



## Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2021 – 04:44 PM EDT

PDB ID : 7RF5  
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution  
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Deposited on : 2021-07-13  
Resolution : 2.23 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

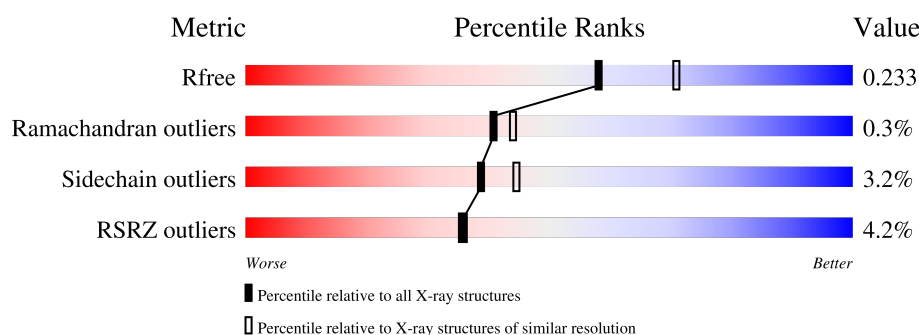
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



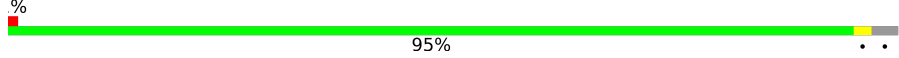
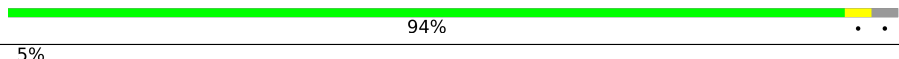
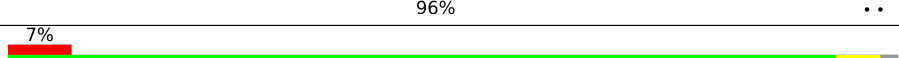
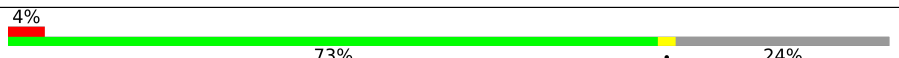
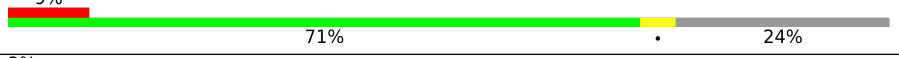
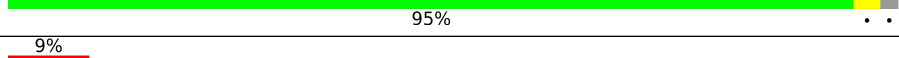
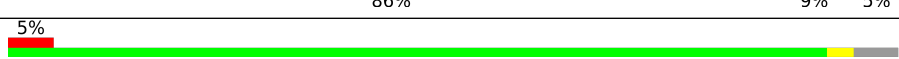



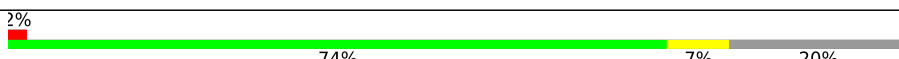
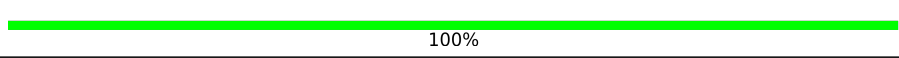
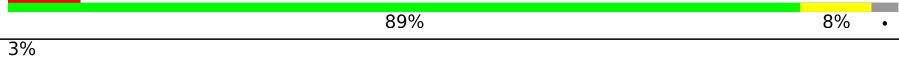

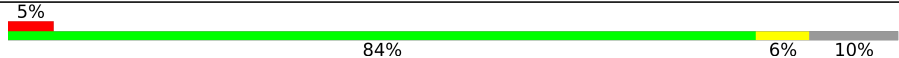


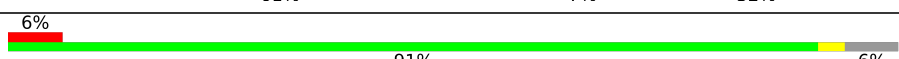
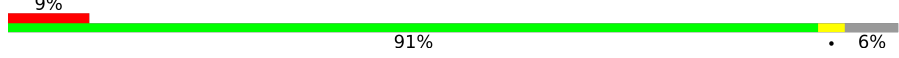




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2391 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	461	
3	c	461	

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Mol	Chain	Length	Quality of chain
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	41	
14	r	41	
15	T	32	
15	t	32	
16	U	134	

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Mol	Chain	Length	Quality of chain
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
24	CLA	A	604	X	-	-	-
24	CLA	A	605	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	612	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	H	101	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	613	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
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24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105562 atoms, of which 52760 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	66	0
			6098	2030	2985	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6086	2027	2976	513	551	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	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	14	0
			6941	2302	3432	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7086	2343	3503	602	624	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	2	0
			5368	1809	2637	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5380	1813	2643	446	466	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	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	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
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	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			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0
			620	202	316	48	53	1		
11	l	36	Total	C	H	N	O		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	S	0	0
			525	171	269	37	47	1		
12	m	32	Total	C	H	N	O	S	0	0
			518	168	267	36	46	1		

- 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	S	0	1
			3700	1168	1830	313	385	4		0
13	o	244	Total	C	H	N	O	S	0	0
			3720	1170	1846	317	383	4		0

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- 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		

- 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
			1547	491	773	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1547	491	773	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
			2135	675	1071	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2135	675	1071	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			

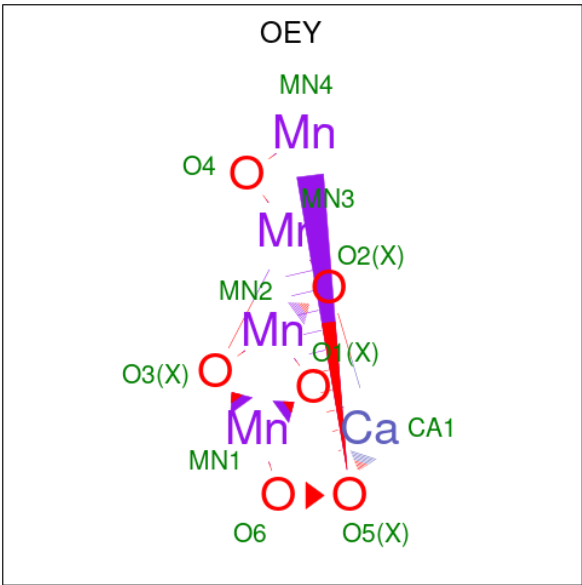
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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

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

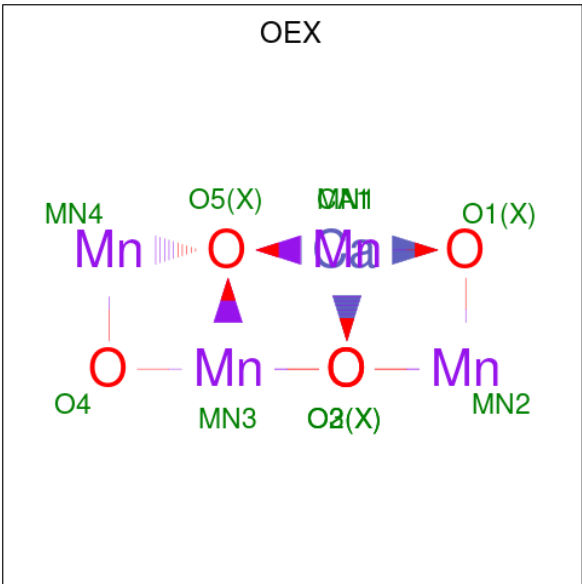
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		
20	z	62	Total	C	H	N	O	S	0	0
			986	326	509	72	77	2		

- Molecule 21 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula:  $\text{CaMn}_4\text{O}_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ) (labeled as "Ligand of Interest" by depositor).



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

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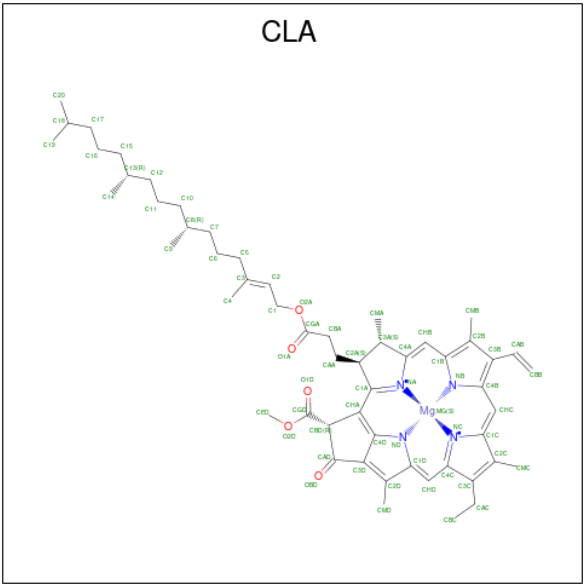
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 23 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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

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

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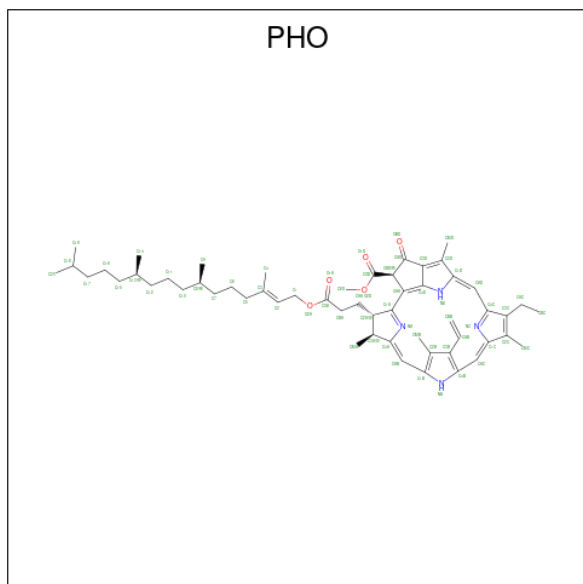
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total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

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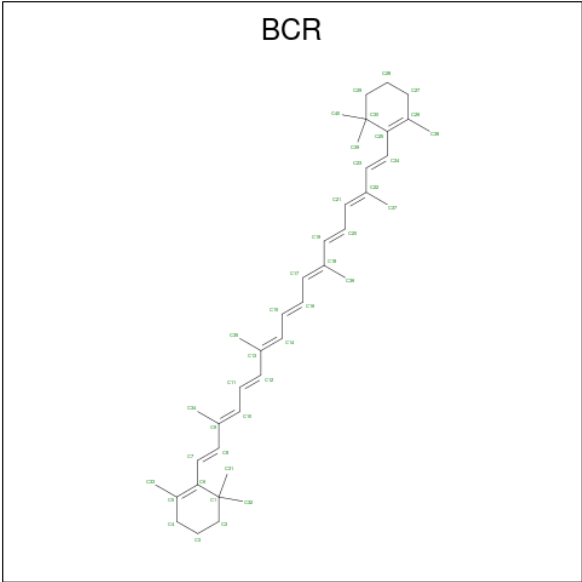
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



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

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



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

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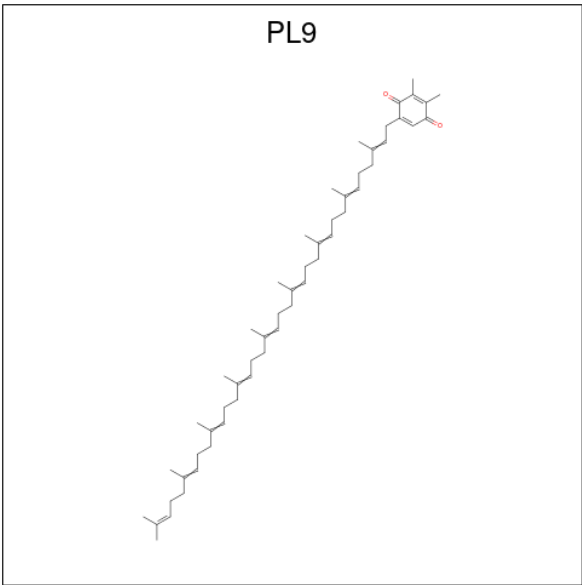
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40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

- Molecule 27 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

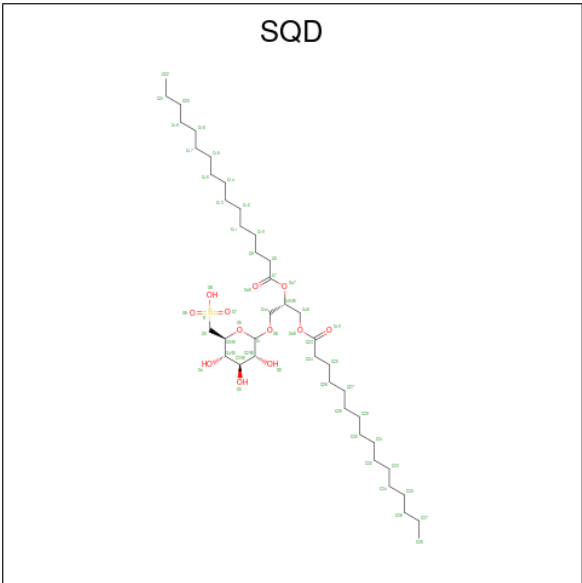
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	2	Total	Cl	0	0
			2	2		
27	a	2	Total	Cl	0	0
			2	2		

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: C<sub>53</sub>H<sub>80</sub>O<sub>2</sub>).



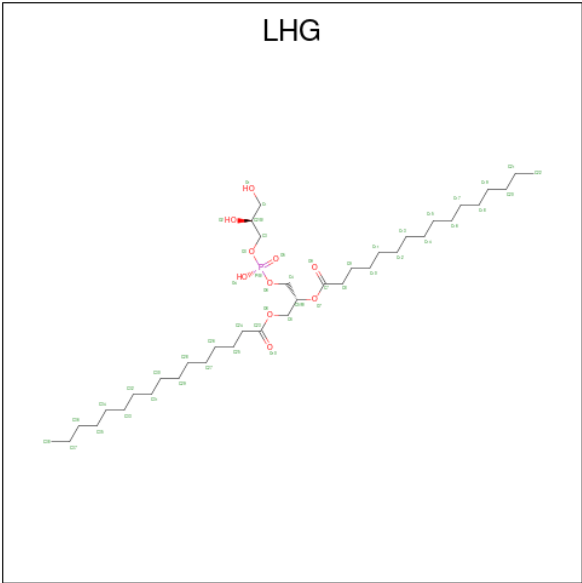
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			135	53	80	2		
28	D	1	Total	C	H	O	0	0
			135	53	80	2		
28	a	1	Total	C	H	O	0	0
			135	53	80	2		
28	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



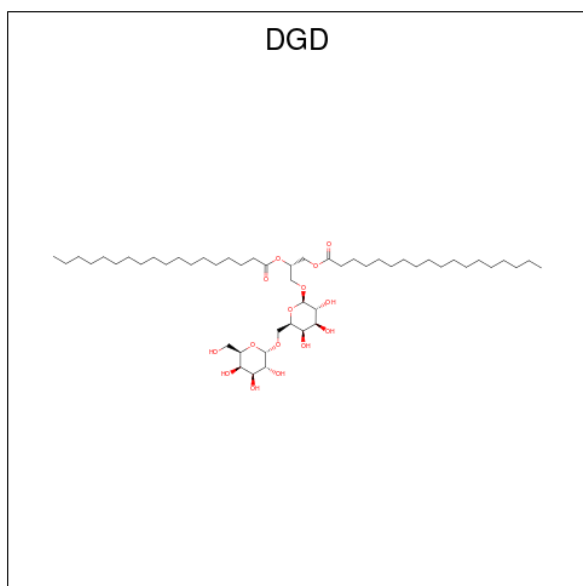
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	a	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
30	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
30	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



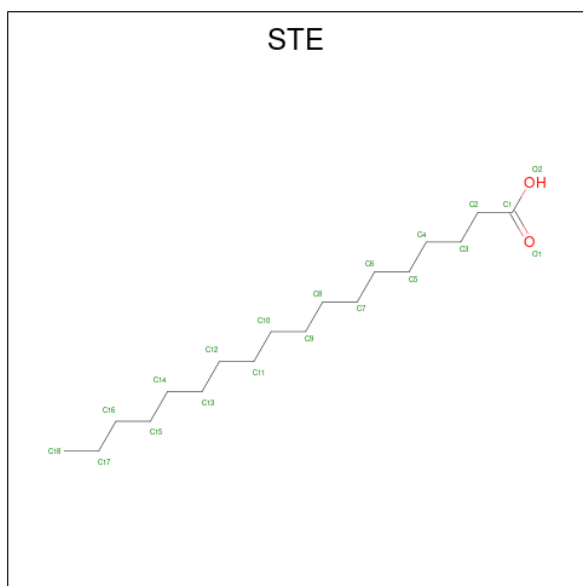
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 32 is STEARIC ACID (three-letter code: STE) (formula: C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>).



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

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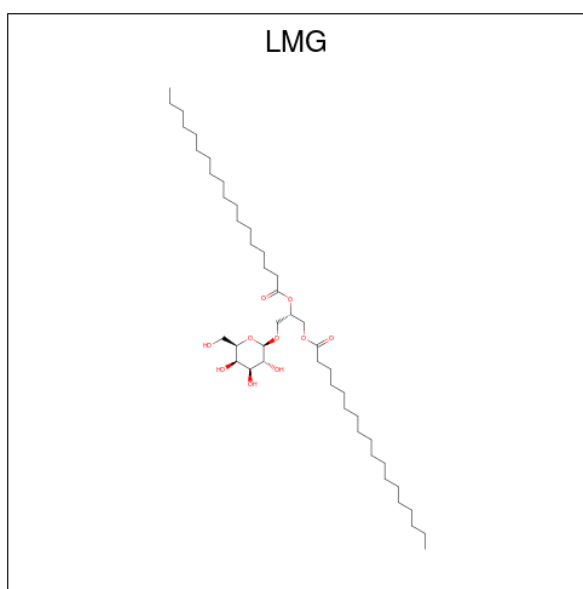
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	R	1	Total C H O 28 10 16 2	0	0
32	T	1	Total C H 47 16 31	0	0
32	T	1	Total C H 44 15 29	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	c	1	Total	C	H	O	0	0
			55	18	35	2		
32	c	1	Total	C	H	O	0	0
			28	10	16	2		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	h	1	Total	C	H		0	0
			41	14	27			
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



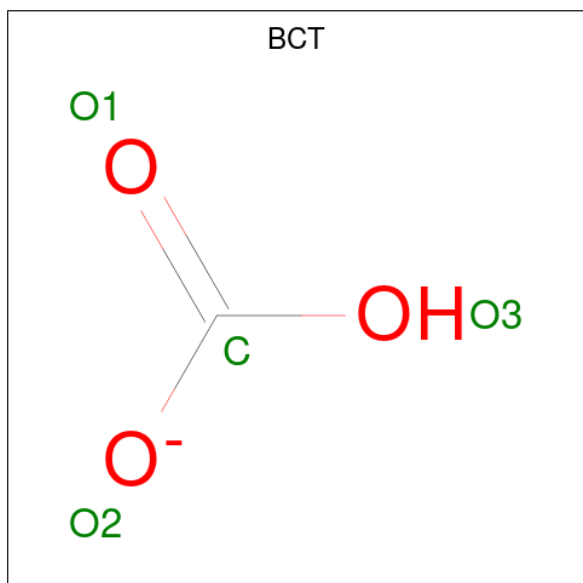
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			122	41	71	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		

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

- Molecule 34 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



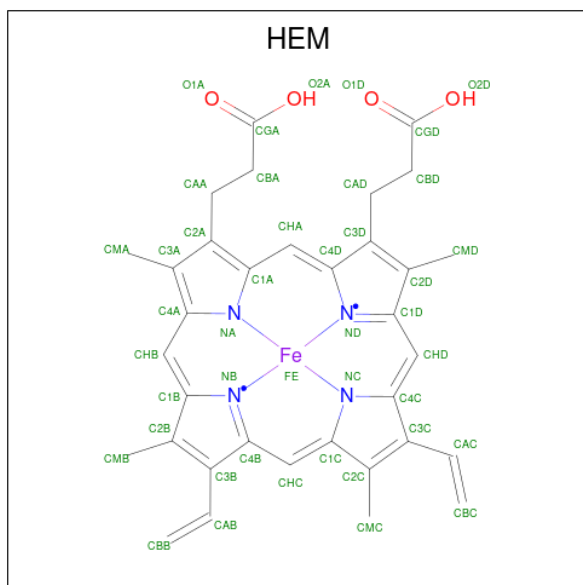
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		

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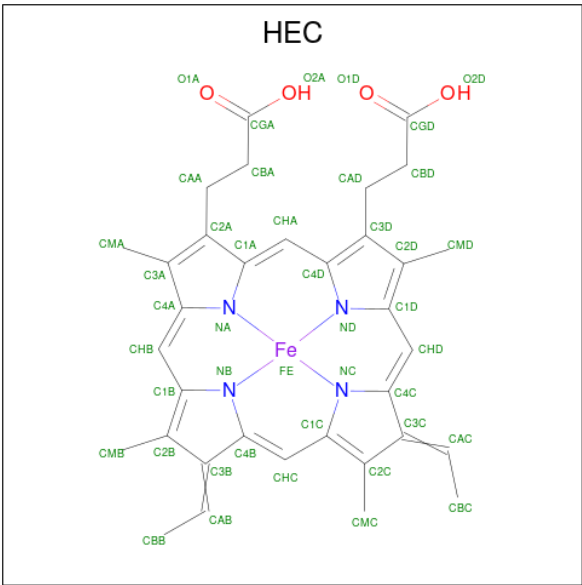
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

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



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

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



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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	118	Total	O	0	0
			118	118		
37	B	141	Total	O	0	0
			141	141		
37	C	114	Total	O	0	0
			114	114		
37	D	100	Total	O	0	0
			100	100		
37	E	20	Total	O	0	0
			20	20		
37	F	3	Total	O	0	0
			3	3		
37	H	29	Total	O	0	0
			29	29		
37	I	7	Total	O	0	0
			7	7		
37	J	6	Total	O	0	0
			6	6		
37	K	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	10	Total O 10 10	0	0
37	M	5	Total O 5 5	0	0
37	O	71	Total O 71 71	0	0
37	R	1	Total O 1 1	0	0
37	T	5	Total O 5 5	0	0
37	U	33	Total O 33 33	0	0
37	V	49	Total O 49 49	0	0
37	X	7	Total O 7 7	0	0
37	Y	4	Total O 4 4	0	0
37	Z	2	Total O 2 2	0	0
37	a	117	Total O 117 117	0	0
37	b	131	Total O 131 131	0	0
37	c	118	Total O 118 118	0	0
37	d	100	Total O 100 100	0	0
37	e	10	Total O 10 10	0	0
37	f	2	Total O 2 2	0	0
37	h	19	Total O 19 19	0	0
37	i	8	Total O 8 8	0	0
37	j	11	Total O 11 11	0	0
37	k	4	Total O 4 4	0	0
37	l	10	Total O 10 10	0	0

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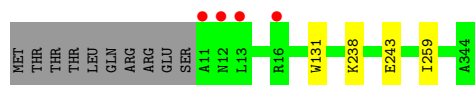
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	5	Total 5	O 5	0	0
37	o	65	Total 65	O 65	0	0
37	r	1	Total 1	O 1	0	0
37	t	5	Total 5	O 5	0	0
37	u	41	Total 41	O 41	0	0
37	v	36	Total 36	O 36	0	0
37	x	8	Total 8	O 8	0	0
37	y	1	Total 1	O 1	0	0
37	z	2	Total 2	O 2	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



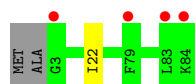
- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



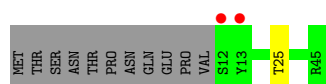
- Molecule 5: Cytochrome b559 subunit alpha



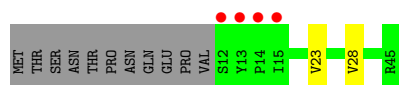
- Molecule 5: Cytochrome b559 subunit alpha



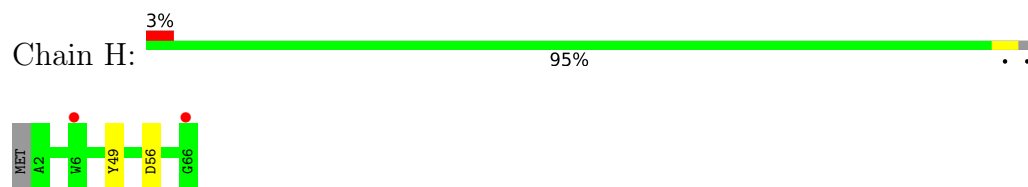
- Molecule 6: Cytochrome b559 subunit beta



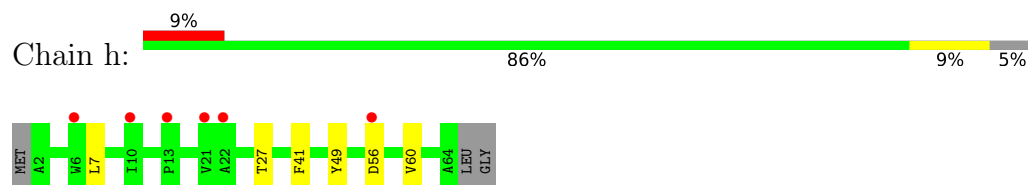
- Molecule 6: Cytochrome b559 subunit beta



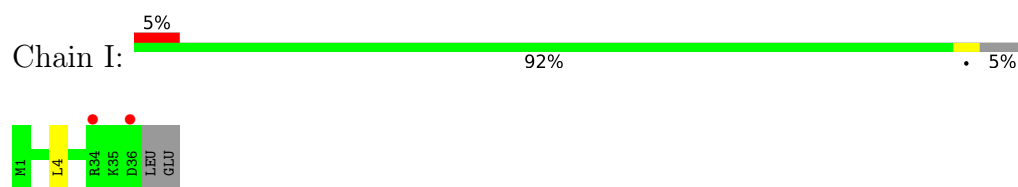
- Molecule 7: Photosystem II reaction center protein H



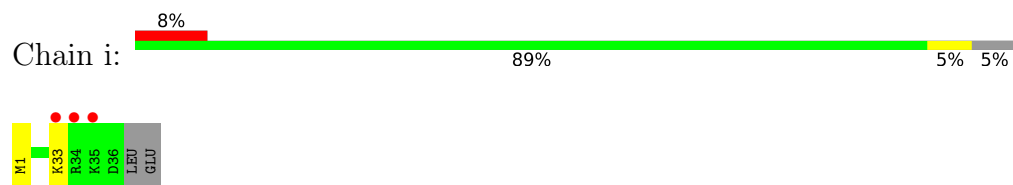
- Molecule 7: Photosystem II reaction center protein H



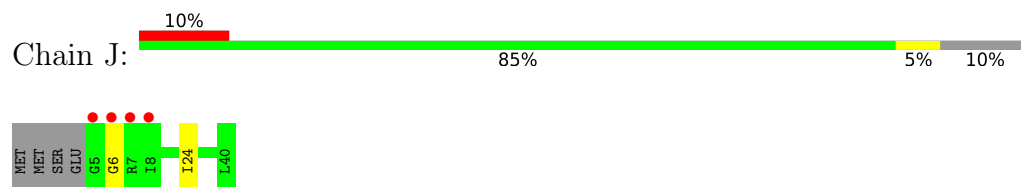
- Molecule 8: Photosystem II reaction center protein I



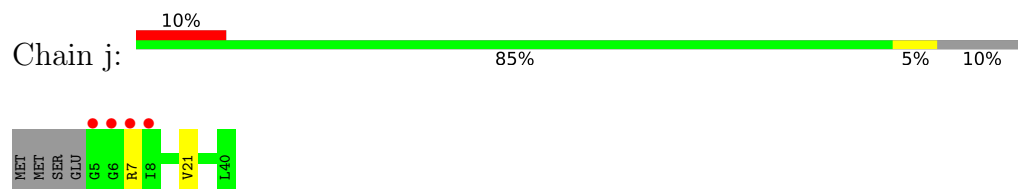
- Molecule 8: Photosystem II reaction center protein I



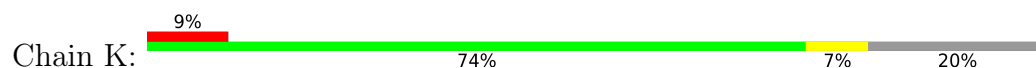
- Molecule 9: Photosystem II reaction center protein J

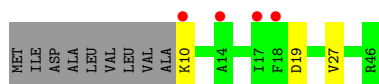


- Molecule 9: Photosystem II reaction center protein J

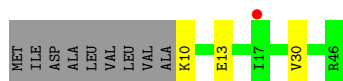
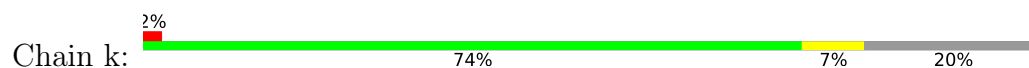


- Molecule 10: Photosystem II reaction center protein K





- Molecule 10: Photosystem II reaction center protein K

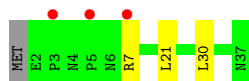
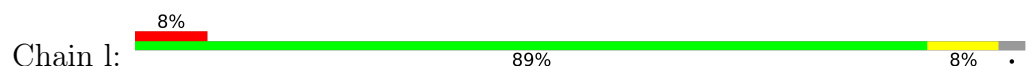


- Molecule 11: Photosystem II reaction center protein L

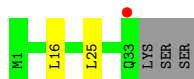
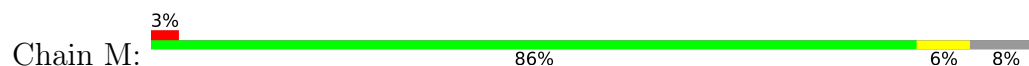


There are no outlier residues recorded for this chain.

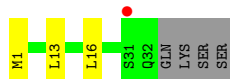
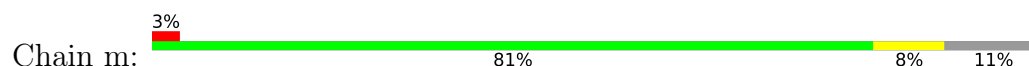
- Molecule 11: Photosystem II reaction center protein L



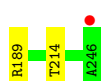
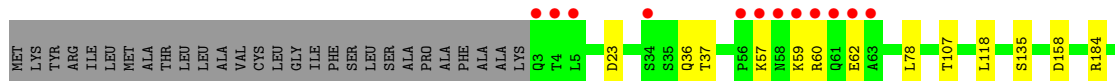
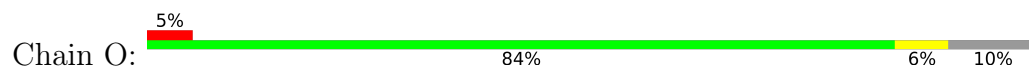
- Molecule 12: Photosystem II reaction center protein M



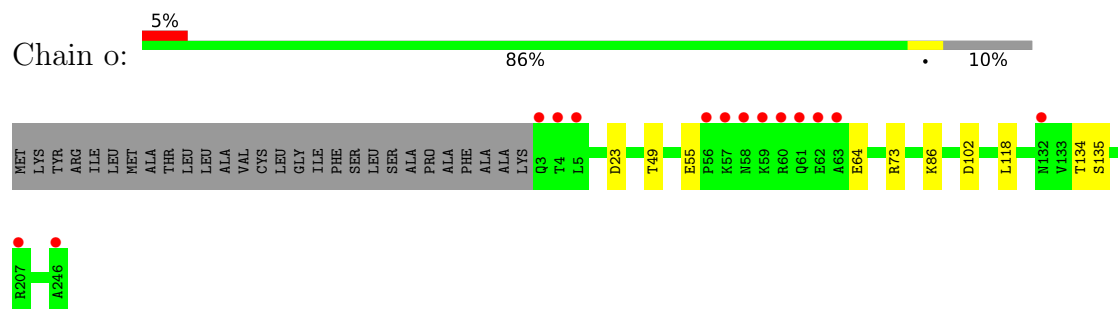
- Molecule 12: Photosystem II reaction center protein M



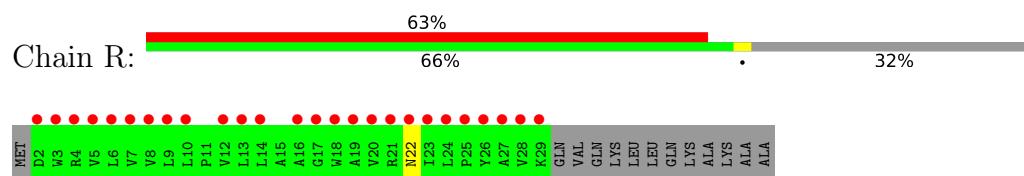
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



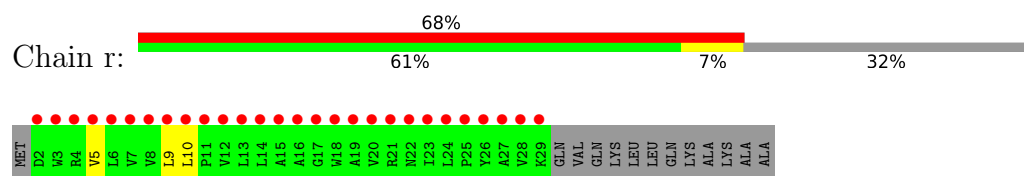
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



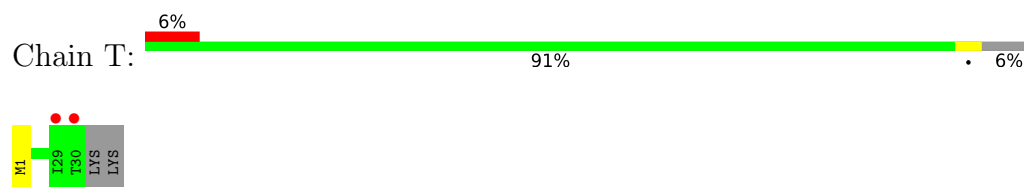
- Molecule 14: Photosystem II protein Y



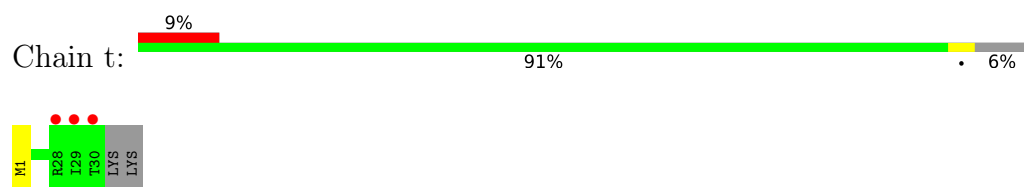
- Molecule 14: Photosystem II protein Y



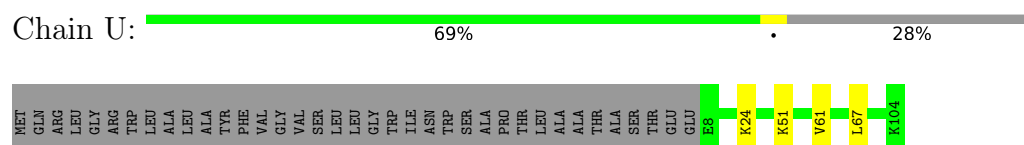
- Molecule 15: Photosystem II reaction center protein T



- Molecule 15: Photosystem II reaction center protein T

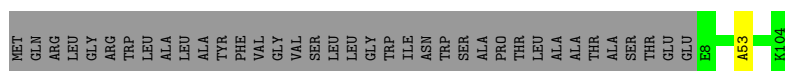


- Molecule 16: Photosystem II 12 kDa extrinsic protein



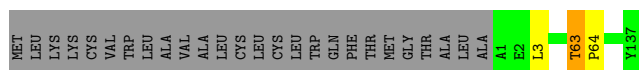
- Molecule 16: Photosystem II 12 kDa extrinsic protein





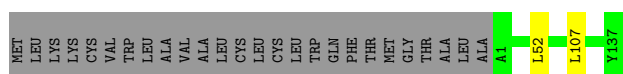
- Molecule 17: Cytochrome c-550

Chain V: 82% 16%



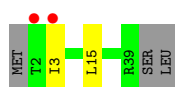
- Molecule 17: Cytochrome c-550

Chain v: 83% 16%



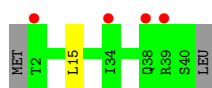
- Molecule 18: Photosystem II reaction center X protein

Chain X: 5% 88% 5% 7%



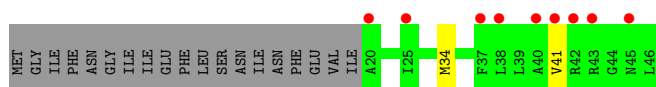
- Molecule 18: Photosystem II reaction center X protein

Chain x: 10% 93% 5%



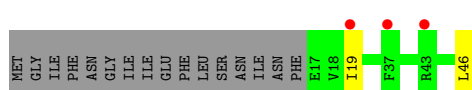
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain Y: 20% 54% 41%



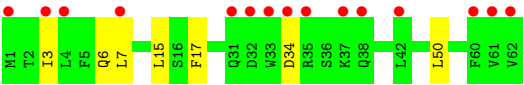
- Molecule 19: Photosystem II reaction center protein Ycf12

Chain y: 7% 61% 35%

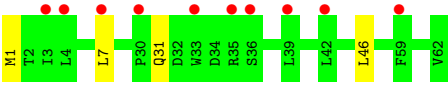


- Molecule 20: Photosystem II reaction center protein Z

Chain Z: 24% 89% 11%



● Molecule 20: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.23 33.70 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.70-2.23) 85.1 (33.70-2.23)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.176 , 0.233 0.176 , 0.233	Depositor DCC
$R_{free}$ test set	3445 reflections (0.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	105562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FE2, OEX, STE, HEC, BCR, CLA, PHO, BCT, DGD, LMG, OEY, CL, FME, PL9, SQD, HEM, LHG

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	0.58	0/3227	0.67	1/4397 (0.0%)
1	a	0.59	0/3224	0.65	0/4393
2	B	0.63	0/4161	0.68	1/5669 (0.0%)
2	b	0.59	0/4118	0.68	1/5611 (0.0%)
3	C	0.61	0/3647	0.67	2/4965 (0.0%)
3	c	0.58	0/3719	0.65	0/5061
4	D	0.66	0/2825	0.69	0/3847
4	d	0.61	0/2834	0.69	1/3859 (0.0%)
5	E	0.54	0/688	0.60	0/940
5	e	0.50	0/683	0.62	0/932
6	F	0.45	0/284	0.59	0/387
6	f	0.50	0/284	0.63	0/387
7	H	0.61	0/523	0.65	0/713
7	h	0.56	0/511	0.68	0/697
8	I	0.61	0/293	0.67	0/396
8	i	0.65	0/293	0.63	0/396
9	J	0.47	0/263	0.61	0/356
9	j	0.50	0/263	0.65	0/356
10	K	0.47	0/303	0.59	0/416
10	k	0.55	0/303	0.64	0/416
11	L	0.72	0/311	0.71	0/422
11	l	0.64	0/303	0.65	0/412
12	M	0.66	0/249	0.67	0/341
12	m	0.68	0/244	0.72	0/334
13	O	0.59	0/1904	0.74	1/2585 (0.0%)
13	o	0.61	0/1905	0.73	2/2583 (0.1%)
14	R	0.40	0/227	0.53	0/313
14	r	0.37	0/227	0.53	0/313
15	T	0.76	0/257	0.69	0/349
15	t	0.75	0/255	0.61	0/346
16	U	0.53	0/785	0.67	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	u	0.60	0/785	0.68	0/1064
17	V	0.59	0/1085	0.70	1/1473 (0.1%)
17	v	0.53	0/1085	0.65	0/1473
18	X	0.48	0/284	0.59	0/384
18	x	0.41	0/289	0.54	0/391
19	Y	0.45	0/197	0.61	0/264
19	y	0.38	0/219	0.59	0/294
20	Z	0.43	0/490	0.52	0/669
20	z	0.42	0/488	0.52	0/666
All	All	0.59	0/44035	0.67	10/59934 (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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	102	ASP	CB-CG-OD1	7.12	124.71	118.30
2	B	380	ASP	CB-CG-OD1	6.06	123.76	118.30
2	b	98	LEU	CA-CB-CG	5.77	128.58	115.30
3	C	396	MET	CG-SD-CE	-5.73	91.04	100.20
17	V	63	THR	C-N-CD	-5.34	108.85	120.60
3	C	315	MET	CG-SD-CE	-5.33	91.68	100.20
1	A	131	TRP	CA-CB-CG	-5.21	103.80	113.70
13	O	158	ASP	CB-CG-OD1	5.19	122.97	118.30
4	d	297	ASP	CB-CG-OD1	5.16	122.95	118.30
13	o	102	ASP	CB-CG-OD2	-5.15	113.66	118.30

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	397/344 (115%)	384 (97%)	12 (3%)	1 (0%)	41	44
1	a	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	488 (97%)	13 (3%)	2 (0%)	34	35
3	C	454/461 (98%)	441 (97%)	12 (3%)	1 (0%)	47	53
3	c	463/461 (100%)	453 (98%)	9 (2%)	1 (0%)	47	53
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	12	7
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	9	5
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	1 (3%)	1 (3%)	4	1
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	4	1
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	226 (93%)	12 (5%)	5 (2%)	7	2
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	34	35
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	14	9
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	22	20
17	v	135/163 (83%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5387/5700 (94%)	5206 (97%)	164 (3%)	17 (0%)	41	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	V	64	PRO
3	c	416	SER
3	C	416	SER
13	O	36	GLN
13	O	59	LYS
13	O	60	ARG
16	u	53	ALA
13	O	57	LYS
13	O	62	GLU
13	o	73	ARG
2	b	127	ARG

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Mol	Chain	Res	Type
2	b	294	SER
5	e	83	LEU
8	i	33	LYS
9	J	6	GLY
1	A	259	ILE
7	h	60	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	322 (99%)	2 (1%)	86	90
1	a	323/280 (115%)	313 (97%)	10 (3%)	40	46
2	B	408/407 (100%)	398 (98%)	10 (2%)	47	54
2	b	402/407 (99%)	395 (98%)	7 (2%)	60	68
3	C	356/362 (98%)	349 (98%)	7 (2%)	55	62
3	c	364/362 (101%)	352 (97%)	12 (3%)	38	43
4	D	277/283 (98%)	271 (98%)	6 (2%)	52	59
4	d	278/283 (98%)	269 (97%)	9 (3%)	39	44
5	E	72/73 (99%)	70 (97%)	2 (3%)	43	49
5	e	71/73 (97%)	68 (96%)	3 (4%)	30	32
6	F	28/39 (72%)	27 (96%)	1 (4%)	35	39
6	f	28/39 (72%)	26 (93%)	2 (7%)	14	11
7	H	54/55 (98%)	52 (96%)	2 (4%)	34	38
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	5
8	I	32/34 (94%)	31 (97%)	1 (3%)	40	46
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	30	32
9	j	24/28 (86%)	22 (92%)	2 (8%)	11	7
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	10	6
12	M	28/32 (88%)	26 (93%)	2 (7%)	14	11
12	m	28/32 (88%)	26 (93%)	2 (7%)	14	11
13	O	206/228 (90%)	197 (96%)	9 (4%)	28	30
13	o	207/228 (91%)	199 (96%)	8 (4%)	32	35
14	R	22/33 (67%)	21 (96%)	1 (4%)	27	29
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	1
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	80 (95%)	4 (5%)	25	25
16	u	84/112 (75%)	84 (100%)	0	100	100
17	V	117/138 (85%)	116 (99%)	1 (1%)	78	84
17	v	117/138 (85%)	115 (98%)	2 (2%)	60	68
18	X	31/34 (91%)	29 (94%)	2 (6%)	17	14
18	x	31/34 (91%)	30 (97%)	1 (3%)	39	44
19	Y	19/37 (51%)	17 (90%)	2 (10%)	7	3
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	6
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	1
20	z	51/52 (98%)	47 (92%)	4 (8%)	12	9
All	All	4451/4654 (96%)	4310 (97%)	141 (3%)	39	44

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LYS
1	A	243	GLU
2	B	87	ASP
2	B	98	LEU
2	B	127	ARG
2	B	246	PHE
2	B	362	PHE
2	B	371	THR
2	B	374	ASN

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Mol	Chain	Res	Type
2	B	385	ARG
2	B	388	SER
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	213	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	26	ARG
4	D	43	LEU
4	D	154	VAL
4	D	180	ARG
4	D	233	ARG
4	D	264	LYS
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	49	TYR
7	H	56	ASP
8	I	4	LEU
9	J	24	ILE
10	K	10	LYS
10	K	19	ASP
10	K	27	VAL
12	M	16	LEU
12	M	25	LEU
13	O	23	ASP
13	O	37	THR
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	184	ARG
13	O	189	ARG
13	O	214	THR
14	R	22	ASN
16	U	24	LYS
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU

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Mol	Chain	Res	Type
17	V	3	LEU
18	X	3	ILE
18	X	15	LEU
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	6	GLN
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	34	ASP
20	Z	50	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	236	THR
2	b	246	PHE
2	b	362	PHE
2	b	506	ARG
3	c	29	GLU
3	c	72	LEU
3	c	79	LYS
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	391[A]	ARG
3	c	391[B]	ARG
3	c	468	SER
4	d	180	ARG

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Mol	Chain	Res	Type
4	d	182	LEU
4	d	230	SER
4	d	233	ARG
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	321	LEU
5	e	4	THR
5	e	8	ARG
5	e	65	LEU
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
7	h	41	PHE
7	h	49	TYR
7	h	56	ASP
9	j	7	ARG
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	30	VAL
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	23	ASP
13	o	49	THR
13	o	55	GLU
13	o	64	GLU
13	o	86	LYS
13	o	118	LEU
13	o	134	THR
13	o	135	SER
14	r	5	VAL
14	r	9	LEU
14	r	10	LEU
17	v	52	LEU
17	v	107	LEU
18	x	15	LEU

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Mol	Chain	Res	Type
19	y	19	ILE
19	y	46	LEU
20	z	1	MET
20	z	7	LEU
20	z	31	GLN
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	409	GLN
3	C	74	HIS
3	C	201	ASN
13	O	88	ASN
13	O	231	HIS
16	U	63	ASN
17	V	86	GLN
20	Z	38	GLN
1	a	19	ASN
1	a	234	ASN
2	b	409	GLN
2	b	490	GLN
13	o	61	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
8	FME	I	1	8	8,9,10	0.94	0	7,9,11	0.89	0
15	FME	T	1	15	8,9,10	1.13	0	7,9,11	1.42	1 (14%)
12	FME	M	1	12	8,9,10	0.84	0	7,9,11	0.88	0
15	FME	t	1	15	8,9,10	1.25	1 (12%)	7,9,11	0.80	0
12	FME	m	1	12	8,9,10	0.90	0	7,9,11	1.04	1 (14%)
8	FME	i	1	8	8,9,10	1.12	1 (12%)	7,9,11	0.85	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
8	FME	I	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.87	1.42	1.46
8	i	1	FME	CA-N	-2.31	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	CA-N-CN	3.03	127.49	122.82
12	m	1	FME	CA-N-CN	-2.06	119.65	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
12	M	1	FME	CB-CA-N-CN
12	m	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
15	t	1	FME	CB-CG-SD-CE
15	T	1	FME	CB-CG-SD-CE
12	M	1	FME	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	B	605	-	56,73,73	1.72	5 (8%)	55,113,113	1.52	12 (21%)
24	CLA	b	615	-	56,73,73	1.65	8 (14%)	55,113,113	1.50	10 (18%)
33	LMG	D	407	-	51,51,55	1.00	3 (5%)	59,59,63	1.35	5 (8%)
31	DGD	C	516	-	63,63,67	1.38	11 (17%)	77,77,81	1.35	11 (14%)
26	BCR	b	617	-	41,41,41	1.04	4 (9%)	56,56,56	1.26	6 (10%)
24	CLA	B	610	-	56,73,73	1.53	9 (16%)	55,113,113	1.50	8 (14%)
24	CLA	C	506	-	56,73,73	1.65	8 (14%)	55,113,113	1.77	9 (16%)
26	BCR	T	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.24	4 (7%)
32	STE	b	621	-	16,19,19	0.38	0	15,19,19	0.94	0
31	DGD	C	517	-	63,63,67	1.12	4 (6%)	77,77,81	1.40	9 (11%)
26	BCR	K	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.21	6 (10%)
26	BCR	b	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.31	9 (16%)
24	CLA	B	608	-	56,73,73	1.54	7 (12%)	55,113,113	1.86	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	606	-	56,73,73	1.62	6 (10%)	55,113,113	2.03	11 (20%)
26	BCR	c	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.23	5 (8%)
24	CLA	c	509	-	56,73,73	1.55	4 (7%)	55,113,113	1.86	10 (18%)
24	CLA	B	604	-	56,73,73	1.37	7 (12%)	55,113,113	1.46	10 (18%)
26	BCR	D	405	-	41,41,41	1.20	2 (4%)	56,56,56	1.13	5 (8%)
22	OEX	A	602[A]	1,3,37	0,15,15	-	-	-	-	-
26	BCR	X	101	-	41,41,41	1.13	1 (2%)	56,56,56	1.39	8 (14%)
24	CLA	B	609	37	56,73,73	1.73	10 (17%)	55,113,113	1.62	10 (18%)
32	STE	B	626	-	8,11,19	0.39	0	7,11,19	0.67	0
30	LHG	D	409	-	48,48,48	1.16	5 (10%)	51,54,54	1.22	5 (9%)
32	STE	b	623	-	12,15,19	0.53	0	11,15,19	0.54	0
31	DGD	c	516	-	63,63,67	1.27	8 (12%)	77,77,81	1.44	15 (19%)
32	STE	B	623	-	17,17,19	0.43	0	16,16,19	0.77	0
32	STE	a	617	-	9,9,19	0.51	0	8,8,19	0.56	0
32	STE	B	619	-	13,16,19	0.41	0	12,16,19	0.87	0
24	CLA	b	612	-	56,73,73	1.41	7 (12%)	55,113,113	2.01	13 (23%)
31	DGD	c	517	-	63,63,67	1.12	6 (9%)	77,77,81	1.32	8 (10%)
24	CLA	b	613	-	56,73,73	1.72	8 (14%)	55,113,113	1.70	12 (21%)
29	SQD	D	408	-	35,36,54	0.96	3 (8%)	42,45,65	1.86	8 (19%)
31	DGD	C	518	-	63,63,67	1.17	9 (14%)	77,77,81	1.39	7 (9%)
33	LMG	c	521	-	48,48,55	1.20	5 (10%)	56,56,63	1.30	5 (8%)
24	CLA	c	513	-	56,73,73	1.61	6 (10%)	55,113,113	1.66	11 (20%)
31	DGD	c	518	-	63,63,67	1.08	8 (12%)	77,77,81	1.40	12 (15%)
24	CLA	d	403	-	56,73,73	1.70	10 (17%)	55,113,113	1.21	5 (9%)
24	CLA	c	511	3	56,73,73	1.83	7 (12%)	55,113,113	1.69	8 (14%)
29	SQD	B	620	-	53,54,54	0.96	2 (3%)	62,65,65	2.18	13 (20%)
33	LMG	D	411	-	31,31,55	1.00	3 (9%)	33,33,63	1.18	3 (9%)
29	SQD	a	616	-	35,35,54	1.05	2 (5%)	37,37,65	1.16	3 (8%)
32	STE	t	102	-	10,13,19	0.48	0	9,13,19	0.72	0
30	LHG	d	406	-	48,48,48	0.80	0	51,54,54	1.18	3 (5%)
24	CLA	C	502	-	56,73,73	1.47	8 (14%)	55,113,113	1.44	8 (14%)
24	CLA	c	510	-	56,73,73	1.74	10 (17%)	55,113,113	1.91	12 (21%)
24	CLA	A	605	37	56,73,73	1.63	7 (12%)	55,113,113	1.60	11 (20%)
34	BCT	D	402	23	0,3,3	-	-	0,3,3	-	-
32	STE	C	521	-	8,11,19	0.47	0	7,11,19	0.73	0
24	CLA	a	607	-	56,73,73	1.55	6 (10%)	55,113,113	1.49	9 (16%)
32	STE	T	103	-	14,14,19	0.40	0	13,13,19	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	C	513	-	56,73,73	1.62	8 (14%)	55,113,113	1.85	10 (18%)
32	STE	j	101	-	8,11,19	0.42	0	7,11,19	0.76	0
33	LMG	C	515	-	48,48,55	1.20	5 (10%)	56,56,63	1.56	12 (21%)
32	STE	d	411	-	16,19,19	0.35	0	15,19,19	0.80	0
22	OEX	a	602[A]	1,3,37	0,15,15	-	-	-		
24	CLA	b	611	-	56,73,73	1.46	9 (16%)	55,113,113	1.67	11 (20%)
26	BCR	B	616	-	41,41,41	1.12	3 (7%)	56,56,56	1.45	8 (14%)
24	CLA	B	601	-	56,73,73	1.65	8 (14%)	55,113,113	1.75	12 (21%)
24	CLA	C	507	37	56,73,73	1.72	10 (17%)	55,113,113	1.81	11 (20%)
24	CLA	B	612	-	56,73,73	1.71	6 (10%)	55,113,113	1.92	12 (21%)
24	CLA	C	503	-	56,73,73	1.82	10 (17%)	55,113,113	1.73	12 (21%)
26	BCR	b	618	-	41,41,41	1.35	3 (7%)	56,56,56	1.39	9 (16%)
24	CLA	c	502	-	56,73,73	1.59	7 (12%)	55,113,113	1.73	10 (18%)
26	BCR	B	618	-	41,41,41	1.15	2 (4%)	56,56,56	1.37	8 (14%)
24	CLA	b	610	37	56,73,73	1.45	8 (14%)	55,113,113	1.67	10 (18%)
24	CLA	c	512	-	56,73,73	1.47	6 (10%)	55,113,113	1.74	13 (23%)
30	LHG	D	410	-	46,46,48	1.14	4 (8%)	49,52,54	1.16	2 (4%)
24	CLA	C	504	37	50,67,73	1.82	8 (16%)	47,105,113	1.44	9 (19%)
24	CLA	b	605	-	56,73,73	1.53	7 (12%)	55,113,113	1.70	9 (16%)
28	PL9	d	405	-	55,55,55	1.48	5 (9%)	68,69,69	1.59	12 (17%)
32	STE	Z	101	-	7,7,19	0.46	0	6,6,19	0.38	0
24	CLA	C	510	-	56,73,73	1.47	8 (14%)	55,113,113	1.60	7 (12%)
26	BCR	B	617	-	41,41,41	1.14	3 (7%)	56,56,56	1.40	7 (12%)
26	BCR	c	515	-	41,41,41	1.26	4 (9%)	56,56,56	1.49	11 (19%)
25	PHO	a	606	-	67,69,69	1.11	7 (10%)	85,99,99	1.12	4 (4%)
26	BCR	d	404	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	4 (7%)
24	CLA	H	101	37	56,73,73	1.76	8 (14%)	55,113,113	1.55	9 (16%)
33	LMG	M	101	-	51,51,55	1.02	4 (7%)	59,59,63	1.40	9 (15%)
24	CLA	B	614	-	56,73,73	1.78	8 (14%)	55,113,113	1.69	7 (12%)
28	PL9	D	406	-	55,55,55	1.24	6 (10%)	68,69,69	1.88	18 (26%)
30	LHG	A	614	-	48,48,48	0.82	2 (4%)	51,54,54	1.22	6 (11%)
24	CLA	B	613	-	56,73,73	1.62	9 (16%)	55,113,113	1.50	12 (21%)
24	CLA	b	603	-	56,73,73	1.64	11 (19%)	55,113,113	1.65	9 (16%)
29	SQD	A	615	-	38,38,54	1.05	3 (7%)	40,40,65	1.45	4 (10%)
32	STE	M	104	-	17,17,19	0.35	0	16,16,19	0.86	0
30	LHG	d	407	-	38,38,48	0.95	2 (5%)	41,44,54	1.16	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	b	608	-	56,73,73	1.95	9 (16%)	55,113,113	1.55	10 (18%)
32	STE	a	618	-	8,11,19	0.46	0	7,11,19	0.67	0
24	CLA	d	402	-	56,73,73	1.32	8 (14%)	55,113,113	1.47	8 (14%)
24	CLA	B	607	-	56,73,73	1.69	11 (19%)	55,113,113	1.87	11 (20%)
24	CLA	C	508	-	56,73,73	1.80	9 (16%)	55,113,113	1.51	7 (12%)
32	STE	d	409	-	13,16,19	0.31	0	12,16,19	0.92	0
24	CLA	C	501	-	56,73,73	1.74	9 (16%)	55,113,113	1.50	9 (16%)
33	LMG	c	519	-	37,37,55	1.24	5 (13%)	45,45,63	1.32	6 (13%)
24	CLA	a	613	37	56,73,73	1.76	7 (12%)	55,113,113	1.40	8 (14%)
32	STE	C	519	-	8,11,19	0.51	0	7,11,19	0.55	0
26	BCR	t	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.43	9 (16%)
32	STE	C	520	-	15,15,19	0.44	0	14,14,19	0.63	0
33	LMG	b	622	-	55,55,55	0.91	3 (5%)	63,63,63	1.51	10 (15%)
33	LMG	a	619	-	55,55,55	1.40	7 (12%)	63,63,63	1.48	10 (15%)
24	CLA	A	604	-	56,73,73	1.61	6 (10%)	55,113,113	1.74	13 (23%)
33	LMG	d	408	-	44,44,55	1.00	4 (9%)	52,52,63	1.25	4 (7%)
24	CLA	D	404	-	56,73,73	1.39	8 (14%)	55,113,113	1.64	9 (16%)
29	SQD	b	620	-	48,49,54	0.98	3 (6%)	57,60,65	2.55	15 (26%)
31	DGD	h	102	-	63,63,67	1.19	8 (12%)	77,77,81	1.36	9 (11%)
24	CLA	C	511	3	56,73,73	1.77	8 (14%)	55,113,113	1.53	7 (12%)
32	STE	R	101	-	8,11,19	0.42	0	7,11,19	0.74	0
25	PHO	D	401	-	67,69,69	1.22	9 (13%)	85,99,99	1.12	5 (5%)
32	STE	X	102	-	16,19,19	0.34	0	15,19,19	0.95	0
24	CLA	C	512	-	56,73,73	1.71	6 (10%)	55,113,113	1.63	12 (21%)
32	STE	c	523	-	8,11,19	0.38	0	7,11,19	0.64	0
26	BCR	K	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.22	3 (5%)
26	BCR	a	608	-	41,41,41	1.13	3 (7%)	56,56,56	1.35	10 (17%)
21	OEY	a	601[B]	1,3,37	0,16,16	-	-	-	-	-
32	STE	b	624	-	16,19,19	0.47	0	15,19,19	0.79	0
36	HEC	V	201	17	26,50,50	2.27	4 (15%)	18,82,82	1.88	6 (33%)
32	STE	d	410	-	16,19,19	0.41	0	15,19,19	0.67	0
24	CLA	b	616	-	51,68,73	1.70	10 (19%)	49,107,113	1.74	12 (24%)
24	CLA	A	612	37	56,73,73	1.32	5 (8%)	55,113,113	1.62	10 (18%)
24	CLA	c	508	-	55,72,73	1.73	6 (10%)	53,111,113	1.69	11 (20%)
32	STE	B	621	-	8,11,19	0.45	0	7,11,19	0.92	0
24	CLA	B	611	-	56,73,73	1.55	6 (10%)	55,113,113	1.89	8 (14%)
24	CLA	b	614	-	56,73,73	1.55	8 (14%)	55,113,113	1.52	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CLA	c	507	37	56,73,73	1.58	7 (12%)	55,113,113	1.76	11 (20%)
24	CLA	c	501	-	56,73,73	1.44	8 (14%)	55,113,113	1.57	9 (16%)
26	BCR	k	102	-	41,41,41	1.12	2 (4%)	56,56,56	1.12	5 (8%)
32	STE	B	622	-	14,17,19	0.45	0	13,17,19	0.75	0
32	STE	h	103	-	13,13,19	0.42	0	12,12,19	0.64	0
33	LMG	m	101	-	51,51,55	1.21	4 (7%)	59,59,63	1.56	8 (13%)
30	LHG	e	101	-	41,41,48	0.99	2 (4%)	44,47,54	1.29	6 (13%)
24	CLA	a	604	-	56,73,73	1.71	10 (17%)	55,113,113	1.56	8 (14%)
36	HEC	v	201	17	26,50,50	2.33	3 (11%)	18,82,82	2.26	6 (33%)
24	CLA	C	505	-	56,73,73	1.67	7 (12%)	55,113,113	1.70	10 (18%)
25	PHO	d	401	-	67,69,69	1.25	8 (11%)	85,99,99	1.27	7 (8%)
24	CLA	c	505	-	56,73,73	1.57	8 (14%)	55,113,113	2.01	15 (27%)
35	HEM	F	101	6,5	27,50,50	1.96	4 (14%)	17,82,82	1.93	4 (23%)
33	LMG	Y	101	-	48,48,55	1.27	7 (14%)	56,56,63	1.29	5 (8%)
24	CLA	a	605	37	56,73,73	1.56	10 (17%)	55,113,113	1.61	10 (18%)
30	LHG	l	101	-	48,48,48	0.77	2 (4%)	51,54,54	1.24	5 (9%)
32	STE	b	625	-	9,9,19	0.40	0	8,8,19	0.51	0
26	BCR	A	608	-	41,41,41	1.22	4 (9%)	56,56,56	1.37	8 (14%)
34	BCT	a	611	23	0,3,3	-	-	0,3,3	-	-
21	OEY	A	601[B]	1,3,37	0,16,16	-	-	-	-	-
24	CLA	B	603	-	56,73,73	1.68	9 (16%)	55,113,113	2.32	13 (23%)
32	STE	B	625	-	14,14,19	0.43	0	13,13,19	0.83	0
33	LMG	D	412	-	20,26,55	0.60	0	18,26,63	1.16	0
32	STE	M	102	-	11,14,19	0.46	0	10,14,19	0.71	0
24	CLA	c	504	37	51,68,73	1.63	7 (13%)	49,107,113	1.61	9 (18%)
29	SQD	A	613	-	51,52,54	1.10	6 (11%)	60,63,65	2.08	13 (21%)
24	CLA	b	604	-	56,73,73	1.58	5 (8%)	55,113,113	2.32	14 (25%)
30	LHG	D	413	-	48,48,48	1.01	3 (6%)	51,54,54	1.32	7 (13%)
24	CLA	c	503	-	56,73,73	1.56	10 (17%)	55,113,113	1.26	4 (7%)
28	PL9	A	611	-	55,55,55	1.27	5 (9%)	68,69,69	1.74	17 (25%)
32	STE	c	520	-	16,19,19	0.38	0	15,19,19	0.84	0
32	STE	I	101	-	14,14,19	0.50	0	13,13,19	0.61	0
32	STE	J	101	-	8,11,19	0.36	0	7,11,19	0.65	0
24	CLA	b	602	-	56,73,73	1.58	9 (16%)	55,113,113	1.78	13 (23%)
24	CLA	B	606	37	56,73,73	1.62	9 (16%)	55,113,113	1.70	7 (12%)
30	LHG	L	101	-	48,48,48	0.74	2 (4%)	51,54,54	1.16	3 (5%)
24	CLA	b	607	37	56,73,73	1.50	7 (12%)	55,113,113	1.54	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	SQD	f	102	-	40,41,54	1.09	4 (10%)	49,52,65	1.85	10 (20%)
32	STE	M	103	-	9,9,19	0.48	0	8,8,19	0.57	0
24	CLA	B	602	-	56,73,73	1.35	8 (14%)	55,113,113	1.47	12 (21%)
24	CLA	B	615	-	51,68,73	1.81	11 (21%)	49,107,113	1.94	10 (20%)
24	CLA	b	601	37	56,73,73	1.61	7 (12%)	55,113,113	1.80	11 (20%)
28	PL9	a	612	-	55,55,55	0.90	1 (1%)	68,69,69	1.54	11 (16%)
26	BCR	k	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.08	4 (7%)
24	CLA	D	403	-	56,73,73	1.49	8 (14%)	55,113,113	1.64	10 (18%)
32	STE	B	624	-	15,15,19	0.50	0	14,14,19	0.57	0
32	STE	L	102	-	8,11,19	0.49	0	7,11,19	0.77	0
33	LMG	c	522	-	49,49,55	0.98	4 (8%)	57,57,63	1.26	3 (5%)
24	CLA	b	609	-	56,73,73	1.66	8 (14%)	55,113,113	1.74	12 (21%)
26	BCR	h	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.33	8 (14%)
24	CLA	c	506	-	56,73,73	1.51	8 (14%)	55,113,113	1.68	10 (18%)
25	PHO	A	606	-	67,69,69	1.27	9 (13%)	85,99,99	1.19	9 (10%)
24	CLA	A	607	-	45,62,73	1.51	10 (22%)	41,99,113	1.92	8 (19%)
26	BCR	C	514	-	41,41,41	1.28	3 (7%)	56,56,56	1.21	5 (8%)
24	CLA	C	509	-	56,73,73	1.60	8 (14%)	55,113,113	1.75	9 (16%)
31	DGD	A	616	-	67,67,67	1.26	9 (13%)	81,81,81	1.46	13 (16%)
35	HEM	f	101	6,5	27,50,50	1.89	4 (14%)	17,82,82	2.01	3 (17%)
26	BCR	K	103	-	41,41,41	1.24	4 (9%)	56,56,56	1.30	7 (12%)
30	LHG	a	614	-	48,48,48	1.06	4 (8%)	51,54,54	1.34	7 (13%)
31	DGD	H	102	-	63,63,67	1.32	9 (14%)	77,77,81	1.40	8 (10%)
29	SQD	a	615	-	53,54,54	0.97	6 (11%)	62,65,65	2.05	11 (17%)
32	STE	T	102	-	15,15,19	0.37	0	14,14,19	0.82	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
24	CLA	B	605	-	1/1/20/20	13/37/115/115	-
24	CLA	b	615	-	1/1/20/20	4/37/115/115	-
33	LMG	D	407	-	-	14/46/66/70	0/1/1/1
31	DGD	C	516	-	-	22/51/91/95	0/2/2/2
26	BCR	b	617	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	610	-	1/1/20/20	6/37/115/115	-
24	CLA	C	506	-	1/1/20/20	14/37/115/115	-
26	BCR	T	101	-	-	11/29/63/63	0/2/2/2
32	STE	b	621	-	-	9/15/17/17	-
31	DGD	C	517	-	-	18/51/91/95	0/2/2/2
26	BCR	K	101	-	-	9/29/63/63	0/2/2/2
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
24	CLA	b	606	-	1/1/20/20	7/37/115/115	-
24	CLA	B	608	-	-	4/37/115/115	-
26	BCR	c	514	-	-	8/29/63/63	0/2/2/2
24	CLA	c	509	-	1/1/20/20	13/37/115/115	-
24	CLA	B	604	-	1/1/20/20	14/37/115/115	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
26	BCR	X	101	-	-	6/29/63/63	0/2/2/2
24	CLA	B	609	37	1/1/20/20	7/37/115/115	-
32	STE	B	626	-	-	4/7/9/17	-
30	LHG	D	409	-	-	21/53/53/53	-
32	STE	b	623	-	-	6/11/13/17	-
31	DGD	c	516	-	-	20/51/91/95	0/2/2/2
32	STE	B	623	-	-	9/15/15/17	-
32	STE	a	617	-	-	4/7/7/17	-
32	STE	B	619	-	-	9/12/14/17	-
24	CLA	b	612	-	1/1/20/20	6/37/115/115	-
31	DGD	c	517	-	-	19/51/91/95	0/2/2/2
24	CLA	b	613	-	1/1/20/20	4/37/115/115	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
31	DGD	C	518	-	-	18/51/91/95	0/2/2/2
33	LMG	c	521	-	-	27/43/63/70	0/1/1/1
24	CLA	c	513	-	1/1/20/20	8/37/115/115	-
31	DGD	c	518	-	-	15/51/91/95	0/2/2/2
24	CLA	d	403	-	1/1/20/20	8/37/115/115	-
24	CLA	c	511	3	1/1/20/20	6/37/115/115	-
29	SQD	B	620	-	-	23/49/69/69	0/1/1/1
33	LMG	D	411	-	-	14/33/33/70	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	a	616	-	-	18/37/37/69	-
32	STE	t	102	-	-	2/9/11/17	-
30	LHG	d	406	-	-	26/53/53/53	-
24	CLA	C	502	-	1/1/20/20	6/37/115/115	-
24	CLA	c	510	-	1/1/20/20	13/37/115/115	-
24	CLA	A	605	37	1/1/20/20	14/37/115/115	-
32	STE	C	521	-	-	2/7/9/17	-
24	CLA	a	607	-	1/1/20/20	11/37/115/115	-
32	STE	T	103	-	-	8/12/12/17	-
24	CLA	C	513	-	1/1/20/20	9/37/115/115	-
32	STE	j	101	-	-	3/7/9/17	-
33	LMG	C	515	-	-	17/43/63/70	0/1/1/1
32	STE	d	411	-	-	11/15/17/17	-
24	CLA	b	611	-	1/1/20/20	4/37/115/115	-
26	BCR	B	616	-	-	7/29/63/63	0/2/2/2
24	CLA	B	601	-	1/1/20/20	8/37/115/115	-
24	CLA	C	507	37	1/1/20/20	7/37/115/115	-
24	CLA	B	612	-	1/1/20/20	12/37/115/115	-
24	CLA	C	503	-	1/1/20/20	5/37/115/115	-
26	BCR	b	618	-	-	2/29/63/63	0/2/2/2
24	CLA	c	502	-	1/1/20/20	8/37/115/115	-
26	BCR	B	618	-	-	6/29/63/63	0/2/2/2
24	CLA	b	610	37	1/1/20/20	7/37/115/115	-
24	CLA	c	512	-	1/1/20/20	16/37/115/115	-
30	LHG	D	410	-	-	21/51/51/53	-
24	CLA	C	504	37	1/1/18/20	8/30/108/115	-
24	CLA	b	605	-	1/1/20/20	6/37/115/115	-
28	PL9	d	405	-	-	12/53/73/73	0/1/1/1
32	STE	Z	101	-	-	2/5/5/17	-
24	CLA	C	510	-	1/1/20/20	8/37/115/115	-
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
26	BCR	c	515	-	-	5/29/63/63	0/2/2/2
25	PHO	a	606	-	-	2/53/103/103	0/5/6/6
26	BCR	d	404	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	H	101	37	1/1/20/20	18/37/115/115	-
33	LMG	M	101	-	-	23/46/66/70	0/1/1/1
24	CLA	B	614	-	1/1/20/20	6/37/115/115	-
28	PL9	D	406	-	-	11/53/73/73	0/1/1/1
30	LHG	A	614	-	-	30/53/53/53	-
24	CLA	B	613	-	1/1/20/20	16/37/115/115	-
24	CLA	b	603	-	1/1/20/20	4/37/115/115	-
29	SQD	A	615	-	-	17/39/39/69	-
32	STE	M	104	-	-	10/15/15/17	-
30	LHG	d	407	-	-	15/43/43/53	-
24	CLA	b	608	-	1/1/20/20	6/37/115/115	-
32	STE	a	618	-	-	4/7/9/17	-
24	CLA	d	402	-	-	6/37/115/115	-
24	CLA	B	607	-	1/1/20/20	4/37/115/115	-
24	CLA	C	508	-	-	7/37/115/115	-
32	STE	d	409	-	-	10/12/14/17	-
24	CLA	C	501	-	1/1/20/20	4/37/115/115	-
33	LMG	c	519	-	-	9/31/51/70	0/1/1/1
24	CLA	a	613	37	1/1/20/20	4/37/115/115	-
32	STE	C	519	-	-	3/7/9/17	-
26	BCR	t	101	-	-	7/29/63/63	0/2/2/2
32	STE	C	520	-	-	7/13/13/17	-
33	LMG	b	622	-	-	25/50/70/70	0/1/1/1
33	LMG	a	619	-	-	36/50/70/70	0/1/1/1
24	CLA	A	604	-	1/1/20/20	9/37/115/115	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1
24	CLA	D	404	-	1/1/20/20	13/37/115/115	-
29	SQD	b	620	-	-	21/44/64/69	0/1/1/1
31	DGD	h	102	-	-	18/51/91/95	0/2/2/2
24	CLA	C	511	3	1/1/20/20	9/37/115/115	-
32	STE	R	101	-	-	4/7/9/17	-
25	PHO	D	401	-	-	3/53/103/103	0/5/6/6
32	STE	X	102	-	-	12/15/17/17	-
24	CLA	C	512	-	1/1/20/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	c	523	-	-	7/7/9/17	-
26	BCR	K	102	-	-	7/29/63/63	0/2/2/2
26	BCR	a	608	-	-	6/29/63/63	0/2/2/2
32	STE	b	624	-	-	9/15/17/17	-
36	HEC	V	201	17	-	0/6/54/54	-
32	STE	d	410	-	-	11/15/17/17	-
24	CLA	b	616	-	1/1/19/20	8/31/109/115	-
24	CLA	A	612	37	1/1/20/20	7/37/115/115	-
24	CLA	c	508	-	1/1/19/20	8/36/114/115	-
32	STE	B	621	-	-	6/7/9/17	-
24	CLA	B	611	-	1/1/20/20	13/37/115/115	-
24	CLA	b	614	-	1/1/20/20	14/37/115/115	-
24	CLA	c	507	37	1/1/20/20	11/37/115/115	-
24	CLA	c	501	-	1/1/20/20	4/37/115/115	-
26	BCR	k	102	-	-	8/29/63/63	0/2/2/2
32	STE	B	622	-	-	8/13/15/17	-
32	STE	h	103	-	-	6/11/11/17	-
33	LMG	m	101	-	-	21/46/66/70	0/1/1/1
30	LHG	e	101	-	-	21/46/46/53	-
24	CLA	a	604	-	1/1/20/20	4/37/115/115	-
36	HEC	v	201	17	-	0/6/54/54	-
24	CLA	C	505	-	1/1/20/20	11/37/115/115	-
25	PHO	d	401	-	-	9/53/103/103	0/5/6/6
24	CLA	c	505	-	1/1/20/20	9/37/115/115	-
35	HEM	F	101	6,5	-	1/6/54/54	-
33	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
24	CLA	a	605	37	-	12/37/115/115	-
30	LHG	l	101	-	-	16/53/53/53	-
32	STE	b	625	-	-	5/7/7/17	-
26	BCR	A	608	-	-	6/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/20/20	13/37/115/115	-
32	STE	B	625	-	-	8/12/12/17	-
33	LMG	D	412	-	-	9/18/22/70	-
32	STE	M	102	-	-	5/10/12/17	-
24	CLA	c	504	37	1/1/19/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	A	613	-	-	22/47/67/69	0/1/1/1
24	CLA	b	604	-	1/1/20/20	13/37/115/115	-
30	LHG	D	413	-	-	15/53/53/53	-
24	CLA	c	503	-	1/1/20/20	7/37/115/115	-
28	PL9	A	611	-	-	21/53/73/73	0/1/1/1
32	STE	c	520	-	-	7/15/17/17	-
32	STE	I	101	-	-	7/12/12/17	-
32	STE	J	101	-	-	2/7/9/17	-
24	CLA	b	602	-	-	8/37/115/115	-
24	CLA	B	606	37	1/1/20/20	14/37/115/115	-
30	LHG	L	101	-	-	19/53/53/53	-
24	CLA	b	607	37	1/1/20/20	13/37/115/115	-
29	SQD	f	102	-	-	17/36/56/69	0/1/1/1
32	STE	M	103	-	-	2/7/7/17	-
24	CLA	B	602	-	1/1/20/20	11/37/115/115	-
24	CLA	B	615	-	1/1/19/20	7/31/109/115	-
24	CLA	b	601	37	1/1/20/20	18/37/115/115	-
28	PL9	a	612	-	-	19/53/73/73	0/1/1/1
26	BCR	k	101	-	-	11/29/63/63	0/2/2/2
24	CLA	D	403	-	-	10/37/115/115	-
32	STE	B	624	-	-	11/13/13/17	-
32	STE	L	102	-	-	3/7/9/17	-
33	LMG	c	522	-	-	26/44/64/70	0/1/1/1
24	CLA	b	609	-	-	8/37/115/115	-
26	BCR	h	101	-	-	6/29/63/63	0/2/2/2
24	CLA	c	506	-	1/1/20/20	15/37/115/115	-
25	PHO	A	606	-	-	3/53/103/103	0/5/6/6
24	CLA	A	607	-	1/1/17/20	2/24/102/115	-
26	BCR	C	514	-	-	7/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/20/20	12/37/115/115	-
31	DGD	A	616	-	-	28/55/95/95	0/2/2/2
35	HEM	f	101	6,5	-	0/6/54/54	-
26	BCR	K	103	-	-	6/29/63/63	0/2/2/2
30	LHG	a	614	-	-	24/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DGD	H	102	-	-	18/51/91/95	0/2/2/2
29	SQD	a	615	-	-	25/49/69/69	0/1/1/1
32	STE	T	102	-	-	9/13/13/17	-

All (859) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C4B-NB	8.42	1.42	1.35
24	B	605	CLA	MG-NA	8.14	2.25	2.06
24	B	613	CLA	C4B-NB	8.10	1.42	1.35
24	H	101	CLA	C4B-NB	8.08	1.42	1.35
24	A	605	CLA	C4B-NB	8.07	1.42	1.35
24	C	503	CLA	C4B-NB	8.02	1.42	1.35
24	B	601	CLA	C4B-NB	7.95	1.42	1.35
24	b	604	CLA	C4B-NB	7.84	1.42	1.35
24	b	608	CLA	C4C-NC	7.83	1.42	1.35
24	b	609	CLA	C4B-NB	7.78	1.42	1.35
24	C	512	CLA	MG-NA	7.74	2.24	2.06
24	b	601	CLA	C4B-NB	7.64	1.42	1.35
24	B	614	CLA	C4B-NB	7.64	1.42	1.35
24	b	613	CLA	C4B-NB	7.62	1.42	1.35
24	B	603	CLA	MG-NA	7.61	2.24	2.06
24	c	513	CLA	C4B-NB	7.56	1.42	1.35
24	C	504	CLA	C4B-NB	7.54	1.41	1.35
24	C	506	CLA	C4B-NB	7.52	1.41	1.35
36	V	201	HEC	C3B-C2B	-7.46	1.33	1.40
24	c	505	CLA	C4B-NB	7.40	1.41	1.35
24	b	607	CLA	C4B-NB	7.35	1.41	1.35
24	C	511	CLA	MG-NA	7.14	2.23	2.06
24	B	609	CLA	C4B-NB	7.09	1.41	1.35
24	C	511	CLA	C4B-NB	7.04	1.41	1.35
24	c	511	CLA	C4B-NB	7.01	1.41	1.35
24	C	505	CLA	MG-NA	6.93	2.22	2.06
24	C	507	CLA	MG-NA	6.88	2.22	2.06
24	a	613	CLA	MG-NA	6.87	2.22	2.06
24	c	510	CLA	C4C-NC	6.82	1.41	1.35
24	c	504	CLA	C4B-NB	6.81	1.41	1.35
24	C	501	CLA	C4B-NB	6.79	1.41	1.35
24	b	608	CLA	MG-NA	6.78	2.22	2.06
24	c	508	CLA	C4B-NB	6.76	1.41	1.35
24	d	403	CLA	C4B-NB	6.73	1.41	1.35
24	a	604	CLA	C4B-NB	6.63	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C4C-NC	6.63	1.41	1.35
24	c	509	CLA	C4B-NB	6.63	1.41	1.35
24	B	611	CLA	C4C-NC	6.62	1.41	1.35
24	C	508	CLA	C4B-NB	6.61	1.41	1.35
24	b	603	CLA	C4B-NB	6.60	1.41	1.35
24	C	508	CLA	MG-NA	6.59	2.21	2.06
36	v	201	HEC	C3B-C2B	-6.59	1.33	1.40
24	c	511	CLA	C4C-NC	6.58	1.41	1.35
24	C	513	CLA	C4B-NB	6.57	1.41	1.35
24	b	606	CLA	C4B-NB	6.57	1.41	1.35
24	c	511	CLA	MG-NA	6.56	2.21	2.06
24	C	504	CLA	C4C-NC	6.50	1.41	1.35
24	b	615	CLA	C4B-NB	6.46	1.41	1.35
24	B	606	CLA	C4B-NB	6.45	1.41	1.35
24	C	510	CLA	C4B-NB	6.45	1.41	1.35
24	c	502	CLA	C4B-NB	6.45	1.41	1.35
24	c	512	CLA	C4B-NB	6.42	1.40	1.35
24	B	615	CLA	MG-NA	6.37	2.21	2.06
24	c	507	CLA	C4B-NB	6.36	1.40	1.35
24	B	615	CLA	C4B-NB	6.34	1.40	1.35
24	B	611	CLA	C4B-NB	6.32	1.40	1.35
28	d	405	PL9	C6-C1	-6.30	1.37	1.48
24	a	607	CLA	C4B-NB	6.26	1.40	1.35
24	c	509	CLA	C4C-NC	6.24	1.40	1.35
24	c	502	CLA	C4C-NC	6.24	1.40	1.35
24	a	613	CLA	C4B-NB	6.23	1.40	1.35
24	c	506	CLA	C4B-NB	6.21	1.40	1.35
24	b	616	CLA	C4B-NB	6.21	1.40	1.35
24	b	612	CLA	C4B-NB	6.17	1.40	1.35
24	C	505	CLA	C4B-NB	6.14	1.40	1.35
24	c	501	CLA	C4B-NB	6.10	1.40	1.35
24	b	602	CLA	C4B-NB	6.09	1.40	1.35
24	b	608	CLA	C4B-NB	6.09	1.40	1.35
36	v	201	HEC	C3C-C2C	-6.02	1.34	1.40
24	c	503	CLA	C4B-NB	5.95	1.40	1.35
24	A	604	CLA	C4B-NB	5.95	1.40	1.35
24	B	614	CLA	MG-NA	5.94	2.20	2.06
24	b	605	CLA	C4C-NC	5.89	1.40	1.35
24	c	510	CLA	C4B-NB	5.88	1.40	1.35
24	B	608	CLA	MG-NA	5.88	2.20	2.06
24	A	604	CLA	C4C-NC	5.85	1.40	1.35
24	C	502	CLA	C4B-NB	5.78	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	C4C-NC	5.78	1.40	1.35
24	H	101	CLA	C4C-NC	5.77	1.40	1.35
24	b	602	CLA	C4C-NC	5.75	1.40	1.35
24	b	614	CLA	C4C-NC	5.75	1.40	1.35
24	C	512	CLA	C4C-NC	5.73	1.40	1.35
35	f	101	HEM	C3B-C2B	-5.72	1.32	1.40
24	C	503	CLA	MG-NA	5.68	2.19	2.06
24	b	610	CLA	C4C-NC	5.68	1.40	1.35
35	F	101	HEM	C3C-C2C	-5.68	1.32	1.40
24	C	507	CLA	C4B-NB	5.67	1.40	1.35
24	b	605	CLA	C4B-NB	5.66	1.40	1.35
24	c	508	CLA	MG-NA	5.61	2.19	2.06
24	c	508	CLA	C4C-NC	5.61	1.40	1.35
24	C	506	CLA	MG-NA	5.58	2.19	2.06
24	c	513	CLA	C4C-NC	5.55	1.40	1.35
24	B	607	CLA	MG-NA	5.54	2.19	2.06
24	B	610	CLA	C4B-NB	5.47	1.40	1.35
24	C	509	CLA	C4B-NB	5.45	1.40	1.35
24	B	610	CLA	C4C-NC	5.43	1.40	1.35
24	C	501	CLA	C4C-NC	5.38	1.40	1.35
24	c	504	CLA	C4C-NC	5.29	1.39	1.35
24	b	613	CLA	C4C-NC	5.27	1.39	1.35
24	B	607	CLA	C4C-NC	5.27	1.39	1.35
24	C	513	CLA	MG-NA	5.26	2.18	2.06
24	b	603	CLA	C4C-NC	5.25	1.39	1.35
24	b	616	CLA	C4C-NC	5.23	1.39	1.35
24	b	606	CLA	MG-NA	5.22	2.18	2.06
24	B	601	CLA	C4C-NC	5.19	1.39	1.35
24	B	609	CLA	C4C-NC	5.14	1.39	1.35
24	C	513	CLA	C4C-NC	5.14	1.39	1.35
24	c	510	CLA	MG-NA	5.13	2.18	2.06
24	B	604	CLA	C4B-NB	5.09	1.39	1.35
24	b	614	CLA	C4B-NB	5.07	1.39	1.35
24	a	607	CLA	C4C-NC	5.06	1.39	1.35
24	B	612	CLA	MG-NA	5.06	2.18	2.06
24	A	612	CLA	C4B-NB	5.06	1.39	1.35
24	a	613	CLA	C4C-NC	5.06	1.39	1.35
28	A	611	PL9	C7-C3	-5.05	1.46	1.51
24	a	604	CLA	MG-NA	5.03	2.18	2.06
24	B	608	CLA	C4B-NB	4.99	1.39	1.35
35	F	101	HEM	C3B-C2B	-4.99	1.33	1.40
24	c	503	CLA	C4C-NC	4.97	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	605	CLA	C4B-NB	4.92	1.39	1.35
24	b	601	CLA	C4C-NC	4.91	1.39	1.35
24	a	605	CLA	C4C-NC	4.90	1.39	1.35
24	C	507	CLA	C4C-NC	4.90	1.39	1.35
24	D	404	CLA	C4C-NC	4.90	1.39	1.35
36	V	201	HEC	C3C-C2C	-4.87	1.35	1.40
24	B	607	CLA	C4B-NB	4.87	1.39	1.35
36	v	201	HEC	C3D-C2D	4.84	1.52	1.37
24	B	613	CLA	C4C-NC	4.81	1.39	1.35
24	c	506	CLA	C4C-NC	4.79	1.39	1.35
24	B	606	CLA	MG-NA	4.76	2.17	2.06
24	c	512	CLA	C4C-NC	4.76	1.39	1.35
24	d	403	CLA	C4C-NC	4.68	1.39	1.35
24	D	403	CLA	C4C-NC	4.68	1.39	1.35
24	a	605	CLA	MG-NA	-4.67	1.95	2.06
24	A	604	CLA	MG-NA	4.65	2.17	2.06
24	b	606	CLA	C4C-NC	4.65	1.39	1.35
26	b	618	BCR	C30-C25	-4.64	1.47	1.53
24	C	508	CLA	C4C-NC	4.64	1.39	1.35
24	d	403	CLA	MG-NA	4.63	2.17	2.06
24	C	511	CLA	C4C-NC	4.63	1.39	1.35
33	a	619	LMG	C4-C5	4.61	1.62	1.53
24	B	615	CLA	C4C-NC	4.58	1.39	1.35
24	a	604	CLA	C4C-NC	4.57	1.39	1.35
24	b	604	CLA	C4C-NC	4.56	1.39	1.35
24	A	605	CLA	C4C-NC	4.55	1.39	1.35
24	C	503	CLA	C4C-NC	4.51	1.39	1.35
24	C	510	CLA	C4C-NC	4.48	1.39	1.35
24	D	404	CLA	C4B-NB	4.48	1.39	1.35
24	A	607	CLA	C4B-NB	4.45	1.39	1.35
24	C	502	CLA	C4C-NC	4.44	1.39	1.35
24	d	402	CLA	C4C-NC	4.43	1.39	1.35
24	C	505	CLA	C4C-NC	4.43	1.39	1.35
36	V	201	HEC	C3D-C2D	4.42	1.50	1.37
24	B	605	CLA	C4B-NB	4.42	1.39	1.35
24	b	610	CLA	C4B-NB	4.39	1.39	1.35
33	Y	101	LMG	C4-C5	4.37	1.62	1.53
24	d	402	CLA	C4B-NB	4.36	1.39	1.35
24	b	613	CLA	MG-NA	4.35	2.16	2.06
26	K	103	BCR	C30-C25	-4.34	1.47	1.53
33	C	515	LMG	C4-C3	4.33	1.63	1.52
24	B	608	CLA	C4C-NC	4.28	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C4C-NC	4.28	1.39	1.35
24	B	614	CLA	C4C-NC	4.24	1.39	1.35
24	b	611	CLA	C4C-NC	4.24	1.39	1.35
24	b	611	CLA	C4B-NB	4.24	1.39	1.35
31	A	616	DGD	C4D-C5D	4.23	1.61	1.53
26	C	514	BCR	C1-C6	-4.21	1.48	1.53
24	b	604	CLA	MG-NA	4.21	2.16	2.06
24	b	611	CLA	MG-NA	4.21	2.16	2.06
24	D	403	CLA	C4B-NB	4.16	1.38	1.35
24	C	501	CLA	MG-NA	4.14	2.16	2.06
24	c	507	CLA	MG-NA	4.13	2.16	2.06
26	t	101	BCR	C30-C25	-4.13	1.48	1.53
24	B	603	CLA	C4B-NB	4.12	1.38	1.35
24	c	501	CLA	C4C-NC	4.08	1.38	1.35
33	m	101	LMG	C4-C3	4.07	1.62	1.52
24	c	505	CLA	MG-NA	4.06	2.15	2.06
24	B	606	CLA	C4C-NC	4.05	1.38	1.35
26	C	514	BCR	C30-C25	-4.05	1.48	1.53
24	B	605	CLA	C3B-C2B	-4.02	1.34	1.40
24	C	512	CLA	C4B-NB	4.02	1.38	1.35
31	C	516	DGD	O5D-C6D	-4.01	1.36	1.43
24	B	612	CLA	C4C-NC	4.01	1.38	1.35
30	a	614	LHG	O7-C5	-3.96	1.36	1.46
35	f	101	HEM	C3C-C2C	-3.95	1.34	1.40
31	H	102	DGD	C4E-C5E	3.94	1.61	1.53
26	D	405	BCR	C1-C6	-3.89	1.48	1.53
26	K	101	BCR	C1-C6	-3.87	1.48	1.53
26	k	102	BCR	C30-C25	-3.86	1.48	1.53
28	a	612	PL9	C53-C6	-3.86	1.42	1.50
24	C	501	CLA	C3B-C2B	-3.82	1.35	1.40
24	D	403	CLA	MG-NA	3.79	2.15	2.06
26	X	101	BCR	C30-C25	-3.79	1.48	1.53
24	B	602	CLA	C3B-C2B	-3.76	1.35	1.40
24	C	508	CLA	C1B-NB	3.75	1.38	1.35
33	D	407	LMG	O2-C2	-3.74	1.34	1.43
28	d	405	PL9	C7-C3	3.74	1.55	1.51
26	B	616	BCR	C1-C6	-3.73	1.48	1.53
24	b	615	CLA	MG-NA	3.73	2.15	2.06
26	d	404	BCR	C1-C6	-3.71	1.48	1.53
33	m	101	LMG	O7-C8	-3.71	1.37	1.46
31	C	517	DGD	C4D-C3D	3.69	1.61	1.52
31	c	516	DGD	O6E-C1E	-3.66	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	515	BCR	C1-C6	-3.64	1.48	1.53
31	A	616	DGD	C3E-C2E	3.64	1.61	1.52
30	D	409	LHG	O8-C6	-3.60	1.36	1.45
26	a	608	BCR	C30-C25	-3.60	1.48	1.53
24	c	505	CLA	C4C-NC	3.60	1.38	1.35
24	C	504	CLA	MG-NA	3.60	2.14	2.06
29	A	615	SQD	O48-C23	3.58	1.43	1.33
29	a	616	SQD	O47-C7	3.57	1.44	1.34
26	k	101	BCR	C30-C25	-3.56	1.48	1.53
29	B	620	SQD	O47-C7	3.56	1.44	1.34
26	d	404	BCR	C30-C25	-3.56	1.48	1.53
24	H	101	CLA	MG-NA	3.55	2.14	2.06
35	F	101	HEM	C3B-CAB	3.55	1.55	1.47
24	B	609	CLA	C1D-C2D	3.54	1.50	1.42
24	b	609	CLA	MG-NA	3.53	2.14	2.06
26	D	405	BCR	C30-C25	-3.52	1.48	1.53
26	K	102	BCR	C1-C6	-3.52	1.48	1.53
30	D	410	LHG	P-O6	3.52	1.73	1.59
24	D	403	CLA	CAA-C2A	-3.50	1.47	1.54
33	m	101	LMG	O1-C7	-3.49	1.37	1.43
25	d	401	PHO	CHC-C1C	3.49	1.45	1.38
24	D	404	CLA	CMD-C2D	-3.48	1.43	1.51
24	B	609	CLA	CMB-C2B	-3.48	1.44	1.51
30	D	409	LHG	O7-C5	-3.47	1.37	1.46
29	b	620	SQD	O48-C23	3.46	1.43	1.33
24	C	502	CLA	C3B-C2B	-3.46	1.35	1.40
24	B	603	CLA	C4C-NC	3.46	1.38	1.35
25	d	401	PHO	C3B-C4B	3.45	1.50	1.43
24	A	612	CLA	C4C-NC	3.45	1.38	1.35
31	H	102	DGD	C1E-C2E	3.41	1.62	1.52
24	b	609	CLA	CMB-C2B	-3.41	1.44	1.51
30	a	614	LHG	C24-C23	3.40	1.60	1.50
26	K	101	BCR	C30-C25	-3.40	1.49	1.53
29	D	408	SQD	O48-C23	3.39	1.43	1.33
31	c	517	DGD	O5D-C1E	3.39	1.46	1.40
24	c	512	CLA	C1D-C2D	3.38	1.50	1.42
24	b	612	CLA	C4C-NC	3.37	1.38	1.35
24	a	613	CLA	CMB-C2B	-3.37	1.44	1.51
24	A	605	CLA	CMD-C2D	-3.36	1.43	1.51
24	A	607	CLA	CMB-C2B	-3.35	1.44	1.51
28	d	405	PL9	C11-C9	-3.34	1.44	1.51
29	B	620	SQD	O48-C23	3.33	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	CMB-C2B	-3.33	1.44	1.51
24	b	615	CLA	C3B-C2B	-3.32	1.35	1.40
33	c	521	LMG	C7-C8	3.31	1.60	1.50
24	B	603	CLA	C3B-C2B	-3.31	1.35	1.40
24	B	602	CLA	C3B-CAB	-3.29	1.41	1.47
24	B	604	CLA	C4C-NC	3.29	1.38	1.35
33	c	521	LMG	C3-C2	3.29	1.60	1.52
24	b	609	CLA	C4C-NC	3.29	1.38	1.35
31	H	102	DGD	O5D-C1E	3.29	1.45	1.40
29	A	615	SQD	O47-C7	3.28	1.43	1.34
29	A	613	SQD	O48-C23	3.27	1.42	1.33
24	b	613	CLA	CMB-C2B	-3.26	1.44	1.51
33	a	619	LMG	C4-C3	3.26	1.60	1.52
33	c	519	LMG	C4-C3	3.25	1.60	1.52
29	a	616	SQD	O48-C23	3.25	1.42	1.33
26	A	608	BCR	C1-C6	-3.24	1.49	1.53
30	e	101	LHG	P-O6	3.23	1.72	1.59
33	D	411	LMG	C7-C8	3.23	1.59	1.51
26	b	619	BCR	C30-C25	-3.23	1.49	1.53
24	b	616	CLA	MG-NA	3.23	2.13	2.06
26	B	618	BCR	C1-C6	-3.23	1.49	1.53
24	B	605	CLA	C3B-CAB	-3.21	1.41	1.47
30	D	413	LHG	O7-C5	-3.21	1.38	1.46
31	c	516	DGD	O3E-C3E	-3.20	1.35	1.43
24	c	510	CLA	CMB-C2B	-3.20	1.45	1.51
24	b	610	CLA	C3B-C2B	-3.20	1.35	1.40
24	b	603	CLA	C3B-C2B	-3.19	1.35	1.40
29	f	102	SQD	O48-C23	3.19	1.42	1.33
24	b	616	CLA	C3B-CAB	-3.19	1.41	1.47
24	B	602	CLA	C4C-NC	3.19	1.38	1.35
24	B	609	CLA	C3B-C2B	-3.17	1.36	1.40
24	b	602	CLA	MG-NA	3.17	2.13	2.06
25	D	401	PHO	C4C-C3C	3.16	1.50	1.45
24	c	507	CLA	C3B-C2B	-3.15	1.36	1.40
24	B	607	CLA	C1D-C2D	3.15	1.49	1.42
30	D	413	LHG	C24-C23	3.15	1.59	1.50
33	a	619	LMG	C7-C8	3.15	1.60	1.50
24	a	604	CLA	CMB-C2B	-3.14	1.45	1.51
26	B	618	BCR	C30-C25	-3.13	1.49	1.53
25	a	606	PHO	C3B-C4B	3.12	1.49	1.43
24	b	615	CLA	CMB-C2B	-3.12	1.45	1.51
31	C	517	DGD	O3E-C3E	-3.12	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	CMB-C2B	-3.11	1.45	1.51
24	C	501	CLA	CMB-C2B	-3.10	1.45	1.51
29	f	102	SQD	O47-C7	3.10	1.43	1.34
29	a	615	SQD	O48-C23	3.09	1.42	1.33
35	f	101	HEM	C3C-CAC	3.08	1.54	1.47
25	A	606	PHO	C1A-NA	3.07	1.43	1.37
24	B	614	CLA	C3B-C2B	-3.07	1.36	1.40
26	B	617	BCR	C30-C25	-3.06	1.49	1.53
26	K	102	BCR	C30-C25	-3.06	1.49	1.53
31	C	516	DGD	O5D-C1E	3.04	1.45	1.40
24	a	607	CLA	CMD-C2D	-3.04	1.44	1.51
24	C	509	CLA	MG-NA	3.04	2.13	2.06
31	C	516	DGD	C6E-C5E	3.04	1.62	1.51
24	B	615	CLA	CMC-C2C	-3.03	1.44	1.51
33	a	619	LMG	C3-C2	3.03	1.60	1.52
29	b	620	SQD	O47-C7	3.01	1.42	1.34
24	b	614	CLA	C3B-C2B	-3.00	1.36	1.40
24	B	607	CLA	CMD-C2D	-2.99	1.44	1.51
24	A	607	CLA	C3B-C2B	-2.98	1.36	1.40
31	A	616	DGD	C1E-C2E	2.98	1.61	1.52
30	D	410	LHG	O3-C3	-2.98	1.33	1.44
26	T	101	BCR	C30-C25	-2.97	1.49	1.53
24	B	610	CLA	CMB-C2B	-2.97	1.45	1.51
24	b	605	CLA	MG-NA	2.95	2.13	2.06
26	k	101	BCR	C1-C6	-2.95	1.49	1.53
31	C	518	DGD	C6D-C5D	2.95	1.60	1.51
33	Y	101	LMG	C1-C2	2.94	1.60	1.52
24	A	607	CLA	C4C-NC	2.93	1.37	1.35
28	A	611	PL9	C21-C19	2.93	1.57	1.51
25	D	401	PHO	CMC-C2C	-2.93	1.44	1.50
24	B	603	CLA	CMB-C2B	-2.93	1.45	1.51
31	h	102	DGD	O1G-C1G	-2.92	1.38	1.45
26	c	515	BCR	C30-C25	-2.92	1.49	1.53
31	h	102	DGD	O2G-C1B	2.91	1.42	1.34
33	m	101	LMG	C1-C2	2.91	1.60	1.52
31	c	516	DGD	C4D-C3D	2.91	1.59	1.52
24	H	101	CLA	CMB-C2B	-2.90	1.45	1.51
24	A	612	CLA	C1D-C2D	2.90	1.49	1.42
24	b	616	CLA	C1D-C2D	2.90	1.49	1.42
31	C	516	DGD	C4E-C3E	2.90	1.59	1.52
24	b	611	CLA	C1D-C2D	2.89	1.49	1.42
30	d	407	LHG	P-O6	2.88	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CMB-C2B	-2.87	1.45	1.51
33	c	521	LMG	O1-C1	2.87	1.45	1.40
24	a	607	CLA	CMC-C2C	-2.86	1.44	1.51
24	B	609	CLA	MG-NA	2.85	2.13	2.06
24	C	507	CLA	C1D-C2D	2.85	1.49	1.42
26	K	103	BCR	C1-C6	-2.85	1.49	1.53
28	D	406	PL9	C52-C5	-2.85	1.44	1.50
29	A	613	SQD	O2-C2	-2.85	1.36	1.43
33	d	408	LMG	O2-C2	-2.85	1.36	1.43
31	H	102	DGD	C4D-C5D	2.84	1.59	1.53
24	C	501	CLA	CMD-C2D	-2.84	1.44	1.51
24	B	607	CLA	C3B-CAB	-2.84	1.42	1.47
31	C	518	DGD	O5D-C1E	2.83	1.45	1.40
24	B	604	CLA	C3B-C2B	-2.83	1.36	1.40
24	b	605	CLA	C4B-CHC	-2.83	1.33	1.41
24	c	503	CLA	C3B-C2B	-2.82	1.36	1.40
31	c	516	DGD	O2G-C2G	-2.81	1.39	1.46
31	C	518	DGD	O1G-C1G	-2.81	1.38	1.45
33	a	619	LMG	O7-C10	2.81	1.42	1.34
24	c	501	CLA	CMB-C2B	-2.80	1.45	1.51
24	c	513	CLA	CMB-C2B	-2.80	1.45	1.51
24	c	501	CLA	C4B-CHC	-2.80	1.33	1.41
24	b	608	CLA	CMB-C2B	-2.80	1.45	1.51
33	Y	101	LMG	C4-C3	2.79	1.59	1.52
31	C	516	DGD	O1G-C1G	-2.79	1.38	1.45
24	a	605	CLA	CMD-C2D	-2.79	1.44	1.51
26	B	616	BCR	C33-C5	-2.78	1.46	1.50
24	C	507	CLA	CMD-C2D	-2.78	1.45	1.51
24	b	610	CLA	CMB-C2B	-2.76	1.45	1.51
24	H	101	CLA	C1D-C2D	2.76	1.48	1.42
30	D	409	LHG	P-O6	2.76	1.70	1.59
24	c	506	CLA	MG-NA	2.76	2.12	2.06
26	b	619	BCR	C1-C6	-2.76	1.50	1.53
35	F	101	HEM	C3C-CAC	2.75	1.53	1.47
24	b	602	CLA	CAC-C3C	-2.74	1.45	1.52
25	A	606	PHO	C4C-NC	2.74	1.42	1.36
31	C	518	DGD	O6D-C5D	-2.74	1.37	1.44
33	b	622	LMG	C4-C3	2.73	1.59	1.52
31	A	616	DGD	C3G-C2G	2.73	1.59	1.50
24	B	608	CLA	C3B-CAB	-2.73	1.42	1.47
24	b	601	CLA	C1D-C2D	2.72	1.48	1.42
24	B	601	CLA	CMB-C2B	-2.72	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C1-C6	-2.72	1.50	1.53
25	d	401	PHO	C4C-NC	2.72	1.42	1.36
26	h	101	BCR	C30-C25	-2.71	1.50	1.53
31	H	102	DGD	C4D-C3D	2.71	1.59	1.52
24	A	612	CLA	OBD-CAD	2.71	1.26	1.22
24	C	501	CLA	C1D-C2D	2.71	1.48	1.42
24	c	504	CLA	CMD-C2D	-2.71	1.45	1.51
31	h	102	DGD	O2D-C2D	-2.71	1.36	1.43
33	c	522	LMG	C4-C5	2.71	1.58	1.53
24	a	604	CLA	C1D-C2D	2.71	1.48	1.42
24	b	614	CLA	MG-NA	2.71	2.12	2.06
24	b	609	CLA	C3B-C2B	-2.70	1.36	1.40
26	b	617	BCR	C1-C6	-2.70	1.50	1.53
24	d	403	CLA	CMD-C2D	-2.70	1.45	1.51
31	c	518	DGD	C6D-C5D	2.70	1.60	1.51
24	b	610	CLA	C1C-C2C	2.70	1.48	1.42
24	b	603	CLA	CMB-C2B	-2.69	1.46	1.51
30	D	410	LHG	C24-C23	-2.69	1.42	1.50
24	C	511	CLA	CMB-C2B	-2.69	1.46	1.51
24	b	603	CLA	CMD-C2D	-2.69	1.45	1.51
24	C	503	CLA	C1D-C2D	2.69	1.48	1.42
24	C	506	CLA	CMC-C2C	-2.69	1.45	1.51
24	C	503	CLA	CMD-C2D	-2.69	1.45	1.51
24	d	403	CLA	C3B-C2B	-2.68	1.36	1.40
24	a	605	CLA	CMB-C2B	-2.68	1.46	1.51
24	c	510	CLA	C3B-C2B	-2.68	1.36	1.40
24	b	604	CLA	C1D-C2D	2.68	1.48	1.42
25	D	401	PHO	CHD-C4C	-2.68	1.34	1.40
24	c	511	CLA	CMB-C2B	-2.67	1.46	1.51
24	a	604	CLA	CAC-C3C	-2.67	1.45	1.52
26	T	101	BCR	C1-C6	-2.67	1.50	1.53
24	A	604	CLA	C3D-C2D	-2.67	1.34	1.39
24	B	611	CLA	C1D-C2D	2.66	1.48	1.42
24	c	509	CLA	CMB-C2B	-2.66	1.46	1.51
33	c	519	LMG	C4-C5	2.66	1.58	1.53
24	d	403	CLA	C3B-CAB	-2.66	1.42	1.47
24	c	502	CLA	CMD-C2D	-2.66	1.45	1.51
31	A	616	DGD	C4E-C5E	2.65	1.58	1.53
24	b	616	CLA	CMB-C2B	-2.65	1.46	1.51
24	B	602	CLA	CMB-C2B	-2.64	1.46	1.51
33	c	519	LMG	O1-C1	2.64	1.44	1.40
33	c	519	LMG	C7-C8	2.64	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	CMB-C2B	-2.64	1.46	1.51
24	c	503	CLA	C1D-C2D	2.64	1.48	1.42
25	A	606	PHO	C3B-C4B	2.64	1.48	1.43
31	h	102	DGD	C4E-C5E	2.63	1.58	1.53
30	A	614	LHG	P-O6	2.63	1.69	1.59
33	Y	101	LMG	O7-C8	-2.63	1.40	1.46
24	C	509	CLA	CMD-C2D	-2.63	1.45	1.51
24	c	513	CLA	C1D-C2D	2.63	1.48	1.42
24	B	613	CLA	CMB-C2B	-2.62	1.46	1.51
25	a	606	PHO	C1C-NC	-2.62	1.33	1.38
24	c	505	CLA	C3B-CAB	-2.62	1.42	1.47
24	c	501	CLA	CMD-C2D	-2.62	1.45	1.51
24	C	513	CLA	CMB-C2B	-2.61	1.46	1.51
26	b	618	BCR	C1-C6	-2.61	1.50	1.53
31	c	516	DGD	O3G-C3G	-2.61	1.39	1.43
25	A	606	PHO	CHC-C1C	2.60	1.43	1.38
24	D	404	CLA	CMB-C2B	-2.60	1.46	1.51
24	b	603	CLA	CAC-C3C	-2.60	1.45	1.52
24	c	504	CLA	C3B-C2B	-2.60	1.36	1.40
24	B	602	CLA	CMC-C2C	-2.60	1.45	1.51
26	c	515	BCR	C33-C5	-2.60	1.46	1.50
24	d	402	CLA	CMB-C2B	-2.60	1.46	1.51
24	C	510	CLA	MG-NA	2.60	2.12	2.06
33	M	101	LMG	C4-C3	2.60	1.58	1.52
24	a	607	CLA	CMB-C2B	-2.59	1.46	1.51
31	A	616	DGD	C4D-C3D	2.59	1.58	1.52
24	b	613	CLA	CMD-C2D	-2.59	1.45	1.51
24	A	607	CLA	CAC-C3C	-2.59	1.45	1.52
24	C	508	CLA	C1D-C2D	2.59	1.48	1.42
24	c	512	CLA	CMB-C2B	-2.59	1.46	1.51
24	B	610	CLA	C1D-C2D	2.59	1.48	1.42
24	C	506	CLA	C4C-NC	2.58	1.37	1.35
25	D	401	PHO	O2D-CGD	2.58	1.39	1.33
26	a	608	BCR	C38-C26	-2.58	1.46	1.50
33	M	101	LMG	O1-C1	2.58	1.44	1.40
24	d	402	CLA	C1D-C2D	2.58	1.48	1.42
24	c	511	CLA	C1D-C2D	2.58	1.48	1.42
24	C	501	CLA	C1C-C2C	2.57	1.48	1.42
29	a	615	SQD	O3-C3	-2.57	1.36	1.43
25	a	606	PHO	C4C-C3C	2.57	1.49	1.45
33	d	408	LMG	C7-C8	2.57	1.58	1.50
24	A	605	CLA	CMB-C2B	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	C3B-CAB	-2.57	1.42	1.47
24	B	602	CLA	C4B-NB	2.57	1.37	1.35
31	C	517	DGD	C6D-C5D	2.57	1.59	1.51
24	b	612	CLA	CAC-C3C	-2.57	1.45	1.52
24	b	616	CLA	CAC-C3C	-2.57	1.45	1.52
29	a	615	SQD	O2-C2	-2.56	1.37	1.43
30	a	614	LHG	P-O6	2.56	1.69	1.59
24	b	608	CLA	C1D-C2D	2.55	1.48	1.42
26	c	514	BCR	C30-C25	-2.55	1.50	1.53
24	b	603	CLA	CMC-C2C	-2.55	1.45	1.51
24	a	604	CLA	O2D-CED	-2.55	1.39	1.45
24	B	615	CLA	CMD-C2D	-2.55	1.45	1.51
33	d	408	LMG	O7-C8	-2.55	1.40	1.46
35	f	101	HEM	C3B-CAB	2.54	1.53	1.47
31	c	516	DGD	C4E-C3E	2.54	1.58	1.52
24	b	606	CLA	CMB-C2B	-2.54	1.46	1.51
24	B	604	CLA	C1D-C2D	2.54	1.48	1.42
26	k	102	BCR	C1-C6	-2.54	1.50	1.53
24	B	604	CLA	CMB-C2B	-2.54	1.46	1.51
24	B	614	CLA	CAC-C3C	-2.53	1.45	1.52
31	C	516	DGD	C3D-C2D	2.53	1.58	1.52
24	C	505	CLA	CMB-C2B	-2.53	1.46	1.51
24	B	601	CLA	C1D-C2D	2.53	1.48	1.42
24	C	512	CLA	C1D-C2D	2.53	1.48	1.42
29	A	613	SQD	O3-C3	-2.52	1.37	1.43
26	C	514	BCR	C33-C5	-2.52	1.46	1.50
24	b	614	CLA	CMC-C2C	-2.52	1.45	1.51
29	A	613	SQD	O4-C4	-2.52	1.37	1.43
24	B	613	CLA	C3B-C2B	-2.52	1.36	1.40
24	A	604	CLA	CMB-C2B	-2.51	1.46	1.51
24	B	609	CLA	CMC-C2C	-2.51	1.45	1.51
26	h	101	BCR	C33-C5	-2.51	1.46	1.50
26	a	608	BCR	C1-C6	-2.51	1.50	1.53
31	C	517	DGD	C1E-C2E	2.51	1.59	1.52
24	b	603	CLA	C1D-C2D	2.51	1.48	1.42
33	c	519	LMG	C3-C2	2.51	1.58	1.52
24	b	607	CLA	MG-NA	2.51	2.12	2.06
29	f	102	SQD	O2-C2	-2.50	1.37	1.43
24	A	607	CLA	CMD-C2D	-2.50	1.45	1.51
31	c	517	DGD	O3E-C3E	-2.50	1.37	1.43
24	a	613	CLA	CAC-C3C	-2.50	1.46	1.52
24	A	607	CLA	C4B-CHC	-2.50	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	518	DGD	O2E-C2E	-2.50	1.37	1.43
24	B	607	CLA	CMB-C2B	-2.50	1.46	1.51
25	d	401	PHO	CMD-C2D	-2.49	1.45	1.50
24	B	612	CLA	CMB-C2B	-2.49	1.46	1.51
28	d	405	PL9	C3-C4	-2.49	1.45	1.49
24	H	101	CLA	C3B-C2B	-2.49	1.36	1.40
24	a	613	CLA	C3B-C2B	-2.49	1.36	1.40
24	B	611	CLA	CMC-C2C	-2.49	1.45	1.51
24	c	508	CLA	CMD-C2D	-2.49	1.45	1.51
24	C	502	CLA	C1D-C2D	2.49	1.48	1.42
24	b	601	CLA	MG-NA	2.49	2.12	2.06
24	c	503	CLA	C3B-CAB	-2.49	1.42	1.47
24	B	612	CLA	C3B-CAB	-2.48	1.42	1.47
24	B	615	CLA	CMB-C2B	-2.48	1.46	1.51
24	B	611	CLA	CMD-C2D	-2.48	1.45	1.51
24	C	510	CLA	CAC-C3C	-2.48	1.46	1.52
24	C	507	CLA	CMC-C2C	-2.48	1.45	1.51
24	B	606	CLA	C3B-CAB	-2.47	1.42	1.47
24	C	503	CLA	CMB-C2B	-2.47	1.46	1.51
24	b	601	CLA	C1B-NB	2.47	1.37	1.35
31	c	517	DGD	C6D-C5D	2.47	1.59	1.51
30	D	410	LHG	O8-C23	2.47	1.40	1.33
24	H	101	CLA	C3B-CAB	-2.47	1.42	1.47
24	c	505	CLA	CMC-C2C	-2.46	1.45	1.51
25	d	401	PHO	CHD-C1D	2.46	1.43	1.38
28	D	406	PL9	C3-C4	-2.46	1.45	1.49
24	b	613	CLA	C1D-C2D	2.46	1.48	1.42
31	c	518	DGD	C2A-C1A	-2.46	1.43	1.50
26	A	608	BCR	C30-C25	-2.45	1.50	1.53
24	B	613	CLA	C3B-CAB	-2.45	1.42	1.47
24	B	606	CLA	C1D-C2D	2.45	1.48	1.42
24	B	607	CLA	C3B-C2B	-2.44	1.37	1.40
24	a	605	CLA	CAC-C3C	-2.44	1.46	1.52
24	c	506	CLA	CMB-C2B	-2.44	1.46	1.51
24	A	605	CLA	CAA-C2A	-2.43	1.49	1.54
24	C	503	CLA	C3B-CAB	-2.43	1.43	1.47
24	b	608	CLA	CMD-C2D	-2.43	1.45	1.51
24	C	506	CLA	C1D-C2D	2.43	1.48	1.42
29	A	615	SQD	O47-C45	-2.43	1.42	1.47
24	C	505	CLA	CMC-C2C	-2.43	1.45	1.51
24	b	602	CLA	CMD-C2D	-2.43	1.45	1.51
33	a	619	LMG	C1-C2	2.42	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	101	LHG	P-O6	2.42	1.69	1.59
24	c	504	CLA	C1D-C2D	2.42	1.48	1.42
24	c	502	CLA	C4B-CHC	-2.42	1.34	1.41
25	D	401	PHO	CAC-C3C	-2.41	1.44	1.51
24	B	606	CLA	CAC-C3C	-2.41	1.46	1.52
24	b	608	CLA	C3B-CAB	-2.41	1.43	1.47
24	C	507	CLA	C3B-C2B	-2.40	1.37	1.40
24	b	612	CLA	CMC-C2C	-2.40	1.45	1.51
24	C	504	CLA	C1D-C2D	2.40	1.48	1.42
26	b	617	BCR	C30-C25	-2.40	1.50	1.53
31	c	518	DGD	O6D-C5D	-2.40	1.38	1.44
24	b	603	CLA	MG-NA	2.40	2.12	2.06
25	D	401	PHO	C1C-NC	-2.39	1.33	1.38
24	a	607	CLA	MG-NA	2.39	2.12	2.06
24	D	403	CLA	C1D-C2D	2.39	1.48	1.42
24	C	509	CLA	C1D-C2D	2.39	1.48	1.42
24	c	502	CLA	CMB-C2B	-2.39	1.46	1.51
24	C	511	CLA	C1D-C2D	2.39	1.48	1.42
24	B	609	CLA	CMD-C2D	-2.38	1.45	1.51
24	B	610	CLA	C3B-C2B	-2.38	1.37	1.40
24	b	614	CLA	C1D-C2D	2.38	1.48	1.42
24	B	601	CLA	O2D-CGD	2.38	1.39	1.33
24	c	504	CLA	CAC-C3C	-2.38	1.46	1.52
24	b	607	CLA	CMD-C2D	-2.38	1.45	1.51
31	A	616	DGD	O2G-C2G	-2.38	1.40	1.46
24	d	403	CLA	CMB-C2B	-2.38	1.46	1.51
24	B	603	CLA	CMC-C2C	-2.38	1.45	1.51
24	b	612	CLA	CMD-C2D	-2.38	1.45	1.51
31	c	518	DGD	O2G-C2G	-2.38	1.40	1.46
24	b	615	CLA	CMC-C2C	-2.37	1.45	1.51
31	h	102	DGD	C6D-C5D	2.37	1.59	1.51
24	B	615	CLA	C3B-C2B	-2.37	1.37	1.40
33	c	522	LMG	C7-C8	2.37	1.58	1.50
24	C	502	CLA	CAC-C3C	-2.36	1.46	1.52
24	c	513	CLA	CMC-C2C	-2.36	1.45	1.51
24	c	503	CLA	CMB-C2B	-2.36	1.46	1.51
24	B	608	CLA	CMD-C2D	-2.36	1.45	1.51
33	a	619	LMG	C9-C8	2.36	1.57	1.50
24	C	506	CLA	CAC-C3C	-2.36	1.46	1.52
24	C	503	CLA	C3B-C2B	-2.36	1.37	1.40
24	b	607	CLA	C1D-C2D	2.36	1.47	1.42
24	b	603	CLA	C3B-CAB	-2.35	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	CMB-C2B	-2.35	1.46	1.51
24	B	610	CLA	CMC-C2C	-2.35	1.46	1.51
24	b	611	CLA	CMD-C2D	-2.35	1.46	1.51
24	c	507	CLA	CAC-C3C	-2.35	1.46	1.52
24	C	504	CLA	CAC-C3C	-2.35	1.46	1.52
26	K	101	BCR	C33-C5	-2.35	1.47	1.50
33	c	521	LMG	O7-C10	2.35	1.40	1.34
29	A	613	SQD	O47-C7	2.34	1.40	1.34
24	b	616	CLA	CMD-C2D	-2.34	1.46	1.51
24	B	603	CLA	O2D-CED	-2.34	1.39	1.45
24	c	506	CLA	O2D-CGD	2.33	1.38	1.33
29	A	613	SQD	O48-C46	-2.33	1.39	1.45
24	b	602	CLA	CMC-C2C	-2.33	1.46	1.51
28	D	406	PL9	C36-C34	2.32	1.56	1.51
24	d	403	CLA	CMC-C2C	-2.32	1.46	1.51
33	C	515	LMG	C6-C5	2.32	1.59	1.51
26	T	101	BCR	C38-C26	-2.32	1.47	1.50
24	C	511	CLA	CMC-C2C	-2.31	1.46	1.51
24	C	503	CLA	CMC-C2C	-2.31	1.46	1.51
24	C	501	CLA	CMC-C2C	-2.31	1.46	1.51
25	A	606	PHO	CMB-C2B	-2.31	1.45	1.50
31	H	102	DGD	O3D-C3D	-2.30	1.37	1.43
24	B	615	CLA	C4B-CHC	-2.30	1.34	1.41
28	d	405	PL9	C53-C6	-2.30	1.45	1.50
24	b	614	CLA	C5-C3	-2.30	1.46	1.51
24	b	608	CLA	C1B-NB	2.30	1.37	1.35
24	B	604	CLA	C1B-NB	-2.30	1.33	1.35
24	c	507	CLA	C3B-CAB	-2.30	1.43	1.47
24	b	609	CLA	C1D-C2D	2.30	1.47	1.42
26	A	608	BCR	C33-C5	-2.29	1.47	1.50
24	B	601	CLA	C4B-CHC	-2.29	1.34	1.41
30	D	413	LHG	P-O4	-2.29	1.44	1.55
24	c	505	CLA	C3B-C2B	-2.29	1.37	1.40
24	b	615	CLA	CMD-C2D	-2.29	1.46	1.51
24	B	609	CLA	CAC-C3C	-2.29	1.46	1.52
24	C	512	CLA	CMD-C2D	-2.29	1.46	1.51
31	H	102	DGD	O2D-C2D	-2.29	1.37	1.43
33	Y	101	LMG	C3-C2	2.28	1.58	1.52
31	C	516	DGD	C4D-C3D	2.28	1.58	1.52
33	C	515	LMG	C3-C2	2.28	1.58	1.52
31	A	616	DGD	O5D-C6D	-2.28	1.39	1.43
24	b	601	CLA	O2A-CGA	2.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	O2D-CGD	2.27	1.38	1.33
24	B	603	CLA	CAC-C3C	-2.27	1.46	1.52
24	C	508	CLA	CMB-C2B	-2.27	1.46	1.51
24	B	602	CLA	CMD-C2D	-2.27	1.46	1.51
24	B	615	CLA	C1D-C2D	2.27	1.47	1.42
24	c	501	CLA	C3B-CAB	-2.27	1.43	1.47
24	C	503	CLA	CAC-C3C	-2.27	1.46	1.52
24	B	608	CLA	CMC-C2C	-2.26	1.46	1.51
24	A	605	CLA	C1D-C2D	2.26	1.47	1.42
31	C	518	DGD	C6E-C5E	2.26	1.59	1.51
29	a	615	SQD	O47-C7	2.26	1.40	1.34
24	C	513	CLA	C4B-CHC	-2.26	1.34	1.41
24	B	601	CLA	C1C-C2C	2.26	1.47	1.42
33	Y	101	LMG	C6-C5	2.26	1.59	1.51
24	B	606	CLA	C3B-C2B	-2.26	1.37	1.40
24	b	602	CLA	C4B-CHC	-2.26	1.34	1.41
24	c	504	CLA	CMB-C2B	-2.25	1.47	1.51
24	b	616	CLA	C1B-NB	2.25	1.37	1.35
24	C	513	CLA	CMC-C2C	-2.25	1.46	1.51
26	K	103	BCR	C33-C5	-2.25	1.47	1.50
24	C	508	CLA	C4B-CHC	-2.24	1.34	1.41
24	c	506	CLA	C1D-C2D	2.24	1.47	1.42
33	M	101	LMG	C9-C8	2.24	1.57	1.50
24	C	513	CLA	C1D-C2D	2.24	1.47	1.42
25	a	606	PHO	C1B-C2B	2.24	1.50	1.45
31	h	102	DGD	C4E-C3E	2.24	1.58	1.52
24	C	510	CLA	CMD-C2D	-2.24	1.46	1.51
33	M	101	LMG	O4-C4	-2.24	1.37	1.43
24	b	607	CLA	CAC-C3C	-2.24	1.46	1.52
24	c	501	CLA	CMC-C2C	-2.23	1.46	1.51
24	c	505	CLA	C1D-C2D	2.23	1.47	1.42
24	c	509	CLA	C1D-C2D	2.23	1.47	1.42
24	C	511	CLA	CMD-C2D	-2.23	1.46	1.51
25	A	606	PHO	C1C-NC	-2.23	1.33	1.38
24	d	402	CLA	CAC-C3C	-2.23	1.46	1.52
29	D	408	SQD	O3-C3	-2.23	1.37	1.43
24	H	101	CLA	C1C-C2C	2.23	1.47	1.42
24	C	509	CLA	O2D-CGD	2.23	1.38	1.33
24	b	602	CLA	C1D-C2D	2.22	1.47	1.42
24	c	502	CLA	CMC-C2C	-2.22	1.46	1.51
30	L	101	LHG	O7-C5	-2.22	1.41	1.46
30	l	101	LHG	O8-C23	2.22	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C	515	LMG	O1-C7	-2.22	1.39	1.43
26	B	616	BCR	C30-C25	-2.22	1.50	1.53
33	c	522	LMG	C6-C5	2.22	1.59	1.51
24	C	502	CLA	CMB-C2B	-2.22	1.47	1.51
24	c	503	CLA	CMC-C2C	-2.21	1.46	1.51
24	b	611	CLA	CMB-C2B	-2.21	1.47	1.51
24	b	611	CLA	CMC-C2C	-2.21	1.46	1.51
24	a	604	CLA	CMD-C2D	-2.21	1.46	1.51
33	c	522	LMG	C3-C2	2.21	1.57	1.52
30	D	409	LHG	P-O3	2.20	1.68	1.59
24	b	614	CLA	O2D-CGD	2.20	1.38	1.33
30	D	409	LHG	O6-C4	-2.20	1.36	1.44
24	B	614	CLA	CMD-C2D	-2.20	1.46	1.51
24	b	608	CLA	O2A-CGA	2.20	1.39	1.33
24	b	610	CLA	C1D-C2D	2.20	1.47	1.42
24	c	506	CLA	CAC-C3C	-2.20	1.46	1.52
25	d	401	PHO	C1C-NC	-2.20	1.33	1.38
25	a	606	PHO	CHD-C4C	-2.20	1.35	1.40
24	B	601	CLA	CAC-C3C	-2.19	1.46	1.52
24	b	605	CLA	C1D-C2D	2.19	1.47	1.42
24	D	403	CLA	CAC-C3C	-2.19	1.46	1.52
24	C	502	CLA	CMD-C2D	-2.19	1.46	1.51
25	A	606	PHO	CAA-C2A	-2.19	1.50	1.54
24	B	614	CLA	C1D-C2D	2.19	1.47	1.42
24	B	607	CLA	CMC-C2C	-2.19	1.46	1.51
24	D	404	CLA	C3B-C2B	-2.19	1.37	1.40
26	k	101	BCR	C33-C5	-2.18	1.47	1.50
25	d	401	PHO	CMC-C2C	-2.18	1.46	1.50
25	A	606	PHO	O2D-CGD	2.18	1.38	1.33
24	D	404	CLA	C4B-CHC	-2.18	1.34	1.41
24	B	610	CLA	CAA-C2A	-2.18	1.50	1.54
24	b	609	CLA	CMC-C2C	-2.18	1.46	1.51
24	C	507	CLA	CMB-C2B	-2.18	1.47	1.51
24	A	607	CLA	C1D-C2D	2.18	1.47	1.42
26	b	617	BCR	C33-C5	-2.18	1.47	1.50
24	c	510	CLA	CAC-C3C	-2.18	1.46	1.52
24	B	602	CLA	O2D-CGD	2.18	1.38	1.33
24	C	502	CLA	MG-NA	2.18	2.11	2.06
26	K	103	BCR	C27-C26	-2.18	1.46	1.51
24	b	607	CLA	C3B-C2B	-2.17	1.37	1.40
24	b	606	CLA	CAC-C3C	-2.17	1.46	1.52
24	C	504	CLA	CMD-C2D	-2.17	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	516	DGD	O1G-C1A	2.17	1.39	1.33
26	b	617	BCR	C4-C5	-2.17	1.46	1.51
24	a	604	CLA	CMC-C2C	-2.17	1.46	1.51
24	d	402	CLA	CMC-C2C	-2.16	1.46	1.51
33	C	515	LMG	C7-C8	2.16	1.57	1.50
24	b	610	CLA	CMD-C2D	-2.16	1.46	1.51
33	c	521	LMG	C4-C5	2.16	1.57	1.53
31	h	102	DGD	C4D-C3D	2.16	1.57	1.52
24	d	402	CLA	CMD-C2D	-2.16	1.46	1.51
24	B	607	CLA	C4B-CHC	-2.15	1.35	1.41
28	D	406	PL9	C26-C24	-2.15	1.46	1.51
24	c	508	CLA	CMB-C2B	-2.15	1.47	1.51
24	c	505	CLA	CMB-C2B	-2.15	1.47	1.51
24	b	612	CLA	CMB-C2B	-2.14	1.47	1.51
26	B	617	BCR	C1-C6	-2.14	1.50	1.53
30	l	101	LHG	O7-C5	-2.14	1.41	1.46
24	b	611	CLA	C3B-C2B	-2.14	1.37	1.40
31	h	102	DGD	C1G-C2G	2.14	1.57	1.50
25	D	401	PHO	CMD-C2D	-2.14	1.46	1.50
24	D	403	CLA	C1A-CHA	-2.14	1.34	1.43
24	a	605	CLA	C4B-CHC	-2.14	1.35	1.41
24	C	511	CLA	CAC-C3C	-2.14	1.46	1.52
25	A	606	PHO	CMD-C2D	-2.13	1.46	1.50
31	C	518	DGD	O4E-C4E	-2.13	1.38	1.43
24	a	613	CLA	C1D-C2D	2.13	1.47	1.42
24	b	616	CLA	CMC-C2C	-2.13	1.46	1.51
24	b	602	CLA	CMB-C2B	-2.13	1.47	1.51
25	d	401	PHO	C1A-NA	2.12	1.41	1.37
24	c	510	CLA	CMD-C2D	-2.12	1.46	1.51
24	B	615	CLA	C3B-CAB	-2.12	1.43	1.47
24	a	605	CLA	CMC-C2C	-2.12	1.46	1.51
25	D	401	PHO	C4C-NC	2.12	1.41	1.36
29	a	615	SQD	O4-C4	-2.12	1.38	1.43
24	a	605	CLA	C3B-C2B	-2.12	1.37	1.40
26	B	617	BCR	C33-C5	-2.12	1.47	1.50
24	C	512	CLA	CMB-C2B	-2.12	1.47	1.51
24	b	605	CLA	O2D-CED	-2.12	1.40	1.45
33	Y	101	LMG	O1-C7	-2.12	1.39	1.43
33	D	411	LMG	C9-C8	2.12	1.57	1.50
26	c	515	BCR	C38-C26	-2.11	1.47	1.50
26	t	101	BCR	C27-C26	-2.11	1.46	1.51
24	C	508	CLA	CMD-C2D	-2.11	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	407	LHG	O7-C5	-2.11	1.41	1.46
24	B	608	CLA	O2D-CGD	2.11	1.38	1.33
24	c	512	CLA	C3B-CAB	-2.11	1.43	1.47
25	D	401	PHO	C3B-C4B	2.11	1.47	1.43
24	A	607	CLA	CMC-C2C	-2.11	1.46	1.51
24	B	611	CLA	CMB-C2B	-2.11	1.47	1.51
24	b	613	CLA	CAA-C2A	-2.11	1.50	1.54
31	C	516	DGD	O2G-C1B	2.11	1.40	1.34
24	B	613	CLA	C1A-CHA	-2.11	1.34	1.43
30	a	614	LHG	O8-C23	2.10	1.39	1.33
31	C	518	DGD	C4D-C5D	2.10	1.57	1.53
24	d	403	CLA	O2D-CGD	2.10	1.38	1.33
24	B	613	CLA	C4B-CHC	-2.10	1.35	1.41
26	A	608	BCR	C14-C13	-2.10	1.33	1.35
24	C	507	CLA	C3B-CAB	-2.10	1.43	1.47
24	C	506	CLA	C3B-C2B	-2.10	1.37	1.40
24	c	503	CLA	CAC-C3C	-2.10	1.47	1.52
24	b	607	CLA	C3B-CAB	-2.10	1.43	1.47
24	C	505	CLA	CMD-C2D	-2.10	1.46	1.51
24	c	503	CLA	C4-C3	-2.10	1.45	1.50
24	C	510	CLA	C1D-C2D	2.10	1.47	1.42
24	C	504	CLA	CMB-C2B	-2.10	1.47	1.51
24	B	603	CLA	CMD-C2D	-2.10	1.46	1.51
24	b	610	CLA	C4B-CHC	-2.09	1.35	1.41
24	c	503	CLA	C4B-CHC	-2.09	1.35	1.41
24	C	507	CLA	C4B-CHC	-2.09	1.35	1.41
31	c	518	DGD	C3E-C2E	2.09	1.57	1.52
31	c	518	DGD	O4E-C4E	-2.09	1.38	1.43
24	b	601	CLA	CAC-C3C	-2.09	1.47	1.52
31	C	518	DGD	O3D-C3D	-2.09	1.38	1.43
24	c	501	CLA	C1D-C2D	2.08	1.47	1.42
31	H	102	DGD	O3E-C3E	-2.08	1.38	1.43
24	c	511	CLA	C1C-C2C	2.08	1.47	1.42
28	A	611	PL9	C35-C34	-2.08	1.45	1.50
24	c	510	CLA	CMC-C2C	-2.08	1.46	1.51
33	b	622	LMG	C3-C2	2.08	1.57	1.52
24	d	402	CLA	C1C-C2C	2.08	1.47	1.42
24	C	506	CLA	C3B-CAB	-2.08	1.43	1.47
24	b	609	CLA	C3B-CAB	-2.08	1.43	1.47
24	A	612	CLA	CAC-C3C	-2.08	1.47	1.52
24	b	611	CLA	CAC-C3C	-2.08	1.47	1.52
24	c	513	CLA	C3B-C2B	-2.07	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C4B-CHC	-2.07	1.35	1.41
24	c	508	CLA	CMC-C2C	-2.07	1.46	1.51
29	f	102	SQD	O3-C3	-2.07	1.38	1.43
31	C	516	DGD	C6D-C5D	2.06	1.58	1.51
24	b	605	CLA	CMB-C2B	-2.06	1.47	1.51
30	e	101	LHG	C4-C5	2.06	1.57	1.50
31	C	516	DGD	O1A-C1A	2.06	1.28	1.22
31	A	616	DGD	O2G-C1B	2.06	1.40	1.34
33	b	622	LMG	O6-C1	2.06	1.47	1.41
29	D	408	SQD	O2-C2	-2.05	1.38	1.43
25	a	606	PHO	CAA-C2A	-2.05	1.50	1.54
33	D	407	LMG	C4-C5	2.05	1.57	1.53
24	A	607	CLA	C3B-CAB	-2.05	1.43	1.47
24	b	615	CLA	CAC-C3C	-2.05	1.47	1.52
24	c	510	CLA	C1C-C2C	2.05	1.47	1.42
24	B	615	CLA	O2D-CED	-2.05	1.40	1.45
24	B	604	CLA	O2D-CED	-2.05	1.40	1.45
31	c	517	DGD	C4E-C5E	2.04	1.57	1.53
31	c	516	DGD	C4D-C5D	2.04	1.57	1.53
28	D	406	PL9	C12-C13	2.04	1.57	1.50
28	D	406	PL9	C7-C3	-2.04	1.49	1.51
24	B	606	CLA	CMA-C3A	-2.04	1.48	1.53
24	c	506	CLA	CMD-C2D	-2.04	1.46	1.51
24	b	612	CLA	C1C-C2C	2.04	1.47	1.42
24	B	613	CLA	O2D-CED	-2.04	1.40	1.45
24	A	604	CLA	C1C-C2C	2.04	1.47	1.42
31	c	517	DGD	C1E-C2E	2.04	1.58	1.52
24	B	612	CLA	O2D-CED	-2.04	1.40	1.45
24	a	604	CLA	O2D-CGD	2.04	1.38	1.33
31	c	517	DGD	O4D-C4D	-2.04	1.38	1.43
29	a	615	SQD	O47-C45	-2.03	1.41	1.46
30	A	614	LHG	O8-C23	2.03	1.39	1.33
24	B	607	CLA	O2A-CGA	2.03	1.39	1.33
24	B	610	CLA	CMD-C2D	-2.03	1.46	1.51
24	c	512	CLA	CMC-C2C	-2.03	1.46	1.51
28	A	611	PL9	C37-C38	2.03	1.57	1.50
31	c	518	DGD	C1E-C2E	2.03	1.58	1.52
24	a	605	CLA	C3B-CAB	-2.03	1.43	1.47
24	b	613	CLA	CAC-C3C	-2.02	1.47	1.52
24	c	507	CLA	C4B-CHC	-2.02	1.35	1.41
26	b	618	BCR	C33-C5	-2.02	1.47	1.50
31	c	518	DGD	O1G-C1G	-2.02	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	V	201	HEC	C1C-NC	2.02	1.40	1.36
33	D	411	LMG	O8-C28	2.02	1.39	1.33
24	C	510	CLA	O1D-CGD	2.02	1.26	1.21
24	D	404	CLA	CAC-C3C	-2.02	1.47	1.52
28	A	611	PL9	C41-C39	2.02	1.55	1.51
24	D	404	CLA	CMC-C2C	-2.02	1.46	1.51
24	B	609	CLA	CMA-C3A	-2.01	1.48	1.53
31	H	102	DGD	O6E-C1E	2.01	1.47	1.41
24	C	513	CLA	CMD-C2D	-2.01	1.46	1.51
24	c	511	CLA	CMD-C2D	-2.01	1.46	1.51
24	C	504	CLA	O2D-CGD	2.01	1.38	1.33
33	d	408	LMG	C4-C5	2.01	1.57	1.53
24	C	510	CLA	CMB-C2B	-2.01	1.47	1.51
31	c	516	DGD	C3G-C2G	2.01	1.56	1.50
24	b	606	CLA	C1B-NB	2.01	1.37	1.35
29	b	620	SQD	O3-C3	-2.01	1.38	1.43
24	B	613	CLA	CMC-C2C	-2.01	1.46	1.51
24	d	403	CLA	C1B-NB	2.01	1.37	1.35
24	C	509	CLA	CMC-C2C	-2.00	1.46	1.51
24	B	610	CLA	C3B-CAB	-2.00	1.43	1.47
24	A	605	CLA	CAC-C3C	-2.00	1.47	1.52
24	C	508	CLA	CMC-C2C	-2.00	1.46	1.51
24	c	510	CLA	C1D-C2D	2.00	1.47	1.42
25	a	606	PHO	CHC-C1C	2.00	1.42	1.38
33	D	407	LMG	O1-C1	2.00	1.43	1.40
24	c	502	CLA	CAC-C3C	-2.00	1.47	1.52

All (1244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4A-NA-C1A	11.93	112.07	106.71
29	b	620	SQD	O6-C1-C2	11.85	126.80	108.30
24	b	604	CLA	C4A-NA-C1A	11.25	111.76	106.71
24	b	606	CLA	C4A-NA-C1A	9.39	110.93	106.71
29	B	620	SQD	O6-C1-C2	9.11	122.52	108.30
24	c	505	CLA	C4A-NA-C1A	9.09	110.79	106.71
24	B	606	CLA	C4A-NA-C1A	8.56	110.55	106.71
29	a	615	SQD	O6-C1-C2	8.53	121.62	108.30
24	c	511	CLA	C4A-NA-C1A	8.53	110.54	106.71
24	b	601	CLA	C4A-NA-C1A	8.47	110.51	106.71
24	B	614	CLA	C4A-NA-C1A	8.34	110.45	106.71
24	C	507	CLA	C4A-NA-C1A	8.28	110.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C4A-NA-C1A	8.22	110.40	106.71
24	B	608	CLA	C4A-NA-C1A	7.92	110.27	106.71
24	B	611	CLA	C4A-NA-C1A	7.75	110.19	106.71
24	B	612	CLA	C4A-NA-C1A	7.67	110.16	106.71
24	C	513	CLA	C4A-NA-C1A	7.58	110.12	106.71
24	c	509	CLA	C4A-NA-C1A	7.47	110.06	106.71
24	c	507	CLA	C4A-NA-C1A	7.46	110.06	106.71
24	c	508	CLA	C4A-NA-C1A	7.00	109.85	106.71
24	B	615	CLA	C4A-NA-C1A	6.72	109.73	106.71
29	A	613	SQD	O6-C1-C2	6.69	118.75	108.30
24	H	101	CLA	C4A-NA-C1A	6.63	109.69	106.71
29	b	620	SQD	O7-S-C6	6.43	114.58	106.94
24	C	503	CLA	C4A-NA-C1A	6.34	109.56	106.71
24	c	510	CLA	C4A-NA-C1A	6.31	109.54	106.71
24	C	510	CLA	C4A-NA-C1A	6.15	109.47	106.71
24	C	509	CLA	CMB-C2B-C1B	-6.14	119.02	128.46
28	a	612	PL9	C7-C3-C4	6.13	121.86	116.88
24	C	506	CLA	C4A-NA-C1A	6.11	109.45	106.71
29	D	408	SQD	O9-S-C6	6.10	114.19	106.94
24	b	605	CLA	C4A-NA-C1A	6.01	109.41	106.71
29	f	102	SQD	O7-S-C6	5.89	113.94	106.94
29	a	615	SQD	O7-S-C6	5.88	113.93	106.94
24	A	604	CLA	C4A-NA-C1A	5.85	109.34	106.71
24	b	614	CLA	C4A-NA-C1A	5.81	109.32	106.71
29	A	613	SQD	O7-S-C6	5.79	113.82	106.94
24	B	601	CLA	CMB-C2B-C1B	-5.78	119.58	128.46
24	C	511	CLA	C4A-NA-C1A	5.77	109.30	106.71
24	c	512	CLA	C4A-NA-C1A	5.75	109.29	106.71
24	b	612	CLA	CMB-C2B-C1B	-5.69	119.72	128.46
24	A	607	CLA	CMB-C2B-C1B	-5.64	119.79	128.46
24	b	608	CLA	CMB-C2B-C1B	-5.60	119.85	128.46
28	D	406	PL9	C36-C34-C33	-5.60	109.78	121.12
29	A	613	SQD	C1-C2-C3	-5.59	98.36	110.00
24	b	603	CLA	C4A-NA-C1A	5.58	109.21	106.71
28	d	405	PL9	C7-C3-C4	5.57	121.41	116.88
24	C	505	CLA	CMB-C2B-C1B	-5.57	119.90	128.46
24	D	404	CLA	CMB-C2B-C1B	-5.54	119.95	128.46
24	c	506	CLA	CMB-C2B-C1B	-5.49	120.03	128.46
24	A	612	CLA	C4A-NA-C1A	5.47	109.17	106.71
24	B	615	CLA	O2D-CGD-O1D	-5.42	113.25	123.84
24	C	509	CLA	CMB-C2B-C3B	5.41	134.81	124.68
24	B	612	CLA	CMB-C2B-C1B	-5.41	120.14	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	602	CLA	C4A-NA-C1A	5.41	109.14	106.71
24	c	503	CLA	C4A-NA-C1A	5.38	109.12	106.71
24	c	501	CLA	O2D-CGD-O1D	-5.36	113.36	123.84
24	c	502	CLA	CMB-C2B-C1B	-5.36	120.23	128.46
31	C	518	DGD	O3G-C3G-C2G	-5.25	98.23	110.90
35	f	101	HEM	CBA-CAA-C2A	-5.24	102.82	112.49
29	b	620	SQD	C1-C2-C3	-5.19	99.20	110.00
24	b	613	CLA	CMB-C2B-C1B	-5.18	120.50	128.46
24	B	611	CLA	CMB-C2B-C1B	-5.17	120.51	128.46
24	b	612	CLA	OBD-CAD-CBD	-5.13	118.56	125.89
24	A	605	CLA	CMB-C2B-C1B	-5.10	120.62	128.46
36	v	201	HEC	CMC-C2C-C1C	-5.10	120.62	128.46
29	f	102	SQD	O6-C1-C2	5.09	116.24	108.30
28	D	406	PL9	C7-C3-C4	5.05	120.98	116.88
24	b	609	CLA	C4A-NA-C1A	5.04	108.97	106.71
24	c	504	CLA	CMB-C2B-C1B	-5.03	120.74	128.46
29	B	620	SQD	C1-C2-C3	-5.02	99.54	110.00
35	f	101	HEM	CBD-CAD-C3D	-4.99	103.28	112.48
24	b	607	CLA	C4A-NA-C1A	4.97	108.94	106.71
29	D	408	SQD	O6-C1-C2	4.96	116.05	108.30
24	b	604	CLA	OBD-CAD-CBD	-4.94	118.84	125.89
24	C	505	CLA	CMB-C2B-C3B	4.89	133.82	124.68
24	C	509	CLA	C4A-NA-C1A	4.87	108.90	106.71
24	c	513	CLA	C4A-NA-C1A	4.87	108.90	106.71
24	B	601	CLA	CMB-C2B-C3B	4.86	133.76	124.68
28	A	611	PL9	C7-C3-C4	4.84	120.81	116.88
24	B	609	CLA	C4A-NA-C1A	4.83	108.88	106.71
24	C	508	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
24	a	605	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
24	a	607	CLA	C4A-NA-C1A	4.80	108.86	106.71
24	C	512	CLA	C4A-NA-C1A	4.79	108.86	106.71
24	D	403	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
24	a	604	CLA	C4A-NA-C1A	4.77	108.85	106.71
24	b	608	CLA	CMB-C2B-C3B	4.75	133.57	124.68
24	B	613	CLA	O2D-CGD-O1D	-4.73	114.58	123.84
29	a	615	SQD	C1-C2-C3	-4.71	100.18	110.00
29	A	615	SQD	C45-O47-C7	4.70	123.92	117.88
24	C	506	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
24	C	511	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
24	B	601	CLA	O2D-CGD-CBD	4.67	119.56	111.27
24	c	502	CLA	CMB-C2B-C3B	4.64	133.36	124.68
24	D	404	CLA	CMB-C2B-C3B	4.62	133.32	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	H	102	DGD	O3G-C3G-C2G	-4.62	99.75	110.90
24	c	506	CLA	CMB-C2B-C3B	4.62	133.32	124.68
24	c	510	CLA	CMB-C2B-C1B	-4.61	121.37	128.46
24	c	506	CLA	C4A-NA-C1A	4.57	108.76	106.71
24	b	612	CLA	CMB-C2B-C3B	4.57	133.23	124.68
24	C	513	CLA	CMB-C2B-C1B	-4.56	121.46	128.46
29	a	615	SQD	C1-O5-C5	-4.55	104.75	113.69
24	a	613	CLA	C4A-NA-C1A	4.55	108.75	106.71
24	c	510	CLA	O2D-CGD-O1D	-4.55	114.95	123.84
24	A	605	CLA	CMB-C2B-C3B	4.55	133.18	124.68
29	A	613	SQD	O47-C7-C8	4.54	121.29	111.50
24	A	607	CLA	CMB-C2B-C3B	4.54	133.16	124.68
29	b	620	SQD	O2-C2-C1	4.54	121.06	110.05
24	b	611	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
25	d	401	PHO	O2D-CGD-O1D	-4.49	115.07	123.84
24	b	611	CLA	O2D-CGD-O1D	-4.48	115.07	123.84
24	a	604	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
24	C	508	CLA	C4A-NA-C1A	4.45	108.71	106.71
24	c	513	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
29	A	613	SQD	O8-S-C6	4.45	112.83	105.74
24	b	602	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
29	B	620	SQD	O8-S-C6	4.43	112.79	105.74
24	A	612	CLA	CMB-C2B-C3B	4.38	132.87	124.68
24	a	605	CLA	CMB-C2B-C3B	4.37	132.86	124.68
24	b	604	CLA	C4D-C3D-CAD	-4.36	106.04	108.47
24	C	502	CLA	C4A-NA-C1A	4.35	108.66	106.71
24	b	605	CLA	O1D-CGD-CBD	4.35	133.39	124.48
24	b	610	CLA	O2D-CGD-O1D	-4.35	115.34	123.84
24	b	616	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
24	B	607	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
24	A	612	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
24	C	510	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
29	A	613	SQD	O47-C7-O49	-4.31	113.30	123.70
35	F	101	HEM	CBD-CAD-C3D	-4.30	104.56	112.48
24	B	603	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
26	b	618	BCR	C36-C18-C17	-4.26	116.95	122.92
29	b	620	SQD	O9-S-C6	4.26	112.00	106.94
24	c	509	CLA	CHB-C4A-NA	4.24	130.37	124.51
24	b	607	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
30	A	614	LHG	O4-P-O5	4.22	133.11	112.24
29	a	615	SQD	O47-C7-C8	4.22	120.60	111.50
30	d	406	LHG	O4-P-O5	4.22	133.09	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	CMD-C2D-C3D	4.21	132.56	124.68
24	b	612	CLA	C4D-C3D-CAD	-4.21	106.12	108.47
30	D	409	LHG	O4-P-O5	4.20	133.01	112.24
31	C	517	DGD	O3G-C3G-C2G	-4.19	100.79	110.90
28	A	611	PL9	C40-C39-C41	4.18	122.30	115.27
24	B	611	CLA	CMB-C2B-C3B	4.18	132.49	124.68
24	b	610	CLA	CHB-C4A-NA	4.17	130.28	124.51
24	b	616	CLA	CMB-C2B-C3B	4.16	132.46	124.68
24	b	606	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
24	C	501	CLA	C4A-NA-C1A	4.16	108.58	106.71
24	B	605	CLA	C4A-NA-C1A	4.11	108.55	106.71
24	c	511	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
24	b	610	CLA	C4A-NA-C1A	4.10	108.55	106.71
36	v	201	HEC	CBA-CAA-C2A	-4.09	104.93	112.48
30	e	101	LHG	O4-P-O5	4.09	132.48	112.24
24	B	608	CLA	CMD-C2D-C3D	4.09	132.32	124.68
24	C	508	CLA	CMB-C2B-C3B	4.09	132.32	124.68
24	c	509	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
24	A	604	CLA	CHB-C4A-NA	4.07	130.14	124.51
24	b	616	CLA	C4A-NA-C1A	4.07	108.53	106.71
24	d	403	CLA	C4A-NA-C1A	4.06	108.53	106.71
24	C	501	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
24	D	404	CLA	C4A-NA-C1A	4.05	108.53	106.71
24	c	502	CLA	O2D-CGD-O1D	-4.03	115.97	123.84
24	C	506	CLA	CMB-C2B-C3B	4.02	132.21	124.68
24	C	502	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
24	C	505	CLA	OBD-CAD-CBD	-4.02	120.15	125.89
24	b	602	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
26	B	616	BCR	C2-C1-C6	4.01	116.66	110.48
24	B	609	CLA	CHB-C4A-NA	4.01	130.05	124.51
24	A	604	CLA	CMB-C2B-C1B	-4.00	122.31	128.46
24	b	601	CLA	CHB-C4A-NA	4.00	130.04	124.51
24	B	615	CLA	O2D-CGD-CBD	4.00	118.38	111.27
26	a	608	BCR	C37-C22-C21	-3.98	117.34	122.92
24	B	612	CLA	CMB-C2B-C3B	3.98	132.12	124.68
29	B	620	SQD	O47-C7-C8	3.98	120.07	111.50
29	f	102	SQD	O9-S-O7	-3.97	100.19	113.95
33	m	101	LMG	O6-C1-O1	-3.97	100.57	109.97
24	B	608	CLA	C4D-C3D-CAD	-3.97	106.26	108.47
29	B	620	SQD	C1-O5-C5	-3.97	105.89	113.69
36	v	201	HEC	C1D-C2D-C3D	-3.96	104.24	107.00
24	a	605	CLA	C4A-NA-C1A	3.96	108.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	408	SQD	O8-S-C6	3.95	112.04	105.74
24	c	504	CLA	CMB-C2B-C3B	3.95	132.07	124.68
30	L	101	LHG	O4-P-O5	3.95	131.78	112.24
33	a	619	LMG	C1-C2-C3	-3.94	101.79	110.00
24	C	513	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
30	d	407	LHG	O4-P-O5	3.93	131.67	112.24
24	b	602	CLA	O2D-CGD-CBD	3.92	118.23	111.27
24	c	512	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
30	l	101	LHG	O4-P-O5	3.90	131.54	112.24
36	V	201	HEC	CMC-C2C-C1C	-3.90	122.47	128.46
24	c	510	CLA	CMB-C2B-C3B	3.89	131.96	124.68
24	D	403	CLA	CMB-C2B-C3B	3.89	131.95	124.68
35	F	101	HEM	CBA-CAA-C2A	-3.88	105.33	112.49
24	A	607	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
30	D	413	LHG	O4-P-O5	3.88	131.42	112.24
24	B	607	CLA	CMB-C2B-C3B	3.86	131.90	124.68
25	D	401	PHO	CMB-C2B-C1B	-3.86	119.12	125.06
24	b	615	CLA	CMD-C2D-C3D	3.86	131.90	124.68
29	B	620	SQD	O7-S-C6	3.85	111.51	106.94
24	c	505	CLA	C4D-C3D-CAD	-3.83	106.33	108.47
24	B	608	CLA	OBD-CAD-CBD	-3.83	120.42	125.89
24	B	604	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
24	B	610	CLA	CMB-C2B-C1B	-3.82	122.58	128.46
24	B	610	CLA	C4A-NA-C1A	3.82	108.42	106.71
24	b	609	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
24	a	604	CLA	CMB-C2B-C3B	3.80	131.79	124.68
24	C	513	CLA	CMB-C2B-C3B	3.80	131.78	124.68
33	b	622	LMG	C1-O6-C5	-3.79	106.24	113.69
24	B	607	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
24	b	602	CLA	CMB-C2B-C3B	3.79	131.77	124.68
24	C	510	CLA	CMB-C2B-C3B	3.78	131.76	124.68
24	c	512	CLA	C1-C2-C3	-3.75	119.55	126.04
28	D	406	PL9	C30-C29-C31	-3.75	108.96	115.27
24	b	603	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
24	c	501	CLA	O2D-CGD-CBD	3.74	117.91	111.27
29	A	615	SQD	O47-C7-C8	3.73	119.55	111.50
24	c	509	CLA	O2A-CGA-O1A	-3.73	114.17	123.59
26	B	616	BCR	C37-C22-C21	-3.73	117.69	122.92
24	b	604	CLA	OBD-CAD-C3D	3.73	134.17	127.98
24	C	507	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
24	a	605	CLA	CHB-C4A-NA	3.72	129.65	124.51
24	b	603	CLA	OBD-CAD-CBD	-3.71	120.59	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	OBD-CAD-CBD	-3.70	120.61	125.89
30	a	614	LHG	O4-P-O5	3.70	130.54	112.24
24	B	608	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
24	A	604	CLA	CMB-C2B-C3B	3.69	131.59	124.68
24	B	608	CLA	CMB-C2B-C3B	3.69	131.59	124.68
33	C	515	LMG	O6-C5-C4	-3.69	103.00	109.69
33	m	101	LMG	O7-C10-O9	-3.66	114.86	123.70
30	D	410	LHG	O4-P-O5	3.65	130.28	112.24
28	D	406	PL9	C20-C19-C21	3.65	121.41	115.27
26	T	101	BCR	C7-C8-C9	-3.64	120.73	126.23
24	C	512	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
29	B	620	SQD	O2-C2-C1	3.64	118.89	110.05
28	d	405	PL9	C40-C39-C41	3.64	121.39	115.27
26	B	617	BCR	C15-C16-C17	-3.64	116.02	123.47
31	h	102	DGD	O3G-C3G-C2G	-3.64	102.12	110.90
24	b	609	CLA	C4D-C3D-CAD	-3.64	106.44	108.47
24	B	611	CLA	C11-C12-C13	-3.63	104.18	115.92
24	b	614	CLA	C1-C2-C3	-3.63	119.76	126.04
29	B	620	SQD	C3-C4-C5	3.63	116.71	110.24
26	b	617	BCR	C2-C1-C6	3.62	116.06	110.48
33	b	622	LMG	O1-C1-C2	-3.62	102.65	108.30
24	C	512	CLA	CMB-C2B-C3B	3.62	131.44	124.68
24	C	509	CLA	CHB-C4A-NA	3.61	129.51	124.51
33	a	619	LMG	C1-O6-C5	-3.61	106.60	113.69
24	A	607	CLA	C1B-CHB-C4A	-3.60	122.98	130.12
29	A	613	SQD	C1-O5-C5	-3.60	106.62	113.69
24	B	605	CLA	C4D-C3D-CAD	-3.60	106.46	108.47
24	b	607	CLA	CMB-C2B-C3B	3.59	131.40	124.68
24	b	612	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
24	c	513	CLA	O2D-CGD-O1D	-3.59	116.81	123.84
24	B	609	CLA	C1B-CHB-C4A	-3.56	123.06	130.12
24	B	603	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
24	B	607	CLA	O2D-CGD-CBD	3.55	117.58	111.27
24	B	615	CLA	CMB-C2B-C1B	-3.53	123.03	128.46
24	b	613	CLA	OBD-CAD-CBD	-3.53	120.85	125.89
24	c	513	CLA	CMB-C2B-C3B	3.53	131.28	124.68
24	c	513	CLA	CHB-C4A-NA	3.53	129.39	124.51
28	a	612	PL9	C7-C3-C2	-3.53	118.66	123.30
24	b	613	CLA	C4D-C3D-CAD	-3.53	106.50	108.47
29	b	620	SQD	C3-C4-C5	3.53	116.53	110.24
24	d	402	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
26	t	101	BCR	C15-C16-C17	-3.52	116.27	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CMB-C2B-C3B	3.51	131.25	124.68
26	B	617	BCR	C37-C22-C21	-3.51	118.00	122.92
24	b	615	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
24	b	606	CLA	O2D-CGD-CBD	3.51	117.50	111.27
26	A	608	BCR	C37-C22-C21	-3.50	118.01	122.92
24	a	607	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
26	B	618	BCR	C36-C18-C17	-3.49	118.04	122.92
24	C	513	CLA	C4-C3-C5	3.49	121.13	115.27
24	B	615	CLA	CMB-C2B-C3B	3.48	131.19	124.68
24	C	503	CLA	C1-O2A-CGA	3.48	125.57	116.44
24	b	610	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
24	c	507	CLA	OBD-CAD-CBD	-3.47	120.94	125.89
31	A	616	DGD	C4E-C3E-C2E	-3.46	104.78	110.82
24	C	512	CLA	C1-C2-C3	-3.46	120.07	126.04
24	c	502	CLA	O1D-CGD-CBD	3.45	131.55	124.48
24	b	601	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
24	c	507	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
28	a	612	PL9	C22-C23-C24	-3.44	119.37	127.66
24	b	612	CLA	OBD-CAD-C3D	3.44	133.70	127.98
24	b	611	CLA	C4A-NA-C1A	3.44	108.25	106.71
24	c	501	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
24	b	611	CLA	CMB-C2B-C3B	3.43	131.10	124.68
24	c	508	CLA	O2D-CGD-CBD	3.43	117.36	111.27
24	c	510	CLA	CMD-C2D-C3D	3.43	131.10	124.68
26	b	617	BCR	C3-C4-C5	-3.43	107.95	114.08
24	B	615	CLA	CHB-C4A-NA	3.43	129.25	124.51
24	D	403	CLA	C4-C3-C5	3.42	121.03	115.27
33	m	101	LMG	O8-C28-O10	-3.42	114.96	123.59
26	d	404	BCR	C38-C26-C25	-3.42	120.69	124.53
24	b	613	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
24	b	615	CLA	C4A-NA-C1A	3.42	108.24	106.71
24	B	613	CLA	C4A-NA-C1A	3.41	108.24	106.71
24	c	505	CLA	CMD-C2D-C3D	3.41	131.06	124.68
24	C	511	CLA	CMB-C2B-C3B	3.41	131.05	124.68
24	A	612	CLA	CHB-C4A-NA	3.39	129.19	124.51
24	d	402	CLA	C4A-NA-C1A	3.38	108.23	106.71
24	c	512	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
24	c	505	CLA	OBD-CAD-CBD	-3.38	121.06	125.89
24	d	402	CLA	CMB-C2B-C3B	3.38	131.00	124.68
28	A	611	PL9	O1-C4-C3	-3.38	117.00	120.72
26	K	103	BCR	C15-C16-C17	-3.37	116.56	123.47
24	C	504	CLA	CMB-C2B-C1B	-3.37	123.28	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	C11-C12-C13	-3.37	105.02	115.92
30	a	614	LHG	O8-C23-C24	3.37	122.48	111.91
24	b	613	CLA	C1-C2-C3	-3.37	120.22	126.04
24	c	501	CLA	CMC-C2C-C3C	3.36	131.28	124.94
29	f	102	SQD	O5-C5-C4	3.36	115.80	109.69
28	a	612	PL9	C20-C19-C21	3.36	120.92	115.27
26	B	616	BCR	C37-C22-C23	3.35	123.36	118.08
24	D	404	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
24	B	603	CLA	C4D-C3D-CAD	-3.35	106.60	108.47
24	B	614	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
33	C	515	LMG	O6-C1-O1	-3.34	102.06	109.97
24	B	603	CLA	OBD-CAD-CBD	-3.34	121.12	125.89
24	b	616	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
29	B	620	SQD	O48-C23-C24	3.33	122.34	111.91
24	B	603	CLA	CMB-C2B-C3B	3.32	130.90	124.68
24	b	610	CLA	CAA-CBA-CGA	-3.32	103.55	113.25
24	c	502	CLA	CMC-C2C-C3C	3.31	131.19	124.94
24	a	607	CLA	O2D-CGD-CBD	3.30	117.14	111.27
26	X	101	BCR	C27-C26-C25	3.30	127.52	122.73
24	a	607	CLA	CMB-C2B-C3B	3.30	130.85	124.68
26	K	102	BCR	C37-C22-C21	-3.30	118.30	122.92
24	B	609	CLA	CMB-C2B-C1B	-3.30	123.40	128.46
29	f	102	SQD	O9-S-C6	3.29	110.85	106.94
24	b	606	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
24	b	606	CLA	CMB-C2B-C3B	3.29	130.83	124.68
24	b	615	CLA	CHB-C4A-NA	3.28	129.05	124.51
24	C	501	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
24	B	611	CLA	C4D-C3D-CAD	-3.28	106.64	108.47
24	D	403	CLA	C1-C2-C3	-3.28	120.37	126.04
24	A	612	CLA	CMC-C2C-C3C	3.27	131.11	124.94
24	b	605	CLA	C4D-C3D-CAD	-3.27	106.65	108.47
26	B	618	BCR	C2-C1-C6	3.27	115.51	110.48
24	B	614	CLA	CHB-C4A-NA	3.26	129.02	124.51
24	B	603	CLA	CMD-C2D-C3D	3.26	130.77	124.68
31	c	517	DGD	O6D-C1D-O3G	-3.25	102.28	109.97
24	A	605	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
24	b	605	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
24	C	501	CLA	OBD-CAD-CBD	-3.24	121.27	125.89
24	D	403	CLA	O2A-CGA-O1A	-3.24	115.42	123.59
26	B	617	BCR	C15-C14-C13	-3.23	122.69	127.31
33	m	101	LMG	O3-C3-C2	-3.23	102.88	110.35
28	A	611	PL9	C27-C28-C29	-3.23	119.88	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	502	CLA	CMD-C2D-C3D	3.23	130.72	124.68
26	K	103	BCR	C37-C22-C21	-3.23	118.41	122.92
25	A	606	PHO	C1B-NB-C4B	3.22	112.58	106.51
29	b	620	SQD	O48-C23-C24	3.22	122.02	111.91
26	C	514	BCR	C36-C18-C17	-3.22	118.41	122.92
24	b	603	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
24	c	504	CLA	C4-C3-C5	3.22	120.68	115.27
24	b	603	CLA	CMB-C2B-C3B	3.22	130.69	124.68
24	A	607	CLA	C4-C3-C5	3.21	120.68	115.27
24	C	505	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
24	c	502	CLA	O2A-CGA-O1A	-3.20	115.50	123.59
24	B	602	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
24	B	609	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
24	c	505	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
36	V	201	HEC	CMC-C2C-C3C	3.20	129.58	125.82
24	b	604	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
24	b	601	CLA	O2D-CGD-CBD	3.20	116.95	111.27
31	A	616	DGD	C3G-C2G-C1G	-3.20	104.23	111.79
24	c	504	CLA	C4A-NA-C1A	3.19	108.14	106.71
30	D	413	LHG	O8-C23-C24	3.18	121.89	111.91
31	c	518	DGD	O3G-C3G-C2G	-3.18	103.22	110.90
24	b	612	CLA	C1-C2-C3	-3.18	120.54	126.04
24	c	509	CLA	CMB-C2B-C3B	3.17	130.61	124.68
31	c	518	DGD	C6D-O5D-C1E	3.17	119.93	113.74
24	c	501	CLA	CMB-C2B-C3B	3.16	130.60	124.68
25	a	606	PHO	C1-C2-C3	-3.16	120.57	126.04
24	c	512	CLA	CMB-C2B-C3B	3.16	130.59	124.68
31	C	518	DGD	O6D-C1D-O3G	-3.16	102.48	109.97
26	B	617	BCR	C36-C18-C17	-3.16	118.50	122.92
24	B	610	CLA	C14-C13-C15	-3.15	99.87	111.29
31	C	517	DGD	O5D-C6D-C5D	-3.15	103.21	109.05
33	Y	101	LMG	O6-C1-O1	-3.15	102.51	109.97
28	D	406	PL9	C42-C43-C44	-3.15	120.08	127.66
29	b	620	SQD	O5-C1-C2	-3.15	103.69	110.35
24	C	503	CLA	C4D-C3D-CAD	-3.15	106.72	108.47
24	c	506	CLA	OBD-CAD-CBD	-3.14	121.41	125.89
25	A	606	PHO	C1-C2-C3	-3.14	120.61	126.04
26	c	514	BCR	C2-C1-C6	3.14	115.31	110.48
29	B	620	SQD	O9-S-C6	3.14	110.67	106.94
24	C	512	CLA	CHB-C4A-NA	3.13	128.85	124.51
28	A	611	PL9	C7-C3-C2	-3.13	119.18	123.30
24	B	606	CLA	C1-C2-C3	-3.13	120.63	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	522	LMG	O6-C1-O1	-3.13	102.56	109.97
24	b	616	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
31	A	616	DGD	O3G-C3G-C2G	-3.13	103.35	110.90
24	c	512	CLA	CHB-C4A-NA	3.12	128.82	124.51
24	B	602	CLA	C4D-C3D-CAD	-3.12	106.73	108.47
33	m	101	LMG	O1-C1-C2	-3.11	103.44	108.30
31	C	516	DGD	O5D-C6D-C5D	-3.11	103.29	109.05
24	D	404	CLA	C4-C3-C5	3.11	120.50	115.27
24	B	610	CLA	CMB-C2B-C3B	3.11	130.50	124.68
24	b	605	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
26	c	515	BCR	C2-C1-C6	3.10	115.26	110.48
24	b	610	CLA	O2D-CGD-CBD	3.10	116.77	111.27
24	B	601	CLA	CHB-C4A-NA	3.10	128.79	124.51
24	C	503	CLA	CMD-C2D-C3D	3.09	130.47	124.68
24	B	613	CLA	O2D-CGD-CBD	3.09	116.77	111.27
29	a	616	SQD	O48-C23-O10	-3.09	115.79	123.59
26	X	101	BCR	C37-C22-C23	3.09	122.95	118.08
29	f	102	SQD	O47-C7-C8	3.09	119.41	110.80
24	B	612	CLA	CMC-C2C-C3C	3.09	130.76	124.94
24	B	603	CLA	CHB-C4A-NA	3.08	128.77	124.51
36	v	201	HEC	CBD-CAD-C3D	-3.08	106.81	112.49
24	b	605	CLA	CMD-C2D-C3D	3.08	130.44	124.68
28	D	406	PL9	C22-C23-C24	-3.07	120.26	127.66
28	A	611	PL9	C36-C34-C33	-3.07	114.91	121.12
24	C	505	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
24	b	609	CLA	O1D-CGD-CBD	3.06	130.75	124.48
26	X	101	BCR	C30-C25-C26	-3.06	118.31	122.61
29	a	615	SQD	O48-C23-C24	3.06	121.51	111.91
26	c	514	BCR	C38-C26-C25	-3.06	121.09	124.53
24	B	606	CLA	CMB-C2B-C3B	3.06	130.40	124.68
24	b	615	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
26	A	608	BCR	C40-C30-C25	3.05	115.25	110.30
29	B	620	SQD	O9-S-O7	-3.05	103.39	113.95
24	A	605	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
24	B	606	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
29	B	620	SQD	O48-C23-O10	-3.04	115.91	123.59
31	c	516	DGD	O3G-C3G-C2G	-3.04	103.56	110.90
24	D	404	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
24	B	615	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
25	A	606	PHO	CMB-C2B-C1B	-3.04	120.39	125.06
24	d	402	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
24	b	614	CLA	O2A-CGA-O1A	-3.03	115.94	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	DGD	O6D-C1D-O3G	-3.03	102.80	109.97
24	C	512	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
31	C	516	DGD	O3G-C3G-C2G	-3.03	103.60	110.90
24	B	605	CLA	CMD-C2D-C3D	3.02	130.34	124.68
29	b	620	SQD	O8-S-O7	-3.02	103.90	111.27
31	A	616	DGD	O5D-C6D-C5D	-3.01	103.47	109.05
28	d	405	PL9	C7-C8-C9	-3.01	121.77	126.79
25	d	401	PHO	C1-C2-C3	-3.01	120.83	126.04
24	b	609	CLA	CMB-C2B-C3B	3.01	130.31	124.68
28	D	406	PL9	C7-C8-C9	-3.01	121.78	126.79
24	c	507	CLA	CMB-C2B-C3B	3.00	130.30	124.68
24	B	604	CLA	C4D-C3D-CAD	-3.00	106.80	108.47
29	a	616	SQD	O48-C23-C24	3.00	121.33	111.91
24	b	615	CLA	C11-C10-C8	-3.00	106.22	115.92
24	C	507	CLA	CMB-C2B-C3B	3.00	130.29	124.68
28	D	406	PL9	C35-C34-C36	3.00	120.31	115.27
24	b	606	CLA	CMD-C2D-C3D	3.00	130.29	124.68
24	c	509	CLA	CMD-C2D-C3D	3.00	130.29	124.68
24	b	601	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
24	c	508	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
26	h	101	BCR	C36-C18-C17	-2.99	118.73	122.92
29	a	616	SQD	O47-C7-C8	2.99	117.95	111.50
24	C	506	CLA	CMD-C2D-C3D	2.99	130.27	124.68
24	H	101	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
24	H	101	CLA	O2D-CGD-CBD	2.98	116.57	111.27
28	D	406	PL9	C31-C29-C28	2.98	127.16	121.12
29	b	620	SQD	O47-C7-C8	2.98	117.93	111.50
26	d	404	BCR	C27-C26-C25	2.98	127.06	122.73
33	C	515	LMG	C1-O6-C5	-2.98	107.83	113.69
26	b	619	BCR	C29-C30-C25	2.98	115.07	110.48
26	X	101	BCR	C37-C22-C21	-2.98	118.75	122.92
24	a	607	CLA	CHB-C4A-NA	2.98	128.63	124.51
29	a	615	SQD	O8-S-C6	2.97	110.47	105.74
24	d	402	CLA	CMD-C2D-C3D	2.97	130.23	124.68
26	T	101	BCR	C27-C26-C25	2.97	127.04	122.73
24	c	505	CLA	OBD-CAD-C3D	2.97	132.90	127.98
26	c	515	BCR	C27-C26-C25	2.96	127.03	122.73
24	c	502	CLA	C1-C2-C3	-2.96	120.92	126.04
24	C	508	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	B	604	CLA	CMB-C2B-C3B	2.95	130.19	124.68
24	a	607	CLA	CMD-C2D-C3D	2.95	130.19	124.68
24	B	612	CLA	C1-C2-C3	-2.95	120.95	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C15-C16-C17	-2.94	117.44	123.47
26	c	515	BCR	C15-C16-C17	-2.93	117.46	123.47
24	D	403	CLA	CMD-C2D-C3D	2.93	130.17	124.68
28	A	611	PL9	C40-C39-C38	-2.93	116.16	123.68
24	b	610	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
33	a	619	LMG	O7-C10-O9	-2.93	116.62	123.70
24	c	510	CLA	O1D-CGD-CBD	2.93	130.48	124.48
33	b	622	LMG	C1-C2-C3	-2.93	103.89	110.00
26	b	619	BCR	C2-C1-C6	2.93	114.99	110.48
24	a	605	CLA	CMD-C2D-C3D	2.93	130.15	124.68
24	C	503	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
26	a	608	BCR	C27-C26-C25	2.92	126.97	122.73
24	B	613	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	t	101	BCR	C36-C18-C19	2.91	122.67	118.08
24	b	608	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	B	607	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
24	c	509	CLA	C4D-C3D-CAD	-2.91	106.85	108.47
26	h	101	BCR	C37-C22-C21	-2.91	118.85	122.92
24	B	605	CLA	O2A-CGA-O1A	-2.91	116.26	123.59
24	C	511	CLA	CMD-C2D-C3D	2.90	130.10	124.68
24	c	506	CLA	C4-C3-C5	2.90	120.14	115.27
24	C	504	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
28	A	611	PL9	C12-C13-C14	-2.89	120.69	127.66
24	b	602	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
25	d	401	PHO	O1D-CGD-CBD	2.89	130.41	124.48
24	A	604	CLA	CAA-CBA-CGA	-2.89	104.81	113.25
24	A	607	CLA	O2D-CGD-CBD	2.89	116.40	111.27
24	B	605	CLA	OBD-CAD-CBD	-2.89	121.77	125.89
24	c	508	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	a	613	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
31	C	516	DGD	O3E-C3E-C2E	-2.88	103.69	110.35
24	B	602	CLA	CMB-C2B-C3B	2.88	130.06	124.68
31	h	102	DGD	O3E-C3E-C2E	-2.87	103.70	110.35
24	C	513	CLA	CMD-C2D-C3D	2.87	130.05	124.68
24	b	611	CLA	O2D-CGD-CBD	2.87	116.37	111.27
24	c	507	CLA	CMC-C2C-C3C	2.87	130.35	124.94
29	D	408	SQD	C1-C2-C3	-2.87	104.02	110.00
24	C	501	CLA	O2D-CGD-CBD	2.87	116.37	111.27
36	v	201	HEC	CAD-CBD-CGD	-2.87	107.86	112.67
24	A	605	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
24	b	605	CLA	CMB-C2B-C3B	2.86	130.04	124.68
31	c	517	DGD	O3G-C3G-C2G	-2.86	103.99	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	a	606	PHO	O2D-CGD-O1D	-2.85	118.26	123.84
24	A	604	CLA	C7-C6-C5	-2.85	105.62	113.36
26	K	101	BCR	C15-C16-C17	-2.85	117.64	123.47
24	a	613	CLA	C4D-C3D-CAD	-2.84	106.88	108.47
24	c	507	CLA	C4D-C3D-CAD	-2.84	106.88	108.47
24	b	614	CLA	C1B-CHB-C4A	-2.84	124.48	130.12
29	A	615	SQD	O48-C23-C24	2.84	120.83	111.91
24	c	507	CLA	CMD-C2D-C3D	2.84	130.00	124.68
29	A	613	SQD	O8-S-O7	-2.84	104.34	111.27
25	a	606	PHO	CMB-C2B-C1B	-2.84	120.69	125.06
26	b	619	BCR	C37-C22-C21	-2.84	118.95	122.92
31	c	518	DGD	O5D-C1E-C2E	2.83	112.72	108.30
24	C	512	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
24	D	403	CLA	C4A-NA-C1A	2.83	107.98	106.71
26	c	515	BCR	C8-C9-C10	2.83	123.28	118.94
26	C	514	BCR	C15-C16-C17	-2.83	117.68	123.47
24	b	608	CLA	OBD-CAD-CBD	-2.83	121.86	125.89
24	c	511	CLA	CMB-C2B-C3B	2.82	129.96	124.68
24	b	616	CLA	CHB-C4A-NA	2.82	128.42	124.51
24	C	507	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
26	D	405	BCR	C27-C26-C25	2.82	126.83	122.73
24	b	608	CLA	O2D-CGD-CBD	2.82	116.28	111.27
30	A	614	LHG	O8-C23-C24	2.82	120.74	111.91
24	C	505	CLA	CMD-C2D-C3D	2.81	129.94	124.68
24	B	601	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
31	c	516	DGD	O6D-C1D-O3G	-2.81	103.32	109.97
24	C	505	CLA	OBD-CAD-C3D	2.81	132.65	127.98
31	h	102	DGD	C3E-C4E-C5E	-2.81	105.23	110.24
30	D	413	LHG	C11-C10-C9	-2.80	100.19	114.42
31	c	516	DGD	C3E-C4E-C5E	-2.80	105.24	110.24
24	c	508	CLA	CMD-C2D-C3D	2.80	129.92	124.68
24	b	609	CLA	OBD-CAD-CBD	-2.80	121.90	125.89
24	b	609	CLA	CHA-C1A-NA	-2.80	119.99	126.40
28	d	405	PL9	C22-C23-C24	-2.79	120.94	127.66
24	B	601	CLA	C16-C15-C13	-2.79	106.90	115.92
33	Y	101	LMG	O8-C28-O10	-2.79	116.55	123.59
25	d	401	PHO	C1B-NB-C4B	2.79	111.76	106.51
24	B	605	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
29	b	620	SQD	O8-S-C6	2.78	110.17	105.74
24	b	604	CLA	CHB-C4A-NA	2.78	128.35	124.51
24	b	604	CLA	CAA-CBA-CGA	-2.78	105.14	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	C6-C7-C8	-2.77	106.95	115.92
24	B	609	CLA	CMB-C2B-C3B	2.77	129.86	124.68
24	b	606	CLA	CMC-C2C-C3C	2.77	130.16	124.94
29	a	615	SQD	O9-S-O7	-2.77	104.37	113.95
26	b	618	BCR	C15-C16-C17	-2.77	117.81	123.47
24	C	506	CLA	CHB-C4A-NA	2.76	128.34	124.51
24	c	506	CLA	OBD-CAD-C3D	2.76	132.57	127.98
24	b	612	CLA	CHB-C4A-NA	2.76	128.33	124.51
24	B	614	CLA	CMD-C2D-C3D	2.76	129.84	124.68
30	D	413	LHG	O8-C23-O10	-2.76	116.63	123.59
24	B	608	CLA	OBD-CAD-C3D	2.76	132.56	127.98
26	K	102	BCR	C27-C26-C25	2.75	126.73	122.73
26	B	616	BCR	C3-C4-C5	-2.75	109.17	114.08
31	H	102	DGD	O2D-C2D-C1D	-2.75	103.37	110.05
24	b	603	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
31	c	516	DGD	C3G-C2G-C1G	-2.75	105.29	111.79
24	B	606	CLA	C2A-C1A-CHA	2.75	128.66	123.86
31	c	518	DGD	O6E-C1E-O5D	-2.74	103.48	109.97
33	C	515	LMG	C9-C8-C7	-2.74	105.30	111.79
28	A	611	PL9	C35-C34-C36	2.74	119.87	115.27
30	D	409	LHG	C18-C17-C16	-2.73	100.54	114.42
24	b	605	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	a	605	CLA	CMC-C2C-C3C	2.73	130.09	124.94
26	c	515	BCR	C35-C13-C14	-2.73	119.10	122.92
24	c	508	CLA	C4D-C3D-CAD	-2.73	106.95	108.47
29	A	613	SQD	O5-C1-O6	2.73	116.43	109.97
26	b	619	BCR	C15-C16-C17	-2.72	117.89	123.47
24	B	607	CLA	C11-C10-C8	-2.72	107.11	115.92
26	b	618	BCR	C35-C13-C14	-2.72	119.11	122.92
25	A	606	PHO	C5-C3-C2	2.72	126.62	121.12
28	A	611	PL9	C31-C32-C33	-2.72	102.95	111.88
24	a	605	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
24	c	505	CLA	CMC-C2C-C3C	2.72	130.06	124.94
24	a	605	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
31	A	616	DGD	O6D-C1D-O3G	-2.71	103.55	109.97
24	C	503	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
31	h	102	DGD	C1D-C2D-C3D	-2.71	104.35	110.00
24	b	616	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
24	b	615	CLA	C4D-C3D-CAD	-2.71	106.96	108.47
28	A	611	PL9	C11-C9-C8	-2.71	115.64	121.12
24	c	505	CLA	CMB-C2B-C3B	2.70	129.74	124.68
26	c	515	BCR	C37-C22-C21	-2.70	119.14	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	C4D-C3D-CAD	-2.70	106.96	108.47
26	h	101	BCR	C27-C26-C25	2.69	126.64	122.73
24	C	501	CLA	OBD-CAD-C3D	2.69	132.45	127.98
30	a	614	LHG	C20-C19-C18	-2.69	100.76	114.42
24	B	610	CLA	C7-C6-C5	-2.69	106.05	113.36
24	b	602	CLA	CHB-C4A-NA	2.69	128.23	124.51
33	d	408	LMG	O6-C1-O1	-2.69	103.61	109.97
24	c	513	CLA	C4-C3-C5	2.69	119.79	115.27
24	b	606	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
30	e	101	LHG	O8-C23-C24	2.69	120.33	111.91
31	C	517	DGD	C6D-O5D-C1E	2.68	118.98	113.74
33	c	521	LMG	O3-C3-C2	-2.68	104.14	110.35
28	D	406	PL9	C40-C39-C41	2.68	119.78	115.27
24	b	616	CLA	OBD-CAD-CBD	-2.68	122.06	125.89
28	A	611	PL9	C22-C23-C24	-2.68	121.20	127.66
24	C	513	CLA	CHB-C4A-NA	2.68	128.21	124.51
24	B	605	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
24	c	507	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
24	d	402	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
31	h	102	DGD	O6D-C1D-O3G	-2.67	103.66	109.97
24	b	609	CLA	C5-C3-C2	2.67	126.51	121.12
28	D	406	PL9	C7-C3-C2	-2.66	119.80	123.30
24	c	506	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
24	C	503	CLA	O1D-CGD-CBD	2.66	129.93	124.48
26	t	101	BCR	C1-C6-C5	-2.66	118.87	122.61
24	d	403	CLA	OBD-CAD-CBD	-2.66	122.10	125.89
24	C	504	CLA	C4A-NA-C1A	2.66	107.90	106.71
29	A	615	SQD	O47-C45-C46	2.66	112.28	106.13
33	M	101	LMG	O7-C10-O9	-2.65	117.29	123.70
28	d	405	PL9	C12-C13-C14	-2.65	121.27	127.66
28	D	406	PL9	C27-C28-C29	-2.65	121.27	127.66
31	C	516	DGD	O6D-C1D-O3G	-2.65	103.70	109.97
24	a	613	CLA	CMD-C2D-C3D	2.65	129.63	124.68
26	A	608	BCR	C27-C26-C25	2.65	126.57	122.73
24	H	101	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
24	c	502	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
26	B	616	BCR	C27-C26-C25	2.64	126.57	122.73
28	a	612	PL9	C32-C33-C34	-2.64	121.30	127.66
26	B	617	BCR	C29-C30-C25	2.64	114.55	110.48
33	a	619	LMG	C9-C8-C7	-2.64	105.54	111.79
33	M	101	LMG	O3-C3-C2	-2.64	104.24	110.35
29	D	408	SQD	C44-O6-C1	2.64	118.22	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	408	SQD	C3-C4-C5	2.64	114.95	110.24
24	c	505	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
33	D	407	LMG	O1-C7-C8	-2.64	104.54	110.90
24	c	502	CLA	C4A-NA-C1A	2.64	107.89	106.71
24	B	613	CLA	CMD-C2D-C3D	2.63	129.61	124.68
33	C	515	LMG	C3-C4-C5	-2.63	105.55	110.24
24	C	506	CLA	OBD-CAD-CBD	-2.63	122.14	125.89
24	b	604	CLA	C11-C10-C8	-2.63	107.43	115.92
24	b	602	CLA	C4D-C3D-CAD	-2.63	107.01	108.47
25	A	606	PHO	C2B-C1B-NB	-2.63	105.83	109.79
28	D	406	PL9	C12-C13-C14	-2.62	121.34	127.66
31	c	516	DGD	O3E-C3E-C2E	-2.62	104.28	110.35
24	b	604	CLA	CMD-C2D-C3D	2.62	129.58	124.68
24	b	609	CLA	CMC-C2C-C3C	2.62	129.88	124.94
33	a	619	LMG	O8-C28-O10	-2.62	116.98	123.59
24	C	501	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
33	M	101	LMG	C40-C39-C38	-2.62	101.14	114.42
24	B	615	CLA	CMC-C2C-C3C	2.62	129.88	124.94
24	b	604	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
24	B	612	CLA	CMD-C2D-C3D	2.62	129.57	124.68
24	c	504	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
26	b	618	BCR	C27-C26-C25	2.61	126.53	122.73
24	C	508	CLA	CMC-C2C-C3C	2.61	129.87	124.94
33	m	101	LMG	O1-C7-C8	-2.61	104.60	110.90
26	a	608	BCR	C2-C1-C6	2.61	114.50	110.48
35	F	101	HEM	CMD-C2D-C1D	-2.61	124.46	128.46
28	d	405	PL9	C7-C3-C2	-2.60	119.87	123.30
29	D	408	SQD	O9-S-O7	-2.60	104.94	113.95
24	B	610	CLA	C1-C2-C3	-2.60	121.55	126.04
28	A	611	PL9	O2-C1-C2	-2.60	115.83	121.78
36	V	201	HEC	CBD-CAD-C3D	-2.59	107.70	112.49
24	c	509	CLA	OBD-CAD-CBD	-2.59	122.19	125.89
33	b	622	LMG	C3-C4-C5	-2.59	105.62	110.24
33	b	622	LMG	C4-C3-C2	-2.59	106.30	110.82
24	C	507	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	a	613	CLA	CHB-C4A-NA	2.58	128.08	124.51
24	B	603	CLA	C11-C10-C8	-2.58	107.58	115.92
30	d	407	LHG	O8-C23-C24	2.58	120.00	111.91
24	b	607	CLA	C1-O2A-CGA	2.58	123.21	116.44
30	a	614	LHG	O8-C23-O10	-2.58	117.09	123.59
24	B	610	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
24	B	601	CLA	O2D-CGD-O1D	-2.57	118.82	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	615	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
24	c	510	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	b	612	CLA	CAA-CBA-CGA	-2.56	105.76	113.25
31	c	518	DGD	O6D-C1D-O3G	-2.56	103.90	109.97
26	B	617	BCR	C2-C1-C6	2.56	114.43	110.48
24	b	601	CLA	CMB-C2B-C3B	2.56	129.47	124.68
33	M	101	LMG	C1-O6-C5	-2.56	108.66	113.69
29	b	620	SQD	O5-C5-C4	2.56	114.34	109.69
24	B	611	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	B	612	CLA	OBD-CAD-CBD	-2.56	122.24	125.89
24	c	505	CLA	C11-C10-C8	-2.56	107.66	115.92
31	C	516	DGD	CDB-CCB-CBB	-2.55	101.45	114.42
26	a	608	BCR	C37-C22-C23	2.55	122.10	118.08
28	a	612	PL9	C26-C24-C23	-2.55	115.96	121.12
24	c	509	CLA	CMC-C2C-C3C	2.55	129.75	124.94
31	C	516	DGD	CBB-CAB-C9B	-2.55	101.49	114.42
24	C	507	CLA	CMC-C2C-C3C	2.55	129.74	124.94
24	A	612	CLA	C3D-CAD-CBD	-2.54	104.26	107.61
33	M	101	LMG	O6-C1-O1	-2.54	103.95	109.97
31	H	102	DGD	C3D-C4D-C5D	-2.54	105.70	110.24
33	c	519	LMG	C9-C8-C7	-2.54	105.78	111.79
31	C	516	DGD	O1G-C1A-C2A	-2.54	103.94	111.91
24	D	403	CLA	C6-C5-C3	2.54	120.11	113.45
36	v	201	HEC	CMB-C2B-C1B	-2.54	124.56	128.46
24	B	613	CLA	C1-C2-C3	-2.54	121.66	126.04
26	k	102	BCR	C27-C26-C25	2.54	126.41	122.73
24	b	612	CLA	C4A-NA-C1A	2.54	107.85	106.71
24	D	403	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
24	B	614	CLA	C11-C10-C8	-2.53	107.73	115.92
24	B	607	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	b	613	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	A	604	CLA	C1-C2-C3	-2.52	121.68	126.04
31	A	616	DGD	C1D-C2D-C3D	-2.52	104.75	110.00
29	b	620	SQD	O9-S-O7	-2.52	105.23	113.95
24	b	614	CLA	CHB-C4A-NA	2.52	127.99	124.51
31	C	516	DGD	C6D-O5D-C1E	2.52	118.66	113.74
26	B	618	BCR	C36-C18-C19	2.52	122.04	118.08
29	A	613	SQD	O9-S-O7	-2.51	105.25	113.95
24	b	604	CLA	CMC-C2C-C3C	2.51	129.68	124.94
24	B	612	CLA	C4D-C3D-CAD	-2.51	107.07	108.47
24	d	402	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
28	A	611	PL9	C20-C19-C21	2.51	119.50	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	401	PHO	C1B-NB-C4B	2.51	111.24	106.51
24	B	604	CLA	OBD-CAD-CBD	-2.51	122.31	125.89
24	C	504	CLA	C4-C3-C5	2.51	119.49	115.27
31	A	616	DGD	O1G-C1A-O1A	-2.50	117.27	123.59
24	b	609	CLA	CMD-C2D-C3D	2.50	129.35	124.68
24	C	508	CLA	OBD-CAD-CBD	-2.49	122.33	125.89
24	b	611	CLA	C1-C2-C3	-2.49	121.73	126.04
24	b	611	CLA	CMD-C2D-C3D	2.49	129.34	124.68
24	c	510	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
36	V	201	HEC	C4B-C3B-C2B	2.49	109.04	106.35
24	C	512	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
30	l	101	LHG	C5-O7-C7	-2.48	111.68	117.79
25	A	606	PHO	O2D-CGD-O1D	-2.48	118.99	123.84
24	B	605	CLA	O2D-CGD-CBD	2.48	115.67	111.27
24	c	513	CLA	CMD-C2D-C3D	2.48	129.32	124.68
24	B	603	CLA	C6-C5-C3	-2.48	106.96	113.45
24	B	602	CLA	C1-C2-C3	-2.48	121.76	126.04
24	B	605	CLA	CHA-C1A-NA	-2.48	120.73	126.40
24	C	502	CLA	O1D-CGD-CBD	2.48	129.55	124.48
26	K	103	BCR	C27-C26-C25	2.48	126.33	122.73
24	C	512	CLA	CMC-C2C-C3C	2.47	129.61	124.94
24	C	510	CLA	OBD-CAD-CBD	-2.47	122.36	125.89
24	c	508	CLA	CMB-C2B-C3B	2.47	129.30	124.68
24	B	604	CLA	OBD-CAD-C3D	2.47	132.08	127.98
24	B	604	CLA	CMD-C2D-C3D	2.47	129.30	124.68
24	b	604	CLA	O2D-CGD-CBD	2.47	115.65	111.27
33	m	101	LMG	O6-C1-C2	2.46	115.56	110.35
31	c	518	DGD	C3G-C2G-C1G	-2.46	105.96	111.79
28	D	406	PL9	C37-C38-C39	-2.46	121.73	127.66
26	K	101	BCR	C38-C26-C25	-2.46	121.76	124.53
28	d	405	PL9	C41-C39-C38	-2.46	116.14	121.12
31	A	616	DGD	CDB-CCB-CBB	-2.46	101.96	114.42
33	c	519	LMG	C40-C39-C38	-2.45	101.97	114.42
26	t	101	BCR	C7-C8-C9	-2.45	122.53	126.23
24	b	603	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
30	l	101	LHG	C20-C19-C18	-2.45	102.00	114.42
26	c	514	BCR	C3-C4-C5	-2.45	109.71	114.08
31	A	616	DGD	O5D-C1E-C2E	2.45	112.12	108.30
36	V	201	HEC	CMD-C2D-C1D	-2.45	124.70	128.46
24	c	512	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
26	b	618	BCR	C30-C25-C26	-2.45	119.17	122.61
24	c	513	CLA	O2A-CGA-O1A	-2.44	117.42	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C15-C14-C13	-2.44	123.82	127.31
24	A	607	CLA	CMC-C2C-C3C	2.44	129.55	124.94
31	c	517	DGD	O2E-C2E-C1E	-2.44	104.11	110.05
24	c	504	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
33	D	407	LMG	O1-C1-C2	-2.44	104.49	108.30
24	b	607	CLA	OBD-CAD-CBD	-2.44	122.41	125.89
24	B	612	CLA	C2A-C1A-CHA	2.44	128.12	123.86
33	C	515	LMG	O7-C10-C11	2.43	116.75	111.50
31	h	102	DGD	CDB-CCB-CBB	-2.43	102.08	114.42
33	m	101	LMG	C38-C37-C36	-2.43	102.08	114.42
26	K	103	BCR	C36-C18-C17	-2.43	119.52	122.92
24	B	603	CLA	O2D-CGD-CBD	2.43	115.58	111.27
24	a	607	CLA	CAA-CBA-CGA	-2.43	106.16	113.25
26	k	101	BCR	C38-C26-C25	-2.43	121.80	124.53
26	B	616	BCR	C29-C30-C25	2.42	114.21	110.48
31	A	616	DGD	CBB-CAB-C9B	-2.42	102.11	114.42
24	b	613	CLA	C4A-NA-C1A	2.42	107.80	106.71
24	A	605	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	C	506	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
26	b	619	BCR	C36-C18-C17	-2.42	119.53	122.92
24	B	601	CLA	CHA-C1A-NA	-2.42	120.85	126.40
24	B	613	CLA	C4D-C3D-CAD	-2.42	107.12	108.47
24	B	612	CLA	C4-C3-C5	2.42	119.33	115.27
26	t	101	BCR	C36-C18-C17	-2.42	119.54	122.92
24	B	605	CLA	CMC-C2C-C3C	2.41	129.49	124.94
24	B	606	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	C	503	CLA	C4-C3-C5	2.41	119.33	115.27
24	B	604	CLA	C7-C6-C5	-2.41	106.81	113.36
24	a	607	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
24	c	508	CLA	CHB-C4A-NA	2.41	127.84	124.51
33	D	411	LMG	O8-C28-O10	-2.41	117.52	123.59
24	a	604	CLA	CMC-C2C-C3C	2.41	129.48	124.94
24	C	507	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
24	d	402	CLA	C1-C2-C3	-2.40	121.89	126.04
31	c	518	DGD	CBB-CAB-C9B	-2.40	102.25	114.42
26	a	608	BCR	C38-C26-C25	-2.40	121.83	124.53
26	k	102	BCR	C2-C1-C6	2.40	114.17	110.48
33	D	407	LMG	O2-C2-C3	-2.40	104.81	110.35
33	c	519	LMG	O6-C1-O1	-2.40	104.30	109.97
26	K	101	BCR	C2-C1-C6	2.40	114.17	110.48
24	b	616	CLA	C2A-C3A-C4A	2.39	105.74	101.87
24	C	503	CLA	CMB-C2B-C3B	2.39	129.16	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	604	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	b	603	CLA	OBD-CAD-C3D	2.39	131.95	127.98
24	B	607	CLA	C11-C12-C13	-2.39	108.19	115.92
30	D	409	LHG	C20-C19-C18	-2.39	102.29	114.42
24	A	604	CLA	CMD-C2D-C3D	2.39	129.15	124.68
24	b	601	CLA	CMD-C2D-C3D	2.39	129.15	124.68
24	c	512	CLA	CMD-C2D-C3D	2.39	129.15	124.68
24	c	511	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	A	607	CLA	CAA-CBA-CGA	-2.39	106.28	113.25
24	B	602	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
33	b	622	LMG	O6-C5-C6	2.38	112.36	106.44
24	B	611	CLA	CMD-C2D-C3D	2.38	129.14	124.68
24	c	508	CLA	C1-C2-C3	-2.38	121.92	126.04
24	B	609	CLA	CMD-C2D-C3D	2.38	129.14	124.68
24	b	606	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
24	c	512	CLA	C4D-C3D-CAD	-2.38	107.14	108.47
24	H	101	CLA	CMB-C2B-C3B	2.38	129.13	124.68
29	A	613	SQD	O3-C3-C4	2.38	115.85	110.35
26	c	515	BCR	C37-C22-C23	2.37	121.82	118.08
24	b	611	CLA	CMC-C2C-C3C	2.37	129.42	124.94
30	D	410	LHG	O8-C23-C24	2.37	119.35	111.91
24	C	505	CLA	CHA-C1A-NA	-2.37	120.97	126.40
28	D	406	PL9	C8-C7-C3	2.37	118.68	111.98
24	B	612	CLA	CHA-C1A-NA	-2.37	120.97	126.40
26	X	101	BCR	C36-C18-C17	-2.37	119.61	122.92
31	H	102	DGD	C4D-C3D-C2D	-2.37	106.69	110.82
24	b	611	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	c	506	CLA	C4-C3-C2	-2.37	117.61	123.68
28	d	405	PL9	C37-C38-C39	-2.37	121.97	127.66
24	b	602	CLA	OBD-CAD-CBD	-2.36	122.52	125.89
26	D	405	BCR	C16-C15-C14	-2.36	118.63	123.47
24	d	403	CLA	CHA-C1A-NA	-2.36	120.99	126.40
24	C	504	CLA	O2D-CGD-CBD	2.36	115.47	111.27
24	a	607	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
26	b	618	BCR	C36-C18-C19	2.36	121.79	118.08
24	a	605	CLA	C4D-C3D-CAD	-2.35	107.16	108.47
29	b	620	SQD	O47-C45-C46	2.35	116.91	108.40
24	b	610	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
31	C	518	DGD	O5D-C6D-C5D	-2.35	104.70	109.05
25	D	401	PHO	CED-O2D-CGD	2.35	121.24	115.94
26	d	404	BCR	C16-C15-C14	-2.34	118.68	123.47
30	d	407	LHG	O8-C23-O10	-2.34	117.69	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	CMB-C2B-C3B	2.34	129.06	124.68
33	c	521	LMG	O2-C2-C1	-2.34	104.36	110.05
26	C	514	BCR	C2-C1-C6	2.34	114.08	110.48
31	C	518	DGD	CDB-CCB-CBB	-2.34	102.55	114.42
24	b	613	CLA	CMD-C2D-C3D	2.34	129.05	124.68
33	C	515	LMG	O3-C3-C2	-2.34	104.95	110.35
30	l	101	LHG	O8-C23-C24	2.33	119.23	111.91
26	T	101	BCR	C1-C6-C5	-2.33	119.33	122.61
24	c	503	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
30	a	614	LHG	C11-C10-C9	-2.33	102.59	114.42
24	B	611	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	d	401	PHO	C2B-C1B-NB	-2.33	106.28	109.79
24	B	603	CLA	O2A-C1-C2	2.33	114.75	108.64
33	a	619	LMG	O6-C1-C2	-2.33	105.42	110.35
33	b	622	LMG	O7-C10-O9	-2.33	118.08	123.70
33	c	521	LMG	C9-C8-C7	-2.32	106.29	111.79
29	f	102	SQD	C3-C4-C5	2.32	114.38	110.24
24	C	511	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
26	a	608	BCR	C20-C21-C22	-2.32	124.00	127.31
30	a	614	LHG	C18-C17-C16	-2.32	102.65	114.42
24	B	604	CLA	C4A-NA-C1A	2.32	107.75	106.71
35	F	101	HEM	CMB-C2B-C3B	2.31	129.01	124.68
24	b	613	CLA	CMC-C2C-C3C	2.31	129.31	124.94
26	C	514	BCR	C34-C9-C10	-2.31	119.68	122.92
24	C	513	CLA	O2D-CGD-CBD	2.31	115.38	111.27
31	c	516	DGD	O1G-C1A-C2A	-2.31	104.65	111.91
24	C	510	CLA	CMD-C2D-C3D	2.31	129.00	124.68
24	C	509	CLA	CMC-C2C-C3C	2.31	129.30	124.94
24	b	602	CLA	CMD-C2D-C3D	2.31	129.00	124.68
24	b	614	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
24	a	613	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
24	C	506	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
33	c	519	LMG	C38-C37-C36	-2.31	102.72	114.42
26	B	616	BCR	C15-C16-C17	-2.31	118.75	123.47
24	b	602	CLA	C16-C15-C13	-2.31	108.47	115.92
33	Y	101	LMG	O1-C7-C8	-2.31	105.33	110.90
24	B	613	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
31	c	517	DGD	CDB-CCB-CBB	-2.30	102.72	114.42
31	c	516	DGD	O3G-C1D-C2D	-2.30	104.71	108.30
24	b	609	CLA	C1-O2A-CGA	2.29	122.46	116.44
33	c	522	LMG	O8-C28-O10	-2.29	117.80	123.59
33	D	411	LMG	C38-C37-C36	-2.29	102.78	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	a	619	LMG	O7-C10-C11	2.29	116.44	111.50
24	A	605	CLA	CMD-C2D-C3D	2.29	128.97	124.68
26	b	617	BCR	C36-C18-C19	2.29	121.69	118.08
26	c	515	BCR	C1-C6-C5	-2.29	119.39	122.61
24	c	505	CLA	C3A-C2A-C1A	2.29	104.77	101.34
24	b	604	CLA	CGD-CBD-CAD	-2.29	103.32	110.73
24	b	608	CLA	CMC-C2C-C3C	2.29	129.25	124.94
24	D	404	CLA	CMD-C2D-C3D	2.29	128.96	124.68
31	C	517	DGD	O6E-C1E-O5D	-2.29	104.56	109.97
24	D	403	CLA	CMC-C2C-C3C	2.28	129.25	124.94
24	B	606	CLA	CHA-C1A-NA	-2.28	121.17	126.40
24	b	614	CLA	OBD-CAD-CBD	-2.28	122.64	125.89
26	B	618	BCR	C29-C30-C25	2.28	113.99	110.48
25	a	606	PHO	O2A-CGA-O1A	-2.28	117.84	123.59
24	b	613	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
24	B	602	CLA	O2D-CGD-CBD	2.28	115.31	111.27
24	C	502	CLA	C4D-C3D-CAD	-2.28	107.20	108.47
31	C	516	DGD	C9B-C8B-C7B	-2.27	102.88	114.42
24	a	604	CLA	OBD-CAD-CBD	-2.27	122.65	125.89
24	c	511	CLA	CMC-C2C-C3C	2.27	129.23	124.94
24	c	510	CLA	C11-C12-C13	-2.27	108.58	115.92
31	c	518	DGD	CDB-CCB-CBB	-2.27	102.91	114.42
31	h	102	DGD	O5E-C6E-C5E	-2.27	103.51	111.29
31	c	516	DGD	O4D-C4D-C5D	-2.27	103.66	109.30
24	b	606	CLA	CHB-C4A-NA	2.27	127.65	124.51
24	c	505	CLA	C6-C7-C8	-2.27	108.59	115.92
24	C	512	CLA	CMD-C2D-C3D	2.27	128.92	124.68
30	D	413	LHG	C18-C17-C16	-2.27	102.92	114.42
33	b	622	LMG	C9-C8-C7	-2.27	106.43	111.79
33	d	408	LMG	O2-C2-C1	-2.27	104.54	110.05
30	e	101	LHG	C20-C19-C18	-2.26	102.93	114.42
29	B	620	SQD	C46-C45-C44	-2.26	106.43	111.79
24	b	615	CLA	CMB-C2B-C3B	2.26	128.91	124.68
25	A	606	PHO	O1D-CGD-CBD	2.26	129.11	124.48
26	t	101	BCR	C1-C6-C7	2.26	122.17	115.78
24	c	511	CLA	C4D-C3D-CAD	-2.26	107.21	108.47
25	A	606	PHO	CBD-CHA-C4D	-2.26	105.99	108.54
24	c	512	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
28	A	611	PL9	C25-C24-C26	2.25	119.06	115.27
31	c	516	DGD	CCB-CBB-CAB	-2.25	102.99	114.42
24	A	605	CLA	C1-C2-C3	-2.25	122.15	126.04
24	C	510	CLA	O2A-CGA-O1A	-2.25	117.91	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	C11-C12-C13	-2.25	108.65	115.92
31	h	102	DGD	CBB-CAB-C9B	-2.25	103.01	114.42
26	b	617	BCR	C29-C30-C25	2.25	113.94	110.48
26	h	101	BCR	C37-C22-C23	2.24	121.61	118.08
24	A	605	CLA	CAA-CBA-CGA	-2.24	106.70	113.25
24	C	503	CLA	C7-C6-C5	-2.24	107.27	113.36
28	A	611	PL9	C36-C37-C38	-2.24	104.51	111.88
26	d	404	BCR	C11-C10-C9	-2.24	124.11	127.31
24	b	601	CLA	CMC-C2C-C3C	2.24	129.17	124.94
26	K	101	BCR	C27-C26-C25	2.24	125.99	122.73
24	C	513	CLA	C4D-C3D-CAD	-2.24	107.22	108.47
26	k	101	BCR	C27-C26-C25	2.24	125.98	122.73
24	A	612	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
24	B	610	CLA	CHB-C4A-NA	2.24	127.61	124.51
24	B	601	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
24	b	603	CLA	O2A-C1-C2	-2.24	102.75	108.64
31	c	516	DGD	O2D-C2D-C1D	-2.23	104.62	110.05
30	A	614	LHG	C11-C10-C9	-2.23	103.08	114.42
33	b	622	LMG	C40-C39-C38	-2.23	103.09	114.42
24	b	607	CLA	CMD-C2D-C3D	2.23	128.85	124.68
26	h	101	BCR	C2-C1-C6	2.23	113.92	110.48
33	M	101	LMG	C38-C37-C36	-2.23	103.11	114.42
31	A	616	DGD	O5E-C6E-C5E	-2.23	103.65	111.29
33	Y	101	LMG	O2-C2-C1	-2.23	104.64	110.05
24	B	604	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
24	C	507	CLA	C2A-C1A-CHA	2.22	127.75	123.86
26	B	618	BCR	C38-C26-C25	-2.22	122.03	124.53
26	h	101	BCR	C38-C26-C25	-2.22	122.04	124.53
26	c	515	BCR	C7-C8-C9	-2.22	122.88	126.23
31	C	517	DGD	C3E-C4E-C5E	-2.22	106.28	110.24
24	b	613	CLA	O1D-CGD-CBD	2.22	129.02	124.48
24	c	504	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
28	d	405	PL9	C8-C7-C3	2.22	118.24	111.98
30	l	101	LHG	C11-C10-C9	-2.21	103.21	114.42
33	D	407	LMG	O6-C1-O1	-2.21	104.74	109.97
33	d	408	LMG	C3-C4-C5	-2.21	106.30	110.24
28	D	406	PL9	C16-C14-C13	2.21	125.58	121.12
26	b	619	BCR	C36-C18-C19	2.21	121.56	118.08
24	b	616	CLA	OBD-CAD-C3D	2.21	131.65	127.98
28	a	612	PL9	C27-C28-C29	-2.21	122.35	127.66
24	C	507	CLA	O1D-CGD-CBD	2.21	129.00	124.48
29	f	102	SQD	O48-C23-C24	2.21	118.83	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	CMC-C2C-C3C	2.21	129.10	124.94
24	b	611	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
24	C	504	CLA	C4D-C3D-CAD	-2.21	107.24	108.47
24	A	605	CLA	CMC-C2C-C3C	2.20	129.10	124.94
26	A	608	BCR	C16-C15-C14	-2.20	118.96	123.47
24	b	608	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
24	B	608	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
33	M	101	LMG	O2-C2-C3	-2.20	105.26	110.35
24	c	507	CLA	OBD-CAD-C3D	2.20	131.64	127.98
33	a	619	LMG	O1-C1-C2	2.20	111.74	108.30
33	c	521	LMG	C6-C5-C4	-2.20	107.85	113.00
33	M	101	LMG	C37-C36-C35	-2.20	103.26	114.42
24	c	510	CLA	O2A-C1-C2	-2.20	102.86	108.64
24	B	602	CLA	C3B-C4B-NB	-2.20	106.37	109.21
24	C	501	CLA	CAA-CBA-CGA	-2.20	106.83	113.25
26	t	101	BCR	C4-C5-C6	2.20	125.92	122.73
30	a	614	LHG	C15-C14-C13	-2.20	103.28	114.42
24	c	512	CLA	OBD-CAD-CBD	-2.19	122.76	125.89
24	c	512	CLA	O1D-CGD-CBD	2.19	128.97	124.48
29	D	408	SQD	O5-C5-C4	2.19	113.68	109.69
26	b	618	BCR	C1-C6-C5	-2.19	119.52	122.61
26	K	102	BCR	C30-C25-C26	-2.19	119.53	122.61
30	d	406	LHG	C20-C19-C18	-2.19	103.29	114.42
24	c	507	CLA	O1A-CGA-CBA	2.19	132.29	123.73
26	b	617	BCR	C36-C18-C17	-2.19	119.85	122.92
26	A	608	BCR	C8-C7-C6	-2.19	121.05	127.20
24	b	604	CLA	CMB-C2B-C3B	2.19	128.77	124.68
26	h	101	BCR	C36-C18-C19	2.18	121.52	118.08
24	C	504	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
24	B	607	CLA	CMD-C2D-C3D	2.18	128.76	124.68
24	B	613	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
24	B	601	CLA	OBD-CAD-CBD	-2.18	122.78	125.89
31	H	102	DGD	C6D-C5D-C4D	2.18	116.64	112.09
30	D	413	LHG	C20-C19-C18	-2.18	103.36	114.42
31	H	102	DGD	C3E-C4E-C5E	-2.18	106.35	110.24
26	b	618	BCR	C37-C22-C21	-2.18	119.87	122.92
26	t	101	BCR	C34-C9-C10	-2.18	119.87	122.92
24	b	606	CLA	C4D-C3D-CAD	-2.18	107.26	108.47
24	B	613	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
24	a	613	CLA	CHA-C1A-NA	-2.18	121.42	126.40
24	B	602	CLA	CMB-C2B-C1B	-2.18	125.12	128.46
28	a	612	PL9	C21-C19-C18	-2.17	116.72	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	608	BCR	C15-C16-C17	-2.17	119.02	123.47
24	a	604	CLA	CHB-C4A-NA	2.17	127.52	124.51
29	a	615	SQD	O10-C23-C24	-2.17	115.25	123.73
26	a	608	BCR	C29-C30-C25	2.17	113.83	110.48
24	C	509	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
30	D	413	LHG	C15-C14-C13	-2.17	103.40	114.42
24	c	501	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
28	d	405	PL9	C40-C39-C38	-2.17	118.12	123.68
31	H	102	DGD	C3G-C2G-C1G	-2.17	106.66	111.79
26	A	608	BCR	C37-C22-C23	2.17	121.49	118.08
24	A	604	CLA	C11-C12-C13	-2.17	108.92	115.92
33	D	411	LMG	O1-C7-C8	-2.17	106.04	111.78
31	C	516	DGD	C7A-C6A-C5A	-2.17	103.43	114.42
24	c	511	CLA	CMD-C2D-C3D	2.16	128.73	124.68
24	d	403	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	A	612	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
24	c	501	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
26	k	102	BCR	C8-C7-C6	-2.16	121.14	127.20
24	b	602	CLA	CMC-C2C-C3C	2.16	129.01	124.94
30	d	406	LHG	C27-C26-C25	-2.16	103.47	114.42
28	d	405	PL9	C20-C19-C21	2.16	118.90	115.27
24	B	614	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
26	k	102	BCR	C37-C22-C21	-2.16	119.90	122.92
29	a	615	SQD	O9-S-C6	2.15	109.50	106.94
24	d	403	CLA	CMD-C2D-C3D	2.15	128.71	124.68
24	c	510	CLA	OBD-CAD-CBD	-2.15	122.82	125.89
24	B	605	CLA	CMB-C2B-C3B	2.15	128.70	124.68
26	t	101	BCR	C12-C13-C14	-2.15	115.64	118.94
26	b	619	BCR	C38-C26-C25	-2.15	122.11	124.53
24	A	604	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
24	C	505	CLA	C16-C15-C13	-2.15	108.97	115.92
28	a	612	PL9	O2-C1-C2	-2.15	116.86	121.78
24	B	608	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
29	b	620	SQD	O10-C23-C24	-2.15	115.35	123.73
24	B	609	CLA	O1A-CGA-CBA	2.15	132.11	123.73
31	c	518	DGD	C5B-C4B-C3B	-2.15	103.53	114.42
31	c	516	DGD	O2G-C1B-C2B	-2.15	106.88	111.50
24	B	602	CLA	OBD-CAD-C3D	2.15	131.54	127.98
24	C	503	CLA	OBD-CAD-CBD	-2.15	122.83	125.89
25	D	401	PHO	C2B-C1B-NB	-2.14	106.56	109.79
24	C	504	CLA	CMB-C2B-C3B	2.14	128.68	124.68
30	A	614	LHG	C27-C26-C25	-2.14	103.57	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
24	C	509	CLA	C1-C2-C3	-2.14	122.35	126.04
24	C	512	CLA	O2D-CGD-CBD	2.14	115.06	111.27
31	c	516	DGD	CAB-C9B-C8B	-2.13	103.60	114.42
26	A	608	BCR	C15-C14-C13	-2.13	124.27	127.31
24	c	508	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
29	A	613	SQD	O5-C1-C2	-2.13	105.84	110.35
26	X	101	BCR	C1-C6-C5	-2.13	119.62	122.61
30	L	101	LHG	C27-C26-C25	-2.13	103.63	114.42
26	D	405	BCR	C38-C26-C25	-2.13	122.14	124.53
24	C	506	CLA	OBD-CAD-C3D	2.13	131.51	127.98
24	b	609	CLA	O2D-CGD-CBD	-2.12	107.49	111.27
29	a	615	SQD	O5-C1-O6	2.12	115.00	109.97
24	C	502	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
24	D	404	CLA	O2D-CGD-CBD	2.12	115.04	111.27
33	Y	101	LMG	O6-C5-C6	2.12	111.71	106.44
24	C	513	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	K	103	BCR	C7-C8-C9	-2.12	123.03	126.23
31	c	518	DGD	C3D-C4D-C5D	-2.12	106.46	110.24
26	B	618	BCR	C33-C5-C6	-2.12	122.15	124.53
24	B	601	CLA	CMD-C2D-C3D	2.12	128.64	124.68
25	A	606	PHO	CAC-C3C-C4C	-2.12	122.91	125.22
24	C	501	CLA	CMB-C2B-C3B	2.12	128.64	124.68
24	c	505	CLA	O2D-CGD-CBD	2.12	115.03	111.27
24	C	509	CLA	C4D-C3D-CAD	-2.12	107.29	108.47
33	M	101	LMG	O2-C2-C1	-2.12	104.91	110.05
31	h	102	DGD	C3G-C2G-C1G	-2.11	106.79	111.79
31	A	616	DGD	C8B-C7B-C6B	-2.11	103.70	114.42
31	C	517	DGD	O2D-C2D-C1D	-2.11	104.92	110.05
24	C	503	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
24	B	601	CLA	C4D-C3D-CAD	-2.11	107.29	108.47
24	c	511	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
24	c	513	CLA	CAA-CBA-CGA	-2.11	107.09	113.25
29	A	613	SQD	O48-C23-C24	2.11	118.52	111.91
24	b	605	CLA	CMC-C2C-C3C	2.11	128.91	124.94
26	c	514	BCR	C27-C26-C25	2.10	125.79	122.73
24	b	608	CLA	CMD-C2D-C3D	2.10	128.62	124.68
26	D	405	BCR	C15-C16-C17	-2.10	119.16	123.47
31	c	518	DGD	CAB-C9B-C8B	-2.10	103.74	114.42
26	a	608	BCR	C36-C18-C17	-2.10	119.98	122.92
30	D	409	LHG	C27-C26-C25	-2.10	103.76	114.42
26	h	101	BCR	C7-C8-C9	-2.10	123.06	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C4D-C3D-CAD	-2.10	107.30	108.47
30	e	101	LHG	C11-C10-C9	-2.10	103.78	114.42
26	K	101	BCR	C11-C10-C9	-2.10	124.32	127.31
24	C	511	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
24	c	509	CLA	C2A-C3A-C4A	2.09	105.25	101.87
24	A	605	CLA	C7-C6-C5	-2.09	107.67	113.36
36	V	201	HEC	C3B-C4B-NB	-2.09	107.00	110.94
24	A	612	CLA	C16-C15-C13	-2.09	109.16	115.92
33	D	407	LMG	O3-C3-C2	-2.09	105.52	110.35
24	B	612	CLA	CHB-C4A-NA	2.09	127.40	124.51
31	C	518	DGD	O3D-C3D-C4D	-2.09	105.52	110.35
24	c	505	CLA	C16-C15-C13	-2.09	109.16	115.92
24	H	101	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
24	A	612	CLA	C4D-C3D-CAD	2.09	109.64	108.47
24	c	506	CLA	CMD-C2D-C3D	2.09	128.58	124.68
24	B	615	CLA	C2A-C3A-C4A	2.08	105.23	101.87
33	C	515	LMG	O8-C28-O10	-2.08	118.34	123.59
31	c	516	DGD	CDB-CCB-CBB	-2.08	103.86	114.42
24	a	613	CLA	C2A-C1A-CHA	2.08	127.50	123.86
24	C	502	CLA	CMC-C2C-C3C	2.08	128.86	124.94
24	b	611	CLA	OBD-CAD-CBD	-2.08	122.92	125.89
25	d	401	PHO	C3C-C4C-NC	-2.08	107.06	110.28
30	e	101	LHG	C5-O7-C7	-2.08	112.68	117.79
24	c	504	CLA	O2D-CGD-CBD	2.08	114.96	111.27
30	A	614	LHG	O8-C23-O10	-2.08	118.35	123.59
24	B	614	CLA	CMB-C2B-C3B	2.08	128.56	124.68
24	B	615	CLA	CMD-C2D-C3D	2.08	128.56	124.68
30	e	101	LHG	O8-C23-O10	-2.08	118.36	123.59
24	B	607	CLA	C6-C7-C8	-2.07	109.22	115.92
31	A	616	DGD	C5B-C4B-C3B	-2.07	103.92	114.42
31	C	516	DGD	C7B-C6B-C5B	-2.07	103.92	114.42
26	a	608	BCR	C39-C30-C25	-2.07	106.94	110.30
28	a	612	PL9	C35-C34-C36	2.07	118.75	115.27
31	c	517	DGD	CBB-CAB-C9B	-2.06	103.94	114.42
24	b	601	CLA	C4D-C3D-CAD	-2.06	107.32	108.47
31	C	517	DGD	C1D-C2D-C3D	-2.06	105.70	110.00
24	b	616	CLA	C1-C2-C3	-2.06	122.47	126.04
26	B	617	BCR	C8-C7-C6	-2.06	121.41	127.20
26	k	102	BCR	C38-C26-C25	-2.06	122.21	124.53
24	c	507	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
30	A	614	LHG	C20-C19-C18	-2.06	103.97	114.42
24	B	602	CLA	C1B-CHB-C4A	-2.06	126.04	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
24	B	605	CLA	C2A-C1A-CHA	2.06	127.46	123.86
30	L	101	LHG	C20-C19-C18	-2.06	103.98	114.42
24	A	604	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
24	c	505	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
24	c	506	CLA	CHB-C4A-NA	2.06	127.36	124.51
29	f	102	SQD	O5-C1-C2	-2.06	106.00	110.35
24	B	602	CLA	CMC-C2C-C3C	2.06	128.82	124.94
33	C	515	LMG	C38-C37-C36	-2.06	103.99	114.42
26	a	608	BCR	C30-C25-C26	-2.06	119.72	122.61
28	a	612	PL9	C12-C13-C14	-2.05	122.71	127.66
24	b	601	CLA	CBA-CAA-C2A	2.05	119.93	113.86
24	b	608	CLA	C11-C10-C8	-2.05	109.28	115.92
31	c	518	DGD	O3G-C1D-C2D	-2.05	105.10	108.30
24	C	504	CLA	O1A-CGA-CBA	2.05	131.74	123.73
26	T	101	BCR	C31-C1-C6	2.05	113.63	110.30
26	D	405	BCR	C24-C23-C22	-2.05	123.14	126.23
26	k	101	BCR	C7-C8-C9	-2.05	123.14	126.23
28	d	405	PL9	C15-C14-C13	-2.05	118.42	123.68
26	b	619	BCR	C20-C21-C22	-2.05	124.39	127.31
26	K	103	BCR	C20-C21-C22	-2.05	124.39	127.31
26	K	103	BCR	C2-C1-C6	2.05	113.64	110.48
24	C	507	CLA	C3A-C2A-C1A	2.05	104.41	101.34
35	f	101	HEM	C4C-C3C-C2C	2.04	108.33	106.90
33	C	515	LMG	C35-C34-C33	-2.04	104.05	114.42
30	D	409	LHG	O8-C23-C24	2.04	118.32	111.91
24	b	602	CLA	CGD-CBD-CAD	-2.04	104.11	110.73
24	A	604	CLA	C11-C10-C8	-2.04	109.31	115.92
24	D	404	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	C	509	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
31	C	517	DGD	O3G-C1D-C2D	-2.04	105.12	108.30
24	b	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
24	c	502	CLA	CMD-C2D-C3D	2.04	128.50	124.68
33	c	519	LMG	O8-C28-O10	-2.04	118.44	123.59
26	X	101	BCR	C16-C15-C14	-2.04	119.30	123.47
26	k	101	BCR	C8-C7-C6	-2.04	121.47	127.20
31	C	518	DGD	O3G-C1D-C2D	-2.04	105.12	108.30
33	c	521	LMG	O7-C10-O9	-2.04	118.78	123.70
24	B	613	CLA	O1D-CGD-CBD	2.04	128.65	124.48
28	A	611	PL9	O2-C1-C6	2.04	124.12	120.59
24	A	604	CLA	CMC-C2C-C3C	2.04	128.78	124.94
26	c	515	BCR	C38-C26-C25	-2.04	122.24	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	605	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
33	d	408	LMG	O2-C2-C3	-2.04	105.64	110.35
24	b	614	CLA	CMB-C2B-C3B	2.03	128.49	124.68
31	c	517	DGD	C3E-C4E-C5E	-2.03	106.61	110.24
26	c	514	BCR	C15-C16-C17	-2.03	119.31	123.47
24	b	608	CLA	C4D-C3D-CAD	-2.03	107.34	108.47
24	B	603	CLA	CGD-CBD-CAD	-2.03	104.15	110.73
26	C	514	BCR	C37-C22-C21	-2.03	120.08	122.92
24	C	502	CLA	OBD-CAD-CBD	-2.03	122.99	125.89
31	c	517	DGD	O2D-C2D-C1D	-2.03	105.11	110.05
26	X	101	BCR	C38-C26-C25	-2.03	122.25	124.53
24	H	101	CLA	C3D-CAD-CBD	-2.03	104.93	107.61
24	c	503	CLA	CMA-C3A-C4A	2.03	117.22	111.77
24	c	503	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
24	c	501	CLA	OBD-CAD-CBD	-2.03	123.00	125.89
26	b	617	BCR	C24-C23-C22	-2.03	123.17	126.23
24	C	510	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
24	b	601	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
24	b	610	CLA	CAA-C2A-C3A	-2.02	107.24	112.78
26	K	101	BCR	C24-C23-C22	-2.02	123.18	126.23
31	c	516	DGD	O3D-C3D-C2D	-2.02	105.68	110.35
31	c	517	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
26	b	619	BCR	C28-C27-C26	-2.02	110.47	114.08
24	b	616	CLA	CMD-C2D-C3D	2.02	128.46	124.68
33	C	515	LMG	O2-C2-C1	-2.02	105.14	110.05
24	c	501	CLA	O1D-CGD-CBD	2.02	128.61	124.48
33	c	522	LMG	O7-C10-O9	-2.02	118.83	123.70
24	b	615	CLA	C3B-C4B-NB	-2.02	106.60	109.21
24	B	609	CLA	C4-C3-C2	-2.02	118.50	123.68
33	c	519	LMG	C8-O7-C10	2.02	121.65	117.90
24	B	613	CLA	C4-C3-C2	-2.01	118.51	123.68
24	b	607	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
28	D	406	PL9	C21-C19-C18	-2.01	117.05	121.12
24	H	101	CLA	C1-C2-C3	-2.01	122.56	126.04
24	H	101	CLA	CHB-C4A-NA	2.01	127.29	124.51
25	d	401	PHO	CMD-C2D-C1D	2.01	128.16	125.06
26	c	515	BCR	C34-C9-C10	-2.01	120.11	122.92
26	B	616	BCR	C36-C18-C19	2.01	121.25	118.08
28	D	406	PL9	O2-C1-C2	-2.01	117.17	121.78
24	C	511	CLA	CHB-C4A-NA	2.01	127.29	124.51
29	f	102	SQD	O47-C7-O49	-2.01	118.85	123.70
31	C	518	DGD	C6B-C5B-C4B	-2.01	104.22	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C8-C7-C6	-2.01	121.56	127.20
24	c	512	CLA	O2D-CGD-CBD	2.01	114.84	111.27
31	H	102	DGD	CAB-C9B-C8B	-2.01	104.23	114.42
33	C	515	LMG	C12-C11-C10	-2.01	106.32	113.62
31	c	516	DGD	CEB-CDB-CCB	-2.01	104.23	114.42
24	c	508	CLA	C7-C6-C5	-2.01	107.91	113.36
33	a	619	LMG	O7-C8-C7	2.01	115.67	108.40
24	a	604	CLA	CMD-C2D-C3D	2.01	128.43	124.68
25	D	401	PHO	C1-C2-C3	-2.01	122.57	126.04
24	B	604	CLA	CHB-C4A-NA	2.00	127.28	124.51
33	a	619	LMG	C33-C32-C31	-2.00	104.25	114.42
24	b	614	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
33	b	622	LMG	O8-C28-O10	-2.00	118.54	123.59
24	c	513	CLA	O2D-CGD-CBD	2.00	114.83	111.27

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	607	CLA	ND
24	A	612	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	609	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	C	501	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	507	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	404	CLA	ND
24	H	101	CLA	ND
24	a	604	CLA	ND
24	a	607	CLA	ND
24	a	613	CLA	ND
24	b	601	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	c	501	CLA	ND
24	c	502	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	d	403	CLA	ND

All (1880) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	604	CLA	C2C-C3C-CAC-CBC
24	A	612	CLA	CHA-CBD-CGD-O1D
24	A	612	CLA	CHA-CBD-CGD-O2D
24	B	613	CLA	CHA-CBD-CGD-O1D
24	B	613	CLA	CHA-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O1D
24	C	503	CLA	C11-C10-C8-C9
24	D	404	CLA	C4-C3-C5-C6
24	H	101	CLA	C1A-C2A-CAA-CBA
24	H	101	CLA	C3A-C2A-CAA-CBA
24	H	101	CLA	CHA-CBD-CGD-O1D
24	H	101	CLA	CHA-CBD-CGD-O2D
24	H	101	CLA	CAD-CBD-CGD-O1D
24	a	605	CLA	CHA-CBD-CGD-O1D
24	a	605	CLA	CHA-CBD-CGD-O2D
24	a	613	CLA	CHA-CBD-CGD-O1D
24	a	613	CLA	CHA-CBD-CGD-O2D
24	b	601	CLA	C1A-C2A-CAA-CBA
24	b	601	CLA	CAD-CBD-CGD-O1D
24	b	601	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	C2C-C3C-CAC-CBC
24	b	614	CLA	CHA-CBD-CGD-O1D
24	b	614	CLA	CHA-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	C11-C12-C13-C15
24	b	616	CLA	C11-C10-C8-C9
24	c	504	CLA	C2-C3-C5-C6
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CBD-CGD-O2D-CED
24	c	509	CLA	C6-C7-C8-C9
24	d	403	CLA	C11-C10-C8-C9
25	d	401	PHO	C1A-C2A-CAA-CBA
25	d	401	PHO	CHA-CBD-CGD-O1D
25	d	401	PHO	CHA-CBD-CGD-O2D
25	d	401	PHO	CBD-CGD-O2D-CED
26	B	616	BCR	C1-C6-C7-C8
26	B	617	BCR	C16-C17-C18-C36
26	B	617	BCR	C37-C22-C23-C24
26	C	514	BCR	C36-C18-C19-C20
26	C	514	BCR	C37-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	D	405	BCR	C23-C24-C25-C30
26	K	101	BCR	C7-C8-C9-C34
26	K	101	BCR	C16-C17-C18-C36
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C7-C8-C9-C34
26	K	102	BCR	C11-C12-C13-C35
26	K	102	BCR	C20-C21-C22-C37
26	K	102	BCR	C37-C22-C23-C24
26	K	103	BCR	C1-C6-C7-C8
26	K	103	BCR	C10-C11-C12-C13
26	K	103	BCR	C11-C12-C13-C35
26	T	101	BCR	C7-C8-C9-C10
26	b	617	BCR	C1-C6-C7-C8
26	b	618	BCR	C35-C13-C14-C15
26	b	619	BCR	C37-C22-C23-C24
26	c	514	BCR	C1-C6-C7-C8
26	c	514	BCR	C11-C12-C13-C14
26	c	514	BCR	C11-C12-C13-C35
26	c	515	BCR	C11-C12-C13-C35
26	c	515	BCR	C35-C13-C14-C15
26	c	515	BCR	C20-C21-C22-C37
26	d	404	BCR	C37-C22-C23-C24
26	h	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C37-C22-C23-C24
26	k	102	BCR	C11-C12-C13-C35
26	k	102	BCR	C37-C22-C23-C24
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C10-C9-C34
26	t	101	BCR	C11-C12-C13-C35
28	A	611	PL9	C12-C13-C14-C16
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C25-C24-C26-C27
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C37-C38-C39-C41
28	A	611	PL9	C43-C44-C46-C47
28	D	406	PL9	C32-C33-C34-C35
28	D	406	PL9	C35-C34-C36-C37
28	a	612	PL9	C12-C13-C14-C16
28	a	612	PL9	C20-C19-C21-C22
28	a	612	PL9	C22-C23-C24-C26

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Mol	Chain	Res	Type	Atoms
28	a	612	PL9	C39-C41-C42-C43
28	a	612	PL9	C47-C48-C49-C51
28	d	405	PL9	C32-C33-C34-C35
28	d	405	PL9	C32-C33-C34-C36
28	d	405	PL9	C37-C38-C39-C41
28	d	405	PL9	C38-C39-C41-C42
29	A	615	SQD	C44-C45-C46-O48
29	B	620	SQD	O5-C1-O6-C44
29	B	620	SQD	O6-C44-C45-O47
29	B	620	SQD	O49-C7-O47-C45
29	B	620	SQD	C8-C7-O47-C45
29	B	620	SQD	O10-C23-O48-C46
29	B	620	SQD	C24-C23-O48-C46
29	D	408	SQD	C45-C44-O6-C1
29	a	616	SQD	O49-C7-O47-C45
29	a	616	SQD	C8-C7-O47-C45
29	b	620	SQD	C8-C7-O47-C45
29	b	620	SQD	O10-C23-O48-C46
29	f	102	SQD	C2-C1-O6-C44
29	f	102	SQD	O5-C1-O6-C44
30	A	614	LHG	O1-C1-C2-C3
30	A	614	LHG	C4-O6-P-O4
30	D	409	LHG	O2-C2-C3-O3
30	D	409	LHG	C3-O3-P-O5
30	D	409	LHG	C4-O6-P-O4
30	D	413	LHG	C1-C2-C3-O3
30	D	413	LHG	C3-O3-P-O4
30	D	413	LHG	C3-O3-P-O5
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O4
30	a	614	LHG	O1-C1-C2-C3
30	d	406	LHG	O1-C1-C2-C3
30	d	406	LHG	C3-O3-P-O6
30	d	406	LHG	C4-O6-P-O5
30	e	101	LHG	C1-C2-C3-O3
30	e	101	LHG	C3-O3-P-O5
31	A	616	DGD	C2B-C1B-O2G-C2G
31	A	616	DGD	O1B-C1B-O2G-C2G
32	B	619	STE	C1-C2-C3-C4
32	B	621	STE	C1-C2-C3-C4
32	B	626	STE	C1-C2-C3-C4
32	L	102	STE	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	R	101	STE	C1-C2-C3-C4
32	b	624	STE	C1-C2-C3-C4
32	c	520	STE	C1-C2-C3-C4
32	c	523	STE	C1-C2-C3-C4
32	d	410	STE	C1-C2-C3-C4
33	C	515	LMG	O9-C10-O7-C8
33	D	411	LMG	O1-C7-C8-C9
33	D	411	LMG	O1-C7-C8-O7
33	D	411	LMG	C11-C10-O7-C8
33	D	412	LMG	C28-C29-C30-C31
33	Y	101	LMG	C2-C1-O1-C7
33	Y	101	LMG	O6-C1-O1-C7
33	b	622	LMG	C2-C1-O1-C7
33	b	622	LMG	O6-C1-O1-C7
33	c	521	LMG	C11-C10-O7-C8
33	c	522	LMG	O6-C1-O1-C7
24	B	615	CLA	O1D-CGD-O2D-CED
24	b	601	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	CBD-CGD-O2D-CED
24	B	615	CLA	CBD-CGD-O2D-CED
24	C	501	CLA	CBD-CGD-O2D-CED
24	b	601	CLA	CBD-CGD-O2D-CED
33	c	521	LMG	O10-C28-O8-C9
33	c	522	LMG	O10-C28-O8-C9
33	c	519	LMG	C11-C10-O7-C8
29	b	620	SQD	C24-C23-O48-C46
33	c	521	LMG	C29-C28-O8-C9
33	c	522	LMG	C29-C28-O8-C9
24	b	609	CLA	CBD-CGD-O2D-CED
24	c	512	CLA	CBD-CGD-O2D-CED
29	a	616	SQD	O10-C23-O48-C46
30	A	614	LHG	O10-C23-O8-C6
33	M	101	LMG	O10-C28-O8-C9
24	c	509	CLA	O1D-CGD-O2D-CED
24	B	613	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
25	d	401	PHO	O1D-CGD-O2D-CED
33	D	411	LMG	O9-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
29	f	102	SQD	O10-C23-O48-C46
24	B	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C3-C5-C6-C7
24	C	512	CLA	C3-C5-C6-C7
24	b	602	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	b	604	CLA	C3-C5-C6-C7
24	b	614	CLA	C3-C5-C6-C7
29	f	102	SQD	C24-C23-O48-C46
33	M	101	LMG	C29-C28-O8-C9
33	C	515	LMG	C11-C10-O7-C8
33	Y	101	LMG	C11-C10-O7-C8
33	c	519	LMG	O9-C10-O7-C8
24	A	607	CLA	C4-C3-C5-C6
24	B	604	CLA	C4-C3-C5-C6
24	c	504	CLA	C4-C3-C5-C6
24	B	604	CLA	C2-C3-C5-C6
24	D	404	CLA	C2-C3-C5-C6
28	D	406	PL9	C33-C34-C36-C37
28	a	612	PL9	C18-C19-C21-C22
24	B	605	CLA	C2A-CAA-CBA-CGA
24	b	606	CLA	C2A-CAA-CBA-CGA
24	C	506	CLA	C3-C5-C6-C7
24	b	601	CLA	C3-C5-C6-C7
30	A	614	LHG	C24-C23-O8-C6
33	a	619	LMG	C29-C28-O8-C9
24	C	501	CLA	O1D-CGD-O2D-CED
28	a	612	PL9	C47-C48-C49-C50
28	a	612	PL9	C22-C23-C24-C25
29	f	102	SQD	O49-C7-O47-C45
28	D	406	PL9	C32-C33-C34-C36
29	D	408	SQD	O10-C23-O48-C46
30	e	101	LHG	O10-C23-O8-C6
31	C	516	DGD	O6E-C5E-C6E-O5E
29	A	615	SQD	C46-C45-O47-C7
24	C	510	CLA	CBD-CGD-O2D-CED
24	H	101	CLA	CBD-CGD-O2D-CED
30	D	413	LHG	O2-C2-C3-O3
30	e	101	LHG	O2-C2-C3-O3
29	a	616	SQD	C24-C23-O48-C46
33	c	521	LMG	O6-C5-C6-O5
29	f	102	SQD	C8-C7-O47-C45
24	b	607	CLA	CBD-CGD-O2D-CED
32	b	624	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	c	522	LMG	O6-C5-C6-O5
24	C	509	CLA	C3-C5-C6-C7
31	c	518	DGD	O1A-C1A-O1G-C1G
24	C	513	CLA	C4-C3-C5-C6
28	A	611	PL9	C40-C39-C41-C42
24	C	513	CLA	C2-C3-C5-C6
28	A	611	PL9	C23-C24-C26-C27
28	A	611	PL9	C38-C39-C41-C42
31	A	616	DGD	O6D-C1D-O3G-C3G
28	A	611	PL9	C19-C21-C22-C23
28	A	611	PL9	C39-C41-C42-C43
28	D	406	PL9	C29-C31-C32-C33
28	a	612	PL9	C34-C36-C37-C38
28	a	612	PL9	C44-C46-C47-C48
24	B	602	CLA	O1D-CGD-O2D-CED
28	A	611	PL9	C12-C13-C14-C15
24	c	512	CLA	O1D-CGD-O2D-CED
30	A	614	LHG	C1-C2-C3-O3
29	b	620	SQD	O49-C7-O47-C45
24	a	605	CLA	C3-C5-C6-C7
24	c	506	CLA	CBA-CGA-O2A-C1
29	D	408	SQD	C24-C23-O48-C46
30	e	101	LHG	C24-C23-O8-C6
33	Y	101	LMG	C29-C28-O8-C9
30	D	409	LHG	C30-C31-C32-C33
30	d	407	LHG	C30-C31-C32-C33
32	B	625	STE	C5-C6-C7-C8
32	c	520	STE	C2-C3-C4-C5
24	B	605	CLA	C15-C16-C17-C18
24	b	603	CLA	C10-C11-C12-C13
33	c	522	LMG	C4-C5-C6-O5
29	A	615	SQD	C44-C45-O47-C7
30	A	614	LHG	C27-C28-C29-C30
24	b	611	CLA	C13-C15-C16-C17
30	A	614	LHG	O2-C2-C3-O3
29	B	620	SQD	C2-C1-O6-C44
33	c	522	LMG	C2-C1-O1-C7
24	C	504	CLA	C4-C3-C5-C6
24	A	607	CLA	C2-C3-C5-C6
28	A	611	PL9	C33-C34-C36-C37
28	D	406	PL9	C38-C39-C41-C42
24	A	605	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C6-C7-C8-C9
24	B	605	CLA	C11-C12-C13-C14
24	B	606	CLA	C14-C13-C15-C16
24	B	610	CLA	C11-C12-C13-C14
24	C	507	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	D	403	CLA	C14-C13-C15-C16
24	H	101	CLA	C14-C13-C15-C16
24	b	601	CLA	C11-C10-C8-C9
24	b	604	CLA	C6-C7-C8-C9
24	b	607	CLA	C11-C10-C8-C9
24	b	610	CLA	C14-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C9
24	c	510	CLA	C14-C13-C15-C16
24	c	512	CLA	C6-C7-C8-C9
26	A	608	BCR	C11-C12-C13-C35
26	B	616	BCR	C37-C22-C23-C24
26	D	405	BCR	C37-C22-C23-C24
26	b	619	BCR	C7-C8-C9-C34
24	c	506	CLA	O1A-CGA-O2A-C1
33	a	619	LMG	O10-C28-O8-C9
24	B	606	CLA	C10-C11-C12-C13
24	b	614	CLA	C8-C10-C11-C12
33	m	101	LMG	O6-C5-C6-O5
24	C	503	CLA	C5-C6-C7-C8
24	C	505	CLA	C10-C11-C12-C13
24	b	601	CLA	C8-C10-C11-C12
24	b	605	CLA	C10-C11-C12-C13
24	b	611	CLA	C8-C10-C11-C12
24	b	614	CLA	C13-C15-C16-C17
24	c	509	CLA	C13-C15-C16-C17
29	A	613	SQD	C7-C8-C9-C10
30	a	614	LHG	C7-C8-C9-C10
33	c	522	LMG	C10-C11-C12-C13
24	B	607	CLA	C13-C15-C16-C17
24	B	615	CLA	C5-C6-C7-C8
24	C	502	CLA	C13-C15-C16-C17
24	a	605	CLA	C10-C11-C12-C13
24	b	602	CLA	C15-C16-C17-C18
24	b	608	CLA	C5-C6-C7-C8
24	c	508	CLA	C10-C11-C12-C13
24	d	403	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	D	406	PL9	C22-C23-C24-C25
28	D	406	PL9	C37-C38-C39-C40
29	A	613	SQD	C23-C24-C25-C26
29	A	615	SQD	C23-C24-C25-C26
30	a	614	LHG	C23-C24-C25-C26
31	c	517	DGD	C1B-C2B-C3B-C4B
33	D	407	LMG	C10-C11-C12-C13
33	M	101	LMG	C10-C11-C12-C13
33	b	622	LMG	C10-C11-C12-C13
33	d	408	LMG	C28-C29-C30-C31
33	a	619	LMG	O6-C5-C6-O5
32	M	104	STE	C2-C3-C4-C5
24	B	602	CLA	C8-C10-C11-C12
24	B	611	CLA	C10-C11-C12-C13
24	C	509	CLA	C5-C6-C7-C8
24	C	509	CLA	C8-C10-C11-C12
24	b	611	CLA	C15-C16-C17-C18
24	b	613	CLA	C15-C16-C17-C18
24	D	403	CLA	C3-C5-C6-C7
32	B	626	STE	C4-C5-C6-C7
33	c	521	LMG	C41-C42-C43-C44
24	b	609	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	C2-C1-O2A-CGA
24	C	504	CLA	C8-C10-C11-C12
24	b	607	CLA	C10-C11-C12-C13
29	a	616	SQD	C7-C8-C9-C10
31	C	518	DGD	C1A-C2A-C3A-C4A
33	c	521	LMG	C4-C5-C6-O5
24	B	601	CLA	C11-C12-C13-C15
24	B	605	CLA	C11-C12-C13-C15
24	C	508	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C15
24	b	602	CLA	C11-C12-C13-C15
24	b	604	CLA	C6-C7-C8-C10
24	b	609	CLA	C11-C12-C13-C15
24	c	506	CLA	C11-C12-C13-C15
24	c	510	CLA	C12-C13-C15-C16
26	K	101	BCR	C13-C14-C15-C16
24	C	510	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	C13-C15-C16-C17
24	C	512	CLA	C8-C10-C11-C12
24	H	101	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	603	CLA	CBD-CGD-O2D-CED
31	C	517	DGD	O6E-C1E-O5D-C6D
24	B	613	CLA	O1D-CGD-O2D-CED
28	A	611	PL9	C34-C36-C37-C38
28	A	611	PL9	C44-C46-C47-C48
28	a	612	PL9	C24-C26-C27-C28
26	B	617	BCR	C18-C19-C20-C21
26	B	618	BCR	C10-C11-C12-C13
26	d	404	BCR	C10-C11-C12-C13
26	t	101	BCR	C18-C19-C20-C21
24	A	605	CLA	C10-C11-C12-C13
24	B	606	CLA	C5-C6-C7-C8
24	B	606	CLA	C15-C16-C17-C18
24	B	613	CLA	C5-C6-C7-C8
24	b	614	CLA	C5-C6-C7-C8
31	c	517	DGD	C1A-C2A-C3A-C4A
24	A	612	CLA	C15-C16-C17-C18
24	B	606	CLA	C8-C10-C11-C12
24	B	613	CLA	C15-C16-C17-C18
24	C	513	CLA	C15-C16-C17-C18
24	b	607	CLA	C8-C10-C11-C12
24	c	505	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
24	c	512	CLA	C13-C15-C16-C17
24	d	403	CLA	C13-C15-C16-C17
30	a	614	LHG	C10-C11-C12-C13
33	b	622	LMG	C11-C10-O7-C8
24	B	605	CLA	C8-C10-C11-C12
24	B	610	CLA	C8-C10-C11-C12
24	b	607	CLA	C5-C6-C7-C8
30	A	614	LHG	C4-O6-P-O3
30	D	410	LHG	C3-O3-P-O6
30	D	413	LHG	C3-O3-P-O6
30	a	614	LHG	C3-O3-P-O6
30	d	406	LHG	C4-O6-P-O3
24	c	512	CLA	CBA-CGA-O2A-C1
32	d	411	STE	C9-C10-C11-C12
24	C	506	CLA	C8-C10-C11-C12
24	a	605	CLA	C13-C15-C16-C17
24	c	503	CLA	C15-C16-C17-C18
24	C	511	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
28	A	611	PL9	C45-C44-C46-C47
24	c	512	CLA	C8-C10-C11-C12
24	b	601	CLA	C2A-CAA-CBA-CGA
31	C	516	DGD	C4E-C5E-C6E-O5E
24	C	511	CLA	CBA-CGA-O2A-C1
31	c	518	DGD	C2A-C1A-O1G-C1G
24	B	604	CLA	C13-C15-C16-C17
31	C	518	DGD	CCA-CDA-CEA-CFA
32	B	622	STE	C3-C4-C5-C6
32	J	101	STE	C6-C7-C8-C9
32	b	621	STE	C13-C14-C15-C16
32	d	409	STE	C2-C3-C4-C5
33	C	515	LMG	C14-C15-C16-C17
26	A	608	BCR	C35-C13-C14-C15
26	A	608	BCR	C20-C21-C22-C37
26	B	616	BCR	C11-C10-C9-C34
26	B	616	BCR	C16-C17-C18-C36
26	B	617	BCR	C11-C10-C9-C34
26	B	618	BCR	C35-C13-C14-C15
26	C	514	BCR	C16-C17-C18-C36
26	K	101	BCR	C35-C13-C14-C15
26	K	103	BCR	C20-C21-C22-C37
26	T	101	BCR	C20-C21-C22-C37
26	a	608	BCR	C11-C10-C9-C34
26	b	617	BCR	C20-C21-C22-C37
26	b	619	BCR	C35-C13-C14-C15
26	c	515	BCR	C16-C17-C18-C36
26	k	102	BCR	C11-C10-C9-C34
29	A	615	SQD	C9-C10-C11-C12
29	a	615	SQD	C12-C13-C14-C15
29	f	102	SQD	C28-C29-C30-C31
30	A	614	LHG	C11-C10-C9-C8
31	A	616	DGD	C2B-C3B-C4B-C5B
31	C	518	DGD	C6A-C7A-C8A-C9A
31	c	518	DGD	CCB-CDB-CEB-CFB
31	h	102	DGD	C9A-CAA-CBA-CCA
32	B	623	STE	C3-C4-C5-C6
32	c	523	STE	C4-C5-C6-C7
33	C	515	LMG	C33-C34-C35-C36
33	D	407	LMG	C35-C36-C37-C38
33	D	411	LMG	C34-C35-C36-C37
33	M	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
33	c	521	LMG	C29-C30-C31-C32
33	c	522	LMG	C32-C33-C34-C35
24	a	604	CLA	C16-C17-C18-C20
24	b	604	CLA	C16-C17-C18-C20
29	A	613	SQD	C10-C11-C12-C13
29	A	615	SQD	C10-C11-C12-C13
29	B	620	SQD	C13-C14-C15-C16
29	a	615	SQD	C28-C29-C30-C31
30	A	614	LHG	C33-C34-C35-C36
30	D	410	LHG	C24-C25-C26-C27
30	d	406	LHG	C28-C29-C30-C31
31	A	616	DGD	CAA-CBA-CCA-CDA
31	C	517	DGD	C5A-C6A-C7A-C8A
31	C	518	DGD	C9A-CAA-CBA-CCA
31	h	102	DGD	C2B-C3B-C4B-C5B
31	h	102	DGD	C5B-C6B-C7B-C8B
32	B	619	STE	C11-C12-C13-C14
32	B	622	STE	C11-C10-C9-C8
32	B	622	STE	C10-C11-C12-C13
32	J	101	STE	C5-C6-C7-C8
33	C	515	LMG	C13-C14-C15-C16
33	C	515	LMG	C35-C36-C37-C38
33	C	515	LMG	C38-C39-C40-C41
33	Y	101	LMG	C17-C18-C19-C20
33	a	619	LMG	C12-C13-C14-C15
33	a	619	LMG	C13-C14-C15-C16
33	c	521	LMG	C32-C33-C34-C35
33	c	522	LMG	C18-C19-C20-C21
29	b	620	SQD	C46-C45-O47-C7
33	b	622	LMG	C9-C8-O7-C10
31	h	102	DGD	O6E-C5E-C6E-O5E
30	A	614	LHG	C23-C24-C25-C26
29	A	613	SQD	C34-C35-C36-C37
30	A	614	LHG	C12-C13-C14-C15
30	D	413	LHG	C28-C29-C30-C31
30	l	101	LHG	C14-C15-C16-C17
31	C	516	DGD	C8A-C9A-CAA-CBA
32	d	410	STE	C13-C14-C15-C16
33	a	619	LMG	C33-C34-C35-C36
33	b	622	LMG	C16-C17-C18-C19
33	b	622	LMG	C40-C41-C42-C43
33	c	522	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	B	620	SQD	C25-C26-C27-C28
30	A	614	LHG	C13-C14-C15-C16
30	D	409	LHG	C32-C33-C34-C35
30	D	410	LHG	C11-C12-C13-C14
30	D	410	LHG	C26-C27-C28-C29
30	L	101	LHG	C29-C30-C31-C32
30	a	614	LHG	C11-C10-C9-C8
30	d	407	LHG	C27-C28-C29-C30
31	c	518	DGD	C9B-CAB-CBB-CCB
32	B	623	STE	C5-C6-C7-C8
32	C	519	STE	C3-C4-C5-C6
32	T	103	STE	C11-C10-C9-C8
32	X	102	STE	C5-C6-C7-C8
32	b	621	STE	C14-C15-C16-C17
32	b	625	STE	C2-C3-C4-C5
32	c	523	STE	C3-C4-C5-C6
29	A	615	SQD	C12-C13-C14-C15
30	a	614	LHG	C14-C15-C16-C17
31	C	518	DGD	C4A-C5A-C6A-C7A
32	B	621	STE	C2-C3-C4-C5
32	B	624	STE	C11-C10-C9-C8
32	T	103	STE	C9-C10-C11-C12
32	d	411	STE	C6-C7-C8-C9
33	a	619	LMG	C40-C41-C42-C43
33	m	101	LMG	C16-C17-C18-C19
26	A	608	BCR	C12-C13-C14-C15
26	B	616	BCR	C20-C21-C22-C23
26	B	618	BCR	C11-C10-C9-C8
26	B	618	BCR	C12-C13-C14-C15
26	C	514	BCR	C20-C21-C22-C23
26	K	101	BCR	C11-C10-C9-C8
26	K	101	BCR	C16-C17-C18-C19
26	T	101	BCR	C12-C13-C14-C15
26	X	101	BCR	C11-C10-C9-C8
26	b	618	BCR	C12-C13-C14-C15
26	h	101	BCR	C11-C10-C9-C8
26	k	102	BCR	C20-C21-C22-C23
29	a	615	SQD	C2-C1-O6-C44
31	C	517	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
33	M	101	LMG	C2-C1-O1-C7
31	c	518	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
32	B	624	STE	C14-C15-C16-C17
32	d	409	STE	C5-C6-C7-C8
24	A	612	CLA	C16-C17-C18-C20
24	B	607	CLA	C16-C17-C18-C20
24	b	616	CLA	C11-C12-C13-C14
29	a	615	SQD	C30-C31-C32-C33
31	C	518	DGD	C5A-C6A-C7A-C8A
31	h	102	DGD	CBB-CCB-CDB-CEB
32	B	625	STE	C11-C10-C9-C8
33	D	407	LMG	C30-C31-C32-C33
33	D	412	LMG	C29-C30-C31-C32
28	a	612	PL9	C33-C34-C36-C37
24	B	603	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C12-C13-C14
24	c	506	CLA	C11-C10-C8-C9
24	c	510	CLA	C11-C12-C13-C14
30	L	101	LHG	C12-C13-C14-C15
30	d	407	LHG	C25-C26-C27-C28
31	A	616	DGD	C4B-C5B-C6B-C7B
31	C	517	DGD	C6A-C7A-C8A-C9A
31	H	102	DGD	C6B-C7B-C8B-C9B
32	B	619	STE	C6-C7-C8-C9
32	B	621	STE	C5-C6-C7-C8
32	Z	101	STE	C11-C12-C13-C14
32	a	617	STE	C5-C6-C7-C8
33	Y	101	LMG	C18-C19-C20-C21
33	c	522	LMG	C14-C15-C16-C17
24	D	404	CLA	C5-C6-C7-C8
24	c	502	CLA	C15-C16-C17-C18
30	D	409	LHG	C18-C19-C20-C21
30	D	410	LHG	C27-C28-C29-C30
30	L	101	LHG	C18-C19-C20-C21
30	d	406	LHG	C11-C10-C9-C8
31	c	516	DGD	CBA-CCA-CDA-CEA
31	h	102	DGD	C7A-C8A-C9A-CAA
32	b	625	STE	C3-C4-C5-C6
32	t	102	STE	C6-C7-C8-C9
30	D	409	LHG	O1-C1-C2-C3
30	D	410	LHG	O1-C1-C2-C3
30	d	407	LHG	O1-C1-C2-C3
26	A	608	BCR	C11-C12-C13-C14
24	c	507	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	a	619	LMG	C11-C10-O7-C8
30	D	410	LHG	C14-C15-C16-C17
31	H	102	DGD	CCB-CDB-CEB-CFB
31	c	516	DGD	C4A-C5A-C6A-C7A
32	B	624	STE	C5-C6-C7-C8
32	B	624	STE	C9-C10-C11-C12
32	b	624	STE	C14-C15-C16-C17
32	d	410	STE	C11-C12-C13-C14
29	A	613	SQD	C12-C13-C14-C15
29	A	615	SQD	C11-C10-C9-C8
29	b	620	SQD	C27-C28-C29-C30
30	A	614	LHG	C14-C15-C16-C17
30	D	413	LHG	C29-C30-C31-C32
30	e	101	LHG	C11-C10-C9-C8
30	e	101	LHG	C27-C28-C29-C30
30	l	101	LHG	C27-C28-C29-C30
31	C	517	DGD	CBA-CCA-CDA-CEA
31	H	102	DGD	C5A-C6A-C7A-C8A
31	c	516	DGD	C4B-C5B-C6B-C7B
31	c	518	DGD	CCA-CDA-CEA-CFA
32	B	619	STE	C2-C3-C4-C5
32	B	621	STE	C4-C5-C6-C7
32	B	624	STE	C7-C8-C9-C10
32	C	519	STE	C2-C3-C4-C5
32	I	101	STE	C11-C10-C9-C8
32	T	103	STE	C11-C12-C13-C14
32	X	102	STE	C4-C5-C6-C7
32	Z	101	STE	C13-C14-C15-C16
33	D	412	LMG	C32-C33-C34-C35
33	M	101	LMG	C32-C33-C34-C35
33	M	101	LMG	C33-C34-C35-C36
33	Y	101	LMG	C11-C12-C13-C14
33	Y	101	LMG	C35-C36-C37-C38
33	m	101	LMG	C31-C32-C33-C34
33	m	101	LMG	C34-C35-C36-C37
24	B	601	CLA	C16-C17-C18-C19
24	B	601	CLA	C16-C17-C18-C20
24	a	604	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C20
31	c	517	DGD	O6E-C1E-O5D-C6D
33	M	101	LMG	O6-C1-O1-C7
24	C	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	615	CLA	C15-C16-C17-C18
29	a	616	SQD	C11-C10-C9-C8
30	d	407	LHG	C26-C27-C28-C29
31	c	517	DGD	CCA-CDA-CEA-CFA
31	h	102	DGD	C7B-C8B-C9B-CAB
32	T	103	STE	C14-C15-C16-C17
32	X	102	STE	C6-C7-C8-C9
32	h	103	STE	C11-C12-C13-C14
33	D	407	LMG	C15-C16-C17-C18
29	A	613	SQD	C11-C10-C9-C8
29	B	620	SQD	C9-C10-C11-C12
29	a	616	SQD	C12-C13-C14-C15
30	A	614	LHG	C18-C19-C20-C21
30	D	410	LHG	C33-C34-C35-C36
30	d	406	LHG	C29-C30-C31-C32
32	B	626	STE	C2-C3-C4-C5
32	I	101	STE	C10-C11-C12-C13
32	X	102	STE	C11-C12-C13-C14
32	b	623	STE	C3-C4-C5-C6
33	D	407	LMG	C21-C22-C23-C24
33	c	521	LMG	C15-C16-C17-C18
24	a	607	CLA	C5-C6-C7-C8
24	c	512	CLA	O1A-CGA-O2A-C1
31	C	517	DGD	CCB-CDB-CEB-CFB
32	M	104	STE	C7-C8-C9-C10
32	c	520	STE	C9-C10-C11-C12
24	a	607	CLA	CBA-CGA-O2A-C1
31	c	516	DGD	O6D-C5D-C6D-O5D
29	D	408	SQD	C32-C33-C34-C35
32	a	617	STE	C4-C5-C6-C7
32	c	520	STE	C7-C8-C9-C10
32	d	409	STE	C9-C10-C11-C12
24	b	601	CLA	C3A-C2A-CAA-CBA
25	d	401	PHO	C3A-C2A-CAA-CBA
24	b	608	CLA	C13-C15-C16-C17
24	d	403	CLA	C8-C10-C11-C12
29	b	620	SQD	C25-C26-C27-C28
29	f	102	SQD	C29-C30-C31-C32
30	D	410	LHG	C29-C30-C31-C32
30	L	101	LHG	C33-C34-C35-C36
31	C	516	DGD	C9A-CAA-CBA-CCA
31	c	518	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
31	c	518	DGD	C3B-C4B-C5B-C6B
32	X	102	STE	C13-C14-C15-C16
33	D	407	LMG	C12-C13-C14-C15
33	b	622	LMG	C31-C32-C33-C34
33	c	522	LMG	C33-C34-C35-C36
24	A	605	CLA	C16-C17-C18-C20
24	B	609	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
30	D	410	LHG	C9-C10-C11-C12
31	H	102	DGD	CCA-CDA-CEA-CFA
30	e	101	LHG	C4-C5-C6-O8
30	D	409	LHG	C15-C16-C17-C18
30	D	413	LHG	C14-C15-C16-C17
30	a	614	LHG	C15-C16-C17-C18
31	C	518	DGD	CBA-CCA-CDA-CEA
32	T	103	STE	C10-C11-C12-C13
33	D	407	LMG	C36-C37-C38-C39
33	c	519	LMG	C30-C31-C32-C33
33	c	521	LMG	C34-C35-C36-C37
24	b	608	CLA	O2A-C1-C2-C3
33	D	407	LMG	O6-C5-C6-O5
31	A	616	DGD	C1B-C2B-C3B-C4B
31	C	516	DGD	C1B-C2B-C3B-C4B
29	A	615	SQD	C16-C17-C18-C19
29	a	615	SQD	C24-C25-C26-C27
32	T	102	STE	C7-C8-C9-C10
24	C	511	CLA	O1A-CGA-O2A-C1
28	D	406	PL9	C28-C29-C31-C32
31	c	516	DGD	C4D-C5D-C6D-O5D
33	c	522	LMG	C11-C10-O7-C8
29	D	408	SQD	C31-C32-C33-C34
29	b	620	SQD	C9-C10-C11-C12
30	a	614	LHG	C32-C33-C34-C35
30	A	614	LHG	O1-C1-C2-O2
30	D	410	LHG	O1-C1-C2-O2
29	f	102	SQD	C26-C27-C28-C29
30	d	406	LHG	C15-C16-C17-C18
31	H	102	DGD	C7B-C8B-C9B-CAB
32	B	623	STE	C13-C14-C15-C16
32	b	621	STE	C11-C10-C9-C8
32	c	523	STE	C6-C7-C8-C9
32	d	411	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	D	412	LMG	C33-C34-C35-C36
24	b	604	CLA	C16-C17-C18-C19
32	b	621	STE	C3-C4-C5-C6
30	L	101	LHG	C13-C14-C15-C16
30	l	101	LHG	C16-C17-C18-C19
29	D	408	SQD	C30-C31-C32-C33
30	D	413	LHG	C25-C26-C27-C28
32	M	102	STE	C9-C10-C11-C12
32	b	624	STE	C10-C11-C12-C13
33	a	619	LMG	C23-C24-C25-C26
29	B	620	SQD	C11-C12-C13-C14
31	A	616	DGD	C5B-C6B-C7B-C8B
31	C	516	DGD	CBA-CCA-CDA-CEA
32	C	520	STE	C7-C8-C9-C10
32	d	409	STE	C10-C11-C12-C13
32	d	410	STE	C3-C4-C5-C6
33	Y	101	LMG	O9-C10-O7-C8
31	A	616	DGD	C5A-C6A-C7A-C8A
32	B	619	STE	C9-C10-C11-C12
32	B	625	STE	C4-C5-C6-C7
33	m	101	LMG	C18-C19-C20-C21
24	B	613	CLA	C8-C10-C11-C12
24	c	506	CLA	C13-C15-C16-C17
29	B	620	SQD	C11-C10-C9-C8
29	B	620	SQD	C33-C34-C35-C36
30	d	406	LHG	C33-C34-C35-C36
32	b	624	STE	C12-C13-C14-C15
32	d	411	STE	C13-C14-C15-C16
33	Y	101	LMG	C33-C34-C35-C36
26	B	616	BCR	C5-C6-C7-C8
26	C	514	BCR	C23-C24-C25-C26
26	C	514	BCR	C23-C24-C25-C30
26	K	102	BCR	C1-C6-C7-C8
26	K	103	BCR	C5-C6-C7-C8
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	c	514	BCR	C5-C6-C7-C8
26	k	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C23-C24-C25-C26
26	k	101	BCR	C23-C24-C25-C30
30	L	101	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
32	d	410	STE	C9-C10-C11-C12
24	C	506	CLA	CBA-CGA-O2A-C1
24	H	101	CLA	CBA-CGA-O2A-C1
24	B	609	CLA	C8-C10-C11-C12
24	C	506	CLA	C15-C16-C17-C18
24	C	513	CLA	C10-C11-C12-C13
24	a	607	CLA	C10-C11-C12-C13
24	c	513	CLA	C10-C11-C12-C13
29	b	620	SQD	C10-C11-C12-C13
32	B	625	STE	C10-C11-C12-C13
33	M	101	LMG	C13-C14-C15-C16
33	a	619	LMG	C41-C42-C43-C44
30	e	101	LHG	C7-C8-C9-C10
31	c	517	DGD	CAB-CBB-CCB-CDB
28	A	611	PL9	C47-C48-C49-C50
24	b	603	CLA	C13-C15-C16-C17
33	c	519	LMG	O6-C5-C6-O5
29	a	615	SQD	C14-C15-C16-C17
30	d	406	LHG	C13-C14-C15-C16
32	B	622	STE	C5-C6-C7-C8
33	a	619	LMG	C30-C31-C32-C33
24	C	505	CLA	C4-C3-C5-C6
28	D	406	PL9	C30-C29-C31-C32
24	B	603	CLA	C11-C10-C8-C7
24	C	505	CLA	C2-C3-C5-C6
24	C	506	CLA	C2-C3-C5-C6
24	a	607	CLA	C11-C10-C8-C7
24	b	605	CLA	C11-C12-C13-C15
24	b	607	CLA	C11-C10-C8-C7
24	b	610	CLA	C12-C13-C15-C16
24	c	505	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	511	CLA	C6-C7-C8-C10
28	a	612	PL9	C38-C39-C41-C42
24	C	506	CLA	O1A-CGA-O2A-C1
24	a	607	CLA	O1A-CGA-O2A-C1
33	M	101	LMG	C39-C40-C41-C42
33	a	619	LMG	C39-C40-C41-C42
24	B	605	CLA	C10-C11-C12-C13
24	c	510	CLA	C16-C17-C18-C19
24	b	612	CLA	C10-C11-C12-C13
29	a	615	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
33	D	412	LMG	C31-C32-C33-C34
24	H	101	CLA	O1D-CGD-O2D-CED
32	d	410	STE	C6-C7-C8-C9
32	d	411	STE	C7-C8-C9-C10
33	M	101	LMG	C19-C20-C21-C22
33	a	619	LMG	C10-C11-C12-C13
24	C	511	CLA	C8-C10-C11-C12
24	C	504	CLA	C11-C12-C13-C14
29	B	620	SQD	C35-C36-C37-C38
31	C	516	DGD	C4B-C5B-C6B-C7B
33	a	619	LMG	C38-C39-C40-C41
33	b	622	LMG	C32-C33-C34-C35
33	c	522	LMG	C17-C18-C19-C20
30	e	101	LHG	C16-C17-C18-C19
32	j	101	STE	C4-C5-C6-C7
26	B	617	BCR	C22-C23-C24-C25
26	d	404	BCR	C22-C23-C24-C25
24	B	605	CLA	C16-C17-C18-C19
31	c	516	DGD	O6E-C1E-O5D-C6D
24	B	609	CLA	C15-C16-C17-C18
29	D	408	SQD	C25-C26-C27-C28
30	D	410	LHG	C25-C26-C27-C28
31	C	516	DGD	CAB-CBB-CCB-CDB
32	C	520	STE	C12-C13-C14-C15
32	b	621	STE	C11-C12-C13-C14
33	d	408	LMG	C37-C38-C39-C40
29	A	615	SQD	C7-C8-C9-C10
33	m	101	LMG	C11-C10-O7-C8
26	K	101	BCR	C18-C19-C20-C21
30	l	101	LHG	C32-C33-C34-C35
31	c	518	DGD	C4B-C5B-C6B-C7B
24	b	602	CLA	C8-C10-C11-C12
31	A	616	DGD	C4A-C5A-C6A-C7A
31	C	517	DGD	C9A-CAA-CBA-CCA
31	H	102	DGD	C4B-C5B-C6B-C7B
33	c	522	LMG	C12-C13-C14-C15
33	c	522	LMG	O9-C10-O7-C8
32	d	409	STE	C11-C10-C9-C8
29	A	613	SQD	O6-C44-C45-O47
29	a	615	SQD	O6-C44-C45-O47
31	A	616	DGD	O2G-C2G-C3G-O3G
33	c	521	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
33	b	622	LMG	O6-C5-C6-O5
33	d	408	LMG	O6-C5-C6-O5
24	c	501	CLA	CBA-CGA-O2A-C1
29	a	615	SQD	C15-C16-C17-C18
33	D	407	LMG	C33-C34-C35-C36
24	B	611	CLA	C16-C17-C18-C20
24	b	616	CLA	C11-C12-C13-C15
30	A	614	LHG	C34-C35-C36-C37
24	c	506	CLA	C4-C3-C5-C6
29	a	615	SQD	C23-C24-C25-C26
24	C	504	CLA	C2-C3-C5-C6
28	D	406	PL9	C4-C3-C7-C8
28	a	612	PL9	C4-C3-C7-C8
24	B	601	CLA	C11-C12-C13-C14
24	B	612	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	508	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C14
24	b	605	CLA	C11-C12-C13-C14
24	c	505	CLA	C11-C10-C8-C9
24	c	506	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	c	511	CLA	C6-C7-C8-C9
30	e	101	LHG	C12-C13-C14-C15
24	c	501	CLA	C2A-CAA-CBA-CGA
24	c	512	CLA	C2A-CAA-CBA-CGA
32	d	411	STE	C12-C13-C14-C15
26	T	101	BCR	C11-C12-C13-C35
31	H	102	DGD	CAB-CBB-CCB-CDB
32	B	619	STE	C11-C10-C9-C8
26	k	101	BCR	C7-C8-C9-C10
24	H	101	CLA	O1A-CGA-O2A-C1
24	B	603	CLA	C1A-C2A-CAA-CBA
24	C	503	CLA	C1A-C2A-CAA-CBA
24	a	605	CLA	C1A-C2A-CAA-CBA
24	a	613	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	c	513	CLA	C1A-C2A-CAA-CBA
24	A	605	CLA	C16-C17-C18-C19
24	B	605	CLA	C16-C17-C18-C20
29	a	615	SQD	C32-C33-C34-C35
29	f	102	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	c	517	DGD	C4B-C5B-C6B-C7B
32	B	623	STE	C14-C15-C16-C17
32	a	617	STE	C2-C3-C4-C5
33	M	101	LMG	C14-C15-C16-C17
26	k	102	BCR	C9-C10-C11-C12
24	b	601	CLA	C10-C11-C12-C13
25	d	401	PHO	C8-C10-C11-C12
30	D	409	LHG	C3-O3-P-O6
30	D	409	LHG	C4-O6-P-O3
30	d	407	LHG	C31-C32-C33-C34
32	I	101	STE	C2-C3-C4-C5
32	T	102	STE	C12-C13-C14-C15
33	c	522	LMG	C37-C38-C39-C40
24	d	402	CLA	C3-C5-C6-C7
29	A	615	SQD	C15-C16-C17-C18
33	C	515	LMG	C16-C17-C18-C19
24	c	504	CLA	C8-C10-C11-C12
24	c	507	CLA	C5-C6-C7-C8
29	a	615	SQD	C17-C18-C19-C20
32	C	521	STE	C6-C7-C8-C9
29	A	613	SQD	C14-C15-C16-C17
32	M	104	STE	C13-C14-C15-C16
32	b	624	STE	C2-C3-C4-C5
24	B	609	CLA	C16-C17-C18-C19
24	c	510	CLA	C16-C17-C18-C20
29	a	616	SQD	C17-C18-C19-C20
30	l	101	LHG	C29-C30-C31-C32
32	d	411	STE	C4-C5-C6-C7
33	a	619	LMG	C32-C33-C34-C35
29	f	102	SQD	C27-C28-C29-C30
30	D	409	LHG	C12-C13-C14-C15
30	D	409	LHG	C25-C26-C27-C28
31	C	517	DGD	C3A-C4A-C5A-C6A
32	B	623	STE	C6-C7-C8-C9
30	D	409	LHG	C1-C2-C3-O3
24	b	614	CLA	C4-C3-C5-C6
28	d	405	PL9	C43-C44-C46-C47
32	b	624	STE	C11-C12-C13-C14
33	a	619	LMG	C35-C36-C37-C38
30	D	410	LHG	C32-C33-C34-C35
33	C	515	LMG	C11-C12-C13-C14
33	D	407	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	C29-C30-C31-C32
30	D	410	LHG	C17-C18-C19-C20
31	A	616	DGD	C1G-C2G-C3G-O3G
31	C	516	DGD	O1G-C1G-C2G-C3G
33	Y	101	LMG	O1-C7-C8-C9
33	c	521	LMG	O1-C7-C8-C9
33	c	522	LMG	O1-C7-C8-C9
33	m	101	LMG	C32-C33-C34-C35
30	L	101	LHG	C10-C11-C12-C13
30	d	406	LHG	C35-C36-C37-C38
32	M	103	STE	C3-C4-C5-C6
31	C	517	DGD	C2G-C3G-O3G-C1D
31	C	517	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C2G-C3G-O3G-C1D
31	c	517	DGD	C5D-C6D-O5D-C1E
33	a	619	LMG	C8-C7-O1-C1
29	A	613	SQD	C17-C18-C19-C20
30	L	101	LHG	C19-C20-C21-C22
32	T	102	STE	C13-C14-C15-C16
24	H	101	CLA	C8-C10-C11-C12
33	m	101	LMG	C4-C5-C6-O5
32	L	102	STE	C7-C8-C9-C10
31	c	516	DGD	O6E-C5E-C6E-O5E
29	D	408	SQD	C28-C29-C30-C31
31	c	518	DGD	CDA-CEA-CFA-CGA
32	a	618	STE	C4-C5-C6-C7
32	d	410	STE	C2-C3-C4-C5
24	c	507	CLA	C16-C17-C18-C20
30	D	410	LHG	C35-C36-C37-C38
31	c	517	DGD	C9A-CAA-CBA-CCA
31	c	518	DGD	C5B-C6B-C7B-C8B
24	C	513	CLA	CBD-CGD-O2D-CED
30	a	614	LHG	O1-C1-C2-O2
30	D	410	LHG	C12-C13-C14-C15
32	R	101	STE	C7-C8-C9-C10
33	c	521	LMG	C42-C43-C44-C45
33	c	522	LMG	C29-C30-C31-C32
30	l	101	LHG	C7-C8-C9-C10
29	a	616	SQD	C18-C19-C20-C21
29	a	616	SQD	C19-C20-C21-C22
32	C	519	STE	C7-C8-C9-C10
33	D	407	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C11-C10-C9-C34
26	b	617	BCR	C35-C13-C14-C15
26	b	619	BCR	C20-C21-C22-C37
26	h	101	BCR	C35-C13-C14-C15
26	k	101	BCR	C20-C21-C22-C37
24	c	505	CLA	C4-C3-C5-C6
28	d	405	PL9	C30-C29-C31-C32
30	d	407	LHG	C35-C36-C37-C38
32	h	103	STE	C5-C6-C7-C8
33	b	622	LMG	C18-C19-C20-C21
24	c	503	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C19
33	m	101	LMG	C29-C28-O8-C9
30	A	614	LHG	C17-C18-C19-C20
33	a	619	LMG	C15-C16-C17-C18
24	C	512	CLA	C13-C15-C16-C17
32	b	621	STE	C2-C3-C4-C5
29	B	620	SQD	C46-C45-O47-C7
33	D	411	LMG	C9-C8-O7-C10
24	C	505	CLA	C5-C6-C7-C8
24	b	616	CLA	C2-C1-O2A-CGA
24	c	506	CLA	C2-C1-O2A-CGA
30	L	101	LHG	C11-C12-C13-C14
33	M	101	LMG	C36-C37-C38-C39
24	b	607	CLA	O1D-CGD-O2D-CED
29	A	613	SQD	C25-C26-C27-C28
29	b	620	SQD	C28-C29-C30-C31
30	l	101	LHG	C19-C20-C21-C22
32	C	520	STE	C11-C10-C9-C8
32	T	103	STE	C12-C13-C14-C15
32	B	623	STE	C1-C2-C3-C4
32	T	102	STE	C9-C10-C11-C12
33	Y	101	LMG	C40-C41-C42-C43
31	C	516	DGD	O1G-C1A-C2A-C3A
24	B	614	CLA	C16-C17-C18-C20
31	C	518	DGD	C3B-C4B-C5B-C6B
33	b	622	LMG	C19-C20-C21-C22
31	C	518	DGD	O1A-C1A-O1G-C1G
33	d	408	LMG	C10-C11-C12-C13
24	b	604	CLA	C15-C16-C17-C18
26	b	617	BCR	C12-C13-C14-C15
26	k	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
29	a	616	SQD	C31-C32-C33-C34
30	D	413	LHG	C19-C20-C21-C22
33	a	619	LMG	C36-C37-C38-C39
33	a	619	LMG	C42-C43-C44-C45
33	M	101	LMG	O1-C7-C8-O7
33	c	521	LMG	O7-C8-C9-O8
31	A	616	DGD	CDB-CEB-CFB-CGB
32	M	103	STE	C1-C2-C3-C4
29	A	615	SQD	O49-C7-O47-C45
31	c	516	DGD	O1B-C1B-O2G-C2G
24	A	612	CLA	C13-C15-C16-C17
24	c	501	CLA	O1A-CGA-O2A-C1
31	C	517	DGD	CDA-CEA-CFA-CGA
28	d	405	PL9	C22-C23-C24-C25
30	D	409	LHG	C11-C10-C9-C8
24	A	604	CLA	C12-C13-C15-C16
24	A	605	CLA	C12-C13-C15-C16
24	B	602	CLA	C6-C7-C8-C10
24	B	612	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	a	607	CLA	C12-C13-C15-C16
24	b	601	CLA	C11-C12-C13-C15
24	b	608	CLA	C11-C12-C13-C15
24	b	609	CLA	C12-C13-C15-C16
24	b	612	CLA	C12-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C10
24	b	615	CLA	C11-C12-C13-C15
24	c	506	CLA	C6-C7-C8-C10
24	c	510	CLA	C6-C7-C8-C10
24	c	512	CLA	C6-C7-C8-C10
29	f	102	SQD	C25-C26-C27-C28
32	M	104	STE	C10-C11-C12-C13
24	B	601	CLA	C14-C13-C15-C16
24	B	602	CLA	C6-C7-C8-C9
24	B	611	CLA	C11-C10-C8-C9
24	C	506	CLA	C14-C13-C15-C16
24	a	607	CLA	C14-C13-C15-C16
24	b	605	CLA	C11-C10-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	b	608	CLA	C11-C12-C13-C14
24	b	609	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	609	CLA	C14-C13-C15-C16
24	b	612	CLA	C14-C13-C15-C16
24	c	507	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	d	402	CLA	C6-C7-C8-C9
26	c	514	BCR	C14-C15-C16-C17
31	c	516	DGD	C9B-CAB-CBB-CCB
32	I	101	STE	C1-C2-C3-C4
32	d	411	STE	C5-C6-C7-C8
32	h	103	STE	C10-C11-C12-C13
33	c	521	LMG	C11-C12-C13-C14
24	c	503	CLA	C5-C6-C7-C8
29	a	615	SQD	C34-C35-C36-C37
32	b	621	STE	C6-C7-C8-C9
33	a	619	LMG	C37-C38-C39-C40
33	c	521	LMG	C30-C31-C32-C33
30	D	413	LHG	O10-C23-O8-C6
31	A	616	DGD	CBB-CCB-CDB-CEB
30	a	614	LHG	C18-C19-C20-C21
32	M	104	STE	C15-C16-C17-C18
24	C	507	CLA	C13-C15-C16-C17
31	C	516	DGD	C5B-C6B-C7B-C8B
31	H	102	DGD	C9A-CAA-CBA-CCA
32	L	102	STE	C2-C3-C4-C5
33	D	412	LMG	C17-C18-C19-C20
24	B	603	CLA	C10-C11-C12-C13
24	B	604	CLA	C8-C10-C11-C12
29	A	615	SQD	C32-C33-C34-C35
30	d	406	LHG	C16-C17-C18-C19
31	A	616	DGD	C2A-C3A-C4A-C5A
29	D	408	SQD	C29-C30-C31-C32
31	A	616	DGD	C7B-C8B-C9B-CAB
32	B	622	STE	C13-C14-C15-C16
24	B	604	CLA	C16-C17-C18-C20
31	C	517	DGD	O6D-C1D-O3G-C3G
32	b	623	STE	C9-C10-C11-C12
33	D	411	LMG	C14-C15-C16-C17
33	Y	101	LMG	C12-C13-C14-C15
33	c	522	LMG	C19-C20-C21-C22
30	L	101	LHG	C23-C24-C25-C26
29	a	615	SQD	C11-C12-C13-C14
31	h	102	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
32	X	102	STE	C7-C8-C9-C10
24	B	602	CLA	C5-C6-C7-C8
24	B	606	CLA	C13-C15-C16-C17
29	b	620	SQD	C13-C14-C15-C16
31	A	616	DGD	CBA-CCA-CDA-CEA
33	b	622	LMG	C38-C39-C40-C41
33	m	101	LMG	C17-C18-C19-C20
24	B	613	CLA	C4-C3-C5-C6
33	Y	101	LMG	C10-C11-C12-C13
30	L	101	LHG	O10-C23-O8-C6
32	a	618	STE	C2-C3-C4-C5
33	c	519	LMG	C39-C40-C41-C42
33	m	101	LMG	C22-C23-C24-C25
24	D	404	CLA	C10-C11-C12-C13
33	M	101	LMG	C28-C29-C30-C31
30	d	406	LHG	C31-C32-C33-C34
32	B	624	STE	C3-C4-C5-C6
32	d	411	STE	C15-C16-C17-C18
32	h	103	STE	C6-C7-C8-C9
33	a	619	LMG	C17-C18-C19-C20
24	a	605	CLA	C3A-C2A-CAA-CBA
24	a	604	CLA	C15-C16-C17-C18
31	c	517	DGD	C6B-C7B-C8B-C9B
29	f	102	SQD	C33-C34-C35-C36
30	A	614	LHG	C35-C36-C37-C38
31	c	518	DGD	C6B-C7B-C8B-C9B
32	B	619	STE	C12-C13-C14-C15
33	C	515	LMG	C31-C32-C33-C34
31	A	616	DGD	CCB-CDB-CEB-CFB
32	R	101	STE	C3-C4-C5-C6
33	c	521	LMG	C12-C13-C14-C15
24	c	507	CLA	C16-C17-C18-C19
24	c	507	CLA	CBA-CGA-O2A-C1
33	m	101	LMG	C33-C34-C35-C36
24	c	513	CLA	C5-C6-C7-C8
29	A	613	SQD	O6-C44-C45-C46
29	B	620	SQD	O6-C44-C45-C46
29	a	615	SQD	O6-C44-C45-C46
29	a	616	SQD	C44-C45-C46-O48
30	A	614	LHG	C4-C5-C6-O8
30	d	407	LHG	C4-C5-C6-O8
33	M	101	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	M	101	LMG	C7-C8-C9-O8
33	b	622	LMG	O1-C7-C8-C9
33	c	521	LMG	C33-C34-C35-C36
30	d	406	LHG	C17-C18-C19-C20
32	B	625	STE	C13-C14-C15-C16
33	c	521	LMG	C31-C32-C33-C34
33	M	101	LMG	C15-C16-C17-C18
24	C	511	CLA	C3-C5-C6-C7
29	b	620	SQD	C7-C8-C9-C10
29	A	615	SQD	C28-C29-C30-C31
24	c	503	CLA	C16-C17-C18-C19
24	b	614	CLA	C2-C3-C5-C6
29	a	615	SQD	C19-C20-C21-C22
32	B	622	STE	C2-C3-C4-C5
32	c	523	STE	C2-C3-C4-C5
33	b	622	LMG	C41-C42-C43-C44
30	l	101	LHG	C34-C35-C36-C37
31	c	517	DGD	CDA-CEA-CFA-CGA
33	D	412	LMG	C35-C36-C37-C38
32	M	104	STE	C6-C7-C8-C9
30	d	407	LHG	O1-C1-C2-O2
24	b	604	CLA	C10-C11-C12-C13
32	B	625	STE	C3-C4-C5-C6
30	e	101	LHG	O6-C4-C5-O7
30	D	413	LHG	C27-C28-C29-C30
24	A	612	CLA	C16-C17-C18-C19
24	B	606	CLA	C16-C17-C18-C19
24	B	614	CLA	C16-C17-C18-C19
24	b	602	CLA	C16-C17-C18-C19
33	C	515	LMG	C39-C40-C41-C42
32	B	621	STE	C7-C8-C9-C10
33	Y	101	LMG	O10-C28-O8-C9
30	a	614	LHG	C25-C26-C27-C28
32	B	625	STE	C2-C3-C4-C5
29	A	615	SQD	O47-C45-C46-O48
31	c	516	DGD	C2E-C1E-O5D-C6D
29	B	620	SQD	C24-C25-C26-C27
31	C	516	DGD	C6A-C7A-C8A-C9A
32	B	625	STE	C6-C7-C8-C9
32	M	102	STE	C3-C4-C5-C6
29	a	616	SQD	O47-C45-C46-O48
29	a	615	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	D	412	LMG	C37-C38-C39-C40
24	B	607	CLA	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C19
24	c	504	CLA	C11-C12-C13-C15
33	c	522	LMG	C11-C12-C13-C14
32	C	520	STE	C3-C4-C5-C6
32	d	410	STE	C12-C13-C14-C15
24	d	402	CLA	C2-C1-O2A-CGA
28	d	405	PL9	C28-C29-C31-C32
32	a	618	STE	C3-C4-C5-C6
24	C	508	CLA	C11-C10-C8-C9
24	C	509	CLA	C14-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C9
24	H	101	CLA	C6-C7-C8-C9
24	a	607	CLA	C11-C10-C8-C9
24	b	601	CLA	C11-C12-C13-C14
24	b	604	CLA	C14-C13-C15-C16
24	c	502	CLA	C14-C13-C15-C16
25	D	401	PHO	C14-C13-C15-C16
29	b	620	SQD	C30-C31-C32-C33
33	a	619	LMG	C16-C17-C18-C19
30	a	614	LHG	C29-C30-C31-C32
31	h	102	DGD	C8B-C9B-CAB-CBB
32	b	623	STE	C11-C10-C9-C8
24	B	614	CLA	C10-C11-C12-C13
24	D	403	CLA	C10-C11-C12-C13
29	f	102	SQD	C32-C33-C34-C35
30	d	407	LHG	C29-C30-C31-C32
32	M	102	STE	C4-C5-C6-C7
32	b	624	STE	C6-C7-C8-C9
24	B	610	CLA	C16-C17-C18-C20
26	B	617	BCR	C23-C24-C25-C26
26	B	617	BCR	C23-C24-C25-C30
26	d	404	BCR	C23-C24-C25-C26
26	d	404	BCR	C23-C24-C25-C30
26	h	101	BCR	C23-C24-C25-C26
24	b	610	CLA	C8-C10-C11-C12
32	b	625	STE	C1-C2-C3-C4
33	b	622	LMG	C39-C40-C41-C42
33	d	408	LMG	C32-C33-C34-C35
26	K	103	BCR	C17-C18-C19-C20
26	T	101	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	k	101	BCR	C21-C22-C23-C24
24	b	616	CLA	C5-C6-C7-C8
30	e	101	LHG	C8-C7-O7-C5
33	Y	101	LMG	C37-C38-C39-C40
33	c	519	LMG	C35-C36-C37-C38
24	B	606	CLA	C16-C17-C18-C20
31	C	517	DGD	C8B-C9B-CAB-CBB
31	h	102	DGD	C9B-CAB-CBB-CCB
24	C	513	CLA	O1D-CGD-O2D-CED
30	A	614	LHG	O6-C4-C5-C6
30	d	406	LHG	O6-C4-C5-C6
30	e	101	LHG	O6-C4-C5-C6
30	a	614	LHG	C9-C10-C11-C12
31	C	518	DGD	C4B-C5B-C6B-C7B
32	B	624	STE	C10-C11-C12-C13
33	d	408	LMG	C14-C15-C16-C17
24	B	601	CLA	C12-C13-C15-C16
24	B	602	CLA	C12-C13-C15-C16
24	B	604	CLA	C11-C10-C8-C7
24	B	606	CLA	C12-C13-C15-C16
24	B	611	CLA	C11-C10-C8-C7
24	B	612	CLA	C12-C13-C15-C16
24	C	503	CLA	C11-C10-C8-C7
24	C	504	CLA	C11-C10-C8-C7
24	C	506	CLA	C12-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C7
24	C	509	CLA	C11-C10-C8-C7
24	C	509	CLA	C12-C13-C15-C16
24	C	510	CLA	C11-C10-C8-C7
24	C	511	CLA	C6-C7-C8-C10
24	D	403	CLA	C6-C7-C8-C10
24	D	403	CLA	C12-C13-C15-C16
24	D	404	CLA	C12-C13-C15-C16
24	H	101	CLA	C2-C3-C5-C6
24	a	605	CLA	C6-C7-C8-C10
24	b	607	CLA	C6-C7-C8-C10
24	b	607	CLA	C11-C12-C13-C15
24	b	616	CLA	C11-C10-C8-C7
24	c	505	CLA	C2-C3-C5-C6
24	c	505	CLA	C6-C7-C8-C10
24	c	507	CLA	C6-C7-C8-C10
24	c	508	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	C6-C7-C8-C10
24	d	402	CLA	C6-C7-C8-C10
31	A	616	DGD	CEA-CFA-CGA-CHA
33	a	619	LMG	C22-C23-C24-C25
32	b	625	STE	C7-C8-C9-C10
33	m	101	LMG	C35-C36-C37-C38
24	C	507	CLA	C10-C11-C12-C13
25	d	401	PHO	C5-C6-C7-C8
29	a	616	SQD	C15-C16-C17-C18
29	b	620	SQD	C16-C17-C18-C19
33	c	521	LMG	C16-C17-C18-C19
24	A	604	CLA	C4C-C3C-CAC-CBC
26	a	608	BCR	C35-C13-C14-C15
31	c	517	DGD	CCB-CDB-CEB-CFB
32	b	623	STE	C5-C6-C7-C8
24	B	604	CLA	C16-C17-C18-C19
24	B	611	CLA	CBA-CGA-O2A-C1
31	A	616	DGD	C2A-C1A-O1G-C1G
33	M	101	LMG	C34-C35-C36-C37
31	H	102	DGD	C8B-C9B-CAB-CBB
32	b	624	STE	C13-C14-C15-C16
33	c	521	LMG	C36-C37-C38-C39
24	B	610	CLA	C13-C15-C16-C17
32	M	104	STE	C12-C13-C14-C15
32	X	102	STE	C10-C11-C12-C13
24	C	503	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
24	d	403	CLA	CAD-CBD-CGD-O2D
25	A	606	PHO	CAD-CBD-CGD-O2D
25	a	606	PHO	CAD-CBD-CGD-O2D
33	a	619	LMG	C9-C8-O7-C10
33	c	522	LMG	C9-C8-O7-C10
31	c	516	DGD	CDA-CEA-CFA-CGA
31	c	517	DGD	C7A-C8A-C9A-CAA
33	D	407	LMG	C34-C35-C36-C37
33	c	522	LMG	C39-C40-C41-C42
32	B	619	STE	C4-C5-C6-C7
32	T	103	STE	C13-C14-C15-C16
24	H	101	CLA	C4-C3-C5-C6
28	d	405	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
29	A	615	SQD	C31-C32-C33-C34
30	L	101	LHG	C27-C28-C29-C30
33	m	101	LMG	C15-C16-C17-C18
29	b	620	SQD	O5-C1-O6-C44
24	A	605	CLA	C2C-C3C-CAC-CBC
30	l	101	LHG	C4-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-C3G
31	c	516	DGD	O1A-C1A-O1G-C1G
32	d	411	STE	C2-C3-C4-C5
30	A	614	LHG	O6-C4-C5-O7
24	c	513	CLA	C8-C10-C11-C12
24	d	403	CLA	C15-C16-C17-C18
24	c	511	CLA	CBA-CGA-O2A-C1
24	A	604	CLA	C16-C17-C18-C20
32	b	623	STE	C10-C11-C12-C13
32	c	520	STE	C6-C7-C8-C9
24	B	606	CLA	CHA-CBD-CGD-O1D
24	B	606	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
30	e	101	LHG	C28-C29-C30-C31
24	B	611	CLA	O1A-CGA-O2A-C1
24	c	507	CLA	O1A-CGA-O2A-C1
32	B	626	STE	C5-C6-C7-C8
33	M	101	LMG	C12-C13-C14-C15
26	h	101	BCR	C20-C21-C22-C23
30	A	614	LHG	O7-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-O2G
33	M	101	LMG	O7-C8-C9-O8
33	a	619	LMG	O7-C8-C9-O8
30	a	614	LHG	C31-C32-C33-C34
32	b	621	STE	C5-C6-C7-C8
32	j	101	STE	C7-C8-C9-C10
24	c	511	CLA	C16-C17-C18-C20
30	D	409	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
30	d	406	LHG	O1-C1-C2-O2
29	A	613	SQD	C16-C17-C18-C19
32	B	624	STE	C4-C5-C6-C7
28	d	405	PL9	C35-C34-C36-C37
29	a	615	SQD	O10-C23-O48-C46
30	D	413	LHG	C23-C24-C25-C26
28	A	611	PL9	C4-C3-C7-C8
30	a	614	LHG	C27-C28-C29-C30
33	C	515	LMG	C40-C41-C42-C43
24	B	602	CLA	C14-C13-C15-C16
24	C	510	CLA	C11-C10-C8-C9
24	a	605	CLA	C6-C7-C8-C9
24	b	607	CLA	C14-C13-C15-C16
32	T	102	STE	C6-C7-C8-C9
31	h	102	DGD	CAB-CBB-CCB-CDB
30	D	409	LHG	C13-C14-C15-C16
25	A	606	PHO	C2C-C3C-CAC-CBC
26	B	618	BCR	C37-C22-C23-C24
24	D	404	CLA	C15-C16-C17-C18
31	C	516	DGD	CDA-CEA-CFA-CGA
31	c	518	DGD	C2A-C3A-C4A-C5A
33	c	519	LMG	C37-C38-C39-C40
26	d	404	BCR	C21-C22-C23-C24
32	M	102	STE	C2-C3-C4-C5
32	T	102	STE	C10-C11-C12-C13
32	d	411	STE	C1-C2-C3-C4
24	b	608	CLA	C16-C17-C18-C19
30	e	101	LHG	O9-C7-O7-C5
30	A	614	LHG	C29-C30-C31-C32
29	a	615	SQD	C9-C10-C11-C12
32	B	622	STE	C4-C5-C6-C7
26	A	608	BCR	C9-C10-C11-C12
24	B	611	CLA	C8-C10-C11-C12
30	l	101	LHG	C4-O6-P-O3
29	b	620	SQD	C19-C20-C21-C22
32	C	521	STE	C2-C3-C4-C5
30	D	410	LHG	O2-C2-C3-O3
30	d	407	LHG	C24-C25-C26-C27
24	c	510	CLA	C4-C3-C5-C6
24	B	613	CLA	C2-C3-C5-C6
31	c	516	DGD	C6B-C7B-C8B-C9B
32	j	101	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	H	102	DGD	O1A-C1A-O1G-C1G
30	A	614	LHG	C4-O6-P-O5
30	D	409	LHG	C4-O6-P-O5
30	D	410	LHG	C3-O3-P-O5
30	a	614	LHG	C3-O3-P-O5
30	d	406	LHG	C3-O3-P-O5
24	B	613	CLA	C16-C17-C18-C20
24	b	615	CLA	C16-C17-C18-C20
33	m	101	LMG	C28-C29-C30-C31
33	a	619	LMG	C11-C12-C13-C14
33	a	619	LMG	C21-C22-C23-C24
33	m	101	LMG	C38-C39-C40-C41
24	b	616	CLA	C10-C11-C12-C13
29	A	613	SQD	C9-C10-C11-C12
29	b	620	SQD	C12-C13-C14-C15
32	T	102	STE	C4-C5-C6-C7
33	a	619	LMG	C34-C35-C36-C37
31	H	102	DGD	CDA-CEA-CFA-CGA
32	c	523	STE	C5-C6-C7-C8
29	A	613	SQD	C32-C33-C34-C35
30	d	406	LHG	C9-C10-C11-C12
24	a	607	CLA	C16-C17-C18-C20
30	a	614	LHG	C26-C27-C28-C29
31	H	102	DGD	C9B-CAB-CBB-CCB
31	H	102	DGD	CBB-CCB-CDB-CEB
24	B	606	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	513	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CAA-CBA-CGA-O2A
29	f	102	SQD	C30-C31-C32-C33
30	L	101	LHG	C16-C17-C18-C19
29	B	620	SQD	C23-C24-C25-C26
30	d	407	LHG	C23-C24-C25-C26
31	h	102	DGD	C2A-C3A-C4A-C5A
32	B	619	STE	C7-C8-C9-C10
24	C	509	CLA	C10-C11-C12-C13
32	X	102	STE	C9-C10-C11-C12
24	A	605	CLA	C11-C12-C13-C15
24	B	603	CLA	C12-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	B	610	CLA	C11-C12-C13-C15
24	B	614	CLA	C12-C13-C15-C16
24	C	505	CLA	C6-C7-C8-C10
24	C	505	CLA	C11-C12-C13-C15
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C12-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C10
24	b	601	CLA	C11-C10-C8-C7
24	c	503	CLA	C6-C7-C8-C10
24	c	504	CLA	C11-C10-C8-C7
29	f	102	SQD	C23-C24-C25-C26
30	d	406	LHG	O6-C4-C5-O7
31	C	516	DGD	C1A-C2A-C3A-C4A
33	m	101	LMG	C10-C11-C12-C13
32	B	621	STE	C6-C7-C8-C9
30	d	406	LHG	C26-C27-C28-C29
31	c	516	DGD	CCB-CDB-CEB-CFB
33	d	408	LMG	C33-C34-C35-C36
26	T	101	BCR	C13-C14-C15-C16
29	a	615	SQD	C18-C19-C20-C21
33	c	522	LMG	C13-C14-C15-C16
24	c	509	CLA	C16-C17-C18-C19
29	A	613	SQD	C31-C32-C33-C34
30	A	614	LHG	C24-C25-C26-C27
33	a	619	LMG	O8-C28-C29-C30
31	C	517	DGD	C4A-C5A-C6A-C7A
31	c	516	DGD	C1G-C2G-C3G-O3G
32	b	623	STE	C4-C5-C6-C7
33	c	521	LMG	C7-C8-C9-O8
29	b	620	SQD	O6-C44-C45-O47
29	f	102	SQD	O47-C45-C46-O48
30	e	101	LHG	O7-C5-C6-O8
31	C	516	DGD	O1G-C1G-C2G-O2G
33	Y	101	LMG	O1-C7-C8-O7
33	b	622	LMG	O1-C7-C8-O7
33	c	522	LMG	O1-C7-C8-O7
30	d	406	LHG	C25-C26-C27-C28
30	e	101	LHG	C26-C27-C28-C29
24	d	402	CLA	C16-C17-C18-C20
24	B	612	CLA	C8-C10-C11-C12
24	D	404	CLA	C13-C15-C16-C17
32	B	623	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
32	X	102	STE	C15-C16-C17-C18
32	d	409	STE	C11-C12-C13-C14
24	c	511	CLA	O1A-CGA-O2A-C1
30	d	407	LHG	O10-C23-O8-C6
24	B	604	CLA	CBA-CGA-O2A-C1
31	C	516	DGD	CDB-CEB-CFB-CGB
32	C	520	STE	C11-C12-C13-C14
32	T	102	STE	C5-C6-C7-C8
33	m	101	LMG	C11-C12-C13-C14
24	A	605	CLA	C11-C12-C13-C14
24	B	612	CLA	C11-C12-C13-C14
24	B	612	CLA	C14-C13-C15-C16
24	C	502	CLA	C11-C12-C13-C14
24	C	504	CLA	C11-C10-C8-C9
24	C	513	CLA	C6-C7-C8-C9
24	D	403	CLA	C6-C7-C8-C9
24	D	404	CLA	C14-C13-C15-C16
24	b	602	CLA	C11-C12-C13-C14
24	b	607	CLA	C6-C7-C8-C9
26	C	514	BCR	C22-C23-C24-C25
32	B	623	STE	C11-C10-C9-C8
30	d	407	LHG	C32-C33-C34-C35
32	M	102	STE	C11-C10-C9-C8
32	X	102	STE	C3-C4-C5-C6
33	c	521	LMG	C39-C40-C41-C42
30	d	406	LHG	C14-C15-C16-C17
31	h	102	DGD	CDA-CEA-CFA-CGA
33	m	101	LMG	C13-C14-C15-C16
31	C	516	DGD	O1A-C1A-O1G-C1G
30	d	406	LHG	C30-C31-C32-C33
32	b	625	STE	C5-C6-C7-C8
32	c	520	STE	C3-C4-C5-C6
24	d	402	CLA	C16-C17-C18-C19
29	A	613	SQD	C11-C12-C13-C14
33	Y	101	LMG	C32-C33-C34-C35
32	C	520	STE	C10-C11-C12-C13
31	C	517	DGD	C3B-C4B-C5B-C6B
33	a	619	LMG	C24-C25-C26-C27
24	A	604	CLA	C15-C16-C17-C18
29	A	615	SQD	C27-C28-C29-C30
31	c	517	DGD	C3A-C4A-C5A-C6A
32	d	409	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	b	610	CLA	C2A-CAA-CBA-CGA
32	X	102	STE	C2-C3-C4-C5
24	A	604	CLA	O1D-CGD-O2D-CED
30	A	614	LHG	C10-C11-C12-C13
31	C	516	DGD	C6B-C7B-C8B-C9B
31	C	517	DGD	CDB-CEB-CFB-CGB
31	C	518	DGD	C7B-C8B-C9B-CAB
24	c	505	CLA	C16-C17-C18-C20
24	b	612	CLA	C13-C15-C16-C17
28	a	612	PL9	C15-C14-C16-C17
26	X	101	BCR	C23-C24-C25-C26
26	a	608	BCR	C23-C24-C25-C30
26	c	514	BCR	C23-C24-C25-C26
26	c	514	BCR	C23-C24-C25-C30
24	c	506	CLA	C2-C3-C5-C6
31	C	517	DGD	O1B-C1B-O2G-C2G
32	T	102	STE	C15-C16-C17-C18
29	a	616	SQD	C29-C30-C31-C32
32	I	101	STE	C5-C6-C7-C8
32	d	409	STE	C7-C8-C9-C10
33	a	619	LMG	C4-C5-C6-O5
24	B	612	CLA	C5-C6-C7-C8
24	B	612	CLA	C15-C16-C17-C18
26	T	101	BCR	C16-C17-C18-C19
31	A	616	DGD	O1G-C1G-C2G-O2G
33	Y	101	LMG	C36-C37-C38-C39
31	A	616	DGD	O6D-C5D-C6D-O5D
24	c	509	CLA	C5-C6-C7-C8
33	D	412	LMG	C30-C31-C32-C33
33	c	521	LMG	C38-C39-C40-C41
30	a	614	LHG	C13-C14-C15-C16
31	C	518	DGD	C5B-C6B-C7B-C8B
32	d	409	STE	C12-C13-C14-C15
30	D	410	LHG	C4-C5-C6-O8
31	A	616	DGD	O1G-C1G-C2G-C3G
32	t	102	STE	C11-C10-C9-C8
24	C	502	CLA	C11-C12-C13-C15
24	C	510	CLA	C6-C7-C8-C10
24	b	605	CLA	C11-C10-C8-C7
24	b	606	CLA	C12-C13-C15-C16
24	c	510	CLA	C2-C3-C5-C6
28	a	612	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
29	B	620	SQD	C29-C30-C31-C32
31	C	518	DGD	C8A-C9A-CAA-CBA
24	B	603	CLA	C14-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C9
24	C	505	CLA	C6-C7-C8-C9
24	b	601	CLA	C14-C13-C15-C16
24	c	505	CLA	C6-C7-C8-C9
24	B	603	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	C16-C17-C18-C20
32	b	621	STE	C12-C13-C14-C15
26	a	608	BCR	C37-C22-C23-C24
24	B	610	CLA	C16-C17-C18-C19
30	A	614	LHG	C2-C3-O3-P
30	D	410	LHG	C2-C3-O3-P
24	B	613	CLA	O1A-CGA-O2A-C1
29	A	613	SQD	C30-C31-C32-C33
32	B	624	STE	C6-C7-C8-C9
33	M	101	LMG	C17-C18-C19-C20
33	c	521	LMG	C14-C15-C16-C17
33	D	411	LMG	C36-C37-C38-C39
24	A	604	CLA	C16-C17-C18-C19
24	a	607	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C19
24	B	613	CLA	CBA-CGA-O2A-C1
31	H	102	DGD	O2G-C1B-C2B-C3B
32	d	409	STE	C6-C7-C8-C9
24	b	606	CLA	C15-C16-C17-C18
31	C	518	DGD	O6D-C5D-C6D-O5D
24	B	604	CLA	O1A-CGA-O2A-C1
30	D	410	LHG	C10-C11-C12-C13
29	a	615	SQD	O5-C1-O6-C44
26	X	101	BCR	C9-C10-C11-C12
24	b	603	CLA	C8-C10-C11-C12
30	L	101	LHG	C15-C16-C17-C18
30	e	101	LHG	C14-C15-C16-C17
31	C	518	DGD	CAB-CBB-CCB-CDB
30	D	413	LHG	C7-C8-C9-C10
24	c	504	CLA	C11-C12-C13-C14
30	L	101	LHG	C9-C10-C11-C12
24	b	604	CLA	C8-C10-C11-C12
31	A	616	DGD	CCA-CDA-CEA-CFA
33	d	408	LMG	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C15-C16-C17-C18
29	a	616	SQD	C10-C11-C12-C13
30	a	614	LHG	C19-C20-C21-C22
32	T	103	STE	C4-C5-C6-C7
32	a	617	STE	C1-C2-C3-C4
24	D	403	CLA	C2-C1-O2A-CGA
33	a	619	LMG	C29-C30-C31-C32
33	c	522	LMG	C20-C21-C22-C23
31	C	517	DGD	C2D-C1D-O3G-C3G
29	A	613	SQD	C35-C36-C37-C38
24	b	604	CLA	C13-C15-C16-C17
24	b	602	CLA	C2A-CAA-CBA-CGA
29	b	620	SQD	O47-C45-C46-O48
30	d	407	LHG	C2-C3-O3-P
29	D	408	SQD	O10-C23-C24-C25
32	B	622	STE	C6-C7-C8-C9
29	a	615	SQD	C35-C36-C37-C38
30	l	101	LHG	C26-C27-C28-C29
33	b	622	LMG	C36-C37-C38-C39
31	H	102	DGD	C7A-C8A-C9A-CAA
33	Y	101	LMG	C15-C16-C17-C18
24	C	510	CLA	C2-C3-C5-C6
24	D	403	CLA	C11-C10-C8-C9
24	C	508	CLA	C16-C17-C18-C19
29	B	620	SQD	C34-C35-C36-C37
30	D	409	LHG	C28-C29-C30-C31
30	a	614	LHG	C12-C13-C14-C15
33	d	408	LMG	C30-C31-C32-C33
33	b	622	LMG	C34-C35-C36-C37
26	D	405	BCR	C16-C17-C18-C36
26	X	101	BCR	C16-C17-C18-C36
33	a	619	LMG	O1-C7-C8-C9
24	B	603	CLA	C16-C17-C18-C19
24	C	512	CLA	O2A-C1-C2-C3
25	D	401	PHO	O2A-C1-C2-C3
25	a	606	PHO	O2A-C1-C2-C3
31	A	616	DGD	C4E-C5E-C6E-O5E
32	B	623	STE	C10-C11-C12-C13
26	T	101	BCR	C7-C8-C9-C34
29	A	613	SQD	C15-C16-C17-C18
24	c	512	CLA	C4-C3-C5-C6
24	c	512	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	c	510	CLA	C11-C12-C13-C15
30	a	614	LHG	C33-C34-C35-C36
26	t	101	BCR	C13-C14-C15-C16
30	L	101	LHG	C4-O6-P-O3
24	C	512	CLA	C10-C11-C12-C13
31	H	102	DGD	CDB-CEB-CFB-CGB
33	b	622	LMG	C11-C12-C13-C14
33	Y	101	LMG	C38-C39-C40-C41
30	l	101	LHG	C8-C7-O7-C5
24	H	101	CLA	C16-C17-C18-C19
24	b	611	CLA	C10-C11-C12-C13
31	c	517	DGD	CBB-CCB-CDB-CEB
31	h	102	DGD	CAA-CBA-CCA-CDA
24	B	615	CLA	O1A-CGA-O2A-C1
31	h	102	DGD	C4A-C5A-C6A-C7A
24	c	511	CLA	C16-C17-C18-C19
26	B	616	BCR	C12-C13-C14-C15
30	l	101	LHG	O7-C5-C6-O8
33	a	619	LMG	O1-C7-C8-O7
24	B	612	CLA	C13-C15-C16-C17
26	k	101	BCR	C19-C20-C21-C22
31	A	616	DGD	CFB-CGB-CHB-CIB
31	C	516	DGD	C7B-C8B-C9B-CAB
33	D	407	LMG	C39-C40-C41-C42
30	e	101	LHG	C9-C10-C11-C12
31	h	102	DGD	C5A-C6A-C7A-C8A
24	A	604	CLA	C2-C1-O2A-CGA
24	B	605	CLA	C11-C10-C8-C9
24	C	510	CLA	C6-C7-C8-C9
24	a	605	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C10-C8-C9
24	b	609	CLA	C15-C16-C17-C18
32	B	624	STE	C11-C12-C13-C14
32	M	104	STE	C1-C2-C3-C4
30	D	409	LHG	C33-C34-C35-C36
33	D	407	LMG	C17-C18-C19-C20
24	a	607	CLA	C15-C16-C17-C18
24	b	605	CLA	C5-C6-C7-C8
24	b	601	CLA	O1A-CGA-O2A-C1
26	B	618	BCR	C23-C24-C25-C30
26	K	101	BCR	C23-C24-C25-C30
26	K	102	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
26	h	101	BCR	C23-C24-C25-C30
26	k	102	BCR	C23-C24-C25-C30
26	t	101	BCR	C1-C6-C7-C8
24	B	611	CLA	C13-C15-C16-C17
31	c	517	DGD	CAA-CBA-CCA-CDA
33	a	619	LMG	C7-C8-C9-O8
26	c	515	BCR	C13-C14-C15-C16
32	C	520	STE	C4-C5-C6-C7
32	M	104	STE	C11-C10-C9-C8
24	B	602	CLA	C4-C3-C5-C6
33	Y	101	LMG	O6-C5-C6-O5
24	c	502	CLA	C13-C15-C16-C17
29	B	620	SQD	C45-C44-O6-C1
33	C	515	LMG	C8-C7-O1-C1
32	a	618	STE	C6-C7-C8-C9
30	e	101	LHG	C15-C16-C17-C18
31	h	102	DGD	CCA-CDA-CEA-CFA
33	d	408	LMG	C15-C16-C17-C18
24	C	511	CLA	C16-C17-C18-C19
24	D	403	CLA	C16-C17-C18-C19
33	C	515	LMG	C30-C31-C32-C33
24	c	504	CLA	C10-C11-C12-C13
24	c	506	CLA	C8-C10-C11-C12
35	F	101	HEM	C3D-CAD-CBD-CGD
32	d	410	STE	C10-C11-C12-C13
29	D	408	SQD	O48-C23-C24-C25
24	b	601	CLA	CBA-CGA-O2A-C1
31	C	516	DGD	O6D-C5D-C6D-O5D
24	A	605	CLA	C15-C16-C17-C18
24	c	509	CLA	C8-C10-C11-C12
29	a	616	SQD	C27-C28-C29-C30
24	c	508	CLA	C4-C3-C5-C6
24	B	605	CLA	C6-C7-C8-C10
24	B	608	CLA	C2-C3-C5-C6
24	D	403	CLA	C11-C12-C13-C15
24	b	612	CLA	C11-C10-C8-C7
28	A	611	PL9	C13-C14-C16-C17
30	d	406	LHG	C34-C35-C36-C37
33	C	515	LMG	C36-C37-C38-C39
29	a	615	SQD	O47-C45-C46-O48
33	Y	101	LMG	C30-C31-C32-C33
24	B	604	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	B	608	CLA	C3-C5-C6-C7
31	h	102	DGD	O2G-C1B-C2B-C3B
26	a	608	BCR	C16-C17-C18-C36
30	D	413	LHG	C11-C12-C13-C14
29	a	615	SQD	O47-C7-C8-C9
24	c	513	CLA	C4-C3-C5-C6
28	a	612	PL9	C45-C44-C46-C47
24	c	512	CLA	C2-C3-C5-C6
24	B	604	CLA	C11-C10-C8-C9
24	B	609	CLA	C14-C13-C15-C16
24	C	501	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	C	512	CLA	C11-C10-C8-C9
24	D	404	CLA	C6-C7-C8-C9
24	b	604	CLA	C11-C12-C13-C14
24	c	502	CLA	C6-C7-C8-C9
24	c	504	CLA	C11-C10-C8-C9
24	c	508	CLA	C6-C7-C8-C9
29	D	408	SQD	C44-C45-C46-O48
24	D	404	CLA	C3A-C2A-CAA-CBA
24	d	403	CLA	C3A-C2A-CAA-CBA
32	X	102	STE	C14-C15-C16-C17
33	d	408	LMG	C35-C36-C37-C38
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	CAD-CBD-CGD-O2D
24	B	608	CLA	CAD-CBD-CGD-O2D
24	B	609	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	b	604	CLA	CAD-CBD-CGD-O2D
24	b	607	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	512	CLA	CAD-CBD-CGD-O2D
24	c	513	CLA	CAD-CBD-CGD-O2D
25	D	401	PHO	CAD-CBD-CGD-O2D
24	B	613	CLA	C2A-CAA-CBA-CGA
24	b	613	CLA	CAA-CBA-CGA-O2A
31	C	516	DGD	O2G-C1B-C2B-C3B
33	b	622	LMG	O7-C10-C11-C12
33	m	101	LMG	O8-C28-C29-C30
31	C	518	DGD	CDB-CEB-CFB-CGB
24	b	606	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	c	523	STE	C7-C8-C9-C10
32	h	103	STE	C11-C10-C9-C8
28	d	405	PL9	C33-C34-C36-C37
29	A	613	SQD	O47-C7-C8-C9
26	D	405	BCR	C21-C22-C23-C24
24	D	404	CLA	C2C-C3C-CAC-CBC
24	a	613	CLA	C2C-C3C-CAC-CBC
24	c	502	CLA	C2C-C3C-CAC-CBC
24	B	603	CLA	O2A-C1-C2-C3
24	B	612	CLA	O2A-C1-C2-C3
24	B	615	CLA	O2A-C1-C2-C3
24	D	404	CLA	O2A-C1-C2-C3
33	D	411	LMG	C32-C33-C34-C35
32	I	101	STE	C3-C4-C5-C6
24	A	604	CLA	CBD-CGD-O2D-CED
24	A	605	CLA	CHA-CBD-CGD-O1D
24	A	605	CLA	CHA-CBD-CGD-O2D
24	B	605	CLA	CHA-CBD-CGD-O1D
24	B	605	CLA	CHA-CBD-CGD-O2D
24	B	609	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	606	CLA	CHA-CBD-CGD-O1D
24	b	606	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	C2-C3-C5-C6
25	d	401	PHO	C2C-C3C-CAC-CBC
30	l	101	LHG	O6-C4-C5-C6
26	d	404	BCR	C16-C17-C18-C19
33	D	411	LMG	C13-C14-C15-C16
29	B	620	SQD	O47-C7-C8-C9
32	d	410	STE	C5-C6-C7-C8
33	C	515	LMG	C28-C29-C30-C31
32	d	410	STE	C11-C10-C9-C8
24	c	506	CLA	C10-C11-C12-C13
24	B	605	CLA	C5-C6-C7-C8
29	A	613	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	I	101	STE	C12-C13-C14-C15
24	A	605	CLA	C11-C10-C8-C7
24	B	604	CLA	C6-C7-C8-C10
24	H	101	CLA	C6-C7-C8-C10
24	H	101	CLA	C12-C13-C15-C16
24	b	604	CLA	C12-C13-C15-C16
24	b	610	CLA	C11-C12-C13-C15
24	B	612	CLA	CAA-CBA-CGA-O2A
31	c	516	DGD	O1G-C1A-C2A-C3A
24	B	614	CLA	C14-C13-C15-C16
24	C	505	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C10-C8-C9
24	a	605	CLA	C14-C13-C15-C16
25	A	606	PHO	C14-C13-C15-C16
26	K	101	BCR	C9-C10-C11-C12
24	b	610	CLA	CBD-CGD-O2D-CED
32	h	103	STE	C7-C8-C9-C10
24	C	501	CLA	C2A-CAA-CBA-CGA
24	B	611	CLA	CAA-CBA-CGA-O2A
32	M	104	STE	C4-C5-C6-C7
33	b	622	LMG	C42-C43-C44-C45
24	b	601	CLA	C16-C17-C18-C20
32	B	624	STE	C15-C16-C17-C18
28	A	611	PL9	C12-C11-C9-C10
31	c	518	DGD	O6E-C5E-C6E-O5E
31	A	616	DGD	C9A-CAA-CBA-CCA
33	D	411	LMG	C29-C28-O8-C9
33	c	519	LMG	C29-C28-O8-C9
30	a	614	LHG	C17-C18-C19-C20
24	B	601	CLA	C1A-C2A-CAA-CBA
24	d	403	CLA	C1A-C2A-CAA-CBA
24	c	503	CLA	C8-C10-C11-C12
28	d	405	PL9	C21-C22-C23-C24
30	D	409	LHG	C31-C32-C33-C34
24	C	513	CLA	C5-C6-C7-C8
31	c	516	DGD	C2A-C3A-C4A-C5A
24	c	505	CLA	O1A-CGA-O2A-C1
24	c	509	CLA	C2A-CAA-CBA-CGA
33	D	411	LMG	C12-C13-C14-C15
24	b	613	CLA	C13-C15-C16-C17
30	A	614	LHG	C32-C33-C34-C35
30	d	406	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
24	b	613	CLA	CAA-CBA-CGA-O1A
29	a	615	SQD	O49-C7-C8-C9
26	k	102	BCR	C22-C23-C24-C25
24	b	609	CLA	C8-C10-C11-C12
30	A	614	LHG	C31-C32-C33-C34
33	m	101	LMG	C20-C21-C22-C23
30	l	101	LHG	C4-O6-P-O4
29	B	620	SQD	O49-C7-C8-C9
24	a	604	CLA	C13-C15-C16-C17
26	X	101	BCR	C11-C10-C9-C34
26	a	608	BCR	C23-C24-C25-C26
26	k	102	BCR	C23-C24-C25-C26
26	t	101	BCR	C5-C6-C7-C8
28	A	611	PL9	C9-C11-C12-C13
33	c	519	LMG	C33-C34-C35-C36
24	c	510	CLA	C13-C15-C16-C17
29	A	613	SQD	C13-C14-C15-C16
33	D	411	LMG	C15-C16-C17-C18
33	M	101	LMG	C22-C23-C24-C25
29	a	616	SQD	C30-C31-C32-C33
31	C	518	DGD	O1G-C1A-C2A-C3A
31	C	518	DGD	C7A-C8A-C9A-CAA
33	d	408	LMG	C11-C12-C13-C14
30	D	409	LHG	C23-C24-C25-C26
24	C	510	CLA	C4-C3-C5-C6
31	c	516	DGD	CAB-CBB-CCB-CDB
24	A	605	CLA	CAD-CBD-CGD-O1D
24	B	611	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	512	CLA	C3-C5-C6-C7
29	b	620	SQD	C11-C10-C9-C8
30	l	101	LHG	C17-C18-C19-C20
24	C	505	CLA	C8-C10-C11-C12
24	A	605	CLA	C11-C10-C8-C9
24	b	612	CLA	C11-C10-C8-C9
24	c	512	CLA	C11-C12-C13-C14
33	Y	101	LMG	C31-C32-C33-C34
24	c	510	CLA	CAA-CBA-CGA-O2A
33	D	411	LMG	C35-C36-C37-C38
28	a	612	PL9	C12-C13-C14-C15

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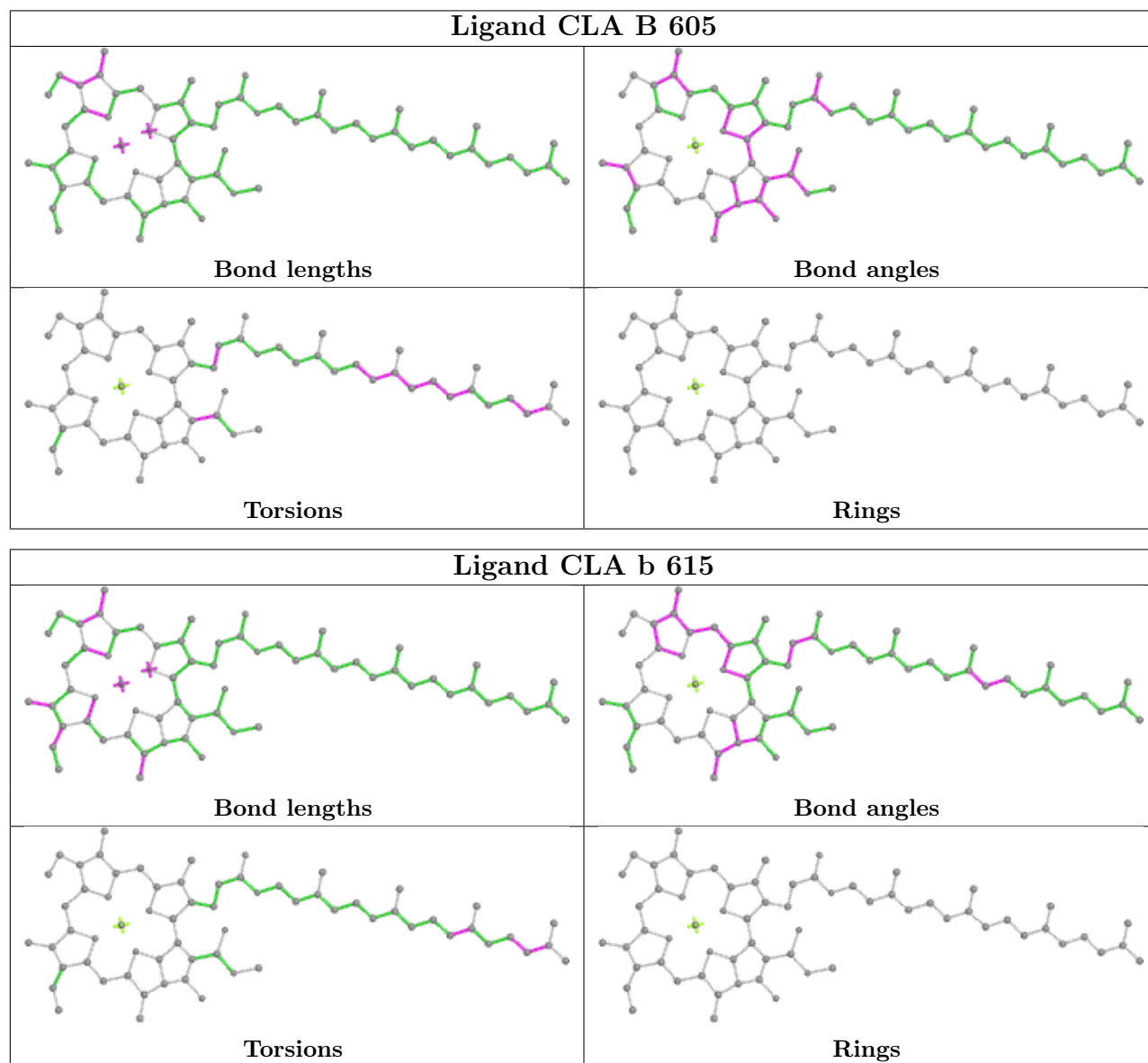
Mol	Chain	Res	Type	Atoms
33	b	622	LMG	C30-C31-C32-C33
30	L	101	LHG	O7-C7-C8-C9
24	B	608	CLA	C4-C3-C5-C6
32	c	520	STE	C4-C5-C6-C7
28	a	612	PL9	C42-C43-C44-C46
24	B	601	CLA	C3A-C2A-CAA-CBA
24	B	607	CLA	C11-C12-C13-C15
24	a	605	CLA	C11-C10-C8-C7
24	c	508	CLA	C12-C13-C15-C16
24	c	512	CLA	C11-C12-C13-C15
30	a	614	LHG	O6-C4-C5-O7
31	C	516	DGD	O1B-C1B-C2B-C3B
31	A	616	DGD	C4D-C5D-C6D-O5D
31	c	518	DGD	O1G-C1A-C2A-C3A
31	H	102	DGD	C1B-C2B-C3B-C4B
33	c	521	LMG	C10-C11-C12-C13
26	c	514	BCR	C21-C22-C23-C24
24	B	611	CLA	CAA-CBA-CGA-O1A
31	c	517	DGD	O1A-C1A-C2A-C3A
26	X	101	BCR	C15-C16-C17-C18
30	d	406	LHG	C11-C12-C13-C14
32	R	101	STE	C6-C7-C8-C9
31	c	517	DGD	O6D-C1D-O3G-C3G
33	C	515	LMG	O6-C1-O1-C7
24	A	612	CLA	O1D-CGD-O2D-CED
24	C	506	CLA	C13-C15-C16-C17
33	b	622	LMG	C13-C14-C15-C16
24	B	612	CLA	CAA-CBA-CGA-O1A
24	B	614	CLA	C5-C6-C7-C8
31	H	102	DGD	C8A-C9A-CAA-CBA
24	B	613	CLA	C13-C15-C16-C17

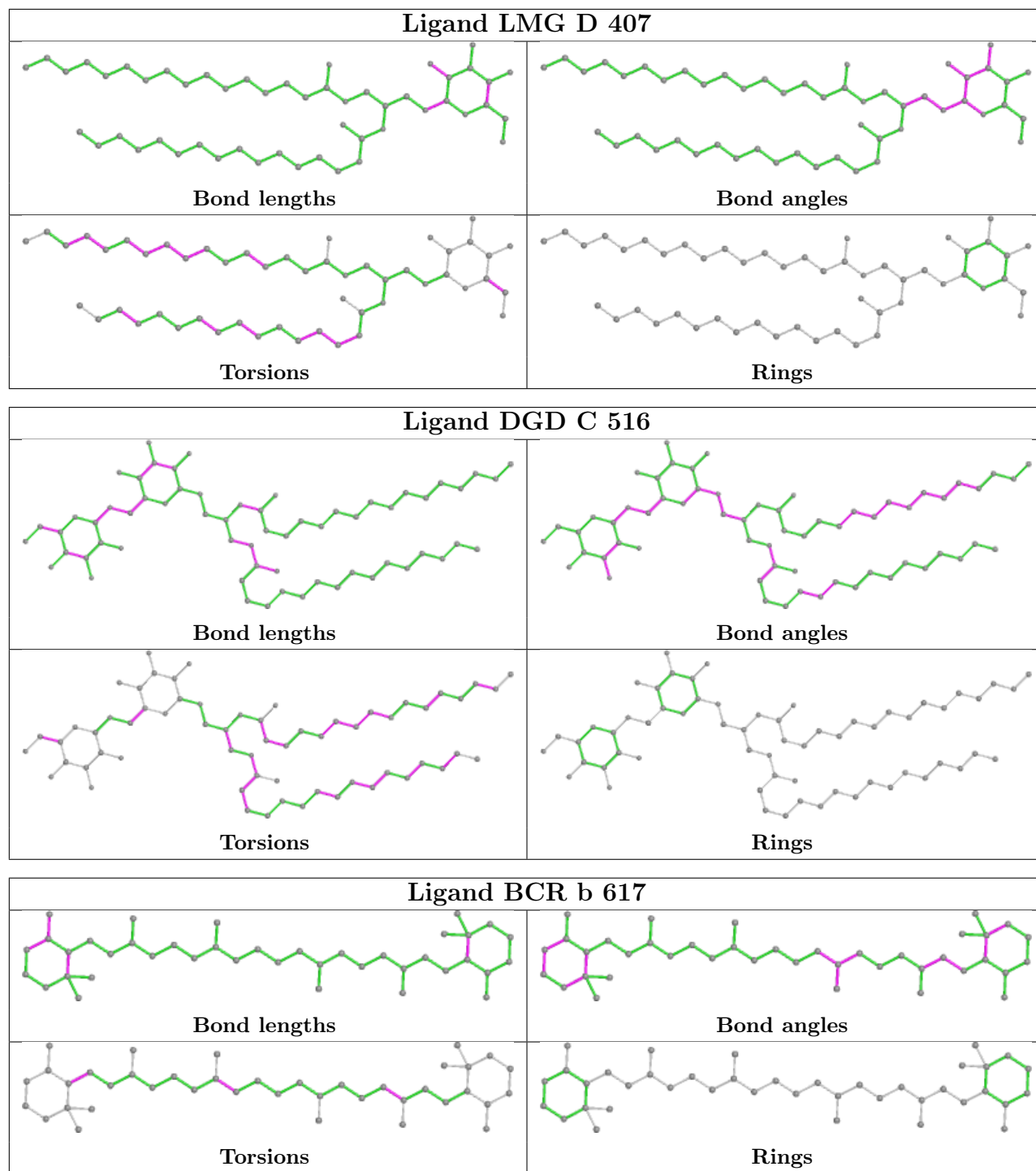
There are no ring outliers.

No monomer is involved in short contacts.

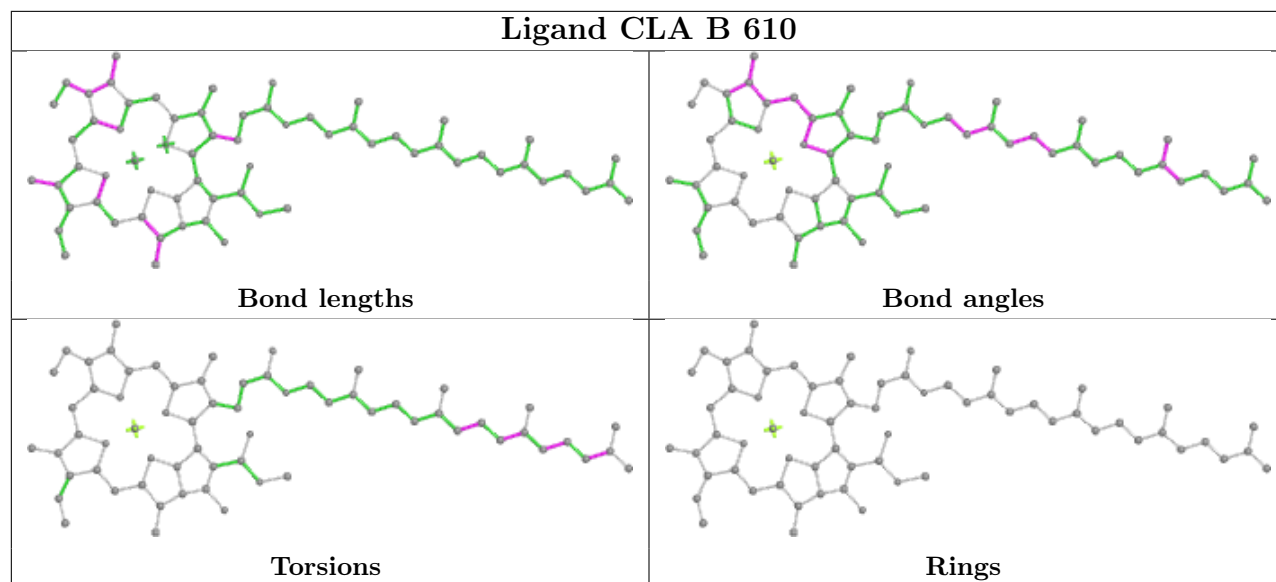
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

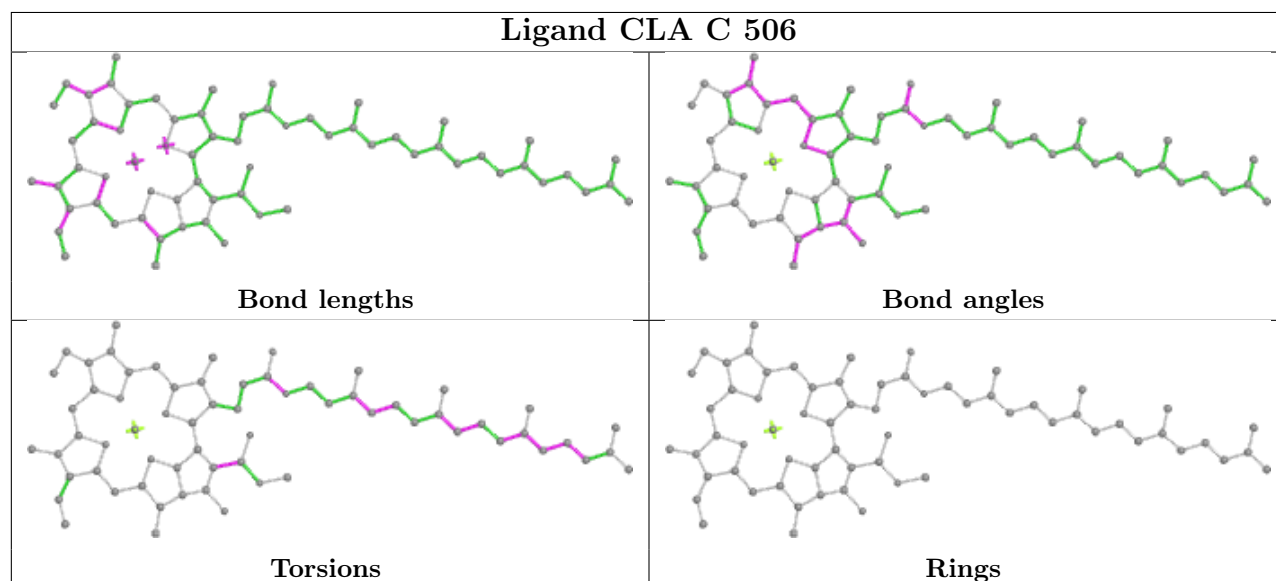




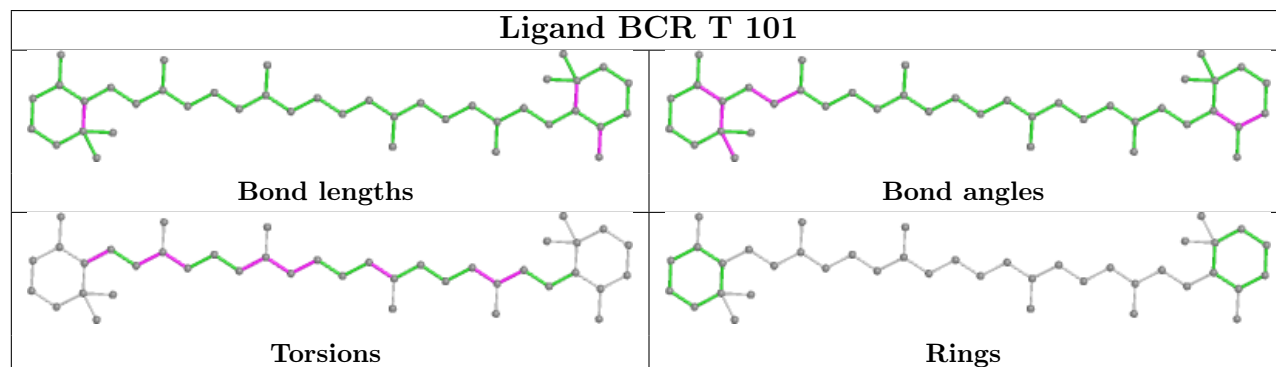
## Ligand CLA B 610

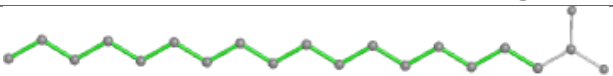
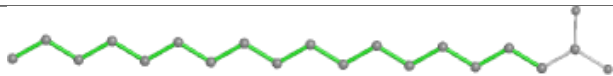
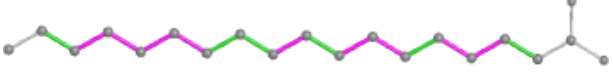
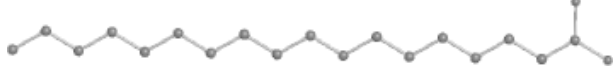


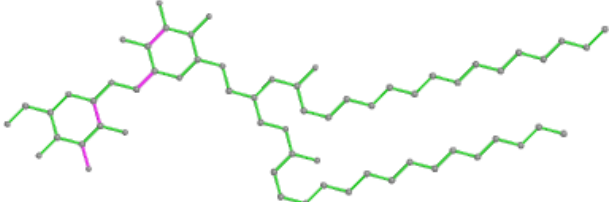
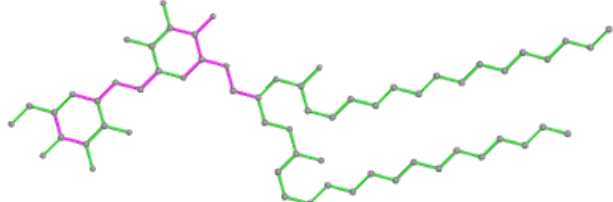
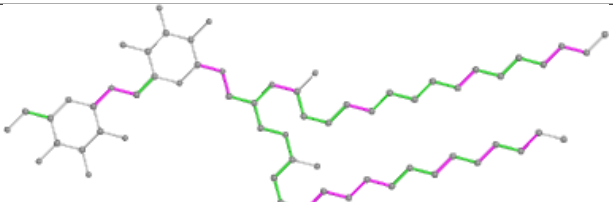
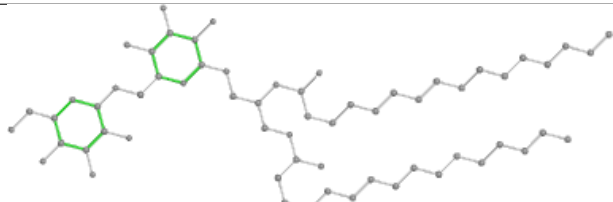
## Ligand CLA C 506

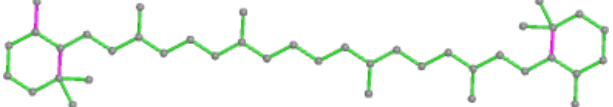
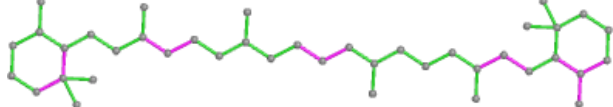
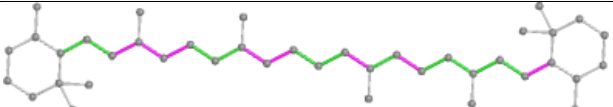
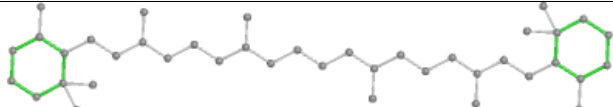


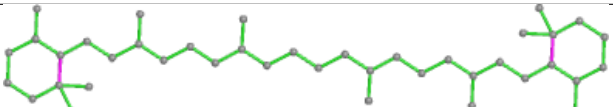
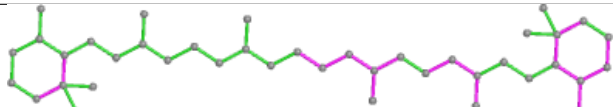
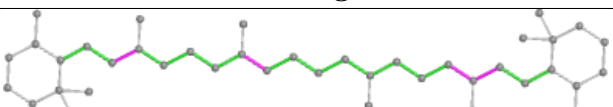
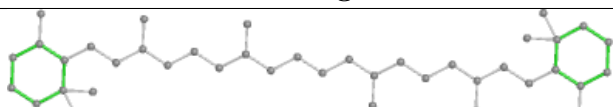
## Ligand BCR T 101



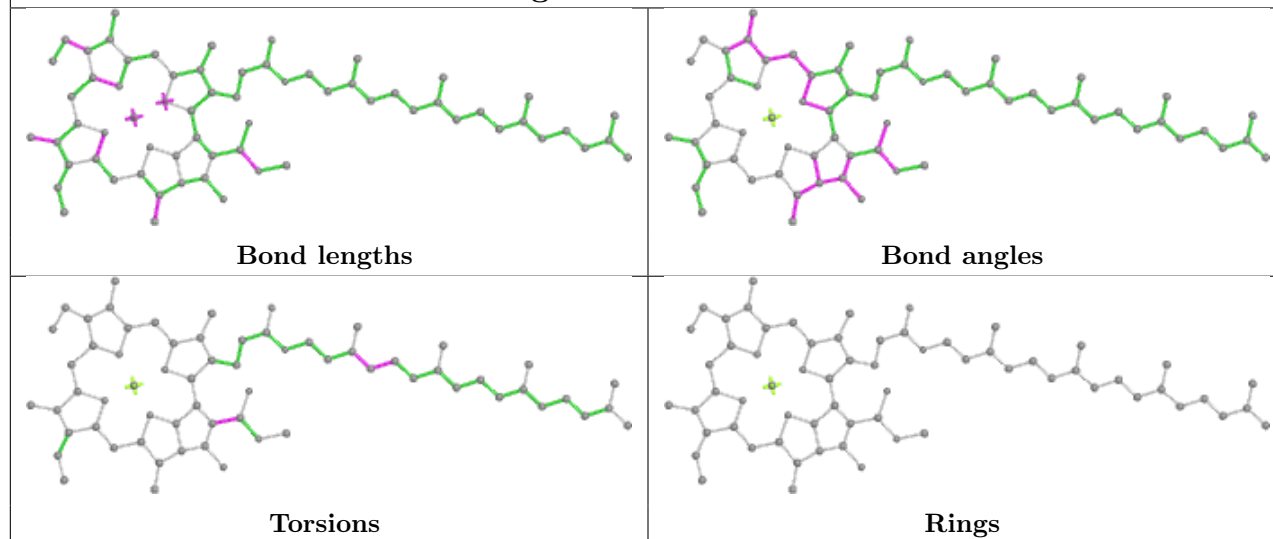
Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD C 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

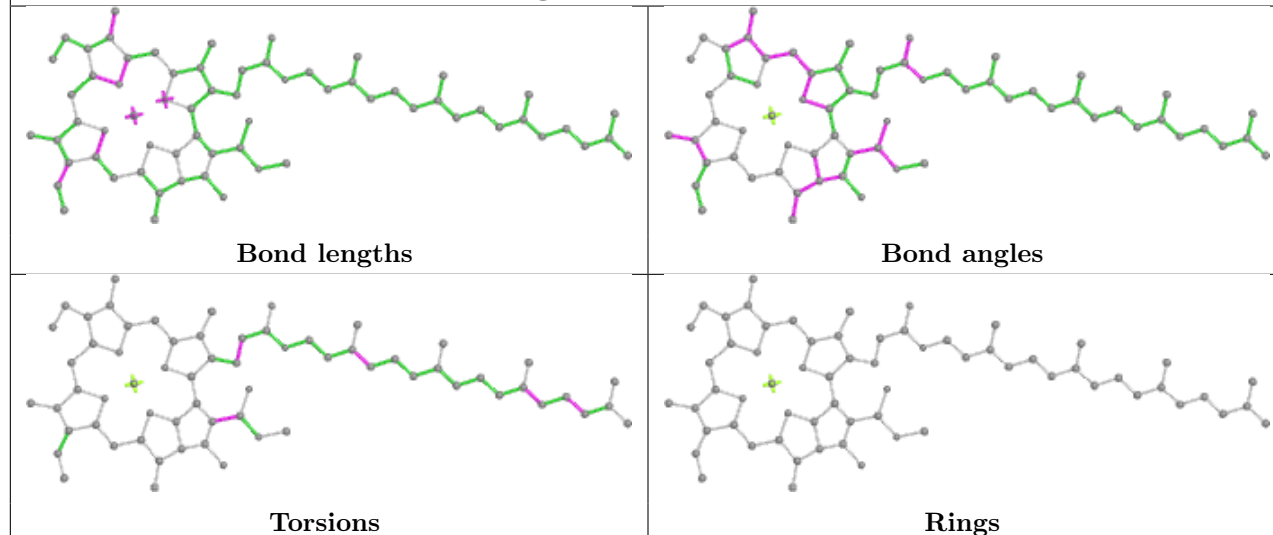
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

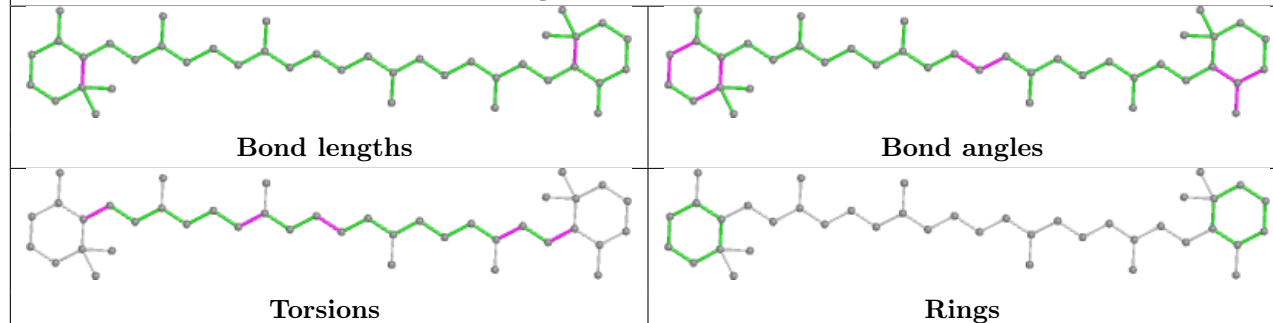
## Ligand CLA B 608



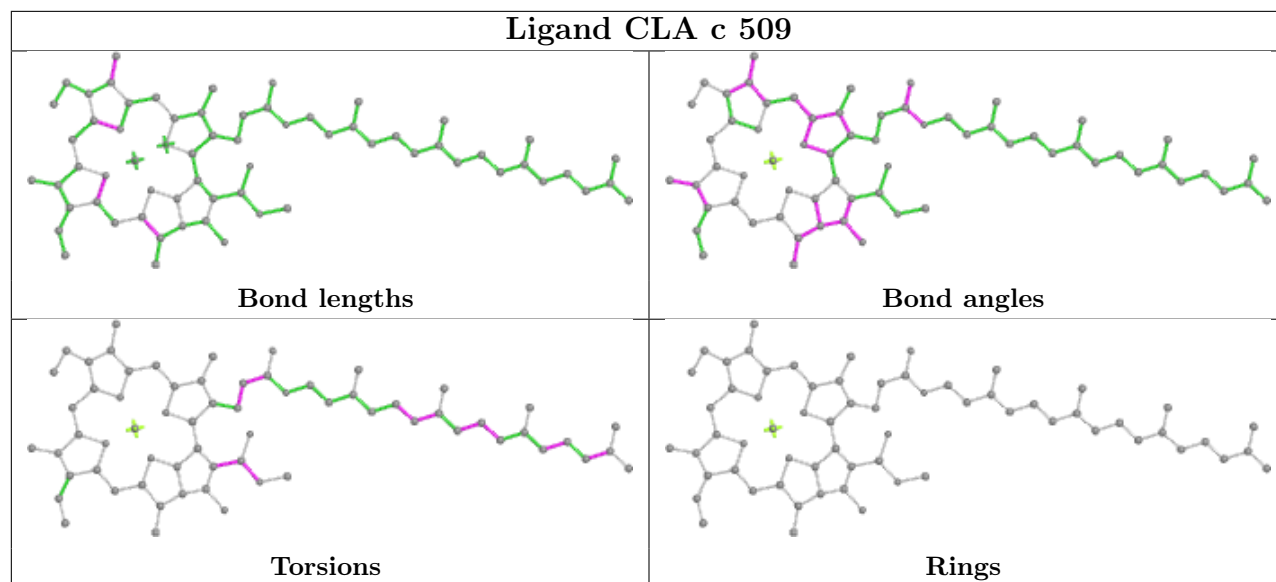
## Ligand CLA b 606



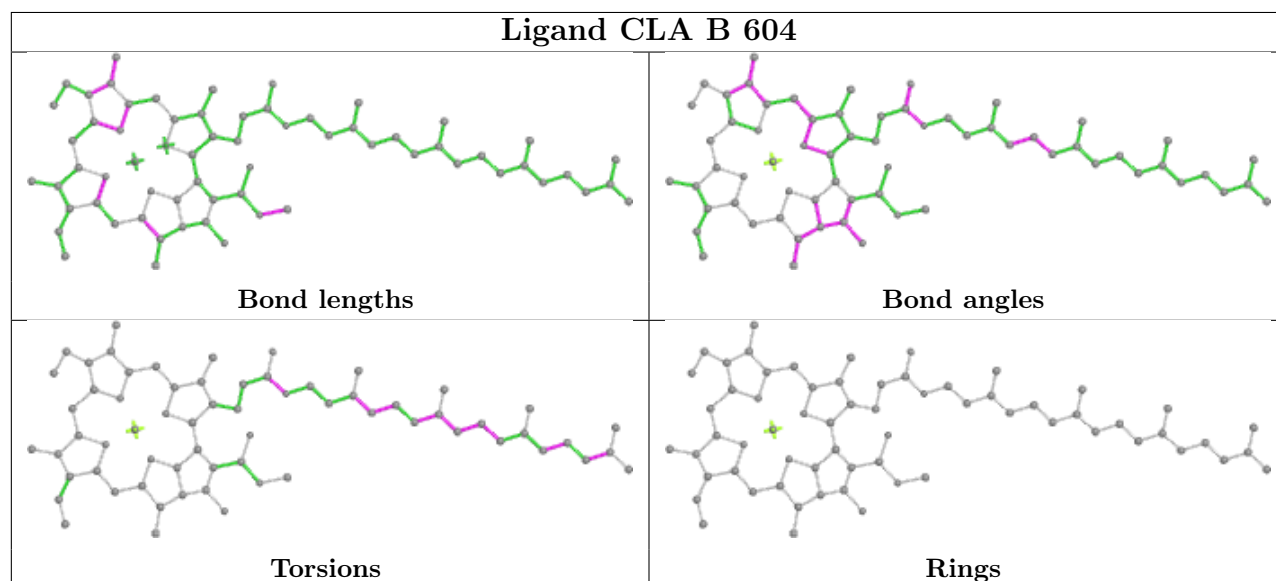
## Ligand BCR c 514



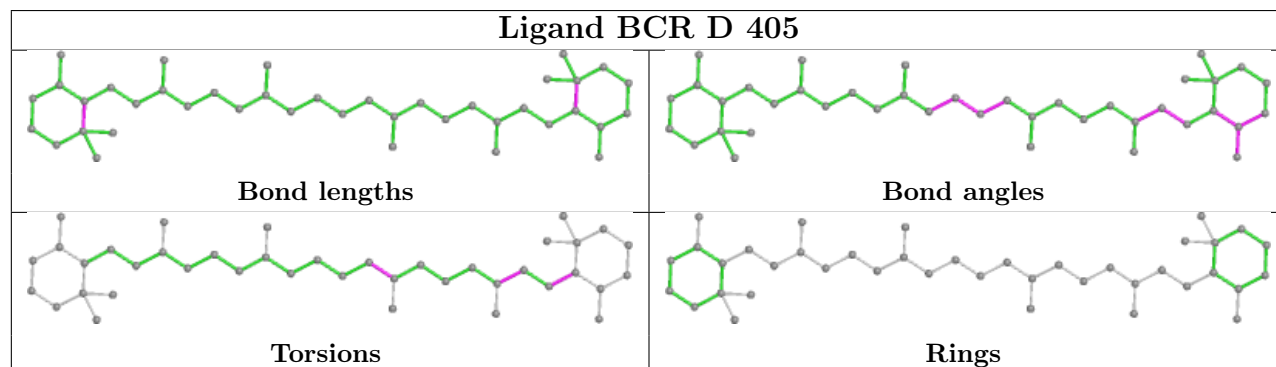
## Ligand CLA c 509

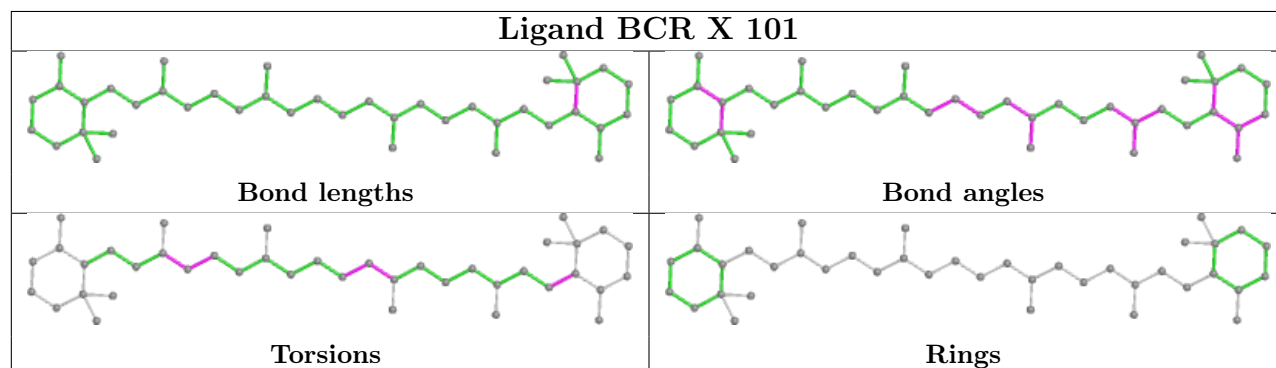
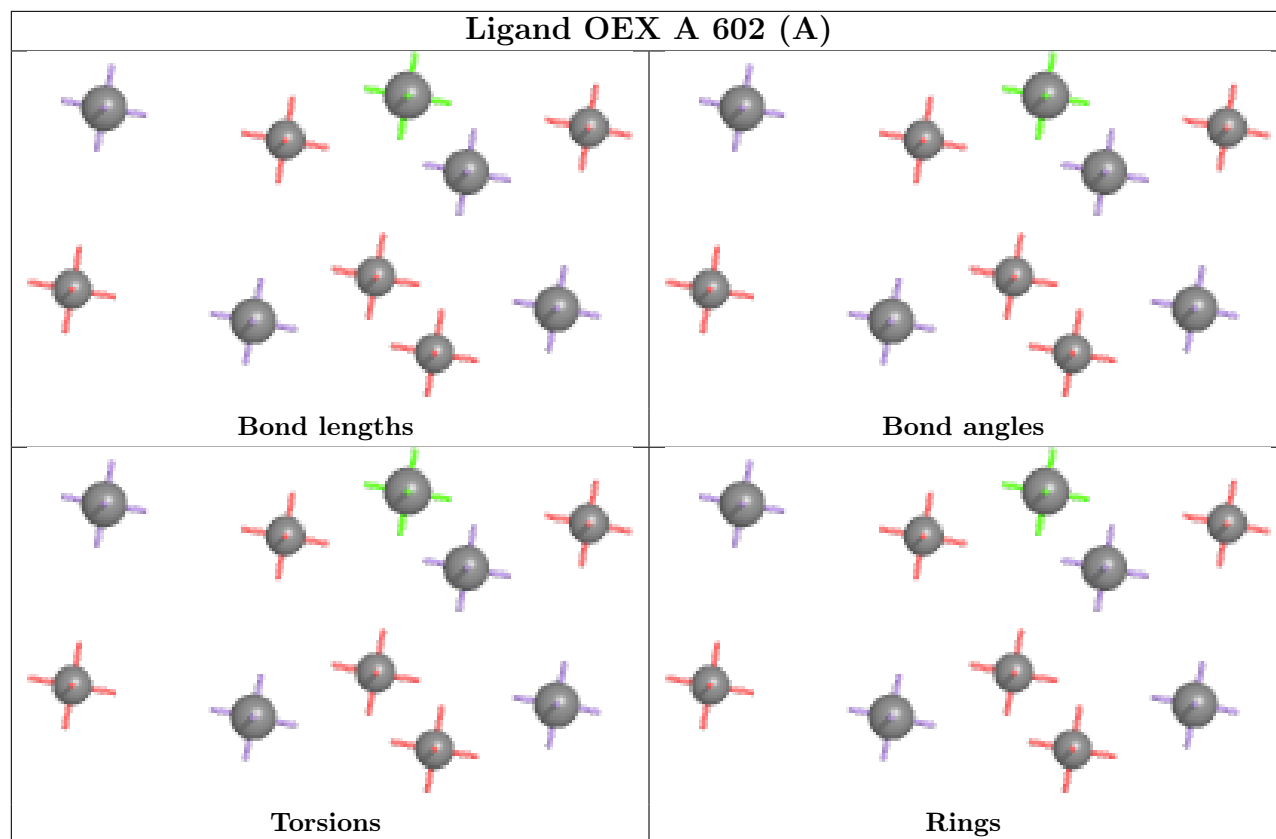


## Ligand CLA B 604

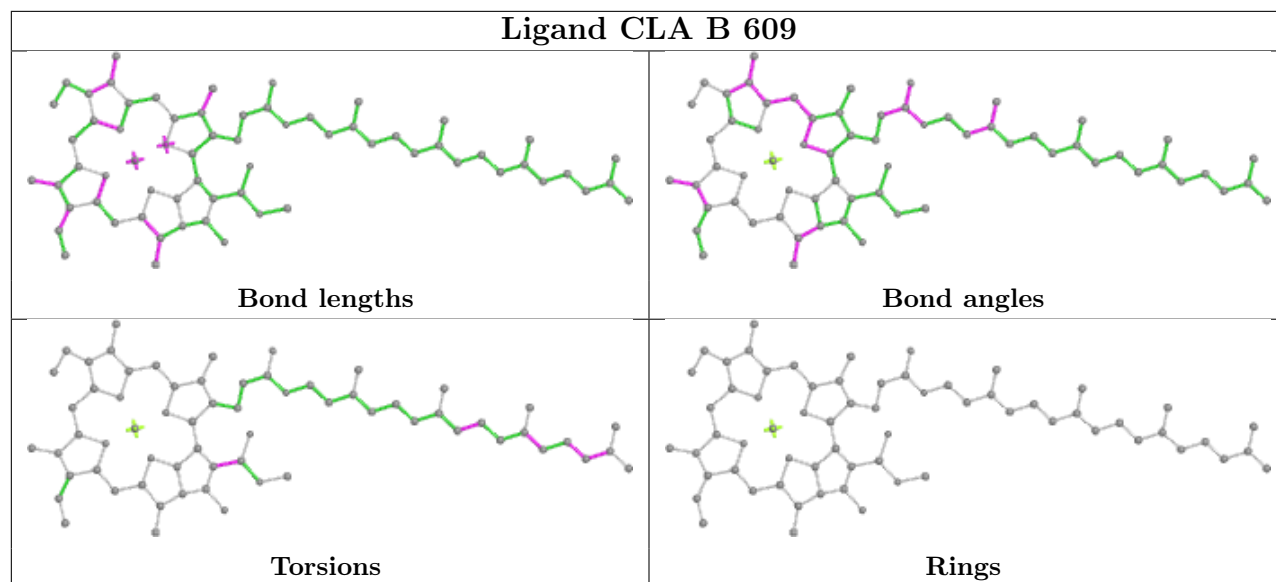


## Ligand BCR D 405

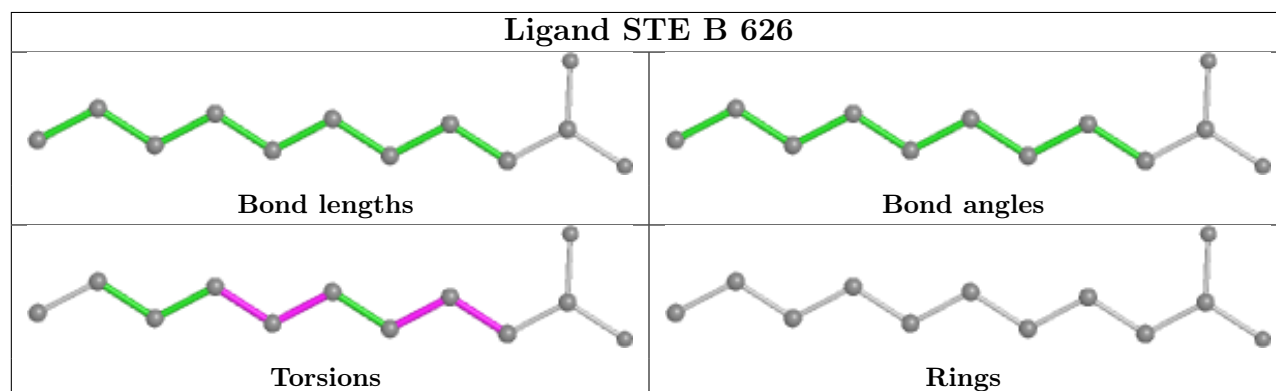


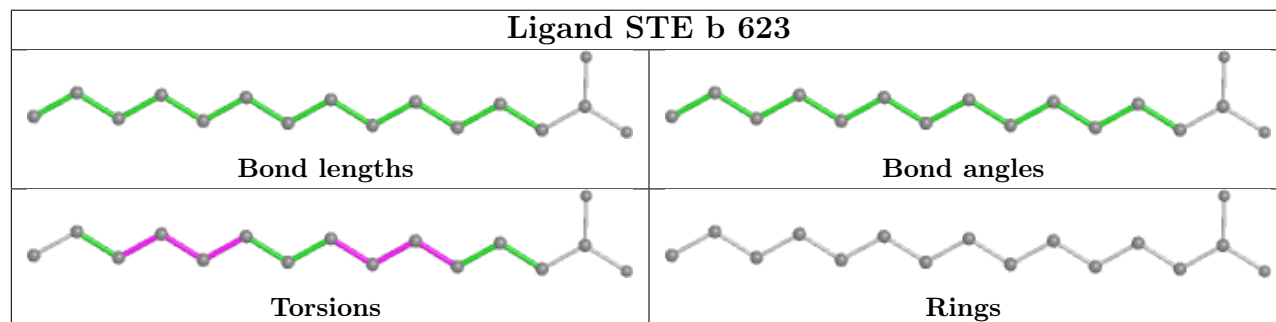
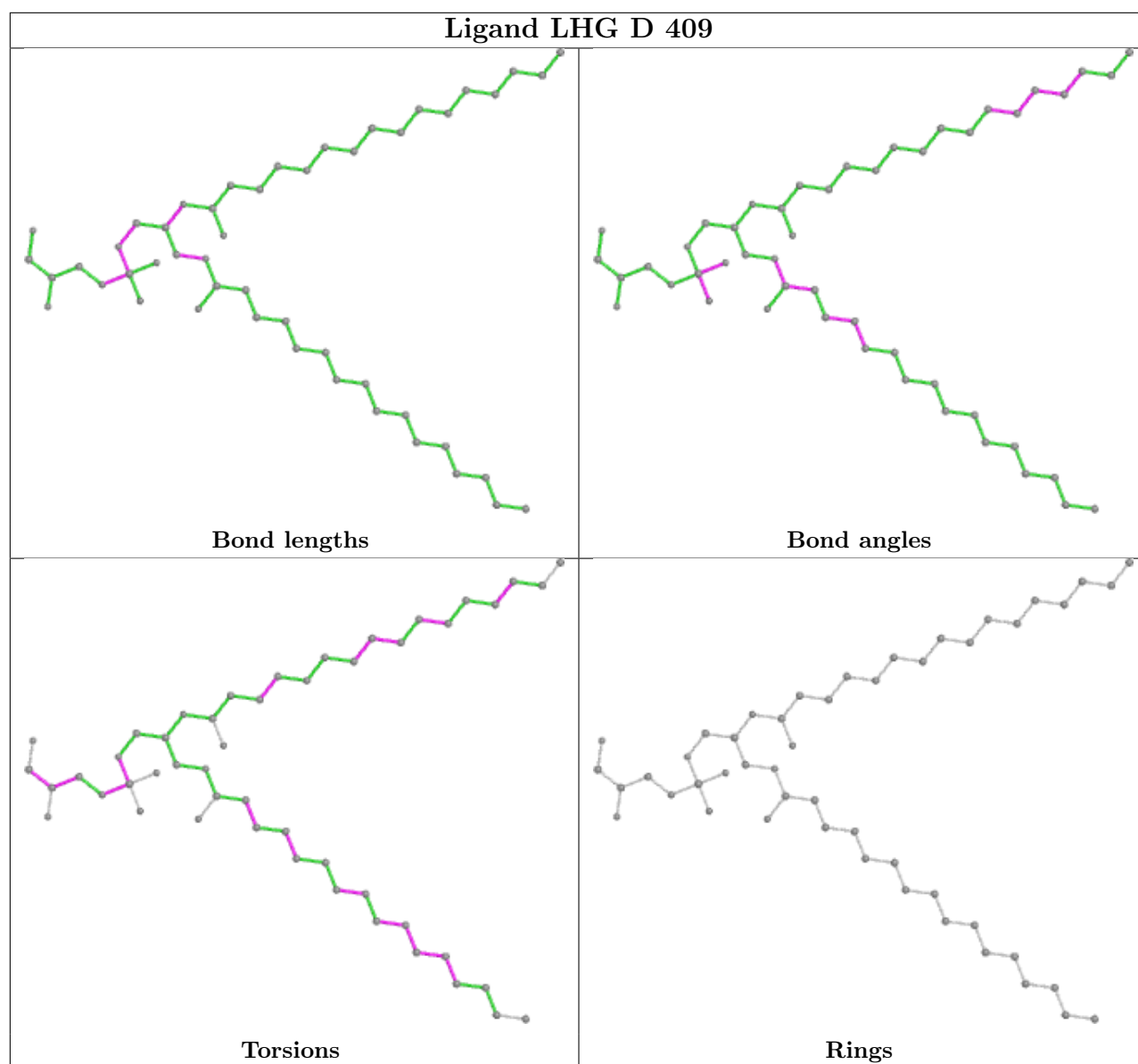


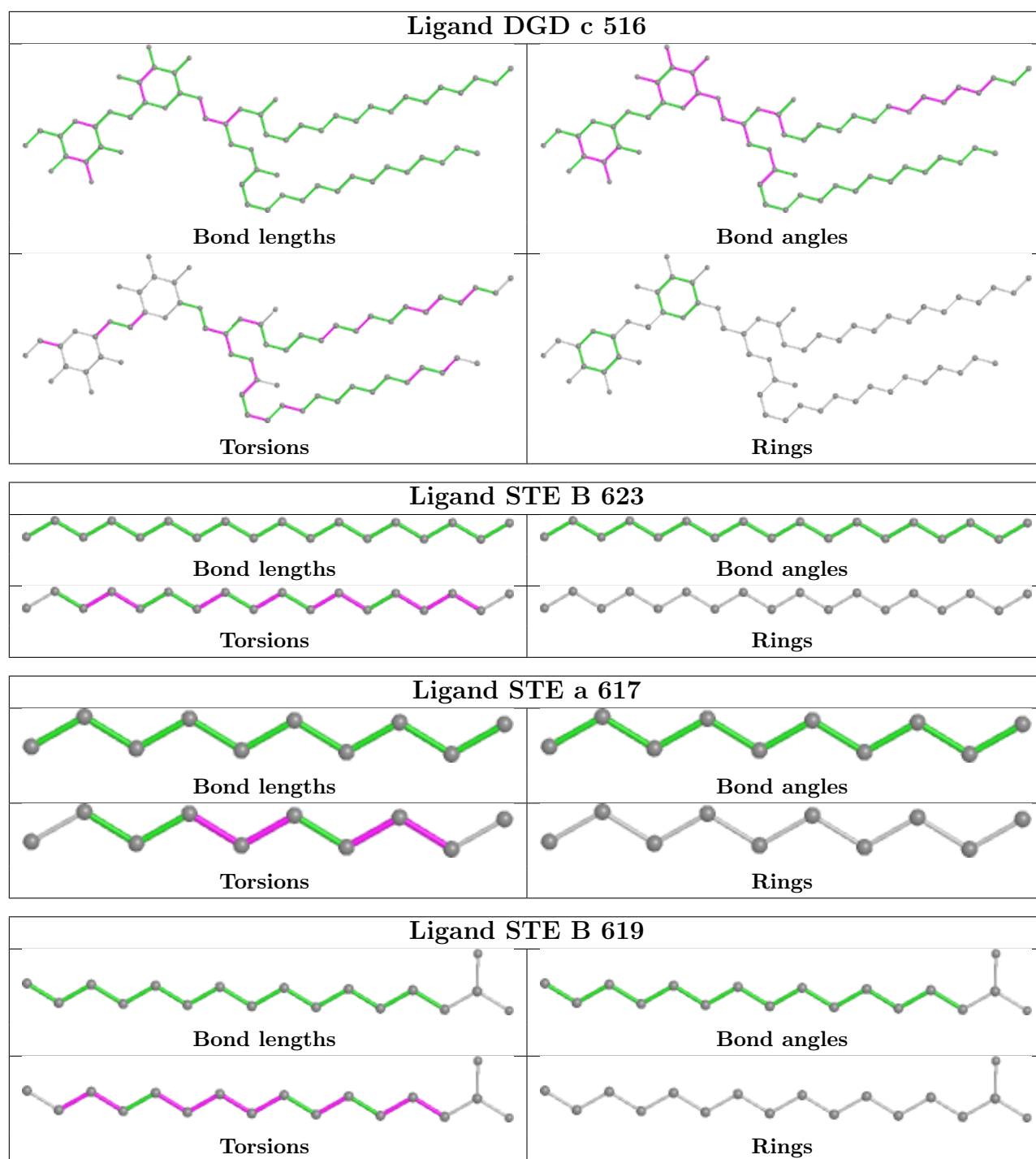
## Ligand CLA B 609



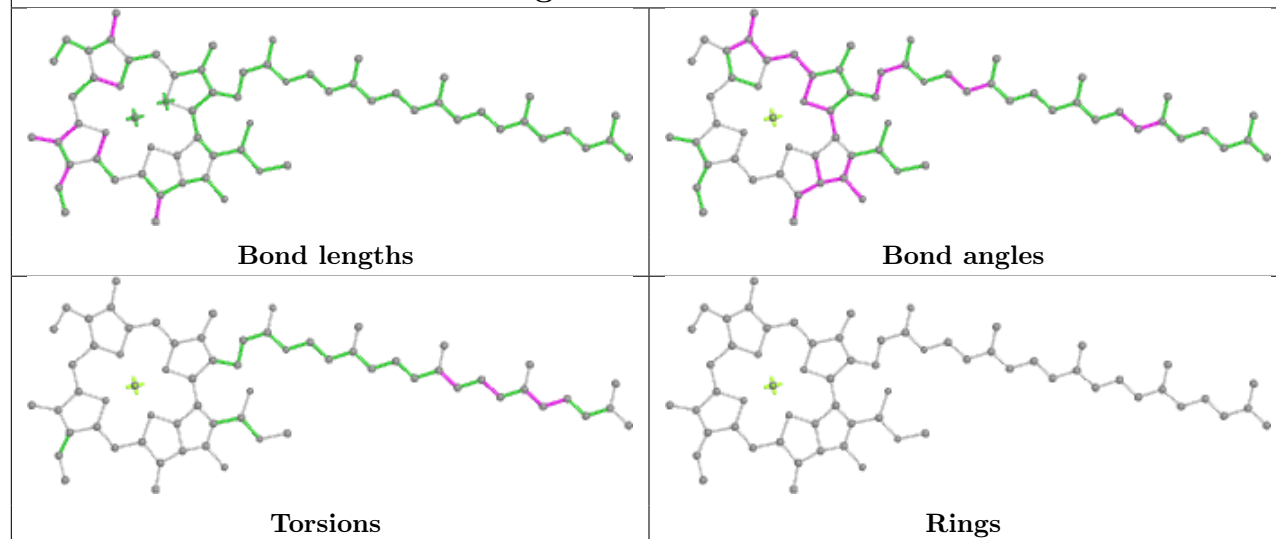
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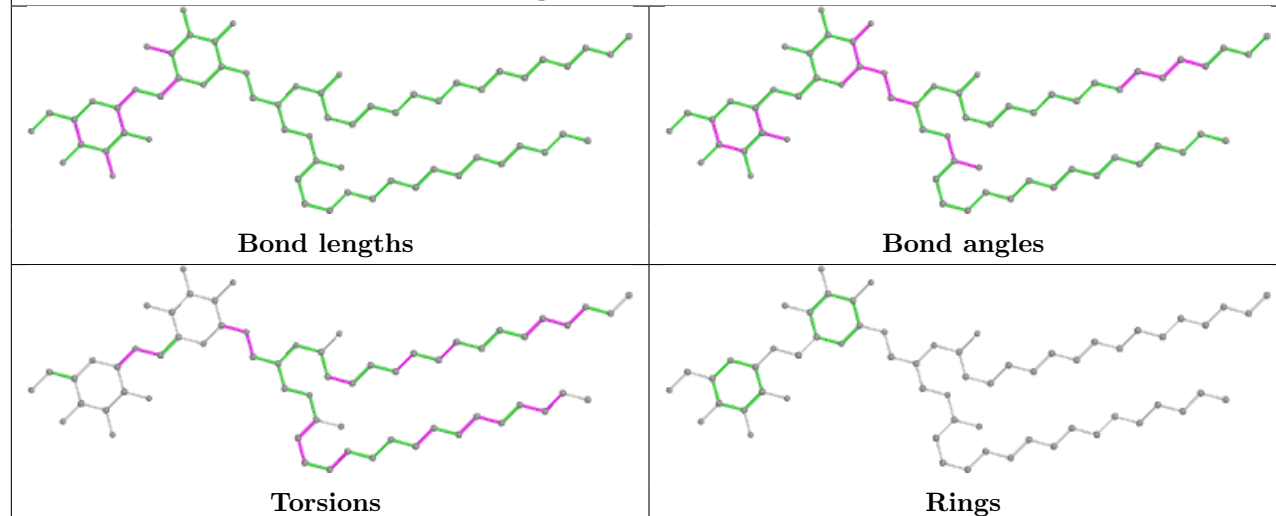




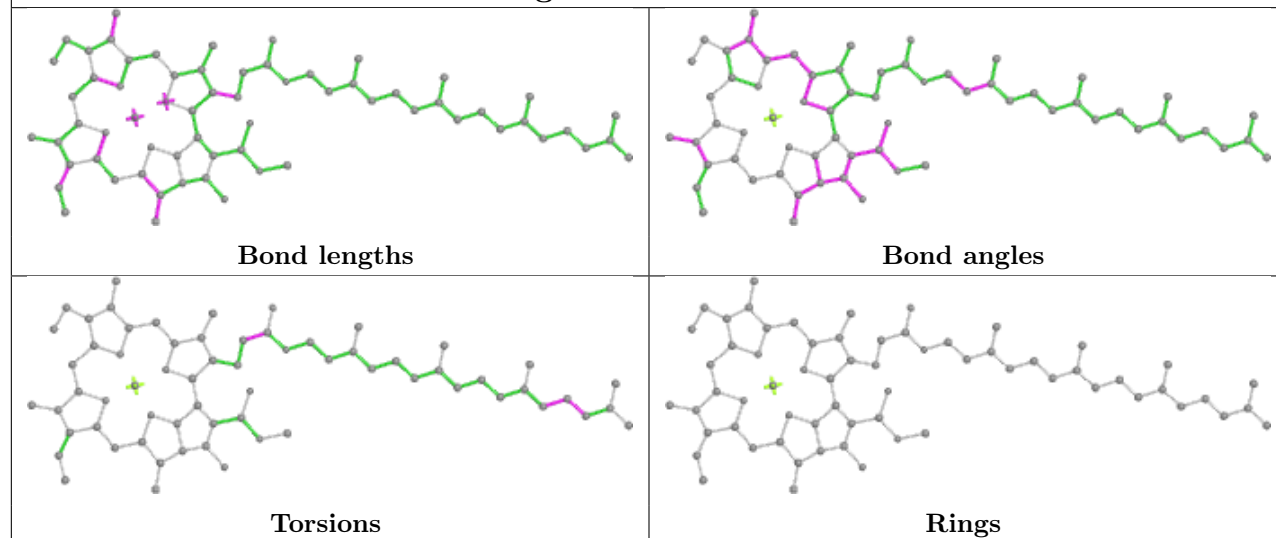
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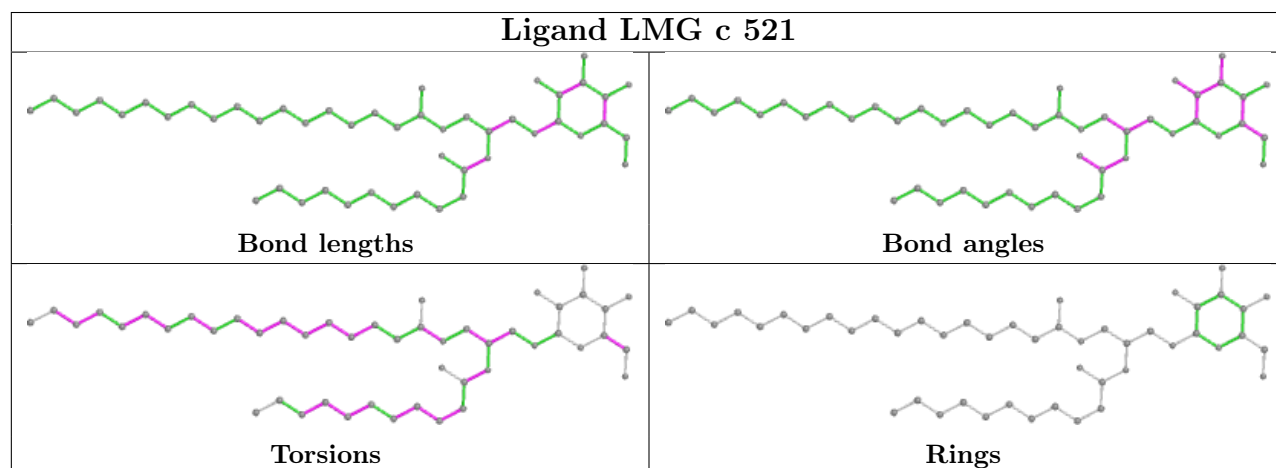
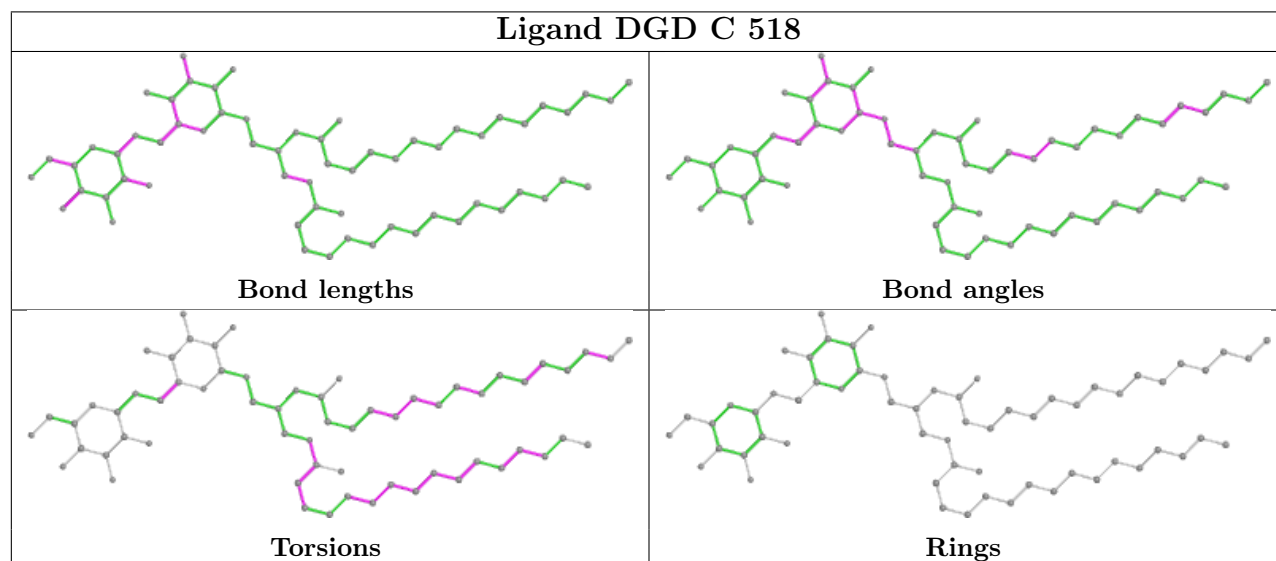
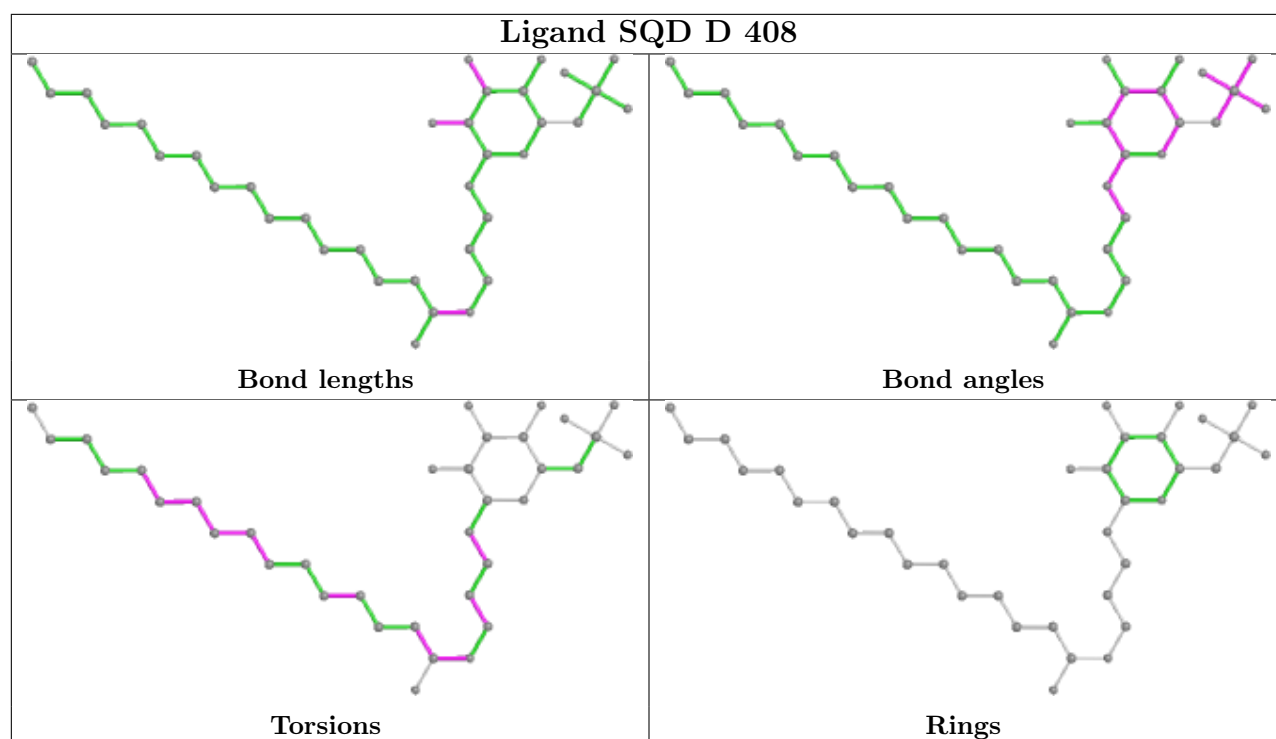


## Ligand DGD c 517

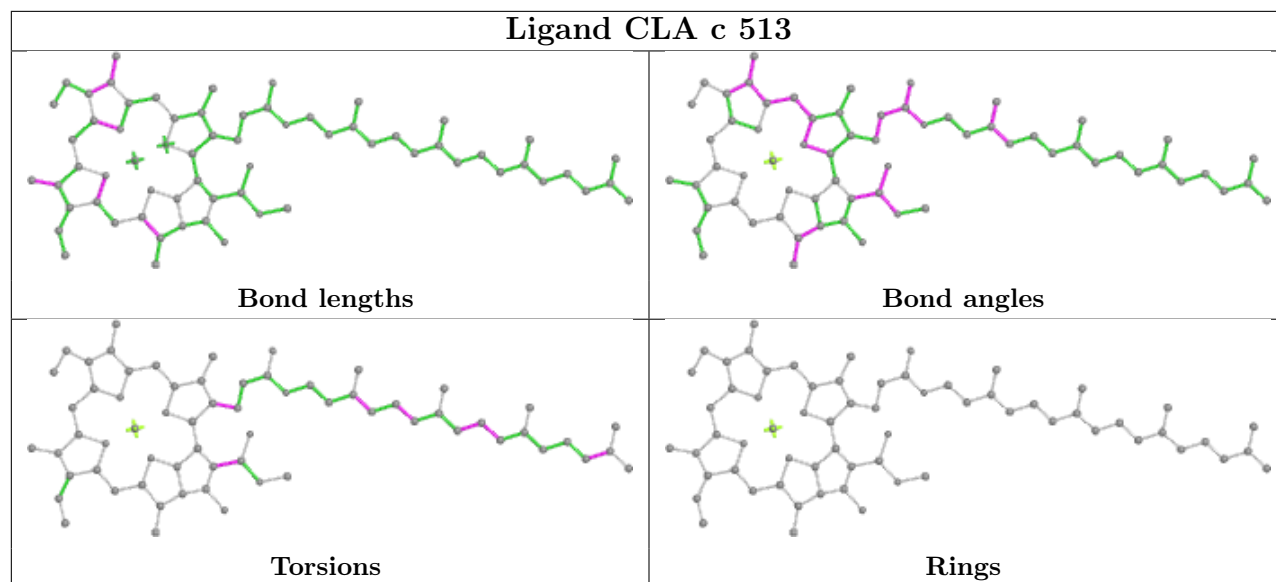


## Ligand CLA b 613

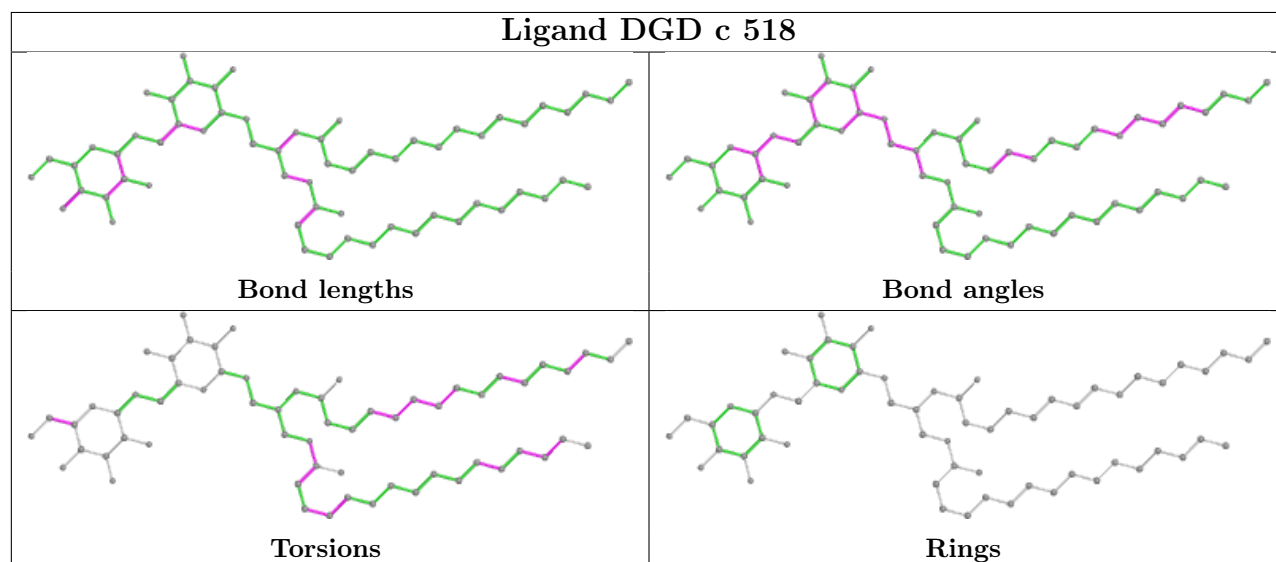




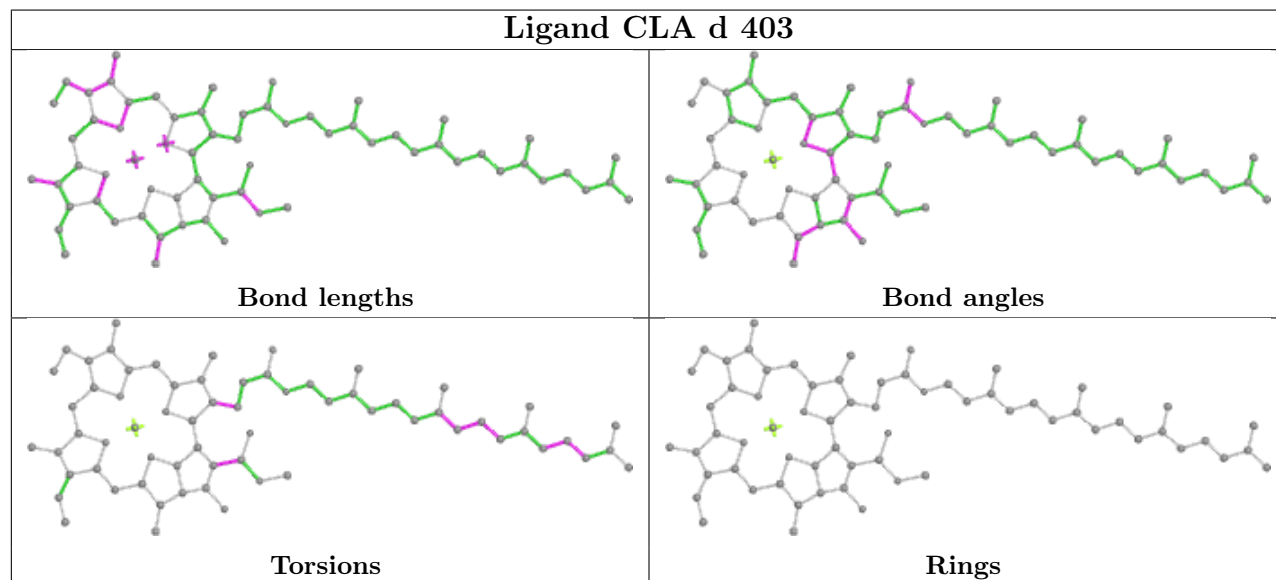
## Ligand CLA c 513



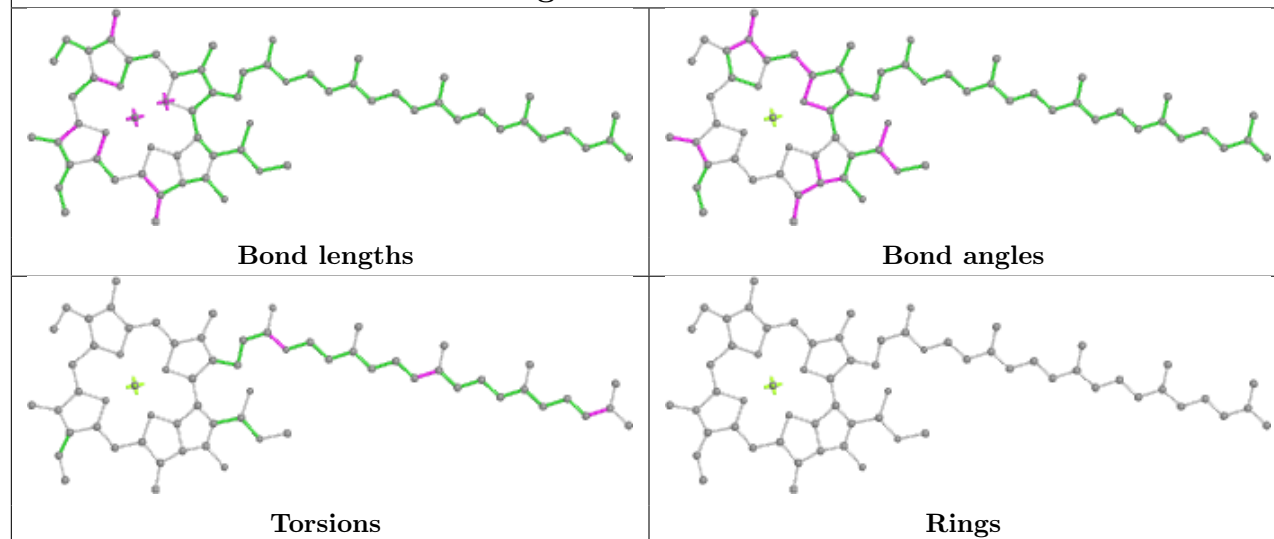
## Ligand DGD c 518



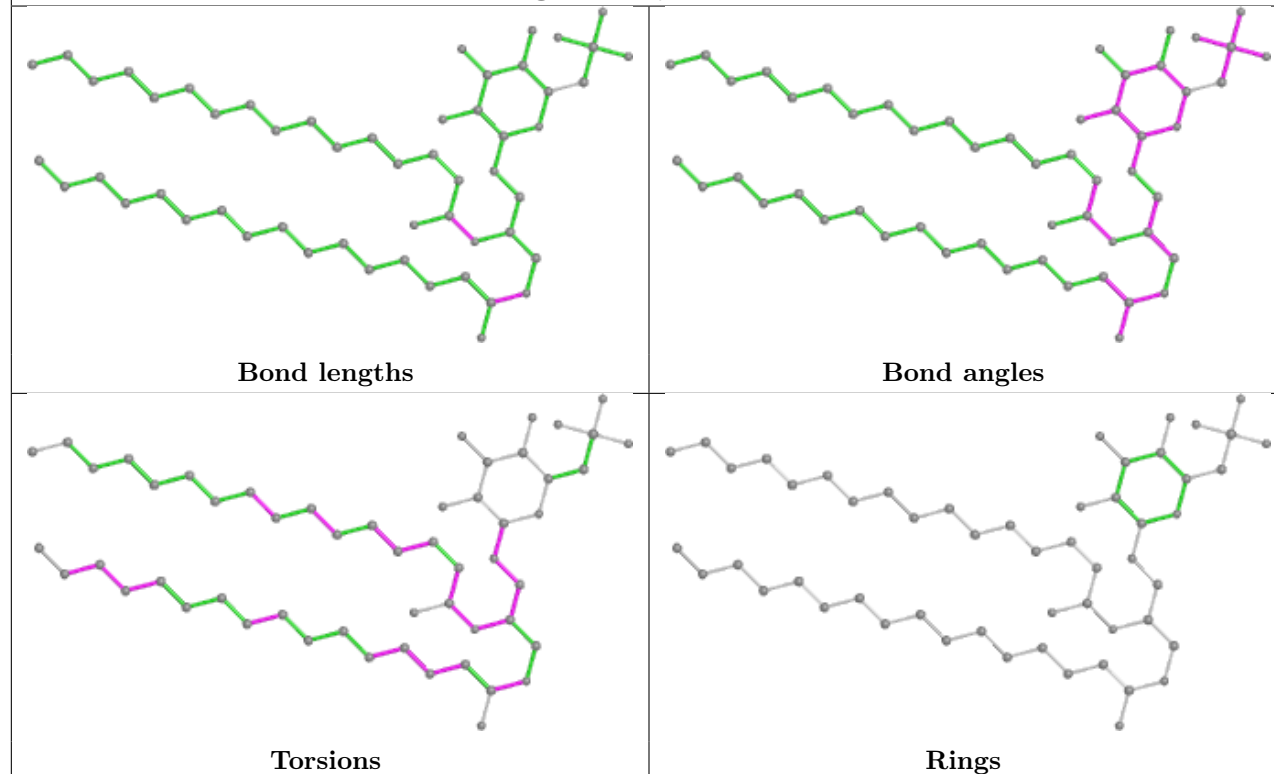
## Ligand CLA d 403

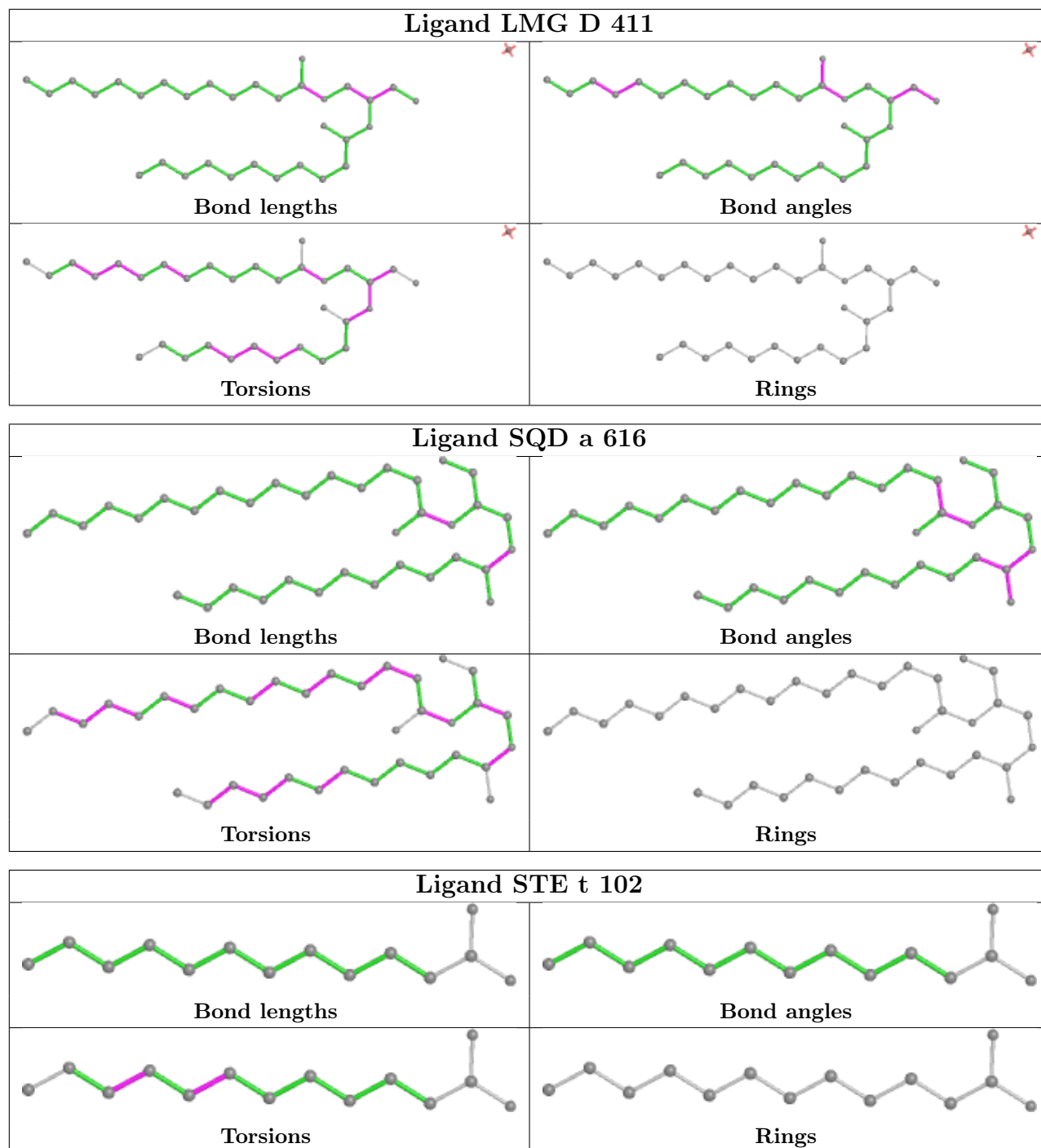


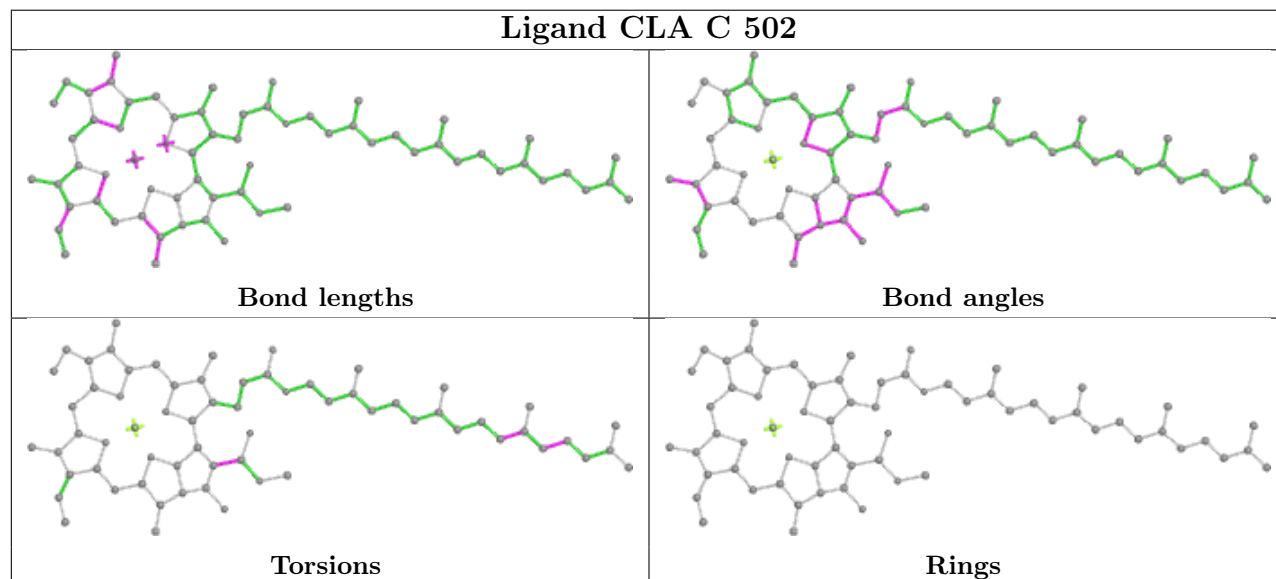
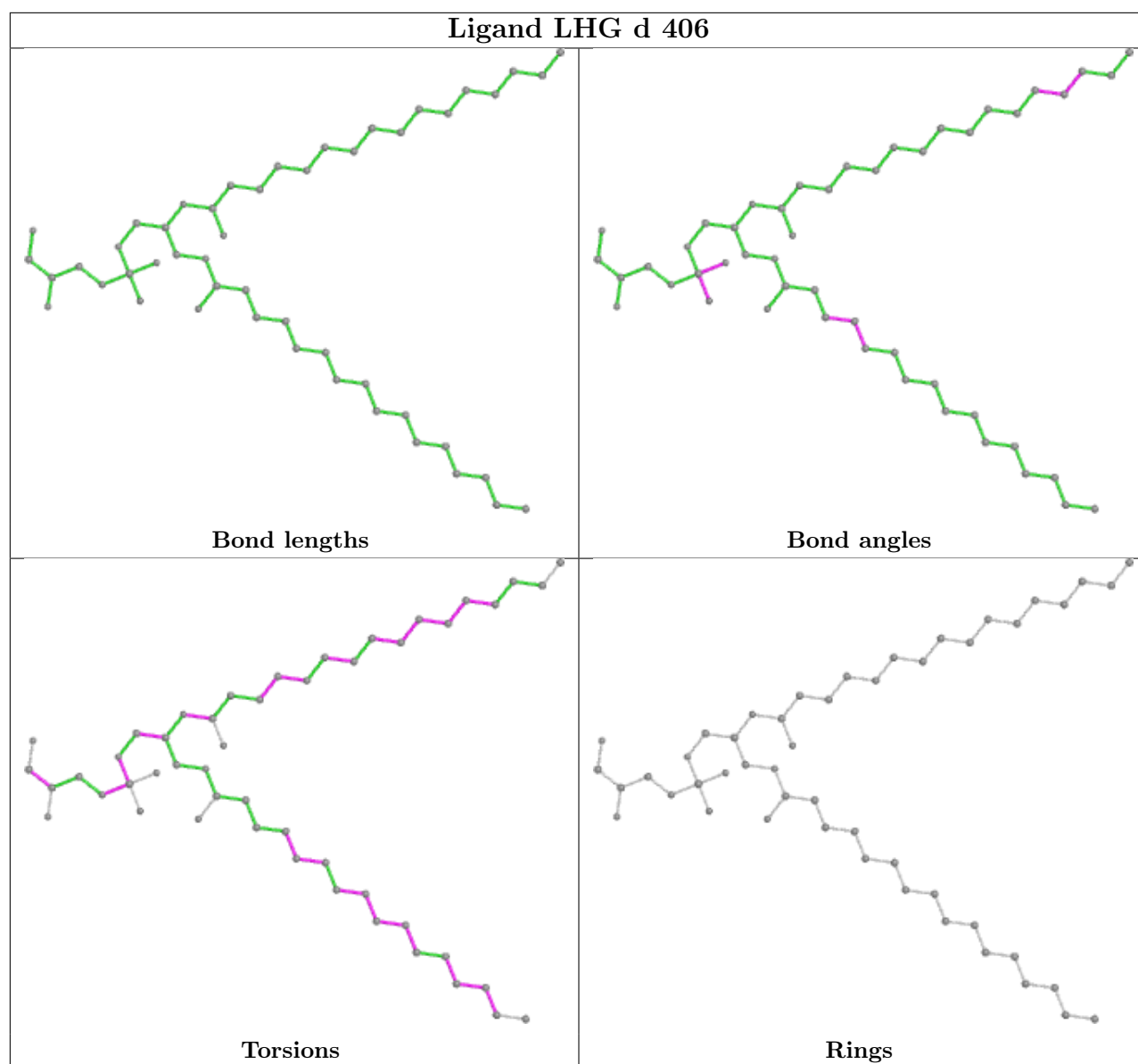
## Ligand CLA c 511



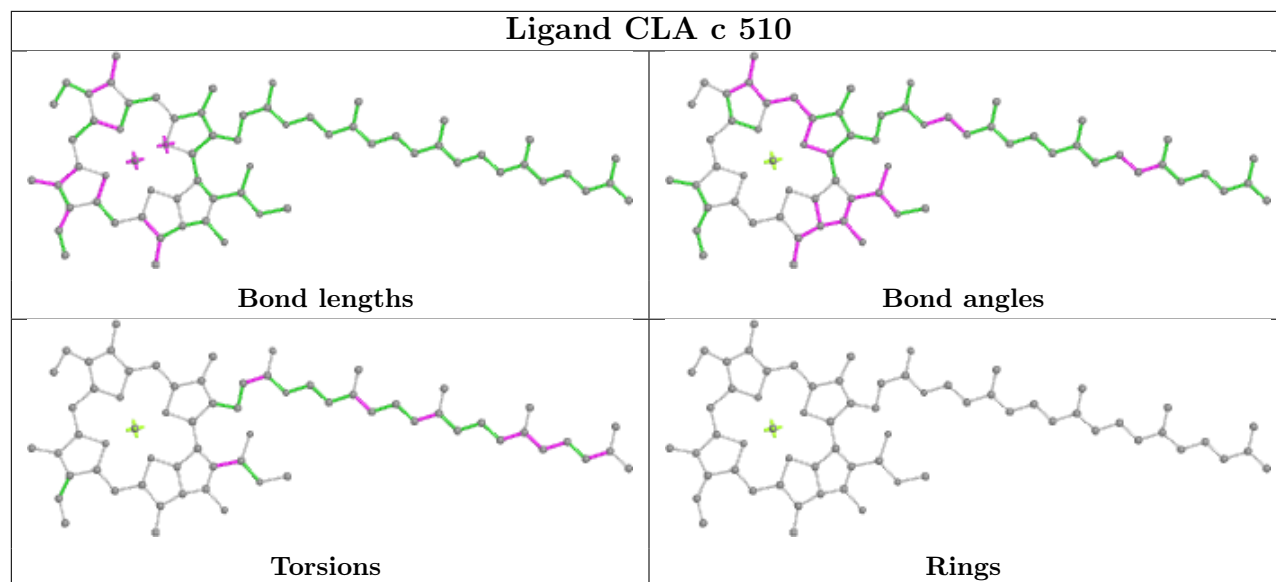
## Ligand SQD B 620



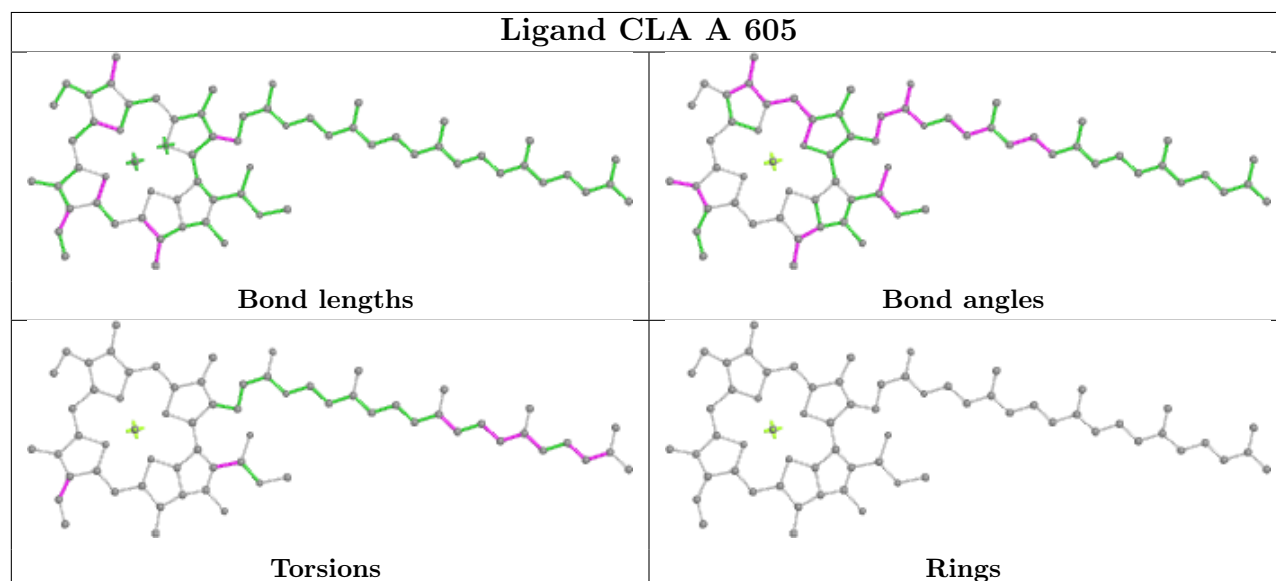




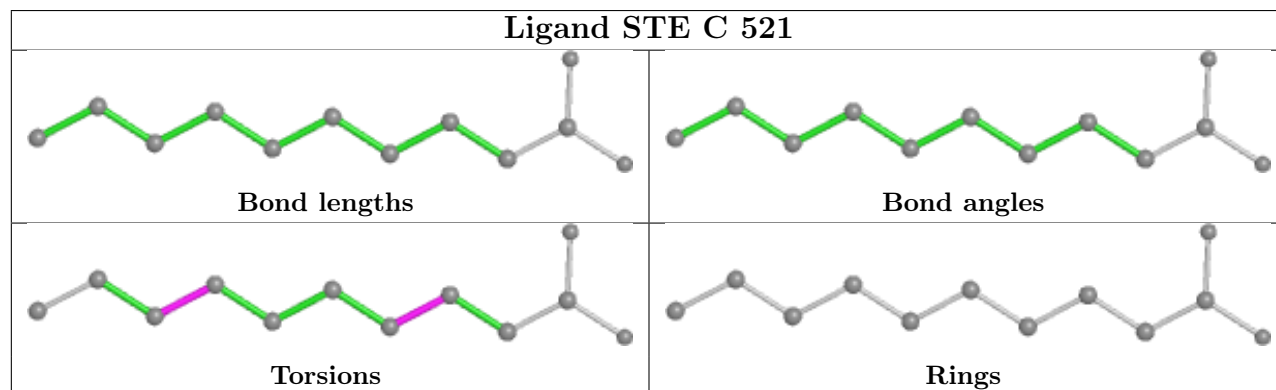
## Ligand CLA c 510



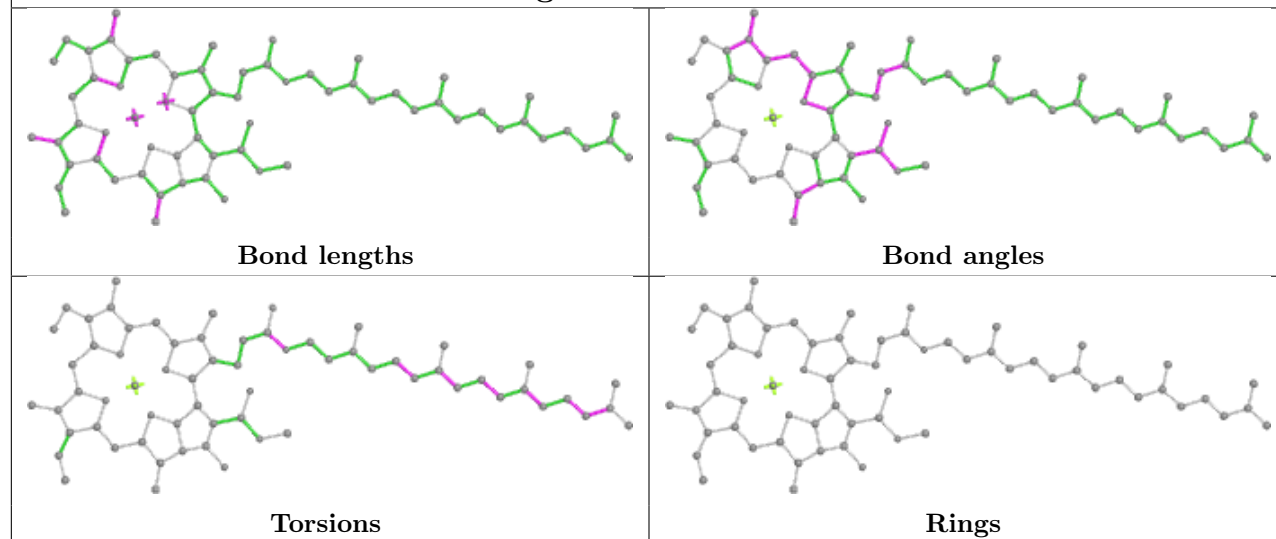
## Ligand CLA A 605



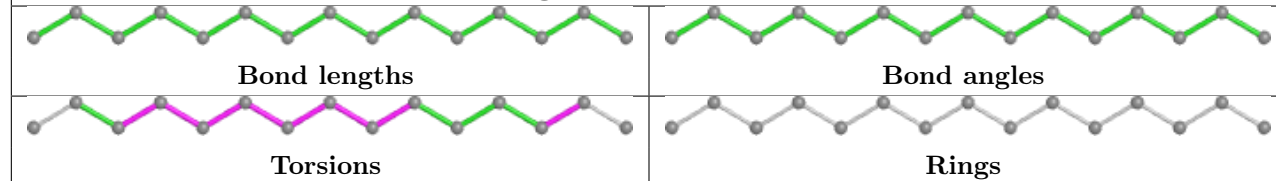
## Ligand STE C 521



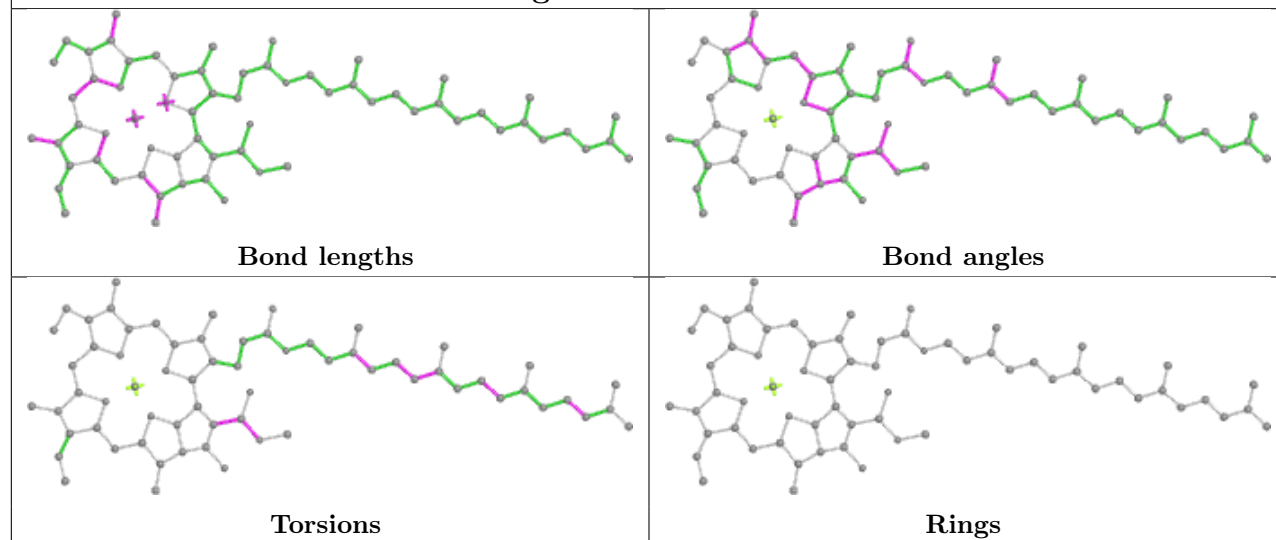
## Ligand CLA a 607

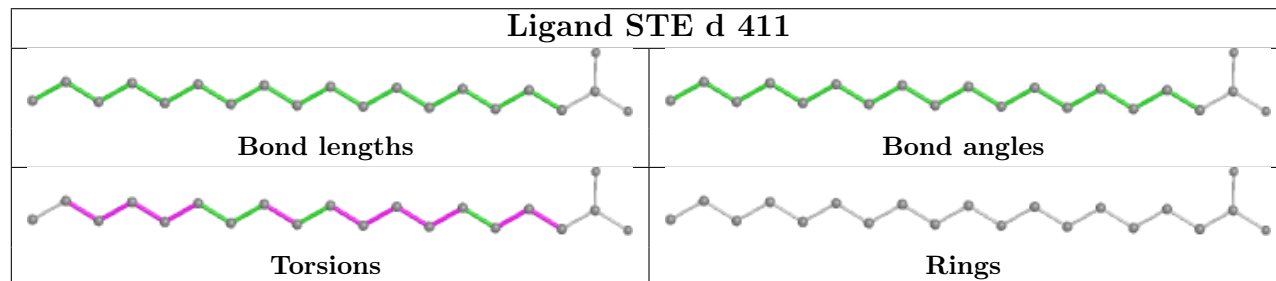
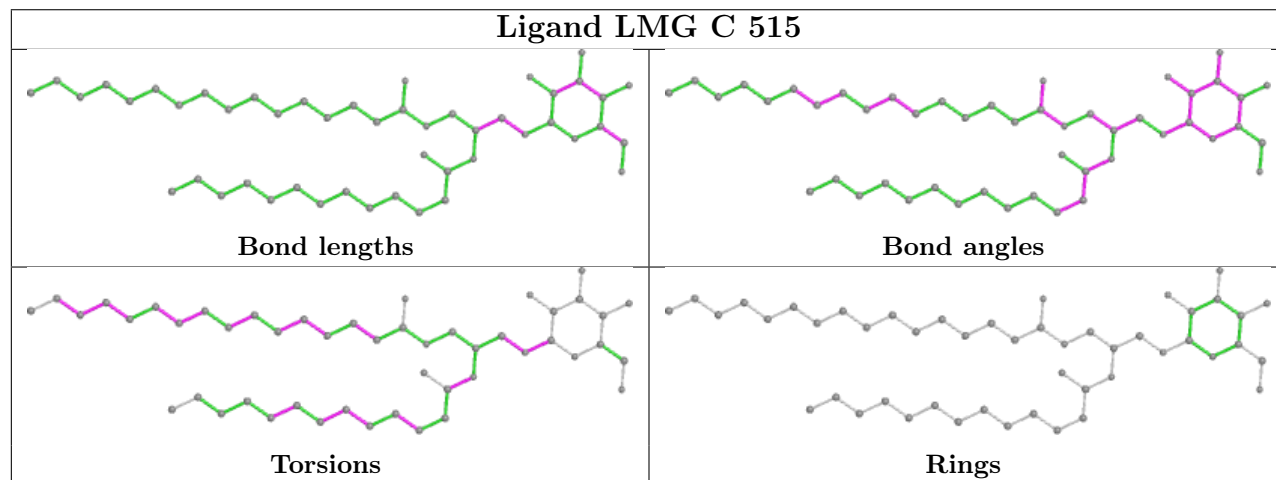
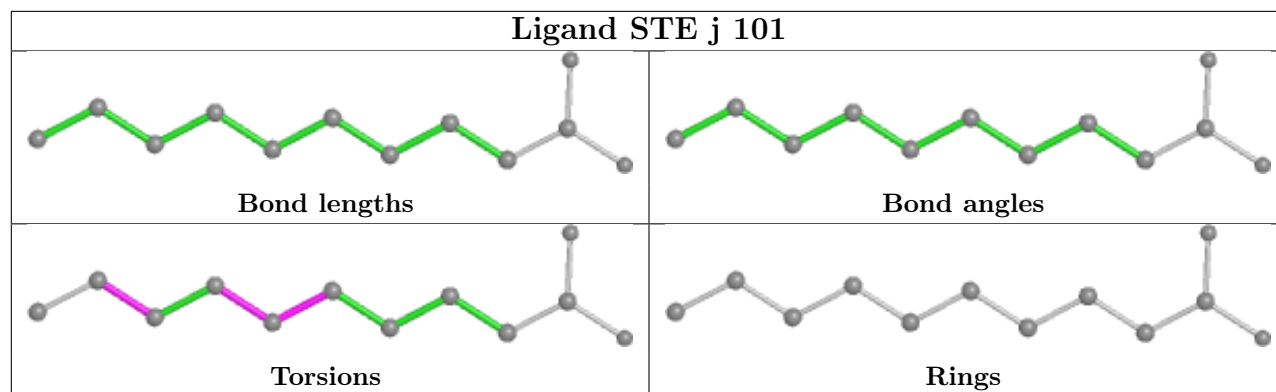


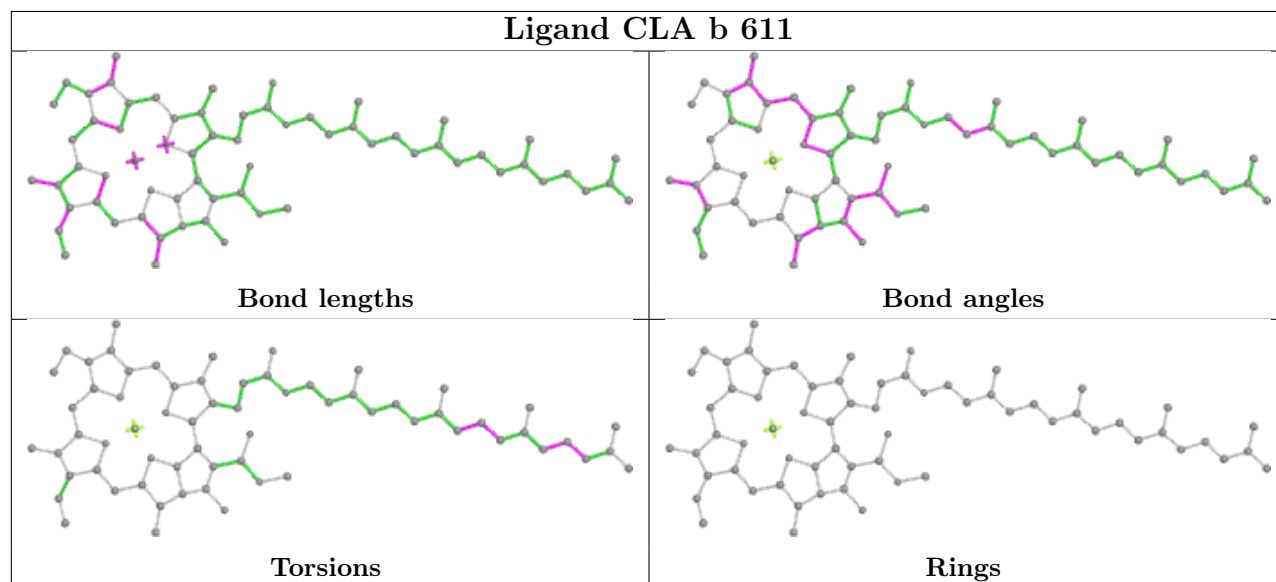
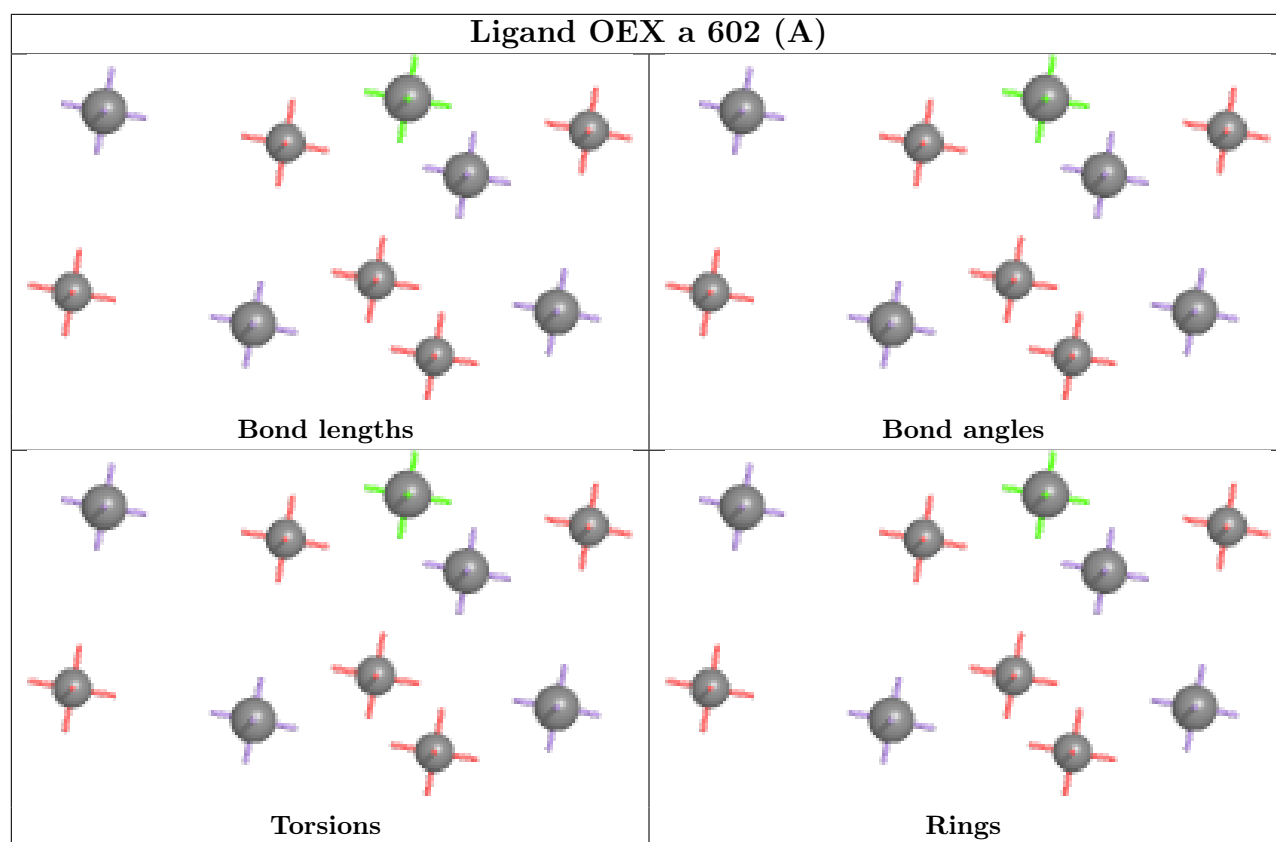
## Ligand STE T 103

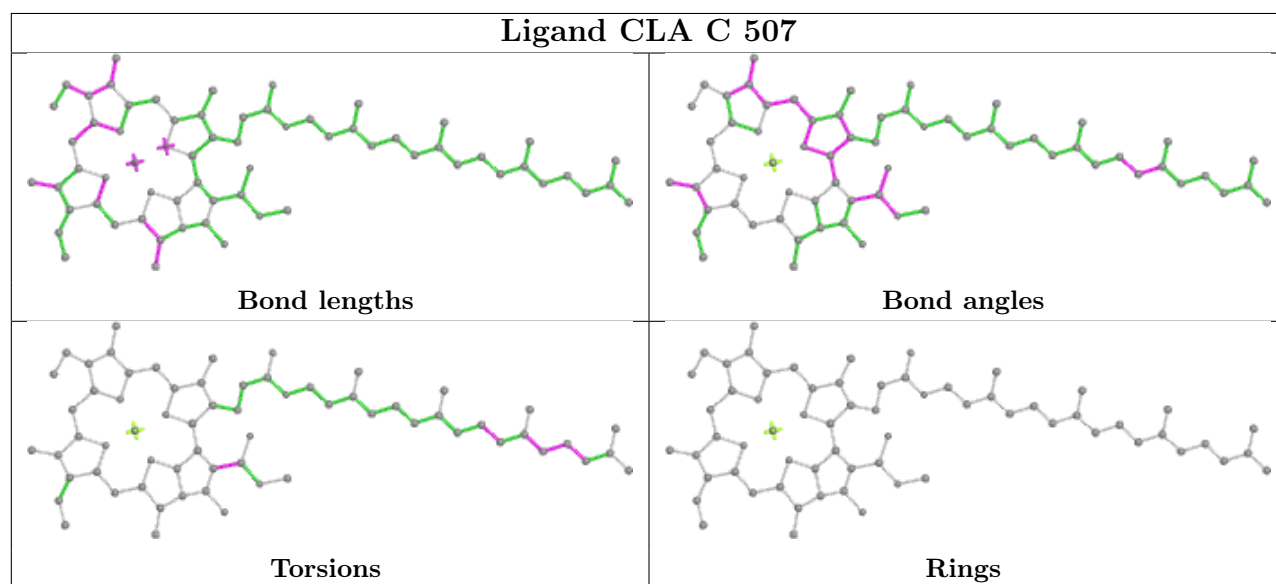
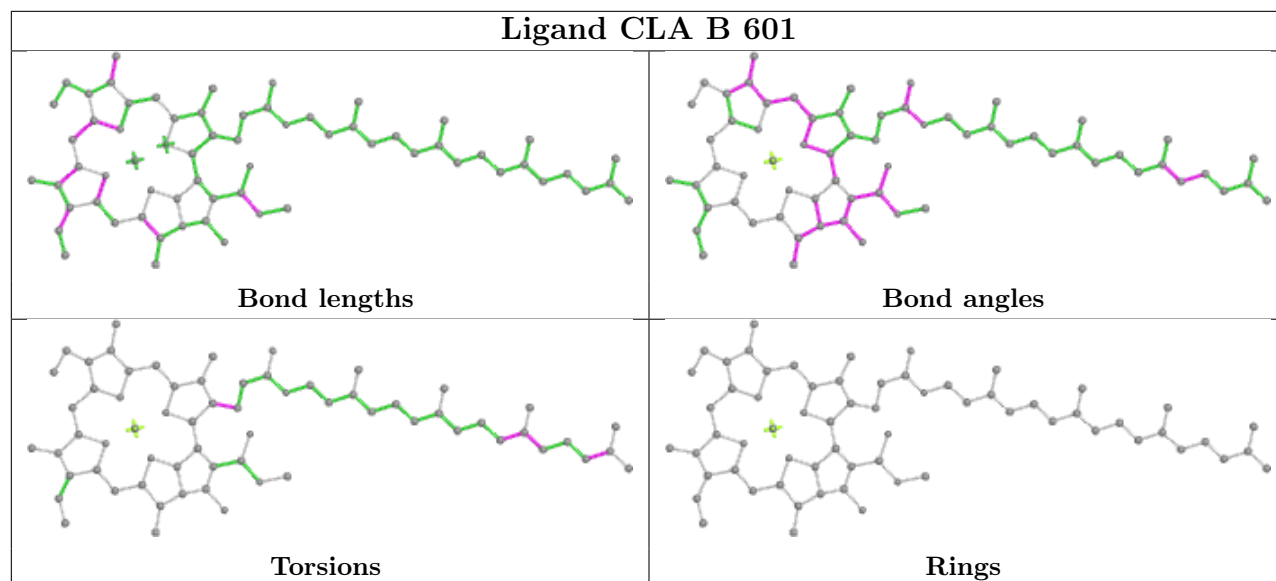
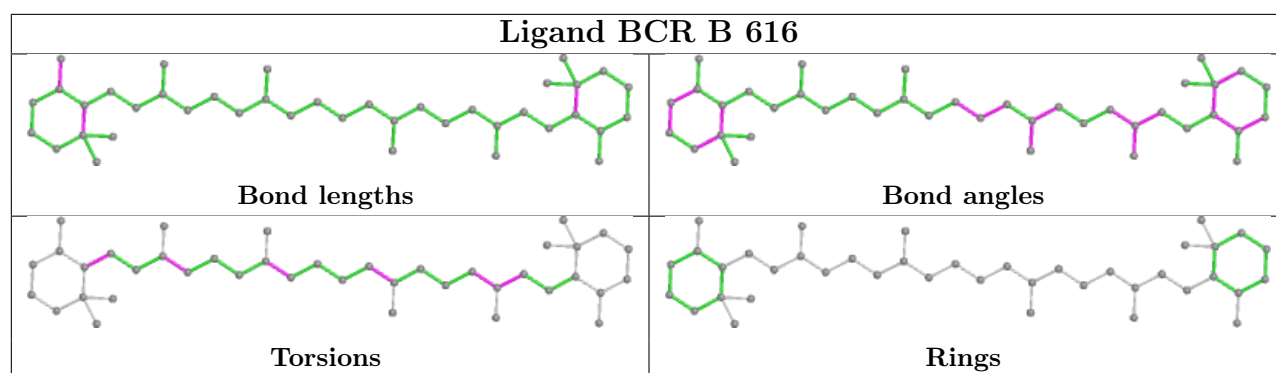


## Ligand CLA C 513

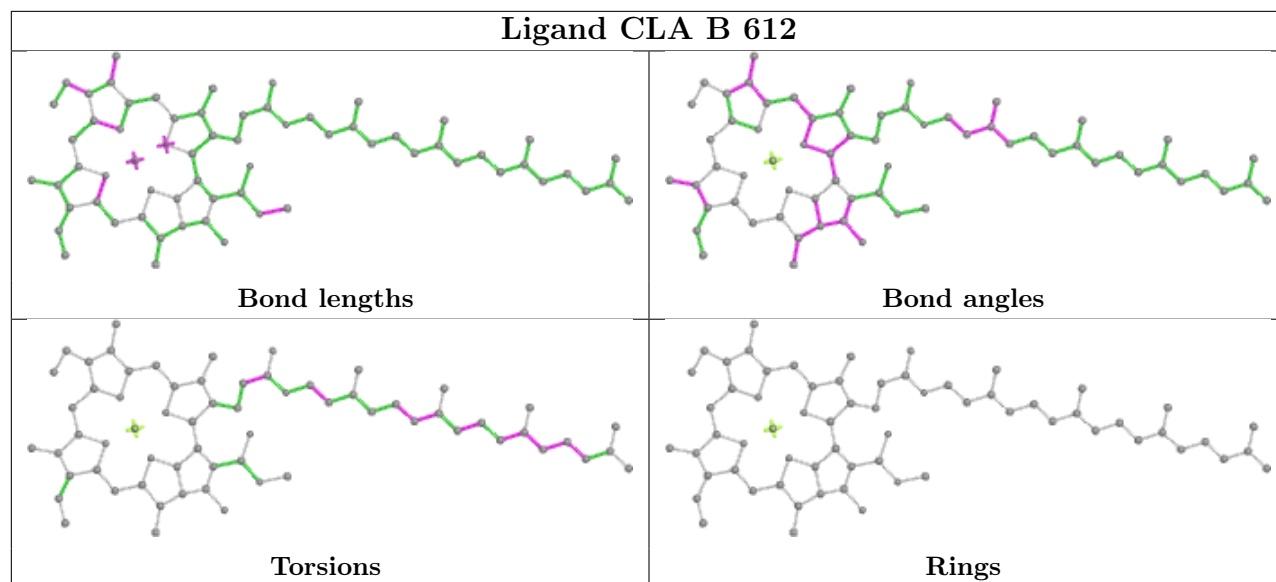




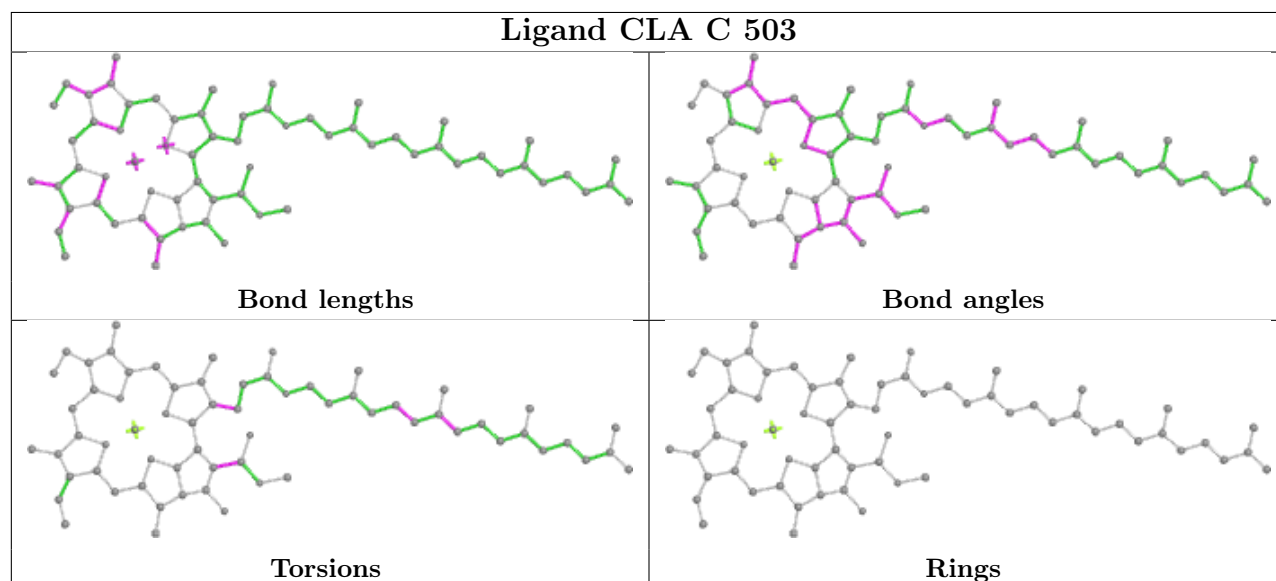




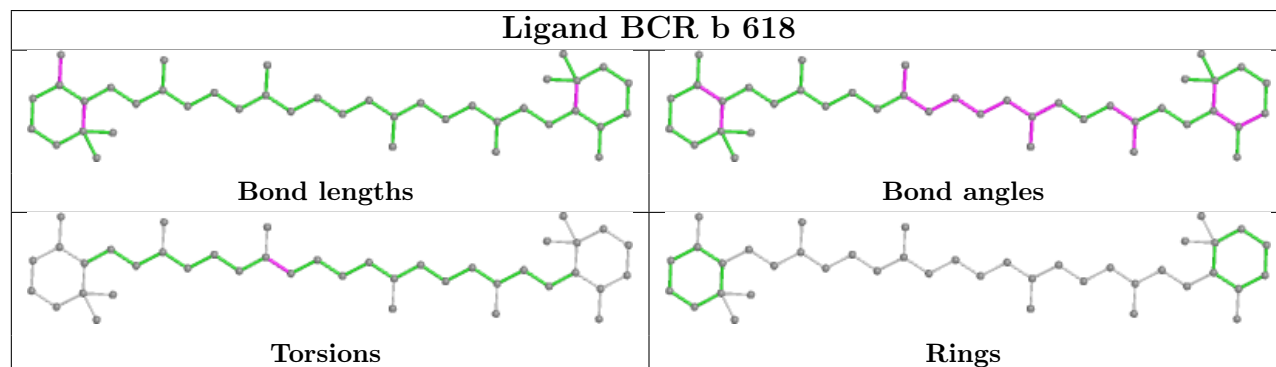
## Ligand CLA B 612



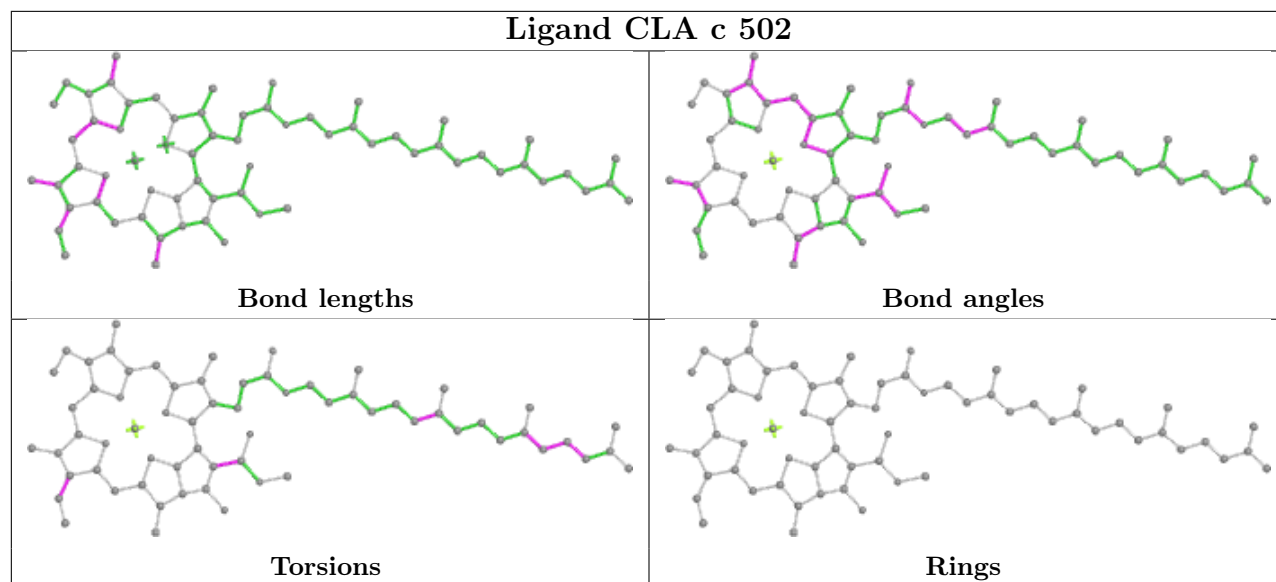
## Ligand CLA C 503



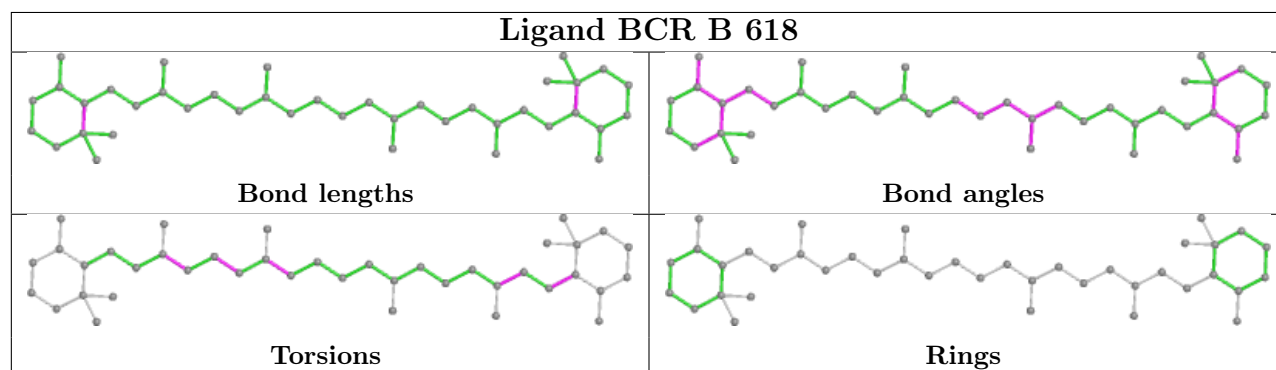
## Ligand BCR b 618



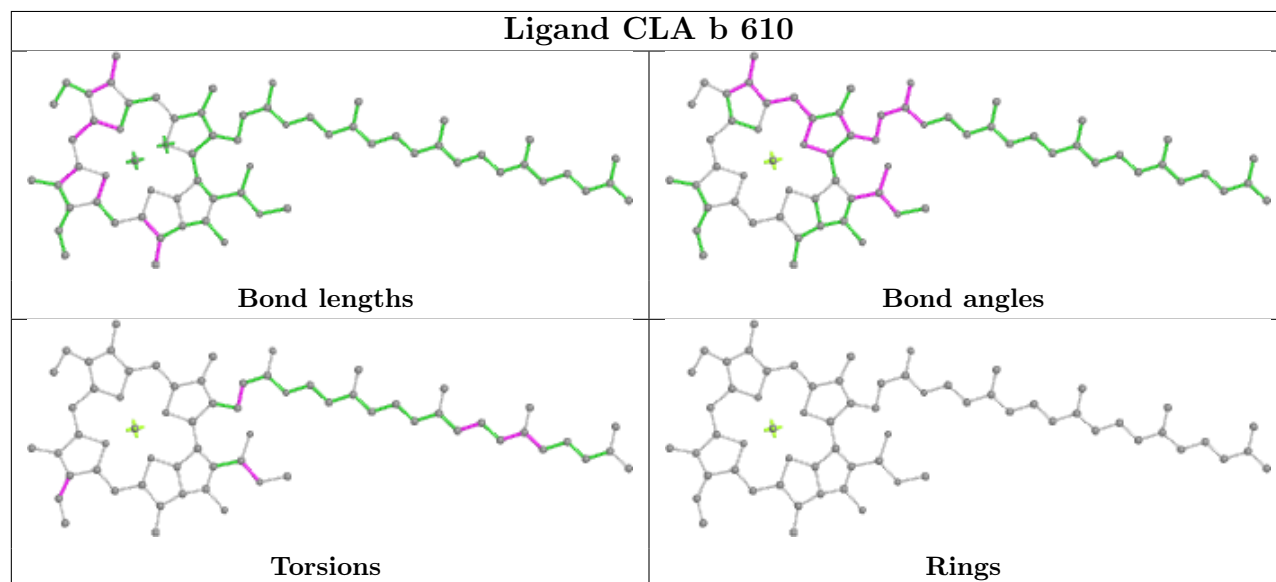
## Ligand CLA c 502



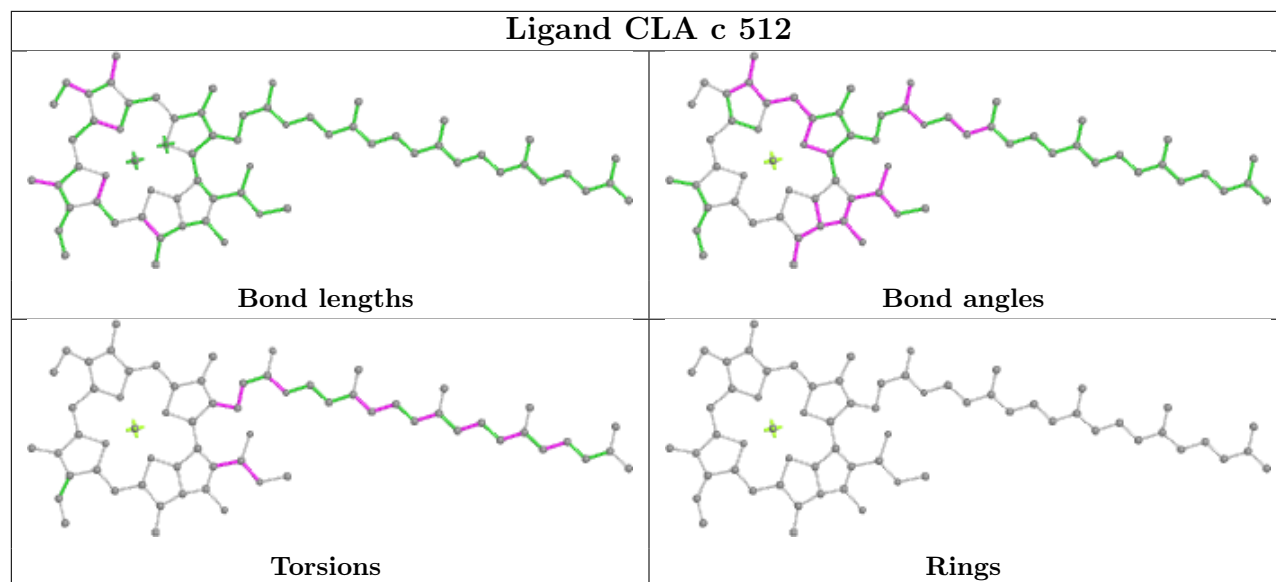
## Ligand BCR B 618



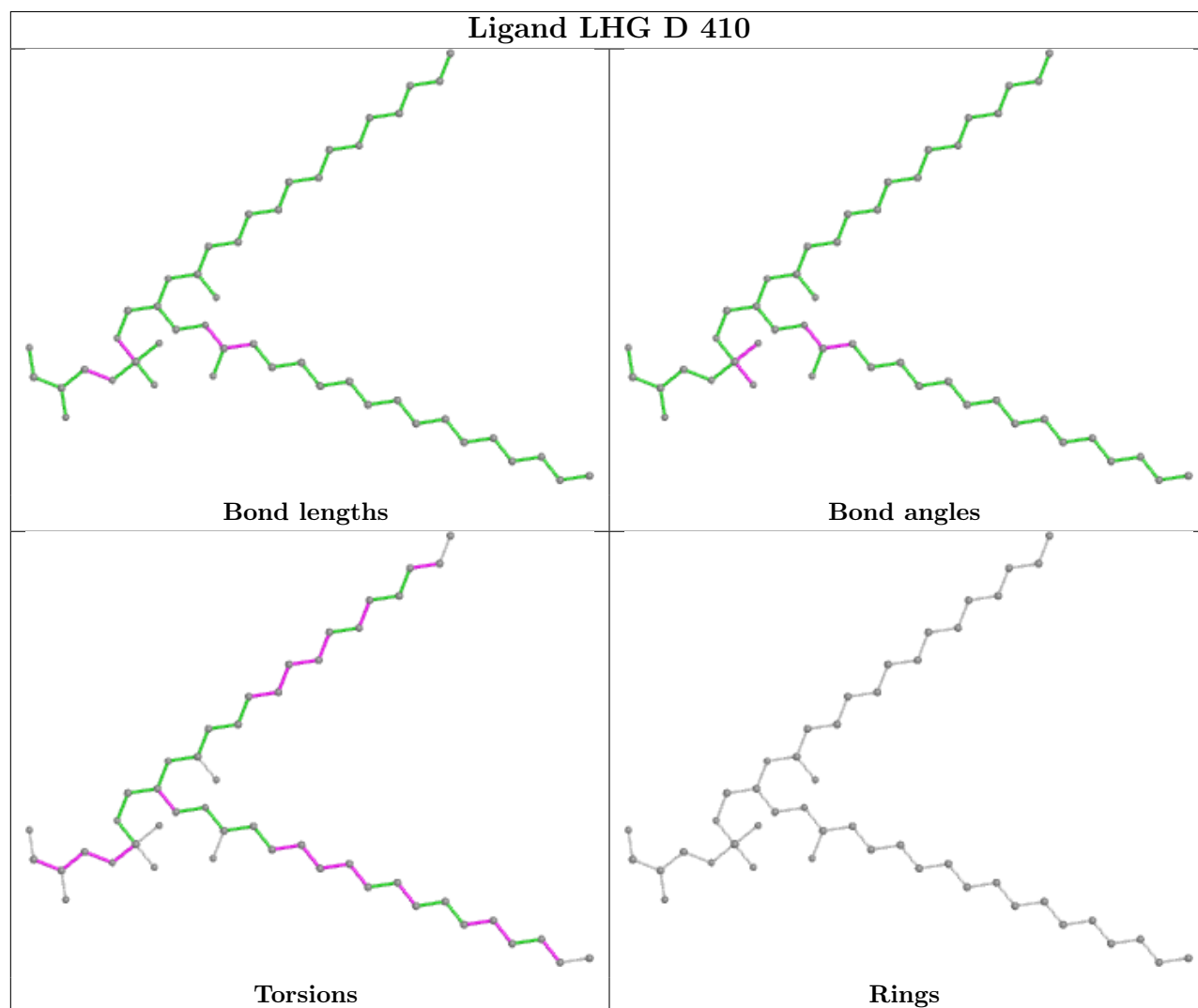
## Ligand CLA b 610

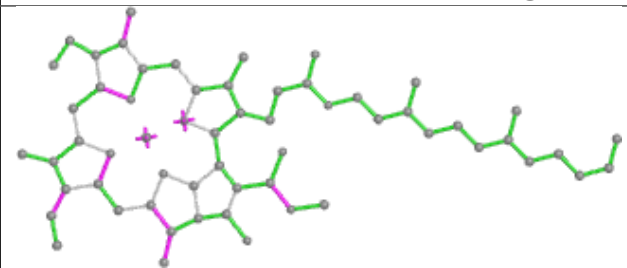
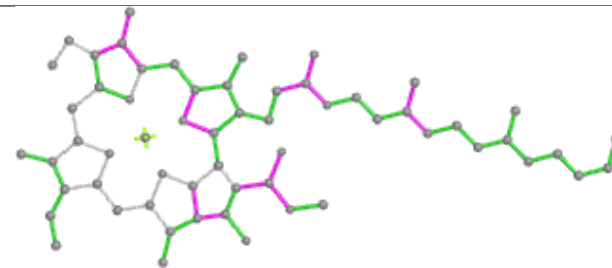
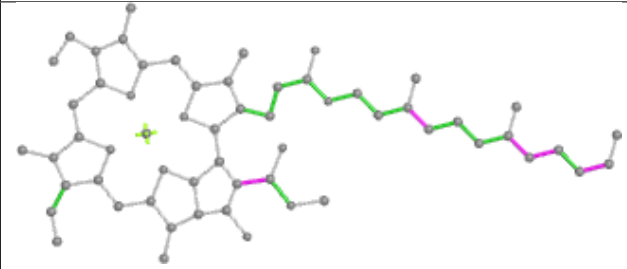
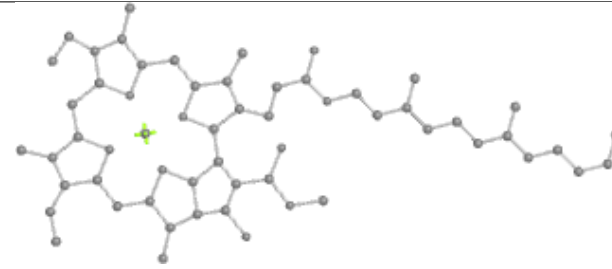


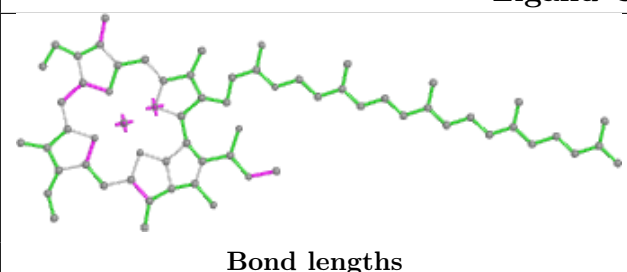
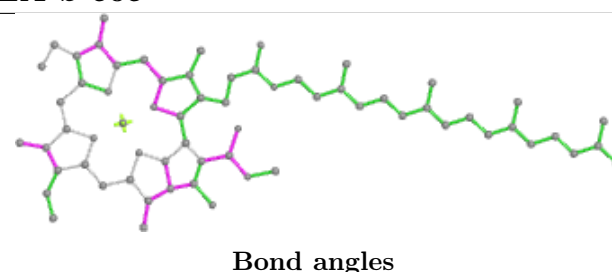
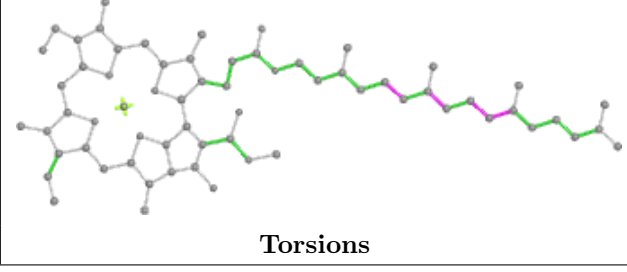
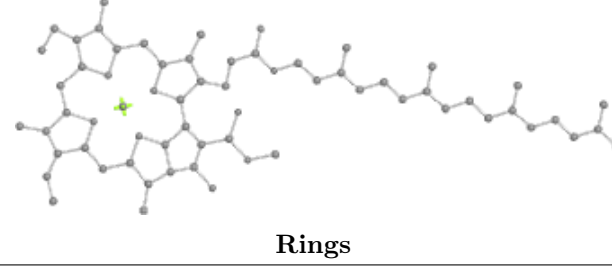
## Ligand CLA c 512

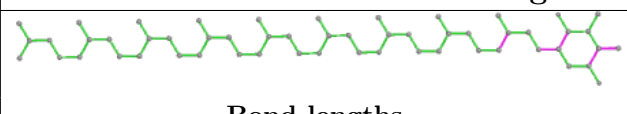
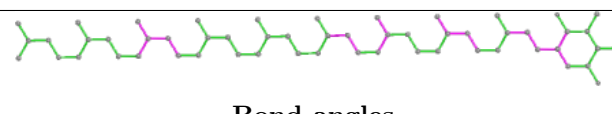
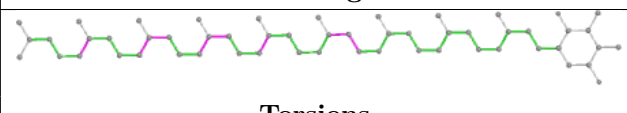
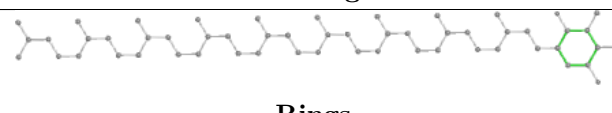


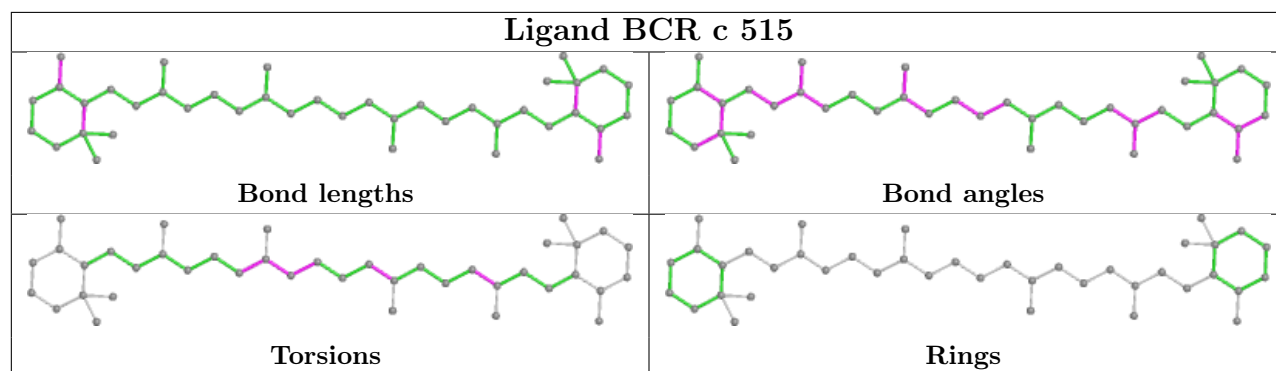
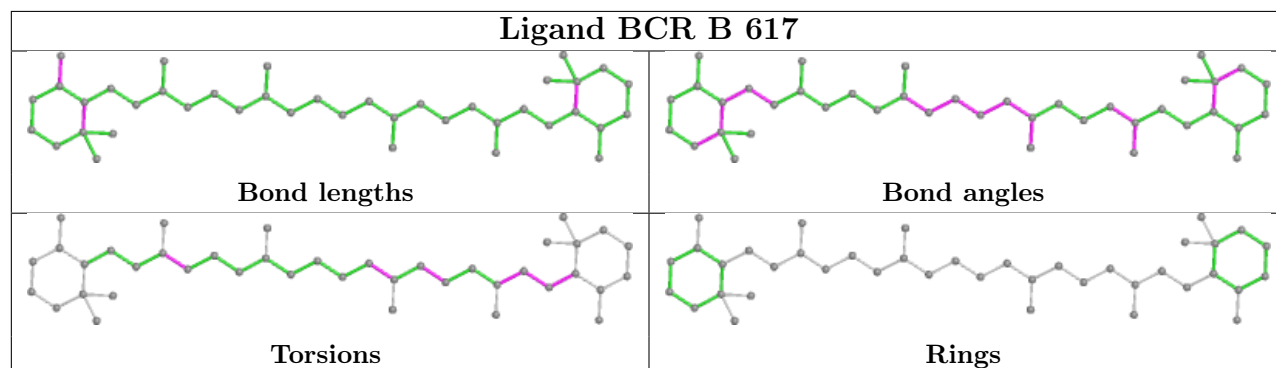
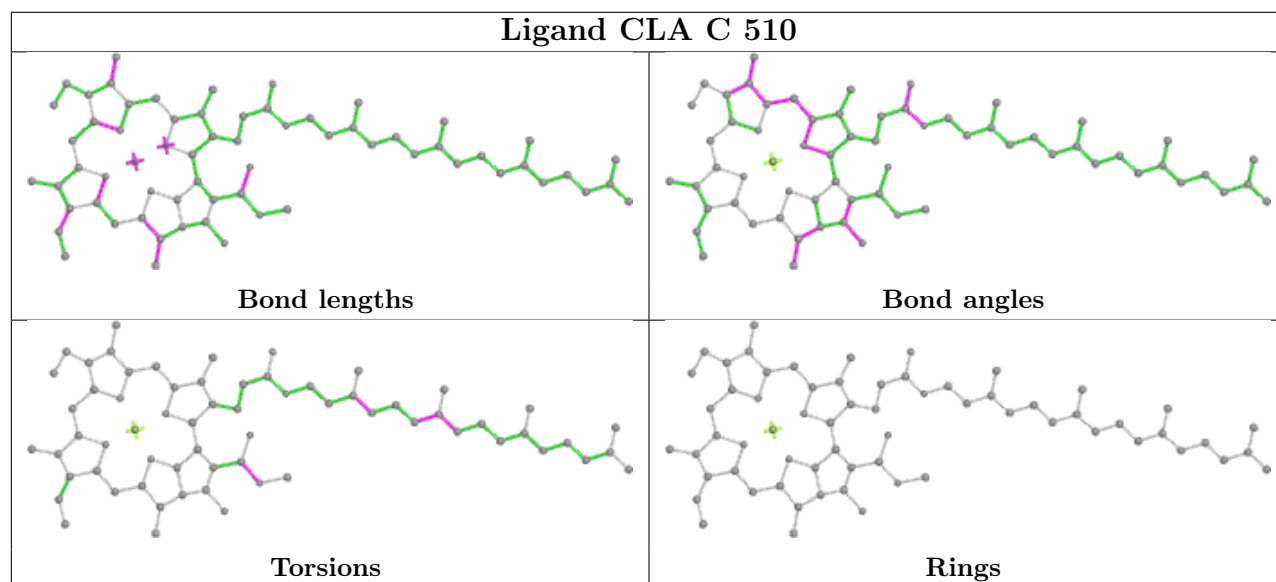
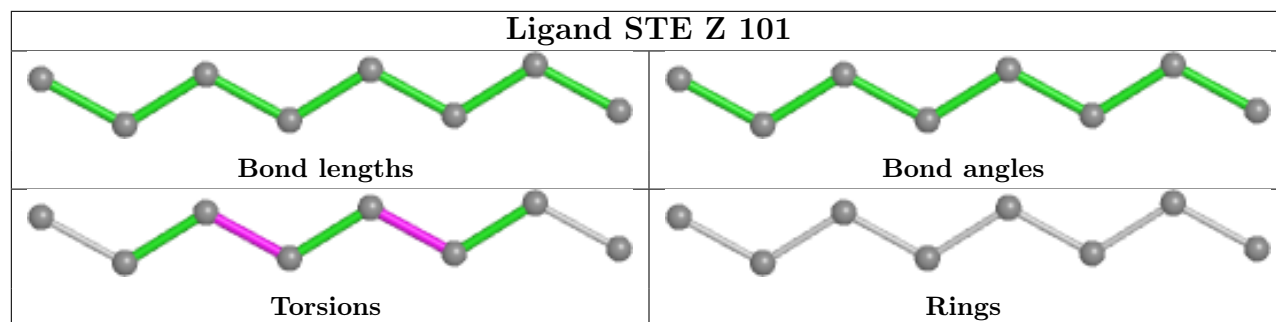
## Ligand LHG D 410



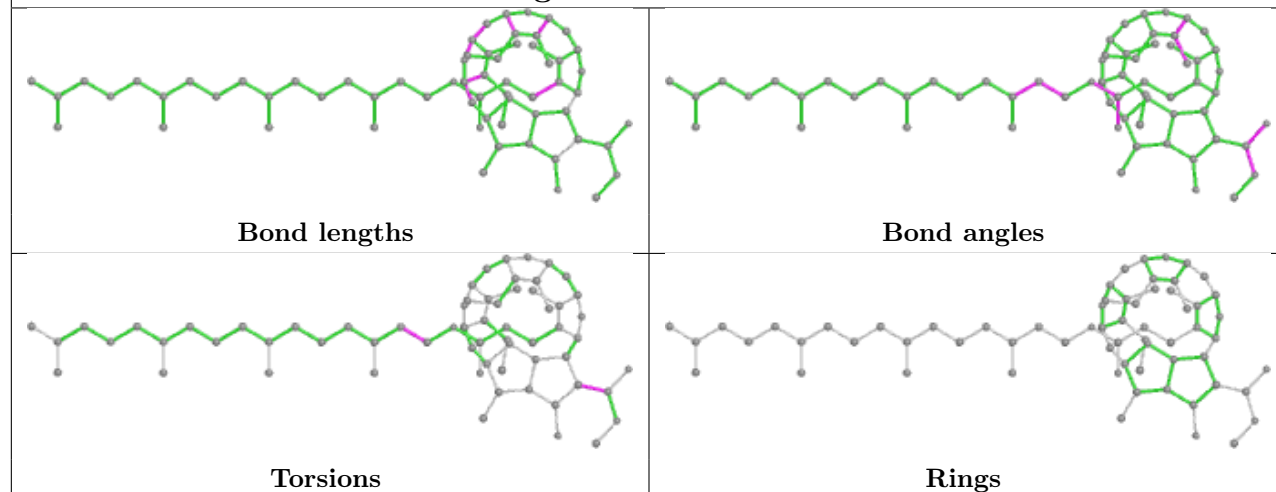
Ligand CLA C 504	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

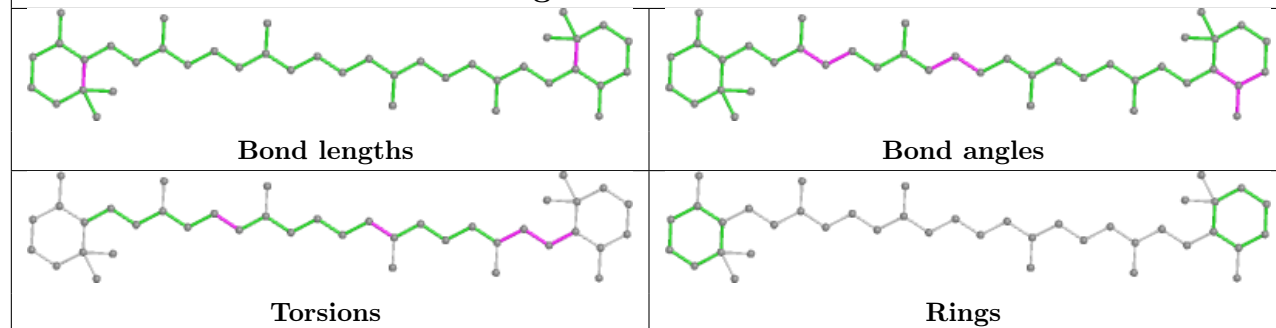
Ligand PL9 d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings



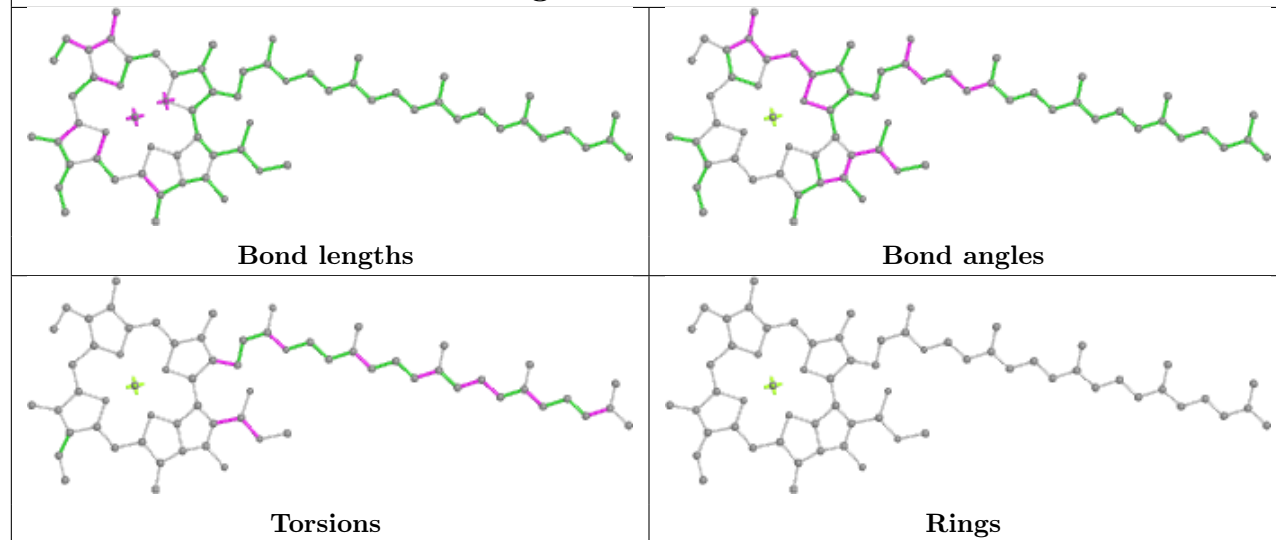
## Ligand PHO a 606

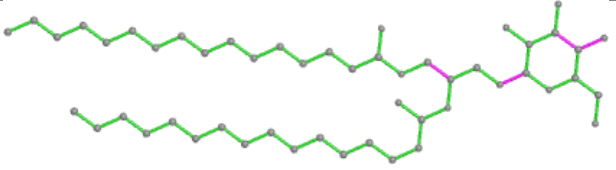
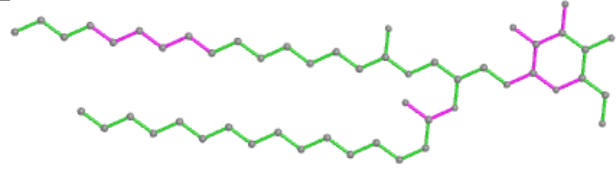
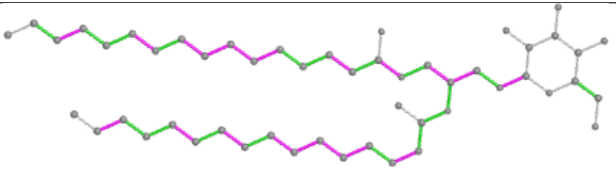
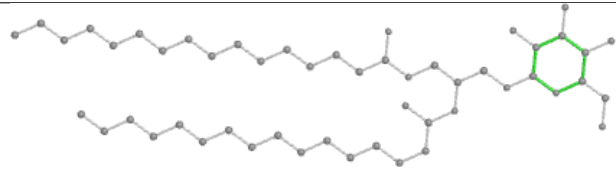


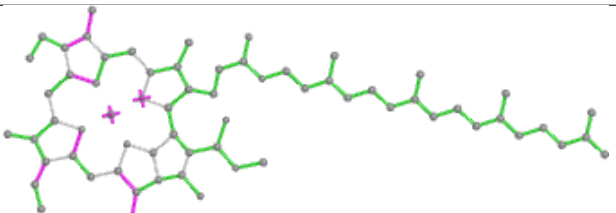
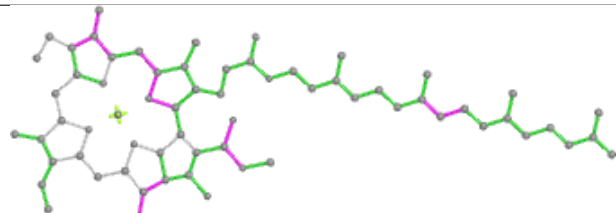
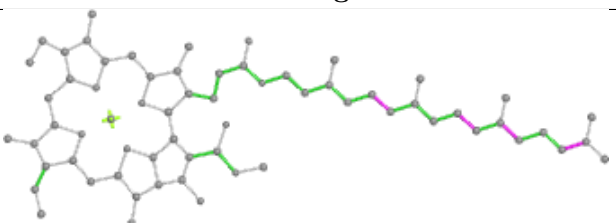
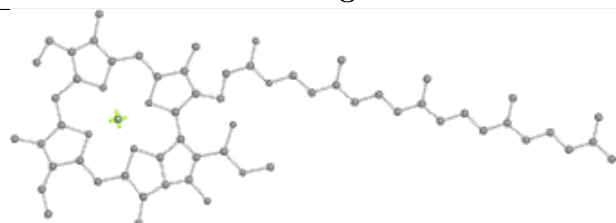
## Ligand BCR d 404

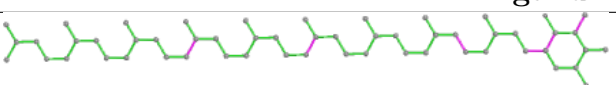
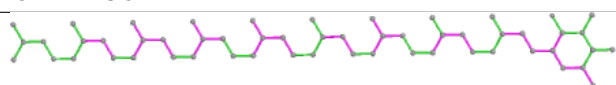
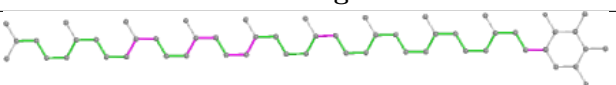
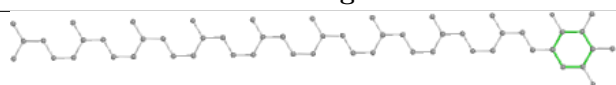


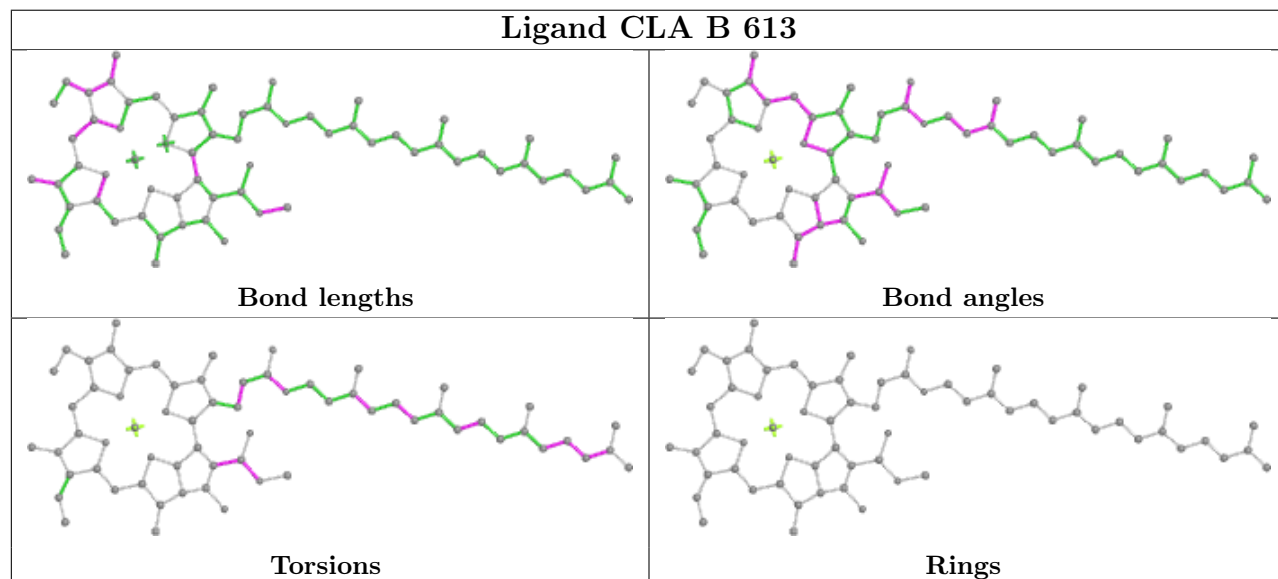
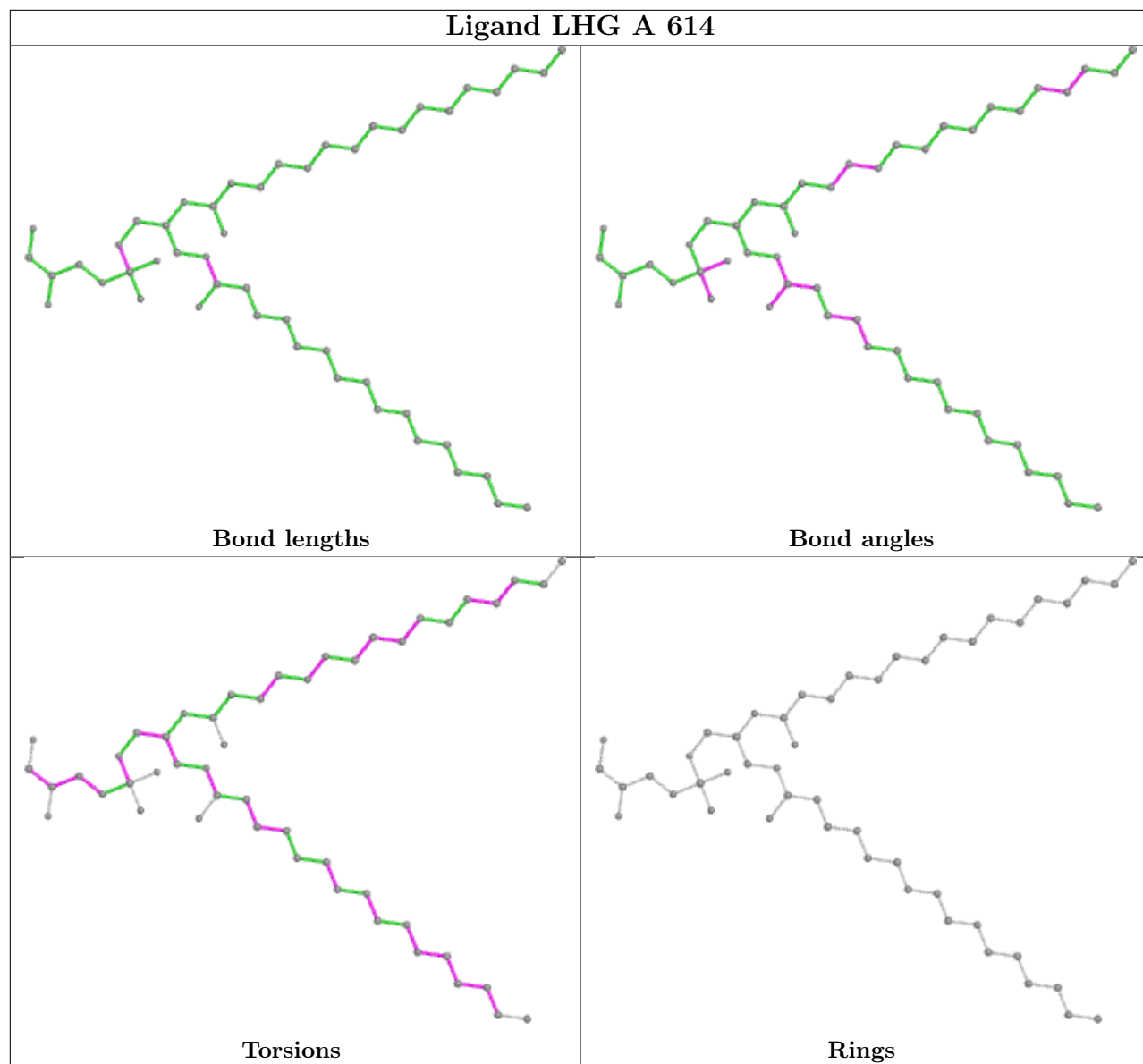
## Ligand CLA H 101



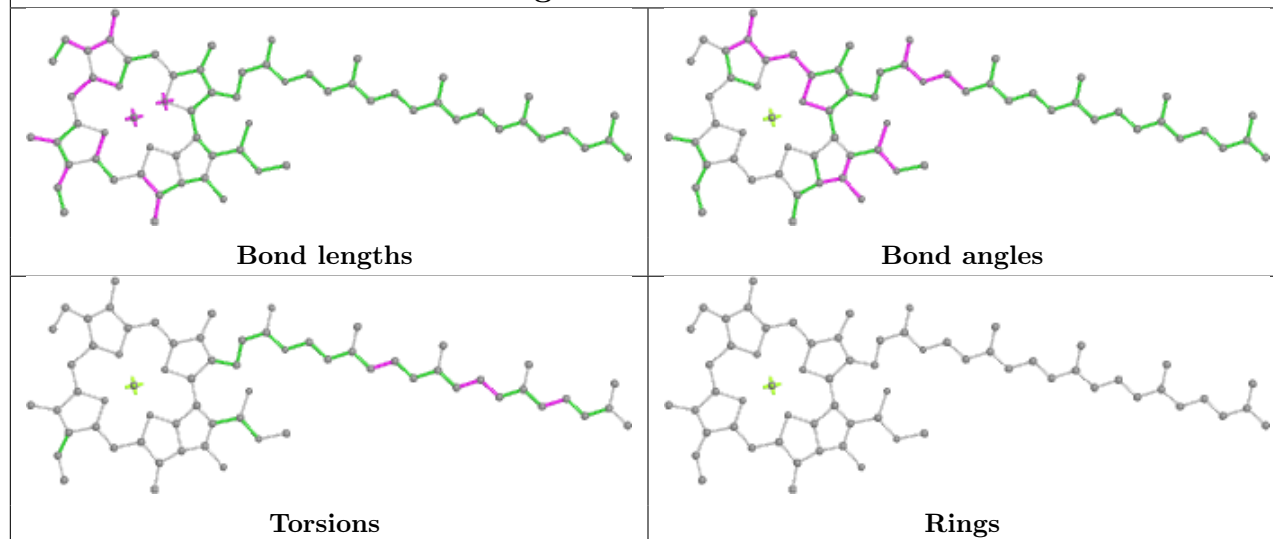
Ligand LMG M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

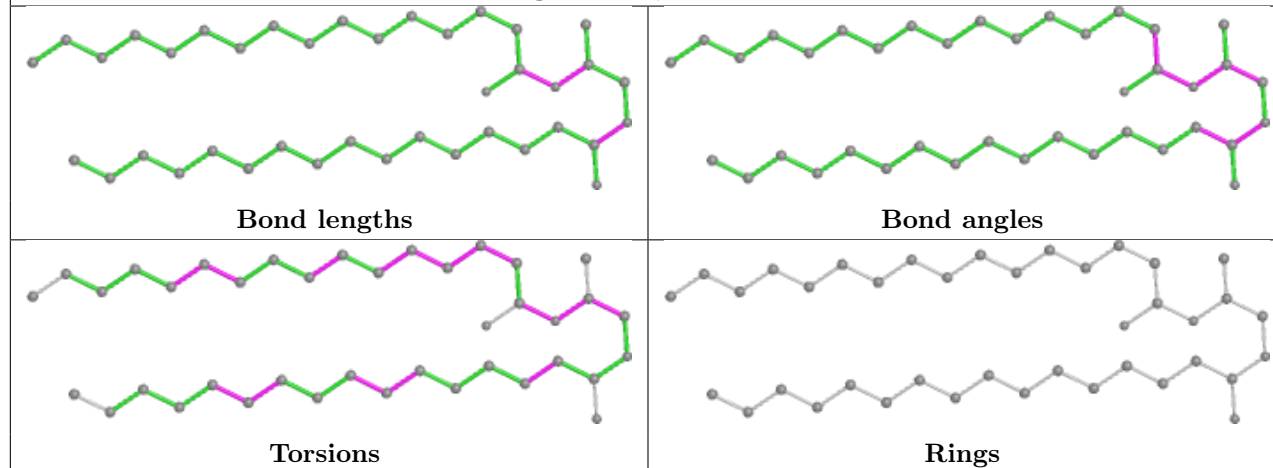
Ligand PL9 D 406	
	
Bond lengths	Bond angles
	
Torsions	Rings



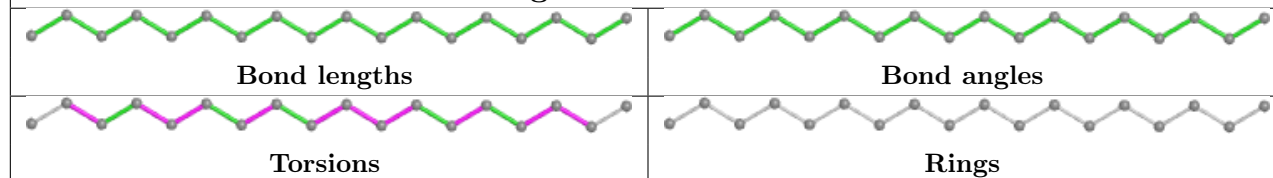
## Ligand CLA b 603

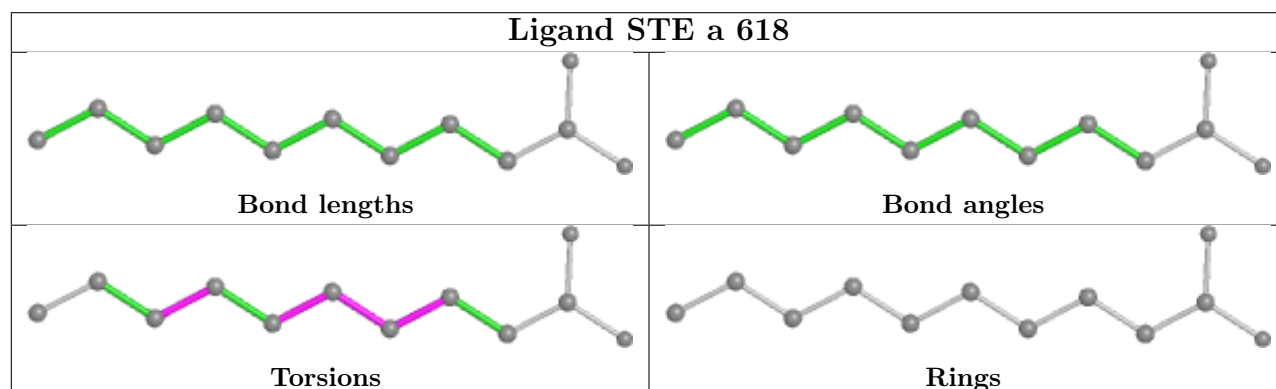
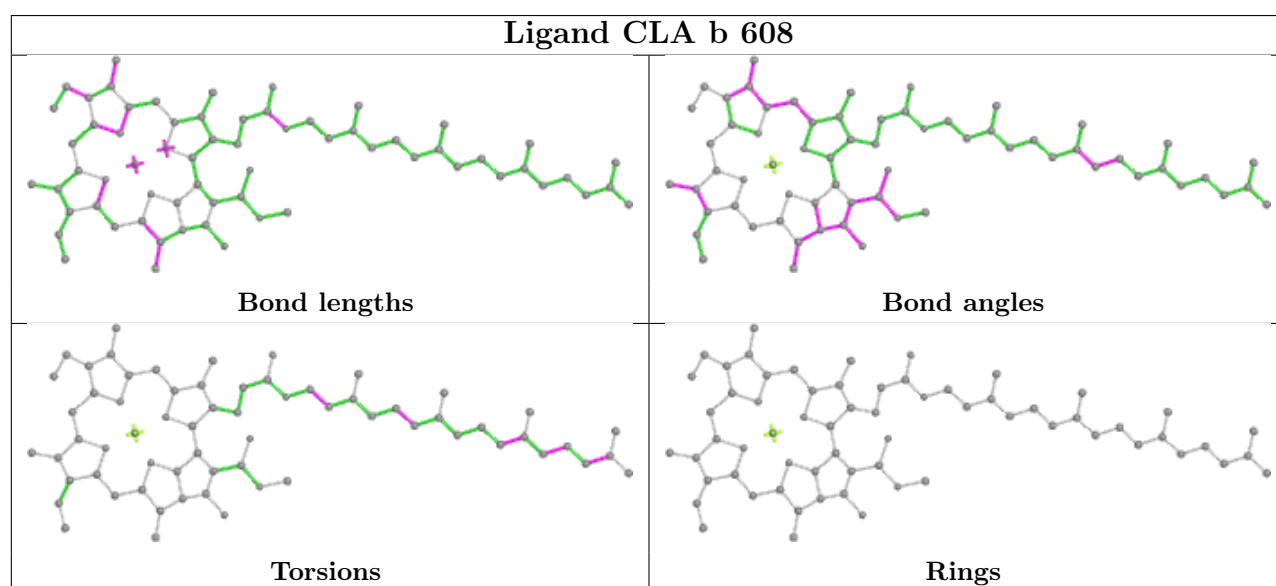
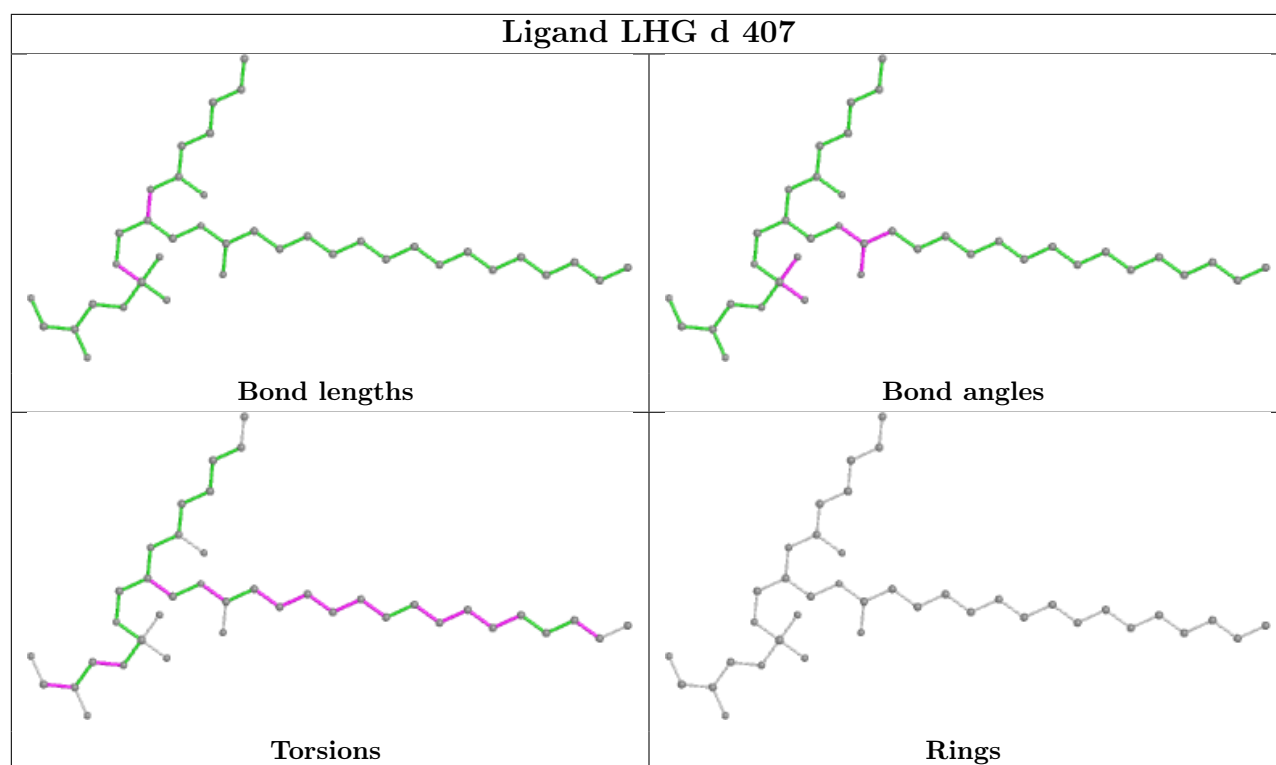


## Ligand SQD A 615

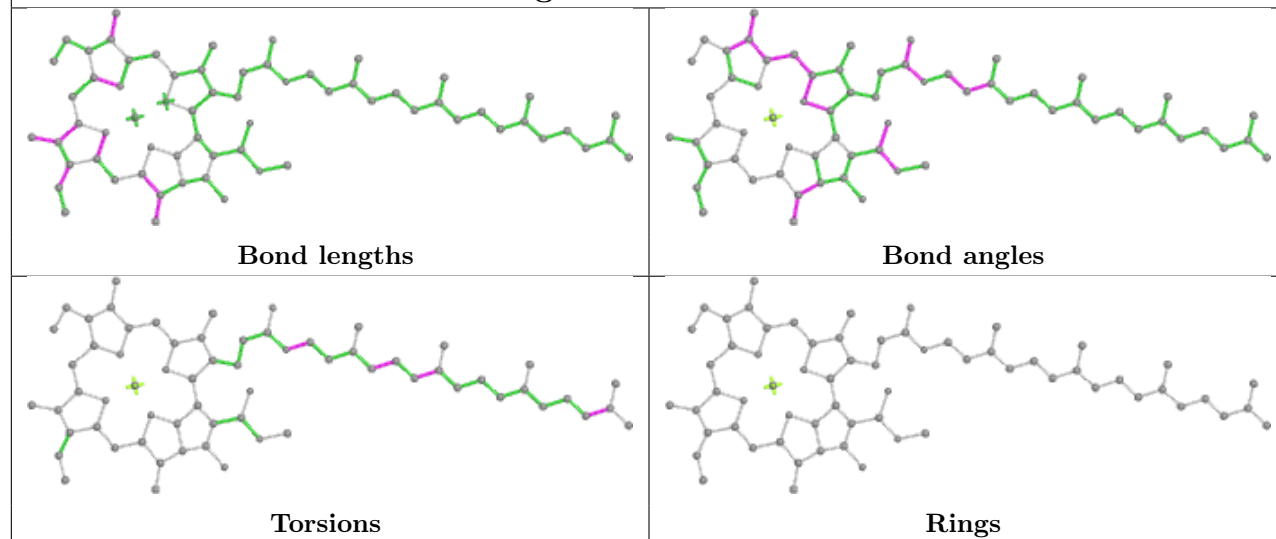


## Ligand STE M 104

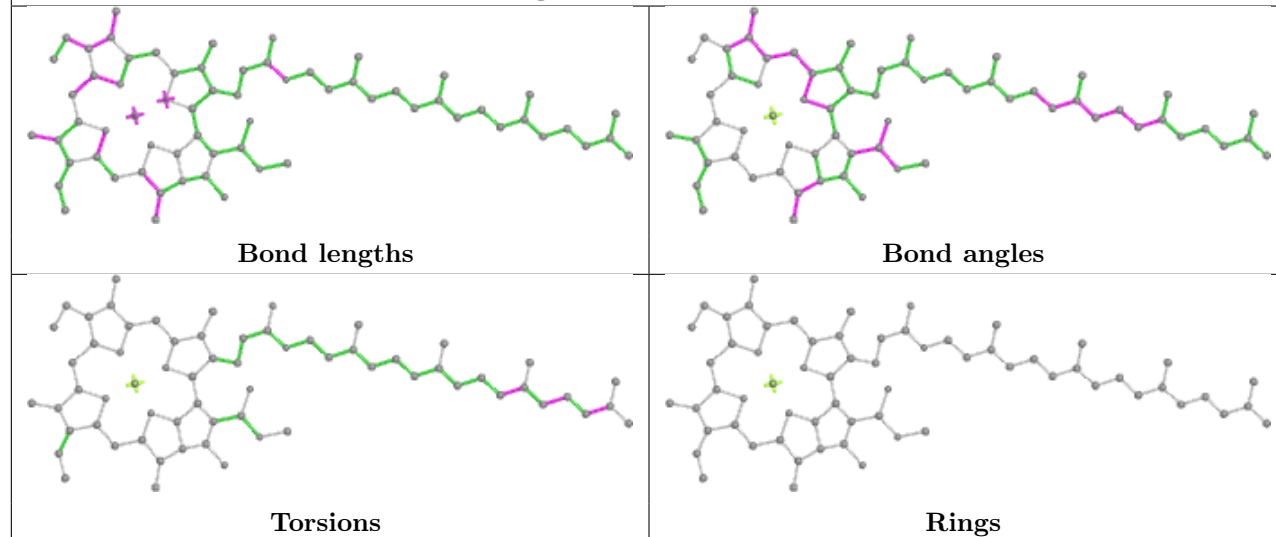




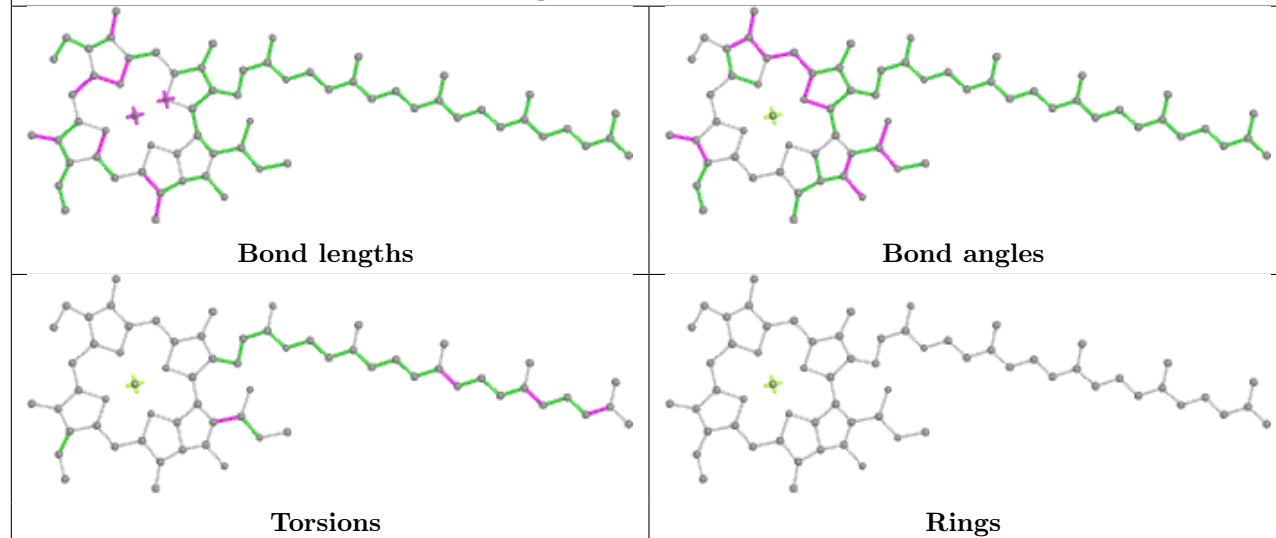
## Ligand CLA d 402

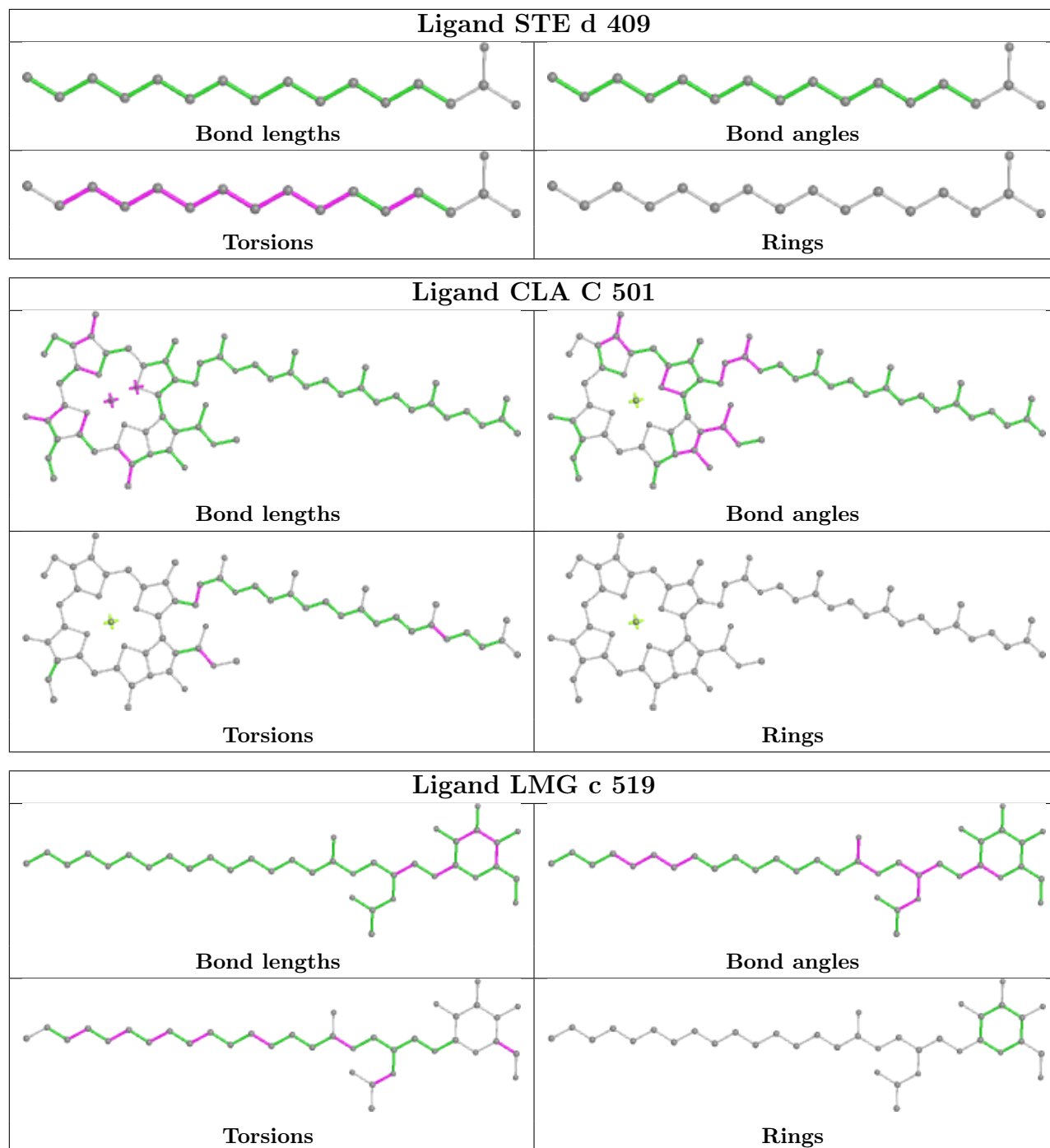


## Ligand CLA B 607

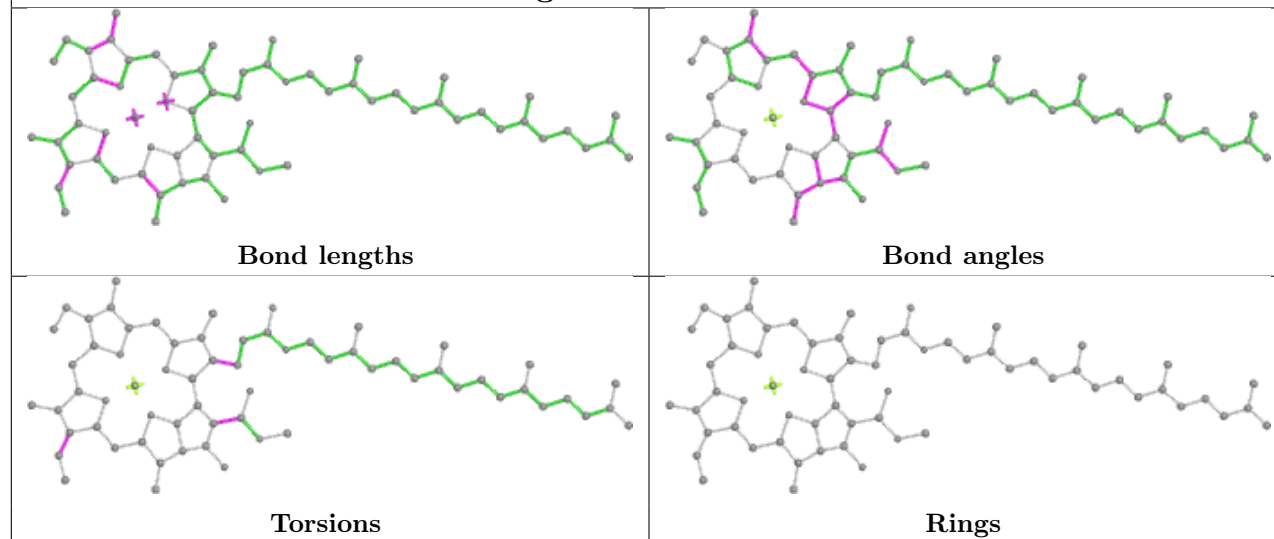


## Ligand CLA C 508

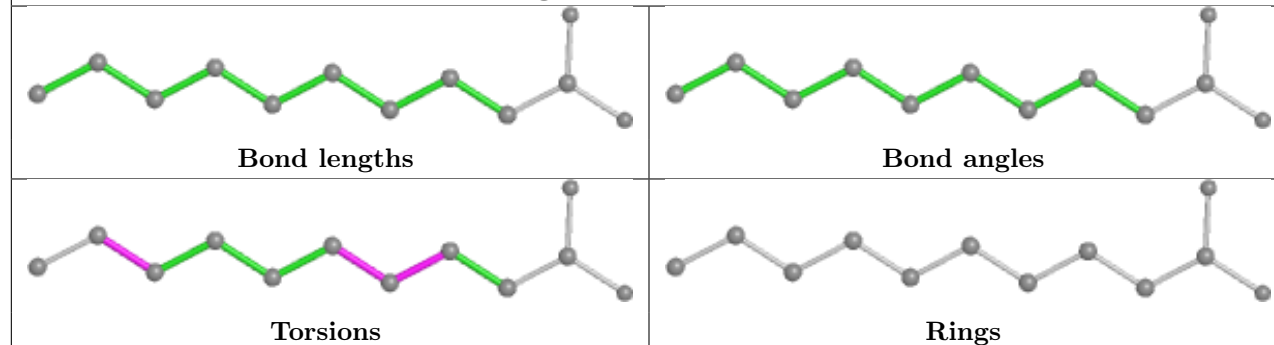




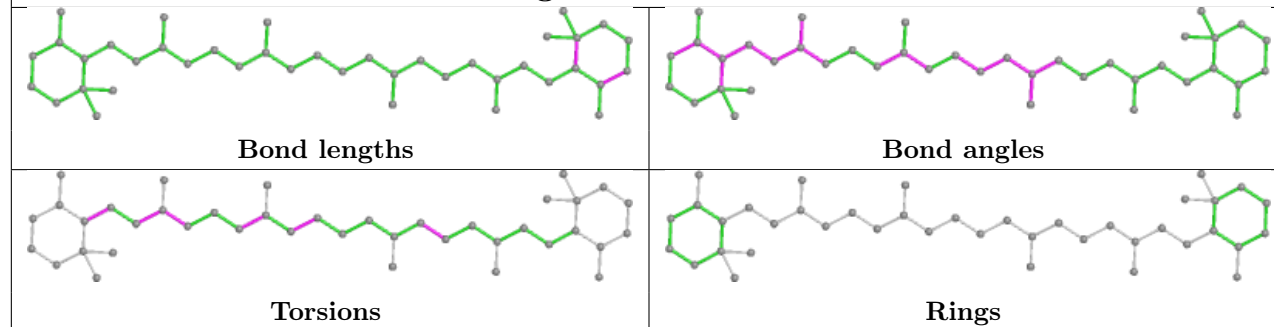
## Ligand CLA a 613



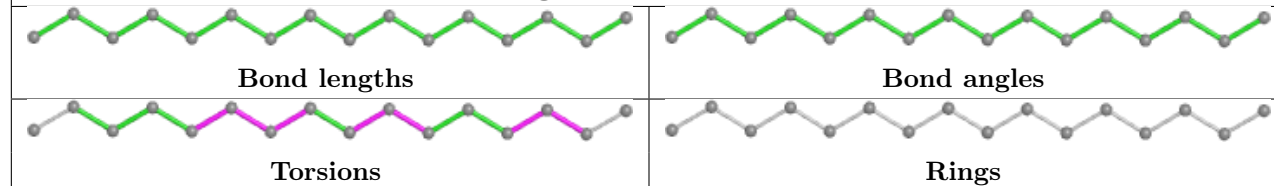
## Ligand STE C 519

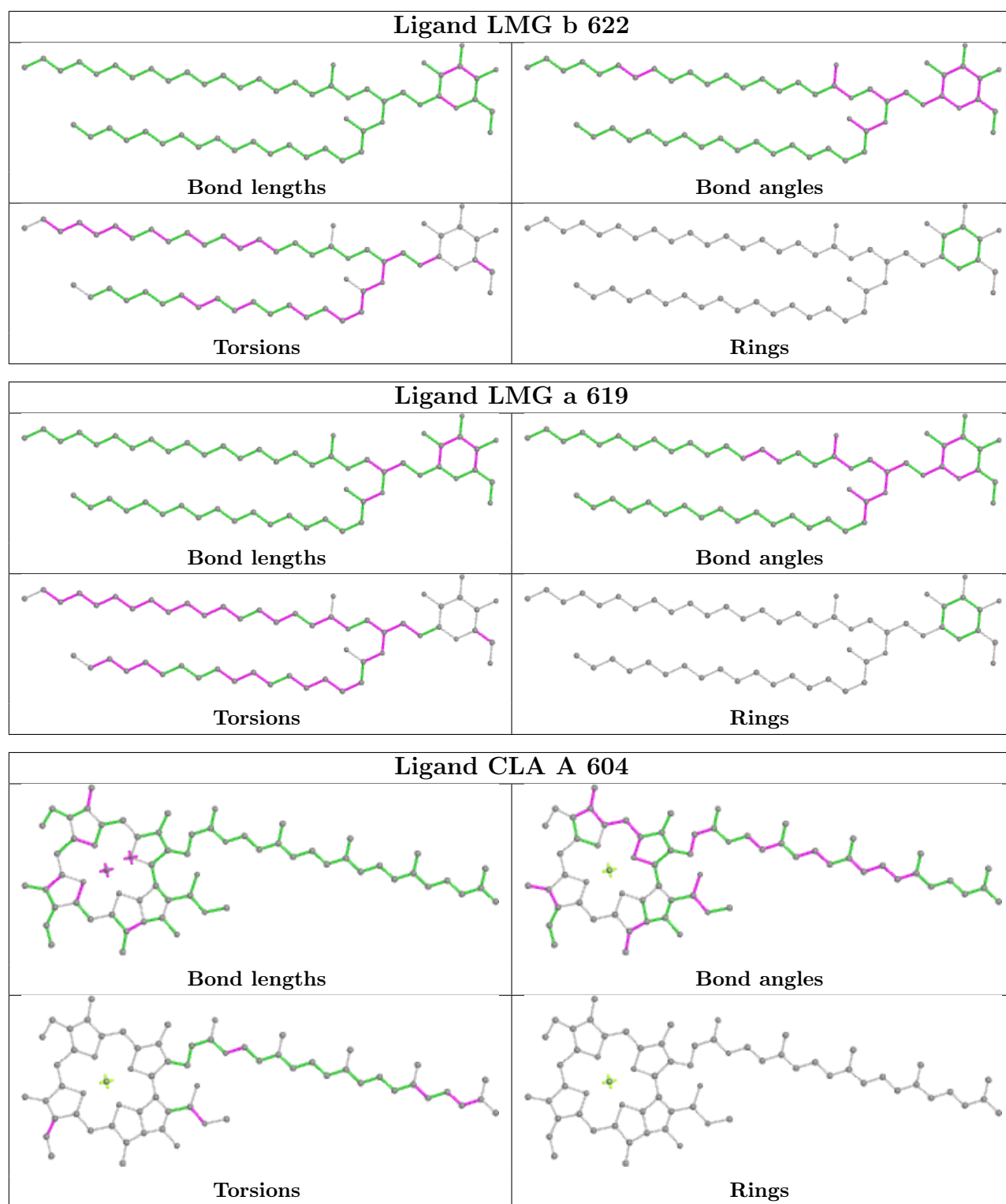


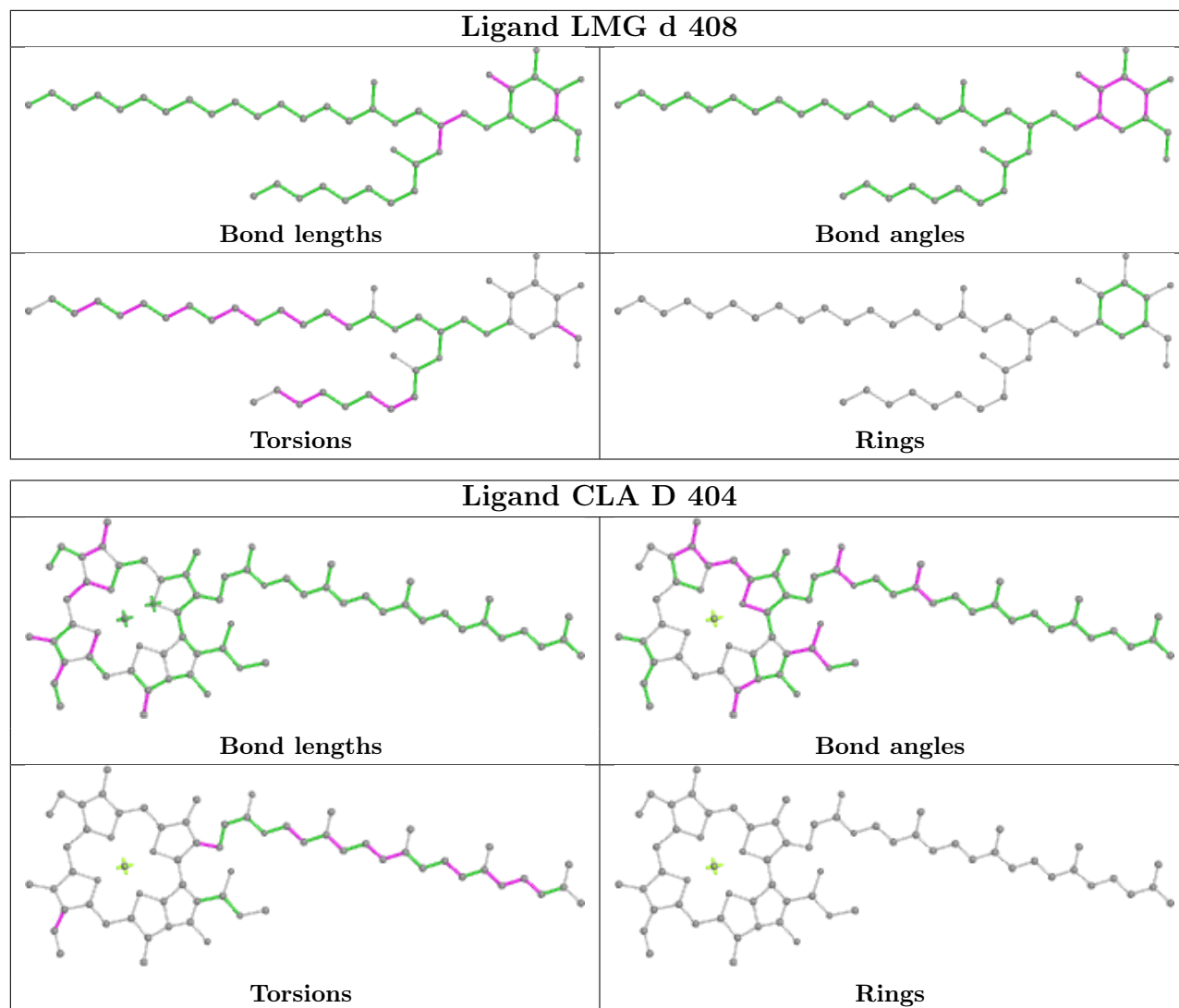
## Ligand BCR t 101

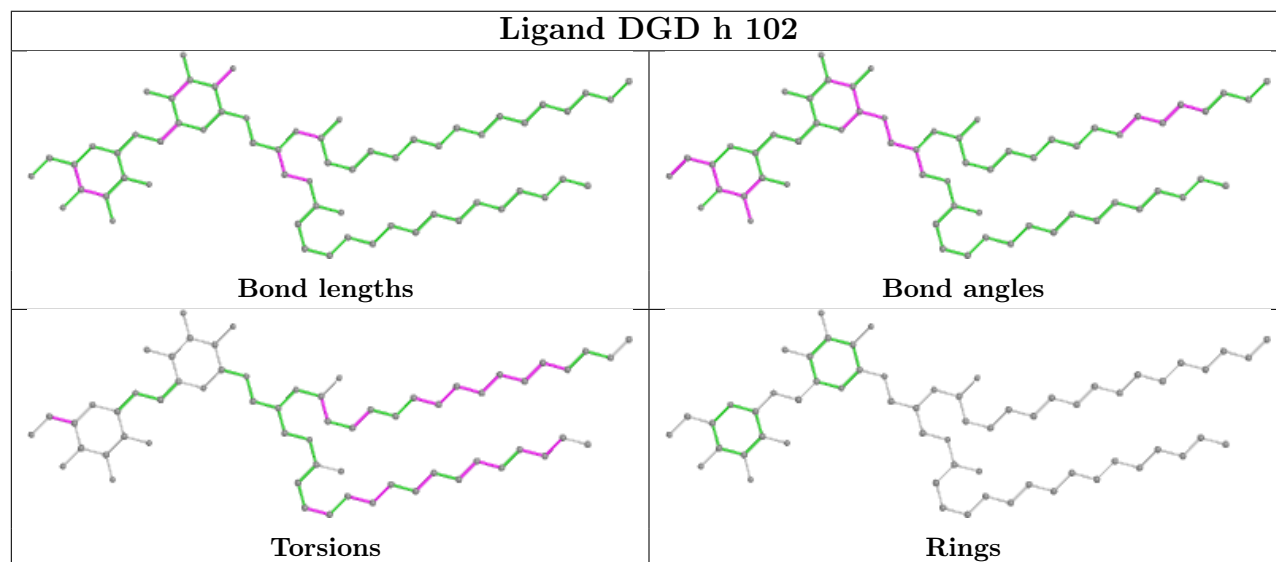
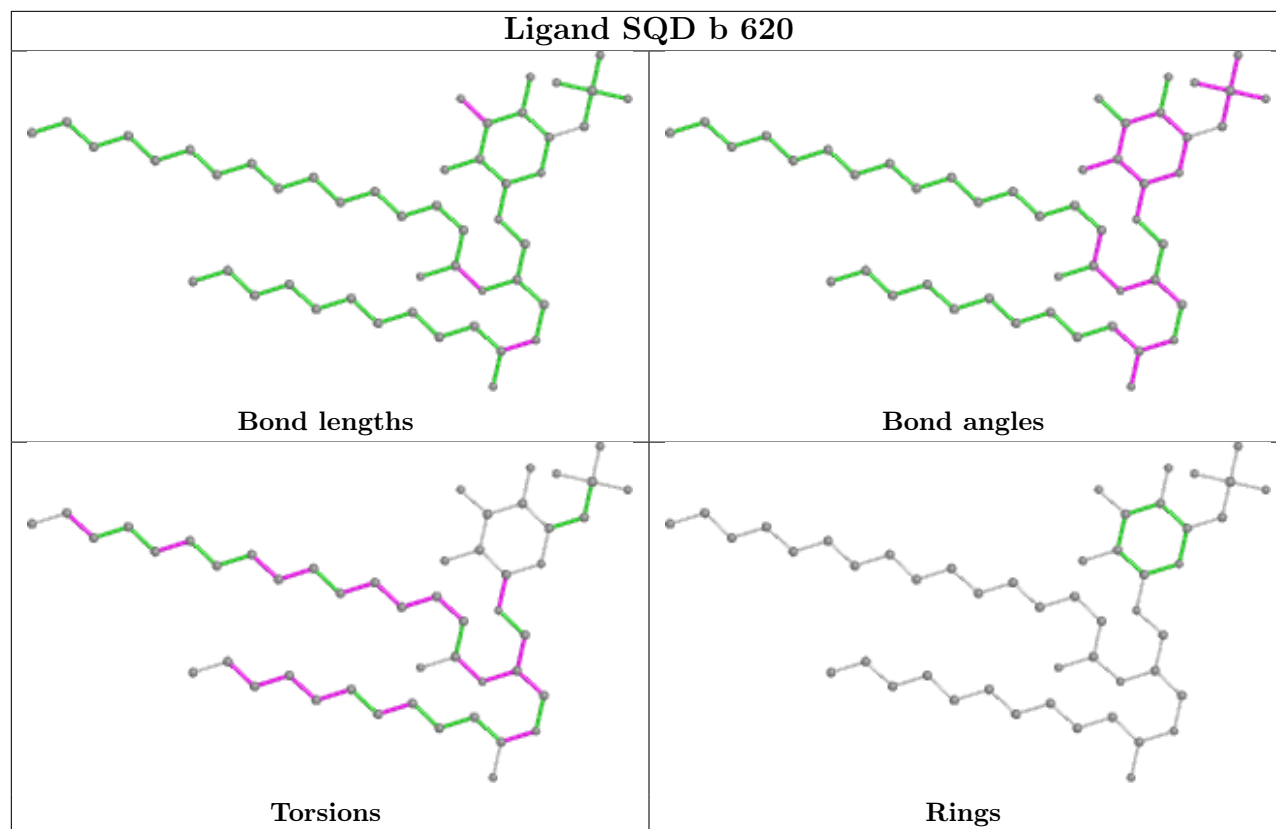


## Ligand STE C 520

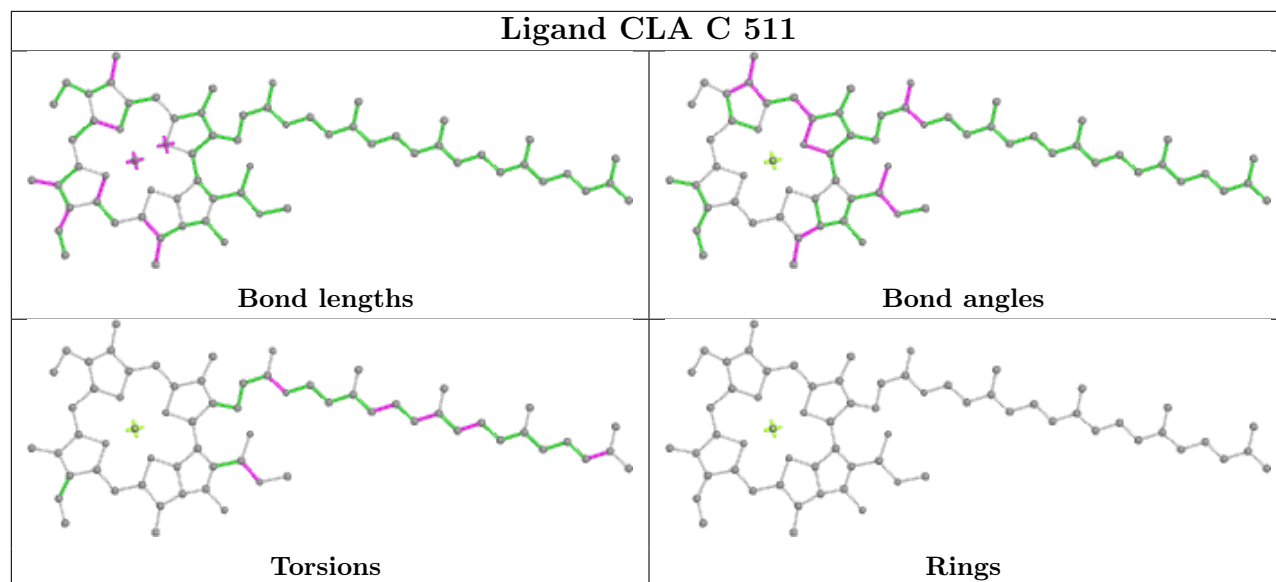




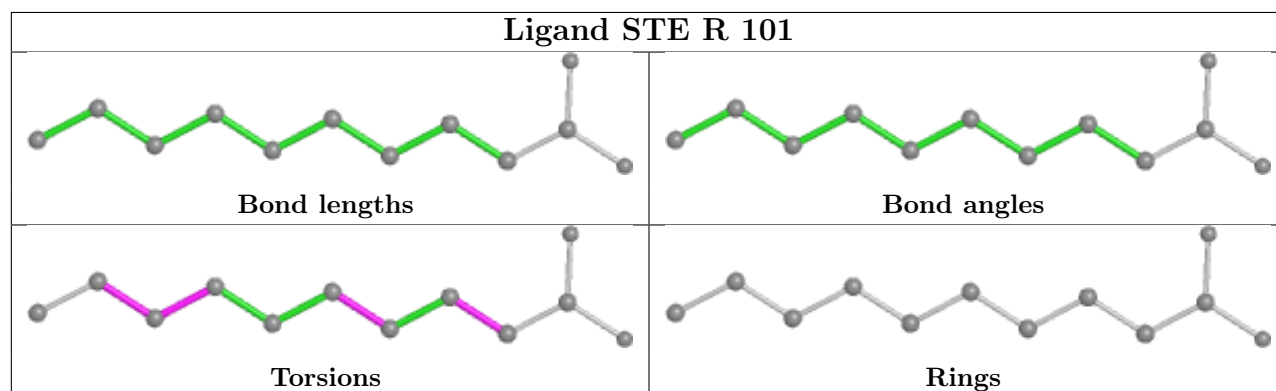




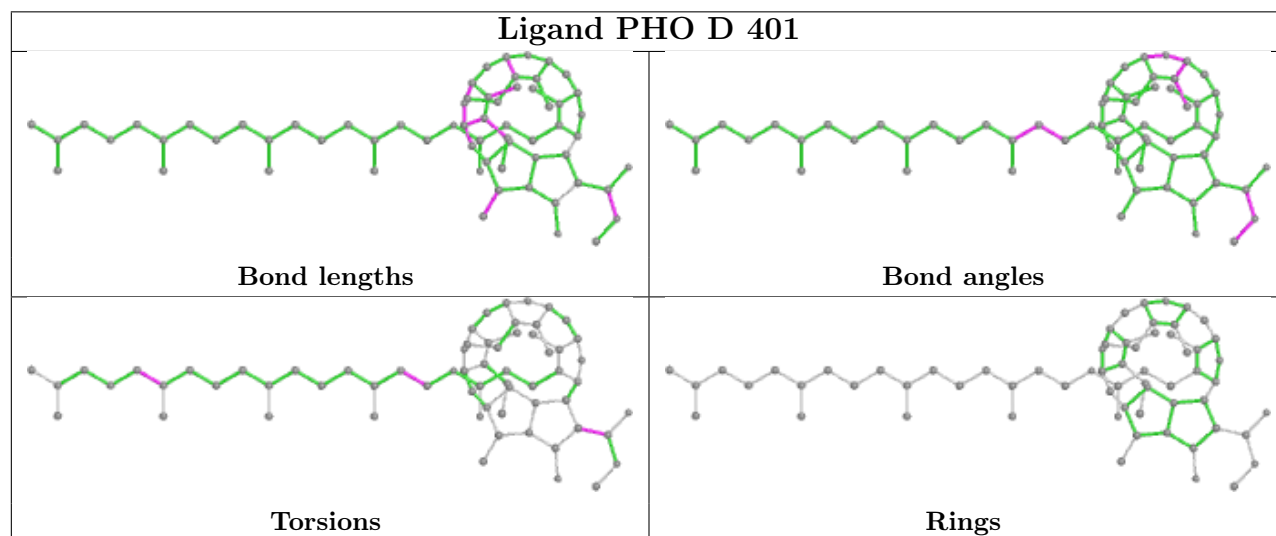
## Ligand CLA C 511

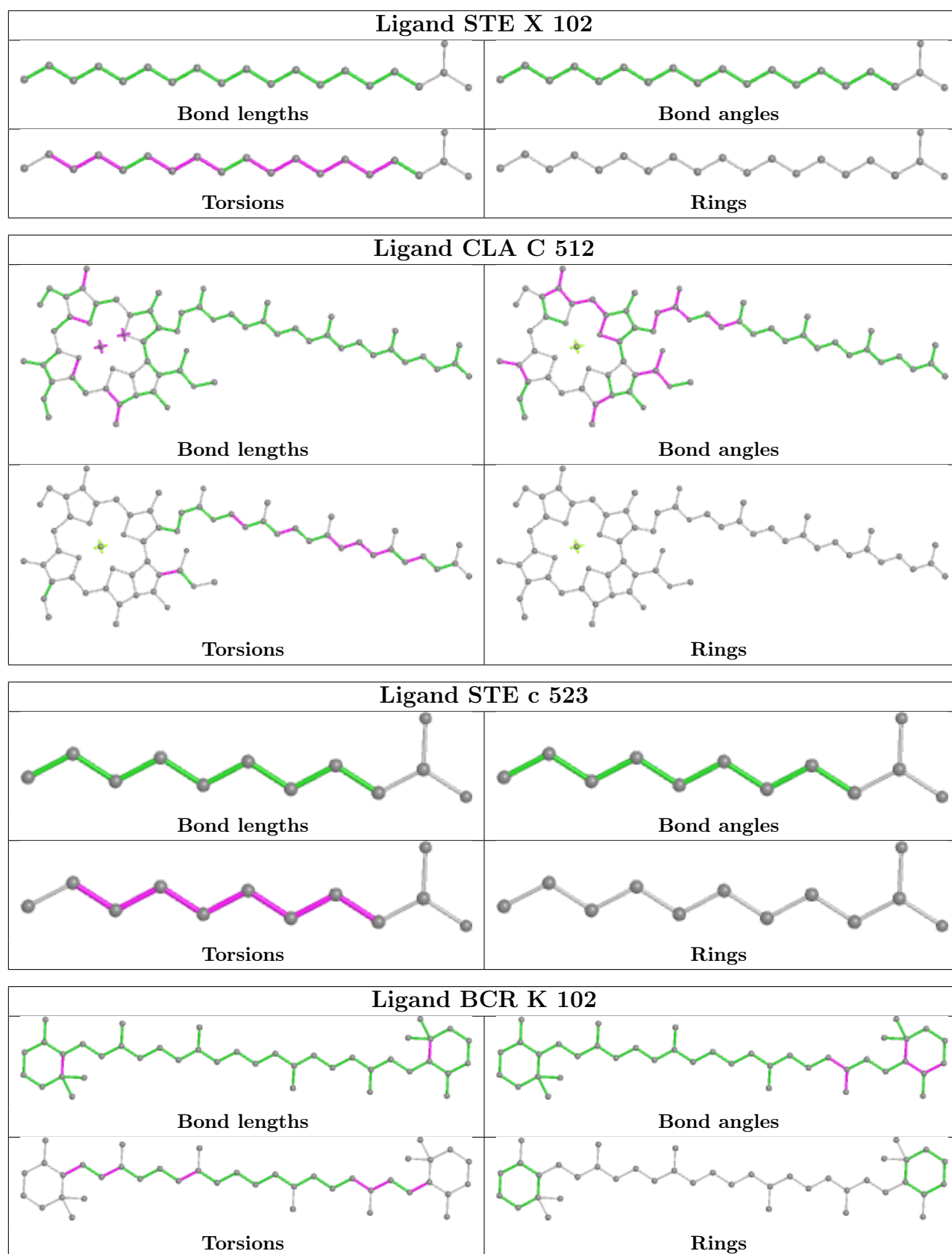


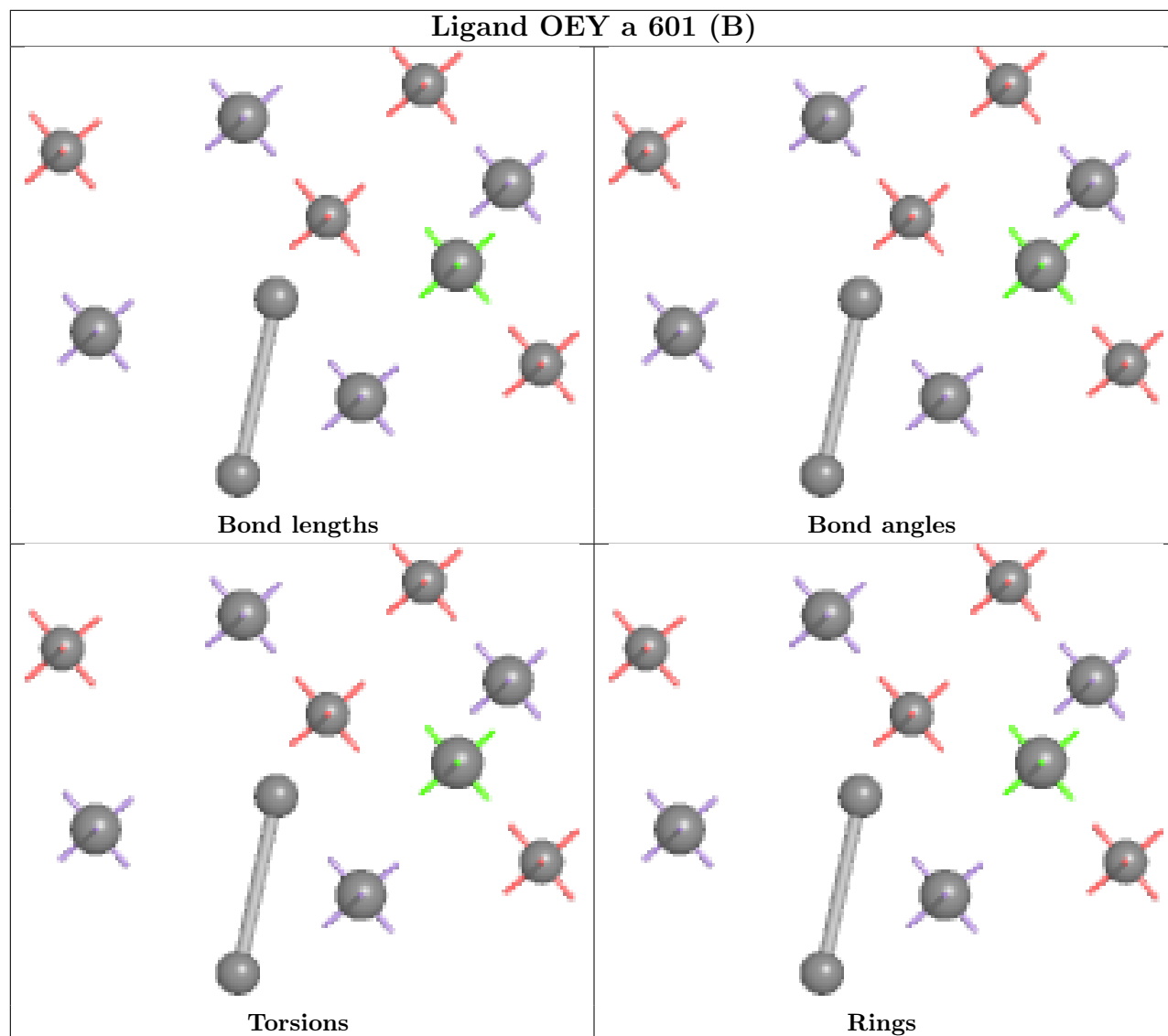
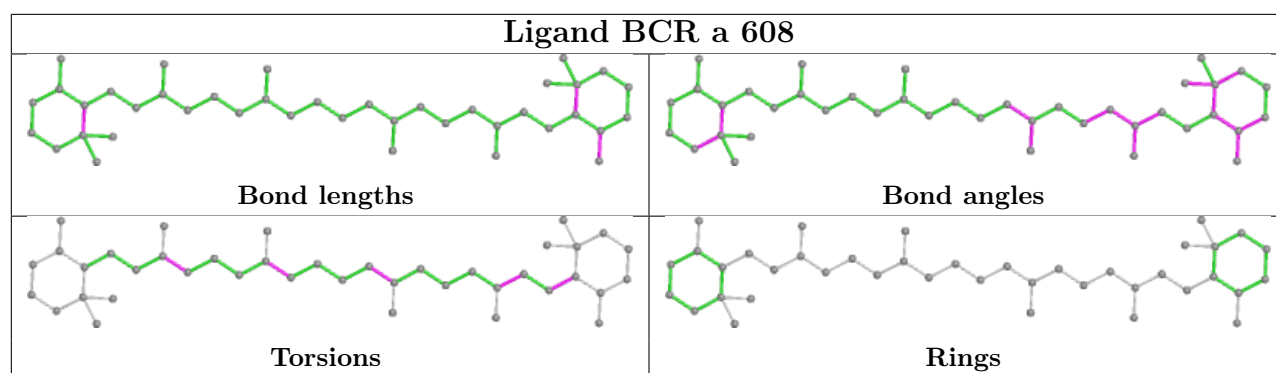
## Ligand STE R 101



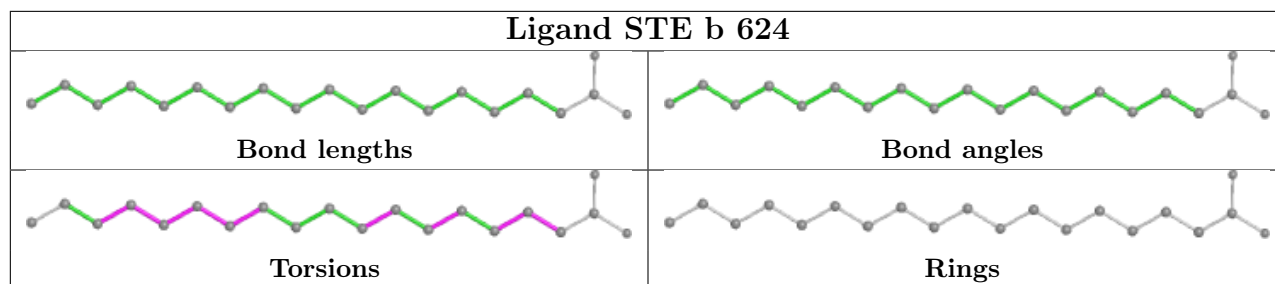
## Ligand PHO D 401



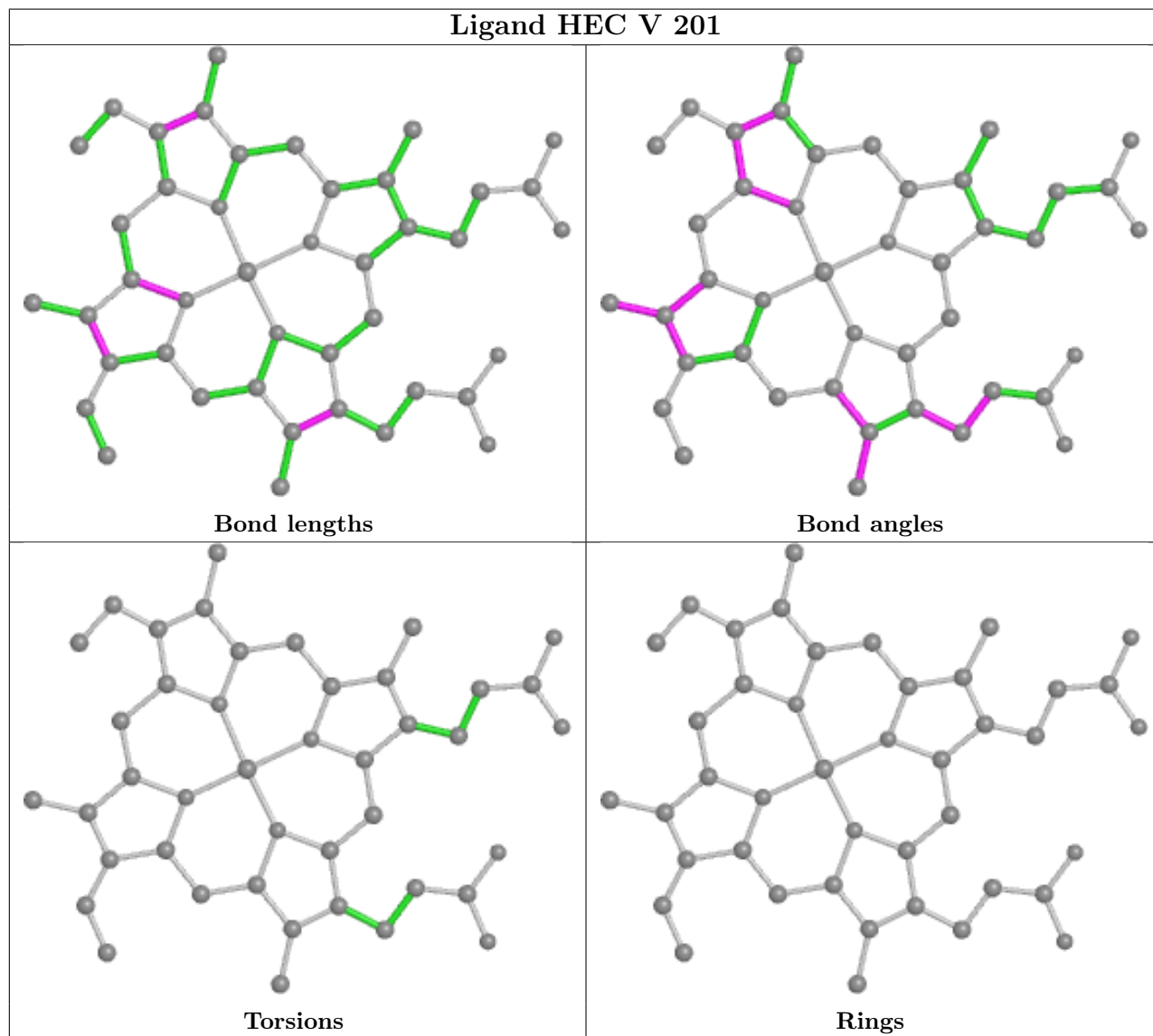




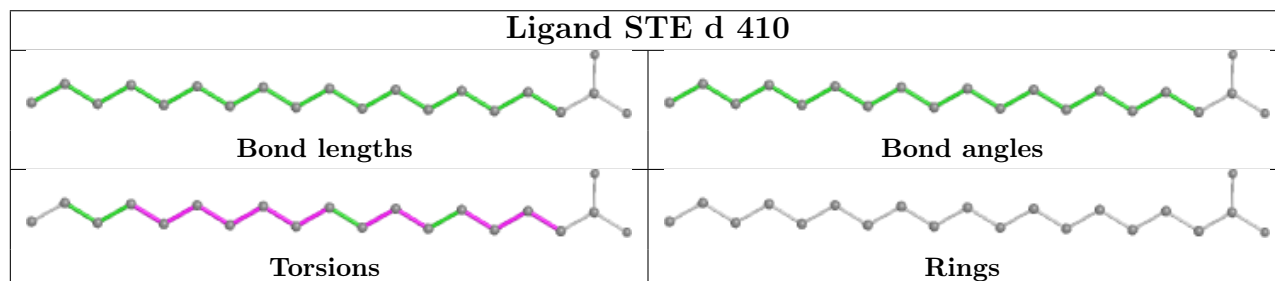
## Ligand STE b 624



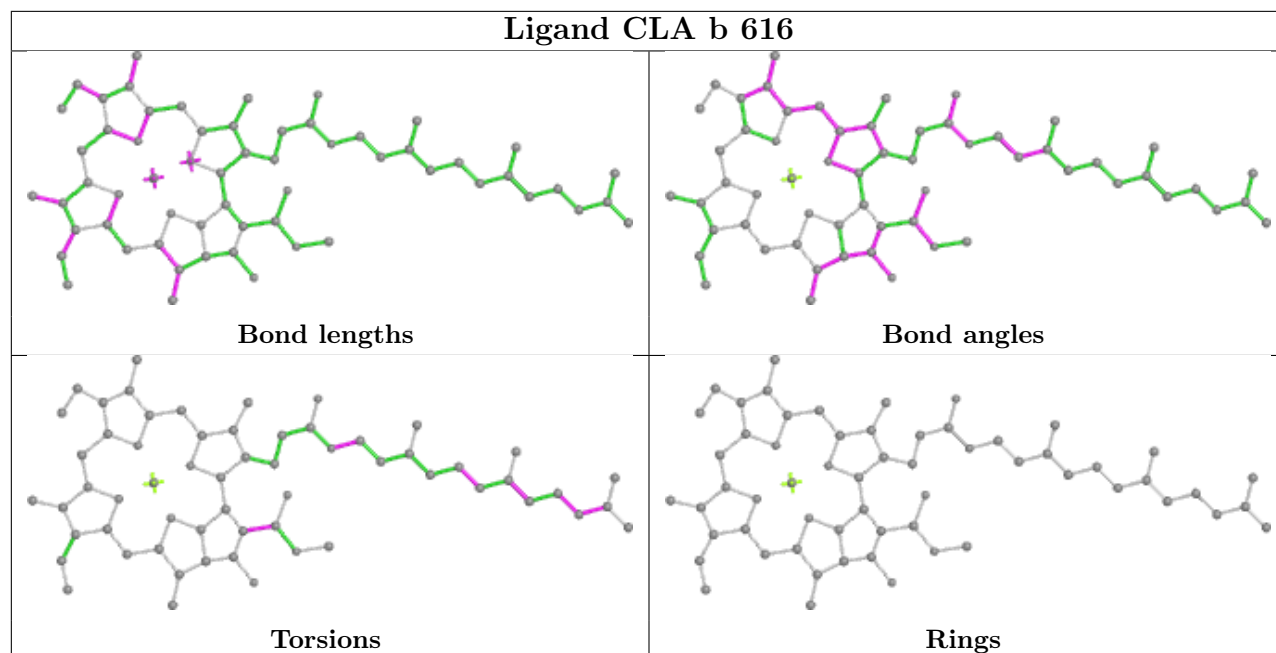
## Ligand HEC V 201



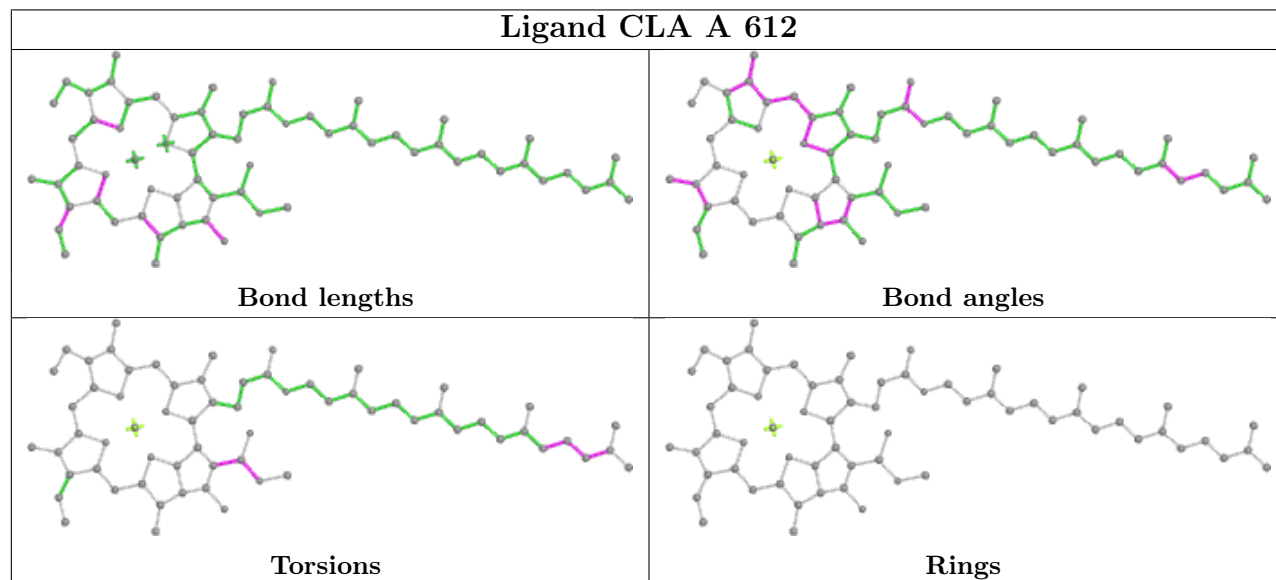
## Ligand STE d 410



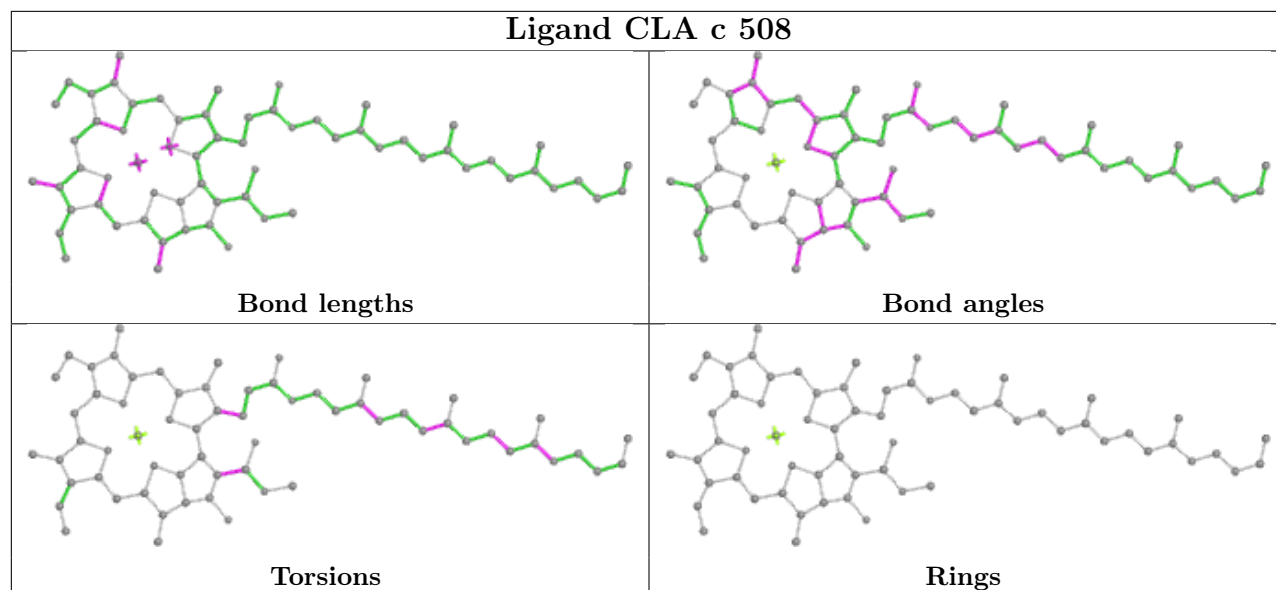
## Ligand CLA b 616



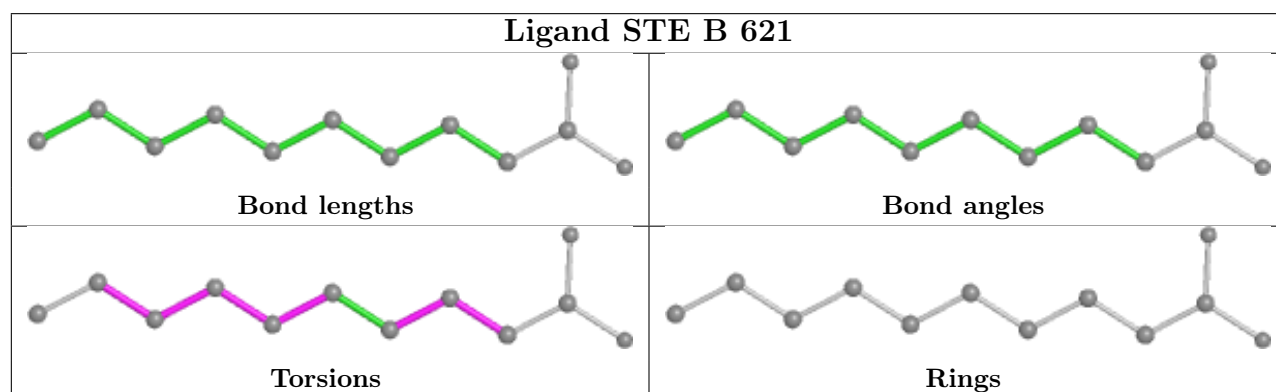
## Ligand CLA A 612



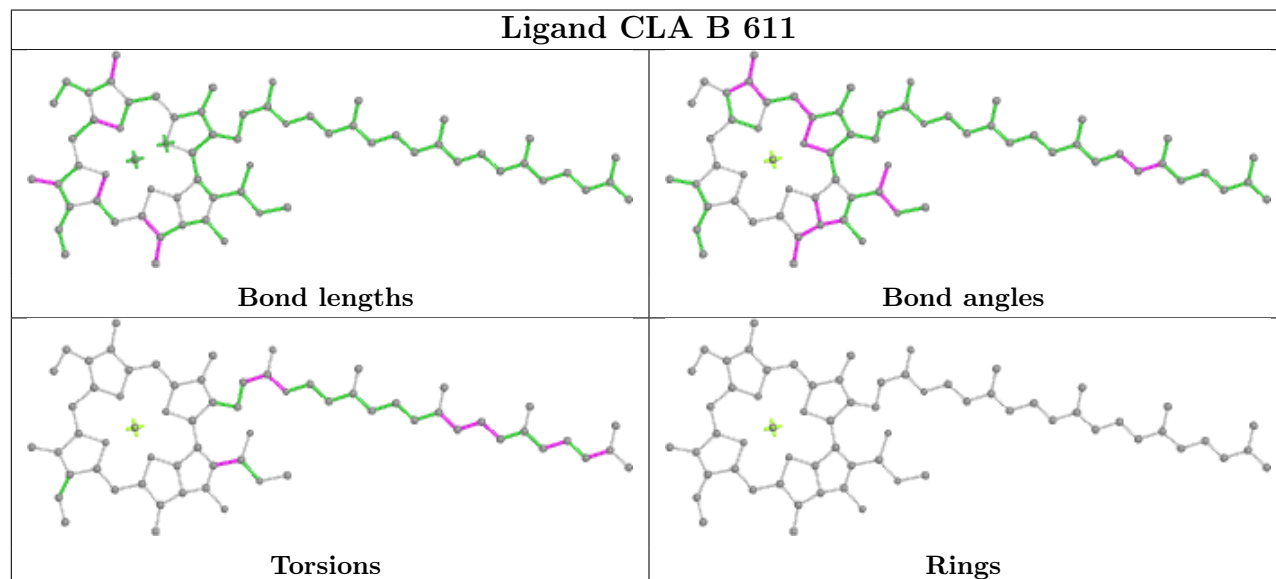
## Ligand CLA c 508



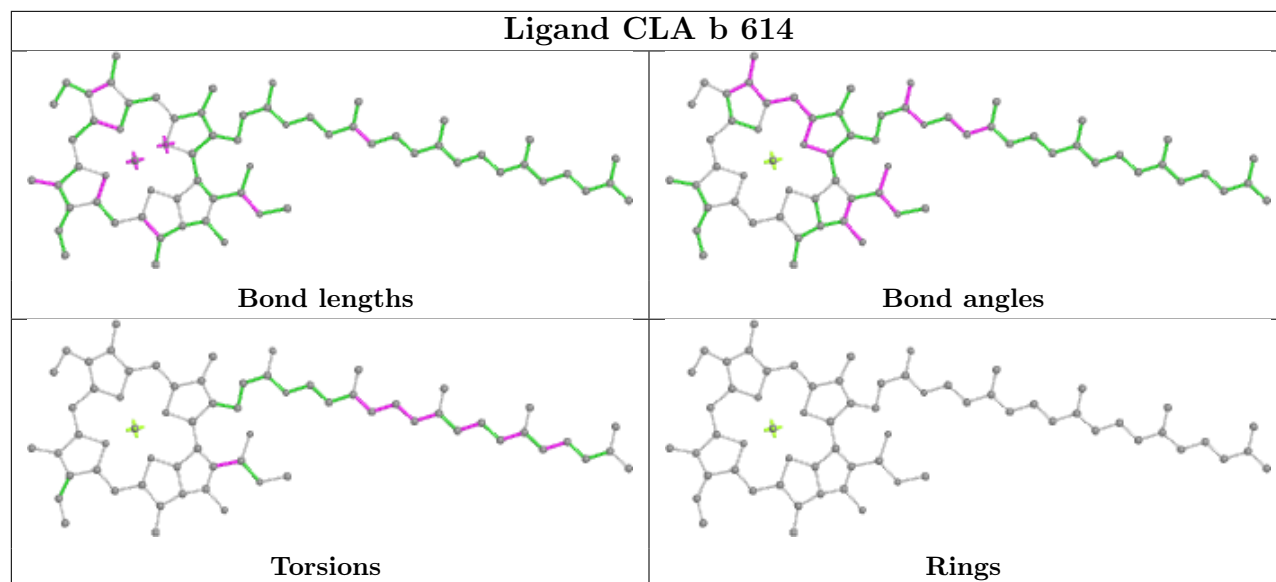
## Ligand STE B 621



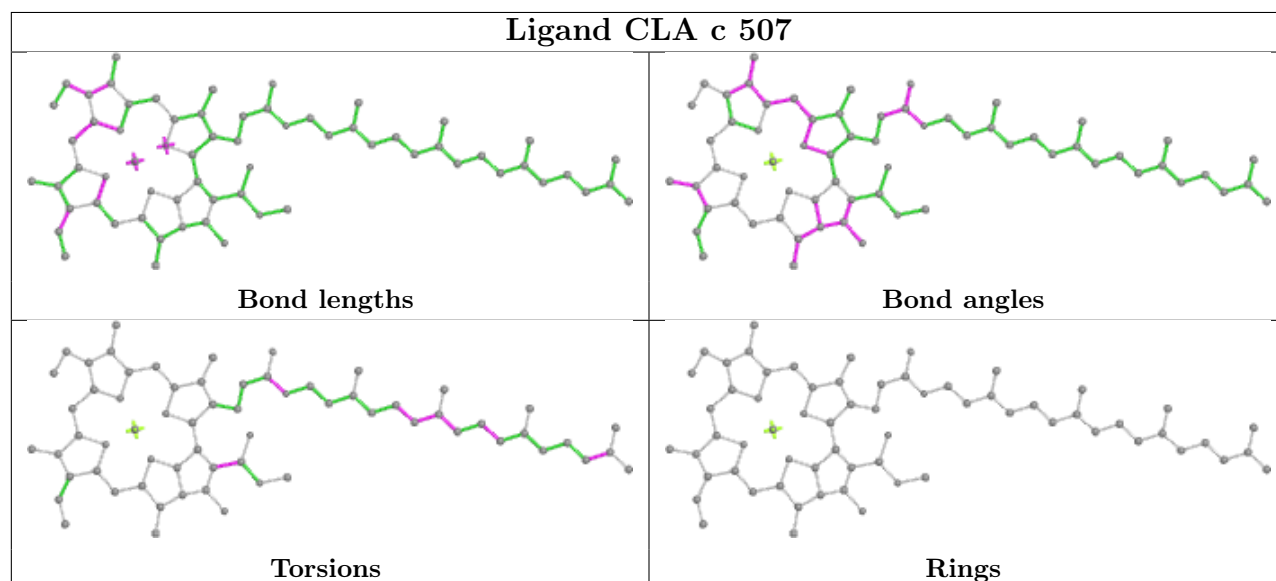
## Ligand CLA B 611



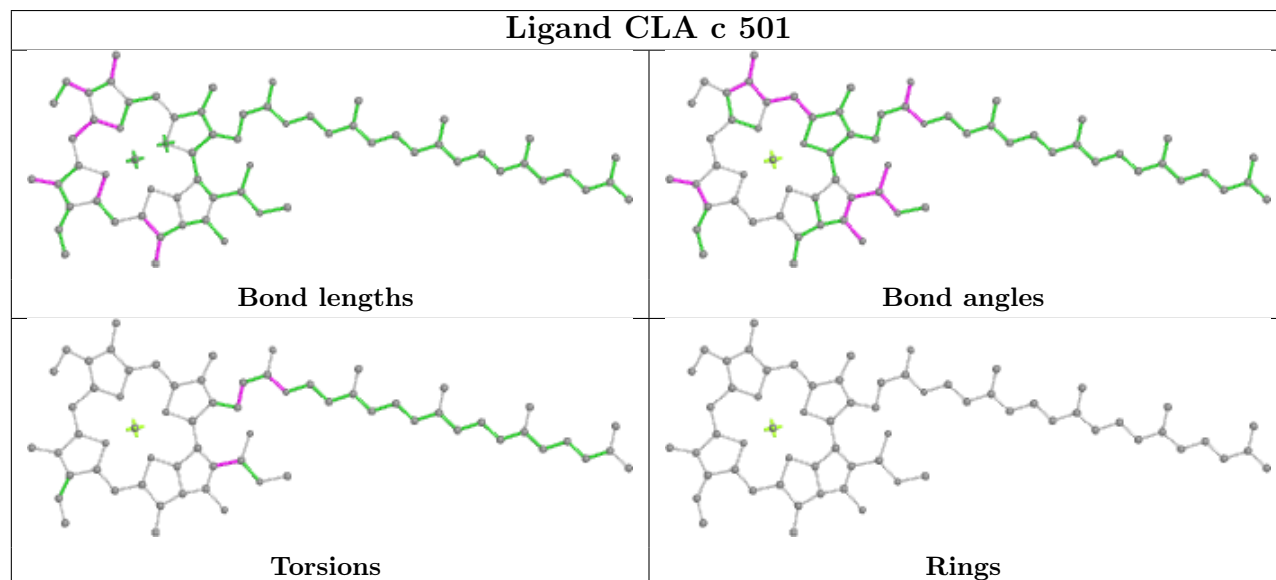
## Ligand CLA b 614

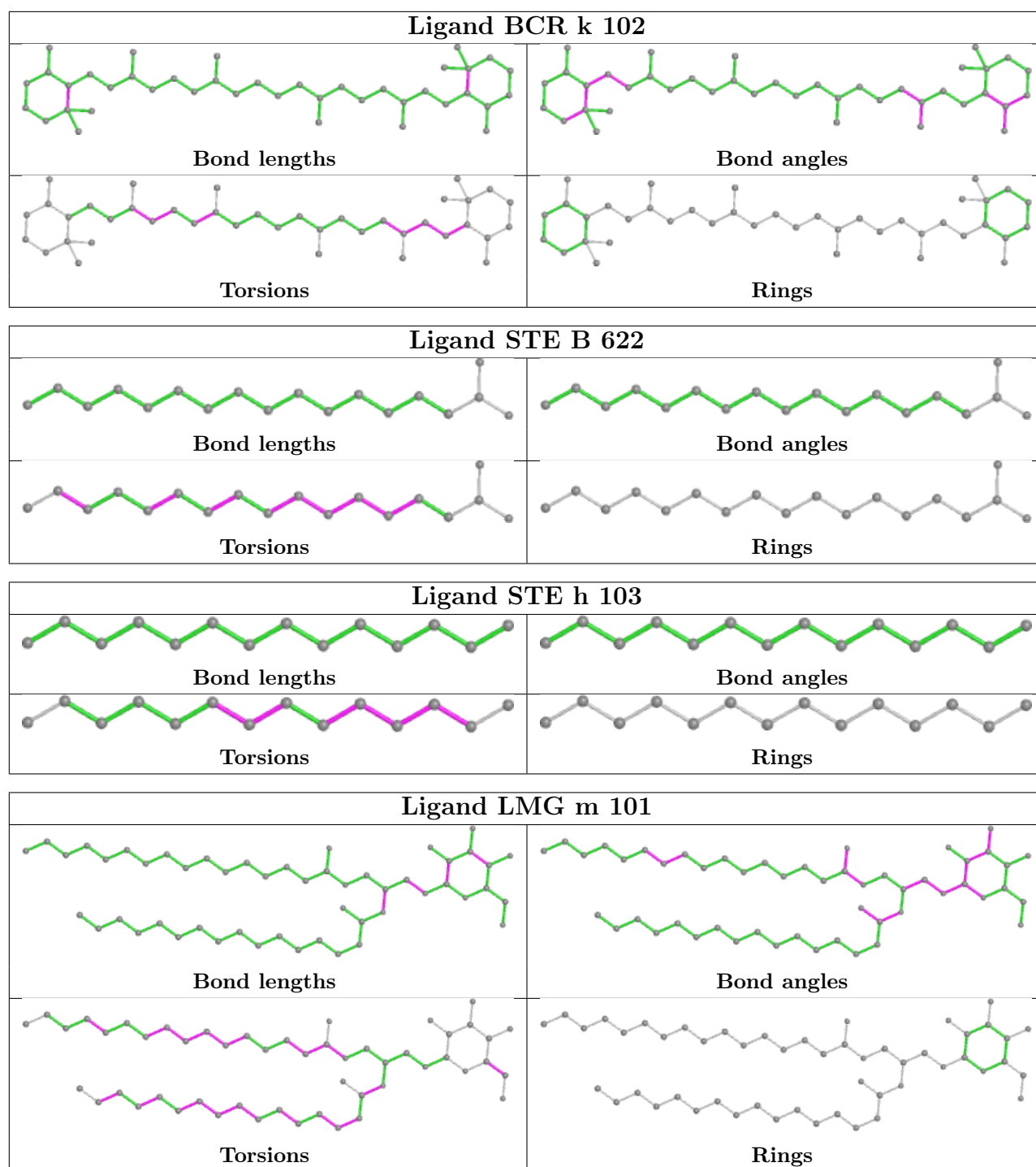


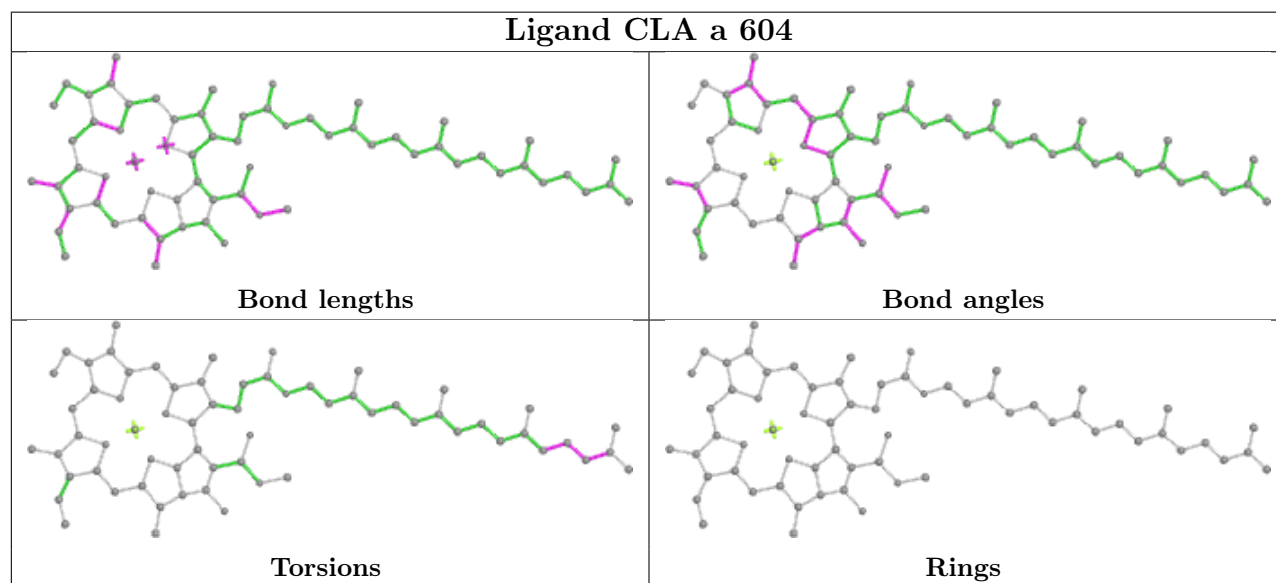
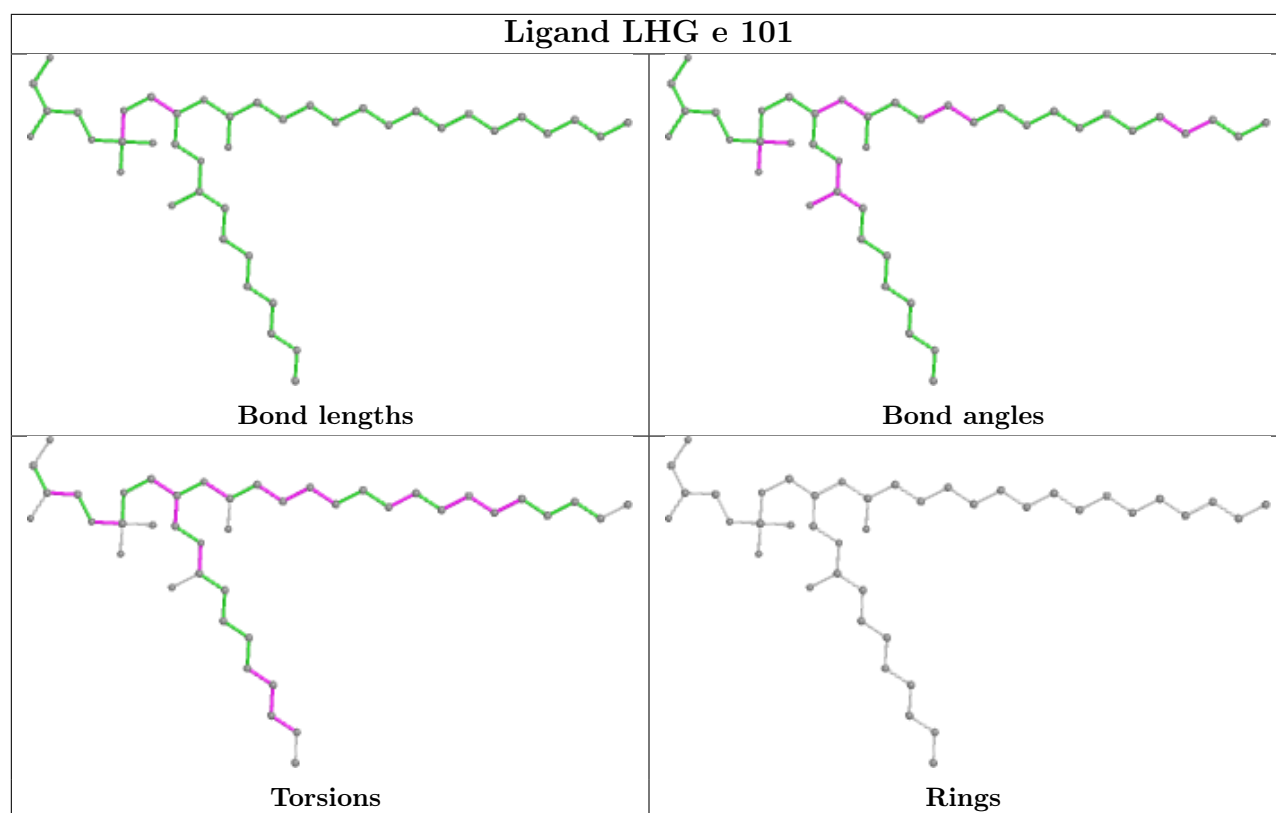
## Ligand CLA c 507



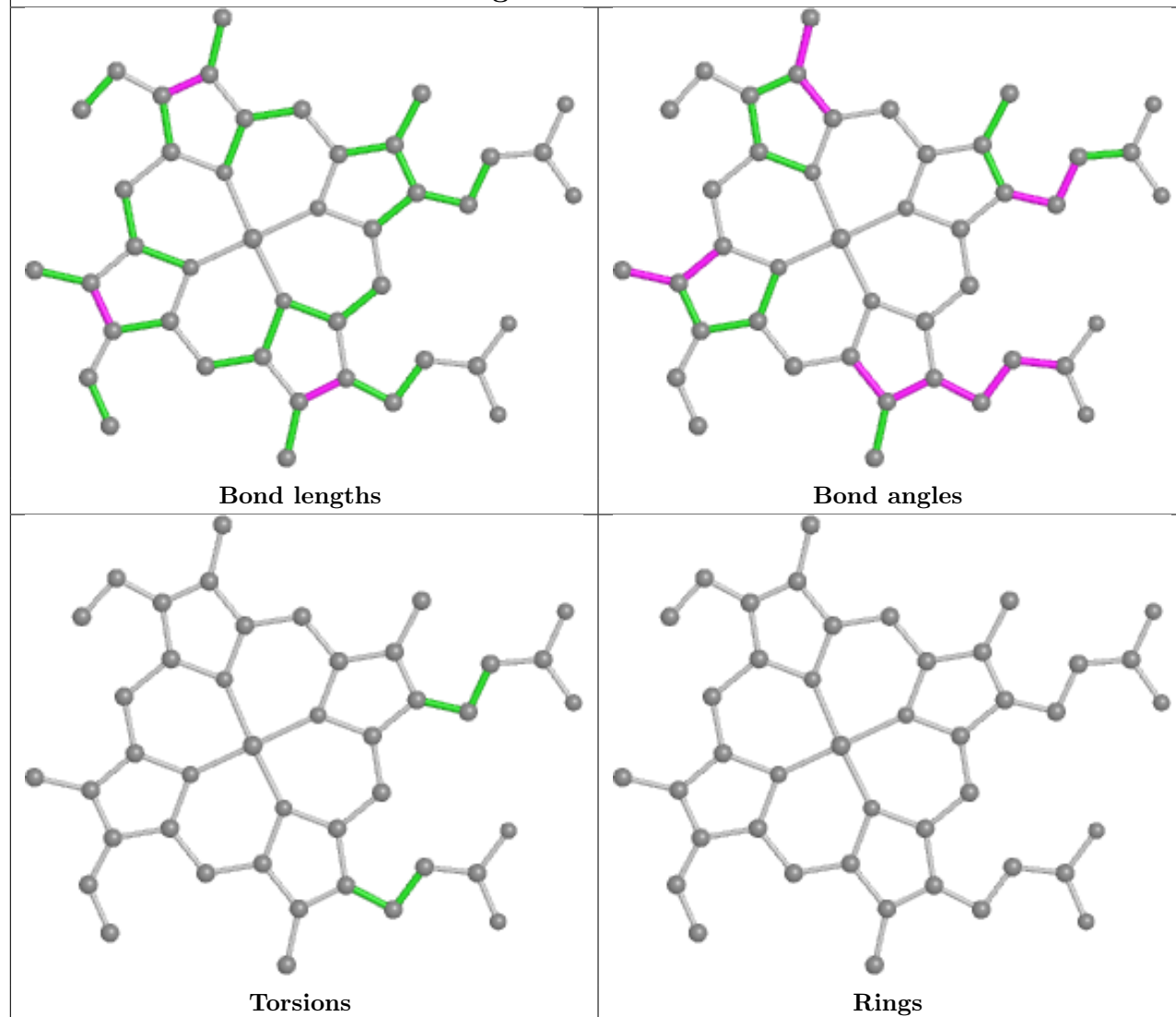
## Ligand CLA c 501



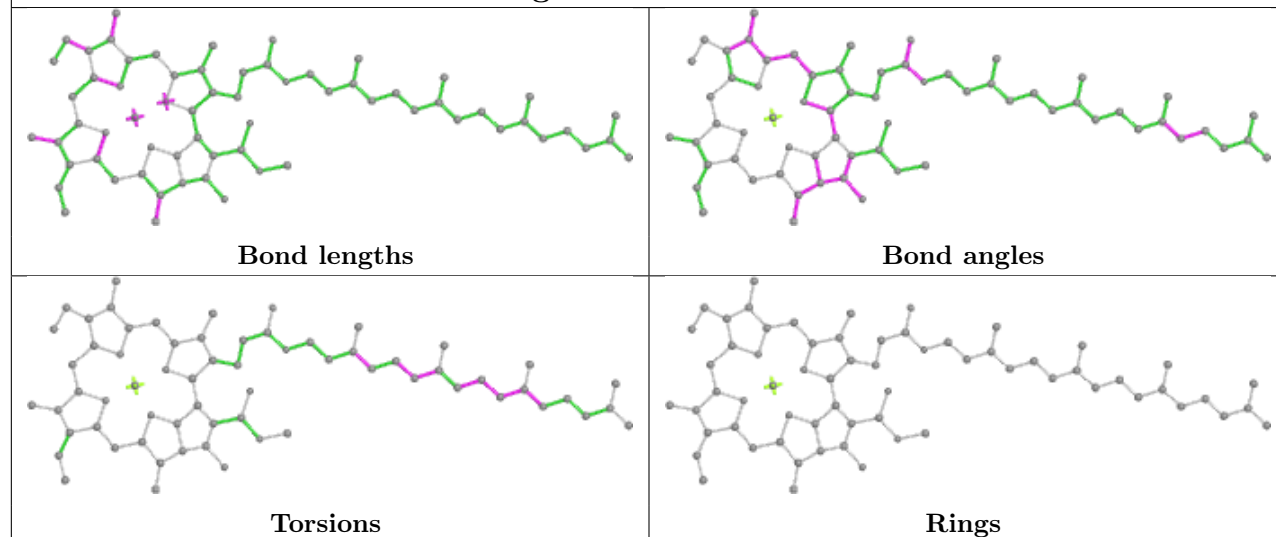


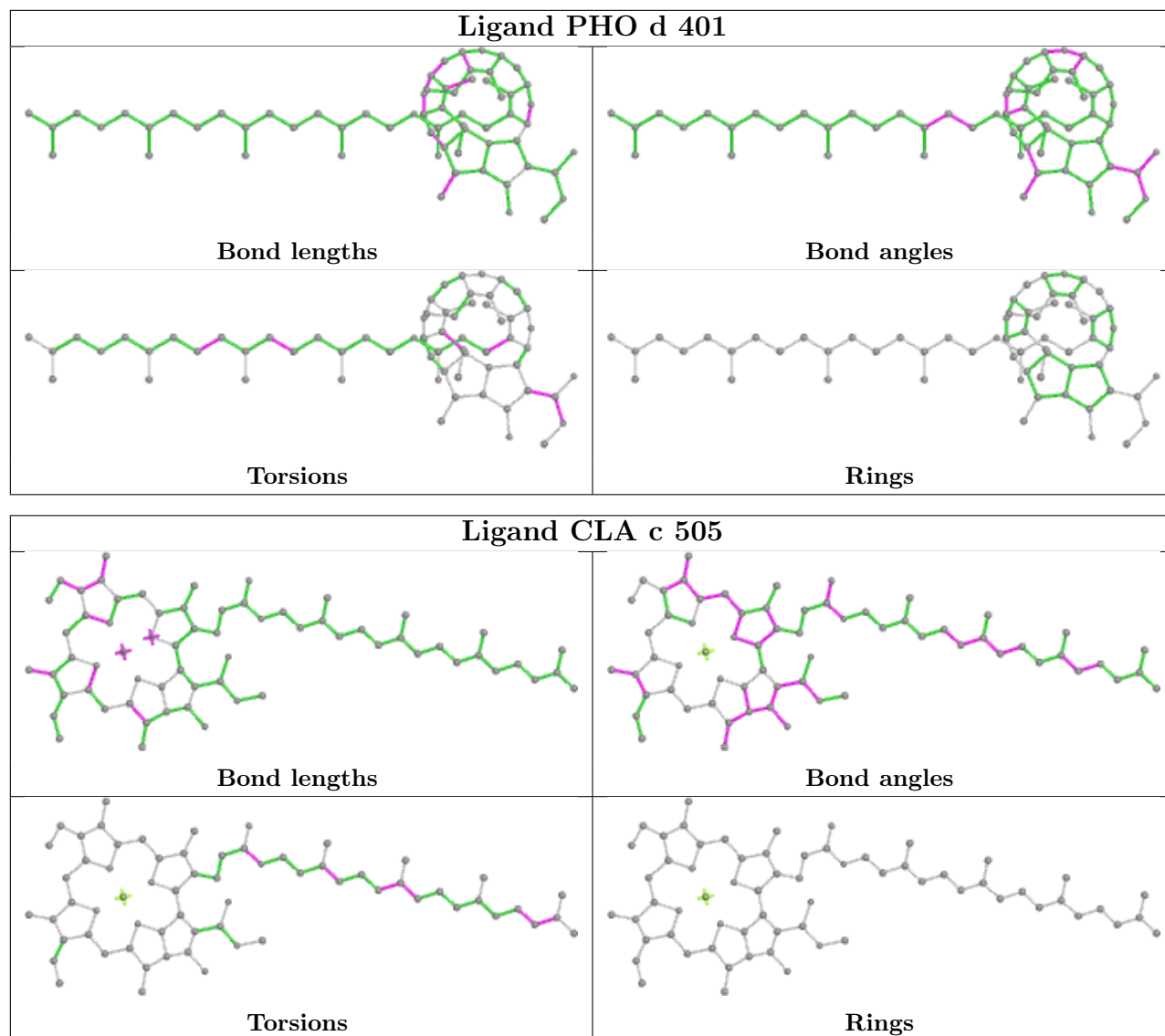


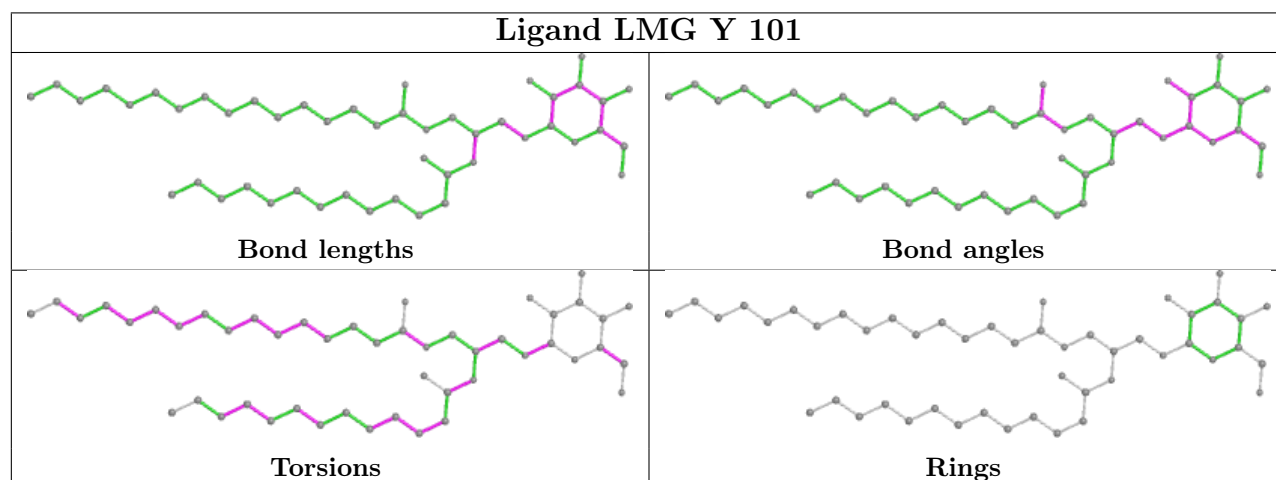
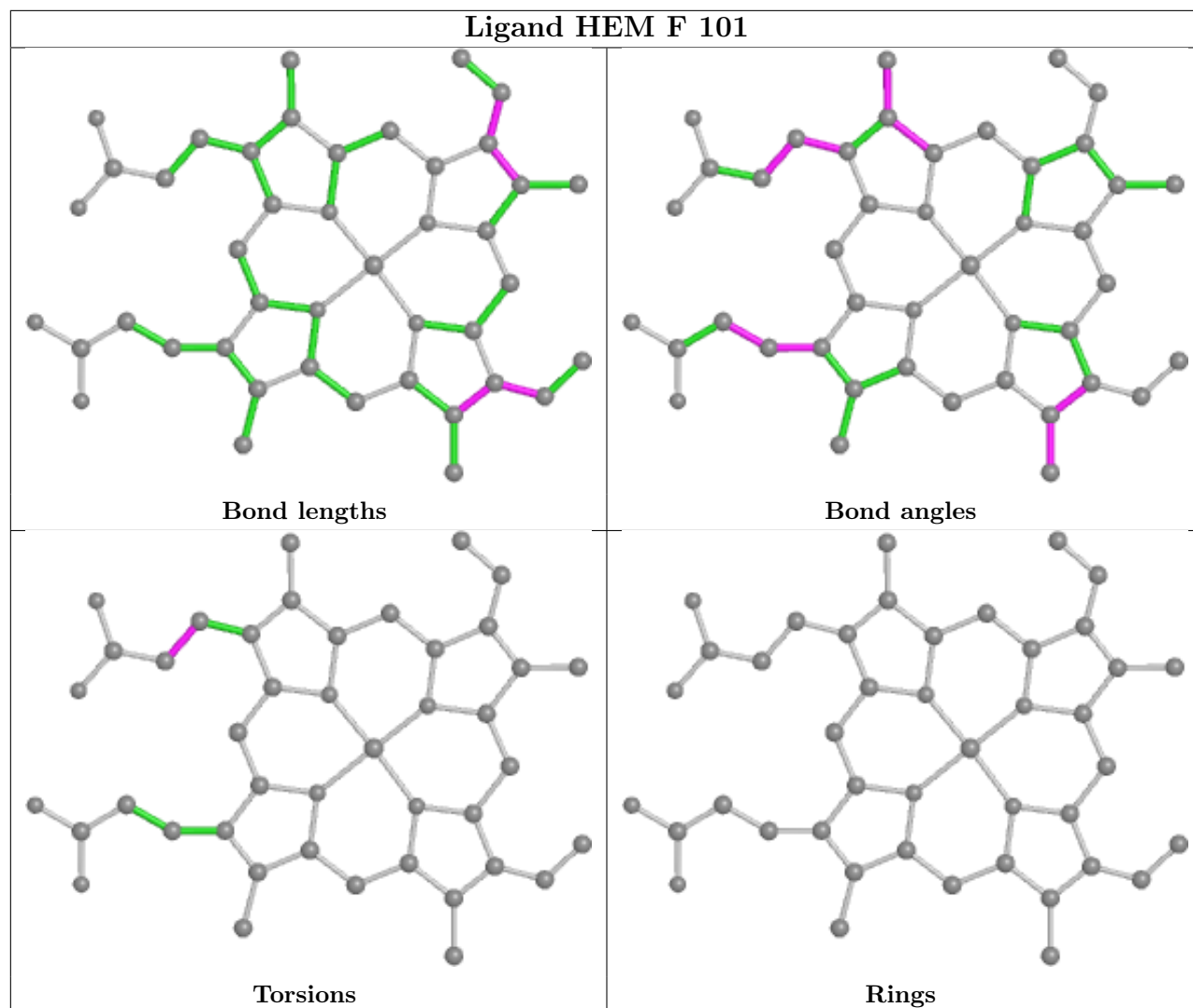
## Ligand HEC v 201



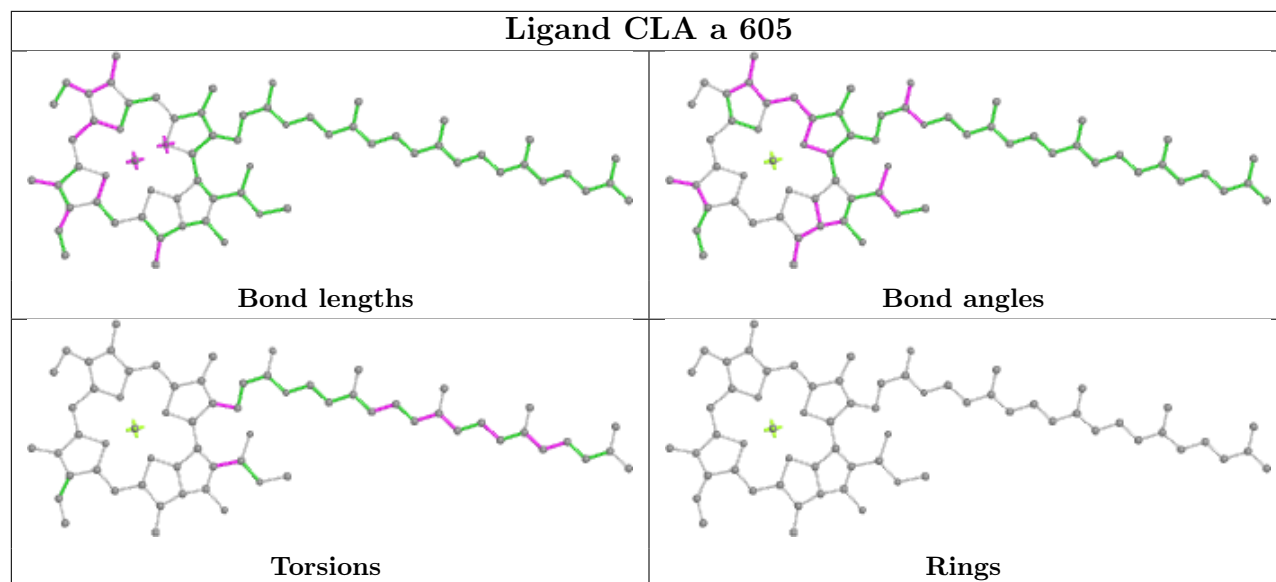
## Ligand CLA C 505



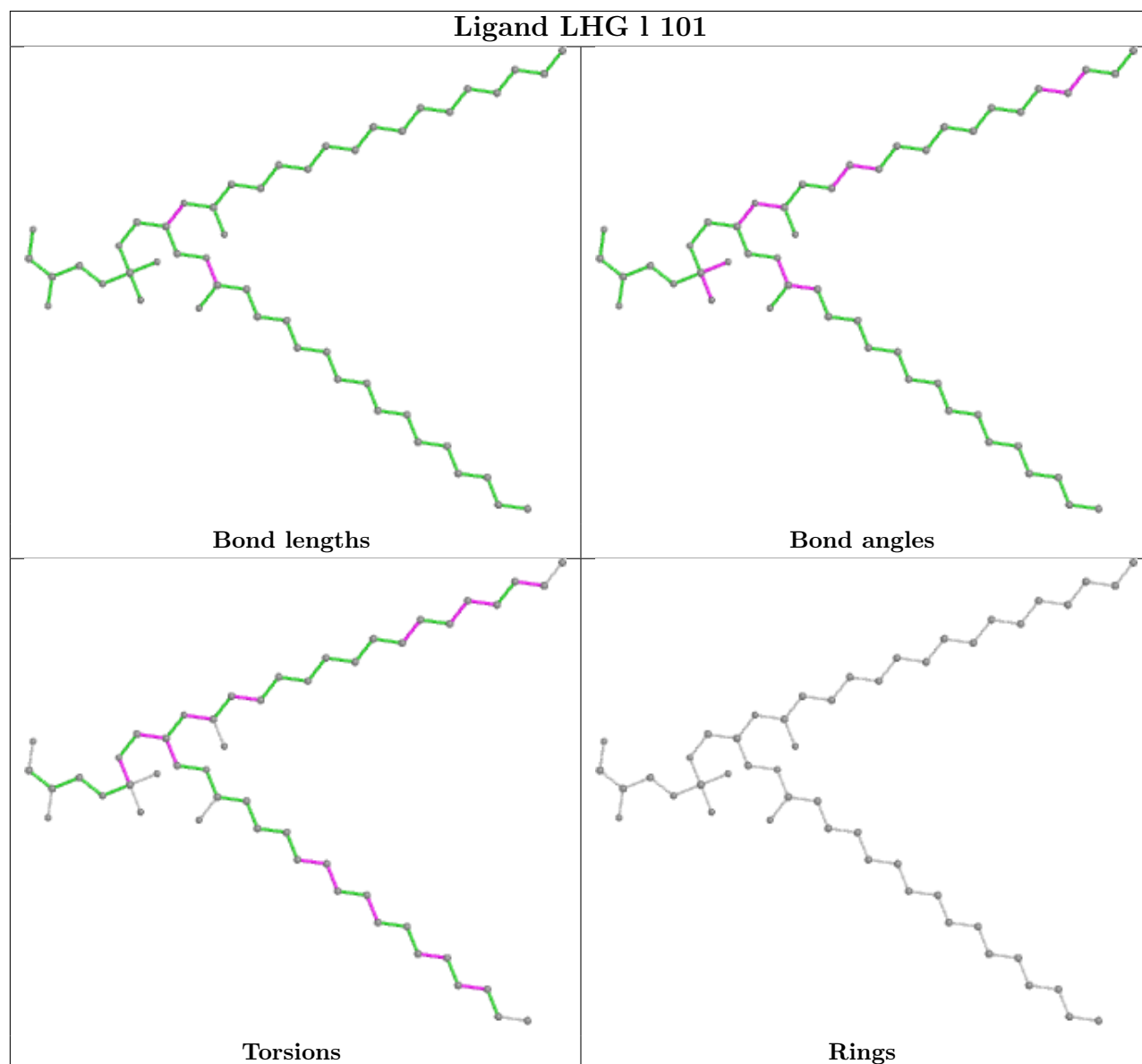


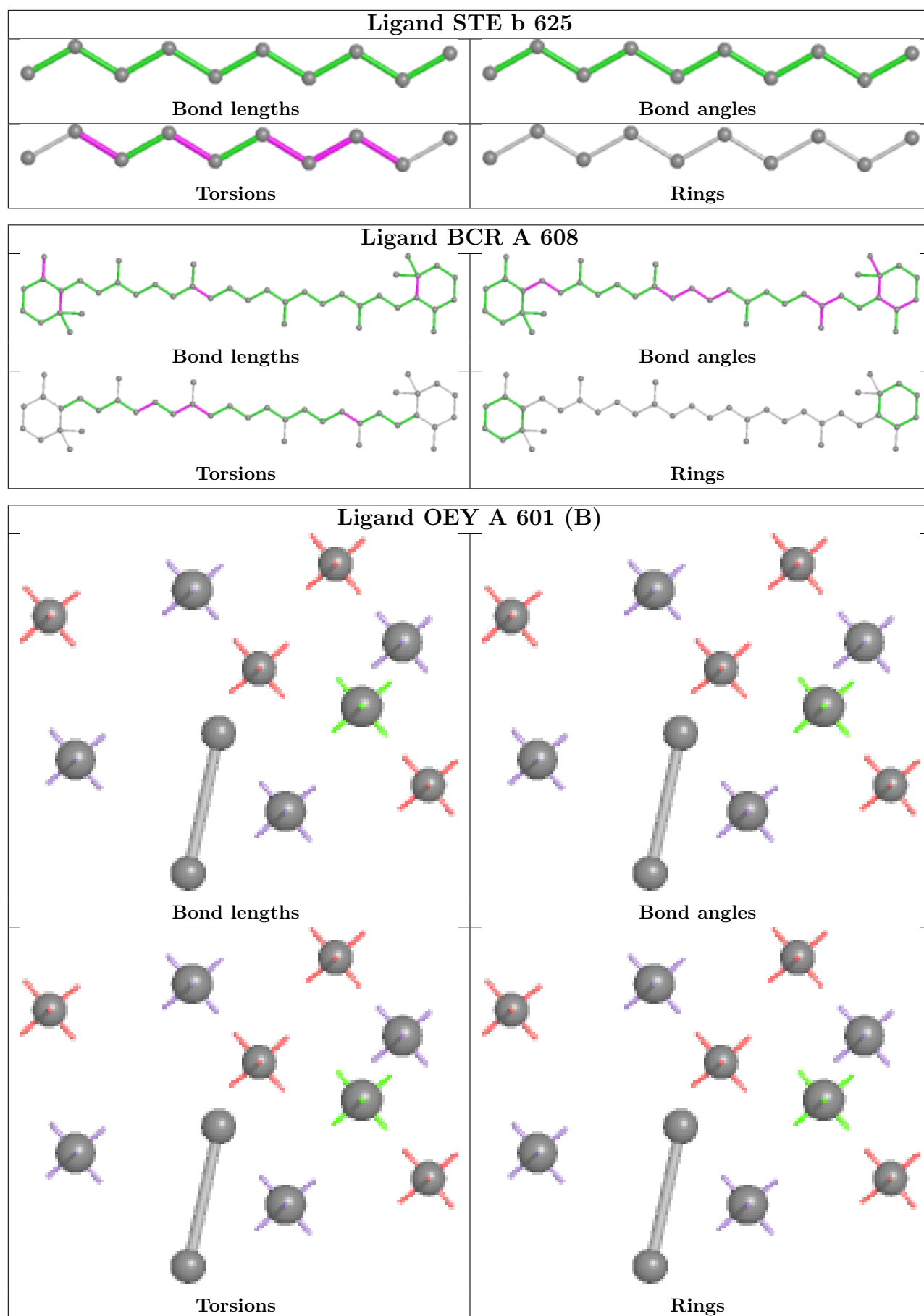


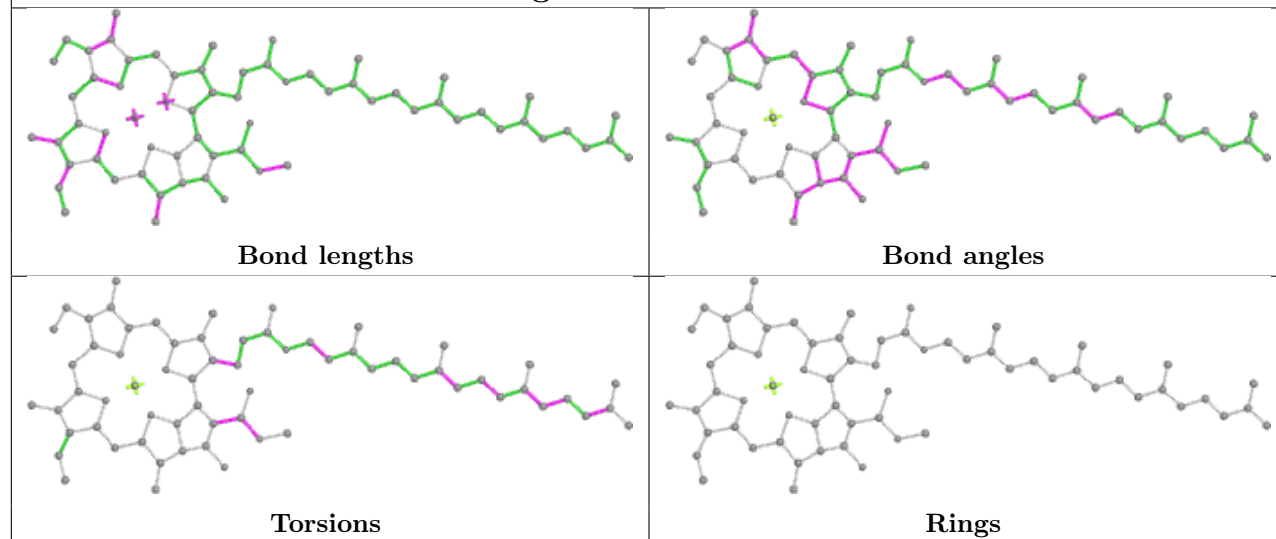
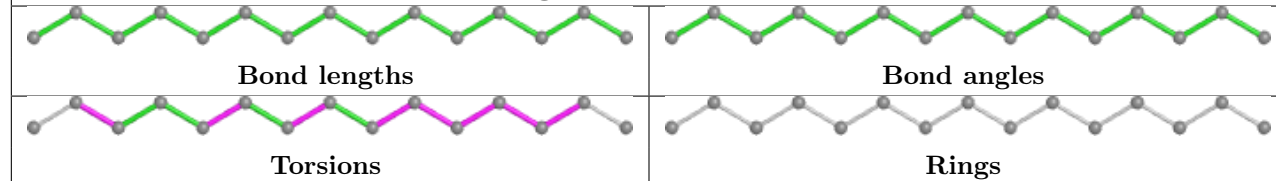
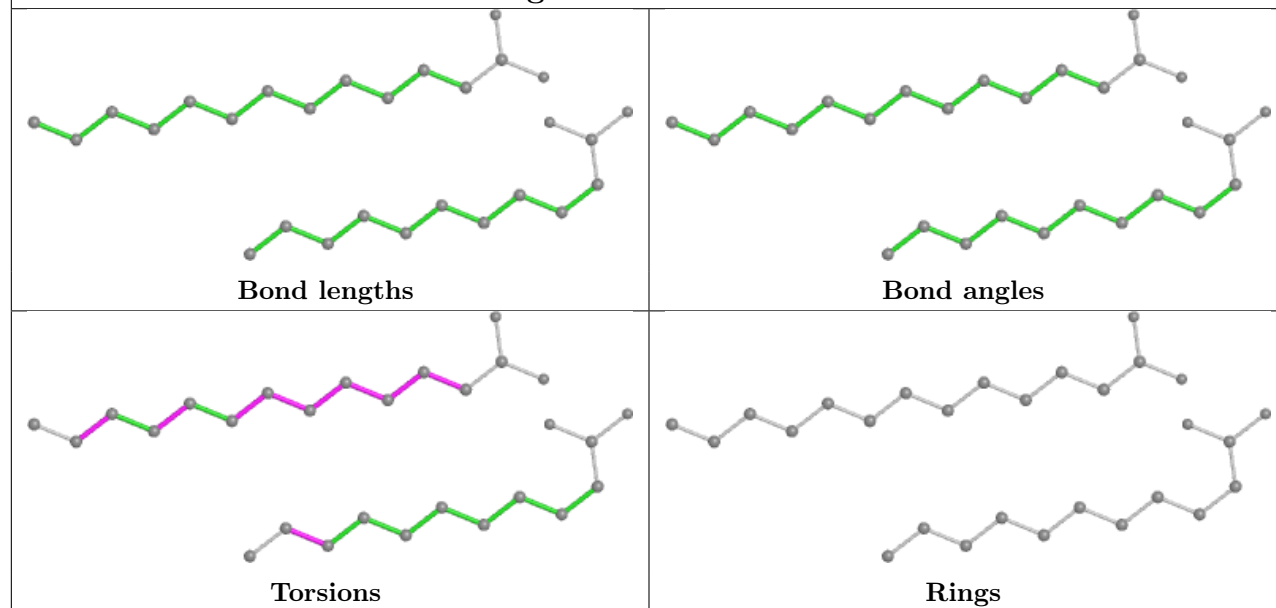
## Ligand CLA a 605



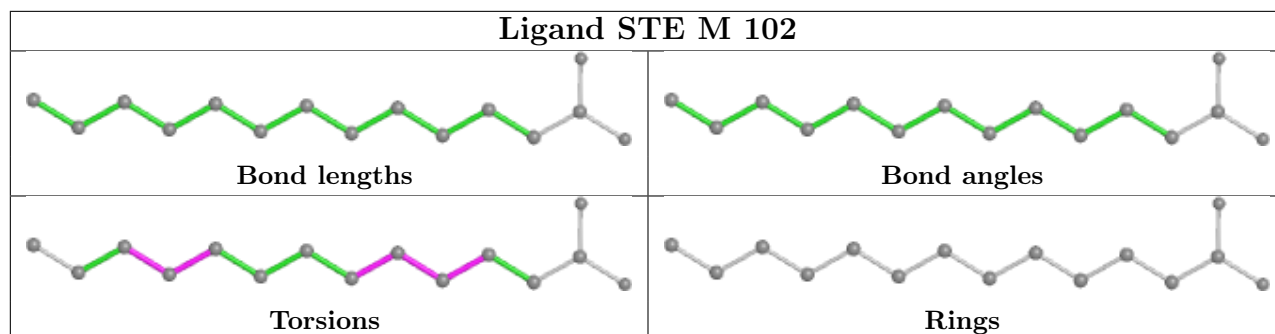
## Ligand LHG 1 101



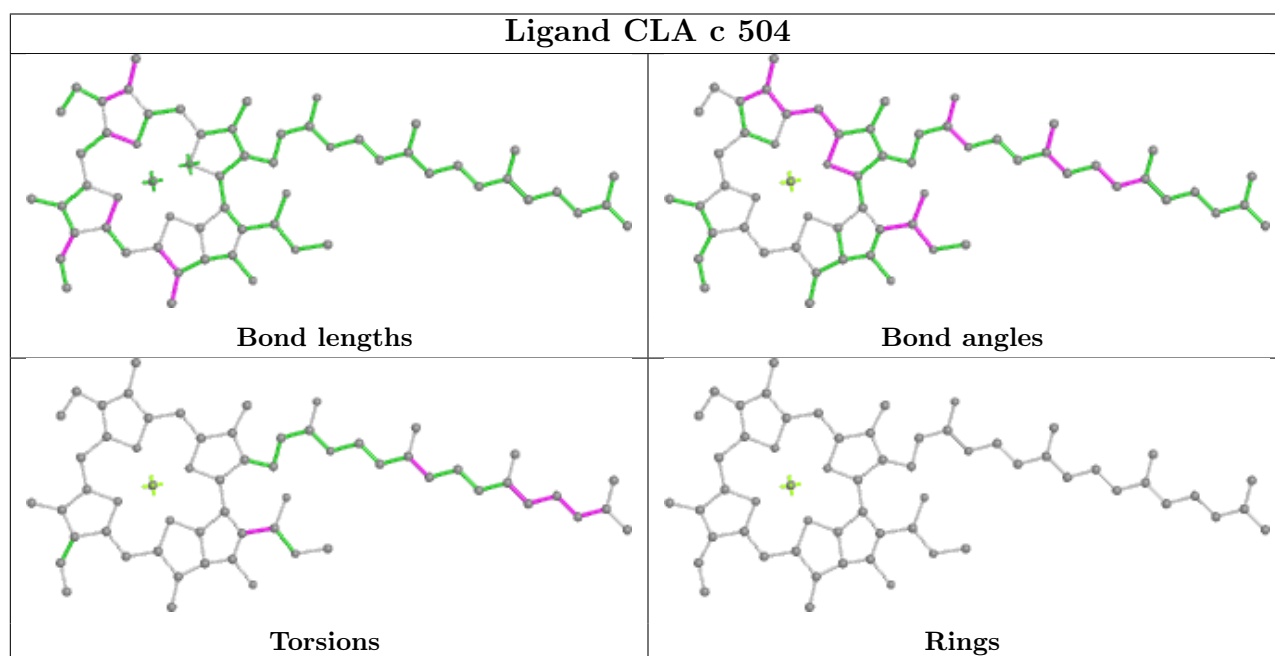


**Ligand CLA B 603****Ligand STE B 625****Ligand LMG D 412**

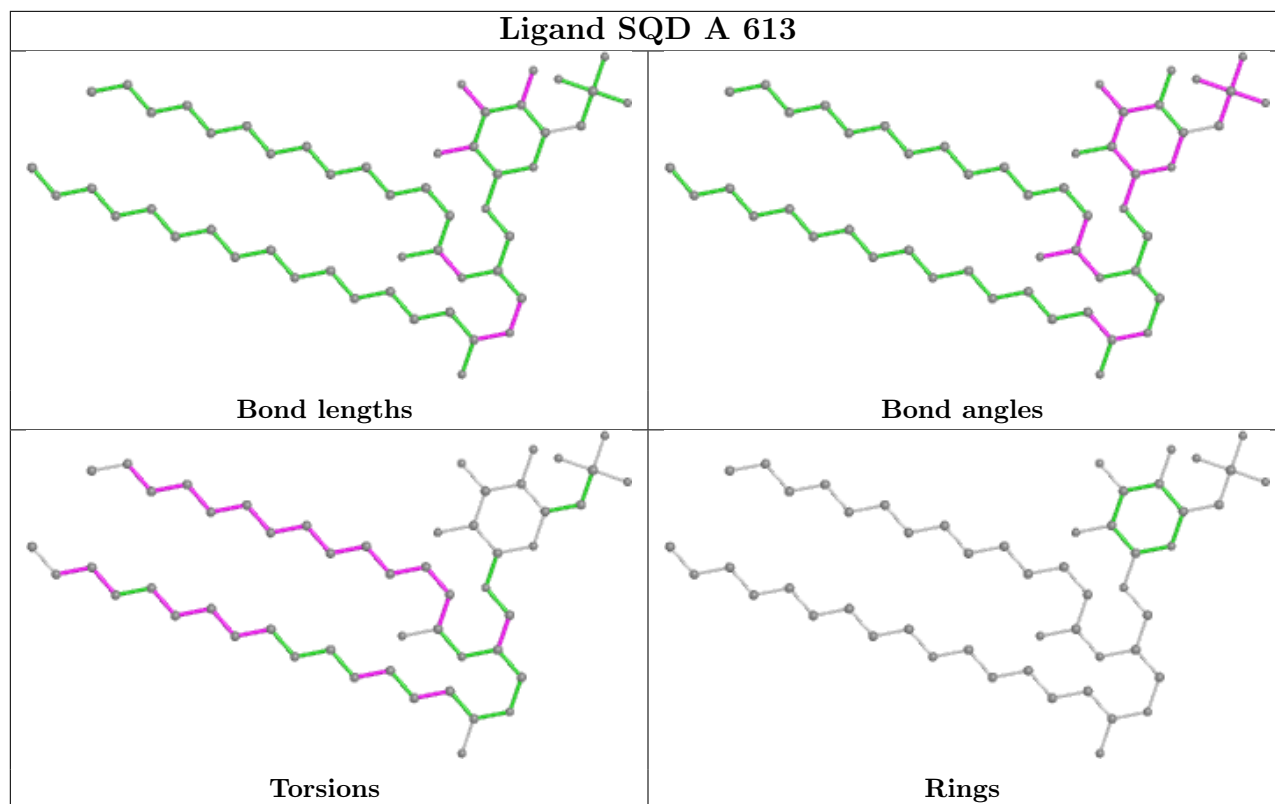
## Ligand STE M 102



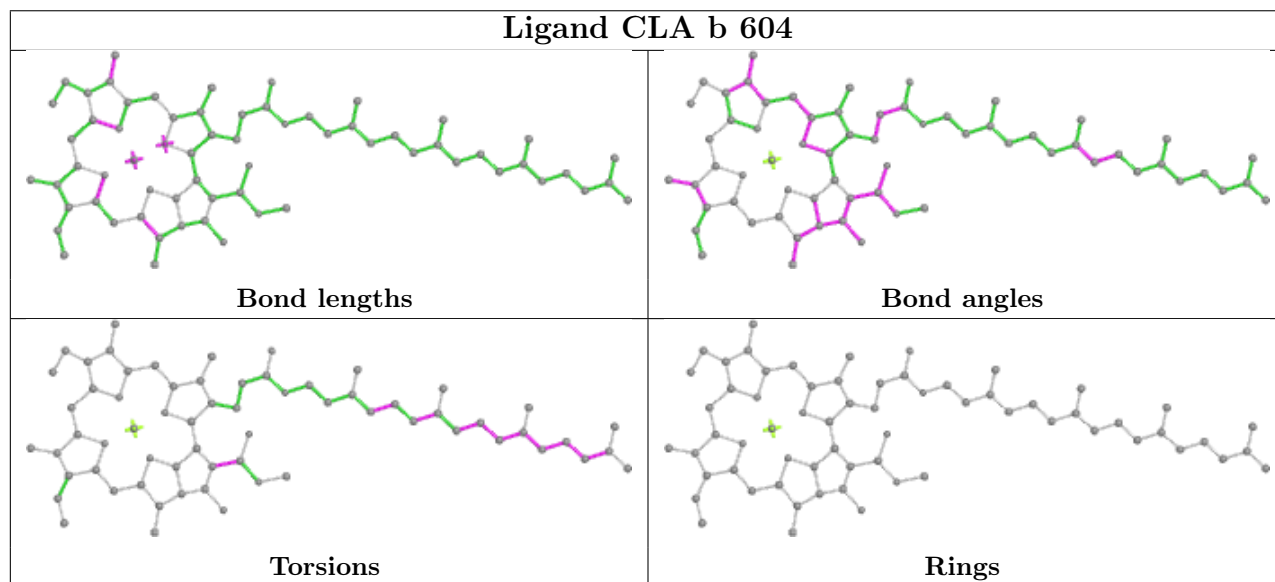
## Ligand CLA c 504

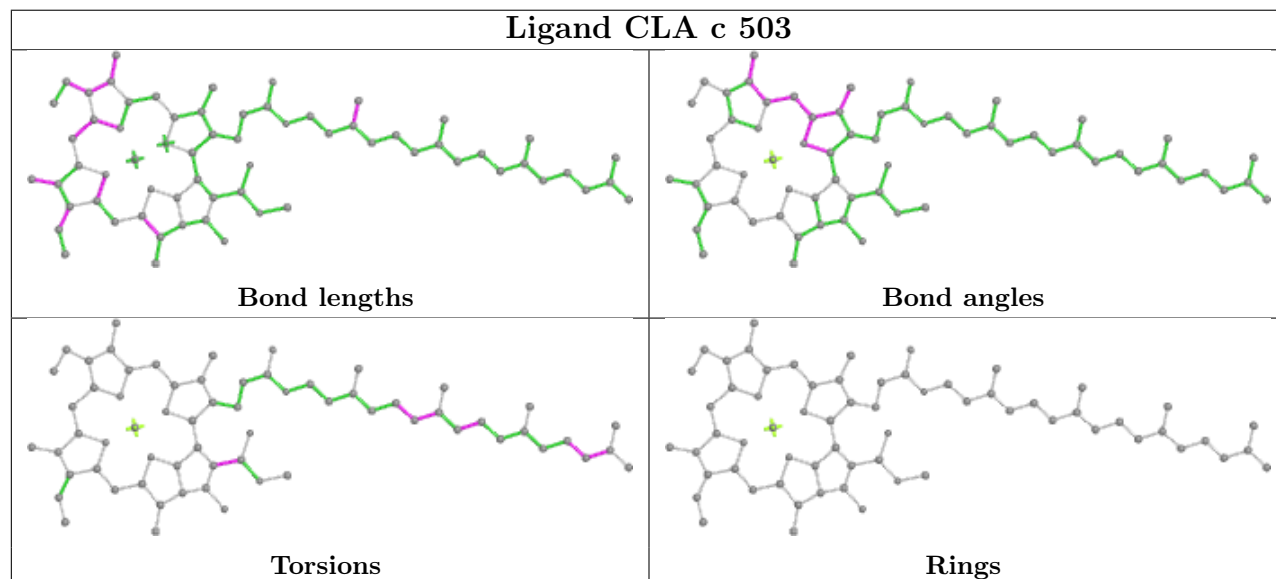
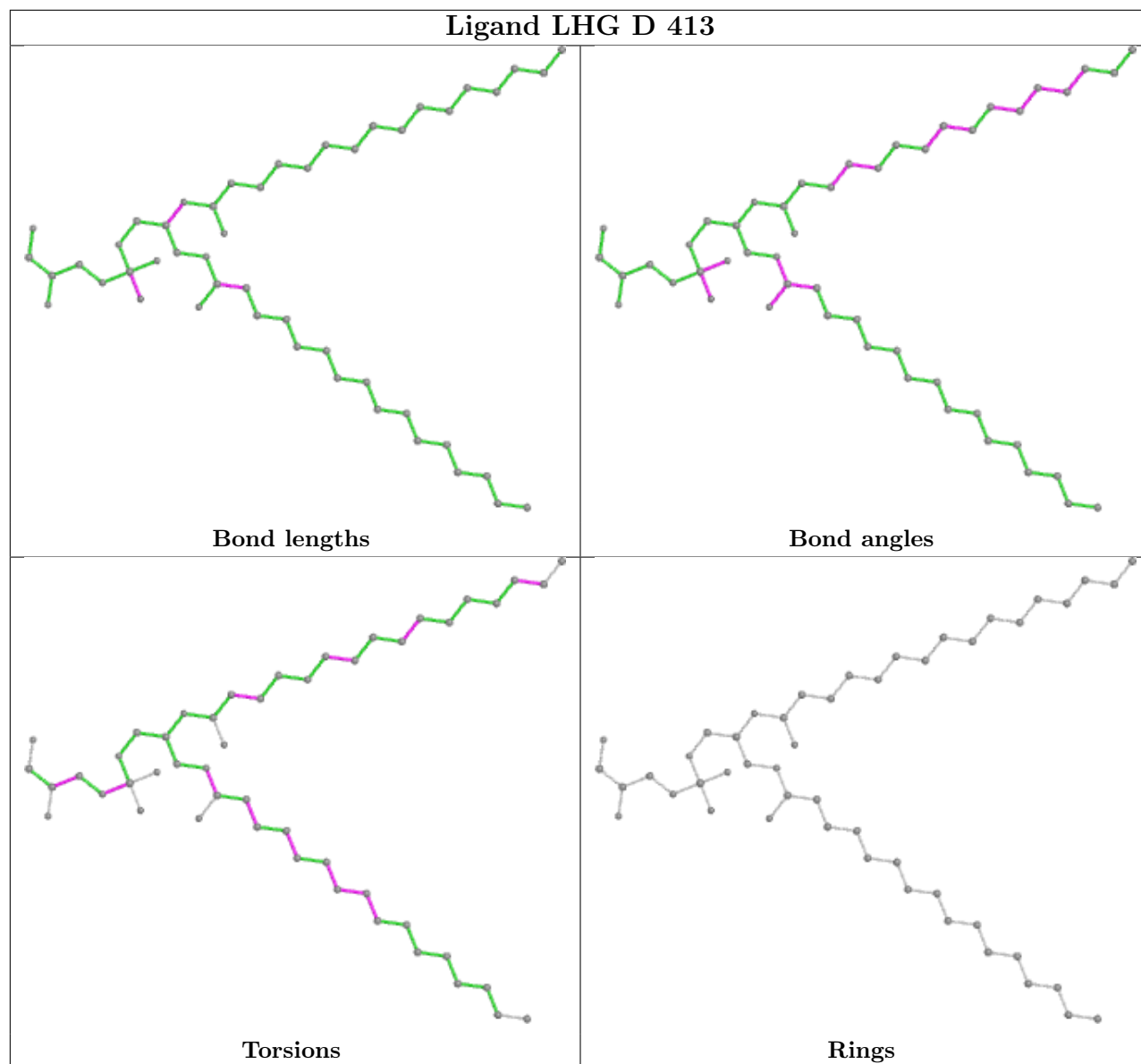


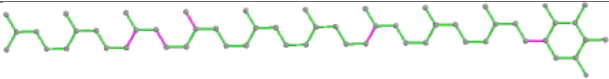
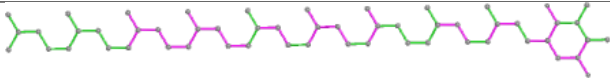
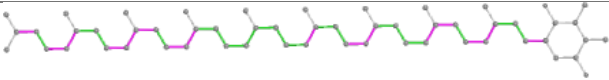
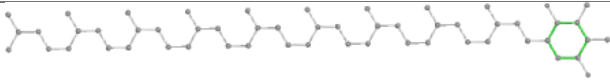
## Ligand SQD A 613

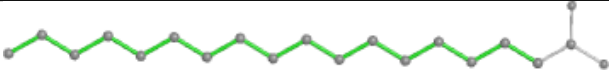
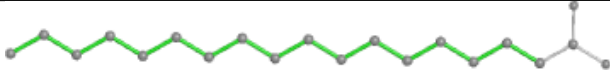
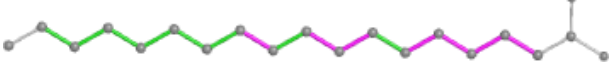
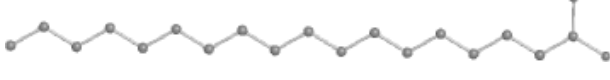



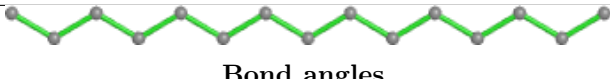


## Ligand CLA b 604

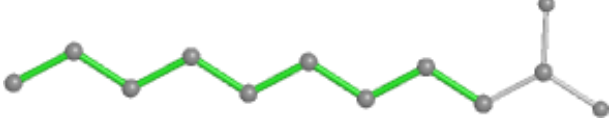
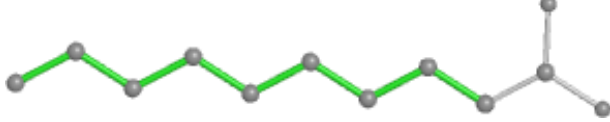
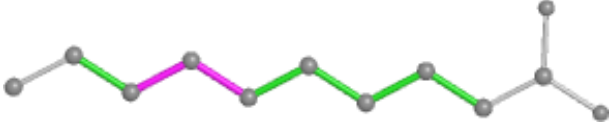
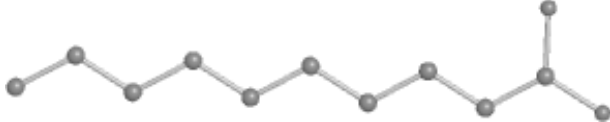




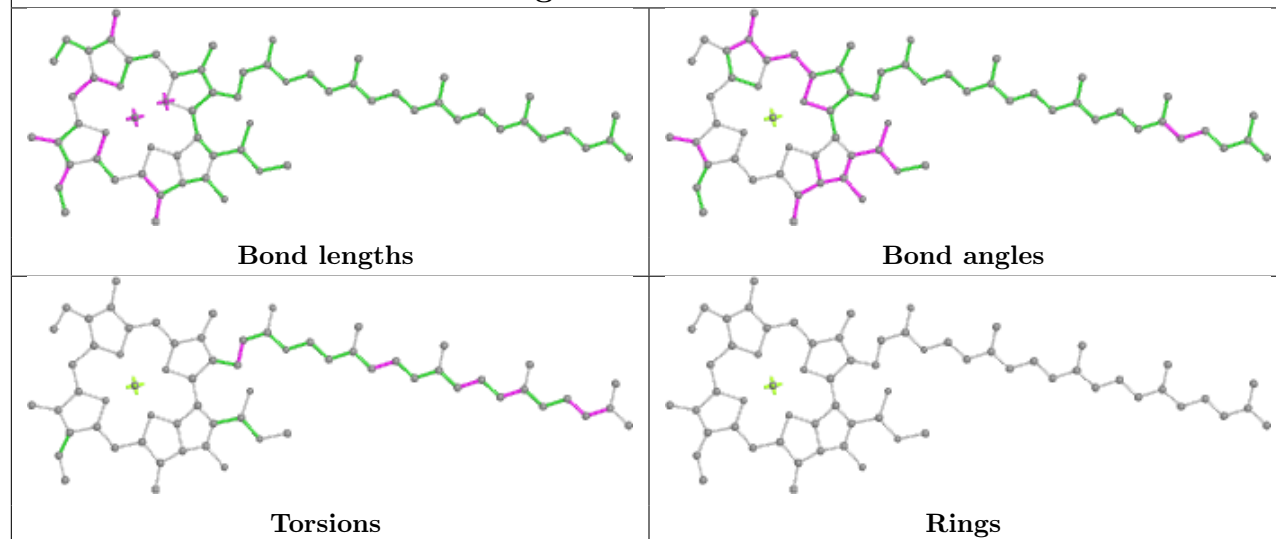
Ligand PL9 A 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand STE c 520	
 Bond lengths	 Bond angles
 Torsions	 Rings

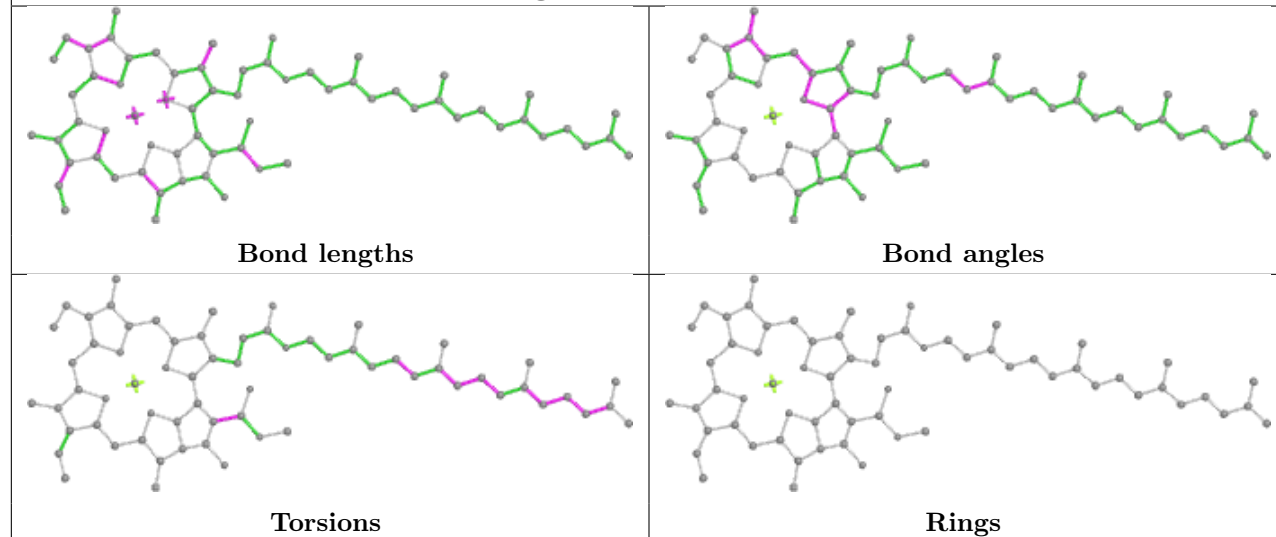
Ligand STE I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

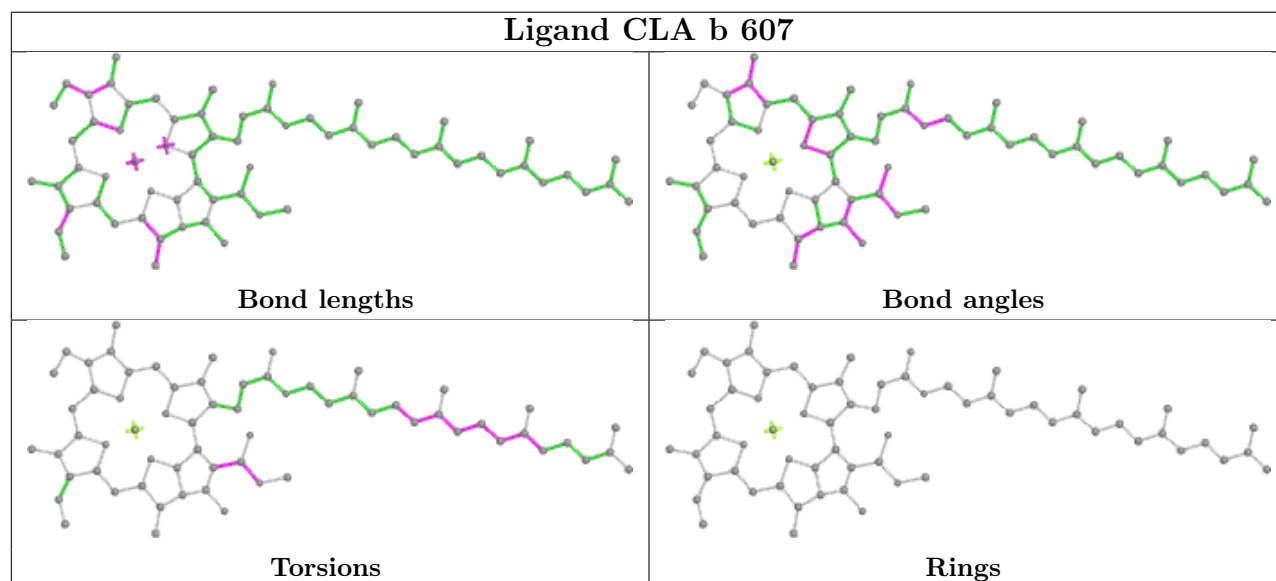
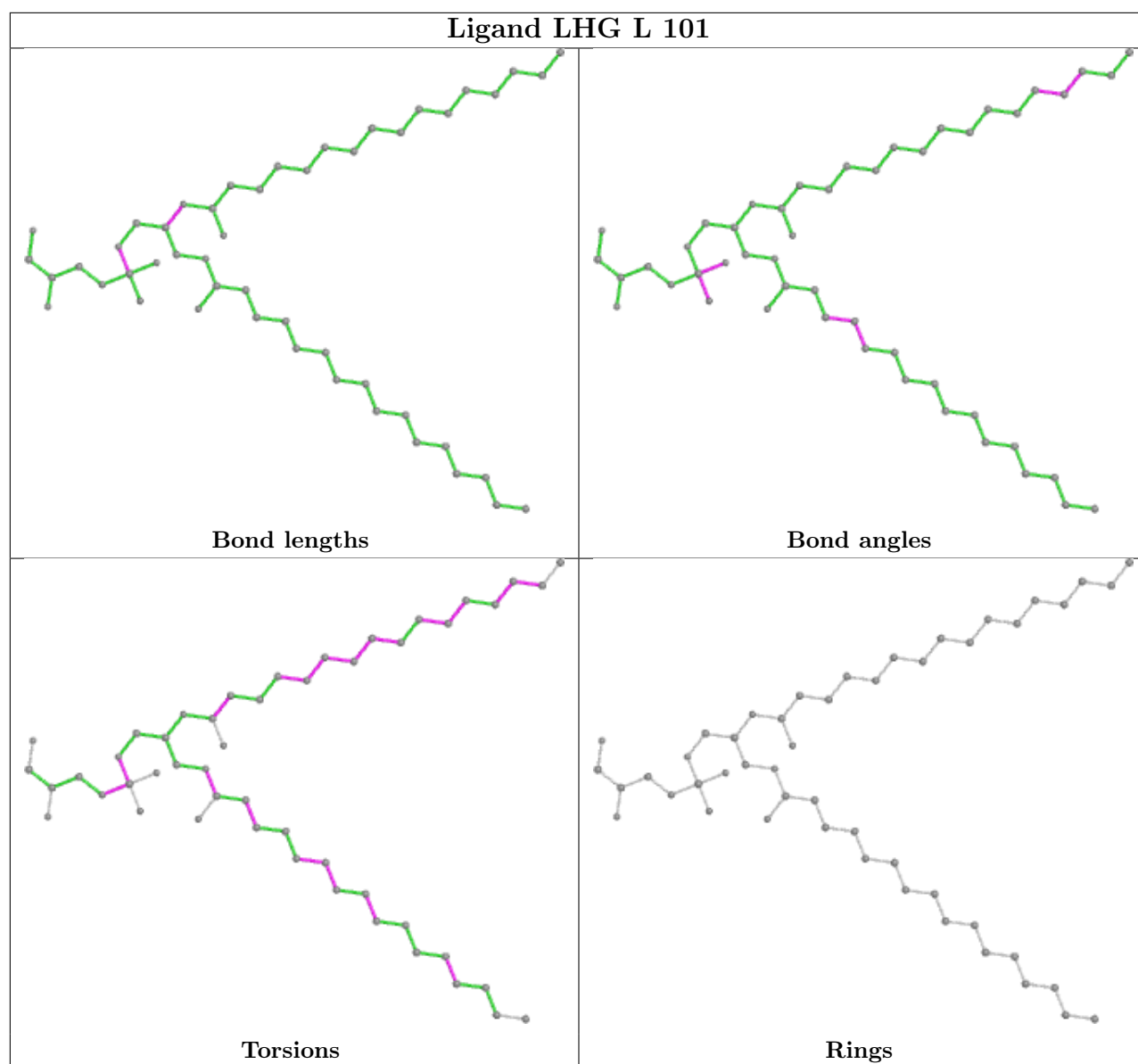
Ligand STE J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

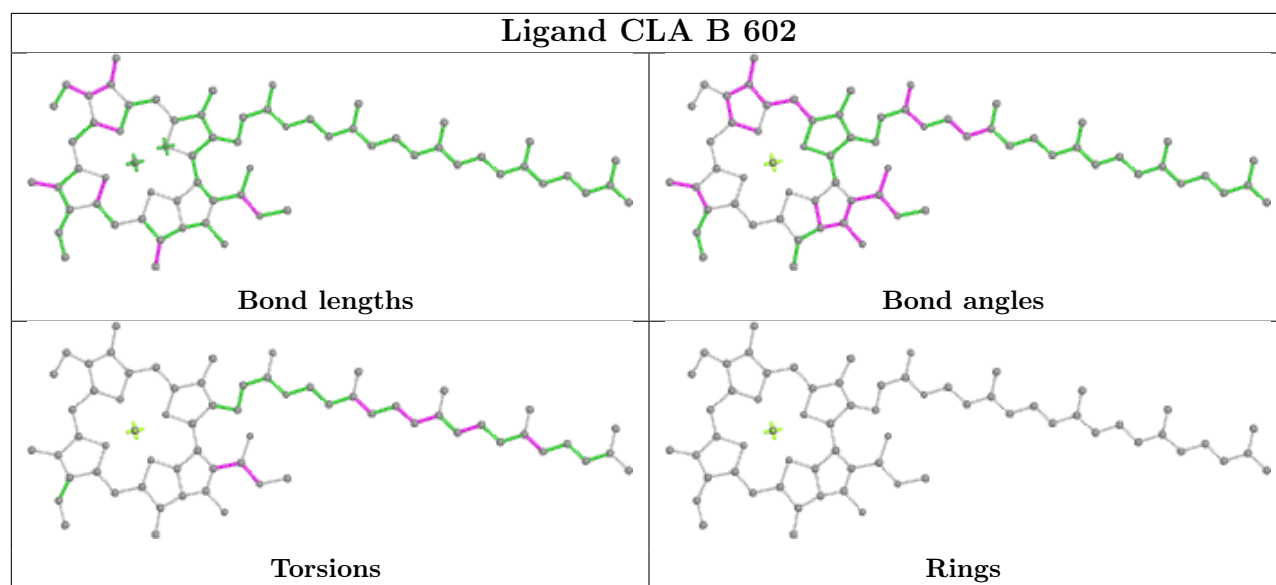
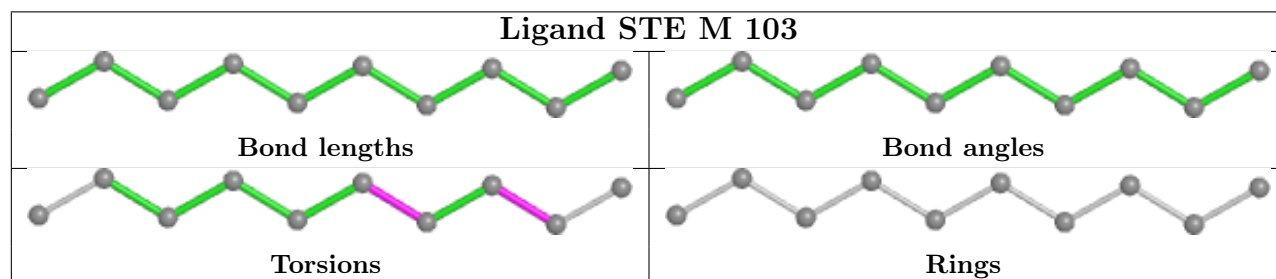
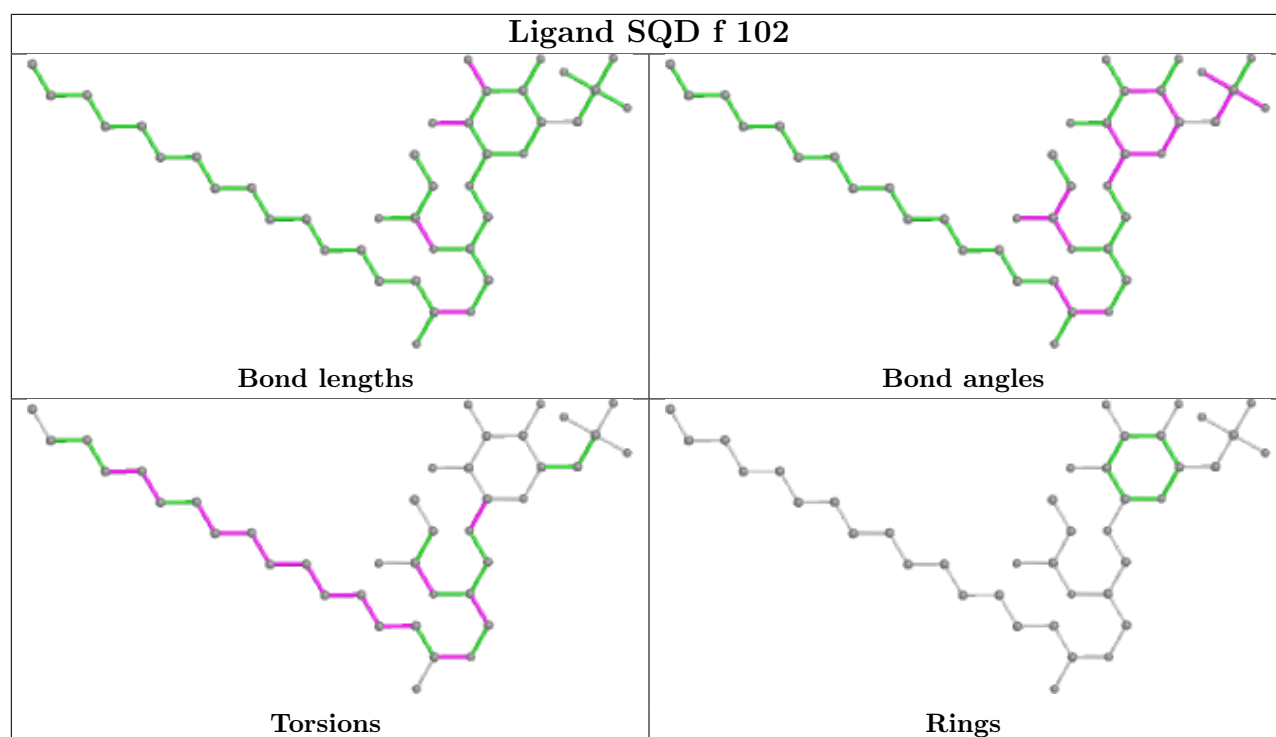
## Ligand CLA b 602

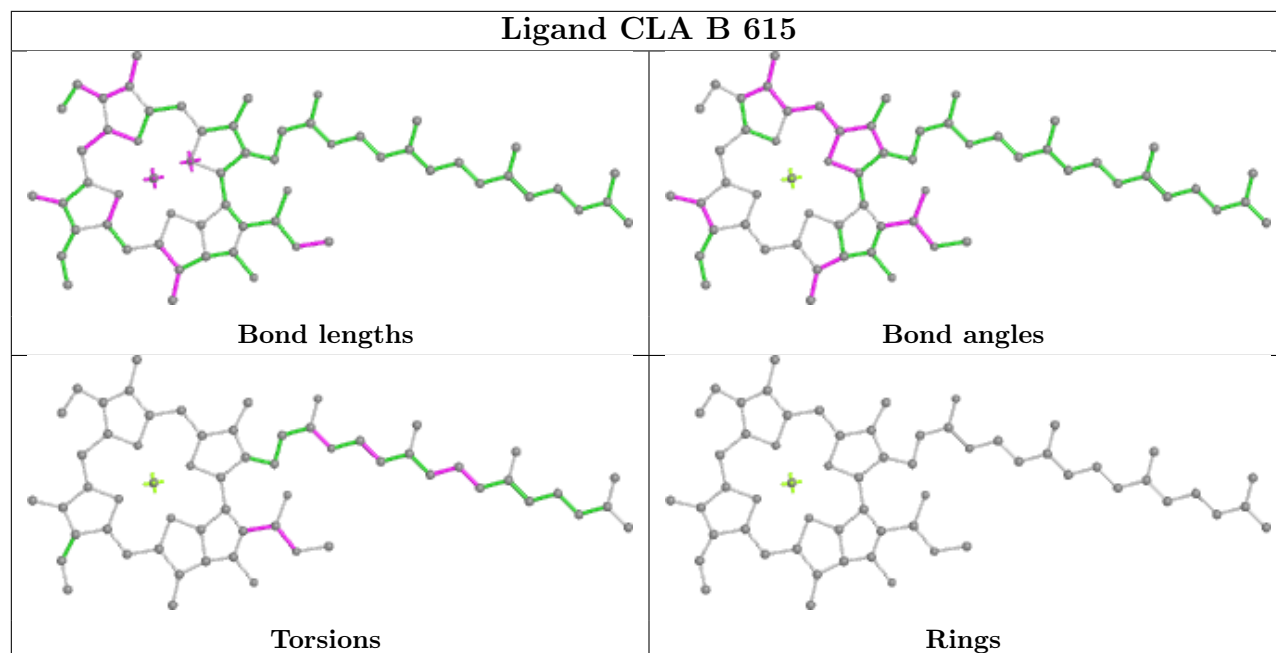
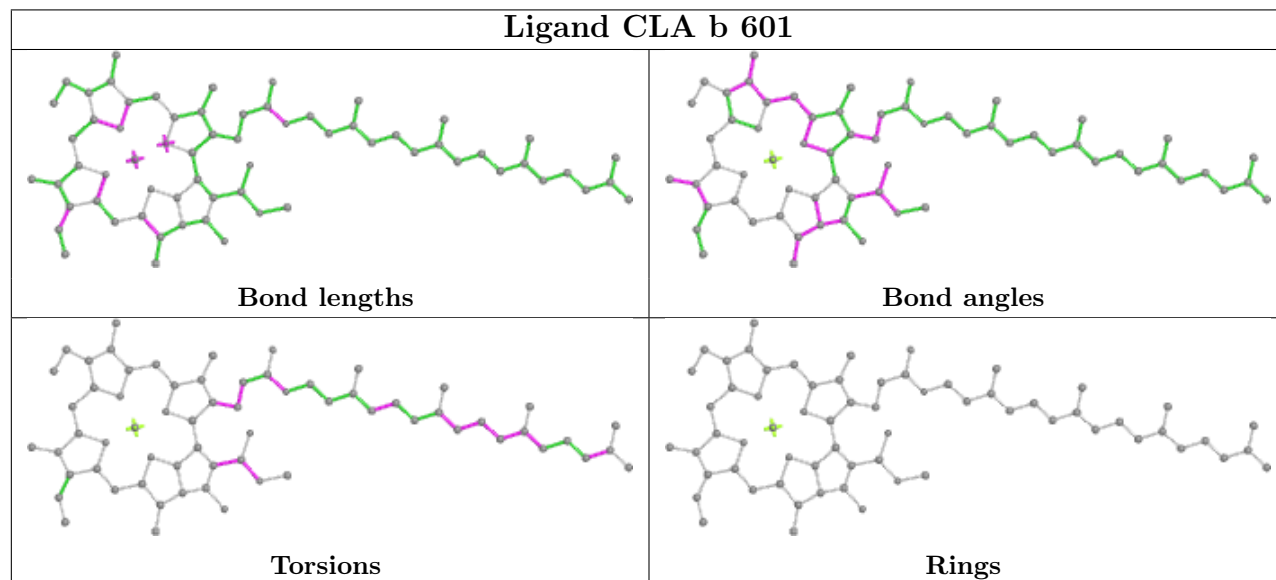
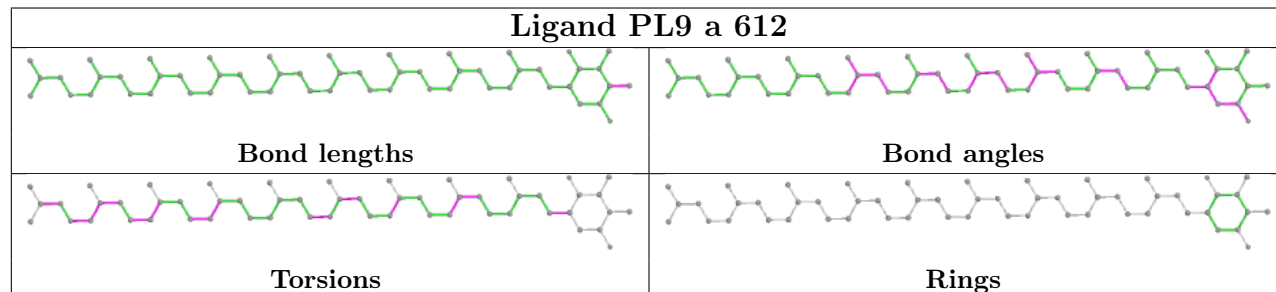


## Ligand CLA B 606

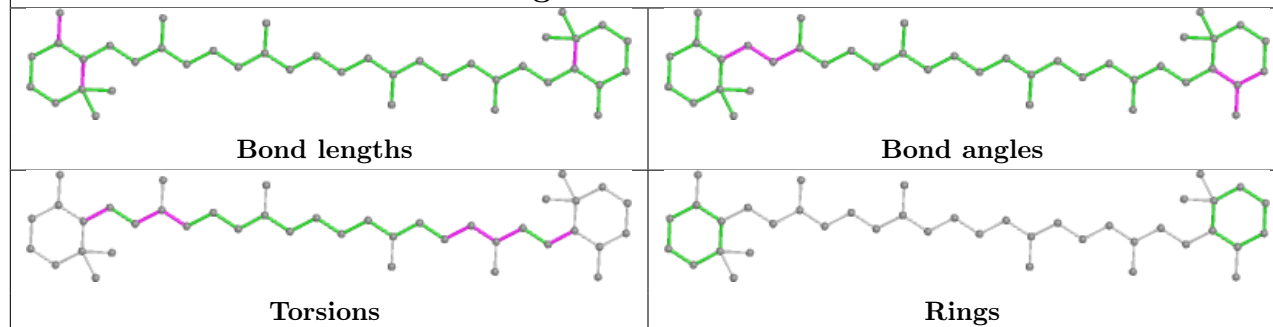




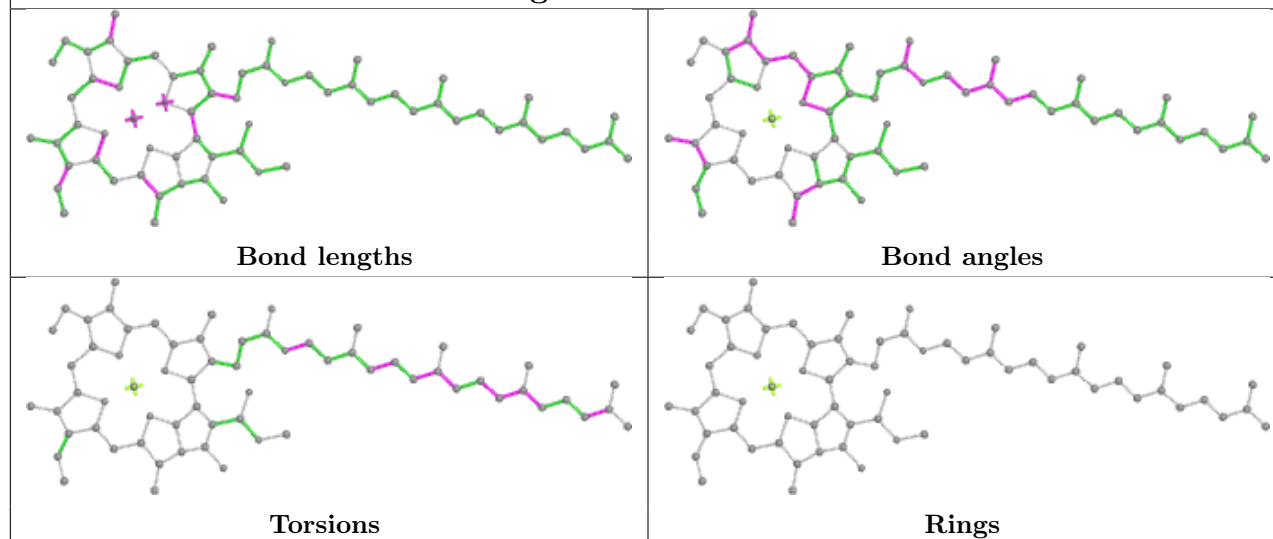


**Ligand CLA B 615****Ligand CLA b 601****Ligand PL9 a 612**

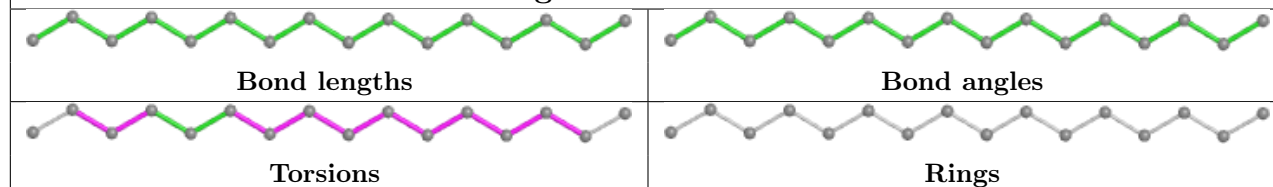
## Ligand BCR k 101



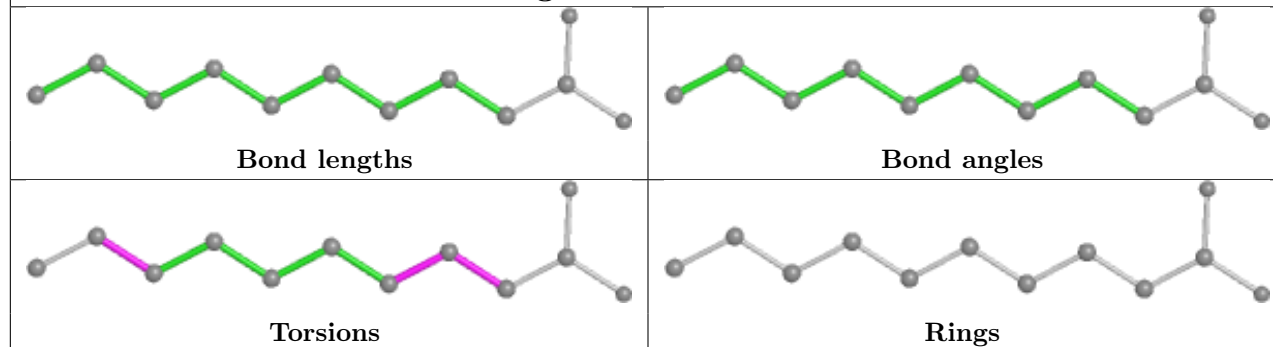
## Ligand CLA D 403

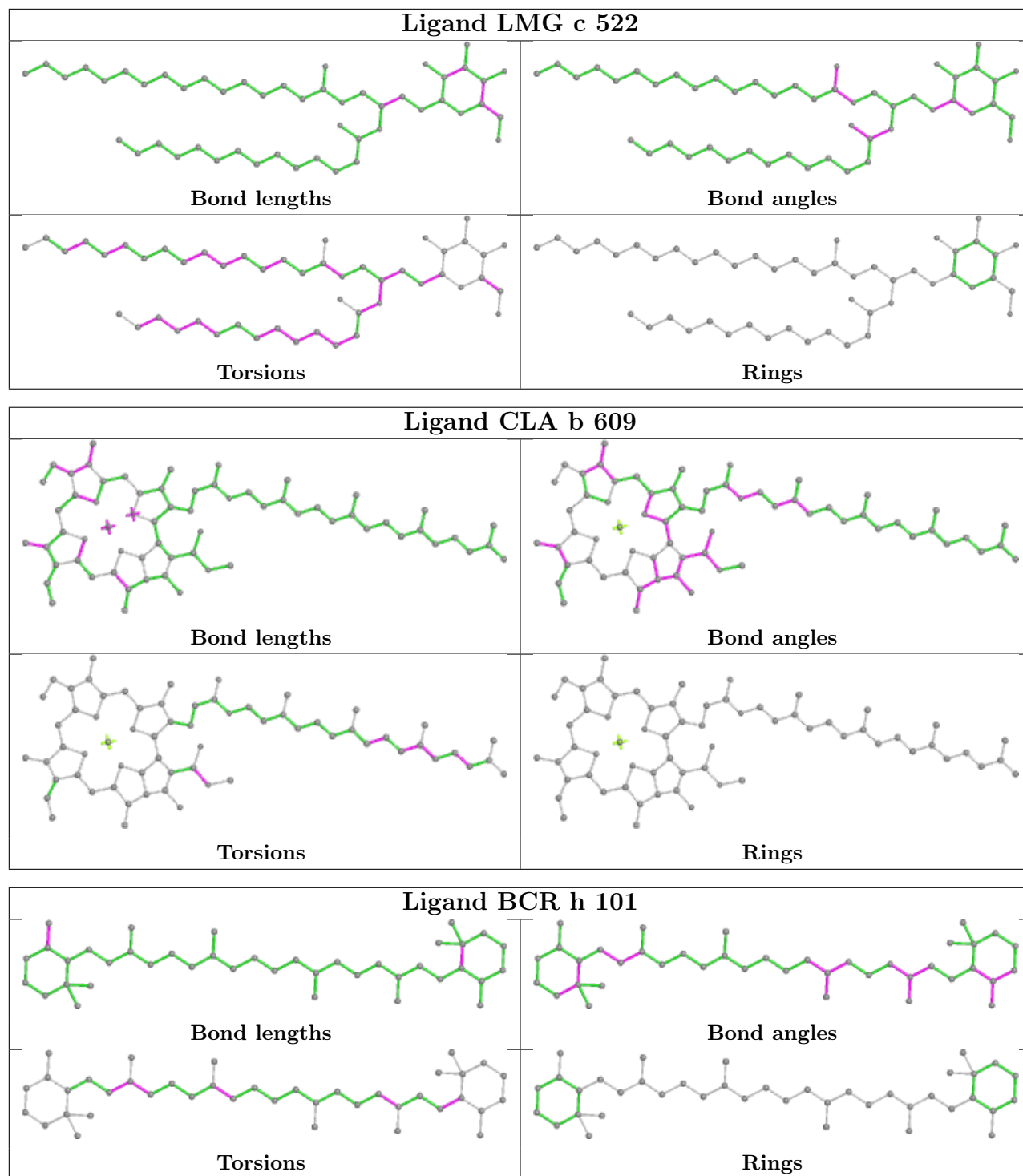


## Ligand STE B 624

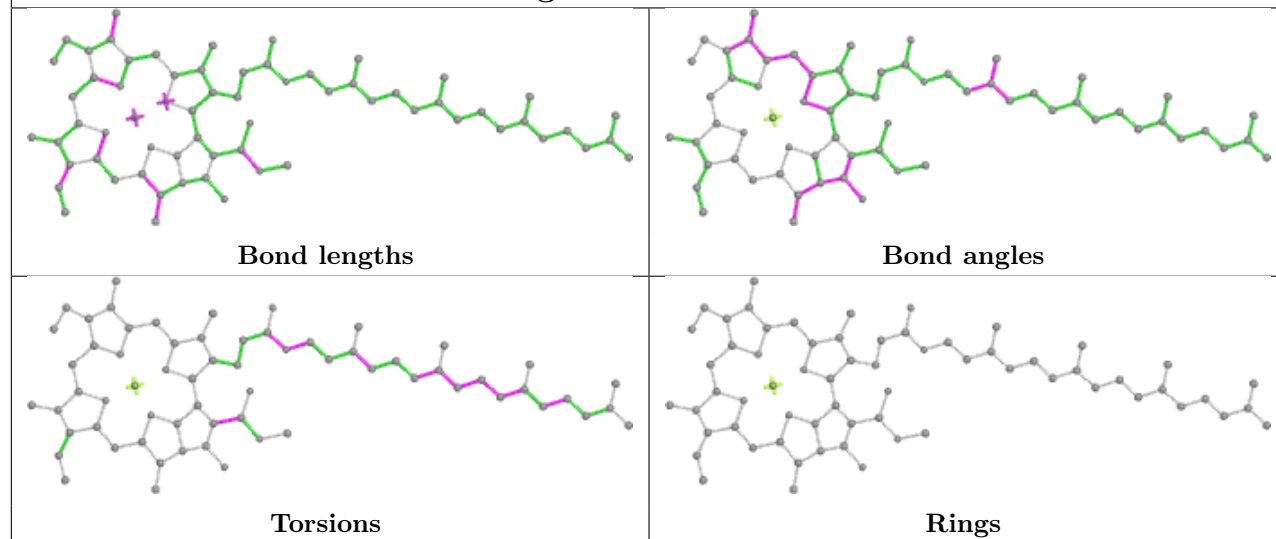


## Ligand STE L 102

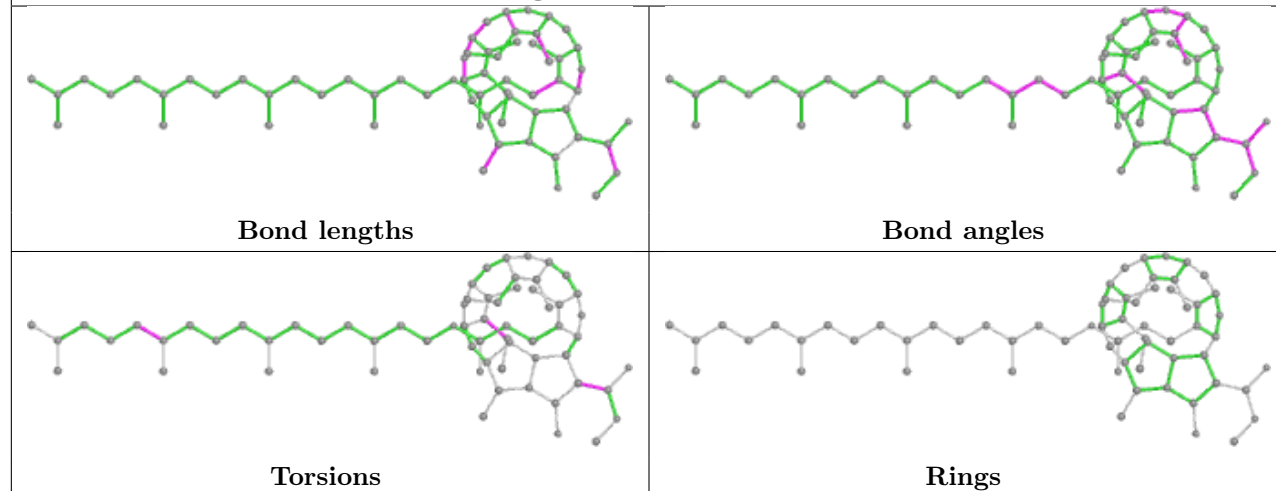




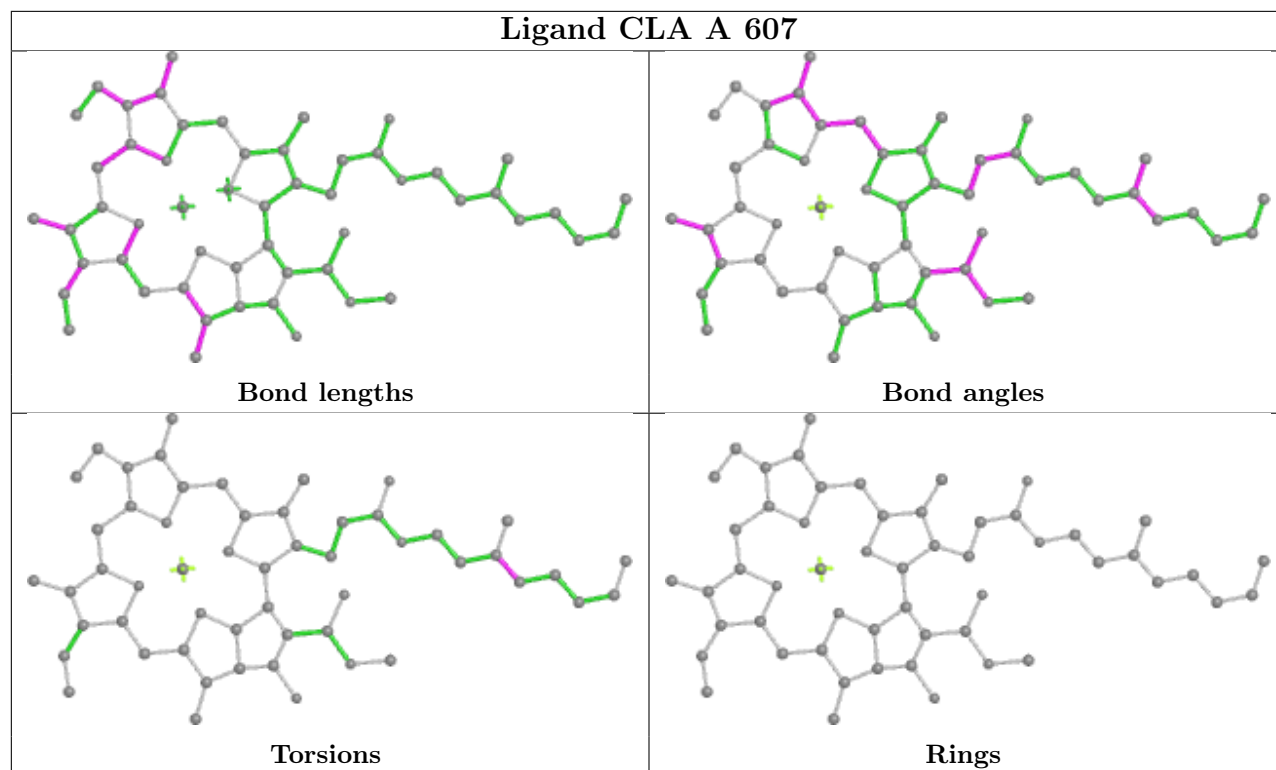
## Ligand CLA c 506



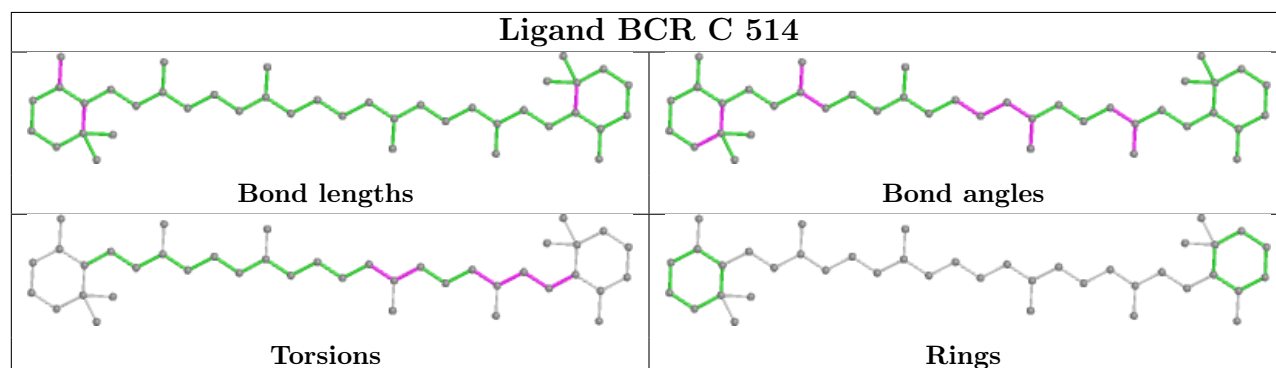
## Ligand PHO A 606



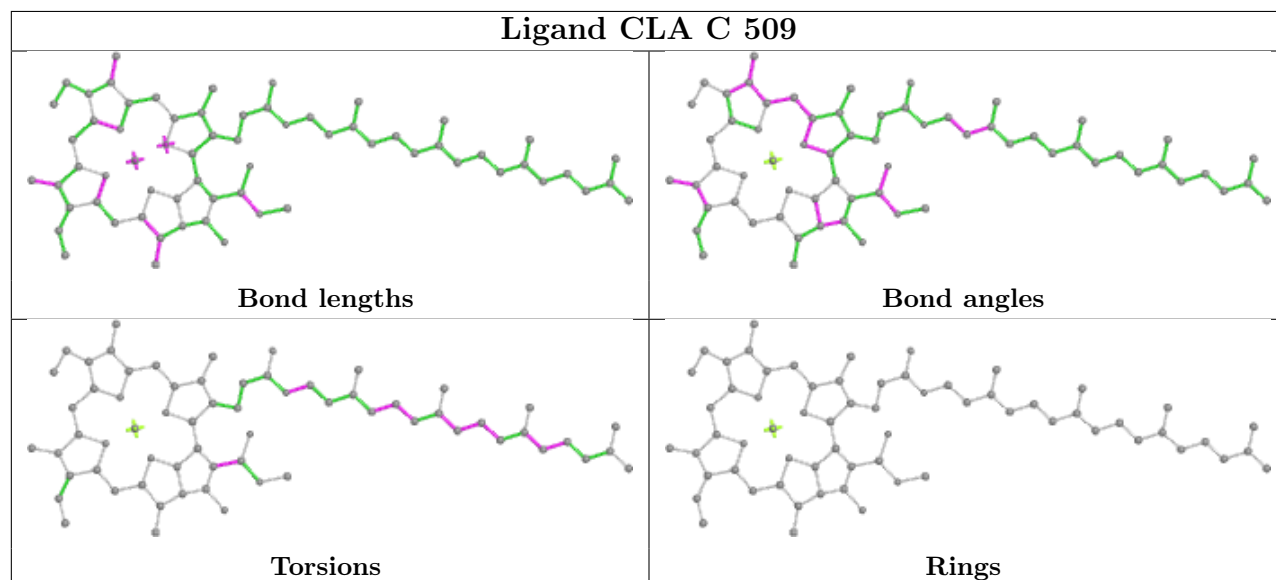
## Ligand CLA A 607

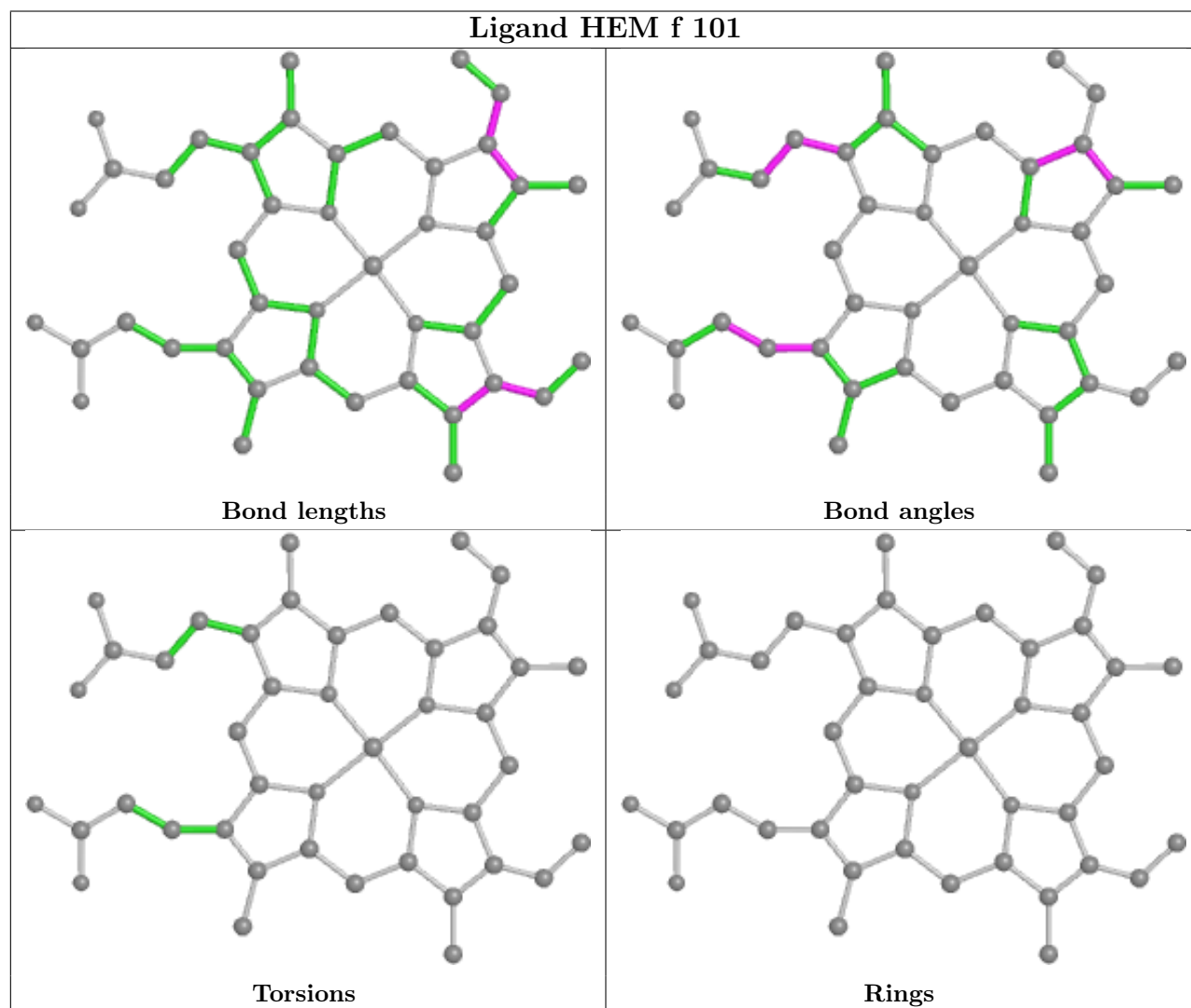
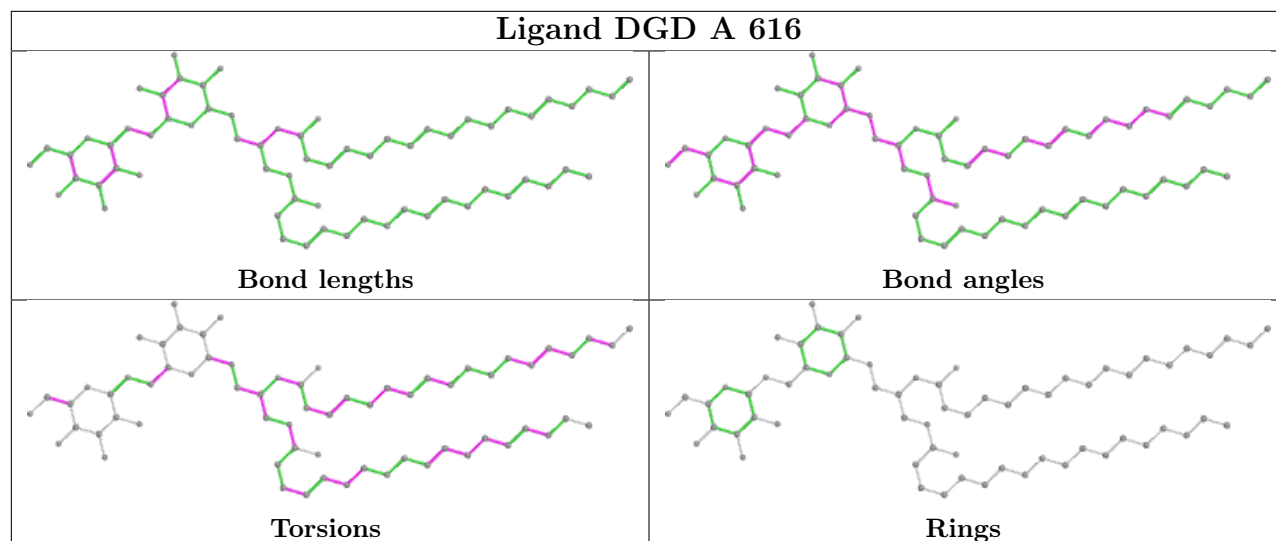


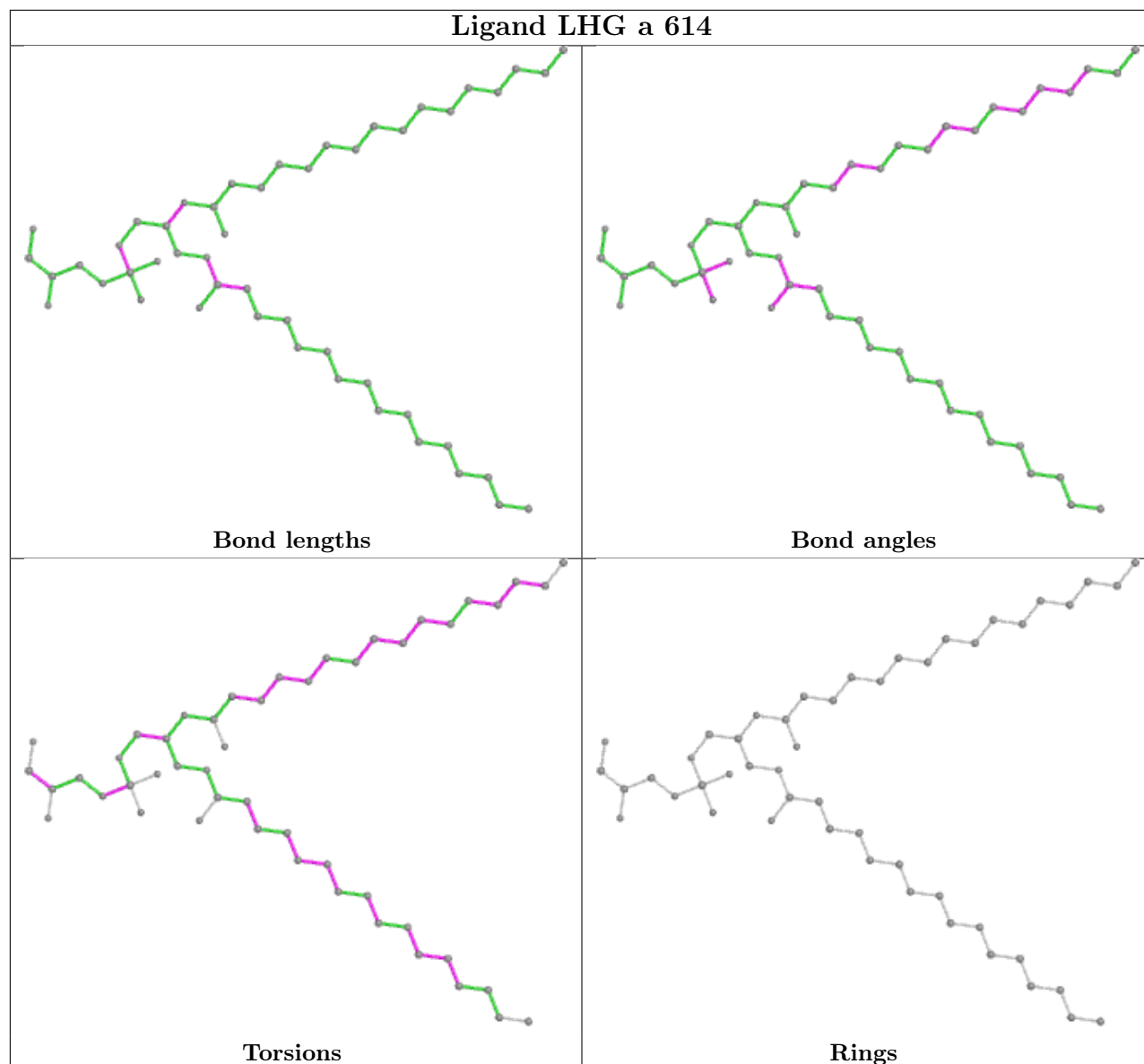
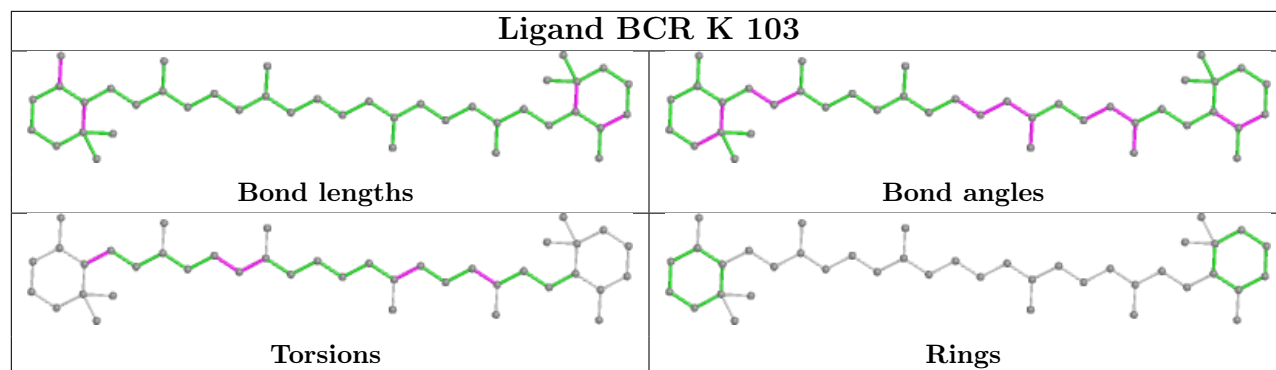
## Ligand BCR C 514

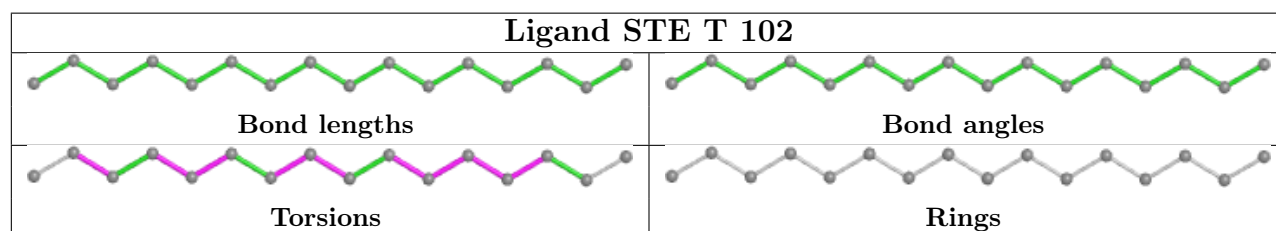
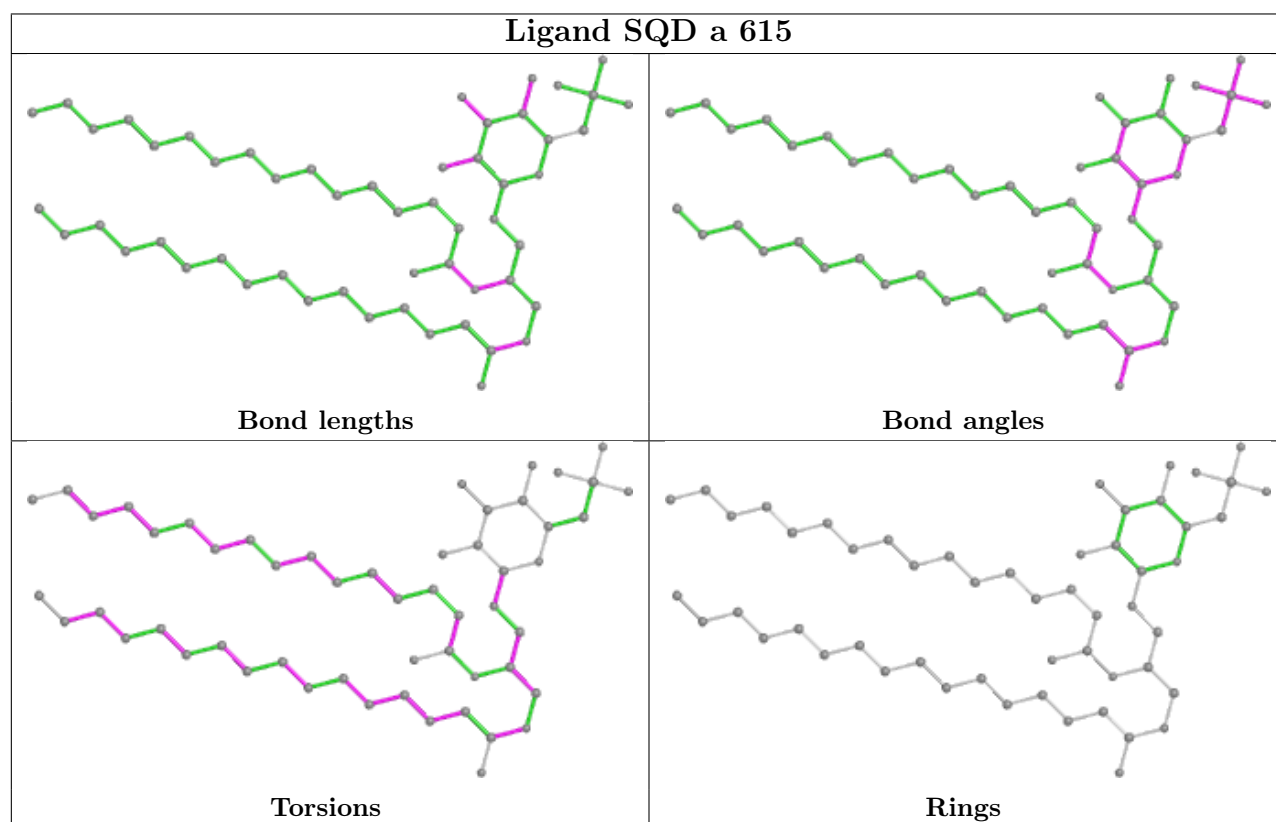
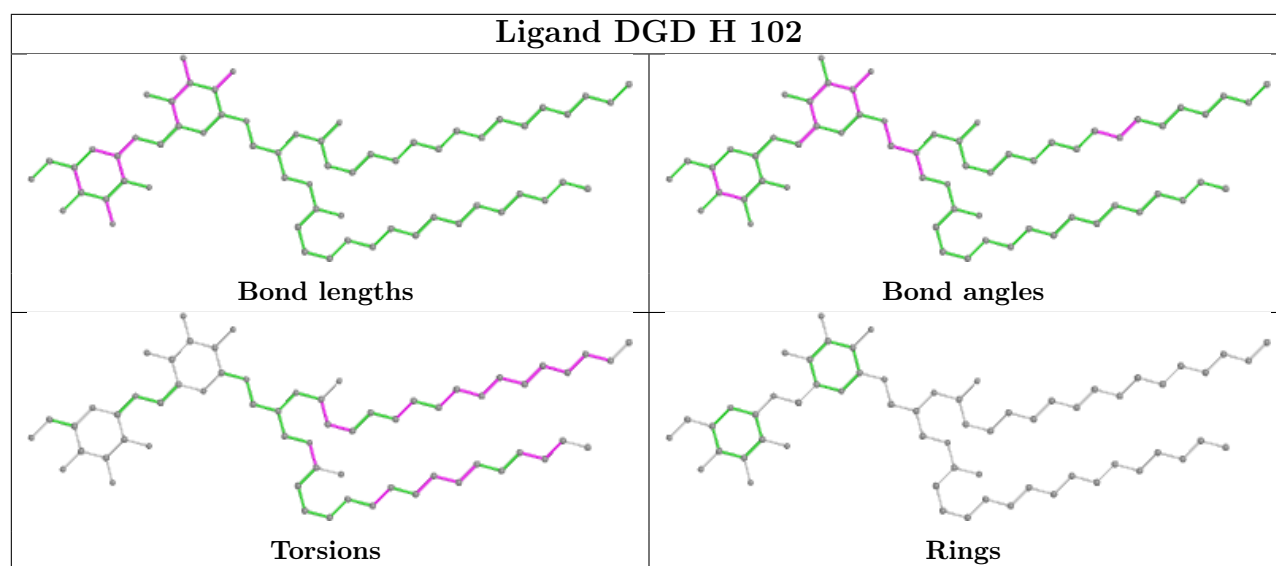


## Ligand CLA C 509









## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.39	4 (1%) 79 80	25, 33, 53, 84	0
1	a	334/344 (97%)	-0.36	1 (0%) 94 94	24, 35, 61, 85	0
2	B	505/510 (99%)	-0.40	6 (1%) 79 80	27, 37, 64, 93	0
2	b	505/510 (99%)	-0.23	16 (3%) 47 47	28, 39, 74, 106	0
3	C	442/461 (95%)	-0.31	8 (1%) 68 69	29, 40, 56, 78	0
3	c	451/461 (97%)	-0.25	8 (1%) 68 69	29, 43, 63, 97	0
4	D	341/352 (96%)	-0.41	3 (0%) 84 84	26, 34, 54, 82	0
4	d	341/352 (96%)	-0.34	0 100 100	27, 38, 63, 84	0
5	E	82/84 (97%)	-0.02	4 (4%) 29 29	37, 55, 74, 87	0
5	e	82/84 (97%)	0.19	6 (7%) 15 14	40, 64, 84, 93	0
6	F	34/45 (75%)	-0.30	2 (5%) 22 21	41, 48, 71, 97	0
6	f	34/45 (75%)	-0.17	4 (11%) 4 3	45, 54, 92, 109	0
7	H	65/66 (98%)	-0.12	2 (3%) 49 49	37, 45, 62, 77	0
7	h	63/66 (95%)	0.25	6 (9%) 8 7	44, 55, 66, 69	0
8	I	35/38 (92%)	-0.33	2 (5%) 23 23	35, 42, 70, 89	0
8	i	35/38 (92%)	-0.18	3 (8%) 10 10	36, 43, 72, 80	0
9	J	36/40 (90%)	0.02	4 (11%) 5 4	39, 54, 84, 92	0
9	j	36/40 (90%)	0.07	4 (11%) 5 4	42, 57, 94, 101	0
10	K	37/46 (80%)	0.16	4 (10%) 5 5	48, 56, 76, 86	0
10	k	37/46 (80%)	-0.10	1 (2%) 54 55	51, 59, 76, 84	0
11	L	37/37 (100%)	-0.56	0 100 100	28, 33, 62, 71	0
11	l	36/37 (97%)	-0.27	3 (8%) 11 11	28, 34, 65, 88	0
12	M	32/36 (88%)	-0.18	1 (3%) 49 49	29, 36, 63, 74	0
12	m	31/36 (86%)	-0.31	1 (3%) 47 47	30, 37, 58, 71	0

*Continued on next page...*

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	244/272 (89%)	-0.12	13 (5%) 26 26	29, 45, 82, 128	0
13	o	244/272 (89%)	-0.19	14 (5%) 23 23	29, 44, 80, 121	0
14	R	28/41 (68%)	3.55	26 (92%) 0 0	77, 89, 101, 107	0
14	r	28/41 (68%)	5.75	28 (100%) 0 0	86, 118, 129, 134	0
15	T	29/32 (90%)	-0.40	2 (6%) 16 16	30, 35, 60, 81	0
15	t	29/32 (90%)	-0.24	3 (10%) 6 5	31, 36, 71, 78	0
16	U	97/134 (72%)	-0.39	0 100 100	36, 46, 69, 89	0
16	u	97/134 (72%)	-0.47	0 100 100	34, 44, 60, 85	0
17	V	137/163 (84%)	-0.64	0 100 100	31, 44, 59, 76	0
17	v	137/163 (84%)	-0.28	0 100 100	37, 51, 69, 81	0
18	X	38/41 (92%)	0.22	2 (5%) 26 26	45, 55, 75, 79	0
18	x	39/41 (95%)	0.47	4 (10%) 6 5	49, 65, 92, 106	0
19	Y	27/46 (58%)	1.35	9 (33%) 0 0	58, 76, 89, 93	0
19	y	30/46 (65%)	0.60	3 (10%) 7 6	63, 76, 92, 97	0
20	Z	62/62 (100%)	0.78	15 (24%) 0 0	59, 74, 112, 126	0
20	z	62/62 (100%)	0.73	10 (16%) 1 1	61, 73, 108, 120	0
All	All	5293/5700 (92%)	-0.19	222 (4%) 36 35	24, 41, 77, 134	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	r	14	LEU	10.8
14	r	9	LEU	10.2
13	o	58	ASN	8.8
14	r	10	LEU	8.7
14	r	3	TRP	8.1
14	r	28	VAL	8.1
2	b	495	PHE	7.7
14	R	3	TRP	7.6
14	r	13	LEU	7.4
14	r	18	TRP	7.4
13	o	3	GLN	6.9
14	r	19	ALA	6.1
14	r	25	PRO	6.0
14	r	6	LEU	6.0
14	r	26	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
14	r	15	ALA	6.0
13	O	56	PRO	6.0
13	o	60	ARG	5.9
14	r	22	ASN	5.8
2	b	502	VAL	5.8
1	A	13	LEU	5.7
14	R	20	VAL	5.7
13	O	60	ARG	5.7
14	r	7	VAL	5.7
14	R	6	LEU	5.5
13	O	3	GLN	5.5
14	r	24	LEU	5.5
6	F	12	SER	5.4
13	O	4	THR	5.3
9	J	5	GLY	5.3
14	r	4	ARG	5.2
14	R	26	TYR	5.2
14	R	13	LEU	5.1
14	r	29	LYS	5.0
14	R	25	PRO	4.9
14	r	12	VAL	4.9
14	r	11	PRO	4.9
13	o	4	THR	4.8
13	o	57	LYS	4.8
13	O	61	GLN	4.7
3	c	23	ALA	4.7
14	R	21	ARG	4.7
6	f	12	SER	4.7
5	e	79	PHE	4.7
9	j	7	ARG	4.7
20	z	30	PRO	4.6
14	r	5	VAL	4.6
20	z	35	ARG	4.5
20	Z	1	MET	4.5
2	b	127	ARG	4.5
1	A	11	ALA	4.4
20	Z	34	ASP	4.4
13	O	62	GLU	4.4
9	j	6	GLY	4.3
13	o	56	PRO	4.3
14	r	27	ALA	4.3
14	r	2	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
14	R	28	VAL	4.2
3	c	24	THR	4.1
13	O	59	LYS	4.1
2	b	487	SER	4.1
10	k	17	ILE	4.1
14	r	23	ILE	4.1
13	o	61	GLN	4.1
9	J	6	GLY	4.0
14	R	14	LEU	4.0
19	Y	41	VAL	4.0
2	b	486	LEU	4.0
20	z	33	TRP	3.9
15	t	29	ILE	3.9
20	Z	33	TRP	3.9
13	o	62	GLU	3.9
19	Y	43	ARG	3.9
2	b	505	ARG	3.8
7	h	21	VAL	3.8
11	l	3	PRO	3.7
20	Z	62	VAL	3.7
13	o	132	ASN	3.7
3	C	146	PHE	3.7
14	R	24	LEU	3.7
18	X	2	THR	3.6
19	y	19	ILE	3.6
14	R	27	ALA	3.6
8	i	35	LYS	3.6
20	Z	32	ASP	3.6
2	b	496	TYR	3.6
5	E	79	PHE	3.6
5	e	61	ARG	3.6
20	Z	35	ARG	3.6
20	Z	31	GLN	3.6
13	o	59	LYS	3.5
2	b	503	THR	3.5
2	B	505	ARG	3.5
14	r	21	ARG	3.5
13	O	246	ALA	3.5
8	I	34	ARG	3.4
14	R	29	LYS	3.4
9	J	7	ARG	3.4
3	c	143	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
14	r	16	ALA	3.3
20	Z	7	LEU	3.3
15	T	30	THR	3.3
18	X	3	ILE	3.3
14	R	18	TRP	3.3
19	Y	40	ALA	3.3
14	r	17	GLY	3.2
20	z	3	ILE	3.2
18	x	38	GLN	3.2
15	t	30	THR	3.2
9	j	8	ILE	3.2
14	R	17	GLY	3.1
14	r	8	VAL	3.1
2	b	491	VAL	3.1
14	R	10	LEU	3.1
19	Y	37	PHE	3.1
14	R	2	ASP	3.1
13	O	57	LYS	3.0
2	B	127	ARG	3.0
2	b	292	LEU	3.0
7	H	66	GLY	3.0
7	h	10	ILE	3.0
14	r	20	VAL	3.0
9	J	8	ILE	3.0
2	B	495	PHE	3.0
14	R	5	VAL	3.0
5	e	74	GLN	3.0
2	b	506	ARG	3.0
19	Y	42	ARG	3.0
14	R	7	VAL	3.0
2	b	490	GLN	2.9
20	Z	38	GLN	2.9
3	c	146	PHE	2.9
6	F	13	TYR	2.9
1	a	11	ALA	2.9
20	Z	4	LEU	2.9
14	R	23	ILE	2.8
13	O	5	LEU	2.8
8	i	34	ARG	2.8
11	l	7	ARG	2.8
5	e	82	GLN	2.8
13	O	63	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	57	ALA	2.8
3	C	143	TYR	2.7
14	R	8	VAL	2.7
20	Z	3	ILE	2.7
20	z	42	LEU	2.7
7	h	6	TRP	2.7
3	C	145	SER	2.7
13	o	207	ARG	2.7
14	R	9	LEU	2.7
13	o	246	ALA	2.6
13	o	5	LEU	2.6
11	l	5	PRO	2.6
4	D	227	GLU	2.6
14	R	19	ALA	2.6
10	K	10	LYS	2.6
15	t	28	ARG	2.6
18	x	2	THR	2.5
20	z	59	PHE	2.5
19	Y	20	ALA	2.5
19	y	43	ARG	2.5
2	b	489	GLU	2.5
20	z	4	LEU	2.5
19	y	37	PHE	2.5
5	e	4	THR	2.5
5	E	84	LYS	2.5
19	Y	25	ILE	2.5
5	E	83	LEU	2.5
14	R	12	VAL	2.4
20	Z	37	LYS	2.4
3	c	262	ARG	2.4
6	f	15	ILE	2.4
5	e	84	LYS	2.4
8	I	36	ASP	2.4
2	b	295	GLY	2.4
14	R	16	ALA	2.4
7	h	56	ASP	2.4
13	O	34	SER	2.4
7	h	13	PRO	2.3
13	O	58	ASN	2.3
20	Z	61	VAL	2.3
3	c	25	ASN	2.3
3	c	459	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
10	K	17	ILE	2.3
8	i	33	LYS	2.2
10	K	18	PHE	2.2
20	Z	60	PHE	2.2
7	h	22	ALA	2.2
18	x	39	ARG	2.2
9	j	5	GLY	2.2
13	o	63	ALA	2.2
19	Y	45	ASN	2.2
3	C	62	PHE	2.2
3	C	58	GLY	2.2
14	R	22	ASN	2.2
19	Y	38	LEU	2.2
2	b	85	GLY	2.2
5	E	3	GLY	2.2
6	f	13	TYR	2.1
18	x	34	ILE	2.1
20	Z	42	LEU	2.1
20	z	39	LEU	2.1
3	c	191	PRO	2.1
12	M	33	GLN	2.1
12	m	31	SER	2.1
20	z	36	SER	2.1
4	D	12	ARG	2.1
10	K	14	ALA	2.1
1	A	12	ASN	2.1
7	H	6	TRP	2.1
2	b	128	THR	2.1
2	B	486	LEU	2.1
2	B	502	VAL	2.1
6	f	14	PRO	2.1
14	R	4	ARG	2.1
2	B	293	ALA	2.1
3	C	59	LEU	2.0
20	z	7	LEU	2.0
3	C	122	SER	2.0
15	T	29	ILE	2.0
1	A	16	ARG	2.0
4	D	229	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
15	FME	T	1	10/11	0.94	0.10	37,46,65,67	0
15	FME	t	1	10/11	0.95	0.10	34,48,77,77	0
12	FME	M	1	10/11	0.96	0.10	45,54,73,74	0
8	FME	i	1	10/11	0.97	0.17	46,57,67,70	0
12	FME	m	1	10/11	0.97	0.14	39,54,76,81	0
8	FME	I	1	10/11	0.97	0.16	45,56,68,71	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
32	STE	R	101	12/20	0.66	0.29	66,87,95,107	0
32	STE	a	618	12/20	0.77	0.29	40,72,79,81	0
32	STE	B	623	18/20	0.78	0.33	54,80,90,94	0
32	STE	h	103	14/20	0.78	0.28	60,77,87,92	0
33	LMG	c	521	48/55	0.79	0.24	43,78,104,111	0
32	STE	b	623	16/20	0.80	0.20	50,67,85,92	0
32	STE	d	411	20/20	0.80	0.21	54,78,96,100	0
30	LHG	e	101	42/49	0.80	0.29	59,92,114,126	0
26	BCR	X	101	40/40	0.80	0.17	34,52,70,73	0
26	BCR	h	101	40/40	0.81	0.18	42,63,87,92	0
30	LHG	A	614	49/49	0.81	0.25	51,87,115,118	0
32	STE	B	625	15/20	0.81	0.19	46,67,82,96	0
24	CLA	b	601	65/65	0.82	0.21	54,74,95,108	0
32	STE	b	621	20/20	0.82	0.22	45,62,80,86	0
32	STE	B	624	16/20	0.82	0.24	38,69,90,91	0
32	STE	B	626	12/20	0.83	0.43	57,71,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	STE	b	624	20/20	0.83	0.20	42,67,87,89	0
32	STE	c	520	20/20	0.83	0.24	43,68,86,100	0
28	PL9	A	611	55/55	0.83	0.27	38,69,87,92	0
29	SQD	a	616	36/54	0.83	0.19	31,69,93,98	0
33	LMG	D	411	33/55	0.83	0.19	44,61,84,94	0
33	LMG	b	622	55/55	0.83	0.29	54,76,98,109	0
32	STE	B	622	18/20	0.83	0.17	45,66,89,89	0
28	PL9	a	612	55/55	0.84	0.21	43,77,95,103	0
32	STE	L	102	12/20	0.84	0.20	54,70,85,93	0
24	CLA	c	512	65/65	0.84	0.17	47,65,93,98	0
32	STE	T	103	15/20	0.84	0.19	46,65,87,88	0
32	STE	a	617	10/20	0.84	0.23	37,70,76,81	0
24	CLA	C	512	65/65	0.85	0.19	41,62,97,102	0
32	STE	B	619	17/20	0.85	0.17	35,53,73,77	0
32	STE	B	621	12/20	0.85	0.12	38,62,74,78	0
32	STE	I	101	15/20	0.85	0.17	45,62,89,90	0
24	CLA	c	513	65/65	0.85	0.21	47,75,105,109	0
26	BCR	K	102	40/40	0.85	0.15	44,62,77,85	0
33	LMG	c	522	49/55	0.85	0.17	36,61,90,107	0
32	STE	d	410	20/20	0.86	0.24	50,65,79,81	0
24	CLA	C	513	65/65	0.86	0.21	50,69,101,107	0
31	DGD	A	616	66/66	0.86	0.17	46,68,85,98	0
24	CLA	H	101	65/65	0.86	0.16	44,68,98,103	0
32	STE	C	521	12/20	0.86	0.14	36,54,66,68	0
32	STE	X	102	20/20	0.86	0.18	38,57,80,83	0
32	STE	Z	101	8/20	0.86	0.18	50,64,77,77	0
29	SQD	f	102	41/54	0.87	0.23	64,94,114,118	0
33	LMG	Y	101	48/55	0.87	0.19	47,75,101,104	0
32	STE	M	104	18/20	0.87	0.16	39,52,86,91	0
32	STE	c	523	12/20	0.87	0.19	58,75,87,90	0
33	LMG	C	515	48/55	0.87	0.16	31,61,83,93	0
29	SQD	B	620	54/54	0.88	0.15	41,62,87,95	0
33	LMG	a	619	55/55	0.88	0.16	39,61,83,85	0
32	STE	C	519	12/20	0.88	0.14	43,63,75,76	0
32	STE	M	103	10/20	0.88	0.17	44,55,60,69	0
29	SQD	A	615	39/54	0.88	0.18	45,65,95,96	0
26	BCR	D	405	40/40	0.89	0.14	35,51,89,97	0
33	LMG	D	412	28/55	0.89	0.14	39,56,67,75	0
29	SQD	b	620	49/54	0.89	0.14	40,62,90,107	0
32	STE	C	520	16/20	0.89	0.12	47,59,68,73	0
32	STE	b	625	10/20	0.89	0.28	47,58,68,69	0
32	STE	t	102	14/20	0.89	0.14	42,54,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	STE	M	102	15/20	0.89	0.15	42,58,67,69	0
26	BCR	k	102	40/40	0.90	0.19	45,61,74,77	0
24	CLA	a	607	65/65	0.90	0.14	23,41,90,102	0
26	BCR	c	514	40/40	0.90	0.18	45,65,82,84	0
24	CLA	C	502	65/65	0.90	0.16	32,47,64,67	0
26	BCR	k	101	40/40	0.90	0.13	40,67,79,81	0
33	LMG	M	101	51/55	0.91	0.13	34,53,80,85	0
32	STE	j	101	12/20	0.91	0.16	49,65,78,78	0
26	BCR	d	404	40/40	0.91	0.13	40,59,99,107	0
24	CLA	c	502	65/65	0.91	0.16	33,48,67,71	0
24	CLA	D	404	65/65	0.91	0.14	24,47,107,122	0
26	BCR	K	101	40/40	0.91	0.15	45,64,76,82	0
33	LMG	m	101	51/55	0.91	0.14	37,55,75,85	0
24	CLA	d	403	65/65	0.92	0.15	31,55,98,106	0
24	CLA	c	508	64/65	0.92	0.15	36,53,99,120	0
33	LMG	D	407	51/55	0.92	0.18	31,64,87,89	0
33	LMG	c	519	37/55	0.92	0.15	48,69,83,87	0
24	CLA	b	616	60/65	0.92	0.15	33,50,93,101	0
24	CLA	b	615	65/65	0.92	0.15	30,46,69,80	0
32	STE	T	102	16/20	0.92	0.14	43,58,78,83	0
24	CLA	c	506	65/65	0.93	0.13	35,55,90,101	0
26	BCR	K	103	40/40	0.93	0.16	42,59,74,83	0
24	CLA	C	508	65/65	0.93	0.14	31,49,105,118	0
29	SQD	D	408	36/54	0.93	0.19	57,78,93,96	0
26	BCR	b	617	40/40	0.93	0.12	33,49,64,65	0
26	BCR	b	619	40/40	0.93	0.10	33,54,68,72	0
24	CLA	B	615	60/65	0.93	0.14	27,46,103,111	0
24	CLA	B	614	65/65	0.93	0.14	28,43,63,67	0
24	CLA	C	505	65/65	0.93	0.16	25,48,71,77	0
26	BCR	C	514	40/40	0.93	0.11	27,47,60,72	0
31	DGD	C	517	62/66	0.93	0.13	38,58,106,117	0
31	DGD	c	518	62/66	0.93	0.14	32,59,84,90	0
32	STE	d	409	17/20	0.93	0.12	43,58,66,77	0
24	CLA	C	507	65/65	0.93	0.15	31,47,67,70	0
33	LMG	d	408	44/55	0.93	0.15	37,61,93,102	0
24	CLA	c	503	65/65	0.93	0.15	36,50,65,65	0
24	CLA	b	602	65/65	0.94	0.15	29,48,67,71	0
24	CLA	b	604	65/65	0.94	0.15	26,41,79,98	0
24	CLA	b	606	65/65	0.94	0.12	29,46,76,85	0
24	CLA	b	609	65/65	0.94	0.14	34,51,74,79	0
24	CLA	b	614	65/65	0.94	0.12	29,44,78,91	0
31	DGD	C	518	62/66	0.94	0.12	28,53,75,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DGD	H	102	62/66	0.94	0.11	32,49,62,71	0
31	DGD	c	517	62/66	0.94	0.12	36,56,97,103	0
26	BCR	T	101	40/40	0.94	0.10	26,47,62,63	0
31	DGD	h	102	62/66	0.94	0.12	35,53,66,79	0
24	CLA	C	510	65/65	0.94	0.15	33,51,68,70	0
24	CLA	C	511	65/65	0.94	0.12	38,55,72,78	0
24	CLA	B	605	65/65	0.94	0.11	22,41,70,73	0
24	CLA	C	503	65/65	0.94	0.15	36,49,61,63	0
24	CLA	c	505	65/65	0.94	0.18	30,48,69,76	0
24	CLA	B	608	65/65	0.94	0.13	27,45,63,72	0
24	CLA	c	507	65/65	0.94	0.14	32,49,62,74	0
24	CLA	C	506	65/65	0.94	0.12	28,47,91,95	0
24	CLA	c	509	65/65	0.94	0.19	34,55,70,75	0
28	PL9	D	406	55/55	0.94	0.12	25,39,50,65	0
24	CLA	c	511	65/65	0.94	0.12	41,60,78,81	0
32	STE	J	101	12/20	0.94	0.13	50,62,78,78	0
29	SQD	A	613	52/54	0.94	0.16	36,63,92,97	0
24	CLA	a	605	65/65	0.94	0.14	30,45,99,110	0
24	CLA	B	601	65/65	0.94	0.16	27,41,63,71	0
24	CLA	B	603	65/65	0.94	0.14	23,38,77,86	0
29	SQD	a	615	54/54	0.94	0.15	45,70,92,96	0
26	BCR	B	616	40/40	0.94	0.13	31,44,61,67	0
26	BCR	B	618	40/40	0.94	0.11	29,46,61,71	0
26	BCR	c	515	40/40	0.95	0.12	32,50,72,73	0
24	CLA	b	612	65/65	0.95	0.17	23,39,55,56	0
31	DGD	c	516	62/66	0.95	0.12	28,45,75,84	0
24	CLA	b	613	65/65	0.95	0.15	23,41,81,88	0
24	CLA	C	509	65/65	0.95	0.18	30,50,66,77	0
26	BCR	A	608	40/40	0.95	0.09	29,40,48,49	0
26	BCR	t	101	40/40	0.95	0.10	29,44,55,58	0
24	CLA	B	613	65/65	0.95	0.16	25,42,82,92	0
26	BCR	B	617	40/40	0.95	0.10	29,44,58,59	0
24	CLA	C	504	59/65	0.95	0.12	34,47,85,97	0
28	PL9	d	405	55/55	0.95	0.12	27,41,52,54	0
24	CLA	A	607	54/65	0.95	0.11	20,36,69,78	0
24	CLA	A	605	65/65	0.95	0.14	24,39,100,106	0
24	CLA	c	504	60/65	0.95	0.11	36,52,83,88	0
24	CLA	b	605	65/65	0.95	0.15	28,42,56,59	0
24	CLA	C	501	65/65	0.95	0.12	29,41,55,61	0
24	CLA	b	608	65/65	0.95	0.15	30,48,71,80	0
24	CLA	B	602	65/65	0.95	0.17	22,38,61,72	0
26	BCR	a	608	40/40	0.95	0.09	26,39,47,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
24	CLA	b	610	65/65	0.95	0.17	27,43,54,62	0
30	LHG	D	410	47/49	0.95	0.14	33,53,93,98	0
30	LHG	a	614	49/49	0.95	0.12	33,54,72,75	0
26	BCR	b	618	40/40	0.95	0.11	28,46,61,65	0
30	LHG	l	101	49/49	0.95	0.12	34,51,61,71	0
24	CLA	c	510	65/65	0.95	0.15	38,54,70,72	0
31	DGD	C	516	62/66	0.95	0.13	27,43,82,94	0
24	CLA	b	611	65/65	0.95	0.14	25,38,62,75	0
30	LHG	D	413	49/49	0.96	0.12	34,47,70,76	0
30	LHG	L	101	49/49	0.96	0.13	32,46,60,67	0
24	CLA	D	403	65/65	0.96	0.12	19,33,57,66	0
30	LHG	d	407	39/49	0.96	0.11	38,54,74,77	0
24	CLA	B	607	65/65	0.96	0.12	24,40,63,68	0
24	CLA	b	607	65/65	0.96	0.11	22,43,71,75	0
24	CLA	B	604	65/65	0.96	0.15	25,38,51,54	0
24	CLA	a	604	65/65	0.96	0.11	24,35,49,57	0
24	CLA	B	609	65/65	0.96	0.14	22,36,48,51	0
24	CLA	B	611	65/65	0.96	0.14	23,37,51,60	0
24	CLA	a	613	65/65	0.96	0.13	23,37,48,53	0
24	CLA	B	612	65/65	0.96	0.14	22,39,78,86	0
24	CLA	A	612	65/65	0.96	0.11	22,34,54,58	0
24	CLA	b	603	65/65	0.96	0.15	26,42,74,82	0
24	CLA	B	606	65/65	0.96	0.11	22,37,71,79	0
24	CLA	d	402	65/65	0.96	0.12	25,40,67,76	0
24	CLA	c	501	65/65	0.96	0.13	31,45,60,63	0
25	PHO	A	606	64/64	0.96	0.14	25,37,46,48	0
25	PHO	D	401	64/64	0.96	0.10	21,34,45,47	0
25	PHO	a	606	64/64	0.96	0.13	23,35,43,45	0
25	PHO	d	401	64/64	0.96	0.10	27,43,53,64	0
35	HEM	f	101	43/43	0.96	0.14	49,67,93,97	0
30	LHG	D	409	49/49	0.97	0.10	29,42,55,71	0
24	CLA	B	610	65/65	0.97	0.15	21,35,51,55	0
30	LHG	d	406	49/49	0.97	0.10	28,45,61,66	0
34	BCT	a	611	4/4	0.97	0.23	35,36,48,53	0
35	HEM	F	101	43/43	0.97	0.11	42,58,73,76	0
24	CLA	A	604	65/65	0.97	0.10	19,33,50,61	0
36	HEC	V	201	43/43	0.97	0.12	28,38,45,53	0
36	HEC	v	201	43/43	0.97	0.13	32,41,54,58	0
27	CL	A	609	1/1	0.99	0.12	34,34,34,34	0
27	CL	A	610	1/1	0.99	0.03	37,37,37,37	0
27	CL	a	609	1/1	0.99	0.04	32,32,32,32	0
34	BCT	D	402	4/4	0.99	0.14	34,36,43,47	0

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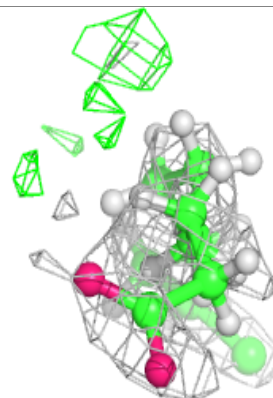
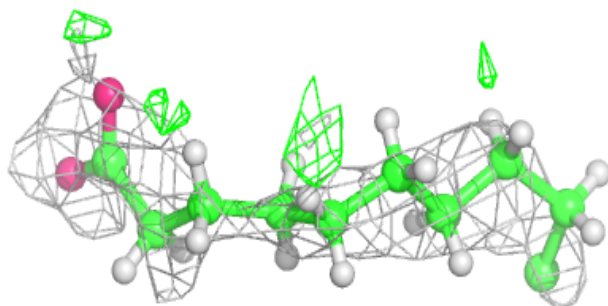
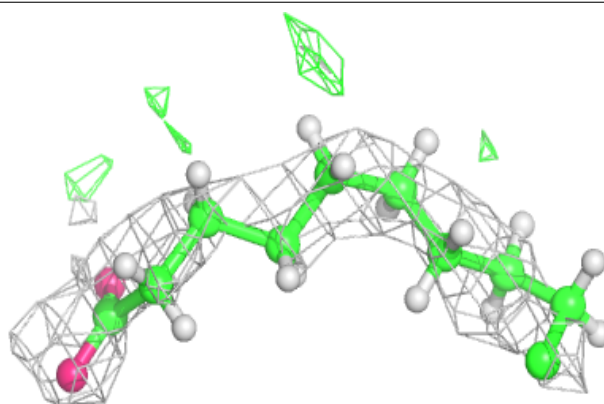
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
27	CL	a	610	1/1	0.99	0.03	35,35,35,35	0
21	OEY	A	601[B]	11/11	0.99	0.14	21,25,29,31	11
21	OEY	a	601[B]	11/11	0.99	0.12	21,26,32,32	11
22	OEX	A	602[A]	10/10	0.99	0.14	33,36,40,40	10
22	OEX	a	602[A]	10/10	0.99	0.12	31,36,39,40	10
23	FE2	a	603	1/1	1.00	0.05	32,32,32,32	0
23	FE2	A	603	1/1	1.00	0.08	31,31,31,31	0

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

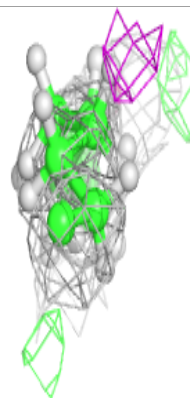
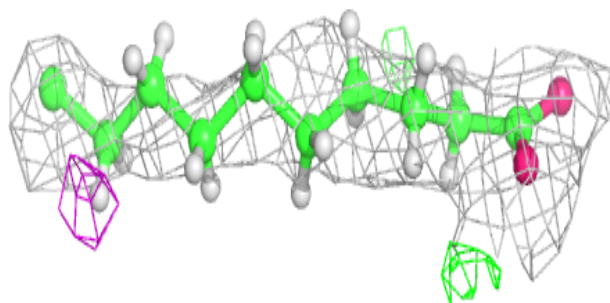
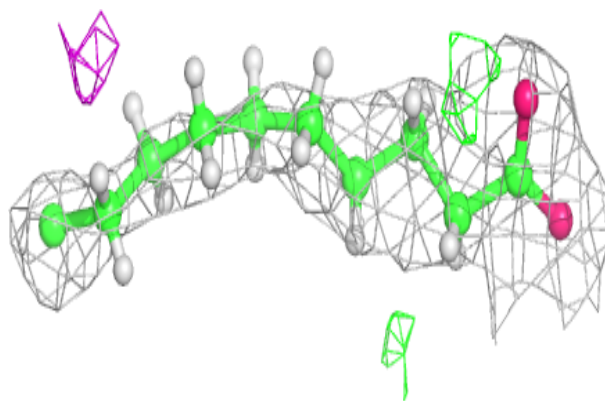
**Electron density around STE R 101:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

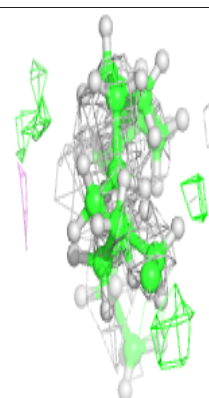
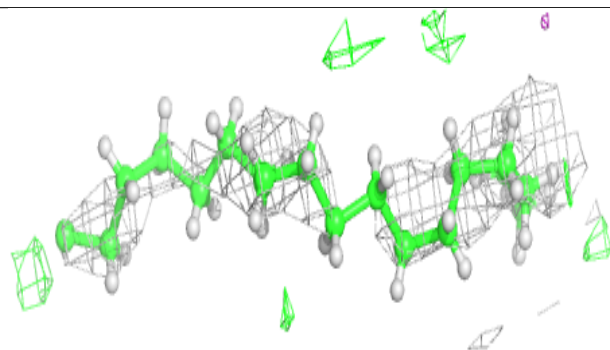
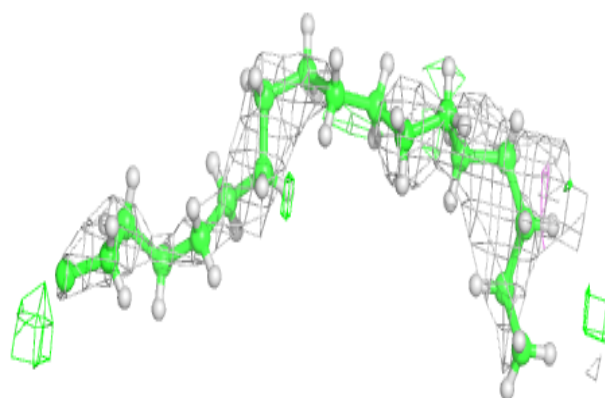


**Electron density around STE a 618:**

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

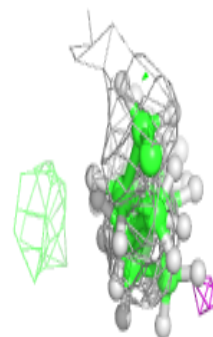
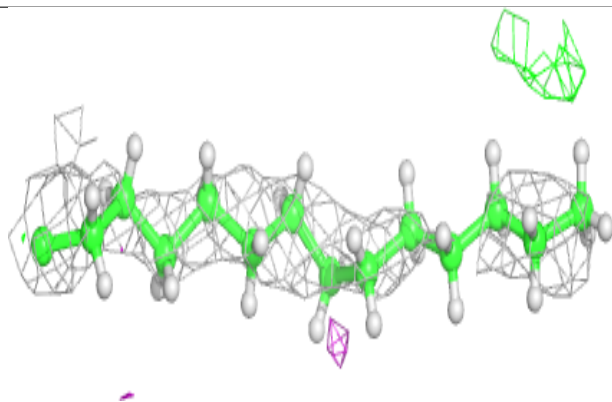
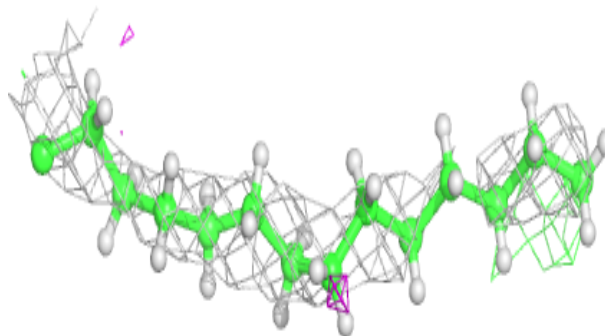
**Electron density around STE B 623:**

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

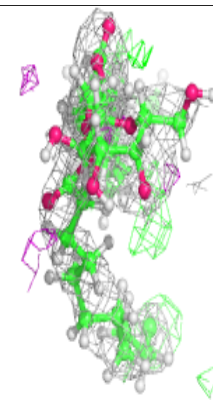
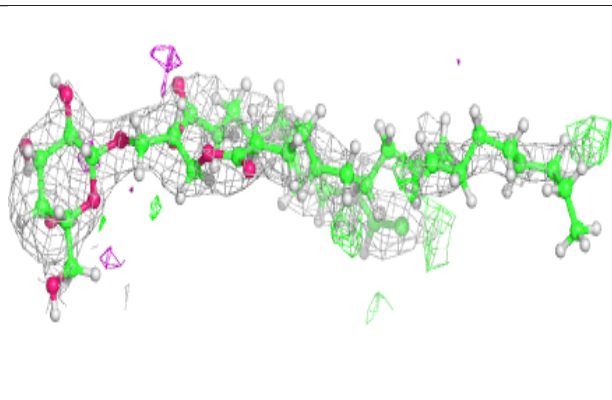
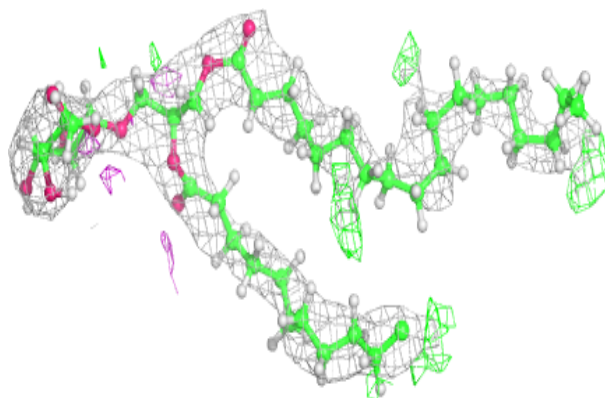


**Electron density around STE h 103:**

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

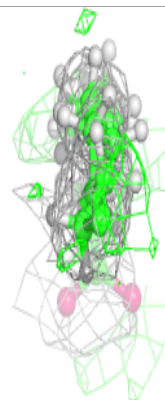
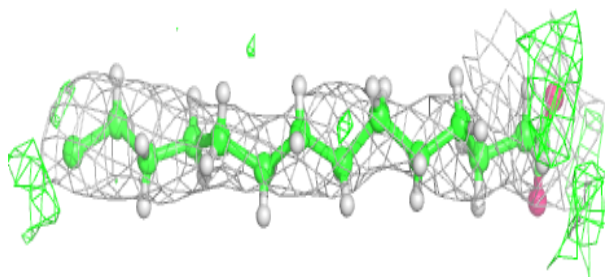
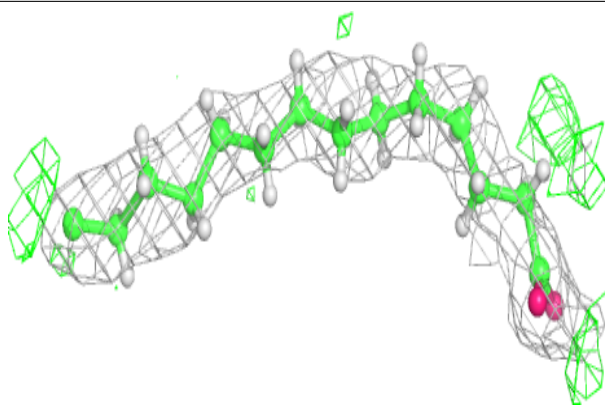
**Electron density around LMG c 521:**

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

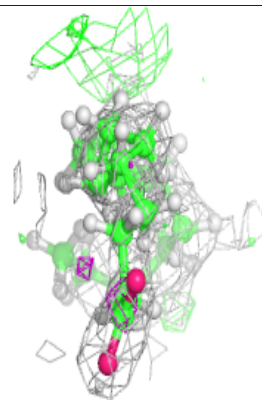
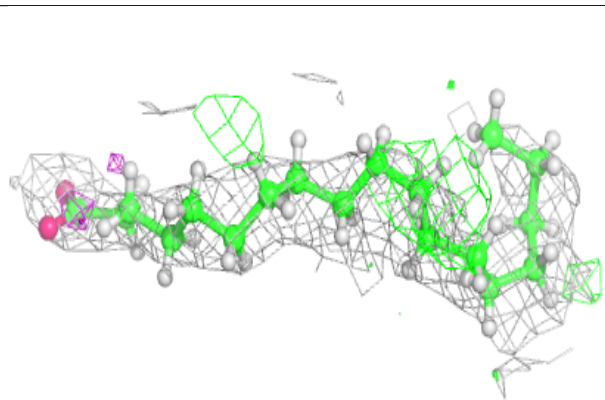
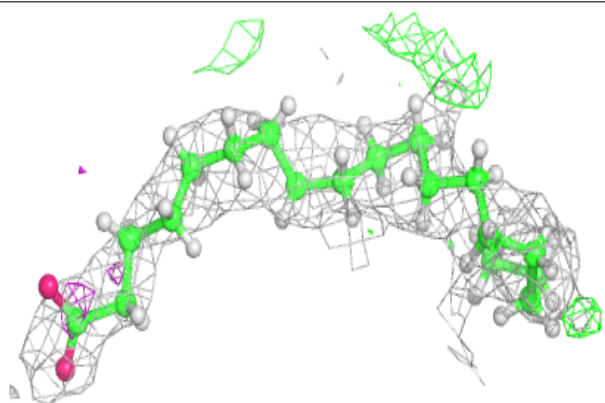


**Electron density around STE b 623:**

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

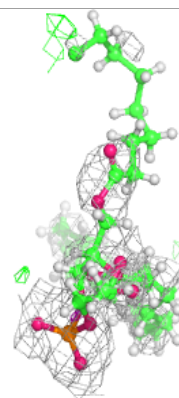
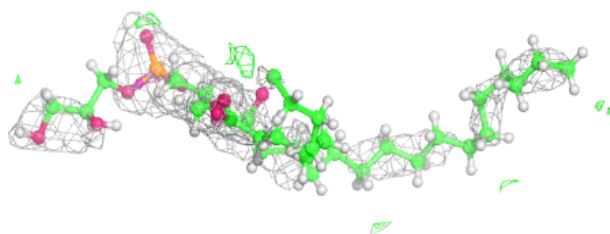
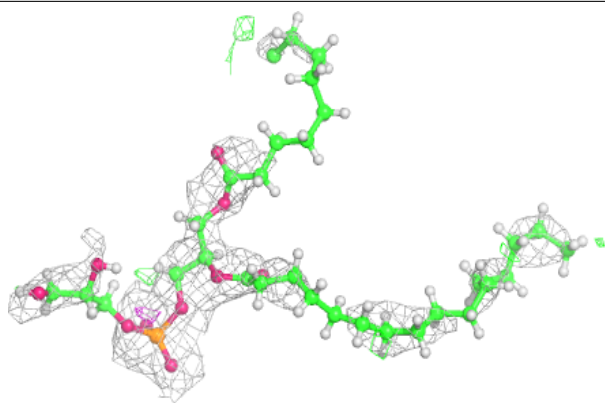
**Electron density around STE d 411:**

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

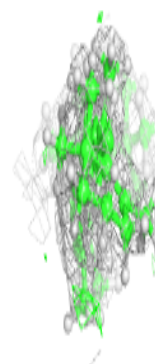
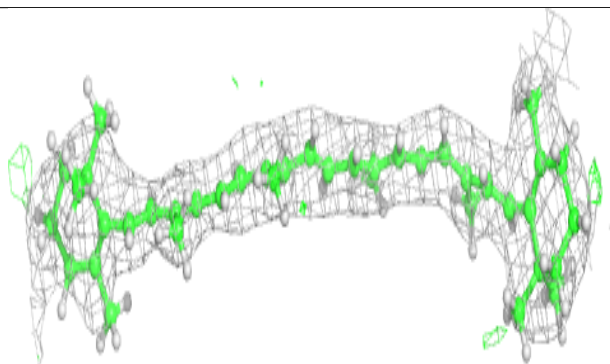
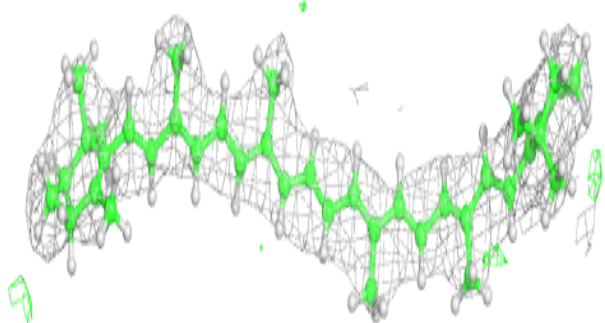


**Electron density around LHG e 101:**

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

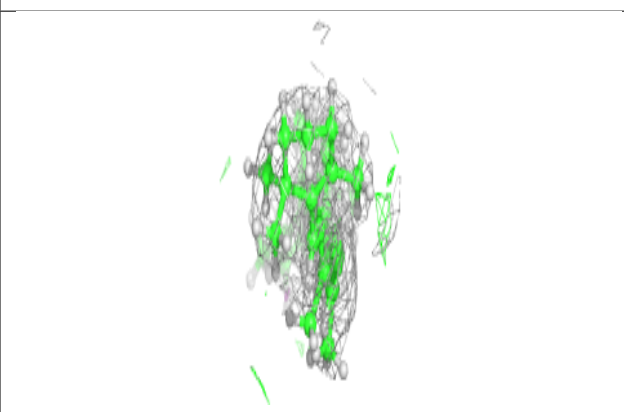
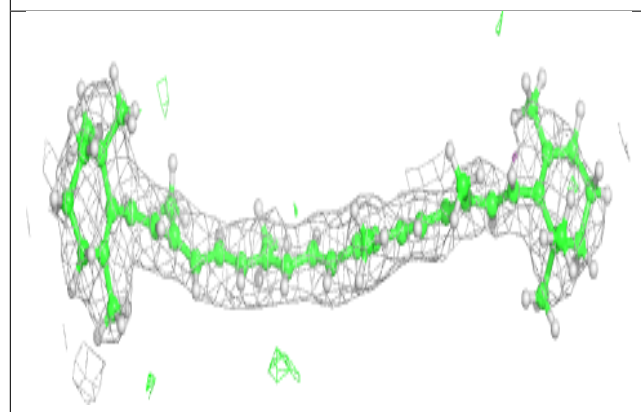
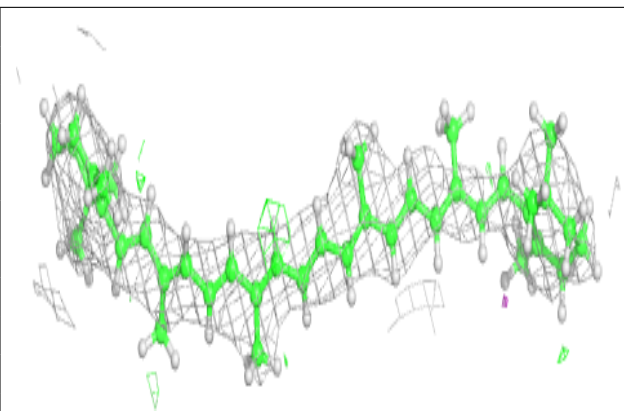
**Electron density around BCR X 101:**

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



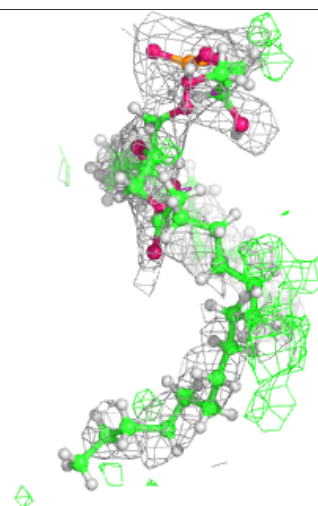
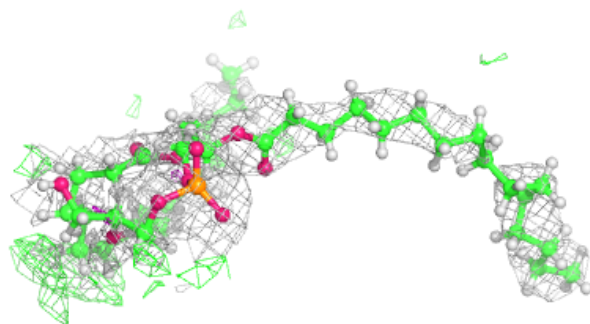
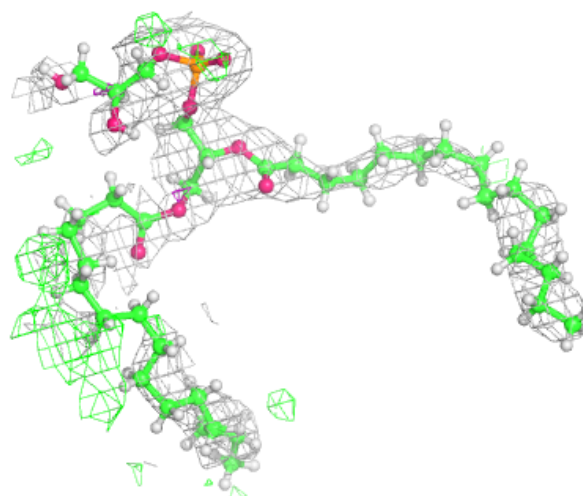
**Electron density around BCR h 101:**

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



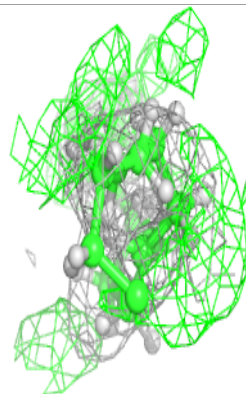
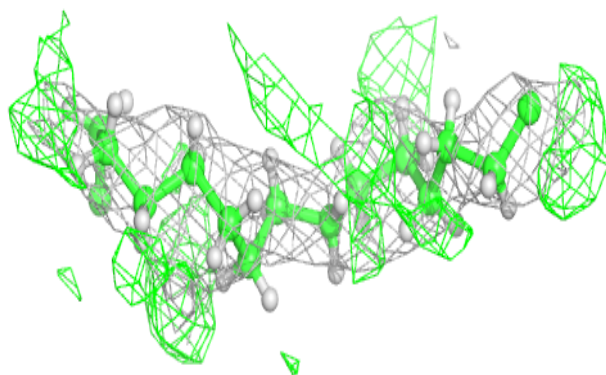
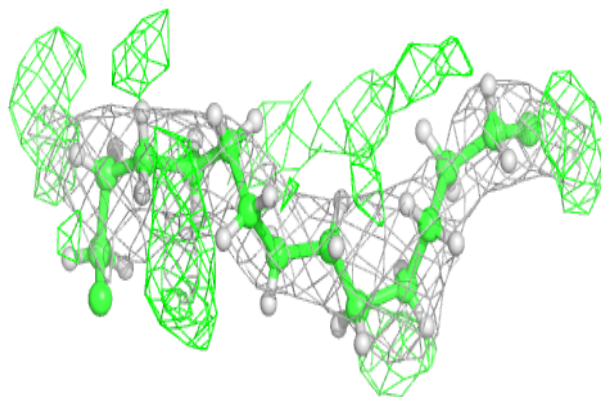
**Electron density around LHG A 614:**

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and green (positive)

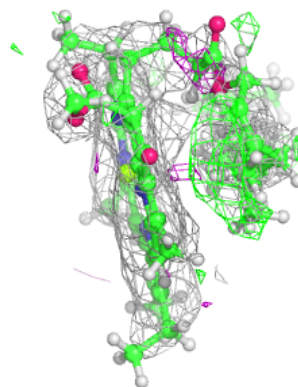
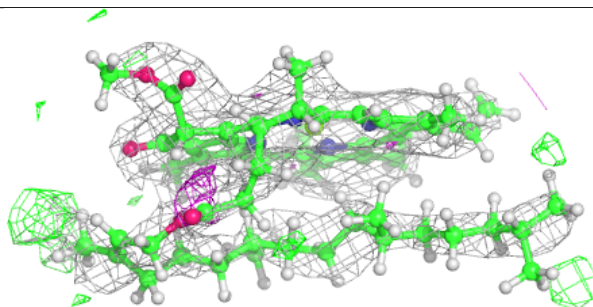
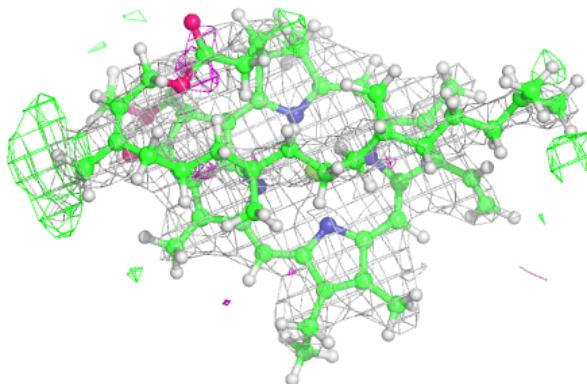


**Electron density around STE B 625:**

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

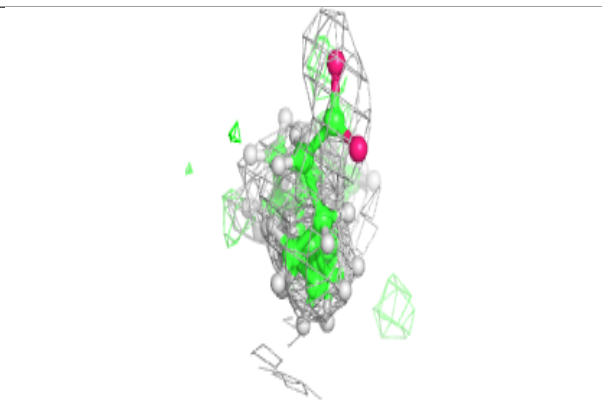
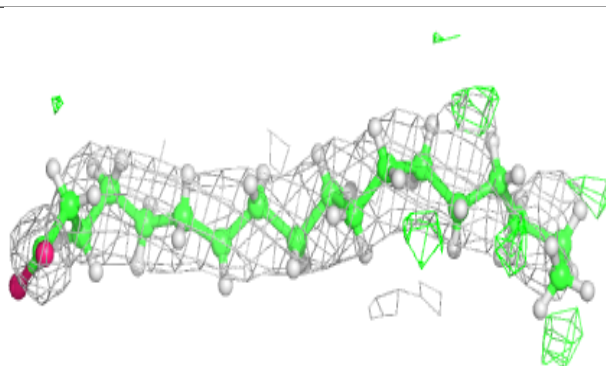
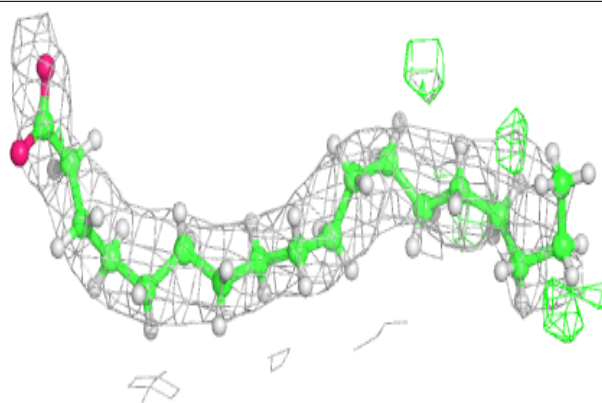
**Electron density around CLA b 601:**

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

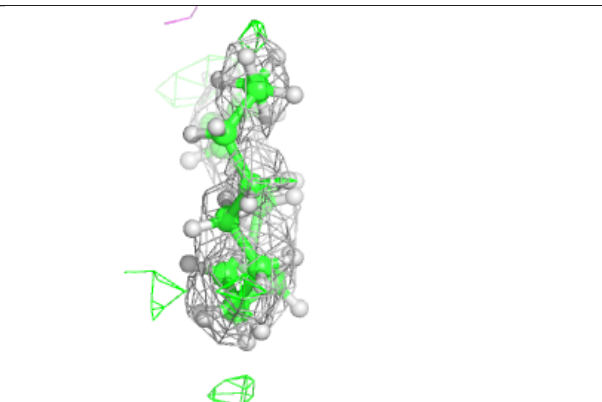
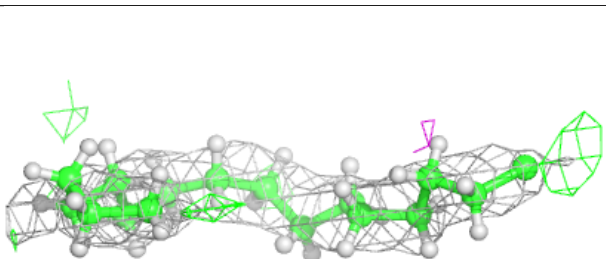
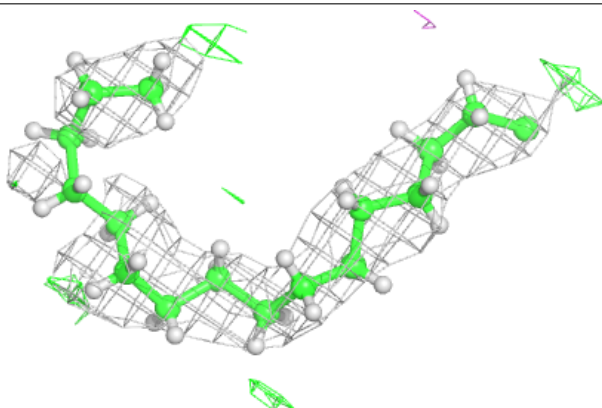


**Electron density around STE b 621:**

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

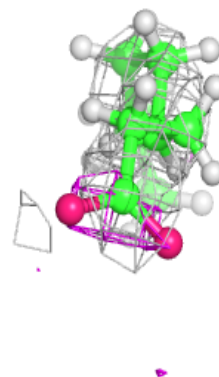
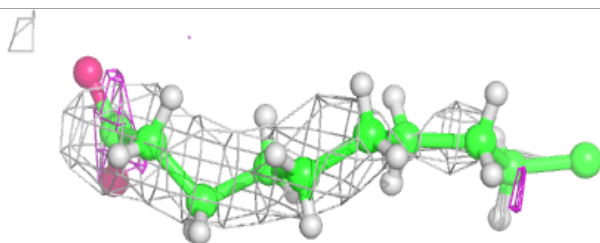
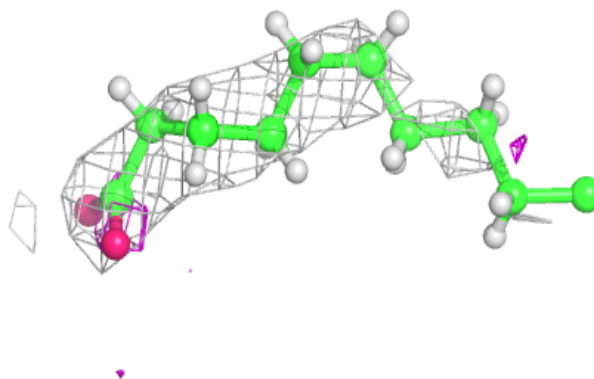
**Electron density around STE B 624:**

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

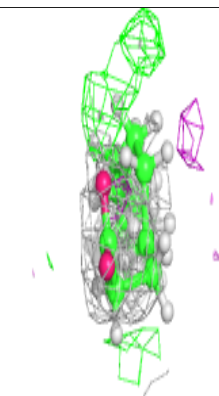
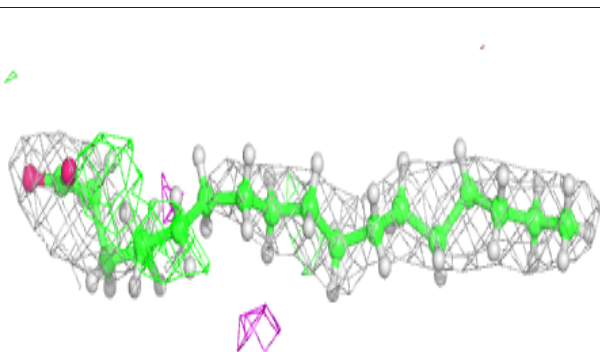
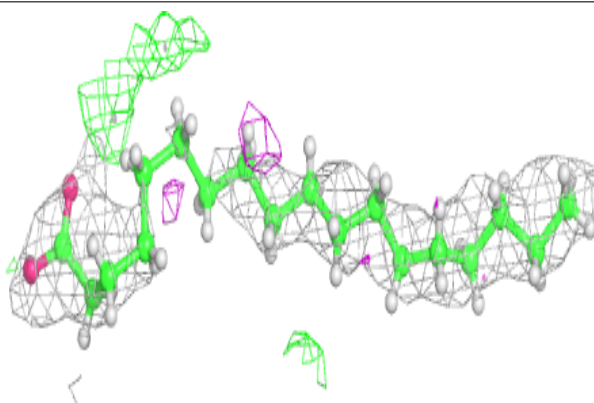


**Electron density around STE B 626:**

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

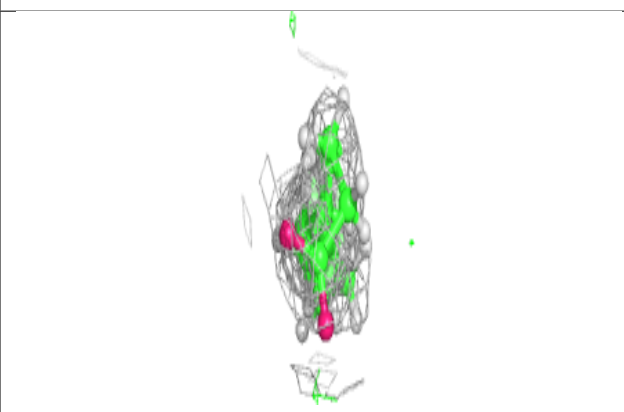
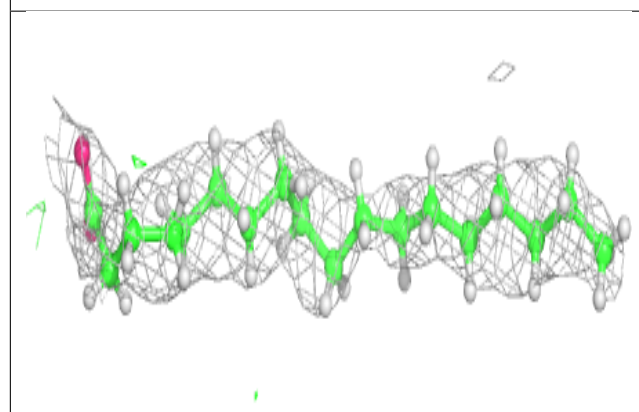
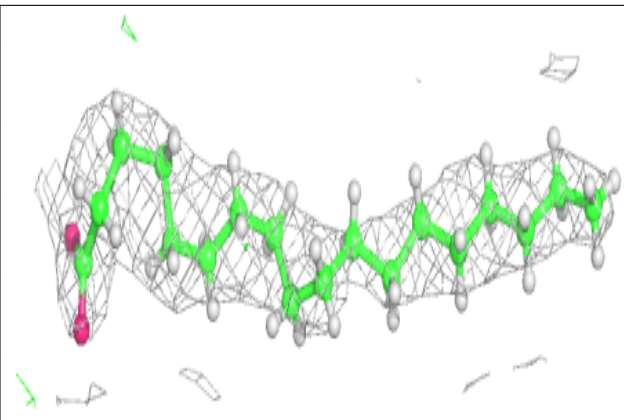
**Electron density around STE b 624:**

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

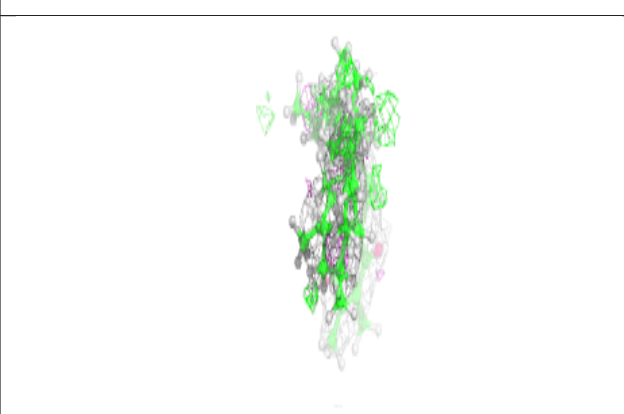
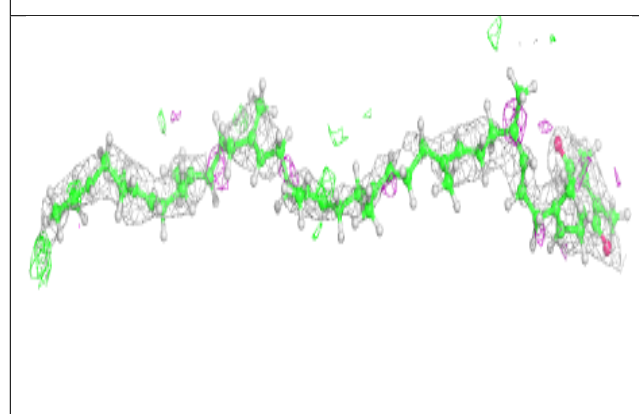
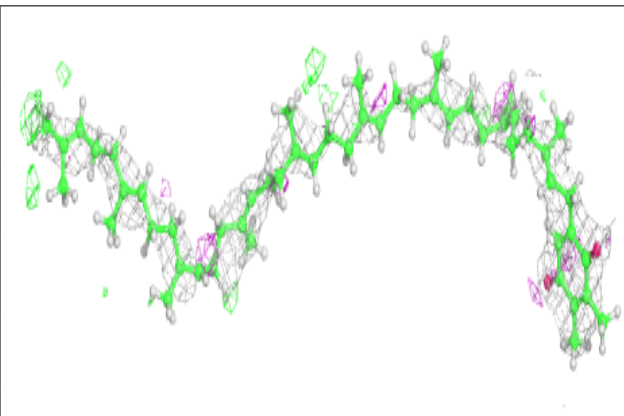


**Electron density around STE c 520:**

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and green (positive)

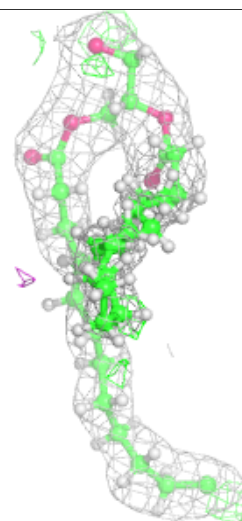
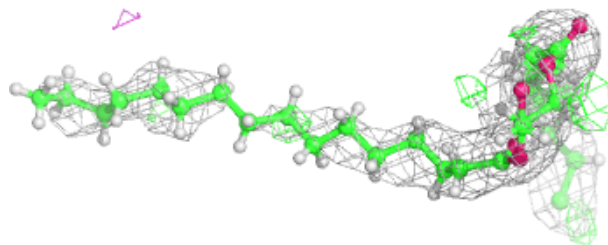
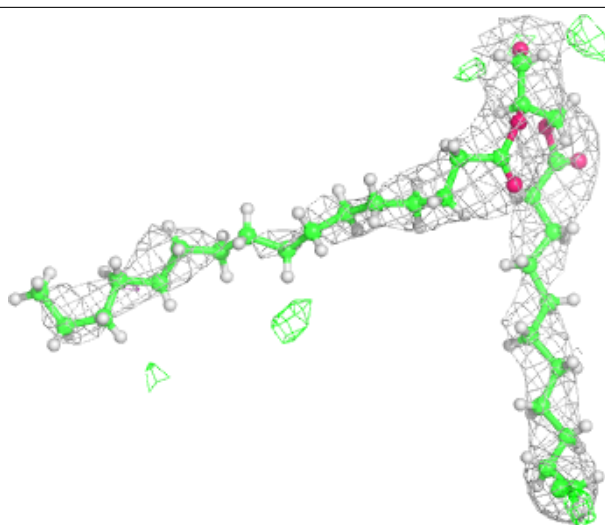
**Electron density around PL9 A 611:**

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



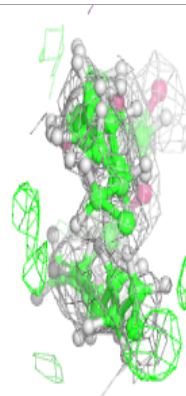
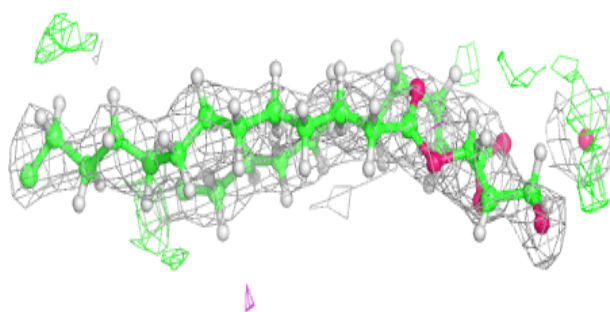
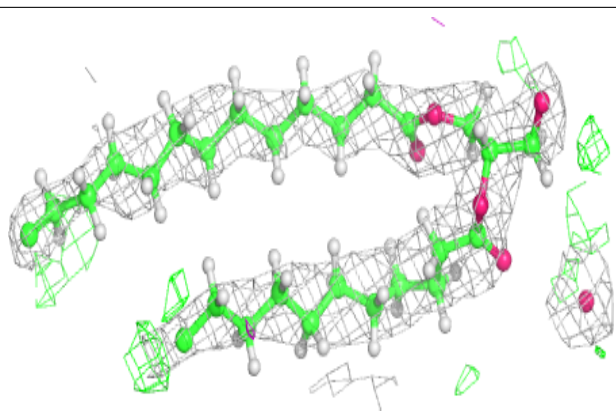
**Electron density around SQD a 616:**

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

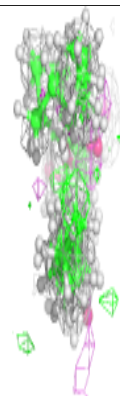
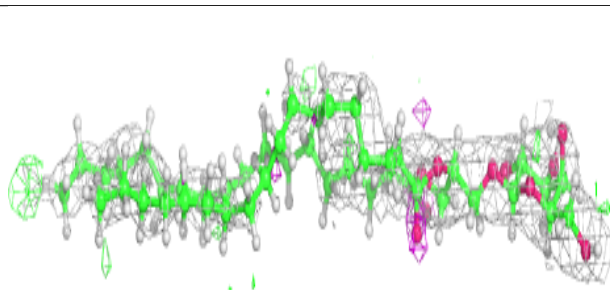
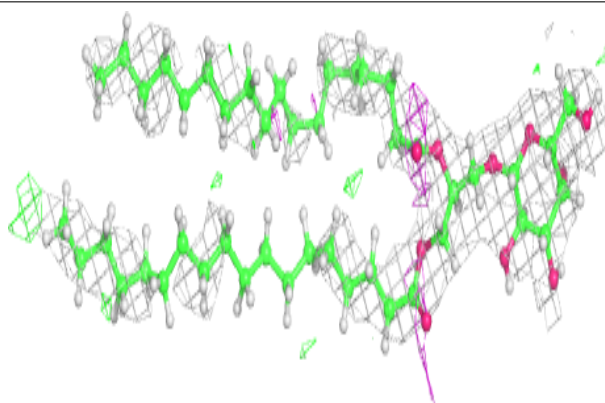


**Electron density around LMG D 411:**

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

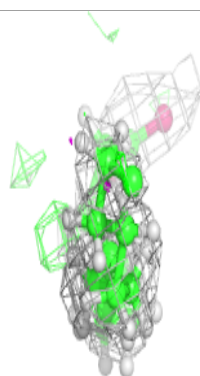
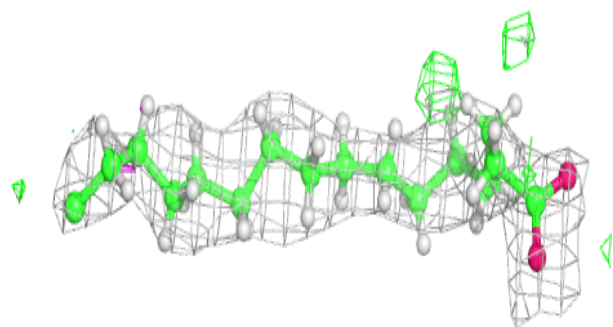
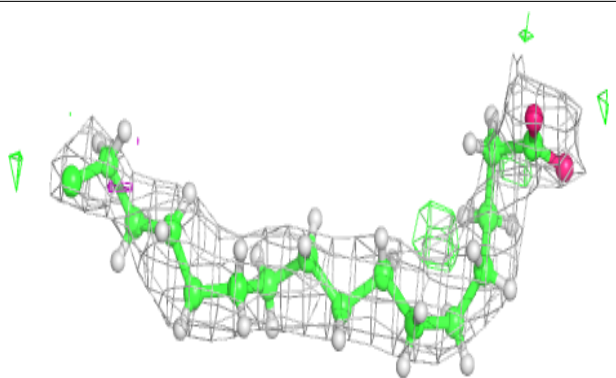
**Electron density around LMG b 622:**

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

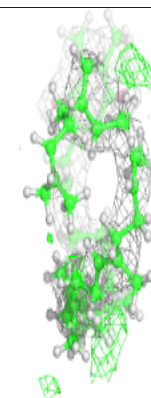
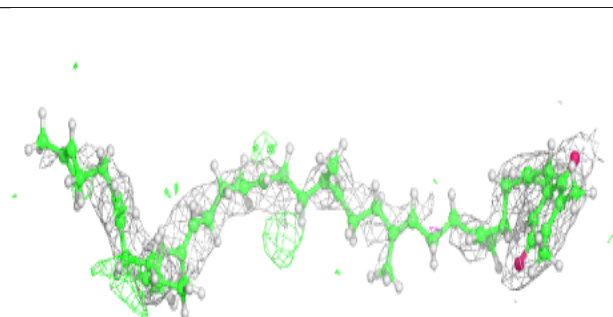
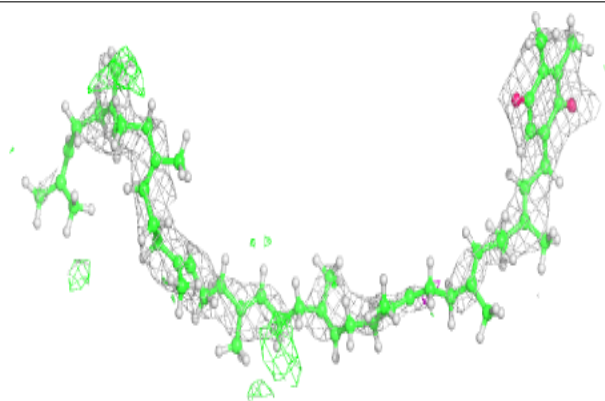


**Electron density around STE B 622:**

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

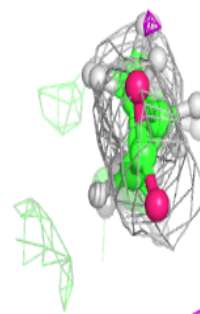
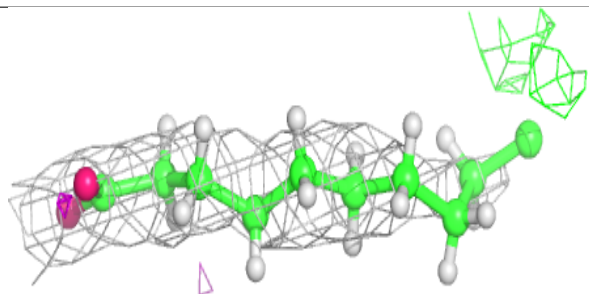
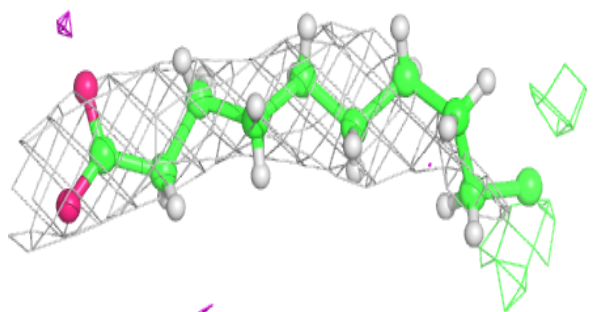
**Electron density around PL9 a 612:**

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



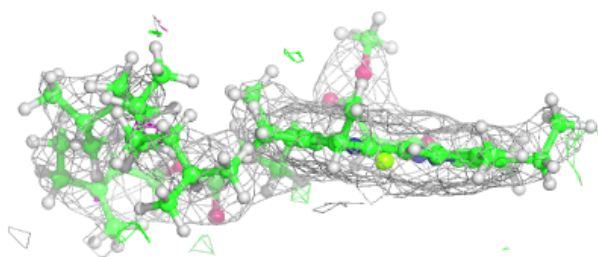
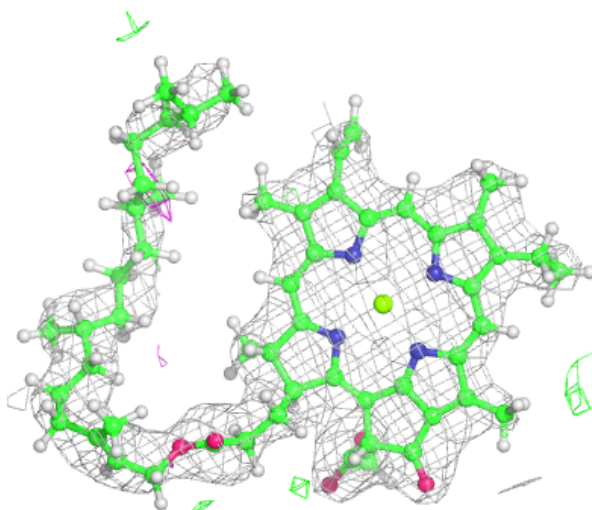
**Electron density around STE L 102:**

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



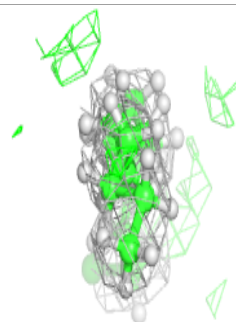
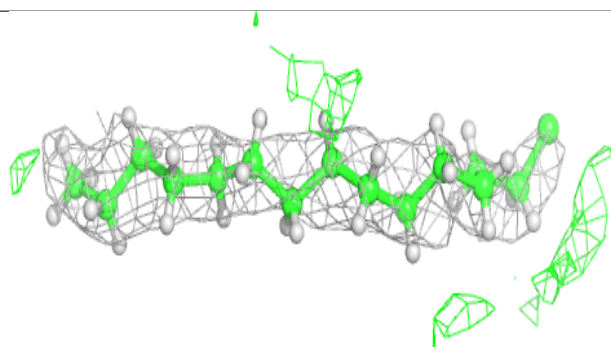
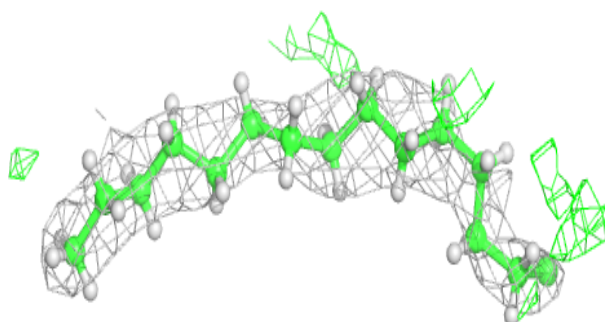
**Electron density around CLA c 512:**

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

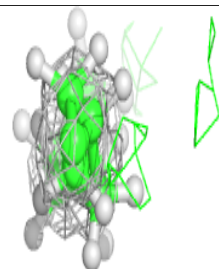
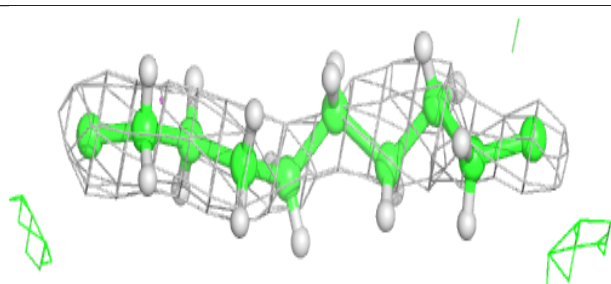
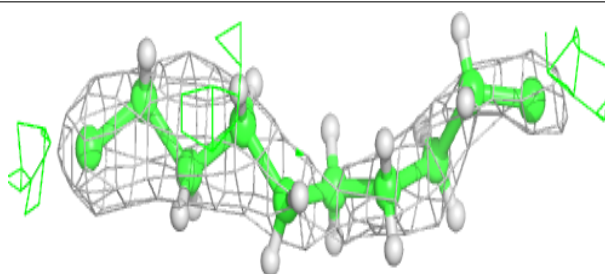


**Electron density around STE T 103:**

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

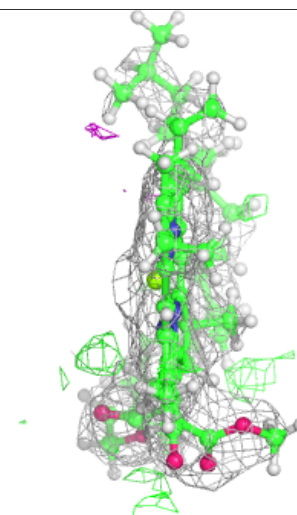
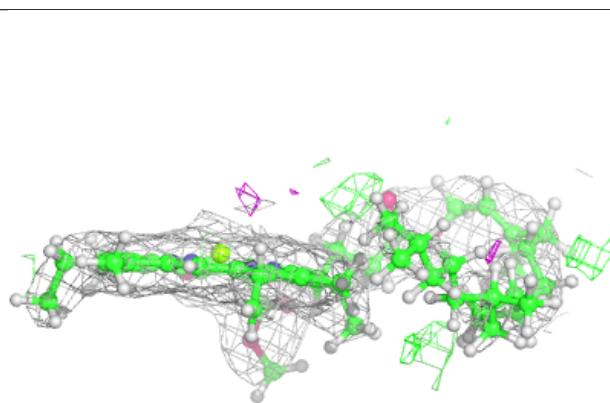
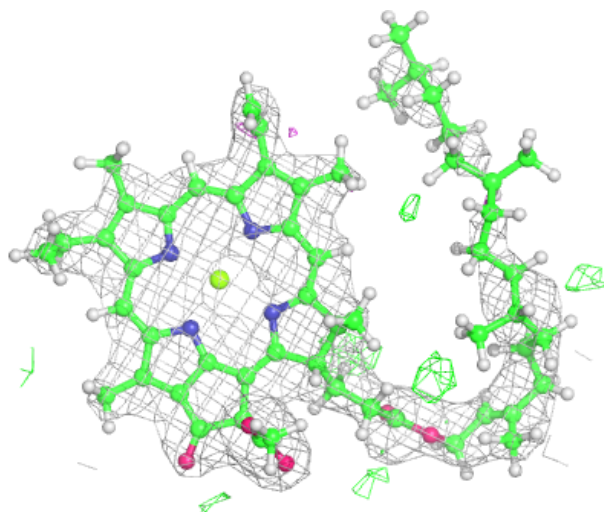
**Electron density around STE a 617:**

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



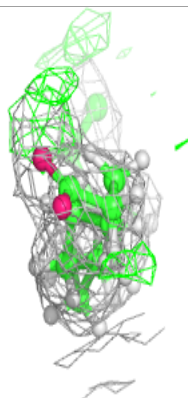
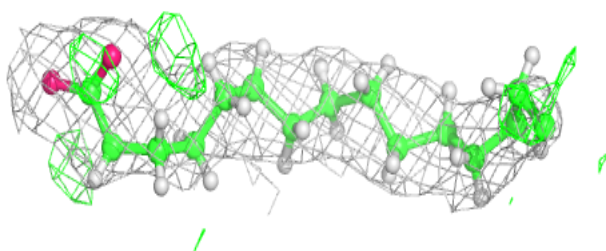
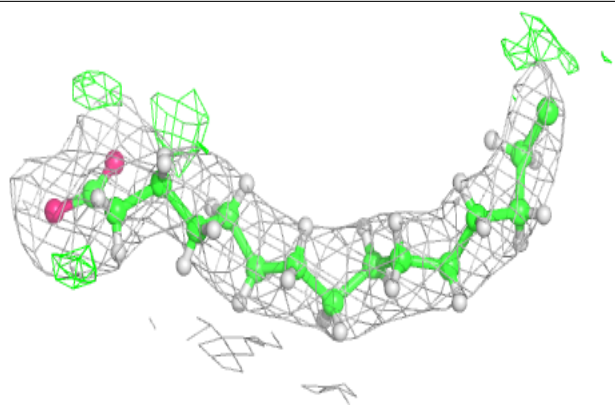
**Electron density around CLA C 512:**

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

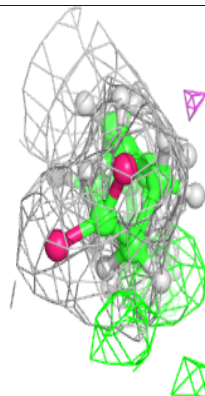
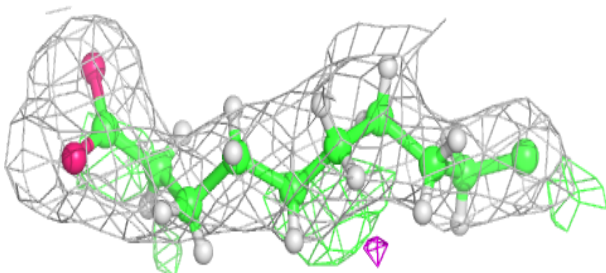
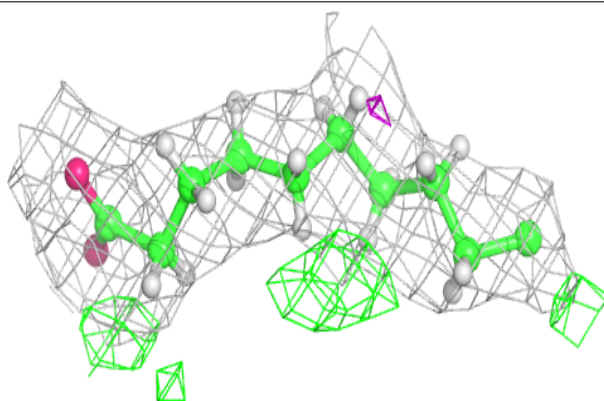


**Electron density around STE B 619:**

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

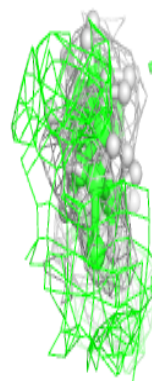
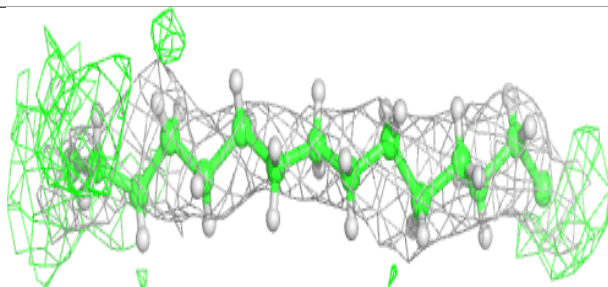
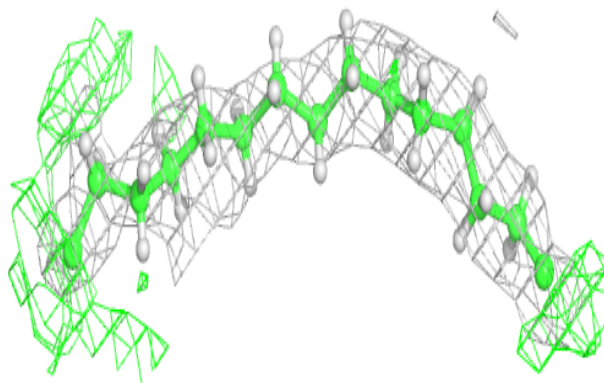
**Electron density around STE B 621:**

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

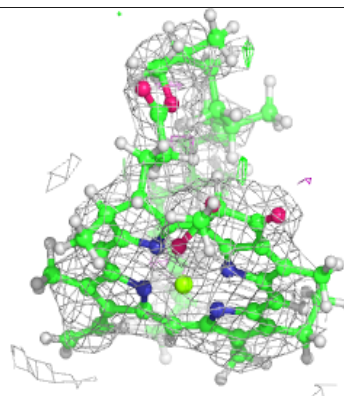
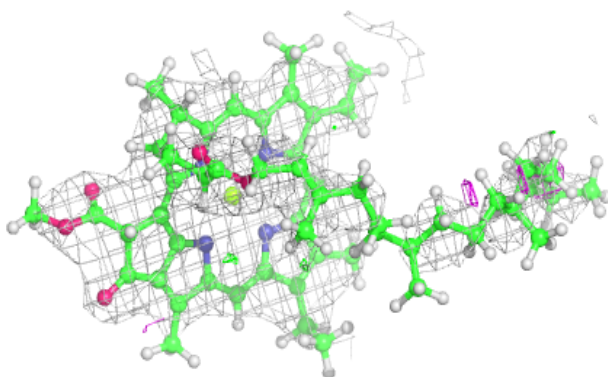
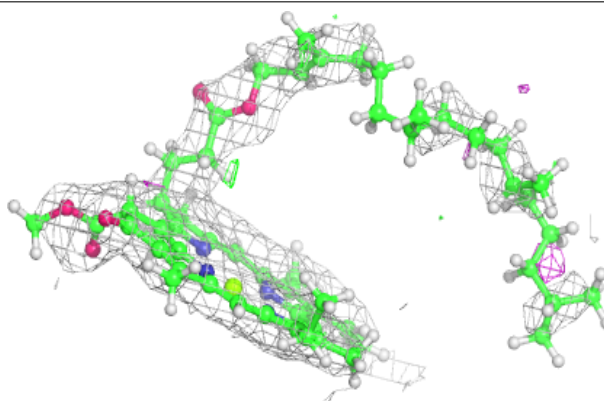


**Electron density around STE I 101:**

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

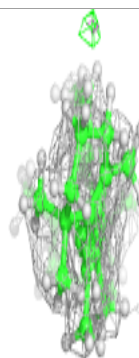
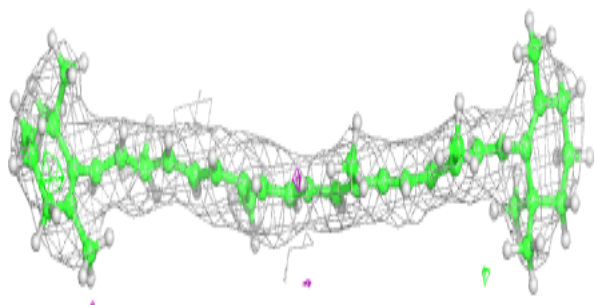
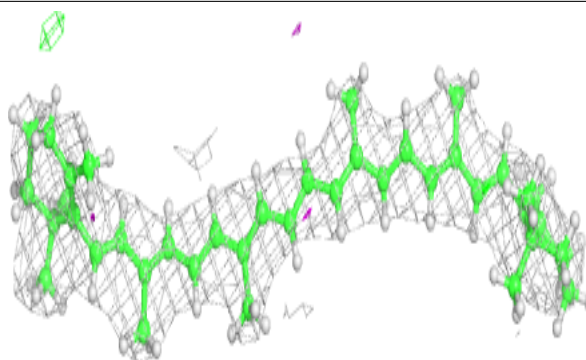
**Electron density around CLA c 513:**

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

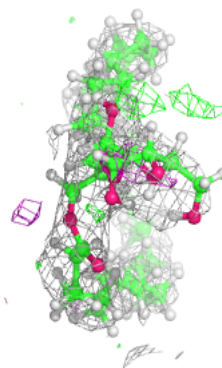
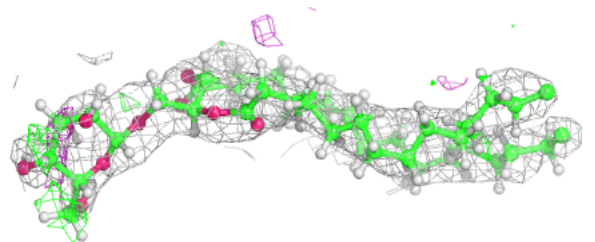
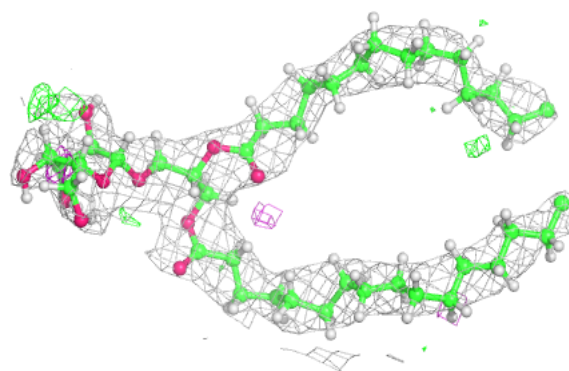


**Electron density around BCR K 102:**

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

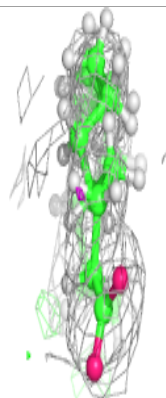
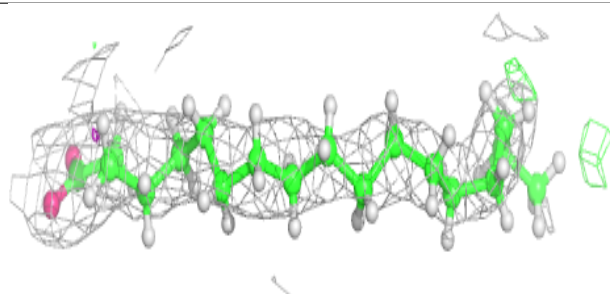
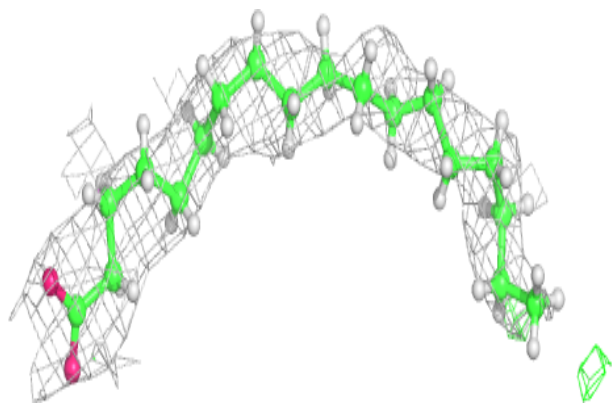
**Electron density around LMG c 522:**

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

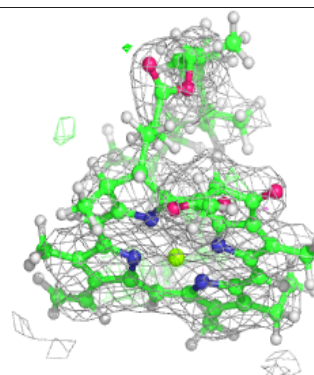
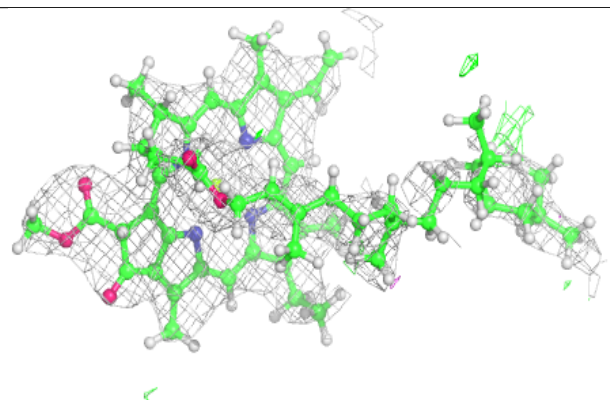
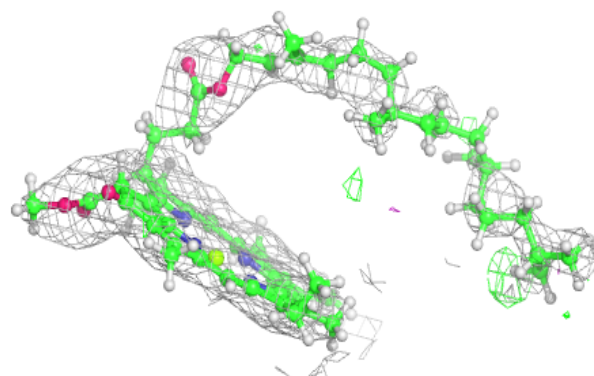


**Electron density around STE d 410:**

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

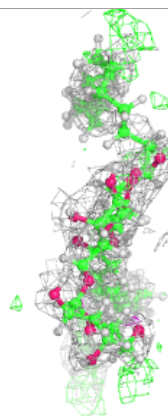
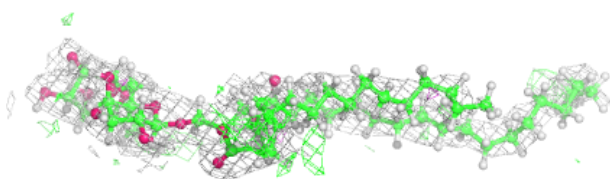
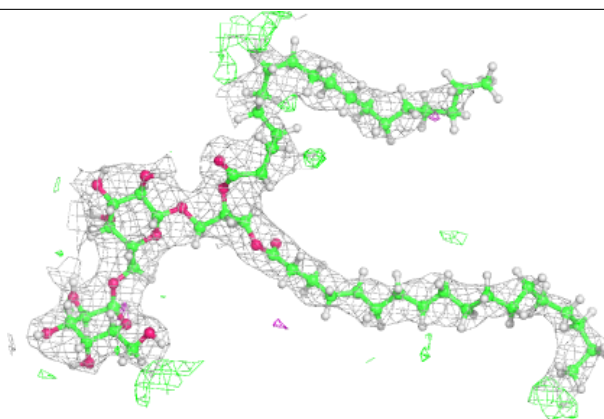
**Electron density around CLA C 513:**

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

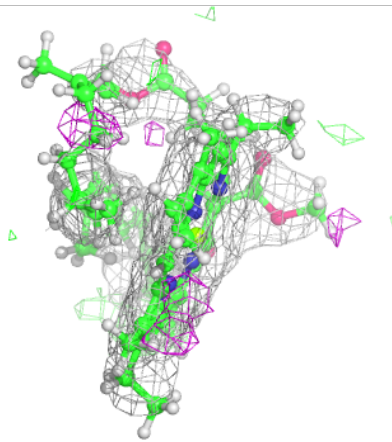
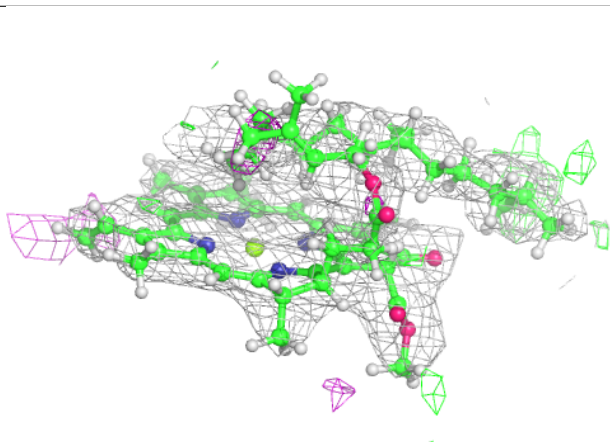
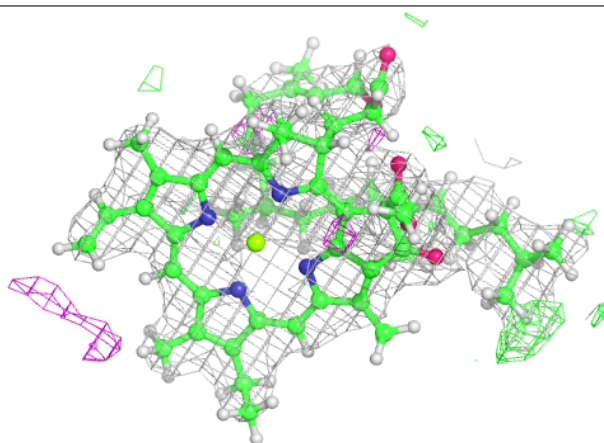


**Electron density around DGD A 616:**

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

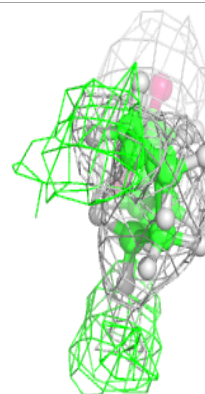
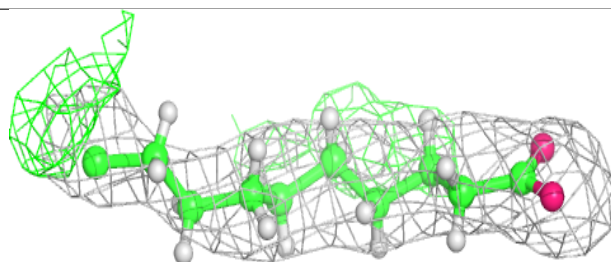
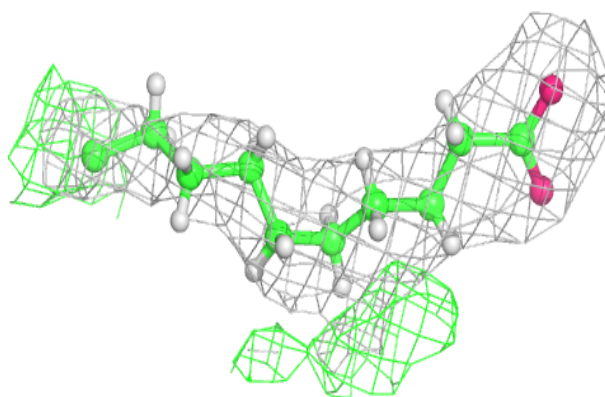
**Electron density around CLA H 101:**

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

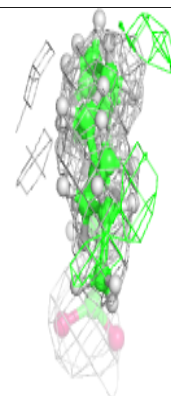
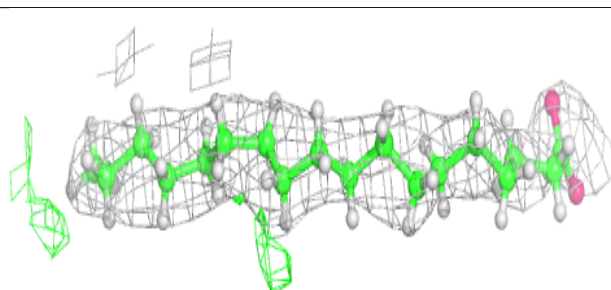
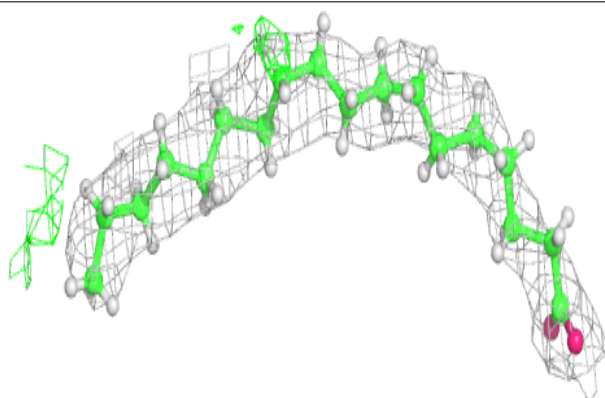


**Electron density around STE C 521:**

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

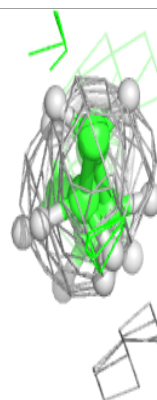
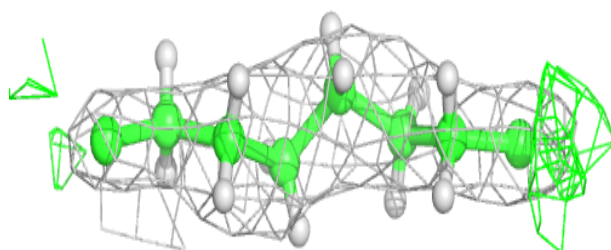
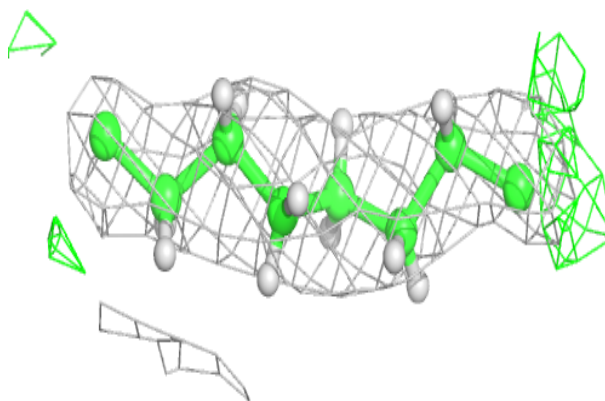
**Electron density around STE X 102:**

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

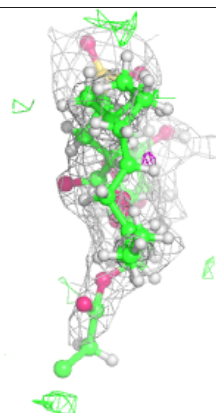
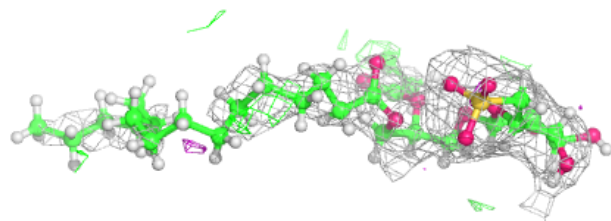
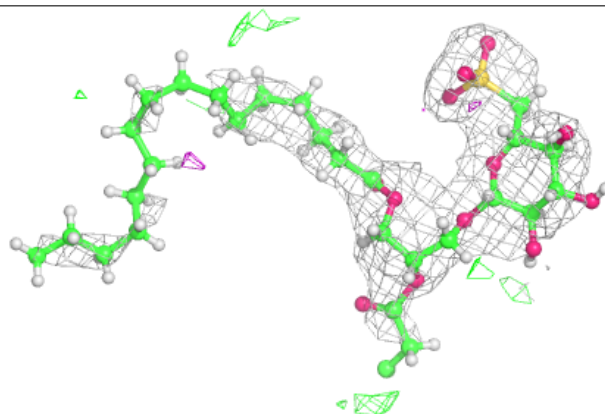


**Electron density around STE Z 101:**

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

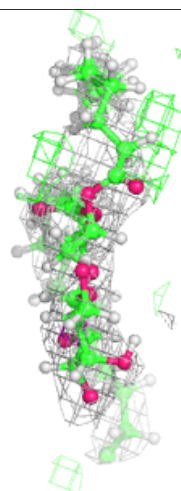
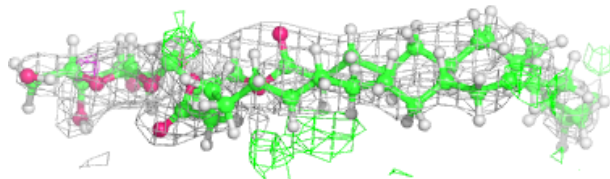
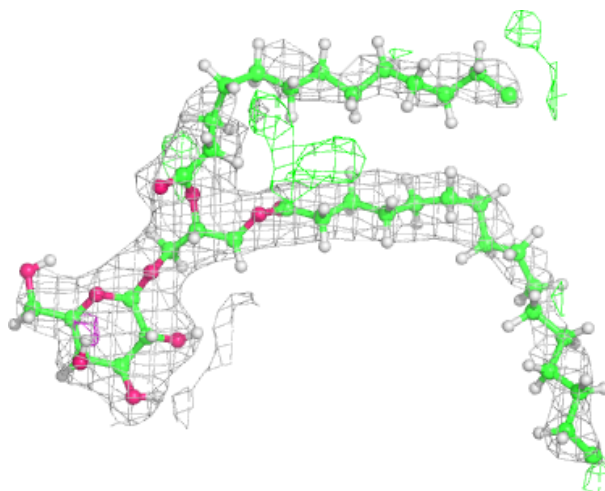
**Electron density around SQD f 102:**

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



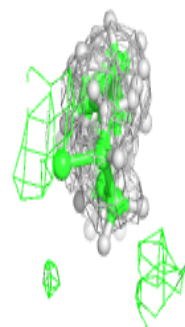
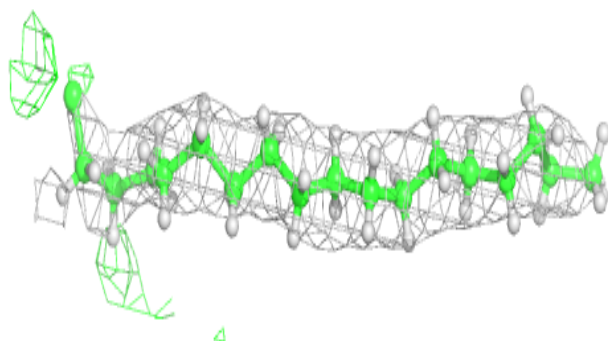
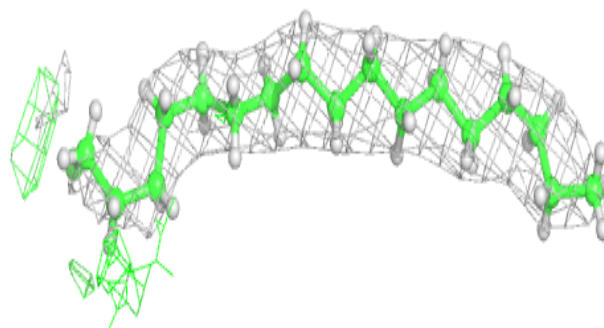
**Electron density around LMG Y 101:**

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

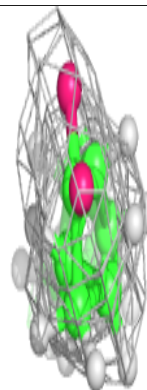
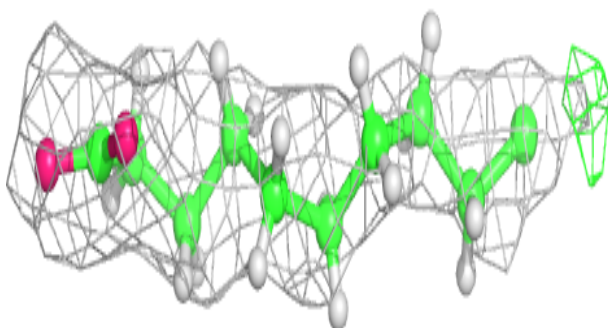
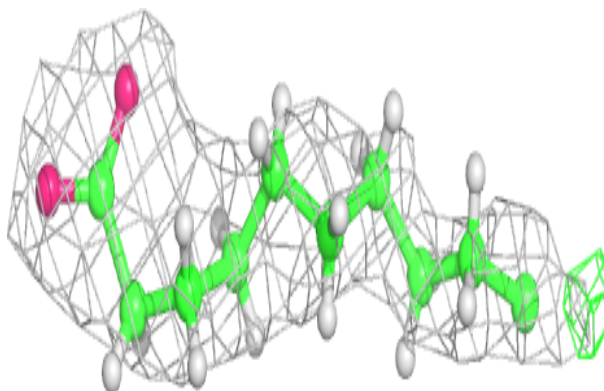


**Electron density around STE M 104:**

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

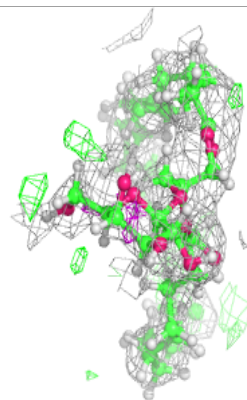
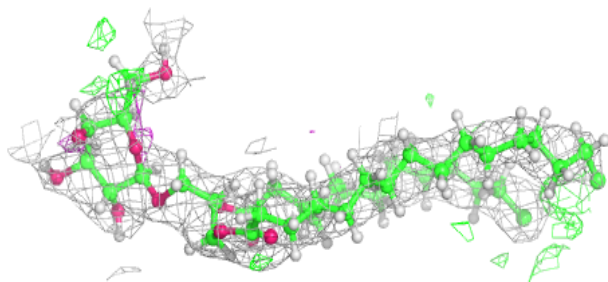
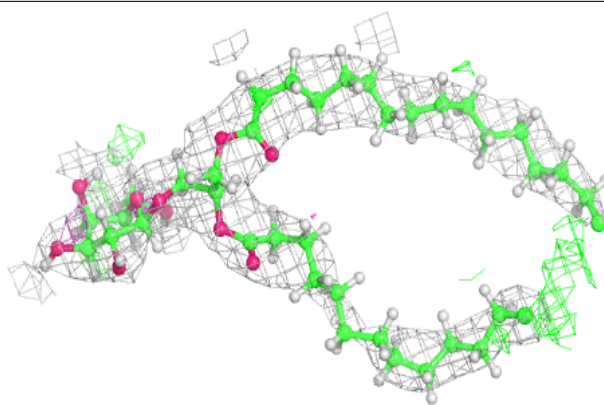
**Electron density around STE c 523:**

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

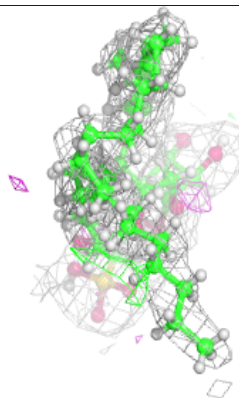
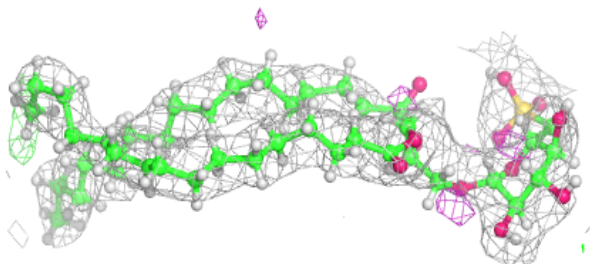
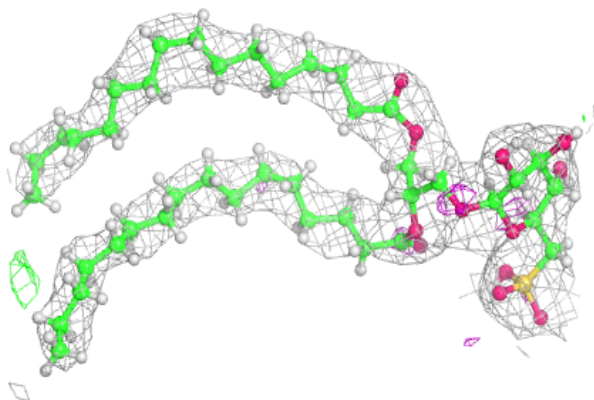


**Electron density around LMG C 515:**

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

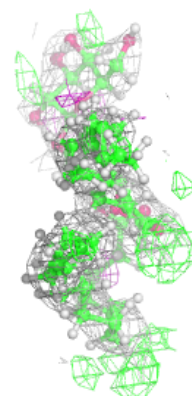
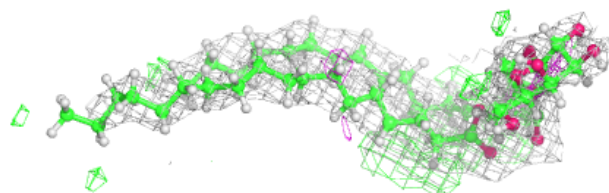
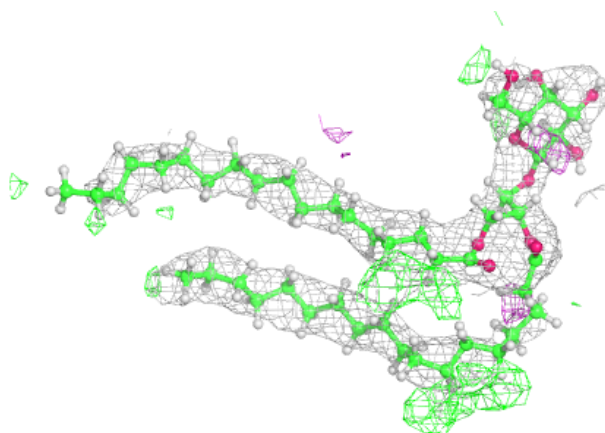
**Electron density around SQD B 620:**

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

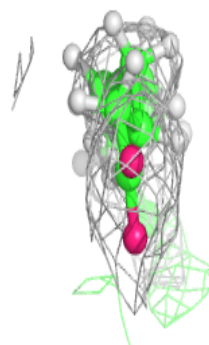
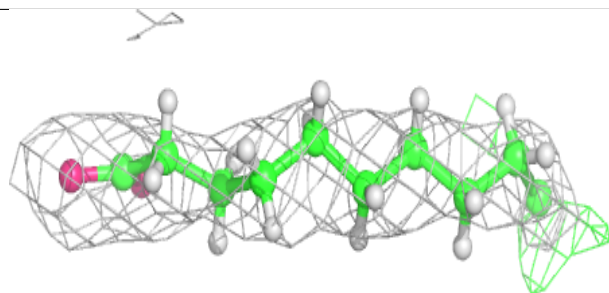
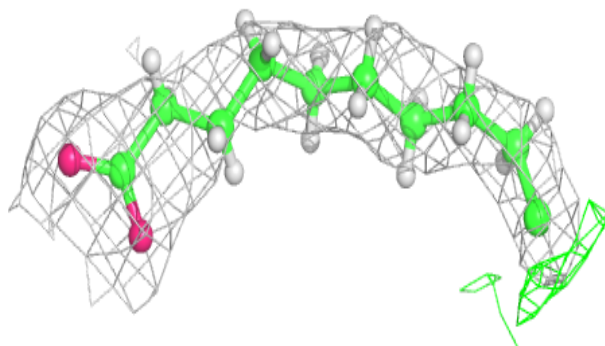


**Electron density around LMG a 619:**

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

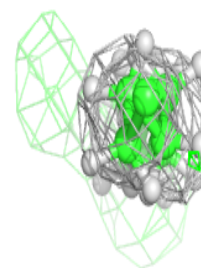
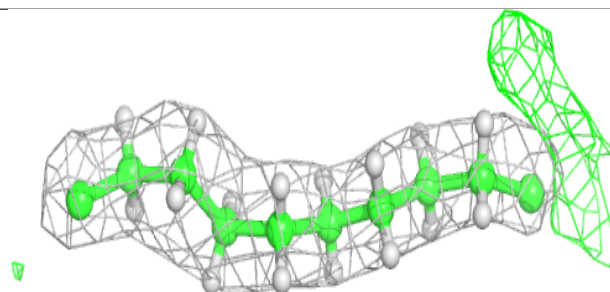
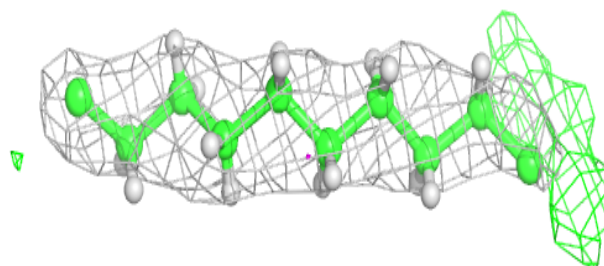
**Electron density around STE C 519:**

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



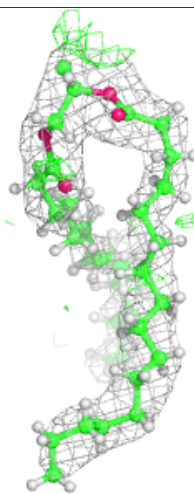
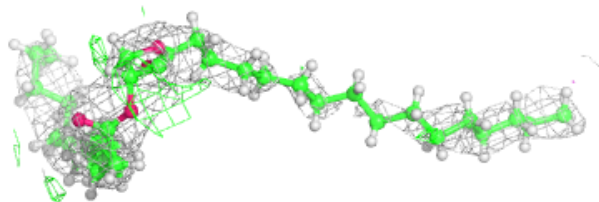
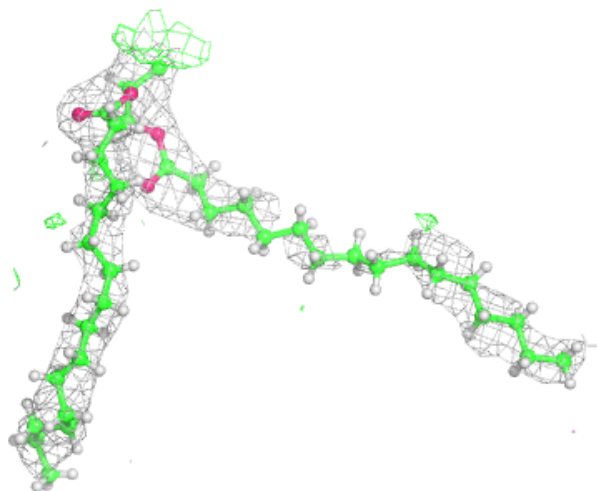
**Electron density around STE M 103:**

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



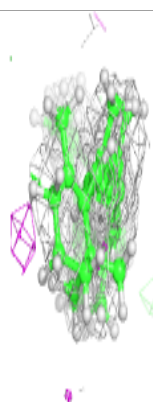
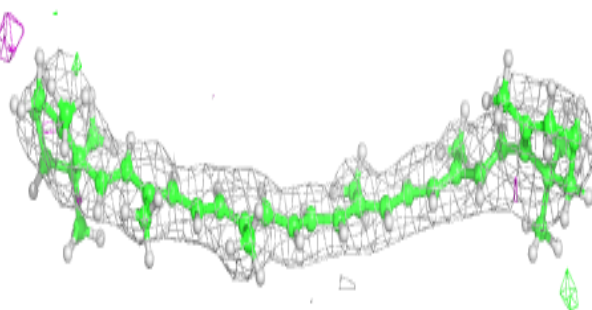
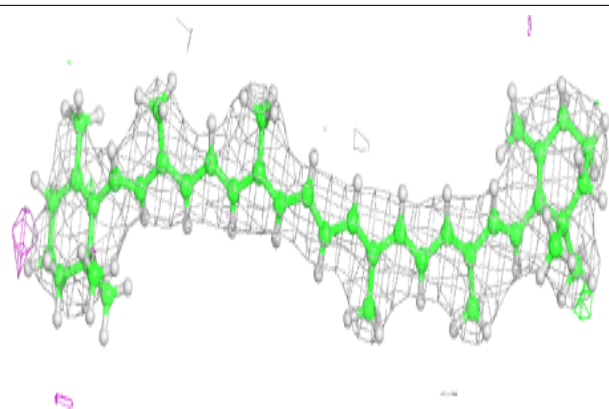
**Electron density around SQD A 615:**

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

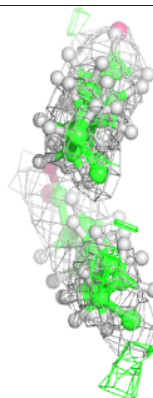
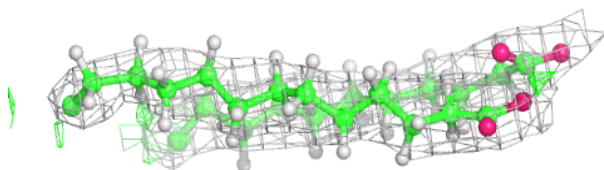
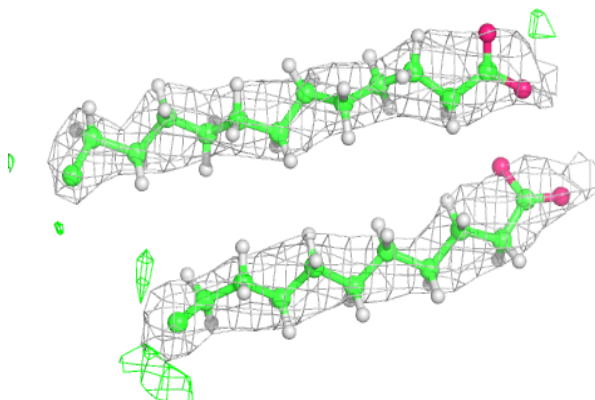


**Electron density around BCR D 405:**

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

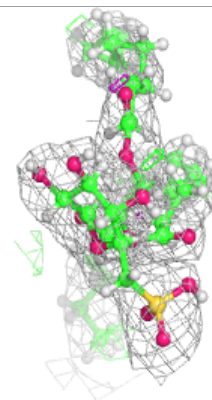
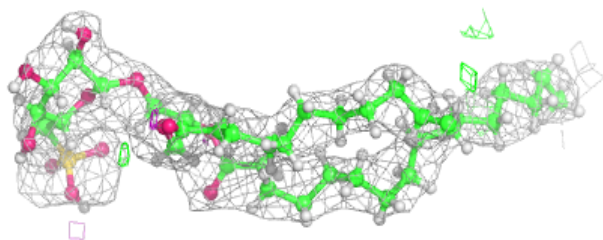
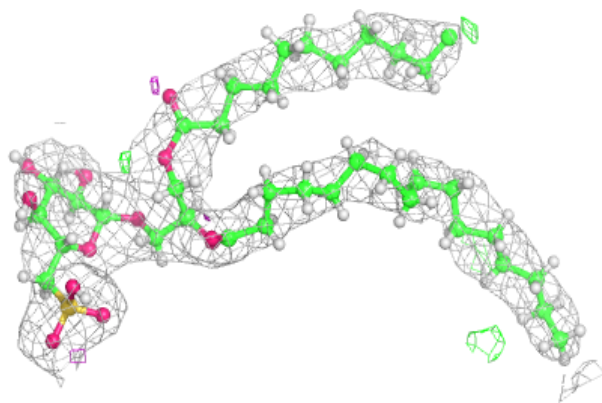
**Electron density around LMG D 412:**

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

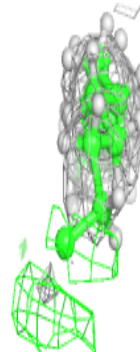
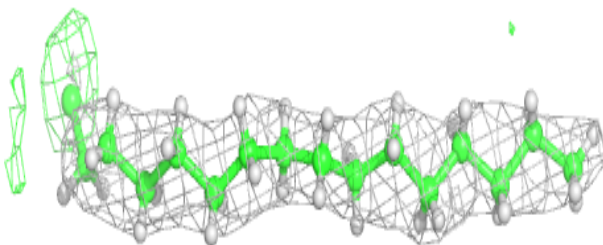
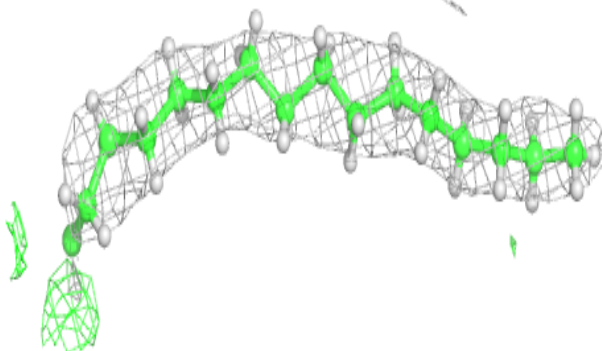


**Electron density around SQD b 620:**

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

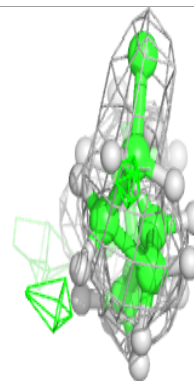
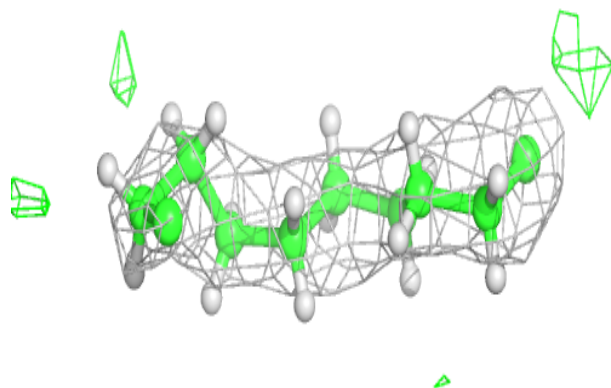
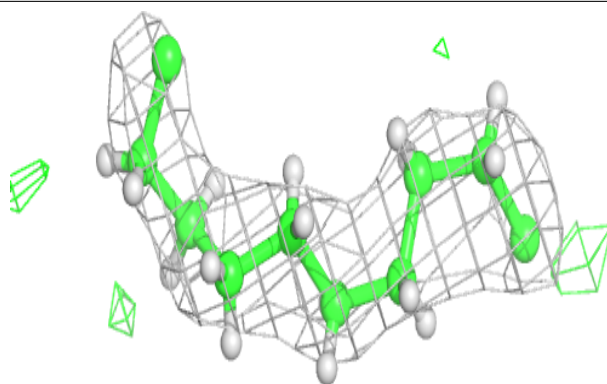
**Electron density around STE C 520:**

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

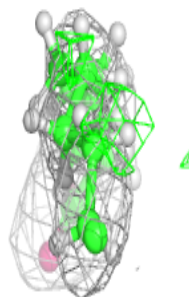
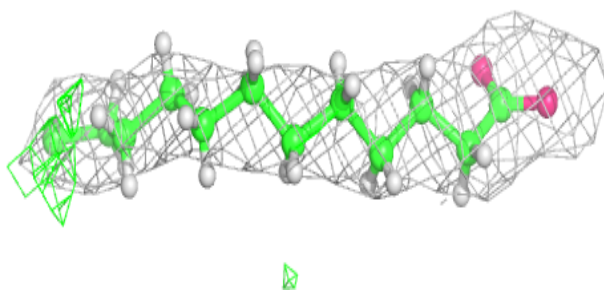
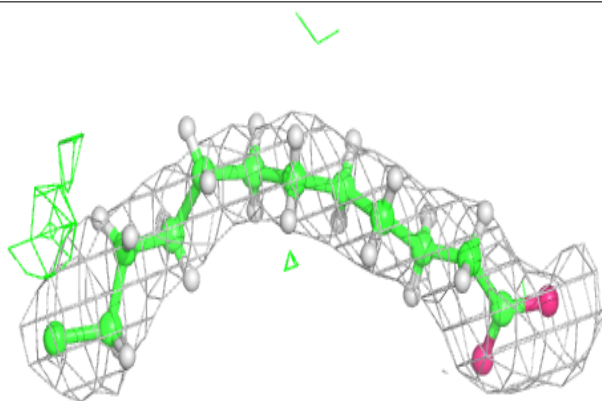


**Electron density around STE b 625:**

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

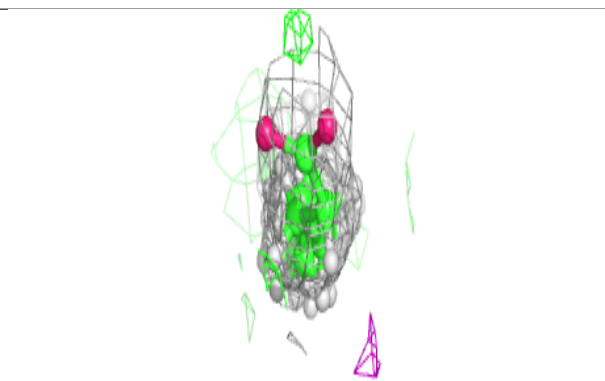
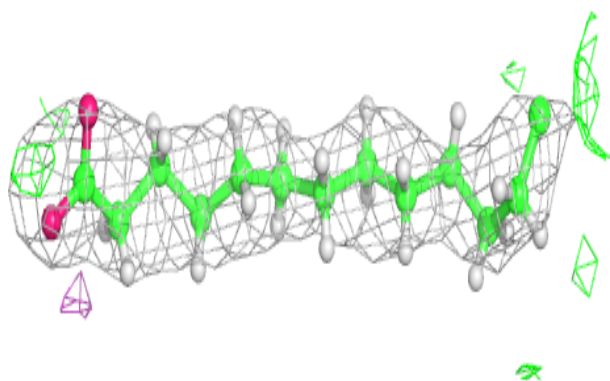
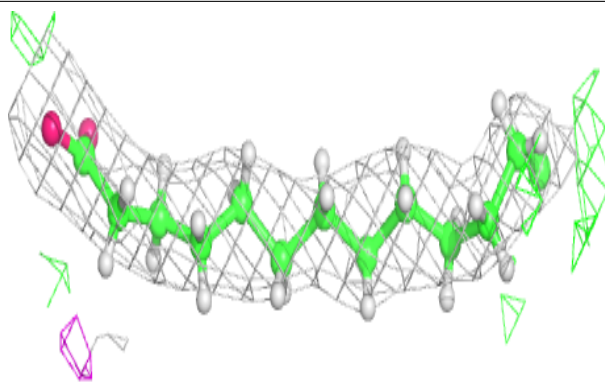
**Electron density around STE t 102:**

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

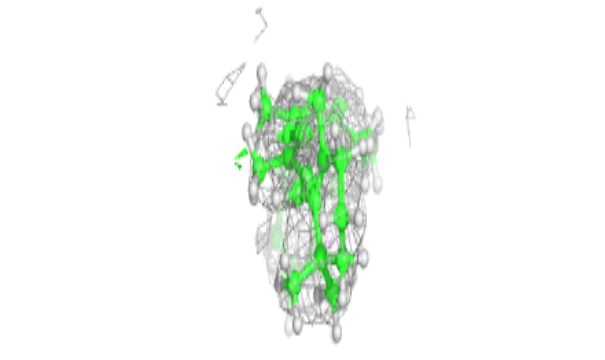
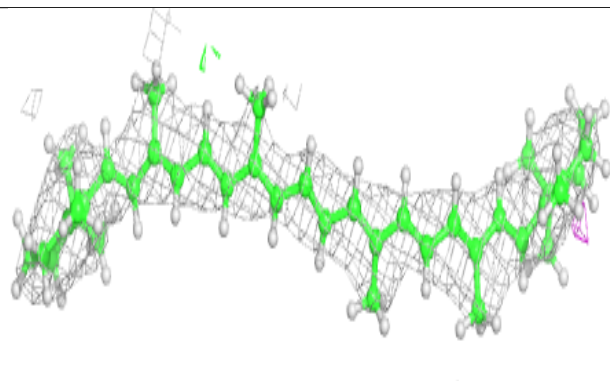
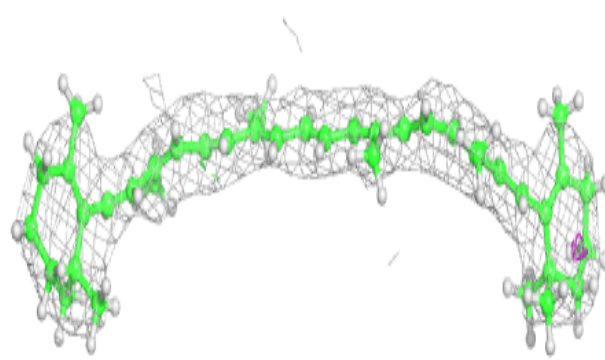


**Electron density around STE M 102:**

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

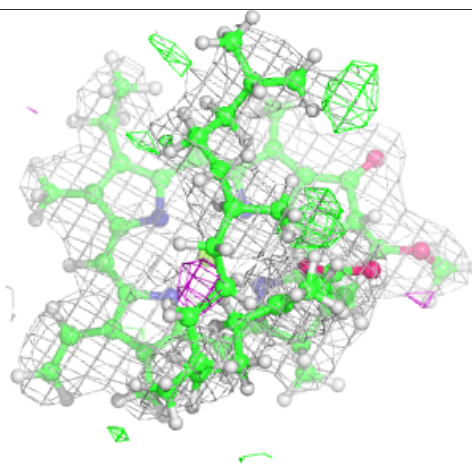
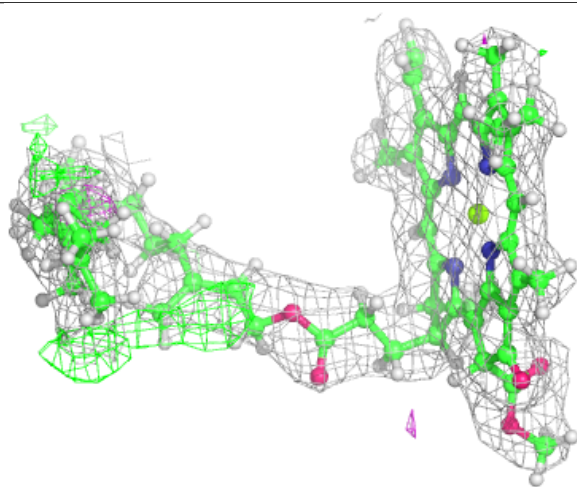
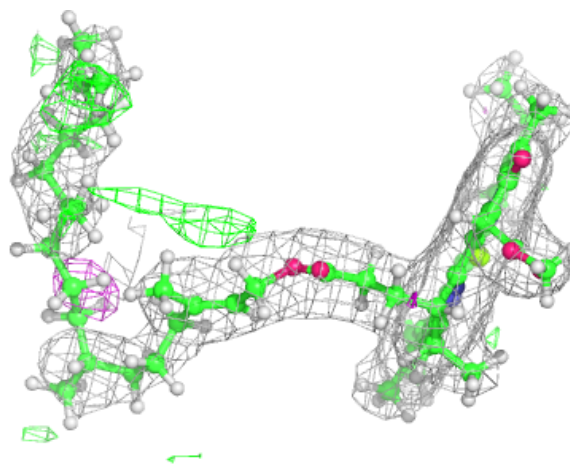
**Electron density around BCR k 102:**

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



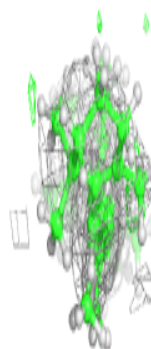
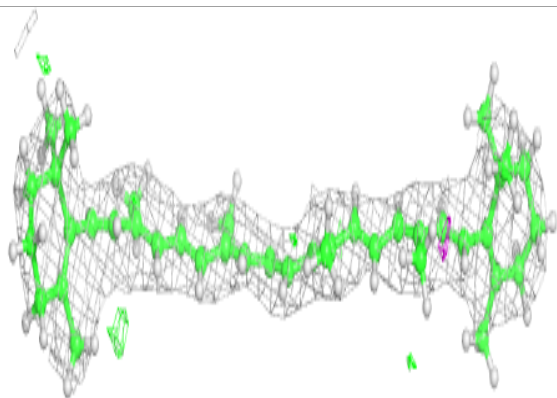
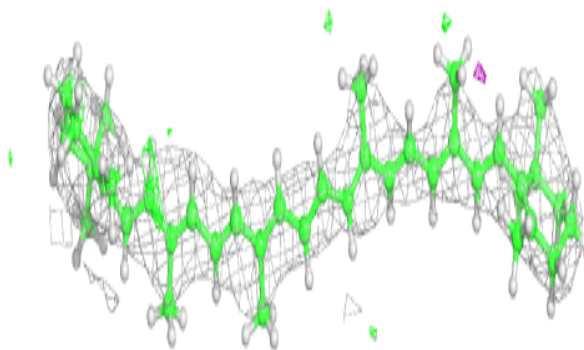
**Electron density around CLA a 607:**

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

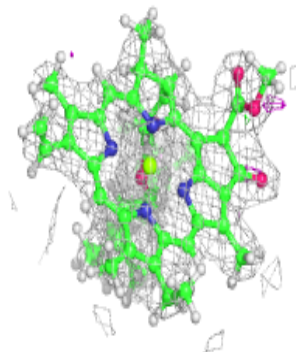
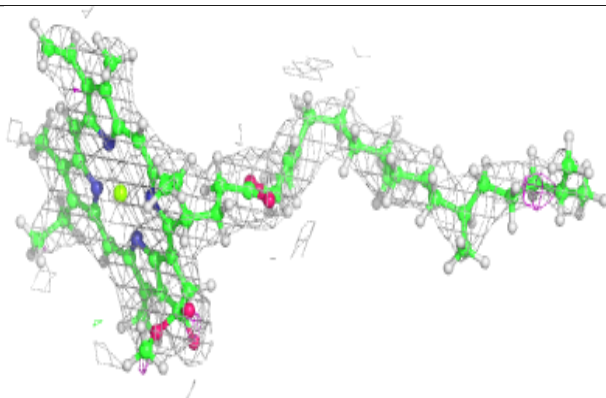
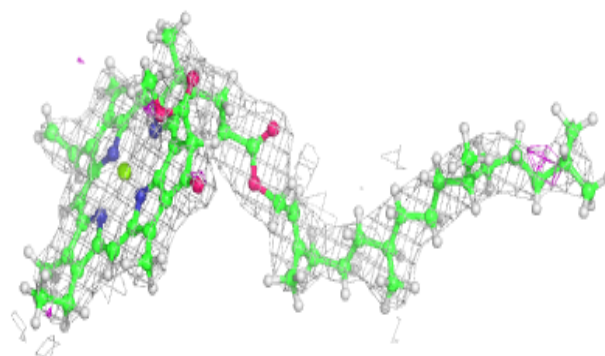


**Electron density around BCR c 514:**

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

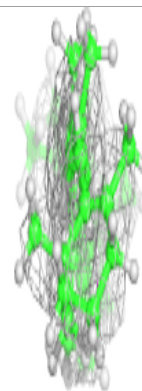
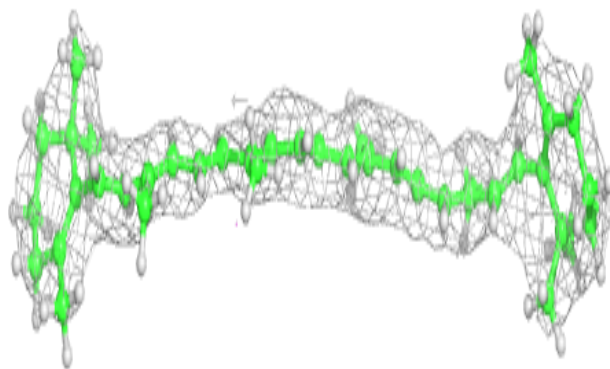
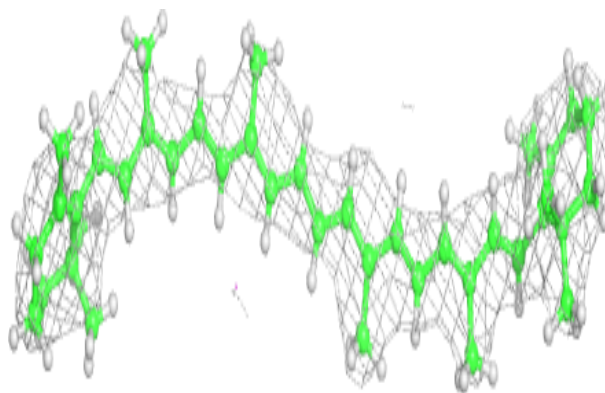
**Electron density around CLA C 502:**

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

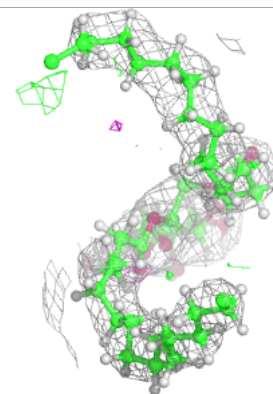
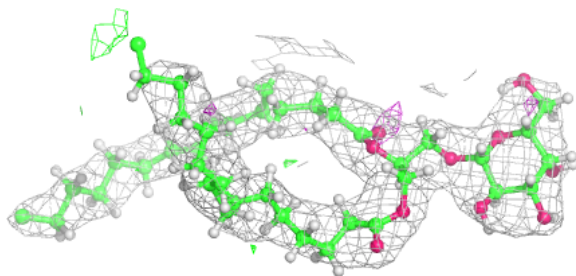
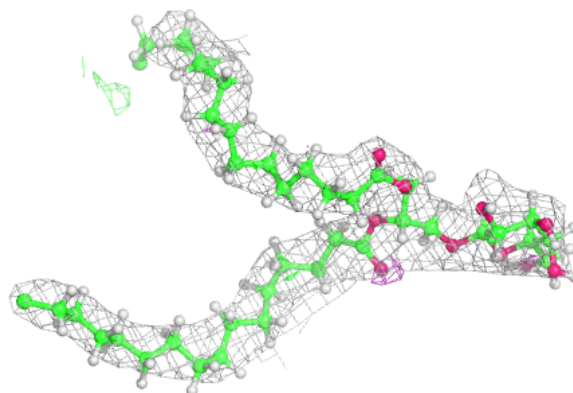


**Electron density around BCR k 101:**

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

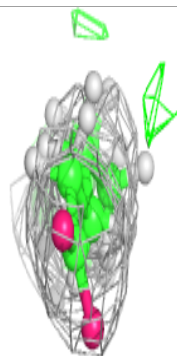
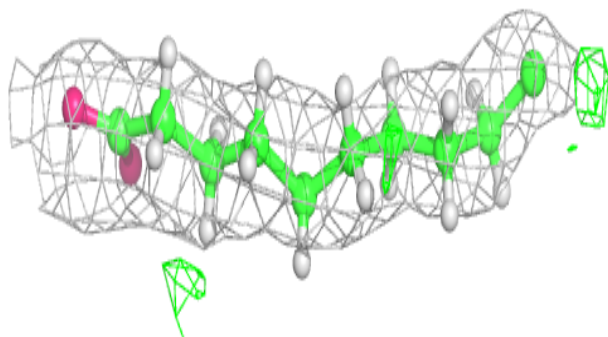
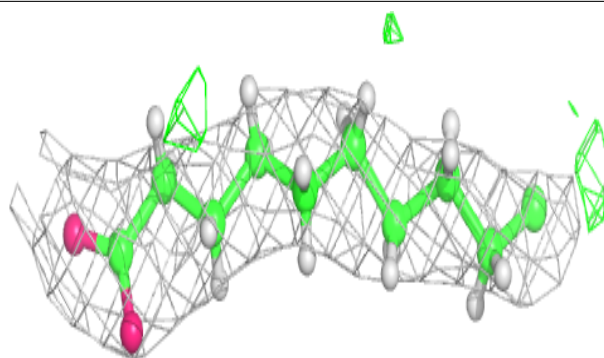
**Electron density around LMG M 101:**

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

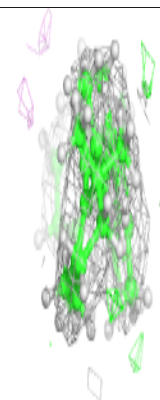
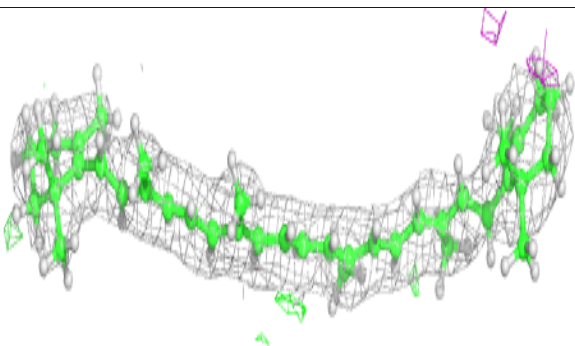
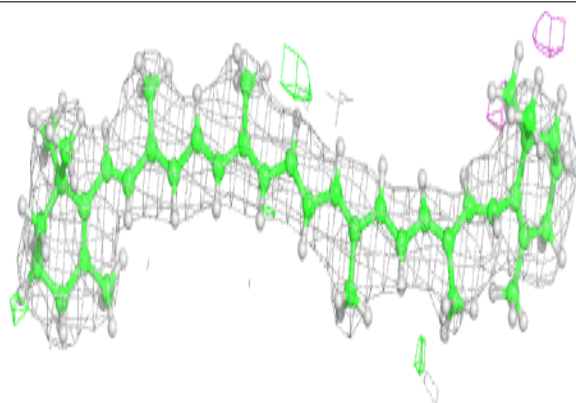


**Electron density around STE j 101:**

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

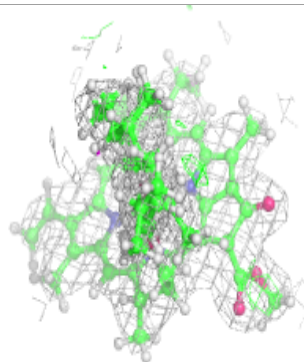
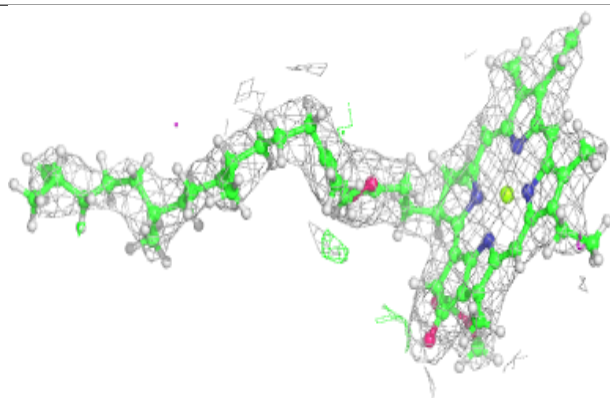
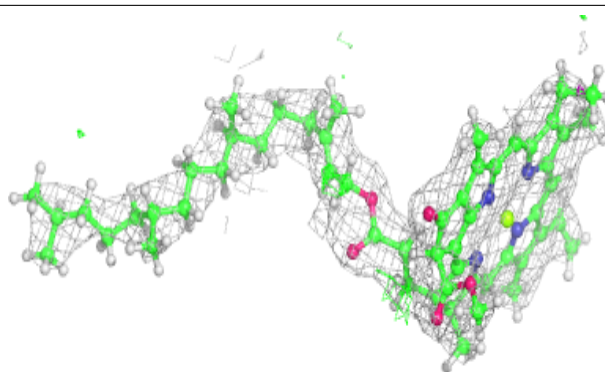
**Electron density around BCR d 404:**

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

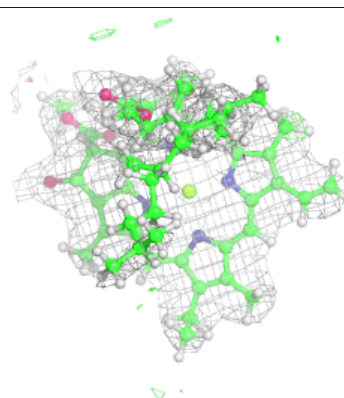
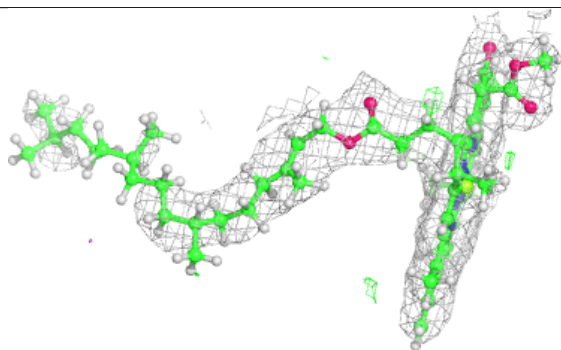
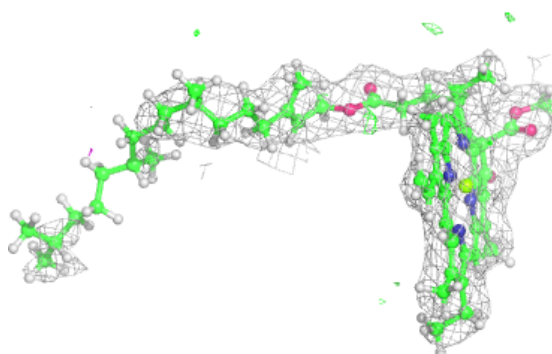


**Electron density around CLA c 502:**

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

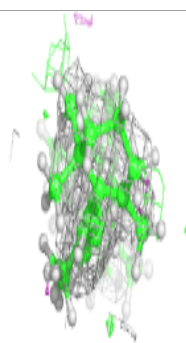
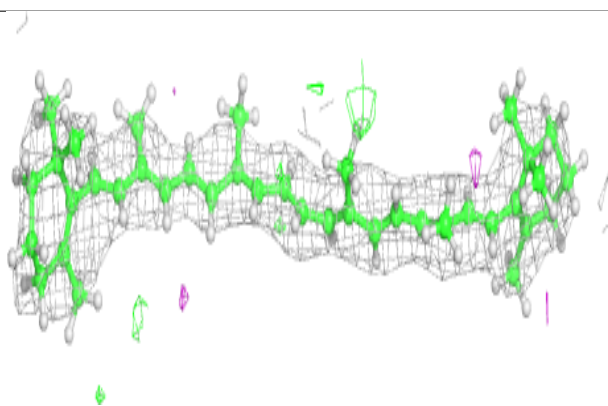
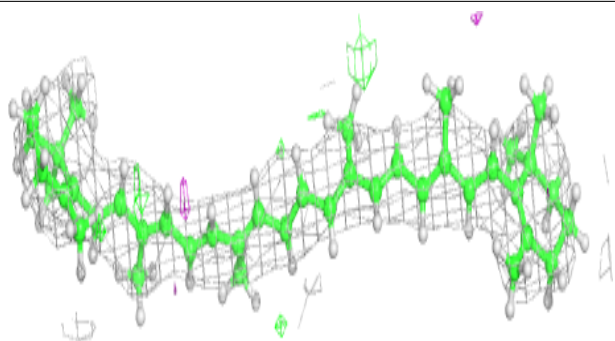
**Electron density around CLA D 404:**

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

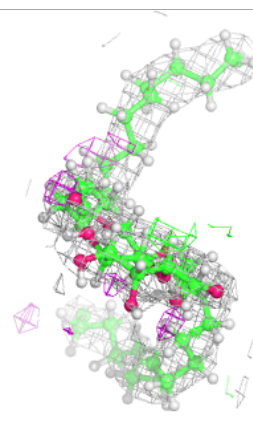
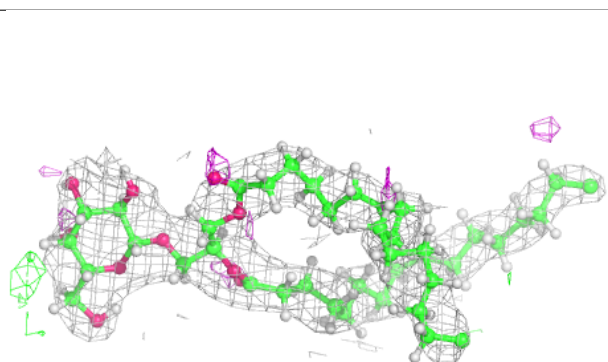
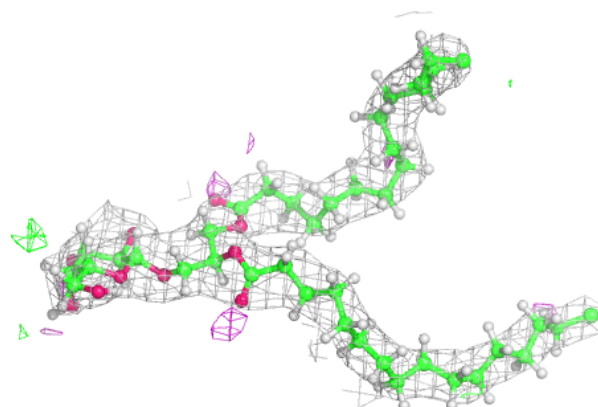


**Electron density around BCR K 101:**

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

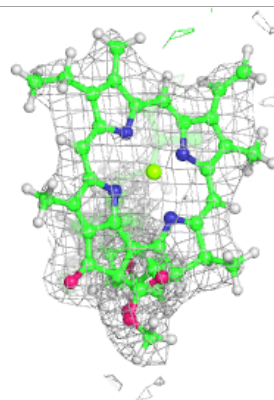
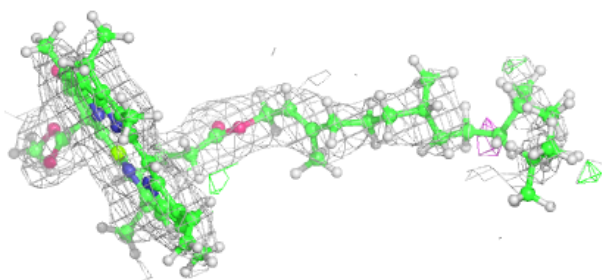
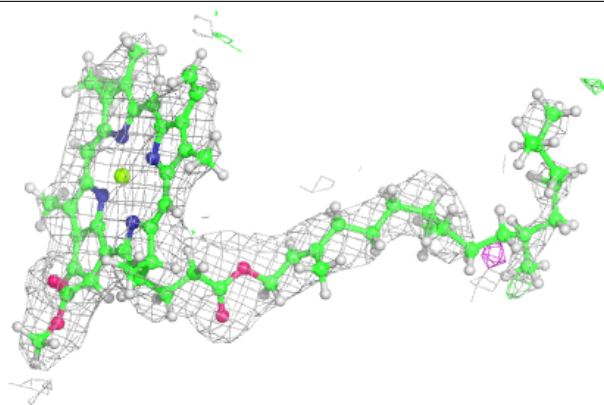
**Electron density around LMG m 101:**

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

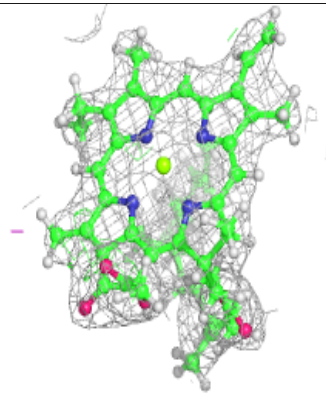
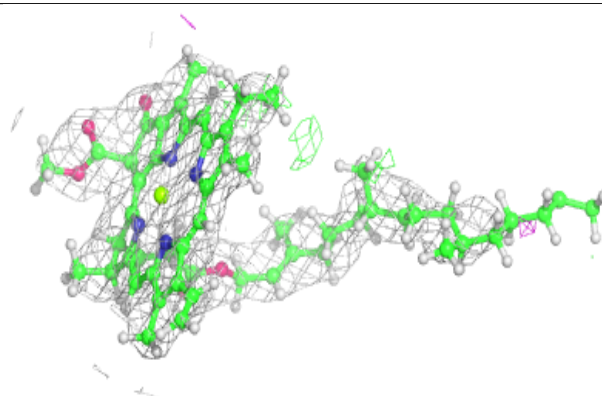
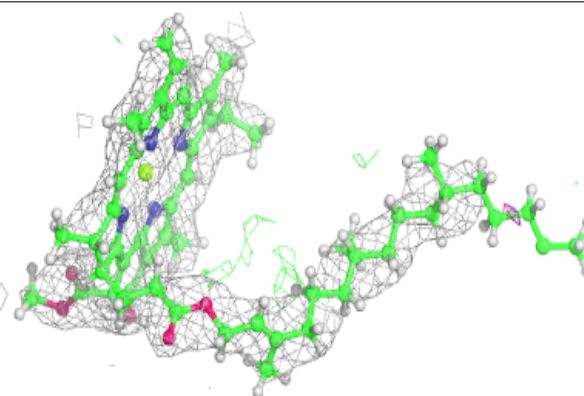


**Electron density around CLA d 403:**

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

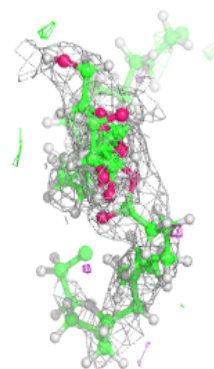
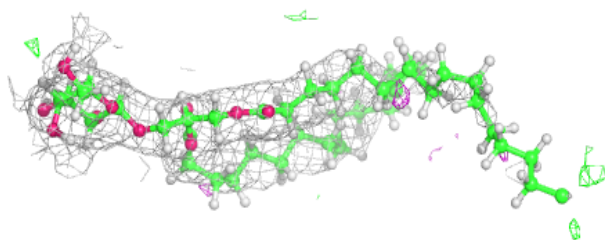
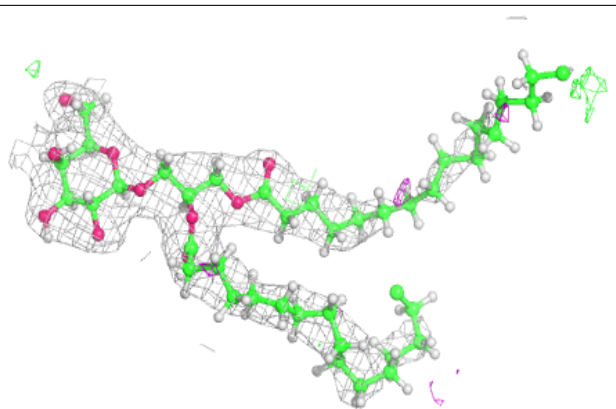
**Electron density around CLA c 508:**

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

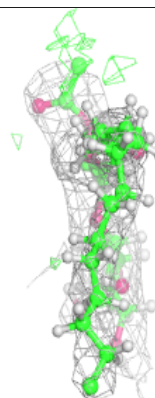
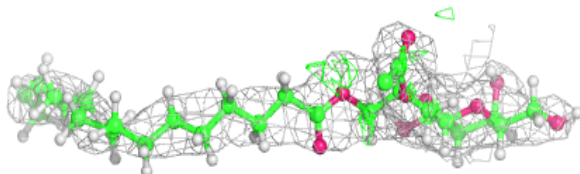
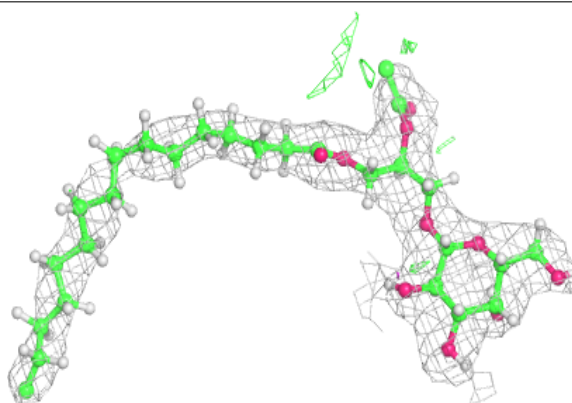


**Electron density around LMG D 407:**

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

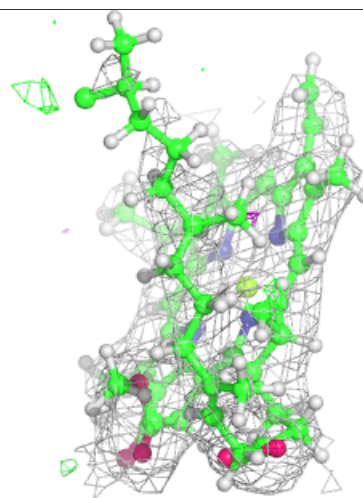
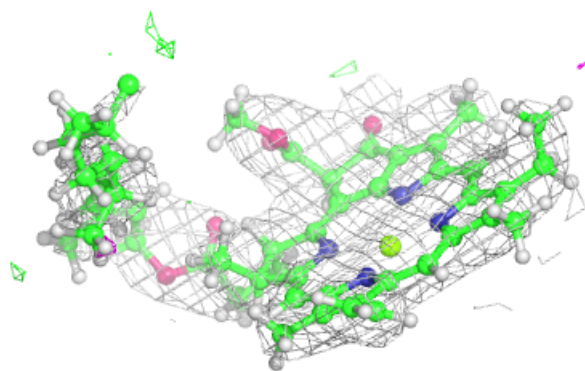
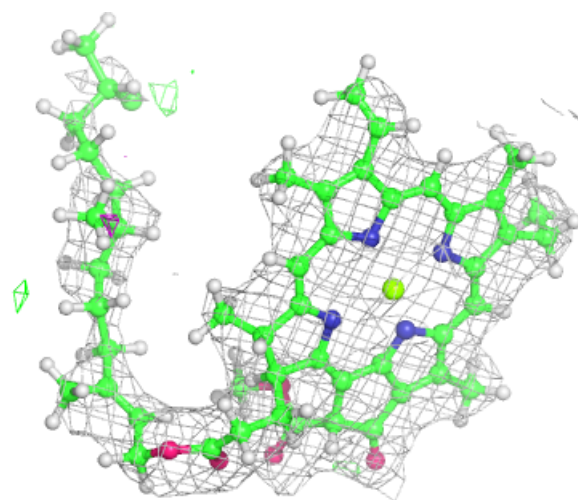
**Electron density around LMG c 519:**

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



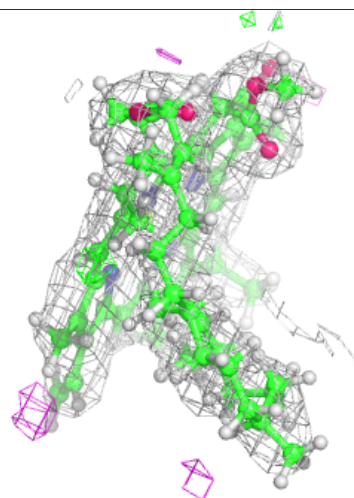
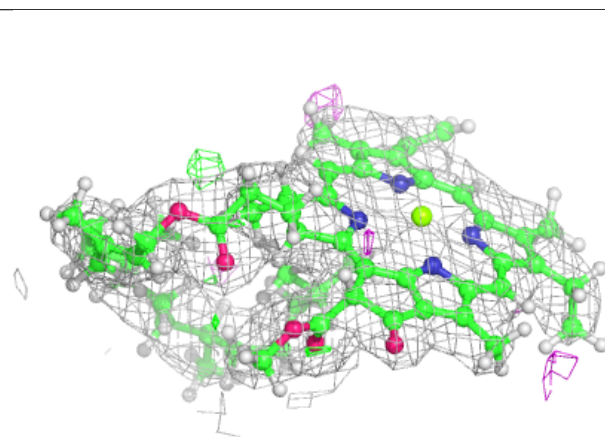
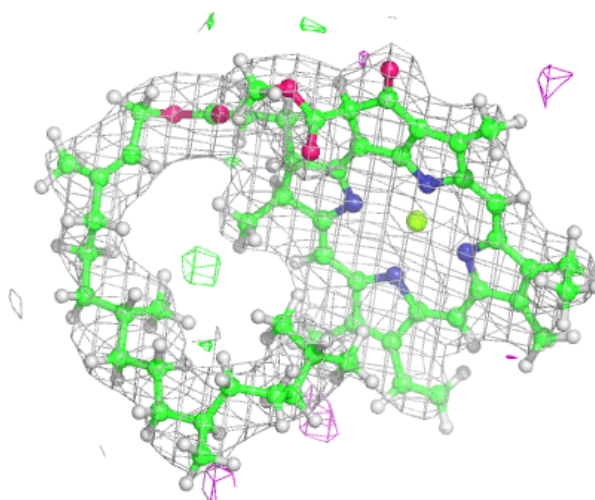
**Electron density around CLA b 616:**

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



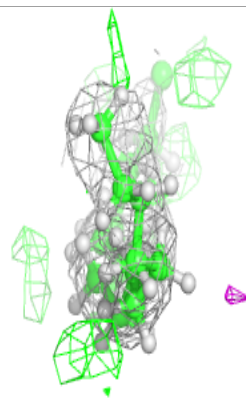
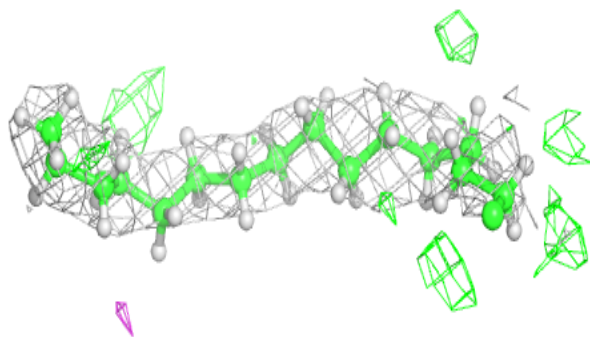
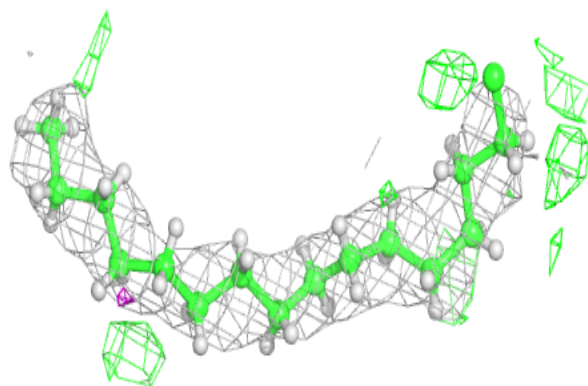
**Electron density around CLA b 615:**

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



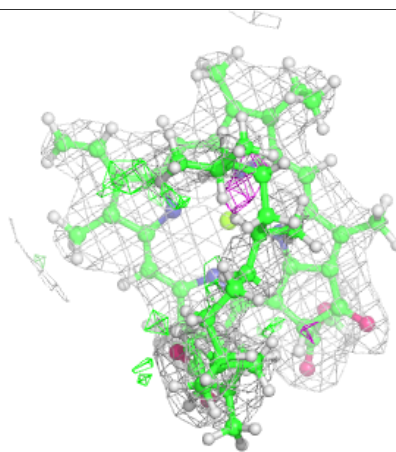
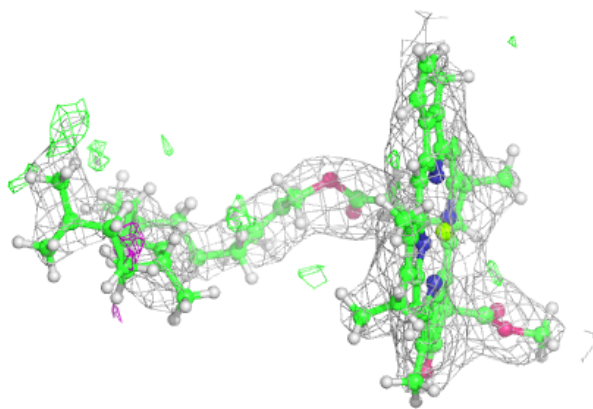
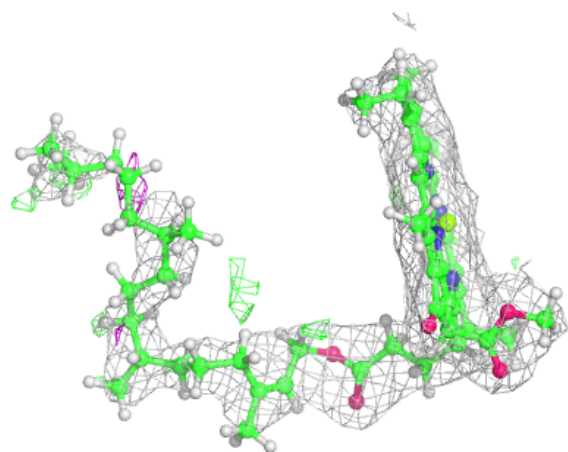
**Electron density around STE T 102:**

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



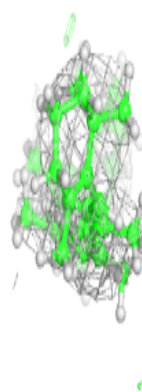
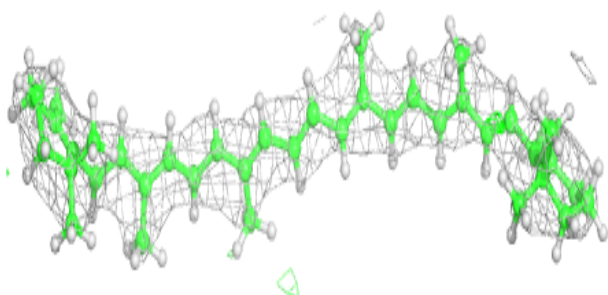
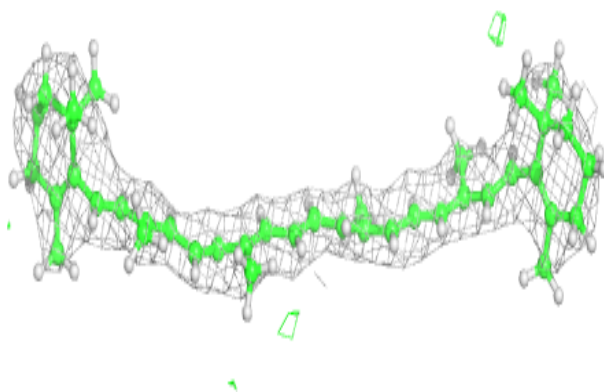
**Electron density around CLA c 506:**

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

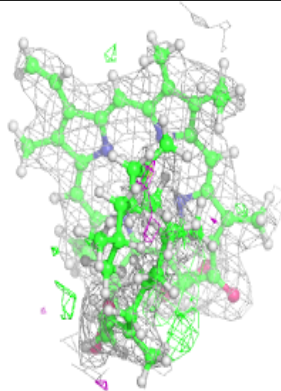
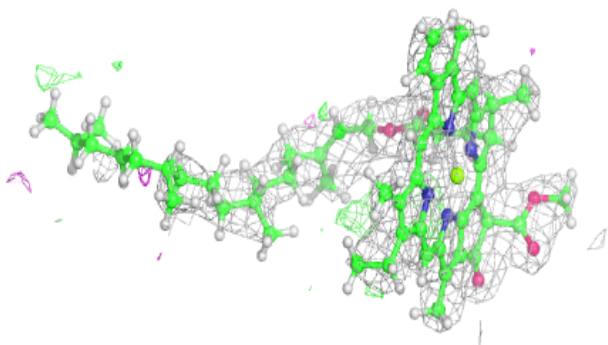
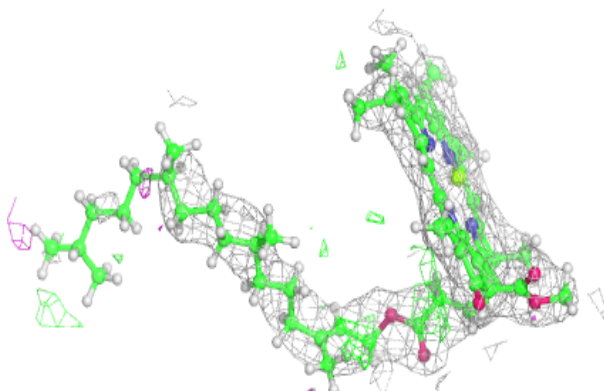


**Electron density around BCR K 103:**

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

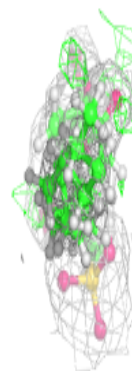
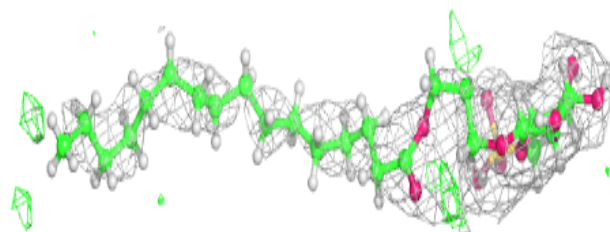
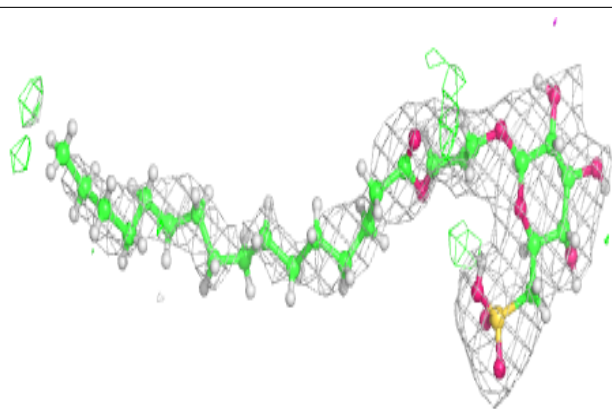
**Electron density around CLA C 508:**

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

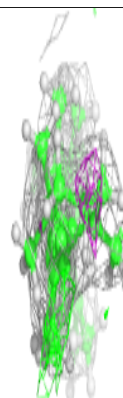
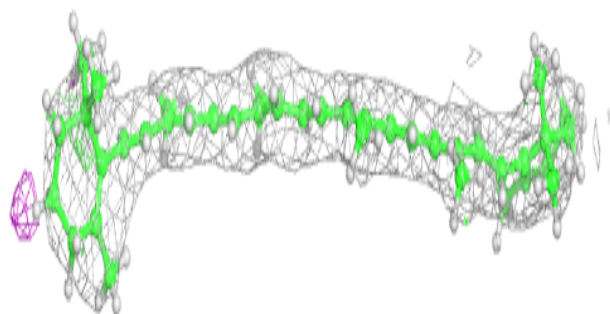
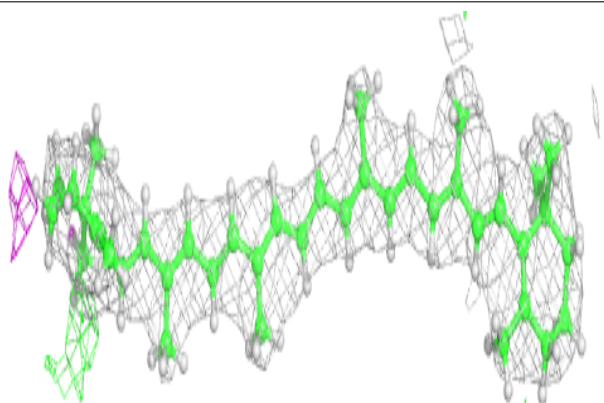


**Electron density around SQD D 408:**

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

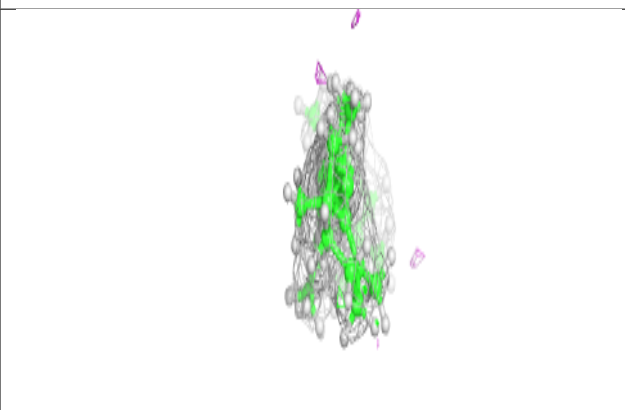
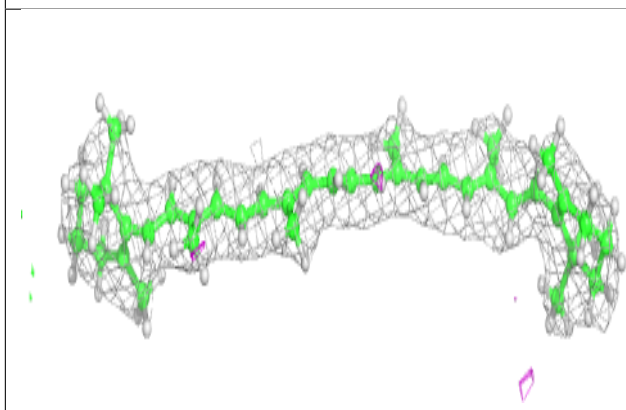
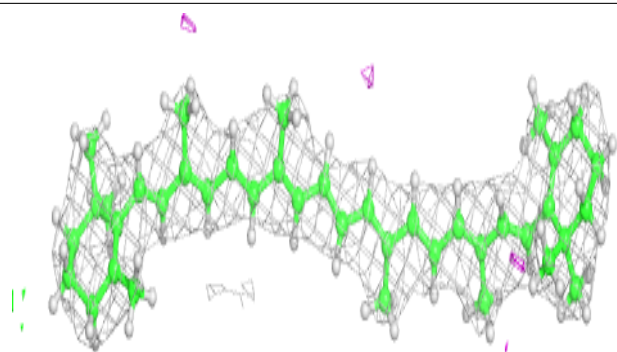
**Electron density around BCR b 617:**

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



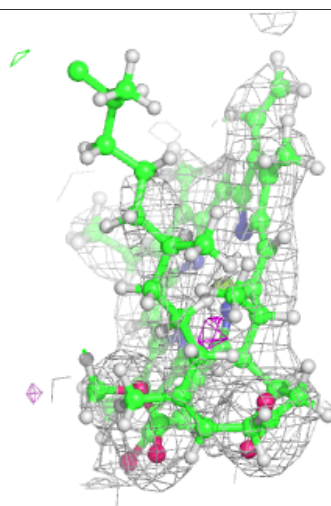
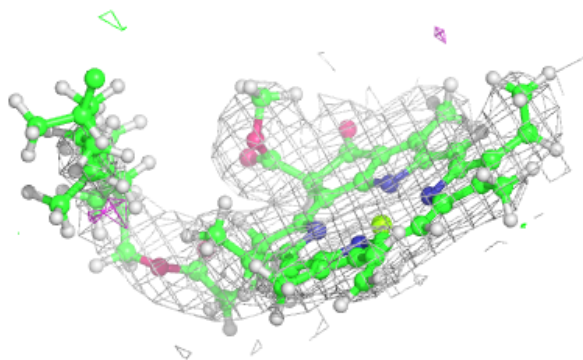
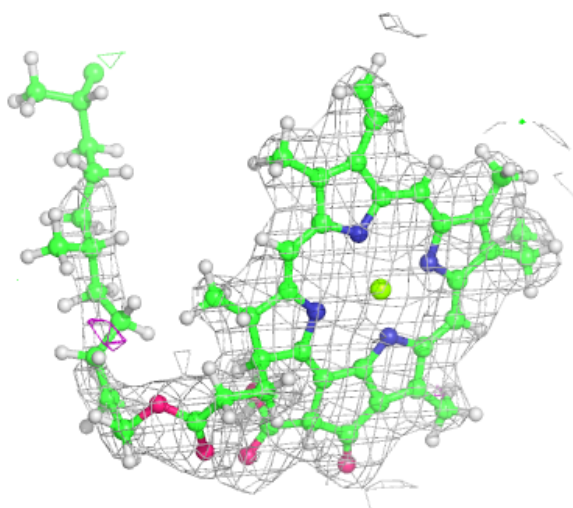
**Electron density around BCR b 619:**

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



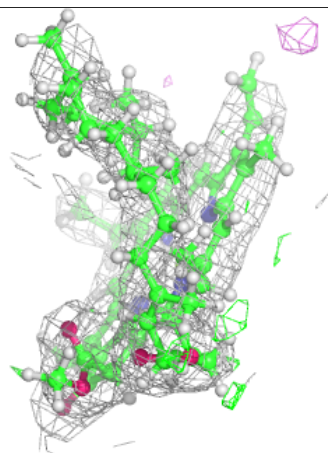
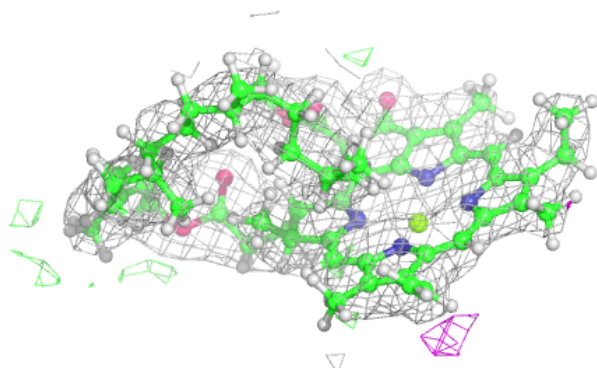
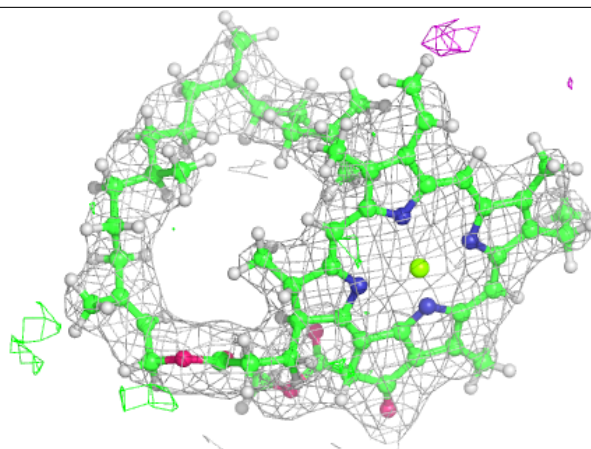
**Electron density around CLA B 615:**

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

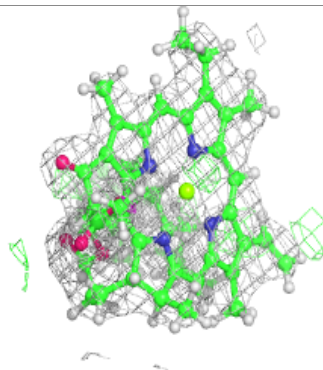
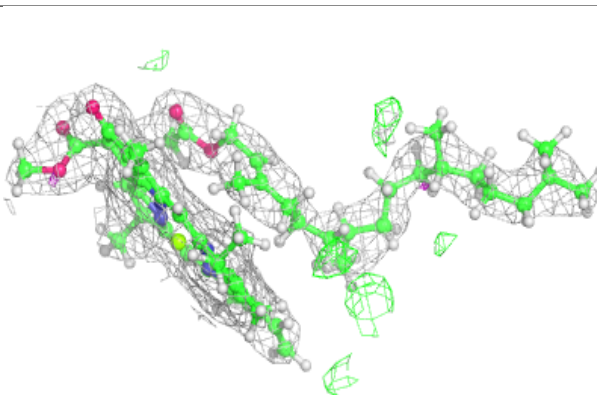
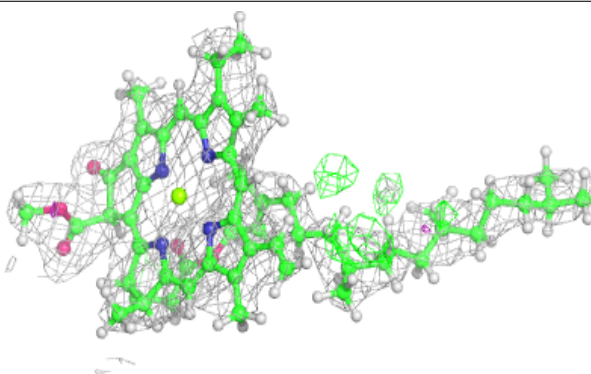


**Electron density around CLA B 614:**

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

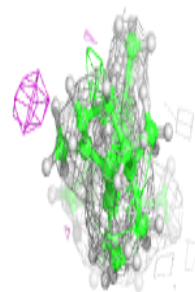
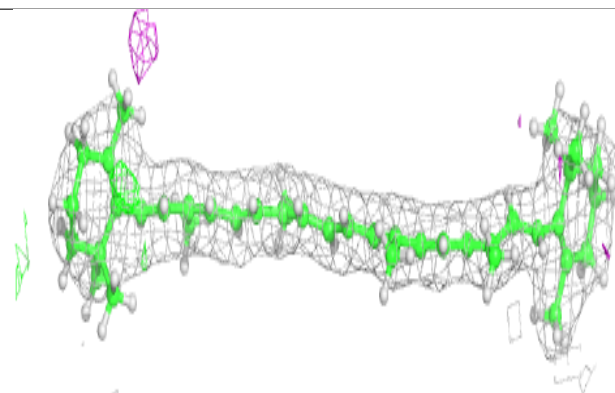
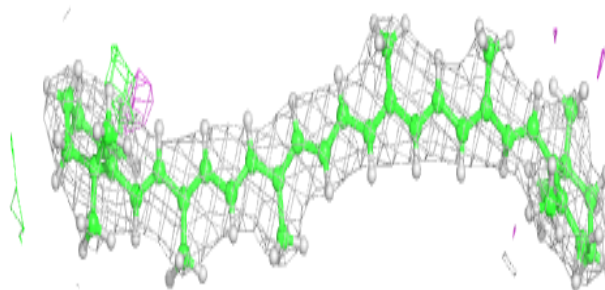
**Electron density around CLA C 505:**

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



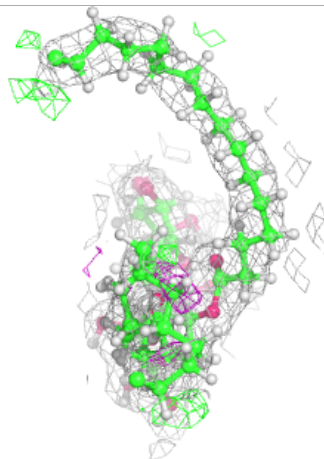
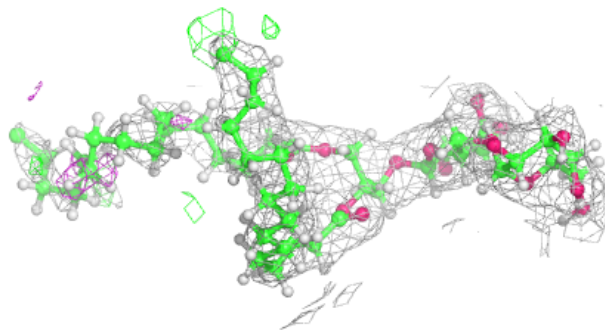
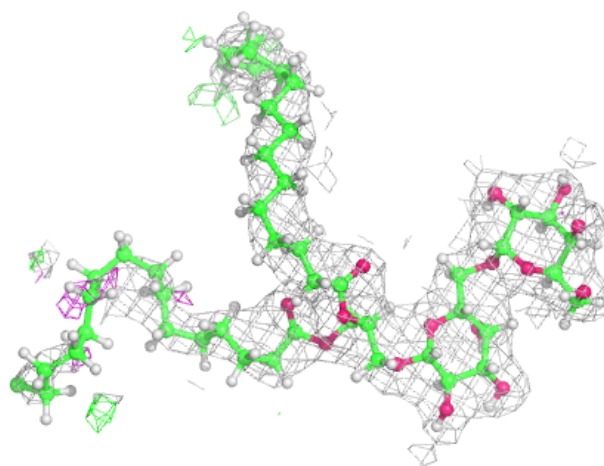
**Electron density around BCR C 514:**

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



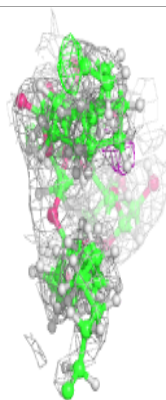
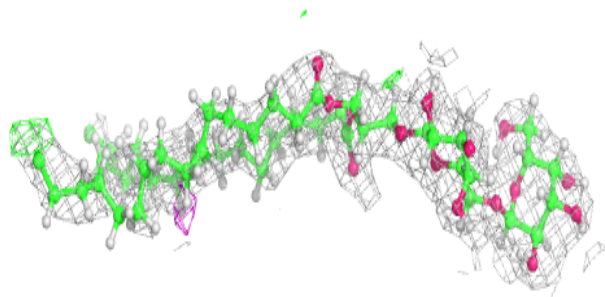
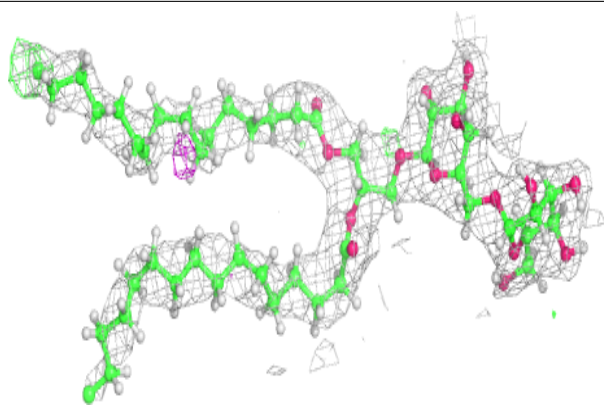
**Electron density around DGD C 517:**

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

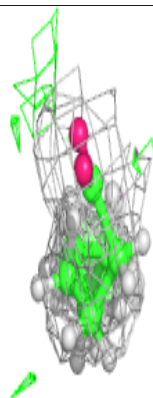
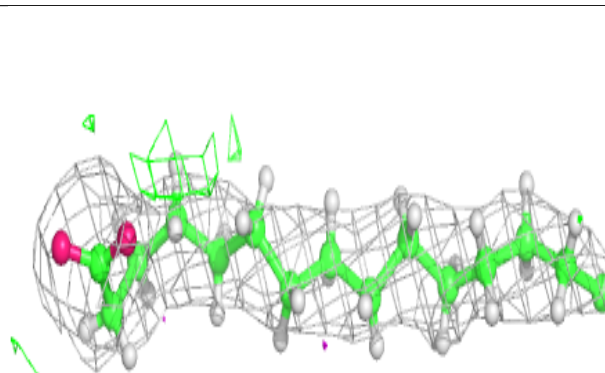
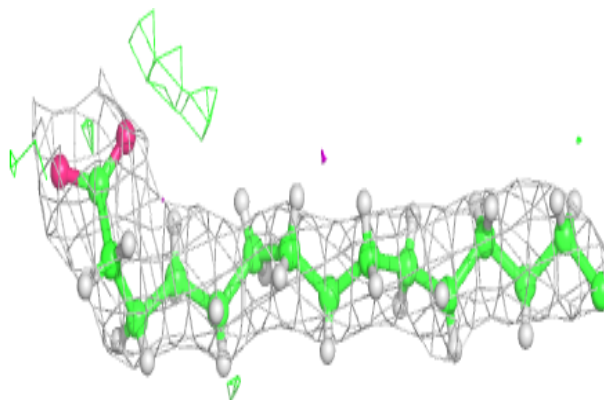


**Electron density around DGD c 518:**

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

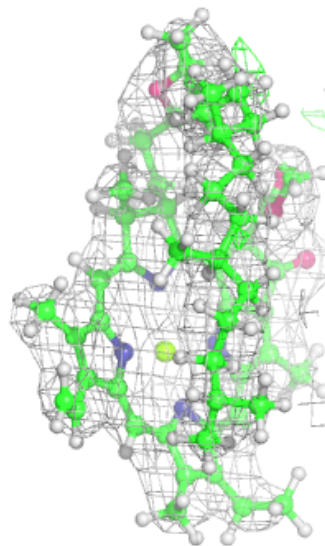
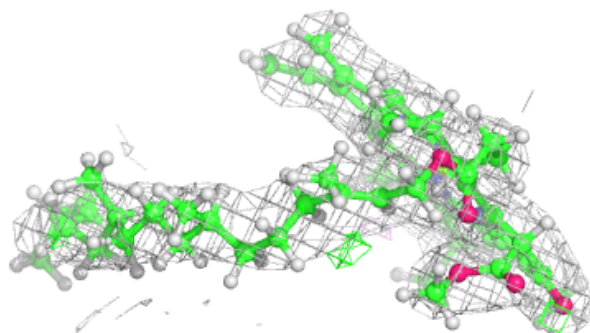
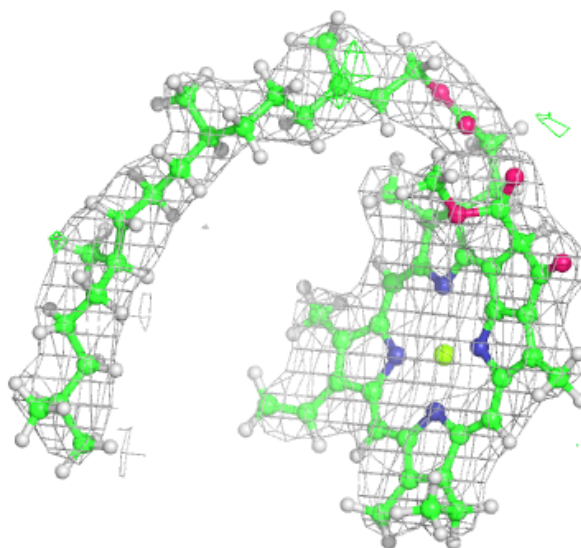
**Electron density around STE d 409:**

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



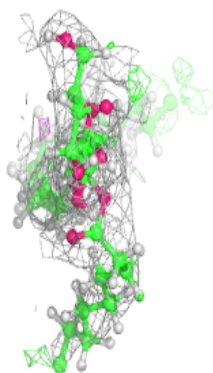
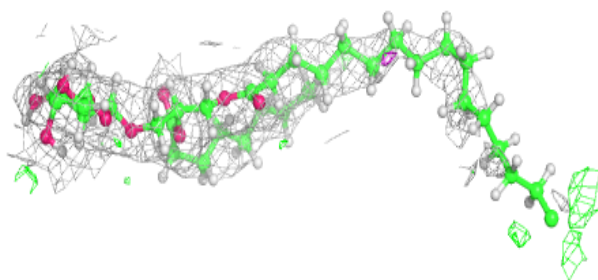
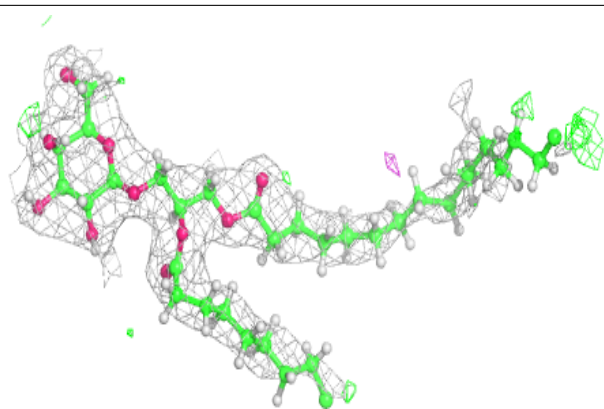
**Electron density around CLA C 507:**

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



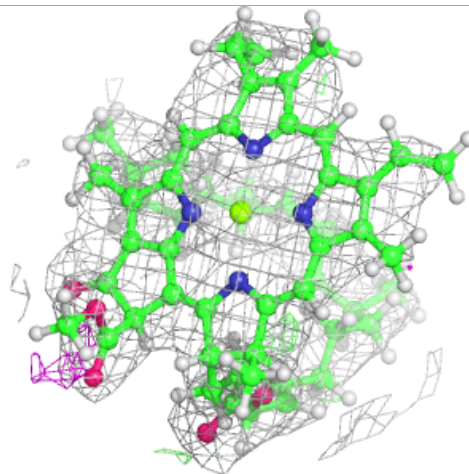
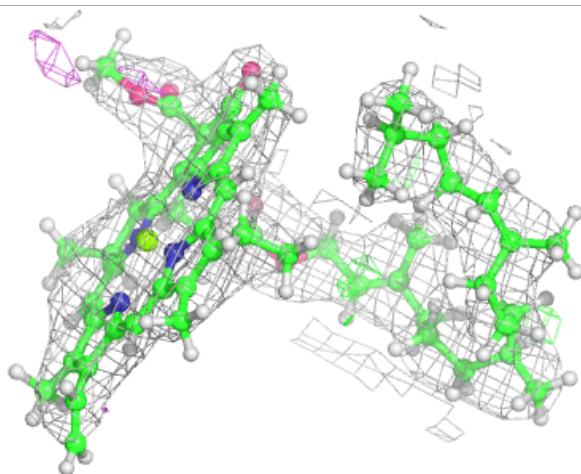
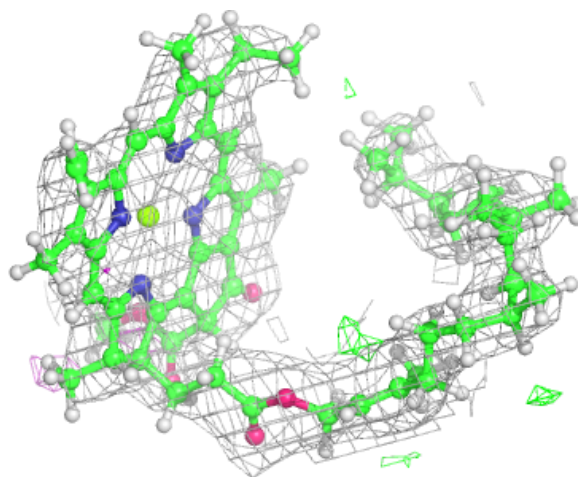
**Electron density around LMG d 408:**

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



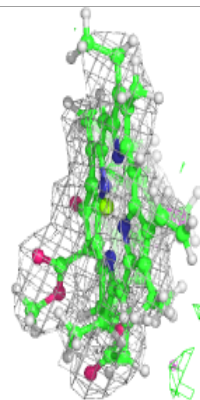
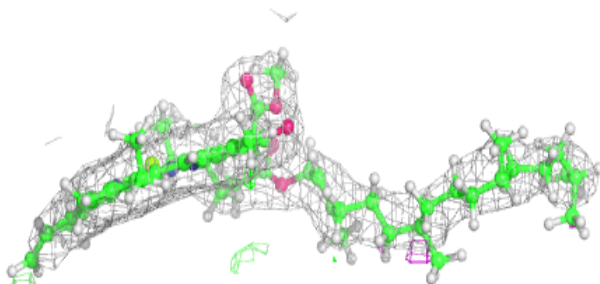
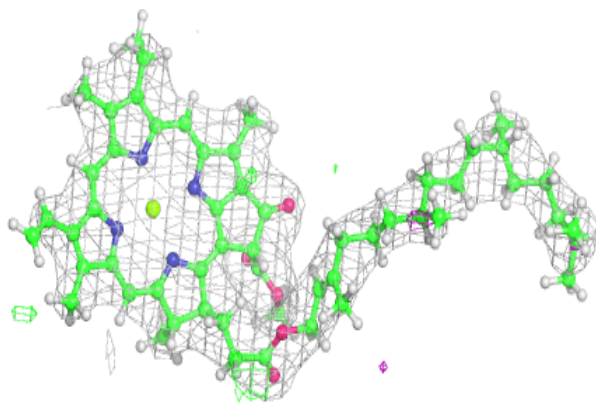
**Electron density around CLA c 503:**

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

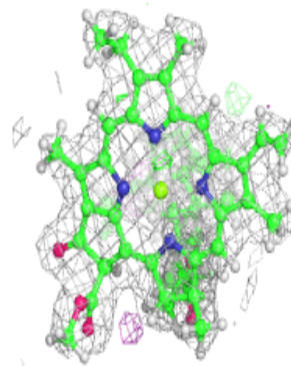
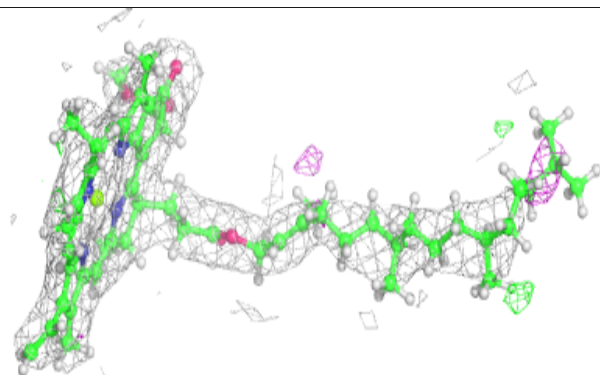
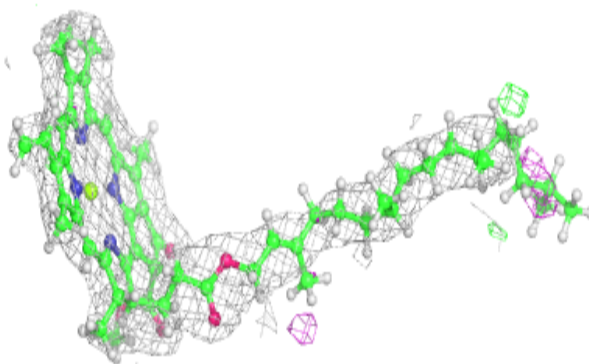


**Electron density around CLA b 602:**

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

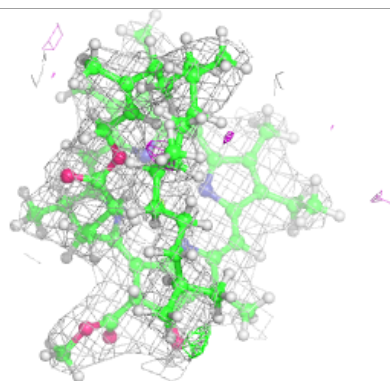
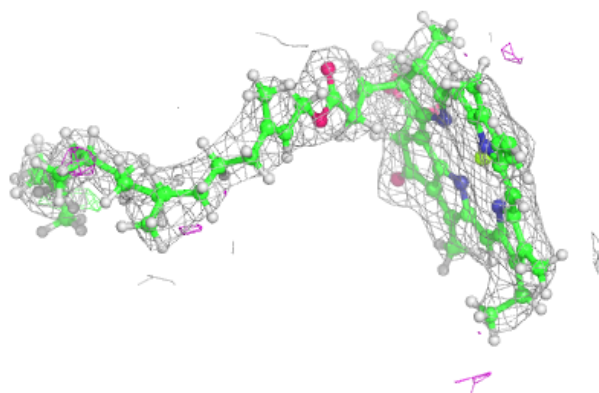
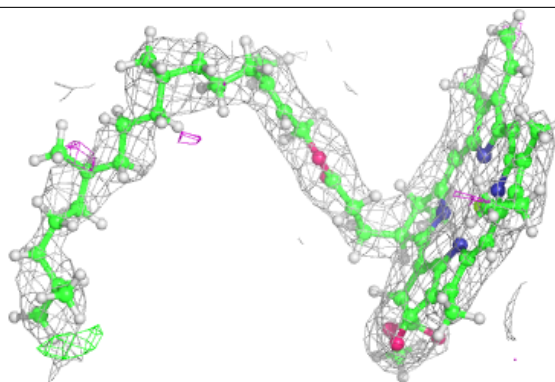
**Electron density around CLA b 604:**

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

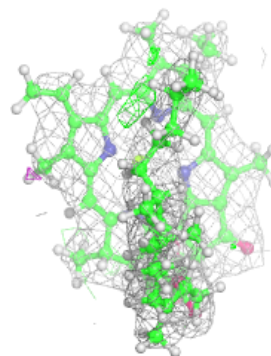
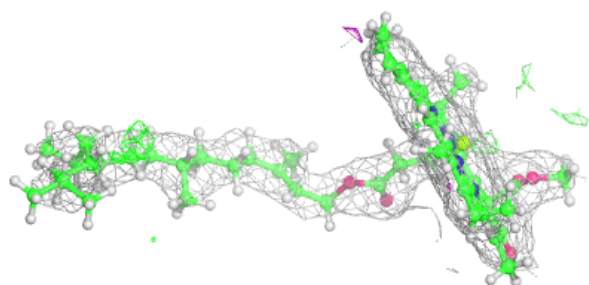
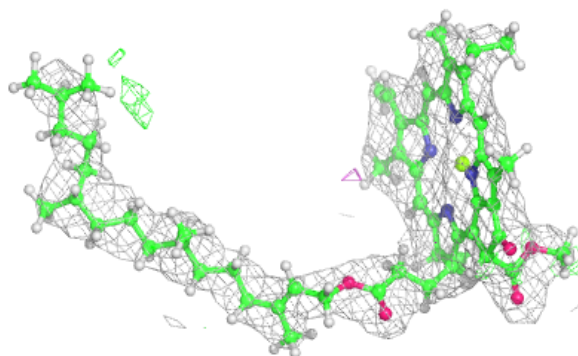


**Electron density around CLA b 606:**

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

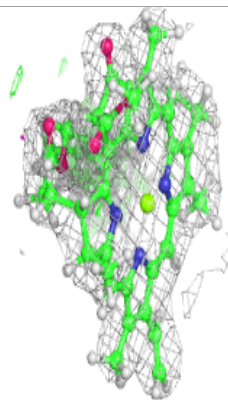
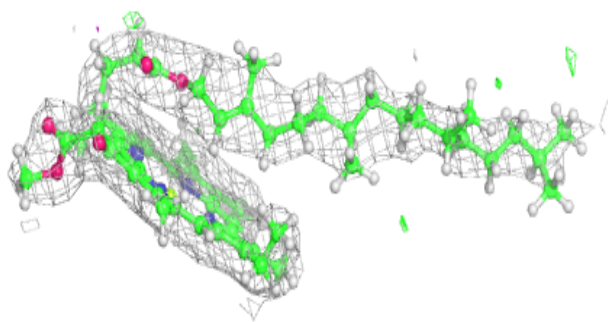
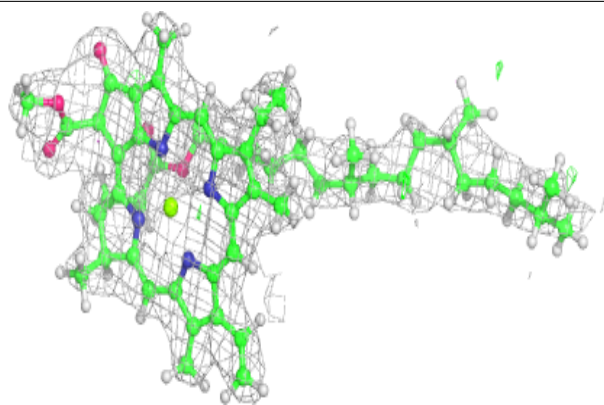
**Electron density around CLA b 609:**

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

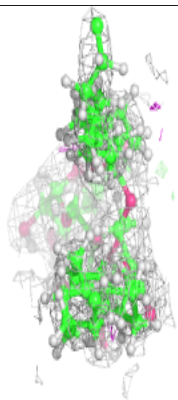
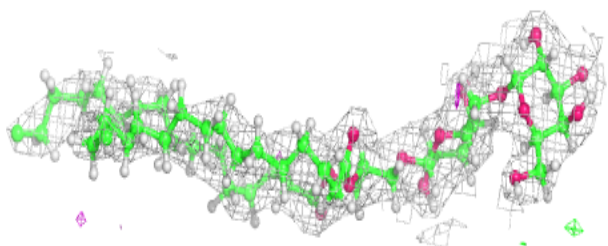
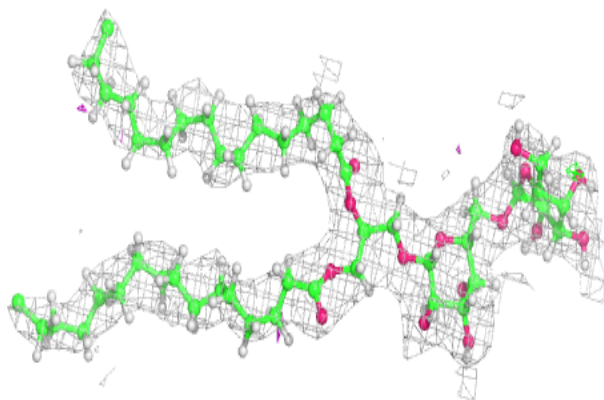


**Electron density around CLA b 614:**

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

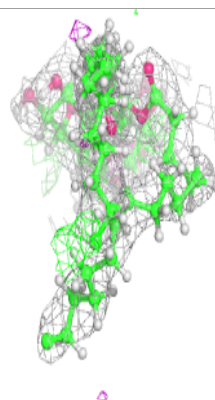
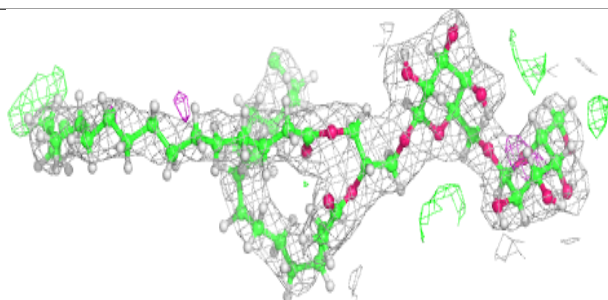
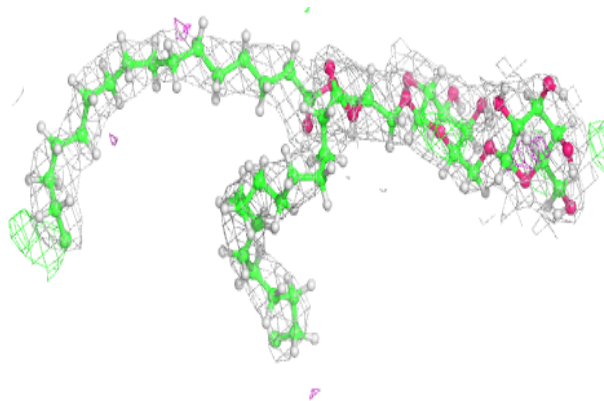
**Electron density around DGD C 518:**

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

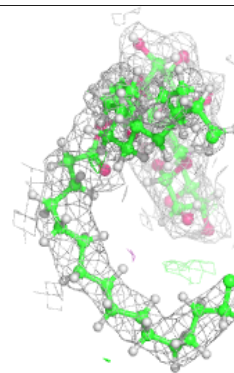
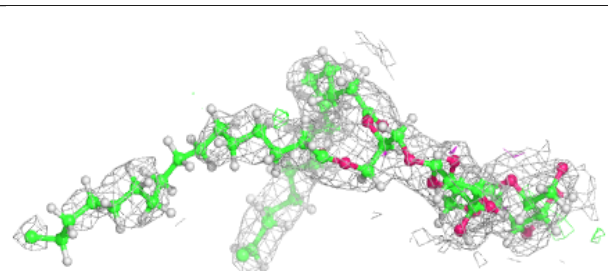
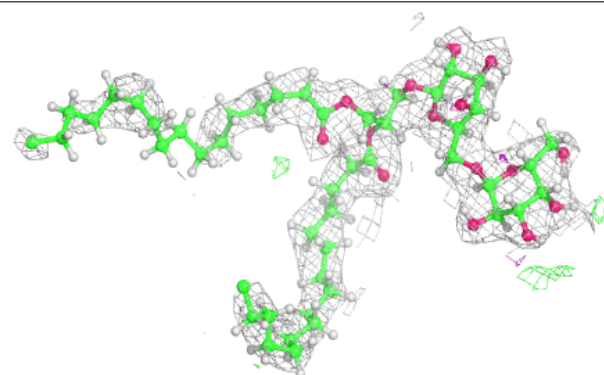


**Electron density around DGD H 102:**

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

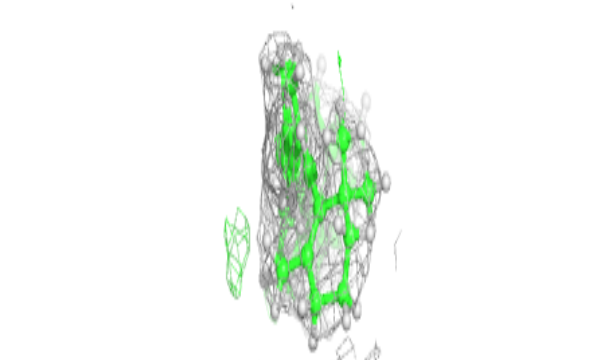
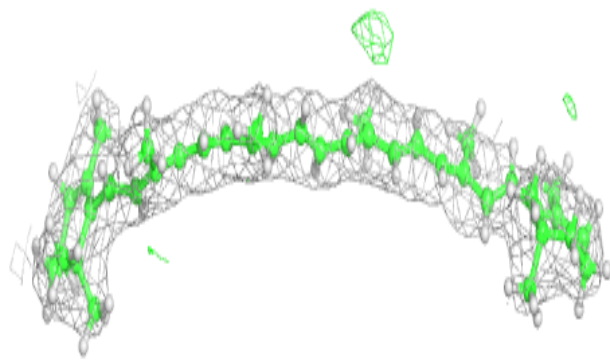
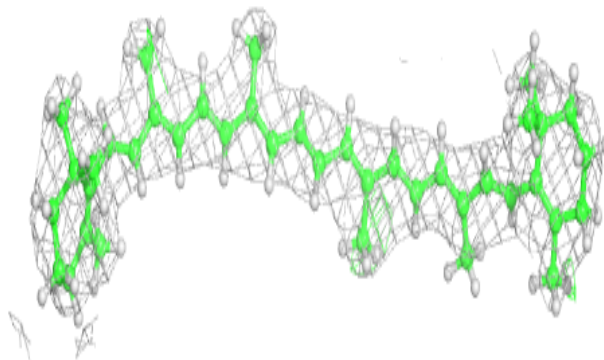
**Electron density around DGD c 517:**

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

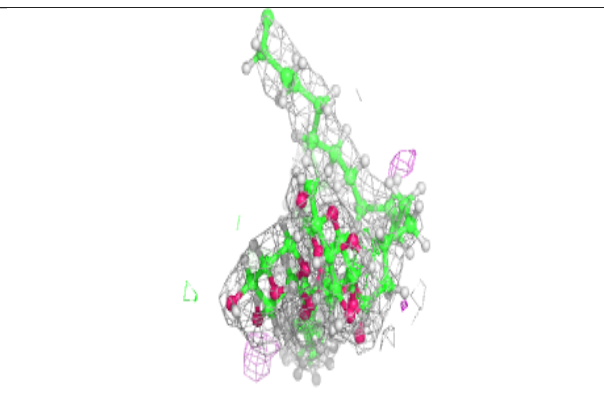
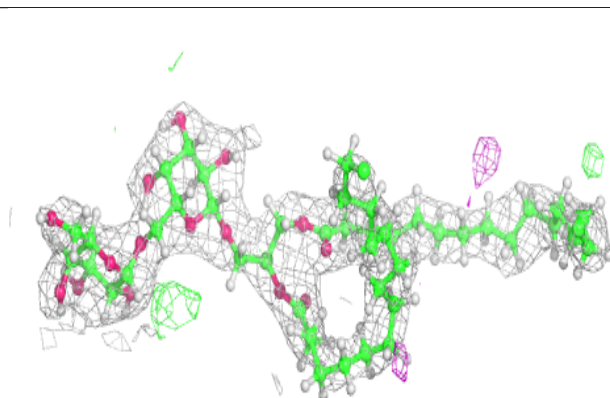
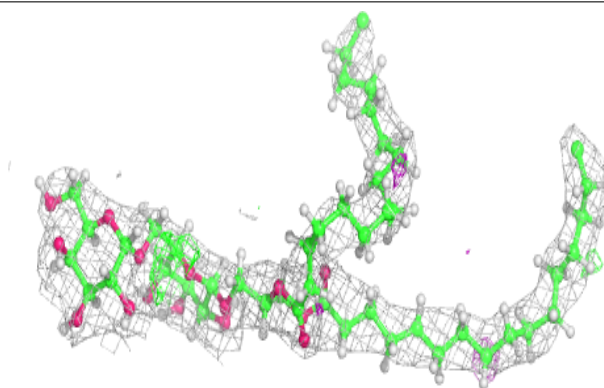


**Electron density around BCR T 101:**

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

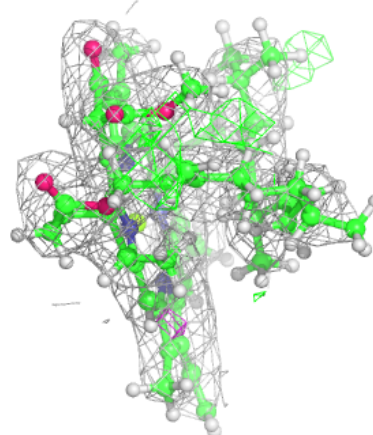
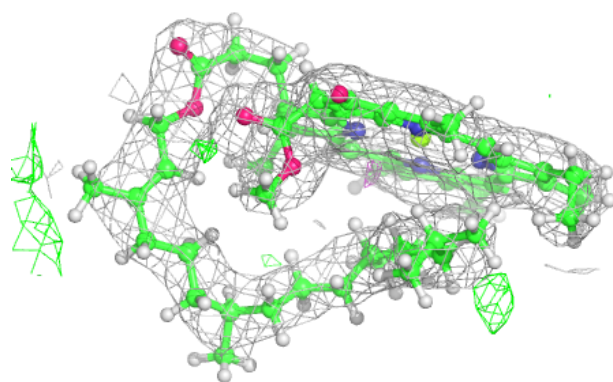
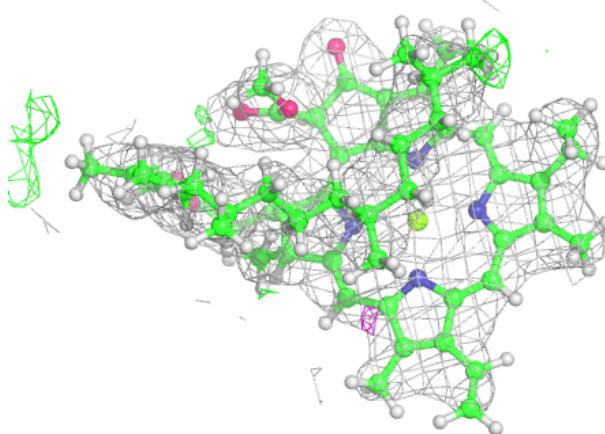
**Electron density around DGD h 102:**

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



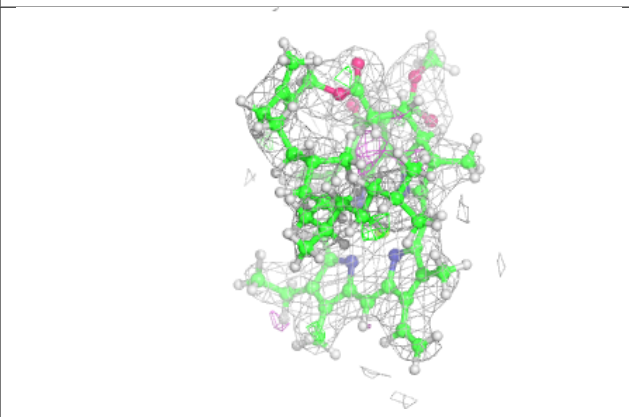
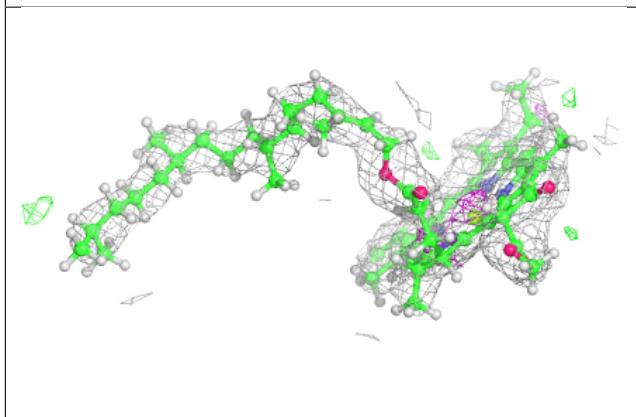
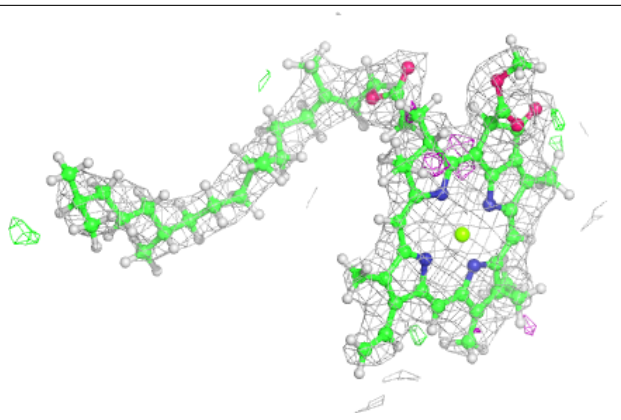
**Electron density around CLA C 510:**

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

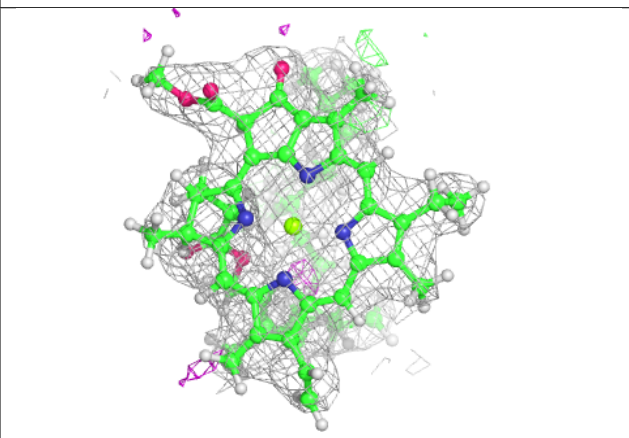
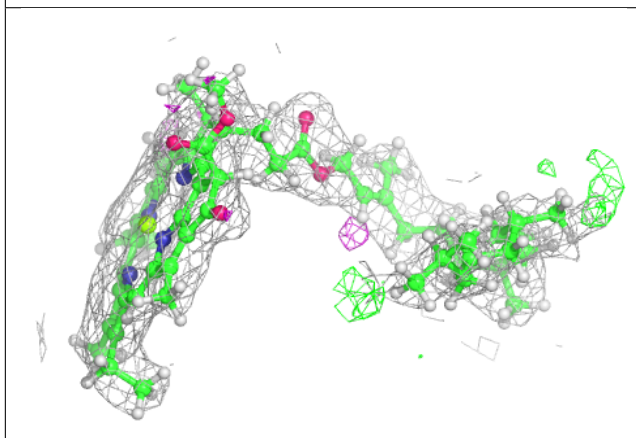
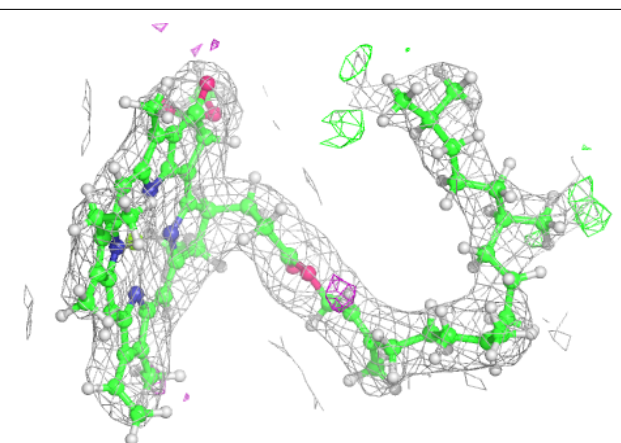


**Electron density around CLA C 511:**

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

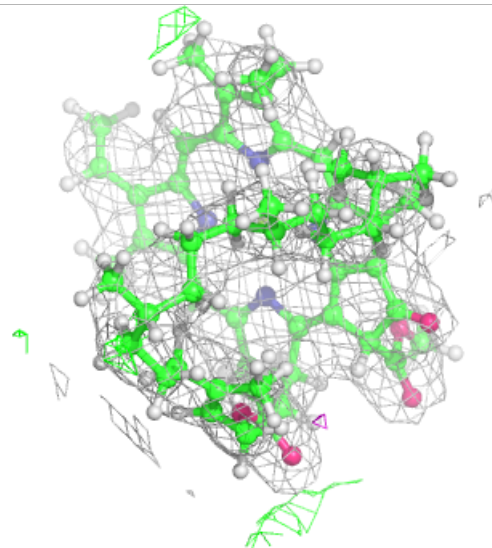
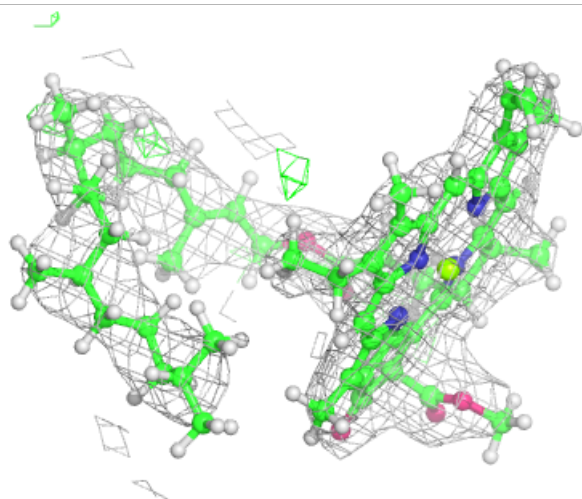
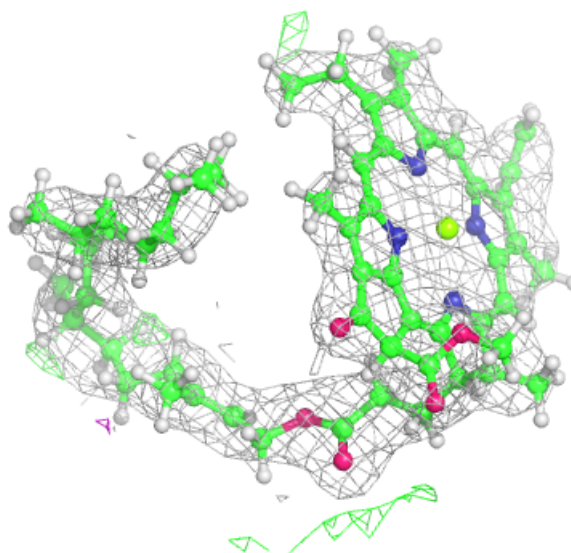
**Electron density around CLA B 605:**

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



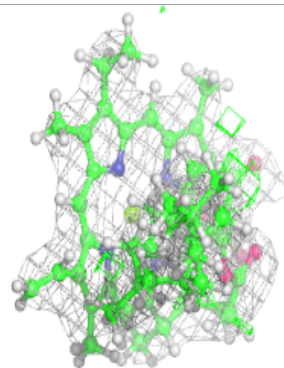
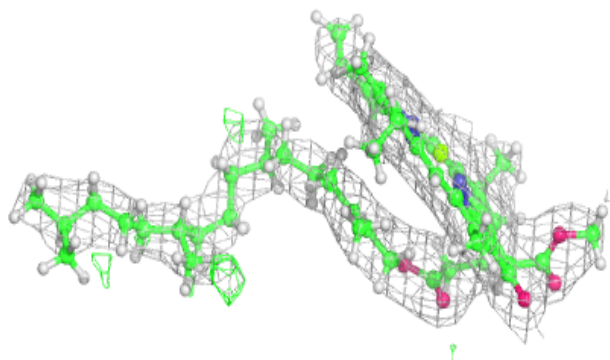
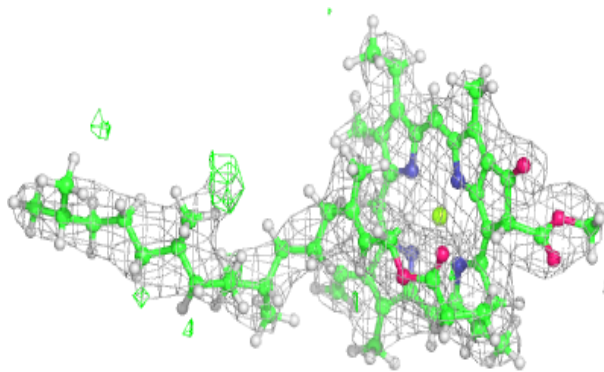
**Electron density around CLA C 503:**

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

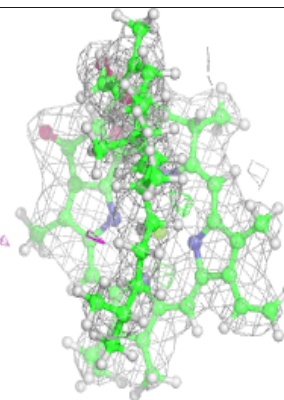
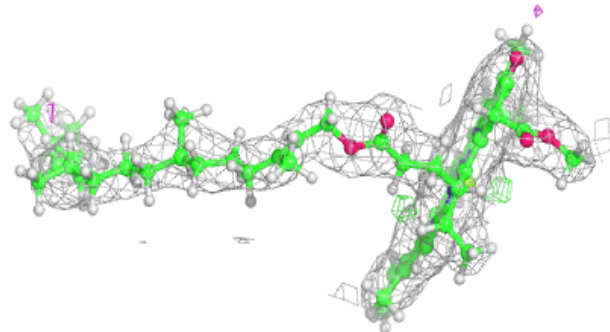
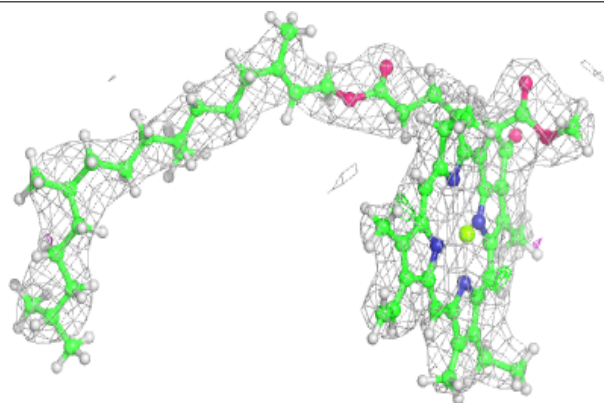


**Electron density around CLA c 505:**

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

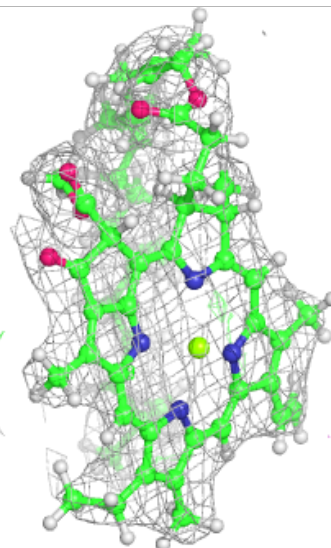
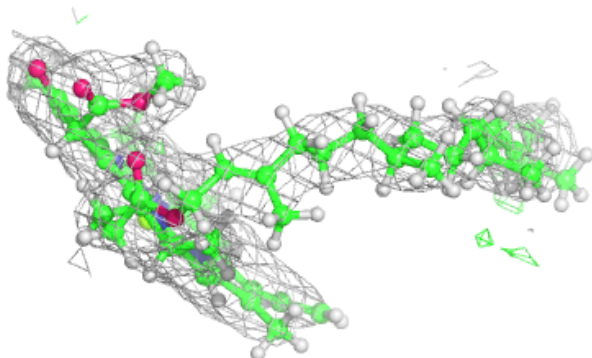
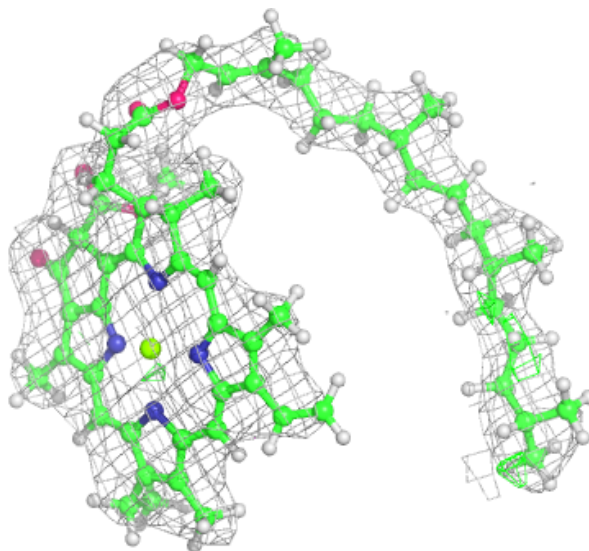
**Electron density around CLA B 608:**

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



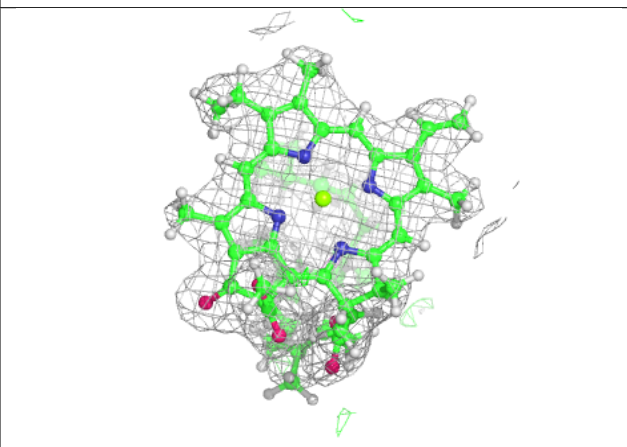
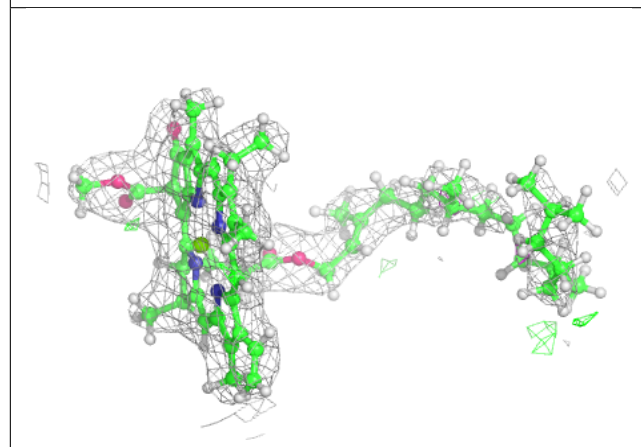
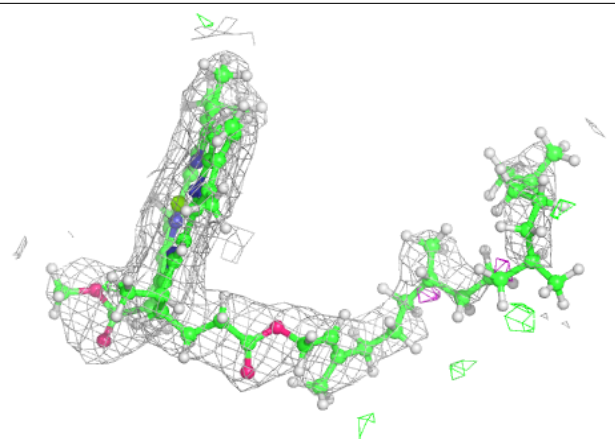
**Electron density around CLA c 507:**

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



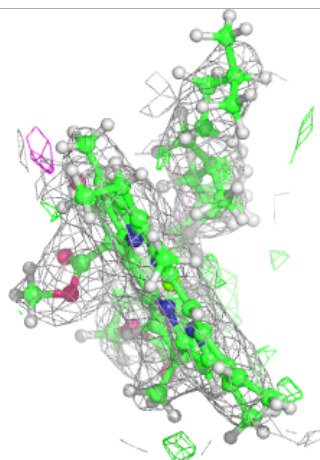
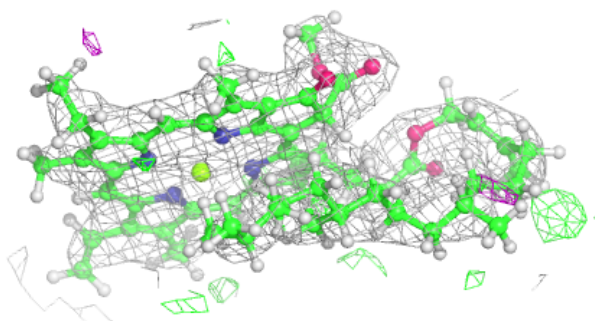
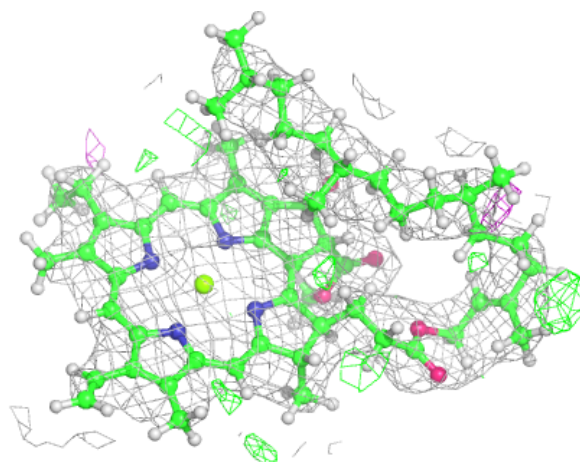
**Electron density around CLA C 506:**

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



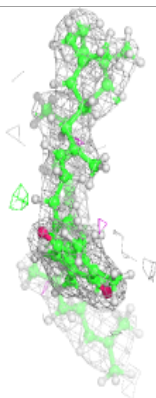
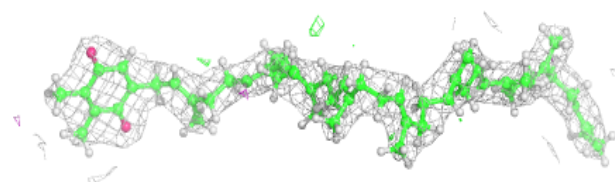
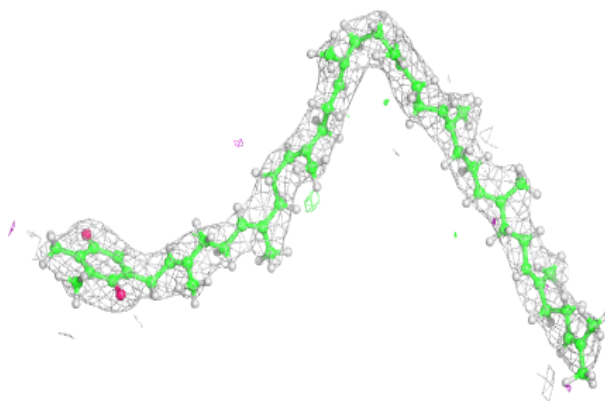
**Electron density around CLA c 509:**

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

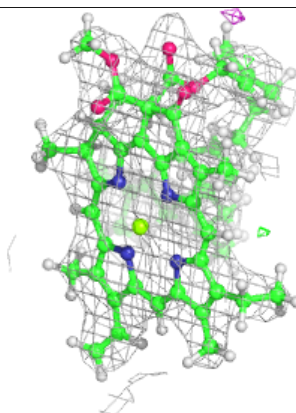
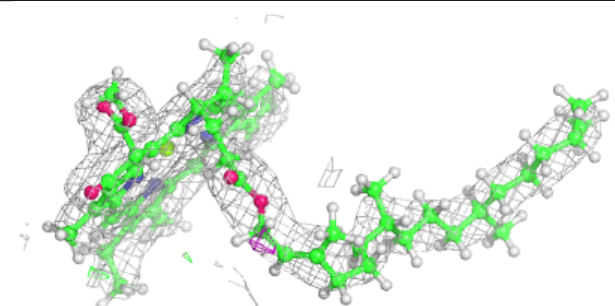
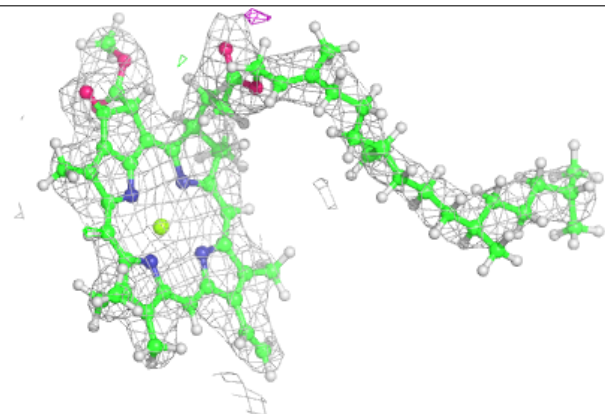


**Electron density around PL9 D 406:**

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

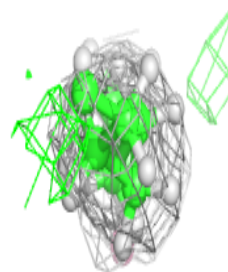
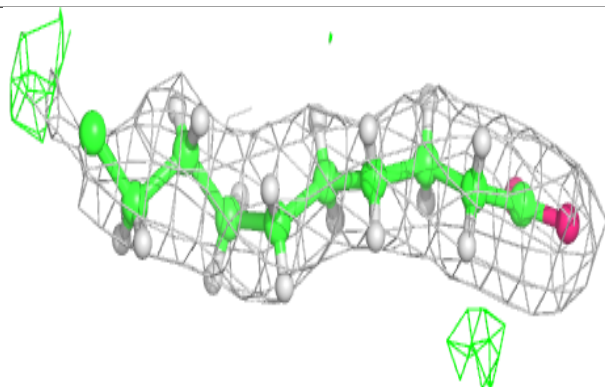
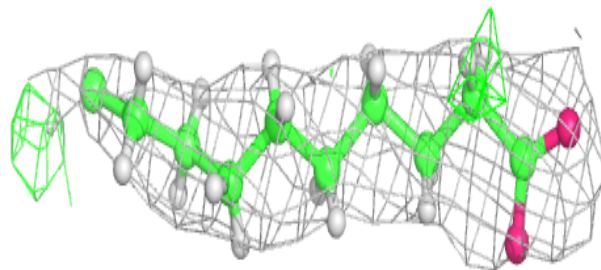
**Electron density around CLA c 511:**

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

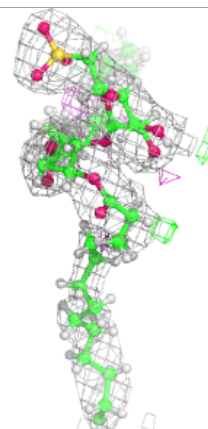
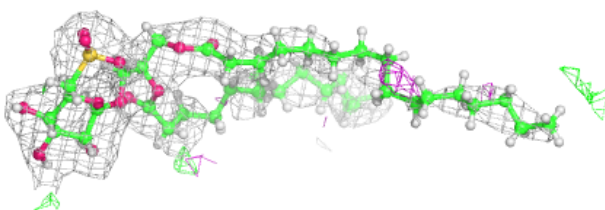
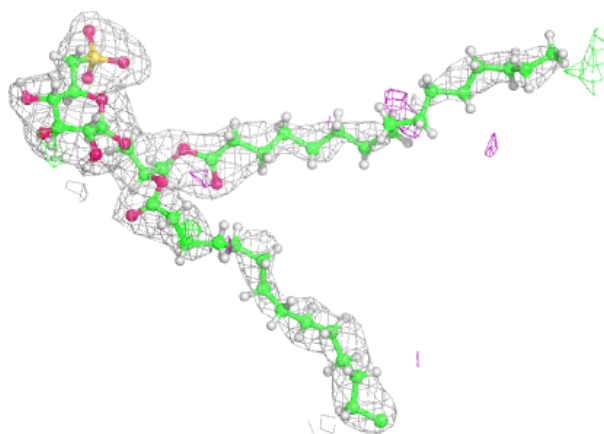


**Electron density around STE J 101:**

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

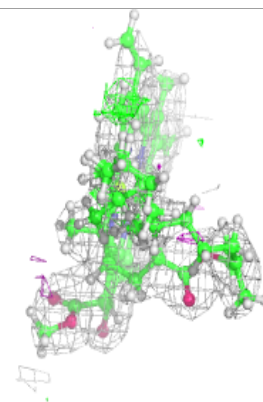
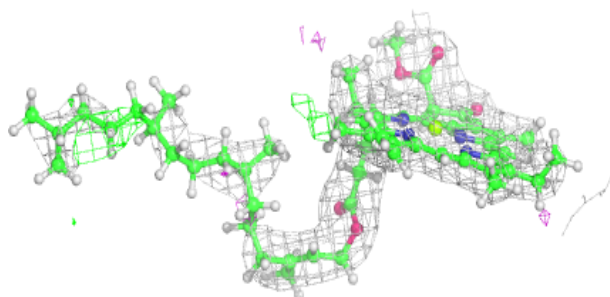
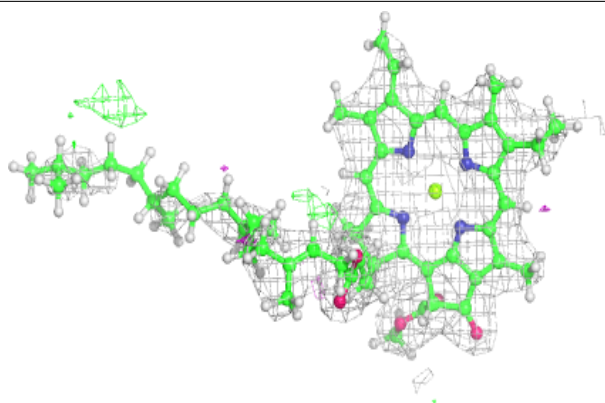
**Electron density around SQD A 613:**

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

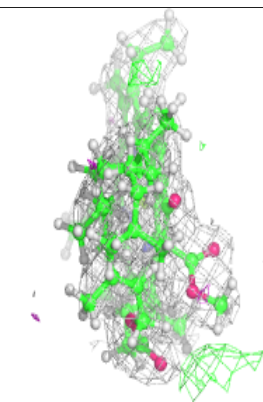
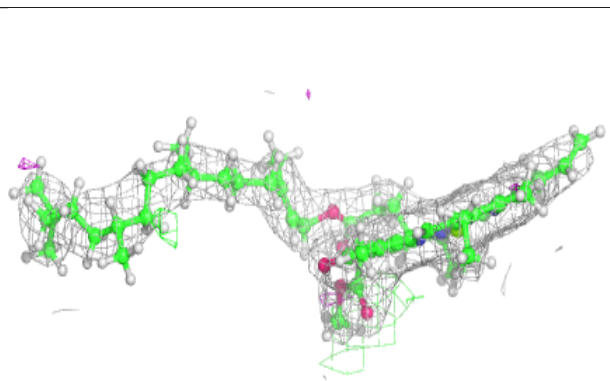
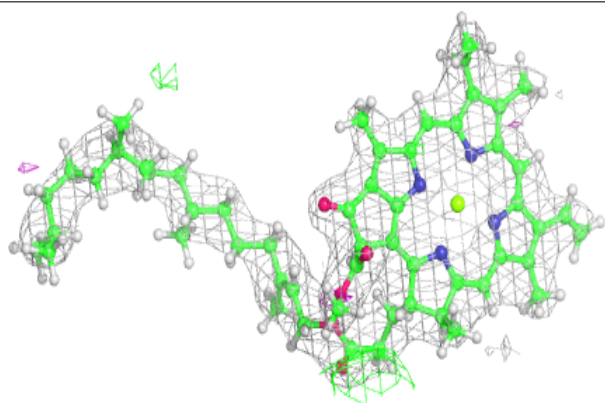


**Electron density around CLA a 605:**

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

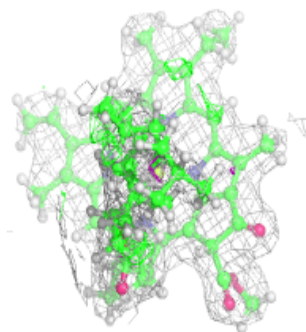
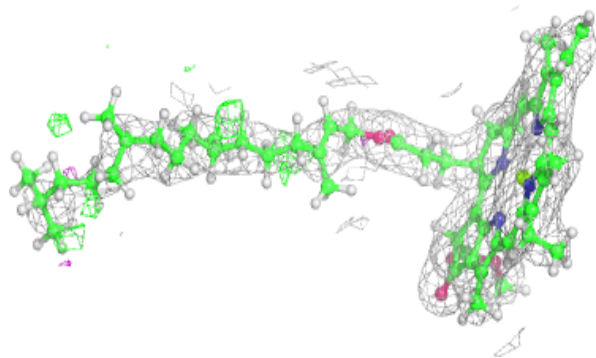
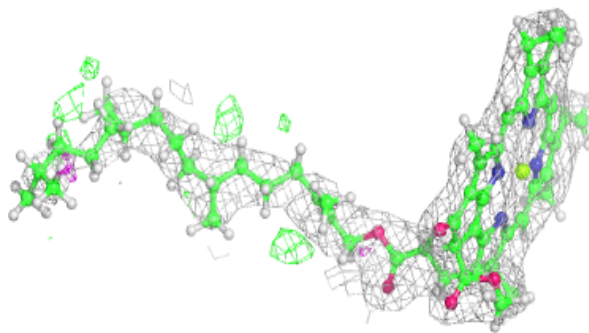
**Electron density around CLA B 601:**

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



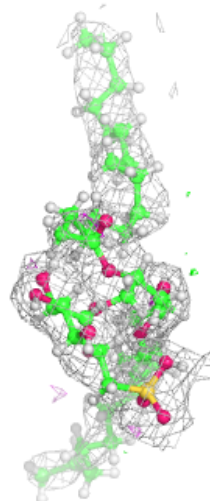
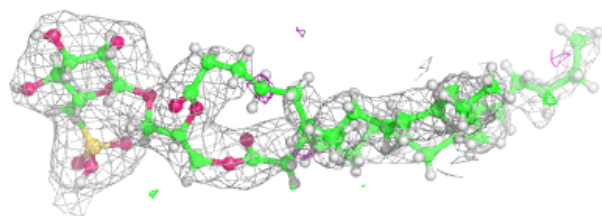
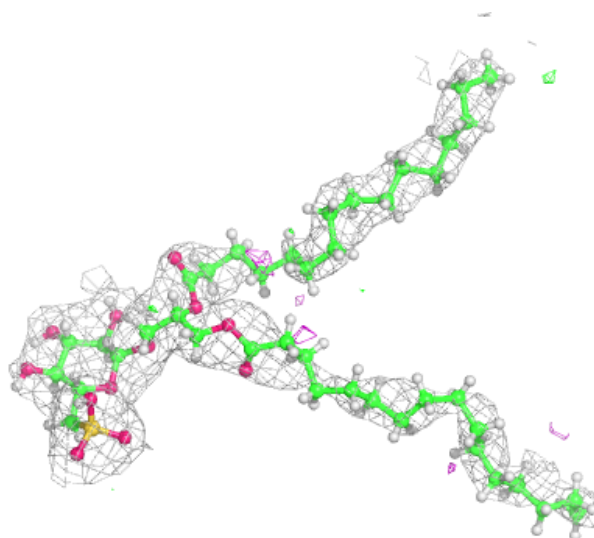
**Electron density around CLA B 603:**

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



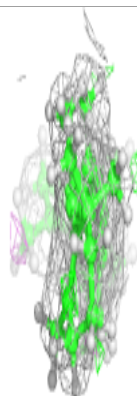
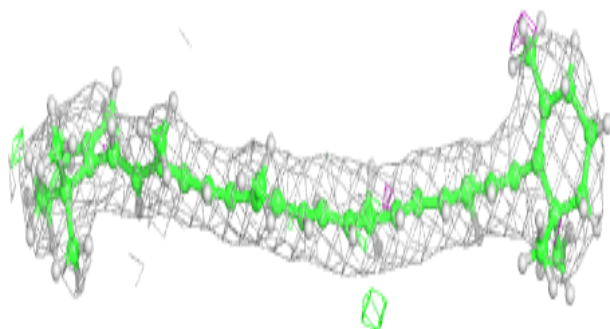
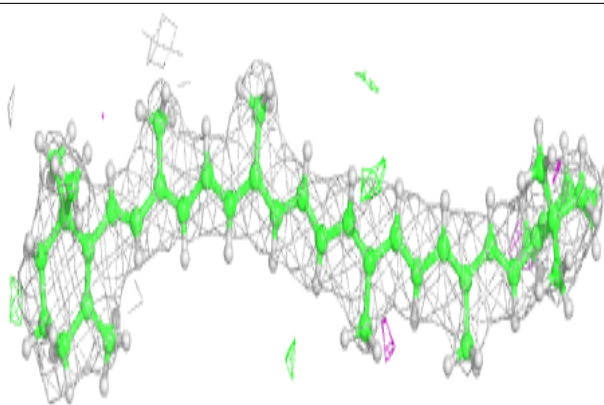
**Electron density around SQD a 615:**

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

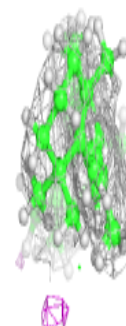
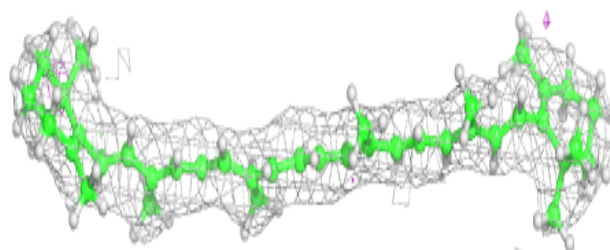
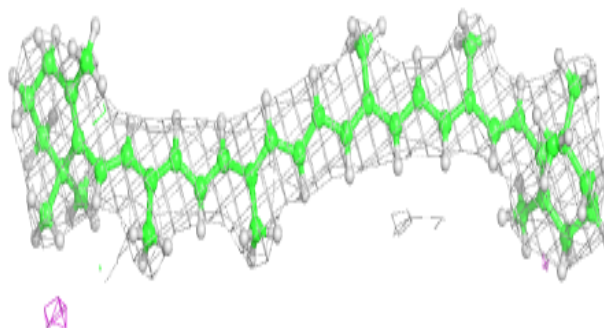


**Electron density around BCR B 616:**

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

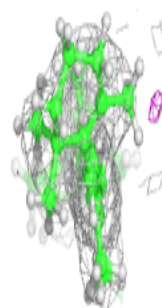
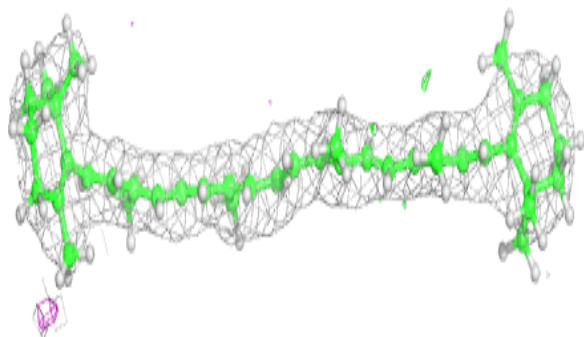
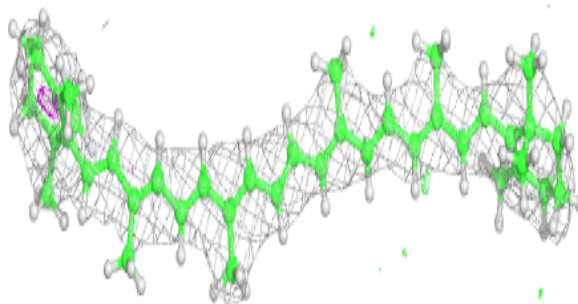
**Electron density around BCR B 618:**

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

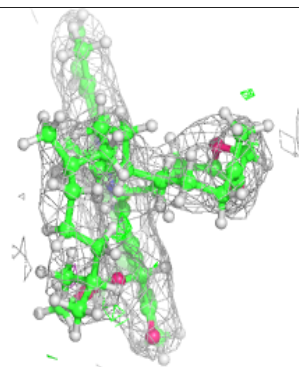
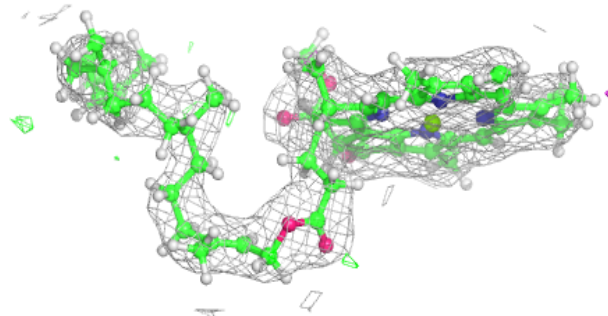
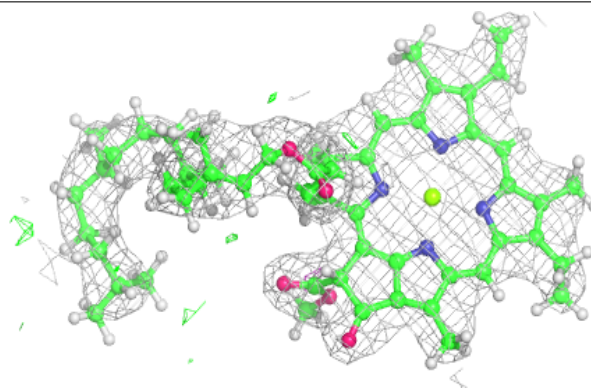


**Electron density around BCR c 515:**

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

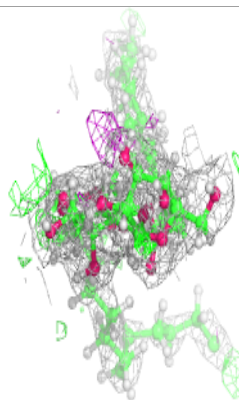
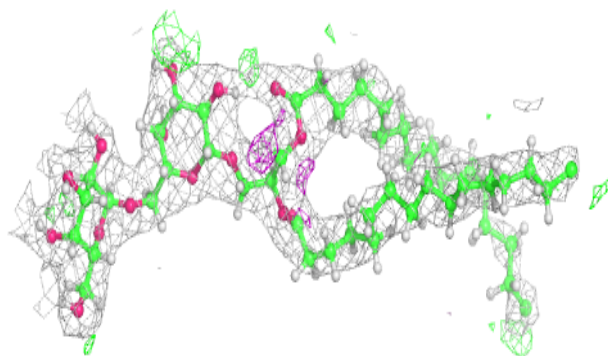
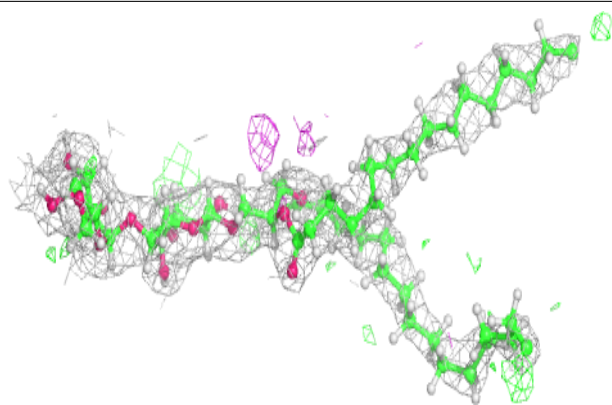
**Electron density around CLA b 612:**

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



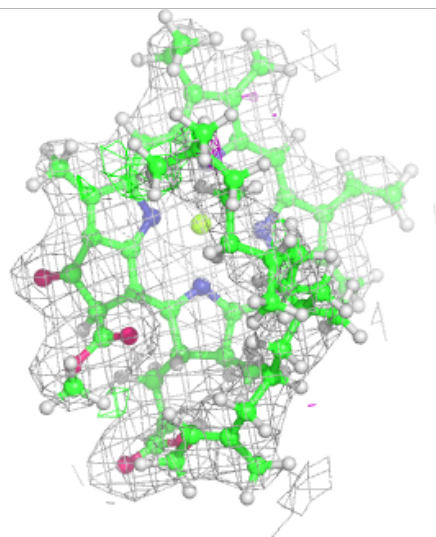
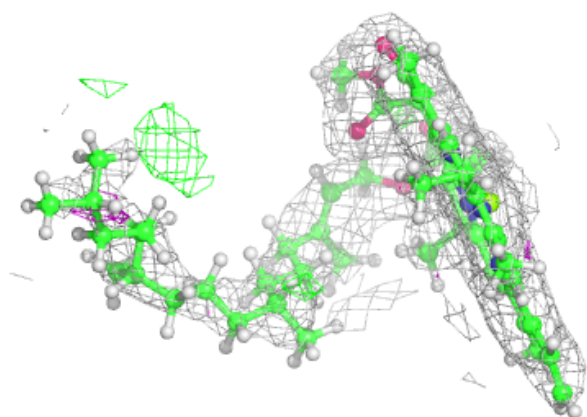
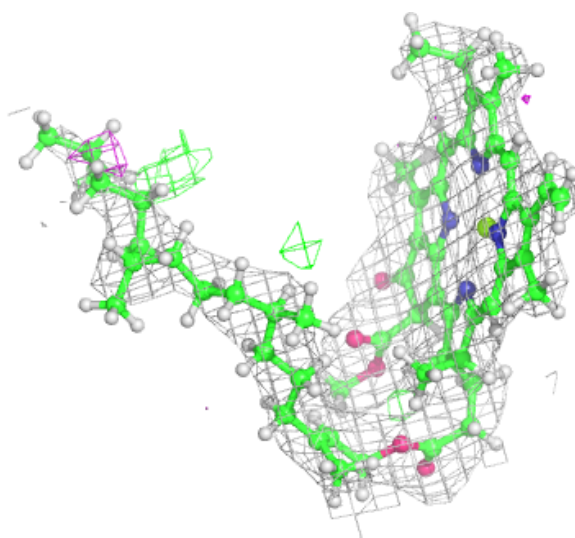
**Electron density around DGD c 516:**

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



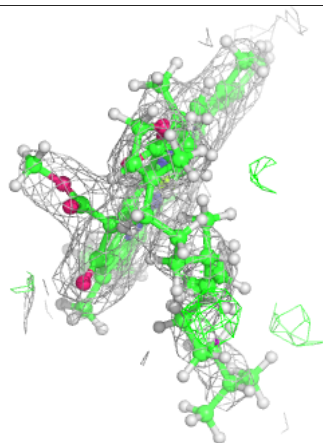
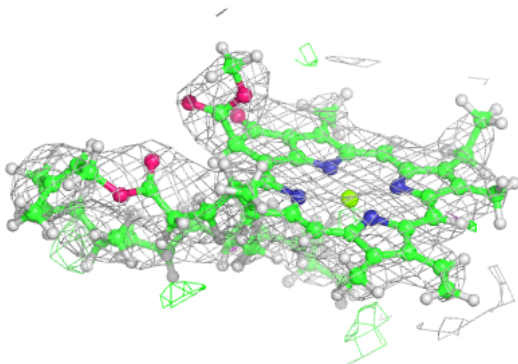
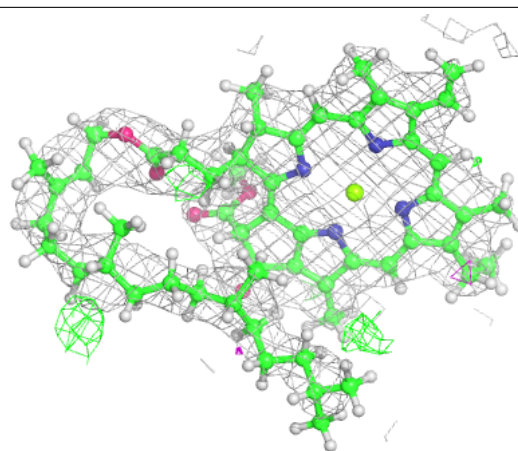
**Electron density around CLA b 613:**

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

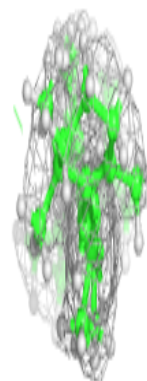
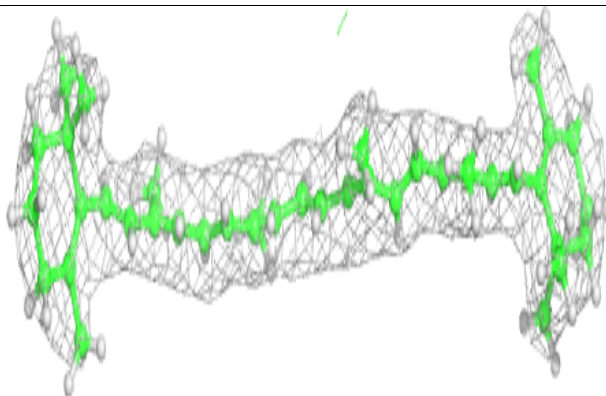
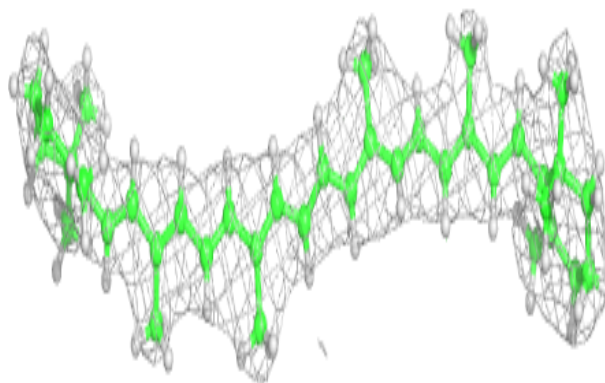


**Electron density around CLA C 509:**

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

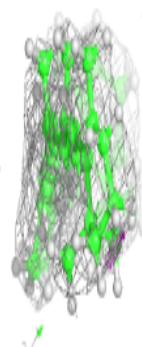
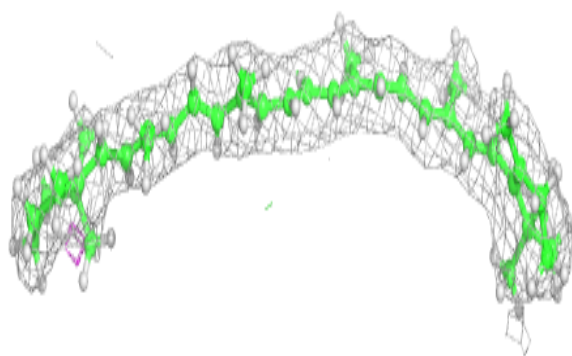
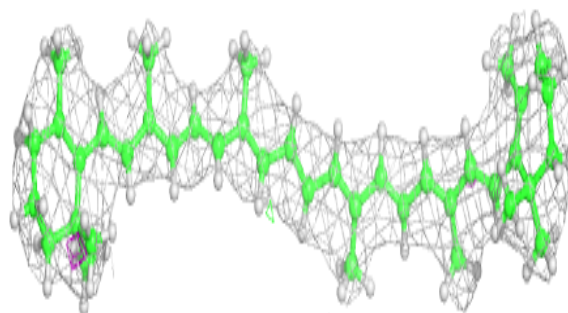
**Electron density around BCR A 608:**

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

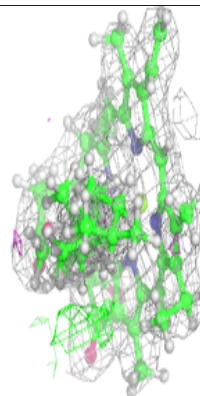
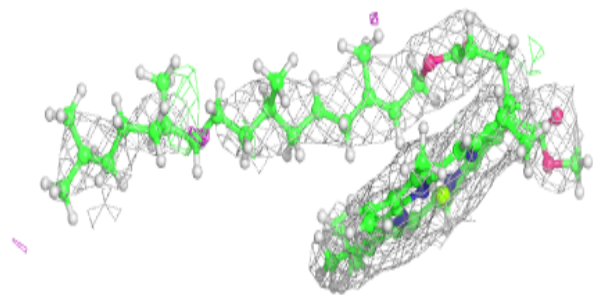
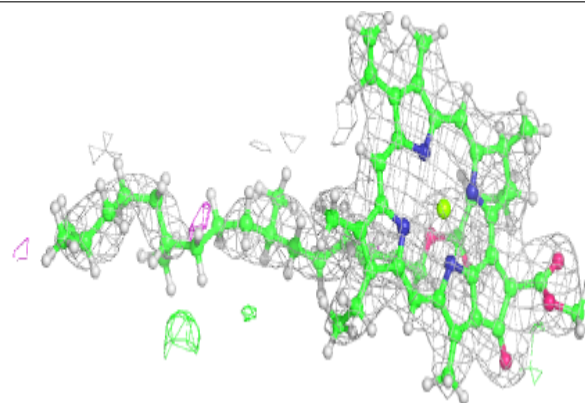


**Electron density around BCR t 101:**

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

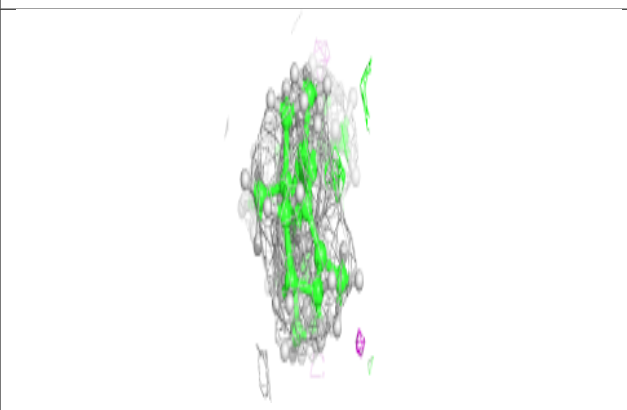
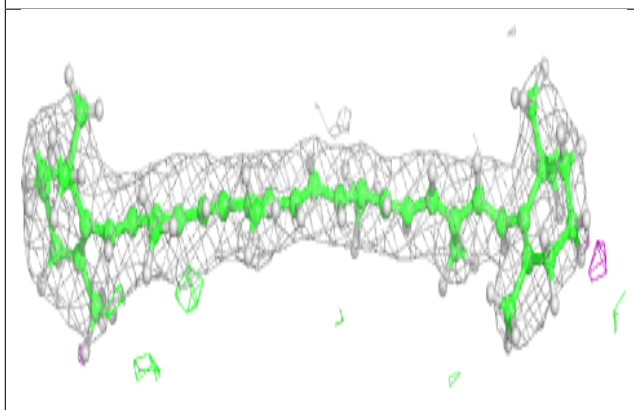
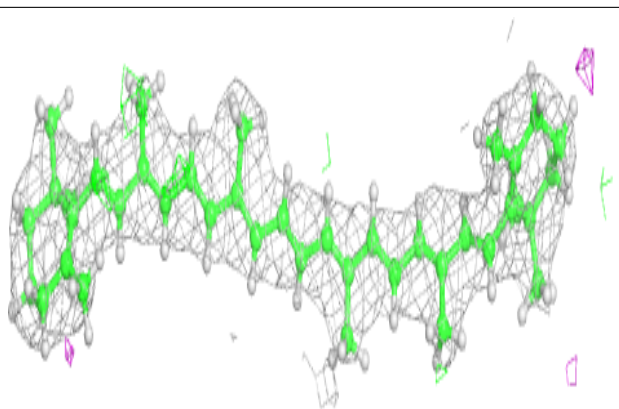
**Electron density around CLA B 613:**

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

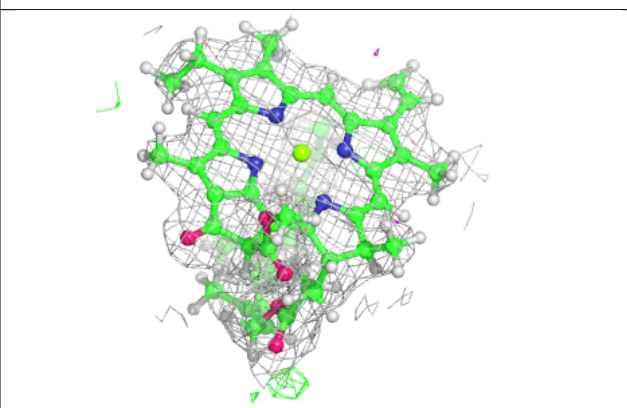
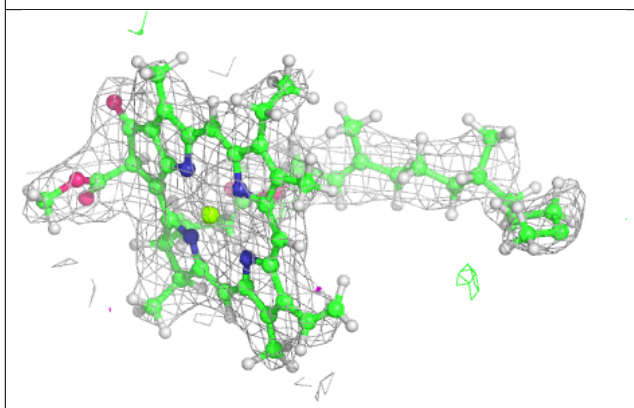
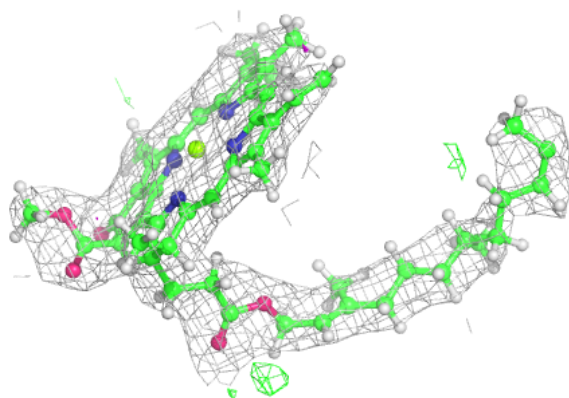


**Electron density around BCR B 617:**

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

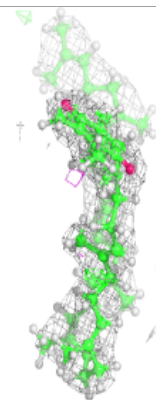
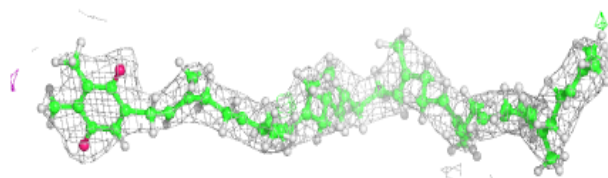
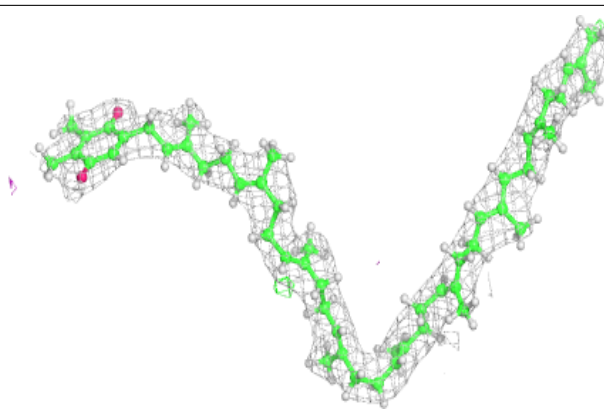
**Electron density around CLA C 504:**

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



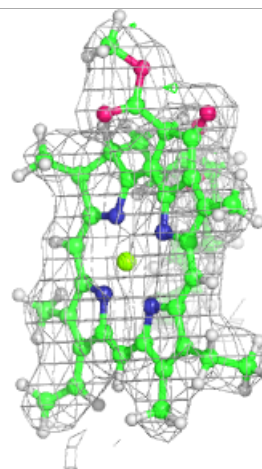
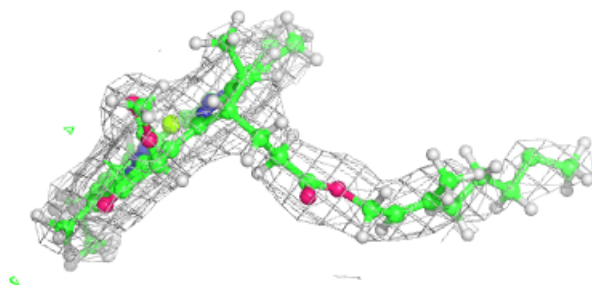
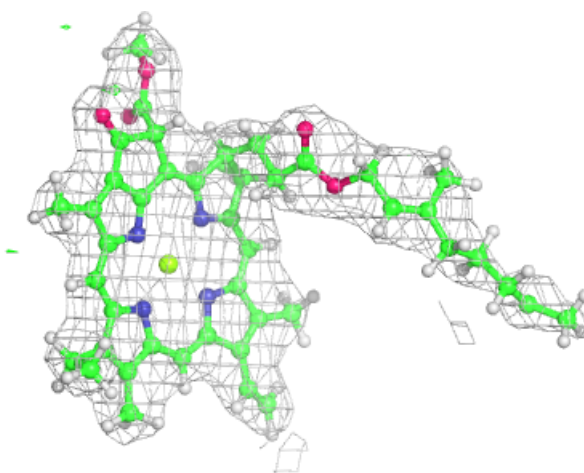
**Electron density around PL9 d 405:**

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



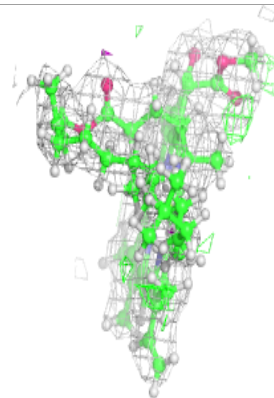
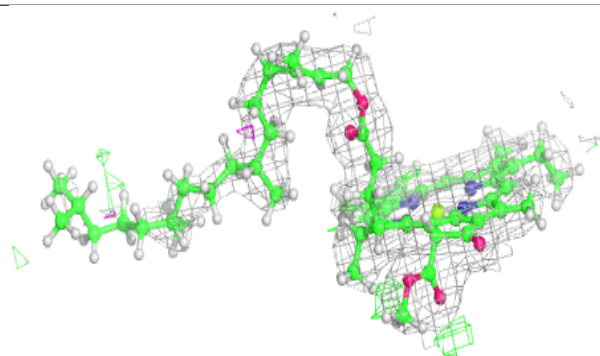
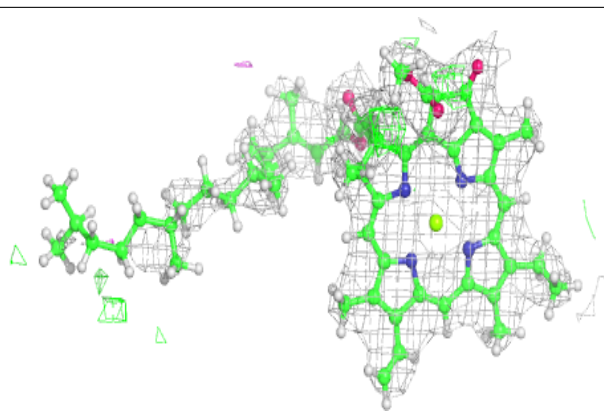
**Electron density around CLA A 607:**

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

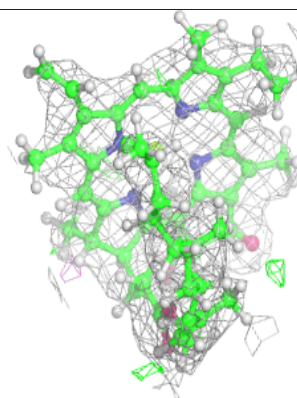
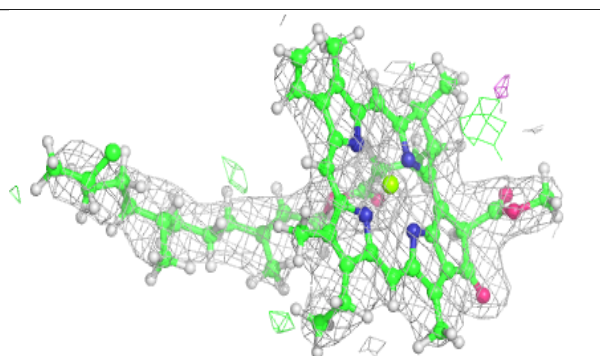
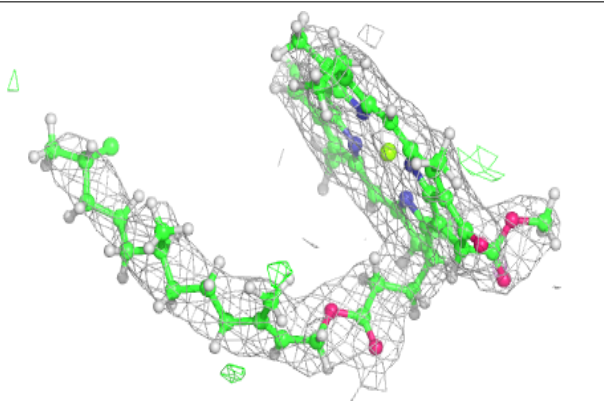


**Electron density around CLA A 605:**

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

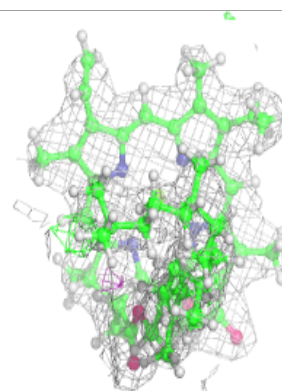
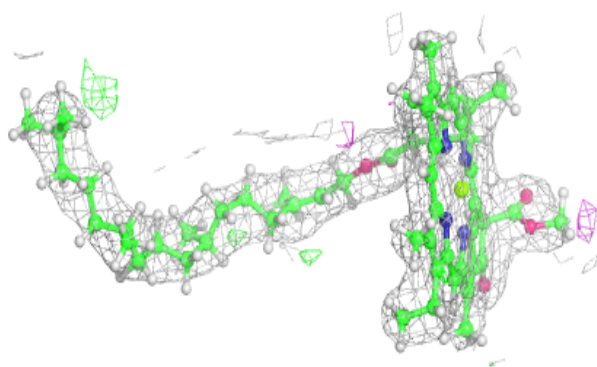
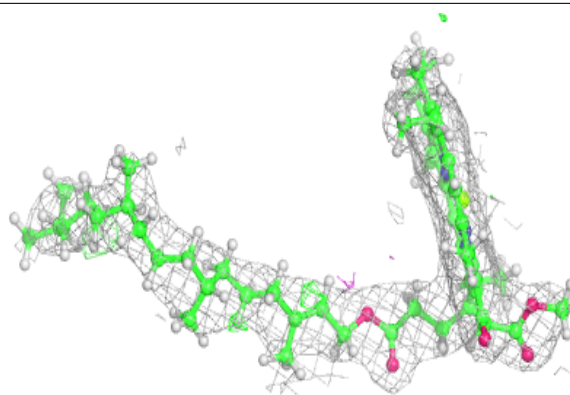
**Electron density around CLA c 504:**

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

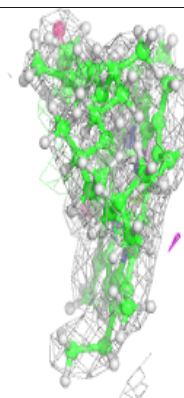
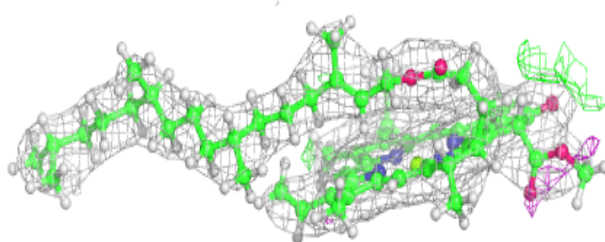
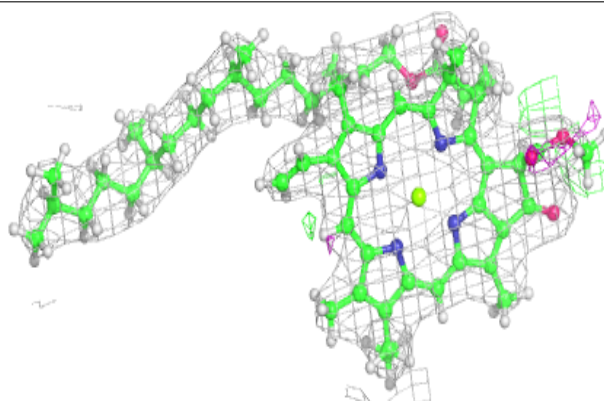


**Electron density around CLA b 605:**

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

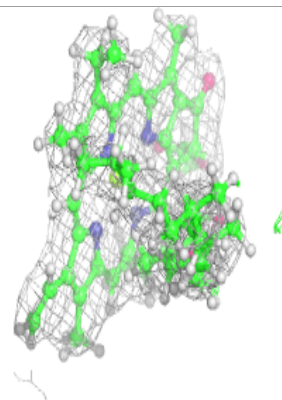
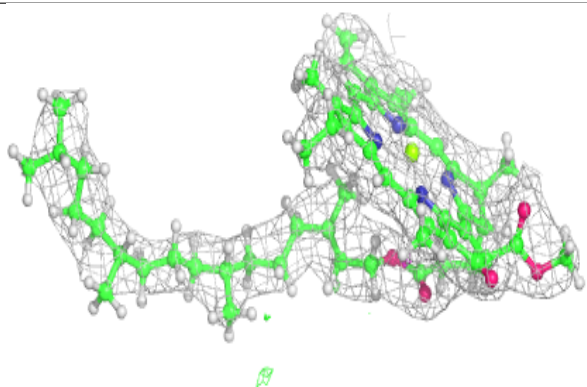
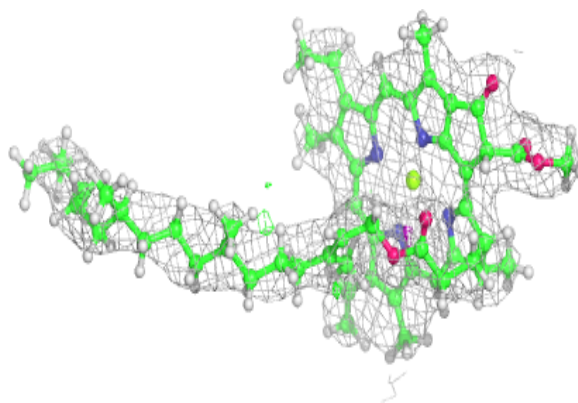
**Electron density around CLA C 501:**

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

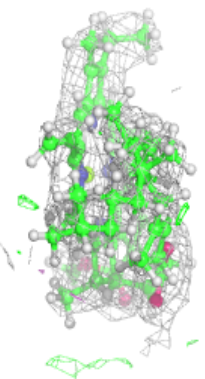
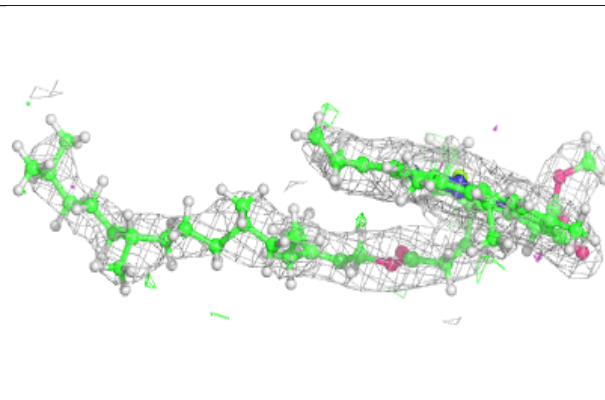
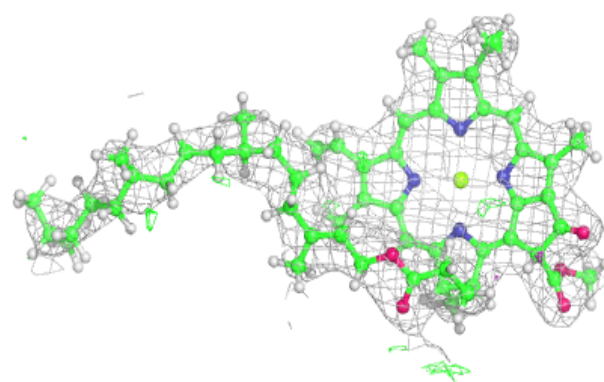


**Electron density around CLA b 608:**

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

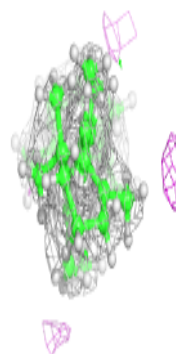
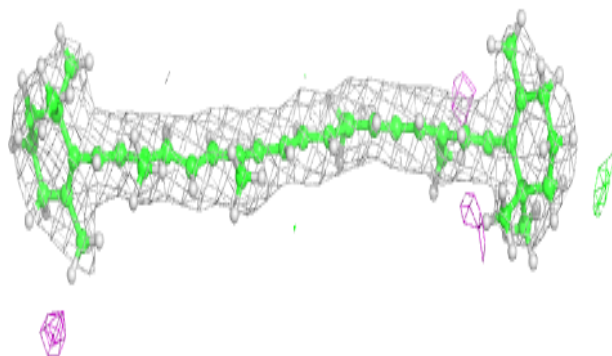
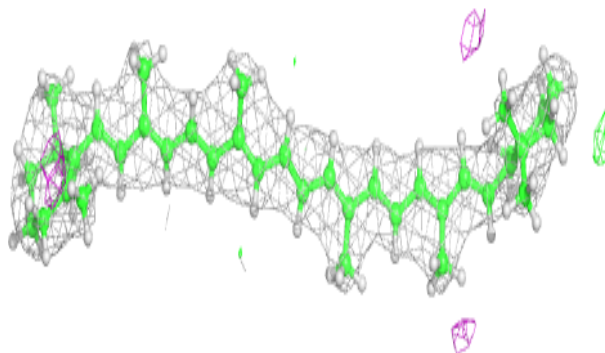
**Electron density around CLA B 602:**

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



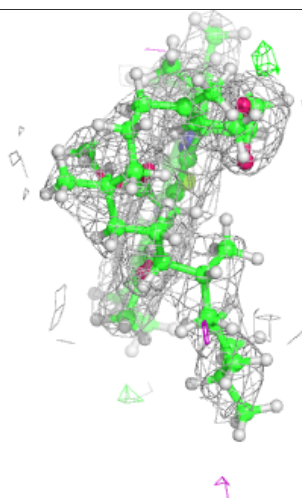
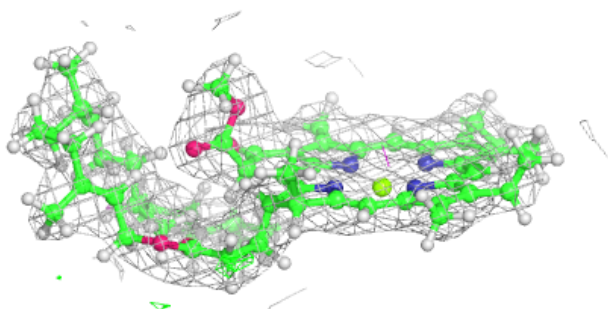
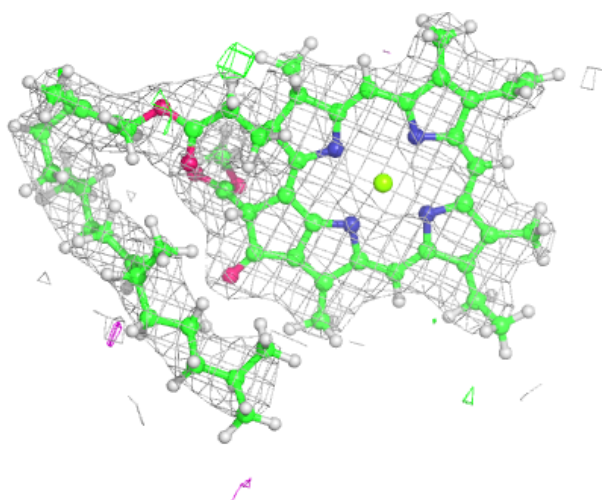
**Electron density around BCR a 608:**

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



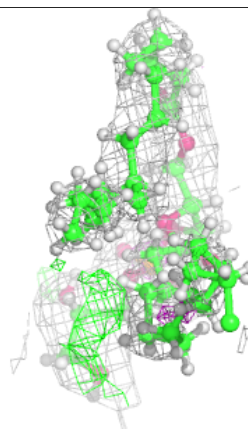
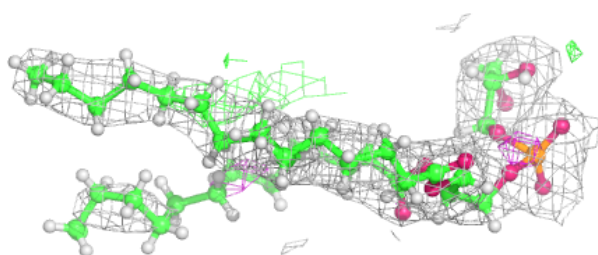
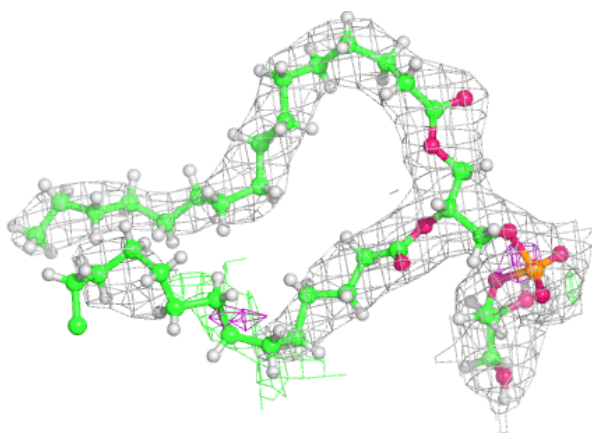
**Electron density around CLA b 610:**

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

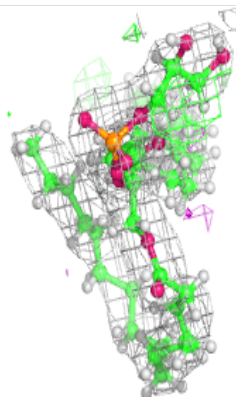
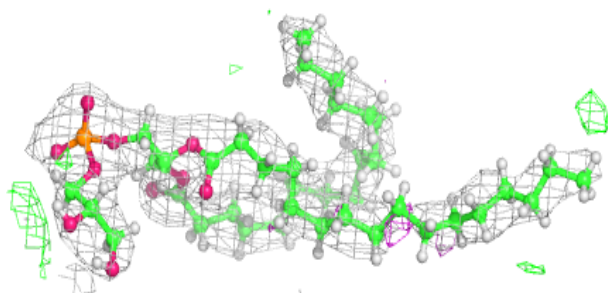
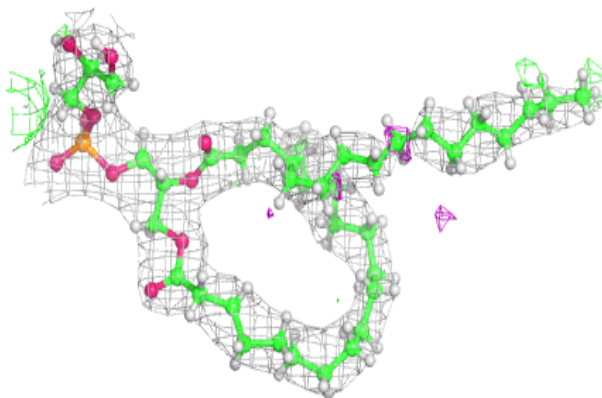


**Electron density around LHG D 410:**

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

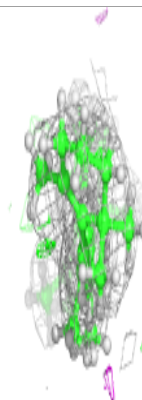
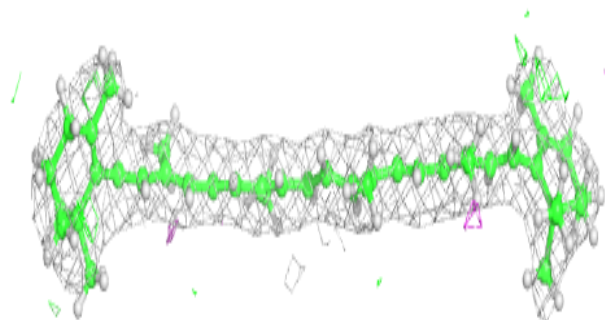
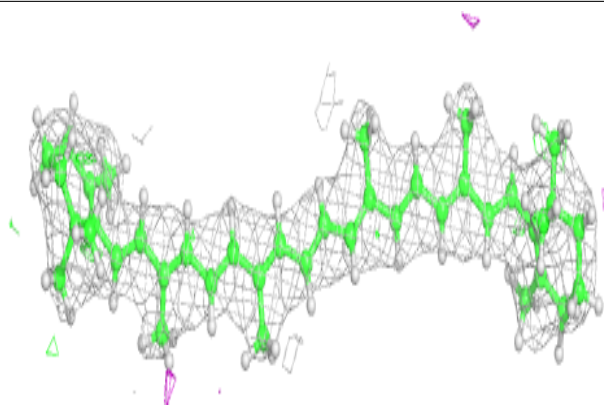
**Electron density around LHG a 614:**

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



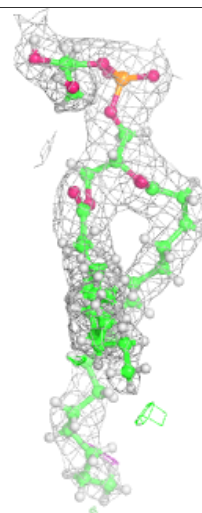
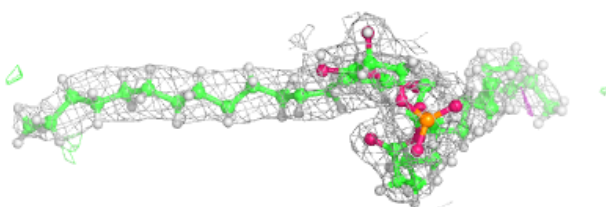
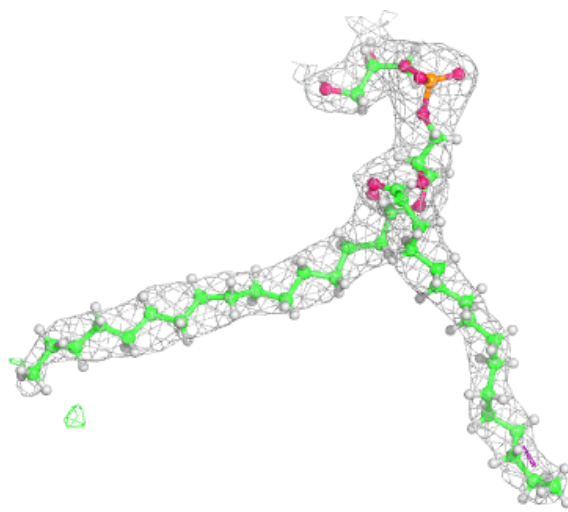
**Electron density around BCR b 618:**

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



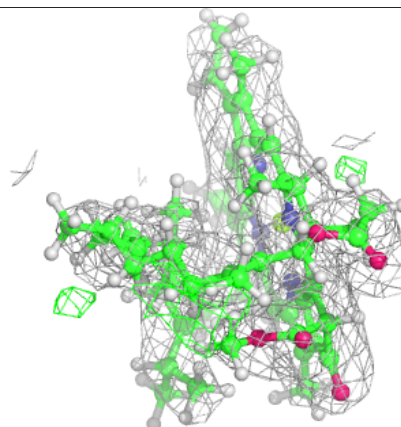
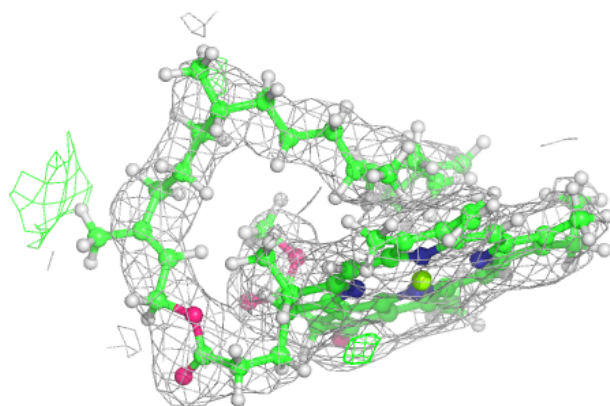
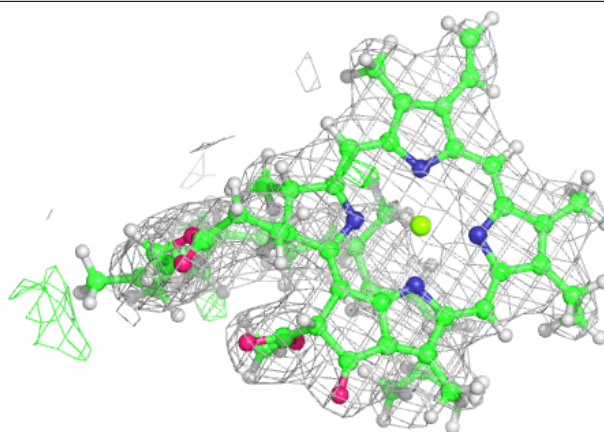
**Electron density around LHG 1 101:**

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

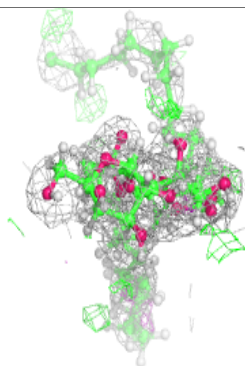
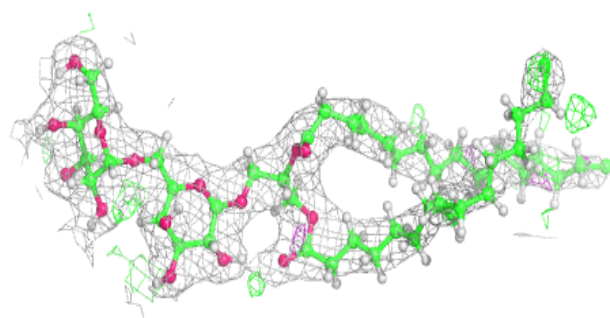
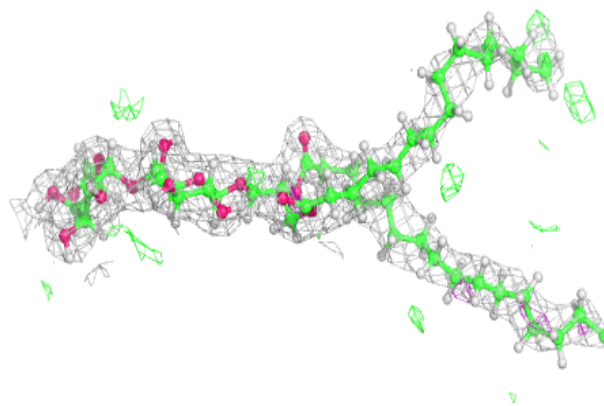


**Electron density around CLA c 510:**

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

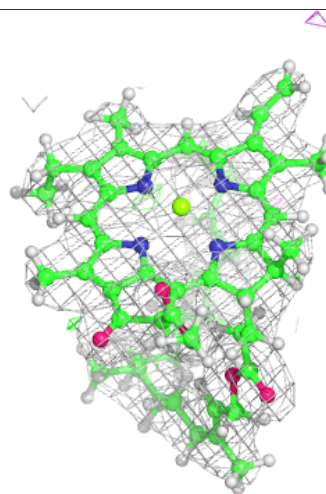
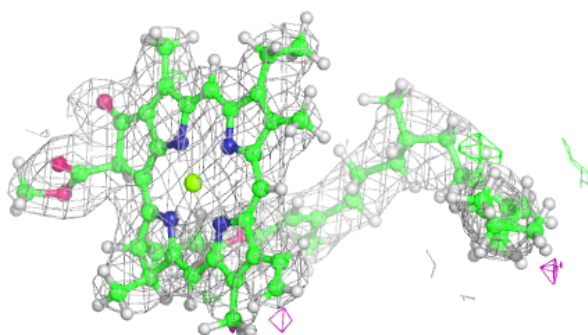
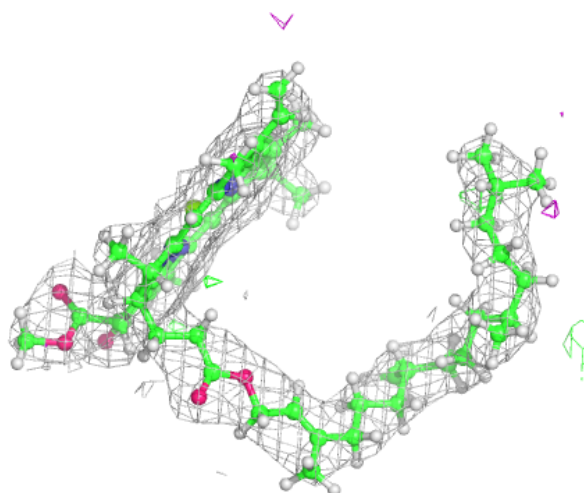
**Electron density around DGD C 516:**

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



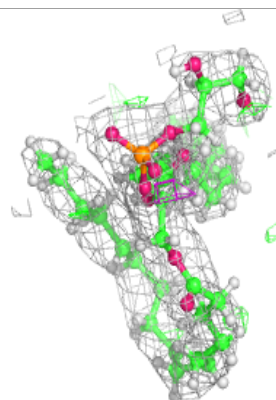
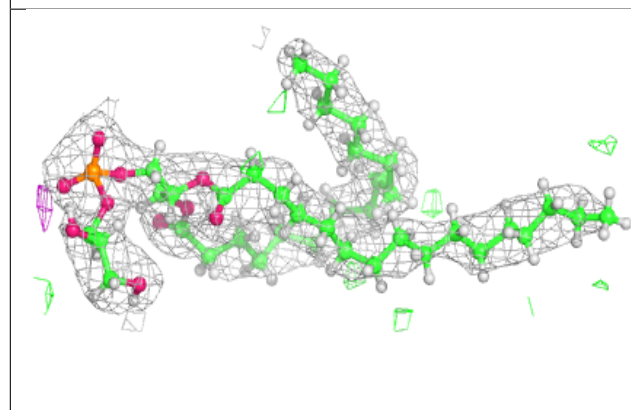
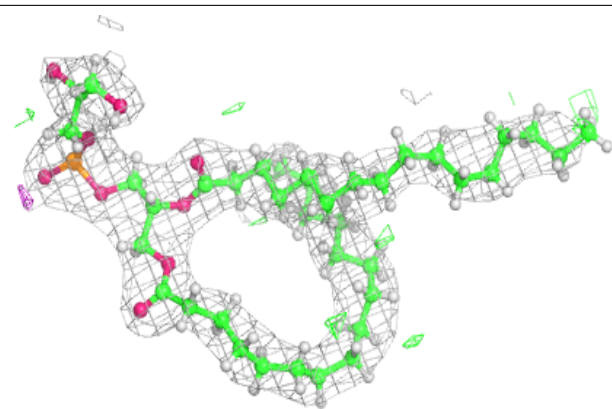
**Electron density around CLA b 611:**

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



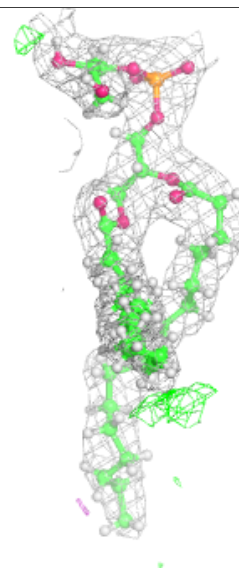
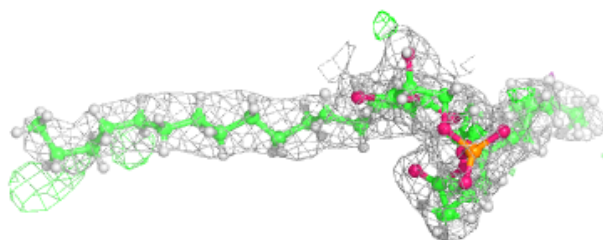
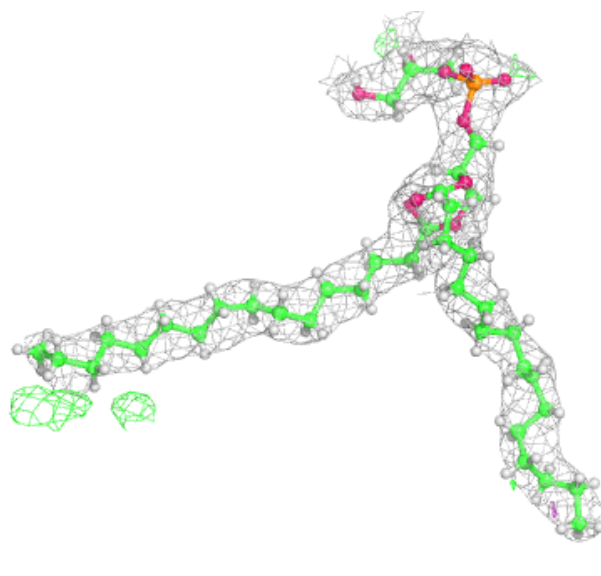
**Electron density around LHG D 413:**

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



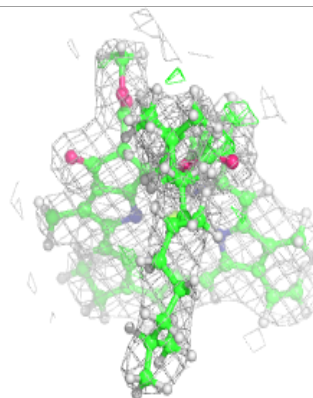
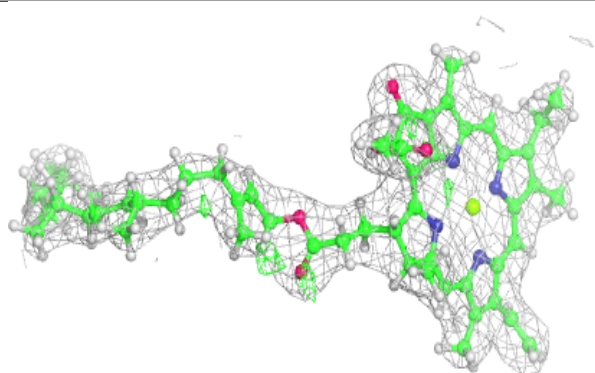
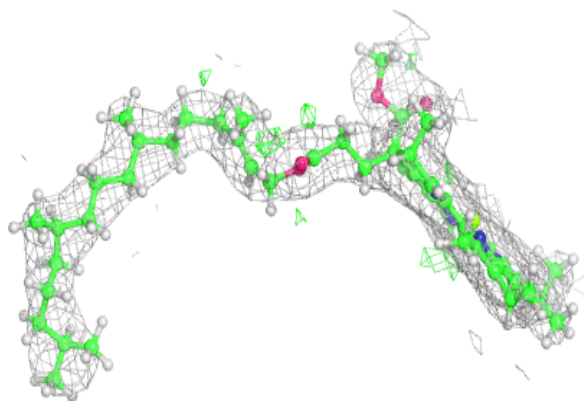
**Electron density around LHG L 101:**

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

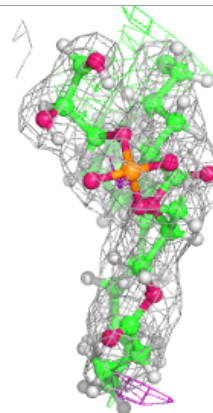
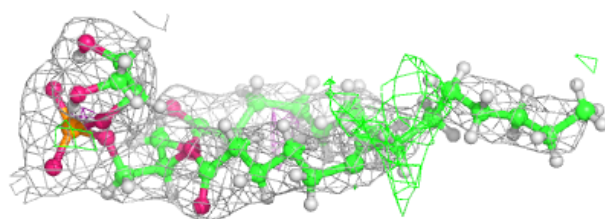
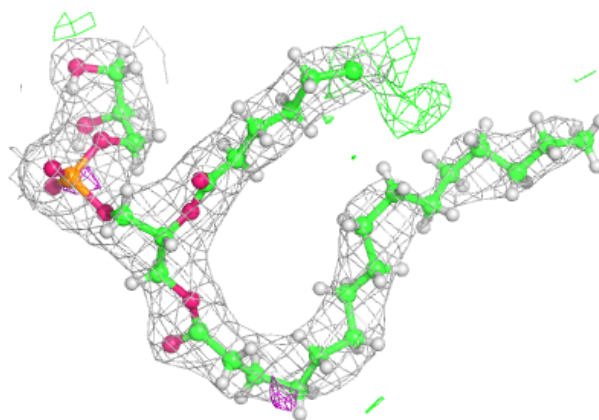


**Electron density around CLA D 403:**

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

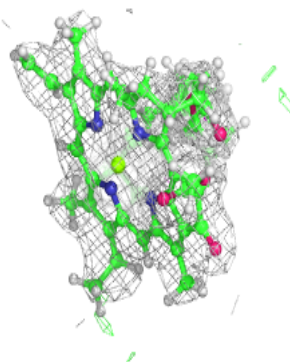
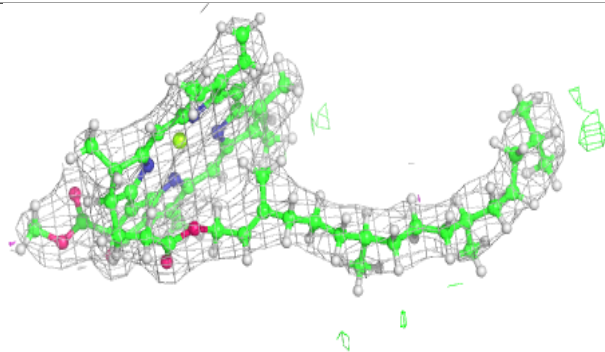
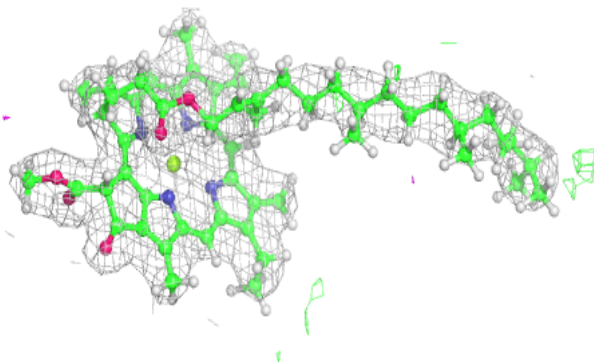
**Electron density around LHG d 407:**

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

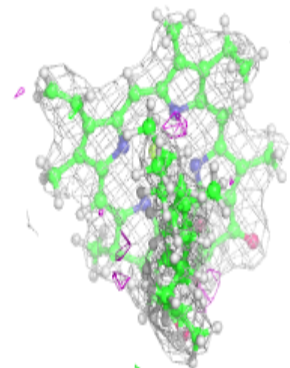
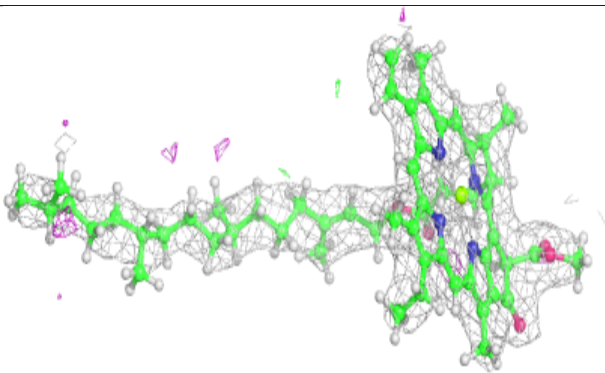
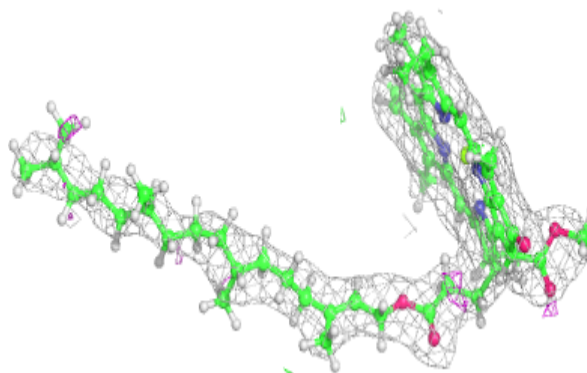


**Electron density around CLA B 607:**

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

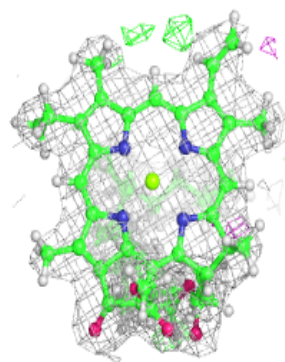
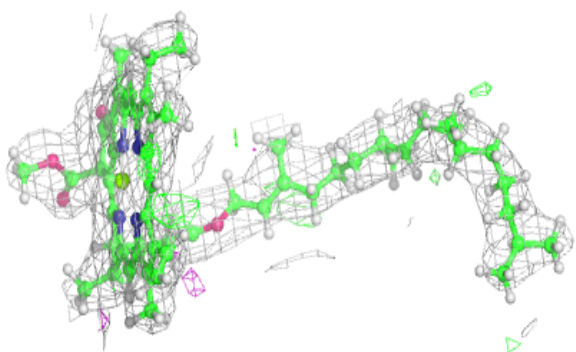
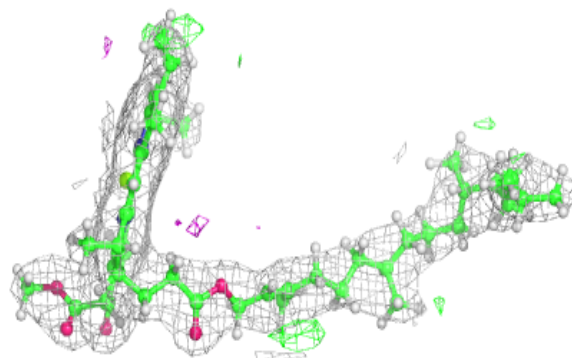
**Electron density around CLA b 607:**

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

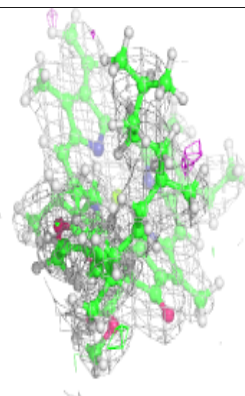
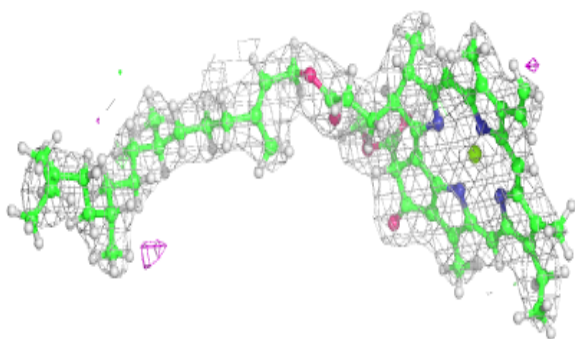
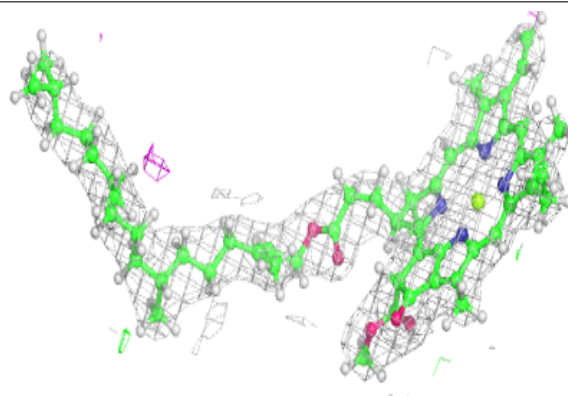


**Electron density around CLA B 604:**

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

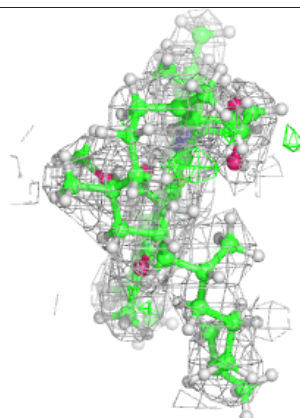
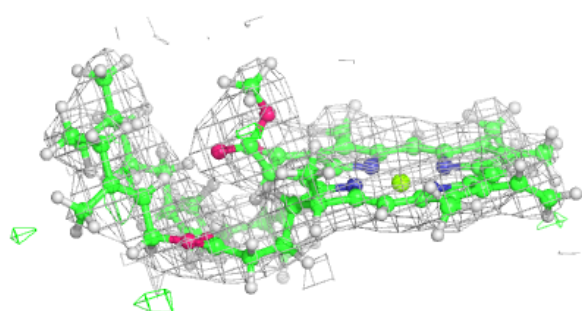
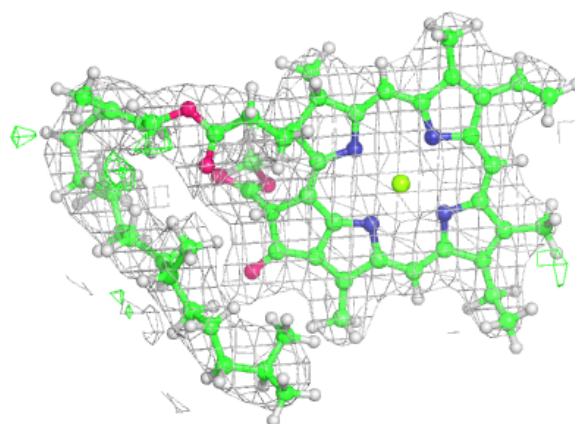
**Electron density around CLA a 604:**

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



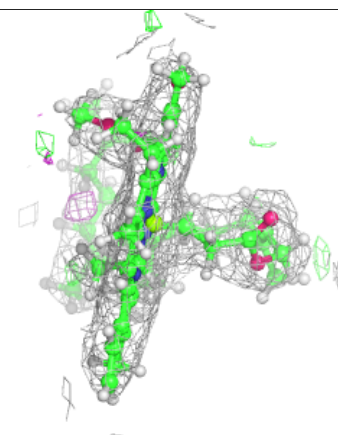
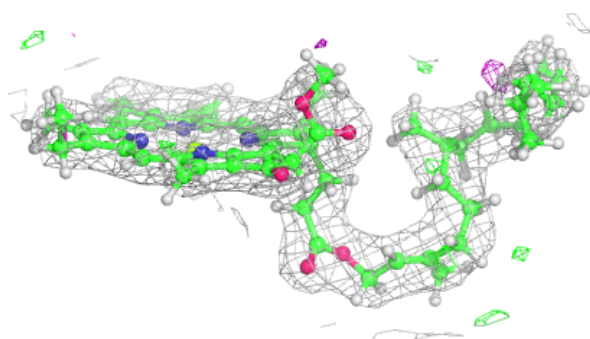
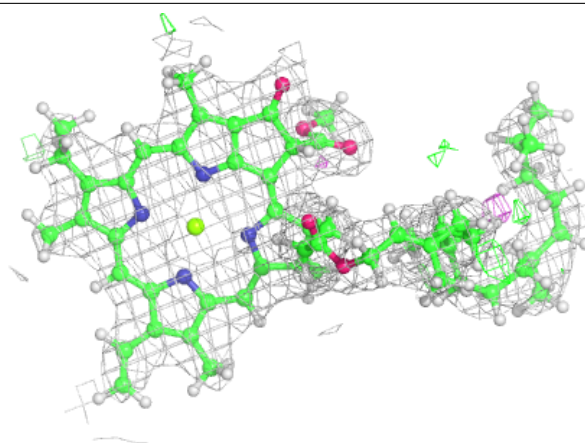
**Electron density around CLA B 609:**

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

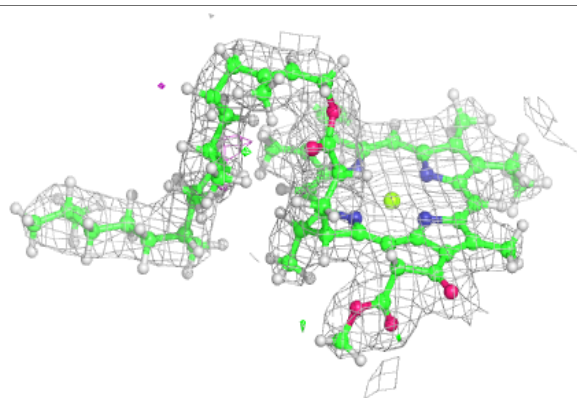
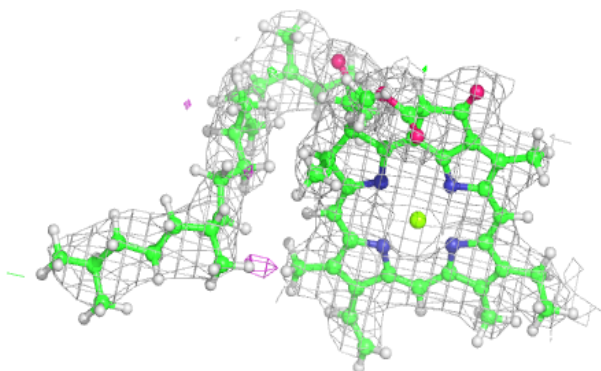


**Electron density around CLA B 611:**

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

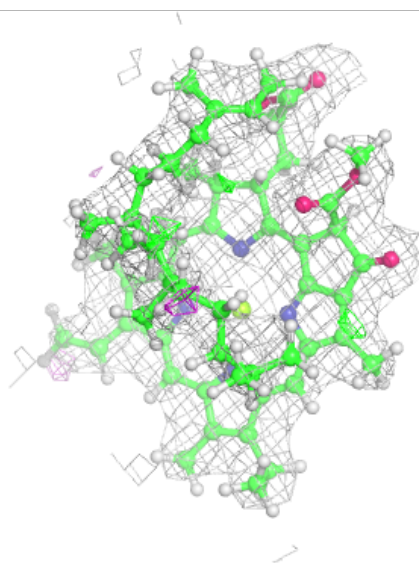
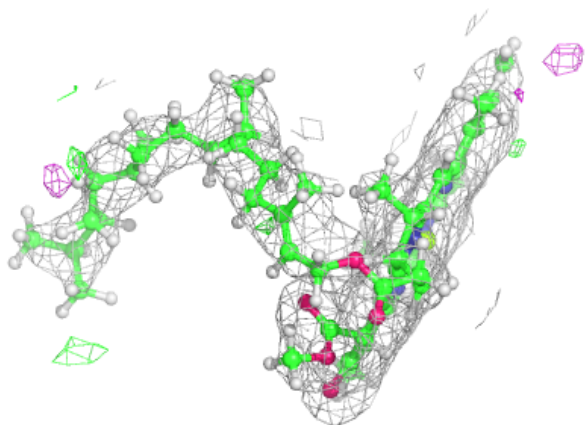
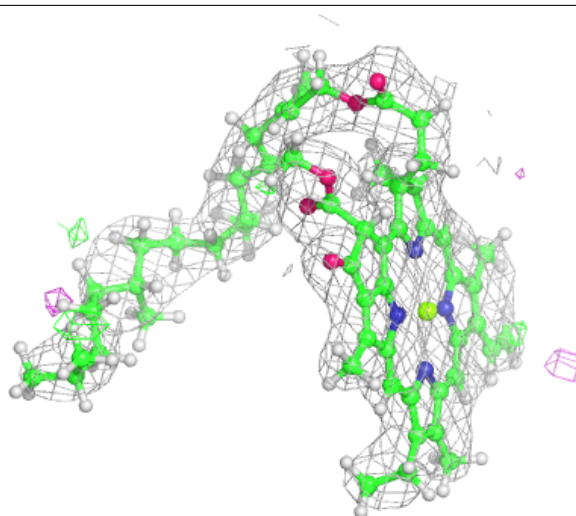
**Electron density around CLA a 613:**

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



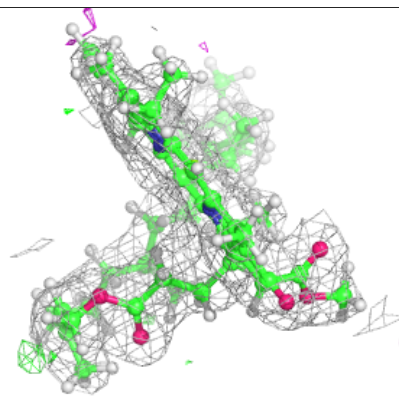
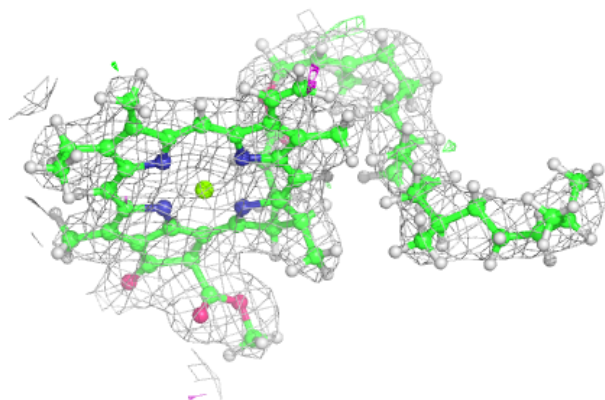
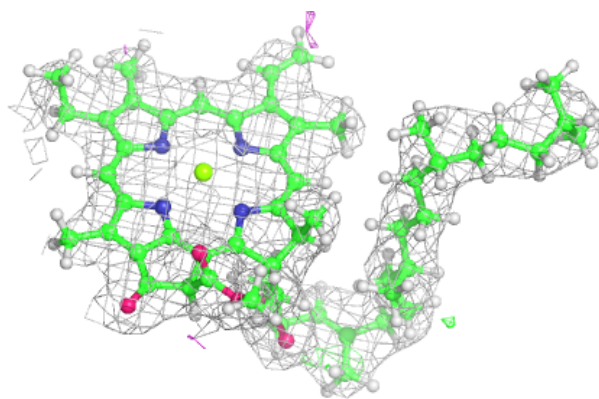
**Electron density around CLA B 612:**

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

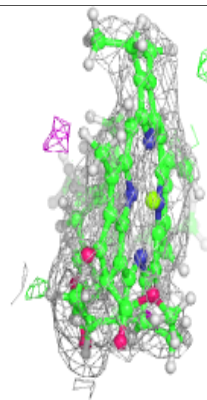
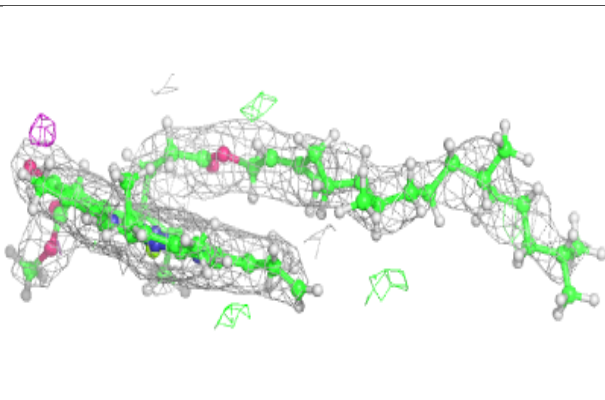
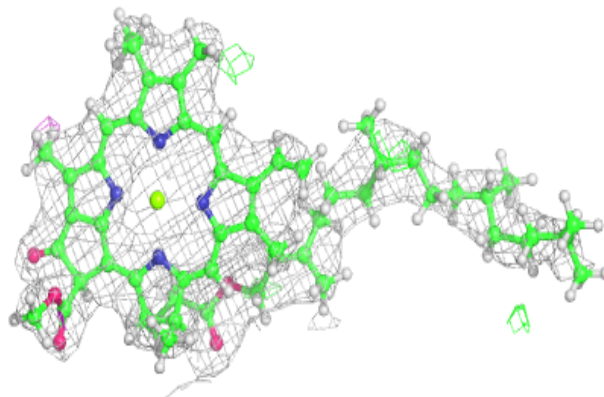


**Electron density around CLA A 612:**

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

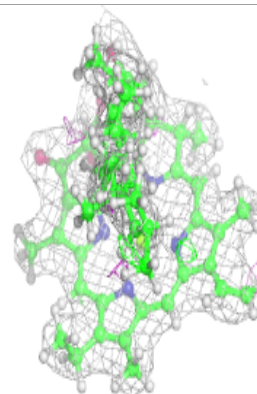
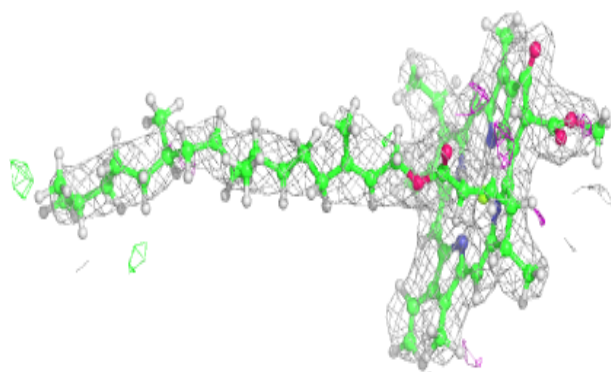
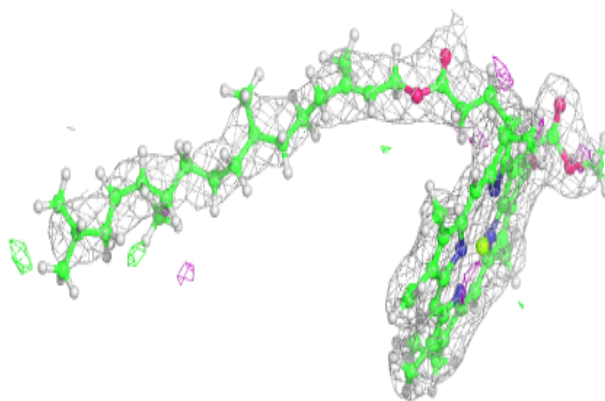
**Electron density around CLA b 603:**

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

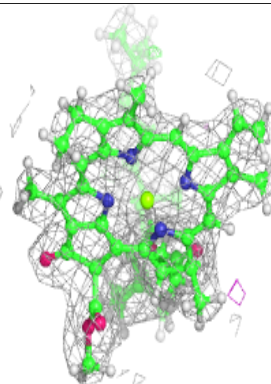
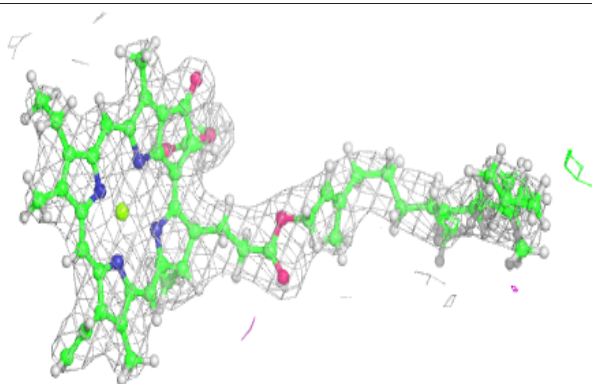
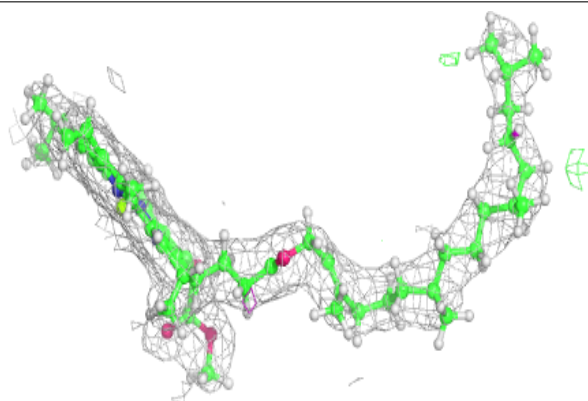


**Electron density around CLA B 606:**

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

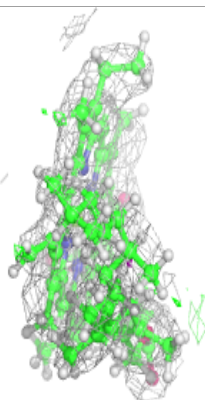
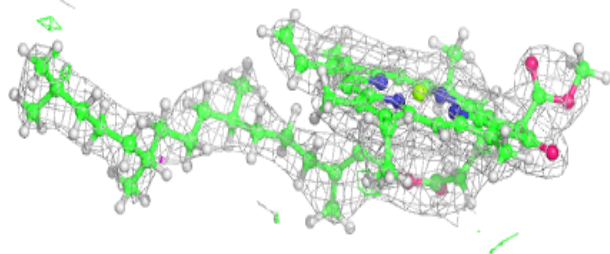
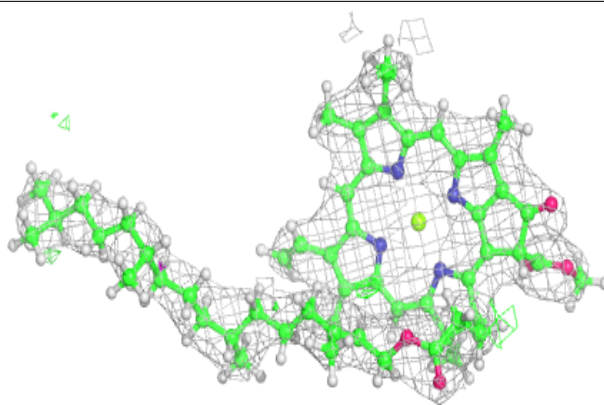
**Electron density around CLA d 402:**

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

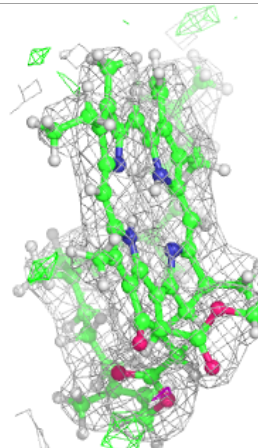
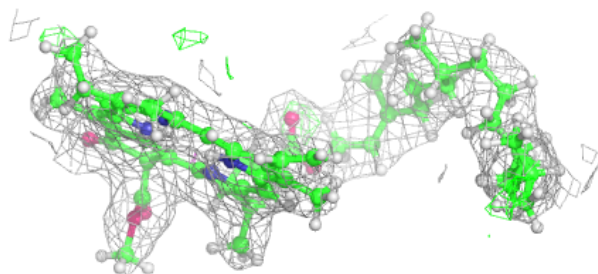
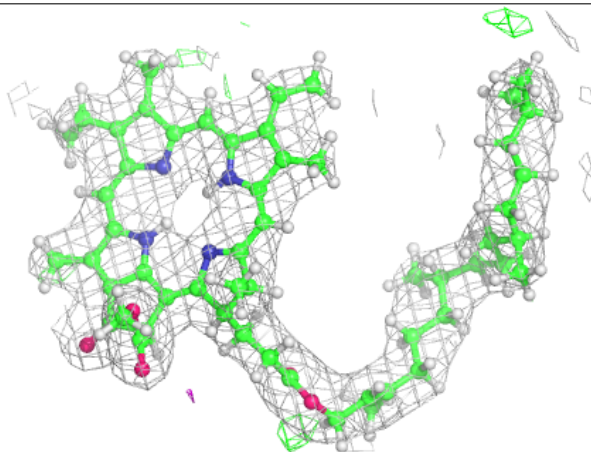


**Electron density around CLA c 501:**

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

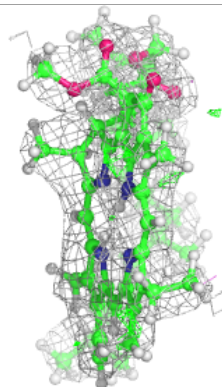
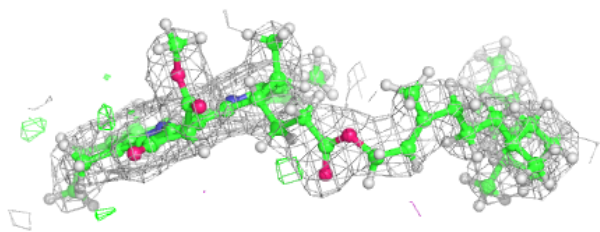
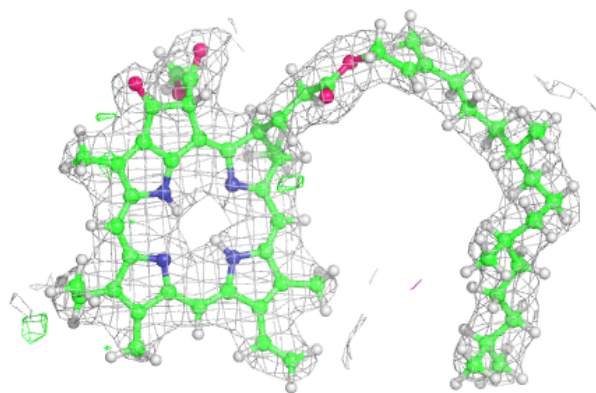
**Electron density around PHO A 606:**

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

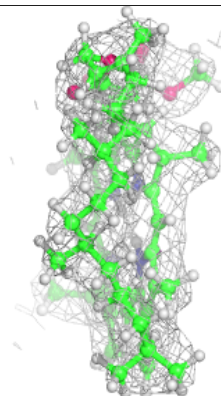
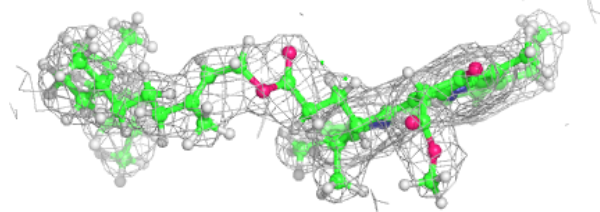
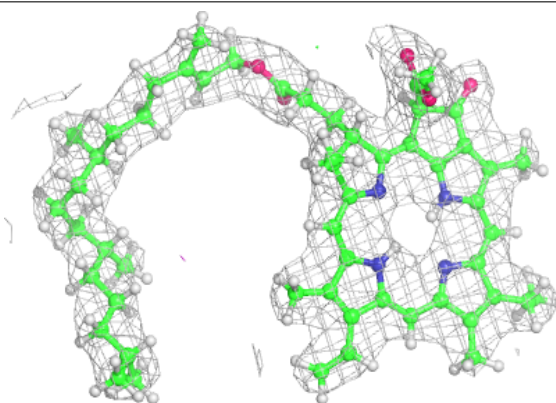


**Electron density around PHO D 401:**

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

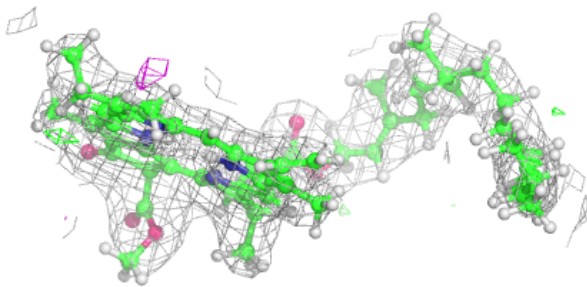
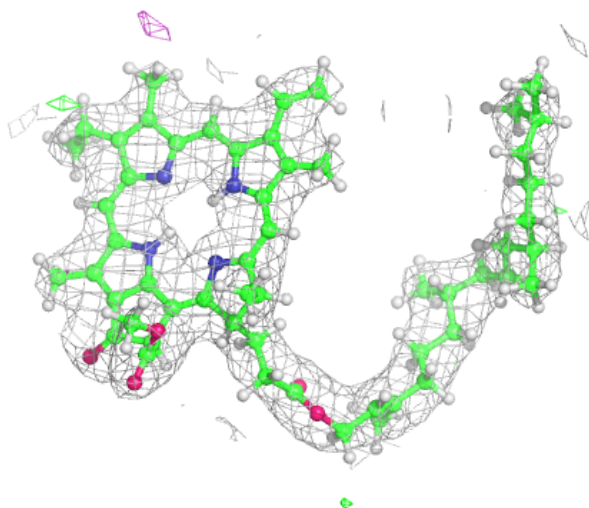
**Electron density around PHO a 606:**

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



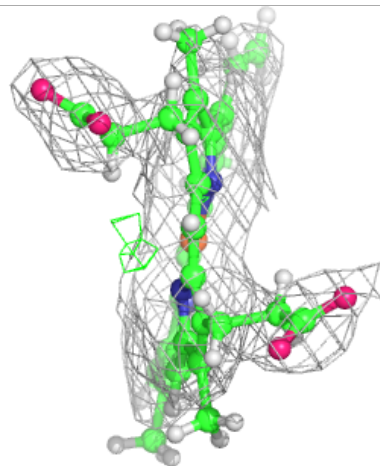
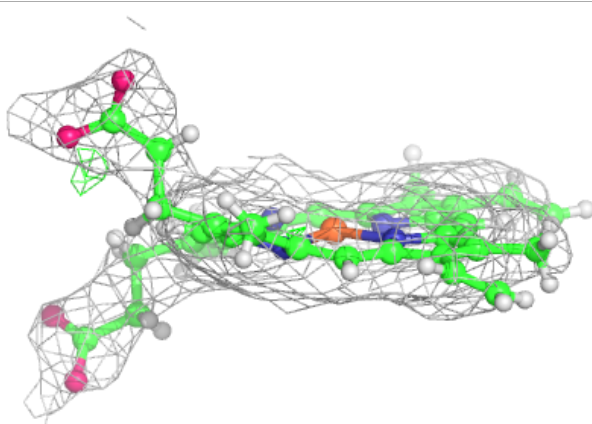
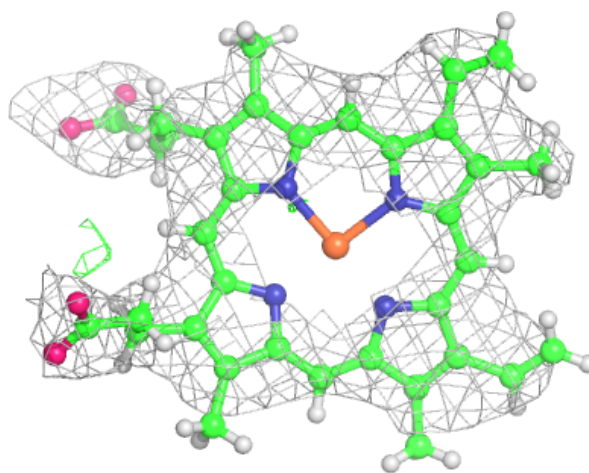
**Electron density around PHO d 401:**

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



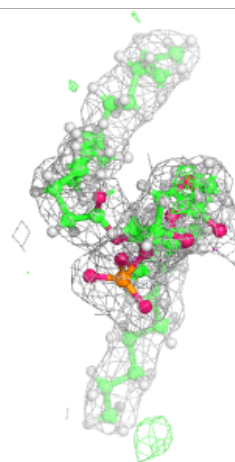
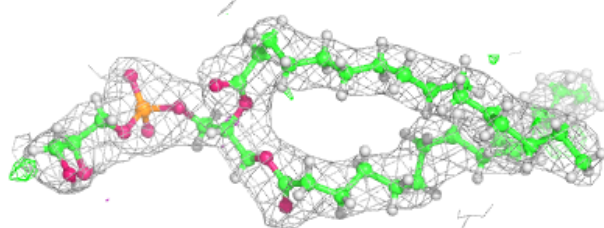
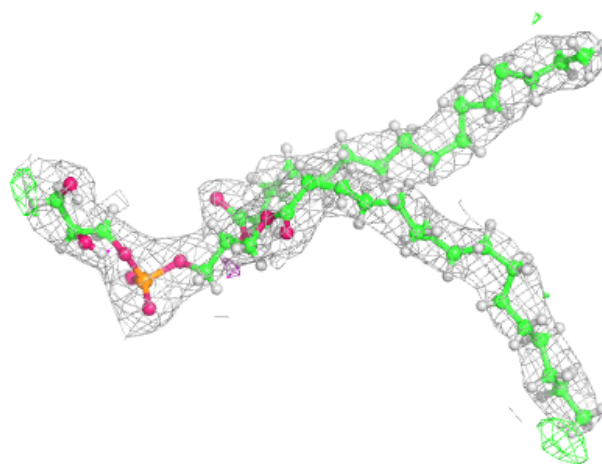
**Electron density around HEM f 101:**

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



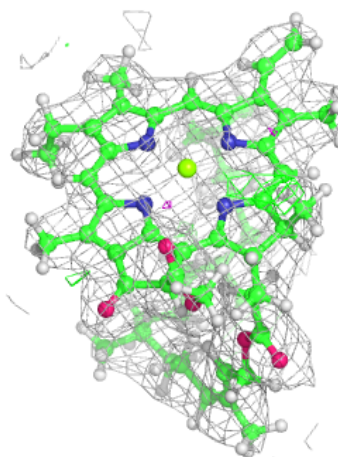
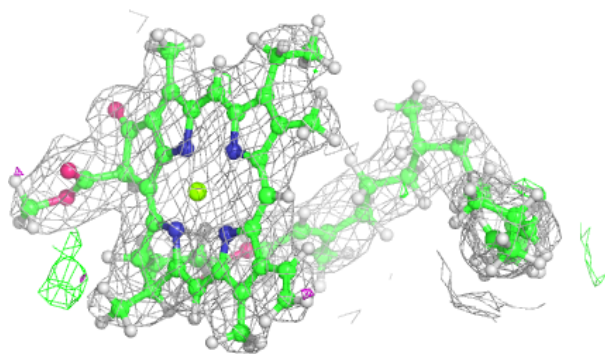
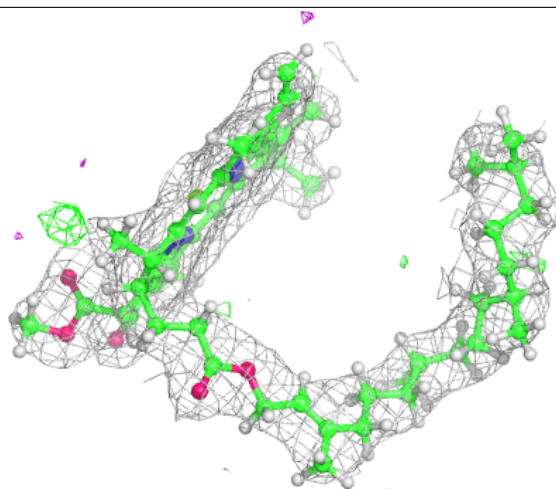
**Electron density around LHG D 409:**

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



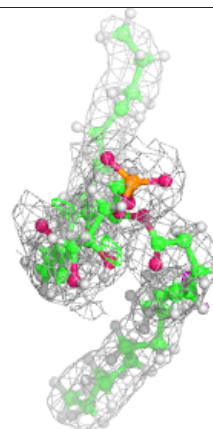
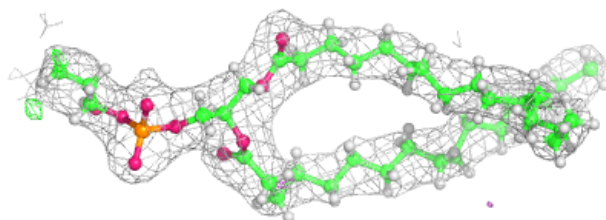
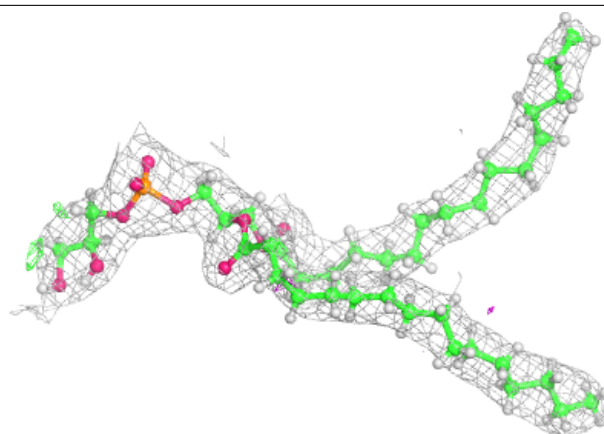
**Electron density around CLA B 610:**

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



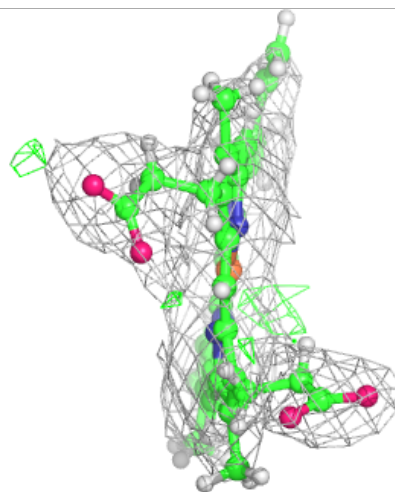
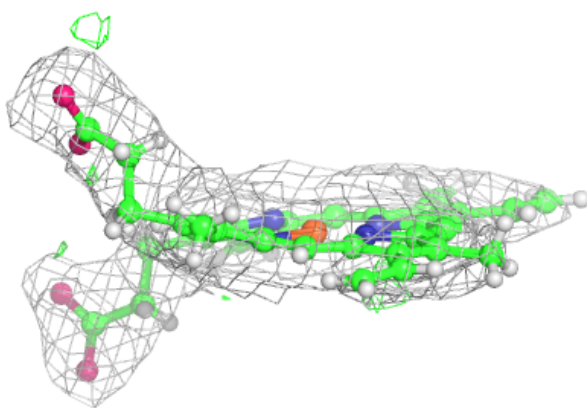
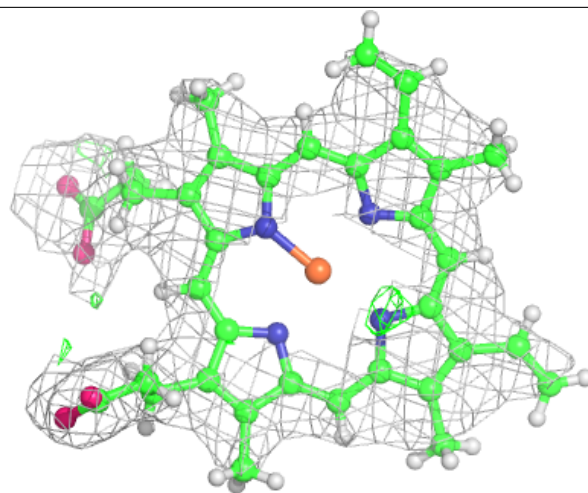
**Electron density around LHG d 406:**

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



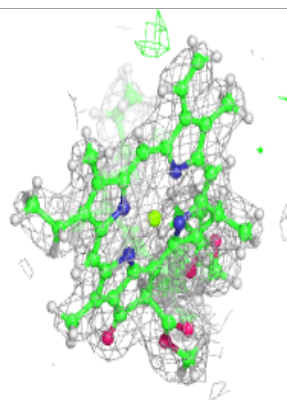
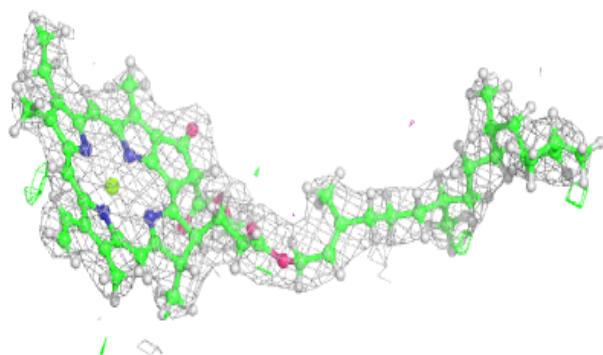
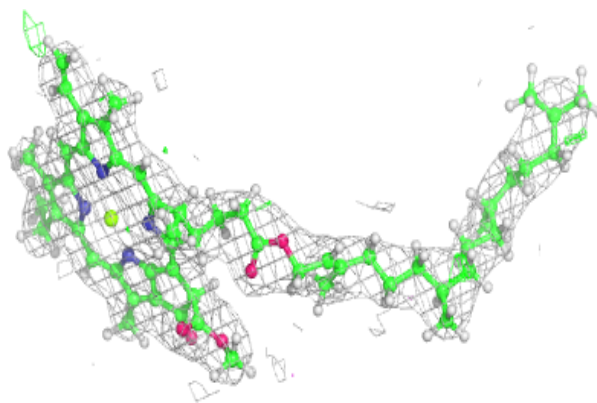
**Electron density around HEM F 101:**

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



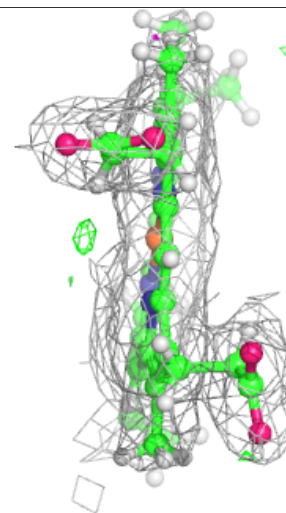
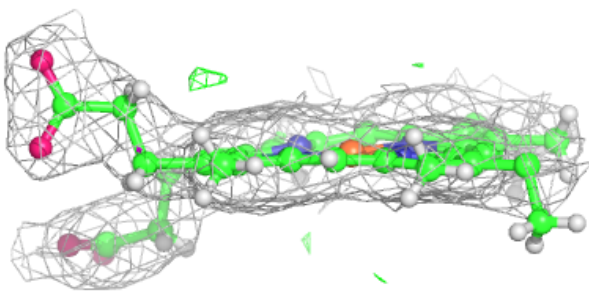
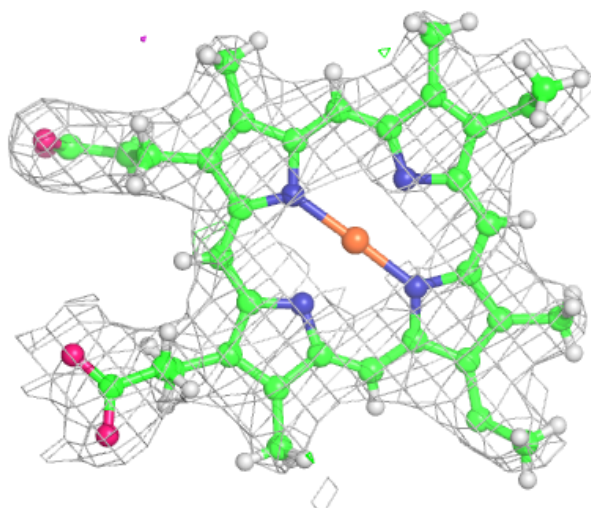
**Electron density around CLA A 604:**

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



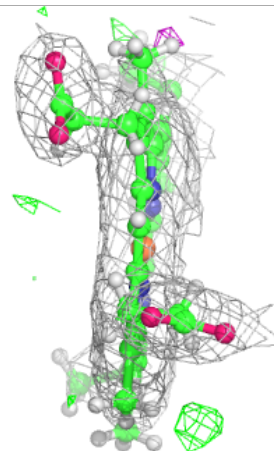
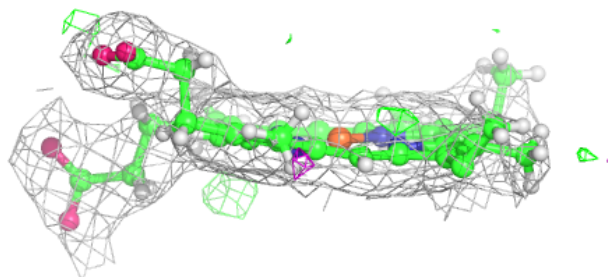
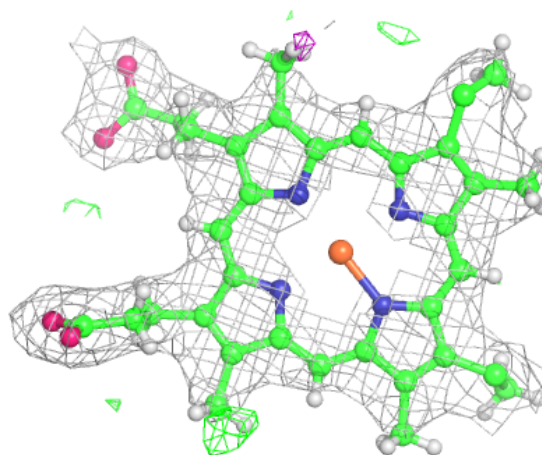
**Electron density around HEC V 201:**

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



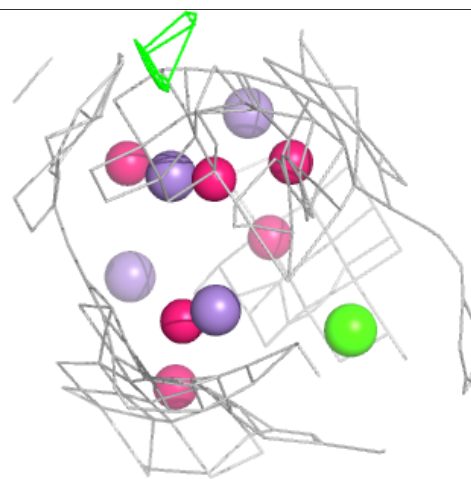
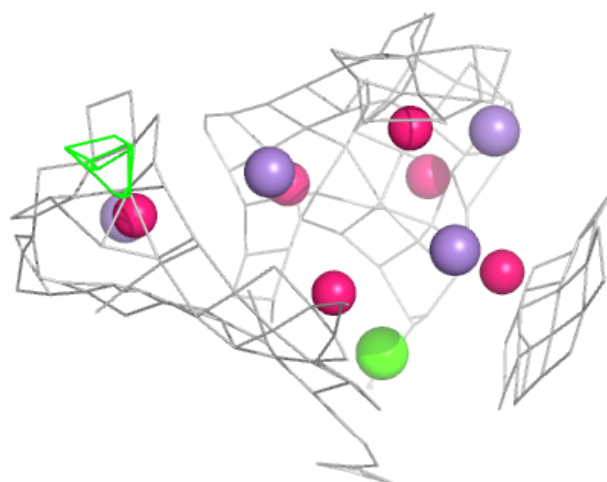
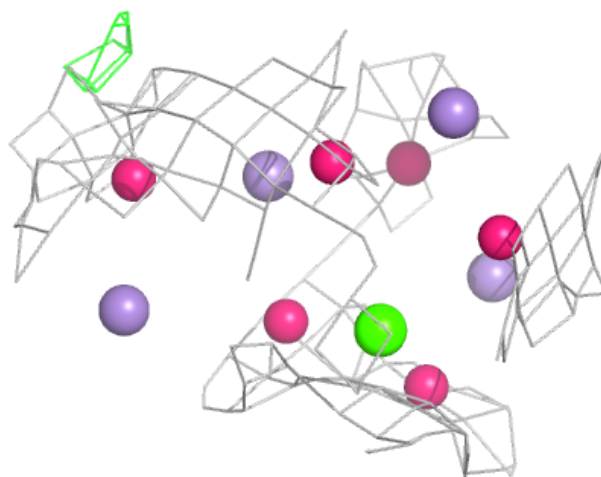
**Electron density around HEC v 201:**

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



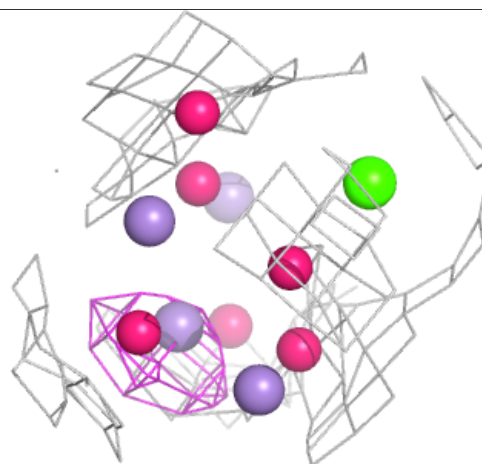
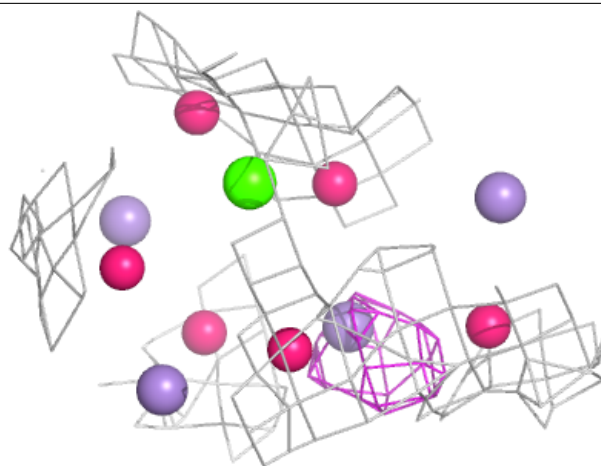
**Electron density around OEY A 601 (B):**

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



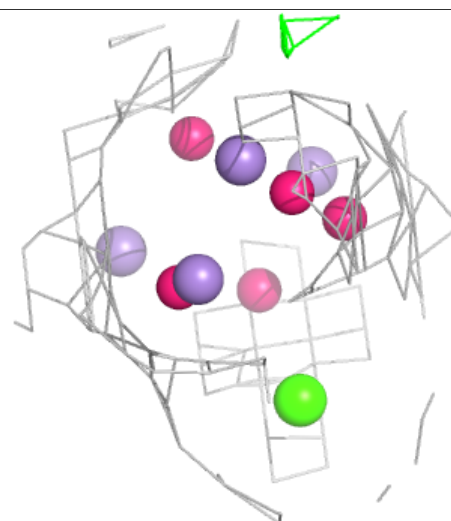
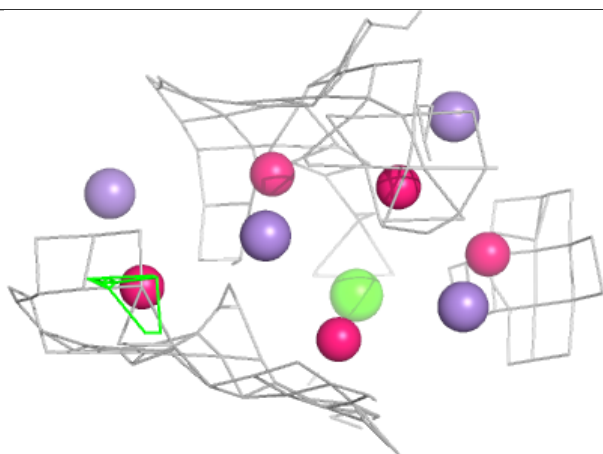
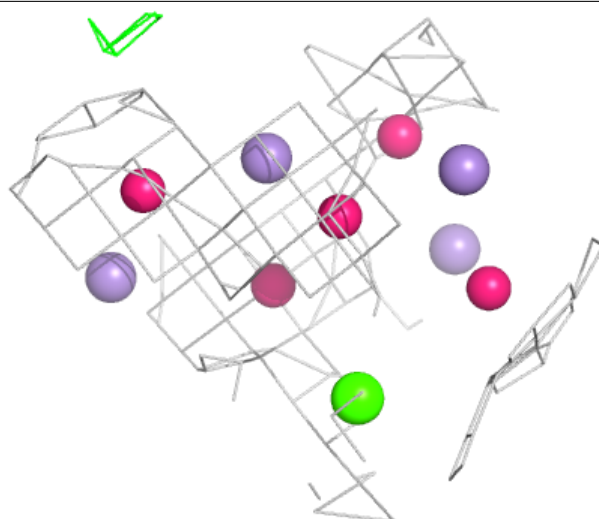
**Electron density around OEY a 601 (B):**

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



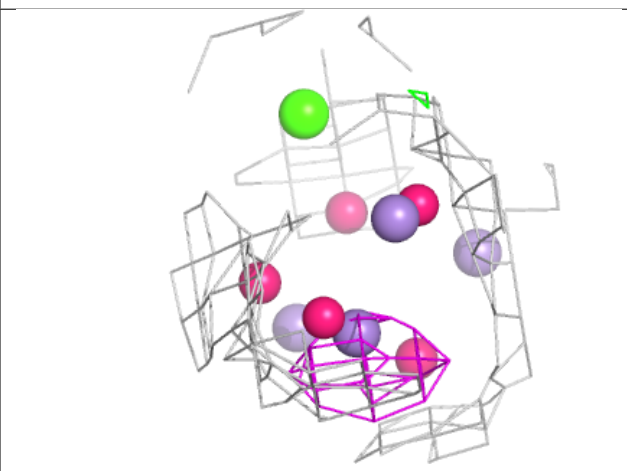
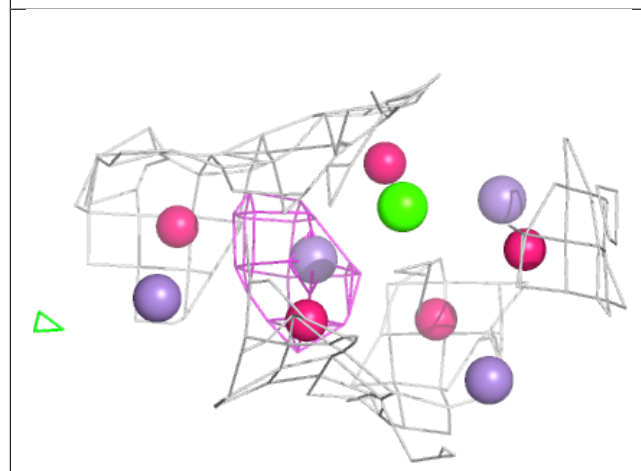
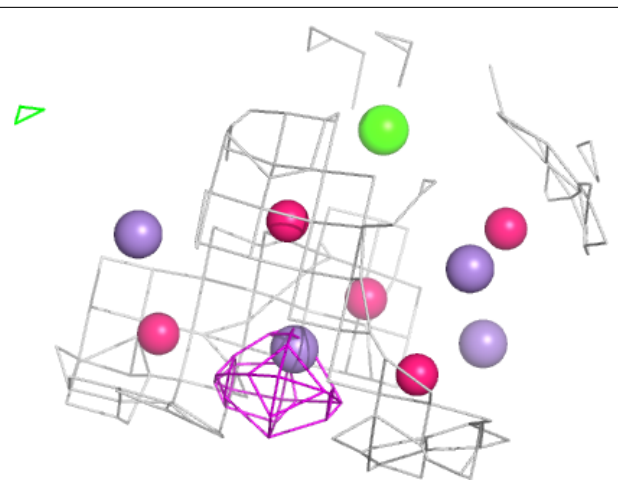
**Electron density around OEX A 602 (A):**

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



**Electron density around OEX a 602 (A):**

$2mF_o-DF_c$  (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.