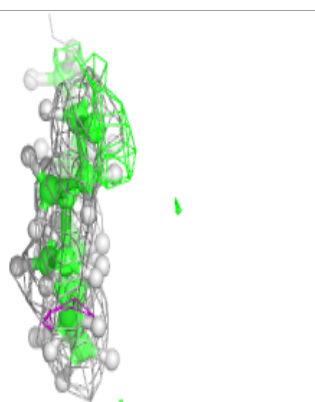
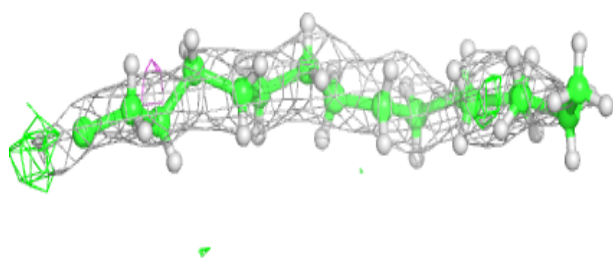
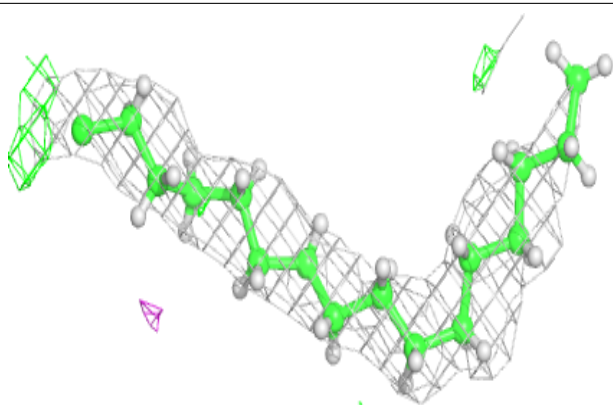
**Electron density around STE B 627:**

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

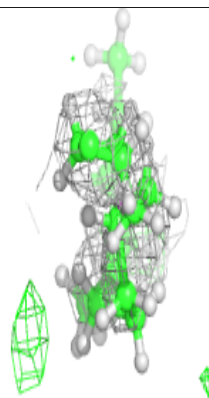
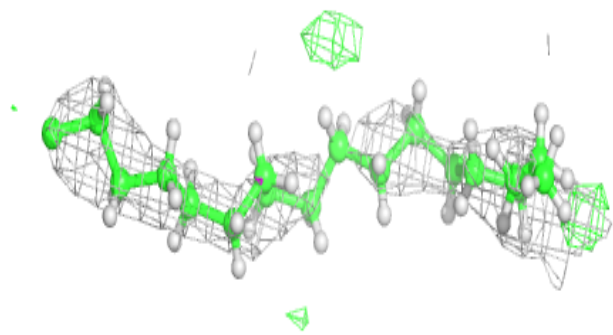
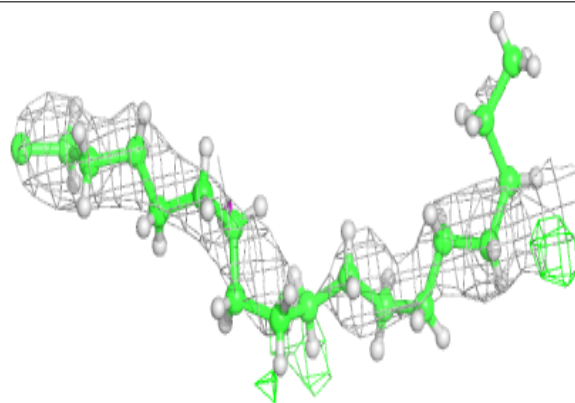


Electron density around STE B 626:

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

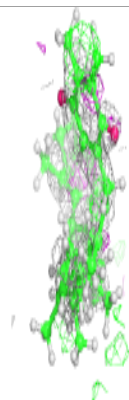
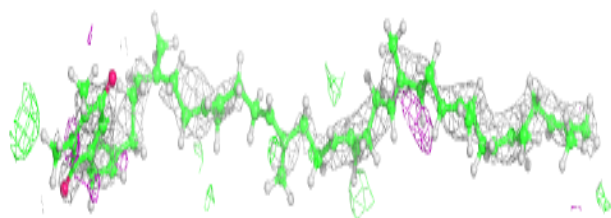
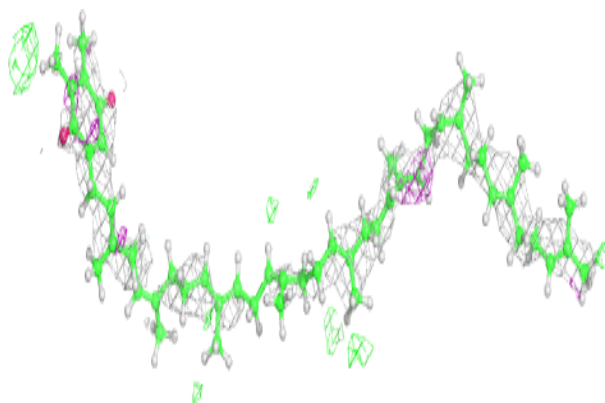
**Electron density around STE H 104:**

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

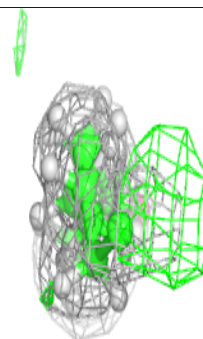
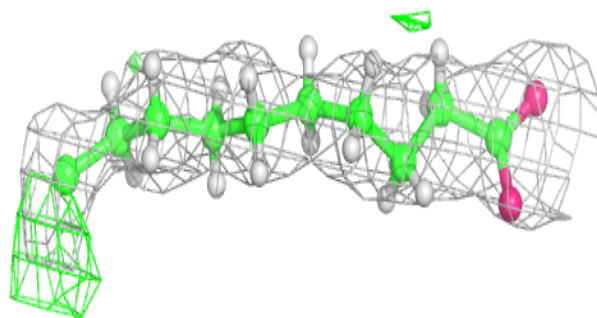
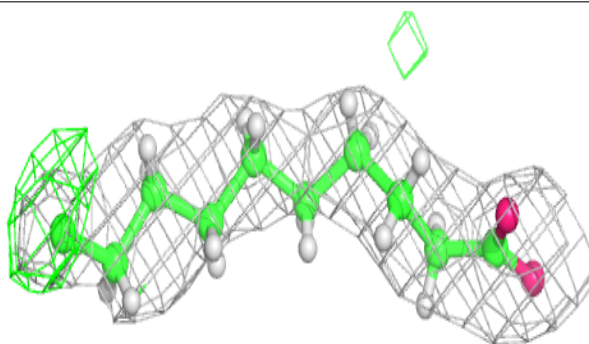


Electron density around PL9 A 409:

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

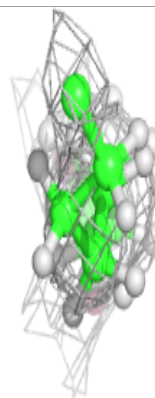
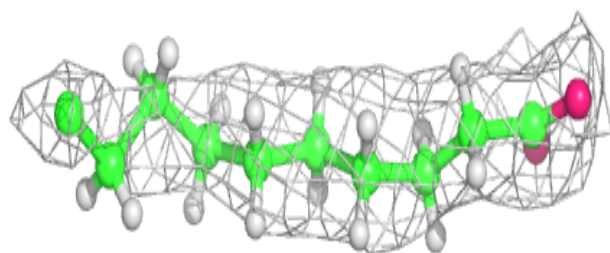
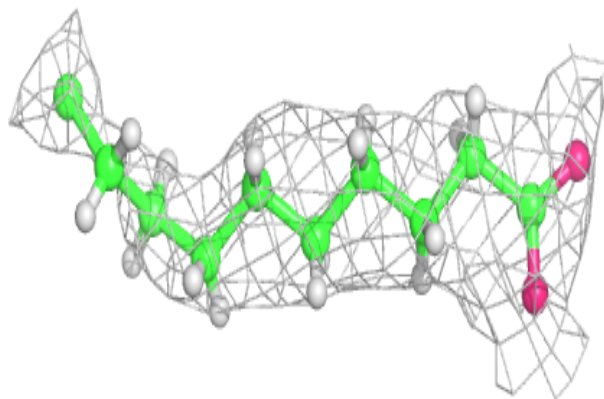
**Electron density around STE j 101:**

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

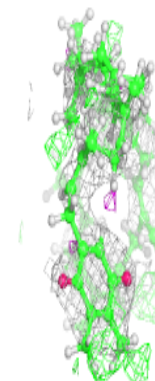
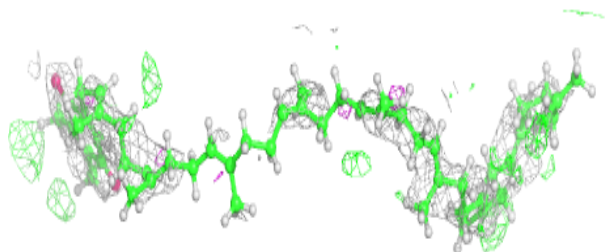
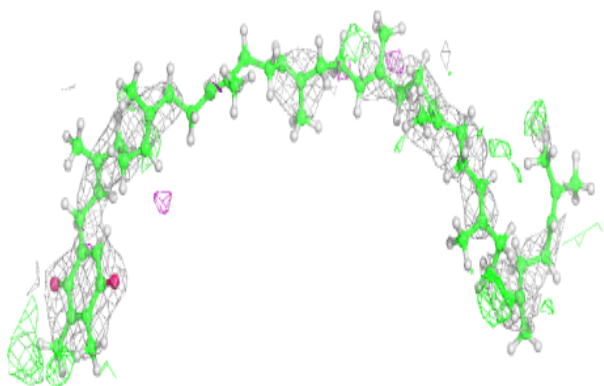


Electron density around STE c 501:

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

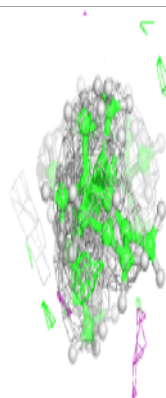
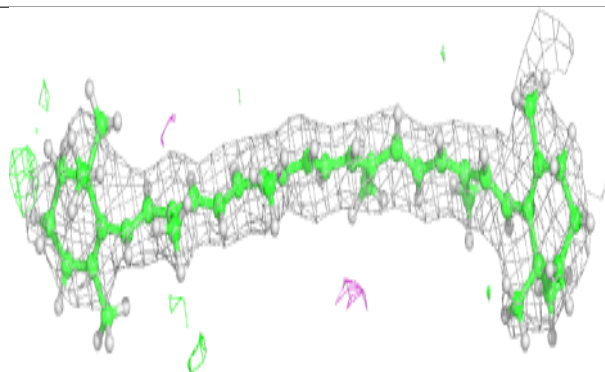
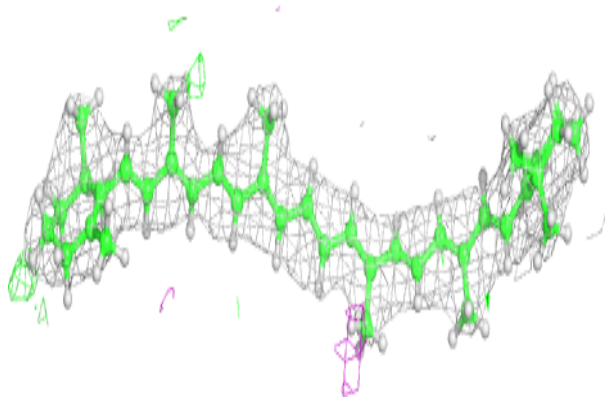
**Electron density around PL9 a 409:**

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

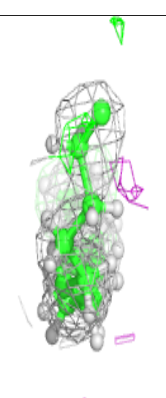
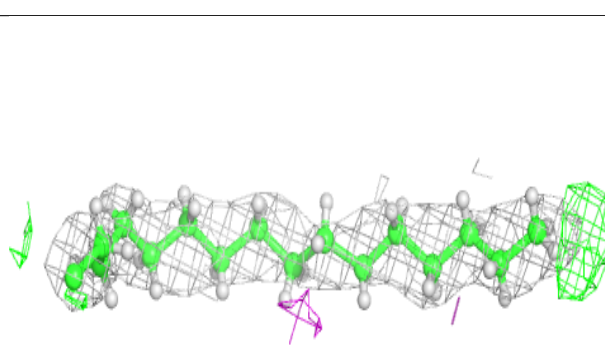
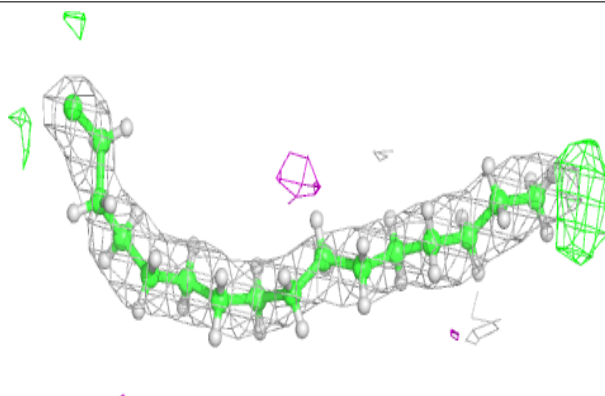


Electron density around BCR H 102:

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

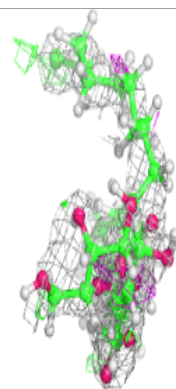
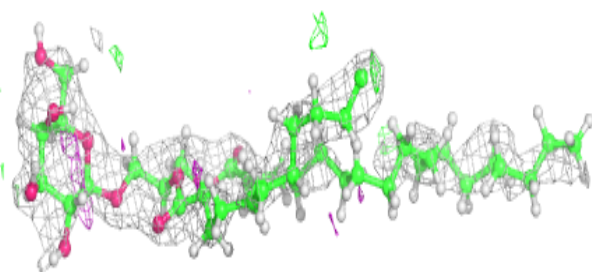
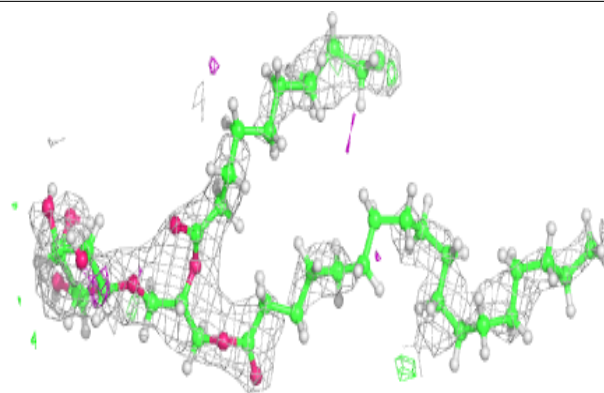
**Electron density around STE C 519:**

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

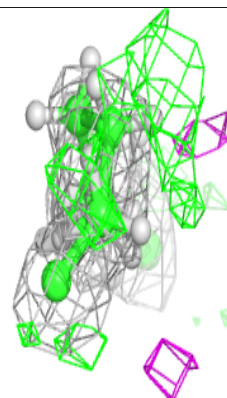
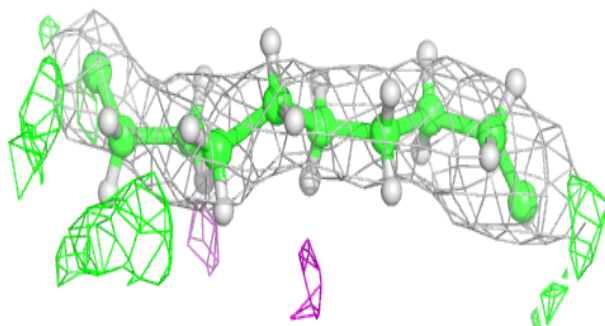
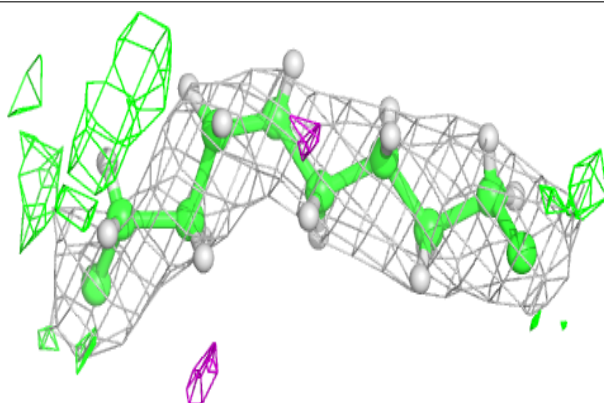


Electron density around LMG c 522:

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

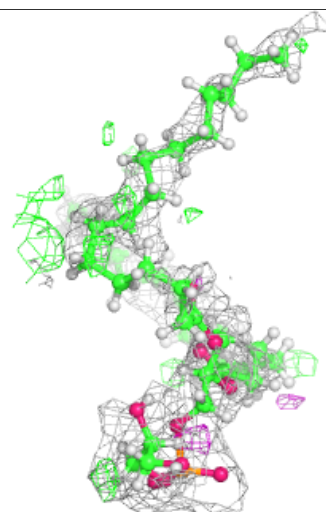
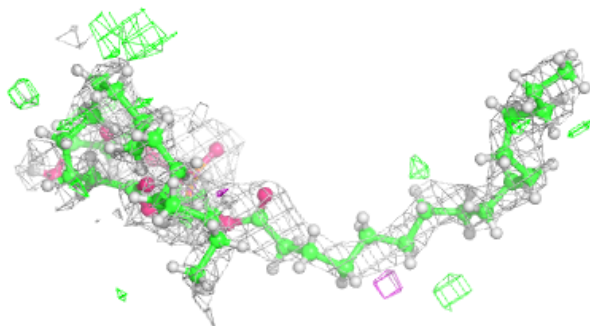
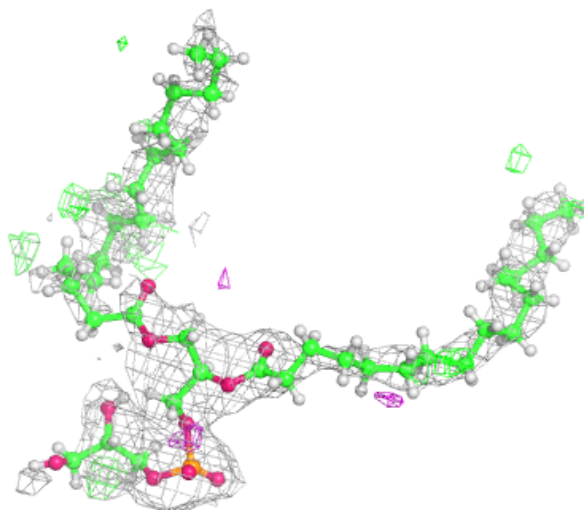
**Electron density around STE b 625:**

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



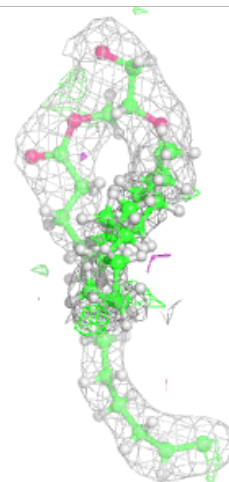
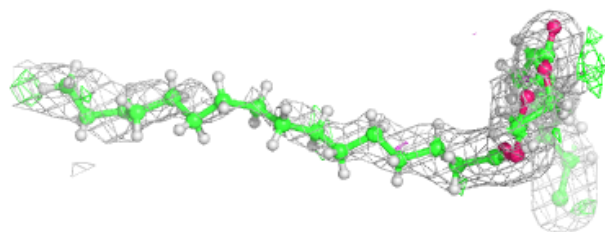
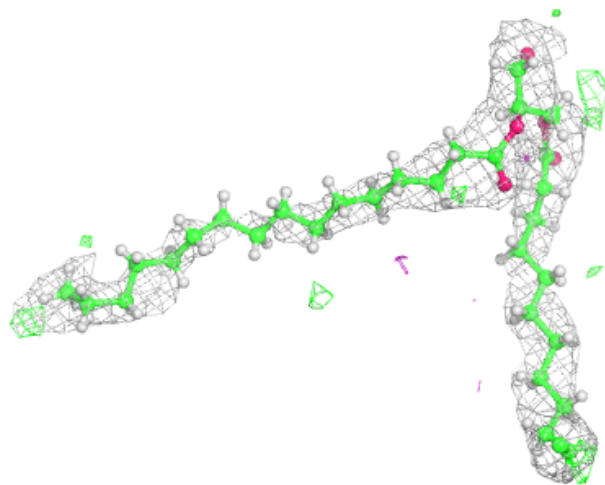
Electron density around LHG E 101:

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



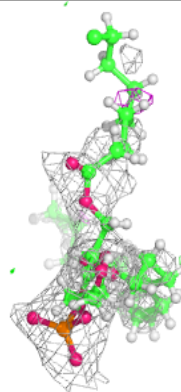
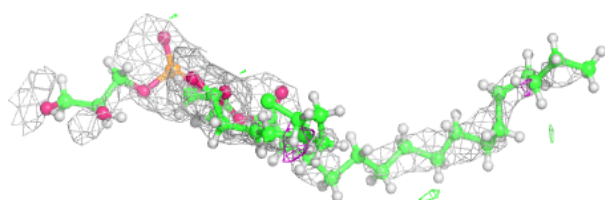
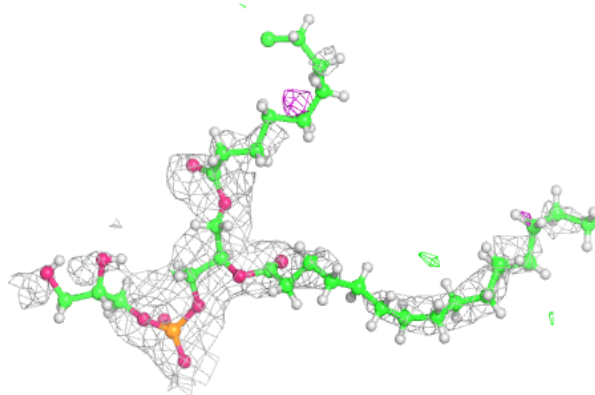
Electron density around SQD a 412:

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

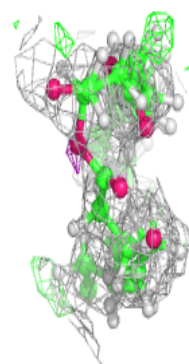
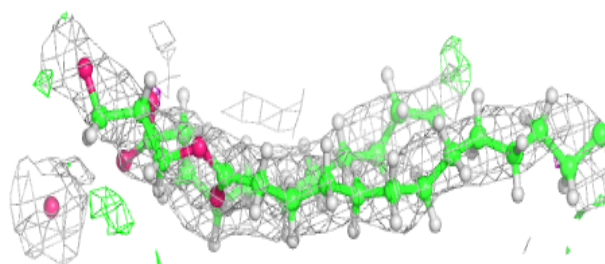
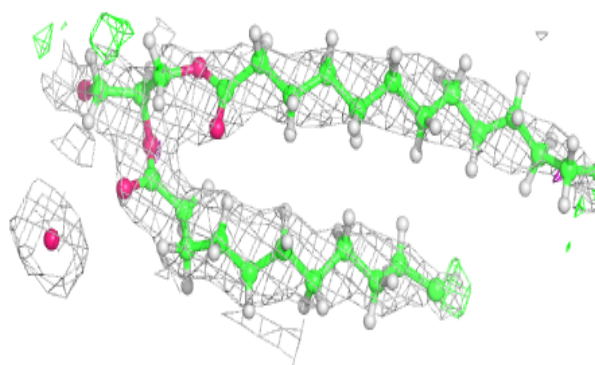


Electron density around LHG e 101:

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

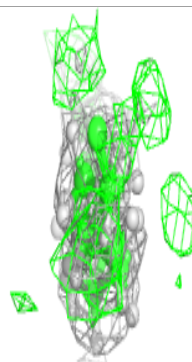
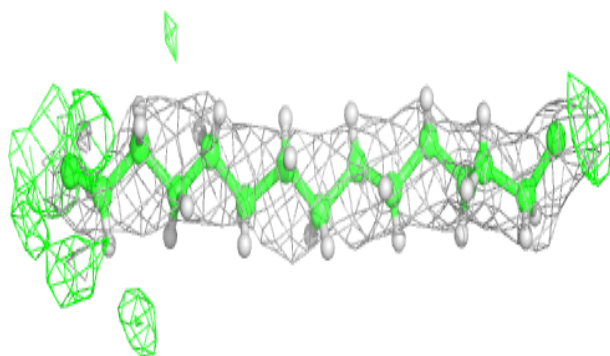
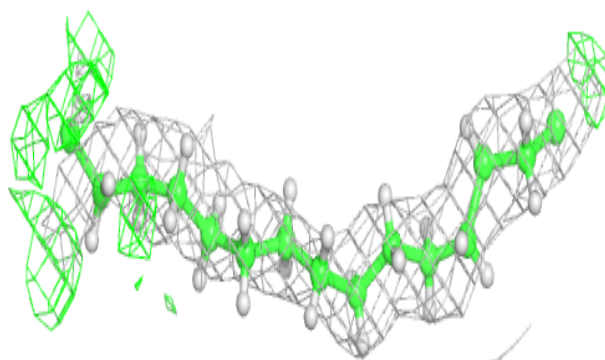
**Electron density around LMG D 411:**

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

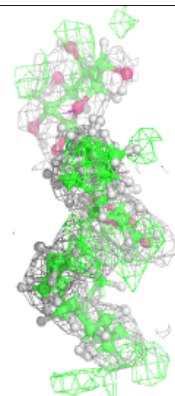
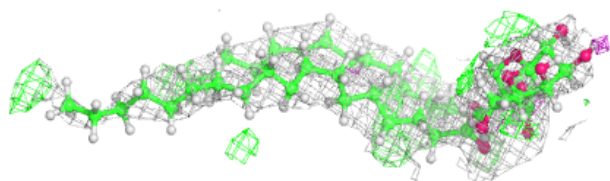
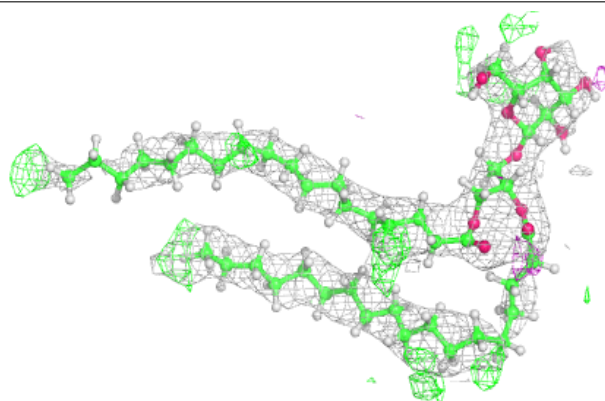


Electron density around STE I 101:

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

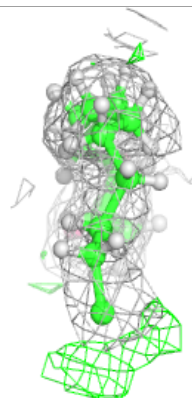
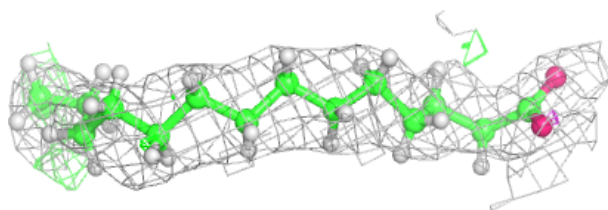
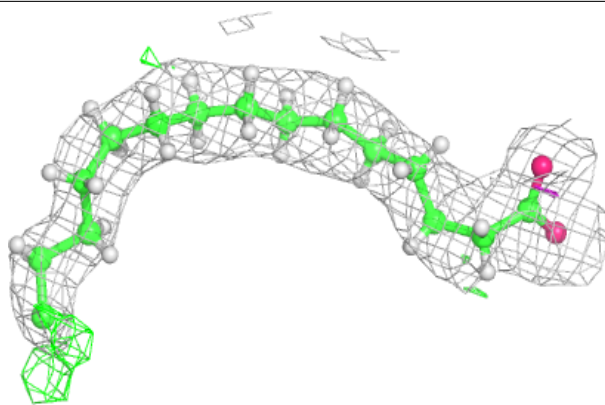
**Electron density around LMG a 415:**

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

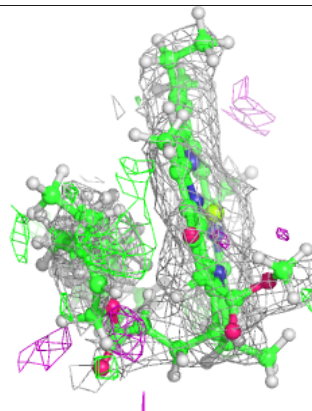
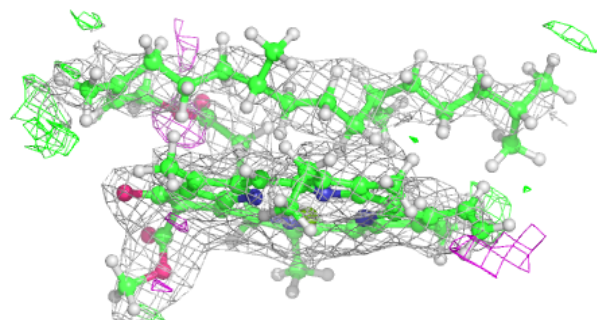
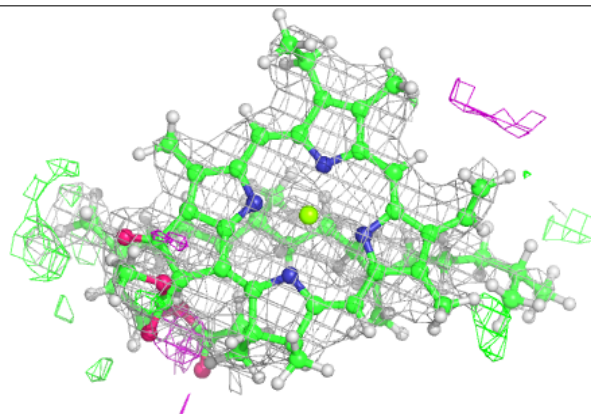


Electron density around STE B 620:

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

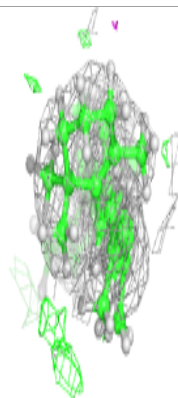
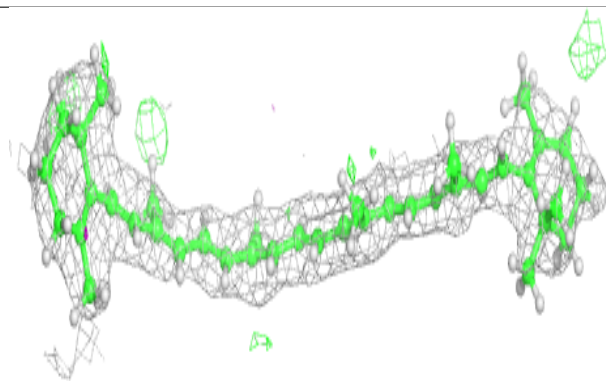
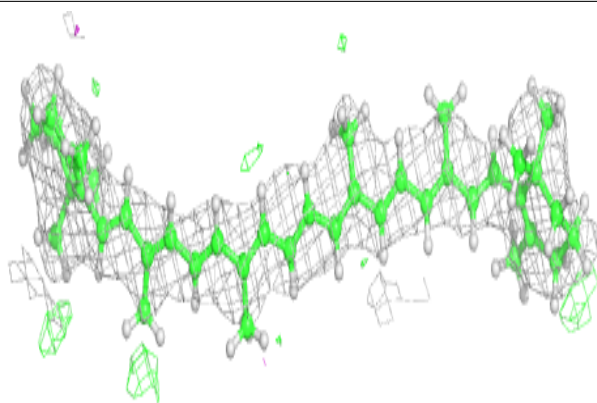
**Electron density around CLA b 601:**

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

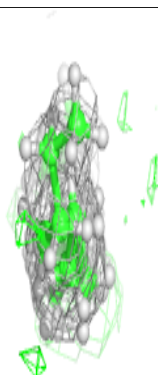
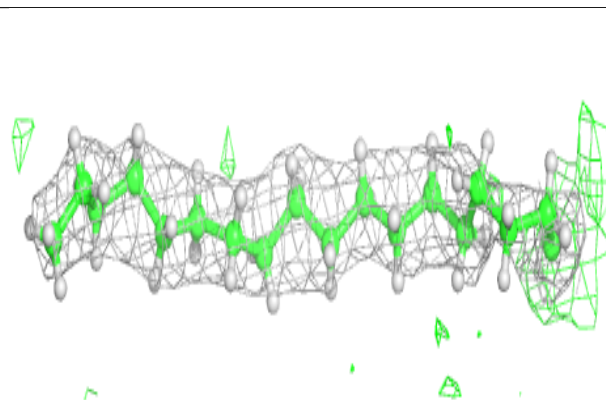
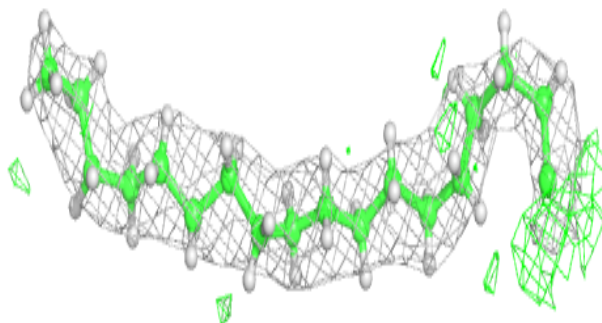


Electron density around BCR h 101:

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

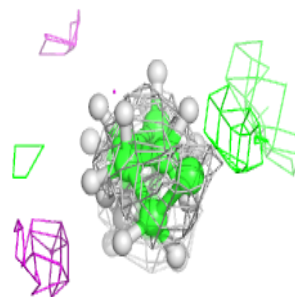
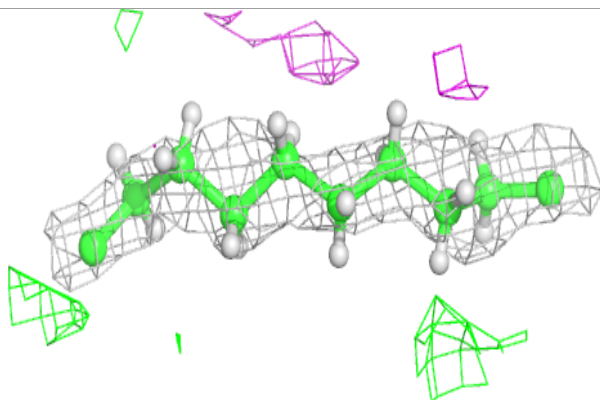
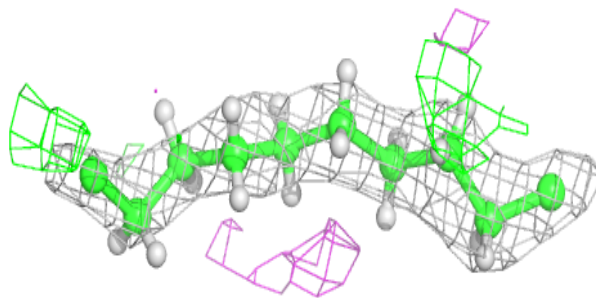
**Electron density around STE m 101:**

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

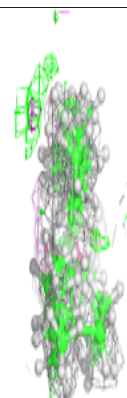
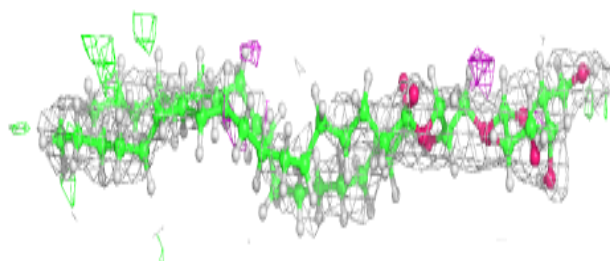
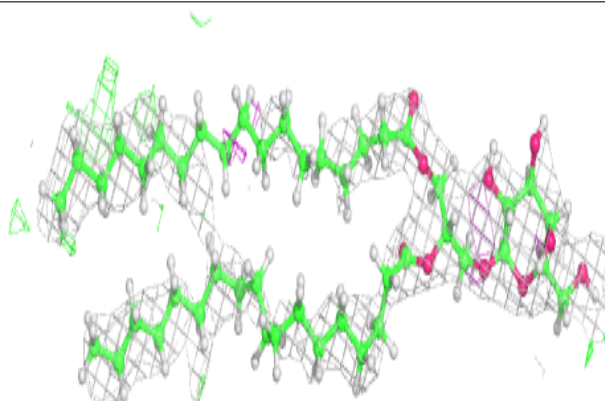


Electron density around STE a 413:

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

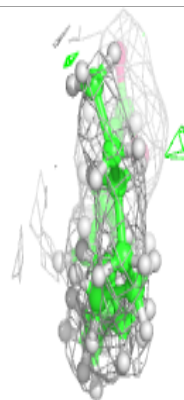
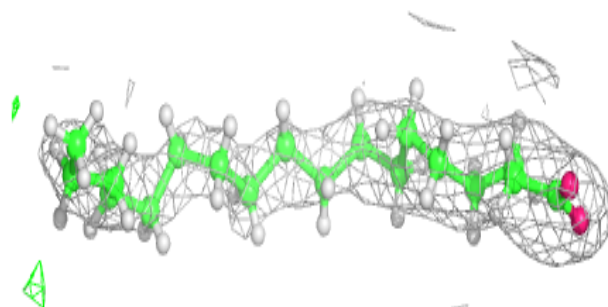
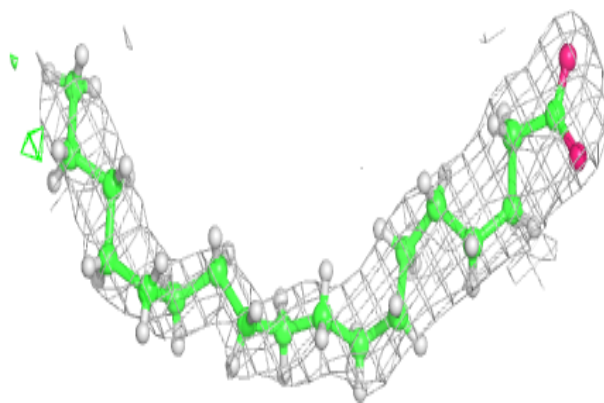
**Electron density around LMG b 623:**

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



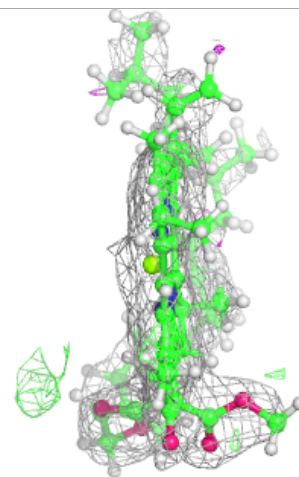
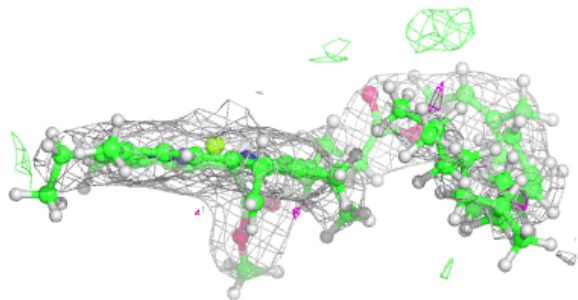
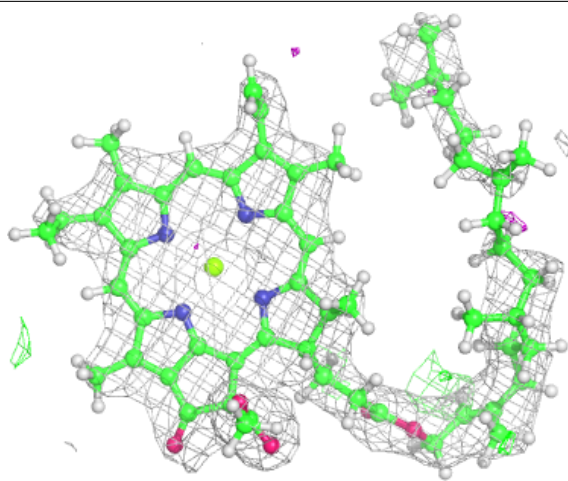
Electron density around STE d 413:

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



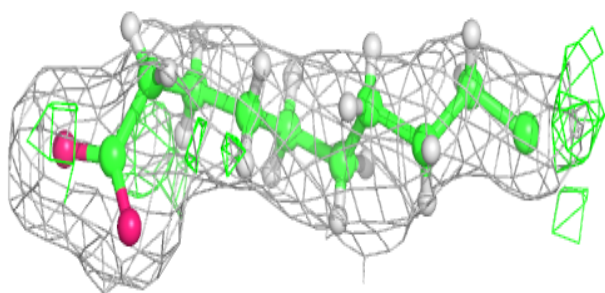
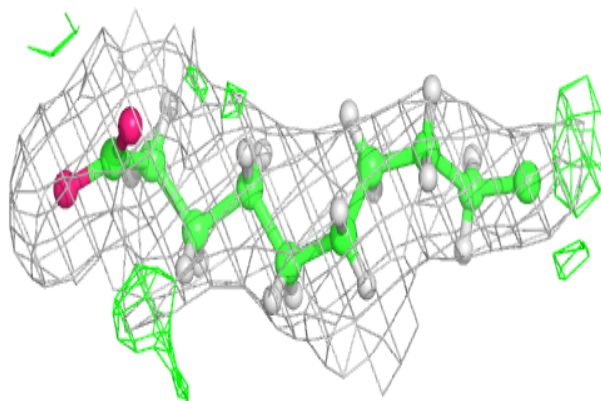
Electron density around CLA C 512:

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

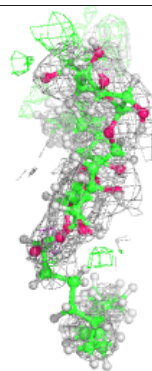
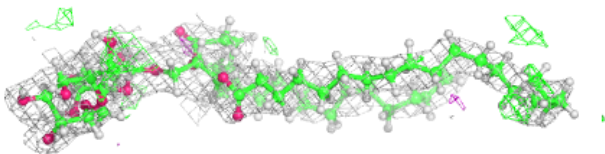
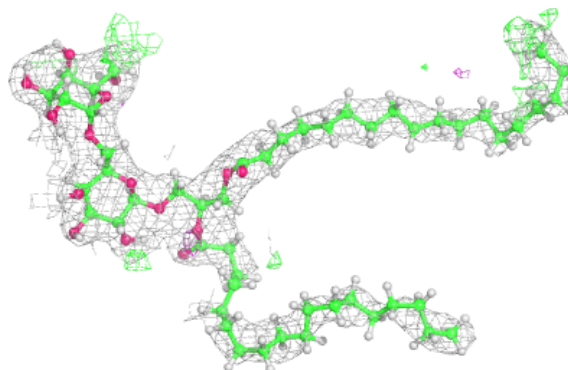


Electron density around STE B 624:

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

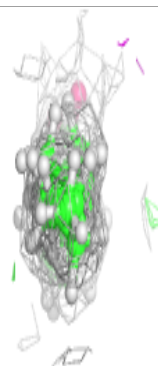
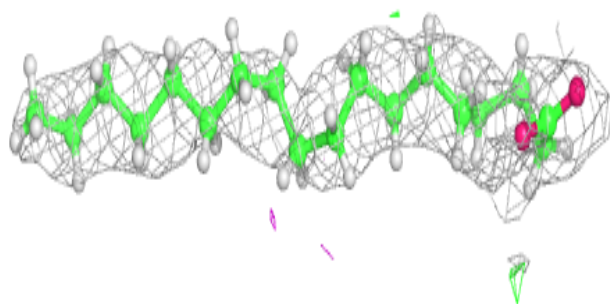
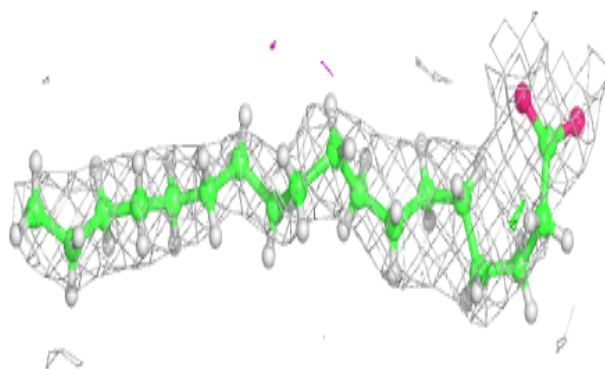
**Electron density around DGD A 413:**

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

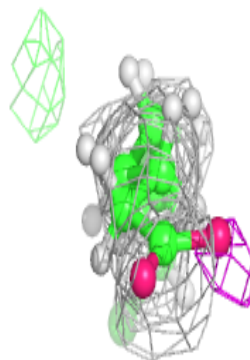
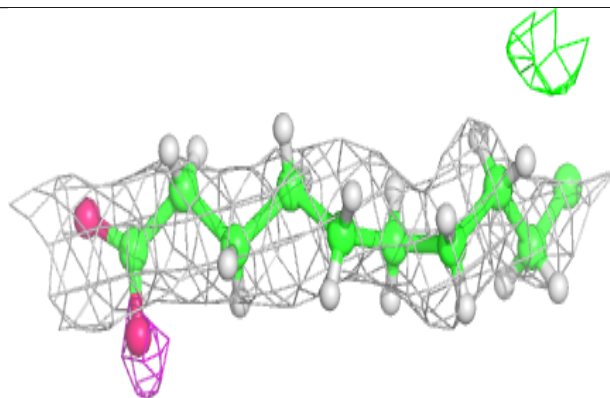
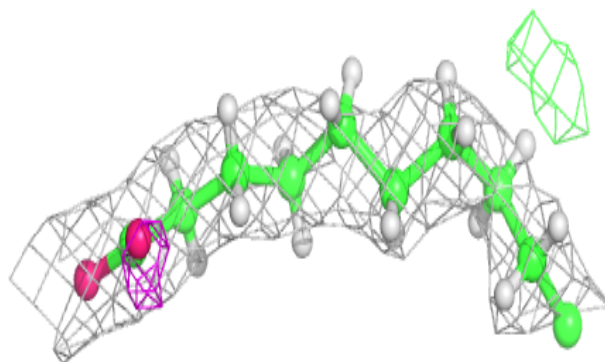


Electron density around STE c 521:

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

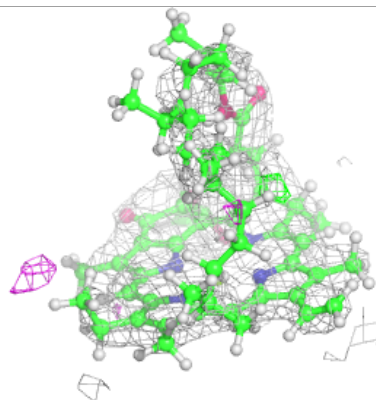
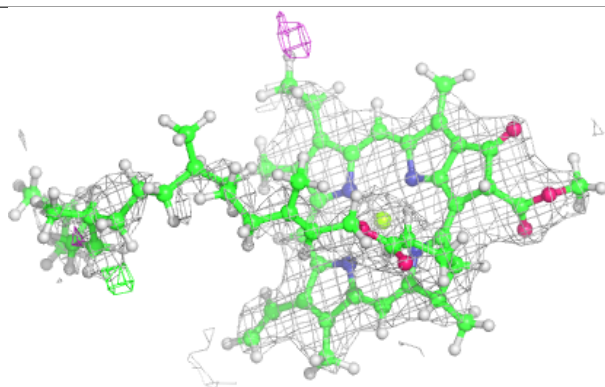
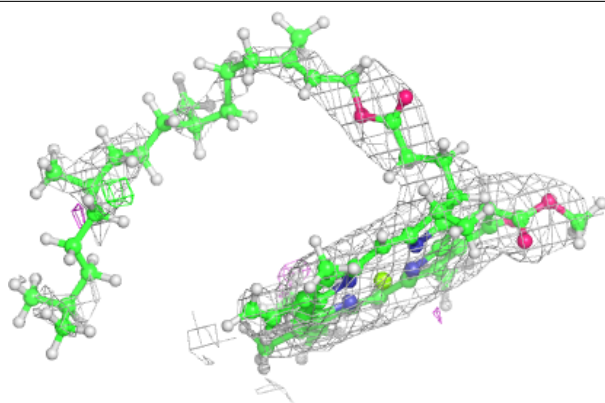
**Electron density around STE m 102:**

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

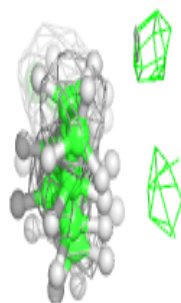
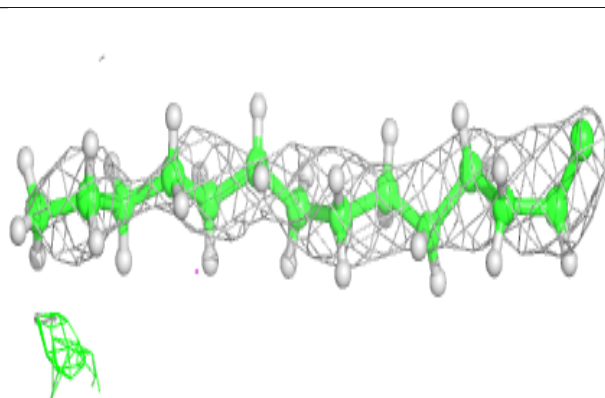
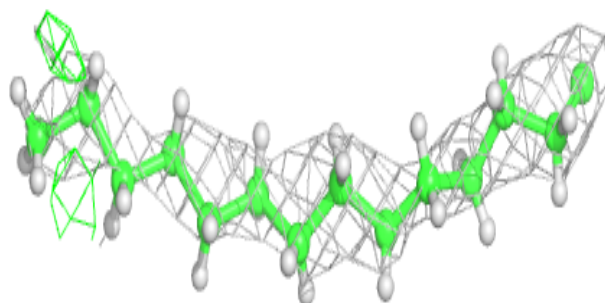


Electron density around CLA c 514:

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

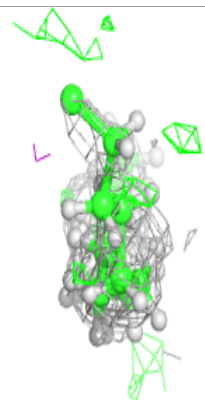
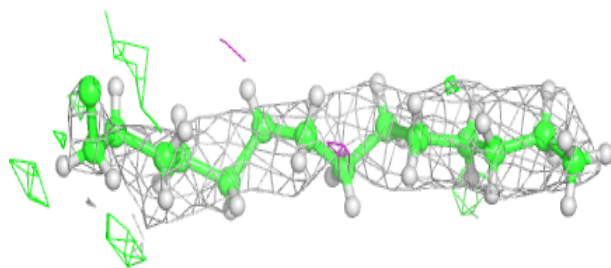
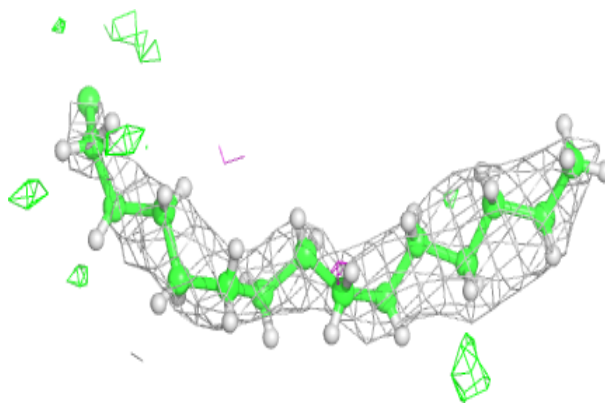
**Electron density around STE b 626:**

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

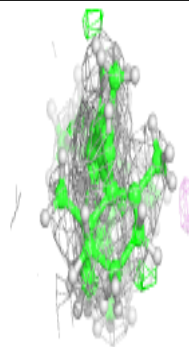
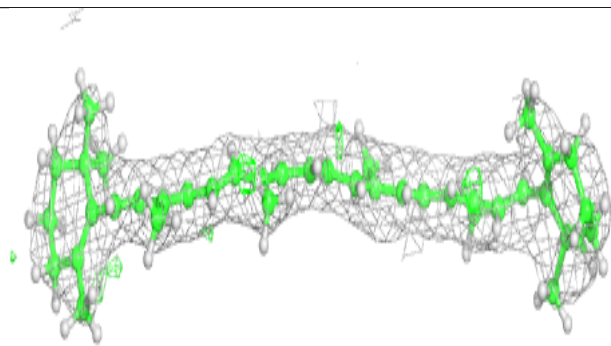
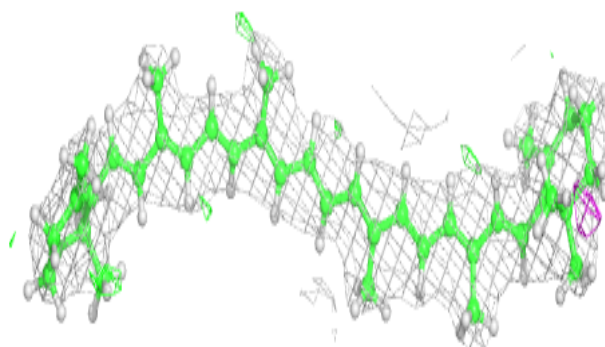


Electron density around STE T 102:

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

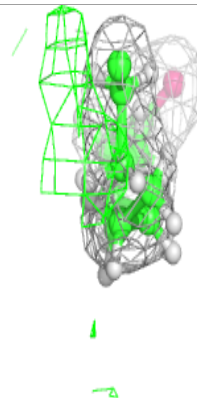
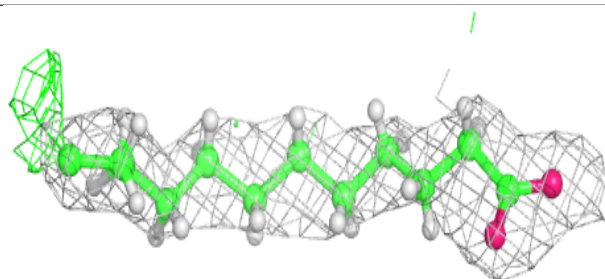
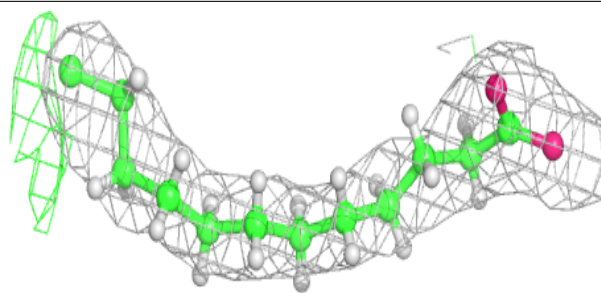
**Electron density around BCR K 102:**

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



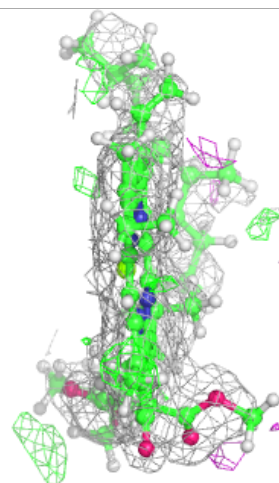
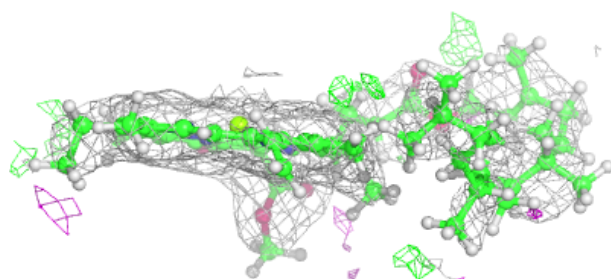
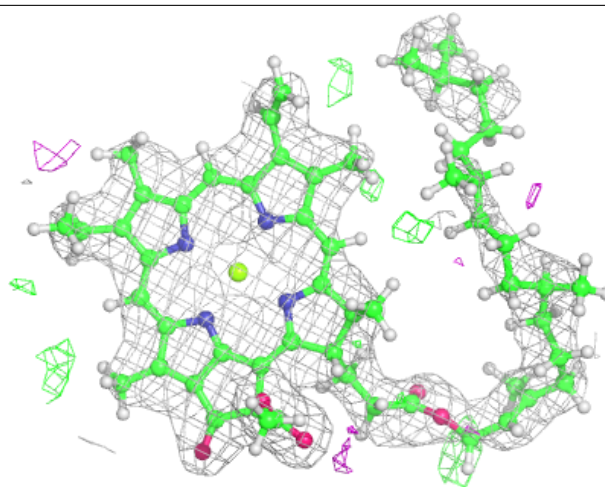
Electron density around STE B 623:

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



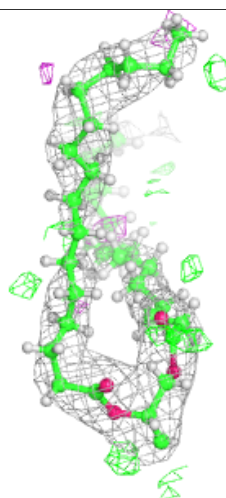
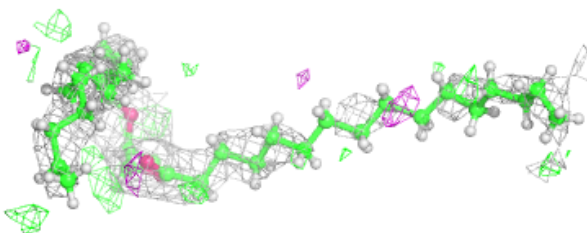
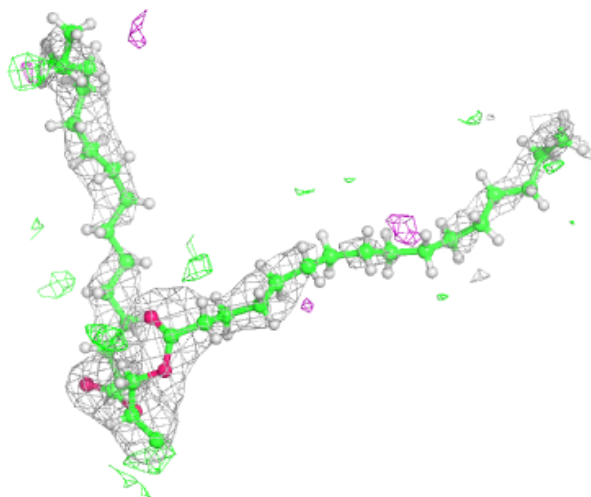
Electron density around CLA c 513:

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



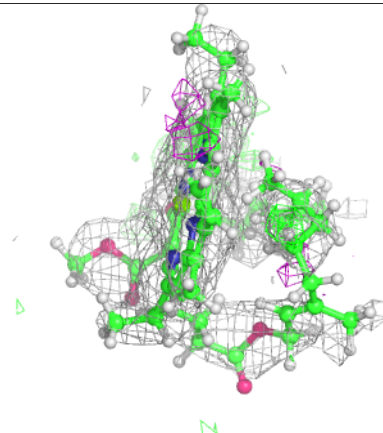
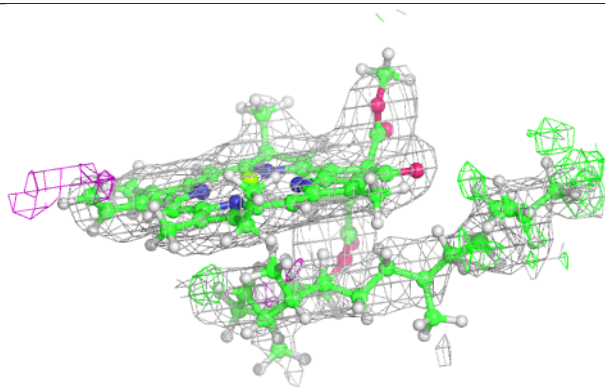
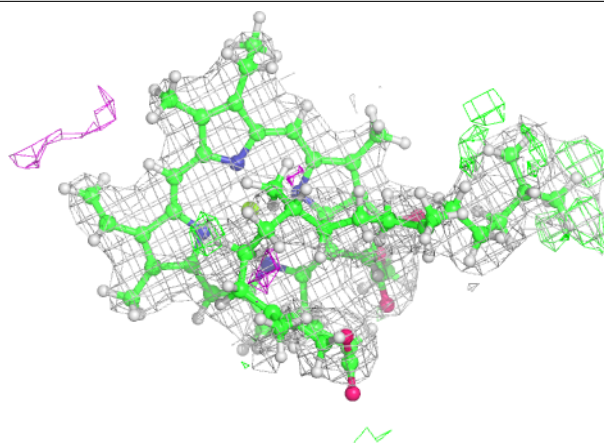
Electron density around SQD A 412:

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

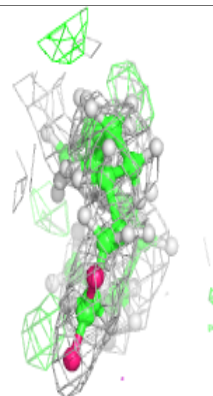
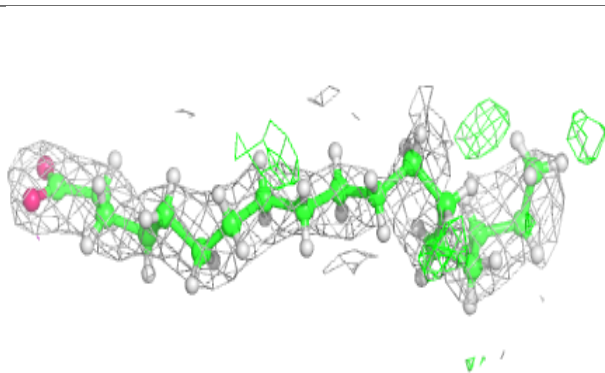
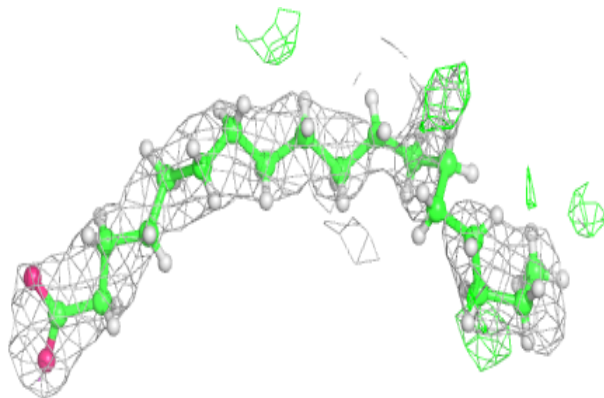


Electron density around CLA H 101:

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

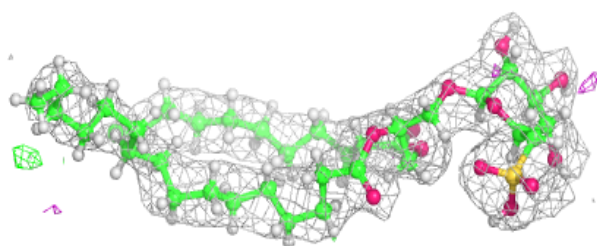
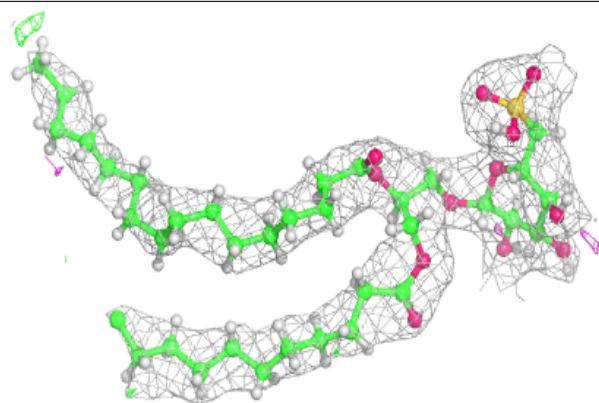
**Electron density around STE b 627:**

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

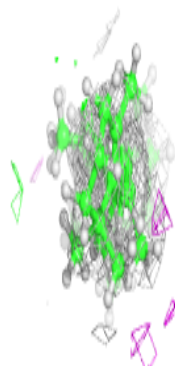
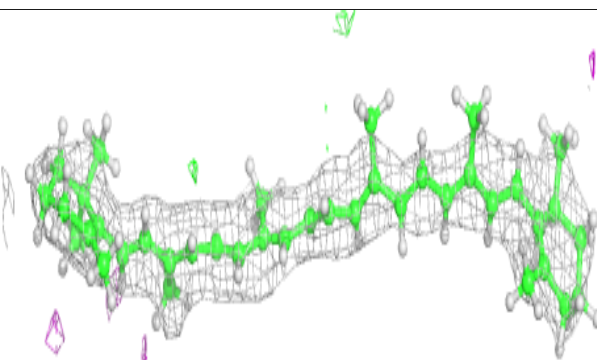
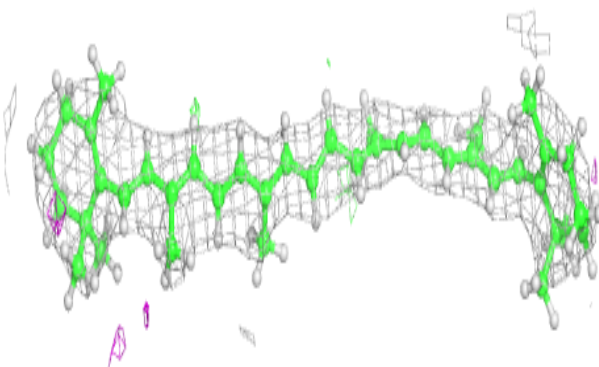


Electron density around SQD L 101:

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

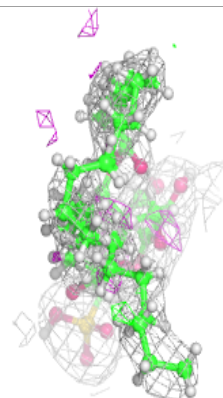
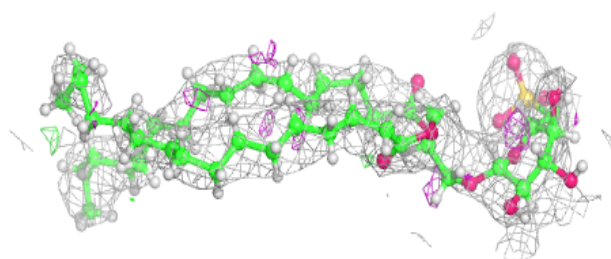
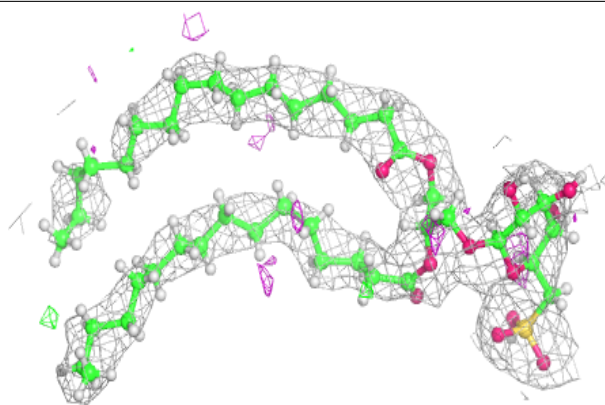
**Electron density around BCR K 101:**

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

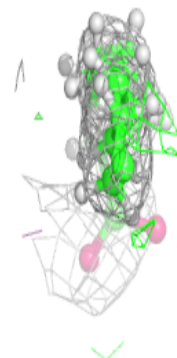
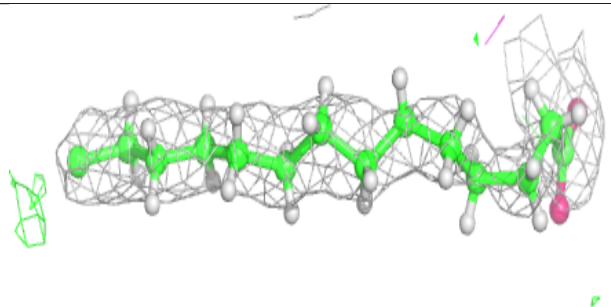
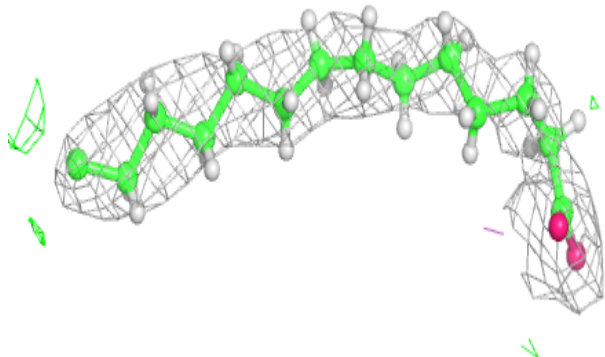


Electron density around SQD B 622:

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

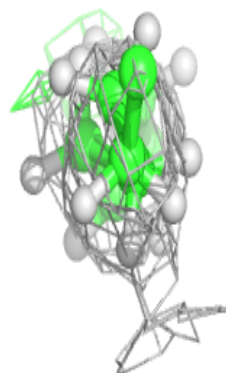
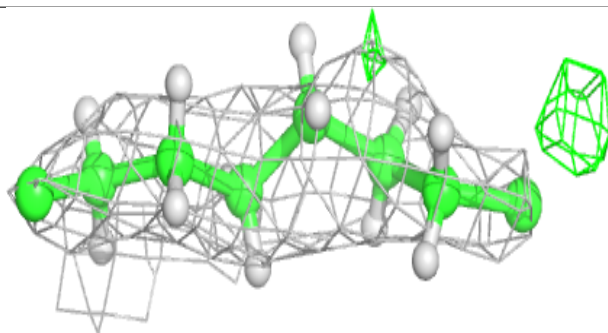
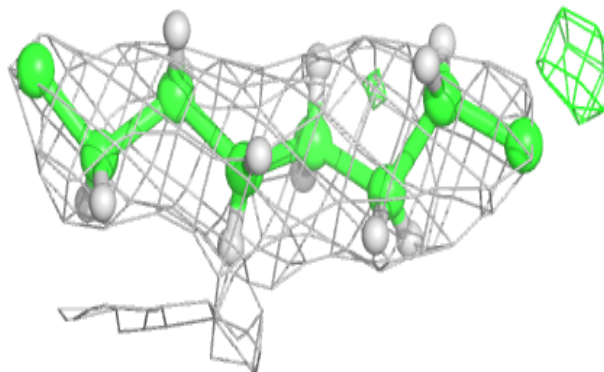
**Electron density around STE d 411:**

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

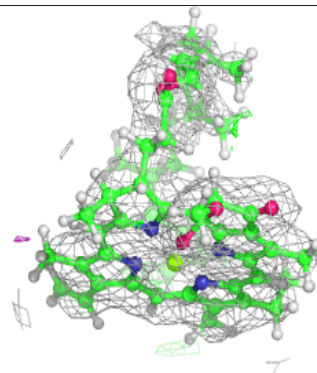
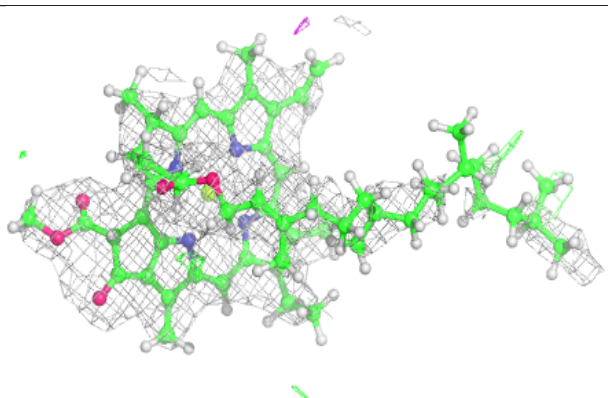
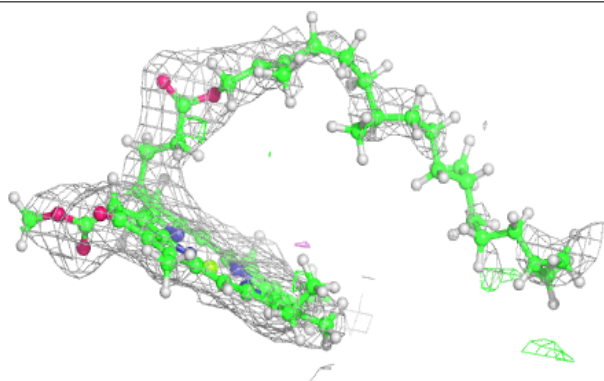


Electron density around STE Z 101:

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

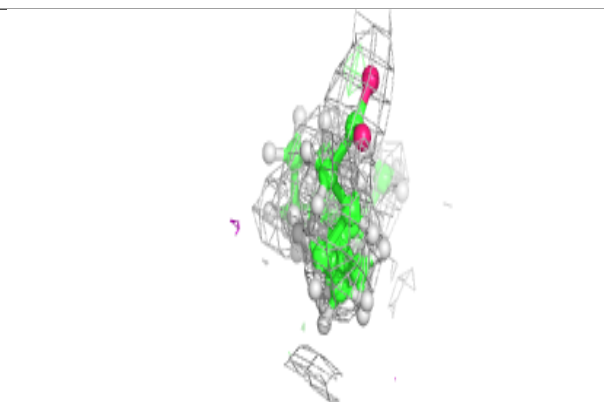
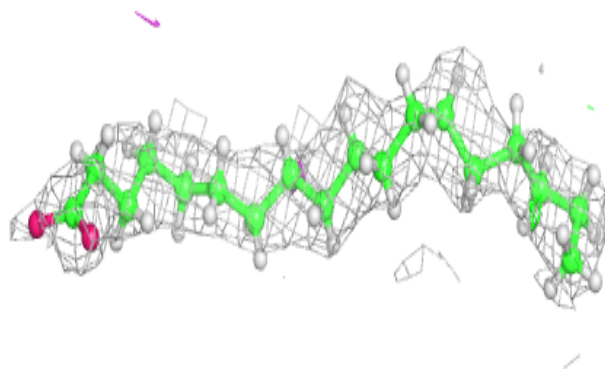
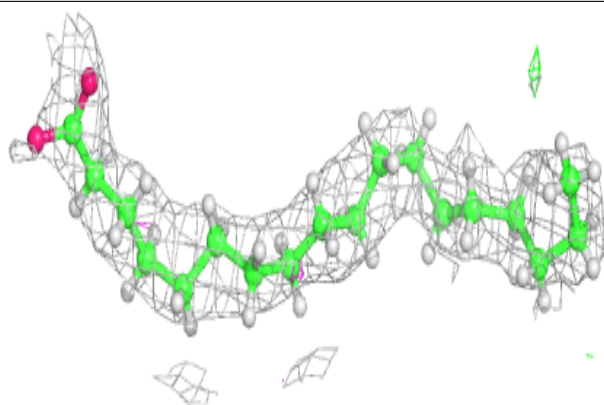
**Electron density around CLA C 513:**

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

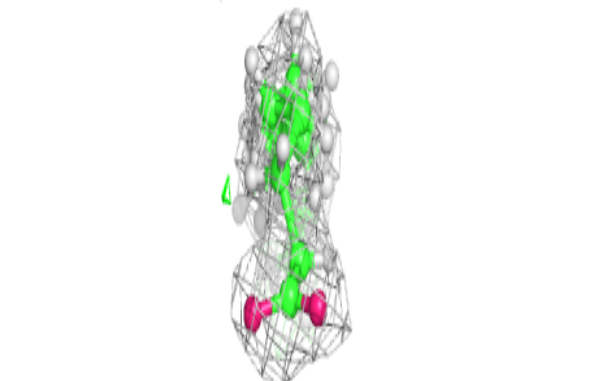
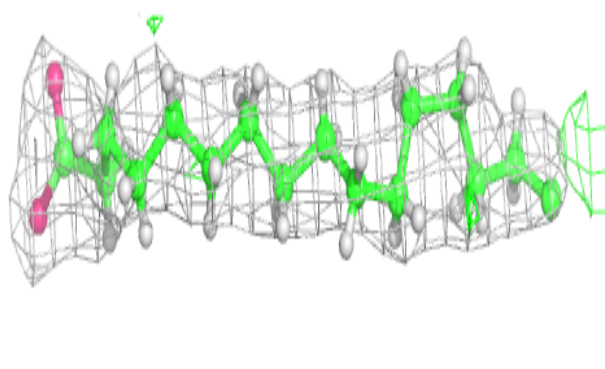
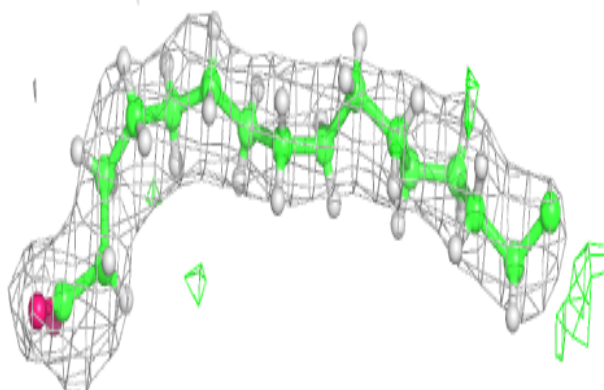


Electron density around STE b 622:

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

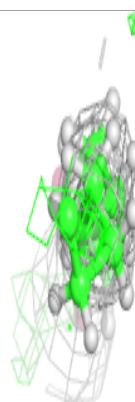
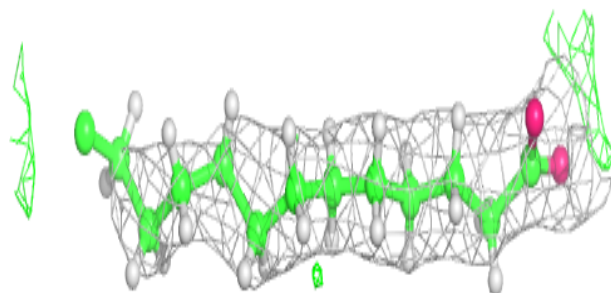
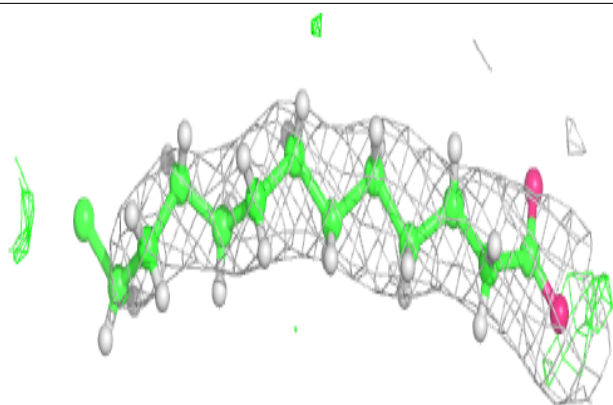
**Electron density around STE B 625:**

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

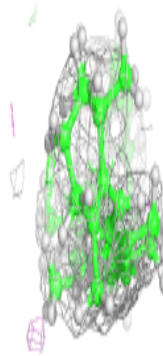
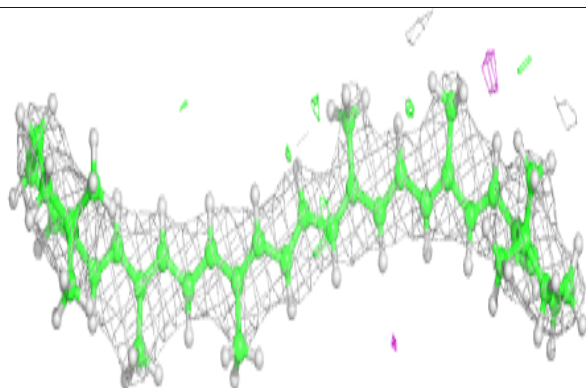
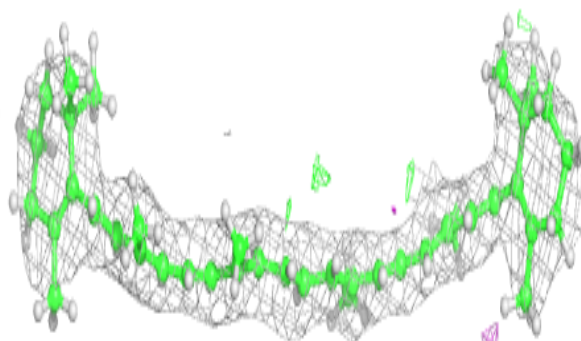


Electron density around STE M 102:

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

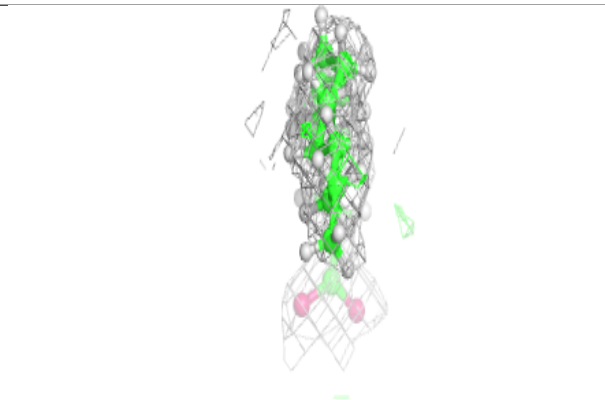
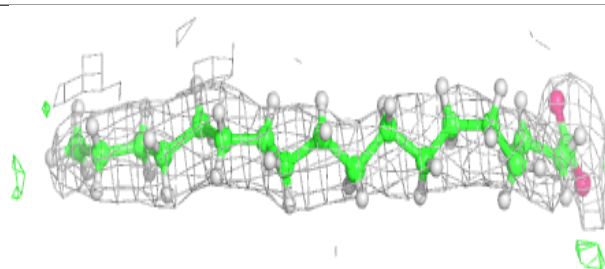
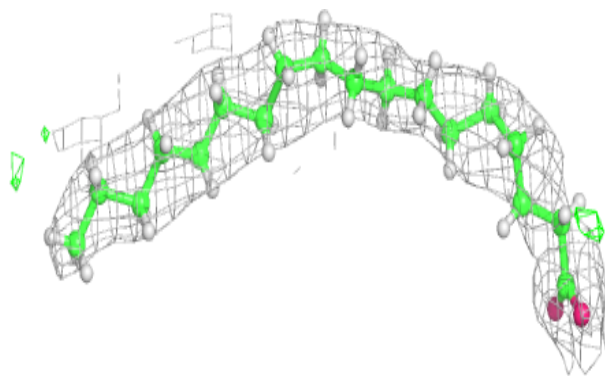
**Electron density around BCR k 102:**

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

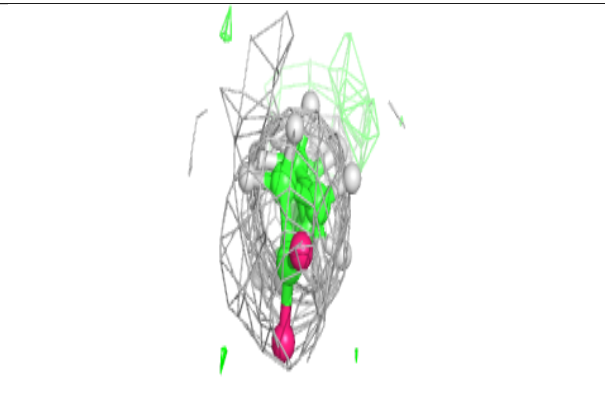
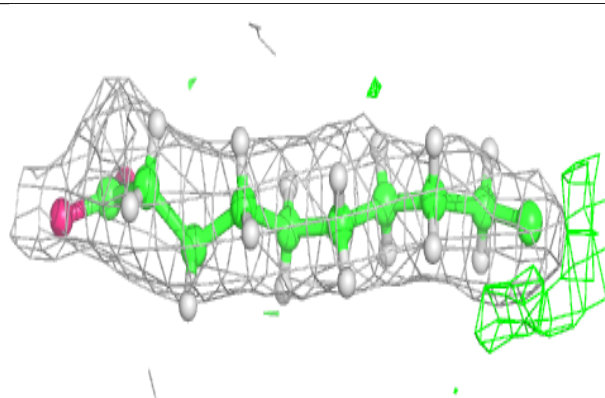
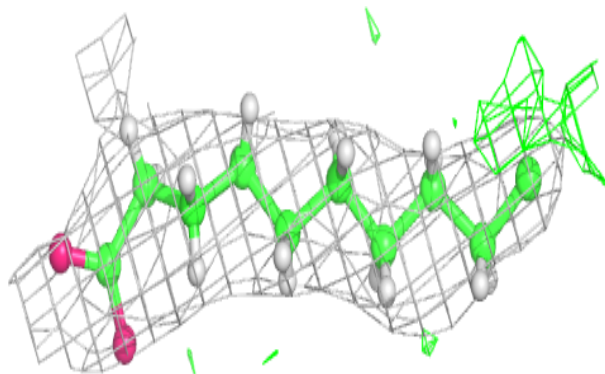


Electron density around STE D 413:

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

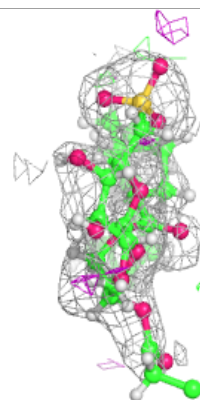
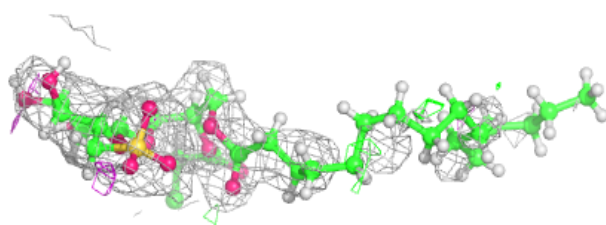
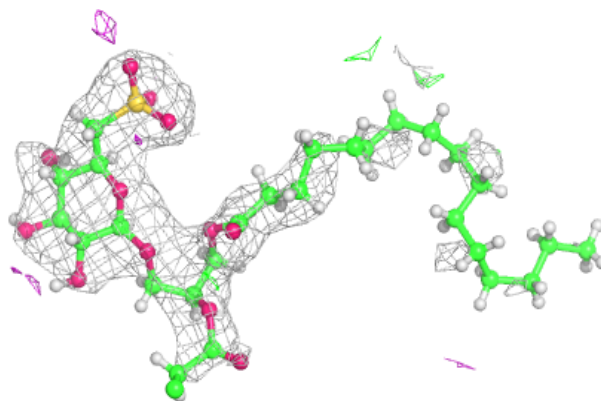
**Electron density around STE J 101:**

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

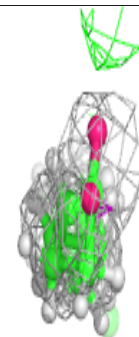
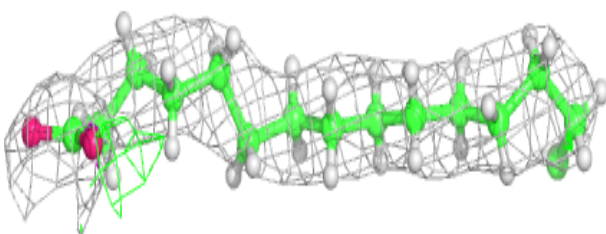
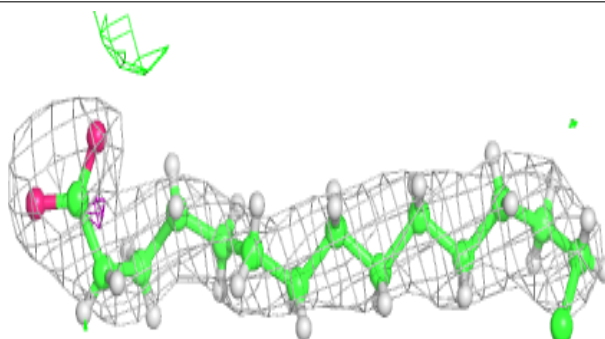


Electron density around SQD f 102:

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

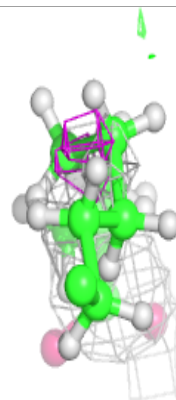
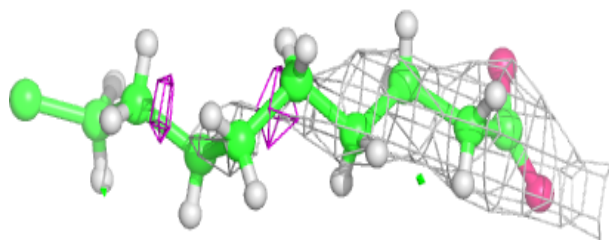
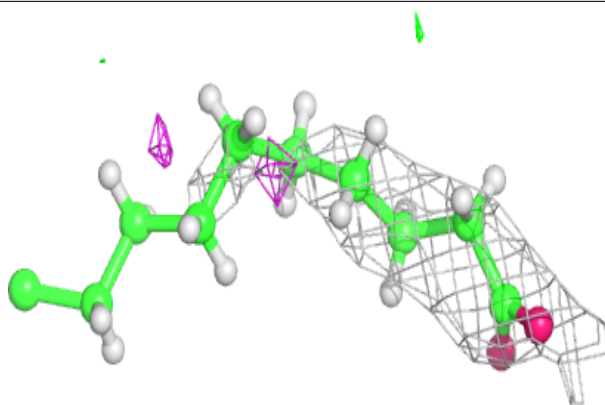
**Electron density around STE d 412:**

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



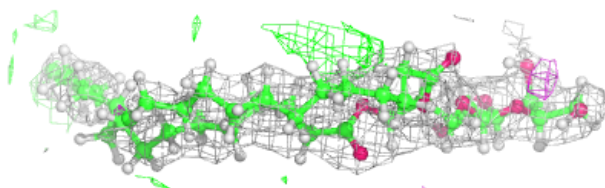
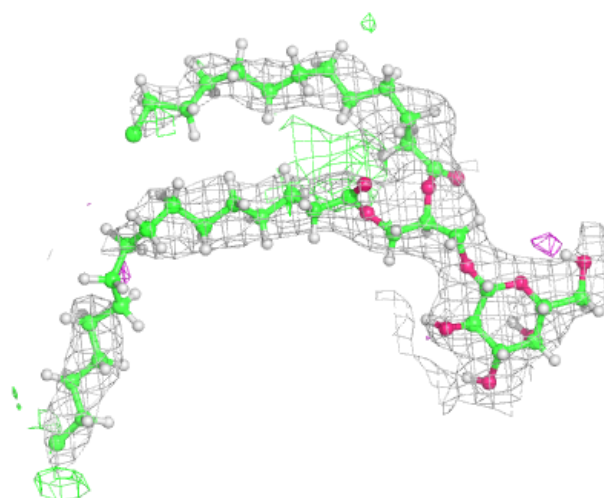
Electron density around STE B 601:

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



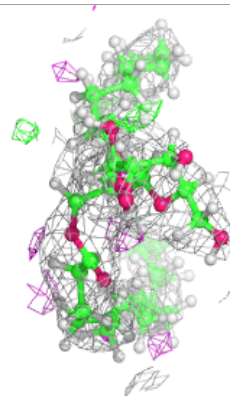
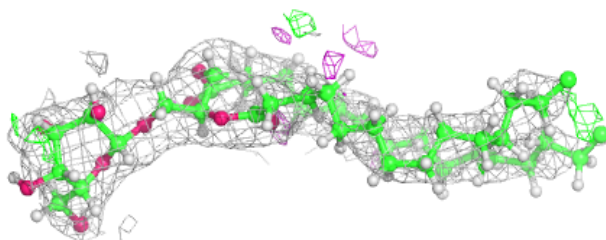
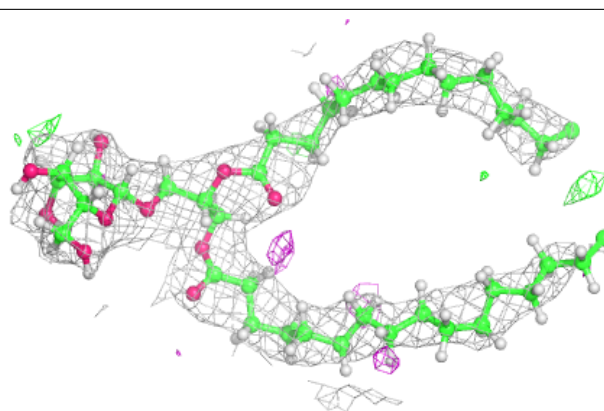
Electron density around LMG Y 101:

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

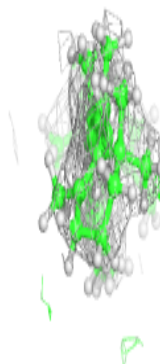
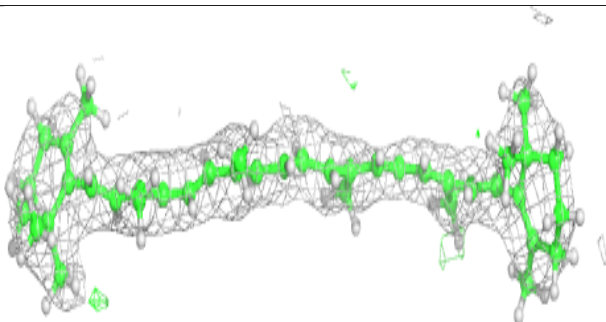
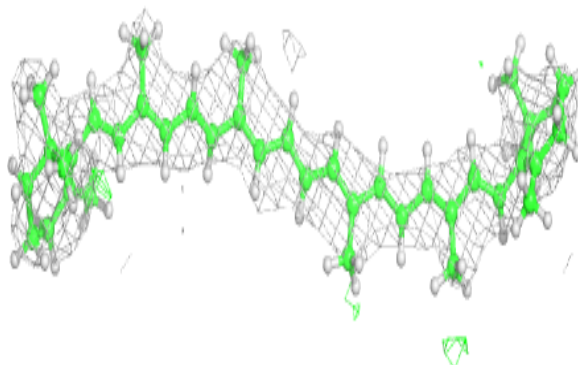


Electron density around LMG c 523:

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

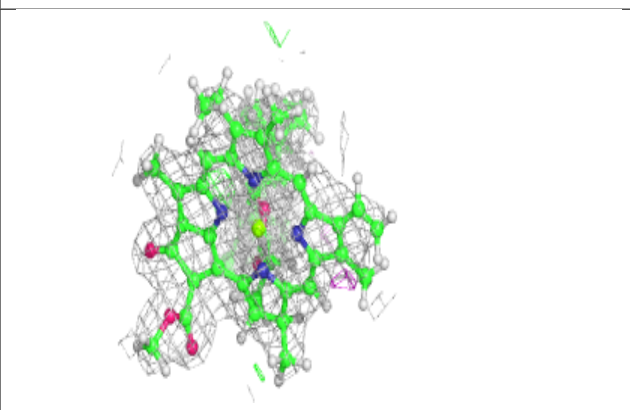
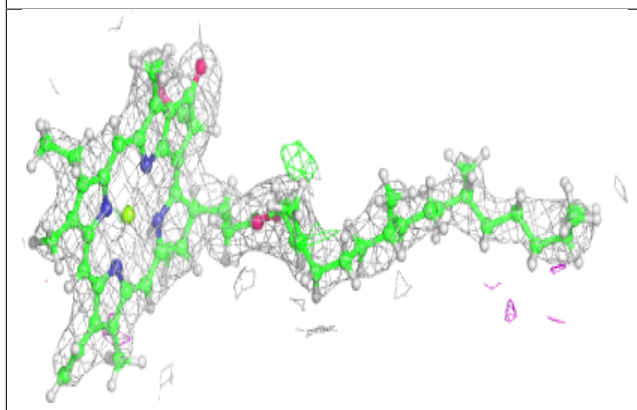
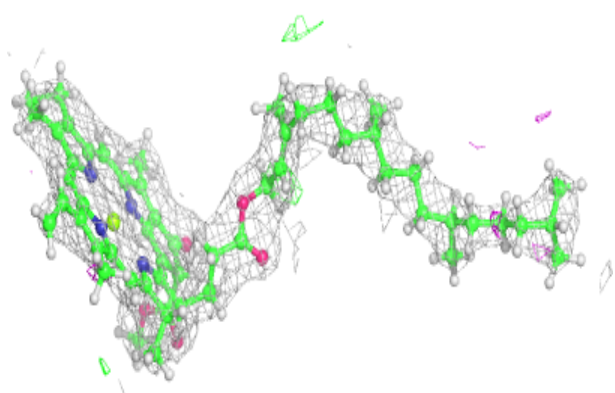
**Electron density around BCR k 101:**

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

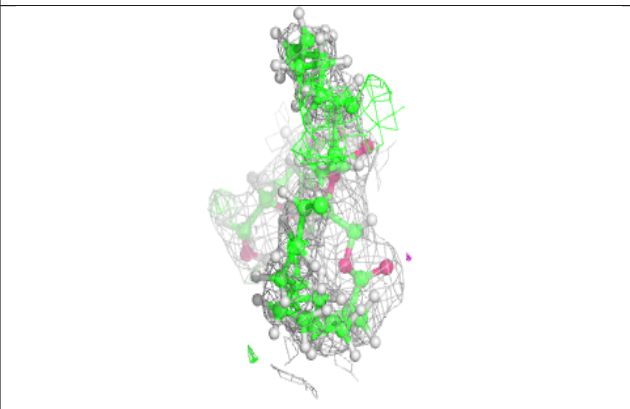
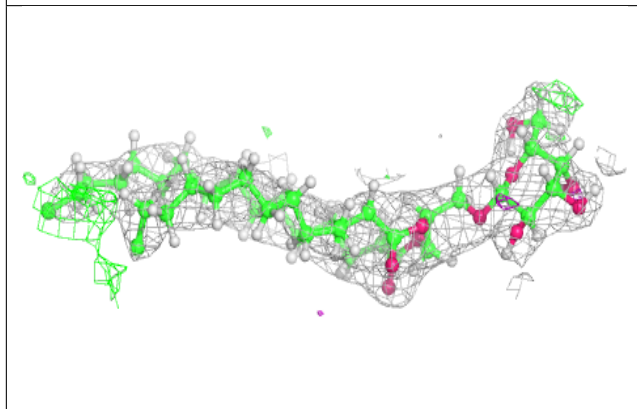
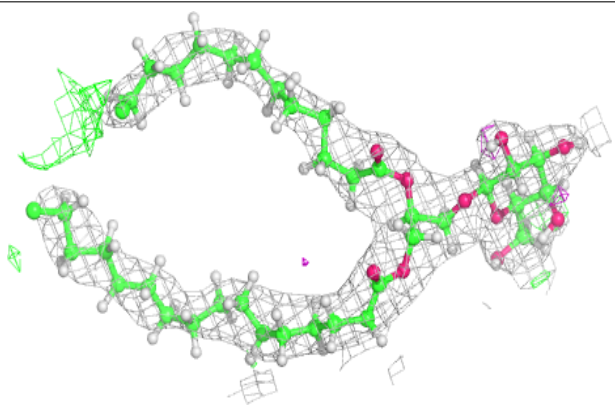


Electron density around CLA c 503:

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

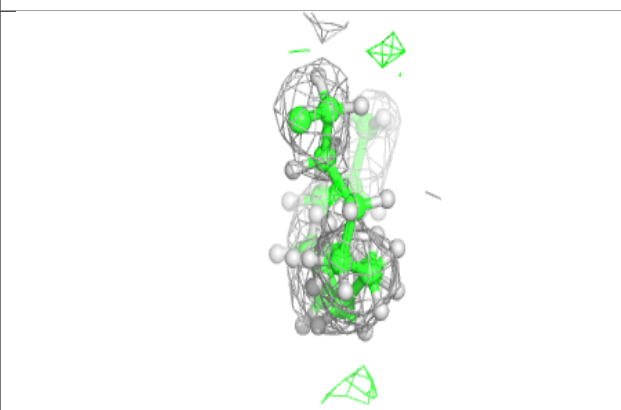
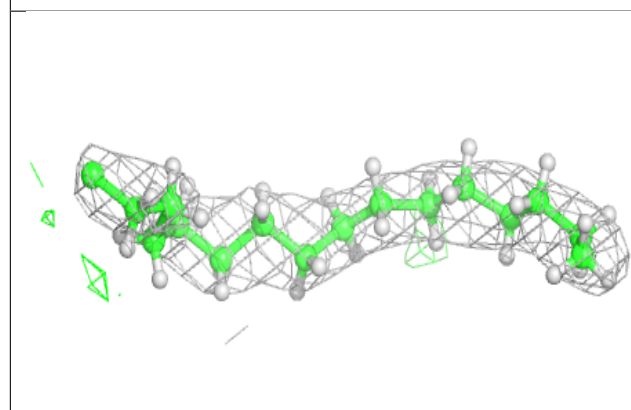
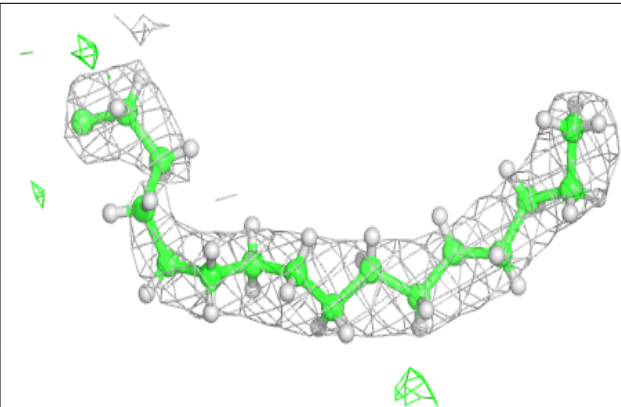
**Electron density around LMG A 410:**

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

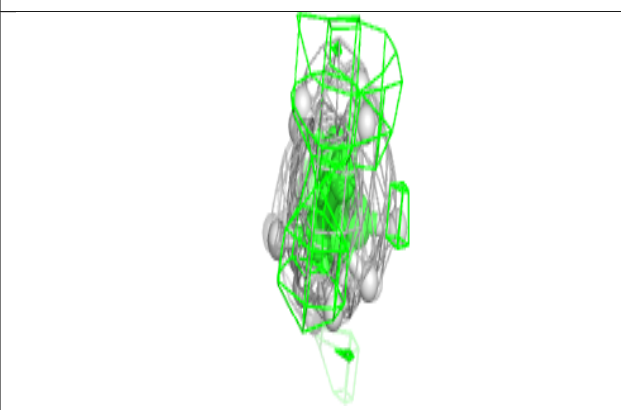
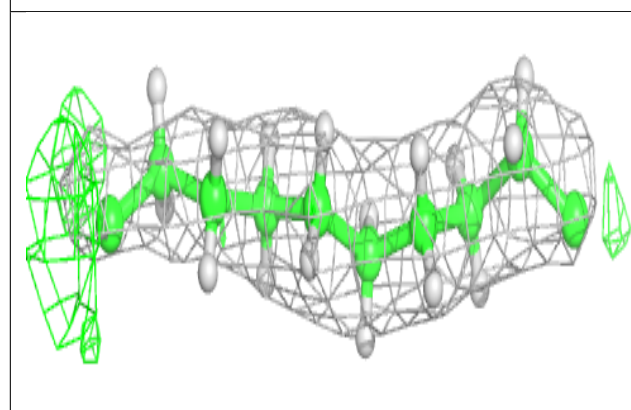
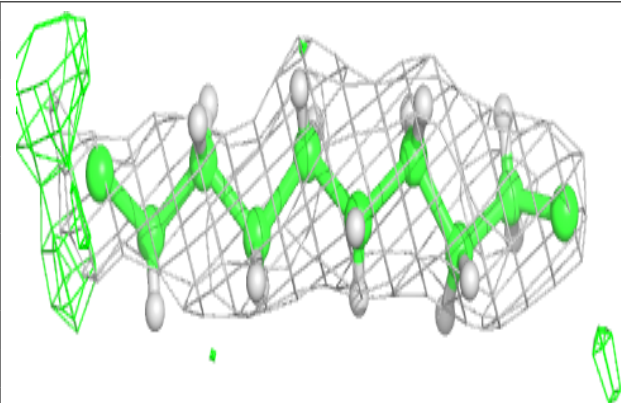


Electron density around STE b 620:

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

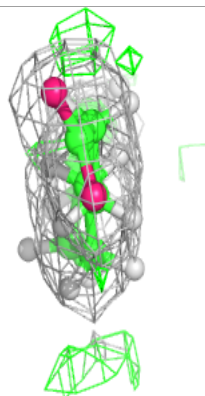
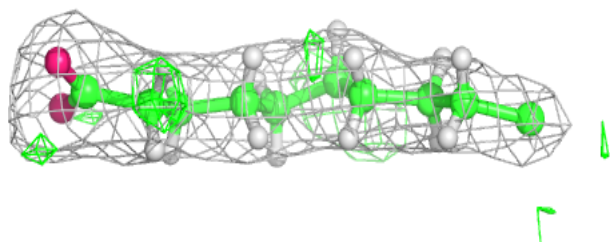
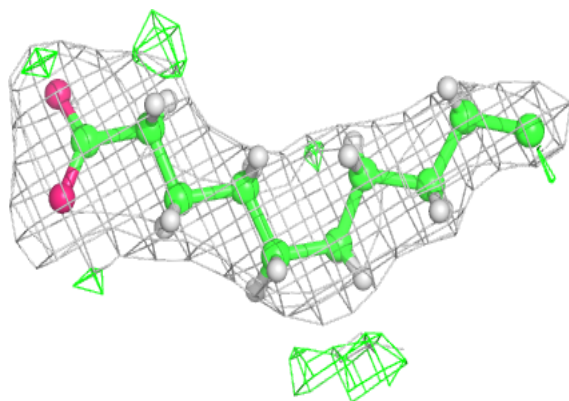
**Electron density around STE M 103:**

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

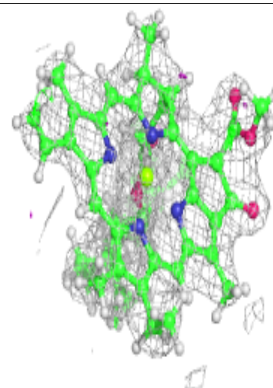
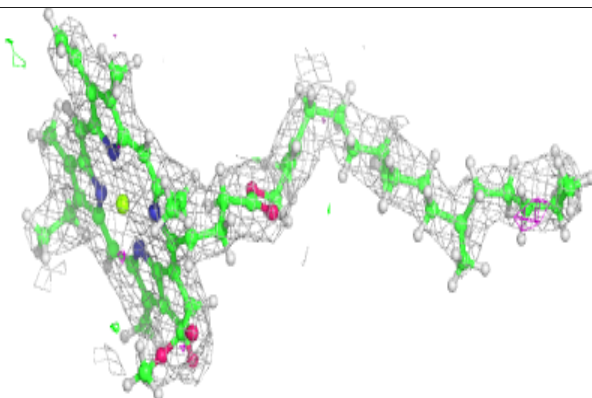
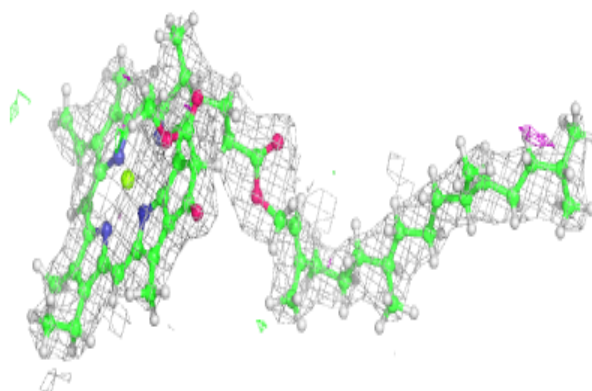


Electron density around STE C 520:

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

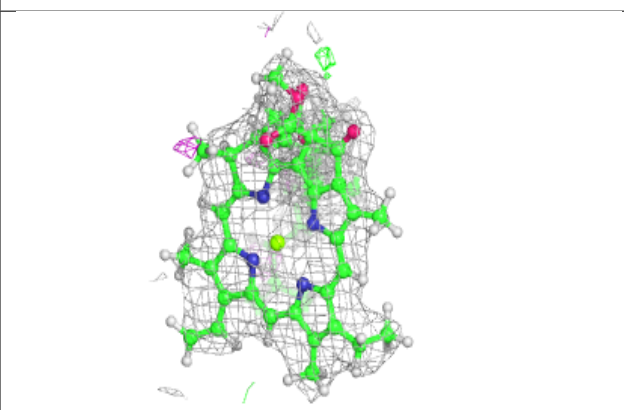
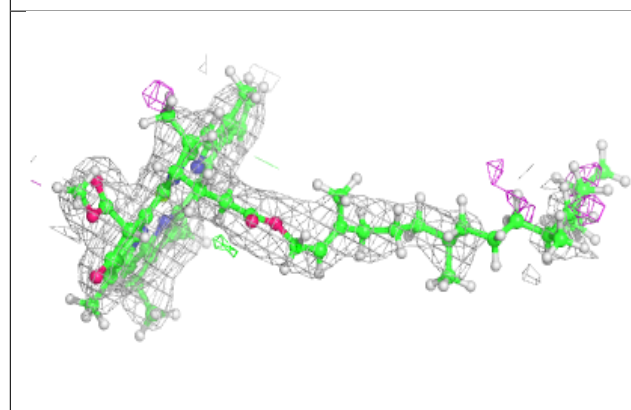
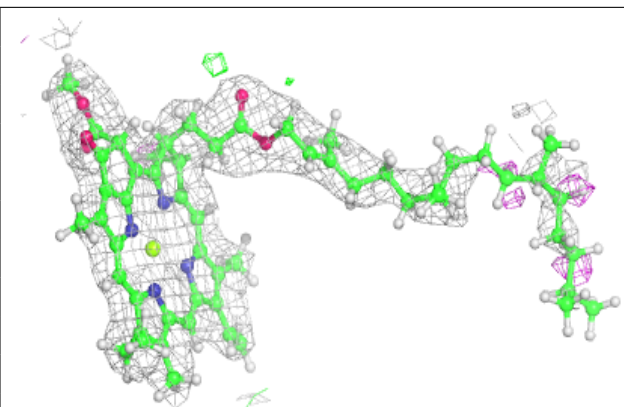
**Electron density around CLA C 502:**

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

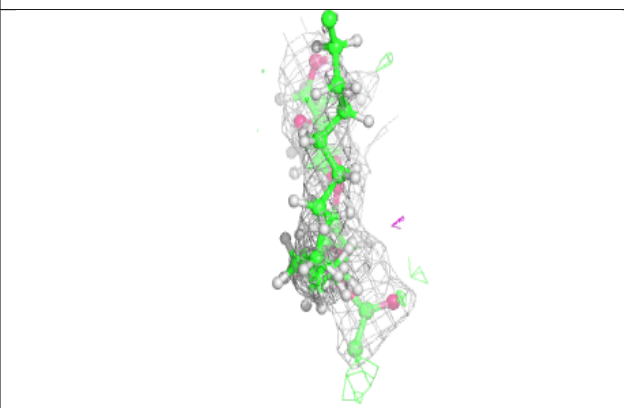
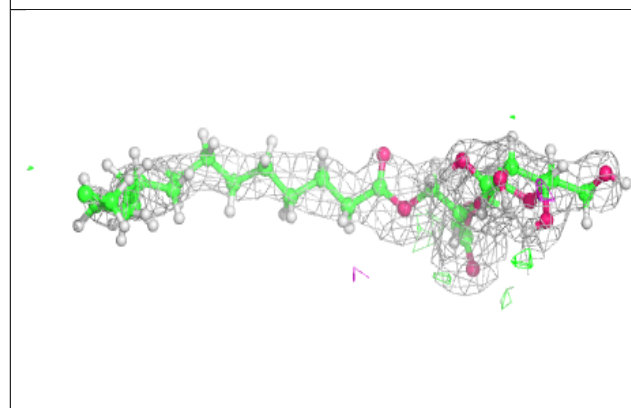
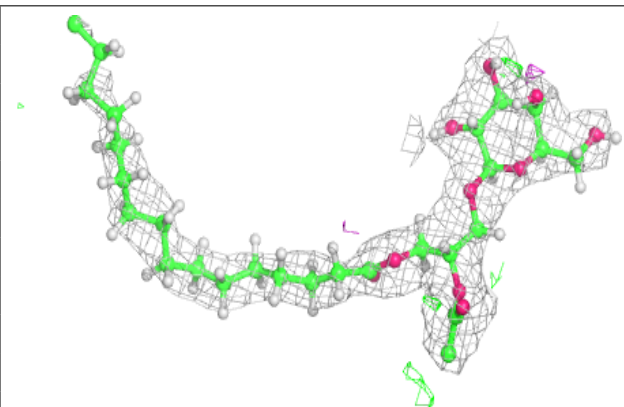


Electron density around CLA d 404:

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

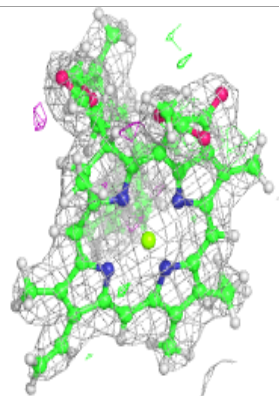
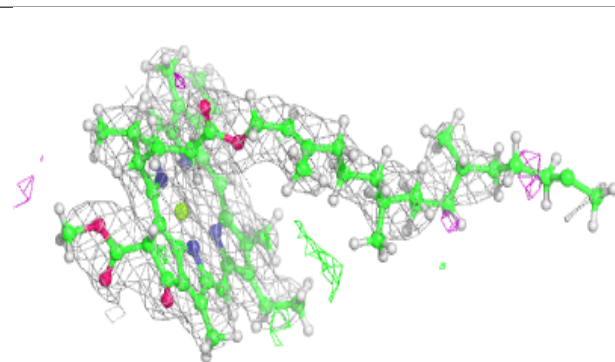
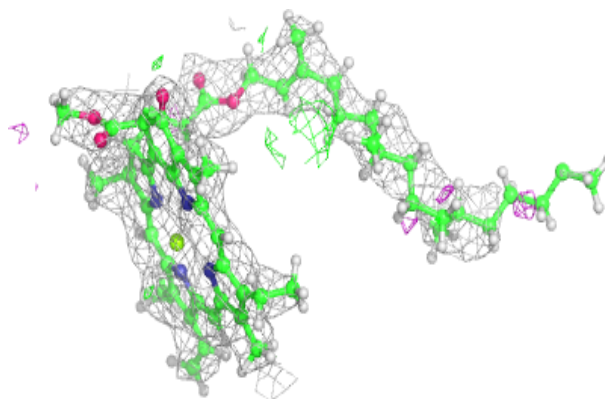
**Electron density around LMG c 520:**

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

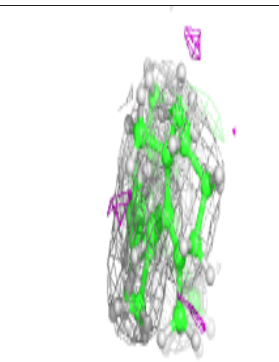
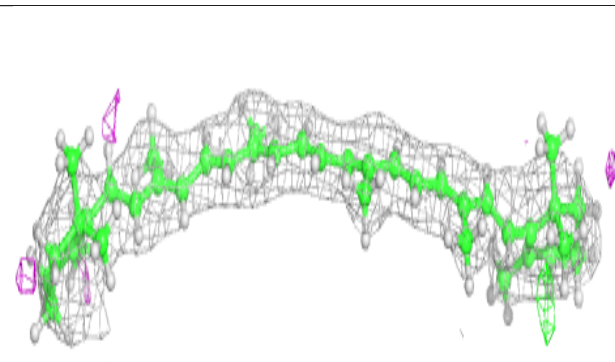
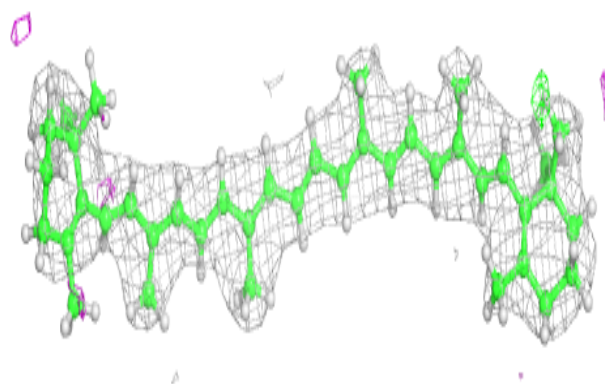


Electron density around CLA c 509:

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

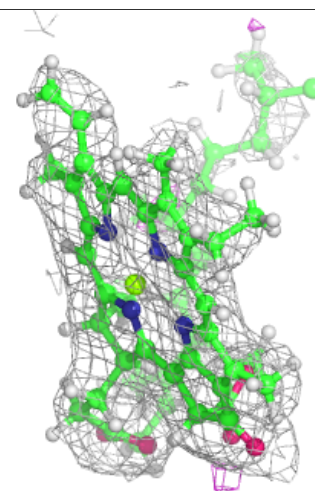
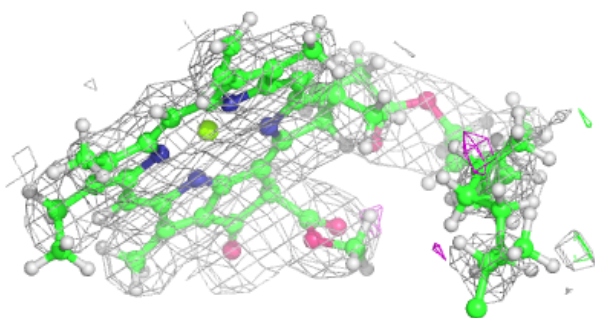
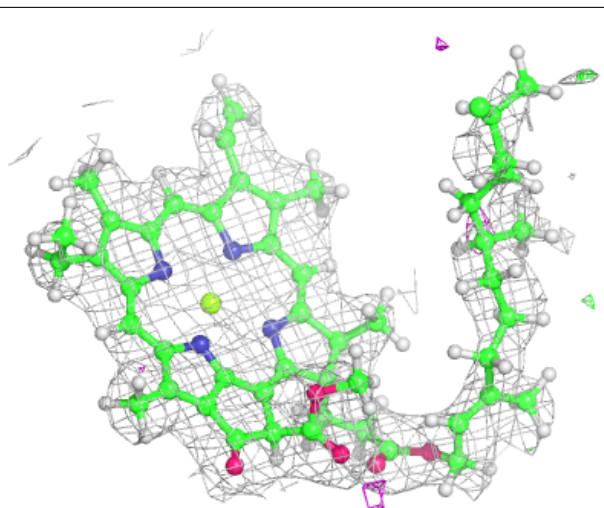
**Electron density around BCR F 101:**

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



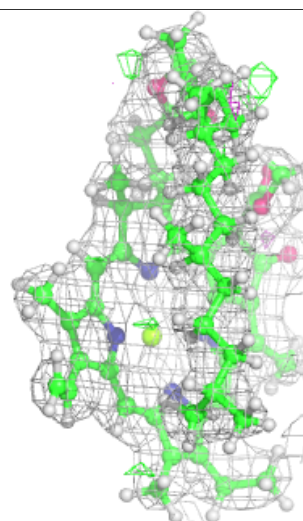
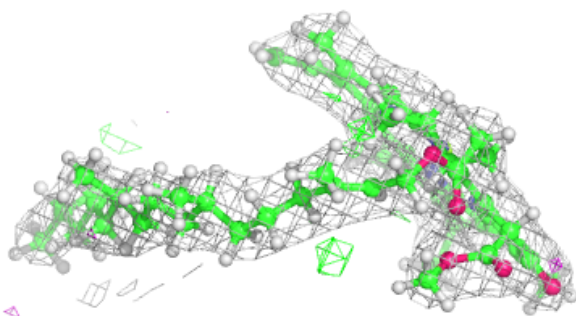
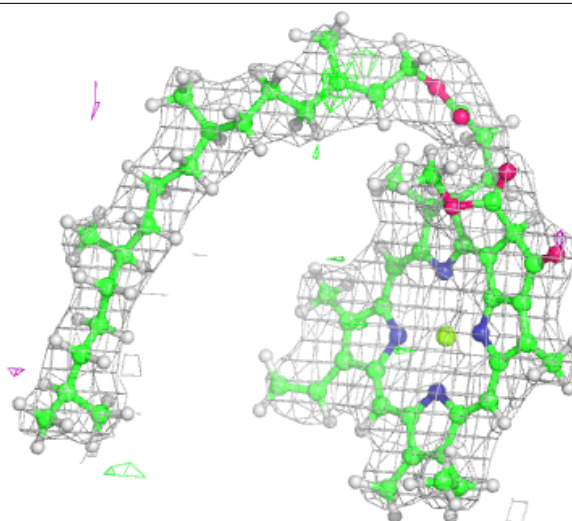
Electron density around CLA b 616:

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



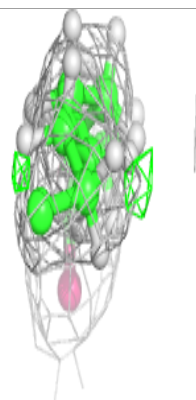
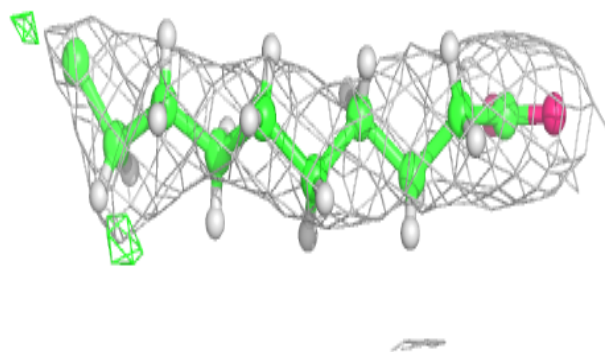
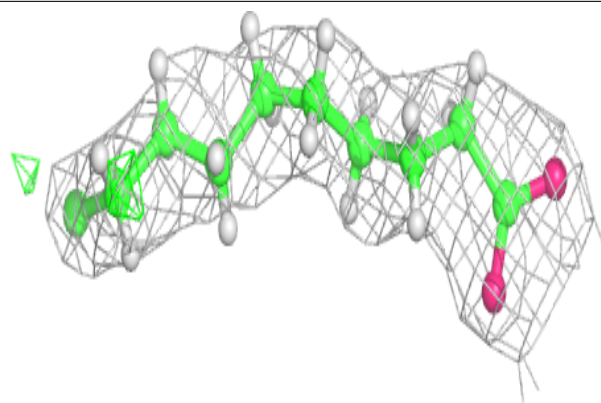
Electron density around CLA C 507:

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

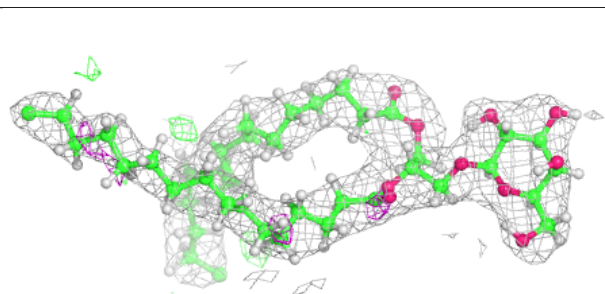
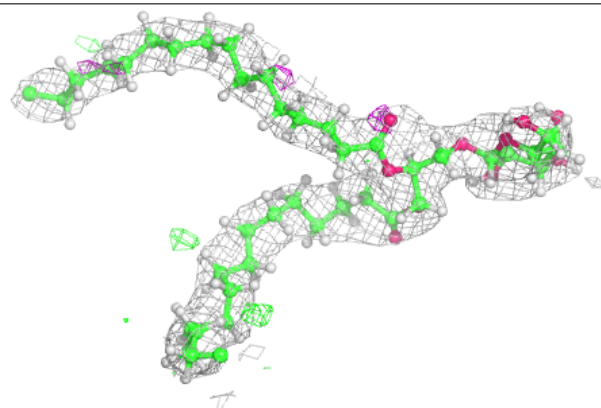


Electron density around STE C 518:

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

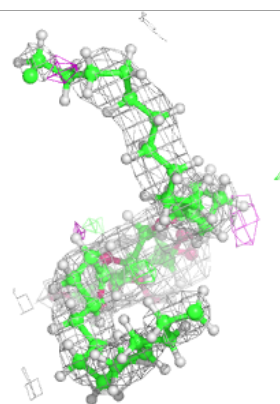
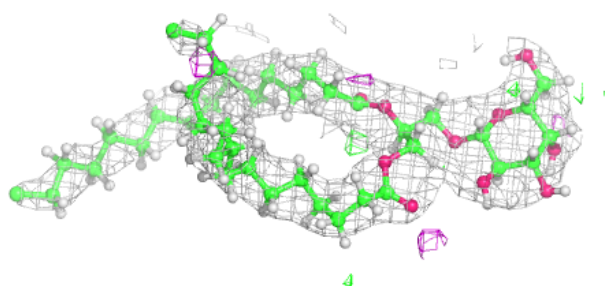
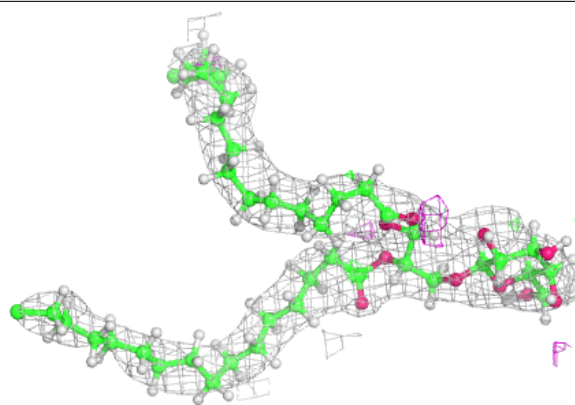
**Electron density around LMG M 101:**

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



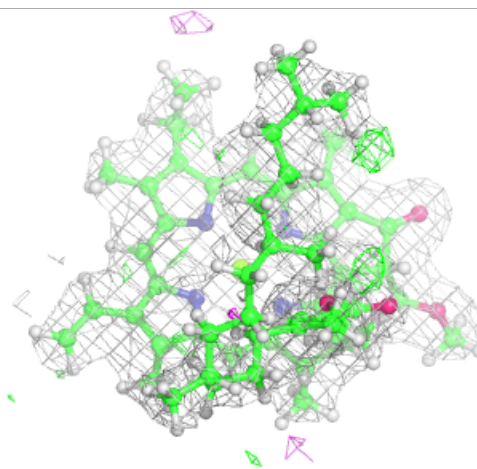
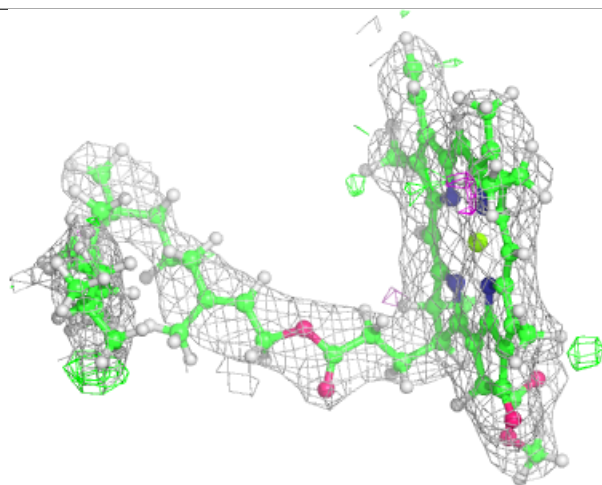
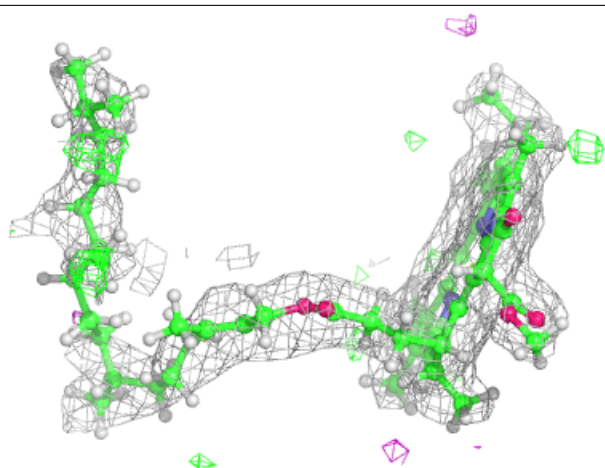
Electron density around LMG b 621:

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



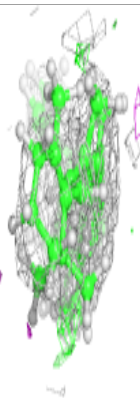
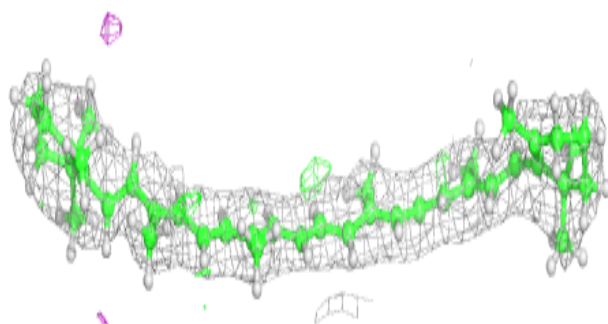
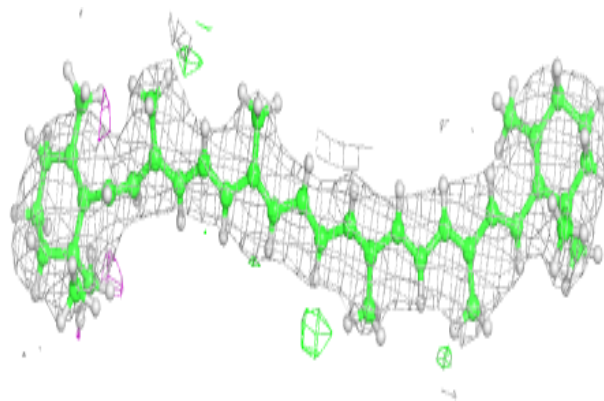
Electron density around CLA a 405:

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

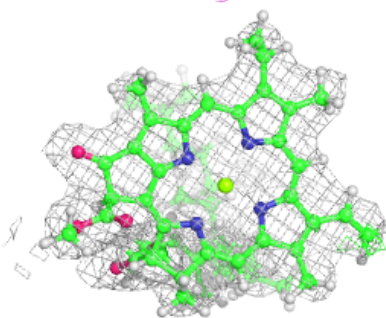
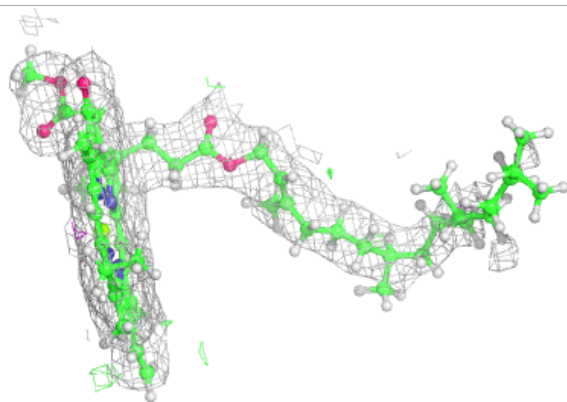
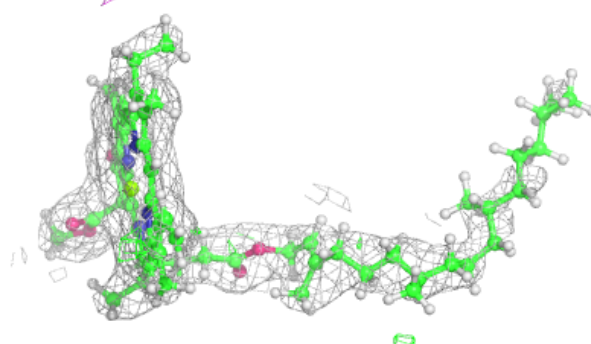


Electron density around BCR d 405:

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

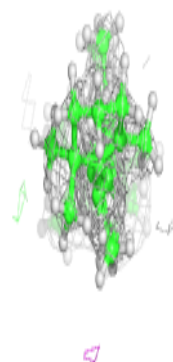
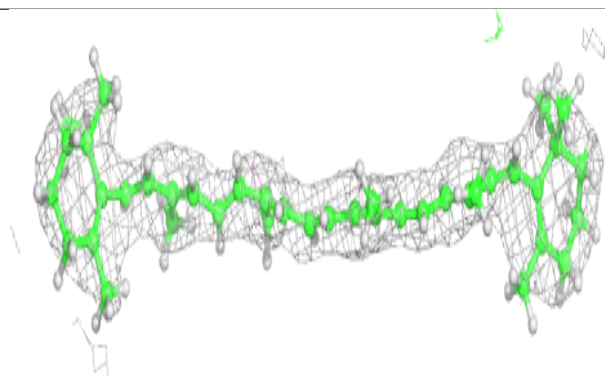
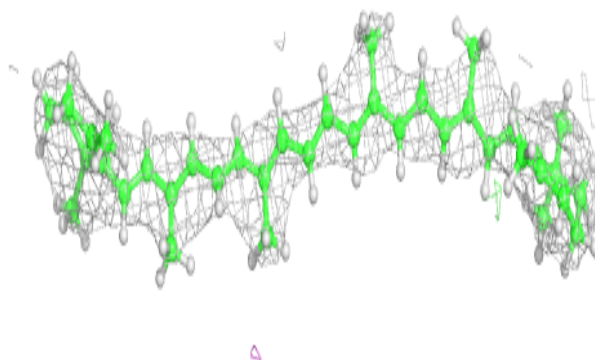
**Electron density around CLA D 405:**

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

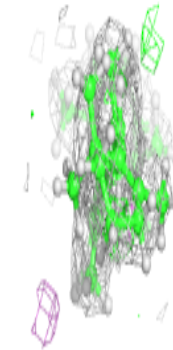
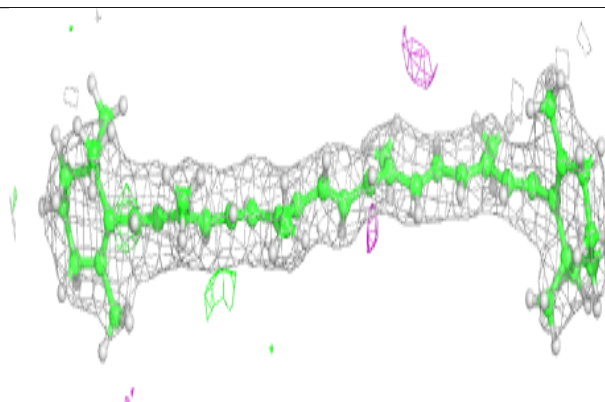
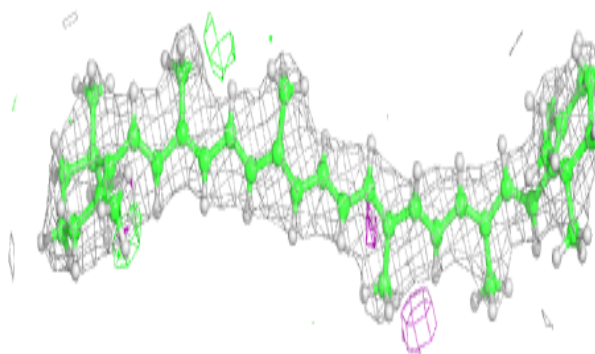


Electron density around BCR c 515:

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

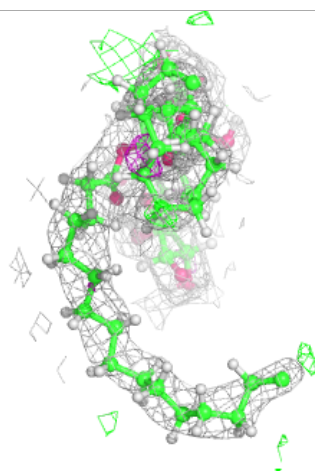
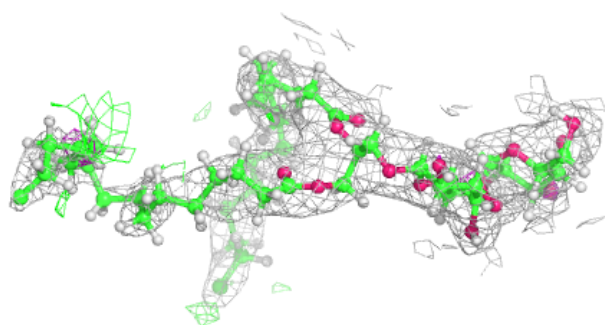
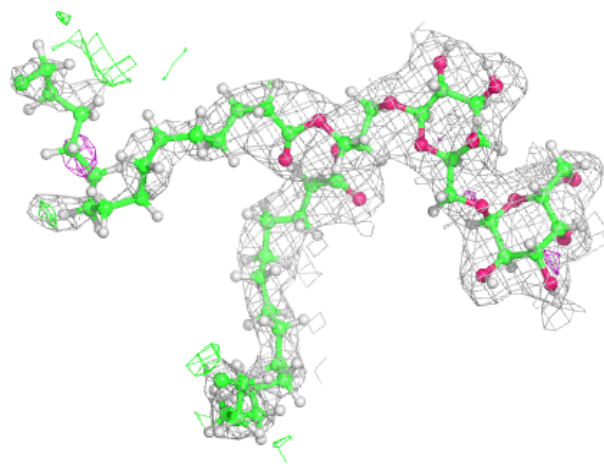
**Electron density around BCR C 514:**

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



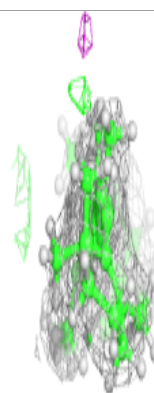
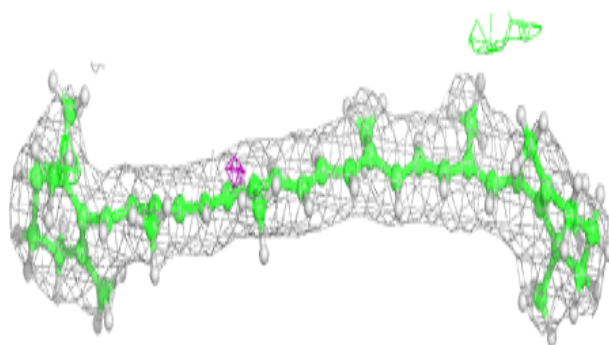
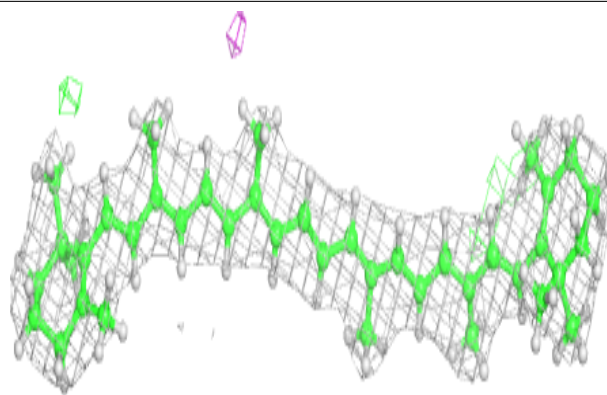
Electron density around DGD C 516:

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



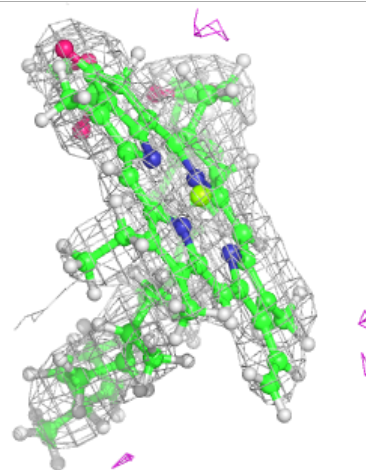
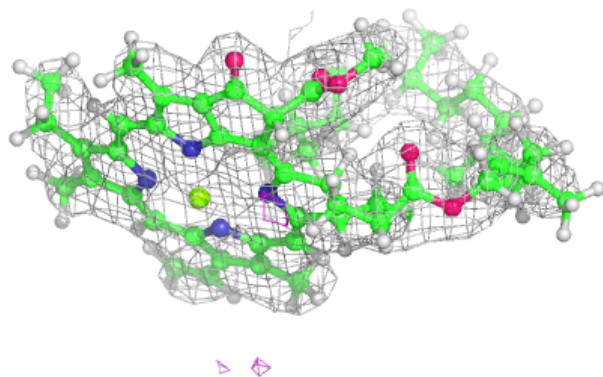
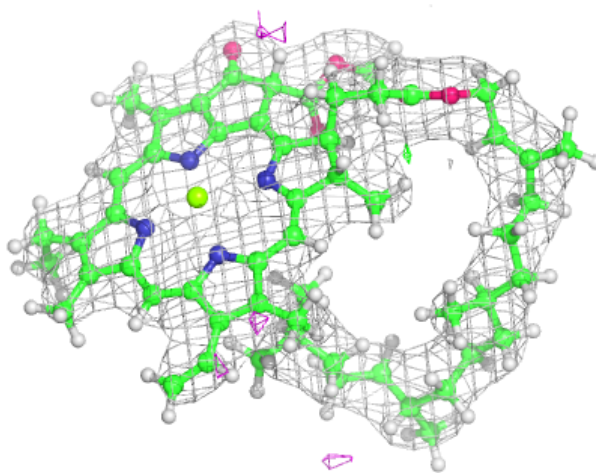
Electron density around BCR B 619:

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



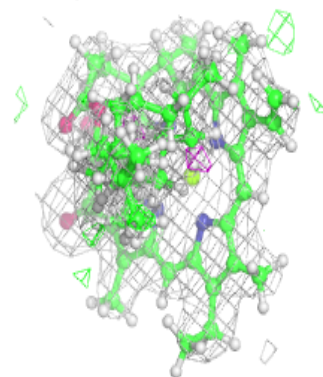
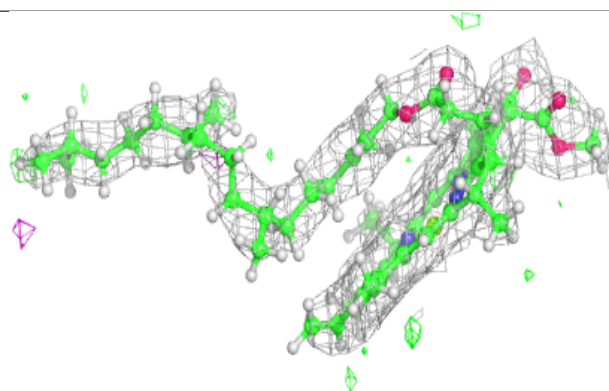
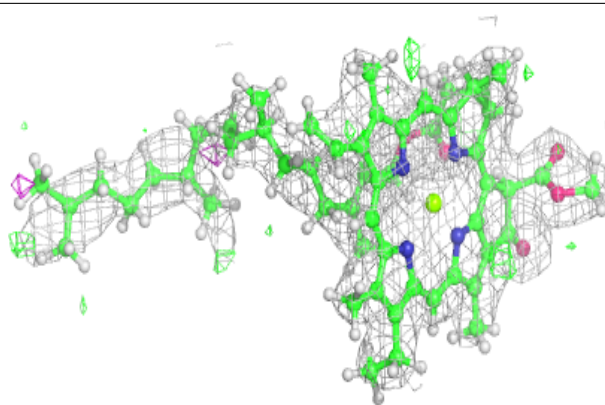
Electron density around CLA b 615:

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

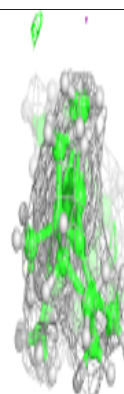
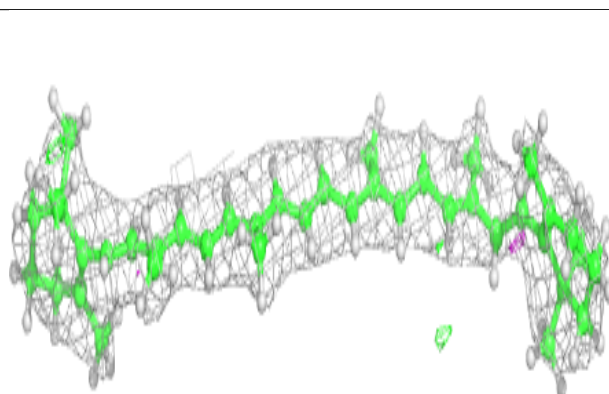
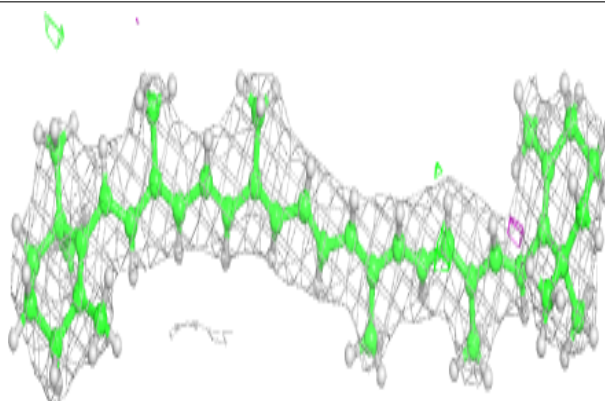


Electron density around CLA c 506:

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

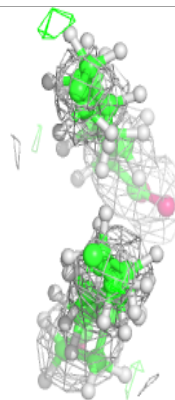
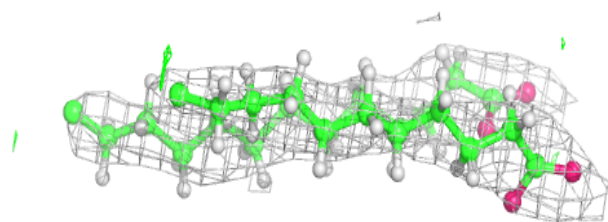
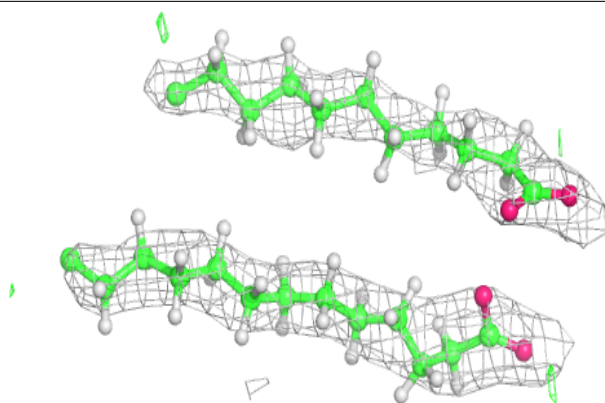
**Electron density around BCR b 619:**

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

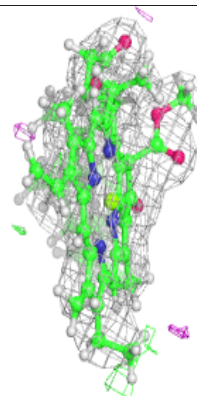
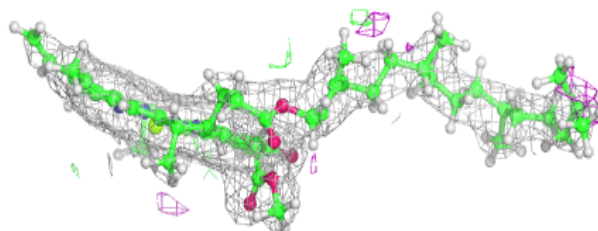
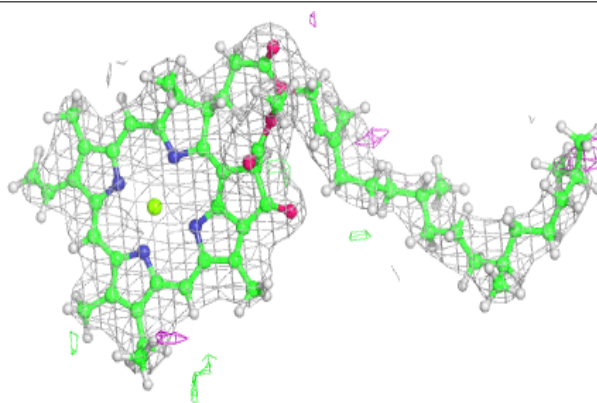


Electron density around LMG B 621:

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

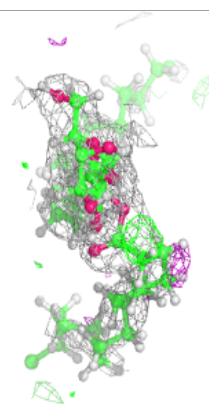
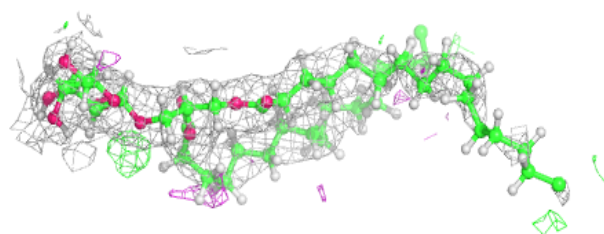
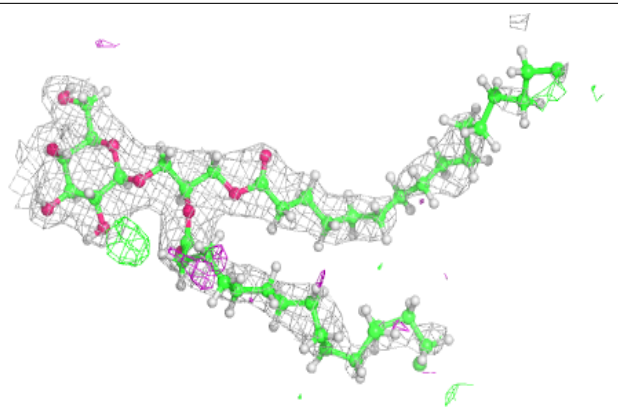
**Electron density around CLA b 602:**

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

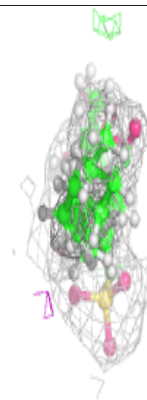
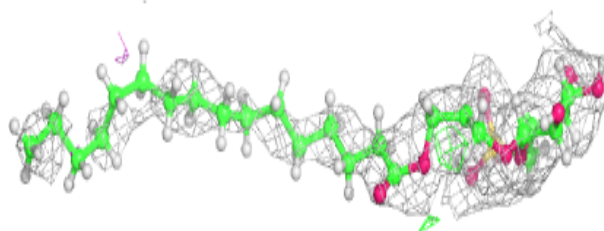
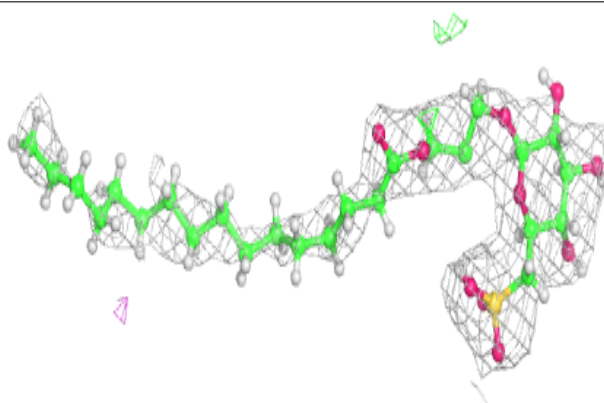


Electron density around LMG D 407:

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

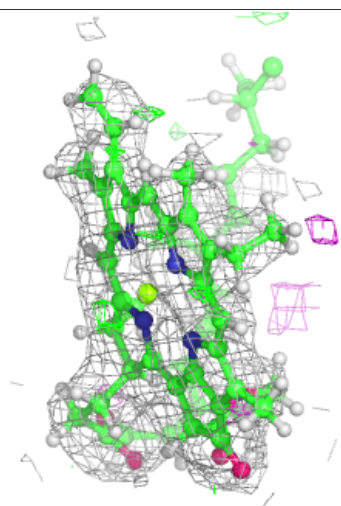
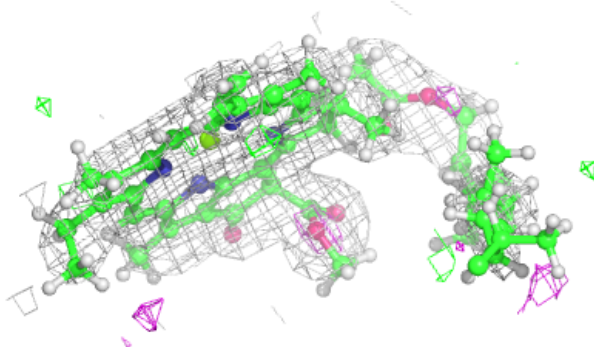
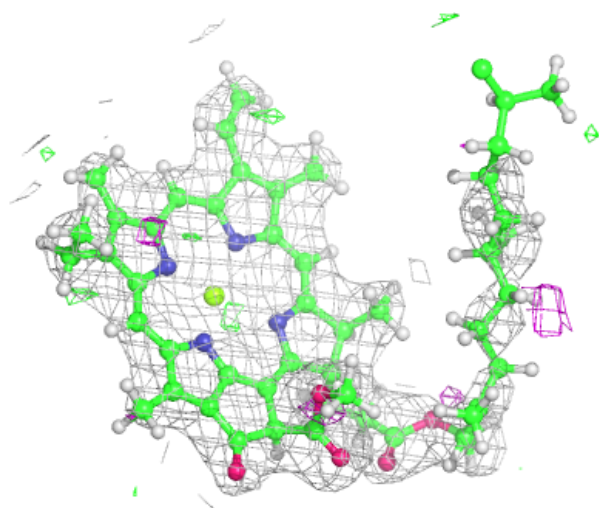
**Electron density around SQD D 408:**

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



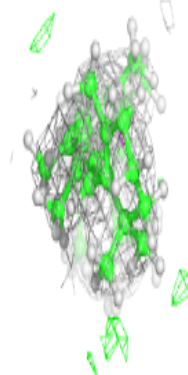
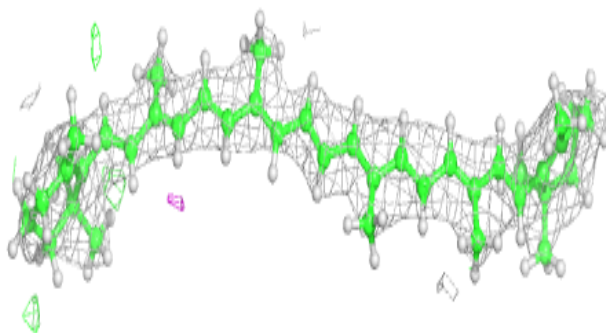
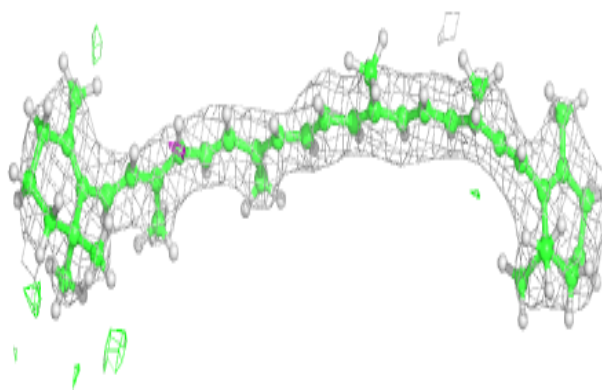
Electron density around CLA B 616:

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

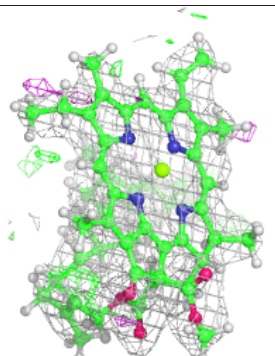
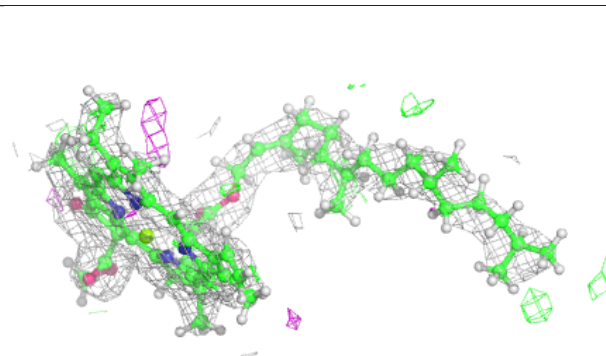
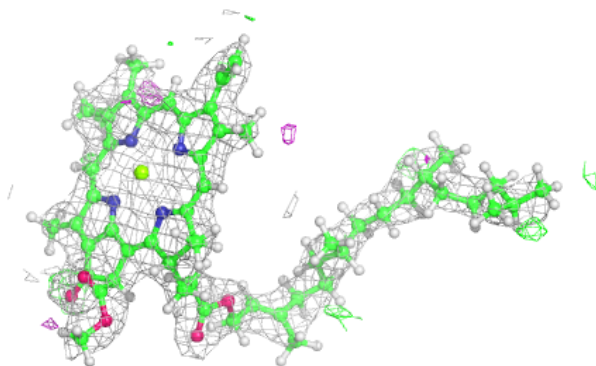


Electron density around BCR K 103:

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

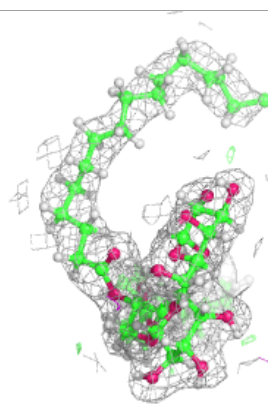
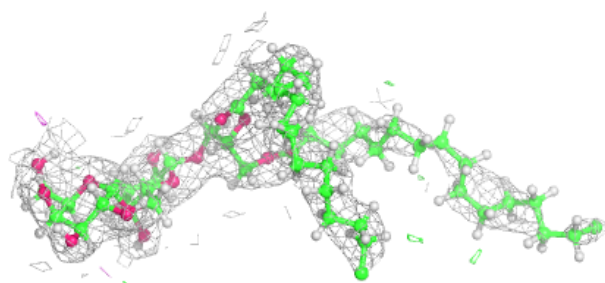
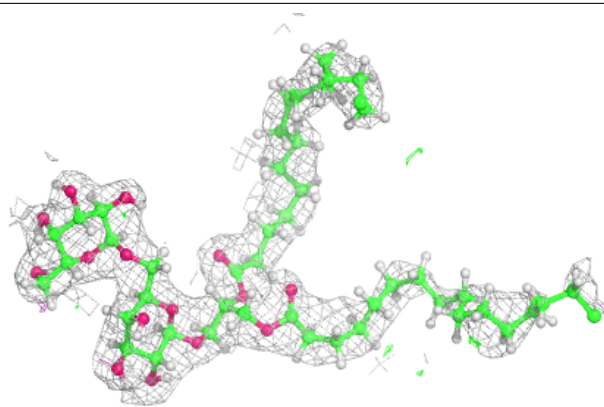
**Electron density around CLA c 512:**

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



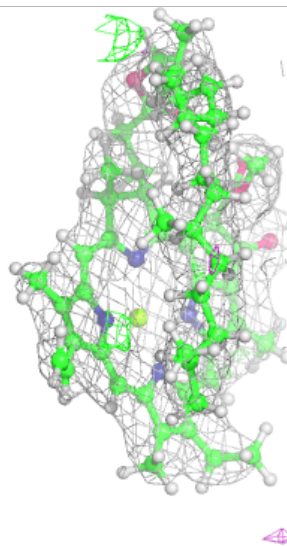
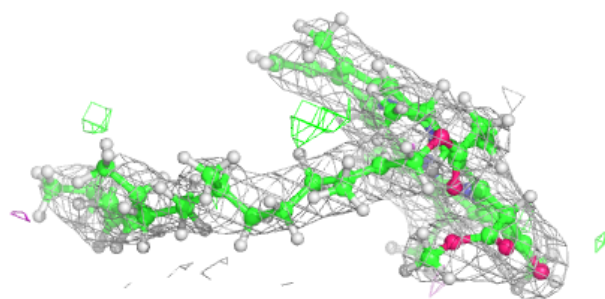
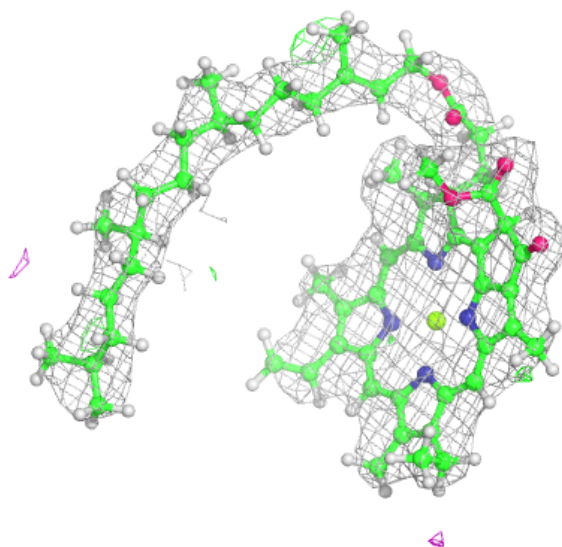
Electron density around DGD c 518:

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



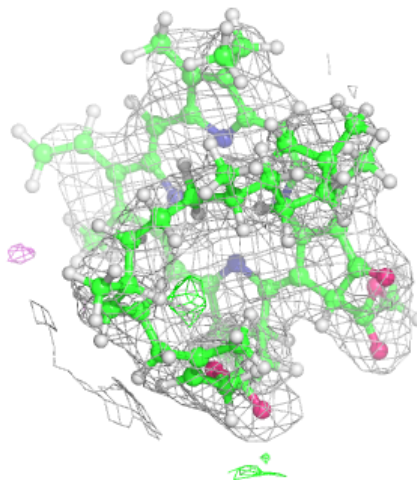
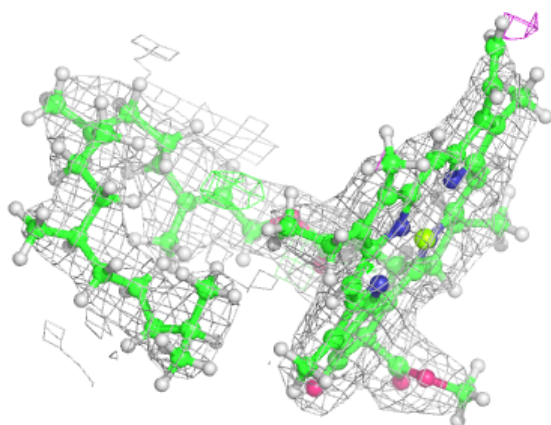
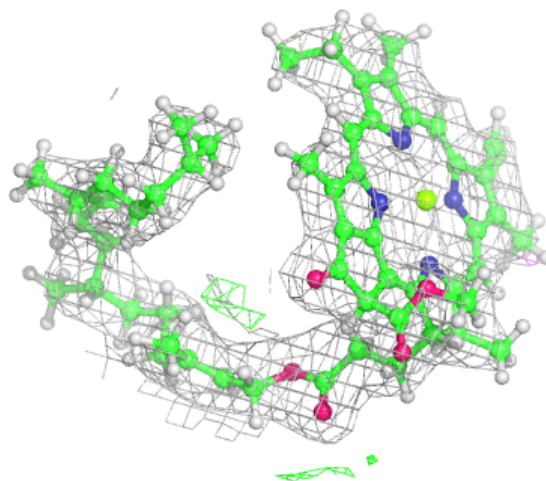
Electron density around CLA c 508:

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



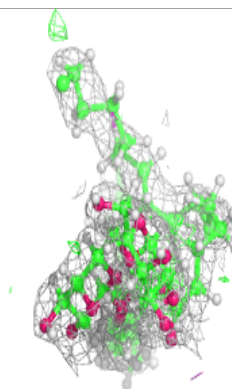
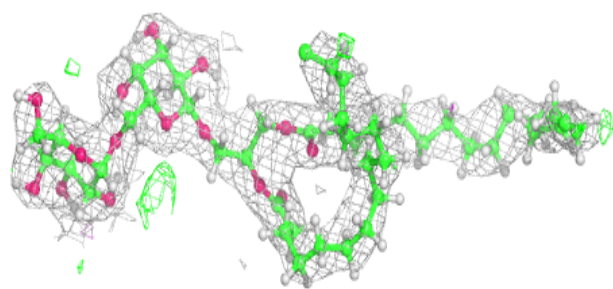
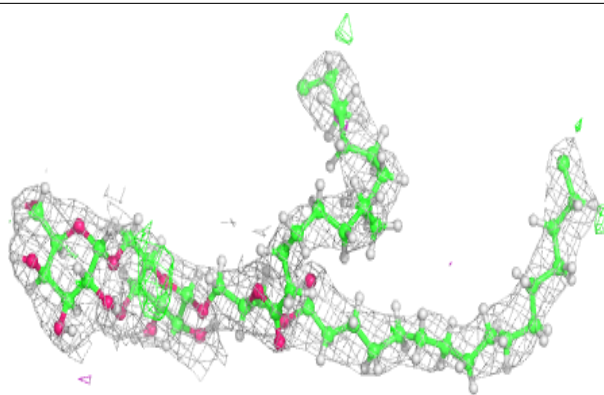
Electron density around CLA c 504:

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



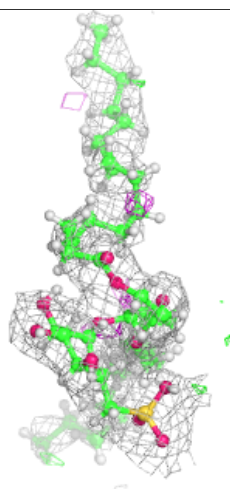
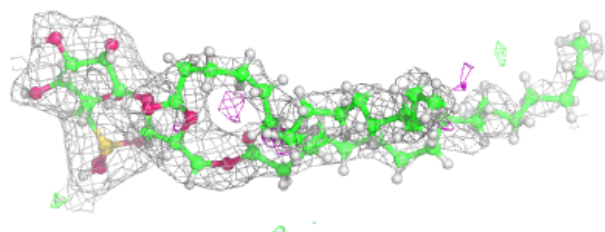
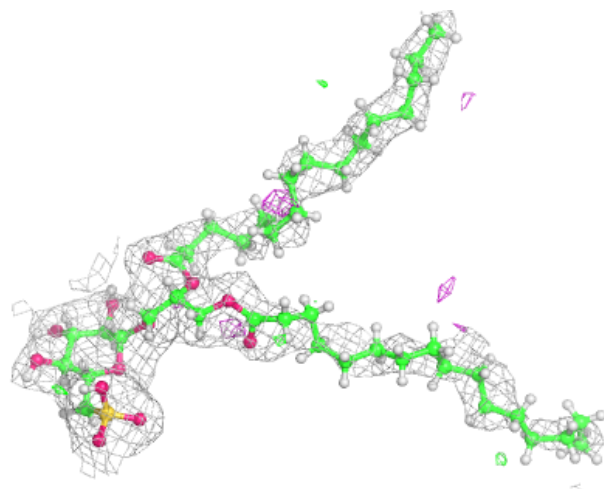
Electron density around DGD h 102:

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



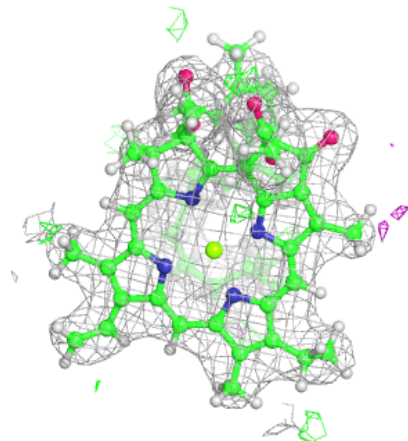
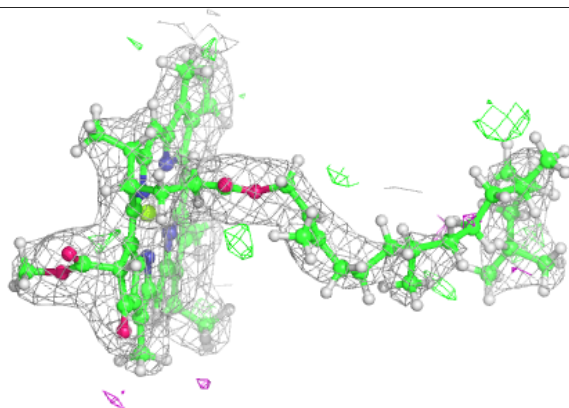
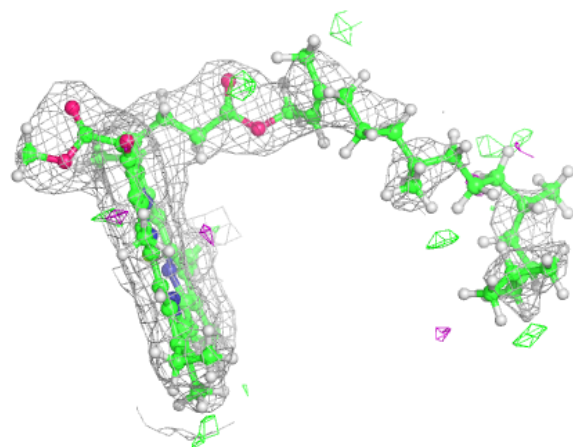
Electron density around SQD a 411:

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



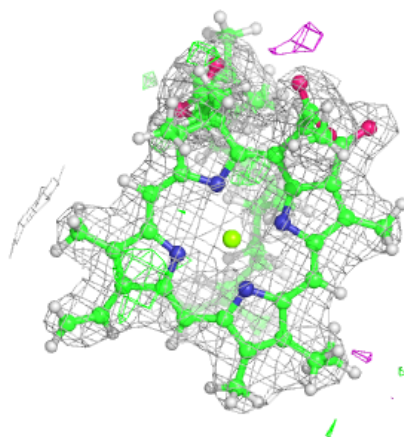
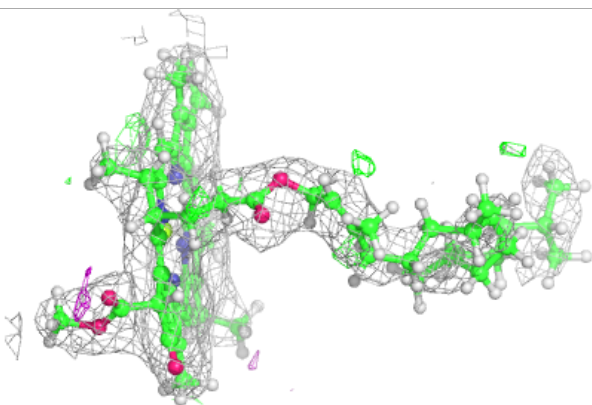
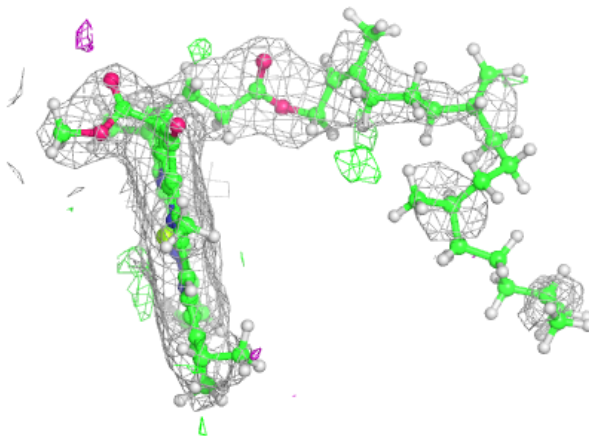
Electron density around CLA C 506:

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



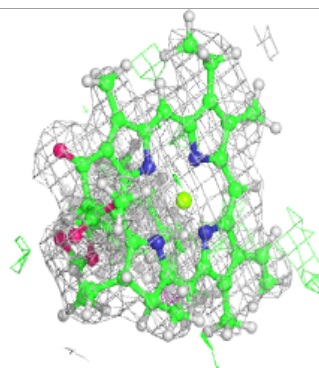
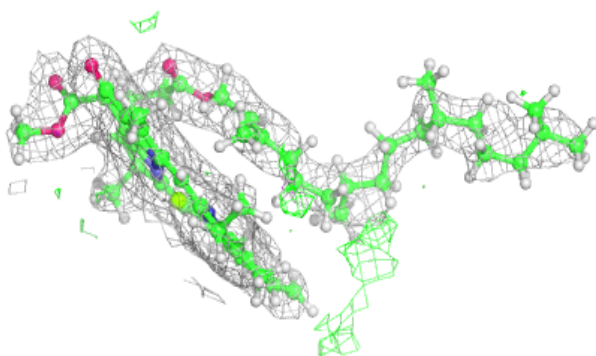
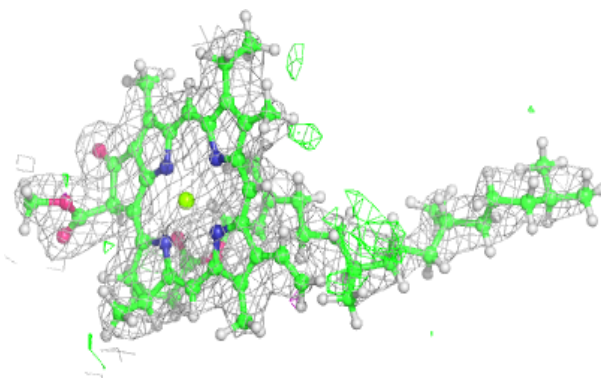
Electron density around CLA c 507:

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

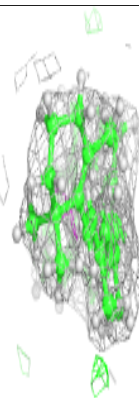
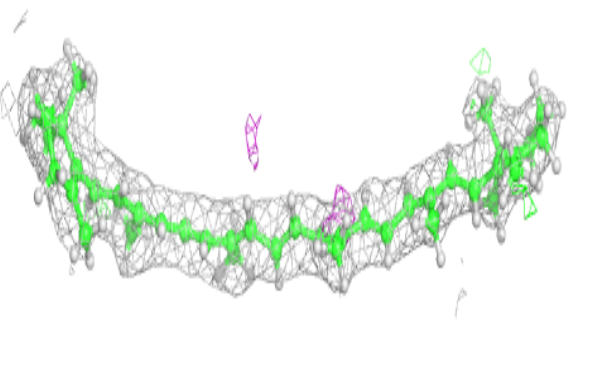
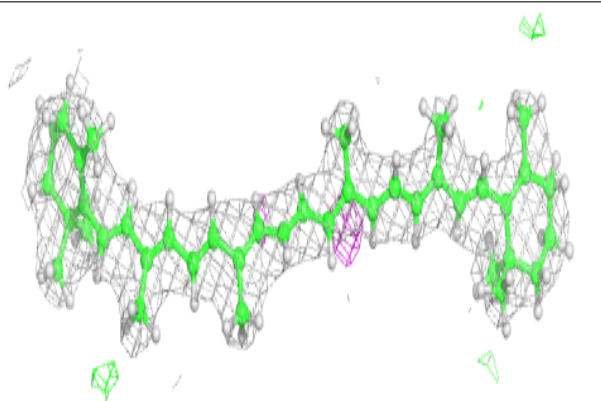


Electron density around CLA C 505:

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

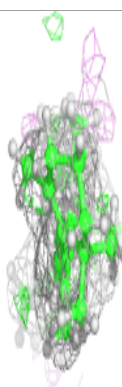
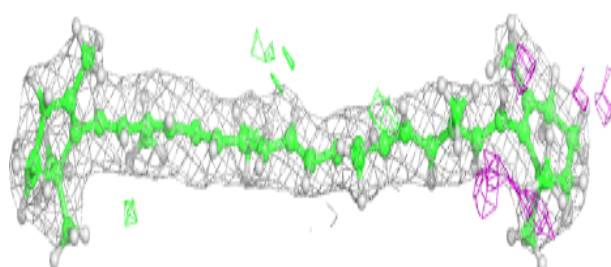
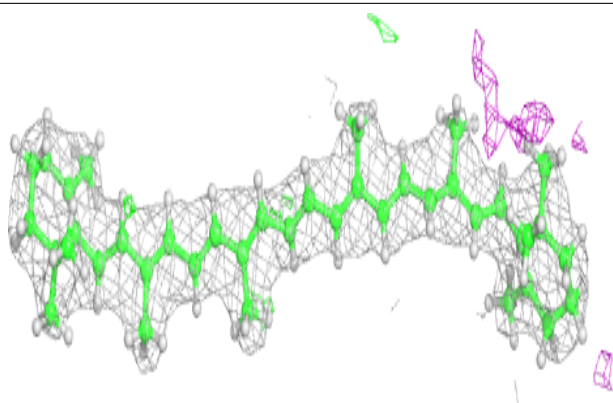
**Electron density around BCR T 101:**

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

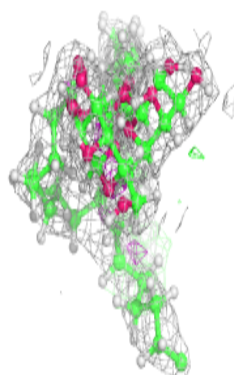
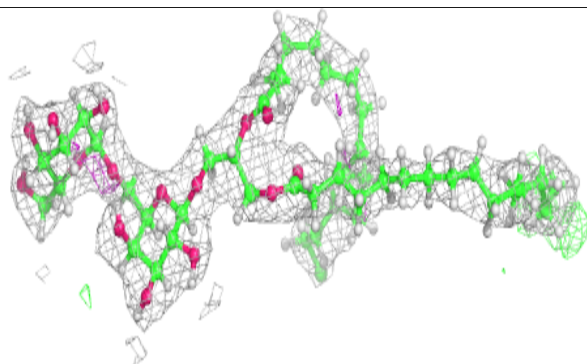
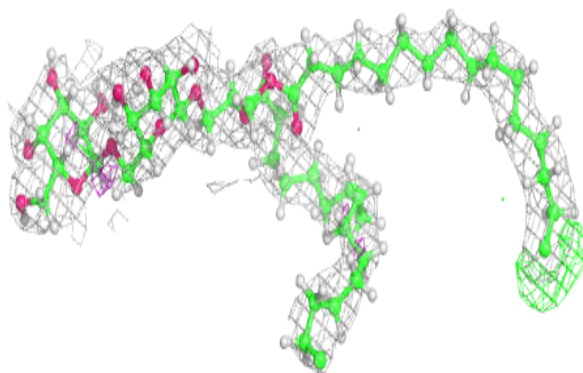


Electron density around BCR B 618:

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

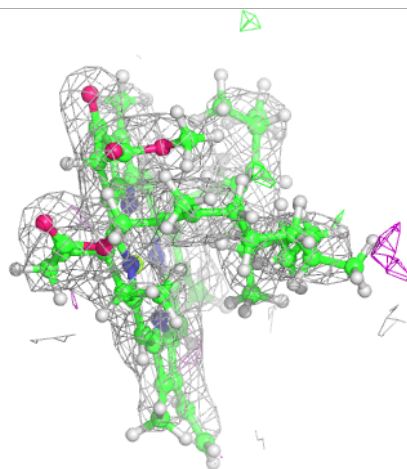
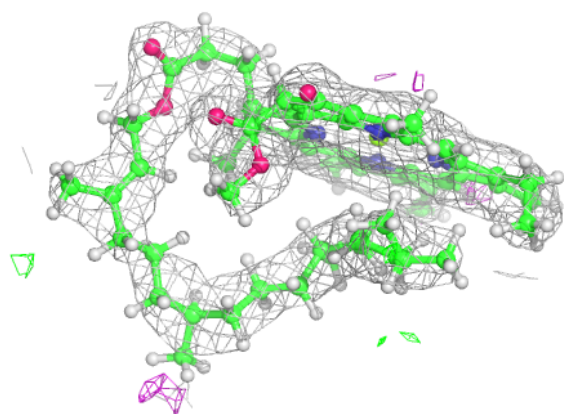
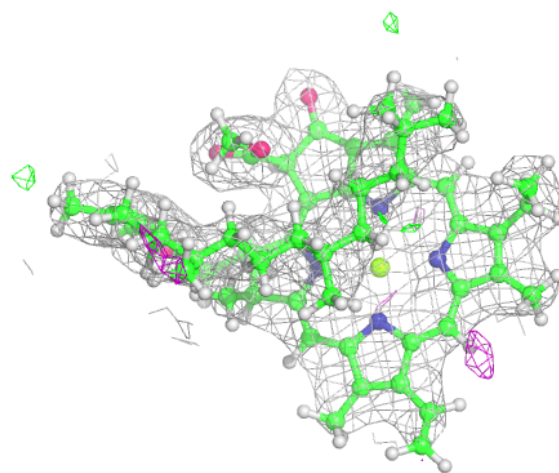
**Electron density around DGD H 103:**

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



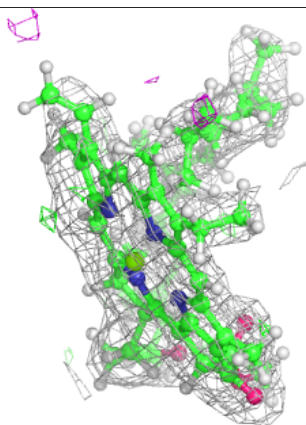
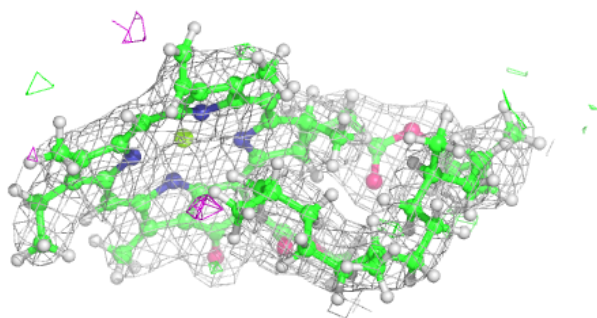
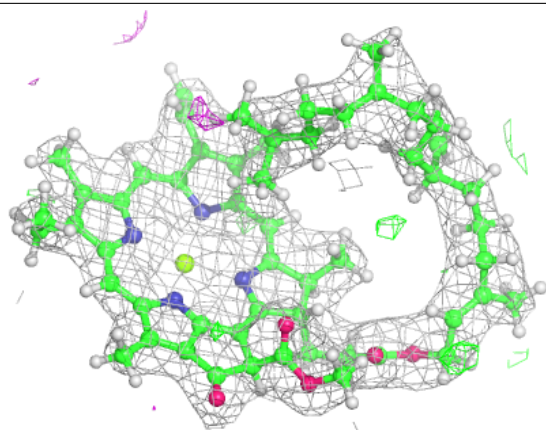
Electron density around CLA C 510:

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

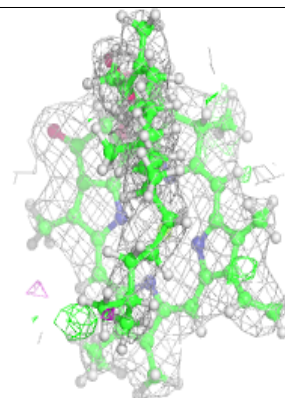
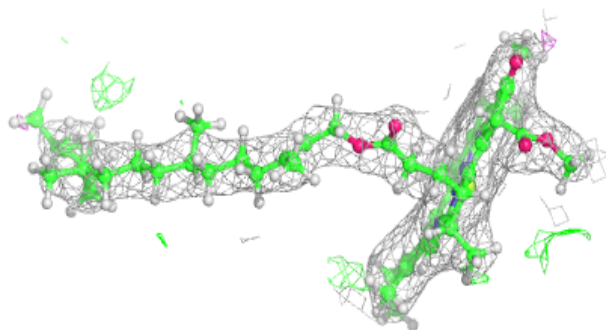
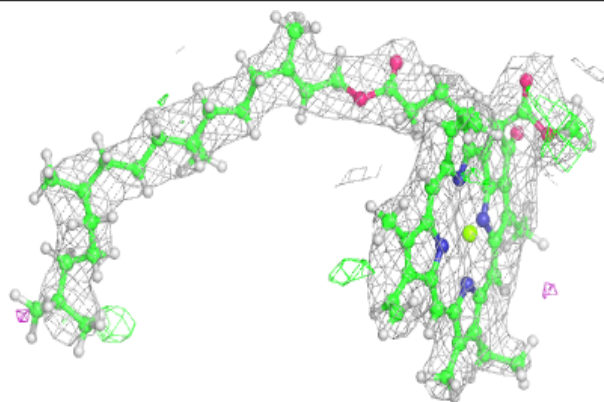


Electron density around CLA B 615:

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

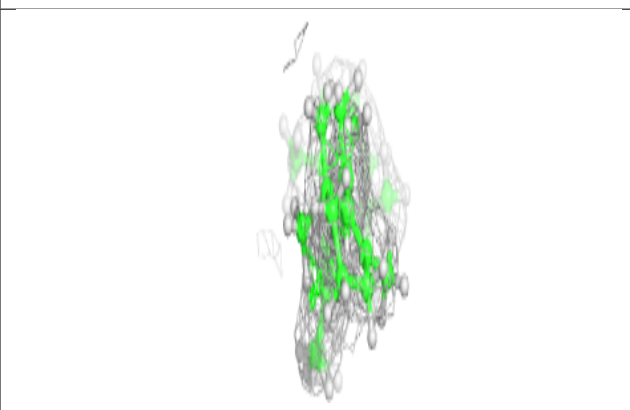
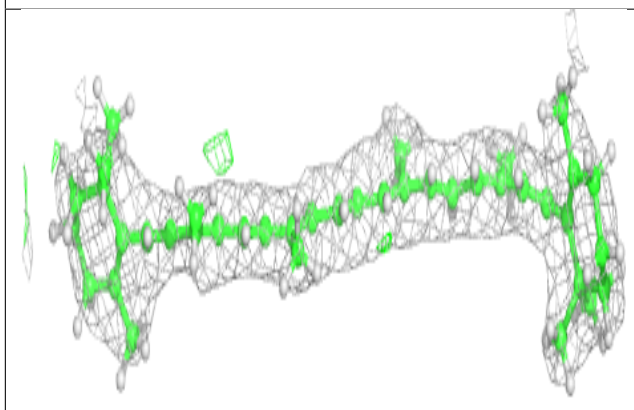
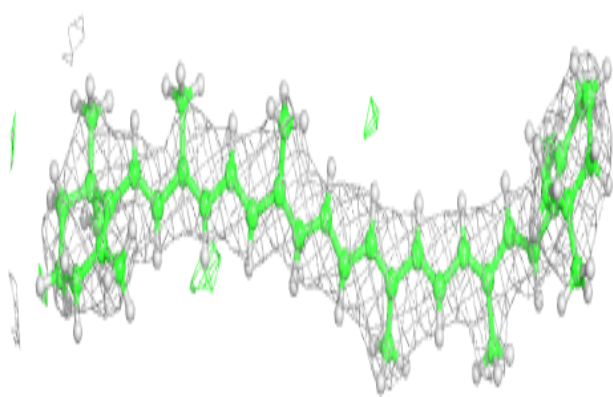
**Electron density around CLA b 609:**

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

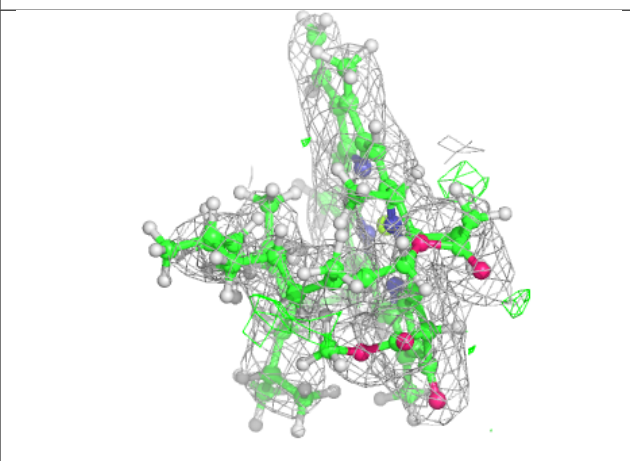
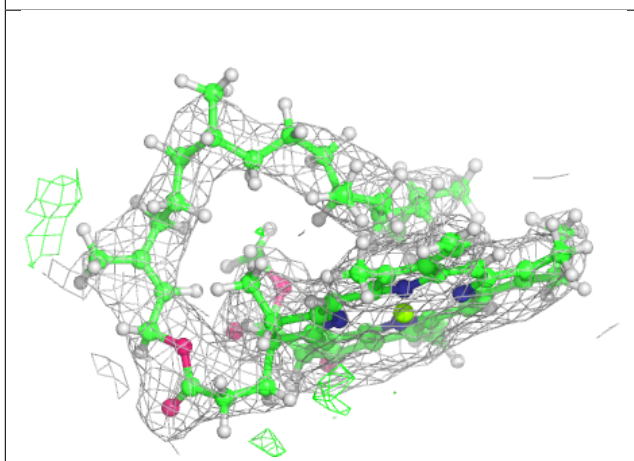
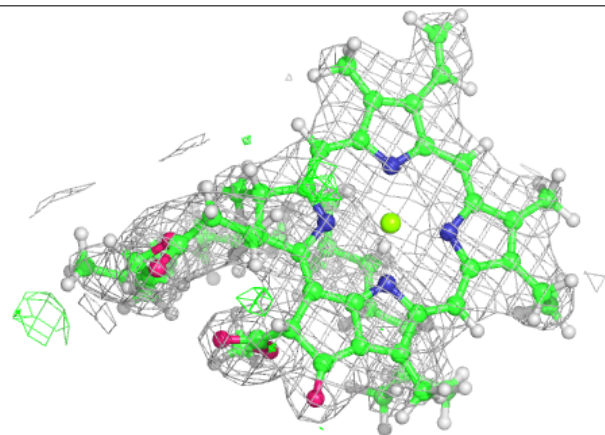


Electron density around BCR c 516:

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

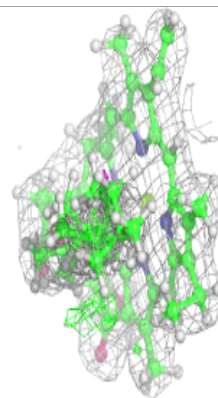
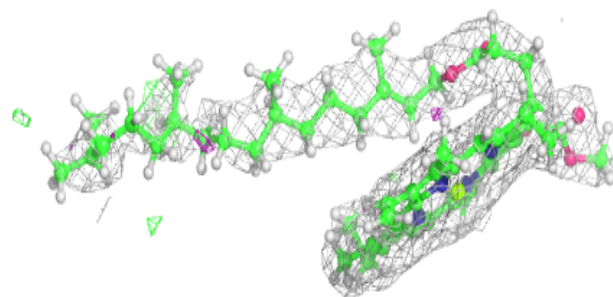
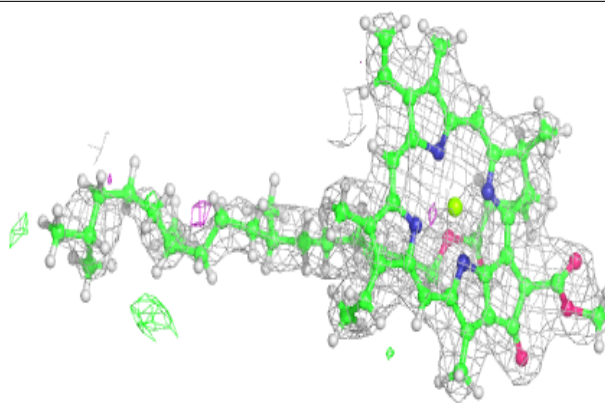
**Electron density around CLA c 511:**

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



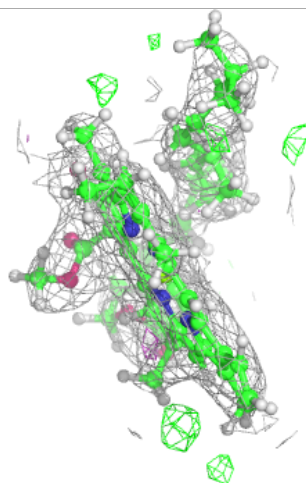
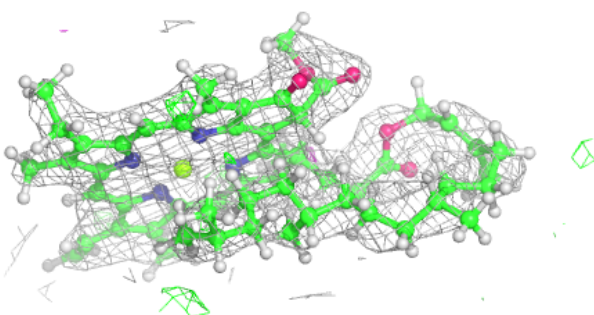
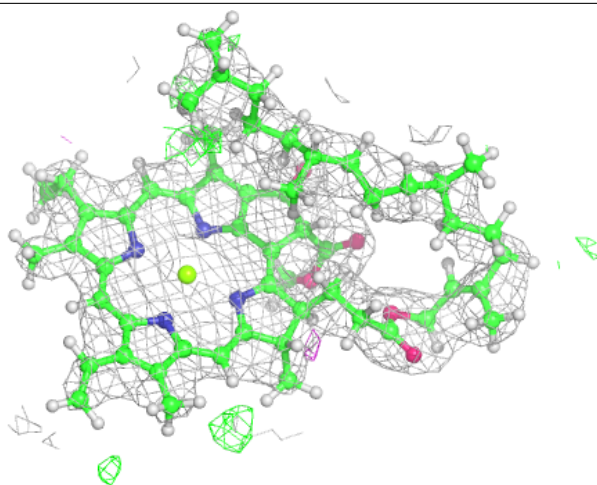
Electron density around CLA B 614:

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



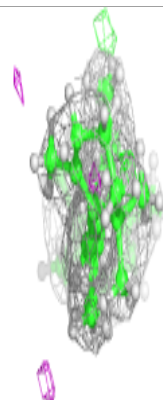
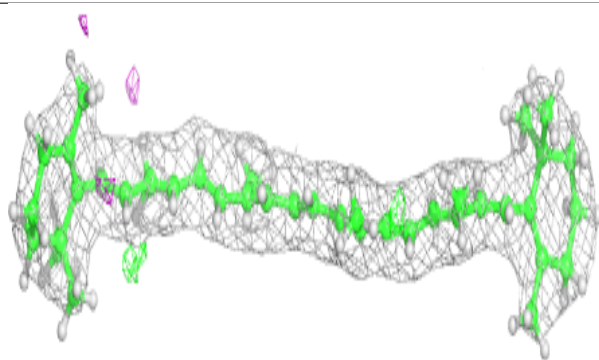
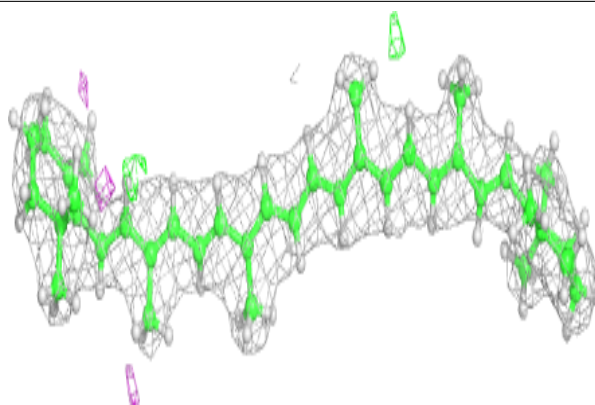
Electron density around CLA c 510:

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



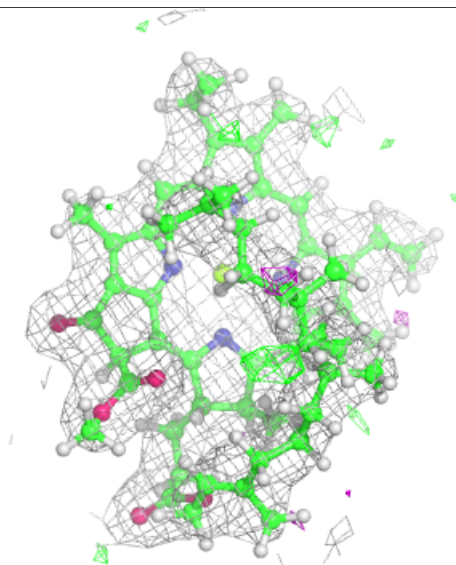
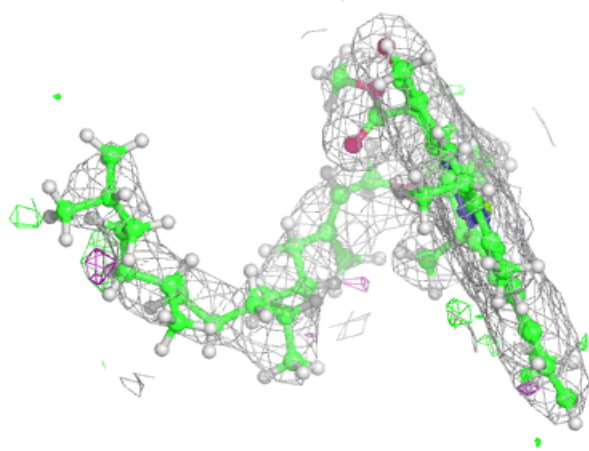
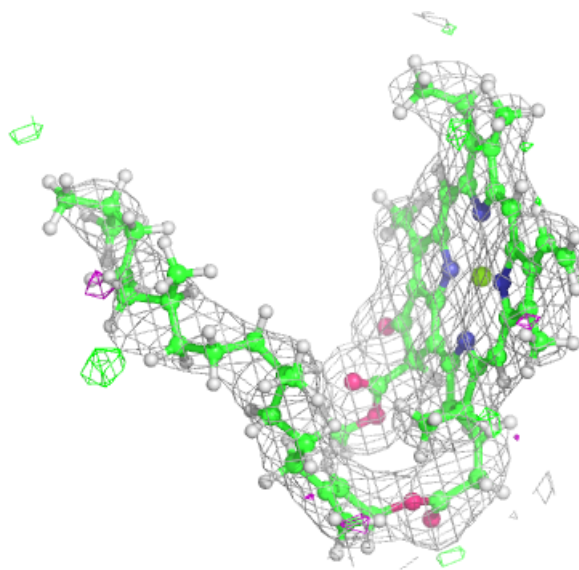
Electron density around BCR A 406:

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



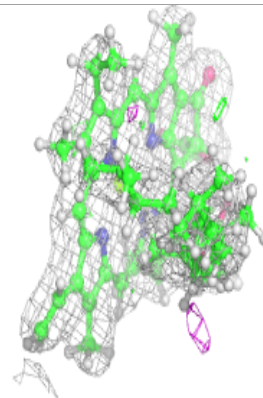
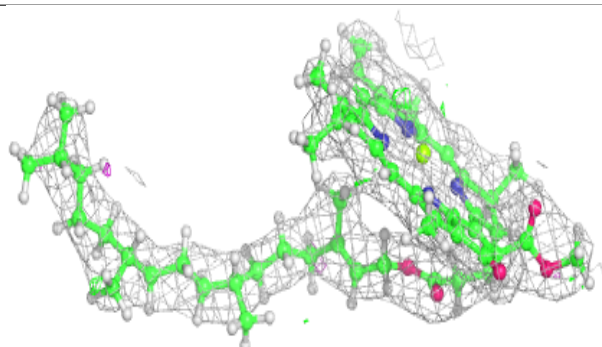
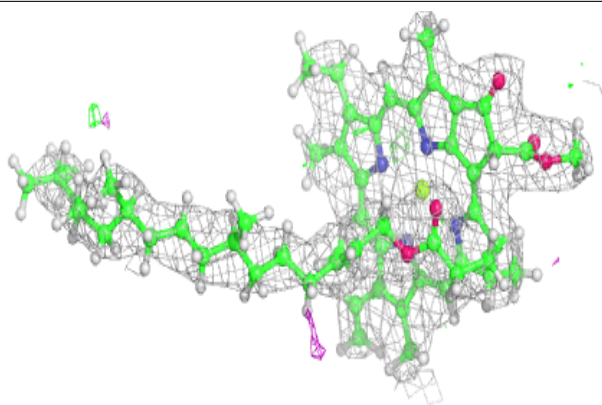
Electron density around CLA B 613:

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

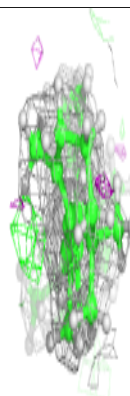
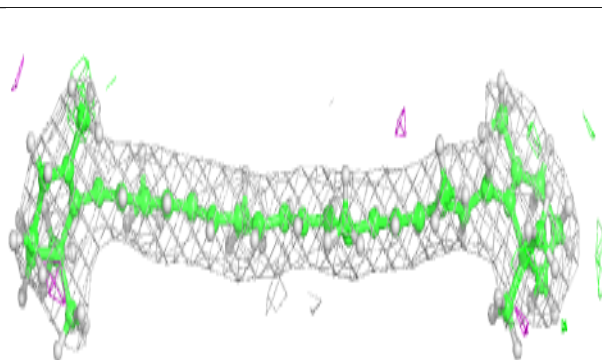
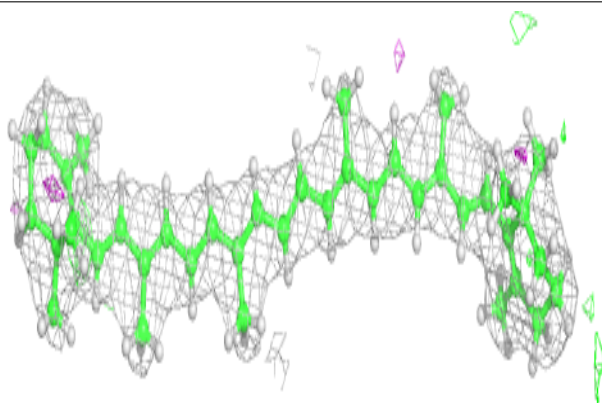


Electron density around CLA b 608:

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

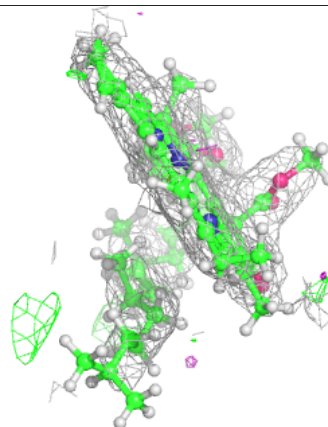
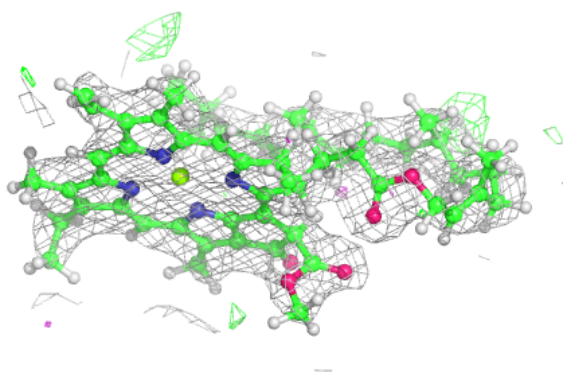
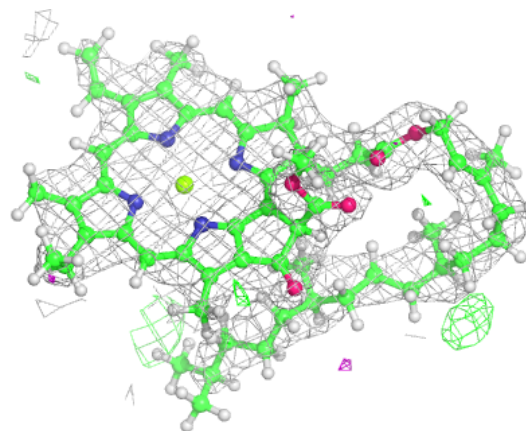
**Electron density around BCR b 618:**

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

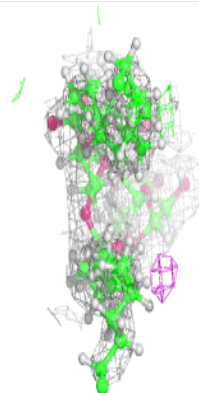
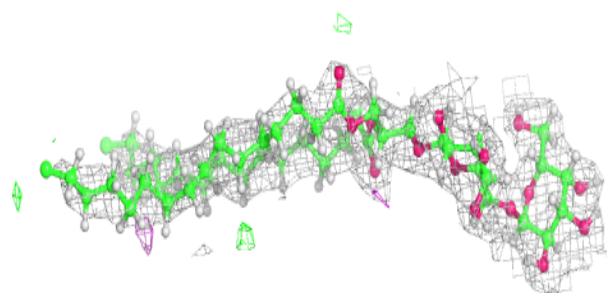
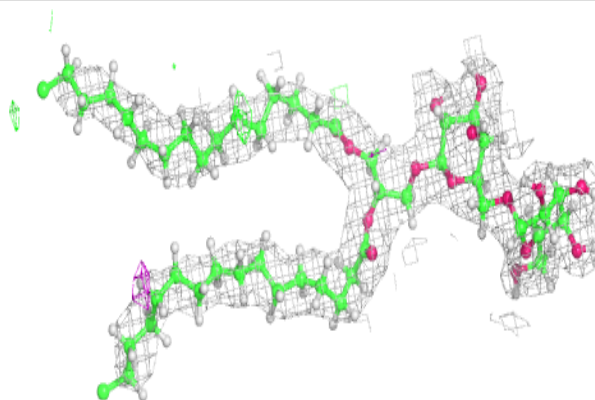


Electron density around CLA C 509:

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

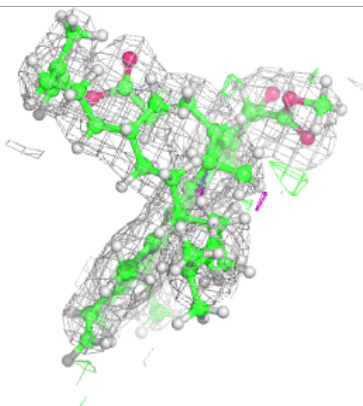
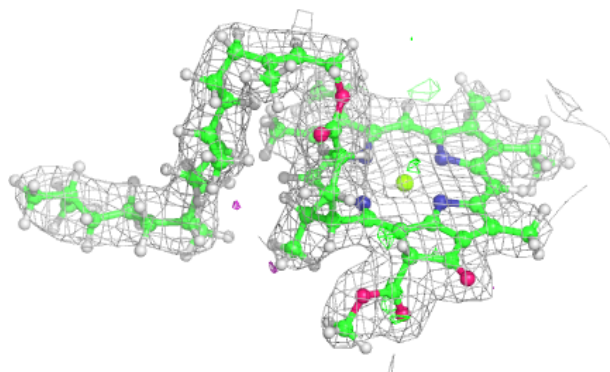
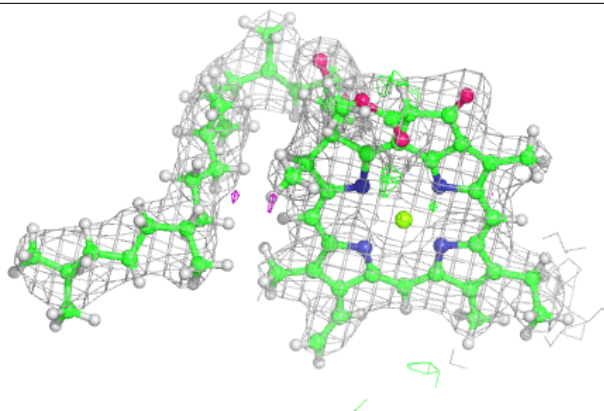
**Electron density around DGD C 517:**

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

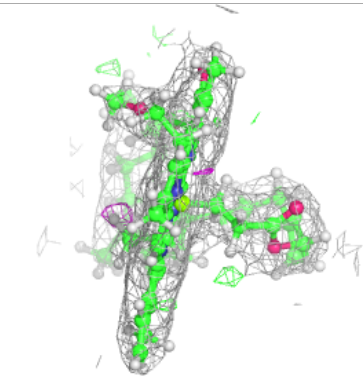
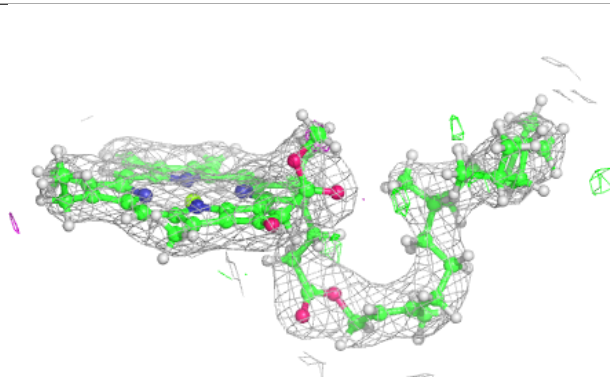
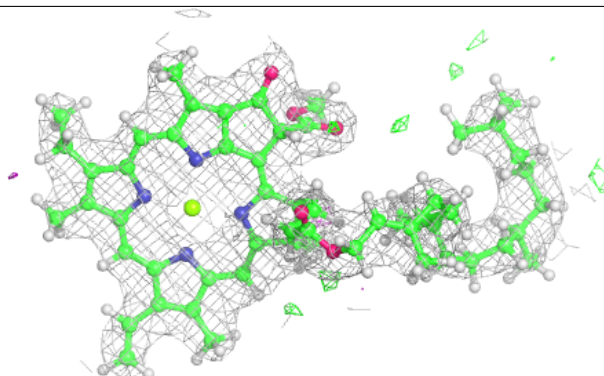


Electron density around CLA a 410:

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

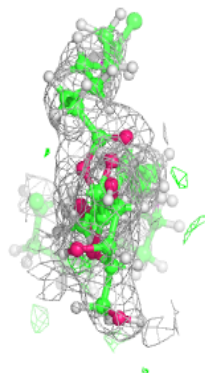
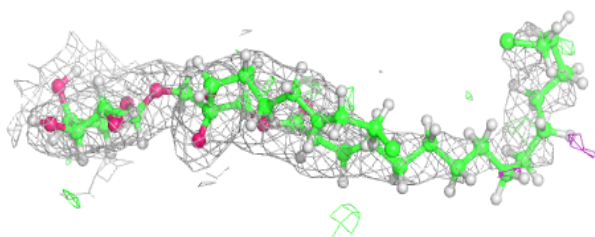
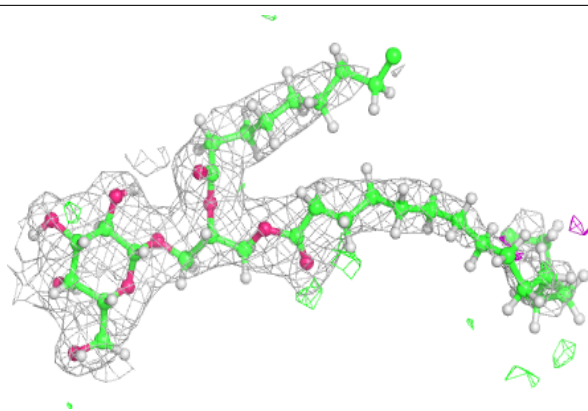
**Electron density around CLA b 612:**

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

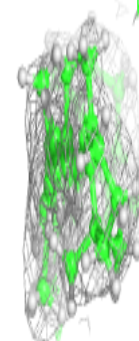
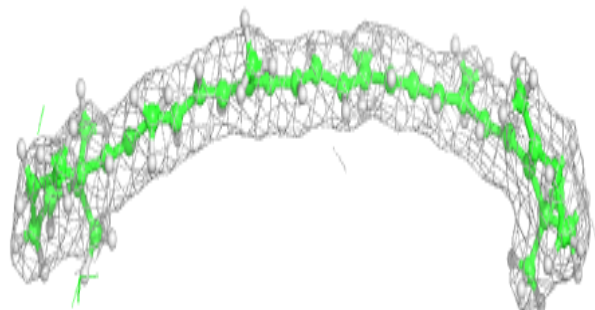
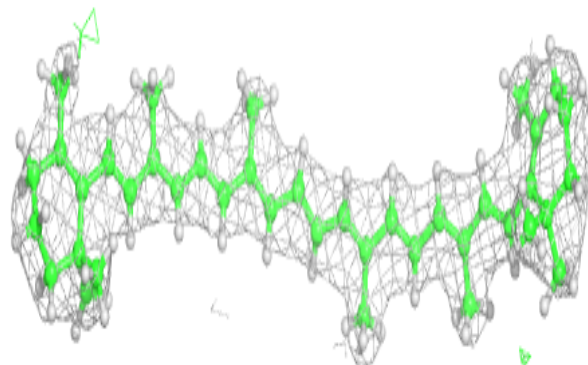


Electron density around LMG d 410:

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

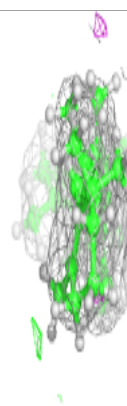
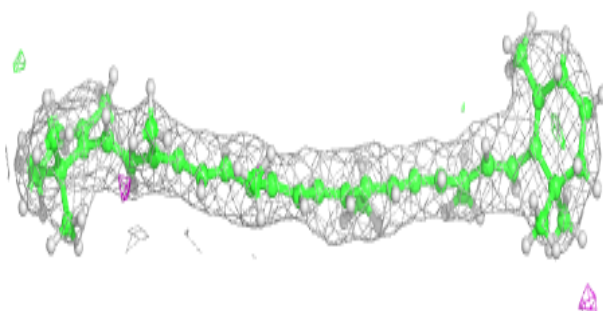
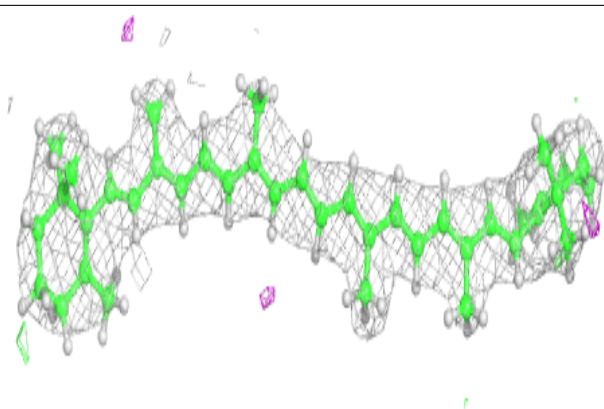
**Electron density around BCR t 101:**

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

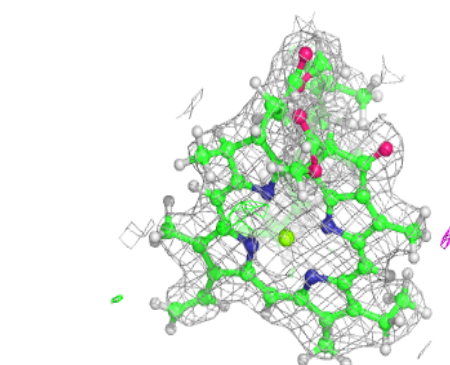
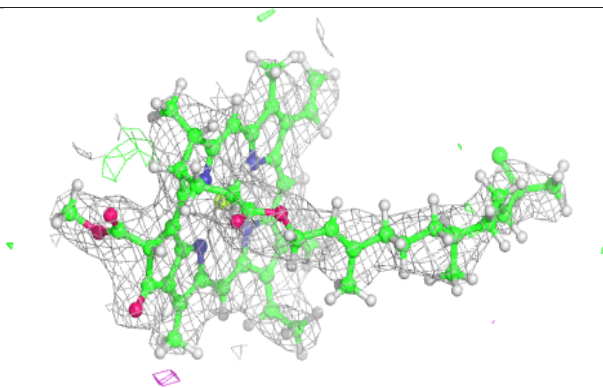
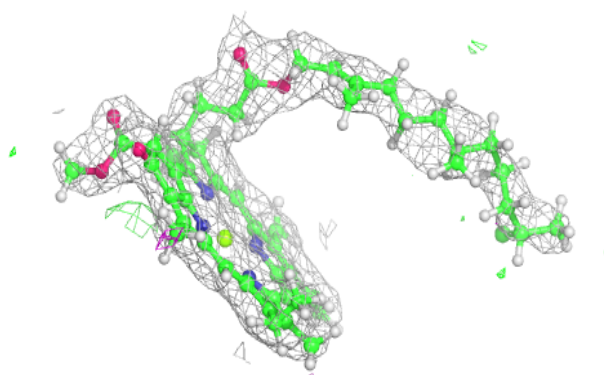


Electron density around BCR b 617:

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

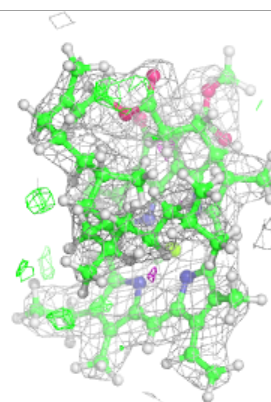
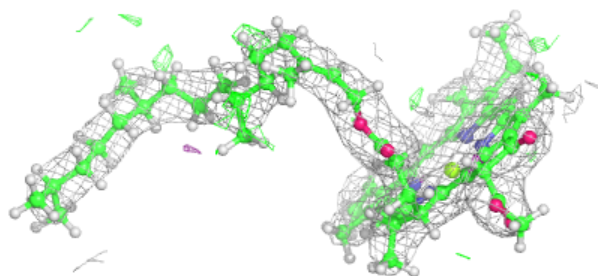
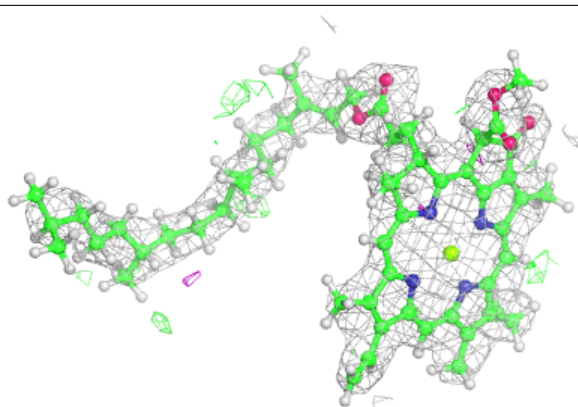
**Electron density around CLA c 505:**

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



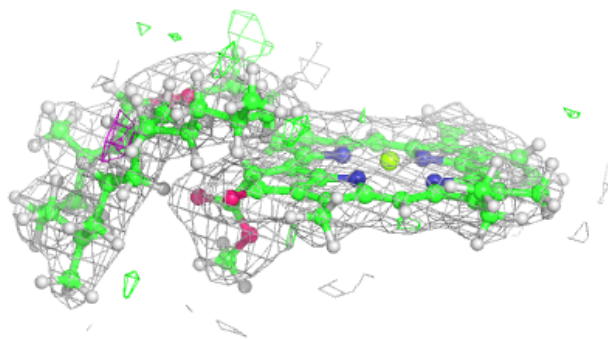
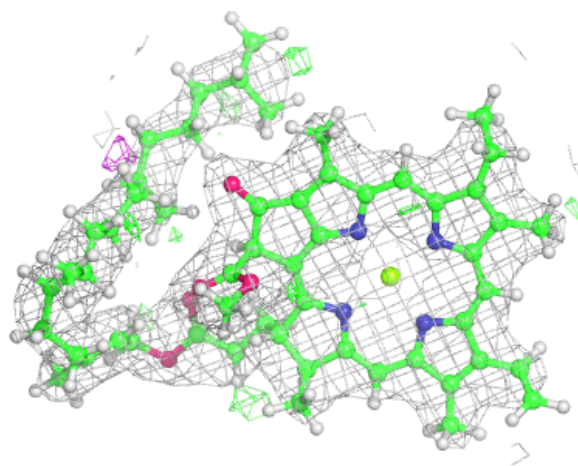
Electron density around CLA C 511:

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



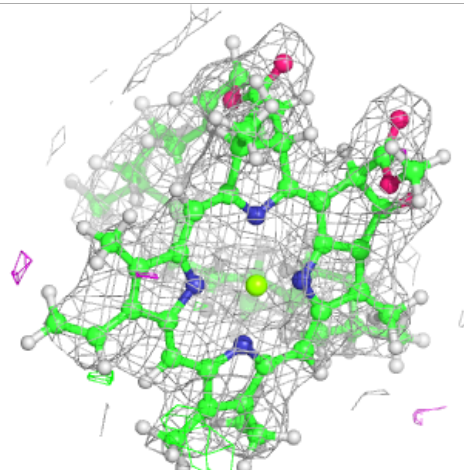
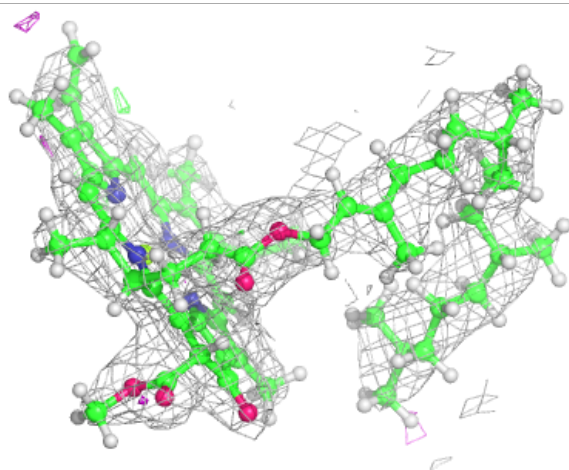
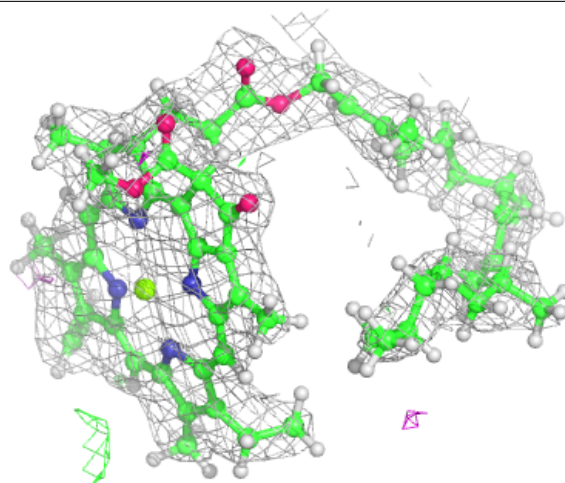
Electron density around CLA b 610:

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



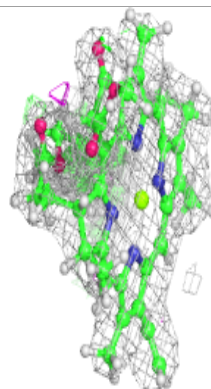
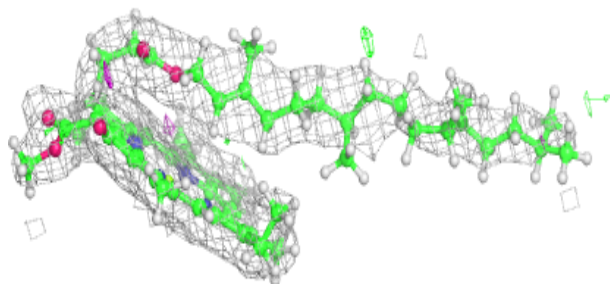
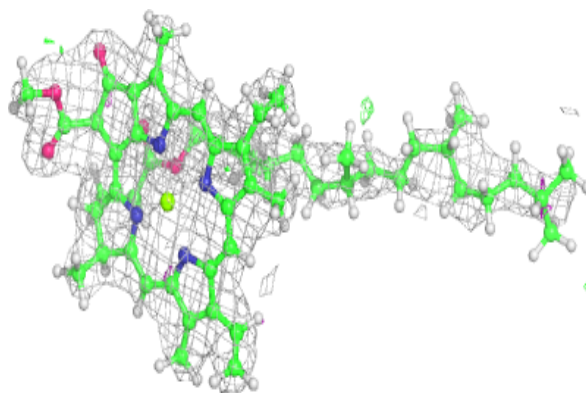
Electron density around CLA C 503:

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

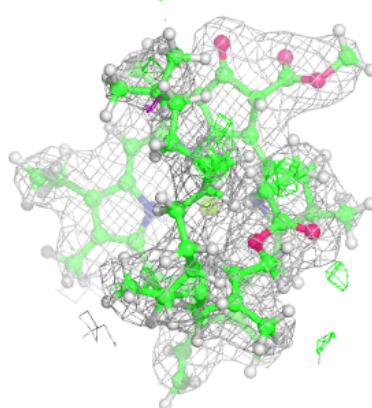
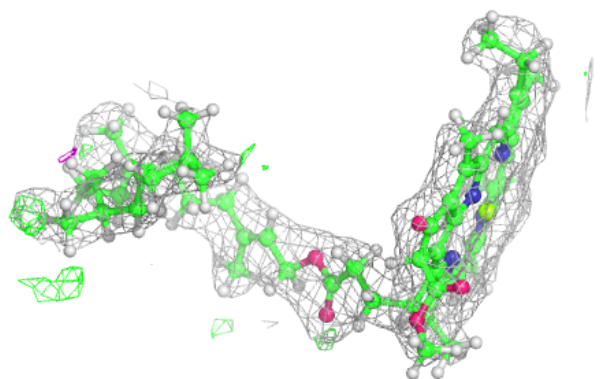
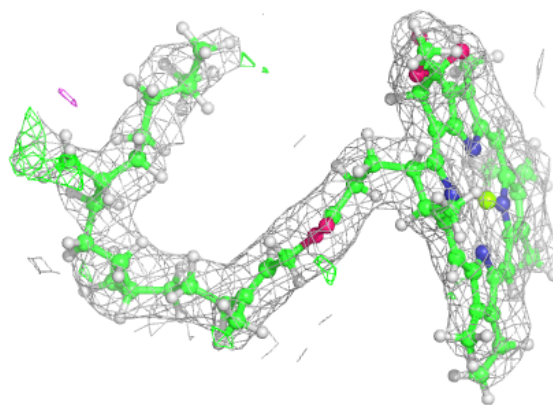


Electron density around CLA b 614:

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

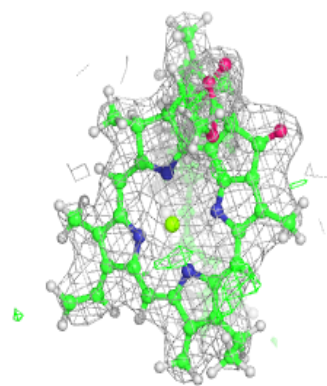
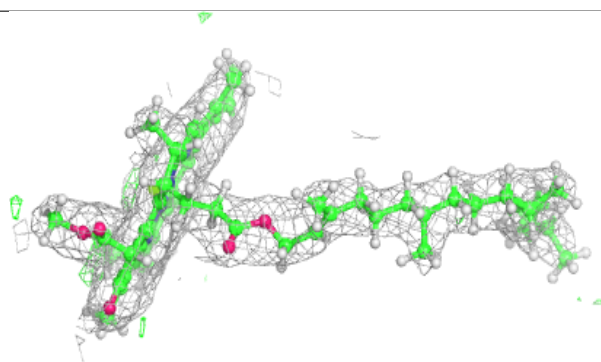
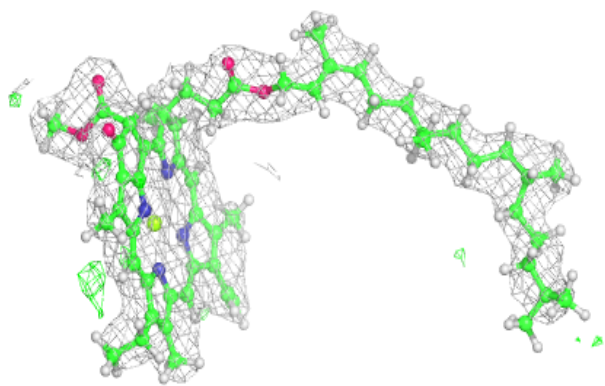
**Electron density around CLA B 606:**

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

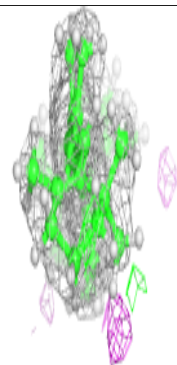
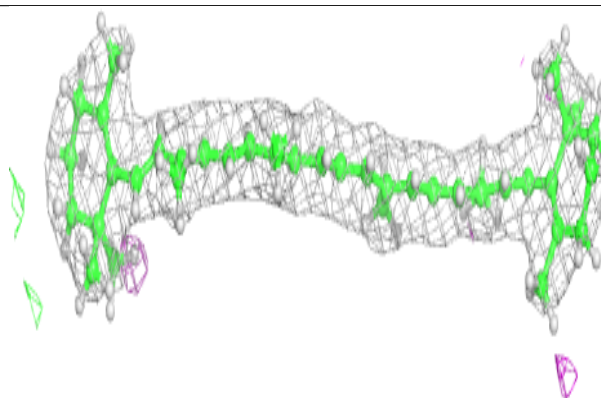
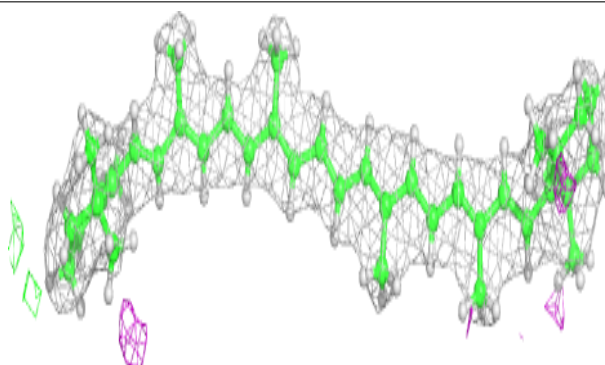


Electron density around CLA B 609:

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

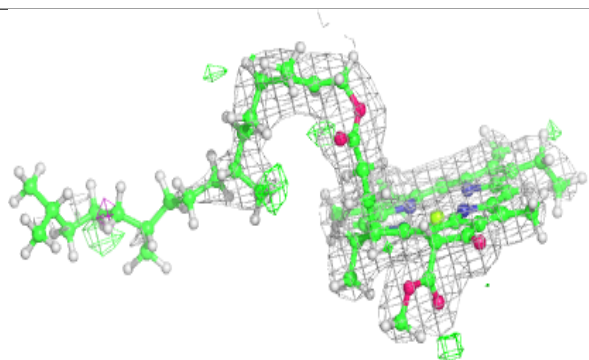
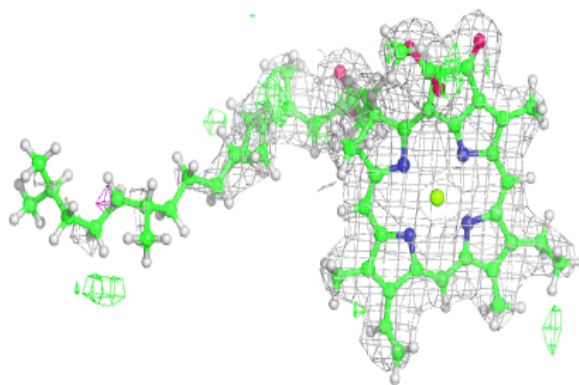
**Electron density around BCR a 406:**

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

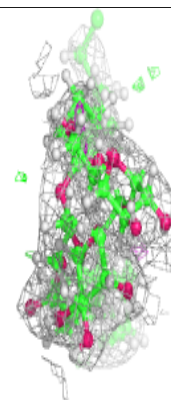
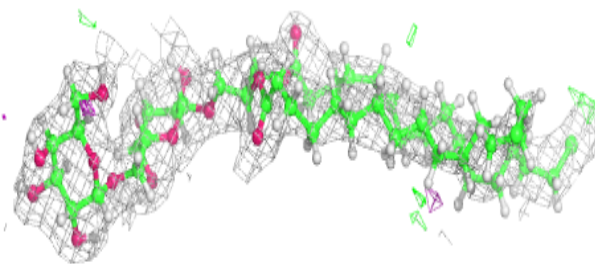
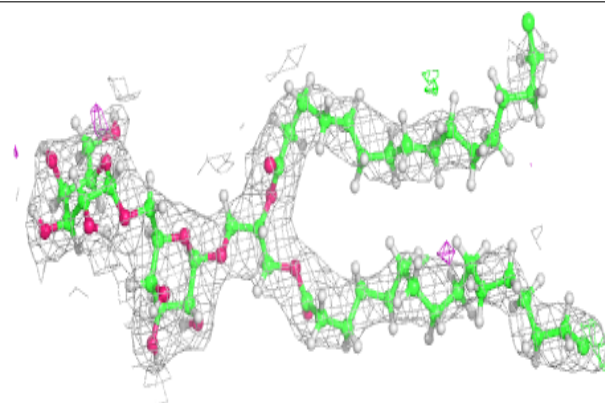


Electron density around CLA A 403:

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

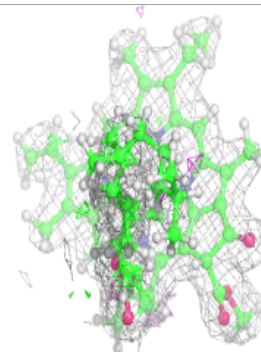
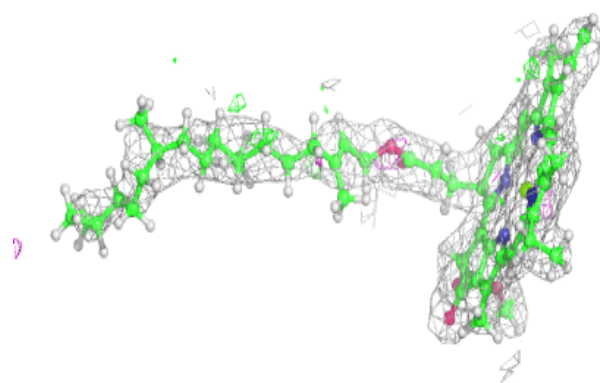
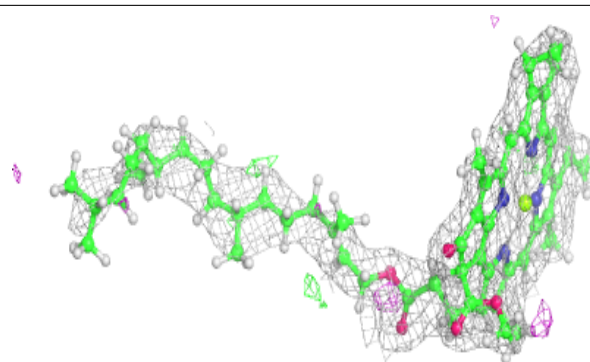
**Electron density around DGD c 519:**

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

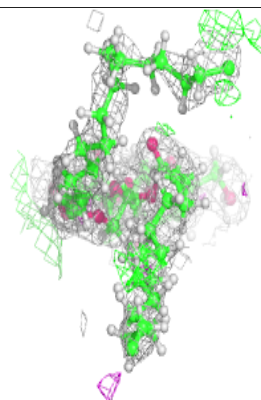
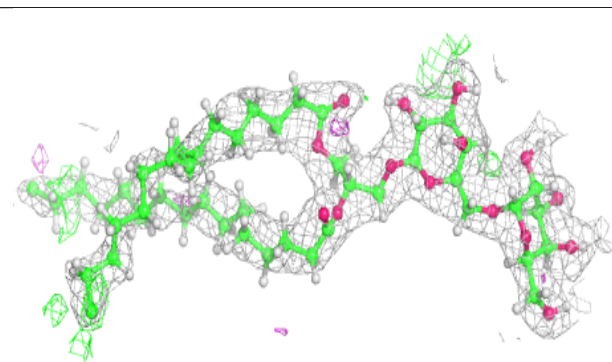
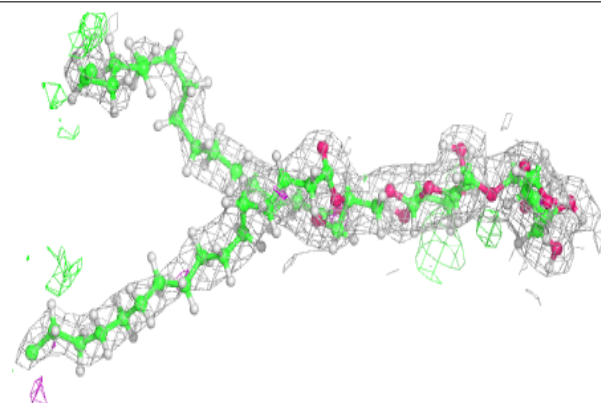


Electron density around CLA B 604:

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

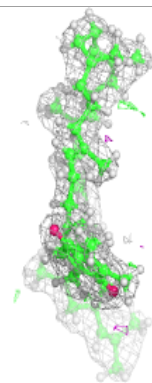
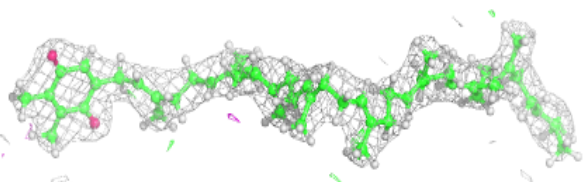
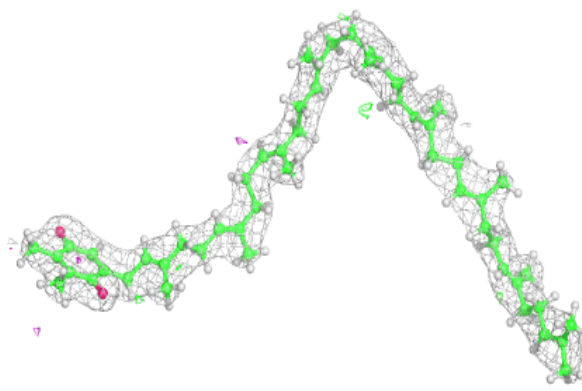
**Electron density around DGD C 515:**

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

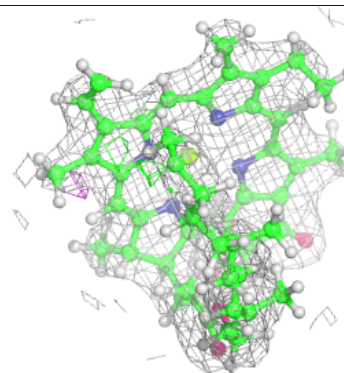
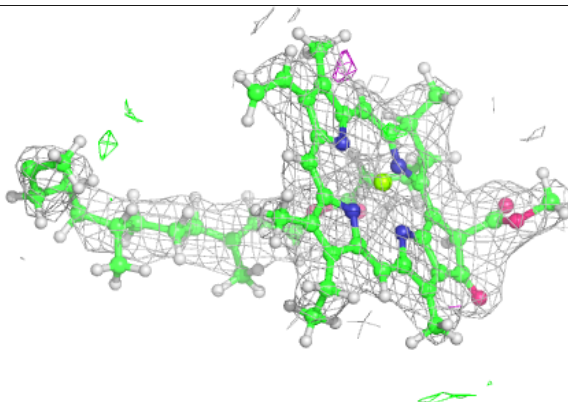
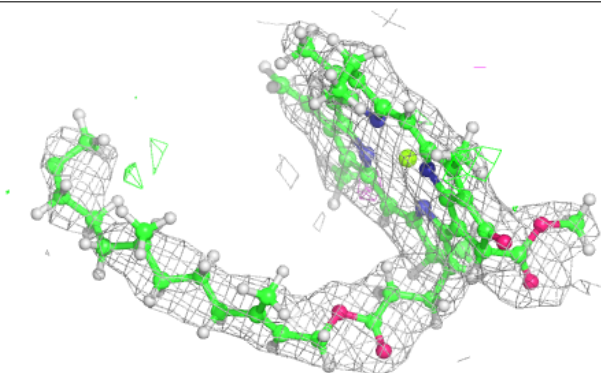


Electron density around PL9 D 406:

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

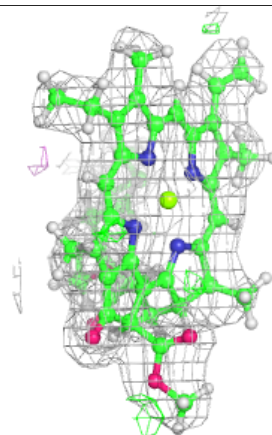
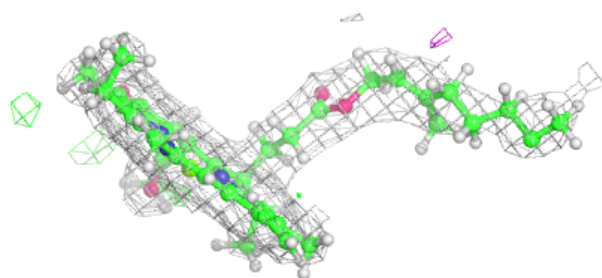
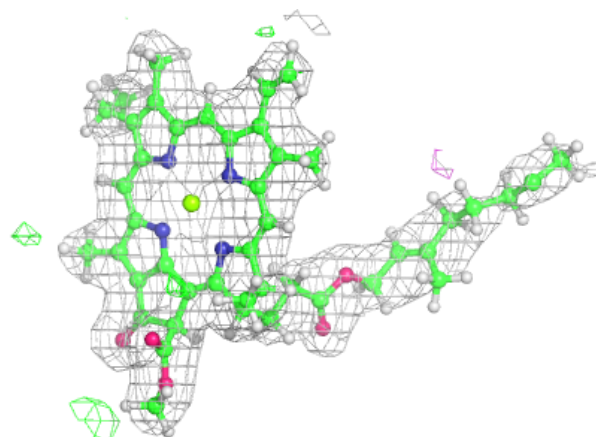
**Electron density around CLA C 504:**

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

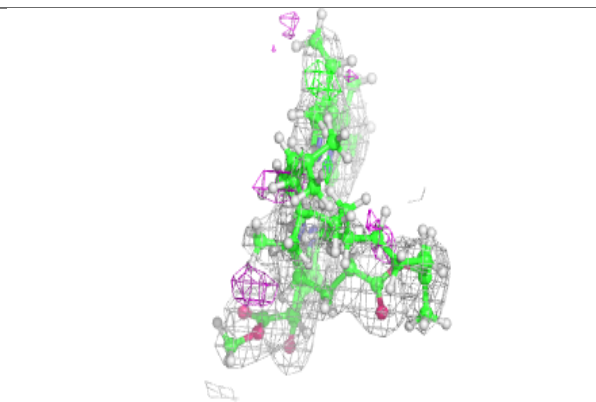
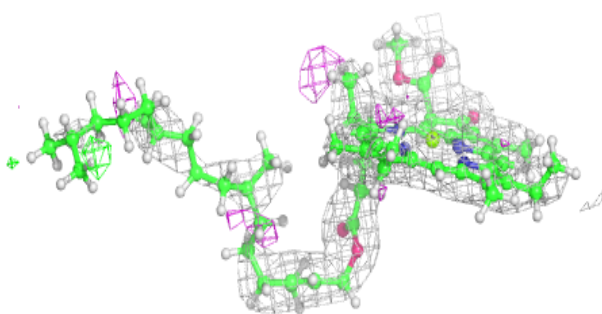
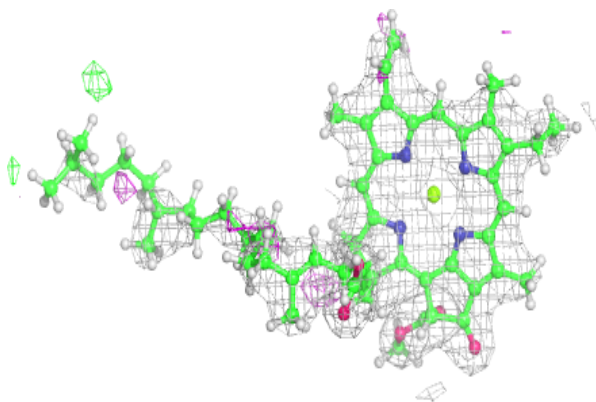


Electron density around CLA A 405:

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

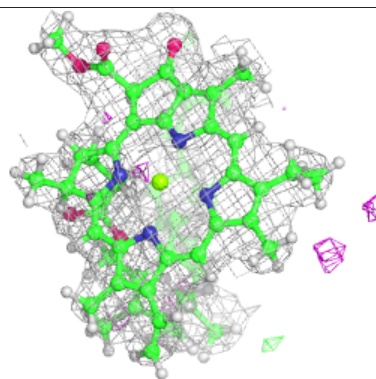
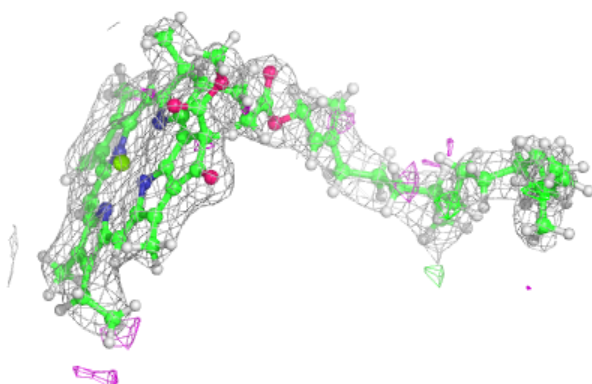
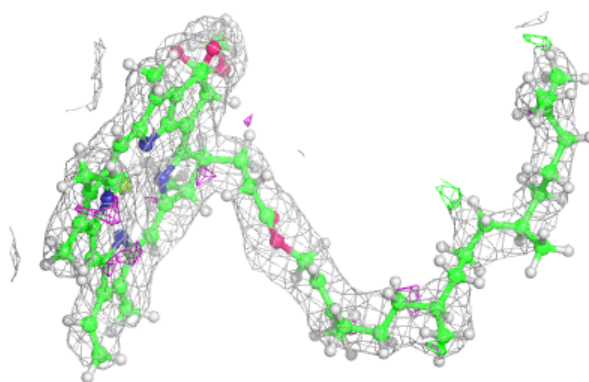
**Electron density around CLA a 403:**

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

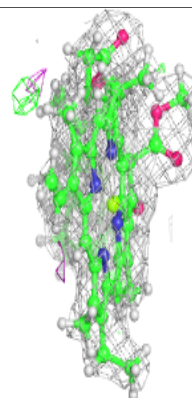
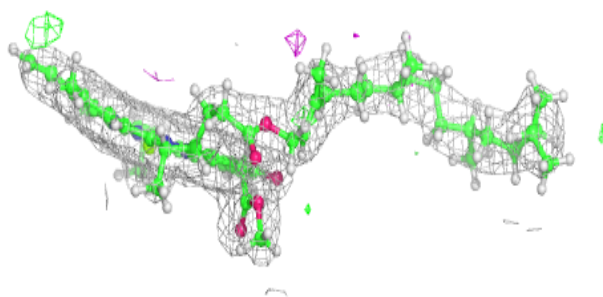
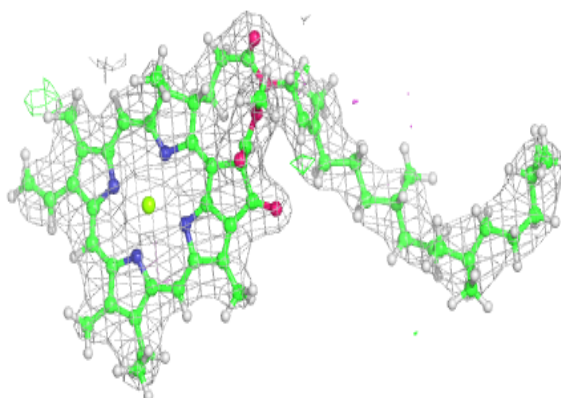


Electron density around CLA b 606:

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

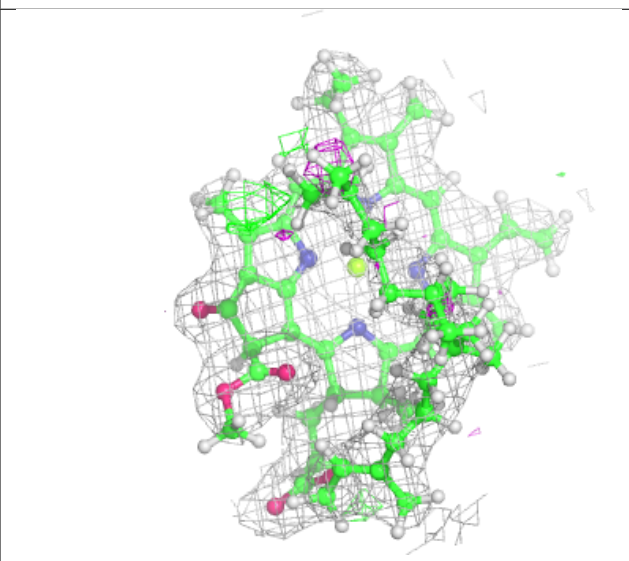
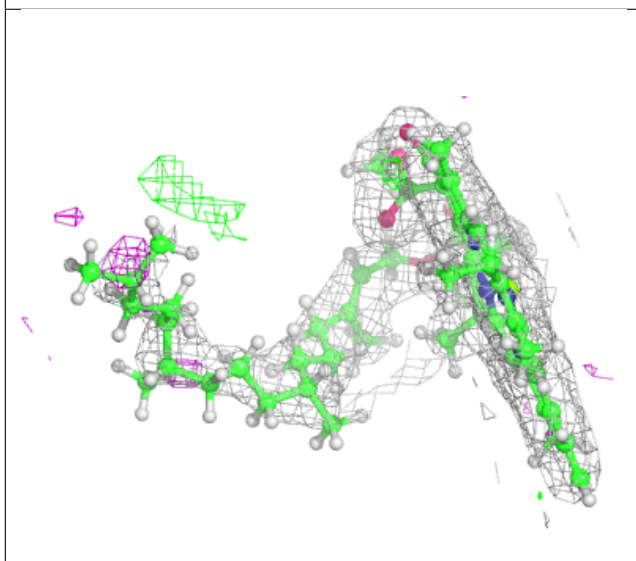
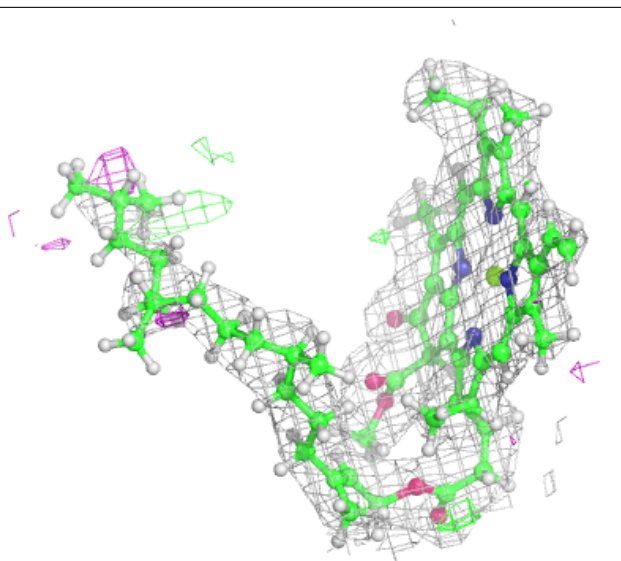
**Electron density around CLA B 602:**

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



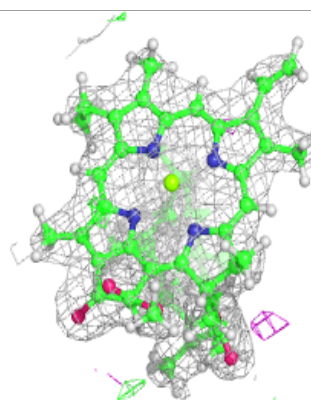
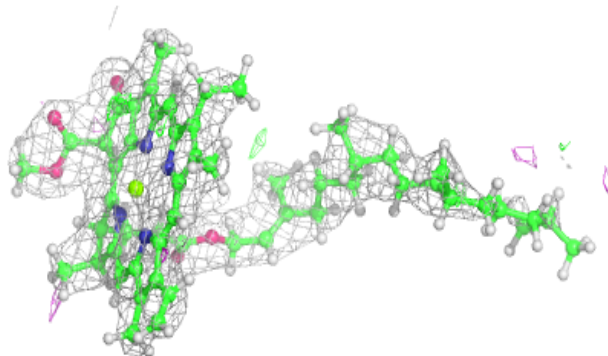
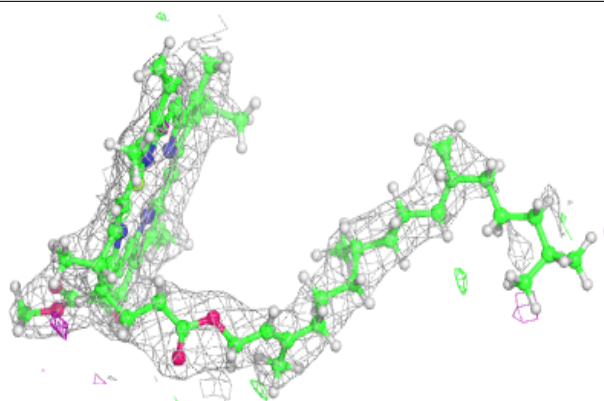
Electron density around CLA b 613:

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

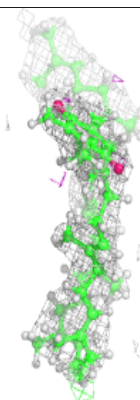
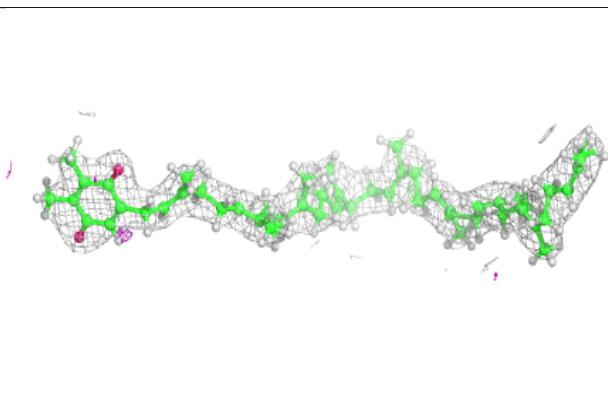
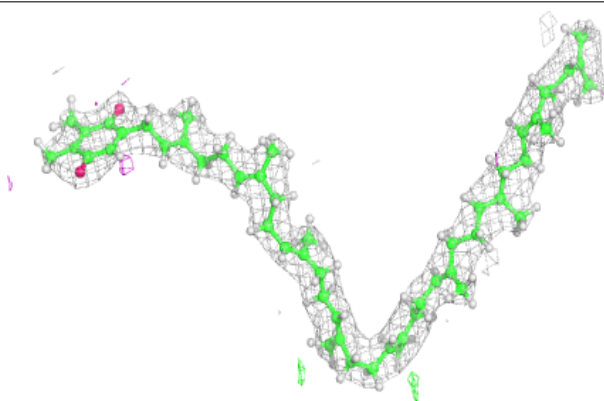


Electron density around CLA C 508:

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

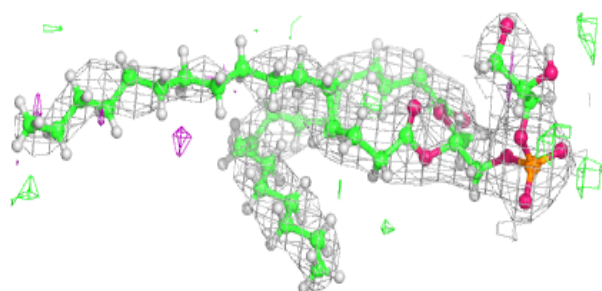
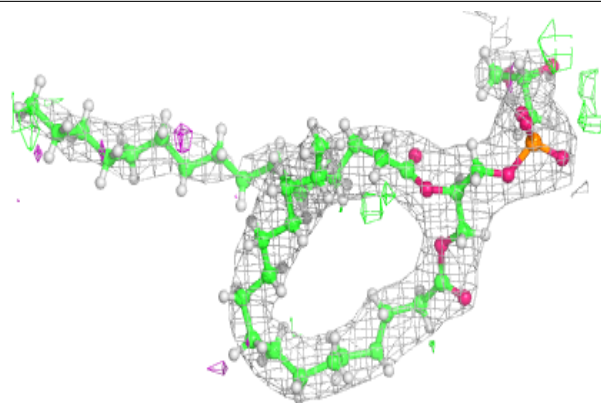
**Electron density around PL9 d 406:**

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

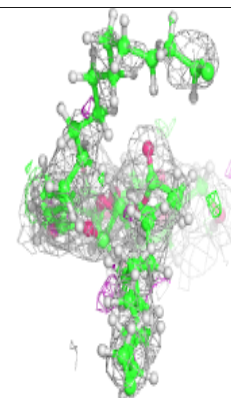
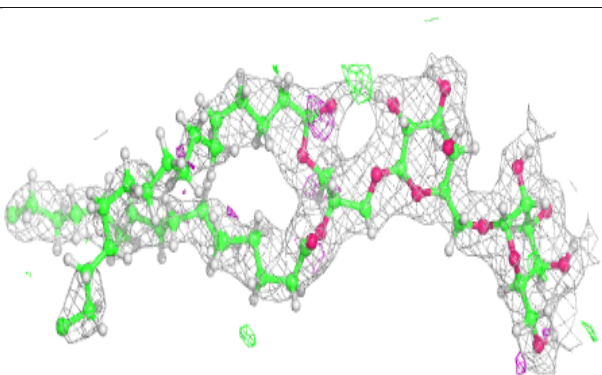
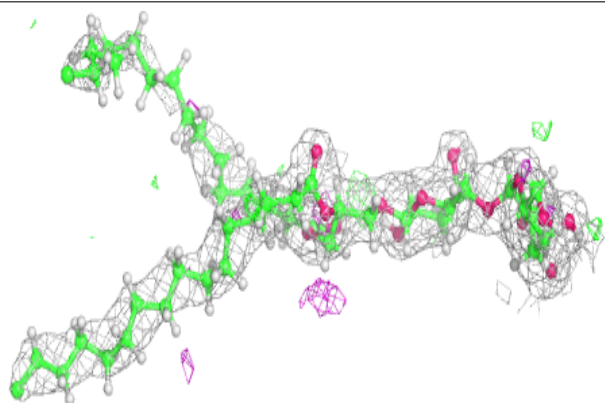


Electron density around LHG d 407:

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

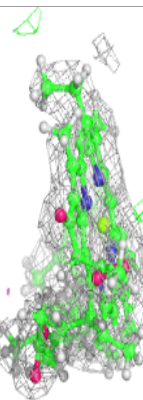
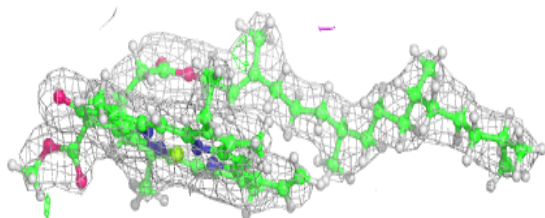
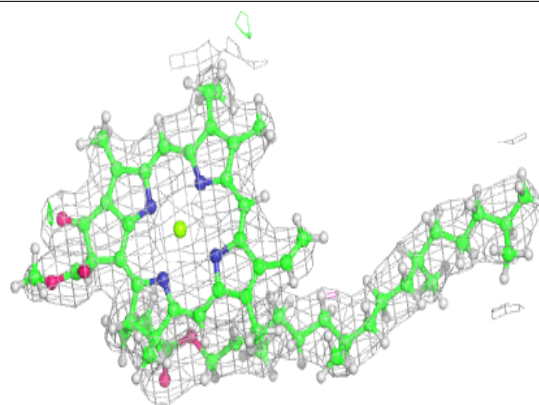
**Electron density around DGD c 517:**

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

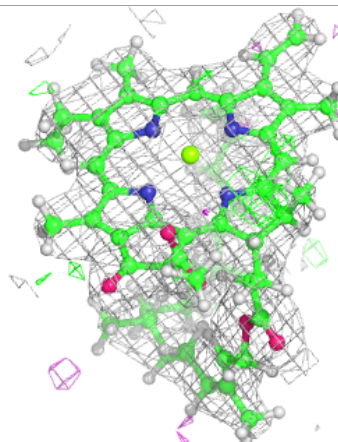
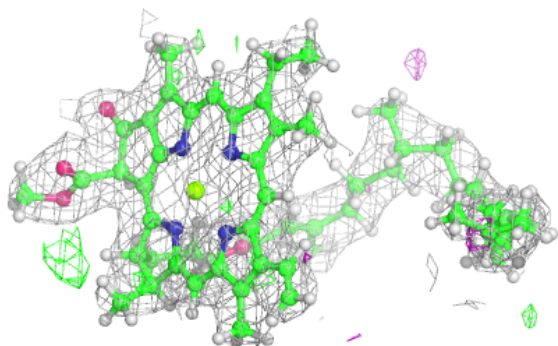
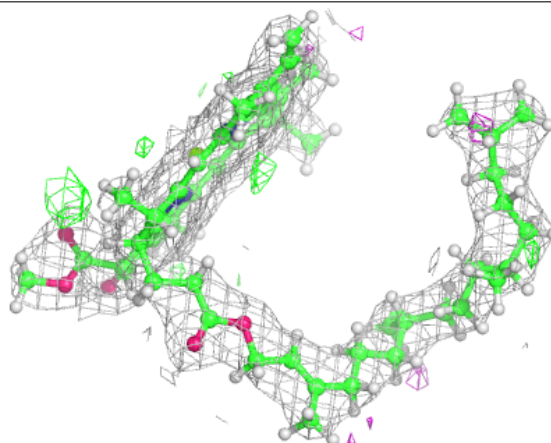


Electron density around CLA C 501:

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

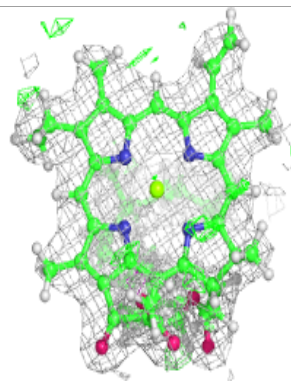
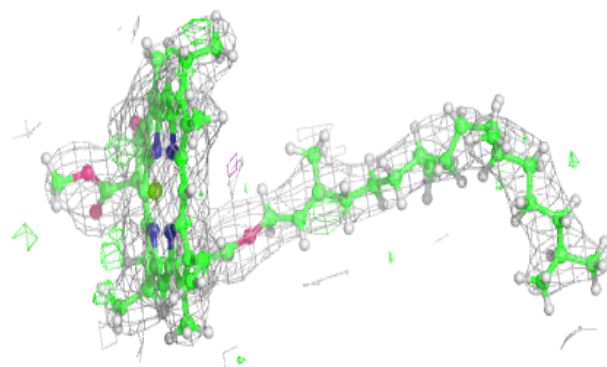
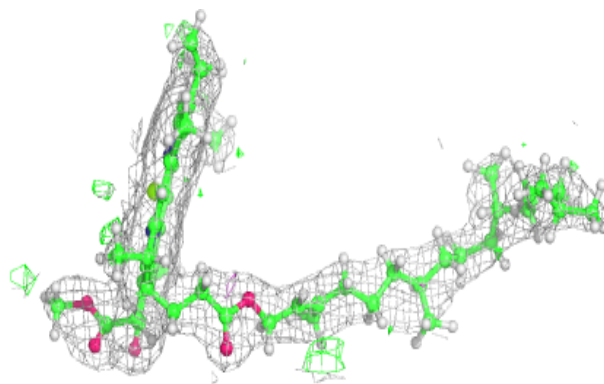
**Electron density around CLA b 611:**

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



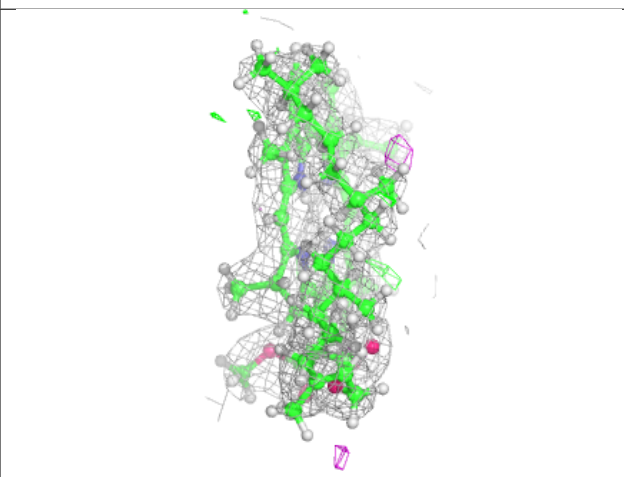
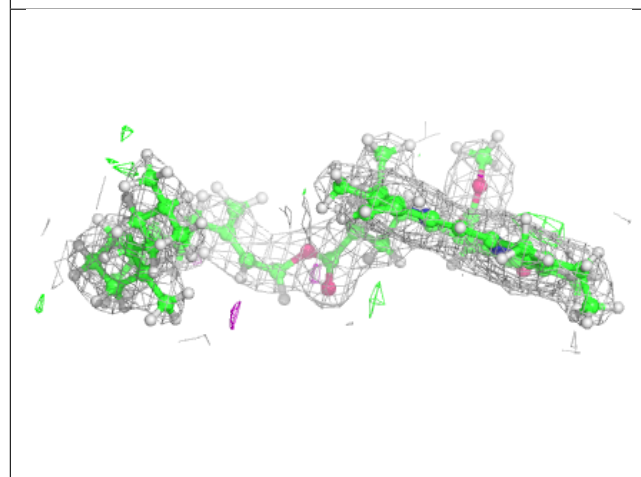
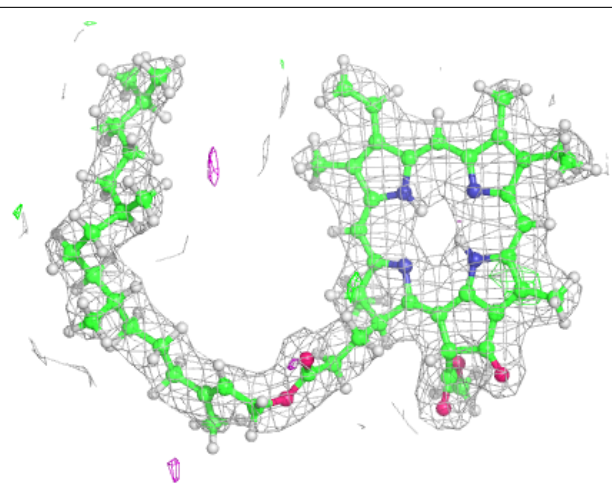
Electron density around CLA B 605:

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



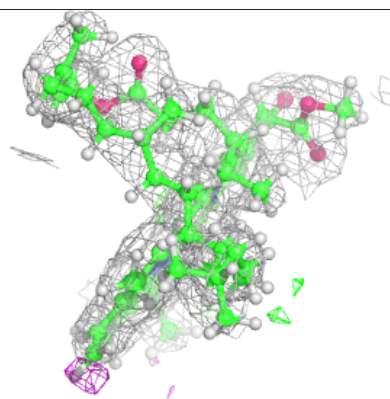
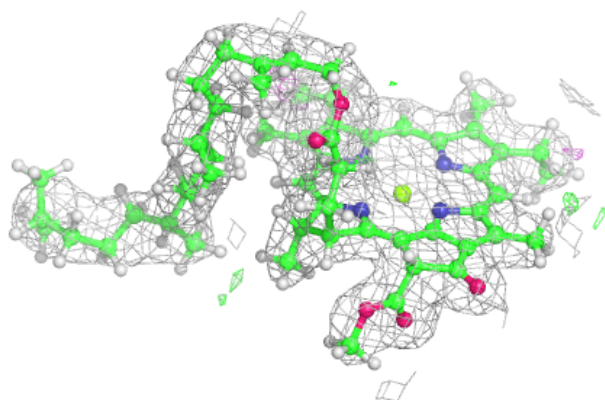
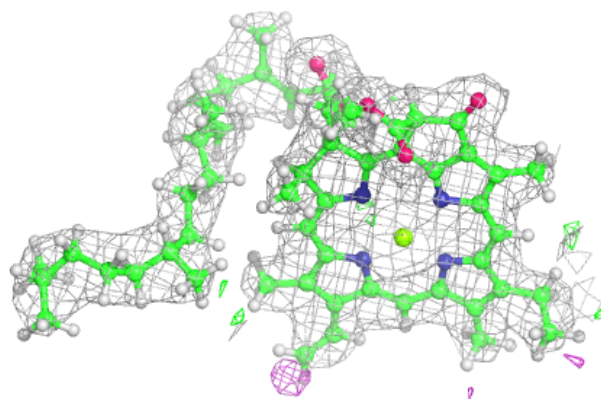
Electron density around PHO A 404:

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

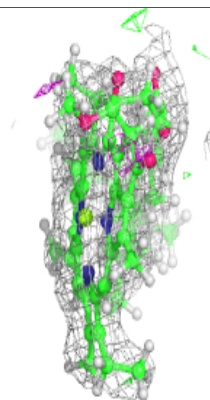
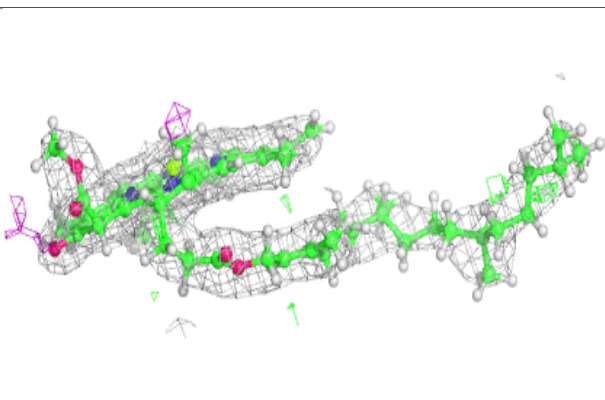
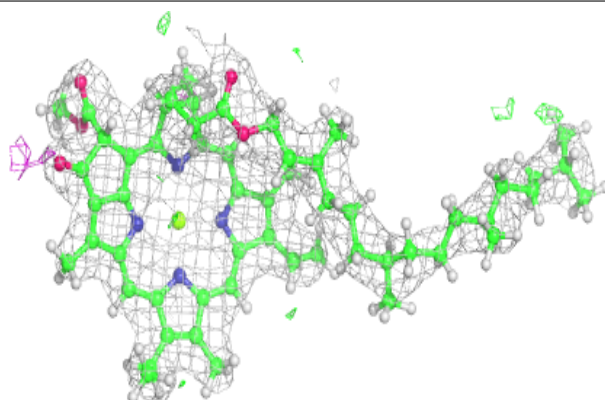


Electron density around CLA D 404:

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

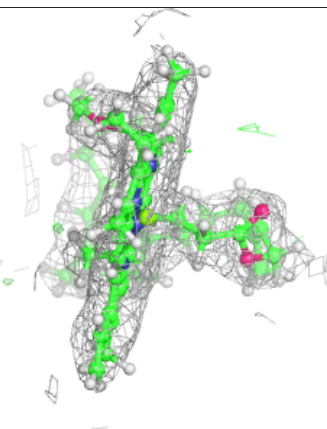
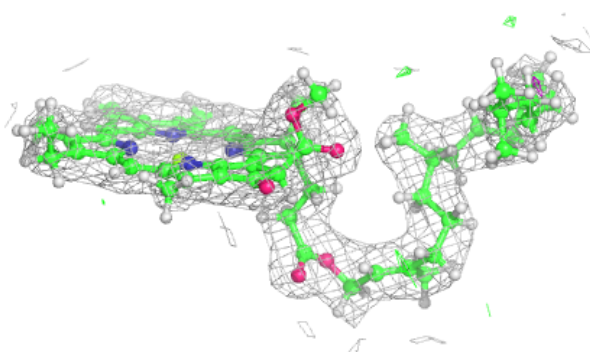
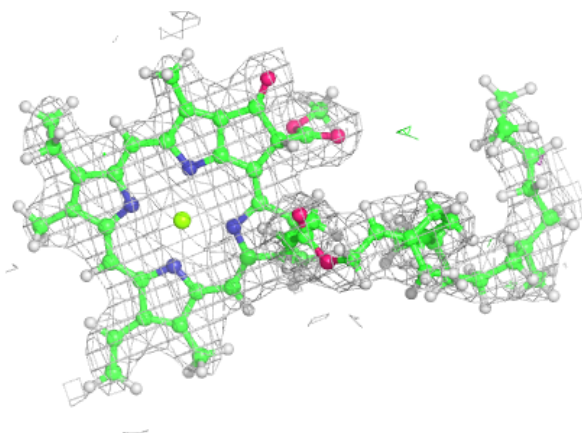
**Electron density around CLA B 603:**

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

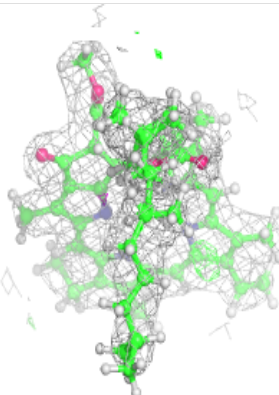
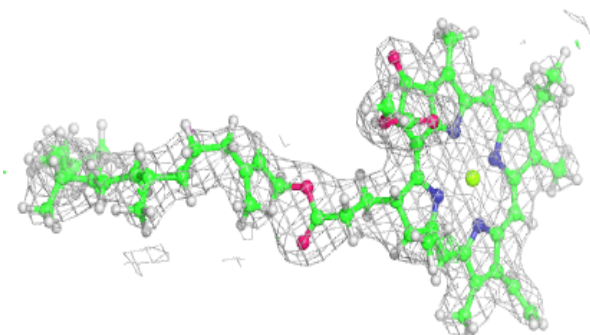
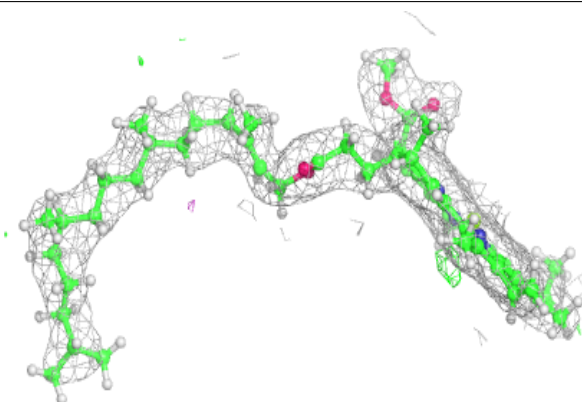


Electron density around CLA B 612:

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

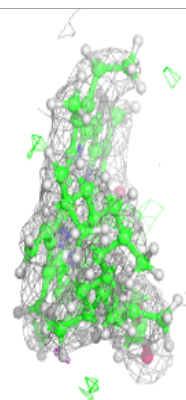
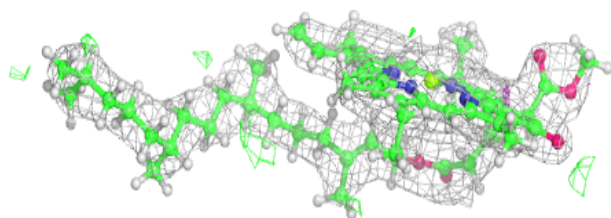
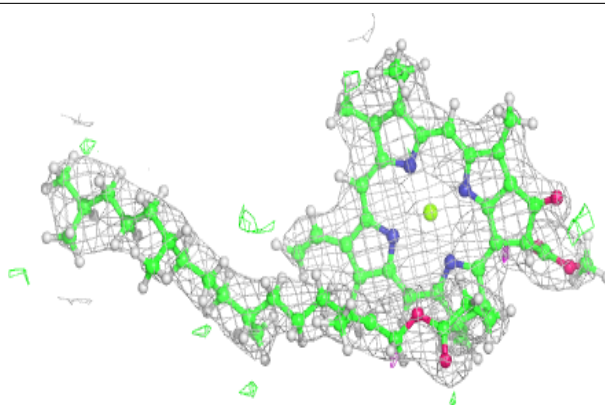
**Electron density around CLA d 403:**

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

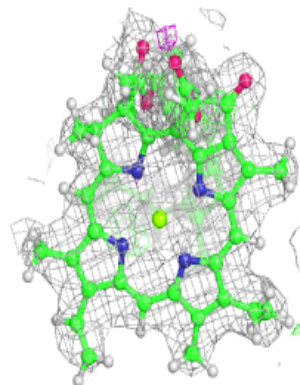
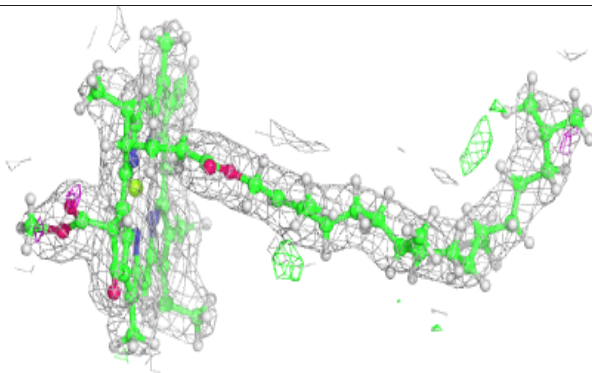
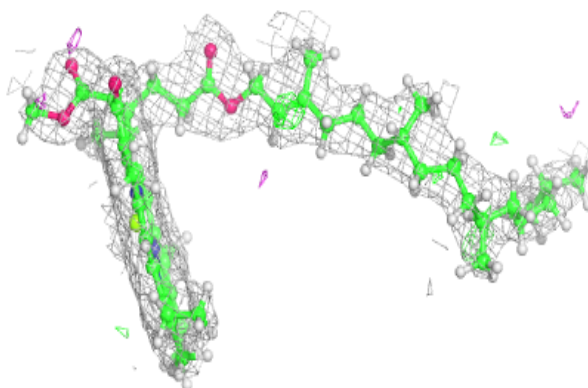


Electron density around CLA c 502:

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

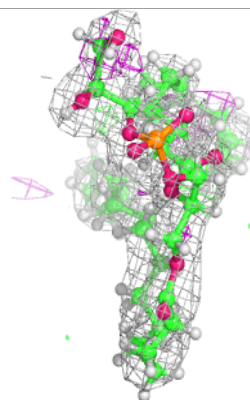
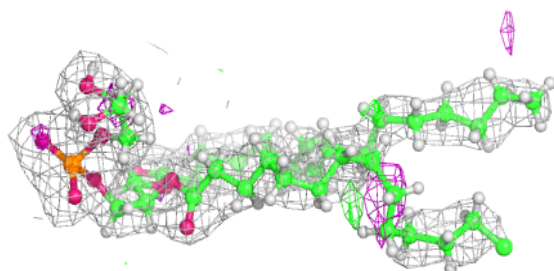
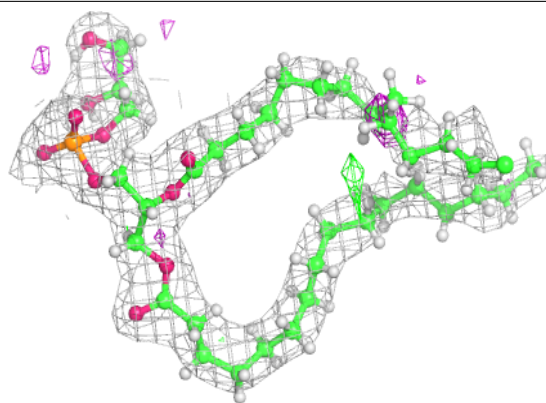
**Electron density around CLA b 605:**

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

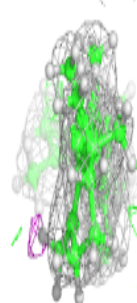
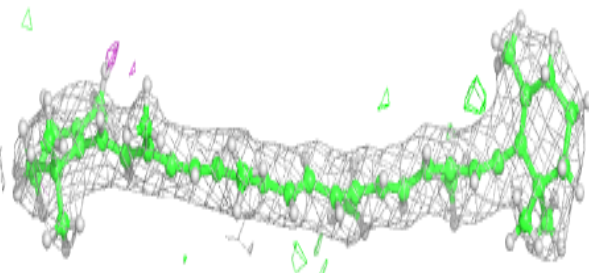
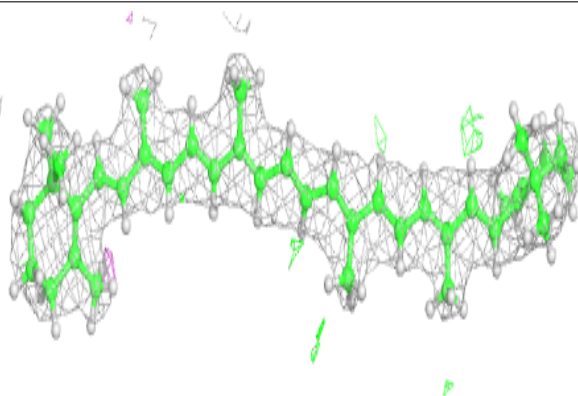


Electron density around LHG D 410:

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

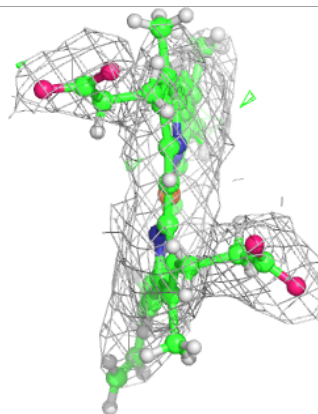
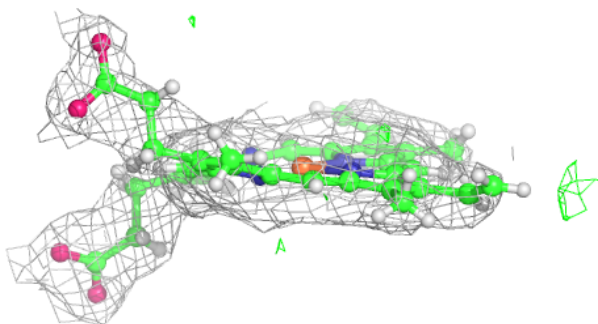
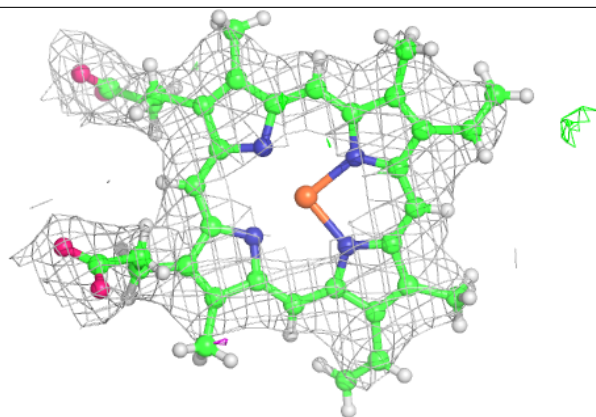
**Electron density around BCR B 617:**

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

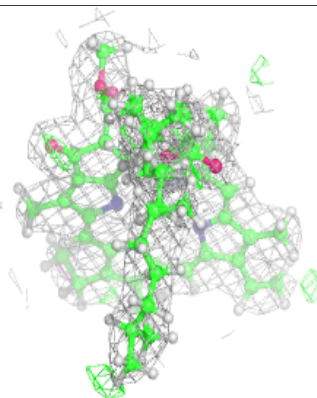
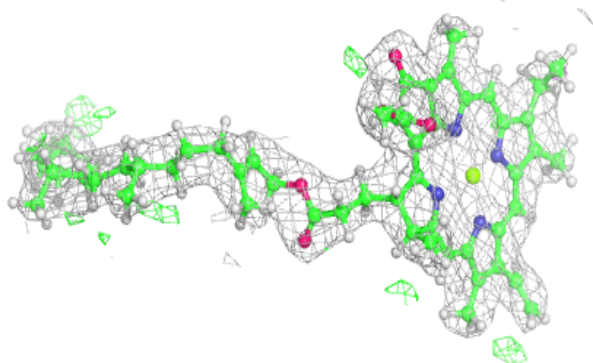
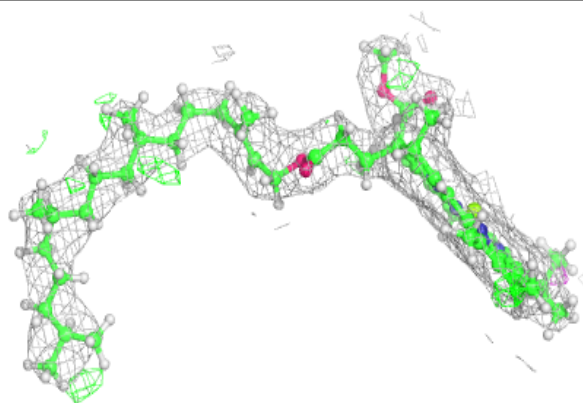


Electron density around HEC F 102:

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

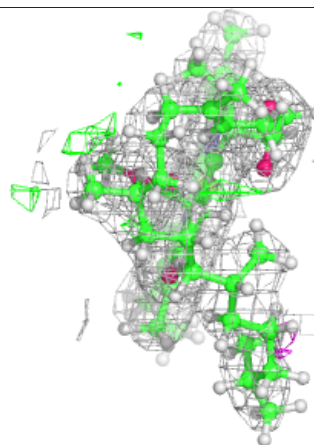
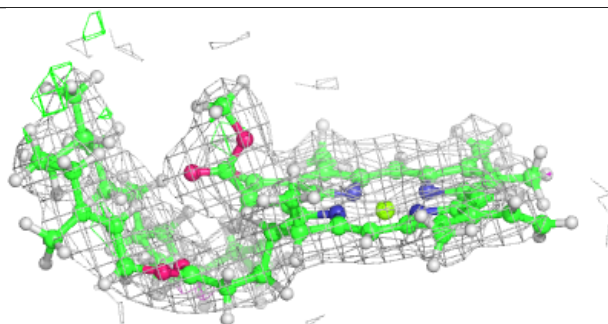
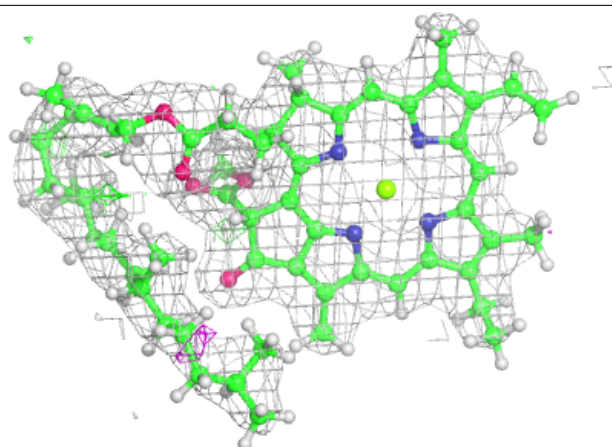
**Electron density around CLA D 403:**

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

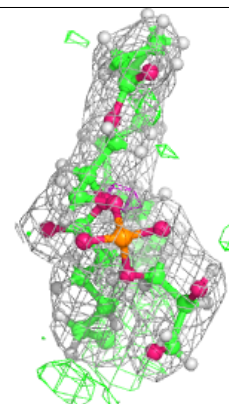
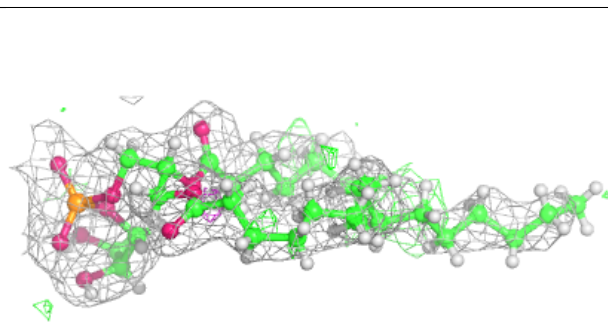
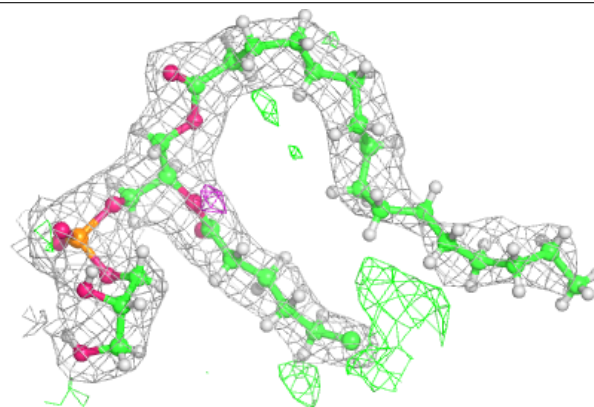


Electron density around CLA B 610:

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

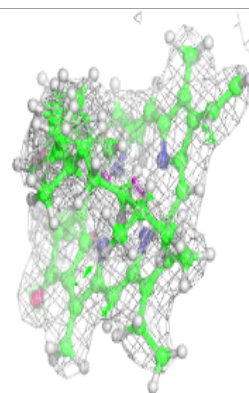
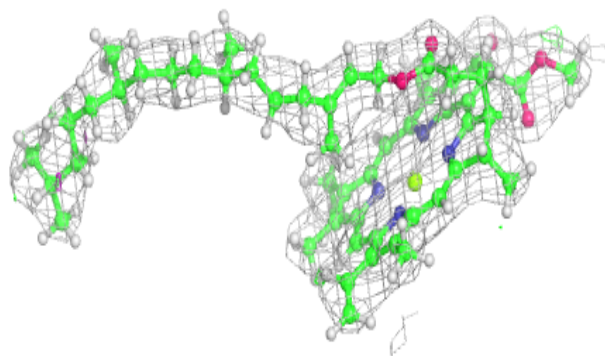
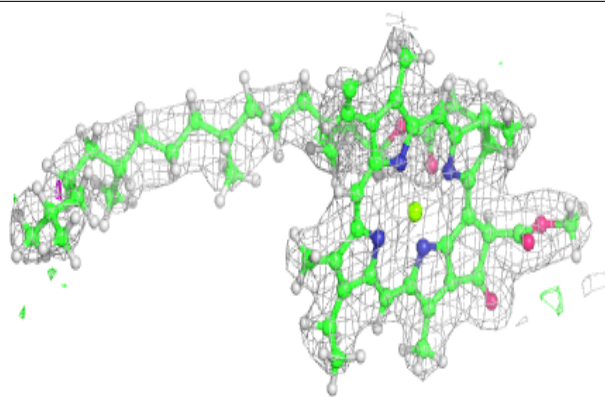
**Electron density around LHG d 409:**

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

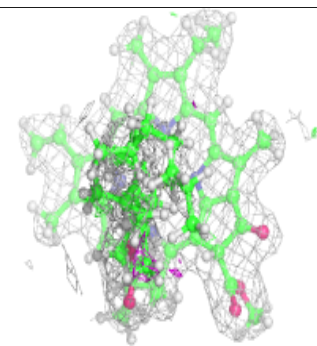
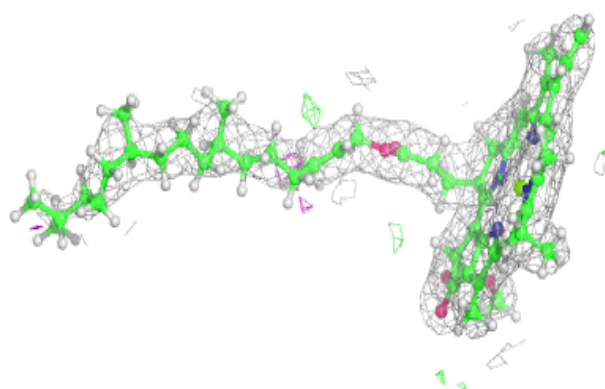
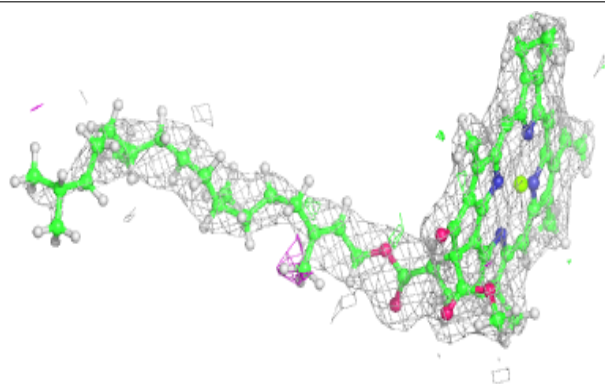


Electron density around CLA B 608:

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

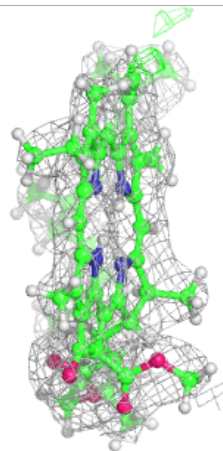
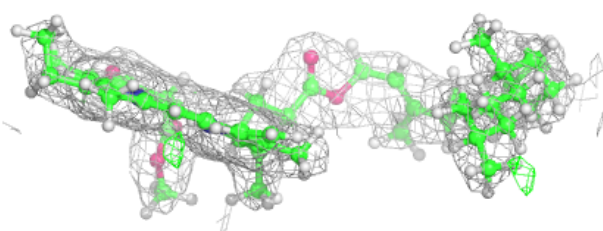
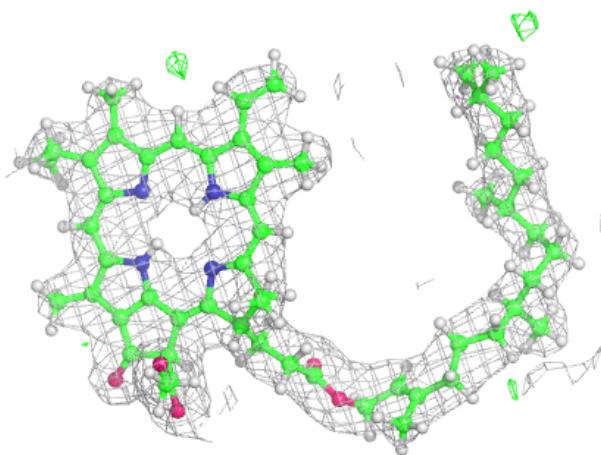
**Electron density around CLA b 604:**

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



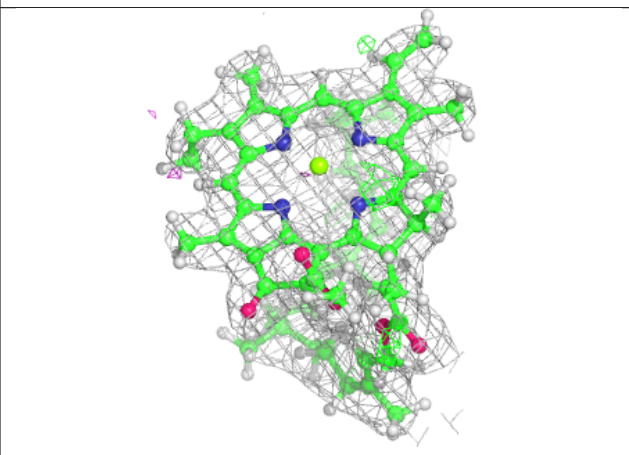
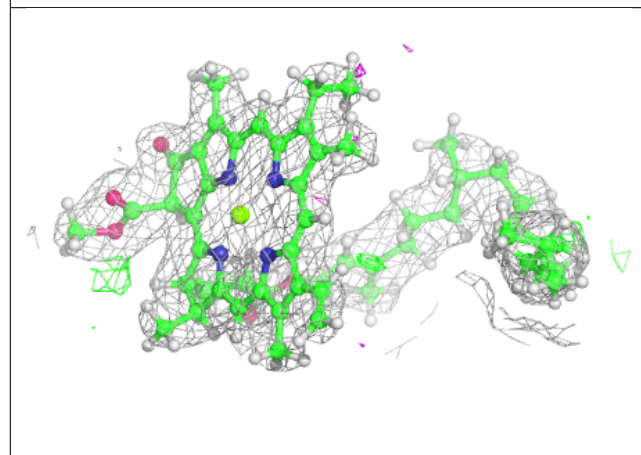
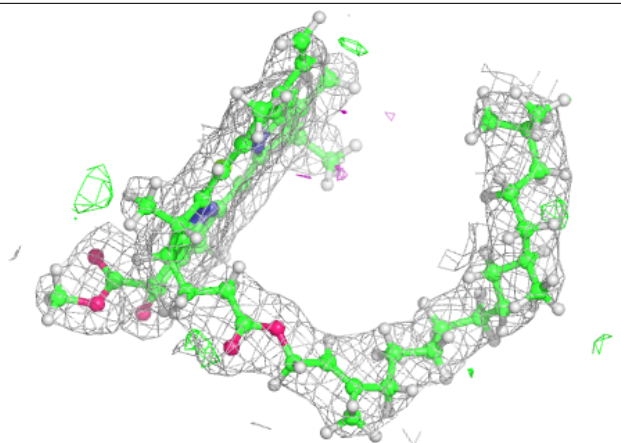
Electron density around PHO a 404:

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



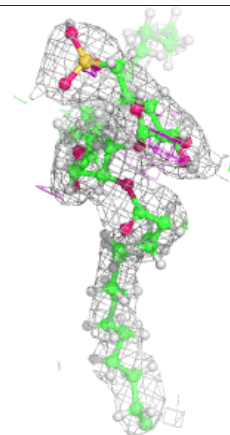
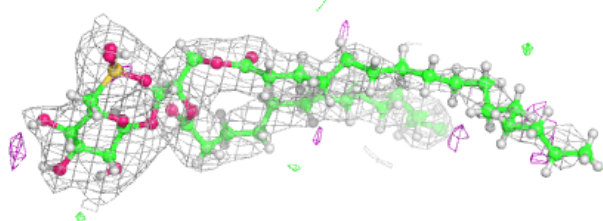
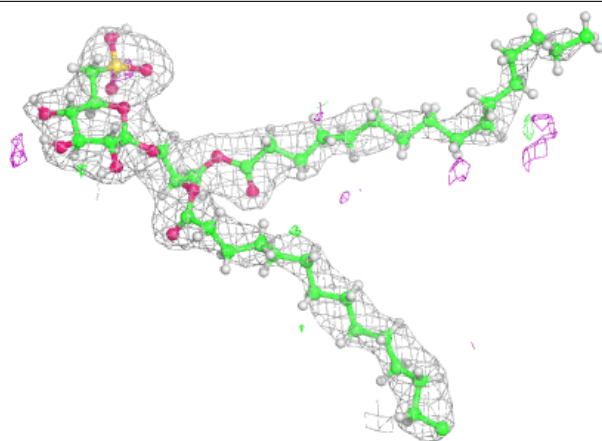
Electron density around CLA B 611:

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

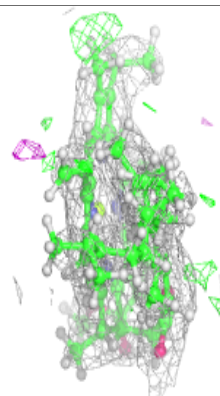
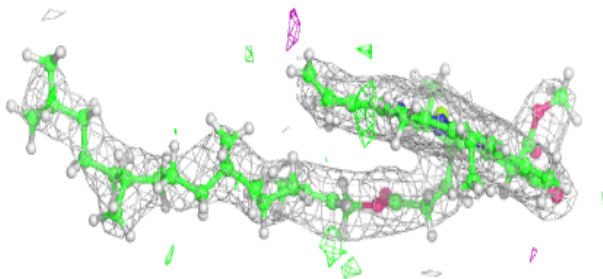
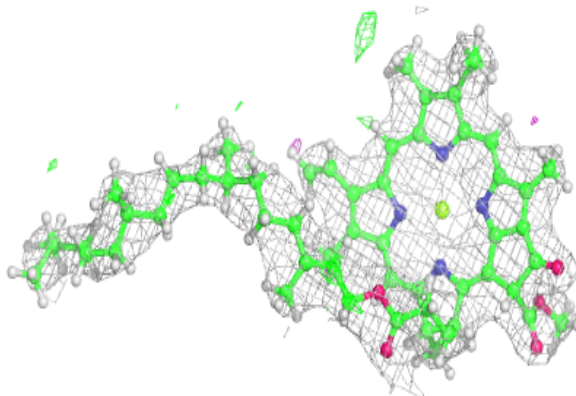


Electron density around SQD A 411:

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

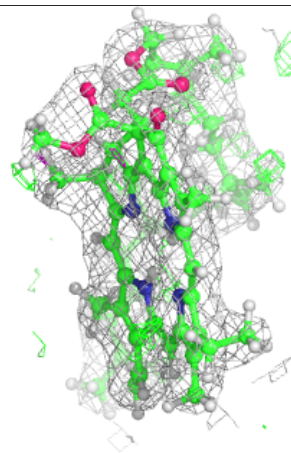
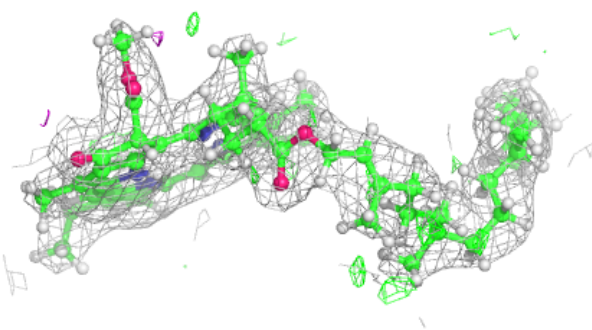
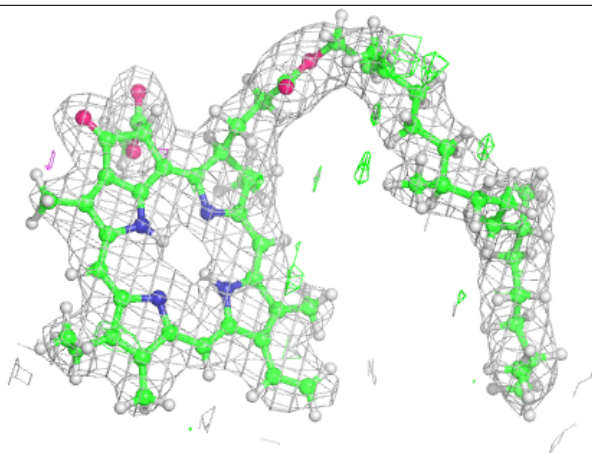
**Electron density around CLA b 603:**

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



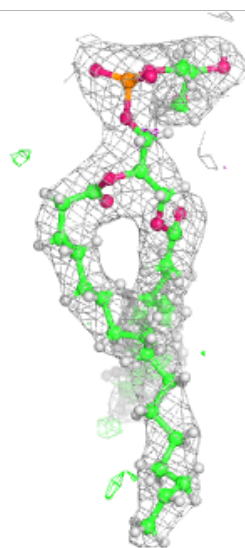
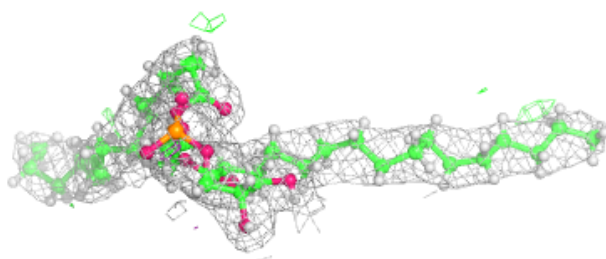
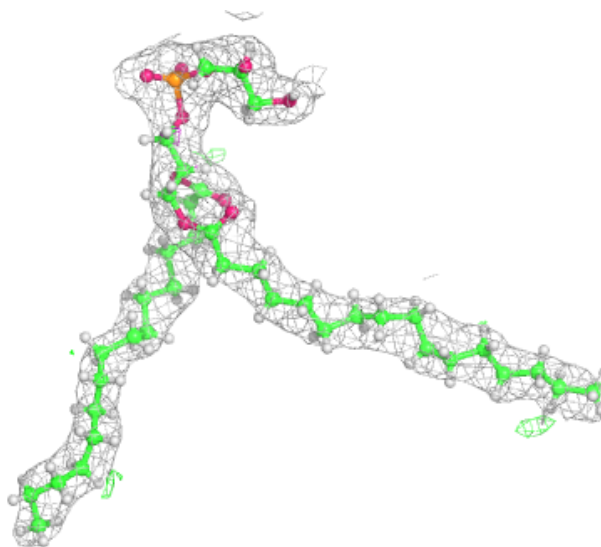
Electron density around PHO D 401:

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



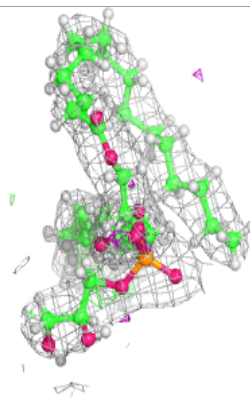
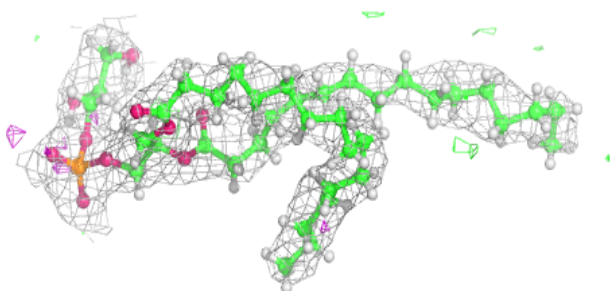
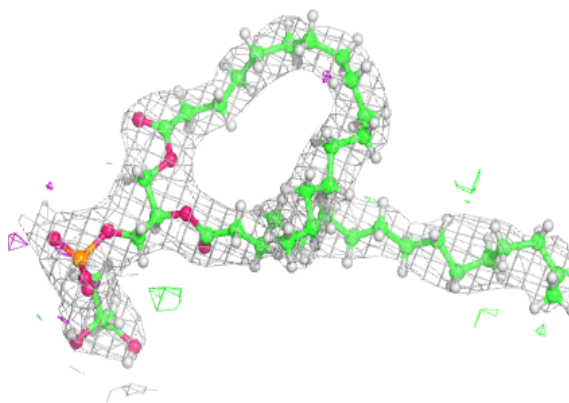
Electron density around LHG L 102:

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

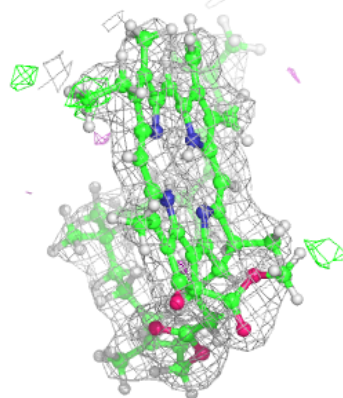
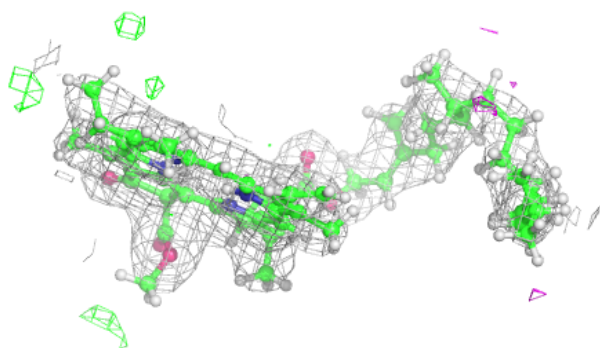
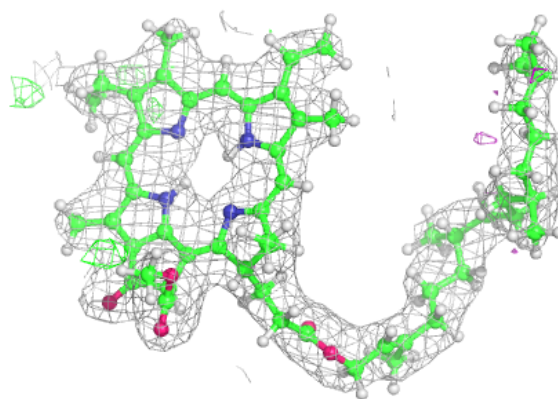


Electron density around LHG D 412:

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

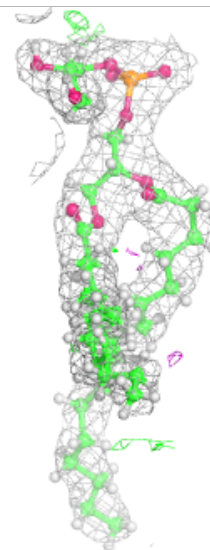
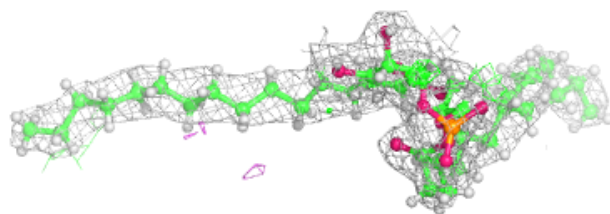
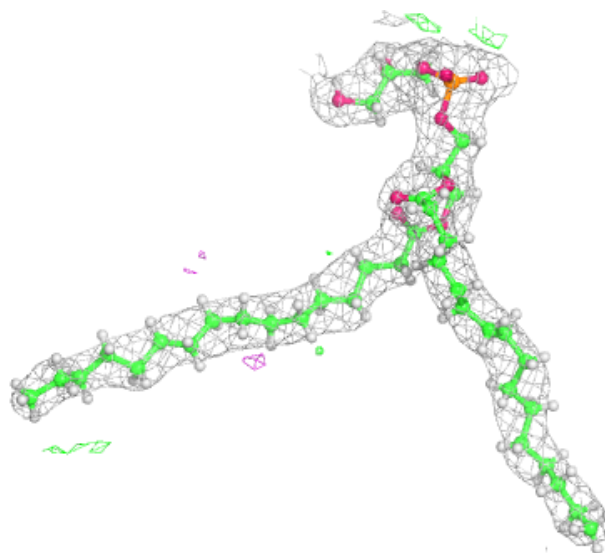
**Electron density around PHO d 401:**

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



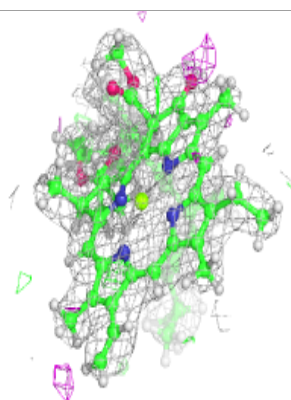
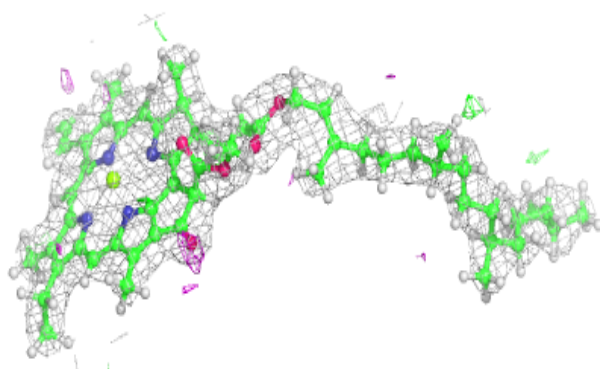
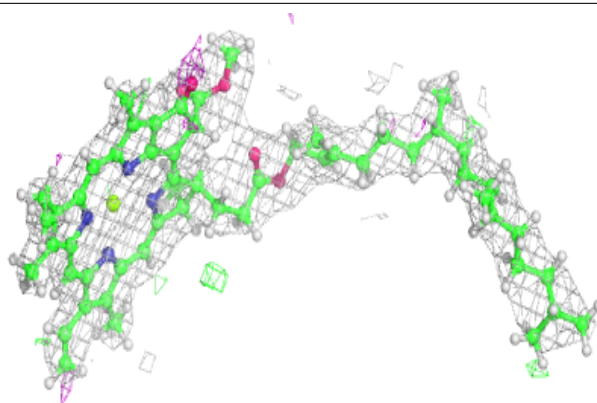
Electron density around LHG 1 101:

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

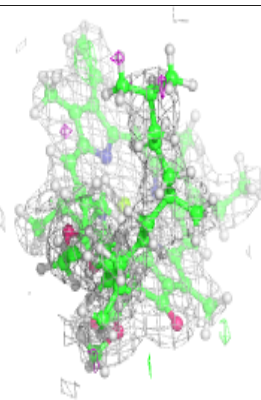
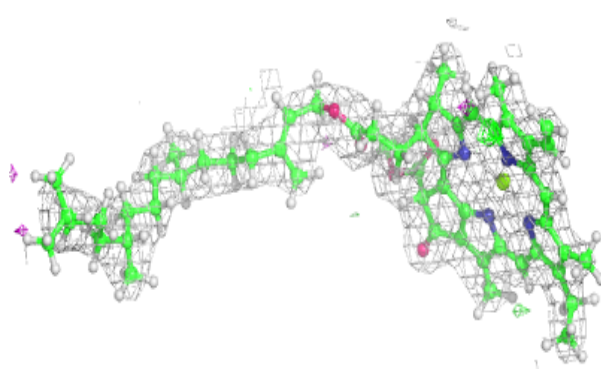
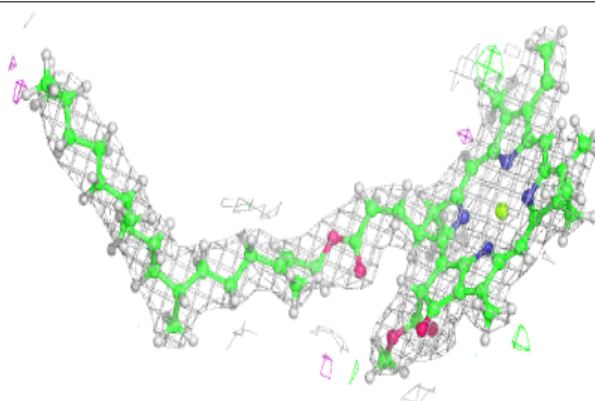


Electron density around CLA A 402:

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

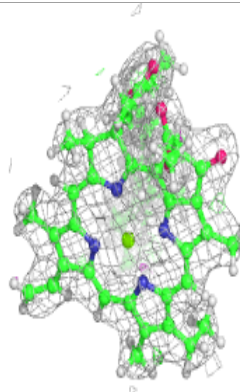
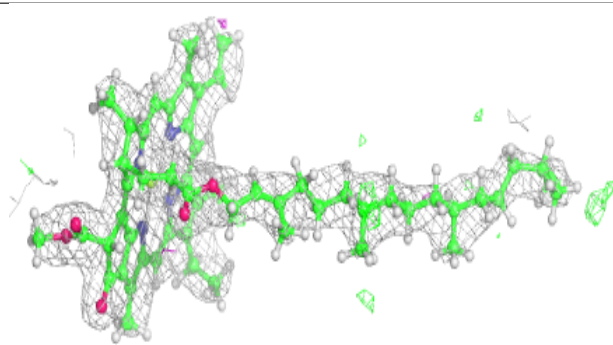
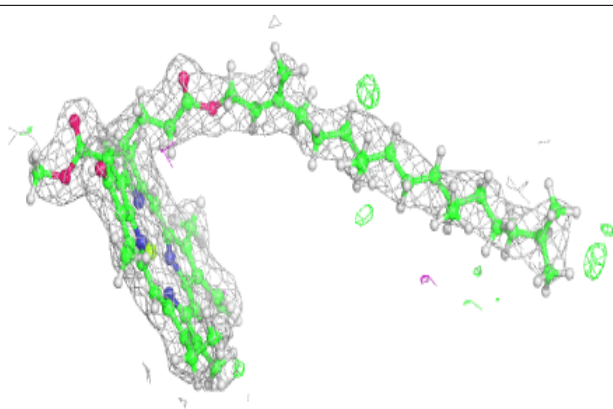
**Electron density around CLA a 402:**

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

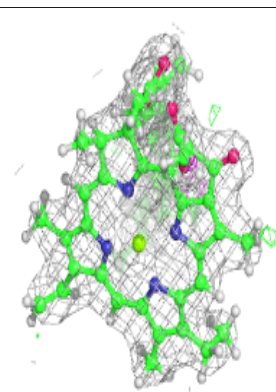
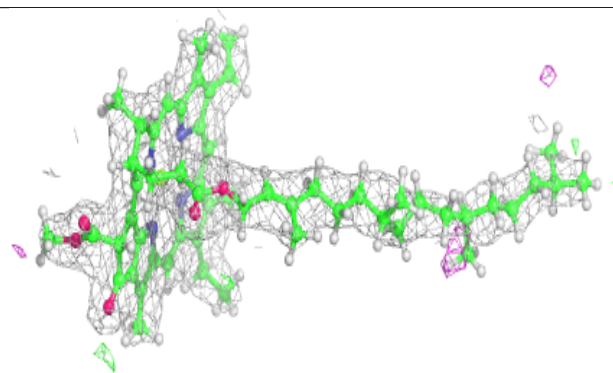
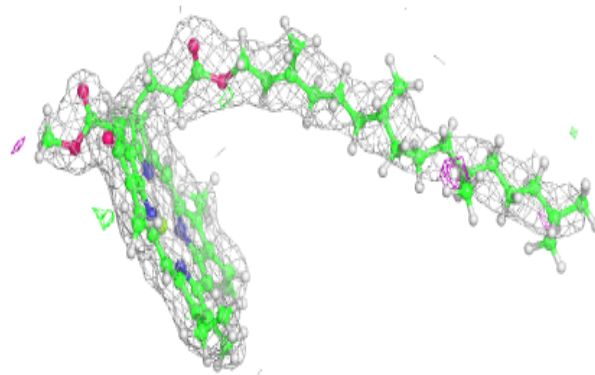


Electron density around CLA B 607:

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

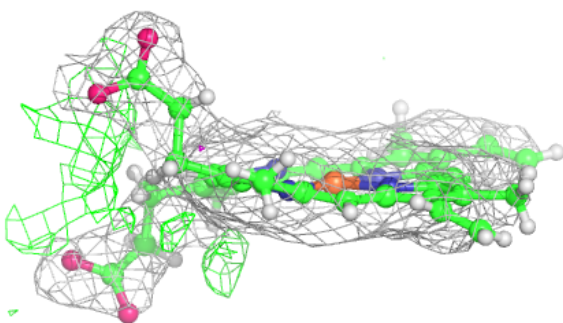
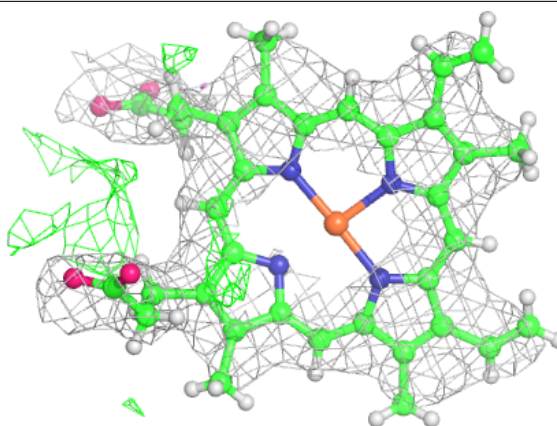
**Electron density around CLA b 607:**

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



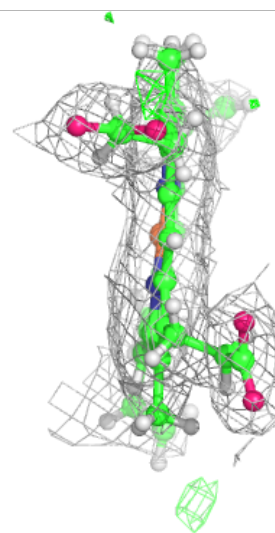
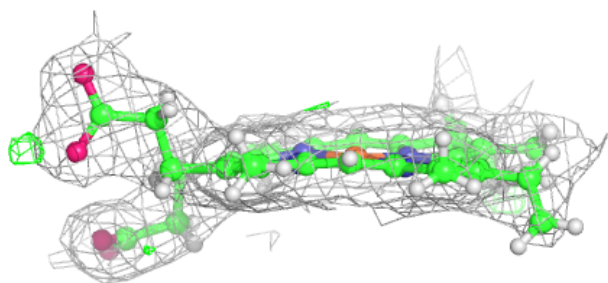
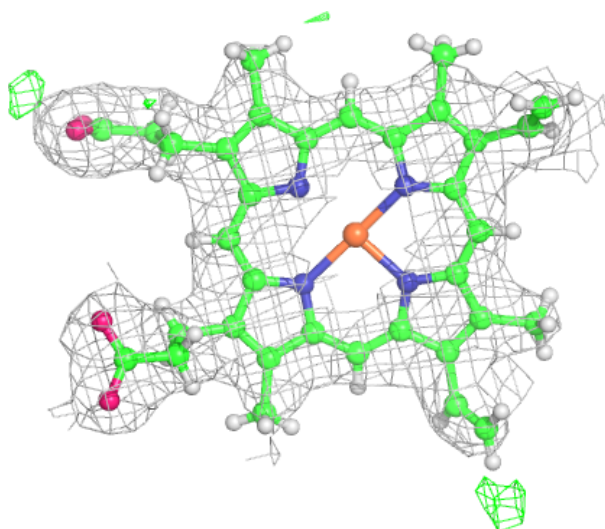
Electron density around HEC f 101:

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



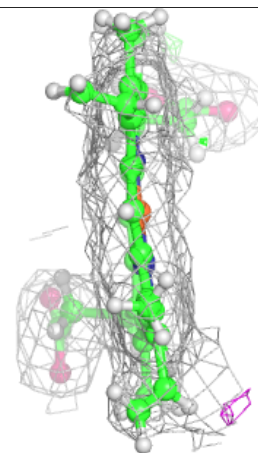
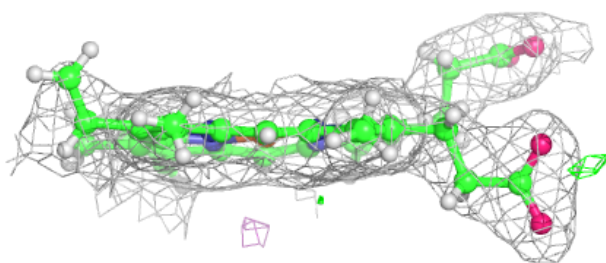
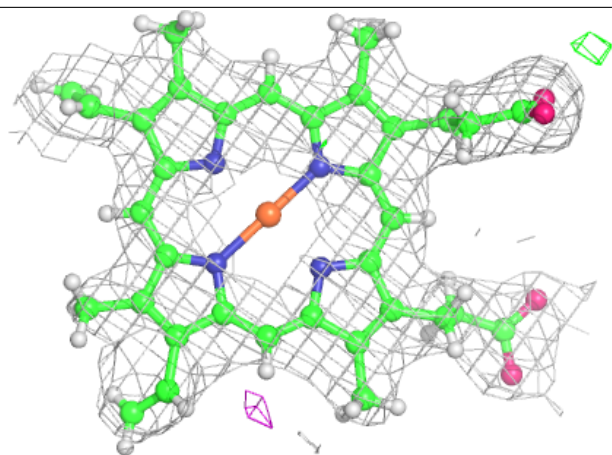
Electron density around HEC v 201:

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



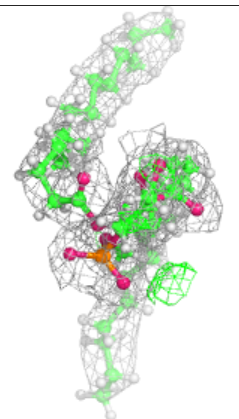
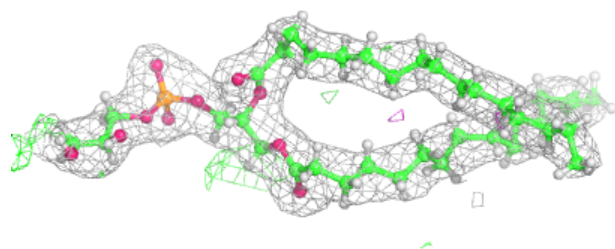
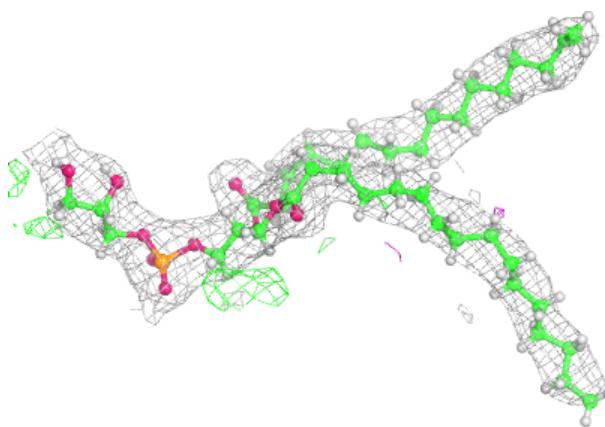
Electron density around HEC V 201:

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



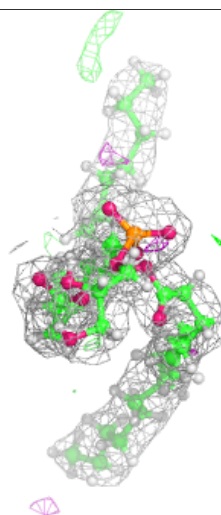
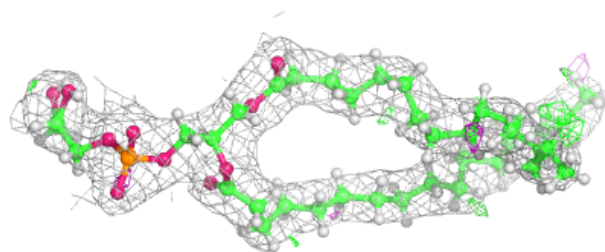
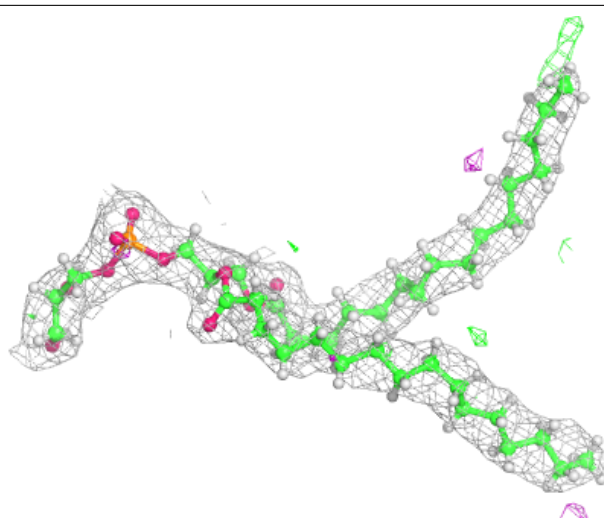
Electron density around LHG d 408:

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



Electron density around LHG D 409:

$2mF_o-DF_c$ (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.